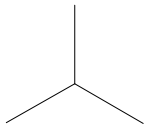
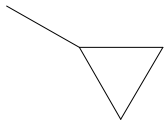
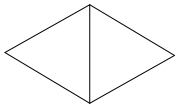
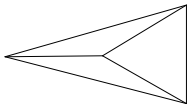
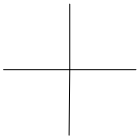
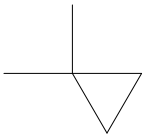
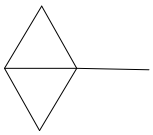
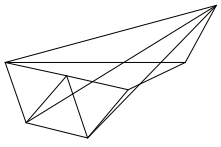
Table 3: GENSMI Structures, No Constraints

SMILES	*Branching*	*Complexity*	*Cyclization*	*Mass*	*History*	*ID*
	3	6	0	58	S(6).N1(6/1).N1(6/1).N1(6/1).	5
	2.33	9.6	1	56	S(6).N1(6/1).N1(6/1).N1(6/1).E2-3.	6
	2.5	13.2	1.5	54	S(6).N1(6/1).N1(6/1).N1(6/1).E2-3.E2-4.	7
	3	20.38	2.25	52	S(6).N1(6/1).N1(6/1).N1(6/1).E2-3.E2-4.E3-4.	8
	4	7.4	0	72	S(6).N1(6/1).N1(6/1).N1(6/1).N1(6/1).	9
	2.67	11	1	70	S(6).N1(6/1).N1(6/1).N1(6/1).N1(6/1).E2-3.	10
	2.75	14.6	1.5	68	S(6).N1(6/1).N1(6/1).N1(6/1).N1(6/1).E2-3.E2-4.	11
	3.71	87.21	3.14	86	S(6).N1(6/1).N1(6/1).N1(6/1).N1(6/1).N2(6/1).N2(6/1).E2-3.E3-4.E3-6.E4-5.E4-6.E5-7.E6-7.	100

tablet 4.83 Daylight CIS