

Structural Studies on Ethyl Isovalerate by Microwave Spectroscopy and Quantum Chemical Calculations

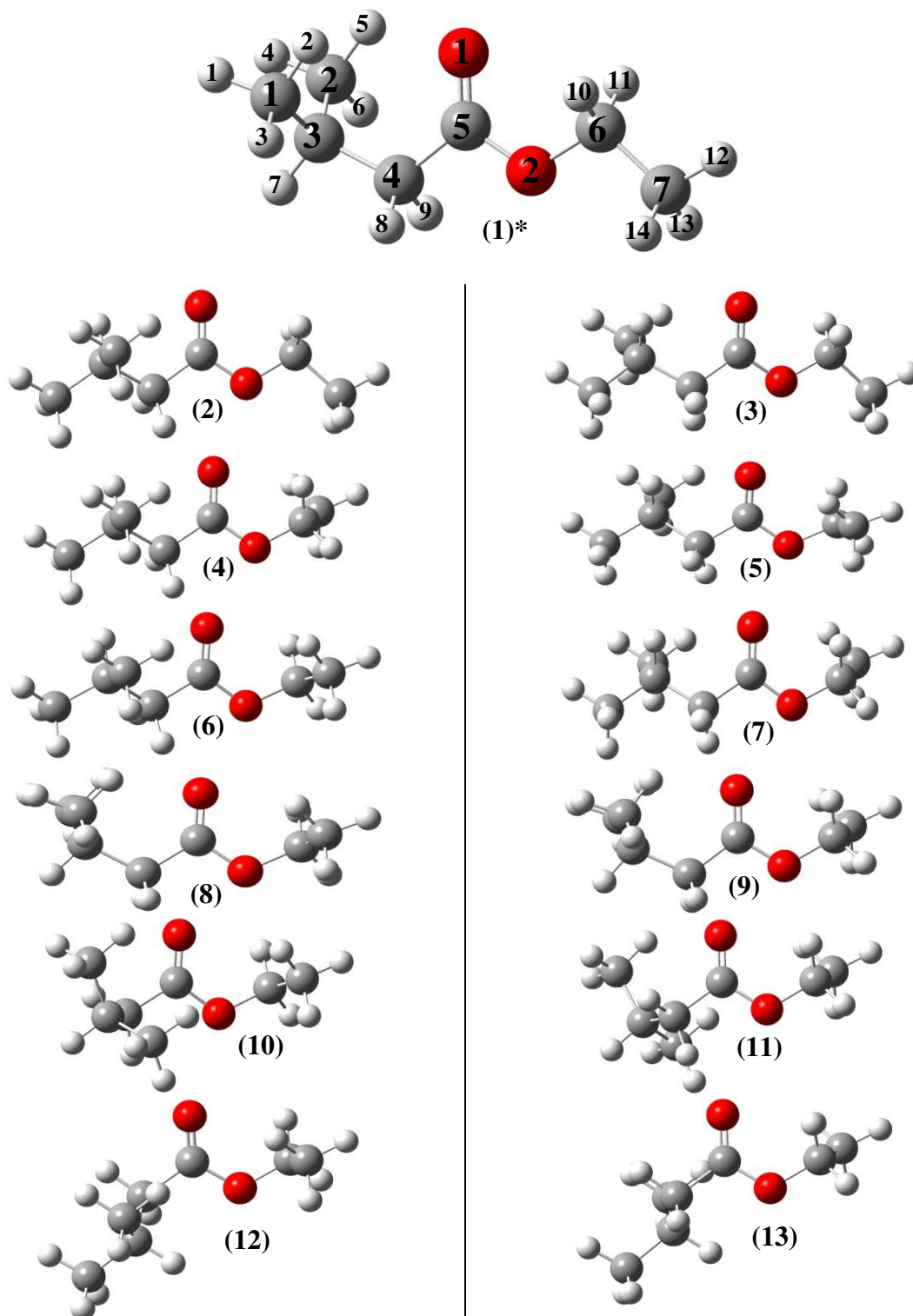
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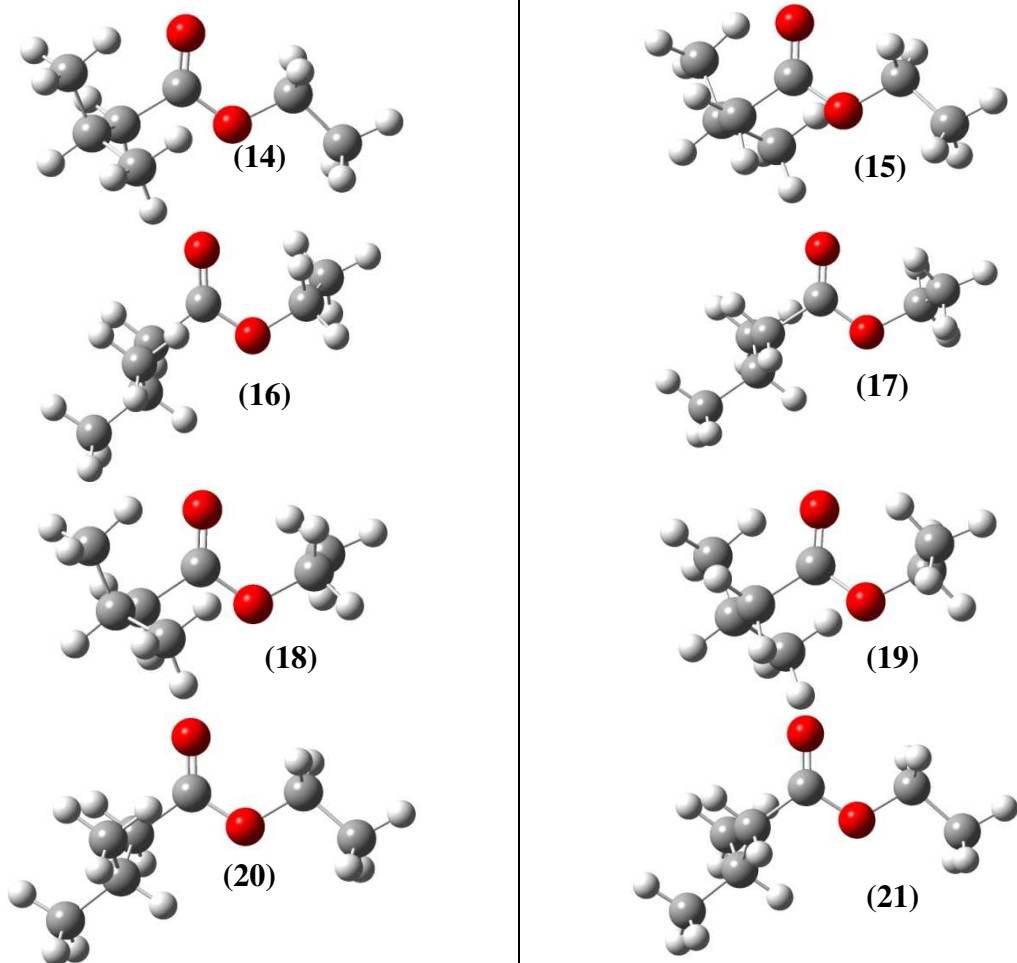
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SUPPORTING INFORMATION

Supporting Information 1: Conformers of ethyl isovalerate optimized at B3LYP/6-311++G** level. Conformer 1 has C_s symmetry, while the other conformers have C_1 symmetry and appear as enantiomeric pairs. They are referred to as conformer 2/3, conformer 4/5, etc. throughout the text.





*Note: The optimized structure of conformer 1 does not have full C_s symmetry. However, by enforcing full C_s symmetry an energy value which is only 16 J/mol lower than without enforcing C_s symmetry was obtained.

Supporting Information 2: Frequency list of the observed conformer of ethyl isovalerate.

Upper level			Lower level			Frequency [GHz]	obs-calc. ^a
J	K _a	K _c	J	K _a	K _c		
2	2	1	1	1	0	12.6897563	-3.3
2	2	0	1	1	1	12.7223439	1.0
3	0	3	2	0	2	3.9917569	0.2
2	2	0	2	1	1	9.9958418	-3.5
4	0	4	3	0	3	5.3212411	0.7
3	2	2	3	1	2	9.9472269	-2.6
3	2	1	3	1	2	9.9483988	-1.4
5	0	5	4	0	4	6.6497816	0.4
5	1	4	4	0	4	10.2470526	3.6
4	2	3	4	1	3	9.8828104	-1.5
4	2	2	4	1	3	9.8863233	-0.2
5	2	3	4	1	3	16.5449469	1.0
4	2	3	4	1	4	10.2063230	6.9
4	2	2	4	1	4	10.2098334	5.6
6	0	6	5	0	5	7.9771470	0.2
6	1	6	5	0	5	10.9984317	-3.3
6	1	5	5	0	5	11.6777722	0.7
6	1	5	5	1	4	8.0805035	-0.2
5	2	4	5	1	4	9.8024411	1.4
5	2	3	5	1	4	9.8106311	-0.3
5	2	4	5	1	5	10.2876964	2.3
5	2	3	5	1	5	10.2958910	5.2
7	0	7	6	0	6	9.3031100	-0.4
7	1	7	6	0	6	12.2212171	-1.5
7	1	6	6	0	6	13.1269443	4.2
7	1	6	6	1	5	9.4263159	0.5
6	2	5	6	1	5	9.7062140	-4.8
6	2	4	6	1	5	9.7225963	1.9
7	1	7	6	1	6	9.1999307	0.3
6	2	5	6	1	6	10.3855604	5.1
8	0	8	7	0	7	10.6274540	0.3
7	2	6	7	1	6	9.5942835	1.3
7	2	5	7	1	6	9.6237344	-0.6
8	1	7	7	1	6	10.7716778	-0.7
7	2	6	7	1	7	10.5000040	0.3
8	1	8	7	1	7	10.5130401	-0.4
7	2	5	7	1	7	10.5294552	-1.4
8	2	6	7	2	5	10.6637657	0.0
8	2	7	7	2	6	10.6441900	0.3

^a Obs-Calc is the observed-minus-calculated frequency in kHz.

Upper level			Lower level		
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J	K _a	K _c	J	K _a	K _c	Frequency [GHz]	obs-calc. ^a
8	3	6	7	3	5	10.6497144	0.0
8	4	4	7	4	3	10.6486604	-1.5
8	3	5	7	3	4	10.6499801	-0.6
8	5	4	7	5	3	10.6481355	-2.5
8	6	3	7	6	2	10.6478500	1.7
9	0	9	8	0	8	11.9499726	0.6
8	2	6	8	1	7	9.5158234	1.2
9	1	8	8	1	7	12.1165176	-0.1
8	2	7	8	1	8	10.6311527	-0.2
8	2	6	8	1	8	10.6801827	1.0
9	1	9	8	1	8	11.8257054	0.6
9	2	7	8	2	6	12.0015561	-0.8
9	2	8	8	2	7	11.9736747	0.1
9	3	6	8	3	5	11.9820265	-0.2
9	3	7	8	3	6	11.9815387	0.1
9	4	6	8	4	5	11.9800966	0.5
10	0	10	9	0	9	13.2704806	0.2
9	2	7	9	1	8	9.4008633	1.9
10	1	9	9	1	8	13.4607542	1.0
10	0	10	9	1	9	10.5910536	1.0
9	2	8	9	1	9	10.7791236	0.9
9	2	7	9	1	9	10.8560322	-1.6
10	1	10	9	1	9	13.1378811	0.9
10	2	9	9	2	8	13.3027930	0.0
8	4	5	9	3	6	11.4494431	-1.9
10	5	6	9	5	5	13.3106498	-2.9
11	0	11	10	0	10	14.5888203	-0.2
10	2	8	10	1	9	9.2810778	-1.5
11	1	10	10	1	9	14.8042997	-0.7
10	2	9	10	1	10	10.9440327	-2.9
11	0	11	10	1	10	12.0419940	1.2
12	0	12	11	0	11	15.9048687	0.4
11	2	9	11	1	10	9.1588987	-2.9
12	1	11	11	1	10	16.1470689	0.1
11	2	10	11	1	11	11.1260118	-0.5
12	1	12	11	1	11	15.7606131	0.4
13	0	13	12	0	12	17.2185418	0.2
12	2	10	12	1	11	9.0369232	-1.2
13	1	12	12	1	11	17.4889614	-0.5
12	2	11	12	1	12	11.3251682	0.3
13	1	13	12	1	12	17.0711046	-1.2
13	1	12	12	2	10	8.4520358	-1.7
13	1	12	12	2	11	8.6830647	-3.6

^a Obs-Calc is the observed-minus-calculated frequency in kHz.

Upper level	Lower level
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J	K _a	K _c	J	K _a	K _c	Frequency [GHz]	obs-calc. ^a
14	0	14	13	0	13	18.5298053	-0.8
13	2	11	13	1	12	8.9178766	-0.8
14	1	13	13	1	12	18.8298773	0.9
13	2	12	13	1	13	11.5416052	-1.6
14	1	14	13	1	13	18.3809821	-0.1
14	1	13	13	2	11	9.9119998	0.8
14	1	13	13	2	12	10.2253957	-4.3
15	0	15	14	0	14	19.8386806	0.3
14	2	12	14	1	13	8.8045813	-0.9
15	1	14	14	1	13	20.1697027	0.3
14	2	13	14	1	14	11.7754203	1.6
15	1	15	14	1	14	19.6902228	0.5
15	1	14	14	2	13	11.7803064	-1.9
16	0	16	15	0	15	21.1452369	0.1
15	2	13	15	1	14	8.6999028	-2.6
16	1	15	15	1	14	21.5083246	2.2
15	2	14	15	1	15	12.0266735	0.0
16	1	16	15	1	15	20.9988116	0.0
16	1	15	15	2	13	12.8084193	2.2
16	1	15	15	2	14	13.3471554	1.8
17	0	17	16	0	16	22.4496004	0.4
16	2	14	16	1	15	8.6067083	-2.0
16	2	15	16	1	16	12.2954193	2.2
17	1	16	16	2	14	14.2389064	4.4
17	1	16	16	2	15	14.9252095	-1.3
17	2	15	17	1	16	8.5278091	-2.0
17	2	16	17	1	17	12.5816629	-4.0
18	1	17	17	2	16	16.5136594	-1.7
18	2	16	18	1	17	8.4659289	-2.2
18	2	17	18	1	18	12.8854076	-0.2
19	1	18	18	2	17	18.1115858	0.2
19	2	17	19	1	18	8.4236668	-2.9
19	2	18	19	1	19	13.2065933	4.8
20	1	19	19	2	18	19.7179577	-1.3
20	2	18	20	1	19	8.4034779	-2.0
20	2	19	20	1	20	13.5451164	-2.1
21	2	19	21	1	20	8.4076527	-3.1
21	2	20	21	1	21	13.9008623	-3.1
22	2	20	22	1	21	8.4383298	-0.7
23	2	21	23	1	22	8.4974800	-1.6
23	2	22	23	1	23	14.6632584	-0.2
24	2	22	24	1	23	8.5869412	0.6
24	2	23	24	1	24	15.0694158	-0.4

^a Obs-Calc is the observed-minus-calculated frequency in kHz.

Upper level	Lower level
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J	K _a	K _c	J	K _a	K _c	Frequency [GHz]	obs-calc. ^a
25	2	24	25	1	25	15.4918114	-1.2
26	3	24	26	2	25	17.9037141	3.9
27	3	25	27	2	26	18.0714893	3.5

^a Obs-Calc is the observed-minus-calculated frequency in kHz.

Supporting Information 3: Cartesian coordinates of conformer 1 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.041120	1.278471	0.043188
O-2	1.474494	-0.455419	-0.026441
C-1	-2.657878	0.149599	1.291734
C-2	-2.686198	0.265958	-1.249677
C-3	-2.288064	-0.561891	-0.018474
C-4	-0.814427	-1.006875	-0.054287
C-5	0.235308	0.087403	-0.005871
C-6	2.589746	0.469226	0.012984
C-7	3.864640	-0.349298	0.000659
H-1	-3.733997	0.341722	1.331943
H-2	-2.139378	1.106122	1.379865
H-3	-2.398790	-0.461928	2.162204
H-4	-3.763061	0.458218	-1.248743
H-5	-2.169858	1.227599	-1.261596
H-6	-2.445961	-0.263085	-2.177692
H-7	-2.864286	-1.495537	-0.054886
H-8	-0.602939	-1.685470	0.779557
H-9	-0.617566	-1.592056	-0.959773
H-10	2.504211	1.081983	0.913260
H-11	2.521686	1.134973	-0.850589
H-12	4.730370	0.317608	0.034594
H-13	3.933509	-0.954672	-0.905965
H-14	3.910940	-1.015517	0.865066

Supporting Information 4: Cartesian coordinates of conformer 2 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.332998	1.332386	-0.751672
O-2	1.445957	-0.448197	0.063719
C-1	-3.396142	-0.911525	-0.310171
C-2	-2.326228	0.792851	1.225497
C-3	-2.219617	0.054102	-0.115572
C-4	-0.886883	-0.700692	-0.236329
C-5	0.329173	0.197324	-0.338472
C-6	2.693869	0.280986	-0.049349
C-7	3.799680	-0.621410	0.458542
H-1	-4.350376	-0.381086	-0.247188
H-2	-3.399517	-1.690814	0.460026
H-3	-3.352907	-1.406163	-1.285306
H-4	-3.269045	1.343004	1.292363
H-5	-2.293055	0.087860	2.064011
H-6	-1.513737	1.512361	1.350347
H-7	-2.245769	0.800451	-0.916350
H-8	-0.745946	-1.394334	0.598139
H-9	-0.884955	-1.315457	-1.145466
H-10	2.614270	1.201065	0.533969
H-11	2.840313	0.561357	-1.095135
H-12	4.759659	-0.102960	0.387321
H-13	3.860525	-1.538128	-0.132317
H-14	3.634100	-0.894120	1.503236

Supporting Information 5: Cartesian coordinates of conformer 3 optimized at DFT/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.333346	1.333533	-0.751304
O-2	-1.445390	-0.448305	0.062580
C-1	3.396778	-0.909290	-0.311055
C-2	2.323731	0.788739	1.229475
C-3	2.219474	0.055001	-0.114521
C-4	0.887283	-0.700037	-0.240038
C-5	-0.329042	0.197882	-0.339718
C-6	-2.693487	0.280888	-0.048403
C-7	-3.798778	-0.622427	0.458983
H-1	4.350650	-0.378633	-0.244560
H-2	3.399344	-1.691551	0.456121
H-3	3.355258	-1.400150	-1.288168
H-4	3.266233	1.338984	1.299891
H-5	2.289481	0.080602	2.065289
H-6	1.510794	1.507504	1.355800
H-7	2.246345	0.804344	-0.912466
H-8	0.745808	-1.397395	0.591210
H-9	0.886801	-1.310675	-1.151957
H-10	-2.613544	1.200086	0.536255
H-11	-2.840777	0.562836	-1.093643
H-12	-4.758867	-0.103958	0.389405
H-13	-3.860038	-1.538212	-0.133275
H-14	-3.632281	-0.896780	1.503102

Supporting Information 6: Cartesian coordinates of conformer 4 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.547871	0.816572	1.030966
O-2	-1.389519	-0.274129	-0.757375
C-1	3.344345	-0.979156	0.172061
C-2	2.414392	1.272778	-0.513625
C-3	2.151514	-0.019264	0.272051
C-4	0.867124	-0.714573	-0.205290
C-5	-0.404333	0.045424	0.112194
C-6	-2.694125	0.321781	-0.535424
C-7	-3.529263	-0.509762	0.424012
H-1	4.261197	-0.498933	0.525128
H-2	3.513829	-1.293859	-0.863692
H-3	3.186335	-1.879778	0.773055
H-4	3.317801	1.770949	-0.150648
H-5	2.558040	1.060083	-1.579166
H-6	1.585678	1.977795	-0.414109
H-7	2.007022	0.247177	1.324182
H-8	0.900728	-0.917670	-1.279734
H-9	0.764158	-1.690428	0.286458
H-10	-3.143758	0.355747	-1.528202
H-11	-2.556495	1.337880	-0.164205
H-12	-4.529680	-0.075738	0.510823
H-13	-3.080157	-0.527697	1.418699
H-14	-3.632450	-1.535531	0.062033

Supporting Information 7: Cartesian coordinates of conformer 5 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.546695	0.826264	1.021626
O-2	1.391073	-0.280157	-0.755817
C-1	-3.343195	-0.980841	0.177127
C-2	-2.417075	1.270624	-0.515020
C-3	-2.151274	-0.019441	0.273004
C-4	-0.866961	-0.714166	-0.204945
C-5	0.404366	0.047573	0.109052
C-6	2.695625	0.316877	-0.536654
C-7	3.528582	-0.507093	0.431133
H-1	-4.259812	-0.501208	0.531609
H-2	-3.514743	-1.297224	-0.857784
H-3	-3.182838	-1.880455	0.779014
H-4	-3.320326	1.768611	-0.151409
H-5	-2.562612	1.055332	-1.579786
H-6	-1.588867	1.976617	-0.418613
H-7	-2.005515	0.249520	1.324325
H-8	-0.901833	-0.919253	-1.279000
H-9	-0.762125	-1.689248	0.287946
H-10	3.147005	0.342264	-1.528903
H-11	2.557961	1.336114	-0.174189
H-12	4.529027	-0.072760	0.516088
H-13	3.077755	-0.516616	1.425164
H-14	3.632023	-1.535836	0.077786

Supporting Information 8: Cartesian coordinates of conformer 6 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.545052	0.288380	1.339814
O-2	-1.416439	-0.749373	-0.465650
C-1	3.451081	-0.582677	-0.204948
C-2	2.058426	1.523468	-0.379888
C-3	2.132975	0.098819	0.186020
C-4	0.938721	-0.752454	-0.271037
C-5	-0.393230	-0.321641	0.308279
C-6	-2.764209	-0.472754	-0.003862
C-7	-3.250142	0.882807	-0.489124
H-1	4.308881	0.005684	0.132589
H-2	3.532799	-0.692601	-1.292053
H-3	3.534837	-1.579521	0.238489
H-4	2.901644	2.125089	-0.028961
H-5	2.092383	1.511931	-1.475334
H-6	1.140658	2.029012	-0.070783
H-7	2.087420	0.165659	1.277984
H-8	0.859376	-0.774178	-1.362158
H-9	1.078873	-1.794907	0.042288
H-10	-2.781647	-0.534261	1.084835
H-11	-3.361579	-1.283068	-0.423022
H-12	-4.291905	1.028407	-0.188567
H-13	-3.196711	0.948458	-1.578471
H-14	-2.655679	1.688771	-0.055358

Supporting Information 9: Cartesian coordinates of conformer 7 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.543597	0.303137	1.334951
O-2	1.417598	-0.753362	-0.458437
C-1	-3.450413	-0.587911	-0.202840
C-2	-2.062714	1.520826	-0.385261
C-3	-2.133846	0.097974	0.185539
C-4	-0.937760	-0.752088	-0.268869
C-5	0.393319	-0.316896	0.309166
C-6	2.764853	-0.473160	0.002736
C-7	3.253236	0.876248	-0.496890
H-1	-4.309520	-0.000840	0.133650
H-2	-3.532539	-0.700924	-1.289607
H-3	-3.531405	-1.583802	0.243273
H-4	-2.907343	2.121675	-0.036379
H-5	-2.096808	1.505357	-1.480668
H-6	-1.146102	2.029513	-0.077947
H-7	-2.088297	0.168710	1.277262
H-8	-0.858147	-0.776510	-1.359964
H-9	-1.075712	-1.794111	0.046820
H-10	2.780119	-0.522283	1.092096
H-11	3.362112	-1.288866	-0.406020
H-12	4.294346	1.024422	-0.195264
H-13	3.202723	0.929482	-1.587045
H-14	2.658401	1.687663	-0.073885

Supporting Information 10: Cartesian coordinates of conformer 8 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.245838	0.242372	1.116278
O-2	-1.456185	-0.638315	-0.571251
C-1	2.356947	1.479092	-0.238100
C-2	2.731087	-0.822588	0.779277
C-3	2.257254	-0.038511	-0.453787
C-4	0.862261	-0.477021	-0.935903
C-5	-0.300748	-0.232901	0.007199
C-6	-2.678441	-0.481011	0.193871
C-7	-3.294110	0.892260	-0.017357
H-1	3.386959	1.765263	-0.006351
H-2	1.721717	1.801216	0.589137
H-3	2.055278	2.028272	-1.135966
H-4	3.767187	-0.566751	1.019348
H-5	2.114941	-0.596002	1.651349
H-6	2.689797	-1.902239	0.602124
H-7	2.932945	-0.294266	-1.280285
H-8	0.612937	0.020375	-1.879829
H-9	0.860263	-1.548533	-1.166095
H-10	-2.458940	-0.659646	1.247085
H-11	-3.330786	-1.271086	-0.179438
H-12	-4.248823	0.952233	0.513430
H-13	-3.481005	1.076402	-1.078037
H-14	-2.640904	1.676558	0.369205

Supporting Information 11: Cartesian coordinates of conformer 9 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.246379	0.269618	1.107833
O-2	1.455582	-0.645459	-0.562156
C-1	-2.373634	1.470691	-0.239025
C-2	-2.720435	-0.833128	0.783127
C-3	-2.258346	-0.046121	-0.452509
C-4	-0.860243	-0.471343	-0.937465
C-5	0.301275	-0.223141	0.006410
C-6	2.676946	-0.482234	0.203127
C-7	3.300202	0.884281	-0.028604
H-1	-3.406097	1.746174	-0.005161
H-2	-1.739635	1.801022	0.585860
H-3	-2.080230	2.021458	-1.138664
H-4	-3.759277	-0.589755	1.024246
H-5	-2.105954	-0.596582	1.653773
H-6	-2.665835	-1.912627	0.608670
H-7	-2.933576	-0.310387	-1.276709
H-8	-0.614858	0.034587	-1.878070
H-9	-0.850015	-1.541035	-1.175069
H-10	2.454178	-0.642863	1.258554
H-11	3.325956	-1.281589	-0.155960
H-12	4.253904	0.947930	0.503566
H-13	3.490628	1.050360	-1.091638
H-14	2.650039	1.677973	0.343649

Supporting Information 12: Cartesian coordinates of conformer 10 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.408115	-1.360112	0.743698
O-2	-1.252685	-0.006765	-0.852756
C-1	1.639827	1.725315	-0.066014
C-2	2.625718	-0.359751	0.993352
C-3	2.119377	0.286696	-0.302540
C-4	1.046166	-0.571803	-1.023777
C-5	-0.256144	-0.708054	-0.263237
C-6	-2.562986	-0.062478	-0.231265
C-7	-2.717488	0.996414	0.847928
H-1	2.450241	2.338686	0.337590
H-2	0.814684	1.758264	0.652418
H-3	1.293737	2.191653	-0.992804
H-4	3.434313	0.237998	1.424389
H-5	1.829338	-0.444306	1.736029
H-6	3.012161	-1.366453	0.810322
H-7	2.962785	0.330426	-1.002746
H-8	0.837979	-0.145185	-2.006563
H-9	1.437036	-1.583811	-1.163723
H-10	-2.715615	-1.064131	0.172396
H-11	-3.255834	0.106464	-1.056133
H-12	-3.738006	0.972008	1.241298
H-13	-2.531228	1.994790	0.445043
H-14	-2.030615	0.812563	1.675708

Supporting Information 13: Cartesian coordinates of conformer 11 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.409766	-1.362073	0.741727
O-2	1.251799	-0.005161	-0.852981
C-1	-1.640150	1.725275	-0.067243
C-2	-2.623723	-0.359244	0.995342
C-3	-2.119265	0.286199	-0.301768
C-4	-1.046586	-0.572572	-1.023452
C-5	0.256397	-0.708544	-0.264013
C-6	2.562399	-0.060314	-0.232119
C-7	2.715658	0.995849	0.849924
H-1	-2.450270	2.338575	0.337072
H-2	-0.813873	1.759380	0.649820
H-3	-1.295785	2.190980	-0.994997
H-4	-3.432444	0.238258	1.426475
H-5	-1.826563	-0.442189	1.737383
H-6	-3.009355	-1.366534	0.813887
H-7	-2.963537	0.328848	-1.001003
H-8	-0.839275	-0.146464	-2.006647
H-9	-1.437518	-1.584676	-1.162501
H-10	2.716930	-1.062815	0.168700
H-11	3.254554	0.112072	-1.056859
H-12	3.736108	0.971226	1.243463
H-13	2.528636	1.995158	0.449714
H-14	2.028795	0.809122	1.677063

Supporting Information 14: Cartesian coordinates of conformer 12 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.936989	-1.235928	1.138639
O-2	-1.085945	-0.142416	-0.831313
C-1	1.807775	1.081004	1.146547
C-2	3.253856	0.179360	-0.723259
C-3	1.818551	0.403355	-0.229996
C-4	1.052306	-0.939749	-0.211397
C-5	-0.413703	-0.807654	0.137333
C-6	-2.509972	0.057465	-0.639936
C-7	-2.796649	1.325612	0.146664
H-1	2.338413	2.036595	1.111079
H-2	2.300284	0.451691	1.895428
H-3	0.791617	1.277592	1.498539
H-4	3.803305	1.124147	-0.765315
H-5	3.799796	-0.492110	-0.051767
H-6	3.269854	-0.261642	-1.724212
H-7	1.310570	1.060844	-0.943907
H-8	1.122472	-1.405449	-1.199418
H-9	1.498294	-1.617886	0.519785
H-10	-2.922137	-0.820240	-0.140826
H-11	-2.908846	0.119375	-1.652987
H-12	-3.877541	1.483602	0.206075
H-13	-2.351355	2.196379	-0.340590
H-14	-2.409147	1.250770	1.164316

Supporting Information 15: Cartesian coordinates of conformer 13 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.938944	-1.235923	1.138501
O-2	1.084727	-0.142241	-0.831539
C-1	-1.806797	1.084269	1.144131
C-2	-3.254363	0.177298	-0.721948
C-3	-1.818669	0.402667	-0.230469
C-4	-1.052450	-0.940296	-0.208578
C-5	0.414036	-0.807620	0.138064
C-6	2.508905	0.058177	-0.641865
C-7	2.796344	1.324656	0.147199
H-1	-2.336841	2.040094	1.106207
H-2	-2.299319	0.457418	1.895066
H-3	-0.790319	1.281238	1.495009
H-4	-3.803952	1.121917	-0.765934
H-5	-3.799681	-0.492530	-0.048316
H-6	-3.271149	-0.266238	-1.721772
H-7	-1.311272	1.058121	-0.946645
H-8	-1.123621	-1.409112	-1.195096
H-9	-1.497665	-1.616361	0.525003
H-10	2.922474	-0.820569	-0.145680
H-11	2.906073	0.122936	-1.655385
H-12	3.877304	1.482658	0.205292
H-13	2.350410	2.196378	-0.337818
H-14	2.410187	1.247737	1.165156

Supporting Information 16: Cartesian coordinates of conformer 14 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.130581	-1.633782	-0.400654
O-2	1.243226	0.155862	0.393805
C-1	-1.652379	1.704912	-0.520120
C-2	-2.885665	-0.512623	-0.563984
C-3	-2.141483	0.507987	0.306713
C-4	-0.994667	-0.134396	1.133291
C-5	0.156518	-0.642928	0.291766
C-6	2.403634	-0.228862	-0.384782
C-7	3.495320	0.786209	-0.114406
H-1	-2.494666	2.206236	-1.005088
H-2	-0.960659	1.388877	-1.307571
H-3	-1.135088	2.440252	0.102536
H-4	-3.726762	-0.034473	-1.074661
H-5	-2.228813	-0.947582	-1.320689
H-6	-3.281306	-1.334708	0.039313
H-7	-2.850409	0.887964	1.052730
H-8	-0.612793	0.592214	1.852860
H-9	-1.390659	-0.991842	1.684397
H-10	2.121881	-0.258044	-1.439947
H-11	2.699947	-1.238872	-0.092547
H-12	4.389305	0.526677	-0.687878
H-13	3.761077	0.803393	0.944994
H-14	3.179486	1.789925	-0.407659

Supporting Information 17: Cartesian coordinates of conformer 15 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.128687	-1.628356	-0.402554
O-2	-1.246201	0.157240	0.394058
C-1	1.658595	1.700629	-0.528057
C-2	2.888702	-0.519047	-0.555420
C-3	2.143310	0.507613	0.307010
C-4	0.992463	-0.127841	1.133322
C-5	-0.157271	-0.638352	0.291012
C-6	-2.405719	-0.230207	-0.384604
C-7	-3.500314	0.781479	-0.113214
H-1	2.502842	2.196685	-1.015021
H-2	0.967183	1.381440	-1.314529
H-3	1.142447	2.441235	0.089293
H-4	3.732122	-0.045071	-1.066163
H-5	2.233493	-0.957447	-1.311488
H-6	3.281355	-1.338155	0.053877
H-7	2.850281	0.890735	1.053272
H-8	0.609933	0.603293	1.847937
H-9	1.384709	-0.983201	1.690414
H-10	-2.124105	-0.257705	-1.439842
H-11	-2.699017	-1.241302	-0.093137
H-12	-4.393358	0.520228	-0.687418
H-13	-3.766552	0.796552	0.946080
H-14	-3.187138	1.786442	-0.405036

Supporting Information 18: Cartesian coordinates of conformer 16 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.908736	1.520685	-0.532476
O-2	1.031778	-0.590459	0.258574
C-1	-2.212911	0.793594	1.157963
C-2	-3.250027	-0.889004	-0.422371
C-3	-1.946398	-0.379755	0.205979
C-4	-0.941293	0.003244	-0.904210
C-5	0.418001	0.425530	-0.392078
C-6	2.349569	-0.332683	0.807389
C-7	3.439679	-0.586834	-0.220483
H-1	-2.914285	0.501447	1.944643
H-2	-2.647276	1.643051	0.620253
H-3	-1.296938	1.142861	1.642188
H-4	-3.961475	-1.193928	0.350222
H-5	-3.728043	-0.108307	-1.023983
H-6	-3.071295	-1.750603	-1.072404
H-7	-1.501891	-1.197999	0.782627
H-8	-0.796634	-0.855259	-1.568446
H-9	-1.331569	0.831637	-1.499910
H-10	2.382040	0.694019	1.173772
H-11	2.428054	-1.021532	1.649191
H-12	4.420913	-0.456930	0.245466
H-13	3.378726	-1.606353	-0.608822
H-14	3.363195	0.115425	-1.052422

Supporting Information 19: Cartesian coordinates of conformer 17 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.908868	1.520648	-0.533001
O-2	-1.031844	-0.590201	0.258790
C-1	2.213765	0.794595	1.157034
C-2	3.249520	-0.890229	-0.421901
C-3	1.946321	-0.379520	0.206204
C-4	0.941266	0.003059	-0.904075
C-5	-0.418030	0.425613	-0.392113
C-6	-2.349575	-0.332218	0.807522
C-7	-3.439679	-0.587377	-0.220105
H-1	2.914694	0.502583	1.944168
H-2	2.649041	1.643078	0.618524
H-3	1.298002	1.145241	1.640675
H-4	3.961371	-1.193697	0.350886
H-5	3.727290	-0.110816	-1.025375
H-6	3.070280	-1.753104	-1.070092
H-7	1.501426	-1.196924	0.783749
H-8	0.796490	-0.855658	-1.568016
H-9	1.331542	0.831201	-1.500145
H-10	-2.382201	0.694780	1.173077
H-11	-2.427903	-1.020403	1.649885
H-12	-4.420929	-0.457332	0.245776
H-13	-3.378536	-1.607169	-0.607694
H-14	-3.363392	0.114264	-1.052591

Supporting Information 20: Cartesian coordinates of conformer 18 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.438742	-1.351051	-0.450508
O-2	1.160928	0.670254	0.248179
C-1	-2.064103	1.483810	-0.521407
C-2	-2.755917	-0.956197	-0.437891
C-3	-2.215131	0.237082	0.360820
C-4	-0.905427	-0.097127	1.124572
C-5	0.282207	-0.359115	0.222995
C-6	2.348455	0.552275	-0.577317
C-7	3.469412	-0.157167	0.164313
H-1	-3.026755	1.762869	-0.958881
H-2	-1.367834	1.305576	-1.347099
H-3	-1.692390	2.339379	0.049450
H-4	-3.713962	-0.700614	-0.900156
H-5	-2.063799	-1.255406	-1.228141
H-6	-2.914473	-1.825680	0.206536
H-7	-2.947112	0.471449	1.143595
H-8	-0.659801	0.722380	1.802272
H-9	-1.061356	-1.001910	1.718726
H-10	2.086559	0.027428	-1.496645
H-11	2.615404	1.583527	-0.810497
H-12	4.371769	-0.165338	-0.454105
H-13	3.701832	0.355402	1.100851
H-14	3.198561	-1.191489	0.383508

Supporting Information 21: Cartesian coordinates of conformer 19 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.439302	-1.351624	-0.449510
O-2	-1.160535	0.670490	0.247803
C-1	2.064458	1.484099	-0.520742
C-2	2.755144	-0.956277	-0.438928
C-3	2.215144	0.236706	0.360678
C-4	0.905511	-0.097256	1.124646
C-5	-0.282286	-0.359299	0.223304
C-6	-2.348112	0.552471	-0.577634
C-7	-3.469174	-0.156662	0.164134
H-1	3.026939	1.762432	-0.959052
H-2	1.367159	1.307015	-1.345806
H-3	1.694176	2.339733	0.050951
H-4	3.713461	-0.701015	-0.900803
H-5	2.062956	-1.254303	-1.229563
H-6	2.912908	-1.826431	0.204783
H-7	2.947463	0.470292	1.143389
H-8	0.660054	0.722385	1.802250
H-9	1.061473	-1.001962	1.718902
H-10	-2.086287	0.027405	-1.496862
H-11	-2.614915	1.583713	-0.811018
H-12	-4.371616	-0.164553	-0.454161
H-13	-3.701317	0.355984	1.100700
H-14	-3.198598	-1.191061	0.383288

Supporting Information 22: Cartesian coordinates of conformer 20 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.696858	1.920385	0.099783
O-2	1.131199	-0.254484	-0.296125
C-1	-2.015198	-0.077329	1.499250
C-2	-3.153745	-0.885729	-0.611553
C-3	-1.812923	-0.548539	0.053156
C-4	-1.057445	0.504090	-0.788746
C-5	0.328085	0.833585	-0.277593
C-6	2.491492	-0.065325	0.166641
C-7	3.195812	-1.404001	0.083365
H-1	-2.536810	-0.839311	2.085231
H-2	-2.613711	0.839251	1.533229
H-3	-1.064219	0.131060	1.997147
H-4	-3.690415	-1.649690	-0.041930
H-5	-3.797396	-0.001204	-0.668643
H-6	-3.012750	-1.263542	-1.628502
H-7	-1.200449	-1.456408	0.069375
H-8	-0.955677	0.136352	-1.815320
H-9	-1.618652	1.440913	-0.819175
H-10	2.463348	0.320904	1.188101
H-11	2.970657	0.689992	-0.460670
H-12	4.229255	-1.297761	0.424198
H-13	3.210513	-1.776624	-0.943357
H-14	2.702192	-2.147126	0.713769

Supporting Information 23: Cartesian coordinates of conformer 21 optimized at B3LYP/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.698265	1.921123	0.102131
O-2	-1.130241	-0.253854	-0.295723
C-1	2.013639	-0.082909	1.499643
C-2	3.153908	-0.883362	-0.613264
C-3	1.812568	-0.548609	0.051606
C-4	1.057884	0.507348	-0.786767
C-5	-0.328199	0.834972	-0.275845
C-6	-2.491065	-0.066350	0.166176
C-7	-3.194340	-1.405411	0.080343
H-1	2.535093	-0.846926	2.083111
H-2	2.611813	0.833741	1.537553
H-3	1.062204	0.123206	1.997625
H-4	3.689858	-1.649858	-0.046369
H-5	3.797884	0.001195	-0.666119
H-6	3.013741	-1.256890	-1.631913
H-7	1.199970	-1.456447	0.063844
H-8	0.956957	0.143725	-1.814911
H-9	1.619116	1.444276	-0.813113
H-10	-2.970250	0.689544	-0.460416
H-11	-2.464031	0.318394	1.188228
H-12	-4.228132	-1.300432	0.420505
H-13	-2.700687	-2.149130	0.710023
H-14	-3.207949	-1.776507	-0.946948

Supporting Information 24: Cartesian coordinates of conformer 2 optimized at HF/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.322987	1.295383	-0.732578
O-2	1.455148	-0.412613	0.088564
C-1	-3.345848	-0.993815	-0.289626
C-2	-2.408281	0.900136	1.087012
C-3	-2.209030	0.022280	-0.151726
C-4	-0.860079	-0.701754	-0.118959
C-5	0.342423	0.196125	-0.288935
C-6	2.685746	0.285601	-0.068707
C-7	3.793239	-0.617373	0.427741
H-1	-4.308657	-0.492712	-0.326732
H-2	-3.364271	-1.681508	0.553581
H-3	-3.243512	-1.583071	-1.197066
H-4	-3.358656	1.423753	1.036647
H-5	-2.411332	0.297449	1.993662
H-6	-1.626033	1.645824	1.175563
H-7	-2.217402	0.665869	-1.026228
H-8	-0.737437	-1.267330	0.799876
H-9	-0.798961	-1.426684	-0.928684
H-10	2.640969	1.209045	0.494805
H-11	2.815731	0.539193	-1.113432
H-12	4.749792	-0.114249	0.321850
H-13	3.825202	-1.539428	-0.142841
H-14	3.649731	-0.865413	1.473989

Supporting Information 25: Cartesian coordinates of conformer 3 optimized at HF/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.322917	1.295431	-0.732285
O-2	-1.455286	-0.412599	0.088663
C-1	3.345858	-0.994224	-0.289357
C-2	2.408613	0.900626	1.086312
C-3	2.209139	0.022086	-0.151904
C-4	0.860048	-0.701740	-0.118662
C-5	-0.342431	0.196162	-0.288722
C-6	-2.685871	0.285584	-0.068795
C-7	-3.793451	-0.617372	0.427545
H-1	4.308773	-0.493323	-0.326435
H-2	3.364073	-1.681744	0.554004
H-3	3.243590	-1.583680	-1.196672
H-4	3.358805	1.424494	1.035305
H-5	2.412211	0.298370	1.993240
H-6	1.626188	1.646126	1.174828
H-7	2.217485	0.665217	-1.026737
H-8	0.737466	-1.266895	0.800428
H-9	0.798702	-1.426986	-0.928096
H-10	-2.641154	1.209051	0.494673
H-11	-2.815695	0.539132	-1.113545
H-12	-4.750000	-0.114270	0.321504
H-13	-3.825336	-1.539454	-0.142994
H-14	-3.650091	-0.865360	1.473823

Supporting Information 26: Cartesian coordinates of conformer 2 optimized at MP2/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.409718	-1.588206	0.668552
O-2	-1.288447	0.179844	-0.435779
C-1	3.432971	0.236865	-0.551511
C-2	1.737732	1.208300	1.039987
C-3	2.112442	-0.001333	0.181492
C-4	0.997714	-0.318238	-0.827373
C-5	-0.285729	-0.669973	-0.116092
C-6	-2.541083	-0.083741	0.232709
C-7	-3.526556	0.962005	-0.243342
H-1	4.240173	0.442818	0.158834
H-2	3.347930	1.098680	-1.224144
H-3	3.717673	-0.635431	-1.149031
H-4	2.534295	1.435207	1.756030
H-5	1.584961	2.092193	0.409145
H-6	0.818146	1.032046	1.607773
H-7	2.220013	-0.875526	0.835471
H-8	0.833508	0.533324	-1.495002
H-9	1.285479	-1.186523	-1.431412
H-10	-2.381013	-0.034463	1.313401
H-11	-2.866595	-1.097748	-0.015092
H-12	-4.494830	0.800383	0.239333
H-13	-3.663166	0.899013	-1.325385
H-14	-3.175783	1.965417	0.008897

Supporting Information 27: Cartesian coordinates of conformer 3 optimized at MP2/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.409780	-1.588194	0.668593
O-2	1.288464	0.179877	-0.435720
C-1	-3.433015	0.236612	-0.551511
C-2	-1.737879	1.208533	1.039802
C-3	-2.112444	-0.001307	0.181521
C-4	-0.997717	-0.318234	-0.827292
C-5	0.285747	-0.669944	-0.116019
C-6	2.541139	-0.083783	0.232672
C-7	3.526603	0.961973	-0.243375
H-1	-4.240152	0.442968	0.158790
H-2	-3.347972	1.098088	-1.224580
H-3	-3.717808	-0.635966	-1.148574
H-4	-2.534356	1.435298	1.755978
H-5	-1.585495	2.092391	0.408813
H-6	-0.818112	1.032599	1.607388
H-7	-2.219930	-0.875395	0.835655
H-8	-0.833505	0.533285	-1.494973
H-9	-1.285478	-1.186547	-1.431301
H-10	2.381143	-0.034577	1.313379
H-11	2.866611	-1.097782	-0.015223
H-12	4.494923	0.800277	0.239182
H-13	3.663099	0.899075	-1.325438
H-14	3.175885	1.965370	0.008995

Supporting Information 28: Cartesian coordinates of conformer 2 optimized at MP3/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.330535	1.295696	-0.765827
O-2	1.440719	-0.460969	0.071971
C-1	-3.393447	-0.900209	-0.273671
C-2	-2.287763	0.831617	1.195682
C-3	-2.205308	0.058279	-0.126822
C-4	-0.887600	-0.719721	-0.225986
C-5	0.330924	0.173026	-0.338971
C-6	2.659474	0.286019	-0.054538
C-7	3.785285	-0.591719	0.461773
H-1	-4.341359	-0.356395	-0.207834
H-2	-3.382881	-1.654533	0.522790
H-3	-3.366000	-1.422425	-1.236142
H-4	-3.223912	1.396231	1.255104
H-5	-2.257691	0.138495	2.045869
H-6	-1.460133	1.539795	1.295181
H-7	-2.227650	0.780028	-0.950653
H-8	-0.758238	-1.387537	0.632786
H-9	-0.886983	-1.355120	-1.121539
H-10	2.571944	1.211513	0.520996
H-11	2.805459	0.555790	-1.104187
H-12	4.735563	-0.055694	0.380193
H-13	3.854469	-1.513657	-0.121461
H-14	3.621367	-0.852098	1.510686

Supporting Information 29: Cartesian coordinates of conformer 3 optimized at MP3/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.330673	1.295883	-0.765603
O-2	-1.440742	-0.460879	0.072056
C-1	3.393399	-0.900489	-0.273736
C-2	2.288121	0.831665	1.195503
C-3	2.205425	0.058228	-0.126913
C-4	0.887564	-0.719582	-0.225936
C-5	-0.330990	0.173178	-0.338855
C-6	-2.659585	0.285922	-0.054641
C-7	-3.785331	-0.591884	0.461734
H-1	4.341404	-0.356807	-0.208176
H-2	3.382820	-1.654617	0.522912
H-3	3.365688	-1.422924	-1.236074
H-4	3.224754	1.395477	1.255135
H-5	2.257189	0.138705	2.045791
H-6	1.461088	1.540576	1.294671
H-7	2.227740	0.779913	-0.950805
H-8	0.758248	-1.387370	0.632863
H-9	0.886844	-1.354962	-1.121509
H-10	-2.572199	1.211507	0.520767
H-11	-2.805521	0.555514	-1.104342
H-12	-4.735679	-0.056002	0.380010
H-13	-3.854341	-1.513924	-0.121359
H-14	-3.621422	-0.852056	1.510701

Supporting Information 30: Cartesian coordinates of conformer 2 optimized at MP4/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.333368	1.317958	-0.756201
O-2	1.435997	-0.461639	0.057121
C-1	-3.398547	-0.881412	-0.286001
C-2	-2.266445	0.783131	1.238788
C-3	-2.205314	0.066361	-0.115903
C-4	-0.891739	-0.710016	-0.266601
C-5	0.328576	0.184318	-0.351227
C-6	2.659904	0.284567	-0.043608
C-7	3.776714	-0.608719	0.464864
H-1	-4.344523	-0.337580	-0.186157
H-2	-3.380993	-1.668308	0.479311
H-3	-3.385822	-1.364587	-1.269928
H-4	-3.201266	1.346397	1.336714
H-5	-2.224474	0.054801	2.059569
H-6	-1.436230	1.486850	1.356759
H-7	-2.237849	0.822855	-0.909203
H-8	-0.755697	-1.418381	0.558854
H-9	-0.903739	-1.302187	-1.192251
H-10	2.569659	1.198906	0.550647
H-11	2.815623	0.574933	-1.087223
H-12	4.731118	-0.075392	0.403246
H-13	3.847431	-1.519512	-0.136924
H-14	3.601823	-0.890107	1.507408

Supporting Information 31: Cartesian coordinates of conformer 3 optimized at MP4/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	-0.333185	1.317890	-0.756308
O-2	-1.435891	-0.461238	0.058055
C-1	3.398437	-0.882026	-0.285692
C-2	2.266483	0.783866	1.237937
C-3	2.205397	0.066091	-0.116227
C-4	0.891664	-0.710079	-0.266287
C-5	-0.328505	0.184426	-0.350781
C-6	-2.659940	0.284702	-0.043283
C-7	-3.776931	-0.609092	0.463898
H-1	4.344572	-0.338475	-0.185723
H-2	3.380449	-1.668731	0.479815
H-3	3.385866	-1.365461	-1.269499
H-4	3.201012	1.347716	1.335293
H-5	2.225001	0.056085	2.059216
H-6	1.435878	1.487227	1.355484
H-7	2.238008	0.822084	-0.910000
H-8	0.755743	-1.418237	0.559370
H-9	0.903204	-1.302542	-1.191789
H-10	-2.570392	1.198787	0.551486
H-11	-2.814913	0.575535	-1.086877
H-12	-4.731500	-0.076175	0.401262
H-13	-3.846564	-1.519862	-0.138056
H-14	-3.603087	-0.890500	1.506616

Supporting Information 32: Cartesian coordinates of conformer 2 optimized at CCSD/6-311++G** level in the principal axes of inertia system.

Atom	a/Å	b/Å	c/Å
O-1	0.337809	1.345657	-0.736820
O-2	1.427635	-0.466866	0.033817
C-1	-3.410047	-0.843958	-0.304417
C-2	-2.226699	0.705358	1.303446
C-3	-2.203460	0.080401	-0.097909
C-4	-0.900113	-0.695430	-0.329405
C-5	0.325437	0.196239	-0.368453
C-6	2.655963	0.283646	-0.027829
C-7	3.765485	-0.627634	0.465559
H-1	-4.348855	-0.299219	-0.147916
H-2	-3.384175	-1.680934	0.406925
H-3	-3.422931	-1.260790	-1.319221
H-4	-3.153492	1.270289	1.460300
H-5	-2.173969	-0.077235	2.073255
H-6	-1.385555	1.392364	1.449135
H-7	-2.244819	0.889266	-0.838417
H-8	-0.757247	-1.464487	0.439405
H-9	-0.934253	-1.214615	-1.298150
H-10	2.556763	1.178485	0.595099
H-11	2.823038	0.607227	-1.060498
H-12	4.721779	-0.093127	0.433142
H-13	3.843151	-1.519181	-0.165130
H-14	3.577159	-0.942556	1.497058