Electronic Supplementary Information

Unexpected Different Chemoselectivity in the Aerobic Oxidation of Methylated Planar Catechin and Bent Epicatechin Derivatives Catalyzed by the *Trametes villosa* Laccase/1-Hydroxybenzotriazole System

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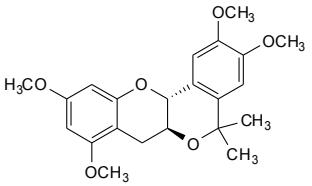
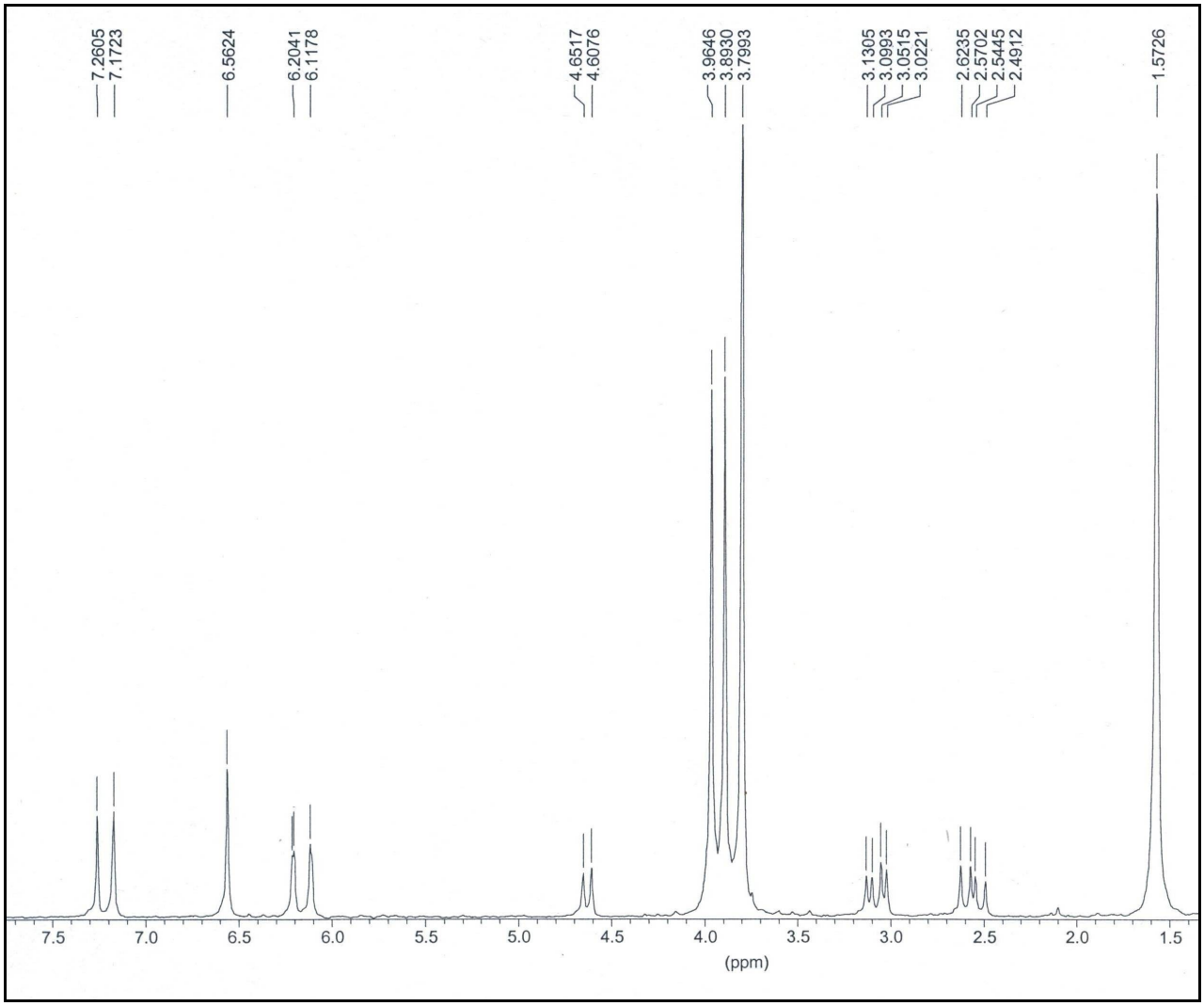
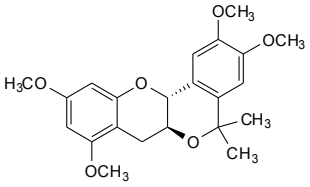
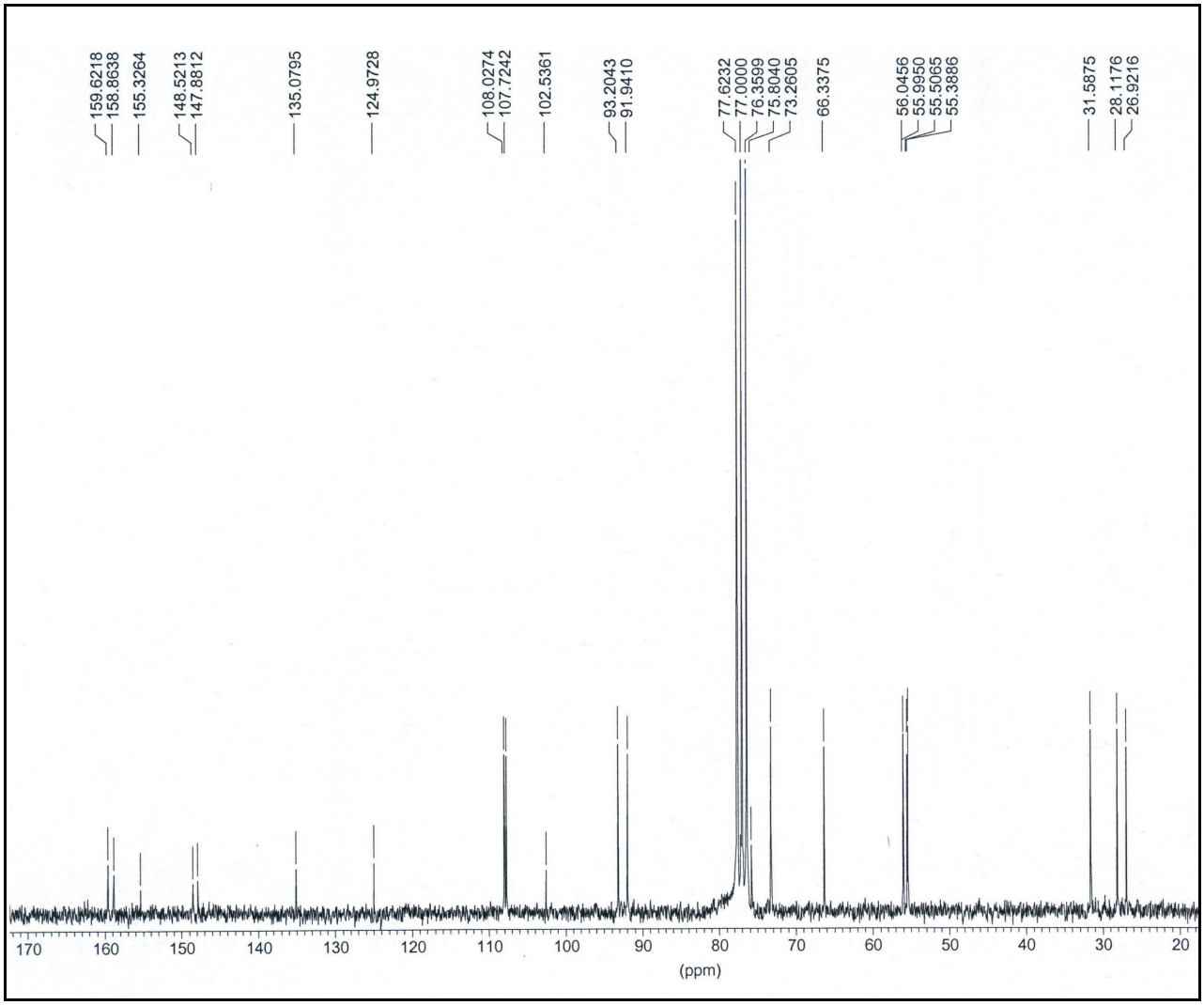




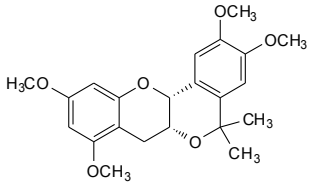
Methylated planar catechin **5**

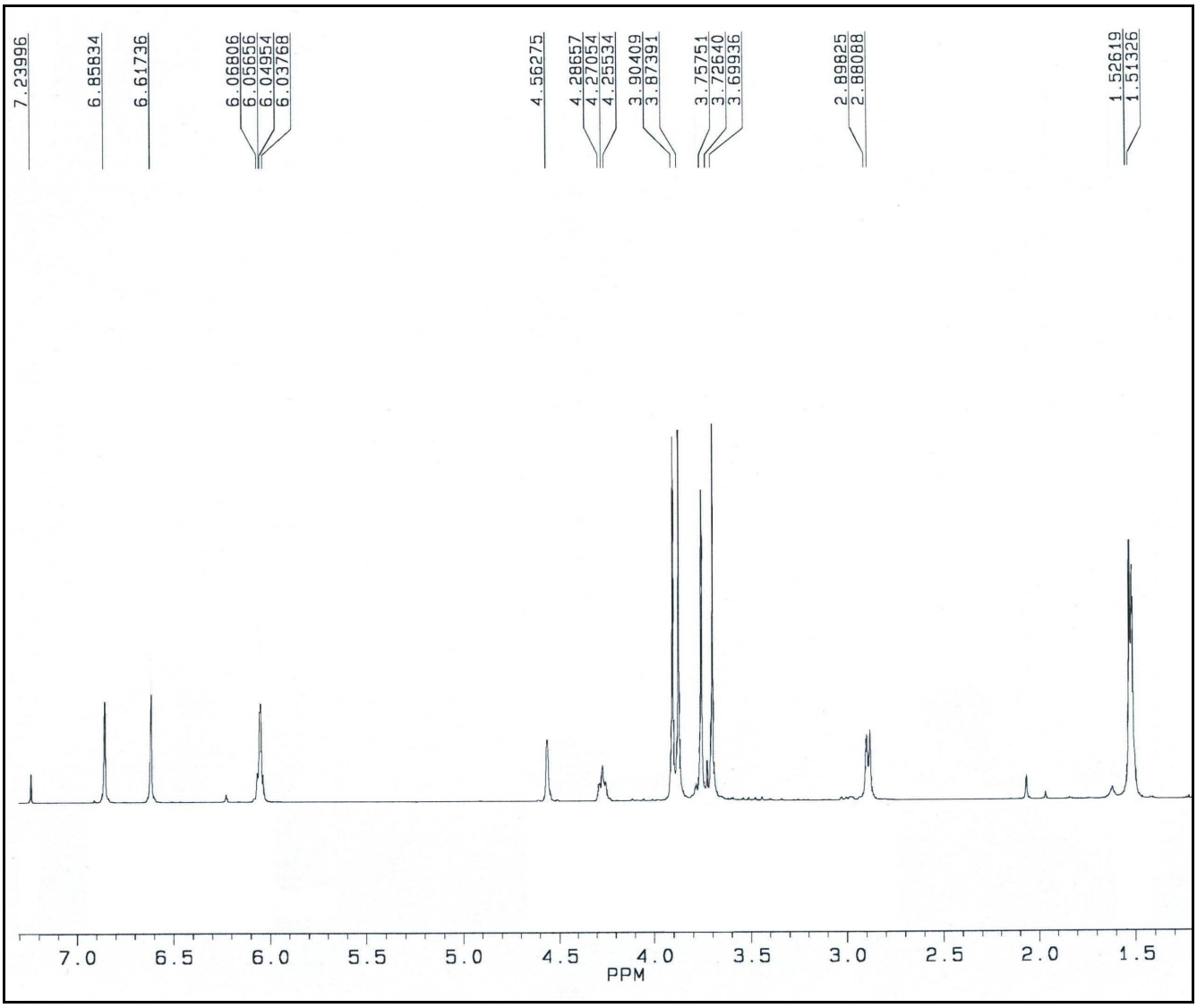
^{13}C-NMR ($CDCl_3$)





Methylated bent epicatechin **6**
^{1}H-NMR ($CDCl_3$)





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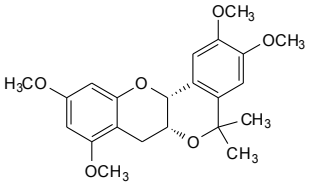

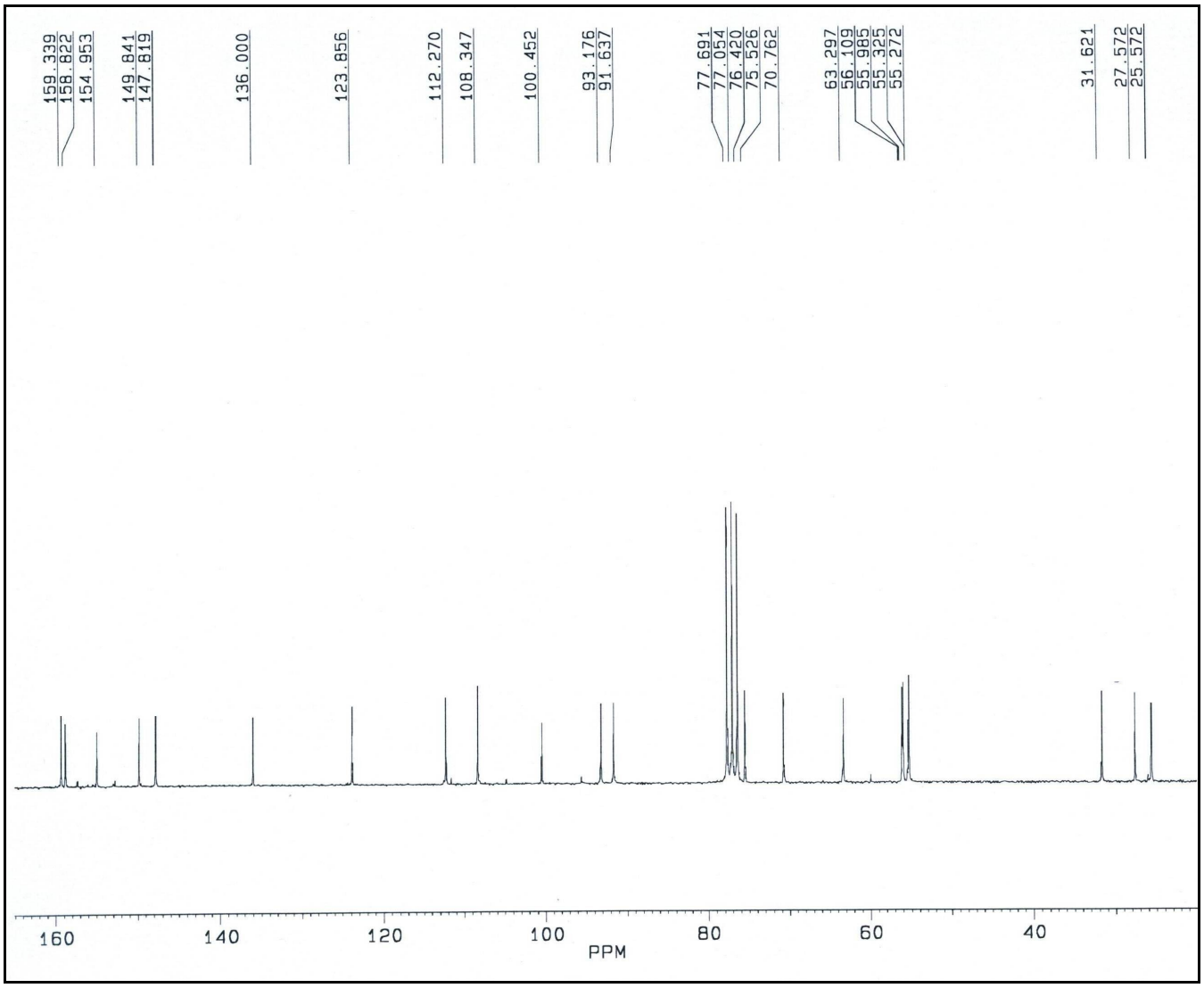

(S)-3-(2-Hydroxy-4,6-dimethoxybenzyl)-6,7-dimethoxy-1,1-dimethylisochroman-4-one **7**.
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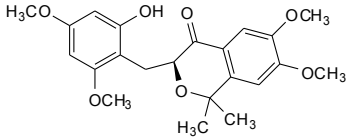

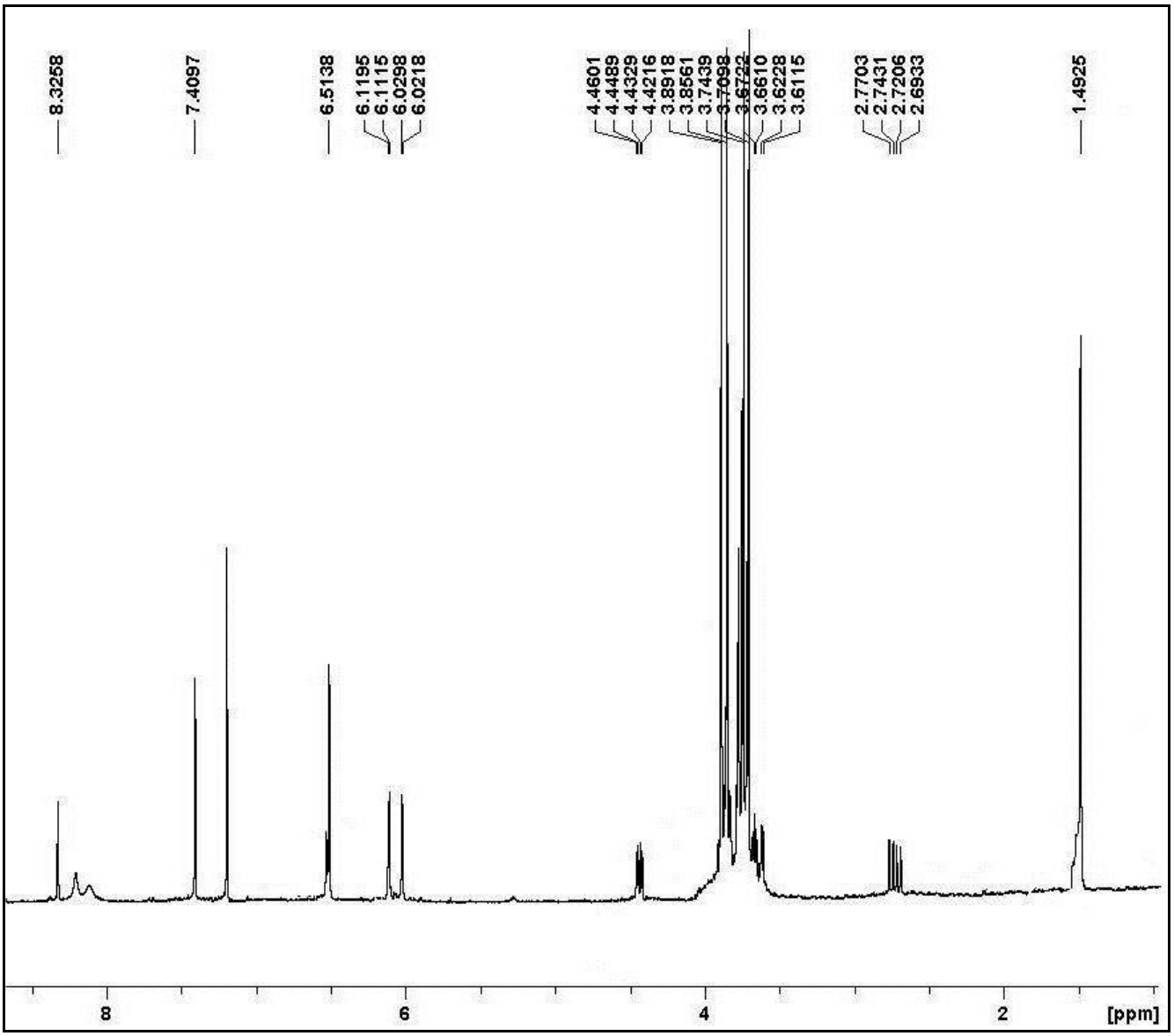

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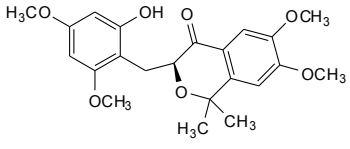

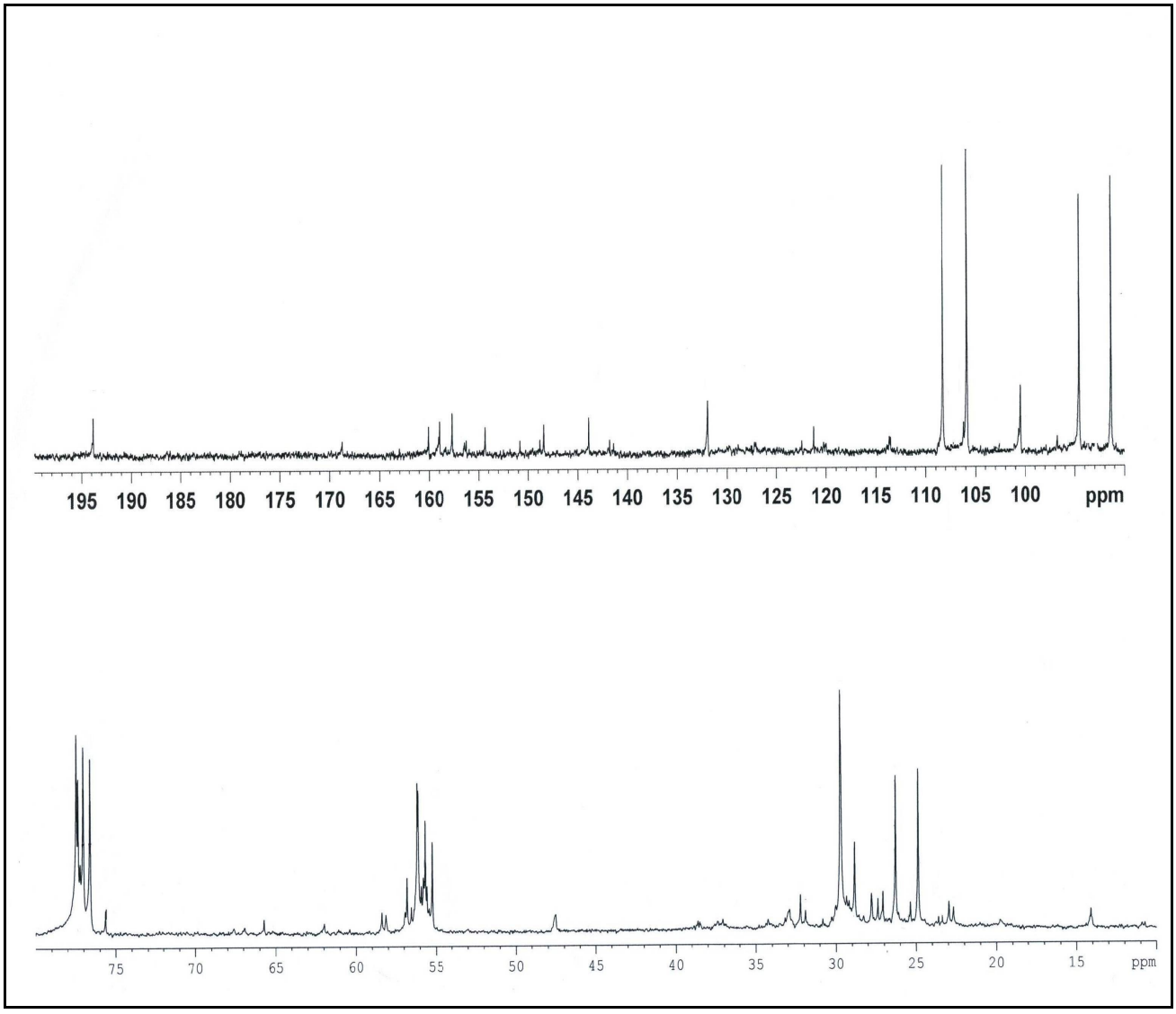

(6aS,12aR)-2,3,8,10-tetramethoxy-5,5-dimethyl-6a,12a-dihydroisochromeno[4,3-b]chromen-7(5H)-one **8**.
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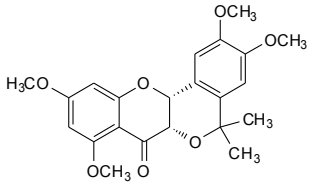

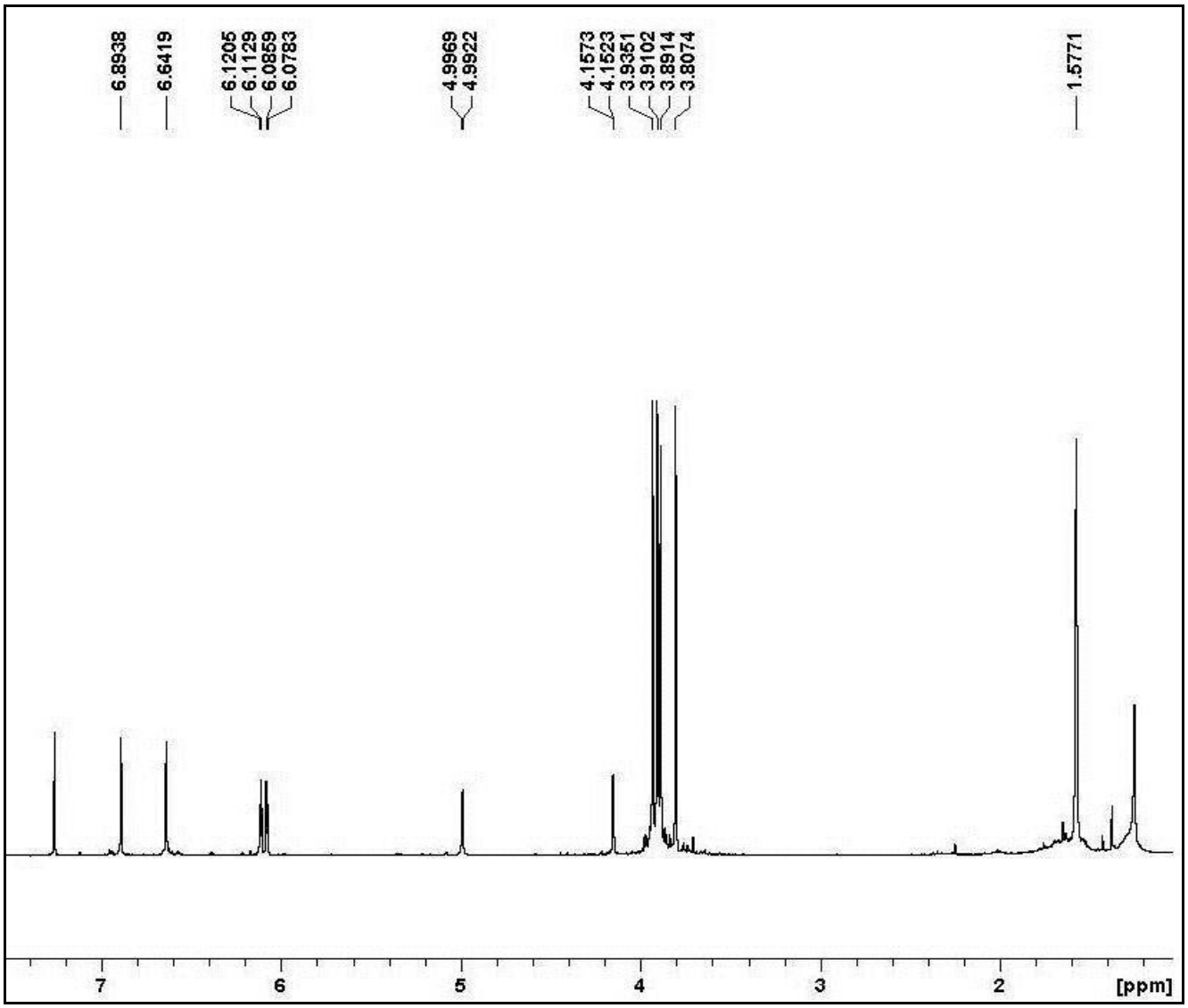

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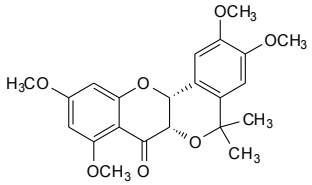

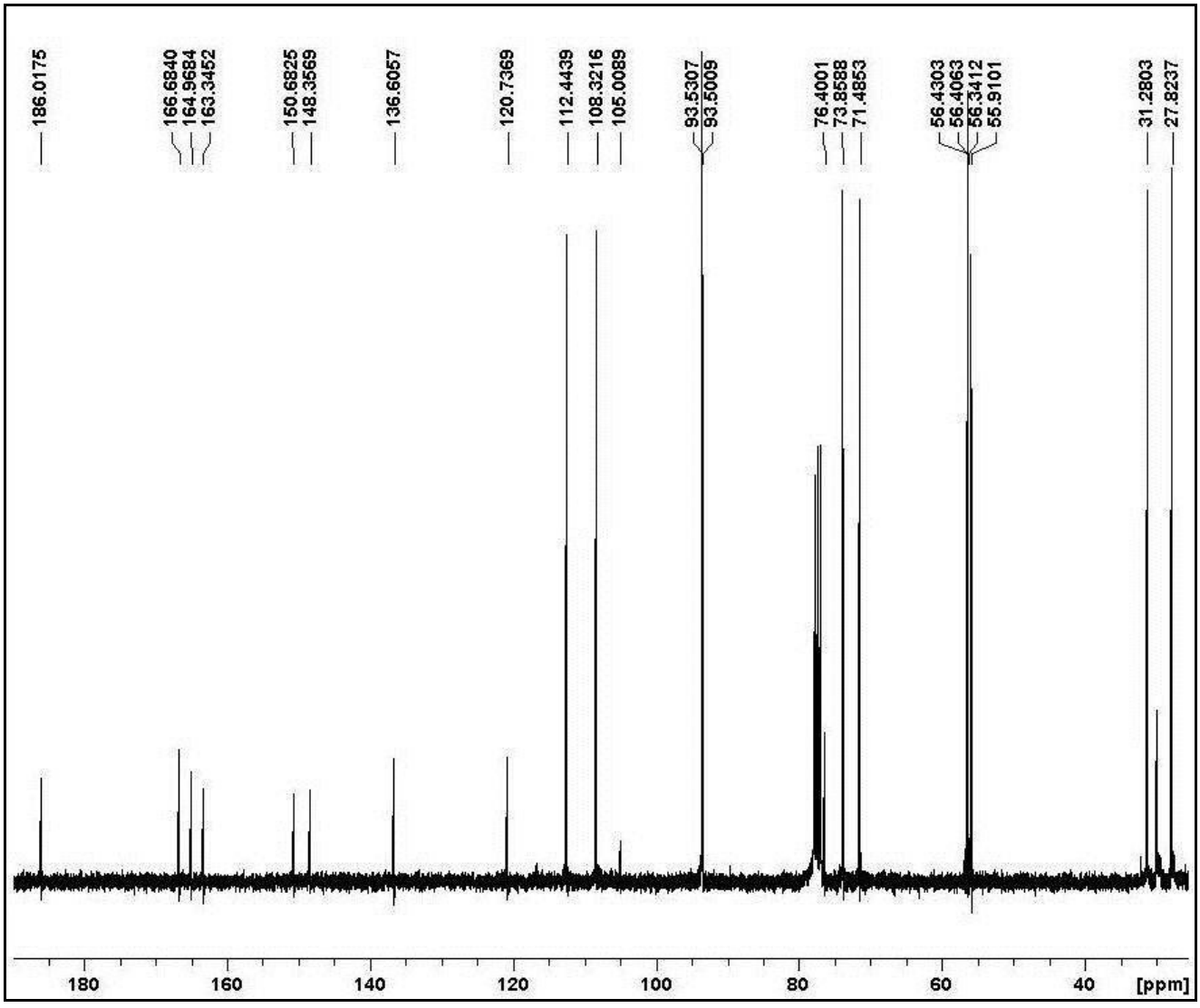

(6aR,12aR)-7-hydroxy-2,3,10-trimethoxy-5,5-dimethyl-6a,7-dihydroisochromeno[4,3-b]chromene-8,11(5H,12aH)-dione **9**.

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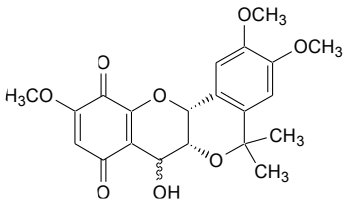

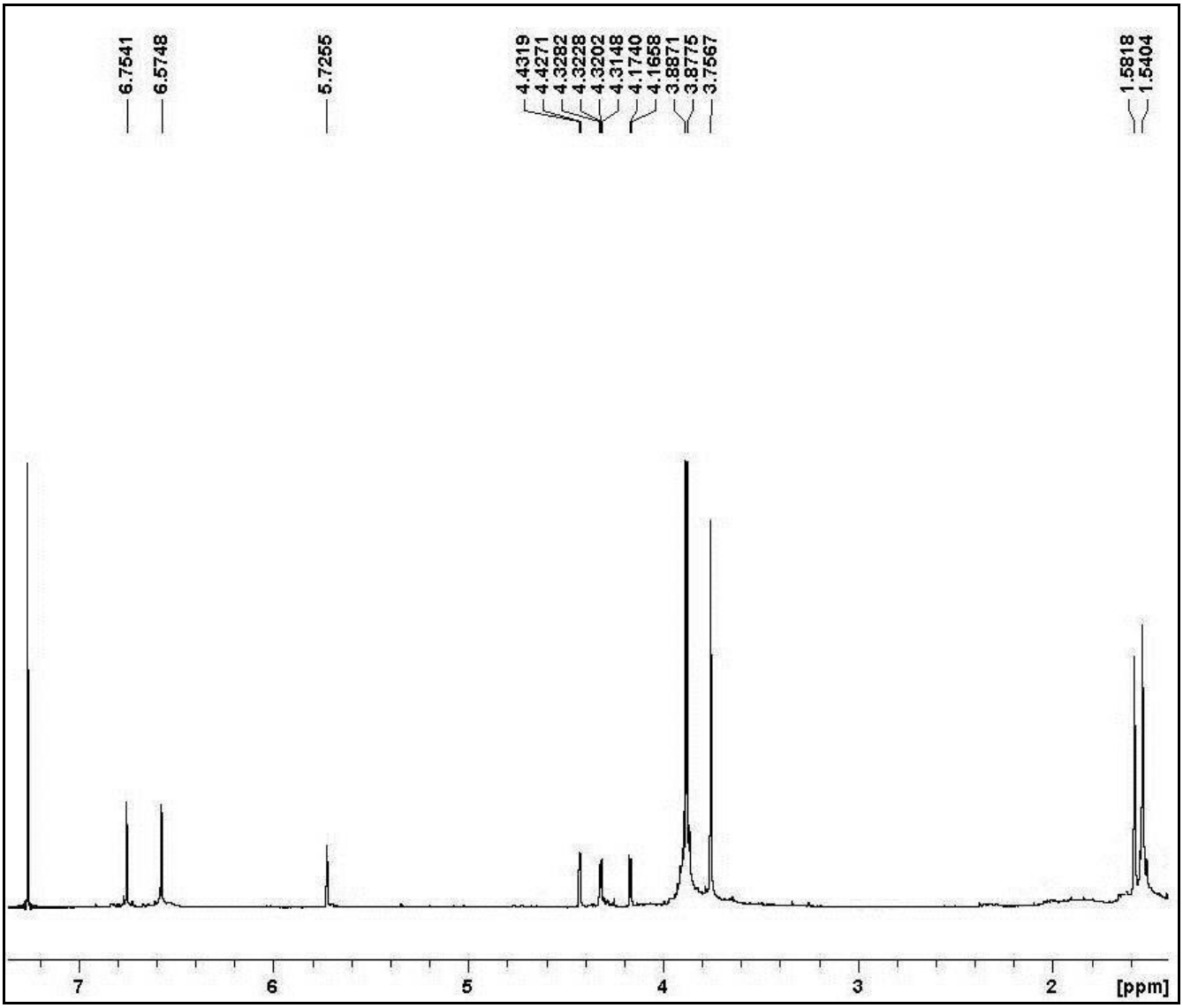

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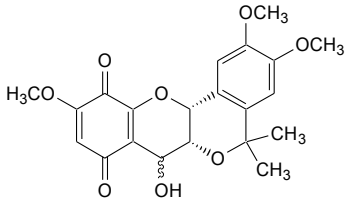

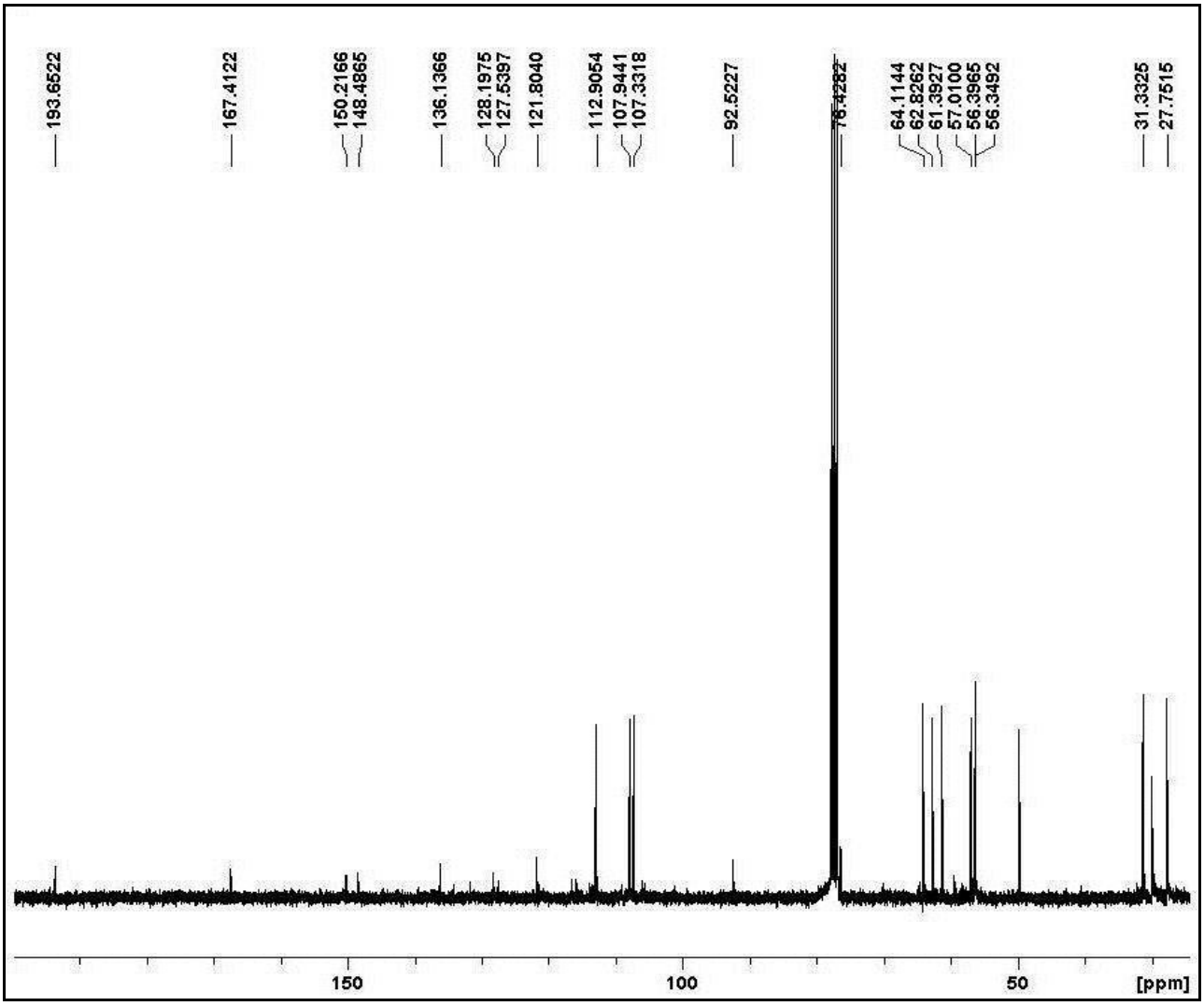

Computational methods

All calculations were performed with the software package SPARTAN 08 (Wavefunction, Inc., Irvine, CA, USA). Structures of catechin derivatives **5** (just one conformation, owing to the rigidity of the structure involving a *trans*-junction between the rings C and D) and **6** (two geometries, namely **6a** and **6b**, due to the residual conformational flexibility arising from the *cis*-junction between the rings C and D) were modeled in two steps, first performing a SCF structure optimization at the HF/3-21G(*) level of theory, next by refining the obtained geometries through B3LYP/6-31G(d) calculations. Conformation **6a** was found 9.78 kJ mol^{-1} more stable than that of **6b**, an energy difference corresponding to Boltzmann populations of 98% for **6a** and 2% for **6b**, at room temperature, so that **6a** should be much more significant in determining the chemical properties of **6**. Radicals at the positions C-2 and C-4 of **5**, **6a** and **6b** were also optimized by the same above procedure, to afford the $\mathbf{5}_{C\text{-}2}$, $\mathbf{5}_{C\text{-}4}$, $\mathbf{6a}_{C\text{-}2}$, $\mathbf{6a}_{C\text{-}4}$, $\mathbf{6b}_{C\text{-}2}$ and $\mathbf{6b}_{C\text{-}4}$ final geometries. All the above generated geometries, with exclusion of **6b**, $\mathbf{6b}_{C\text{-}2}$ and $\mathbf{6b}_{C\text{-}4}$, were also submitted to single point energy calculations at the B3LYP/6-311+G(d,p) level of theory. The obtained energies were employed in the assessment of $BDE_{C\text{-}H}$ values (Table 1 of main text), according to the equation $BDE_{C\text{-}H} = \Delta H°_f (R^{\cdot}) + \Delta H°_f (H^{\cdot}) - \Delta H°_f (R\text{-}H)$. The average absolute difference found among $BDE_{C\text{-}H}$ values coming from calculations of type B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) and B3LYP/6-311+G(d,p)//HF/3-21G(*) amounts to only 3.27 kJ mol^{-1}, while an even smaller average discrepance (i.e. 2.73 kJ mol^{-1}) was found among $BDE_{C\text{-}H}$ values coming from calculations of type B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) and B3LYP/6-31G(d) (**Table 2** of the manuscript). This confirmed that geometries obtained through HF/3-21G(*) optimizations are suitable to be employed in reliable estimations of reaction energy changes, provided they are submitted to single point energy calculations performed at a properly high level of theory (i.e. the B3LYP/6-311+G(d,p) method, in the present case). For this reason, in the present study all next energy evaluations conceived to perform assessments of differential C-2/C-4 reactivity in compounds **5** and **6** have been performed on structures optimized by the HF/3-21G(*) method and next submitted to single point energy calculations at the B3LYP/6-311+G(d,p) level of theory.

The H-abstraction from the positions either C-2 or C-4 of the already modelled ground state geometries of **5** and **6a** (calculations on **6b** were not performed owing to its negligible Boltzmann population) has been simulated by generating four relevant adducts with BTNO (i.e. the transition states denoted as TS_$\mathbf{5}_{C\text{-}2}$-BTNO, TS_$\mathbf{5}_{C\text{-}4}$-BTNO, TS_$\mathbf{6a}_{C\text{-}2}$-BTNO, TS_$\mathbf{6a}_{C\text{-}4}$-BTNO). The approximate disposition attributed to BTNO inside each TS-complex was suggested by those ones present within the similar TS structures found in the study performed on catechins **3** and **4** and reported in reference.[1] These TS geometries were then optimized through the HF/3-21G(*) method and validated as saddle points by chegking the presence among the evaluated vibrational modes of only one imaginary frequency, just corresponding to the migration of the benzylic hydrogen from carbon C-2 or C-4 of **5** or **6** towards BTNO. As already mentioned above, all such structures were eventually submitted to single point energy calculations performed at the B3LYP/6-311+G(d,p) level of theory. The hybrid Hartree-Fock/Density Functional Theory B3LYP method was chosen as a good compromise to obtain reliable kinetic data of radical hydrogen abstraction (as suggested by relevant theoretical studies reported elsewere)[2] at a reasonable computational expense. This is expected to be particularly true in the present case, in consideration that the required kinetic information are represented by energy differences between isomeric transition states. In other words, errors associated to the absolute values of the calculated activation energies (deriving from the adopted approximations or from the possible difficulty of the method to take into proper account the extent of dispersive forces) are expected to be roughly cancelled one to each other at level of the mathematical differences $\Delta\Delta E^{x}_{C\text{-}2\,-\,C\text{-}4}$ (with x equal to **5** or **6**), and so their effects significantly mitigated. However, for sake of comparison, single point energy calculations were also performed at the much higher level of theory M06-2x/6-311+G(d,p), being the M06-2x method a meta-hybrid GGA DFT functional, which is known to have a very good response under dispersion forces,

improving one of the biggest deficiencies in DFT methods[2c]. Finally, starting from the structures of TS_**5**$_{C\text{-}2}$-BTNO and TS_**6a**$_{C\text{-}4}$-BTNO, the related two ground states having the oxygen atom of BTNO roughly equidistant from the hydrogens linked to carbons C-2 and C-4 (the adducts denoted **5**:BTNO and **6a**:BTNO, respectively) were generated by equilibrium geometry optimization with the HF/3-21G(*) method. Their stability was also assessed by single point energy calculations at the both B3LYP/6-311+G(d,p) and M06-2x/6-311+G(d,p) levels of theory. As expected, by comparison of the energy differences $\Delta\Delta E^{5}_{C\text{-}2\,-\,C\text{-}4}$ and $\Delta\Delta E^{6}_{C\text{-}2\,-\,C\text{-}4}$ (see main text for their definition) obtained at the two levels of theory B3LYP/6-311+G(d,p) and M06-2x/6-311+G(d,p) it may be concluded that their relevant values do not undergo significant deviations, as the change amount just to 0.9 kcal mol^{-1} in the case of $\Delta\Delta E^{5}_{C\text{-}2\,-\,C\text{-}4}$ and -1.4 kcal mol^{-1} in the case of $\Delta\Delta E^{6}_{C\text{-}2\,-\,C\text{-}4}$ (that is, in the order of the computational error).

Visual inspection of HAT transition states TS_**5**$_{C\text{-}2}$-BTNO, TS_**5**$_{C\text{-}4}$-BTNO, TS_**6a**$_{C\text{-}2}$-BTNO, and TS_**6a**$_{C\text{-}4}$-BTNO suggests why the observed chemoselective reactivity may originate from the forced coplanar or bent disposition assumed by rings C and D. In **5**, the coplanar conformation allows the structure of BTNO to approach the hydrogen in the C-2 position by establishing additive favorable interactions with the molecular framework related to cycle D. However, this is not possible in **6** due to the tilted geometry that cycle D assumes with respect to C (Figure S2).

Table S1

Substrate	Energy (a.u.)				
	HF [a]	DFT2//HF [b]	M06-2x//HF [c]	DFT [d]	DFT2//DFT [e]
H atom	-0.496199	-0.502156		-0.500273	-0.502156
BTNO	-464.978160	-470.519510			
5	-1290.194118	-1305.634452		-1305.291008	-1305.642032
$5_{C\text{-}2}$	-1289.599022	-1304.996774		-1304.653324	-1305.002873
$5_{C\text{-}4}$	-1289.586922	-1304.987505		-1304.643965	-1304.994407
5:BTNO	-1755.19044	-1776.155253	-1775.445208		
TS_$5_{C\text{-}2}$-BTNO	-1755.140551	-1776.138083	-1775.432223		
TS_$5_{C\text{-}4}$-BTNO	-1755.139109	-1776.131932	-1775.427537		
6a	-1290.188412	-1305.632598		-1305.288959	-1305.640497
$6a_{C\text{-}2}$	-1289.599024	-1304.996884		-1304.653646	-1305.003016
$6a_{C\text{-}4}$	-1289.581975	-1304.989334		-1304.644359	-1304.996182
6a:BTNO	-1755.185263	-1776.153116	-1775.443957		
TS_$6a_{C\text{-}2}$-BTNO	-1755.126330	-1776.133564	-1775.426145		
TS_$6a_{C\text{-}4}$-BTNO	-1755.134552	-1776.139944	-1775.430278		
6b	-1290.192417			-1305.285235	
$6b_{C\text{-}2}$	-1289.593861			-1304.648343	
$6b_{C\text{-}4}$	-1289.589066			-1304.641941	

[a] HF/3-21G(*); [b] B3LYP/6-311+G(d,p)// HF/3-21G(*); [c] M06-2x/6-311+G(d,p)//HF/3-21G(*) [d] B3LYP/6-31G(d); [e] B3LYP/6-311+G(d,p)// B3LYP/6-31G(d).

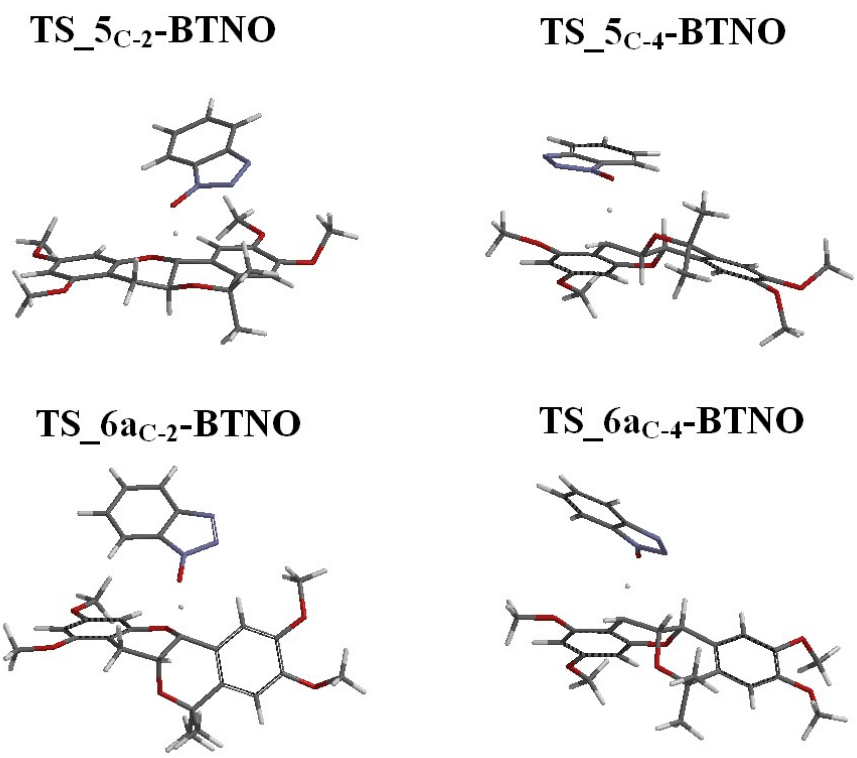

Figure S1. Calculated structures of the H-abstraction transition states of catechins **5** and **6** with BTNO.

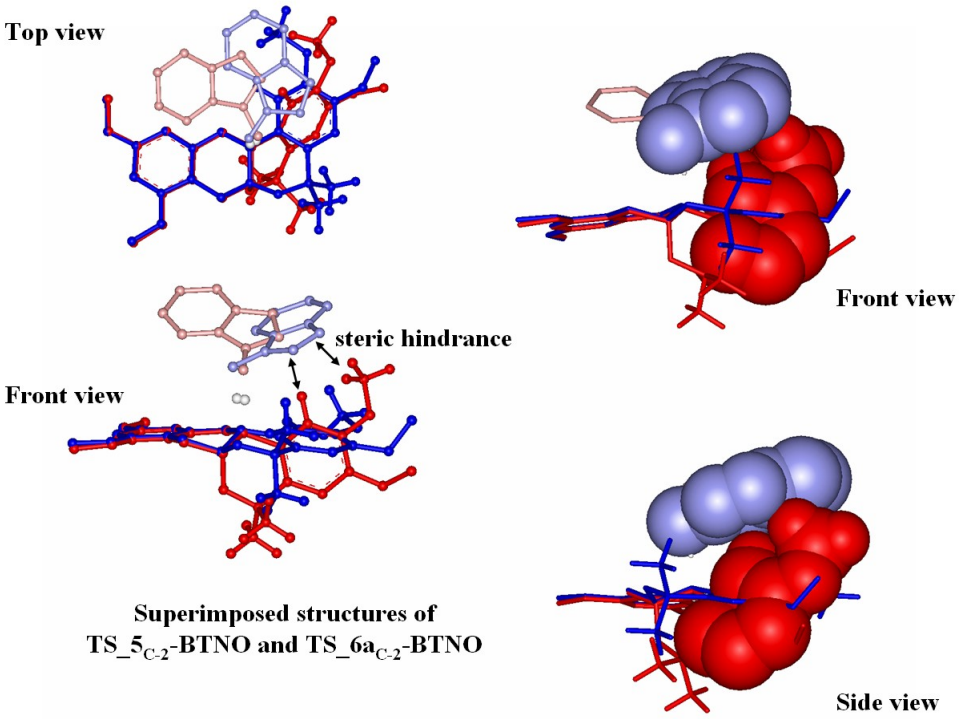

Figure S2. Superimposed structures of the optimized transition states TS_5$_{C\text{-}2}$-BTNO (blue geometry) and TS_6a$_{C\text{-}2}$-BTNO (red geometry). For sake of clarity the only plotted hydrogens are those ones either involved in the HAT process or responsible for possible steric hindrance with respect to the BTNO approach. On the right side of the figure they are emphasized, through space fill representation, the unfavorable steric interactions that BTNO would establish with the catechin framework in TS_6a$_{C\text{-}2}$-BTNO by preserving the same favourable disposition displayed in TS_5$_{C\text{-}2}$-BTNO.

Cartesian coordinates of all structures reported in Table S1 (coordinates in Angström).

Compound BTNO, HF/3-21G(*)

H	0.398267	0.044853	-0.082685
C	0.178833	-0.035896	0.976454
C	-0.397747	-0.246916	3.760097
C	-0.079531	-1.285550	1.556434
C	0.145879	1.099550	1.798533
C	-0.137412	0.992757	3.164420
C	-0.357825	-1.359279	2.916243
H	0.343942	2.078181	1.365840
H	-0.155975	1.892312	3.777689
H	-0.618375	-0.339417	4.818466
N	-0.114747	-2.544996	1.006248
N	-0.405975	-3.406984	1.975815
N	-0.545570	-2.692142	3.092277
O	-0.852770	-3.352159	4.259023

Compound BTNO, B3LYP/6-31G*

H	-1.891342	-2.255158	0.000000
C	-1.585137	-1.230403	0.000000
C	-0.722530	1.473123	0.000000
C	-0.244475	-0.894727	0.000000
C	-2.494814	-0.191278	0.000000
C	-2.063098	1.143471	0.000000
C	0.173958	0.417718	0.000000
H	-3.544457	-0.402002	0.000000
H	-2.794228	1.926421	0.000000
H	-0.385890	2.487723	0.000000
N	0.905697	-1.727452	0.000000
N	1.954149	-1.019299	0.000000
N	1.547183	0.345481	0.000000
O	2.422912	1.343060	0.000000

Compound **5**, HF/3-21G(*)

H	-2.306304	-2.753020	-0.008984
C	-2.838413	-1.829006	0.007239
C	-4.095006	0.632543	0.029799
C	-2.104998	-0.654355	-0.117680
C	-4.202016	-1.753397	0.145180
C	-4.838435	-0.515319	0.153350
C	-2.705584	0.584010	-0.102456

H	-5.899704	-0.504386	0.257758
O	-4.633595	1.888412	0.030306
O	-5.022248	-2.838279	0.275782
C	-6.051101	2.086617	0.165946
H	-6.589609	1.620165	-0.648704
H	-6.196156	3.153805	0.135385
H	-6.411775	1.694169	1.107914
C	-4.479832	-4.169576	0.285479
H	-3.975782	-4.393635	-0.645976
H	-5.326530	-4.824627	0.407874
H	-3.790383	-4.305288	1.108859
O	-0.741893	-0.804336	-0.248872
C	-1.906037	1.867006	-0.216078
C	-0.449065	1.578316	0.110439
H	-0.318638	1.406467	1.171271
C	0.021040	0.352565	-0.649912
H	-0.135100	0.531807	-1.706768
O	0.355740	2.665543	-0.362302
C	1.477708	0.104864	-0.360904
C	4.157292	-0.344437	0.139937
C	2.310113	1.182632	-0.095877
C	1.984724	-1.184414	-0.370667
C	3.316027	-1.413846	-0.124534
C	3.652366	0.934036	0.159072
H	1.332824	-2.011340	-0.549214
H	4.333415	1.731832	0.370627
O	5.506887	-0.549699	0.377288
O	3.807810	-2.710220	-0.123744
C	5.836606	-1.210313	1.635252
H	5.513757	-0.604213	2.471751
H	6.910346	-1.306450	1.642964
H	5.366659	-2.179314	1.676992
C	4.670982	-3.056464	-1.246458
H	4.125823	-2.973178	-2.177540
H	4.968229	-4.079955	-1.084064
H	5.532709	-2.408489	-1.263323
H	-2.307218	2.610858	0.456347
H	-1.953084	2.267331	-1.222408
C	1.774779	2.615247	-0.049915
C	2.418562	3.477506	-1.140448
H	3.486351	3.564809	-0.989172
H	1.971674	4.463342	-1.118464

H	2.230073	3.033708	-2.108695
C	1.980617	3.230357	1.341655
H	3.033612	3.310823	1.576460
H	1.505822	2.624568	2.103092
H	1.538695	4.218627	1.356427

Compound **5**, B3LYP/6-31G*

H	-2.331995	-2.753434	0.141565
C	-2.864381	-1.812069	0.104762
C	-4.122655	0.679145	-0.020799
C	-2.118206	-0.632121	-0.038861
C	-4.249340	-1.720223	0.189884
C	-4.891129	-0.472187	0.121328
C	-2.713344	0.630386	-0.096567
H	-5.971012	-0.448218	0.184853
O	-4.652027	1.938210	-0.090217
O	-5.084829	-2.791551	0.334601
C	-6.058674	2.084254	0.008841
H	-6.575446	1.567897	-0.810479
H	-6.253772	3.156310	-0.059163
H	-6.436054	1.705052	0.967507
C	-4.503727	-4.082247	0.422792
H	-3.947286	-4.337937	-0.488669
H	-5.336223	-4.778070	0.544931
H	-3.831986	-4.163314	1.287416
O	-0.756881	-0.808311	-0.092178
C	-1.891412	1.898488	-0.203069
C	-0.432941	1.596112	0.109644
H	-0.301860	1.457528	1.193924
C	-0.005392	0.307830	-0.585416
H	-0.213951	0.417283	-1.661800
O	0.376231	2.653173	-0.377466
C	1.465077	0.062255	-0.352784
C	4.189726	-0.389738	0.114466
C	2.308271	1.152218	-0.078749
C	1.990721	-1.232746	-0.411024
C	3.343137	-1.471805	-0.190633
C	3.665563	0.899158	0.159945
H	1.339558	-2.076034	-0.614298
H	4.354688	1.706432	0.389042
O	5.540164	-0.565869	0.327251
O	3.811950	-2.767511	-0.229085

C	5.870816	-1.246417	1.543485
H	5.525957	-0.672849	2.413795
H	6.960899	-1.315978	1.565447
H	5.433532	-2.249616	1.571080
C	4.672246	-3.059490	-1.336021
H	4.144270	-2.910355	-2.286911
H	4.947904	-4.111967	-1.236499
H	5.572068	-2.436280	-1.316090
H	-2.277491	2.665842	0.476462
H	-1.950363	2.326760	-1.213430
C	1.772822	2.589324	-0.020429
C	2.459210	3.470300	-1.074015
H	3.529918	3.571962	-0.872395
H	2.005621	4.466941	-1.065816
H	2.329989	3.038004	-2.070565
C	1.948788	3.193423	1.387132
H	3.003452	3.225820	1.678936
H	1.413933	2.606139	2.140615
H	1.553667	4.214586	1.397847

Compound $\mathbf{5}_{C\text{-}2}$, HF/3-21G(*)

H	-2.398894	-2.684144	0.753814
C	-2.894270	-1.789339	0.451477
C	-4.054692	0.606656	-0.337979
C	-2.120687	-0.665292	0.191885
C	-4.260347	-1.696483	0.306281
C	-4.844365	-0.494133	-0.088424
C	-2.666717	0.536903	-0.197281
H	-5.906235	-0.471061	-0.186516
O	-4.546265	1.820446	-0.731657
O	-5.129308	-2.728734	0.529606
C	-5.957332	2.021167	-0.922408
H	-6.344301	1.365140	-1.691353
H	-6.061790	3.047655	-1.232615
H	-6.503149	1.859294	-0.001825
C	-4.643720	-4.019708	0.934865
H	-3.983049	-4.441691	0.188224
H	-5.520023	-4.638393	1.036152
H	-4.125095	-3.963189	1.883498
O	-0.756578	-0.811622	0.345071
C	-1.776494	1.722772	-0.483758
C	-0.528529	1.649043	0.400420

H	-0.806449	1.854773	1.429390
C	0.087027	0.287211	0.293661
O	0.388296	2.634052	-0.088832
C	1.451945	0.074545	0.128573
C	4.212566	-0.329914	-0.142704
C	2.343240	1.191871	0.146539
C	1.980096	-1.233462	-0.043803
C	3.339872	-1.426012	-0.176418
C	3.707023	0.960843	0.020236
H	1.319958	-2.072818	-0.061706
H	4.411020	1.766107	0.034841
O	5.580381	-0.510835	-0.280193
O	3.843619	-2.709595	-0.333371
C	6.247638	-1.175277	0.832718
H	6.156102	-0.582454	1.733789
H	7.284860	-1.253922	0.549012
H	5.820633	-2.152642	0.988135
C	4.367935	-3.019004	-1.657486
H	3.582654	-2.946156	-2.398591
H	4.728205	-4.033723	-1.602211
H	5.172066	-2.343868	-1.903638
H	-2.309477	2.641504	-0.297539
H	-1.444919	1.721133	-1.514704
C	1.766103	2.584478	0.371907
C	2.448821	3.656955	-0.479886
H	3.483277	3.792993	-0.195100
H	1.919892	4.590553	-0.340954
H	2.393520	3.379933	-1.523630
C	1.836891	2.938256	1.865131
H	2.871556	3.014186	2.174901
H	1.359562	2.178050	2.471190
H	1.342421	3.886835	2.037804

Compound **5**$_{C\text{-}2}$, B3LYP/6-31G*

H	-2.430631	-2.652893	0.694558
C	-2.924461	-1.738090	0.396786
C	-4.080716	0.690621	-0.388396
C	-2.141483	-0.611341	0.115000
C	-4.306438	-1.622629	0.275893
C	-4.893490	-0.406978	-0.115432
C	-2.675588	0.613464	-0.277551
H	-5.972121	-0.364718	-0.195530

O	-4.558732	1.908280	-0.780818
O	-5.187405	-2.636694	0.516905
C	-5.962330	2.077493	-0.901830
H	-6.383380	1.408162	-1.663066
H	-6.111922	3.114211	-1.208883
H	-6.473173	1.902880	0.054132
C	-4.666871	-3.891686	0.924266
H	-4.005476	-4.321628	0.160755
H	-5.531481	-4.543801	1.061410
H	-4.118166	-3.812097	1.871853
O	-0.780425	-0.801852	0.235188
C	-1.768490	1.783752	-0.564164
C	-0.496181	1.653788	0.279870
H	-0.767127	1.861934	1.332816
C	0.067306	0.270994	0.166834
O	0.434718	2.614377	-0.188610
C	1.446412	0.023693	0.047677
C	4.226825	-0.401962	-0.159441
C	2.348871	1.133705	0.096495
C	1.974135	-1.284785	-0.131113
C	3.337321	-1.495910	-0.238312
C	3.713057	0.891546	-0.001550
H	1.306318	-2.136786	-0.187358
H	4.431501	1.703935	0.045976
O	5.590151	-0.566925	-0.274939
O	3.807265	-2.785726	-0.378458
C	6.211427	-1.227899	0.833001
H	6.077207	-0.647232	1.755314
H	7.276211	-1.286227	0.594164
H	5.806055	-2.234884	0.973780
C	4.351223	-3.080194	-1.668988
H	3.587016	-2.959031	-2.448074
H	4.669515	-4.125029	-1.634316
H	5.209429	-2.438802	-1.896957
H	-2.270302	2.729312	-0.342171
H	-1.474314	1.817484	-1.621799
C	1.779799	2.533594	0.334362
C	2.523245	3.615017	-0.457121
H	3.556185	3.727631	-0.114915
H	2.010822	4.572892	-0.323555
H	2.529601	3.368941	-1.522793
C	1.787384	2.870083	1.839147

H	2.815588	2.909299	2.213782
H	1.253492	2.115388	2.425535
H	1.314068	3.844309	2.007398

Compound $\mathbf{5}_{C\text{-}4}$, HF/3-21G(*)

H	-2.403931	-2.779015	0.017803
C	-2.903080	-1.836201	0.052836
C	-4.118785	0.685784	0.119712
C	-2.124574	-0.689753	0.087846
C	-4.286968	-1.721576	0.061284
C	-4.889524	-0.454178	0.087284
C	-2.697197	0.606006	0.135016
H	-5.956354	-0.420531	0.083373
O	-4.622182	1.959815	0.151728
O	-5.154239	-2.785388	0.034142
C	-6.040715	2.190508	0.142535
H	-6.495506	1.795065	-0.756755
H	-6.159011	3.261196	0.169127
H	-6.514546	1.748992	1.010031
C	-4.654781	-4.132137	0.018212
H	-4.062184	-4.321870	-0.868046
H	-5.527563	-4.764299	0.011352
H	-4.060643	-4.342037	0.898835
O	-0.747753	-0.843255	0.064469
C	-1.884921	1.750536	0.207161
C	-0.410591	1.540072	0.351048
H	-0.140500	1.413695	1.394604
C	0.001863	0.294096	-0.414046
H	-0.227634	0.461819	-1.458832
O	0.318446	2.619999	-0.247259
C	1.472573	0.059400	-0.218993
C	4.184974	-0.342318	0.101319
C	2.309509	1.158084	-0.076422
C	1.989420	-1.224553	-0.196275
C	3.338536	-1.430600	-0.038665
C	3.669347	0.932694	0.088404
H	1.333870	-2.063686	-0.280118
H	4.356637	1.744866	0.202829
O	5.550923	-0.524530	0.246309
O	3.843109	-2.721328	-0.003184
C	5.982242	-1.110263	1.510696
H	5.714921	-0.460700	2.334035

H	7.054678	-1.196469	1.442811
H	5.529235	-2.079364	1.641719
C	4.624039	-3.124482	-1.166538
H	4.009818	-3.098546	-2.057152
H	4.944576	-4.134769	-0.969487
H	5.474404	-2.472082	-1.284694
H	-2.298849	2.733642	0.235980
C	1.763879	2.590139	-0.069762
C	2.293993	3.382041	-1.269308
H	3.370590	3.480793	-1.225444
H	1.843026	4.366188	-1.268181
H	2.018592	2.876746	-2.185120
C	2.093022	3.294268	1.254147
H	3.162313	3.394999	1.383730
H	1.697565	2.737431	2.094226
H	1.643917	4.279272	1.246640

Compound **5**$_{C\text{-}4}$, B3LYP/6-31G*

H	-2.421040	-2.761501	0.134568
C	-2.919386	-1.800928	0.115513
C	-4.131917	0.738174	0.030955
C	-2.138254	-0.648352	0.089084
C	-4.310128	-1.672294	0.106349
C	-4.917910	-0.400397	0.054615
C	-2.697820	0.664241	0.063827
H	-5.999298	-0.358276	0.038362
O	-4.626487	2.007259	-0.007604
O	-5.180963	-2.722277	0.131137
C	-6.033850	2.182601	-0.020066
H	-6.487276	1.721116	-0.906948
H	-6.200999	3.260982	-0.046965
H	-6.497596	1.763167	0.882306
C	-4.645670	-4.035680	0.182980
H	-4.035136	-4.256371	-0.702566
H	-5.505270	-4.708293	0.206688
H	-4.038804	-4.187175	1.085273
O	-0.778349	-0.826040	0.114261
C	-1.869176	1.799603	0.114474
C	-0.402298	1.582025	0.248245
H	-0.115094	1.514659	1.314799
C	-0.022350	0.266381	-0.429528
H	-0.279938	0.363973	-1.494992

O	0.334867	2.616454	-0.389979
C	1.453507	0.024939	-0.260437
C	4.204253	-0.377939	0.063892
C	2.302370	1.138530	-0.132033
C	1.982155	-1.268894	-0.242759
C	3.348478	-1.483882	-0.092193
C	3.673967	0.909638	0.036970
H	1.325287	-2.127287	-0.333501
H	4.369897	1.735224	0.151955
O	5.567557	-0.532934	0.198004
O	3.827196	-2.776138	-0.054472
C	5.986362	-1.108980	1.441105
H	5.702389	-0.462758	2.281937
H	7.075395	-1.179241	1.390835
H	5.555380	-2.104818	1.583739
C	4.601839	-3.157133	-1.197024
H	3.990120	-3.123667	-2.108097
H	4.925134	-4.184920	-1.016289
H	5.476006	-2.509520	-1.319980
H	-2.277051	2.801997	0.133686
C	1.762111	2.577352	-0.162859
C	2.343229	3.347374	-1.357721
H	3.429123	3.453703	-1.271591
H	1.895539	4.345820	-1.400860
H	2.115701	2.825579	-2.291987
C	2.066839	3.316288	1.155580
H	3.144034	3.381440	1.339458
H	1.614236	2.804295	2.010751
H	1.661044	4.331541	1.103051

Compound **5**:BTNO

H	0.194027	-3.771174	-1.021398
C	-0.550659	-3.325450	-0.401436
C	-2.401144	-2.054791	1.205879
C	-0.256065	-2.100951	0.189451
C	-1.774306	-3.907524	-0.169797
C	-2.713535	-3.264292	0.633200
C	-1.155499	-1.457091	1.014732
H	-3.658846	-3.739240	0.769447
O	-3.280666	-1.337214	1.984914
O	-2.169718	-5.107008	-0.693907
C	-4.490994	-1.948738	2.473155

H	-5.178625	-2.151819	1.663109
H	-4.924142	-1.230953	3.150605
H	-4.273386	-2.867357	3.001648
C	-1.288986	-5.860709	-1.543738
H	-1.038241	-5.305575	-2.438623
H	-1.836088	-6.750124	-1.809176
H	-0.379997	-6.132646	-1.022358
O	0.983213	-1.569784	-0.088872
C	-0.821616	-0.148793	1.704524
H	-1.307917	0.676683	1.204899
H	-1.159154	-0.175095	2.730527
C	0.678738	0.096243	1.636288
H	1.212175	-0.547329	2.324218
O	0.920597	1.483521	1.897549
C	2.642210	0.155030	0.136027
C	5.343798	0.780164	-0.072948
C	3.459173	-0.540389	-0.754423
C	3.170318	1.160541	0.939784
C	4.528443	1.459144	0.811371
C	4.802018	-0.238128	-0.867093
H	3.019371	-1.326561	-1.326877
O	6.682474	1.110439	-0.115663
C	7.212485	1.624509	-1.367699
H	7.145409	0.875358	-2.136629
H	8.242729	1.870231	-1.165816
H	6.675971	2.516266	-1.668894
C	-6.029956	3.108698	-1.439587
C	-4.453684	1.280085	0.096779
C	-6.572122	2.433730	-0.352153
C	-5.797234	1.535435	0.401604
C	-3.935354	1.966016	-0.981200
H	-7.595453	2.598129	-0.082308
H	-6.245208	1.030630	1.233474
H	-3.879247	0.585567	0.673069
H	-6.600246	3.794931	-2.029208
N	-3.907121	3.389120	-2.756284
N	-2.662458	2.869546	-2.677250
N	-2.676979	1.994306	-1.585999
C	2.310279	1.910361	1.957090
C	-4.689307	2.857312	-1.741277
O	-1.605255	1.312327	-1.203965
C	1.176705	-0.169859	0.227928
C	2.243990	3.405592	1.630313
H	3.223399	3.861564	1.690206

H	1.580397	3.890801	2.334824
H	1.847207	3.538891	0.632873
C	2.826111	1.673216	3.383521
H	3.826827	2.067020	3.500972
H	2.847700	0.615370	3.613251
H	2.165769	2.169471	4.083760
H	4.988018	2.219096	1.408212
O	5.668428	-0.879496	-1.721277
C	5.236283	-2.035502	-2.457245
H	6.107151	-2.380909	-2.990106
H	4.454305	-1.784203	-3.162896
H	4.883222	-2.813076	-1.791862
H	0.595656	0.429819	-0.460729

Compound TS_**5**$_{C\text{-}2}$-BTNO, HF/3-21G(*): 1 imaginary frequency at 2915.828 cm^{-1}

H	-2.626850	-2.073691	1.673195
C	-3.208782	-1.338442	1.164785
C	-4.602112	0.649787	-0.172735
C	-2.550800	-0.236164	0.630177
C	-4.574361	-1.429584	1.021863
C	-5.275551	-0.431736	0.347920
C	-3.215544	0.769969	-0.034776
H	-6.332381	-0.545151	0.258782
O	-5.209942	1.671420	-0.845564
O	-5.332307	-2.460460	1.504040
C	-6.630013	1.669052	-1.075071
H	-6.928638	0.807781	-1.658371
H	-6.832427	2.571633	-1.627235
H	-7.176283	1.680293	-0.140750
C	-4.725303	-3.537333	2.236916
H	-4.008686	-4.072143	1.626299
H	-5.534979	-4.195238	2.505937
H	-4.236020	-3.175215	3.132268
O	-1.178778	-0.207961	0.811117
C	-2.484561	1.960757	-0.619071
H	-2.272976	1.805187	-1.670081
H	-3.092735	2.847000	-0.524669
C	-1.156726	2.146356	0.103084
H	-1.316063	2.536399	1.103015
O	-0.332494	3.002782	-0.684910
C	0.938211	0.917071	0.694079
C	3.581355	1.090291	1.553208
C	1.553874	-0.180185	1.317704

C	1.646536	2.112145	0.492639
C	2.966052	2.170542	0.939432
C	2.864305	-0.105013	1.740480
H	0.974022	-1.065022	1.457798
O	4.882465	1.234197	1.979289
C	5.893331	0.393237	1.354414
H	5.717629	-0.639937	1.597327
H	6.834818	0.724755	1.761663
H	5.887122	0.530553	0.280234
C	3.279767	-3.219851	-1.935998
C	0.459865	-2.935503	-1.561412
C	2.494107	-4.298857	-1.550977
C	1.102853	-4.157204	-1.366328
C	1.257036	-1.865537	-1.945230
H	2.947083	-5.257341	-1.396640
H	0.526296	-5.012191	-1.074718
H	-0.594022	-2.817601	-1.423326
H	4.335435	-3.308796	-2.084252
N	3.161964	-0.769251	-2.501595
N	2.173943	0.127091	-2.558509
N	1.001574	-0.557342	-2.215381
C	1.004505	3.316279	-0.194137
C	2.637364	-1.992174	-2.130031
O	-0.224783	0.077009	-2.211565
H	-0.318434	0.507811	-1.045010
C	-0.430842	0.820841	0.207835
C	1.770887	3.686528	-1.468214
H	2.767436	4.036610	-1.232561
H	1.230671	4.470695	-1.982941
H	1.837879	2.820317	-2.111098
C	0.898074	4.501900	0.773246
H	1.880646	4.823118	1.092605
H	0.325249	4.233920	1.652665
H	0.403067	5.323434	0.270953
H	3.551504	3.057758	0.820707
O	3.539938	-1.134527	2.348175
C	2.889518	-2.397594	2.569309
H	3.625215	-3.018533	3.053559
H	2.585111	-2.851138	1.634476
H	2.027874	-2.285912	3.215246

Compound TS_**5**$_{C\text{-}4}$-BTNO, HF/3-21G(*): 1 imaginary frequency at 3039.963 cm^{-1}

H	-1.134757	-3.021129	1.030303
C	-1.646650	-2.116046	1.268584
C	-2.889181	0.307552	1.863535
C	-0.958379	-0.920484	1.117489
C	-2.957167	-2.091616	1.711809
C	-3.579856	-0.875056	2.006693
C	-1.554508	0.309419	1.410456
H	-4.591250	-0.905226	2.345154
O	-3.401874	1.538267	2.147019
O	-3.728032	-3.206825	1.892099
C	-4.825718	1.740385	2.278460
H	-5.343799	1.374693	1.404431
H	-4.954147	2.806454	2.357351
H	-5.202488	1.256701	3.169910
C	-3.202517	-4.515987	1.616105
H	-2.917208	-4.612538	0.576244
H	-4.004500	-5.200523	1.837715
H	-2.350084	-4.737351	2.245775
O	0.347049	-1.000205	0.675016
C	-0.830558	1.561307	1.227253
C	0.663589	1.364602	1.132503
H	1.074903	1.140879	2.110560
C	0.955755	0.214639	0.186068
H	0.525066	0.469333	-0.773175
O	1.262682	2.522672	0.550440
C	2.441897	0.023642	0.069618
C	5.185646	-0.300493	-0.200439
C	2.979766	-1.241955	-0.145877
C	3.275761	1.139790	0.174877
C	4.651967	0.955152	0.030500
C	4.345133	-1.407711	-0.284859
H	2.337342	-2.093708	-0.196136
O	6.558079	-0.444475	-0.324609
C	7.041919	-0.802496	-1.653162
H	6.606264	-1.737948	-1.964545
H	8.112149	-0.892742	-1.560764
H	6.797000	-0.023491	-2.363430
C	-4.747620	-0.761338	-2.806390
C	-1.931918	-0.283930	-2.816685
C	-4.186902	0.319507	-2.117405
C	-3.881813	-1.597671	-3.497216
C	-2.492455	-1.359914	-3.502566

C	-2.806213	0.542226	-2.122749
H	-4.271340	-2.435344	-4.039583
H	-1.851915	-2.021433	-4.050534
H	-0.879149	-0.098786	-2.826178
H	-5.805364	-0.920906	-2.794432
N	-4.803990	1.303998	-1.371339
N	-3.877456	2.145385	-0.910136
N	-2.645017	1.662017	-1.362549
O	-1.472526	2.354916	-1.113231
H	-1.165923	2.384613	1.832909
H	-1.136357	1.996658	0.033491
C	2.716953	2.535256	0.462572
C	2.999417	3.494831	-0.697263
H	2.534721	4.448846	-0.484628
H	2.569646	3.098307	-1.607070
H	4.063249	3.637208	-0.834168
C	3.268713	3.079440	1.787328
H	2.810058	4.038764	1.990302
H	4.341931	3.204744	1.734950
H	3.044010	2.405296	2.604369
H	5.332964	1.777460	0.102320
O	4.867932	-2.670955	-0.513128
C	5.614828	-3.254163	0.595321
H	6.449577	-2.621424	0.851223
H	5.959021	-4.213897	0.245098
H	4.969801	-3.383802	1.454485

Compound **6a**, HF/3-21G(*)

H	-2.090878	-2.439000	0.924725
C	-2.659906	-1.620641	0.545267
C	-4.015101	0.550608	-0.492892
C	-1.980688	-0.625316	-0.151106
C	-4.017305	-1.510804	0.715012
C	-4.705676	-0.420320	0.190270
C	-2.634976	0.463248	-0.670849
H	-5.760457	-0.378757	0.342114
O	-4.602766	1.656510	-1.043782
O	-4.785054	-2.427486	1.379588
C	-6.012330	1.893083	-0.895185
H	-6.591652	1.101365	-1.352196
H	-6.203742	2.824158	-1.403092
H	-6.285204	1.981742	0.148334

C	-4.184620	-3.592627	1.968293
H	-3.710535	-4.211479	1.217060
H	-4.995346	-4.134504	2.426981
H	-3.455190	-3.320257	2.720499
O	-0.628879	-0.806673	-0.291995
C	-1.890306	1.558630	-1.393642
C	-0.399209	1.485346	-1.088986
C	0.124151	0.060589	-1.175509
H	0.035364	-0.307012	-2.189309
O	-0.241218	1.915602	0.269970
C	1.552577	-0.000966	-0.705216
C	4.173387	-0.152558	0.164405
C	2.010882	0.905460	0.236928
C	2.407319	-0.969709	-1.207372
C	3.710555	-1.052922	-0.781700
C	3.329335	0.812209	0.661497
H	2.060940	-1.678000	-1.932253
H	3.727496	1.489977	1.387258
O	5.485705	-0.203708	0.603443
O	4.544585	-2.036288	-1.289318
C	5.835910	-1.357600	1.425256
H	5.251397	-1.358409	2.335844
H	6.882227	-1.243680	1.658340
H	5.664403	-2.267922	0.874443
C	5.609745	-1.570169	-2.169310
H	5.189769	-1.095875	-3.046748
H	6.160847	-2.451273	-2.455358
H	6.246490	-0.877065	-1.643509
H	-2.258244	2.519554	-1.066847
H	-2.045831	1.481852	-2.465141
C	1.099284	1.986497	0.813084
C	1.657366	3.386338	0.514698
H	2.619394	3.531501	0.987728
H	0.962752	4.126275	0.891441
H	1.775825	3.532413	-0.552267
C	0.891734	1.770740	2.316066
H	1.824961	1.853774	2.857606
H	0.465348	0.789591	2.473597
H	0.195917	2.514056	2.683593
H	0.163495	2.110828	-1.771490

Compound **6a**, B3LYP/6-31G*

H	-2.117061	-2.695433	0.481433
C	-2.696816	-1.823279	0.208333
C	-4.082241	0.486109	-0.529371
C	-2.010965	-0.677010	-0.225582
C	-4.085846	-1.788438	0.266336
C	-4.792760	-0.633318	-0.108569
C	-2.673011	0.492853	-0.592022
H	-5.873365	-0.653301	-0.055007
O	-4.672703	1.661225	-0.908611
O	-4.866726	-2.836403	0.667709
C	-6.083945	1.764588	-0.817189
H	-6.585385	1.047356	-1.480260
H	-6.331054	2.780478	-1.131661
H	-6.432788	1.606006	0.211518
C	-4.218448	-4.029274	1.076430
H	-3.632673	-4.471365	0.259402
H	-5.013996	-4.719418	1.364542
H	-3.557789	-3.855029	1.936120
O	-0.645275	-0.785838	-0.237934
C	-1.914863	1.731283	-1.004900
C	-0.431242	1.619562	-0.666166
C	0.098835	0.216261	-0.957051
H	0.013519	0.002620	-2.033350
O	-0.275004	1.884288	0.719835
C	1.533640	0.111571	-0.510190
C	4.203675	-0.080024	0.304581
C	1.997264	0.938136	0.523722
C	2.403760	-0.786994	-1.134807
C	3.735860	-0.889968	-0.747489
C	3.337972	0.825212	0.914668
H	2.049748	-1.421113	-1.943323
H	3.744583	1.437810	1.713570
O	5.517080	-0.121415	0.717972
O	4.553062	-1.802991	-1.377603
C	5.901577	-1.331549	1.381966
H	5.317960	-1.469902	2.301378
H	6.957197	-1.214045	1.637617
H	5.770488	-2.201868	0.731566
C	5.565703	-1.224234	-2.208603
H	5.112511	-0.636536	-3.017543
H	6.121691	-2.061140	-2.637296
H	6.241237	-0.586777	-1.629189

H	-2.324360	2.616101	-0.506391
H	-2.022159	1.911834	-2.084028
C	1.074312	1.944113	1.220209
C	1.593689	3.384517	1.037553
H	2.592820	3.509752	1.467688
H	0.910612	4.081626	1.533664
H	1.653215	3.652772	-0.022785
C	0.926084	1.601114	2.709580
H	1.882800	1.673926	3.236928
H	0.538532	0.584143	2.819347
H	0.217426	2.295218	3.173261
H	0.142881	2.339875	-1.269996

Compound **6a**$_{C\text{-}2}$, HF/3-21G(*)

H	-2.458985	-2.796958	-0.691198
C	-2.972292	-1.906576	-0.405653
C	-4.179743	0.478383	0.345355
C	-2.219586	-0.767549	-0.148197
C	-4.341292	-1.834081	-0.278059
C	-4.948972	-0.636993	0.097161
C	-2.789177	0.429416	0.222530
H	-6.012326	-0.630036	0.182484
O	-4.694501	1.688286	0.721347
O	-5.191893	-2.881958	-0.500794
C	-6.110519	1.870208	0.894121
H	-6.643669	1.691460	-0.030827
H	-6.233175	2.898114	1.192541
H	-6.496695	1.216304	1.665613
C	-4.682650	-4.171698	-0.879862
H	-4.152768	-4.122565	-1.822732
H	-5.548797	-4.804231	-0.982820
H	-4.025989	-4.573137	-0.118465
O	-0.851914	-0.893728	-0.284275
C	-1.922078	1.632439	0.509856
C	-0.659832	1.569376	-0.354980
C	-0.025830	0.217875	-0.226759
O	0.235552	2.572379	0.138076
C	1.340329	0.027357	-0.045583
C	4.102929	-0.333737	0.262537
C	2.214828	1.157903	-0.060696
C	1.888011	-1.273454	0.121060
C	3.248345	-1.444132	0.276233

C	3.579100	0.949143	0.095818
H	1.240384	-2.122535	0.132497
H	4.271371	1.764963	0.084175
O	5.472654	-0.495347	0.403903
O	3.769351	-2.718435	0.452205
C	5.927575	-0.914941	1.724200
H	5.678545	-0.164408	2.463440
H	6.998433	-1.013907	1.648141
H	5.476002	-1.857652	1.987359
C	4.529761	-3.246851	-0.673182
H	3.896194	-3.336590	-1.546096
H	4.871418	-4.222414	-0.365748
H	5.367193	-2.602547	-0.888847
H	-1.605693	1.646259	1.546346
H	-2.467745	2.540392	0.306950
C	1.620081	2.540271	-0.304235
C	1.707430	2.883328	-1.799519
H	2.745490	2.969371	-2.095623
H	1.203778	3.824141	-1.987719
H	1.248363	2.112184	-2.405868
C	2.274818	3.629973	0.548460
H	3.311499	3.778675	0.278415
H	2.206623	3.361747	1.593824
H	1.735065	4.554853	0.393212
H	-0.924999	1.761662	-1.390119

Compound **6a**$_{C\text{-}2}$, B3LYP/6-31G*

H	-2.449385	-2.784022	-0.712852
C	-2.970964	-1.885005	-0.412171
C	-4.197930	0.505545	0.379666
C	-2.221611	-0.737052	-0.126080
C	-4.355549	-1.810756	-0.291235
C	-4.977980	-0.614377	0.103414
C	-2.791195	0.470162	0.269007
H	-6.057049	-0.605069	0.184241
O	-4.710769	1.706993	0.777002
O	-5.205839	-2.850040	-0.535802
C	-6.119252	1.835280	0.895648
H	-6.622430	1.652732	-0.062908
H	-6.298691	2.865461	1.209108
H	-6.523208	1.149283	1.651543
C	-4.646176	-4.090790	-0.936711

H	-4.098625	-3.998758	-1.884094
H	-5.490474	-4.769378	-1.072523
O	-0.855592	-0.888669	-0.243987
C	-1.919285	1.665906	0.560559
C	-0.638156	1.572560	-0.275865
C	-0.038799	0.206141	-0.156581
O	0.263348	2.558952	0.197283
C	1.343726	-0.004647	-0.015164
C	4.125387	-0.352825	0.284443
C	2.217328	1.127983	-0.052462
C	1.903653	-1.300948	0.151110
C	3.268879	-1.474637	0.290594
C	3.582537	0.925300	0.101273
H	1.259811	-2.172651	0.171471
H	4.278082	1.758204	0.084608
O	5.491163	-0.483902	0.410117
O	3.767571	-2.747997	0.476426
C	5.933891	-0.906729	1.705258
H	5.653149	-0.169961	2.469548
H	7.023249	-0.971880	1.647830
H	5.515827	-1.883388	1.968080
C	4.505306	-3.258602	-0.638337
H	3.865932	-3.324147	-1.528729
H	4.832565	-4.261552	-0.353418
H	5.377172	-2.634169	-0.861176
H	-1.631972	1.707695	1.619991
H	-2.446361	2.596074	0.335503
C	1.615054	2.508942	-0.313397
C	1.629544	2.826128	-1.822199
H	2.660543	2.890582	-2.185595
H	1.131013	3.784568	-2.007727
H	1.124840	2.050211	-2.406797
C	2.320566	3.622734	0.467990
H	3.353298	3.759063	0.133989
H	2.321469	3.396236	1.538142
H	1.783414	4.563632	0.312511
H	-0.907705	1.772193	-1.330718
H	-3.973316	-4.496615	-0.169824

Compound **6a**$_{C\text{-}4}$, HF/3-21G(*)

H	-2.127724	-2.742573	0.350807
C	-2.705014	-1.871744	0.132736

C	-4.127600	0.465225	-0.456413
C	-2.024932	-0.691918	-0.130273
C	-4.093314	-1.879578	0.108997
C	-4.801015	-0.706150	-0.193337
C	-2.705369	0.509945	-0.423173
H	-5.866565	-0.766887	-0.205241
O	-4.735385	1.656781	-0.757729
O	-4.867547	-2.986578	0.356421
C	-6.168021	1.767544	-0.768791
H	-6.604945	1.122204	-1.520248
H	-6.376518	2.797182	-1.008976
H	-6.586450	1.526448	0.200078
C	-4.255468	-4.238070	0.705602
H	-3.622161	-4.603390	-0.093213
H	-5.070822	-4.925133	0.863031
H	-3.672284	-4.151249	1.613809
O	-0.648715	-0.722465	-0.098425
C	-1.991645	1.695590	-0.642109
C	-0.497707	1.688055	-0.514500
C	0.070632	0.309890	-0.823079
H	-0.028316	0.120998	-1.884518
O	-0.187267	2.016723	0.854548
C	1.512329	0.199447	-0.403577
C	4.175489	-0.057847	0.302325
C	2.052509	1.056478	0.539840
C	2.305838	-0.782725	-0.980173
C	3.626612	-0.919693	-0.635618
C	3.393233	0.913911	0.877049
H	1.892969	-1.457834	-1.701788
H	3.854330	1.558477	1.595769
O	5.510532	-0.159615	0.655351
O	4.397007	-1.915271	-1.215347
C	5.873803	-1.342205	1.429466
H	5.349560	-1.343868	2.376031
H	6.936177	-1.267559	1.596075
H	5.636436	-2.234216	0.873016
C	5.417642	-1.460486	-2.152163
H	4.957177	-0.956829	-2.992193
H	5.924175	-2.350378	-2.489245
H	6.106035	-0.796182	-1.654933
H	-2.510116	2.615548	-0.799397
C	1.210330	2.137909	1.209309

C	1.710121	3.535647	0.812427
H	2.723005	3.692303	1.159788
H	1.063278	4.281179	1.257784
H	1.698339	3.662415	-0.263212
C	1.199623	1.963213	2.732163
H	2.188365	2.088969	3.152984
H	0.824926	0.977952	2.972491
H	0.533043	2.700802	3.159995
H	-0.050037	2.402948	-1.193251

Compound **6a**$_{C\text{-}4}$, B3LYP/6-31G*

H	-2.220288	-2.652809	0.715745
C	-2.777280	-1.780620	0.398285
C	-4.141890	0.529225	-0.452935
C	-2.067042	-0.646131	0.010624
C	-4.172961	-1.747076	0.359275
C	-4.857751	-0.591971	-0.073966
C	-2.706195	0.553399	-0.415114
H	-5.939405	-0.623105	-0.093429
O	-4.711717	1.692341	-0.877305
O	-4.978299	-2.791258	0.707194
C	-6.127313	1.782401	-0.891339
H	-6.569586	1.054323	-1.584006
H	-6.359570	2.793367	-1.231246
H	-6.547537	1.627296	0.110767
C	-4.366148	-3.985603	1.169018
H	-3.721112	-4.430695	0.400311
H	-5.184089	-4.671823	1.396505
H	-3.774582	-3.809203	2.076682
O	-0.707157	-0.713063	0.092898
C	-1.945574	1.688013	-0.732538
C	-0.459128	1.627431	-0.634171
C	0.032998	0.187386	-0.764263
H	-0.121724	-0.145451	-1.801630
O	-0.055851	2.160926	0.634873
C	1.491100	0.071864	-0.401932
C	4.221194	-0.164857	0.178874
C	2.127483	1.079022	0.338134
C	2.221637	-1.037049	-0.845710
C	3.577350	-1.169145	-0.569446
C	3.495934	0.942141	0.610427
H	1.733996	-1.818016	-1.422979

H	4.033416	1.696851	1.176520
O	5.569281	-0.225573	0.455297
O	4.252694	-2.288874	-1.005695
C	5.947965	-1.250408	1.382455
H	5.475813	-1.081384	2.358974
H	5.675599	-2.243470	1.011726
C	5.182343	-2.046285	-2.067654
H	4.661720	-1.674604	-2.960072
H	5.644275	-3.010208	-2.293598
H	5.951563	-1.327439	-1.767241
H	-2.428843	2.626054	-0.973399
C	1.359675	2.305971	0.841464
C	1.854979	3.588904	0.142543
H	2.915713	3.767179	0.348741
H	1.278563	4.446419	0.504681
H	1.738520	3.525426	-0.944423
C	1.483733	2.443165	2.366507
H	2.519101	2.620266	2.673561
H	1.120427	1.533713	2.853439
H	0.870817	3.285381	2.703584
H	-0.000397	2.212772	-1.447640
H	7.032896	-1.177526	1.487687

Compound **6a**:BTNO

H	-0.075392	-2.778202	-2.418205
C	-0.763640	-2.607114	-1.621457
C	-2.459537	-2.059544	0.483377
C	-0.387320	-1.716181	-0.620722
C	-1.988817	-3.225300	-1.548008
C	-2.853091	-2.943203	-0.492532
C	-1.210036	-1.445840	0.448819
H	-3.804358	-3.425961	-0.484596
O	-3.262423	-1.693979	1.543309
O	-2.458416	-4.118495	-2.472137
C	-4.424101	-2.477496	1.879255
H	-5.191660	-2.381523	1.122687
H	-4.781353	-2.080099	2.815559
H	-4.164322	-3.520898	1.998058
C	-1.652915	-4.489799	-3.603225
H	-1.436280	-3.632819	-4.228317
H	-2.242584	-5.202753	-4.155671
H	-0.724153	-4.948739	-3.289074

O	0.837986	-1.118051	-0.767494
C	-0.773283	-0.539541	1.575970
H	-0.972327	-1.018749	2.523274
C	0.719860	-0.248687	1.487308
C	1.137513	0.043388	0.054305
H	0.599864	0.898890	-0.328779
O	1.389963	-1.446140	1.898784
C	2.624191	0.230554	-0.011607
C	5.381867	0.564166	-0.128906
C	3.188682	1.128658	-0.916218
C	3.433012	-0.505020	0.845753
C	4.813706	-0.316273	0.772885
C	4.558471	1.301726	-0.987687
H	2.539977	1.681028	-1.563913
O	6.756727	0.663785	-0.168062
C	7.353615	1.950017	0.152198
H	7.052029	2.691047	-0.566942
H	8.419190	1.791485	0.110266
H	7.069328	2.261676	1.150239
C	-6.150710	3.498524	-0.287127
C	-4.486853	1.360454	0.636164
C	-4.775853	3.475809	-0.532385
C	-6.683750	2.434810	0.431841
C	-5.866217	1.384796	0.883519
C	-3.979683	2.429124	-0.071996
H	-7.733192	2.411093	0.644256
H	-6.308092	0.577633	1.431686
H	-3.882422	0.545646	0.975796
H	-6.752966	4.307006	-0.643780
N	-3.995694	4.396563	-1.216852
N	-2.710502	3.980418	-1.213602
N	-2.696355	2.771820	-0.508188
O	-1.582399	2.087158	-0.297581
H	-1.318274	0.393291	1.534395
C	2.839086	-1.522662	1.815720
C	3.111285	-2.939741	1.298285
H	2.651343	-3.657839	1.965721
H	4.174565	-3.133025	1.236097
H	2.664574	-3.036512	0.318625
C	3.369123	-1.322816	3.241791
H	3.156606	-0.317620	3.586088
H	4.436049	-1.491392	3.296896

H	2.868630	-2.025383	3.895225
H	5.484576	-0.864404	1.399915
O	5.184255	2.168650	-1.851812
C	4.448248	2.789331	-2.919561
H	3.957295	2.048351	-3.537624
H	5.180576	3.322356	-3.503277
H	3.712219	3.486049	-2.538658
H	0.985393	0.593021	2.115397

Compound TS_**6a**$_{C\text{-}2}$-BTNO, HF/3-21G(*): 1 imaginary frequency at 2911.977 cm-1

H	1.870746	0.035833	2.417098
C	2.307126	-0.566247	1.652638
C	3.318883	-2.116475	-0.413461
C	1.534891	-0.866070	0.535761
C	3.592547	-1.054863	1.721545
C	4.103521	-1.833495	0.682964
C	2.010907	-1.633550	-0.501529
H	5.104330	-2.190309	0.779225
O	3.737025	-2.864732	-1.480696
O	4.448889	-0.826622	2.763703
C	5.032627	-3.488891	-1.482655
H	5.822642	-2.749725	-1.448157
H	5.087113	-4.036116	-2.409196
H	5.138915	-4.169477	-0.647857
C	4.031005	-0.041496	3.893702
H	3.775932	0.967655	3.596073
H	4.877841	-0.021615	4.559662
H	3.184154	-0.494352	4.393315
O	0.261814	-0.334537	0.521661
C	1.153577	-1.945551	-1.703125
H	1.408825	-1.286223	-2.526377
H	1.323280	-2.965078	-2.012490
C	-0.322275	-1.777096	-1.373045
O	-0.694612	-2.871540	-0.515694
C	-2.028186	-0.436473	-0.138892
C	-4.680215	-0.285626	0.662793
C	-2.633603	0.802411	0.054798
C	-2.738682	-1.612415	0.065577
C	-4.072907	-1.508697	0.458369
C	-3.950551	0.891753	0.456574
H	-2.067824	1.689369	-0.127682
O	-5.988881	-0.276273	1.091143

C	-6.981172	0.383662	0.257239
H	-6.765745	1.434231	0.181862
H	-7.924856	0.221364	0.752494
H	-7.003633	-0.064370	-0.729089
C	2.562480	4.701561	0.118981
C	2.869527	2.194831	-1.220993
C	3.814751	4.129180	-0.053661
C	3.964493	2.892098	-0.714090
C	1.621055	2.775845	-1.040332
H	4.684521	4.631533	0.318499
H	4.945300	2.476145	-0.826214
H	2.980218	1.253329	-1.714176
H	2.427283	5.639890	0.614664
N	0.121220	4.335225	-0.363074
N	-0.572086	3.375165	-0.980701
N	0.351917	2.409525	-1.377949
C	-2.096845	-2.983037	-0.140914
C	1.460272	4.002747	-0.387587
O	-0.039094	1.344744	-2.180586
H	-0.349773	0.472980	-1.417137
C	-0.599057	-0.528149	-0.567172
C	-2.823676	-3.767132	-1.242843
H	-3.849386	-3.964226	-0.961233
H	-2.313179	-4.708810	-1.399965
H	-2.827195	-3.212690	-2.173443
C	-2.056505	-3.769143	1.173023
H	-3.054988	-3.964650	1.540713
H	-1.506270	-3.201431	1.910636
H	-1.545437	-4.708716	1.005716
H	-4.669113	-2.379581	0.632794
O	-4.608063	2.077466	0.660240
C	-3.881179	3.324247	0.624253
H	-4.609499	4.085043	0.851330
H	-3.448258	3.502531	-0.349856
H	-3.094875	3.333793	1.367622
H	-0.921912	-1.757357	-2.272462

Compound TS_**6a**$_{C\text{-}4}$-BTNO, HF/3-21G(*): 1 imaginary frequency at 2884.395 cm^{-1}

H	0.656730	-0.488233	3.145809
C	1.242474	-0.859443	2.335337
C	2.685221	-1.791352	0.147086
C	0.705289	-0.770837	1.056710

C	2.495271	-1.415713	2.510791
C	3.222592	-1.880500	1.410220
C	1.404577	-1.240989	-0.054333
H	4.189300	-2.291688	1.595529
O	3.319755	-2.209474	-0.992163
O	3.115793	-1.549023	3.722792
C	4.610097	-2.842088	-0.920740
H	5.352072	-2.163602	-0.521140
H	4.860591	-3.101770	-1.936296
H	4.572012	-3.737277	-0.313813
C	2.478051	-1.087278	4.926081
H	2.289286	-0.022183	4.885169
H	3.172532	-1.303372	5.721147
H	1.547341	-1.611325	5.102164
O	-0.539897	-0.220331	0.940973
C	0.820798	-1.174339	-1.380217
C	-0.657323	-0.843453	-1.413872
C	-1.010711	0.204444	-0.371434
H	-0.541248	1.144689	-0.615868
O	-1.344625	-2.060247	-1.084675
C	-2.502053	0.344732	-0.250205
C	-5.261076	0.648946	0.012451
C	-3.045791	1.534636	0.232553
C	-3.342811	-0.707927	-0.589186
C	-4.724480	-0.534622	-0.458242
C	-4.408072	1.702650	0.364407
H	-2.408522	2.353008	0.498316
O	-6.606900	0.873839	0.172725
C	-7.572788	-0.059408	-0.336392
H	-7.435812	-0.225100	-1.397632
H	-8.533655	0.396086	-0.162145
H	-7.521246	-1.006481	0.186172
C	5.116623	2.901166	0.217879
C	4.785645	0.989182	-1.880590
C	3.851851	2.589810	-0.295038
C	6.208513	2.246109	-0.335083
C	6.044945	1.302639	-1.369852
C	3.706325	1.653982	-1.321301
H	7.194090	2.458280	0.027021
H	6.910787	0.818432	-1.775374
H	4.647844	0.271544	-2.660705
H	5.221565	3.618918	1.003986

N	2.608546	3.079541	0.055723
N	1.680795	2.492748	-0.721364
N	2.359918	1.621146	-1.554102
O	1.715364	0.903517	-2.538974
H	1.117654	-1.962138	-2.050720
H	1.343712	-0.135155	-1.971065
C	-2.794585	-2.035760	-1.104807
C	-3.260843	-2.296519	-2.545301
H	-2.809116	-3.214005	-2.900977
H	-2.964462	-1.485594	-3.199465
H	-4.337696	-2.392618	-2.591561
C	-3.179476	-3.189161	-0.172291
H	-2.715793	-4.098590	-0.532315
H	-4.252305	-3.326364	-0.135354
H	-2.806704	-2.979210	0.820620
H	-5.377879	-1.338078	-0.723874
O	-4.894719	2.913336	0.810115
C	-5.589692	2.925824	2.086912
H	-6.483826	2.329096	2.030664
H	-5.835592	3.959079	2.272029
H	-4.943378	2.556276	2.873823
H	-0.942692	-0.477988	-2.391568

Compound **6b**, HF/3-21G(*)

H	2.748316	-1.988180	1.808449
C	2.880310	-1.265094	1.035656
C	3.107953	0.673089	-0.921641
C	1.944874	-0.241444	0.933748
C	3.925830	-1.303221	0.147215
C	4.043181	-0.329004	-0.840586
C	2.039728	0.736467	-0.024600
H	4.869587	-0.400181	-1.510640
O	3.142339	1.667675	-1.858339
O	4.902521	-2.259123	0.150181
C	4.199854	1.731519	-2.830454
H	5.164577	1.841222	-2.351555
H	3.988137	2.602353	-3.428621
H	4.207158	0.849338	-3.457501
C	4.884390	-3.321337	1.118496
H	4.958270	-2.933137	2.126378
H	5.747574	-3.927191	0.897837
H	3.986259	-3.918428	1.027907

O	0.932814	-0.262717	1.868201
C	1.014326	1.840535	-0.124382
C	0.331907	2.025706	1.229100
C	-0.150156	0.684871	1.775564
H	-0.496751	0.812905	2.790119
O	-0.785459	2.921529	1.203800
C	-1.266477	0.160950	0.903149
C	-3.332703	-0.808214	-0.657234
C	-2.159106	1.049891	0.324591
C	-1.414594	-1.201029	0.702207
C	-2.439370	-1.689613	-0.071230
C	-3.185935	0.544950	-0.460890
H	-0.719607	-1.883957	1.140058
H	-3.897613	1.192148	-0.928651
O	-4.382059	-1.275962	-1.431158
O	-2.564547	-3.055170	-0.273515
C	-4.010531	-1.861057	-2.714812
H	-3.532987	-1.117748	-3.339925
H	-4.933634	-2.185098	-3.167338
H	-3.347359	-2.696486	-2.560671
C	-3.697735	-3.689573	0.389006
H	-3.610873	-3.584100	1.462535
H	-3.651888	-4.731547	0.116427
H	-4.620139	-3.247703	0.047464
H	0.278837	1.587308	-0.876527
C	-2.039624	2.550909	0.563693
C	-3.117468	2.999377	1.561138
H	-4.107289	2.828665	1.157940
H	-2.989425	4.053531	1.771929
H	-3.012128	2.447063	2.485689
C	-2.140599	3.363505	-0.735323
H	-3.131415	3.296123	-1.164404
H	-1.418845	3.020484	-1.464054
H	-1.930981	4.399201	-0.502087
H	1.493919	2.760649	-0.423352
H	1.032204	2.463386	1.925215

Compound **6b**, B3LYP/6-31G*

H	2.841024	-1.862200	1.848996
C	2.932775	-1.141468	1.047254
C	3.060201	0.776429	-0.979059
C	1.965161	-0.129037	0.948254

C	3.964234	-1.171644	0.115643
C	4.034908	-0.213218	-0.909508
C	2.004298	0.848714	-0.043670
H	4.851786	-0.280081	-1.615792
O	3.038342	1.751012	-1.938028
O	4.964845	-2.101975	0.105988
C	4.077899	1.769871	-2.902454
H	5.061087	1.904364	-2.432500
H	3.867448	2.621251	-3.552614
H	4.089239	0.849322	-3.500554
C	4.954460	-3.101435	1.112063
H	5.029836	-2.664322	2.116681
H	5.829862	-3.726095	0.923239
H	4.048180	-3.719160	1.057565
O	0.998782	-0.160358	1.925467
C	0.962213	1.939976	-0.118596
C	0.252751	2.080274	1.232054
C	-0.133440	0.707664	1.791584
H	-0.485251	0.842280	2.820985
O	-0.889907	2.923944	1.226330
C	-1.236870	0.113185	0.940060
C	-3.286019	-0.948346	-0.646146
C	-2.169133	0.979991	0.346773
C	-1.343890	-1.267578	0.751044
C	-2.362239	-1.809991	-0.026816
C	-3.182698	0.426234	-0.447118
H	-0.622780	-1.937677	1.206648
H	-3.923458	1.054159	-0.932057
O	-4.321211	-1.432202	-1.417308
O	-2.412641	-3.174978	-0.209900
C	-3.917919	-2.001288	-2.668431
H	-3.431541	-1.244907	-3.298118
H	-4.834144	-2.343264	-3.155439
H	-3.237490	-2.845772	-2.520301
C	-3.518133	-3.822927	0.428995
H	-3.476848	-3.676630	1.516275
H	-3.417849	-4.887202	0.203639
H	-4.474296	-3.450658	0.046767
H	0.233788	1.711948	-0.906312
C	-2.117728	2.489719	0.588807
C	-3.222717	2.886008	1.586201
H	-4.216670	2.687040	1.171724

H	-3.142962	3.953646	1.816840
H	-3.116051	2.321288	2.517606
C	-2.269033	3.303236	-0.710242
H	-3.258625	3.170402	-1.159302
H	-1.515330	3.018484	-1.449610
H	-2.139718	4.364993	-0.478814
H	1.422171	2.894828	-0.392211
H	0.938044	2.558749	1.940496

Compound **6b**$_{C\text{-}2}$, HF/3-21G(*)

H	-2.415540	-2.793562	-0.326131
C	-2.895978	-1.854076	-0.170440
C	-4.015183	0.654058	0.224398
C	-2.113778	-0.706397	-0.188657
C	-4.248728	-1.727492	0.050843
C	-4.812222	-0.468516	0.249716
C	-2.640395	0.553081	-0.002237
H	-5.864139	-0.420476	0.419064
O	-4.486644	1.924158	0.410993
O	-5.123143	-2.777962	0.093754
C	-5.885080	2.168669	0.639799
H	-6.482475	1.832120	-0.197633
H	-5.975976	3.236895	0.746787
H	-6.223780	1.679896	1.544220
C	-4.659003	-4.124679	-0.100677
H	-4.220029	-4.249116	-1.082610
H	-5.534371	-4.746608	-0.012131
H	-3.935387	-4.403112	0.654753
O	-0.760429	-0.896459	-0.399971
C	-1.756876	1.781235	-0.040103
C	-0.544677	1.478619	-0.930657
C	0.086786	0.197248	-0.491754
O	0.388609	2.559907	-0.986704
C	1.447506	0.024505	-0.275088
C	4.204619	-0.276572	0.106877
C	2.290217	1.175910	-0.234695
C	2.015575	-1.265330	-0.098702
C	3.375777	-1.407105	0.085357
C	3.654798	0.997690	-0.041930
H	1.386632	-2.128506	-0.114819
H	4.324487	1.830201	0.003030
O	5.573778	-0.408321	0.279575

O	3.921683	-2.671658	0.253185
C	6.008683	-0.848009	1.599973
H	5.724816	-0.121533	2.350474
H	7.083126	-0.919243	1.546523
H	5.574335	-1.807210	1.830742
C	4.717541	-3.164152	-0.864146
H	4.105753	-3.246877	-1.753166
H	5.069218	-4.139277	-0.567750
H	5.547634	-2.500672	-1.046934
H	-1.421693	2.040960	0.956400
C	1.639137	2.552815	-0.242935
C	2.471509	3.604102	-0.981708
H	3.405322	3.803727	-0.473534
H	1.895765	4.518621	-1.030422
H	2.671713	3.267689	-1.989421
C	1.379633	2.987322	1.209312
H	2.320844	3.123041	1.726874
H	0.805139	2.238488	1.739227
H	0.830094	3.920692	1.213398
H	-2.309864	2.617590	-0.439695
H	-0.907974	1.346542	-1.944856

Compound **6b**C-2, B3LYP/6-31G*

H	2.841024	-1.862200	1.848996
C	2.932775	-1.141468	1.047254
C	3.060201	0.776429	-0.979059
C	1.965161	-0.129037	0.948254
C	3.964234	-1.171644	0.115643
C	4.034908	-0.213218	-0.909508
C	2.004298	0.848714	-0.043670
H	4.851786	-0.280081	-1.615792
O	3.038342	1.751012	-1.938028
O	4.964845	-2.101975	0.105988
C	4.077899	1.769871	-2.902454
H	5.061087	1.904364	-2.432500
H	3.867448	2.621251	-3.552614
H	4.089239	0.849322	-3.500554
C	4.954460	-3.101435	1.112063
H	5.029836	-2.664322	2.116681
H	5.829862	-3.726095	0.923239
H	4.048180	-3.719160	1.057565
O	0.998782	-0.160358	1.925467

C	0.962213	1.939976	-0.118596
C	0.252751	2.080274	1.232054
C	-0.133440	0.707664	1.791584
O	-0.889907	2.923944	1.226330
C	-1.236870	0.113185	0.940060
C	-3.286019	-0.948346	-0.646146
C	-2.169133	0.979991	0.346773
C	-1.343890	-1.267578	0.751044
C	-2.362239	-1.809991	-0.026816
C	-3.182698	0.426234	-0.447118
H	-0.622780	-1.937677	1.206648
H	-3.923458	1.054159	-0.932057
O	-4.321211	-1.432202	-1.417308
O	-2.412641	-3.174978	-0.209900
C	-3.917919	-2.001288	-2.668431
H	-3.431541	-1.244907	-3.298118
H	-4.834144	-2.343264	-3.155439
H	-3.237490	-2.845772	-2.520301
C	-3.518133	-3.822927	0.428995
H	-3.476848	-3.676630	1.516275
H	-3.417849	-4.887202	0.203639
H	-4.474296	-3.450658	0.046767
H	0.233788	1.711948	-0.906312
C	-2.117728	2.489719	0.588807
C	-3.222717	2.886008	1.586201
H	-4.216670	2.687040	1.171724
H	-3.142962	3.953646	1.816840
H	-3.116051	2.321288	2.517606
C	-2.269033	3.303236	-0.710242
H	-3.258625	3.170402	-1.159302
H	-1.515330	3.018484	-1.449610
H	-2.139718	4.364993	-0.478814
H	1.422171	2.894828	-0.392211
H	0.938044	2.558749	1.940496

Compound **6b**$_{C\text{-}4}$, HF/3-21G(*)

H	2.495296	-1.969478	1.828213
C	2.642267	-1.216685	1.086075
C	2.949309	0.809079	-0.820872
C	1.840445	-0.087560	1.134253
C	3.599839	-1.330070	0.086052
C	3.745648	-0.312475	-0.869543

C	1.968055	0.961478	0.199516
H	4.491448	-0.450737	-1.620533
O	3.023915	1.851842	-1.707947
O	4.449190	-2.398861	-0.058237
C	3.985104	1.838527	-2.776463
H	4.996739	1.802138	-2.392212
H	3.832992	2.760249	-3.313500
H	3.821508	0.998531	-3.439628
C	4.378427	-3.512613	0.846546
H	4.583153	-3.206198	1.864935
H	5.138636	-4.201883	0.517394
H	3.408899	-3.993058	0.803771
O	0.911302	0.001126	2.156127
C	1.159844	2.101089	0.297696
C	0.216925	2.239858	1.457068
C	-0.230700	0.866212	1.958861
H	-0.672637	0.963031	2.938417
O	-0.950480	3.025973	1.185350
C	-1.221249	0.248271	0.997242
C	-3.044755	-0.952405	-0.703583
C	-2.030498	1.037039	0.199026
C	-1.339883	-1.133449	0.949260
C	-2.241157	-1.736499	0.109470
C	-2.933269	0.415594	-0.655613
H	-0.712145	-1.744321	1.561158
H	-3.573735	0.987030	-1.294203
O	-3.970548	-1.534959	-1.553687
O	-2.332647	-3.119320	0.066312
C	-3.416423	-2.263607	-2.689170
H	-2.855954	-1.592199	-3.326339
H	-4.263998	-2.659078	-3.224967
H	-2.780040	-3.060273	-2.340595
C	-3.550969	-3.688362	0.630170
H	-3.624407	-3.447786	1.682735
H	-3.464047	-4.755053	0.501510
H	-4.413333	-3.311621	0.103906
H	1.298294	2.920485	-0.372345
C	-1.952411	2.556833	0.243171
C	-3.256599	3.142068	0.801488
H	-4.094634	2.906831	0.159045
H	-3.154605	4.216971	0.879719
H	-3.439750	2.739267	1.788552

C	-1.647298	3.142524	-1.144058
H	-2.482038	2.986868	-1.814892
H	-0.768141	2.684257	-1.573647
H	-1.476931	4.206633	-1.039412
H	0.710975	2.765337	2.265266

Compound **6b**C-4, B3LYP/6-31G*

H	2.841024	-1.862200	1.848996
C	2.932775	-1.141468	1.047254
C	3.060201	0.776429	-0.979059
C	1.965161	-0.129037	0.948254
C	3.964234	-1.171644	0.115643
C	4.034908	-0.213218	-0.909508
C	2.004298	0.848714	-0.043670
H	4.851786	-0.280081	-1.615792
O	3.038342	1.751012	-1.938028
O	4.964845	-2.101975	0.105988
C	4.077899	1.769871	-2.902454
H	5.061087	1.904364	-2.432500
H	3.867448	2.621251	-3.552614
H	4.089239	0.849322	-3.500554
C	4.954460	-3.101435	1.112063
H	5.029836	-2.664322	2.116681
H	5.829862	-3.726095	0.923239
H	4.048180	-3.719160	1.057565
O	0.998782	-0.160358	1.925467
C	0.962213	1.939976	-0.118596
C	0.252751	2.080274	1.232054
C	-0.133440	0.707664	1.791584
H	-0.485251	0.842280	2.820985
O	-0.889907	2.923944	1.226330
C	-1.236870	0.113185	0.940060
C	-3.286019	-0.948346	-0.646146
C	-2.169133	0.979991	0.346773
C	-1.343890	-1.267578	0.751044
C	-2.362239	-1.809991	-0.026816
C	-3.182698	0.426234	-0.447118
H	-0.622780	-1.937677	1.206648
H	-3.923458	1.054159	-0.932057
O	-4.321211	-1.432202	-1.417308
O	-2.412641	-3.174978	-0.209900
C	-3.917919	-2.001288	-2.668431

H	-3.431541	-1.244907	-3.298118
H	-4.834144	-2.343264	-3.155439
H	-3.237490	-2.845772	-2.520301
C	-3.518133	-3.822927	0.428995
H	-3.476848	-3.676630	1.516275
H	-3.417849	-4.887202	0.203639
H	-4.474296	-3.450658	0.046767
H	0.233788	1.711948	-0.906312
C	-2.117728	2.489719	0.588807
C	-3.222717	2.886008	1.586201
H	-4.216670	2.687040	1.171724
H	-3.142962	3.953646	1.816840
H	-3.116051	2.321288	2.517606
C	-2.269033	3.303236	-0.710242
H	-3.258625	3.170402	-1.159302
H	-1.515330	3.018484	-1.449610
H	-2.139718	4.364993	-0.478814
H	0.938044	2.558749	1.940496

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