

## Additional Figures and Tables

Table 1 list the names and applied concentrations of all 63 chemicals in the data set. The experiment began by applying highest concentration chosen by the researchers to a cell culture. This was then diluted by 1/3 for the subsequent culture continuing for 10 dilutions to achieve the 11 original concentration levels. The maximal concentration was intended to be chosen to be just large enough to kill off all of the cells in the culture. The chemicals in this table are separated into MOA groups indicating the cell structure or function targeted by that class of chemicals.

Table 1: A list of chemicals in MOA groups I - X and maximal/minimal concentrations.

	Group I: DNA/RNA-Nucleic Acid Targets	Concentration(1:3)
1	5-Fluorouracil (5-FU)	200 $\mu$ M to 3.39 nM
2	Gemcitabine HCl	1650 $\mu$ M to 27.94 nM
3	Etoposide phosphate	200 $\mu$ M to 3.39 nM
4	Doxorubicin	100 $\mu$ M to 1.69 nM
5	Merbarone	200 $\mu$ M to 3.39 nM
6	Clofarabine	25 $\mu$ M to 0.42 nM
7	Hydroxyurea	10 $\mu$ M to 169 nM
8	SN-38	200 $\mu$ M to 3.39 nM
9	Topotecan	95 $\mu$ M to 1.61 nM
10	Irinotecan	160 $\mu$ M to 2.71 nM
11	Cytosine	8950 $\mu$ M to 151.57 nM

12	ABT-888	308 $\mu$ M to 5.22 nM
13	Mitoxantrone dihydrochloride	150 $\mu$ M to 2.54 nM
14	CRT0044876	194 $\mu$ M to 3.29 nM
15	NU7026	20 $\mu$ M to 0.34 nM
16	Mitomycin C	200 $\mu$ M to 3.39 nM
17	Cordycepin	200 $\mu$ M to 3.39 nM
18	Actinomycin D	2 $\mu$ M to 0.0339 nM
19	Cisplatin H <sub>2</sub> O	$\mu$ M to 2.54 nM
20	Ochratoxin A	10 $\mu$ M to 0.17 nM
Group II: Transport Protein-Primary Active transporter Targets		Concentration(1:3)
21	Brefeldin A	40 $\mu$ M to 0.68 nM
22	Exo 1	300 $\mu$ M to 5.08 nM
23	Leptomycin B	20 nM to 0.000339 nM
24	Concanamycin A	0.2 $\mu$ M to 0.003 nM
25	Thapsigargin	2 $\mu$ M to 0.0339 nM
26	BHQ	400 $\mu$ M to 7 nM
Group III: Protein-Actin Targets		Concentration(1:3)
27	Bafilomycin A1	0.3212 $\mu$ M to 0.01 nM
28	Cytochalasin D	20 $\mu$ M to 0.339 nM
29	Cytochalasin B	20 $\mu$ M to 0.339 nM
30	Latrunculin A	2 $\mu$ M to 0.0339 nM
31	Latrunculin B	2 $\mu$ M to 0.0339 nM
Group IV: Protein-Tubulin Targets		Concentration(1:3)
32	Docetaxel	1 $\mu$ M to 0.02 nM
33	Paclitaxel	20 $\mu$ M to 0.339 nM
34	Vincristine Sulfate	250 $\mu$ M to 4.23 nM

35	Vinblastine sulfate	40 $\mu$ M to 0.68 nM
Group V: Ribosome-50S Subunit Targets		Concentration(1:3)
36	Emetine	50 $\mu$ M to 0.847 nM
37	Puromycin	1000 $\mu$ M to 17 nM
38	Anisomycin	10 $\mu$ M to 0.17 nM
Group VI: Transport Proteins-Electrochemical Potential-driven Transporters		Concentration(1:3)
39	Oligomycin	20 $\mu$ M to 0.339 nM
40	Antimycin A	200 $\mu$ M to 3.387 nM
41	Rotenone	200 $\mu$ M to 3.387 nM
42	CCCP	100 $\mu$ M to 1.69 nM
Group VII: Ion Channel Targets		Concentration(1:3)
43	Valproic acid	50 mM to 847 nM
44	BAPT-am	60 $\mu$ M to 1 nM
Group VIII: Enzyme Targets		Concentration(1:3)
45	Cyclosporin A	100 $\mu$ M to 1.69 nM
46	FK-506	50 $\mu$ M to 1 nM
47	(S)-HDAC-42	128 $\mu$ M to 2.17 nM
48	SAHA	151 $\mu$ M to 2.56 nM
49	W7 HCl	200 $\mu$ M to 3.39 nM
Group IX: Receptors		Concentration(1:3)
50	benzo[a]pyrene	100 $\mu$ M to 1.69 nM
Group X: Protein- Motor Targets		Concentration(1:3)
51	Monastrol	100 $\mu$ M to 1.69 nM
52	S-trityl-cysteine	100 $\mu$ M to 1.69 nM
53	Dimethylenastron	40 $\mu$ M to 0.68 nM
54	Y-27632	188 $\mu$ M to 3.18 nM

55	HA1100 hydrochloride	1000 $\mu$ M to 16.94 nM
56	Ro32-3555	200 $\mu$ M to 3.39 nM
57	Batimastat	200 $\mu$ M to 3.39 nM
58	MLCKInhibPep18	94.5 $\mu$ M to 1.6 nM
59	Blebbistatin	100 $\mu$ M to 1.69 nM
60	ML7 hydrochloride	100 $\mu$ M to 1.69 nM
61	FAKInhibitor14	2500 $\mu$ M to 42.34 nM
62	PF573228	40 $\mu$ M to 0.68 nM
63	PF431396	5 $\mu$ M to 0.08 nM

Table 2 displays all of the fitted coefficients from the B-spline model of Section ???. Of note for the cytotoxicity data is the second half of the table, which details the differences in B-spline coefficients between MOA group 10 and group 1. For each of the  $\hat{\beta}$ 's, the first index corresponds to the concentration level with 1 = *high*, 2 = *medium*, and 3 = *low*. The second index is for MOA group 1 or 10. The third indicates the specific cubic B-spline, which are temporally ordered meaning that 1 is for the beginning of the experiment whereas 4 is for the end. Glancing at the p-values, we see that B-spline 1 does not yield significant differences between the MOA groups mainly because all cell cultures began from the same starting point. Meanwhile, B-splines 3 and 4 at high and medium concentration yield significant differences. At low concentration, MOA group differences are not noticeable.

Table 2: All of the estimated coefficients from the functional mixed effects model using B-splines.

fixed effects:	Estimate	Std. Error	t value	Pr(>  t )
$\hat{\mu}$	3.75	0.28	13.19	<2e-16
$\hat{\beta}_{1,1,1}$	-2.79	0.29	-9.80	3.35e-16
$\hat{\beta}_{2,1,1}$	-2.88	0.29	-10.09	< 2e-16
$\hat{\beta}_{3,1,1}$	-2.89	0.29	-10.11	< 2e-16
$\hat{\beta}_{1,1,2}$	-0.88	0.35	-2.56	0.011



Table 3: The performance of SOMs on the fPCA coefficients under different parameter settings for the SOMs algorithm.

neigh_func	topology	structure	grid	accuracy rate
Gaussian	rectangular	Toroidal	$6 \times 5$	<b>88.24%</b>
			$4 \times 3$	<b>88.24%</b>
		Planar	$6 \times 5$	64.71%
			$4 \times 3$	<b>88.24%</b>
		Toroidal	$6 \times 5$	<b>88.24%</b>
			$4 \times 3$	<b>88.24%</b>
	hexagonal	Planar	$6 \times 5$	<b>88.24%</b>
			$4 \times 3$	82.35%
		Toroidal	$6 \times 5$	85.29%
			$4 \times 3$	82.35%
	rectangular	Planar	$6 \times 5$	67.65%
			$4 \times 3$	82.35%
		Toroidal	$6 \times 5$	82.35%
			$4 \times 3$	82.35%

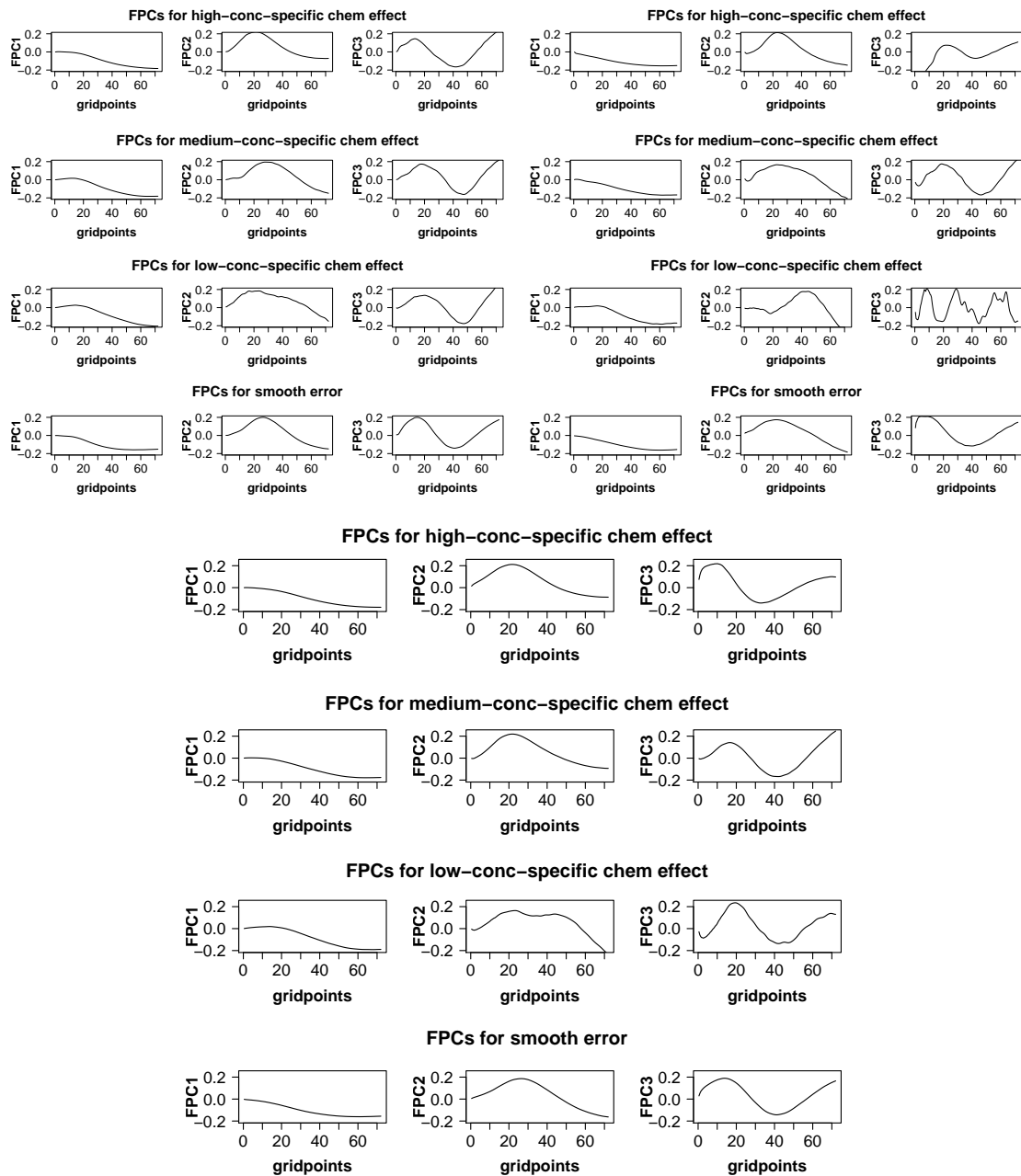


Figure 1: The first three estimated functional principal components for MOA group 1 (top left), MOA group 10 (top right), and for all the chemicals (bottom) for concentration levels high, medium, low, and for the smooth errors.