Supporting Information

***Rec. Nat. Prod.* X:X (202X) XX-XX**

Aspilactonol J, A New Cytotoxic Polyketide Isolated from the Marine-Derived Fungus *Aspergillus* sp. w2-13

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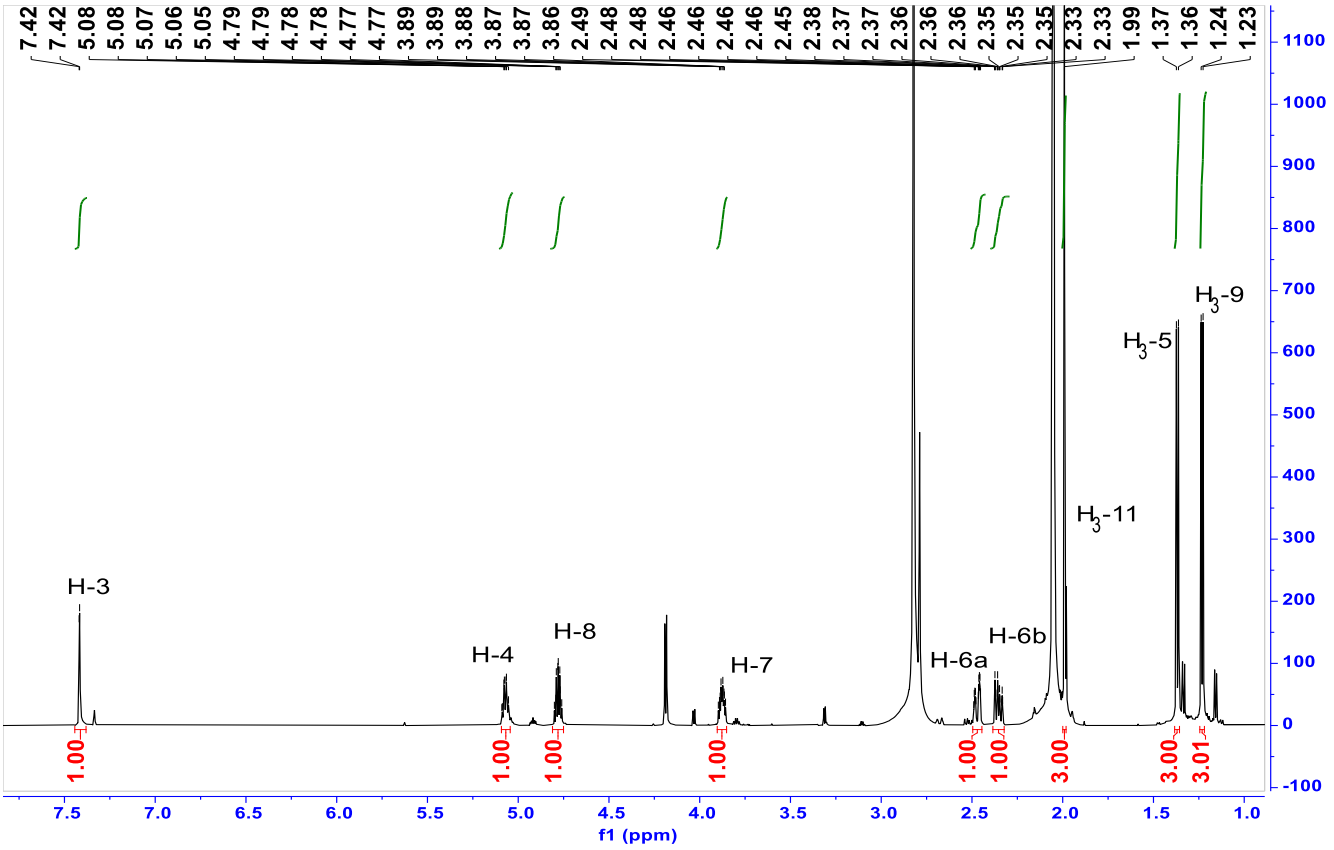


Figure S1: ^{1}H-NMR spectrum of **1**

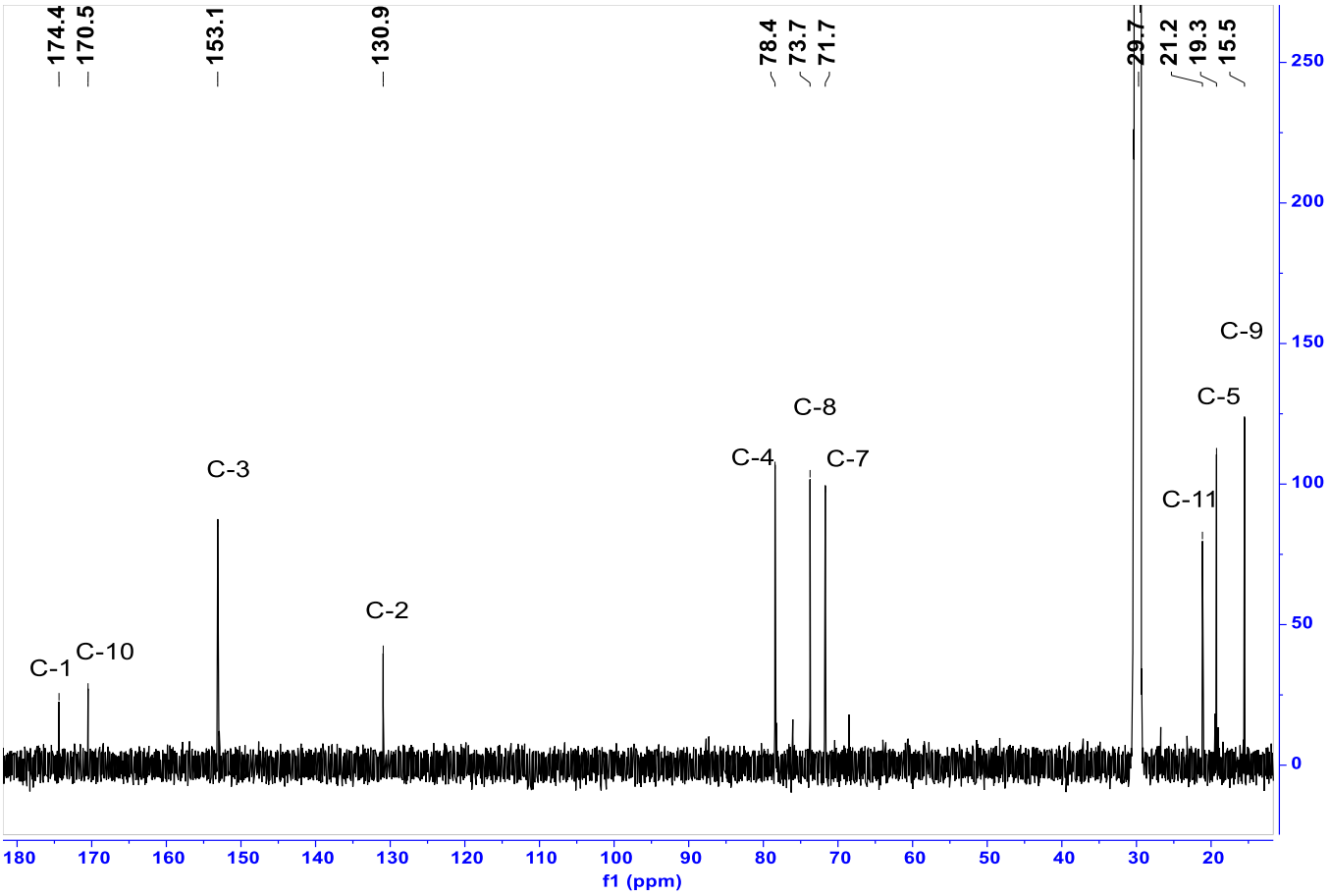


Figure S2: ^{13}C-NMR spectrum of **1**

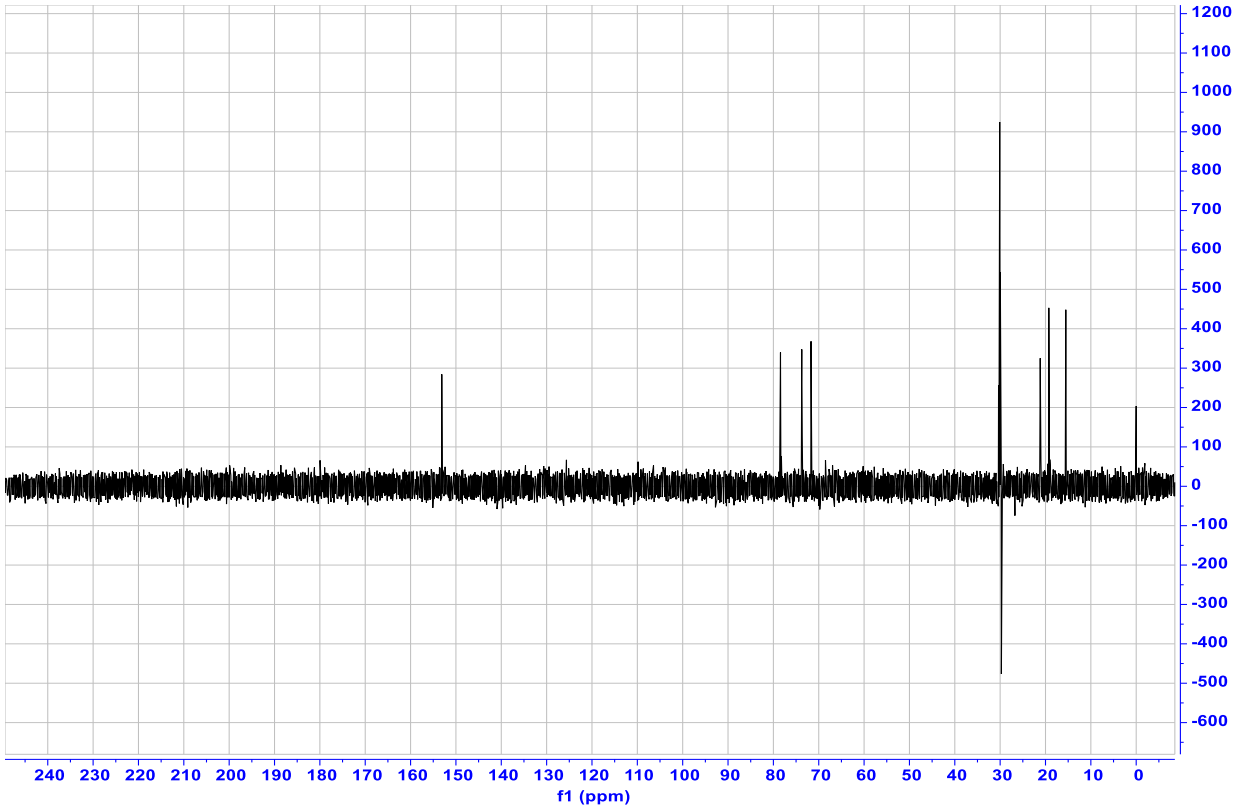


Figure S3: DEPT spectrum of **1**

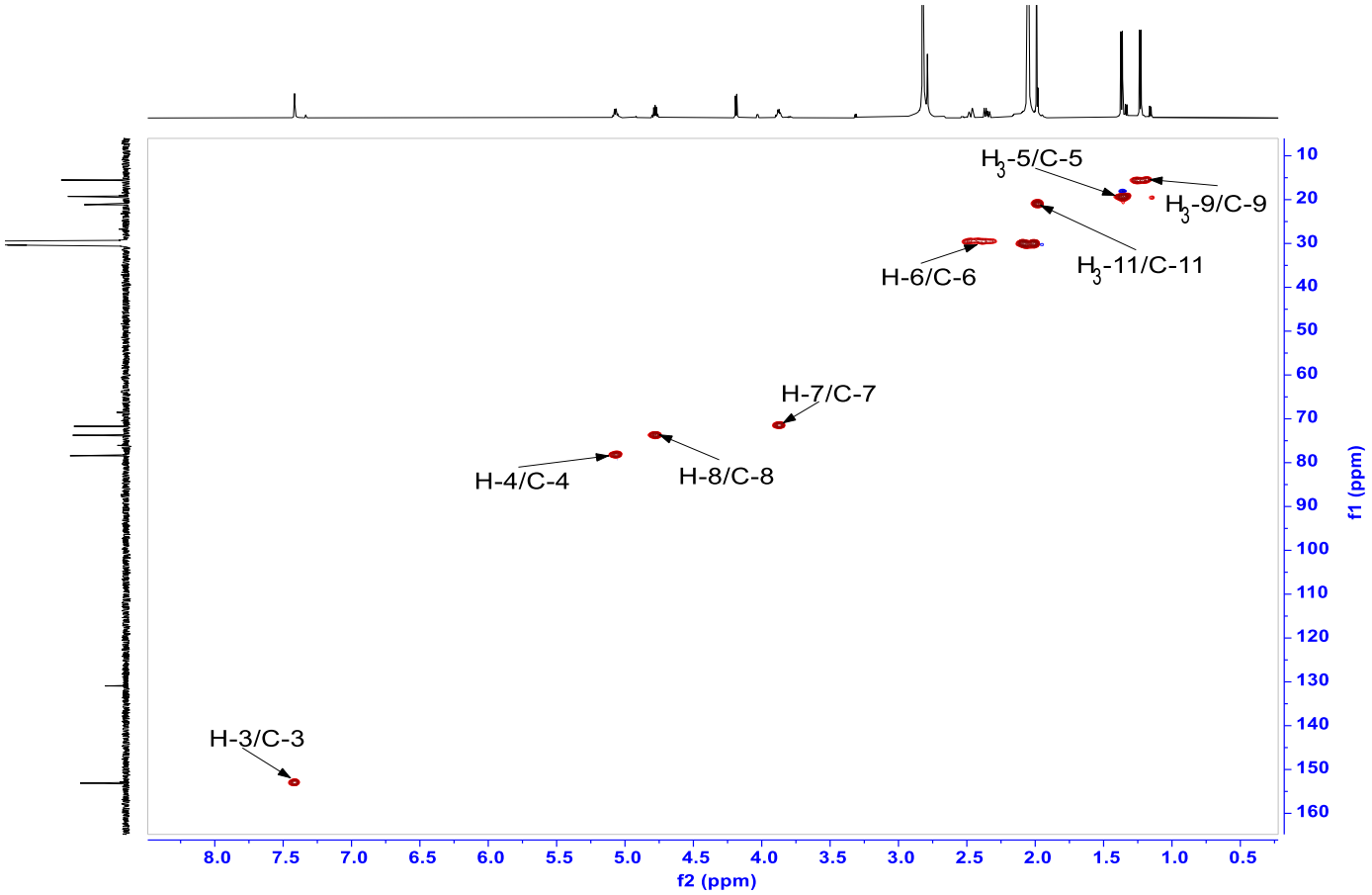


Figure S4: HSQC spectrum of **1**

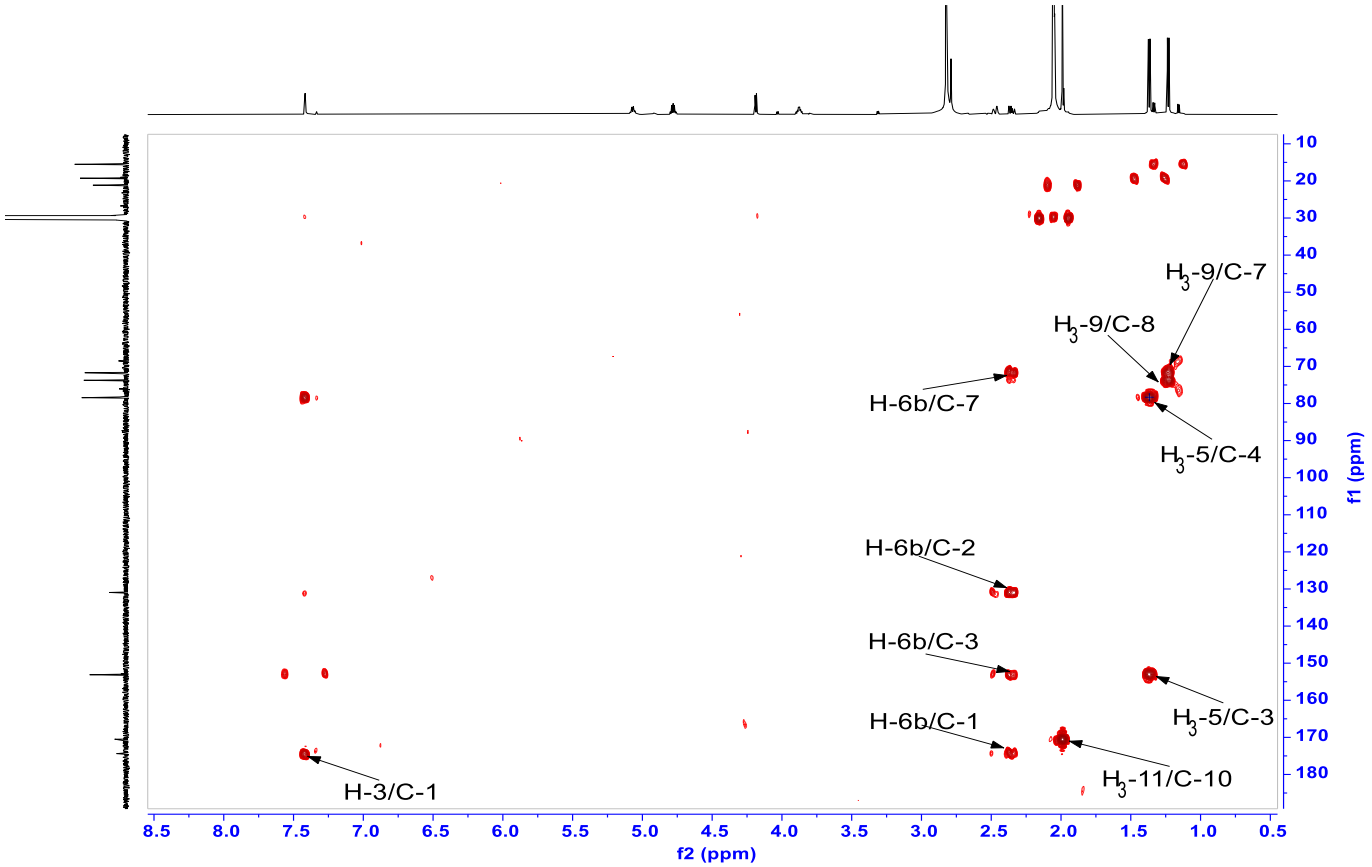


Figure S5: HMBC spectrum of **1**

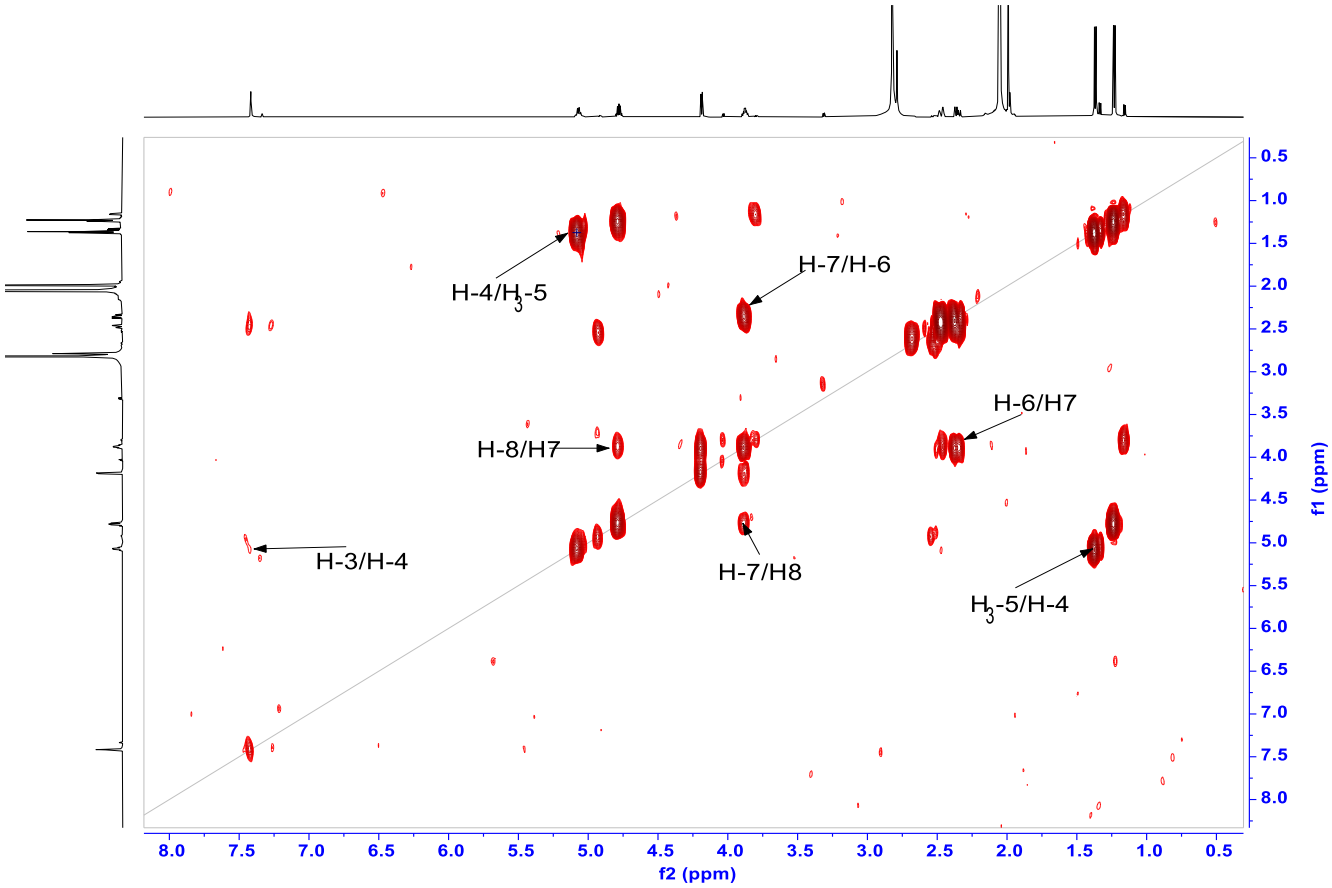


Figure S6: COSY spectrum of **1**

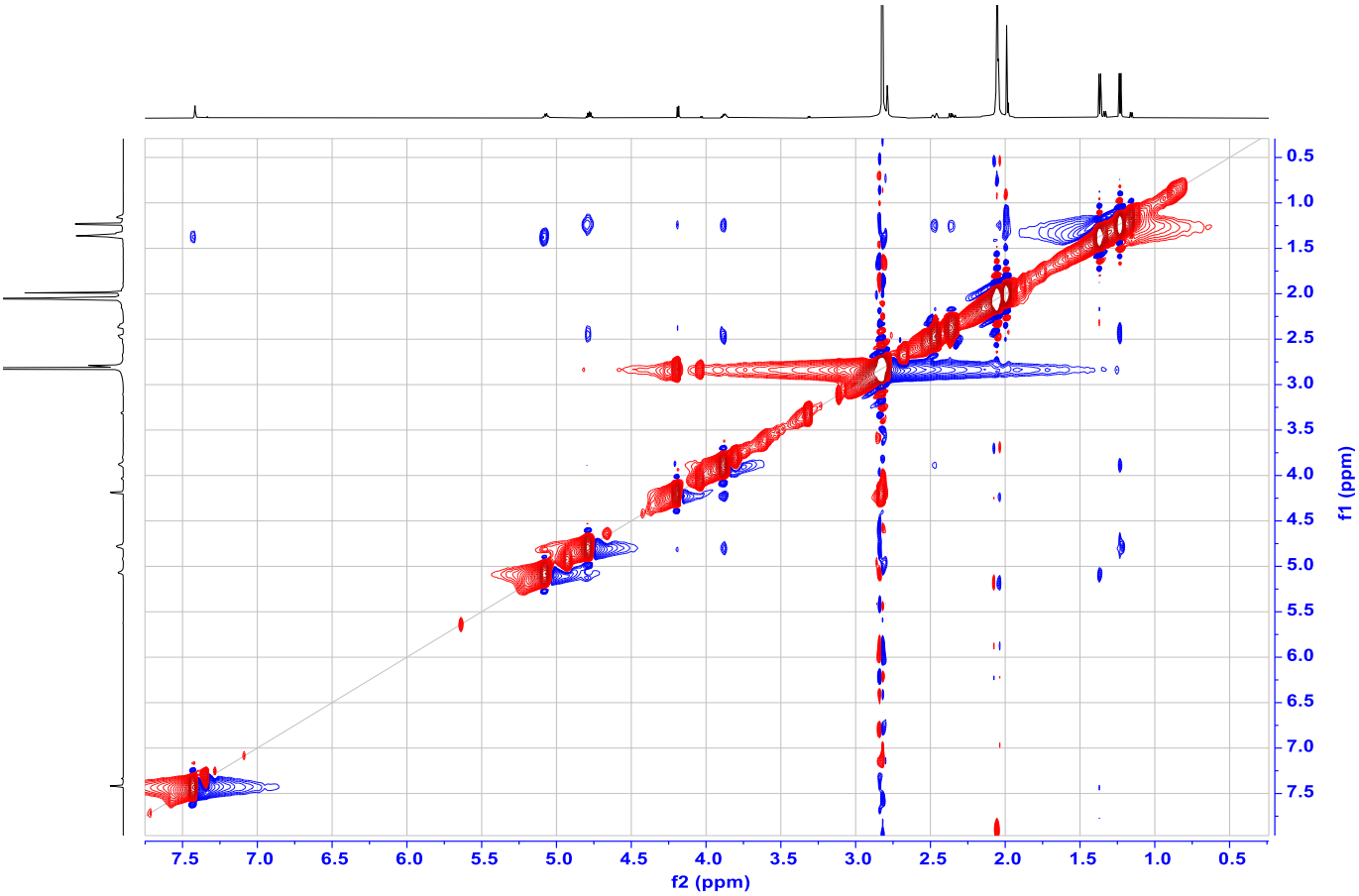


Figure S7: NOESY spectrum of **1**

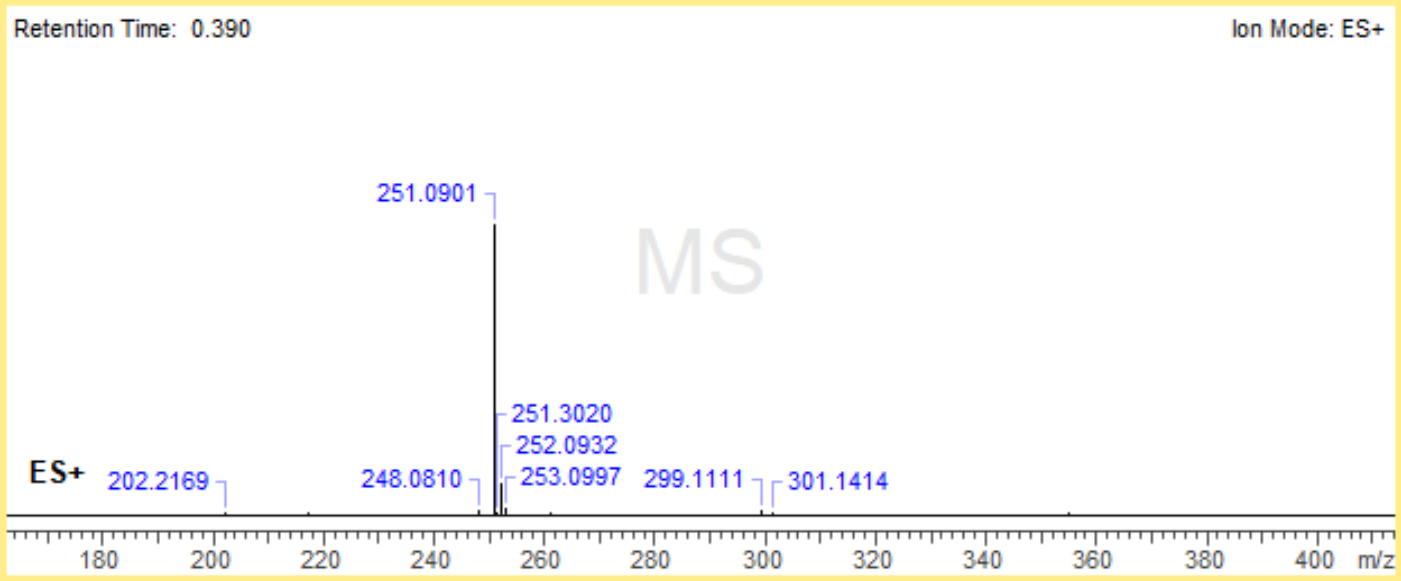


Figure S8: MS spectrum of **1**

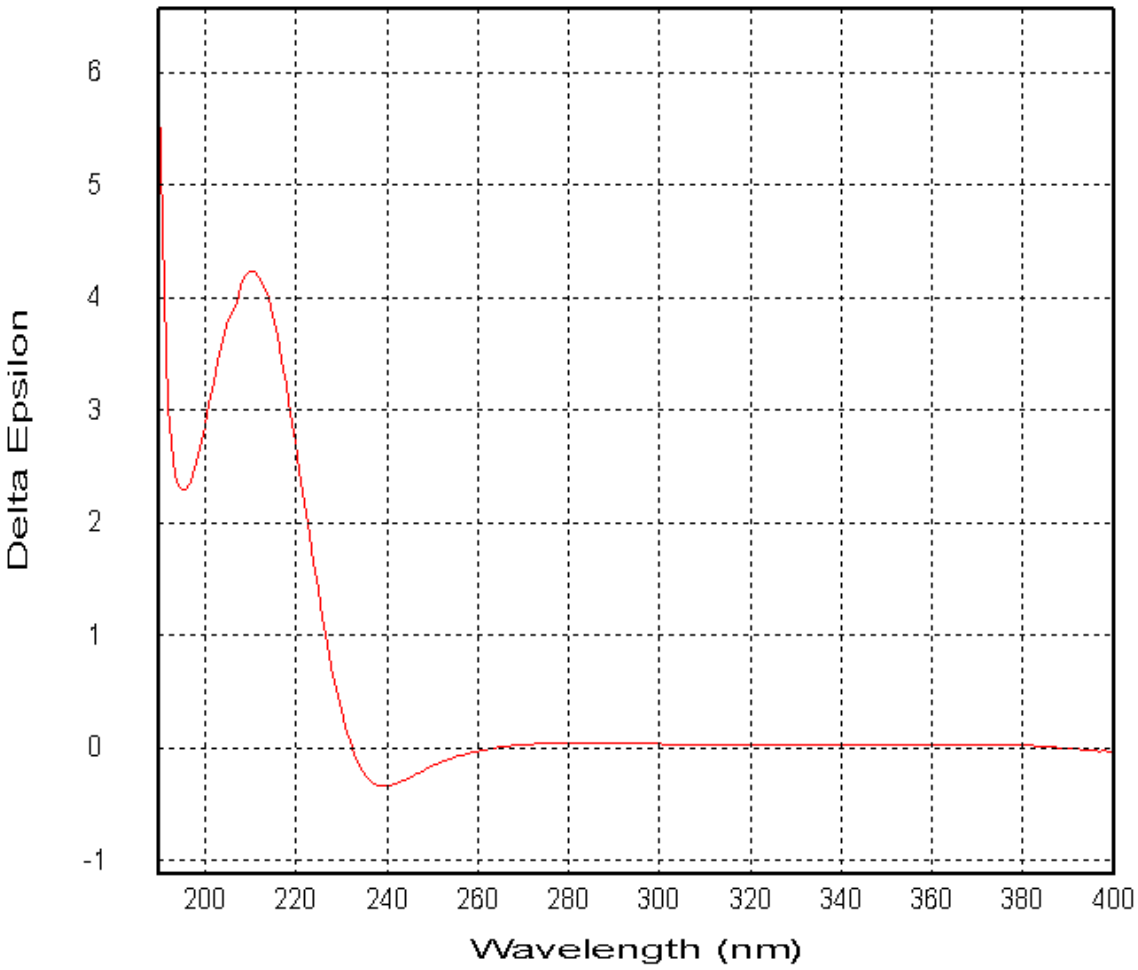


Figure S9: ECD spectrum of **1**

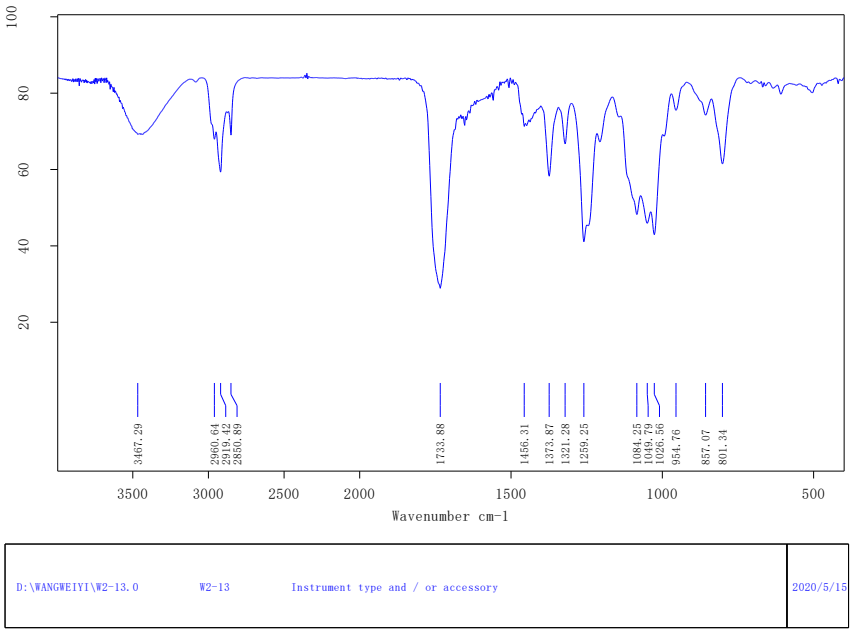


Figure S10: IR spectrum of **1**

Table S1: Experimental and calculated ^{13}C-NMR chemical shifts of **1a** and **1b**

No.	δexptl.	1a-δcalcd.	1b-δcalcd.
1	174.4	174.4	174.4
2	130.9	129.8	130.4
3	153.1	156.6	156.5
4	78.4	81.0	80.4
5	19.3	19.4	19.4
6	29.7	32.2	32.5
7	71.7	73.4	73.5
8	73.7	72.1	72.6
9	15.5	18.3	18.6
10	170.5	169.7	170.1
11	21.2	22.9	23.1

Table S2: Experimental and calculated ^{1}H-NMR chemical shifts of **1a** and **1b**

No.	δexptl.	1a-δcalcd.	1b-δcalcd.
3	7.42	7.73	7.74
4	5.07	5.11	5.12
5	1.37	1.37	1.26
6a	2.47	2.52	2.45
6b	2.35	2.45	2.42
7	3.87	3.57	3.53
8	4.78	4.78	4.77
9	1.23	1.16	1.17
11	1.99	1.92	1.92

Functional	Solvent?	Basis Set	Type of Data
mPW1PW91	PCM	6-31+G(d,p)	Unscaled Shifts

1a 1b

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	36.76%	63.24%	-	-	-	-
sDP4+ (C data)	23.04%	76.96%	-	-	-	-
sDP4+ (all data)	14.82%	85.18%	-	-	-	-
uDP4+ (H data)	49.65%	50.35%	-	-	-	-
uDP4+ (C data)	46.59%	53.41%	-	-	-	-
uDP4+ (all data)	46.24%	53.76%	-	-	-	-
DP4+ (H data)	36.43%	63.57%	-	-	-	-
DP4+ (C data)	20.71%	79.29%	-	-	-	-
DP4+ (all data)	13.02%	86.98%	-	-	-	-

Figure S11: Result of DP4+ analysis

Table S3: Comparison of key parameters of ^{13}C NMR computation between 1a and 1b

Atom_type	Parameters	1a	1b
13C	R^2	0.9993	0.9994
	MAE	1.7	1.5
	CMAE	1.3	1.2

Table S4: Conformational analysis of the B3LYP/6-31G(d) optimized conformers of 1a in the gas phase (T=298.15 K)

Conformer	E[a] (Hartree)	C[b] (Hartree)	G[c] (kcal/mol)	ΔG[d] (kcal/mol)	Population[e]
1a-1	-804.880801	0.214564	-504928.063423	0.0	35.39%
1a-2	-804.88156	0.215924	-504927.686494	0.376929	18.73%
1a-3	-804.881559	0.215933	-504927.680036	0.383387	18.52%
1a-4	-804.88156	0.215938	-504927.67783	0.385592	18.45%
1a-5	-804.877898	0.213617	-504926.836186	1.227236	4.45%
1a-6	-804.877898	0.213618	-504926.835462	1.227961	4.45%

[a]Electronic energy obtained at M062X/6-311+G(2d,p) level of theory; [b]Thermal correction to Gibbs free energy obtained at B3LYP/6-31G(d) level of theory; [c]Gibbs free energy (E + C); [d]The relative Gibbs free energy; [e]The Boltzmann distribution of each conformer.

Table S5: Atomic coordinates (Å) of **1a**-1 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	2.434650	0.605920	-0.525249	H	3.655675	-2.169870	1.873647
C	1.127479	-0.035576	-0.812440	H	2.107304	-1.338423	2.160069
C	1.224684	-1.323033	-0.462138	H	2.119523	-3.031611	1.616982
C	2.599872	-1.598589	0.073729	H	3.143526	-2.309833	-0.561537
C	2.624366	-2.064349	1.525624	H	0.440343	-2.069230	-0.496616
C	-0.002918	0.767370	-1.375121	H	0.398770	1.427924	-2.153725
C	-0.708725	1.650882	-0.323324	H	-0.740748	0.116899	-1.852448
C	-1.521508	0.824751	0.683097	H	1.029142	2.543839	-0.071070
C	-2.146596	1.671808	1.777886	H	-1.414347	2.305282	-0.861581
C	-2.633229	-1.145854	-0.167514	H	-4.764205	-1.283025	-0.369595
C	-3.866883	-1.589855	-0.916721	H	-3.904685	-1.107230	-1.898521
O	-1.782432	-1.893850	0.271051	H	-3.854841	-2.673890	-1.031737
O	3.289273	-0.330212	-0.034859	H	-0.892709	0.038685	1.104596
O	-2.609593	0.196572	-0.055418	H	-2.825191	2.416797	1.348514
O	2.746586	1.771156	-0.676704	H	-2.713596	1.041207	2.469911
O	0.204822	2.421129	0.436991	H	-1.360383	2.193276	2.327662

Table S6: Atomic coordinates (Å) of **1a**-2 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	1.139571	-1.613841	-0.323244	H	3.602321	1.827384	0.080128
C	0.725606	-0.855302	0.889521	H	3.968970	0.821936	-1.337519
C	1.733101	-0.025519	1.187419	H	2.313871	1.444822	-1.090197
C	2.859170	-0.193238	0.211002	H	3.756475	-0.589155	0.704877
C	3.205366	1.057167	-0.590869	H	1.770003	0.686973	2.004712
C	-0.587939	-1.046874	1.589251	H	-0.589037	-2.013338	2.109132
C	-1.850631	-1.044321	0.691392	H	-0.685150	-0.267544	2.351009
C	-1.840747	0.075433	-0.361606	H	-1.255157	-2.520351	-0.418842
C	-3.173024	0.233908	-1.071501	H	-2.709139	-0.886953	1.355399
C	-0.582775	2.115220	-0.203841	H	0.152521	2.974357	1.613230
C	-0.326254	3.308015	0.685561	H	0.327333	4.013853	0.172268
O	-0.007294	1.892304	-1.248951	H	-1.267676	3.792069	0.960357
O	2.388289	-1.227652	-0.683068	H	-1.048045	-0.111163	-1.088600
O	-1.523579	1.315306	0.335962	H	-3.457805	-0.723357	-1.515369
O	0.515388	-2.445511	-0.954876	H	-3.952172	0.536637	-0.363102
O	-2.077055	-2.289233	0.064058	H	-3.101967	0.988242	-1.860989

Table S7: Atomic coordinates (Å) of **1a**-3 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	1.139963	-1.613724	-0.323101	H	3.602390	1.827947	0.079759
C	0.725838	-0.855127	0.889579	H	3.968637	0.822370	-1.337878
C	1.733169	-0.025127	1.187396	H	2.313611	1.445268	-1.090238
C	2.859259	-0.192662	0.210975	H	3.756623	-0.588376	0.704906
C	3.205217	1.057685	-0.591053	H	1.769910	0.687510	2.004577
C	-0.587701	-1.046939	1.589213	H	-0.588600	-2.013348	2.109204
C	-1.850378	-1.044709	0.691320	H	-0.685182	-0.267577	2.350912
C	-1.840738	0.075061	-0.361667	H	-1.254552	-2.520683	-0.418835
C	-3.173058	0.233187	-1.071566	H	-2.708897	-0.887521	1.355358
C	-0.583338	2.115270	-0.203832	H	0.326351	4.014042	0.172514
C	-0.327191	3.308063	0.685656	H	-1.268740	3.791851	0.960479
O	-0.007733	1.892583	-1.248926	H	0.151519	2.974417	1.613380
O	2.388579	-1.227284	-0.683017	H	-1.047945	-0.111311	-1.088615
O	-1.523936	1.315053	0.335905	H	-3.102146	0.987333	-1.861247
O	0.515975	-2.445647	-0.954605	H	-3.457774	-0.724226	-1.515157
O	-2.076545	-2.289653	0.063960	H	-3.952164	0.536041	-0.363171

Table S8: Atomic coordinates (Å) of **1a**-4 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	1.140050	-1.613754	-0.323037	H	3.968669	0.822491	-1.337844
C	0.725849	-0.855118	0.889592	H	2.313560	1.445281	-1.090392
C	1.733088	-0.024985	1.187346	H	3.602189	1.828146	0.079688
C	2.859218	-0.192519	0.210971	H	3.756581	-0.588151	0.704981
C	3.205159	1.057796	-0.591113	H	1.769755	0.687695	2.004493
C	-0.587688	-1.046994	1.589221	H	-0.588586	-2.013428	2.109166
C	-1.850334	-1.044767	0.691292	H	-0.685180	-0.267656	2.350940
C	-1.840682	0.075016	-0.361687	H	-1.254440	-2.520756	-0.418802
C	-3.172969	0.233066	-1.071669	H	-2.708877	-0.887598	1.355301
C	-0.583400	2.115281	-0.203815	H	0.150649	2.974358	1.613775
C	-0.327379	3.308066	0.685726	H	0.326659	4.013812	0.172893
O	-0.007812	1.892655	-1.248917	H	-1.268957	3.792169	0.959909
O	2.388640	-1.227202	-0.682973	H	-1.047854	-0.111338	-1.088606
O	-1.523991	1.314993	0.335901	H	-3.952189	0.535702	-0.363303
O	0.516149	-2.445769	-0.954493	H	-3.102074	0.987351	-1.861221
O	-2.076469	-2.289715	0.063920	H	-3.457518	-0.724312	-1.515442

Table S9: Atomic coordinates (Å) of **1a**-5 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	2.313388	1.033854	-0.558123	H	5.291883	-0.947323	0.924471
C	1.400575	-0.138425	-0.612235	H	3.704842	-0.970841	1.733163
C	2.149022	-1.241666	-0.529036	H	4.302808	-2.425586	0.902520
C	3.600575	-0.866031	-0.421652	H	4.173988	-1.215766	-1.290590
C	4.269304	-1.331223	0.868102	H	1.803903	-2.269077	-0.503957
C	-0.075412	0.062563	-0.630086	H	-0.315389	0.911377	-1.279686
C	-0.587166	0.340758	0.803703	H	-0.582653	-0.823569	-1.023032
C	-2.007463	0.946737	0.811586	H	-1.228390	-1.371530	1.403608
C	-1.998000	2.457570	0.640184	H	0.067769	1.096318	1.251526
C	-3.259376	-0.824168	-0.261880	H	-3.844021	-0.780390	-2.324209
C	-4.257249	-1.092172	-1.360019	H	-4.502979	-2.153968	-1.380535
O	-2.869543	-1.664498	0.531324	H	-5.164581	-0.503752	-1.188575
O	3.601537	0.576873	-0.469792	H	-2.486436	0.660959	1.753579
O	-2.858456	0.453273	-0.275007	H	-1.517528	2.924089	1.505287
O	2.027668	2.208482	-0.575338	H	-1.439127	2.749052	-0.254848
O	-0.468041	-0.800155	1.627733	H	-3.018594	2.841419	0.556650

Table S10: Atomic coordinates (Å) of **1a**-6 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	2.313488	1.033876	-0.558053	H	3.704412	-0.971071	1.733209
C	1.400551	-0.138292	-0.612277	H	4.302284	-2.425891	0.902629
C	2.148855	-1.241632	-0.529113	H	5.291569	-0.947767	0.924735
C	3.600440	-0.866199	-0.421607	H	4.173909	-1.215985	-1.290486
C	4.268945	-1.331524	0.868224	H	1.803578	-2.268992	-0.504098
C	-0.075436	0.062779	-0.630187	H	-0.315378	0.911486	-1.279948
C	-0.587188	0.341283	0.803520	H	-0.582678	-0.823409	-1.023000
C	-2.007613	0.946952	0.811346	H	-1.227999	-1.370994	1.403850
C	-1.998547	2.457752	0.639566	H	0.067637	1.097072	1.251112
C	-3.259146	-0.824512	-0.261692	H	-4.502673	-2.154732	-1.379946
C	-4.256966	-1.092925	-1.359782	H	-5.164317	-0.504460	-1.188585
O	-2.869072	-1.664604	0.531625	H	-3.843694	-0.781461	-2.324055
O	3.601608	0.576706	-0.469696	H	-2.486421	0.661314	1.753467
O	-2.858584	0.453056	-0.275040	H	-3.019268	2.841344	0.556399
O	2.027945	2.208534	-0.575208	H	-1.517771	2.924610	1.504312
O	-0.467810	-0.799382	1.627892	H	-1.440190	2.749102	-0.255830

Table S11: Conformational analysis of the B3LYP/6-31G(d) optimized conformers of **1b** in the gas phase (T=298.15 K)

Conformer	**E[a] (Hartree)**	**C[b] (Hartree)**	**G[c] (kcal/mol)**	**ΔG[d] (kcal/mol)**	**Population[e]**
1b-1	-804.880747	0.214987	-504927.764258	0.0	34.68%
1b-2	-804.880764	0.215677	-504927.341829	0.422429	16.99%
1b-3	-804.880763	0.215683	-504927.337756	0.426502	16.88%
1b-4	-804.88076	0.215687	-504927.333259	0.430999	16.75%
1b-5	-804.877734	0.213435	-504926.847353	0.916904	7.37%
1b-6	-804.877734	0.213441	-504926.843927	0.920331	7.33%

[a]Electronic energy obtained at M062X/6-311+G(2d,p) level of theory; [b]Thermal correction to Gibbs free energy obtained at B3LYP/6-31G(d) level of theory; [c]Gibbs free energy (E + C); [d]The relative Gibbs free energy; [e]The Boltzmann distribution of each conformer.

Table S12: Atomic coordinates (Å) of **1b**-1 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	2.332985	-0.841160	-0.285472	H	3.726103	2.176775	-0.892112
C	1.129780	-0.003293	-0.515574	H	3.244774	3.251326	0.442277
C	1.334251	1.170781	0.092382	H	4.626858	2.150128	0.642553
C	2.695411	1.181603	0.726309	H	2.623186	1.250145	1.819591
C	3.634850	2.258322	0.195212	H	0.642370	2.001946	0.151434
C	-0.021267	-0.533533	-1.312136	H	-0.636266	0.285135	-1.694553
C	-0.911790	-1.518574	-0.523671	H	0.382378	-1.068526	-2.180948
C	-1.748485	-0.818331	0.556563	H	0.694533	-2.640341	-0.323771
C	-2.544200	-1.789640	1.411137	H	-1.615597	-1.974030	-1.240226
C	-2.574472	1.376151	-0.034938	H	-4.656547	1.827876	-0.276124
C	-3.703825	2.070212	-0.758433	H	-3.543523	3.148419	-0.737825
O	-1.673914	1.944643	0.549457	H	-3.763947	1.716476	-1.792390
O	3.242192	-0.124937	0.427260	H	-1.103043	-0.189917	1.172843
O	-2.708511	0.039077	-0.127190	H	-3.123597	-1.246750	2.164525
O	2.529373	-1.985744	-0.645443	H	-3.235723	-2.371123	0.791795
O	-0.156794	-2.517251	0.137753	H	-1.860159	-2.479083	1.909967

Table S13: Atomic coordinates (Å) of **1b**-2 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	-1.242627	-1.313966	-0.447911	H	-4.375687	1.327745	0.770951
C	-0.818602	-0.572049	0.770786	H	-4.763723	0.347308	-0.659413
C	-1.652215	0.466386	0.900433	H	-4.286672	-0.447745	0.859263
C	-2.653441	0.476560	-0.214802	H	-2.473065	1.334406	-0.875083
C	-4.113070	0.420469	0.216357	H	-1.626443	1.231491	1.669135
C	0.363827	-0.955457	1.609031	H	0.528715	-0.166708	2.349456
C	1.679244	-1.209891	0.827518	H	0.153698	-1.881523	2.158403
C	1.936770	-0.179176	-0.286170	H	0.938490	-2.644824	-0.248570
C	3.328868	-0.294270	-0.881039	H	2.497975	-1.145117	1.554185
C	0.955620	2.020772	-0.307094	H	0.288637	4.039722	-0.070214
C	0.923381	3.324956	0.454237	H	0.535036	3.153888	1.464375
O	0.310707	1.785943	-1.307470	H	1.935265	3.727538	0.560450
O	-2.330560	-0.706453	-0.980517	H	1.182666	-0.287837	-1.067499
O	1.789070	1.147881	0.296900	H	3.449265	0.398028	-1.720034
O	-0.741804	-2.300653	-0.954360	H	4.089366	-0.066605	-0.125836
O	1.747132	-2.515378	0.291391	H	3.483589	-1.316491	-1.235200

Table S14: Atomic coordinates (Å) of **1b**-3 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	-1.242035	-1.314025	-0.448060	H	-4.286473	-0.448963	0.859144
C	-0.818343	-0.572351	0.770866	H	-4.376032	1.326502	0.771036
C	-1.652261	0.465815	0.900717	H	-4.763560	0.346144	-0.659498
C	-2.653399	0.475999	-0.214611	H	-2.473168	1.334041	-0.874669
C	-4.113040	0.419377	0.216365	H	-1.626742	1.230765	1.669581
C	0.364189	-0.955535	1.609074	H	0.528849	-0.166810	2.349580
C	1.679637	-1.209578	0.827475	H	0.154340	-1.881704	2.158374
C	1.936763	-0.178702	-0.286157	H	0.939372	-2.644497	-0.248907
C	3.328956	-0.293193	-0.880879	H	2.498399	-1.144596	1.554091
C	0.954728	2.020839	-0.307072	H	0.286652	4.039377	-0.070130
C	0.922019	3.325042	0.454157	H	0.534210	3.153861	1.464475
O	0.309869	1.785751	-1.307445	H	1.933710	3.728251	0.559841
O	-2.330106	-0.706753	-0.980589	H	1.182779	-0.287681	-1.067549
O	1.788446	1.148248	0.296972	H	3.484262	-1.315419	-1.234774
O	-0.740830	-2.300411	-0.954788	H	3.449086	0.398960	-1.720033
O	1.747842	-2.515014	0.291330	H	4.089256	-0.064920	-0.125654

Table S15: Atomic coordinates (Å) of **1b**-4 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	-1.241620	-1.313912	-0.448181	H	-4.763610	0.344980	-0.659721
C	-0.818248	-0.572356	0.770931	H	-4.286520	-0.450075	0.858949
C	-1.652554	0.465474	0.900940	H	-4.376710	1.325354	0.770955
C	-2.653611	0.475570	-0.214468	H	-2.473535	1.333747	-0.874379
C	-4.113271	0.418364	0.216262	H	-1.627357	1.230308	1.669929
C	0.364383	-0.955268	1.609106	H	0.528932	-0.166445	2.349530
C	1.679865	-1.209224	0.827499	H	0.154735	-1.881408	2.158535
C	1.936963	-0.178435	-0.286234	H	0.939884	-2.644177	-0.248949
C	3.329266	-0.292846	-0.880711	H	2.498608	-1.144084	1.554128
C	0.954253	2.020821	-0.307094	H	0.285752	4.039199	-0.070488
C	0.921138	3.325054	0.454025	H	0.532992	3.153844	1.464221
O	0.309137	1.785461	-1.307275	H	1.932703	3.728458	0.560092
O	-2.329816	-0.706991	-0.980644	H	1.183109	-0.287537	-1.067720
O	1.788481	1.148616	0.296695	H	4.089386	-0.064183	-0.125420
O	-0.739995	-2.300044	-0.955073	H	3.484837	-1.315154	-1.234253
O	1.748188	-2.514709	0.291571	H	3.449448	0.399063	-1.720059

Table S16: Atomic coordinates (Å) of **1b**-5 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	-2.309298	1.006289	-0.357094	H	-4.278951	-1.452695	-1.588030
C	-1.430545	-0.183180	-0.203678	H	-4.649630	-2.556333	-0.241663
C	-2.188016	-1.196351	0.225075	H	-5.599944	-1.069367	-0.459233
C	-3.618010	-0.748377	0.345485	H	-3.954128	-0.783911	1.390525
C	-4.600007	-1.504371	-0.543211	H	-1.864859	-2.203363	0.463383
C	0.036719	-0.064460	-0.433414	H	0.477067	-1.044551	-0.639408
C	0.723150	0.540563	0.814876	H	0.212880	0.579650	-1.301725
C	2.135080	1.082014	0.501227	H	1.426525	-0.995407	1.735546
C	2.107880	2.505477	-0.032498	H	0.131507	1.404379	1.137145
C	3.233892	-0.938530	-0.250579	H	4.323912	-2.541306	-1.150299
C	4.084158	-1.499319	-1.362464	H	3.552150	-1.419942	-2.315544
O	2.942607	-1.548157	0.764700	H	5.006480	-0.916519	-1.454570
O	-3.591370	0.642328	-0.040792	H	2.728331	1.017365	1.418993
O	2.840839	0.311212	-0.526603	H	3.109945	2.822096	-0.335086
O	-2.003259	2.126768	-0.692442	H	1.437286	2.590724	-0.893576
O	0.704390	-0.358814	1.903335	H	1.745755	3.183954	0.745607

Table S17: Atomic coordinates (Å) of **1b**-6 obtained at the B3LYP/6-31G(d) level of theory in the gas phase

C	-2.309249	1.006252	-0.356924	H	-5.600007	-1.069215	-0.459273
C	-1.430546	-0.183276	-0.203639	H	-4.279060	-1.452532	-1.588130
C	-2.188069	-1.196466	0.224974	H	-4.649791	-2.556269	-0.241856
C	-3.618043	-0.748437	0.345443	H	-3.954146	-0.784056	1.390486
C	-4.600103	-1.504283	-0.543309	H	-1.864966	-2.203529	0.463149
C	0.036721	-0.064602	-0.433382	H	0.477068	-1.044738	-0.639170
C	0.723151	0.540676	0.814789	H	0.212902	0.579326	-1.301825
C	2.135063	1.082089	0.501002	H	1.426623	-0.995079	1.735727
C	2.107806	2.505473	-0.032937	H	0.131485	1.404526	1.136920
C	3.233944	-0.938535	-0.250453	H	5.006070	-0.916321	-1.455160
C	4.084089	-1.499536	-1.362325	H	4.324426	-2.541288	-1.149653
O	2.942813	-1.547939	0.764998	H	3.551634	-1.421026	-2.315232
O	-3.591338	0.642308	-0.040693	H	2.728349	1.017585	1.418754
O	2.840757	0.311122	-0.526741	H	1.745804	3.184061	0.745129
O	-2.003158	2.126748	-0.692175	H	3.109834	2.822030	-0.335715
O	0.704440	-0.358517	1.903403	H	1.437078	2.590606	-0.893923

Table S18: Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer **1b**-1 at the CAM-B3LYP/6-311G(d) level of theory in MeOH with IEFPCM solvent model

***Num*[a]**	***Transition*[b]**	***CI-coeff*[b]**	***ΔE (eV)*[d]**	***λ (nm)*[e]**	***f*[f]**	***R_{vel}*[g]**	***R_{len}*[h]**
1	58->62	0.6342	5.5189	224.66	0.0014	-10.6655	-10.3518
2	59->63	0.65785	5.9747	207.51	0.0018	-20.8666	-21.001
3	61->62	0.67037	6.1282	202.32	0.2707	38.9507	35.2156
4	60->62	0.67529	6.5225	190.09	0.0072	11.189	12.5771
5	56->62	0.66324	6.9786	177.66	0.0805	-1.703	-1.2914
6	59->62	0.65298	7.2367	171.33	0.0025	4.8176	7.1155
7	53->62	0.53585	7.5140	165.00	0.0059	22.3567	24.1936
	57->62	-0.26709					
8	53->62	0.26323	7.6604	161.85	0.0188	0.2821	-0.058
	57->62	0.57134					
9	57->63	-0.41507	7.9637	155.69	0.1033	-2.282	-2.8789
	60->63	0.45945					
	61->63	-0.25278					
10	51->62	-0.36911	8.0305	154.39	0.0082	-17.3085	-17.8365
	52->62	0.36947					
11	60->64	0.23241	8.1631	151.88	0.0426	27.1868	28.9367
	61->63	0.3671					
	61->64	0.30004					
12	54->62	0.27916	8.2757	149.82	0.0029	15.5729	13.4019
13	60->64	-0.30023	8.3024	149.34	0.0406	-18.3603	-28.6234
	61->63	0.43895					
14	54->62	0.25553	8.4329	147.02	0.0451	-64.4193	-56.6786
	60->64	-0.22998					
	61->64	0.36711					
15	55->63	0.45909	8.5013	145.84	0.0096	-21.4861	-19.1419
	60->63	-0.27391					
16	54->62	0.4936	8.5627	144.80	0.0152	-20.179	-16.3339

17	55->63	0.2548	8.6306	143.66	0.0171	24.1563	21.8898
	57->63	0.34162					
	60->63	0.33415					
18	55->62	0.53667	8.7560	141.60	0.0344	-10.0702	-9.7813
19	59->64	0.51707	8.8368	140.30	0.0682	-11.8795	-13.4727
	59->65	-0.2362					
20	61->65	0.29028	8.9333	138.79	0.0063	-0.9555	-1.7874
	61->66	0.47479					
21	46->62	-0.25209	8.9552	138.45	0.0021	-3.5978	-3.3055
	49->62	0.30443					
	52->62	0.26315					
	55->62	-0.26289					
22	57->64	-0.2832	9.1731	135.16	0.0872	14.6829	14.8712
	60->64	0.22828					
	61->65	0.33158					
23	48->62	0.54215	9.2197	134.48	0.0234	-20.6998	-21.2808
24	60->67	0.25332	9.2809	133.59	0.0231	0.5434	3.5095
	60->70	0.30338					
25	45->62	-0.29373	9.3422	132.71	0.0085	2.4549	1.7861
	50->62	0.25755					
	52->62	0.30569					
26	57->64	-0.25771	9.3663	132.37	0.0119	14.9974	14.8798
	60->66	0.30787					
	60->67	0.29401					
27	58->63	0.62403	9.4398	131.34	0.0327	39.4485	40.3705
28	61->68	0.29125	9.5134	130.33	0.0752	22.8432	30.3614
29	61->67	0.38471	9.5543	129.77	0.0177	42.8486	44.3128
	61->69	-0.23483					
	61->71	0.22669					
30	57->64	0.32299	9.5654	129.62	0.0786	-11.7687	-20.3295
31	56->64	0.25014	9.6242	128.83	0.0067	-20.2587	-20.3524
32	56->64	0.22815	9.6523	128.45	0.0315	-13.9213	-18.9424
33	60->69	0.38456	9.7166	127.60	0.0280	-1.4152	3.1115
34	59->65	0.28427	9.7592	127.04	0.0195	3.916	2.5819
	59->67	0.26365					
35	60->68	0.35212	9.8124	126.35	0.1022	38.7327	43.0158
36	56->66	0.2351	9.8447	125.94	0.1011	-59.297	-60.7409
	58->68	0.23882					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength;[f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S19: Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer **1b**-2 at the CAM-B3LYP/6-311G(d) level of theory in MeOH with IEFPCM solvent model

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*f*[f]	R_{vel}[g]	R_{len}[h]
1	58->62	0.59964	5.4988	225.47	0.0029	-17.8632	-18.1514
	61->62	-0.25518					
2	59->63	0.58583	5.9523	208.30	0.0253	24.5356	22.1921
	61->62	-0.22587					
3	59->63	0.24452	6.0799	203.92	0.2165	1.1494	-0.5618
	60->62	-0.27556					
	61->62	0.53526					
4	60->62	0.61446	6.4495	192.24	0.0481	15.382	16.929
	61->62	0.29439					
5	57->62	0.261	6.8399	181.27	0.0076	-7.095	-7.6229
	59->62	0.59106					
6	56->62	-0.31264	6.9217	179.12	0.0587	-12.1448	-12.9402
	57->62	0.52091					
	59->62	-0.31872					
7	53->62	0.29516	7.3208	169.36	0.0038	3.5347	5.501
	55->62	0.46169					
	56->62	-0.28165					
8	51->62	0.27384	7.6571	161.92	0.0087	1.3082	0.3151
	55->62	0.39377					
	56->62	0.32467					
	57->62	0.27678					
9	53->62	0.38757	7.7614	159.75	0.0360	38.6649	37.5592
	56->62	0.33913					
10	61->63	0.5694	7.8406	158.13	0.0512	-1.5051	-2.1505
11	60->63	0.58275	8.0574	153.88	0.0270	-18.1603	-21.0045
12	58->65	-0.26989	8.2572	150.15	0.0190	-3.281	-1.7572
	61->64	-0.23731					
	61->65	0.38731					
13	61->64	0.40204	8.3469	148.54	0.0163	-44.4438	-42.2854
14	54->62	0.41099	8.4183	147.28	0.0026	8.1271	8.6202
	54->63	-0.27732					
15	60->64	0.36898	8.5347	145.27	0.0103	4.6079	4.0134
	61->64	-0.23174					
	61->65	-0.30868					
16	54->63	0.28685	8.5959	144.24	0.0035	9.2782	10.1768
	60->64	0.25632					
17	60->65	0.42502	8.6140	143.93	0.1720	-2.6479	2.9145
	61->65	-0.25916					
18	54->62	0.42394	8.7186	142.21	0.0038	-14.8322	-16.23
19	56->63	0.22546	8.8245	140.50	0.0428	29.2634	29.9853
	59->64	0.41326					
20	59->64	0.47097	8.8529	140.05	0.0612	26.0533	23.1537
21	52->62	0.55768	8.9888	137.93	0.0099	1.2373	-0.156
22	60->64	-0.2511	9.0327	137.26	0.0043	3.2644	5.5021
	61->69	0.29771					
23	58->63	0.63278	9.0577	136.88	0.0004	-0.7471	-0.1213

24	61->67	0.36386	9.1392	135.66	0.0016	2.4622	2.47
	61->69	0.22437					
25	49->62	-0.26577	9.1699	135.21	0.0132	-27.7228	-22.4245
	61->66	0.3428					
26	49->62	0.33542	9.1868	134.96	0.0039	-11.8522	-12.9819
27	43->62	0.23692	9.2944	133.40	0.0072	10.7237	11.2948
	45->62	0.25207					
	49->62	0.29532					
28	60->66	0.40305	9.3324	132.85	0.0100	9.7449	8.8046
	61->69	0.2443					
29	46->62	0.29721	9.4423	131.31	0.0010	-9.3273	-12.1009
	50->62	-0.28579					
	51->62	-0.27025					
30	50->62	-0.26172	9.5208	130.22	0.0490	16.4573	7.8682
	61->67	0.27252					
31	60->67	0.24939	9.5253	130.16	0.0542	-88.0646	-84.6546
	61->67	0.33637					
32	56->63	0.40254	9.5706	129.55	0.0035	8.5443	6.615
	57->63	-0.29242					
33	55->63	0.31181	9.6045	129.09	0.0289	-2.0564	-2.7663
	57->63	-0.30628					
34	61->70	0.36811	9.6387	128.63	0.0275	33.8394	29.3909
35	61->70	0.30296	9.6769	128.12	0.0600	0.4061	0.1302
36	50->62	0.29622	9.7073	127.72	0.0340	-18.1264	-19.1718
	55->63	-0.27676					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength;[f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S20: Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer **1b**-3 at the CAM-B3LYP/6-311G(d) level of theory in MeOH with IEFPCM solvent model.

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*f*[f]	R_{vel}[g]	R_{len}[h]
1	58->62	0.59959	5.4986	225.48	0.0029	-17.8615	-18.15
	61->62	-0.25524					
2	59->63	0.58568	5.9520	208.31	0.0253	24.5397	22.1983
	61->62	-0.22605					
3	59->63	0.24466	6.0798	203.93	0.2164	1.1388	-0.5721
	60->62	-0.27539					
	61->62	0.53525					
4	60->62	0.6145	6.4493	192.24	0.0482	15.4157	16.9633
	61->62	0.29422					
5	57->62	0.26084	6.8396	181.27	0.0076	-7.0977	-7.6252
	59->62	0.59109					
6	56->62	-0.31259	6.9216	179.13	0.0587	-12.1621	-12.9598
	57->62	0.52102					
	59->62	-0.31851					
7	53->62	0.29499	7.3206	169.36	0.0038	3.5241	5.4895
	55->62	0.46136					
	56->62	-0.28223					
8	51->62	0.27374	7.6569	161.93	0.0087	1.3138	0.3181
	55->62	0.39416					
	56->62	0.32448					
	57->62	0.27672					
9	53->62	0.38771	7.7611	159.75	0.0360	38.675	37.5729
	56->62	0.33892					
10	61->63	0.56956	7.8404	158.13	0.0512	-1.506	-2.1515
11	60->63	0.58283	8.0573	153.88	0.0271	-18.1735	-21.0228
12	58->65	-0.26987	8.2572	150.15	0.0190	-3.2851	-1.7615
	61->64	-0.23713					
	61->65	0.38737					
13	61->64	0.40178	8.3468	148.54	0.0163	-44.4641	-42.3111
14	54->62	0.41088	8.4180	147.28	0.0026	8.1417	8.6357
	54->63	-0.27711					
15	60->64	0.36842	8.5346	145.27	0.0103	4.4901	3.9157
	61->64	-0.23202					
	61->65	-0.30901					
16	54->63	0.28701	8.5959	144.24	0.0034	7.9448	8.833
	60->64	0.25603					
17	60->65	0.42559	8.6140	143.93	0.1720	-1.2233	4.3323
	61->65	-0.25828					
18	54->62	0.42364	8.7186	142.21	0.0038	-14.8028	-16.2009
19	56->63	0.22545	8.8244	140.50	0.0428	29.2433	29.9605
	59->64	0.41294					
20	59->64	0.47121	8.8528	140.05	0.0613	26.0287	23.1333
21	52->62	0.55777	8.9887	137.93	0.0099	1.2566	-0.1347
22	60->64	-0.25113	9.0327	137.26	0.0043	3.2839	5.5151
	61->69	0.29765					

23	58->63	0.63246	9.0573	136.89	0.0004	-0.7093	-0.0789
24	61->67	0.36389	9.1393	135.66	0.0016	2.4522	2.4617
	61->69	0.22438					
25	49->62	-0.26725	9.1698	135.21	0.0132	-27.7693	-22.4705
	61->66	0.34155					
26	49->62	0.3338	9.1866	134.96	0.0039	-11.7672	-12.8906
	61->66	0.22378					
27	43->62	0.23702	9.2943	133.40	0.0072	10.6694	11.2398
	45->62	0.25196					
	49->62	0.29568					
28	60->66	0.40315	9.3324	132.85	0.0100	9.7597	8.8164
	61->69	0.24438					
29	46->62	0.29708	9.4420	131.31	0.0010	-9.409	-12.1737
	50->62	-0.28613					
	51->62	-0.27055					
30	50->62	-0.26338	9.5207	130.23	0.0499	15.3745	6.7711
	61->67	0.26833					
31	60->67	0.24897	9.5251	130.17	0.0533	-87.0097	-83.586
	61->67	0.33969					
32	56->63	0.40321	9.5703	129.55	0.0036	8.6193	6.6873
	57->63	-0.29316					
33	55->63	0.31232	9.6042	129.09	0.0288	-2.0981	-2.8034
	57->63	-0.30563					
34	61->70	0.3673	9.6387	128.63	0.0275	33.7596	29.3295
35	61->70	0.30416	9.6768	128.12	0.0599	0.5575	0.2561
36	50->62	0.29612	9.7072	127.72	0.0342	-18.1722	-19.2125
	55->63	-0.27656					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength;[f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S21: Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer **1b**-4 at the CAM-B3LYP/6-311G(d) level of theory in MeOH with IEFPCM solvent model

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*f*[f]	R_{vel}[g]	R_{len}[h]
1	58->62	0.59951	5.4985	225.49	0.0029	-17.8533	-18.1414
	61->62	-0.25534					
2	59->63	0.58576	5.9519	208.31	0.0252	24.5398	22.1983
	61->62	-0.22568					
3	59->63	0.24432	6.0798	203.93	0.2165	1.1551	-0.5564
	60->62	-0.27557					
	61->62	0.53529					
4	60->62	0.6144	6.4491	192.25	0.0481	15.4076	16.9538
	61->62	0.29434					
5	57->62	-0.25918	6.8392	181.28	0.0075	-7.0556	-7.5804
	59->62	0.5921					
6	56->62	0.313	6.9218	179.12	0.0589	-12.226	-13.0283
	57->62	0.52191					
	59->62	0.31663					
7	53->62	0.29471	7.3206	169.36	0.0038	3.5353	5.498
	55->62	0.46086					
	56->62	-0.28314					
8	51->62	0.27419	7.6571	161.92	0.0087	1.285	0.2895
	55->62	0.39471					
	56->62	0.32339					
	57->62	-0.27631					
9	53->62	0.38761	7.7612	159.75	0.0361	38.7253	37.62
	56->62	0.33922					
10	61->63	0.56957	7.8405	158.13	0.0512	-1.5695	-2.2119
11	60->63	0.58284	8.0568	153.89	0.0270	-18.1258	-20.9792
12	58->65	-0.26988	8.2572	150.15	0.0190	-3.2829	-1.757
	61->64	-0.23727					
	61->65	0.38741					
13	61->64	0.40191	8.3469	148.54	0.0163	-44.4636	-42.3148
14	54->62	0.41088	8.4181	147.28	0.0026	8.104	8.5964
	54->63	-0.27728					
15	60->64	0.36883	8.5346	145.27	0.0103	4.513	3.9325
	61->64	-0.2317					
	61->65	-0.30904					
16	54->63	0.28712	8.5959	144.24	0.0035	8.5642	9.4555
	60->64	0.25602					
17	60->65	0.4253	8.6140	143.93	0.1719	-1.8328	3.7337
	61->65	-0.25854					
18	54->62	0.42385	8.7187	142.20	0.0038	-14.8225	-16.2188
19	56->63	0.22585	8.8243	140.50	0.0428	29.2551	29.9697
	59->64	0.41243					
20	59->64	0.47163	8.8527	140.05	0.0613	25.9408	23.0425
21	52->62	0.55764	8.9889	137.93	0.0099	1.2218	-0.1737
22	60->64	-0.2511	9.0327	137.26	0.0043	3.3211	5.5656
	61->69	0.29737					

23	58->63	0.63224	9.0568	136.90	0.0004	-0.6345	-0.0052
24	61->67	0.36397	9.1394	135.66	0.0016	2.4677	2.4806
	61->69	0.2246					
25	49->62	-0.26523	9.1698	135.21	0.0132	-27.676	-22.3726
	61->66	0.34273					
26	49->62	0.33481	9.1866	134.96	0.0039	-11.8484	-12.98
27	43->62	0.23676	9.2943	133.40	0.0073	10.6886	11.2581
	45->62	0.25167					
	49->62	0.29591					
28	60->66	0.40305	9.3323	132.86	0.0100	9.6863	8.7387
	61->69	0.24422					
29	46->62	0.29698	9.4419	131.31	0.0010	-9.4745	-12.2439
	50->62	-0.28607					
	51->62	-0.27043					
30	50->62	0.26502	9.5206	130.23	0.0506	14.4013	5.7933
	61->67	-0.26449					
31	60->67	0.24857	9.5250	130.17	0.0524	-85.7593	-82.3339
	61->67	0.34265					
32	56->63	0.40343	9.5701	129.55	0.0036	8.706	6.7778
	57->63	0.29258					
33	55->63	0.31261	9.6041	129.09	0.0288	-2.3192	-3.0226
	57->63	0.3064					
34	61->70	0.36624	9.6386	128.63	0.0276	33.4949	29.0818
35	61->70	0.30547	9.6769	128.12	0.0600	0.8287	0.5058
36	50->62	0.2962	9.7071	127.72	0.0343	-18.2628	-19.3015
	55->63	-0.27614					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength;[f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S22: Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer **1b**-5 at the CAM-B3LYP/6-311G(d) level of theory in MeOH with IEFPCM solvent model

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*f*[f]	R_{vel}[g]	R_{len}[h]
1	59->62	0.64601	5.4146	228.98	0.0002	-4.7821	-4.3272
2	56->63	-0.24644	6.0291	205.64	0.0018	-1.0452	-0.9319
	58->63	0.56528					
	60->63	-0.30483					
3	61->62	0.68193	6.1562	201.40	0.3451	17.2357	17.4562
4	58->62	0.20919	6.8184	181.84	0.0588	37.9415	40.4539
	60->62	0.61707					
5	56->62	0.22859	6.9708	177.86	0.0449	-3.9208	-3.8229
	57->62	0.63654					
6	60->63	-0.32013	7.4994	165.33	0.0236	11.6728	5.1214
	61->63	0.56834					
7	54->62	0.49592	7.5441	164.35	0.0047	-6.6771	-7.3915
	55->62	0.22561					
	58->62	-0.26627					
8	53->62	0.27918	7.7241	160.52	0.0091	-2.5267	-1.2899
	54->62	0.27131					
	56->62	0.20031					
	58->62	0.44189					
9	56->63	0.53879	8.0521	153.98	0.0718	-41.4843	-48.1538
	57->63	-0.24029					
	58->63	0.24906					
10	52->62	0.38257	8.1090	152.90	0.0011	-1.796	-2.0056
	53->62	0.22994					
	58->62	-0.29513					
11	55->63	0.35355	8.3286	148.87	0.0197	21.5075	23.4305
	60->63	0.38469					
	61->63	0.28005					
12	56->62	0.38778	8.4132	147.37	0.0055	29.4134	30.6808
	59->67	-0.29307					
13	51->62	0.23811	8.4979	145.90	0.0052	-22.6968	-23.641
	56->62	0.41375					
	59->67	0.2232					
14	61->64	0.45527	8.5152	145.60	0.0231	0.9472	1.0552
	61->65	0.36285					
	61->68	-0.20683					
15	55->63	0.23775	8.7158	142.25	0.1032	-26.621	-34.3307
	60->64	0.27177					
	61->64	-0.21454					
	61->65	0.20692					
16	55->63	-0.24885	8.7731	141.32	0.0191	26.382	27.9586
	60->63	0.26849					
	61->65	0.24653					
	61->66	-0.2435					
17	61->67	0.51235	8.8150	140.65	0.1618	31.3637	33.1555
18	45->62	-0.26043	8.9157	139.06	0.0054	-0.2829	0.1067
	51->62	0.22553					
	52->62	0.3489					
	59->67	-0.20843					

19	61->65	0.21251	8.9652	138.29	0.0250	-2.0915	-1.3479
	61->66	0.41808					
	61->69	0.21822					
20	55->62	0.28383	9.0745	136.63	0.0382	-24.9302	-23.4866
	58->64	0.41289					
	60->64	-0.24943					
21	55->62	0.53167	9.0983	136.27	0.0164	-18.7514	-19.6809
22	59->63	0.60879	9.1268	135.85	0.0149	0.2312	-1.0912
23	61->64	0.20969	9.1448	135.58	0.0096	-1.5042	0.7968
	61->70	0.20751					
24	48->62	-0.25584	9.2959	133.37	0.0196	-20.4462	-19.738
	49->62	0.53133					
25	60->64	0.21336	9.3461	132.66	0.0425	45.5927	42.579
	60->66	0.20999					
	61->69	0.43958					
26	46->62	0.31817	9.4416	131.32	0.0053	-14.1604	-13.7869
	51->62	0.25965					
	53->62	0.20488					
	60->66	0.20039					
27	59->64	0.2711	9.4522	131.17	0.0280	47.7975	43.6968
	59->66	0.26025					
	59->69	0.22365					
28	46->62	-0.20312	9.4949	130.58	0.0415	-6.1118	-1.7781
	59->64	-0.20696					
	60->66	0.28891					
29	60->67	0.29155	9.5049	130.44	0.0244	-1.8959	-1.7528
	61->66	-0.23366					
	61->68	0.22602					
30	52->63	-0.22193	9.5711	129.54	0.0886	44.655	48.3738
	53->63	0.40954					
	54->63	-0.25497					
	55->63	-0.28936					
31	56->64	0.38471	9.5903	129.28	0.0003	0.3709	0.5581
	57->64	-0.20101					
32	56->64	0.25964	9.6400	128.61	0.0282	-18.1775	-16.0162
	58->64	0.2343					
	60->64	0.22531					
	60->69	0.22215					
33	50->63	0.30367	9.7119	127.66	0.0720	4.5593	6.2745
	51->63	0.2572					
	57->63	-0.26571					
34	60->67	0.22259	9.7475	127.20	0.0198	5.7923	11.1508
	61->70	0.3729					
	61->71	0.20878					
35	50->63	-0.21112	9.7808	126.76	0.0201	-25.3211	-31.0803
	57->65	0.3533					
36	57->65	-0.23757	9.8341	126.08	0.0500	21.0379	17.9444
	57->67	0.28036					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

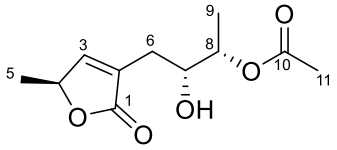
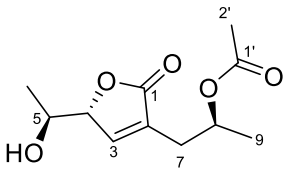
Table S23: Key transitions, oscillator strengths, and rotatory strengths in the ECD spectrum of conformer **1b**-6 at the CAM-B3LYP/6-311G(d) level of theory in MeOH with IEFPCM solvent model.

Num[a]	*Transition*[b]	*CI-coeff*[b]	*ΔE (eV)*[d]	*λ (nm)*[e]	*f*[f]	R_{vel}[g]	R_{len}[h]
1	59->62	0.64601	5.4146	228.98	0.0002	-4.7799	-4.3252
2	56->63	-0.24645	6.0290	205.64	0.0018	-1.042	-0.9315
	58->63	0.56527					
	60->63	-0.30482					
3	61->62	0.68193	6.1562	201.40	0.3451	17.2292	17.4489
4	58->62	0.20918	6.8184	181.84	0.0589	37.9478	40.4612
	60->62	0.61708					
5	56->62	0.22869	6.9708	177.86	0.0449	-3.9137	-3.816
	57->62	0.63651					
6	60->63	-0.32011	7.4993	165.33	0.0236	11.6656	5.1108
	61->63	0.56836					
7	54->62	0.49597	7.5442	164.34	0.0047	-6.6631	-7.3761
	55->62	0.22541					
	58->62	-0.26628					
8	53->62	0.27923	7.7242	160.51	0.0091	-2.5406	-1.3041
	54->62	0.27127					
	56->62	0.20031					
	58->62	0.44184					
9	56->63	0.53874	8.0520	153.98	0.0718	-41.5132	-48.185
	57->63	-0.24035					
	58->63	0.24905					
10	52->62	0.38258	8.1091	152.90	0.0011	-1.7668	-1.9742
	53->62	0.2299					
	58->62	-0.29514					
11	55->63	0.35362	8.3286	148.86	0.0197	21.5177	23.4437
	60->63	0.3847					
	61->63	0.27998					
12	56->62	0.38772	8.4132	147.37	0.0055	29.3972	30.6655
	59->67	-0.2931					
13	51->62	0.23806	8.4979	145.90	0.0052	-22.711	-23.6559
	56->62	0.41378					
	59->67	0.22321					
14	61->64	0.45534	8.5152	145.60	0.0231	0.9604	1.0695
	61->65	0.36278					
	61->68	-0.20683					
15	55->63	0.23778	8.7159	142.25	0.1032	-26.6194	-34.3338
	60->64	0.27179					
	61->64	-0.21451					
	61->65	0.20693					
16	55->63	-0.24878	8.7731	141.32	0.0190	26.3433	27.9169
	60->63	0.26839					
	61->65	0.24675					
	61->66	-0.24362					
17	61->67	0.51235	8.8150	140.65	0.1620	31.409	33.2072
18	45->62	-0.26044	8.9158	139.06	0.0054	-0.2814	0.1082
	51->62	0.22552					
	52->62	0.34895					
	59->67	-0.20837					

19	61->65	0.2127	8.9652	138.29	0.0249	-2.0868	-1.338
	61->66	0.4181					
	61->69	0.21828					
20	55->62	0.28297	9.0745	136.63	0.0382	-24.9863	-23.5483
	58->64	0.41322					
	60->64	-0.2497					
21	55->62	0.53224	9.0983	136.27	0.0164	-18.701	-19.6306
22	59->63	0.60888	9.1267	135.85	0.0149	0.2307	-1.0884
23	61->64	0.20965	9.1448	135.58	0.0096	-1.5288	0.7652
	61->70	0.20752					
24	48->62	-0.25625	9.2960	133.37	0.0196	-20.4444	-19.7362
	49->62	0.53114					
25	60->64	0.21332	9.3461	132.66	0.0425	45.5894	42.5783
	60->66	0.20993					
	61->69	0.4396					
26	46->62	0.31854	9.4416	131.32	0.0053	-14.1887	-13.816
	51->62	0.25994					
	53->62	0.20519					
27	59->64	0.27072	9.4522	131.17	0.0280	47.9026	43.8012
	59->66	0.26013					
	59->69	0.22355					
28	46->62	-0.20275	9.4949	130.58	0.0414	-6.1571	-1.8144
	59->64	-0.20698					
	60->66	0.28914					
29	60->67	0.29171	9.5049	130.44	0.0244	-1.9079	-1.7704
	61->66	-0.23363					
	61->68	0.22568					
30	52->63	-0.22192	9.5711	129.54	0.0886	44.6899	48.4114
	53->63	0.40949					
	54->63	-0.25513					
	55->63	-0.28928					
31	56->64	0.38464	9.5903	129.28	0.0003	0.3724	0.5587
	57->64	-0.20107					
32	56->64	0.25967	9.6401	128.61	0.0282	-18.1919	-16.0302
	58->64	0.23431					
	60->64	0.22533					
	60->69	0.22222					
33	50->63	0.30353	9.7119	127.66	0.0719	4.593	6.3125
	51->63	0.25724					
	57->63	-0.26571					
34	60->67	0.22256	9.7475	127.20	0.0199	5.8269	11.1787
	61->70	0.37295					
	61->71	0.2087					
35	50->63	-0.21104	9.7808	126.76	0.0201	-25.3583	-31.1136
	57->65	0.35316					
36	57->65	-0.23772	9.8341	126.08	0.0500	21.0605	17.9653
	57->67	0.28037					

[a]Number of the excited states; [b]Only transitions with contribution over 10.0% were listed; [c]Configuration-interaction coefficient; [d]Excitation energy; [e]Wavelength; [f]Oscillator strength; [g]Rotatory strength in velocity form (10^{-40} cgs); [h]Rotatory strength in length form (10^{-40} cgs).

Table S24: Comparison table of compound **1** with its most similar compound

Sturctures	 **1**	

No.	δ_H (Multiplicity, *J*, nH)	δ_C	δ_H (Multiplicity, *J*, nH)	δ_C
1	-	174.4	-	173.7
2	-	130.9	-	129.8
3	7.42 (d, 1.5 Hz, 1H)	153.1	7.47 (d, 1.4 Hz, 1H)	150.3
4	5.07 (qd, 6.8, 1.7 Hz, 1H)	78.4	4.86 (dd, 4.8, 1.5 Hz, 1H)	85.4
5	1.37 (d, 6.8 Hz, 3H)	19.3	3.74 (m, 1H)	66.9
6a	2.47 (ddt, 15.1, 3.6, 1.7 Hz, 1H)	29.7	1.10 (d, 6.4 Hz, 3H)	19.4
6b	2.35 (ddt, 15.1, 8.8, 1.4 Hz, 1H)	29.7		
7	3.87 (m, 1H)	71.7	2.47 (d, 6.4 Hz, 2H)	31.4
8	4.78 (qd, 6.4, 5.0 Hz, 1H)	73.7	5.01 (m, 1H)	68.5
9	1.23 (d, 6.4 Hz, 3H)	15.5	1.18 (d, 6.3 Hz, 3H)	19.9
10	-	170.5		
11	1.99 (s, 3H)	21.2		
1'			-	170.3
2'			1.96 (s, 3H)	21.4

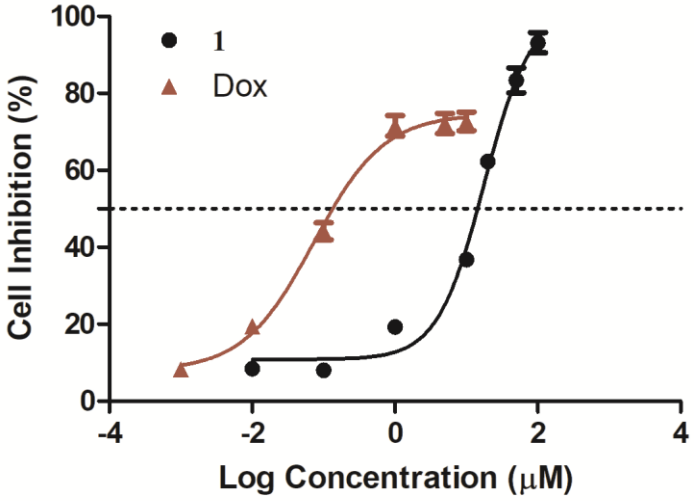
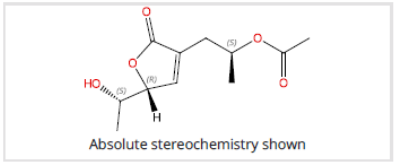


Figure S12: Compound **1** inhibited the proliferation of HepG2 cells in the CCK8 assay

1 Similarity Score: **99**

3020686-93-2



Absolute stereochemistry shown

$C_{11}H_{16}O_5$

2(5*H*)-Furanone, 3-[(2*S*)-2-(acetyloxy)propyl]-5-[(1*S*)-1-hydroxyethyl]-, (5*R*)-

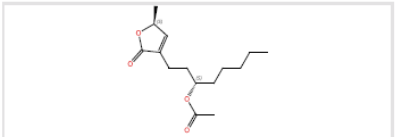
1 Reference | 0 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	228.24	-
Boiling Point (Predicted)	401.6±30.0 °C	Press: 760 Torr
Density (Predicted)	1.191±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.58±0.20	Most Acidic Temp: 25 °C

Figure S13: Scifinder search report for compound **1** with a similarity score of 99

2 Similarity Score: **95**

168418-97-1



Absolute stereochemistry shown, Rotation (+)

$C_{15}H_{24}O_4$

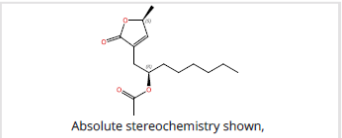
2(5*H*)-Furanone, 3-[3-(acetyloxy)octyl]-5-methyl-, [*S*-(*R**,*R**)]-

1 Reference | 4 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	268.35	-
Boiling Point (Predicted)	401.8±28.0 °C	Press: 760 Torr
Density (Predicted)	1.028±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr

3 Similarity Score: **95**

168418-96-0



Absolute stereochemistry shown, Rotation (+)

$C_{15}H_{24}O_4$

2(5*H*)-Furanone, 3-[2-(acetyloxy)octyl]-5-methyl-, [*S*-(*R**,*S**)]-

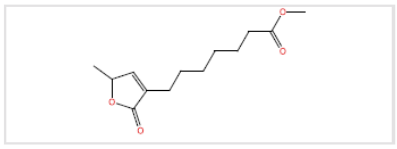
1 Reference | 5 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	268.35	-
Boiling Point (Predicted)	396.6±25.0 °C	Press: 760 Torr
Density (Predicted)	1.028±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr

Figure S14: Scifinder search report for compound **1** with a similarity score of 95

4 Similarity Score: **94**

352007-97-7



$C_{13}H_{20}O_4$

Methyl 2,5-dihydro-5-methyl-2-oxo-3-furanheptanoate

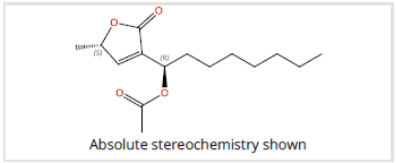
3 References | 11 Reactions | 2 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	240.30	-
Boiling Point (Predicted)	364.7±25.0 °C	Press: 760 Torr
Density (Predicted)	1.055±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr
Spectra		

Figure S15: Scifinder search report for compound **1** with a similarity score of 94

5 Similarity Score: **93**

165602-21-1



$C_{15}H_{24}O_4$

2(5*H*)-Furanone, 3-[1-(acetyloxy)octyl]-5-methyl-, [*S*-(*R**,*S**)]-

1 Reference | 8 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	268.35	-
Boiling Point (Predicted)	389.5±25.0 °C	Press: 760 Torr
Density (Predicted)	1.037±0.06 g/cm^3	Temp: 20 °C; Press: 760 Torr

Figure S16: Scifinder search report for compound **1** with a similarity score of 93

S1: *NMR and ECD Calculations*

The molecular conformers were optimized and analyzed using the following process and parameters. We optimized the conformers that fell within a 10 kcal/mol energy window using the B3LYP/6-31G(d) level of theory, incorporating Grimme's D3 dispersion correction via the "EmpiricalDispersion=GD3" setting in the input files. A frequency analysis was carried out for these conformations at the same theoretical level to verify their status as true local minima on the potential energy surface. Subsequently, the energy of each optimized conformation was assessed using the M062X/6-311+G(2d,p) method with D3 dispersion adjustment. Additionally, the Gibbs free energies for the conformers were determined by summing the "Thermal correction to Gibbs Free Energy" from the frequency analysis with the electronic energies derived at the M062X/6-311+G(2d,p) level. Equilibrium populations at room temperature (298.15 K) were then computed based on the Boltzmann distribution law, focusing further calculations only on those conformers that constituted more than 2% of the population.

In terms of NMR data, shielding constants were computed via the GIAO approach at the mPW1PW91-SCRF/6-31+G(d,p) level using chloroform as the solvent in the IEFPCM model. These constants were then transformed into chemical shifts relative to TMS at 0 ppm ($\delta cal = \sigma TMS - \sigma cal$), where σTMS represents the TMS shielding constant calculated at this same level [1]. Additionally, the EXCEL spreadsheet by Sarotti et al [2] was employed to compute DP4+ probabilities for each candidate. We also calculated various statistical parameters for each candidate, such as the correlation coefficient R^2, the mean absolute error (MAE), and the corrected mean absolute error (CMAE), where $\delta corr = (\delta cal - b)/a$.

References

[1] P. H. Willoughby, M. J. Jansma and T. R. Hoye (2014). A guide to small-molecule structure assignment through computation of ^{1}H and ^{13}C NMR chemical shifts, *Nat. Protocol.* **9**, 643-660.

[2] N. Grimblat, M. M. Zanardi and A. M. Sarotti (2015). Beyond DP4: an improved probability for the stereochemical assignment of isomeric compounds using quantum chemical calculations of NMR shifts, *J. Org. Chem.* **80**, 12526-12534.