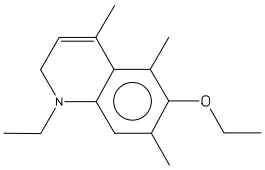
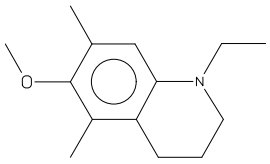
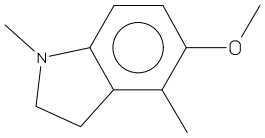
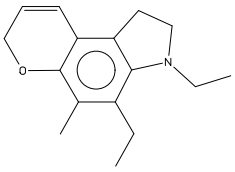
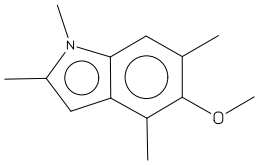
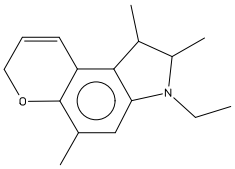
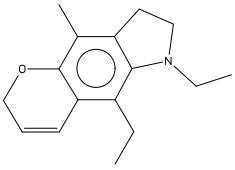
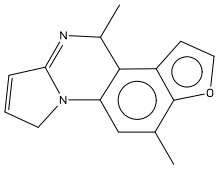
Table 7: GENSMI Structures, Approx. Mass 150-250, Top and Worst Similarities to WDI 03.4

SMILES	*Branching*	*Complexity*	*Cyclization*	*Mass*	*History*	*Similarity*
	2.54	35.5	1.2	245	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N9(6/1).N10(6/1).N11(6/1).N13(6/1).E11=15.	0.8101
	2.5	31.8	1.2	219	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N9(6/1).N10(6/1).E11-15.	0.8089
	2.5	28.3	1.22	177	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).E9-11.	0.8088
	2.47	42.385	1.31	243	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N9(6/1).N10(6/1).N11(6/1).N13(6/1).E8-15.E14=18.	0.8081
	2.7	33.2	1.22	203	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N9(6/1).E9=11.	0.8011
	2.57	43.085	1.31	243	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N9(6/1).N10(6/1).N11(6/1).N12(6/2).E9-11.E13-18.	0.7974
	2.47	42.385	1.31	243	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N9(6/1).N10(6/1).N11(6/1).N12(6/2).E8-15.E13-18.	0.7967
	2.5	59.3	1.38	238	S(Nc1ccc(O)cc1).N1(6/1).N1(6/1).N3(6/1).N4(6/1).N6(6/1).N7(6/1).N9(6/1).N10(6/1).N11(6/1).N11(7/1).E9=18.E12=13.E15=16.	0.3744

tablet 4.83 Daylight CIS