Electronic Supplementary Material (ESI) for RSC Advances.

- SUPPLEMENTARY INFORMATION -

Fluoxetine Scaffold to Design Tandem Molecular Antioxidants and Green Catalysts

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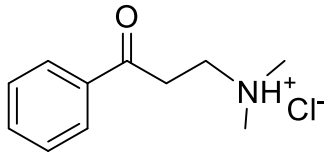
Chemistry

NMR and ESI-MS spectra

Compound 2



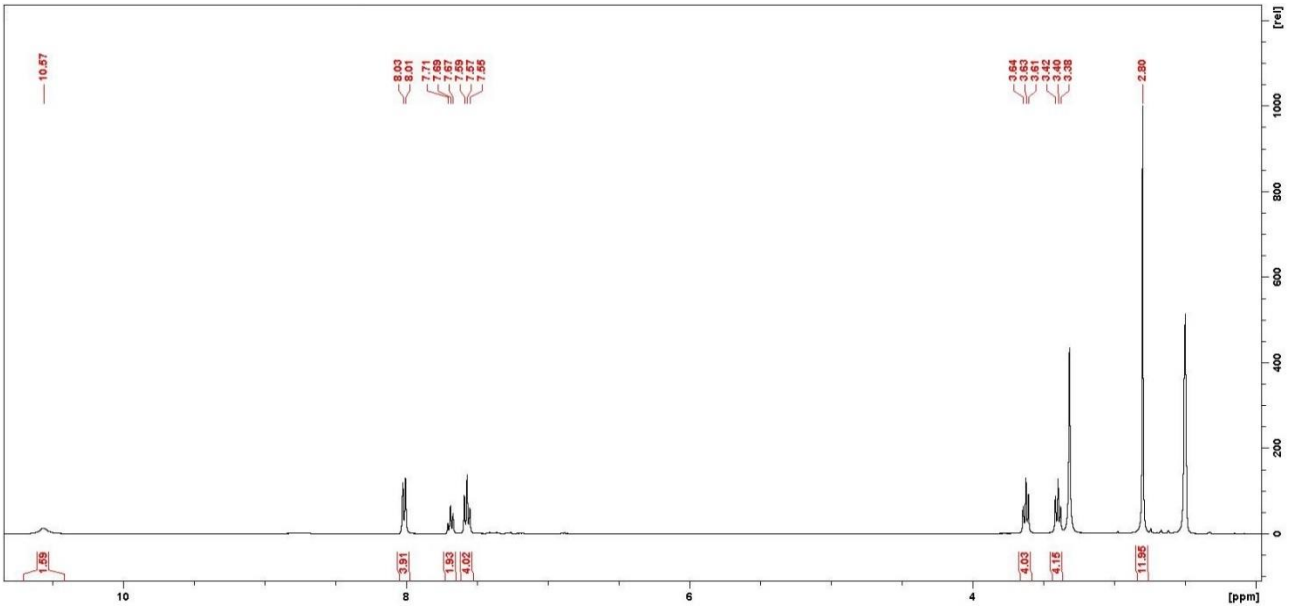


Figure S1. 1H-NMR spectrum of compound 2.

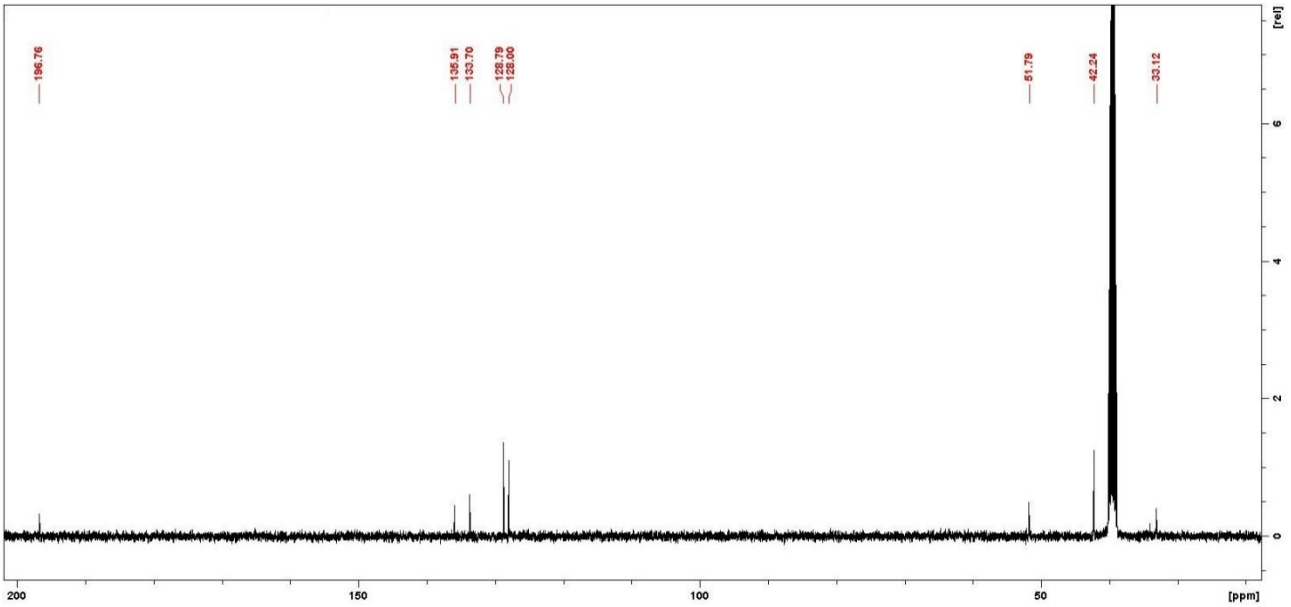


Figure S2. ^{13}C-NMR spectrum of compound 2.

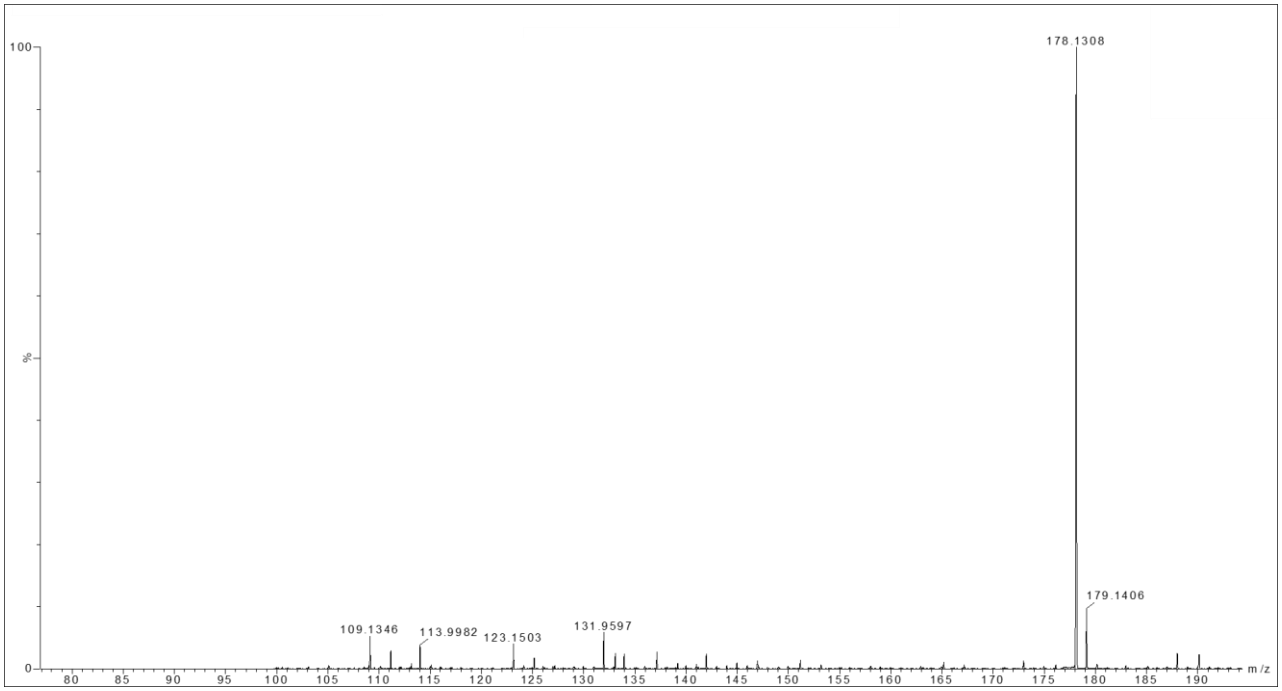
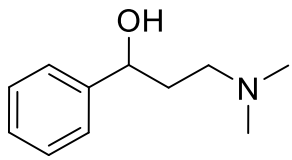


Figure S3. HRMS ESI spectrum of compound 2.

Compound 3



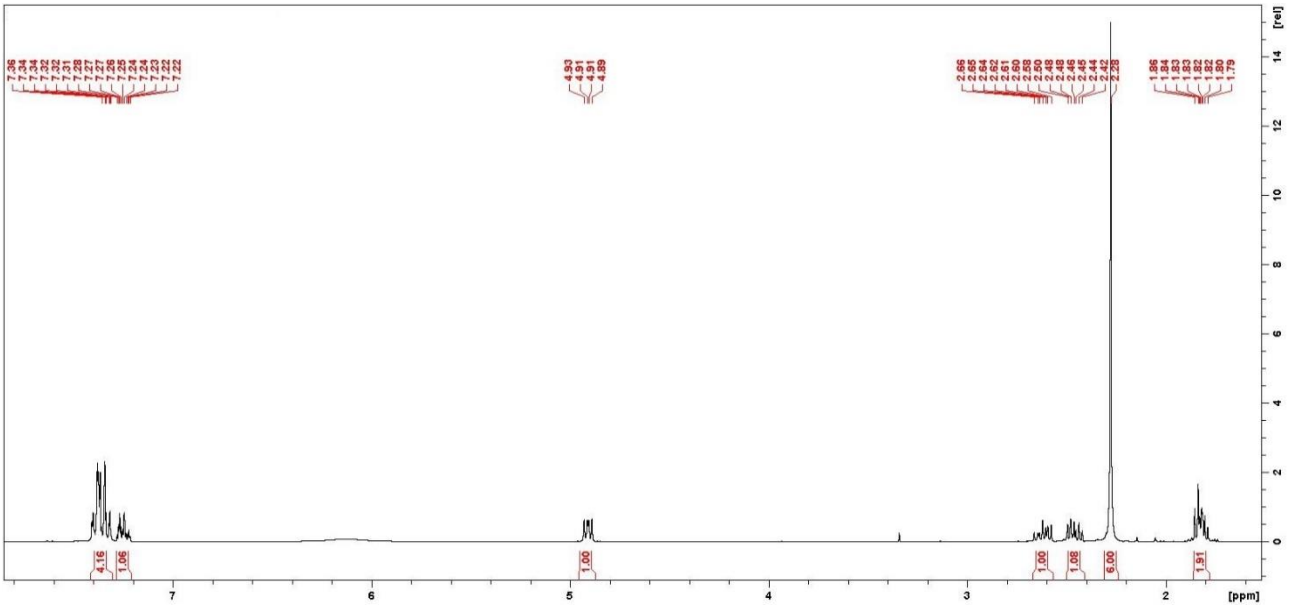


Figure S4. ^{1}H-NMR spectrum of compound 3.

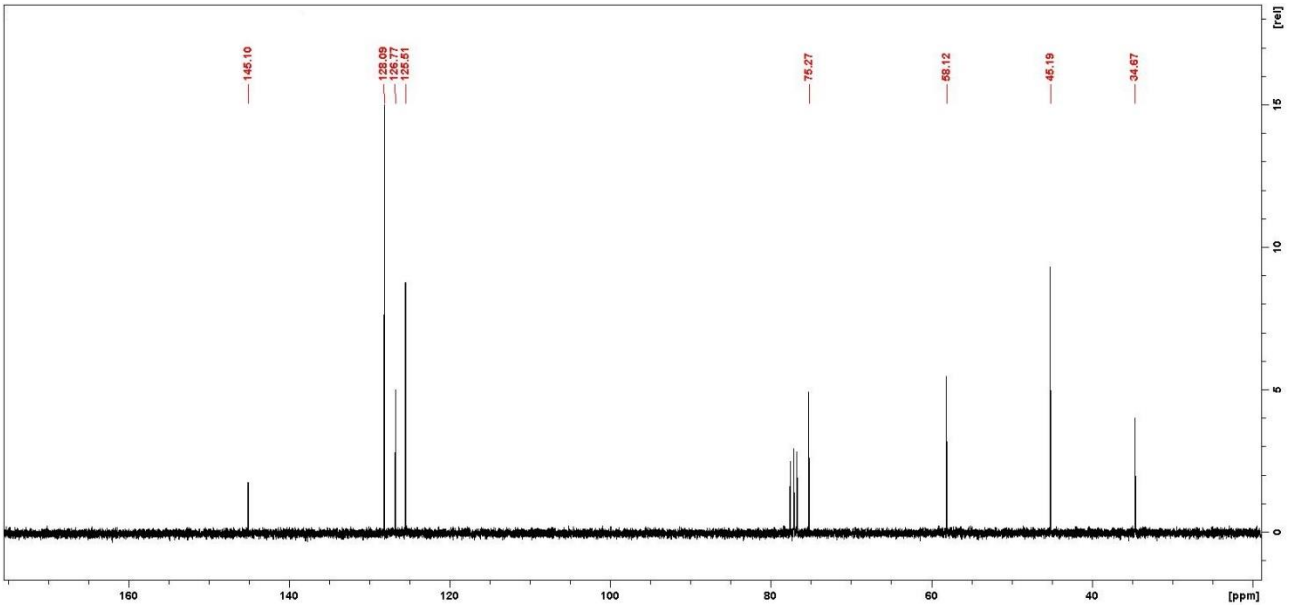


Figure S5. ^{13}C-NMR spectrum of compound 3.

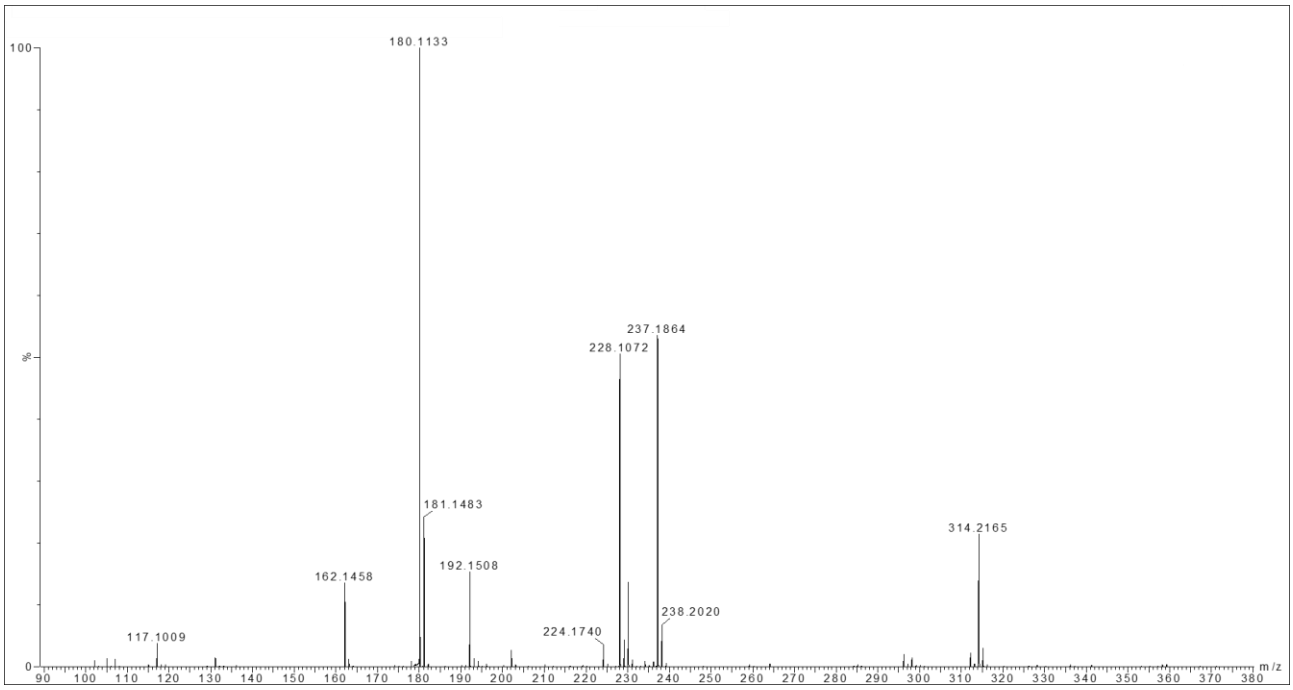
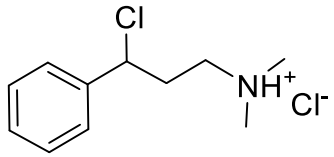


Figure S6. HRMS ESI spectrum of compound 3.

Compound 4



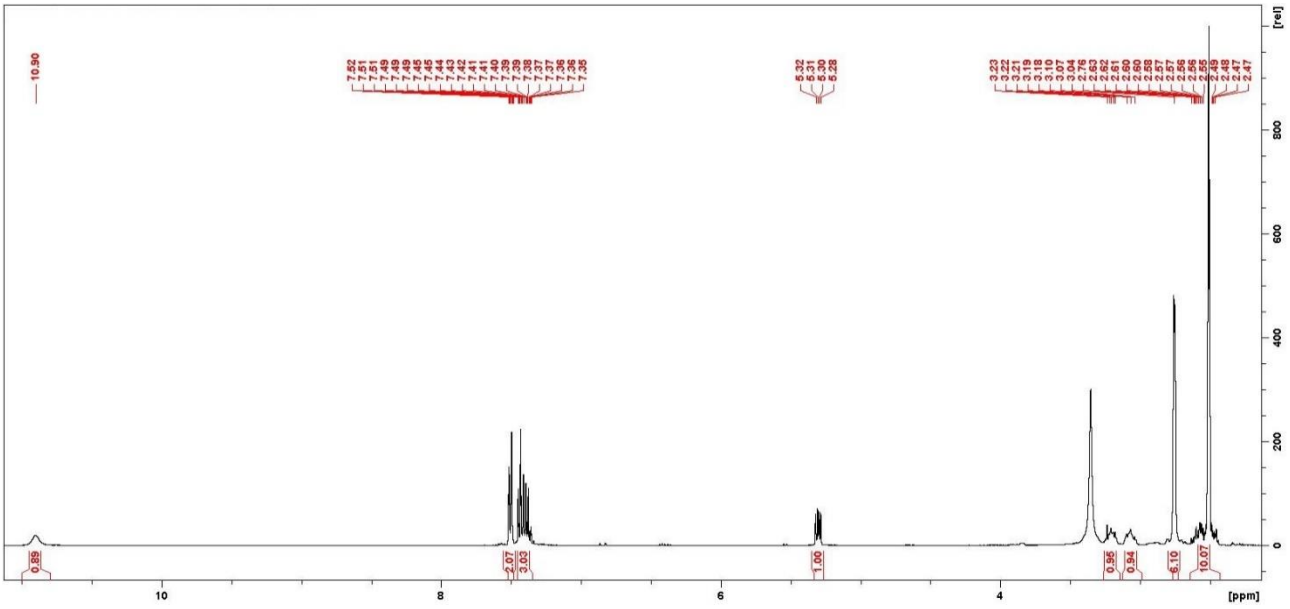


Figure S7. ^{1}H-NMR spectrum of compound 4.

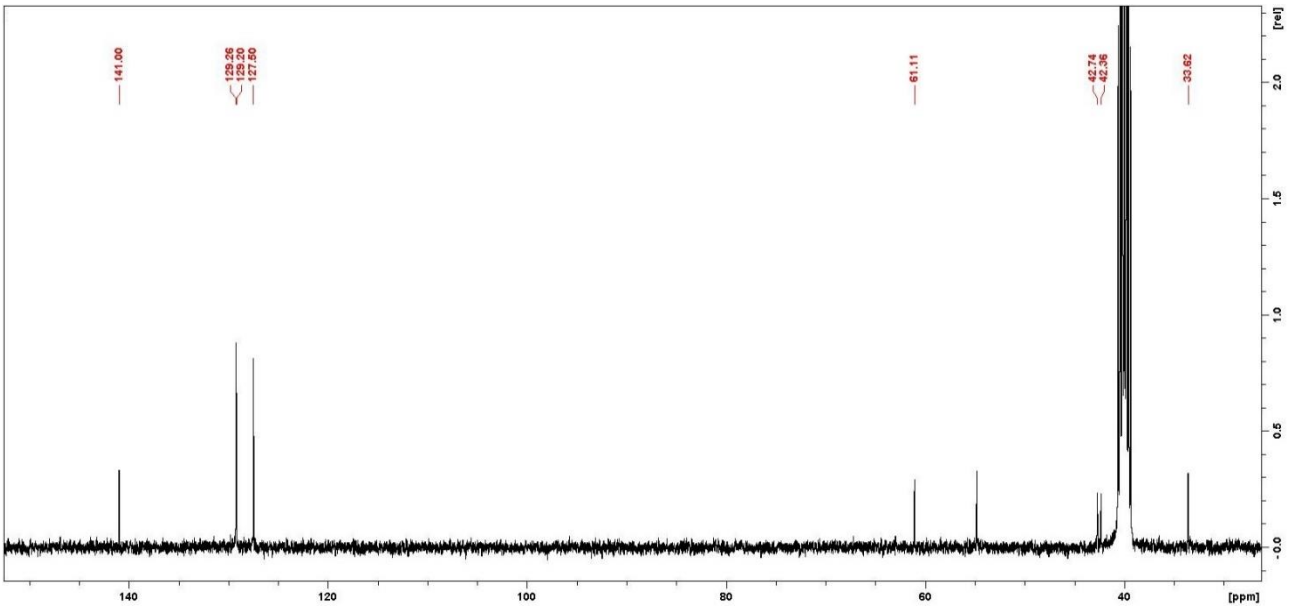


Figure S8. ^{13}C-NMR spectrum of compound 4.

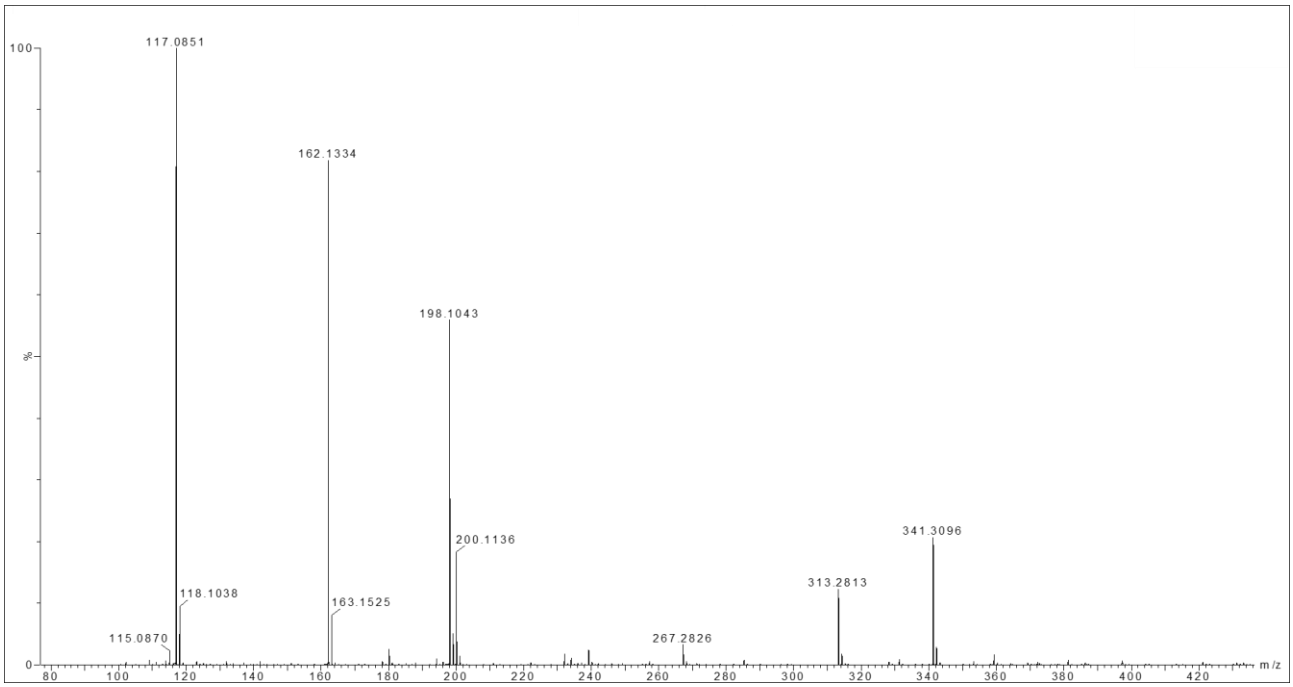
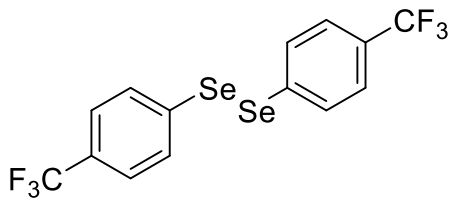


Figure S9. HRMS ESI spectrum of compound 4.

Compound 5



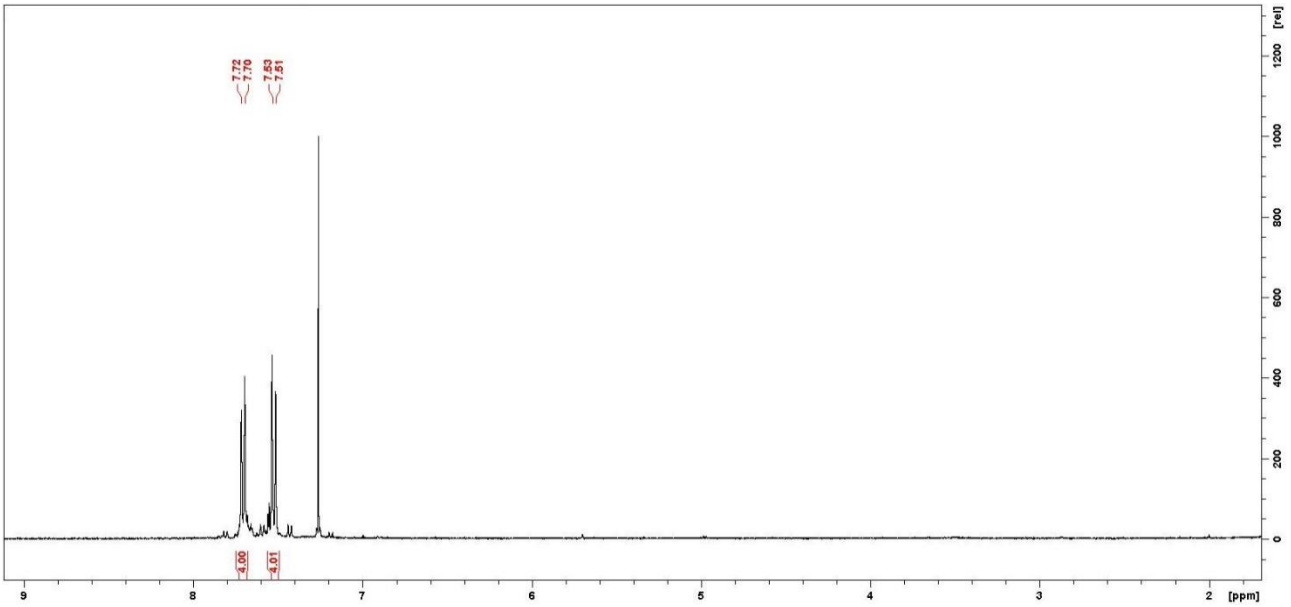


Figure S10. ^{1}H-NMR spectrum of compound 5.

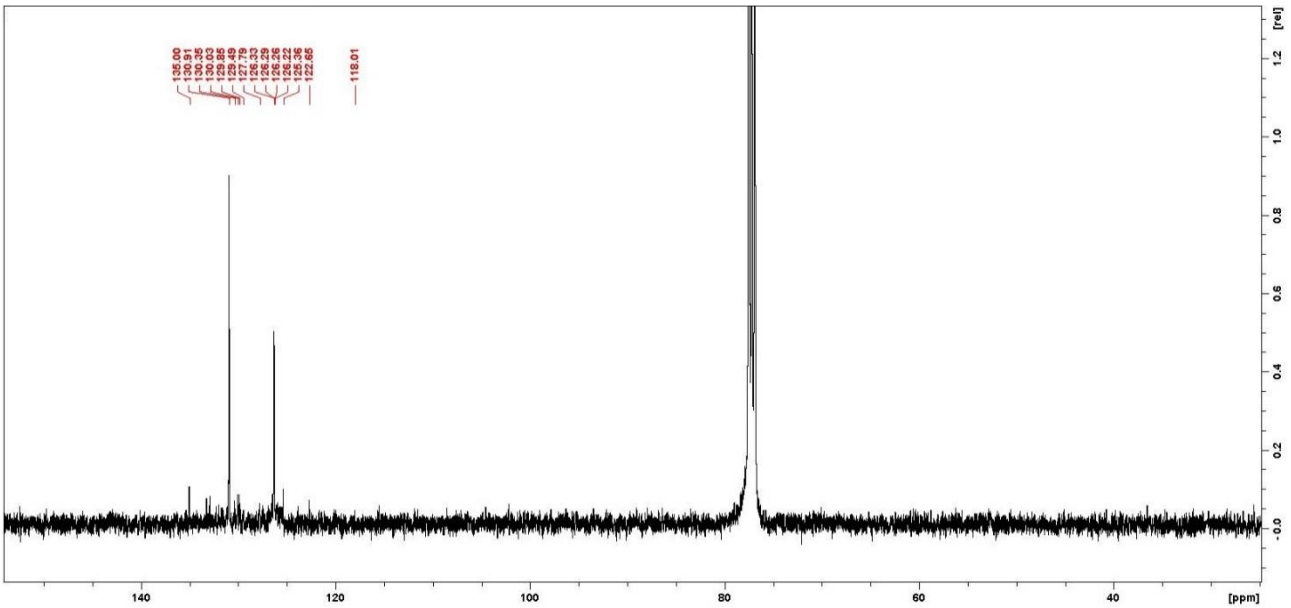


Figure S11. ^{13}C-NMR spectrum of compound 5.

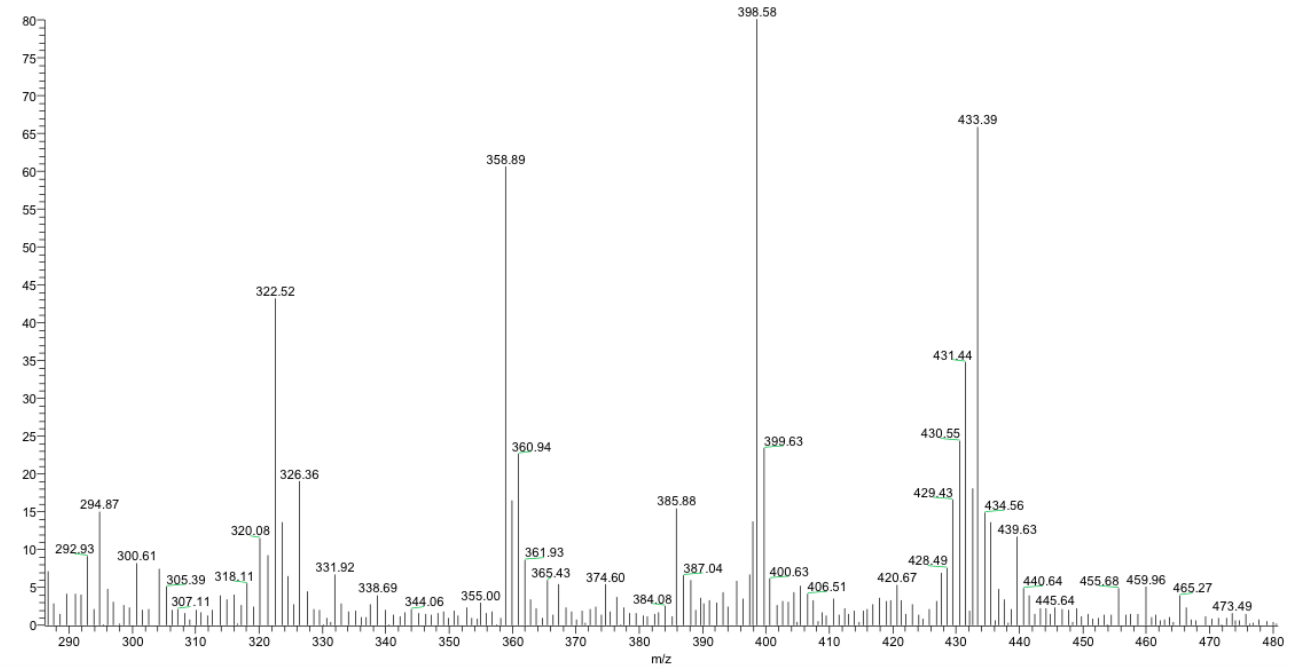
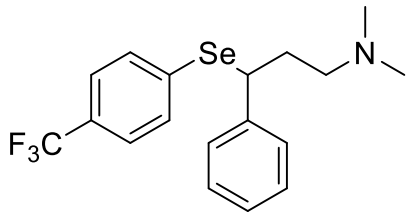


Figure S12. ESI-MS spectrum of compound 5.

Compound 1-CF_3



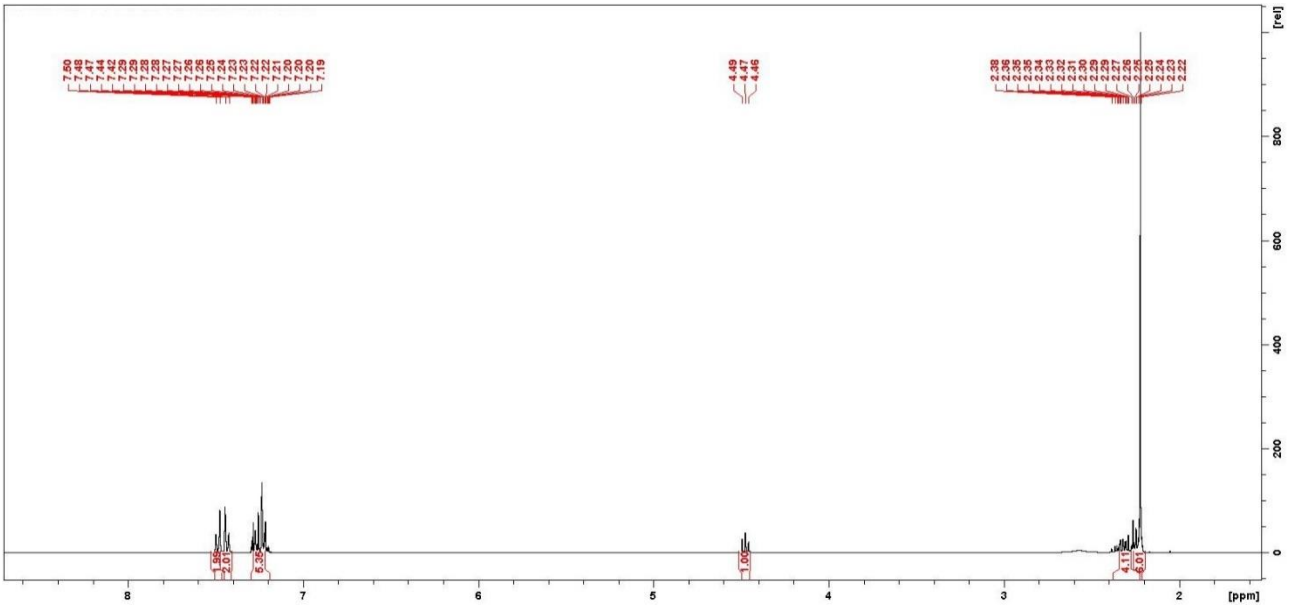


Figure S13. 1H-NMR spectrum of compound 1-CF3.

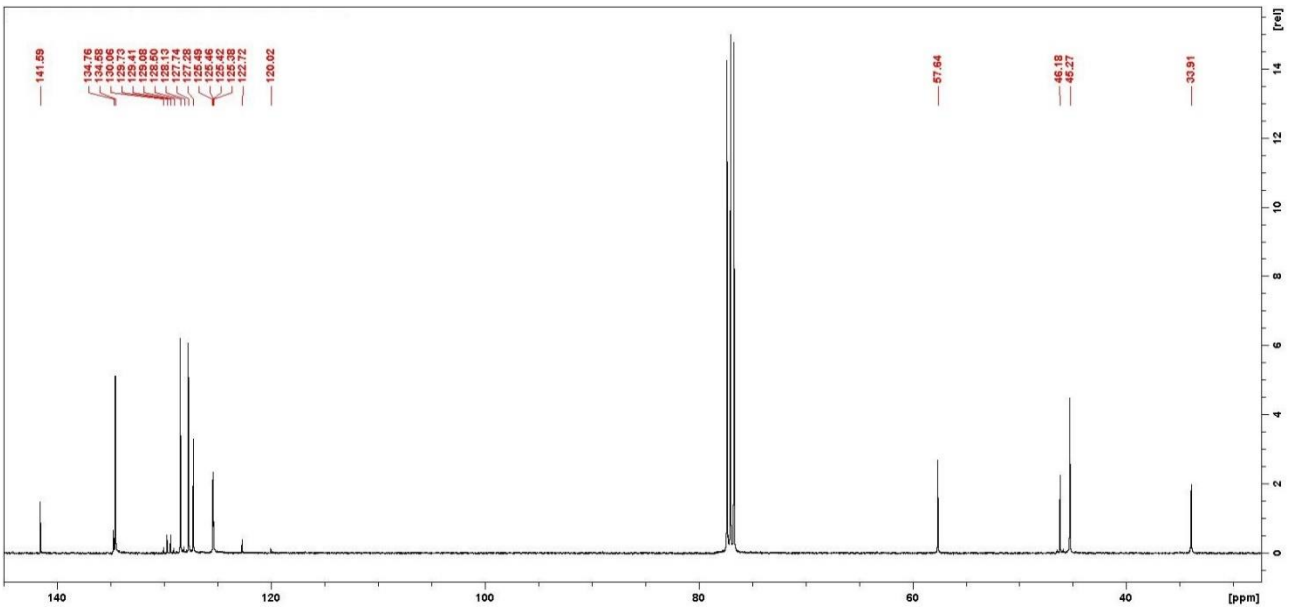


Figure S14. 13C-NMR spectrum of compound 1-CF3.

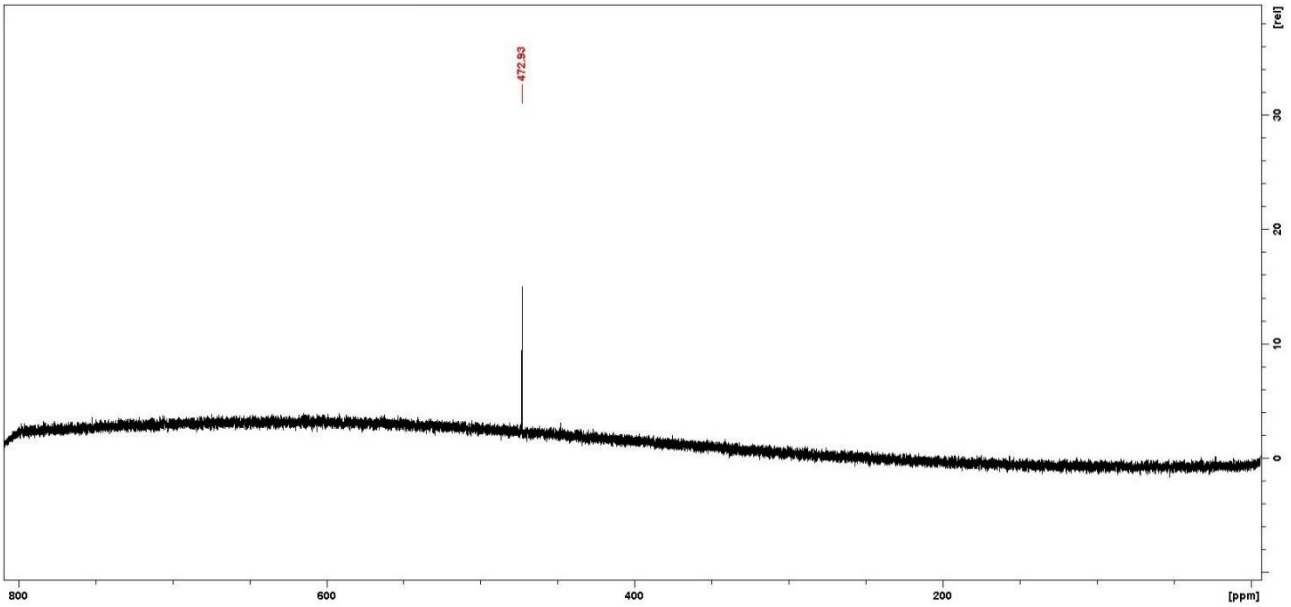


Figure S15. ^{77}Se-NMR spectrum of compound 1-CF_3.

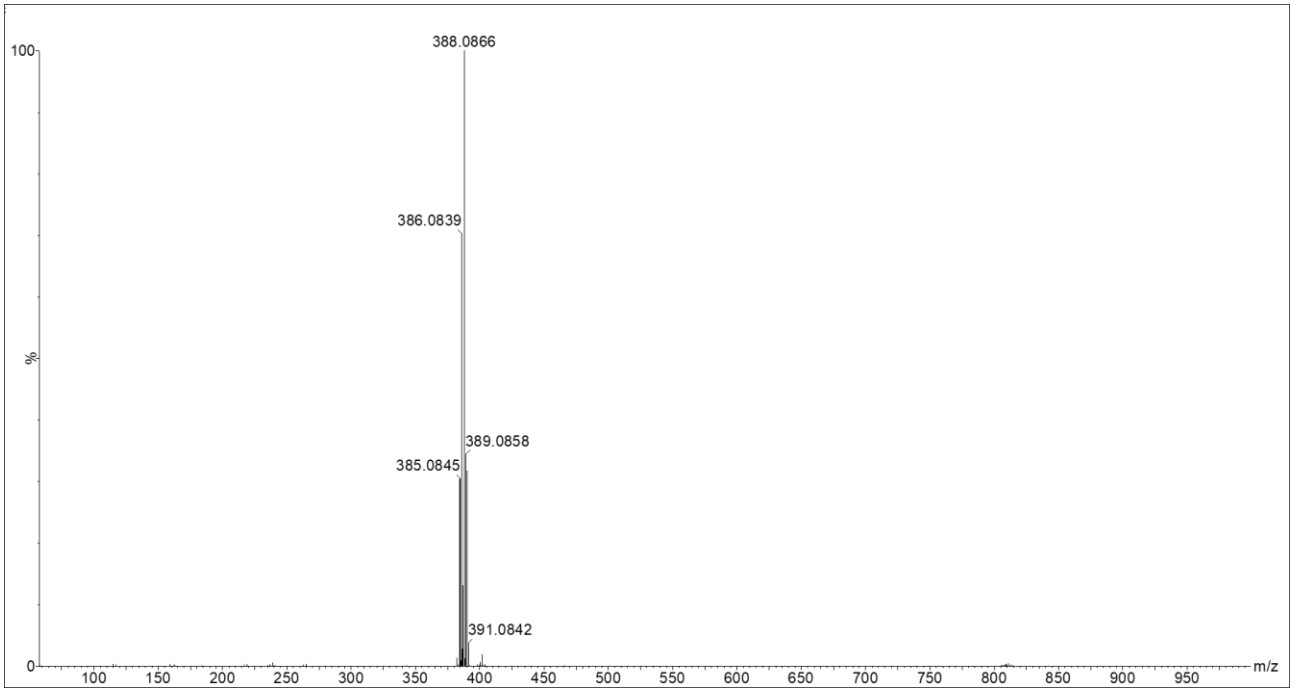


Figure S16. HRMS ESI spectrum of compound 1-CF_3.

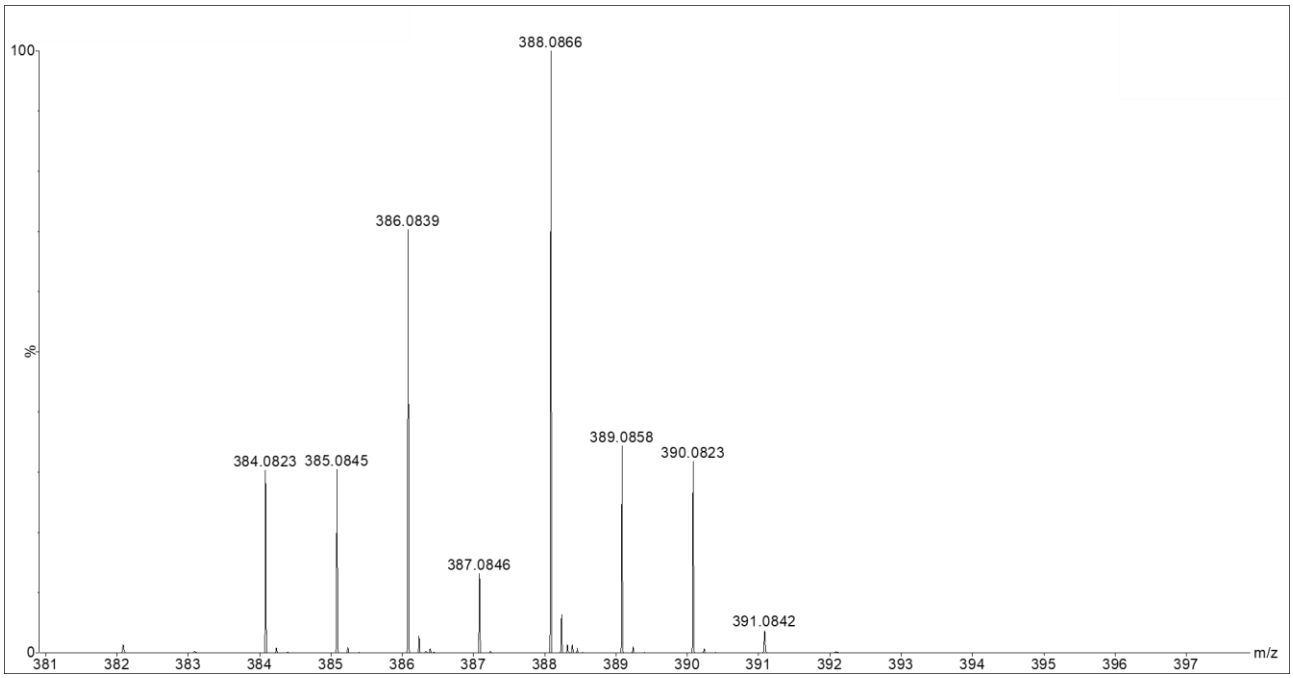
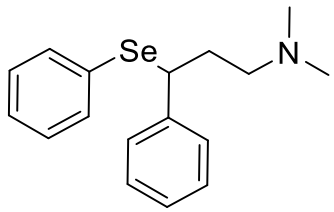


Figure S17. Detailed HRMS spectrum showing the isotopic distribution of compound 1-CF_3.

Compound 1-H



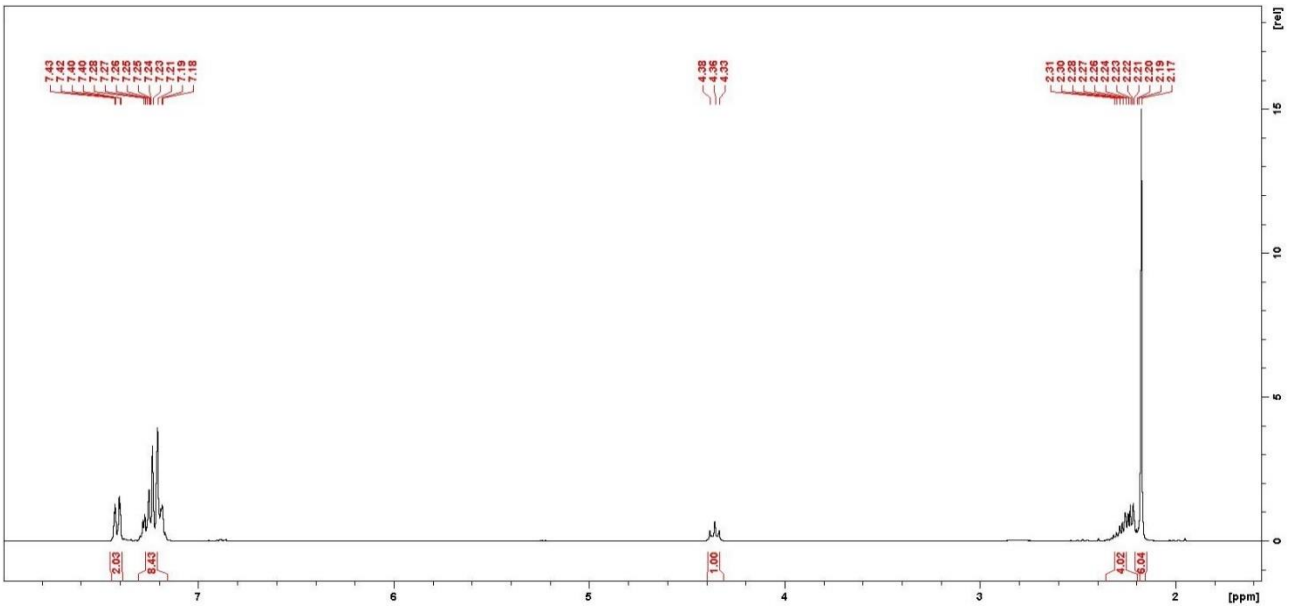


Figure S18. ^{1}H-NMR spectrum of compound 1-H.

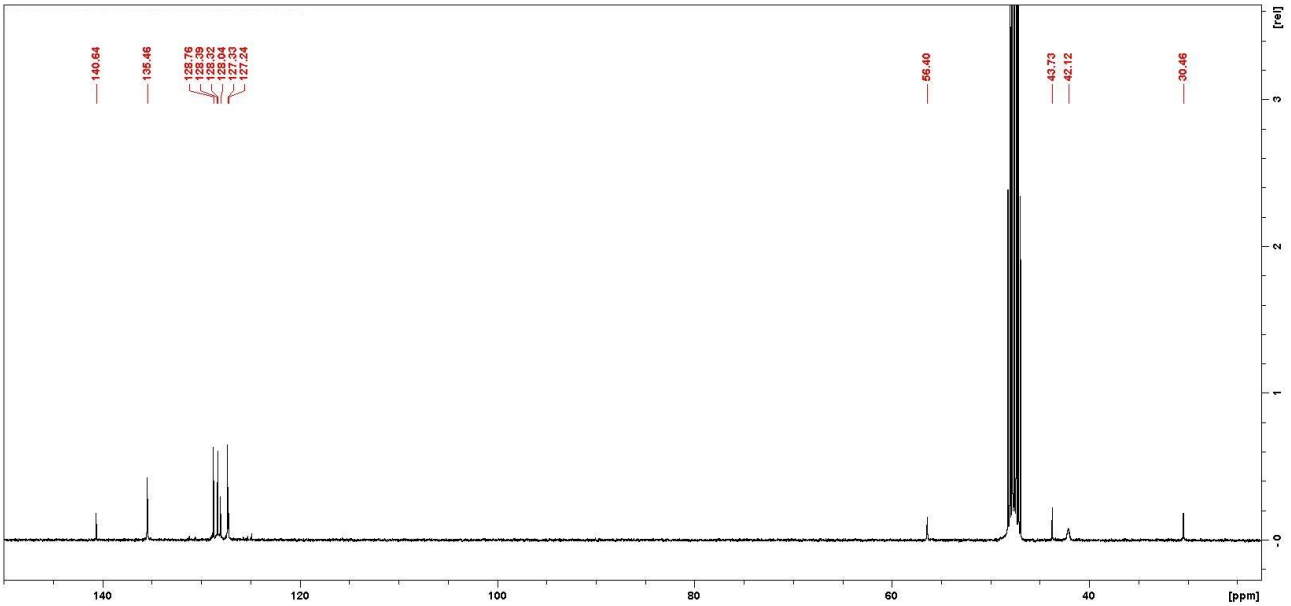


Figure S19. ^{13}C-NMR spectrum of compound 1-H.

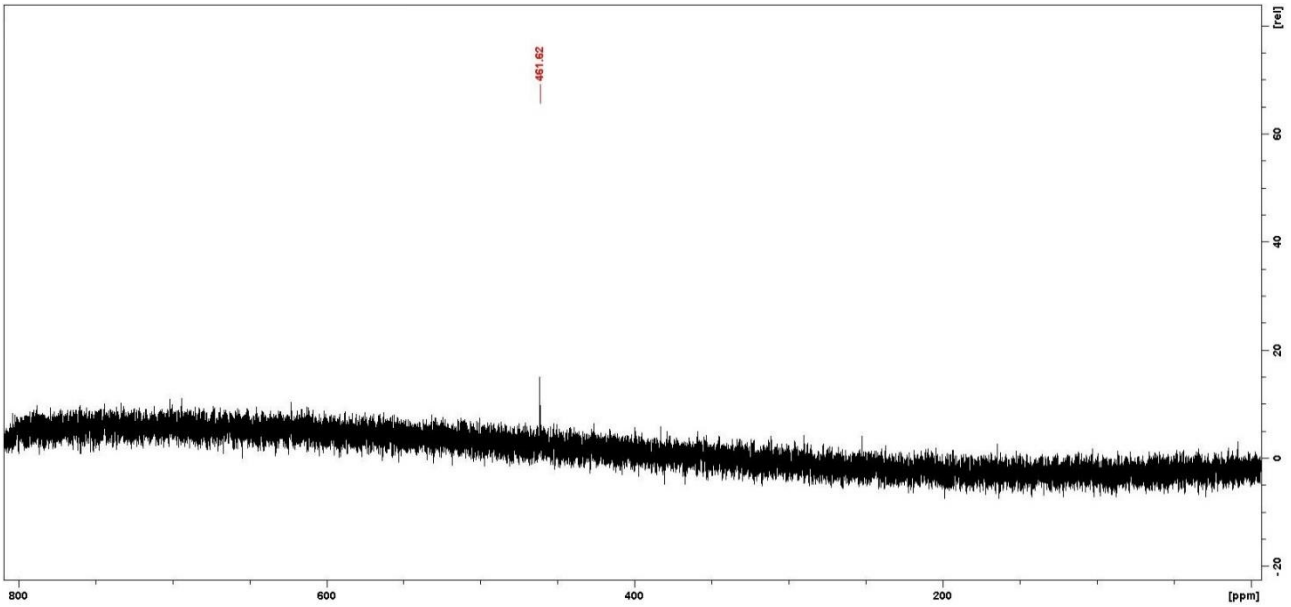


Figure S20. ^{77}Se-NMR spectrum of compound 1-H.

Figure S21. HRMS ESI spectrum of compound 1-H.

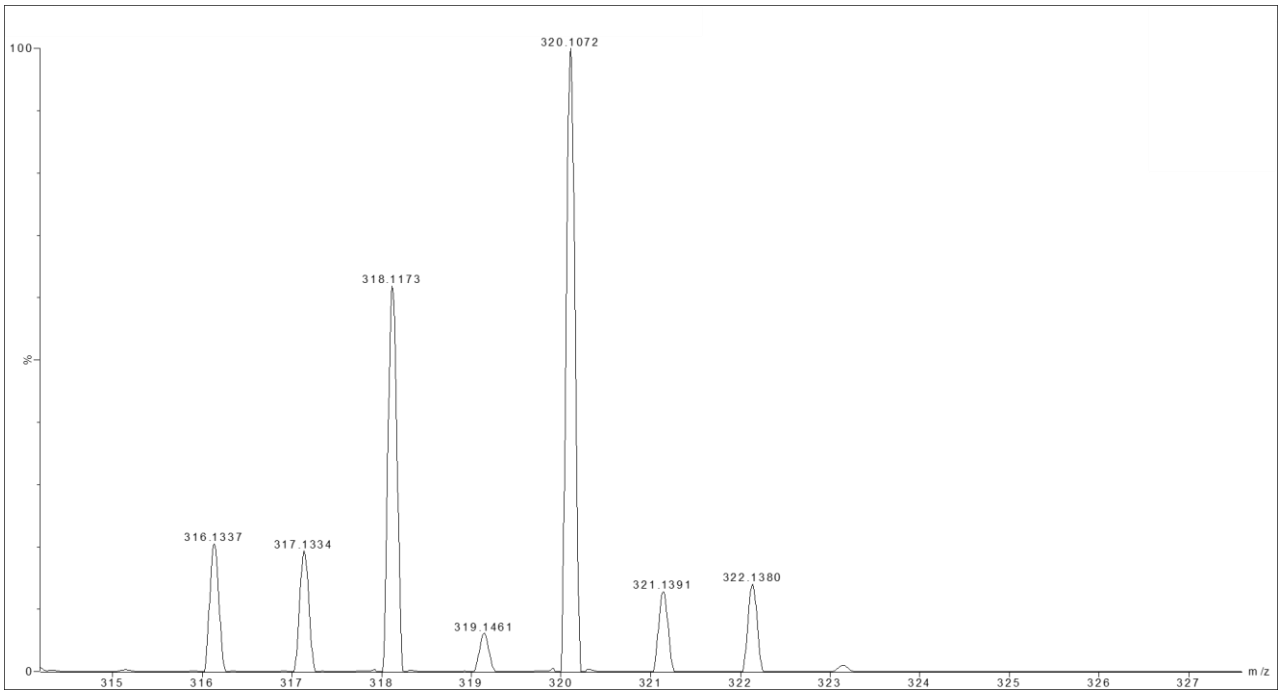


Figure S22. Detailed HRMS spectrum showing the isotopic distribution of compound 1-H.

NMR study of the reaction with H_2O_2

Compound 1-CF_3

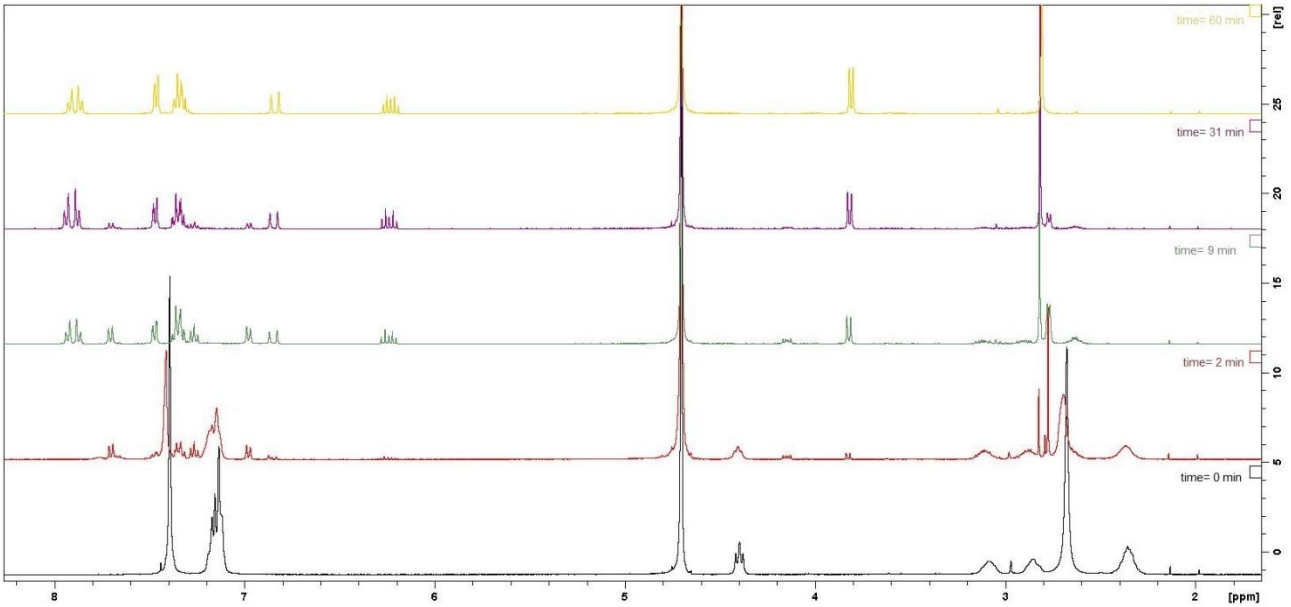


Figure S23. Variation over time of the 1H-NMR spectra during the oxidation-reaction of compound 1-CF3.

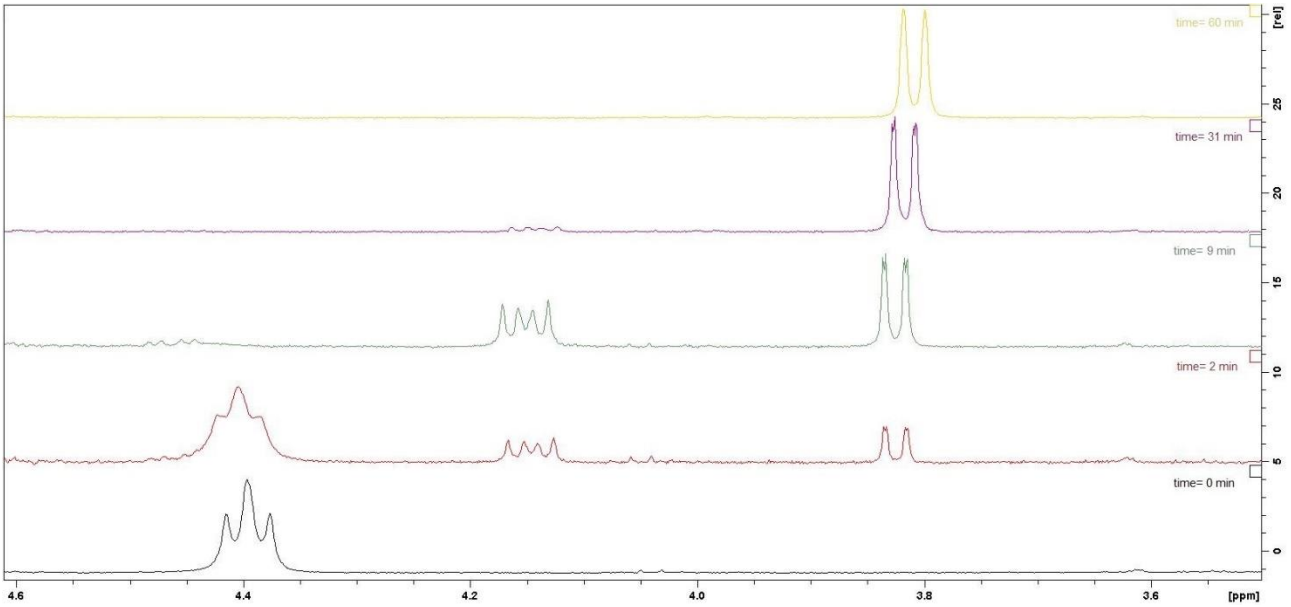


Figure S24. Variation over time of the ^{1}H-NMR spectra during the oxidation-reaction of compound 1-CF_3, focus on the region between 4.6 and 3.5 ppm (area of interest to integrate for relative abundance over time calculation).

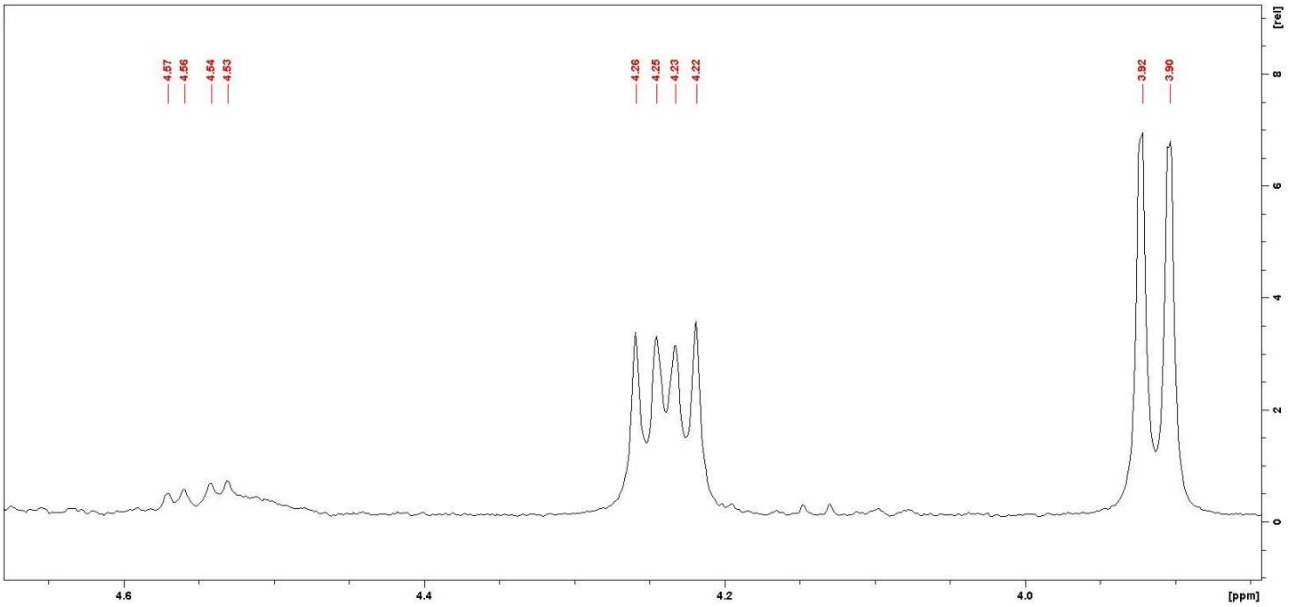


Figure S25. ^{1}H-NMR spectrum during the oxidation-reaction of compound 1-CF_3 at t= 9 min, focus on the region between 4.6 and 3.5 ppm (the signal corresponding to the other diastereoisomer of the selenoxide is detectable at 4.46 ppm after the disappearance of the starting material).

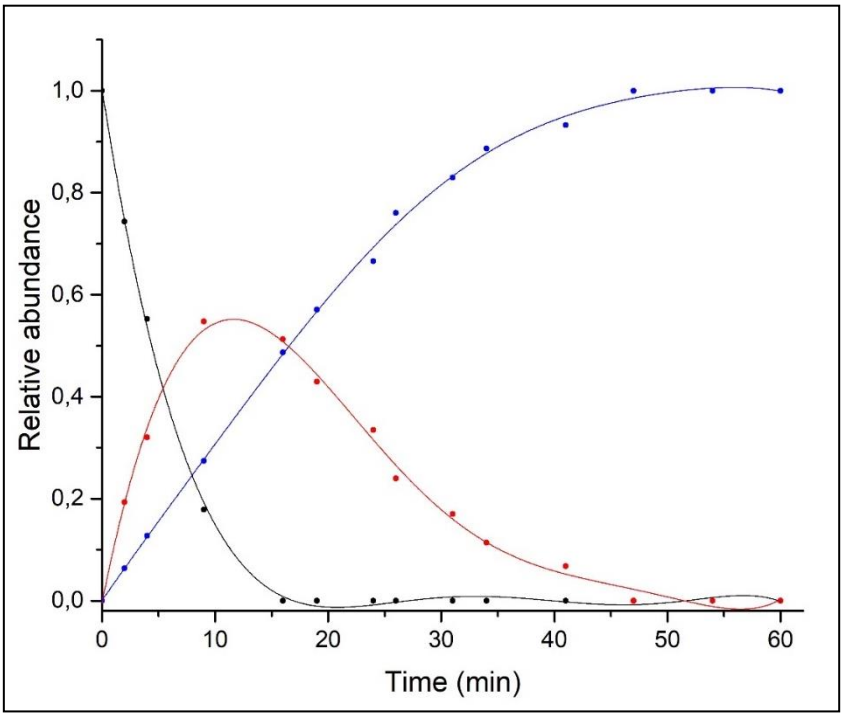


Figure S26. 1H-NMR study of the reaction with H2O2 of compound 1-CF3. This graph was obtained by integration of the α-hydrogen signals for the starting material and the two diastereoisomers and the allylic-hydrogens signals for the cinnamylamine in the 1H-NMR spectra acquired at different time points (• starting material, • diastereoisomer R-R/S-S, • amine).

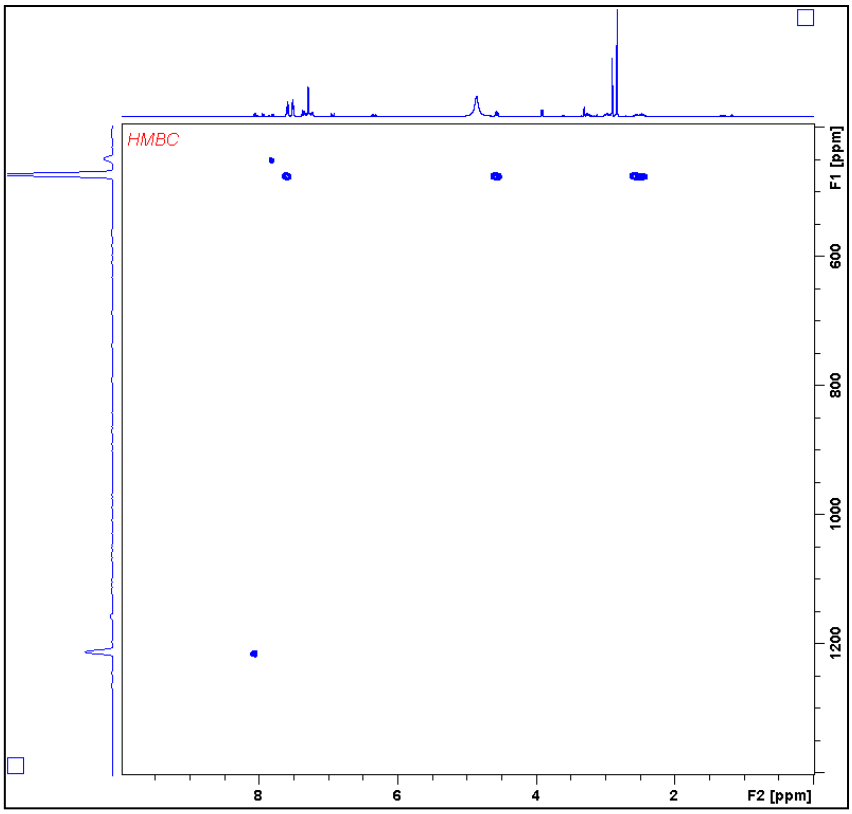


Figure S27. Mid-reaction $^{1}H^{77}Se$ HMBC NMR spectrum of compound 1-CF_3 after dilution 1:1 in MeOD.

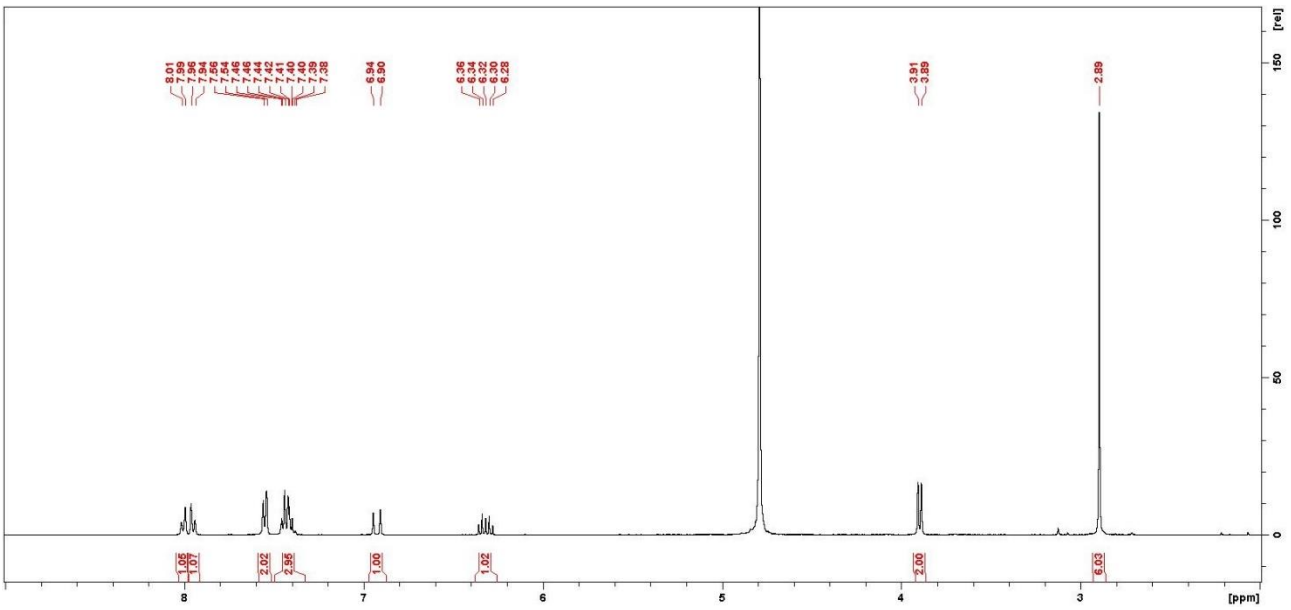


Figure S28. ^{1}H-NMR spectrum of cinnamylamine 6 and seleninic acid 7 after the oxidation reaction of 1-CF_3 in D_2O, 400 MHz. The doublets at 8.00 ppm and at 7.95 ppm are referred to the seleninic acid 7. Cinnamylamine 6: δ_H (ppm) 7.55 (d, J = 6.7 Hz, 2H), 7.46 – 7.38 (m, 3H), 6.92 (d, J = 15.8 Hz, 1H), 6.32 (m, 1H), 3.90 (d, J = 7.5 Hz, 2H), 2.89 (s, 6H).

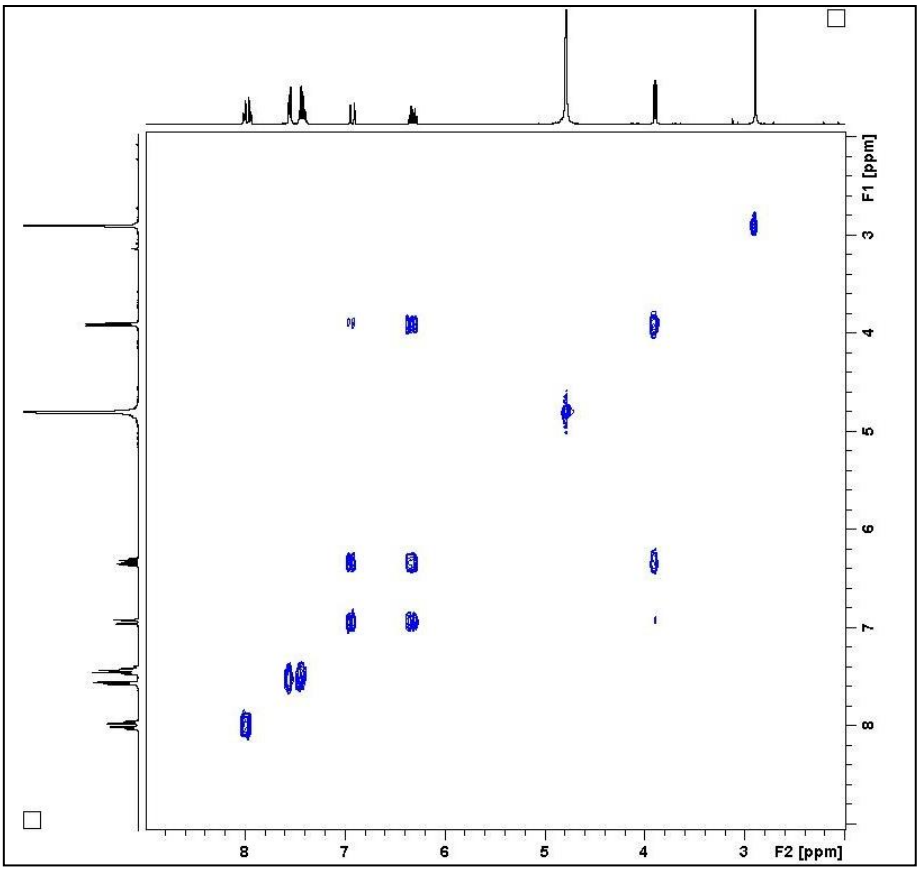


Figure S29. COSY-NMR spectrum of cinnamylamine 6 and seleninic acid 7 after the oxidation reaction of 1-CF_3 in D_2O, 400 MHz.

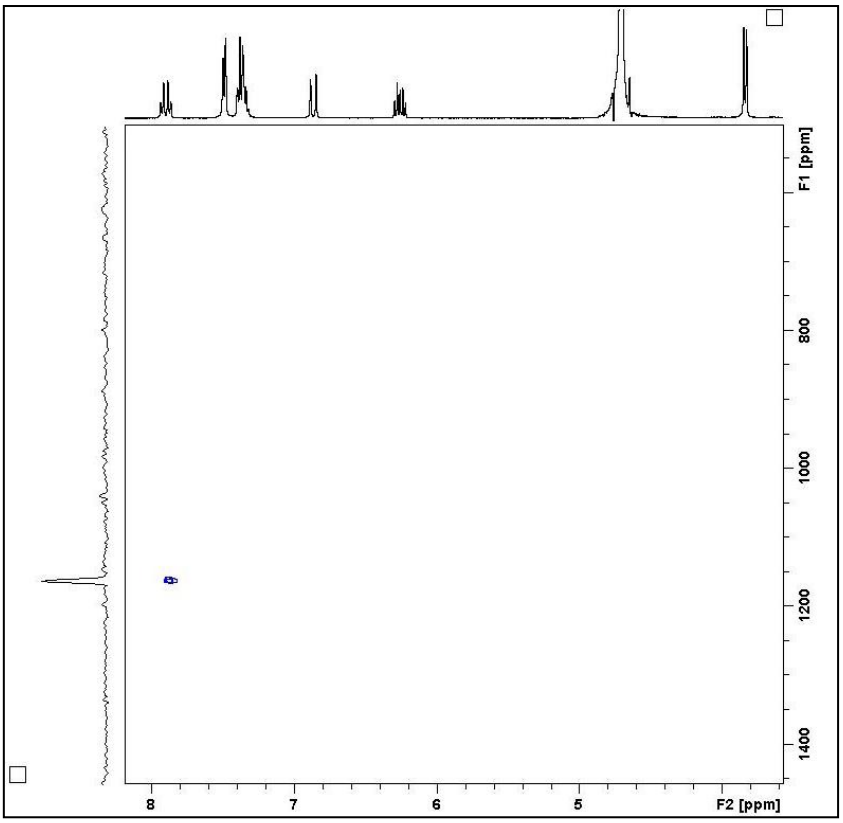


Figure S30. $^{1}H^{77}Se$ HMBC NMR spectrum of compound 1-CF_3 at the end of the reaction.

Compound 1-H

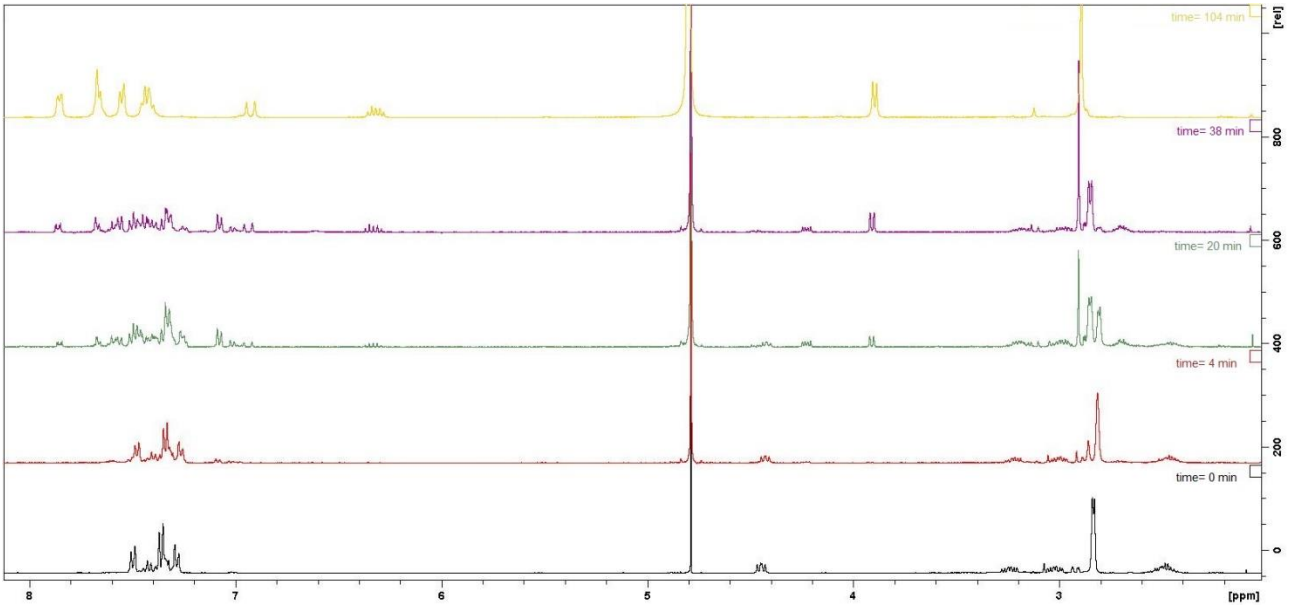


Figure S31. Variation over time of the ^{1}H-NMR spectra during the oxidation-reaction of compound 1-H.

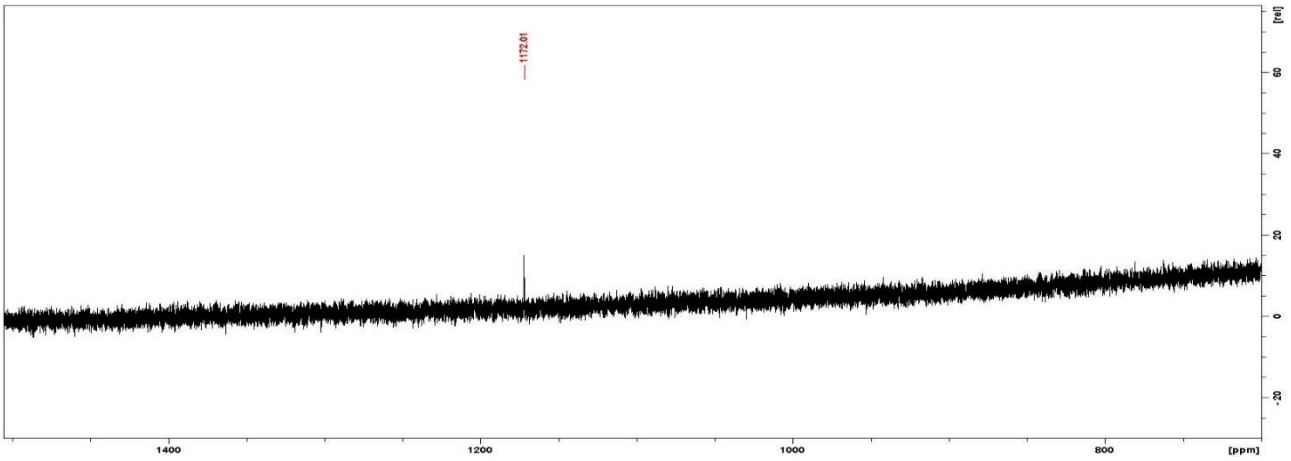


Figure S32. ^{77}Se-NMR spectrum of compound 1-H at the end of the reaction, showing the presence of seleninic acid 8.

ESI-MS study of the reaction with H_2O_2

Compound 1-H

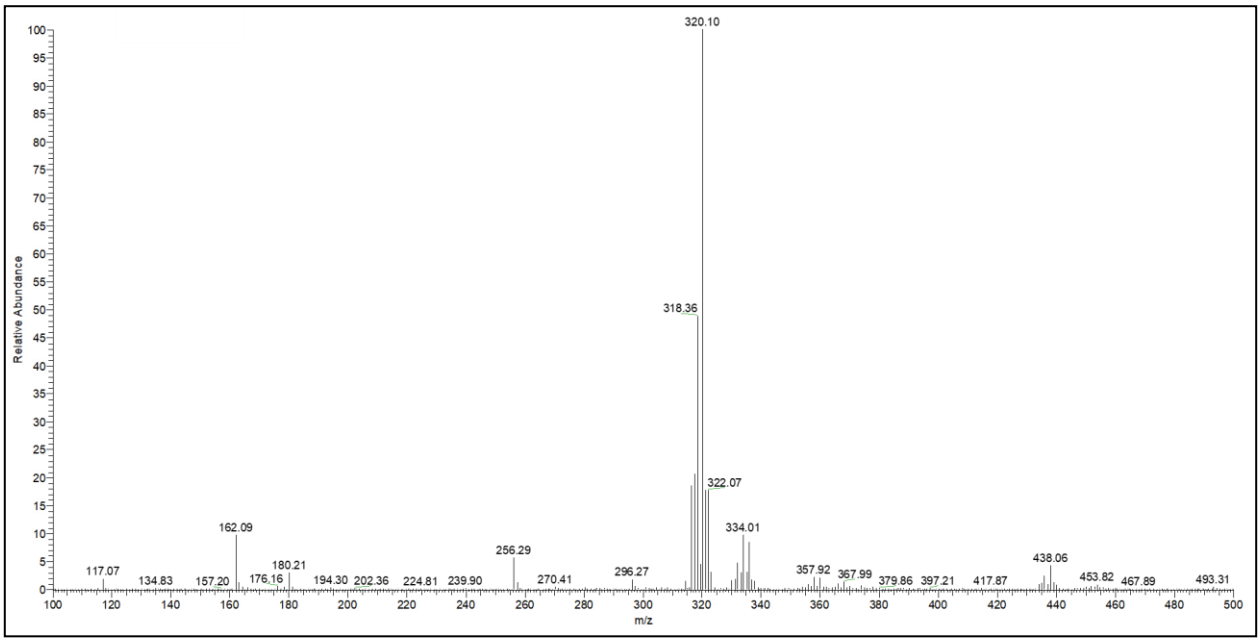


Figure S33. ESI-MS study of the reaction of compound 1-H with H2O2 (positive ionization mode, t = 5 min). The peaks corresponding to the starting material (m/z = 318), the selenoxide (m/z = 334) and the cinnamylamine 6 (m/z = 162) were detected.

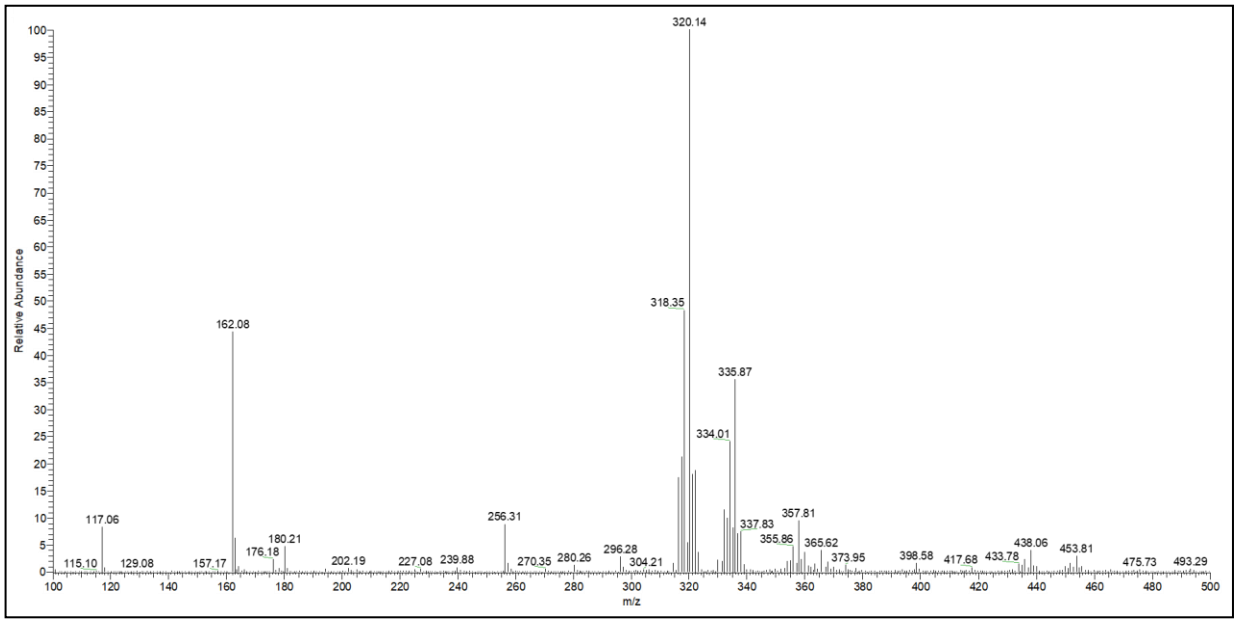


Figure S34. ESI-MS study of the reaction of compound 1-H with H2O2 (positive ionization mode, t = 20 min). The peaks corresponding to the starting material (m/z = 318), the selenoxide and its sodium adduct (m/z = 334 and m/z = 357) and the cinnamylamine 6 (m/z = 162) were detected.

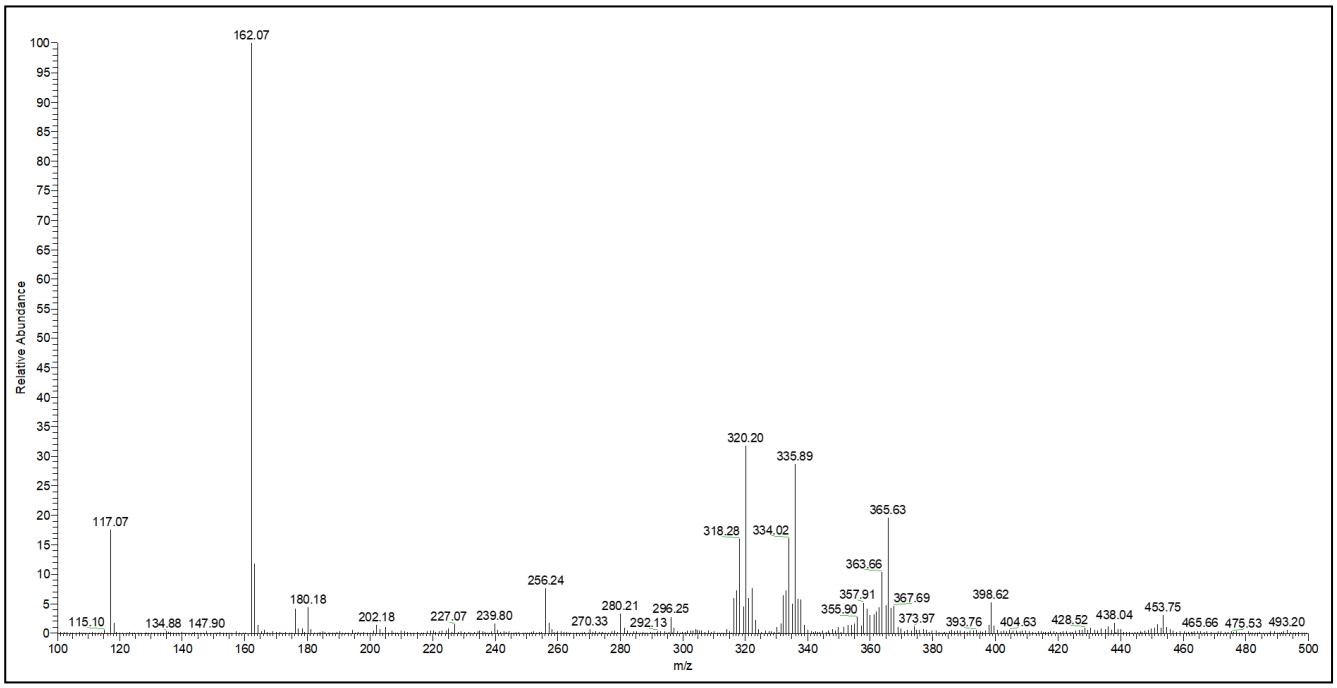


Figure S35. ESI-MS study of the reaction of compound 1-H with H2O2 (positive ionization mode, t = 60 min). The peaks corresponding to the starting material (m/z = 318), the selenoxide and its sodium and methanol adduct (m/z = 334, m/z = 357, m/z = 365), together with the cinnamylamine 6 (m/z = 162) were detected.

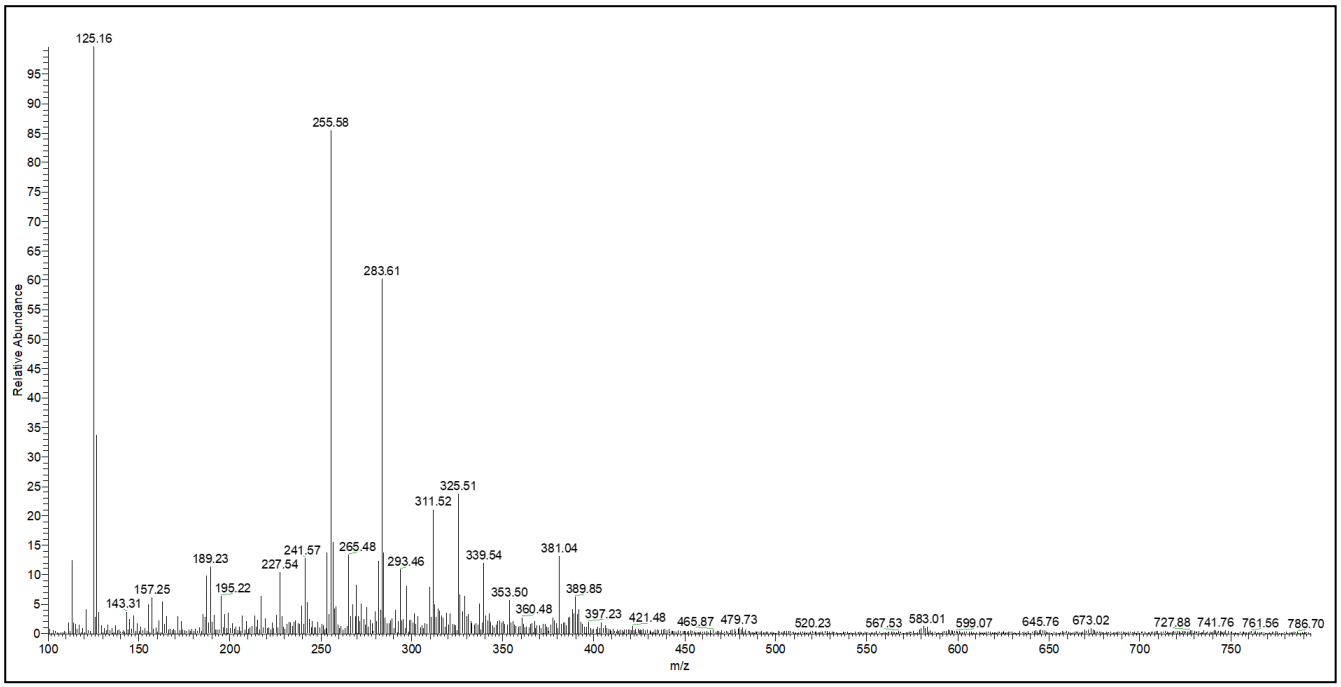


Figure S36. ESI-MS study of the reaction of compound 1-H with H2O2 (negative ionization mode, t = 10 min). The seleninic acid 8 (m/z = 189) is detectable.

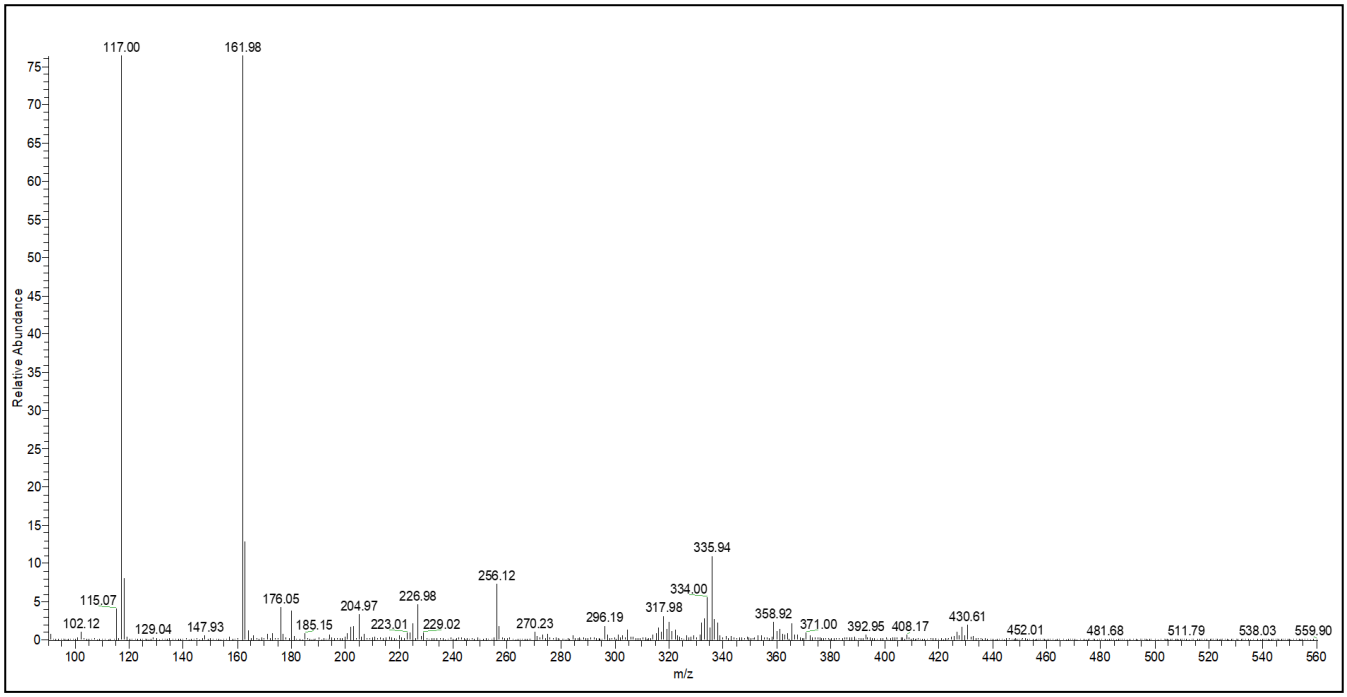


Figure S37. ESI-MS characterization of the NMR sample of compound 1-H used for the NMR study (positive ionization mode, final timepoint). Cinnamylamine 6 (m/z = 162), selenoxide (m/z = 334) and diphenyl diselenide (m/z = 316) are clearly detectable.

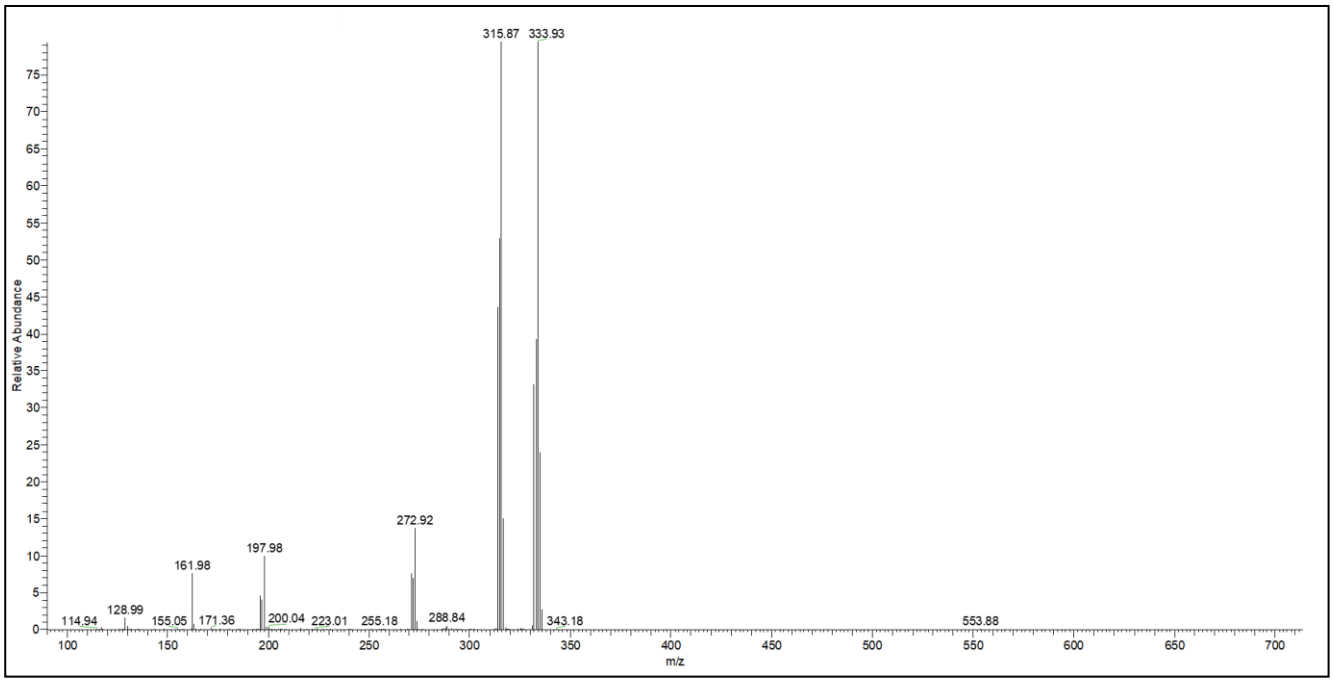


Figure S38. CID experiment showing the fragmentation pattern of the selenoxide (from compound 1-H, positive ionization mode, parent ion m/z = 334, NCE = 16). The fragmentation promotes the formation of diphenyl diselenide (m/z = 315) and of the cinnamylamine 6 (m/z = 162).

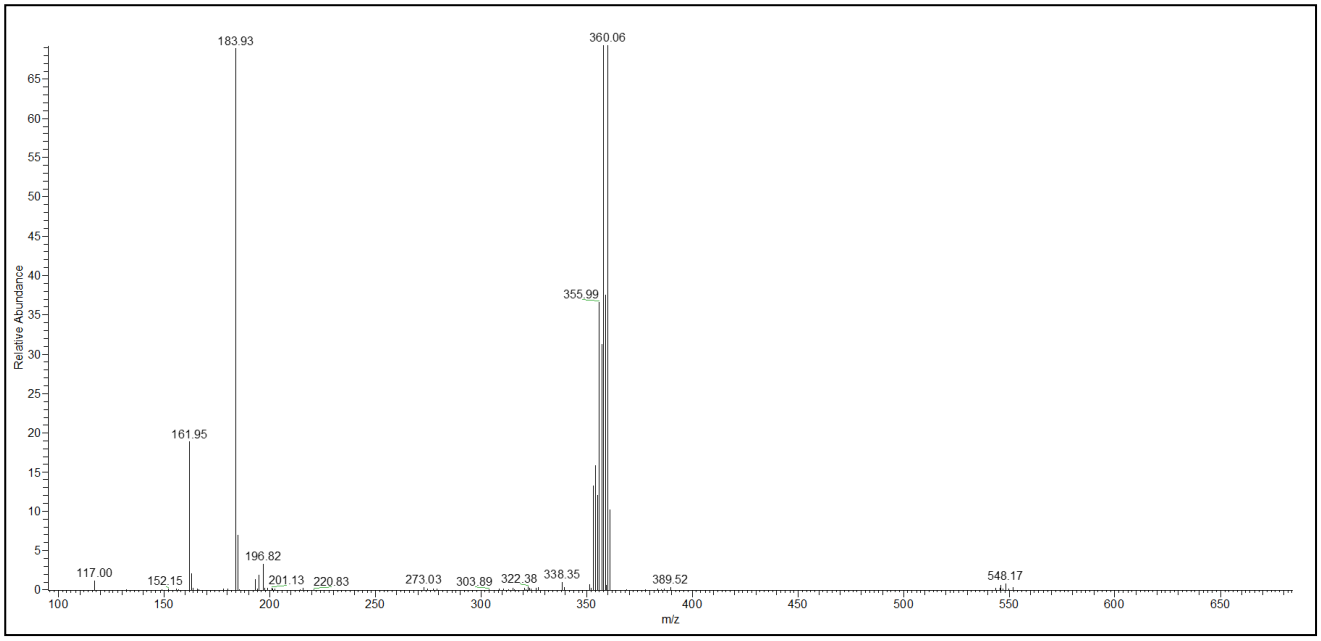


Figure S39. CID experiment showing the fragmentation pattern of the sodium adduct of the selenoxide (from compound 1-H, positive ionization mode, parent ion m/z = 357, NCE = 16). The fragmentation promotes the formation of the cinnamylamine 6 (m/z = 162) and of the cinnamylamine sodium adduct (m/z = 184).

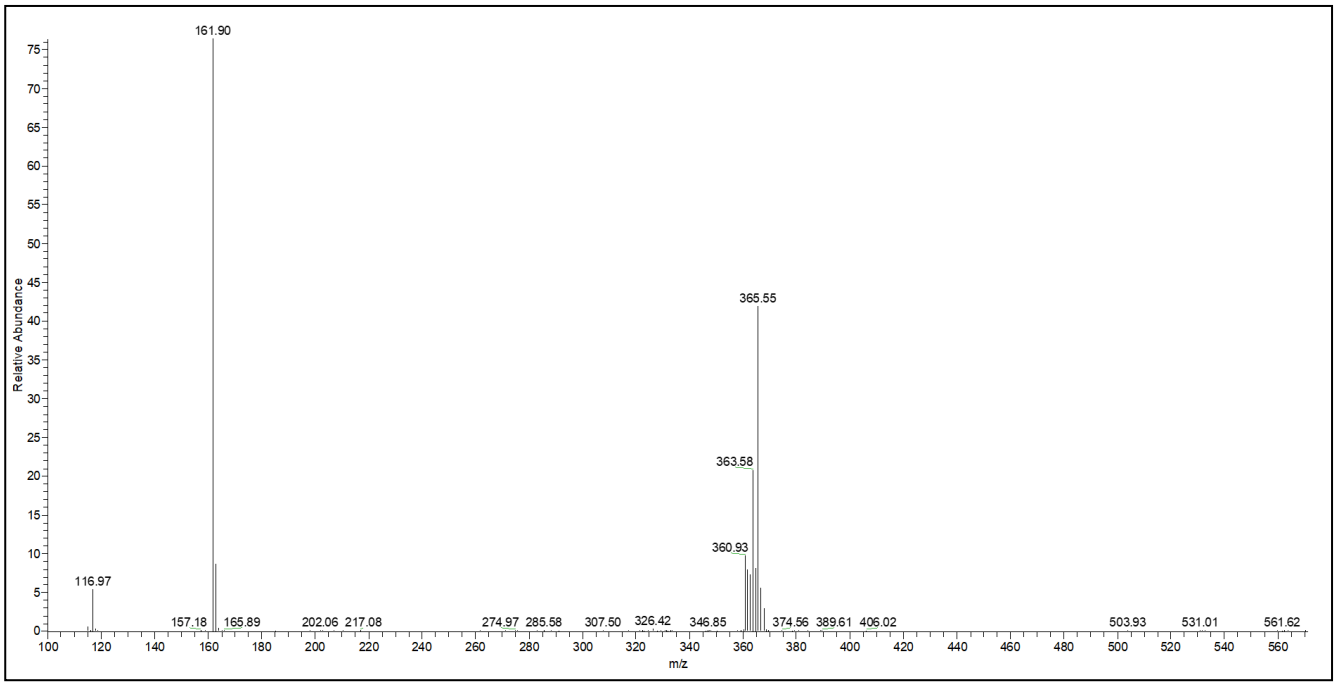


Figure S40. CID experiment showing the fragmentation pattern of the methanol adduct of the selenoxide (from compound 1-H, positive ionization mode, parent ion m/z = 365, NCE = 12). The fragmentation promotes the formation of the cinnamylamine 6 (m/z = 162).

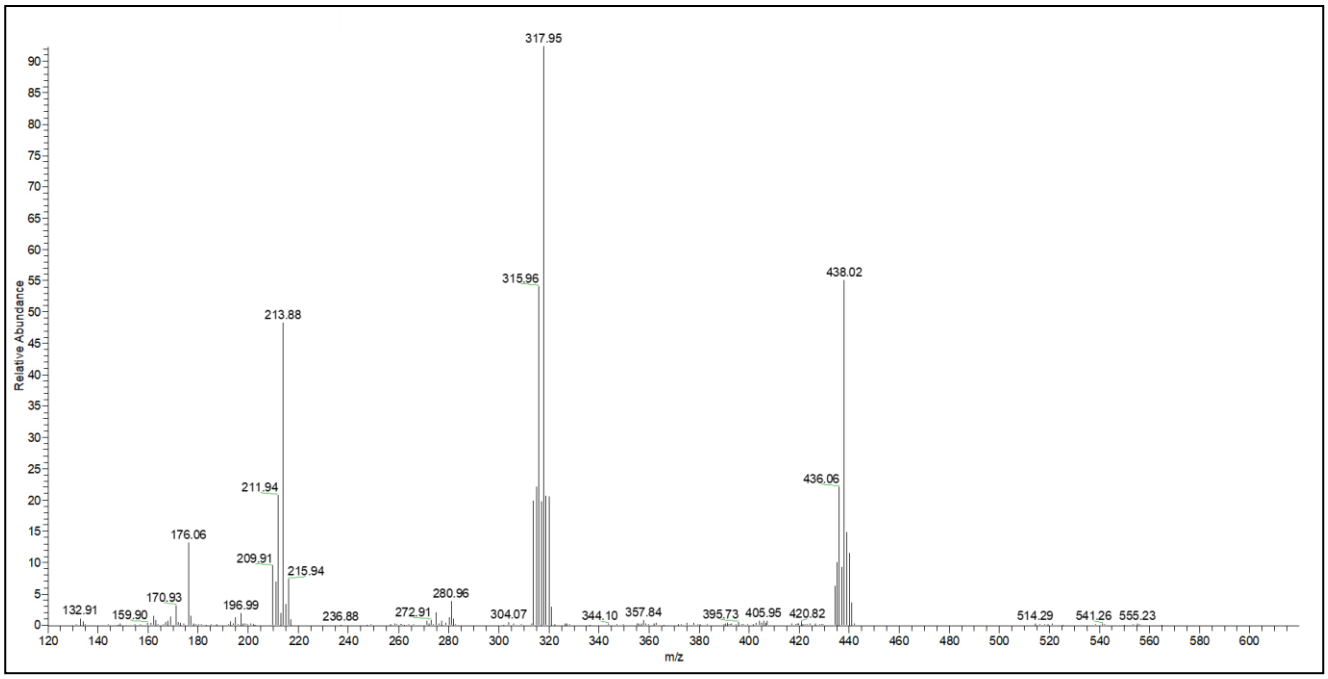


Figure S41. CID experiment showing the fragmentation pattern of the ion with m/z = 438 (from compound 1-H, positive ionization mode, NCE = 24). The fragmentation promotes the formation of two Se-containing species (m/z = 316 and m/z = 212).

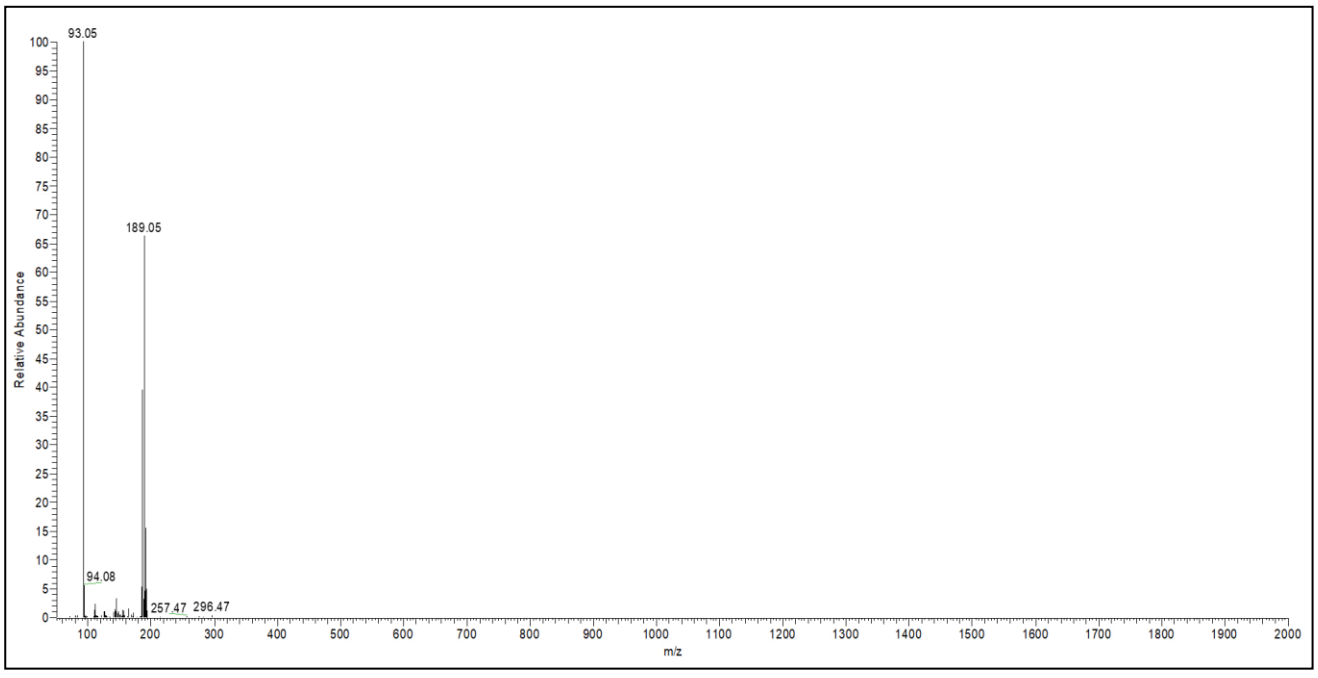


Figure S42. CID experiment showing the fragmentation pattern of the seleninic acid 8 (from compound 1-H, negative ionization mode, parent ion m/z = 189, NCE = 25). The fragmentation promotes the formation of phenol (m/z = 93).

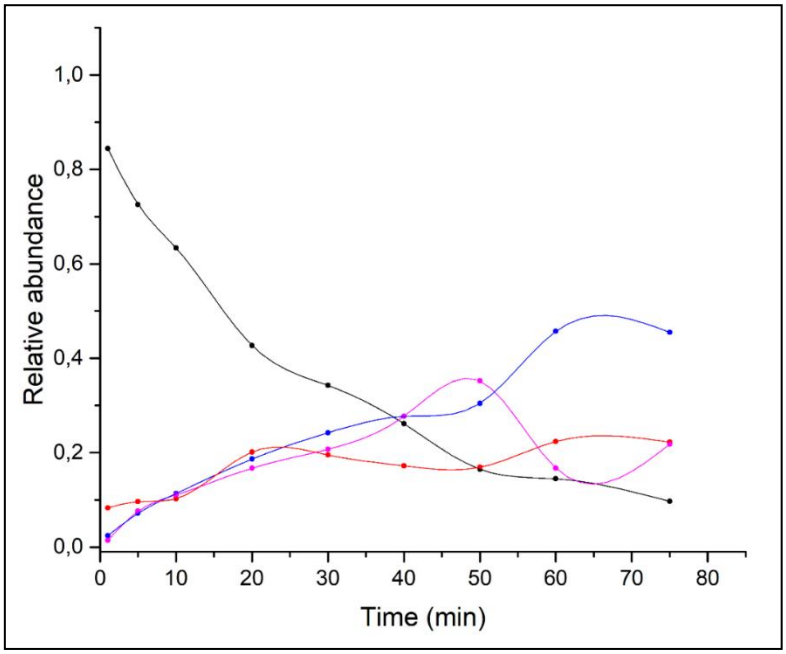


Figure S43. ESI-MS study of the reaction with H_2O_2 of compound 1-H. This graph was obtained using the relative intensities of the signals in the m/z spectra acquired at different time points (• starting material, • selenoxide, • seleninic acid, • cinnamylamine).

Compound 1-CF_3

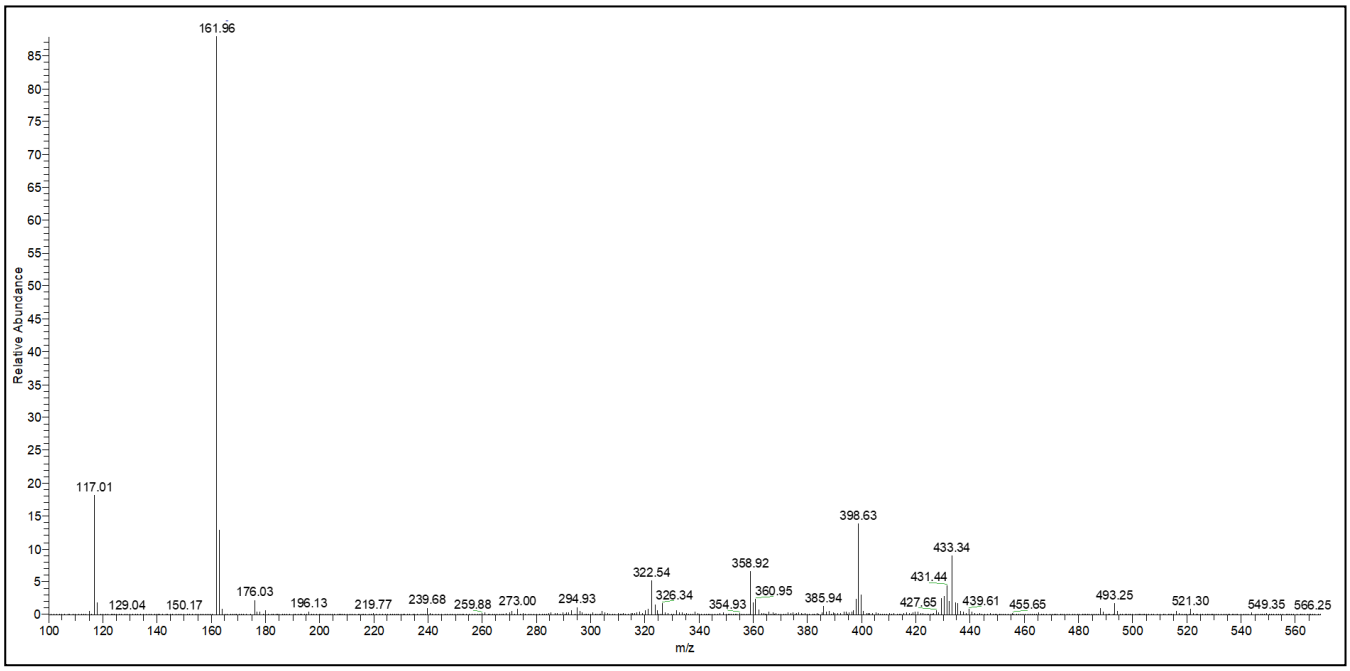


Figure S44. ESI-MS characterization of the NMR sample of compound 1-CF3 used for the study of the reaction (positive ionization mode, final timepoint). Cinnamylamine 6 (m/z = 162) and oxidised selenium species are clearly detectable.

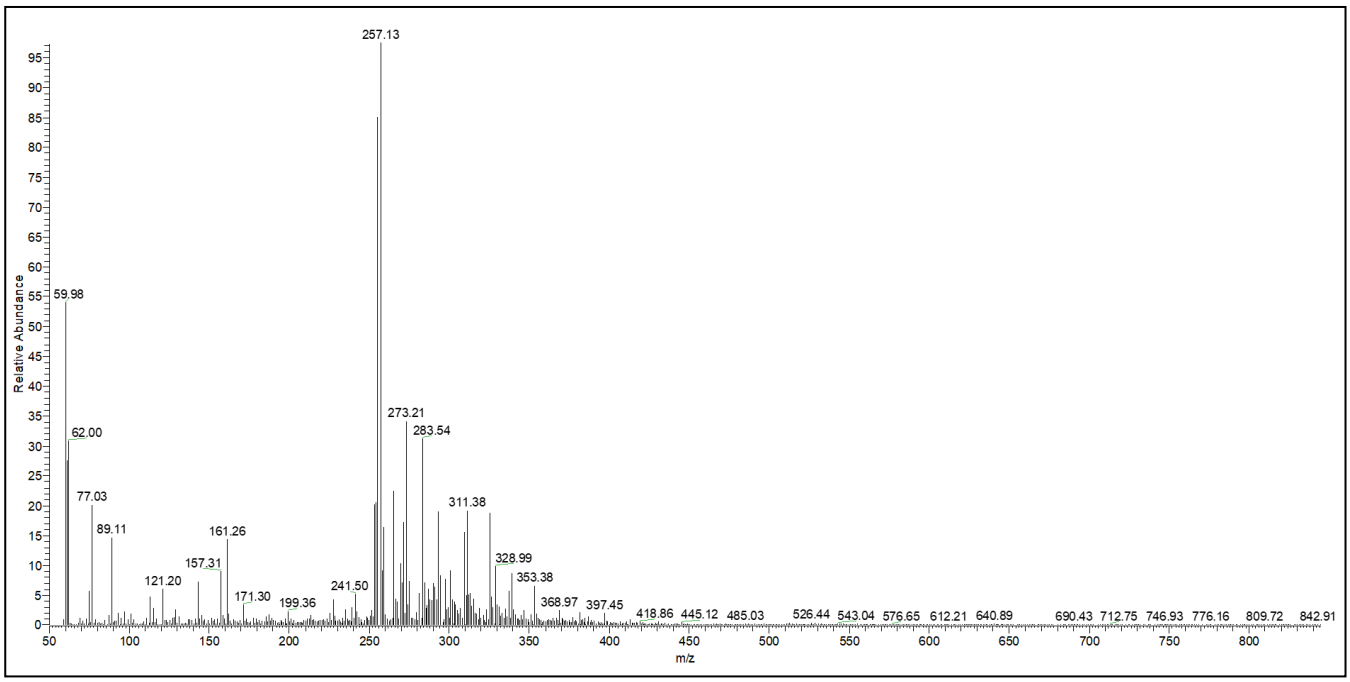


Figure S45. ESI-MS characterization of the NMR sample of compound 1-CF_3 used for the study of the reaction (negative ionization mode, final timepoint). Seleninic acid 7 (m/z = 255) was detected.

Computational methodology

Tables

Table S1. $\Delta G°_{HAT}$ (kcal mol^{-1}) in the gas phase, in benzene, and in water for the scavenging of HO•, HOO• and CH_2=CHOO• from non-aromatic sites of selenofluoxetine. Level of theory: (SMD)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d).

Site	Gas Phase	Benzene	Water	Gas Phase	Benzene	Water	Gas Phase	Benzene	Water
	HO•			HOO•			CH_2CHOO•		
C7	-28.06	-28.43	-29.87	3.54	3.62	2.59	2.24	2.15	0.31
C14	-18.94	-19.39	-21.83	12.65	12.66	10.63	11.35	11.18	8.34
C15	-26.81	-28.04	-30.93	4.79	4.00	1.53	3.49	2.53	-0.76
N16	-24.98	-25.70	-32.01	6.62	6.35	0.45	5.32	4.88	-1.84
C17	-25.43	-26.05	-28.16	6.17	5.99	4.30	4.87	4.52	2.02

Table S2. Relative electronic energies for the stationary points of the oxidation and elimination reactions of selenofluoxetine derivatives. Level of theory OLYP/TZ2P.

Selenofluoxetine R=H, R'=CF_3. E in kcal mol^{-1}			
	ΔE		ΔE
1+H_2O_2	0.0	1+H_2O_2	0.0
R-*S*-RCox	-3.1	*R*-*R*-RCox	-2.5
R-*S*-TSox	16.5	*R*-*R*-TSox	17.9
R-*S*-PCox	-42.1	*R*-*R*-PCox	-41.7
R-*S*-Ox+H_2O	-37.9	*R*-*R*-Ox+H_2O	-36.8
R-*S*-TSelim+H_2O	-24.0	*R*-*R*-TSelim+H_2O	-24.8
R-*S*-PCelim+H_2O	-49.1	*R*-*R*-PCelim+H_2O	-49.1
6'+7+H_2O	-47.5	6'+7+H_2O	-47.5

1-CF$_3$ R=CH$_3$, R'=CF$_3$. E in kcal mol^{-1}			
	ΔE		ΔE
1-CF$_3$ +H$_2$O$_2$	0.0	1-CF$_3$ +H$_2$O$_2$	0.0
R-*S*-RCox	-3.0	*R*-*R*-RCox	-2.5
R-*S*-TSox	16.6	*R*-*R*-TSox	18.0
R-*S*-PCox	-42.5	*R*-*R*-PCox	-41.7
R-*S*-Ox+H$_2$O	-37.9	*R*-*R*-Ox+H$_2$O	-36.8
R-*S*-TSelim+H$_2$O	-21.7	*R*-*R*-TSelim+H$_2$O	-22.9
R-*S*-PCelim+H$_2$O	-49.3	*R*-*R*-PCelim+H$_2$O	-49.2
6+7+H$_2$O	-47.5	6+7+H$_2$O	-47.5

1-H R=CH$_3$, R'=H, E in kcal mol^{-1}			
	ΔE		ΔE
1-H+H$_2$O$_2$	0.0	**1-H** +H$_2$O$_2$	0.0
R-*S*-RCox	-3.3	*R*-*R*-RCox	-2.9
R-*S*-TSox	15.5	*R*-*R*-TSox	16.9
R-*S*-PCox	-43.2	*R*-*R*-PCox	-42.4
R-*S*-Ox+H$_2$O	-38.4	*R*-*R*-Ox+H$_2$O	-37.3
R-*S*-TSelim	-21.6	*R*-*R*-TSelim+H$_2$O	-22.7
R-*S*-PCelim	-48.7	*R*-*R*-PCelim+H$_2$O	-48.7
6+8+H$_2$O	-46.7	6+8+H$_2$O	-46.7

Structure and energies of the optimised selenofluoxetine radicals. Level of theory M06-2X/6-31G(d,p)

Selenofluoxetine (SeFl)

Bond Energy -3411.95597389 a.u.

F	5.644535	-0.339833	0.350695
C	4.641628	0.495918	0.663447
F	4.706992	0.696996	1.988637
F	4.899817	1.665248	0.062315
C	3.309201	-0.065587	0.257197
C	2.689841	0.365489	-0.911030
C	1.476818	-0.199621	-1.294158
C	0.889669	-1.190869	-0.509472
C	1.519735	-1.619602	0.660594
C	2.728906	-1.056032	1.047521
H	3.221507	-1.377863	1.959767
H	1.052837	-2.393850	1.261120
Se	-0.784094	-1.959611	-1.016901
C	-1.903474	-0.731292	0.037223
C	-1.807855	0.693161	-0.451880
C	-1.882161	1.006433	-1.812424
C	-1.871294	2.331927	-2.233145
C	-1.776242	3.362903	-1.299450
C	-1.695058	3.058528	0.056219
C	-1.712285	1.730550	0.477845
H	-1.672904	1.486581	1.536284
H	-1.615287	3.855689	0.789297
H	-1.760603	4.397177	-1.629091
H	-1.929028	2.561627	-3.292989
H	-1.912812	0.194879	-2.535133
C	-3.340316	-1.269498	-0.021128
C	-4.306889	-0.400765	0.779965
N	-3.854971	-0.250659	2.156251
H	-3.869327	-1.162759	2.609738
C	-4.684095	0.677626	2.909244
H	-4.354290	0.704793	3.950836
H	-5.768	0.435458	2.888500
H	-4.558208	1.681226	2.489288
H	-5.326825	-0.818561	0.706017
H	-4.342047	0.601402	0.335992
H	-3.678526	-1.314493	-1.063969
H	-3.348010	-2.298578	0.361799
H	-1.546105	-0.787932	1.067076
H	0.975895	0.136323	-2.195977
H	3.148878	1.142961	-1.511920

SeFl-TS-C7

Bond Energy -3487.65670998 a.u.

F	4.752916	1.732002	0.234942
C	4.715807	0.455017	0.648866
F	5.728765	-0.179995	0.039764
F	4.976181	0.465595	1.964452
C	3.393661	-0.188195	0.347735
C	3.203177	-0.837519	-0.867772
C	1.956674	-1.373396	-1.171519
C	0.913658	-1.280194	-0.250857
C	1.109723	-0.637241	0.973573
C	2.349748	-0.081625	1.264094
H	2.512282	0.421170	2.211816
H	0.299780	-0.565678	1.694866
Se	-0.766587	-2.065274	-0.689310
C	-1.914264	-0.603863	-0.131935
C	-1.468374	0.739354	-0.642138
C	-1.103276	0.905198	-1.982537
C	-0.772916	2.164099	-2.469348
C	-0.790546	3.270464	-1.620969
C	-1.133130	3.107545	-0.282329
C	-1.469047	1.847203	0.208182
H	-1.715459	1.701239	1.256236
H	-1.129935	3.961681	0.388092
H	-0.524467	4.251933	-2.974
H	-0.490141	2.281417	-3.511085
H	-1.049345	0.027669	-2.621938
C	-3.354248	-0.966270	-0.518990
C	-4.403401	0.035337	-0.039408
N	-4.583495	-0.003305	1.413558
H	-4.957259	-0.917745	1.666178
C	-5.503074	1.032332	1.876776
H	-5.673436	0.919024	2.949677
H	-6.474312	1.012049	1.359227
H	-5.046475	2.011444	1.705094
H	-5.353082	-0.156135	-0.565582
H	-4.089728	1.050455	-0.308032
H	-3.411743	-1.026448	-1.613444
H	-3.591592	-1.967424	-0.134060
H	-1.837817	-0.627070	1.043418
H	1.789286	-1.859542	-2.127585
H	4.021897	-0.915841	-1.575405
O	-1.963940	-0.366440	2.402506
H	-2.920284	-0.116114	2.304107

SeFl-C7-rad

Bond Energy -3411.31263177 a.u.

F	5.349629	-0.231673	-0.329421
C	4.391095	0.102940	0.547301
F	4.625159	-0.573776	1.681996
F	4.559075	1.404578	0.831738
C	3.018407	-0.175797	0.008940
C	2.798972	-0.192434	-1.364702
C	1.510872	-0.387895	-1.850853
C	0.453935	-0.587614	-0.962984
C	0.674889	-0.580031	0.414853
C	1.960285	-0.365023	0.896144
H	2.148014	-0.360607	1.965270
H	-0.154757	-0.770960	1.089597
Se	-1.285412	-0.896906	-1.696341
C	-2.406393	-0.040955	-0.447126
C	-2.186418	1.315076	-0.043830
C	-1.285464	2.165636	-0.729123
C	-1.093520	3.475463	-0.325332
C	-1.785661	3.989293	0.772928
C	-2.684096	3.171560	1.458658
C	-2.886585	1.859638	1.060104
H	-3.581525	1.238102	1.616026
H	-3.229319	3.560879	2.313151
H	-1.629333	5.015897	1.087768
H	-0.402295	4.106668	-0.875237
H	-0.766564	1.778322	-1.599340
C	-3.547403	-0.882605	0.043934
C	-3.223424	-1.695795	1.310366
N	-1.947491	-2.381604	1.198396
H	-1.837213	-2.777614	0.266741
C	-1.768110	-3.397732	2.219388
H	-0.805455	-3.895242	2.077871
H	-2.562716	-4.162923	2.230570
H	-1.757106	-2.918563	3.204290
H	-4.063957	-2.388773	1.499818
H	-3.166264	-1.022863	2.176647
H	-4.427120	-0.259669	0.241225
H	-3.833437	-1.585879	-0.748570
H	1.324530	-0.379221	-2.920776
H	3.627909	-0.046041	-2.049050

SeFl-TS-C14

Bond Energy -3487.65162647 a.u

F	4.900509	-0.478954	2.029184
C	4.777593	0.068959	0.811697
F	5.025325	1.380856	0.928050
F	5.753023	-0.449403	0.049811
C	3.420457	-0.192399	0.221595
C	2.849482	0.738537	-0.640990
C	1.617582	0.466807	-1.227455
C	0.964238	-0.732388	-0.946666
C	1.539804	-1.659999	-0.077921
C	2.771303	-1.390934	0.507602
H	3.224922	-2.102598	1.189635
H	1.021028	-2.588530	0.138600
Se	-0.739457	-1.097269	-1.727183
C	-1.780106	-0.313162	-0.255573
C	-1.725157	1.197063	-0.229345
C	-1.759841	1.962715	-1.397569
C	-1.784093	3.351969	-1.328164
C	-1.764147	3.992205	-0.090664
C	-1.725646	3.234911	1.077098
C	-1.707599	1.843990	1.009193
H	-1.720	1.242656	1.915452
H	-1.706538	3.727040	2.044762
H	-1.775527	5.076447	-0.037901
H	-1.811215	3.936329	-2.242943
H	-1.743202	1.457406	-2.359382
C	-3.214866	-0.817819	-0.371658
C	-4.076768	-0.504190	0.837409
N	-3.418688	-0.962387	2.049568
H	-3.196041	-1.951286	1.932550
C	-4.239748	-0.761733	3.231590
H	-3.731483	-1.175316	4.105922
H	-5.241445	-1.217903	3.160701
H	-4.373460	0.312892	3.397061
H	-5.076458	-0.950890	0.691076
H	-4.220981	0.583770	0.911168
H	-3.688955	-0.538868	-1.319108
H	-3.150287	-2.023150	-0.377602
H	-1.352571	-0.713123	0.665891
H	1.155058	1.187739	-1.893450
H	3.361548	1.672904	-0.844795
O	-2.650640	-3.223117	-0.007950
H	-1.801548	-3.086377	-0.481276

SeFl-C14-rad

Bond Energy -3411.28738748 a.u.

F	4.931932	0.605814	1.884710
C	4.677284	0.637372	0.568178
F	4.732585	1.917655	0.174216
F	5.688251	-0.003038	-0.039679
C	3.351203	0.010883	0.243497
C	2.881707	-1.043731	1.022390

C	1.679278	-1.657391	0.690040
C	0.951198	-1.219217	-0.416850
C	1.428954	-0.162466	-1.192592
C	2.638	0.455798	-0.860941
H	3.003013	1.285581	-1.452034
H	0.850997	0.181215	-2.044304
Se	-0.710646	-2.057452	-0.846804
C	-1.835316	-0.829374	0.216321
C	-1.849661	0.565584	-0.369344
C	-2.091239	0.763532	-1.732265
C	-2.173273	2.049637	-2.253585
C	-2.005844	3.154853	-1.419365
C	-1.760898	2.963657	-0.063092
C	-1.686057	1.673685	0.460341
H	-1.523690	1.520539	1.523209
H	-1.626430	3.819161	0.591937
H	-2.063299	4.159275	-1.827448
H	-2.362214	2.191301	-3.313515
H	-2.184821	-0.105945	-2.377736
C	-3.204884	-1.427821	0.286578
C	-4.339495	-0.556718	0.716089
N	-4.057090	0.031327	2.030189
H	-4.071469	-0.710069	2.727749
C	-5.019778	1.061848	2.389072
H	-4.820380	1.411015	3.405370
H	-6.071812	0.735226	2.331585
H	-4.891787	1.911279	1.709700
H	-5.291514	-1.112209	0.688171
H	-4.439380	0.284979	0.016162
H	-3.290075	-2.509225	0.336434
H	-1.375010	-0.799019	1.213188
H	1.294939	-2.478710	1.286476
H	3.450506	-1.374987	1.885028

SeFl-TS-C15

Bond Energy -3487.64796514 a.u.

F	5.714921	0.548249	-0.338851
C	4.800803	0.651789	0.637984
F	5.342842	0.143115	1.752242
F	4.608032	1.963641	0.845579
C	3.519028	-0.036339	0.263843
C	2.837676	0.407510	-0.868458
C	1.652028	-0.210406	-1.244083
C	1.146053	-1.267172	-0.483119
C	1.834397	-1.705736	0.646468
C	3.025059	-1.090327	1.023773
H	3.566438	-1.426684	1.900952
H	1.433376	-2.531466	1.225633
Se	-0.498438	-2.106319	-0.973739
C	-1.654833	-0.911034	0.084052
C	-1.575033	0.510263	-0.408363
C	-1.789133	0.819221	-1.755555
C	-1.792990	2.141028	-2.183966
C	-1.561502	3.173418	-1.273992
C	-1.323628	2.872705	0.065046
C	-1.335182	1.545667	0.496398
H	-1.186314	1.308772	1.545756
H	-1.135968	3.669766	0.777826
H	-1.562819	4.205751	-1.609196
H	-1.976961	2.369239	-3.229073
H	-1.930407	0.008338	-2.465599
C	-3.075076	-1.490317	0.013507
C	-4.089983	-0.661588	0.781549
N	-3.652608	-0.314568	2.099356
H	-3.311394	-1.136141	2.595813
C	-4.666862	0.390483	2.868554
H	-4.265037	0.663304	3.847064
H	-5.590813	-0.192491	3.012658
H	-4.924412	1.302025	2.322424
H	-5.096598	-1.114920	0.736394
H	-4.282395	0.359032	0.204917
H	-3.398430	-1.563871	-1.031749
H	-3.052659	-2.516348	0.408502
H	-1.289384	-0.960937	1.112042
H	1.107161	0.128930	-2.118904
H	3.236744	1.233240	-1.449924
O	-4.602668	1.656744	-0.197561
H	-3.700727	2.027285	-0.105978

SeFl-C15-rad

Bond Energy -3411.29886394 a.u.

F	5.709460	-0.314265	0.276133
C	4.704275	0.511508	0.605860
F	4.875286	0.867159	1.887758
F	4.860242	1.622711	-0.131965
C	3.366616	-0.127311	0.376365
C	3.193387	-0.982948	-0.708205
C	1.941389	-1.527055	-0.963692
C	0.862620	-1.240602	-0.123219
C	1.047545	-0.389329	0.967432
C	2.293863	0.174894	1.210091
H	2.437707	0.838455	2.056254
H	0.219202	-0.158916	1.629541
Se	-0.811347	-2.059937	-0.501867
C	-2.041545	-0.646718	0.089626
C	-1.711896	0.713272	-0.474883
C	-1.219132	0.880480	-1.770690

C	-1.006388	2.155675	-2.283779
C	-1.274693	3.279796	-1.505670
C	-1.760198	3.121227	-0.210547
C	-1.977688	1.844519	0.300967
H	-2.372066	1.714674	1.306879
H	-1.967294	3.991954	0.404391
H	-1.099492	4.273958	-1.905023
H	-0.619853	2.271771	-3.291725
H	-0.981956	-0.002528	-2.357798
C	-3.463164	-1.116425	-0.322057
C	-4.532865	-0.212700	0.193502
N	-4.665888	-0.120068	1.577090
H	-4.621585	-1.021371	2.044047
C	-5.717855	0.737444	2.093098
H	-5.659433	0.774419	3.182946
H	-6.724863	0.410885	1.798570
H	-5.561062	1.750199	1.709858
H	-4.732190	0.715063	-0.336122
H	-3.514775	-1.171237	-1.414609
H	-3.607323	-2.139264	0.058983
H	-2.007794	-0.614407	1.182043
H	1.795345	-2.175226	-1.822503
H	4.033927	-1.214926	-1.354426

SeFl-TS-N16

Bond Energy -3487.65104459 a.u.

F	5.560473	0.810196	0.246850
C	4.802804	-0.049625	0.941912
F	5.526731	-1.161447	1.140058
F	4.594702	0.497271	2.150256
C	3.508495	-0.350496	0.241695
C	2.978832	0.559336	-0.667984
C	1.755985	0.290829	-1.275417
C	1.066015	-0.881054	-0.966866
C	1.605635	-1.789740	-0.054765
C	2.827971	-1.526017	0.551501
H	3.258712	-2.231326	1.255037
H	1.062260	-2.702110	0.169660
Se	-0.623124	-1.252241	-1.778941
C	-1.711316	-0.394325	-0.382261
C	-1.484701	1.096196	-0.321283
C	-1.498804	1.881901	-1.478225
C	-1.367129	3.263486	-1.395062
C	-1.208427	3.879398	-0.153962
C	-1.184058	3.103853	1.995
C	-1.323433	1.719515	0.917236
H	-1.320428	1.111833	1.818585
H	-1.052110	3.574724	1.970527
H	-1.097659	4.957479	-0.090534
H	-1.379101	3.861749	-2.301262
H	-1.575771	1.389356	-2.444312
C	-3.176124	-0.751749	-0.674334
C	-4.132541	-0.115830	0.327348
N	-3.777948	-0.483252	1.687289
H	-3.658426	-1.528143	1.791107
C	-4.649698	0.078730	2.698036
H	-4.411049	-0.354026	3.671537
H	-5.720792	-0.077972	2.488205
H	-4.480467	1.160377	2.746931
H	-5.167999	-0.404932	0.084325
H	-4.077164	0.978803	0.261087
H	-3.445570	-0.413924	-1.682679
H	-3.297259	-1.840584	-0.644600
H	-1.411351	-0.850436	0.563967
H	1.329315	0.993226	-1.983829
H	3.522646	1.467797	-0.903776
O	-4.505412	-2.755903	1.547471
H	-5.396849	-2.486344	1.837349

SeFl-N16-rad

Bond Energy -3411.30084271 a.u.

F	5.634152	-0.123166	0.035934
C	4.623979	0.584562	0.565542
F	4.836166	0.635681	1.888838
F	4.729726	1.833201	0.088525
C	3.290818	-0.025706	0.239210
C	2.621868	0.358515	-0.919500
C	1.413825	-0.247303	-1.248788
C	0.877825	-1.231269	-0.417984
C	1.554584	-1.610315	0.742042
C	2.762680	-1.007682	1.073575
H	3.291339	-1.292053	1.977482
H	1.125638	-2.376196	1.380317
Se	-0.792196	-2.054650	-0.846075
C	-1.908077	-0.783788	0.157407
C	-1.854482	0.604990	-0.429600
C	-2.031205	0.824856	-1.799236
C	-2.067178	2.118670	-2.307243
C	-1.915260	3.211926	-1.454722
C	-1.726088	3.001368	-0.092344
C	-1.697134	1.703905	0.416693
H	-1.560411	1.535952	1.482589
H	-1.595328	3.846456	0.576931
H	-1.936490	4.221326	-1.853664
H	-2.205681	2.275791	-3.372792
H	-2.103824	-0.033817	-2.462032
C	-3.333805	-1.353040	0.184368

C	-4.298633	-0.403294	0.890873
N	-3.819841	-0.058128	2.207355
C	-4.564709	1.043075	2.760461
H	-4.294871	1.198707	3.807066
H	-5.652276	0.887482	2.685406
H	-4.336109	1.962619	2.197141
H	-5.289305	-0.879488	0.988120
H	-4.453885	0.502771	0.281413
H	-3.687444	-1.529851	-0.839329
H	-3.314758	-2.319291	0.699767
H	-1.523688	-0.766303	1.179681
H	0.875869	0.050189	-2.142896
H	3.040328	1.132441	-1.554328

SeFl-TS-C17

Bond Energy -3487.64707333 a.u.

F	5.071361	1.694733	0.766326
C	4.923922	0.379207	0.979640
F	5.967313	-0.230389	0.395473
F	5.035483	0.166088	2.298935
C	3.616413	-0.128445	0.441806
C	3.064045	0.463038	-0.691031
C	1.883192	-0.042265	-1.224276
C	1.256295	-1.132920	-0.620968
C	1.815981	-1.719147	0.514757
C	2.997862	-1.218127	1.048942
H	3.436066	-1.665348	1.935042
H	1.317993	-2.567001	0.974265
Se	-0.378031	-1.823404	-1.330018
C	-1.567476	-0.680710	-0.257155
C	-1.438089	0.778755	-0.618337
C	-1.436032	1.201734	-1.951129
C	-1.395686	2.556556	-2.261715
C	-1.346752	3.507979	-1.243518
C	-1.340820	3.094571	0.085200
C	-1.387998	1.736718	0.395986
H	-1.403527	1.409510	1.432482
H	-1.295641	3.828931	0.883833
H	-1.307318	4.565255	-1.486795
H	-1.393477	2.871554	-3.300931
H	-1.428341	0.451923	-2.738255
C	-2.997185	-1.203174	-0.460372
C	-4.019534	-0.396881	0.333652
N	-3.682520	-0.370409	1.750892
H	-3.684308	-1.316931	2.125894
C	-4.538667	0.474156	2.520039
H	-4.309111	0.409169	3.586193
H	-5.651379	0.173909	2.406446
H	-4.450887	1.511961	2.181452
H	-5.034136	-0.796977	0.176436
H	-4.016420	0.641162	-0.020866
H	-3.260647	-1.159886	-1.524435
H	-3.034791	-2.259985	-0.165982
H	-1.279686	-0.825885	0.786315
H	1.436644	0.415609	-2.100726
H	3.552168	1.318076	-1.147017
O	-6.951250	-0.428208	1.830357
H	-7.156746	0.309055	1.222437

SeFl-C17-rad

Bond Energy -3411.29739238 a.u.

F	5.616266	-0.211152	0.057628
C	4.614495	0.505356	0.591236
F	4.807694	0.515936	1.918443
F	4.754795	1.763351	0.149878
C	3.273097	-0.066376	0.230134
C	2.618862	0.376348	-0.915779
C	1.402312	-0.193649	-1.276320
C	0.843365	-1.200563	-0.489476
C	1.506367	-1.639422	0.657375
C	2.722393	-1.072272	1.020473
H	3.240502	-1.403011	1.914717
H	1.061099	-2.424668	1.260038
Se	-0.837612	-1.974912	-0.963756
C	-1.940871	-0.738775	0.098032
C	-1.858179	0.681107	-0.406051
C	-1.976568	0.979716	-1.767004
C	-1.980842	2.300502	-2.201774
C	-1.857475	3.341580	-1.282381
C	-1.731485	3.052017	0.072853
C	-1.732805	1.728286	0.508700
H	-1.654872	1.500320	1.568845
H	-1.629540	3.856489	0.794958
H	-1.854685	4.372258	-1.623255
H	-2.072868	2.518877	-3.261525
H	-2.028856	0.160688	-2.480025
C	-3.377094	-1.281265	0.071068
C	-4.337896	-0.399780	0.865876
N	-3.879019	-0.227821	2.235525
H	-3.861496	-1.099995	2.754792
C	-4.381242	0.846911	2.962967
H	-4.106783	0.879602	4.010985
H	-4.435098	1.786366	2.421507
H	-5.354969	-0.816981	0.819731
H	-4.377106	0.596954	0.413766
H	-3.731599	-1.345929	-0.965249
H	-3.377465	-2.303418	0.471721
H	-1.562653	-0.785069	1.121574

H	0.875876	0.149988	-2.160543
H	3.055051	1.167731	-1.51612

Structure and energies of the optimised selenofluoxetine derivatives. Level of theory ZORA-OLYP/TZ2P

SeFl

Bond Energy -8.57122944 a.u.

F	5.545011	0.756206	0.344867
C	4.578575	0.354221	1.207948
F	5.139573	-0.572982	2.029114
F	4.277951	1.432880	1.989574
C	3.350770	-0.176515	0.502340
C	3.070796	0.189759	-0.814731
C	1.907926	-0.263867	-1.435169
C	1.017806	-1.097336	-0.751576
C	1.309619	-1.471760	0.565604
C	2.460514	-1.005822	1.192402
H	2.672713	-1.304538	2.214309
H	0.644009	-2.140420	1.102821
Se	-0.536095	-1.783638	-1.668578
C	-2.019352	-0.907414	-0.602664
C	-2.009211	0.594355	-0.727675
C	-2.275738	1.251687	-1.938690
C	-2.282747	2.641310	-2.014155
C	-2.016773	3.411281	-0.879999
C	-1.744289	2.774264	0.328249
C	-1.741636	1.381048	0.400990
H	-1.534451	0.897719	1.352358
H	-1.532189	3.360120	1.219406
H	-2.018928	4.496653	-0.941049
H	-2.491576	3.127028	-2.964497
H	-2.462439	0.673950	-2.839375
C	-3.319951	-1.600405	-1.043005
C	-4.527874	-1.302941	-0.143732
N	-4.367450	-1.851535	1.199604
H	-4.274670	-2.861645	1.133455
C	-5.473735	-1.537044	2.095687
H	-5.318806	-2.044	3.055296
H	-6.469313	-1.827727	1.711585
H	-5.495960	-0.458490	2.287660
H	-5.433803	-1.683934	-0.654286
H	-4.662997	-0.219562	-0.049774
H	-3.577935	-1.311724	-2.066769
H	-3.155678	-2.685093	-1.063693
H	-1.813322	-1.185474	0.430269
H	1.691331	0.039170	-2.454696
H	3.751912	0.834513	-1.360213

H_2O_2

Bond Energy -0.65281998 a.u.

O	-0.015407	-0.730641	-0.690438
O	0.015407	0.730641	-0.690438
H	0.800760	0.883499	-0.140076
H	-0.800760	-0.883499	-0.140076

***R*-*S*-SeFl-RCox**

Bond Energy -9.22904476 a.u.

F	5.609249	0.945069	0.448017
C	4.641500	0.372935	1.206730
F	5.215257	-0.669491	1.864092
F	4.294777	1.288621	2.157634
C	3.441687	-0.058322	0.392077
C	3.180056	0.517109	-0.851729
C	2.043102	0.146883	-1.568303
C	1.163404	-0.809667	-1.054271
C	1.434030	-1.392570	0.189253
C	2.559530	-1.010863	0.912174
H	2.757266	-1.469809	1.875925
H	0.775038	-2.153777	0.594485
Se	-0.356391	-1.355045	-2.116016
C	-1.888069	-0.733011	-0.937408
C	-1.939152	0.768045	-0.820326
C	-2.237489	1.598743	-1.911377
C	-2.304341	2.980900	-1.762810
C	-2.069635	3.568771	-0.518279
C	-1.766879	2.758426	0.573414
C	-1.702530	1.373244	0.421559
H	-1.473703	0.752444	1.283906
H	-1.579894	3.202093	1.548333
H	-2.120083	4.648621	-0.403812
H	-2.536990	3.603624	-2.623409
H	-2.404668	1.165927	-2.893590
C	-3.157366	-1.402448	-1.490516

C	-4.357957	-1.341649	-0.535041
N	-4.115593	-2.076984	0.700816
H	-3.908069	-3.046667	0.477327
C	-5.229896	-2.031109	1.638584
H	-5.001368	-2.659551	2.504865
H	-6.195830	-2.365849	1.216281
H	-5.365742	-1.005496	2.293
H	-5.244555	-1.710472	-1.087159
H	-4.573345	-0.299692	-0.270944
H	-3.451218	-0.943101	-2.439332
H	-2.944454	-2.454819	-1.710180
H	-1.666843	-1.166474	0.036882
H	1.840317	0.610815	-2.528458
H	3.855077	1.259285	-1.264725
O	-0.747872	-5.043395	0.014239
O	-0.957600	-4.877232	-1.422785
H	-0.636469	-3.960690	-1.546187
H	-0.021289	-5.687113	0.004712

***R*-*R*-SeFl-RCox**

Bond Energy -9.22801464 a.u.

F	5.468356	1.127552	0.632624
C	4.579	0.535314	1.458239
F	5.242517	-0.408482	2.167392
F	4.172764	1.486044	2.353582
C	3.388112	-0.044295	0.710965
C	3.006380	0.478351	-0.525673
C	1.886841	-0.027050	-1.184294
C	1.140387	-1.061594	-0.613562
C	1.530277	-1.587865	0.623029
C	2.642740	-1.077739	1.285771
H	2.934943	-1.495741	2.243895
H	0.970100	-2.404812	1.067582
Se	-0.370193	-1.819103	-1.553275
C	-1.917058	-0.916815	-0.586861
C	-1.885825	0.584884	-0.685233
C	-2.123128	1.270409	-1.886753
C	-2.110776	2.661597	-1.930549
C	-1.858572	3.402866	-0.774722
C	-1.617539	2.736951	0.424928
C	-1.630674	1.342995	0.466269
H	-1.447051	0.836140	1.410315
H	-1.417702	3.300683	1.332979
H	-1.847359	4.489285	-0.811840
H	-2.293742	3.169055	-2.874573
H	-2.304170	0.720691	-2.804942
C	-3.188294	-1.598391	-1.118193
C	-4.444376	-1.315570	-0.281442
N	-4.360523	-1.891788	1.057122
H	-4.274505	-2.901430	0.976192
C	-5.509544	-1.582639	1.900100
H	-5.409810	-2.105372	2.856424
H	-6.486149	-1.855578	1.458816
H	-5.531386	-0.507801	2.111632
H	-5.320647	-1.682423	-0.850470
H	-4.581338	-0.233862	-0.173401
H	-3.386211	-1.288426	-2.148572
H	-3.026625	-2.683439	-1.150101
H	-1.770919	-1.214384	0.451157
H	1.597462	0.392371	-2.142059
H	3.577513	1.280578	-0.981133
O	-1.400364	-0.504148	-5.486609
O	-0.028052	-0.583018	-4.990730
H	-0.186855	-0.900242	-4.079206
H	-1.394300	-1.241626	-6.117788

***R*-*S*-SeFl-TSox**

Bond Energy -9.19767611 a.u.

F	5.434269	1.245720	0.508609
C	4.561344	0.525074	1.256034
F	5.262529	-0.486966	1.824883
F	4.148206	1.337169	2.271477
C	3.383880	0.021266	0.446144
C	2.986984	0.690914	-0.712574
C	1.874946	0.249451	-1.426545
C	1.160521	-0.861546	-0.974964
C	1.556470	-1.543722	0.176915
C	2.665588	-1.093877	0.887607
H	2.976150	-1.626951	1.780549
H	1.018416	-2.430231	0.496176
Se	-0.343403	-1.493244	-2.021482
C	-1.903146	-0.829437	-0.906400
C	-1.905962	0.672687	-0.821810
C	-2.193960	1.488504	-1.927094
C	-2.213127	2.875399	-1.806613
C	-1.945737	3.478815	-0.576753
C	-1.657037	2.681823	0.529103
C	-1.635072	1.293321	0.405701
H	-1.416358	0.682278	1.277219
H	-1.448067	3.139348	1.492865
H	-1.962497	4.561633	-0.483148
H	-2.438032	3.487960	-2.676258
H	-2.399321	1.042676	-2.896341
C	-3.165942	-1.487728	-1.479962
C	-4.394081	-1.352167	-0.566491
N	-4.189082	-1.978868	0.732160
H	-3.943634	-2.956401	0.601444

C	-5.342642	-1.885473	1.617561
H	-5.135945	-2.434792	2.540895
H	-6.281663	-2.278621	1.185525
H	-5.516618	-0.837593	1.887577
H	-5.260435	-1.768908	-1.117028
H	-4.620093	-0.292594	-0.397594
H	-3.418744	-1.059574	-2.454997
H	-2.963894	-2.551069	-1.641795
H	-1.685403	-1.264092	0.068689
H	1.572063	0.775898	-2.326360
H	3.541201	1.554216	-1.065072
O	-0.339999	-5.283790	-0.425126
O	-0.531273	-3.394180	-1.122031
H	0.035994	-4.001265	-1.633560
H	-1.256214	-5.530478	-0.619364

***R*-*R*-SeFl-TSox**

Bond Energy -9.19546902 a.u.

F	5.418257	1.269472	0.084459
C	4.601943	0.757586	1.037736
F	5.351911	-0.078672	1.799979
F	4.232501	1.796034	1.840966
C	3.389926	0.063805	0.449271
C	2.876868	0.468910	-0.784719
C	1.735375	-0.136648	-1.305015
C	1.102569	-1.146506	-0.580774
C	1.614183	-1.562004	0.651541
C	2.755193	-0.952982	1.167062
H	3.150991	-1.279189	2.123281
H	1.133709	-2.359198	1.211157
Se	-0.446850	-2.054058	-1.302444
C	-2.001175	-0.988909	-0.498501
C	-1.838267	0.501978	-0.554949
C	-1.999980	1.243021	-1.737143
C	-1.885891	2.630972	-1.720437
C	-1.610551	3.307756	-0.531820
C	-1.443915	2.583408	0.647390
C	-1.554328	1.194779	0.632488
H	-1.431954	0.641293	1.560343
H	-1.229622	3.097631	1.580990
H	-1.525699	4.391625	-0.525246
H	-2.010399	3.185890	-2.647003
H	-2.187206	0.740750	-2.679184
C	-3.257410	-1.576273	-1.156425
C	-4.551534	-1.233165	-0.404396
N	-4.603881	-1.850375	0.918071
H	-4.608115	-2.861073	0.807979
C	-5.772761	-1.460245	1.699701
H	-5.780907	-2.016150	2.642282
H	-6.738944	-1.631118	1.190734
H	-5.711339	-0.394223	1.944696
H	-5.402490	-1.524427	-1.048694
H	-4.624664	-0.148222	-0.272762
H	-3.340919	-1.230070	-2.188607
H	-3.167879	-2.669850	-1.207207
H	-1.956887	-1.320719	0.540454
H	1.343678	0.166122	-2.269154
H	3.367403	1.254767	-1.349573
O	-0.894278	-0.782661	-5.175376
O	-0.589101	-1.191909	-3.225045
H	-0.537974	-1.949903	-3.837112
H	-0.069413	-0.285328	-5.277678

***R*-*S*-SeFl-PCox**

Bond Energy -9.29112167 a.u.

F	5.255740	0.876982	1.004005
C	4.344196	0.131480	1.679447
F	5.005742	-0.928543	2.204808
F	3.919953	0.891322	2.731644
C	3.181202	-0.286636	0.803682
C	2.739682	0.562284	-0.214705
C	1.640572	0.205201	-0.992868
C	0.982359	-0.995895	-0.736679
C	1.423078	-1.856173	0.263238
C	2.521913	-1.496163	1.039859
H	2.869133	-2.165239	1.820396
H	0.920578	-2.806619	0.418562
Se	-0.528928	-1.572332	-1.877218
C	-2.042948	-0.675141	-0.761370
C	-2.046525	0.801961	-1.011983
C	-2.393565	1.349646	-2.259024
C	-2.393343	2.727459	-2.463248
C	-2.050367	3.593179	-1.424361
C	-1.703116	3.066487	-0.180992
C	-1.696608	1.687720	0.019704
H	-1.426915	1.290539	0.994739
H	-1.436510	3.730284	0.637783
H	-2.054939	4.668461	-1.583154
H	-2.663969	3.126301	-3.437834
H	-2.666686	0.698265	-3.084730
C	-3.325585	-1.446495	-1.076564
C	-4.448758	-1.216035	-0.052652
N	-4.094958	-1.705353	1.274650
H	-3.896646	-2.700682	1.218137
C	-5.129137	-1.481380	2.277318
H	-4.821540	-1.936068	3.223977
H	-6.121950	-1.886664	2.007237
H	-5.247578	-0.405773	2.450562

H	-5.367457	-1.687514	-0.452983
H	-4.666323	-0.144472	0.030642
H	-3.708258	-1.179067	-2.066734
H	-3.091063	-2.516627	-1.109593
H	-1.730761	-0.892930	0.260243
H	1.313729	0.867273	-1.789821
H	3.255012	1.497023	-0.410312
O	1.277128	-5.157992	-2.647144
O	-0.701913	-3.188032	-1.515424
H	0.597823	-4.555425	-2.298889
H	0.778256	-5.932554	-2.931306

***R*-*R*-SeFl-PCox**

Bond Energy -9.29051152 a.u.

F	5.426354	1.235948	0.831805
C	4.491907	0.641802	1.613655
F	5.134191	-0.289625	2.365572
F	4.036814	1.594958	2.477633
C	3.356426	0.043698	0.809369
C	3.040799	0.550195	-0.453650
C	1.965344	0.027047	-1.168886
C	1.206055	-0.993321	-0.609154
C	1.518643	-1.516391	0.644607
C	2.592934	-0.991369	1.358133
H	2.839478	-1.395299	2.334803
H	0.941649	-2.331845	1.074971
Se	-0.261406	-1.778674	-1.669091
C	-1.857767	-0.850011	-0.692455
C	-1.778109	0.641262	-0.724921
C	-2.034294	1.382038	-1.891272
C	-1.963503	2.773432	-1.879113
C	-1.641141	3.456964	-0.707198
C	-1.383649	2.735102	0.458130
C	-1.447288	1.344376	0.445803
H	-1.250544	0.794604	1.362753
H	-1.134449	3.254965	1.379991
H	-1.592566	4.543020	-0.701210
H	-2.162054	3.325999	-2.794216
H	-2.279507	0.876578	-2.818013
C	-3.121730	-1.500135	-1.267950
C	-4.368858	-1.285479	-0.397085
N	-4.267232	-1.967416	0.890960
H	-4.219507	-2.969570	0.726109
C	-5.386073	-1.694782	1.787036
H	-5.278151	-2.294875	2.695914
H	-6.380411	-1.904778	1.352025
H	-5.370467	-0.640118	2.083257
H	-5.251733	-1.605416	-0.982105
H	-4.501441	-0.215695	-0.201649
H	-3.328769	-1.123079	-2.271962
H	-2.962746	-2.581244	-1.381124
H	-1.695451	-1.217453	0.324581
H	1.715564	0.401560	-2.157205
H	3.633386	1.350244	-0.885077
O	-2.229772	-1.442883	-5.186968
O	-0.102959	-1.045257	-3.152733
H	-1.461636	-1.342156	-4.596854
H	-1.847461	-1.460550	-6.071734

***R*-*S*-SeFl-Ox**

Bond Energy -8.76950646 a.u.

F	5.217759	0.882612	1.022200
C	4.364011	0.038959	1.656127
F	5.092715	-1.028430	2.069675
F	3.940641	0.684121	2.782417
C	3.194713	-0.364168	0.782837
C	2.728234	0.505414	-0.206278
C	1.620934	0.155555	-0.977100
C	0.979444	-1.058963	-0.743931
C	1.445976	-1.939116	0.227056
C	2.551618	-1.587168	0.997273
H	2.916462	-2.270426	1.757639
H	0.951281	-2.897181	0.363358
Se	-0.547658	-1.640542	-1.870164
C	-2.044403	-0.722176	-0.728549
C	-2.070048	0.747719	-1.010095
C	-2.452872	1.265876	-2.259669
C	-2.470184	2.638771	-2.493935
C	-2.109166	3.530671	-1.483605
C	-1.726445	3.034143	-0.238155
C	-1.702998	1.660247	-0.007558
H	-1.406138	1.287195	0.969161
H	-1.445926	3.718060	0.559242
H	-2.127464	4.602108	-1.665828
H	-2.768737	3.013470	-3.470034
H	-2.740260	0.594045	-3.063858
C	-3.323949	-1.515384	-0.994516
C	-4.420675	-1.289893	0.058553
N	-4.023049	-1.760921	1.380309
H	-3.806628	-2.752584	1.326074
C	-5.034876	-1.548517	2.407512
H	-4.694347	-1.989036	3.349683
H	-6.026592	-1.974900	2.166801
H	-5.169845	-0.473905	2.575249
H	-5.343871	-1.778495	-0.309937
H	-4.651214	-0.220603	0.137787
H	-3.740132	-1.267090	-1.976196
H	-3.073400	-2.582411	-1.022265

H	-1.703475	-0.914761	0.288848
H	1.273719	0.835649	-1.749995
H	3.229166	1.451447	-0.383875
O	-0.708561	-3.251186	-1.514066

***R*-*R*-SeFl-Ox**

Bond Energy -8.76769791 a.u.

F	5.330906	1.138458	0.239928
C	4.467771	0.598381	1.134733
F	5.173561	-0.289954	1.883279
F	4.092399	1.604887	1.976789
C	3.265847	-0.041039	0.472449
C	2.869801	0.348912	-0.808981
C	1.735366	-0.213360	-1.391635
C	0.998064	-1.153801	-0.683007
C	1.391403	-1.561427	0.590666
C	2.524242	-0.998459	1.172272
H	2.833144	-1.312163	2.164405
H	0.831516	-2.316259	1.138525
Se	-0.553196	-2.002208	-1.574725
C	-2.063102	-0.972583	-0.560388
C	-1.937269	0.511812	-0.667588
C	-2.178628	1.200336	-1.868716
C	-2.063400	2.587459	-1.929747
C	-1.710235	3.319824	-0.796766
C	-1.464487	2.650202	0.401812
C	-1.572462	1.263367	0.462062
H	-1.383209	0.755146	1.404242
H	-1.188927	3.208239	1.293400
H	-1.626855	4.402588	-0.847053
H	-2.249213	3.098530	-2.871365
H	-2.437539	0.651505	-2.766953
C	-3.371546	-1.598598	-1.057508
C	-4.588737	-1.272704	-0.178927
N	-4.487825	-1.870955	1.149413
H	-4.477903	-2.882975	1.052883
C	-5.577424	-1.496669	2.044325
H	-5.473830	-2.038867	2.989346
H	-6.587620	-1.696525	1.641867
H	-5.516567	-0.426096	2.268998
H	-5.498630	-1.591377	-0.723035
H	-4.670775	-0.187496	-0.053423
H	-3.584155	-1.273753	-2.079585
H	-3.262451	-2.690982	-1.105494
H	-1.873537	-1.297903	0.465952
H	1.421294	0.068407	-2.392768
H	3.445398	1.087412	-1.357290
O	-0.520213	-1.402073	-3.116690

***R*-*S*-SeFl-TSelim**

Bond Energy -8.74737682 a.u.

F	4.974279	-0.936514	2.552980
C	3.950175	-1.826286	2.484698
F	4.502790	-3.061114	2.370316
F	3.323180	-1.791079	3.698138
C	2.991781	-1.515912	1.357868
C	2.776211	-0.190808	0.966118
C	1.853896	0.101498	-0.033361
C	1.136511	-0.930389	-0.647453
C	1.355155	-2.255126	-0.265327
C	2.275862	-2.544126	0.737854
H	2.443695	-3.576488	1.028294
H	0.813232	-3.055037	-0.760863
Se	-0.103394	-0.488504	-2.074563
C	-2.507573	0.208310	-0.736915
C	-2.807188	1.429418	-1.465811
C	-3.494587	1.457645	-2.698803
C	-3.783154	2.661755	-3.329502
C	-3.404539	3.875621	-2.751050
C	-2.726495	3.871055	-1.530485
C	-2.428194	2.668379	-0.902199
H	-1.899914	2.675945	0.048351
H	-2.430126	4.809344	-1.067937
H	-3.635920	4.814700	-3.246880
H	-4.309178	2.655628	-4.281060
H	-3.796043	0.530138	-3.174930
C	-3.049324	-1.087630	-0.974848
C	-3.372299	-1.998783	0.219211
N	-2.306893	-2.070706	1.208581
H	-1.481141	-2.474554	0.778753
C	-2.659093	-2.852460	2.387295
H	-1.790536	-2.919774	3.049582
H	-3.004973	-3.879784	2.167795
H	-3.458272	-2.346551	2.940944
H	-3.658152	-2.990327	-0.180783
H	-4.265087	-1.606692	0.726381
H	-3.860868	-1.116569	-1.706191
H	-2.140764	-1.649624	-1.609425
H	-1.996	0.346473	0.208727
H	1.698206	1.137997	-0.324386
H	3.326400	0.615547	1.440355
O	-0.965184	-1.947387	-2.323290

***R*-*R*-SeFl-TSelim**

Bond Energy -8.74867977 a.u.

F	5.237694	-0.091881	-1.457381
C	4.511313	0.603518	-0.544723
F	5.297017	0.761053	0.552150
F	4.322097	1.851834	-1.068828
C	3.196279	-0.066812	-0.221391
C	2.537030	-0.827578	-1.191612
C	1.302581	-1.406616	-0.913591
C	0.717130	-1.221499	0.339555
C	1.371046	-0.460838	1.313726
C	2.605273	0.115372	1.032700
H	3.107113	0.704742	1.793244
H	0.927443	-0.310754	2.295374
Se	-0.976993	-2.046051	0.786641
C	-2.880478	-0.098313	-0.170963
C	-2.167471	1.162717	-0.104884
C	-1.426364	1.703150	-1.178630
C	-0.810886	2.943869	-1.070634
C	-0.916350	3.689024	0.105869
C	-1.643827	3.174364	1.181056
C	-2.253435	1.930709	1.078817
H	-2.817423	1.538194	1.921803
H	-1.735215	3.746320	2.101208
H	-0.435269	4.660494	0.183605
H	-0.242590	3.335598	-1.910606
H	-1.327075	1.147256	-2.105048
C	-3.123961	-0.900338	-1.322835
C	-4.479560	-1.617731	-1.444980
N	-4.768518	-2.481065	-0.307647
H	-4.061252	-3.209119	-0.268112
C	-6.089165	-3.094347	-0.361591
H	-6.204775	-3.780262	0.483326
H	-6.293019	-3.658140	-1.290977
H	-6.861098	-2.321750	-0.268319
H	-4.483984	-2.160925	-2.409021
H	-5.281967	-0.869965	-1.510250
H	-2.827838	-0.449211	-2.272270
H	-2.318878	-1.831536	-1.191219
H	-3.463237	-0.345249	0.712932
H	0.796094	-2.009742	-1.660574
H	2.990319	-0.978403	-2.166311
O	-1.441897	-2.808940	-0.676512

***R*-*S*-SeFl-PCelim**

Bond Energy -8.78737727 a.u.

F	4.962890	-2.012189	3.002109
C	3.756043	-2.543778	2.680695
F	3.934967	-3.883717	2.541169
F	2.951950	-2.373060	3.773269
C	3.155859	-1.914323	1.446275
C	3.496112	-0.610443	1.075129
C	2.892055	-0.013644	-0.026474
C	1.946282	-0.720955	-0.779245
C	1.608765	-2.028027	-0.415432
C	2.205589	-2.613810	0.696387
H	1.936427	-3.629441	0.969880
H	0.887226	-2.587875	-1.863
Se	1.197935	0.149884	-2.321883
C	-3.233716	0.413258	-0.472023
C	-3.461909	1.528873	-1.401146
C	-4.014412	1.384554	-2.688392
C	-4.206345	2.486007	-3.514960
C	-3.854161	3.767389	-3.084321
C	-3.305451	3.931854	-1.813802
C	-3.111938	2.827619	-0.987531
H	-2.683126	2.969305	0.001852
H	-3.026122	4.922547	-1.463313
H	-4.005834	4.625534	-3.733955
H	-4.633724	2.344959	-4.504895
H	-4.297284	0.402430	-3.055158
C	-3.554091	-0.881183	-0.638395
C	-3.330186	-1.988775	0.351356
N	-2.541516	-1.627656	1.516670
H	-1.615157	-1.339645	1.216013
C	-2.411257	-2.706602	2.488263
H	-1.741397	-2.389281	3.292799
H	-2.021875	-3.653584	2.070023
H	-3.388381	-2.919438	2.936118
H	-2.916913	-2.861475	-0.198636
H	-4.317038	-2.329037	0.704952
H	-4.046752	-1.212218	-1.551972
H	-0.967416	-0.553130	-2.177366
H	-2.774167	0.696724	0.472855
H	3.158010	1.008621	-0.285293
H	4.227001	-0.051027	1.649789
O	-0.223417	-0.933682	-2.670730

***R*-*R*-SeFl-PCelim**

Bond Energy -8.78733884 a.u.

F	5.623680	-0.081533	-1.832517
C	5.313246	0.222269	-0.546097
F	6.353629	-0.195453	0.223404
F	5.295057	1.586368	-0.462224
C	3.999862	-0.380499	-0.109224
C	3.003511	-0.671897	-1.043332
C	1.775008	-1.184389	-0.634557

C	1.530299	-1.457	0.722934
C	2.524196	-1.105196	1.665462
C	3.749961	-0.600318	1.249631
H	4.512221	-0.377208	1.989380
H	2.351535	-1.263154	2.727761
Se	-0.122369	-2.123166	1.386316
C	-3.801787	0.296856	-0.462936
C	-3.004308	1.528209	-0.371731
C	-2.356870	2.131113	-1.467514
C	-1.617018	3.297859	-1.311331
C	-1.497657	3.900681	-0.056832
C	-2.128891	3.318898	1.040971
C	-2.868777	2.149503	0.883648
H	-3.356111	1.705261	1.748546
H	-2.044349	3.774716	2.024510
H	-0.915947	4.811192	0.061071
H	-1.125792	3.740743	-2.174515
H	-2.424863	1.684956	-2.455169
C	-4.130388	-0.393163	-1.568457
C	-4.964255	-1.641649	-1.625666
N	-5.228658	-2.265595	-0.339418
H	-4.346564	-2.567821	0.063954
C	-6.125855	-3.411919	-0.424540
H	-6.212788	-3.876144	0.562447
H	-5.806792	-4.189498	-1.143088
H	-7.126107	-3.076314	-0.720445
H	-4.492797	-2.335096	-2.353557
H	-5.933877	-1.380183	-2.079836
H	-3.803460	-0.046270	-2.547954
H	-1.584806	-1.394576	-0.214450
H	-4.186509	-0.070731	0.486719
H	1.015607	-1.419807	-1.372086
H	3.183345	-0.508003	-2.100950
O	-1.101479	-2.233188	-0.144768

Compound 6'

Bond Energy -5.14894703 a.u.

C	-3.256798	0.425114	-0.447819
C	-3.465263	1.533505	-1.388627
C	-3.948462	1.371799	-2.701340
C	-4.130634	2.465663	-3.540243
C	-3.833194	3.757226	-3.098760
C	-3.346523	3.938467	-1.805316
C	-3.163878	2.841704	-0.966449
H	-2.784237	2.997039	0.040935
H	-3.106699	4.936767	-1.446879
H	-3.975227	4.609420	-3.758450
H	-4.503309	2.310347	-4.550145
H	-4.176829	0.379743	-3.079079
C	-3.625243	-0.857224	-0.595070
C	-3.396625	-1.968972	0.388078
N	-2.528322	-1.633915	1.504618
H	-1.620671	-1.356109	1.142505
C	-2.353435	-2.725609	2.453422
H	-1.630921	-2.427636	3.219373
H	-2.005160	-3.673593	2.001826
H	-3.303905	-2.930250	2.959191
H	-3.044572	-2.857417	-0.179058
H	-4.373156	-2.272304	0.799890
H	-4.153354	-1.175749	-1.492824
H	-2.766335	0.704143	0.482622

Compound 7

Bond Energy -3.63585314 a.u.

Se	-0.425902	1.868544	0.712233
C	-1.766419	0.526881	0.390634
C	-3.035623	0.969160	-0.004977
C	-4.054763	0.050668	-0.225523
C	-3.820761	-1.318726	-0.060639
C	-2.552300	-1.753606	0.328803
C	-1.528679	-0.838310	0.561408
H	-3.239403	2.028078	-0.147536
H	-5.034295	0.405641	-0.529928
H	-2.356450	-2.812438	0.463625
H	-0.553307	-1.189026	0.880643
O	1.042504	0.828234	1.007607
H	1.462651	0.723379	0.140827
C	-4.919048	-2.310959	-0.361369
F	-4.736461	-3.497850	0.270891
F	-4.994261	-2.588069	-1.697331
F	-6.144148	-1.848790	0.004769

1-H

Bond Energy -8.51449492 a.u.

C	3.353566	-0.167137	0.545062
C	2.968038	0.409967	-0.664155
C	1.826750	-0.043243	-1.327551
C	1.067574	-1.086362	-0.786643
C	1.463432	-1.671872	0.421865
C	2.597586	-1.207170	1.087443
H	2.896197	-1.667168	2.026649
H	0.890800	-2.496231	0.836977
Se	-0.463318	-1.765800	-1.753209
C	-1.976467	-0.964874	-0.669007
C	-2.015862	0.539214	-0.752392

C	-2.326565	1.220633	-1.939518
C	-2.378476	2.610902	-1.977412
C	-2.113627	3.359023	-0.828392
C	-1.795562	2.698649	0.356043
C	-1.748287	1.304790	0.390789
H	-1.503328	0.802812	1.323423
H	-1.582446	3.267120	1.258315
H	-2.151629	4.445067	-0.859773
H	-2.621802	3.114554	-2.910141
H	-2.512939	0.661435	-2.851881
C	-3.252927	-1.690246	-1.125157
C	-4.482112	-1.429073	-0.238296
N	-4.352859	-1.895353	1.142589
C	-5.306808	-1.239081	2.025840
H	-5.128956	-1.554527	3.058920
H	-6.364133	-1.465531	1.782245
H	-5.173801	-0.154384	1.977850
H	-5.363184	-1.880219	-0.738084
H	-4.666369	-0.351720	-0.205282
H	-3.518971	-1.388239	-2.143561
H	-3.050609	-2.764209	-1.175667
H	-1.755584	-1.261858	0.356045
H	1.523623	0.415048	-2.263783
H	3.552397	1.220486	-1.093401
H	4.241445	0.188866	1.061747
C	-4.429195	-3.343885	1.271463
H	-4.269041	-3.626771	2.316339
H	-5.406514	-3.758658	0.952643
H	-3.649674	-3.827885	0.678979

***R*-*S*-1-H-RCox**

Bond Energy -9.17259827 a.u.

C	3.426242	0.031069	0.377229
C	3.039882	0.709072	-0.777975
C	1.919862	0.289888	-1.497178
C	1.185827	-0.819758	-1.065965
C	1.580282	-1.507229	0.087591
C	2.693155	-1.074983	0.808748
H	2.992258	-1.611969	1.705912
H	1.028264	-2.381044	0.419487
Se	-0.319912	-1.423755	-2.120514
C	-1.872249	-0.840297	-0.947754
C	-1.934885	0.657225	-0.796689
C	-2.250629	1.510323	-1.865494
C	-2.325788	2.888465	-1.685661
C	-2.081012	3.450950	-0.431393
C	-1.758925	2.618646	0.638141
C	-1.687068	1.237756	0.454729
H	-1.440476	0.599657	1.299441
H	-1.562466	3.042116	1.620274
H	-2.138313	4.527652	-0.292490
H	-2.572888	3.528135	-2.529739
H	-2.425354	1.098219	-2.855182
C	-3.125702	-1.507689	-1.535845
C	-4.370502	-1.407218	-0.636570
N	-4.242768	-2.068618	0.660950
C	-5.220208	-1.570418	1.618571
H	-5.043619	-2.030186	2.596127
H	-6.269486	-1.783432	1.331710
H	-5.114113	-0.487444	1.731995
H	-5.233269	-1.799868	-1.212001
H	-4.581735	-0.350752	-0.449064
H	-3.383314	-1.054612	-2.498782
H	-2.907400	-2.558196	-1.746240
H	-1.657970	-1.292490	0.020208
H	1.614598	0.826906	-2.389910
H	3.605723	1.572109	-1.120649
O	-0.060380	-5.233645	-0.194885
O	-0.632092	-4.964027	-1.512297
H	-0.418291	-4.012576	-1.612990
H	0.706974	-5.770610	-0.450313
C	-4.285318	-3.523403	0.575099
H	-4.128444	-3.951081	1.569797
H	-5.250989	-3.905513	0.188236
H	-3.489359	-3.901455	-0.068767
H	4.296856	0.361038	0.938545

***R*-*R*-1-H-RCox**

Bond Energy -9.17186777 a.u.

C	3.411879	-0.045282	0.724896
C	2.985478	0.567574	-0.452645
C	1.878009	0.072964	-1.142782
C	1.193283	-1.045173	-0.655575
C	1.627283	-1.664779	0.522147
C	2.730188	-1.161104	1.211560
H	3.060692	-1.647799	2.126161
H	1.108752	-2.543282	0.895035
Se	-0.295890	-1.791643	-1.638624
C	-1.874622	-0.979346	-0.646632
C	-1.900891	0.525102	-0.698057
C	-2.181720	1.237872	-1.874171
C	-2.223001	2.629255	-1.875241
C	-1.981625	3.344624	-0.700947
C	-1.695846	2.651993	0.473544
C	-1.655580	1.257968	0.471779
H	-1.435534	0.729909	1.396229
H	-1.502443	3.195200	1.395543

H	-2.012871	4.431346	-0.704582
H	-2.439412	3.157566	-2.800635
H	-2.355450	0.709638	-2.806246
C	-3.119179	-1.694262	-1.195795
C	-4.396434	-1.452066	-0.373081
N	-4.343296	-1.949513	1.001806
C	-5.336688	-1.304169	1.849388
H	-5.214660	-1.643873	2.882843
H	-6.381570	-1.515878	1.546729
H	-5.192809	-0.219984	1.832673
H	-5.247433	-1.890937	-0.931870
H	-4.582052	-0.375578	-0.327065
H	-3.325299	-1.369025	-2.220366
H	-2.915326	-2.767666	-1.257159
H	-1.713552	-1.300608	0.382431
H	1.548108	0.559163	-2.055100
H	3.512823	1.436711	-0.838396
O	-1.419486	-0.490093	-5.494878
O	-0.043196	-0.423666	-5.008691
H	-0.158698	-0.766019	-4.098671
H	-1.343141	-1.229501	-6.119095
C	-4.438005	-3.399859	1.093588
H	-4.333659	-3.707677	2.138451
H	-5.401048	-3.798084	0.715987
H	-3.633261	-3.877919	0.530571
H	4.274849	0.342675	1.260354

***R*-*S*-1-H-TSox**

Bond Energy -9.14253720 a.u.

C	3.385486	0.026386	0.522768
C	3.015980	0.724089	-0.626594
C	1.922347	0.300540	-1.382239
C	1.204419	-0.827407	-0.976008
C	1.574539	-1.541631	0.165929
C	2.665705	-1.103076	0.915038
H	2.959161	-1.656747	1.803470
H	1.031780	-2.438713	0.445721
Se	-0.269704	-1.432429	-2.076351
C	-1.856723	-0.880850	-0.940430
C	-1.925092	0.619257	-0.831893
C	-2.262421	1.436609	-1.922076
C	-2.339714	2.819771	-1.783372
C	-2.081456	3.418999	-0.549581
C	-1.743095	2.620844	0.541323
C	-1.663598	1.236208	0.399386
H	-1.404859	0.624445	1.259292
H	-1.547	3.074838	1.508132
H	-2.143466	4.498869	-0.441534
H	-2.602438	3.432622	-2.642203
H	-2.460826	0.994631	-2.894455
C	-3.093552	-1.586044	-1.513162
C	-4.335055	-1.474179	-0.608707
N	-4.165423	-2.013506	0.737483
C	-5.206857	-1.536784	1.637227
H	-5.006100	-1.893663	2.652051
H	-6.223724	-1.876151	1.356064
H	-5.210456	-0.442704	1.659525
H	-5.175737	-1.960024	-1.145252
H	-4.603438	-0.418527	-0.507567
H	-3.364430	-1.162816	-2.486097
H	-2.850786	-2.635548	-1.686561
H	-1.611962	-1.317735	0.027349
H	1.632731	0.848241	-2.274181
H	3.576343	1.601554	-0.939347
O	-0.250984	-5.353604	-0.808390
O	-0.439375	-3.419259	-1.355074
H	0.238435	-3.928644	-1.835484
H	-1.083807	-5.627232	-1.220447
C	-4.058158	-3.468421	0.774714
H	-3.910195	-3.792589	1.808714
H	-4.961533	-3.977507	0.384502
H	-3.194606	-3.812603	0.203913
H	4.238691	0.358234	1.108994

***R*-*R*-1-H-TSox**

Bond Energy -9.14042289 a.u.

C	3.397532	0.097568	0.490096
C	2.889647	0.528329	-0.735265
C	1.763777	-0.081939	-1.287940
C	1.148416	-1.127439	-0.598033
C	1.655377	-1.572917	0.626657
C	2.780953	-0.953275	1.169383
H	3.176651	-1.297975	2.121484
H	1.182939	-2.397246	1.153602
Se	-0.370049	-2.050738	-1.362390
C	-1.966875	-1.062449	-0.550735
C	-1.854366	0.434732	-0.567663
C	-2.032632	1.199854	-1.731950
C	-1.964617	2.590035	-1.680
C	-1.719340	3.245880	-0.473225
C	-1.535338	2.497661	0.688392
C	-1.599830	1.106954	0.637957
H	-1.462018	0.534395	1.551982
H	-1.343077	2.994896	1.636033
H	-1.670764	4.331537	-0.439181
H	-2.101167	3.163307	-2.593667
H	-2.195815	0.715447	-2.687739
C	-3.195182	-1.677294	-1.234977

C	-4.514803	-1.374293	-0.504362
N	-4.602185	-1.923624	0.849529
C	-5.592591	-1.222291	1.656663
H	-5.573556	-1.610315	2.680020
H	-6.627541	-1.327259	1.275978
H	-5.353047	-0.155851	1.696737
H	-5.343760	-1.732368	-1.145693
H	-4.629904	-0.289773	-0.430945
H	-3.279407	-1.309208	-2.259938
H	-3.063503	-2.761709	-1.315891
H	-1.921790	-1.416269	0.481230
H	1.369905	0.240269	-2.245048
H	3.371023	1.343857	-1.269204
O	-0.847276	-0.666653	-5.198723
O	-0.534903	-1.139867	-3.264237
H	-0.445167	-1.883299	-3.887694
H	-0.045333	-0.128080	-5.267725
C	-4.834176	-3.361978	0.871156
H	-4.042677	-3.891674	0.335856
H	-4.824715	-3.718776	1.905510
H	-5.802716	-3.653135	0.418883
H	4.276698	0.576411	0.913700

***R*-*S*-1-H-PCox**

Bond Energy -9.23622177 a.u.

C	3.335169	-0.186056	0.567986
C	2.855099	0.747650	-0.350136
C	1.767546	0.430855	-1.165640
C	1.165520	-0.820961	-1.043590
C	1.644015	-1.767610	-0.140725
C	2.731861	-1.440756	0.669271
H	3.110297	-2.173122	1.378343
H	1.186053	-2.749602	-0.078282
Se	-0.319623	-1.285898	-2.261558
C	-1.886703	-0.773003	-0.985051
C	-1.979860	0.720661	-0.908482
C	-2.389905	1.503501	-2.001535
C	-2.470104	2.890755	-1.902607
C	-2.145272	3.531588	-0.706903
C	-1.734744	2.770205	0.386835
C	-1.648993	1.383619	0.284178
H	-1.330602	0.802276	1.145366
H	-1.480574	3.256553	1.325544
H	-2.212692	4.613706	-0.628802
H	-2.789876	3.473165	-2.763364
H	-2.651304	1.030439	-2.944019
C	-3.116633	-1.533836	-1.482254
C	-4.315845	-1.474683	-0.516441
N	-4.068482	-2.038587	0.808129
C	-5.034184	-1.557586	1.786125
H	-4.772181	-1.938884	2.778055
H	-6.075773	-1.869833	1.570682
H	-5.011522	-0.464392	1.829128
H	-5.172046	-1.968941	-1.019188
H	-4.602589	-0.427764	-0.380365
H	-3.459953	-1.133449	-2.442584
H	-2.832976	-2.572146	-1.670477
H	-1.560179	-1.185864	-0.030162
H	1.402075	1.158720	-1.885553
H	3.328495	1.722445	-0.438527
O	-0.464168	-5.174486	-0.392484
O	-0.340367	-2.949432	-2.301749
H	-0.422905	-4.462891	-1.057467
H	-0.177013	-5.959296	-0.873430
C	-3.995354	-3.495563	0.812349
H	-3.759120	-3.843888	1.822010
H	-4.944437	-3.974445	0.499407
H	-3.200634	-3.851848	0.156093
H	4.185226	0.060659	1.199146

***R*-*R*-1-H-PCox**

Bond Energy -9.23490329 a.u.

C	3.289629	-0.052036	1.036973
C	3.014450	0.508802	-0.210616
C	1.967866	0.014158	-0.989503
C	1.202473	-1.039317	-0.501073
C	1.474869	-1.620593	0.736946
C	2.521643	-1.117190	1.509974
H	2.740306	-1.562336	2.477559
H	0.888445	-2.460436	1.104240
Se	-0.216796	-1.795763	-1.638487
C	-1.866920	-0.920934	-0.701317
C	-1.812650	0.571801	-0.696330
C	-2.054935	1.336176	-1.850457
C	-2.008334	2.727978	-1.804109
C	-1.723491	3.389188	-0.609925
C	-1.478383	2.643767	0.543278
C	-1.518284	1.252936	0.496926
H	-1.329278	0.684613	1.404126
H	-1.257253	3.145568	1.482301
H	-1.693927	4.475540	-0.577536
H	-2.195985	3.298441	-2.710573
H	-2.271104	0.849712	-2.794376
C	-3.093657	-1.582464	-1.339516
C	-4.391186	-1.372455	-0.538739
N	-4.384897	-1.970372	0.797857
C	-5.359873	-1.341470	1.679441
H	-5.271652	-1.763554	2.685681

H	-6.408329	-1.477683	1.348245
H	-5.163045	-0.267661	1.746777
H	-5.233315	-1.750920	-1.150523
H	-4.555189	-0.298019	-0.421060
H	-3.260395	-1.196993	-2.348268
H	-2.909717	-2.655578	-1.461561
H	-1.734491	-1.307488	0.313126
H	1.743933	0.430264	-1.967420
H	3.616353	1.334996	-0.581494
O	-2.100355	-1.186140	-5.169058
O	-0.016236	-1.012844	-3.093152
H	-1.345051	-1.163288	-4.553014
H	-1.694036	-1.145583	-6.042213
C	-4.555514	-3.416988	0.777898
H	-3.774669	-3.892029	0.179284
H	-4.473187	-3.810091	1.795881
H	-5.535004	-3.734004	0.368275
H	4.107623	0.335490	1.639011

***R*-*S*-1-H-Ox**

Bond Energy -11.01446300 a.u.

C	3.233436	-0.328599	0.765608
C	2.758577	0.551826	-0.206934
C	1.656982	0.202845	-0.990344
C	1.036098	-1.027606	-0.780529
C	1.510760	-1.921943	0.174579
C	2.611694	-1.564357	0.953224
H	2.988339	-2.256026	1.703253
H	1.028571	-2.889470	0.287486
Se	-0.471401	-1.600171	-1.931176
C	-2.007685	-0.776330	-0.769449
C	-2.074963	0.702781	-0.988416
C	-2.482648	1.262642	-2.212062
C	-2.537766	2.643106	-2.389314
C	-2.189582	3.502221	-1.346640
C	-1.780520	2.964593	-0.126820
C	-1.719979	1.583499	0.046511
H	-1.400962	1.178370	1.003246
H	-1.507926	3.622246	0.695168
H	-2.237407	4.579447	-1.484256
H	-2.855525	3.049448	-3.346595
H	-2.759704	0.617330	-3.041094
C	-3.258433	-1.596623	-1.083029
C	-4.384429	-1.428799	-0.045893
N	-4.035547	-1.851924	1.309248
C	-4.945341	-1.293494	2.299383
H	-4.607965	-1.566927	3.304203
H	-5.990782	-1.644745	2.188449
H	-4.947578	-0.201401	2.231045
H	-5.274171	-1.970752	-0.426219
H	-4.665200	-0.372204	0.002273
H	-3.673288	-1.317397	-2.057384
H	-2.973986	-2.649316	-1.162817
H	-1.670101	-1.102	0.242896
H	1.296562	0.889415	-1.752051
H	3.247547	1.510595	-0.362134
O	-0.598083	-3.229612	-1.648121
C	-3.924172	-3.298282	1.451584
H	-3.611631	-3.539780	2.472027
H	-4.877266	-3.827814	1.253299
H	-3.167495	-3.697659	0.773735
H	4.094323	-0.055573	1.370788

***R*-*R*-1-H-Ox**

Bond Energy -8.71172911

C	3.279413	-0.051604	0.558513
C	2.892016	0.422384	-0.695435
C	1.773740	-0.113367	-1.335342
C	1.049302	-1.118201	-0.703239
C	1.433518	-1.612563	0.542752
C	2.551717	-1.069703	1.176887
H	2.857458	-1.447337	2.149702
H	0.878606	-2.416321	1.022927
Se	-0.467450	-1.942883	-1.666172
C	-2.027460	-1.015253	-0.627636
C	-1.960772	0.475097	-0.690302
C	-2.233094	1.188258	-1.870349
C	-2.169871	2.579885	-1.892914
C	-1.838194	3.293086	-0.741473
C	-1.560333	2.599243	0.436274
C	-1.616460	1.208266	0.457753
H	-1.399519	0.680736	1.383215
H	-1.299734	3.141898	1.341888
H	-1.795511	4.379263	-0.761627
H	-2.378831	3.109568	-2.819340
H	-2.474815	0.655609	-2.782897
C	-3.303309	-1.683246	-1.152511
C	-4.549372	-1.413153	-0.290239
N	-4.475666	-1.948825	1.069898
C	-5.389753	-1.264410	1.974771
H	-5.248931	-1.640479	2.993175
H	-6.457417	-1.399529	1.710971
H	-5.175350	-0.191896	1.979866
H	-5.432687	-1.803726	-0.833636
H	-4.688808	-0.331548	-0.213686
H	-3.522251	-1.339119	-2.167449
H	-3.143160	-2.764051	-1.235620

H	-1.828265	-1.362205	0.389873
H	1.462081	0.232397	-2.317075
H	3.462756	1.211181	-1.179911
O	-0.432749	-1.258416	-3.173735
C	-4.664433	-3.391837	1.128337
H	-3.922802	-3.906026	0.512490
H	-4.531515	-3.737662	2.158018
H	-5.668832	-3.713522	0.787959
H	4.153253	0.366497	1.051909

***R*-*S*-1-H-TSelim**

Bond Energy -8.68675303 a.u.

C	3.314624	-1.182595	1.104863
C	2.882019	0.106629	0.791402
C	1.877756	0.298722	-0.156802
C	1.306876	-0.806589	-0.796794
C	1.743246	-2.097559	-0.495469
C	2.742403	-2.280048	0.459575
H	3.081022	-3.286619	0.694647
H	1.304821	-2.948379	-1.007134
Se	-0.016541	-0.476017	-2.181047
C	-2.412847	0.077905	-0.785
C	-2.717887	1.348263	-1.427593
C	-3.400601	1.462183	-2.657820
C	-3.699449	2.706817	-3.199493
C	-3.336881	3.879148	-2.532225
C	-2.664376	3.789852	-1.312051
C	-2.356375	2.546587	-0.772853
H	-1.832002	2.490158	0.178318
H	-2.379591	4.693949	-0.779105
H	-3.576363	4.849882	-2.958379
H	-4.221917	2.764748	-4.151435
H	-3.692212	0.569738	-3.202302
C	-2.940986	-1.199294	-1.103654
C	-3.404253	-2.134719	0.035181
N	-2.453157	-2.342078	1.123334
C	-3.063679	-2.289221	2.443126
H	-2.283448	-2.352234	3.208793
H	-3.786438	-3.107822	2.633618
H	-3.586725	-1.337723	2.578206
H	-3.713180	-3.091814	-0.418345
H	-4.317033	-1.696191	0.455134
H	-3.687001	-1.200411	-1.903339
H	-1.955958	-1.749106	-1.697093
H	-1.906364	0.156853	0.174631
H	1.543078	1.307831	-0.388167
H	3.321776	0.967208	1.290104
O	-0.819782	-1.982175	-2.388861
C	-1.648779	-3.544341	0.951297
H	-0.849101	-3.565529	1.698073
H	-2.241581	-4.474552	1.057482
H	-1.187223	-3.547157	-0.036014
H	4.095551	-1.330643	1.846221

***R*-*R*-1-H-TSelim**

Bond Energy -8.68849359 a.u.

C	3.244808	0.445902	-0.321525
C	2.663557	-0.370961	-1.292452
C	1.501744	-1.088771	-1.010783
C	0.919556	-0.982327	0.253081
C	1.495352	-0.166678	1.232292
C	2.657778	0.544869	0.940890
H	3.103662	1.179883	1.702779
H	1.045874	-0.080326	2.219429
Se	-0.659797	-2.003576	0.721831
C	-2.802260	-0.299876	-0.193698
C	-2.222905	1.028016	-0.105279
C	-1.544922	1.662941	-1.168610
C	-1.070330	2.962709	-1.041920
C	-1.257338	3.675736	0.143979
C	-1.923584	3.067456	1.210033
C	-2.392524	1.765794	1.088489
H	-2.909871	1.301735	1.925109
H	-2.078032	3.611991	2.138524
H	-0.887685	4.693703	0.236213
H	-0.549354	3.426173	-1.876270
H	-1.384748	1.135166	-2.102816
C	-2.962630	-1.108572	-1.351038
C	-4.301830	-1.856698	-1.553913
N	-4.811421	-2.577455	-0.389945
C	-6.251979	-2.449656	-0.225178
H	-6.556318	-2.929758	0.710658
H	-6.837172	-2.913583	-1.044207
H	-6.532313	-1.393639	-0.164818
H	-4.191839	-2.522039	-2.427786
H	-5.046078	-1.104801	-1.840060
H	-2.655288	-0.639897	-2.289775
H	-2.083601	-1.986612	-1.196110
H	-3.370599	-0.611804	0.679598
H	1.051008	-1.735526	-1.757322
H	3.119584	-0.455796	-2.276330
O	-1.070259	-2.803370	-0.739917
C	-4.389305	-3.972711	-0.344295
H	-4.678618	-4.412431	0.615881
H	-4.844763	-4.584095	-1.148217
H	-3.305546	-4.043289	-0.435604
H	4.152162	1.670	-0.545875

***R*-*S*-1-H-PCelim**

Bond Energy -8.73004929 a.u.

C	3.380181	-1.371575	0.723709
C	3.997114	-0.223444	0.224948
C	3.530991	0.377059	-0.943329
C	2.449748	-0.186670	-1.631964
C	1.831330	-1.339506	-1.141981
C	2.295816	-1.919746	0.038383
H	1.807765	-2.814488	0.418317
H	0.996127	-1.778866	-1.677416
Se	1.915252	0.656903	-3.281210
C	-3.386925	-0.092477	-0.131473
C	-3.146211	1.051395	-1.019541
C	-3.326790	1.018379	-2.416622
C	-3.086889	2.142850	-3.199915
C	-2.656005	3.337140	-2.616302
C	-2.465459	3.389122	-1.236631
C	-2.705067	2.262394	-0.453593
H	-2.551618	2.316752	0.621671
H	-2.127011	4.309385	-0.766616
H	-2.468738	4.212912	-3.232134
H	-3.235701	2.087722	-4.275844
H	-3.655651	0.104504	-2.902203
C	-3.908055	-1.286834	-0.449882
C	-4.173044	-2.424635	0.502002
N	-3.486810	-2.355752	1.786439
C	-4.173718	-3.112489	2.822645
H	-3.659092	-2.973211	3.778571
H	-4.219830	-4.201467	2.621281
H	-5.197874	-2.744595	2.937057
H	-3.963091	-3.378668	-0.026569
H	-5.255231	-2.444748	0.696472
H	-4.221209	-1.495918	-1.472153
H	-0.355353	0.446631	-3.127504
H	-3.113208	0.068380	0.909501
H	4.008229	1.285079	-1.306113
H	4.838672	0.218867	0.752941
O	0.291691	-0.124314	-3.569226
C	-2.083092	-2.736323	1.688973
H	-1.585910	-2.558228	2.647547
H	-1.943463	-3.803336	1.424467
H	-1.580389	-2.131732	0.932028
H	3.739915	-1.832093	1.639922

***R*-*R*-1-H-PCelim**

Bond Energy -8.72993513 a.u.

C	4.845889	0.325141	-0.199881
C	3.768421	-0.022365	-1.014586
C	2.614990	-0.586932	-0.469546
C	2.535185	-0.791668	0.909742
C	3.608541	-0.436721	1.736158
C	4.761195	0.111742	1.176743
H	5.591349	0.383192	1.824680
H	3.551546	-0.577973	2.813589
Se	1.002112	-1.603600	1.752153
C	-4.183677	-0.084548	-0.588631
C	-3.215145	1.013170	-0.479892
C	-2.671911	1.699909	-1.583511
C	-1.757762	2.732848	-1.409093
C	-1.350147	3.114277	-0.128339
C	-1.871202	2.445492	0.977809
C	-2.788012	1.410690	0.802093
H	-3.192007	0.901026	1.674110
H	-1.563868	2.728213	1.981779
H	-0.632262	3.919654	0.002706
H	-1.354022	3.243437	-2.280312
H	-2.959253	1.421396	-2.592740
C	-4.786299	-0.544871	-1.694988
C	-5.797252	-1.660825	-1.756388
N	-5.848969	-2.538259	-0.593425
C	-7.141131	-3.192602	-0.450804
H	-7.151276	-3.783867	0.470229
H	-7.389838	-3.873276	-1.289514
H	-7.933976	-2.442118	-0.375792
H	-5.631845	-2.230315	-2.695468
H	-6.788425	-1.200373	-1.878932
H	-4.588784	-0.083798	-2.662034
H	-0.665549	-0.712158	0.468849
H	-4.436539	-0.570517	0.351766
H	1.785663	-0.865709	-1.111130
H	3.823486	0.139165	-2.088824
O	-0.211310	-1.565218	0.391681
C	-4.756591	-3.504461	-0.575613
H	-4.771543	-4.059081	0.367655
H	-4.817331	-4.237559	-1.403878
H	-3.795833	-2.991630	-0.648639
H	5.742715	0.760666	-0.632231

Compound 6

27
C11NH15

C	-3.237979	0.472901	-0.478519
C	-3.500629	1.588371	-1.396151
C	-3.910706	1.428481	-2.733899
C	-4.150628	2.529235	-3.548821

C	-3.986012	3.826626	-3.057485
C	-3.573275	4.007001	-1.738467
C	-3.331979	2.903378	-0.923758
H	-3.010104	3.057666	0.103676
H	-3.436367	5.010096	-1.341391
H	-4.172799	4.684397	-3.698538
H	-4.464127	2.375387	-4.578852
H	-4.035446	0.433107	-3.149476
C	-3.482081	-0.831183	-0.676757
C	-3.232615	-1.943302	0.309608
N	-2.316610	-1.634095	1.401410
C	-2.538242	-2.477983	2.566124
H	-1.874899	-2.162509	3.377660
H	-2.350496	-3.554119	2.377868
H	-3.569571	-2.369301	2.915303
H	-2.911566	-2.845406	-0.253195
H	-4.202433	-2.217736	0.749496
H	-3.940843	-1.169229	-1.605254
H	-2.804691	0.756757	0.478832
C	-0.921173	-1.660821	0.981266
H	-0.283450	-1.310360	1.798798
H	-0.577835	-2.673308	0.690273
H	-0.772041	-0.995949	0.128278

Compound 8

Bond Energy -3.00447930 a.u.

Se	-0.229018	1.753446	0.064112
C	-1.666618	0.470224	0.042457
C	-2.974497	0.948980	-0.100560
C	-4.038711	0.051509	-0.198858
C	-3.808511	-1.320855	-0.116205
C	-2.505574	-1.796860	0.047901
C	-1.434347	-0.908971	0.108841
H	-3.162713	2.018903	-0.122957
H	-5.051255	0.430170	-0.316024
H	-4.639913	-2.018545	-0.175312
H	-2.320356	-2.866534	0.111672
H	-0.422480	-1.290547	0.208833
O	0.664358	1.259933	1.594612
H	1.391704	0.698247	1.292068

1-CF_3

Bond Energy -9.14466765 a.u.

C	3.342526	-0.137005	0.519233
C	3.065777	0.288526	-0.780358
C	1.921248	-0.163297	-1.435774
C	1.051010	-1.059060	-0.807931
C	1.344182	-1.498541	0.488841
C	2.475356	-1.034412	1.151419
H	2.686277	-1.380289	2.158725
H	0.693720	-2.214272	0.982224
Se	-0.477926	-1.735523	-1.773181
C	-1.990935	-0.955886	-0.674016
C	-2.028865	0.549454	-0.736201
C	-2.327376	1.247337	-1.916718
C	-2.377580	2.638042	-1.935018
C	-2.123770	3.369061	-0.772673
C	-1.819234	2.691960	0.405799
C	-1.773271	1.297713	0.421121
H	-1.540448	0.782781	1.349741
H	-1.615650	3.247317	1.318248
H	-2.159920	4.455418	-0.789007
H	-2.610811	3.155355	-2.862727
H	-2.505622	0.701526	-2.838764
C	-3.266051	-1.675988	-1.142473
C	-4.488443	-1.438098	-0.239433
N	-4.342172	-1.933358	1.129427
C	-5.281370	-1.292271	2.040034
H	-5.089668	-1.629957	3.063472
H	-6.342503	-1.510339	1.806920
H	-5.145167	-0.207298	2.012896
H	-5.371919	-1.881935	-0.740854
H	-4.676138	-0.362392	-0.182374
H	-3.539005	-1.350719	-2.151677
H	-3.061588	-2.748132	-1.217774
H	-1.774119	-1.269057	0.346885
H	1.702361	0.191625	-2.437912
H	3.730116	0.984663	-1.281433
C	-4.423061	-3.384370	1.228713
H	-4.248008	-3.690107	2.264651
H	-5.406903	-3.787825	0.916417
H	-3.655130	-3.859208	0.613961
C	4.593696	0.318990	1.236074
F	4.362222	0.582090	2.550596
F	5.568190	-0.636266	1.198462
F	5.127344	1.442445	0.695220

***R*-*S*-1-CF_3-RCox**

Bond Energy -9.80232087 a.u.

C	3.412620	0.045227	0.357916
C	3.081145	0.664891	-0.847256
C	1.960364	0.246481	-1.562927
C	1.170800	-0.804452	-1.089066

C	1.515528	-1.435665	0.111708
C	2.624764	-1.007644	0.834087
H	2.878757	-1.501752	1.766861
H	0.927465	-2.268665	0.483249
Se	-0.333798	-1.404300	-2.144696
C	-1.883228	-0.837911	-0.958418
C	-1.945946	0.657967	-0.792193
C	-2.257073	1.521871	-1.853578
C	-2.331845	2.898065	-1.659429
C	-2.091694	3.446931	-0.398286
C	-1.775484	2.603521	0.664249
C	-1.703825	1.224560	0.466746
H	-1.463529	0.577639	1.306547
H	-1.583580	3.016567	1.651601
H	-2.148250	4.522133	-0.248453
H	-2.575037	3.546830	-2.497581
H	-2.428703	1.120341	-2.848150
C	-3.135635	-1.502129	-1.552326
C	-4.377342	-1.412257	-0.647180
N	-4.240295	-2.081825	0.644878
C	-5.209892	-1.588686	1.613667
H	-5.025743	-2.054940	2.586650
H	-6.261300	-1.799101	1.333710
H	-5.101844	-0.506609	1.733258
H	-5.240398	-1.804172	-1.222301
H	-4.591633	-0.357824	-0.452225
H	-3.396398	-1.039337	-2.509707
H	-2.916043	-2.550353	-1.772893
H	-1.667409	-1.301284	0.003824
H	1.698626	0.747194	-2.489647
H	3.684223	1.482904	-1.226775
O	-0.046352	-5.164540	-0.127780
O	-0.607605	-4.961682	-1.461703
H	-0.398174	-4.015718	-1.603506
H	0.716918	-5.722279	-0.348848
C	-4.285491	-3.536248	0.549857
H	-4.120631	-3.970601	1.540278
H	-5.254817	-3.914329	0.168762
H	-3.495404	-3.911193	-0.103032
C	4.643208	0.463554	1.132859
F	4.420651	0.478469	2.474156
F	5.681673	-0.396123	0.920932
F	5.082391	1.699640	0.789519

***R*-*R*-1-CF_3-RCox**

Bond Energy -9.80146839 a.u.

C	3.382708	-0.016477	0.718446
C	2.997713	0.540609	-0.501391
C	1.895102	0.031967	-1.186607
C	1.174195	-1.044199	-0.662780
C	1.571799	-1.609141	0.554585
C	2.665676	-1.095814	1.244165
H	2.961325	-1.541009	2.189144
H	1.030522	-2.456969	0.963336
Se	-0.311248	-1.803118	-1.640480
C	-1.886304	-0.984787	-0.645299
C	-1.901547	0.519699	-0.694433
C	-2.169876	1.236207	-1.871138
C	-2.200783	2.627848	-1.869579
C	-1.961401	3.338914	-0.692284
C	-1.688678	2.642364	0.482970
C	-1.658627	1.248092	0.478776
H	-1.450189	0.716962	1.404191
H	-1.497713	3.182443	1.407198
H	-1.984244	4.425776	-0.694021
H	-2.407614	3.159683	-2.795061
H	-2.342172	0.711055	-2.805318
C	-3.133399	-1.692537	-1.197690
C	-4.404682	-1.454702	-0.363902
N	-4.341165	-1.965151	1.005501
C	-5.320811	-1.320239	1.869963
H	-5.190063	-1.670719	2.898653
H	-6.370127	-1.521503	1.576553
H	-5.168977	-0.237073	1.862009
H	-5.260024	-1.886506	-0.921128
H	-4.587393	-0.378249	-0.307148
H	-3.343679	-1.356296	-2.217721
H	-2.933251	-2.766015	-1.269538
H	-1.728774	-1.310404	0.382909
H	1.597961	0.483188	-2.127414
H	3.547263	1.377483	-0.919064
O	-1.400297	-0.469132	-5.535965
O	-0.029622	-0.429672	-5.031144
H	-0.162674	-0.784858	-4.129590
H	-1.321840	-1.189613	-6.181806
C	-4.446567	-3.415842	1.084572
H	-4.332649	-3.734466	2.125113
H	-5.416960	-3.802443	0.714409
H	-3.652349	-3.895164	0.507742
C	4.598171	0.499223	1.458741
F	4.389410	0.557600	2.801437
F	5.678286	-0.312148	1.268374
F	4.965748	1.741469	1.059880

***R*-*S*-1-CF_3-TSox**

Bond Energy -9.77103164 a.u.

C	3.377339	0.025944	0.485679
C	2.978328	0.746370	-0.641645

C	1.886255	0.317405	-1.392806
C	1.193545	-0.832879	-1.010473
C	1.593726	-1.566423	0.107891
C	2.682324	-1.128662	0.857066
H	2.995373	-1.701045	1.724348
H	1.075083	-2.482153	0.372249
Se	-0.287266	-1.439377	-2.103488
C	-1.862609	-0.888690	-0.947611
C	-1.922414	0.610241	-0.823808
C	-2.264556	1.440237	-1.902918
C	-2.333576	2.822194	-1.748790
C	-2.062247	3.406802	-0.510769
C	-1.719592	2.595837	0.569287
C	-1.648351	1.212405	0.412137
H	-1.387318	0.590434	1.264061
H	-1.506624	3.038593	1.539064
H	-2.117632	4.485728	-0.390929
H	-2.600309	3.445532	-2.598717
H	-2.473701	1.009637	-2.878166
C	-3.104628	-1.584274	-1.520231
C	-4.339842	-1.473438	-0.606429
N	-4.162142	-2.023809	0.734001
C	-5.187045	-1.540494	1.649774
H	-4.978369	-1.907077	2.659446
H	-6.211014	-1.865324	1.378393
H	-5.176481	-0.446735	1.679837
H	-5.186097	-1.950947	-1.141263
H	-4.602052	-0.417300	-0.495921
H	-3.379184	-1.152243	-2.488168
H	-2.867351	-2.633760	-1.702466
H	-1.612191	-1.337586	0.013310
H	1.580629	0.884195	-2.266842
H	3.515280	1.640507	-0.940126
O	-0.183359	-5.351318	-0.834970
O	-0.419906	-3.417408	-1.365613
H	0.204235	-3.946923	-1.896655
H	-1.058577	-5.625928	-1.146344
C	-4.073297	-3.480118	0.759609
H	-3.914118	-3.813943	1.788801
H	-4.988225	-3.974983	0.378587
H	-3.222551	-3.830268	0.173129
C	4.529845	0.519694	1.336578
F	4.084621	1.309966	2.355915
F	5.222772	-0.498158	1.904166
F	5.416821	1.260452	0.625901

***R*-*R*-1-CF_3-TSox**

Bond Energy -9.76884926 a.u.

C	3.368883	0.121459	0.489617
C	2.868447	0.533036	-0.746989
C	1.750244	-0.090859	-1.296245
C	1.132874	-1.130322	-0.601628
C	1.636489	-1.556957	0.630431
C	2.753063	-0.929145	1.175153
H	3.139691	-1.260511	2.133502
H	1.167103	-2.375676	1.167957
Se	-0.382575	-2.061225	-1.364271
C	-1.977056	-1.064535	-0.551175
C	-1.855298	0.431324	-0.566542
C	-2.027425	1.198626	-1.730377
C	-1.950012	2.588231	-1.676778
C	-1.701396	3.240833	-0.468933
C	-1.524281	2.490458	0.692423
C	-1.598127	1.100318	0.640537
H	-1.467009	0.526139	1.554583
H	-1.330222	2.985582	1.640693
H	-1.645023	4.325993	-0.433688
H	-2.081918	3.163581	-2.589749
H	-2.193475	0.716388	-2.686753
C	-3.205165	-1.674453	-1.239499
C	-4.522820	-1.372607	-0.503981
N	-4.605620	-1.928367	0.847194
C	-5.587200	-1.225506	1.664388
H	-5.563732	-1.619141	2.685417
H	-6.624822	-1.322830	1.289631
H	-5.341368	-0.160691	1.708672
H	-5.353319	-1.726715	-1.145244
H	-4.636146	-0.288267	-0.425702
H	-3.289802	-1.300629	-2.262301
H	-3.076213	-2.758835	-1.325401
H	-1.934880	-1.421656	0.479781
H	1.363611	0.222398	-2.259105
H	3.344738	1.344498	-1.287088
O	-0.824501	-0.688679	-5.203044
O	-0.525662	-1.147599	-3.262650
H	-0.456441	-1.886622	-3.895845
H	-0.008	-0.174188	-5.285768
C	-4.846089	-3.365710	0.862402
H	-4.061439	-3.897327	0.318879
H	-4.831749	-3.728248	1.894626
H	-5.819229	-3.648343	0.415105
C	4.611609	0.766350	1.069694
F	4.556631	0.851275	2.424336
F	5.728754	0.046141	0.766867
F	4.812259	2.021101	0.599109

***R*-*S*-1-CF_3-PCox**

Bond Energy -9.86519385 a.u.

C	3.322806	-0.192062	0.590137
C	2.822109	0.761850	-0.299363
C	1.739214	0.449325	-1.118236
C	1.158976	-0.815360	-1.038147
C	1.661870	-1.779474	-0.169329
C	2.744771	-1.463310	0.648266
H	3.134364	-2.211162	1.331336
H	1.224063	-2.771772	-0.133028
Se	-0.323139	-1.280612	-2.265989
C	-1.890659	-0.768340	-0.988490
C	-1.984861	0.725407	-0.913860
C	-2.384576	1.507100	-2.011512
C	-2.466641	2.894307	-1.913654
C	-2.154701	3.535400	-0.714635
C	-1.755682	2.774919	0.383959
C	-1.667604	1.388331	0.282539
H	-1.359780	0.807434	1.147928
H	-1.512648	3.261711	1.325287
H	-2.223610	4.617435	-0.637535
H	-2.778057	3.476381	-2.777608
H	-2.636743	1.033582	-2.956324
C	-3.118019	-1.531832	-1.487951
C	-4.316373	-1.475464	-0.520336
N	-4.063541	-2.035068	0.804670
C	-5.027553	-1.553604	1.784740
H	-4.760988	-1.931287	2.776730
H	-6.068683	-1.869380	1.573523
H	-5.007637	-0.460278	1.824498
H	-5.170447	-1.974565	-1.021560
H	-4.607432	-0.429477	-0.386724
H	-3.462202	-1.130887	-2.447652
H	-2.832782	-2.569742	-1.676125
H	-1.565356	-1.181145	-0.033098
H	1.360546	1.197554	-1.809144
H	3.272068	1.747685	-0.356492
O	-0.427624	-5.152205	-0.360162
O	-0.332122	-2.942607	-2.305119
H	-0.406053	-4.464778	-1.049836
H	-0.158363	-5.955362	-0.820851
C	-3.987149	-3.492088	0.812629
H	-3.748102	-3.837043	1.822690
H	-4.935563	-3.973858	0.502762
H	-3.192639	-3.848369	0.155952
C	4.531950	0.134531	1.442
F	4.576257	1.447059	1.789008
F	4.562316	-0.582458	2.592774
F	5.693049	-0.134650	0.779154

***R*-*R*-1-CF_3-PCox**

Bond Energy -9.86390092 a.u.

C	3.275175	-0.018661	1.043791
C	3.011754	0.512424	-0.220718
C	1.969859	0.126	-0.991723
C	1.196430	-1.038716	-0.488765
C	1.461648	-1.590786	0.763658
C	2.501253	-1.075968	1.533135
H	2.707840	-1.499067	2.511096
H	0.872712	-2.419403	1.150559
Se	-0.217833	-1.808329	-1.628770
C	-1.868422	-0.924077	-0.699282
C	-1.806275	0.568270	-0.695398
C	-2.038283	1.332657	-1.851573
C	-1.983762	2.724184	-1.805833
C	-1.701397	3.384432	-0.610550
C	-1.467850	2.638925	0.545
C	-1.515657	1.248331	0.499509
H	-1.337532	0.682	1.408976
H	-1.249944	3.140324	1.484876
H	-1.665247	4.470528	-0.578861
H	-2.163507	3.295110	-2.713527
H	-2.253204	0.846913	-2.796132
C	-3.093541	-1.582295	-1.343826
C	-4.390709	-1.373902	-0.541476
N	-4.382829	-1.978329	0.791901
C	-5.350434	-1.347800	1.681092
H	-5.260279	-1.775660	2.684624
H	-6.400809	-1.476153	1.353635
H	-5.146804	-0.275601	1.753148
H	-5.232935	-1.748581	-1.155087
H	-4.553376	-0.299805	-0.419224
H	-3.258334	-1.192244	-2.350979
H	-2.911324	-2.655331	-1.469238
H	-1.743110	-1.311769	0.315793
H	1.756163	0.398399	-1.979239
H	3.613376	1.328766	-0.606478
O	-2.116952	-1.171191	-5.156188
O	-0.003157	-1.033262	-3.083856
H	-1.347492	-1.160618	-4.559194
H	-1.732133	-1.149641	-6.039744
C	-4.563139	-3.423991	0.765012
H	-3.788539	-3.901148	0.159893
H	-4.478323	-3.823072	1.780384
H	-5.546601	-3.732060	0.358641
C	4.431786	0.500106	1.872666
F	4.812653	1.749469	1.511172
F	5.529679	-0.299444	1.748181
F	4.130176	0.542781	3.197533

***R*-*S*-1-CF_3-Ox**

Bond Energy -9.34293670 a.u.

C	3.232578	-0.334087	0.730452
C	2.731702	0.564419	-0.215156
C	1.628825	0.216070	-0.992783
C	1.025762	-1.026452	-0.809545
C	1.526687	-1.934492	0.117571
C	2.628068	-1.584139	0.894691
H	3.020	-2.289531	1.620535
H	1.062432	-2.912445	0.213789
Se	-0.488500	-1.605741	-1.953876
C	-2.012846	-0.783531	-0.776778
C	-2.075266	0.697443	-0.985790
C	-2.476205	1.266461	-2.207315
C	-2.527923	2.648346	-2.374305
C	-2.183781	3.498669	-1.323110
C	-1.782661	2.951633	-0.104863
C	-1.724961	1.569147	0.058300
H	-1.413446	1.156531	1.014347
H	-1.514314	3.602626	0.723676
H	-2.229022	4.576926	-1.452829
H	-2.840180	3.062636	-3.329898
H	-2.751107	0.627846	-3.042283
C	-3.267867	-1.597901	-1.089640
C	-4.385636	-1.430558	-0.042979
N	-4.025899	-1.860073	1.306946
C	-4.919160	-1.295280	2.309119
H	-4.572544	-1.574387	3.309112
H	-5.968741	-1.636571	2.209330
H	-4.911809	-0.203097	2.243459
H	-5.279417	-1.968257	-0.419213
H	-4.662672	-0.373353	0.010907
H	-3.687040	-1.310774	-2.059767
H	-2.989045	-2.651580	-1.175775
H	-1.671613	-1.016461	0.232378
H	1.255254	0.918917	-1.732282
H	3.202911	1.531979	-0.354063
O	-0.598129	-3.234057	-1.665317
C	-3.927181	-3.308075	1.444612
H	-3.604821	-3.555101	2.460580
H	-4.887655	-3.827445	1.256476
H	-3.182644	-3.713556	0.756896
C	4.397522	0.065504	1.611150
F	3.966153	0.661999	2.761056
F	5.153069	-0.998008	1.983961
F	5.227722	0.950067	1.001991

***R*-*R*-1-CF_3-Ox**

Bond Energy -9.34113692 a.u.

C	3.255626	-0.028329	0.556660
C	2.877727	0.422369	-0.710171
C	1.765071	-0.127276	-1.344708
C	1.035164	-1.121171	-0.704688
C	1.414585	-1.593368	0.550927
C	2.524860	-1.042338	1.184771
H	2.820253	-1.403115	2.165011
H	0.859889	-2.388168	1.044981
Se	-0.478598	-1.952857	-1.672416
C	-2.035442	-1.019117	-0.633782
C	-1.962099	0.471103	-0.694772
C	-2.229278	1.186629	-1.874467
C	-2.160421	2.578019	-1.894628
C	-1.828412	3.287887	-0.741240
C	-1.556754	2.591611	0.436492
C	-1.618513	1.200829	0.455765
H	-1.408261	0.671466	1.381778
H	-1.296995	3.132021	1.343565
H	-1.781057	4.373822	-0.759664
H	-2.365554	3.110084	-2.820455
H	-2.472222	0.656579	-2.788233
C	-3.312934	-1.682714	-1.160258
C	-4.554457	-1.413813	-0.290476
N	-4.472987	-1.955724	1.066440
C	-5.374286	-1.268607	1.982731
H	-5.226873	-1.650375	2.997981
H	-6.444906	-1.395120	1.727827
H	-5.152137	-0.197721	1.990799
H	-5.440551	-1.800651	-0.831563
H	-4.691690	-0.332323	-0.209074
H	-3.534331	-1.332558	-2.172502
H	-3.155883	-2.763571	-1.248435
H	-1.838848	-1.369075	0.383330
H	1.461969	0.206393	-2.333204
H	3.445829	1.204046	-1.203644
O	-0.431405	-1.267231	-3.177670
C	-4.672239	-3.397858	1.122
H	-3.940630	-3.914974	0.494582
H	-4.531992	-3.749472	2.146670
H	-5.682151	-3.710033	0.787900
C	4.487469	0.528809	1.238087
F	4.309887	0.667367	2.579148
F	5.563440	-0.293172	1.071102
F	4.844711	1.744743	0.757260

***R*-*S*-1-CF_3-TSelim**

Bond Energy -9.31710873 a.u.

C	3.315421	-1.165684	1.222681
C	2.963789	0.130656	0.835280
C	2.013861	0.327890	-0.162328
C	1.405890	-0.771092	-0.778255
C	1.759583	-2.066555	-0.398883
C	2.706623	-2.260808	0.601322
H	2.979402	-3.271158	0.890090
H	1.298726	-2.916771	-0.890384
Se	0.146007	-0.439491	-2.216197
C	-2.325587	0.044432	-0.894899
C	-2.628404	1.324991	-1.514685
C	-3.275535	1.459326	-2.762242
C	-3.571588	2.712707	-3.284235
C	-3.241796	3.872790	-2.579413
C	-2.605747	3.763233	-1.341401
C	-2.300193	2.511465	-0.821384
H	-1.803664	2.438648	0.143500
H	-2.347444	4.657969	-0.780143
H	-3.478673	4.850481	-2.990765
H	-4.065789	2.787466	-4.249889
H	-3.540658	0.576602	-3.335254
C	-2.810382	-1.235639	-1.269997
C	-3.281556	-2.222877	-0.175922
N	-2.369512	-2.415652	0.947617
C	-2.983597	-2.198238	2.248781
H	-2.215123	-2.238980	3.027638
H	-3.760969	-2.945394	2.504503
H	-3.443419	-1.206375	2.287718
H	-3.510654	-3.179771	-0.668358
H	-4.240436	-1.847677	0.202549
H	-3.531151	-1.228282	-2.092721
H	-1.803632	-1.748034	-1.826496
H	-1.846155	0.105525	0.079768
H	1.752433	1.343431	-0.451522
H	3.428934	0.988515	1.309887
O	-0.612217	-1.955538	-2.482681
C	-1.648008	-3.679027	0.890263
H	-0.867827	-3.695916	1.657574
H	-2.303049	-4.557880	1.051284
H	-1.165900	-3.789710	-0.082141
C	4.303208	-1.386376	2.344641
F	3.671373	-1.518036	3.549582
F	5.039789	-2.514521	2.170559
F	5.178462	-0.356772	2.477911

***R*-*R*-1-CF_3-TSelim**

Bond Energy -9.31910635 a.u.

C	3.208953	0.484273	-0.297828
C	2.643742	-0.350439	-1.266007
C	1.497251	-1.085684	-0.979296
C	0.910249	-0.990181	0.282820
C	1.476081	-0.163038	1.258533
C	2.621602	0.569497	0.968827
H	3.052028	1.213863	1.728804
H	1.029192	-0.079632	2.246622
Se	-0.659697	-2.025732	0.740443
C	-2.800524	-0.296540	-0.217902
C	-2.214716	1.027487	-0.145642
C	-1.534766	1.645979	-1.218064
C	-1.050268	2.943202	-1.106142
C	-1.230021	3.669571	0.072973
C	-1.899526	3.078701	1.146876
C	-2.378048	1.779449	1.040659
H	-2.897485	1.328122	1.882869
H	-2.048387	3.635089	2.069100
H	-0.851894	4.685313	0.153694
H	-0.527787	3.394645	-1.945964
H	-1.382206	1.107678	-2.147528
C	-2.951392	-1.127173	-1.362567
C	-4.292636	-1.877680	-1.555276
N	-4.795841	-2.587073	-0.382591
C	-6.231937	-2.438607	-0.194943
H	-6.527098	-2.908850	0.748700
H	-6.836397	-2.899212	-1.001344
H	-6.496945	-1.378562	-0.136458
H	-4.182275	-2.551008	-2.422270
H	-5.036997	-1.128681	-1.847799
H	-2.644460	-0.670111	-2.307272
H	-2.083493	-1.995214	-1.195682
H	-3.368863	-0.597770	0.659237
H	1.059850	-1.738684	-1.728052
H	3.096421	-0.428887	-2.249275
O	-1.050504	-2.825083	-0.723896
C	-4.390034	-3.987301	-0.335916
H	-4.670512	-4.418691	0.630540
H	-4.864208	-4.596962	-1.129892
H	-3.308472	-4.071347	-0.442145
C	4.479412	1.248100	-0.589468
F	4.649636	1.489160	-1.914950
F	5.585505	0.563894	-0.172556
F	4.512396	2.453225	0.048

***R*-*S*-1-CF_3-PCelim**

Bond Energy -9.36103445 a.u.

C	3.320044	-1.135276	0.719499
C	4.082243	-0.179213	0.039853
C	3.639278	0.341259	-1.170047
C	2.427939	-0.096522	-1.721773

C	1.667922	-1.057572	-1.051822
C	2.115275	-1.570448	0.162523
H	1.515434	-2.314796	0.676208
H	0.732901	-1.407213	-1.475331
Se	1.902038	0.656488	-3.410140
C	-3.344318	-0.192135	-0.099912
C	-3.037381	0.956885	-0.960468
C	-3.240490	0.976954	-2.354797
C	-2.932758	2.103926	-3.110766
C	-2.409231	3.247875	-2.501685
C	-2.197149	3.247050	-1.124196
C	-2.505757	2.118209	-0.368720
H	-2.335272	2.131792	0.705234
H	-1.789285	4.127832	-0.634171
H	-2.171132	4.126270	-3.095829
H	-3.105620	2.092113	-4.184553
H	-3.644476	0.104589	-2.859557
C	-3.915473	-1.354583	-0.449519
C	-4.248156	-2.496330	0.476079
N	-3.584814	-2.479934	1.773906
C	-4.327310	-3.217533	2.785829
H	-3.824473	-3.117552	3.752760
H	-4.422408	-4.299626	2.566494
H	-5.334143	-2.801333	2.887317
H	-4.070629	-3.449141	-0.066276
H	-5.333831	-2.471296	0.649224
H	-4.221384	-1.530220	-1.480272
H	-0.372527	0.502785	-3.263209
H	-3.077332	-0.065698	0.947513
H	4.242957	1.093238	-1.673397
H	5.020600	0.170741	0.458117
O	0.271001	-0.114294	-3.645235
C	-2.199529	-2.926838	1.696840
H	-1.712439	-2.787638	2.666833
H	-2.105521	-3.994692	1.417076
H	-1.655310	-2.334899	0.958383
C	3.826935	-1.729508	2.011077
F	4.547386	-0.838311	2.742665
F	2.820809	-2.175482	2.808147
F	4.647877	-2.798949	1.788097

***R*-*R*-1-CF_3-PCelim**

Bond Energy -9.36088410 a.u.

C	4.700939	0.273896	-0.351356
C	3.509144	-0.049297	-1.004367
C	2.410591	-0.515649	-0.287663
C	2.494404	-0.653425	1.099553
C	3.685512	-0.326199	1.760767
C	4.780072	0.133056	1.038097
H	5.697470	0.381852	1.561904
H	3.769832	-0.423493	2.840914
Se	1.039481	-1.309921	2.171221
C	-4.107861	-0.102786	-0.597323
C	-3.134061	0.981393	-0.421557
C	-2.474435	1.630864	-1.483539
C	-1.564075	2.654806	-1.246629
C	-1.276180	3.064139	0.057763
C	-1.913213	2.432124	1.124244
C	-2.825859	1.405768	0.885995
H	-3.323664	0.927260	1.726700
H	-1.701731	2.738630	2.145888
H	-0.561771	3.863065	0.237785
H	-1.069517	3.136780	-2.086742
H	-2.667132	1.329751	-2.508673
C	-4.626388	-0.565466	-1.744589
C	-5.647942	-1.665431	-1.876196
N	-5.807569	-2.528085	-0.712085
C	-7.118432	-3.159230	-0.665973
H	-7.212	-3.739262	0.257457
H	-7.311521	-3.845318	-1.514676
H	-7.901361	-2.394790	-0.661994
H	-5.417405	-2.248025	-2.793179
H	-6.617785	-1.190035	-2.082947
H	-4.344509	-0.117353	-2.696704
H	-0.741953	-0.629327	0.913778
H	-4.446169	-0.572846	0.324135
H	1.495898	-0.775560	-0.809056
H	3.433144	0.053255	-2.082202
O	-0.269586	-1.476654	0.919610
C	-4.737368	-3.512131	-0.597174
H	-4.837436	-4.055771	0.347268
H	-4.744121	-4.253337	-1.420344
H	-3.765016	-3.015960	-0.597835
C	5.872353	0.828823	-1.124780
F	5.844533	2.195017	-1.171863
F	7.066142	0.488172	-0.571219
F	5.894855	0.399587	-2.413239

Compound 7

Bond Energy -3.63585314 a.u.

Se	-0.425902	1.868544	0.712233
C	-1.766419	0.526881	0.390634
C	-3.035623	0.969160	-0.004977
C	-4.054763	0.050668	-0.225523
C	-3.820761	-1.318726	-0.060639
C	-2.552300	-1.753606	0.328803
C	-1.528679	-0.838310	0.561408
H	-3.239403	2.028078	-0.147536
H	-5.034295	0.405641	-0.529928
H	-2.356450	-2.812438	0.463625

H	-0.553307	-1.189026	0.880643	F	-4.736461	-3.497850	0.270891
O	1.042504	0.828234	1.007607	F	-4.994261	-2.588069	-1.697331
H	1.462651	0.723379	0.140827	F	-6.144148	-1.848790	0.00476
C	-4.919048	-2.310959	-0.361369				