

SUPPLEMENTARY INFORMATION

Structured plant metabolomics for the simultaneous exploration of multiple factors

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R code for design generation

```
require(DoE.base)

show.oas(factors = list(nlevels=c(2,3,4), number=c(12,1,1)), show = "all", showmetrics=TRUE)

Experimental.plan<- oa.design(ID=L96.2.19.3.1.4.23,
nlevels=c(2,2,2,2,2,4,3,2,2,2,2,2,2,2), columns="min34",
  factor.names=list(
    KNO3=c("-", "+"), NH4NO3=c("-", "+"), CaCl2=c("-", "+"), KH2PO4=c("-", "+"),
    MgSO4=c("-", "+"),
    auxins=c("IAA", "IBA", "NAA", "2.4-D"),
    cytokinins=c("kinetin", "DH-zeatin", "BAP"),
    MeJa=c("MeJa-", "MeJa+"),
    SA=c("-", "+"),
    GA3=c("-", "+"),
    Ethephon=c("-", "+"), Cyclanilide=c("-", "+"),
    AbscA=c("-", "+"),
    Light=c("Lght-", "Lght+")),
  seed = 49, randomize=TRUE)

Experimental.plan
```

Table S1. Factor levels.

	Low level (-)	High level (+)
<i>Nutrients</i>		
NH₄NO₃	4.24 mM	20.61 mM
KNO₃	18.79 mM	70.16 mM
CaCl₂	2.99 mM	10.84 mM
KH₂PO₄	1.25 mM	2.72 mM
MgSO₄	1.5 mM	3.0 mM
<i>Auxins</i>		
<i>(10 μM of chosen one; reference level underlined)</i>		
	IAA	<u>IBA</u> NAA 2,4-D
<i>Cytokinins</i>		
<i>(10 μM of chosen one; reference level underlined)</i>		
	Kinetin	DHZ <u>BAP</u>
<i>Elicitors</i>		
MeJa	0 μM	10 μM
Salicylic acid	0 μM	10 μM
GA₃	0 μM	10 μM
Ethephon	0 μM	10 μM
Cyclanilide	0 μM	10 μM
Absciscic acid	0 μM	10 μM
Light	11.5 μmol/s	35.62 μmol/s

Table S2. Experimental design in coded values.

Run name	KNO ₃	NH ₄ NO ₃	CaCl ₂	KH ₂ PO ₄	MgSO ₄	Auxins	Cytokinins	MeJa	SA	GA ₃	Ethephon	Cyclanilide	ABA	Light
1	-	+	-	+	+	IAA	DHZ	MeJa+	+	+	-	+	+	Lght+
2	-	+	+	+	+	NAA	Kinetin	MeJa+	-	+	+	+	+	Lght+
3	-	+	-	-	-	2,4-D	Kinetin	MeJa-	+	+	+	+	+	Lght+
4	+	-	-	+	-	IAA	Kinetin	MeJa+	-	+	-	-	+	Lght+
5	-	-	-	-	+	IAA	DHZ	MeJa-	+	+	+	-	+	Lght+
6	-	+	-	-	-	IAA	BAP	MeJa+	+	+	+	-	-	Lght+
7	-	+	-	-	-	NAA	DHZ	MeJa-	+	-	-	+	+	Lght+
8	-	-	-	+	-	IAA	BAP	MeJa+	+	-	+	-	+	Lght-
9	+	+	+	+	+	2,4-D	DHZ	MeJa-	+	+	+	-	+	Lght+
10	+	-	+	+	+	NAA	DHZ	MeJa+	-	+	-	-	-	Lght-
11	-	-	+	+	+	NAA	DHZ	MeJa-	+	-	+	+	+	Lght-
12	-	+	+	-	-	NAA	DHZ	MeJa-	-	+	+	+	-	Lght-
13	-	-	-	+	+	IBA	Kinetin	MeJa-	-	-	-	+	+	Lght-
14	+	-	-	+	-	IBA	DHZ	MeJa-	-	+	+	+	-	Lght-
15	+	+	-	+	-	IBA	BAP	MeJa+	+	-	-	-	+	Lght+
16	-	-	-	-	-	2,4-D	DHZ	MeJa+	-	-	+	+	+	Lght-
17	+	-	-	-	+	IBA	Kinetin	MeJa+	-	+	+	+	+	Lght+
18	-	-	+	-	+	2,4-D	Kinetin	MeJa-	-	+	+	-	-	Lght-
19	-	+	+	-	-	IBA	DHZ	MeJa-	-	+	-	+	+	Lght+
20	+	+	+	+	+	IBA	Kinetin	MeJa+	+	+	-	+	-	Lght-
21	+	+	+	-	-	IBA	Kinetin	MeJa+	+	+	+	-	-	Lght-
22	+	-	+	-	+	IBA	Kinetin	MeJa-	+	+	-	-	+	Lght+
23	+	+	-	-	+	IBA	DHZ	MeJa-	+	-	+	+	+	Lght-
24	+	-	-	+	+	NAA	DHZ	MeJa+	+	-	+	-	-	Lght+
25	-	-	-	+	+	2,4-D	BAP	MeJa-	-	-	-	-	+	Lght+
26	+	-	+	-	-	NAA	Kinetin	MeJa+	-	-	+	-	+	Lght-

Run name	KNO ₃	NH ₄ NO ₃	CaCl ₂	KH ₂ PO ₄	MgSO ₄	Auxins	Cytokinins	MeJa	SA	GA ₃	Ethephon	Cyclanilide	ABA	Light
27	+	-	+	-	-	2,4-D	DHZ	MeJa-	-	-	+	-	-	Lght+
28	-	-	-	+	+	NAA	BAP	MeJa+	-	+	-	-	+	Lght-
29	+	-	+	-	+	IAA	DHZ	MeJa+	+	+	+	+	-	Lght-
30	+	+	-	+	+	2,4-D	BAP	MeJa+	-	+	+	+	+	Lght-
31	-	+	+	+	-	NAA	BAP	MeJa+	+	+	-	+	-	Lght+
32	+	+	+	-	+	IAA	BAP	MeJa-	-	-	-	-	+	Lght+
33	-	-	-	+	-	IBA	BAP	MeJa-	+	+	+	+	+	Lght-
34	-	+	-	+	+	2,4-D	DHZ	MeJa+	+	+	+	+	-	Lght-
35	+	+	+	+	-	IAA	DHZ	MeJa+	-	-	+	+	+	Lght-
36	-	+	-	+	+	NAA	Kinetin	MeJa-	+	+	-	-	+	Lght+
37	+	-	-	-	+	IAA	DHZ	MeJa+	-	-	-	+	+	Lght+
38	+	-	+	-	-	IAA	DHZ	MeJa-	-	-	-	-	-	Lght-
39	+	+	-	-	-	NAA	DHZ	MeJa+	-	+	+	-	+	Lght+
40	+	-	+	+	-	2,4-D	BAP	MeJa+	+	+	+	-	-	Lght+
41	-	+	-	+	-	IAA	DHZ	MeJa-	-	-	+	-	-	Lght+
42	+	-	+	-	+	2,4-D	DHZ	MeJa+	+	+	-	+	+	Lght+
43	+	+	+	+	-	IBA	BAP	MeJa+	-	-	+	+	-	Lght+
44	-	-	+	-	-	NAA	BAP	MeJa+	+	-	-	-	+	Lght+
45	+	-	-	+	-	NAA	DHZ	MeJa-	-	+	-	+	+	Lght+
46	-	+	+	-	+	IAA	Kinetin	MeJa-	+	-	+	-	+	Lght-
47	+	-	-	-	-	NAA	Kinetin	MeJa-	+	-	-	-	-	Lght+
48	-	-	+	-	+	IAA	BAP	MeJa+	-	+	+	+	+	Lght-
49	-	+	+	+	+	2,4-D	DHZ	MeJa+	-	-	-	+	+	Lght+
50	-	-	+	+	-	2,4-D	Kinetin	MeJa-	-	+	-	+	-	Lght-
51	-	+	+	+	+	IBA	BAP	MeJa-	-	+	+	-	-	Lght+
52	-	-	+	+	-	IBA	DHZ	MeJa+	-	+	+	-	+	Lght+
53	+	-	-	-	-	2,4-D	DHZ	MeJa-	+	+	-	-	-	Lght-
54	-	+	-	+	-	IBA	Kinetin	MeJa+	-	-	+	-	+	Lght-

Run name	KNO ₃	NH ₄ NO ₃	CaCl ₂	KH ₂ PO ₄	MgSO ₄	Auxins	Cytokinins	MeJa	SA	GA ₃	Ethephon	Cyclanilide	ABA	Light
55	-	+	-	+	-	2,4-D	DHZ	MeJa-	-	-	-	-	-	Lght-
56	-	-	+	+	+	2,4-D	BAP	MeJa-	+	-	+	+	-	Lght+
57	+	-	+	+	+	2,4-D	Kinetin	MeJa+	-	-	-	-	-	Lght+
58	+	-	-	+	+	2,4-D	Kinetin	MeJa-	+	-	+	-	+	Lght-
59	+	+	-	-	-	IAA	Kinetin	MeJa-	-	+	-	+	-	Lght-
60	-	+	+	-	+	NAA	DHZ	MeJa+	+	-	-	-	-	Lght-
61	-	-	+	-	-	IAA	Kinetin	MeJa+	+	-	-	+	+	Lght-
62	-	+	+	-	+	IBA	DHZ	MeJa+	+	-	+	-	-	Lght+
63	-	-	-	-	-	IBA	Kinetin	MeJa-	-	-	+	+	-	Lght+
64	+	-	+	+	+	IAA	BAP	MeJa-	-	+	-	+	-	Lght+
65	-	-	+	+	-	IAA	BAP	MeJa+	-	-	-	+	-	Lght-
66	+	+	+	+	+	NAA	BAP	MeJa-	+	-	-	+	-	Lght-
67	+	+	+	-	-	2,4-D	BAP	MeJa+	+	-	+	-	+	Lght-
68	+	+	-	-	-	2,4-D	BAP	MeJa+	-	-	-	+	-	Lght-
69	-	-	-	+	-	NAA	Kinetin	MeJa+	+	+	+	-	-	Lght-
70	+	-	-	+	+	IBA	DHZ	MeJa+	+	-	-	-	-	Lght-
71	+	+	+	-	-	NAA	BAP	MeJa-	+	+	+	+	+	Lght-
72	+	+	-	+	+	NAA	BAP	MeJa-	-	-	+	-	+	Lght-
73	+	+	+	+	-	NAA	Kinetin	MeJa-	-	-	+	+	-	Lght+
74	+	-	-	-	-	IBA	BAP	MeJa+	+	+	-	+	-	Lght+
75	+	+	+	-	+	NAA	Kinetin	MeJa-	-	-	-	+	+	Lght-
76	-	-	-	-	-	NAA	BAP	MeJa+	-	-	+	+	-	Lght+
77	-	-	-	-	+	IBA	BAP	MeJa-	+	-	-	+	-	Lght-
78	+	+	-	-	+	2,4-D	Kinetin	MeJa+	+	-	+	+	-	Lght+
79	+	+	-	-	+	IAA	BAP	MeJa-	+	-	+	+	-	Lght+
80	-	+	-	-	+	2,4-D	BAP	MeJa-	-	+	-	+	-	Lght+
81	+	-	+	+	-	IAA	Kinetin	MeJa-	+	+	+	+	+	Lght+
82	-	+	-	-	+	IBA	DHZ	MeJa+	-	+	-	-	-	Lght-

Run name	KNO ₃	NH ₄ NO ₃	CaCl ₂	KH ₂ PO ₄	MgSO ₄	Auxins	Cytokinins	MeJa	SA	GA ₃	Ethephon	Cyclanilide	ABA	Light
83	+	+	-	+	-	IAA	BAP	MeJa-	+	+	-	-	+	Lght-
84	+	+	-	+	+	IAA	Kinetin	MeJa-	-	+	+	-	-	Lght-
85	-	-	+	-	+	IBA	BAP	MeJa-	-	-	+	-	+	Lght-
86	-	+	+	-	-	2,4-D	Kinetin	MeJa+	-	+	-	-	+	Lght+
87	-	+	-	-	+	IAA	Kinetin	MeJa+	-	-	-	-	-	Lght+
88	-	-	+	-	-	2,4-D	BAP	MeJa-	+	+	-	-	+	Lght-
89	-	-	-	-	+	NAA	Kinetin	MeJa+	+	+	-	+	-	Lght-
90	+	+	-	+	-	2,4-D	Kinetin	MeJa+	+	-	-	+	+	Lght-
91	-	+	+	+	-	IAA	DHZ	MeJa-	+	+	-	-	-	Lght-
92	+	-	+	+	-	IBA	DHZ	MeJa-	+	-	-	+	+	Lght+
93	+	-	-	-	+	NAA	BAP	MeJa-	-	+	+	-	-	Lght+
94	+	+	+	-	+	IBA	BAP	MeJa+	-	+	-	-	+	Lght-
95	-	-	+	+	+	IAA	Kinetin	MeJa+	+	-	+	+	-	Lght+
96	-	+	+	+	-	IBA	Kinetin	MeJa-	+	-	-	-	-	Lght+

Figure S1. NH_4NO_3 S-plot



Figure S2. CaCl₂ S-plot

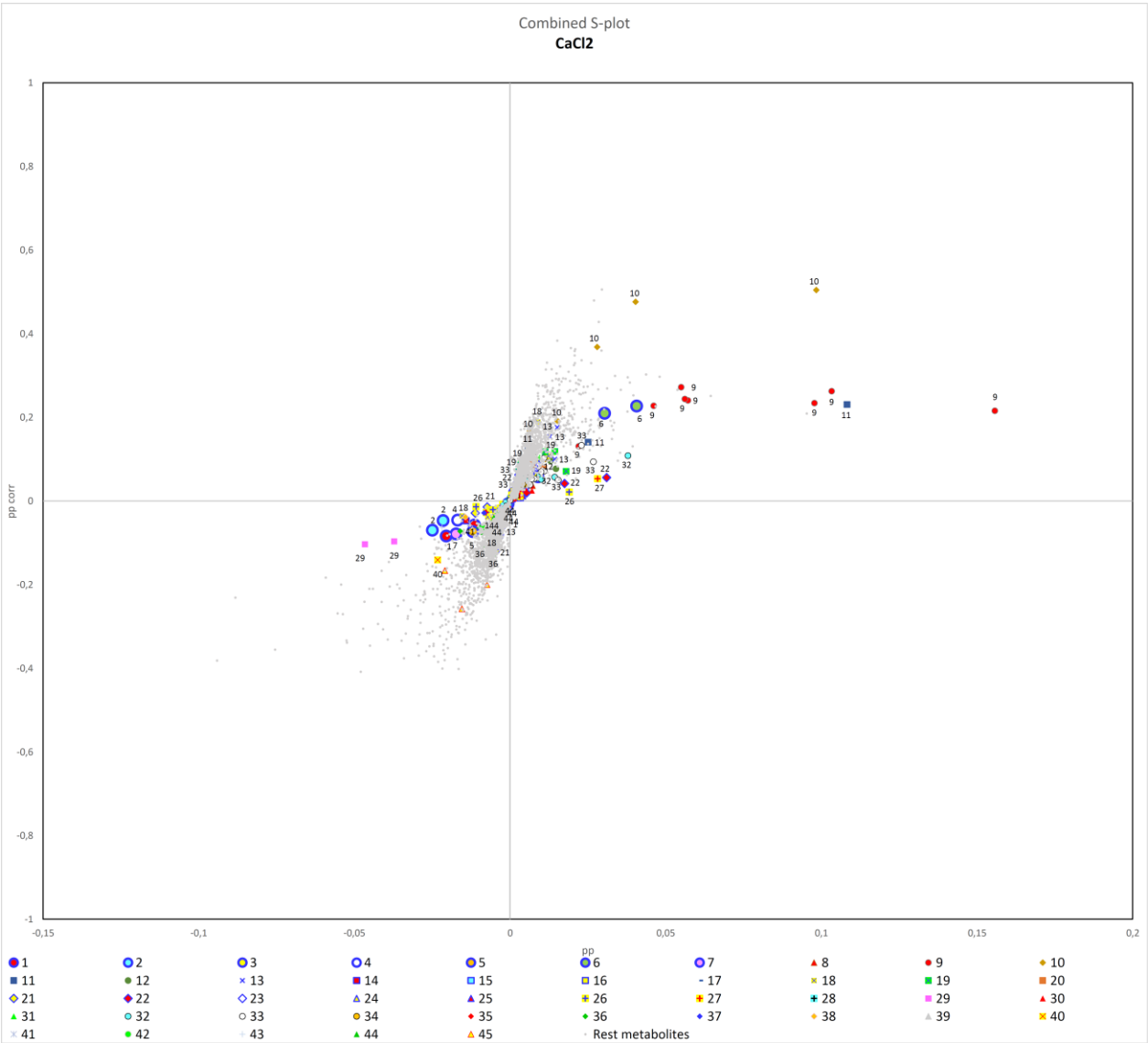


Figure S3. IAA S-plot

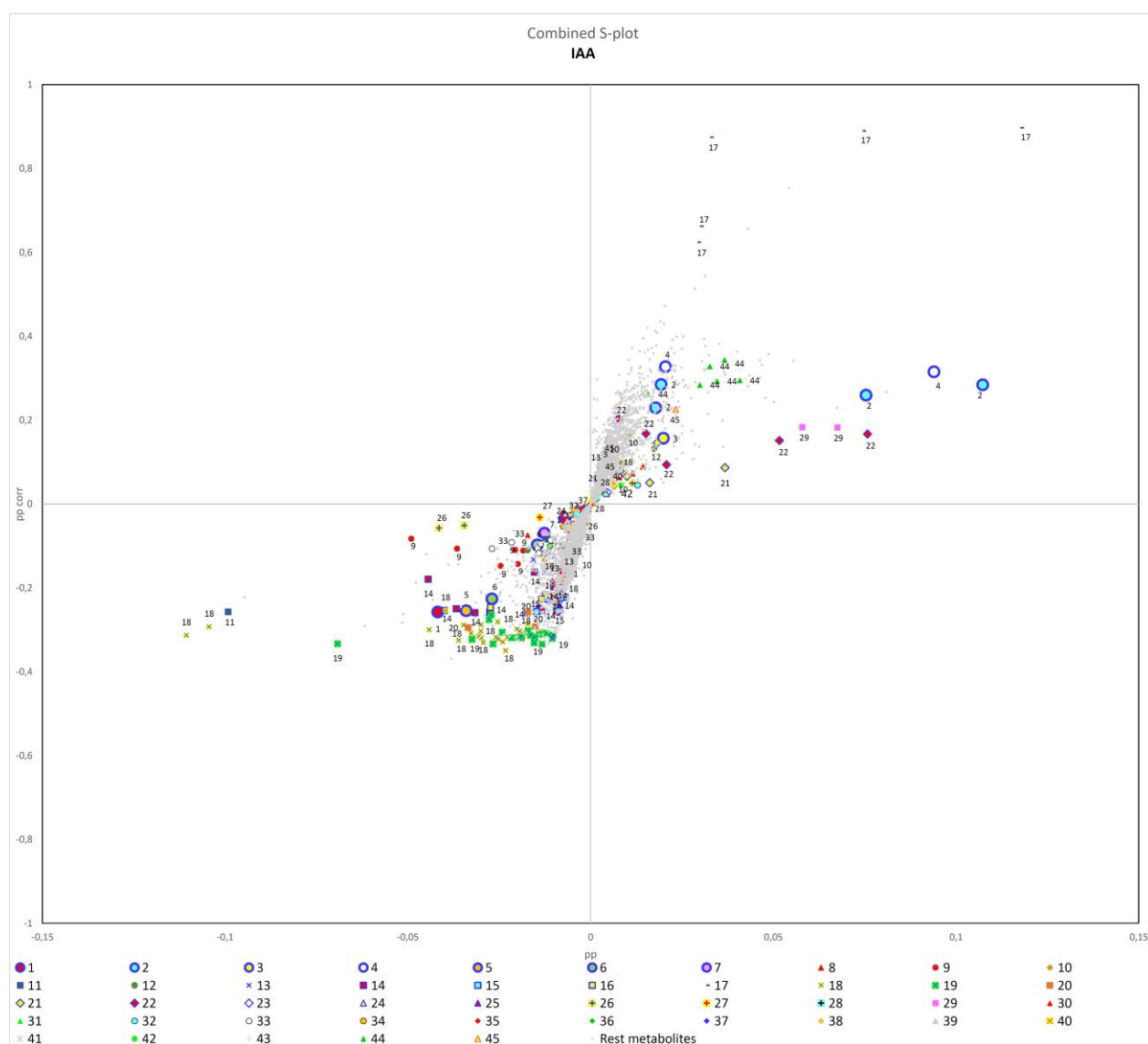


Figure S4. IBA S-plot



Figure S5. NAA S-plot

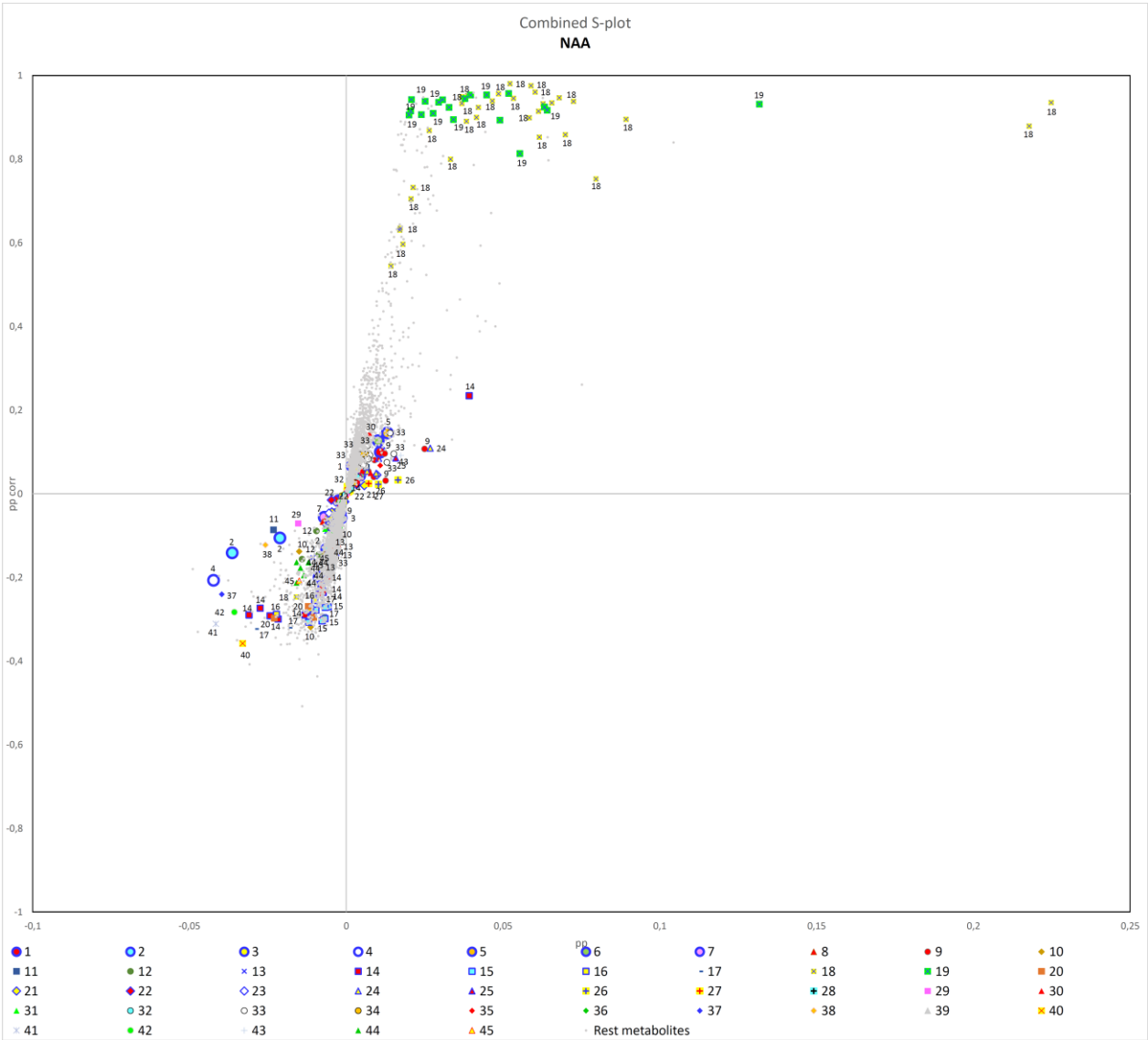


Figure S6. 2,4-D S-plot

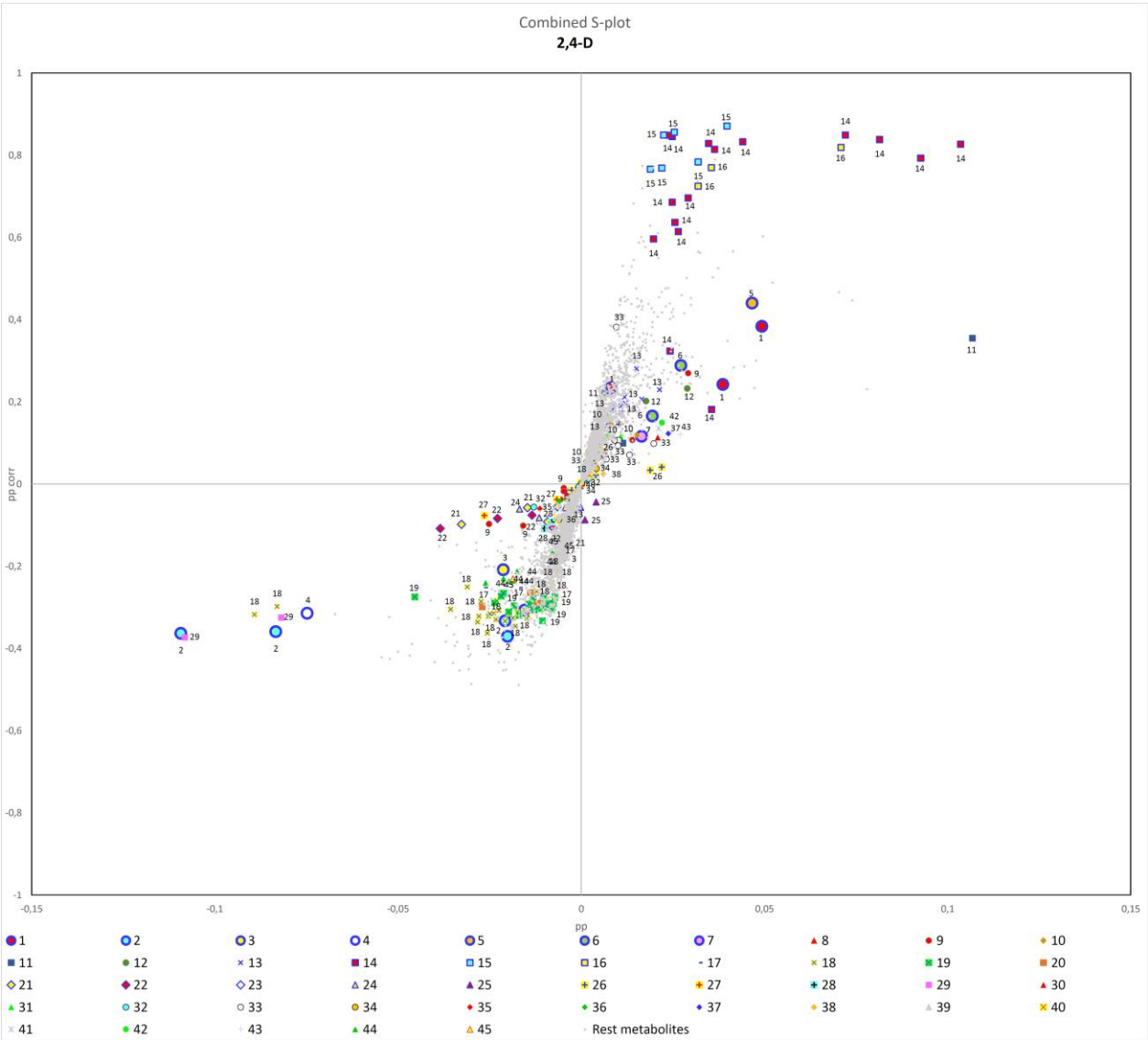


Figure S7. Kinetin S-plot



Figure S8. DHZ S-plot

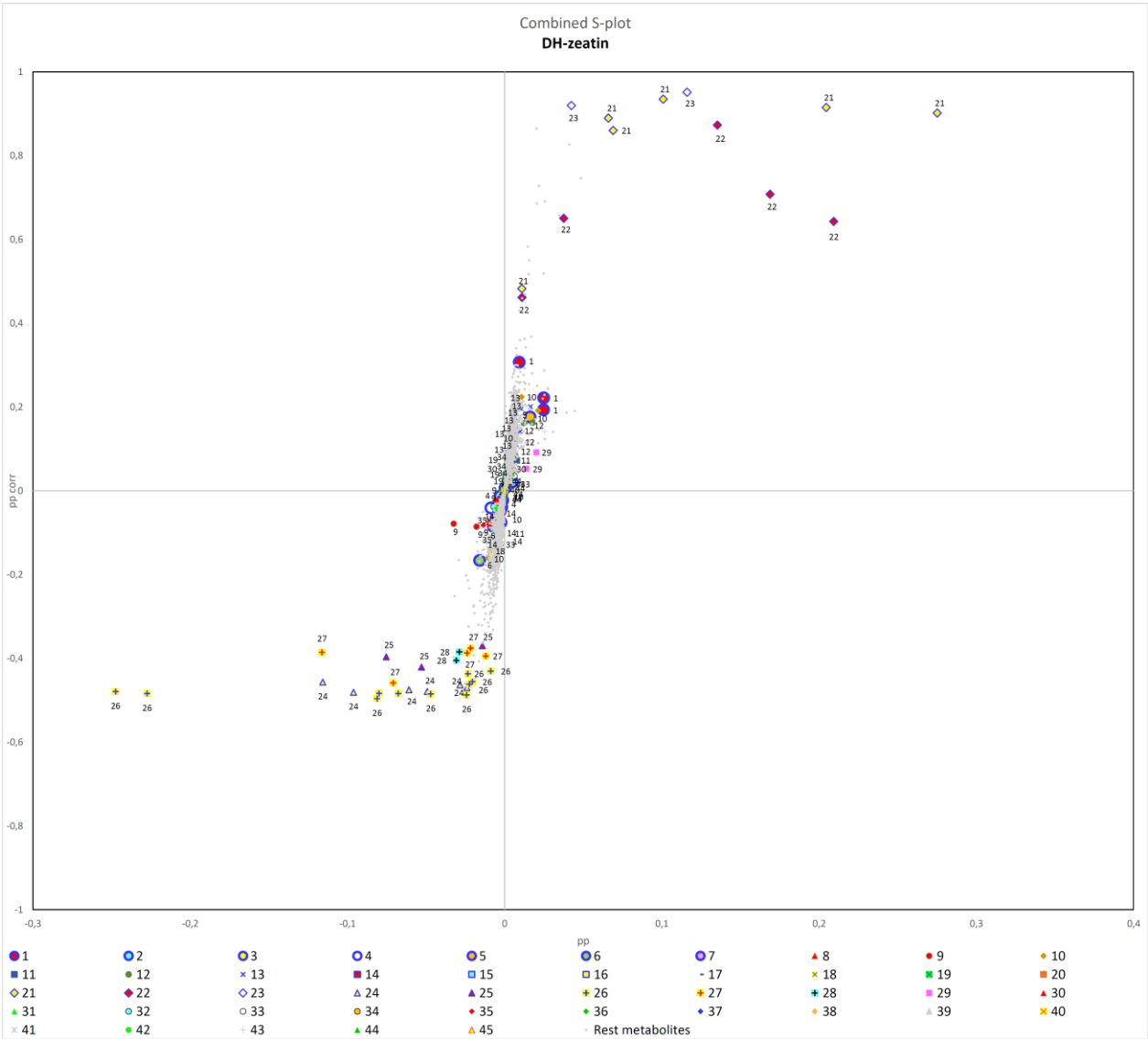


Figure S9. BAP S-plot

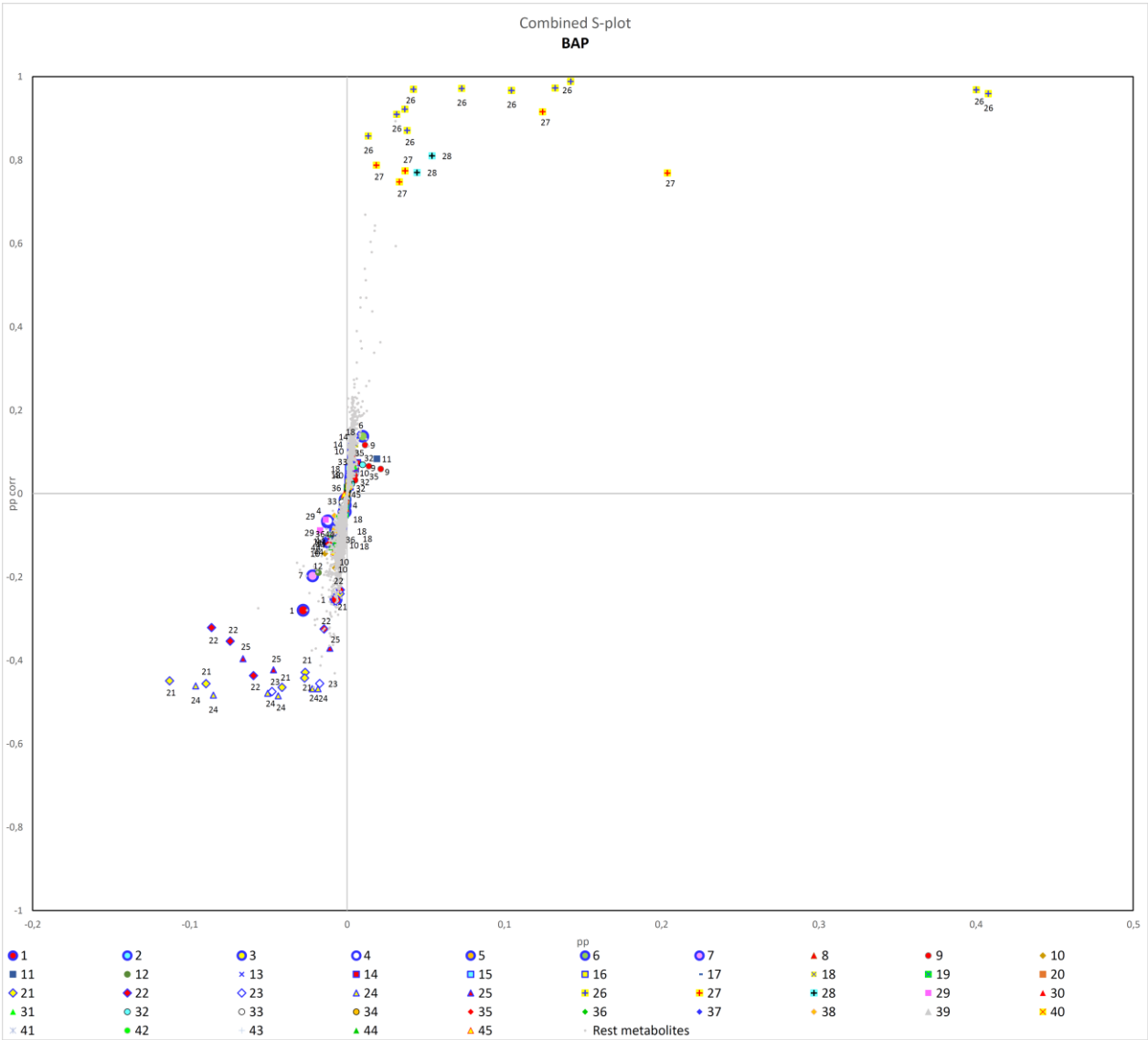


Figure S10. Methyl jasmonate S-plot

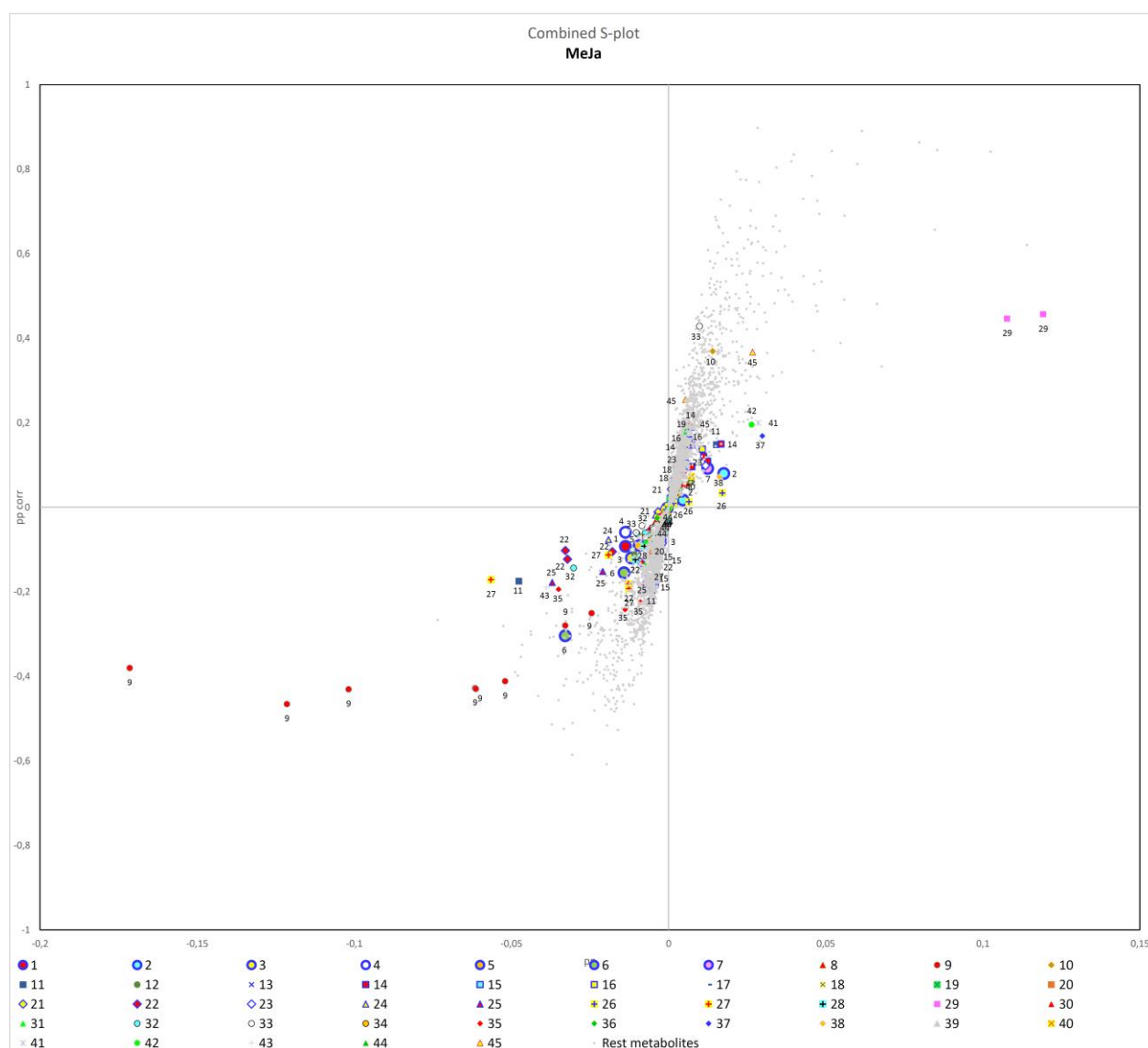


Figure S11. Salicylic acid S-plot

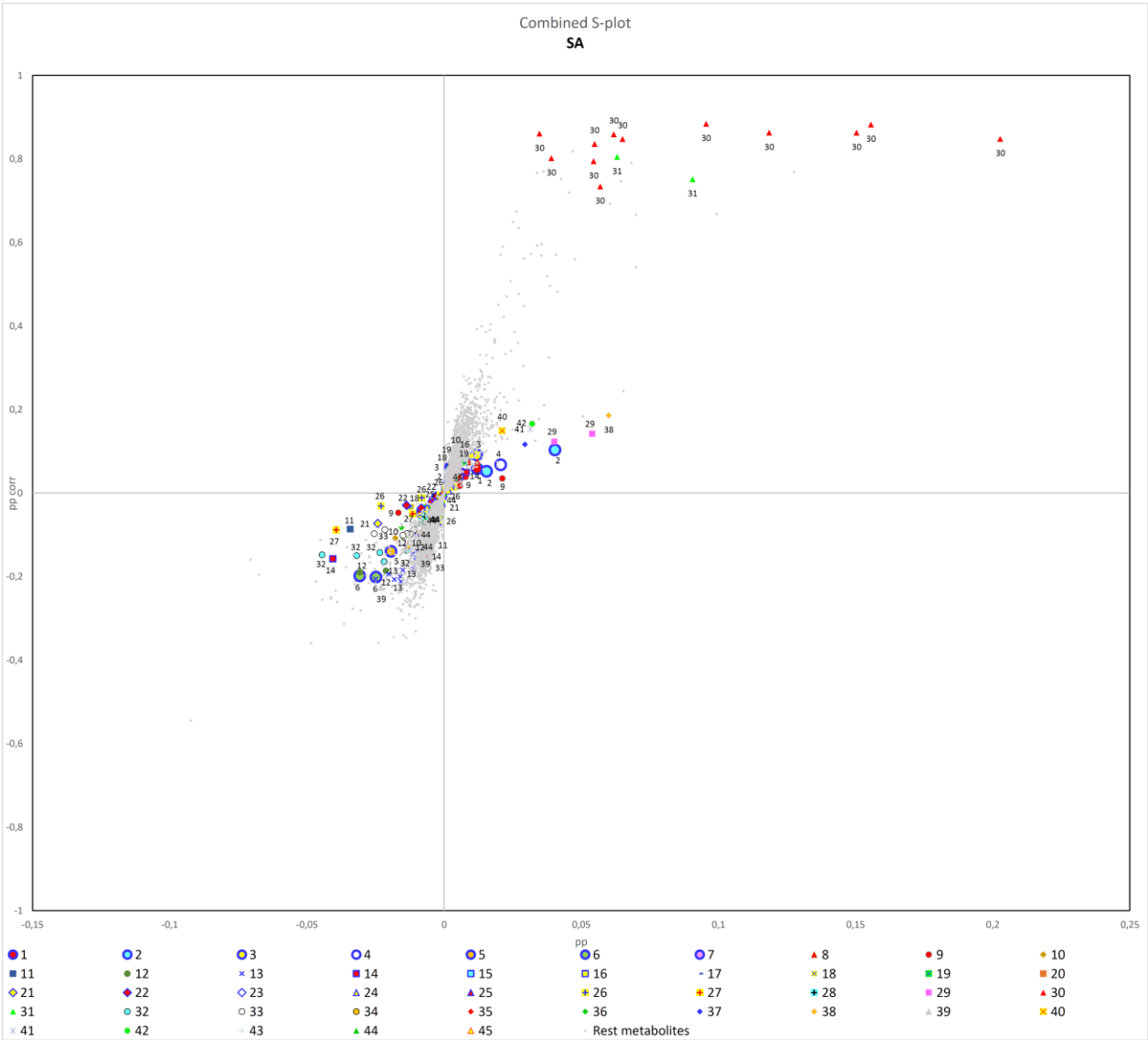


Figure S12. GA₃ S-plot

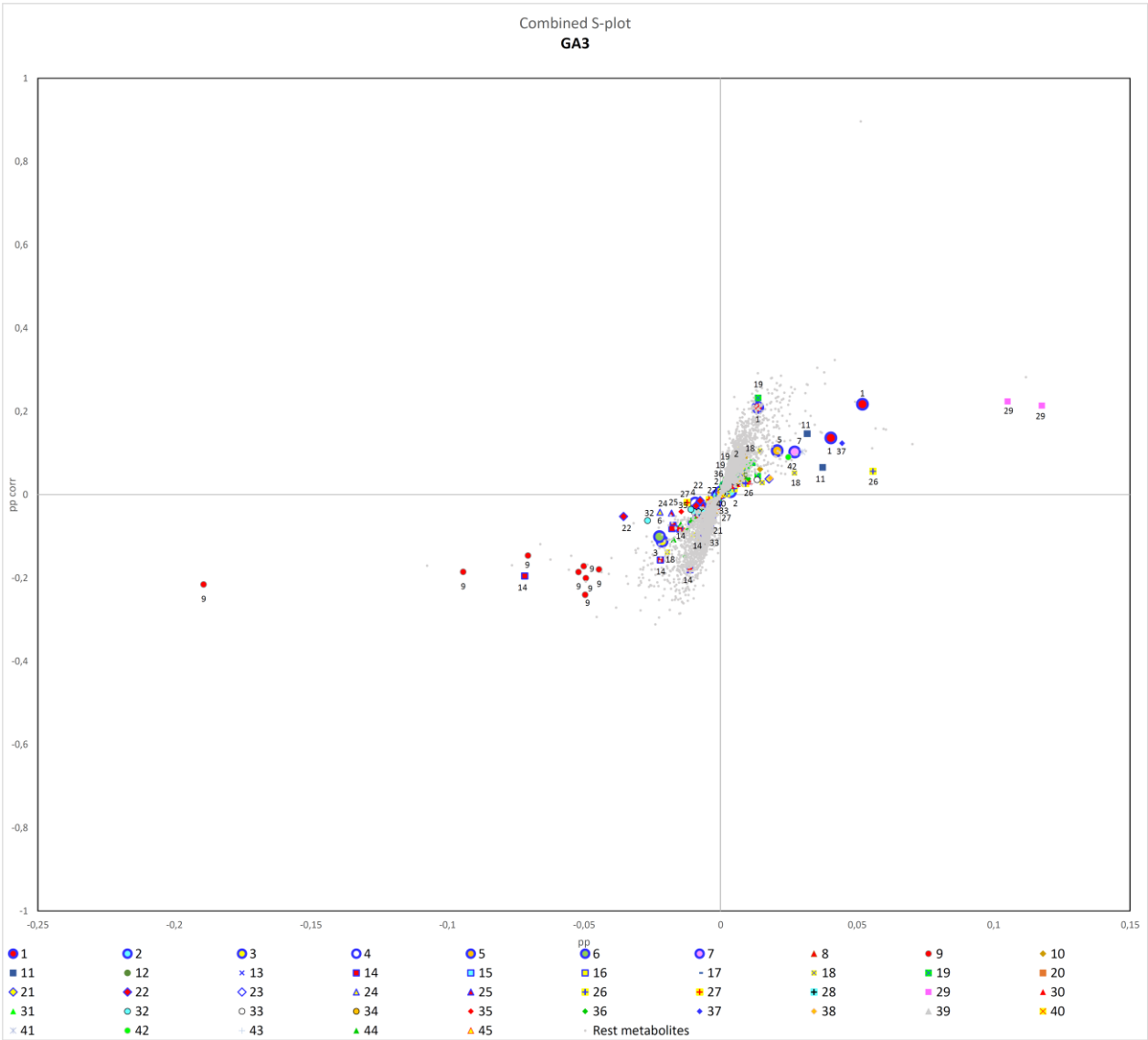


Figure S13. Ethephon S-plot

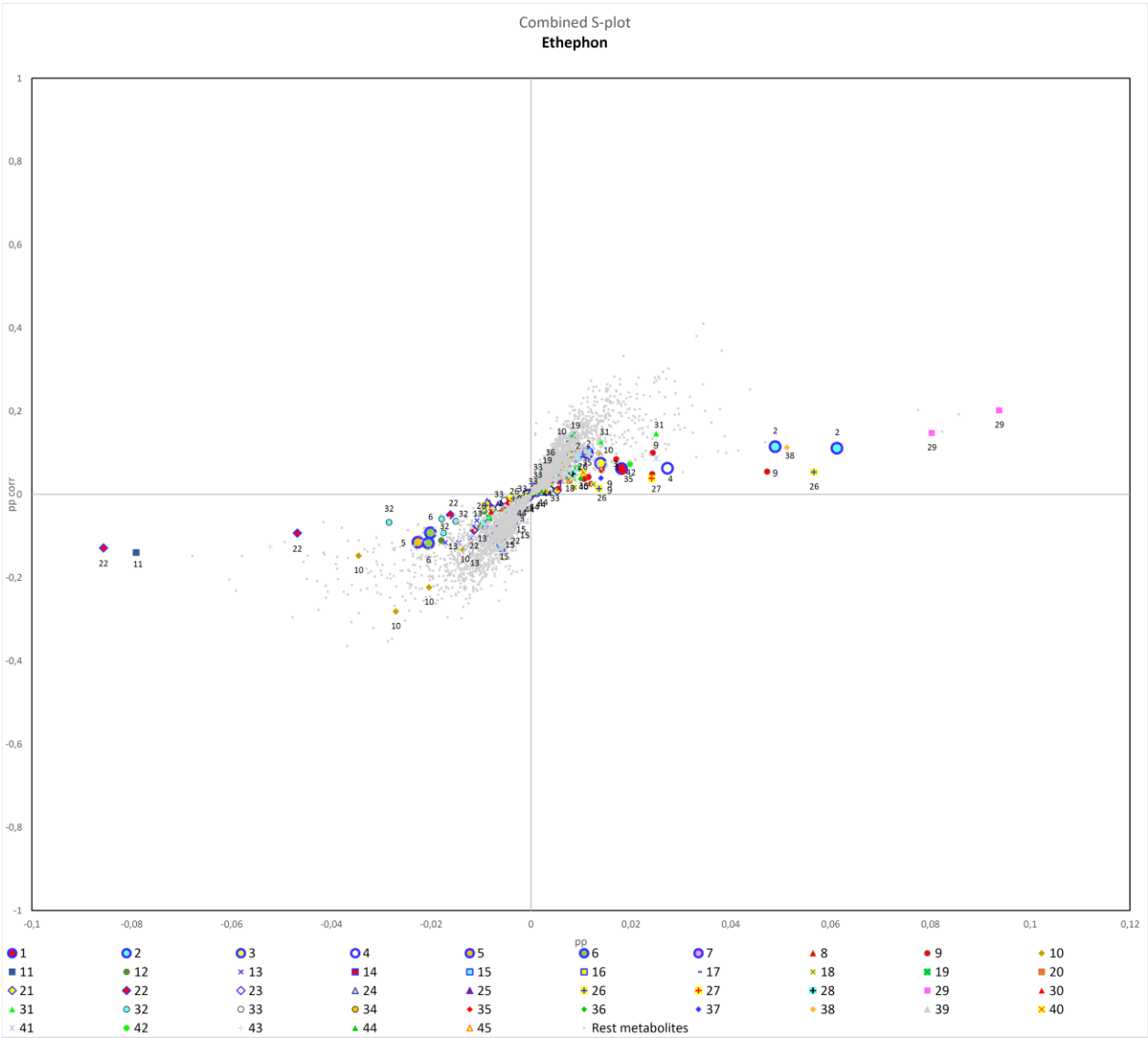


Figure S14. Cyclanilide S-plot

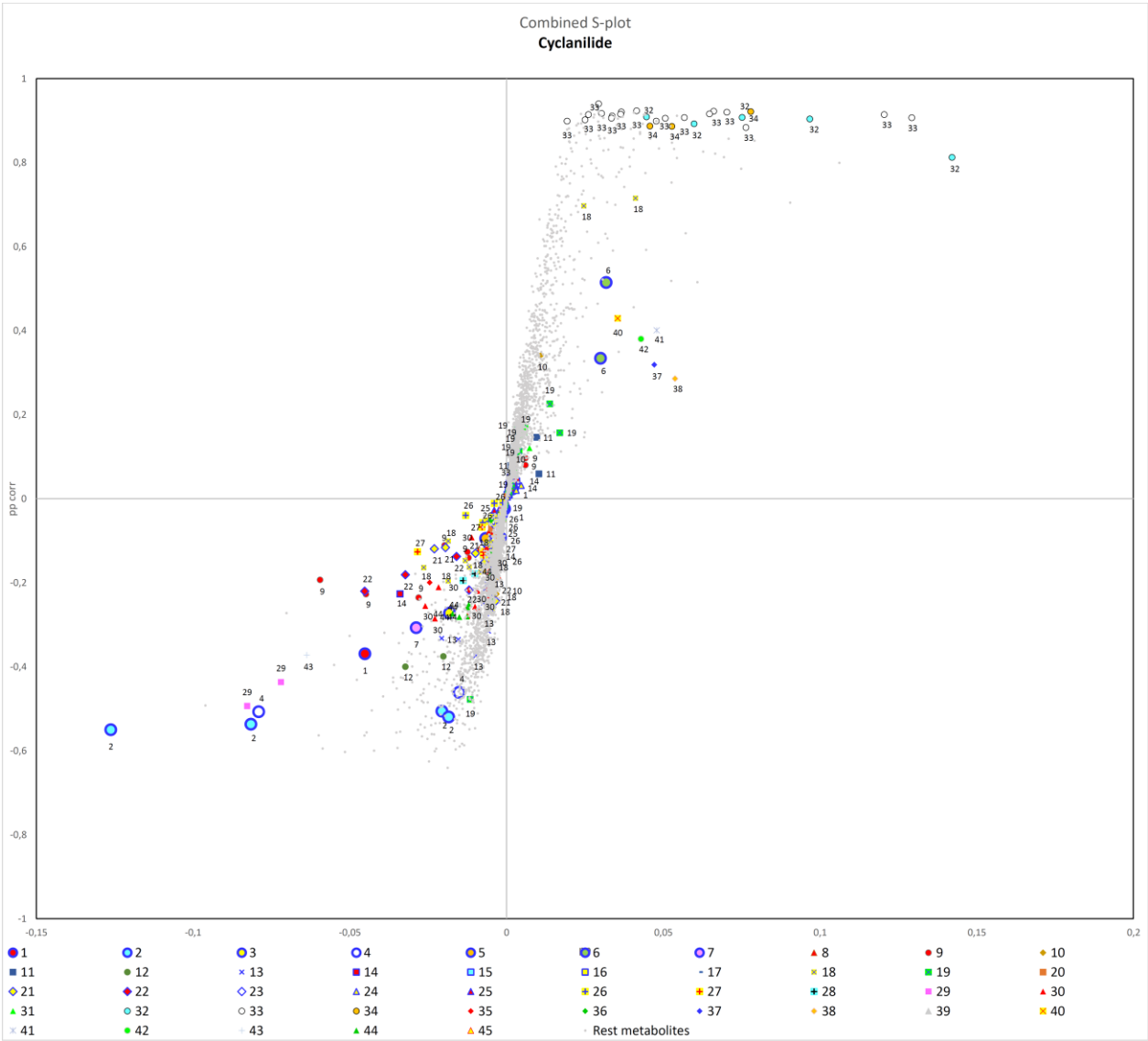


Figure S15. ABA S-plot

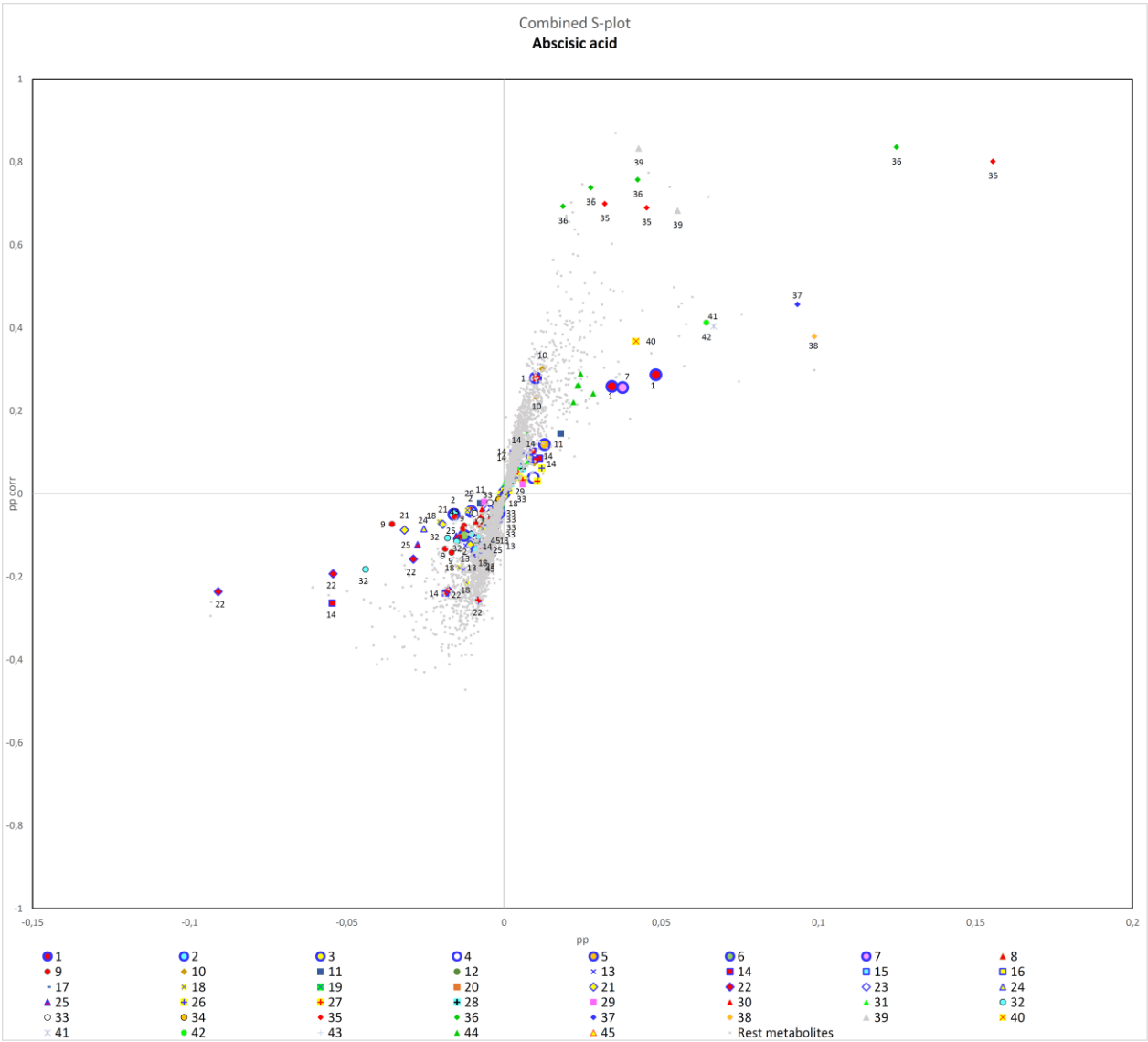


Figure S16. Light S-plot

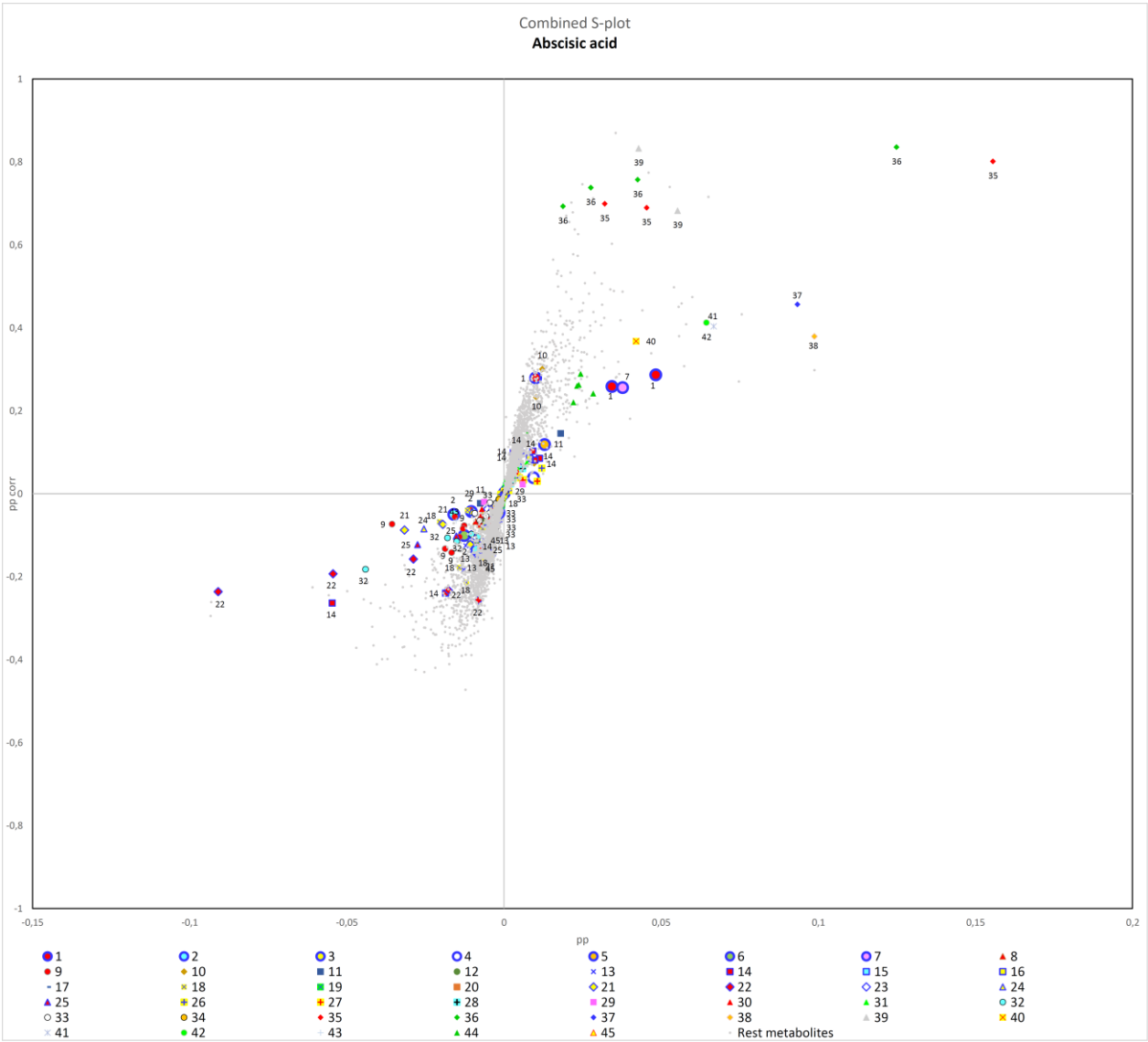


Figure S17. Plot of absolute correlations showing potentially relevant confounding between main effects and two-factor interactions in terms of triples of factor comparisons

