

# Supplementary Material

## ROS-Scavenging Selenofluoxetine Derivatives Inhibit *In Vivo* Serotonin Reuptake

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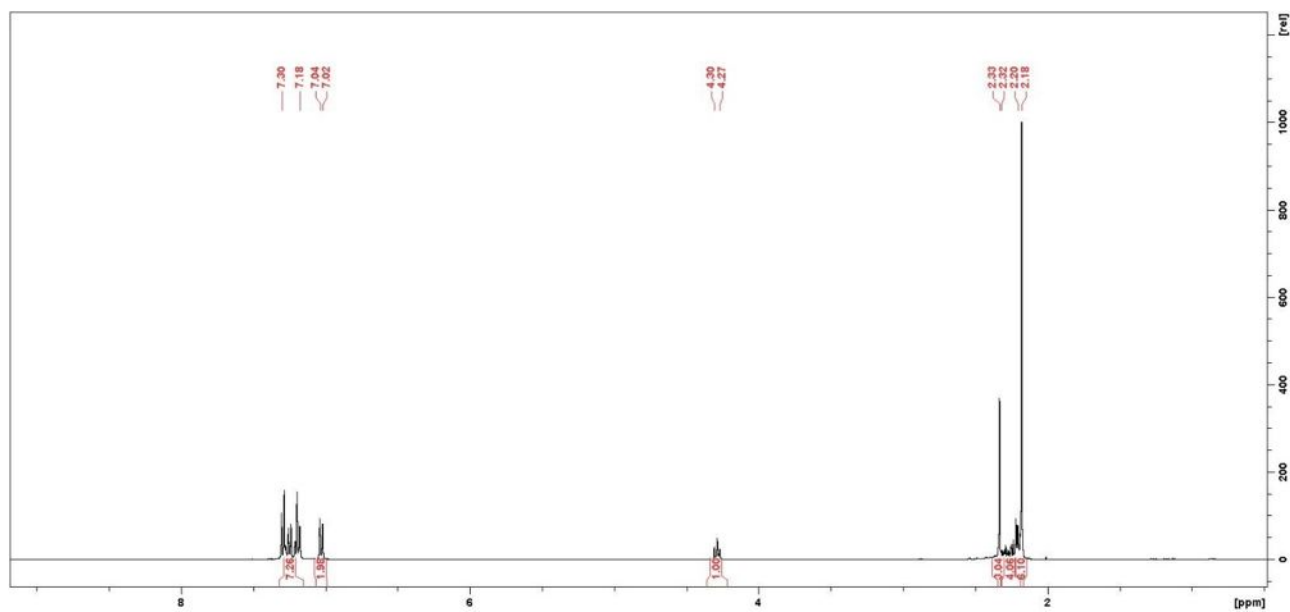
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†These authors equally contributed to this work

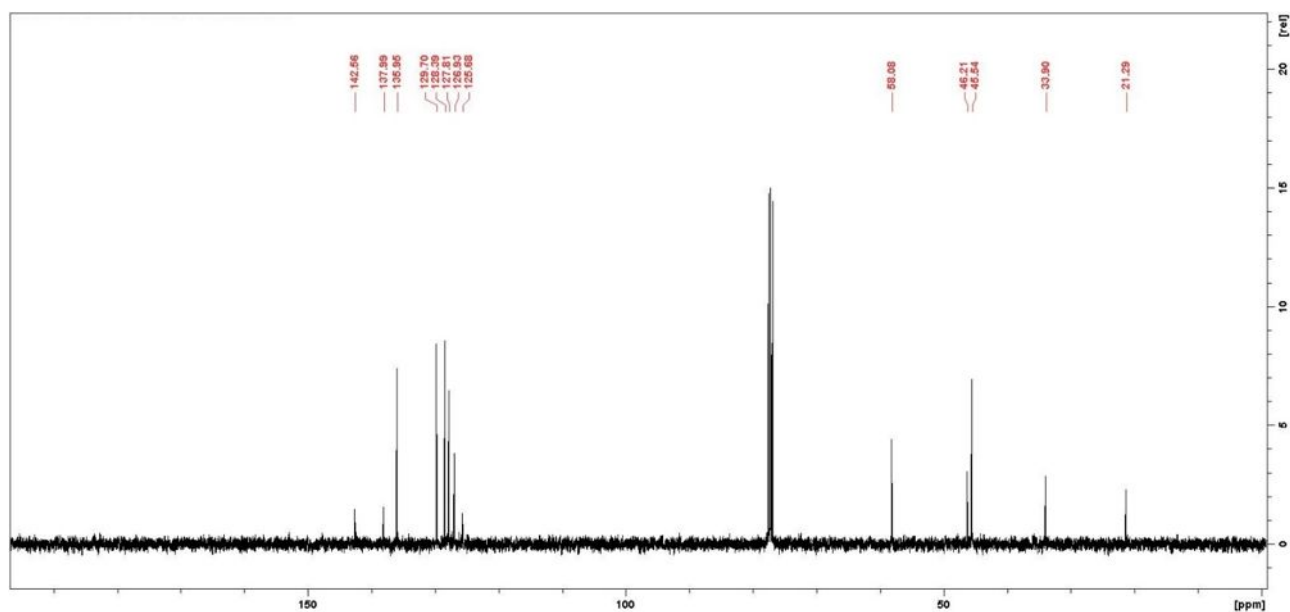
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## Chemistry

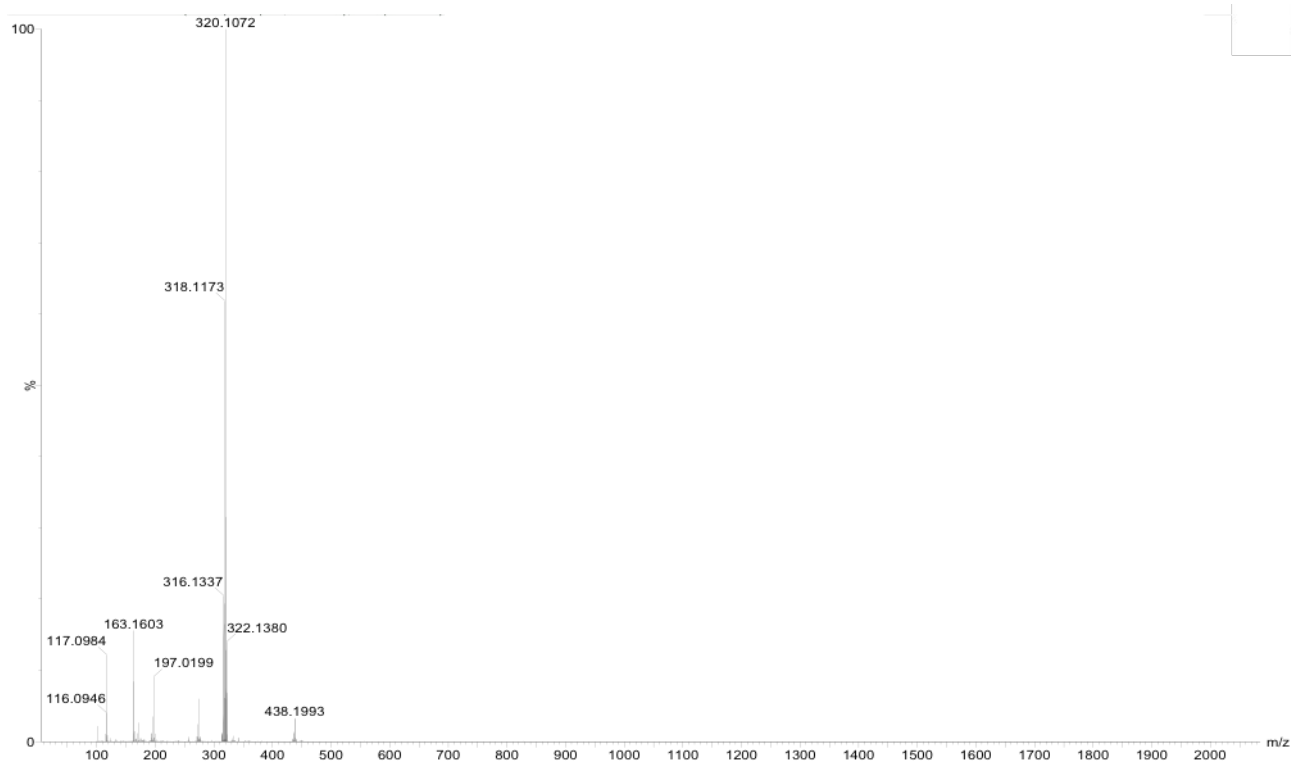
*<sup>1</sup>H-NMR, <sup>13</sup>C-NMR and ESI-MS spectra of the final compounds*



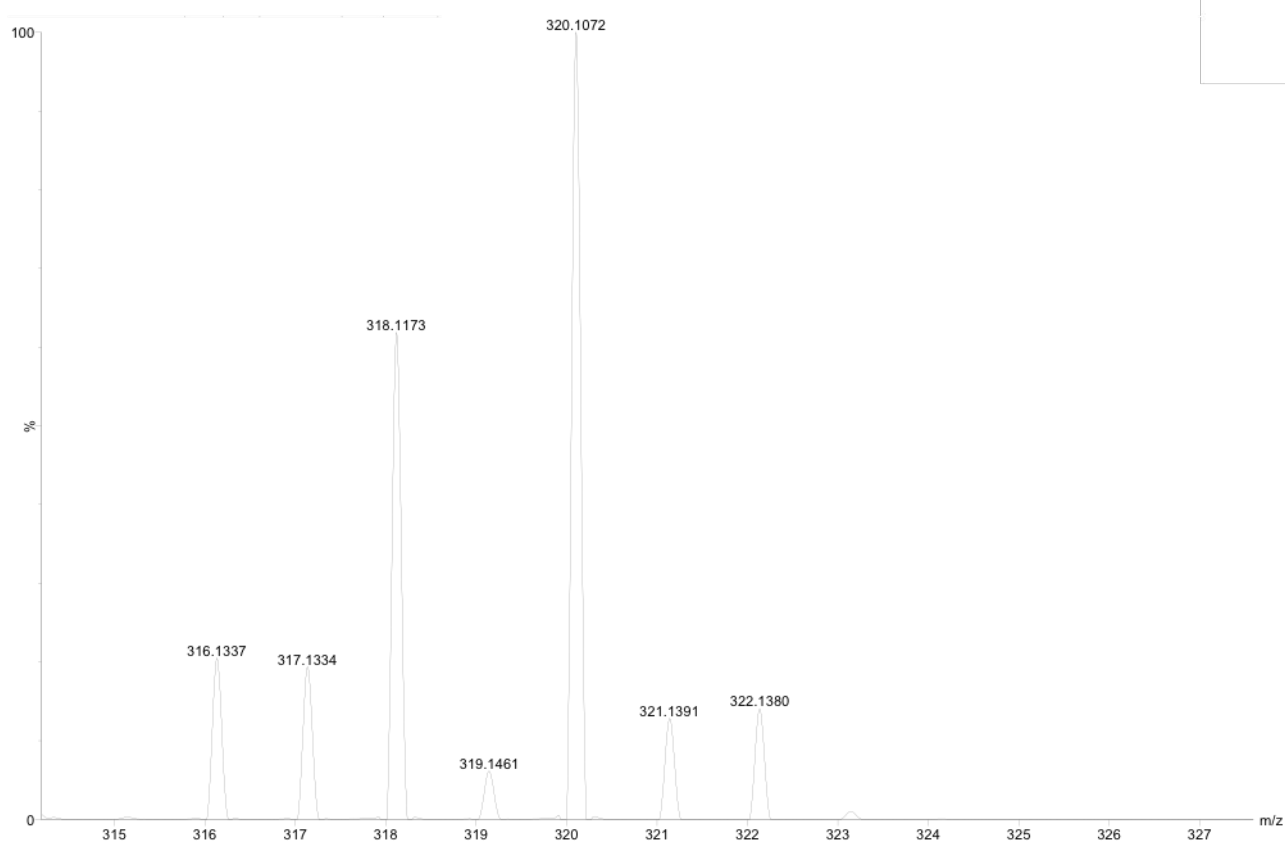
**Figure S1.** <sup>1</sup>H-NMR spectrum of compound 1-CH<sub>3</sub>.



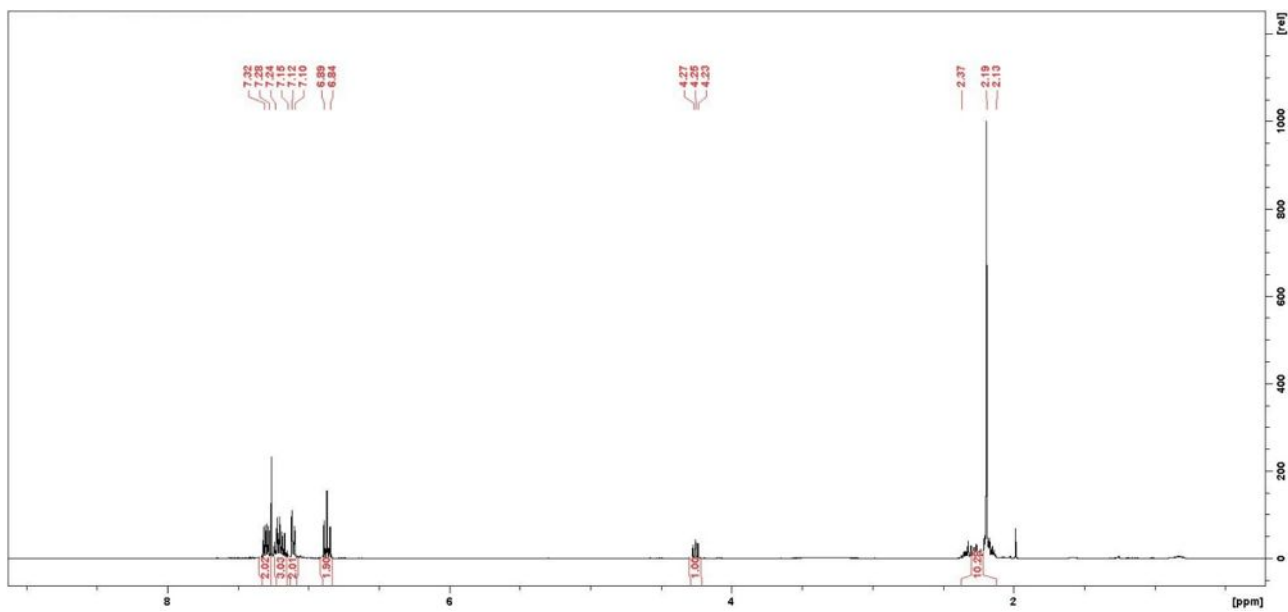
**Figure S2.** <sup>13</sup>C-NMR spectrum of compound 1-CH<sub>3</sub>.



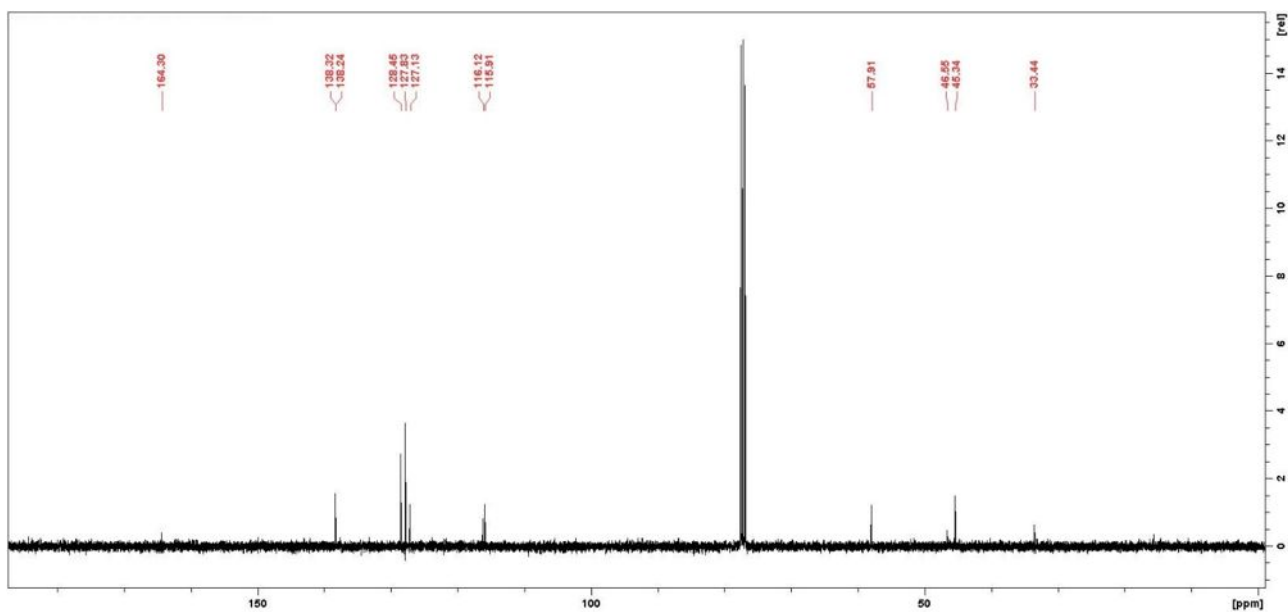
**Figure S3.** ESI-MS spectrum of compound 1-CH<sub>3</sub> (positive ionization mode).



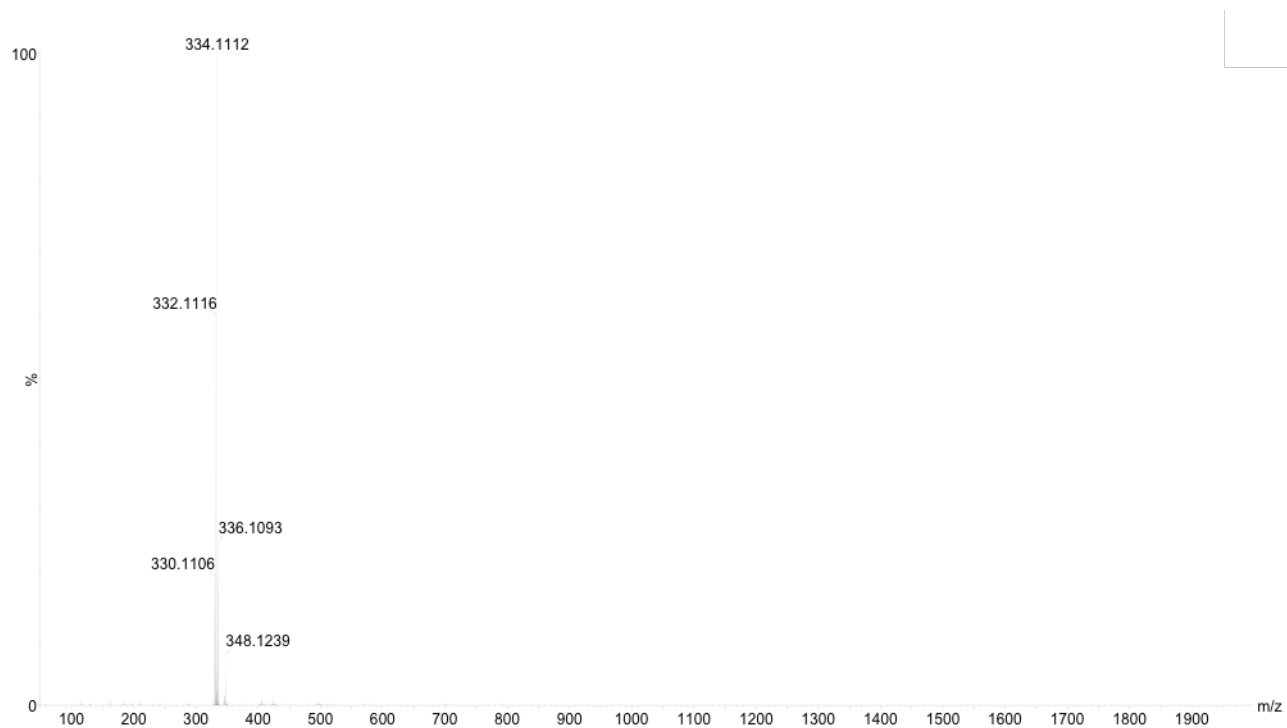
**Figure S4.** Detailed view of the peak of compound 1-CH<sub>3</sub>, showing the isotopic distribution, in the ESI-MS spectrum (positive ionization mode).



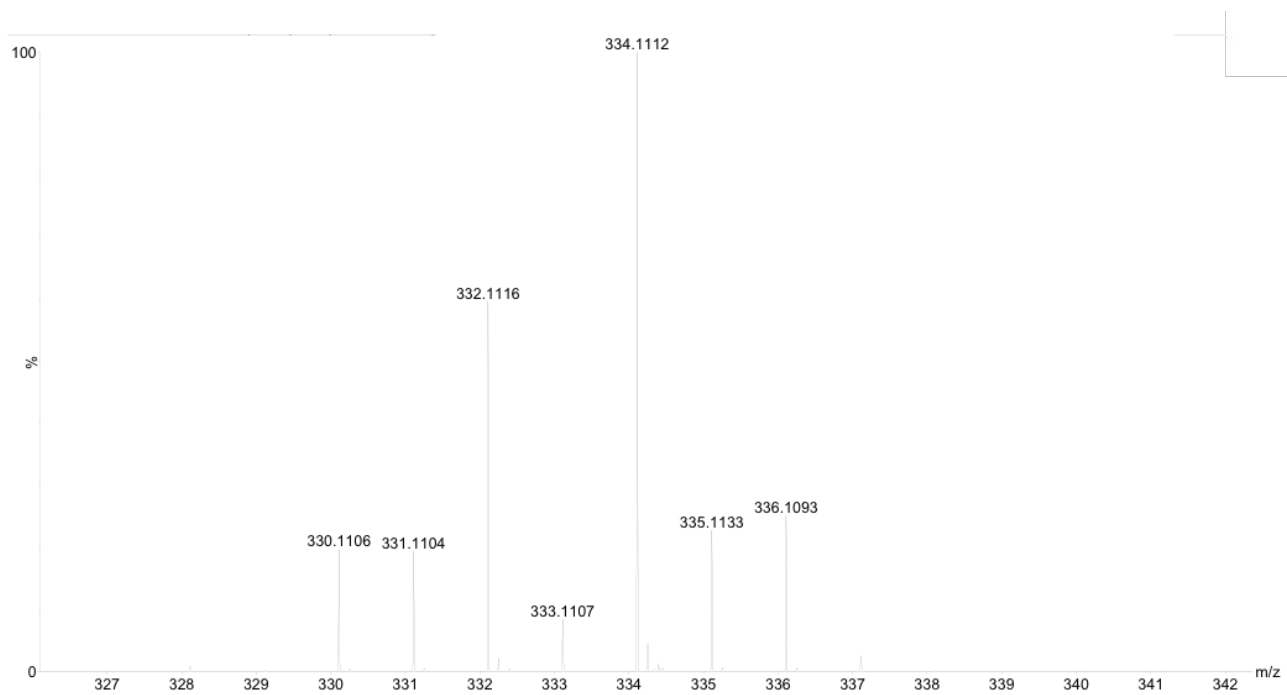
**Figure S5.**  $^1\text{H}$ -NMR spectrum of compound **1-F**.



**Figure S6.**  $^{13}\text{C}$ -NMR spectrum of compound **1-F**.

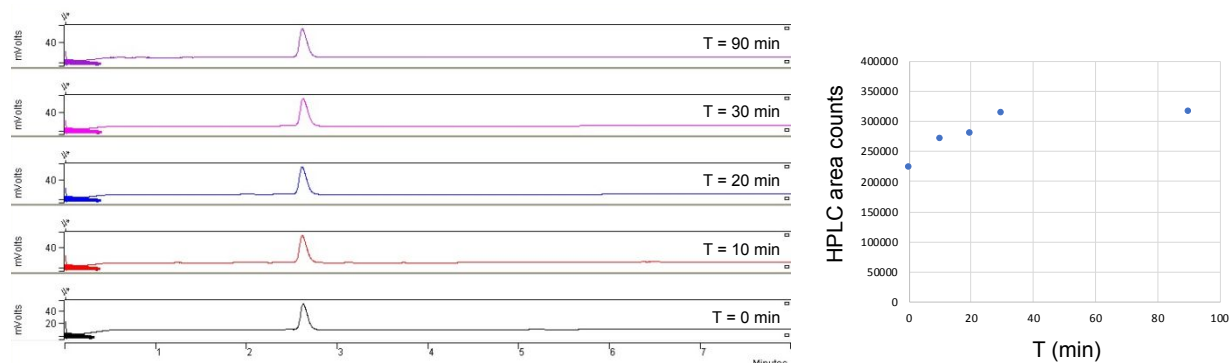


**Figure S7.** ESI-MS spectrum of compound **1-F** (positive ionization mode).

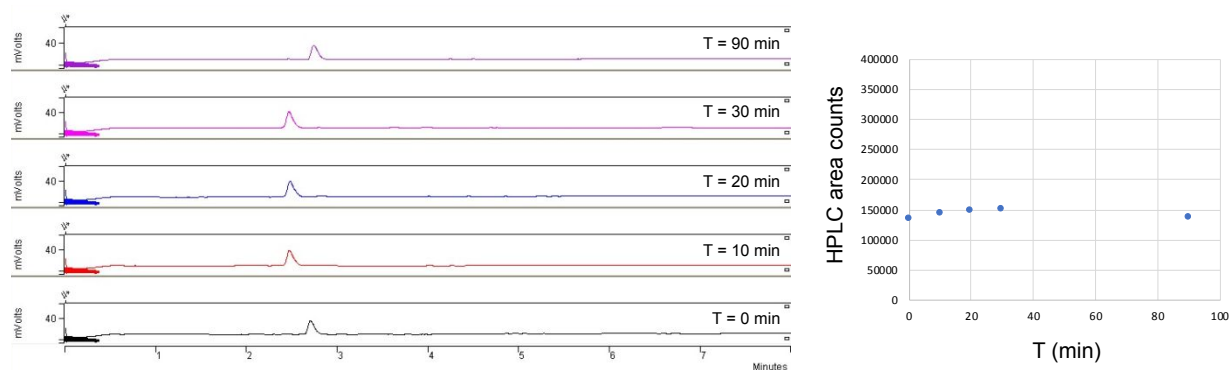


**Figure S8.** Detailed view of the peak of compound **1-F**, showing the isotopic distribution, in the ESI-MS spectrum (positive ionization mode).

### HPLC analysis and stability study



**Figure S9.** HPLC analysis at different time points for compound **1-CH<sub>3</sub>**. Chromatograms were acquired by injecting a 0.2 mg/mL solution of the compound in water.



**Figure S10.** HPLC analysis at different time points for compound **1-F**. Chromatograms were acquired by injecting a 0.2 mg/mL solution of the compound in water.

**Table S1.** Coordinates of the optimized structures of selenofluoxetine derivatives. Level of theory M06-2X/6-31G(d,p).

1-F				1-F			
Energy=-3213.5141677 Ha				C	-2.0975685011	2.4632146067	-1.9153198548
NImag=0				C	-2.2654585659	3.1352951287	-0.70545196
C	3.0868678202	-0.1998310386	0.563746953	C	-2.2858496233	2.4140774443	0.4846513357
C	2.5494993625	0.6017823604	-0.4322422415	C	-2.1449376606	1.0277413302	0.4661811479
C	1.485822386	0.1093246266	-1.1817380807	H	-2.1836779804	0.4568715304	1.3899999918
C	0.9734107661	-1.1641062227	-0.9281879903	H	-2.409224482	2.930414391	1.432057076
C	1.5362712968	-1.9482399393	0.080180102	H	-2.3738776935	4.2154762313	-0.6919775504
C	2.6009032253	-1.4700395287	0.83671104	H	-2.0730675154	3.019329046	-2.8478023192
H	3.0565992428	-2.0588236298	1.6249464399	H	-1.7741116633	0.5532387408	-2.8667249204
H	1.1336961729	-2.9386787555	0.2678776552	C	-3.2294012979	-1.7973936792	-1.1970600571
Se	-0.4982181565	-1.839252131	-1.9373385607	C	-4.3989598523	-1.3585666553	-0.3154776318
C	-1.9082136583	-1.1608197369	-0.745803386	N	-4.1315778237	-1.5378842335	1.1058301372
C	-1.9791963223	0.347565879	-0.7419342252	C	-5.128142655	-0.8460911463	-1.903262747
C	-1.9502986333	1.0804009317	-1.9324864674	H	-4.8950602698	-0.9636836588	2.9657827133
				H	-6.1525890556	-1.2256304562	1.7311221336
				H	-5.1089925946	0.2213790366	1.6622871973
				H	-5.3156865437	-1.8982521671	-0.6241729103
				H	-4.5794620038	-0.2909567945	-0.4829139953

H	-3.4467827485	-1.5035192359	-2.2316982789
H	-3.1192869357	-2.8879294954	-1.1983600417
H	-1.6642461472	-1.5178292732	0.7524324952
H	1.0420424763	0.7196177821	-1.9616083255
H	2.9643443075	1.5884657934	-0.60508853
C	-4.0620243876	-2.9419286853	1.4694676352
H	-3.8695236101	-3.0313129724	2.5424215645
H	-4.9974424859	-3.4855629972	1.2382004669
H	-3.2405015179	-3.4334900294	0.940354722
F	4.1133932817	0.2685696671	1.2879387065

### 1-F C7 Radical

Energy=-3212.8707494 Ha

NImag=0

C	2.3152139075	-0.7965824281	0.9527459726
C	2.5993911175	-1.0231708316	-0.3848555263
C	1.5393815237	-1.2185011537	-1.2648329684
C	0.2251308369	-1.2083630609	-0.7974437277
C	-0.0397394748	-0.983382114	0.5541716383
C	1.0149685747	-0.7674639558	1.4352324842
H	0.8444108363	-0.5840036541	2.4905894321
H	-1.068633015	-0.986918496	0.9102534666
Se	-1.1805002678	-1.5476104645	-2.0490455392
C	-2.5718668246	-0.4528446711	-1.3916071961
C	-2.4144422991	0.9705316439	-1.3075935343
C	-1.2362281266	1.6228969637	-1.7467139713
C	-1.0995775396	2.9968176221	-1.6519924009
C	-2.1282964914	3.7793385451	-1.1248245665
C	-3.3072251566	3.1629132025	-0.7062713943
C	-3.4529007117	1.7873296854	-0.7963415476
H	-4.3847949082	1.3367240595	-0.472667479
H	-4.121593149	3.7610823273	-0.3086625153
H	-2.0164669594	4.856246434	-1.051369368
H	-0.1846684038	3.4658634984	-2.0008267159
H	-0.447517372	1.0258986237	-2.1898159753
C	-3.8739258559	-1.1515700084	-1.1138296422
C	-4.2136257289	-1.3324102575	0.3790742422
N	-3.1503942097	-1.92122358	1.1777438884
C	-3.5442876941	-1.956710199	2.57589465
H	-2.715630021	-2.3370463839	3.1802536473
H	-4.4256345454	-2.6006863799	2.7529222312
H	-3.7841811087	-0.9458302616	2.9187649886
H	-5.1415929938	-1.9362868839	0.4427182671
H	-4.4370977349	-0.354779869	0.8196787255
H	-4.7051687209	-0.5930676118	-1.5648335825
H	-3.8643741368	-2.1334886537	-1.5981224632
H	1.7362118817	-1.3735005431	-2.3217445698
H	3.6303455525	-1.0293315612	-0.7206253429
C	-2.7660553524	-3.2468217309	0.7151147262
H	-2.0511057578	-3.6759263714	1.423124781
H	-3.6275088423	-3.934717724	0.6317493523
H	-2.2655669197	-3.1636949513	-0.2517687276
F	3.3306000441	-0.5949087414	1.8067761935

### 1-F C14 Radical

Energy=-3212.8521503 Ha

NImag=0

C	2.7599076804	-0.518859708	0.8023281858
C	2.4340244266	0.1923558734	-0.3429452964
C	1.2946528459	-0.174144373	-1.0521392976
C	0.5009050159	-1.2351911146	-0.6126287765
C	0.8522740789	-1.9306214092	0.5459481002
C	1.990011549	-1.5767976155	1.2633143986
H	2.2877302774	-2.1006164276	2.1648087374
H	0.2295433934	-2.7534452801	0.8833563803
Se	-1.0789608445	-1.7249410466	-1.5611145138
C	-2.2932691227	-0.4947697041	-0.5741611507
C	-1.9944680566	0.9482485571	-0.9187633851

C	-1.8329783859	1.3684976422	-2.2427831526
C	-1.6271880441	2.7116850251	-2.5348882934
C	-1.56042686	3.6520413716	-1.5070194083
C	-1.7037107721	3.2385343735	-0.186529247
C	-1.9210001557	1.8932062319	0.1047504415
H	-2.0355198936	1.5706300479	1.1366154504
H	-1.6422209329	3.9616955131	0.62111015138
H	-1.3904260548	4.6994323648	-1.736249884
H	-1.5074521868	3.0259234702	-3.5674722096
H	-1.8412835772	0.6246749183	-3.0350071213
C	-3.6885020184	-0.8882943006	-0.8948418238
C	-4.6660285253	-1.2767020314	0.16879873
N	-4.05295495	-1.9435476182	1.3091867379
C	-5.0161684857	-2.0964522997	2.3848263645
H	-4.5293957058	-2.5577062643	3.248728218
H	-5.8776550912	-2.7279172582	2.0972758756
H	-5.3953357295	-1.1158199378	2.6872546028
H	-5.4685337052	-1.8963424666	-0.2812695636
H	-5.1654218118	-0.3709778499	0.5538385348
H	-4.0721525747	-0.6543733892	-1.8836042975
H	-2.1040390391	-0.6792976016	0.4867096129
H	1.0120201306	0.3707303088	-1.9472001118
H	3.0671766057	1.0135382159	-0.6596903822
C	-3.4935583426	-3.2356117239	0.9360947711
H	-3.0599554803	-3.7083238067	1.8225779772
H	-4.2575377151	-3.9182411211	0.5189774135
H	-2.7002459301	-3.1029488456	0.195988927
F	3.8582229409	-0.1720996562	1.4885583711

### 1-F C15 Radical

Energy=-3212.8589215 Ha

NImag=0

C	2.8824299463	-0.4363499803	0.7689059522
C	2.5343358403	0.2519921017	-0.3836703224
C	1.4143254768	-0.1652686266	-1.0954273831
C	0.6598622199	-1.2526642162	-0.651628501
C	1.0351192466	-1.9261653199	0.512147256
C	2.1538684653	-1.5217009225	1.2329241542
H	2.4684418076	-2.0278535387	2.1387594966
H	0.4474218491	-2.7738829453	0.8509262796
Se	-0.8903747398	-1.8171200904	-1.6077797952
C	-2.1661837586	-0.6824244571	-0.6449842515
C	-1.9948983278	0.7905341648	-0.913037886
C	-1.7116219897	1.2789094249	-2.1924177224
C	-1.6504529782	2.6476731114	-2.4277101562
C	-1.8611643613	3.5495636592	-1.38252665146
C	-2.1350590538	3.0718093809	-0.107522283
C	-2.2006454963	1.6995682613	0.1259708806
H	-2.4172440983	1.3242931015	1.123443264
H	-2.294052682	3.7667192006	0.7116116985
H	-1.8065183851	4.6181329498	-1.5689574015
H	-1.4313035697	3.0130647929	-3.4266542246
H	-1.5224316177	0.5671935432	-2.991770749
C	-3.6008189089	-1.1828465674	-1.0054882097
C	-4.5041370435	-1.1876883006	0.1809969025
N	-4.1203147349	-1.9269950972	1.2965896691
C	-5.0783372016	-1.9703245878	2.3838730617
H	-4.5832927153	-2.3139749784	3.2966967789
H	-5.9234242825	-2.6422284904	2.1674121628
H	-5.4717395717	-0.9659136247	2.5602993689
H	-5.0724496761	-0.2917874862	0.4160943314
H	-4.0179085818	-0.5337452582	-1.7801676933
H	-3.5345747282	-2.189126497	-1.4436583164
H	-1.9872439055	-0.8776487588	0.4160810099
H	1.1173650318	0.3608427632	-1.9967612315
H	3.135722724	1.095411112	-0.7038359962
C	-3.4416994528	-3.1935008497	1.0702061677
H	-3.0701478176	-3.5704433247	2.0271416319
H	-4.1131747071	-3.9509701568	0.6339440799
H	-2.5871311343	-3.0611515696	0.3996990776
F	3.9621068654	-0.0407708587	1.4581643466

### 1-F C17 Radical

Energy=-3212.8553992 Ha

NImag=0

C	3.0622628791	-0.2084699097	0.5831936894
C	2.5240593106	0.5962233106	-0.4099273851
C	1.4644088209	0.1033735628	-1.1646354531
C	0.9562885754	-1.1732594756	-0.9183371729
C	1.5194814968	-1.9604562135	0.0874269638
C	2.5807057327	-1.4820078351	0.8485704431
H	3.0371198165	-2.0730671541	1.6346646736
H	1.1205428578	-2.9534787046	0.269155936
Se	-0.5098178874	-1.8477596173	-1.9358201502
C	-1.9264329764	-1.1629354203	-0.7552402116
C	-1.9833722836	0.3454744866	-0.7449590085
C	-1.9624057196	1.0794166043	-1.9354786543
C	-2.0965463979	2.4631016659	-1.9147481548
C	-2.2433864221	3.1350623393	-0.7016412229
C	-2.2550299301	2.4130507792	0.4876469904
C	-2.1265405036	1.0252696676	0.4655996669
H	-2.1552872879	0.4584174347	1.3925330126
H	-2.3626163131	2.9285209907	1.4372837577
H	-2.3423930341	4.2160552655	-0.6856124
H	-2.0786631866	3.0203635452	-2.8466408191
H	-1.8016900866	0.5520779517	-2.872482476
C	-3.2478123564	-1.7862747786	-1.2228705804
C	-4.4265452542	-1.3456316363	-0.3539778603
N	-4.1816744149	-1.5493451533	1.067224858
C	-4.891903047	-0.7275569296	1.9324320595
H	-4.7561611956	-0.9245734423	2.9905481742
H	-5.0062353797	0.3034138214	1.6141342323
H	-5.3401078456	-1.87523962	-0.672142363
H	-4.5985763045	-0.2753325339	-0.5026358925
H	-3.4536143604	-1.4848129183	-2.257541714
H	-3.1472646616	-2.8778404133	-1.2303056329
H	-1.6933218771	-1.5267373417	0.2489359946
H	1.0204932513	0.7156118063	-1.9428979456
H	2.935658014	1.585266052	-0.5768969454
C	-4.0544320571	-2.9382397285	1.4651484179
H	-3.8338713664	-2.9857987126	2.5341031257
H	-4.9767576973	-3.5084740835	1.2720724692
H	-3.2300592488	-3.4149763129	0.9269757061
F	4.0851012936	0.2600417153	1.3119618042

### 1-F TS@C7

Energy=-3289.2145755 Ha

NImag=1 (-969.09 cm<sup>-1</sup>)

C	3.855342311	-0.0867928064	1.0720963469
C	3.6739380646	0.4853671103	-0.1778479072
C	2.6042018318	0.053859591	-0.9555449488
C	1.7486918309	-0.9403442141	-0.4827011295
C	1.956321565	-1.5055695006	0.7767729476
C	3.0134594519	-1.0713286615	1.5688932885
H	3.1948741881	-1.4819704696	2.5557083281
H	1.2736748435	-2.2660264418	1.1425261562
Se	0.267308084	-1.5111127779	-1.5378540936
C	-1.0878116395	-0.566482628	-0.5141084099
C	-0.7772990791	0.8948483493	-0.351574282
C	-0.5585250223	1.693494732	-1.4803868413
C	-0.3310042677	3.0572975516	-1.3431914982
C	-0.3051312036	3.6382909089	-0.0752288109
C	-0.5014843002	2.8451153587	1.0504479297
C	-0.7369437955	1.4775844781	0.915466745
H	-0.8702785504	0.843710714	1.7871620262
H	-0.4638163125	3.2880396694	2.0411621933
H	-0.1629385895	3.6679480079	-2.2253272868
H	-0.5312559132	1.2212195055	-2.459707062
C	-2.4626630111	-0.8529696833	-1.1203155669
C	-3.6182380655	-0.1933393166	-0.3668572648
N	-3.800374197	-0.6745225297	1.0044576167

C	-4.7139513773	0.2032872164	1.7242846736
H	-4.830849667	-0.1523342042	2.7515657216
H	-5.7117835852	0.242525145	1.2537266148
H	-4.3001521792	1.2150574525	1.7516908544
H	-4.5502328951	-0.3358375918	-0.9448591774
H	-3.4288266994	0.8843781887	-0.3174843937
H	-2.4808186822	-0.4639990646	-2.1474067795
H	-2.6044051678	-1.9369418563	-1.1987583206
H	-1.0282157787	-1.1004262073	0.5335716374
H	2.4235367844	0.4973035914	-1.9292859883
H	4.3560697573	1.2568125409	-0.5168746394
O	-1.2347220049	-1.5135099618	1.847922679
H	-2.1488150955	-1.1307902582	1.8539914765
H	-0.1203553564	4.7027431819	0.031926023
F	4.8806792923	0.3291719823	1.8296547822
C	-4.2841500094	-2.0512118809	1.027629003
H	-3.5328642876	-2.7207726397	0.6031993407
H	-4.4515536368	-2.3569251162	2.0640699956
H	-5.229608172	-2.1662510903	0.469988925

### 1-F TS@C14

Energy=-3289.2085238 Ha

NImag= 1 (-1374.05 cm<sup>-1</sup>)

C	4.053758656	-0.0816480353	1.0356005971
C	3.5445472836	0.9945863351	0.3240008081
C	2.474138669	0.7759815791	-0.5370947864
C	1.931863469	-0.5026089317	-0.6726738021
C	2.460170786	-1.5670153896	0.0587596065
C	3.5321830521	-1.3622294667	0.9205474274
H	3.9655576361	-2.1694199865	1.5002776175
H	2.0304565149	-2.5581178203	-0.0483881825
Se	0.4443934455	-0.791496085	-1.8280190863
C	-0.9216552631	-0.4115276795	-0.4643106672
C	-1.042206508	1.0712858552	-0.1907344425
C	-1.1099842182	1.9990989385	-1.2345294786
C	-1.3003437373	3.350505999	-0.9668196205
C	-1.4108170049	3.7950628372	0.3496735082
C	-1.3303652434	2.8788431639	1.3944811927
C	-1.1489508138	1.5235479707	1.1261769765
H	-1.1111198684	0.8002524634	1.9355679579
H	-1.4061573614	3.2179401797	2.4233178054
H	-1.5528180731	4.8509000745	0.5584741439
H	-1.35369599	4.0597897218	-1.7872282145
H	-0.9826459077	1.6541023784	-2.2572044561
C	-2.2431135832	-1.0105105204	-0.9358923446
C	-3.3981635635	-0.7649821737	0.0233711555
N	-3.0559249364	-1.0542461051	1.4074098939
C	-3.9782767815	-0.3941655241	2.3143982434
H	-3.6896219388	-0.6115493629	3.3471165391
H	-5.0245592965	-0.7232106729	2.1750796659
H	-3.9294209827	0.6892636334	2.1636384814
H	-4.2884108201	-1.3301648892	-0.311195032
H	-3.6526659741	0.3016253662	-0.0415495116
H	-2.5039893157	-0.6990088885	-1.9544153821
H	-2.0571090129	-2.2071655229	-1.0413522377
H	-0.6054191479	-0.9306162905	0.4435153894
H	2.0501302019	1.6006046124	-1.101159605
H	3.9854231566	1.976657491	0.4527035576
O	-1.4573273883	-3.3969398223	-1.1093208468
H	-0.5844910337	-3.0499279111	-1.3932648432
F	5.0864562945	0.1221156732	1.8641953244
C	-3.0125565397	-2.4874127708	1.6637780495
H	-2.6991218734	-2.6585194251	2.6979520125
H	-3.9999566496	-2.963676321	1.5182919727
H	-2.2967933339	-2.9737288423	0.9967807834

### 1-F TS@C15

Energy=-3289.2056544 Ha

NImag= 1 (-1222.94 cm<sup>-1</sup>)

C	4.1492093261	0.6277625778	0.9696695263
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C	3.5428217041	1.238361479	-0.118025972	H	-4.196770123	-1.0955227765	-0.4728019738
C	2.5218833179	0.561453923	-0.7773051171	H	-3.3298545762	0.4512723691	-0.3447825259
C	2.1190370243	-0.7030936817	-0.3444009787	H	-2.1747125336	-0.9266789286	-1.9488683176
C	2.7495071728	-1.2931128754	0.7523797168	H	-2.0509703823	-2.287965218	-0.8438361418
C	3.7728875644	-0.6290839487	1.4203677374	H	-0.5952212574	-0.9897437491	0.6737891336
H	4.2800884136	-1.0649287777	2.2738122634	H	2.4133048782	0.9732599528	-1.4441322487
H	2.4336926681	-2.2790854585	1.0786846168	H	4.2999083782	1.7748077293	0.0009005506
Se	0.7056299405	-1.6263692674	-1.2322977253	O	-6.3296859272	-1.06060526	1.0561161561
C	-0.7508536241	-0.9074112034	-0.1210342402	H	-6.4333057494	-0.4097354557	0.3342514924
C	-0.8995452709	0.5831911418	-0.2879281459	F	5.2280668739	0.4723907074	2.0226478696
C	-0.9835195485	1.1638680255	-1.5578364906	C	-3.1962927863	-2.1528349977	1.7477358563
C	-1.2107142731	2.5281065952	-1.6967179853	H	-4.1626593978	-2.6094401491	1.4771544786
C	-1.338404891	3.3363071161	-0.5660120296	H	-2.385474121	-2.7281576428	1.2931116864
C	-1.232963332	2.769536794	0.7021728434	H	-3.0771877479	-2.1993435478	2.8334226163
C	-1.0182513843	1.3978612576	0.8396695768				
H	-0.9731836584	0.944955479	1.8257777718				
H	-1.3261134784	3.3921129584	1.5866594629				
H	-1.5151998363	4.4017181277	-0.6746637829				
H	-1.2893097717	2.9640026129	-2.6877683641				
H	-0.8466124455	0.5336188869	-2.4327125196				
C	-2.0249658405	-1.6744830178	-0.5009469247				
C	-3.2308240163	-1.2617974901	0.3269674743				
N	-2.9861176265	-1.1598849751	1.7387538147				
C	-4.148511664	-0.6221651851	2.4300991783				
H	-3.9009502319	-0.4530681972	3.4820472114				
H	-5.0157007496	-1.3052582009	2.3815801154				
H	-4.4289848499	0.3252653773	1.9644542274				
H	-4.1198646625	-1.8722963652	0.0760106566				
H	-3.5880246807	-0.1835619992	-0.0494174942				
H	-2.2609971026	-1.5024401667	-1.5582737369				
H	-1.8355052401	-2.7514096394	-0.3967457513				
H	-0.4839626244	-1.1290390648	0.9147418381				
H	2.026306377	1.0195232935	-1.6271351616				
H	3.873225787	2.2226122564	-0.4303592412				
O	-4.0947810742	1.0453485009	-0.3749145817				
H	-3.2920775528	1.5717824082	-0.1816523188				
F	5.135014066	1.2738729886	1.6075457127				
C	-2.5660651566	-2.4244402541	2.3279951243				
H	-2.3826674476	-2.2764141225	3.3959277665				
H	-3.3308359712	-3.2136227247	2.2134894362				
H	-1.6374363652	-2.777143848	1.8708394414				

### 1-F TS@C17

Energy=-3289.2064877 Ha

NImag=1 (-587.81 cm<sup>-1</sup>)

C	4.2203332957	0.0401564273	1.2516146493
C	3.8062175641	0.8278089412	0.1878626386
C	2.7614399223	0.3727193998	-0.6100275118
C	2.1456045465	-0.8499278924	-0.3370333911
C	2.5855493016	-1.6216373896	0.7397664517
C	3.6298317085	-1.1802282819	1.5454478064
H	3.9916627769	-1.7604186889	2.3869156097
H	2.1042368131	-2.5734063367	0.9417427404
Se	0.7007697302	-1.4706464483	-1.4168066212
C	-0.7352627626	-0.6474779416	-0.3546541282
C	-0.6844458433	0.8606109387	-0.3960862624
C	-0.5368005587	1.5484326303	-1.6048312349
C	-0.5735385637	2.9381800629	-1.636008691
C	-0.7472995996	3.6615961372	-0.45668598
C	-0.8838955408	2.9848779722	0.7516254602
C	-0.8540222316	1.5917139449	0.7809653041
H	-0.9790760728	1.0587969896	1.7198661639
H	-1.0107228633	3.5407551064	1.6758443666
H	-0.7689629242	4.7467545489	-0.4807286141
H	-0.4574324705	3.4593771091	-2.581626264
H	-0.3554358746	0.9780511965	-2.5124213293
C	-2.0656546661	-1.1932921432	-0.8901827894
C	-3.2597488523	-0.6207720779	-0.1287551949
N	-3.13486842	-0.7645920278	1.3165040296
C	-4.0802299987	0.046135623	2.0090321833
H	-3.9673325373	-0.0518739937	3.0925718078
H	-5.1608732011	-0.299751981	1.772248994
H	-3.98829297	1.0950900868	1.7111842267