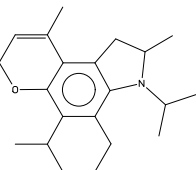
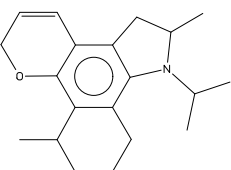
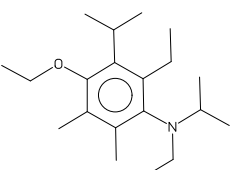
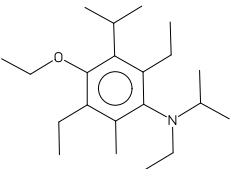
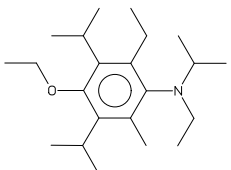
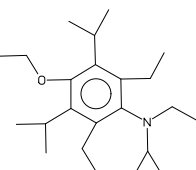
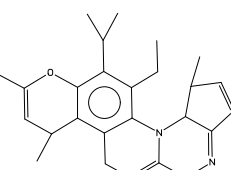


Table 8: GENSMI Structures, Approx. Mass 250-400, Top and Worst Similarities to WDI 03.4

SMILES	Branching	Complexity	Cyclization	Mass	History	Similarity
	2.69	47.685	1.31	313	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N8(6/1).N9(6/1).N9(6/1).N10(6/1).N11(6/1).N12(6/1).N12(6/1).N13(6/1).N14(6/1).E10-15.E14=22.	0.8411
	2.62	46.285	1.31	299	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N8(6/1).N9(6/1).N9(6/1).N10(6/1).N11(6/1).N12(6/1).N12(6/1).N13(6/1).E10-15.E14=22.	0.8172
	2.69	27.1	1	305	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N8(6/1).N9(6/1).N9(6/1).N10(6/1).N11(6/1).N12(6/1).N12(6/1).N13(6/1).	0.8012
	2.64	26.8	1	319	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N8(6/1).N9(6/1).N9(6/1).N10(6/1).N11(6/1).N12(6/1).N12(6/1).N13(6/1).N14(6/1).	0.7919
	2.71	28.2	1	333	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N8(6/1).N9(6/1).N9(6/1).N10(6/1).N11(6/1).N12(6/1).N12(6/1).N13(6/1).N14(6/1).N14(6/1).	0.7919
	2.67	27.9	1	347	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N8(6/1).N9(6/1).N9(6/1).N10(6/1).N11(6/1).N12(6/1).N12(6/1).N13(6/1).N14(6/1).N14(6/1).N15(6/1).	0.7919
	2.61	79.3219	1.38	388	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N8(6/1).N9(6/1).N9(6/1).N10(6/1).N11(6/1).N12(6/1).N12(6/1).N13(6/1).N14(6/1).N14(6/1).N15(6/1).N16(6/1).N16(6/1).N17(6/1).N18(7/1).E10=19.E13=20.E17=29.E26=28.	0.3448