A switchable intramolecular hydrogen bond in 5-nitrosopyrimidines

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Figure S1. The temperature dependence of ¹H NMR spectra of the compound 5e. The NH region (top) and the region of aromatic protons (bottom).

Figure S2. The dependence of the percentage of rotamer A found in DMSO solution of compounds 4 – 7 as a function of the nature of the substituents R¹ and R².

Figure S3. The transition state of compound **5e** and the computational details: Cartesian coordinates of optimized structures.

Atomic number	x	y	z
6	-0.788028	-0.806794	-0.088458
6	0.421320	-0.081748	-0.079817
6	-1.988343	-0.072387	-0.137530
7	0.422059	1.255743	-0.154401
7	-1.979908	1.266273	-0.215481
6	-0.776896	1.856704	-0.221967
7	-3.203528	-0.707908	-0.093104
1	-3.208681	-1.697170	-0.294077
7	-0.811604	-2.237508	0.192358
8	-0.775778	-2.945662	-0.802171
7	1.610417	-0.769129	0.011763
6	2.950374	-0.337261	0.076408
1	1.513320	-1.773363	0.050374
6	3.919590	-1.345526	0.242876
6	5.273394	-1.028430	0.309364
6	5.692721	0.302050	0.213151
6	3.369558	0.999773	-0.022341
6	4.732249	1.301293	0.047804
7	-0.769251	3.219890	-0.340737
1	3.605774	-2.384321	0.322154
1	6.000365	-1.825116	0.438003
1	6.747712	0.552444	0.264710
1	2.634157	1.778443	-0.154870
1	5.040499	2.340179	-0.031753
1	-1.640449	3.701093	-0.180839
1	0.089717	3.702593	-0.129252
6	-4.451816	-0.014510	-0.262811
6	-5.103527	0.628614	0.933141
6	-5.673012	-0.646592	0.353530
1	-4.572412	0.491335	-1.219218
1	-4.573382	0.559172	1.877247
1	-5.637856	1.560191	0.774313
1	-6.602600	-0.601527	-0.205133
1	-5.532730	-1.561298	0.922819

Figure S4. Compound **3e** dissolved in different solvents and have different electronic spectra (solvatochromic effect). Solutions of compound **3e** in acetone, DMSO, ethanol and methanol (from left to right).

Table S1. The calculated (B3LYP/6-31+g(d,p)//TD-B3LYP/6-31+g(d,p)/PCM) electronic transitions of compounds **3a** – **3h**.

Compound	Transition	Orbitals	Orbitals		λ_{max}	Oscillator strength
3a	1	70→71	HOMO → LUMO	n→ π^*	619	0.0006
	2	69→71	HOMO-1 → LUMO	π → π^*	378	0.3805
	3	66→71	HOMO-4 → LUMO	π → π^*	317	0.0000
	4	68→71	HOMO-2 → LUMO	π → π^*	311	0.3257
	5	70→72	HOMO → LUMO+1	n→ π^*	311	0.0000
3b	1	80→81	HOMO → LUMO	n→ π^*	615	0.0007
	2	79→81	HOMO-1 → LUMO	π → π^*	373	0.2821
	3	76→81	HOMO-4 → LUMO	π → π^*	315	0.0000
	4	78→81	HOMO-2 → LUMO	π → π^*	307	0.3609
	5	77→81	HOMO-3 → LUMO	π → π^*	296	0.0006
3c	1	79→80	HOMO → LUMO	n→ π^*	617	0.0006
	2	78→80	HOMO-1 → LUMO	π → π^*	383	0.3793
	3	75→80	HOMO-4 → LUMO	π → π^*	317	0.0000
	4	79→81	HOMO → LUMO+1	n→ π^*	311	0.0000
	5	77→80	HOMO-2 → LUMO	π → π^*	311	0.3187
3d	1	72→73	HOMO → LUMO	n→ π^*	609	0.0007
	2	71→73	HOMO-1 → LUMO	π → π^*	396	0.2726
	3	68→73	HOMO-4 → LUMO	π → π^*	313	0.0000
	4	70→73	HOMO-2 → LUMO	π → π^*	305	0.3631
	5	69→73	HOMO-3 → LUMO	π → π^*	296	0.0040
3e	1	64→65	HOMO → LUMO	n→ π^*	608	0.0007
	2	63→65	HOMO-1 → LUMO	π → π^*	392	0.2342
	3	60→65	HOMO-4 → LUMO	π → π^*	313	0.0000
	4	61→65	HOMO-3 → LUMO	π → π^*	313	0.0241
	5	62→65	HOMO-2 → LUMO	π → π^*	304	0.3481
3f	1	67→69	HOMO-1 → LUMO	n→ π^*	606	0.0007
	2	68→69	HOMO → LUMO	π → π^*	409	0.2512
	3	65→69	HOMO-3 → LUMO	π → π^*	315	0.0149
	4	64→69	HOMO-4 → LUMO	π → π^*	313	0.0000
	5	66→69	HOMO-2 → LUMO	π → π^*	303	0.3535
3g	1	67→69	HOMO-1 → LUMO	n→ π^*	602	0.0007
	2	68→69	HOMO → LUMO	π → π^*	431	0.2382

	3	64→69	HOMO-4 → LUMO	$\pi \rightarrow \pi^*$	311	0.0000
	4	66→69	HOMO-2 → LUMO	$\pi \rightarrow \pi^*$	304	0.2202
	5	65→69	HOMO-3 → LUMO	$\pi \rightarrow \pi^*$	302	0.1405
3h	1	67→69	HOMO-1 → LUMO	$n \rightarrow \pi^*$	598	0.0007
	2	68→69	HOMO → LUMO	$\pi \rightarrow \pi^*$	483	0.2567
	3	63→69	HOMO-5 → LUMO	$\pi \rightarrow \pi^*$	310	0.0010
	4	65→69	HOMO-3 → LUMO	$\pi \rightarrow \pi^*$	309	0.0085
	5	66→69	HOMO-2 → LUMO	$\pi \rightarrow \pi^*$	304	0.3234

Table S2. Graphical representation of molecular orbitals of compounds **3e** and **3h**.

	3e	3h
LUMO+1		
LUMO		
HOMO		
HOMO-1		

HOMO-2

HOMO-3

HOMO-4

HOMO-5

Figure S5. The NMR spectra of compound **3a**.

060313servisHR_7+ #60-68 RT: 1.67-1.90 AV: 9 NL: 2.52E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S6. The HR-MS spectrum (top) and electronic spectra (bottom) of compound **3a**.

Figure S7. The NMR spectra of the compound **3b**.

130313servisHR_7+ #60-73 RT: 1.68-2.05 AV: 14 NL: 8.39E4
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S8. The HR-MS spectrum (top) and electronic spectra (bottom) of compound **3b**.

Figure S9. The NMR spectra of compound **3c**.

040413servisHR_29+ #58-60 RT: 1.62-1.68 AV: 3 NL: 2.90E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S10. The HR-MS spectrum (top) and electronic spectra (bottom) of compound **3c**.

Figure S11. The NMR spectra of compound **3d**.

060213servisHR_32+ #61-69 RT: 1.70-1.93 AV: 9 NL: 1.55E8
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S12. The HR-MS spectrum (top) and electronic spectra (bottom) of compound **3d**.

Figure S13. The NMR spectra of compound **3e**.

070113servisHR_22+ #59-72 RT: 1.65-2.02 AV: 14 NL: 2.39E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S14. The HR-MS spectrum (top) and electronic spectra (bottom) of compound **3e**.

Figure S15. The NMR spectra of compound **3f**.

070113servisHR_27+ #60-70 RT: 1.68-1.96 AV: 11 NL: 1.62E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S16. The HR-MS spectrum (top) and electronic spectra (bottom) of compound **3f**.

Figure S17. The NMR spectra of compound **3g**.

090213servisHR_10_130215124104 #62-65 RT: 1.71-1.80 AV: 4 NL: 2.52E6
T: FTMS + p ESI Full ms [60.00-800.00]

Figure S18. The HR-MS spectrum (top) and electronic spectra (bottom) of compound **3g**.

Figure S19. The NMR spectra of compound **3h**.

060213servisHR_30+ #61-66 RT: 1.70-1.84 AV: 6 NL: 6.41E6
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S20. The HR-MS spectrum (top) and electronic spectra (bottom) of compound **3h**.

Figure S21. The NMR spectra of compound **3i**.

210613servisHR_40 #57-89 RT: 1.66-2.03 AV: 13 NL: 3.43E4
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S22. The HR-MS spectrum (top) and electronic spectra (bottom) of compound **3i**.

Figure S23. The NMR spectra of compound **4a**.

060313servisHR_6+ #59-89 RT: 1.64-1.93 AV: 11 NL: 2.39E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S24. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **4a**.

Figure S25. The NMR spectra of compound **4b**.

130313servisHR_6+ #59-74 RT: 1.65-2.08 AV: 16 NL: 4.44E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S26. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **4b**.

Figure S27. The NMR spectra of compound **4c**.

060313servisHR_2+ #59-80 RT: 1.64-1.87 AV: 2 NL: 3.43E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S28. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **4c**.

Figure S29. The NMR spectra of compound **4d**.

060213servisHR_27+ #67-70 RT: 1.87-1.96 AV: 4 NL: 2.78E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S30. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **4d**.

Figure S31. The NMR spectra of compound **4e**.

070113servisHR_25+ #63-64 RT: 1.76-1.79 AV: 2 NL: 2.14E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S32. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **4e**.

Figure S33. The NMR spectra of compound **4f**.

090213servisHR_12_130215124940 #60-67 RT: 1.66-1.85 AV: 8 NL: 8.85E5
T: FTMS + p ESI Full ms [60.00-800.00]

Figure S34. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **4f**.

Figure S35. The NMR spectra of compound **4g**.

070113servisHR_26+ #60-62 RT: 1.68-1.73 AV: 3 NL: 1.92E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S36. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **4g**.

Figure S37. The NMR spectra of compound **4h**.

060213servisHR_28+ #60-87 RT: 1.67-1.87 AV: 8 NL: 3.52E6
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S38. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **4h**.

Figure S39. The NMR spectrum of compound **5a**.

060313servisHR_5+ #59-87 RT: 1.64-1.87 AV: 0 NL: 1.18E6
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S40. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **5a**.

Figure S41. The NMR spectra of compound **5b**.

070313servisHR_7+ #61-69 RT: 1.70-1.93 AV: 9 NL: 1.98E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S42. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **5b**.

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060213servisHR_31+ #60-66 RT: 1.67-1.84 AV: 7 NL: 8.28E6
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S44. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **5c**.

Figure S45. The NMR spectra of the compound **5d**.

060213servisHR_29+ #60-67 RT: 1.67-1.87 AV: 8 NL: 6.38E6
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S46. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **5d**.

Figure S47. The NMR spectra of the compound **5e**.

070113servisHR_24+ #60-71 RT: 1.68-1.99 AV: 12 NL: 2.80E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S48. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **5e**.

060313servisHR_8+ #04-86 RT: 1.78-1.84 AV: 3 NL: 2.62E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S50. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **5f**.

Figure S51. The NMR spectra of the compound **5g**.

070113servisHR_23+ #59-61 RT: 1.65-1.70 AV: 3 NL: 4.80E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S52. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **5g**.

Figure S53. The NMR spectra of the compound **5h**.

060213servisHR_26+ #60-67 RT: 1.67-1.87 AV: 8 NL: 7.70E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S54. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **5h**.

Figure S55. The NMR spectra of compound **6a**.

130313servisHR_9+ #60-78 RT: 1.68-2.19 AV: 19 NL: 1.04E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S56. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **6a**.

Figure S57. The NMR spectra of compound **6b**.

130313servisHR_8+ #59-75 RT: 1.65-2.11 AV: 17 NL: 4.01E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S58. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **6b**.

Figure S59. The NMR spectra of compound **6c**.

090213servisHR_13_130215125359 #60-67 RT: 1.66-1.85 AV: 8 NL: 5.47E5
T: FTMS + p ESI Full ms [60.00-800.00]

Figure S60. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **6c**.

Figure S61. The NMR spectra of compound **6d**.

090213servisHR_14_130215125817 #59-69 RT: 1.63-1.91 AV: 11 NL: 4.48E5
T: FTMS + p ESI Full ms [60.00-800.00]

Figure S62. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **6d**.

Figure S63. The NMR spectra of compound **6e**.

090213servisHR_09 #61-66 RT: 1.69-1.83 AV: 6 NL: 1.88E6
T: FTMS + p ESI Full ms [60.00-800.00]

Figure S64. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **6e**.

Figure S65. The NMR spectra of compound **6f**.

060313servisHR_4+ #59-88 RT: 1.64-1.90 AV: 10 NL: 5.39E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S66. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **6f**.

Figure S67. The NMR spectra of compound **6g**.

090213servisHR_08 #62-66 RT: 1.71-1.82 AV: 5 NL: 2.88E6
T: FTMS + p ESI Full ms [60.00-800.00]

Figure S68. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **6g**.

Figure S69. The NMR spectra of compound **6h**.

060313servisHR_3+ #58-71 RT: 1.61-1.98 AV: 14 NL: 5.98E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S70. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **6h**.

Figure S71. The NMR spectra of compound **6i**.

210613servisHR_41 #56-64 RT: 1.65-1.89 AV: 9 NL: 5.29E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S72. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **6i**.

Figure S73. The NMR spectra of compound **7a**.

300413servisHR_13 #54-57 RT: 1.63-1.72 AV: 4 NL: 1.07E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S74. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **7a**.

Figure S75. The NMR spectra of compound **7b**.

160513servisHR_12 #57-58 RT: 1.72-1.75 AV: 2 NL: 2.00E3
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S76. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **7b**.

Figure S77. The NMR spectra of compound **7c**.

100513servisHR_13 #56-71 RT: 1.89-2.16 AV: 16 NL: 8.37E4
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S78. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound 7c.

300413servisHR_12 #55-58 RT: 1.66-1.75 AV: 4 NL: 1.41E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S80. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **7d**.

Figure S81. The NMR spectra of compound 7e.

100413servisHR_8+ #59-79 RT: 1.65-2.22 AV: 21 NL: 5.18E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S82. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **7e**.

Figure S83. The NMR spectra of compound **7f**.

100413servisHR_9+ #60-77 RT: 1.68-2.16 AV: 18 NL: 1.02E6
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure S84. The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **7f**.

Figure S85. The NMR spectra of compound **7i**.

210613servisHR_42 #58-70 RT: 1.71-2.08 AV: 13 NL: 1.20E5
T: FTMS + p ESI Full ms [200.00-2000.00]

Figure 86: The HR-MS spectrum (top) and electronic spectrum (bottom) of compound **7i**.

Tables S3. Computational details: Cartesian coordinates of optimized structures

Compound 3a

Atomic number	x	y	z
6	-2.072631	-0.879134	0.000000
6	-0.833771	-0.129664	0.000000
6	-3.263104	-0.079134	0.000000
7	-0.823012	1.209437	0.000001
7	-3.242262	1.242541	0.000000
6	-2.017309	1.820957	0.000001
7	-2.234215	-2.241958	0.000000
8	-1.195689	-2.953910	0.000000
7	0.320635	-0.837801	0.000000
6	1.665297	-0.442253	0.000000
1	0.121408	-1.851112	0.000000
6	2.612267	-1.487395	0.000001
6	3.971760	-1.215372	0.000001
6	4.423894	0.117318	0.000000
6	2.115947	0.890248	-0.000001
6	3.481535	1.158766	-0.000001
7	-2.008943	3.171278	0.000001
1	2.270679	-2.518514	0.000002
1	4.688929	-2.029131	0.000002
1	1.397652	1.695428	-0.000002
1	3.824119	2.188305	-0.000003
1	-2.882516	3.672650	0.000002
1	-1.132597	3.667426	0.000002
6	-5.634292	0.074982	-0.000001
1	-5.681384	0.703836	0.891900
1	-6.440915	-0.657024	-0.000003
1	-5.681382	0.703839	-0.891900
6	5.826739	0.408461	0.000000
7	6.966662	0.646679	0.000000
8	-4.428565	-0.712792	-0.000001

Compound 3b

Atomic number	x	y	z
6	2.869636	-0.874178	-0.000002
6	1.615536	-0.148977	-0.000002
6	4.044066	-0.05123	0.000000
7	1.579888	1.190434	0.000000
7	3.998157	1.269726	0.000003
6	2.761718	1.824122	0.000003
7	3.058006	-2.233189	-0.000003
8	2.033565	-2.965679	-0.000004
7	0.475943	-0.877772	-0.000004
6	-0.878235	-0.506934	-0.000004
1	0.692971	-1.886918	-0.000003
6	-1.803882	-1.571011	0.000008
6	-3.16826	-1.322665	0.000008
6	-3.641862	-0.003361	-0.000005
6	-1.355669	0.813448	-0.000017
6	-2.73071	1.053302	-0.000017
7	2.727934	3.174477	0.000007
1	-1.442378	-2.595324	0.000018
1	-3.866278	-2.15363	0.000018
1	-0.655247	1.634194	-0.000027
1	-3.089703	2.076437	-0.000028
1	3.591859	3.692162	0.000012
1	1.842142	3.653487	0.000011
6	6.411715	0.148963	0.000003
1	6.446667	0.778798	-0.891823
1	7.232799	-0.566874	0.000002
1	6.446665	0.778795	0.891831
6	-5.124257	0.238125	0.000001
8	5.222129	-0.662325	0.000000
9	-5.441292	1.555372	-0.000051
9	-5.730662	-0.313869	-1.087152
9	-5.730637	-0.313775	1.087217

Compound 3c

Atomic number	x	y	z
6	2.888841	-0.893239	0.000000
6	1.650942	-0.139799	0.000000
6	4.081478	-0.096776	0.000000

7	1.646829	1.200268	0.000001
7	4.06611	1.224691	0.000000
6	2.841886	1.8068	0.000001
7	3.047506	-2.255838	0.000000
8	2.007254	-2.966003	0.000000
7	0.494646	-0.841316	0.000000
6	-0.851102	-0.440824	0.000000
1	0.687128	-1.85496	0.000000
6	-1.799336	-1.484228	0.000002
6	-3.159241	-1.207299	0.000001
6	-3.610293	0.12276	0.000000
6	-1.299188	0.892498	-0.000002
6	-2.665762	1.157702	-0.000002
7	2.838481	3.157796	0.000002
1	-1.457889	-2.515729	0.000003
1	-3.876424	-2.019744	0.000003
1	-0.580417	1.697171	-0.000003
1	-3.019688	2.183331	-0.000003
1	3.713553	3.656253	0.000003
1	1.963181	3.655875	0.000003
6	6.452702	0.050476	-0.000001
1	6.501606	0.679645	0.891698
8	-5.859732	-0.607192	0.000001
6	-7.273267	-0.337597	0.000000
1	-7.754176	-1.315524	0.000001
1	-7.553193	0.230734	0.890298
1	-7.553193	0.230733	-0.890299
6	-5.052717	0.48089	-0.000001
8	-5.482906	1.621225	-0.000002
1	6.501603	0.679649	-0.891698
1	7.258173	-0.682971	-0.000004
8	5.24602	-0.734513	-0.000001

Compound 3d

Atomic number	x	y	z
6	-0.008317	0.000016	-0.034312
6	-0.006453	0.000004	1.415686
6	1.291021	0.000009	-0.640854
7	1.139116	-0.000012	2.114542
7	2.412976	-0.000007	0.057423
6	2.276011	-0.000017	1.406447
7	-1.091284	0.000034	-0.874506
8	-2.237887	0.000040	-0.350762
7	-1.203189	0.000010	2.039655
6	-1.556825	0.000002	3.401782
1	-1.970362	0.000024	1.349166
6	-2.937222	0.000015	3.677616
6	-3.406350	0.000008	4.987038
6	-2.490878	-0.000012	6.040823
6	-0.649140	-0.000018	4.473420
6	-1.120929	-0.000025	5.787451
7	3.431434	-0.000033	2.107833
1	-3.648800	0.000031	2.856556
1	-4.472075	0.000019	5.186713
1	0.411771	-0.000028	4.275011
1	-0.417247	-0.000041	6.612801
1	4.310081	-0.000037	1.615805
1	3.406030	-0.000040	3.114432
6	2.646563	0.000012	-2.591977
1	3.209999	0.891672	-2.307544
1	2.437310	0.000021	-3.661088
1	3.209984	-0.891662	-2.307556
17	-3.073429	-0.000021	7.699789
8	1.349711	0.000019	-1.967481

Compound 3e

Atomic number	x	y	z
6	-0.008832	0.000146	-0.034648
6	-0.006859	0.000104	1.416319
6	1.289909	0.000111	-0.641904
7	1.140873	0.000039	2.113209
7	2.412754	0.000046	0.054681
6	2.275962	0.000014	1.404321
7	-1.090908	0.000213	-0.875615
8	-2.238188	0.000245	-0.353280

7	-1.201620	0.000134	2.041410
6	-1.558897	0.000108	3.405126
1	-1.969841	0.000185	1.353287
6	-2.941462	0.000161	3.671993
6	-3.409155	0.000141	4.982830
6	-2.508588	0.000068	6.053039
6	-0.652349	0.000035	4.478005
6	-1.137941	0.000016	5.788166
7	3.432838	-0.000052	2.104612
1	-3.645072	0.000218	2.843665
1	-4.479403	0.000182	5.166916
1	-2.871397	0.000052	7.076286
1	0.408427	-0.000005	4.279180
1	-0.427612	-0.000041	6.610243
1	4.310869	-0.000071	1.611736
1	3.407536	-0.000077	3.111175
6	2.644058	0.000112	-2.593646
1	3.207986	0.891611	-2.309420
1	2.435025	0.000148	-3.662887
1	3.207916	-0.891446	-2.309467
8	1.347697	0.000146	-1.969381

Compound 3f

Atomic number	x	y	z
6	-1.847170	-0.895382	-0.000047
6	-0.617862	-0.123764	-0.000200
6	-3.050754	-0.116385	0.000295
7	-0.636461	1.219660	0.000229
7	-3.056116	1.204860	0.000694
6	-1.839112	1.805023	0.000760
7	-1.985278	-2.258360	-0.000170
8	-0.932761	-2.953138	-0.000415
7	0.545590	-0.803068	-0.000695
6	1.890446	-0.378895	-0.000812
1	0.371409	-1.819581	-0.000584
6	2.856470	-1.403299	0.001033
6	4.212622	-1.099430	0.000146
6	4.662030	0.231374	-0.002118
6	2.321735	0.955292	-0.004133
6	3.690652	1.238317	-0.004959
7	-1.860236	3.157545	0.001313
1	2.534891	-2.441618	0.002154
1	4.934949	-1.912145	0.000641
1	1.594272	1.752698	-0.006932
1	4.004414	2.279469	-0.008492
1	-2.744133	3.639731	0.002436
1	-0.993821	3.670445	0.002240
6	-5.423469	-0.003238	0.000584
1	-5.481424	0.625428	0.892249
1	-6.219461	-0.747177	0.000429
1	-5.481599	0.625987	-0.890675
1	6.658170	0.063192	-0.826331
6	6.138119	0.552951	0.005095
1	6.616253	0.211394	0.931215
1	6.310676	1.629662	-0.080280
8	-4.207156	-0.771529	0.000223

Compound 3g

Atomic number	x	y	z
6	-0.009500	0.000002	-0.034375
6	-0.007619	0.000001	1.417224
6	1.289305	0.000001	-0.641271
7	1.142038	-0.000002	2.115047
7	2.412025	-0.000001	0.055291
6	2.275496	-0.000002	1.405557
7	-1.091966	0.000005	-0.872809
8	-2.238996	0.000006	-0.346681
7	-1.199541	0.000002	2.042255
6	-1.552988	0.000001	3.407957
1	-1.968411	0.000004	1.353787
6	-2.933476	0.000003	3.686891
6	-3.403378	0.000002	4.993734
6	-2.495381	-0.000001	6.058535
6	-0.648664	-0.000003	4.480004
6	-1.124099	-0.000004	5.793593

7	3.434681	-0.000005	2.103505
1	-3.644575	0.000006	2.865163
1	-4.467822	0.000005	5.202632
1	0.412766	-0.000005	4.283620
1	-0.411279	-0.000007	6.615662
1	4.311252	-0.000005	1.608148
1	3.412237	-0.000005	3.109976
6	2.643951	0.000001	-2.592552
1	3.207892	0.891475	-2.308138
1	2.435557	0.000002	-3.661949
1	3.207890	-0.891475	-2.308139
8	-3.011523	-0.000002	7.329056
1	-2.295155	-0.000005	7.977221
8	1.347486	0.000002	-1.969020

Compound 3h

Atomic number	x	y	z
6	-1.836983	-0.899086	0.004090
6	-0.607420	-0.125874	-0.001820
6	-3.040999	-0.120686	0.003448
7	-0.628301	1.220063	-0.008486
7	-3.047974	1.200169	-0.003716
6	-1.830561	1.802163	-0.010405
7	-1.972045	-2.260533	0.010500
8	-0.915582	-2.952930	0.009965
7	0.554783	-0.801704	-0.000866
6	1.900104	-0.375781	-0.003744
1	0.380132	-1.818969	0.001003
6	2.870743	-1.393358	-0.031571
6	4.227158	-1.094240	-0.031213
6	4.667421	0.240953	-0.001033
6	2.333072	0.959380	0.024337
6	3.695446	1.253839	0.025238
7	-1.856755	3.155709	-0.016208
1	2.555212	-2.433232	-0.052931
1	4.952982	-1.902839	-0.059216
1	1.604020	1.755366	0.046441
1	4.008907	2.294972	0.042283
1	-2.742458	3.633593	-0.043665
1	-0.992582	3.671117	-0.049144
6	-5.413498	-0.009209	0.008365
1	-5.469931	0.624914	0.896335
1	-6.209610	-0.753110	0.014262
1	-5.474036	0.615049	-0.886306
1	6.290160	1.460139	0.295223
7	6.029612	0.549323	-0.057142
1	6.659596	-0.176908	0.255014
8	-4.197483	-0.777054	0.009782

Compound 3i

Atomic number	x	y	z
6	-2.59407	-0.88268	0.010962
6	-1.33686	-0.15515	-0.01337
6	-3.76843	-0.06024	0.018766
7	-1.30876	1.191142	-0.03015
7	-3.72724	1.259775	0.001988
6	-2.48829	1.816569	-0.02344
7	-2.77896	-2.23789	0.027836
8	-1.74808	-2.96857	0.020125
7	-0.20019	-0.87222	-0.01939
6	1.159069	-0.49515	-0.03813
1	-0.41136	-1.88249	-0.00885
6	2.094724	-1.54286	-0.06743
6	3.461303	-1.29755	-0.08005
6	3.967859	0.024009	-0.07402
6	1.645481	0.820148	-0.01536
6	3.0166	1.068359	-0.02802
7	-2.46555	3.170459	-0.04033
1	1.745075	-2.57216	-0.07499
1	4.131768	-2.14726	-0.0964
1	0.94963	1.645188	0.01736
1	3.339959	2.101496	-0.00201
1	-3.33361	3.679933	-0.06055
1	-1.58353	3.653583	-0.08614
6	-6.13488	0.138879	0.052696
1	-6.15625	0.780507	0.936849

1	-6.95801	-0.57477	0.074046
1	-6.18416	0.759285	-0.84538
7	5.335459	0.280533	-0.12607
8	-4.94849	-0.67353	0.043834
6	5.811191	1.628268	0.144856
6	6.268531	-0.81413	0.094024
1	6.89629	1.65159	0.03199
1	5.392506	2.342234	-0.57225
1	5.560186	1.974894	1.160965
1	7.287633	-0.43859	-0.01152
1	6.167964	-1.26846	1.093418
1	6.131771	-1.6017	-0.65443

Compound 4a

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	2.057893	-0.850253	-0.000010	6	1.992585	-0.797886	0.000000
6	0.818664	-0.104551	-0.000013	6	0.738987	-0.078912	0.000000
6	3.268874	-0.055923	-0.000012	6	3.185789	0.018752	0.000000
7	0.806009	1.230124	-0.000013	7	0.689053	1.248290	0.000000
7	3.234351	1.279862	-0.000001	7	3.115438	1.359488	0.000000
6	2.010550	1.842034	-0.000008	6	1.884410	1.891383	0.000000
7	4.461525	-0.668935	-0.000034	7	4.386688	-0.568357	0.000000
1	4.431394	-1.680739	0.000034	1	4.352505	-1.589779	0.000000
7	2.229789	-2.195851	0.000006	7	1.917923	-2.153099	0.000000
8	1.212275	-2.948152	0.000008	8	2.985769	-2.824523	0.000000
7	-0.329074	-0.827121	-0.000012	7	-0.396507	-0.831819	0.000000
6	-1.675664	-0.442570	-0.000007	6	-1.753352	-0.490950	0.000000
1	-0.120934	-1.838816	-0.000009	1	-0.183099	-1.826948	0.000000
6	-2.617335	-1.492700	-0.000009	6	-2.668025	-1.564248	-0.000001
6	-3.978108	-1.227458	-0.000003	6	-4.035284	-1.334136	-0.000001
6	-4.437227	0.102996	0.000005	6	-4.529158	-0.016486	0.000000
6	-2.133225	0.887872	0.000001	6	-2.245207	0.827172	0.000001
6	-3.500058	1.149350	0.000007	6	-3.618085	1.052922	0.000001
7	1.983613	3.193204	-0.000008	7	1.815918	3.241204	-0.000001
1	-2.270154	-2.521959	-0.000015	1	-2.297385	-2.585749	-0.000002
1	-4.691280	-2.044769	-0.000005	1	-4.726643	-2.170000	-0.000001
1	-1.417573	1.695701	0.000003	1	-1.550410	1.653107	0.000001
1	-3.847966	2.177131	0.000013	1	-3.991563	2.071685	0.000002
1	2.851227	3.704775	0.000004	1	2.667226	3.779521	-0.000001
1	1.100626	3.676910	-0.000004	1	0.918395	3.697242	-0.000002
6	5.734375	0.034803	0.000047	6	5.642350	0.166178	0.000001
1	5.832899	0.669525	-0.885937	1	5.724098	0.803438	-0.885804
1	6.533655	-0.707878	-0.000446	1	6.458148	-0.558068	0.000001
1	5.833276	0.668746	0.886556	1	5.724098	0.803438	0.885806
6	-5.841515	0.386515	0.000011	6	-5.940091	0.230484	0.000000
7	-6.982887	0.618132	0.000017	7	-7.087234	0.431815	0.000000

Compound 4b

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	2.855026	-0.846090	-0.000007	6	2.795834	-0.797722	-0.000335
6	1.601620	-0.123134	-0.000022	6	1.530935	-0.096916	-0.007015
6	4.051202	-0.029942	0.000012	6	3.976981	0.036174	0.005898
7	1.565924	1.211915	-0.000017	7	1.463427	1.230236	-0.007634
7	3.993114	1.304853	0.000018	7	3.888036	1.375701	0.005318
6	2.758718	1.844610	0.000005	6	2.648966	1.889544	-0.001314
7	5.254887	-0.621853	0.000025	7	5.186218	-0.534125	0.012493
1	5.242227	-1.634009	0.000022	1	5.165770	-1.556082	0.012482
7	3.051853	-2.187957	-0.000007	7	2.741685	-2.153389	-0.000384
8	2.048388	-2.959273	-0.000021	8	3.819791	-2.809339	0.005406
7	0.468034	-0.864763	-0.000037	7	0.407121	-0.864084	-0.012429
6	-0.887452	-0.503250	-0.000044	6	-0.956619	-0.540906	-0.018962
1	0.692629	-1.872417	-0.000031	1	0.632630	-1.856318	-0.009740
6	-1.809052	-1.571007	0.000004	6	-1.855976	-1.625243	-0.016708
6	-3.174323	-1.327777	0.000000	6	-3.228015	-1.411002	-0.024421
6	-3.653152	-0.010219	-0.000055	6	-3.733221	-0.105567	-0.037446
6	-1.370068	0.815523	-0.000100	6	-1.466499	0.768902	-0.030898
6	-2.745919	1.050048	-0.000103	6	-2.844943	0.973324	-0.038521
7	2.708219	3.195516	0.000014	7	2.561761	3.238658	-0.002027
1	-1.443296	-2.593824	0.000043	1	-1.472462	-2.642012	-0.011354

1	-3.869261	-2.161365	0.000037	1	-3.904758	-2.258506	-0.026671
1	-0.671312	1.637970	-0.000141	1	-0.784241	1.605130	-0.036289
1	-3.108868	2.071813	-0.000150	1	-3.228667	1.987980	-0.051682
1	3.566728	3.722095	0.000044	1	3.405443	3.788694	0.004659
1	1.816668	3.663186	0.000022	1	1.657757	3.681651	-0.004286
6	6.514847	0.104223	0.000050	6	6.431135	0.218038	0.019316
1	6.602566	0.740346	-0.886139	1	6.509079	0.856263	-0.866202
1	7.327249	-0.624160	0.000052	1	7.257199	-0.494534	0.024233
1	6.602543	0.740327	0.886254	1	6.498995	0.856817	0.905262
6	-5.136112	0.225366	0.000021	6	-5.214643	0.132858	0.008968
9	-5.458911	1.541311	-0.000519	9	-5.571476	1.289435	-0.606128
9	-5.741031	-0.328494	1.087493	9	-5.681419	0.222369	1.287951
9	-5.741302	-0.329469	-1.086794	9	-5.917819	-0.866720	-0.582089

Compound 4c

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-2.874262	-0.864670	-0.000017	6	2.811405	-0.817232	-0.000001
6	-1.637282	-0.113204	-0.000021	6	1.566838	-0.079555	-0.000039
6	-4.088729	-0.075783	-0.000017	6	4.016318	-0.017658	0.000011
7	-1.633382	1.222504	-0.000026	7	1.539131	1.249134	-0.000050
7	-4.061896	1.259760	0.000004	7	3.967025	1.323683	-0.000007
6	-2.839472	1.827490	-0.000018	6	2.742727	1.873217	-0.000033
7	-5.278811	-0.695527	-0.000059	7	5.208439	-0.623547	0.000053
1	-5.242546	-1.707077	0.000040	1	5.157156	-1.644556	0.000083
7	-3.041579	-2.210425	0.000007	7	2.718949	-2.170447	0.000006
8	-2.021433	-2.959771	0.000010	8	3.778461	-2.857171	0.000033
7	-0.486484	-0.827444	-0.000019	7	0.421247	-0.812766	-0.000057
6	0.860688	-0.436156	-0.000011	6	-0.933148	-0.452397	-0.000062
1	-0.686423	-1.839812	-0.000017	1	0.617375	-1.811174	-0.000052
6	1.805029	-1.483330	-0.000035	6	-1.860175	-1.514511	-0.000071
6	3.165867	-1.211458	-0.000026	6	-3.225470	-1.265524	-0.000047
6	3.622226	0.116996	0.000005	6	-3.704442	0.054651	-0.000002
6	1.313972	0.895686	0.000023	6	-1.408610	0.871574	-0.000036
6	2.681435	1.155632	0.000029	6	-2.780044	1.108170	-0.000001
7	-2.819791	3.179376	-0.000028	7	2.694739	3.224391	-0.000057
1	1.459329	-2.513427	-0.000061	1	-1.499941	-2.540137	-0.000097
1	3.880063	-2.026559	-0.000044	1	-3.925588	-2.092765	-0.000056
1	0.596843	1.702107	0.000046	1	-0.704908	1.689860	-0.000040
1	3.039231	2.179932	0.000054	1	-3.154268	2.126596	0.000027
1	-3.689833	3.686538	-0.000056	1	3.553797	3.750015	0.000028
1	-1.938662	3.666566	-0.000081	1	1.803487	3.692715	0.000001
6	-6.554766	0.001581	0.000100	6	6.474642	0.091778	0.000087
1	-6.656803	0.636318	-0.885614	1	6.566308	0.728035	0.885771
8	5.868760	-0.622449	0.000016	8	-5.937889	-0.722555	-0.000006
6	7.282960	-0.357933	0.000017	6	-7.356263	-0.481433	0.000038
1	7.760527	-1.337553	0.000035	1	-7.817637	-1.468799	-0.000012
1	7.565203	0.209416	-0.890224	1	-7.647881	0.081125	0.890288
1	7.565197	0.209448	0.890238	1	-7.647918	0.081230	-0.890134
6	5.065581	0.469167	0.000011	6	-5.152821	0.382575	0.000042
8	5.501407	1.607489	0.000011	8	-5.607874	1.513395	0.000117
1	-6.657315	0.635137	0.886614	1	6.566353	0.728037	-0.885589
1	-7.350551	-0.745002	-0.000626	1	7.279642	-0.644598	0.000108

Compound 4d

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	2.205213	-0.853813	-0.000005	6	-2.141882	-0.801737	-0.000001
6	0.961031	-0.113014	-0.000005	6	-0.883389	-0.086076	-0.000002
6	3.412703	-0.054598	-0.000008	6	-3.332278	0.018862	0.000000
7	0.946359	1.224535	-0.000006	7	-0.833529	1.243701	-0.000003
7	3.374652	1.280530	0.000002	7	-3.259950	1.359184	-0.000001
6	2.147046	1.838126	-0.000003	6	-2.025977	1.887244	-0.000004
7	4.607941	-0.664601	-0.000027	7	-4.534605	-0.566716	0.000003
1	4.579629	-1.676416	0.000019	1	-4.499970	-1.588624	0.000003
7	2.382428	-2.197344	0.000004	7	-2.073563	-2.155650	0.000001
8	1.366472	-2.954042	0.000006	8	-3.145242	-2.824407	0.000002
7	-0.181431	-0.835071	-0.000005	7	0.247549	-0.836144	-0.000001
6	-1.534286	-0.451380	-0.000003	6	1.610950	-0.493959	-0.000001
1	0.026878	-1.846070	-0.000003	1	0.036486	-1.831296	-0.000001
6	-2.473450	-1.500039	-0.000002	6	2.524566	-1.564186	-0.000009
6	-3.839555	-1.238283	0.000001	6	3.897046	-1.335537	-0.000008

6	-4.281604	0.085736	0.000002	6	4.371560	-0.023239	0.000001
6	-1.995826	0.875209	-0.000002	6	2.104467	0.820814	0.000009
6	-3.367202	1.136813	0.000000	6	3.481797	1.048805	0.000010
7	2.118800	3.190533	-0.000002	7	-1.956763	3.238137	-0.000007
1	-2.127806	-2.530102	-0.000002	1	2.157079	-2.587138	-0.000017
1	-4.553338	-2.054478	0.000001	1	4.590307	-2.169259	-0.000015
1	-1.284231	1.686991	-0.000003	1	1.412578	1.649548	0.000016
1	-3.720271	2.162343	0.000001	1	3.858770	2.065802	0.000018
1	2.985838	3.702708	0.000012	1	-2.807736	3.776666	-0.000014
1	1.234978	3.672461	0.000008	1	-1.058631	3.692746	-0.000017
6	5.878065	0.042802	0.000023	6	-5.788490	0.169750	0.000006
1	5.975182	0.678099	-0.885882	1	-5.869606	0.807519	0.885667
1	6.679951	-0.697253	-0.000346	1	-6.605819	-0.552956	0.000001
1	5.975476	0.677527	0.886312	1	-5.869604	0.807529	-0.885648
17	-6.006948	0.427123	0.000004	17	6.104935	0.276629	0.000002

Compound 4e

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	1.401737	-0.879275	0.000049	6	1.345103	-0.814502	-0.000010
6	0.201613	-0.067436	0.000054	6	0.113127	-0.051553	-0.000009
6	2.653650	-0.151882	0.000013	6	2.565679	-0.039325	-0.000004
7	0.266877	1.269480	0.000052	7	0.115902	1.279952	-0.000007
7	2.694401	1.182963	0.000044	7	2.545116	1.302589	-0.000010
6	1.500432	1.810854	0.000053	6	1.331111	1.876522	-0.000009
7	3.811548	-0.831259	-0.000079	7	3.744994	-0.670744	0.000012
1	3.723498	-1.839625	-0.000056	1	3.670257	-1.690755	0.000008
7	1.502339	-2.230521	0.000054	7	1.227252	-2.164485	-0.000013
8	0.445463	-2.928942	0.000080	8	2.274087	-2.872978	-0.000013
7	-0.980353	-0.720228	0.000050	7	-1.044341	-0.756753	-0.000009
6	-2.312310	-0.261697	0.000010	6	-2.397423	-0.367224	-0.000002
1	-0.833043	-1.741117	0.000061	1	-0.871737	-1.759171	-0.000010
6	-3.303906	-1.261556	-0.000009	6	-3.343057	-1.409897	0.000007
6	-4.653150	-0.919917	-0.000052	6	-4.706742	-1.129472	0.000014
6	-5.040707	0.424112	-0.000079	6	-5.155128	0.195099	0.000013
6	-2.698713	1.088914	-0.000015	6	-2.844429	0.964209	-0.000003
6	-4.057314	1.415104	-0.000060	6	-4.216364	1.228497	0.000004
7	1.552152	3.163204	0.000063	7	1.313917	3.229618	-0.000011
1	-3.007341	-2.307169	0.000011	1	-3.002454	-2.442556	0.000008
1	-5.402165	-1.706317	-0.000066	1	-5.418863	-1.949467	0.000020
1	-6.092709	0.692500	-0.000115	1	-6.218043	0.415745	0.000019
1	-1.941586	1.858305	0.000000	1	-2.123059	1.767341	-0.000011
1	-4.344635	2.462918	-0.000082	1	-4.549690	2.262588	0.000003
1	2.447763	3.623356	0.000049	1	2.184737	3.735227	0.000009
1	0.697785	3.695553	0.000050	1	0.433356	3.717363	0.000013
6	5.120610	-0.199649	-0.000163	6	5.025682	0.017378	0.000033
1	5.254823	0.429281	-0.885864	1	5.131109	0.652056	-0.885385
1	5.877975	-0.985323	-0.000905	1	5.815132	-0.735787	-0.000240
1	5.255533	0.428249	0.886180	1	5.131309	0.651615	0.885744

Compound 4f

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-1.833103	-0.863961	-0.000032	6	-1.770496	-0.807335	0.000047
6	-0.602871	-0.097929	-0.000208	6	-0.519921	-0.074133	0.000016
6	-3.056492	-0.089547	0.000312	6	-2.971870	-0.002640	0.000240
7	-0.618094	1.241338	0.000200	7	-0.491169	1.257828	0.000313
7	-3.047136	1.245691	0.000714	7	-2.919243	1.338280	0.000571
6	-1.829836	1.828157	0.000744	6	-1.691312	1.882774	0.000659
7	-4.239296	-0.725043	0.000263	7	-4.166036	-0.605863	0.000102
1	-4.188836	-1.735962	0.000043	1	-4.115163	-1.627479	-0.000088
7	-1.984372	-2.210106	-0.000139	7	-1.685776	-2.159330	-0.000165
8	-0.953604	-2.947477	-0.000384	8	-2.749857	-2.842629	-0.000218
7	0.553299	-0.793138	-0.000708	7	0.619913	-0.804996	-0.000255
6	1.901043	-0.381739	-0.000806	6	1.981953	-0.444435	-0.000421
1	0.368952	-1.807974	-0.000552	1	0.425461	-1.803317	-0.000121
6	2.860414	-1.412458	0.000933	6	2.908166	-1.504129	0.000848
6	4.218546	-1.117164	-0.000029	6	4.275440	-1.252110	-0.000225
6	4.676563	0.210727	-0.002328	6	4.775757	0.059923	-0.002105
6	2.340992	0.949839	-0.004217	6	2.463746	0.872111	-0.003183
6	3.711681	1.224006	-0.005136	6	3.842585	1.102376	-0.004164
7	-1.831463	3.181845	0.001237	7	-1.642437	3.235405	0.001021

1	2.531892	-2.448621	0.001994	1	2.549847	-2.530914	0.001659
1	4.935792	-1.934446	0.000343	1	4.965740	-2.092290	-0.000089
1	1.617274	1.750919	-0.007058	1	1.765729	1.695811	-0.005409
1	4.032252	2.263132	-0.008786	1	4.195120	2.131109	-0.007166
1	-2.709356	3.674863	0.002625	1	-2.501177	3.761196	0.002118
1	-0.957837	3.681893	0.002421	1	-0.750595	3.702140	0.002086
6	-5.523437	-0.044493	0.000658	6	-5.429842	0.112542	0.000209
1	-5.634304	0.588273	0.886920	1	-5.520443	0.749170	0.885912
1	-6.309990	-0.800979	0.000368	1	-6.237069	-0.621582	-0.000062
1	-5.634405	0.589058	-0.885025	1	-5.520296	0.749664	-0.885153
1	6.673448	0.024072	-0.821532	1	6.763228	-0.176886	-0.832378
6	6.154792	0.522735	0.005496	6	6.263269	0.325125	0.004165
1	6.629206	0.184685	0.934899	1	6.730862	-0.040538	0.926491
1	6.334417	1.597760	-0.086869	1	6.476001	1.395262	-0.073690

Compound 4g

rotamer A				rotamer B			
Atomic number	x	y	z	Atomic number	x	y	z
6	1.813876	-0.866627	-0.000001	6	-1.752784	-0.809104	-0.000001
6	0.584223	-0.099581	-0.000003	6	-0.501272	-0.077010	-0.000011
6	3.037816	-0.093250	-0.000001	6	-2.953265	-0.003359	-0.000001
7	0.600335	1.241024	-0.000004	7	-0.471438	1.256122	-0.000025
7	3.029423	1.241947	-0.000002	7	-2.899483	1.337582	-0.000015
6	1.812570	1.825882	-0.000004	6	-1.671132	1.881276	-0.000031
7	4.219901	-0.729965	-0.000002	7	-4.147826	-0.605677	0.000011
1	4.168227	-1.740851	0.000006	1	-4.097474	-1.627418	0.000039
7	1.962421	-2.212465	0.000001	7	-1.669150	-2.160834	0.000015
8	0.928860	-2.947249	0.000001	8	-2.733802	-2.843676	0.000031
7	-0.571294	-0.793167	-0.000002	7	0.637096	-0.807323	-0.000007
6	-1.918977	-0.379449	-0.000001	6	2.000176	-0.445312	-0.000004
1	-0.386619	-1.808639	-0.000002	1	0.442718	-1.805665	-0.000006
6	-2.882380	-1.406769	-0.000007	6	2.929730	-1.502085	-0.000076
6	-4.241097	-1.118646	-0.000005	6	4.297698	-1.257818	-0.000067
6	-4.668841	0.213685	0.000002	6	4.768700	0.059248	0.000012
6	-2.354923	0.953805	0.000006	6	2.478646	0.872630	0.000076
6	-3.722179	1.240488	0.000008	6	3.854779	1.114925	0.000082
7	1.817574	3.179989	-0.000006	7	-1.622926	3.234313	-0.000050
1	-2.557396	-2.443745	-0.000012	1	2.574673	-2.529666	-0.000139
1	-4.978890	-1.913898	-0.000009	1	5.008789	-2.077055	-0.000122
1	-1.628072	1.752138	0.000011	1	1.777952	1.694111	0.000131
1	-4.046345	2.279201	0.000014	1	4.210896	2.143060	0.000145
1	2.696946	3.670340	-0.000008	1	-2.482214	3.759192	-0.000081
1	0.945697	3.682835	-0.000010	1	-0.731790	3.702126	-0.000096
6	5.504840	-0.050965	0.000010	6	-5.411127	0.113589	0.000032
1	5.616494	0.582092	-0.885945	1	-5.501292	0.750442	0.885623
1	6.290503	-0.808372	-0.000043	1	-6.218856	-0.619977	-0.000065
1	5.616530	0.582007	0.886022	1	-5.501208	0.750601	-0.885449
8	-6.021410	0.443504	0.000003	8	6.128780	0.244931	0.000016
1	-6.194741	1.393878	0.000009	1	6.333179	1.189053	0.000080

Compound 4h

rotamer A				rotamer B			
Atomic number	x	y	z	Atomic number	x	y	z
6	-1.823099	-0.866936	0.003653	6	-1.761986	-0.809780	0.003746
6	-0.592568	-0.100076	-0.001862	6	-0.509216	-0.077598	-0.002397
6	-3.046634	-0.092628	0.003371	6	-2.962107	-0.003035	0.002508
7	-0.609497	1.241799	-0.007519	7	-0.480596	1.256641	-0.008956
7	-3.038481	1.242113	-0.003153	7	-2.908688	1.337566	-0.005615
6	-1.820387	1.825868	-0.008911	6	-1.679221	1.880877	-0.011577
7	-4.229023	-0.729834	0.009018	7	-4.156631	-0.606093	0.008797
1	-4.176559	-1.740651	0.012573	1	-4.104698	-1.628019	0.013544
7	-1.972336	-2.211897	0.009090	7	-1.680183	-2.160716	0.009962
8	-0.937863	-2.947377	0.008671	8	-2.746208	-2.843508	0.015817
7	0.562165	-0.792209	-0.001479	7	0.628238	-0.805976	-0.001446
6	1.910578	-0.379253	-0.004215	6	1.992632	-0.444412	-0.003950
1	0.377331	-1.807701	0.000089	1	0.434565	-1.804430	-0.000965
6	2.874448	-1.403306	-0.028980	6	2.922676	-1.497455	-0.037137
6	4.232930	-1.112771	-0.028415	6	4.290729	-1.250401	-0.035879
6	4.681725	0.219514	-0.001124	6	4.782244	0.065639	-0.000204
6	2.352195	0.953302	0.020752	6	2.476168	0.872476	0.029811
6	3.716533	1.238780	0.021860	6	3.849434	1.113861	0.030933
7	-1.826625	3.180739	-0.012047	7	-1.631946	3.234558	-0.016467

1	2.551871	-2.441079	-0.048014	1	2.570195	-2.525843	-0.063398
1	4.953712	-1.926032	-0.054055	1	4.984295	-2.086770	-0.068328
1	1.626912	1.753050	0.040479	1	1.776906	1.694993	0.055765
1	4.036881	2.277898	0.036522	1	4.201724	2.142451	0.052097
1	-2.706156	3.669385	-0.047924	1	-2.491385	3.757870	-0.052679
1	-0.955198	3.682701	-0.054049	1	-0.741194	3.701280	-0.059256
6	-5.513672	-0.050977	0.008238	6	-5.419888	0.112680	0.007844
1	-5.623289	0.587416	0.890687	1	-5.507639	0.755616	0.889338
1	-6.299527	-0.808262	0.014643	1	-6.227589	-0.620983	0.015093
1	-5.627882	0.577092	-0.881060	1	-5.513103	0.743967	-0.881513
1	6.311402	1.428540	0.295615	1	6.448720	1.219400	0.307069
7	6.046797	0.518958	-0.057188	7	6.157644	0.322436	-0.057508
1	6.670118	-0.210143	0.261869	1	6.755206	-0.427478	0.263139

Compound 5a

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-1.444521	-0.826707	-0.120597	6	-1.382129	-0.789054	-0.116037
6	-0.199888	-0.090284	-0.081087	6	-0.126211	-0.073858	-0.084562
6	-2.648671	-0.023802	-0.165683	6	-2.571738	0.031070	-0.163233
7	-0.177221	1.243893	-0.091929	7	-0.071564	1.252740	-0.100011
7	-2.603984	1.309921	-0.184565	7	-2.496451	1.370101	-0.186683
6	-1.376838	1.863320	-0.145735	6	-1.264616	1.898330	-0.152659
7	-3.846050	-0.637405	-0.193085	7	-3.775263	-0.558992	-0.193106
1	-3.812417	-1.649304	-0.243533	1	-3.738681	-1.581294	-0.212840
7	-1.624701	-2.171704	-0.130623	7	-1.308566	-2.144927	-0.104278
8	-0.612947	-2.930305	-0.089192	8	-2.375541	-2.816767	-0.130796
7	0.941803	-0.821009	-0.034886	7	1.006192	-0.830194	-0.038032
6	2.290481	-0.445822	0.003561	6	2.363342	-0.493019	0.000532
1	0.726582	-1.831131	-0.036653	1	0.789610	-1.824632	-0.036090
6	3.224201	-1.502453	0.038875	6	3.274665	-1.568788	0.030510
6	4.586205	-1.246709	0.078211	6	4.641920	-1.342431	0.071546
6	5.054672	0.080478	0.083461	6	5.139281	-0.026136	0.083916
6	2.757393	0.881372	0.009179	6	2.858736	0.823769	0.012741
6	4.125449	1.133308	0.048626	6	4.231608	1.045740	0.054030
7	-1.341194	3.214131	-0.163270	7	-1.192710	3.247864	-0.173420
1	2.869909	-2.529271	0.034852	1	2.901364	-2.589274	0.021208
1	5.293175	-2.068964	0.104858	1	5.330618	-2.180189	0.094092
1	2.047875	1.694158	-0.017589	1	2.166594	1.651610	-0.010250
1	4.480533	2.158623	0.052491	1	4.607745	2.063485	0.063464
1	-2.205792	3.729727	-0.197782	1	-2.043003	3.786910	-0.205138
1	-0.456129	3.693193	-0.135108	1	-0.294978	3.702663	-0.146364
6	-5.102900	0.046521	-0.323931	6	-5.017598	0.157048	-0.290073
6	-5.800841	0.572696	0.906293	6	-5.733252	0.593439	0.966821
6	-6.328983	-0.653418	0.196015	6	-6.266590	-0.558323	0.143727
1	-5.197648	0.633226	-1.234523	1	-5.075721	0.821792	-1.147547
1	-5.299595	0.426749	1.857630	1	-5.257559	0.357620	1.913443
1	-6.345892	1.507062	0.814509	1	-6.257918	1.543637	0.942498
1	-7.241863	-0.573375	-0.385458	1	-7.165013	-0.411681	-0.447256
1	-6.191930	-1.614100	0.685103	1	-6.157501	-1.559272	0.552147
6	6.460326	0.354191	0.123841	6	6.550217	0.217038	0.126606
7	7.602812	0.577846	0.156724	7	7.697357	0.415381	0.161503

Compound 5b

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-2.246234	-0.834705	-0.124394	6	-2.189571	-0.796932	-0.124819
6	-0.990595	-0.115472	-0.093289	6	-0.925299	-0.094136	-0.109759
6	-3.439345	-0.015466	-0.163126	6	-3.371320	0.034896	-0.160396
7	-0.950893	1.219098	-0.106399	7	-0.859216	1.232580	-0.130973
7	-3.377260	1.317341	-0.184066	7	-3.283860	1.372941	-0.190338
6	-2.141791	1.853836	-0.153823	6	-2.045978	1.888775	-0.173565
7	-4.645175	-0.613455	-0.182461	7	-4.580745	-0.544155	-0.172865
1	-4.624573	-1.625734	-0.231967	1	-4.552908	-1.566980	-0.189551
7	-2.445411	-2.176708	-0.131294	7	-2.130417	-2.152935	-0.109782
8	-1.444170	-2.949752	-0.094803	8	-3.205088	-2.814024	-0.121338
7	0.140318	-0.860115	-0.052549	7	0.199166	-0.859588	-0.072908
6	1.496381	-0.502194	-0.021093	6	1.562057	-0.534249	-0.046021
1	-0.086935	-1.867086	-0.051410	1	-0.025152	-1.852066	-0.066612
6	2.414515	-1.572432	0.012258	6	2.462620	-1.618200	-0.032956
6	3.780021	-1.332996	0.045550	6	3.833379	-1.402325	-0.003272
6	4.262615	-0.016805	0.046327	6	4.337636	-0.095820	0.012326

6	1.982745	0.815204	-0.020128	6	2.070486	0.775577	-0.030311
6	3.358851	1.045897	0.013277	6	3.449071	0.981880	0.000665
7	-2.088757	3.204442	-0.173912	7	-1.961702	3.237797	-0.202452
1	2.045839	-2.594203	0.011848	1	2.080163	-2.635254	-0.048995
1	4.472212	-2.168476	0.071150	1	4.511254	-2.249227	0.001774
1	1.286678	1.639546	-0.045353	1	1.387742	1.611335	-0.044195
1	3.724769	2.066604	0.013601	1	3.831435	1.996868	0.010322
1	-2.946747	3.731111	-0.204083	1	-2.807123	3.784589	-0.229468
1	-1.197124	3.671476	-0.152498	1	-1.059177	3.683643	-0.191416
6	-5.893598	0.086409	-0.306449	6	-5.817296	0.182916	-0.256817
6	-6.580895	0.617276	0.927868	6	-6.517058	0.624045	1.007468
6	-7.126251	-0.600251	0.215649	6	-7.068295	-0.522048	0.188105
1	-5.984629	0.677273	-1.214743	1	-5.877995	0.849425	-1.112736
1	-6.078093	0.462321	1.876968	1	-6.034228	0.382870	1.949121
1	-7.115142	1.558348	0.840916	1	-7.033848	1.578716	0.989413
1	-8.040279	-0.507547	-0.362163	1	-7.971172	-0.366835	-0.393866
1	-6.998926	-1.564016	0.701312	1	-6.963985	-1.524467	0.594183
6	5.745779	0.214737	0.082216	6	5.819189	0.130187	0.097815
9	6.072085	1.529809	0.088383	9	6.184713	1.357869	-0.348677
9	6.375944	-0.342608	-0.989067	9	6.521052	-0.782275	-0.624255
9	6.322345	-0.339873	1.184522	9	6.280389	0.033928	1.378174

Compound 5c

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-2.258982	-0.834654	-0.123884	6	-2.199841	-0.794593	-0.121108
6	-1.016732	-0.091826	-0.091400	6	-0.951070	-0.063533	-0.096438
6	-3.467339	-0.037784	-0.158987	6	-3.399673	0.011283	-0.158077
7	-1.003660	1.243488	-0.099831	7	-0.915819	1.264600	-0.109261
7	-3.431285	1.295763	-0.175703	7	-3.342649	1.350867	-0.179041
6	-2.205530	1.855405	-0.144136	6	-2.116039	1.893990	-0.152224
7	-4.662035	-0.658883	-0.179048	7	-4.595992	-0.594932	-0.180815
1	-4.621847	-1.670296	-0.233442	1	-4.544711	-1.616823	-0.203871
7	-2.433911	-2.179949	-0.135855	7	-2.111492	-2.148739	-0.113504
8	-1.418841	-2.935075	-0.102917	8	-3.171846	-2.833329	-0.134608
7	0.128769	-0.813648	-0.054397	7	0.190160	-0.802792	-0.059307
6	1.478119	-0.431063	-0.024500	6	1.545917	-0.449030	-0.029057
1	-0.077664	-1.824606	-0.056277	1	-0.011249	-1.800138	-0.057988
6	2.415214	-1.484333	0.004755	6	2.467587	-1.515594	-0.006643
6	3.777435	-1.221350	0.035274	6	3.833677	-1.273229	0.025951
6	4.242549	0.104057	0.037177	6	4.318949	0.044610	0.037071
6	1.940175	0.897771	-0.022127	6	2.027755	0.872633	-0.018234
6	3.308981	1.148779	0.008209	6	3.399917	1.102571	0.014487
7	-2.178070	3.207008	-0.159242	7	-2.061791	3.244831	-0.170551
1	2.062835	-2.512157	0.003112	1	2.102543	-2.539478	-0.015069
1	4.485979	-2.041062	0.057539	1	4.529566	-2.103859	0.042871
1	1.228655	1.708852	-0.044191	1	1.328247	1.694321	-0.035469
1	3.673508	2.170700	0.009860	1	3.778950	2.119179	0.023338
1	-3.045647	3.717778	-0.186046	1	-2.918898	3.773185	-0.193837
1	-1.294979	3.690052	-0.135594	1	-1.169152	3.709905	-0.147251
6	-5.922823	0.017929	-0.303148	6	-5.847541	0.105147	-0.268797
6	-6.617497	0.539735	0.930741	6	-6.560017	0.532303	0.993000
6	-7.142533	-0.689052	0.222475	6	-7.084490	-0.626087	0.173219
1	-6.026134	0.605082	-1.212642	1	-5.920627	0.769724	-1.125362
1	-6.110246	0.396189	1.879247	1	-6.074538	0.302452	1.936116
1	-7.168350	1.471053	0.842303	1	-7.097000	1.475729	0.972677
1	-8.058933	-0.613650	-0.354143	1	-7.988918	-0.490612	-0.411311
1	-6.997615	-1.649280	0.710194	1	-6.959719	-1.625713	0.580369
8	6.483369	-0.650051	0.097635	8	6.548045	-0.743158	0.093290
6	7.898878	-0.394662	0.129975	6	7.967043	-0.508562	0.129480
1	8.369789	-1.377310	0.149052	1	8.423783	-1.498035	0.138995
1	8.206405	0.163976	-0.757380	1	8.283631	0.054625	-0.751778
1	8.163152	0.177753	1.022491	1	8.238665	0.050798	1.028056
6	5.687823	0.446762	0.068989	6	5.768394	0.365648	0.072688
8	6.131224	1.582149	0.070030	8	6.228689	1.494306	0.083187

Compound 5d

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-1.594032	-0.831639	-0.121174	6	-1.533628	-0.793796	-0.116260
6	-0.345040	-0.099133	-0.083057	6	-0.273068	-0.081435	-0.085877
6	-2.795327	-0.024894	-0.164686	6	-2.720762	0.029759	-0.162895

7	-0.321437	1.237935	-0.094489	7	-0.219028	1.247763	-0.102548
7	-2.748296	1.308116	-0.184165	7	-2.644052	1.368315	-0.187612
6	-1.517741	1.858003	-0.147158	6	-1.409420	1.893257	-0.155127
7	-3.994912	-0.636606	-0.189900	7	-3.925641	-0.559219	-0.191171
1	-3.962076	-1.648429	-0.241891	1	-3.888360	-1.582007	-0.210824
7	-1.778474	-2.174708	-0.131300	7	-1.465787	-2.148375	-0.104500
8	-0.767650	-2.936840	-0.091159	8	-2.536242	-2.818052	-0.130147
7	0.791929	-0.828461	-0.037848	7	0.855048	-0.834472	-0.039337
6	2.146680	-0.453238	-0.000669	6	2.218713	-0.495470	-0.002597
1	0.577204	-1.838050	-0.039263	1	0.641179	-1.829023	-0.036656
6	3.078632	-1.507793	0.033734	6	3.129547	-1.567793	0.022483
6	4.445852	-1.254662	0.071849	6	4.502000	-1.342351	0.061703
6	4.896334	0.066551	0.076074	6	4.979353	-0.031156	0.076368
6	2.616639	0.870417	0.004416	6	2.715108	0.818164	0.012653
6	3.989140	1.123358	0.042644	6	4.092410	1.042938	0.052014
7	-1.481969	3.210029	-0.165789	7	-1.337402	3.243829	-0.177853
1	2.726545	-2.535666	0.030215	1	2.759933	-2.589913	0.010924
1	5.154093	-2.075277	0.097863	1	5.193091	-2.177662	0.080446
1	1.910608	1.686641	-0.021668	1	2.025438	1.648523	-0.006558
1	4.348754	2.146615	0.046224	1	4.471514	2.059074	0.063830
1	-2.346489	3.725491	-0.198823	1	-2.187647	3.782690	-0.208749
1	-0.596463	3.688081	-0.138527	1	-0.439255	3.697621	-0.151439
6	-5.249628	0.049621	-0.322115	6	-5.166407	0.158292	-0.288797
6	-5.947232	0.578833	0.907000	6	-5.881523	0.597586	0.967377
6	-6.477606	-0.647179	0.197858	6	-6.416551	-0.554733	0.145803
1	-5.343582	0.636066	-1.233098	1	-5.224416	0.822475	-1.146834
1	-5.446335	0.433068	1.858539	1	-5.405750	0.362482	1.914135
1	-6.490606	1.514106	0.813965	1	-6.405201	1.548354	0.941910
1	-7.390247	-0.565879	-0.383909	1	-7.315025	-0.407581	-0.445068
1	-6.342560	-1.607622	0.687970	1	-6.308607	-1.555331	0.555373
17	6.623203	0.397175	0.123989	17	6.712732	0.264721	0.125926

Compound 5e

rotamer A				rotamer B			
Atomic number	x	y	z	Atomic number	x	y	z
6	-0.813107	-0.815948	-0.118049	6	0.753004	-0.780265	-0.109803
6	0.407723	-0.036678	-0.063805	6	-0.489753	-0.035456	-0.064283
6	-2.043776	-0.055557	-0.169656	6	1.960507	0.012630	-0.165951
7	0.378164	1.301182	-0.068308	7	-0.507103	1.295594	-0.075475
7	-2.048568	1.278090	-0.182851	7	1.919403	1.352581	-0.184938
6	-0.839504	1.874105	-0.130052	6	0.698321	1.908817	-0.137314
7	-3.219240	-0.713362	-0.208445	7	3.149417	-0.608127	-0.208999
1	-3.146092	-1.722746	-0.266501	1	3.083886	-1.629651	-0.232374
7	-0.947807	-2.164731	-0.137615	7	0.651840	-2.132281	-0.102715
8	0.089568	-2.889862	-0.091315	8	1.705469	-2.828931	-0.142048
7	1.570903	-0.720370	-0.011022	7	-1.635582	-0.757497	-0.009530
6	2.913418	-0.296623	0.039563	6	-2.993192	-0.387217	0.039061
1	1.397296	-1.736939	-0.019006	1	-1.448398	-1.757282	-0.011732
6	3.877870	-1.321815	0.082192	6	-3.923306	-1.443186	0.074351
6	5.234612	-1.015250	0.132192	6	-5.289910	-1.182156	0.124203
6	5.657005	0.318196	0.140993	6	-5.756906	0.135882	0.140185
6	3.334854	1.043442	0.048792	6	-3.458943	0.937721	0.055121
6	4.700532	1.334308	0.099209	6	-4.833577	1.182504	0.105432
7	-0.856346	3.227212	-0.141520	7	0.662051	3.261448	-0.153856
1	3.554452	-2.359410	0.075225	1	-3.568441	-2.470938	0.062082
1	5.962228	-1.820869	0.164129	1	-5.989787	-2.012223	0.150423
1	6.714917	0.559103	0.179812	1	-6.822151	0.341345	0.179027
1	2.598927	1.832467	0.016376	1	-2.749609	1.751060	0.028075
1	5.014823	2.374326	0.105544	1	-5.181296	2.211774	0.117392
1	-1.739900	3.708942	-0.176778	1	1.525901	3.777892	-0.187034
1	0.009843	3.738253	-0.097841	1	-0.223722	3.737749	-0.111180
6	-4.497410	-0.075472	-0.353460	6	4.407019	0.076946	-0.318975
6	-5.221126	0.436503	0.867545	6	5.642376	-0.667243	0.105740
6	-5.702298	-0.813205	0.164602	6	5.144396	0.499988	0.929763
1	-4.608353	0.500779	-1.269210	1	4.474995	0.738245	-1.178635
1	-4.720324	0.316173	1.822650	1	5.512210	-1.664010	0.518137
1	-5.797887	1.350525	0.764713	1	6.539121	-0.544199	-0.493268
1	-6.613893	-0.769211	-0.422860	1	5.692138	1.436929	0.897793
1	-5.535087	-1.764682	0.662205	1	4.671013	0.278940	1.881092

Compound 5f

rotamer A				rotamer B			

Atomic number	x	y	z	Atomic number	x	y	z
6	-1.227317	-0.826462	-0.119472	6	1.166202	-0.789312	-0.114780
6	0.012293	-0.076197	-0.075159	6	-0.089006	-0.064022	-0.078132
6	-2.439695	-0.036963	-0.165828	6	2.361185	0.022779	-0.164762
7	0.014098	1.262824	-0.084253	7	-0.126811	1.267340	-0.092695
7	-2.413242	1.296181	-0.183302	7	2.299261	1.361758	-0.187267
6	-1.189521	1.863585	-0.140591	6	1.068780	1.898673	-0.149001
7	-3.630677	-0.667192	-0.195497	7	3.559994	-0.579599	-0.198334
1	-3.581229	-1.678129	-0.251184	1	3.509990	-1.602185	-0.219926
7	-1.393882	-2.171333	-0.133720	7	1.086978	-2.142318	-0.105354
8	-0.372807	-2.920434	-0.091462	8	2.152231	-2.822469	-0.136583
7	1.158789	-0.785628	-0.026969	7	-1.223201	-0.802054	-0.028153
6	2.510818	-0.390666	0.015349	6	-2.586717	-0.449651	0.013779
1	0.962193	-1.798032	-0.031046	1	-1.022352	-1.799105	-0.027522
6	3.456833	-1.433003	0.051843	6	-3.506183	-1.514748	0.043103
6	4.817763	-1.154314	0.095449	6	-4.874227	-1.270810	0.088286
6	5.292007	0.167825	0.104138	6	-5.382030	0.038195	0.105517
6	2.967007	0.935430	0.025100	6	-3.076050	0.864062	0.031828
6	4.340232	1.192836	0.069127	6	-4.455444	1.086188	0.077278
7	-1.175396	3.217014	-0.157331	7	1.012175	3.250843	-0.169893
1	3.115802	-2.465094	0.046650	1	-3.142115	-2.539438	0.031473
1	5.524387	-1.980302	0.123980	1	-5.559154	-2.115061	0.111212
1	2.253649	1.745355	-0.000691	1	-2.383210	1.691869	0.011434
1	4.673372	2.227979	0.076922	1	-4.813682	2.112842	0.091855
1	-2.047794	3.718719	-0.190442	1	1.868300	3.780104	-0.200050
1	-0.297258	3.707931	-0.123313	1	0.118914	3.713576	-0.135562
6	-4.894151	0.000140	-0.335172	6	4.807462	0.124632	-0.300605
6	-5.603181	0.525005	0.889133	6	6.051296	-0.600111	0.133021
6	-6.114048	-0.711657	0.183922	6	5.529942	0.560063	0.952612
1	-4.994334	0.581555	-1.248883	1	4.871144	0.786258	-1.160351
1	-5.102794	0.390747	1.842611	1	5.933694	-1.598451	0.545397
1	-6.159584	1.452018	0.790270	1	6.950109	-0.463781	-0.460007
1	-7.026000	-0.645628	-0.400933	1	6.063556	1.505228	0.923465
1	-5.966952	-1.667999	0.678549	1	5.053522	0.332607	1.900908
6	6.773514	0.461572	0.141578	6	-6.870610	0.294690	0.144104
1	7.261628	-0.049034	0.979754	1	-7.358402	-0.042373	-0.778788
1	7.270671	0.123874	-0.776043	1	-7.347583	-0.238267	0.974721
1	6.963553	1.533657	0.246506	1	-7.086958	1.360369	0.262782

Compound 5g

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-1.210334	-0.827903	-0.118990	6	1.150199	-0.791287	-0.112480
6	0.029159	-0.077423	-0.073698	6	-0.105960	-0.067163	-0.075662
6	-2.422744	-0.038651	-0.166045	6	2.344157	0.021924	-0.164383
7	0.030923	1.262953	-0.082055	7	-0.145004	1.265339	-0.091592
7	-2.396405	1.294454	-0.182796	7	2.280936	1.360881	-0.188375
6	-1.172802	1.862545	-0.138737	6	1.050026	1.896927	-0.149766
7	-3.613387	-0.669325	-0.197043	7	3.543343	-0.579540	-0.198423
1	-3.563342	-1.680246	-0.253008	1	3.493802	-1.602282	-0.218788
7	-1.375029	-2.172396	-0.133623	7	1.072146	-2.144018	-0.101891
8	-0.351643	-2.919608	-0.090822	8	2.137973	-2.823701	-0.133279
7	1.174587	-0.785932	-0.025440	7	-1.238620	-0.804641	-0.024230
6	2.526810	-0.389423	0.016916	6	-2.603228	-0.450752	0.016582
1	0.977067	-1.798844	-0.029798	1	-1.037870	-1.801709	-0.023117
6	3.476284	-1.428925	0.055299	6	-3.526247	-1.513003	0.039167
6	4.837889	-1.158153	0.097556	6	-4.894972	-1.276905	0.082059
6	5.282785	0.168552	0.102614	6	-5.373422	0.037305	0.103435
6	2.979881	0.938104	0.022772	6	-3.089173	0.864297	0.038728
6	4.350029	1.207323	0.065309	6	-4.466067	1.098385	0.081443
7	-1.161175	3.216433	-0.154918	7	0.993921	3.249471	-0.172316
1	3.138177	-2.461682	0.051337	1	-3.165476	-2.538449	0.022477
1	5.564884	-1.962772	0.126593	1	-5.600967	-2.100368	0.098946
1	2.263926	1.745710	-0.006195	1	-2.393610	1.689950	0.021636
1	4.687347	2.241812	0.069002	1	-4.827934	2.124376	0.097905
1	-2.034852	3.716062	-0.185261	1	1.850461	3.777896	-0.204924
1	-0.284613	3.709593	-0.116584	1	0.101275	3.713208	-0.139155
6	-4.877088	-0.002596	-0.337388	6	4.790204	0.125389	-0.302994
6	-5.587483	0.521156	0.886617	6	6.035259	-0.598511	0.128468
6	-6.097094	-0.715308	0.180155	6	5.514735	0.561489	0.948838
1	-4.976768	0.579321	-1.250835	1	4.851928	0.786913	-1.162958
1	-5.087905	0.386508	1.840464	1	5.919000	-1.596844	0.541233

1	-6.144286	1.447942	0.787854	1	6.932896	-0.461764	-0.466238
1	-7.008542	-0.649351	-0.405489	1	6.047753	1.506959	0.918553
1	-5.949978	-1.671892	0.674300	1	5.040249	0.333863	1.898062
8	6.637530	0.380844	0.144675	8	-6.733967	0.214886	0.145305
1	6.823439	1.328844	0.143650	1	-6.943695	1.157761	0.157326

Compound 5h

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-1.218557	-0.828082	-0.121270	6	-1.158534	-0.791332	-0.116314
6	0.021678	-0.077826	-0.071918	6	0.098819	-0.067244	-0.074502
6	-2.430572	-0.037884	-0.166308	6	-2.352121	0.023078	-0.164628
7	0.022442	1.263881	-0.074801	7	0.136545	1.266486	-0.083066
7	-2.404689	1.294821	-0.176941	7	-2.289381	1.361835	-0.179696
6	-1.179990	1.862749	-0.128663	6	-1.057460	1.897406	-0.136351
7	-3.621504	-0.669132	-0.200750	7	-3.551337	-0.578868	-0.203458
1	-3.570366	-1.679686	-0.261905	1	-3.500454	-1.601679	-0.229787
7	-1.383740	-2.171672	-0.141565	7	-1.082145	-2.143340	-0.113210
8	-0.359424	-2.919569	-0.099843	8	-2.149172	-2.822937	-0.149711
7	1.166423	-0.784826	-0.025272	7	1.230588	-0.802921	-0.025940
6	2.519269	-0.388969	0.019408	6	2.596492	-0.449747	0.017737
1	0.968884	-1.797761	-0.031081	1	1.030423	-1.800084	-0.025099
6	3.468502	-1.424954	0.082895	6	3.518637	-1.508542	0.077911
6	4.829917	-1.151684	0.124429	6	4.887525	-1.269927	0.120257
6	5.296629	0.174532	0.102417	6	5.387993	0.043111	0.103121
6	2.978720	0.937643	-0.000153	6	3.088968	0.864193	0.002228
6	4.345947	1.205773	0.041007	6	4.463052	1.097104	0.044808
7	-1.169727	3.217509	-0.141528	7	-1.002376	3.250773	-0.153006
1	3.132222	-2.458420	0.098511	1	3.159350	-2.534823	0.090632
1	5.538889	-1.973857	0.179085	1	5.574580	-2.110663	0.172493
1	2.264940	1.746441	-0.049072	1	2.395934	1.691056	-0.044198
1	4.679961	2.240615	0.029537	1	4.822056	2.123563	0.037138
1	-2.044811	3.715518	-0.137665	1	-1.860317	3.777887	-0.147381
1	-0.295165	3.709934	-0.065194	1	-0.111763	3.713625	-0.077367
6	-4.884686	-0.002204	-0.341326	6	-4.797906	0.126405	-0.305216
6	-5.596539	0.519149	0.882828	6	-5.523545	0.556028	0.948208
6	-6.105501	-0.715874	0.173213	6	-6.043380	-0.599776	0.121320
1	-4.983703	0.582007	-1.253471	1	-4.859305	0.792780	-1.161517
1	-5.097852	0.382547	1.836857	1	-5.049725	0.323494	1.896577
1	-6.153246	1.446154	0.785343	1	-6.056697	1.501586	0.922452
1	-7.016374	-0.648528	-0.413222	1	-6.940663	-0.459948	-0.473259
1	-5.958955	-1.673524	0.665456	1	-5.927280	-1.600251	0.528909
7	6.662892	0.456991	0.200661	7	6.762438	0.291294	0.204627
1	6.950586	1.360360	-0.150013	1	7.070364	1.187205	-0.148511
1	7.286799	-0.282448	-0.092404	1	7.365319	-0.461599	-0.098617

Compound 6a

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-2.386071	0.923864	0.000000	6	2.352261	-0.758291	-0.000003
6	-1.171276	0.137067	0.000000	6	1.090656	-0.052957	-0.000002
6	-3.616986	0.173013	0.000000	6	3.532175	0.068302	-0.000001
7	-1.204499	-1.196714	0.000000	7	1.027895	1.273598	-0.000001
7	-3.631748	-1.161103	0.000000	7	3.451964	1.405869	0.000001
6	-2.429198	-1.767664	0.000000	6	2.216378	1.928694	0.000000
7	-4.795723	0.817003	0.000000	7	4.745077	-0.496810	0.000000
1	-4.808657	1.826648	0.000000	1	4.792636	-1.513380	0.000006
7	-2.517543	2.277290	0.000000	7	2.295824	-2.118085	0.000000
8	-1.476919	2.993014	0.000000	8	3.369368	-2.773001	0.000002
7	0.000000	0.820178	0.000000	7	-0.036434	-0.817576	-0.000003
6	1.333371	0.390248	0.000000	6	-1.397298	-0.490141	-0.000002
1	-0.171454	1.837643	0.000000	1	0.185629	-1.810623	-0.000003
6	2.309478	1.408218	0.000000	6	-2.300764	-1.572638	0.000000
6	3.660611	1.097422	0.000000	6	-3.670294	-1.356221	0.000001
6	4.074380	-0.247763	0.000000	6	-4.177204	-0.043588	0.000001
6	1.745372	-0.954790	0.000000	6	-1.901952	0.822927	-0.000003
6	3.102685	-1.262030	0.000000	6	-3.277078	1.034950	-0.000002
7	-2.451102	-3.118300	0.000000	7	2.137972	3.277250	0.000001
1	1.997012	2.448589	0.000000	1	-1.920026	-2.590411	0.000001
1	4.400886	1.890236	0.000000	1	-4.353245	-2.198949	0.000003
1	1.003124	-1.738201	0.000000	1	-1.215552	1.655826	-0.000004
1	3.415940	-2.300887	0.000000	1	-3.660769	2.049888	-0.000002

1	-3.336729	-3.598259	0.000000	1	2.985263	3.822085	0.000003
1	-1.586324	-3.633884	0.000000	1	1.237112	3.726725	0.000001
1	-5.647739	0.278518	0.000000	1	5.558626	0.101231	0.000014
6	5.468377	-0.578518	0.000000	6	-5.590639	0.189137	0.000002
7	6.601305	-0.848199	0.000000	7	-6.739736	0.378690	0.000003

Compound 6b

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	3.212490	-0.815997	-0.000001	6	-3.149112	-0.753306	0.003710
6	1.952841	-0.101831	-0.000002	6	-1.878402	-0.062624	-0.006640
6	4.397089	0.005739	0.000002	6	-4.319243	0.086972	0.011162
7	1.909205	1.232407	0.000000	7	-1.801787	1.263907	-0.009792
7	4.334414	1.338332	0.000003	7	-4.224250	1.423514	0.007479
6	3.097856	1.873241	0.000003	6	-2.982244	1.931740	-0.003181
7	5.611688	-0.568550	0.000002	7	-5.538591	-0.464575	0.021936
1	5.682878	-1.575731	0.000002	1	-5.596784	-1.480724	0.024429
7	3.423573	-2.159015	-0.000001	7	-3.109241	-2.113163	0.005700
8	2.426756	-2.934981	-0.000003	8	-4.190856	-2.755714	0.015214
7	0.824212	-0.850469	-0.000004	7	-0.760958	-0.838232	-0.013297
6	-0.533998	-0.497062	-0.000005	6	0.605714	-0.524785	-0.020371
1	1.052959	-1.856102	-0.000003	1	-0.992390	-1.828920	-0.010898
6	-1.448810	-1.570403	0.000004	6	1.496364	-1.616557	-0.032662
6	-2.815548	-1.335381	0.000004	6	2.869391	-1.412633	-0.039730
6	-3.302132	-0.020725	-0.000006	6	3.384983	-0.110607	-0.036770
6	-1.024139	0.818745	-0.000015	6	1.125311	0.780567	-0.017367
6	-2.401399	1.044994	-0.000015	6	2.505914	0.974831	-0.023586
7	3.041106	3.223287	0.000005	7	-2.888914	3.279719	-0.007700
1	-1.077117	-2.591088	0.000012	1	1.104908	-2.630288	-0.039130
1	-3.505432	-2.173138	0.000011	1	3.539735	-2.265360	-0.053557
1	-0.330457	1.645439	-0.000022	1	0.449792	1.622225	-0.011905
1	-2.770520	2.064530	-0.000023	1	2.897332	1.986393	-0.023793
1	3.897133	3.754093	0.000010	1	-3.730016	3.833925	-0.004732
1	2.147429	3.686911	0.000008	1	-1.982907	3.718554	-0.017781
1	6.430721	0.018760	0.000005	1	-6.345207	0.142695	0.027113
6	-4.786663	0.206148	0.000002	6	4.870183	0.104373	0.009323
9	-5.116901	1.520136	-0.000056	9	5.233342	1.323475	-0.461952
9	-5.388010	-0.351715	1.087205	9	5.546901	-0.822520	-0.717799
9	-5.388038	-0.351819	-1.087132	9	5.361471	0.021400	1.279189

Compound 6c

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	3.235403	-0.852273	-0.000003	6	3.169366	-0.792160	-0.000036
6	1.995058	-0.104313	0.000002	6	1.920497	-0.061356	-0.000089
6	4.441732	-0.062599	-0.000005	6	4.365534	0.011169	-0.000028
7	1.988677	1.230819	0.000010	7	1.887052	1.267099	-0.000049
7	4.415742	1.270996	0.000005	7	4.313437	1.349857	0.000140
6	3.193411	1.838977	0.000014	6	3.087395	1.896862	0.000109
7	5.640565	-0.670027	-0.000033	7	5.566619	-0.579556	-0.000487
1	5.683806	-1.678742	-0.000036	1	5.590499	-1.597182	-0.000973
7	3.411315	-2.200240	0.000004	7	3.087782	-2.149736	0.000067
8	2.394587	-2.950208	0.000005	8	4.149565	-2.825813	0.000170
7	0.846238	-0.821119	-0.000002	7	0.779147	-0.800343	-0.000153
6	-0.502362	-0.432784	-0.000002	6	-0.577557	-0.446150	-0.000121
1	1.046485	-1.832398	-0.000003	1	0.978718	-1.797893	-0.000114
6	-1.443891	-1.482231	0.000015	6	-1.499179	-1.512682	0.000001
6	-2.805407	-1.213564	0.000014	6	-2.865693	-1.270144	0.000035
6	-3.264677	0.113788	-0.000006	6	-3.350700	0.047732	-0.000056
6	-0.958349	0.897937	-0.000021	6	-1.058876	0.875503	-0.000218
6	-2.326486	1.154672	-0.000023	6	-2.431472	1.105648	-0.000186
7	3.173132	3.190253	0.000029	7	3.036608	3.247232	0.000276
1	-1.095940	-2.511586	0.000031	1	-1.134230	-2.536641	0.000074
1	-3.517722	-2.030286	0.000027	1	-3.561945	-2.100617	0.000135
1	-0.243277	1.706168	-0.000034	1	-0.359202	1.697218	-0.000316
1	-2.686731	2.178099	-0.000039	1	-2.810548	2.122265	-0.000262
1	4.042962	3.697994	0.000030	1	3.894562	3.774874	0.000271
1	2.291853	3.677190	0.000035	1	2.144404	3.713785	0.000195
8	-5.509398	-0.630864	0.000012	8	-5.580506	-0.739737	0.000139
6	-6.924429	-0.370076	0.000012	6	-7.000169	-0.505496	0.000191
1	-7.399329	-1.350970	0.000029	1	-7.456672	-1.495099	0.000327
1	-7.208035	0.196527	0.890270	1	-7.294348	0.055779	0.890385

1	-7.208041	0.196501	-0.890260	1	-7.294447	0.055578	-0.890097
6	-4.709123	0.462601	-0.000008	6	-4.800865	0.368951	-0.000018
8	-5.147211	1.599959	-0.000025	8	-5.260726	1.497730	-0.000112
1	6.475174	-0.105186	-0.000008	1	6.392341	0.001368	0.000777

Compound 6d

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-2.333196	1.353284	0.000000	6	-2.499553	-0.761586	-0.000014
6	-1.266046	0.372910	0.000000	6	-1.233374	-0.059205	-0.000010
6	-3.672634	0.819994	0.000000	6	-3.677002	0.068414	-0.000002
7	-1.526993	-0.938521	0.000000	7	-1.171047	1.269927	-0.000009
7	-3.913148	-0.491860	0.000000	7	-3.595168	1.405680	0.000000
6	-2.828297	-1.292496	0.000000	6	-2.356912	1.925033	-0.000009
7	-4.726141	1.654625	0.000000	7	-4.891129	-0.495431	0.000037
1	-4.566758	2.651633	0.000000	1	-4.937484	-1.512443	0.000007
7	-2.235427	2.708172	0.000000	7	-2.448829	-2.119977	0.000001
8	-1.087846	3.238872	0.000000	8	-3.525739	-2.772748	0.000001
7	0.000000	0.844975	0.000000	7	-0.110535	-0.820670	-0.000010
6	1.245900	0.191826	0.000000	6	1.256695	-0.491647	-0.000006
1	0.005704	1.876168	0.000000	1	-0.330103	-1.813816	-0.000014
6	2.379665	1.026030	0.000000	6	2.159554	-1.570770	-0.000018
6	3.663193	0.490083	0.000000	6	3.534173	-1.355389	-0.000013
6	3.824727	-0.896445	0.000000	6	4.021419	-0.047734	0.000004
6	1.425663	-1.201023	0.000000	6	1.762624	0.818246	0.000012
6	2.714393	-1.737957	0.000000	6	3.142089	1.032908	0.000017
7	-3.080910	-2.620800	0.000000	7	-2.278082	3.274697	-0.000019
1	2.252579	2.105083	0.000000	1	1.782325	-2.590168	-0.000032
1	4.529017	1.142786	0.000000	1	4.219341	-2.195758	-0.000023
1	0.563124	-1.850107	0.000000	1	1.078947	1.653740	0.000022
1	2.849726	-2.814108	0.000000	1	3.528812	2.046222	0.000031
1	-4.035342	-2.942277	0.000000	1	-3.125125	3.819588	-0.000009
1	-2.316214	-3.275518	0.000000	1	-1.376705	3.722889	-0.000021
1	-5.656773	1.267971	0.000000	1	-5.703710	0.103752	0.000086
17	5.443284	-1.583881	0.000000	17	5.757345	0.235223	0.000010

Compound 6e

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-1.745729	-0.905225	-0.000001	6	1.695670	-0.797732	-0.000040
6	-0.552441	-0.081538	-0.000001	6	0.458770	-0.042445	-0.000074
6	-2.998600	-0.192514	0.000000	6	2.907069	-0.017836	-0.000070
7	-0.631990	1.254031	-0.000001	7	0.454732	1.288932	-0.000053
7	-3.056970	1.139739	-0.000002	7	2.882621	1.321536	0.000076
6	-1.871237	1.782969	-0.000001	6	1.666478	1.892096	0.000065
7	-4.157395	-0.874520	0.000004	7	4.096091	-0.633433	-0.000514
1	-4.136365	-1.883592	0.000003	1	4.096824	-1.651687	0.000888
7	-1.837594	-2.260375	0.000000	7	1.589484	-2.152345	0.000091
8	-0.775303	-2.946111	-0.000001	8	2.639201	-2.849527	0.000175
7	0.635866	-0.722166	0.000000	7	-0.694039	-0.754543	-0.000106
6	1.963493	-0.249931	0.000000	6	-2.049813	-0.372577	-0.000056
1	0.500850	-1.743779	0.000000	1	-0.516947	-1.756021	-0.000068
6	2.964902	-1.239772	-0.000002	6	-2.989183	-1.420710	0.000042
6	4.310587	-0.884421	-0.000002	6	-4.354440	-1.147998	0.000086
6	4.684254	0.463513	0.000001	6	-4.810210	0.174024	0.000033
6	2.335711	1.104509	0.000003	6	-2.504028	0.956255	-0.000109
6	3.690923	1.444510	0.000003	6	-3.877451	1.212795	-0.000066
7	-1.939539	3.133978	-0.000002	7	1.645469	3.244440	0.000220
1	2.679150	-2.288406	-0.000004	1	-2.642828	-2.451452	0.000084
1	5.067606	-1.663084	-0.000004	1	-5.061935	-1.971962	0.000163
1	5.733446	0.742627	0.000001	1	-5.874353	0.388606	0.000066
1	1.570864	1.866208	0.000005	1	-1.787419	1.763630	-0.000185
1	3.967575	2.495159	0.000005	1	-4.216613	2.244955	-0.000111
1	-2.840843	3.583122	-0.000003	1	2.514886	3.752685	0.000118
1	-1.091911	3.677001	-0.000004	1	0.763569	3.729803	0.000080
1	-5.025775	-0.363772	0.000005	1	4.933534	-0.069679	0.000706

Compound 6f

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-2.190493	-0.858312	0.000087	6	2.127114	-0.775315	0.000034

6	-0.957676	-0.094462	-0.000111	6	0.869372	-0.054062	-0.000069
6	-3.406607	-0.084277	0.000445	6	3.316496	0.037780	0.000315
7	-0.971689	1.244224	0.000221	7	0.829393	1.277477	0.000179
7	-3.399340	1.249088	0.000784	7	3.255570	1.375892	0.000593
6	-2.182799	1.832980	0.000742	6	2.023816	1.912886	0.000561
7	-4.597697	-0.708682	0.000465	7	4.522146	-0.545124	0.000328
1	-4.625467	-1.717898	0.000286	1	4.550742	-1.563112	0.000149
7	-2.348846	-2.206907	-0.000014	7	2.058570	-2.131891	-0.000152
8	-1.320737	-2.943888	-0.000265	8	3.127364	-2.800380	-0.000119
7	0.197311	-0.791162	-0.000574	7	-0.263261	-0.795400	-0.000380
6	1.546039	-0.381546	-0.000733	6	-1.628973	-0.446890	-0.000470
1	0.013611	-1.805114	-0.000439	1	-0.061107	-1.792031	-0.000255
6	2.503625	-1.413760	0.000721	6	-2.545279	-1.514983	0.000598
6	3.862150	-1.120461	-0.000280	6	-3.914725	-1.275258	-0.000215
6	4.321980	0.206805	-0.002289	6	-4.426766	0.032261	-0.001753
6	1.987521	0.949351	-0.003774	6	-2.122229	0.865243	-0.002746
6	3.358638	1.221530	-0.004742	6	-3.503127	1.083156	-0.003509
7	-2.185141	3.186086	0.001161	7	1.966605	3.264506	0.000871
1	2.173701	-2.449494	0.001591	1	-2.177882	-2.538549	0.001257
1	4.578200	-1.938755	-0.000110	1	-4.597455	-2.121565	-0.000057
1	1.265082	1.751569	-0.006303	1	-1.431710	1.695226	-0.004623
1	3.680736	2.260147	-0.008090	1	-3.864897	2.108641	-0.005983
1	-3.063348	3.678764	0.002319	1	2.822076	3.795806	0.001713
1	-1.311859	3.686752	0.002062	1	1.071907	3.725780	0.001534
1	6.317472	0.020355	-0.824565	1	-6.139199	1.352617	-0.061827
1	-5.439949	-0.155579	0.000787	1	5.343770	0.041441	0.000531
6	5.800648	0.516537	0.005089	6	-5.916625	0.283676	0.003694
1	6.275519	0.173907	0.932539	1	-6.383157	-0.097646	0.920124
1	5.981851	1.591606	-0.083177	1	-6.409607	-0.212757	-0.840322

Compound 6g

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-2.320701	0.259939	0.000000	6	2.108542	-0.776478	0.000003
6	-0.930405	-0.152582	0.000000	6	0.849593	-0.056887	-0.000002
6	-3.290106	-0.806597	0.000000	6	3.296697	0.038134	0.000005
7	-0.591091	-1.449151	0.000000	7	0.807950	1.275803	-0.000013
7	-2.932312	-2.091018	0.000000	7	3.234055	1.376247	-0.000008
6	-1.604885	-2.334952	0.000000	6	2.001655	1.911922	-0.000021
7	-4.603483	-0.517815	0.000000	7	4.502935	-0.543442	0.000023
1	-4.896548	0.448000	0.000000	1	4.532275	-1.561489	0.000062
7	-2.826688	1.519365	0.000000	7	2.041625	-2.132820	0.000008
8	-2.026207	2.499686	0.000000	8	3.111245	-2.800406	0.000014
7	0.000000	0.822145	0.000000	7	-0.281302	-0.798110	0.000003
6	1.409605	0.779182	0.000000	6	-1.648149	-0.448607	0.000001
1	-0.444490	1.752433	0.000000	1	-0.078860	-1.794688	0.000001
6	2.067251	2.024483	0.000000	6	-2.567604	-1.514038	-0.000056
6	3.453726	2.105166	0.000000	6	-3.937710	-1.282392	-0.000054
6	4.218203	0.933038	0.000000	6	-4.420887	0.030326	0.000005
6	2.181942	-0.391667	0.000000	6	-2.138506	0.864834	0.000061
6	3.576265	-0.307357	0.000000	6	-3.516782	1.094462	0.000062
7	-1.253394	-3.642063	0.000000	7	1.944505	3.263924	-0.000039
1	1.480396	2.939070	0.000000	1	-2.203218	-2.538342	-0.000103
1	3.955476	3.066938	0.000000	1	-4.641239	-2.108119	-0.000098
1	1.691484	-1.353484	0.000000	1	-1.445582	1.692865	0.000106
1	4.163012	-1.223646	0.000000	1	-3.882257	2.119264	0.000109
1	-1.972757	-4.346666	0.000000	1	2.800256	3.794754	-0.000074
1	-0.279988	-3.897994	0.000000	1	1.050284	3.725856	-0.000084
8	5.583133	1.068789	0.000000	8	-5.782375	0.203147	0.000004
1	6.001869	0.198194	0.000000	1	-5.996098	1.145219	0.000052
1	-5.270462	-1.272811	0.000000	1	5.324018	0.043887	0.000051

Compound 6h

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	2.179571	-0.862431	0.004412	6	2.118189	-0.777474	0.004418
6	0.946753	-0.097302	-0.001056	6	0.858123	-0.057546	-0.001623
6	3.396197	-0.089000	0.004721	6	3.306186	0.037900	0.003723
7	0.962920	1.244012	-0.006035	7	0.817934	1.276281	-0.007470
7	3.390558	1.243919	-0.001096	7	3.244133	1.375719	-0.003497
6	2.173438	1.829533	-0.006851	6	2.010731	1.911226	-0.009428
7	4.586629	-0.715605	0.010467	7	4.512253	-0.544674	0.009793

1	4.611674	-1.724881	0.013971	1	4.539442	-1.562994	0.014694
7	2.335334	-2.209908	0.009498	7	2.052718	-2.132946	0.010136
8	1.303256	-2.944628	0.008649	8	3.123423	-2.800899	0.015834
7	-0.207054	-0.790515	-0.001253	7	-0.272034	-0.796610	-0.001291
6	-1.556261	-0.378959	-0.004356	6	-1.640110	-0.447386	-0.004122
1	-0.023172	-1.805154	0.000178	1	-0.070426	-1.793337	-0.000868
6	-2.518747	-1.404258	-0.026573	6	-2.560276	-1.509039	-0.034246
6	-3.877501	-1.115321	-0.026370	6	-3.930463	-1.274470	-0.033373
6	-4.327791	0.216600	-0.002061	6	-4.433973	0.037208	-0.001126
6	-1.999088	0.953139	0.017497	6	-2.135377	0.865118	0.026108
6	-3.363693	1.237069	0.018296	6	-3.510728	1.094038	0.026925
7	2.180872	3.183761	-0.010026	7	1.954752	3.263847	-0.014403
1	-2.195139	-2.441773	-0.043266	1	-2.198604	-2.534292	-0.057780
1	-4.597330	-1.929456	-0.049934	1	-4.616373	-2.117193	-0.063393
1	-1.274884	1.753898	0.035174	1	-1.443785	1.694153	0.049663
1	-3.685176	2.275834	0.030536	1	-3.872280	2.119427	0.045293
1	3.060932	3.672032	-0.039937	1	2.810804	3.793293	-0.043397
1	1.309887	3.686906	-0.046313	1	1.060879	3.725177	-0.049953
1	-5.959099	1.424690	0.290907	1	-6.111127	1.176764	0.302124
1	5.429866	-0.164158	0.010175	1	5.333663	0.042111	0.009232
7	-5.692811	0.514273	-0.058313	7	-5.811292	0.281232	-0.058734
1	-6.316017	-0.214892	0.260671	1	-6.402649	-0.473308	0.262433

Compound 6i

Atomic number	x	rotamer A y	z	Atomic number	x	rotamer B y	z
6	2.940562	-0.823819	0.017026	6	2.875561	-0.760507	0.015778
6	1.678059	-0.108885	-0.007595	6	1.599320	-0.069283	-0.008991
6	4.124934	-0.001859	0.027216	6	4.044654	0.081899	0.023688
7	1.640904	1.232531	-0.021676	7	1.529438	1.263740	-0.024682
7	4.066259	1.329565	0.012557	7	3.952603	1.417797	0.006830
6	2.826336	1.865751	-0.012177	6	2.707112	1.925032	-0.017442
7	5.339448	-0.580436	0.051653	7	5.263499	-0.473310	0.047836
1	5.404179	-1.587881	0.062612	1	5.313194	-1.490844	0.059304
7	3.150470	-2.163660	0.032372	7	2.841259	-2.116748	0.029131
8	2.148281	-2.939296	0.023606	8	3.927116	-2.760291	0.051417
7	0.552771	-0.846719	-0.016301	7	0.486170	-0.832631	-0.016203
6	-0.810965	-0.488333	-0.036970	6	-0.888942	-0.513522	-0.037852
1	0.776226	-1.853310	-0.006510	1	0.709028	-1.824799	-0.007436
6	-1.735044	-1.546169	-0.063658	6	-1.787648	-1.590942	-0.075936
6	-3.104249	-1.315227	-0.078688	6	-3.162850	-1.391463	-0.091615
6	-3.624654	0.000918	-0.078053	6	-3.713533	-0.088699	-0.081186
6	-1.311048	0.821980	-0.019528	6	-1.418459	0.784035	-0.009357
6	-2.684692	1.055474	-0.034664	6	-2.797632	0.985558	-0.025872
7	2.779973	3.219522	-0.025386	7	2.621165	3.276268	-0.033379
1	-1.374476	-2.571740	-0.067128	1	-1.406434	-2.609522	-0.087806
1	-3.765701	-2.172056	-0.092782	1	-3.803518	-2.263784	-0.114633
1	-0.622641	1.653540	0.011046	1	-0.749472	1.630982	0.030178
1	-3.019101	2.085176	-0.012896	1	-3.154824	2.007363	0.004028
1	3.640101	3.742446	-0.045997	1	3.465439	3.824600	-0.053579
1	1.889898	3.686938	-0.073592	1	1.717470	3.716976	-0.079853
1	6.159909	0.004237	0.058923	1	6.071360	0.131937	0.053020
7	-4.995307	0.242913	-0.133124	7	-5.091000	0.123071	-0.140037
6	-5.916271	-0.860667	0.092655	6	-5.983974	-1.003426	0.084103
1	-6.939441	-0.497034	-0.015442	1	-7.015909	-0.665664	-0.025177
1	-5.770462	-1.650645	-0.651509	1	-5.817631	-1.788210	-0.661107
1	-5.811282	-1.308680	1.094547	1	-5.869323	-1.450552	1.085678
6	-5.485140	1.585850	0.136754	6	-5.609923	1.448696	0.159931
1	-5.238999	1.935494	1.153065	1	-5.373882	1.780332	1.184887
1	-5.072766	2.303726	-0.580044	1	-5.211623	2.191507	-0.539023
1	-6.570295	1.598055	0.022287	1	-6.694857	1.440445	0.042221

Compound 7a

Atomic number	x	rotamer A y	z	Atomic number	x	rotamer B y	z
6	-1.480329	-0.750858	-0.000008	6	1.416995	-0.732251	0.000085
6	-0.215914	-0.045559	-0.000005	6	0.144509	-0.040310	0.000067
6	-2.661584	0.080775	-0.000007	6	2.589565	0.112378	0.000119
7	-0.166626	1.288457	-0.000002	7	0.069335	1.286513	0.000072
7	-2.595540	1.396979	-0.000004	7	2.496244	1.432401	0.000142
6	-1.351159	1.931143	-0.000001	6	1.249596	1.947597	0.000107
7	-3.874491	-0.567424	-0.000011	7	3.807657	-0.511946	0.000140

1	-3.774345	-1.579296	-0.000009	1	3.712725	-1.535114	0.000265
7	-1.692971	-2.094496	-0.000010	7	1.353877	-2.092439	0.000033
8	-0.701971	-2.875158	-0.000010	8	2.418063	-2.765018	0.000056
7	0.910019	-0.798478	-0.000005	7	-0.975091	-0.812056	0.000038
6	2.268736	-0.450307	-0.000002	6	-2.340024	-0.494783	0.000007
1	0.679327	-1.803174	-0.000007	1	-0.746648	-1.803606	0.000024
6	3.179460	-1.526578	0.000000	6	-3.232838	-1.585562	-0.000041
6	4.547230	-1.299369	0.000003	6	-4.604390	-1.381658	-0.000069
6	5.042668	0.017753	0.000004	6	-5.122685	-0.073637	-0.000051
6	2.761894	0.866736	-0.000001	6	-2.855652	0.813570	0.000026
6	4.135622	1.090073	0.000002	6	-4.232799	1.013162	-0.000003
7	-1.309208	3.277310	0.000003	7	1.180955	3.292384	0.000118
1	2.804435	-2.546019	-0.000001	1	-2.843115	-2.599926	-0.000055
1	5.237426	-2.136095	0.000004	1	-5.279779	-2.230403	-0.000106
1	2.069964	1.694869	-0.000002	1	-2.177741	1.653282	0.000061
1	4.511966	2.107686	0.000003	1	-4.625633	2.024535	0.000011
1	-2.176983	3.791181	0.000003	1	2.038318	3.823578	0.000106
1	-0.423543	3.756880	0.000005	1	0.285789	3.754008	0.000077
6	-5.179237	-0.041560	-0.000004	6	5.102670	0.047724	-0.000153
8	-5.436787	1.143453	-0.000014	8	5.332915	1.238218	-0.000491
6	-6.238964	-1.130559	0.000037	6	6.184419	-1.017471	-0.000016
1	-6.143532	-1.769260	-0.885285	1	6.098801	-1.658544	0.884416
1	-7.220811	-0.658323	-0.000147	1	7.157073	-0.526468	-0.000191
1	-6.143730	-1.768956	0.885601	1	6.098671	-1.658898	-0.884179
6	6.454613	0.261821	0.000007	6	-6.538364	0.146307	-0.000080
7	7.601914	0.460949	0.000010	7	-7.689016	0.325367	-0.000104

Compound 7b

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	2.276373	-0.756540	0.000002	6	-2.219916	-0.739340	-0.004714
6	1.004440	-0.063544	0.000003	6	-0.940582	-0.058228	-0.010314
6	3.449389	0.086379	0.000001	6	-3.385109	0.115382	0.000977
7	0.943468	1.270764	0.000005	7	-0.855665	1.268742	-0.010396
7	3.371461	1.401754	0.000003	7	-3.281360	1.434456	0.000923
6	2.121381	1.923847	0.000006	6	-2.029838	1.938864	-0.004649
7	4.668539	-0.551095	-0.000002	7	-4.608570	-0.499245	0.006750
1	4.576643	-1.563791	-0.000002	1	-4.521170	-1.523342	0.006230
7	2.502332	-2.097662	0.000002	7	-2.169164	-2.099551	-0.005280
8	1.519142	-2.888454	0.000003	8	-3.239609	-2.763176	-0.000521
7	-0.113390	-0.825648	0.000002	7	0.171773	-0.837427	-0.015263
6	-1.477506	-0.489320	0.000001	6	1.541420	-0.529874	-0.020456
1	0.125113	-1.828053	0.000003	1	-0.062869	-1.827322	-0.013224
6	-2.376846	-1.575167	0.000009	6	2.425293	-1.626226	-0.018037
6	-3.746704	-1.358616	0.000006	6	3.800116	-1.430043	-0.024303
6	-4.250443	-0.050597	-0.000005	6	4.321789	-0.131228	-0.035837
6	-1.984300	0.819757	-0.000010	6	2.067118	0.773006	-0.031054
6	-3.364565	1.027348	-0.000012	6	3.448346	0.959342	-0.037196
7	2.067396	3.269971	0.000011	7	-1.950565	3.283408	-0.004417
1	-1.991758	-2.590880	0.000017	1	2.028686	-2.637966	-0.013667
1	-4.425253	-2.205531	0.000012	1	4.465785	-2.286243	-0.026505
1	-1.302617	1.656289	-0.000017	1	1.396972	1.618823	-0.036570
1	-3.747506	2.041723	-0.000021	1	3.845474	1.968730	-0.049353
1	2.930455	3.791585	0.000014	1	-2.803602	3.821364	0.000628
1	1.177212	3.741046	0.000017	1	-1.051536	3.737401	-0.007168
6	5.968202	-0.014659	-0.000005	6	-5.898607	0.070103	0.013774
8	6.216888	1.172449	-0.000006	8	-6.120762	1.262333	0.014357
6	7.037042	-1.095041	-0.000008	6	-6.988585	-0.986951	0.020971
1	6.946975	-1.734403	0.885409	1	-6.911289	-1.631675	-0.861563
1	8.014985	-0.614752	-0.000017	1	-7.957483	-0.488553	0.023404
1	6.946961	-1.734414	-0.885415	1	-6.904205	-1.626084	0.906936
6	-5.738509	0.156748	-0.000003	6	5.807072	0.087362	0.011893
9	-6.085160	1.466063	-0.000052	9	6.177466	1.245959	-0.589887
9	-6.331069	-0.409152	1.087283	9	6.495356	-0.914562	-0.591808
9	-6.331084	-0.409239	-1.087234	9	6.274060	0.154816	1.291429

Compound 7c

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	-2.289240	-0.757296	-0.000116	6	-2.229824	-0.736889	-0.000005
6	-1.030824	-0.039227	-0.000099	6	-0.967126	-0.023950	-0.000005
6	-3.478586	0.062595	-0.000092	6	-3.415818	0.089128	-0.000003

7	-0.997669	1.296307	-0.000073	7	-0.916345	1.304972	-0.000005
7	-3.427615	1.379000	-0.000062	7	-3.345518	1.410103	-0.000002
6	-2.187391	1.925633	-0.000056	6	-2.106078	1.945273	-0.000003
7	-4.685039	-0.599764	-0.000103	7	-4.623692	-0.556507	-0.000001
1	-4.571660	-1.610313	-0.000097	1	-4.509397	-1.578208	-0.000003
7	-2.489847	-2.102347	-0.000134	7	-2.146446	-2.095058	-0.000006
8	-1.491829	-2.874633	-0.000152	8	-3.201010	-2.784845	-0.000005
7	0.102374	-0.777704	-0.000107	7	0.164093	-0.774284	-0.000006
6	1.459892	-0.415433	-0.000071	6	1.526366	-0.435117	-0.000005
1	-0.114723	-1.784548	-0.000128	1	-0.045451	-1.769743	-0.000007
6	2.379136	-1.483893	-0.000052	6	2.433614	-1.513378	-0.000003
6	3.745924	-1.242617	-0.000009	6	3.803227	-1.288072	-0.000001
6	4.231244	0.075146	0.000014	6	4.304206	0.023561	0.000000
6	1.941598	0.905782	-0.000051	6	2.023348	0.880283	-0.000004
6	3.314736	1.134915	-0.000010	6	3.398897	1.093128	-0.000002
7	-2.160018	3.272762	-0.000028	7	-2.060246	3.291484	-0.000003
1	2.011005	-2.506196	-0.000067	1	2.056026	-2.532730	-0.000003
1	4.441874	-2.073274	0.000008	1	4.489147	-2.127058	0.000001
1	1.243734	1.728835	-0.000067	1	1.334915	1.711329	-0.000006
1	3.695608	2.150796	0.000007	1	3.790869	2.104800	-0.000002
1	-3.032943	3.777523	-0.000021	1	-2.926135	3.808389	-0.000002
1	-1.278837	3.760607	-0.000026	1	-1.172270	3.766921	-0.000004
6	-5.994898	-0.090844	0.000068	6	-5.927299	-0.020882	0.000007
8	-6.269431	1.090766	0.000047	8	-6.181190	1.165214	0.000011
6	-7.041008	-1.193643	0.000440	6	-6.989807	-1.105938	0.000013
1	-6.937310	-1.831497	-0.884563	1	-6.892369	-1.745532	-0.884255
1	-8.028821	-0.733968	0.000047	1	-7.971280	-0.632736	0.000052
1	-6.937579	-1.830437	0.886246	1	-6.892318	-1.745576	0.884243
8	6.142164	1.524136	0.000079	8	6.231265	1.450399	0.000002
8	6.460942	-0.713404	0.000098	8	6.524372	-0.790793	0.000006
6	5.683233	0.395353	0.000065	6	5.759058	0.327029	0.000003
6	7.881431	-0.481146	0.000154	6	7.947309	-0.574367	0.000010
1	8.336270	-1.471417	0.000165	1	8.391161	-1.569633	0.000016
1	8.175952	0.079628	-0.890166	1	8.248130	-0.016925	-0.890297
1	8.175882	0.079614	0.890507	1	8.248124	-0.016917	0.890315

Compound 7d

Atomic number	x	rotamer A y	z	Atomic number	x	rotamer B y	z
6	-1.628820	-0.753484	0.000022	6	-1.567464	-0.734981	0.000111
6	-0.360666	-0.051577	0.000033	6	-0.290836	-0.045395	0.000082
6	-2.807412	0.081468	0.000008	6	-2.737818	0.112689	0.000148
7	-0.310924	1.285292	0.000037	7	-0.216624	1.284130	0.000089
7	-2.739846	1.396976	0.000010	7	-2.643711	1.432162	0.000177
6	-1.492386	1.928160	0.000027	6	-1.394406	1.944649	0.000137
7	-4.022137	-0.565984	-0.000011	7	-3.957068	-0.511463	0.000174
1	-3.920864	-1.577863	-0.000001	1	-3.860126	-1.535193	0.000320
7	-1.845015	-2.095175	0.000025	7	-1.509358	-2.093739	0.000056
8	-0.854708	-2.878865	0.000036	8	-2.576639	-2.764804	0.000088
7	0.761022	-0.802591	0.000037	7	0.824891	-0.813480	0.000042
6	2.125216	-0.454152	0.000025	6	2.195884	-0.494347	0.000003
1	0.531116	-1.806925	0.000039	1	0.599238	-1.805263	0.000032
6	3.034747	-1.528050	0.000010	6	3.088481	-1.581612	-0.000026
6	4.407259	-1.303011	-0.000011	6	4.464863	-1.378399	-0.000058
6	4.884722	0.008793	-0.000017	6	4.963506	-0.074938	-0.000059
6	2.621000	0.859613	0.000025	6	2.712434	0.811084	-0.000005
6	3.998777	1.084195	0.000003	6	4.093696	1.013518	-0.000036
7	-1.450767	3.275540	0.000035	7	-1.326379	3.290501	0.000161
1	2.662244	-2.548704	0.000013	1	2.702477	-2.597712	-0.000022
1	5.098926	-2.137948	-0.000023	1	5.142690	-2.224652	-0.000080
1	1.932353	1.690842	0.000040	1	2.036960	1.653112	0.000010
1	4.379091	2.099837	0.000003	1	4.489308	2.023336	-0.000043
1	-2.318533	3.789017	0.000029	1	-2.183906	3.821077	0.000160
1	-0.564852	3.754375	0.000053	1	-0.431060	3.751579	0.000133
6	-5.325398	-0.041204	-0.000047	6	-5.250821	0.046679	-0.000192
8	-5.585753	1.143721	-0.000073	8	-5.484428	1.237055	-0.000554
6	-6.385132	-1.130996	-0.000043	6	-6.332122	-1.019754	-0.000084
1	-6.289468	-1.769669	-0.885365	1	-6.245522	-1.661390	-0.884008
1	-7.367185	-0.659117	-0.000162	1	-7.305231	-0.529580	-0.000536
1	-6.289609	-1.769501	0.885417	1	-6.246003	-1.660688	0.884398
17	6.617218	0.303522	-0.000053	17	6.700887	0.192672	-0.000097

Compound 7e

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	0.223359	0.007680	0.055173	6	-0.794839	-0.725330	-0.000001
6	0.134289	0.000936	1.502732	6	0.469511	-0.010864	0.000000
6	1.560181	-0.009609	-0.491180	6	-1.981421	0.099613	-0.000001
7	1.237429	-0.020093	2.260713	7	0.515506	1.320752	0.000002
7	2.634345	-0.030218	0.270533	7	-1.914162	1.420423	0.000002
6	2.412365	-0.034326	1.608729	6	-0.674182	1.956827	0.000003
7	1.664822	-0.003519	-1.864395	7	-3.188484	-0.549031	-0.000002
1	0.755772	0.012869	-2.320045	1	-3.070002	-1.570860	0.000000
7	-0.791315	0.028179	-0.848581	7	-0.711796	-2.082263	-0.000002
8	-1.984664	0.044030	-0.435650	8	-1.766936	-2.773694	-0.000003
7	-1.099553	0.016669	2.046959	7	1.599178	-0.755290	-0.000001
6	-1.541816	0.015907	3.386224	6	2.967003	-0.412997	0.000000
1	-1.824419	0.031791	1.315939	1	1.393858	-1.751360	-0.000002
6	-2.937619	0.036130	3.568242	6	3.873023	-1.489706	-0.000003
6	-3.483110	0.037268	4.848733	6	5.245944	-1.258940	-0.000003
6	-2.648481	0.018289	5.970896	6	5.741588	0.048580	0.000001
6	-0.700948	-0.003181	4.510915	6	3.460877	0.901334	0.000003
6	-1.264444	-0.001757	5.789386	6	4.841489	1.115698	0.000004
7	3.527774	-0.055540	2.366480	7	-0.633297	3.304289	0.000005
1	-3.590293	0.050924	2.699308	1	3.495649	-2.509452	-0.000006
1	-4.562310	0.053022	4.968418	1	5.927968	-2.104017	-0.000005
1	-3.072379	0.019149	6.970330	1	6.811759	0.230436	0.000001
1	0.369874	-0.018723	4.376286	1	2.770038	1.730750	0.000006
1	-0.605046	-0.016621	6.652582	1	5.212138	2.136859	0.000006
1	4.426375	-0.066661	1.909497	1	-1.501100	3.817675	0.000004
1	3.455865	-0.060066	3.370906	1	0.253104	3.782252	0.000005
6	2.804729	-0.016284	-2.683856	6	-4.492456	-0.017733	-0.000007
8	3.945621	-0.035972	-2.270925	8	-4.751739	1.167621	-0.000025
6	2.451000	-0.002596	-4.162533	6	-5.551988	-1.106242	0.000021
1	1.846756	-0.877317	-4.428197	1	-5.452437	-1.745719	-0.884086
1	3.374950	-0.013559	-4.739893	1	-6.534936	-0.636040	-0.000084
1	1.873962	0.893195	-4.418293	1	-5.452549	-1.745541	0.884270

Compound 7f

		rotamer A				rotamer B	
Atomic number	x	y	z	Atomic number	x	y	z
6	1.266219	-0.748325	0.000265	6	1.203161	-0.730882	-0.000023
6	0.004529	-0.032513	0.000287	6	-0.070122	-0.031270	-0.000063
6	2.453660	0.073709	0.000285	6	2.379727	0.108366	0.000152
7	-0.027888	1.306603	0.000605	7	-0.131421	1.300551	0.000181
7	2.402294	1.389497	0.000582	7	2.297113	1.428148	0.000404
6	1.159422	1.934348	0.000861	6	1.050331	1.949858	0.000477
7	3.661343	-0.589010	-0.000032	7	3.594325	-0.526606	0.000056
1	3.545788	-1.599457	-0.000239	1	3.486758	-1.549872	-0.000105
7	1.469020	-2.091573	0.000118	7	1.136757	-2.088228	-0.000180
8	0.470522	-2.865730	0.000116	8	2.200514	-2.767390	-0.000212
7	-1.124737	-0.767688	-0.000008	7	-1.190485	-0.787172	-0.000326
6	-2.487830	-0.404133	-0.000262	6	-2.562344	-0.458070	-0.000358
1	-0.909108	-1.774480	0.000122	1	-0.975248	-1.781089	-0.000228
6	-3.408189	-1.469329	0.001100	6	-3.461101	-1.540656	0.000809
6	-4.775945	-1.223230	0.000049	6	-4.834021	-1.322357	0.000277
6	-5.281365	0.087378	-0.002074	6	-5.366137	-0.022821	-0.001204
6	-2.974461	0.910767	-0.003073	6	-3.075180	0.846274	-0.002353
6	-4.354018	1.135231	-0.004087	6	-4.459231	1.042600	-0.002833
7	1.134792	3.283110	0.001403	7	0.994593	3.297090	0.000867
1	-3.043113	-2.493172	0.002201	1	-3.078004	-2.558430	0.001623
1	-5.463257	-2.065686	0.000406	1	-5.503535	-2.179055	0.000760
1	-2.281070	1.738156	-0.005155	1	-2.398515	1.687480	-0.003964
1	-4.711873	2.161962	-0.007016	1	-4.836869	2.062228	-0.004839
1	2.008691	3.785735	0.001799	1	1.856680	3.819930	0.001225
1	0.254361	3.771804	0.001983	1	0.102892	3.765013	0.001177
6	4.970173	-0.082344	-0.000177	6	4.891970	0.018806	0.000122
8	5.248541	1.098926	0.000136	8	5.138884	1.206938	0.000344
6	6.015354	-1.186785	-0.000833	6	5.963417	-1.058170	-0.000135
1	5.911063	-1.824600	0.884132	1	5.871001	-1.698735	0.883970
1	7.003766	-0.728308	-0.000609	1	6.941199	-0.577308	-0.000258
1	5.910986	-1.823522	-0.886568	1	5.870709	-1.698617	-0.884295
6	-6.769754	0.345193	0.003023	6	-6.859638	0.204898	0.002533
1	-7.263819	-0.149964	-0.840997	1	-7.340464	-0.281535	-0.854236

1	-6.988397	1.414849	-0.062271	1	-7.099259	1.271169	-0.041637
1	-7.237060	-0.035246	0.919337	1	-7.323673	-0.203509	0.908328

Compound 7g

rotamer A				rotamer B			
Atomic number	x	y	z	Atomic number	x	y	z
6	-1.249580	-0.749893	-0.000001	6	1.187435	-0.733100	0.000074
6	0.012230	-0.034318	-0.000001	6	-0.086975	-0.035066	0.000091
6	-2.436762	0.072362	-0.000001	6	2.362716	0.107729	0.000040
7	0.045188	1.306139	0.000000	7	-0.149958	1.297890	0.000098
7	-2.385021	1.388078	0.000000	7	2.278411	1.427445	0.000058
6	-1.142001	1.933191	0.000000	6	1.031021	1.947894	0.000090
7	-3.644386	-0.590346	-0.000001	7	3.578030	-0.525762	-0.000027
1	-3.528711	-1.600810	0.000001	1	3.471516	-1.549251	-0.000044
7	-1.451106	-2.092724	-0.000001	7	1.122690	-2.090178	0.000067
8	-0.450498	-2.865434	-0.000002	8	2.187335	-2.768435	0.000032
7	1.140331	-0.768930	-0.000001	7	-1.205740	-0.790733	0.000090
6	2.503539	-0.404376	0.000000	6	-2.578564	-0.460613	0.000043
1	0.923393	-1.776092	-0.000002	1	-0.990272	-1.784613	0.000088
6	3.427376	-1.467095	-0.000005	6	-3.480673	-1.540567	0.000031
6	4.795452	-1.229270	-0.000004	6	-4.853975	-1.330339	-0.000029
6	5.272184	0.086663	0.000001	6	-5.357435	-0.025024	-0.000079
6	2.987511	0.911978	0.000005	6	-3.088576	0.845161	-0.000002
6	4.364058	1.148101	0.000005	6	-4.470018	1.053355	-0.000063
7	-1.119381	3.282412	0.000001	7	0.975462	3.295515	0.000113
1	3.065019	-2.491605	-0.000009	1	-3.100605	-2.559136	0.000067
1	5.503551	-2.050993	-0.000007	1	-5.544729	-2.166715	-0.000040
1	2.291605	1.737330	0.000008	1	-2.409377	1.684368	0.000008
1	4.725876	2.174089	0.000010	1	-4.851304	2.072253	-0.000100
1	-1.994293	3.783245	-0.000001	1	1.837902	3.817757	0.000088
1	-0.240181	3.773058	-0.000001	1	0.084306	3.764211	0.000126
6	-4.953183	-0.083652	-0.000003	6	4.874937	0.021359	-0.000166
8	-5.231389	1.097678	-0.000013	8	5.120205	1.209856	-0.000254
6	-5.998461	-1.187963	0.000014	6	5.947894	-1.054072	-0.000048
1	-5.894164	-1.825290	-0.885300	1	5.857141	-1.693564	0.885007
1	-6.986837	-0.729407	-0.000021	1	6.924993	-0.571814	-0.001555
1	-5.894198	-1.825221	0.885382	1	5.855398	-1.695849	-0.883252
8	6.631000	0.264916	0.000002	8	-6.720455	0.125908	-0.000141
1	6.842494	1.207640	0.000005	1	-6.950637	1.064169	-0.000178

Compound 7h

rotamer A				rotamer B			
Atomic number	x	y	z	Atomic number	x	y	z
6	1.257775	-0.749331	-0.000506	6	-1.195697	-0.733068	-0.000056
6	-0.004749	-0.033808	-0.004347	6	0.079901	-0.034840	-0.004357
6	2.444562	0.073784	0.000104	6	-2.370655	0.108812	-0.000599
7	-0.036793	1.308051	-0.008240	7	0.141657	1.299392	-0.009295
7	2.393423	1.389006	-0.004245	7	-2.286878	1.428083	-0.006436
6	1.149108	1.934142	-0.009519	6	-1.038217	1.948333	-0.011894
7	3.652340	-0.590139	0.005210	7	-3.585976	-0.525788	0.004960
1	3.534547	-1.600440	0.007580	1	-3.477313	-1.549515	0.008301
7	1.459789	-2.091198	0.003630	7	-1.132689	-2.089215	0.004897
8	0.458069	-2.864526	0.003044	8	-2.198678	-2.767685	0.009510
7	-1.132190	-0.766872	-0.003746	7	1.197820	-0.788456	-0.003009
6	-2.495879	-0.403297	-0.004736	6	2.571822	-0.459076	-0.004035
1	-0.914878	-1.774088	-0.003122	1	0.982904	-1.782466	-0.003097
6	-3.420432	-1.462899	-0.023726	6	3.474546	-1.535530	-0.031819
6	-4.788322	-1.223010	-0.021495	6	4.847975	-1.322903	-0.029460
6	-5.286197	0.092333	0.001618	6	5.372146	-0.018933	0.001917
6	-2.985656	0.912308	0.015952	6	3.087117	0.845642	0.025508
6	-4.359081	1.147209	0.018843	6	4.465554	1.052801	0.027897
7	1.128025	3.284021	-0.015685	7	-0.983974	3.296462	-0.019841
1	-3.060363	-2.488321	-0.039538	1	3.096927	-2.555011	-0.054767
1	-5.478497	-2.062391	-0.042623	1	5.520471	-2.176312	-0.057700
1	-2.291351	1.739106	0.031009	1	2.409453	1.686037	0.047233
1	-4.717391	2.173716	0.030092	1	4.843214	2.072254	0.045685
1	2.003334	3.783856	-0.023918	1	-1.846780	3.817827	-0.029150
1	0.249069	3.774872	-0.029738	1	-0.092964	3.765213	-0.034646
6	4.960969	-0.085827	0.006817	6	-4.882697	0.019338	0.006251
8	5.242383	1.095037	0.004252	8	-5.130856	1.207516	0.002628
6	6.004771	-1.191993	0.012198	6	-5.954447	-1.057711	0.012940
1	5.896236	-1.828085	0.897888	1	-5.864479	-1.701174	-0.869307

1	6.993864	-0.734945	0.015204	1	-6.932224	-0.576782	0.014234
1	5.902754	-1.830231	-0.872737	1	-5.859237	-1.695376	0.898834
1	-6.960659	1.243221	0.287448	1	7.067958	1.095888	0.298721
7	-6.659261	0.340296	-0.051977	7	6.751538	0.202952	-0.053805
1	-7.258829	-0.410166	0.262239	1	7.333778	-0.560424	0.262506

Compound 7i

	rotamer A				rotamer B		
Atomic number	x	y	z	Atomic number	x	y	z
6	1.996417	-0.757312	-0.004699	6	-1.937672	-0.740388	-0.003449
6	0.720108	-0.066621	-0.022134	6	-0.653078	-0.058279	-0.022560
6	3.166678	0.089098	0.002811	6	-3.101748	0.116714	0.001909
7	0.662198	1.275019	-0.032756	7	-0.574904	1.275631	-0.036420
7	3.090276	1.402862	-0.008024	7	-3.001624	1.434593	-0.012571
6	1.835088	1.923612	-0.026926	6	-1.746006	1.938861	-0.032865
7	4.387142	-0.551762	0.022292	7	-4.324795	-0.503069	0.022941
1	4.287913	-1.564094	0.029016	1	-4.227744	-1.528188	0.031765
7	2.224727	-2.094612	0.006962	7	-1.892547	-2.096809	0.008508
8	1.237804	-2.887539	0.000680	8	-2.967620	-2.761650	0.026574
7	-0.392817	-0.820733	-0.027366	7	0.455104	-0.824936	-0.026033
6	-1.762685	-0.483676	-0.040460	6	1.832797	-0.512645	-0.040911
1	-0.156310	-1.823651	-0.020790	1	0.228586	-1.816377	-0.019314
6	-2.669021	-1.556910	-0.061358	6	2.724273	-1.596084	-0.077361
6	-4.041480	-1.348540	-0.068832	6	4.100453	-1.405549	-0.086204
6	-4.583104	-0.040410	-0.065612	6	4.659202	-0.105792	-0.069893
6	-2.283180	0.818750	-0.021275	6	2.369623	0.781767	-0.007100
6	-3.659959	1.029911	-0.028769	6	3.749694	0.974643	-0.016715
7	1.788553	3.273213	-0.040311	7	-1.675585	3.286460	-0.050584
1	-2.292042	-2.576554	-0.066345	1	2.336643	-2.612179	-0.093492
1	-4.689235	-2.215794	-0.078569	1	4.735984	-2.281599	-0.108143
1	-1.608801	1.661813	0.004431	1	1.706569	1.633339	0.030941
1	-4.011307	2.053846	-0.006075	1	4.113461	1.993934	0.017107
1	2.654215	3.789522	-0.041659	1	-2.532036	3.818176	-0.054448
1	0.900424	3.746882	-0.062507	1	-0.778964	3.743902	-0.075440
6	5.685596	-0.023320	0.035304	6	-5.614555	0.057065	0.033775
8	5.945750	1.162544	0.027287	8	-5.849574	1.248010	0.022352
6	6.749745	-1.109815	0.062433	6	-6.698621	-1.007410	0.063004
1	6.649131	-1.732197	0.958782	1	-6.621366	-1.666251	-0.809017
1	7.730202	-0.634502	0.061819	1	-7.670838	-0.515321	0.062588
1	6.663450	-1.765377	-0.811423	1	-6.605223	-1.631631	0.958647
7	-5.955633	0.179128	-0.110449	7	6.036285	0.097211	-0.119593
6	-6.859967	-0.940488	0.103715	6	6.923644	-1.036269	0.091677
1	-7.888514	-0.590509	0.003674	1	6.755729	-1.810693	-0.664146
1	-6.704948	-1.719211	-0.650597	1	7.957300	-0.701870	-0.009936
1	-6.745038	-1.398573	1.099601	1	6.803910	-1.495310	1.086947
6	-6.467762	1.516413	0.146986	6	6.564054	1.421353	0.172037
1	-6.219673	1.881513	1.156974	1	6.176052	2.161594	-0.535587
1	-6.074133	2.233307	-0.581475	1	6.324107	1.762713	1.192553
1	-7.553731	1.507576	0.041868	1	7.649501	1.403385	0.061763

Table S3. The calculated NH...O hydrogen-bond lengths in compounds **3a–7i** (Å).

Compound	Rotamer A $d_{\text{NH}\cdots\text{O}}$	Rotamer B $d_{\text{NH}\cdots\text{O}}$	Compound	Rotamer A $d_{\text{NH}\cdots\text{O}}$	Rotamer B $d_{\text{NH}\cdots\text{O}}$
3a	1.718	-	6a	1.743	1.901
3b	1.721	-	6b	1.747	1.898
3c	1.725	-	6c	1.751	1.894
3d	1.721	-	6d	1.747	1.892
3e	1.728	-	6e	1.753	1.887
3f	1.728	-	6f	1.754	1.886
3g	1.722	-	6g	1.749	1.885
3h	1.722	-	6h	1.749	1.881
3i	1.723	-	6i	1.750	1.880
4a	1.734	1.842	7a	1.748	1.786
4b	1.738	1.839	7b	1.752	1.783
4c	1.743	1.836	7c	1.756	1.780
4d	1.738	1.834	7d	1.752	1.777
4e	1.745	1.829	7e	1.759	1.773
4f	1.746	1.828	7f	1.759	1.771
4g	1.740	1.827	7g	1.753	1.771
4h	1.740	1.823	7h	1.753	1.766
5a	1.734	1.842	7i	1.754	1.763
5b	1.737	1.838			
5c	1.742	1.836			
5d	1.737	1.834			
5e	1.745	1.829			
5f	1.745	1.827			
5g	1.739	1.827			
5h	1.740	1.823			