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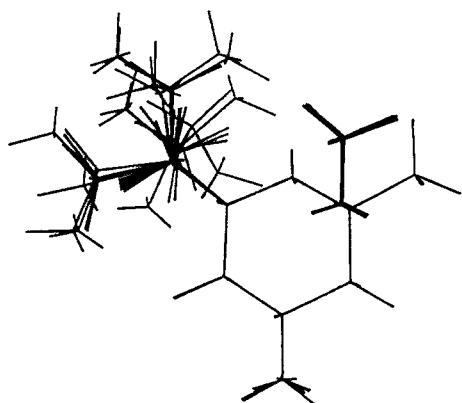


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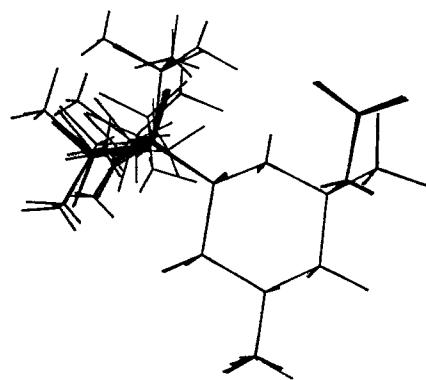
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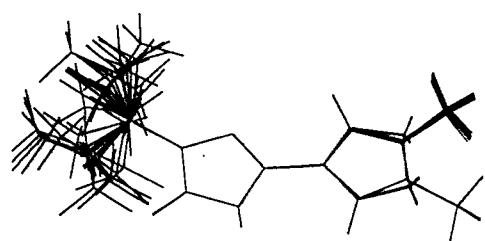
**Figure 1.** Overlayed conformational structures that were generated by Macromodel for fragments I–III in both enantiomeric configurations.



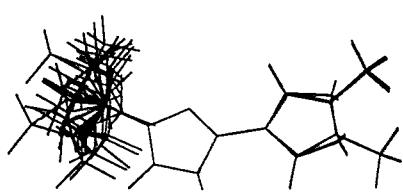
Fragment I, (2*R*,4*R*,6*R*) configuration



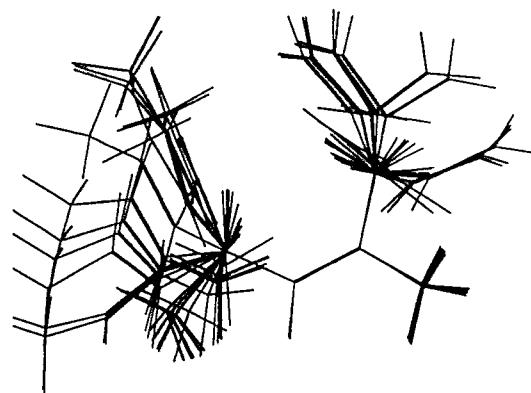
Fragment I, (2*S*,4*S*,6*S*) configuration



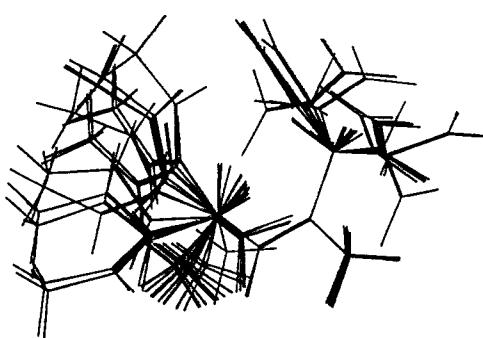
Fragment II, (8*R*) configuration



Fragment II, (8*S*) configuration



Fragment III, (22*R*) configuration



Fragment III, (22*S*) configuration

Table A1. Molar rotation angles, steric energies for conformational isomers, and Boltzmann averaged sum of fragments (I - III) for a single calculation.

Fragment I, (2R,6R,8R)			Fragment I, (2S,6S,8S)		
E (kJ/mol)	[M]D	Boltzmann Average.	E (kJ/mol)	[M]D	Boltzmann Average
-131.32	-184.42	-184.42	-131.83	197.14	197.14
-127.77	-126.24	-173.55	-127.64	130.18	187.11
-127.75	-91.17	-160.68	-127.28	102.95	177.49
-123.51	-163.43	-160.75	-126.54	91.59	170.83
-123.50	-122.08	-159.76	-123.54	53.59	168.26
-123.46	-62.04	-157.37	-123.47	62.00	166.05
-123.22	-119.39	-156.55	-122.93	120.83	165.31
-122.91	-120.76	-155.88	-120.78	110.65	164.95
-122.56	-109.40	-155.14	-120.28	120.15	164.71
-120.79	-110.66	-154.80	-120.14	140.06	164.58
-120.28	-120.84	-154.60	-119.18	91.57	164.33
-118.77	-109.64	-154.45	-117.69	82.94	164.18
-117.60	-84.48	-154.31	-117.47	86.44	164.06
-116.13	-62.96	-154.21	-116.26	90.31	163.98
-113.41	-	108.29	-116.15	62.98	163.88

Fragment II, (8 R)			Fragment II, (8 S)		
E(kJ/mol)	[M]D	Boltzmann Average.	E(kJ/mol)	[M]D	Boltzmann Average.
109.81	190.77	190.77	109.78	-210.31	-210.31
110.09	134.11	164.08	110.47	-71.21	-150.64
110.47	55.38	132.89	111.52	26.97	-112.04
113.68	-13.33	122.58	113.66	13.14	-101.75
113.83	60.23	118.71	113.82	-60.19	-98.79
114.14	53.67	115.33	117.24	15.87	-96.84
114.17	48.72	112.09	118.38	-9.49	-95.92
115.14	35.59	109.68	118.51	187.57	-93.13
116.57	1.26	107.82	118.85	39.18	-92.01
118.39	6.48	107.01	118.89	82.33	-90.56

Fragment III, (22 R)			Fragment III, (22 S)		
E(kJ/mol)	[M]D	Boltzmann Average.	E(kJ/mol)	[M]D	Boltzmann Average.
-3.72	346.68	346.68	-3.73	-356.47	-356.47
-3.41	243.06	298.18	-3.36	-252.77	-308.62
-2.78	-327.73	132.33	-2.80	326.65	-138.15
-2.43	366.88	175.95	-2.42	-357.83	-179.12
-2.05	238.50	184.53	-1.97	-218.49	-184.39
-1.87	196.75	185.91	-1.95	-211.90	-187.62
-1.81	9.99	168.46	-0.88	145.44	-164.37
-1.52	356.87	183.72	-0.59	-580.68	-188.71
-1.47	-174.62	157.39	-0.49	273.13	-164.22
-0.87	-145.96	140.94	-0.20	198.30	-147.95
-0.55	551.99	159.59	-0.19	-173.59	-149.05
-0.49	-268.95	141.45	-0.13	-238.67	-152.65
-0.20	175.22	142.67	-0.07	-218.70	-155.14
-0.08	215.62	145.10	-0.01	-256.18	-158.72