Supporting information for

Tropolone-Isobutylamine Complex: A Hydrogen-Bonded Troponoid without Dominant π-π Interactions

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Table S1 Atomic coordinates (in $\text{Å} \times 10^4$) and equivalent isotropic displacement parameters (in $\text{Å}^2 \times 10^3$) are presented for the heavy (non-hydrogen) atoms of TrOH·iBA as deduced from X-ray crystallographic analyses, where $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	*x*	*y*	*z*	$U(\text{eq})$
O_1	4232(1)	3940(1)	5768(1)	35(1)
O_2	807(1)	4708(1)	6224(1)	28(1)
N_1	7805(2)	3976(1)	5113(1)	26(1)
C_1	3744(2)	3312(1)	6352(1)	26(1)
C_2	5110(2)	2330(1)	6725(1)	31(1)
C_3	4945(2)	1468(1)	7341(1)	33(1)
C_4	3332(2)	1296(1)	7770(1)	34(1)
C_5	1501(2)	2021(1)	7692(1)	34(1)
C_6	834(2)	3081(1)	7195(1)	30(1)
C_7	1736(2)	3720(1)	6597(1)	24(1)
C_8	8700(2)	2631(1)	4890(1)	28(1)
C_9	7512(2)	1970(1)	4204(1)	32(1)
C_{10}	8596(2)	619(1)	4015(1)	43(1)
C_{11}	5289(2)	1698(1)	4326(1)	42(1)

Table S2 Bond lengths (in Å) and bond angles (in deg.) are tabulated for TrOH·iBA as deduced from X-ray crystallographic analyses.

Coordinate	Bond Length
O_1-C_1	1.2710(14)
O_2-C_7	1.2737(13)
N_1-C_8	1.4848(14)
N_1-H_{1a}	0.938(16)
N_1-H_{1b}	1.001(17)
N_1-H_{1c}	0.956(17)
C_1-C_2	1.4161(16)
C_1-C_7	1.4863(16)
C_2-C_3	1.3856(18)
C_2-H_2	0.9500
C_3-C_4	1.3822(19)
C_3-H_3	0.9500
C_4-C_5	1.3835(18)
C_4-H_4	0.9500
C_5-C_6	1.3868(17)
C_5-H_5	0.9500
C_6-C_7	1.4125(17)
C_6-H_6	0.9500
C_8-C_9	1.5187(16)
C_8-H_{8a}	0.9900
C_8-H_{8b}	0.9900
C_9-C_{11}	1.5231(18)
C_9-C_{10}	1.5287(18)
C_9-H_9	1.0000
C_{10}-H_{10a}	0.9800
C_{10}-H_{10b}	0.9800
C_{10}-H_{10c}	0.9800
C_{11}-H_{11a}	0.9800
C_{11}-H_{11b}	0.9800
C_{11}-H_{11c}	0.9800

Coordinate	Bond Angle
C_8-N_1-H_{1a}	109.3(9)
C_8-N_1-H_{1b}	113.3(9)
H_{1a}-N_1-H_{1b}	104.2(13)
C_8-N_1-H_{1c}	110.8(10)
H_{1a}-N_1-H_{1c}	108.7(13)
H_{1b}-N_1-H_{1c}	110.3(13)
O_1-C_1-C_2	119.77(11)
O_1-C_1-C_7	115.17(10)
C_2-C_1-C_7	125.04(10)
C_3-C_2-C_1	131.92(12)
C_3-C_2-H_2	114.0
C_1-C_2-H_2	114.0
C_4-C_3-C_2	129.69(12)
C_4-C_3-H_3	115.2
C_2-C_3-H_3	115.2
C_3-C_4-C_5	126.53(12)
C_3-C_4-H_4	116.7
C_5-C_4-H_4	116.7
C_4-C_5-C_6	130.04(12)
C_4-C_5-H_5	115.0
C_6-C_5-H_5	115.0
C_5-C_6-C_7	131.98(12)
C_5-C_6-H_6	114.0
C_7-C_6-H_6	114.0
O_2-C_7-C_6	119.88(11)
O_2-C_7-C_1	115.65(10)
C_6-C_7-C_1	124.47(10)
N_1-C_8-C_9	113.05(9)
N_1-C_8-H_{8a}	109.0
C_9-C_8-H_{8a}	109.0

Coordinate	Bond Angle
N_1-C_8-H_{8b}	109.0
C_9-C_8-H_{8b}	109.0
H_{8a}-C_8-H_{8b}	107.8
C_8-C_9-C_{11}	112.12(11)
C_8-C_9-C_{10}	108.44(10)
C_{11}-C_9-C_{10}	111.37(11)
C_8-C_9-H_9	108.3
C_{11}-C_9-H_9	108.3
C_{10}-C_9-H_9	108.3
C_9-C_{10}-H_{10a}	109.5
C_9-C_{10}-H_{10b}	109.5
H_{10a}-C_{10}-H_{10b}	109.5
C_9-C_{10}-H_{10c}	109.5
H_{10a}-C_{10}-H_{10c}	109.5
H_{10b}-C_{10}-H_{10c}	109.5
C_9-C_{11}-H_{11a}	109.5
C_9-C_{11}-H_{11b}	109.5
H_{11a}-C_{11}-H_{11b}	109.5
C_9-C_{11}-H_{11c}	109.5
H_{11a}-C_{11}-H_{11c}	109.5
H_{11b}-C_{11}-H_{11c}	109.5

Table S3 Anisotropic displacement parameters (in $\text{Å}^2 \times 10^3$) are presented for TrOH·iBA as deduced from X-ray crystallographic analyses, where the exponent for the anisotropic displacement factor takes the form $-2\pi^2\left(h^2a^{*2}U^{11}+\ldots+2hka^*b^*U^{12}\right)$.

atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O_1	34(1)	35(1)	36(1)	12(1)	12(1)	6(1)
O_2	32(1)	25(1)	27(1)	0(1)	3(1)	4(1)
N_1	29(1)	23(1)	27(1)	2(1)	3(1)	2(1)
C_1	30(1)	23(1)	26(1)	0(1)	3(1)	-2(1)
C_2	30(1)	30(1)	34(1)	2(1)	2(1)	2(1)
C_3	39(1)	27(1)	32(1)	2(1)	-5(1)	3(1)
C_4	51(1)	26(1)	25(1)	4(1)	0(1)	-1(1)
C_5	47(1)	30(1)	26(1)	1(1)	10(1)	-5(1)
C_6	33(1)	29(1)	29(1)	-1(1)	7(1)	0(1)
C_7	30(1)	20(1)	22(1)	-4(1)	1(1)	-2(1)
C_8	32(1)	24(1)	30(1)	0(1)	1(1)	3(1)
C_9	38(1)	27(1)	28(1)	3(1)	-1(1)	-2(1)
C_{10}	55(1)	34(1)	40(1)	-8(1)	-1(1)	1(1)
C_{11}	40(1)	36(1)	47(1)	5(1)	-3(1)	-8(1)

Table S4 Hydrogen coordinates (in in $\text{Å} \times 10^4$) and isotropic displacement parameters (in $\text{Å}^2 \times 10^3$) are tabulated for TrOH·iBA as deduced from X-ray crystallographic analyses.

atom	x	y	z	$U(\text{eq})$
H_{1a}	8680(20)	4389(15)	5499(9)	43(4)
H_{1b}	6490(30)	3858(16)	5340(9)	54(5)
H_{1c}	7630(20)	4608(17)	4696(9)	50(4)
H_2	6373	2246	6515	37
H_3	6116	914	7490	40
H_4	3497	611	8158	41
H_5	553	1750	8032	41
H_6	-473	3445	7270	36
H_{8a}	8741	1968	5317	34
H_{8b}	10125	2797	4780	34
H_9	7539	2628	3769	38
H_{10a}	10035	820	3962	65
H_{10b}	7939	233	3541	65
H_{10c}	8511	-63	4421	65
H_{11a}	5232	1124	4778	62
H_{11b}	4609	1202	3888	62
H_{11c}	4595	2591	4389	62

Table S5 Torsion angles (in deg.) are compiled for TrOH·iBA as deduced from X-ray crystallographic analyses.

Dihedral Coordinate	Torsion Angle
O_1-C_1-C_2-C_3	-177.01(12)
C_7-C_1-C_2-C_3	4.6(2)
C_1-C_2-C_3-C_4	1.5(2)
C_2-C_3-C_4-C_5	-3.1(2)
C_3-C_4-C_5-C_6	-1.2(2)
C_4-C_5-C_6-C_7	3.0(2)
C_5-C_6-C_7-O_2	-178.90(12)
C_5-C_6-C_7-C_1	1.8(2)
O_1-C_1-C_7-O_2	-4.22(14)
C_2-C_1-C_7-O_2	174.21(10)
O_1-C_1-C_7-C_6	175.13(10)
C_2-C_1-C_7-C_6	-6.45(18)
N_1-C_8-C_9-C_{11}	-57.99(13)
N_1-C_8-C_9-C_{10}	178.63(10)

Table S6 Cartesian coordinates (in Å) are tabulated for the minimum-energy (equilibrium) geometries predicted by M06-2X/apVDZ quantum-chemical calculations performed on the core quad complex for TrOH·iBA (*cf.*, Fig. 4), with the independent results obtained for fully-relaxed and $\bar{1}$–constrained optimization procedures being presented.

		M06-2X/apVDZ; Fully Relaxed			**M06-2X/apVDZ; $\bar{1}$ Constrained**		
	Atom	***x***	***y***	***z***	***x***	***y***	***z***
Tropolone Monomer 1	O	-1.582549	1.031682	0.704217	0.767481	0.451021	1.752034
	O	-2.526775	1.622997	-1.664434	-1.484233	1.332229	2.746356
	C	-2.810799	0.731641	0.487114	0.528417	0.148732	2.977584
	C	-3.553627	0.107828	1.50142	1.453638	-0.634687	3.682493
	H	-2.983416	-0.003303	2.426284	2.33208	-0.881941	3.083301
	C	-4.869967	-0.381405	1.543422	1.457586	-1.135881	4.994163
	H	-5.152627	-0.83225	2.496824	2.340462	-1.725873	5.247654
	C	-5.850239	-0.375865	0.574022	0.526407	-0.994616	6.001779
	H	-6.810153	-0.819777	0.832566	0.744048	-1.477298	6.953117
	C	-5.729202	0.164896	-0.722798	-0.68275	-0.276087	5.916444
	H	-6.624292	0.08105	-1.342761	-1.286575	-0.278408	6.826344
	C	-3.553627	0.107828	1.50142	-0.774177	0.670013	3.522889
	C	-4.665262	0.783839	-1.334215	-1.227877	0.428923	4.869136
	H	-4.820181	1.11882	-2.360312	-2.193042	0.902682	5.050989
Isobutylamine Monomer 1	N	-0.326802	-1.347557	1.428749	0.985395	-1.560687	-0.086639
	H	-0.431648	-1.255135	2.438367	1.906346	-1.563153	-0.523399
	H	-0.740152	-0.48367	1.019188	0.979149	-0.880644	0.708249
	H	0.735689	-1.4004	1.231265	0.347854	-1.179034	-0.857545
	C	-0.986023	-2.59347	0.954072	0.560004	-2.930498	0.297316
	H	-2.058326	-2.524921	1.179254	1.033679	-3.187903	1.253552
	H	-0.549838	-3.418826	1.528393	0.927343	-3.61196	-0.477272
	C	-0.765829	-2.815307	-0.538082	-0.958689	-3.028274	0.404079
	H	0.315356	-2.763117	-0.723061	-1.368378	-2.781847	-0.585504
	C	-1.455792	-1.738334	-1.371151	-1.518311	-2.037745	1.422652
	H	-1.073781	-0.737843	-1.144093	-1.311963	-0.997912	1.144262
	H	-1.284981	-1.916211	-2.438799	-2.605706	-2.145538	1.502426
	H	-2.541045	-1.746951	-1.193595	-1.08497	-2.214175	2.417859
	C	-1.277451	-4.206419	-0.908058	-1.341543	-4.462682	0.760678
	H	-1.121596	-4.398207	-1.975903	-2.431725	-4.570776	0.793844
	H	-0.759246	-4.990278	-0.341556	-0.950233	-5.178309	0.02669
	H	-2.354863	-4.288709	-0.706124	-0.946251	-4.732081	1.750073

Table S6 (continued).

		M06-2X/apVDZ; Fully Relaxed		M06-2X/apVDZ; $\bar{1}$ Constrained		
	Atom	*x*	*y*	*x*	*y*	*x*	*y*
Tropolone Monomer 2	O	1.453916	-0.492115	-0.720643	-0.767481	-0.451021	-1.752034
	O	2.23573	-1.759929	1.407116	1.484233	-1.332229	-2.746356
	C	2.706775	-0.562983	-0.557702	-0.528417	-0.148732	-2.977584
	C	3.582407	0.055569	-1.485601	-1.453638	0.634687	-3.682493
	H	3.042111	0.538439	-2.302296	-2.33208	0.881941	-3.083301
	C	4.970878	0.137581	-1.550454	-1.457586	1.135881	-4.994163
	H	5.351099	0.695415	-2.408612	-2.340462	1.725873	-5.247654
	C	5.940626	-0.384054	-0.7026	-0.526407	0.994616	-6.001779
	H	6.980709	-0.194626	-0.96231	-0.744048	1.477298	-6.953117
	C	5.701363	-1.134942	0.451336	0.68275	0.276087	-5.916444
	H	6.595246	-1.462164	0.986392	1.286575	0.278408	-6.826344
	C	3.149941	-1.308929	0.667563	0.774177	-0.670013	-3.522889
	C	4.508217	-1.528989	1.034793	1.227877	-0.428923	-4.869136
	H	4.589082	-2.109061	1.954322	2.193042	-0.902682	-5.050989
Isobutylamine Monomer 2	N	0.160119	1.81081	-1.130132	-0.985395	1.560687	0.086639
	H	-0.272936	1.883277	-2.049344	-1.906346	1.563153	0.523399
	H	0.759674	0.944454	-1.093735	-0.979149	0.880644	-0.708249
	H	-0.660751	1.615292	-0.474756	-0.347854	1.179034	0.857545
	C	0.893838	3.040305	-0.742527	-0.560004	2.930498	-0.297316
	H	1.900937	2.998954	-1.178294	-1.033679	3.187903	-1.253552
	H	0.362266	3.896984	-1.170727	-0.927343	3.61196	0.477272
	C	0.974614	3.183775	0.774769	0.958689	3.028274	-0.404079
	H	-0.057038	3.22814	1.151746	1.368378	2.781847	0.585504
	C	1.671848	1.987935	1.420092	1.518311	2.037745	-1.422652
	H	1.740506	2.129428	2.504531	2.605706	2.145538	-1.502426
	H	1.129884	1.054496	1.234402	1.311963	0.997912	-1.144262
	H	2.692168	1.872732	1.026134	1.08497	2.214175	-2.417859
	C	1.688378	4.489886	1.115421	1.341543	4.462682	-0.760678
	H	1.183242	5.354929	0.667256	0.950233	5.178309	-0.02669
	H	1.718224	4.638102	2.201031	2.431725	4.570776	-0.793844
	H	2.72467	4.468713	0.750154	0.946251	4.732081	-1.750073

Table S7 Cartesian coordinates (in Å) are tabulated for the minimum-energy (equilibrium) geometries predicted by M06-2X/apVDZ (CP) quantum-chemical calculations performed on the core quad complex for TrOH·iBA (*cf.*, Fig. 4), with the independent results obtained for fully-relaxed and $\bar{1}$–constrained optimization procedures being presented.

		M06-2X/apVDZ (CP); Fully Relaxed			**M06-2X/apVDZ (CP); $\bar{1}$ Constrained**		
	Atom	***x***	***y***	***z***	***x***	***y***	***z***
Tropolone Monomer 1	O	-1.661796	0.782999	0.765409	0.756574	0.384876	1.797339
	O	-2.699946	1.484386	-1.536989	-1.475578	1.347661	2.768840
	C	-2.866221	0.403668	0.540349	0.518315	0.138469	3.035989
	C	-3.544049	-0.343801	1.517765	1.437397	-0.625762	3.770456
	H	-2.950819	-0.474889	2.425951	2.307734	-0.912510	3.176385
	C	-4.820347	-0.929415	1.543456	1.443252	-1.068694	5.102627
	H	-5.053227	-1.459689	2.469258	2.320964	-1.657638	5.376349
	C	-5.814093	-0.936076	0.587139	0.519006	-0.873580	6.108078
	H	-6.734140	-1.466515	0.827355	0.736250	-1.317771	7.078211
	C	-5.751838	-0.310188	-0.674137	-0.683070	-0.147902	5.996726
	H	-6.644479	-0.427124	-1.292455	-1.284327	-0.106157	6.907471
	C	-3.432219	0.806154	-0.797504	-0.772430	0.701749	3.566409
	C	-4.747520	0.429073	-1.253370	-1.224654	0.518165	4.921999
	H	-4.941988	0.814821	-2.255126	-2.184845	1.009119	5.086667
Isobutylamine Monomer 1	N	-0.162454	-1.497986	1.399842	0.942051	-1.570906	-0.124412
	H	-0.313261	-1.505060	2.407544	1.862321	-1.547516	-0.563456
	H	-0.623550	-0.635728	1.043459	0.938483	-0.945325	0.711485
	H	0.906128	-1.473031	1.231251	0.307634	-1.146701	-0.878329
	C	-0.701469	-2.741735	0.787678	0.523680	-2.964950	0.165278
	H	-1.787613	-2.768655	0.948494	1.051601	-3.307661	1.065218
	H	-0.235792	-3.580011	1.318870	0.839141	-3.575440	-0.688069
	C	-0.375665	-2.819509	-0.700141	-0.986261	-3.066207	0.356535
	H	0.709126	-2.675483	-0.804455	-1.454557	-2.743188	-0.584633
	C	-1.094671	-1.729557	-1.490944	-1.478681	-2.159208	1.482802
	H	-0.800658	-0.728660	-1.156900	-1.311164	-1.096902	1.264706
	H	-0.850856	-1.809021	-2.557235	-2.555245	-2.295790	1.639418
	H	-2.185274	-1.825517	-1.381928	-0.966004	-2.394895	2.427482
	C	-0.749655	-4.208390	-1.214677	-1.355605	-4.524339	0.620712
	H	-0.513604	-4.296914	-2.281586	-2.442910	-4.635295	0.704907
	H	-0.205258	-4.996238	-0.678805	-1.007733	-5.180898	-0.186946
	H	-1.827441	-4.388322	-1.093272	-0.908121	-4.870234	1.563217

Table S7 (continued).

		M06-2X/apVDZ (CP); Fully Relaxed		M06-2X/apVDZ (CP); $\bar{1}$ Constrained		
	Atom	*x*	*y*	*x*	*y*	*x*	*y*
Tropolone Monomer 2	O	1.648305	-0.090243	-0.371171	-0.756573	-0.384863	-1.797333
	O	2.394230	-1.939618	1.294061	1.475565	-1.347676	-2.768839
	C	2.895510	-0.284578	-0.296084	-0.518318	-0.138466	-3.035985
	C	3.790608	0.507528	-1.060879	-1.437395	0.625771	-3.770453
	H	3.268205	1.250688	-1.667743	-2.307726	0.912532	-3.176378
	C	5.176658	0.498911	-1.184459	-1.443252	1.068696	-5.102626
	H	5.573101	1.249944	-1.871019	-2.320959	1.657648	-5.376347
	C	6.126991	-0.316732	-0.580246	-0.519014	0.873565	-6.108080
	H	7.169313	-0.141138	-0.841119	-0.736257	1.317753	-7.078215
	C	5.864496	-1.341536	0.331345	0.683055	0.147874	-5.996730
	H	6.743809	-1.876078	0.696886	1.284307	0.106117	-6.907479
	C	3.317523	-1.370397	0.652105	0.772419	-0.701763	-3.566409
	C	4.662801	-1.788564	0.857720	1.224638	-0.518192	-4.922003
	H	4.724744	-2.608815	1.574009	2.184822	-1.009158	-5.086672
Isobutylamine Monomer 2	N	-0.057334	1.886718	-1.028956	-0.942046	1.570918	0.124417
	H	-0.455448	1.708760	-1.950589	-1.862316	1.547530	0.563463
	H	0.783535	1.278833	-0.883439	-0.938482	0.945336	-0.711480
	H	-0.810730	1.518454	-0.361577	-0.307630	1.146712	0.878334
	C	0.165291	3.333789	-0.810170	-0.523673	2.964961	-0.165276
	H	1.031862	3.652394	-1.405588	-1.051595	3.307672	-1.065215
	H	-0.726905	3.853166	-1.177786	-0.839131	3.575453	0.688071
	C	0.388662	3.642971	0.666364	0.986267	3.066214	-0.356537
	H	-0.514837	3.320767	1.204717	1.454565	2.743196	0.584631
	C	1.588185	2.879712	1.225718	1.478684	2.159213	-1.482804
	H	1.764022	3.160840	2.271014	2.555247	2.295794	-1.639423
	H	1.438485	1.793787	1.189584	1.311167	1.096908	-1.264705
	H	2.498630	3.117208	0.655324	0.966005	2.394900	-2.427482
	C	0.559378	5.150371	0.840716	1.355615	4.524345	-0.620715
	H	-0.302874	5.702338	0.445523	1.007745	5.180906	0.186942
	H	0.669075	5.404416	1.901485	2.442920	4.635299	-0.704912
	H	1.460746	5.498968	0.316729	0.908130	4.870239	-1.563221

Table S8 Cartesian coordinates (in Å) are tabulated for the minimum-energy geometry predicted by M06-2X/apVDZ (PCB) quantum-chemical calculations performed on the TrOH·iBA unit cell, with the crystalline lattice specified by translation vectors $\mathbf{v}_1 \equiv (7.09112, 0, 0)$, $\mathbf{v}_2 \equiv (0.000675, 10.06927, 0)$, and $\mathbf{v}_3 \equiv (-1.92403, -0.00043, 17.90432)$.

Atom	x	y	z	x	y	z	Atom
O	-0.47356768	-0.82601071	0.95318834	-3.52781835	-2.21630726	-0.94338282	H
O	-2.9703983	-0.31040846	1.38458838	1.71788148	-2.95246456	-1.79093174	C
C	-1.01344935	-1.49282862	1.89049368	1.73349389	-2.21038742	-2.60844248	H
C	-0.25188759	-2.45117383	2.6060632	2.41311256	-4.22114378	-2.27200327	C
H	0.78201138	-2.51089638	2.25246092	-3.63856938	-4.0241037	-2.57966739	H
C	-0.57345027	-3.32233345	3.64044671	1.8874397	-4.65850208	-3.13327909	H
H	0.25254718	-3.96077599	3.97043539	2.43752252	5.08281048	-1.47731511	H
C	-1.77986896	-3.51086753	4.30969248	0.26636149	-3.22332342	-1.41024537	C
H	-1.79085755	-4.26094944	5.1029921	0.20863911	-3.94815189	-0.58100509	H
C	-2.96708186	-2.82078462	4.06681366	-0.28485142	-3.6403769	-2.26675576	H
H	-3.80934532	-3.11480451	4.70202208	-0.25641222	-2.31058194	-1.08746654	H
C	-3.2459008	-1.8185851	3.14413496	-2.62798015	4.008767	8.01897747	N
H	2.8261454	-1.41969068	3.17414803	-3.31543367	4.41447527	7.34102647	H
C	-2.45751256	-1.18916033	2.14179794	-1.6876244	3.97808394	7.55210032	H
O	-0.1366343	4.20911515	6.84375166	-0.61978079	4.64489401	-9.05506001	H
O	2.36053395	4.72271891	6.41250151	-1.19890143	2.68420652	-9.46407648	C
C	0.40265532	3.54198707	5.9063648	-3.11301008	2.01718942	7.56153084	H
C	-0.35965344	2.58424627	5.19075773	-2.24760127	2.81705645	-9.16259842	H
H	-1.39356079	2.52520382	5.54444099	-0.40121544	2.08258976	-8.31568021	C
C	-0.03881267	1.71301288	4.15622617	-0.41694659	2.82487962	-7.49836465	H
H	-0.86527946	1.07515342	3.82626747	-1.09528726	0.81352998	-7.83395262	C
C	1.16738899	1.52382196	3.48675814	-2.13471838	1.00985089	-7.5258511	H
H	1.17774041	0.77385587	2.69333056	-0.56887485	0.37679028	-6.97281437	H
C	2.35507869	2.21311506	3.72954187	-1.11883178	0.04798872	-8.62842301	H
H	3.19702822	1.91867695	3.09410137	1.05033537	1.81266563	-8.69693526	C
C	2.63472218	3.21492655	4.65240489	1.10822132	1.0876991	-9.52604507	H
H	-3.43706518	3.61313213	4.6223227	1.60218863	1.39618311	-7.84056107	H
C	1.84694437	3.84458277	5.65505177	1.57231855	2.72570315	-9.0201253	H
O	0.82688862	0.66356653	-2.10821508	-1.66503932	0.86287238	-0.93350381	N

Table S8 (continued).

Atom	x	y	z	x	y	z	Atom
O	3.32372423	0.14804229	-2.53966913	-2.35209061	0.45641365	-1.61142983	H
C	1.36672628	1.33039145	-3.04553842	-0.7246449	0.89419432	-1.40021343	H
C	0.60511152	2.28870366	-3.76110194	-1.58053416	0.22743864	-0.1030111	H
H	-0.42878345	2.34838821	-3.40747566	-2.16123126	2.18760715	-0.51284768	C
C	0.9266132	3.15986927	-4.79550245	-2.15134804	2.8539478	-1.39175501	H
H	0.10058075	3.79828181	-5.12547113	-3.20998472	2.05400608	-0.21189792	H
C	2.13301489	3.34844635	-5.46476922	-1.36462155	2.79012939	0.635802	C
H	2.14397949	4.09852526	-6.25807484	-1.38035995	2.04810924	1.45335974	H
C	3.32026679	2.65842845	-5.2218874	-2.05983463	4.0588776	1.11671453	C
H	4.16250925	2.95249233	-5.85710382	-3.09933469	3.86193452	1.42420465	H
C	3.59915074	1.65625493	-4.2991977	-1.53427477	4.4962219	1.97806435	H
H	4.61824454	1.25742551	-4.32920377	-2.08337513	4.82416735	0.32199737	H
C	2.81079749	1.02677715	-3.29686469	0.08695344	3.06088325	0.25525163	C
O	0.48873323	-4.37150533	-7.99924639	0.14480682	3.78563272	-0.57404866	H
O	-2.00840201	-4.88503409	-7.56765023	0.63809036	3.47798572	1.11178502	H
C	-0.05038239	-3.70444724	-7.06171253	0.60971715	2.14808776	-0.0673832	H
C	0.71211137	-2.74687045	-6.34608346	1.05607825	-4.17162292	8.73007298	N
H	1.74599072	-2.687908	-6.69986772	1.74341478	-4.5773942	9.40809098	H
C	0.3914876	-1.87569406	-5.31142991	0.1156395	-4.14097186	9.19680613	H
H	1.21807339	-1.2379776	-4.98148521	0.97207072	-4.80722019	7.89970228	H
C	-0.81463206	-1.68640314	-4.64184288	1.55116236	-2.8466007	8.30906275	C
H	-0.82483047	-0.93649005	-3.8483593	1.54105519	-2.18011235	9.1878526	H
C	-2.00243676	-2.37552524	-4.88459461	2.59993021	-2.97944963	8.00781869	H
H	-2.84429729	-2.08101613	-4.24906811	0.75375137	-2.24482294	7.16056448	C
C	-2.28228125	-3.37724473	-5.80749662	0.76957452	-2.9870388	6.34318592	H
H	-3.30166089	-3.77531331	-5.77736343	1.4480322	-0.97578516	6.67907989	C
C	-1.49466644	-4.00696095	-6.8102445	2.48749531	-1.17218307	6.37113537	H
N	2.01836626	-1.02528055	-0.22155793	0.92181078	-0.53890546	5.81789863	H
H	2.70543254	-0.61882883	0.45636009	1.47152171	-0.2103269	7.47363228	H
H	1.07799283	-1.05665549	0.24518468	-0.69784144	-1.97481381	7.54159253	C
H	1.93379209	-0.38980582	-1.05201464	-0.75580139	-1.24996827	8.37080334	H
C	2.51457919	-2.34997133	-0.64232706	-1.24950871	-1.55815829	6.68518434	H
H	2.50481097	-3.01635897	0.23654427	-1.21996362	-2.88785132	7.86455857	H