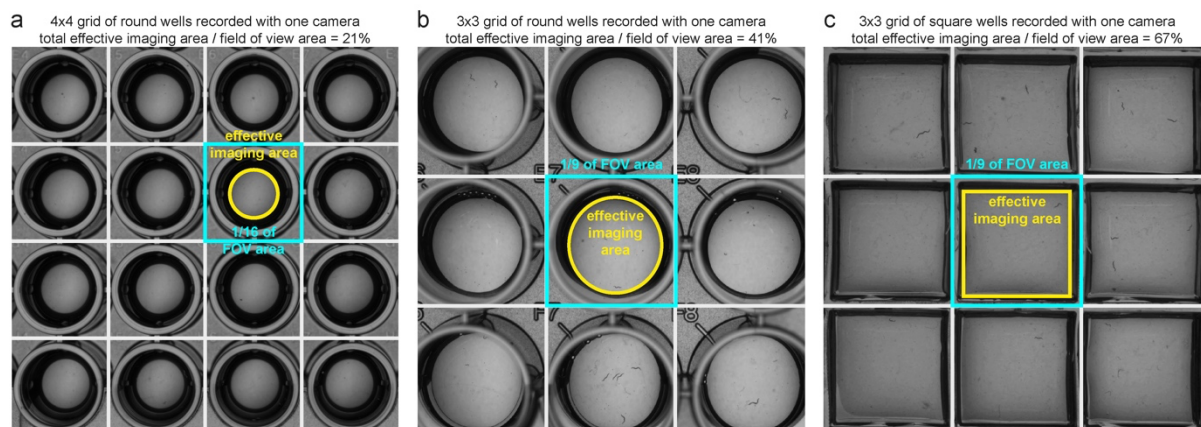
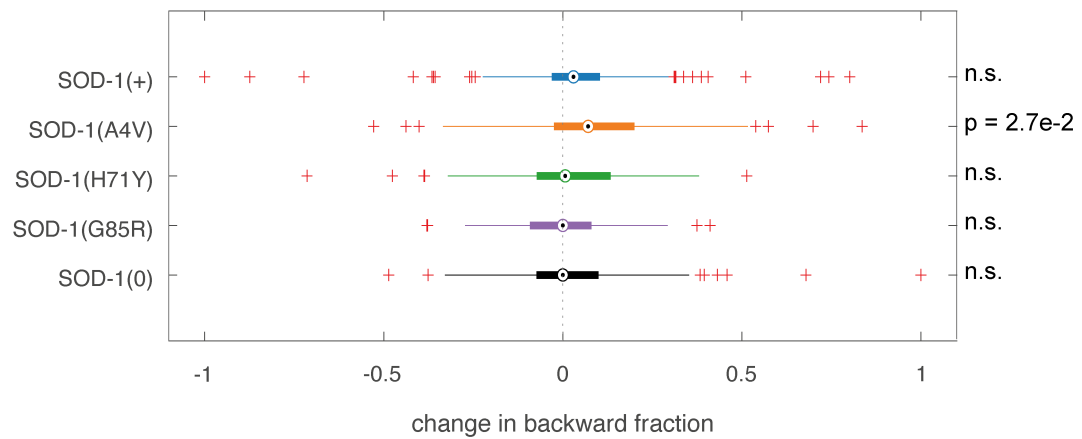


## Supplementary figures and tables

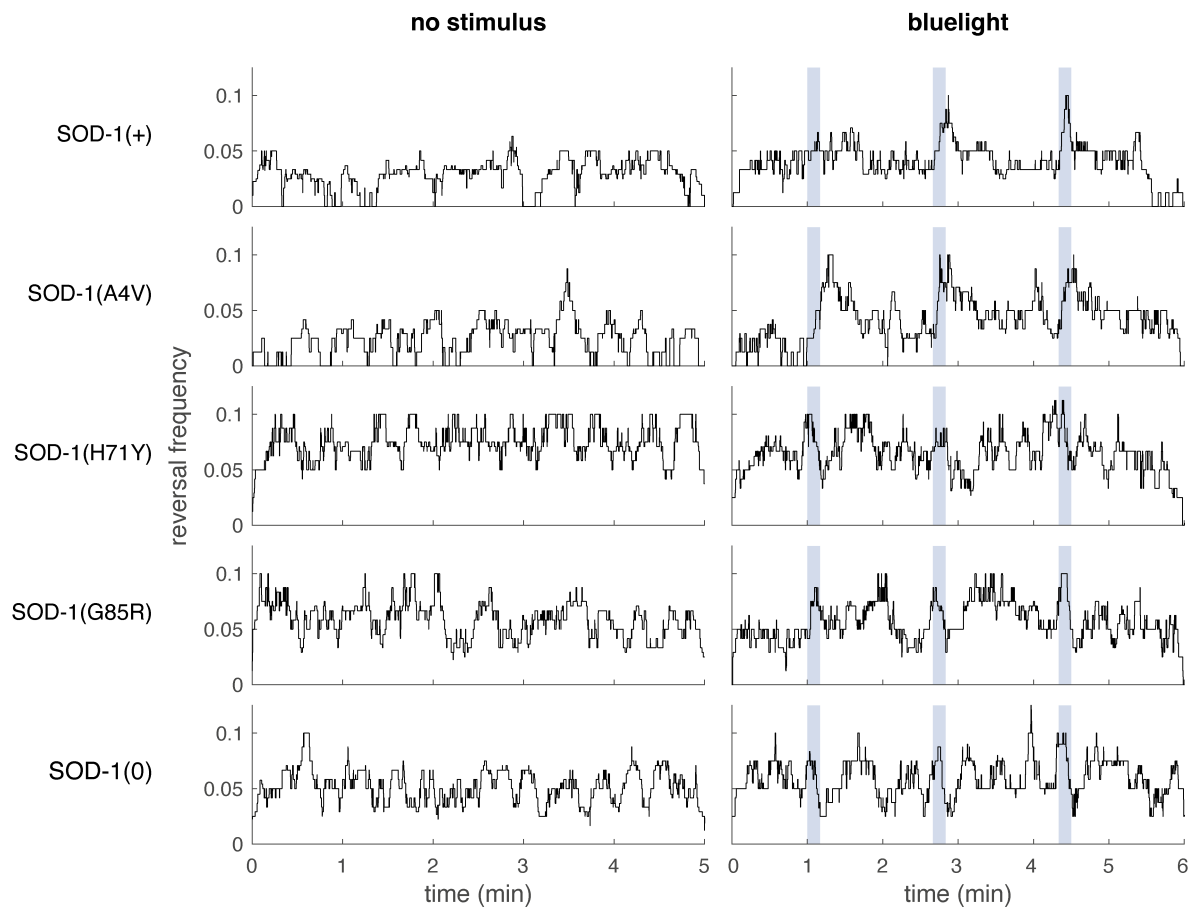


**Supplementary Figure 1: Alternative plate designs investigated.** **a)** Round wells are less optimal than square wells as a large part of the field of view is lost to the area between wells, thus reducing the effective area for behaviour. Round wells further lose more effective area due to the shadows cast by the separators. **b)** Using larger round wells (here a 48 multiwell plate) yields an increase in the effective area available for imaging, relative to the field of view. Throughput is however negatively affected, as fewer wells are imaged at the same time. **c)** A prototype custom made 54 multiwell plate. Custom plates with shallow wells and thin separators are the best option to maximise effective imaging area, but this comes with increased manufacturing costs and undermines interoperability with established automated liquid handling instruments.

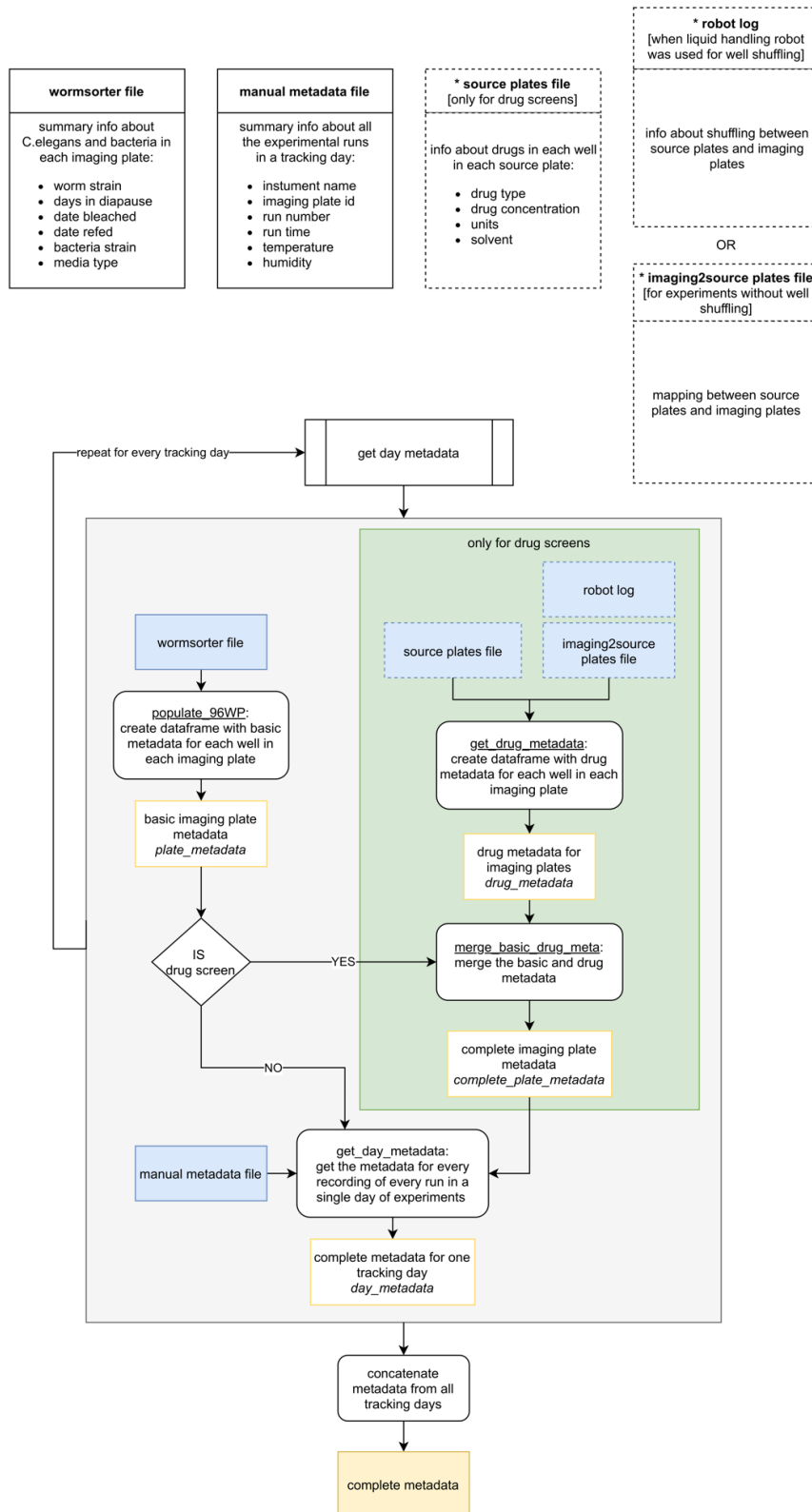
a



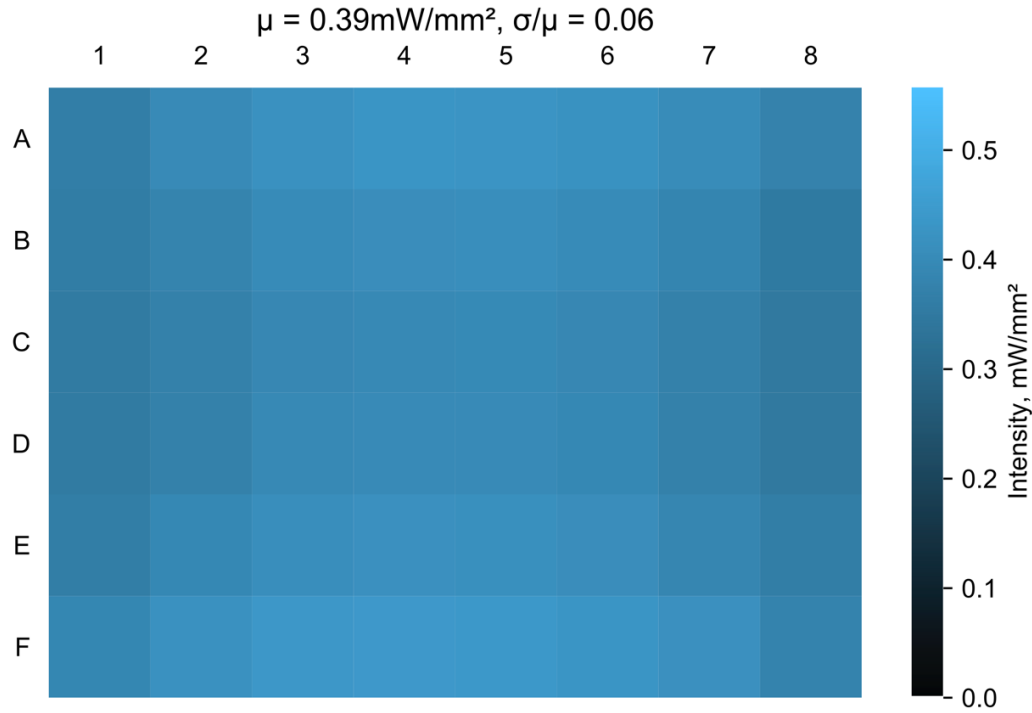
b



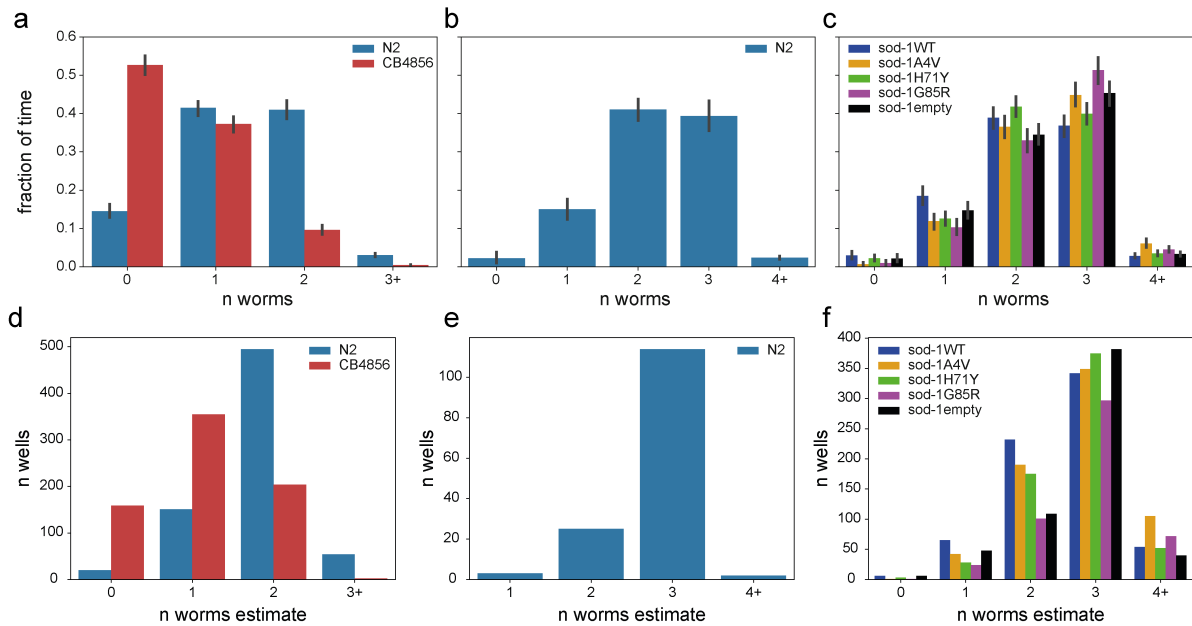
**Supplementary Figure 2: Backward locomotion in ALS disease models. a)** Changes in the overall fraction of backward locomotion upon blue light stimulation. The difference was calculated by subtracting the average feature values over the  $t = 50-60$  second pre-stimulus window from those over the  $t = 65-75$  second first blue light pulse window (these correspond to the first and the second time points in Figure 3d, respectively). Two sample t-test against SOD-1(+) control strain (n.s. not significant). Boxes show median and 25<sup>th</sup> and 75<sup>th</sup> percentiles. **b)** Reversal frequency per worm per second, calculated for each frame at 25 fps. A reversal was detected when a worm changes its motion state from forward or paused to backwards. A 10 second sliding window was used to calculate reversal frequency, then the data was smoothed over a 3 second window. A random sample of 20 independent experiments was used to generate the left and the right column plots for each strain.



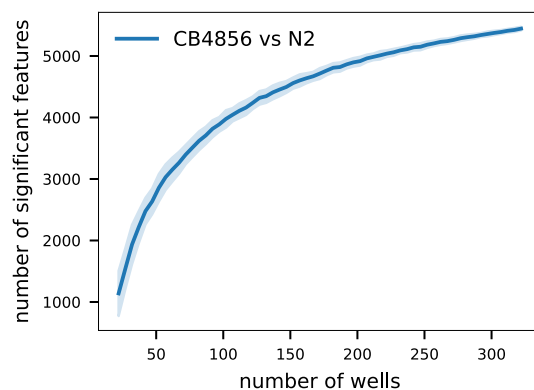
**Supplementary Figure 3:** Flow chart of the full metadata compilation based on standardised experimental records when imaging with the Kastl - HighRes. As mentioned in the methods section “Data provenance”, experiments with multiwell plates pose challenges in terms of keeping track of data provenance. Our pipeline to handle the automatic creation of metadata can flexibly accommodate different experimental needs (objects marked with \* and surrounded by dashed boxes are optional and only present in some experimental designs).



**Supplementary Figure 4:** Representative heatmap showing the intensity of the blue light emitted by the blue LEDs, built by taking 48 measurements in a 6-by-8 grid spanning the sample area, using a Coherent® Fieldmaster power meter (Coherent Inc, USA).



**Supplementary Figure 5:** Worms can crawl into the shaded area at the edge of the well, preventing perfect tracking of all worms throughout the video. **a)** Fraction of time in which  $n$  worms are simultaneously tracked, in an experiment with a nominal 2 worms per well. Three worms are occasionally observed either because of loading errors or cases where non-worm objects are not correctly filtered by the CNN worm classifier. **b, c)** Dispensing 3 worms per well significantly decreases the fraction of time in which 0 or 1 worms are tracked. Values shown are averages across all wells in each experiment, and error bars show 95% confidence interval via bootstrapping. **d, e, f)** Number of wells in which  $n$  worms were imaged simultaneously. The nominal number of worms is 2, 3, and 3 in the three panels respectively.



**Supplementary Figure 6:** The number of features deemed to be significantly different between the Hawaiian strain and the N2 control (Kruskal-Wallis with Benjamin-Yekutieli correction for multiple comparison, false discovery rate 0.05) increases as a function of the number of wells imaged. This figure was obtained by repeatedly sampling an ever-increasing number of wells from the full dataset featured in Figure 3a,b) Solid line is the mean, shaded area is the standard deviation across 100 random samplings without substitution.

**Supplementary Table 1:** List of strains in this study

| Strain name | Genotype                                                                                                    |
|-------------|-------------------------------------------------------------------------------------------------------------|
| N2          | Bristol wild-type reference strain                                                                          |
| CB4856      | Wild isolate                                                                                                |
| CX11314     | Wild isolate                                                                                                |
| DL238       | Wild isolate                                                                                                |
| ED3017      | Wild isolate                                                                                                |
| EG4725      | Wild isolate                                                                                                |
| JT11398     | Wild isolate                                                                                                |
| JU258       | Wild isolate                                                                                                |
| JU775       | Wild isolate                                                                                                |
| LKC34       | Wild isolate                                                                                                |
| MY16        | Wild isolate                                                                                                |
| MY23        | Wild isolate                                                                                                |
| HA2427      | sod-1(tm776) II; unc-119(ed3) III; rtSi001[sod-1p::sod-1(WT); Cbr-unc-119(+)] IV                            |
| HA2464      | sod-1(tm776) II; unc-119(+) III; rtSi008 [sod-1p::sod-1A4V <sup>M</sup> ::sod-1 3'UTR + Cbr-unc-119(+)] IV  |
| HA2425      | sod-1(tm776) II; unc-119(+) III; rtSi007 [sod-1p::sod-1H71Y <sup>M</sup> ::sod-1 3'UTR + Cbr-unc-119(+)] IV |
| HA2426      | sod-1(tm776) II; unc-119(+) III; rtSi006 [sod-1p::sod-1G85R <sup>M</sup> ::sod-1 3'UTR + Cbr-unc-119(+)] IV |
| HA2622      | sod-1(tm776) II; unc-119(+) III; rtSi026 [Cbr-unc-119(+)] IV                                                |

**Supplementary Table 2:** detailed protocols

| Figure panel                           | Protocol                                                                                                          | Number of worms per well | Acclimatisation time (hours) |
|----------------------------------------|-------------------------------------------------------------------------------------------------------------------|--------------------------|------------------------------|
| Figure 2                               | <a href="https://dx.doi.org/10.17504/protocols.io.bn5zmg76">https://dx.doi.org/10.17504/protocols.io.bn5zmg76</a> | 3                        | 4.5                          |
| Figure 3a-b                            | <a href="https://dx.doi.org/10.17504/protocols.io.9vqh65w">https://dx.doi.org/10.17504/protocols.io.9vqh65w</a>   | 2                        | 4.5                          |
| Figure 3c-e                            | <a href="https://dx.doi.org/10.17504/protocols.io.bsicncaw">https://dx.doi.org/10.17504/protocols.io.bsicncaw</a> | 3                        | 1.5                          |
| Figure 4,<br>Supplementary<br>Figure 2 | <a href="https://dx.doi.org/10.17504/protocols.io.bsicncaw">https://dx.doi.org/10.17504/protocols.io.bsicncaw</a> | 3                        | 1.5                          |
| Figure 5                               | <a href="https://dx.doi.org/10.17504/protocols.io.bs6znhf6">https://dx.doi.org/10.17504/protocols.io.bs6znhf6</a> | 3                        | 4.5                          |

Note: Acclimatisation time is defined here as time of imaging – (start time on COPAS worm sorting + end time on COPAS worm sorting) / 2.

**Supplementary Table 3:** Sample size for all experiments involving multiple strains.

| Figure         | worm strain | n wells | across n plates | across n days | worms per well |
|----------------|-------------|---------|-----------------|---------------|----------------|
| Fig 2          | N2          | 34      | 32              | 3             | 3              |
| Fig 2          | JT11398     | 21      | 19              | 3             | 3              |
| Fig 2          | MY16        | 27      | 24              | 3             | 3              |
| Fig 2          | EG4725      | 29      | 26              | 3             | 3              |
| Fig 2          | JU258       | 25      | 23              | 3             | 3              |
| Fig 2          | JU775       | 25      | 21              | 4             | 3              |
| Fig 2          | LKC34       | 27      | 26              | 3             | 3              |
| Fig 2          | CB4856      | 29      | 27              | 4             | 3              |
| Fig 2          | DL238       | 16      | 15              | 3             | 3              |
| Fig 2          | ED3017      | 20      | 20              | 3             | 3              |
| Fig 2          | MY23        | 23      | 22              | 3             | 3              |
| Fig 3a (left)  | N2          | 377     | 149             | 6             | 2              |
| Fig 3a (left)  | CB4856      | 115     | 82              | 6             | 2              |
| Fig 3a (right) | N2          | 398     | 152             | 6             | 2              |
| Fig 3a (right) | CB4856      | 98      | 73              | 6             | 2              |
| Fig 3b         | N2          | 529     | 155             | 6             | 2              |
| Fig 3b         | CB4856      | 396     | 152             | 6             | 2              |
| Fig 3c-e       | N2          | 144     | 4               | 4             | 3              |
| Fig 4, S2      | sod-1(+)    | 232     | 15              | 3             | 3              |
| Fig 4, S2      | sod-1(A4V)  | 228     | 15              | 3             | 3              |
| Fig 4, S2      | sod-1(H71Y) | 211     | 15              | 3             | 3              |
| Fig 4, S2      | sod-1(G85R) | 165     | 13              | 3             | 3              |
| Fig 4, S2      | sod-1(0)    | 195     | 13              | 3             | 3              |

**Supplementary Table 4:** Sample size for each compound and concentration featured in Figure 5. Three N2 worms were dispensed in each well.

| compound and concentration (μM)              | wells | plates | days | compound and concentration (μM)                 | wells | plates | days |
|----------------------------------------------|-------|--------|------|-------------------------------------------------|-------|--------|------|
| Adenosine 5'-monophosphate monohydrate_1.0   | 8     | 8      | 3    | Labetalol hydrochloride_1.0                     | 6     | 6      | 3    |
| Adenosine 5'-monophosphate monohydrate_10.0  | 8     | 8      | 3    | Labetalol hydrochloride_10.0                    | 6     | 6      | 3    |
| Adenosine 5'-monophosphate monohydrate_100.0 | 8     | 8      | 3    | Labetalol hydrochloride_100.0                   | 7     | 7      | 4    |
| Adiphenine hydrochloride_1.0                 | 7     | 7      | 3    | Laudanosine (R,S)_1.0                           | 7     | 7      | 3    |
| Adiphenine hydrochloride_10.0                | 7     | 7      | 3    | Laudanosine (R,S)_10.0                          | 7     | 7      | 3    |
| Adiphenine hydrochloride_100.0               | 7     | 7      | 3    | Laudanosine (R,S)_100.0                         | 6     | 6      | 3    |
| Agmatine sulfate_0.25                        | 5     | 5      | 2    | Lomefloxacin hydrochloride_0.5                  | 4     | 4      | 2    |
| Agmatine sulfate_2.5                         | 8     | 8      | 3    | Lomefloxacin hydrochloride_5.0                  | 2     | 2      | 1    |
| Agmatine sulfate_25.0                        | 7     | 7      | 3    | Lomefloxacin hydrochloride_50.0                 | 3     | 3      | 2    |
| Alverine citrate salt_1.0                    | 8     | 8      | 3    | Loperamide hydrochloride_1.0                    | 7     | 7      | 3    |
| Alverine citrate salt_10.0                   | 8     | 8      | 3    | Loperamide hydrochloride_10.0                   | 6     | 6      | 2    |
| Alverine citrate salt_100.0                  | 7     | 7      | 3    | Loperamide hydrochloride_100.0                  | 7     | 7      | 3    |
| Ambroxol hydrochloride_1.0                   | 7     | 7      | 3    | Mebeverine hydrochloride_1.0                    | 5     | 5      | 3    |
| Ambroxol hydrochloride_10.0                  | 7     | 7      | 3    | Mebeverine hydrochloride_10.0                   | 6     | 6      | 3    |
| Ambroxol hydrochloride_100.0                 | 7     | 7      | 3    | Mebeverine hydrochloride_100.0                  | 8     | 8      | 3    |
| Amikacin_1.0                                 | 6     | 6      | 3    | Meclofenamic acid sodium salt monohydrate_1.0   | 4     | 4      | 2    |
| Amikacin_10.0                                | 7     | 7      | 2    | Meclofenamic acid sodium salt monohydrate_10.0  | 7     | 7      | 3    |
| Amikacin_100.0                               | 7     | 7      | 3    | Meclofenamic acid sodium salt monohydrate_100.0 | 6     | 6      | 3    |
| Amiodarone hydrochloride_0.5                 | 8     | 8      | 3    | Melatonin_1.0                                   | 7     | 7      | 3    |
| Amiodarone hydrochloride_5.0                 | 7     | 7      | 3    | Melatonin_10.0                                  | 6     | 6      | 3    |
| Amiodarone hydrochloride_50.0                | 5     | 5      | 3    | Melatonin_100.0                                 | 7     | 7      | 3    |
| Amoxicillin_0.5                              | 7     | 7      | 2    | Mepenzolate bromide_1.0                         | 6     | 6      | 3    |
| Amoxicillin_5.0                              | 8     | 8      | 3    | Mepenzolate bromide_10.0                        | 8     | 8      | 3    |
| Amoxicillin_50.0                             | 6     | 6      | 3    | Mepenzolate bromide_100.0                       | 6     | 6      | 3    |
| Ampicillin trihydrate_1.0                    | 7     | 7      | 3    | Mesoridazine besylate_1.0                       | 6     | 6      | 2    |
| Ampicillin trihydrate_10.0                   | 5     | 5      | 2    | Mesoridazine besylate_10.0                      | 7     | 7      | 3    |
| Ampicillin trihydrate_100.0                  | 3     | 3      | 2    | Mesoridazine besylate_100.0                     | 7     | 7      | 3    |
| Antazoline hydrochloride_1.0                 | 6     | 6      | 3    | Metaraminol bitartrate_1.0                      | 7     | 7      | 2    |
| Antazoline hydrochloride_10.0                | 7     | 7      | 4    | Metaraminol bitartrate_10.0                     | 6     | 6      | 2    |
| Antazoline hydrochloride_100.0               | 6     | 6      | 3    | Metaraminol bitartrate_100.0                    | 8     | 8      | 3    |
| Arecoline hydrobromide_1.0                   | 8     | 8      | 3    | Metformin hydrochloride_1.0                     | 8     | 8      | 3    |
| Arecoline hydrobromide_10.0                  | 7     | 7      | 2    | Metformin hydrochloride_10.0                    | 6     | 6      | 3    |
| Arecoline hydrobromide_100.0                 | 7     | 7      | 3    | Metformin hydrochloride_100.0                   | 7     | 7      | 3    |
| Ascorbic acid_1.0                            | 6     | 6      | 3    | Methapyrilene hydrochloride_1.0                 | 5     | 5      | 3    |
| Ascorbic acid_10.0                           | 7     | 7      | 3    | Methapyrilene hydrochloride_10.0                | 6     | 6      | 3    |
| Ascorbic acid_100.0                          | 7     | 7      | 3    | Methapyrilene hydrochloride_100.0               | 6     | 6      | 3    |
| Atropine sulfate monohydrate_1.0             | 7     | 7      | 3    | Methocarbamol_1.0                               | 7     | 7      | 3    |
| Atropine sulfate monohydrate_10.0            | 4     | 4      | 3    | Methocarbamol_10.0                              | 7     | 7      | 3    |
| Atropine sulfate monohydrate_100.0           | 6     | 6      | 3    | Methocarbamol_100.0                             | 7     | 7      | 3    |
| Bacampicillin hydrochloride_1.0              | 7     | 7      | 3    | Metoprolol-(+,-) (+)-tartrate salt_1.0          | 7     | 7      | 3    |
| Bacampicillin hydrochloride_10.0             | 6     | 6      | 2    | Metoprolol-(+,-) (+)-tartrate salt_10.0         | 8     | 8      | 3    |
| Bacampicillin hydrochloride_100.0            | 7     | 7      | 3    | Metoprolol-(+,-) (+)-tartrate salt_100.0        | 6     | 6      | 3    |
| Benfluorex hydrochloride_1.0                 | 8     | 8      | 3    | Metronidazole_1.0                               | 8     | 4      | 3    |
| Benfluorex hydrochloride_10.0                | 7     | 7      | 3    | Metronidazole_10.0                              | 8     | 4      | 3    |
| Benfluorex hydrochloride_100.0               | 5     | 5      | 3    | Metronidazole_100.0                             | 6     | 3      | 2    |
| Benoxinate hydrochloride_1.0                 | 7     | 7      | 3    | Mexiletine hydrochloride_1.0                    | 5     | 5      | 3    |
| Benoxinate hydrochloride_10.0                | 5     | 5      | 3    | Mexiletine hydrochloride_10.0                   | 7     | 7      | 4    |
| Benoxinate hydrochloride_100.0               | 7     | 7      | 3    | Mexiletine hydrochloride_100.0                  | 4     | 4      | 3    |
| Benzydamine hydrochloride_1.0                | 6     | 6      | 3    | Midodrine hydrochloride_1.0                     | 7     | 7      | 2    |
| Benzydamine hydrochloride_10.0               | 7     | 7      | 3    | Midodrine hydrochloride_10.0                    | 7     | 7      | 2    |
| Benzydamine hydrochloride_100.0              | 8     | 8      | 3    | Midodrine hydrochloride_100.0                   | 6     | 6      | 2    |
| Brompheniramine maleate_1.0                  | 5     | 5      | 2    | Minoxidil_0.25                                  | 8     | 8      | 3    |
| Brompheniramine maleate_10.0                 | 7     | 7      | 3    | Minoxidil_2.5                                   | 7     | 7      | 2    |
| Brompheniramine maleate_100.0                | 4     | 4      | 2    | Minoxidil_25.0                                  | 8     | 8      | 3    |
| Buflomedil hydrochloride_1.0                 | 8     | 8      | 3    | Molsidomine_1.0                                 | 7     | 7      | 3    |
| Buflomedil hydrochloride_10.0                | 8     | 8      | 3    | Molsidomine_10.0                                | 7     | 7      | 3    |
| Buflomedil hydrochloride_100.0               | 8     | 8      | 3    | Molsidomine_100.0                               | 5     | 5      | 3    |

| compound and concentration (µM)                  | wells | plates | days | compound and concentration (µM)          | wells | plates | days |
|--------------------------------------------------|-------|--------|------|------------------------------------------|-------|--------|------|
| Bupivacaine hydrochloride _1.0                   | 7     | 7      | 3    | Nalidixic acid sodium salt hydrate _0.25 | 6     | 6      | 2    |
| Bupivacaine hydrochloride _10.0                  | 8     | 8      | 3    | Nalidixic acid sodium salt hydrate _2.5  | 7     | 7      | 3    |
| Bupivacaine hydrochloride _100.0                 | 5     | 5      | 3    | Nalidixic acid sodium salt hydrate _25.0 | 5     | 5      | 2    |
| Buspirone hydrochloride _0.5                     | 8     | 8      | 3    | Naphazoline hydrochloride _0.5           | 7     | 7      | 3    |
| Buspirone hydrochloride _5.0                     | 8     | 8      | 3    | Naphazoline hydrochloride _5.0           | 5     | 5      | 3    |
| Buspirone hydrochloride _50.0                    | 8     | 8      | 3    | Naphazoline hydrochloride _50.0          | 7     | 7      | 3    |
| CSAA466656 _1.0                                  | 3     | 2      | 2    | Nefopam hydrochloride _1.0               | 6     | 6      | 4    |
| CSAA466656 _10.0                                 | 1     | 1      | 1    | Nefopam hydrochloride _10.0              | 6     | 6      | 4    |
| CSAA466656 _100.0                                | 3     | 3      | 3    | Nefopam hydrochloride _100.0             | 6     | 6      | 4    |
| Captopril _1.0                                   | 7     | 7      | 3    | Neostigmine bromide _1.0                 | 6     | 6      | 3    |
| Captopril _10.0                                  | 6     | 6      | 2    | Neostigmine bromide _10.0                | 6     | 6      | 2    |
| Captopril _100.0                                 | 7     | 7      | 3    | Neostigmine bromide _100.0               | 6     | 6      | 2    |
| Carbenicillin disodium salt _1.0                 | 7     | 7      | 3    | Nitrofurantoin _1.0                      | 7     | 7      | 3    |
| Carbenicillin disodium salt _10.0                | 6     | 6      | 2    | Nitrofurantoin _10.0                     | 7     | 7      | 3    |
| Carbenicillin disodium salt _100.0               | 6     | 6      | 3    | Nitrofurantoin _100.0                    | 7     | 7      | 3    |
| Cefadroxil _0.5                                  | 8     | 8      | 3    | Nortriptyline hydrochloride _1.0         | 6     | 6      | 3    |
| Cefadroxil _5.0                                  | 7     | 7      | 3    | Nortriptyline hydrochloride _10.0        | 5     | 5      | 2    |
| Cefadroxil _50.0                                 | 8     | 8      | 3    | Nortriptyline hydrochloride _100.0       | 5     | 5      | 2    |
| Chenodiol _1.0                                   | 7     | 7      | 3    | Olanzapine _1.0                          | 7     | 4      | 3    |
| Chenodiol _10.0                                  | 7     | 7      | 3    | Olanzapine _10.0                         | 7     | 4      | 3    |
| Chenodiol _100.0                                 | 7     | 7      | 3    | Olanzapine _100.0                        | 7     | 4      | 3    |
| Chloroquine diphosphate _0.5                     | 6     | 6      | 3    | Ornidazole _1.0                          | 7     | 7      | 3    |
| Chloroquine diphosphate _5.0                     | 7     | 7      | 3    | Ornidazole _10.0                         | 7     | 7      | 3    |
| Chloroquine diphosphate _50.0                    | 7     | 7      | 3    | Ornidazole _100.0                        | 7     | 7      | 3    |
| Chlorpheniramine maleate _1.0                    | 7     | 7      | 3    | Orphenadrine hydrochloride _1.0          | 5     | 5      | 2    |
| Chlorpheniramine maleate _10.0                   | 7     | 7      | 3    | Orphenadrine hydrochloride _10.0         | 5     | 5      | 3    |
| Chlorpheniramine maleate _100.0                  | 7     | 7      | 3    | Orphenadrine hydrochloride _100.0        | 4     | 4      | 2    |
| Chlorpromazine _1.0                              | 7     | 4      | 3    | Oxethazaine _1.0                         | 7     | 7      | 3    |
| Chlorpromazine _10.0                             | 8     | 4      | 3    | Oxethazaine _10.0                        | 6     | 6      | 3    |
| Chlorpromazine _100.0                            | 3     | 2      | 2    | Oxethazaine _100.0                       | 7     | 7      | 3    |
| Chlorzoxazone _1.0                               | 6     | 6      | 3    | Oxolinic acid _0.25                      | 6     | 6      | 2    |
| Chlorzoxazone _10.0                              | 7     | 7      | 3    | Oxolinic acid _2.5                       | 7     | 7      | 2    |
| Chlorzoxazone _100.0                             | 7     | 7      | 3    | Oxolinic acid _25.0                      | 5     | 5      | 2    |
| Ciclopirox ethanolamine _1.0                     | 7     | 7      | 3    | Oxymetazoline hydrochloride _1.0         | 4     | 4      | 3    |
| Ciclopirox ethanolamine _10.0                    | 5     | 5      | 2    | Oxymetazoline hydrochloride _10.0        | 6     | 6      | 4    |
| Ciclopirox ethanolamine _100.0                   | 5     | 5      | 2    | Oxymetazoline hydrochloride _100.0       | 6     | 6      | 4    |
| Cinoxacin _0.5                                   | 7     | 4      | 3    | Pentoxifylline _1.0                      | 7     | 7      | 3    |
| Cinoxacin _5.0                                   | 4     | 3      | 2    | Pentoxifylline _10.0                     | 7     | 7      | 2    |
| Cinoxacin _50.0                                  | 6     | 3      | 2    | Pentoxifylline _100.0                    | 7     | 7      | 2    |
| Clarithromycin _0.5                              | 6     | 6      | 2    | Phenacetin _1.0                          | 8     | 8      | 3    |
| Clarithromycin _5.0                              | 7     | 7      | 3    | Phenacetin _10.0                         | 8     | 8      | 3    |
| Clarithromycin _50.0                             | 6     | 6      | 3    | Phenacetin _100.0                        | 6     | 6      | 3    |
| Clomiphene citrate (Z,E) _1.0                    | 6     | 6      | 2    | Pheniramine maleate _1.0                 | 8     | 8      | 3    |
| Clomiphene citrate (Z,E) _10.0                   | 8     | 8      | 3    | Pheniramine maleate _10.0                | 6     | 6      | 3    |
| Clomiphene citrate (Z,E) _100.0                  | 5     | 5      | 3    | Pheniramine maleate _100.0               | 5     | 5      | 3    |
| Colistin sulfate _0.5                            | 4     | 4      | 2    | Phenylpropanolamine hydrochloride _1.0   | 8     | 8      | 3    |
| Colistin sulfate _5.0                            | 6     | 6      | 2    | Phenylpropanolamine hydrochloride _10.0  | 8     | 8      | 3    |
| Colistin sulfate _50.0                           | 5     | 5      | 2    | Phenylpropanolamine hydrochloride _100.0 | 8     | 8      | 3    |
| Convolamine hydrochloride _0.5                   | 6     | 6      | 3    | Pimozide _0.25                           | 6     | 6      | 3    |
| Convolamine hydrochloride _5.0                   | 6     | 6      | 3    | Pimozide _2.5                            | 7     | 7      | 3    |
| Convolamine hydrochloride _50.0                  | 5     | 5      | 2    | Pimozide _25.0                           | 7     | 7      | 3    |
| Dehydrocholic acid _1.0                          | 7     | 7      | 3    | Pipenzolate bromide _1.0                 | 6     | 6      | 3    |
| Dehydrocholic acid _10.0                         | 6     | 6      | 2    | Pipenzolate bromide _10.0                | 7     | 7      | 3    |
| Dehydrocholic acid _100.0                        | 7     | 7      | 3    | Pipenzolate bromide _100.0               | 7     | 7      | 3    |
| Dextromethorphan hydrobromide monohydrate _1.0   | 7     | 7      | 3    | Piracetam _1.0                           | 7     | 7      | 3    |
| Dextromethorphan hydrobromide monohydrate _10.0  | 7     | 7      | 2    | Piracetam _10.0                          | 7     | 7      | 3    |
| Dextromethorphan hydrobromide monohydrate _100.0 | 8     | 8      | 3    | Piracetam _100.0                         | 8     | 8      | 3    |
| Dicloxacillin sodium salt hydrate _1.0           | 7     | 7      | 3    | Praziquantel _1.0                        | 7     | 7      | 4    |
| Dicloxacillin sodium salt hydrate _10.0          | 7     | 7      | 3    | Praziquantel _10.0                       | 7     | 7      | 4    |
| Dicloxacillin sodium salt hydrate _100.0         | 7     | 7      | 3    | Praziquantel _100.0                      | 7     | 7      | 4    |
| Diethylcarbazine citrate _1.0                    | 7     | 7      | 3    | Prednisone _1.0                          | 7     | 7      | 3    |

| compound and concentration (µM)     | wells | plates | days | compound and concentration (µM)       | wells | plates | days |
|-------------------------------------|-------|--------|------|---------------------------------------|-------|--------|------|
| Diethylcarbamazine citrate_10.0     | 8     | 8      | 3    | Prednisone_10.0                       | 7     | 7      | 3    |
| Diethylcarbamazine citrate_100.0    | 8     | 8      | 3    | Prednisone_100.0                      | 7     | 7      | 3    |
| Dihydrostreptomycin sulfate_0.5     | 7     | 7      | 3    | Prilocaine hydrochloride_1.0          | 8     | 8      | 3    |
| Dihydrostreptomycin sulfate_5.0     | 6     | 6      | 3    | Prilocaine hydrochloride_10.0         | 7     | 7      | 3    |
| Dihydrostreptomycin sulfate_50.0    | 5     | 5      | 3    | Prilocaine hydrochloride_100.0        | 7     | 7      | 2    |
| Diltiazem hydrochloride_1.0         | 7     | 7      | 3    | Probenecid_1.0                        | 7     | 7      | 3    |
| Diltiazem hydrochloride_10.0        | 7     | 7      | 3    | Probenecid_10.0                       | 6     | 6      | 3    |
| Diltiazem hydrochloride_100.0       | 6     | 6      | 2    | Probenecid_100.0                      | 5     | 5      | 3    |
| Diphenhydramine hydrochloride_1.0   | 6     | 6      | 3    | Procaine hydrochloride_1.0            | 8     | 8      | 3    |
| Diphenhydramine hydrochloride_10.0  | 7     | 7      | 3    | Procaine hydrochloride_10.0           | 8     | 8      | 3    |
| Diphenhydramine hydrochloride_100.0 | 7     | 7      | 3    | Procaine hydrochloride_100.0          | 7     | 7      | 2    |
| Diprophylline_1.0                   | 8     | 8      | 3    | Proglumide_1.0                        | 6     | 6      | 3    |
| Diprophylline_10.0                  | 5     | 5      | 3    | Proglumide_10.0                       | 6     | 6      | 3    |
| Diprophylline_100.0                 | 7     | 7      | 3    | Proglumide_100.0                      | 6     | 6      | 3    |
| Disopyramide_1.0                    | 7     | 7      | 4    | Propafenone hydrochloride_1.0         | 7     | 7      | 3    |
| Disopyramide_10.0                   | 6     | 6      | 3    | Propafenone hydrochloride_10.0        | 7     | 7      | 3    |
| Disopyramide_100.0                  | 5     | 5      | 2    | Propafenone hydrochloride_100.0       | 4     | 4      | 3    |
| Doxylamine succinate_1.0            | 6     | 6      | 4    | Pyrazinamide_1.0                      | 7     | 7      | 3    |
| Doxylamine succinate_10.0           | 6     | 6      | 3    | Pyrazinamide_10.0                     | 7     | 7      | 3    |
| Doxylamine succinate_100.0          | 4     | 4      | 2    | Pyrazinamide_100.0                    | 7     | 7      | 3    |
| Droperidol_1.0                      | 8     | 8      | 3    | Pyrilamine maleate_1.0                | 8     | 8      | 3    |
| Droperidol_10.0                     | 8     | 8      | 3    | Pyrilamine maleate_10.0               | 8     | 8      | 3    |
| Droperidol_100.0                    | 8     | 8      | 3    | Pyrilamine maleate_100.0              | 8     | 8      | 3    |
| Dropropizine (R,S)_1.0              | 5     | 5      | 2    | Pyrrithione sodium salt_1.0           | 7     | 7      | 3    |
| Dropropizine (R,S)_10.0             | 6     | 6      | 3    | Pyrrithione sodium salt_10.0          | 7     | 7      | 3    |
| Dropropizine (R,S)_100.0            | 5     | 5      | 2    | Pyrrithione sodium salt_100.0         | 7     | 7      | 3    |
| Dyclonine hydrochloride_0.5         | 6     | 6      | 4    | Scopolamin-N-oxide hydrobromide_1.0   | 5     | 5      | 3    |
| Dyclonine hydrochloride_5.0         | 7     | 7      | 4    | Scopolamin-N-oxide hydrobromide_10.0  | 5     | 5      | 3    |
| Dyclonine hydrochloride_50.0        | 7     | 7      | 4    | Scopolamin-N-oxide hydrobromide_100.0 | 6     | 6      | 4    |
| Epiandrosterone_1.0                 | 6     | 6      | 2    | Strophantine octahydrate_1.0          | 6     | 6      | 2    |
| Epiandrosterone_10.0                | 5     | 5      | 2    | Strophantine octahydrate_10.0         | 6     | 6      | 2    |
| Epiandrosterone_100.0               | 6     | 6      | 3    | Strophantine octahydrate_100.0        | 5     | 5      | 2    |
| Estradiol-17 beta_1.0               | 6     | 6      | 3    | Sulfadiazine_1.0                      | 6     | 6      | 4    |
| Estradiol-17 beta_10.0              | 5     | 5      | 2    | Sulfadiazine_10.0                     | 6     | 6      | 4    |
| Estradiol-17 beta_100.0             | 5     | 5      | 2    | Sulfadiazine_100.0                    | 5     | 5      | 3    |
| Fenbufen_1.0                        | 7     | 7      | 2    | Sulfaguanidine_1.0                    | 7     | 7      | 3    |
| Fenbufen_10.0                       | 7     | 7      | 3    | Sulfaguanidine_10.0                   | 6     | 6      | 2    |
| Fenbufen_100.0                      | 7     | 7      | 2    | Sulfaguanidine_100.0                  | 7     | 7      | 3    |
| Fenoterol hydrobromide_1.0          | 7     | 7      | 3    | Sulfathiazole_1.0                     | 7     | 7      | 3    |
| Fenoterol hydrobromide_10.0         | 7     | 7      | 3    | Sulfathiazole_10.0                    | 7     | 7      | 3    |
| Fenoterol hydrobromide_100.0        | 8     | 8      | 3    | Sulfathiazole_100.0                   | 7     | 7      | 3    |
| Flavoxate hydrochloride_0.5         | 6     | 6      | 3    | Sulfisoxazole_1.0                     | 5     | 5      | 2    |
| Flavoxate hydrochloride_5.0         | 5     | 5      | 2    | Sulfisoxazole_10.0                    | 5     | 5      | 2    |
| Flavoxate hydrochloride_50.0        | 7     | 7      | 4    | Sulfisoxazole_100.0                   | 5     | 5      | 2    |
| Flufenamic acid_1.0                 | 6     | 6      | 3    | Suxibuzone_1.0                        | 8     | 8      | 3    |
| Flufenamic acid_10.0                | 7     | 7      | 3    | Suxibuzone_10.0                       | 8     | 8      | 3    |
| Flufenamic acid_100.0               | 8     | 8      | 3    | Suxibuzone_100.0                      | 7     | 7      | 3    |
| Flunarizine dihydrochloride_0.25    | 6     | 6      | 3    | Tamoxifen citrate_1.0                 | 7     | 7      | 3    |
| Flunarizine dihydrochloride_2.5     | 8     | 8      | 3    | Tamoxifen citrate_10.0                | 7     | 7      | 3    |
| Flunarizine dihydrochloride_25.0    | 5     | 5      | 2    | Tamoxifen citrate_100.0               | 6     | 6      | 3    |
| Fusaric acid_1.0                    | 6     | 6      | 2    | Thiamphenicol_1.0                     | 3     | 3      | 2    |
| Fusaric acid_10.0                   | 6     | 6      | 2    | Thiamphenicol_10.0                    | 6     | 6      | 3    |
| Fusaric acid_100.0                  | 6     | 6      | 2    | Thiamphenicol_100.0                   | 3     | 3      | 1    |
| Gabazine bromide_1.0                | 6     | 6      | 2    | Thyroxine (L)_1.0                     | 8     | 8      | 3    |
| Gabazine bromide_10.0               | 6     | 6      | 3    | Thyroxine (L)_10.0                    | 8     | 8      | 3    |
| Gabazine bromide_100.0              | 5     | 5      | 2    | Thyroxine (L)_100.0                   | 8     | 8      | 3    |
| Glibenclamide_1.0                   | 8     | 8      | 3    | Todalazine hydrochloride_1.0          | 7     | 7      | 3    |
| Glibenclamide_10.0                  | 6     | 6      | 3    | Todalazine hydrochloride_10.0         | 8     | 8      | 3    |
| Glibenclamide_100.0                 | 5     | 5      | 2    | Todalazine hydrochloride_100.0        | 6     | 6      | 2    |
| Gramine_1.0                         | 5     | 5      | 2    | Tolazoline hydrochloride_1.0          | 5     | 5      | 2    |
| Gramine_10.0                        | 6     | 6      | 3    | Tolazoline hydrochloride_10.0         | 6     | 6      | 3    |
| Gramine_100.0                       | 5     | 5      | 3    | Tolazoline hydrochloride_100.0        | 5     | 5      | 3    |
| Guaifenesin_1.0                     | 8     | 8      | 3    | Tolfenamic acid_1.0                   | 6     | 6      | 3    |
| Guaifenesin_10.0                    | 7     | 7      | 3    | Tolfenamic acid_10.0                  | 7     | 7      | 3    |
| Guaifenesin_100.0                   | 8     | 8      | 3    | Tolfenamic acid_100.0                 | 7     | 7      | 2    |

| compound and concentration (μM)          | wells | plates | days | compound and concentration (μM)        | wells | plates | days |
|------------------------------------------|-------|--------|------|----------------------------------------|-------|--------|------|
| Guanethidine sulfate_0.25                | 5     | 5      | 3    | Tranexamic acid_0.5                    | 7     | 7      | 3    |
| Guanethidine sulfate_2.5                 | 5     | 5      | 3    | Tranexamic acid_5.0                    | 7     | 7      | 3    |
| Guanethidine sulfate_25.0                | 8     | 8      | 3    | Tranexamic acid_50.0                   | 7     | 7      | 3    |
| Haloperidol_1.0                          | 7     | 4      | 3    | Trazodone hydrochloride_0.5            | 8     | 8      | 3    |
| Haloperidol_10.0                         | 8     | 4      | 3    | Trazodone hydrochloride_5.0            | 7     | 7      | 3    |
| Haloperidol_100.0                        | 7     | 4      | 3    | Trazodone hydrochloride_50.0           | 8     | 8      | 3    |
| Hemicholinium bromide_1.0                | 7     | 7      | 3    | Trigonelline hydrochloride_0.5         | 6     | 6      | 3    |
| Hemicholinium bromide_10.0               | 7     | 7      | 3    | Trigonelline hydrochloride_5.0         | 7     | 7      | 3    |
| Hemicholinium bromide_100.0              | 6     | 6      | 2    | Trigonelline hydrochloride_50.0        | 7     | 7      | 3    |
| Homatropine hydrobromide (R,S)_1.0       | 7     | 7      | 3    | Trihexyphenidyl-D,L Hydrochloride_0.5  | 7     | 7      | 3    |
| Homatropine hydrobromide (R,S)_10.0      | 6     | 6      | 3    | Trihexyphenidyl-D,L Hydrochloride_5.0  | 7     | 7      | 3    |
| Homatropine hydrobromide (R,S)_100.0     | 7     | 7      | 3    | Trihexyphenidyl-D,L Hydrochloride_50.0 | 8     | 8      | 3    |
| Homochlorcyclizine dihydrochloride_1.0   | 6     | 6      | 3    | Trimethadione_1.0                      | 7     | 7      | 3    |
| Homochlorcyclizine dihydrochloride_10.0  | 8     | 8      | 3    | Trimethadione_10.0                     | 7     | 7      | 3    |
| Homochlorcyclizine dihydrochloride_100.0 | 2     | 2      | 1    | Trimethadione_100.0                    | 6     | 6      | 3    |
| Hydroquinine hydrobromide hydrate_1.0    | 8     | 8      | 3    | Tripolidine hydrochloride_1.0          | 6     | 6      | 3    |
| Hydroquinine hydrobromide hydrate_10.0   | 7     | 7      | 3    | Tripolidine hydrochloride_10.0         | 7     | 7      | 4    |
| Hydroquinine hydrobromide hydrate_100.0  | 8     | 8      | 3    | Tripolidine hydrochloride_100.0        | 7     | 7      | 4    |
| Hydroxyzine dihydrochloride_1.0          | 6     | 6      | 2    | Troleandomycin_1.0                     | 7     | 7      | 2    |
| Hydroxyzine dihydrochloride_10.0         | 6     | 6      | 3    | Troleandomycin_10.0                    | 7     | 7      | 2    |
| Hydroxyzine dihydrochloride_100.0        | 6     | 6      | 3    | Troleandomycin_100.0                   | 4     | 4      | 2    |
| Isoxsuprine hydrochloride_1.0            | 6     | 6      | 3    | Valsartan_1.0                          | 8     | 8      | 3    |
| Isoxsuprine hydrochloride_10.0           | 7     | 7      | 3    | Valsartan_10.0                         | 8     | 8      | 3    |
| Isoxsuprine hydrochloride_100.0          | 7     | 7      | 3    | Valsartan_100.0                        | 8     | 8      | 3    |
| Kanamycin A sulfate_0.5                  | 8     | 8      | 3    | Verapamil hydrochloride_1.0            | 6     | 6      | 3    |
| Kanamycin A sulfate_5.0                  | 6     | 6      | 3    | Verapamil hydrochloride_10.0           | 7     | 7      | 3    |
| Kanamycin A sulfate_50.0                 | 7     | 7      | 2    | Verapamil hydrochloride_100.0          | 7     | 7      | 3    |
| Ketoprofen_1.0                           | 8     | 8      | 3    | Xylometazoline hydrochloride_1.0       | 8     | 8      | 3    |
| Ketoprofen_10.0                          | 8     | 8      | 3    | Xylometazoline hydrochloride_10.0      | 8     | 8      | 3    |
| Ketoprofen_100.0                         | 8     | 8      | 3    | Xylometazoline hydrochloride_100.0     | 7     | 7      | 2    |
| DMSO_0                                   | 50    | 36     | 4    | Yohimbine hydrochloride_0.5            | 7     | 7      | 3    |
| DMSO_1                                   | 50    | 34     | 4    | Yohimbine hydrochloride_5.0            | 7     | 7      | 3    |
| DMSO_2                                   | 49    | 36     | 4    | Yohimbine hydrochloride_50.0           | 7     | 7      | 3    |
| DMSO_3                                   | 49    | 35     | 4    | DMSO_5                                 | 49    | 37     | 4    |
| DMSO_4                                   | 49    | 36     | 4    |                                        |       |        |      |

Note: the numerous control data points (DMSO) were randomly partitioned into 6 groups using scikit-learn's StratifiedKFold to maintain the correct imaging day distribution.