Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary Information

Influence of phenylpropanoid units of lignin and its oxidized derivatives on the stability and βO4 binding properties: DFT and QTAIM approach

Carlos A.C. Kramer[*‡], Amison R.L da Silva [†], Luciene S. de Carvalho*[*‡]*

‡ Energy Technology Laboratory, Institute of Chemistry, Federal University of Rio Grande do Norte, Natal, Rio Grande do Norte 59075-000, Brazil

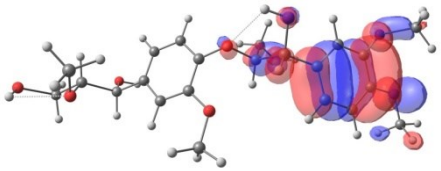
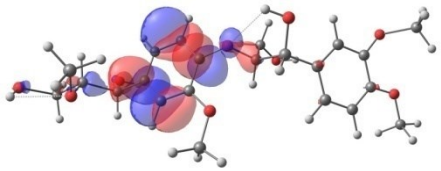
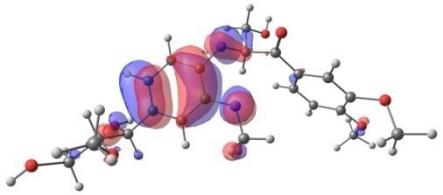
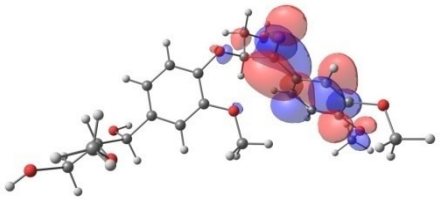
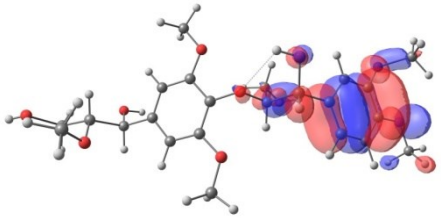
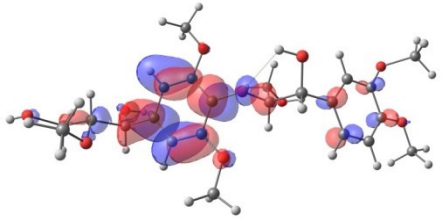
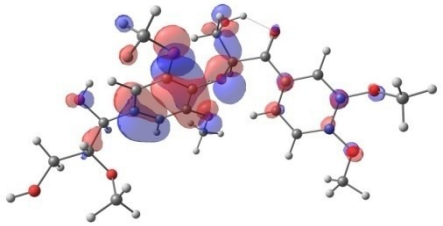
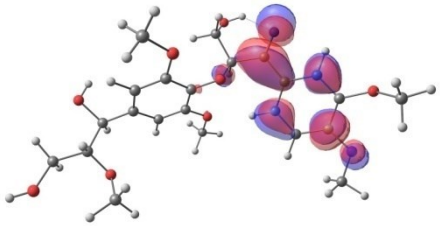
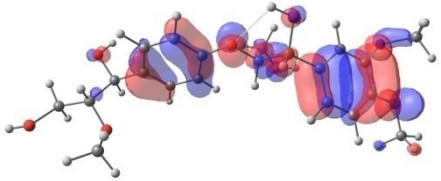
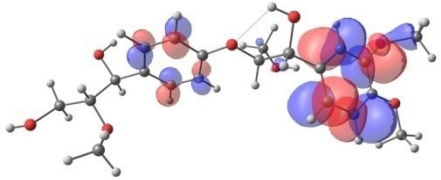
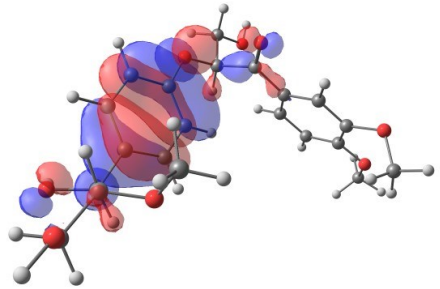
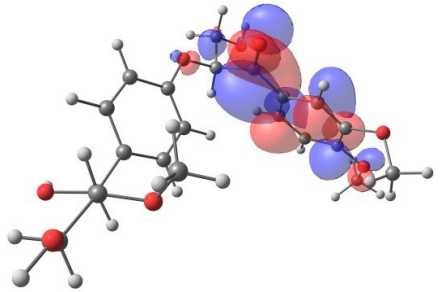
†Theory Chemistry Group, Analytical Chemistry and Chemical Physics Department, Federal University of Ceará, Fortaleza, Ceará 60455-900, Brazil

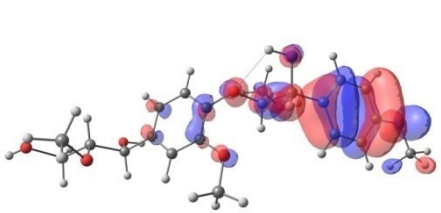
Corresponding author

*Email: carlosaugustokramer@gmail.com or amison.rick@gmail.com

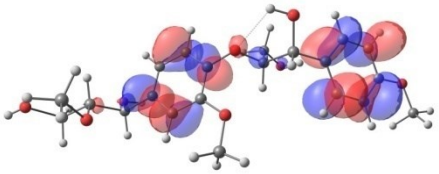
Contents

Table S1: Images of the HOMO and LUMO orbital densities for the lignin models and their oxidized pairs in their respective optimized geometries

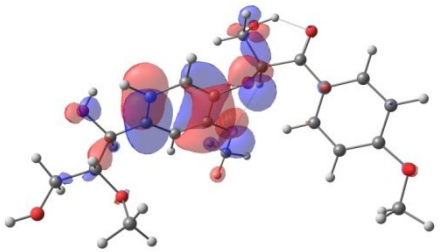
B3LYP			
GG-HOMO	**GG-LUMO**	**GGOX-HOMO**	**GGOX-LUMO**
			
GS-HOMO	**GS-LUMO**	**GSOX-HOMO**	**GSOX-LUMO**
			
GH-HOMO	**GH-LUMO**	**GHOX-HOMO**	**GHOX-LUMO**
			
HG-HOMO	**HG-LUMO**	**HGOX-HOMO**	**HGOX-LUMO**



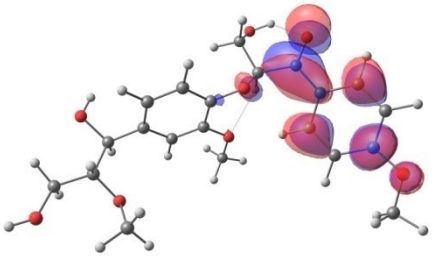
HS-HOMO



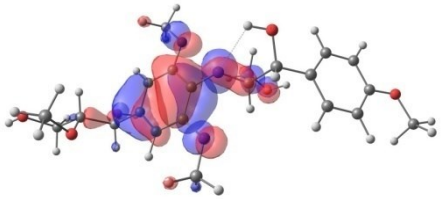
HS-LUMO



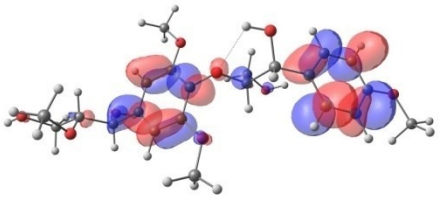
HSOX-HOMO



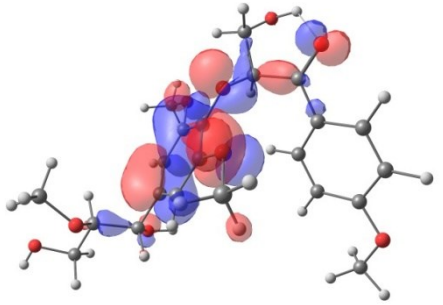
HSOX-LUMO



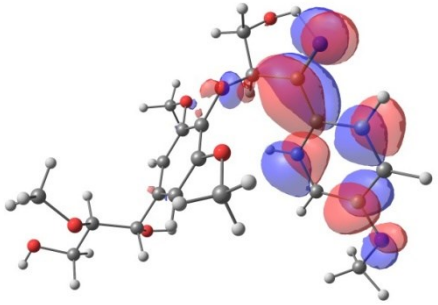
HH-HOMO



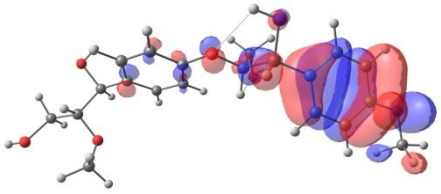
HH-LUMO



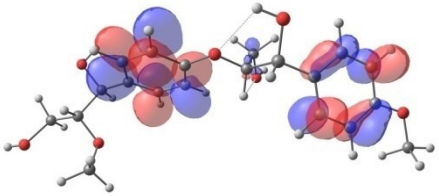
HHOX-HOMO



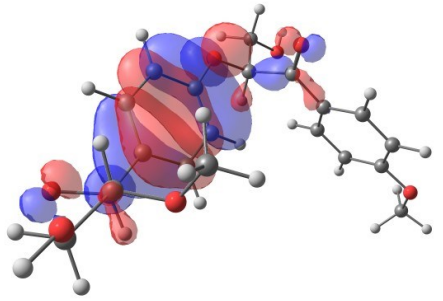
HHOX-LUMO



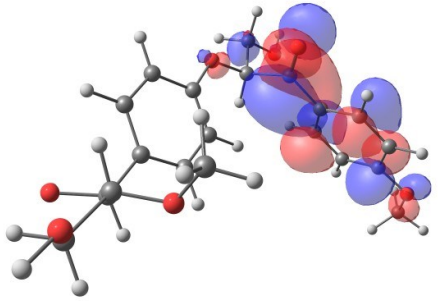
SG-HOMO



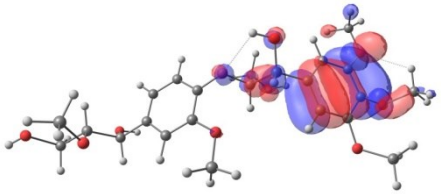
SG-LUMO



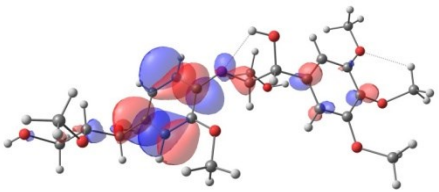
SGOX-HOMO



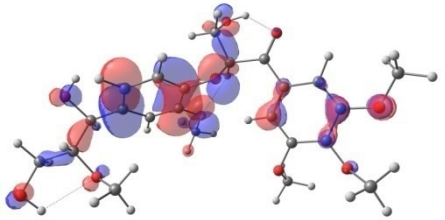
SGOX-LUMO



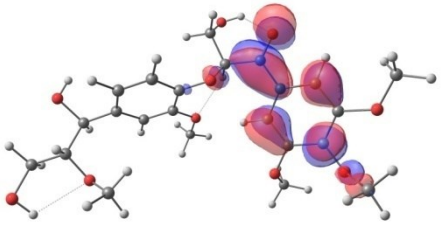
SS-HOMO



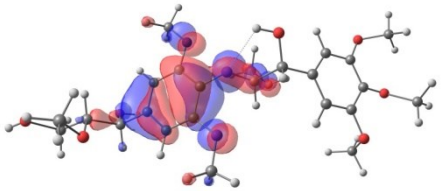
SS-LUMO



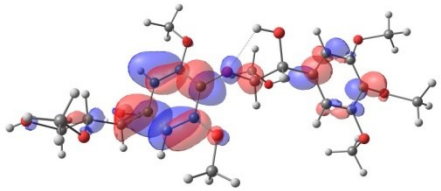
SSOX-HOMO



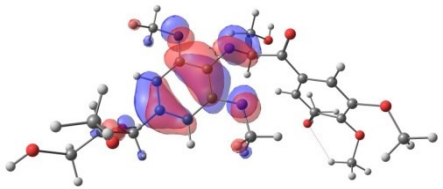
SSOX-LUMO



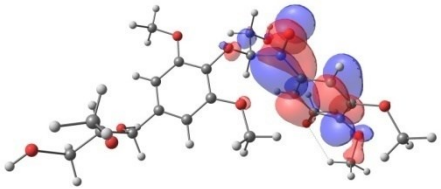
SH-HOMO



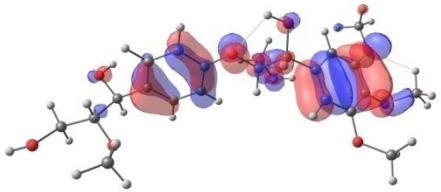
SH-LUMO



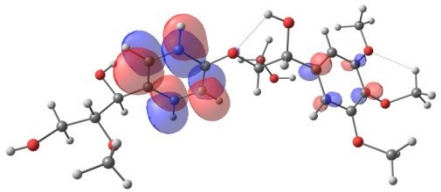
SHOX-HOMO



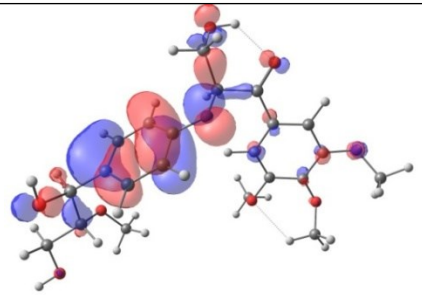
SHOX-LUMO



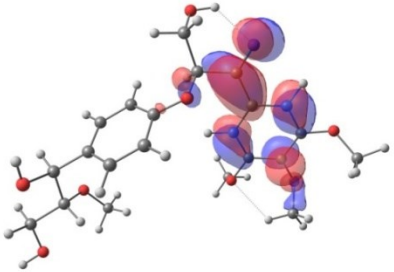
GG-HOMO



GG-LUMO

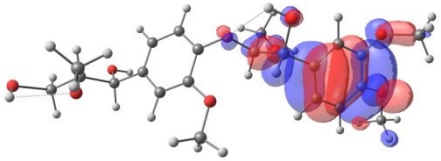


GGOX-HOMO

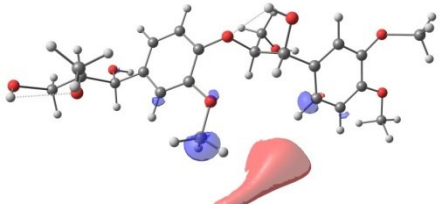


GGOX-LUMO

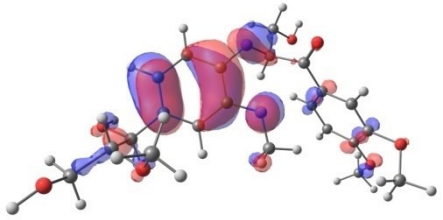
M062X



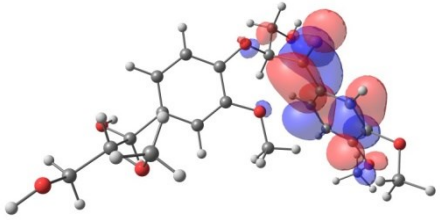
GS-HOMO



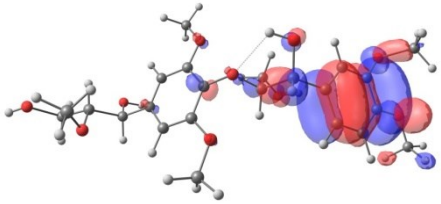
GS-LUMO



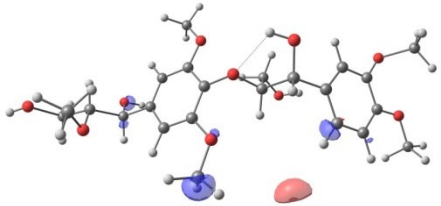
GSOX-HOMO



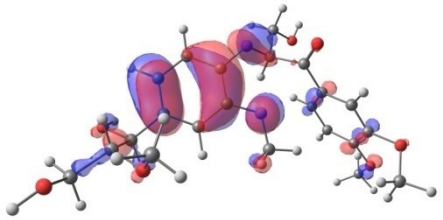
GSOX-LUMO



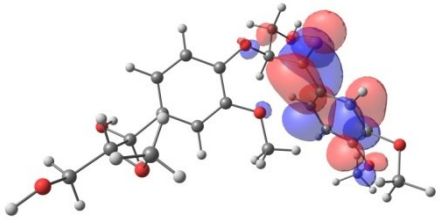
GH-HOMO



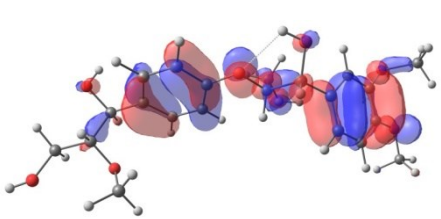
GH-LUMO



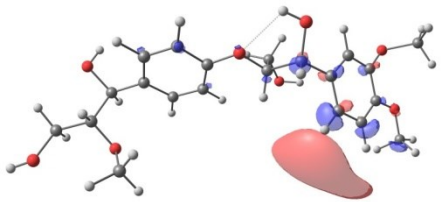
GHOX-HOMO



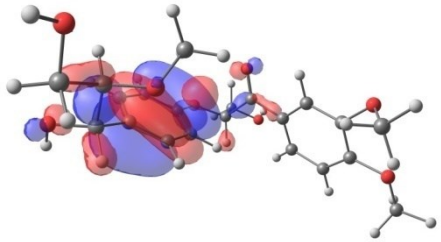
GHOX-LUMO



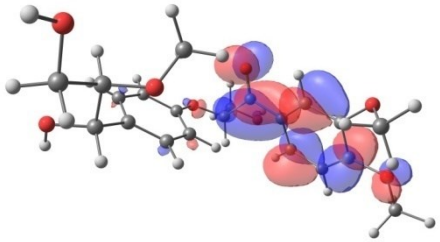
HG-HOMO



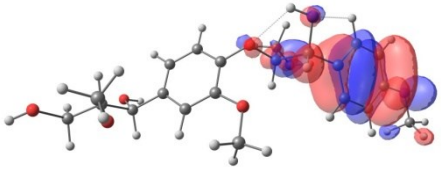
HG-LUMO



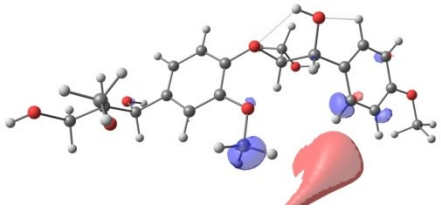
HGOX-HOMO



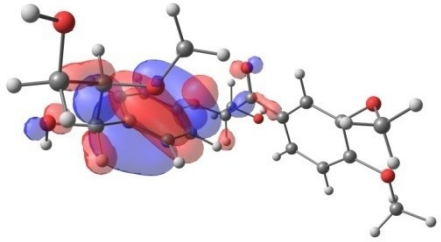
HGOX-LUMO



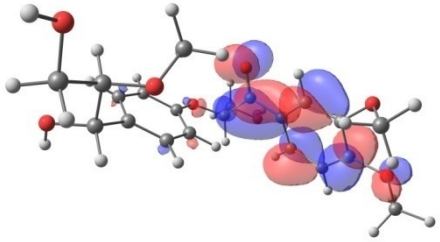
HS-HOMO



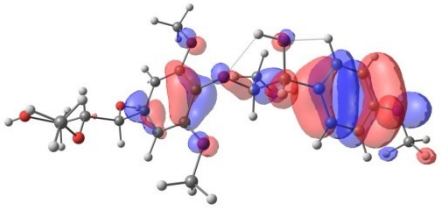
HS-LUMO



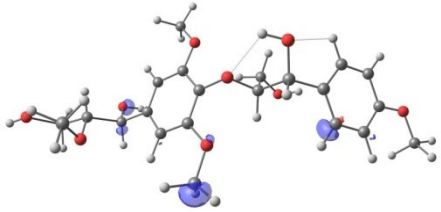
HSOX-HOMO



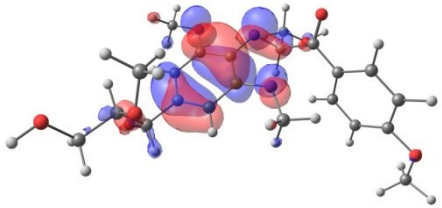
HSOX-LUMO



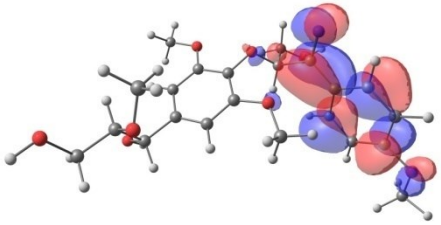
HH-HOMO



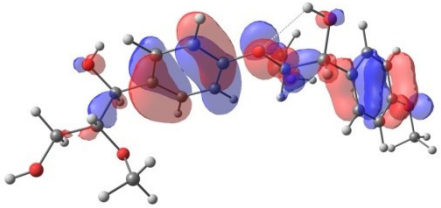
HH-LUMO



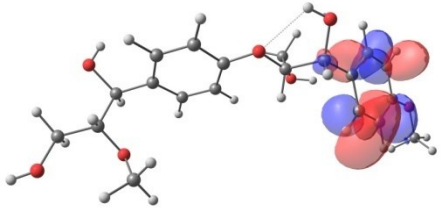
HHOX-HOMO



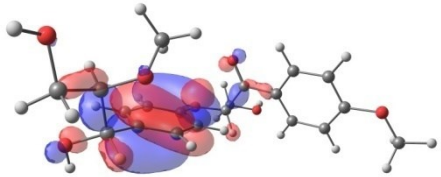
HHOX-LUMO



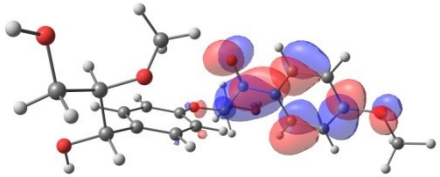
SG-HOMO



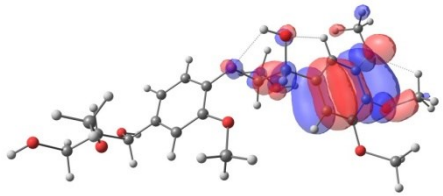
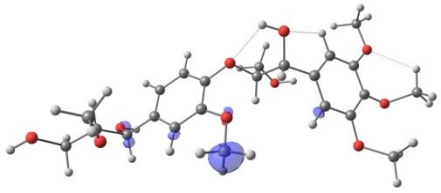
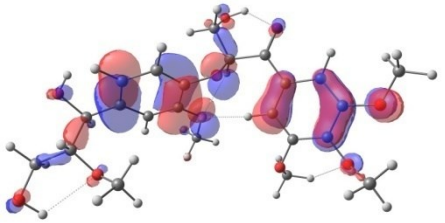
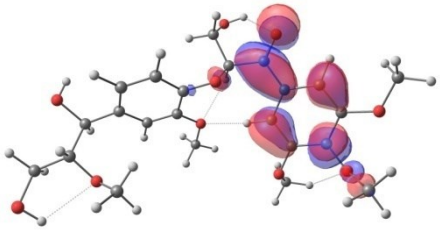
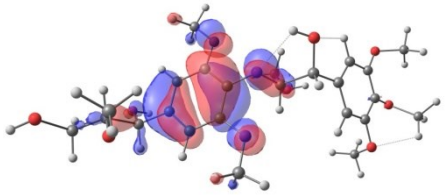
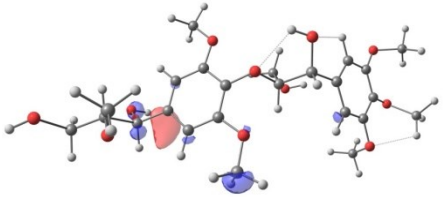
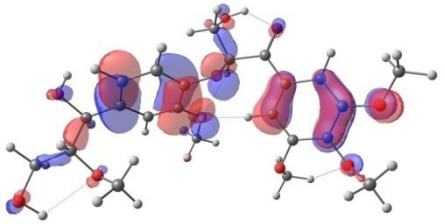
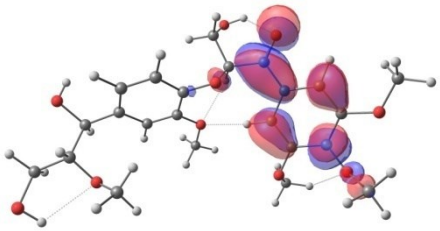
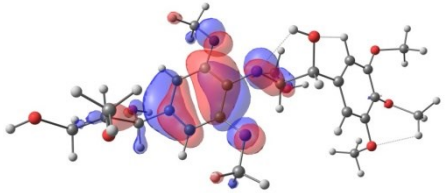
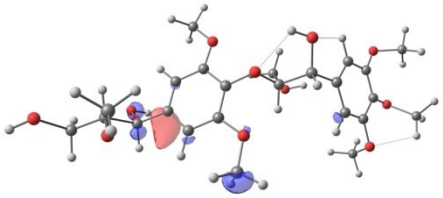
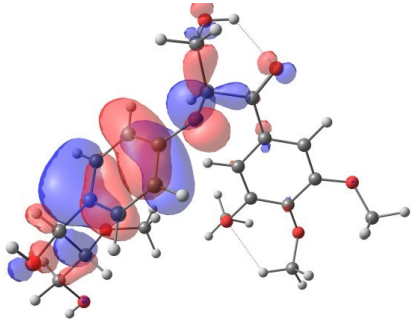
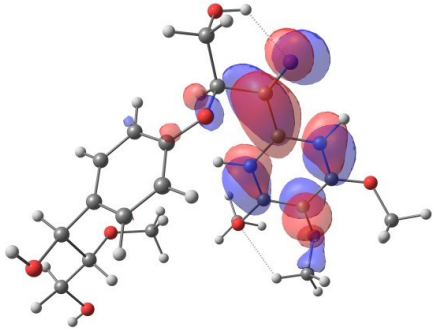
SG-LUMO



SGOX-HOMO



SGOX-LUMO

			
SS-HOMO	**SS-LUMO**	**SSOX-HOMO**	**SSOX-LUMO**
			
SH-HOMO	**SH-LUMO**	**SHOX-HOMO**	**SHOX-LUMO**
			

Subtitle:
Red Atom: Oxygen
White Atom: Hydrogen
Gray Atom: Carbon

Table S2: Atomic coordinates and details of the optimized structure of the SS model calculated with B3LYP functional

MODEL	SS	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000017	**RMS FORCE**	0.000004
MAXIMUM DISPLACEMENT	0.001736	**RMS DISPLACEMENT**	0.000373
PREDICTED ENERGY CHANGE (Hartree)	$-1.91.10^{-8}$	**NUMBER OF STEPS**	13
Atom	Coordinates (Angstroms)		
	X	Y	Z
C	4.962996	1.378405	-0.104775
C	3.694931	1.080125	-0.593456
C	3.313860	-0.252674	-0.799977
C	4.229596	-1.270273	-0.530057
C	5.521307	-0.979595	-0.062488
C	5.905054	0.359049	0.150575
H	3.014232	1.901681	-0.795827
H	3.968135	-2.306287	-0.709572
C	1.917192	-0.562511	-1.304688
H	1.663344	0.166274	-2.088900
C	0.827226	-0.416760	-0.218897
H	0.789637	0.622484	0.121761
C	0.980607	-1.344236	0.996685
H	0.016988	-1.411347	1.507194
O	1.894574	-1.877359	-1.849713
H	0.967818	-2.079827	-2.047786
O	-0.391013	-0.741086	-0.941422
C	-1.596035	-0.412278	-0.372424
C	-2.468006	-1.441840	0.030586
C	-2.019837	0.926098	-0.277761
C	-3.73645	-1.133708	0.537565
C	-3.282225	1.230439	0.247860
C	-4.139258	0.202544	0.648145
H	-4.412751	-1.916684	0.857843
H	-3.618000	2.257195	0.320990
O	-1.128411	1.860253	-0.725238
O	-1.983519	-2.709228	-0.111484
C	-1.509901	3.232040	-0.694056
H	-1.686402	3.574543	0.332962
H	-0.669246	3.781273	-1.119782
H	-2.406381	3.409794	-1.299732
C	-2.818433	-3.799859	0.261694
H	-2.234948	-4.698859	0.059612
H	-3.073529	-3.763491	1.327997
H	-3.739128	-3.820866	-0.334134

C	-5.518247	0.535208	1.194694
H	-5.532172	1.595252	1.488185
C	-6.635244	0.340809	0.145174
H	-6.574208	-0.682709	-0.253058
C	-8.023038	0.546252	0.747919
H	-8.131360	-0.085866	1.635842
H	-8.127328	1.601178	1.040489
O	-5.860205	-0.287037	2.318966
H	-5.121777	-0.269240	2.942319
O	-6.374673	1.288092	-0.883847
O	-8.993191	0.199311	-0.248494
H	-9.876349	0.325920	0.118841
C	-6.654452	0.848422	-2.209679
H	-6.060372	-0.042037	-2.461382
H	-7.718395	0.627219	-2.342512
H	-6.362145	1.666602	-2.872391
O	6.303980	-2.065758	0.218703
O	7.139375	0.652972	0.687558
O	5.305032	2.699581	0.108954
C	7.699364	-2.054801	-0.099549
H	7.865980	-1.643317	-1.102486
H	8.274393	-1.487014	0.634468
H	8.007497	-3.102184	-0.087177
C	8.033992	1.399875	-0.154454
H	7.596253	2.359071	-0.441831
H	8.937052	1.562111	0.437286
H	8.284728	0.823717	-1.053846
C	5.261413	3.107602	1.485679
H	4.246707	2.996394	1.886634
H	5.963017	2.524036	2.091321
H	5.546776	4.161310	1.499432
H	1.260846	-2.353044	0.670871
O	1.896809	-0.829343	1.960631
H	2.794326	-0.926444	1.613558

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

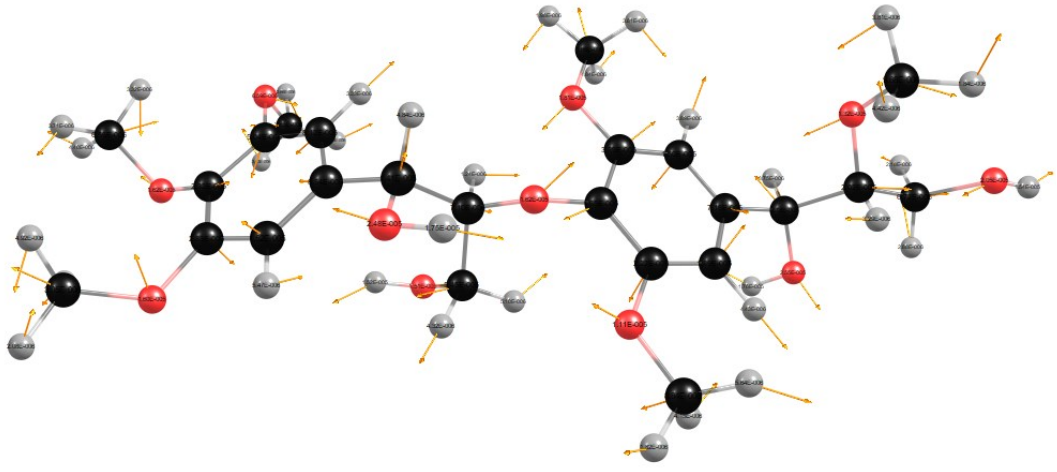


Table S3: Atomic coordinates and details of the optimized structure of the SSOX model calculated with B3LYP functional

MODEL	SSOX	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000009	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001428	**RMS DISPLACEMENT**	0.000222
PREDICTED ENERGY CHANGE (Hartree)	$-2.92.10^{-9}$	**NUMBER OF STEPS**	31
Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-4.243346	-0.222683	1.177005
C	-3.201648	0.560388	0.689365
C	-2.983974	0.653438	-0.693381
C	-3.818715	-0.055915	-1.565622
C	-4.846982	-0.869205	-1.085902
C	-5.067666	-0.965588	0.306723
H	-2.613492	1.121064	1.405251
H	-3.666106	0.021952	-2.636159
C	-1.907851	1.501192	-1.295549
C	-0.796804	2.106549	-0.407456
H	-0.750304	1.617331	0.567911
C	-1.013673	3.611129	-0.224571
H	-0.160378	4.023311	0.327322
O	-1.892192	1.746628	-2.490948
O	0.463023	1.961003	-1.082240
C	1.436275	1.227627	-0.455432
C	2.627098	1.863602	-0.055984
C	1.305980	-0.162137	-0.283050
C	3.671345	1.113344	0.500656
C	2.343260	-0.905464	0.294479
C	3.526914	-0.268638	0.675471
H	4.592498	1.590153	0.811918
H	2.252843	-1.977372	0.419182
O	0.121436	-0.687762	-0.709387
O	2.669441	3.213827	-0.248620
C	-0.085864	-2.091182	-0.593992
H	-0.056430	-2.414009	0.454091
H	-1.079744	-2.274380	-1.003319
H	0.659179	-2.650134	-1.172556
C	3.873980	3.903363	0.061784
H	3.691390	4.946649	-0.199158
H	4.115707	3.832363	1.129881
H	4.716282	3.522759	-0.528822
C	4.665293	-1.079551	1.272973
H	4.266660	-2.048397	1.608277

C	5.782059	-1.379760	0.248649
H	6.121530	-0.432225	-0.194803
C	6.979711	-2.069444	0.897709
H	7.314959	-1.483060	1.760030
H	6.668952	-3.067780	1.238444
O	5.285440	-0.400493	2.374598
H	4.588407	-0.093951	2.969725
O	5.189762	-2.207423	-0.745253
O	8.017055	-2.170880	-0.086239
H	8.777503	-2.615621	0.307187
C	5.616131	-1.963695	-2.082560
H	5.394847	-0.929451	-2.382913
H	6.686713	-2.158910	-2.203345
H	5.043266	-2.644964	-2.716303
O	-5.634352	-1.469696	-2.030469
O	-6.136372	-1.686585	0.778752
O	-4.467376	-0.277786	2.539960
C	-6.050741	-2.828087	-1.859683
H	-5.221284	-3.447564	-1.496212
H	-6.897423	-2.905265	-1.174594
H	-6.343122	-3.170623	-2.854348
C	-5.836923	-2.798553	1.640684
H	-5.276613	-2.476018	2.520960
H	-6.801989	-3.211928	1.939225
H	-5.266833	-3.560071	1.093874
C	-5.478977	0.629218	3.006141
H	-5.191644	1.666316	2.796159
H	-6.445812	0.412110	2.538258
H	-5.548464	0.480125	4.085407
H	-1.055863	4.073761	-1.218051
O	-2.237082	3.789602	0.496103
H	-2.514785	4.710648	0.426661

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

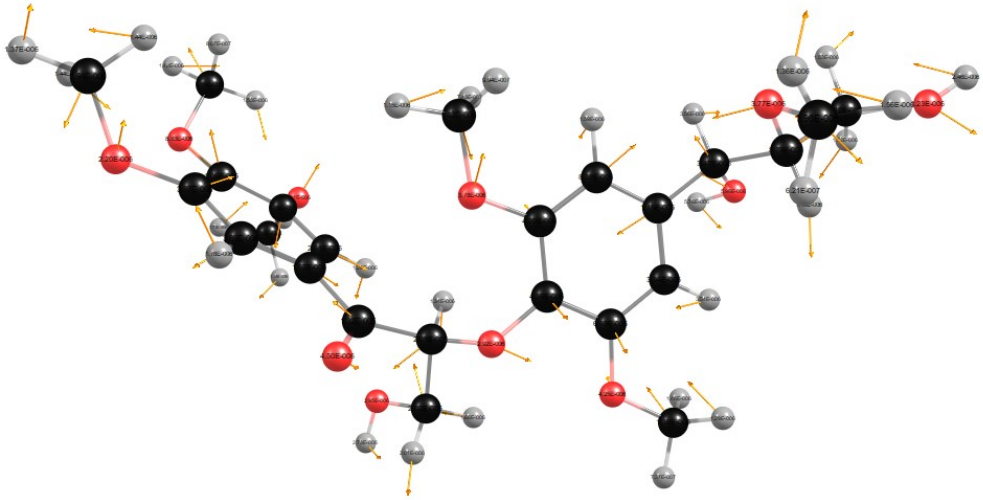


Table S4: Atomic coordinates and details of the optimized structure of the SG model calculated with B3LYP functional

MODEL	SG	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000006	**RMS FORCE**	0.000001
MAXIMUM DISPLACEMENT	0.001280	**RMS DISPLACEMENT**	0.000214
PREDICTED ENERGY CHANGE (Hartree)	$-2.93.10^{-9}$	**NUMBER OF STEPS**	16
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	4.612938	1.485880	0.212411
C	3.359812	1.119365	-0.300726
C	3.109350	-0.185934	-0.713319
C	4.125636	-1.149523	-0.622545
C	5.375498	-0.796216	-0.104352
C	5.638981	0.528938	0.317652
H	2.598196	1.889630	-0.369303
H	3.928530	-2.150596	-0.981049
C	1.736760	-0.553726	-1.244681
H	1.355507	0.288533	-1.838618
C	0.691350	-0.797766	-0.133107
H	0.529515	0.132848	0.417357
C	1.019017	-1.924703	0.858178
H	0.091952	-2.223234	1.354794
O	1.851207	-1.710024	-2.072554
H	0.951510	-1.950996	-2.337990
O	-0.513419	-1.162327	-0.863437
C	-1.729253	-0.821224	-0.313257
C	-2.613339	-1.828843	0.062805
C	-2.129396	0.530208	-0.206654
C	-3.884963	-1.521870	0.555836
C	-3.393578	0.831013	0.307788
C	-4.279560	-0.187587	0.688359
H	-4.562367	-2.319105	0.844998
H	-3.717227	1.861540	0.392451
O	-1.225042	1.462885	-0.631997
C	-1.589670	2.838777	-0.570539
H	-1.769967	3.157694	0.463309
H	-0.739330	3.388123	-0.976066
H	-2.479470	3.041486	-1.178274
C	-5.656220	0.168983	1.224875
H	-5.639495	1.213169	1.571735
C	-6.755698	0.069883	0.143958
H	-6.723393	-0.934272	-0.303799
C	-8.147352	0.299095	0.728918

H	-8.299416	-0.376346	1.577593
H	-8.215944	1.339561	1.078551
O	-6.052677	-0.694544	2.297627
H	-5.325333	-0.745077	2.932066
O	-6.434830	1.056585	-0.830265
O	-9.109305	0.048542	-0.303608
H	-9.994852	0.171899	0.058988
C	-6.714977	0.700397	-2.181120
H	-6.163073	-0.205558	-2.470510
H	-7.786304	0.540981	-2.339563
H	-6.371130	1.535554	-2.796315
O	6.407020	-1.678831	0.055672
O	6.824826	0.862305	0.928036
O	4.710368	2.779998	0.642250
C	6.194877	-3.043948	-0.292137
H	5.383670	-3.483258	0.300483
H	5.970378	-3.154679	-1.359650
H	7.130542	-3.554583	-0.061110
C	8.016804	0.786150	0.132792
H	7.935794	1.436105	-0.748151
H	8.825463	1.142028	0.774299
H	8.217847	-0.239845	-0.182697
C	5.924958	3.518042	0.473369
H	6.661153	3.259326	1.236307
H	6.348953	3.348785	-0.523676
H	5.639899	4.567965	0.568135
H	1.410470	-2.796980	0.317818
O	1.899035	-1.512279	1.898451
H	2.768985	-1.331931	1.514904
H	-2.290374	-2.859576	-0.045453

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

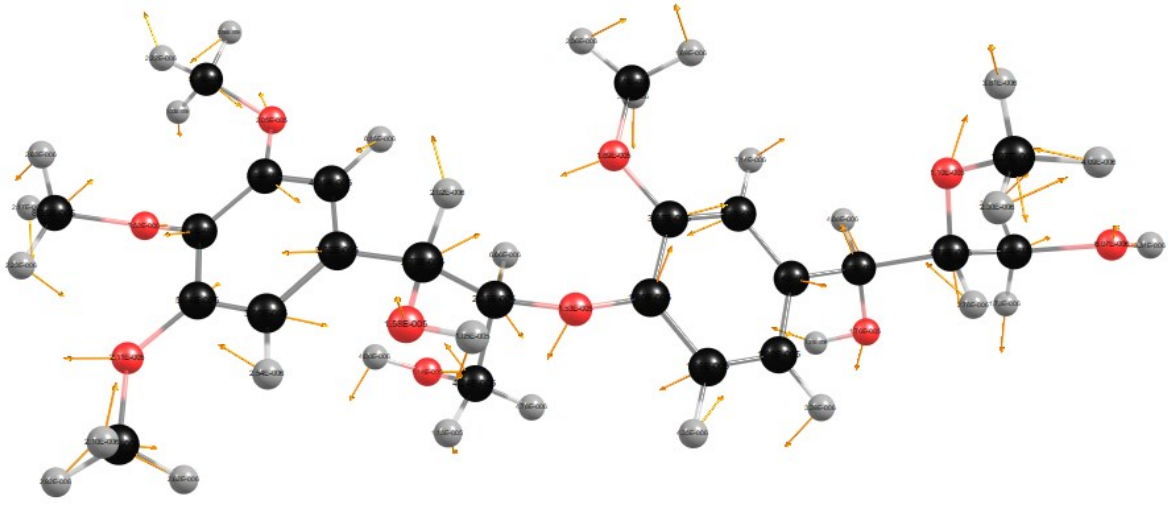


Table S5: Atomic coordinates and details of the optimized structure of the SGOX model calculated with B3LYP functional

MODEL	SGOX	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000014	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.000989	**RMS DISPLACEMENT**	0.000257
PREDICTED ENERGY CHANGE (Hartree)	$-8.19.10^{-9}$	**NUMBER OF STEPS**	30
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-3.163442	-1.493167	0.483654
C	-2.471322	-0.279524	0.482536
C	-3.079717	0.867043	-0.041532
C	-4.388003	0.798866	-0.556721
C	-5.074331	-0.411441	-0.569768
C	-4.454830	-1.580785	-0.062114
H	-1.464395	-0.261005	0.879770
H	-4.836101	1.711014	-0.928730
C	-2.418726	2.198928	-0.034833
C	-0.922334	2.330096	0.308863
H	-0.782611	2.046714	1.359442
C	-0.423689	3.768598	0.110584
H	0.653888	3.797727	0.292582
O	-3.058901	3.222089	-0.273509
O	-0.217373	1.414154	-0.556123
C	1.129142	1.207061	-0.341649
C	2.013371	1.499246	-1.378498
C	1.624444	0.622382	0.845243
C	3.379114	1.233144	-1.258251
C	2.996360	0.380942	0.969385
C	3.881188	0.674684	-0.078484
H	4.053040	1.468923	-2.075715
H	3.390091	-0.063333	1.876253
O	0.700054	0.323937	1.809074
C	1.145304	-0.284414	3.019375
H	1.837317	0.370866	3.561501
H	0.247768	-0.439299	3.618785
H	1.625686	-1.249990	2.823336
C	5.360196	0.366923	0.075577
H	5.579421	0.235581	1.146213
C	5.807823	-0.928429	-0.636108
H	5.599114	-0.845080	-1.711374
C	7.302906	-1.196117	-0.436175
H	7.892019	-0.414771	-0.917610

H	7.529851	-1.188034	0.641581
O	6.184568	1.404451	-0.469775
H	5.890698	2.252763	-0.111656
O	5.111703	-2.053185	-0.088415
O	7.686276	-2.432592	-1.022709
H	7.107922	-3.108228	-0.639882
C	4.071657	-2.590295	-0.902747
H	3.259277	-1.870511	-1.054366
H	4.460523	-2.906723	-1.880268
H	3.681821	-3.462511	-0.372628
O	-6.341897	-0.577907	-1.047796
O	-5.112607	-2.779028	-0.031105
O	-2.520727	-2.612077	0.957951
C	-7.031430	0.567296	-1.542793
H	-7.146757	1.328545	-0.762302
H	-6.512923	1.002635	-2.405487
H	-8.014368	0.208701	-1.849907
C	-5.332467	-3.415242	-1.302097
H	-4.374150	-3.620185	-1.792864
H	-5.838734	-4.355771	-1.079227
H	-5.964350	-2.797032	-1.945143
C	-3.064070	-3.189049	2.154515
H	-3.021386	-2.466848	2.980040
H	-4.094808	-3.520129	2.002196
H	-2.429384	-4.045943	2.388108
H	-0.606944	4.080100	-0.926245
O	-1.018192	4.661670	1.038775
H	-1.953215	4.723885	0.789810
H	1.605579	1.935366	-2.284952

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

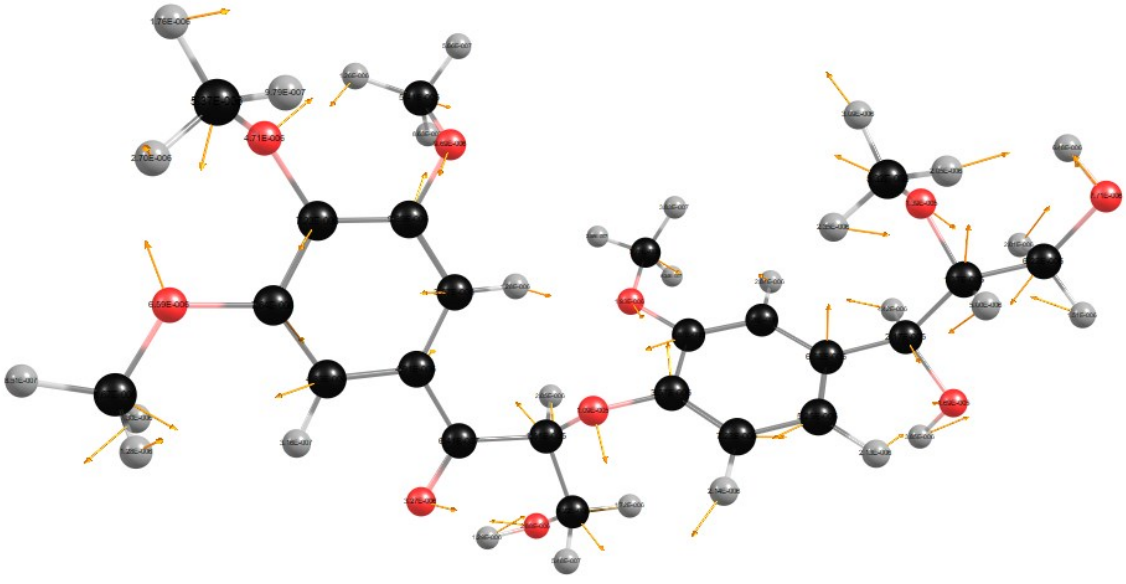


Table S6: Atomic coordinates and details of the optimized structure of the SH model calculated with B3LYP functional

MODEL	SH	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000009	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001005	**RMS DISPLACEMENT**	0.000298
PREDICTED ENERGY CHANGE (Hartree)	$-5.80.10^{-9}$	**NUMBER OF STEPS**	15
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	4.366980	1.684107	-0.066712
C	3.154832	1.180899	-0.563667
C	2.976081	-0.184453	-0.764766
C	4.022966	-1.072938	-0.475043
C	5.232250	-0.582203	0.027254
C	5.423130	0.804974	0.236146
H	2.370183	1.895552	-0.792061
H	3.883504	-2.127174	-0.671142
C	1.644713	-0.698109	-1.281107
H	1.252919	0.023968	-2.012294
C	0.573936	-0.818195	-0.169673
H	0.376632	0.182484	0.230974
C	0.944152	-1.765652	0.987016
H	0.026365	-2.120755	1.461324
O	1.843836	-1.959270	-1.913479
H	0.970060	-2.288417	-2.169321
O	-0.586390	-1.317405	-0.862724
C	-1.849501	-1.081366	-0.374854
C	-2.901734	-1.580448	-1.157105
C	-2.132182	-0.394724	0.811174
C	-4.219988	-1.384229	-0.760215
C	-3.465303	-0.209973	1.194965
C	-4.525132	-0.691938	0.424036
H	-5.025873	-1.778036	-1.373158
H	-3.675136	0.330148	2.114099
C	-5.964764	-0.477591	0.851435
H	-5.973493	-0.143373	1.899525
C	-6.676505	0.613978	0.022936
H	-6.590895	0.363911	-1.045104
C	-8.157314	0.722611	0.378427
H	-8.621826	-0.266606	0.304551
H	-8.245212	1.086992	1.412233
O	-6.745398	-1.675347	0.713697

H	-6.259006	-2.401233	1.126485
O	-5.986162	1.825739	0.304265
O	-8.767200	1.643320	-0.535747
H	-9.704396	1.721236	-0.320189
C	-5.856982	2.729651	-0.788591
H	-5.320516	2.259433	-1.625687
H	-6.833617	3.083221	-1.134702
H	-5.267590	3.573018	-0.420637
O	6.288620	-1.377558	0.371441
O	6.563920	1.287140	0.831082
O	4.391607	3.032763	0.147046
C	6.150063	-2.789572	0.240546
H	5.331142	-3.167577	0.864010
H	5.981002	-3.079858	-0.803156
H	7.094258	-3.210510	0.587996
C	7.795743	1.139169	0.109261
H	7.731121	1.631679	-0.869534
H	8.556645	1.633829	0.716066
H	8.053322	0.086262	-0.023091
C	5.584418	3.791860	-0.078721
H	6.284783	3.694648	0.752422
H	6.070910	3.485226	-1.012269
H	5.252387	4.827941	-0.170756
H	1.476585	-2.640158	0.591725
O	1.687925	-1.114396	2.010058
H	2.568672	-0.906056	1.667379
H	-1.342020	-0.011473	1.445718
H	-2.666145	-2.113361	-2.072962

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

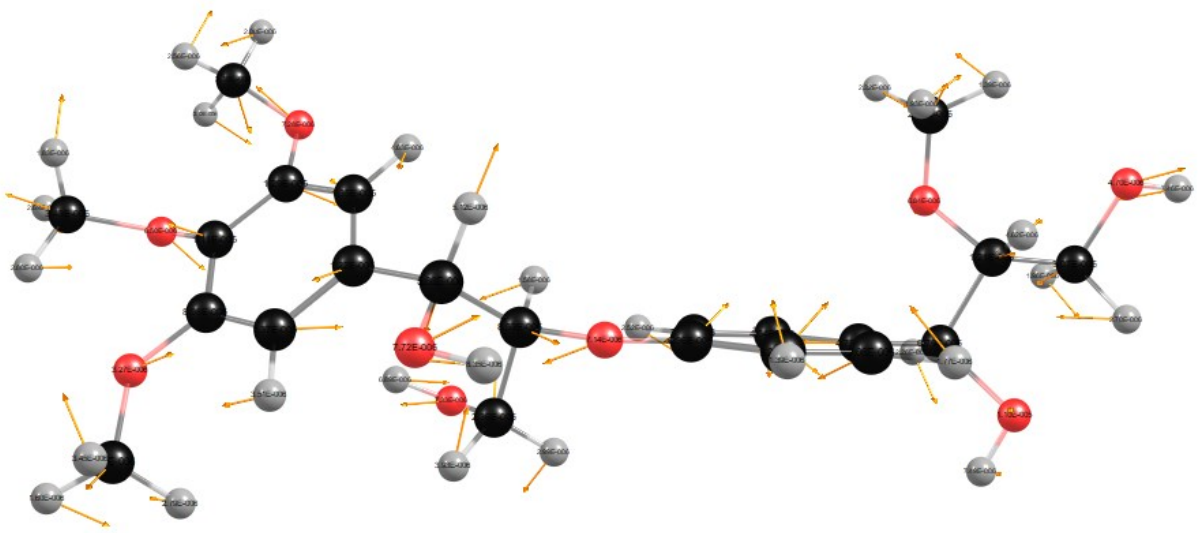


Table S7: Atomic coordinates and details of the optimized structure of the SHOX model calculated with B3LYP functional

MODEL	SHOX	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000033	**RMS FORCE**	0.000004
MAXIMUM DISPLACEMENT	0.001171	**RMS DISPLACEMENT**	0.000301
PREDICTED ENERGY CHANGE (Hartree)	$-1.13.10^{-8}$	**NUMBER OF STEPS**	15
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-2.544226	-1.407578	0.387134
C	-2.076647	-0.098064	0.409357
C	-2.956073	0.963073	0.138201
C	-4.295994	0.684992	-0.162854
C	-4.767399	-0.626786	-0.221465
C	-3.883779	-1.697174	0.047705
H	-1.033052	0.061626	0.650223
H	-4.984760	1.497852	-0.362033
C	-2.540203	2.390443	0.198845
C	-1.048408	2.757594	0.351661
H	-0.722718	2.392284	1.335901
C	-0.832253	4.277125	0.281641
H	0.240265	4.485852	0.300104
O	-3.368422	3.296121	0.167653
O	-0.336683	2.100144	-0.699082
C	0.984417	1.753608	-0.535157
C	1.558544	1.067599	-1.615784
C	1.754093	2.029686	0.599810
C	2.885481	0.657267	-1.553933
C	3.088663	1.609054	0.642658
C	3.674191	0.919004	-0.420319
H	3.320344	0.130177	-2.398450
H	3.677272	1.823193	1.530501
C	5.120395	0.465433	-0.356803
H	5.610573	0.972878	0.487352
C	5.258319	-1.053232	-0.113879
H	4.686284	-1.590995	-0.884580
C	6.713548	-1.509848	-0.182508
H	7.157329	-1.167237	-1.123451
C	7.262470	-1.063962	0.659590
O	5.823033	0.753407	-1.575527
H	5.654252	1.675310	-1.811226
O	4.700872	-1.293035	1.173220
O	6.734431	-2.940868	-0.098395
H	7.649810	-3.242094	-0.145800
C	3.990437	-2.518796	1.317371
H	3.149751	-2.570977	0.610265

H	4.646370	-3.382687	1.168592
H	3.596252	-2.526015	2.336631
O	-6.102091	-0.780358	-0.470569
O	-4.364204	-2.979643	0.072193
O	-1.673817	-2.436901	0.681912
C	-6.550881	-1.795305	-1.377003
H	-5.908340	-1.835065	-2.264927
H	-6.582258	-2.774928	-0.896305
H	-7.556449	-1.493605	-1.676040
C	-3.788293	-3.909670	-0.865655
H	-2.707676	-3.988802	-0.730836
H	-4.266230	-4.869099	-0.661596
H	-4.014206	-3.598233	-1.892561
C	-1.786574	-2.946987	2.020694
H	-1.557825	-2.161560	2.750899
H	-2.790229	-3.344033	2.207836
H	-1.049521	-3.747616	2.103557
H	-1.237732	4.651711	-0.666480
O	-1.402325	4.940632	1.397563
H	-2.363665	4.881109	1.288345
H	1.347011	2.575658	1.442840
H	0.946167	0.864635	-2.488401

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

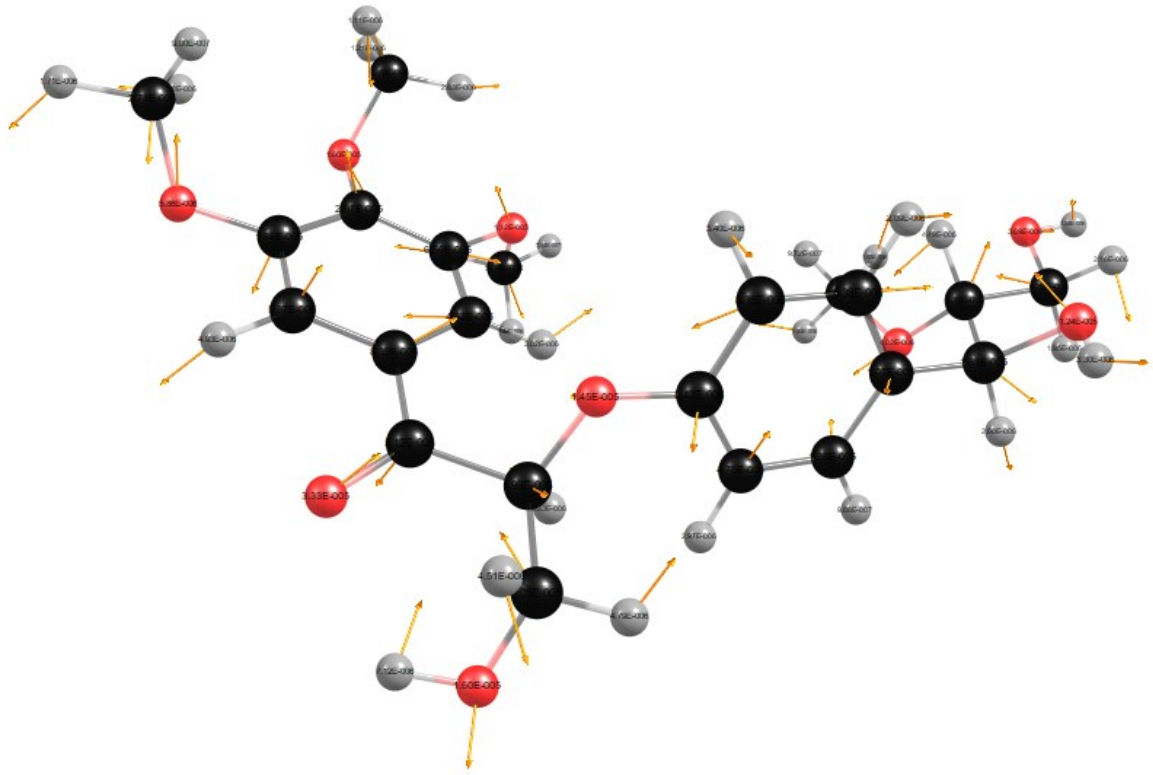


Table S8: Atomic coordinates and details of the optimized structure of the GS model calculated with B3LYP functional

MODEL	GS	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000012	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001697	**RMS DISPLACEMENT**	0.000359
PREDICTED ENERGY CHANGE (Hartree)	$-5.11.10^{-9}$	**NUMBER OF STEPS**	14
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-5.341838	-1.793079 -	0.035896
C	-4.080786	-1.487437	-0.556990
C	-3.691521	-0.163504	-0.773906
C	-4.609129	0.857144	-0.482573
C	-5.873177	0.569790	0.030680
C	-6.247322	-0.771564	0.272488
H	-3.397696	-2.299667	-0.791759
H	-4.350810	1.893549	-0.668749
C	-2.306196	0.149585	-1.304869
H	-2.037651	-0.613815	-2.050546
C	-1.204913	0.093142	-0.221981
H	-1.127015	-0.927508	0.165323
C	-1.387052	1.065729	0.954128
H	-0.417260	1.219822	1.433092
O	-2.321711	1.433853	-1.921038
H	-1.399880	1.655861	-2.122036
O	-0.004163	0.425758	-0.971215
C	1.217871	0.220659	-0.381676
C	2.026259	1.333181	-0.078715
C	1.721588	-1.075376	-0.167120
C	3.311125	1.150011	0.447514
C	2.999897	-1.253617	0.377773
C	3.793388	-0.143919	0.677942
H	3.938273	1.998368	0.691654
H	3.396902	-2.247262	0.543158
O	0.889014	-2.098916	-0.523179
O	1.465342	2.550726	-0.332727
C	1.350250	-3.436224	-0.360530
H	1.544376	-3.666584	0.694186
H	0.544070	-4.072557	-0.727728
H	2.256729	-3.619447	-0.949560
C	2.231312	3.719469	-0.062390
H	1.594179	4.559363	-0.341906
H	2.486595	3.794660	1.001825
H	3.149849	3.743100	-0.661445
C	5.189400	-0.341935	1.246247
H	5.266553	-1.367904	1.635428

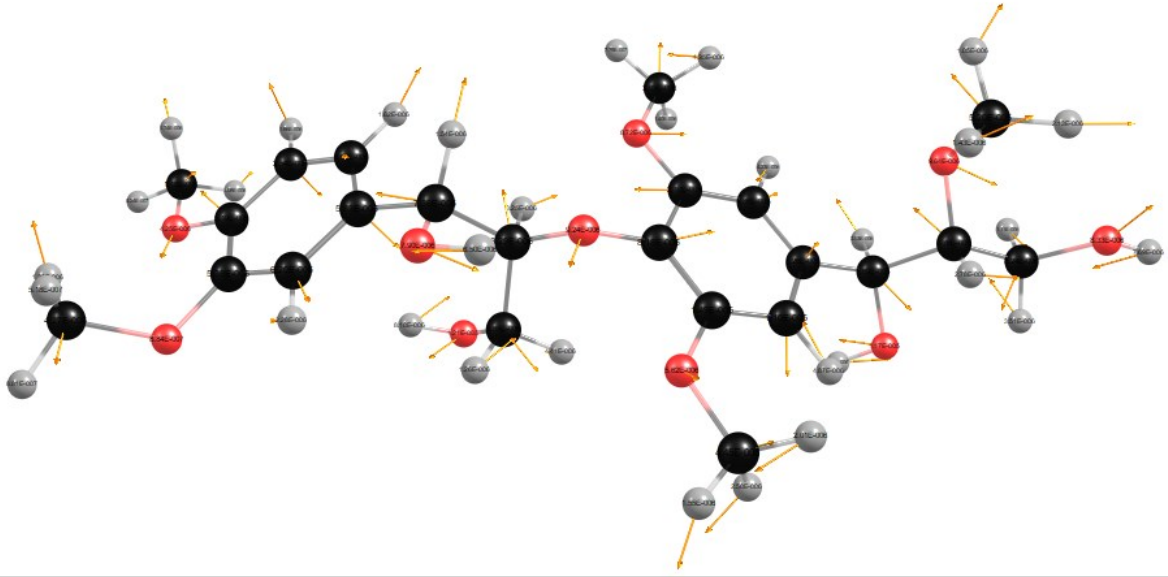
C	6.293773	-0.177921	0.178414
H	6.172042	0.799489	-0.311177
C	7.690851	-0.244218	0.790901
H	7.760781	0.472529	1.616179
H	7.857558	-1.259543	1.179060
O	5.480350	0.598755	2.289069
H	4.743649	0.593956	2.914684
O	6.091964	-1.229087	-0.758911
O	8.639283	0.066060	-0.238015
H	9.528157	0.026547	0.135123
C	6.342143	-0.894622	-2.120792
H	5.692464	-0.070022	-2.448099
H	7.389828	-0.619651	-2.280011
C	6.101952	-1.786320	-2.704956
O	-6.702766	1.615196	0.359481
O	-7.491988	-0.970227	0.801205
C	-7.880837	1.763125	-0.444119
H	-7.609652	1.920100	-1.495854
H	-8.535784	0.891628	-0.353056
H	-8.392670	2.649541	-0.064898
C	-7.889695	-2.299261	1.115861
H	-7.213051	-2.754187	1.849786
H	-8.887875	-2.215248	1.547372
H	-7.932890	-2.928647	0.217956
H	-1.742464	2.038179	0.592627
O	-2.239469	0.537190	1.967583
H	-3.150737	0.552634	1.644208
H	-5.607708	-2.830383	0.129737
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S9: Atomic coordinates and details of the optimized structure of the GSOX model calculated with B3LYP functional

MODEL	GSOX	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000006	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001697	**RMS DISPLACEMENT**	0.000320
PREDICTED ENERGY CHANGE (Hartree)	$-5.34.10^{-9}$	**NUMBER OF STEPS**	57
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-3.603709 -	1.802088	0.457832
C	-2.877365	-0.614271	0.557429
C	-3.461356	0.608363	0.197766
C	-4.789672	0.612160	-0.275397
C	-5.515202	-0.560939	-0.395677
C	-4.922175	-1.792308	-0.014550
H	-1.857347	-0.649338	0.918421
H	-5.260658	1.551568	-0.543288
C	-2.768660	1.913298	0.328510
C	-1.270924	1.986647	0.688839
H	-1.156311	1.658281	1.731263
C	-0.737052	3.421336	0.561523
H	0.342130	3.412823	0.735298
O	-3.385401	2.970273	0.192257
O	-0.568887	1.084066	-0.192298
C	0.771428	0.877564	0.038287
C	1.703212	1.327743	-0.918076
C	1.228453	0.147658	1.149780
C	3.067888	1.058361	-0.753274
C	2.595919	-0.099660	1.322941
C	3.511883	0.348163	0.368369
H	3.793231	1.405293	-1.478635
H	2.952858	-0.664457	2.174948
O	0.256294	-0.283551	2.013546
O	1.179176	2.024012	-1.964630
C	0.651855	-0.992439	3.184936
H	1.296158	-0.376326	3.823299
H	-0.272241	-1.221596	3.717070
H	1.169393	-1.924813	2.930184
C	2.060716	2.493163	-2.978435
H	1.427043	3.004865	-3.703656
H	2.796916	3.199565	-2.575237
H	2.581640	1.662999	-3.471051
C	4.993184	0.054118	0.542412
H	5.174780	-0.219772	1.592226
C	5.467718	-1.133076	-0.324911
H	5.197273	-0.937280	-1.372941

C	6.979642	-1.329145	-0.241012
H	7.482205	-0.383104	-0.469239
H	7.238718	-1.638200	0.782090
O	5.807379	1.178437	0.183120
H	5.462186	1.959564	0.635695
O	4.771917	-2.275644	0.159992
O	7.346465	-2.344106	-1.184170
H	8.301684	-2.474584	-1.146124
C	4.374594	-3.218996	-0.830648
H	3.707994	-2.753313	-1.570936
H	5.240383	-3.653309	-1.340805
H	3.824992	-4.003407	-0.304491
O	-6.827232	-0.503767	-0.800401
O	-5.705909	-2.895897	-0.135675
C	-7.103726	-1.030850	-2.104461
H	-6.538029	-0.482254	-2.868197
H	-6.867758	-2.098074	-2.160210
H	-8.172709	-0.882769	-2.267764
C	-5.182143	-4.157814	0.269532
H	-4.914246	-4.152185	1.332651
H	-5.984309	-4.876851	0.100959
H	-4.307422	-4.437052	-0.329980
H	-0.920058	3.791625	-0.454360
O	-1.300395	4.277434	1.544181
H	-2.238406	4.363206	1.312607
H	-3.134389	-2.733077	0.752534

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

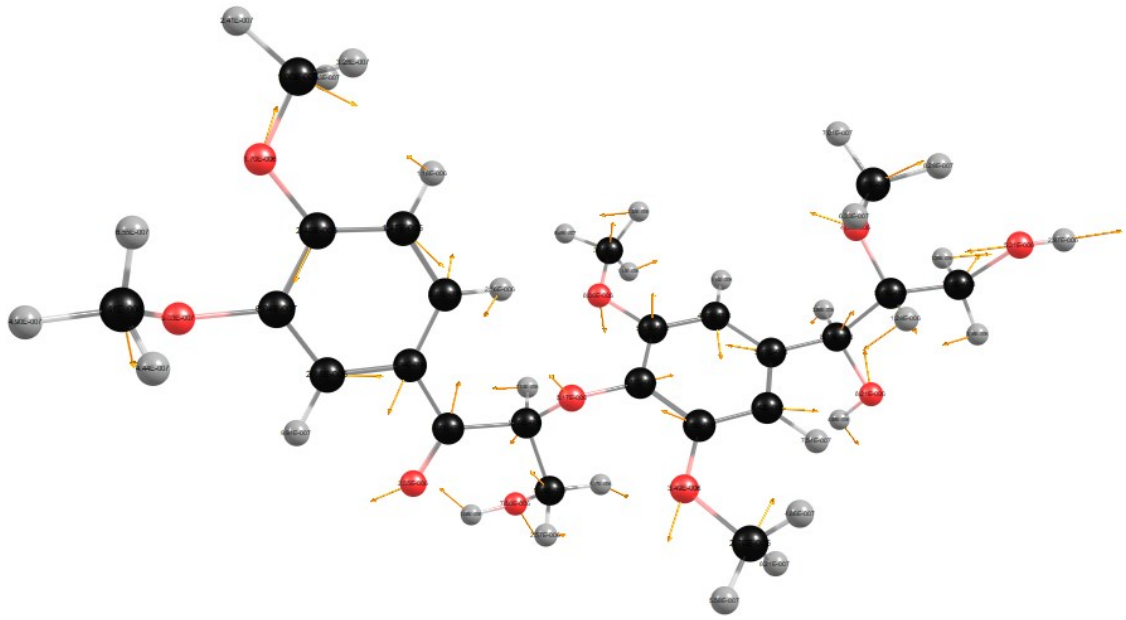


Table S10: Atomic coordinates and details of the optimized structure of the GG model calculated with B3LYP functional

MODEL	GG	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000013	**RMS FORCE**	0.000003
MAXIMUM DISPLACEMENT	0.001309	**RMS DISPLACEMENT**	0.000266
PREDICTED ENERGY CHANGE (Hartree)	$-2.72.10^{-8}$	**NUMBER OF STEPS STEPS**	9
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	4.949323	1.744747	0.101250
C	3.708392	1.335959	-0.396971
C	3.459523	-0.004559	-0.700591
C	4.496399	-0.932684	-0.520353
C	5.741990	-0.541225	-0.031185
C	5.975016	0.813467	0.299360
H	2.929800	2.079917	-0.544280
H	4.348155	-1.975910	-0.775796
C	2.095176	-0.434568	-1.203333
H	1.708748	0.343135	-1.878064
C	1.044979	-0.583283	-0.079456
H	0.85732	0.396230	0.369240
C	1.388038	-1.589867	1.029538
H	0.461548	-1.865184	1.540622
O	2.229525	-1.662111	-1.915314
H	1.335977	-1.942429	-2.161549
O	-0.147151	-1.046006	-0.777123
C	-1.374748	-0.712435	-0.253193
C	-2.212732	-1.721444	0.216519
C	-1.835494	0.624123	-0.263808
C	-3.497088	-1.430890	0.684687
C	-3.114230	0.910883	0.224308
C	-3.954651	-0.109811	0.694572
H	-4.136326	-2.228457	1.049810
H	-3.481182	1.930854	0.225224
O	-0.972773	1.556687	-0.767043
C	-1.402662	2.913194	-0.833826
H	-1.605444	3.317642	0.165377
H	-0.576902	3.462819	-1.286989
H	-2.296512	3.016864	-1.460454
C	-5.348591	0.232177	1.190959
H	-5.389154	1.312334	1.398828
C	-6.469536	-0.071503	0.173221
H	-6.461579	-1.142798	-0.069716
C	-7.849186	0.306473	0.721399
H	-8.095844	-0.318558	1.580350
H	-7.831196	1.357515	1.050213

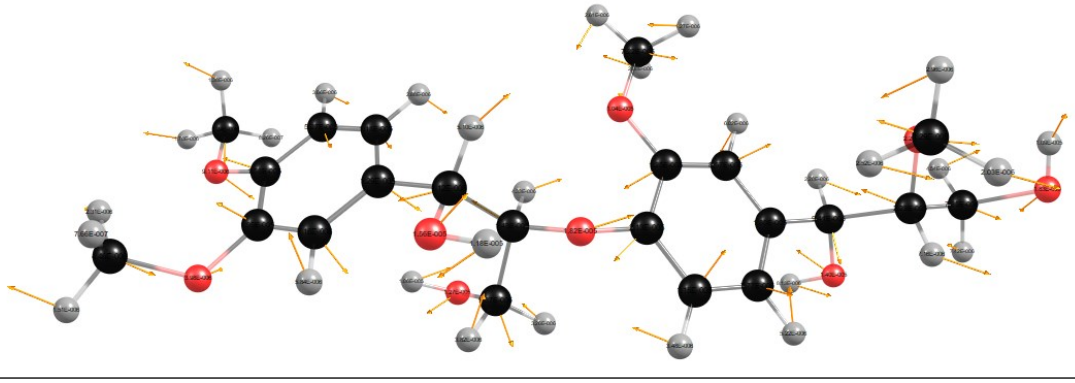
O	-5.695584	-0.506746	2.368763
H	-4.979510	-0.417284	3.011803
O	-6.274705	0.701032	-1.016510
O	-8.863111	0.100445	-0.252921
H	-8.596178	0.602787	-1.036430
C	-5.772989	-0.016577	-2.141453
H	-4.766972	-0.410882	-1.957977
H	-6.441859	-0.845619	-2.410299
H	-5.732984	0.694534	-2.970112
O	6.693922	-1.506994	0.188257
O	7.210545	1.113606	0.798781
C	7.851678	-1.459744	-0.656837
H	7.561125	-1.564930	-1.709777
H	8.410151	-0.530176	-0.513807
H	8.470251	-2.31006	-0.364069
C	7.472393	2.453053	1.201261
H	6.781668	2.773477	1.990890
H	8.491196	2.451104	1.590474
H	7.407650	3.146581	0.353389
H	1.818366	-2.500332	0.592986
O	2.233604	-1.036251	2.032538
H	3.125926	-0.944661	1.670890
H	-1.842048	-2.741602	0.200739
H	5.105545	2.790822	0.336634
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S11: Atomic coordinates and details of the optimized structure of the GGOX model calculated with B3LYP functional

MODEL	GGOX	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000009	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001116	**RMS DISPLACEMENT**	0.000197
PREDICTED ENERGY CHANGE (Hartree)	$-3.07.10^{-9}$	**NUMBER OF STEPS**	15
ATOM	Coordinates (Angstroms)		

	X	Y	Z
C	-4.312890	-0.208096	1.556845
C	-3.321477	0.596028	0.989405
C	-3.141628	0.640142	-0.398137
C	-3.980437	-0.149145	-1.209338
C	-4.959617	-0.963082	-0.661968
C	-5.141833	-0.990747	0.744331
H	-2.719911	1.211300	1.647330
H	-3.866541	-0.112399	-2.287401
C	-2.125969	1.495498	-1.075598
C	-1.060137	2.256116	-0.251873
H	-0.935412	1.826532	0.743964
C	-1.429836	3.738472	-0.129830
H	-0.600613	4.264939	0.361118
O	-2.123708	1.637894	-2.289274
O	0.190534	2.226179	-0.957253
C	1.257611	1.586856	-0.374606
C	2.450959	2.290394	-0.228472
C	1.210073	0.222142	-0.011137
C	3.594332	1.668201	0.280650
C	2.349538	-0.387856	0.520576
C	3.548965	0.324770	0.665569
H	4.516897	2.230880	0.383766
H	2.327845	-1.435914	0.795205
O	0.017449	-0.409577	-0.220082
C	-0.086230	-1.796351	0.082573
H	0.084493	-1.985867	1.149776
H	-1.106983	-2.077399	-0.177734
H	0.622235	-2.384759	-0.512520
C	4.780932	-0.370765	1.219900
H	4.462146	-1.274923	1.760173
C	5.752238	-0.828761	0.109310
H	5.997991	0.034941	-0.525614
C	7.047906	-1.395088	0.685120
H	7.485013	-0.668767	1.378775
H	6.816154	-2.321435	1.230785
O	5.527979	0.482112	2.098114
H	4.909658	0.898636	2.712994
O	5.050193	-1.812462	-0.642352
O	7.938171	-1.660709	-0.406218
H	8.765907	-2.010619	-0.055156
C	5.283220	-1.792768	-2.048001
H	4.995843	-0.823453	-2.479866
H	6.332036	-2.001472	-2.282592
H	4.647751	-2.572167	-2.475534
O	-5.798671	-1.659773	-1.498267
O	-6.142447	-1.789718	1.204804

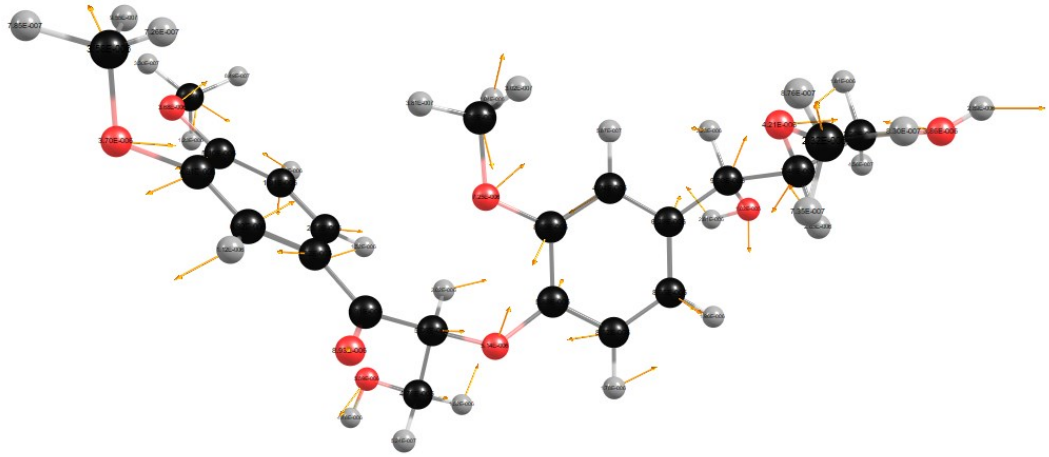
C	-5.643989	-3.084033	-1.503286
H	-4.630844	-3.359018	-1.823969
H	-5.853003	-3.511149	-0.517603
H	-6.367636	-3.462389	-2.227515
C	-6.417066	-1.806026	2.602646
H	-6.690826	-0.807806	2.964155
H	-7.262817	-2.482660	2.728708
H	-5.559419	-2.182102	3.173728
H	-1.563247	4.144879	-1.139932
O	-2.627475	3.830455	0.643109
H	-3.016711	4.705355	0.527583
H	2.468650	3.331874	-0.533810
H	-4.442846	-0.205640	2.632449
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S12: Atomic coordinates and details of the optimized structure of the GH model calculated with B3LYP functional

MODEL	GH	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000013	**RMS FORCE**	0.000006
MAXIMUM DISPLACEMENT	0.001268	**RMS DISPLACEMENT**	0.000344
PREDICTED ENERGY CHANGE (Hartree)	$-8.81.10^{-9}$	**NUMBER OF STEPS**	12
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	4.689131	1.939781	-0.350391
C	3.495705	1.352405	-0.781785
C	3.338871	-0.035451	-0.793434
C	4.419850	-0.832985	-0.388001
C	5.619182	-0.264280	0.038453
C	5.758448	1.142624	0.073382
H	2.683252	1.995406	-1.110662
H	4.345110	-1.914254	-0.416484
C	2.022250	-0.652051	-1.223744

H	1.605282	-0.048685	-2.044218
C	0.959156	-0.649080	-0.098720
H	0.730360	0.391248	0.159487
C	1.361724	-1.410366	1.178787
H	0.456030	-1.733780	1.697229
O	2.257481	-1.980736	-1.678401
H	1.393922	-2.369967	-1.878367
O	-0.187574	-1.275466	-0.706335
C	-1.455287	-1.015421	-0.244847
C	-2.493771	-1.653278	-0.940064
C	-1.756051	-0.179313	0.836223
C	-3.815967	-1.447710	-0.561821
C	-3.092943	0.012875	1.203007
C	-4.139266	-0.607272	0.517181
H	-4.610511	-1.950790	-1.105756
H	-3.316836	0.668071	2.040432
C	-5.582998	-0.386728	0.926761
H	-5.597119	0.099394	1.913584
C	-6.345316	0.540121	-0.044916
H	-6.258462	0.136767	-1.064901
C	-7.826277	0.641919	0.312244
H	-8.249780	-0.364974	0.392936
H	-7.920218	1.152277	1.281794
O	-6.315758	-1.621037	0.979430
H	-5.794840	-2.259500	1.484339
O	-5.702233	1.806271	0.042383
O	-8.482318	1.391290	-0.719038
H	-9.421446	1.455738	-0.507409
C	-5.627895	2.545071	-1.172771
H	-5.088126	1.977637	-1.945018
H	-6.623429	2.808504	-1.544343
H	-5.065828	3.454051	-0.944739
O	6.615589	-1.095583	0.487770
O	6.952085	1.623712	0.529284
C	7.805249	-1.151607	-0.311929
H	7.567673	-1.494633	-1.326770
H	8.302608	-0.178368	-0.352454
H	8.457568	-1.879162	0.174161
C	7.120703	3.033263	0.633863
H	6.381405	3.472735	1.314572
H	8.121299	3.181674	1.041385
H	7.050908	3.518984	-0.347450
H	1.933174	-2.307994	0.912410
O	2.070995	-0.588307	2.099361
H	2.971348	-0.458573	1.770607
H	-0.97189	0.313382	1.404437
H	-2.244285	-2.301347	-1.774345

H	4.774001	3.019905	-0.344946
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			

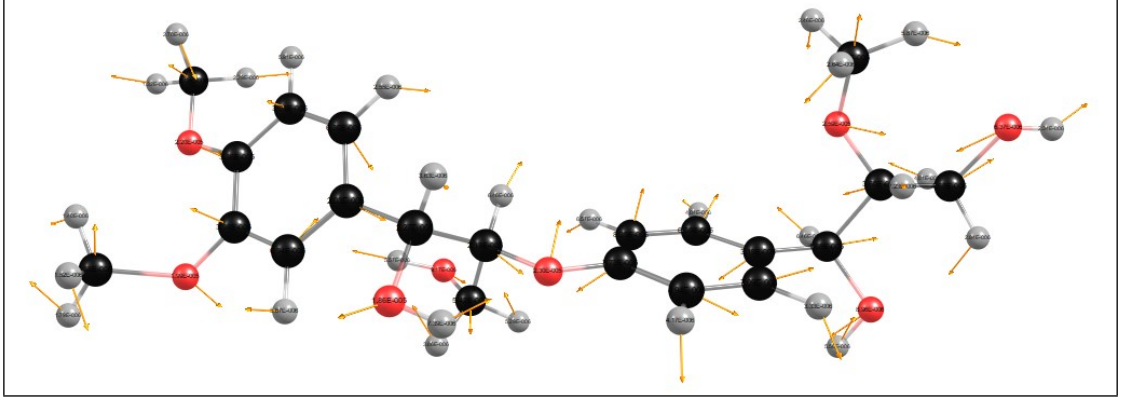


Table S13: Atomic coordinates and details of the optimized structure of the GHOX model calculated with B3LYP functional

MODEL	GHOX	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000006	**RMS FORCE**	0.000001
MAXIMUM DISPLACEMENT	0.001186	**RMS DISPLACEMENT**	0.000230
PREDICTED ENERGY CHANGE (Hartree)	$-2.09.10^{-9}$	**NUMBER OF STEPS**	29
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-4.277497	-0.260934	1.299323
C	-3.398520	0.710243	0.815676
C	-2.751207	0.539567	-0.415455
C	-3.003563	-0.635059	-1.152881
C	-3.861738	-1.614040	-0.680273
C	-4.520447	-1.426962	0.562978
H	-3.263599	1.616787	1.393167
H	-2.521208	-0.775658	-2.114064
C	-1.813215	1.535532	-0.999069
C	-1.296586	2.726419	-0.143672
H	-1.404367	2.531097	0.928940
C	-2.050915	4.013263	-0.496505
H	-1.558567	4.850785	0.013931
O	-1.420251	1.448068	-2.153295
O	0.060901	3.017791	-0.448559
C	1.056289	2.179705	-0.017949
C	2.359424	2.567111	-0.364319
C	0.855053	1.015603	0.730545
C	3.444496	1.795876	0.035596
C	1.960405	0.255461	1.130020
C	3.263676	0.624559	0.792208
H	4.449030	2.107301	-0.237013

H	1.793790	-0.652697	1.702980
C	4.450587	-0.216823	1.220640
H	4.116403	-0.929433	1.989449
C	5.041716	-1.048533	0.061695
H	5.276685	-0.376002	-0.776403
C	6.319846	-1.774293	0.474003
H	7.025090	-1.053774	0.902189
H	6.067499	-2.528151	1.233918
O	5.519381	0.592410	1.737852
H	5.141316	1.225144	2.362788
O	4.025486	-1.971042	-0.313626
O	6.871189	-2.398176	-0.693082
H	7.680406	-2.861458	-0.445444
C	3.913455	-2.227240	-1.710380
H	3.698706	-1.301814	-2.263715
H	4.824089	-2.688181	-2.107110
H	3.070816	-2.912551	-1.829937
O	-4.126865	-2.710415	-1.462866
O	-5.366788	-2.417983	0.946612
C	-3.599397	-3.959989	-0.996955
H	-2.505713	-3.910848	-0.923601
H	-4.027309	-4.235650	-0.028296
H	-3.880172	-4.701683	-1.746650
C	-6.099635	-2.264657	2.159690
H	-6.743559	-1.378168	2.123334
H	-6.717181	-3.159144	2.244863
H	-5.428730	-2.198841	3.024616
H	-1.989764	4.168711	-1.580580
O	-3.399124	3.857246	-0.056665
H	-3.943848	4.552034	-0.445020
H	-0.139809	0.683235	1.002483
H	2.495673	3.470815	-0.949405
H	-4.780471	-0.093902	2.244122

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

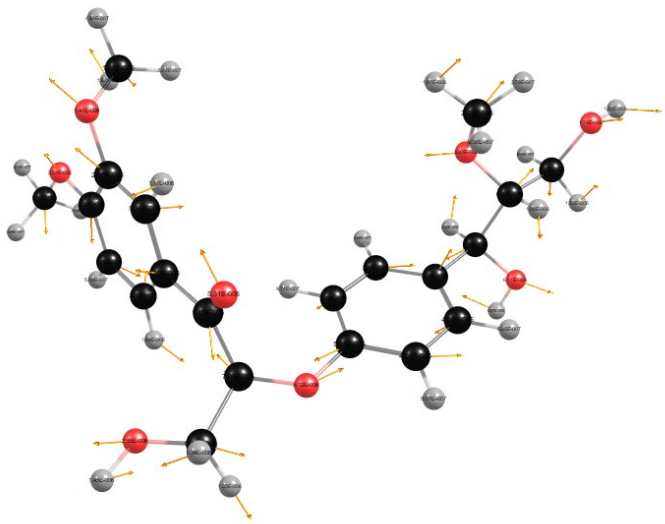


Table S14: Atomic coordinates and details of the optimized structure of the HS model calculated with B3LYP functional

MODEL	HS	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000011	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001613	**RMS DISPLACEMENT**	0.000374
PREDICTED ENERGY CHANGE (Hartree)	$-4.83.10^{-9}$	**NUMBER OF STEPS**	14
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	5.906581	-1.404796	-0.013070
C	4.632088	-1.159594	0.507751
C	4.191375	0.137166	0.789033
C	5.076294	1.202858	0.554390
C	6.349815	0.975687	0.038120
C	6.772272	-0.329471	-0.253159
H	3.973833	-2.004341	0.696917
H	4.763219	2.211781	0.799825
C	2.791641	0.368245	1.324430
H	2.553938	-0.430883	2.042740
C	1.697106	0.301153	0.235199
H	1.664049	-0.708473	-0.186159
C	1.843133	1.319686	-0.906372
H	0.870860	1.448237	-1.387589
O	2.748202	1.630403	1.983945
H	1.817638	1.801806	2.193689
O	0.480135	0.558078	0.987125
C	-0.728438	0.303523	0.388858
C	-1.590735	1.379355	0.102691
C	-1.165.46	-1.012122	0.149502
C	-2.863396	1.141371	-0.431354
C	-2.432122	-1.244471	-0.403135
C	-3.279526	-0.170738	-0.686363
H	-3.531765	1.961442	-0.662434
H	-2.778309	-2.253666	-0.587478
O	-0.283972	-1.998789	0.490378
O	-1.092791	2.618923	0.380508
C	-0.679339	-3.354578	0.307859
H	-0.860156	-3.579328	-0.750428
H	0.156132	-3.956090	0.668201
H	-1.576900	-3.589768	0.892023
C	-1.917157	3.751941	0.130667
H	-1.324356	4.617769	0.428053
H	-2.174249	3.834578	-0.932574
H	-2.836689	3.716959	0.727606
C	-4.662324	-0.428418	-1.263055

H	-4.686026	-1.449062	-1.672633
C	-5.776174	-0.342404	-0.195946
H	-5.706793	0.630549	0.312476
C	-7.166259	-0.469652	-0.814872
H	-7.270792	0.257842	-1.626988
H	-7.278767	-1.484807	-1.222498
O	-4.998642	0.516647	-2.288083
H	-4.262249	0.560118	-2.912554
O	-5.521090	-1.399203	0.721711
O	-8.132779	-0.228311	0.215658
H	-9.017211	-0.305273	-0.162178
C	-5.799754	-1.108186	2.088126
H	-5.204411	-0.251754	2.436365
H	-6.863281	-0.901401	2.245187
H	-5.508296	-1.994928	2.656270
O	8.038506	-0.449772	-0.755226
C	8.525380	-1.748611	-1.068241
H	7.911233	-2.231445	-1.838906
H	9.536335	-1.602857	-1.450705
H	8.562783	-2.387841	-0.177034
H	2.153536	2.293617	-0.508724
O	2.724334	0.864630	-1.931277
H	3.628631	0.876721	-1.588600
H	6.208708	-2.424958	-0.217655
H	7.037037	1.796954	-0.138499

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

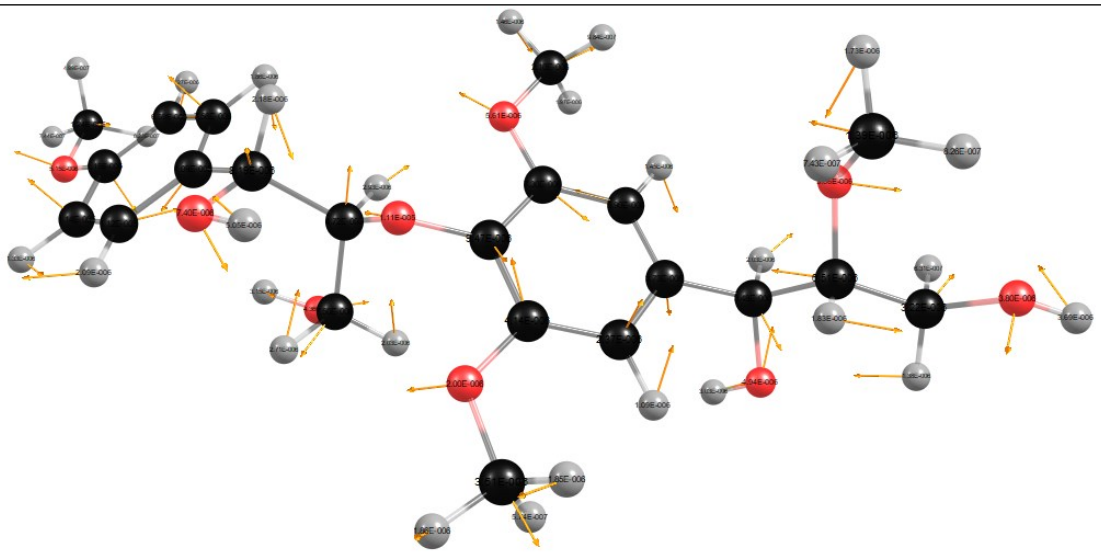


Table S15: Atomic coordinates and details of the optimized structure of the HSOX model calculated with B3LYP functional

MODEL	HSOX	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000032	**RMS FORCE**	0.000003
MAXIMUM DISPLACEMENT	0.001776	**RMS DISPLACEMENT**	0.000413
PREDICTED ENERGY CHANGE (Hartree)	$-1.66.10^{-8}$	**NUMBER OF STEPS**	34
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	2.776004	-2.05531	-1.07188
C	2.646305	-0.69155	-0.79856
C	3.507256	-0.04205	0.096515
C	4.517861	-0.80378	0.721596
C	4.652752	-2.15724	0.469495
C	3.781376	-2.79439	-0.43431
H	1.860438	-0.14253	-1.3044
H	5.18962	-0.30195	1.409844
C	3.439359	1.412832	0.38777
C	2.210975	2.239974	-0.04987
H	1.940454	2.015539	-1.08414
C	2.466878	3.742344	0.089717
H	1.584402	4.274276	-0.27028
O	4.351912	1.976041	0.990407
O	1.124626	1.91624	0.848797
C	0.062461	1.164081	0.420893
C	-0.75702	1.55319	-0.65693
C	-0.28683	0.023822	1.171904
C	-1.88059	0.792987	-1.00411
C	-1.41693	-0.7287	0.823894
C	-2.21107	-0.34582	-0.25963
H	-2.51087	1.083196	-1.83555
H	-1.69719	-1.60014	1.402192
O	0.535495	-0.2644	2.21622
O	-0.37457	2.695889	-1.30453
C	0.230971	-1.38936	3.031849
H	0.263156	-2.32267	2.45574
H	1.005108	-1.4119	3.799622
H	-0.75219	-1.2851	3.506828
C	-1.18053	3.178315	-2.37518
H	-0.69743	4.094316	-2.71691
H	-1.22214	2.458037	-3.20132
H	-2.19785	3.405429	-2.0351
C	-3.44922	-1.15215	-0.61626
H	-3.36364	-2.1477	-0.15612
C	-4.74877	-0.51461	-0.07532
H	-4.80424	0.527691	-0.42236

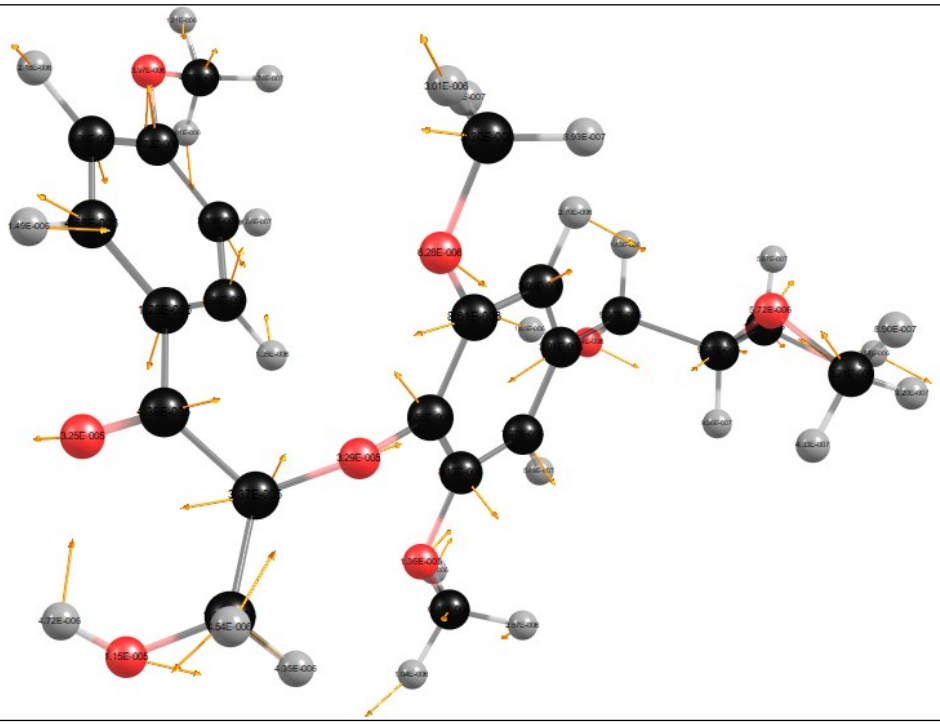
C	-5.99207	-1.25572	-0.56206
H	-5.96158	-1.34148	-1.65365
H	-5.99706	-2.26289	-0.12051
O	-3.61269	-1.28325	-2.03576
H	-2.76811	-1.56474	-2.41147
O	-4.64515	-0.55967	1.34245
O	-7.14182	-0.512	-0.13948
H	-7.93703	-0.97333	-0.43227
C	-5.17632	0.566711	2.034703
H	-4.67102	1.492436	1.723786
H	-6.25422	0.665651	1.870757
H	-4.97843	0.395976	3.095617
O	3.996832	-4.12459	-0.62178
C	3.164738	-4.83568	-1.53368
H	3.251996	-4.43136	-2.54932
H	3.524251	-5.86491	-1.52049
H	2.115118	-4.81155	-1.2165
H	2.615441	3.982652	1.148962
O	3.569021	4.16339	-0.70335
H	4.365969	3.829329	-0.26559
H	2.098065	-2.5219	-1.77613
H	5.424005	-2.74896	0.951756
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S16: Atomic coordinates and details of the optimized structure of the HG model calculated with B3LYP functional

MODEL	HG	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000012	**RMS FORCE**	0.000003
MAXIMUM DISPLACEMENT	0.001421	**RMS DISPLACEMENT**	0.000330
PREDICTED ENERGY CHANGE (Hartree)	$-5.83.10^{-9}$	**NUMBER OF STEPS**	14
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-5.56983	1.359504	-0.35575
C	-4.31062	1.101592	0.195046
C	-4.01165	-0.12233	0.801294
C	-5.02393	-1.09463	0.865334
C	-6.28396	-0.85295	0.323328
C	-6.56452	0.374403	-0.29468
H	-3.5506	1.877901	0.147034
H	-4.82047	-2.03664	1.36273
C	-2.62571	-0.37788	1.360849
H	-2.26503	0.542003	1.84382
C	-1.57938	-0.72846	0.27877
H	-1.43524	0.13586	-0.37574
H	-1.89356	-1.96475	-0.57759
H	-0.96311	-2.30981	-1.03615
O	-2.70243	-1.4251	2.325229
C	-1.79537	-1.60837	2.610701
O	-0.36509	-0.98351	1.03874
C	0.843817	-0.72621	0.431351
C	1.718745	-1.77998	0.180998
C	1.248726	0.596507	0.141435
C	2.985044	-1.54893	-0.36426
C	2.507601	0.818971	-0.42339
C	3.384034	-0.2464	-0.67687
H	3.655201	-2.3816	-0.55294
H	2.835342	1.827109	-0.64727
O	0.353998	1.58374	0.4498
C	0.737121	2.937553	0.228302
H	0.912856	3.134185	-0.83653
H	-0.10137	3.542662	0.575236
H	1.635277	3.19541	0.801876
C	4.755307	0.027894	-1.27245
H	4.737323	1.015296	-1.75795
C	5.867177	0.07234	-0.20057
H	5.836723	-0.8608	0.380959
C	7.252581	0.212112	-0.8272
H	7.392789	-0.57531	-1.57546
H	7.320108	1.193587	-1.31886

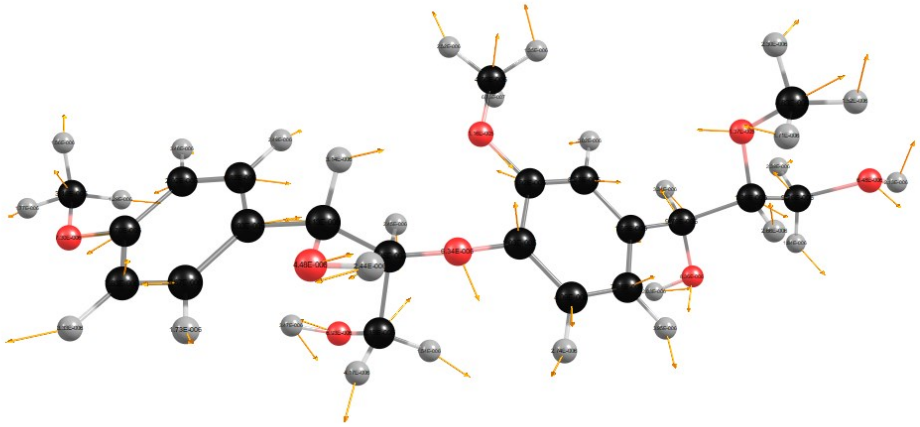
O	5.136855	-0.97511	-2.222
H	4.401464	-1.10987	-2.83448
O	5.561285	1.184859	0.63275
O	8.225561	0.103169	0.219404
H	9.107369	0.166899	-0.16693
C	5.856888	1.015771	2.016399
H	5.306836	0.159778	2.433242
H	6.929718	0.87582	2.182628
H	5.521956	1.9284	2.515505
O	-7.82879	0.516362	-0.79466
C	-8.17528	1.739724	-1.43182
H	-7.54431	1.926286	-2.30999
H	-9.21235	1.625803	-1.74957
H	-8.09844	2.587446	-0.73926
H	-2.28035	-2.77329	0.056273
O	-2.7745	-1.67829	-1.65997
H	-3.65714	-1.50643	-1.3038
H	1.393196	-2.78521	0.429886
H	-5.76008	2.321037	-0.81735
H	-7.06904	-1.6004	0.376774
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S17: Atomic coordinates and details of the optimized structure of the HGOX model calculated with B3LYP functional

MODEL	HGOX	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000007	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.000756	**RMS DISPLACEMENT**	0.000167
PREDICTED ENERGY CHANGE (Hartree)	$-2.49.10^{-9}$	**NUMBER OF STEPS**	41
ATOM	Coordinates (Angstroms)		
	X	Y	Z

C	-3.818013	-1.952361	0.206710
C	-3.21133	-0.69544	0.204579
C	-3.8814	0.429768	-0.30014
C	-5.18684	0.263048	-0.81147
C	-5.79387	-0.97981	-0.82613
C	-5.11141	-2.09998	-0.31492
H	-2.20895	-0.59853	0.603419
H	-5.70766	1.133642	-1.19569
C	-3.30444	1.793641	-0.28561
C	-1.8311	2.024158	0.106794
H	-1.719	1.78429	1.171868
C	-1.4112	3.483749	-0.1202
H	-0.34411	3.582976	0.095605
O	-3.99755	2.777224	-0.5495
O	-1.03118	1.125581	-0.69321
C	0.314891	1.019334	-0.40831
C	1.230035	1.350742	-1.40492
C	0.78712	0.498065	0.816633
C	2.603298	1.191873	-1.20358
C	2.163145	0.366623	1.022661
C	3.07993	0.706096	0.017728
H	3.301312	1.456409	-1.99154
H	2.53886	-0.03263	1.957163
O	-0.16632	0.140343	1.734209
C	0.259179	-0.35507	3.001366
H	0.854534	0.391995	3.539638
H	-0.65461	-0.56109	3.559915
H	0.839226	-1.27904	2.892353
C	4.569686	0.528317	0.260215
H	4.747165	0.482511	1.345322
C	5.113154	-0.78662	-0.34213
H	4.852379	-0.82168	-1.41009
C	6.630662	-0.88701	-0.20635
H	7.092045	0.013193	-0.62625
H	6.885548	-0.95909	0.861089
O	5.336581	1.593147	-0.31487
H	4.942001	2.433263	-0.04546
O	4.460064	-1.83776	0.361348
O	7.061972	-2.05917	-0.90906
H	8.023281	-2.11996	-0.85341
C	4.134746	-2.98674	-0.41593
H	3.46855	-2.72067	-1.2493
H	5.033679	-3.47277	-0.80818
H	3.607993	-3.67119	0.253714
O	-5.78901	-3.27717	-0.37107
C	-5.16155	-4.45902	0.119372
H	-4.93302	-4.37308	1.188445

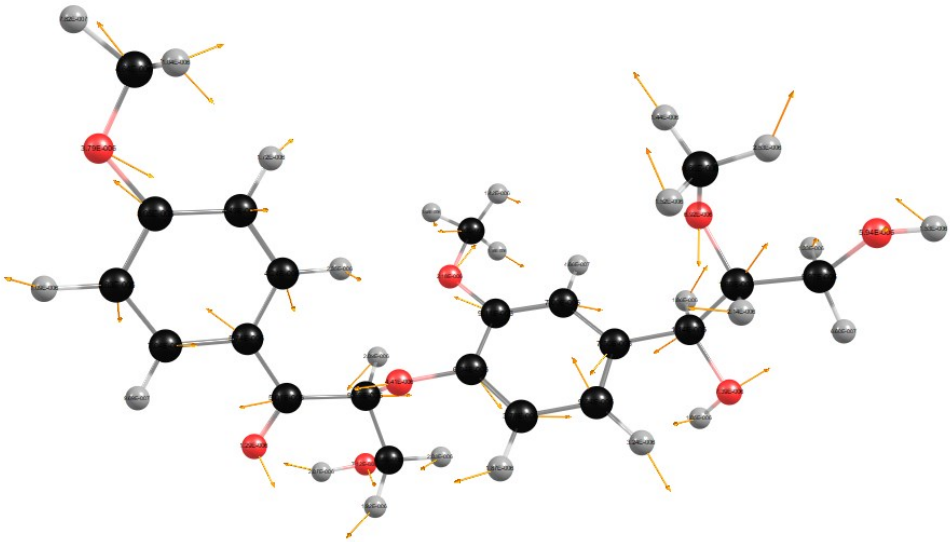
H	-5.88349	-5.26146	-0.03423
H	-4.24352	-4.68145	-0.43742
H	-1.57708	3.752513	-1.17195
O	-2.08904	4.367057	0.758795
H	-3.0192	4.351996	0.483829
H	-3.27644	-2.80068	0.607357
H	-6.7938	-1.11746	-1.22424
H	0.842161	1.733808	-2.34351
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S18: Atomic coordinates and details of the optimized structure of the HH model calculated with B3LYP functional

MODEL	HH	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000006	**RMS FORCE**	0.000001
MAXIMUM DISPLACEMENT	0.001073	**RMS DISPLACEMENT**	0.000139
PREDICTED ENERGY CHANGE (Hartree)	$-1.78.10^{-9}$	**NUMBER OF STEPS**	15
Atom	Coordinates (Angstroms)		
	X	Y	Z
C	5.295660	-1.638756	0.379258
C	4.104216	1.020766	-0.770897
C	3.956870	-0.368645	-0.745555
C	5.050188	-1.144372	-0.331412
C	6.244766	-0.545714	0.058234
C	6.373851	0.850157	0.042388
H	3.279874	1.647161	-1.104501
H	4.964974	-2.225360	-0.336537

C	2.641675	-0.999281	-1.158035
H	2.283172	-0.506512	-2.074293
C	1.529560	-0.813289	-0.101353
H	1.345943	0.258805	0.034554
C	1.853427	-1.428540	1.272558
H	1.046880	-2.115325	1.559063
O	2.844684	-2.387023	-1.412173
H	1.982879	-2.763099	-1.641004
O	0.376263	-1.429467	-0.703992
C	-0.885373	-1.120405	-0.256668
C	-1.941744	-1.687737	-0.985313
C	-1.158677	-0.302747	0.845750
C	-3.258088	-1.428071	-0.620115
C	-2.491089	-0.055721	1.197108
C	-3.555925	-0.602810	0.478036
H	-4.067903	-1.874452	-1.190469
H	-2.696539	0.585560	2.050049
C	-4.993175	-0.320472	0.871817
H	-4.998930	0.140607	1.870675
C	-5.693084	0.667871	-0.086077
H	-5.606820	0.289041	-1.115401
C	-7.173753	0.831410	0.248286
H	-7.647006	-0.155426	0.292109
H	-7.261142	1.318075	1.230555
O	-5.787615	-1.517719	0.882274
H	-5.300532	-2.197335	1.366738
O	-4.993198	1.899378	0.047868
O	-7.773232	1.641015	-0.771930
H	-8.711412	1.747400	-0.573515
C	-4.853668	2.661999	-1.146549
H	-4.320912	2.088248	-1.918953
H	-5.826224	2.980425	-1.535738
H	-4.256292	3.538153	-0.882643
O	7.584801	1.343410	0.444960
C	7.780341	2.751697	0.439988
H	7.078431	3.256139	1.116142
H	8.799989	2.911746	0.792673
H	7.676080	3.167094	-0.570393
H	2.787283	-1.998544	1.222042
O	1.962313	-0.353168	2.211905
H	2.389676	-0.674212	3.015500
H	-0.361738	0.127057	1.441460
H	-1.710882	-2.321444	-1.835900
H	5.368542	2.719154	-0.413212
H	7.094606	-1.143468	0.372090
H	7.094606	-1.143468	0.372090
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			

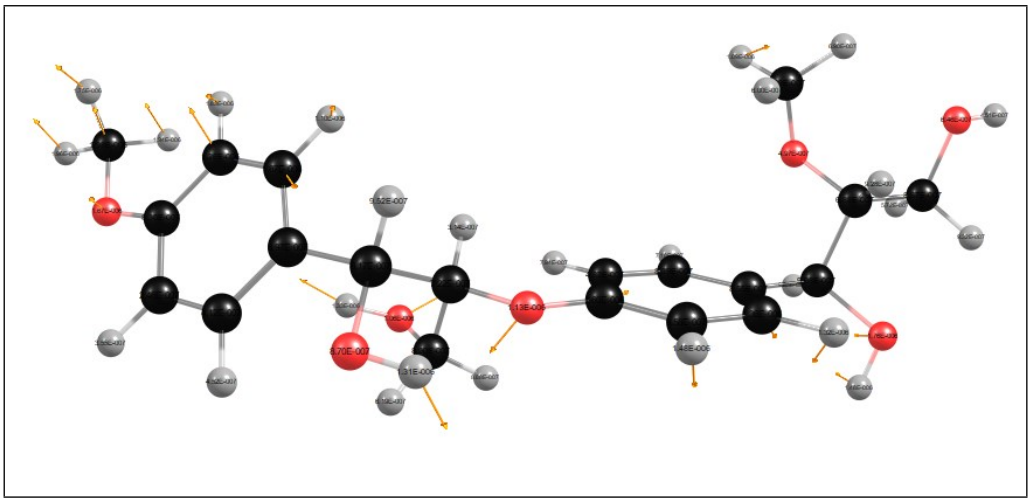


Table S19: Atomic coordinates and details of the optimized structure of the HHOX model calculated with B3LYP functional

MODEL	HHOX	**FUNCTIONAL**	B3LYP
MAXIMUM FORCE	0.000009	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.000857	**RMS DISPLACEMENT**	0.000209
PREDICTED ENERGY CHANGE (Hartree)	$-6.57.10^{-9}$	**NUMBER OF STEPS**	13
Atom	Coordinates (Angstroms)		
	X	Y	Z
C	4.572617	-1.09469	-0.94545
C	3.772931	0.001243	-0.61495
C	3.064065	0.045284	0.594675
C	3.180341	-1.04877	1.47924
C	3.961463	-2.14526	1.160469
C	4.664759	-2.17668	-0.05861
H	3.743889	0.8401	-1.30047
H	2.638005	-1.01248	2.418142
C	2.205505	1.186661	1.005477
C	1.82414	2.294148	-0.01702
H	1.938059	1.946378	-1.04985
C	2.687584	3.543722	0.189507
H	2.289613	4.344686	-0.44641
O	1.773063	1.287308	2.144951
O	0.493848	2.746134	0.197257
C	-0.56639	1.9533	-0.15836
C	-1.83442	2.506115	0.075368
C	-0.45915	0.682402	-0.73196
C	-2.97811	1.792244	-0.26295
C	-1.62193	-0.01872	-1.07199
C	-2.89169	0.515113	-0.84482
H	-3.95457	2.231869	-0.07954
H	-1.52889	-1.00976	-1.50779

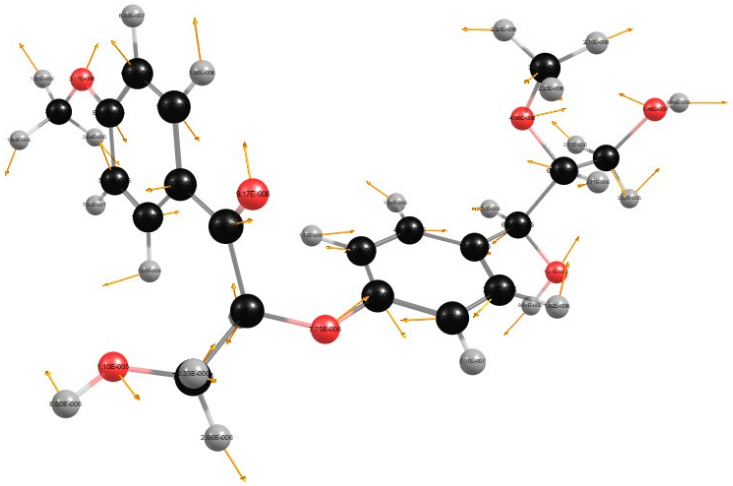
O	-4.14294	-0.26147	-1.20758
H	-3.85796	-1.10307	-1.8564
C	-4.85075	-0.86291	0.025945
H	-5.04349	-0.06053	0.753297
C	-6.18155	-1.51471	-0.34088
H	-6.79691	-0.79825	-0.89575
H	-5.98187	-2.38886	-0.97757
O	-5.10829	0.565486	-1.87779
H	-4.64923	1.064745	-2.56616
O	-3.9444	-1.81605	0.568436
O	-6.82985	-1.91226	0.874509
H	-7.67051	-2.33209	0.655805
C	-3.90211	-1.88473	1.990517
H	-3.61353	-0.91567	2.422308
H	-4.86614	-2.1977	2.405066
H	-3.13615	-2.62326	2.239165
O	5.405045	-3.2948	-0.2827
C	6.148826	-3.39849	-1.49395
H	6.89735	-2.60075	-1.57003
H	6.651256	-4.36505	-1.44956
H	5.488722	-3.3696	-2.36912
H	2.613687	3.850393	1.240082
O	4.026277	3.209094	-0.17364
H	4.621785	3.905605	0.127286
H	0.505431	0.222795	-0.91235
H	-1.8979	3.491475	0.525511
H	5.116584	-1.0901	-1.88211
H	4.048081	-2.99307	1.832109
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S20: Atomic coordinates and details of the optimized structure of the SS model calculated with M062-X functional

MODEL	SS	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000001	**RMS FORCE**	0.000000
MAXIMUM DISPLACEMENT	0.000034	**RMS DISPLACEMENT**	0.000008
PREDICTED ENERGY CHANGE (Hartree)	$-1.26.10^{-11}$	**NUMBER OF STEPS**	1
Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-4.784451	-1.395187	0.013107
C	-3,55644	-1,12219	-0,57176
C	-3,22339	0,19112	-0,91401
C	-4,13878	1,214759	-0,68961
C	-5,39086	0,940886	-0,12681
C	-5,72384	-0,37246	0,234334
H	-2,86265	-1,94398	-0,72643
H	-3,90177	2,236121	-0,96552
C	-1,8472	0,488746	-1,46049
H	-1,58681	-0,26905	-2,21491
C	-0,77645	0,407857	-0,362
H	-0,69176	-0,62486	-0,0029
C	-1,01782	1,338971	0,828653
H	-0,06447	1,501357	1,338697
O	-1,84369	1,775421	-2,04
H	-0,92116	1,998509	-2,22665
O	0,427592	0,791298	-1,04788
C	1,602059	0,463887	-0,43183
C	2,394383	1,472818	0,13063
C	2,050085	-0,86416	-0,41764
C	3,627607	1,154674	0,708313
C	3,272586	-1,18557	0,176854
C	4,054447	-0,17308	0,729534
H	4,264985	1,919378	1,136691
H	3,643497	-2,20353	0,18496
O	1,220351	-1,76323	-1,00743
O	1,875788	2,724088	0,064469
C	1,652734	-3,10944	-1,06477
H	1,771091	-3,52953	-0,05949
H	0,872239	-3,65175	-1,59708
H	2,598535	-3,19532	-1,6117
C	2,63876	3,778119	0,618817
H	2,051307	4,682693	0,467373
H	2,805067	3,624442	1,691322
H	3,60399	3,877822	0,109453
C	5,423167	-0,50662	1,288927
H	5,426599	-1,55586	1,622693

C	6,494437	-0,36677	0,198208
H	6,481796	0,670117	-0,17049
C	7,889243	-0,67085	0,710196
H	8,084294	-0,0847	1,615133
H	7,943944	-1,74257	0,949361
O	5,802818	0,356112	2,347851
H	5,120407	0,32956	3,028913
O	6,178134	-1,27226	-0,83847
O	8,788231	-0,3319	-0,33345
H	9,676449	-0,61382	-0,0949
C	5,875783	-0,66151	-2,0762
H	4,998681	-0,00457	-1,99035
H	6,734264	-0,08717	-2,44468
H	5,650191	-1,4656	-2,77913
O	-6,20832	2,006489	0,094179
O	-6,91068	-0,63328	0,867608
O	-5,08211	-2,68259	0,384372
C	-7,58439	1,886821	-0,24632
H	-7,69813	1,341801	-1,19103
H	-8,14828	1,38427	0,541594
H	-7,9489	2,90663	-0,37541
C	-7,81472	-1,46632	0,141964
H	-7,37438	-2,44794	-0,05013
H	-8,7024	-1,5678	0,767553
H	-8,08817	-0,99285	-0,8085
C	-5,01866	-2,88929	1,795959
H	-4,01042	-2,66781	2,163841
H	-5,74827	-2,25864	2,313952
H	-5,24892	-3,94194	1,962969
H	-1,37815	2,312678	0,47161
O	-1,89146	0,768351	1,784609
H	-2,79575	0,824496	1,451806

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

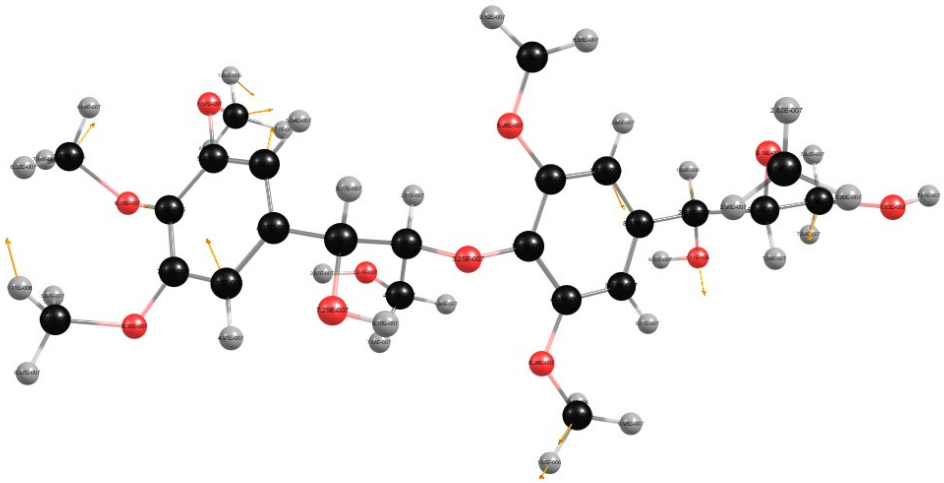


Table S21: Atomic coordinates and details of the optimized structure of the SSOX model calculated with M062-X functional

MODEL	SSOX	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000014	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001658	**RMS DISPLACEMENT**	0.000295
PREDICTED ENERGY CHANGE (Hartree)	$-5.17.10^{-9}$	**NUMBER OF STEPS**	73
Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-3.982113	-0.255441	1.134354
C	-3,06172	0,689628	0,70051
C	-2,81881	0,835859	-0,66759
C	-3,50461	0,043078	-1,58661
C	-4,40816	-0,92585	-1,15518
C	-4,64863	-1,08859	0,219827
H	-2,58899	1,321385	1,444514
H	-3,31992	0,162102	-2,64894
C	-1,80779	1,798119	-1,20633
C	-0,7377	2,399921	-0,27856
H	-0,70951	1,891519	0,68927
C	-1,02624	3,87919	-0,07723
H	-0,22854	4,320806	0,532131
O	-1,80484	2,119247	-2,37451
O	0,532177	2,308332	-0,91317
C	1,43902	1,465649	-0,34078
C	2,695734	1,97143	0,020163
C	1,157096	0,106895	-0,14609
C	3,660836	1,118497	0,564315
C	2,109451	-0,73875	0,427107
C	3,359635	-0,2289	0,76868
H	4,645306	1,482498	0,834505
H	1,906787	-1,79401	0,568269
O	-0,08048	-0,28412	-0,54728
O	2,875387	3,298439	-0,1914
C	-0,506	-1,59251	-0,21322
H	-0,45842	-1,75238	0,870306
H	-1,54204	-1,66261	-0,54897
H	0,102185	-2,34501	-0,7274
C	4,147473	3,838479	0,103377
H	4,090434	4,894905	-0,1561
H	4,386499	3,735402	1,168502
H	4,930055	3,356678	-0,49394
C	4,433703	-1,16101	1,291019
H	3,951837	-2,03247	1,761113
C	5,302101	-1,68152	0,13674
H	5,776188	-0,81995	-0,35758

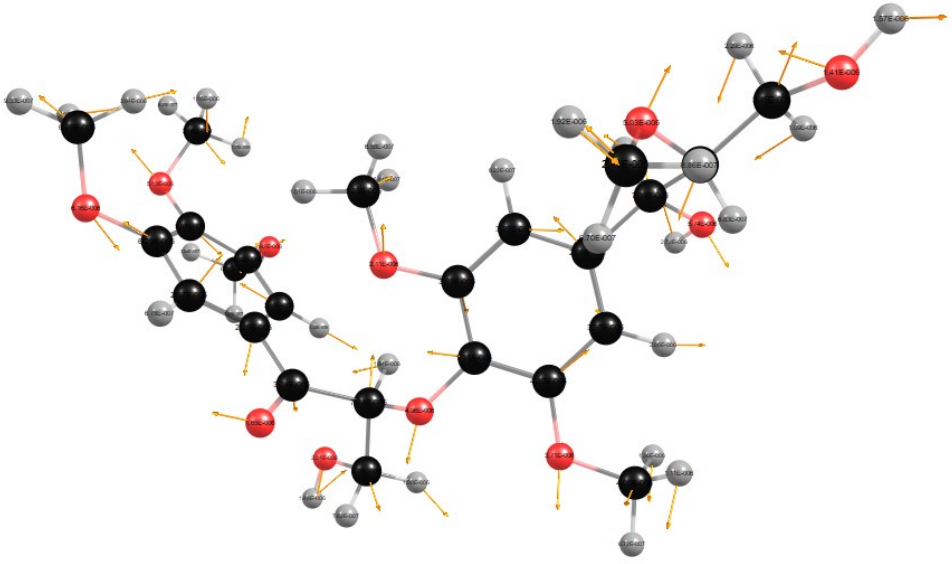
C	6,397414	-2,6166	0,612007
H	6,949097	-2,14789	1,434631
H	5,927785	-3,54473	0,968124
O	5,309993	-0,52162	2,205219
H	4,784011	-0,11866	2,905939
O	4,464403	-2,37827	-0,76117
O	7,237861	-2,86254	-0,50385
H	7,872514	-3,55019	-0,28116
C	4,341931	-1,77696	-2,03459
H	3,910161	-0,76929	-1,95945
H	5,317681	-1,72565	-2,53278
H	3,670283	-2,40808	-2,61912
O	-5,05834	-1,64799	-2,10937
O	-5,5856	-1,99013	0,642868
O	-4,24109	-0,37914	2,476906
C	-5,10712	-3,06137	-1,95844
H	-4,14586	-3,43991	-1,5882
H	-5,90918	-3,36313	-1,28207
H	-5,28902	-3,46361	-2,95571
C	-5,08289	-3,05914	1,445002
H	-4,62282	-2,6798	2,360572
H	-5,9414	-3,68686	1,686061
H	-4,34934	-3,64436	0,876895
C	-5,50134	0,169654	2,86309
H	-5,52701	1,242887	2,644678
H	-6,32111	-0,3352	2,341912
H	-5,58879	0,011857	3,938415
H	-1,04087	4,360013	-1,06263
O	-2,28719	3,948597	0,570965
H	-2,64398	4,838806	0,497128
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S22: Atomic coordinates and details of the optimized structure of the SG model calculated with M062-X functional

MODEL	SG	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000010	**RMS FORCE**	0.000003
MAXIMUM DISPLACEMENT	0.001065	**RMS DISPLACEMENT**	0.000260
PREDICTED ENERGY CHANGE (Hartree)	$-1.33.10^{-8}$	**NUMBER OF STEPS**	17
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	4,360803	1,519689	0,310645
C	3,136055	1,118415	-0,23342
C	2,976479	-0,16406	-0,73787
C	4,042739	-1,07012	-0,70966
C	5,259808	-0,68048	-0,151
C	5,43329	0,620758	0,363786
H	2,322835	1,838351	-0,24765
H	3,897556	-2,05719	-1,1298
C	1,625754	-0,59727	-1,25539
H	1,162056	0,234856	-1,80342
C	0,667636	-0,95739	-0,11054
H	0,439179	-0,05918	0,473055
C	1,17021	-2,05176	0,833352
H	0,300185	-2,48196	1,338399
O	1,790104	-1,71434	-2,1073
H	0,90312	-2,02073	-2,34004
O	-0,51589	-1,44407	-0,77194
C	-1,71163	-1,05296	-0,2289
C	-2,57034	-1,99494	0,312839
C	-2,09585	0,302545	-0,27945
C	-3,81501	-1,611	0,819343
C	-3,32511	0,685258	0,247479
C	-4,18905	-0,27126	0,796411
H	-4,49303	-2,35367	1,227814
H	-3,64854	1,719392	0,212669
O	-1,20279	1,148012	-0,86074
C	-1,56584	2,512525	-0,95787
H	-1,70172	2,955849	0,035112
H	-0,74018	3,007033	-1,46854
H	-2,48529	2,633096	-1,54199
C	-5,55027	0,161805	1,304761
H	-5,4772	1,187473	1,69922
C	-6,568	0,191673	0,157414
H	-6,57114	-0,79369	-0,33334
C	-7,97486	0,498822	0,638321
H	-8,26873	-0,22818	1,402981
H	-7,98201	1,508533	1,073595

O	-6,06642	-0,71447	2,290745
H	-5,41822	-0,79965	2,999848
O	-6,13652	1,193767	-0,74006
O	-8,82027	0,428781	-0,50036
H	-9,71823	0,662179	-0,24605
C	-6,13423	0,799871	-2,09831
H	-5,42784	-0,02653	-2,26046
H	-7,13726	0,500441	-2,42011
H	-5,80815	1,666177	-2,67712
O	6,336434	-1,50047	-0,03113
O	6,58967	0,977393	1,000039
O	4,408942	2,778956	0,821324
C	6,184261	-2,84514	-0,44603
H	5,383006	-3,33947	0,114948
H	5,971843	-2,90669	-1,51903
H	7,134597	-3,33246	-0,23183
C	7,756754	1,043045	0,185057
H	7,594595	1,719446	-0,6632
H	8,547914	1,440829	0,822111
H	8,035903	0,053355	-0,18162
C	5,580915	3,560716	0,624085
H	6,345226	3,329011	1,367301
H	5,983463	3,400729	-0,38304
H	5,263271	4,599623	0,722729
H	1,654422	-2,84813	0,250591
O	2,012871	-1,5541	1,851235
H	2,853822	-1,28455	1,460431
H	-2,25171	-3,03254	0,321609

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

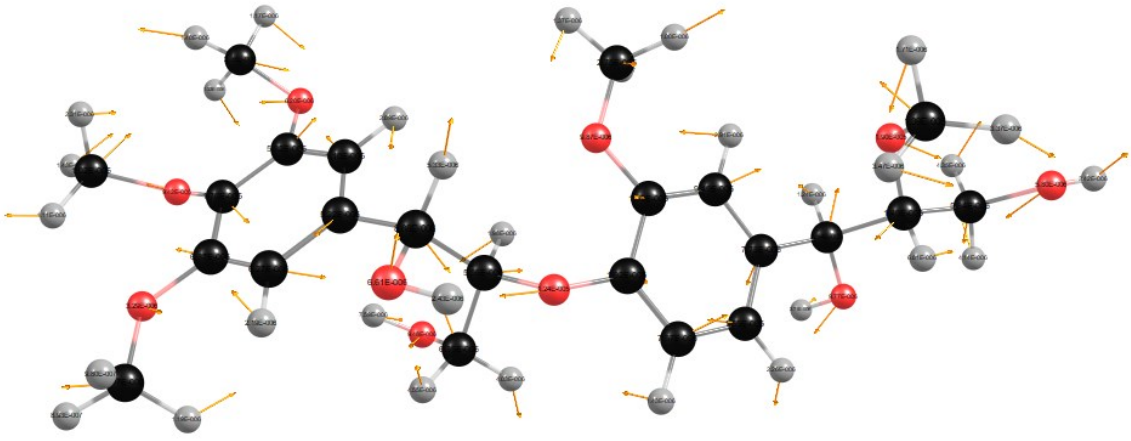


Table S23: Atomic coordinates and details of the optimized structure of the SGOX model calculated with M062-X functional

MODEL	SGOX	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000019	**RMS FORCE**	0.000004
MAXIMUM DISPLACEMENT	0.001498	**RMS DISPLACEMENT**	0.000315
PREDICTED ENERGY CHANGE (Hartree)	$-1.67.10^{-8}$	**NUMBER OF STEPS**	30
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-4,13217	461787 0.	440904
C	-2,42242	-0,261855	0,452385
C	-3,02981	0,89295	-0,035114
C	-4,34098	0,86203	-0,531847
C	-5,04093	-0,337406	-0,5527
C	-4,43217	-1,514211	-0,066684
H	-1,40377	-0,262239	0,823639
H	-4,77718	1,788935	-0,883832
C	-2,34086	2,211844	-0,001384
C	-0,85325	2,28068	0,370994
H	-0,73043	1,912686	1,39948
C	-0,33392	3,714328	0,281588
H	0,738575	3,717731	0,494514
O	-2,94361	3,244593	-0,243293
O	-0,17497	1,425521	-0,553336
C	1,166667	1,229654	-0,330879
C	2,086239	1,719144	-1,246794
C	1,611729	0,475123	0,771796
C	3,450765	1,472836	-1,086504
C	2,975541	0,250387	0,942261
C	3,896666	0,740462	0,010344
H	4,166959	1,842132	-1,814043
H	3,337777	-0,337559	1,778844
O	0,644693	0,006755	1,604505
C	1,029192	-0,896289	2,625842
H	1,670366	-0,404471	3,365505
H	0,103338	-1,219438	3,101012
H	1,547749	-1,763594	2,202423
C	5,360695	0,389589	0,160433
H	5,572608	0,194606	1,223711
C	5,718144	-0,884718	-0,615202
H	5,543051	-0,711579	-1,687584
C	7,172895	-1,285625	-0,403441
H	7,835137	-0,530216	-0,828379
H	7,369427	-1,35525	0,677944

O	6,220259	1,395599	-0,345017
H	6,014708	2,232086	0,088679
O	4,918966	-1,96388	-0,155208
O	7,448007	-2,509636	-1,047851
H	6,803325	-3,146521	-0,713075
C	3,881191	-2,350777	-1,039907
H	3,185729	-1,525243	-1,233124
H	4,296927	-2,703388	-1,992692
H	3,341781	-3,166976	-0,555987
O	-6,30608	-0,489694	-1,018668
O	-5,11404	-2,693693	-0,055316
O	-2,52056	-2,602004	0,887567
C	-6,96535	0,668755	-1,495156
H	-7,05868	1,420574	-0,703604
H	-6,43317	1,101636	-2,349841
H	-7,95619	0,341699	-1,807231
C	-5,22616	-3,309556	-1,338814
H	-4,23007	-3,541062	-1,731001
H	-5,78677	-4,231759	-1,186446
H	-5,76578	-2,657701	-2,0316
C	-3,06216	-3,11857	2,101012
H	-2,94985	-2,383455	2,90734
H	-4,11683	-3,378624	1,978863
H	-2,48394	-4,012318	2,337619
H	-0,48593	4,088213	-0,739764
O	-0,94887	4,539182	1,243091
H	-1,86478	4,660758	0,959586
H	1,70821	2,286466	-2,091576

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

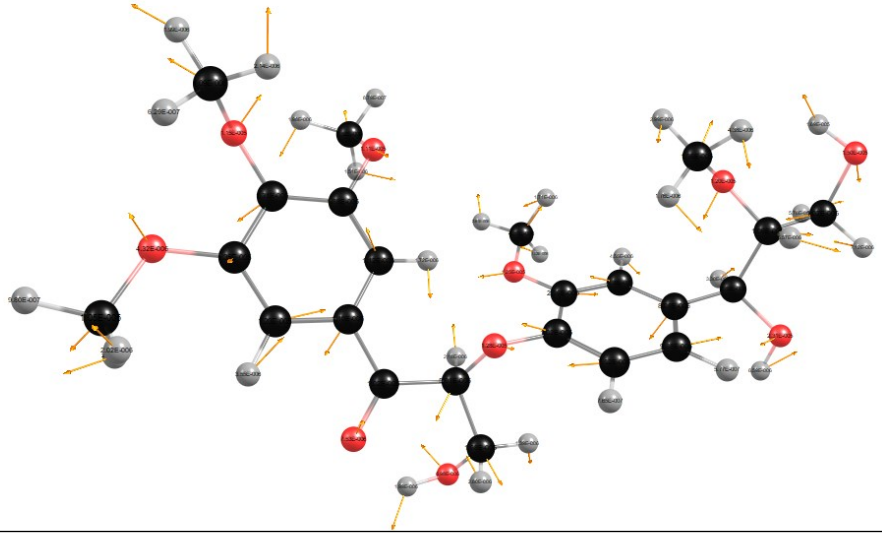


Table S24: Atomic coordinates and details of the optimized structure of the SH model calculated with M062-X functional

MODEL	SH	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000009	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001630	**RMS DISPLACEMENT**	0.000241
PREDICTED ENERGY CHANGE (Hartree)	$-9.09.10^{-9}$	**NUMBER OF STEPS**	20
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	4,274385	1,642301	-0,212023
C	3,107902	1,114681	-0,777142
C	2,934171	-0,25841	-0,879455
C	3,927704	-1,13019	-0,420896
C	5,0847	-0,60923	0,157793
C	5,271538	0,784175	0,268231
H	2,355409	1,812815	-1,131901
H	3,778704	-2,19627	-0,533446
C	1,634363	-0,80792	-1,421372
H	1,302039	-0,18506	-2,264607
C	0,533915	-0,75717	-0,348528
H	0,320325	0,293556	-0,112822
C	0,909596	-1,49882	0,942759
H	0,001044	-1,88917	1,408111
O	1,832301	-2,13992	-1,846819
H	0,963808	-2,50031	-2,070306
O	-0,59318	-1,36706	-0,971919
C	-1,84159	-1,13594	-0,460644
C	-2,89867	-1,73796	-1,149391
C	-2,09742	-0,35402	0,667909
C	-4,20391	-1,55259	-0,715448
C	-3,41648	-0,18277	1,091098
C	-4,47995	-0,77299	0,413841
H	-5,02518	-2,01337	-1,257872
H	-3,61701	0,433949	1,962754
C	-5,90919	-0,53262	0,84962
H	-5,9199	-0,2725	1,919446
C	-6,51208	0,653753	0,088736
H	-6,41952	0,459961	-0,991366
C	-7,97826	0,871107	0,415928
H	-8,53816	-0,0516	0,228341
H	-8,06069	1,138486	1,479149
O	-6,74701	-1,65051	0,598736
H	-6,35425	-2,42878	1,010887
O	-5,76267	1,791783	0,457682
O	-8,43027	1,932091	-0,412934
H	-9,33795	2,152421	-0,182734

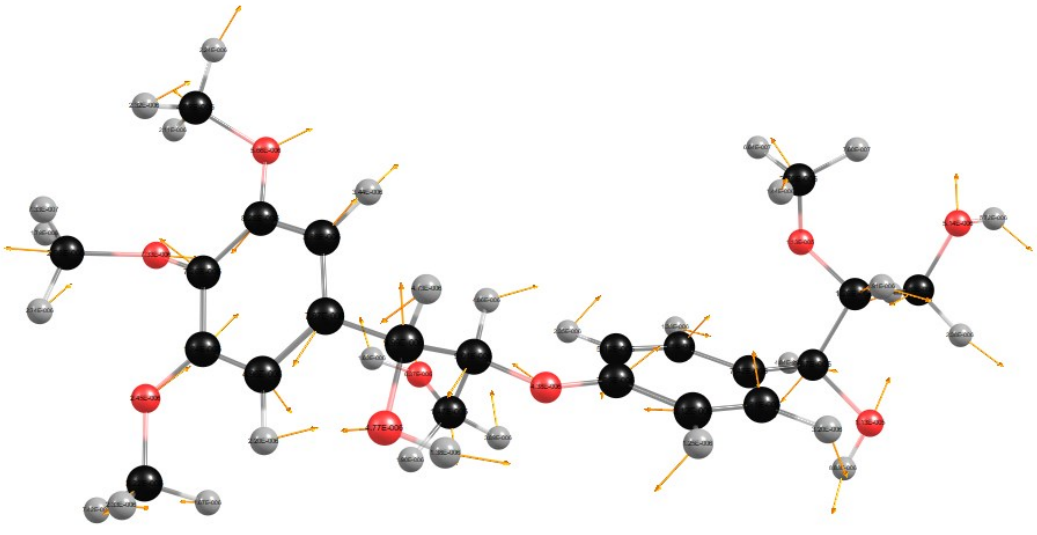
C	-5,3435	2,593217	-0,628754
H	-4,66714	2,029614	-1,287052
H	-6,20379	2,955406	-1,202036
H	-4,80225	3,440684	-0,20467
O	6,082517	-1,37115	0,675465
O	6,354154	1,299233	0,923677
O	4,33368	2,995844	-0,110347
C	5,904919	-2,77556	0,670672
H	5,008843	-3,0585	1,234575
H	5,831883	-3,16152	-0,352032
H	6,78776	-3,18916	1,156338
C	7,620636	1,085845	0,305179
H	7,614988	1,470626	-0,721948
H	8,344435	1,644785	0,899669
H	7,881532	0,025861	0,300308
C	5,567044	3,656663	-0,369749
H	6,212717	3,655205	0,509536
H	6,08555	3,183203	-1,211573
H	5,302347	4,679528	-0,640434
H	1,553626	-2,35396	0,698076
O	1,509713	-0,64163	1,890877
H	2,396912	-0,40918	1,586579
H	-1,29429	0,109563	1,230105
H	-2,67465	-2,33907	-2,024591
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S25: Atomic coordinates and details of the optimized structure of the SHOX model calculated with M062-X functional

MODEL	SHOX	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000004	**RMS FORCE**	0.000001
MAXIMUM DISPLACEMENT	0.001630	**RMS**	0.000241

		DISPLACEMENT	
PREDICTED ENERGY CHANGE (Hartree)	$-9.09.10^{-9}$	**NUMBER OF STEPS**	67
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-1.687151	-1,372865	0,428596
C	-1,58024	0,010903	0,444216
C	-2,70635	0,793002	0,161445
C	-3,92141	0,18156	-0,14562
C	-4,02509	-1,20598	-0,19825
C	-2,8996	-1,99864	0,089419
H	-0,61527	0,437684	0,701594
H	-4,79785	0,785055	-0,35575
C	-2,66848	2,282375	0,216292
C	-1,30042	2,974019	0,286459
H	-0,81147	2,646004	1,213133
C	-1,43511	4,492975	0,297755
H	-0,43422	4,934463	0,285715
O	-3,68643	2,949844	0,213993
O	-0,57831	2,555653	-0,86012
C	0,726986	2,167635	-0,73791
C	1,22831	1,40298	-1,7957
C	1,542017	2,482345	0,349676
C	2,525244	0,913675	-1,73786
C	2,841883	1,975134	0,393764
C	3,339625	1,174432	-0,62945
H	2,906759	0,289689	-2,54182
H	3,464689	2,185693	1,258901
C	4,668782	0,472513	-0,48208
H	5,278334	1,005108	0,265008
C	4,444401	-0,96115	0,029378
H	3,887256	-1,51674	-0,74073
C	5,750653	-1,68662	0,284432
H	6,410268	-1,5627	-0,5823
C	6,222873	-1,24081	1,171521
O	5,367692	0,355729	-1,71132
H	5,469485	1,234289	-2,09546
O	3,714189	-0,90706	1,236833
O	5,433199	-3,05125	0,503886
H	6,222778	-3,52044	0,789824
C	2,374333	-1,34772	1,135789
H	1,797593	-0,7533	0,415729
H	2,333125	-2,40384	0,838688
H	1,927522	-1,23217	2,126085
O	-5,24876	-1,72869	-0,47564
O	-3,02485	-3,35705	0,120854

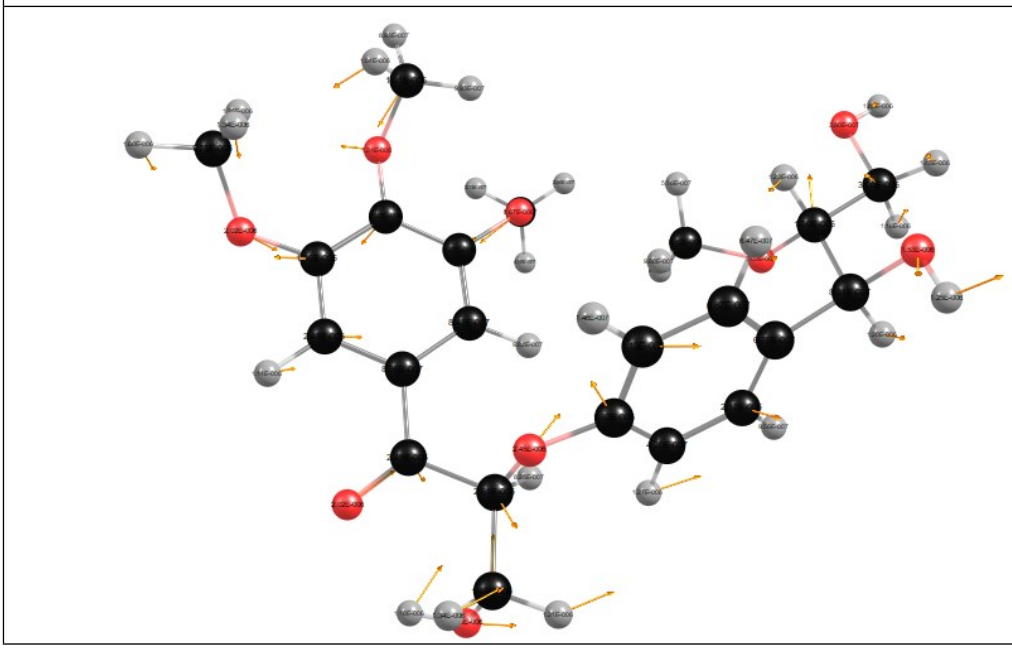
O	-0,59214	-2,1356	0,747739
C	-5,33272	-2,79906	-1,41102
H	-4,62279	-2,64615	-2,23254
H	-5,14357	-3,76106	-0,93178
H	-6,34883	-2,77057	-1,80583
C	-2,22929	-4,07529	-0,82581
H	-1,16463	-3,89247	-0,66432
H	-2,45965	-5,12975	-0,67243
H	-2,50412	-3,78352	-1,846
C	-0,68277	-2,75859	2,030565
H	-0,73931	-1,99548	2,815181
H	-1,5582	-3,41323	2,08568
H	0,229765	-3,34328	2,1527
H	-1,96115	4,809686	-0,61117
O	-2,08156	4,936301	1,467014
H	-3,01346	4,694135	1,382943
H	1,1862	3,112192	1,157819
H	0,571922	1,182638	-2,6309
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S26: Atomic coordinates and details of the optimized structure of the GS model calculated with M062-X functional

MODEL	GS	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000005	**RMS FORCE**	0.000001
MAXIMUM DISPLACEMENT	0.001227	**RMS DISPLACEMENT**	0.000270
PREDICTED ENERGY CHANGE (Hartree)	$-1.81.10^{-9}$	**NUMBER OF STEPS**	20
ATOM	Coordinates (Angstroms)		
	X	Y	Z

C	-5.144865 -	1,803874	0,279641
C	-3,92754	-1,55774	-0,35779
C	-3,60243	-0,28485	-0,81615
C	-4,53053	0,749321	-0,65016
C	-5,74727	0,518228	-0,02136
C	-6,06171	-0,76808	0,460657
H	-3,22156	-2,37457	-0,48541
H	-4,3108	1,747584	-1,0146
C	-2,24617	-0,01728	-1,42372
H	-1,96919	-0,85867	-2,07701
C	-1,15304	0,089319	-0,34999
H	-1,01615	-0,88392	0,137138
C	-1,41743	1,154296	0,717904
H	-0,46248	1,439594	1,167246
O	-2,30261	1,180549	-2,16976
H	-1,39163	1,416321	-2,39429
O	0,020402	0,428241	-1,10939
C	1,217963	0,277522	-0,46965
C	1,94557	1,411338	-0,08751
C	1,75314	-0,9994	-0,25229
C	3,198738	1,269773	0,516784
C	2,996366	-1,14289	0,367806
C	3,711203	-0,00741	0,744832
H	3,784613	2,133063	0,809594
H	3,433209	-2,12011	0,534344
O	0,98244	-2,03316	-0,67993
O	1,34516	2,600402	-0,34437
C	1,500597	-3,34009	-0,52196
H	1,646233	-3,58219	0,536961
H	0,756636	-4,01062	-0,95051
H	2,449874	-3,45425	-1,05761
C	2,038795	3,776162	0,024359
H	1,393418	4,605358	-0,26251
H	2,216954	3,807914	1,105525
H	2,994546	3,854581	-0,50626
C	5,092385	-0,16151	1,352016
H	5,144071	-1,12357	1,884613
C	6,160259	-0,19408	0,251499
H	6,052187	0,709879	-0,36736
C	7,571874	-0,23012	0,808203
H	7,722683	0,615681	1,487686
H	7,704025	-1,17088	1,361674
O	5,427158	0,907612	2,220471
H	4,743925	0,981256	2,897241
O	5,921333	-1,35536	-0,51554
O	8,44874	-0,16598	-0,30664
H	9,357113	-0,26196	-0,00483

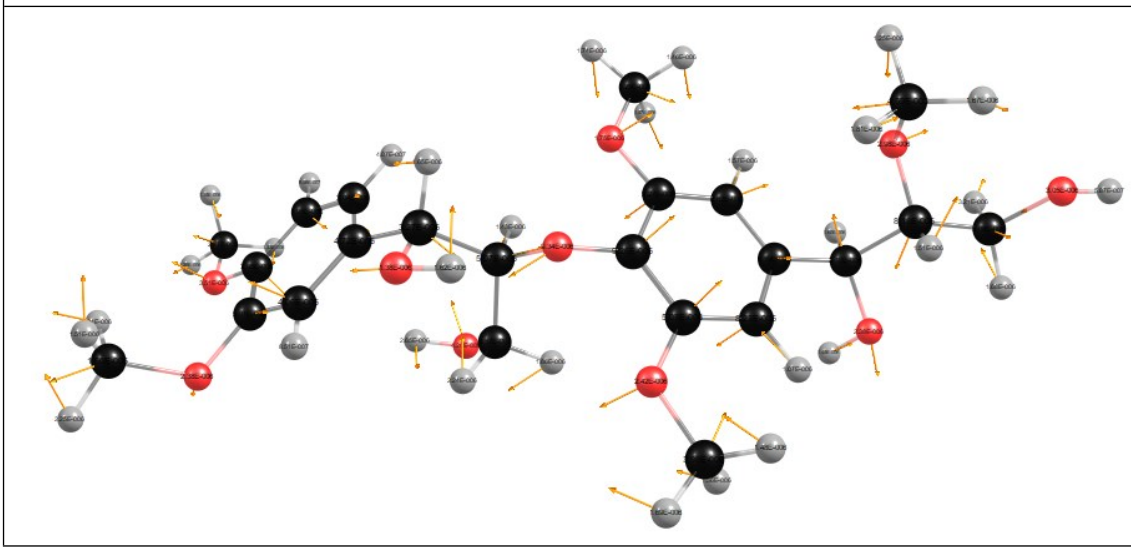
C	5,867973	-1,13203	-1,9105
H	5,032163	-0,465	-2,16517
H	6,809524	-0,70505	-2,27305
C	5,703348	-2,10378	-2,37971
O	-6,61133	1,560363	0,171171
O	-7,26491	-0,897	1,079411
C	-7,78282	1,508456	-0,63712
H	-7,51094	1,531766	-1,69897
H	-8,36852	0,610539	-0,42017
H	-8,36467	2,396552	-0,38941
C	-7,58612	-2,16006	1,625508
H	-6,84979	-2,46161	2,37954
H	-8,56172	-2,04445	2,096025
H	-7,64511	-2,92694	0,843973
H	-1,84937	2,049768	0,251681
O	-2,22268	0,663847	1,772488
H	-3,13665	0,604554	1,467765
H	-5,36531	-2,80286	0,636432
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S27: Atomic coordinates and details of the optimized structure of the GSOX model calculated with M062-X functional

MODEL	GSOX	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000009	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.000687	**RMS DISPLACEMENT**	0.000154
PREDICTED ENERGY CHANGE (Hartree)	$-4.55.10^{-9}$	**NUMBER OF STEPS**	63
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-4.284338	-0,278401	1,540095
C	-3,36709	0,634661	1,015843
C	-3,15547	0,716554	-0,35783

C	-3,8806	-0,12606	-1,21278
C	-4,77978	-1,04589	-0,70614
C	-4,99255	-1,1268	0,688513
H	-2,85062	1,304354	1,694948
H	-3,73267	-0,06095	-2,28633
C	-2,16722	1,645641	-0,97841
C	-1,08002	2,313468	-0,11721
H	-0,99562	1,840199	0,865508
C	-1,40385	3,790746	0,047094
H	-0,58833	4,277006	0,595872
O	-2,19413	1,895118	-2,16484
O	0,166051	2,242441	-0,79932
C	1,117494	1,43103	-0,25649
C	2,380462	1,970519	0,025948
C	0,877884	0,070581	-0,0205
C	3,392951	1,149927	0,53271
C	1,878953	-0,74257	0,515634
C	3,134303	-0,19934	0,778427
H	4,382417	1,54071	0,740068
H	1,708965	-1,79945	0,685262
O	-0,37013	-0,35518	-0,34606
O	2,519101	3,296192	-0,22172
C	-0,74229	-1,67149	0,017093
H	-0,62273	-1,82672	1,095741
H	-1,7954	-1,76707	-0,25196
H	-0,14901	-2,41161	-0,53143
C	3,79367	3,868345	-0,01081
H	3,699374	4,917454	-0,28852
H	4,094519	3,793699	1,040992
H	4,551689	3,389563	-0,64133
C	4,256304	-1,09836	1,256208
H	3,821143	-1,96806	1,772848
C	5,064928	-1,62864	0,063628
H	5,487651	-0,76969	-0,47939
C	6,20866	-2,52759	0,492432
H	6,800298	-2,02558	1,266193
H	5,783357	-3,45543	0,901091
O	5,171977	-0,42178	2,102524
H	4,679862	-0,00969	2,822262
O	4,189732	-2,36537	-0,76381
O	6,982583	-2,78578	-0,66792
H	7,643925	-3,45537	-0,46912
C	3,982786	-1,80374	-2,04438
H	3,53882	-0,80115	-1,97231
H	4,926687	-1,75191	-2,60048
H	3,288933	-2,46205	-2,57004
O	-5,50012	-1,83708	-1,55777

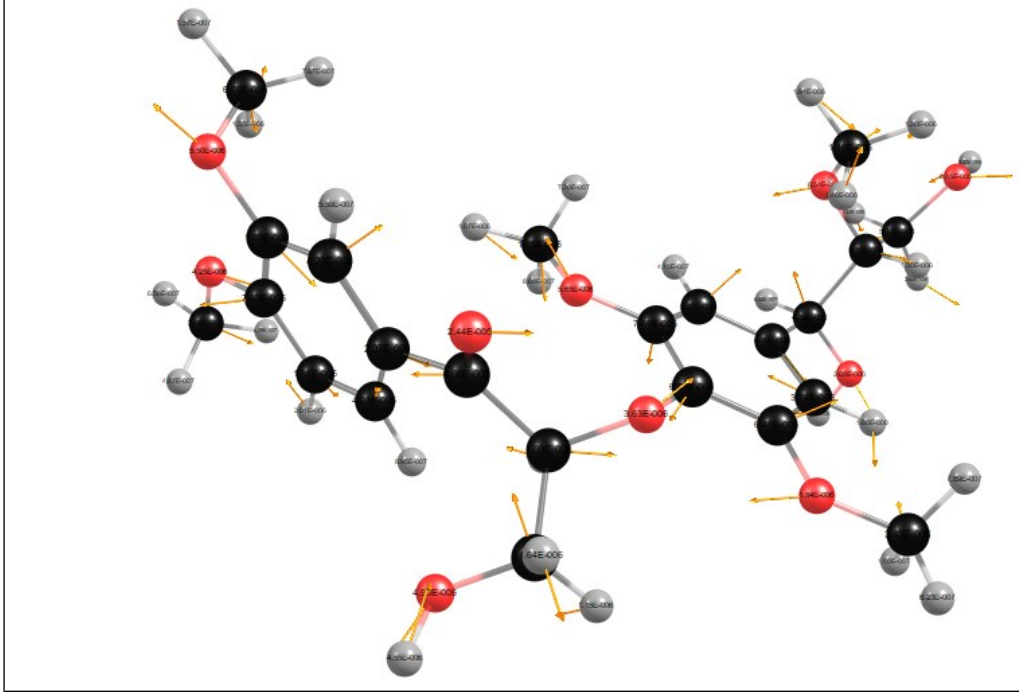
O	-5,90291	-2,0442	1,095283
C	-5,09672	-3,20154	-1,56672
H	-4,05272	-3,28582	-1,89331
H	-5,21699	-3,65262	-0,57702
H	-5,74328	-3,70931	-2,28272
C	-6,19178	-2,11684	2,477933
H	-6,5828	-1,16237	2,847851
H	-6,95327	-2,88821	2,584407
H	-5,30199	-2,39698	3,053783
H	-1,48386	4,234269	-0,95255
O	-2,62935	3,852064	0,760319
H	-3,03339	4,717061	0,643817
H	-4,44757	-0,31112	2,610562
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S28: Atomic coordinates and details of the optimized structure of the GG model calculated with M062-X functional

MODEL	GG	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000039	**RMS FORCE**	0.000006
MAXIMUM DISPLACEMENT	0.001657	**RMS DISPLACEMENT**	0.000339
PREDICTED ENERGY CHANGE (Hartree)	$-4.56.10^{-8}$	**NUMBER OF STEPS**	12
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	4.685319	1.765225	0,212156
C	3,474879	1,308953	-0,31251
C	3,319004	-0,01572	-0,7086

C	4,408119	-0,88706	-0,59533
C	5,619716	-0,44619	-0,07824
C	5,765196	0,891376	0,341743
H	2,639997	2,000285	-0,39991
H	4,320715	-1,92099	-0,91334
C	1,975932	-0,51136	-1,18658
H	1,515855	0,247198	-1,83666
C	1,006116	-0,73528	-0,01777
H	0,760184	0,226985	0,44453
C	1,507333	-1,69298	1,06506
H	0,63563	-2,06513	1,61208
O	2,155669	-1,72025	-1,89617
H	1,274689	-2,06163	-2,10037
O	-0,16603	-1,31315	-0,62628
C	-1,36982	-0,9001	-0,12281
C	-2,19677	-1,79993	0,531455
C	-1,79541	0,429131	-0,32399
C	-3,45144	-1,40006	0,99799
C	-3,03668	0,829987	0,162091
C	-3,86964	-0,08544	0,817427
H	-4,10485	-2,10859	1,497759
H	-3,39091	1,844046	0,010836
O	-0,9294	1,230566	-0,99928
C	-1,34096	2,558367	-1,26402
H	-1,49816	3,115887	-0,33359
H	-0,5315	3,015911	-1,8318
H	-2,26073	2,572828	-1,85983
C	-5,2528	0,349921	1,24974
H	-5,24852	1,440068	1,408594
C	-6,30392	0,052681	0,173238
H	-6,35004	-1,0342	0,008527
C	-7,68404	0,557553	0,575823
H	-8,04545	0,006353	1,444919
H	-7,60978	1,623281	0,843375
O	-5,70063	-0,32308	2,413008
H	-5,04877	-0,20643	3,114173
O	-5,95391	0,717144	-1,0316
O	-8,60791	0,3619	-0,47189
H	-8,23262	0,791685	-1,25151
C	-5,44464	-0,13	-2,04702
H	-4,53649	-0,65089	-1,72062
H	-6,19765	-0,87037	-2,34694
H	-5,20493	0,508119	-2,89954
O	6,648282	-1,33423	0,068231
O	6,97788	1,228361	0,852834
C	7,731145	-1,13492	-0,83574
H	7,383773	-1,23908	-1,87032

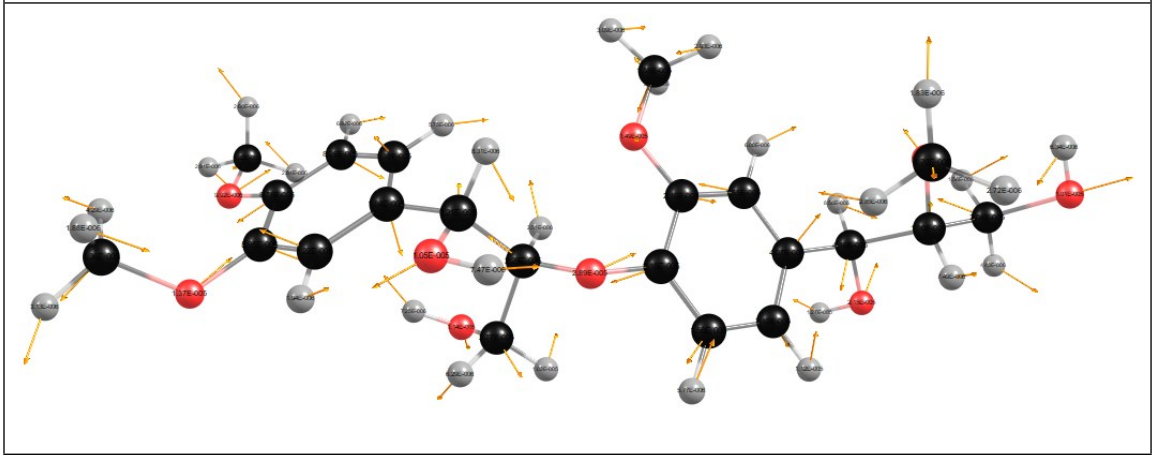
H	8,185912	-0,15099	-0,6904
H	8,460586	-1,91439	-0,61493
C	7,138915	2,544977	1,340972
H	6,426426	2,755608	2,146896
H	8,154681	2,598355	1,730552
H	7,014958	3,283025	0,539615
H	2,009211	-2,55144	0,598369
O	2,330158	-1,05112	2,017063
H	3,201599	-0,90007	1,630081
H	-1,84391	-2,81859	0,65825
H	4,773696	2,79921	0,523395
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S29: Atomic coordinates and details of the optimized structure of the GGOX model calculated with M062-X functional

MODEL	GGOX	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000020	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001315	**RMS DISPLACEMENT**	0.000329
PREDICTED ENERGY CHANGE (Hartree)	$-1.50.10^{-8}$	**NUMBER OF STEPS**	11
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-4.075531 -	0,27684	1,521498
C	-3,23506	0,691485	0,968952
C	-2,98678	0,715363	-0,40088
C	-3,59627	-0,24315	-1,22332
C	-4,41833	-1,21704	-0,68742
C	-4,66917	-1,23849	0,703074
H	-2,80939	1,447027	1,620299
H	-3,4188	-0,22619	-2,29421
C	-2,07123	1,69842	-1,04827
C	-1,09234	2,52815	-0,1963
H	-0,97291	2,109407	0,807242
C	-1,60461	3,958619	-0,10163

H	-0,87384	4,56638	0,446294
O	-2,07606	1,87235	-2,24835
O	0,168326	2,597969	-0,8503
C	1,20384	1,886467	-0,30936
C	2,423248	2,523251	-0,13441
C	1,081113	0,519155	0,011085
C	3,524475	1,827315	0,368256
C	2,171265	-0,16307	0,543181
C	3,398581	0,48641	0,720078
H	4,480383	2,328485	0,484828
H	2,097029	-1,21704	0,787063
O	-0,13217	-0,03918	-0,23989
C	-0,35369	-1,37312	0,176744
H	-0,19042	-1,47677	1,255948
H	-1,39708	-1,58846	-0,05901
H	0,301582	-2,06555	-0,36375
C	4,59141	-0,29712	1,230195
H	4,237431	-1,09353	1,903681
C	5,322393	-0,98179	0,068582
H	5,582752	-0,2177	-0,67976
C	6,595902	-1,67803	0,513379
H	7,249468	-0,95991	1,020288
H	6,327294	-2,48307	1,212616
O	5,540623	0,524129	1,888623
H	5,087829	1,031863	2,572152
O	4,4238	-1,92641	-0,47476
O	7,205237	-2,20201	-0,65714
H	7,997258	-2,69056	-0,41332
C	4,305868	-1,87696	-1,88354
H	3,90435	-0,90582	-2,20502
H	5,27433	-2,05678	-2,36246
H	3,605125	-2,66374	-2,16903
O	-5,02855	-2,12337	-1,50964
O	-5,49913	-2,2165	1,138881
C	-4,49501	-3,43973	-1,4235
H	-3,43658	-3,43903	-1,71219
H	-4,60705	-3,84284	-0,41239
H	-5,06295	-4,04897	-2,12688
C	-5,82437	-2,23927	2,515263
H	-6,3181	-1,30879	2,817196
H	-6,51035	-3,07487	2,64683
H	-4,93076	-2,3972	3,13027
H	-1,71108	4,349425	-1,12087
O	-2,84643	3,894904	0,579634
H	-3,34669	4,70223	0,427307
H	2,492054	3,571456	-0,40657
H	-4,27026	-0,26479	2,587112

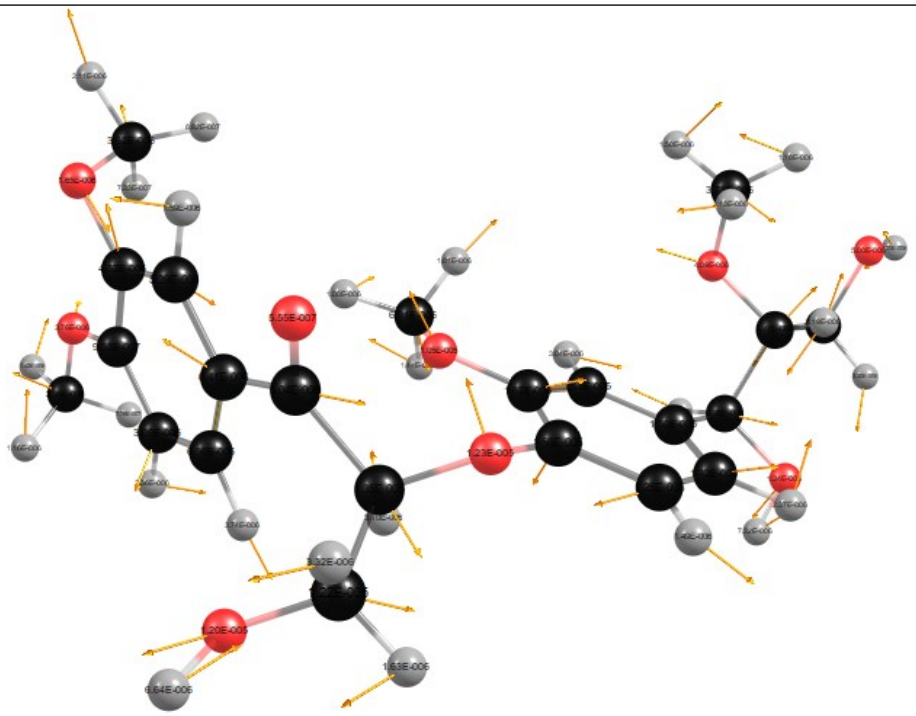
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES


Table S30: Atomic coordinates and details of the optimized structure of the GH model calculated with M062-X functional

MODEL	GH	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000019	**RMS FORCE**	0.000004
MAXIMUM DISPLACEMENT	0.001199	**RMS DISPLACEMENT**	0.000310
PREDICTED ENERGY CHANGE (Hartree)	$-1.36.10^{-8}$	**NUMBER OF STEPS**	17
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	4.565060	1.847352	-0,590105
C	3,422627	1,182057	-1,03931
C	3,286806	-0,19418	-0,88407
C	4,329191	-0,91231	-0,28741
C	5,473042	-0,26471	0,16076
C	5,596168	1,132726	0,020231
H	2,628039	1,756048	-1,50961
H	4,260641	-1,98904	-0,17123
C	2,004664	-0,88286	-1,2887
H	1,644901	-0,45343	-2,23579
C	0,908092	-0,65578	-0,23535
H	0,655537	0,412562	-0,21498
C	1,317638	-1,10237	1,175769
H	0,426198	-1,42029	1,722553
O	2,249971	-2,26439	-1,44148
H	1,395623	-2,69444	-1,5795
O	-0,19954	-1,41839	-0,70704

C	-1,45316	-1,12745	-0,2426
C	-2,49199	-1,88933	-0,78588
C	-1,73215	-0,14104	0,70599
C	-3,8016	-1,66015	-0,38794
C	-3,05526	0,071512	1,096678
C	-4,10054	-0,67628	0,561861
H	-4,60863	-2,24723	-0,81812
H	-3,27383	0,845166	1,827466
C	-5,53589	-0,39725	0,951972
H	-5,55276	0,076084	1,945966
C	-6,18001	0,588119	-0,02981
H	-6,08308	0,181008	-1,04844
C	-7,65206	0,819374	0,259469
H	-8,18084	-0,13996	0,266172
H	-7,74179	1,292432	1,247865
O	-6,33696	-1,56889	0,942647
H	-5,91984	-2,23208	1,504847
O	-5,46843	1,801342	0,092298
O	-8,14125	1,676638	-0,76182
H	-9,05808	1,901859	-0,57704
C	-5,08548	2,380886	-1,13879
H	-4,39533	1,718504	-1,68052
H	-5,96191	2,592832	-1,76076
H	-4,57041	3,313279	-0,9011
O	6,449769	-0,98711	0,785857
O	6,738955	1,682797	0,504409
C	7,647895	-1,13703	0,029256
H	7,438258	-1,66213	-0,90991
H	8,103639	-0,16486	-0,17839
H	8,321781	-1,73697	0,641005
C	6,871873	3,088483	0,429874
H	6,067357	3,58929	0,980608
H	7,82977	3,323823	0,891688
H	6,872889	3,431774	-0,61133
H	1,992493	-1,96518	1,10651
O	1,890134	-0,04347	1,915857
H	2,793601	0,101318	1,606429
H	-0,94294	0,450676	1,156524
H	-2,25015	-2,64887	-1,52212
H	4,638183	2,920876	-0,71603
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			

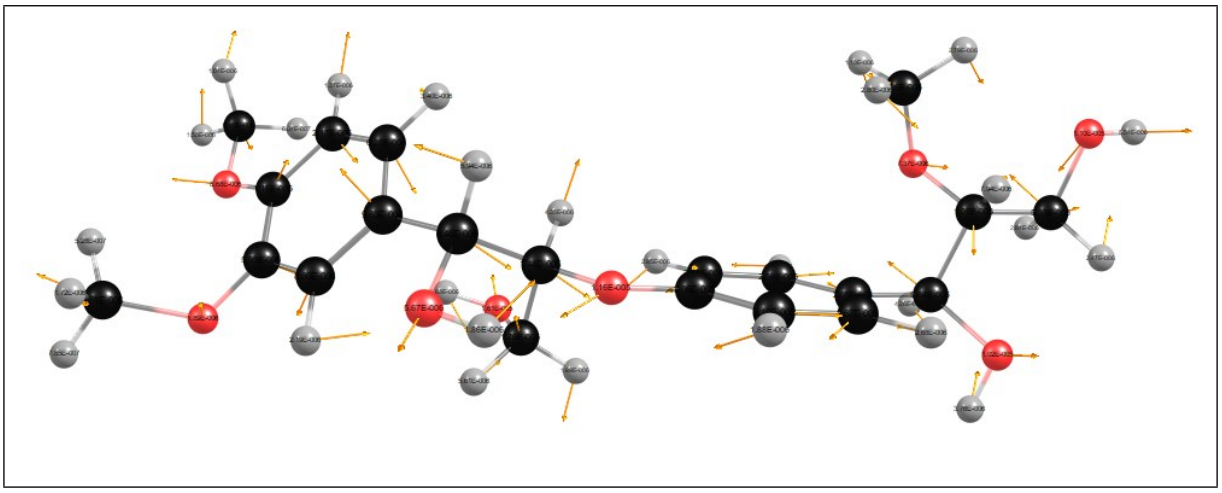


Table S31: Atomic coordinates and details of the optimized structure of the GHOX model calculated with M062-X functional

MODEL	GHOX	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000013	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001721	**RMS DISPLACEMENT**	0.000314
PREDICTED ENERGY CHANGE (Hartree)	$-2.13.10^{-9}$	**NUMBER OF STEPS**	75
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-4.189310	-0,318462	1,085412
C	-3,37061	0,727497	0,657645
C	-2,5102	0,553518	-0,42547
C	-2,47372	-0,68742	-1,08123
C	-3,26828	-1,73447	-0,65835
C	-4,14429	-1,55329	0,43706
H	-3,45018	1,690442	1,150372
H	-1,81535	-0,82977	-1,9325
C	-1,60488	1,622189	-0,92595
C	-1,29675	2,854582	-0,04368
H	-1,51898	2,657978	1,012839
C	-2,11586	4,046904	-0,52131
H	-1,79714	4,936328	0,035215
O	-1,06734	1,549788	-2,01133
O	0,04755	3,24556	-0,19943
C	1,024323	2,375035	0,1924
C	2,331018	2,737186	-0,14635
C	0,787172	1,194776	0,898675
C	3,390274	1,91275	0,205454
C	1,865348	0,382712	1,252849
C	3,170336	0,721957	0,908622
H	4,403765	2,18226	-0,07971
H	1,678323	-0,54792	1,781669

C	4,313675	-0,22719	1,189102
H	4,047863	-0,86793	2,044676
C	4,547025	-1,14714	-0,0179
H	4,789072	-0,5217	-0,89068
C	5,691971	-2,11647	0,202861
H	6,578482	-1,5659	0,53725
H	5,391928	-2,834	0,980098
O	5,537464	0,449194	1,432246
H	5,398334	1,096327	2,133466
O	3,360674	-1,88109	-0,23867
O	5,921709	-2,76936	-1,03559
H	6,56796	-3,47099	-0,91195
C	2,717382	-1,60258	-1,46672
H	2,415035	-0,54804	-1,52964
H	3,371875	-1,85156	-2,31078
H	1,824287	-2,22917	-1,50429
O	-3,24832	-2,92277	-1,33203
O	-4,89633	-2,62613	0,77218
C	-2,59424	-3,97944	-0,63572
H	-1,54383	-3,72169	-0,45602
H	-3,09504	-4,19134	0,3136
H	-2,6501	-4,85403	-1,28391
C	-5,82084	-2,48024	1,833632
H	-6,55561	-1,69922	1,608644
H	-6,32601	-3,44076	1,923666
H	-5,3085	-2,24444	2,773365
H	-1,91214	4,195079	-1,58876
O	-3,4744	3,732462	-0,27513
H	-4,04252	4,356809	-0,73661
H	-0,21714	0,887571	1,17027
H	2,486175	3,65684	-0,70025
H	-4,86592	-0,15685	1,915665

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES

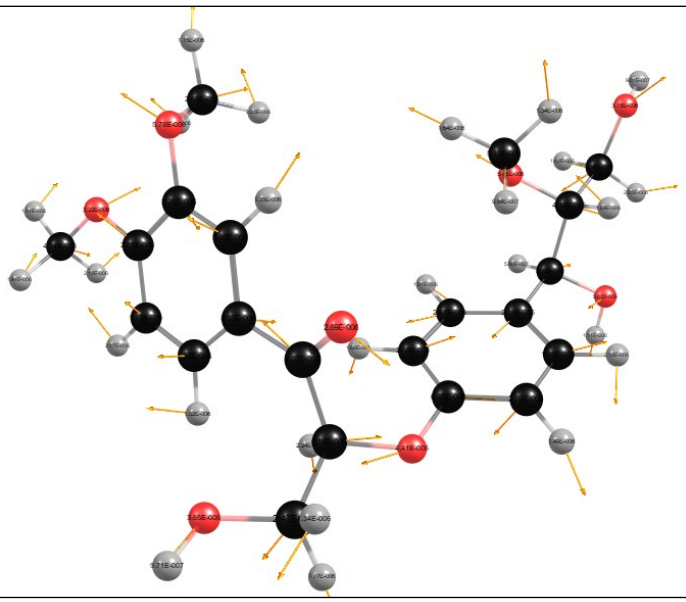


Table S32: Atomic coordinates and details of the optimized structure of the HS model calculated with M062-X functional

MODEL	HS	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000026	**RMS FORCE**	0.000005
MAXIMUM DISPLACEMENT	0.001375	**RMS DISPLACEMENT**	0.000288
PREDICTED ENERGY CHANGE (Hartree)	$-2.13.10^{-8}$	**NUMBER OF STEPS**	16
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-5,71749	1,426747	-0,28992
C	4,484338	-1,25776	0,341132
C	4,099249	-0,02739	0,867966
C	4,988371	1,050261	0,771064
C	6,220109	0,89849	0,147186
C	6,589765	-0,33962	-0,38992
H	3,808887	-2,10732	0,413817
H	4,703497	2,005758	1,199041
C	2,7249	0,145547	1,469271
H	2,478924	-0,73811	2,077729
C	1,639792	0,255084	0,38739
H	1,550281	-0,69936	-0,14589
C	1,869454	1,379305	-0,62633
H	0,908666	1,642248	-1,07664
O	2,716374	1,307139	2,272926
H	1,792934	1,488127	2,497318
O	0,444378	0,508554	1,14538
C	-0,73926	0,330737	0,486903
C	-1,51508	1,445273	0,144929
C	-1,21439	-0,95901	0,213174
C	-2,75661	1,272145	-0,47487
C	-2,44593	-1,13295	-0,42227
C	-3,2094	-0,01643	-0,75823
H	-3,37955	2,119312	-0,73658
H	-2,83711	-2,12133	-0,63107
O	-0,40032	-1,97353	0,604924
O	-0,97156	2,648907	0,455564
C	-0,85872	-3,29508	0,392643
H	-0,98765	-3,50194	-0,67587
H	-0,0879	-3,9481	0,800234
H	-1,80484	-3,47207	0,916631
C	-1,71724	3,805858	0,13163
H	-1,11298	4,651152	0,458352
H	-1,89062	3,875415	-0,94855
H	-2,67861	3,817129	0,657698
C	-4,57938	-0,2076	-1,3802

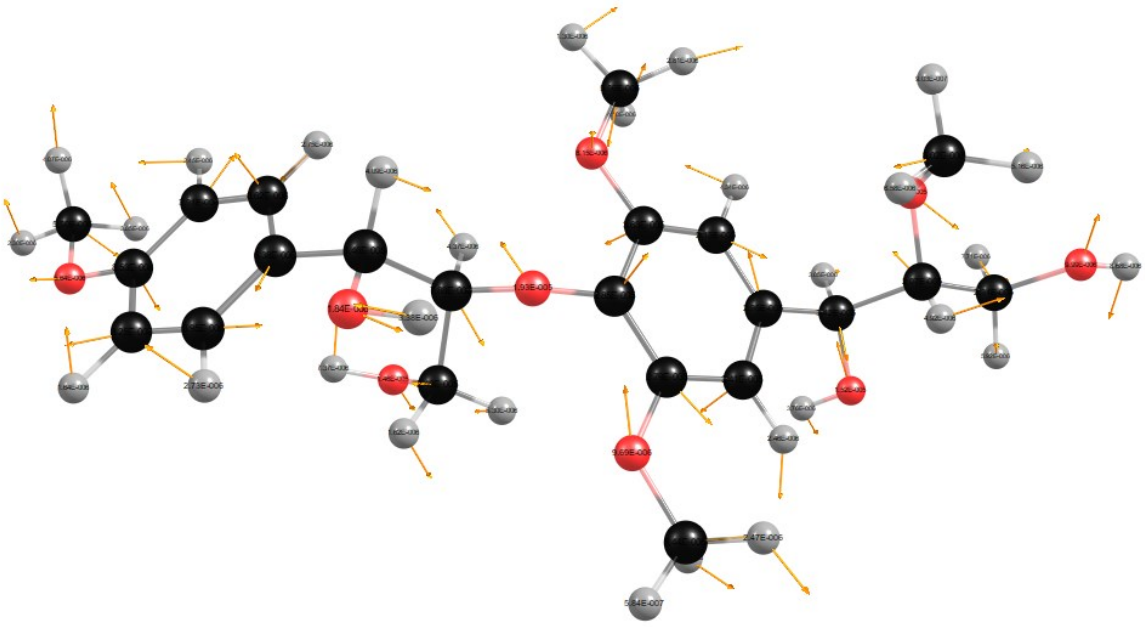
H	-4,58481	-1,14785	-1,95272
C	-5,64931	-0,33524	-0,2885
H	-5,58481	0,545273	0,36908
C	-7,05547	-0,41069	-0,85517
H	-7,24163	0,456742	-1,49762
H	-7,14225	-1,33088	-1,45062
O	-4,95903	0,88071	-2,2052
H	-4,27915	1,01077	-2,87682
O	-5,36086	-1,51631	0,429553
O	-7,9393	-0,43617	0,255677
H	-8,84137	-0,55625	-0,05623
C	-5,32875	-1,35223	1,833431
H	-4,52793	-0,6579	2,124889
H	-6,29238	-0,98698	2,205252
H	-5,12108	-2,33473	2,261389
O	7,813448	-0,38991	-0,98121
C	8,222733	-1,61974	-1,54221
H	7,538804	-1,93945	-2,33742
H	9,211993	-1,44444	-1,96319
H	8,285307	-2,40303	-0,77739
H	2,253559	2,270357	-0,11182
O	2,709935	0,977358	-1,691
H	3,61701	0,913098	-1,36691
H	5,981456	-2,39766	-0,6912
H	6,918711	1,724762	0,067623
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S33: Atomic coordinates and details of the optimized structure of the HSOX model calculated with M062-X functional

MODEL	HSOX	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.00008	**RMS FORCE**	0.000002

MAXIMUM DISPLACEMENT	0.001709	**RMS DISPLACEMENT**	0.000288
PREDICTED ENERGY CHANGE (Hartree)	$-5.37.10^{-9}$	**NUMBER OF STEPS**	58
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-4,55647	-1,1242	1,145947
C	3,719812	-0,06895	-0,78004
C	3,522548	0,261247	0,560178
C	4,191155	-0,48297	1,546112
C	5,011366	-1,54046	1,200685
C	5,197618	-1,86814	-0,15165
H	3,24298	0,507718	-1,56568
H	4,037878	-0,21423	2,586617
C	2,622154	1,3616	1,00851
C	1,634779	2,018906	0,030707
H	1,541632	1,447982	-0,89717
C	2,102127	3,441667	-0,27262
H	1,417509	3,894892	-0,99315
O	2,673871	1,789684	2,144597
O	0,361622	2,137124	0,65622
C	-0,63801	1,347983	0,168765
C	-1,82507	1,954595	-0,26543
C	-0,52155	-0,0478	0,136251
C	-2,88666	1,164998	-0,71846
C	-1,56958	-0,83558	-0,34515
C	-2,75043	-0,22339	-0,75889
H	-3,82105	1,610064	-1,04024
H	-1,49652	-1,91685	-0,35705
O	0,662095	-0,53224	0,593727
O	-1,84375	3,308548	-0,21114
C	0,912279	-1,91912	0,459197
H	0,834094	-2,22929	-0,58945
H	1,933201	-2,07319	0,811127
H	0,215988	-2,50332	1,0709
C	-3,04034	3,959798	-0,58683
H	-2,85482	5,024737	-0,45275
H	-3,28898	3,760644	-1,63597
H	-3,87621	3,650397	0,051082
C	-3,93067	-1,0759	-1,17826
H	-3,55838	-2,0461	-1,54267
C	-4,84534	-1,35519	0,022941
H	-5,20994	-0,39289	0,413361
C	-6,04762	-2,20181	-0,34839
H	-6,54778	-1,76715	-1,22113
H	-5,69407	-3,21321	-0,59503
O	-4,73256	-0,44655	-2,16466

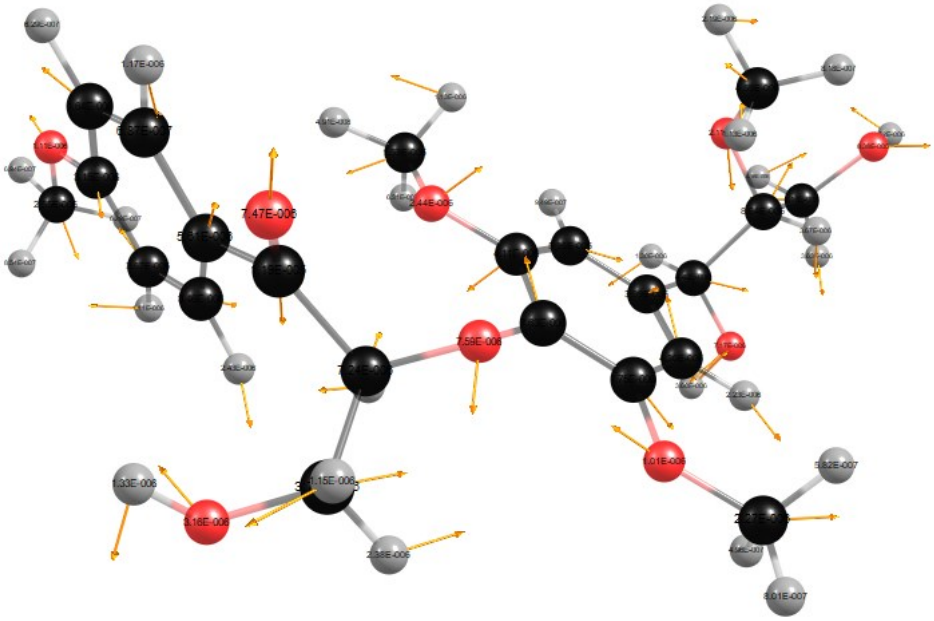
H	-4,16804	-0,18851	-2,90274
O	-4,08863	-2,03968	0,998788
O	-6,90087	-2,21874	0,784543
H	-7,6091	-2,854	0,642857
C	-3,88828	-1,31772	2,197405
H	-3,34326	-0,38171	2,012049
H	-4,8479	-1,09816	2,680932
H	-3,28995	-1,95292	2,852922
O	6,018776	-2,91759	-0,39435
C	6,255134	-3,27911	-1,74133
H	6,723485	-2,45663	-2,29374
H	6,93479	-4,12935	-1,70858
H	5,324364	-3,57325	-2,23991
H	2,065504	4,019103	0,658258
O	3,394384	3,437597	-0,85394
H	4,058058	3,388565	-0,1564
H	4,699715	-1,34916	-2,19564
H	5,52598	-2,13209	1,950334
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S34: Atomic coordinates and details of the optimized structure of the HG model calculated with M062-X functional

MODEL	HG	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000013	**RMS FORCE**	0.000003
MAXIMUM DISPLACEMENT	0.000776	**RMS DISPLACEMENT**	0.000144
PREDICTED ENERGY CHANGE (Hartree)	$-9.87.10^{-9}$	**NUMBER OF STEPS**	16
ATOM	Coordinates (Angstroms)		

	X	Y	Z
C	-5,28037	1,378383	-0,59998
C	-4,05275	1,132885	0,016113
C	-3,85752	0,020622	0,831342
C	-4,93215	-0,85222	1,042665
C	-6,16092	-0,62185	0,437096
C	-6,34065	0,49226	-0,39032
H	-3,22933	1,823609	-0,15365
H	-4,79333	-1,70906	1,693812
C	-2,49314	-0,26203	1,411478
H	-2,04309	0,675894	1,768455
C	-1,53516	-0,83526	0,35711
H	-1,3187	-0,0703	-0,39687
H	-2,0307	-2,10092	-0,34535
H	-1,15966	-2,6141	-0,76393
O	-2,62746	-1,17741	2,480236
C	-1,73346	-1,41277	2,762834
O	-0,34206	-1,16511	1,093323
C	0,845187	-0,91281	0,458234
C	1,685657	-1,95785	0,111907
C	1,241725	0,41813	0,215977
C	2,923674	-1,70404	-0,48468
C	2,464664	0,666947	-0,39872
C	3,310014	-0,39393	-0,74888
H	3,587639	-2,52425	-0,7387
H	2,798321	1,681356	-0,58584
O	0,36622	1,378059	0,619956
C	0,756573	2,727291	0,44896
H	0,885698	2,969771	-0,61213
H	-0,05096	3,328557	0,865587
H	1,687454	2,937842	0,98772
C	4,665479	-0,0944	-1,3586
H	4,595237	0,828646	-1,95529
C	5,705663	0,157414	-0,25976
H	5,707793	-0,7049	0,424487
C	7,106007	0,337603	-0,81788
H	7,376903	-0,53694	-1,41903
H	7,115244	1,234242	-1,4543
O	5,153297	-1,16248	-2,15084
H	4,488563	-1,38678	-2,81269
O	5,302449	1,329778	0,417599
O	7,972755	0,494247	0,295738
H	8,869128	0,649977	-0,01693
C	5,323401	1,226006	1,827925
H	4,611307	0,461873	2,170287
H	6,329363	0,98485	2,187264
H	5,018822	2,198284	2,220028

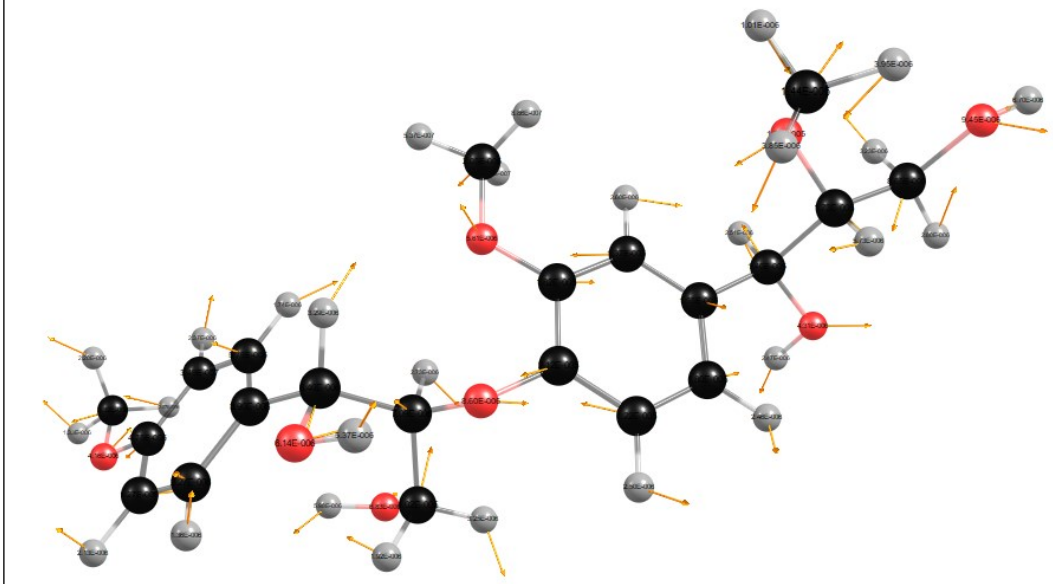
O	-7,577	0,63258	-0,93826
C	-7,79878	1,739217	-1,78756
H	-7,13187	1,710692	-2,65745
H	-8,83295	1,660782	-2,12047
H	-7,65912	2,685038	-1,25066
H	-2,50183	-2,7704	0,387444
O	-2,88712	-1,82106	-1,43393
H	-3,74341	-1,53198	-1,09439
H	1,358711	-2,97016	0,327791
H	-5,39467	2,251751	-1,23049
H	-7,00195	-1,28902	0,594073
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S35: Atomic coordinates and details of the optimized structure of the HGOX model calculated with M062-X functional

MODEL	HGOX	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000010	**RMS FORCE**	0.000002
MAXIMUM DISPLACEMENT	0.001305	**RMS DISPLACEMENT**	0.000263
PREDICTED ENERGY CHANGE (Hartree)	$-5.34.10^{-9}$	**NUMBER OF STEPS**	34
ATOM	Coordinates (Angstroms)		
	X	Y	Z
C	-3.807420	-1,900357	0,137444
C	-3,17484	-0,65876	0,175108
C	-3,83555	0,491638	-0,26051
C	-5,15167	0,384006	-0,74187
C	-5,78537	-0,84112	-0,79272
C	-5,11381	-1,99272	-0,35151

H	-2,15663	-0,59513	0,544556
H	-5,65887	1,284884	-1,07193
C	-3,21997	1,838126	-0,19771
C	-1,74412	1,98403	0,198602
H	-1,62806	1,646337	1,238368
C	-1,28945	3,438541	0,088566
H	-0,2209	3,495403	0,313351
O	-3,87242	2,844539	-0,42991
O	-1,00144	1,140015	-0,6873
C	0,34576	1,035557	-0,43701
C	1,248859	1,531946	-1,36392
C	0,818656	0,372281	0,711713
C	2,62373	1,394457	-1,16306
C	2,189726	0,260436	0,924176
C	3,096536	0,768843	-0,01313
H	3,325769	1,771616	-1,89992
H	2,57716	-0,25049	1,798267
O	-0,13329	-0,12921	1,547524
C	0,305543	-0,81553	2,705708
H	0,877894	-0,15135	3,362632
H	-0,59762	-1,14511	3,218357
H	0,91777	-1,68414	2,438014
C	4,583851	0,57614	0,208971
H	4,789562	0,581322	1,290938
C	5,036194	-0,78735	-0,32894
H	4,73238	-0,86616	-1,38412
C	6,54056	-0,97292	-0,24064
H	7,042564	-0,15909	-0,77464
H	6,833351	-0,94846	0,818961
O	5,36331	1,55773	-0,45038
H	5,067446	2,431253	-0,16825
O	4,381914	-1,76617	0,45196
O	6,832134	-2,23566	-0,82056
H	7,776136	-2,40802	-0,75212
C	3,795267	-2,8136	-0,29585
H	3,003643	-2,4243	-0,95158
H	4,548778	-3,33755	-0,89307
H	3,353907	-3,50552	0,424171
O	-5,81419	-3,14755	-0,43828
C	-5,18635	-4,3415	-0,01268
H	-4,92367	-4,29122	1,050159
H	-5,91477	-5,13552	-0,17043
H	-4,28698	-4,546	-0,60448
H	-1,44617	3,786517	-0,94136
O	-1,95283	4,252159	1,027118
H	-2,87354	4,310245	0,737789
H	-3,27461	-2,77824	0,481615

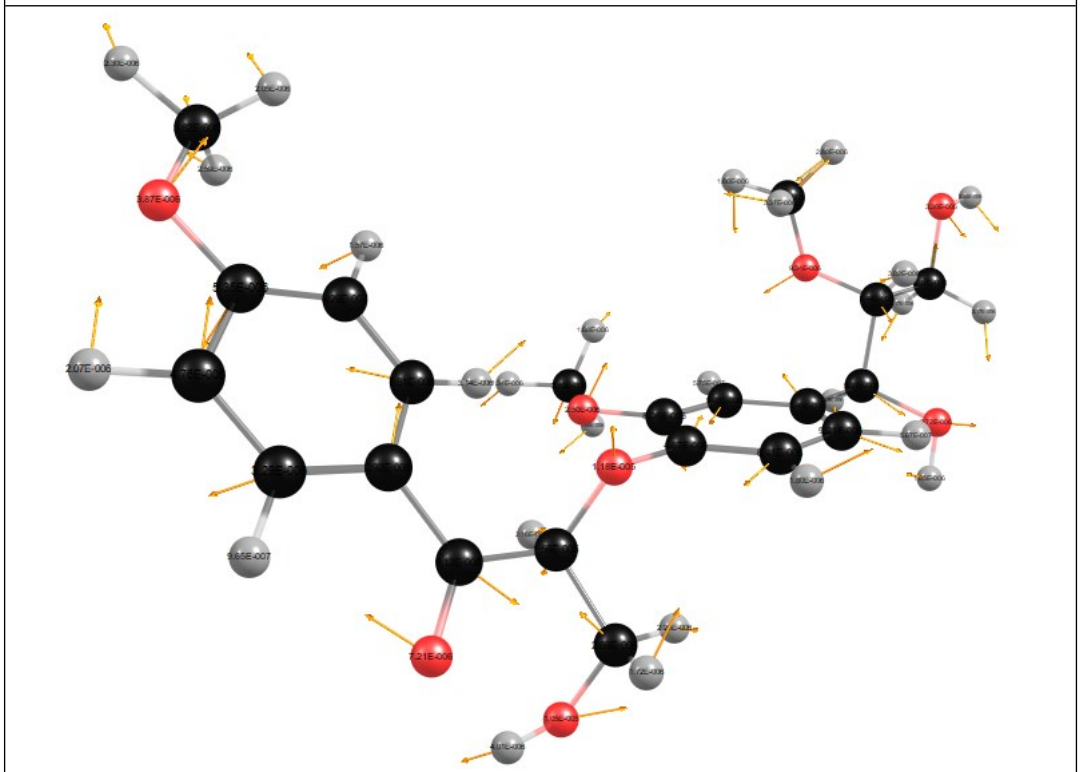
H	-6,7985	-0,94582	-1,1655
H	0,851605	2,024824	-2,24571
OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES			
			

Table S36: Atomic coordinates and details of the optimized structure of the HH model calculated with M062-X functional

MODEL	HH	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000001	**RMS FORCE**	0.000000
MAXIMUM DISPLACEMENT	0.000087	**RMS DISPLACEMENT**	0.000020
PREDICTED ENERGY CHANGE (Hartree)	$-2.02.10^{-11}$	**NUMBER OF STEPS**	1
Atom	Coordinates (Angstroms)		
	X	Y	Z
C	5,19078	-1,58061	0,535475
C	4,035899	0,935203	-0,97977
C	3,854441	-0,4345	-0,80359
C	4,87056	-1,17057	-0,18118
C	6,026319	-0,54387	0,265497
C	6,191425	0,83573	0,094652
H	3,261997	1,522088	-1,46969
H	4,748057	-2,24211	-0,06196
C	2,553773	-1,08574	-1,21063
H	2,220323	-0,66654	-2,17192
C	1,453114	-0,79653	-0,17664
H	1,237248	0,280113	-0,18383
C	1,832232	-1,22387	1,248792

H	0,925081	-1,49491	1,794796
O	2,751315	-2,47848	-1,3286
H	1,88454	-2,88035	-1,47377
O	0,325063	-1,53133	-0,64339
C	-0,92277	-1,18787	-0,19952
C	-1,98119	-1,92651	-0,73684
C	-1,17787	-0,17136	0,723706
C	-3,28629	-1,64478	-0,35802
C	-2,49683	0,094157	1,095412
C	-3,56132	-0,63042	0,566489
H	-4,10823	-2,21412	-0,78377
H	-2,69655	0,891204	1,806176
C	-4,99016	-0,29562	0,936276
H	-5,00057	0,197087	1,920907
C	-5,59137	0,691956	-0,07018
H	-5,49756	0,263271	-1,08027
C	-7,05788	0,97617	0,199867
H	-7,6178	0,034821	0,217242
H	-7,14159	1,468654	1,179268
O	-5,83022	-1,43959	0,941091
H	-5,44074	-2,10571	1,519412
O	-4,84065	1,882661	0,037977
O	-7,50907	1,831391	-0,84042
H	-8,41961	2,089784	-0,66836
C	-4,43612	2,433398	-1,19956
H	-3,76618	1,742006	-1,73027
H	-5,30354	2,66503	-1,82698
H	-3,89191	3,351757	-0,97245
O	7,35379	1,357445	0,565353
C	7,560684	2,747526	0,416755
H	6,789624	3,320744	0,944897
H	8,534191	2,955508	0,858628
H	7,570856	3,035165	-0,64112
H	2,474339	-2,1132	1,205502
O	2,438166	-0,17077	1,970608
H	3,340012	-0,04851	1,646486
H	-0,37376	0,404099	1,168889
H	-1,75787	-2,7101	-1,45346
H	5,296092	2,64774	-0,68831
H	6,821806	-1,10293	0,746695
H	5,19078	-1,58061	0,535475

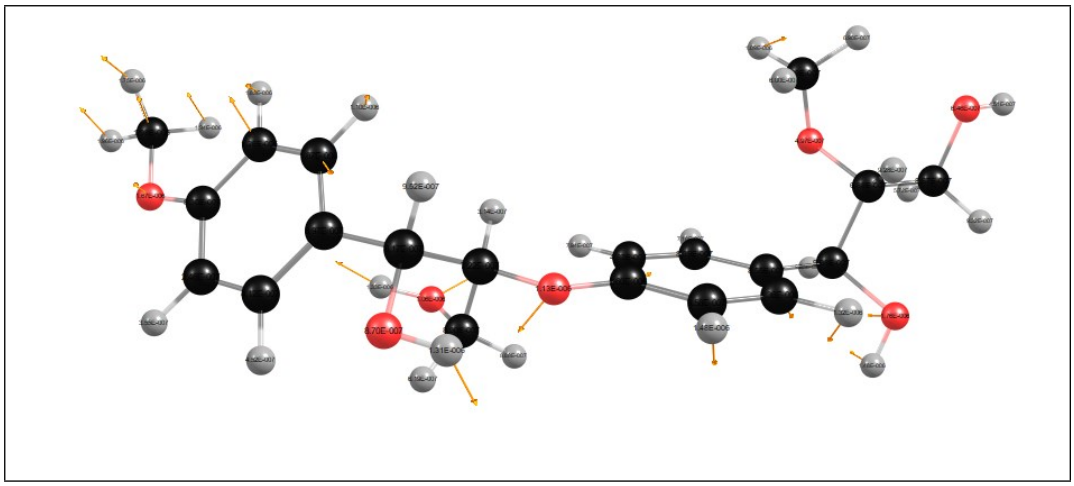
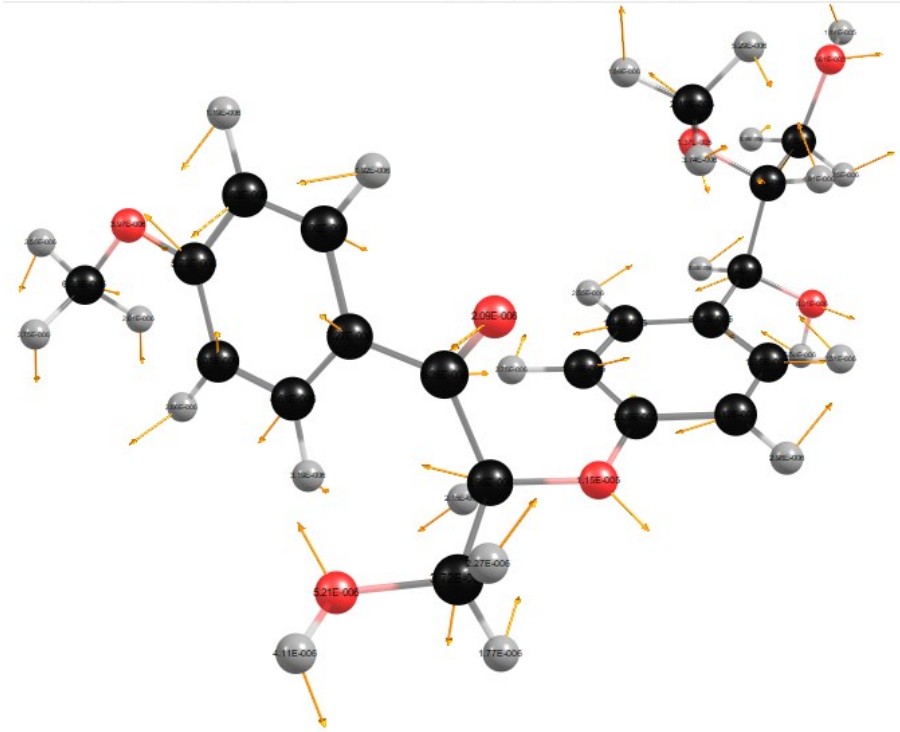


Table S37: Atomic coordinates and details of the optimized structure of the HHOX model calculated with M062-X functional

MODEL	HHOX	**FUNCTIONAL**	M062-X
MAXIMUM FORCE	0.000020	**RMS FORCE**	0.000004
MAXIMUM DISPLACEMENT	0.001546	**RMS DISPLACEMENT**	0.000406
PREDICTED ENERGY CHANGE (Hartree)	$-2.72.10^{-08}$	**NUMBER OF STEPS**	31
Atom	Coordinates (Angstroms)		
	X	Y	Z
C	4.445358	-1.053011	-0,872576
C	3,673752	0,062871	-0,55007
C	2,816916	0,047752	0,551616
C	2,742426	-1,11385	1,339419
C	3,493656	-2,22901	1,026235
C	4,350861	-2,20413	-0,08546
H	3,783911	0,961457	-1,14765
H	2,077192	-1,11446	2,197067
C	1,967519	1,204079	0,940056
C	1,741657	2,370185	-0,04981
H	1,933132	2,06074	-1,08532
C	2,654128	3,536406	0,31192
H	2,397866	4,390574	-0,3261
O	1,418433	1,260334	2,02129
O	0,435186	2,879987	0,075167
C	-0,6136	2,076635	-0,26971
C	-1,88462	2,609501	-0,03538
C	-0,4816	0,807677	-0,83538
C	-3,01427	1,871542	-0,3577
C	-1,62923	0,082971	-1,16131
C	-2,90095	0,59682	-0,9265
H	-4,00201	2,278696	-0,15828
H	-1,5262	-0,91349	-1,5822

O	-4,13414	-0,23878	-1,1883
H	-3,90031	-0,99373	-1,9554
C	-4,54844	-0,99173	0,083439
H	-4,75596	-0,25417	0,873731
C	-5,79332	-1,83398	-0,11799
H	-6,58478	-1,21959	-0,5618
H	-5,54429	-2,65913	-0,80049
O	-5,24925	0,545953	-1,5829
H	-4,98909	1,097403	-2,32995
O	-3,47773	-1,83569	0,451641
O	-6,16978	-2,32207	1,160093
H	-6,87137	-2,97235	1,060053
C	-2,8829	-1,52127	1,695025
H	-2,45715	-0,50828	1,688309
H	-3,61473	-1,6105	2,506997
H	-2,07855	-2,24228	1,851043
O	5,047025	-3,34196	-0,31437
C	5,928826	-3,37241	-1,42011
H	6,715218	-2,616	-1,31774
H	6,376203	-4,36526	-1,41904
H	5,387538	-3,21525	-2,36
H	2,469288	3,799768	1,360508
O	3,984252	3,1016	0,097034
H	4,599116	3,725296	0,495117
H	0,492047	0,366506	-1,02077
H	-1,9581	3,595302	0,411258
H	5,11143	-1,00962	-1,72536
H	3,442312	-3,13663	1,617844

OPTIMIZED STRUCTURE IMAGE WITH FORCE LINES



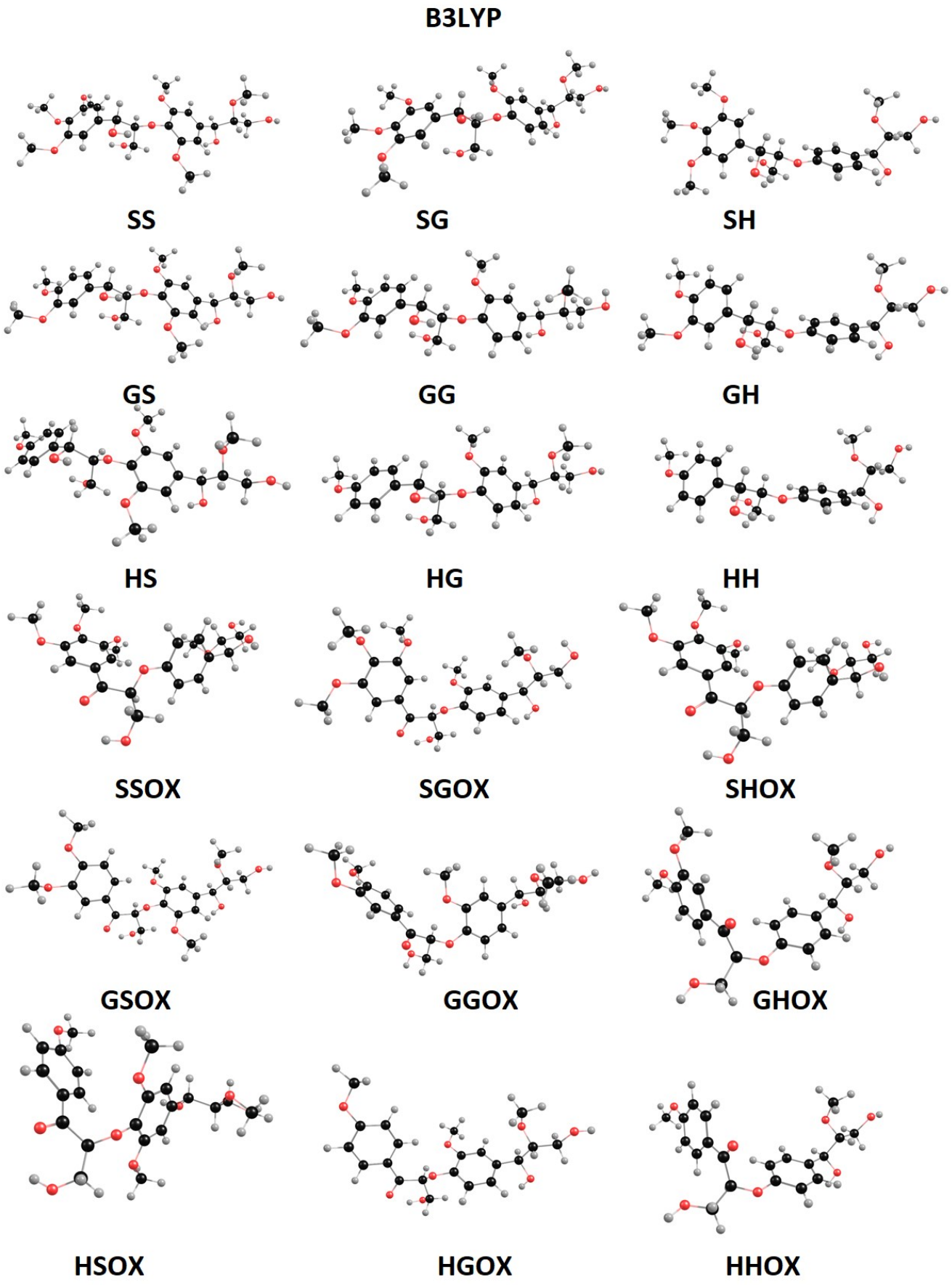


Fig. S1 Optimized structures images - B3LYP

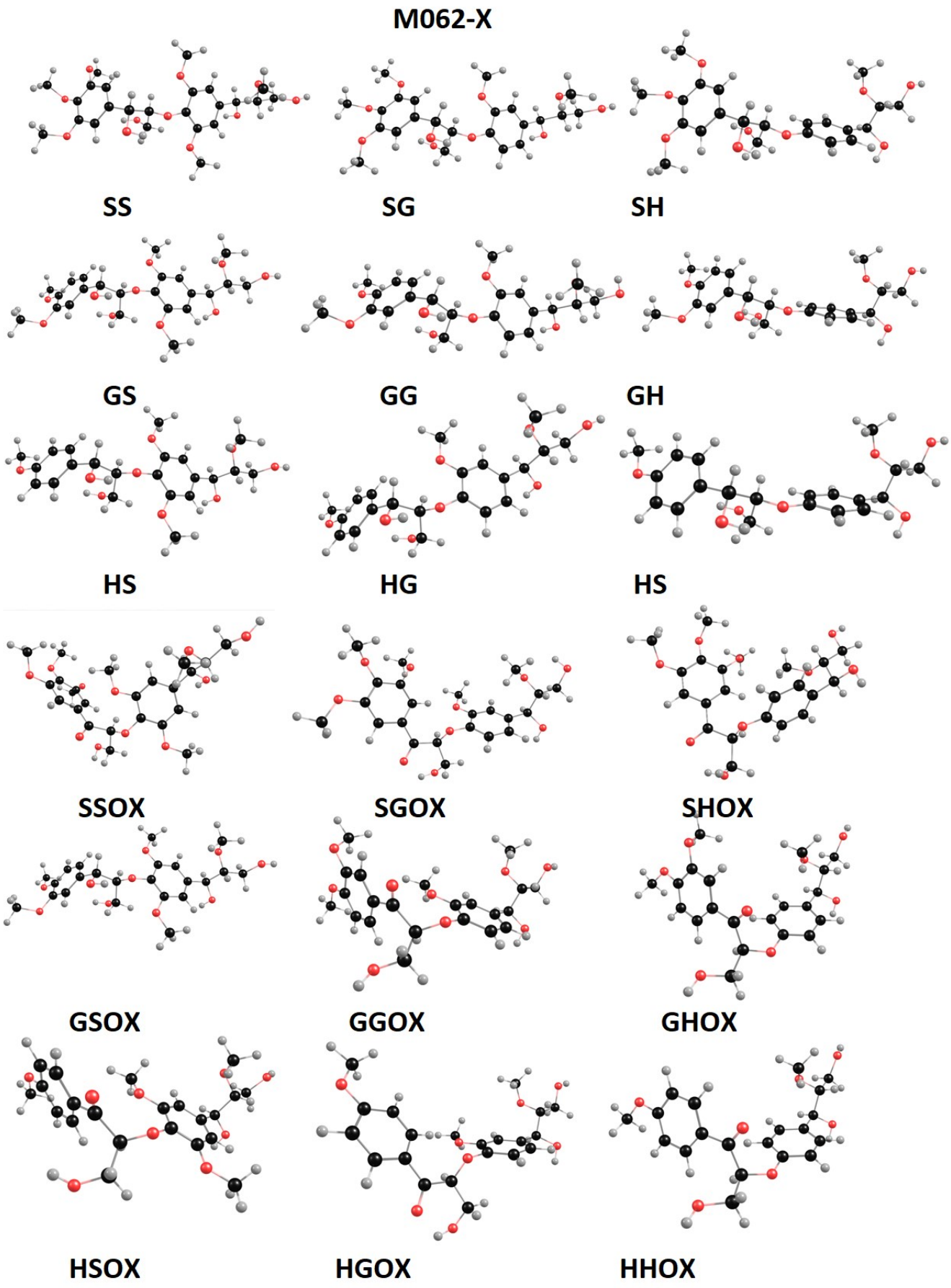


Fig. S2 Optimized structures images - M062-X