
Supplementary information

Heat flows enrich prebiotic building blocks and enhance their reactivity

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Supplementary Discussions

Supplementary Discussion 1: *Stability of the thermogravitational accumulation against temporal fluctuations of the temperature gradient and behaviour in the limit of small temperature gradients.*

While the stability of thermogravitational accumulation to changes in chamber geometry⁴¹ as well as spatial fluctuations in heat flux⁴² has already been demonstrated, we here explore the stability of the process to temporal fluctuations in heat flux.

Using finite element simulations (Comsol 5.4), we simulate a 2-dimensional closed heat flow chamber with a height of 50 mm and a width of 0.17 mm. To show the temporal stability to heat flux fluctuations, we simulate a proxy species with a diffusion coefficient of $D = 800 \times 10^{-12} \text{ m}^2/\text{s}$ and a Soret coefficient of $S_T = 5.7 \times 10^{-3} \text{ 1/K}$, which is in the range of the compounds studied in this work. The simulated differential equations correspond to those given in the method section (Determination of thermophoretic strength) but are now solved simultaneously to account for the time variance of the applied temperature difference. The cold side is kept at a constant 30 °C, while the warm side is varied as shown in Supplementary Fig. 12. The simulation is run for 14 h.

The results depicted in Supplementary Fig. 12 for constant temperature differences of $\Delta T = 10 \text{ K}$ and $\Delta T = 20 \text{ K}$ show, as expected, a non-linear increase of the strength of the thermogravitational accumulation with ΔT at the point of maximum accumulation (cold, lower corner). If instead a variable temperature difference is applied, here exemplarily with a sinusoidal function of amplitude 10 K (thus varying between 0 and 20 K) and periodicity (Supplementary Fig. 12: black solid line), the average accumulation characteristic is the same as for a constant temperature difference of 12 K (Supplementary Fig. 12: orange).

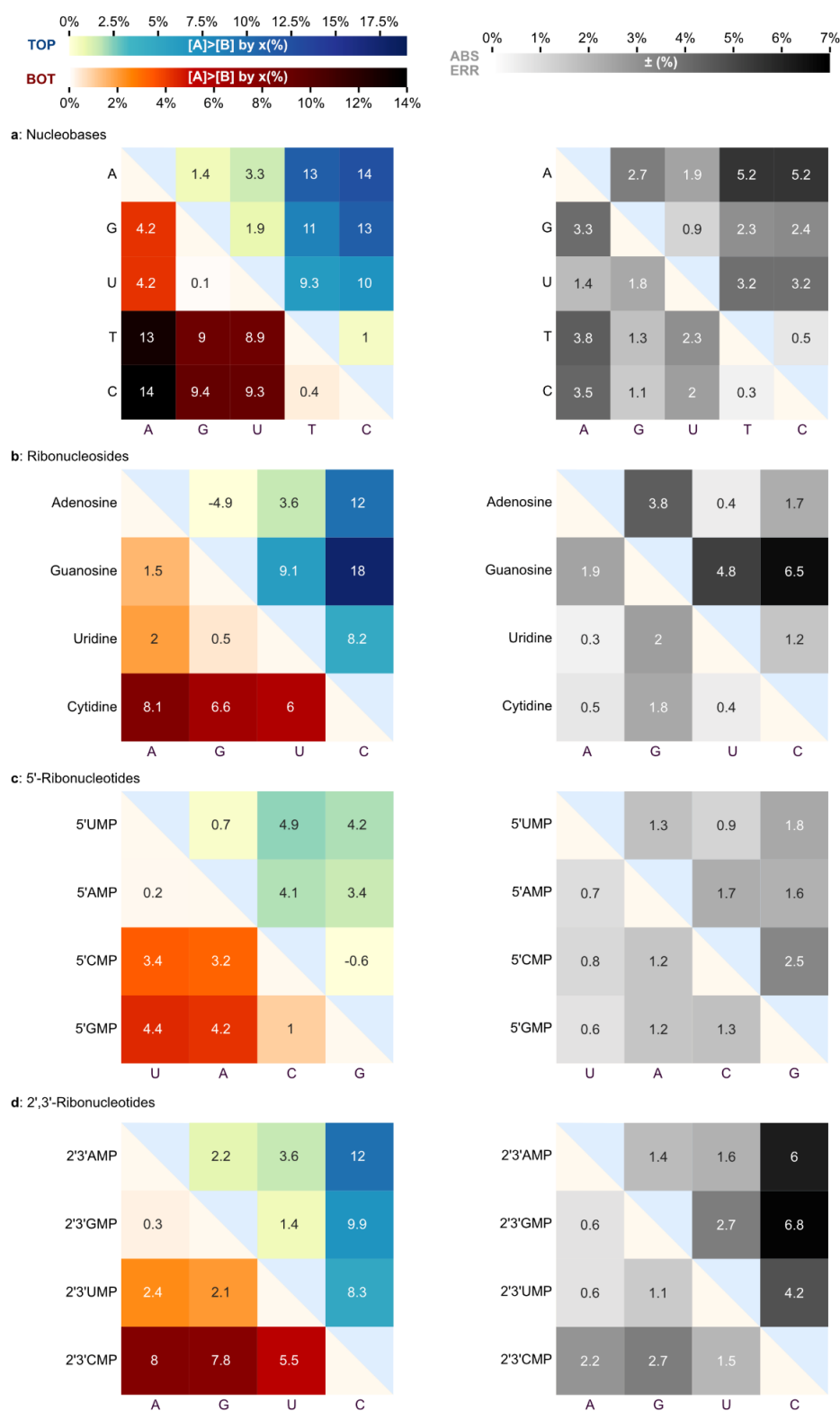
The time-averaged temperature difference gives a value of 10 K. The deviation from the accumulation with a constant temperature difference of 10 K (Supplementary Fig. 12: blue) is due to the nonlinear dependence of the thermogravitational accumulation on the temperature difference. Temperature differences above 10 K therefore contribute disproportionately more to the accumulation compared to those below 10 K. Despite the very strong temporal fluctuations of the heat flux, the accumulation process under consideration shows to be extremely stable.

The exact determination of the temperature gradients occurring in natural systems, for example in fissures in basaltic glass, is difficult. Therefore, a discussion of the possible enrichments by heat flux driven chambers at very small temperature differences as well as the natural conditions, which also make larger temperature gradients appear realistic, is relevant. As shown in the main text in Figure 4f, even in small networks with very moderate temperature gradients of only 2 K, an enhancement of e.g. I vs N of (3.5 ± 0.2) -fold can be achieved.

Figure 4f shows that these values can be further boosted by the size of the system, but our calculations here are limited by the measurement accuracy of the Soret coefficients involved. Due to the accumulating error of the heat flux chambers connected in series, a calculation of systems $N > 30$ is no longer reliably possible. However, we expect here a continuation of the behavior shown in Figure 4f and thus a compensation of the smaller temperature differences discussed here.

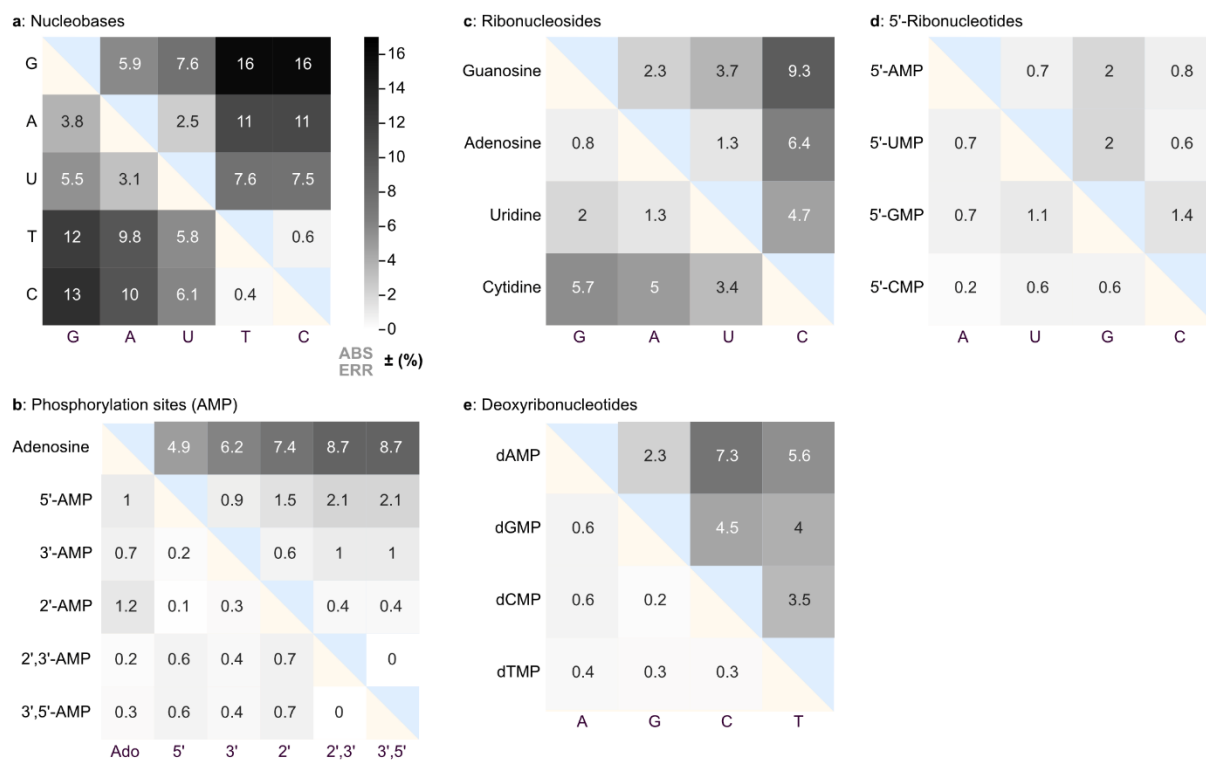
Even larger temperature gradients are likely to be realistic within natural systems. Varying across orders of magnitude in fracture size and associated widely varying flow velocities, fast flows can serve as effective heat sources and sinks for narrower adjacent channels^{49,55}, implementing a wide range of possible temperature differences in which the effects shown can take place. Also, it should be noted here that the temperature gradients shown here, as discussed above, need not act all the time and could also fluctuate over the local dimension (for a stability analysis over local fluctuations, see reference 42). In summary, the systems discussed here may well be considered realistic and thus may have made a relevant contribution to prebiotic chemistry.

Supplementary Figures



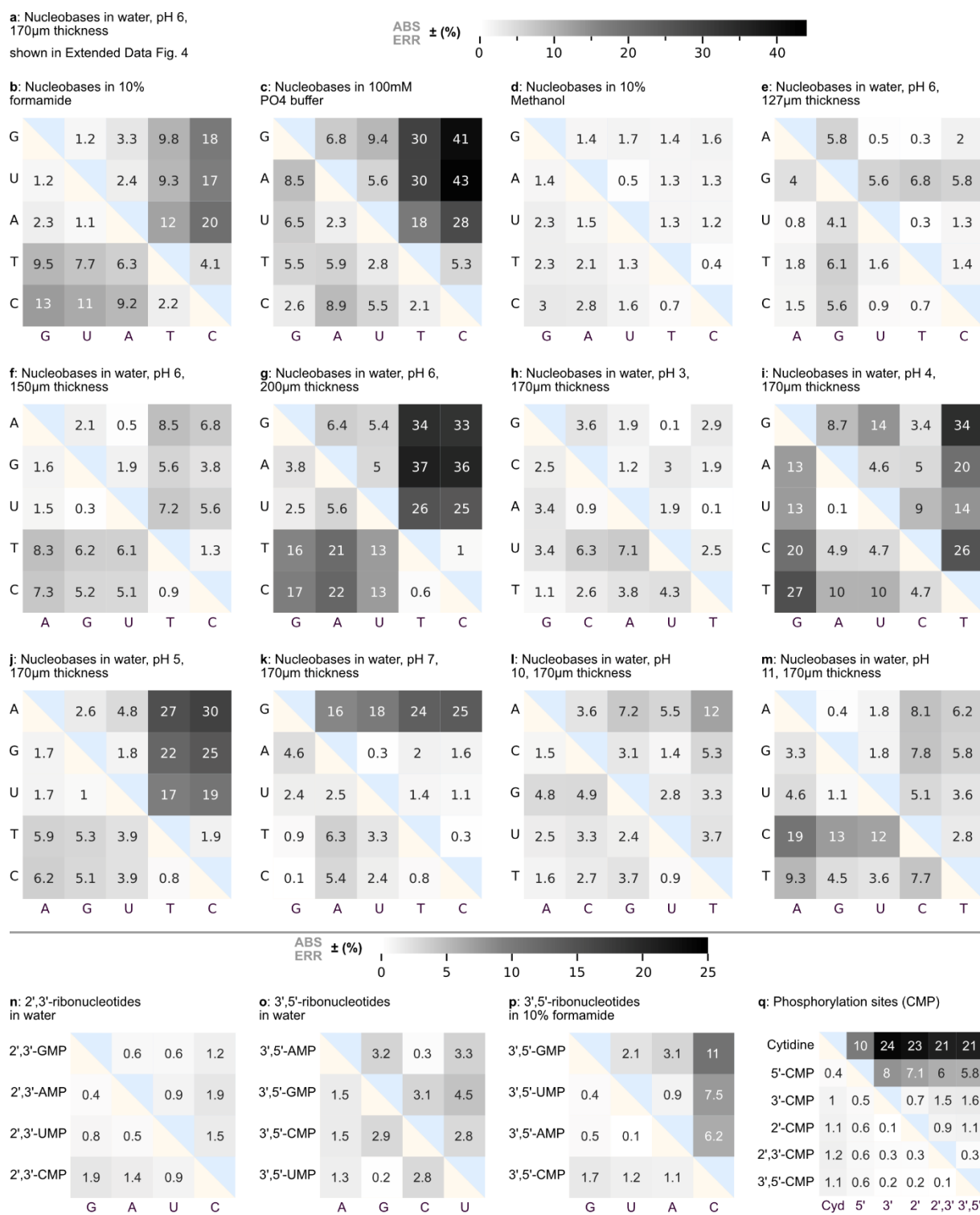
Supplementary Figure 1: Enrichment of nucleobases, nucleosides, 5'-nucleotides and 2',3'-cyclic nucleotides after 6 h.

The tendencies are the same as after 18 h (Fig. 3a/c/d, main text and Extended Data Fig. 5n) though at lowered amplitudes. Error maps show s.d. (3 repeats, for raw data see Supplementary Tables 5-65).

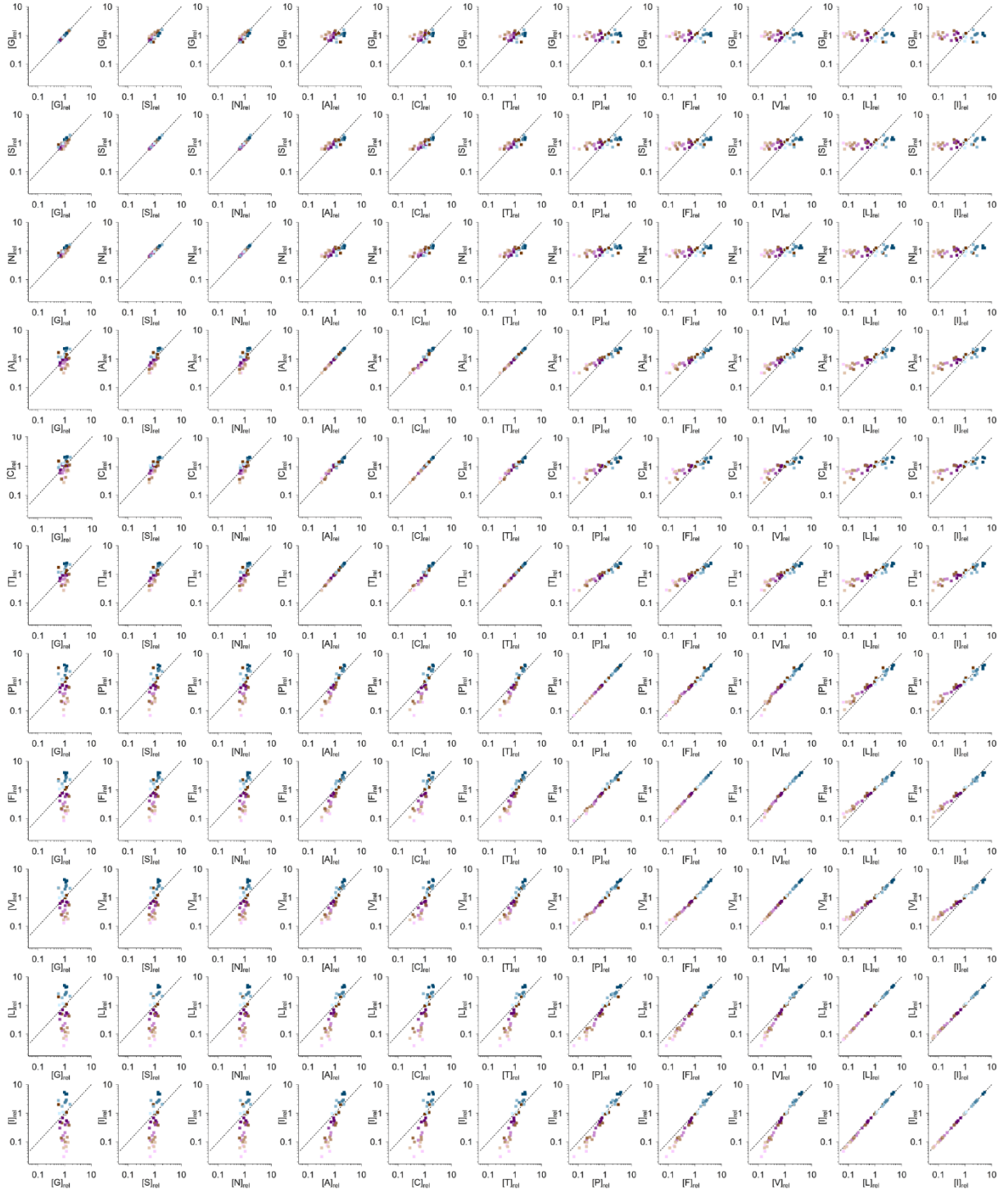


Supplementary Figure 2: Error maps for Figure 3.

Error maps show s.d. (3 repeats, for raw data see Supplementary Tables 5-65).

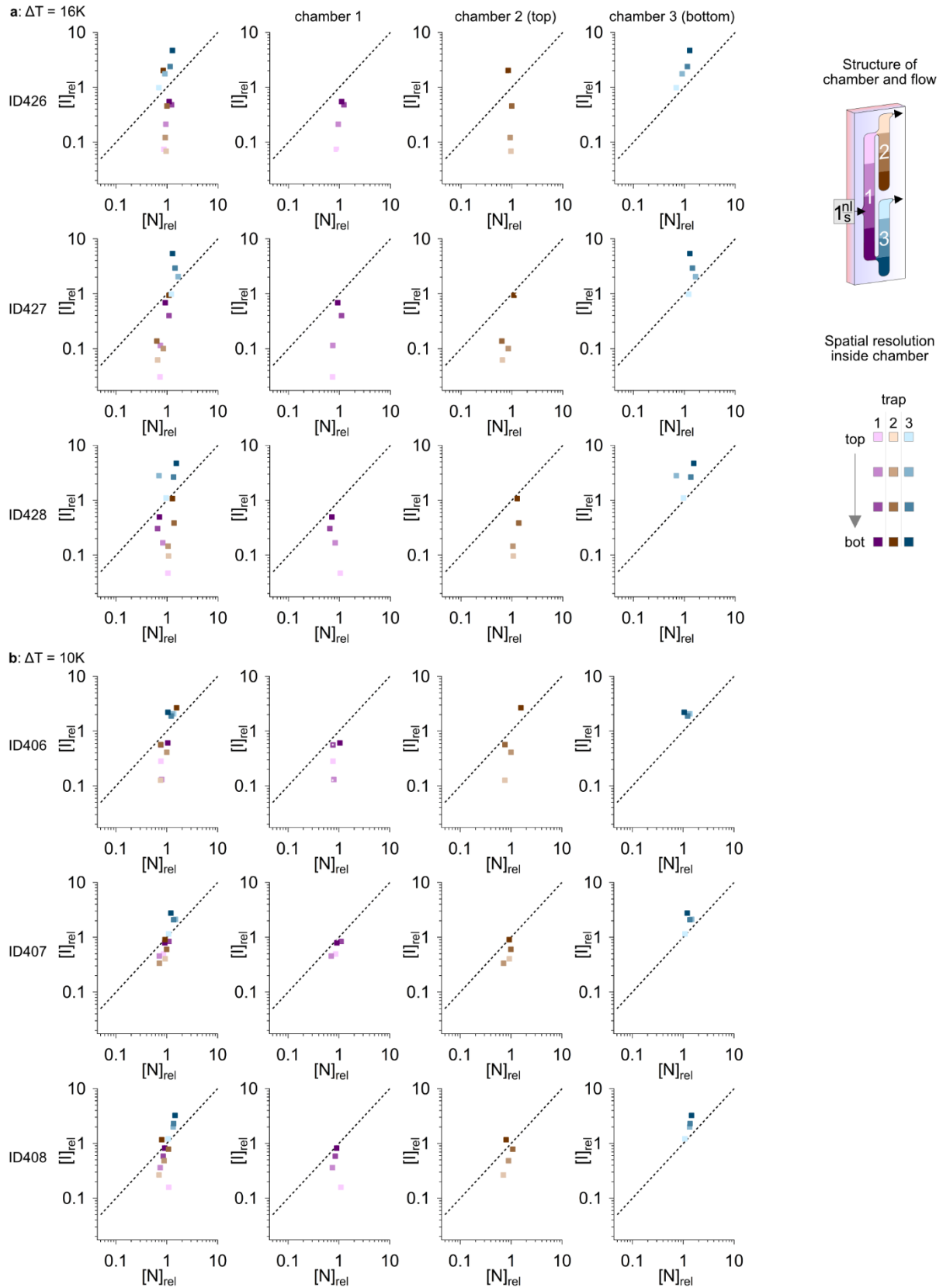


Supplementary Figure 3: Error maps for Extended Data Fig. 5.
Error maps show s.d. (3 repeats, for raw data see Supplementary Tables 5-65).



Supplementary Figure 4: Separation of amino acids in experimental network

Experimental setup of a small network of three interconnected chambers with an volume-inflow of 1 nl/s of the same AA-mixture used in Figure 4 and $\Delta T=16$ K. After 60 h, the chamber contents from 3 repeats were frozen and divided into individual parts according to the colour gradations shown in Supplementary Figure 5 and measured by HPLC. In addition to examples shown in the main text Fig. 4 and Extended Data Fig. 6, we show various combinations of pairs. For instance, thermophoretically different AAs glycine (G) and isoleucine (I) separate readily while mass-identical leucine (L) and I only show minor concentration differences in our experimental system.



Supplementary Figure 5: Individual experiments and per-chamber depiction of network experiments

Experimental setup of a small network of three interconnected chambers with an volume-inflow of 1 nl/s of the same AA-mixture used in Figure 4 with a ΔT of (a) 16K and (b) 10K. After 60 h, the chamber contents from 3 repeats at each temperature gradient were frozen and

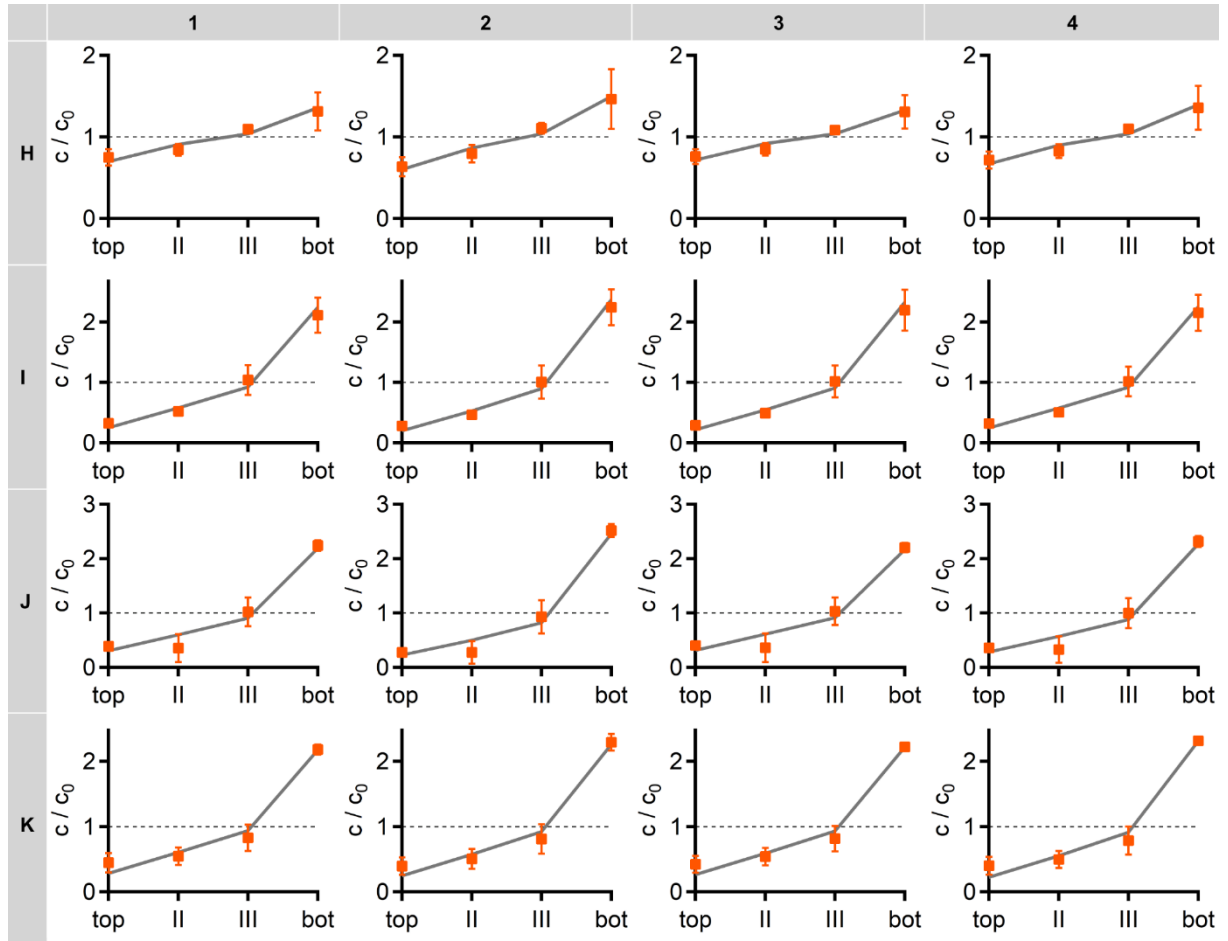
divided into individual parts according to the colour gradations shown on the right side. For the AA pair I vs N, the concentrations per repeat and per individual chambers are shown.

3'	0.1			
2'	2.7	2.6		
2',3'	8.8	8.7	6.0	
3',5'	9.3	9.2	6.4	0.4
	5'	3'	2'	2',3'

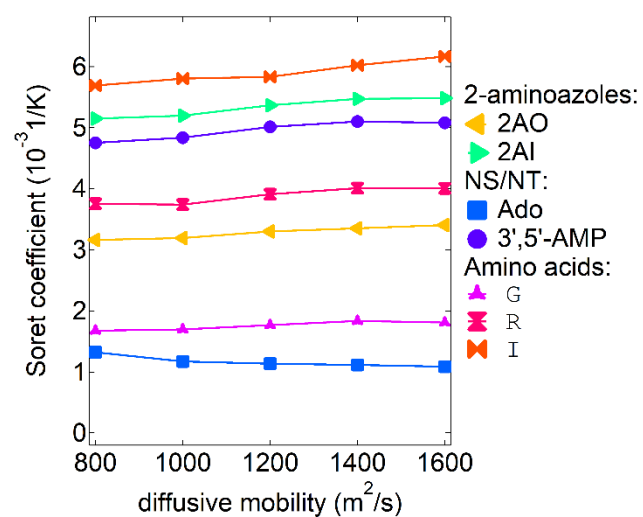
3'	5.2			
2'	5.3	0.1		
2',3'	7.3	2.0	1.9	
3',5'	7.3	2.0	1.9	0.0
	5'	3'	2'	2',3'

[illegible]

As shown in Extended Data Fig. 2, the experimental restriction to average over 25 % of the heat flux chamber results in lowered enrichment values. The maximal pairwise separation values shown here are calculated by numerically finding the steady state solution for a set temperature gradient of 5 K, fixing the top of a chamber to 1 and taking the value from the lowest mm of the chamber. **(a/b)** shows the maximal pairwise separation for adenosine and cytidine monophosphates, showing separation of up to 5 % between species of identical mass. **(c)** Similarly, for amino acids, up to 90 % separation are feasible.

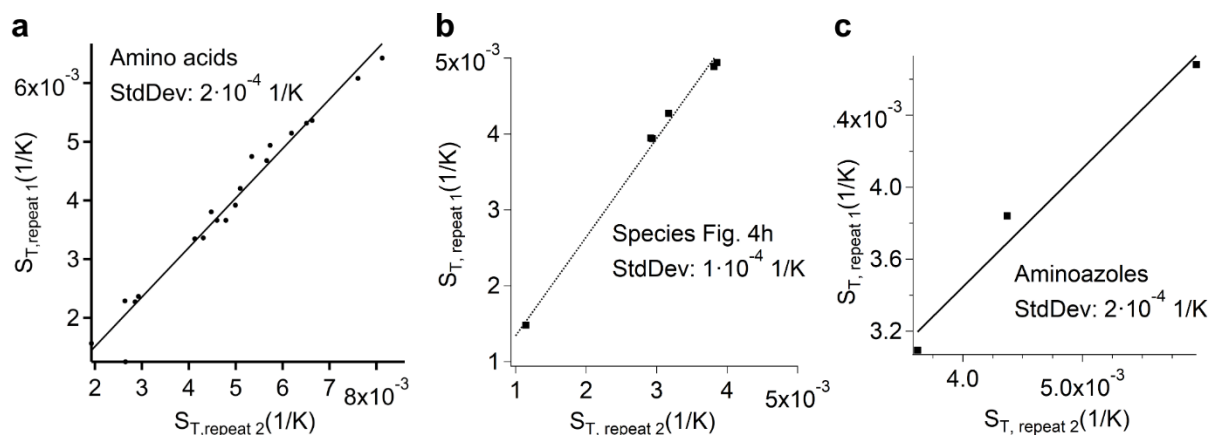


Supplementary Figure 7: Concentration profiles in heat flux cell and fit for Soret coefficient. In addition to data shown in Extended Data Fig. 8 (errors=s.d., 3 repeats). **H1:** Adenosine, **H2:** Cytidine, **H3:** Guanosine, **H4:** Uridine, **I1:** 5'-AMP, **I2:** 5'-CMP, **I3:** 5'-GMP, **I4:** 5'-UMP, **J1:** 2',3'-AMP, **J2:** 2',3'-CMP, **J3:** 2',3'-GMP, **J4:** 2',3'-UMP, **K1:** 3',5'-AMP, **K2:** 3',5'-CMP, **K3:** 3',5'-GMP, **K4:** 3',5'-UMP.



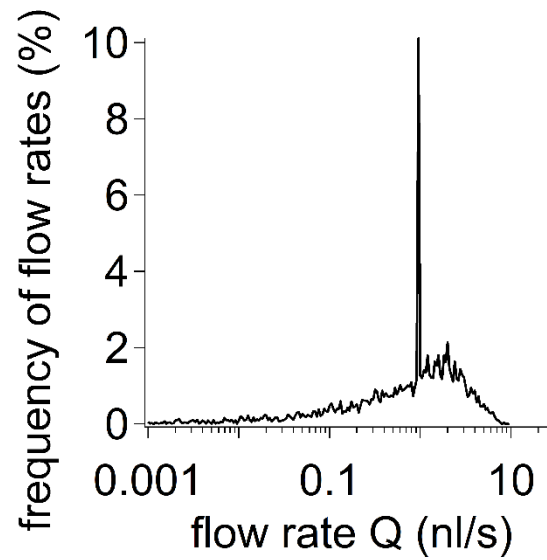
Supplementary Figure 8: Influence of diffusion constant on determination of Soret coefficient for different exemplary species.

For details on determination of the Soret coefficient, see Methods.



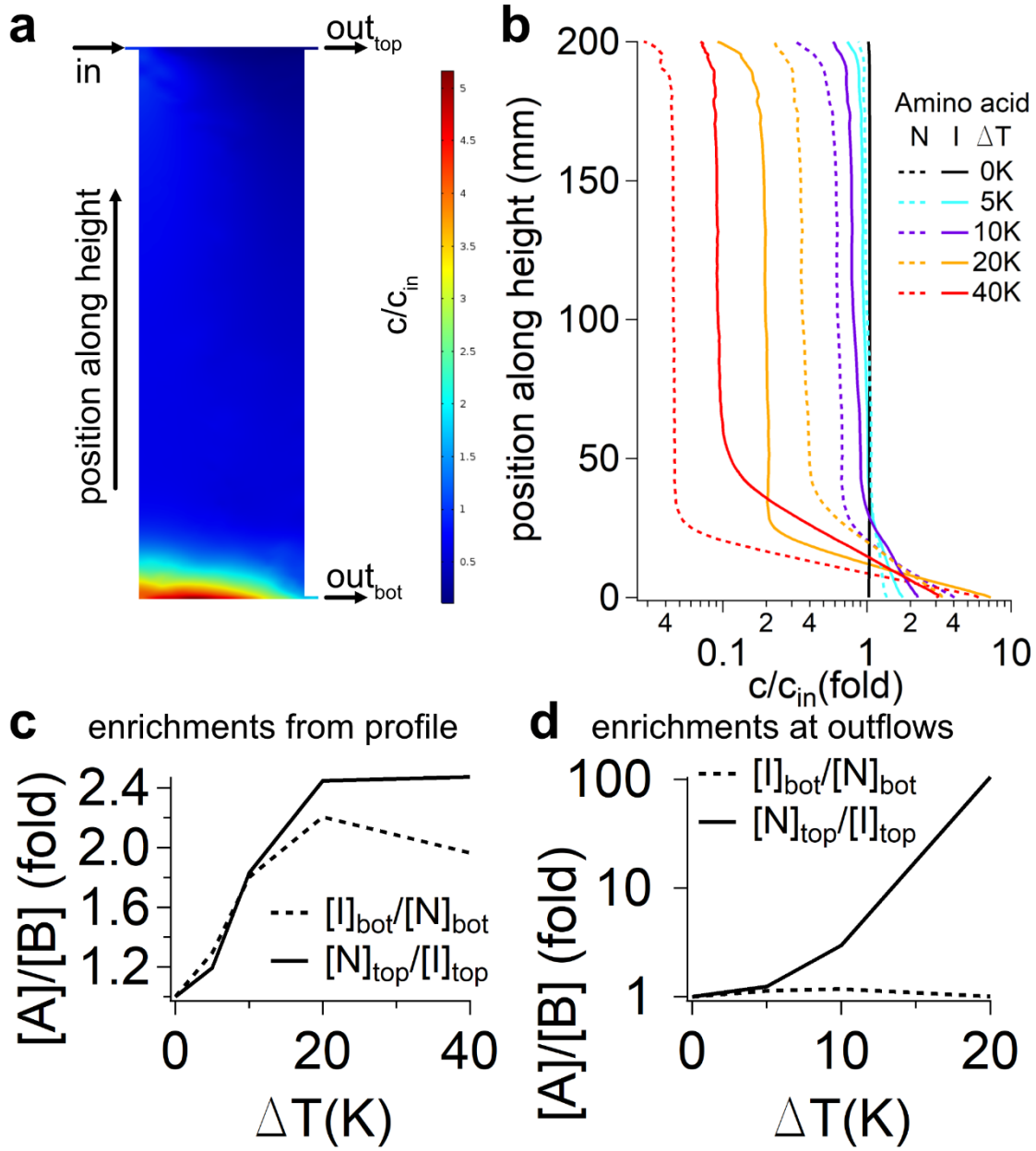
Supplementary Figure 9: Errors in Soret coefficients for network models.

To separate random from systematic errors, measurements of Soret coefficients for each of 2 repeats are shown in **a-c**. Systematic errors here are smaller differences in the temperature gradients between different measurements. These deviations affect the Soret coefficients of all species present in the respective mixtures equally, so they lead to a slope different from 1 in these correlation plots. The random error, e.g. by the integral determination of the peaks, then results from the standard deviation of the linear fits of these correlations (shown here as solid lines).



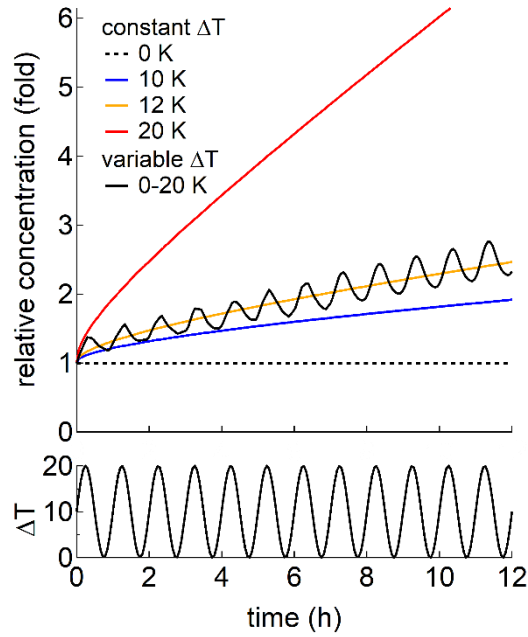
Supplementary Figure 10: Example distribution of flow rates for a network.

Example for system of 20 by 20 heat flux traps over 30 iterations. The input flow rate was set to 1 nl/s, which is why it is the most common. The maximum flow rates were limited to 10 nl/s, the smallest to $1 \cdot 10^{-3}$ nl/s.



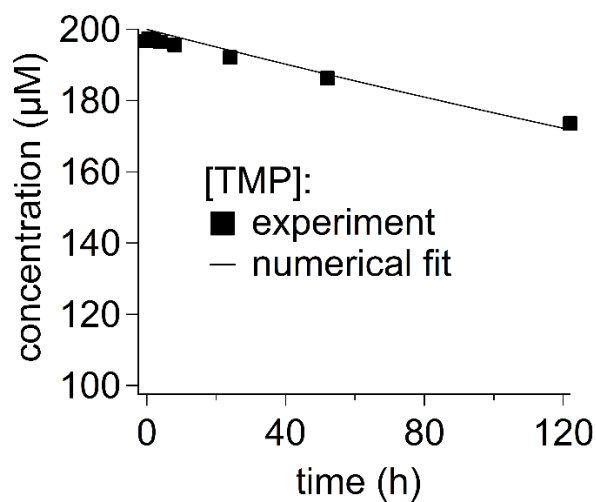
Supplementary Figure 11: Example of enrichment behavior in a single heat-flow chamber as used in the network simulation.

As in main text Figures 4 and 5 ($\Delta T = 10$ K, $v_{in} = 1 \frac{nl}{s}$, $v_{out,bot} = 0.5 \frac{nl}{s}$, height=200 mm, width=60mm, thickness=0.17mm, amino acids: I and N). **(a)** Concentration of AA I within the complete heat flow chamber. The concentration distribution is distorted by the fluid flow toward to top and bottom outlet. **(b)** Projection of concentrations of AAs I (solid) and N (dashed) relative to the inflow concentration (c_{in}) along the height axis of the chamber for different temperature differences ΔT . **(c)** Increasing temperature differences lead to larger concentration ratios between AAs I and N at the top position of the chamber (at 200mm) compared to the bottom section of the chamber (at 0 mm). **(d)** Concentration ratios between the AAs I and N at the top and bottom outlet positions. The outward fluid flow toward the bottom and top change the concentration ratios to even more extreme values. This effect leads to the observed dependence on the temperature difference in a larger network and scales with the network size.



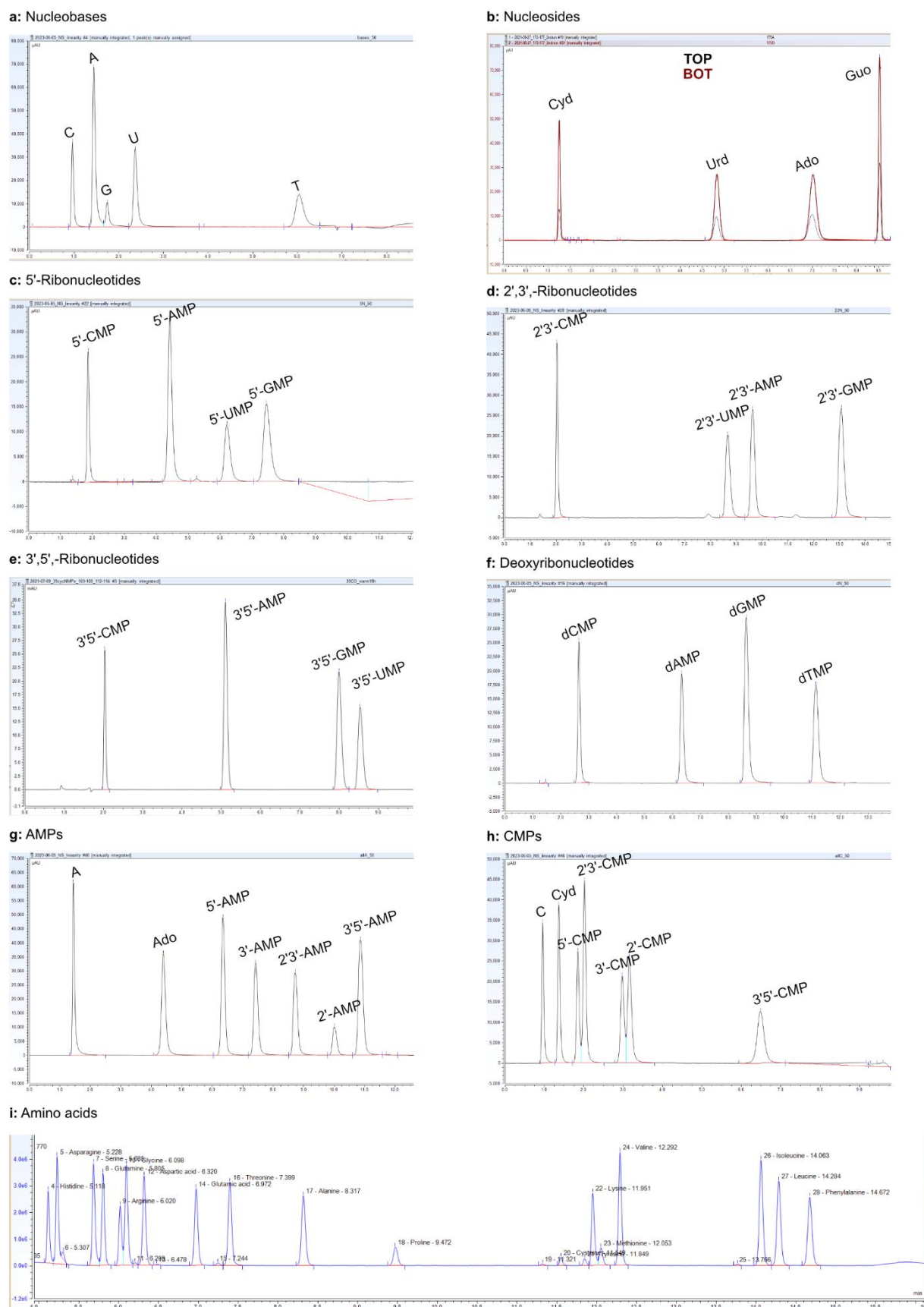
Supplementary Figure 12: Stability of thermogravitational accumulation against fluctuations of the applied temperature gradients.

Relative concentration increase at the bottom/cold spot of the heat flow chamber is plotted versus the accumulation time. Plots that show scenarios with constant temperature difference (blue, orange, red, dashed black) show the exponential increase in accumulation efficiency. The solid black plot shows the scenario with a varying temperature difference (sine function with 10 K amplitude and 1 h periodicity).



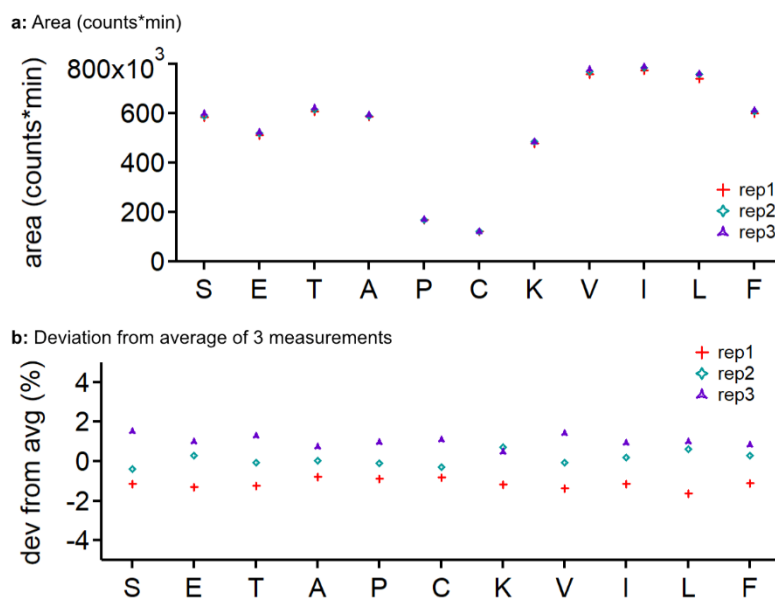
Supplementary Figure 13: TMP hydrolysis under reaction conditions

Time series at 90 °C and at an initial concentration of 200 μM and pH 10.5 (as indicated in Methods) over a period of 120 h (errors=s.d., 3 repeats). The numerical fit corresponds to the solution of Eq. 18. The reaction rate was determined to be $k_4 = 3.5 \cdot 10^{-7}$ (1/s)(±19%).



Supplementary Figure 14: Separation of molecules in LC methods

In (b) we show exemplary chromatograms for the extracted top (black) and bottom (red) fractions.



Supplementary Figure 15: Reproducibility of amino acid detection in LC method described in Methods.

We separated a sample of amino acids into 3 parts and prepared each individually according to the pre-column derivatization introduced in Methods to check for potential errors. For a selection of amino acids, we show **(a)** the measured peak integral and **(b)** the deviation from the average peak integral of the 3 measurements.

Supplementary Tables

Supplementary Table 1: List of abbreviations used.

Abbreviation	Full name
2AO	2-aminooxazole
2AI	2-aminoimidazole
2AT	2-aminothiazole
A	Adenine
C	Cytosine
G	Guanine
T	Thymine
U	Uracil
Ado	D-Adenosine
Cyd / D-Cyd	D-Cytidine (dextrorotary)
L-Cyd	L-Cytidine (levorotary)
Guo	D-Guanosine
Urd	D-Uridine
2',3'-AMP	2',3'-cyclic Adenosine monophosphate
2',3'-CMP	2',3'-cyclic Cytidine monophosphate
2',3'-GMP	2',3'-cyclic Guanosine monophosphate
2',3'-UMP	2',3'-cyclic Uridine monophosphate
2'-AMP	Adenosine 2'-monophosphate
2'-CMP	Cytidine 2'-monophosphate
3',5'-AMP	3',5'-cyclic Adenosine monophosphate
3',5'-CMP	3',5'-cyclic Cytidine monophosphate
3',5'-GMP	3',5'-cyclic Guanosine monophosphate
3',5'-UMP	3',5'-cyclic Uridine monophosphate
3'-AMP	Adenosine 3'-monophosphate
3'-CMP	Cytidine 3'-monophosphate
5'-AMP	Adenosine 5'-monophosphate
5'-CMP	Cytidine 5'-monophosphate
5'-GMP	Guanosine 5'-monophosphate
5'-UMP	Uridine 5'-monophosphate
dAMP	2'-Deoxyadenosine 5'-monophosphate
dCMP	2'-Deoxycytidine 5'-monophosphate
dGMP	2'-Deoxyguanosine 5'-monophosphate
dTMP	Thymidine 5'-monophosphate
PO ₄	Orthophosphate (PO ₄)
diPO ₄	Pyrophosphate (P ₂ O ₇)
TMP	Trimetaphosphate (P ₃ O ₉)
triPO ₄	Triphosphate (P ₃ O ₁₀)
Extended Data Fig. 2 and Supplementary Tables 23-28	
Ans	Anserine
Arg	Arginine
Asp	Aspartic acid
Car	Carnosine
Cit	Citrulline
Cre	Creatinine

Cys	Cysteine
Cth	Cystathionine
ETA	Ethanolamine
Glu	Glutamic acid
AABA	Homoalanine
Hcy	Homocysteine
His	Histidine
Hyl	Hydroxylysine
Hyp	Hydroxyproline
Leu-Ile	Leucine + Isoleucine
Lys	Lysine
Met	Methionine
3-MH	Methylhistidine
Orn	Ornithine
Phe	Phenylalanine
Pro	Proline
Sar	Sarcosine
Ser	Serine
Tau	Taurine
Thr	Threonine
Tyr	Tyrosine
Val	Valine

Supplementary Table 2: Enrichment against mean concentration of set of molecules.

When not stated, conditions are: 18 h in water. Starting from a mean concentration of $\bar{c}_0$, at the top ($j=top$), the average concentration $\bar{c}_{top} = \frac{1}{S} \sum_i \bar{c}_{i,top}$ (see Methods, Eq. 3) of all species $i: 1, 2, \dots, S$ decreases as the solutes are enriched by thermophoretic accumulation at the bottom. The average bottom concentration $\bar{c}_{bot} = \frac{1}{S} \sum_i c_{i,bot}$ increases accordingly (see Methods, Eq. 3). Errors=s.d., 3 repeats.

2-aminoazoles, different temperature gradients							
Setting	fract ion j	$\bar{c}_j/\bar{c}_0$	2AI	2AO	2AT		
5K	top	0.79	(-6.3±0.4)%	(6.9±1.2)%	(-0.5±1.6)%		
	bot	1.26	(2.8±1.2)%	(-3.1±1.5)%	(0.3±2.7)%		
10K	top	0.65	(-9.2±8.1)%	(10.9±6.2)%	(-1.7±4.1)%		
	bot	1.51	(5.5±3.8)%	(-6.8±2.5)%	(1.2±1.3)%		
18K	top	0.29	(-43±14)%	(29.5±0.9)%	(14±13)%		
	bot	2.08	(16.5±4.0)%	(-11.9±0.8)%	(-4.7±4.6)%		
Nucleobases, nucleosides, nucleotides							
Setting	fract ion j	$\bar{c}_j/\bar{c}_0$	A	C	G	T	U
NB	top	0.69	(16.3±3.5)%	(-20.4±4.4)%	(18.1±7.2)%	(-19.7±4.6)%	(5.7±1.4)%
	bot	1.46	(-11.6±3.6)%	(14.7±4.7)%	(-12.4±5.0)%	(14.3±4.4)%	(-5.1±1.0)%
rNS	top	0.72	(5.0±0.9)%	(-11.5±3.9)%	(6.5±3.3)%		(0.1±0.4)%
	bot	1.36	(-3.3±1.4)%	(7.0±3.3)%	(-3.5±1.9)%		(-0.2±0.1)%
5'-NMP	top	0.30	(6.1±0.7)%	(-7.3±0.1)%	(-4.2±1.2)%		(5.3±0.7)%
	bot	2.18	(-2.9±0.3)%	(3.1±0.1)%	(0.8±0.6)%		(-1.0±0.5)%
dNMP	top	0.19	(11.1±3.2)%	(-7.6±3.0)%	(5.1±1.2)%	(-8.6±2.1)%	
	bot	2.73	(-3.1±0.4)%	(2.1±0.2)%	(-1.8±0.2)%	(2.8±0.1)%	
2',3'-NMP	top	0.36	(8.9±0.6)%	(-22.4±0.7)%	(13.0±0.0)%		(0.5±0.5)%
	bot	2.32	(-3.4±0.4)%	(8.5±1.0)%	(-5.0±0.7)%		(-0.1±0.1)%
3',5'-NMP	top	0.41	(6.9±1.2)%	(-5.3±0.8)%	(1.9±2.4)%		(-3.5±2.3)%
	bot	2.27	(-3.2±0.3)%	(1.7±1.8)%	(-1.4±1.1)%		(2.9±1.0)%
3',5'-NMP 10% Form.	top	0.16	(2.6±0.5)%	(-23.1±3.5)%	(14.5±2.9)%		(6.0±0.7)%
	bot	3.14	(-0.5±0.1)%	(4.5±1.0)%	(-2.7±0.6)%		(-1.2±0.3)%
Nucleobases in various pH & buffers							
Setting	fract ion j	$\bar{c}_j/\bar{c}_0$	A	C	G	T	U
pH3	top	0.65	(8.8±0.6)%	(0.4±1.8)%	(20.6±1.4)%	(-31.0±0.3)%	(1.2±1.3)%
	bot	1.34	(-10.9±2.3)%	(-13.9±1.5)%	(-16.8±0.5)%	(34.9±0.1)%	(6.7±3.5)%
pH4	top	0.80	(3.8±0.5)%	(0.6±5.4)%	(16.9±9.7)%	(-20±12)%	(-1.8±3.8)%
	bot	1.27	(-3.3±1.1)%	(8.0±3.5)%	(-16±10)%	(13.4±8.7)%	(-2.1±1.0)%
pH5	top	0.47	(26.6±7.2)%	(-30.7±6.9)%	(25.0±4.0)%	(-30.3±6.0)%	(9.4±1.7)%
	bot	1.59	(-15.1±2.1)%	(17.9±2.3)%	(-13.6±1.7)%	(17.4±2.3)%	(-6.6±1.0)%
pH7	top	0.68	(16.3±3.7)%	(-20.3±3.4)%	(17.2±14.6)%	(-17.3±3.8)%	(4.0±3.6)%
	bot	1.29	(-8.4±3.1)%	(9.8±1.2)%	(-8.4±1.0)%	(9.1±2.0)%	(-2.2±1.1)%
pH10	top	0.48	(33.1±4.5)%	(-10.0±1.0)%	(10.7±2.9)%	(-27.1±2.5)%	(-6.7±0.4)%

	bot	1.97	(-20.0±1.0)%	(-4.6±2.2)%	(-4.0±2.6)%	(19.6±0.5)%	(9.1±0.7)%
pH11	top	0.79	(17.7±2.5)%	(-10.1±3.6)%	(10.0±2.4)%	(-14.2±2.2)%	(-3.4±0.6)%
	bot	1.25	(-21.2±4.1)%	(14.7±8.7)%	(-11.3±2.4)%	(16.2±2.0)%	(1.6±2.9)%
127µm	top	0.80	(9.3±1.8)%	(-12.5±0.7)%	(10.4±4.6)%	(-11.1±1.2)%	(3.9±1.2)%
	bot	1.22	(-7.1±0.5)%	(9.2±1.2)%	(-6.9±3.4)%	(8.1±1.8)%	(-3.3±0.3)%
150µm	top	0.65	(17.2±2.6)%	(-22.0±1.8)%	(19.0±0.4)%	(-20.9±2.8)%	(6.7±1.9)%
	bot	1.49	(-11.9±2.9)%	(14.3±2.7)%	(-10.0±1.6)%	(13.5±3.6)%	(-5.9±1.8)%
200µm	top	0.54	(27.0±9.8)%	(-32.9±8.7)%	(30.6±6.7)%	(-31.5±9.6)%	(6.8±3.9)%
	bot	1.38	(-13.9±7.4)%	(17.1±8.0)%	(-14.0±4.9)%	(15.6±7.6)%	(-4.9±3.5)%
10% Forma mide	top	0.26	(7.2±4.8)%	(-29.6±5.6)%	(27.7±2.1)%	(-15.0±4.0)%	(9.7±2.7)%
	bot	2.29	(-5.0±2.3)%	(17.4±6.0)%	(-13.0±4.0)%	(8.4±3.4)%	(-7.7±3.2)%
100mM PO4	top	0.40	(34.2±7.9)%	(-33.2±9.2)%	(9±10)%	(-29.1±6.6)%	(19.1±2.5)%
	bot	1.81	(-14.3±3.7)%	(21.9±2.5)%	(-16.2±3.2)%	(17.6±0.5)%	(-9.0±1.9)%
10% Methan ol	top	0.94	(1.4±0.7)%	(-2.0±0.7)%	(1.9±1.1)%	(-1.5±0.7)%	(0.2±0.8)%
	bot	1.10	(-1.6±1.3)%	(2.4±1.5)%	(-2.4±1.5)%	(1.9±0.8)%	(-0.3±0.8)%
Nucleobases, nucleotides after 6 hours							
Setting	fract ion j	$\overline{c_j/c_0}$	A	C	G	T	U
NB	top	0.84	(6.0±2.7)%	(-7.1±1.9)%	(4.6±0.4)%	(-6.1±1.9)%	(2.6±1.0)%
	bot	1.21	(-6.6±2.0)%	(6.3±0.9)%	(-2.8±1.1)%	(5.9±1.2)%	(-2.7±0.9)%
rNS	top	0.70	(2.3±0.7)%	(-8.7±2.0)%	(7.7±3.6)%		(-1.3±1.0)%
	bot	1.30	(-2.8±0.5)%	(5.1±0.4)%	(-1.4±1.4)%		(-0.9±0.6)%
5'- NMP	top	0.65	(1.7±0.8)%	(-2.4±1.2)%	(-1.7±1.4)%		(2.4±0.6)%
	bot	1.56	(-1.8±0.7)%	(1.4±0.7)%	(2.3±0.7)%		(-2.0±0.1)%
2',3'- NMPs	top	0.57	(4.3±1.5)%	(-6.9±3.7)%	(2.0±2.5)%		(0.6±0.4)%
	bot	1.67	(-2.6±0.6)%	(5.2±1.5)%	(-2.3±1.0)%		(-0.3±0.1)%

Supplementary Table 3: List of coefficients of determination, slopes and standard deviations of linear fits of LC and IC methods

The coefficient of determination is calculated as $R^2 = 1 - \frac{\sum_{i=1}^n (y_i - f(x_i))^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$ with y_i the measured values, $f(x_i)$ the predicted value from the fitted slope, $\bar{y}$ the mean value of the measured slope and $i=1 \dots n$ the individual calibration measurements. The values are used for measurements of nucleobases, nucleosides, nucleotides, 2-aminoazoles and trimetaphosphate as described in Methods.

Set of molecules	Species	R ² (linear fit)	Slope (linear fit)	Error (linear fit)
Nucleobases (μAU*s/μM)	A	0.999946	6817.31	25.10
	C	0.999991	2729.11	4.00
	G	0.999861	1295.07	7.64
	U	0.999958	4331.60	13.97
	T	0.999992	3820.38	5.38
Nucleosides (μAU*s/μM)	A	0.999969	8478.40	23.59
	C	0.999966	3545.42	10.37
	G	0.999954	7947.92	26.81
	U	0.999960	5435.43	17.15
5'- Ribonucleotides (μAU*s/μM)	A	0.999963	6266.74	19.04
	C	0.999958	2773.21	8.99
	G	0.999969	5044.92	14.06
	U	0.999975	3047.74	7.68
2',3'- Ribonucleotides (μAU*s/μM)	A	0.999984	6285.21	12.51
	C	0.999974	4551.70	11.50
	G	0.999976	7937.32	19.31
	U	0.999981	5272.32	11.57
3',5'- Ribonucleotides (μAU*s/μM)	A	0.999971	8257.57	25.88
	C	0.999980	3428.16	8.93
	G	0.998556	5910.68	129.79
	U	0.997852	6211.76	166.41
Deoxyribo- nucleotides (μAU*s/μM)	A	0.999981	3402.14	7.41
	C	0.999981	3171.54	6.87
	G	0.999956	6302.40	20.87
	T	0.999968	4478.07	12.57
AMPs (μAU*s/μM)	2'-AMP	0.999980	2050.85	4.64
	3'-AMP	0.999981	6633.92	14.35
CMPs (μAU*s/μM)	2'-CMP	0.999934	3878.25	18.24
	3'-CMP	0.999957	2745.52	10.42
2AZ (nAU*min/μM)	2AI	0.975984	8492.38	769.13
	2AO	0.994395	8922.18	386.75
	2AT	0.999316	2222.47	33.57

Supplementary Table 4: List of coefficients of determination, slopes and standard deviations of linear fits of LC methods for amino acids.

Exemplary sets of calibrations are shown on pages 135-165. ED refers to Extended Data; S refers to the Supplementary Information. In each category, F references to figures, T to tables. The calibration used for the analysis of Glycine dimerization is partially shown here and partially at the end of the Supplementary Information. R^2 is defined as in Supplementary Table 3.

for measurements:			Species	R^2	slope (linear fit) counts*min/ μ M, W / Y: mAU*min/ μ M Gly / GlyGly: μ AU*min/mM	range of calibration (μ M)	
Fig.	Ext.	Suppl.				min	max
2	EDF3 EDF8 EDT1	SF7 ST6 ST29 ST32	A	0.984	4753	5	75
			C	0.984	415	5	75
			D	0.973	4625	5	75
			E	0.982	4335	5	75
			F	0.992	5432	5	75
			G	0.989	5555	5	75
			H	0.991	3299	5	75
			I	0.989	6911	5	75
			K	0.980	3632	5	75
			L	0.989	5928	5	75
			M	0.993	1106	5	75
			N	0.988	5076	5	75
			P	0.989	1452	5	75
			Q	0.990	4727	5	75
			R	0.991	3134	5	75
			S	0.990	4926	5	75
			T	0.991	5476	5	75
			V	0.982	6529	5	75
			W	0.987	0.0076	5	75
			Y	0.991	0.0080	5	75
4 (0K 16K)	EDF6	SF4 SF5 ST14 ST15	A	0.985	11963	2	500
			C	0.977	1507	2	500
			F	0.986	15084	2	500
			G	0.987	15002	2	500
			I	0.993	17736	2	500
			L	0.987	18440	2	500
			N	0.995	13338	2	500
			P	0.987	3898	2	500
			S	0.992	14064	2	500
			T	0.987	16080	2	500
			V	0.992	16030	2	500
4 (10K)		SF5 ST14 ST15	A	0.997	18781	2	500
			C	0.978	3558	2	500
			F	0.997	19950	2	500
			I	0.997	26016	2	500
			L	0.998	23086	2	500
			N	0.998	17121	2	500

			P	0.998	5922	2	500
			T	0.997	20305	2	500
			V	0.992	23707	2	500
			A	0.969	14386	5	60
			C	0.975	1385	5	60
			D	0.966	11099	5	60
			E	0.970	10808	5	60
			F	0.977	15219	5	60
			H	0.956	8977	5	60
			I	0.976	20888	5	60
			K	0.975	10569	5	60
			L	0.951	18271	5	60
			N	0.979	11051	5	60
			P	0.976	4190	5	60
			Q	0.974	11513	5	60
			S	0.948	14032	5	60
			T	0.972	15502	5	60
			V	0.974	19218	5	60
5c left		ST18	Gly	0.995	617.4	500	20000
			GlyGly	0.981	341.3	2.5	10000
5b		ST17	Gly	0.998	see pages 166-167 (in counts*min vs mM)		
5c right		ST20	GlyGly	0.992			

Supplementary Table 5: Raw data Fig. 2a – 2-aminoazoles in water, 170 μ m, 18 h, 18 K.

Per repeat (k), fraction ($j \in \{\text{top, II, III, bot}\}$) and species, we analyse the HPLC data to obtain “measured values”. Using the calibration shown in Supplementary Table 3, we calculate the corresponding “concentration (μ M)” $[A]_{j,k,HPLC}$. Per species and repeat, we calculate an average total concentration over all fraction (c_0) which we use to normalize our data (“ $[A]_{j,k}$ concentration ($\times c_0$)”) to be able to compare runs and species with different concentrations. Per fraction, we can thus determine a mean concentration $\bar{c}_{j,k}$. Against this mean concentration, we calculate the “ratio species vs mean” (as introduced in Eq. 4 in the Methods). The averages and errors of those are shown in Supplementary Table 2. Furthermore, we directly compare species against species (right-most columns) for the top and bottom fraction. The average and standard deviations of those are shown in the heat maps in Fig. 2-3, Extended Data Fig. 2-5 and Supplementary Fig. 1-3.

repeat k	species	measured values (mAU*min)				concentration (μ M) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 3				c_0 (μ M)	Normalization (Eq. 1) $[A]_{j,k}$ concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)		Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)							
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)				bot part (red shade)			
1	2AO	0.143	0.278	0.329	0.647	15.98	31.17	36.92	72.5	39.14	0.41	0.8	0.94	1.85	29.08	-10.72	2AO	0	1.61	194.19	2AO	0	0.15	-26.56
	2AT	0.031	0.051	0.082	0.141	13.81	23.13	36.99	63.58	34.38	0.4	0.67	1.08	1.85	27.04	-10.85	2AT	-1.58	0	189.52	2AT	-0.15	0	-26.67
	2AI	0.050	0.204	0.279	0.910	5.9	24.02	32.9	107.2	42.51	0.14	0.57	0.77	2.52	-56.12	21.57	2AI	-66.01	-65.46	0	2AI	36.16	36.37	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.32	0.68	0.93	2.07				2AO	2AT	2AI		2AO	2AT	2AI
2	2AO	0.179	0.309	0.494	0.752	20.03	34.62	55.42	84.34	48.6	0.41	0.71	1.14	1.74	28.76	-12.19	2AO	0	34.73	70.15	2AO	0	-12.45	-21.53
	2AT	0.027	0.050	0.102	0.176	12.19	22.41	45.85	79.01	39.87	0.31	0.56	1.15	1.98	-4.43	0.29	2AT	-25.77	0	26.3	2AT	14.22	0	-10.38
	2AI	0.125	0.234	0.563	1.141	14.71	27.58	66.33	134.3	60.73	0.24	0.45	1.09	2.21	-24.33	11.9	2AI	-41.23	-20.82	0	2AI	27.44	11.58	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.32	0.58	1.13	1.98				2AO	2AT	2AI		2AO	2AT	2AI
3	2AO	0.150	0.284	0.550	0.910	16.81	31.8	61.64	102.03	53.07	0.32	0.6	1.16	1.92	30.77	-12.68	2AO	0	9.92	160.23	2AO	0	-9.52	-24.84
	2AT	0.030	0.049	0.115	0.220	13.41	22.05	51.79	98.85	46.52	0.29	0.47	1.11	2.12	18.97	-3.49	2AT	-9.02	0	136.74	2AT	10.52	0	-16.93
	2AI	0.070	0.162	0.595	1.467	8.22	19.08	70.07	172.7	67.52	0.12	0.28	1.04	2.56	-49.75	16.18	2AI	-61.57	-57.76	0	2AI	33.05	20.38	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.24	0.45	1.1	2.2				2AO	2AT	2AI		2AO	2AT	2AI

Supplementary Table 6: Raw data Fig. 2b and Extended Data Fig. 3 – AA in water, 170 μ m, 18 h, pH 7.4.

Samples were injected 2-3 times and the mean concentration was used to calculate the normalized concentrations and enrichments (following tables). Calibrations are shown in Supplementary Table 4 and at the end of the Supplementary Information (pages 135-154).

repeat k	species	measured values (counts*min) for W and Y: mAU*min				measured values (counts*min) for W and Y: mAU*min				measured values (counts*min) for W and Y: mAU*min				concentration (μ M) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 4				c_0 (μ M)	Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)	
		top	II	III	bot	top	II	III	bot	top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot
1	H	34236	65431	113293	132221	36382	67925	118823	138230					10.70	20.21	35.18	40.98	26.77	0.40	0.75	1.31	1.53	11.3	-3.7
	N	68489	105096	169019	166371	71260	110150	178744	173497					13.77	21.20	34.26	33.48	25.68	0.54	0.83	1.33	1.30	49.3	-18.0
	S	73581	114278	178598	181273	76036	120354	187252	190450					15.19	23.81	37.13	37.73	28.46	0.53	0.84	1.30	1.33	48.5	-16.7
	Q	63435	97669	157164	154095	64696	102286	164591	161260					13.55	21.15	34.03	33.36	25.52	0.53	0.83	1.33	1.31	47.8	-17.8
	R	30462	63237	109290	141583	31657	65929	113552	148480					9.91	20.60	35.55	46.27	28.08	0.35	0.73	1.27	1.65	-1.8	3.6
	G	91090	135703	185619	182435	95079	141649	195603	192302					16.76	24.96	34.31	33.73	27.44	0.61	0.91	1.25	1.23	70.0	-22.7
	D	35610	62979	163833	172103	37590	65133	172021	182014					7.91	13.85	36.31	38.28	24.09	0.33	0.57	1.51	1.59	-8.5	-0.1
	E	29726	57542	155133	170993	30598	61041	164472	178843					6.96	13.68	36.86	40.35	24.46	0.28	0.56	1.51	1.65	-20.8	3.7
	T	54663	99848	192941	214999	53579	104756	203098	224493					9.88	18.68	36.16	40.13	26.21	0.38	0.71	1.38	1.53	5.0	-3.7
	A	47345	83438	170334	175737	50012	87447	178964	183333					10.24	17.98	36.75	37.77	25.69	0.40	0.70	1.43	1.47	11.0	-7.5
	P	8710	20337	50488	64711	9326	21305	52630	66842					6.21	14.34	35.50	45.29	25.33	0.25	0.57	1.40	1.79	-31.8	12.4
	C	4076	8385	15561	17618	4181	8545	16678	19315					9.95	20.41	38.86	44.52	28.44	0.35	0.72	1.37	1.57	-2.5	-1.6
	K	31694	56463	134067	129117	32450	58361	138858	134901					8.83	15.81	37.57	36.34	24.64	0.36	0.64	1.52	1.48	-0.2	-7.2
	M	6888	16098	38357	45872	7019	16598	40168	48109					6.29	14.79	35.51	42.50	24.77	0.25	0.60	1.43	1.72	-29.3	7.9
	V	49349	103411	246673	292075	44521	88469	226343	297284					7.19	14.70	36.23	45.14	25.81	0.28	0.57	1.40	1.75	-22.5	10.0
	I	29670	79746	234895	330117	30791	84457	247654	346622					4.37	11.88	34.91	48.96	25.03	0.17	0.47	1.39	1.96	-51.3	23.0
	L	28663	73764	203375	278285	29959	77718	214416	289835					4.94	12.78	35.24	47.92	25.22	0.20	0.51	1.40	1.90	-45.4	19.5
	F	35543	84698	186591	262090	37403	88338	196470	274163					6.71	15.93	35.26	49.36	26.82	0.25	0.59	1.31	1.84	-30.3	15.7
	Y	0.1188	0.1912	0.2877	0.3170	0.1274	0.1990	0.3057	0.3325					15.33	24.30	36.95	40.44	29.26	0.52	0.83	1.26	1.38	45.9	-13.1
	W	0.0387	0.1114	0.2711	0.3642	0.0408	0.1147	0.2789	0.3730					5.25	14.94	36.34	48.71	26.31	0.20	0.57	1.38	1.85	-44.4	16.4

	mean concentration per fraction $\bar{c}_{j,k}$																		0.36	0.68	1.38	1.59		
2	H	43629	60589	93184	194818	25819	43891	90408	207775	46676	64625	98510	205958	11.73	17.08	28.50	61.48	29.70	0.40	0.58	0.96	2.07	11.4	-7.1
	N	90482	115634	153551	248928	62984	91687	156481	254336	97421	122929	161592	262087	16.48	21.69	30.97	50.26	29.85	0.55	0.73	1.04	1.68	55.7	-24.5
	S	95317	123204	164412	254838	90422	102615	163231	260112	102092	131070	172767	268052	19.48	24.15	33.86	52.98	32.62	0.60	0.74	1.04	1.62	68.4	-27.1
	Q	83358	107017	144161	234753	55562	82727	145056	237905	88579	114626	150951	247805	16.04	21.46	31.04	50.81	29.84	0.54	0.72	1.04	1.70	51.7	-23.6
	R	35737	51001	86741	203339	18669	34963	84069	222142	38662	55318	89470	214384	9.90	15.02	27.68	68.05	30.16	0.33	0.50	0.92	2.26	-7.4	1.2
	G	123544	146465	179840	239970	114254	128383	180146	248600	132831	154857	188421	252725	22.24	25.78	32.91	44.48	31.35	0.71	0.82	1.05	1.42	100.1	-36.4
	D	46298	73032	129731	308275	26408	44469	113589	291130	49836	77235	134498	324495	8.83	14.03	27.23	66.58	29.17	0.30	0.48	0.93	2.28	-14.6	2.4
	E	38821	62346	115078	313900	19239	34829	97313	285283	40848	64954	120228	326894	7.61	12.47	25.58	71.21	29.22	0.26	0.43	0.88	2.44	-26.6	9.3
	T	70161	98107	158385	349426	39464	66395	150411	351760	72379	101213	166505	369338	11.08	16.17	28.93	65.16	30.34	0.37	0.53	0.95	2.15	3.0	-3.7
	A	67293	92053	145650	295295	43869	65056	137537	284783	71008	97650	153592	310232	12.78	17.87	30.63	62.44	30.93	0.41	0.58	0.99	2.02	16.5	-9.4
	P	12134	18734	35990	111473	5475	9982	31678	106404	13131	18853	37702	117014	7.05	10.92	24.18	76.86	29.75	0.24	0.37	0.81	2.58	-33.1	15.9
	C	5710	7225	12602	28045	2544	4845	12659	31132	5540	7922	12610	28322	11.09	16.07	30.44	70.32	31.98	0.35	0.50	0.95	2.20	-2.2	-1.4
	K	48300	67309	112484	243019	31150	48685	108965	234861	50704	70400	117969	257243	11.94	17.10	31.15	67.46	31.91	0.37	0.54	0.98	2.11	5.6	-5.2
	M	12164	15570	29897	77878	6872	10858	27181	77624	12180	17351	33883	80715	9.41	13.20	27.43	71.22	30.31	0.31	0.44	0.90	2.35	-12.4	5.4
	V	50087	74047	178470	538090	29094	54198	120561	468598	47095	74663	173715	581482	6.45	10.36	24.14	81.09	30.51	0.21	0.34	0.79	2.66	-40.4	19.2
	I	39149	64450	142840	594453	15019	29241	115029	541826	41558	68166	150649	627295	4.62	7.81	19.70	85.06	29.30	0.16	0.27	0.67	2.90	-55.5	30.2
	L	37666	60526	130280	496892	15492	29806	107533	459164	40127	62812	136081	523036	5.25	8.61	21.02	83.17	29.51	0.18	0.29	0.71	2.82	-49.9	26.4
	F	42452	65479	130634	414791	17710	35356	114510	417078	44966	69669	135717	437900	6.45	10.46	23.37	77.92	29.55	0.22	0.35	0.79	2.64	-38.4	18.3
	Y																							
	W	0.0731	0.1049	0.2152	0.5432	0.0250	0.0662	0.1840	0.5677	0.0668	0.1049	0.2136	0.5636	7.27	12.15	26.99	73.76	30.04	0.24	0.40	0.90	2.46	-31.8	10.1
	mean concentration per fraction $\bar{c}_{j,k}$																		0.35	0.51	0.91	2.23		
3	H	35350	73935	103728	175591	36558	77148	110076	186128					10.90	22.90	32.40	54.82	30.25	0.36	0.76	1.07	1.81	11.2	-8.2
	N	81941	132925	167352	222500	85843	139006	177123	236965					16.53	26.79	33.93	45.26	30.63	0.54	0.87	1.11	1.48	66.5	-25.2
	S	93402	136689	192163	246511	97023	142205	202762	259661					19.33	28.31	40.08	51.37	34.77	0.56	0.81	1.15	1.48	71.5	-25.2
	Q	73063	123660	156793	211947	75909	127758	165093	221778					15.76	26.59	34.05	45.88	30.57	0.52	0.87	1.11	1.50	59.1	-24.0
	R	27317	65857	95518	181800	28193	68498	100065	190266					8.85	21.43	31.20	59.35	30.21	0.29	0.71	1.03	1.96	-9.5	-0.5

	G	121545	154734	196642	221589	124914	161870	206731	233403					22.18	28.50	36.31	40.95	31.98	0.69	0.89	1.14	1.28	114.0	-35.1
	D	42114	103188	154527	311047	42916	107627	161062	326898					9.19	22.79	34.11	68.96	33.76	0.27	0.67	1.01	2.04	-16.0	3.4
	E	30518	88417	140549	305997	30976	89566	149182	321422					7.09	20.53	33.42	72.37	33.35	0.21	0.62	1.00	2.17	-34.4	9.9
	T	56282	122256	178663	321170	56449	127759	188812	334837					10.29	22.83	33.55	59.90	31.64	0.33	0.72	1.06	1.89	0.4	-4.1
	A	59467	115234	167029	281046	60598	120031	176522	294781					12.63	24.75	36.14	60.58	33.53	0.38	0.74	1.08	1.81	16.3	-8.5
	P	9099	25360	40619	102215	9667	26562	42898	106486					6.46	17.87	28.75	71.84	31.23	0.21	0.57	0.92	2.30	-36.2	16.5
	C	4219	10235	14776	27015	4420	10921	15432	26913					10.42	25.50	36.42	65.01	34.34	0.30	0.74	1.06	1.89	-6.4	-4.1
	K	37249	87710	124982	233825	37523	90725	132188	243587					10.29	24.56	35.40	65.72	33.99	0.30	0.72	1.04	1.93	-6.6	-2.1
	M	7032	19225	29882	69113	7263	20065	32168	70894					6.47	17.77	28.06	63.32	28.90	0.22	0.61	0.97	2.19	-31.0	11.0
	V	49902	113462	173147	475252	33435	107393	189191	483698					6.38	16.91	27.75	73.44	31.12	0.21	0.54	0.89	2.36	-36.7	19.5
	I	22592	90859	163044	536241	24144	94571	170034	563344					3.38	13.42	24.10	79.55	30.11	0.11	0.45	0.80	2.64	-65.3	33.8
	L	23437	83940	146347	448525	23688	88143	152199	468736					3.97	14.51	25.18	77.37	30.26	0.13	0.48	0.83	2.56	-59.5	29.5
	F	28822	89481	143122	368553	28586	91937	150325	386964					5.28	16.70	27.01	69.55	29.64	0.18	0.56	0.91	2.35	-45.0	18.9
	Y	0.1420	0.2239	0.2962	0.4419	0.1475	0.2360	0.3183	0.4660					18.03	28.64	38.26	56.54	35.37	0.51	0.81	1.08	1.60	57.3	-19.0
	W	0.0378	0.1355	0.2259	0.4963	0.0342	0.1349	0.2123	0.4979					4.76	17.87	28.96	65.69	29.32	0.16	0.61	0.99	2.24	-49.9	13.5
	mean concentration per fraction $\bar{c}_{j,k}$																		0.32	0.69	1.01	1.97		
4	H	45825	85648	88616	148568	47842	89163	93376	157360					14.19	26.49	27.58	46.36	28.66	0.50	0.92	0.96	1.62	13.4	-4.8
	N	74937	131331	122000	180905	79025	138552	129201	191844					15.17	26.59	24.75	36.72	25.80	0.59	1.03	0.96	1.42	34.6	-16.3
	S	77666	132596	124999	191592	81677	139553	131414	203252					16.17	27.62	26.02	40.07	27.47	0.59	1.01	0.95	1.46	34.8	-14.2
	Q	68950	124182	114137	171366	73007	128812	119140	179753					15.02	26.76	24.68	37.14	25.90	0.58	1.03	0.95	1.43	32.8	-15.6
	R	42921	84426	95049	170742	44641	89001	100092	179842					13.97	27.66	31.13	55.92	32.17	0.43	0.86	0.97	1.74	-0.6	2.3
	G	98021	144752	141205	193846	104081	150061	148111	204671					18.19	26.54	26.04	35.87	26.66	0.68	1.00	0.98	1.35	56.3	-20.8
	D	43266	109459	88802	181863	45505	114368	94100	191598					9.60	24.20	19.77	40.37	23.48	0.41	1.03	0.84	1.72	-6.4	1.2
	E	38122	104017	85082	181290	39488	107962	89152	191252					8.95	24.45	20.10	42.97	24.12	0.37	1.01	0.83	1.78	-15.0	4.8
	T	66431	141188	132638	233667	69393	148258	139691	244864					12.40	26.43	24.87	43.69	26.85	0.46	0.98	0.93	1.63	5.8	-4.2
	A	54449	116983	105478	181257	57956	123308	110571	190832					11.83	25.28	22.73	39.14	24.74	0.48	1.02	0.92	1.58	9.4	-6.9
	P	13645	34311	33444	69074	14044	35694	35403	72416					9.53	24.10	23.70	48.71	26.51	0.36	0.91	0.89	1.84	-17.7	8.1

	C	5453	12645	12359	21289	5702	12977	12485	22114					13.45	30.89	29.95	52.32	31.65	0.42	0.98	0.95	1.65	-2.7	-2.7
	K	32266	87705	70471	134611	33523	90963	73529	140568					9.06	24.59	19.82	37.88	22.84	0.40	1.08	0.87	1.66	-9.2	-2.4
	M	10610	25518	25436	50758	10880	27832	27958	52680					9.72	24.13	24.15	46.78	26.19	0.37	0.92	0.92	1.79	-15.0	5.1
	V	57791	188823	144903	324768	55011	155562	151191	330095					8.64	26.38	22.68	50.15	26.96	0.32	0.98	0.84	1.86	-26.6	9.5
	I	50777	150472	146717	368152	53103	158181	154632	389284					7.52	22.33	21.80	54.80	26.61	0.28	0.84	0.82	2.06	-35.3	21.2
	L	46307	132160	128911	308729	48924	138774	135242	325708					8.03	22.85	22.28	53.51	26.67	0.30	0.86	0.84	2.01	-31.0	18.1
	F	57999	136276	145757	313618	60901	142057	152601	328707					10.94	25.62	27.46	59.13	30.79	0.36	0.83	0.89	1.92	-18.6	13.0
	Y	0.1457	0.2411	0.2609	0.4034	0.1480	0.2561	0.2756	0.4251					18.29	30.96	33.41	51.60	33.56	0.54	0.92	1.00	1.54	24.8	-9.5
	W	0.0633	0.1845	0.2065	0.4332	0.0689	0.1974	0.2205	0.4531					8.74	25.23	28.21	58.56	30.19	0.29	0.84	0.93	1.94	-33.7	14.2
	mean concentration per fraction $\bar{c}_{j,k}$																			0.44	0.95	0.91	1.70	

Supplementary Table 7: Raw data Fig. 2b and Extended Data Fig. 3 – AA in water, 170 μ m, 18 h, pH 7.4 – enrichments in top fraction
Shown in the top right triangle.

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)																				
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
1	A	H	0.0	-25.4	-25.1	-24.7	13.3	-34.5	21.7	40.6	6.0	0.3	63.1	14.2	11.6	57.5	43.5	128.8	103.9	59.7	-23.7	100.3
		N	34.1	0.0	0.5	1.0	51.9	-12.2	63.2	88.5	42.2	34.5	118.7	53.2	49.6	111.2	92.5	206.8	173.5	114.1	2.3	168.6
		S	33.4	-0.5	0.0	0.5	51.2	-12.6	62.4	87.6	41.5	33.8	117.7	52.4	48.9	110.1	91.5	205.3	172.1	113.1	1.8	167.2
		Q	32.8	-1.0	-0.5	0.0	50.5	-13.0	61.6	86.7	40.8	33.2	116.6	51.7	48.2	109.2	90.7	203.9	170.8	112.1	1.3	166.0
		R	-11.7	-34.2	-33.9	-33.5	0.0	-42.2	7.4	24.1	-6.4	-11.5	44.0	0.8	-1.5	39.0	26.7	101.9	80.0	40.9	-32.7	76.8
		G	52.7	13.9	14.5	15.0	73.1	0.0	85.9	114.7	62.0	53.1	149.1	74.5	70.4	140.5	119.2	249.4	211.5	143.9	16.5	205.9
		D	-17.8	-38.7	-38.4	-38.1	-6.9	-46.2	0.0	15.5	-12.9	-17.6	34.0	-6.1	-8.3	29.4	18.0	88.0	67.6	31.2	-37.3	64.6
		E	-28.9	-46.9	-46.7	-46.4	-19.4	-53.4	-13.4	0.0	-24.6	-28.7	16.0	-18.7	-20.6	12.0	2.1	62.8	45.1	13.6	-45.7	42.5
		T	-5.7	-29.7	-29.3	-29.0	6.8	-38.3	14.8	32.6	0.0	-5.4	53.8	7.7	5.2	48.5	35.4	115.8	92.3	50.6	-28.0	88.9
		A	-0.3	-25.6	-25.3	-24.9	13.0	-34.7	21.4	40.2	5.8	0.0	62.7	13.9	11.3	57.1	43.2	128.2	103.4	59.2	-23.9	99.8
		P	-38.7	-54.3	-54.1	-53.8	-30.5	-59.9	-25.4	-13.8	-35.0	-38.5	0.0	-30.0	-31.6	-3.5	-12.0	40.3	25.0	-2.1	-53.2	22.8
		C	-12.4	-34.7	-34.4	-34.1	-0.8	-42.7	6.6	23.1	-7.2	-12.2	42.8	0.0	-2.3	37.9	25.7	100.3	78.5	39.8	-33.2	75.4
		K	-10.4	-33.2	-32.8	-32.5	1.6	-41.3	9.1	26.0	-4.9	-10.1	46.2	2.4	0.0	41.2	28.7	105.1	82.8	43.1	-31.6	79.5
		M	-36.5	-52.6	-52.4	-52.2	-28.1	-58.4	-22.7	-10.7	-32.7	-36.3	3.6	-27.5	-29.2	0.0	-8.8	45.3	29.5	1.4	-51.5	27.2
		V	-30.3	-48.1	-47.8	-47.5	-21.1	-54.4	-15.2	-2.1	-26.1	-30.2	13.6	-20.4	-22.3	9.7	0.0	59.4	42.1	11.2	-46.8	39.5
		I	-56.3	-67.4	-67.2	-67.1	-50.5	-71.4	-46.8	-38.6	-53.7	-56.2	-28.7	-50.1	-51.2	-31.2	-37.3	0.0	-10.9	-30.2	-66.6	-12.5
		L	-51.0	-63.4	-63.2	-63.1	-44.4	-67.9	-40.3	-31.1	-48.0	-50.8	-20.0	-44.0	-45.3	-22.8	-29.6	12.2	0.0	-21.7	-62.6	-1.8
		F	-37.4	-53.3	-53.1	-52.8	-29.0	-59.0	-23.8	-12.0	-33.6	-37.2	2.2	-28.5	-30.1	-1.4	-10.1	43.3	27.7	0.0	-52.2	25.4
		Y	31.1	-2.3	-1.8	-1.3	48.5	-14.2	59.5	84.2	39.0	31.4	113.8	49.7	46.2	106.4	88.1	199.8	167.2	109.3	0.0	162.5
		W	-50.1	-62.8	-62.6	-62.4	-43.4	-67.3	-39.2	-29.8	-47.1	-49.9	-18.6	-43.0	-44.3	-21.4	-28.3	14.2	1.8	-20.3	-61.9	0.0
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
		B																				
2	A	H	0.0	-28.4	-33.8	-26.5	20.4	-44.3	30.5	51.7	8.2	-4.4	66.6	13.9	5.5	27.2	86.9	150.7	122.3	80.9		63.3
		N	39.7	0.0	-7.6	2.7	68.2	-22.2	82.3	112.0	51.1	33.6	132.8	59.2	47.5	77.8	161.2	250.2	210.6	152.8		128.2
		S	51.2	8.2	0.0	11.1	82.0	-15.8	97.2	129.4	63.5	44.6	151.8	72.2	59.5	92.3	182.5	278.9	236.0	173.5		146.9
		Q	36.1	-2.6	-10.0	0.0	63.9	-24.2	77.6	106.5	47.2	30.2	126.8	55.1	43.7	73.2	154.4	241.2	202.5	146.3		122.3
		R	-16.9	-40.6	-45.0	-39.0	0.0	-53.7	8.4	26.0	-10.1	-20.6	38.4	-5.3	-12.3	5.7	55.3	108.2	84.6	50.3		35.7
		G	79.6	28.5	18.8	31.9	116.2	0.0	134.3	172.5	94.2	71.7	199.1	104.6	89.5	128.5	235.6	350.1	299.1	224.9		193.3
		D	-23.4	-45.1	-49.3	-43.7	-7.7	-57.3	0.0	16.3	-17.1	-26.7	27.7	-12.7	-19.1	-2.5	43.3	92.1	70.3	38.7		25.2
		E	-34.1	-52.8	-56.4	-51.6	-20.7	-63.3	-14.0	0.0	-28.7	-37.0	9.8	-24.9	-30.4	-16.2	23.2	65.2	46.5	19.2		7.6
		T	-7.6	-33.8	-38.8	-32.1	11.3	-48.5	20.6	40.3	0.0	-11.6	54.0	5.3	-2.4	17.6	72.8	131.7	105.5	67.3		51.0
		A	4.6	-25.2	-30.8	-23.2	25.9	-41.8	36.4	58.7	13.1	0.0	74.2	19.2	10.4	33.0	95.5	162.1	132.4	89.2		70.8
		P	-40.0	-57.0	-60.3	-55.9	-27.7	-66.6	-21.7	-8.9	-35.1	-42.6	0.0	-31.6	-36.6	-23.6	12.2	50.5	33.4	8.6		-2.0
		C	-12.2	-37.2	-41.9	-35.5	5.6	-51.1	14.5	33.2	-5.1	-16.1	46.2	0.0	-7.4	11.7	64.0	120.0	95.0	58.8		43.3
		K	-5.3	-32.2	-37.3	-30.4	14.1	-47.2	23.6	43.8	2.5	-9.4	57.8	8.0	0.0	20.5	77.1	137.5	110.6	71.4		54.7
		M	-21.4	-43.8	-48.0	-42.3	-5.4	-56.2	2.5	19.3	-15.0	-24.8	30.9	-10.4	-17.0	0.0	46.9	97.0	74.7	42.2		28.4

		V	-46.5	-61.7	-64.6	-60.7	-35.6	-70.2	-30.2	-18.8	-42.1	-48.8	-10.9	-39.0	-43.5	-31.9	0.0	34.1	18.9	-3.2		-12.6
		I	-60.1	-71.4	-73.6	-70.7	-52.0	-77.8	-47.9	-39.5	-56.8	-61.8	-33.5	-54.5	-57.9	-49.2	-25.4	0.0	-11.3	-27.8		-34.8
		L	-55.0	-67.8	-70.2	-66.9	-45.8	-74.9	-41.3	-31.7	-51.3	-57.0	-25.0	-48.7	-52.5	-42.8	-15.9	12.8	0.0	-18.6		-26.5
		F	-44.7	-60.4	-63.4	-59.4	-33.5	-69.2	-27.9	-16.1	-40.2	-47.2	-7.9	-37.0	-41.7	-29.7	3.3	38.5	22.8	0.0		-9.7
		Y																				
		W	-38.8	-56.2	-59.5	-55.0	-26.3	-65.9	-20.1	-7.1	-33.8	-41.4	2.0	-30.2	-35.4	-22.1	14.5	53.5	36.1	10.8		0.0
			H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
			B																			
3	A	H	0.0	-33.3	-35.2	-30.1	22.9	-48.1	32.3	69.4	10.7	-4.4	74.1	18.8	19.0	61.0	75.6	220.8	174.2	102.0	-29.3	122.0
		N	49.8	0.0	-2.9	4.7	84.1	-22.2	98.2	153.8	65.9	43.2	160.9	77.9	78.2	141.3	163.1	380.6	310.8	202.6	5.9	232.5
		S	54.3	3.0	0.0	7.8	89.6	-19.9	104.2	161.4	70.9	47.5	168.7	83.2	83.6	148.5	171.0	395.0	323.1	211.7	9.0	242.5
		Q	43.1	-4.5	-7.3	0.0	75.9	-25.7	89.3	142.4	58.5	36.8	149.2	69.9	70.2	130.5	151.4	359.1	292.4	189.1	1.1	217.6
		R	-18.6	-45.7	-47.3	-43.1	0.0	-57.7	7.7	37.8	-9.9	-22.2	41.7	-3.4	-3.2	31.0	42.9	161.0	123.1	64.4	-42.5	80.6
		G	92.5	28.5	24.8	34.5	136.6	0.0	154.8	226.1	113.2	84.1	235.3	128.7	129.1	210.1	238.2	517.6	428.0	288.9	36.1	327.3
		D	-24.4	-49.6	-51.0	-47.2	-7.1	-60.7	0.0	28.0	-16.3	-27.7	31.6	-10.3	-10.1	21.7	32.7	142.4	107.2	52.7	-46.6	67.7
		E	-41.0	-60.6	-61.7	-58.7	-27.4	-69.3	-21.9	0.0	-34.6	-43.6	2.8	-29.9	-29.8	-4.9	3.7	89.4	61.9	19.3	-58.3	31.0
		T	-9.7	-39.7	-41.5	-36.9	11.0	-53.1	19.5	53.0	0.0	-13.7	57.3	7.2	7.4	45.4	58.6	189.7	147.6	82.4	-36.2	100.4
		A	4.6	-30.2	-32.2	-26.9	28.5	-45.7	38.4	77.2	15.8	0.0	82.1	24.2	24.4	68.4	83.7	235.5	186.8	111.3	-26.1	132.1
		P	-42.6	-61.7	-62.8	-59.9	-29.4	-70.2	-24.0	-2.7	-36.4	-45.1	0.0	-31.8	-31.7	-7.5	0.9	84.2	57.5	16.0	-59.4	27.5
		C	-15.8	-43.8	-45.4	-41.2	3.5	-56.3	11.4	42.6	-6.8	-19.5	46.6	0.0	0.2	35.6	47.9	170.1	130.9	70.1	-40.5	86.9
		K	-15.9	-43.9	-45.5	-41.3	3.3	-56.3	11.2	42.4	-6.9	-19.6	46.4	-0.2	0.0	35.4	47.6	169.6	130.5	69.8	-40.6	86.6
		M	-37.9	-58.6	-59.8	-56.6	-23.7	-67.7	-17.8	5.2	-31.2	-40.6	8.1	-26.3	-26.1	0.0	9.1	99.2	70.3	25.4	-56.1	37.8
		V	-43.1	-62.0	-63.1	-60.2	-30.0	-70.4	-24.7	-3.6	-37.0	-45.6	-0.9	-32.4	-32.3	-8.3	0.0	82.6	56.1	15.0	-59.8	26.4
		I	-68.8	-79.2	-79.8	-78.2	-61.7	-83.8	-58.8	-47.2	-65.5	-70.2	-45.7	-63.0	-62.9	-49.8	-45.2	0.0	-14.5	-37.0	-78.0	-30.8
		L	-63.5	-75.7	-76.4	-74.5	-55.2	-81.1	-51.7	-38.2	-59.6	-65.1	-36.5	-56.7	-56.6	-41.3	-35.9	17.0	0.0	-26.3	-74.2	-19.1
		F	-50.5	-67.0	-67.9	-65.4	-39.2	-74.3	-34.5	-16.2	-45.2	-52.7	-13.8	-41.2	-41.1	-20.3	-13.0	58.8	35.7	0.0	-65.0	9.9
		Y	41.5	-5.5	-8.3	-1.1	73.9	-26.5	87.2	139.7	56.7	35.3	146.4	68.0	68.3	127.9	148.6	353.9	288.0	185.9	0.0	214.1
		W	-54.9	-69.9	-70.8	-68.5	-44.6	-76.6	-40.4	-23.7	-50.1	-56.9	-21.5	-46.5	-46.4	-27.4	-20.9	44.5	23.5	-9.0	-68.2	0.0
4	A		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
			B																			
		H	0.0	-15.7	-15.9	-14.6	14.1	-27.4	21.2	33.4	7.2	3.6	37.8	16.6	24.9	33.5	54.6	75.4	64.5	39.3	-9.1	71.2
		N	18.7	0.0	-0.2	1.4	35.4	-13.9	43.8	58.3	27.2	23.0	63.5	38.3	48.2	58.4	83.4	108.1	95.1	65.3	7.9	103.1
		S	18.8	0.2	0.0	1.5	35.6	-13.7	44.1	58.6	27.4	23.2	63.7	38.6	48.5	58.7	83.7	108.4	95.4	65.6	8.0	103.4
		Q	17.1	-1.4	-1.5	0.0	33.5	-15.0	41.9	56.2	25.5	21.3	61.3	36.5	46.2	56.3	80.9	105.3	92.5	63.1	6.4	100.4
		R	-12.3	-26.1	-26.2	-25.1	0.0	-36.4	6.2	17.0	-6.0	-9.2	20.7	2.2	9.5	17.0	35.5	53.7	44.2	22.1	-20.3	50.0
		G	37.8	16.1	15.9	17.7	57.2	0.0	67.0	83.8	47.7	42.8	89.8	60.6	72.1	83.9	112.9	141.6	126.6	92.0	25.2	135.8
		D	-17.5	-30.5	-30.6	-29.5	-5.9	-40.1	0.0	10.1	-11.5	-14.5	13.6	-3.8	3.1	10.1	27.5	44.7	35.7	15.0	-25.0	41.2
		E	-25.1	-36.8	-36.9	-36.0	-14.5	-45.6	-9.2	0.0	-19.6	-22.3	3.2	-12.6	-6.4	0.0	15.8	31.4	23.2	4.4	-31.9	28.3
		T	-6.7	-21.4	-21.5	-20.3	6.4	-32.3	13.0	24.4	0.0	-3.3	28.5	8.7	16.5	24.5	44.2	63.6	53.4	29.9	-15.2	59.6
		A	-3.5	-18.7	-18.8	-17.6	10.1	-30.0	17.0	28.8	3.5	0.0	32.9	12.5	20.5	28.8	49.1	69.2	58.7	34.4	-12.3	65.1
		P	-27.4	-38.8	-38.9	-38.0	-17.2	-47.3	-12.0	-3.1	-22.2	-24.8	0.0	-15.4	-9.3	-3.1	12.2	27.3	19.4	1.2	-34.0	24.3
		C	-14.2	-27.7	-27.8	-26.7	-2.1	-37.7	4.0	14.5	-8.0	-11.1	18.2	0.0	7.1	14.5	32.6	50.4	41.1	19.5	-22.0	46.8

	K	-19.9	-32.5	-32.6	-31.6	-8.7	-41.9	-3.0	6.8	-14.2	-17.0	10.3	-6.7	0.0	6.9	23.8	40.4	31.7	11.6	-27.2	37.0
	M	-25.1	-36.9	-37.0	-36.0	-14.5	-45.6	-9.2	0.0	-19.7	-22.4	3.2	-12.7	-6.4	0.0	15.8	31.4	23.2	4.4	-31.9	28.2
	V	-35.3	-45.5	-45.6	-44.7	-26.2	-53.0	-21.6	-13.7	-30.6	-33.0	-10.9	-24.6	-19.2	-13.6	0.0	13.5	6.4	-9.9	-41.2	10.7
	I	-43.0	-52.0	-52.0	-51.3	-35.0	-58.6	-30.9	-23.9	-38.9	-40.9	-21.5	-33.5	-28.8	-23.9	-11.9	0.0	-6.2	-20.6	-48.2	-2.4
	L	-39.2	-48.8	-48.8	-48.1	-30.6	-55.9	-26.3	-18.9	-34.8	-37.0	-16.2	-29.1	-24.0	-18.8	-6.0	6.6	0.0	-15.3	-44.7	4.1
	F	-28.2	-39.5	-39.6	-38.7	-18.1	-47.9	-13.0	-4.2	-23.0	-25.6	-1.1	-16.3	-10.4	-4.2	10.9	25.9	18.0	0.0	-34.8	22.8
	Y	10.0	-7.3	-7.4	-6.0	25.5	-20.1	33.4	46.8	18.0	14.0	51.6	28.3	37.4	46.9	70.1	93.0	80.9	53.3	0.0	88.3
	W	-41.6	-50.8	-50.8	-50.1	-33.3	-57.6	-29.2	-22.0	-37.4	-39.4	-19.5	-31.9	-27.0	-22.0	-9.7	2.5	-3.9	-18.6	-46.9	0.0
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
		B																			

Supplementary Table 8: Raw data Fig. 2b and Extended Data Fig. 3 – AA in water, 170 μm, 18 h, pH 7.4 – enrichments in bottom fraction
Shown in the bottom left triangle.

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)																				
1	A	H	0.0	17.4	15.5	17.2	-7.1	24.6	-3.7	-7.2	0.0	4.1	-14.4	-2.2	3.8	-10.8	-12.4	-21.7	-19.4	-16.8	10.8	-17.3
		N	-14.8	0.0	-1.6	-0.2	-20.9	6.1	-18.0	-21.0	-14.8	-11.3	-27.1	-16.7	-11.6	-24.0	-25.4	-33.3	-31.4	-29.2	-5.7	-29.6
		S	-13.4	1.7	0.0	1.4	-19.6	7.8	-16.6	-19.6	-13.4	-9.9	-25.9	-15.3	-10.1	-22.7	-24.2	-32.2	-30.2	-28.0	-4.1	-28.4
		Q	-14.6	0.2	-1.4	0.0	-20.7	6.3	-17.8	-20.8	-14.6	-11.1	-26.9	-16.5	-11.4	-23.8	-25.3	-33.2	-31.2	-29.0	-5.5	-29.4
		R	7.6	26.4	24.3	26.1	0.0	34.0	3.7	-0.1	7.6	12.0	-7.8	5.2	11.7	-4.0	-5.8	-15.8	-13.3	-10.5	19.2	-11.0
		G	-19.7	-5.7	-7.3	-5.9	-25.4	0.0	-22.7	-25.5	-19.7	-16.4	-31.2	-21.5	-16.7	-28.4	-29.7	-37.2	-35.3	-33.2	-11.1	-33.6
		D	3.8	21.9	19.9	21.6	-3.5	29.3	0.0	-3.7	3.8	8.1	-11.1	1.5	7.7	-7.4	-9.1	-18.7	-16.4	-13.7	15.0	-14.2
		E	7.7	26.5	24.5	26.2	0.1	34.2	3.8	0.0	7.8	12.2	-7.7	5.4	11.8	-3.9	-5.7	-15.7	-13.2	-10.4	19.3	-10.9
		T	0.0	17.4	15.5	17.1	-7.1	24.5	-3.7	-7.2	0.0	4.1	-14.4	-2.2	3.8	-10.8	-12.5	-21.7	-19.4	-16.8	10.7	-17.3
		A	-3.9	12.8	11.0	12.5	-10.7	19.6	-7.5	-10.8	-3.9	0.0	-17.7	-6.1	-0.3	-14.3	-15.9	-24.8	-22.6	-20.1	6.4	-20.6
		P	16.8	37.1	34.9	36.8	8.5	45.4	12.5	8.4	16.8	21.6	0.0	14.2	21.2	4.2	2.2	-8.6	-5.9	-2.9	29.3	-3.4
		C	2.3	20.1	18.1	19.8	-5.0	27.4	-1.5	-5.1	2.3	6.5	-12.4	0.0	6.1	-8.7	-10.5	-20.0	-17.6	-14.9	13.3	-15.4
		K	-3.7	13.1	11.3	12.9	-10.5	20.0	-7.2	-10.6	-3.6	0.3	-17.5	-5.8	0.0	-14.0	-15.6	-24.6	-22.4	-19.9	6.7	-20.3
		M	12.1	31.6	29.4	31.3	4.1	39.6	8.0	4.0	12.1	16.7	-4.0	9.6	16.3	0.0	-1.9	-12.3	-9.7	-6.8	24.1	-7.3
		V	14.2	34.1	31.9	33.8	6.1	42.3	10.0	6.0	14.2	18.9	-2.2	11.7	18.5	1.9	0.0	-10.6	-8.0	-5.0	26.5	-5.5
		I	27.7	50.0	47.6	49.7	18.7	59.1	23.1	18.6	27.8	33.0	9.4	24.9	32.6	14.0	11.9	0.0	2.9	6.3	41.5	5.7
		L	24.1	45.7	43.4	45.4	15.3	54.6	19.6	15.2	24.1	29.2	6.3	21.4	28.8	10.7	8.7	-2.9	0.0	3.2	37.4	2.6
		F	20.2	41.2	38.9	40.8	11.7	49.8	15.8	11.6	20.2	25.2	3.0	17.6	24.8	7.3	5.3	-5.9	-3.1	0.0	33.2	-0.6
		Y	-9.7	6.0	4.3	5.8	-16.1	12.5	-13.0	-16.2	-9.7	-6.0	-22.7	-11.7	-6.3	-19.4	-20.9	-29.3	-27.2	-24.9	0.0	-25.3
	W	20.9	42.0	39.7	41.7	12.4	50.6	16.5	12.2	20.9	25.9	3.6	18.2	25.5	7.9	5.9	-5.4	-2.6	0.6	33.9	0.0	
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
		B																				
2	A	H	0.0	22.9	27.4	21.6	-8.2	45.9	-9.3	-15.1	-3.6	2.5	-19.9	-5.9	-2.1	-11.9	-22.1	-28.7	-26.5	-21.5		-15.7
		N	-18.7	0.0	3.7	-1.1	-25.4	18.7	-26.2	-30.9	-21.6	-16.6	-34.8	-23.4	-20.3	-28.3	-36.6	-42.0	-40.2	-36.1		-31.4
		S	-21.5	-3.5	0.0	-4.6	-28.0	14.5	-28.8	-33.4	-24.4	-19.5	-37.1	-26.1	-23.2	-30.9	-38.9	-44.1	-42.4	-38.4		-33.8
		Q	-17.7	1.1	4.8	0.0	-24.5	20.0	-25.4	-30.1	-20.7	-15.7	-34.1	-22.6	-19.4	-27.5	-35.9	-41.4	-39.6	-35.4		-30.6
		R	9.0	34.0	38.9	32.5	0.0	59.0	-1.2	-7.4	5.0	11.8	-12.7	2.6	6.7	-4.0	-15.1	-22.3	-19.9	-14.4		-8.1
		G	-31.5	-15.7	-12.7	-16.7	-37.1	0.0	-37.8	-41.8	-34.0	-29.7	-45.1	-35.5	-32.9	-39.6	-46.6	-51.1	-49.7	-46.2		-42.2
		D	10.3	35.6	40.5	34.1	1.2	60.9	0.0	-6.4	6.3	13.1	-11.6	3.8	8.0	-2.8	-14.1	-21.4	-19.0	-13.4		-7.0
		E	17.7	44.8	50.1	43.2	8.0	71.8	6.8	0.0	13.5	20.7	-5.6	10.8	15.3	3.7	-8.3	-16.0	-13.5	-7.6		-0.7
		T	3.8	27.6	32.2	26.2	-4.8	51.4	-5.9	-11.9	0.0	6.4	-16.8	-2.3	1.6	-8.6	-19.2	-26.0	-23.8	-18.5		-12.5
		A	-2.5	19.9	24.3	18.6	-10.5	42.3	-11.6	-17.2	-6.0	0.0	-21.8	-8.2	-4.5	-14.1	-24.0	-30.5	-28.4	-23.4		-17.8
		P	24.8	53.4	59.0	51.7	14.5	82.1	13.2	6.0	20.3	28.0	0.0	17.5	22.2	10.0	-2.8	-11.0	-8.3	-2.0		5.2
		C	6.2	30.6	35.4	29.2	-2.5	55.0	-3.7	-9.8	2.4	8.9	-14.9	0.0	4.0	-6.4	-17.3	-24.3	-22.0	-16.6		-10.4
		K	2.1	25.5	30.1	24.1	-6.3	49.0	-7.4	-13.3	-1.6	4.7	-18.2	-3.9	0.0	-10.0	-20.5	-27.2	-25.0	-19.8		-13.9
		M	13.5	39.5	44.6	38.0	4.1	65.6	2.9	-3.6	9.4	16.4	-9.0	6.8	11.1	0.0	-11.6	-19.1	-16.6	-10.9		-4.3

		V	28.4	57.8	63.6	56.1	17.8	87.3	16.4	9.0	23.7	31.7	2.9	20.9	25.7	13.1	0.0	-8.5	-5.7	0.8		8.3
		I	40.3	72.4	78.7	70.5	28.7	104.6	27.2	19.1	35.2	43.8	12.4	32.0	37.4	23.6	9.2	0.0	3.0	10.1		18.3
		L	36.1	67.4	73.5	65.5	24.9	98.6	23.5	15.6	31.2	39.6	9.1	28.1	33.3	19.9	6.0	-2.9	0.0	6.9		14.8
		F	27.4	56.6	62.3	54.9	16.9	85.9	15.5	8.2	22.8	30.6	2.1	19.9	24.7	12.2	-0.8	-9.2	-6.4	0.0		7.4
		Y																				
		W	18.6	45.8	51.1	44.2	8.8	73.0	7.6	0.7	14.3	21.6	-5.0	11.6	16.1	4.5	-7.6	-15.4	-12.9	-6.9		0.0
			H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
			B																			
3	A	H	0.0	22.6	22.6	20.7	-7.8	41.5	-11.3	-16.5	-4.3	0.3	-21.2	-4.3	-6.3	-17.3	-23.2	-31.4	-29.1	-22.8	13.3	-19.1
		N	-18.4	0.0	0.0	-1.5	-24.8	15.4	-27.6	-31.9	-21.9	-18.2	-35.8	-21.9	-23.6	-32.5	-37.4	-44.1	-42.2	-37.0	-7.6	-34.0
		S	-18.5	0.0	0.0	-1.6	-24.8	15.4	-27.7	-31.9	-22.0	-18.2	-35.8	-22.0	-23.6	-32.6	-37.4	-44.1	-42.2	-37.0	-7.6	-34.1
		Q	-17.2	1.6	1.6	0.0	-23.6	17.2	-26.5	-30.8	-20.7	-16.9	-34.8	-20.7	-22.4	-31.5	-36.4	-43.2	-41.3	-36.0	-6.1	-33.0
		R	8.4	32.9	33.0	30.9	0.0	53.4	-3.8	-9.5	3.8	8.7	-14.6	3.8	1.6	-10.3	-16.7	-25.6	-23.2	-16.3	22.9	-12.3
		G	-29.3	-13.4	-13.3	-14.7	-34.8	0.0	-37.3	-41.0	-32.4	-29.1	-44.3	-32.4	-33.8	-41.6	-45.7	-51.5	-49.9	-45.4	-19.9	-42.9
		D	12.7	38.2	38.2	36.1	4.0	59.5	0.0	-5.9	7.9	13.0	-11.2	7.9	5.6	-6.8	-13.4	-22.7	-20.1	-13.0	27.8	-8.8
		E	19.8	46.8	46.9	44.6	10.4	69.5	6.2	0.0	14.6	20.1	-5.7	14.6	12.2	-1.0	-8.1	-17.9	-15.1	-7.5	35.7	-3.2
		T	4.5	28.1	28.1	26.1	-3.7	47.8	-7.3	-12.8	0.0	4.8	-17.7	0.0	-2.1	-13.6	-19.8	-28.4	-26.0	-19.3	18.4	-15.5
		A	-0.3	22.3	22.3	20.4	-8.0	41.1	-11.5	-16.7	-4.5	0.0	-21.4	-4.6	-6.5	-17.5	-23.4	-31.6	-29.3	-23.0	13.0	-19.4
		P	27.0	55.7	55.7	53.3	17.1	79.7	12.6	6.0	21.5	27.3	0.0	21.5	19.0	5.0	-2.5	-12.9	-10.0	-2.0	43.9	2.7
		C	4.5	28.1	28.2	26.2	-3.6	47.9	-7.3	-12.7	0.0	4.8	-17.7	0.0	-2.1	-13.6	-19.8	-28.3	-25.9	-19.3	18.4	-15.5
		K	6.7	30.8	30.9	28.8	-1.6	51.0	-5.3	-10.9	2.1	7.0	-16.0	2.1	0.0	-11.8	-18.1	-26.8	-24.4	-17.6	20.9	-13.7
		M	20.9	48.2	48.3	46.0	11.5	71.1	7.3	1.0	15.7	21.2	-4.8	15.7	13.3	0.0	-7.2	-17.1	-14.3	-6.6	37.0	-2.2
		V	30.2	59.7	59.7	57.2	20.1	84.3	15.5	8.8	24.7	30.6	2.6	24.6	22.1	7.7	0.0	-10.7	-7.7	0.6	47.6	5.3
		I	45.8	78.8	78.8	76.0	34.5	106.3	29.4	21.8	39.6	46.2	14.8	39.5	36.7	20.6	12.0	0.0	3.3	12.6	65.3	17.9
		L	41.1	73.0	73.1	70.4	30.1	99.7	25.2	17.8	35.1	41.5	11.1	35.0	32.3	16.7	8.3	-3.2	0.0	9.0	59.9	14.1
		F	29.5	58.8	58.8	56.4	19.4	83.3	14.9	8.2	24.0	29.9	2.0	23.9	21.4	7.1	-0.6	-11.2	-8.2	0.0	46.8	4.7
		Y	-11.8	8.2	8.2	6.5	-18.6	24.9	-21.7	-26.3	-15.5	-11.5	-30.5	-15.6	-17.3	-27.0	-32.3	-39.5	-37.5	-31.9	0.0	-28.7
		W	23.7	51.6	51.7	49.3	14.0	75.0	9.7	3.3	18.4	24.0	-2.6	18.3	15.9	2.3	-5.0	-15.2	-12.4	-4.5	40.2	0.0
4	A		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
			B																			
		H	0.0	13.7	10.9	12.8	-6.9	20.2	-5.9	-9.2	-0.6	2.3	-11.9	-2.1	-2.5	-9.4	-13.0	-21.4	-19.4	-15.8	5.2	-16.6
		N	-12.0	0.0	-2.4	-0.8	-18.1	5.8	-17.2	-20.1	-12.6	-10.0	-22.6	-13.9	-14.2	-20.3	-23.5	-30.9	-29.1	-25.9	-7.4	-26.7
		S	-9.8	2.5	0.0	1.7	-16.1	8.4	-15.1	-18.1	-10.4	-7.8	-20.6	-11.8	-12.1	-18.3	-21.6	-29.2	-27.3	-24.0	-5.1	-24.8
		Q	-11.4	0.8	-1.7	0.0	-17.5	6.6	-16.6	-19.5	-11.9	-9.3	-21.9	-13.2	-13.5	-19.7	-22.9	-30.4	-28.5	-25.3	-6.7	-26.1
		R	7.4	22.2	19.2	21.2	0.0	29.2	1.1	-2.4	6.8	9.9	-5.4	5.2	4.8	-2.7	-6.6	-15.6	-13.4	-9.5	13.1	-10.4
		G	-16.8	-5.4	-7.8	-6.2	-22.6	0.0	-21.7	-24.5	-17.3	-14.9	-26.8	-18.6	-18.9	-24.7	-27.7	-34.7	-32.9	-29.9	-12.5	-30.6
		D	6.3	20.8	17.9	19.9	-1.1	27.8	0.0	-3.5	5.6	8.7	-6.4	4.0	3.6	-3.7	-7.6	-16.5	-14.3	-10.5	11.8	-11.4
		E	10.1	25.2	22.1	24.2	2.5	32.4	3.6	0.0	9.5	12.6	-3.0	7.8	7.4	-0.2	-4.2	-13.5	-11.2	-7.2	15.9	-8.2
		T	0.6	14.4	11.6	13.5	-6.4	21.0	-5.3	-8.7	0.0	2.9	-11.4	-1.5	-1.9	-8.9	-12.5	-21.0	-18.9	-15.3	5.9	-16.1
		A	-2.2	11.2	8.5	10.3	-9.0	17.6	-8.0	-11.2	-2.8	0.0	-13.9	-4.3	-4.6	-11.4	-15.0	-23.2	-21.2	-17.6	2.9	-18.5
		P	13.6	29.1	26.0	28.1	5.7	36.6	6.9	3.1	12.9	16.1	0.0	11.1	10.8	2.9	-1.2	-10.8	-8.4	-4.3	19.5	-5.3
		C	2.2	16.2	13.3	15.3	-4.9	22.9	-3.8	-7.2	1.6	4.5	-10.0	0.0	-0.3	-7.4	-11.1	-19.7	-17.6	-13.9	7.5	-14.8

	K	2.5	16.6	13.7	15.7	-4.6	23.3	-3.5	-6.9	1.9	4.8	-9.7	0.3	0.0	-7.1	-10.8	-19.5	-17.3	-13.6	7.9	-14.5
	M	10.4	25.5	22.4	24.5	2.7	32.7	3.9	0.2	9.7	12.9	-2.8	8.0	7.7	0.0	-4.0	-13.3	-11.0	-7.0	16.2	-7.9
	V	15.0	30.7	27.5	29.7	7.0	38.3	8.2	4.4	14.3	17.6	1.2	12.5	12.2	4.2	0.0	-9.7	-7.3	-3.1	21.0	-4.1
	I	27.3	44.7	41.2	43.6	18.5	53.0	19.8	15.6	26.5	30.2	12.1	24.6	24.2	15.3	10.7	0.0	2.6	7.2	34.0	6.1
	L	24.0	41.0	37.6	39.9	15.4	49.1	16.7	12.6	23.3	26.8	9.2	21.4	21.0	12.4	7.9	-2.6	0.0	4.5	30.5	3.4
	F	18.7	35.0	31.7	33.9	10.5	42.7	11.7	7.8	18.0	21.4	4.5	16.2	15.8	7.5	3.2	-6.7	-4.3	0.0	24.9	-1.0
	Y	-5.0	8.0	5.4	7.2	-11.6	14.3	-10.6	-13.7	-5.5	-2.8	-16.3	-7.0	-7.3	-13.9	-17.4	-25.3	-23.4	-20.0	0.0	-20.8
	W	19.9	36.3	33.0	35.3	11.6	44.2	12.9	8.9	19.2	22.6	5.6	17.4	17.0	8.6	4.3	-5.8	-3.3	1.0	26.2	0.0
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
		B																			

Supplementary Table 9: Raw data Fig. 3a and Extended Data Fig. 5a – nucleobases in water, 170µm, 18h

rep	eat	spe	k	measured values (µAU*min)				concentration (µM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (µM)	Normalization (Eq. 1)				Ratio species vs mean (Eq. 4)		Ratio species against species (shown in heat maps), Eq. 2											
													concentration (x c ₀)				[A] _{j,k} /c̄ _{j,k} – 1 (%)		[A] _{j,k} /[B] _{j,k} – 1 (%)											
				top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)						bot part (red shade)					
1	C			663.99	928.45	1173.02	2148.73	14.6	20.41	25.79	47.24	27.01	0.54	0.76	0.95	1.75	-22.82	18.78	C	0	-32.92	-39	-25.79	-0.04	C	0	37.07	45.68	25.74	0.17
	A			2384.36	2718.93	2957.58	3775.75	20.99	23.93	26.03	33.23	26.04	0.81	0.92	1	1.28	15.07	-13.35	A	49.09	0	-9.05	10.63	49.03	A	-27.05	0	6.28	-8.27	-26.92
	G			669.47	707.5	738.41	907.17	31.02	32.78	34.21	42.03	35.01	0.89	0.94	0.98	1.2	26.52	-18.47	G	63.93	9.95	0	21.65	63.86	G	-31.36	-5.91	0	-13.69	-31.24
	U			1385.64	1682.96	1895.22	2646.42	19.19	23.31	26.25	36.66	26.35	0.73	0.88	1	1.39	4.01	-5.54	U	34.75	-9.61	-17.8	0	34.7	U	-20.47	9.01	15.86	0	-20.34
	T			966.27	1361.15	1700.63	3120.4	15.18	21.38	26.71	49.01	28.07	0.54	0.76	0.95	1.75	-22.79	18.58	T	0.04	-32.9	-38.97	-25.76	0	T	-0.17	36.84	45.44	25.53	0
	mean concentration per fraction c̄ _{j,k}												0.7	0.85	0.98	1.47				C	A	G	U	T		C	A	G	U	T
2	C			522.74	745.92	881.15	2074.36	11.49	16.4	19.37	45.61	23.22	0.49	0.71	0.83	1.96	-24.12	17.28	C	0	-37.29	-36.18	-29.29	-1.28	C	0	37.79	34.03	24.83	0.95
	A			2105.14	2464.35	2296.27	3801.61	18.53	21.69	20.21	33.46	23.47	0.79	0.92	0.86	1.43	21.01	-14.89	A	59.47	0	1.77	12.75	57.44	A	-27.43	0	-2.73	-9.41	-26.74
	G			517.24	607.52	565.33	977.31	23.96	28.15	26.19	45.28	30.89	0.78	0.91	0.85	1.47	18.91	-12.5	G	56.7	-1.74	0	10.79	54.7	G	-25.39	2.81	0	-6.86	-24.68
	U			1185.18	1466.37	1456.3	2663.82	16.42	20.31	20.17	36.9	23.45	0.7	0.87	0.86	1.57	7.33	-6.05	U	41.43	-11.31	-9.74	0	39.63	U	-19.89	10.38	7.36	0	-19.13
	T			776.13	1108.52	1295.27	3011.8	12.19	17.41	20.34	47.3	24.31	0.5	0.72	0.84	1.95	-23.13	16.17	T	1.29	-36.48	-35.36	-28.38	0	T	-0.95	36.49	32.76	23.65	0
	mean concentration per fraction c̄ _{j,k}												0.65	0.82	0.85	1.67				C	A	G	U	T		C	A	G	U	T
3	C			682.94	996.45	1284.95	1480.68	15.01	21.91	28.25	32.55	24.43	0.61	0.9	1.16	1.33	-14.3	8.19	C	0	-24.05	-21.36	-18.89	-1.29	C	0	15.83	15.3	12.3	-0.06
	A			2221.35	2653.78	2948.17	3157.98	19.55	23.36	25.95	27.79	24.16	0.81	0.97	1.07	1.15	12.84	-6.6	A	31.66	0	3.54	6.79	29.96	A	-13.67	0	-0.46	-3.05	-13.72
	G			490.41	604.4	690.17	725.23	22.72	28	31.98	33.6	29.07	0.78	0.96	1.1	1.16	8.98	-6.17	G	27.16	-3.42	0	3.14	25.52	G	-13.27	0.46	0	-2.6	-13.32
	U			1323.38	1667.43	1923.32	2072.46	18.33	23.1	26.64	28.71	24.19	0.76	0.95	1.1	1.19	5.66	-3.66	U	23.29	-6.36	-3.04	0	21.7	U	-10.95	3.15	2.67	0	-11
	T			1007.24	1445.85	1861.29	2156.92	15.82	22.71	29.23	33.88	25.41	0.62	0.89	1.15	1.33	-13.18	8.25	T	1.31	-23.06	-20.33	-17.83	0	T	0.06	15.9	15.37	12.36	0
	mean concentration per fraction c̄ _{j,k}												0.72	0.93	1.12	1.23				C	A	G	U	T		C	A	G	U	T

Supplementary Table 10: Raw data Fig. 3b – adenosine and AMPs in water, 170µm, 18h

Due to technical problems, for the third replicate the temperature gradient was not applied for the entire duration of the experiment, which is why we do not take it into account for the calculation of the heat flow-driven enrichment.

rep eat k	spe cies	measured values (μAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				C ₀ (μM)	Normalization (Eq. 1) concentration (x C ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} /C̄ _{j,k} − 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} − 1 (%)															
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)								bot part (red shade)							
1	Ad o	3745.69	4798.81	4859.08	5498.03	26.51	33.96	34.39	38.91	33.44	0.79	1.02	1.03	1.16	33.99	-26.22	Ad o	0	44.21	56.97	47.54	71.64	72.96	Ad o	0	-29.43	-32.14	-29.61	-37.91	-38.28		
	5'	2233.92	3330.98	3991.21	6700.22	21.39	31.89	38.21	64.15	38.91	0.55	0.82	0.98	1.65	-7.09	4.54	5'	-30.66	0	8.85	2.31	19.02	19.94	5'	41.7	0	-3.85	-0.26	-12.02	-12.54		
	2'	534.36	846.23	1037.77	1814.44	15.63	24.76	30.36	53.08	30.96	0.5	0.8	0.98	1.71	-14.65	8.73	2'	-36.3	-8.13	0	-6.01	9.34	10.18	2'	47.37	4	0	3.73	-8.5	-9.04		
	3'	1247.72	1917.85	2285.14	3838.79	11.28	17.35	20.67	34.72	21	0.54	0.83	0.98	1.65	-9.19	4.82	3'	-32.22	-2.26	6.39	0	16.34	17.23	3'	42.07	0.26	-3.6	0	-11.79	-12.32		
	2',3'	1800.09	2826.62	3660.37	7304.36	17.18	26.98	34.94	69.73	37.21	0.46	0.73	0.94	1.87	-21.94	18.83	2',3'	-41.74	-15.98	-8.55	-14.04	0	0.77	2',3'	61.06	13.67	9.29	13.37	0	-0.59		
	3',5'	2531.16	3981.59	5167.52	10411.38	18.39	28.93	37.55	75.65	40.13	0.46	0.72	0.94	1.89	-22.53	19.54	3',5'	-42.18	-16.62	-9.24	-14.7	-0.76	0	3',5'	62.02	14.34	9.94	14.05	0.6	0		
	mean concentration per fraction C̄ _{j,k}										0.55	0.82	0.98	1.66				Ado	5'	2'	3'	2',3'	3',5'		Ado	5'	2'	3'	2',3'	3',5'		
2	Ad o	3862.07	3931.11	4175.67	5972.89	27.33	27.82	29.55	42.27	31.74	0.86	0.88	0.93	1.33	26.66	-26.65	Ad o	0	34.37	42.17	35.05	54.33	55.5	Ad o	0	-30.36	-33.22	-30.28	-38.1	-38.48		
	5'	2392.86	2568.85	2834.82	7140.5	22.91	24.6	27.14	68.37	35.75	0.64	0.69	0.76	1.91	-5.74	5.33	5'	-25.58	0	5.8	0.5	14.86	15.72	5'	43.6	0	-4.1	0.12	-11.12	-11.66		
	2'	583.69	636.98	712.66	1921.77	17.08	18.64	20.85	56.22	28.2	0.61	0.66	0.74	1.99	-10.91	9.84	2'	-29.66	-5.49	0	-5.01	8.56	9.37	2'	49.74	4.28	0	4.4	-7.31	-7.88		
	3'	1372.67	1484.13	1643.05	4111.9	12.41	13.42	14.86	37.19	19.47	0.64	0.69	0.76	1.91	-6.21	5.21	3'	-25.95	-0.5	5.27	0	14.28	15.14	3'	43.43	-0.12	-4.22	0	-11.22	-11.76		
	2',3'	1999.27	2169.7	2455.97	7709.24	19.09	20.71	23.45	73.59	34.21	0.56	0.61	0.69	2.15	-17.93	18.51	2',3'	-35.2	-12.93	-7.88	-12.5	0	0.75	2',3'	61.55	12.51	7.89	12.64	0	-0.61		
	3',5'	2807.7	3048.19	3451.08	10975.17	20.4	22.15	25.08	79.75	36.84	0.55	0.6	0.68	2.16	-18.55	19.24	3',5'	-35.69	-13.59	-8.57	-13.15	-0.75	0	3',5'	62.55	13.2	8.55	13.33	0.61	0		
	mean concentration per fraction C̄ _{j,k}										0.64	0.69	0.76	1.91				Ado	5'	2'	3'	2',3'	3',5'		Ado	5'	2'	3'	2',3'	3',5'		

Supplementary Table 11: Raw data Fig. 3c – Ribonucleosides in water, 170µm, 18h

rep	eat	spe	cies	measured values (µAU*s)				concentration (µM) $[A]_{j,k,HPLC}$				c_0 (µM)	Normalization (Eq. 1) concentration (x c_0)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)		Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)									
				top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)					bot part (red shade)				
1	C			42856	57126	87630	160202	12.09	16.11	24.72	45.19	24.53	0.49	0.66	1.01	1.84	-16.9	11.65	C	0	-16.51	-21.79	-25.22	C	0	12.04	17.68	19
	U			79997	97939	141268	222829	14.72	18.02	25.99	41	24.93	0.59	0.72	1.04	1.64	-0.47	-0.35	U	19.78	0	-6.32	-10.43	U	-10.75	0	5.03	6.21
	A			131148	156721	218736	325815	15.47	18.48	25.8	38.43	24.55	0.63	0.75	1.05	1.57	6.25	-5.12	A	27.87	6.75	0	-4.39	A	-15.02	-4.79	0	1.12
	G			115509	133861	180304	271329	14.53	16.84	22.69	34.14	22.05	0.66	0.76	1.03	1.55	11.12	-6.18	G	33.73	11.65	4.59	0	G	-15.97	-5.85	-1.11	0
	mean concentration per fraction $\bar{c}_{j,k}$												0.59	0.72	1.03	1.65				C	U	A	G		C	U	A	G
2	C			57422	74318	97539	110893	16.2	20.96	27.51	31.28	23.99	0.68	0.87	1.15	1.3	-9.75	5.01	C	0	-10.06	-13.77	-13.83	C	0	5.32	7.94	7.15
	U			100453	118881	150246	165666	18.48	21.87	27.64	30.48	24.62	0.75	0.89	1.12	1.24	0.34	-0.3	U	11.18	0	-4.13	-4.2	U	-5.05	0	2.48	1.73
	A			161163	184416	229067	248644	19.01	21.75	27.02	29.33	24.28	0.78	0.9	1.11	1.21	4.66	-2.72	A	15.97	4.3	0	-0.08	A	-7.36	-2.42	0	-0.73
	G			138500	158232	195151	215097	17.43	19.91	24.55	27.06	22.24	0.78	0.9	1.1	1.22	4.74	-2	G	16.05	4.38	0.08	0	G	-6.67	-1.7	0.74	0
	mean concentration per fraction $\bar{c}_{j,k}$												0.75	0.89	1.12	1.24				C	U	A	G		C	U	A	G
3	C			61659	71020	96802	102497	17.39	20.03	27.3	28.91	23.41	0.74	0.86	1.17	1.23	-7.93	4.22	C	0	-8.23	-11.54	-11.04	C	0	4.26	6.3	6.61
	U			106884	115185	149675	156395	19.66	21.19	27.54	28.77	24.29	0.81	0.87	1.13	1.18	0.33	-0.04	U	8.96	0	-3.62	-3.07	U	-4.09	0	1.95	2.25
	A			171403	179162	228648	237098	20.22	21.13	26.97	27.96	24.07	0.84	0.88	1.12	1.16	4.09	-1.95	A	13.05	3.75	0	0.56	A	-5.93	-1.92	0	0.29
	G			146640	155741	196546	203394	18.45	19.6	24.73	25.59	22.09	0.84	0.89	1.12	1.16	3.51	-2.24	G	12.42	3.17	-0.56	0	G	-6.2	-2.2	-0.29	0
	mean concentration per fraction $\bar{c}_{j,k}$												0.81	0.87	1.13	1.18				C	U	A	G		C	U	A	G

Supplementary Table 12: Raw data Fig. 3d – 5'-Ribonucleotides in water, 170µm, 18h

rep	eat	spe	cies	measured values (µAU*min)				concentration (µM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				C ₀ (µM)	Normalization (Eq. 1) concentration (x C ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} /C̄ _{j,k} – 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} – 1 (%)									
				top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)					bot part (red shade)				
1	C			311.46	448.32	1079.66	2466.9	6.74	9.7	23.36	53.37	23.29	0.29	0.42	1	2.29	-7.38	2.99	C	0	-13.42	-11.9	-2.81	C	0	6.37	3.47	2.31
	A			846.94	1193.24	2638.36	5460.1	8.11	11.42	25.26	52.28	24.27	0.33	0.47	1.04	2.15	6.97	-3.18	A	15.5	0	1.76	12.25	A	-5.99	0	-2.73	-3.81
	U			372.11	510.79	1140.31	2509.58	7.33	10.06	22.45	49.41	22.31	0.33	0.45	1.01	2.21	5.12	-0.46	U	13.5	-1.73	0	10.31	U	-3.35	2.81	0	-1.12
	G			482.99	721.47	1651.98	3633.94	5.74	8.58	19.65	43.22	19.3	0.3	0.44	1.02	2.24	-4.71	0.66	G	2.89	-10.92	-9.35	0	G	-2.26	3.96	1.13	0
	mean concentration per fraction C̄ _{j,k}												0.31	0.45	1.02	2.22				C	A	U	G		C	A	U	G
2	C			383.2	538.23	1426.77	2146.23	8.29	11.64	30.87	46.43	24.31	0.34	0.48	1.27	1.91	-7.33	3.23	C	0	-11.96	-11.37	-4.96	C	0	5.92	4.1	3.07
	A			1020.27	1397.84	3367.33	4749.7	9.77	13.38	32.24	45.48	25.22	0.39	0.53	1.28	1.8	5.26	-2.54	A	13.59	0	0.67	7.96	A	-5.59	0	-1.72	-2.69
	U			458.55	617.08	1504.48	2186.51	9.03	12.15	29.62	43.05	23.46	0.38	0.52	1.26	1.83	4.56	-0.84	U	12.83	-0.67	0	7.24	U	-3.94	1.75	0	-1
	G			601.16	841.33	2153.96	3104.92	7.15	10.01	25.62	36.93	19.93	0.36	0.5	1.29	1.85	-2.5	0.16	G	5.21	-7.37	-6.75	0	G	-2.97	2.77	1.01	0
	mean concentration per fraction C̄ _{j,k}												0.37	0.51	1.27	1.85				C	A	U	G		C	A	U	G
3	C			239.91	550.05	820.73	2802.29	5.19	11.9	17.76	60.63	23.87	0.22	0.5	0.74	2.54	-7.07	3.14	C	0	-12.5	-12.48	-1.85	C	0	6.19	4.99	1.61
	A			649.78	1464.37	2089.86	6253.99	6.22	14.02	20.01	59.88	25.03	0.25	0.56	0.8	2.39	6.21	-2.87	A	14.29	0	0.02	12.18	A	-5.83	0	-1.13	-4.31
	U			296.19	646.46	941.68	2883.92	5.83	12.73	18.54	56.77	23.47	0.25	0.54	0.79	2.42	6.18	-1.77	U	14.26	-0.02	0	12.15	U	-4.75	1.14	0	-3.22
	G			375.24	889.94	1275.76	4233.75	4.46	10.58	15.17	50.35	20.14	0.22	0.53	0.75	2.5	-5.32	1.5	G	1.88	-10.85	-10.83	0	G	-1.59	4.5	3.33	0
	mean concentration per fraction C̄ _{j,k}												0.23	0.53	0.77	2.46				C	A	U	G		C	A	U	G

Supplementary Table 13: Raw data Fig. 3e – Deoxyribonucleotides in water, 170μm, 18h

rep eat k	spe cies	measured values (μAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)									
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)					bot part (red shade)				
1	C	397.27	584.32	813.84	4692.53	7.52	11.05	15.4	88.77	30.69	0.24	0.36	0.5	2.89	-4.26	1.89	C	0	-11.39	-7.49	3.26	C	0	5	3.81	-0.99
	A	479.93	706.15	975.11	4783.78	8.46	12.45	17.2	84.37	30.62	0.28	0.41	0.56	2.76	8.05	-2.96	A	12.86	0	4.4	16.54	A	-4.76	0	-1.14	-5.71
	G	823.52	1246.19	1703.29	8668.96	7.84	11.86	16.22	82.53	29.61	0.26	0.4	0.55	2.79	3.49	-1.84	G	8.1	-4.22	0	11.62	G	-3.67	1.15	0	-4.62
	T	529.37	779.82	1096.56	6521.43	7.09	10.45	14.69	87.38	29.9	0.24	0.35	0.49	2.92	-7.28	2.91	T	-3.16	-14.19	-10.41	0	T	1	6.05	4.85	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.26	0.38	0.53	2.84				C	A	G	T		C	A	G	T
2	C	185.64	508.5	1537.77	4445.32	3.51	9.62	29.09	84.1	31.58	0.11	0.3	0.92	2.66	-12.09	2.37	C	0	-23.34	-16.33	-4.83	C	0	6.1	3.96	-0.31
	A	256.15	640.58	1734.58	4431.7	4.52	11.3	30.59	78.16	31.14	0.15	0.36	0.98	2.51	14.67	-3.52	A	30.44	0	9.14	24.14	A	-5.75	0	-2.02	-6.04
	G	415.02	1077.38	2998.93	7998.59	3.95	10.26	28.55	76.15	29.73	0.13	0.35	0.96	2.56	5.06	-1.53	G	19.52	-8.38	0	13.74	G	-3.81	2.06	0	-4.1
	T	266.83	698.93	2068.55	6099.3	3.58	9.36	27.72	81.72	30.59	0.12	0.31	0.91	2.67	-7.63	2.68	T	5.08	-19.45	-12.08	0	T	0.31	6.43	4.28	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.13	0.33	0.94	2.6				C	A	G	T		C	A	G	T
3	C	382.19	571.29	805.98	4714.74	7.23	10.81	15.25	89.19	30.62	0.24	0.35	0.5	2.91	-5.61	1.98	C	0	-12.51	-9.99	1.63	C	0	4.65	4.24	-0.74
	A	467.95	689.43	951.67	4825.79	8.25	12.16	16.78	85.11	30.58	0.27	0.4	0.55	2.78	7.89	-2.55	A	14.31	0	2.89	16.17	A	-4.44	0	-0.39	-5.15
	G	816.07	1237.11	1696.87	8693.16	7.77	11.78	16.15	82.76	29.62	0.26	0.4	0.55	2.79	4.86	-2.17	G	11.1	-2.81	0	12.91	G	-4.07	0.4	0	-4.78
	T	520.02	776.52	1087.61	6568.59	6.97	10.4	14.57	88.01	29.99	0.23	0.35	0.49	2.93	-7.13	2.74	T	-1.61	-13.92	-11.43	0	T	0.75	5.43	5.02	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.25	0.37	0.52	2.86				C	A	G	T		C	A	G	T
4	C	166.63	492.33	1542.28	4503.33	3.15	9.31	29.18	85.19	31.71	0.1	0.29	0.92	2.69	-8.55	2.28	C	0	-19.65	-14.46	4.15	C	0	5.76	4.15	-0.51
	A	216.14	607.39	1726.22	4437.74	3.81	10.71	30.44	78.26	30.81	0.12	0.35	0.99	2.54	13.82	-3.29	A	24.46	0	6.46	29.62	A	-5.45	0	-1.52	-5.93
	G	358.92	1036.52	2990.87	7967.02	3.42	9.87	28.47	75.85	29.4	0.12	0.34	0.97	2.58	6.91	-1.79	G	16.91	-6.07	0	21.75	G	-3.98	1.55	0	-4.47
	T	215.96	662.45	2061.8	6109.74	2.89	8.88	27.63	81.86	30.31	0.1	0.29	0.91	2.7	-12.19	2.8	T	-3.98	-22.85	-17.87	0	T	0.51	6.3	4.68	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.11	0.32	0.95	2.63				C	A	G	T		C	A	G	T

Supplementary Table 14: Raw data Fig. 4b-c – Experimental network, raw data

After recovery in fractions, we pre-column derivatized the samples and recorded the chromatograms in the fluorescence channel.

The sample designation corresponds to the scheme ‘#id#_#chamber#_#fraction# of #totalFractions#’, where #id# is the sample ID, #chamber# is the chamber number as shown in Figure 4a, #fraction# is the fraction number inside each chamber as shown in Figure 4a, and #totalFractions# is the total number of all fractions in the chamber.

dT	repeat	part	[N] (counts* min)	[S] (counts* min)	[G] (counts* min)	[T] (counts* min)	[A] (counts* min)	[P] (counts* min)	[C] (counts* min)	[V] (counts* min)	[I] (counts* min)	[L] (counts* min)	[F] (counts* min)
16.2	1	426_1_1 of 4	386057	390545	447855	296107	268060	36270	37194	165200	86755	102568	118872
16.2	1	426_1_2 of 4	420592	425577	439650	410337	365227	72446	48966	348217	248051	272722	268441
16.2	1	426_1_3 of 4	543682	551062	564611	580260	504453	125414	64069	626755	560455	578038	479063
16.2	1	426_1_4 of 4	489651	502696	501468	557997	485488	130563	59605	662280	638148	644313	509763
16.2	1	426_2_1 of 4	424517	426962	493041	322202	297955	36680	40458	198093	79708	98558	125302
16.2	1	426_2_2 of 4	409130	410934	389395	401430	360047	60568	45493	284374	141244	164799	198089
16.2	1	426_2_3 of 4	440892	460104	336199	687084	577043	148571	66710	675674	531442	583427	558549
16.2	1	426_2_4 of 4	374875	409883	250848	1038859	840339	574867	90600	2034305	2352434	2318265	1634601
16.2	1	426_3_1 of 4	306484	313259	268868	474214	398265	151375	66601	935018	1149305	1199211	788346
16.2	1	426_3_2 of 4	402010	416796	341176	649771	551818	225421	73846	1435239	2049713	2141321	1196869
16.2	1	426_3_3 of 4	508612	546603	440907	880019	749505	314895	78774	1853411	2773988	2759113	1480086
16.2	1	426_3_4 of 4	564675	613123	465040	1166703	996510	528393	87520	3250451	5458502	5016061	2338004
16.2	2	427_1_1 of 4	364139	350458	515004	167405	163999	12947	21881	139530	39328	46719	62827
16.2	2	427_1_2 of 4	369075	360537	440941	261604	241090	38645	32073	257877	146773	158395	153512
16.2	2	427_1_3 of 4	545416	549829	584706	530090	465496	107300	63783	563806	512603	526271	431141
16.2	2	427_1_4 of 4	459455	471755	461977	541281	464349	146611	60595	803797	885687	840095	567383
16.2	2	427_2_1 of 4	325474	322344	502583	161624	162398	20802	15376	180416	79539	85508	82993
16.2	2	427_2_2 of 4	422213	412597	585221	247127	232061	34037	22989	230402	129092	140829	138753
16.2	2	427_2_3 of 4	314764	322276	414719	233103	217403	40489	20147	273158	176969	185896	163244
16.2	2	427_2_4 of 4	545157	572529	581549	679090	588584	199526	56811	1061621	1205985	1143048	776106
16.2	2	427_3_1 of 4	605243	638724	590778	820788	704628	242101	74243	1216493	1256573	1254077	906721
16.2	2	427_3_2 of 4	825395	995216	868281	1294407	1123040	448685	111267	2278408	2623105	2529371	1695863
16.2	2	427_3_3 of 4	718783	772179	640355	1275168	1067895	520852	110972	2832286	3767652	3441098	2071985
16.2	2	427_3_4 of 4	638684	698600	538723	1397922	1148661	748321	111235	4572469	6950136	5915358	2960126
16.2	3	428_1_1 of 4	599466	600615	700248	410592	384435	38156	53982	186198	60489	78932	114888
16.2	3	428_1_2 of 4	474217	487674	520166	462320	409507	74410	48280	343657	216600	244822	252438
16.2	3	428_1_3 of 4	374134	377966	392137	399811	351043	86107	38610	469319	392622	399853	322379
16.2	3	428_1_4 of 4	407899	421993	404778	502100	432397	122199	49615	662383	639266	639491	491229
16.2	3	428_2_1 of 4	615344	611861	798217	369549	335273	40468	45531	191411	123953	138119	149039
16.2	3	428_2_2 of 4	603090	610203	744848	418593	381161	52368	48962	295287	188010	204034	200645
16.2	3	428_2_3 of 4	788182	801372	871516	692928	625363	124728	72600	585185	495473	521763	464474
16.2	3	428_2_4 of 4	734969	770151	702589	940036	841864	268428	95577	1287144	1383074	1339855	958924

16.2	3	428_3_1 of 4	551060	576864	511823	781146	674594	225784	78861	1233332	1412651	1421117	975243
16.2	3	428_3_2 of 4	399233	432416	346139	808124	695063	375996	59129	2323165	3612057	3155797	1606449
16.2	3	428_3_3 of 4	772294	812925	650814	1325134	1126790	476698	117400	2602380	3412954	3266290	2017916
16.2	3	428_3_4 of 4	876530	928230	715837	1683877	1397961	700837	140324	4115048	6024215	5495404	3066482
0	1	436_1_1 of 4	372672	323976	310101	370744	148599	52599	52922	277665	306083	307367	446996
0	1	436_1_2 of 4	263333	213093	195795	247777	85111	31936	40357	165715	179132	180113	333918
0	1	436_1_3 of 4	286968	235075	223182	273917	98450	36160	40518	192279	210817	207933	353187
0	1	436_1_4 of 4	315923	258256	239896	301362	104402	39883	46950	199120	215734	213658	392491
0	1	436_2_1 of 4	323293	265432	253327	307666	106715	40856	46503	208341	225965	225589	400680
0	1	436_2_2 of 4	306688	250011	239885	292636	108496	40447	41148	210458	231000	230458	373282
0	1	436_2_3 of 4	317517	258978	236746	303910	100767	37992	45293	199673	218677	217641	406682
0	1	436_2_4 of 4	342886	284485	270422	333569	120868	45167	48902	233024	255819	255353	418016
0	1	436_3_1 of 4	317991	264071	251433	305431	112689	42304	45263	216126	236489	237384	388715
0	1	436_3_2 of 4	308219	259149	244823	294979	113718	42068	44017	218584	239036	239099	366024
0	1	436_3_3 of 4	324094	264704	253420	307918	109878	42425	47272	214678	237358	237170	408869
0	1	436_3_4 of 4	323747	268593	256792	312363	114806	42789	46069	221745	241969	242200	395922
0	2	437_1_1 of 4	516070	528121	549846	573313	497105	136645	55231	708634	686261	682061	526698
0	2	437_1_2 of 4	523464	536660	556955	579703	511427	139496	57013	734052	696888	693118	533340
0	2	437_1_3 of 4	496072	504269	522211	553161	466016	130485	53868	674218	651528	642475	498559
0	2	437_1_4 of 4	487106	495030	515774	538851	450252	126934	53488	651159	633433	624415	486570
0	2	437_2_1 of 4	512456	524452	543735	567743	482409	136691	56122	691237	675555	670068	526401
0	2	437_2_2 of 4	530787	543879	567863	586586	515433	143793	58086	719057	701476	692389	531592
0	2	437_2_3 of 4	547914	560457	582130	606885	495866	144651	60385	709216	710060	705212	567366
0	2	437_2_4 of 4	437017	440261	450299	475488	371335	108839	49641	552301	536522	529856	458598
0	2	437_3_1 of 4	504008	517301	537748	560433	488523	133251	54713	710984	672428	667907	512269
0	2	437_3_2 of 4	508494	516824	536915	562803	453969	131551	56727	663191	648630	640181	512174
0	2	437_3_3 of 4	496981	509263	522400	552392	481576	131890	56599	709920	681875	679364	522457
0	2	437_3_4 of 4	529358	540972	561292	584334	508711	139150	57381	728576	700132	695567	535303
0	3	438_1_1 of 4	642056	671060	714761	723730	593229	175002	61793	792573	862741	853148	648638
0	3	438_1_2 of 4	469947	480290	500434	520576	429490	124401	52966	584037	623245	616334	472485
0	3	438_1_3 of 4	458701	462542	475481	500960	346239	109223	50704	519584	564072	559013	461951
0	3	438_1_4 of 4	446126	449112	459836	483283	320846	104075	49321	492872	533461	530754	448278
0	3	438_2_1 of 4	461625	467317	482703	505390	351500	112070	46978	523553	569428	564119	465950
0	3	438_2_2 of 4	444672	450925	465225	484395	391163	115976	47549	541996	573887	568074	442976
0	3	438_2_3 of 4	477413	491291	511301	530296	441876	127443	52576	598827	634091	630741	486054
0	3	438_2_4 of 4	475794	491798	502858	532189	454853	127272	54338	622637	650646	647316	504297
0	3	438_3_1 of 4	513516	528646	544710	579799	487327	137582	55852	647101	686363	677088	516111
0	3	438_3_2 of 4	553898	571475	593775	622611	538086	150215	62779	706289	745302	735899	562520
0	3	438_3_3 of 4	539123	554315	573595	601322	527618	144475	59441	701956	721372	714356	545357
0	3	438_3_4 of 4	577245	596126	613084	642695	566565	156759	64403	782875	773367	765426	576825
10.4	1	406_1_1 of 4	418024			349318	342384	74422	63257	344233	261566	243084	246405
10.4	1	406_1_2 of 4	433848			315012	317945	50846	68157	173821	121210	128520	167179

10.4	1	406_1_3 of 4	418137			458698	426601	118392	83995	566311	518335	463487	414675
10.4	1	406_1_4 of 4	571427			587802	545800	139218	110691	566131	564380	523550	489744
10.4	1	406_2_1 of 4	412407			263792	281100	46313	45890	210075	117984	117763	141260
10.4	1	406_2_2 of 4	546804			512908	491863	114563	92253	433651	381421	364325	378104
10.4	1	406_2_3 of 4	414746			475039	427174	125028	87502	513294	526201	483846	448397
10.4	1	406_2_4 of 4	855003			1282750	1128903	444194	232204	2078961	2476525	2123126	1666738
10.4	1	406_3_1 of 4	757316			1046167	918746	349857	201935	1678901	1919196	1668481	1302750
10.4	1	406_3_2 of 4	720884			998893	891776	343064	185325	1609374	1921281	1671277	1246038
10.4	1	406_3_3 of 4	670081			927426	832235	312327	174523	1480357	1744591	1490445	1141678
10.4	1	406_3_4 of 4	574319			868303	754675	319502	167348	1625632	2043176	1693117	1215611
10.4	2	407_1_1 of 4	467144			474589	444474	120878	97275	488363	512512	472264	431782
10.4	2	407_1_2 of 4	383867			410870	381600	108882	86045	442907	472477	433470	383414
10.4	2	407_1_3 of 4	598913			681528	630001	188761	130680	797553	868439	785257	667897
10.4	2	407_1_4 of 4	493803			581044	528493	166405	124825	722340	822270	734769	610839
10.4	2	407_2_1 of 4	504693			471479	444124	107072	91381	421544	420365	394913	381731
10.4	2	407_2_2 of 4	385882			370922	353844	87753	72027	353088	348045	335180	315018
10.4	2	407_2_3 of 4	538463			546254	514121	135858	107977	576745	627706	591684	542104
10.4	2	407_2_4 of 4	501469			607757	562492	183884	112999	837428	938422	829154	676045
10.4	2	407_3_1 of 4	589342			764410	691617	241249	142136	1055258	1197975	1049458	853487
10.4	2	407_3_2 of 4	801286			1148726	1012995	395639	221645	1859624	2196057	1914301	1446095
10.4	2	407_3_3 of 4	736986			1071687	913569	377451	217863	1751908	2166862	1821732	1385496
10.4	2	407_3_4 of 4	652315			1047126	917516	426625	216511	2201960	2874289	2352583	1601250
10.4	3	408_1_1 of 4	552084			284888	243643	45601	45733	155514	128590	129402	160323
10.4	3	408_1_2 of 4	376283			349473	331738	77032	67086	367640	294267	279027	280968
10.4	3	408_1_3 of 4	428469			444098	408609	111027	84547	457503	473249	435860	405737
10.4	3	408_1_4 of 4	456216			525814	447823	139503	102618	604345	663922	597855	539944
10.4	3	408_2_1 of 4	355032			271204	269824	57779	45714	236053	216135	206495	205411
10.4	3	408_2_2 of 4	447839			389727	376142	94882	65260	384683	392716	366239	336981
10.4	3	408_2_3 of 4	543954			533674	498586	139487	85905	605940	638358	589854	513585
10.4	3	408_2_4 of 4	401882			507421	460614	165772	81252	805956	946780	830934	614344
10.4	3	408_3_1 of 4	537992			667220	614842	202156	114854	919924	983975	913444	714654
10.4	3	408_3_2 of 4	674797			918396	795979	304122	157181	1371028	1610876	1385181	1090385
10.4	3	408_3_3 of 4	685488			944806	825732	333227	165620	1558088	1869797	1579267	1201335
10.4	3	408_3_4 of 4	732679			1109491	980919	425955	207745	2064843	2631999	2185245	1512471

Supplementary Table 15: Raw data Fig. 4b-c – Experimental network, concentrations (μM)

From data shown in Supplementary Table 14, concentrations are calculated according to calibrations for amino acids.

The sample designation corresponds to the scheme ‘#id#_#chamber#_#fraction# of #totalFractions#’, where #id# is the sample ID, #chamber# is the chamber number as shown in Figure 4a, #fraction# is the fraction number inside each chamber as shown in Figure 4a, and #totalFractions# is the total number of all fractions in the chamber. Calibrations are shown in Supplementary Table 4 and at the end of the Supplementary Information (pages 155-165)

dT	rep eat	part	[N] (μM)	[S] (μM)	[G] (μM)	[T] (μM)	[A] (μM)	[P] (μM)	[C] (μM)	[V] (μM)	[I] (μM)	[L] (μM)	[F] (μM)
16.2	1	426_1_1 of 4	28.95	27.77	29.85	18.41	22.41	9.31	24.68	10.31	4.89	5.56	7.88
16.2	1	426_1_2 of 4	31.53	30.26	29.31	25.52	30.53	18.59	32.49	21.72	13.99	14.79	17.80
16.2	1	426_1_3 of 4	40.76	39.18	37.64	36.08	42.17	32.18	42.51	39.10	31.60	31.35	31.76
16.2	1	426_1_4 of 4	36.71	35.74	33.43	34.70	40.58	33.50	39.55	41.31	35.98	34.94	33.79
16.2	1	426_2_1 of 4	31.83	30.36	32.87	20.04	24.91	9.41	26.84	12.36	4.49	5.34	8.31
16.2	1	426_2_2 of 4	30.68	29.22	25.96	24.96	30.10	15.54	30.18	17.74	7.96	8.94	13.13
16.2	1	426_2_3 of 4	33.06	32.71	22.41	42.73	48.23	38.12	44.26	42.15	29.96	31.64	37.03
16.2	1	426_2_4 of 4	28.11	29.14	16.72	64.60	70.24	147.48	60.11	126.90	132.64	125.72	108.37
16.2	1	426_3_1 of 4	22.98	22.27	17.92	29.49	33.29	38.84	44.19	58.33	64.80	65.03	52.26
16.2	1	426_3_2 of 4	30.14	29.63	22.74	40.41	46.13	57.83	48.99	89.53	115.57	116.13	79.35
16.2	1	426_3_3 of 4	38.13	38.86	29.39	54.73	62.65	80.79	52.26	115.62	156.40	149.63	98.12
16.2	1	426_3_4 of 4	42.34	43.59	31.00	72.55	83.30	135.56	58.07	202.77	307.76	272.03	155.00
16.2	2	427_1_1 of 4	27.30	24.92	34.33	10.41	13.71	3.32	14.52	8.70	2.22	2.53	4.17
16.2	2	427_1_2 of 4	27.67	25.63	29.39	16.27	20.15	9.91	21.28	16.09	8.28	8.59	10.18
16.2	2	427_1_3 of 4	40.89	39.09	38.98	32.97	38.91	27.53	42.32	35.17	28.90	28.54	28.58
16.2	2	427_1_4 of 4	34.45	33.54	30.79	33.66	38.81	37.61	40.20	50.14	49.94	45.56	37.61
16.2	2	427_2_1 of 4	24.40	22.92	33.50	10.05	13.57	5.34	10.20	11.25	4.48	4.64	5.50
16.2	2	427_2_2 of 4	31.66	29.34	39.01	15.37	19.40	8.73	15.25	14.37	7.28	7.64	9.20
16.2	2	427_2_3 of 4	23.60	22.91	27.64	14.50	18.17	10.39	13.37	17.04	9.98	10.08	10.82
16.2	2	427_2_4 of 4	40.87	40.71	38.76	42.23	49.20	51.19	37.69	66.23	68.00	61.99	51.45
16.2	2	427_3_1 of 4	45.38	45.41	39.38	51.04	58.90	62.11	49.26	75.89	70.85	68.01	60.11
16.2	2	427_3_2 of 4	61.89	70.76	57.88	80.50	93.87	115.11	73.82	142.13	147.90	137.17	112.43
16.2	2	427_3_3 of 4	53.89	54.90	42.68	79.30	89.26	133.63	73.63	176.68	212.43	186.61	137.36
16.2	2	427_3_4 of 4	47.89	49.67	35.91	86.93	96.02	191.98	73.80	285.24	391.87	320.79	196.24
16.2	3	428_1_1 of 4	44.95	42.70	46.68	25.53	32.13	9.79	35.82	11.62	3.41	4.28	7.62
16.2	3	428_1_2 of 4	35.56	34.67	34.67	28.75	34.23	19.09	32.03	21.44	12.21	13.28	16.74
16.2	3	428_1_3 of 4	28.05	26.87	26.14	24.86	29.34	22.09	25.62	29.28	22.14	21.68	21.37
16.2	3	428_1_4 of 4	30.58	30.00	26.98	31.22	36.14	31.35	32.92	41.32	36.04	34.68	32.57
16.2	3	428_2_1 of 4	46.14	43.50	53.21	22.98	28.03	10.38	30.21	11.94	6.99	7.49	9.88
16.2	3	428_2_2 of 4	45.22	43.39	49.65	26.03	31.86	13.44	32.48	18.42	10.60	11.06	13.30
16.2	3	428_2_3 of 4	59.10	56.98	58.09	43.09	52.27	32.00	48.17	36.50	27.94	28.30	30.79
16.2	3	428_2_4 of 4	55.11	54.76	46.83	58.46	70.37	68.87	63.41	80.29	77.98	72.66	63.57

16.2	3	428_3_1 of 4	41.32	41.02	34.12	48.58	56.39	57.93	52.32	76.94	79.65	77.07	64.65
16.2	3	428_3_2 of 4	29.93	30.75	23.07	50.26	58.10	96.46	39.23	144.92	203.66	171.14	106.50
16.2	3	428_3_3 of 4	57.90	57.80	43.38	82.41	94.19	122.30	77.89	162.34	192.43	177.13	133.78
16.2	3	428_3_4 of 4	65.72	66.00	47.72	104.72	116.85	179.80	93.10	256.70	339.66	298.02	203.29
0	1	436_1_1 of 4	27.94	23.04	20.67	23.06	12.42	13.49	35.11	17.32	17.26	16.67	29.63
0	1	436_1_2 of 4	19.74	15.15	13.05	15.41	7.11	8.19	26.78	10.34	10.10	9.77	22.14
0	1	436_1_3 of 4	21.52	16.71	14.88	17.03	8.23	9.28	26.88	11.99	11.89	11.28	23.41
0	1	436_1_4 of 4	23.69	18.36	15.99	18.74	8.73	10.23	31.15	12.42	12.16	11.59	26.02
0	1	436_2_1 of 4	24.24	18.87	16.89	19.13	8.92	10.48	30.85	13.00	12.74	12.23	26.56
0	1	436_2_2 of 4	22.99	17.78	15.99	18.20	9.07	10.38	27.30	13.13	13.02	12.50	24.75
0	1	436_2_3 of 4	23.81	18.41	15.78	18.90	8.42	9.75	30.05	12.46	12.33	11.80	26.96
0	1	436_2_4 of 4	25.71	20.23	18.03	20.74	10.10	11.59	32.44	14.54	14.42	13.85	27.71
0	1	436_3_1 of 4	23.84	18.78	16.76	18.99	9.42	10.85	30.03	13.48	13.33	12.87	25.77
0	1	436_3_2 of 4	23.11	18.43	16.32	18.34	9.51	10.79	29.20	13.64	13.48	12.97	24.27
0	1	436_3_3 of 4	24.30	18.82	16.89	19.15	9.18	10.88	31.36	13.39	13.38	12.86	27.11
0	1	436_3_4 of 4	24.27	19.10	17.12	19.43	9.60	10.98	30.56	13.83	13.64	13.13	26.25
0	2	437_1_1 of 4	38.69	37.55	36.65	35.65	41.55	35.06	36.64	44.21	38.69	36.99	34.92
0	2	437_1_2 of 4	39.25	38.16	37.13	36.05	42.75	35.79	37.83	45.79	39.29	37.59	35.36
0	2	437_1_3 of 4	37.19	35.85	34.81	34.40	38.95	33.48	35.74	42.06	36.73	34.84	33.05
0	2	437_1_4 of 4	36.52	35.20	34.38	33.51	37.64	32.57	35.49	40.62	35.71	33.86	32.26
0	2	437_2_1 of 4	38.42	37.29	36.24	35.31	40.32	35.07	37.23	43.12	38.09	36.34	34.90
0	2	437_2_2 of 4	39.80	38.67	37.85	36.48	43.08	36.89	38.54	44.86	39.55	37.55	35.24
0	2	437_2_3 of 4	41.08	39.85	38.80	37.74	41.45	37.11	40.06	44.24	40.04	38.24	37.61
0	2	437_2_4 of 4	32.77	31.30	30.02	29.57	31.04	27.92	32.93	34.45	30.25	28.73	30.40
0	2	437_3_1 of 4	37.79	36.78	35.85	34.85	40.84	34.19	36.30	44.35	37.91	36.22	33.96
0	2	437_3_2 of 4	38.13	36.75	35.79	35.00	37.95	33.75	37.64	41.37	36.57	34.72	33.95
0	2	437_3_3 of 4	37.26	36.21	34.82	34.35	40.25	33.84	37.55	44.29	38.45	36.84	34.64
0	2	437_3_4 of 4	39.69	38.46	37.41	36.34	42.52	35.70	38.07	45.45	39.48	37.72	35.49
0	3	438_1_1 of 4	48.14	47.71	47.64	45.01	49.59	44.90	41.00	49.44	48.64	46.27	43.00
0	3	438_1_2 of 4	35.24	34.15	33.36	32.37	35.90	31.92	35.14	36.43	35.14	33.42	31.32
0	3	438_1_3 of 4	34.39	32.89	31.69	31.15	28.94	28.02	33.64	32.41	31.80	30.32	30.63
0	3	438_1_4 of 4	33.45	31.93	30.65	30.05	26.82	26.70	32.72	30.75	30.08	28.78	29.72
0	3	438_2_1 of 4	34.61	33.23	32.18	31.43	29.38	28.75	31.17	32.66	32.11	30.59	30.89
0	3	438_2_2 of 4	33.34	32.06	31.01	30.12	32.70	29.75	31.55	33.81	32.36	30.81	29.37
0	3	438_2_3 of 4	35.79	34.93	34.08	32.98	36.94	32.70	34.88	37.36	35.75	34.21	32.22
0	3	438_2_4 of 4	35.67	34.97	33.52	33.10	38.02	32.65	36.05	38.84	36.69	35.10	33.43
0	3	438_3_1 of 4	38.50	37.59	36.31	36.06	40.74	35.30	37.06	40.37	38.70	36.72	34.22
0	3	438_3_2 of 4	41.53	40.63	39.58	38.72	44.98	38.54	41.65	44.06	42.02	39.91	37.29
0	3	438_3_3 of 4	40.42	39.41	38.23	37.39	44.10	37.07	39.44	43.79	40.67	38.74	36.15
0	3	438_3_4 of 4	43.28	42.39	40.87	39.97	47.36	40.22	42.73	48.84	43.60	41.51	38.24
10.4	1	406_1_1 of 4	24.42			17.20	18.23	12.57	17.78	14.52	10.05	10.53	12.35
10.4	1	406_1_2 of 4	25.34			15.51	16.93	8.59	19.16	7.33	4.66	5.57	8.38

10.4	1	406_1_3 of 4	24.42			22.59	22.71	19.99	23.61	23.89	19.92	20.08	20.79
10.4	1	406_1_4 of 4	33.38			28.95	29.06	23.51	31.11	23.88	21.69	22.68	24.55
10.4	1	406_2_1 of 4	24.09			12.99	14.97	7.82	12.90	8.86	4.54	5.10	7.08
10.4	1	406_2_2 of 4	31.94			25.26	26.19	19.34	25.93	18.29	14.66	15.78	18.95
10.4	1	406_2_3 of 4	24.22			23.40	22.74	21.11	24.60	21.65	20.23	20.96	22.48
10.4	1	406_2_4 of 4	49.94			63.18	60.11	75.00	65.27	87.69	95.19	91.96	83.55
10.4	1	406_3_1 of 4	44.23			51.52	48.92	59.07	56.76	70.82	73.77	72.27	65.30
10.4	1	406_3_2 of 4	42.11			49.20	47.48	57.93	52.09	67.89	73.85	72.39	62.46
10.4	1	406_3_3 of 4	39.14			45.68	44.31	52.74	49.06	62.44	67.06	64.56	57.23
10.4	1	406_3_4 of 4	33.54			42.76	40.18	53.95	47.04	68.57	78.54	73.34	60.93
10.4	2	407_1_1 of 4	27.28			23.37	23.67	20.41	27.34	20.60	19.70	20.46	21.64
10.4	2	407_1_2 of 4	22.42			20.24	20.32	18.38	24.19	18.68	18.16	18.78	19.22
10.4	2	407_1_3 of 4	34.98			33.57	33.54	31.87	36.73	33.64	33.38	34.01	33.48
10.4	2	407_1_4 of 4	28.84			28.62	28.14	28.10	35.09	30.47	31.61	31.83	30.62
10.4	2	407_2_1 of 4	29.48			23.22	23.65	18.08	25.69	17.78	16.16	17.11	19.13
10.4	2	407_2_2 of 4	22.54			18.27	18.84	14.82	20.25	14.89	13.38	14.52	15.79
10.4	2	407_2_3 of 4	31.45			26.90	27.37	22.94	30.35	24.33	24.13	25.63	27.17
10.4	2	407_2_4 of 4	29.29			29.93	29.95	31.05	31.76	35.32	36.07	35.92	33.89
10.4	2	407_3_1 of 4	34.42			37.65	36.83	40.73	39.95	44.51	46.05	45.46	42.78
10.4	2	407_3_2 of 4	46.80			56.57	53.94	66.80	62.30	78.44	84.41	82.92	72.49
10.4	2	407_3_3 of 4	43.05			52.78	48.64	63.73	61.24	73.90	83.29	78.91	69.45
10.4	2	407_3_4 of 4	38.10			51.57	48.85	72.04	60.86	92.88	110.48	101.90	80.27
10.4	3	408_1_1 of 4	32.25			14.03	12.97	7.70	12.86	6.56	4.94	5.61	8.04
10.4	3	408_1_2 of 4	21.98			17.21	17.66	13.01	18.86	15.51	11.31	12.09	14.08
10.4	3	408_1_3 of 4	25.03			21.87	21.76	18.75	23.76	19.30	18.19	18.88	20.34
10.4	3	408_1_4 of 4	26.65			25.90	23.84	23.56	28.84	25.49	25.52	25.90	27.07
10.4	3	408_2_1 of 4	20.74			13.36	14.37	9.76	12.85	9.96	8.31	8.94	10.30
10.4	3	408_2_2 of 4	26.16			19.19	20.03	16.02	18.34	16.23	15.10	15.86	16.89
10.4	3	408_2_3 of 4	31.77			26.28	26.55	23.55	24.15	25.56	24.54	25.55	25.74
10.4	3	408_2_4 of 4	23.47			24.99	24.53	27.99	22.84	34.00	36.39	35.99	30.79
10.4	3	408_3_1 of 4	31.42			32.86	32.74	34.13	32.28	38.80	37.82	39.57	35.82
10.4	3	408_3_2 of 4	39.41			45.23	42.38	51.35	44.18	57.83	61.92	60.00	54.66
10.4	3	408_3_3 of 4	40.04			46.53	43.97	56.27	46.55	65.72	71.87	68.41	60.22
10.4	3	408_3_4 of 4	42.79			54.64	52.23	71.92	58.39	87.10	101.17	94.66	75.81

Supplementary Table 16: Raw data Fig. 4b-c – Experimental network, normalization against total concentration of species in chamber network (c_0) per experiment

For comparison between different species in the network, we normalized each concentration from Supplementary Table 15 against the average concentration of this species in the entire network (thus of all 3 chambers as shown in Supplementary Table 15), similar to the normalization done to data shown in heat maps in Fig. 2-3 and Extended Data Figures. The different chamber volumes of chambers and thus of individual fractions is taken into account (chamber 1 has a volume of 24.7 μ l, chambers 2 and 3 have a volume of 14.9 μ l).

The sample designation corresponds to the scheme ‘#id#_#chamber#_#fraction# of #totalFractions#’, where #id# is the sample ID, #chamber# is the chamber number as shown in Figure 4a, #fraction# is the fraction number inside each chamber as shown in Figure 4a, and #totalFractions# is the total number of all fractions in the chamber.

dT	repeat	part	[N] (x_{c0})	[S] (x_{c0})	[G] (x_{c0})	[T] (x_{c0})	[A] (x_{c0})	[P] (x_{c0})	[C] (x_{c0})	[V] (x_{c0})	[I] (x_{c0})	[L] (x_{c0})	[F] (x_{c0})
16.2	1	426_1_1 of 4	0.871	0.853	1.053	0.499	0.526	0.201	0.606	0.177	0.074	0.089	0.164
16.2	1	426_1_2 of 4	0.949	0.930	1.033	0.692	0.716	0.401	0.798	0.373	0.213	0.236	0.371
16.2	1	426_1_3 of 4	1.227	1.204	1.327	0.978	0.989	0.694	1.044	0.672	0.480	0.500	0.661
16.2	1	426_1_4 of 4	1.105	1.098	1.179	0.941	0.952	0.722	0.971	0.710	0.547	0.557	0.704
16.2	1	426_2_1 of 4	0.958	0.933	1.159	0.543	0.584	0.203	0.659	0.212	0.068	0.085	0.173
16.2	1	426_2_2 of 4	0.924	0.898	0.915	0.677	0.706	0.335	0.741	0.305	0.121	0.142	0.273
16.2	1	426_2_3 of 4	0.995	1.005	0.790	1.159	1.132	0.822	1.087	0.724	0.455	0.504	0.771
16.2	1	426_2_4 of 4	0.846	0.895	0.590	1.752	1.648	3.180	1.476	2.180	2.016	2.004	2.257
16.2	1	426_3_1 of 4	0.692	0.684	0.632	0.800	0.781	0.837	1.085	1.002	0.985	1.037	1.088
16.2	1	426_3_2 of 4	0.907	0.911	0.802	1.096	1.082	1.247	1.203	1.538	1.757	1.851	1.652
16.2	1	426_3_3 of 4	1.148	1.194	1.036	1.484	1.470	1.742	1.284	1.987	2.377	2.386	2.043
16.2	1	426_3_4 of 4	1.275	1.339	1.093	1.967	1.954	2.923	1.426	3.484	4.678	4.337	3.228
16.2	2	427_1_1 of 4	0.732	0.674	0.937	0.285	0.322	0.069	0.391	0.131	0.031	0.040	0.085
16.2	2	427_1_2 of 4	0.742	0.694	0.802	0.445	0.473	0.205	0.573	0.242	0.114	0.134	0.208
16.2	2	427_1_3 of 4	1.097	1.058	1.064	0.902	0.913	0.569	1.140	0.530	0.399	0.445	0.584
16.2	2	427_1_4 of 4	0.924	0.907	0.841	0.921	0.911	0.777	1.083	0.756	0.689	0.711	0.768
16.2	2	427_2_1 of 4	0.654	0.620	0.914	0.275	0.319	0.110	0.275	0.170	0.062	0.072	0.112
16.2	2	427_2_2 of 4	0.849	0.794	1.065	0.421	0.455	0.180	0.411	0.217	0.100	0.119	0.188
16.2	2	427_2_3 of 4	0.633	0.620	0.755	0.397	0.427	0.215	0.360	0.257	0.138	0.157	0.221
16.2	2	427_2_4 of 4	1.096	1.101	1.058	1.156	1.155	1.058	1.015	0.998	0.938	0.967	1.051
16.2	2	427_3_1 of 4	1.217	1.229	1.075	1.397	1.383	1.283	1.327	1.143	0.978	1.061	1.228
16.2	2	427_3_2 of 4	1.660	1.914	1.580	2.204	2.204	2.378	1.989	2.142	2.041	2.140	2.296
16.2	2	427_3_3 of 4	1.445	1.485	1.165	2.171	2.096	2.761	1.984	2.662	2.931	2.911	2.805
16.2	2	427_3_4 of 4	1.284	1.344	0.980	2.380	2.254	3.967	1.988	4.298	5.407	5.005	4.008
16.2	3	428_1_1 of 4	1.042	1.013	1.180	0.603	0.647	0.200	0.811	0.177	0.047	0.065	0.148
16.2	3	428_1_2 of 4	0.824	0.823	0.876	0.679	0.689	0.389	0.725	0.327	0.168	0.201	0.324
16.2	3	428_1_3 of 4	0.650	0.638	0.661	0.587	0.591	0.451	0.580	0.446	0.305	0.329	0.414
16.2	3	428_1_4 of 4	0.709	0.712	0.682	0.738	0.728	0.639	0.745	0.630	0.497	0.526	0.631

16.2	3	428_2_1 of 4	1.070	1.032	1.345	0.543	0.564	0.212	0.684	0.182	0.096	0.114	0.191
16.2	3	428_2_2 of 4	1.048	1.029	1.255	0.615	0.642	0.274	0.735	0.281	0.146	0.168	0.258
16.2	3	428_2_3 of 4	1.370	1.352	1.468	1.018	1.053	0.653	1.091	0.557	0.385	0.429	0.597
16.2	3	428_2_4 of 4	1.278	1.299	1.184	1.381	1.417	1.405	1.436	1.224	1.076	1.102	1.232
16.2	3	428_3_1 of 4	0.958	0.973	0.862	1.148	1.136	1.181	1.185	1.173	1.099	1.168	1.252
16.2	3	428_3_2 of 4	0.694	0.729	0.583	1.187	1.170	1.967	0.888	2.210	2.809	2.595	2.063
16.2	3	428_3_3 of 4	1.343	1.371	1.096	1.947	1.897	2.494	1.764	2.475	2.654	2.686	2.592
16.2	3	428_3_4 of 4	1.524	1.566	1.206	2.474	2.353	3.667	2.108	3.914	4.685	4.519	3.938
0	1	436_1_1 of 4	1.181	1.240	1.256	1.222	1.349	1.282	1.166	1.308	1.318	1.326	1.150
0	1	436_1_2 of 4	0.834	0.815	0.793	0.817	0.773	0.778	0.889	0.781	0.771	0.777	0.859
0	1	436_1_3 of 4	0.909	0.900	0.904	0.903	0.894	0.881	0.893	0.906	0.908	0.897	0.908
0	1	436_1_4 of 4	1.001	0.988	0.971	0.994	0.948	0.972	1.034	0.938	0.929	0.922	1.009
0	1	436_2_1 of 4	1.024	1.016	1.026	1.014	0.969	0.996	1.025	0.981	0.973	0.973	1.031
0	1	436_2_2 of 4	0.972	0.957	0.971	0.965	0.985	0.986	0.907	0.991	0.995	0.994	0.960
0	1	436_2_3 of 4	1.006	0.991	0.959	1.002	0.915	0.926	0.998	0.940	0.942	0.939	1.046
0	1	436_2_4 of 4	1.086	1.089	1.095	1.100	1.097	1.101	1.077	1.098	1.102	1.101	1.075
0	1	436_3_1 of 4	1.007	1.010	1.018	1.007	1.023	1.031	0.997	1.018	1.018	1.024	1.000
0	1	436_3_2 of 4	0.976	0.992	0.991	0.973	1.032	1.025	0.970	1.030	1.029	1.031	0.941
0	1	436_3_3 of 4	1.027	1.013	1.026	1.015	0.998	1.034	1.041	1.011	1.022	1.023	1.052
0	1	436_3_4 of 4	1.026	1.028	1.040	1.030	1.042	1.043	1.015	1.044	1.042	1.045	1.018
0	2	437_1_1 of 4	1.018	1.020	1.024	1.021	1.041	1.023	0.993	1.029	1.030	1.033	1.020
0	2	437_1_2 of 4	1.032	1.037	1.037	1.032	1.071	1.044	1.025	1.066	1.046	1.050	1.033
0	2	437_1_3 of 4	0.978	0.974	0.972	0.985	0.976	0.977	0.969	0.979	0.978	0.973	0.965
0	2	437_1_4 of 4	0.960	0.956	0.960	0.959	0.943	0.950	0.962	0.946	0.951	0.946	0.942
0	2	437_2_1 of 4	1.010	1.013	1.012	1.011	1.010	1.023	1.009	1.004	1.014	1.015	1.019
0	2	437_2_2 of 4	1.047	1.050	1.057	1.044	1.079	1.077	1.044	1.044	1.053	1.049	1.029
0	2	437_2_3 of 4	1.080	1.082	1.084	1.080	1.038	1.083	1.086	1.030	1.066	1.068	1.099
0	2	437_2_4 of 4	0.862	0.850	0.838	0.847	0.777	0.815	0.893	0.802	0.805	0.802	0.888
0	2	437_3_1 of 4	0.994	0.999	1.001	0.998	1.023	0.998	0.984	1.033	1.009	1.012	0.992
0	2	437_3_2 of 4	1.003	0.998	1.000	1.002	0.950	0.985	1.020	0.963	0.973	0.970	0.992
0	2	437_3_3 of 4	0.980	0.984	0.973	0.983	1.008	0.987	1.018	1.031	1.023	1.029	1.012
0	2	437_3_4 of 4	1.044	1.045	1.045	1.040	1.065	1.042	1.032	1.058	1.051	1.053	1.036
0	3	438_1_1 of 4	1.272	1.297	1.332	1.292	1.323	1.332	1.130	1.276	1.310	1.308	1.271
0	3	438_1_2 of 4	0.931	0.928	0.932	0.930	0.958	0.947	0.969	0.941	0.946	0.945	0.926
0	3	438_1_3 of 4	0.909	0.894	0.886	0.895	0.772	0.832	0.927	0.837	0.856	0.857	0.905
0	3	438_1_4 of 4	0.884	0.868	0.857	0.863	0.716	0.792	0.902	0.794	0.810	0.814	0.878
0	3	438_2_1 of 4	0.914	0.903	0.899	0.903	0.784	0.853	0.859	0.843	0.864	0.865	0.913
0	3	438_2_2 of 4	0.881	0.871	0.867	0.865	0.872	0.883	0.870	0.873	0.871	0.871	0.868
0	3	438_2_3 of 4	0.946	0.949	0.953	0.947	0.986	0.970	0.962	0.964	0.963	0.967	0.952
0	3	438_2_4 of 4	0.942	0.950	0.937	0.950	1.014	0.969	0.994	1.003	0.988	0.992	0.988
0	3	438_3_1 of 4	1.017	1.022	1.015	1.035	1.087	1.047	1.022	1.042	1.042	1.038	1.011
0	3	438_3_2 of 4	1.097	1.104	1.106	1.112	1.200	1.144	1.148	1.137	1.132	1.128	1.102

0	3	438_3_3 of 4	1.068	1.071	1.069	1.074	1.177	1.100	1.087	1.130	1.095	1.095	1.069
0	3	438_3_4 of 4	1.143	1.152	1.142	1.148	1.264	1.193	1.178	1.261	1.174	1.173	1.130
10.4	1	406_1_1 of 4	0.764			0.555	0.594	0.405	0.536	0.407	0.282	0.300	0.371
10.4	1	406_1_2 of 4	0.793			0.500	0.552	0.277	0.577	0.206	0.131	0.159	0.252
10.4	1	406_1_3 of 4	0.764			0.729	0.740	0.644	0.711	0.670	0.559	0.572	0.624
10.4	1	406_1_4 of 4	1.045			0.934	0.947	0.758	0.938	0.670	0.609	0.646	0.737
10.4	1	406_2_1 of 4	0.754			0.419	0.488	0.252	0.389	0.249	0.127	0.145	0.213
10.4	1	406_2_2 of 4	1.000			0.815	0.854	0.623	0.781	0.513	0.412	0.449	0.569
10.4	1	406_2_3 of 4	0.758			0.755	0.741	0.680	0.741	0.607	0.568	0.597	0.675
10.4	1	406_2_4 of 4	1.563			2.038	1.959	2.417	1.967	2.460	2.673	2.619	2.508
10.4	1	406_3_1 of 4	1.384			1.662	1.594	1.904	1.711	1.987	2.072	2.058	1.960
10.4	1	406_3_2 of 4	1.318			1.587	1.547	1.867	1.570	1.905	2.074	2.062	1.875
10.4	1	406_3_3 of 4	1.225			1.473	1.444	1.700	1.478	1.752	1.883	1.839	1.718
10.4	1	406_3_4 of 4	1.050			1.379	1.310	1.739	1.418	1.924	2.205	2.089	1.829
10.4	2	407_1_1 of 4	0.862			0.724	0.748	0.605	0.745	0.545	0.493	0.519	0.592
10.4	2	407_1_2 of 4	0.708			0.627	0.642	0.545	0.659	0.494	0.455	0.477	0.526
10.4	2	407_1_3 of 4	1.105			1.040	1.060	0.944	1.001	0.890	0.836	0.863	0.916
10.4	2	407_1_4 of 4	0.911			0.887	0.889	0.832	0.956	0.806	0.791	0.808	0.838
10.4	2	407_2_1 of 4	0.931			0.719	0.747	0.536	0.700	0.470	0.405	0.434	0.523
10.4	2	407_2_2 of 4	0.712			0.566	0.595	0.439	0.552	0.394	0.335	0.369	0.432
10.4	2	407_2_3 of 4	0.993			0.834	0.865	0.680	0.827	0.643	0.604	0.651	0.743
10.4	2	407_2_4 of 4	0.925			0.927	0.946	0.920	0.866	0.934	0.903	0.912	0.927
10.4	2	407_3_1 of 4	1.087			1.166	1.163	1.207	1.089	1.177	1.153	1.154	1.170
10.4	2	407_3_2 of 4	1.478			1.753	1.704	1.979	1.698	2.074	2.114	2.105	1.983
10.4	2	407_3_3 of 4	1.359			1.635	1.536	1.888	1.669	1.954	2.085	2.003	1.900
10.4	2	407_3_4 of 4	1.203			1.598	1.543	2.134	1.659	2.456	2.766	2.587	2.196
10.4	3	408_1_1 of 4	1.094			0.521	0.495	0.285	0.471	0.215	0.158	0.181	0.276
10.4	3	408_1_2 of 4	0.746			0.639	0.675	0.481	0.691	0.509	0.363	0.391	0.484
10.4	3	408_1_3 of 4	0.849			0.812	0.831	0.694	0.871	0.633	0.583	0.611	0.700
10.4	3	408_1_4 of 4	0.904			0.962	0.911	0.872	1.057	0.836	0.818	0.838	0.931
10.4	3	408_2_1 of 4	0.703			0.496	0.549	0.361	0.471	0.327	0.266	0.289	0.354
10.4	3	408_2_2 of 4	0.887			0.713	0.765	0.593	0.672	0.532	0.484	0.513	0.581
10.4	3	408_2_3 of 4	1.078			0.976	1.014	0.872	0.885	0.839	0.787	0.826	0.885
10.4	3	408_2_4 of 4	0.796			0.928	0.937	1.036	0.837	1.115	1.167	1.164	1.059
10.4	3	408_3_1 of 4	1.066			1.220	1.250	1.263	1.183	1.273	1.213	1.280	1.232
10.4	3	408_3_2 of 4	1.337			1.680	1.619	1.900	1.619	1.898	1.985	1.940	1.880
10.4	3	408_3_3 of 4	1.358			1.728	1.679	2.082	1.706	2.156	2.304	2.212	2.071
10.4	3	408_3_4 of 4	1.452			2.029	1.995	2.662	2.140	2.858	3.243	3.061	2.608

Supplementary Table 17: Raw data Fig. 5 – Time series of Glycine dimerization

Initial conditions: $[Gly]_{init} = 100 \text{ mM}$, $[TMP]_{init} = 100 \text{ mM}$, $pH_{init} 10.5$ and $90 \text{ }^{\circ}\text{C}$. For calibration see Supplementary Table 4 and pages 166-167.

time (h)	raw data (counts*sec)		concentrations (μM)		yield (%)
	Gly	GlyGly	Gly (G)	GlyGly (GG)	$GG^2/(G+GG^2)$
0	6312720340	9040218	94.43	0.02	0.04
0	6967202216	13981321	104.61	0.04	0.07
0	6166118414	17641697	92.15	0.05	0.10
0.5	6510501172	1047133617	97.50	3.88	7.37
0.5	6687743434	1146289185	100.26	4.25	7.82
0.5	6348718171	1055393674	94.99	3.91	7.60
1	6459441944	1174264345	96.71	4.36	8.27
1	6727673481	1249481314	100.88	4.64	8.43
1	6369976662	1149068656	95.32	4.26	8.21
2	6325995632	1402091140	94.63	5.23	9.94
2	6822661875	1326929661	102.36	4.94	8.80
2	6221412993	1309351882	93.01	4.87	9.48
4	6468439883	1421298682	96.85	5.30	9.86
4	6936828985	1388467887	104.13	5.17	9.04
4	6367673724	1276750915	95.28	4.75	9.06
8	6597753318	1340206864	98.86	4.99	9.17
8	6974769029	1385874327	104.72	5.16	8.98
8	6531154308	1292143800	97.82	4.81	8.95
24	7338413265	1178712620	110.39	4.38	7.34
24	6688639544	1135167978	100.27	4.21	7.75
24	6470860460	1131697184	96.88	4.20	7.97
52	7623634441	1115505084	114.83	4.14	6.72
52	6896860726	1163193182	103.51	4.32	7.70
122	7589395271	1000804052	114.30	3.70	6.08
122	7579834133	973440155	114.15	3.60	5.93

Supplementary Table 18: Raw data Fig. 5 – Variation of TMP concentration

Initial conditions: specified concentrations of Gly ($[Gly]_{init}$) and TMP ($[TMP]_{init}$), pH_{init} 10.5 and 90 °C for 16 h. Samples with $[Gly]_{init} = 100$ mM were diluted 10-fold before injection into LC-MS. For calibration see Supplementary Table 4.

$[Gly]_{init}$ (mM)	$[TMP]_{init}$ (mM)	raw data ($\mu AU \cdot min$)		concentrations (mM)		yield (%)
		Gly	GlyGly	Gly (G)	GlyGly (GG)	$GG \cdot 2 / (G + GG \cdot 2)$
100	0.10	5183.78	0.51	83.96	0.02	0.04
100	0.10	6349.56	0.64	102.84	0.02	0.04
100	0.25	5228.90	0.17	84.69	0.00	0.01
100	0.25	5656.49	0.72	91.61	0.02	0.05
100	0.63	4946.96	0.45	80.12	0.01	0.03
100	1.58	5300.33	6.95	85.84	0.20	0.47
100	1.58	5544.85	8.36	89.81	0.24	0.54
100	3.98	5142.59	24.36	83.29	0.71	1.69
100	3.98	5833.27	28.92	94.48	0.85	1.76
100	10.00	5659.15	97.54	91.66	2.86	5.87
100	25.12	4560.18	152.80	73.86	4.48	10.81
100	25.12	4389.42	158.79	71.09	4.65	11.57
100	63.10	4274.35	171.14	69.23	5.01	12.65
100	63.10	4384.69	179.96	71.02	5.27	12.93
100	158.49	4705.16	194.13	76.21	5.69	12.99
100	158.49	4696.34	200.91	76.06	5.89	13.40
10	0.10	6391.10	0.00	10.35	0.000	0.00
10	0.25	7752.41	0.09	12.56	0.000	0.00
10	0.25	7660.96	0.14	12.41	0.000	0.01
10	0.63	7186.75	0.17	11.64	0.000	0.01
10	0.63	6996.91	0.51	11.33	0.001	0.03
10	1.58	6979.76	3.16	11.31	0.009	0.16
10	1.58	6366.92	1.30	10.31	0.004	0.07
10	3.98	6931.43	9.97	11.23	0.029	0.52
10	3.98	7530.53	11.98	12.20	0.035	0.57
10	10.00	7593.52	41.46	12.30	0.121	1.94
10	25.12	6670.56	36.91	10.80	0.108	1.96
10	25.12	7298.20	37.74	11.82	0.111	1.84
10	63.10	6359.76	45.12	10.30	0.132	2.50
10	63.10	6478.81	44.51	10.49	0.130	2.43
10	158.49	6686.47	48.37	10.83	0.142	2.55
10	158.49	6558.22	45.76	10.62	0.134	2.46

Supplementary Table 19: Raw data Supplementary Figure 13 – TMP degradation

Initial conditions: $[TMP]_{init} = 200\mu\text{M}$ (without Gly), $pH_{init} 10.5$, 90°C for experimental time. To account for evaporation, we normalized the TMP

concentration according to $[TMP]_{normalized} = \frac{[TMP]}{\frac{1}{3}[PO_4] + \frac{2}{3}[diPO_4] + [TMP] + [triPO_4]}$.

time (h)	PO ₄ (μM)	diPO ₄ (μM)	TMP (μM)	triPO ₄ (μM)	TMP _{normalized} (μM)
0	1.50	3.23	210.42	1.06	196.53
0	1.47	3.07	212.20	1.06	196.67
0	1.12	3.09	211.05	0.90	196.89
0.5	1.21	2.94	213.77	0.17	197.66
0.5	1.48	3.24	212.96	0.26	197.30
0.5	1.62	3.14	214.45	0.19	197.40
1	1.31	3.12	211.60	0.49	197.20
1	1.31	3.28	213.31	0.50	197.11
2	1.61	3.26	213.30	0.62	196.93
2	1.61	3.19	216.74	0.69	196.95
2	1.49	3.18	215.33	0.69	196.98
4	2.04	3.26	214.20	1.00	196.46
4	1.80	3.29	214.03	1.04	196.48
4	1.53	3.35	216.28	1.05	196.55
8	2.23	3.58	220.59	1.87	195.57
8	2.41	3.55	217.29	1.55	195.75
8	2.32	3.52	217.53	1.81	195.57
24	8.93	5.56	223.53	2.53	192.09
24	9.19	5.38	223.81	2.29	192.31
24	9.07	5.54	222.65	2.66	191.92
52	24.31	7.67	227.31	2.75	186.87
52	35.11	6.15	247.31	3.62	185.44
52	26.87	7.54	225.93	2.30	186.56

Supplementary Table 20: Raw data Fig. 5 – Glycine dimerization in heat flow chamber

Initial conditions: specified concentration of Gly ($[Gly]_{init}$), $[TMP]_{init} = 1 \text{ mM}$, $pH_{init} = 10.5$, $dT = 10 \text{ K}$ between $75 \text{ }^{\circ}\text{C}$ and $85 \text{ }^{\circ}\text{C}$, $dT = 0 \text{ K}$ (isothermal) at $85 \text{ }^{\circ}\text{C}$, both for 16 h. Due to technical problems, for the third replicate with $[Gly]_{init} = 10 \text{ mM}$, the temperature gradient was not applied for the entire duration of the experiment, which is why we do not take it into account for the calculation of the heat flow-driven enrichment. For calibration see Supplementary Table 4 and pages 166-167.

$[Gly]_{init}$ (mM)	dT (K)	repeat	part in heat flow chamber	raw data (counts*sec)		concentrations (μM)		yield (%)
				Gly	GlyGly	Gly (G)	GlyGly (GG)	$GG^2/(G+GG^2)$
1	10	1	top	802185500	2985868	0.60	0.00	0.18
1	10	1	II	1176008707	5690031	0.88	0.00	0.24
1	10	1	III	1644844965	14388030	1.23	0.00	0.43
1	10	1	bot	1810375377	15005115	1.36	0.00	0.41
1	10	2	top	1328739417	27717693	1.00	0.01	1.02
1	10	2	II	1260566309	19816549	0.94	0.00	0.77
1	10	2	III	1432268457	29163998	1.07	0.01	1.00
1	10	2	bot	2326716092	83442136	1.74	0.02	1.75
1	10	3	top	1135748152	9942536	0.85	0.00	0.43
1	10	3	II	1366989643	11820745	1.02	0.00	0.43
1	10	3	III	1527888876	10097632	1.15	0.00	0.33
1	10	3	bot	1841297149	14902900	1.38	0.00	0.40
1	0	1	top	1467102500	0	1.10	0.00	0.00
1	0	1	II	1517817237	0	1.14	0.00	0.00
1	0	1	III	1367185730	0	1.02	0.00	0.00
1	0	1	bot	1592836350	0	1.19	0.00	0.00
1	0	2	top	1629955701	0	1.22	0.00	0.00
1	0	2	II	1347055154	0	1.01	0.00	0.00
1	0	2	III	1716629737	0	1.29	0.00	0.00
1	0	2	bot	1474382134	0	1.11	0.00	0.00
1	0	3	top	1610370106	0	1.21	0.00	0.00
1	0	3	II	1473755296	0	1.10	0.00	0.00
1	0	3	III	1561244091	0	1.17	0.00	0.00
1	0	3	bot	1393863214	0	1.04	0.00	0.00
10	0	1	full	1238282812	0	9.28	0.00	0.00
10	0	2	full	1400958908	0	10.50	0.00	0.00
10	10	1	top	1014256241	70605118	10.14	0.17	3.33
10	10	1	II	827227886	60344712	8.27	0.15	3.49

10	10	1	III	871205665	62290152	8.71	0.15	3.42
10	10	1	IV	874632626	65897201	8.74	0.16	3.60
10	10	1	bot	1289953582	110420339	12.89	0.27	4.07
10	10	2	top	892728415	26482216	8.92	0.07	1.45
10	10	2	II	1031353717	28558232	10.31	0.07	1.35
10	10	2	III	1040394989	28412444	10.40	0.07	1.33
10	10	2	IV	959940215	26743552	9.59	0.07	1.36
10	10	2	bot	1041392787	69652955	10.41	0.17	3.21

Supplementary Table 21: Raw data Extended Data Fig. 2a – 2-aminoazoles in water, 170 μ m, 18 h, 10 K.

repeat k	species	measured values (mAU*min)				concentration (μ M) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 3				c_0 (μ M)	Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)		Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)							
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)				bot part (red shade)			
1	2AO	0.259	0.330	0.382	0.656	28.97	37	42.86	73.52	45.59	0.64	0.81	0.94	1.61	12.17	-5.9	2AO	0	20.85	18.07	2AO	0	-6.98	-10.15
	2AT	0.050	0.083	0.081	0.163	22.27	37.17	36.54	73.43	42.35	0.53	0.88	0.86	1.73	-7.18	1.17	2AT	-17.25	0	-2.3	2AT	7.51	0	-3.4
	2AI	0.268	0.405	0.423	0.892	31.5	47.71	49.82	105.04	58.52	0.54	0.82	0.85	1.79	-4.99	4.73	2AI	-15.3	2.36	0	2AI	11.3	3.52	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.57	0.83	0.88	1.71				2AO	2AT	2AI		2AO	2AT	2AI
2	2AO	0.287	0.442	0.464	0.568	32.14	49.58	51.95	63.68	49.34	0.65	1	1.05	1.29	17.78	-10.2	2AO	0	14.68	48.13	2AO	0	-9.86	-18.79
	2AT	0.058	0.098	0.107	0.147	26.19	44.14	48.05	66.01	46.1	0.57	0.96	1.04	1.43	2.7	-0.37	2AT	-12.8	0	29.17	2AT	10.94	0	-9.9
	2AI	0.249	0.508	0.608	0.900	29.32	59.85	71.55	105.95	66.67	0.44	0.9	1.07	1.59	-20.49	10.57	2AI	-32.49	-22.58	0	2AI	23.13	10.99	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.55	0.95	1.06	1.44				2AO	2AT	2AI		2AO	2AT	2AI
3	2AO	0.348	0.376	0.385	0.550	39.05	42.11	43.14	61.64	46.49	0.84	0.91	0.93	1.33	2.68	-4.2	2AO	0	3.37	4.78	2AO	0	-6.89	-5.43
	2AT	0.075	0.073	0.089	0.131	33.66	32.94	40.09	58.99	41.42	0.81	0.8	0.97	1.42	-0.67	2.89	2AT	-3.26	0	1.36	2AT	7.4	0	1.57
	2AI	0.387	0.415	0.453	0.677	45.61	48.88	53.29	79.77	56.89	0.8	0.86	0.94	1.4	-2.01	1.3	2AI	-4.56	-1.34	0	2AI	5.74	-1.55	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.82	0.85	0.94	1.38				2AO	2AT	2AI		2AO	2AT	2AI

Supplementary Table 22: Raw data Extended Data Fig. 2a – 2-aminoazoles in water, 170 μ m, 18 h, 5 K.

repeat k	species	measured values (mAU*min)				concentration (μ M) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 3				c_0 (μ M)	Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)		Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)							
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)				bot part (red shade)			
1	2AO	0.349	0.400	0.440	0.543	39.17	44.81	49.34	60.85	48.54	0.81	0.92	1.02	1.25	5.14	-1.15	2AO	0	3.44	12.78	2AO	0	1.59	-4.8
	2AT	0.083	0.099	0.113	0.132	37.53	44.64	50.89	59.35	48.1	0.78	0.93	1.06	1.23	1.64	-2.7	2AT	-3.32	0	9.04	2AT	-1.57	0	-6.3
	2AI	0.392	0.528	0.550	0.722	46.18	62.19	64.82	84.99	64.55	0.72	0.96	1	1.32	-6.78	3.84	2AI	-11.34	-8.29	0	2AI	5.05	6.72	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.77	0.94	1.03	1.27				2AO	2AT	2AI		2AO	2AT	2AI
2	2AO	0.356	0.399	0.418	0.498	39.96	44.74	46.86	55.8	46.84	0.85	0.96	1	1.19	7.72	-4.85	2AO	0	9.28	14.97	2AO	0	-8.31	-5.85
	2AT	0.066	0.080	0.082	0.110	29.65	35.86	37.08	49.36	37.99	0.78	0.94	0.98	1.3	-1.42	3.78	2AT	-8.49	0	5.2	2AT	9.07	0	2.69
	2AI	0.368	0.496	0.492	0.628	43.33	58.45	57.92	73.9	58.4	0.74	1	0.99	1.27	-6.3	1.07	2AI	-13.02	-4.95	0	2AI	6.21	-2.62	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.79	0.97	0.99	1.25				2AO	2AT	2AI		2AO	2AT	2AI
3	2AO	0.363	0.369	0.427	0.500	40.74	41.41	47.89	56.01	46.51	0.88	0.89	1.03	1.2	7.77	-3.29	2AO	0	9.8	14.55	2AO	0	-3.23	-6.42
	2AT	0.071	0.081	0.093	0.111	31.99	36.54	41.98	49.9	40.1	0.8	0.91	1.05	1.24	-1.85	-0.06	2AT	-8.92	0	4.33	2AT	3.34	0	-3.3
	2AI	0.370	0.448	0.496	0.624	43.63	52.78	58.41	73.42	57.06	0.76	0.92	1.02	1.29	-5.92	3.35	2AI	-12.7	-4.15	0	2AI	6.87	3.41	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.81	0.91	1.03	1.25				2AO	2AT	2AI		2AO	2AT	2AI

Supplementary Table 23: Raw data Extended Data Fig. 2b and 2f – mixture of non-proteogenic and proteogenic AA in water, 170 μ m, 18 h, 4 fractions

Due to technical problems, for the third replicate the temperature gradient was not applied for the entire duration of the experiment, which is why we do not take it into account for the calculation of the heat flow-driven enrichment.

repeat k	species	measured values (counts*s)				Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)	
		top	II	III	bot	top	II	III	bot	top	bot
1	Anserine	5661160	14186861	60439034	65311397	0.156	0.39	1.66	1.794	-56.5	15.4
	Arginine	22016377	44274642	153608231	155034889	0.235	0.472	1.639	1.654	-34.3	6.3
	Aspartic acid	122990130	163986536	247094698	235028807	0.64	0.853	1.285	1.222	78.9	-21.4
	Carnosine	9979306	20266295	77231792	82007108	0.211	0.428	1.63	1.731	-41.1	11.3
	Citrulline	117867559	182397721	388083850	381490630	0.441	0.682	1.451	1.426	23.3	-8.3
	Creatinine	125283026	248456331	843952194	849050372	0.242	0.481	1.633	1.643	-32.2	5.6
	Cysteine	4710370	6994902	15602677	23191288	0.373	0.554	1.236	1.837	4.4	18.1
	Cystathionine	35545955	43974432	70715740	62230923	0.669	0.828	1.331	1.172	87.2	-24.7
	Ethanolamine	87566767	153629632	317147701	404955825	0.364	0.638	1.317	1.682	1.7	8.1
	Glutamic acid	160632652	217561571	328811326	317341023	0.627	0.85	1.284	1.239	75.4	-20.3
	Histidine	20491013	34802647	118210601	120636746	0.279	0.473	1.608	1.641	-22.1	5.5
	Homoalanine	355664255	690039385	1955777936	2002729555	0.284	0.552	1.563	1.601	-20.5	2.9
	Homocysteine	62472985	114750157	272380609	286470087	0.339	0.624	1.48	1.557	-5.0	0.1
	Hydroxylysine	24311276	43065626	113774832	110488207	0.333	0.591	1.56	1.515	-6.7	-2.6
	Hydroxyproline	164413172	269219013	575721834	574819884	0.415	0.68	1.454	1.451	16.1	-6.7
	Leu_Isoleu	99494415	257334460	1343860840	1633860520	0.119	0.309	1.612	1.96	-66.6	26.0
	Lysine	16948349	36206710	121302436	120876224	0.23	0.49	1.643	1.637	-35.8	5.3

	Methionine	126216509	298994224	1040431634	937315258	0.21	0.498	1.732	1.56	-41.2	0.3
	Methylhistidine	20519352	57726006	260313528	262878946	0.136	0.384	1.731	1.748	-61.8	12.4
	Ornithine	12608661	19037405	61509756	64691271	0.32	0.482	1.559	1.639	-10.6	5.4
	Phenylalanine	99228691	337584752	1440076029	1605091125	0.114	0.388	1.654	1.844	-68.1	18.5
	Proline	167959106	428909981	1597435540	1599932831	0.177	0.452	1.684	1.687	-50.5	8.4
	Sarcosine	650059441	829292609	1578532943	1444372035	0.578	0.737	1.402	1.283	61.5	-17.5
	Serine	99389885	117112651	172709916	160896091	0.723	0.852	1.256	1.17	102.1	-24.8
	Taurine	33370199	34786476	37685341	33323306	0.959	1	1.083	0.958	168.3	-38.4
	Threonine	91610345	158030941	364403735	365615740	0.374	0.645	1.488	1.493	4.6	-4.0
	Tyrosine	49212648	75668073	191695027	224976919	0.363	0.559	1.416	1.662	1.7	6.8
	Valine	92196100	342808167	1647533619	1613378040	0.1	0.371	1.783	1.746	-72.1	12.3
	mean concentration per fraction $\bar{c}_{j,k}$					0.358	0.581	1.506	1.555		
2	Anserine	6404480	17474518	29985336	95846174	0.171	0.467	0.801	2.561	-58.6	29.0
	Arginine	27485822	62783931	92282637	232426941	0.265	0.605	0.89	2.24	-35.9	12.9
	Aspartic acid	157002104	204312918	221924813	277877904	0.729	0.949	1.031	1.291	76.5	-35.0
	Carnosine	11741861	26339407	41923872	114312753	0.242	0.542	0.863	2.353	-41.5	18.5
	Citrulline	154169887	239605330	298801812	599488263	0.477	0.742	0.925	1.856	15.5	-6.5
	Creatinine	129730202	294549847	527843949	1250163592	0.236	0.535	0.959	2.271	-43.0	14.4
	Cysteine	7921540	7911174	11069908	36479208	0.5	0.499	0.699	2.302	21.0	16.0
	Cystathionine	35166140	50681402	60723148	149900037	0.474	0.684	0.819	2.022	14.9	1.9
	Ethanolamine	147123146	229662500	332703427	462782208	0.502	0.784	1.135	1.579	21.5	-20.5
	Glutamic acid	204632384	268784402	295605805	390310787	0.706	0.927	1.02	1.347	70.9	-32.2
	Histidine	25312291	47300797	81114355	185782898	0.298	0.557	0.956	2.189	-27.8	10.3
	Homoalanine	503607574	904394665	1275829921	2579914641	0.383	0.687	0.97	1.961	-7.4	-1.2

	Homocysteine	82088666	144483585	190180275	364897015	0.42	0.739	0.973	1.867	1.7	-5.9
	Hydroxylysine	31864014	58235170	77978043	148297841	0.403	0.736	0.986	1.875	-2.5	-5.6
	Hydroxyproline	220873325	349506064	435052426	761219465	0.5	0.791	0.985	1.724	21.1	-13.2
	Leu_Isoleu	287471992	340885858	525749398	2051963832	0.359	0.425	0.656	2.56	-13.2	29.0
	Lysine	21651126	48636521	76771640	189021936	0.258	0.579	0.914	2.25	-37.6	13.3
	Methionine	187575370	368927282	547472674	1163121898	0.331	0.651	0.966	2.052	-19.9	3.4
	Methylhistidine	24673653	80214831	135818473	441428608	0.145	0.47	0.796	2.589	-65.0	30.4
	Ornithine	11595276	25018027	38274068	83651840	0.293	0.631	0.966	2.111	-29.2	6.3
	Phenylalanine	173291206	384952919	697423704	1775194935	0.229	0.508	0.92	2.343	-44.6	18.0
	Proline	252436278	549671066	897858212	2014442830	0.272	0.592	0.967	2.169	-34.2	9.3
	Sarcosine	592809379	993915119	1255838065	1799193814	0.511	0.856	1.082	1.55	23.7	-21.9
	Serine	127757429	132936014	162560332	263150074	0.745	0.775	0.947	1.533	80.2	-22.8
	Taurine	35760987	38003994	37791502	39113960	0.949	1.009	1.003	1.038	129.8	-47.7
	Threonine	129423556	197809706	267677576	571881802	0.444	0.678	0.918	1.961	7.4	-1.2
	Tyrosine	74143329	110102016	161703385	222968677	0.521	0.774	1.137	1.568	26.2	-21.0
	Valine	166247816	379689086	726367545	1958382529	0.206	0.47	0.899	2.425	-50.2	22.1
	mean concentration per fraction $\bar{c}_{j,k}$					0.413	0.667	0.935	1.985		

Supplementary Table 24: Raw data Extended Data Fig. 2f – mixture of non-proteogenic and proteogenic AA in water, 170 μ m, 18 h – enrichments in top fraction, 4 fractions

re pe at	specie s	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)																												
		Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val	
1	A	Ans	0.0	-33.8	-75.7	-26.2	-64.7	-35.9	-58.3	-76.8	-57.2	-75.2	-44.2	-45.3	-54.2	-53.4	-62.5	30.3	-32.2	-26.0	14.0	-51.3	36.4	-12.2	-73.1	-78.5	-83.8	-58.4	-57.2	55.9
		Arg	51.0	0.0	-63.3	11.5	-46.7	-3.1	-37.0	-64.9	-35.4	-62.6	-15.7	-17.4	-30.8	-29.6	-43.4	96.8	2.3	11.8	72.1	-26.5	106.1	32.7	-59.3	-67.5	-75.5	-37.2	-35.4	135.4
		Asp	311.3	172.3	0.0	203.6	45.1	163.8	71.4	-4.4	75.9	2.0	129.6	125.0	88.4	91.8	54.1	436.0	178.7	204.5	368.7	100.2	461.1	261.3	10.8	-11.5	-33.3	71.0	76.0	541.1
		Car	35.5	-10.3	-67.1	0.0	-52.2	-13.1	-43.5	-68.5	-42.1	-66.4	-24.4	-25.9	-37.9	-36.8	-49.3	76.5	-8.2	0.3	54.4	-34.1	84.8	19.0	-63.5	-70.9	-78.0	-43.7	-42.0	111.1
		Cit	183.4	87.6	-31.1	109.2	0.0	81.7	18.1	-34.1	21.2	-29.7	58.1	55.0	29.8	32.2	6.2	269.2	92.0	109.8	222.9	37.9	286.6	148.9	-23.7	-39.0	-54.1	17.8	21.2	341.7
		Cre	55.9	3.2	-62.1	15.1	-45.0	0.0	-35.0	-63.8	-33.3	-61.3	-13.0	-14.7	-28.6	-27.3	-41.6	103.2	5.6	15.4	77.7	-24.1	112.7	36.9	-58.0	-66.4	-74.7	-35.2	-33.3	143.0
		Cys	139.9	58.8	-41.7	77.1	-15.3	53.9	0.0	-44.2	2.6	-40.5	33.9	31.2	9.9	11.9	-10.1	212.6	62.5	77.6	173.4	16.8	227.3	110.7	-35.4	-48.4	-61.1	-0.3	2.6	273.9
		Cth	330.3	184.9	4.6	217.7	51.9	176.0	79.4	0.0	84.0	6.7	140.2	135.4	97.1	100.7	61.2	460.7	191.5	218.5	390.4	109.4	487.1	277.9	15.9	-7.4	-30.2	78.9	84.1	570.7
		ETA	133.8	54.8	-43.2	72.6	-17.5	50.0	-2.5	-45.7	0.0	-42.0	30.5	27.9	7.1	9.0	-12.4	204.7	58.4	73.1	166.4	13.8	219.0	105.4	-37.0	-49.7	-62.1	-2.8	0.0	264.4
		Glu	303.3	167.1	-1.9	197.8	42.3	158.7	68.1	-6.3	72.5	0.0	125.1	120.6	84.8	88.1	51.1	425.6	173.3	198.6	359.6	96.3	450.3	254.2	8.6	-13.2	-34.6	67.7	72.6	528.6
		AAB A	79.2	18.6	-56.4	32.3	-36.8	14.9	-25.3	-58.4	-23.4	-55.6	0.0	-2.0	-17.9	-16.4	-32.9	133.5	21.4	32.6	104.2	-12.8	144.5	57.4	-51.8	-61.4	-70.9	-25.5	-23.3	179.3
		Hcy	82.8	21.0	-55.6	35.0	-35.5	17.2	-23.8	-57.5	-21.8	-54.7	2.0	0.0	-16.3	-14.7	-31.5	138.2	23.8	35.3	108.3	-11.0	149.4	60.6	-50.8	-60.7	-70.4	-24.0	-21.8	184.9
		His	118.3	44.5	-46.9	61.2	-23.0	40.0	-9.0	-49.3	-6.6	-45.9	21.8	19.4	0.0	1.8	-18.2	184.5	47.9	61.6	148.8	6.3	197.8	91.7	-41.2	-53.0	-64.6	-9.2	-6.6	240.2
		Hyl	114.4	42.0	-47.9	58.3	-24.3	37.5	-10.6	-50.2	-8.3	-46.8	19.7	17.3	-1.8	0.0	-19.7	179.4	45.3	58.7	144.3	4.4	192.5	88.3	-42.3	-53.9	-65.2	-10.9	-8.3	234.2
		Hyp	166.9	76.7	-35.1	97.1	-5.8	71.2	11.3	-38.0	14.2	-33.8	49.0	46.0	22.3	24.5	0.0	247.8	80.9	97.6	204.2	29.9	264.2	134.5	-28.1	-42.6	-56.7	11.0	14.2	316.0
		Leu- lle	-23.3	-49.2	-81.3	-43.3	-72.9	-50.8	-68.0	-82.2	-67.2	-81.0	-57.2	-58.0	-64.8	-64.2	-71.3	0.0	-48.0	-43.2	-12.5	-62.6	4.7	-32.6	-79.3	-83.5	-87.6	-68.1	-67.2	19.6
		Lys	47.6	-2.3	-64.1	9.0	-47.9	-5.3	-38.5	-65.7	-36.9	-63.4	-17.6	-19.3	-32.4	-31.2	-44.7	92.3	0.0	9.3	68.2	-28.2	101.4	29.6	-60.3	-68.2	-76.1	-38.6	-36.8	130.1
		Met	35.1	-10.6	-67.2	-0.3	-52.3	-13.4	-43.7	-68.6	-42.2	-66.5	-24.6	-26.1	-38.1	-37.0	-49.4	76.0	-8.5	0.0	54.0	-34.2	84.3	18.7	-63.6	-70.9	-78.1	-43.8	-42.2	110.6
		3-MH	-12.3	-41.9	-78.7	-35.2	-69.0	-43.7	-63.4	-79.6	-62.5	-78.2	-51.0	-52.0	-59.8	-59.1	-67.1	14.3	-40.5	-35.0	0.0	-57.3	19.7	-22.9	-76.4	-81.1	-85.8	-63.5	-62.5	36.8
		Orn	105.4	36.0	-50.0	51.7	-27.5	31.8	-14.4	-52.3	-12.1	-49.1	14.7	12.4	-5.9	-4.2	-23.0	167.7	39.2	52.1	134.1	0.0	180.3	80.4	-44.7	-55.8	-66.7	-14.6	-12.1	220.2
		Phe	-26.7	-51.5	-82.2	-45.9	-74.1	-53.0	-69.4	-83.0	-68.7	-81.8	-59.1	-59.9	-66.4	-65.8	-72.5	-4.5	-50.3	-45.7	-16.5	-64.3	0.0	-35.6	-80.3	-84.2	-88.1	-69.5	-68.6	14.2
		Pro	13.8	-24.6	-72.3	-15.9	-59.8	-27.0	-52.5	-73.5	-51.3	-71.8	-36.5	-37.7	-47.8	-46.9	-57.3	48.4	-22.9	-15.7	29.8	-44.6	55.3	0.0	-69.3	-75.5	-81.5	-52.7	-51.3	77.5
		Sar	271.3	145.9	-9.7	174.2	31.1	138.2	54.8	-13.7	58.8	-7.9	107.3	103.2	70.1	73.2	39.1	383.9	151.6	174.9	323.2	80.8	406.7	226.2	0.0	-20.1	-39.8	54.4	58.9	478.8
		Ser	364.7	207.7	13.0	243.1	64.0	198.0	93.7	8.0	98.8	15.2	159.4	154.2	112.9	116.7	74.1	505.5	214.8	244.0	429.6	126.2	534.0	308.1	25.1	0.0	-24.7	93.2	98.8	624.3
		Tau	516.7	308.4	49.9	355.3	117.6	295.6	157.1	43.3	163.8	52.9	244.2	237.4	182.5	187.7	131.0	703.6	317.8	356.5	602.8	200.2	741.4	441.7	66.1	32.7	0.0	156.4	163.9	861.3
		Thr	140.5	59.2	-41.5	77.6	-15.1	54.3	0.3	-44.1	2.9	-40.4	34.2	31.6	10.2	12.2	-9.9	213.4	63.0	78.0	174.1	17.1	228.1	111.2	-35.2	-48.2	-61.0	0.0	2.9	274.9
		Tyr	133.7	54.8	-43.2	72.5	-17.5	49.9	-2.6	-45.7	0.0	-42.1	30.4	27.9	7.1	9.0	-12.4	204.6	58.4	73.0	166.4	13.8	218.9	105.3	-37.1	-49.7	-62.1	-2.8	0.0	264.3
		Val	-35.8	-57.5	-84.4	-52.6	-77.4	-58.8	-73.3	-85.1	-72.6	-84.1	-64.2	-64.9	-70.6	-70.1	-76.0	-16.4	-56.5	-52.5	-26.9	-68.8	-12.5	-43.6	-82.7	-86.2	-89.6	-73.3	-72.5	0.0
			Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val
			B																											
2	A	Ans	0.0	-35.4	-76.5	-29.2	-64.1	-27.4	-65.8	-63.9	-65.9	-75.8	-42.6	-55.3	-59.3	-57.5	-65.8	-52.3	-33.6	-48.3	18.3	-41.5	-25.2	-37.1	-66.5	-77.0	-82.0	-61.4	-67.2	-16.9
		Arg	54.8	0.0	-63.7	9.6	-44.5	12.4	-47.0	-44.2	-47.2	-62.5	-11.2	-30.8	-36.9	-34.2	-47.0	-26.1	2.8	-19.9	83.1	-9.4	15.8	-2.5	-48.1	-64.4	-72.1	-40.3	-49.2	28.7
		Asp	326.2	175.3	0.0	201.7	52.8	209.5	45.9	53.7	45.3	3.3	144.5	90.6	73.6	81.0	45.8	103.3	183.0	120.4	404.1	149.3	218.9	168.3	42.8	-2.0	-23.2	64.4	39.9	254.3
		Car	41.3	-8.8	-66.9	0.0	-49.4	2.6	-51.7	-49.1	-51.9	-65.8	-19.0	-36.8	-42.5	-40.0	-51.7	-32.6	-6.2	-27.0	67.1	-17.4	5.7	-11.1	-52.7	-67.5	-74.5	-45.5	-53.6	17.4

		Cit	178.9	80.1	-34.6	97.5	0.0	102.6	-4.5	0.6	-4.9	-32.4	60.0	24.7	13.6	18.5	-4.6	33.1	85.2	44.2	229.9	63.1	108.7	75.6	-6.6	-35.9	-49.7	7.6	-8.4	131.9
		Cre	37.7	-11.1	-67.7	-2.5	-50.6	0.0	-52.9	-50.3	-53.1	-66.6	-21.0	-38.4	-43.9	-41.5	-52.9	-34.3	-8.6	-28.8	62.9	-19.5	3.0	-13.3	-53.9	-68.4	-75.2	-46.9	-54.8	14.5
		Cys	192.2	88.7	-31.5	106.8	4.7	112.2	0.0	5.4	-0.4	-29.2	67.6	30.6	19.0	24.1	0.0	39.4	94.0	51.1	245.5	70.9	118.6	83.9	-2.1	-32.9	-47.3	12.7	-4.1	142.9
		Cth	177.3	79.1	-34.9	96.3	-0.6	101.4	-5.1	0.0	-5.5	-32.8	59.1	24.0	12.9	17.8	-5.1	32.3	84.1	43.4	227.9	62.2	107.5	74.5	-7.1	-36.3	-50.0	6.9	-9.0	130.5
		ETA	193.4	89.5	-31.2	107.7	5.2	113.1	0.4	5.8	0.0	-28.9	68.3	31.2	19.5	24.6	0.4	40.0	94.8	51.7	247.0	71.6	119.5	84.7	-1.7	-32.6	-47.1	13.1	-3.7	143.9
		Glu	312.6	166.5	-3.2	192.1	47.9	199.6	41.2	48.8	40.6	0.0	136.7	84.5	68.1	75.3	41.2	96.9	174.0	113.3	388.0	141.3	208.7	159.7	38.2	-5.2	-25.6	59.1	35.4	243.0
		AAB A	74.3	12.6	-59.1	23.4	-37.5	26.6	-40.3	-37.1	-40.6	-57.8	0.0	-22.1	-29.0	-26.0	-40.4	-16.9	15.7	-9.9	106.1	1.9	30.4	9.7	-41.6	-59.9	-68.6	-32.8	-42.8	44.9
		Hcy	123.6	44.4	-47.5	58.3	-19.8	62.4	-23.4	-19.3	-23.8	-45.8	28.3	0.0	-8.9	-5.0	-23.5	6.7	48.5	15.6	164.5	30.8	67.3	40.8	-25.1	-48.6	-59.7	-13.7	-26.6	85.9
		His	145.5	58.6	-42.4	73.8	-12.0	78.3	-16.0	-11.5	-16.3	-40.5	40.9	9.8	0.0	4.3	-16.0	17.1	63.0	26.9	190.3	43.6	83.7	54.5	-17.8	-43.6	-55.8	-5.3	-19.4	104.1
		Hyl	135.4	52.1	-44.8	66.7	-15.6	71.0	-19.4	-15.1	-19.8	-42.9	35.1	5.3	-4.1	0.0	-19.4	12.3	56.3	21.7	178.4	37.7	76.2	48.2	-21.1	-45.9	-57.6	-9.2	-22.7	95.7
		Hyp	192.3	88.8	-31.4	106.9	4.8	112.2	0.0	5.4	-0.4	-29.2	67.7	30.7	19.0	24.1	0.0	39.4	94.1	51.1	245.6	70.9	118.7	84.0	-2.1	-32.8	-47.3	12.7	-4.1	143.0
		Leu- lle	109.6	35.4	-50.8	48.4	-24.9	52.2	-28.3	-24.4	-28.6	-49.2	20.3	-6.3	-14.6	-11.0	-28.3	0.0	39.2	8.4	147.9	22.6	56.8	31.9	-29.8	-51.8	-62.2	-19.2	-31.2	74.2
		Lys	50.6	-2.7	-64.7	6.6	-46.0	9.4	-48.5	-45.7	-48.7	-63.5	-13.6	-32.7	-38.7	-36.0	-48.5	-28.2	0.0	-22.1	78.1	-11.9	12.7	-5.2	-49.6	-65.4	-72.9	-41.9	-50.6	25.2
		Met	93.4	24.9	-54.6	36.9	-30.7	40.5	-33.8	-30.2	-34.1	-53.1	11.0	-13.5	-21.2	-17.9	-33.8	-7.7	28.4	0.0	128.7	13.1	44.7	21.7	-35.2	-55.5	-65.1	-25.4	-36.5	60.8
		3-MH	-15.4	-45.4	-80.2	-40.1	-69.7	-38.6	-71.1	-69.5	-71.2	-79.5	-51.5	-62.2	-65.6	-64.1	-71.1	-59.7	-43.9	-56.3	0.0	-50.5	-36.7	-46.8	-71.7	-80.6	-84.8	-67.4	-72.2	-29.7
		Orn	71.0	10.4	-59.9	21.0	-38.7	24.2	-41.5	-38.3	-41.7	-58.6	-1.9	-23.6	-30.4	-27.4	-41.5	-18.4	13.5	-11.6	102.2	0.0	27.9	7.6	-42.7	-60.7	-69.2	-34.1	-43.9	42.1
		Phe	33.7	-13.7	-68.6	-5.4	-52.1	-2.9	-54.3	-51.8	-54.4	-67.6	-23.3	-40.2	-45.6	-43.2	-54.3	-36.2	-11.2	-30.9	58.1	-21.8	0.0	-15.9	-55.2	-69.3	-75.9	-48.5	-56.1	11.1
		Pro	58.9	2.6	-62.7	12.5	-43.0	15.4	-45.6	-42.7	-45.8	-61.5	-8.8	-29.0	-35.3	-32.5	-45.6	-24.2	5.5	-17.9	87.9	-7.1	18.9	0.0	-46.8	-63.5	-71.4	-38.7	-47.9	32.1
		Sar	198.5	92.8	-30.0	111.4	7.0	116.8	2.2	7.7	1.8	-27.6	71.3	33.5	21.6	26.8	2.2	42.4	98.2	54.4	253.1	74.6	123.4	87.9	0.0	-31.4	-46.2	15.1	-2.0	148.2
		Ser	335.1	181.0	2.1	208.0	56.0	216.0	48.9	56.9	48.3	5.4	149.6	94.5	77.2	84.8	48.9	107.6	188.9	125.0	414.6	154.5	225.5	173.9	45.7	0.0	-21.6	67.8	42.8	261.7
Tau	454.8	258.3	30.2	292.8	98.9	302.9	89.9	100.1	89.1	34.5	218.3	148.1	126.0	135.7	89.8	164.7	268.4	186.9	556.2	224.5	315.1	249.2	85.8	27.5	0.0	114.0	82.1	361.2		
Thr	159.3	67.5	-39.2	83.6	-7.0	88.3	-11.2	-6.5	-11.6	-37.2	48.8	15.9	5.6	10.1	-11.3	23.7	72.2	34.1	206.7	51.7	94.0	63.2	-13.1	-40.4	-53.3	0.0	-14.9	115.6		
Tyr	204.6	96.8	-28.5	115.7	9.2	121.2	4.3	9.9	3.8	-26.2	74.8	36.2	24.1	29.4	4.2	45.3	102.3	57.5	260.3	78.2	127.9	91.8	2.0	-30.0	-45.1	17.5	0.0	153.3		
Val	20.3	-22.3	-71.8	-14.8	-56.9	-12.6	-58.8	-56.6	-59.0	-70.8	-31.0	-46.2	-51.0	-48.9	-58.8	-42.6	-20.1	-37.8	42.3	-29.6	-10.0	-24.3	-59.7	-72.4	-78.3	-53.6	-60.5	0.0		
		Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val	
		B																												

Supplementary Table 25: Raw data Extended Data Fig. 2f – mixture of non-proteogenic and proteogenic AA in water, 170 μ m, 18 h – enrichments in bottom fraction, 4 fractions

re pe at	specie s	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)																													
		Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val		
1	A	Ans	0.0	8.5	46.8	3.6	25.8	9.2	-2.3	53.2	6.7	44.8	9.4	12.1	15.3	18.4	23.6	-8.5	9.6	15.0	2.6	9.5	-2.7	6.4	39.8	53.4	87.3	20.2	8.0	2.8	
		Arg	-7.8	0.0	35.3	-4.5	16.0	0.7	-10.0	41.2	-1.6	33.5	0.8	3.3	6.2	9.1	14.0	-15.6	1.0	6.0	-5.4	0.9	-10.3	-1.9	28.9	41.4	72.7	10.8	-0.5	-5.3	
		Asp	-31.9	-26.1	0.0	-29.4	-14.3	-25.6	-33.5	4.3	-27.3	-1.4	-25.5	-23.6	-21.5	-19.3	-15.8	-37.6	-25.3	-21.7	-30.1	-25.4	-33.7	-27.5	-4.7	4.5	27.6	-18.1	-26.4	-30.0	
		Car	-3.5	4.7	41.6	0.0	21.4	5.3	-5.8	47.8	3.0	39.7	5.5	8.1	11.2	14.2	19.3	-11.7	5.7	11.0	-1.0	5.6	-6.1	2.6	34.9	48.0	80.7	16.0	4.2	-0.9	
		Cit	-20.5	-13.8	16.7	-17.6	0.0	-13.2	-22.4	21.7	-15.2	15.1	-13.1	-10.9	-8.4	-5.9	-1.7	-27.2	-12.9	-8.6	-18.4	-13.0	-22.6	-15.4	11.2	21.9	48.9	-4.5	-14.2	-18.3	
		Cre	-8.4	-0.6	34.4	-5.1	15.2	0.0	-10.5	40.3	-2.3	32.6	0.2	2.7	5.6	8.4	13.2	-16.2	0.4	5.3	-6.0	0.2	-10.9	-2.6	28.1	40.5	71.6	10.1	-1.1	-5.9	
		Cys	2.4	11.1	50.3	6.1	28.8	11.8	0.0	56.8	9.2	48.2	12.0	14.8	18.0	21.2	26.6	-6.3	12.2	17.7	5.1	12.1	-0.4	8.9	43.2	57.0	91.8	23.1	10.5	5.2	
		Cth	-34.7	-29.2	-4.2	-32.3	-17.9	-28.7	-36.2	0.0	-30.3	-5.5	-28.6	-26.8	-24.7	-22.7	-19.3	-40.2	-28.4	-24.9	-33.0	-28.5	-36.5	-30.5	-8.7	0.1	22.3	-21.5	-29.5	-32.9	
		ETA	-6.3	1.7	37.6	-2.9	17.9	2.3	-8.5	43.5	0.0	35.7	2.5	5.0	8.0	11.0	15.9	-14.2	2.7	7.8	-3.8	2.6	-8.8	-0.3	31.0	43.7	75.6	12.6	1.2	-3.7	
		Glu	-30.9	-25.1	1.4	-28.4	-13.1	-24.6	-32.5	5.8	-26.3	0.0	-24.5	-22.6	-20.4	-18.2	-14.6	-36.8	-24.3	-20.6	-29.1	-24.4	-32.8	-26.5	-3.4	5.9	29.4	-17.0	-25.4	-29.0	
		AAB A	-8.6	-0.8	34.2	-5.2	15.0	-0.2	-10.7	40.0	-2.4	32.4	0.0	2.5	5.4	8.3	13.0	-16.3	0.2	5.1	-6.2	0.1	-11.0	-2.7	27.8	40.2	71.3	9.9	-1.3	-6.0	
		Hcy	-10.8	-3.2	31.0	-7.5	12.2	-2.6	-12.9	36.6	-4.8	29.2	-2.4	0.0	2.8	5.6	10.3	-18.3	-2.2	2.6	-8.4	-2.3	-13.2	-5.1	24.7	36.8	67.1	7.2	-3.7	-8.3	
		His	-13.2	-5.9	27.4	-10.1	9.1	-5.3	-15.3	32.9	-7.4	25.6	-5.1	-2.8	0.0	2.7	7.3	-20.6	-4.9	-0.2	-11.0	-5.0	-15.6	-7.7	21.3	33.1	62.5	4.3	-6.3	-10.8	
		Hyl	-15.5	-8.4	24.0	-12.5	6.2	-7.8	-17.5	29.3	-9.9	22.3	-7.6	-5.3	-2.7	0.0	4.4	-22.7	-7.4	-2.9	-13.3	-7.6	-17.8	-10.2	18.1	29.5	58.2	1.5	-8.8	-13.2	
		Hyp	-19.1	-12.2	18.7	-16.2	1.8	-11.7	-21.0	23.9	-13.7	17.1	-11.5	-9.3	-6.8	-4.2	0.0	-25.9	-11.3	-7.0	-17.0	-11.5	-21.3	-14.0	13.1	24.1	51.5	-2.8	-12.7	-16.9	
		Leu- lle	9.2	18.5	60.3	13.2	37.4	19.3	6.7	67.3	16.6	58.2	19.5	22.4	25.9	29.3	35.0	0.0	19.7	25.6	12.1	19.6	6.3	16.2	52.7	67.5	104.6	31.3	17.9	12.2	
		Lys	-8.8	-1.0	33.9	-5.4	14.8	-0.4	-10.9	39.7	-2.6	32.1	-0.2	2.3	5.2	8.0	12.8	-16.5	0.0	4.9	-6.4	-0.1	-11.2	-2.9	27.6	39.9	70.9	9.7	-1.5	-6.2	
		Met	-13.0	-5.7	27.6	-9.9	9.4	-5.1	-15.1	33.2	-7.2	25.9	-4.9	-2.5	0.2	3.0	7.5	-20.4	-4.7	0.0	-10.8	-4.8	-15.4	-7.5	21.6	33.4	62.9	4.5	-6.1	-10.6	
		3-MH	-2.6	5.7	43.0	1.0	22.6	6.4	-4.8	49.2	4.0	41.1	6.6	9.2	12.3	15.4	20.5	-10.8	6.8	12.1	0.0	6.6	-5.2	3.7	36.2	49.4	82.5	17.1	5.2	0.1	
		Orn	-8.6	-0.9	34.1	-5.3	14.9	-0.2	-10.8	39.9	-2.5	32.3	-0.1	2.4	5.3	8.2	12.9	-16.4	0.1	5.1	-6.2	0.0	-11.1	-2.8	27.8	40.1	71.2	9.8	-1.3	-6.1	
		Phe	2.8	11.5	50.8	6.5	29.3	12.2	0.4	57.4	9.7	48.8	12.4	15.2	18.4	21.7	27.0	-5.9	12.6	18.2	5.5	12.5	0.0	9.3	43.7	57.6	92.5	23.5	11.0	5.6	
		Pro	-6.0	2.0	38.0	-2.6	18.3	2.6	-8.2	44.0	0.3	36.1	2.8	5.4	8.3	11.3	16.2	-13.9	3.0	8.1	-3.5	2.9	-8.5	0.0	31.4	44.2	76.1	13.0	1.5	-3.4	
		Sar	-28.5	-22.4	5.0	-25.9	-10.0	-21.9	-30.1	9.5	-23.7	3.6	-21.8	-19.8	-17.6	-15.3	-11.6	-34.5	-21.6	-17.8	-26.6	-21.7	-30.4	-23.9	0.0	9.7	34.0	-14.0	-22.8	-26.5	
		Ser	-34.8	-29.3	-4.3	-32.4	-18.0	-28.8	-36.3	-0.1	-30.4	-5.6	-28.7	-26.9	-24.8	-22.8	-19.4	-40.3	-28.5	-25.0	-33.1	-28.6	-36.6	-30.6	-8.8	0.0	22.1	-21.6	-29.6	-33.0	
		Tau	-46.6	-42.1	-21.6	-44.7	-32.8	-41.7	-47.9	-18.2	-43.0	-22.7	-41.6	-40.2	-38.5	-36.8	-34.0	-51.1	-41.5	-38.6	-45.2	-41.6	-48.1	-43.2	-25.4	-18.1	0.0	-35.8	-42.4	-45.1	
		Thr	-16.8	-9.7	22.1	-13.8	4.7	-9.2	-18.7	27.4	-11.2	20.5	-9.0	-6.7	-4.1	-1.5	2.9	-23.8	-8.8	-4.3	-14.6	-8.9	-19.0	-11.5	16.3	27.6	55.9	0.0	-10.2	-14.5	
		Tyr	-7.4	0.5	35.9	-4.0	16.5	1.1	-9.5	41.8	-1.2	34.1	1.3	3.8	6.7	9.7	14.5	-15.2	1.5	6.5	-5.0	1.4	-9.9	-1.5	29.5	42.0	73.5	11.3	0.0	-4.8	
		Val	-2.7	5.6	42.8	0.9	22.4	6.3	-4.9	49.0	3.8	40.9	6.4	9.1	12.2	15.2	20.3	-10.9	6.7	11.9	-0.1	6.5	-5.3	3.5	36.1	49.3	82.3	17.0	5.1	0.0	
				Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val
				B																											
2	A	Ans	0.0	14.3	98.4	8.8	38.0	12.8	11.2	26.6	62.2	90.2	17.0	30.6	37.1	36.6	48.6	0.0	13.8	24.8	-1.1	21.3	9.3	18.0	65.2	67.0	146.6	30.6	63.4	5.6	
		Arg	-12.5	0.0	73.6	-4.8	20.7	-1.3	-2.7	10.8	41.9	66.4	2.4	14.3	20.0	19.5	30.0	-12.5	-0.4	9.2	-13.4	6.2	-4.4	3.3	44.5	46.1	115.8	14.3	42.9	-7.6	
		Asp	-49.6	-42.4	0.0	-45.1	-30.5	-43.2	-43.9	-36.2	-18.3	-4.2	-41.0	-34.2	-30.9	-31.2	-25.1	-49.6	-42.6	-37.1	-50.1	-38.8	-44.9	-40.5	-16.7	-15.8	24.3	-34.2	-17.7	-46.8	
		Car	-8.1	5.0	82.3	0.0	26.8	3.6	2.2	16.3	49.0	74.7	7.5	20.0	26.0	25.5	36.5	-8.1	4.6	14.7	-9.1	11.5	0.4	8.5	51.8	53.4	126.6	20.0	50.1	-3.0	

		Cit	-27.5	-17.2	43.8	-21.1	0.0	-18.3	-19.4	-8.2	17.5	37.8	-15.2	-5.3	-0.6	-1.0	7.7	-27.5	-17.5	-9.6	-28.3	-12.1	-20.8	-14.4	19.7	21.0	78.7	-5.3	18.4	-23.5
		Cre	-11.3	1.4	75.9	-3.5	22.3	0.0	-1.4	12.3	43.8	68.6	3.7	15.8	21.6	21.1	31.7	-11.3	0.9	10.6	-12.3	7.6	-3.1	4.7	46.5	48.1	118.7	15.8	44.8	-6.4
		Cys	-10.1	2.8	78.4	-2.2	24.0	1.4	0.0	13.8	45.8	71.0	5.2	17.4	23.3	22.8	33.6	-10.1	2.3	12.2	-11.1	9.1	-1.7	6.1	48.5	50.1	121.7	17.4	46.9	-5.1
		Cth	-21.0	-9.7	56.7	-14.1	9.0	-10.9	-12.2	0.0	28.1	50.2	-7.6	3.2	8.3	7.9	17.3	-21.0	-10.1	-1.4	-21.9	-4.2	-13.7	-6.8	30.4	31.9	94.8	3.2	29.0	-16.6
		ETA	-38.3	-29.5	22.3	-32.9	-14.9	-30.5	-31.4	-21.9	0.0	17.3	-27.9	-19.5	-15.4	-15.8	-8.4	-38.3	-29.8	-23.1	-39.0	-25.2	-32.6	-27.2	1.8	3.0	52.1	-19.5	0.7	-34.9
		Glu	-47.4	-39.9	4.3	-42.8	-27.4	-40.7	-41.5	-33.4	-14.7	0.0	-38.5	-31.3	-27.9	-28.2	-21.9	-47.4	-40.1	-34.4	-48.0	-36.2	-42.5	-37.9	-13.1	-12.2	29.7	-31.3	-14.1	-44.5
		AAB A	-14.5	-2.3	69.6	-7.0	17.9	-3.6	-4.9	8.2	38.6	62.5	0.0	11.6	17.2	16.7	27.0	-14.5	-2.7	6.7	-15.4	3.7	-6.6	0.9	41.2	42.7	110.8	11.6	39.6	-9.7
		Hcy	-23.4	-12.5	51.9	-16.7	5.6	-13.7	-14.8	-3.1	24.2	45.6	-10.4	0.0	5.0	4.6	13.8	-23.4	-12.9	-4.5	-24.3	-7.1	-16.3	-9.6	26.4	27.8	88.8	0.0	25.1	-19.1
		His	-27.1	-16.7	44.7	-20.6	0.6	-17.8	-18.9	-7.7	18.3	38.7	-14.7	-4.8	0.0	-0.4	8.3	-27.1	-17.0	-9.0	-27.9	-11.5	-20.3	-13.9	20.4	21.8	79.8	-4.8	19.1	-23.0
		Hyl	-26.8	-16.3	45.3	-20.3	1.0	-17.4	-18.6	-7.3	18.7	39.2	-14.3	-4.4	0.4	0.0	8.8	-26.8	-16.7	-8.6	-27.6	-11.2	-20.0	-13.6	20.9	22.3	80.6	-4.4	19.6	-22.7
		Hyp	-32.7	-23.1	33.5	-26.8	-7.1	-24.1	-25.1	-14.8	9.1	28.0	-21.3	-12.1	-7.7	-8.1	0.0	-32.7	-23.4	-16.0	-33.4	-18.3	-26.4	-20.6	11.2	12.4	66.0	-12.1	9.9	-28.9
		Leu- lle	0.0	14.3	98.3	8.8	37.9	12.7	11.2	26.6	62.1	90.1	17.0	30.6	37.1	36.5	48.5	0.0	13.8	24.8	-1.1	21.3	9.3	18.0	65.1	66.9	146.5	30.6	63.3	5.6
		Lys	-12.1	0.4	74.3	-4.4	21.2	-0.9	-2.3	11.2	42.5	67.1	2.8	14.8	20.5	20.0	30.5	-12.1	0.0	9.6	-13.1	6.6	-4.0	3.7	45.1	46.7	116.7	14.8	43.5	-7.2
		Met	-19.9	-8.4	59.0	-12.8	10.6	-9.6	-10.9	1.5	30.0	52.4	-6.2	4.7	9.9	9.5	19.1	-19.8	-8.8	0.0	-20.7	-2.8	-12.4	-5.4	32.4	33.8	97.6	4.7	30.9	-15.4
		3-MH	1.1	15.5	100.5	10.0	39.5	14.0	12.4	28.0	63.9	92.2	18.3	32.0	38.6	38.1	50.2	1.1	15.1	26.1	0.0	22.6	10.5	19.3	67.0	68.8	149.3	32.0	65.1	6.8
		Orn	-17.6	-5.8	63.5	-10.3	13.7	-7.1	-8.3	4.4	33.7	56.7	-3.6	7.7	13.0	12.6	22.5	-17.6	-6.2	2.8	-18.5	0.0	-9.9	-2.7	36.1	37.6	103.3	7.7	34.6	-13.0
		Phe	-8.5	4.6	81.5	-0.4	26.2	3.2	1.8	15.8	48.4	74.0	7.0	19.5	25.5	25.0	35.9	-8.5	4.1	14.2	-9.5	11.0	0.0	8.0	51.1	52.8	125.6	19.5	49.4	-3.4
		Pro	-15.3	-3.2	68.1	-7.8	16.9	-4.5	-5.8	7.3	37.4	61.1	-0.9	10.7	16.2	15.7	25.9	-15.3	-3.6	5.7	-16.2	2.8	-7.4	0.0	39.9	41.5	108.9	10.7	38.4	-10.5
		Sar	-39.5	-30.8	20.1	-34.1	-16.5	-31.7	-32.7	-23.3	-1.8	15.1	-29.2	-20.9	-17.0	-17.3	-10.0	-39.4	-31.1	-24.4	-40.1	-26.5	-33.8	-28.5	0.0	1.1	49.3	-20.9	-1.1	-36.1
		Ser	-40.1	-31.6	18.8	-34.8	-17.4	-32.5	-33.4	-24.2	-2.9	13.9	-29.9	-21.8	-17.9	-18.2	-11.0	-40.1	-31.8	-25.3	-40.8	-27.3	-34.5	-29.3	-1.1	0.0	47.7	-21.8	-2.2	-36.8
		Tau	-59.5	-53.7	-19.6	-55.9	-44.0	-54.3	-54.9	-48.7	-34.2	-22.9	-52.6	-47.0	-44.4	-44.6	-39.8	-59.4	-53.8	-49.4	-59.9	-50.8	-55.7	-52.1	-33.0	-32.3	0.0	-47.0	-33.8	-57.2
		Thr	-23.4	-12.5	51.9	-16.7	5.6	-13.7	-14.8	-3.1	24.2	45.6	-10.4	0.0	5.0	4.6	13.8	-23.4	-12.9	-4.5	-24.3	-7.1	-16.3	-9.6	26.4	27.8	88.8	0.0	25.1	-19.1
		Tyr	-38.8	-30.0	21.5	-33.4	-15.5	-31.0	-31.9	-22.5	-0.7	16.4	-28.4	-20.0	-16.0	-16.4	-9.0	-38.8	-30.3	-23.6	-39.4	-25.7	-33.1	-27.7	1.1	2.2	51.0	-20.0	0.0	-35.3
		Val	-5.3	8.2	87.9	3.0	30.6	6.8	5.3	19.9	53.6	80.1	10.8	23.7	29.9	29.3	40.7	-5.3	7.8	18.2	-6.3	14.9	3.5	11.8	56.4	58.1	133.5	23.7	54.7	0.0
		Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val	
		B																												

Supplementary Table 26: Raw data Extended Data Fig. 2b and 2g – mixture of non-proteogenic and proteogenic AA in water, 170 μ m, 18 h, 12 fractions

Due to technical problems, for the third replicate the temperature gradient was not applied for the entire duration of the experiment, which is why we do not take it into account for the calculation of the heat flow-driven enrichment.

repeat k	species	measured values (counts*s)												Normalization (Eq. 1) concentration (x c ₀)												Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)	
		top	II	III	IV	V	VI	VII	VIII	IX	X	XI	bot	top	II	III	IV	V	VI	VII	VIII	IX	X	XI	bot	top	bot
1	Anserine	9551624	11476674	20504399	17406186	33276686	36216805	18337629	33447667	45194536	46363381	41819528	60292811	0.307	0.368	0.658	0.559	1.068	1.162	0.589	1.074	1.451	1.488	1.342	1.935	-43.6	23.0
	Arginine	37038842	41705006	65839601	52231992	99672725	101961405	55470935	90159454	114588825	119540792	105059990	144486888	0.432	0.487	0.769	0.61	1.164	1.19	0.648	1.053	1.338	1.396	1.227	1.687	-20.4	7.3
	Aspartic acid	150461595	145953487	170605713	117229953	194716385	211639048	103373805	175504822	209882556	223280106	194498068	217398980	0.854	0.828	0.968	0.665	1.105	1.201	0.587	0.996	1.191	1.267	1.104	1.234	57.1	-21.6
	Carnosine	15644775	18652569	29092985	24723017	44303215	47827978	25806768	42895189	53984135	57904881	51951686	66464678	0.392	0.467	0.728	0.619	1.109	1.198	0.646	1.074	1.352	1.45	1.301	1.664	-27.9	5.8
	Citrulline	173661434	168366961	238625378	161742041	314645374	339873622	135081281	273051855	348954715	389212633	328228345	408038849	0.635	0.616	0.873	0.592	1.151	1.244	0.494	0.999	1.277	1.424	1.201	1.493	16.9	-5.1
	Creatinine	230369539	277953525	392167356	298823747	592303027	602632106	298170629	524586207	677118933	749752914	649604378	815272598	0.453	0.546	0.77	0.587	1.164	1.184	0.586	1.03	1.33	1.473	1.276	1.602	-16.7	1.8
	Cysteine	5652566	7090409	9230826	12091505	12926997	16294059	10771118	15849161	16791375	21575517	20445803	20997074	0.4	0.501	0.653	0.855	0.914	1.152	0.762	1.121	1.187	1.526	1.446	1.485	-26.5	-5.6
	Cystathionine	38681187	33522526	45695891	69787202	66514483	71644463	70231078	94328912	82241554	84416868	100225127	104276119	0.539	0.467	0.636	0.972	0.926	0.998	0.978	1.314	1.145	1.176	1.396	1.452	-0.9	-7.7
	Ethanolamine	164469490	192266299	236816469	114752068	280894417	282549134	87294932	167741773	292317598	328833204	257014079	330615813	0.721	0.843	1.039	0.503	1.232	1.239	0.383	0.736	1.282	1.442	1.127	1.45	32.7	-7.8
	Glutamic acid	198724559	190575946	236973157	148872538	266613316	282228759	116294873	216440818	270558073	297281109	247777403	281092701	0.866	0.831	1.033	0.649	1.162	1.23	0.507	0.943	1.179	1.296	1.08	1.225	59.3	-22.1
	Histidine	25641672	36451326	42626390	41036569	75111937	80504779	42706984	71497676	85977437	102075918	91176825	114348725	0.38	0.541	0.632	0.609	1.114	1.194	0.633	1.06	1.275	1.514	1.352	1.696	-30.0	7.8
	Homocysteine	755590904	767010728	1134009322	738195938	1476550145	1555872721	638809096	1215709760	1634329667	1815173852	1521871437	1856091262	0.6	0.609	0.901	0.586	1.173	1.236	0.507	0.966	1.298	1.442	1.209	1.474	10.4	-6.3

Homocysteine	107383361	100618218	148100980	92329779	197606820	215170011	80382959	161502245	226800017	251477796	204447899	262188746	0.629	0.59	0.868	0.541	1.158	1.261	0.471	0.946	1.329	1.473	1.198	1.536	15.8	-2.3
Hydroxyllysine	36695089	41766457	58600097	44801626	79788674	82210006	44579469	72482933	89718354	89764760	83205037	102985535	0.533	0.606	0.851	0.65	1.158	1.193	0.647	1.052	1.302	1.303	1.208	1.495	-2.0	-4.9
Hydroxyproline	230999543	238703170	333174485	193952237	417164113	451025836	163397508	342517945	460111924	507947833	410214193	523280794	0.649	0.67	0.936	0.545	1.172	1.267	0.459	0.962	1.292	1.427	1.152	1.47	19.4	-6.6
Leu_Isoleu	180445360	244097275	508153164	476621534	929786342	958435937	500169818	597497855	961799774	1107059132	821609039	1371678757	0.25	0.338	0.704	0.661	1.289	1.328	0.693	0.828	1.333	1.534	1.139	1.901	-54.0	20.9
Lysine	29643124	36173761	49271978	45236600	80343795	82023569	43937721	76245385	93803659	96038572	88334757	121097695	0.422	0.515	0.702	0.645	1.145	1.169	0.626	1.086	1.337	1.368	1.259	1.726	-22.3	9.7
Methionine	358496252	464716840	682513745	254006117	950430520	950216706	198335078	583075489	980967726	1114155233	829652046	1196169208	0.502	0.651	0.956	0.356	1.332	1.332	0.278	0.817	1.375	1.561	1.163	1.676	-7.6	6.6
Methylhistidine	42020989	49976385	92619620	83740795	166369085	177175651	92373755	161779992	207132319	218050483	207334928	285004146	0.283	0.336	0.623	0.563	1.119	1.192	0.621	1.088	1.394	1.467	1.395	1.918	-48.0	21.9
Ornithine	15404717	19062340	27512897	26649293	39677308	41491457	32993105	48843889	55829498	64160906	64762243	77419630	0.36	0.445	0.643	0.622	0.927	0.969	0.771	1.141	1.304	1.498	1.513	1.808	-33.8	15.0
Phenylalanine	336556629	287560302	574396922	297946928	986507147	965862384	234996973	827994575	1096406449	1143064458	879418361	1397286412	0.447	0.382	0.763	0.396	1.311	1.284	0.312	1.101	1.457	1.519	1.169	1.857	-17.7	18.1
Proline	357262104	427040821	678478008	363839681	980093234	1106185813	332724317	822915982	1206054122	1324371177	1067626639	1507861005	0.421	0.504	0.8	0.429	1.156	1.305	0.392	0.971	1.422	1.562	1.259	1.778	-22.5	13.1
Sarcosine	806392049	1213048885	896549891	809037826	1148113197	1257312600	573200599	1033648453	1467129349	1410783361	1199808131	1682524265	0.717	1.078	0.797	0.719	1.021	1.118	0.51	0.919	1.304	1.254	1.067	1.496	31.9	-4.9
Serine	109047496	97004270	113121655	119126251	147163553	165209739	95910066	155608204	172945632	175340449	175049668	192371302	0.762	0.678	0.79	0.832	1.028	1.154	0.67	1.087	1.208	1.225	1.223	1.344	40.1	-14.6
Taurine	34191182	31754909	30339757	25137711	32156573	33624300	22602410	30761195	33145325	32752528	31723658	32758041	1.106	1.027	0.981	0.813	1.04	1.088	0.731	0.995	1.072	1.06	1.026	1.06	103.5	-32.6
Threonine	145124895	146617765	215176462	157133707	288580720	311839743	138055972	261027744	323288627	361777712	306733010	398295813	0.57	0.576	0.846	0.617	1.134	1.225	0.543	1.026	1.27	1.422	1.205	1.565	4.9	-0.5
Tyrosine	69871890	89906246	117420227	136264091	150470029	151957203	143755320	97907781	130406254	142044129	96282784	145076418	0.57	0.733	0.958	1.111	1.227	1.239	1.172	0.799	1.064	1.158	0.785	1.183	4.8	-24.8
Valine	404369545	409396709	774224716	351429457	1139021352	1310641642	294854542	857446047	1422733809	1598292795	1253505842	1761974587	0.419	0.424	0.802	0.364	1.181	1.358	0.306	0.889	1.475	1.657	1.299	1.826	-22.9	16.1
mean concentration per fraction $\bar{c}_{j,k}$													0.544	0.595	0.81	0.631	1.131	1.204	0.59	1.003	1.294	1.407	1.219	1.573		

2	Anserine	5893436	1777635	9596519	13909351	18794163	19577075	26882871	30097109	37436524	69540104	52022308	147620957	0.163	0.049	0.266	0.385	0.521	0.542	0.745	0.834	1.037	1.927	1.441	4.09	-61.0	41.8
	Arginine	25741098	11335947	35719213	46155927	60948433	64666717	82674249	86448152	105611664	170505033	132032070	340149154	0.266	0.117	0.369	0.477	0.629	0.668	0.854	0.893	1.091	1.761	1.364	3.513	-36.5	21.8
	Aspartic acid	147546584	106701558	163036101	178345913	197359335	179184281	204582259	202414229	220824221	242868700	183494277	265522772	0.773	0.559	0.854	0.934	1.033	0.938	1.071	1.06	1.156	1.272	0.961	1.39	84.5	-51.8
	Carnosine	10174932	4249089	15601240	20588795	27410854	29828470	38043835	40944048	50620354	87610291	68707469	176735955	0.214	0.089	0.328	0.433	0.577	0.627	0.8	0.861	1.065	1.843	1.445	3.717	-48.9	28.9
	Citrulline	142974732	89426104	182313969	209250303	240376389	219355034	264932597	294003491	318710530	473035129	302688186	662135142	0.505	0.316	0.644	0.739	0.849	0.774	0.935	1.038	1.125	1.67	1.069	2.337	20.6	-18.9
	Creatinine	122005096	70672858	192085920	260952070	318718485	344955660	441053782	463539577	602413924	932107917	666217544	1622906987	0.242	0.14	0.382	0.519	0.633	0.686	0.877	0.921	1.197	1.853	1.324	3.226	-42.1	11.9
	Cysteine	12533952	4234829	6624887	7978894	7828999	7598811	8410429	14761395	13676168	44761720	41093117	83682503	0.594	0.201	0.314	0.378	0.371	0.36	0.399	0.7	0.648	2.122	1.948	3.966	41.9	37.6
	Cystathionine	30376600	21268142	38856151	45237709	52692460	44996264	49716072	62523546	56772302	91871419	143764449	173099233	0.449	0.315	0.575	0.669	0.779	0.666	0.735	0.925	0.84	1.359	2.127	2.561	7.3	-11.2
	Ethanolamine	121534573	68890741	155405513	184120215	184568132	225930186	277769657	264785313	317953343	367746591	179564244	450712563	0.521	0.295	0.666	0.789	0.791	0.969	1.191	1.135	1.363	1.577	0.77	1.932	24.5	-33.0
	Glutamic acid	183904806	123680201	216144436	233468222	254968650	234721976	271283286	276216961	296319840	344542801	222700359	374125343	0.728	0.489	0.855	0.924	1.009	0.929	1.074	1.093	1.173	1.364	0.881	1.481	73.9	-48.6
	Histidine	20253569	6631954	29314690	40269780	54073589	46983977	61486271	64445691	76838166	122096109	102073587	255194569	0.276	0.09	0.4	0.549	0.738	0.641	0.839	0.879	1.048	1.666	1.392	3.481	-34.0	20.7
	Homocysteine	513953252	262957208	653701456	813335613	973878964	988096037	1240897824	1260991271	1554986085	2245710458	1482575476	3367520246	0.402	0.205	0.511	0.635	0.761	0.772	0.97	0.985	1.215	1.755	1.158	2.631	-4.1	-8.7
	Homocysteine	75698129	37687986	99653395	131137551	148550490	137347115	180080518	172615333	220271367	285211728	192877532	419534976	0.432	0.215	0.569	0.749	0.849	0.785	1.029	0.986	1.258	1.629	1.102	2.397	3.3	-16.9
	Hydroxylysine	29683061	15956427	39002669	48513812	58876283	60975485	71459882	70753528	88179215	123330844	95390605	200953000	0.394	0.212	0.518	0.645	0.782	0.81	0.95	0.94	1.172	1.639	1.268	2.67	-5.8	-7.4
	Hydroxyproline	197070504	119636578	244120200	280493687	324665431	301087459	370017367	381137680	445431628	620790747	364640876	834635021	0.527	0.32	0.653	0.751	0.869	0.806	0.99	1.02	1.192	1.661	0.976	2.234	26.0	-22.5
	Leu_Isoleu	153838470	56132001	142707886	207160412	307441860	323693601	426589577	496346266	677186961	1343288635	854065230	2795564738	0.237	0.087	0.22	0.319	0.474	0.499	0.658	0.765	1.044	2.071	1.317	4.31	-43.4	49.5
	Lysine	19591776	9095432	28539068	37779401	48674691	50638843	61116952	64672301	77038366	132042954	106476530	261158509	0.262	0.122	0.382	0.506	0.651	0.678	0.818	0.865	1.031	1.767	1.425	3.494	-37.4	21.2

Methionine	249203204	111580491	278773772	368279317	453407789	489613755	628478788	626060033	774924568	1056498126	584427379	1723075822	0.407	0.182	0.455	0.602	0.741	0.8	1.027	1.023	1.266	1.726	0.955	2.815	-2.7	-2.4
Methylhistidine	24430869	5759026	40597265	57272418	74747568	82520511	106654073	120439279	148073347	293619597	227559903	639696507	0.161	0.038	0.267	0.377	0.492	0.544	0.703	0.794	0.976	1.934	1.499	4.215	-61.6	46.2
Ornithine	13084140	5768966	17874367	20617564	28267141	29484986	39460709	43181724	61882255	99850173	81471766	194748577	0.247	0.109	0.337	0.389	0.534	0.557	0.745	0.815	1.168	1.885	1.538	3.676	-41.0	27.5
Phenylalanine	168490779	58052434	249384789	329162778	370053402	445837566	585782730	574601163	792030462	1326223362	672500736	2462725353	0.252	0.087	0.372	0.492	0.553	0.666	0.875	0.858	1.183	1.981	1.004	3.678	-39.9	27.6
Proline	236017583	112343752	341578303	445419052	534546922	533631456	736430931	719891376	990504230	1486432235	856352946	2669210657	0.293	0.14	0.424	0.553	0.664	0.663	0.915	0.894	1.23	1.846	1.064	3.315	-30.0	15.0
Sarcosine	587604443	406777273	882992259	883417416	955085385	910015892	958659058	1129219561	1173964895	1504850937	1131223383	2290601338	0.55	0.381	0.827	0.827	0.894	0.852	0.898	1.057	1.099	1.409	1.059	2.145	31.4	-25.6
Serine	98585505	83941834	116063762	123895698	130329649	113525873	122472672	144839060	138143767	193648287	197692394	277376038	0.68	0.579	0.8	0.854	0.899	0.783	0.844	0.999	0.952	1.335	1.363	1.912	62.4	-33.7
Taurine	29813267	26140438	31144296	30924166	31346749	27242771	29494363	30303265	29546115	31307557	28939314	33941522	0.993	0.871	1.038	1.03	1.044	0.908	0.983	1.01	0.984	1.043	0.964	1.131	137.3	-60.8
Threonine	114850460	66719547	150577075	171032760	198682380	181557707	224398039	257083132	277219339	455860466	321038776	697175909	0.442	0.257	0.58	0.659	0.765	0.699	0.864	0.99	1.068	1.755	1.236	2.685	5.6	-6.9
Tyrosine	61105445	37034865	81402758	88729635	104904749	119317513	138044245	121642939	166391366	192820409	131774055	258525361	0.488	0.296	0.65	0.709	0.838	0.953	1.103	0.972	1.33	1.541	1.053	2.066	16.6	-28.3
Valine	191102105	67784424	260291684	364159224	480303569	546412590	790657861	775506822	1048789881	1813030567	856413117	3156497299	0.222	0.079	0.302	0.422	0.557	0.633	0.917	0.899	1.216	2.102	0.993	3.659	-47.1	26.9
mean concentration per fraction $\bar{c}_{j,k}$													0.419	0.244	0.52	0.618	0.725	0.722	0.886	0.936	1.112	1.696	1.239	2.883		

Supplementary Table 27: Raw data Extended Data Fig. 2g – mixture of non-proteogenic and proteogenic AA in water, 170 μ m, 18 h – enrichments in top fraction, 12 fractions

re pe at	specie s	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)																												
		Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val	
1	A	Ans	0.0	-29.1	-64.1	-21.7	-51.8	-32.3	-23.3	-43.1	-57.5	-64.6	-19.4	-48.9	-51.3	-42.5	-52.8	22.6	-27.4	-39.0	8.4	-14.8	-31.5	-27.2	-57.2	-59.8	-72.3	-46.2	-46.2	-26.9
		Arg	41.1	0.0	-49.4	10.4	-31.9	-4.4	8.2	-19.7	-40.1	-50.1	13.7	-27.9	-31.3	-18.8	-33.3	72.9	2.4	-13.9	53.0	20.2	-3.3	2.6	-39.7	-43.2	-60.9	-24.2	-24.1	3.2
		Asp	178.5	97.4	0.0	118.0	34.4	88.7	113.6	58.5	18.4	-1.4	124.5	42.3	35.7	60.3	31.6	241.4	102.2	70.0	202.0	137.3	90.9	102.6	19.1	12.1	-22.8	49.7	49.8	103.7
		Car	27.8	-9.4	-54.1	0.0	-38.4	-13.4	-2.0	-27.3	-45.7	-54.8	3.0	-34.7	-37.7	-26.5	-39.6	56.6	-7.3	-22.0	38.6	8.9	-12.4	-7.0	-45.4	-48.6	-64.6	-31.3	-31.3	-6.5
		Cit	107.3	46.9	-25.6	62.2	0.0	40.4	59.0	17.9	-11.9	-26.6	67.1	5.9	1.0	19.3	-2.1	154.1	50.4	26.5	124.8	76.6	42.0	50.8	-11.4	-16.6	-42.5	11.4	11.5	51.6
		Cre	47.6	4.6	-47.0	15.5	-28.8	0.0	13.2	-16.0	-37.3	-47.7	19.0	-24.6	-28.1	-15.1	-30.3	80.9	7.1	-9.9	60.1	25.8	1.2	7.4	-36.9	-40.6	-59.1	-20.6	-20.6	8.0
		Cys	30.4	-7.6	-53.2	2.0	-37.1	-11.7	0.0	-25.8	-44.6	-53.9	5.1	-33.4	-36.5	-25.0	-38.4	59.8	-5.4	-20.4	41.4	11.1	-10.7	-5.1	-44.3	-47.5	-63.9	-29.9	-29.9	-4.6
		Cth	75.7	24.6	-36.9	37.5	-15.2	19.1	34.8	0.0	-25.3	-37.8	41.7	-10.2	-14.4	1.1	-17.0	115.4	27.5	7.2	90.6	49.7	20.4	27.9	-24.9	-29.3	-51.3	-5.5	-5.5	28.5
		ETA	135.3	66.8	-15.5	84.2	13.5	59.4	80.5	33.9	0.0	-16.7	89.7	20.2	14.7	35.4	11.2	188.5	70.8	43.6	155.2	100.5	61.3	71.2	0.6	-5.3	-34.8	26.5	26.6	72.1
		Glu	182.5	100.3	1.4	121.1	36.3	91.4	116.7	60.8	20.0	0.0	127.8	44.3	37.6	62.6	33.5	246.3	105.0	72.4	206.3	140.7	93.6	105.5	20.8	13.7	-21.7	51.9	52.0	106.6
		AAB A	24.0	-12.1	-55.5	-2.9	-40.2	-16.0	-4.9	-29.4	-47.3	-56.1	0.0	-36.6	-39.6	-28.6	-41.4	52.0	-10.0	-24.3	34.5	5.7	-15.0	-9.8	-47.0	-50.1	-65.6	-33.3	-33.3	-9.3
		Hcy	95.8	38.8	-29.7	53.2	-5.6	32.6	50.1	11.4	-16.8	-30.7	57.8	0.0	-4.6	12.7	-7.5	139.9	42.1	19.4	112.3	66.8	34.1	42.4	-16.3	-21.2	-45.7	5.2	5.3	43.2
		His	105.2	45.5	-26.3	60.6	-1.0	39.0	57.4	16.8	-12.8	-27.4	65.5	4.8	0.0	18.1	-3.0	151.6	49.0	25.2	122.6	74.9	40.7	49.3	-12.2	-17.4	-43.1	10.3	10.4	50.1
		Hyl	73.8	23.2	-37.6	36.0	-16.2	17.7	33.3	-1.1	-26.2	-38.5	40.1	-11.2	-15.3	0.0	-17.9	113.0	26.1	6.0	88.4	48.1	19.1	26.4	-25.7	-30.1	-51.8	-6.6	-6.5	27.1
		Hyp	111.6	50.0	-24.0	65.6	2.1	43.4	62.3	20.4	-10.1	-25.1	70.6	8.1	3.1	21.8	0.0	159.4	53.6	29.1	129.5	80.3	45.0	54.0	-9.5	-14.8	-41.3	13.8	13.9	54.8
		Leu- lle	-18.4	-42.2	-70.7	-36.2	-60.6	-44.7	-37.4	-53.6	-65.3	-71.1	-34.2	-58.3	-60.2	-53.0	-61.4	0.0	-40.8	-50.2	-11.5	-30.5	-44.1	-40.6	-65.1	-67.2	-77.4	-56.1	-56.1	-40.3
		Lys	37.8	-2.3	-50.5	7.8	-33.5	-6.7	5.7	-21.6	-41.5	-51.2	11.1	-29.6	-32.9	-20.7	-34.9	68.9	0.0	-15.9	49.4	17.4	-5.6	0.2	-41.1	-44.5	-61.8	-25.9	-25.9	0.8
		Met	63.9	16.2	-41.2	28.3	-20.9	11.0	25.7	-6.7	-30.4	-42.0	32.1	-16.3	-20.2	-5.7	-22.6	100.9	18.9	0.0	77.7	39.6	12.3	19.2	-29.9	-34.0	-54.6	-11.9	-11.8	19.9
		3-MH	-7.8	-34.6	-66.9	-27.8	-55.5	-37.5	-29.3	-47.5	-60.8	-67.4	-25.7	-52.9	-55.1	-46.9	-56.4	13.0	-33.1	-43.7	0.0	-21.4	-36.8	-32.9	-60.6	-62.9	-74.4	-50.4	-50.4	-32.5
		Orn	17.4	-16.8	-57.9	-8.2	-43.4	-20.5	-10.0	-33.2	-50.1	-58.5	-5.4	-40.0	-42.8	-32.5	-44.5	43.8	-14.8	-28.4	27.3	0.0	-19.6	-14.6	-49.8	-52.8	-67.5	-36.9	-36.9	-14.2
		Phe	45.9	3.4	-47.6	14.2	-29.6	-1.1	11.9	-17.0	-38.0	-48.3	17.6	-25.5	-28.9	-16.0	-31.1	78.9	5.9	-11.0	58.2	24.3	0.0	6.2	-37.6	-41.3	-59.6	-21.6	-21.5	6.7
		Pro	37.4	-2.6	-50.7	7.6	-33.7	-6.9	5.4	-21.8	-41.6	-51.3	10.8	-29.8	-33.0	-20.9	-35.1	68.5	-0.2	-16.1	49.0	17.1	-5.8	0.0	-41.2	-44.7	-61.9	-26.1	-26.1	0.5
		Sar	133.9	65.8	-16.0	83.0	12.8	58.4	79.4	33.1	-0.6	-17.2	88.5	19.5	13.9	34.6	10.5	186.6	69.7	42.7	153.6	99.3	60.3	70.1	0.0	-5.9	-35.2	25.7	25.8	71.1
		Ser	148.5	76.1	-10.8	94.5	19.9	68.3	90.6	41.4	5.6	-12.0	100.3	26.9	21.1	43.0	17.4	204.5	80.3	51.6	169.4	111.7	70.3	80.8	6.3	0.0	-31.1	33.6	33.7	81.7
		Tau	260.8	155.8	29.5	182.4	74.1	144.4	176.7	105.3	53.3	27.7	190.9	84.3	75.8	107.6	70.5	342.2	161.9	120.2	291.2	207.4	147.2	162.5	54.3	45.2	0.0	93.9	94.1	163.9
		Thr	86.0	31.9	-33.2	45.6	-10.3	26.0	42.7	5.9	-21.0	-34.2	50.0	-5.0	-9.4	7.1	-12.1	128.0	35.0	13.5	101.7	58.5	27.5	35.3	-20.5	-25.1	-48.4	0.0	0.1	36.1
		Tyr	85.9	31.8	-33.3	45.5	-10.3	25.9	42.6	5.8	-21.0	-34.2	49.9	-5.0	-9.4	7.0	-12.2	127.8	34.9	13.4	101.6	58.4	27.4	35.2	-20.5	-25.2	-48.5	-0.1	0.0	36.0
		Val	36.7	-3.1	-50.9	7.0	-34.0	-7.4	4.9	-22.2	-41.9	-51.6	10.2	-30.2	-33.4	-21.3	-35.4	67.6	-0.8	-16.6	48.2	16.5	-6.3	-0.5	-41.5	-45.0	-62.1	-26.5	-26.5	0.0
				Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr
			B																											
2	A	Ans	0.0	-38.6	-78.9	-23.7	-67.7	-32.7	-72.5	-63.7	-68.7	-77.6	-40.9	-59.3	-62.2	-58.6	-69.0	-31.2	-37.7	-59.9	1.4	-33.9	-35.1	-44.3	-70.3	-76.0	-83.6	-63.1	-66.6	-26.3
		Arg	62.8	0.0	-65.6	24.2	-47.3	9.6	-55.3	-40.8	-49.0	-63.5	-3.8	-33.8	-38.5	-32.6	-49.6	12.1	1.4	-34.7	65.2	7.6	5.6	-9.3	-51.7	-60.9	-73.2	-39.9	-45.6	20.0
		Asp	373.2	190.6	0.0	261.0	53.1	218.6	30.0	71.9	48.3	6.1	179.6	92.4	78.7	95.9	46.5	225.7	194.7	89.7	380.0	212.8	207.0	163.6	40.4	13.7	-22.2	74.7	58.2	248.7
		Car	31.1	-19.5	-72.3	0.0	-57.6	-11.7	-64.0	-52.4	-58.9	-70.6	-22.5	-46.7	-50.5	-45.7	-59.4	-9.8	-18.4	-47.4	33.0	-13.4	-15.0	-27.0	-61.1	-68.5	-78.5	-51.6	-56.2	-3.4

		Cit	209.1	89.9	-34.7	135.8	0.0	108.1	-15.0	12.3	-3.1	-30.7	82.7	25.7	16.7	28.0	-4.3	112.8	92.5	24.0	213.6	104.4	100.6	72.2	-8.3	-25.7	-49.2	14.1	3.4	127.8
		Cre	48.5	-8.8	-68.6	13.3	-52.0	0.0	-59.2	-46.0	-53.5	-66.7	-12.2	-39.6	-43.9	-38.5	-54.0	2.2	-7.5	-40.4	50.7	-1.8	-3.6	-17.3	-55.9	-64.3	-75.6	-45.2	-50.3	9.5
		Cys	263.8	123.5	-23.1	177.6	17.7	145.0	0.0	32.2	14.0	-18.4	115.0	47.9	37.4	50.6	12.6	150.5	126.6	45.9	269.1	140.5	136.1	102.7	8.0	-12.6	-40.2	34.3	21.7	168.1
		Cth	175.2	69.0	-41.8	110.0	-11.0	85.3	-24.4	0.0	-13.8	-38.3	62.6	11.9	3.9	13.9	-14.8	89.5	71.4	10.4	179.2	81.9	78.6	53.3	-18.3	-33.9	-54.8	1.6	-8.0	102.8
		ETA	219.1	96.0	-32.6	143.5	3.2	114.9	-12.3	16.0	0.0	-28.4	88.6	29.8	20.5	32.1	-1.2	119.7	98.8	28.0	223.7	111.0	107.1	77.8	-5.3	-23.3	-47.5	17.8	6.7	135.2
		Glu	345.8	173.8	-5.8	240.1	44.2	200.2	22.5	62.0	39.7	0.0	163.4	81.3	68.3	84.5	38.0	206.9	177.6	78.8	352.2	194.7	189.2	148.3	32.3	7.1	-26.7	64.6	49.1	228.5
		AAB A	69.2	3.9	-64.2	29.1	-45.3	13.9	-53.5	-38.5	-47.0	-62.0	0.0	-31.2	-36.1	-30.0	-47.6	16.5	5.4	-32.1	71.7	11.9	9.8	-5.7	-49.8	-59.4	-72.2	-37.5	-43.4	24.7
		Hcy	145.9	51.1	-48.0	87.6	-20.4	65.6	-32.4	-10.6	-22.9	-44.8	45.3	0.0	-7.1	1.8	-23.9	69.3	53.2	-1.4	149.5	62.6	59.6	37.0	-27.0	-40.9	-59.6	-9.2	-17.8	81.3
		His	164.8	62.7	-44.0	102.1	-14.3	78.3	-27.2	-3.8	-17.0	-40.6	56.5	7.7	0.0	9.6	-18.0	82.3	65.0	6.2	168.7	75.1	71.8	47.5	-21.4	-36.4	-56.5	-2.2	-11.4	95.2
		Hyl	141.6	48.4	-48.9	84.3	-21.9	62.7	-33.6	-12.2	-24.3	-45.8	42.8	-1.8	-8.8	0.0	-25.2	66.3	50.5	-3.1	145.0	59.7	56.7	34.6	-28.3	-42.0	-60.3	-10.8	-19.2	78.0
		Hyp	223.0	98.4	-31.7	146.4	4.5	117.5	-11.2	17.4	1.2	-27.5	90.9	31.3	22.0	33.7	0.0	122.4	101.2	29.5	227.7	113.5	109.6	79.9	-4.1	-22.4	-46.9	19.3	8.0	138.1
		Leu- lle	45.3	-10.8	-69.3	10.8	-53.0	-2.2	-60.1	-47.2	-54.5	-67.4	-14.2	-40.9	-45.2	-39.9	-55.0	0.0	-9.5	-41.8	47.3	-4.0	-5.8	-19.1	-56.9	-65.1	-76.1	-46.4	-51.4	7.0
		Lys	60.6	-1.4	-66.1	22.5	-48.1	8.1	-55.9	-41.7	-49.7	-64.0	-5.1	-34.7	-39.4	-33.5	-50.3	10.5	0.0	-35.6	62.9	6.1	4.2	-10.6	-52.4	-61.4	-73.6	-40.7	-46.3	18.3
		Met	149.4	53.2	-47.3	90.3	-19.3	67.9	-31.5	-9.4	-21.9	-44.1	47.4	1.4	-5.8	3.2	-22.8	71.7	55.3	0.0	153.0	64.9	61.8	38.9	-26.0	-40.1	-59.0	-7.9	-16.6	83.8
		3-MH	-1.4	-39.5	-79.2	-24.8	-68.1	-33.6	-72.9	-64.2	-69.1	-77.9	-41.7	-59.9	-62.8	-59.2	-69.5	-32.1	-38.6	-60.5	0.0	-34.8	-36.0	-45.1	-70.7	-76.3	-83.8	-63.6	-67.0	-27.3
		Orn	51.3	-7.1	-68.0	15.4	-51.1	1.9	-58.4	-45.0	-52.6	-66.1	-10.6	-38.5	-42.9	-37.4	-53.2	4.1	-5.8	-39.3	53.4	0.0	-1.8	-15.7	-55.1	-63.7	-75.1	-44.2	-49.4	11.5
		Phe	54.1	-5.3	-67.4	17.6	-50.1	3.8	-57.6	-44.0	-51.7	-65.4	-8.9	-37.3	-41.8	-36.2	-52.3	6.1	-4.0	-38.2	56.3	1.9	0.0	-14.2	-54.3	-63.0	-74.7	-43.1	-48.5	13.6
		Pro	79.5	10.3	-62.1	37.0	-41.9	20.9	-50.7	-34.8	-43.7	-59.7	6.1	-27.0	-32.2	-25.7	-44.4	23.6	11.8	-28.0	82.1	18.7	16.5	0.0	-46.7	-56.9	-70.5	-33.7	-40.0	32.3
		Sar	237.0	107.0	-28.8	157.1	9.0	126.9	-7.4	22.5	5.6	-24.4	99.2	37.0	27.3	39.5	4.3	132.0	109.9	35.1	241.9	122.8	118.7	87.7	0.0	-19.0	-44.6	24.4	12.7	148.4
		Ser	316.3	155.7	-12.0	217.6	34.7	180.3	14.4	51.3	30.4	-6.6	146.0	69.3	57.2	72.3	28.9	186.6	159.3	66.9	322.3	175.2	170.1	131.9	23.5	0.0	-31.6	53.7	39.2	206.8
		Tau	508.4	273.7	28.6	364.2	96.8	309.7	67.2	121.1	90.6	36.5	259.5	147.4	129.7	151.9	88.3	318.9	278.9	144.0	517.2	302.2	294.8	238.9	80.5	46.2	0.0	124.6	103.4	348.4
		Thr	170.9	66.4	-42.8	106.7	-12.4	82.4	-25.6	-1.6	-15.1	-39.2	60.1	10.1	2.3	12.1	-16.1	86.5	68.7	8.6	174.8	79.1	75.8	50.9	-19.6	-34.9	-55.5	0.0	-9.4	99.6
		Tyr	199.1	83.7	-36.8	128.2	-3.3	101.4	-17.8	8.7	-6.3	-32.9	76.7	21.6	12.9	23.8	-7.4	105.9	86.3	19.9	203.4	97.7	94.0	66.6	-11.3	-28.2	-50.8	10.4	0.0	120.4
		Val	35.7	-16.7	-71.3	3.5	-56.1	-8.6	-62.7	-50.7	-57.5	-69.6	-19.8	-44.8	-48.8	-43.8	-58.0	-6.6	-15.5	-45.6	37.6	-10.3	-12.0	-24.4	-59.7	-67.4	-77.7	-49.9	-54.6	0.0
		Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val	
		B																												

Supplementary Table 28: Raw data Extended Data Fig. 2g – mixture of non-proteogenic and proteogenic AA in water, 170 µm, 18 h – enrichments in bottom fraction, 12 fractions

re	pe	specie	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)																														
at		s																															
1	A	Ans	0.0	14.7	56.9	16.3	29.6	20.8	30.3	33.2	33.4	58.0	14.1	31.3	26.0	29.4	31.7	1.8	12.1	15.4	0.9	7.0	4.2	8.8	29.4	44.0	82.6	23.6	63.5	6.0			
		Arg	-12.8	0.0	36.7	1.4	13.0	5.3	13.6	16.2	16.3	37.7	-0.5	14.4	9.8	12.8	14.8	-11.3	-2.2	0.6	-12.0	-6.7	-9.2	-5.1	12.8	25.5	59.2	7.8	42.6	-7.6			
		Asp	-36.2	-26.9	0.0	-25.9	-17.4	-23.0	-16.9	-15.1	-14.9	0.7	-27.2	-16.3	-19.7	-17.5	-16.1	-35.1	-28.5	-26.4	-35.7	-31.8	-33.6	-30.6	-17.5	-8.2	16.4	-21.2	4.3	-32.4			
		Car	-14.0	-1.4	34.9	0.0	11.5	3.9	12.1	14.6	14.7	35.8	-1.9	12.9	8.3	11.3	13.2	-12.5	-3.6	-0.7	-13.2	-8.0	-10.4	-6.4	11.3	23.8	57.0	6.3	40.7	-8.9			
		Cit	-22.8	-11.5	21.0	-10.3	0.0	-6.8	0.6	2.8	2.9	21.9	-12.0	1.3	-2.8	-0.1	1.6	-21.5	-13.5	-10.9	-22.1	-17.4	-19.6	-16.0	-0.2	11.1	40.9	-4.6	26.2	-18.2			
		Cre	-17.2	-5.1	29.8	-3.8	7.3	0.0	7.9	10.3	10.4	30.7	-5.6	8.6	4.2	7.1	9.0	-15.8	-7.2	-4.5	-16.5	-11.4	-13.8	-9.9	7.1	19.2	51.1	2.3	35.4	-12.3			
		Cys	-23.3	-12.0	20.3	-10.8	-0.6	-7.3	0.0	2.2	2.4	21.2	-12.5	0.7	-3.4	-0.7	1.0	-21.9	-14.0	-11.4	-22.6	-17.9	-20.1	-16.5	-0.8	10.5	40.1	-5.1	25.5	-18.7			
		Cth	-24.9	-13.9	17.7	-12.7	-2.7	-9.3	-2.2	0.0	0.1	18.6	-14.4	-1.5	-5.5	-2.9	-1.2	-23.6	-15.8	-13.4	-24.3	-19.7	-21.8	-18.3	-2.9	8.1	37.1	-7.2	22.7	-20.5			
		ETA	-25.1	-14.0	17.6	-12.9	-2.9	-9.4	-2.3	-0.1	0.0	18.4	-14.5	-1.6	-5.6	-3.0	-1.3	-23.7	-16.0	-13.5	-24.4	-19.8	-21.9	-18.5	-3.0	7.9	36.9	-7.3	22.6	-20.6			
		Glu	-36.7	-27.4	-0.7	-26.4	-18.0	-23.5	-17.5	-15.7	-15.5	0.0	-27.8	-16.9	-20.3	-18.1	-16.6	-35.6	-29.0	-26.9	-36.1	-32.2	-34.0	-31.1	-18.1	-8.8	15.6	-21.7	3.5	-32.9			
		AAB A	-12.4	0.5	37.5	1.9	13.6	5.9	14.2	16.8	16.9	38.4	0.0	15.0	10.4	13.4	15.4	-10.8	-1.7	1.2	-11.6	-6.2	-8.7	-4.6	13.4	26.2	60.0	8.3	43.3	-7.1			
		Hcy	-23.8	-12.6	19.5	-11.4	-1.3	-8.0	-0.7	1.5	1.6	20.3	-13.1	0.0	-4.0	-1.4	0.3	-22.5	-14.6	-12.1	-23.1	-18.5	-20.6	-17.1	-1.5	9.7	39.1	-5.8	24.6	-19.3			
		His	-20.6	-8.9	24.5	-7.7	2.9	-4.1	3.5	5.8	5.9	25.4	-9.4	4.2	0.0	2.8	4.5	-19.2	-11.0	-8.4	-19.9	-15.0	-17.3	-13.6	2.7	14.3	45.0	-1.8	29.8	-15.9			
		Hyl	-22.7	-11.4	21.2	-10.2	0.1	-6.6	0.7	2.9	3.1	22.0	-11.8	1.4	-2.7	0.0	1.7	-21.4	-13.4	-10.8	-22.0	-17.3	-19.5	-15.9	-0.1	11.3	41.1	-4.5	26.4	-18.1			
		Hyp	-24.1	-12.9	19.1	-11.7	-1.6	-8.2	-1.0	1.2	1.3	20.0	-13.3	-0.3	-4.3	-1.7	0.0	-22.7	-14.8	-12.3	-23.4	-18.7	-20.9	-17.4	-1.7	9.4	38.7	-6.1	24.2	-19.5			
		Leu- lle	-1.7	12.7	54.1	14.2	27.3	18.7	28.1	30.9	31.1	55.2	12.1	29.0	23.8	27.2	29.4	0.0	10.2	13.4	-0.8	5.2	2.4	6.9	27.1	41.5	79.4	21.5	60.7	4.1			
		Lys	-10.8	2.3	39.9	3.7	15.6	7.7	16.2	18.8	19.0	40.9	1.8	17.1	12.3	15.4	17.4	-9.2	0.0	2.9	-10.0	-4.6	-7.1	-3.0	15.4	28.4	62.8	10.2	45.8	-5.5			
		Met	-13.4	-0.6	35.9	0.7	12.3	4.7	12.9	15.4	15.6	36.8	-1.1	13.7	9.1	12.1	14.1	-11.8	-2.9	0.0	-12.6	-7.3	-9.7	-5.7	12.1	24.7	58.2	7.1	41.7	-8.2			
		3-MH	-0.9	13.7	55.4	15.2	28.4	19.7	29.2	32.0	32.2	56.5	13.1	30.1	24.8	28.3	30.5	0.9	11.1	14.4	0.0	6.0	3.2	7.8	28.2	42.7	80.9	22.5	62.1	5.0			
		Orn	-6.6	7.2	46.6	8.6	21.1	12.9	21.8	24.5	24.7	47.6	6.6	22.7	17.7	20.9	23.0	-4.9	4.8	7.9	-5.7	0.0	-2.6	1.7	20.9	34.6	70.6	15.5	52.8	-1.0			
		Phe	-4.0	10.1	50.5	11.6	24.4	16.0	25.1	27.9	28.1	51.6	9.5	26.0	20.9	24.2	26.4	-2.3	7.6	10.8	-3.1	2.7	0.0	4.4	24.2	38.2	75.3	18.7	57.0	1.7			
		Pro	-8.1	5.4	44.1	6.9	19.1	11.0	19.8	22.4	22.6	45.2	4.9	20.6	15.8	19.0	21.0	-6.5	3.1	6.1	-7.3	-1.6	-4.2	0.0	18.9	32.3	67.8	13.6	50.3	-2.6			
		Sar	-22.7	-11.3	21.2	-10.1	0.2	-6.6	0.8	3.0	3.1	22.1	-11.8	1.5	-2.6	0.1	1.8	-21.3	-13.3	-10.8	-22.0	-17.3	-19.5	-15.9	0.0	11.3	41.2	-4.4	26.4	-18.1			
		Ser	-30.6	-20.3	8.9	-19.3	-10.0	-16.1	-9.5	-7.5	-7.3	9.7	-20.8	-8.8	-12.5	-10.1	-8.6	-29.3	-22.1	-19.8	-29.9	-25.7	-27.6	-24.4	-10.2	0.0	26.8	-14.1	13.6	-26.4			
		Tau	-45.2	-37.2	-14.1	-36.3	-29.0	-33.8	-28.6	-27.0	-26.9	-13.5	-37.5	-28.1	-31.0	-29.1	-27.9	-44.3	-38.6	-36.8	-44.7	-41.4	-42.9	-40.4	-29.2	-21.1	0.0	-32.3	-10.4	-42.0			
		Thr	-19.1	-7.2	26.9	-6.0	4.8	-2.3	5.4	7.8	7.9	27.8	-7.7	6.2	1.9	4.7	6.5	-17.7	-9.3	-6.6	-18.4	-13.4	-15.7	-12.0	4.6	16.5	47.7	0.0	32.3	-14.3			
		Tyr	-38.9	-29.9	-4.1	-28.9	-20.8	-26.1	-20.3	-18.5	-18.4	-3.4	-30.2	-19.7	-23.0	-20.9	-19.5	-37.8	-31.4	-29.4	-38.3	-34.6	-36.3	-33.5	-20.9	-11.9	11.7	-24.4	0.0	-35.2			
		Val	-5.6	8.3	48.0	9.7	22.3	14.0	23.0	25.7	25.9	49.1	7.7	23.9	18.9	22.1	24.3	-3.9	5.8	8.9	-4.8	1.0	-1.7	2.7	22.1	35.9	72.3	16.7	54.3	0.0			
			Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val			
			B																														
2	A	Ans	0.0	16.4	194.2	10.0	75.0	26.8	3.1	59.7	111.6	176.2	17.5	55.4	70.6	53.2	83.1	-5.1	17.0	45.3	-3.0	11.2	11.2	23.4	90.7	113.9	261.6	52.3	98.0	11.8			
		Arg	-14.1	0.0	152.7	-5.5	50.3	8.9	-11.4	37.2	81.8	137.2	0.9	33.5	46.6	31.6	57.3	-18.5	0.5	24.8	-16.7	-4.4	-4.5	6.0	63.8	83.7	210.6	30.8	70.0	-4.0			
		Asp	-66.0	-60.4	0.0	-62.6	-40.5	-56.9	-64.9	-45.7	-28.1	-6.1	-60.1	-47.2	-42.0	-47.9	-37.8	-67.7	-60.2	-50.6	-67.0	-62.2	-62.2	-58.1	-35.2	-27.3	22.9	-48.2	-32.7	-62.0			
		Car	-9.1	5.8	167.4	0.0	59.0	15.2	-6.3	45.2	92.4	151.1	6.8	41.3	55.1	39.2	66.4	-13.7	6.4	32.0	-11.8	1.1	1.1	12.1	73.3	94.4	228.7	38.5	79.9	1.6			

		Cit	-42.8	-33.5	68.1	-37.1	0.0	-27.5	-41.1	-8.7	21.0	57.9	-32.9	-11.2	-2.5	-12.5	4.6	-45.8	-33.1	-17.0	-44.5	-36.4	-36.4	-29.5	9.0	22.2	106.7	-12.9	13.1	-36.1
		Cre	-21.1	-8.2	132.0	-13.2	38.0	0.0	-18.7	26.0	66.9	117.8	-7.3	22.6	34.6	20.8	44.4	-25.2	-7.7	14.6	-23.5	-12.3	-12.3	-2.7	50.4	68.7	185.2	20.1	56.1	-11.9
		Cys	-3.0	12.9	185.3	6.7	69.7	23.0	0.0	54.9	105.3	167.9	13.9	50.7	65.5	48.5	77.6	-8.0	13.5	40.9	-5.9	7.9	7.8	19.6	84.9	107.4	250.7	47.7	92.0	8.4
		Cth	-37.4	-27.1	84.2	-31.1	9.6	-20.6	-35.4	0.0	32.5	72.9	-26.4	-2.7	6.8	-4.1	14.6	-40.6	-26.7	-9.0	-39.2	-30.3	-30.4	-22.8	19.4	33.9	126.4	-4.6	24.0	-30.0
		ETA	-52.8	-45.0	39.0	-48.0	-17.3	-40.1	-51.3	-24.5	0.0	30.5	-44.5	-26.6	-19.4	-27.6	-13.5	-55.2	-44.7	-31.4	-54.2	-47.4	-47.5	-41.7	-9.9	1.0	70.9	-28.0	-6.5	-47.2
		Glu	-63.8	-57.8	6.5	-60.2	-36.7	-54.1	-62.7	-42.2	-23.4	0.0	-57.5	-43.7	-38.2	-44.5	-33.7	-65.6	-57.6	-47.4	-64.9	-59.7	-59.7	-55.3	-31.0	-22.6	30.9	-44.8	-28.3	-59.5
		AAB A	-14.9	-0.9	150.4	-6.4	48.9	7.9	-12.2	35.9	80.2	135.1	0.0	32.3	45.3	30.4	55.8	-19.2	-0.4	23.7	-17.4	-5.3	-5.4	5.0	62.3	82.0	207.8	29.7	68.5	-4.9
		Hcy	-35.7	-25.1	89.3	-29.2	12.6	-18.4	-33.7	2.7	36.2	77.7	-24.4	0.0	9.8	-1.5	17.8	-38.9	-24.7	-6.5	-37.6	-28.4	-28.5	-20.6	22.7	37.6	132.7	-2.0	27.4	-28.1
		His	-41.4	-31.8	72.4	-35.5	2.5	-25.7	-39.6	-6.4	24.0	61.9	-31.2	-8.9	0.0	-10.2	7.3	-44.4	-31.4	-14.9	-43.1	-34.8	-34.8	-27.7	11.7	25.3	111.9	-10.7	16.0	-34.5
		Hyl	-34.7	-24.0	92.1	-28.2	14.2	-17.2	-32.7	4.3	38.2	80.3	-23.3	1.5	11.4	0.0	19.5	-38.0	-23.6	-5.2	-36.6	-27.4	-27.4	-19.4	24.5	39.6	136.1	-0.5	29.3	-27.0
		Hyp	-45.4	-36.4	60.7	-39.9	-4.4	-30.7	-43.7	-12.8	15.6	50.9	-35.8	-15.1	-6.8	-16.3	0.0	-48.2	-36.1	-20.7	-47.0	-39.2	-39.3	-32.6	4.1	16.8	97.5	-16.8	8.1	-39.0
		Leu- lle	5.4	22.7	210.0	15.9	84.4	33.6	8.7	68.3	123.0	191.1	23.8	63.8	79.8	61.4	92.9	0.0	23.3	53.1	2.3	17.2	17.2	30.0	100.9	125.4	281.1	60.5	108.6	17.8
		Lys	-14.6	-0.5	151.4	-6.0	49.5	8.3	-11.9	36.5	80.8	136.0	0.4	32.8	45.8	30.9	56.4	-18.9	0.0	24.1	-17.1	-4.9	-5.0	5.4	62.9	82.7	209.0	30.2	69.2	-4.5
		Met	-31.2	-19.9	102.5	-24.3	20.4	-12.7	-29.0	9.9	45.7	90.1	-19.1	7.0	17.5	5.4	26.0	-34.7	-19.4	0.0	-33.2	-23.4	-23.5	-15.1	31.3	47.2	148.9	4.9	36.3	-23.1
		3-MH	3.1	20.0	203.2	13.4	80.3	30.7	6.3	64.6	118.1	184.6	21.1	60.2	75.9	57.8	88.7	-2.2	20.6	49.7	0.0	14.6	14.6	27.1	96.5	120.4	272.7	57.0	104.0	15.2
		Orn	-10.1	4.7	164.4	-1.1	57.3	14.0	-7.3	43.6	90.3	148.3	5.6	39.7	53.4	37.7	64.6	-14.7	5.2	30.6	-12.8	0.0	0.0	10.9	71.4	92.2	225.1	36.9	78.0	0.5
		Phe	-10.1	4.7	164.6	-1.1	57.4	14.0	-7.3	43.6	90.3	148.4	5.7	39.8	53.5	37.7	64.7	-14.7	5.3	30.6	-12.7	0.0	0.0	11.0	71.5	92.3	225.2	37.0	78.0	0.5
		Pro	-18.9	-5.6	138.4	-10.8	41.8	2.8	-16.4	29.5	71.6	123.9	-4.8	26.0	38.3	24.1	48.4	-23.1	-5.1	17.7	-21.3	-9.8	-9.9	0.0	54.5	73.3	193.1	23.5	60.5	-9.4
		Sar	-47.6	-38.9	54.3	-42.3	-8.2	-33.5	-45.9	-16.2	11.0	44.9	-38.4	-18.5	-10.5	-19.7	-4.0	-50.2	-38.6	-23.8	-49.1	-41.7	-41.7	-35.3	0.0	12.2	89.7	-20.1	3.8	-41.4
		Ser	-53.2	-45.6	37.6	-48.6	-18.2	-40.7	-51.8	-25.3	-1.0	29.2	-45.1	-27.3	-20.2	-28.4	-14.4	-55.6	-45.3	-32.1	-54.6	-48.0	-48.0	-42.3	-10.8	0.0	69.1	-28.8	-7.4	-47.7
		Tau	-72.3	-67.8	-18.7	-69.6	-51.6	-64.9	-71.5	-55.8	-41.5	-23.6	-67.5	-57.0	-52.8	-57.6	-49.4	-73.8	-67.6	-59.8	-73.2	-69.2	-69.3	-65.9	-47.3	-40.9	0.0	-57.9	-45.3	-69.1
		Thr	-34.4	-23.6	93.1	-27.8	14.9	-16.8	-32.3	4.8	38.9	81.3	-22.9	2.0	12.0	0.5	20.2	-37.7	-23.2	-4.6	-36.3	-27.0	-27.0	-19.0	25.2	40.4	137.4	0.0	30.0	-26.6
		Tyr	-49.5	-41.2	48.6	-44.4	-11.6	-36.0	-47.9	-19.3	6.9	39.5	-40.7	-21.5	-13.8	-22.6	-7.5	-52.1	-40.9	-26.6	-51.0	-43.8	-43.8	-37.7	-3.7	8.0	82.7	-23.1	0.0	-43.5
		Val	-10.5	4.2	163.2	-1.6	56.6	13.4	-7.7	42.9	89.4	147.1	5.1	39.1	52.7	37.0	63.8	-15.1	4.7	30.0	-13.2	-0.5	-0.5	10.4	70.6	91.4	223.6	36.3	77.1	0.0
		Ans	Arg	Asp	Car	Cit	Cre	Cys	Cth	ETA	Glu	AAB A	Hcy	His	Hyl	Hyp	Leu- lle	Lys	Met	3-MH	Orn	Phe	Pro	Sar	Ser	Tau	Thr	Tyr	Val	
		B																												

Supplementary Table 29: Raw data Extended Data Fig. 3 – AA in water, 170 μm , 18 h, pH 5.1.

repeat k	species	measured values (counts*min) for W and Y: mAU*min				measured values (counts*min) for W and Y: mAU*min								concentration (μM) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 4				c_0 (μM)	Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)	
		top	II	III	bot	top	II	III	bot					top	II	III	bot		top	II	III	bot	top	bot
1	H	18545	39408	65767	147913	20000	40360	68447	154043					5.84	12.09	20.34	45.76	21.01	0.28	0.58	0.97	2.18	8.8	-7.1
	N	51531	78771	116081	182033	55031	80006	121813	188797					10.50	15.64	23.43	36.53	21.53	0.49	0.73	1.09	1.70	90.7	-27.6
	S	49847	73116	114811	187230	52126	75195	120171	194522					10.35	15.05	23.85	38.75	22.00	0.47	0.68	1.08	1.76	84.0	-24.9
	Q	46514	69925	106850	170929	47987	72085	111472	177674					10.00	15.02	23.09	36.87	21.25	0.47	0.71	1.09	1.74	84.0	-26.0
	R	14681	38761	64098	164343	15811	40109	64714	169066					4.86	12.58	20.55	53.18	22.79	0.21	0.55	0.90	2.33	-16.5	-0.5
	G	84352	108670	133428	194205	87818	112784	140736	201153					15.50	19.93	24.68	35.59	23.92	0.65	0.83	1.03	1.49	153.3	-36.6
	D	12378	16639	68104	166027	12792	18225	72660	172665					2.72	3.77	15.22	36.61	14.58	0.19	0.26	1.04	2.51	-27.0	7.1
	E	9593	15522	61833	165731	10452	15584	64425	170704					2.31	3.59	14.56	38.81	14.82	0.16	0.24	0.98	2.62	-39.0	11.7
	T	24741	49761	100145	221722	26220	51492	104429	232704					4.65	9.25	18.68	41.49	18.52	0.25	0.50	1.01	2.24	-1.7	-4.4
	A	24631	35994	86521	179845	25409	37525	90429	185712					5.26	7.73	18.62	38.46	17.52	0.30	0.44	1.06	2.20	17.5	-6.4
	P	2857	6713	17871	60777	2817	6927	18726	62720					1.95	4.70	12.60	42.51	15.44	0.13	0.30	0.82	2.75	-50.5	17.4
	C	1761	3664	6792	20444	1926	4012	7250	21634					4.45	9.25	16.93	50.73	20.34	0.22	0.45	0.83	2.49	-14.5	6.4
	K	15885	22234	63453	124871	16042	23353	66771	129334					4.39	6.28	17.93	34.99	15.90	0.28	0.39	1.13	2.20	8.1	-6.1
	M	3728	8775	18316	51112	3619	9326	18770	51678					3.32	8.19	16.77	46.49	18.69	0.18	0.44	0.90	2.49	-30.5	6.1
	V	13938	58133	86295	248674	10856	48709	72214	258459					1.90	8.18	12.14	38.84	15.27	0.12	0.54	0.80	2.54	-51.3	8.5
	I	6224	16647	55420	268875	6462	17765	57229	280683					0.92	2.49	8.15	39.76	12.83	0.07	0.19	0.64	3.10	-72.0	32.2
	L	6285	16957	53062	235890	6861	17881	55658	246001					1.11	2.94	9.17	40.65	13.47	0.08	0.22	0.68	3.02	-67.8	28.7
	F	10346	30555	70232	266225	10233	30257	72720	277102					1.89	5.60	13.16	50.01	17.67	0.11	0.32	0.74	2.83	-58.1	20.8
	Y	0.0763	0.1327	0.1942	0.3758	0.0746	0.1323	0.2052	0.3953					9.40	16.50	24.87	48.01	24.70	0.38	0.67	1.01	1.94	48.8	-17.1
	W	0.0126	0.0482	0.1185	0.3879	0.0122	0.0493	0.1167	0.4052					1.64	6.44	15.54	52.40	19.01	0.09	0.34	0.82	2.76	-66.3	17.6
	mean concentration per fraction $\bar{c}_{j,k}$																		0.26	0.47	0.93	2.34		

2	H	34285	67453	117500	170007	35663	70837	121852	174403					10.60	20.96	36.27	52.19	30.01	0.35	0.70	1.21	1.74	8.0	-7.8
	N	86859	143662	184623	205455	89588	136952	175794	209707					17.38	27.64	35.50	40.90	30.36	0.57	0.91	1.17	1.35	75.0	-28.6
	S	85294	129218	167609	210107	89614	134498	175974	216443					17.75	26.77	34.87	43.29	30.67	0.58	0.87	1.14	1.41	76.9	-25.2
	Q	77320	121113	158657	194225	80537	126619	167261	199336					16.70	26.20	34.47	41.63	29.75	0.56	0.88	1.16	1.40	71.6	-25.8
	R	27331	59009	115767	182316	29056	61699	118912	184874					8.99	19.26	37.44	58.57	31.06	0.29	0.62	1.21	1.89	-11.5	0.0
	G	125026	163567	180125	196571	129480	171727	190485	205679					22.91	30.18	33.36	36.21	30.66	0.75	0.98	1.09	1.18	128.4	-37.4
	D	36768	67800	131427	244802	38295	71164	138058	254111					8.11	15.02	29.13	53.93	26.55	0.31	0.57	1.10	2.03	-6.6	7.7
	E	28810	60510	130789	242979	29088	62447	136842	249848					6.68	14.18	30.87	56.84	27.14	0.25	0.52	1.14	2.09	-24.8	11.0
	T	52364	106614	187587	281897	54097	111270	195844	291237					9.72	19.89	35.01	52.33	29.24	0.33	0.68	1.20	1.79	1.6	-5.1
	A	54045	97431	156783	230354	55816	100782	163309	237999					11.56	20.85	33.67	49.27	28.84	0.40	0.72	1.17	1.71	22.5	-9.4
	P	7445	18901	45970	86578	8060	19952	48172	89319					5.34	13.38	32.41	60.55	27.92	0.19	0.48	1.16	2.17	-41.6	15.0
	C	3035	6507	13355	23771	3084	6863	14011	24710					7.38	16.12	32.99	58.44	28.73	0.26	0.56	1.15	2.03	-21.5	7.8
	K	37399	73137	123146	175651	38747	70755	125519	178843					10.48	19.81	34.23	48.80	28.33	0.37	0.70	1.21	1.72	13.1	-8.7
	M	8743	18457	41216	64192	8525	19108	42082	66908					7.81	16.99	37.67	59.29	30.44	0.26	0.56	1.24	1.95	-21.6	3.3
	V	28429	225816	189762	420295	26592	81268	192062	404877					4.21	23.52	29.24	63.20	30.04	0.14	0.78	0.97	2.10	-57.1	11.5
	I	17337	53985	194205	460461	18558	55679	202339	475909					2.60	7.93	28.69	67.74	26.74	0.10	0.30	1.07	2.53	-70.3	34.3
	L	17610	52072	173563	387889	18512	54239	179910	400513					3.05	8.97	29.81	66.50	27.08	0.11	0.33	1.10	2.46	-65.6	30.2
	F	22615	63471	177428	362751	23774	64250	183183	373589					4.27	11.76	33.19	67.78	29.25	0.15	0.40	1.13	2.32	-55.4	22.8
	Y	0.1137	0.1899	0.2942	0.3982	0.1128	0.196	0.2981	0.4166					14.11	24.03	36.89	50.74	31.44	0.45	0.76	1.17	1.61	37.2	-14.4
	W	0.0279	0.0931	0.2529	0.4754	0.0312	0.0977	0.2631	0.5016					3.90	12.60	34.09	64.56	28.79	0.14	0.44	1.18	2.24	-58.5	18.9
	mean concentration per fraction $\bar{c}_{j,k}$																			0.33	0.64	1.15	1.89	
3	H	41315	69842	104906	167749	43152	73890	107842	175221					12.80	21.78	32.24	51.97	29.70	0.43	0.73	1.09	1.75	7.7	-8.3
	N	93246	130411	149665	206780	96038	137980	153403	215862					18.65	26.44	29.85	41.63	29.14	0.64	0.91	1.02	1.43	59.8	-25.2
	S	91403	132542	148454	208062	95550	139126	151499	218120					18.97	27.57	30.44	43.25	30.06	0.63	0.92	1.01	1.44	57.7	-24.6
	Q	84036	121636	139512	194565	88100	127146	142560	202102					18.21	26.32	29.84	41.96	29.08	0.63	0.90	1.03	1.44	56.4	-24.4
	R	33868	62810	108852	169406	34614	65807	111147	174727					10.92	20.52	35.09	54.90	30.36	0.36	0.68	1.16	1.81	-10.1	-5.3
	G	129461	160204	170642	200048	135683	167805	174816	211306					23.87	29.52	31.09	37.03	30.38	0.79	0.97	1.02	1.22	96.2	-36.2

	D	46744	92424	101010	219393	49017	97225	103649	232268					10.35	20.50	22.12	48.82	25.45	0.41	0.81	0.87	1.92	1.6	0.5
	E	39119	83254	102902	217087	40595	87017	103576	229146					9.19	19.64	23.82	51.47	26.03	0.35	0.75	0.91	1.98	-11.8	3.6
	T	60781	113184	157881	288297	64569	117881	161213	300297					11.45	21.10	29.14	53.74	28.86	0.40	0.73	1.01	1.86	-0.9	-2.5
	A	61868	107344	123710	234669	64420	111990	125045	242302					13.29	23.07	26.17	50.18	28.18	0.47	0.82	0.93	1.78	17.8	-6.7
	P	9576	21671	37811	91220	10054	22726	38023	95477					6.76	15.28	26.11	64.27	28.10	0.24	0.54	0.93	2.29	-39.9	19.8
	C	2778	6276	12060	21720	2940	6550	12550	23208					6.89	15.46	29.67	54.16	26.55	0.26	0.58	1.12	2.04	-35.1	6.9
	K	45515	82199	85095	171841	47481	86160	86471	178664					12.80	23.17	23.62	48.25	26.96	0.47	0.86	0.88	1.79	18.6	-6.3
	M	10463	21318	33352	65321	10911	22047	34258	69152					9.67	19.61	30.58	60.82	30.17	0.32	0.65	1.01	2.02	-20.0	5.6
	V	60301	92615	151285	401063	38373	97547	148925	417360					7.56	14.56	22.99	62.68	26.95	0.28	0.54	0.85	2.33	-30.0	21.8
	I	28318	75119	148160	474224	29304	77532	153087	493525					4.17	11.04	21.79	70.01	26.76	0.16	0.41	0.81	2.62	-61.1	37.1
	L	27858	70111	134470	397121	28535	72880	138331	413616					4.76	12.06	23.01	68.38	27.05	0.18	0.45	0.85	2.53	-56.1	32.4
	F	34437	77671	152260	346105	34331	79242	157348	360004					6.33	14.44	28.50	65.00	28.57	0.22	0.51	1.00	2.28	-44.7	19.2
	Y	0.1279	0.1953	0.2727	0.3763	0.1383	0.2153	0.2843	0.399					16.58	25.57	34.69	48.29	31.28	0.53	0.82	1.11	1.54	32.4	-19.2
	W	0.0514	0.1157	0.2208	0.4468	0.0533	0.1218	0.2293	0.4629					6.92	15.69	29.74	60.11	28.11	0.25	0.56	1.06	2.14	-38.5	12.0
mean concentration per fraction $\bar{c}_{j,k}$																			0.40	0.71	0.98	1.91		

Supplementary Table 30: Raw data Extended Data Fig. 3 – AA in water, 170 μm , 18 h, pH 5.1 – enrichments in top fraction

re peat	sp eci es	Ratio species against species (shown in heat maps), Eq. 2																				$[A]_{j,k}/[B]_{j,k} - 1$ (%)	
1	A	H	0.0	-43.0	-40.9	-40.9	30.3	-57.1	49.0	78.2	10.7	-7.5	119.8	27.2	0.6	56.4	123.5	288.7	237.7	159.3	-26.9	222.6	
		N	75.4	0.0	3.7	3.7	128.5	-24.7	161.3	212.5	94.1	62.3	285.5	123.1	76.4	174.4	292.0	581.7	492.2	354.8	28.2	465.7	
		S	69.2	-3.5	0.0	0.0	120.5	-27.4	152.1	201.5	87.2	56.6	271.9	115.3	70.2	164.7	278.2	557.6	471.3	338.8	23.7	445.8	
		Q	69.2	-3.5	0.0	0.0	120.5	-27.4	152.1	201.5	87.2	56.6	271.9	115.3	70.2	164.7	278.2	557.6	471.4	338.8	23.7	445.8	
		R	-23.3	-56.2	-54.6	-54.6	0.0	-67.1	14.3	36.8	-15.1	-29.0	68.7	-2.4	-22.8	20.1	71.5	198.3	159.1	99.0	-43.9	147.6	
		G	133.0	32.8	37.7	37.7	203.6	0.0	247.1	315.1	157.8	115.6	412.1	196.4	134.3	264.4	420.8	805.5	686.7	504.1	70.3	651.5	
		D	-32.9	-61.7	-60.3	-60.3	-12.5	-71.2	0.0	19.6	-25.7	-37.9	47.5	-14.6	-32.5	5.0	50.0	160.9	126.6	74.1	-50.9	116.5	
		E	-43.9	-68.0	-66.8	-66.8	-26.9	-75.9	-16.4	0.0	-37.9	-48.1	23.4	-28.6	-43.6	-12.2	25.4	118.1	89.5	45.5	-59.0	81.0	
		T	-9.6	-48.5	-46.6	-46.6	17.8	-61.2	34.6	61.0	0.0	-16.4	98.6	15.0	-9.1	41.4	102.0	251.2	205.2	134.4	-34.0	191.5	
		A	8.1	-38.4	-36.1	-36.1	40.8	-53.6	61.0	92.6	19.6	0.0	137.6	37.5	8.7	69.1	141.6	320.1	265.0	180.3	-21.0	248.6	
		P	-54.5	-74.1	-73.1	-73.1	-40.7	-80.5	-32.2	-18.9	-49.7	-57.9	0.0	-42.1	-54.2	-28.8	1.7	76.8	53.6	18.0	-66.7	46.8	
		C	-21.4	-55.2	-53.5	-53.5	2.4	-66.3	17.1	40.1	-13.0	-27.3	72.8	0.0	-20.9	23.0	75.7	205.5	165.4	103.8	-42.6	153.6	
		K	-0.6	-43.3	-41.2	-41.2	29.6	-57.3	48.1	77.2	10.0	-8.0	118.5	26.5	0.0	55.5	122.2	286.4	235.7	157.8	-27.3	220.7	
		M	-36.1	-63.6	-62.2	-62.2	-16.7	-72.6	-4.8	13.9	-29.3	-40.9	40.5	-18.7	-35.7	0.0	42.9	148.5	115.9	65.8	-53.3	106.2	
		V	-55.3	-74.5	-73.6	-73.6	-41.7	-80.8	-33.3	-20.3	-50.5	-58.6	-1.7	-43.1	-55.0	-30.0	0.0	73.9	51.1	16.0	-67.3	44.3	
		I	-74.3	-85.3	-84.8	-84.8	-66.5	-89.0	-61.7	-54.2	-71.5	-76.2	-43.4	-67.3	-74.1	-59.8	-42.5	0.0	-13.1	-33.3	-81.2	-17.0	
		L	-70.4	-83.1	-82.5	-82.5	-61.4	-87.3	-55.9	-47.2	-67.2	-72.6	-34.9	-62.3	-70.2	-53.7	-33.8	15.1	0.0	-23.2	-78.4	-4.5	
		F	-61.4	-78.0	-77.2	-77.2	-49.8	-83.4	-42.5	-31.3	-57.3	-64.3	-15.2	-50.9	-61.2	-39.7	-13.8	49.9	30.2	0.0	-71.8	24.4	
		Y	36.8	-22.0	-19.1	-19.1	78.3	-41.3	103.9	143.8	51.4	26.6	200.8	74.1	37.6	114.0	205.8	431.8	362.0	254.8	0.0	341.4	
		W	-69.0	-82.3	-81.7	-81.7	-59.6	-86.7	-53.8	-44.8	-65.7	-71.3	-31.9	-60.6	-68.8	-51.5	-30.7	20.5	4.7	-19.6	-77.3	0.0	
			H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
		B																					
2	A	H	0.0	-38.3	-39.0	-37.1	22.0	-52.7	15.6	43.6	6.3	-11.9	84.8	37.6	-4.5	37.7	151.9	263.8	214.0	142.0	-21.3	160.5	
		N	62.1	0.0	-1.1	2.0	97.8	-23.4	87.3	132.7	72.2	42.9	199.5	123.0	54.8	123.2	308.2	489.6	409.0	292.2	27.6	322.2	
		S	63.8	1.1	0.0	3.1	99.9	-22.5	89.4	135.3	74.1	44.4	202.7	125.5	56.4	125.6	312.7	496.0	414.5	296.5	29.0	326.8	
		Q	58.9	-2.0	-3.0	0.0	93.8	-24.9	83.6	128.1	68.8	40.0	193.6	118.6	51.7	118.8	300.1	477.9	398.9	284.4	25.1	313.8	
		R	-18.0	-49.4	-50.0	-48.4	0.0	-61.2	-5.3	17.7	-12.9	-27.8	51.4	12.8	-21.7	12.9	106.4	198.2	157.4	98.3	-35.5	113.5	
		G	111.5	30.5	29.1	33.1	158.0	0.0	144.4	203.7	124.7	86.4	290.8	191.0	101.9	191.2	432.6	669.3	564.1	411.8	66.5	450.8	
		D	-13.5	-46.6	-47.2	-45.5	5.6	-59.1	0.0	24.2	-8.1	-23.7	59.9	19.0	-17.4	19.1	117.9	214.7	171.7	109.4	-31.9	125.3	
		E	-30.4	-57.0	-57.5	-56.2	-15.0	-67.1	-19.5	0.0	-26.0	-38.6	28.7	-4.2	-33.5	-4.1	75.4	153.3	118.7	68.5	-45.2	81.4	
		T	-5.9	-41.9	-42.6	-40.8	14.8	-55.5	8.8	35.1	0.0	-17.0	73.9	29.5	-10.1	29.6	137.0	242.3	195.5	127.7	-25.9	145.1	
		A	13.4	-30.0	-30.8	-28.6	38.4	-46.4	31.1	62.9	20.5	0.0	109.6	56.1	8.3	56.2	185.7	312.7	256.2	174.5	-10.7	195.5	
		P	-45.9	-66.6	-67.0	-65.9	-34.0	-74.4	-37.4	-22.3	-42.5	-52.3	0.0	-25.5	-48.3	-25.5	36.3	96.9	69.9	31.0	-57.4	41.0	
		C	-27.3	-55.2	-55.6	-54.3	-11.3	-65.6	-16.0	4.3	-22.8	-35.9	34.3	0.0	-30.6	0.1	83.0	164.4	128.2	75.9	-42.8	89.3	
		K	4.7	-35.4	-36.1	-34.1	27.8	-50.5	21.1	50.4	11.3	-7.7	93.5	44.1	0.0	44.2	163.8	281.0	228.9	153.5	-17.6	172.8	
		M	-27.4	-55.2	-55.7	-54.3	-11.4	-65.7	-16.1	4.3	-22.8	-36.0	34.2	-0.1	-30.7	0.0	82.9	164.2	128.0	75.7	-42.8	89.2	
		V	-60.3	-75.5	-75.8	-75.0	-51.6	-81.2	-54.1	-43.0	-57.8	-65.0	-26.6	-45.4	-62.1	-45.3	0.0	44.4	24.7	-3.9	-68.7	3.4	
I	-72.5	-83.0	-83.2	-82.7	-66.5	-87.0	-68.2	-60.5	-70.8	-75.8	-49.2	-62.2	-73.8	-62.1	-30.8	0.0	-13.7	-33.5	-78.4	-28.4			

		L	-68.2	-80.4	-80.6	-80.0	-61.1	-84.9	-63.2	-54.3	-66.2	-71.9	-41.2	-56.2	-69.6	-56.1	-19.8	15.8	0.0	-22.9	-74.9	-17.1
		F	-58.7	-74.5	-74.8	-74.0	-49.6	-80.5	-52.2	-40.7	-56.1	-63.6	-23.6	-43.1	-60.5	-43.1	4.1	50.3	29.8	0.0	-67.5	7.6
		Y	27.0	-21.6	-22.5	-20.0	55.0	-39.9	46.8	82.4	35.0	12.0	134.7	74.8	21.3	74.9	219.9	362.1	298.9	207.4	0.0	230.9
		W	-61.6	-76.3	-76.6	-75.8	-53.2	-81.8	-55.6	-44.9	-59.2	-66.2	-29.1	-47.2	-63.3	-47.1	-3.3	39.7	20.6	-7.1	-69.8	0.0
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
		B																				
3	A	H	0.0	-32.6	-31.7	-31.2	19.8	-45.1	6.0	22.0	8.7	-8.6	79.2	66.0	-9.2	34.5	53.7	176.6	145.1	94.5	-18.7	75.2
		N	48.4	0.0	1.4	2.2	77.8	-18.6	57.3	81.1	61.3	35.7	166.1	146.4	34.7	99.7	128.2	310.6	263.9	188.7	20.7	160.0
		S	46.4	-1.3	0.0	0.8	75.4	-19.7	55.2	78.7	59.1	33.9	162.5	143.1	32.9	97.0	125.1	305.1	259.0	184.9	19.1	156.5
		Q	45.3	-2.1	-0.8	0.0	74.0	-20.3	53.9	77.3	57.9	32.8	160.4	141.1	31.9	95.4	123.3	301.9	256.1	182.6	18.1	154.5
		R	-16.5	-43.8	-43.0	-42.5	0.0	-54.2	-11.5	1.9	-9.3	-23.7	49.7	38.6	-24.2	12.3	28.3	131.0	104.7	62.4	-32.1	46.2
		G	82.3	22.8	24.5	25.5	118.3	0.0	93.2	122.4	98.1	66.6	226.7	202.6	65.5	145.2	180.2	404.2	346.8	254.6	48.2	219.3
		D	-5.6	-36.4	-35.6	-35.0	13.0	-48.2	0.0	15.2	2.5	-13.7	69.2	56.6	-14.3	26.9	45.0	161.1	131.3	83.6	-23.3	65.3
		E	-18.0	-44.8	-44.0	-43.6	-1.8	-55.0	-13.2	0.0	-10.9	-25.1	46.9	36.0	-25.6	10.2	26.0	126.7	100.9	59.4	-33.4	43.5
		T	-8.0	-38.0	-37.2	-36.7	10.2	-49.5	-2.5	12.3	0.0	-15.9	65.0	52.8	-16.5	23.8	41.4	154.6	125.6	79.0	-25.2	61.2
		A	9.4	-26.3	-25.3	-24.7	31.0	-40.0	15.9	33.5	18.9	0.0	96.1	81.6	-0.7	47.2	68.1	202.6	168.2	112.8	-11.0	91.6
		P	-44.2	-62.4	-61.9	-61.6	-33.2	-69.4	-40.9	-31.9	-39.4	-49.0	0.0	-7.4	-49.4	-25.0	-14.3	54.3	36.8	8.5	-54.6	-2.3
		C	-39.8	-59.4	-58.9	-58.5	-27.8	-66.9	-36.2	-26.5	-34.5	-44.9	8.0	0.0	-45.3	-19.0	-7.4	66.7	47.7	17.2	-51.0	5.5
		K	10.2	-25.8	-24.8	-24.2	31.9	-39.6	16.7	34.4	19.7	0.7	97.5	82.9	0.0	48.2	69.3	204.7	170.0	114.3	-10.4	93.0
		M	-25.7	-49.9	-49.2	-48.8	-11.0	-59.2	-21.2	-9.3	-19.2	-32.0	33.3	23.4	-32.5	0.0	14.3	105.6	82.2	44.6	-39.5	30.2
		V	-34.9	-56.2	-55.6	-55.2	-22.1	-64.3	-31.1	-20.6	-29.3	-40.5	16.6	8.0	-40.9	-12.5	0.0	80.0	59.5	26.6	-47.1	14.0
		I	-63.8	-75.6	-75.3	-75.1	-56.7	-80.2	-61.7	-55.9	-60.7	-67.0	-35.2	-40.0	-67.2	-51.4	-44.4	0.0	-11.4	-29.7	-70.6	-36.7
		L	-59.2	-72.5	-72.1	-71.9	-51.1	-77.6	-56.8	-50.2	-55.7	-62.7	-26.9	-32.3	-63.0	-45.1	-37.3	12.8	0.0	-20.6	-66.8	-28.5
		F	-48.6	-65.4	-64.9	-64.6	-38.4	-71.8	-45.5	-37.3	-44.1	-53.0	-7.8	-14.7	-53.3	-30.8	-21.0	42.2	26.0	0.0	-58.2	-10.0
		Y	23.0	-17.2	-16.0	-15.4	47.3	-32.5	30.3	50.0	33.6	12.4	120.4	104.1	11.6	65.4	89.0	240.2	201.4	139.2	0.0	115.4
		W	-42.9	-61.5	-61.0	-60.7	-31.6	-68.7	-39.5	-30.3	-38.0	-47.8	2.3	-5.2	-48.2	-23.2	-12.3	57.9	40.0	11.1	-53.6	0.0
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
		B																				

Supplementary Table 31: Raw data Extended Data Fig. 3 – AA in water, 170 μ m, 18 h, pH 5.1 – enrichments in bottom fraction

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)																				
1	A	H	0.0	28.4	23.7	25.5	-6.6	46.4	-13.3	-16.8	-2.8	-0.8	-20.9	-12.7	-1.0	-12.4	-14.4	-29.7	-27.8	-23.1	12.0	-21.0
		N	-22.1	0.0	-3.6	-2.2	-27.3	14.1	-32.4	-35.2	-24.3	-22.7	-38.4	-32.0	-22.9	-31.8	-33.3	-45.2	-43.8	-40.1	-12.7	-38.4
		S	-19.1	3.8	0.0	1.5	-24.5	18.4	-29.9	-32.8	-21.4	-19.8	-36.0	-29.4	-20.0	-29.2	-30.8	-43.2	-41.7	-37.8	-9.4	-36.1
		Q	-20.3	2.3	-1.5	0.0	-25.6	16.7	-30.9	-33.7	-22.5	-20.9	-37.0	-30.4	-21.2	-30.2	-31.8	-44.0	-42.5	-38.7	-10.7	-37.1
		R	7.1	37.5	32.5	34.4	0.0	56.9	-7.1	-10.9	4.1	6.3	-15.3	-6.5	6.0	-6.2	-8.3	-24.7	-22.7	-17.6	20.0	-15.4
		G	-31.7	-12.3	-15.5	-14.3	-36.2	0.0	-40.8	-43.2	-33.6	-32.2	-46.0	-40.4	-32.4	-40.2	-41.5	-52.0	-50.7	-47.5	-23.5	-46.0
		D	15.3	48.0	42.6	44.7	7.6	68.8	0.0	-4.1	12.1	14.4	-8.8	0.7	14.1	1.0	-1.3	-19.0	-16.8	-11.3	29.2	-8.9
		E	20.2	54.3	48.7	50.9	12.2	76.1	4.3	0.0	16.9	19.3	-4.9	5.0	19.0	5.3	2.9	-15.5	-13.2	-7.5	34.7	-5.0
		T	2.9	32.0	27.2	29.1	-4.0	50.6	-10.8	-14.4	0.0	2.1	-18.6	-10.2	1.8	-9.9	-11.9	-27.7	-25.8	-20.9	15.2	-18.7
		A	0.8	29.4	24.6	26.5	-5.9	47.6	-12.6	-16.2	-2.0	0.0	-20.3	-12.0	-0.3	-11.7	-13.7	-29.2	-27.3	-22.5	12.9	-20.4
		P	26.4	62.3	56.3	58.6	18.0	85.1	9.6	5.1	22.9	25.4	0.0	10.4	25.1	10.7	8.2	-11.2	-8.8	-2.7	41.6	-0.1
		C	14.5	47.0	41.6	43.7	6.9	67.7	-0.7	-4.8	11.3	13.6	-9.4	0.0	13.3	0.3	-2.0	-19.5	-17.4	-11.9	28.3	-9.5
		K	1.1	29.7	25.0	26.8	-5.7	48.0	-12.3	-16.0	-1.8	0.3	-20.1	-11.7	0.0	-11.5	-13.5	-29.0	-27.1	-22.2	13.2	-20.2
		M	14.2	46.5	41.2	43.3	6.6	67.2	-1.0	-5.0	11.0	13.3	-9.7	-0.3	13.0	0.0	-2.3	-19.8	-17.6	-12.2	27.9	-9.8
		V	16.8	49.9	44.5	46.6	9.0	71.0	1.3	-2.8	13.5	15.9	-7.6	2.0	15.6	2.3	0.0	-17.9	-15.7	-10.1	30.9	-7.7
		I	42.3	82.6	76.0	78.6	32.8	108.3	23.4	18.3	38.3	41.2	12.6	24.3	40.8	24.6	21.8	0.0	2.7	9.5	59.4	12.4
		L	38.6	77.9	71.4	73.9	29.4	102.9	20.2	15.3	34.7	37.5	9.6	21.0	37.1	21.4	18.6	-2.6	0.0	6.6	55.2	9.5
		F	30.0	66.8	60.7	63.1	21.3	90.3	12.7	8.1	26.3	29.0	2.8	13.5	28.6	13.8	11.3	-8.7	-6.2	0.0	45.6	2.7
		Y	-10.7	14.6	10.4	12.0	-16.7	30.7	-22.6	-25.8	-13.2	-11.4	-29.4	-22.0	-11.7	-21.8	-23.6	-37.3	-35.6	-31.3	0.0	-29.5
	W	26.6	62.5	56.5	58.9	18.2	85.4	9.8	5.3	23.0	25.6	0.1	10.5	25.3	10.9	8.4	-11.0	-8.7	-2.6	41.8	0.0	
			H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
		B																				
2	A	H	0.0	29.1	23.2	24.3	-7.7	47.3	-14.4	-16.9	-2.8	1.8	-19.8	-14.5	1.0	-10.7	-17.3	-31.3	-29.2	-24.9	7.8	-22.4
		N	-22.5	0.0	-4.6	-3.7	-28.5	14.1	-33.7	-35.7	-24.7	-21.1	-37.9	-33.8	-21.8	-30.8	-36.0	-46.8	-45.1	-41.9	-16.5	-39.9
		S	-18.9	4.8	0.0	0.9	-25.1	19.5	-30.5	-32.6	-21.1	-17.4	-34.9	-30.6	-18.1	-27.5	-32.9	-44.3	-42.5	-39.1	-12.5	-37.1
		Q	-19.6	3.9	-0.9	0.0	-25.8	18.5	-31.1	-33.2	-21.8	-18.1	-35.5	-31.2	-18.8	-28.2	-33.5	-44.8	-43.0	-39.6	-13.3	-37.6
		R	8.4	40.0	33.6	34.8	0.0	59.7	-7.2	-10.0	5.4	10.4	-13.1	-7.3	9.5	-3.2	-10.4	-25.6	-23.2	-18.6	16.8	-15.9
		G	-32.1	-12.4	-16.3	-15.6	-37.4	0.0	-41.9	-43.6	-34.0	-30.9	-45.6	-42.0	-31.5	-39.4	-43.9	-53.4	-51.9	-49.0	-26.8	-47.3
		D	16.8	50.8	43.9	45.2	7.7	72.0	0.0	-3.0	13.5	18.9	-6.3	-0.1	17.9	4.3	-3.4	-19.8	-17.3	-12.3	25.9	-9.4
		E	20.4	55.4	48.4	49.7	11.1	77.4	3.1	0.0	17.0	22.6	-3.4	3.0	21.6	7.5	-0.4	-17.3	-14.7	-9.6	29.8	-6.6
		T	2.9	32.8	26.8	27.9	-5.1	51.6	-11.9	-14.5	0.0	4.8	-17.5	-12.0	3.9	-8.1	-14.9	-29.4	-27.1	-22.8	10.9	-20.2
		A	-1.8	26.8	21.0	22.1	-9.4	44.7	-15.9	-18.4	-4.5	0.0	-21.2	-16.0	-0.8	-12.3	-18.8	-32.6	-30.4	-26.3	5.9	-23.8
		P	24.7	61.0	53.7	55.0	15.0	83.7	6.8	3.6	21.2	26.9	0.0	6.6	25.9	11.4	3.1	-14.4	-11.7	-6.4	34.4	-3.3
		C	16.9	51.0	44.1	45.4	7.9	72.3	0.1	-2.9	13.7	19.1	-6.2	0.0	18.1	4.4	-3.3	-19.7	-17.2	-12.2	26.0	-9.3
		K	-1.0	27.9	22.0	23.1	-8.6	45.9	-15.2	-17.7	-3.8	0.8	-20.6	-15.3	0.0	-11.6	-18.1	-32.0	-29.9	-25.7	6.7	-23.2
		M	12.0	44.6	38.0	39.2	3.3	65.0	-4.1	-7.0	8.8	14.0	-10.2	-4.2	13.1	0.0	-7.4	-23.1	-20.7	-15.9	20.7	-13.1
		V	20.9	56.1	49.0	50.3	11.6	78.1	3.6	0.4	17.5	23.1	-3.0	3.4	22.1	8.0	0.0	-17.0	-14.3	-9.2	30.4	-6.2
I	45.6	88.0	79.5	81.1	34.4	114.5	24.7	21.0	41.5	48.3	16.8	24.5	47.1	30.1	20.4	0.0	3.2	9.3	57.0	13.0		

		L	41.2	82.3	74.0	75.5	30.2	108.0	20.9	17.3	37.2	43.7	13.2	20.7	42.6	26.1	16.7	-3.1	0.0	6.0	52.2	9.5
		F	33.2	72.0	64.2	65.6	22.9	96.2	14.1	10.7	29.5	35.6	6.8	13.9	34.5	19.0	10.2	-8.5	-5.6	0.0	43.6	3.3
		Y	-7.2	19.8	14.3	15.3	-14.4	36.7	-20.6	-22.9	-9.8	-5.5	-25.6	-20.7	-6.3	-17.1	-23.3	-36.3	-34.3	-30.4	0.0	-28.0
		W	28.9	66.4	58.9	60.3	18.9	89.9	10.4	7.1	25.3	31.2	3.4	10.2	30.2	15.1	6.6	-11.5	-8.7	-3.2	39.0	0.0
			H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
3	A	B																				
		H	0.0	22.5	21.6	21.3	-3.2	43.6	-8.8	-11.5	-6.0	-1.7	-23.5	-14.2	-2.2	-13.2	-24.8	-33.1	-30.8	-23.1	13.4	-18.2
		N	-18.4	0.0	-0.7	-1.0	-21.0	17.2	-25.5	-27.8	-23.3	-19.8	-37.5	-30.0	-20.2	-29.1	-38.6	-45.4	-43.5	-37.2	-7.5	-33.2
		S	-17.8	0.7	0.0	-0.3	-20.4	18.1	-25.0	-27.2	-22.7	-19.2	-37.1	-29.5	-19.6	-28.6	-38.1	-45.0	-43.1	-36.8	-6.8	-32.7
		Q	-17.6	1.0	0.3	0.0	-20.2	18.4	-24.8	-27.0	-22.5	-19.0	-36.9	-29.3	-19.4	-28.4	-38.0	-44.9	-42.9	-36.6	-6.5	-32.5
		R	3.3	26.6	25.7	25.3	0.0	48.4	-5.7	-8.5	-2.9	1.5	-20.9	-11.4	1.0	-10.3	-22.3	-30.9	-28.5	-20.5	17.1	-15.4
		G	-30.4	-14.7	-15.3	-15.5	-32.6	0.0	-36.5	-38.4	-34.6	-31.6	-46.7	-40.3	-31.9	-39.5	-47.6	-53.4	-51.8	-46.4	-21.0	-43.0
		D	9.6	34.3	33.3	33.0	6.1	57.4	0.0	-3.0	3.0	7.7	-16.1	-6.0	7.2	-4.8	-17.5	-26.7	-24.1	-15.7	24.3	-10.3
		E	13.0	38.4	37.4	37.0	9.3	62.2	3.1	0.0	6.2	11.0	-13.5	-3.1	10.5	-1.9	-15.0	-24.4	-21.8	-13.1	28.1	-7.5
		T	6.4	30.4	29.4	29.1	3.0	52.8	-2.9	-5.8	0.0	4.6	-18.6	-8.7	4.1	-7.6	-19.9	-28.8	-26.3	-18.1	20.7	-12.9
		A	1.8	24.7	23.8	23.4	-1.5	46.1	-7.2	-9.9	-4.4	0.0	-22.1	-12.7	-0.5	-11.7	-23.4	-31.9	-29.5	-21.7	15.4	-16.7
		P	30.7	60.1	58.9	58.5	26.5	87.6	19.2	15.7	22.8	28.4	0.0	12.1	27.8	13.4	-1.7	-12.6	-9.5	0.5	48.1	7.0
		C	16.6	42.8	41.8	41.4	12.8	67.4	6.3	3.2	9.5	14.6	-10.8	0.0	14.0	1.2	-12.3	-22.0	-19.3	-10.3	32.2	-4.6
		K	2.3	25.3	24.4	24.0	-1.0	46.8	-6.7	-9.5	-3.9	0.5	-21.7	-12.3	0.0	-11.2	-23.1	-31.6	-29.2	-21.3	15.9	-16.3
		M	15.2	41.1	40.1	39.7	11.5	65.4	5.1	2.0	8.2	13.2	-11.8	-1.2	12.6	0.0	-13.3	-23.0	-20.2	-11.4	30.6	-5.7
		V	32.9	62.8	61.6	61.2	28.6	90.8	21.2	17.6	24.9	30.6	1.7	14.0	30.0	15.4	0.0	-11.1	-8.0	2.2	50.7	8.8
		I	49.5	83.2	81.9	81.4	44.7	114.7	36.4	32.3	40.5	46.9	14.4	28.3	46.2	29.8	12.5	0.0	3.5	15.0	69.5	22.4
		L	44.4	76.9	75.7	75.2	39.8	107.4	31.8	27.8	35.7	41.9	10.5	23.9	41.2	25.4	8.7	-3.4	0.0	11.1	63.8	18.2
		F	30.0	59.3	58.1	57.7	25.8	86.7	18.6	15.1	22.2	27.8	-0.5	11.5	27.1	12.9	-2.2	-13.1	-10.0	0.0	47.4	6.4
		Y	-11.8	8.1	7.3	7.0	-14.6	26.6	-19.5	-21.9	-17.1	-13.3	-32.5	-24.3	-13.7	-23.4	-33.6	-41.0	-38.9	-32.2	0.0	-27.8
		W	22.2	49.7	48.6	48.2	18.2	75.4	11.5	8.1	14.8	20.1	-6.5	4.8	19.5	6.1	-8.1	-18.3	-15.4	-6.0	38.5	0.0
			H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
		B																				

Supplementary Table 32: Raw data Extended Data Fig. 3 – AA in water, 170 μ m, 18 h, pH 9.9

repeat k	species	measured values (counts*min) for W and Y: mAU*min				measured values (counts*min) for W and Y: mAU*min								concentration (μ M) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 4				c_0 (μ M)	Normalization (Eq. 1) concentration (x c_0)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)	
		top	II	III	bot	top	II	III	bot					top	II	III	bot		top	II	III	bot	top	bot
1	H	37492	59852	73093	142311	38272	63576	76448	145926					11.48	18.70	22.66	43.68	24.13	0.48	0.78	0.94	1.81	12.3	-8.2
	N	65623	95851	118575	211834	67480	100571	124997	217910					13.11	19.35	23.99	42.33	24.70	0.53	0.78	0.97	1.71	25.3	-13.0
	S	69445	97850	126756	209982	72308	102887	133228	216011					14.39	20.37	26.39	43.24	26.10	0.55	0.78	1.01	1.66	30.1	-16.0
	Q	61819	89919	111376	179279	64020	94601	115498	185135					13.31	19.52	24.00	38.55	23.84	0.56	0.82	1.01	1.62	31.8	-18.0
	R	33445	59857	70928	130058	34692	62995	73413	135572					10.87	19.60	23.03	42.37	23.97	0.45	0.82	0.96	1.77	7.0	-10.3
	G	90651	116019	148208	202637	93530	122986	154348	208261					16.58	21.51	27.23	36.98	25.58	0.65	0.84	1.06	1.45	53.0	-26.6
	D	41931	63302	87320	191248	43126	67317	91591	197930					9.19	14.12	19.34	42.07	21.18	0.43	0.67	0.91	1.99	2.5	0.8
	E	37112	60696	82022	197224	37232	63745	84386	203918					8.58	14.35	19.19	46.27	22.10	0.39	0.65	0.87	2.09	-8.4	6.2
	T	51817	88437	113656	254438	53627	94363	117726	261581					9.63	16.69	21.13	47.12	23.64	0.41	0.71	0.89	1.99	-3.9	1.1
	A	54282	82287	112880	211861	56579	87290	117820	220064					11.66	17.84	24.27	45.44	24.80	0.47	0.72	0.98	1.83	11.0	-7.1
	P	10506	20339	27124	67706	10575	21267	28185	70090					7.26	14.32	19.04	47.44	22.01	0.33	0.65	0.86	2.15	-22.2	9.3
	C	2805	4977	6206	17912	2695	5314	6297	18626					6.63	12.41	15.07	44.05	19.54	0.34	0.63	0.77	2.25	-19.9	14.4
	K	43835	69207	90837	157984	45085	72373	93525	162801					12.24	19.49	25.38	44.16	25.32	0.48	0.77	1.00	1.74	14.1	-11.5
	M	10219	17925	22336	56654	9793	19354	24198	58256					9.05	16.86	21.05	51.97	24.73	0.37	0.68	0.85	2.10	-13.6	6.6
	V	47338	140994	119511	314073	42699	83666	104218	312413					6.90	17.21	17.13	47.98	22.30	0.31	0.77	0.77	2.15	-27.0	9.1
	I	36633	73754	96338	330909	37519	78440	101229	344907					5.36	11.01	14.29	48.89	19.89	0.27	0.55	0.72	2.46	-36.3	24.7
	L	34019	67312	88431	284531	35763	71992	92438	296696					5.89	11.75	15.26	49.02	20.48	0.29	0.57	0.74	2.39	-32.2	21.4
	F	36224	70964	87733	256828	38412	75078	91724	266717					6.87	13.44	16.52	48.19	21.26	0.32	0.63	0.78	2.27	-23.7	15.0
	Y	0.0906	0.1394	0.1702	0.3201	0.1006	0.1477	0.1739	0.3347					11.90	17.88	21.43	40.78	23.00	0.52	0.78	0.93	1.77	22.2	-10.0
	W	0.0536	0.105	0.1167	0.3352	0.0476	0.1088	0.1162	0.3419					6.69	14.12	15.38	44.74	20.23	0.33	0.70	0.76	2.21	-22.0	12.2
	mean concentration per fraction $\bar{c}_{j,k}$																		0.42	0.72	0.89	1.97		
2	H	26452	43548	79378	219504	27531	46968	83139	232566					8.18	13.72	24.63	68.51	28.76	0.28	0.48	0.86	2.38	23.6	-8.5

	N	53751	76085	123718	307981	56404	82111	128917	328618					10.85	15.58	24.89	62.71	28.51	0.38	0.55	0.87	2.20	65.3	-15.5
	S	55133	77863	130425	302309	57773	83916	135485	320108					11.46	16.42	26.99	63.17	29.51	0.39	0.56	0.91	2.14	68.7	-17.8
	Q	51652	73095	117895	258981	53856	78751	122066	275034					11.16	16.06	25.38	56.49	27.27	0.41	0.59	0.93	2.07	77.8	-20.5
	R	22800	40731	78742	201740	23499	43574	79512	213402					7.39	13.45	25.24	66.22	28.08	0.26	0.48	0.90	2.36	14.3	-9.4
	G	88125	102971	144431	268347	91959	111298	153272	283416					16.21	19.29	26.80	49.66	27.99	0.58	0.69	0.96	1.77	151.6	-31.9
	D	22103	50792	99965	353997	23249	54359	103389	376757					4.90	11.37	21.98	78.99	29.31	0.17	0.39	0.75	2.69	-27.3	3.5
	E	18390	42852	92600	363456	18214	45735	95980	385401					4.22	10.22	21.75	86.38	30.64	0.14	0.33	0.71	2.82	-40.1	8.3
	T	32632	60019	120071	409298	34964	64875	124680	433185					6.17	11.40	22.35	76.92	29.21	0.21	0.39	0.77	2.63	-8.2	1.1
	A	36870	64968	120582	342103	37359	68687	125358	362035					7.81	14.06	25.87	74.08	30.45	0.26	0.46	0.85	2.43	11.4	-6.6
	P	5412	12433	28539	118634	5650	13772	30113	125372					3.81	9.02	20.19	84.00	29.25	0.13	0.31	0.69	2.87	-43.5	10.3
	C	2026	4012	7053	33856	2166	3791	8153	35521					5.05	9.41	18.33	83.63	29.11	0.17	0.32	0.63	2.87	-24.6	10.3
	K	26956	53268	97890	255332	28783	57550	102048	268253					7.67	15.25	27.52	72.07	30.63	0.25	0.50	0.90	2.35	8.8	-9.6
	M	5512	10736	25209	93352	5393	11911	26216	98650					4.93	10.24	23.26	86.84	31.32	0.16	0.33	0.74	2.77	-31.6	6.5
	V	24662	55808	114162	567852	18642	45926	112362	580462					3.32	7.79	17.35	87.94	29.10	0.11	0.27	0.60	3.02	-50.5	16.1
	I	14337	37217	99120	632625	14849	40128	103934	669141					2.11	5.60	14.69	94.18	29.14	0.07	0.19	0.50	3.23	-68.5	24.1
	L	13842	35942	92308	531197	14941	38626	96472	561922					2.43	6.29	15.92	92.20	29.21	0.08	0.22	0.55	3.16	-63.9	21.2
	F	16961	39889	93293	449330	17328	41961	97220	476673					3.16	7.53	17.54	85.24	28.37	0.11	0.27	0.62	3.00	-51.7	15.4
	Y	0.0742	0.1091	0.1758	0.5142	0.0763	0.1241	0.1861	0.554					9.37	14.52	22.54	66.52	28.24	0.33	0.51	0.80	2.36	44.2	-9.5
	W	0.0224	0.0554	0.135	0.5669	0.0182	0.0548	0.1387	0.5966					2.68	7.28	18.09	76.87	26.23	0.10	0.28	0.69	2.93	-55.6	12.5
	mean concentration per fraction $\bar{c}_{j,k}$																			0.23	0.40	0.76	2.60	
3	H	34494	39844	68474	235800	36210	45041	71682	246713					10.71	12.86	21.24	73.12	29.48	0.36	0.44	0.72	2.48	13.2	-7.6
	N	64529	72855	114305	333672	67456	81087	118500	349564					13.00	15.16	22.93	67.30	29.60	0.44	0.51	0.77	2.27	36.8	-15.3
	S	71312	90294	125700	329255	74530	100022	130708	345425					14.80	19.32	26.02	68.48	32.15	0.46	0.60	0.81	2.13	43.4	-20.7
	Q	62672	70492	108322	279301	65049	78851	112546	291611					13.51	15.80	23.36	60.39	28.26	0.48	0.56	0.83	2.14	48.9	-20.4
	R	31520	37752	64539	216413	31884	41306	68307	226565					10.11	12.61	21.19	70.66	28.64	0.35	0.44	0.74	2.47	10.0	-8.1
	G	102346	111488	151898	281807	108957	125469	158624	295190					19.02	21.33	27.95	51.93	30.06	0.63	0.71	0.93	1.73	97.1	-35.6
	D	39932	46118	86351	399920	42548	51152	91199	418894					8.92	10.51	19.19	88.51	31.78	0.28	0.33	0.60	2.78	-12.6	3.7

	E	32791	38280	71754	401268	33849	43525	75497	415750					7.69	9.44	16.98	94.24	32.09	0.24	0.29	0.53	2.94	-25.4	9.4
	T	46965	56675	98646	430927	49671	63279	104178	453135					8.82	10.95	18.52	80.72	29.75	0.30	0.37	0.62	2.71	-7.6	1.1
	A	55221	63125	108144	357795	57523	70760	112719	376558					11.86	14.08	23.24	77.25	31.61	0.38	0.45	0.74	2.44	16.9	-8.9
	P	10365	11916	23236	120460	10852	14185	24571	125683					7.30	8.99	16.46	84.73	29.37	0.25	0.31	0.56	2.89	-22.5	7.5
	C	2705	3393	5601	37352	2764	3780	6001	38803					6.59	8.65	13.99	91.81	30.26	0.22	0.29	0.46	3.03	-32.1	13.0
	K	41737	48859	86531	282540	43613	53864	89270	296740					11.75	14.14	24.20	79.74	32.46	0.36	0.44	0.75	2.46	12.8	-8.5
	M	7918	10078	18067	98478	8681	11643	20401	102919					7.51	9.82	17.40	91.09	31.45	0.24	0.31	0.55	2.90	-25.6	7.9
	V	75755	46090	83329	556949	69501	49716	83031	582547					11.12	7.34	12.74	87.27	29.62	0.38	0.25	0.43	2.95	17.0	9.8
	I	30683	37717	69291	640996	31639	41747	72328	667345					4.51	5.75	10.25	94.66	28.79	0.16	0.20	0.36	3.29	-51.2	22.5
	L	28782	35701	64836	543813	30501	39286	67828	565376					5.00	6.32	11.19	93.56	29.02	0.17	0.22	0.39	3.22	-46.3	20.1
	F	30483	36310	65805	469934	32236	40969	68734	489885					5.77	7.11	12.38	88.35	28.41	0.20	0.25	0.44	3.11	-36.7	15.9
	Y	0.0962	0.1155	0.1653	0.6948	0.1017	0.1234	0.1787	0.7349					12.33	14.88	21.42	89.03	34.41	0.36	0.43	0.62	2.59	11.6	-3.6
	W	0.0331	0.0378	0.0898	0.605	0.033	0.044	0.0903	0.6387					4.37	5.40	11.90	82.18	25.96	0.17	0.21	0.46	3.17	-47.6	17.9
	mean concentration per fraction $\bar{c}_{j,k}$																		0.32	0.38	0.62	2.68		

Supplementary Table 33: Raw data Extended Data Fig. 3 – AA in water, 170 μ m, 18 h, pH 9.9 – enrichments in top fraction

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)																				
1	A	H	0.0	-10.4	-13.7	-14.8	4.9	-26.6	9.6	22.6	16.8	1.2	44.3	40.2	-1.6	30.0	53.9	76.4	65.5	47.2	-8.1	43.9
		N	11.6	0.0	-3.7	-4.9	17.1	-18.1	22.3	36.8	30.4	12.9	61.0	56.5	9.8	45.1	71.7	96.8	84.7	64.3	2.6	60.6
		S	15.9	3.8	0.0	-1.2	21.6	-14.9	27.0	42.1	35.4	17.2	67.2	62.5	14.0	50.6	78.3	104.4	91.8	70.6	6.5	66.8
		Q	17.3	5.2	1.3	0.0	23.1	-13.9	28.6	43.9	37.1	18.7	69.3	64.5	15.5	52.5	80.6	107.0	94.2	72.7	7.9	68.9
		R	-4.7	-14.6	-17.7	-18.8	0.0	-30.0	4.5	16.9	11.4	-3.6	37.6	33.7	-6.2	23.9	46.7	68.2	57.8	40.3	-12.4	37.2
		G	36.2	22.1	17.6	16.1	42.9	0.0	49.3	67.0	59.2	37.8	96.6	91.0	34.1	77.1	109.6	140.3	125.5	100.5	25.2	96.1
		D	-8.8	-18.2	-21.3	-22.2	-4.3	-33.0	0.0	11.9	6.6	-7.7	31.7	27.9	-10.2	18.6	40.4	60.9	51.0	34.3	-16.1	31.3
		E	-18.4	-26.9	-29.6	-30.5	-14.4	-40.1	-10.6	0.0	-4.7	-17.5	17.7	14.4	-19.7	6.0	25.5	43.9	35.0	20.1	-25.0	17.4
		T	-14.4	-23.3	-26.1	-27.0	-10.2	-37.2	-6.2	4.9	0.0	-13.4	23.5	20.0	-15.8	11.3	31.7	51.0	41.7	26.0	-21.3	23.2
		A	-1.2	-11.4	-14.7	-15.8	3.7	-27.5	8.3	21.2	15.5	0.0	42.6	38.6	-2.7	28.5	52.1	74.3	63.6	45.5	-9.2	42.2
		P	-30.7	-37.9	-40.2	-40.9	-27.3	-49.1	-24.1	-15.0	-19.1	-29.9	0.0	-2.9	-31.8	-9.9	6.6	22.2	14.7	2.0	-36.3	-0.3
		C	-28.7	-36.1	-38.5	-39.2	-25.2	-47.6	-21.8	-12.6	-16.7	-27.8	2.9	0.0	-29.8	-7.3	9.8	25.8	18.1	5.0	-34.4	2.6
		K	1.6	-8.9	-12.3	-13.4	6.6	-25.4	11.4	24.6	18.7	2.8	46.7	42.5	0.0	32.1	56.4	79.3	68.2	49.6	-6.6	46.3
		M	-23.1	-31.1	-33.6	-34.4	-19.3	-43.5	-15.7	-5.7	-10.1	-22.2	11.0	7.8	-24.3	0.0	18.4	35.7	27.3	13.2	-29.3	10.7
		V	-35.0	-41.8	-43.9	-44.6	-31.8	-52.3	-28.8	-20.3	-24.1	-34.2	-6.2	-8.9	-36.1	-15.5	0.0	14.6	7.6	-4.3	-40.3	-6.5
		I	-43.3	-49.2	-51.1	-51.7	-40.5	-58.4	-37.9	-30.5	-33.8	-42.6	-18.2	-20.5	-44.2	-26.3	-12.8	0.0	-6.2	-16.6	-47.9	-18.4
		L	-39.6	-45.9	-47.9	-48.5	-36.6	-55.7	-33.8	-25.9	-29.4	-38.9	-12.8	-15.3	-40.6	-21.5	-7.0	6.6	0.0	-11.1	-44.5	-13.1
		F	-32.1	-39.1	-41.4	-42.1	-28.7	-50.1	-25.5	-16.7	-20.6	-31.3	-2.0	-4.8	-33.2	-11.7	4.5	19.8	12.5	0.0	-37.6	-2.2
		Y	8.8	-2.5	-6.1	-7.3	14.1	-20.1	19.2	33.4	27.1	10.1	57.0	52.5	7.1	41.4	67.4	91.9	80.1	60.1	0.0	56.6
		W	-30.5	-37.7	-40.0	-40.8	-27.1	-49.0	-23.8	-14.8	-18.8	-29.7	0.3	-2.6	-31.6	-9.7	6.9	22.6	15.0	2.3	-36.1	0.0
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
		B																				
2	A	H	0.0	-25.3	-26.7	-30.5	8.1	-50.9	70.1	106.5	34.6	10.9	118.5	63.9	13.6	80.6	149.6	292.6	242.3	155.6	-14.3	178.2
		N	33.8	0.0	-2.0	-7.0	44.7	-34.3	127.6	176.3	80.2	48.4	192.4	119.2	52.0	141.7	234.0	425.4	358.0	242.1	14.7	272.2
		S	36.5	2.0	0.0	-5.1	47.6	-32.9	132.2	181.8	83.8	51.4	198.3	123.7	55.0	146.6	240.7	436.0	367.2	249.0	17.0	279.8
		Q	43.9	7.5	5.4	0.0	55.6	-29.3	144.7	197.0	93.7	59.6	214.4	135.7	63.4	159.8	259.1	464.8	392.4	267.8	23.3	300.2
		R	-7.5	-30.9	-32.3	-35.7	0.0	-54.6	57.3	90.9	24.5	2.6	102.1	51.5	5.0	67.0	130.8	263.1	216.5	136.4	-20.7	157.3
		G	103.6	52.1	49.1	41.5	120.2	0.0	246.3	320.3	174.1	125.9	344.9	233.6	131.2	267.7	408.2	699.3	596.8	420.5	74.5	466.4
		D	-41.2	-56.1	-56.9	-59.1	-36.4	-71.1	0.0	21.4	-20.8	-34.8	28.5	-3.7	-33.2	6.2	46.8	130.8	101.2	50.3	-49.6	63.6
		E	-51.6	-63.8	-64.5	-66.3	-47.6	-76.2	-17.6	0.0	-34.8	-46.3	5.8	-20.6	-45.0	-12.5	20.9	90.2	65.8	23.8	-58.5	34.7
		T	-25.7	-44.5	-45.6	-48.4	-19.7	-63.5	26.3	53.3	0.0	-17.6	62.3	21.7	-15.7	34.2	85.4	191.6	154.2	89.9	-36.3	106.6
		A	-9.9	-32.6	-34.0	-37.3	-2.5	-55.7	53.3	86.1	21.4	0.0	97.0	47.7	2.4	62.8	125.0	253.9	208.5	130.4	-22.7	150.8
		P	-54.2	-65.8	-66.5	-68.2	-50.5	-77.5	-22.2	-5.5	-38.4	-49.2	0.0	-25.0	-48.0	-17.3	14.2	79.7	56.6	17.0	-60.8	27.3
		C	-39.0	-54.4	-55.3	-57.6	-34.0	-70.0	3.8	26.0	-17.8	-32.3	33.4	0.0	-30.7	10.2	52.3	139.6	108.9	56.0	-47.7	69.8
		K	-11.9	-34.2	-35.5	-38.8	-4.8	-56.7	49.8	81.8	18.6	-2.3	92.4	44.3	0.0	59.1	119.8	245.7	201.4	125.1	-24.5	145.0
		M	-44.6	-58.6	-59.4	-61.5	-40.1	-72.8	-5.8	14.3	-25.5	-38.6	21.0	-9.3	-37.1	0.0	38.2	117.4	89.5	41.5	-52.5	54.0
		V	-59.9	-70.1	-70.7	-72.1	-56.7	-80.3	-31.9	-17.3	-46.1	-55.6	-12.4	-34.4	-54.5	-27.6	0.0	57.3	37.1	2.4	-65.7	11.5
		I	-74.5	-81.0	-81.3	-82.3	-72.5	-87.5	-56.7	-47.4	-65.7	-71.7	-44.3	-58.3	-71.1	-54.0	-36.4	0.0	-12.8	-34.9	-78.2	-29.1

		L	-70.8	-78.2	-78.6	-79.7	-68.4	-85.6	-50.3	-39.7	-60.7	-67.6	-36.1	-52.1	-66.8	-47.2	-27.1	14.7	0.0	-25.3	-75.0	-18.7
		F	-60.9	-70.8	-71.3	-72.8	-57.7	-80.8	-33.5	-19.2	-47.3	-56.6	-14.5	-35.9	-55.6	-29.3	-2.4	53.6	33.9	0.0	-66.5	8.8
		Y	16.7	-12.8	-14.5	-18.9	26.2	-42.7	98.4	140.9	57.1	29.4	155.0	91.2	32.5	110.7	191.2	358.0	299.3	198.3	0.0	224.6
		W	-64.1	-73.1	-73.7	-75.0	-61.1	-82.3	-38.9	-25.8	-51.6	-60.1	-21.4	-41.1	-59.2	-35.1	-10.3	41.1	23.0	-8.1	-69.2	0.0
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
		B																				
3	A	H	0.0	-17.3	-21.1	-24.0	2.9	-42.6	29.5	51.7	22.5	-3.2	46.1	66.8	0.4	52.3	-3.2	132.0	110.9	78.8	1.4	116.1
		N	20.9	0.0	-4.6	-8.1	24.4	-30.6	56.6	83.4	48.1	17.1	76.6	101.6	21.3	84.0	16.9	180.5	154.9	116.1	22.6	161.2
		S	26.7	4.8	0.0	-3.7	30.4	-27.2	64.1	92.2	55.2	22.7	85.1	111.3	27.2	92.9	22.6	193.9	167.1	126.5	28.5	173.7
		Q	31.5	8.8	3.8	0.0	35.4	-24.5	70.4	99.5	61.2	27.4	92.2	119.4	32.0	100.3	27.3	205.2	177.4	135.2	33.4	184.2
		R	-2.8	-19.6	-23.3	-26.1	0.0	-44.2	25.9	47.4	19.1	-5.9	42.0	62.0	-2.5	47.9	-6.0	125.4	104.9	73.7	-1.4	109.9
		G	74.1	44.1	37.5	32.4	79.2	0.0	125.6	164.1	113.4	68.6	154.4	190.4	74.8	165.1	68.5	304.0	267.2	211.3	76.6	276.2
		D	-22.8	-36.1	-39.1	-41.3	-20.6	-55.7	0.0	17.1	-5.4	-25.2	12.8	28.7	-22.5	17.5	-25.3	79.1	62.8	38.0	-21.7	66.8
		E	-34.1	-45.5	-48.0	-49.9	-32.2	-62.1	-14.6	0.0	-19.2	-36.2	-3.7	9.9	-33.8	0.4	-36.2	53.0	39.0	17.9	-33.1	42.4
		T	-18.4	-32.5	-35.6	-38.0	-16.0	-53.1	5.7	23.8	0.0	-21.0	19.2	36.1	-18.1	24.3	-21.0	89.3	72.1	45.9	-17.2	76.3
		A	3.3	-14.6	-18.5	-21.5	6.3	-40.7	33.8	56.6	26.5	0.0	50.9	72.2	3.7	57.2	-0.1	139.6	117.8	84.6	4.8	123.1
		P	-31.6	-43.4	-46.0	-48.0	-29.6	-60.7	-11.3	3.8	-16.1	-33.7	0.0	14.1	-31.3	4.2	-33.8	58.8	44.3	22.4	-30.6	47.9
		C	-40.0	-50.4	-52.7	-54.4	-38.3	-65.6	-22.3	-9.0	-26.5	-41.9	-12.4	0.0	-39.8	-8.7	-42.0	39.1	26.5	7.2	-39.2	29.6
		K	-0.4	-17.6	-21.4	-24.3	2.5	-42.8	29.0	51.1	22.1	-3.5	45.6	66.1	0.0	51.7	-3.6	131.1	110.1	78.1	1.0	115.2
		M	-34.3	-45.7	-48.2	-50.1	-32.4	-62.3	-14.9	-0.4	-19.5	-36.4	-4.0	9.5	-34.1	0.0	-36.5	52.4	38.5	17.4	-33.4	41.9
		V	3.4	-14.5	-18.4	-21.4	6.4	-40.6	33.9	56.8	26.7	0.1	51.0	72.4	3.8	57.4	0.0	139.8	118.0	84.8	4.9	123.3
		I	-56.9	-64.3	-66.0	-67.2	-55.6	-75.2	-44.2	-34.6	-47.2	-58.3	-37.0	-28.1	-56.7	-34.4	-58.3	0.0	-9.1	-22.9	-56.3	-6.9
		L	-52.6	-60.8	-62.6	-63.9	-51.2	-72.8	-38.6	-28.1	-41.9	-54.1	-30.7	-20.9	-52.4	-27.8	-54.1	10.0	0.0	-15.2	-51.9	2.5
		F	-44.1	-53.7	-55.8	-57.5	-42.4	-67.9	-27.5	-15.2	-31.5	-45.8	-18.3	-6.7	-43.9	-14.8	-45.9	29.8	17.9	0.0	-43.3	20.9
		Y	-1.4	-18.4	-22.2	-25.1	1.5	-43.4	27.7	49.5	20.8	-4.5	44.0	64.4	-1.0	50.1	-4.6	128.7	107.9	76.2	0.0	113.0
		W	-53.7	-61.7	-63.5	-64.8	-52.4	-73.4	-40.0	-29.8	-43.3	-55.2	-32.4	-22.8	-53.5	-29.5	-55.2	7.4	-2.4	-17.3	-53.1	0.0
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
		B																				

Supplementary Table 34: Raw data Extended Data Fig. 3 – AA in water, 170 μ m, 18 h, pH 9.9 – enrichments in bottom fraction

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)																				
1	A	H	0.0	5.6	9.2	12.0	2.4	25.2	-8.9	-13.6	-9.2	-1.2	-16.0	-19.7	3.8	-13.9	-15.9	-26.4	-24.4	-20.2	2.1	-18.1
		N	-5.3	0.0	3.5	6.0	-3.1	18.5	-13.7	-18.1	-14.0	-6.4	-20.5	-24.0	-1.7	-18.4	-20.3	-30.3	-28.4	-24.4	-3.3	-22.5
		S	-8.5	-3.3	0.0	2.5	-6.3	14.6	-16.6	-20.9	-16.9	-9.6	-23.1	-26.5	-5.0	-21.2	-23.0	-32.6	-30.8	-26.9	-6.6	-25.1
		Q	-10.7	-5.7	-2.4	0.0	-8.6	11.8	-18.6	-22.8	-18.9	-11.8	-25.0	-28.3	-7.3	-23.1	-24.8	-34.2	-32.5	-28.7	-8.8	-26.9
		R	-2.3	3.1	6.7	9.4	0.0	22.3	-11.0	-15.6	-11.3	-3.5	-17.9	-21.6	1.4	-15.9	-17.8	-28.1	-26.1	-22.0	-0.3	-20.0
		G	-20.1	-15.6	-12.7	-10.6	-18.2	0.0	-27.2	-30.9	-27.4	-21.1	-32.9	-35.9	-17.1	-31.2	-32.8	-41.2	-39.6	-36.2	-18.5	-34.6
		D	9.7	15.9	19.9	22.9	12.3	37.4	0.0	-5.1	-0.3	8.4	-7.8	-11.9	13.9	-5.5	-7.7	-19.2	-17.0	-12.4	12.0	-10.2
		E	15.7	22.2	26.4	29.5	18.4	44.8	5.4	0.0	5.1	14.3	-2.8	-7.1	20.0	-0.4	-2.7	-14.8	-12.5	-7.6	18.1	-5.3
		T	10.1	16.3	20.3	23.3	12.7	37.8	0.3	-4.8	0.0	8.8	-7.5	-11.6	14.3	-5.2	-7.4	-18.9	-16.7	-12.1	12.4	-9.9
		A	1.2	6.9	10.6	13.3	3.6	26.7	-7.8	-12.5	-8.1	0.0	-15.0	-18.7	5.0	-12.8	-14.8	-25.5	-23.5	-19.2	3.3	-17.1
		P	19.0	25.7	30.1	33.3	21.9	49.0	8.5	2.9	8.1	17.6	0.0	-4.4	23.5	2.5	0.2	-12.3	-10.0	-5.0	21.5	-2.5
		C	24.5	31.5	36.1	39.4	27.5	55.9	13.5	7.7	13.1	23.0	4.6	0.0	29.2	7.3	4.8	-8.3	-5.8	-0.6	27.1	2.0
		K	-3.6	1.8	5.3	7.9	-1.3	20.6	-12.2	-16.7	-12.5	-4.8	-19.1	-22.6	0.0	-17.0	-18.9	-29.0	-27.1	-23.1	-1.6	-21.1
		M	16.1	22.6	26.8	30.0	18.9	45.3	5.8	0.4	5.4	14.7	-2.5	-6.8	20.5	0.0	-2.3	-14.5	-12.2	-7.3	18.5	-5.0
		V	18.8	25.5	29.8	33.1	21.7	48.8	8.3	2.7	7.9	17.4	-0.2	-4.6	23.3	2.4	0.0	-12.5	-10.1	-5.1	21.3	-2.7
		I	35.8	43.4	48.4	52.0	39.0	70.0	23.8	17.4	23.3	34.2	14.1	9.0	40.9	17.0	14.3	0.0	2.7	8.4	38.6	11.2
		L	32.3	39.7	44.5	48.1	35.4	65.6	20.5	14.3	20.1	30.7	11.1	6.2	37.2	13.9	11.3	-2.6	0.0	5.6	35.0	8.3
		F	25.3	32.3	36.8	40.2	28.2	56.8	14.1	8.3	13.8	23.8	5.2	0.6	30.0	7.9	5.4	-7.8	-5.3	0.0	27.9	2.5
		Y	-2.0	3.4	7.0	9.7	0.3	22.6	-10.7	-15.3	-11.0	-3.2	-17.7	-21.3	1.7	-15.6	-17.6	-27.9	-25.9	-21.8	0.0	-19.8
	W	22.2	29.0	33.5	36.8	25.1	52.9	11.3	5.6	10.9	20.7	2.6	-1.9	26.8	5.2	2.8	-10.1	-7.6	-2.5	24.7	0.0	
			H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W
		B																				
2	A	H	0.0	8.3	11.3	15.0	1.0	34.3	-11.6	-15.5	-9.5	-2.1	-17.0	-17.1	1.2	-14.1	-21.2	-26.3	-24.5	-20.7	1.1	-18.7
		N	-7.7	0.0	2.8	6.2	-6.7	24.0	-18.4	-22.0	-16.5	-9.6	-23.4	-23.4	-6.5	-20.7	-27.2	-31.9	-30.3	-26.8	-6.6	-24.9
		S	-10.1	-2.7	0.0	3.4	-9.2	20.6	-20.6	-24.1	-18.7	-12.0	-25.4	-25.5	-9.0	-22.8	-29.2	-33.8	-32.2	-28.8	-9.1	-27.0
		Q	-13.1	-5.8	-3.2	0.0	-12.2	16.7	-23.1	-26.5	-21.3	-14.8	-27.9	-27.9	-12.0	-25.3	-31.5	-35.9	-34.4	-31.1	-12.1	-29.3
		R	-1.0	7.2	10.2	13.9	0.0	32.9	-12.5	-16.3	-10.4	-3.0	-17.9	-17.9	0.2	-14.9	-22.0	-27.0	-25.3	-21.5	0.1	-19.5
		G	-25.5	-19.3	-17.1	-14.3	-24.8	0.0	-34.2	-37.1	-32.6	-27.0	-38.2	-38.2	-24.6	-36.0	-41.3	-45.1	-43.8	-40.9	-24.7	-39.5
		D	13.1	22.5	25.9	30.1	14.3	51.9	0.0	-4.4	2.3	10.8	-6.1	-6.2	14.5	-2.8	-10.8	-16.6	-14.6	-10.3	14.4	-8.0
		E	18.3	28.1	31.7	36.1	19.5	58.9	4.6	0.0	7.0	15.9	-1.8	-1.9	19.8	1.7	-6.7	-12.8	-10.7	-6.2	19.7	-3.8
		T	10.5	19.7	23.0	27.1	11.6	48.4	-2.3	-6.6	0.0	8.3	-8.3	-8.4	11.9	-5.0	-12.9	-18.5	-16.6	-12.4	11.8	-10.1
		A	2.1	10.6	13.6	17.4	3.1	37.1	-9.7	-13.7	-7.6	0.0	-15.3	-15.3	3.4	-12.3	-19.5	-24.7	-22.9	-19.1	3.3	-17.0
		P	20.5	30.5	34.1	38.6	21.7	61.8	6.5	1.9	9.0	18.0	0.0	-0.1	22.0	3.6	-5.0	-11.1	-9.0	-4.4	21.9	-2.0
		C	20.6	30.6	34.2	38.7	21.8	61.9	6.6	1.9	9.1	18.1	0.1	0.0	22.1	3.6	-4.9	-11.1	-9.0	-4.4	22.0	-2.0
		K	-1.2	7.0	9.9	13.6	-0.2	32.6	-12.7	-16.5	-10.6	-3.3	-18.1	-18.1	0.0	-15.1	-22.1	-27.2	-25.5	-21.7	-0.1	-19.7
		M	16.4	26.1	29.5	33.9	17.6	56.3	2.9	-1.6	5.3	14.0	-3.4	-3.5	17.8	0.0	-8.3	-14.2	-12.2	-7.7	17.7	-5.4
		V	26.9	37.4	41.2	45.9	28.1	70.3	12.1	7.2	14.8	24.2	5.3	5.2	28.4	9.0	0.0	-6.5	-4.3	0.6	28.3	3.1
I	35.7	46.9	51.0	56.0	37.0	82.1	19.9	14.6	22.7	32.9	12.5	12.5	37.3	16.5	6.9	0.0	2.4	7.5	37.2	10.3		

		L	32.5	43.5	47.4	52.4	33.8	77.9	17.1	12.0	19.9	29.8	9.9	9.9	34.1	13.8	4.4	-2.3	0.0	5.0	34.0	7.7
		F	26.1	36.6	40.4	45.1	27.4	69.3	11.5	6.6	14.1	23.5	4.7	4.6	27.7	8.4	-0.6	-7.0	-4.8	0.0	27.6	2.5
		Y	-1.1	7.1	10.0	13.7	-0.1	32.8	-12.6	-16.4	-10.5	-3.2	-18.0	-18.0	0.1	-15.0	-22.1	-27.1	-25.4	-21.6	0.0	-19.6
		W	23.0	33.2	36.9	41.5	24.2	65.2	8.7	4.0	11.3	20.5	2.1	2.0	24.5	5.7	-3.0	-9.3	-7.2	-2.5	24.4	0.0
				H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y
		B																				
3	A	H	0.0	9.1	16.5	16.1	0.5	43.5	-10.9	-15.6	-8.6	1.5	-14.0	-18.3	0.9	-14.4	-15.8	-24.6	-23.1	-20.3	-4.1	-21.7
		N	-8.3	0.0	6.8	6.4	-7.8	31.6	-18.4	-22.6	-16.2	-7.0	-21.2	-25.1	-7.5	-21.5	-22.8	-30.8	-29.5	-26.9	-12.1	-28.2
		S	-14.1	-6.3	0.0	-0.3	-13.7	23.3	-23.5	-27.5	-21.5	-12.9	-26.2	-29.8	-13.3	-26.5	-27.7	-35.2	-33.9	-31.5	-17.7	-32.7
		Q	-13.8	-6.0	0.3	0.0	-13.4	23.7	-23.3	-27.3	-21.2	-12.6	-25.9	-29.6	-13.0	-26.2	-27.5	-35.0	-33.7	-31.3	-17.4	-32.5
		R	-0.5	8.5	15.8	15.5	0.0	42.8	-11.4	-16.0	-9.1	0.9	-14.5	-18.7	0.4	-14.8	-16.3	-25.0	-23.5	-20.7	-4.6	-22.1
		G	-30.3	-24.0	-18.9	-19.1	-30.0	0.0	-38.0	-41.2	-36.3	-29.3	-40.1	-43.1	-29.7	-40.3	-41.4	-47.4	-46.4	-44.4	-33.2	-45.4
		D	12.3	22.5	30.8	30.3	12.9	61.2	0.0	-5.2	2.6	13.9	-3.5	-8.2	13.4	-3.8	-5.5	-15.3	-13.6	-10.5	7.6	-12.0
		E	18.4	29.2	37.9	37.5	19.1	70.0	5.5	0.0	8.3	20.2	1.8	-3.2	19.5	1.4	-0.3	-10.7	-8.9	-5.6	13.5	-7.2
		T	9.4	19.3	27.4	27.0	10.0	57.0	-2.6	-7.6	0.0	11.0	-6.0	-10.6	10.4	-6.3	-7.9	-17.5	-15.9	-12.8	4.9	-14.3
		A	-1.4	7.5	14.8	14.4	-0.9	41.5	-12.2	-16.8	-9.9	0.0	-15.3	-19.4	-0.5	-15.6	-17.1	-25.7	-24.2	-21.4	-5.5	-22.8
		P	16.3	26.9	35.5	35.0	17.0	67.0	3.6	-1.8	6.3	18.0	0.0	-4.9	17.4	-0.4	-2.1	-12.3	-10.5	-7.2	11.5	-8.9
		C	22.3	33.4	42.5	42.0	23.0	75.6	9.0	3.3	11.8	24.1	5.2	0.0	23.5	4.8	3.0	-7.7	-5.9	-2.5	17.3	-4.1
		K	-0.9	8.1	15.4	15.0	-0.4	42.2	-11.8	-16.4	-9.4	0.5	-14.8	-19.0	0.0	-15.2	-16.6	-25.3	-23.8	-21.0	-5.0	-22.4
		M	16.8	27.4	36.0	35.5	17.4	67.6	4.0	-1.4	6.7	18.5	0.4	-4.6	17.9	0.0	-1.7	-11.9	-10.2	-6.9	11.9	-8.5
		V	18.8	29.6	38.4	37.9	19.4	70.5	5.8	0.3	8.6	20.6	2.1	-2.9	19.9	1.7	0.0	-10.4	-8.6	-5.3	13.9	-6.9
		I	32.6	44.6	54.4	53.9	33.3	90.3	18.1	11.9	21.2	34.5	14.0	8.4	33.8	13.5	11.6	0.0	2.0	5.7	27.1	3.9
		L	30.0	41.8	51.4	50.9	30.7	86.6	15.8	9.8	18.8	31.9	11.8	6.3	31.2	11.3	9.4	-1.9	0.0	3.7	24.6	1.9
		F	25.4	36.8	46.1	45.6	26.1	80.0	11.7	5.9	14.6	27.3	7.8	2.5	26.6	7.4	5.6	-5.4	-3.5	0.0	20.2	-1.7
		Y	4.3	13.8	21.5	21.1	4.9	49.7	-7.1	-11.9	-4.6	5.8	-10.3	-14.7	5.3	-10.7	-12.2	-21.3	-19.8	-16.8	0.0	-18.3
		W	27.6	39.2	48.6	48.2	28.3	83.2	13.7	7.8	16.7	29.5	9.7	4.3	28.8	9.3	7.4	-3.7	-1.8	1.8	22.4	0.0
		H	N	S	Q	R	G	D	E	T	A	P	C	K	M	V	I	L	F	Y	W	
		B																				

Supplementary Table 35: Raw data Extended Data Fig. 4 – AA in water, 170 μm , 18 h, 1 mM NaCl, pH 7.4

repeat k	species	measured values (counts*min)				concentration (μM) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 4				c_0 (μM)	Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)	
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot
1	H	240129	228509	248856	270086	26.75	25.46	27.72	30.09	27.50	0.97	0.93	1.01	1.09	2.8	-2.0
	N	445395	398460	431669	460378	40.30	36.06	39.06	41.66	39.27	1.03	0.92	0.99	1.06	8.5	-5.0
	S	396440	365236	391027	432022	28.25	26.03	27.87	30.79	28.23	1.00	0.92	0.99	1.09	5.8	-2.4
	Q	372695	345029	368662	399270	32.37	29.97	32.02	34.68	32.26	1.00	0.93	0.99	1.08	6.1	-3.7
	D	368979	362075	398502	438519	33.24	32.62	35.90	39.51	35.32	0.94	0.92	1.02	1.12	-0.5	0.2
	E	345228	345953	383664	421874	31.94	32.01	35.50	39.04	34.62	0.92	0.92	1.03	1.13	-2.5	1.0
	T	410640	398772	437069	479041	26.49	25.72	28.19	30.90	27.83	0.95	0.92	1.01	1.11	0.6	-0.6
	A	383676	368233	408779	446861	26.67	25.60	28.41	31.06	27.94	0.95	0.92	1.02	1.11	0.9	-0.4
	P	102069	103787	117429	129617	24.36	24.77	28.03	30.94	27.02	0.90	0.92	1.04	1.14	-4.7	2.5
	C	27079	27023	29840	34156	19.55	19.51	21.54	24.66	21.32	0.92	0.92	1.01	1.16	-3.1	3.6
	K	330308	317788	345357	375746	31.25	30.07	32.68	35.55	32.39	0.96	0.93	1.01	1.10	2.0	-1.7
	V	533798	505323	581994	630861	27.78	26.29	30.28	32.83	29.29	0.95	0.90	1.03	1.12	0.2	0.3
	I	470144	492384	558804	622989	22.51	23.57	26.75	29.83	25.66	0.88	0.92	1.04	1.16	-7.3	4.1
	L	438339	445203	507954	558879	23.99	24.37	27.80	30.59	26.69	0.90	0.91	1.04	1.15	-5.0	2.6
	F	375372	380924	425519	467691	24.67	25.03	27.96	30.73	27.10	0.91	0.92	1.03	1.13	-3.8	1.6
	mean concentration per fraction $\bar{c}_{j,k}$										0.95	0.92	1.02	1.12		
2	H	189131	263141	216165	309541	21.07	29.31	24.08	34.48	27.24	0.77	1.08	0.88	1.27	1.4	-2.4
	N	351665	460045	377286	515134	31.82	41.63	34.14	46.62	38.55	0.83	1.08	0.89	1.21	8.2	-6.8
	S	314792	419321	337242	468966	22.43	29.88	24.03	33.42	27.44	0.82	1.09	0.88	1.22	7.2	-6.1
	Q	291966	392190	317134	435468	25.36	34.07	27.55	37.83	31.20	0.81	1.09	0.88	1.21	6.6	-6.6
	D	297663	410603	346339	501995	26.82	36.99	31.20	45.23	35.06	0.76	1.06	0.89	1.29	0.3	-0.6
	E	279535	393242	332058	492054	25.86	36.39	30.72	45.53	34.63	0.75	1.05	0.89	1.31	-2.1	1.3

	T	328840	456837	378122	545952	21.21	29.47	24.39	35.22	27.57	0.77	1.07	0.88	1.28	0.8	-1.6
	A	311232	426409	349443	505379	21.63	29.64	24.29	35.13	27.67	0.78	1.07	0.88	1.27	2.5	-2.2
	P	83665	121410	100875	155100	19.97	28.98	24.08	37.02	27.51	0.73	1.05	0.88	1.35	-4.9	3.7
	C	22142	31860	25885	39520	15.99	23.00	18.69	28.53	21.55	0.74	1.07	0.87	1.32	-2.8	2.0
	K	262383	360143	300681	428955	24.83	34.08	28.45	40.59	31.98	0.78	1.07	0.89	1.27	1.7	-2.2
	V	428096	567661	517430	773232	22.28	29.54	26.92	40.23	29.74	0.75	0.99	0.91	1.35	-1.8	4.3
	I	383630	563370	486184	767202	18.37	26.97	23.28	36.73	26.34	0.70	1.02	0.88	1.39	-8.6	7.5
	L	363428	493363	446472	677633	19.89	27.00	24.44	37.09	27.10	0.73	1.00	0.90	1.37	-3.8	5.5
	F	303814	434544	369083	564551	19.96	28.55	24.25	37.10	27.47	0.73	1.04	0.88	1.35	-4.7	4.1
	mean concentration per fraction $\bar{c}_{j,k}$										0.76	1.05	0.88	1.30		
3	H	196502	243344	280460	326644	21.89	27.11	31.24	36.39	29.16	0.75	0.93	1.07	1.25	10.8	-5.6
	N	366517	429117	486459	521288	33.17	38.83	44.02	47.17	40.80	0.81	0.95	1.08	1.16	20.0	-12.5
	S	333932	392052	441604	476646	23.80	27.94	31.47	33.97	29.29	0.81	0.95	1.07	1.16	19.9	-12.3
	Q	300096	364856	409761	440921	26.07	31.69	35.59	38.30	32.91	0.79	0.96	1.08	1.16	16.9	-11.9
	D	275173	387515	448942	547803	24.79	34.91	40.45	49.36	37.38	0.66	0.93	1.08	1.32	-2.1	-0.1
	E	254073	371302	428383	541354	23.51	34.36	39.64	50.09	36.90	0.64	0.93	1.07	1.36	-5.9	2.7
	T	317414	427170	493242	586441	20.48	27.56	31.82	37.83	29.42	0.70	0.94	1.08	1.29	2.8	-2.7
	A	303451	399516	458088	539780	21.09	27.77	31.84	37.52	29.56	0.71	0.94	1.08	1.27	5.4	-3.9
	P	74260	108808	133685	174434	17.72	25.97	31.91	41.63	29.31	0.60	0.89	1.09	1.42	-10.7	7.5
	C	20475	28197	33598	43901	14.78	20.36	24.26	31.70	22.77	0.65	0.89	1.07	1.39	-4.2	5.3
	K	256916	344999	391574	453888	24.31	32.64	37.05	42.95	34.24	0.71	0.95	1.08	1.25	4.8	-5.1
	V	370458	577338	648297	857633	19.28	30.04	33.73	44.63	31.92	0.60	0.94	1.06	1.40	-10.8	5.8
	I	316378	524358	625080	898488	15.15	25.10	29.93	43.01	28.30	0.54	0.89	1.06	1.52	-21.0	15.0
	L	307635	480636	564607	779463	16.84	26.31	30.90	42.66	29.18	0.58	0.90	1.06	1.46	-14.8	10.6
	F	268158	407992	475933	630506	17.62	26.81	31.27	41.43	29.28	0.60	0.92	1.07	1.41	-11.2	7.1
	mean concentration per fraction $\bar{c}_{j,k}$										0.68	0.93	1.07	1.32		

Supplementary Table 36: Raw data Extended Data Fig. 4 – AA in water, 170 μm , 18 h, 1 mM NaCl, pH 7.4 – enrichments in top fraction

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)															
1	A	H	0.0	-5.2	-2.8	-3.1	3.3	5.4	2.2	1.9	7.9	6.0	0.8	2.6	10.9	8.2	6.8
		N	5.5	0.0	2.6	2.3	9.0	11.2	7.8	7.5	13.8	11.9	6.4	8.2	17.0	14.2	12.7
		S	2.9	-2.5	0.0	-0.3	6.3	8.5	5.1	4.8	11.0	9.1	3.7	5.5	14.1	11.3	9.9
		Q	3.2	-2.2	0.3	0.0	6.6	8.8	5.4	5.1	11.3	9.4	4.0	5.8	14.4	11.6	10.2
		D	-3.2	-8.3	-5.9	-6.2	0.0	2.0	-1.1	-1.4	4.4	2.6	-2.5	-0.7	7.3	4.7	3.4
		E	-5.1	-10.1	-7.8	-8.1	-2.0	0.0	-3.1	-3.4	2.3	0.6	-4.4	-2.7	5.2	2.6	1.4
		T	-2.1	-7.2	-4.9	-5.1	1.1	3.2	0.0	-0.3	5.6	3.8	-1.4	0.4	8.5	5.9	4.6
		A	-1.8	-7.0	-4.6	-4.9	1.4	3.5	0.3	0.0	5.9	4.1	-1.1	0.7	8.9	6.2	4.9
		P	-7.3	-12.2	-9.9	-10.2	-4.2	-2.3	-5.3	-5.6	0.0	-1.7	-6.6	-4.9	2.8	0.3	-1.0
		C	-5.7	-10.6	-8.3	-8.6	-2.6	-0.6	-3.7	-3.9	1.7	0.0	-5.0	-3.3	4.6	2.0	0.8
		K	-0.8	-6.0	-3.6	-3.8	2.5	4.6	1.4	1.1	7.0	5.2	0.0	1.8	10.0	7.3	6.0
		V	-2.5	-7.6	-5.2	-5.5	0.7	2.8	-0.4	-0.7	5.2	3.4	-1.7	0.0	8.1	5.5	4.2
		I	-9.8	-14.5	-12.4	-12.6	-6.8	-4.9	-7.9	-8.1	-2.7	-4.4	-9.1	-7.5	0.0	-2.4	-3.7
		L	-7.6	-12.4	-10.2	-10.4	-4.5	-2.6	-5.6	-5.8	-0.3	-2.0	-6.8	-5.2	2.5	0.0	-1.2
	F	-6.4	-11.3	-9.0	-9.3	-3.3	-1.3	-4.4	-4.7	1.0	-0.8	-5.7	-4.0	3.8	1.3	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
2	A	H	0.0	-6.3	-5.4	-4.8	1.1	3.6	0.5	-1.0	6.6	4.3	-0.3	3.3	10.9	5.4	6.4
		N	6.7	0.0	1.0	1.5	7.9	10.5	7.3	5.6	13.7	11.3	6.3	10.2	18.4	12.5	13.6
		S	5.7	-1.0	0.0	0.6	6.9	9.4	6.3	4.6	12.6	10.2	5.3	9.2	17.2	11.4	12.5
		Q	5.1	-1.5	-0.6	0.0	6.3	8.8	5.7	4.0	12.0	9.6	4.7	8.5	16.6	10.8	11.8
		D	-1.1	-7.3	-6.4	-5.9	0.0	2.4	-0.6	-2.2	5.4	3.1	-1.5	2.1	9.7	4.2	5.2
		E	-3.4	-9.5	-8.6	-8.1	-2.3	0.0	-2.9	-4.4	2.9	0.7	-3.8	-0.3	7.1	1.8	2.8
		T	-0.5	-6.8	-5.9	-5.4	0.6	3.0	0.0	-1.6	6.0	3.7	-0.9	2.7	10.3	4.8	5.8
		A	1.1	-5.3	-4.4	-3.8	2.2	4.7	1.6	0.0	7.7	5.4	0.7	4.4	12.1	6.5	7.6
		P	-6.2	-12.1	-11.2	-10.7	-5.1	-2.8	-5.6	-7.2	0.0	-2.1	-6.5	-3.1	4.1	-1.1	-0.1
		C	-4.1	-10.1	-9.3	-8.7	-3.0	-0.7	-3.6	-5.1	2.2	0.0	-4.4	-1.0	6.4	1.1	2.1
		K	0.3	-6.0	-5.0	-4.5	1.5	3.9	0.9	-0.7	6.9	4.6	0.0	3.6	11.3	5.8	6.8
		V	-3.2	-9.3	-8.4	-7.9	-2.1	0.3	-2.7	-4.2	3.2	1.0	-3.5	0.0	7.4	2.1	3.0
		I	-9.8	-15.5	-14.7	-14.2	-8.8	-6.6	-9.4	-10.8	-3.9	-6.0	-10.2	-6.9	0.0	-5.0	-4.1
		L	-5.1	-11.1	-10.2	-9.7	-4.1	-1.8	-4.6	-6.1	1.1	-1.1	-5.5	-2.0	5.2	0.0	1.0
	F	-6.0	-11.9	-11.1	-10.6	-5.0	-2.7	-5.5	-7.0	0.1	-2.0	-6.4	-3.0	4.2	-1.0	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
3	A	H	0.0	-7.7	-7.6	-5.2	13.2	17.8	7.9	5.2	24.1	15.7	5.7	24.3	40.3	30.1	24.8
		N	8.3	0.0	0.1	2.6	22.6	27.6	16.8	13.9	34.4	25.2	14.5	34.6	51.9	40.9	35.1
		S	8.2	-0.1	0.0	2.6	22.5	27.5	16.7	13.8	34.3	25.2	14.4	34.5	51.8	40.8	35.0
		Q	5.5	-2.6	-2.5	0.0	19.4	24.3	13.8	11.0	31.0	22.0	11.5	31.1	48.0	37.2	31.6

	D	-11.7	-18.4	-18.4	-16.3	0.0	4.1	-4.7	-7.1	9.7	2.2	-6.6	9.8	23.9	14.9	10.2
	E	-15.1	-21.6	-21.6	-19.6	-3.9	0.0	-8.5	-10.7	5.4	-1.8	-10.3	5.5	19.0	10.4	5.9
	T	-7.3	-14.4	-14.3	-12.1	4.9	9.2	0.0	-2.5	15.1	7.2	-2.0	15.2	30.0	20.6	15.7
	A	-4.9	-12.2	-12.2	-9.9	7.6	12.0	2.5	0.0	18.0	9.9	0.5	18.2	33.3	23.7	18.6
	P	-19.4	-25.6	-25.6	-23.6	-8.8	-5.1	-13.1	-15.3	0.0	-6.8	-14.8	0.1	13.0	4.8	0.5
	C	-13.5	-20.2	-20.1	-18.0	-2.1	1.9	-6.7	-9.0	7.3	0.0	-8.6	7.5	21.3	12.5	7.9
	K	-5.4	-12.7	-12.6	-10.4	7.0	11.4	2.0	-0.5	17.4	9.4	0.0	17.6	32.7	23.0	18.0
	V	-19.6	-25.7	-25.7	-23.7	-9.0	-5.2	-13.2	-15.4	-0.1	-7.0	-14.9	0.0	12.8	4.6	0.4
	I	-28.7	-34.2	-34.1	-32.4	-19.3	-16.0	-23.1	-25.0	-11.5	-17.5	-24.6	-11.4	0.0	-7.2	-11.0
	L	-23.1	-29.0	-29.0	-27.1	-13.0	-9.4	-17.1	-19.1	-4.6	-11.1	-18.7	-4.4	7.8	0.0	-4.1
	F	-19.9	-26.0	-25.9	-24.0	-9.3	-5.6	-13.5	-15.7	-0.5	-7.3	-15.3	-0.4	12.4	4.3	0.0
	H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
	B															

Supplementary Table 37: Raw data Extended Data Fig. 4 – AA in water, 170 μm , 18 h, 1 mM NaCl, pH 7.4 – enrichments in bottom fraction

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)															
1	A	H	0.0	3.1	0.3	1.8	-2.2	-3.0	-1.5	-1.6	-4.4	-5.4	-0.3	-2.4	-5.9	-4.6	-3.5
		N	-3.0	0.0	-2.7	-1.3	-5.2	-5.9	-4.5	-4.6	-7.3	-8.3	-3.4	-5.3	-8.7	-7.4	-6.5
		S	-0.3	2.8	0.0	1.4	-2.5	-3.3	-1.8	-1.9	-4.7	-5.7	-0.7	-2.7	-6.2	-4.9	-3.9
		Q	-1.7	1.3	-1.4	0.0	-3.9	-4.7	-3.2	-3.3	-6.1	-7.1	-2.1	-4.1	-7.5	-6.2	-5.2
		D	2.3	5.4	2.6	4.1	0.0	-0.8	0.7	0.6	-2.3	-3.3	1.9	-0.2	-3.7	-2.4	-1.4
		E	3.1	6.3	3.4	4.9	0.8	0.0	1.5	1.4	-1.5	-2.5	2.7	0.6	-3.0	-1.6	-0.6
		T	1.5	4.7	1.8	3.3	-0.7	-1.5	0.0	-0.1	-3.0	-4.0	1.2	-0.9	-4.4	-3.1	-2.1
		A	1.6	4.8	2.0	3.4	-0.6	-1.4	0.1	0.0	-2.9	-3.9	1.3	-0.8	-4.3	-3.0	-2.0
		P	4.6	7.9	5.0	6.5	2.3	1.5	3.1	3.0	0.0	-1.0	4.3	2.2	-1.5	-0.1	0.9
		C	5.8	9.1	6.1	7.6	3.4	2.6	4.2	4.0	1.1	0.0	5.4	3.2	-0.5	0.9	2.0
		K	0.3	3.5	0.7	2.1	-1.9	-2.6	-1.2	-1.3	-4.1	-5.1	0.0	-2.0	-5.5	-4.2	-3.2
		V	2.4	5.6	2.8	4.2	0.2	-0.6	0.9	0.8	-2.1	-3.1	2.1	0.0	-3.6	-2.2	-1.2
		I	6.2	9.5	6.6	8.1	3.9	3.1	4.6	4.5	1.5	0.5	5.9	3.7	0.0	1.4	2.5
		L	4.8	8.0	5.1	6.6	2.5	1.7	3.2	3.1	0.1	-0.9	4.4	2.3	-1.4	0.0	1.1
		F	3.7	6.9	4.0	5.5	1.4	0.6	2.1	2.0	-0.9	-2.0	3.3	1.2	-2.4	-1.1	0.0
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
2	A	H	0.0	4.7	4.0	4.4	-1.9	-3.7	-0.9	-0.3	-5.9	-4.4	-0.2	-6.4	-9.2	-7.5	-6.3
		N	-4.5	0.0	-0.7	-0.3	-6.3	-8.0	-5.3	-4.7	-10.1	-8.7	-4.7	-10.6	-13.3	-11.6	-10.5
		S	-3.8	0.7	0.0	0.5	-5.6	-7.4	-4.7	-4.1	-9.5	-8.0	-4.0	-10.0	-12.7	-11.0	-9.8
		Q	-4.2	0.3	-0.4	0.0	-6.0	-7.8	-5.1	-4.5	-9.9	-8.4	-4.5	-10.4	-13.1	-11.4	-10.2
		D	1.9	6.7	5.9	6.4	0.0	-1.9	1.0	1.6	-4.1	-2.6	1.7	-4.6	-7.5	-5.7	-4.5
		E	3.9	8.7	8.0	8.5	1.9	0.0	2.9	3.6	-2.3	-0.7	3.6	-2.8	-5.7	-3.9	-2.6
		T	0.9	5.6	4.9	5.4	-1.0	-2.9	0.0	0.6	-5.1	-3.5	0.7	-5.6	-8.4	-6.7	-5.4
		A	0.3	5.0	4.2	4.7	-1.6	-3.5	-0.6	0.0	-5.7	-4.1	0.0	-6.2	-9.0	-7.2	-6.0
		P	6.3	11.3	10.5	11.0	4.3	2.3	5.4	6.0	0.0	1.6	6.0	-0.5	-3.5	-1.7	-0.4
		C	4.6	9.5	8.7	9.2	2.6	0.7	3.6	4.3	-1.6	0.0	4.3	-2.1	-5.1	-3.2	-2.0
		K	0.2	4.9	4.2	4.7	-1.6	-3.5	-0.7	0.0	-5.7	-4.1	0.0	-6.2	-9.0	-7.3	-6.0
		V	6.8	11.9	11.1	11.6	4.9	2.9	5.9	6.6	0.5	2.2	6.6	0.0	-3.0	-1.1	0.2
		I	10.2	15.3	14.5	15.0	8.1	6.1	9.2	9.9	3.6	5.3	9.9	3.1	0.0	1.9	3.3
		L	8.1	13.2	12.4	12.9	6.1	4.1	7.1	7.8	1.7	3.4	7.8	1.2	-1.9	0.0	1.3
		F	6.7	11.7	10.9	11.4	4.7	2.7	5.7	6.4	0.4	2.0	6.4	-0.2	-3.2	-1.3	0.0
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
3	A	H	0.0	7.9	7.6	7.2	-5.5	-8.1	-2.9	-1.7	-12.1	-10.3	-0.5	-10.7	-17.9	-14.6	-11.8
		N	-7.4	0.0	-0.3	-0.6	-12.4	-14.8	-10.1	-8.9	-18.6	-16.9	-7.8	-17.3	-23.9	-20.9	-18.3
		S	-7.1	0.3	0.0	-0.4	-12.2	-14.6	-9.8	-8.7	-18.4	-16.7	-7.6	-17.1	-23.7	-20.7	-18.0
		Q	-6.8	0.6	0.4	0.0	-11.9	-14.3	-9.5	-8.3	-18.1	-16.4	-7.2	-16.8	-23.4	-20.4	-17.8

	D	5.8	14.2	13.9	13.5	0.0	-2.7	2.7	4.0	-7.0	-5.1	5.3	-5.6	-13.1	-9.7	-6.7
	E	8.8	17.4	17.1	16.7	2.8	0.0	5.6	6.9	-4.4	-2.5	8.2	-2.9	-10.7	-7.2	-4.0
	T	3.0	11.2	10.9	10.5	-2.6	-5.3	0.0	1.3	-9.5	-7.6	2.5	-8.0	-15.4	-12.1	-9.1
	A	1.7	9.8	9.5	9.1	-3.9	-6.5	-1.3	0.0	-10.6	-8.8	1.2	-9.2	-16.5	-13.2	-10.3
	P	13.8	22.9	22.5	22.1	7.6	4.6	10.5	11.9	0.0	2.1	13.2	1.6	-6.6	-2.8	0.4
	C	11.5	20.4	20.0	19.6	5.4	2.5	8.2	9.6	-2.0	0.0	11.0	-0.5	-8.4	-4.8	-1.6
	K	0.5	8.5	8.2	7.8	-5.0	-7.6	-2.4	-1.2	-11.7	-9.9	0.0	-10.3	-17.5	-14.2	-11.3
	V	12.0	20.9	20.6	20.1	5.9	3.0	8.7	10.1	-1.6	0.5	11.5	0.0	-8.0	-4.4	-1.2
	I	21.8	31.5	31.1	30.6	15.1	12.0	18.2	19.7	7.0	9.2	21.2	8.7	0.0	4.0	7.4
	L	17.2	26.5	26.1	25.7	10.7	7.7	13.7	15.2	2.9	5.1	16.6	4.6	-3.8	0.0	3.3
	F	13.4	22.4	22.0	21.6	7.1	4.2	10.0	11.5	-0.4	1.7	12.8	1.2	-6.9	-3.2	0.0
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F
		B														

Supplementary Table 38: Raw data Extended Data Fig. 4 – AA in water, 170 μm , 18 h, 10 mM NaCl, pH 7.4

repeat k	species	measured values (counts*min)				concentration (μM) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 4				c_0 (μM)	Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)	
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot
1	H	230724	264264	345433	286340	25.70	29.44	38.48	31.90	31.38	0.82	0.94	1.23	1.02	-4.0	-9.9
	N	423090	473516	475250	484207	38.29	42.85	43.01	43.82	41.99	0.91	1.02	1.02	1.04	6.9	-7.5
	S	373347	428518	409123	441441	26.61	30.54	29.16	31.46	29.44	0.90	1.04	0.99	1.07	6.0	-5.2
	Q	350471	400003	378236	406072	30.44	34.74	32.85	35.27	33.33	0.91	1.04	0.99	1.06	7.1	-6.2
	D	350967	417314	411426	465792	31.62	37.60	37.07	41.97	37.06	0.85	1.01	1.00	1.13	0.0	0.4
	E	327726	395480	391173	451693	30.32	36.59	36.19	41.79	36.23	0.84	1.01	1.00	1.15	-1.8	2.3
	T	394040	463855	454294	509794	25.42	29.92	29.31	32.89	29.38	0.87	1.02	1.00	1.12	1.4	-0.8
	A	364563	427050	415996	467535	25.34	29.68	28.92	32.50	29.11	0.87	1.02	0.99	1.12	2.1	-1.0
	P	99060	118743	120362	141169	23.64	28.34	28.73	33.69	28.60	0.83	0.99	1.00	1.18	-3.1	4.5
	C	27580	30612	32191	37485	19.91	22.10	23.24	27.06	23.08	0.86	0.96	1.01	1.17	1.2	4.0
	K	317978	372212	362733	399125	30.09	35.22	34.32	37.76	34.35	0.88	1.03	1.00	1.10	2.7	-2.5
	V	497143	593948	622721	697719	25.87	30.91	32.40	36.30	31.37	0.82	0.99	1.03	1.16	-3.3	2.6
	I	446752	552150	567144	693409	21.39	26.43	27.15	33.20	27.04	0.79	0.98	1.00	1.23	-7.3	8.9
	L	418348	508346	520782	617461	22.90	27.82	28.50	33.80	28.25	0.81	0.98	1.01	1.20	-5.0	6.1
	F	358733	431875	434511	510095	23.57	28.38	28.55	33.52	28.50	0.83	1.00	1.00	1.18	-3.0	4.3
	mean concentration per fraction $\bar{c}_{j,k}$										0.85	1.00	1.02	1.13		
2	H	222749	258462	221123	317327	24.81	28.79	24.63	35.35	28.40	0.87	1.01	0.87	1.24	4.8	-7.5
	N	420747	479383	401584	499454	38.07	43.38	36.34	45.20	40.75	0.93	1.06	0.89	1.11	12.1	-17.6
	S	377677	439196	361282	468316	26.92	31.30	25.75	33.38	29.33	0.92	1.07	0.88	1.14	10.1	-15.5
	Q	353644	401799	332383	425535	30.72	34.90	28.87	36.96	32.86	0.93	1.06	0.88	1.12	12.1	-16.4
	D	330522	391349	342417	544351	29.78	35.26	30.85	49.04	36.23	0.82	0.97	0.85	1.35	-1.4	0.6
	E	311726	363126	322903	538164	28.84	33.60	29.88	49.80	35.53	0.81	0.95	0.84	1.40	-2.6	4.1

	T	380868	432844	381804	568785	24.57	27.92	24.63	36.69	28.45	0.86	0.98	0.87	1.29	3.6	-4.2
	A	352483	412317	352895	525566	24.50	28.66	24.53	36.53	28.56	0.86	1.00	0.86	1.28	2.9	-4.9
	P	88969	106613	95355	171988	21.24	25.45	22.76	41.05	27.62	0.77	0.92	0.82	1.49	-7.8	10.4
	C	26337	30824	26814	43786	19.02	22.26	19.36	31.61	23.06	0.82	0.97	0.84	1.37	-1.1	1.9
	K	315232	366816	310383	437843	29.83	34.71	29.37	41.43	33.83	0.88	1.03	0.87	1.22	5.8	-9.0
	V	454514	537213	487665	839222	23.65	27.95	25.38	43.67	30.16	0.78	0.93	0.84	1.45	-5.9	7.6
	I	388692	460948	429786	905726	18.61	22.07	20.58	43.36	26.15	0.71	0.84	0.79	1.66	-14.6	23.2
	L	374091	438056	409460	776960	20.47	23.98	22.41	42.52	27.35	0.75	0.88	0.82	1.56	-10.2	15.6
	F	324284	380843	347574	634141	21.31	25.02	22.84	41.67	27.71	0.77	0.90	0.82	1.50	-7.8	11.7
	mean concentration per fraction $\bar{c}_{j,k}$										0.83	0.97	0.85	1.35		
3	H	247326	233094	238582	288036	27.55	25.97	26.58	32.09	28.05	0.98	0.93	0.95	1.14	3.8	-3.2
	N	457553	422836	416762	480712	41.41	38.26	37.71	43.50	40.22	1.03	0.95	0.94	1.08	8.8	-8.5
	S	415340	375742	383445	450700	29.60	26.78	27.33	32.12	28.96	1.02	0.92	0.94	1.11	8.0	-6.1
	Q	388020	354085	350453	406586	33.70	30.76	30.44	35.32	32.55	1.04	0.94	0.94	1.08	9.4	-8.2
	D	373104	366124	381154	470714	33.62	32.99	34.34	42.41	35.84	0.94	0.92	0.96	1.18	-0.9	0.1
	E	364838	348709	366626	463637	33.76	32.27	33.92	42.90	35.71	0.95	0.90	0.95	1.20	-0.1	1.7
	T	421808	403655	418180	512779	27.21	26.04	26.98	33.08	28.33	0.96	0.92	0.95	1.17	1.5	-1.2
	A	393267	372602	384337	472311	27.34	25.90	26.72	32.83	28.20	0.97	0.92	0.95	1.16	2.4	-1.5
	P	103183	102238	108470	143334	24.63	24.40	25.89	34.21	27.28	0.90	0.89	0.95	1.25	-4.6	6.1
	C	29880	28869	29498	36824	21.57	20.84	21.30	26.59	22.58	0.96	0.92	0.94	1.18	1.0	-0.3
	K	347794	329846	338150	400990	32.91	31.21	31.99	37.94	33.51	0.98	0.93	0.95	1.13	3.7	-4.2
	V	501129	537651	541296	713218	26.08	27.98	28.17	37.11	29.83	0.87	0.94	0.94	1.24	-7.6	5.3
	I	463474	485993	533488	708325	22.19	23.27	25.54	33.91	26.23	0.85	0.89	0.97	1.29	-10.6	9.4
	L	424052	452061	481678	619331	23.21	24.74	26.36	33.90	27.05	0.86	0.91	0.97	1.25	-9.4	6.0
	F	376074	377785	407097	518372	24.71	24.82	26.75	34.06	27.59	0.90	0.90	0.97	1.23	-5.4	4.5
	mean concentration per fraction $\bar{c}_{j,k}$										0.95	0.92	0.95	1.18		

Supplementary Table 39: Raw data Extended Data Fig. 4 – AA in water, 170 μm , 18 h, 10 mM NaCl, pH 7.4 – enrichments in top fraction

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)															
1	A	H	0.0	-10.2	-9.4	-10.3	-4.0	-2.1	-5.3	-5.9	-0.9	-5.1	-6.5	-0.7	3.6	1.1	-1.0
		N	11.3	0.0	0.9	-0.2	6.9	8.9	5.4	4.7	10.3	5.7	4.1	10.6	15.3	12.5	10.3
		S	10.3	-0.9	0.0	-1.1	5.9	8.0	4.5	3.8	9.3	4.7	3.2	9.6	14.3	11.5	9.3
		Q	11.5	0.2	1.1	0.0	7.1	9.1	5.6	4.9	10.5	5.9	4.3	10.8	15.5	12.7	10.5
		D	4.2	-6.4	-5.6	-6.6	0.0	1.9	-1.4	-2.0	3.2	-1.1	-2.6	3.5	7.9	5.3	3.2
		E	2.2	-8.2	-7.4	-8.4	-1.9	0.0	-3.2	-3.8	1.3	-3.0	-4.4	1.5	5.8	3.3	1.2
		T	5.6	-5.1	-4.3	-5.3	1.4	3.3	0.0	-0.6	4.6	0.3	-1.2	4.9	9.4	6.7	4.6
		A	6.3	-4.5	-3.7	-4.7	2.0	4.0	0.6	0.0	5.3	0.9	-0.6	5.6	10.1	7.4	5.3
		P	0.9	-9.3	-8.5	-9.5	-3.1	-1.2	-4.4	-5.0	0.0	-4.2	-5.6	0.2	4.5	2.0	0.0
		C	5.3	-5.4	-4.5	-5.5	1.1	3.1	-0.3	-0.9	4.4	0.0	-1.5	4.6	9.1	6.5	4.3
		K	6.9	-3.9	-3.1	-4.1	2.7	4.6	1.3	0.6	6.0	1.5	0.0	6.2	10.8	8.1	5.9
		V	0.7	-9.6	-8.8	-9.7	-3.3	-1.5	-4.7	-5.3	-0.2	-4.4	-5.9	0.0	4.3	1.8	-0.3
		I	-3.4	-13.3	-12.5	-13.4	-7.3	-5.5	-8.6	-9.1	-4.3	-8.3	-9.7	-4.1	0.0	-2.4	-4.4
		L	-1.1	-11.1	-10.3	-11.3	-5.0	-3.2	-6.3	-6.9	-2.0	-6.1	-7.5	-1.7	2.5	0.0	-2.0
	F	1.0	-9.3	-8.5	-9.5	-3.1	-1.2	-4.4	-5.0	0.0	-4.2	-5.6	0.3	4.6	2.0	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
2	A	H	0.0	-6.5	-4.8	-6.5	6.3	7.6	1.2	1.8	13.7	6.0	-0.9	11.4	22.8	16.7	13.6
		N	6.9	0.0	1.8	0.0	13.7	15.1	8.2	8.9	21.5	13.3	6.0	19.2	31.3	24.8	21.5
		S	5.0	-1.8	0.0	-1.8	11.6	13.0	6.3	6.9	19.4	11.3	4.1	17.0	29.0	22.5	19.3
		Q	7.0	0.0	1.9	0.0	13.7	15.1	8.2	8.9	21.6	13.4	6.0	19.2	31.4	24.8	21.6
		D	-5.9	-12.0	-10.4	-12.1	0.0	1.2	-4.8	-4.2	6.9	-0.3	-6.8	4.8	15.5	9.8	6.9
		E	-7.1	-13.1	-11.5	-13.1	-1.2	0.0	-6.0	-5.4	5.6	-1.5	-7.9	3.5	14.1	8.4	5.6
		T	-1.2	-7.6	-5.9	-7.6	5.1	6.4	0.0	0.6	12.3	4.7	-2.1	10.1	21.4	15.3	12.3
		A	-1.8	-8.2	-6.5	-8.2	4.4	5.7	-0.6	0.0	11.6	4.1	-2.7	9.4	20.6	14.6	11.6
		P	-12.0	-17.7	-16.2	-17.8	-6.5	-5.3	-11.0	-10.4	0.0	-6.8	-12.8	-2.0	8.0	2.7	0.0
		C	-5.6	-11.8	-10.1	-11.8	0.3	1.6	-4.5	-3.9	7.3	0.0	-6.5	5.2	15.9	10.1	7.2
		K	0.9	-5.6	-3.9	-5.7	7.3	8.6	2.1	2.7	14.7	6.9	0.0	12.4	23.9	17.7	14.6
		V	-10.3	-16.1	-14.5	-16.1	-4.6	-3.4	-9.2	-8.6	2.0	-4.9	-11.1	0.0	10.2	4.7	2.0
		I	-18.6	-23.9	-22.5	-23.9	-13.4	-12.4	-17.6	-17.1	-7.4	-13.7	-19.3	-9.3	0.0	-5.0	-7.5
		L	-14.3	-19.9	-18.4	-19.9	-8.9	-7.8	-13.3	-12.7	-2.6	-9.2	-15.1	-4.5	5.2	0.0	-2.6
	F	-12.0	-17.7	-16.2	-17.7	-6.4	-5.3	-10.9	-10.4	0.0	-6.7	-12.8	-1.9	8.1	2.7	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
3	A	H	0.0	-4.6	-3.9	-5.1	4.7	3.9	2.3	1.3	8.8	2.8	0.0	12.4	16.1	14.5	9.7
		N	4.8	0.0	0.7	-0.6	9.8	8.9	7.2	6.2	14.0	7.7	4.8	17.8	21.7	20.0	14.9
		S	4.1	-0.7	0.0	-1.3	9.0	8.1	6.4	5.4	13.2	7.0	4.1	16.9	20.8	19.2	14.1
		Q	5.4	0.6	1.3	0.0	10.4	9.5	7.8	6.8	14.7	8.3	5.4	18.4	22.4	20.7	15.6

	D	-4.5	-8.9	-8.2	-9.4	0.0	-0.8	-2.4	-3.3	3.9	-1.8	-4.5	7.3	10.9	9.3	4.7
	E	-3.8	-8.2	-7.5	-8.7	0.8	0.0	-1.6	-2.5	4.7	-1.1	-3.7	8.1	11.7	10.2	5.5
	T	-2.2	-6.7	-6.0	-7.2	2.4	1.6	0.0	-0.9	6.4	0.5	-2.2	9.9	13.5	12.0	7.2
	A	-1.3	-5.8	-5.2	-6.4	3.4	2.6	0.9	0.0	7.4	1.5	-1.3	10.9	14.6	13.0	8.2
	P	-8.1	-12.3	-11.7	-12.8	-3.8	-4.5	-6.0	-6.9	0.0	-5.5	-8.1	3.3	6.7	5.2	0.8
	C	-2.7	-7.2	-6.5	-7.7	1.9	1.1	-0.5	-1.4	5.9	0.0	-2.7	9.3	13.0	11.4	6.7
	K	0.0	-4.6	-3.9	-5.2	4.7	3.9	2.2	1.3	8.8	2.8	0.0	12.3	16.1	14.5	9.6
	V	-11.0	-15.1	-14.5	-15.6	-6.8	-7.5	-9.0	-9.8	-3.2	-8.5	-11.0	0.0	3.3	1.9	-2.4
	I	-13.9	-17.8	-17.2	-18.3	-9.8	-10.5	-11.9	-12.7	-6.3	-11.5	-13.8	-3.2	0.0	-1.4	-5.6
	L	-12.7	-16.7	-16.1	-17.1	-8.5	-9.2	-10.7	-11.5	-5.0	-10.2	-12.6	-1.8	1.4	0.0	-4.2
	F	-8.8	-13.0	-12.4	-13.5	-4.5	-5.2	-6.7	-7.6	-0.8	-6.3	-8.8	2.5	5.9	4.4	0.0
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F
		B														

Supplementary Table 40: Raw data Extended Data Fig. 4 – AA in water, 170 μm , 18 h, 10 mM NaCl, pH 7.4 – enrichments in bottom fraction

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)															
1	A	H	0.0	-2.6	-4.9	-4.0	-10.2	-11.9	-9.2	-8.9	-13.7	-13.3	-7.5	-12.2	-17.2	-15.0	-13.6
		N	2.7	0.0	-2.3	-1.4	-7.8	-9.6	-6.8	-6.5	-11.4	-11.0	-5.1	-9.8	-15.0	-12.8	-11.3
		S	5.1	2.4	0.0	1.0	-5.6	-7.4	-4.5	-4.3	-9.3	-8.9	-2.8	-7.7	-13.0	-10.7	-9.1
		Q	4.1	1.4	-1.0	0.0	-6.5	-8.3	-5.4	-5.2	-10.2	-9.7	-3.7	-8.6	-13.8	-11.5	-10.0
		D	11.4	8.5	6.0	7.0	0.0	-1.9	1.2	1.4	-3.9	-3.4	3.0	-2.2	-7.8	-5.3	-3.7
		E	13.5	10.6	8.0	9.0	1.9	0.0	3.1	3.3	-2.1	-1.6	4.9	-0.3	-6.0	-3.5	-1.9
		T	10.1	7.3	4.7	5.8	-1.2	-3.0	0.0	0.3	-5.0	-4.6	1.8	-3.3	-8.8	-6.4	-4.8
		A	9.8	7.0	4.5	5.5	-1.4	-3.2	-0.3	0.0	-5.2	-4.8	1.5	-3.5	-9.1	-6.7	-5.1
		P	15.9	12.9	10.2	11.3	4.0	2.1	5.3	5.5	0.0	0.5	7.1	1.8	-4.0	-1.5	0.2
		C	15.4	12.4	9.7	10.8	3.6	1.6	4.8	5.0	-0.5	0.0	6.7	1.3	-4.5	-2.0	-0.3
		K	8.2	5.4	2.9	3.9	-2.9	-4.7	-1.8	-1.5	-6.7	-6.2	0.0	-5.0	-10.4	-8.1	-6.5
		V	13.9	10.9	8.3	9.4	2.2	0.3	3.4	3.7	-1.8	-1.3	5.3	0.0	-5.7	-3.2	-1.6
		I	20.8	17.6	14.9	16.0	8.4	6.4	9.7	10.0	4.2	4.7	11.6	6.1	0.0	2.6	4.4
		L	17.7	14.6	11.9	13.0	5.6	3.7	6.9	7.1	1.5	2.0	8.8	3.4	-2.6	0.0	1.7
	F	15.7	12.7	10.0	11.1	3.8	1.9	5.1	5.3	-0.2	0.3	6.9	1.6	-4.2	-1.7	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
2	A	H	0.0	12.2	9.4	10.7	-8.0	-11.2	-3.5	-2.7	-16.2	-9.2	1.7	-14.0	-24.9	-19.9	-17.2
		N	-10.9	0.0	-2.5	-1.4	-18.1	-20.9	-14.0	-13.3	-25.4	-19.1	-9.4	-23.4	-33.1	-28.7	-26.2
		S	-8.6	2.6	0.0	1.2	-15.9	-18.8	-11.8	-11.1	-23.4	-17.0	-7.1	-21.4	-31.4	-26.8	-24.3
		Q	-9.6	1.4	-1.1	0.0	-16.9	-19.7	-12.8	-12.1	-24.3	-18.0	-8.1	-22.3	-32.2	-27.7	-25.2
		D	8.7	22.0	19.0	20.3	0.0	-3.4	5.0	5.8	-8.9	-1.3	10.5	-6.5	-18.4	-13.0	-10.0
		E	12.6	26.4	23.2	24.6	3.5	0.0	8.7	9.6	-5.7	2.2	14.5	-3.2	-15.5	-9.9	-6.8
		T	3.6	16.3	13.3	14.7	-4.7	-8.0	0.0	0.8	-13.2	-5.9	5.3	-10.9	-22.2	-17.1	-14.2
		A	2.8	15.3	12.4	13.7	-5.5	-8.7	-0.8	0.0	-13.9	-6.7	4.5	-11.6	-22.8	-17.7	-14.9
		P	19.4	34.0	30.6	32.1	9.8	6.0	15.2	16.2	0.0	8.4	21.4	2.6	-10.4	-4.4	-1.2
		C	10.1	23.6	20.5	21.9	1.3	-2.2	6.3	7.2	-7.8	0.0	12.0	-5.3	-17.3	-11.8	-8.8
		K	-1.6	10.4	7.6	8.9	-9.5	-12.6	-5.0	-4.3	-17.6	-10.7	0.0	-15.4	-26.1	-21.3	-18.6
		V	16.3	30.5	27.3	28.7	7.0	3.3	12.3	13.2	-2.6	5.6	18.2	0.0	-12.7	-6.9	-3.7
		I	33.2	49.5	45.7	47.4	22.5	18.3	28.6	29.6	11.6	20.9	35.4	14.5	0.0	6.6	10.3
		L	24.9	40.2	36.7	38.3	14.9	11.0	20.6	21.6	4.6	13.4	27.0	7.4	-6.2	0.0	3.4
	F	20.8	35.6	32.2	33.7	11.1	7.3	16.6	17.5	1.2	9.7	22.8	3.9	-9.3	-3.3	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
3	A	H	0.0	5.8	3.1	5.5	-3.3	-4.8	-2.0	-1.7	-8.8	-2.9	1.1	-8.0	-11.5	-8.7	-7.3
		N	-5.5	0.0	-2.5	-0.3	-8.6	-10.0	-7.4	-7.1	-13.7	-8.2	-4.5	-13.1	-16.4	-13.7	-12.4
		S	-3.0	2.6	0.0	2.3	-6.3	-7.7	-5.0	-4.7	-11.5	-5.8	-2.0	-10.8	-14.2	-11.5	-10.2
		Q	-5.2	0.3	-2.2	0.0	-8.3	-9.7	-7.1	-6.8	-13.5	-7.9	-4.2	-12.8	-16.1	-13.4	-12.1

	D	3.4	9.4	6.7	9.1	0.0	-1.5	1.3	1.6	-5.6	0.5	4.5	-4.9	-8.5	-5.6	-4.2
	E	5.0	11.1	8.3	10.7	1.5	0.0	2.9	3.2	-4.2	2.0	6.1	-3.4	-7.1	-4.1	-2.7
	T	2.1	8.0	5.3	7.6	-1.3	-2.8	0.0	0.3	-6.9	-0.8	3.2	-6.1	-9.7	-6.8	-5.4
	A	1.8	7.7	5.0	7.3	-1.6	-3.1	-0.3	0.0	-7.1	-1.1	2.9	-6.4	-9.9	-7.1	-5.7
	P	9.6	15.9	13.0	15.6	6.0	4.4	7.4	7.7	0.0	6.5	10.8	0.8	-3.0	0.1	1.6
	C	2.9	8.9	6.2	8.6	-0.5	-2.0	0.8	1.1	-6.1	0.0	4.0	-5.3	-8.9	-6.0	-4.6
	K	-1.0	4.7	2.1	4.4	-4.3	-5.8	-3.1	-2.8	-9.7	-3.9	0.0	-9.0	-12.4	-9.6	-8.3
	V	8.7	15.0	12.1	14.7	5.1	3.6	6.5	6.8	-0.8	5.6	9.9	0.0	-3.8	-0.7	0.8
	I	13.0	19.5	16.6	19.2	9.3	7.6	10.7	11.0	3.1	9.8	14.2	3.9	0.0	3.2	4.7
	L	9.5	15.9	13.0	15.5	5.9	4.3	7.3	7.6	-0.1	6.4	10.7	0.7	-3.1	0.0	1.5
	F	7.9	14.2	11.3	13.8	4.3	2.8	5.7	6.0	-1.5	4.8	9.1	-0.7	-4.5	-1.5	0.0
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F
		B														

Supplementary Table 41: Raw data Extended Data Fig. 4 – AA in water, 170 μm , 18 h, 100 mM NaCl, pH 7.4

repeat k	species	measured values (counts*min)				concentration (μM) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 4				c_0 (μM)	Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)	
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot
1	H	224736	226101	237934	273864	25.04	25.19	26.51	30.51	26.81	0.93	0.94	0.99	1.14	4.9	-2.7
	N	404928	436605	422385	468544	36.64	39.51	38.22	42.40	39.19	0.93	1.01	0.98	1.08	5.0	-7.5
	S	355640	356018	377900	428608	25.35	25.37	26.93	30.55	27.05	0.94	0.94	1.00	1.13	5.2	-3.4
	Q	332795	333915	346837	401403	28.91	29.00	30.13	34.87	30.73	0.94	0.94	0.98	1.13	5.6	-3.0
	D	339283	355321	375212	442294	30.57	32.01	33.81	39.85	34.06	0.90	0.94	0.99	1.17	0.8	0.1
	E	319897	336739	356551	423171	29.60	31.16	32.99	39.16	33.23	0.89	0.94	0.99	1.18	0.0	0.8
	T	378197	391071	412741	485274	24.40	25.23	26.63	31.30	26.89	0.91	0.94	0.99	1.16	1.9	-0.4
	A	351376	357707	382887	442518	24.42	24.86	26.61	30.76	26.67	0.92	0.93	1.00	1.15	2.8	-1.4
	P	94762	100523	109214	129013	22.62	23.99	26.07	30.79	25.87	0.87	0.93	1.01	1.19	-1.8	1.8
	C	26993	28332	30802	36403	19.49	20.46	22.24	26.28	22.12	0.88	0.92	1.01	1.19	-1.1	1.6
	K	308859	318081	332711	388763	29.22	30.10	31.48	36.78	31.90	0.92	0.94	0.99	1.15	2.9	-1.4
	V	442620	546853	568909	693889	23.03	28.45	29.60	36.11	29.30	0.79	0.97	1.01	1.23	-11.7	5.4
	I	438559	482326	521829	634442	21.00	23.09	24.98	30.37	24.86	0.84	0.93	1.00	1.22	-5.2	4.5
	L	390733	447505	474751	565271	21.39	24.49	25.98	30.94	25.70	0.83	0.95	1.01	1.20	-6.6	2.9
	F	344278	371835	396976	477338	22.62	24.43	26.08	31.37	26.13	0.87	0.94	1.00	1.20	-2.8	2.7
	mean concentration per fraction $\bar{c}_{j,k}$										0.89	0.94	1.00	1.17		
2	H	173643	234142	269606	326096	19.34	26.08	30.03	36.33	27.95	0.69	0.93	1.07	1.30	7.7	-8.3
	N	344979	429659	478056	536715	31.22	38.88	43.26	48.57	40.48	0.77	0.96	1.07	1.20	20.0	-15.4
	S	297362	379885	431805	484546	21.19	27.07	30.77	34.53	28.39	0.75	0.95	1.08	1.22	16.2	-14.2
	Q	276582	354620	395115	456990	24.02	30.80	34.32	39.69	32.21	0.75	0.96	1.07	1.23	16.1	-13.1
	D	253423	346537	415954	557602	22.83	31.22	37.48	50.24	35.44	0.64	0.88	1.06	1.42	0.3	0.0
	E	230767	322996	395515	543256	21.35	29.89	36.60	50.27	34.53	0.62	0.87	1.06	1.46	-3.7	2.7

	T	285932	386391	461744	600370	18.44	24.93	29.79	38.73	27.97	0.66	0.89	1.06	1.38	2.6	-2.3
	A	268712	360876	438305	542960	18.68	25.08	30.47	37.74	27.99	0.67	0.90	1.09	1.35	3.9	-4.9
	P	63488	92714	117230	174168	15.15	22.13	27.98	41.57	26.71	0.57	0.83	1.05	1.56	-11.7	9.8
	C	18765	26449	33121	45501	13.55	19.10	23.91	32.85	22.35	0.61	0.85	1.07	1.47	-5.7	3.7
	K	248476	332383	379532	458116	23.51	31.45	35.91	43.35	33.55	0.70	0.94	1.07	1.29	9.1	-8.9
	V	327178	472185	612570	870233	17.02	24.57	31.87	45.28	29.69	0.57	0.83	1.07	1.53	-10.7	7.6
	I	273433	403674	532452	881870	13.09	19.33	25.49	42.22	25.03	0.52	0.77	1.02	1.69	-18.6	19.0
	L	261361	380338	494177	771590	14.30	20.82	27.05	42.23	26.10	0.55	0.80	1.04	1.62	-14.7	14.1
	F	233426	336543	423390	634890	15.34	22.11	27.82	41.72	26.75	0.57	0.83	1.04	1.56	-10.7	10.0
	mean concentration per fraction $\bar{c}_{j,k}$										0.64	0.88	1.06	1.42		
3	H	155995	225111	245373	293789	17.38	25.08	27.33	32.73	25.63	0.68	0.98	1.07	1.28	11.8	-6.7
	N	324330	410737	435242	495953	29.35	37.17	39.39	44.88	37.70	0.78	0.99	1.04	1.19	28.4	-13.0
	S	283227	364140	405855	449923	20.18	25.95	28.92	32.06	26.78	0.75	0.97	1.08	1.20	24.3	-12.5
	Q	258978	338409	355964	417675	22.50	29.39	30.92	36.28	29.77	0.76	0.99	1.04	1.22	24.6	-11.0
	D	210859	338058	370607	483813	19.00	30.46	33.39	43.59	31.61	0.60	0.96	1.06	1.38	-0.9	0.8
	E	183648	317885	360272	470097	16.99	29.41	33.34	43.50	30.81	0.55	0.95	1.08	1.41	-9.0	3.1
	T	246518	377683	415470	526726	15.90	24.36	26.80	33.98	25.26	0.63	0.96	1.06	1.35	3.8	-1.7
	A	240848	351908	394736	482064	16.74	24.46	27.44	33.51	25.54	0.66	0.96	1.07	1.31	8.1	-4.1
	P	53026	92516	102989	147209	12.66	22.08	24.58	35.14	23.61	0.54	0.94	1.04	1.49	-11.6	8.7
	C	16681	26162	28500	39401	12.04	18.89	20.58	28.45	19.99	0.60	0.94	1.03	1.42	-0.6	4.0
	K	221656	318955	341834	410221	20.97	30.18	32.34	38.81	30.58	0.69	0.99	1.06	1.27	13.1	-7.3
	V	219269	549843	499216	680948	11.41	28.61	25.98	35.43	25.36	0.45	1.13	1.02	1.40	-25.8	2.1
	I	198314	405014	462682	709182	9.49	19.39	22.15	33.95	21.25	0.45	0.91	1.04	1.60	-26.3	16.7
	L	183861	393892	421281	617319	10.06	21.56	23.06	33.79	22.12	0.46	0.97	1.04	1.53	-24.9	11.6
	F	182147	333957	371674	530613	11.97	21.94	24.42	34.87	23.30	0.51	0.94	1.05	1.50	-15.3	9.3
	mean concentration per fraction $\bar{c}_{j,k}$										0.61	0.97	1.05	1.37		

Supplementary Table 42: Raw data Extended Data Fig. 4 – AA in water, 170 μm , 18 h, 100 mM NaCl, pH 7.4 – enrichments in top fraction

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)															
1	A	H	0.0	-0.1	-0.3	-0.7	4.0	4.8	2.9	2.0	6.8	6.0	1.9	18.8	10.6	12.2	7.8
		N	0.1	0.0	-0.2	-0.6	4.2	4.9	3.0	2.1	6.9	6.1	2.0	18.9	10.7	12.4	8.0
		S	0.3	0.2	0.0	-0.4	4.4	5.2	3.3	2.3	7.2	6.3	2.3	19.2	11.0	12.6	8.2
		Q	0.7	0.6	0.4	0.0	4.8	5.6	3.7	2.7	7.6	6.8	2.7	19.7	11.4	13.1	8.7
		D	-3.9	-4.0	-4.2	-4.6	0.0	0.7	-1.1	-2.0	2.6	1.9	-2.0	14.2	6.3	7.9	3.7
		E	-4.6	-4.7	-4.9	-5.3	-0.7	0.0	-1.8	-2.7	1.9	1.1	-2.8	13.3	5.5	7.1	2.9
		T	-2.8	-3.0	-3.2	-3.6	1.1	1.9	0.0	-0.9	3.8	3.0	-1.0	15.4	7.4	9.0	4.8
		A	-1.9	-2.0	-2.3	-2.6	2.1	2.8	0.9	0.0	4.8	3.9	0.0	16.5	8.5	10.1	5.8
		P	-6.4	-6.5	-6.7	-7.1	-2.6	-1.9	-3.6	-4.5	0.0	-0.8	-4.6	11.2	3.5	5.1	1.0
		C	-5.6	-5.7	-6.0	-6.3	-1.8	-1.1	-2.9	-3.8	0.8	0.0	-3.8	12.1	4.3	5.9	1.8
		K	-1.9	-2.0	-2.2	-2.6	2.1	2.8	1.0	0.0	4.8	4.0	0.0	16.6	8.5	10.1	5.8
		V	-15.8	-15.9	-16.1	-16.4	-12.4	-11.8	-13.4	-14.2	-10.1	-10.8	-14.2	0.0	-6.9	-5.5	-9.2
		I	-9.6	-9.7	-9.9	-10.2	-5.9	-5.2	-6.9	-7.8	-3.4	-4.2	-7.8	7.4	0.0	1.5	-2.5
		L	-10.9	-11.0	-11.2	-11.6	-7.3	-6.6	-8.3	-9.2	-4.8	-5.6	-9.2	5.9	-1.5	0.0	-3.9
	F	-7.3	-7.4	-7.6	-8.0	-3.5	-2.8	-4.6	-5.5	-1.0	-1.7	-5.5	10.2	2.5	4.1	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
2	A	H	0.0	-10.2	-7.3	-7.2	7.4	11.9	5.0	3.7	22.0	14.2	-1.2	20.7	32.4	26.3	20.7
		N	11.4	0.0	3.3	3.4	19.7	24.7	16.9	15.6	35.9	27.2	10.1	34.5	47.5	40.7	34.5
		S	7.8	-3.2	0.0	0.1	15.9	20.7	13.2	11.9	31.6	23.1	6.5	30.2	42.7	36.2	30.2
		Q	7.8	-3.3	-0.1	0.0	15.8	20.6	13.1	11.8	31.5	23.1	6.4	30.1	42.6	36.1	30.1
		D	-6.9	-16.5	-13.7	-13.6	0.0	4.2	-2.3	-3.5	13.5	6.3	-8.1	12.3	23.2	17.5	12.3
		E	-10.6	-19.8	-17.1	-17.1	-4.0	0.0	-6.2	-7.3	9.0	2.0	-11.7	7.8	18.3	12.8	7.9
		T	-4.7	-14.5	-11.7	-11.6	2.4	6.6	0.0	-1.2	16.2	8.8	-5.9	15.0	26.1	20.3	15.0
		A	-3.6	-13.5	-10.6	-10.5	3.6	7.9	1.2	0.0	17.6	10.1	-4.8	16.4	27.6	21.7	16.4
		P	-18.0	-26.4	-24.0	-23.9	-11.9	-8.3	-14.0	-15.0	0.0	-6.4	-19.0	-1.1	8.5	3.5	-1.1
		C	-12.4	-21.4	-18.8	-18.7	-5.9	-2.0	-8.1	-9.2	6.8	0.0	-13.5	5.7	15.9	10.6	5.7
		K	1.2	-9.1	-6.1	-6.1	8.8	13.3	6.3	5.0	23.5	15.6	0.0	22.2	34.0	27.8	22.2
		V	-17.2	-25.6	-23.2	-23.1	-11.0	-7.3	-13.0	-14.1	1.1	-5.4	-18.2	0.0	9.7	4.6	0.0
		I	-24.4	-32.2	-29.9	-29.9	-18.8	-15.4	-20.7	-21.6	-7.8	-13.7	-25.4	-8.8	0.0	-4.6	-8.8
		L	-20.8	-28.9	-26.6	-26.5	-14.9	-11.4	-16.9	-17.9	-3.4	-9.6	-21.8	-4.4	4.8	0.0	-4.4
	F	-17.2	-25.6	-23.2	-23.1	-11.0	-7.3	-13.0	-14.1	1.1	-5.4	-18.2	0.0	9.7	4.6	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
3	A	H	0.0	-12.9	-10.0	-10.3	12.8	22.9	7.7	3.4	26.5	12.5	-1.1	50.7	51.7	49.0	32.0
		N	14.8	0.0	3.3	3.0	29.5	41.2	23.7	18.8	45.3	29.2	13.5	73.0	74.2	71.1	51.6
		S	11.2	-3.2	0.0	-0.2	25.4	36.7	19.7	15.0	40.6	25.1	9.9	67.5	68.7	65.6	46.7
		Q	11.4	-3.0	0.2	0.0	25.7	37.0	20.0	15.3	41.0	25.4	10.2	67.9	69.1	66.1	47.1

	D	-11.4	-22.8	-20.3	-20.5	0.0	9.0	-4.5	-8.3	12.1	-0.2	-12.4	33.6	34.5	32.1	17.0
	E	-18.7	-29.2	-26.8	-27.0	-8.2	0.0	-12.4	-15.9	2.9	-8.5	-19.6	22.6	23.4	21.2	7.4
	T	-7.2	-19.1	-16.5	-16.7	4.7	14.1	0.0	-4.0	17.5	4.5	-8.2	39.9	40.9	38.4	22.6
	A	-3.3	-15.8	-13.0	-13.2	9.1	18.9	4.1	0.0	22.3	8.8	-4.4	45.7	46.7	44.1	27.6
	P	-21.0	-31.2	-28.9	-29.1	-10.8	-2.8	-14.9	-18.2	0.0	-11.0	-21.9	19.1	19.9	17.8	4.3
	C	-11.1	-22.6	-20.1	-20.3	0.2	9.2	-4.3	-8.1	12.4	0.0	-12.2	33.9	34.8	32.4	17.3
	K	1.2	-11.9	-9.0	-9.2	14.1	24.4	9.0	4.6	28.0	13.8	0.0	52.4	53.5	50.7	33.5
	V	-33.6	-42.2	-40.3	-40.4	-25.1	-18.4	-28.5	-31.4	-16.0	-25.3	-34.4	0.0	0.7	-1.1	-12.4
	I	-34.1	-42.6	-40.7	-40.9	-25.6	-19.0	-29.0	-31.8	-16.6	-25.8	-34.8	-0.7	0.0	-1.8	-13.0
	L	-32.9	-41.6	-39.6	-39.8	-24.3	-17.5	-27.7	-30.6	-15.1	-24.5	-33.7	1.1	1.8	0.0	-11.4
	F	-24.2	-34.0	-31.8	-32.0	-14.5	-6.9	-18.4	-21.6	-4.2	-14.7	-25.1	14.2	15.0	12.9	0.0
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F
		B														

Supplementary Table 43: Raw data Extended Data Fig. 4 – AA in water, 170 μm , 18 h, 100 mM NaCl, pH 7.4 – enrichments in bottom fraction

re pe at	sp eci es	Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)															
1	A	H	0.0	5.2	0.8	0.3	-2.7	-3.4	-2.3	-1.3	-4.4	-4.2	-1.3	-7.7	-6.9	-5.5	-5.2
		N	-4.9	0.0	-4.2	-4.7	-7.5	-8.2	-7.1	-6.2	-9.1	-9.0	-6.2	-12.2	-11.5	-10.1	-9.9
		S	-0.8	4.4	0.0	-0.5	-3.5	-4.2	-3.0	-2.1	-5.1	-5.0	-2.1	-8.4	-7.6	-6.2	-5.9
		Q	-0.3	4.9	0.5	0.0	-3.0	-3.7	-2.5	-1.6	-4.7	-4.5	-1.6	-7.9	-7.1	-5.7	-5.5
		D	2.8	8.2	3.6	3.1	0.0	-0.7	0.5	1.4	-1.7	-1.5	1.5	-5.1	-4.2	-2.8	-2.5
		E	3.6	8.9	4.4	3.9	0.7	0.0	1.2	2.2	-1.0	-0.8	2.2	-4.4	-3.5	-2.1	-1.8
		T	2.3	7.6	3.1	2.6	-0.5	-1.2	0.0	0.9	-2.2	-2.0	1.0	-5.5	-4.7	-3.3	-3.0
		A	1.4	6.6	2.1	1.7	-1.4	-2.1	-0.9	0.0	-3.1	-2.9	0.0	-6.4	-5.6	-4.2	-3.9
		P	4.6	10.0	5.4	4.9	1.7	1.0	2.2	3.2	0.0	0.2	3.2	-3.4	-2.6	-1.1	-0.8
		C	4.4	9.9	5.2	4.7	1.6	0.8	2.1	3.0	-0.2	0.0	3.0	-3.6	-2.7	-1.3	-1.0
		K	1.3	6.6	2.1	1.6	-1.4	-2.1	-0.9	0.0	-3.1	-3.0	0.0	-6.4	-5.6	-4.2	-3.9
		V	8.3	13.9	9.1	8.6	5.3	4.6	5.9	6.8	3.5	3.7	6.9	0.0	0.9	2.4	2.6
		I	7.4	12.9	8.2	7.7	4.4	3.7	4.9	5.9	2.6	2.8	5.9	-0.9	0.0	1.5	1.8
		L	5.8	11.3	6.6	6.1	2.9	2.2	3.4	4.4	1.1	1.3	4.4	-2.3	-1.5	0.0	0.3
	F	5.5	11.0	6.3	5.8	2.6	1.9	3.1	4.1	0.9	1.0	4.1	-2.6	-1.7	-0.3	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
2	A	H	0.0	8.3	6.9	5.5	-8.3	-10.7	-6.1	-3.6	-16.5	-11.6	0.6	-14.8	-22.9	-19.7	-16.7
		N	-7.7	0.0	-1.4	-2.6	-15.4	-17.6	-13.3	-11.0	-22.9	-18.4	-7.1	-21.3	-28.9	-25.9	-23.1
		S	-6.4	1.4	0.0	-1.3	-14.2	-16.5	-12.2	-9.8	-21.9	-17.2	-5.9	-20.3	-27.9	-24.8	-22.0
		Q	-5.2	2.7	1.3	0.0	-13.1	-15.4	-11.0	-8.6	-20.8	-16.2	-4.6	-19.2	-26.9	-23.8	-21.0
		D	9.0	18.1	16.5	15.0	0.0	-2.6	2.4	5.1	-8.9	-3.6	9.7	-7.1	-16.0	-12.4	-9.1
		E	12.0	21.4	19.7	18.1	2.7	0.0	5.2	8.0	-6.5	-0.9	12.7	-4.5	-13.7	-10.0	-6.7
		T	6.5	15.4	13.8	12.4	-2.3	-4.9	0.0	2.7	-11.0	-5.8	7.2	-9.2	-17.9	-14.4	-11.2
		A	3.7	12.4	10.9	9.4	-4.9	-7.4	-2.6	0.0	-13.4	-8.3	4.4	-11.6	-20.1	-16.7	-13.6
		P	19.7	29.7	28.0	26.3	9.8	6.9	12.4	15.4	0.0	5.9	20.5	2.0	-7.7	-3.8	-0.2
		C	13.1	22.5	20.8	19.3	3.7	0.9	6.1	9.0	-5.6	0.0	13.8	-3.6	-12.9	-9.2	-5.8
		K	-0.6	7.7	6.2	4.8	-8.9	-11.3	-6.7	-4.2	-17.0	-12.1	0.0	-15.3	-23.4	-20.2	-17.2
		V	17.3	27.1	25.4	23.8	7.6	4.8	10.2	13.1	-2.0	3.8	18.1	0.0	-9.6	-5.7	-2.2
		I	29.8	40.6	38.7	36.9	19.0	15.8	21.8	25.1	8.4	14.8	30.6	10.6	0.0	4.2	8.1
		L	24.5	34.9	33.0	31.3	14.2	11.1	16.9	20.0	4.0	10.1	25.3	6.1	-4.1	0.0	3.7
	F	20.0	30.0	28.2	26.6	10.0	7.1	12.6	15.7	0.2	6.1	20.7	2.3	-7.5	-3.6	0.0	
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F	
		B															
3	A	H	0.0	7.3	6.7	4.8	-7.4	-9.6	-5.1	-2.7	-14.2	-10.3	0.6	-8.6	-20.1	-16.4	-14.7
		N	-6.8	0.0	-0.6	-2.3	-13.7	-15.7	-11.5	-9.3	-20.0	-16.3	-6.2	-14.8	-25.5	-22.1	-20.4
		S	-6.2	0.6	0.0	-1.7	-13.2	-15.2	-11.0	-8.8	-19.5	-15.9	-5.7	-14.3	-25.1	-21.6	-20.0
		Q	-4.6	2.4	1.8	0.0	-11.6	-13.7	-9.4	-7.1	-18.1	-14.4	-4.0	-12.8	-23.7	-20.2	-18.6

	D	8.0	15.8	15.2	13.2	0.0	-2.3	2.5	5.1	-7.3	-3.1	8.6	-1.3	-13.7	-9.7	-7.8
	E	10.6	18.6	17.9	15.9	2.4	0.0	5.0	7.6	-5.1	-0.8	11.2	1.0	-11.7	-7.6	-5.7
	T	5.3	13.0	12.3	10.4	-2.5	-4.7	0.0	2.5	-9.6	-5.5	6.0	-3.7	-15.8	-12.0	-10.1
	A	2.8	10.2	9.6	7.7	-4.9	-7.1	-2.4	0.0	-11.8	-7.8	3.4	-6.1	-17.9	-14.1	-12.3
	P	16.5	25.0	24.3	22.1	7.9	5.4	10.6	13.4	0.0	4.6	17.2	6.5	-6.9	-2.6	-0.6
	C	11.4	19.5	18.9	16.8	3.2	0.8	5.8	8.5	-4.4	0.0	12.1	1.8	-10.9	-6.8	-4.9
	K	-0.6	6.6	6.0	4.2	-8.0	-10.1	-5.6	-3.3	-14.7	-10.8	0.0	-9.2	-20.6	-16.9	-15.2
	V	9.4	17.4	16.7	14.7	1.3	-1.0	3.9	6.5	-6.1	-1.8	10.1	0.0	-12.6	-8.5	-6.6
	I	25.1	34.2	33.5	31.1	15.9	13.2	18.8	21.8	7.4	12.3	25.9	14.4	0.0	4.6	6.8
	L	19.6	28.3	27.6	25.4	10.8	8.2	13.6	16.4	2.7	7.3	20.3	9.3	-4.4	0.0	2.1
	F	17.2	25.7	25.0	22.8	8.5	6.0	11.2	14.0	0.6	5.1	17.9	7.1	-6.4	-2.0	0.0
		H	N	S	Q	D	E	T	A	P	C	K	V	I	L	F
		B														

Supplementary Table 44: Raw data Extended Data Fig. 5b – nucleobases in 10 % formamide, 170µm, 18h

rep	eat	species	measured values (µAU*min)				concentration (µM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (µM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} /c̄ _{j,k} – 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} – 1 (%)											
			top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)					bot part (red shade)						
1	C		120.45	545.29	504.07	1746.04	2.65	11.99	11.08	38.39	16.03	0.17	0.75	0.69	2.4	-23.42	23.7	C	0	-25.49	-38.97	-27.87	-13.97	C	0	33.41	49.42	39.49	10.34
	A		496.26	2364.1	2072.88	4017.41	4.37	20.81	18.24	35.36	19.69	0.22	1.06	0.93	1.8	2.78	-7.28	A	34.22	0	-18.08	-3.19	15.46	A	-25.04	0	12	4.56	-17.3
	G		228.53	954.64	840.15	1353.19	10.59	44.23	38.92	62.69	39.11	0.27	1.13	1	1.6	25.47	-17.21	G	63.84	22.07	0	18.18	40.95	G	-33.07	-10.71	0	-6.64	-26.15
	U		299.94	1412.76	1276.39	2248.26	4.15	19.57	17.68	31.14	18.14	0.23	1.08	0.97	1.72	6.16	-11.32	U	38.64	3.29	-15.39	0	19.26	U	-28.31	-4.36	7.11	0	-20.9
	T		242.59	1076.72	990.92	2741.81	3.81	16.91	15.56	43.06	19.84	0.19	0.85	0.78	2.17	-10.99	12.11	T	16.24	-13.39	-29.05	-16.15	0	T	-9.37	20.91	35.42	26.43	0
	mean concentration per fraction c̄ _{j,k}											0.22	0.97	0.87	1.94				C	A	G	U	T		C	A	G	U	T
2	C		128.75	293.36	496.25	1789.68	2.83	6.45	10.91	39.35	14.88	0.19	0.43	0.73	2.64	-36.9	19.3	C	0	-44.61	-51.66	-44.09	-20.73	C	0	26.84	39.03	30.08	9.33
	A		801.53	1542.57	2128.69	4865.74	7.05	13.58	18.73	42.82	20.55	0.34	0.66	0.91	2.08	13.91	-5.94	A	80.53	0	-12.74	0.93	43.1	A	-21.16	0	9.61	2.55	-13.8
	G		359.24	683.84	873.09	1736.06	16.64	31.68	40.45	80.43	42.3	0.39	0.75	0.96	1.9	30.54	-14.19	G	106.8 9	14.6	0	15.67	63.99	G	-28.07	-8.77	0	-6.44	-21.36
	U		472.73	945.11	1316.87	2824.35	6.55	13.09	18.24	39.12	19.25	0.34	0.68	0.95	2.03	12.85	-8.29	U	78.86	-0.92	-13.55	0	41.78	U	-23.12	-2.49	6.88	0	-15.95
	T		298.07	649.75	1017.76	3004	4.68	10.2	15.98	47.18	19.51	0.24	0.52	0.82	2.42	-20.4	9.12	T	26.16	-30.12	-39.02	-29.47	0	T	-8.53	16.01	27.17	18.98	0
	mean concentration per fraction c̄ _{j,k}											0.3	0.61	0.87	2.22				C	A	G	U	T		C	A	G	U	T
3	C		138.48	209.22	425.07	2262.85	3.04	4.6	9.35	49.75	16.68	0.18	0.28	0.56	2.98	-28.46	9.32	C	0	-31.85	-43.7	-34.93	-17.24	C	0	11.39	18.4	13.45	5.28
	A		627.19	814.02	1658.42	6270.06	5.52	7.16	14.6	55.18	20.62	0.27	0.35	0.71	2.68	4.98	-1.86	A	46.74	0	-17.39	-4.52	21.44	A	-10.23	0	6.29	1.84	-5.49
	G		273.61	338.08	639.11	2125.81	12.68	15.66	29.61	98.49	39.11	0.32	0.4	0.76	2.52	27.08	-7.67	G	77.63	21.05	0	15.58	47.01	G	-15.54	-5.92	0	-4.19	-11.08
	U		385.13	495.26	1003.47	3609.56	5.33	6.86	13.9	50	19.02	0.28	0.36	0.73	2.63	9.95	-3.64	U	53.69	4.74	-13.48	0	27.19	U	-11.85	-1.81	4.37	0	-7.2
	T		291.5	451.55	800.99	3744.4	4.58	7.09	12.58	58.81	20.76	0.22	0.34	0.61	2.83	-13.55	3.84	T	20.83	-17.65	-31.98	-21.38	0	T	-5.02	5.81	12.46	7.76	0
	mean concentration per fraction c̄ _{j,k}											0.26	0.35	0.67	2.73				C	A	G	U	T		C	A	G	U	T

Supplementary Table 45: Raw data Extended Data Fig. 5c – nucleobases in 100 mM phosphate buffer, 170μm, 18h

rep eat k	spe cies	measured values (μAU*s)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)					bot part (red shade)						
1	C	13614	28278	59087	168060	4.99	10.36	21.65	61.58	24.65	0.2	0.42	0.88	2.5	-46.09	23.89	C	0	-62.42	-55.78	-54.77	-12.4	C	0	49.8	42.67	38.45	5.83
	A	97457	135393	189061	301763	14.3	19.86	27.73	44.26	26.54	0.54	0.75	1.05	1.67	43.46	-17.3	A	166.1 3	0	17.68	20.37	133.1 4	A	-33.25	0	-4.76	-7.58	-29.36
	G	24668	33469	63044	94385	19.05	25.84	48.68	72.88	41.61	0.46	0.62	1.17	1.75	21.91	-13.16	G	126.1 4	-15.03	0	2.28	98.11	G	-29.91	5	0	-2.96	-25.82
	U	49084	75640	116042	197946	11.33	17.46	26.79	45.7	25.32	0.45	0.69	1.06	1.8	19.19	-10.51	U	121.1	-16.92	-2.23	0	93.69	U	-27.77	8.2	3.05	0	-23.56
	T	26945	54564	109621	275339	7.05	14.28	28.69	72.07	30.53	0.23	0.47	0.94	2.36	-38.46	17.07	T	14.15	-57.11	-49.52	-48.37	0	T	-5.51	41.55	34.81	30.82	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.38	0.59	1.02	2.02				C	A	G	U	T		C	A	G	U	T
2	C	29329	44746	68171	181643	10.75	16.4	24.98	66.56	29.67	0.36	0.55	0.84	2.24	-28.63	23.39	C	0	-47.1	-26.32	-41.53	-4.57	C	0	47.98	44.86	37.55	4.26
	A	138311	165949	197499	306220	20.29	24.34	28.97	44.92	29.63	0.68	0.82	0.98	1.52	34.92	-16.62	A	89.04	0	39.29	10.53	80.41	A	-32.42	0	-2.11	-7.05	-29.54
	G	22565	38363	51600	71086	17.42	29.62	39.84	54.89	35.44	0.49	0.84	1.12	1.55	-3.14	-14.82	G	35.72	-28.21	0	-20.65	29.52	G	-30.97	2.15	0	-5.05	-28.03
	U	77666	97502	121836	204462	17.93	22.51	28.13	47.2	28.94	0.62	0.78	0.97	1.63	22.07	-10.29	U	71.04	-9.52	26.03	0	63.23	U	-27.3	7.58	5.32	0	-24.2
	T	53556	82398	124868	303603	14.02	21.57	32.68	79.47	36.94	0.38	0.58	0.88	2.15	-25.22	18.34	T	4.79	-44.57	-22.79	-38.73	0	T	-4.09	41.93	38.94	31.93	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.51	0.71	0.96	1.82				C	A	G	U	T		C	A	G	U	T
3	C	15404	53622	63211	116411	5.64	19.65	23.16	42.66	22.78	0.25	0.86	1.02	1.87	-24.86	18.4	C	0	-39.49	-30.71	-35.2	-1.57	C	0	30.17	49.04	26.38	0.74
	A	69959	187931	179696	245780	10.26	27.57	26.36	36.05	25.06	0.41	1.1	1.05	1.44	24.16	-9.05	A	65.25	0	14.51	7.09	62.66	A	-23.18	0	14.49	-2.91	-22.61
	G	13322	45215	43666	46809	10.29	34.91	33.72	36.14	28.77	0.36	1.21	1.17	1.26	8.43	-20.56	G	44.31	-12.67	0	-6.48	42.05	G	-32.9	-12.66	0	-15.2	-32.41
	U	39694	111196	110506	153819	9.16	25.67	25.51	35.51	23.96	0.38	1.07	1.06	1.48	15.94	-6.32	U	54.31	-6.62	6.93	0	51.9	U	-20.87	3	17.93	0	-20.29
	T	27598	94565	112548	203790	7.22	24.75	29.46	53.34	28.69	0.25	0.86	1.03	1.86	-23.67	17.53	T	1.59	-38.52	-29.6	-34.17	0	T	-0.73	29.22	47.95	25.45	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.33	1.02	1.07	1.58				C	A	G	U	T		C	A	G	U	T

Supplementary Table 46: Raw data Extended Data Fig. 5d – nucleobases in 10 % methanol, 170μm, 18h

rep eat k	spe cies	measured values (μAU*s)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)						bot part (red shade)					
1	C	78158	85191	52270	84753	28.64	31.22	19.15	31.06	27.52	1.04	1.13	0.7	1.13	-1.72	0.17	C	0	-3.21	-2.58	-2.97	0.27	C	0	0.2	-0.13	1.58	-0.79
	A	158450	165766	99234	165978	23.24	24.32	14.56	24.35	21.62	1.08	1.12	0.67	1.13	1.53	-0.03	A	3.31	0	0.65	0.24	3.59	A	-0.2	0	-0.33	1.38	-0.99
	G	53827	56935	33830	56937	41.56	43.96	26.12	43.96	38.9	1.07	1.13	0.67	1.13	0.88	0.3	G	2.65	-0.64	0	-0.4	2.92	G	0.13	0.33	0	1.71	-0.66
	U	97095	102497	61898	100565	22.42	23.66	14.29	23.22	20.9	1.07	1.13	0.68	1.11	1.29	-1.39	U	3.06	-0.24	0.41	0	3.34	U	-1.56	-1.36	-1.69	0	-2.34
	T	86237	93612	57943	94509	22.57	24.5	15.17	24.74	21.75	1.04	1.13	0.7	1.14	-1.98	0.97	T	-0.26	-3.46	-2.84	-3.23	0	T	0.8	1	0.67	2.39	0
	mean concentration per fraction $\bar{c}_{j,k}$										1.06	1.13	0.68	1.13				C	A	G	U	T		C	A	G	U	T
2	C	77435	79594	81073	90067	28.37	29.16	29.71	33	30.06	0.94	0.97	0.99	1.1	-2.69	3.82	C	0	-4.65	-4.85	-3.23	-0.52	C	0	6.93	6.77	5.06	0.77
	A	157713	159110	156923	163580	23.13	23.34	23.02	23.99	23.37	0.99	1	0.98	1.03	2.05	-2.91	A	4.87	0	-0.22	1.48	4.33	A	-6.48	0	-0.15	-1.75	-5.76
	G	50435	50729	49930	52275	38.94	39.17	38.55	40.36	39.26	0.99	1	0.98	1.03	2.27	-2.76	G	5.1	0.22	0	1.7	4.56	G	-6.34	0.15	0	-1.6	-5.62
	U	95589	97173	96838	102402	22.07	22.43	22.36	23.64	22.62	0.98	0.99	0.99	1.04	0.56	-1.18	U	3.34	-1.46	-1.67	0	2.81	U	-4.82	1.78	1.63	0	-4.08
	T	86426	88920	89788	99238	22.62	23.28	23.5	25.98	23.84	0.95	0.98	0.99	1.09	-2.19	3.03	T	0.52	-4.15	-4.36	-2.73	0	T	-0.77	6.11	5.96	4.26	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.97	0.99	0.99	1.06				C	A	G	U	T		C	A	G	U	T
3	C	69906	72633	74690	85031	25.61	26.61	27.37	31.16	27.69	0.93	0.96	0.99	1.13	-2.03	2.47	C	0	-3.91	-2.67	-2.87	-0.59	C	0	4.54	4.21	3.32	0.45
	A	143021	144255	147053	159901	20.98	21.16	21.57	23.46	21.79	0.96	0.97	0.99	1.08	1.95	-1.98	A	4.07	0	1.29	1.08	3.45	A	-4.35	0	-0.32	-1.17	-3.91
	G	47778	48833	50180	54277	36.89	37.71	38.75	41.91	38.81	0.95	0.97	1	1.08	0.66	-1.67	G	2.74	-1.27	0	-0.2	2.13	G	-4.04	0.32	0	-0.86	-3.61
	U	87054	88633	90374	99551	20.1	20.46	20.86	22.98	21.1	0.95	0.97	0.99	1.09	0.86	-0.82	U	2.95	-1.07	0.2	0	2.34	U	-3.21	1.19	0.87	0	-2.77
	T	78244	80635	83241	94181	20.48	21.11	21.79	24.65	22.01	0.93	0.96	0.99	1.12	-1.44	2.01	T	0.6	-3.33	-2.09	-2.29	0	T	-0.45	4.07	3.74	2.85	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.94	0.97	0.99	1.1				C	A	G	U	T		C	A	G	U	T
4	C	69193	78890	73921	84430	25.35	28.91	27.09	30.94	28.07	0.9	1.03	0.96	1.1	-1.59	1.06	C	0	-1.85	-4.84	-0.58	-0.53	C	0	0.83	4.23	0.33	0.05
	A	137681	155601	141664	163529	20.2	22.82	20.78	23.99	21.95	0.92	1.04	0.95	1.09	0.26	0.23	A	1.88	0	-3.05	1.29	1.34	A	-0.83	0	3.36	-0.5	-0.78
	G	44412	49469	43806	49477	34.29	38.2	33.83	38.2	36.13	0.95	1.06	0.94	1.06	3.41	-3.04	G	5.09	3.15	0	4.48	4.53	G	-4.06	-3.25	0	-3.74	-4.01
	U	83668	95093	88454	101166	19.32	21.95	20.42	23.36	21.26	0.91	1.03	0.96	1.1	-1.02	0.73	U	0.59	-1.27	-4.28	0	0.05	U	-0.33	0.51	3.89	0	-0.28

	T	77238	87689	81616	93704	20.22	22.95	21.36	24.53	22.27	0.91	1.03	0.96	1.1	-1.07	1.02	T	0.53	-1.32	-4.33	-0.05	0	T	-0.05	0.79	4.18	0.28	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.92	1.04	0.95	1.09				C	A	G	U	T		C	A	G	U	T
5	C	73499	77980	79620	101506	26.93	28.57	29.17	37.19	30.47	0.88	0.94	0.96	1.22	-3.1	4.42	C	0	-4.92	-5.93	-3.19	-1.22	C	0	7.61	9.74	3.98	1.41
	A	150313	157392	155633	183417	22.05	23.09	22.83	26.9	23.72	0.93	0.97	0.96	1.13	1.91	-2.97	A	5.17	0	-1.06	1.82	3.89	A	-7.07	0	1.97	-3.37	-5.76
	G	60032	62602	61853	71072	46.35	48.34	47.76	54.88	49.33	0.94	0.98	0.97	1.11	3	-4.85	G	6.3	1.07	0	2.91	5	G	-8.87	-1.94	0	-5.25	-7.59
	U	91144	95514	95440	117192	21.04	22.05	22.03	27.06	23.05	0.91	0.96	0.96	1.17	0.09	0.42	U	3.3	-1.78	-2.83	0	2.04	U	-3.83	3.49	5.54	0	-2.47
	T	81971	86748	87427	110267	21.46	22.71	22.88	28.86	23.98	0.89	0.95	0.95	1.2	-1.9	2.97	T	1.24	-3.74	-4.76	-1.99	0	T	-1.39	6.11	8.21	2.53	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.91	0.96	0.96	1.17				C	A	G	U	T		C	A	G	U	T
6	C	61043	69797	80709	79576	22.37	25.57	29.57	29.16	26.67	0.84	0.96	1.11	1.09	-1.05	2.6	C	0	-1.73	-2.05	-0.63	-0.82	C	0	4.71	5.2	2.23	1.06
	A	122004	139951	160588	149274	17.9	20.53	23.56	21.9	20.97	0.85	0.98	1.12	1.04	0.69	-2.01	A	1.76	0	-0.33	1.11	0.92	A	-4.5	0	0.47	-2.37	-3.49
	G	38231	44079	49886	46405	29.52	34.04	38.52	35.83	34.48	0.86	0.99	1.12	1.04	1.01	-2.47	G	2.09	0.33	0	1.44	1.25	G	-4.94	-0.47	0	-2.83	-3.94
	U	74254	85319	98221	94090	17.14	19.7	22.68	21.72	20.31	0.84	0.97	1.12	1.07	-0.42	0.36	U	0.64	-1.1	-1.42	0	-0.19	U	-2.18	2.43	2.91	0	-1.14
	T	68337	77934	89529	87427	17.89	20.4	23.43	22.88	21.15	0.85	0.96	1.11	1.08	-0.23	1.53	T	0.83	-0.91	-1.23	0.19	0	T	-1.05	3.61	4.1	1.16	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.85	0.97	1.11	1.07				C	A	G	U	T		C	A	G	U	T

Supplementary Table 47: Raw data Extended Data Fig. 5e – nucleobases in water, 127 μ m, 18h

rep eat k	spe cies	measured values (μAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)						bot part (red shade)					
1	C	1212.92	1308.97	1890.54	2132.85	26.67	28.78	41.56	46.89	35.97	0.74	0.8	1.16	1.3	-11.76	8.89	C	0	-18.55	-21.06	-14.65	-0.04	C	0	16.33	17.78	12.84	0.33
	A	5811.7	5625	6953.27	7155.56	51.15	49.51	61.2	62.98	56.21	0.91	0.88	1.09	1.12	8.33	-6.39	A	22.77	0	-3.09	4.78	22.71	A	-14.04	0	1.25	-3	-13.76
	G	1003.53	961.55	1127.11	1182.7	46.49	44.55	52.22	54.79	49.51	0.94	0.9	1.05	1.11	11.78	-7.55	G	26.68	3.19	0	8.11	26.62	G	-15.1	-1.23	0	-4.2	-14.82
	U	1742.74	1731.05	2234.5	2317.84	24.14	23.98	30.95	32.11	27.79	0.87	0.86	1.11	1.16	3.39	-3.49	U	17.17	-4.56	-7.5	0	17.12	U	-11.38	3.1	4.38	0	-11.09
	T	1445.54	1571.36	2247.75	2532.51	22.7	24.68	35.3	39.77	30.61	0.74	0.81	1.15	1.3	-11.73	8.54	T	0.04	-18.51	-21.03	-14.62	0	T	-0.33	15.95	17.4	12.47	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.84	0.85	1.11	1.2				C	A	G	U	T		C	A	G	U	T
2	C	1159.97	1488.63	1774.75	2341.46	25.5	32.73	39.02	51.48	37.18	0.69	0.88	1.05	1.38	-13.48	10.88	C	0	-19.74	-24.86	-15.85	-1.38	C	0	19.69	24.26	14.16	0.7
	A	5558.72	6240.86	6695.57	7524.83	48.92	54.93	58.93	66.23	57.25	0.85	0.96	1.03	1.16	7.79	-7.36	A	24.59	0	-6.38	4.84	22.87	A	-16.45	0	3.82	-4.62	-15.86
	G	903.78	943.6	1009.92	1103.23	41.87	43.72	46.79	51.11	45.87	0.91	0.95	1.02	1.11	15.14	-10.76	G	33.08	6.82	0	11.99	31.25	G	-19.52	-3.68	0	-8.13	-18.96
	U	1685.02	1942.51	2134.34	2507.16	23.34	26.91	29.56	34.73	28.63	0.82	0.94	1.03	1.21	2.82	-2.87	U	18.84	-4.61	-10.7	0	17.2	U	-12.4	4.84	8.85	0	-11.79
	T	1402.12	1775.26	2115.04	2771.75	22.02	27.88	33.22	43.53	31.66	0.7	0.88	1.05	1.37	-12.27	10.11	T	1.4	-18.61	-23.81	-14.68	0	T	-0.7	18.85	23.39	13.36	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.79	0.92	1.04	1.25				C	A	G	U	T		C	A	G	U	T
3	C	1081.12	1433.7	1719.97	2077.44	23.77	31.52	37.81	45.67	34.69	0.69	0.91	1.09	1.32	-12.33	7.91	C	0	-21.64	-15.89	-16.99	-3.23	C	0	16.89	10.64	11.86	2.02
	A	5441.03	5936.8	6506.52	7008.68	47.89	52.25	57.26	61.68	54.77	0.87	0.95	1.05	1.13	11.88	-7.68	A	27.62	0	7.34	5.94	23.5	A	-14.45	0	-5.35	-4.3	-12.73
	G	1293.6	1501	1668.19	1889.65	59.93	69.54	77.29	87.55	73.58	0.81	0.95	1.05	1.19	4.24	-2.47	G	18.9	-6.83	0	-1.3	15.06	G	-9.62	5.65	0	1.11	-7.79
	U	1635.63	1856.95	2102.43	2332.26	22.66	25.72	29.12	32.31	27.45	0.83	0.94	1.06	1.18	5.61	-3.54	U	20.47	-5.6	1.32	0	16.58	U	-10.61	4.49	-1.1	0	-8.8
	T	1349.53	1747.03	2068.44	2459.84	21.19	27.44	32.49	38.63	29.94	0.71	0.92	1.09	1.29	-9.4	5.78	T	3.34	-19.03	-13.09	-14.22	0	T	-1.98	14.58	8.45	9.65	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.78	0.93	1.07	1.22				C	A	G	U	T		C	A	G	U	T

Supplementary Table 48: Raw data Extended Data Fig. 5f – nucleobases in water, 150 μ m, 18h

rep eat k	spe cies	measured values (μAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)						bot part (red shade)					
1	C	859.86	1159.13	1832.82	2756.22	18.9	25.48	40.29	60.6	36.32	0.52	0.7	1.11	1.67	-19.85	14.63	C	0	-29.6	-32.66	-23.21	-2.95	C	0	30.1	28	21.96	0.79
	A	4489.45	5223.05	6789.36	7787.47	39.51	45.97	59.75	68.54	53.44	0.74	0.86	1.12	1.28	13.85	-11.89	A	42.04	0	-4.35	9.08	37.85	A	-23.13	0	-1.61	-6.25	-22.52
	G	760.04	793.91	1097.56	1281.62	35.21	36.78	50.85	59.38	45.55	0.77	0.81	1.12	1.3	19.03	-10.45	G	48.51	4.55	0	14.04	44.12	G	-21.88	1.63	0	-4.72	-21.26
	U	1315.88	1605.43	2188.41	2655.78	18.23	22.24	30.31	36.79	26.89	0.68	0.83	1.13	1.37	4.38	-6.01	U	30.22	-8.32	-12.31	0	26.38	U	-18.01	6.67	4.95	0	-17.36
	T	1045.6	1371.79	2153.59	3227.01	16.42	21.54	33.82	50.68	30.62	0.54	0.7	1.1	1.66	-17.41	13.73	T	3.04	-27.46	-30.61	-20.87	0	T	-0.79	29.07	27	21	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.65	0.78	1.12	1.46				C	A	G	U	T		C	A	G	U	T
2	C	876.27	1631.06	1701.66	2485.39	19.26	35.86	37.41	54.64	36.79	0.52	0.97	1.02	1.49	-21.95	10.88	C	0	-33.68	-34.13	-26.92	-1.21	C	0	21	20.37	15.06	1.72
	A	4971.9	6558.56	5932.42	7729.57	43.76	57.72	52.21	68.03	55.43	0.79	1.04	0.94	1.23	17.67	-8.37	A	50.77	0	-0.68	10.18	48.94	A	-17.36	0	-0.53	-4.91	-15.94
	G	798.78	1044.11	937.02	1239.9	37.01	48.37	43.41	57.44	46.56	0.79	1.04	0.93	1.23	18.48	-7.88	G	51.81	0.69	0	10.93	49.96	G	-16.92	0.53	0	-4.41	-15.5
	U	1427.28	2041.44	1928.25	2571.13	19.77	28.28	26.71	35.61	27.59	0.72	1.02	0.97	1.29	6.8	-3.63	U	36.84	-9.24	-9.86	0	35.18	U	-13.09	5.17	4.61	0	-11.6
	T	1044.13	1941.59	2017.97	2876.19	16.4	30.49	31.69	45.17	30.94	0.53	0.99	1.02	1.46	-21	9.01	T	1.23	-32.86	-33.32	-26.03	0	T	-1.69	18.96	18.34	13.12	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.67	1.01	0.98	1.34				C	A	G	U	T		C	A	G	U	T
3	C	829.95	1023.2	1581.15	3367.89	18.25	22.5	34.76	74.04	37.39	0.49	0.6	0.93	1.98	-24.26	17.36	C	0	-36.97	-36.6	-30.5	0.08	C	0	38.8	32.97	27.56	-0.38
	A	4895.84	4862.88	6512.05	9022.54	43.09	42.8	57.31	79.41	55.65	0.77	0.77	1.03	1.43	20.15	-15.44	A	58.64	0	0.57	10.25	58.77	A	-27.95	0	-4.2	-8.1	-28.23
	G	781.25	746.22	1020.3	1511.52	36.19	34.57	47.27	70.03	47.02	0.77	0.74	1.01	1.49	19.46	-11.73	G	57.74	-0.57	0	9.62	57.87	G	-24.79	4.39	0	-4.07	-25.08
	U	1417.25	1471.14	2050.95	3133.35	19.63	20.38	28.41	43.4	27.96	0.7	0.73	1.02	1.55	8.98	-7.99	U	43.89	-9.3	-8.78	0	44.01	U	-21.61	8.81	4.24	0	-21.9
	T	985.2	1213.99	1865.71	4016.37	15.47	19.07	29.3	63.08	31.73	0.49	0.6	0.92	1.99	-24.33	17.81	T	-0.08	-37.02	-36.66	-30.56	0	T	0.38	39.33	33.47	28.05	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.64	0.69	0.98	1.69				C	A	G	U	T		C	A	G	U	T

Supplementary Table 49: Raw data Extended Data Fig. 5g – nucleobases in water, 200 μ m, 18h

rep eat k	spe cies	measured values (μAU*s)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)					bot part (red shade)						
1	C	29851	75725	140710	169921	10.94	27.75	51.56	62.26	38.13	0.29	0.73	1.35	1.63	-41.11	15.4	C	0	-55.78	-57.91	-45.81	-0.78	C	0	30.78	35.27	20.12	0.36
	A	267376	401379	465079	514578	39.22	58.88	68.22	75.48	60.45	0.65	0.97	1.13	1.25	33.18	-11.76	A	126.16	0	-4.81	22.56	124.39	A	-23.54	0	3.43	-8.16	-23.26
	G	52943	78178	85801	93774	40.88	60.37	66.25	72.41	59.98	0.68	1.01	1.1	1.21	39.91	-14.69	G	137.59	5.05	0	28.76	135.73	G	-26.07	-3.31	0	-11.2	-25.8
	U	67876	118021	152663	174324	15.67	27.25	35.24	40.24	29.6	0.53	0.92	1.19	1.36	8.66	-3.93	U	84.52	-18.41	-22.34	0	83.08	U	-16.75	8.88	12.61	0	-16.45
	T	35609	90747	165867	200390	9.32	23.75	43.42	52.45	32.24	0.29	0.74	1.35	1.63	-40.65	14.98	T	0.79	-55.43	-57.58	-45.38	0	T	-0.36	30.31	34.78	19.68	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.49	0.87	1.22	1.42				C	A	G	U	T		C	A	G	U	T
2	C	49227	104983	131775	151478	18.04	38.47	48.28	55.5	40.07	0.45	0.96	1.2	1.39	-20.81	8.29	C	0	-30.08	-36.39	-21.82	-3.15	C	0	15.3	17.31	9.54	1.59
	A	270630	433283	472666	505007	39.7	63.56	69.33	74.08	61.67	0.64	1.03	1.12	1.2	13.26	-6.08	A	43.02	0	-9.02	11.82	38.52	A	-13.27	0	1.75	-5	-11.89
	G	58792	85466	89999	98099	45.4	65.99	69.49	75.75	64.16	0.71	1.03	1.08	1.18	24.49	-7.69	G	57.2	9.92	0	22.9	52.25	G	-14.76	-1.72	0	-6.63	-13.41
	U	75938	132344	152537	166781	17.53	30.55	35.21	38.5	30.45	0.58	1	1.16	1.26	1.29	-1.14	U	27.91	-10.57	-18.63	0	23.88	U	-8.71	5.26	7.1	0	-7.26
	T	60442	127301	155157	177320	15.82	33.32	40.61	46.41	34.04	0.46	0.98	1.19	1.36	-18.23	6.6	T	3.25	-27.81	-34.32	-19.28	0	T	-1.56	13.5	15.48	7.83	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.57	1	1.15	1.28				C	A	G	U	T		C	A	G	U	T
3	C	34563	61232	112870	181906	12.66	22.44	41.36	66.65	35.78	0.35	0.63	1.16	1.86	-36.78	27.57	C	0	-53.05	-50.41	-42.69	-1.79	C	0	67.3	58.49	41.1	1.83
	A	308651	398003	475136	455906	45.27	58.38	69.7	66.87	60.06	0.75	0.97	1.16	1.11	34.64	-23.75	A	112.97	0	5.62	22.06	109.15	A	-40.23	0	-5.27	-15.66	-39.13
	G	52211	69672	84736	85988	40.32	53.8	65.43	66.4	56.48	0.71	0.95	1.16	1.18	27.47	-19.51	G	101.63	-5.32	0	15.56	98.02	G	-36.9	5.56	0	-10.97	-35.75
	U	78052	109834	150754	166861	18.02	25.36	34.8	38.52	29.18	0.62	0.87	1.19	1.32	10.3	-9.59	U	74.48	-18.07	-13.47	0	71.35	U	-29.13	18.57	12.33	0	-27.83
	T	42282	76418	135915	214615	11.07	20	35.58	56.18	30.71	0.36	0.65	1.16	1.83	-35.63	25.28	T	1.83	-52.19	-49.5	-41.64	0	T	-1.8	64.3	55.64	38.56	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.56	0.81	1.17	1.46				C	A	G	U	T		C	A	G	U	T

Supplementary Table 50: Raw data Extended Data Fig. 5h – nucleobases in water, 170 μm , 18h, pH 3

Due to technical problems, for the third replicate the temperature gradient was not applied for the entire duration of the experiment, which is why we do not take it into account for the calculation of the heat flow-driven enrichment.

rep	eat	k	spe	cies	measured values ($\mu\text{AU}\cdot\text{min}$)				concentration (μM) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 3				c_0 (μM)	Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)		Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)											
					top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)					bot part (red shade)						
1	C				846.79	1460.52	1607.47	1397.6	18.62	32.11	35.34	30.73	29.2	0.64	1.1	1.21	1.05	2.23	-15.42	C	0	-6.52	-14.19	2.29	47.43	C	0	-2.5	1.08	-23.25	-37.26
	A				1951.56	3032.08	3373.53	3088.2	17.18	26.69	29.69	27.18	25.18	0.68	1.06	1.18	1.08	9.36	-13.26	A	6.97	0	-8.21	9.42	57.71	A	2.56	0	3.67	-21.29	-35.65
	G				581.85	823.23	912.01	815.28	26.96	38.14	42.25	37.77	36.28	0.74	1.05	1.16	1.04	19.13	-16.33	G	16.53	8.94	0	19.2	71.81	G	-1.07	-3.54	0	-24.07	-37.93
	U				1317.27	1958.65	2279.63	2897.69	18.25	27.13	31.58	40.14	29.27	0.62	0.93	1.08	1.37	-0.06	10.2	U	-2.24	-8.61	-16.11	0	44.13	U	30.3	27.04	31.7	0	-18.25
	T				814.79	1594.84	1966.43	3160.18	12.8	25.05	30.88	49.63	29.59	0.43	0.85	1.04	1.68	-30.66	34.81	T	-32.17	-36.59	-41.8	-30.62	0	T	59.39	55.41	61.11	22.33	0
	mean concentration per fraction $\bar{c}_{j,k}$													0.62	1	1.14	1.24				C	A	G	U	T		C	A	G	U	T
2	C				850.39	1203.32	1433.84	1605.78	18.7	26.46	31.52	35.3	27.99	0.67	0.95	1.13	1.26	-1.37	-12.35	C	0	-8.86	-19.17	-3.74	43.62	C	0	-4.1	6.02	-15.08	-35.11
	A				2200.16	2711.59	3149.67	3948.02	19.36	23.87	27.72	34.75	26.42	0.73	0.9	1.05	1.31	8.22	-8.61	A	9.73	0	-11.3	5.62	57.59	A	4.27	0	10.55	-11.45	-32.34
	G				794.03	890.45	1016.65	1143.17	36.79	41.25	47.1	52.96	44.53	0.83	0.93	1.06	1.19	22.01	-17.33	G	23.71	12.74	0	19.08	77.67	G	-5.68	-9.54	0	-19.9	-38.8
	U				1354.97	1662.51	1894.14	2900.26	18.77	23.03	26.24	40.17	27.05	0.69	0.85	0.97	1.49	2.46	3.21	U	3.89	-5.32	-16.02	0	49.2	U	17.76	12.93	24.85	0	-23.59
	T				771.97	1117.49	1524.61	3226.26	12.12	17.55	23.94	50.67	26.07	0.47	0.67	0.92	1.94	-31.33	35.07	T	-30.37	-36.54	-43.72	-32.97	0	T	54.11	47.79	63.39	30.87	0
	mean concentration per fraction $\bar{c}_{j,k}$													0.68	0.86	1.02	1.44				C	A	G	U	T		C	A	G	U	T

Supplementary Table 51: Raw data Extended Data Fig. 5i – nucleobases in water, 170 μm , 18h, pH 4

Due to technical problems, for the third replicate the temperature gradient was not applied for the entire duration of the experiment, which is why we do not take it into account for the calculation of the heat flow-driven enrichment.

rep eat k	spe cies	measured values ($\mu\text{AU}\cdot\text{s}$)				concentration (μM) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 3				c_0 (μM)	Normalization (Eq. 1) concentration ($\times c_0$)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)		Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)						bot part (red shade)					
1	C	55180	43628	68083	112994	20.22	15.99	24.95	41.4	25.64	0.79	0.62	0.97	1.61	5.97	11.42	C	0	1.58	-16.31	12.22	54.36	C	0	16.54	50.66	14.99	-8.76
	A	120551	128740	156657	215154	17.68	18.88	22.98	31.56	22.78	0.78	0.83	1.01	1.39	4.33	-4.39	A	-1.55	0	-17.61	10.48	51.96	A	-14.2	0	29.27	-1.33	-21.71
	G	48984	50612	52616	55720	37.82	39.08	40.63	43.02	40.14	0.94	0.97	1.01	1.07	26.62	-26.04	G	19.49	21.37	0	34.09	84.44	G	-33.62	-22.64	0	-23.67	-39.44
	U	68861	81036	104456	137613	15.9	18.71	24.11	31.77	22.62	0.7	0.83	1.07	1.4	-5.57	-3.1	U	-10.89	-9.49	-25.43	0	37.55	U	-13.04	1.35	31.02	0	-20.65
	T	46050	62152	92815	159526	12.05	16.27	24.29	41.76	23.59	0.51	0.69	1.03	1.77	-31.35	22.12	T	-35.22	-34.19	-45.78	-27.3	0	T	9.6	27.73	65.11	26.03	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.74	0.79	1.02	1.45				C	A	G	U	T		C	A	G	U	T
2	C	58200	68579	75452	81354	21.33	25.13	27.65	29.81	25.98	0.82	0.97	1.06	1.15	-4.81	4.51	C	0	-7.8	-11.26	-6.66	3.1	C	0	6.78	11.24	5.65	-0.2
	A	147918	164129	173943	178542	21.7	24.08	25.51	26.19	24.37	0.89	0.99	1.05	1.07	3.24	-2.12	A	8.46	0	-3.75	1.23	11.82	A	-6.35	0	4.18	-1.06	-6.53
	G	38445	41587	43334	42869	29.69	32.11	33.46	33.1	32.09	0.93	1	1.04	1.03	7.26	-6.05	G	12.69	3.9	0	5.18	16.18	G	-10.11	-4.02	0	-5.03	-10.29
	U	94095	105021	112612	116204	21.72	24.25	26	26.83	24.7	0.88	0.98	1.05	1.09	1.98	-1.07	U	7.14	-1.22	-4.92	0	10.46	U	-5.34	1.07	5.3	0	-5.53
	T	79154	97074	107101	114298	20.72	25.41	28.03	29.92	26.02	0.8	0.98	1.08	1.15	-7.67	4.72	T	-3	-10.57	-13.92	-9.47	0	T	0.2	6.99	11.47	5.86	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.86	0.98	1.06	1.1				C	A	G	U	T		C	A	G	U	T

Supplementary Table 52: Raw data Extended Data Fig. 5j – nucleobases in water, 170 μ m, 18h, pH 5

rep	eat	k	spe	cies	measured values (μ AU*min)				concentration (μ M) $[A]_{j,k,HPLC}$ calibration acc. to Supplementary Table 3				c_0 (μ M)	Normalization (Eq. 1) concentration (x c_0)				Ratio species vs mean (Eq. 4) $[A]_{j,k}/\bar{c}_{j,k} - 1$ (%)		Ratio species against species (shown in heat maps), Eq. 2 $[A]_{j,k}/[B]_{j,k} - 1$ (%)											
					top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)					bot part (red shade)						
1	C	587.34	912.57	1270.36	3093.81	12.91	20.06	27.93	68.02	32.23	0.4	0.62	0.87	2.11	-29.27	21.19	C	0	-43.43	-42.7	-34.89	-1.98	C	0	47.78	43.5	31.74	0.69			
	A	2402.21	3027.1	3295.29	4844.31	21.14	26.64	29	42.64	29.86	0.71	0.89	0.97	1.43	25.02	-17.99	A	76.76	0	1.28	15.08	73.26	A	-32.33	0	-2.89	-10.85	-31.86			
	G	380.08	475.55	519.27	799.37	17.61	22.03	24.06	37.03	25.18	0.7	0.87	0.96	1.47	23.45	-15.55	G	74.53	-1.26	0	13.64	71.08	G	-30.32	2.98	0	-8.2	-29.83			
	U	1401.87	1875.82	2185.73	3649.52	19.42	25.98	30.28	50.55	31.56	0.62	0.82	0.96	1.6	8.64	-8.01	U	53.59	-13.11	-12	0	50.55	U	-24.09	12.17	8.93	0	-23.57			
	T	849.17	1308.32	1798.81	4354.33	13.34	20.55	28.25	68.39	32.63	0.41	0.63	0.87	2.1	-27.84	20.35	T	2.02	-42.28	-41.55	-33.58	0	T	-0.69	46.76	42.51	30.83	0			
	mean concentration per fraction $\bar{c}_{j,k}$										0.57	0.77	0.92	1.74				C	A	G	U	T		C	A	G	U	T			
2	C	366.76	915.19	1375.27	2338.75	8.06	20.12	30.24	51.42	27.46	0.29	0.73	1.1	1.87	-23.08	16.22	C	0	-35.16	-36.53	-28.67	1.95	C	0	33.93	34.75	23.88	-0.61			
	A	1427.36	3064.26	3709.26	4406.89	12.56	26.97	32.65	38.79	27.74	0.45	0.97	1.18	1.4	18.62	-13.22	A	54.22	0	-2.12	10	57.22	A	-25.33	0	0.62	-7.5	-25.79			
	G	408.3	864.84	1030.59	1226.34	18.92	40.07	47.75	56.82	40.89	0.46	0.98	1.17	1.39	21.19	-13.75	G	57.56	2.17	0	12.39	60.63	G	-25.79	-0.61	0	-8.07	-26.24			
	U	858.37	1893.45	2436.83	3151.73	11.89	26.23	33.75	43.66	28.88	0.41	0.91	1.17	1.51	7.83	-6.18	U	40.19	-9.09	-11.02	0	42.93	U	-19.28	8.11	8.78	0	-19.77			
	T	508.67	1294.28	1933.9	3327.34	7.99	20.33	30.37	52.26	27.74	0.29	0.73	1.1	1.88	-24.55	16.94	T	-1.91	-36.4	-37.75	-30.03	0	T	0.62	34.75	35.58	24.64	0			
	mean concentration per fraction $\bar{c}_{j,k}$										0.38	0.87	1.14	1.61				C	A	G	U	T		C	A	G	U	T			
3	C	362.27	1068.77	1630.54	2183.51	7.96	23.5	35.85	48	28.83	0.28	0.82	1.24	1.67	-39.74	16.33	C	0	-55.7	-53.82	-46.09	-1.98	C	0	35.46	31.38	23.17	1.34			
	A	2052.56	3219.03	3847.39	4045.81	18.06	28.33	33.86	35.61	28.97	0.62	0.98	1.17	1.23	36.02	-14.12	A	125.7 3	0	4.25	21.69	121.2 6	A	-26.18	0	-3.01	-9.07	-25.19			
	G	310.91	511.87	597.37	658.71	14.4	23.71	27.68	30.52	24.08	0.6	0.98	1.15	1.27	30.47	-11.45	G	116.5 3	-4.08	0	16.73	112.2 4	G	-23.88	3.11	0	-6.25	-22.87			
	U	1109.56	2028.86	2594.78	2927.05	15.37	28.1	35.94	40.54	29.99	0.51	0.94	1.2	1.35	11.77	-5.55	U	85.5	-17.83	-14.33	0	81.82	U	-18.81	9.98	6.67	0	-17.73			
	T	525.62	1536.89	2332.33	3064.29	8.25	24.14	36.63	48.13	29.29	0.28	0.82	1.25	1.64	-38.52	14.8	T	2.02	-54.8	-52.88	-45	0	T	-1.32	33.67	29.65	21.55	0			
	mean concentration per fraction $\bar{c}_{j,k}$										0.46	0.91	1.2	1.43				C	A	G	U	T		C	A	G	U	T			

Supplementary Table 53: Raw data Extended Data Fig. 5k – nucleobases in water, 170 μm , 18h, pH 7

Due to technical problems, for the third replicate the temperature gradient was not applied for the entire duration of the experiment, which is why we do not take it into account for the calculation of the heat flow-driven enrichment.

rep eat k	spe cies	measured values (μAU*s)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)					bot part (red shade)						
1	C	38356	61527	91932	102887	14.05	22.54	33.69	37.7	27	0.52	0.84	1.25	1.4	-23.71	8.61	C	0	-32.25	-42.11	-24.03	-3.31	C	0	14.59	19.94	9.81	1.39
	A	128238	162307	173584	203371	18.81	23.81	25.46	29.83	24.48	0.77	0.97	1.04	1.22	12.61	-5.21	A	47.61	0	-14.55	12.14	42.72	A	-12.73	0	4.67	-4.17	-11.52
	G	35672	49091	27718	46187	27.54	37.91	21.4	35.66	30.63	0.9	1.24	0.7	1.16	31.78	-9.44	G	72.74	17.02	0	31.23	67.02	G	-16.62	-4.46	0	-8.45	-15.47
	U	75869	100297	125881	140802	17.52	23.15	29.06	32.51	25.56	0.69	0.91	1.14	1.27	0.42	-1.09	U	31.63	-10.82	-23.8	0	27.27	U	-8.93	4.36	9.23	0	-7.67
	T	56704	89706	129779	145055	14.84	23.48	33.97	37.97	27.57	0.54	0.85	1.23	1.38	-21.1	7.13	T	3.43	-29.93	-40.13	-21.43	0	T	-1.37	13.02	18.3	8.3	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.68	0.96	1.07	1.29				C	A	G	U	T		C	A	G	U	T
2	C	39219	60681	79652	100721	14.37	22.23	29.19	36.91	25.67	0.56	0.87	1.14	1.44	-16.85	10.95	C	0	-30.71	-19.02	-22.75	-3.91	C	0	25.36	19.8	14.65	-0.18
	A	130685	159701	171198	185488	19.17	23.43	25.11	27.21	23.73	0.81	0.99	1.06	1.15	20.01	-11.5	A	44.33	0	16.88	11.49	38.68	A	-20.23	0	-4.44	-8.54	-20.38
	G	32468	45106	53962	56366	25.07	34.83	41.67	43.52	36.27	0.69	0.96	1.15	1.2	2.67	-7.38	G	23.48	-14.44	0	-4.61	18.65	G	-16.53	4.65	0	-4.29	-16.68
	U	76278	99060	113760	131982	17.61	22.87	26.26	30.47	24.3	0.72	0.94	1.08	1.25	7.64	-3.23	U	29.46	-10.31	4.84	0	24.39	U	-12.78	9.34	4.49	0	-12.94
	T	57560	85949	109445	142298	15.07	22.5	28.65	37.25	25.86	0.58	0.87	1.11	1.44	-13.47	11.15	T	4.07	-27.89	-15.72	-19.61	0	T	0.18	25.59	20.02	14.86	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.67	0.92	1.11	1.3				C	A	G	U	T		C	A	G	U	T

Supplementary Table 54: Raw data Extended Data Fig. 5l – nucleobases in water, 170 μ m, 18h, pH 10

rep eat k	spe cies	measured values (μAU*s)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)						bot part (red shade)					
1	C	29587	50455	70242	118956	10.84	18.49	25.74	43.59	24.66	0.44	0.75	1.04	1.77	-10.37	-5.14	C	0	-32.94	-19.98	-3.69	25.15	C	0	18.11	-0.31	-13.28	-21.12
	A	104484	137461	157117	238505	15.33	20.16	23.05	34.99	23.38	0.66	0.86	0.99	1.5	33.67	-19.68	A	49.13	0	19.33	43.63	86.64	A	-15.33	0	-15.6	-26.57	-33.21
	G	34489	47055	58281	111305	26.63	36.33	45	85.95	48.48	0.55	0.75	0.93	1.77	12.02	-4.84	G	24.97	-16.2	0	20.36	56.41	G	0.32	18.48	0	-13	-20.87
	U	47694	69292	88061	212958	11.01	16	20.33	49.16	24.13	0.46	0.66	0.84	2.04	-6.94	9.39	U	3.83	-30.38	-16.92	0	29.94	U	15.31	36.19	14.95	0	-9.04
	T	33568	56593	78001	214131	8.79	14.81	20.42	56.05	25.02	0.35	0.59	0.82	2.24	-28.38	20.26	T	-20.1	-46.42	-36.06	-23.04	0	T	26.78	49.73	26.38	9.94	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.49	0.72	0.92	1.86				C	A	G	U	T		C	A	G	U	T
2	C	28394	42891	64863	145029	10.4	15.72	23.77	53.14	25.76	0.4	0.61	0.92	2.06	-8.59	-6.98	C	0	-33.94	-14.29	-1.61	29.35	C	0	18.32	-6.52	-15.28	-21.86
	A	100903	123827	147618	287744	14.8	18.16	21.65	42.21	24.21	0.61	0.75	0.89	1.74	38.37	-21.38	A	51.37	0	29.75	48.93	95.81	A	-15.49	0	-21	-28.4	-33.96
	G	31542	39595	48863	147727	24.36	30.57	37.73	114.07	51.68	0.47	0.59	0.73	2.21	6.65	-0.48	G	16.67	-22.93	0	14.79	50.91	G	6.98	26.58	0	-9.36	-16.41
	U	44987	57351	69134	266836	10.39	13.24	15.96	61.6	25.3	0.41	0.52	0.63	2.44	-7.09	9.8	U	1.64	-32.86	-12.88	0	31.47	U	18.03	39.66	10.33	0	-7.77
	T	31334	45612	59488	264935	8.2	11.94	15.57	69.35	26.27	0.31	0.45	0.59	2.64	-29.33	19.05	T	-22.69	-48.93	-33.74	-23.94	0	T	27.97	51.42	19.63	8.43	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.44	0.59	0.75	2.22				C	A	G	U	T		C	A	G	U	T
3	C	28808	45790	62642	113481	10.56	16.78	22.95	41.58	22.97	0.46	0.73	1	1.81	-10.9	-1.78	C	0	-29.99	-21.44	-5.05	16.68	C	0	21.3	5.33	-9.1	-17.81
	A	100158	129649	152746	227717	14.69	19.02	22.41	33.4	22.38	0.66	0.85	1	1.49	27.27	-19.03	A	42.84	0	12.21	35.62	66.67	A	-17.56	0	-13.16	-25.06	-32.24
	G	34649	45533	54923	101799	26.75	35.16	42.41	78.6	45.73	0.59	0.77	0.93	1.72	13.42	-6.75	G	27.29	-10.88	0	20.86	48.53	G	-5.06	15.16	0	-13.7	-21.97
	U	46407	64984	81145	190956	10.71	15	18.73	44.08	22.13	0.48	0.68	0.85	1.99	-6.16	8.05	U	5.32	-26.27	-17.26	0	22.89	U	10.01	33.45	15.88	0	-9.58
	T	33459	51081	68119	187121	8.76	13.37	17.83	48.98	22.23	0.39	0.6	0.8	2.2	-23.64	19.51	T	-14.3	-40	-32.67	-18.63	0	T	21.67	47.59	28.16	10.6	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.52	0.73	0.92	1.84				C	A	G	U	T		C	A	G	U	T

Supplementary Table 55: Raw data Extended Data Fig. 5m – nucleobases in water, 170 μm, 18h, pH 11

rep eat k	spe cies	measured values (μAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ – 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} – 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)						bot part (red shade)					
1	C	847.2	1044.95	1175.07	1924.17	18.63	22.97	25.83	42.3	27.43	0.68	0.84	0.94	1.54	-7.73	6.73	C	0	-21.23	-15.31	-4.46	8.5	C	0	33.77	18.07	1.88	-9.81
	A	2852.06	3217.89	3351.72	3814.29	25.1	28.32	29.5	33.57	29.12	0.86	0.97	1.01	1.15	17.14	-20.22	A	26.95	0	7.52	21.29	37.74	A	-25.25	0	-11.74	-23.84	-32.58
	G	767.81	873.76	938.77	1250.91	35.57	40.48	43.49	57.95	44.37	0.8	0.91	0.98	1.31	8.95	-9.6	G	18.07	-6.99	0	12.8	28.11	G	-15.3	13.3	0	-13.71	-23.61
	U	1471.72	1732.71	1944.93	3134.5	20.39	24	26.94	43.42	28.69	0.71	0.84	0.94	1.51	-3.42	4.76	U	4.67	-17.55	-11.35	0	13.57	U	-1.84	31.3	15.89	0	-11.47
	T	1078.88	1333.57	1536.5	2947.67	16.94	20.94	24.13	46.29	27.08	0.63	0.77	0.89	1.71	-14.95	18.33	T	-7.83	-27.4	-21.94	-11.95	0	T	10.87	48.31	30.91	12.96	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.74	0.87	0.95	1.44				C	A	G	U	T		C	A	G	U	T
2	C	1074.82	1323.56	1516.1	2060.58	23.63	29.1	33.33	45.3	32.84	0.72	0.89	1.01	1.38	-15.14	26.82	C	0	-29.84	-25.12	-12.8	1.62	C	0	72.97	48.56	29.72	8.65
	A	3416.61	3549.74	3702.11	2656.81	30.07	31.24	32.58	23.38	29.32	1.03	1.07	1.11	0.8	20.96	-26.68	A	42.54	0	6.73	24.29	44.84	A	-42.19	0	-14.11	-25	-37.19
	G	900.08	996.78	980.14	869.76	41.7	46.18	45.41	40.3	43.4	0.96	1.06	1.05	0.93	13.33	-14.63	G	33.55	-6.31	0	16.45	35.7	G	-32.69	16.43	0	-12.68	-26.87
	U	1922.98	2297.05	2623.34	2478.06	26.64	31.82	36.34	34.33	32.28	0.83	0.99	1.13	1.06	-2.68	-2.24	U	14.68	-19.54	-14.13	0	16.54	U	-22.91	33.34	14.52	0	-16.25
	T	1492.98	1960.11	2303.71	2676.99	23.45	30.78	36.18	42.04	33.11	0.71	0.93	1.09	1.27	-16.49	16.73	T	-1.59	-30.96	-26.31	-14.19	0	T	-7.96	59.2	36.73	19.4	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.85	0.99	1.08	1.09				C	A	G	U	T		C	A	G	U	T
3	C	915.17	1156.35	1271.71	1702.06	20.12	25.42	27.96	37.42	27.73	0.73	0.92	1.01	1.35	-7.29	10.49	C	0	-19.37	-13.99	-3.22	4.47	C	0	32.68	22.31	8.03	-2.76
	A	2829.36	3306.38	3242.91	3197.66	24.9	29.1	28.54	28.14	27.67	0.9	1.05	1.03	1.02	14.98	-16.72	A	24.03	0	6.68	20.03	29.58	A	-24.63	0	-7.81	-18.58	-26.71
	G	744.93	894.14	919	974.27	34.51	41.42	42.58	45.14	40.91	0.84	1.01	1.04	1.1	7.78	-9.67	G	16.26	-6.26	0	12.51	21.46	G	-18.24	8.48	0	-11.67	-20.5
	U	1547.06	1955.65	2173.75	2577.41	21.43	27.09	30.11	35.7	28.58	0.75	0.95	1.05	1.25	-4.21	2.27	U	3.33	-16.69	-11.12	0	7.96	U	-7.44	22.81	13.22	0	-9.99
	T	1256.39	1607.21	1862.28	2510.52	19.73	25.24	29.25	39.43	28.41	0.69	0.89	1.03	1.39	-11.26	13.63	T	-4.28	-22.83	-17.67	-7.37	0	T	2.84	36.45	25.78	11.1	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.78	0.96	1.03	1.22				C	A	G	U	T		C	A	G	U	T

Supplementary Table 56: Raw data Extended Data Fig. 5n – 2',3'-Ribonucleotides in water, 170µm, 18h

rep	eat	species	measured values (mAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)									
			top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)				bot part (red shade)					
1	C	0.461	0.854	1.775	4.786	6.08	11.26	23.39	63.08	25.95	0.23	0.43	0.9	2.43	-21.54	8.83	C	0	-21.52	-27.71	-30.59	C	0	8.78	12.96	14.84	
	U	0.677	1.138	2.190	5.069	7.71	12.95	24.92	57.68	25.82	0.3	0.5	0.97	2.23	-0.02	0.05	U	27.42	0	-7.88	-11.55	U	-8.07	0	3.84	5.56	
	A	0.858	1.419	2.615	5.695	8.19	13.55	24.96	54.36	25.27	0.32	0.54	0.99	2.15	8.53	-3.65	A	38.32	8.56	0	-3.98	A	-11.47	-3.7	0	1.66	
	G	1.139	1.858	3.360	7.145	8.61	14.05	25.4	54.01	25.52	0.34	0.55	1	2.12	13.03	-5.23	G	44.06	13.06	4.15	0	G	-12.92	-5.27	-1.63	0	
	mean concentration per fraction $\bar{c}_{j,k}$										0.3	0.51	0.96	2.23				C	U	A	G		C	U	A	G	
2	C	0.434	0.556	1.101	4.556	5.72	7.33	14.52	60.05	21.91	0.26	0.33	0.66	2.74	-23.15	9.54	C	0	-23.49	-29.97	-31.96	C	0	9.73	13.8	16.08	
	U	0.674	0.806	1.487	4.935	7.67	9.17	16.92	56.16	22.48	0.34	0.41	0.75	2.5	0.45	-0.17	U	30.71	0	-8.47	-11.07	U	-8.87	0	3.7	5.78	
	A	0.867	1.016	1.817	5.603	8.28	9.7	17.34	53.48	22.2	0.37	0.44	0.78	2.41	9.75	-3.74	A	42.81	9.25	0	-2.84	A	-12.12	-3.57	0	2	
	G	1.145	1.339	2.403	7.044	8.65	10.12	18.16	53.25	22.55	0.38	0.45	0.81	2.36	12.95	-5.63	G	46.98	12.45	2.92	0	G	-13.85	-5.47	-1.97	0	
	mean concentration per fraction $\bar{c}_{j,k}$										0.34	0.41	0.75	2.5				C	U	A	G		C	U	A	G	
3	C	0.607	0.098	2.198	4.354	8.01	1.29	28.98	57.4	23.92	0.33	0.05	1.21	2.4	-22.48	7.19	C	0	-23.37	-28.46	-31.39	C	0	7.47	10.43	11.67	
	U	0.911	0.136	2.638	4.657	10.37	1.55	30.02	53	23.73	0.44	0.07	1.26	2.23	1.15	-0.26	U	30.49	0	-6.65	-10.47	U	-6.95	0	2.75	3.9	
	A	1.130	0.173	3.110	5.250	10.79	1.65	29.69	50.12	23.06	0.47	0.07	1.29	2.17	8.35	-2.93	A	39.78	7.12	0	-4.1	A	-9.45	-2.68	0	1.12	
	G	1.508	0.224	3.988	6.642	11.4	1.69	30.15	50.21	23.36	0.49	0.07	1.29	2.15	12.98	-4.01	G	45.75	11.69	4.27	0	G	-10.45	-3.76	-1.11	0	
	mean concentration per fraction $\bar{c}_{j,k}$										0.43	0.07	1.26	2.24				C	U	A	G		C	U	A	G	

Supplementary Table 57: Raw data Extended Data Fig. 5o – 3',5'-Ribonucleotides in water, 170μm, 18h

rep	eat	spe	cies	measured values (mAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				C ₀ (μM)	Normalization (Eq. 1) concentration (x C ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{C}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
				top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)						bot part (red shade)																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									

Supplementary Table 58: Raw data Extended Data Fig. 5p – 3',5'-Ribonucleotides in 10 % formamide, 170μm, 18h

rep eat k	spe cies	measured values (μAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)				bot part (red shade)							
1	C	210.9	226.38	898.32	5455.3	3.69	3.96	15.72	95.48	29.71	0.12	0.13	0.53	3.21	-20.26	3.24	C	0	-21.9	-29.29	-24.33	C	0	3.62	5.34	4.15		
	A	530.08	549.65	1916.11	10335.3	3.85	3.99	13.92	75.1	24.22	0.16	0.16	0.57	3.1	2.1	-0.37	A	28.04	0	-9.46	-3.11	A	-3.49	0	1.66	0.52		
	G	474.41	487.03	1603.12	8237.32	4.82	4.94	16.27	83.62	27.41	0.18	0.18	0.59	3.05	12.78	-2	G	41.42	10.45	0	7.02	G	-5.07	-1.64	0	-1.13		
	U	334.7	344.35	1186.14	6290.47	3.23	3.33	11.46	60.76	19.69	0.16	0.17	0.58	3.09	5.38	-0.88	U	32.15	3.21	-6.56	0	U	-3.99	-0.51	1.14	0		
	mean concentration per fraction $\bar{c}_{j,k}$										0.16	0.16	0.57	3.11				C	A	G	U		C	A	G	U		
2	C	209.7	242.48	473.76	4047.95	3.67	4.24	8.29	70.85	21.76	0.17	0.2	0.38	3.26	-21	4.65	C	0	-23.51	-29.53	-25.19	C	0	5.26	7.6	6.05		
	A	551.76	614.38	1104.48	7740.06	4.01	4.46	8.03	56.24	18.18	0.22	0.25	0.44	3.09	3.28	-0.58	A	30.73	0	-7.87	-2.21	A	-5	0	2.22	0.75		
	G	489.96	549.66	955.58	6194.96	4.97	5.58	9.7	62.89	20.78	0.24	0.27	0.47	3.03	12.1	-2.74	G	41.9	8.54	0	6.15	G	-7.06	-2.17	0	-1.44		
	U	343.21	386.68	686.53	4673.27	3.32	3.74	6.63	45.14	14.71	0.23	0.25	0.45	3.07	5.61	-1.32	U	33.68	2.25	-5.79	0	U	-5.71	-0.75	1.46	0		
	mean concentration per fraction $\bar{c}_{j,k}$										0.21	0.24	0.43	3.11				C	A	G	U		C	A	G	U		
3	C	80.02	160.9	453.03	3774.96	1.4	2.82	7.93	66.07	19.55	0.07	0.14	0.41	3.38	-28.09	5.58	C	0	-29.79	-39.4	-32.8	C	0	6.25	9.38	7.15		
	A	238.28	470.59	1206.02	7428.57	1.73	3.42	8.76	53.98	16.97	0.1	0.2	0.52	3.18	2.42	-0.63	A	42.43	0	-13.69	-4.28	A	-5.88	0	2.95	0.85		
	G	229.2	444.43	1093.1	5990.42	2.33	4.51	11.1	60.81	19.69	0.12	0.23	0.56	3.09	18.67	-3.48	G	65.02	15.86	0	10.9	G	-8.58	-2.87	0	-2.04		
	U	153.36	301.69	763.24	4537.76	1.48	2.91	7.37	43.83	13.9	0.11	0.21	0.53	3.15	7	-1.47	U	48.8	4.48	-9.83	0	U	-6.67	-0.84	2.09	0		
	mean concentration per fraction $\bar{c}_{j,k}$										0.1	0.2	0.5	3.2				C	A	G	U		C	A	G	U		

Supplementary Table 59: Raw data Extended Data Fig. 5q – cytidine and CMPs in water, 170μm, 18h

rep eat k	spe cies	measured values (μAU*s)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)													
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)								bot part (red shade)					
1	Cyd	42272	51612	96405	150254	11.92	14.56	27.19	42.38	24.01	0.5	0.61	1.13	1.76	38.55	-16.19	Cyd	0	40.71	70.98	74.9	71.78	70.85	Cyd	0	-15.76	-23.83	-21.86	-22.05	-23.86
	5'	27246	37613	82222	161771	9.82	13.56	29.65	58.33	27.84	0.35	0.49	1.06	2.1	-1.53	-0.5	5'	-28.93	0	21.51	24.3	22.08	21.42	5'	18.71	0	-9.58	-7.24	-7.46	-9.62
	2',3'	38228	54265	129048	305021	8.4	11.92	28.35	67.01	28.92	0.29	0.41	0.98	2.32	-18.96	10.04	2',3'	-41.51	-17.7	0	2.29	0.47	-0.08	2',3'	31.29	10.59	0	2.59	2.34	-0.04
	3'	21969	32865	79928	174786	8	11.97	29.11	63.66	28.19	0.28	0.42	1.03	2.26	-20.78	7.26	3'	-42.83	-19.55	-2.24	0	-1.78	-2.32	3'	27.97	7.8	-2.52	0	-0.24	-2.56
	2'	30647	45424	107994	240051	7.9	11.71	27.85	61.9	27.34	0.29	0.43	1.02	2.26	-19.34	7.52	2'	-41.79	-18.09	-0.47	1.82	0	-0.54	2'	28.28	8.06	-2.29	0.24	0	-2.33
	3',5'	28104	39954	94591	224158	8.2	11.65	27.59	65.39	28.21	0.29	0.41	0.98	2.32	-18.9	10.08	3',5'	-41.47	-17.64	0.08	2.37	0.55	0	3',5'	31.34	10.64	0.04	2.63	2.39	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.33	0.46	1.03	2.17				Cyd	5'	2',3'	3'	2'	3',5'		Cyd	5'	2',3'	3'	2'	3',5'
2	Cyd	51275	66015	85799	127640	14.46	18.62	24.2	36	23.32	0.62	0.8	1.04	1.54	28.2	-15.99	Cyd	0	28.18	47.21	49.8	46.28	48.09	Cyd	0	-15.52	-23.4	-21.13	-21.13	-23.37
	5'	35711	51897	72768	134876	12.88	18.71	26.24	48.64	26.62	0.48	0.7	0.99	1.83	0.02	-0.56	5'	-21.99	0	14.84	16.86	14.12	15.53	5'	18.37	0	-9.33	-6.65	-6.65	-9.29
	2',3'	52960	79518	117025	253354	11.64	17.47	25.71	55.66	27.62	0.42	0.63	0.93	2.02	-12.91	9.68	2',3'	-32.07	-12.92	0	1.76	-0.63	0.6	2',3'	30.55	10.29	0	2.96	2.96	0.04
	3'	30308	48361	70868	143297	11.04	17.61	25.81	52.19	26.66	0.41	0.66	0.97	1.96	-14.41	6.52	3'	-33.24	-14.43	-1.73	0	-2.35	-1.14	3'	26.79	7.12	-2.87	0	0	-2.83
	2'	42779	66345	96993	197515	11.03	17.11	25.01	50.93	26.02	0.42	0.66	0.96	1.96	-12.36	6.52	2'	-31.64	-12.37	0.63	2.4	0	1.24	2'	26.79	7.12	-2.87	0	0	-2.83
	3',5'	38507	58379	85695	185237	11.23	17.03	25	54.03	26.82	0.42	0.63	0.93	2.01	-13.43	9.63	3',5'	-32.47	-13.44	-0.6	1.15	-1.22	0	3',5'	30.49	10.24	-0.04	2.92	2.92	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.46	0.68	0.97	1.89				Cyd	5'	2',3'	3'	2'	3',5'		Cyd	5'	2',3'	3'	2'	3',5'
	Cyd	31562	52630	111168	128850	8.9	14.84	31.36	36.34	22.86	0.39	0.65	1.37	1.59	49.43	-15.12	Cyd	0	53.5	98.74	109.27	101.86	98.9	Cyd	0	-15.08	-22.19	-20.38	-20.44	-22.29
	5'	18328	35547	99873	135250	6.61	12.82	36.01	48.77	26.05	0.25	0.49	1.38	1.87	-2.65	-0.05	5'	-34.85	0	29.47	36.33	31.5	29.58	5'	17.76	0	-8.38	-6.24	-6.31	-8.5
	2',3'	24293	49911	168414	253322	5.34	10.97	37	55.65	27.24	0.2	0.4	1.36	2.04	-24.81	9.09	2',3'	-49.68	-22.76	0	5.3	1.57	0.08	2',3'	28.52	9.14	0	2.33	2.26	-0.13
	3'	13258	29386	100092	142260	4.83	10.7	36.46	51.82	25.95	0.19	0.41	1.4	2	-28.59	6.61	3'	-52.21	-26.65	-5.03	0	-3.54	-4.95	3'	25.6	6.66	-2.28	0	-0.07	-2.4
	2'	19069	41558	137263	197511	4.92	10.72	35.39	50.93	25.49	0.19	0.42	1.39	2	-25.97	6.68	2'	-50.46	-23.96	-1.54	3.67	0	-1.46	2'	25.69	6.74	-2.21	0.07	0	-2.33
	3',5'	17852	36472	123870	186550	5.21	10.64	36.13	54.42	26.6	0.2	0.4	1.36	2.05	-24.87	9.23	3',5'	-49.72	-22.82	-0.08	5.21	1.49	0	3',5'	28.69	9.29	0.13	2.46	2.39	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.24	0.46	1.38	1.93				Cyd	5'	2',3'	3'	2'	3',5'		Cyd	5'	2',3'	3'	2'	3',5'

Supplementary Table 60: Raw data Extended Data Fig. 5r – Deoxy- vs 5'-Ribonucleotides in water, 170μm, 18h

repeat k	species	measured values (μAU*min)				concentration (μM)				c ₀ (μM)	Normalization (Eq. 1)			
		top	II	III	bot	top	II	III	bot		concentration (x c ₀)			
1	5'CMP	169.74	424.53	839.37	3350.67	3.67	9.19	18.16	72.49	25.88	0.14	0.35	0.7	2.8
	dCMP	175.41	461.99	958.96	4073.06	3.32	8.74	18.14	77.06	26.81	0.12	0.33	0.68	2.87
	5'GMP	346.97	784.07	1329.61	4453.89	4.13	9.33	15.81	52.97	20.56	0.2	0.45	0.77	2.58
	dGMP	511.85	1208.13	2131.29	7815.32	4.87	11.5	20.29	74.4	27.77	0.18	0.41	0.73	2.68
	5'AMP	1317.97	1984.17	3279.2	7064.98	12.62	19	31.4	67.64	32.66	0.39	0.58	0.96	2.07
	dAMP	571.02	858.51	1432.45	3071.21	10.07	15.14	25.26	54.16	26.16	0.38	0.58	0.97	2.07
	5'UMP	549.3	837.71	1430.5	3220.96	10.81	16.49	28.16	63.41	29.72	0.36	0.55	0.95	2.13
	dTMP	390.43	618.95	1109.22	2846.79	5.23	8.29	14.86	38.14	16.63	0.31	0.5	0.89	2.29
	mean concentration per fraction $\bar{c}_{j,k}$										0.26	0.47	0.83	2.44
2	5'CMP	347.18	704.67	1116	3159.95	7.51	15.25	24.15	68.37	28.82	0.26	0.53	0.84	2.37
	dCMP	398.3	819.88	1312.14	3827.4	7.54	15.51	24.82	72.41	30.07	0.25	0.52	0.83	2.41
	5'GMP	540.73	1015.7	1718.89	4146.49	6.43	12.08	20.44	49.31	22.07	0.29	0.55	0.93	2.23
	dGMP	845.22	1671.92	2820.86	7391.98	8.05	15.92	26.86	70.37	30.3	0.27	0.53	0.89	2.32
	5'AMP	1534.83	1588.98	2664.24	5930.75	14.7	15.21	25.51	56.78	28.05	0.52	0.54	0.91	2.02
	dAMP	696.47	699.71	1161.9	2576.55	12.28	12.34	20.49	45.44	22.64	0.54	0.55	0.91	2.01
	5'UMP	671.53	686.52	1147.4	2710.09	13.22	13.52	22.59	53.35	25.67	0.52	0.53	0.88	2.08
	dTMP	485.15	489.83	853.87	2383.49	6.5	6.56	11.44	31.94	14.11	0.46	0.47	0.81	2.26
	mean concentration per fraction $\bar{c}_{j,k}$										0.39	0.52	0.87	2.21
3	5'CMP	1127.31	1294.99	1410.79	1684.55	24.39	28.02	30.52	36.45	29.84	0.82	0.94	1.02	1.22
	dCMP	1335.34	1545.51	1689.73	2018.81	25.26	29.24	31.97	38.19	31.16	0.81	0.94	1.03	1.23
	5'GMP	1560.59	1729.83	1894.02	2331.29	18.56	20.57	22.53	27.73	22.35	0.83	0.92	1.01	1.24
	dGMP	2661.51	2988.6	3285.33	4048.55	25.34	28.45	31.28	38.54	30.9	0.82	0.92	1.01	1.25
	5'AMP	1819.02	2778.42	3823.17	6974.22	17.42	26.6	36.6	66.77	36.85	0.47	0.72	0.99	1.81

	dAMP	776.81	1200.06	1677.78	3036.55	13.7	21.16	29.59	53.55	29.5	0.46	0.72	1	1.82
	5'UMP	776.61	1210.37	1702.05	3175.12	15.29	23.83	33.51	62.51	33.78	0.45	0.71	0.99	1.85
	dTMP	585.64	951.06	1401.87	2761.97	7.85	12.74	18.78	37.01	19.09	0.41	0.67	0.98	1.94
	mean concentration per fraction $\bar{c}_{j,k}$										0.63	0.82	1.01	1.54

Supplementary Table 61: Raw data Extended Data Fig. 5s-u – Chirality of amino acids and nucleoside in water, 170µm, 18h
Each compound was analysed in a separate run. Due to technical problems, for the third replicate of cytidine chiral separation the temperature gradient was not applied for the entire duration of the experiment, which is why we do not take it into account for the calculation of the heat flow-driven enrichment.

		Raw data (counts*min for Amino acids, µAU*min for cytidine)			concentrations (µM)			Normalization (Eq. 1) concentration (x c ₀)		
		Repeat 1	Repeat 2	Repeat 3	Repeat 1	Repeat 2	Repeat 3	Repeat 1	Repeat 2	Repeat 3
L-Serine	top	357762.18	389775.31	392169.21	72.55	79.01	79.49	0.88	0.91	0.95
	II	399559.36	425184.41	392717.48	80.99	86.16	79.60	0.98	0.99	0.95
	III	439297.54	435742.96	429217.61	89.01	88.29	86.97	1.08	1.02	1.04
	bottom	437473.30	465881.68	443719.48	88.64	94.37	89.90	1.07	1.09	1.07
	c ₀ (µM)				82.79	86.96	83.99			
D-Serine	top	361647.23	378348.22	414610.32	73.33	76.70	84.02	0.93	0.93	1.04
	II	385201.82	399703.98	405301.24	78.09	81.01	82.14	0.99	0.98	1.01
	III	389921.03	422252.97	347992.72	79.04	85.57	70.57	1.00	1.03	0.87
	bottom	422312.42	433740.64	430845.06	85.58	87.89	87.30	1.08	1.06	1.08
	c ₀ (µM)				79.01	82.79	81.01			
L-Threonine	top	387210.64	364486.05	390897.41	70.63	66.51	71.30	0.92	0.90	0.90
	II	412346.73	399252.18	405525.21	75.20	72.82	73.96	0.98	0.98	0.93
	III	432729.36	407077.01	460181.63	78.90	74.24	83.88	1.03	1.00	1.06
	bottom	451308.93	456273.54	480216.74	82.27	83.17	87.51	1.07	1.12	1.11
	c ₀ (µM)				76.75	74.18	79.16			
D-Threonine	top	343706.88	419771.78	370256.49	62.74	76.54	67.56	0.81	0.98	0.82
	II	407149.61	431178.24	440857.08	74.25	78.61	80.37	0.96	1.01	0.97
	III	509280.53	436664.40	484323.39	82.78	79.61	88.26	1.07	1.02	1.07
	bottom	487535.27	425516.43	518873.29	88.84	77.59	94.52	1.15	0.99	1.14
	c ₀ (µM)				77.15	78.09	82.68			
L-Cytidine	top	628.48	603.99		10.64	10.22		0.36	0.41	
	II	950.74	994.42		16.09	16.83		0.54	0.68	
	III	2251.66	1231.55		38.11	20.84		1.27	0.84	
	bottom	3248.43	3007.97		54.97	50.90		1.84	2.06	
	c ₀ (µM)				29.95	24.70				
D-Cytidine	top	796.67	619.49		13.48	10.48		0.55	0.44	
	II	791.50	788.39		13.39	13.34		0.55	0.57	
	III	1609.61	1485.40		27.24	25.14		1.11	1.07	
	bottom	2594.78	2681.85		43.91	45.39		1.79	1.92	
	c ₀ (µM)				24.51	23.59				

Supplementary Table 62: Raw data Supplementary Fig. 1a – nucleobases in water, 170µm, 6h

rep eat k	spe cies	measured values (μAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)											
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)						bot part (red shade)					
1	C	864.79	975.25	1002.41	1259.33	19.01	21.44	22.04	27.69	22.54	0.84	0.95	0.98	1.23	-7.05	6.16	C	0	-11.12	-11.61	-9.5	-1.73	C	0	11.98	10.79	8.93	0.39
	A	2412.8	2528.86	2441.54	2788.88	21.24	22.26	21.49	24.55	22.38	0.95	0.99	0.96	1.1	4.58	-5.2	A	12.51	0	-0.56	1.82	10.56	A	-10.7	0	-1.06	-2.72	-10.36
	G	605.61	606.41	623.29	703.54	28.06	28.09	28.88	32.59	29.41	0.95	0.96	0.98	1.11	5.17	-4.18	G	13.14	0.56	0	2.39	11.18	G	-9.74	1.07	0	-1.68	-9.39
	U	1504.64	1580.34	1553.3	1820.32	20.84	21.89	21.52	25.21	22.37	0.93	0.98	0.96	1.13	2.71	-2.54	U	10.5	-1.78	-2.34	0	8.59	U	-8.2	2.8	1.71	0	-7.85
	T	1284.43	1420.57	1450.77	1831.01	20.17	22.31	22.78	28.76	23.51	0.86	0.95	0.97	1.22	-5.41	5.76	T	1.76	-9.55	-10.06	-7.91	0	T	-0.38	11.55	10.37	8.51	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.91	0.97	0.97	1.16				C	A	G	U	T		C	A	G	U	T
2	C	816.79	851.82	1066.63	1345.31	17.96	18.73	23.45	29.58	22.43	0.8	0.84	1.05	1.32	-4.81	5.25	C	0	-8.14	-8.55	-6.09	-0.58	C	0	11.06	8.18	7.1	0.81
	A	2273.86	2305.06	2758.81	3097.88	20.01	20.29	24.28	27.26	22.96	0.87	0.88	1.06	1.19	3.62	-5.23	A	8.86	0	-0.46	2.23	8.22	A	-9.96	0	-2.59	-3.57	-9.23
	G	659.46	651.61	783.55	918.13	30.55	30.19	36.3	42.54	34.89	0.88	0.87	1.04	1.22	4.09	-2.71	G	9.35	0.46	0	2.7	8.71	G	-7.56	2.66	0	-1	-6.82
	U	1404.32	1421.75	1734.34	2028.18	19.45	19.69	24.02	28.09	22.82	0.85	0.86	1.05	1.23	1.36	-1.73	U	6.48	-2.18	-2.63	0	5.86	U	-6.63	3.7	1.01	0	-5.88
	T	1197.28	1252.66	1551.7	1944.81	18.8	19.67	24.37	30.54	23.35	0.81	0.84	1.04	1.31	-4.25	4.41	T	0.59	-7.6	-8.02	-5.54	0	T	-0.8	10.17	7.32	6.24	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.84	0.86	1.05	1.25				C	A	G	U	T		C	A	G	U	T
3	C	768.53	1011.98	1147.02	1443.66	16.9	22.25	25.22	31.74	24.03	0.7	0.93	1.05	1.32	-9.37	7.51	C	0	-17.5	-13.24	-12.59	-0.79	C	0	18.81	9.21	11.86	0.04
	A	2322.49	2709.67	2836.66	3029.33	20.44	23.85	24.97	26.66	23.98	0.85	0.99	1.04	1.11	9.86	-9.52	A	21.21	0	5.16	5.95	20.25	A	-15.84	0	-8.08	-5.85	-15.8
	G	551.09	624.69	721.21	822.36	25.53	28.94	33.41	38.1	31.5	0.81	0.92	1.06	1.21	4.47	-1.56	G	15.26	-4.91	0	0.76	14.35	G	-8.43	8.79	0	2.43	-8.4
	U	1405.7	1703.18	1816.61	2063.46	19.47	23.59	25.16	28.58	24.2	0.8	0.97	1.04	1.18	3.68	-3.89	U	14.4	-5.62	-0.75	0	13.49	U	-10.6	6.22	-2.37	0	-10.57
	T	1140.79	1492	1679.14	2125.05	17.92	23.43	26.37	33.37	25.27	0.71	0.93	1.04	1.32	-8.64	7.46	T	0.8	-16.84	-12.55	-11.89	0	T	-0.04	18.77	9.17	11.82	0
	mean concentration per fraction $\bar{c}_{j,k}$										0.78	0.95	1.05	1.23				C	A	G	U	T		C	A	G	U	T

Supplementary Table 63: Raw data Supplementary Fig. 1b – Ribonucleosides in water, 170μm, 6h

rep eat k	spe cies	measured values (μAU*s)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / <c̄<sub>j,k - 1 (%)</c̄<sub>		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)									
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)				bot part (red shade)					
1	C	43670	60769	79848	103677	12.32	17.14	22.52	29.24	20.31	0.61	0.84	1.11	1.44	-6.32	4.53	C	0	-6.21	-9.11	-9.36	C	0	6.03	7.72	4.69
	U	72563	98382	125445	152384	13.35	18.1	23.08	28.04	20.64	0.65	0.88	1.12	1.36	-0.12	-1.42	U	6.62	0	-3.09	-3.36	U	-5.69	0	1.59	-1.27
	A	116192	153813	193612	232747	13.7	18.14	22.84	27.45	20.53	0.67	0.88	1.11	1.34	3.07	-2.96	A	10.03	3.19	0	-0.28	A	-7.17	-1.57	0	-2.81
	G	94862	119535	157580	194984	11.94	15.04	19.83	24.53	17.83	0.67	0.84	1.11	1.38	3.36	-0.15	G	10.33	3.48	0.28	0	G	-4.48	1.28	2.9	0
	mean concentration per fraction c̄ _{j,k}										0.65	0.86	1.11	1.38				C	U	A	G		C	U	A	G
2	C	45386	53015	83308	102582	12.8	14.95	23.5	28.93	20.05	0.64	0.75	1.17	1.44	-8.69	5.21	C	0	-7.68	-10.75	-15.06	C	0	6.44	8.84	5.96
	U	77828	87844	131826	152584	14.32	16.16	24.25	28.07	20.7	0.69	0.78	1.17	1.36	-1.1	-1.16	U	8.31	0	-3.33	-8	U	-6.05	0	2.26	-0.44
	A	124498	137146	203619	230750	14.68	16.18	24.02	27.22	20.52	0.72	0.79	1.17	1.33	2.3	-3.34	A	12.04	3.44	0	-4.83	A	-8.12	-2.21	0	-2.64
	G	108841	111938	161113	197196	13.69	14.08	20.27	24.81	18.22	0.75	0.77	1.11	1.36	7.49	-0.71	G	17.73	8.69	5.08	0	G	-5.63	0.45	2.71	0
	mean concentration per fraction c̄ _{j,k}										0.7	0.77	1.16	1.37				C	U	A	G		C	U	A	G
3	C	54968	80890	95863	100879	15.5	22.82	27.04	28.45	23.45	0.66	0.97	1.15	1.21	-11.1	5.45	C	0	-8.75	-12.33	-20.83	C	0	5.53	7.7	9.01
	U	94953	130666	147991	150686	17.47	24.04	27.23	27.72	24.11	0.72	1	1.13	1.15	-2.58	-0.08	U	9.58	0	-3.93	-13.24	U	-5.24	0	2.05	3.3
	A	152403	202532	225824	227672	17.98	23.89	26.64	26.85	23.84	0.75	1	1.12	1.13	1.4	-2.09	A	14.07	4.09	0	-9.69	A	-7.15	-2.01	0	1.22
	G	136090	162275	172172	181384	17.12	20.42	21.66	22.82	20.51	0.84	1	1.06	1.11	12.29	-3.27	G	26.31	15.27	10.73	0	G	-8.27	-3.19	-1.2	0
	mean concentration per fraction c̄ _{j,k}										0.74	0.99	1.11	1.15				C	U	A	G		C	U	A	G

Supplementary Table 64: Raw data Supplementary Fig. 1c – 5'-Ribonucleotides in water, 170μm, 6h

rep	eat	spe	cies	measured values (μAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / $\bar{c}_{j,k}$ - 1 (%)		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)									
				top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)				bot part (red shade)					
1	C	696.45	845.29	1434.23	1860	15.07	18.29	31.03	40.24	26.16	0.58	0.7	1.19	1.54	-2.26	1.28	C	0	-4.86	-4.1	0.11	C	0	3.95	3.22	-1.84		
	A	1708.37	2052.63	3349.07	4175.74	16.36	19.65	32.07	39.98	27.01	0.61	0.73	1.19	1.48	2.73	-2.57	A	5.11	0	0.8	5.23	A	-3.8	0	-0.7	-5.58		
	U	759.45	902.05	1511.3	1884.44	14.95	17.76	29.75	37.1	24.89	0.6	0.71	1.2	1.49	1.91	-1.88	U	4.28	-0.79	0	4.39	U	-3.12	0.71	0	-4.91		
	G	1047.5	1269.42	2111.62	2853.39	12.46	15.1	25.11	33.94	21.65	0.58	0.7	1.16	1.57	-2.38	3.18	G	-0.11	-4.97	-4.21	0	G	1.88	5.9	5.16	0		
	mean concentration per fraction $\bar{c}_{j,k}$										0.59	0.71	1.18	1.52				C	A	U	G		C	A	U	G		
2	C	615.85	823.69	1033.93	1937.44	13.32	17.82	22.37	41.92	23.86	0.56	0.75	0.94	1.76	-3.86	2.32	C	0	-5.31	-5.85	-4.05	C	0	4.15	4.44	0.85		
	A	1512.3	1991.69	2426.84	4325.17	14.48	19.07	23.24	41.41	24.55	0.59	0.78	0.95	1.69	1.54	-1.76	A	5.61	0	-0.57	1.34	A	-3.99	0	0.28	-3.18		
	U	677.73	883.36	1087	1921.89	13.34	17.39	21.4	37.84	22.49	0.59	0.77	0.95	1.68	2.12	-2.03	U	6.22	0.57	0	1.92	U	-4.26	-0.28	0	-3.45		
	G	941.98	1204.25	1507.81	2819.62	11.2	14.32	17.93	33.53	19.25	0.58	0.74	0.93	1.74	0.2	1.46	G	4.22	-1.32	-1.88	0	G	-0.84	3.28	3.57	0		
	mean concentration per fraction $\bar{c}_{j,k}$										0.58	0.76	0.94	1.72				C	A	U	G		C	A	U	G		
3	C	805.06	795.1	1085.33	1504.84	17.42	17.2	23.48	32.56	22.67	0.77	0.76	1.04	1.44	-0.99	0.53	C	0	-1.69	-4.05	2	C	0	1.51	2.52	-1.8		
	A	1934.27	1919.71	2542.18	3501.43	18.52	18.38	24.34	33.52	23.69	0.78	0.78	1.03	1.42	0.72	-0.97	A	1.72	0	-2.4	3.75	A	-1.49	0	0.99	-3.27		
	U	874.1	846.43	1115.75	1529.18	17.21	16.66	21.97	30.1	21.49	0.8	0.78	1.02	1.4	3.19	-1.94	U	4.22	2.46	0	6.3	U	-2.46	-0.98	0	-4.22		
	G	1182.45	1194.79	1604.51	2295.72	14.06	14.21	19.08	27.3	18.66	0.75	0.76	1.02	1.46	-2.92	2.38	G	-1.96	-3.61	-5.93	0	G	1.83	3.38	4.4	0		
	mean concentration per fraction $\bar{c}_{j,k}$										0.78	0.77	1.03	1.43				C	A	U	G		C	A	U	G		

Supplementary Table 65: Raw data Supplementary Fig. 1d – 2',3'-Ribonucleotides in water, 170μm, 6h

rep eat k	spe cies	measured values (mAU*min)				concentration (μM) [A] _{j,k,HPLC} calibration acc. to Supplementary Table 3				c ₀ (μM)	Normalization (Eq. 1) concentration (x c ₀)				Ratio species vs mean (Eq. 4) [A] _{j,k} / <c̄<sub>j,k - 1 (%)</c̄<sub>		Ratio species against species (shown in heat maps), Eq. 2 [A] _{j,k} /[B] _{j,k} - 1 (%)									
		top	II	III	bot	top	II	III	bot		top	II	III	bot	top	bot	top part (blue shade)				bot part (red shade)					
1	C	0.991	1.289	1.631	4.296	13.07	17	21.5	56.63	27.05	0.48	0.63	0.79	2.09	-8.1	6.25	C	0	-8.2	-11.82	-11.43	C	0	6.41	9.26	9.94
	U	1.254	1.599	1.988	4.687	14.27	18.2	22.63	53.34	27.11	0.53	0.67	0.83	1.97	0.11	-0.15	U	8.93	0	-3.94	-3.52	U	-6.02	0	2.68	3.32
	A	1.533	1.919	2.378	5.361	14.63	18.32	22.7	51.18	26.71	0.55	0.69	0.85	1.92	4.22	-2.76	A	13.4	4.11	0	0.44	A	-8.48	-2.61	0	0.62
	G	2.027	2.555	3.206	7.079	15.33	19.31	24.24	53.51	28.1	0.55	0.69	0.86	1.9	3.76	-3.35	G	12.9	3.65	-0.44	0	G	-9.04	-3.21	-0.61	0
	mean concentration per fraction c̄ _{j,k}										0.53	0.67	0.84	1.97				C	U	A	G		C	U	A	G
2	C	0.723	1.252	1.722	3.291	9.53	16.51	22.69	43.38	23.03	0.41	0.72	0.99	1.88	-10.8	6.35	C	0	-11.55	-16	-14.03	C	0	6.74	9.91	9.34
	U	0.961	1.552	2.081	3.628	10.94	17.66	23.69	41.29	23.4	0.47	0.75	1.01	1.76	0.84	-0.36	U	13.05	0	-5.04	-2.81	U	-6.31	0	2.98	2.44
	A	1.197	1.877	2.484	4.167	11.43	17.92	23.71	39.78	23.21	0.49	0.77	1.02	1.71	6.2	-3.24	A	19.05	5.31	0	2.35	A	-9.02	-2.89	0	-0.52
	G	1.574	2.551	3.324	5.636	11.9	19.28	25.13	42.61	24.73	0.48	0.78	1.02	1.72	3.76	-2.74	G	16.32	2.89	-2.29	0	G	-8.54	-2.38	0.52	0
	mean concentration per fraction c̄ _{j,k}										0.46	0.76	1.01	1.77				C	U	A	G		C	U	A	G
3	C	1.101	1.270	1.767	2.004	14.51	16.73	23.29	26.42	20.24	0.72	0.83	1.15	1.31	-1.91	3.04	C	0	-2.82	-4.24	-0.47	C	0	3.38	4.93	4
	U	1.387	1.586	2.174	2.374	15.78	18.05	24.74	27.02	21.4	0.74	0.84	1.16	1.26	0.93	-0.33	U	2.9	0	-1.46	2.42	U	-3.27	0	1.49	0.6
	A	1.686	1.912	2.608	2.801	16.09	18.25	24.9	26.74	21.49	0.75	0.85	1.16	1.24	2.43	-1.8	A	4.43	1.48	0	3.94	A	-4.7	-1.47	0	-0.88
	G	2.224	2.592	3.658	3.876	16.81	19.6	27.65	29.3	23.34	0.72	0.84	1.18	1.26	-1.45	-0.92	G	0.47	-2.36	-3.79	0	G	-3.85	-0.59	0.89	0
	mean concentration per fraction c̄ _{j,k}										0.73	0.84	1.16	1.27				C	U	A	G		C	U	A	G

Supplementary Table 66: Raw data Supplementary Fig. 15

	area (counts * min)			deviation from mean (%)		
	repeat 1	repeat 2	repeat 3	repeat 1	repeat 2	repeat 3
S	585228	589553	600901	-1.13	-0.40	1.52
E	511421	519610	523440	-1.30	0.28	1.02
T	608092	615182	623499	-1.22	-0.07	1.28
A	585935	590815	594969	-0.79	0.04	0.74
P	168516	169837	171658	-0.88	-0.10	0.97
C	121011	121676	123355	-0.82	-0.28	1.10
K	477430	486495	485441	-1.18	0.70	0.48
V	758800	768624	780076	-1.35	-0.07	1.42
I	773793	784323	789932	-1.14	0.21	0.93
L	740480	757193	760091	-1.61	0.61	1.00
F	600381	608858	612207	-1.11	0.28	0.83

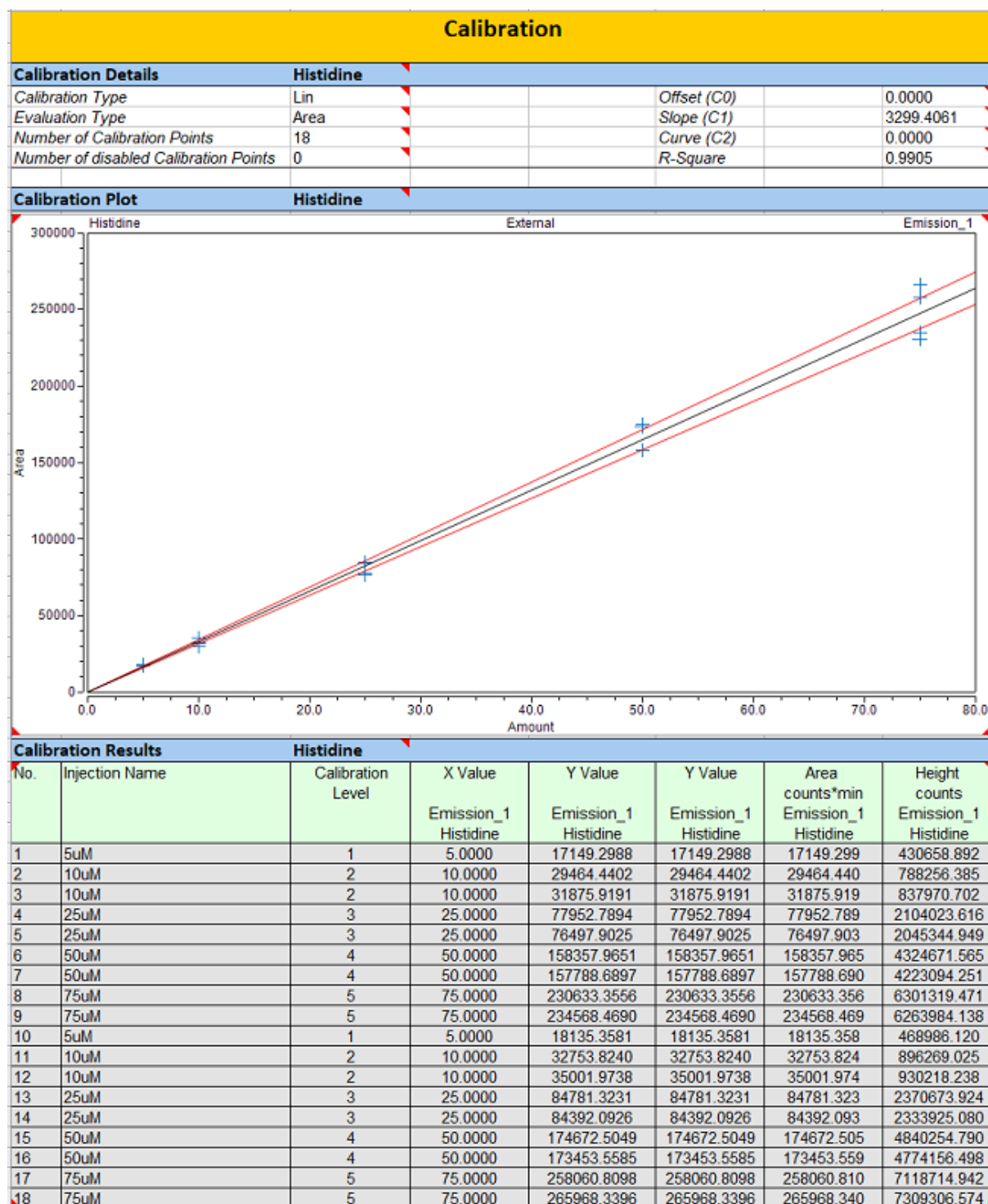
Supplementary references

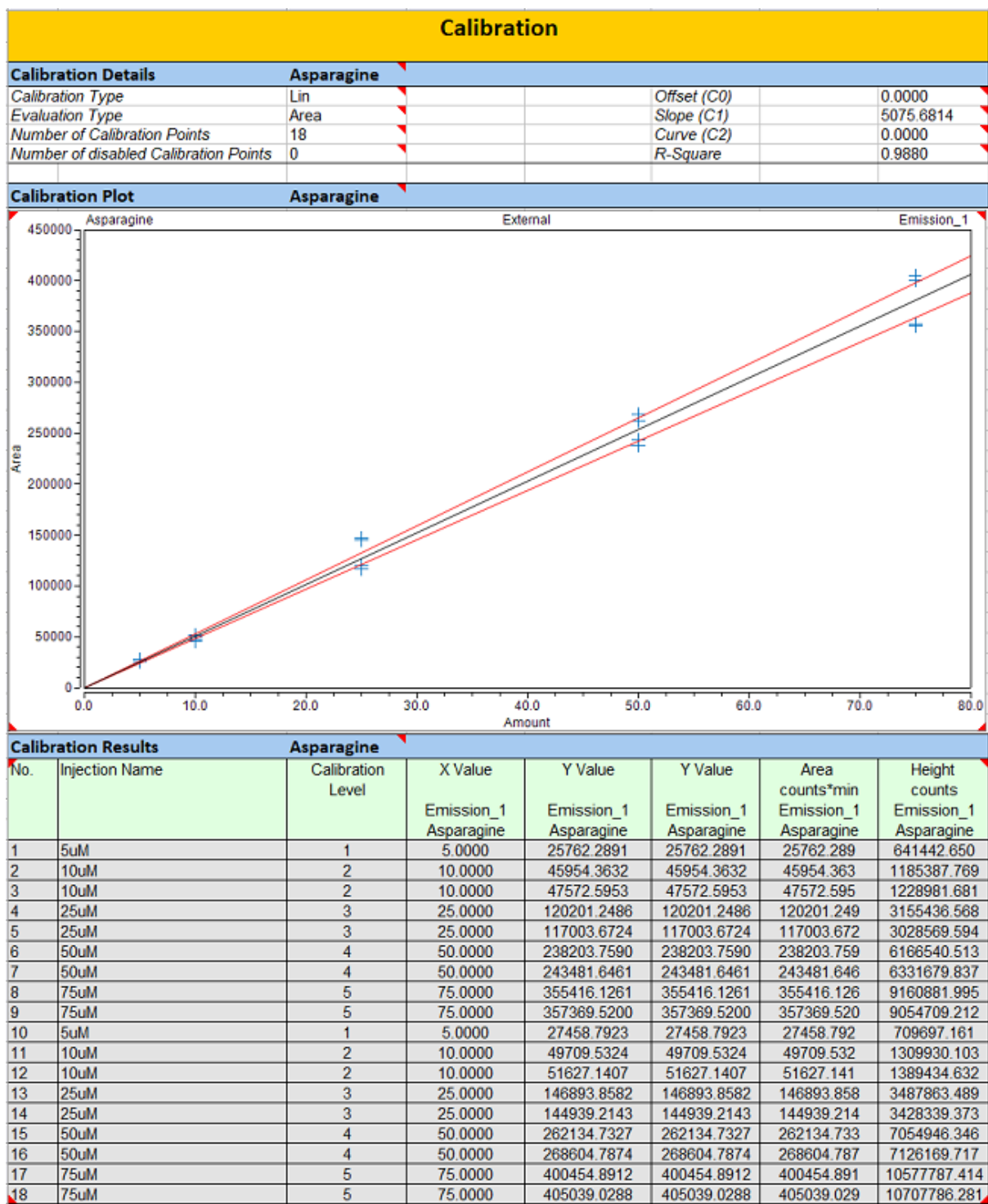
References 41, 42 and 49 are also referenced in the main text.

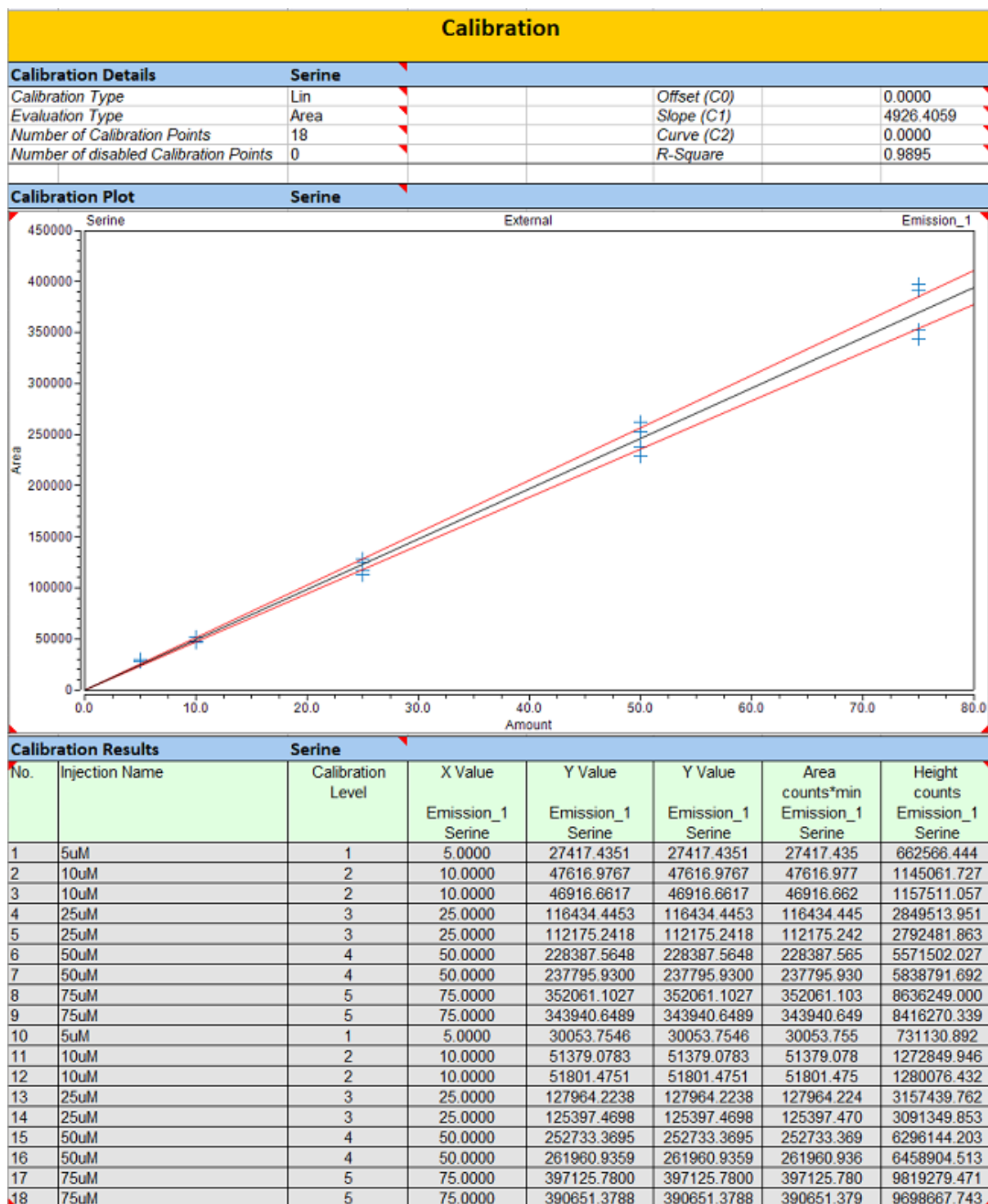
- 41. Keil, L., Hartmann, M., Lanzmich, S. & Braun, D. Probing of molecular replication and accumulation in shallow heat gradients through numerical simulations. *Phys. Chem. Chem. Phys.* **18**, 20153–20159 (2016).
- 42. Matreux, T. *et al.* Heat flows in rock cracks naturally optimize salt compositions for ribozymes. *Nat. Chem.* **13**, 1038–1045 (2021).
- 49. Bai, L., Baker, D. R. & Hill, R. J. Permeability of vesicular Stromboli basaltic glass: Lattice Boltzmann simulations and laboratory measurements. *J. Geophys. Res.* **115**, B07201 (2010).
- 55. Viswanathan, H. S. *et al.* From Fluid Flow to Coupled Processes in Fractured Rock: Recent Advances and New Frontiers. *Reviews of Geophysics* **60**, (2022).

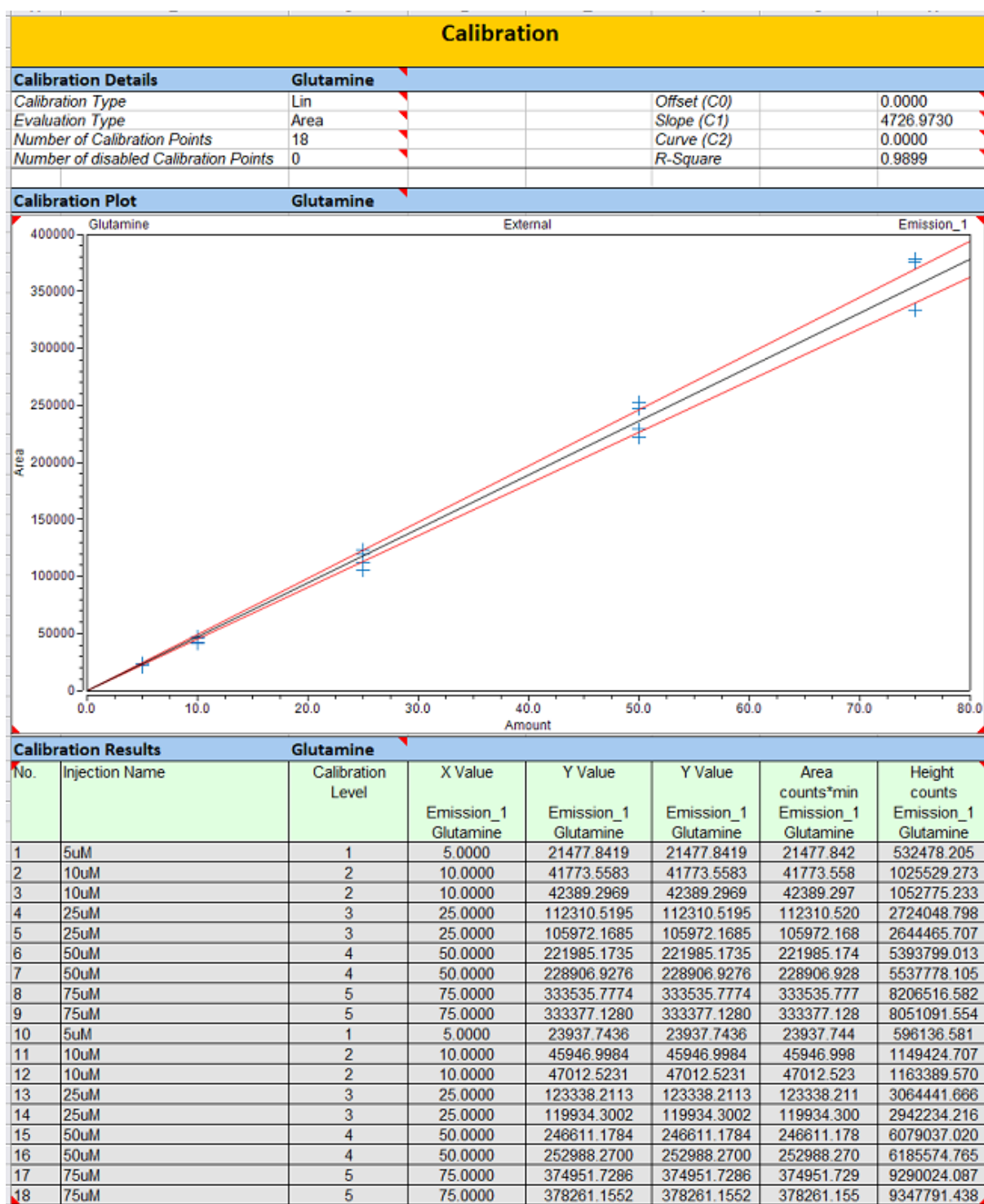
Calibration data amino acids (Fig. 2)

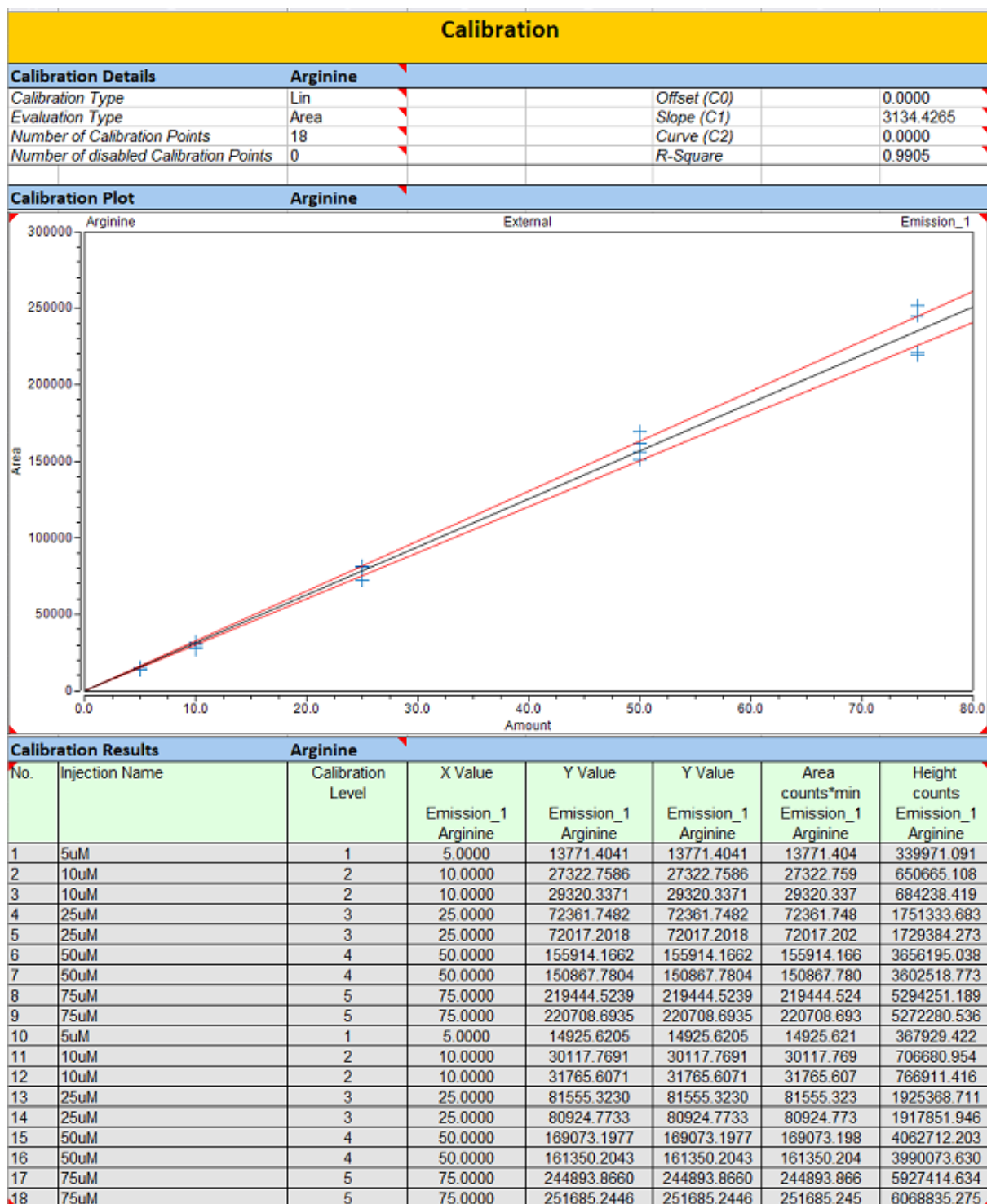
Fluorescence channel for all amino acids except for tryptophan and tyrosine, where the UV-channel is used (see Methods for details).

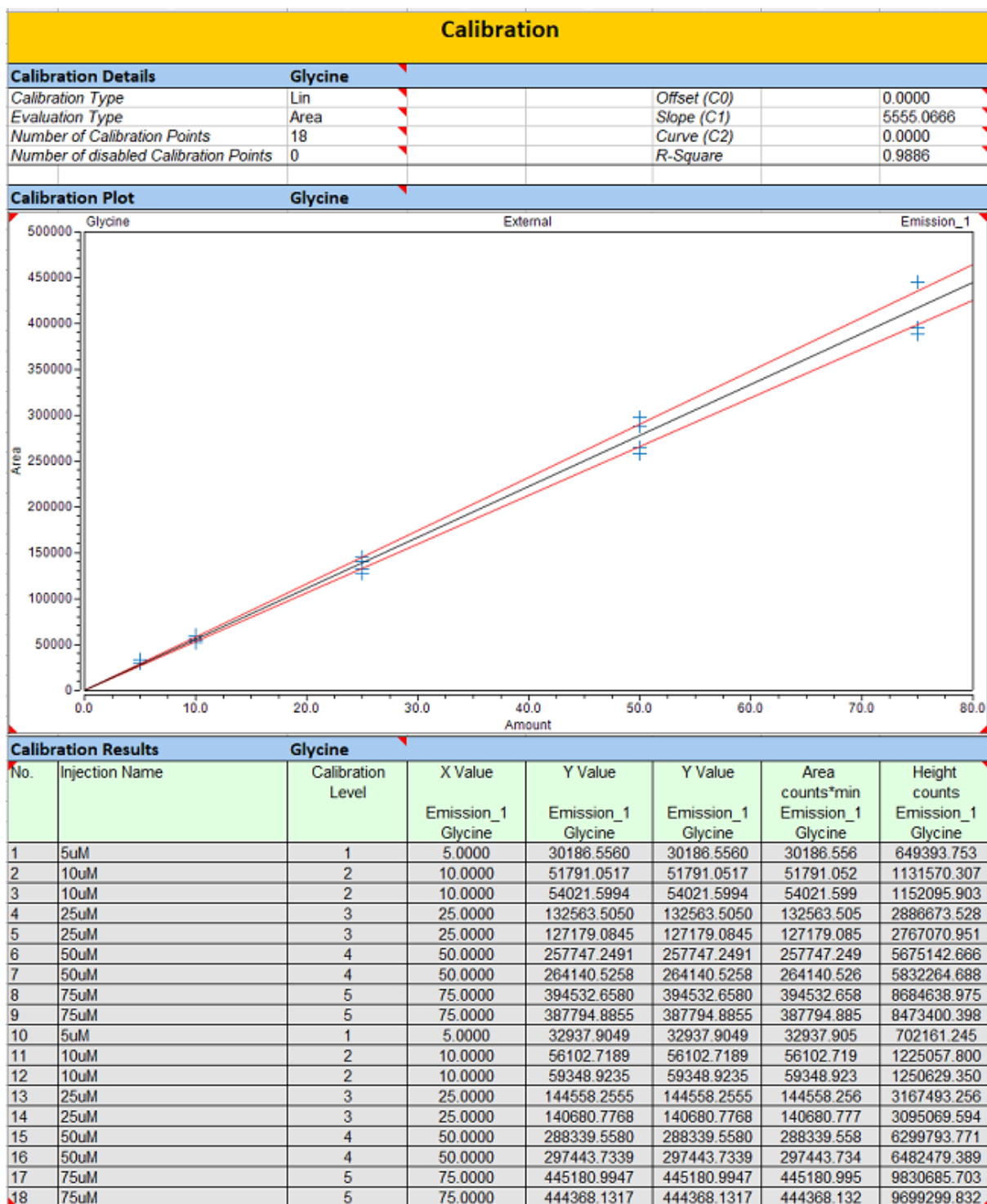


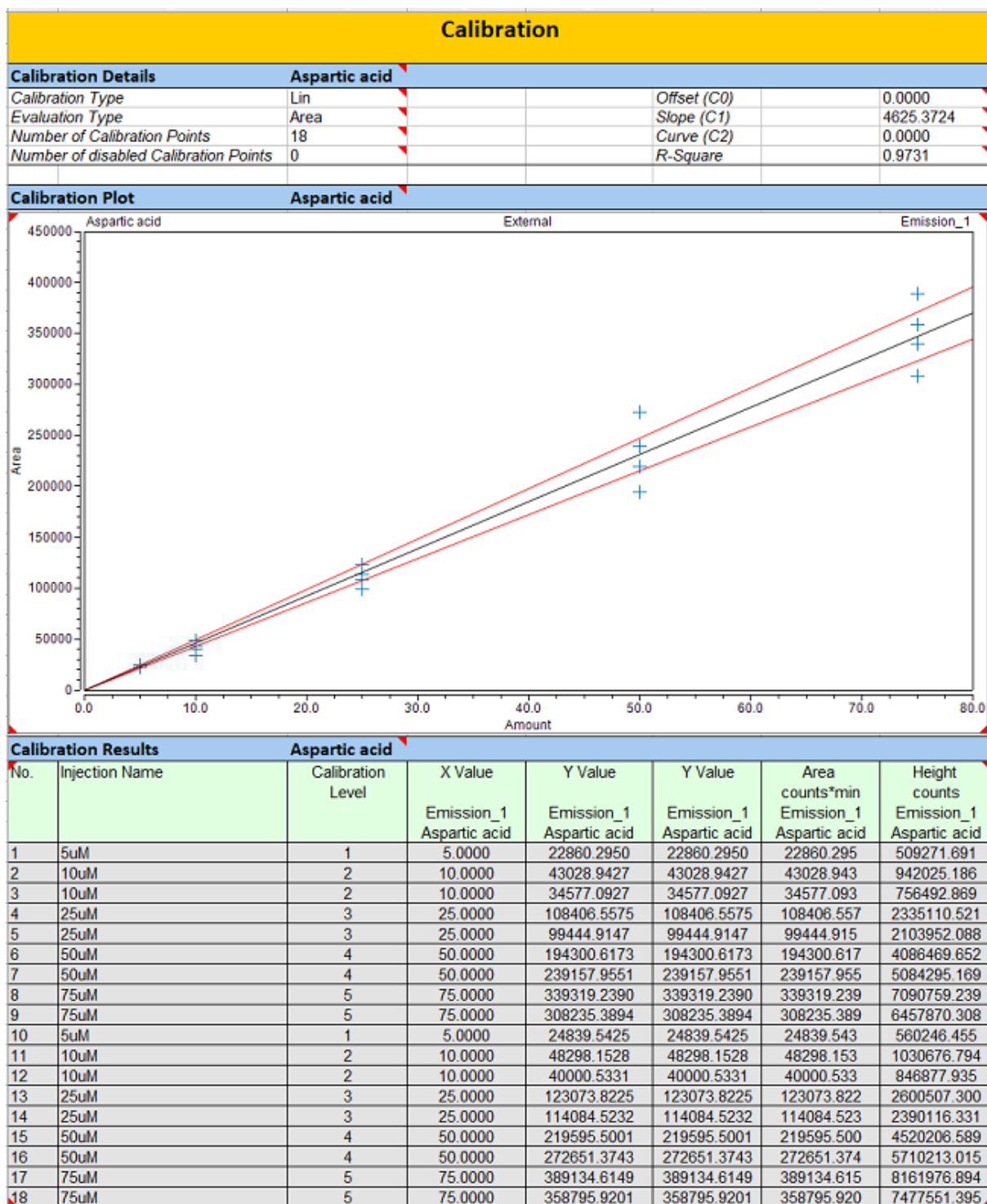


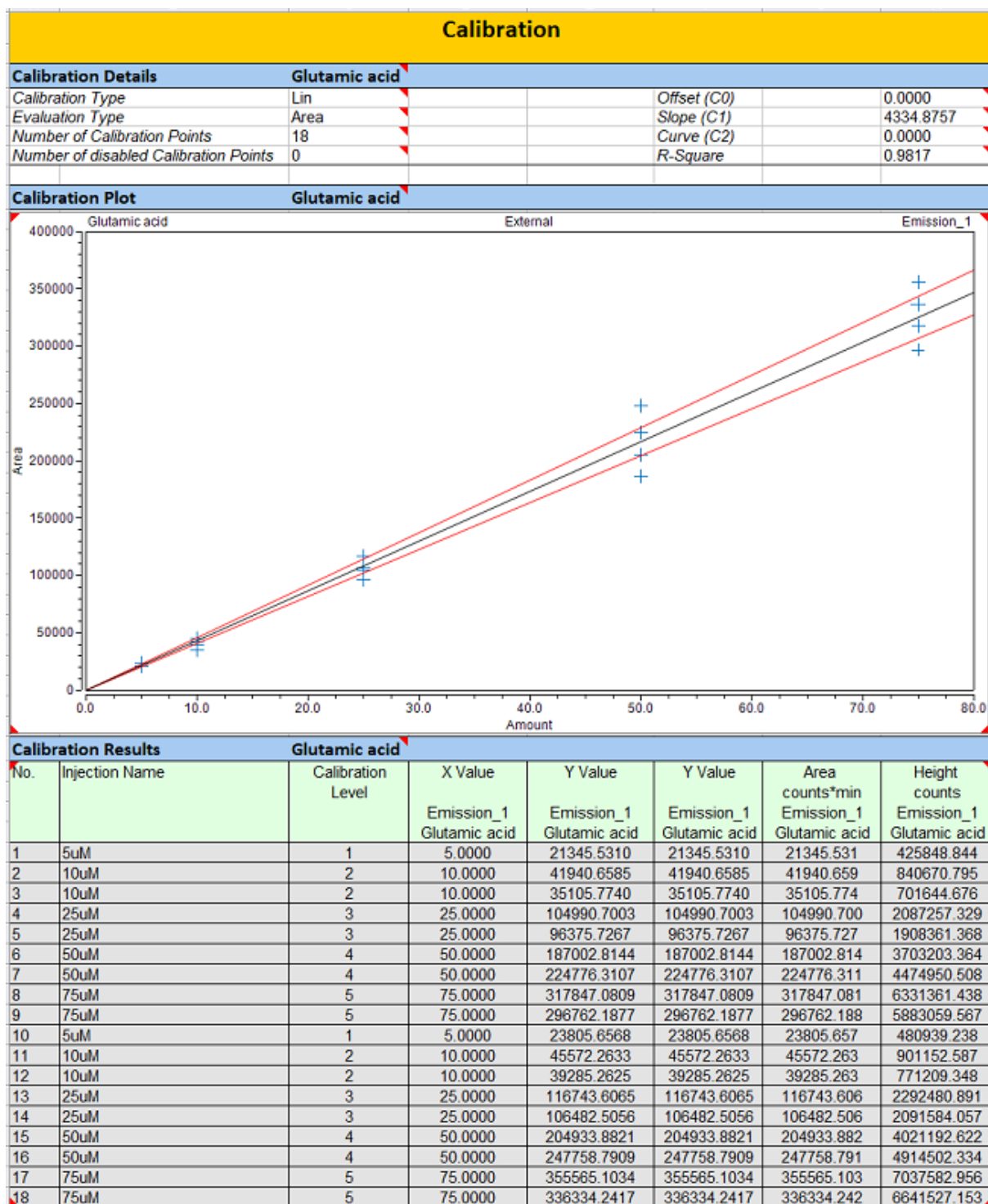


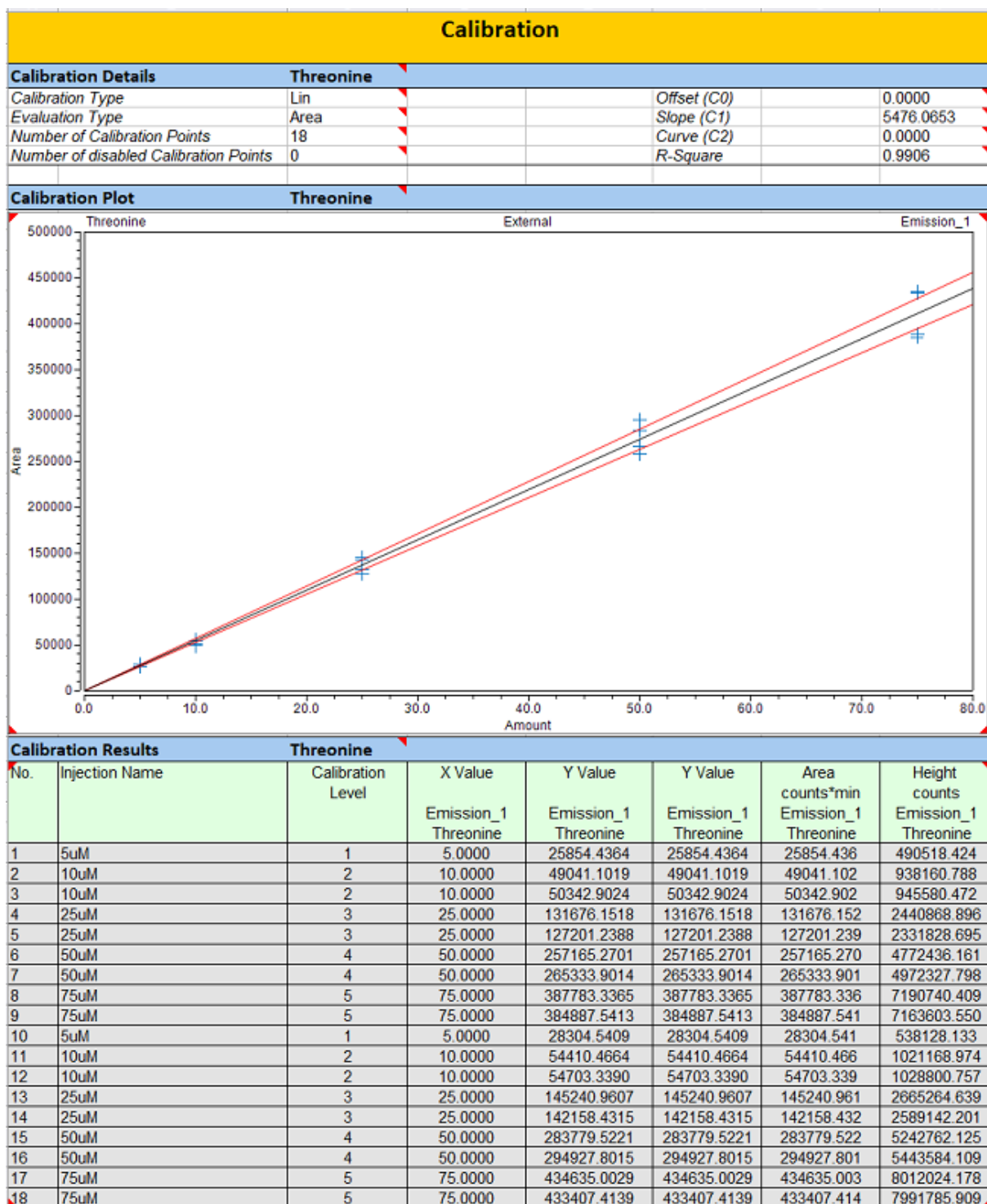


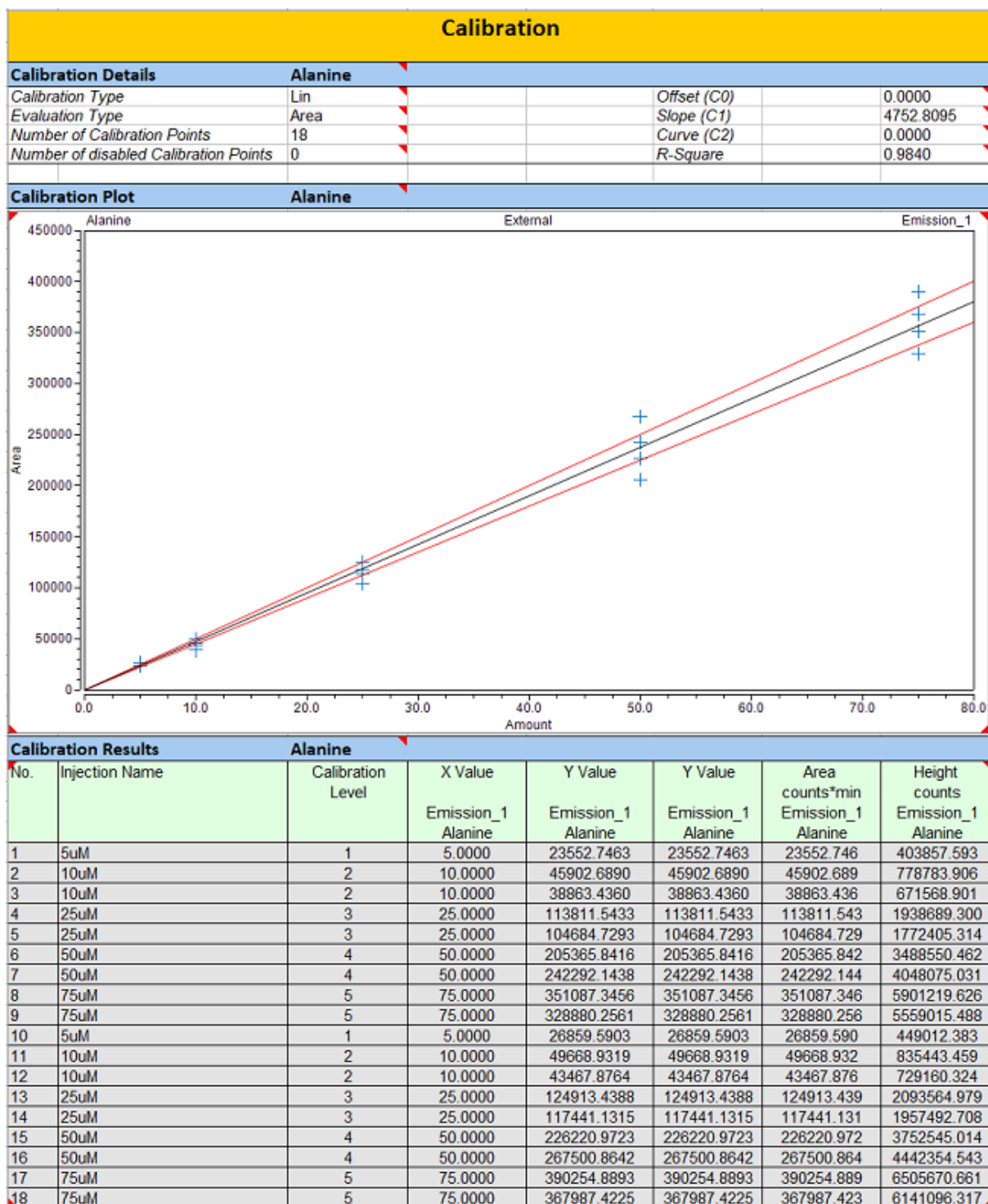






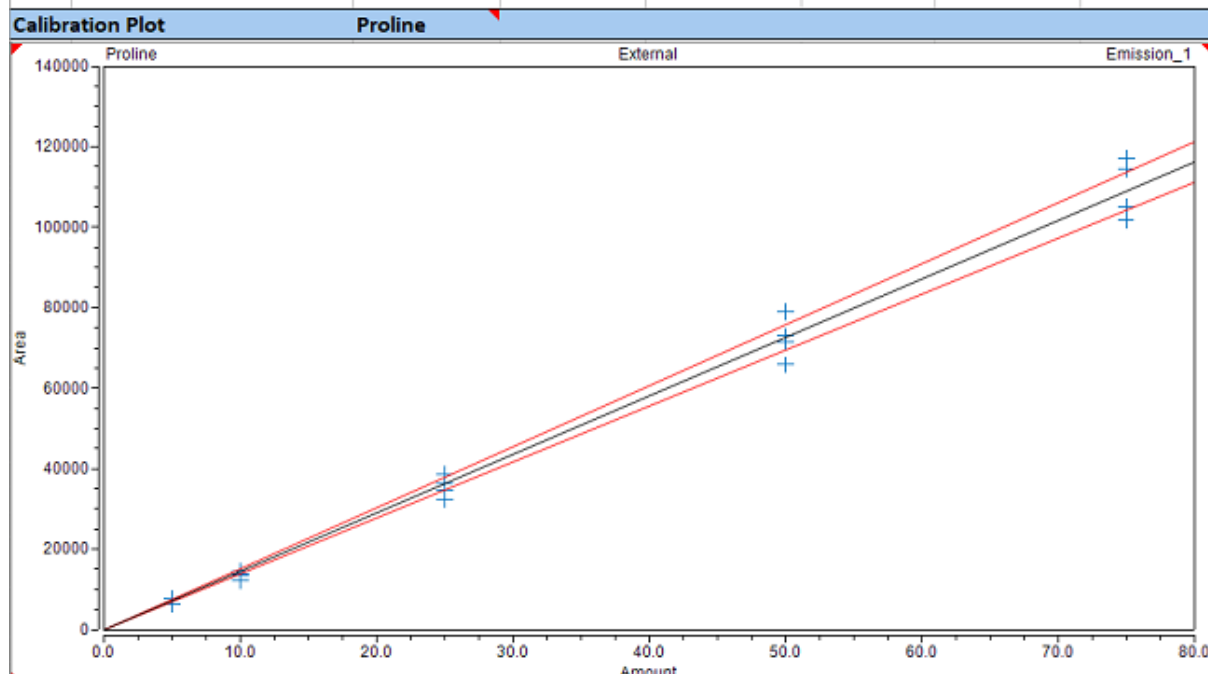




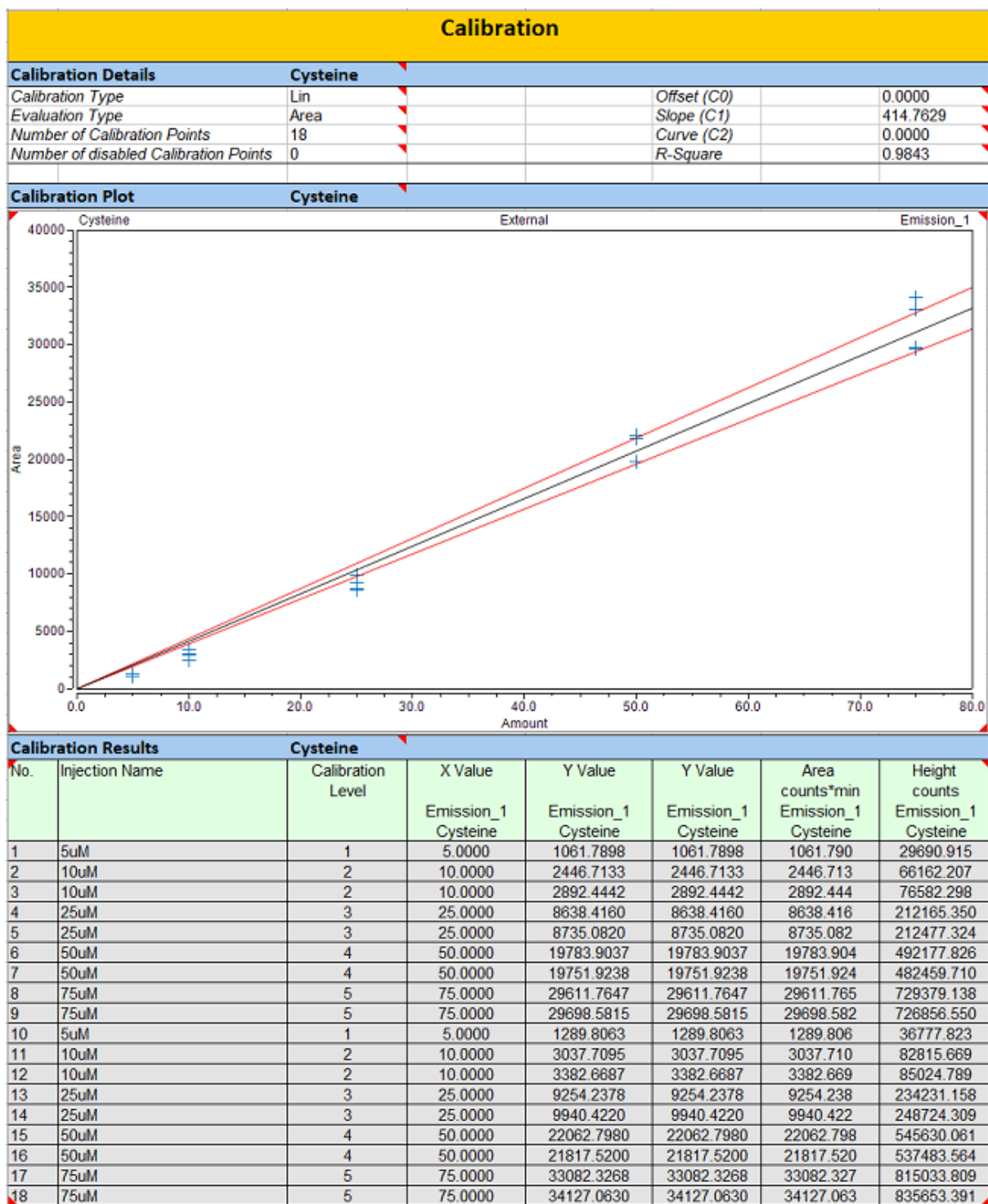


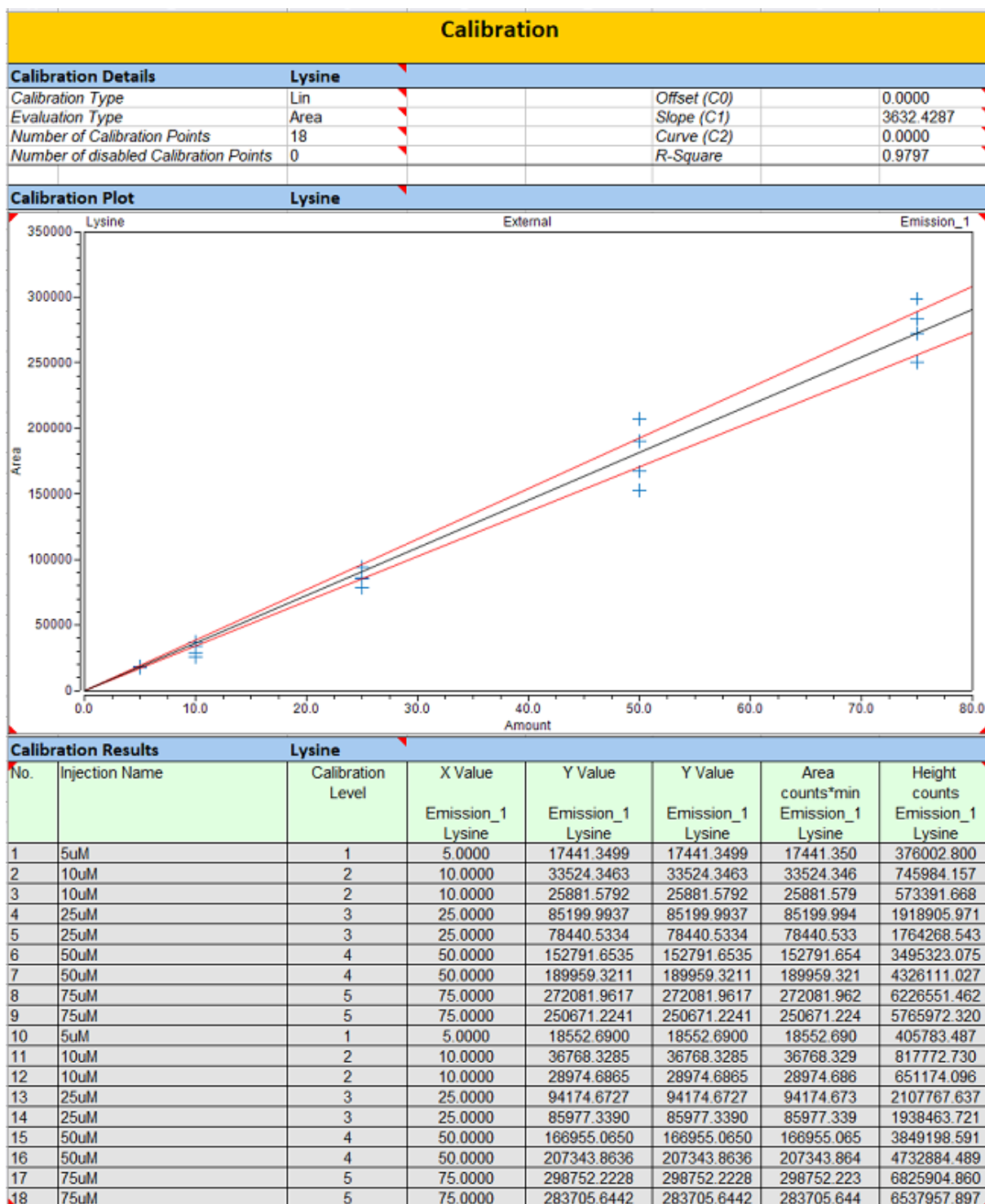
Calibration

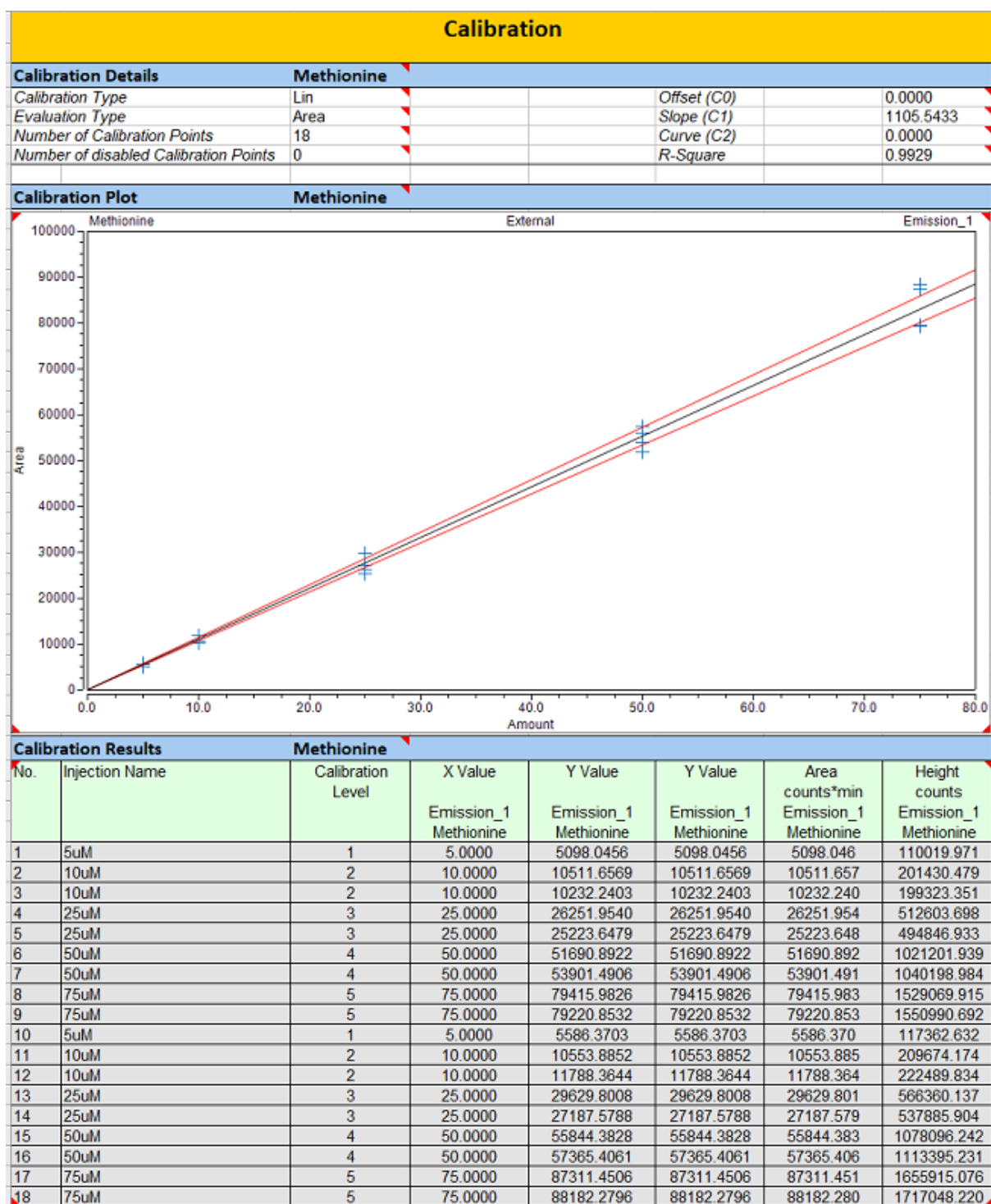
Calibration Details		Proline	
Calibration Type	Lin	Offset (C0)	0.0000
Evaluation Type	Area	Slope (C1)	1452.4449
Number of Calibration Points	18	Curve (C2)	0.0000
Number of disabled Calibration Points	0	R-Square	0.9892



Calibration Results		Proline					
No.	Injection Name	Calibration Level	X Value Emission_1 Proline	Y Value Emission_1 Proline	Y Value Emission_1 Proline	Area counts*min Emission_1 Proline	Height counts Emission_1 Proline
1	5uM	1	5.0000	6382.8285	6382.8285	6382.829	106026.328
2	10uM	2	10.0000	13622.0075	13622.0075	13622.008	212169.718
3	10uM	2	10.0000	12114.3152	12114.3152	12114.315	193487.207
4	25uM	3	25.0000	34612.3600	34612.3600	34612.360	536443.624
5	25uM	3	25.0000	32327.8353	32327.8353	32327.835	498072.002
6	50uM	4	50.0000	65798.8457	65798.8457	65798.846	1005963.498
7	50uM	4	50.0000	71596.4068	71596.4068	71596.407	1092256.079
8	75uM	5	75.0000	105149.9258	105149.9258	105149.926	1604543.430
9	75uM	5	75.0000	101611.4607	101611.4607	101611.461	1556146.818
10	5uM	1	5.0000	7671.5000	7671.5000	7671.500	119755.432
11	10uM	2	10.0000	14448.8987	14448.8987	14448.899	227690.233
12	10uM	2	10.0000	13776.3500	13776.3500	13776.350	213514.033
13	25uM	3	25.0000	38657.5741	38657.5741	38657.574	575889.745
14	25uM	3	25.0000	36448.3534	36448.3534	36448.353	544994.106
15	50uM	4	50.0000	72951.0697	72951.0697	72951.070	1097795.188
16	50uM	4	50.0000	79061.3791	79061.3791	79061.379	1196905.446
17	75uM	5	75.0000	117017.7342	117017.7342	117017.734	1764419.524
18	75uM	5	75.0000	114324.1618	114324.1618	114324.162	1754953.251



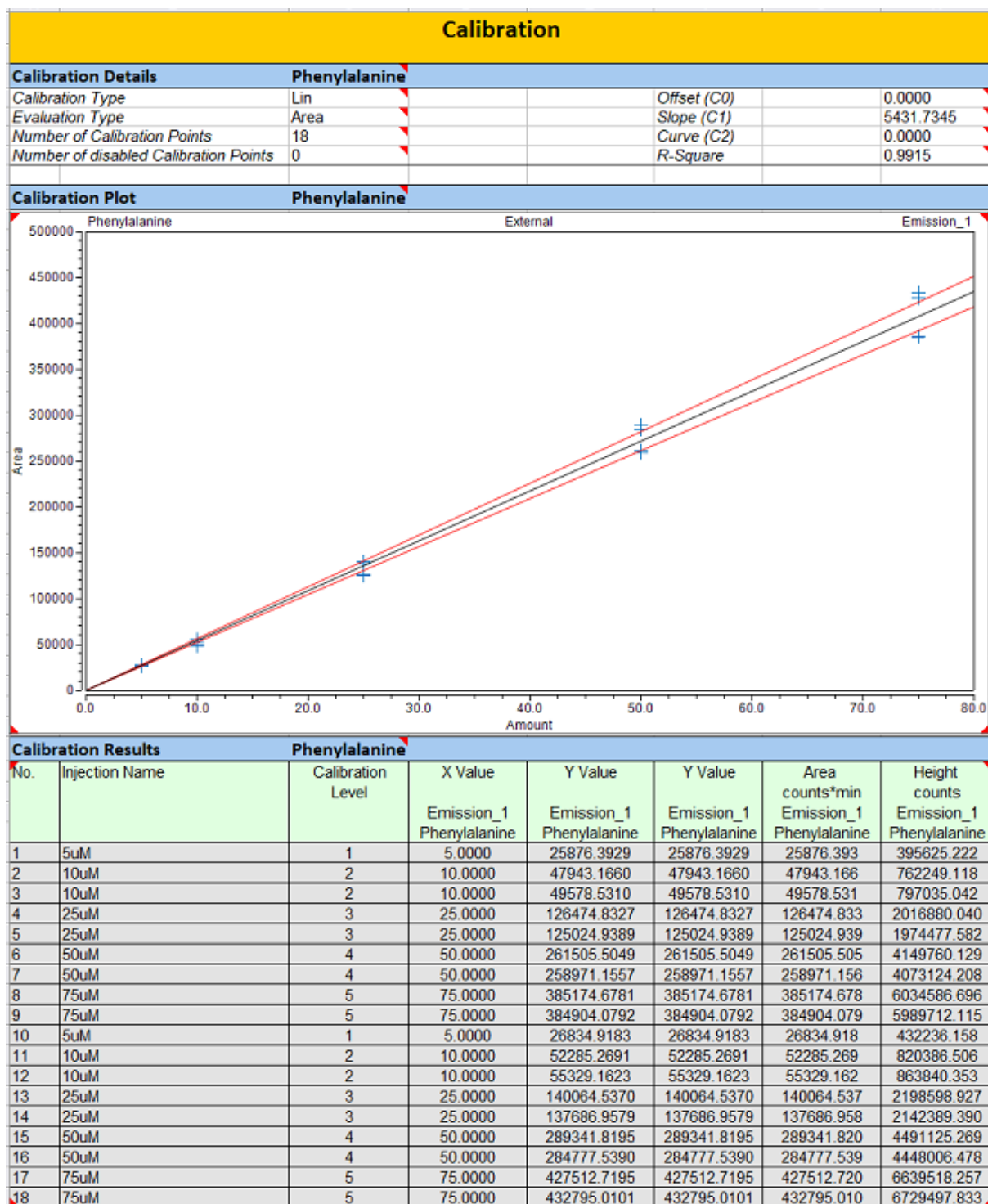


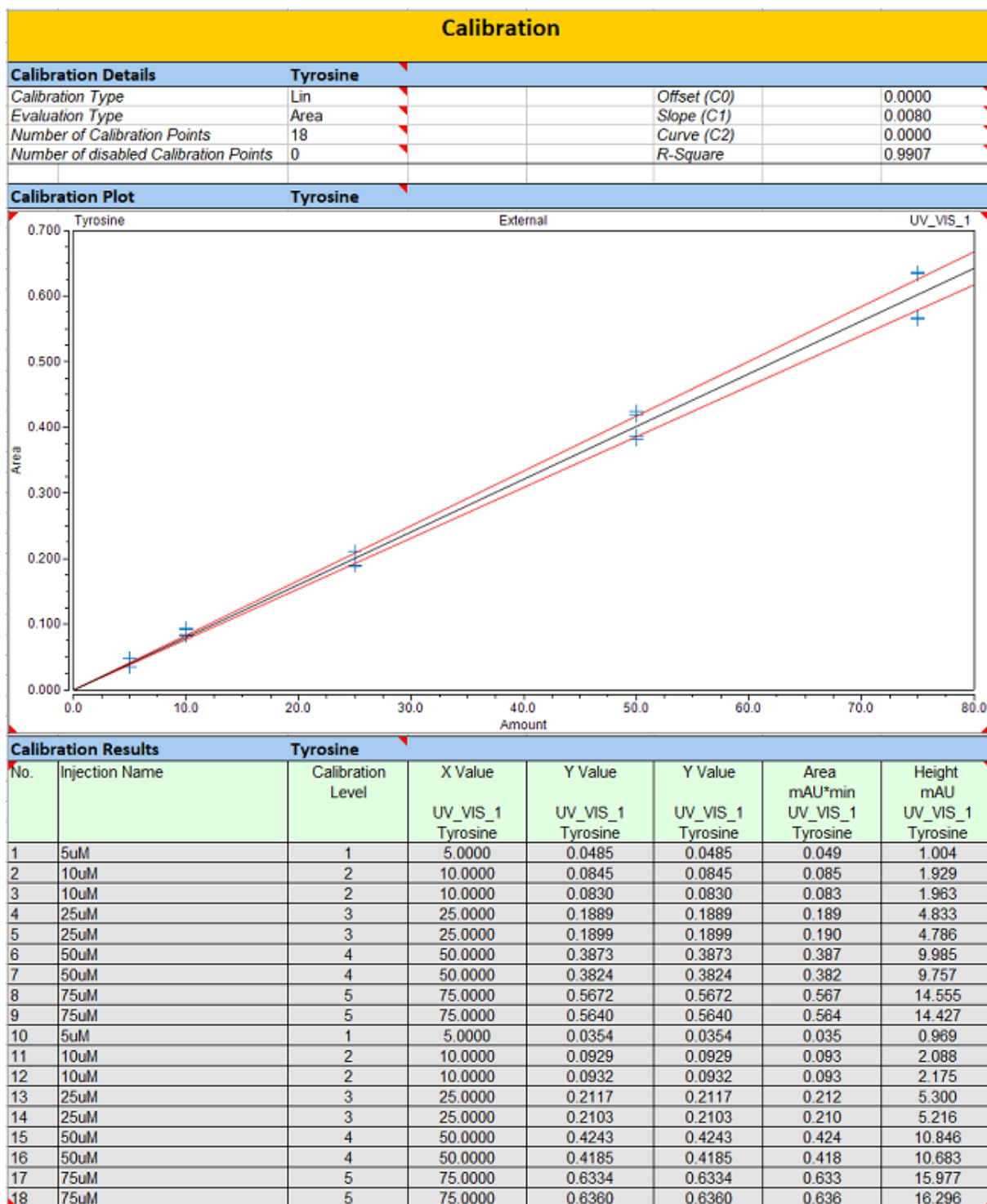


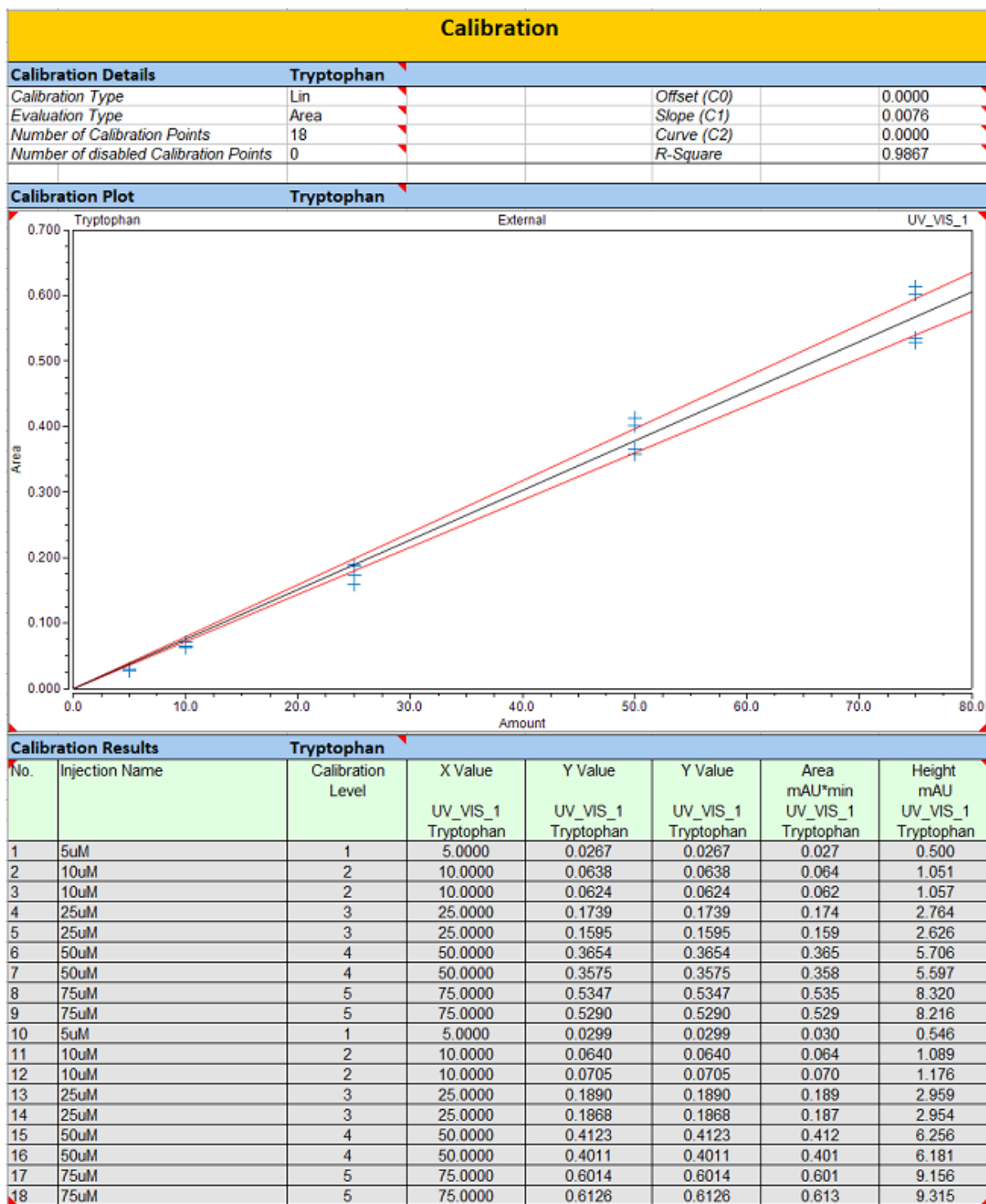






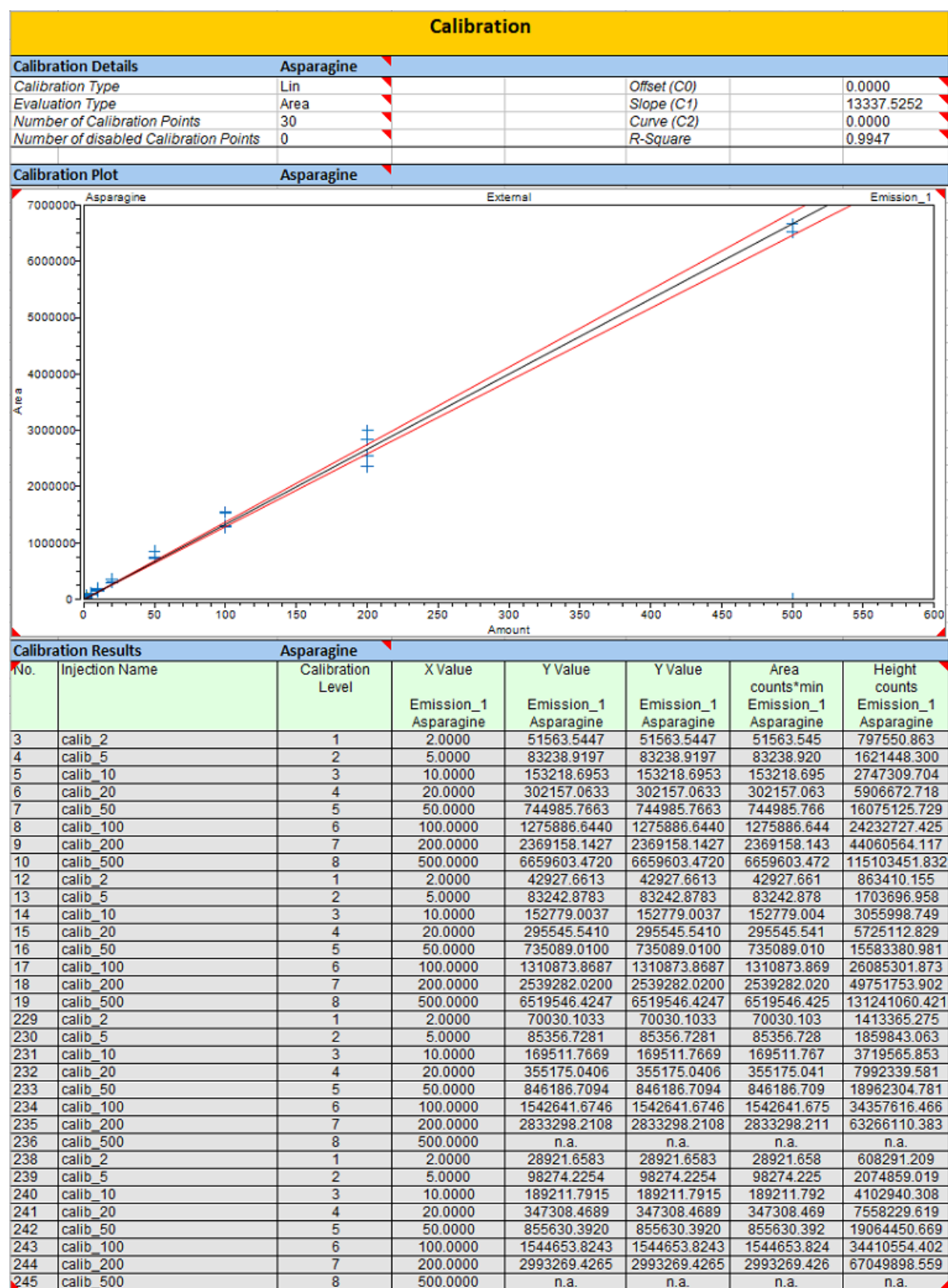


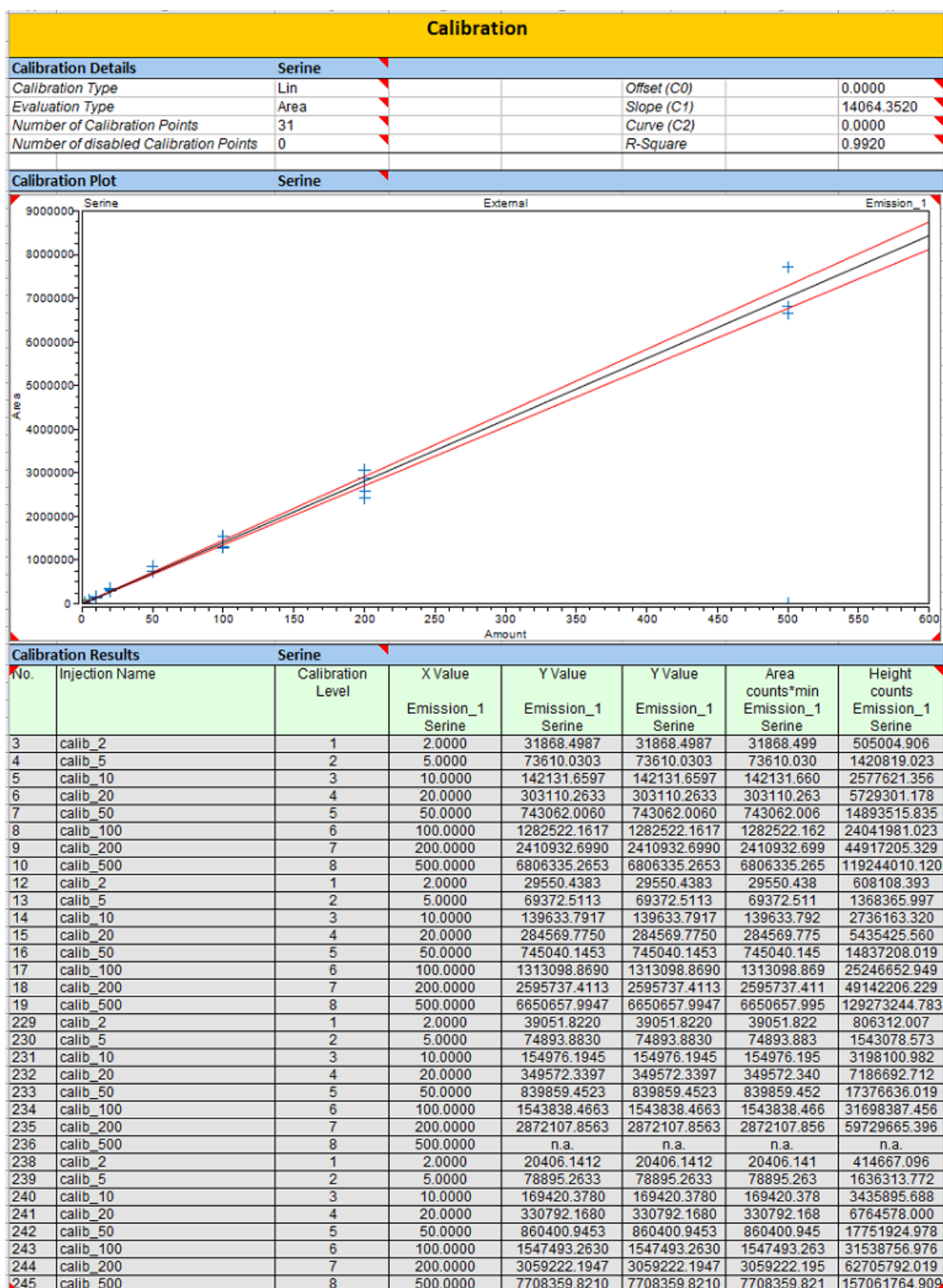


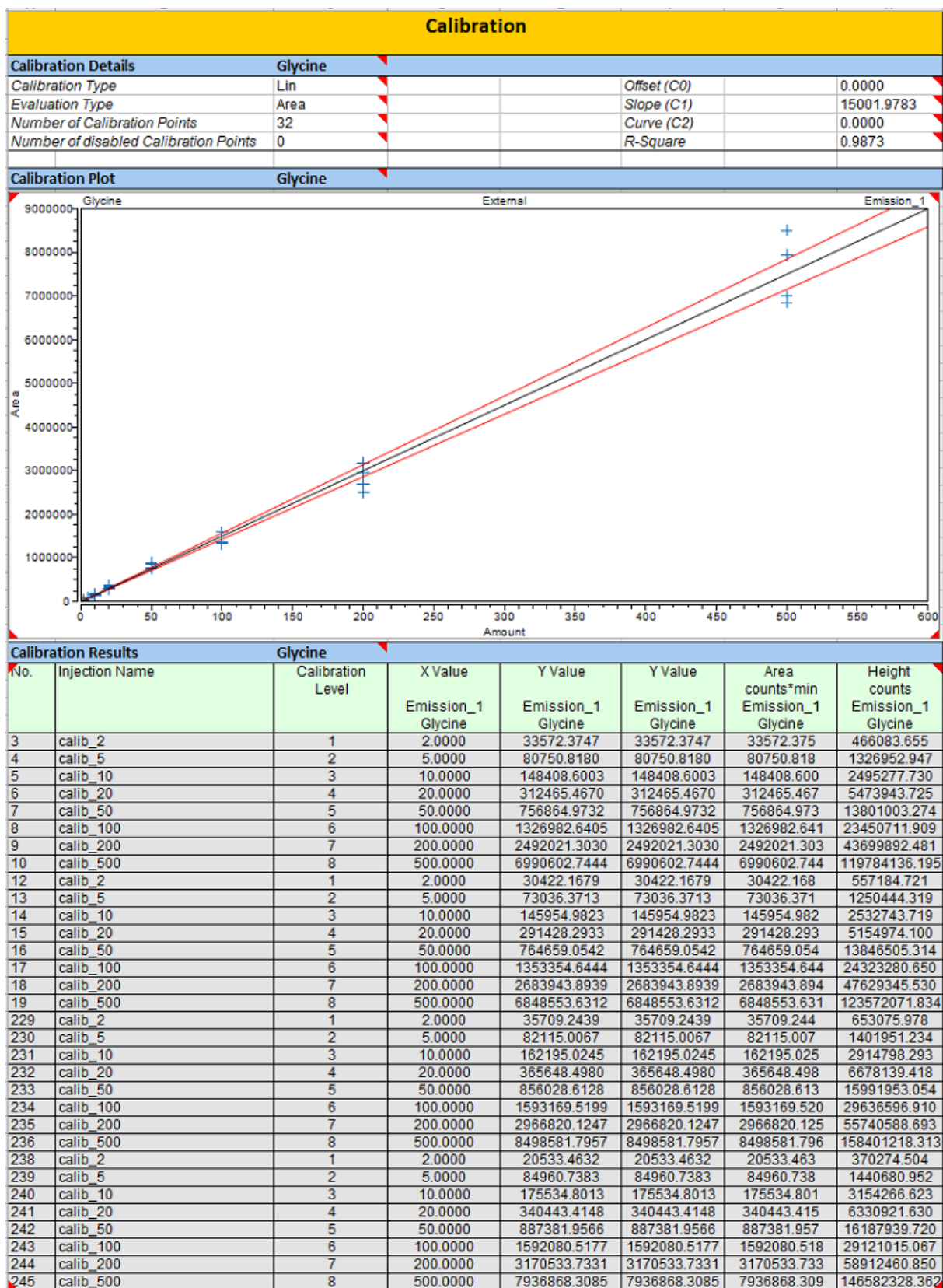


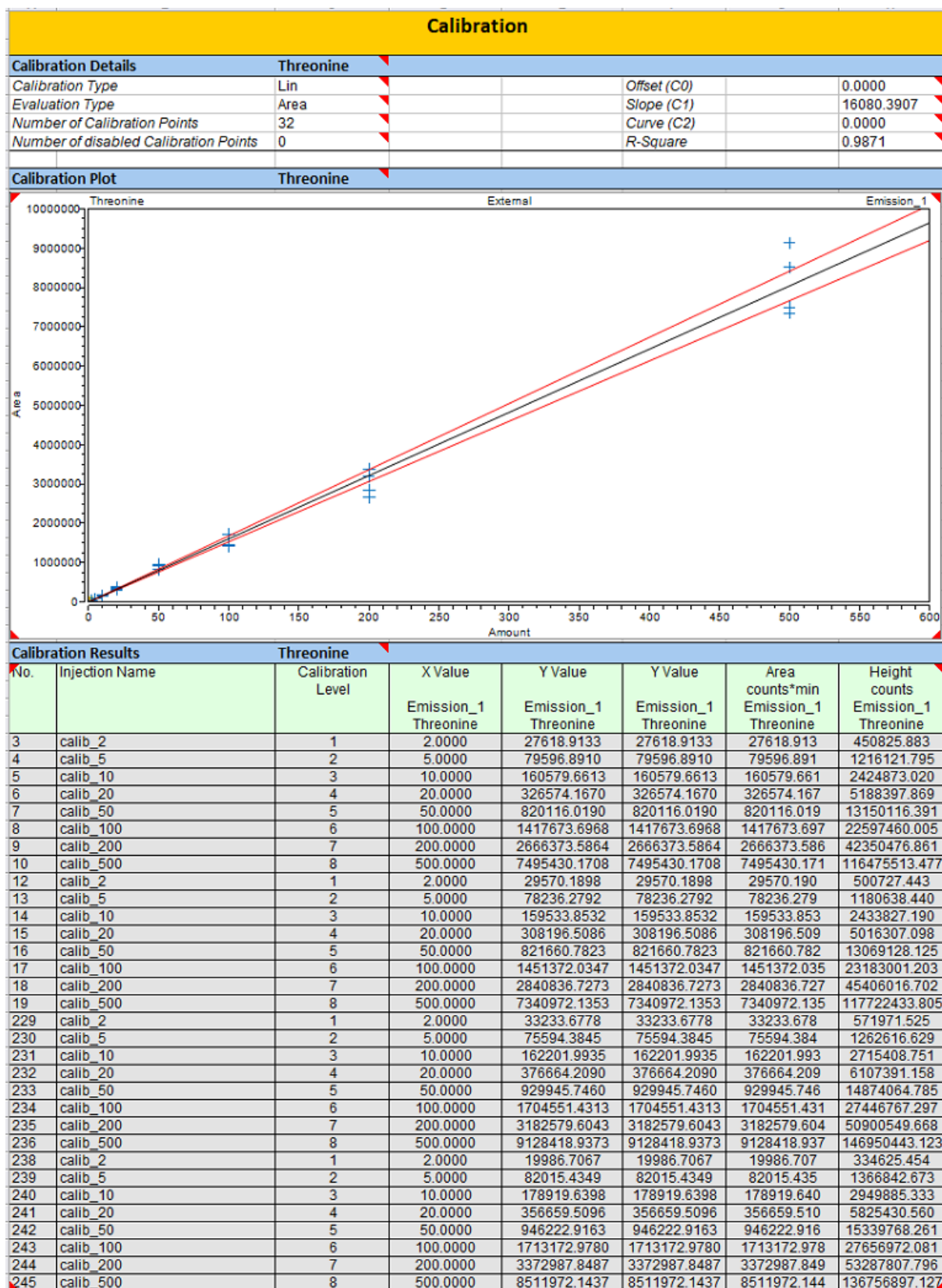
Calibration data amino acids (Fig. 4 – 0 K and 16 K)

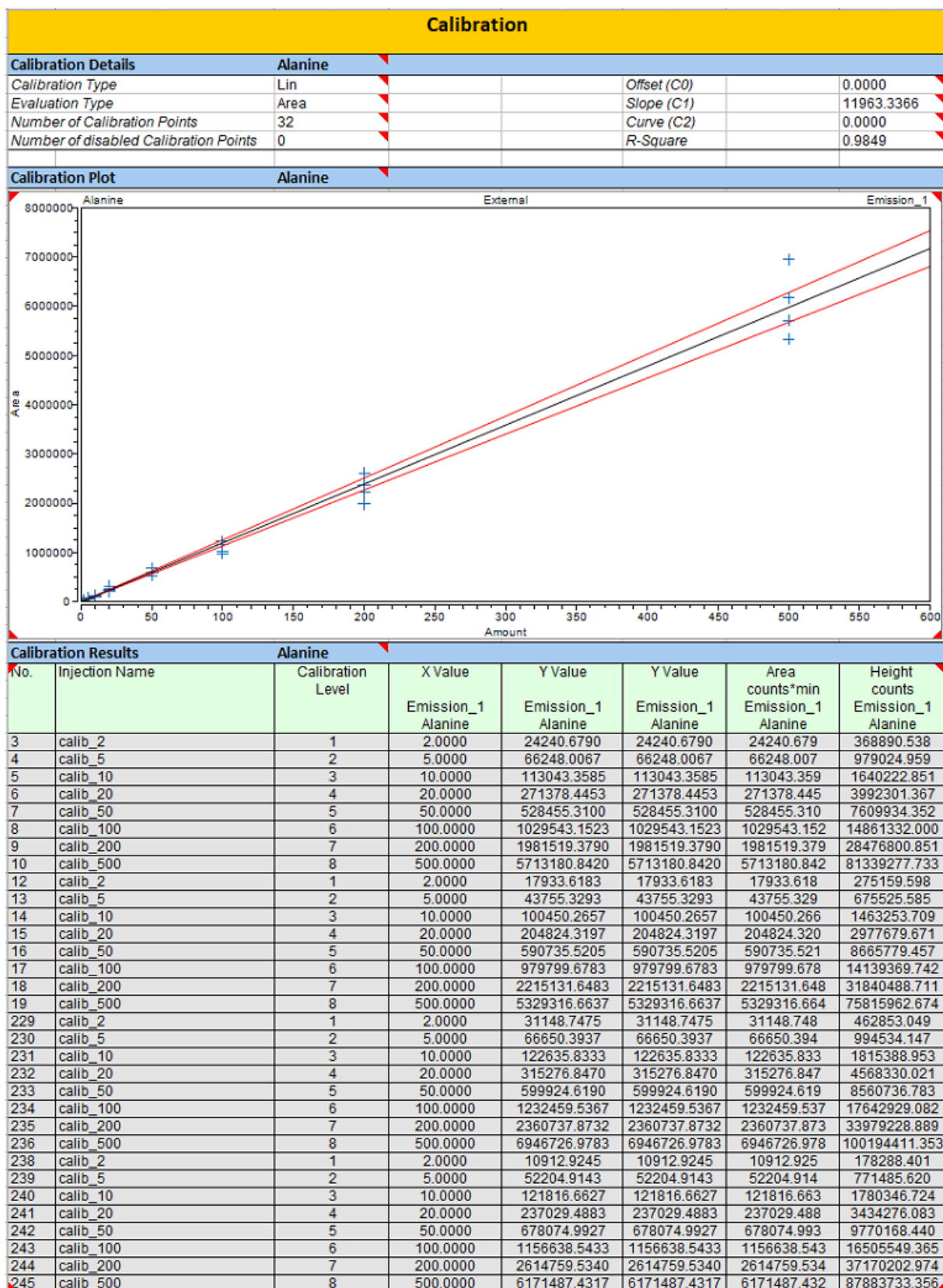
Fluorescence channel for all amino acids (see Methods for details).

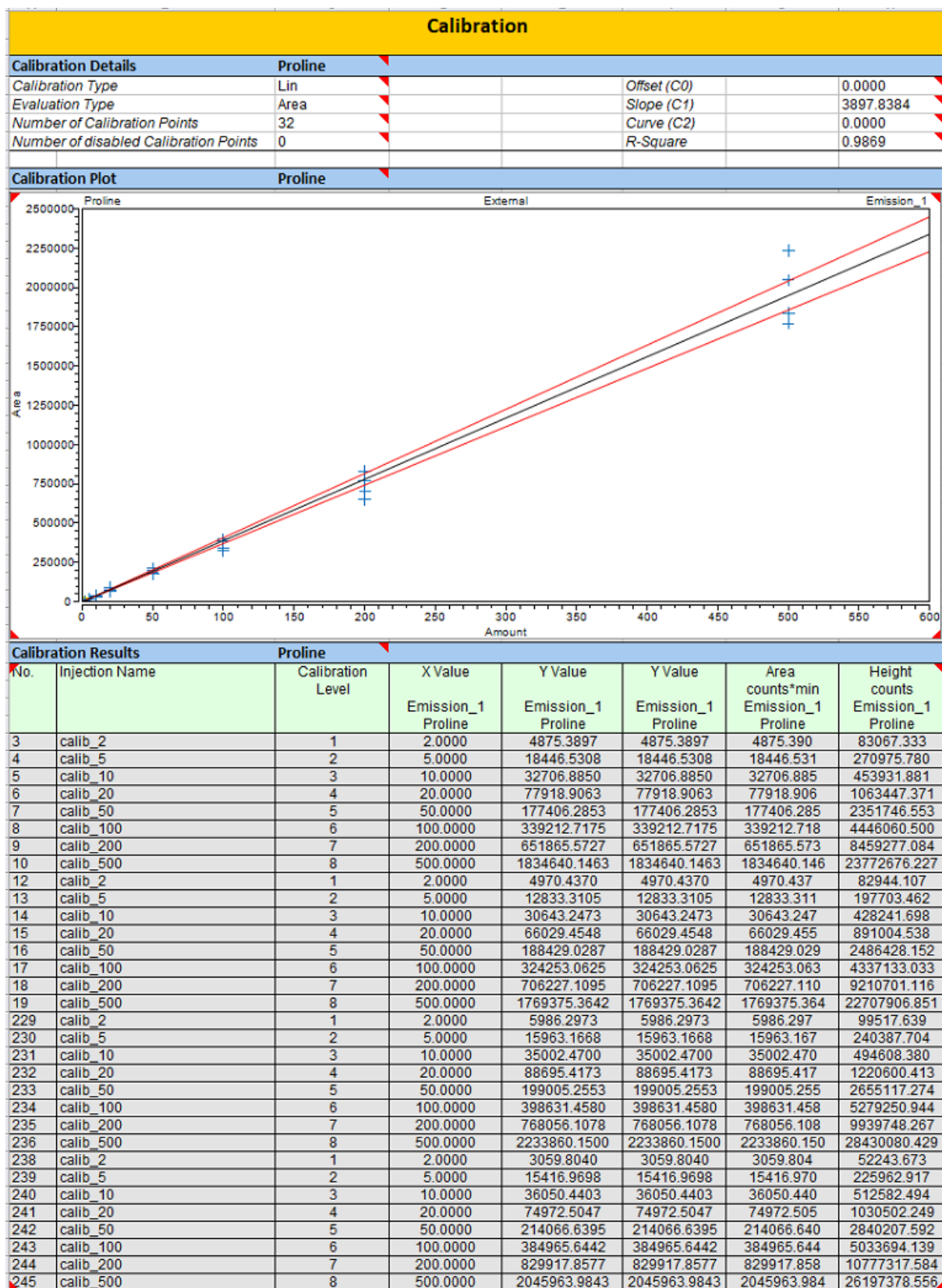


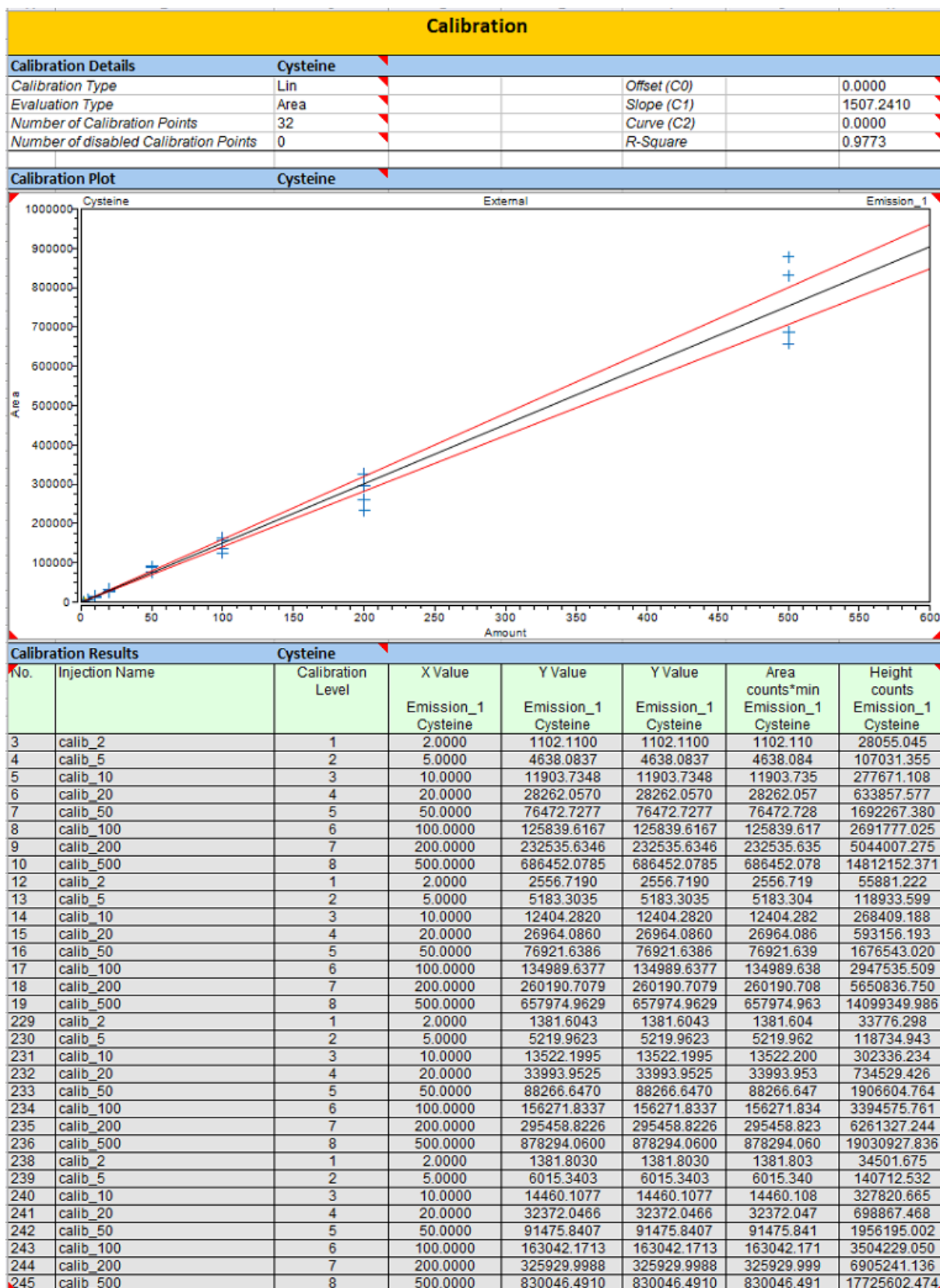


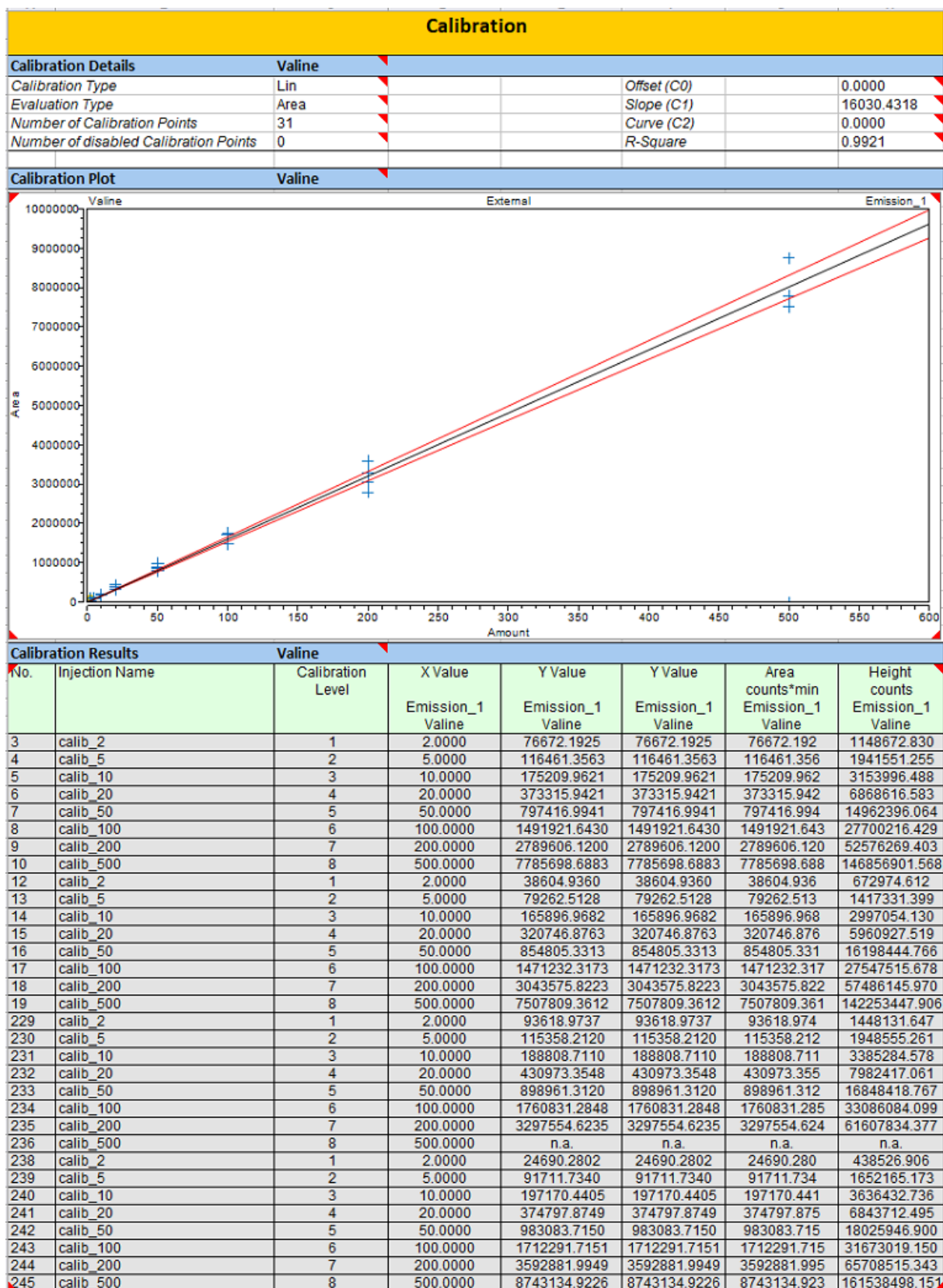


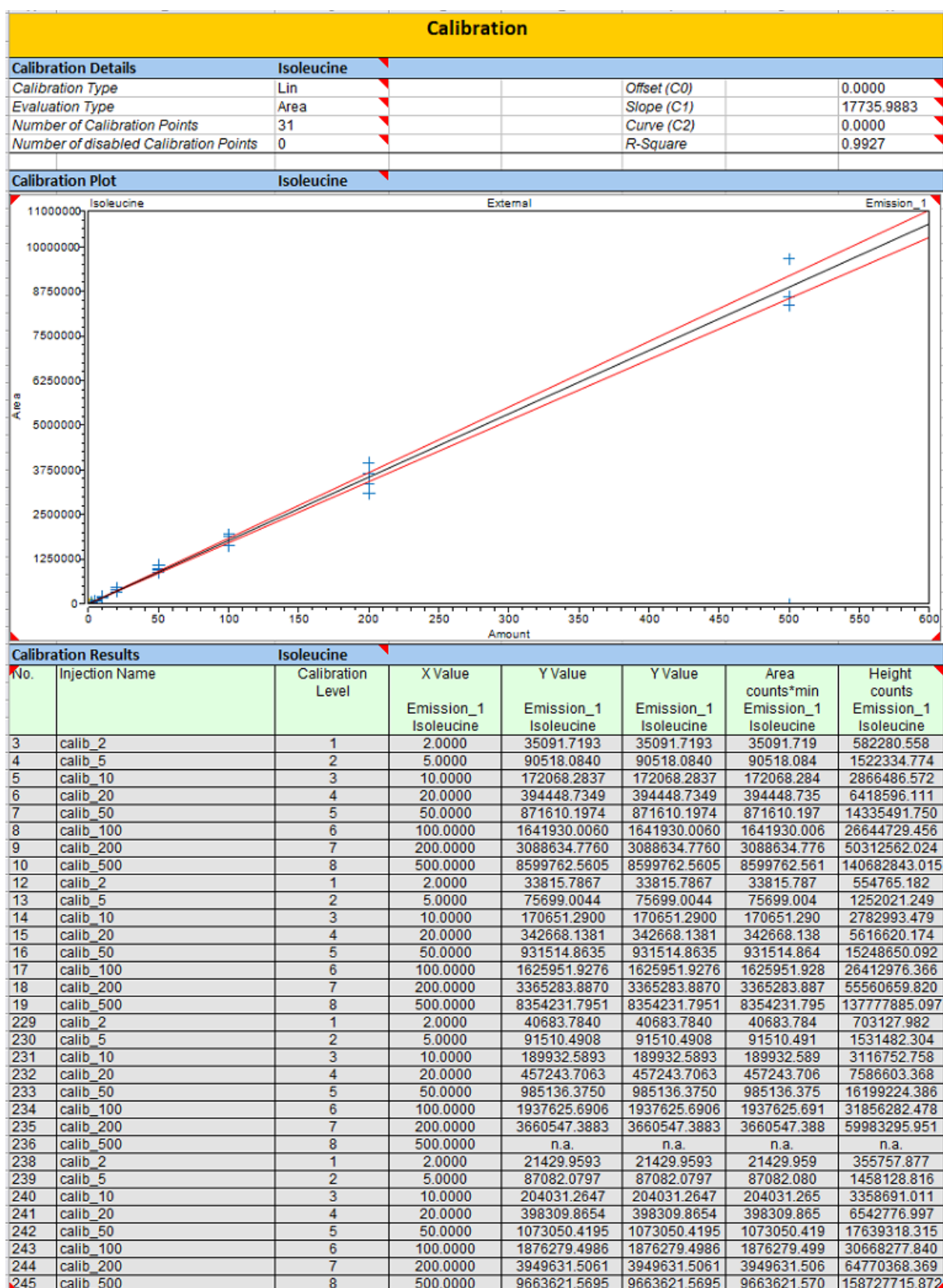


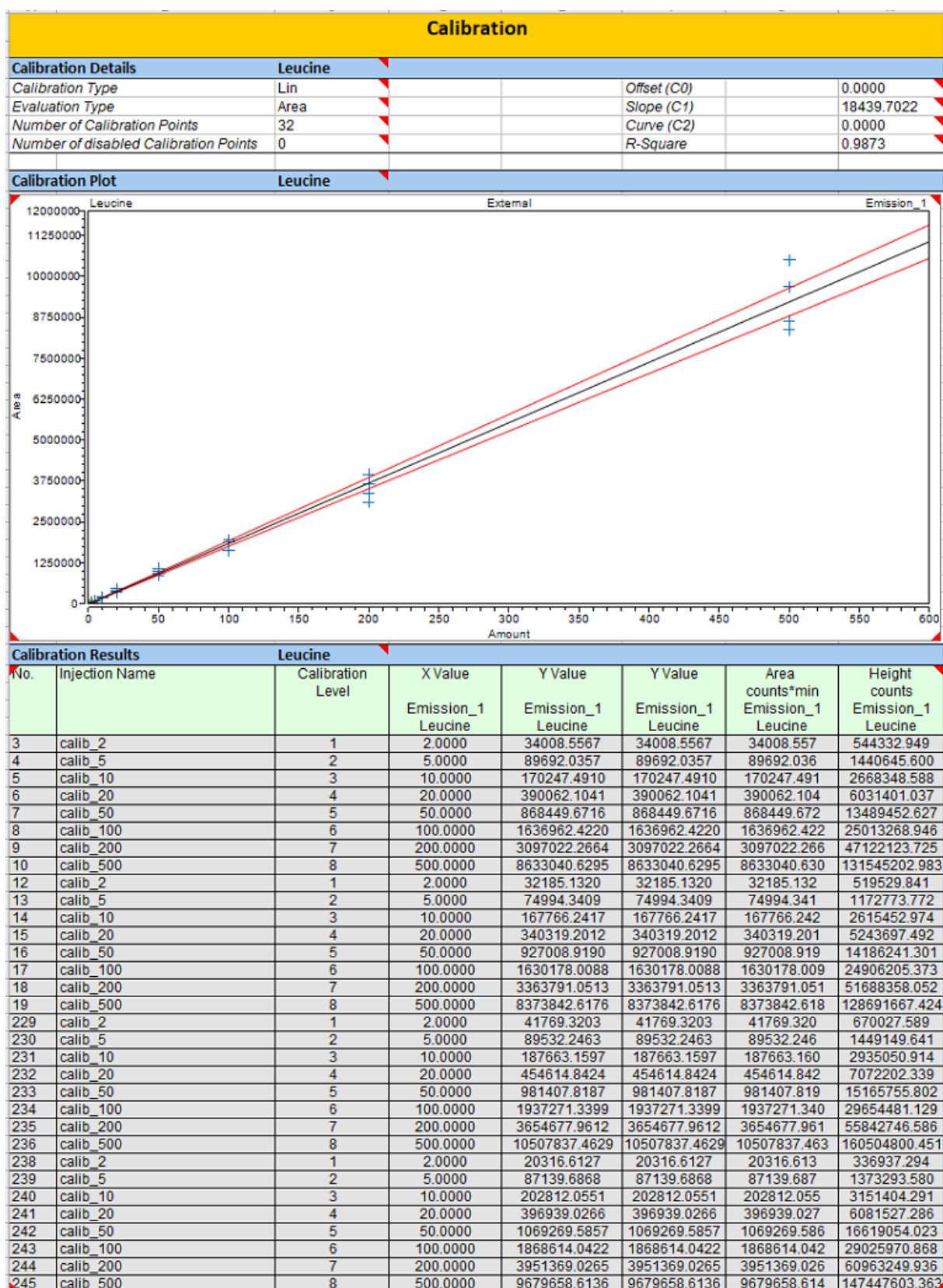


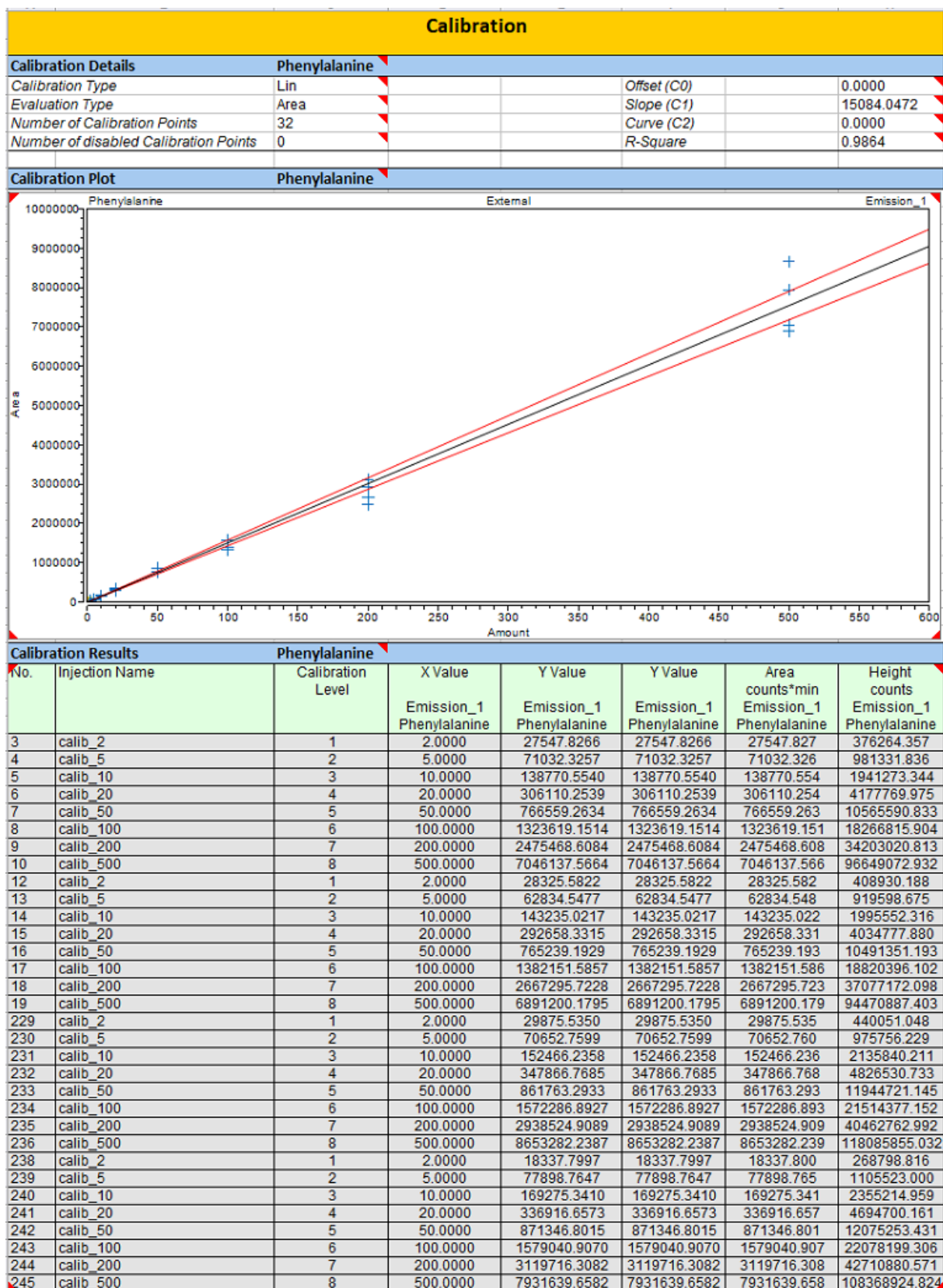






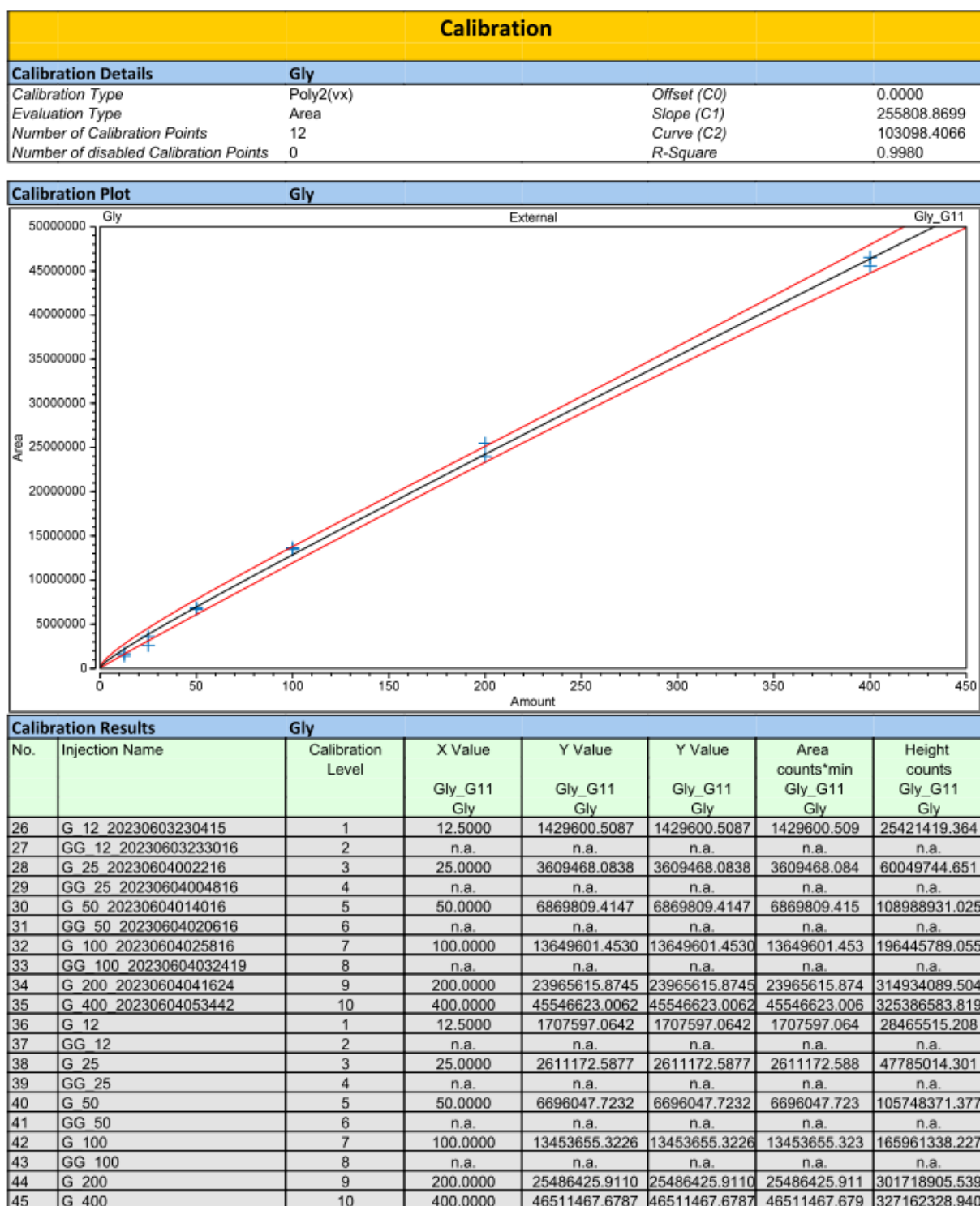




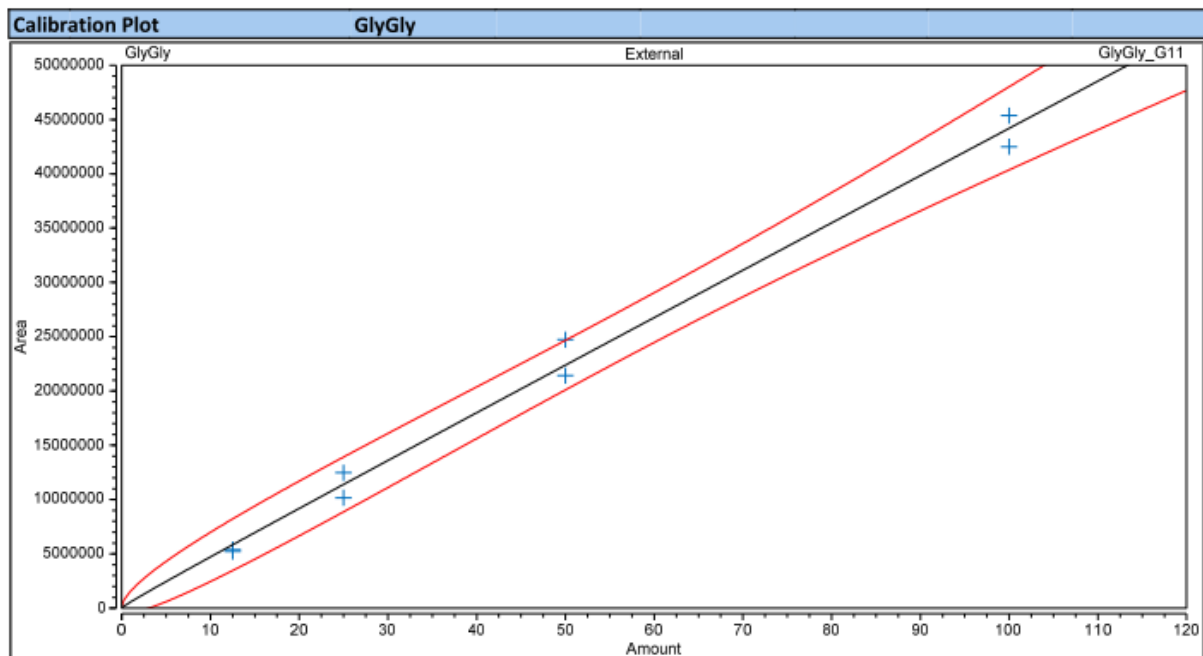


Calibration data dimerization of glycine (Fig. 5)

Detection with mass spectrometry (see Methods for details).



Calibration			
Calibration Details		GlyGly	
Calibration Type	Poly2(vx)	Offset (C0)	0.0000
Evaluation Type	Area	Slope (C1)	139176.2585
Number of Calibration Points	8	Curve (C2)	427965.4347
Number of disabled Calibration Points	0	R-Square	0.9921



Calibration Results		GlyGly					
No.	Injection Name	Calibration Level	X Value GlyGly_G11 GlyGly	Y Value GlyGly_G11 GlyGly	Y Value GlyGly_G11 GlyGly	Area counts*min GlyGly_G11 GlyGly	Height counts GlyGly_G11 GlyGly
26	G 12 20230603230415	1	n.a.	n.a.	n.a.	n.a.	n.a.
27	GG 12 20230603233016	2	12.5000	5384754.0942	5384754.0942	5384754.094	97637773.424
28	G 25 20230604002216	3	n.a.	n.a.	n.a.	n.a.	n.a.
29	GG 25 20230604004816	4	25.0000	12477607.2745	12477607.2745	12477607.275	196759190.800
30	G 50 20230604014016	5	n.a.	n.a.	n.a.	n.a.	n.a.
31	GG 50 20230604020616	6	50.0000	21412660.7238	21412660.7238	21412660.724	356168404.774
32	G 100 20230604025816	7	n.a.	n.a.	n.a.	n.a.	n.a.
33	GG 100 20230604032419	8	100.0000	42500409.6149	42500409.6149	42500409.615	677670184.695
34	G 200 20230604041624	9	n.a.	n.a.	n.a.	n.a.	n.a.
35	G 400 20230604053442	10	n.a.	n.a.	n.a.	n.a.	n.a.
36	G 12	1	n.a.	n.a.	n.a.	n.a.	n.a.
37	GG 12	2	12.5000	5219763.2798	5219763.2798	5219763.280	90770186.825
38	G 25	3	n.a.	n.a.	n.a.	n.a.	n.a.
39	GG 25	4	25.0000	10165642.4339	10165642.4339	10165642.434	199402806.172
40	G 50	5	n.a.	n.a.	n.a.	n.a.	n.a.
41	GG 50	6	50.0000	24719767.7495	24719767.7495	24719767.749	438024122.537
42	G 100	7	n.a.	n.a.	n.a.	n.a.	n.a.
43	GG 100	8	100.0000	45363923.8196	45363923.8196	45363923.820	646217894.684
44	G 200	9	n.a.	n.a.	n.a.	n.a.	n.a.
45	G 400	10	n.a.	n.a.	n.a.	n.a.	n.a.