

Supplementary Table 3 Rankings of the correct MDDR activity class for each PubChem MeSH pharmacological action set by SEA and by MPS

	MeSH Pharmacological Action	Rank of top matching MDDR activity class	
		SEA	MPS
1	Adrenergic α -Antagonists	1	10
2	Adrenergic β -Agonists	1	1
3	Adrenergic β -Antagonists	1	2
4	Androgen Antagonists	3	13
5	Androgens	1	1
6	Aromatase Inhibitors	2	2
7	Carbonic Anhydrase Inhibitors	1	1
8	Cholinergic Antagonists	1	1
9	Cholinesterase Inhibitors	1	8
10	Cyclooxygenase Inhibitors	2	57
11	Dopamine Agonists	1	5
12	Estrogen Antagonists	1	1
13	Estrogens	1	1
14	Glucocorticoids	1	1
15	Histamine H2 Antagonists	1	1
16	HIV Protease Inhibitors	1	6
17	Lipoxygenase Inhibitors	1	42
18	Muscarinic Antagonists	2	1
19	Nicotinic Agonists	1	6
20	Phosphodiesterase Inhibitors	1	4
21	Protease Inhibitors	4	11
22	Reverse Transcriptase Inhibitors	2	18
23	Trypsin Inhibitors	1	10
	Average	1.4	8.2