Supporting Information

Analgesic monoterpene indole alkaloids from *Gelsemium elegans*

stems

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Figure S18. HMBC spectrum of **2** (¹H: 400 MHz, ¹³C: 100 MHz, chloroform-*d*).



Figure S19. ¹H-¹H COSY (400 MHz, chloroform-*d*) spectrum of **2**.



Figure S20. NOESY (400 MHz, chloroform-*d*) spectrum of 2.

Table S1. Important thermodynamic parameters (a.u.) and Boltzmann distributions of

Conformation	Gibbs free energies	Boltzmann distribution
	(Hartree)	
1	-1036.12	94.16%
2	-1036.11	0.97%
3	-1036.12	4.86%

the optimized 19*S**-1 at B3LYP/6-31G (d) level in methanol.

Confor	mation 1						
Atom	Χ	Y	Z	Atom	Χ	Y	Z
С	-0.70728	-1.43699	-0.85572	Н	С	-4.14219	0.847123
С	-0.9289	-1.08975	0.458824	Н	С	-4.61257	0.877903
С	0.50301	-2.06979	-1.49181	Н	С	-3.88443	0.298239
Ν	1.216853	0.709386	1.862231	Н	Н	0.060232	-2.49863
С	1.339737	-0.75355	1.701924	Н	Н	-0.59411	-1.09862
С	-0.06418	-1.41204	1.651024	Н	Н	2.370585	-1.46691
С	1.513042	-0.97617	-1.93343	Н	Н	1.045531	-0.33745
С	1.917729	-0.21312	-0.69979	Н	Н	3.131541	1.469373
С	1.840196	1.106117	-0.46568	Н	Н	1.750157	2.569688
С	2.055109	1.527463	0.972163	Н	Н	3.152394	-2.76273
С	2.258717	-1.09256	0.492341	Н	Н	2.355053	-3.21756
С	2.269718	-2.57215	0.094003	Н	Н	1.139653	1.686666
0	1.090845	-3.00576	-0.58412	Н	Н	2.052665	3.997267
С	1.395558	2.164108	-1.44998	Н	Н	3.337679	2.776343
С	2.462704	3.224328	-1.72388	Н	Н	2.783452	3.707067
Н	0.197337	-2.65182	-2.37362	Н	Н	2.31539	0.988001
Н	3.283871	-0.85789	0.818864	Н	Н	0.590915	0.579899
Н	1.845739	-1.17622	2.589098	Н	Н	1.059572	2.199814
С	1.309573	1.135682	3.247717	Н	Н	-0.37073	2.201162
0	0.25339	2.865312	-0.94282	Н	Н	-1.86264	-1.16063
С	-2.67167	-0.31501	-0.85061	Н	Н	-2.58799	0.218483
С	-2.17985	-0.36926	0.483309	Н	Н	-4.73292	1.314851
Ν	-1.74335	-0.95536	-1.64629	Н	Н	-5.55773	1.365757
С	-2.93904	0.231911	1.5034	Н	Н	-4.24403	0.324628
Confor	mation 2						
Atom	Χ	Y	Z	Atom	Χ	Y	Z
С	-0.4159	-1.57404	-0.68509	C	-4.02998	0.406718	1.363307
С	-0.59838	-1.09145	0.594481	С	-4.5863	0.200207	0.084021
С	0.836706	-2.07651	-1.35605	С	-3.84465	-0.38672	-0.93465
Ν	1.774515	1.071575	1.845392	Н	0.612014	-2.17787	1.967622

Table S2. Optimized coordinate of 19S*-1 at B3LYP/6-31G (d) level in methanol

С	1.747117	-0.37828	1.668692	Н	-0.14364	-0.75908	2.646254
С	0.371883	-1.12899	1.752088	Н	2.556457	-1.26725	-2.41454
С	1.638459	-0.88001	-1.95303	Н	1.047376	-0.42294	-2.74928
С	1.902843	0.05035	-0.79508	Н	1.901114	2.846158	0.767774
С	1.37465	1.275485	-0.6272	Н	0.26301	2.227451	0.881807
С	1.313986	1.913639	0.743676	Н	3.605249	-2.26618	-0.61634
C	2.553222	-0.66482	0.387662	Н	3.041054	-2.69424	1.001791
C	2.767805	-2.15346	0.089333	Н	0.68846	1.477266	-2.65377
0	1.613888	-2.82269	-0.41783	Н	0.763634	3.915797	-2.81564
C	0.661708	2.057894	-1.7216	Н	2.353853	3.280583	-2.32596
C	1.312553	3.411933	-2.01351	Н	1.28883	4.059717	-1.13182
Н	0.57264	-2.7724	-2.16635	Н	1.651792	2.602707	3.258299
Н	3.551383	-0.23834	0.561782	Н	1.783282	0.969553	3.934493
Н	2.324858	-0.77692	2.516635	Н	0.229323	1.542923	3.270639
С	1.327853	1.561825	3.132239	Н	-1.12925	1.509787	-1.12015
0	-0.69925	2.343085	-1.376	Н	-1.72022	-1.71066	-2.36488
С	-2.52883	-0.76141	-0.64171	Н	-2.31403	0.190186	2.643015
С	-1.94625	-0.57374	0.643338	Н	-4.63567	0.87208	2.13609
N	-1.56383	-1.34933	-1.43576	Н	-5.61006	0.507465	-0.11027
С	-2.72557	0.026563	1.650398	Н	-4.27092	-0.54581	-1.92188
Confor	mation 3						
Atom	X	Y	Ζ	Atom	Χ	Y	Z
Atom C	X 0.562719	Y 0.239098	Z 1.568877	Atom C	X 4.251368	Y -0.84934	Z -0.95593
AtomCC	X 0.562719 0.855547	Y 0.239098 -0.8615	Z 1.568877 0.79377	Atom C C	X 4.251368 4.679462	Y -0.84934 0.401359	Z -0.95593 -0.4658
Atom C C C	X 0.562719 0.855547 -0.70328	Y 0.239098 -0.8615 0.593294	Z 1.568877 0.79377 2.304638	Atom C C C	X 4.251368 4.679462 3.870059	Y -0.84934 0.401359 1.157797	Z -0.95593 -0.4658 0.374788
Atom C C C N	X 0.562719 0.855547 -0.70328 -1.14771	Y 0.239098 -0.8615 0.593294 -1.50382	Z 1.568877 0.79377 2.304638 -1.5449	Atom C C C H	X 4.251368 4.679462 3.870059 -0.18103	Y -0.84934 0.401359 1.157797 -2.58023	Z -0.95593 -0.4658 0.374788 1.547203
Atom C C C N C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714	Atom C C H H	X 4.251368 4.679462 3.870059 -0.18103 0.585671	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927
Atom C C N C C C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364	Atom C C H H H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706
Atom C C C N C C C C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998	Atom C C H H H H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265
Atom C C N C C C C C C C C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236	Atom C C H H H H H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446
Atom C C N C C C C C C C C C C C C C C C C C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699	Atom C C H H H H H H H H H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844
Atom C C N C C C C C C C C C C C C C C C C C C C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349	Atom C C H H H H H H H H H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686
Atom C C N C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016 -2.32802	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378 -0.91636	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349 0.564868	Atom C C H H H H H H H H H H H H H H H H H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371
Atom C C N C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016 -2.32802 -2.43406	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378 -0.91636 -1.09225	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349 0.564868 2.083468	Atom C C H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933 -2.00923	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088 2.162869	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371 -2.71906
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Atom C C N C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016 -2.32802 -2.43406 -1.31018 -1.50844	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378 -0.91636 -1.09225 -0.60134 2.12824	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349 0.564868 2.083468 2.810555 -1.73452	Atom C C H H H H H H H H H H H H H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933 -2.00923 0.202888 0.381787	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088 2.162869 3.217199 1.446317	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371 -2.71906 -2.49102 -2.56747
Atom C C N C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016 -2.32802 -2.43406 -1.31018 -1.50844 -0.00324	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378 -0.91636 -1.09225 -0.60134 2.12824 2.27709	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349 0.564868 2.083468 2.810555 -1.73452 -1.9684	Atom C C H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933 -2.00923 0.202888 0.381787 0.529276	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088 2.162869 3.217199 1.446317 2.278039	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371 -2.71906 -2.49102 -2.56747 -1.01314
Atom C C N C H	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016 -2.32802 -2.43406 -1.31018 -1.50844 -0.00324 -0.4567	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378 -0.91636 -1.09225 -0.60134 2.12824 2.27709 1.202141	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349 0.564868 2.083468 2.810555 -1.73452 -1.9684 3.186736	Atom C C H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933 -2.00923 0.202888 0.381787 0.529276 -2.15056	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088 2.162869 3.217199 1.446317 2.278039 -3.11872	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371 -2.71906 -2.49102 -2.56747 -1.01314 -2.55361
Atom C C N C H H	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016 -2.32802 -2.43406 -1.31018 -1.50844 -0.00324 -0.4567 -3.32713	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378 -0.91636 -1.09225 -0.60134 2.12824 2.27709 1.202141 -1.15122	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349 0.564868 2.083468 2.810555 -1.73452 -1.9684 3.186736 0.16445	Atom C C H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933 -2.00923 0.202888 0.381787 0.529276 -2.15056 -0.44598	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088 2.162869 3.217199 1.446317 2.278039 -3.11872 -3.39311	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371 -2.71906 -2.49102 -2.56747 -1.01314 -2.55361 -2.12054
Atom C C N C H H H	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016 -2.32802 -2.43406 -1.31018 -1.50844 -0.00324 -0.4567 -3.32713 -1.85121	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378 -0.91636 -1.09225 -0.60134 2.12824 2.27709 1.202141 -1.15122 -2.88853	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349 0.564868 2.083468 2.810555 -1.73452 -1.73452 -1.9684 3.186736 0.16445 -0.10852	Atom C C H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933 -2.00923 0.202888 0.381787 0.529276 -2.15056 -0.44598 -0.8454	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088 2.162869 3.217199 1.446317 2.278039 -3.11872 -3.39311 -2.30627	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371 -2.71906 -2.49102 -2.56747 -1.01314 -2.55361 -2.12054 -3.45702
Atom C C N C C C C C C C C C C C C C C C C H H C	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016 -2.32802 -2.43406 -1.31018 -1.31018 -1.50844 -0.00324 -0.4567 -3.32713 -1.85121 -1.15811	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378 -0.91636 -1.09225 -0.60134 2.12824 2.27709 1.202141 -1.15122 -2.88853 -2.63263	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349 0.564868 2.083468 2.810555 -1.73452 -1.73452 -1.9684 3.186736 0.16445 -0.10852 -2.45837	Atom C C H	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933 -2.00923 0.202888 0.381787 0.529276 -2.15056 -0.44598 -0.8454 -2.85405	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088 2.162869 3.217199 1.446317 2.278039 -3.11872 -3.39311 -2.30627 3.13397	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371 -2.71906 -2.49102 -2.56747 -1.01314 -2.55361 -2.12054 -3.45702 -0.74709
Atom C C N C C C C C C C C C C C C C C C H H C O	X 0.562719 0.855547 -0.70328 -1.14771 -1.35154 0.009251 -1.66922 -1.99666 -1.86453 -1.98016 -2.32802 -2.43406 -1.31018 -1.31018 -1.50844 -0.00324 -0.4567 -3.32713 -1.85121 -1.15811 -1.91777	Y 0.239098 -0.8615 0.593294 -1.50382 -1.90263 -2.09094 1.397018 0.524882 0.797818 -0.39378 -0.91636 -1.09225 -0.60134 2.12824 2.27709 1.202141 -1.15122 -2.88853 -2.63263 3.264022	Z 1.568877 0.79377 2.304638 -1.5449 -0.13714 0.58364 1.395998 0.210236 -1.09699 -2.02349 0.564868 2.083468 2.810555 -1.73452 -1.73452 -1.9684 3.186736 0.16445 -0.10852 -2.45837 -0.96737	Atom C C H H H H H H H H H H H H H <td>X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933 -2.00923 0.202888 0.381787 0.529276 -2.15056 -0.44598 -0.8454 -2.85405 1.669826</td> <td>Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088 2.162869 3.217199 1.446317 2.278039 -3.11872 -3.39311 -2.30627 3.13397 2.000855</td> <td>Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371 -2.71906 -2.49102 -2.56747 -1.01314 -2.55361 -2.12054 -3.45702 -0.74709 2.036629</td>	X 4.251368 4.679462 3.870059 -0.18103 0.585671 -2.56365 -1.21034 -3.04629 -1.62918 -3.35143 -2.51933 -2.00923 0.202888 0.381787 0.529276 -2.15056 -0.44598 -0.8454 -2.85405 1.669826	Y -0.84934 0.401359 1.157797 -2.58023 -2.81123 1.645636 2.338205 -0.68981 -0.12847 -0.59272 -2.15088 2.162869 3.217199 1.446317 2.278039 -3.11872 -3.39311 -2.30627 3.13397 2.000855	Z -0.95593 -0.4658 0.374788 1.547203 -0.00927 1.98706 1.090265 -2.14446 -3.02844 2.432686 2.352371 -2.71906 -2.49102 -2.56747 -1.01314 -2.55361 -2.12054 -3.45702 -0.74709 2.036629

С	2.167329	-0.63071	0.23854	Н	4.906502	-1.4141	-1.61397
N	1.615561	1.142753	1.509303	Н	5.656648	0.782118	-0.75042
С	3.009316	-1.36841	-0.61202	Н	4.197405	2.123618	0.75186

Table S3. Important thermodynamic parameters (a.u.) and Boltzmann distributions of the optimized $19R^*-1$ at B3LYP/6-31G (d) level in methanol.

Conformation	Gibbs free energies	Boltzmann distribution
	(Hartree)	
1	-1036.12	77.60%
2	-1036.11	13.05%
3	-1036.12	9.34%

Table S4. Optimized coordinate of $19R^*-1$ at B3LYP/6-31G (d) level in methanol

Confor	mation 1						
Atom	Χ	Y	Z	Atom	X	Y	Z
С	1.230997	1.059339	-0.53507	С	4.911764	-1.54913	0.344563
С	1.497625	0.158738	0.485476	С	5.344982	-0.92928	-0.84573
С	-0.09777	1.712232	-0.37745	С	4.540072	-0.01261	-1.51205
N	-1.56287	-1.27772	1.258866	Н	0.932299	0.741149	2.4612
С	-0.98592	-0.04428	1.827363	Н	0.925281	-0.98047	2.206432
С	0.626721	-0.03352	1.742831	Н	-1.70354	2.870111	-1.33521
С	-1.41436	1.822916	-1.19641	Н	-1.3829	1.335187	-2.17348
С	-2.26515	1.013742	-0.18139	Н	-3.65816	-0.80932	1.495868
С	-2.87604	-0.15264	-0.44229	Н	-3.27231	-2.10308	0.369087
С	-2.93358	-1.12415	0.717932	Н	-1.91297	3.356747	1.341695
С	-1.84095	1.202789	1.30173	Н	-0.78431	2.677461	2.529139
С	-1.16486	2.567469	1.505273	Н	-3.27015	0.188697	-2.51905
0	-0.06628	2.762979	0.597736	Н	-2.68897	-2.08578	-3.32726
С	-3.26551	-0.65669	-1.81513	Н	-1.31173	-1.33937	-2.47419
С	-2.32559	-1.73438	-2.35589	Н	-2.27926	-2.59139	-1.6773
Н	-0.39683	0.843513	0.152485	Н	-2.07276	-2.27556	3.093859
Н	-2.7469	1.210187	1.92026	Н	-0.43612	-2.58134	2.467223
Н	-1.14604	-0.035	2.923726	Н	-1.82702	-3.31593	1.665711
С	-1.47502	-2.40969	2.170124	Н	-5.18352	-0.57621	-1.4374
0	-4.57409	-1.24938	-1.78031	Н	2.339301	1.693905	-2.241
С	3.288463	0.276022	-0.95934	Н	3.346786	-1.75136	1.807646
С	2.821705	-0.34648	0.239691	Н	5.56661	-2.25973	0.841755
N	2.303227	1.142437	-1.39799	Н	6.324928	-1.17043	-1.24849
С	3.666337	-1.26567	0.889025	Н	4.875223	0.467733	-2.42803
Confor	mation 2						
Atom	X	Y	Z	Atom	X	Y	Z
С	1.222486	1.025898	-0.59604	C	4.891699	-1.53269	0.461704

С	1.482632	0.19162	0.481246	С	5.331693	-0.99051	-0.76351
C	-0.10526	1.690913	-0.48709	C	4.532103	-0.11566	-1.48984
N	-1.58529	-1.18458	1.345804	Н	0.913184	0.90485	2.411324
С	-1.00628	0.084896	1.826446	Н	0.90045	-0.83077	2.271864
С	0.606972	0.084658	1.745695	Н	-1.70899	2.785509	-1.5201
С	-1.41986	1.749125	-1.3157	Н	-1.38601	1.203395	-2.26164
С	-2.27378	1.005477	-0.25578	Н	-3.6852	-0.69951	1.524173
C	-2.88377	-0.17405	-0.44083	Н	-3.28547	-2.06681	0.495006
C	-2.95148	-1.06625	0.77989	Н	-1.92781	3.444559	1.108133
С	-1.85741	1.292802	1.213391	Н	-0.80734	2.845738	2.345956
С	-1.18166	2.667848	1.329343	Н	-3.30417	0.031355	-2.52643
0	-0.07592	2.802388	0.418016	Н	-2.5012	-2.24484	-3.21269
С	-3.23542	-0.77511	-1.78119	Н	-1.2149	-1.33287	-2.40068
С	-2.19461	-1.80033	-2.25572	Н	-2.07883	-2.60537	-1.5238
Н	-0.40848	0.859924	0.097833	Н	-2.12756	-2.03639	3.24391
Н	-2.767	1.341141	1.824521	Н	-0.48252	-2.39421	2.668899
Н	-1.16781	0.171658	2.919074	Н	-1.86449	-3.18485	1.905076
С	-1.5161	-2.24309	2.342829	Н	-4.71602	-1.86553	-2.45097
0	-4.52278	-1.3904	-1.62765	Н	2.341851	1.552476	-2.33144
С	3.279154	0.210871	-0.96181	Н	3.320638	-1.63697	1.92838
С	2.805818	-0.33262	0.272718	Н	5.542349	-2.21232	1.005562
N	2 207823	1 0/0/08	1 45007	Ц	6 21 26 91	1 25002	1 1/1506
IN	2.291023	1.049400	-1.43907	п	0.512081	-1.23902	-1.14390
C	3.645104	-1.21148	0.982065	H	4.872413	0.305121	-2.43286
C C Confor	3.645104 mation 3	-1.21148	0.982065	H	4.872413	0.305121	-2.43286
C Confor Atom	2.237823 3.645104 mation 3 X	-1.21148 Y	-1.43907 0.982065 Z	H H Atom	4.872413 X	0.305121 Y	-2.43286
C Confor Atom C	2.237823 3.645104 mation 3 X -1.10298	-1.21148 Y -0.91851	0.982065 Z 0.699318	H Atom C	4.872413 X -4.99989	0.305121 Y 0.792266	-2.43286 Z -1.03733
C Confor Atom C C	2.297823 3.645104 mation 3 X -1.10298 -1.47	-1.21148 Y -0.91851 0.376624	-1.43907 0.982065 Z 0.699318 0.363167	H Atom C C	4.872413 X -4.99989 -5.34469	Y 0.792266 -0.5744	-2.43286 Z -1.03733 -0.99311
C Confor Atom C C C	2.237823 3.645104 mation 3 X -1.10298 -1.47 0.265746	-1.21148 Y -0.91851 0.376624 -0.98274	Image: 1.43907 0.982065 Z 0.699318 0.363167 1.283225	H Atom C C C	0.312081 4.872413 X -4.99989 -5.34469 -4.44996	Y 0.792266 -0.5744 -1.52559	-2.43286 Z -1.03733 -0.99311 -0.51676
C Confor Atom C C C N	2.237823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849	-1.21148 -1.21148 Y -0.91851 0.376624 -0.98274 1.869111	-1.43907 0.982065 Z 0.699318 0.363167 1.283225 -0.75399	H Atom C C C H	0.312081 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472	Y 0.792266 -0.5744 -1.52559 1.912885	-1.14390 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609
C Confor Atom C C C N C	2.237823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143	-1.21148 -1.21148 Y -0.91851 0.376624 -0.98274 1.869111 1.814037	Z 0.699318 0.363167 1.283225 -0.75399 0.638028	H Atom C C C H H	0.312081 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386	•1.23902 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223	-1.14390 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609 0.0928
C Confor Atom C C C N C C	2.237823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548	Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522	-1.43907 0.982065 Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781	H Atom C C C H H H	0.312081 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991	Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106	-2.43286 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141
C Confor Atom C C C N C C C C	2.237823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921	Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709	Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128	H H C C C H H H H	0.312081 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087	Y 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233	-1.14390 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984
C Confor Atom C C C C C C C C C	2.297823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035	I.049408 -1.21148 Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.37146	Z 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263	н Н С С С Н Н Н Н Н Н	0.312081 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087 3.549202	Y 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117	-1.14390 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562
C Confor Atom C C C C C C C C C C	2.237823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035 2.909045	Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.37146 -0.05766	Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263 -0.56129	н Н С С С Н Н Н Н Н Н Н	0.312081 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087 3.549202 3.118421	Y 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117 1.571172	-1.14390 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562 -1.95996
NCAtomCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	2.297823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035 2.909045 2.845742	I.049408 -1.21148 Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.37146 -0.05766 1.417285	Z 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263 -0.56129 -0.91053	н Н Аtom С С С Н Н Н Н Н Н Н Н	0.312081 4.872413 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087 3.549202 3.118421 2.143673	Y 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117 1.571172 -0.06358	Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562 -1.95996 3.413472
NCConforAtomCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	2.297823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035 2.909045 2.845742 1.913946	Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.37146 -0.05766 1.417285 0.850689	-1.43907 0.982065 Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263 -0.56129 -0.91053 1.476005	н Н С С С Н Н Н Н Н Н Н Н Н Н	0.312081 4.872413 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087 3.549202 3.118421 2.143673 0.94248	Y 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117 1.571172 -0.06358 1.241393	-1.14390 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562 -1.95996 3.413472 3.399373
NCConforAtomCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	2.297823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035 2.909045 2.845742 1.913946 1.335681	Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.05766 1.417285 0.850689 0.393304	-1.43907 0.982065 Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263 -0.56129 -0.91053 1.476005 2.823547	н Н С С С Н Н Н Н Н Н Н Н Н Н	0.312081 4.872413 4.872413 X -4.99989 -5.34469 -0.91472 -1.04386 1.982991 1.575087 3.549202 3.118421 2.143673 0.94248 3.680289	Y 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117 1.571172 -0.06358 1.241393 -0.4762	Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562 -1.95996 3.413472 3.399373 -2.5046
NCConforAtomCCCCCCCCCCCCO	2.297823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035 2.909045 2.845742 1.913946 1.335681 0.273466	I.049408 -1.21148 Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.37146 -0.05766 1.417285 0.850689 0.393304 -0.55963	-1.43907 0.982065 Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263 -0.56129 -0.91053 1.476005 2.823547 2.653634	н Н Аtom С С Н Н Н Н Н Н Н Н Н Н Н Н	0.312081 4.872413 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087 3.549202 3.118421 2.143673 0.94248 3.680289 4.415479	Y 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117 1.571172 -0.06358 1.241393 -0.4762 -2.80512	Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562 -1.95996 3.413472 3.399373 -2.5046 -2.11121
NCConforAtomCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	2.297823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035 2.909045 2.845742 1.913946 1.335681 0.273466 3.243384	Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.37146 -0.05766 1.417285 0.850689 0.393304 -0.55963 -1.04785	-1.43907 0.982065 Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263 -0.56129 -0.91053 1.476005 2.823547 2.653634 -1.66972	н Н Аtom С С С Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н Н	0.312081 4.872413 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087 3.549202 3.118421 2.143673 0.94248 3.680289 4.415479 5.206511	Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117 1.571172 -0.06358 1.241393 -0.4762 -2.80512 -1.66633	-1.14390 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562 -1.95996 3.413472 3.399373 -2.5046 -2.11121 -0.99538
NCConforAtomCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	2.297823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035 2.909045 2.845742 1.913946 1.335681 0.273466 3.243384 4.250122	I.049408 -1.21148 Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.37146 -0.05766 1.417285 0.850689 0.393304 -0.55963 -1.04785 -2.12345	-1.43907 0.982065 Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263 -0.56129 -0.91053 1.476005 2.823547 2.653634 -1.66972 -1.27029	н H Atom С С Н H H H H H H H H H H H H H	0.312081 4.872413 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087 3.549202 3.118421 2.143673 0.94248 3.680289 4.415479 5.206511 3.890802	-1.23902 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117 1.5771172 -0.06358 1.241393 -0.4762 -2.80512 -1.66633 -2.70727	-1.14390 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562 -1.95996 3.413472 3.399373 -2.5046 -2.11121 -0.99538 -0.41781
NCConforAtomCCCCCCCCCCCCCCCCCCCCCCCCCCCCH	2.297823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035 2.909045 2.845742 1.913946 1.335681 0.273466 3.243384 4.250122 0.482922	Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.37146 -0.05766 1.417285 0.850689 0.393304 -0.55963 -1.04785 -2.12345 -0.11139	-1.43907 0.982065 Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263 -0.56129 -0.91053 1.476005 2.823547 2.653634 -1.66972 -1.27029 0.717492	н H Atom С С Н H H H H H H H H H H H H H	0.312081 4.872413 -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087 3.549202 3.118421 2.143673 0.94248 3.680289 4.415479 5.206511 3.890802 1.799688	-1.23902 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117 1.571172 -0.06358 1.241393 -0.4762 -2.80512 -1.66633 -2.70727 3.985586	-2.43286 -2.43286 Z -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562 -1.95996 3.413472 3.399373 -2.5046 -2.11121 -0.99538 -0.41781 -0.87637
NCConforAtomCCCCCCCCCCCCCCCCCCCCCCCCCHH	2.297823 3.645104 mation 3 X -1.10298 -1.47 0.265746 1.439849 0.947143 -0.65548 1.608921 2.366035 2.909045 2.845742 1.913946 1.335681 0.273466 3.243384 4.250122 0.482922 2.797447	I.049408 -1.21148 Y -0.91851 0.376624 -0.98274 1.869111 1.814037 1.638522 -1.68709 -0.37146 -0.05766 1.417285 0.850689 0.393304 -0.55963 -1.04785 -2.12345 -0.11139 1.458415	-1.43907 0.982065 Z 0.699318 0.363167 1.283225 -0.75399 0.638028 0.70781 0.952128 0.628263 -0.56129 -0.91053 1.476005 2.823547 2.653634 -1.66972 -1.27029 0.717492 1.706798	н H Atom С С Н H H H H H H H H H H H H H	0.312081 4.872413 4.872413 X -4.99989 -5.34469 -4.44996 -0.91472 -1.04386 1.982991 1.575087 3.549202 3.118421 2.143673 0.94248 3.680289 4.415479 5.206511 3.890802 1.799688 0.16964	-1.23902 0.305121 Y 0.792266 -0.5744 -1.52559 1.912885 2.458223 -2.25106 -2.33233 2.033117 1.5771172 -0.06358 1.241393 -0.4762 -2.80512 -1.66633 -2.70727 3.985586 3.442559	-1.14390 -2.43286 -2.43286 -2.43286 -1.03733 -0.99311 -0.51676 1.740609 0.0928 1.813141 0.073984 -0.31562 -1.95996 3.413472 3.399373 -2.5046 -2.11121 -0.99538 -0.41781 -0.87637 -1.33759

С	1.229353	3.173221	-1.36876	Н	1.369775	-1.06616	-2.23754
0	2.072037	-1.73228	-2.15339	Н	-2.09618	-2.79591	0.549148
С	-3.19873	-1.08004	-0.07967	Н	-3.50439	2.289817	-0.64821
С	-2.82038	0.297735	-0.12575	Н	-5.72411	1.510563	-1.41226
N	-2.13723	-1.79366	0.447801	Н	-6.32679	-0.88968	-1.33474
С	-3.75453	1.232464	-0.60922	Н	-4.71682	-2.57885	-0.47911

Table S5 DP4+ probability of 13 C NMR chemical shift of compound 1.

Functional	Solvent?		Basis Set		Type of Data		
mP V 1P V 91	P(6-311G (d, p)		6-311G(d,p) Shielding Tenso		g Tensors
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6	
sDP4+ (H data)	-	-	1	1	-	-	
sDP4+ (C data)	d100.00%	ⅆ 0.00%	1	1	-	-	
sDP4+ (all data)	d 100.00%	d 0. 00 %	Ι	Ι	Ι	-	
uDP4+ (H data)	-	-	-	-	-	-	
uDP4+ (C data)	d 100.00%	d 0. 00 %	I	Ι	-	-	
uDP4+ (all data)	📶 00. 00 %	d 0. 00 %	I	Ι	-	-	
DP4+ (H data)	-	-	-	-	-	-	
DP4+ (C data)	d 100.00%	1 0.00%	_	_	_	_	
DP4+ (all data)	d 100.00%	1 0.00%	_	_	_	_	