Supporting Information

Computational Insight into the Reaction Intermediates in the Glycosylation Reaction

Assisted by Donor Heteroatoms

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Tables of optimised geometries for
compounds 11-15 and ions 9,10 17-23.

Structure number: 9

Energy= -3.50376150 a.u.

Atom (Å)	X	Y	Z
S	0.0309	-0.1238	0.1791
C	2.3223	-0.0763	-0.1198
O	2.9508	1.0453	-0.2641
C	3.0807	1.9575	0.9134
C	3.1310	1.1635	2.1926
C	1.8529	0.3356	2.3477
C	1.6365	-0.5183	1.0965
H	1.6966	-1.6043	1.2513
H	0.9950	1.0102	2.5011
H	1.9045	-0.3189	3.2294
H	4.0250	0.5161	2.1903
H	3.2391	1.8626	3.0366
H	4.0003	2.5112	0.6926
H	2.2140	2.6334	0.8497
H	2.4011	-0.7269	-0.9959
C	-0.3843	-1.7431	-0.5888
H	-1.3320	-1.5643	-1.1153
H	0.3750	-2.0532	-1.3163
H	-0.5267	-2.4924	0.1994

Structure number: 10 R=Me

Energy= -2.57904695 a.u.

Atom (Å)	X	Y	Z
S	-0.0029	0.0079	0.0111
C	1.8670	-0.0023	-0.0197
C	1.7402	1.4468	-0.0071
O	1.9451	2.0956	1.1014
C	1.6506	3.5419	1.1015
H	2.1441	3.9288	1.9957
H	2.0668	3.9937	0.1951
H	0.5643	3.6698	1.1578
H	1.5611	2.0041	-0.9335
H	2.2085	-0.4368	-0.9656
H	2.3122	-0.4649	0.8675
C	-0.3030	0.0377	1.8213
H	-0.0126	-0.9289	2.2503
H	0.2527	0.8642	2.2843
H	-1.3829	0.2010	1.9338

Structure number: 12 Y=SeH

Energy= -3.51411376 a.u.

Atom (Å)	X	Y	Z
Se	-0.2070	-0.0750	-0.2646
C	1.7861	0.0253	0.0027
C	2.3123	1.4531	0.0639
O	2.1277	1.9015	1.4202
C	1.8347	0.7647	2.2647
C	2.6851	0.8734	3.5163
O	2.3248	-0.2252	4.3655
H	2.8400	-0.1422	5.1942
H	3.7523	0.8348	3.2288
H	2.4839	1.8448	4.0007
C	2.1113	-0.4728	1.4121
H	3.1858	-0.7257	1.4627
H	1.5395	-1.3555	1.7296
H	0.7685	0.8022	2.5568
H	3.3930	1.4576	-0.1836
H	1.7897	2.1498	-0.6060
H	2.2492	-0.5760	-0.7910
H	-0.1473	0.4286	-1.656

Structure number: 11 Y=SH

Energy= -3.54420230 a.u.

Atom (Å)	X	Y	Z
S	-0.1644	-0.0974	-0.4312
C	1.6689	-0.0094	-0.0738
C	2.2142	1.4107	0.0035
O	1.9838	1.8753	1.3438
C	1.7003	0.7485	2.2036
C	2.6104	0.8445	3.4159
O	2.2812	-0.2483	4.2868
H	2.8676	-0.1918	5.0695
H	3.6620	0.7901	3.0760
H	2.4494	1.8190	3.9096
C	1.9186	-0.5056	1.3547
H	2.9675	-0.8393	1.4371
H	1.2746	-1.3440	1.6539
H	0.6471	0.8142	2.5328
H	3.3023	1.3959	-0.2056
H	1.7256	2.1101	-0.6893
H	2.1888	-0.6202	-0.8248
H	-0.1037	0.5525	-1.6307

Structure number: 13 Y=I

Energy= -3.31596357 a.u.

Atom (Å)	X	Y	Z
I	-0.2607	-0.0725	-0.2921
C	1.9663	0.0361	0.1610
C	2.4662	1.4670	0.2172
O	2.2452	1.9257	1.5598
C	1.9928	0.7838	2.4170
C	2.8340	0.9393	3.6712
O	2.5386	-0.1778	4.5180
H	3.0031	-0.0378	5.3695
H	3.9051	0.9702	3.3909
H	2.5708	1.8980	4.1535
C	2.3009	-0.4462	1.5663
H	3.3923	-0.6454	1.5851
H	1.7821	-1.3563	1.8913
H	0.9235	0.7814	2.7017
H	3.5569	1.4502	0.0003
H	1.9819	2.1605	-0.4822
H	2.4107	-0.5587	-0.6470

Structure number: 14 Y=S

Energy= -3.53893862 a.u.

Atom (Å)	X	Y	Z
S	-0.1247	-0.0055	-0.3477
C	1.7301	-0.0135	-0.1028
C	1.1738	1.3446	-0.0033
O	1.2838	1.8439	1.2842
C	1.5203	0.7027	2.1617
C	2.3093	1.2095	3.3505
O	2.4493	0.1052	4.2512
H	2.9643	0.4159	5.0247
H	3.2919	1.5790	3.0014
H	1.7592	2.0490	3.8118
C	2.2244	-0.3470	1.2898
H	3.3203	-0.2004	1.3215
H	1.9982	-1.3725	1.6126
H	0.5412	0.3204	2.4941
H	1.2426	2.1143	-0.7714
H	2.3062	-0.3331	-0.9751

Structure number: 15 Y=Se

Energy= -3.51170007 a.u.

Atom (Å)	X	Y	Z
Se	-0.1764	-0.0493	-0.2854
C	1.8087	0.0147	0.0260
C	1.2787	1.3775	0.1191
O	1.3681	1.8770	1.3985
C	1.6066	0.7429	2.2891
C	2.4230	1.2600	3.4552
O	2.6068	0.1542	4.3464
H	3.1562	0.4649	5.0957
H	3.3879	1.6431	3.0748
H	1.8780	2.0896	3.9390
C	2.2931	-0.3213	1.4227
H	3.3906	-0.1929	1.4578
H	2.0486	-1.3412	1.7480
H	0.6258	0.3798	2.6368
H	1.3445	2.1436	-0.6528
H	2.4009	-0.2992	-0.8376

Structure number: 17 Y=SH

Energy= -3.49283460 a.u.

Atom (Å)	X	Y	Z
S	0.1162	0.2929	-0.1430
C	1.9965	-0.2747	-0.0662
C	1.8468	1.1834	-0.0996
H	1.5874	2.6053	1.5552
H	3.2375	2.0536	1.1828
C	2.1814	1.7293	1.2650
C	2.0752	0.5176	2.2113
C	2.9663	0.6145	3.4421
O	2.8270	-0.6237	4.1301
H	3.3616	-0.5880	4.9530
H	4.0125	0.7833	3.1194
H	2.6511	1.4710	4.0635
C	2.4101	-0.6929	1.3139
H	3.5083	-0.8327	1.2542
H	1.9848	-1.6463	1.6544
H	1.0324	0.4142	2.5661
H	1.9847	1.7773	-1.0069
H	2.2239	-0.8754	-0.9512
H	0.0488	0.2548	-1.5114

Structure number: 17 Y=SeH

Energy= -3.46852959 a.u.

Atom (Å)	X	Y	Z
Se	0.0137	0.1289	-0.0693
C	2.0636	-0.2832	-0.0704
C	1.8301	1.1624	-0.0819
H	1.5570	2.5652	1.5885
H	3.2187	2.0794	1.1777
C	2.1767	1.7134	1.2762
C	2.1262	0.4891	2.2068
C	2.9641	0.6104	3.4700
O	2.8049	-0.6231	4.1649
H	3.2879	-0.5696	5.0173
H	4.0215	0.7876	3.1946
H	2.6106	1.4684	4.0689
C	2.5491	-0.6825	1.2965
H	3.6544	-0.7267	1.2172
H	2.2095	-1.6703	1.6348
H	1.0824	0.3201	2.5350
H	1.8938	1.7678	-0.9900
H	2.3147	-0.8532	-0.9695
H	-0.0492	0.1177	-1.5547

Structure number: 17 Y=I

Energy= -3.24683954 a.u.

Atom (Å)	X	Y	Z
I	-0.2048	-0.2056	-0.1438
C	2.1502	0.1109	0.0914
C	2.5875	1.5369	0.0155
C	1.8758	2.2355	1.1863
C	2.5931	3.4602	1.7390
O	1.7953	3.9082	2.8311
H	2.1827	4.7377	3.1864
H	3.6150	3.1880	2.0687
H	2.6732	4.2268	0.9481
C	1.6934	1.1054	2.2189
C	1.6172	-0.1457	1.4159
H	1.6034	-1.1479	1.8580
H	2.6321	0.9740	2.8082
H	0.8933	1.2540	2.9564
H	0.8756	2.5680	0.8574
H	2.4734	2.0061	-0.9722
H	3.6840	1.4787	0.2118
H	2.5749	-0.6810	-0.5345

Structure number: 18 Y=SH

Energy= -3.12969071 a.u.

Atom (Å)	X	Y	Z
S	-0.0603	-0.0632	0.0134
C	2.3339	0.0232	0.0057
O	2.8176	1.2165	-0.0073
C	2.3150	1.9803	1.1958
C	3.5023	2.7014	1.8110
O	2.9671	3.2697	2.9981
H	3.6274	3.8901	3.3784
H	4.3027	1.9663	2.0212
H	3.8850	3.4592	1.1077
C	1.6737	0.9090	2.0795
C	1.4535	-0.2696	1.1351
H	1.4758	-1.2741	1.5699
H	2.3740	0.5970	2.8714
H	0.7539	1.2617	2.5653
H	1.5908	2.6942	0.7733
H	2.6388	-0.6425	-0.8062
H	-0.0575	-1.3577	-0.4316

Structure number: 18 Y=SMe (R=COCF₃)

Energy= -4.92644697 a.u.

Atom (Å)	X	Y	Z
S	0.1154	-0.1145	0.1553
C	2.3920	0.0457	-0.0684
O	2.8262	1.2728	-0.1169
C	2.3989	1.9940	1.1304
C	3.5579	2.8687	1.5643
O	3.0518	3.5336	2.7447
C	3.9388	4.4081	3.2979
O	5.0447	4.6374	2.8918
C	3.2985	5.0659	4.5431
F	4.1610	5.9208	5.0995
F	2.1723	5.7302	4.1880
F	2.9673	4.1098	5.4484
H	4.4480	2.2715	1.8156
H	3.8206	3.6064	0.7929
C	1.9879	0.8783	2.0919
C	1.6976	-0.2985	1.1672
H	1.7918	-1.3111	1.5747
H	2.8298	0.6000	2.7476
H	1.1356	1.1601	2.7246
H	1.5478	2.6141	0.8069
H	2.6581	-0.6002	-0.9075
C	-0.2062	-1.8652	-0.3142
H	0.6361	-2.2914	-0.8713
H	-0.4315	-2.4427	0.5901
H	-1.0873	-1.8203	-0.9683

Structure number: 18 Y=SMe

Energy= -3.73269409 a.u.

Atom (Å)	X	Y	Z
S	-0.0562	0.0021	0.0286
C	2.2524	-0.0068	0.0028
O	2.7773	1.1814	-0.0020
C	2.3044	1.9350	1.2113
C	3.4873	2.6940	1.7812
O	2.9635	3.2983	2.9569
H	3.6325	3.9211	3.3166
H	4.3043	1.9812	2.0026
H	3.8438	3.4325	1.0442
C	1.7113	0.8578	2.1201
C	1.4205	-0.2947	1.1665
H	1.4019	-1.3112	1.5744
H	2.4591	0.5215	2.8573
H	0.8262	1.2096	2.6665
H	1.5456	2.6315	0.8208
H	2.5385	-0.6722	-0.8143
C	-0.4550	-1.7223	-0.4754
H	-0.7761	-2.2906	0.4053
H	-1.2857	-1.6210	-1.1864
H	0.3940	-2.1982	-0.9795

Structure number: 18 Y=SPh

Energy= -5.60597041 a.u.

Atom (Å)	X	Y	Z
S	-0.5972	0.1547	-0.1093
C	1.6009	-0.2585	0.6013
O	2.4323	0.7029	0.3301
C	1.9263	1.9741	0.9559
C	3.1197	2.7166	1.5253
O	2.5541	3.8916	2.0873
H	3.2796	4.4546	2.4387
H	3.6132	2.0821	2.2860
H	3.8384	2.9309	0.7153
C	0.8743	1.5105	1.9614
C	0.4946	0.1203	1.4623
H	0.1024	-0.6060	2.1818
H	1.3142	1.4126	2.9682
H	0.0231	2.2024	2.0277
H	1.4897	2.5322	0.1118
H	1.8271	-1.2473	0.1978
C	-1.1814	-1.5494	-0.1670
C	-0.7983	-2.3551	-1.2428
C	-1.3053	-3.6501	-1.3278
C	-2.1785	-4.1270	-0.3496
C	-2.5640	-3.3069	0.7126
C	-2.0743	-2.0075	0.8067
H	-2.4008	-1.3529	1.6152
H	-3.2618	-3.6744	1.4653
H	-2.5701	-5.1422	-0.4199
H	-1.0172	-4.2867	-2.1644
H	-0.1244	-1.9719	-2.0094

Structure number: 18 Y=S^tBu (R= COCF₃)

Energy= -6.72665032 a.u.

Atom (Å)	X	Y	Z
S	0.1393	-0.0304	0.0369
C	2.3877	-0.0189	-0.0615
O	2.8910	1.1909	-0.0774
C	2.4438	1.9175	1.1558
C	3.6196	2.7382	1.6449
O	3.0962	3.4170	2.8112
C	3.9930	4.2483	3.4076
O	5.1245	4.4370	3.0526
C	3.3276	4.9241	4.6301
F	4.2026	5.7328	5.2355
F	2.2515	5.6454	4.2319
F	2.9091	3.9788	5.5105
H	4.4719	2.1015	1.9278
H	3.9463	3.4699	0.8926
C	1.9486	0.8155	2.0943
C	1.6312	-0.3322	1.1436
H	1.6463	-1.3531	1.5379
H	2.7546	0.4914	2.7737
H	1.0892	1.1344	2.6988
H	1.6309	2.5762	0.8119
H	2.6823	-0.6839	-0.8738
C	-0.5036	-1.7983	-0.3958
C	0.5717	-2.6148	-1.0965
H	0.9246	-2.1267	-2.0165
H	1.4252	-2.8454	-0.4407
H	0.1301	-3.5835	-1.3852
C	-0.9832	-2.4447	0.8957
H	-0.1619	-2.6579	1.5954
H	-1.7395	-1.8315	1.4057
H	-1.4477	-3.4125	0.6433
C	-1.6673	-1.4765	-1.3329
H	-1.3281	-0.9845	-2.2559
H	-2.1531	-2.4245	-1.6133
H	-2.4275	-0.8471	-0.8465

Structure number: 18 Y=S[†]Bu

Energy= -5.53208259 a.u.

Atom (Å)	X	Y	Z
S	0.0446	-0.0622	0.0337
C	2.3292	0.0064	0.0374
O	2.8007	1.2220	0.0379
C	2.2839	1.9472	1.2499
C	3.4272	2.7588	1.8276
O	2.8833	3.3186	3.0168
H	3.4963	4.0099	3.3491
H	4.2811	2.0858	2.0341
H	3.7423	3.5256	1.1009
C	1.7427	0.8409	2.1567
C	1.5021	-0.3163	1.1941
H	1.5249	-1.3344	1.5957
H	2.5069	0.5376	2.8915
H	0.8418	1.1510	2.7023
H	1.4914	2.6053	0.8615
H	2.6635	-0.6529	-0.7642
C	-0.5204	-1.8455	-0.4137
C	0.6103	-2.6328	-1.0607
H	0.2140	-3.6163	-1.3641
H	0.9899	-2.1360	-1.9654
H	1.4398	-2.8321	-0.3651
C	-1.0384	-2.5063	0.8566
H	-1.4512	-3.4933	0.5895
H	-0.2448	-2.6813	1.5977
H	-1.8413	-1.9193	1.3244
C	-1.6502	-1.5699	-1.4061
H	-2.0915	-2.5349	-1.7018
H	-2.4514	-0.9623	-0.9594
H	-1.2845	-1.0713	-2.3153

Structure number: 18 Y=SeH

Energy= -3.10478411 a.u.

Atom (Å)	X	Y	Z
Se	0.0251	0.0926	0.0328
C	2.4862	-0.0515	-0.0584
O	3.0661	1.1060	0.0161
C	2.6400	1.7818	1.2931
C	3.8381	2.5069	1.8743
O	3.3293	3.0616	3.0799
H	4.0236	3.6243	3.4881
H	4.6530	1.7808	2.0538
H	4.1879	3.2745	1.1639
C	2.0710	0.6460	2.1411
C	1.6862	-0.4030	1.1065
H	1.6285	-1.4517	1.4153
H	2.8574	0.2179	2.7868
H	1.2437	0.9708	2.7859
H	1.8723	2.5049	0.9711
H	2.7115	-0.6593	-0.9382
H	-0.0868	-1.2603	-0.5665

Structure number: 18 Y=SeMe (R=COCF₃)

Energy= -4.90206394 a.u.

Atom (Å)	X	Y	Z
Se	-0.0461	-0.2485	-0.3314
C	2.3329	-0.2241	-0.2723
O	2.8622	0.9715	-0.1931
C	2.4048	1.6269	1.0735
C	3.6010	2.3562	1.6570
O	3.0951	2.9403	2.8784
C	3.7816	4.0391	3.3055
O	4.7437	4.5229	2.7760
C	3.1220	4.5752	4.6007
F	3.7558	5.6789	5.0103
F	1.8162	4.8673	4.3695
F	3.1855	3.6325	5.5740
H	4.4186	1.6575	1.8943
H	3.9721	3.1379	0.9802
C	1.8286	0.4818	1.9146
C	1.5456	-0.6068	0.8883
H	1.5319	-1.6527	1.2126
H	2.5852	0.0974	2.6199
H	0.9481	0.7886	2.4950
H	1.6368	2.3503	0.7552
H	2.6466	-0.8359	-1.1198
C	-0.3197	-2.1017	-0.9724
H	0.5898	-2.4804	-1.4524
H	-0.6323	-2.7241	-0.1261
H	-1.1247	-2.0227	-1.7166

Structure number: 18 Y=SeMe

Energy= -3.70840524 a.u.

Atom (Å)	X	Y	Z
Se	-0.0230	-0.0303	-0.0236
C	2.3805	0.0816	-0.0127
O	2.8631	1.2935	0.0178
C	2.3997	1.9743	1.2734
C	3.5747	2.7471	1.8430
O	3.0719	3.2824	3.0607
H	3.7467	3.8863	3.4412
H	4.4189	2.0505	2.0059
H	3.8859	3.5288	1.1301
C	1.8735	0.8389	2.1541
C	1.6095	-0.2873	1.1638
H	1.6379	-1.3223	1.5206
H	2.6562	0.5045	2.8563
H	0.9952	1.1339	2.7434
H	1.6063	2.6630	0.9412
H	2.6921	-0.5442	-0.8508
C	-0.2355	-1.9144	-0.5905
H	0.6617	-2.2600	-1.1165
H	-0.4616	-2.5257	0.2906
H	-1.0878	-1.9033	-1.2843

Structure number: 18 Y=SePh

Energy= -5.58065667 a.u.

Atom (Å)	X	Y	Z
Se	-0.4851	0.1658	-0.1724
C	1.7613	-0.2620	0.6896
O	2.6165	0.6944	0.4452
C	2.1062	1.9631	1.0595
C	3.2881	2.7175	1.6366
O	2.7070	3.8937	2.1851
H	3.4252	4.4642	2.5367
H	3.7783	2.0921	2.4061
H	4.0128	2.9342	0.8337
C	1.0461	1.5007	2.0604
C	0.6562	0.1230	1.5407
H	0.2303	-0.6135	2.2285
H	1.4904	1.3778	3.0635
H	0.2096	2.2072	2.1444
H	1.6725	2.5252	0.2157
H	2.0056	-1.2539	0.3052
C	-1.1087	-1.6684	-0.1760
C	-0.7223	-2.5045	-1.2279
C	-1.2693	-3.7842	-1.2998
C	-2.1812	-4.2129	-0.3361
C	-2.5609	-3.3657	0.7058
C	-2.0330	-2.0792	0.7886
H	-2.3600	-1.4021	1.5781
H	-3.2867	-3.6989	1.4480
H	-2.6103	-5.2131	-0.4034
H	-0.9848	-4.4450	-2.1189
H	-0.0214	-2.1599	-1.9885

Structure number: 18 Y=SeSiMe₃

Energy= -5.40378742 a.u.

Atom (Å)	X	Y	Z
Se	0.0002	-0.0957	0.0555
Si	2.4101	0.0410	-0.0316
C	2.8093	1.8714	-0.1676
H	2.4340	2.3184	-1.1000
H	2.3939	2.4364	0.6800
H	3.9043	2.0049	-0.1565
C	2.9883	-0.9624	-1.5164
H	2.6482	-0.5480	-2.4777
H	4.0918	-0.9425	-1.5397
H	2.6847	-2.0174	-1.4437
C	2.8534	-0.7309	1.6213
H	2.4128	-0.1811	2.4670
H	2.5348	-1.7823	1.6813
H	3.9489	-0.7040	1.7466
C	-0.4814	0.4601	-1.8457
C	-0.5246	-0.9719	-2.0873
O	-1.7342	-1.4681	-2.1638
C	-2.7191	-0.3822	-1.8539
C	-3.9029	-0.5513	-2.7862
O	-4.7542	0.5431	-2.4673
H	-5.5849	0.4542	-2.9833
H	-3.5472	-0.5160	-3.8331
H	-4.3810	-1.5282	-2.6020
C	-1.9235	0.9135	-2.0191
H	-2.0438	1.3107	-3.0422
H	-2.2367	1.6913	-1.3104
H	-3.0193	-0.5620	-0.8091
H	0.2942	-1.6416	-2.3500
H	0.3152	1.0567	-2.2980

Structure number: 18 Y=SePhOMe₂

Energy= -7.23017992 a.u.

Atom (Å)	X	Y	Z
Se	0.1411	-0.0975	0.0321
C	2.5496	0.0787	0.1357
O	2.9973	1.3081	0.1135
C	2.4314	2.0433	1.2890
C	3.5148	2.9488	1.8407
O	2.9104	3.5610	2.9739
H	3.5091	4.2644	3.3067
H	4.3949	2.3364	2.1135
H	3.8111	3.6801	1.0702
C	1.9395	0.9407	2.2287
C	1.7593	-0.2516	1.3017
H	1.7868	-1.2689	1.7035
H	2.7192	0.6879	2.9682
H	1.0330	1.2277	2.7778
H	1.6045	2.6420	0.8726
H	2.9000	-0.5897	-0.6527
C	0.1270	-1.9223	-0.6136
C	0.5877	-2.1615	-1.9047
C	0.5039	-3.4735	-2.3971
C	-0.0432	-4.4938	-1.6091
C	-0.5130	-4.2092	-0.3200
C	-0.4271	-2.9070	0.1990
H	-0.8191	-2.7031	1.1937
H	-0.1112	-5.5029	-2.0009
H	0.9809	-1.3763	-2.5476
O	-1.0722	-5.1238	0.5045
C	-1.2295	-6.4677	0.0115
H	-1.8710	-6.4763	-0.8804
H	-0.2501	-6.9148	-0.2076
H	-1.7148	-7.0171	0.8231
O	0.9788	-3.6495	-3.6513
C	0.9340	-4.9753	-4.2115
H	-0.1050	-5.3218	-4.2974
H	1.3764	-4.8815	-5.2074
H	1.5290	-5.6705	-3.6033

Structure number: 18 Y=SePhSnMe₃

Energy= -7.71669571 a.u.

Atom (Å)	X	Y	Z
Se	0.0195	0.1213	-0.3188
C	1.9729	-0.5541	0.9442
O	2.9816	0.2741	0.8437
C	2.5474	1.6165	1.3449
C	3.7020	2.2230	2.1176
O	3.1913	3.4661	2.5840
H	3.9274	3.9756	2.9874
H	3.9801	1.5453	2.9465
H	4.5690	2.3451	1.4469
C	1.2775	1.3313	2.1495
C	0.8044	-0.0021	1.5902
H	0.1586	-0.6509	2.1890
H	1.5207	1.1908	3.2170
H	0.5402	2.1414	2.0739
H	2.3457	2.2042	0.4340
H	2.1487	-1.5851	0.6333
C	-0.7836	-1.6300	-0.4587
C	-0.1913	-2.5726	-1.3039
C	-0.8495	-3.7814	-1.5257
C	-2.0932	-4.0630	-0.9389
C	-2.6535	-3.0914	-0.0939
C	-2.0158	-1.8764	0.1537
H	-2.4876	-1.1259	0.7892
H	-3.6247	-3.2628	0.3747
Sn	-3.1915	-5.9486	-1.4304
H	-0.3782	-4.5014	-2.1971
H	0.7549	-2.3596	-1.8019
C	-2.8328	-6.2537	-3.5792
H	-3.4309	-7.1031	-3.9374
H	-3.1215	-5.3524	-4.1372
H	-1.7713	-6.4714	-3.7621
C	-5.2853	-5.5001	-0.9380
H	-5.9279	-6.3314	-1.2601
H	-5.4064	-5.3668	0.1460
H	-5.6038	-4.5864	-1.4590
C	-2.3320	-7.5582	-0.2027
H	-1.2735	-7.6992	-0.4609
H	-2.4157	-7.3039	0.8625
H	-2.8745	-8.4944	-0.3934

Structure number: 18 Y=SePhOMe

Energy= -6.40907794 a.u.

Atom (Å)	X	Y	Z
Se	0.1431	-0.1117	0.0334
C	2.5962	0.1272	0.0553
O	2.9984	1.3725	0.0634
C	2.4569	2.0403	1.2916
C	3.5398	2.9418	1.8504
O	2.9678	3.4697	3.0417
H	3.5476	4.1876	3.3773
H	4.4452	2.3385	2.0512
H	3.7855	3.7246	1.1139
C	2.0232	0.8845	2.1958
C	1.8500	-0.2698	1.2215
H	1.9109	-1.3028	1.5751
H	2.8284	0.6249	2.9047
H	1.1232	1.1219	2.7783
H	1.6038	2.6380	0.9314
H	2.9294	-0.4914	-0.7793
C	0.0537	-1.8987	-0.6461
C	0.3695	-2.1405	-1.9941
C	0.2124	-3.4091	-2.5143
C	-0.2776	-4.4524	-1.7055
C	-0.6040	-4.2050	-0.3621
C	-0.4396	-2.9290	0.1626
H	-0.7163	-2.7385	1.1993
H	-0.9961	-4.9942	0.2751
O	-0.4060	-5.6423	-2.3177
H	0.4457	-3.6242	-3.5575
H	0.7224	-1.3331	-2.6357
C	-0.9621	-6.7418	-1.5655
H	-0.9890	-7.5813	-2.2653
H	-0.3168	-6.9855	-0.7113
H	-1.9799	-6.4973	-1.2334

Structure number: 18 Y=SePhNO₂

Energy= -6.11885197 a.u.

Atom (Å)	X	Y	Z
Se	0.0799	-0.0443	-0.0043
C	2.5401	0.0313	0.0876
O	3.0303	1.2367	0.0966
C	2.4983	1.9697	1.2977
C	3.6330	2.7818	1.8935
O	3.0684	3.3350	3.0749
H	3.6706	4.0309	3.4177
H	4.4850	2.1094	2.1093
H	3.9561	3.5514	1.1735
C	1.9353	0.8657	2.1944
C	1.7087	-0.2900	1.2303
H	1.7048	-1.3161	1.6111
H	2.6886	0.5528	2.9378
H	1.0362	1.1830	2.7392
H	1.7164	2.6314	0.8906
H	2.8596	-0.6274	-0.7227
C	-0.0615	-1.8721	-0.6400
C	0.2072	-2.1415	-1.9847
C	0.0449	-3.4403	-2.4582
C	-0.3864	-4.4220	-1.5765
N	-0.5536	-5.8127	-2.0805
O	-0.9981	-6.6382	-1.2827
O	-0.2313	-6.0194	-3.2506
C	-0.6753	-4.1608	-0.2430
C	-0.5145	-2.8641	0.2339
H	-0.7619	-2.6321	1.2696
H	-1.0314	-4.9675	0.3966
H	0.2448	-3.7004	-3.4972
H	0.5296	-1.3512	-2.6624

Structure number: 18 Y=SePhMe₃

Energy= -7.36769512 a.u.

Atom (Å)	X	Y	Z
Se	0.1869	0.1601	0.0118
C	2.5372	-0.0465	-0.0692
O	3.1212	1.1200	-0.2030
C	2.8293	1.9694	0.9945
C	4.1215	2.6606	1.3903
O	3.7730	3.4100	2.5470
H	4.5502	3.9439	2.8223
H	4.8918	1.8933	1.5979
H	4.4660	3.2981	0.5580
C	2.2572	0.9951	2.0265
C	1.8051	-0.1922	1.1899
H	1.7300	-1.1751	1.6649
H	3.0517	0.6499	2.7118
H	1.4555	1.4411	2.6314
H	2.0921	2.7131	0.6528
H	2.7759	-0.7856	-0.8332
C	-0.8673	-1.5291	-0.0989
C	-0.3545	-2.8284	-0.1733
C	-1.2837	-3.8707	-0.2740
C	-2.6563	-3.6511	-0.3365
C	-3.1146	-2.3314	-0.2932
C	-2.2481	-1.2482	-0.1732
C	-2.8065	0.1491	-0.1456
H	-3.9012	0.1201	-0.2151
H	-2.5519	0.6733	0.7883
H	-2.4468	0.7511	-0.9952
H	-4.1865	-2.1335	-0.3570
C	-3.6253	-4.7909	-0.4449
H	-3.1352	-5.7048	-0.8054
H	-4.0672	-5.0089	0.5411
H	-4.4479	-4.5445	-1.1313
H	-0.9025	-4.8935	-0.3283
C	1.0982	-3.2094	-0.1771
H	1.3552	-3.7839	0.7269
H	1.3175	-3.8485	-1.0456
H	1.7678	-2.3506	-0.2343

Structure number: 18 Y=SePh(OMe)₃

Energy= -8.05309783 a.u.

Atom (Å)	X	Y	Z
Se	0.0985	-0.0434	-0.0270
C	2.4709	0.0482	0.0889
O	2.9348	1.2784	0.1063
C	2.3603	1.9923	1.2856
C	3.4459	2.8732	1.8702
O	2.8289	3.4922	2.9937
H	3.4340	4.1826	3.3413
H	4.3077	2.2428	2.1596
H	3.7742	3.6032	1.1115
C	1.8415	0.8787	2.1982
C	1.6575	-0.2971	1.2481
H	1.6740	-1.3195	1.6323
H	2.6092	0.6043	2.9421
H	0.9315	1.1673	2.7405
H	1.5477	2.6144	0.8764
H	2.8281	-0.6135	-0.6976
C	-0.3042	-1.8332	-0.6509
C	0.5758	-2.9210	-0.7811
C	0.1106	-4.1151	-1.3068
C	-1.2257	-4.2297	-1.7192
C	-2.1102	-3.1533	-1.6156
C	-1.6348	-1.9562	-1.0844
O	-2.3811	-0.8265	-0.9448
C	-3.7512	-0.8549	-1.3943
H	-4.1405	0.1484	-1.1989
H	-3.7939	-1.0705	-2.4701
H	-4.3235	-1.5958	-0.8206
H	-3.1403	-3.2405	-1.9403
O	-1.5613	-5.4440	-2.2093
H	0.7487	-4.9875	-1.4160
O	1.8661	-2.7270	-0.3730
C	-2.9194	-5.6480	-2.6389
H	-2.9618	-6.6876	-2.9761
H	-3.6137	-5.5002	-1.8002
H	-3.1647	-4.9760	-3.4728
C	2.7597	-3.8581	-0.4569
H	2.8794	-4.1769	-1.5009
H	3.7183	-3.5048	-0.0637
H	2.3879	-4.6866	0.1611

Structure number: 18 Y=Se^tBu (R=COCF₃)

Energy= -6.70283208 a.u.

Atom (Å)	X	Y	Z
Se	-0.0050	-0.0146	-0.0038
C	2.3506	-0.0027	0.0424
O	2.8714	1.2043	0.0150
C	2.3919	1.9626	1.2121
C	3.5617	2.7953	1.6954
O	3.0352	3.5284	2.8267
C	3.9343	4.3942	3.3695
O	5.0622	4.5628	2.9925
C	3.2797	5.1360	4.5585
F	4.1552	5.9863	5.1036
F	2.1921	5.8240	4.1330
F	2.8823	4.2404	5.4981
H	4.4041	2.1625	2.0144
H	3.9073	3.4929	0.9194
C	1.8732	0.8856	2.1677
C	1.5765	-0.2860	1.2390
H	1.5716	-1.2998	1.6516
H	2.6667	0.5742	2.8690
H	1.0076	1.2230	2.7530
H	1.5869	2.6130	0.8333
H	2.6788	-0.6900	-0.7374
C	-0.5349	-1.9704	-0.4710
C	0.6493	-2.7032	-1.0775
H	1.0234	-2.2081	-1.9852
H	1.4719	-2.8492	-0.3612
H	0.3098	-3.7124	-1.3702
C	-1.0404	-2.6216	0.8064
H	-0.2481	-2.7517	1.5577
H	-1.8732	-2.0634	1.2568
H	-1.4114	-3.6298	0.5526
C	-1.6516	-1.7478	-1.4874
H	-1.2914	-1.2524	-2.4009
H	-2.0490	-2.7352	-1.7767
H	-2.4908	-1.1712	-1.0685

Structure number: 18 Y=Se^tBu

Energy= -5.50814206 a.u.

Atom (Å)	X	Y	Z
Se	-0.0383	0.0133	0.0259
C	1.9901	0.0640	-0.0246
C	1.8130	1.5055	0.0335
O	2.0539	2.0278	1.2108
C	2.3669	0.9236	2.1755
C	3.5056	1.3938	3.0598
O	3.7822	0.2754	3.8945
H	4.4471	0.5426	4.5659
H	4.3680	1.6663	2.4227
H	3.1866	2.2815	3.6312
C	2.6734	-0.2860	1.2905
H	3.7594	-0.3643	1.1097
H	2.3311	-1.2296	1.7353
H	1.4462	0.7932	2.7665
H	1.6417	2.2051	-0.7849
H	2.3546	-0.3934	-0.9498
C	-0.5038	-0.2859	-1.9696
C	0.1006	0.8181	-2.8220
H	1.2007	0.7912	-2.8335
H	-0.2262	0.6619	-3.8649
H	-0.2465	1.8150	-2.5142
C	-0.0011	-1.6689	-2.3538
H	1.0960	-1.7430	-2.3293
H	-0.4256	-2.4553	-1.7142
H	-0.3147	-1.8735	-3.3921
C	-2.0294	-0.2160	-1.9459
H	-2.3949	0.7751	-1.6394
H	-2.3965	-0.4078	-2.9680
H	-2.4726	-0.9827	-1.2917

Structure number: 18 Y=I

Energy= -3.16513072 a.u.

Atom (Å)	X	Y	Z
I	-0.2705	-0.2779	-0.1447
C	2.4484	0.2919	0.1510
O	2.7214	1.5444	0.0732
C	1.9628	2.2924	1.1575
C	2.8737	3.3760	1.7043
O	2.1073	3.9201	2.7738
H	2.5613	4.7257	3.1129
H	3.8256	2.9327	2.0501
H	3.0807	4.1136	0.9117
C	1.5604	1.1803	2.1177
C	1.5386	-0.0559	1.2320
H	1.6662	-1.0390	1.6998
H	2.3546	1.0261	2.8747
H	0.6226	1.3841	2.6498

H 1.1065 2.7357 0.6249

H 2.9246 -0.3646 -0.5848

Structure number: 19 Y=SPh (R¹=CH₂OCOCF₃)

Energy= -7.40201393 a.u.

Atom (Å)	X	Y	Z
S	-0.1070	-0.0262	0.8087
C	2.1619	-0.3787	0.5444
O	2.9510	0.6442	0.3940
C	3.1940	1.5460	1.5642
C	3.1472	0.7492	2.8457
C	1.7733	0.0945	3.0113
C	1.4244	-0.7033	1.7568
H	1.2736	-1.7809	1.8917
H	1.0120	0.8682	3.2004
H	1.7622	-0.5788	3.8800
H	3.9471	-0.0124	2.8270
H	3.3573	1.4273	3.6864
C	4.5298	2.1964	1.2459
O	4.7149	3.1815	2.2891
C	5.8550	3.9100	2.1486
O	6.6553	3.8004	1.2595
C	5.9819	4.9014	3.3308
F	6.1099	4.2064	4.4918
F	4.8761	5.6815	3.4170
F	7.0582	5.6772	3.1610
H	5.3524	1.4658	1.2703
H	4.5094	2.6856	0.2619
H	2.3888	2.2991	1.5177
H	2.1462	-1.0465	-0.3225
C	-0.7402	-1.4962	-0.0174
C	-0.7539	-1.5378	-1.4154
C	-1.3411	-2.6306	-2.0496
C	-1.8975	-3.6631	-1.2947
C	-1.8822	-3.6079	0.1003
C	-1.3111	-2.5179	0.7493
H	-1.3304	-2.4530	1.8377
H	-2.3323	-4.4091	0.6867
H	-2.3568	-4.5152	-1.7971
H	-1.3663	-2.6721	-3.1384
H	-0.3307	-0.7194	-1.9983

Structure number: 20 Y=SeH

Energy= -2.87607979 a.u.

Atom (Å)	X	Y	Z
Se	-0.0661	-0.0066	-0.0297
C	2.3913	-0.0122	0.0359
O	3.0392	1.1061	0.0275
C	2.9907	1.9730	1.2428
C	2.8814	1.1276	2.4851
C	1.6039	0.2854	2.4415
C	1.5491	-0.4974	1.1252
H	1.5660	-1.5906	1.2206
H	0.7256	0.9417	2.5480
H	1.5666	-0.4261	3.2790
H	3.7747	0.4850	2.5681
H	2.8752	1.7899	3.3646
H	3.9210	2.5472	1.1705
H	2.1296	2.6415	1.0872
H	2.5944	-0.6302	-0.8451
H	-0.0248	-1.2648	-0.8192

Structure number: 20 Y=SeMe

Energy= -3.47941493 a.u.

Atom (Å)	X	Y	Z
Se	-0.0660	0.0165	-0.0235
C	2.3441	0.0051	0.0373
O	3.0167	1.1170	0.0249
C	3.0289	1.9612	1.2540
C	2.9139	1.1056	2.4893
C	1.6083	0.3076	2.4556
C	1.5266	-0.4785	1.1452
H	1.5339	-1.5726	1.2379
H	0.7544	0.9974	2.5526
H	1.5447	-0.3933	3.3001
H	3.7853	0.4312	2.5514
H	2.9437	1.7586	3.3755
H	3.9796	2.5000	1.1728
H	2.1930	2.6678	1.1340
H	2.5319	-0.6132	-0.8451
C	-0.3175	-1.6997	-0.9761
H	-1.1941	-1.5305	-1.6179
H	0.5534	-1.9284	-1.6006
H	-0.5246	-2.4873	-0.2426

Structure number: 20 Y=SePh

Energy= -5.35346212 a.u.

Atom (Å)	X	Y	Z
Se	-0.1000	-0.0347	-0.0185
C	2.3714	-0.1050	0.0476
O	3.0675	0.9779	-0.1112
C	3.2132	1.9177	1.0501
C	3.0945	1.1708	2.3538
C	1.7333	0.4707	2.4388
C	1.5424	-0.3922	1.2020
H	1.4450	-1.4741	1.3755
H	0.9439	1.2344	2.5089
H	1.6598	-0.1588	3.3375
H	3.9171	0.4402	2.4393
H	3.2102	1.8908	3.1788
H	4.2033	2.3553	0.8782
H	2.4352	2.6811	0.9137
H	2.5056	-0.8308	-0.7602
C	-0.1769	1.8979	0.0176
C	-0.8713	2.5303	1.0564
C	-1.0142	3.9157	1.0258
C	-0.4788	4.6511	-0.0323
C	0.1944	4.0085	-1.0722
C	0.3452	2.6234	-1.0587
H	0.8497	2.1153	-1.8804
H	0.5897	4.5854	-1.9089
H	-0.6056	5.7341	-0.0574
H	-1.5624	4.4194	1.8225
H	-1.3215	1.9483	1.8608

Structure number: 20 Y=Se^tBu

Energy= -5.27775354 a.u.

Atom (Å)	X	Y	Z
Se	0.0221	0.0861	-0.0070
C	2.4049	0.1471	0.0103
O	2.9895	1.3123	0.0854
C	2.8825	2.0580	1.3672
C	2.9470	1.1033	2.5327
C	1.7670	0.1267	2.4891
C	1.6468	-0.4793	1.0885
H	1.6850	-1.5750	1.0400
H	0.8383	0.6490	2.7661
H	1.9047	-0.6853	3.2188
H	3.9059	0.5593	2.4969
H	2.9339	1.6792	3.4709
H	3.7248	2.7564	1.3201
H	1.9359	2.6184	1.3154
H	2.6443	-0.3904	-0.9102
C	-0.4659	-1.6916	-0.9684
C	-1.6151	-1.2761	-1.8838
H	-1.3679	-0.3898	-2.4883
H	-1.8087	-2.1016	-2.5903
H	-2.5445	-1.0919	-1.3241
C	0.7215	-2.2251	-1.7550
H	0.9834	-1.5740	-2.6032
H	1.6084	-2.3993	-1.1271
H	0.4348	-3.2085	-2.1653
C	-0.9313	-2.6603	0.1100
H	-0.1353	-2.9187	0.8247
H	-1.7904	-2.2635	0.6686
H	-1.2462	-3.6015	-0.3718

Structure number: 21 Y=SPh (R¹=CH₂OCOCF₃)

Energy= -7.37720251 a.u.

Atom (Å)	X	Y	Z
Se	-0.2539	0.0760	0.5585
C	2.1472	-0.3191	0.5623
O	2.9798	0.6704	0.3892
C	3.1961	1.6398	1.5071
C	3.0068	0.9512	2.8377
C	1.5904	0.3784	2.9354
C	1.3312	-0.5347	1.7406
H	1.1557	-1.5961	1.9543
H	0.8628	1.2057	2.9664
H	1.4554	-0.1933	3.8643
H	3.7615	0.1521	2.9438
H	3.1868	1.6845	3.6383
C	4.5929	2.1815	1.2484
O	4.7709	3.2236	2.2363
C	5.9912	3.8217	2.1794
O	6.8675	3.5629	1.3995
C	6.0923	4.8933	3.2925
F	5.9765	4.2994	4.5095
F	5.0962	5.8038	3.1623
F	7.2740	5.5160	3.2187
H	5.3589	1.4029	1.3813
H	4.6756	2.6021	0.2363
H	2.4492	2.4365	1.3474
H	2.1852	-1.0567	-0.2451
C	-0.7574	-1.6116	-0.2472
C	-0.5823	-1.7794	-1.6245
C	-1.0426	-2.9512	-2.2214
C	-1.6662	-3.9320	-1.4503
C	-1.8411	-3.7487	-0.0777
C	-1.3938	-2.5808	0.5351
H	-1.5609	-2.4204	1.6003
H	-2.3446	-4.5106	0.5180
H	-2.0299	-4.8438	-1.9252
H	-0.9196	-3.0929	-3.2954
H	-0.1103	-1.0029	-2.2268

Structure number: 22 Y=I

Energy= -2.66367356 a.u.

Atom (Å)	X	Y	Z
I	-0.1622	-0.0370	-0.0788
C	2.5994	0.0358	0.1307
O	3.2446	1.1431	0.1298
C	3.1576	2.0369	1.3359
C	3.0537	1.1956	2.5795
C	1.7943	0.3185	2.5337
C	1.7202	-0.4203	1.1982
H	1.7219	-1.5180	1.2592
H	0.9017	0.9409	2.6904
H	1.8115	-0.4271	3.3429
H	3.9653	0.5809	2.6767
H	3.0204	1.8618	3.4560
H	4.0767	2.6285	1.2618
H	2.2806	2.6747	1.1500
H	2.7997	-0.5871	-0.7501

Structure number: 23 Y=I ($R^1=CH_2OCOCF_3$)

Energy= -4.68587574 a.u.

Atom (Å)	X	Y	Z
I	0.1415	0.2625	-0.0688
C	2.8243	-0.3126	0.2916
O	3.6352	0.6836	0.2992
C	3.4810	1.6982	1.4079
C	3.2879	0.9436	2.6999
C	1.9864	0.1289	2.6591
C	1.8068	-0.5540	1.3034
H	1.5392	-1.6184	1.3439
H	1.1242	0.7692	2.8925
H	2.0088	-0.6618	3.4263
H	4.1635	0.2878	2.8545
H	3.2684	1.6639	3.5327
C	4.6967	2.6055	1.3173
O	4.2476	3.8203	1.9603
C	4.9979	4.9196	1.6656
O	5.9909	4.9335	0.9912
C	4.3483	6.1650	2.3184
F	4.3166	6.0213	3.6662
F	3.0733	6.3031	1.8698
F	5.0466	7.2603	2.0036
H	5.5718	2.2030	1.8494
H	4.9674	2.8073	0.2707
H	2.5868	2.2765	1.1193
H	2.9962	-1.0136	-0.5353