

## Additional File: 63 chemicals in 10 MOA clusters

<b>Cluster I: DNA/RNA-Nucleic Acid Targets</b>	Solvent	Concentration(1:3)
5-Fluorouracil (5-FU)	DMSO	200 $\mu$ M to 3.39 nM
Gemcitabine HCl	H <sub>2</sub> O	1650 $\mu$ M to 27.94 nM
Etoposide phosphate	DMSO	200 $\mu$ M to 3.39 nM
Doxorubicin	H <sub>2</sub> O	100 $\mu$ M to 1.69 nM
Merbarone	DMSO	200 $\mu$ M to 3.39 nM
Clofarabine	H <sub>2</sub> O	25 $\mu$ M to 0.42 nM
Hydroxyurea	H <sub>2</sub> O	10 $\mu$ M to 169 nM
SN-38	DMSO	200 $\mu$ M to 3.39 nM
Topotecan	DMSO	95 $\mu$ M to 1.61 nM
Irinotecan	DMSO	160 $\mu$ M to 2.71 nM
Cytosine	H <sub>2</sub> O	8950 $\mu$ M to 151.57 nM
ABT-888	DMSO	308 $\mu$ M to 5.22 nM
Mitoxantrone dihydrochloride	DMSO	150 $\mu$ M to 2.54 nM
CRT0044876	DMSO	194 $\mu$ M to 3.29 nM
NU7026	DMSO	20 $\mu$ M to 0.34 nM
Mitomycin C	DMSO	200 $\mu$ M to 3.39 nM
Cordycepin	DMSO	200 $\mu$ M to 3.39 nM
Actinomycin D	DMSO	2 $\mu$ M to 0.0339 nM
Cisplatin	H <sub>2</sub> O	150 $\mu$ M to 2.54 nM
Ochratoxin A	DMSO	10 $\mu$ M to 0.17 nM
<b>Cluster II: Transport Protein-Primary Activetransporter Targets</b>	Solvent	Concentration(1:3)
Brefeldin A	DMSO	40 $\mu$ M to 0.68 nM
Exo 1	DMSO	300 $\mu$ M to 5.08 nM
Leptomycin B	DMSO	20 nM to 0.000339 nM
Concanamycin A	DMSO	0.2 $\mu$ M to 0.003 nM
Thapsigargin	DMSO	2 $\mu$ M to 0.0339 nM
BHQ	DMSO	400 $\mu$ M to 7 nM
<b>Cluster III: Protein-Actin Targets</b>		
Bafilomycin A1	DMSO	0.3212 $\mu$ M to 0.01 nM
Cytochalasin D	DMSO	20 $\mu$ M to 0.339 nM
Cytochalasin B	DMSO	20 $\mu$ M to 0.339 nM
Latrunculin A	DMSO	2 $\mu$ M to 0.0339 nM
Latrunculin B	DMSO	2 $\mu$ M to 0.0339 nM
<b>Cluster IV: Protein-Tubulin Targets</b>		
Docetaxel	DMSO	1 $\mu$ M to 0.02 nM
Paclitaxel	DMSO	20 $\mu$ M to 0.339 nM
Vincristine Sulfate	H <sub>2</sub> O	250 $\mu$ M to 4.23 nM
Vinblastine sulfate	H <sub>2</sub> O	40 $\mu$ M to 0.68 nM
<b>Cluster V: Ribosome-50S Subunit Targets</b>		
Emetine	H <sub>2</sub> O	50 $\mu$ M to 0.847 nM
Puromycin	H <sub>2</sub> O	1000 $\mu$ M to 17 nM
Anisomycin	H <sub>2</sub> O	10 $\mu$ M to 0.17 nM
<b>Cluster VI: Transport Proteins-Electrochemical Potential-driven Transporters</b>		
Oligomycin	DMSO	20 $\mu$ M to 0.339 nM
Antimycin A	DMSO	200 $\mu$ M to 3.387 nM
Rotenone	DMSO	200 $\mu$ M to 3.387 nM
CCCP	DMSO	100 $\mu$ M to 1.69 nM

<b>Cluster VII: Ion Channel Targets</b>	Solvent	Concentration(1:3)
Valproic acid	H <sub>2</sub> O	50 mM to 847 nM
BAPT-am	DMSO	60 $\mu$ M to 1 nM
<b>Cluster VIII: Enzyme Targets</b>		
Cyclosporin A	DMSO	100 $\mu$ M to 1.69 nM
FK-506	DMSO	50 $\mu$ M to 1 nM
(S)-HDAC-42	DMSO	128 $\mu$ M to 2.17 nM
SAHA	DMSO	151 $\mu$ M to 2.56 nM
W7 HCl	DMSO	200 $\mu$ M to 3.39 nM
<b>Cluster IX: Receptors</b>		
benzo[a]pyrene	DMSO	100 $\mu$ M to 1.69 nM
<b>Cluster X: Protein- Motor Targets</b>		
Monastrol	DMSO	100 $\mu$ M to 1.69 nM
S-trityl-cysteine	DMSO	100 $\mu$ M to 1.69 nM
Dimethylnastron	DMSO	40 $\mu$ M to 0.68 nM
Y-27632	DMSO	188 $\mu$ M to 3.18 nM
HA1100 hydrochloride	H <sub>2</sub> O	1000 $\mu$ M to 16.94 nM
Ro32-3555	DMSO	200 $\mu$ M to 3.39 nM
Batimastat	DMSO	200 $\mu$ M to 3.39 nM
MLCKInhibPep18	H <sub>2</sub> O	94.5 $\mu$ M to 1.6 nM
Blebbistatin	DMSO	100 $\mu$ M to 1.69 nM
ML7 hydrochloride	DMSO	100 $\mu$ M to 1.69 nM
FAKInhibitor14	H <sub>2</sub> O	2500 $\mu$ M to 42.34 nM
PF573228	DMSO	40 $\mu$ M to 0.68 nM
PF431396	DMSO	5 $\mu$ M to 0.08 nM