Highly Enantioselective (–)-Sparteine-Mediated Lateral Metalation-Functionalization of Remote Silyl Protected *ortho*-Ethyl Phenyl Dialkyl-O-carbamates

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Supporting Information

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Computational Details

All structures and energies reported were determined at the PM3 level with SMD diethylether solvation using GAMESS [1 May 2012 (R1)]. Cartesian coordinates are given in Ångström.

Path A

R (A)

Energy: -633030.0972 kJ mol^{-1}

C	-3.037453	0.106549	0.824733
C	-1.713103	-0.296636	0.906653
C	-0.690873	0.640153	0.710113
C	-0.970753	1.987650	0.429156
C	-2.315961	2.354667	0.318955
C	-3.333516	1.429703	0.515055
O	0.606316	0.220483	1.013143
C	1.480555	-0.149221	0.022464
N	2.687791	-0.596315	0.622247
C	3.903532	-0.720088	-0.252982
C	4.500958	0.633083	-0.631304
C	0.110185	3.001512	0.235566
C	-0.303043	4.406512	0.617577
Si	-4.411687	-1.078814	1.172077
C	-5.354073	-1.449612	-0.425585
O	1.168887	-0.184973	-1.166729
C	-5.599920	-0.304186	2.427743
C	-3.733016	-2.701194	1.876825
C	2.812945	-0.405982	2.117778
C	2.880705	-1.766384	2.804573
C	3.981138	0.472052	2.542512
C	4.972619	-1.610988	0.369855
Li	1.056138	0.207348	-3.054719
C	1.275329	2.284290	-3.578280
C	2.371866	2.793283	-2.695690
C	0.018299	3.103021	-3.491759
C	0.090538	4.420779	-4.244252
H	3.850753	1.196385	-1.328160
H	5.465588	0.494893	-1.138210
H	4.678301	1.271673	0.250707
H	3.537946	-1.228115	-1.190032
H	5.546256	-1.078086	1.148376
H	5.685618	-1.942224	-0.395922
H	4.546087	-2.508657	0.847536
H	1.855903	0.103191	2.429946
H	3.027648	-1.641163	3.885284

H	3.712746	-2.383144	2.423532
H	1.957069	-2.342543	2.662414
H	3.864607	0.784267	3.587947
H	4.065018	1.381091	1.923920
H	4.945277	-0.059773	2.461185
H	-2.551965	3.405475	0.084514
H	-4.382052	1.745007	0.436613
H	-1.474969	-1.342581	1.145388
H	0.432101	2.971265	-0.842849
H	1.010879	2.717970	0.816652
H	-1.263275	4.682606	0.150570
H	0.448032	5.138457	0.295799
H	-0.428252	4.516238	1.702476
H	-3.091869	-3.213105	1.153144
H	-4.552735	-3.377404	2.136595
H	-3.143090	-2.525643	2.780964
H	-4.672749	-1.808193	-1.209665
H	-5.857938	-0.556496	-0.805518
H	-6.112881	-2.219370	-0.259468
H	-5.120355	-0.182793	3.402822
H	-6.482818	-0.935319	2.563620
H	-5.937927	0.681644	2.094671
H	0.290302	4.267891	-5.313129
H	0.889383	5.066320	-3.855025
H	-0.847400	4.986402	-4.167612
H	-0.838609	2.514523	-3.893280
H	-0.229764	3.302043	-2.423104
H	2.025734	2.898320	-1.649842
H	2.753826	3.783563	-2.997648
H	3.242392	2.104059	-2.690660
H	1.614851	2.191998	-4.634710
C	-3.333953	-2.005334	-3.460223
C	-3.194730	-0.573299	-3.945511
C	-1.847839	0.002549	-3.521415
N	-0.675011	-0.797091	-4.016552
C	-0.495953	-0.625792	-5.506493
C	0.540099	-1.568442	-6.131432
H	0.458650	-1.458125	-7.241222
C	0.226951	-3.008590	-5.735370
C	0.313568	-3.103080	-4.214542
H	0.135754	-4.161315	-3.898706
C	-0.802195	-2.241501	-3.586475
H	-0.680430	-2.236723	-2.470995
C	-2.170723	-2.860118	-3.928207
C	1.719903	-2.720959	-3.731233
N	2.216190	-1.392940	-4.251327
C	2.004957	-1.281234	-5.750874

H	2.629411	-2.071447	-6.257173
C	2.495957	0.081534	-6.249579
C	3.978659	0.246373	-5.948146
C	4.237439	0.076164	-4.458900
C	3.689623	-1.255758	-3.956239
H	-4.286837	-2.439434	-3.821496
H	-3.405937	-2.021300	-2.348223
H	-4.011908	0.050584	-3.535014
H	-3.304924	-0.529726	-5.049906
H	-1.780114	0.043361	-2.410072
H	-1.735173	1.056652	-3.876316
H	-0.194870	0.431823	-5.679594
H	-1.471100	-0.769968	-6.028543
H	-0.794203	-3.294555	-6.074666
H	0.922193	-3.721132	-6.219742
H	-2.236194	-3.031472	-5.028304
H	-2.237991	-3.866055	-3.468819
H	2.419633	-3.537647	-4.023941
H	1.743408	-2.671718	-2.620028
H	2.312651	0.162545	-7.338456
H	1.918184	0.913426	-5.770699
H	4.574461	-0.487965	-6.527399
H	4.324094	1.243783	-6.281254
H	5.324193	0.122293	-4.250542
H	3.781040	0.919421	-3.877850
H	4.265623	-2.097661	-4.404408
H	3.833086	-1.335633	-2.853471

TS1 (A)

Energy: -632950.8066 kJ mol^{-1}
Imaginary frequency: 1075.18i cm^{-1}

C	-3.009729	-0.036081	0.809053
C	-1.723141	-0.501492	1.026046
C	-0.631045	0.302626	0.687542
C	-0.786649	1.585645	0.110172
C	-2.115314	2.026299	-0.075532
C	-3.196331	1.232477	0.259260
O	0.616610	-0.167607	1.122588
C	1.580703	-0.441786	0.196610
N	2.837392	-0.689508	0.804794
C	4.058723	-0.545901	-0.064618
C	4.349944	0.909057	-0.429401
C	0.325515	2.399579	-0.316808
C	0.150823	3.883975	-0.218616

Si	-4.476182	-1.066258	1.208364
C	-5.399305	-1.476617	-0.396621
O	1.326331	-0.598158	-1.004923
C	-5.631618	-0.106814	2.365882
C	-3.966590	-2.687807	2.050123
C	2.903179	-0.484015	2.301006
C	3.245102	-1.804916	2.982297
C	3.859749	0.614415	2.742367
C	5.287640	-1.191159	0.564469
Li	0.928812	0.054380	-2.727772
C	1.106897	2.412309	-3.101744
C	2.386802	3.135520	-2.768156
C	0.027630	3.320818	-3.650409
C	0.321968	3.878249	-5.030145
H	3.579246	1.348109	-1.094474
H	5.307293	0.982126	-0.963130
H	4.416893	1.554538	0.463374
H	3.820122	-1.111948	-1.010172
H	5.727756	-0.552567	1.350528
H	6.061843	-1.359866	-0.194685
H	5.056366	-2.160985	1.036023
H	1.856659	-0.184681	2.597988
H	3.361420	-1.657553	4.063948
H	4.186528	-2.236246	2.600140
H	2.458737	-2.556689	2.835445
H	3.668436	0.891633	3.786625
H	3.761411	1.523857	2.126173
H	4.913918	0.293597	2.672275
H	-2.255536	3.033913	-0.497215
H	-4.217758	1.599621	0.098172
H	-1.570984	-1.491962	1.476364
H	0.604336	2.134040	-1.704678
H	1.300215	2.096324	0.102815
H	-0.832092	4.197174	-0.609103
H	0.932332	4.392305	-0.809936
H	0.220961	4.253321	0.814141
H	-3.321306	-3.285964	1.400431
H	-4.848028	-3.287362	2.294178
H	-3.421095	-2.496342	2.978458
H	-4.703939	-1.840476	-1.166218
H	-5.901871	-0.591976	-0.797420
H	-6.155245	-2.248118	-0.229195
H	-5.160309	0.060916	3.337960
H	-6.562463	-0.655883	2.531849
H	-5.884621	0.869151	1.941209
H	0.462017	3.075803	-5.769490
H	1.237188	4.485778	-5.039007

H	-0.495619	4.515523	-5.391371
H	-0.927955	2.746063	-3.690429
H	-0.156426	4.156941	-2.944982
H	2.231558	3.846772	-1.936916
H	2.805231	3.707388	-3.610149
H	3.160759	2.403861	-2.452914
H	1.343569	1.658106	-3.910601
C	-3.489170	-1.802704	-3.566166
C	-3.294553	-0.335167	-3.906392
C	-1.927438	0.151428	-3.438620
N	-0.780959	-0.659168	-3.980316
C	-0.547716	-0.355952	-5.441667
C	0.479813	-1.273156	-6.117218
H	0.449852	-1.050614	-7.212791
C	0.089462	-2.729024	-5.880186
C	0.122517	-2.981139	-4.375744
H	-0.114273	-4.055715	-4.174258
C	-0.973644	-2.133394	-3.691606
H	-0.878427	-2.238144	-2.577190
C	-2.358142	-2.652968	-4.116008
C	1.533280	-2.722966	-3.824244
N	2.079513	-1.357493	-4.168520
C	1.937937	-1.081480	-5.654630
H	2.561864	-1.832294	-6.216481
C	2.476513	0.312715	-5.989418
C	3.937229	0.433573	-5.581884
C	4.106860	0.115461	-4.104212
C	3.531256	-1.259269	-3.771241
H	-4.455796	-2.160829	-3.971431
H	-3.570192	-1.926828	-2.460890
H	-4.084447	0.274023	-3.425264
H	-3.416142	-0.175275	-4.998009
H	-1.868324	0.119806	-2.323756
H	-1.766511	1.223808	-3.718124
H	-0.214442	0.705859	-5.511315
H	-1.505497	-0.421493	-6.007417
H	-0.933645	-2.928449	-6.272220
H	0.766570	-3.421112	-6.416836
H	-2.409297	-2.700615	-5.229214
H	-2.475454	-3.699057	-3.770234
H	2.211103	-3.519358	-4.208238
H	1.535151	-2.818301	-2.715496
H	2.363916	0.499117	-7.075326
H	1.867992	1.100668	-5.478195
H	4.563533	-0.246627	-6.194086
H	4.305858	1.455459	-5.795164
H	5.180491	0.131160	-3.830630

H	3.631991	0.915317	-3.474620
H	4.133925	-2.053751	-4.266881
H	3.607707	-1.450044	-2.673316

INT (A)

Energy: -572328.0704 kJ mol^{-1}

C	-2.845646	0.254360	0.779471
C	-1.555546	-0.122746	1.113703
C	-0.465556	0.509641	0.512406
C	-0.620857	1.496671	-0.510863
C	-1.963343	1.929994	-0.721133
C	-3.033659	1.318122	-0.107320
O	0.784600	0.146154	1.040101
C	1.643215	-0.553034	0.246446
N	2.820888	-0.993166	0.910778
C	4.074890	-1.057711	0.078239
C	4.666200	0.325553	-0.189877
C	0.455982	2.004124	-1.289023
C	0.267853	3.207225	-2.148873
Si	-4.297978	-0.728573	1.304576
C	-5.015328	-1.557045	-0.251180
O	1.382239	-0.861033	-0.925524
C	-5.623950	0.394866	2.064568
C	-3.823167	-2.064922	2.563555
C	2.872498	-0.843187	2.411919
C	2.904415	-2.233023	3.044011
C	4.029242	0.001333	2.928120
C	5.120200	-1.976890	0.697239
Li	0.693336	0.116302	-2.463354
H	3.992246	0.946982	-0.800490
H	5.612023	0.235796	-0.740665
H	4.874630	0.882242	0.739434
H	3.767610	-1.494014	-0.916731
H	5.661565	-1.481324	1.522356
H	5.863287	-2.274770	-0.052913
H	4.673190	-2.893140	1.118291
H	1.915757	-0.337582	2.712373
H	3.020099	-2.157189	4.133045
H	3.742195	-2.840604	2.659497
H	1.980091	-2.792262	2.849412
H	3.873133	0.259707	3.983182
H	4.144712	0.941097	2.363518
H	4.992120	-0.534657	2.858089
H	-2.126533	2.743826	-1.444480

H	-4.056147	1.651542	-0.326733
H	-1.400213	-0.923717	1.849649
H	1.465868	1.938776	-0.842751
H	-0.785122	3.351598	-2.447214
H	0.865241	3.134571	-3.071572
H	0.581131	4.132766	-1.640518
H	-3.062665	-2.739023	2.159727
H	-4.695789	-2.665323	2.835206
H	-3.421868	-1.616379	3.476500
H	-4.227792	-2.024830	-0.861128
H	-5.516285	-0.816664	-0.882645
H	-5.742782	-2.327674	0.014311
H	-5.270146	0.839998	2.998267
H	-6.534873	-0.168674	2.283298
H	-5.884121	1.208929	1.381817
C	-3.349630	-2.430664	-3.391418
C	-3.465704	-0.941012	-3.656596
C	-2.213622	-0.222443	-3.167975
N	-0.929272	-0.733943	-3.759961
C	-0.768553	-0.235108	-5.176117
C	0.372404	-0.894630	-5.957592
H	0.277245	-0.572961	-7.024444
C	0.246990	-2.410826	-5.870896
C	0.377408	-2.808323	-4.404027
H	0.335966	-3.922850	-4.316291
C	-0.820824	-2.239202	-3.609555
H	-0.652700	-2.414611	-2.512477
C	-2.094885	-2.991509	-4.034976
C	1.745232	-2.369131	-3.863955
N	2.000456	-0.893308	-4.033686
C	1.773777	-0.469662	-5.474215
H	2.528527	-0.989755	-6.126961
C	1.976732	1.044225	-5.613997
C	3.360460	1.457194	-5.134484
C	3.609206	0.968487	-3.714946
C	3.406663	-0.542592	-3.620664
H	-4.239680	-2.961369	-3.781350
H	-3.356553	-2.609197	-2.289463
H	-4.349437	-0.529761	-3.127533
H	-3.643026	-0.750475	-4.734860
H	-2.134432	-0.314321	-2.056976
H	-2.291265	0.868373	-3.370674
H	-0.565479	0.861150	-5.116154
H	-1.716199	-0.361989	-5.746120
H	-0.741152	-2.744271	-6.261826
H	1.013619	-2.913383	-6.491329
H	-2.181871	-2.963069	-5.146684

H	-1.987994	-4.062546	-3.772339
H	2.536901	-2.960842	-4.378392
H	1.828633	-2.613028	-2.781595
H	1.841230	1.333476	-6.675087
H	1.176247	1.586776	-5.051844
H	4.135353	1.053230	-5.817274
H	3.462625	2.558504	-5.181088
H	4.639310	1.219761	-3.393469
H	2.932934	1.499669	-2.999761
H	4.156674	-1.075446	-4.247741
H	3.573973	-0.896455	-2.571272

TS2 (A)

Energy: -640051.5212 kJ mol^{-1}
Imaginary frequency: 26.33i cm^{-1}

C	-3.148994	0.042050	0.457146
C	-1.901713	-0.465657	0.774688
C	-0.745745	0.162048	0.291025
C	-0.801082	1.287717	-0.578729
C	-2.102340	1.810242	-0.813914
C	-3.235214	1.207405	-0.309712
O	0.445556	-0.304774	0.868036
C	1.415291	-0.806921	0.052835
N	2.627654	-1.218287	0.695889
C	3.864457	-0.770087	-0.051166
C	3.970301	0.754246	-0.095042
C	0.346891	1.922277	-1.173727
C	0.272021	3.401267	-1.365958
Si	-4.687144	-0.851432	0.928569
C	-5.384602	-1.669114	-0.633190
O	1.228191	-0.954693	-1.160916
C	-5.979063	0.347996	1.624760
C	-4.328833	-2.190504	2.221989
C	2.630077	-1.328928	2.201614
C	3.112556	-2.724255	2.591888
C	3.448562	-0.258494	2.913883
C	5.144898	-1.381112	0.498441
Li	0.331565	-0.010287	-2.574048
H	3.072555	1.219729	-0.545873
H	4.838812	1.064182	-0.689044
H	4.082400	1.186444	0.914652
H	3.730279	-1.159602	-1.103047
H	5.474291	-0.886343	1.428846
H	5.957252	-1.280803	-0.232674

H	5.027887	-2.452524	0.731836
H	1.570273	-1.235621	2.552097
H	3.186105	-2.809802	3.684083
H	4.106710	-2.955927	2.172481
H	2.423668	-3.505966	2.246144
H	3.176953	-0.208059	3.975720
H	3.297640	0.742792	2.477003
H	4.531560	-0.466819	2.860150
H	-2.176017	2.724298	-1.425658
H	-4.224070	1.634689	-0.520761
H	-1.824847	-1.353507	1.418166
H	-0.692703	3.714594	-1.798683
H	1.076736	3.761760	-2.028917
H	0.382526	3.938031	-0.410660
H	-3.675202	-2.969070	1.818417
H	-5.257829	-2.666246	2.548702
H	-3.839359	-1.765632	3.102844
H	-4.630933	-2.320294	-1.099152
H	-5.675836	-0.918342	-1.373352
H	-6.263087	-2.276598	-0.401371
H	-5.634919	0.799043	2.559409
H	-6.918991	-0.172878	1.827741
H	-6.186147	1.157505	0.918399
C	-3.080977	-3.235745	-2.962446
C	-3.088201	-1.997793	-3.839857
C	-1.860914	-1.148848	-3.527923
N	-0.562736	-1.870692	-3.804218
C	-0.359478	-2.007544	-5.293657
C	0.694995	-3.023459	-5.748429
H	0.544895	-3.177406	-6.845957
C	0.519043	-4.348264	-5.020630
C	0.666363	-4.071037	-3.528589
H	0.594363	-5.034324	-2.963880
C	-0.509039	-3.185195	-3.057467
H	-0.348464	-2.904958	-1.983975
C	-1.801480	-4.025923	-3.158173
C	2.056811	-3.492370	-3.238185
N	2.404417	-2.309825	-4.085004
C	2.150646	-2.562318	-5.544217
H	2.826456	-3.388622	-5.900708
C	2.457694	-1.313370	-6.371490
C	3.885437	-0.850802	-6.138077
C	4.138489	-0.617362	-4.658488
C	3.805115	-1.856738	-3.836433
H	-3.954033	-3.876348	-3.197046
H	-3.214971	-2.941539	-1.895395
H	-4.012097	-1.411330	-3.672365

H	-3.084787	-2.280021	-4.916514
H	-1.882735	-0.844991	-2.447271
H	-1.876667	-0.207737	-4.127550
H	-0.062951	-0.997038	-5.675657
H	-1.336537	-2.268988	-5.768902
H	-0.478253	-4.790725	-5.238821
H	1.261946	-5.095595	-5.361587
H	-1.837395	-4.534193	-4.150071
H	-1.751906	-4.841881	-2.410154
H	2.809050	-4.303711	-3.367787
H	2.122067	-3.165403	-2.180239
H	2.302725	-1.538761	-7.445328
H	1.721700	-0.508821	-6.125764
H	4.597244	-1.604429	-6.531715
H	4.083093	0.076777	-6.708887
H	5.197043	-0.339838	-4.488938
H	3.539360	0.256404	-4.310987
H	4.537950	-2.666004	-4.052652
H	3.895820	-1.629743	-2.748474
S	-0.031801	1.582133	-6.125024
S	0.494748	1.877878	-4.182508
C	-0.671811	3.131794	-6.807096
C	2.152564	2.623683	-4.157226
H	2.955690	1.872056	-4.200313
H	2.236267	3.181401	-3.207668
H	2.304974	3.330599	-4.980018
H	0.091282	3.915202	-6.868773
H	-1.519558	3.535888	-6.243903
H	-1.015713	2.914836	-7.826450
H	1.349461	1.622104	-0.793405

C3 (A)

Energy: -640159.5837 kJ mol^{-1}

C	-3.069058	0.189156	0.169919
C	-1.811523	-0.256066	0.545460
C	-0.672078	0.391089	0.052621
C	-0.756187	1.471734	-0.848261
C	-2.046851	1.919460	-1.171779
C	-3.179304	1.289960	-0.673862
O	0.535924	-0.002772	0.644393
C	1.449878	-0.695744	-0.088192
N	2.660855	-1.042390	0.610739
C	3.900531	-0.578870	-0.119932
C	3.957013	0.943454	-0.240734

C	0.432632	2.126144	-1.448979
C	0.422095	3.631019	-1.283952
Si	-4.575479	-0.721735	0.725038
C	-5.140077	-1.843699	-0.693123
O	1.216788	-1.060237	-1.241094
C	-5.967037	0.488742	1.155227
C	-4.190494	-1.786811	2.244700
C	2.616922	-1.074079	2.120176
C	3.148513	-2.424582	2.596706
C	3.362006	0.068026	2.800584
C	5.185816	-1.109427	0.498610
Li	0.921030	-0.849645	-3.117819
H	3.079717	1.351834	-0.777902
H	4.852705	1.253969	-0.793574
H	3.985990	1.433383	0.748326
H	3.809262	-1.027789	-1.151817
H	5.462145	-0.556548	1.413638
H	6.017874	-1.009372	-0.210058
H	5.105041	-2.172421	0.780448
H	1.542754	-1.017614	2.432137
H	3.185705	-2.452409	3.693750
H	4.166822	-2.629889	2.224404
H	2.509427	-3.254209	2.267399
H	3.056371	0.157272	3.850563
H	3.177198	1.038238	2.309806
H	4.454744	-0.090278	2.787244
H	-2.148718	2.782347	-1.843259
H	-4.175297	1.656943	-0.954084
H	-1.717325	-1.105299	1.236849
H	-0.494079	4.086495	-1.685167
H	1.280536	4.070299	-1.822368
H	0.501388	3.927840	-0.229628
H	-3.512350	-2.607615	1.993207
H	-5.109014	-2.222420	2.648543
H	-3.721480	-1.195803	3.036290
H	-4.325662	-2.499493	-1.034937
H	-5.467673	-1.252522	-1.553948
H	-5.974884	-2.476658	-0.380636
H	-5.702417	1.103920	2.019729
H	-6.886192	-0.052915	1.396562
H	-6.182140	1.160132	0.318315
C	-3.192113	-3.537708	-3.211676
C	-3.205967	-2.186910	-3.906125
C	-1.937804	-1.407495	-3.579359
N	-0.671593	-2.137963	-3.934444
C	-0.460556	-2.150127	-5.431149
C	0.693535	-3.047348	-5.894738

H	0.645189	-3.095297	-7.011007
C	0.513537	-4.447277	-5.313893
C	0.564200	-4.331562	-3.793239
H	0.484220	-5.351685	-3.340979
C	-0.650468	-3.514143	-3.302629
H	-0.553666	-3.338231	-2.198310
C	-1.937285	-4.319012	-3.556230
C	1.912545	-3.749634	-3.345018
N	2.274501	-2.445428	-4.017939
C	2.105080	-2.551855	-5.523462
H	2.832497	-3.320676	-5.909885
C	2.449832	-1.211316	-6.178930
C	3.895187	-0.841872	-5.877544
C	4.132940	-0.793225	-4.376301
C	3.706066	-2.089834	-3.694473
H	-4.087097	-4.123811	-3.497753
H	-3.276731	-3.387708	-2.109500
H	-4.089263	-1.602310	-3.578745
H	-3.318049	-2.316401	-5.002554
H	-1.903442	-1.184446	-2.487442
H	-1.919989	-0.414184	-4.099890
H	-0.285612	-1.085887	-5.741424
H	-1.391526	-2.480009	-5.947332
H	-0.465485	-4.877329	-5.624994
H	1.289241	-5.142934	-5.688010
H	-1.963059	-4.645639	-4.622489
H	-1.903497	-5.253051	-2.961273
H	2.701839	-4.512965	-3.535162
H	1.906661	-3.573061	-2.246994
H	2.298205	-1.291089	-7.273500
H	1.754292	-0.406360	-5.832935
H	4.583818	-1.571725	-6.350019
H	4.139932	0.137959	-6.331221
H	5.205583	-0.612399	-4.166269
H	3.591974	0.078910	-3.929802
H	4.395077	-2.915279	-3.984165
H	3.797142	-1.980726	-2.586304
S	-0.454690	1.449822	-5.079048
S	0.596301	1.741023	-3.344463
C	-0.973718	3.042319	-5.774994
C	2.328964	2.316560	-3.578633
H	3.084966	1.585030	-3.260501
H	2.467098	3.236374	-2.988929
H	2.505693	2.547320	-4.633203
H	-0.198398	3.810012	-5.682091
H	-1.875502	3.429454	-5.290191
H	-1.196268	2.922440	-6.840733

H	1.378646	1.747258	-0.981971

Path B

R (B)

Energy: -633029.1674 kJ mol^{-1}

C	-2.908630	0.199654	0.697805
C	-1.584456	-0.204895	0.775436
C	-0.566363	0.753509	0.709299
C	-0.849684	2.118427	0.542409
C	-2.193739	2.496645	0.465667
C	-3.207958	1.549383	0.549159
O	0.734373	0.345071	1.008934
C	1.562292	-0.144631	0.031695
N	2.760847	-0.605284	0.635459
C	3.939435	-0.880596	-0.255143
C	4.623680	0.394774	-0.740652
C	0.218051	3.159663	0.439051
C	0.779099	3.529621	1.796206
Si	-4.283295	-1.032910	0.783927
C	-5.402256	-0.800047	-0.724381
O	1.217941	-0.255377	-1.143944
C	-5.280959	-0.761775	2.369316
C	-3.602074	-2.801024	0.761848
C	2.938792	-0.304033	2.107166
C	2.917665	-1.607156	2.900112
C	4.184209	0.505554	2.437453
C	4.953676	-1.804664	0.409749
Li	1.070189	0.121112	-3.025386
C	1.326724	2.192145	-3.525224
C	2.442318	2.675065	-2.652472
C	0.083415	3.031329	-3.428947
C	0.151758	4.318023	-4.234648
H	3.973772	0.988235	-1.412810
H	5.529495	0.145905	-1.310209
H	4.924205	1.050837	0.093677
H	3.516546	-1.421266	-1.149631
H	5.589338	-1.261757	1.131188
H	5.615988	-2.249483	-0.343690
H	4.472022	-2.625519	0.966952
H	2.033744	0.307461	2.393770
H	3.107383	-1.410879	3.963404
H	3.685860	-2.317456	2.548431
H	1.947001	-2.114808	2.827258

H	4.119577	0.906406	3.456886
H	4.324790	1.354430	1.747885
H	5.100214	-0.108266	2.379809
H	-2.448338	3.556359	0.337894
H	-4.257844	1.865383	0.492274
H	-1.344590	-1.270786	0.893203
H	-0.194190	4.063939	-0.055467
H	1.030140	2.804603	-0.242469
H	-0.002292	3.906116	2.468970
H	1.540963	4.314412	1.704482
H	1.251898	2.669934	2.291480
H	-3.025557	-2.986492	-0.150331
H	-4.419899	-3.526648	0.795399
H	-2.948917	-2.991594	1.618187
H	-4.893933	-1.169152	-1.627112
H	-5.649376	0.253570	-0.881490
H	-6.337444	-1.354463	-0.610022
H	-4.684977	-0.994088	3.256168
H	-6.166381	-1.403826	2.381639
H	-5.616887	0.275788	2.452629
H	0.341505	4.122157	-5.298418
H	0.956247	4.975440	-3.878577
H	-0.783387	4.889885	-4.172108
H	-0.791258	2.439402	-3.786312
H	-0.136626	3.275398	-2.367849
H	2.128502	2.759908	-1.594047
H	2.822303	3.670012	-2.942037
H	3.309690	1.982272	-2.682929
H	1.656367	2.092577	-4.585080
C	-3.356055	-2.044234	-3.442748
C	-3.170195	-0.636909	-3.982012
C	-1.845969	-0.064314	-3.488361
N	-0.670406	-0.876989	-3.955406
C	-0.511115	-0.748100	-5.452270
C	0.516553	-1.707225	-6.062511
H	0.425907	-1.624555	-7.173912
C	0.206777	-3.136944	-5.627920
C	0.299773	-3.193182	-4.105341
H	0.117656	-4.242003	-3.761925
C	-0.808183	-2.310232	-3.490274
H	-0.680067	-2.279077	-2.375841
C	-2.181603	-2.934565	-3.808398
C	1.713104	-2.808451	-3.644796
N	2.213539	-1.496945	-4.201565
C	1.983664	-1.409075	-5.699968
H	2.604810	-2.204131	-6.202677
C	2.466364	-0.049949	-6.217771

C	3.956950	0.106580	-5.952230
C	4.246601	-0.050290	-4.467370
C	3.692385	-1.366433	-3.930468
H	-4.291926	-2.484034	-3.840571
H	-3.501281	-2.001019	-2.337061
H	-4.008225	0.012425	-3.664824
H	-3.182062	-0.645706	-5.095519
H	-1.823332	-0.034622	-2.375163
H	-1.708359	0.991564	-3.828855
H	-0.213997	0.303193	-5.662258
H	-1.502920	-0.903551	-5.946022
H	-0.814156	-3.434159	-5.957454
H	0.901882	-3.860495	-6.096141
H	-2.228249	-3.190213	-4.893050
H	-2.267496	-3.900771	-3.273141
H	2.404438	-3.636932	-3.924161
H	1.747906	-2.732661	-2.535153
H	2.256516	0.027441	-7.301927
H	1.907052	0.788714	-5.727196
H	4.534286	-0.637941	-6.537079
H	4.302422	1.097908	-6.302975
H	5.338102	-0.015938	-4.282469
H	3.813828	0.806160	-3.888305
H	4.254314	-2.222979	-4.368482
H	3.849748	-1.423769	-2.827371

TS1 (B)

Energy: -632938.9157 kJ mol^{-1}
Imaginary frequency: 1050.06i cm^{-1}

C	-2.905463	-0.212367	0.784949
C	-1.587226	-0.514610	1.076606
C	-0.565146	0.353609	0.672965
C	-0.821966	1.555137	-0.027114
C	-2.184956	1.815328	-0.311308
C	-3.194390	0.957722	0.083653
O	0.713315	-0.004626	1.125064
C	1.645512	-0.379849	0.203892
N	2.893211	-0.690712	0.811759
C	4.116265	-0.538133	-0.053258
C	4.425564	0.923253	-0.369878
C	0.168395	2.500572	-0.495789
C	1.334765	2.825235	0.388493
Si	-4.281404	-1.333414	1.258945
C	-5.263480	-1.791709	-0.299300

O	1.374613	-0.557607	-0.990331
C	-5.435987	-0.444846	2.471176
C	-3.625216	-2.918262	2.066171
C	2.964684	-0.502711	2.310133
C	3.282772	-1.841211	2.968464
C	3.944892	0.568362	2.766868
C	5.334689	-1.222819	0.553266
Li	0.900597	0.045831	-2.719517
C	1.271645	2.375142	-3.162022
C	2.612692	2.969767	-2.822512
C	0.301540	3.375071	-3.753367
C	0.699068	3.896295	-5.121550
H	3.569240	1.448239	-0.848778
H	5.275613	0.991675	-1.061410
H	4.680630	1.497729	0.537394
H	3.864722	-1.069213	-1.015896
H	5.788061	-0.615985	1.356981
H	6.103696	-1.383204	-0.212655
H	5.085874	-2.200774	0.998504
H	1.926379	-0.183555	2.613874
H	3.414387	-1.713520	4.050790
H	4.209887	-2.287434	2.568272
H	2.477893	-2.572426	2.818585
H	3.754274	0.842313	3.811988
H	3.872472	1.484400	2.155881
H	4.991172	0.221650	2.700214
H	-2.438806	2.728744	-0.863419
H	-4.239948	1.192595	-0.153329
H	-1.351090	-1.437143	1.625139
H	-0.310463	3.428374	-0.860441
H	0.674416	2.155899	-1.787019
H	1.134558	2.654682	1.455428
H	1.628818	3.878303	0.278060
H	2.232222	2.231151	0.124503
H	-2.935832	-3.445571	1.400777
H	-4.449378	-3.596471	2.304643
H	-3.090356	-2.698319	2.994395
H	-4.593710	-1.949091	-1.155703
H	-5.962005	-0.994480	-0.568789
H	-5.838442	-2.708538	-0.145259
H	-4.914443	-0.194159	3.398734
H	-6.293643	-1.073401	2.725856
H	-5.814680	0.484215	2.035373
H	0.804291	3.078172	-5.849325
H	1.660430	4.427108	-5.093423
H	-0.047235	4.595323	-5.520747
H	-0.698629	2.885026	-3.836701

H	0.159463	4.224523	-3.055515
H	2.534321	3.723028	-2.024878
H	3.105239	3.458445	-3.677630
H	3.300128	2.175828	-2.459664
H	1.446311	1.583458	-3.950164
C	-3.603852	-1.474769	-3.681199
C	-3.292113	-0.033538	-4.045952
C	-1.903523	0.361161	-3.555462
N	-0.807185	-0.549395	-4.039143
C	-0.500889	-0.295141	-5.496331
C	0.474065	-1.302311	-6.118944
H	0.499098	-1.099647	-7.218513
C	-0.038347	-2.718051	-5.871530
C	-0.075255	-2.942742	-4.363022
H	-0.403196	-3.991290	-4.152069
C	-1.122795	-1.998447	-3.731611
H	-1.071018	-2.088728	-2.613128
C	-2.529303	-2.417158	-4.192606
C	1.331592	-2.785575	-3.765853
N	1.997033	-1.475505	-4.114474
C	1.926033	-1.216473	-5.608529
H	2.506522	-2.024434	-6.136784
C	2.585034	0.124009	-5.947569
C	4.036659	0.136989	-5.492639
C	4.134417	-0.171329	-4.006544
C	3.439448	-1.489431	-3.673900
H	-4.587231	-1.767388	-4.098002
H	-3.709554	-1.575733	-2.575445
H	-4.043809	0.643993	-3.596300
H	-3.378430	0.110635	-5.142960
H	-1.879082	0.361485	-2.436982
H	-1.652739	1.409758	-3.860522
H	-0.084377	0.736166	-5.573639
H	-1.440637	-0.298504	-6.094941
H	-1.060864	-2.843453	-6.294656
H	0.598796	-3.471650	-6.373023
H	-2.551844	-2.474310	-5.306214
H	-2.736773	-3.446859	-3.839935
H	1.956091	-3.641551	-4.110029
H	1.287492	-2.856924	-2.656091
H	2.523482	0.297275	-7.039775
H	2.026678	0.968985	-5.471681
H	4.627398	-0.598583	-6.075444
H	4.490082	1.124194	-5.705934
H	5.196858	-0.236978	-3.698365
H	3.705697	0.672315	-3.401288
H	3.989544	-2.337851	-4.140489

H	3.469308	-1.667298	-2.571839

INT (B)

Energy: -572328.4367 kJ mol^{-1}

C	-2.798027	0.355068	0.754176
C	-1.490945	0.037527	1.072248
C	-0.429372	0.668054	0.406007
C	-0.643618	1.603810	-0.637379
C	-1.997322	1.985772	-0.834510
C	-3.041469	1.371422	-0.169745
O	0.833556	0.317658	0.920244
C	1.608977	-0.510940	0.165023
N	2.711251	-1.159252	0.808406
C	4.016209	-1.038337	0.058150
C	4.578229	0.380434	0.113891
C	0.348218	2.179320	-1.537068
C	1.647228	2.663766	-0.968587
Si	-4.203459	-0.660597	1.364241
C	-4.952392	-1.512443	-0.160684
O	1.340855	-0.750130	-1.016755
C	-5.512580	0.434889	2.183633
C	-3.620933	-1.979493	2.593499
C	2.674889	-1.335469	2.305519
C	2.705469	-2.832720	2.612881
C	3.786666	-0.616367	3.058241
C	5.049283	-2.051681	0.530407
Li	0.730212	0.250680	-2.523411
H	3.884767	1.110017	-0.344495
H	5.528415	0.438920	-0.431924
H	4.766119	0.714223	1.148748
H	3.771518	-1.269652	-1.020543
H	5.526897	-1.741092	1.476136
H	5.843597	-2.165934	-0.217932
H	4.605526	-3.045267	0.711010
H	1.697458	-0.935238	2.676936
H	2.764011	-3.000916	3.696208
H	3.574007	-3.333445	2.150374
H	1.804107	-3.343344	2.249297
H	3.561638	-0.578172	4.131546
H	3.929481	0.417798	2.703969
H	4.757656	-1.129684	2.943250
H	-2.221274	2.772199	-1.566762
H	-4.077959	1.666965	-0.378104
H	-1.291584	-0.725644	1.838485

H	-0.093861	2.966478	-2.174345
H	1.498240	3.284235	-0.070890
H	2.187010	3.285243	-1.698895
H	2.347915	1.857067	-0.679680
H	-2.883489	-2.646445	2.137546
H	-4.463493	-2.590350	2.929899
H	-3.160779	-1.523292	3.474528
H	-4.178205	-2.024794	-0.752053
H	-5.430350	-0.779120	-0.817631
H	-5.703290	-2.251267	0.129475
H	-5.134791	0.870341	3.112692
H	-6.409524	-0.142812	2.423741
H	-5.805492	1.255461	1.522124
C	-3.189256	-2.573875	-3.196269
C	-3.401640	-1.143324	-3.650663
C	-2.196344	-0.284019	-3.288082
N	-0.873025	-0.782694	-3.805740
C	-0.730694	-0.459981	-5.274948
C	0.437142	-1.158765	-5.978668
H	0.324126	-0.973936	-7.075949
C	0.380575	-2.655798	-5.705457
C	0.541735	-2.856444	-4.201899
H	0.556793	-3.951741	-3.973986
C	-0.677993	-2.250528	-3.469930
H	-0.494750	-2.277217	-2.361592
C	-1.905411	-3.126724	-3.783392
C	1.890652	-2.288718	-3.743544
N	2.052985	-0.825650	-4.075871
C	1.821907	-0.620288	-5.563473
H	2.597542	-1.208468	-6.128757
C	1.975446	0.853109	-5.947280
C	3.308787	1.420178	-5.484611
C	3.572051	1.136239	-4.013045
C	3.436007	-0.352870	-3.710346
H	-4.045596	-3.205514	-3.502724
H	-3.177607	-2.611932	-2.080982
H	-4.304597	-0.721303	-3.163916
H	-3.603238	-1.108922	-4.740965
H	-2.109411	-0.201092	-2.177802
H	-2.370569	0.746286	-3.659613
H	-0.575810	0.640653	-5.366894
H	-1.671701	-0.700714	-5.818647
H	-0.593881	-3.078843	-6.039653
H	1.164354	-3.197233	-6.269234
H	-2.002098	-3.239089	-4.889215
H	-1.728261	-4.149081	-3.394930
H	2.705040	-2.884013	-4.218720

H	2.015067	-2.425205	-2.646906
H	1.894159	0.949513	-7.049246
H	1.108953	1.425440	-5.545128
H	4.127153	0.991065	-6.098289
H	3.336650	2.511443	-5.669739
H	4.592214	1.471967	-3.740489
H	2.882567	1.727535	-3.364021
H	4.216482	-0.930515	-4.255678
H	3.608337	-0.553890	-2.622013

TS2 (B)

Energy: -640054.0259 kJ mol^{-1}
Imaginary frequency: 31.67i cm^{-1}

C	-2.914102	-0.183918	0.489202
C	-1.632068	-0.524015	0.887025
C	-0.522912	0.084130	0.287852
C	-0.647632	1.029717	-0.768051
C	-1.990432	1.374528	-1.106637
C	-3.079167	0.782272	-0.503954
O	0.696163	-0.277800	0.879801
C	1.632974	-0.905019	0.112358
N	2.739047	-1.355633	0.889152
C	4.050006	-1.502762	0.164842
C	4.640265	-0.156638	-0.250238
C	0.406598	1.673887	-1.488043
C	1.690313	2.071962	-0.837673
Si	-4.355375	-1.100827	1.157771
C	-4.346046	-2.839969	0.395591
O	1.482793	-1.131668	-1.093799
C	-5.980853	-0.232961	0.704539
C	-4.243632	-1.239619	3.045718
C	2.690147	-1.028970	2.363363
C	2.698928	-2.326459	3.165344
C	3.792246	-0.094588	2.842700
C	5.064373	-2.306284	0.968148
Li	0.840659	-0.278110	-2.755039
H	3.956779	0.405804	-0.914295
H	5.582157	-0.301931	-0.794458
H	4.849411	0.489870	0.619350
H	3.805391	-2.084446	-0.769219
H	5.534427	-1.696847	1.760119
H	5.865759	-2.673314	0.314886
H	4.606245	-3.175642	1.468887
H	1.697895	-0.514913	2.514614

H	2.730901	-2.111014	4.241280
H	3.573588	-2.954944	2.923227
H	1.801637	-2.930113	2.976900
H	3.546079	0.313813	3.830809
H	3.949521	0.752622	2.154442
H	4.761460	-0.616270	2.931401
H	-2.152407	2.125008	-1.890864
H	-4.095835	1.067814	-0.804505
H	-1.492937	-1.273292	1.678785
H	1.615391	2.109182	0.259672
H	2.001682	3.076517	-1.163484
H	2.539842	1.399896	-1.074910
H	-3.269119	-1.627791	3.355966
H	-5.014255	-1.912088	3.432396
H	-4.381373	-0.262845	3.517281
H	-4.119818	-2.793935	-0.679304
H	-5.316650	-3.327300	0.517070
H	-3.587794	-3.469408	0.868780
H	-5.973785	0.810577	1.031518
H	-6.829413	-0.730518	1.182020
H	-6.147789	-0.244331	-0.376303
C	-3.253000	-2.890111	-3.325794
C	-3.181711	-1.555123	-4.043784
C	-1.895431	-0.825096	-3.674805
N	-0.635739	-1.598165	-3.959229
C	-0.340912	-1.590861	-5.440218
C	0.742205	-2.574603	-5.893394
H	0.721461	-2.598788	-7.011270
C	0.441839	-3.965223	-5.348225
C	0.462273	-3.877819	-3.825644
H	0.297111	-4.896706	-3.393853
C	-0.702943	-2.983105	-3.349056
H	-0.612748	-2.820729	-2.242441
C	-2.023951	-3.724062	-3.633794
C	1.840637	-3.409694	-3.345962
N	2.275191	-2.105744	-3.959950
C	2.169187	-2.178669	-5.469365
H	2.865052	-2.981682	-5.842203
C	2.599317	-0.854752	-6.104150
C	4.006476	-0.470208	-5.673993
C	4.129211	-0.463236	-4.157774
C	3.695427	-1.801970	-3.574147
H	-4.164864	-3.440032	-3.630295
H	-3.357574	-2.734609	-2.226106
H	-4.051370	-0.925666	-3.773056
H	-3.250574	-1.705334	-5.141506
H	-1.903094	-0.579416	-2.583624

H	-1.837029	0.149293	-4.208792
H	-0.017193	-0.552110	-5.702533
H	-1.270374	-1.798752	-6.017635
H	-0.556504	-4.316174	-5.694383
H	1.175025	-4.708783	-5.715848
H	-2.039366	-4.050690	-4.700299
H	-2.048740	-4.657517	-3.037322
H	2.581633	-4.211245	-3.572014
H	1.843347	-3.289727	-2.241751
H	2.553259	-0.947029	-7.207389
H	1.865572	-0.054632	-5.837030
H	4.743208	-1.174766	-6.110240
H	4.265687	0.527190	-6.080837
H	5.174325	-0.252402	-3.857234
H	3.518275	0.362065	-3.720586
H	4.387344	-2.608139	-3.908600
H	3.761304	-1.779536	-2.460254
S	0.026007	2.203296	-6.358538
S	0.681849	2.099647	-4.435445
C	-0.676337	3.843765	-6.657225
C	2.344289	2.820384	-4.374124
H	3.051964	2.337467	-5.059750
H	2.714198	2.678094	-3.346058
H	2.343970	3.894431	-4.588956
H	0.072206	4.642581	-6.621643
H	-1.478614	4.106520	-5.959479
H	-1.101085	3.823437	-7.669485
H	0.034528	2.452021	-2.184718

C3 (B)

Energy: -640148.6609 kJ mol^{-1}

C	-2.907821	0.062660	0.202035
C	-1.613374	-0.320965	0.506585
C	-0.524244	0.418843	0.019567
C	-0.697469	1.549791	-0.801213
C	-2.032866	1.907882	-1.080765
C	-3.110179	1.185216	-0.594131
O	0.705155	0.034278	0.571313
C	1.592038	-0.677820	-0.179121
N	2.696787	-1.145966	0.591685
C	4.029678	-1.121905	-0.109721
C	4.517373	0.305640	-0.350301
C	0.351634	2.420162	-1.394796
C	1.571448	2.670215	-0.538534

Si	-4.309044	-0.927958	0.879994
C	-4.158708	-2.708348	0.252169
O	1.394688	-0.957742	-1.363885
C	-5.972042	-0.198525	0.346560
C	-4.199280	-0.930044	2.771804
C	2.594369	-0.960882	2.088862
C	2.661288	-2.331392	2.755794
C	3.631536	-0.022901	2.690386
C	5.079913	-1.937359	0.632722
Li	1.049640	-0.672001	-3.211659
H	3.750973	0.926858	-0.852721
H	5.414651	0.306270	-0.981375
H	4.768314	0.821495	0.592884
H	3.850313	-1.615475	-1.108201
H	5.494697	-1.386191	1.495222
H	5.915355	-2.183665	-0.034436
H	4.668876	-2.880732	1.030667
H	1.574975	-0.516008	2.264483
H	2.671300	-2.225495	3.848335
H	3.570741	-2.885452	2.463751
H	1.798609	-2.957336	2.493665
H	3.337189	0.273164	3.705048
H	3.762112	0.894966	2.093233
H	4.624708	-0.500761	2.759787
H	-2.221215	2.792557	-1.703702
H	-4.135524	1.497321	-0.833090
H	-1.446876	-1.199487	1.146360
H	1.303902	2.975225	0.481231
H	2.186573	3.472752	-0.983262
H	2.245216	1.796828	-0.459497
H	-3.211221	-1.260191	3.105939
H	-4.944213	-1.604925	3.202715
H	-4.375503	0.069237	3.178920
H	-4.055836	-2.737644	-0.840969
H	-5.041622	-3.293232	0.523717
H	-3.280806	-3.200441	0.680874
H	-6.102023	0.814983	0.737307
H	-6.797855	-0.811928	0.718402
H	-6.053928	-0.149160	-0.743157
C	-3.215375	-3.155433	-3.430437
C	-3.152239	-1.763816	-4.034951
C	-1.840137	-1.080672	-3.668074
N	-0.617700	-1.859443	-4.071718
C	-0.407753	-1.793527	-5.566913
C	0.690378	-2.726697	-6.090636
H	0.635665	-2.703593	-7.207430
C	0.432368	-4.146482	-5.593919

C	0.488169	-4.124173	-4.069327
H	0.350387	-5.163313	-3.678446
C	-0.678935	-3.271118	-3.528563
H	-0.577669	-3.171449	-2.415556
C	-2.008874	-3.982310	-3.835639
C	1.865315	-3.646288	-3.588996
N	2.313180	-2.335432	-4.192998
C	2.129270	-2.339075	-5.700122
H	2.806935	-3.124087	-6.140834
C	2.553741	-0.982167	-6.269751
C	4.026158	-0.736270	-5.972137
C	4.289302	-0.809646	-4.476076
C	3.770770	-2.109453	-3.869228
H	-4.144412	-3.668000	-3.746815
H	-3.278747	-3.082537	-2.319874
H	-3.998831	-1.149860	-3.671226
H	-3.272176	-1.818048	-5.137140
H	-1.790360	-0.925345	-2.565128
H	-1.767751	-0.060873	-4.130119
H	-0.168803	-0.724431	-5.809692
H	-1.356264	-2.036627	-6.098704
H	-0.568587	-4.502094	-5.928180
H	1.168408	-4.860804	-6.010523
H	-2.053127	-4.230806	-4.921980
H	-2.029152	-4.956646	-3.308600
H	2.607539	-4.446927	-3.812575
H	1.863355	-3.522093	-2.483763
H	2.379785	-0.973409	-7.363776
H	1.920478	-0.158067	-5.854956
H	4.654418	-1.476515	-6.508019
H	4.331661	0.254175	-6.361290
H	5.375543	-0.726176	-4.275274
H	3.822963	0.067542	-3.963994
H	4.392423	-2.964905	-4.218754
H	3.878642	-2.079939	-2.757905
S	-0.198772	1.758237	-4.998835
S	0.796551	1.957585	-3.229695
C	-0.611509	3.385690	-5.686053
C	2.603808	2.293127	-3.347199
H	3.235316	1.421706	-3.122706
H	2.876986	3.090835	-2.639897
H	2.844632	2.630858	-4.360036
H	0.085184	4.167727	-5.366796
H	-1.617101	3.700583	-5.388434
H	-0.588205	3.345824	-6.780174
H	-0.120639	3.417922	-1.570586

Butane

Energy: -60713.0062 kJ mol^{-1}

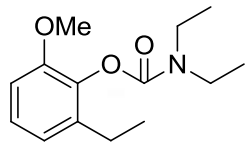
C	-1.434013	2.776748	-0.064692
C	0.072226	2.657512	-0.122248
H	-1.823885	2.508434	0.926341
H	-1.921547	2.116971	-0.794779
H	-1.761475	3.802075	-0.278940
C	0.531628	1.233809	0.148899
H	0.535796	3.348321	0.610013
H	0.441131	2.988146	-1.113618
H	0.162727	0.903177	1.140271
C	2.037868	1.114572	0.091337
H	0.068055	0.542999	-0.583359
H	2.525405	1.774355	0.821416
H	2.427735	1.382877	-0.899701
H	2.365330	0.089246	0.305591

Dimethyl disulfide

Energy: -67767.2269 kJ mol^{-1}

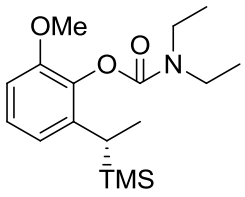
S	-1.065513	0.654587	0.024600
S	0.955141	0.584524	-0.071356
C	-1.696701	-0.923584	0.632589
C	1.658472	1.042520	1.526208
H	1.310097	2.010752	1.901647
H	2.743655	1.112519	1.364290
H	1.482351	0.296341	2.308611
H	-1.390302	-1.151197	1.659477
H	-1.420449	-1.776749	0.003684
H	-2.792270	-0.834275	0.619860

^{1}H and ^{13}C NMR Spectra



5

(300 MHz, $CDCl_3$)



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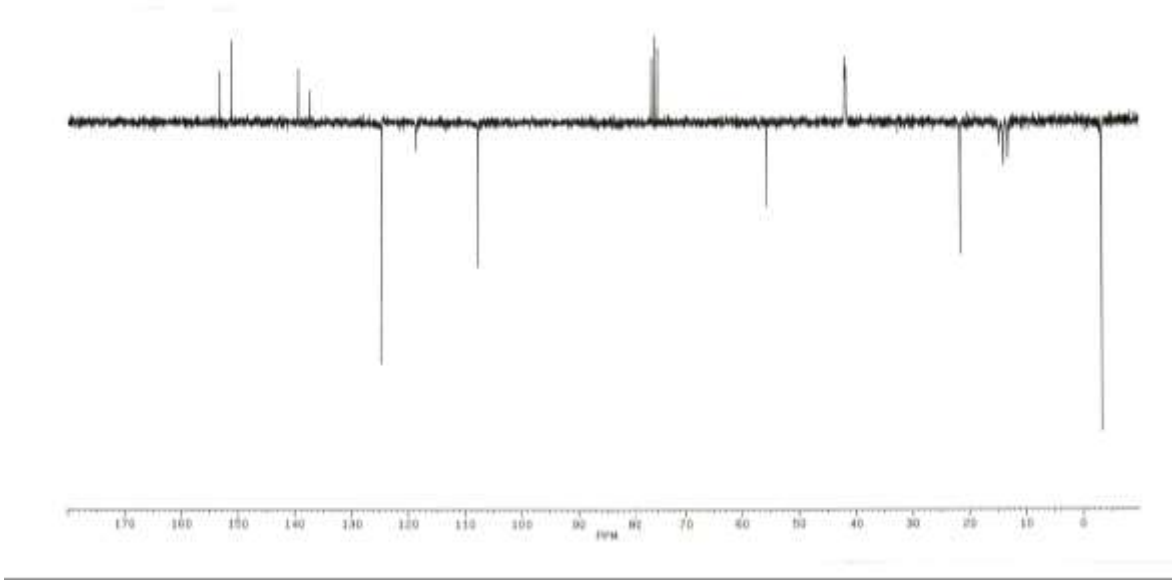
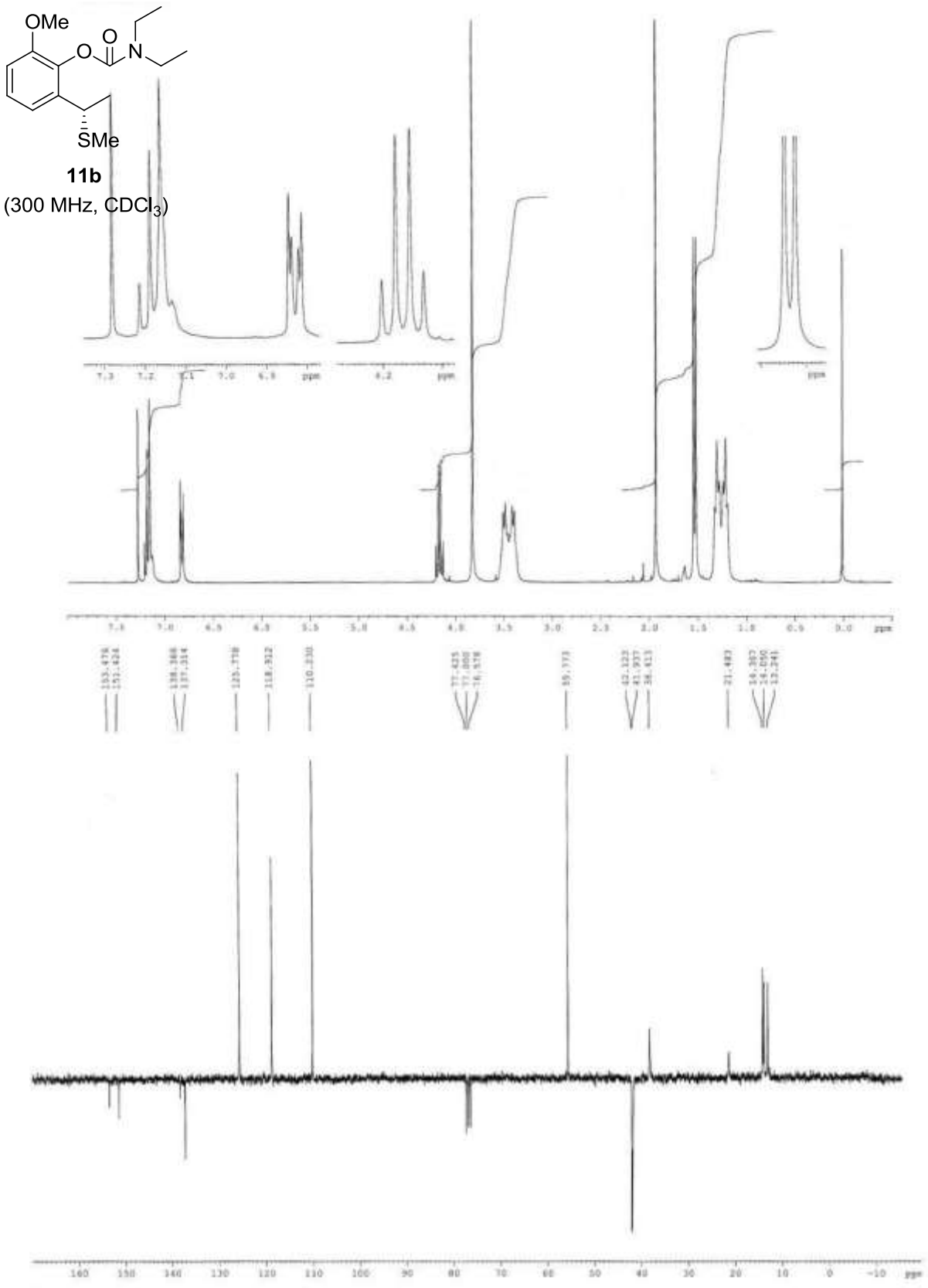
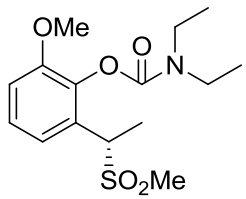
(300 MHz, $CDCl_3$)

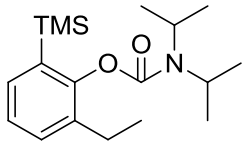



OMe
O
O
N
SMe
11b
(300 MHz, CDCl3)



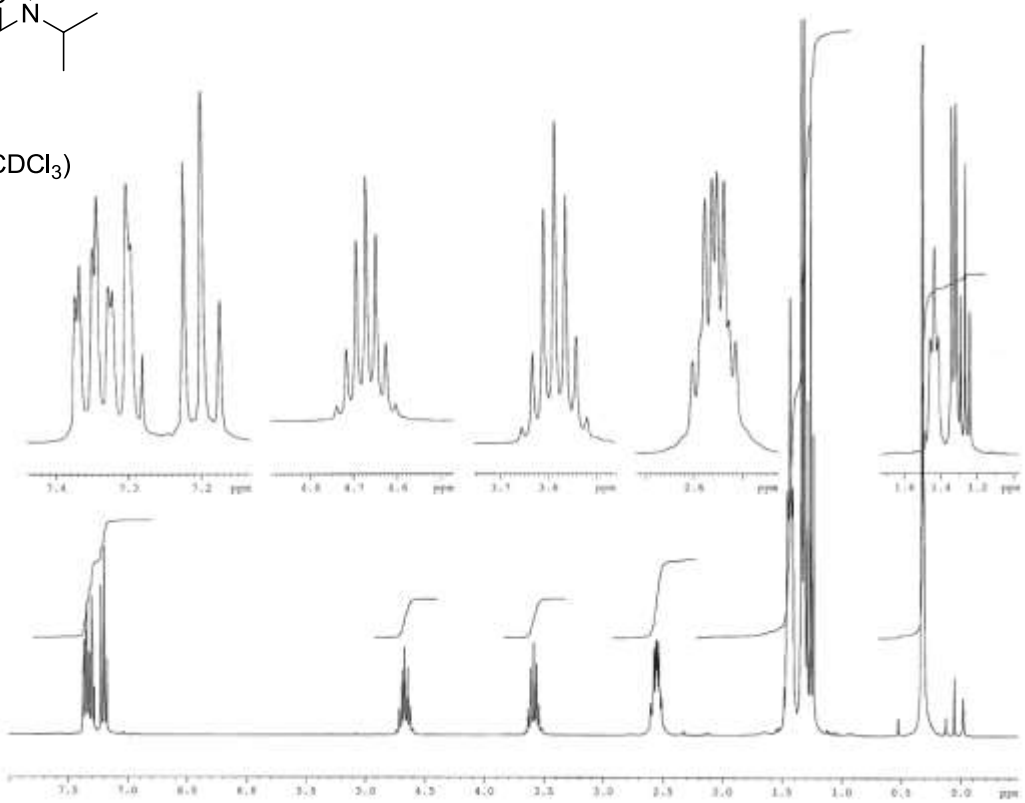
11c

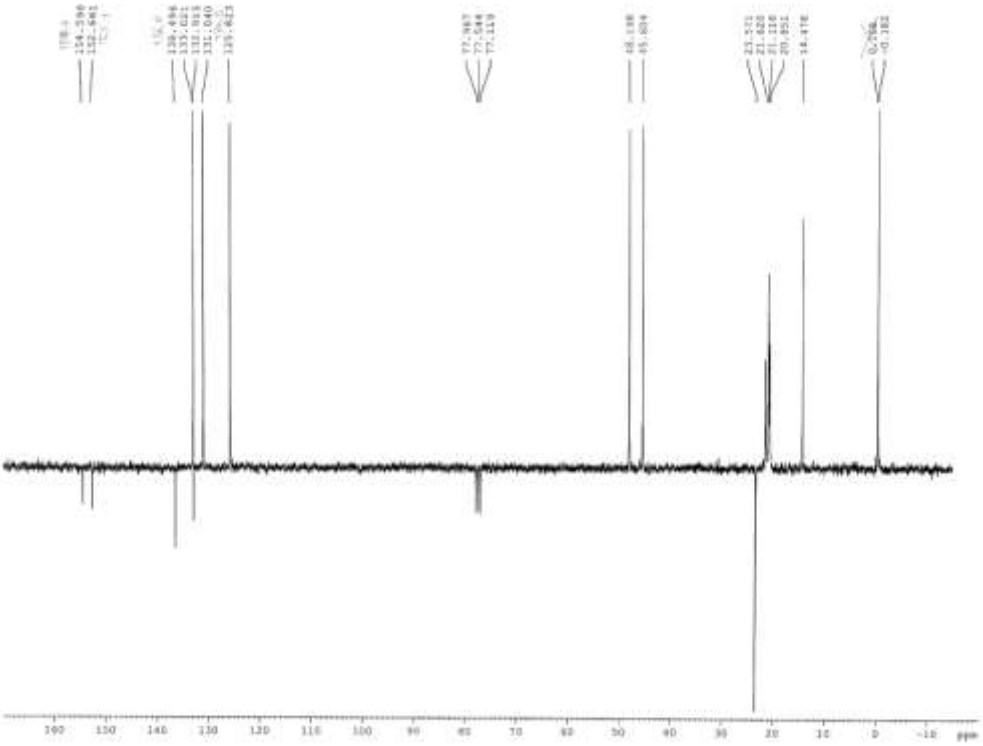
(300 MHz, $CDCl_3$)

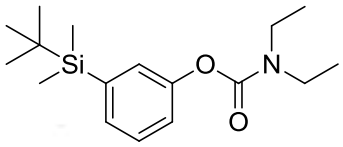


7

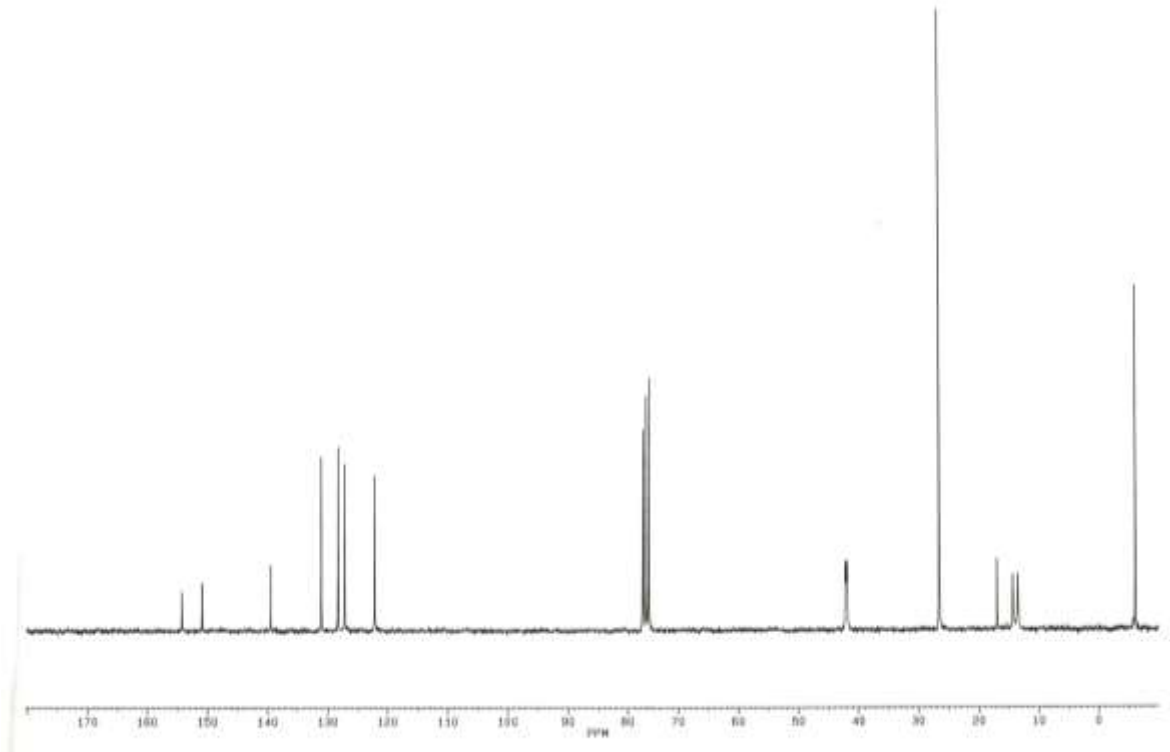
(300 MHz, $CDCl_3$)

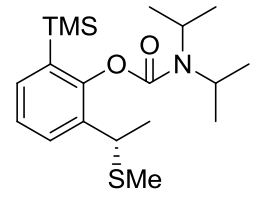






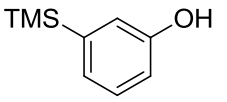
(300 MHz, $CDCl_3$)



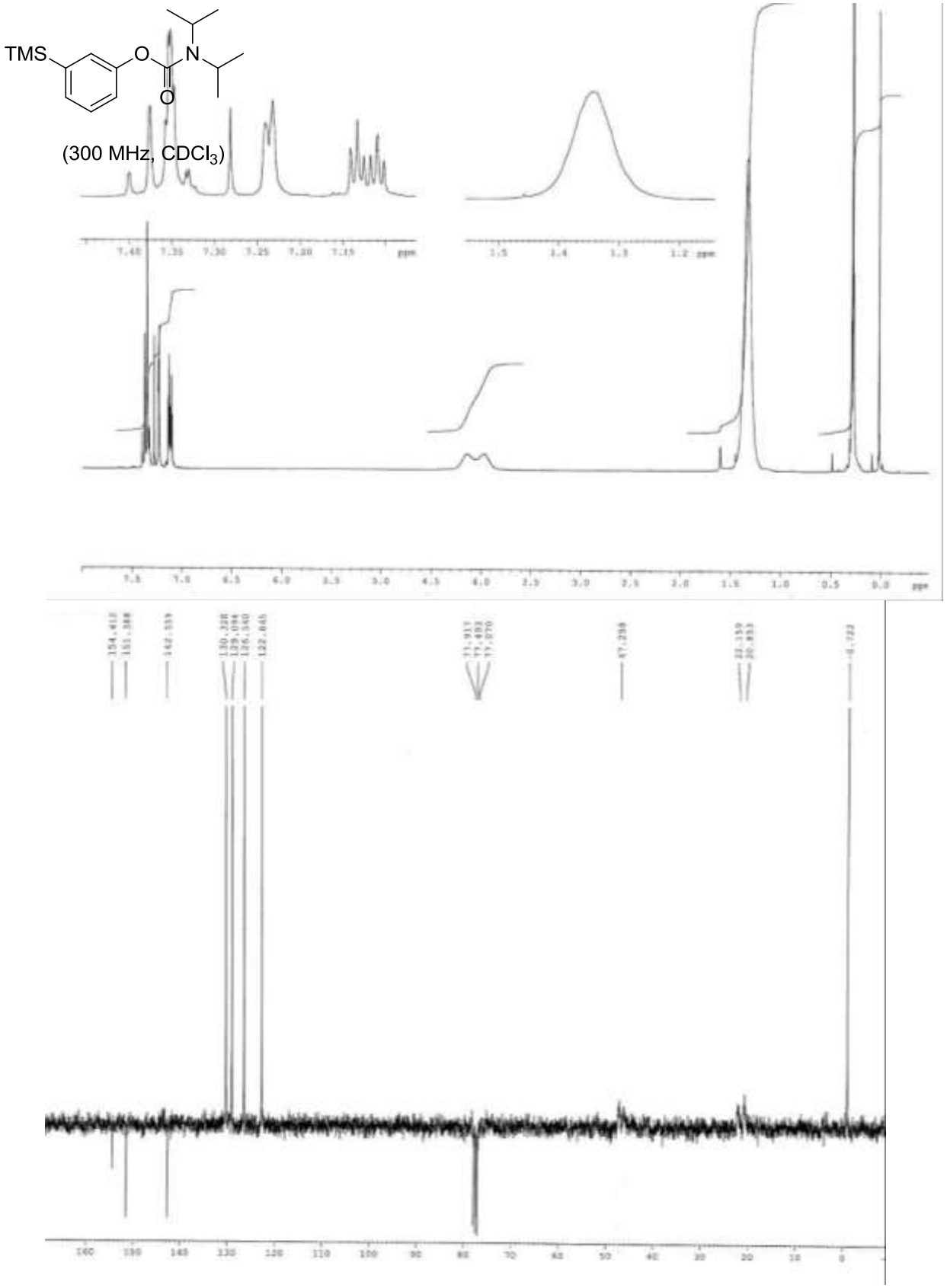


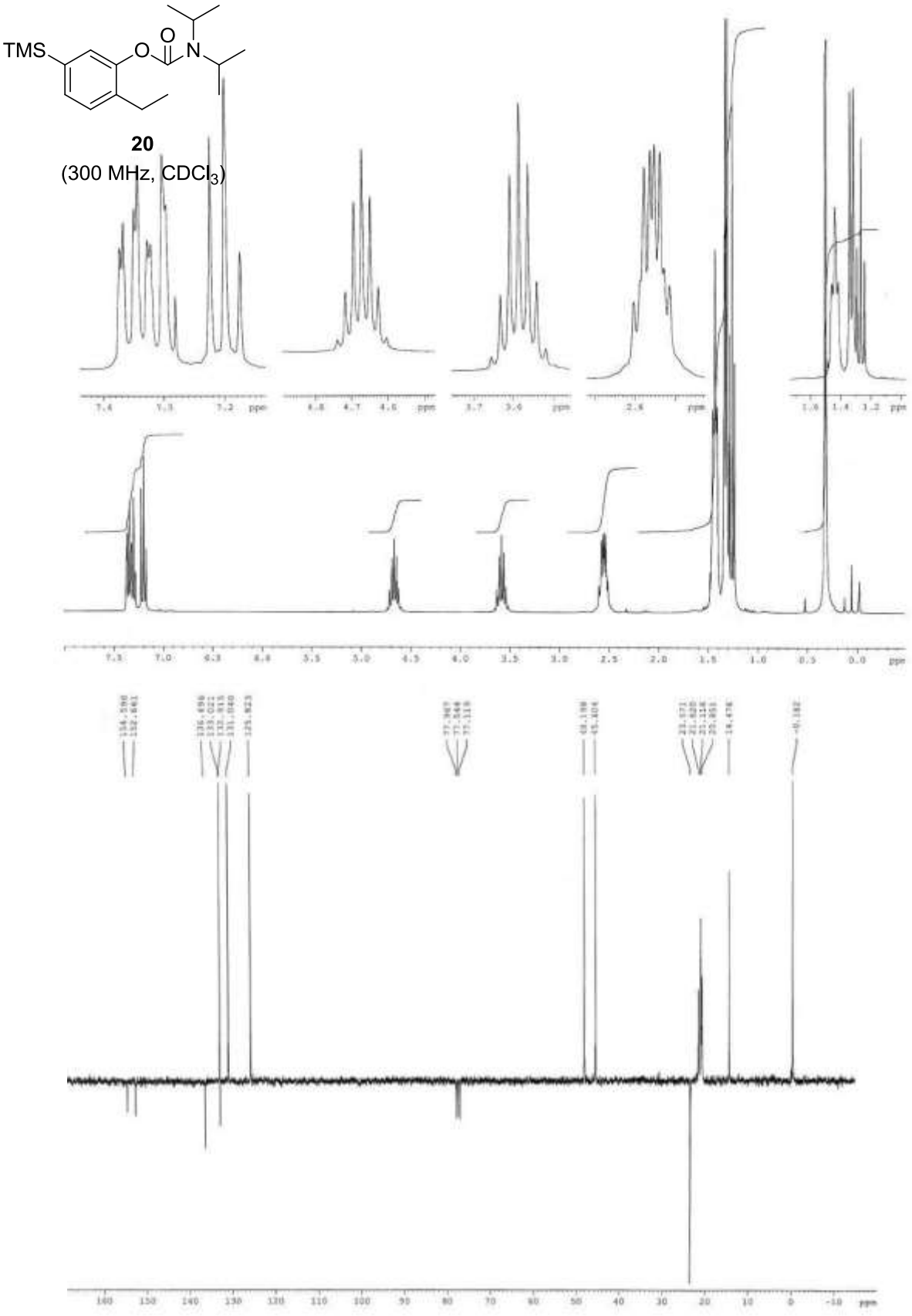
13a

(300 MHz, $CDCl_3$)



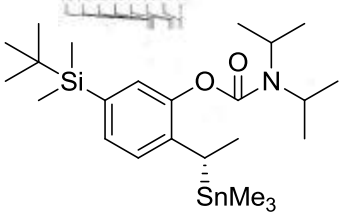
(300 MHz, $CDCl_3$)


TMS
O
N
O
(300 MHz, CDCl3)



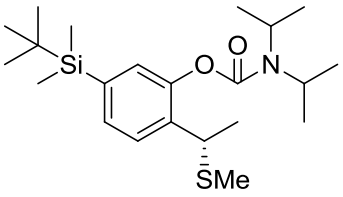
20

(300 MHz, $CDCl_3$)



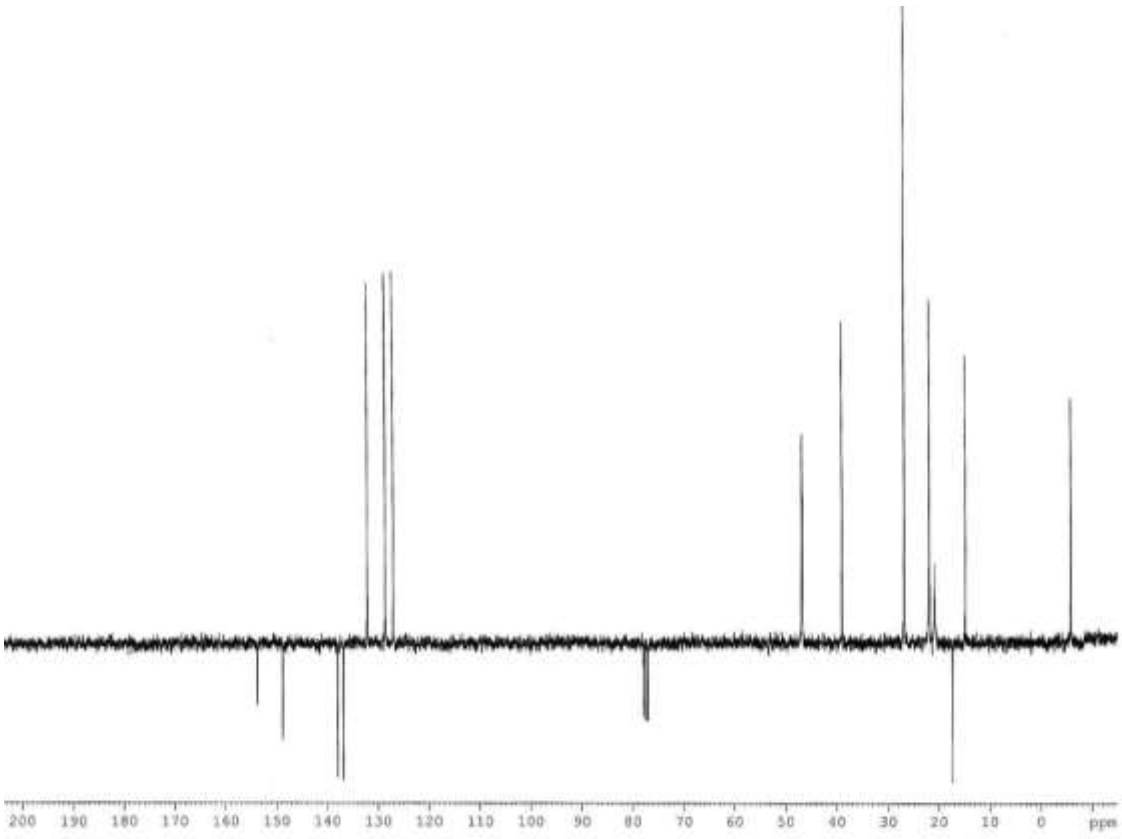
17e

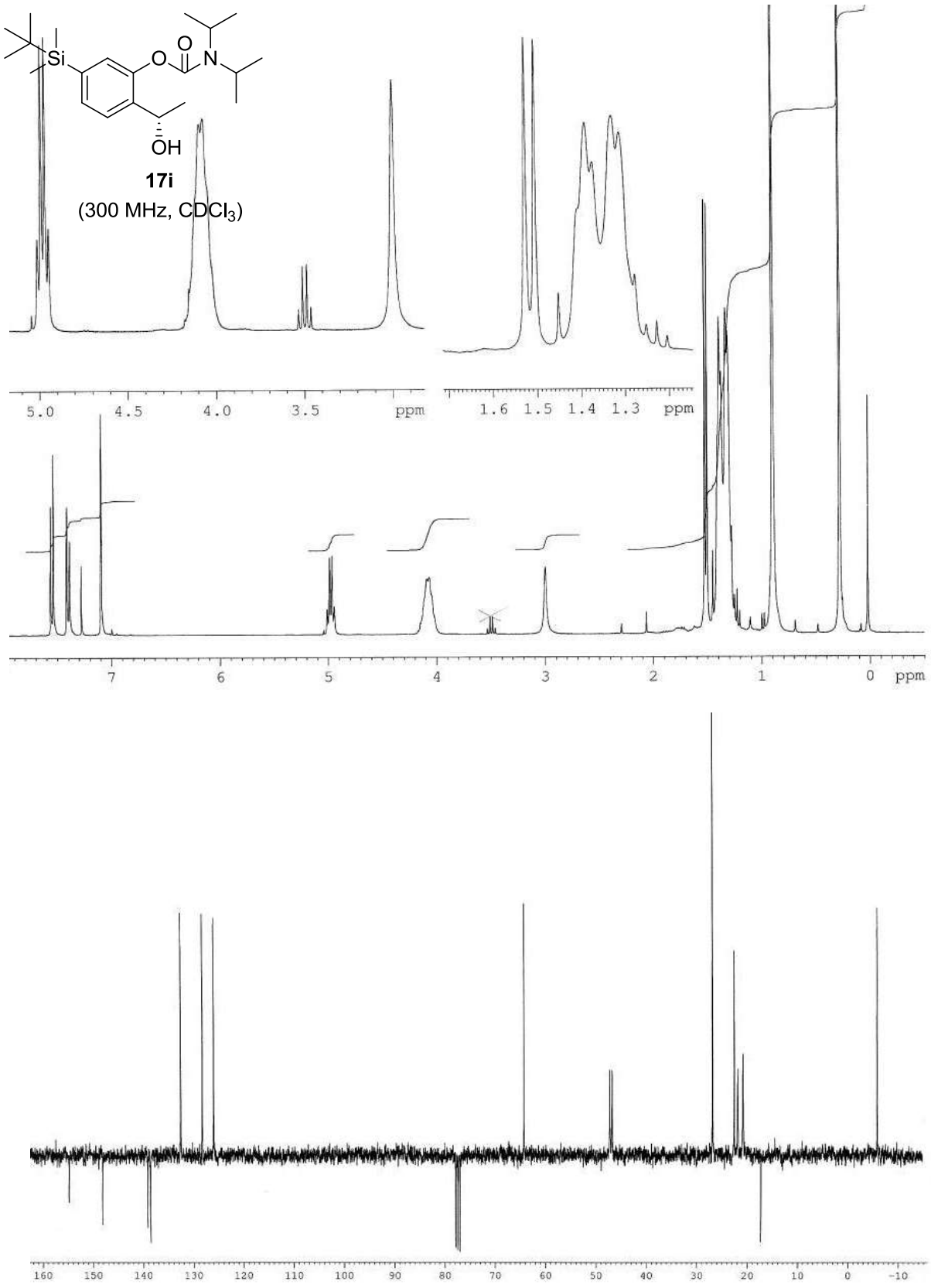
(400 MHz, $CDCl_3$)

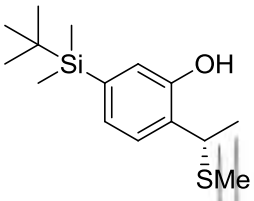


17g

(300 MHz, $CDCl_3$)

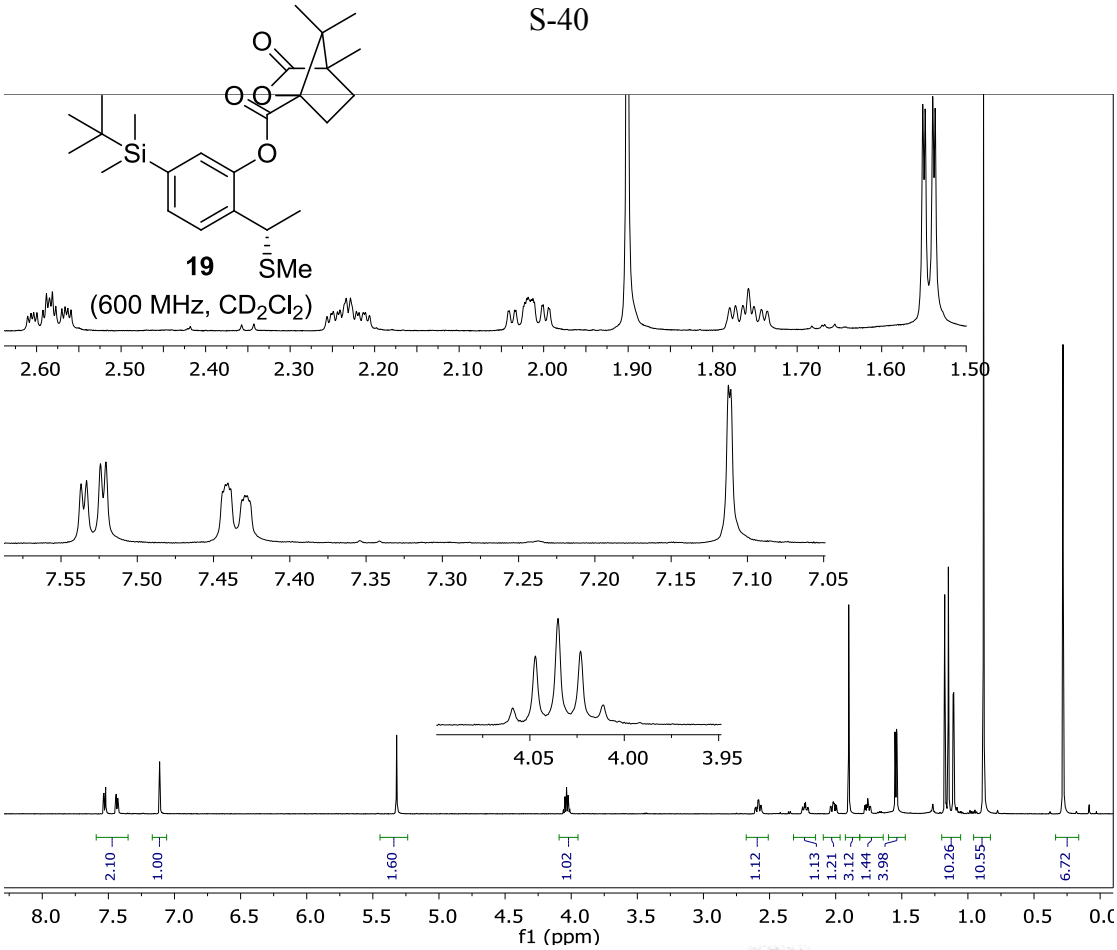


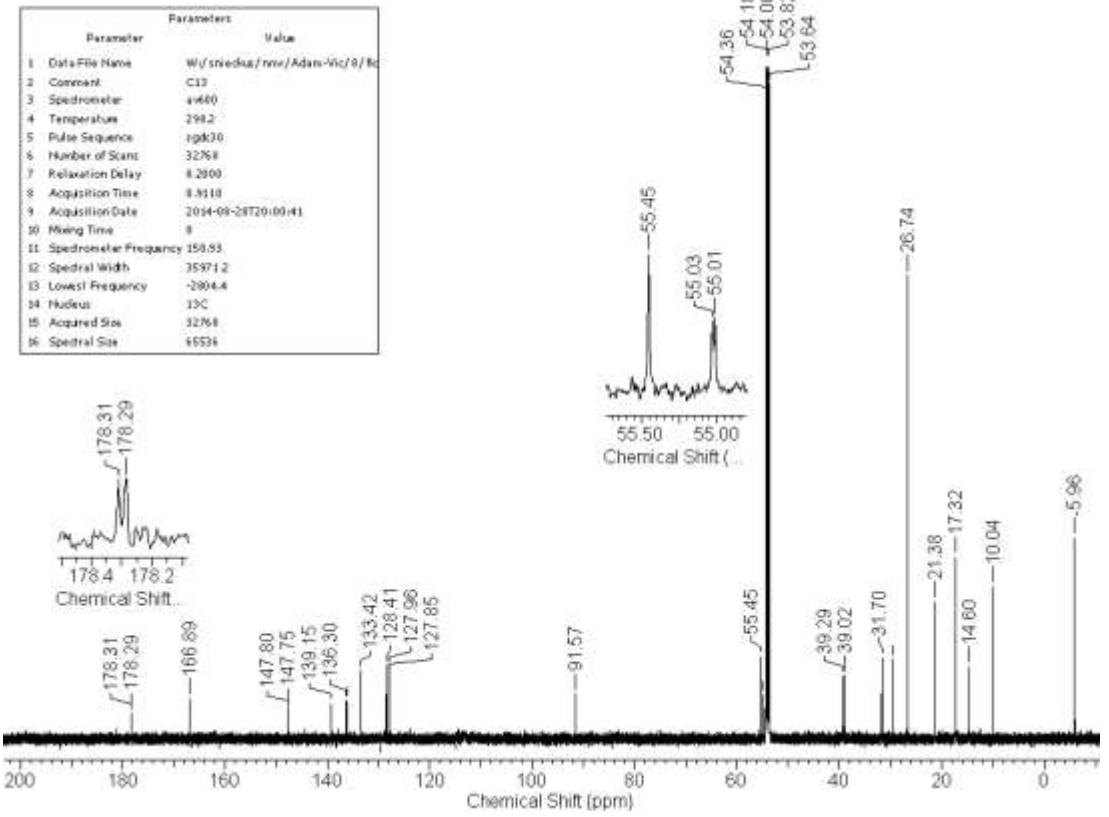

Si
O
O
N
OH
17i
(300 MHz, CDCl3)
5.0
4.5
4.0
3.5
ppm
1.6
1.5
1.4
1.3
ppm
7
6
5
4
3
2
1
0
ppm
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

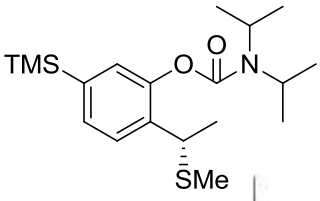


18

(300 MHz, $CDCl_3$)

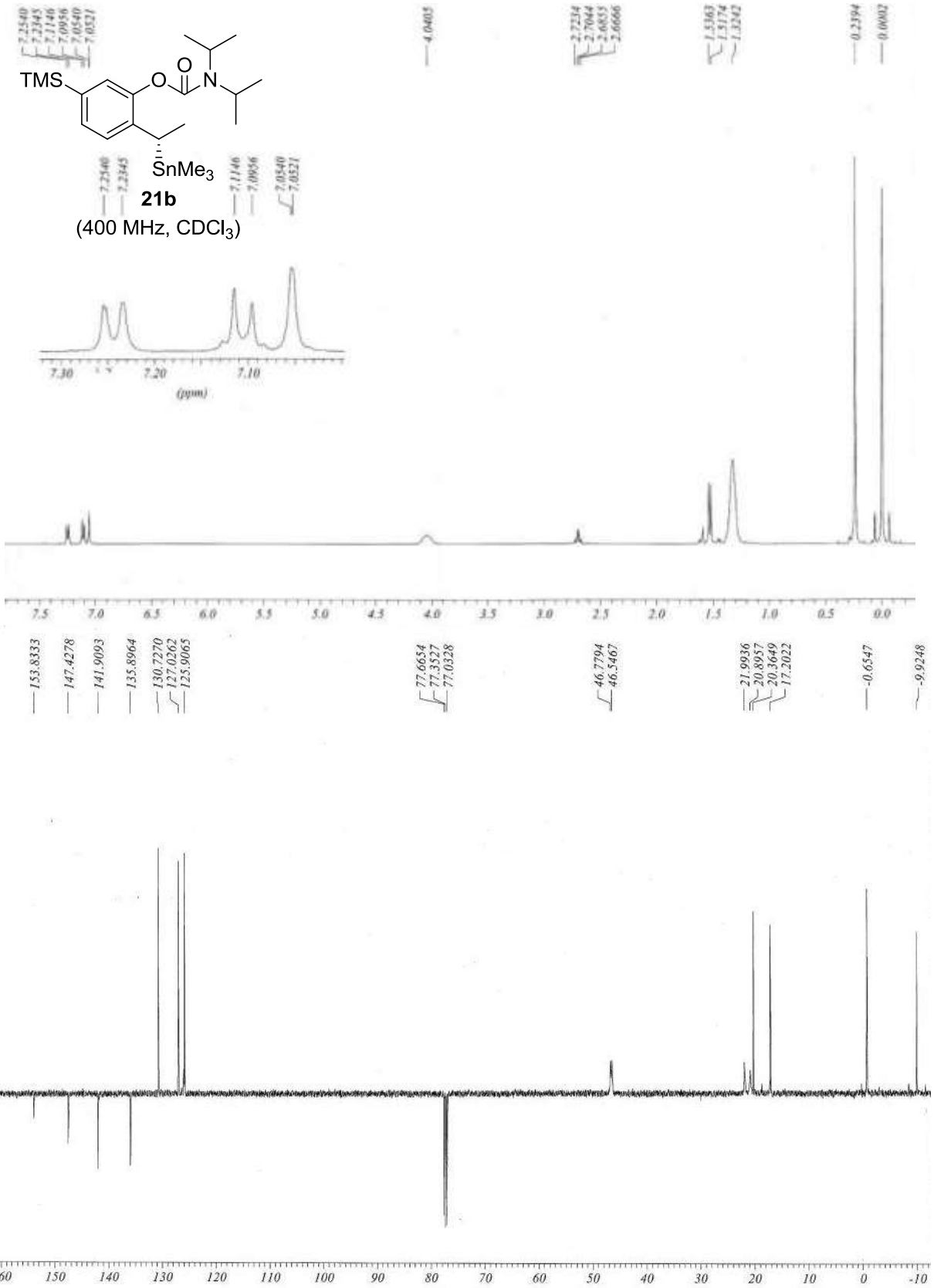

19
SMe
(600 MHz, CD_2Cl_2)
f1 (ppm)

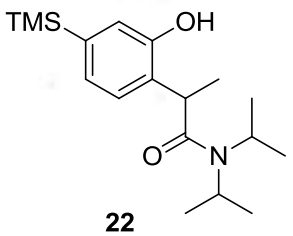

Parameters
Chemical Shift (ppm)



21a

(300 MHz, $CDCl_3$)


TMS
O
O
N
SnMe3
21b
(400 MHz, CDCl3)
7.30
7.20
7.10
(ppm)



22

(400 MHz, $CDCl_3$)

X-Ray Data

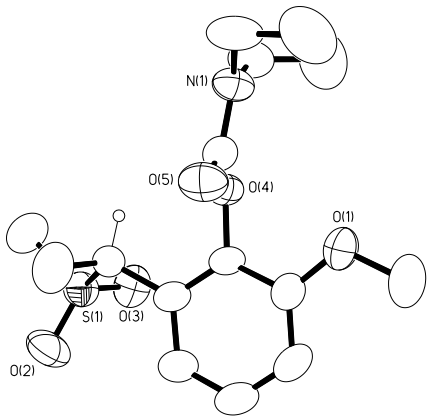


Figure S1. Molecular Structure of **11c**.

X-Ray Diffraction Analysis Report for Compound 11c

The crystal of the compound was mounted on a glass fiber with epoxy glue. The data for the compound were collected on a CCD-detector-equipped SMART system with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) operated at 50 kV and 35 mA at 23°C over the 2θ range of 4-56°. No significant decay was observed for the crystal.

The data were processed on a Pentium PC using Siemens SHELXTL (version 5.0) software package. The data were corrected for Lorentz-polarization effects. Neutral atoms scattering factors were taken from Cromer and Waber. The structure was solved by direct method. Full-matrix least-square refinements minimizing the function $\sum w(F_o^2 - F_c^2)^2$ were applied to the compound. The positions of hydrogen were calculated and refined successfully.

Enantiomer I (correct one): R1 = 0.0409 for 1688 Fo > 4sig(Fo) and 0.1071 for all 3440 data. wR2 = 0.0746, GooF = S = 0.779, Restrained GooF = 0.779 for all data. Flack x parameter = 0.1840 with esd 0.0775

Enantiomer II (for comparing purpose): R1 = 0.0412 for 1688 Fo > 4sig(Fo) and 0.1076 for all 3440 data. wR2 = 0.0772, GooF = S = 0.780, Restrained GooF = 0.780 for all data. Flack x parameter = 0.9411 with esd 0.1231

Table S1. Crystal Data and Structure Refinement for **11c**.

Identification code	023	
Empirical formula	C15 H23 N O5 S	
Formula weight	329.40	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 20.529(18) Å	α= 90°.
	b = 6.669(6) Å	β= 95.761(13)°.
	c = 12.889(11) Å	γ = 90°.
Volume	1756(3) $Å^3$	
Z	4	
Density (calculated)	1.246 Mg/m^3	
Absorption coefficient	0.205 mm^{-1}	
F(000)	704	
Crystal size	0.1 x 0.3 x0 .4 mm^3	
Theta range for data collection	1.59 to 28.32°.	
Index ranges	-25<=h<=27, -8<=k<=8, -16<=l<=15	
Reflections collected	6047	
Independent reflections	3440 [R(int) = 0.0379]	
Completeness to theta = 28.32°	94.4 %	
Absorption correction	Empirical (Bruker SADABS)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3440 / 1 / 199	

Goodness-of-fit on F^2	0.778
Final R indices [I>2sigma(I)]	R1 = 0.0407, wR2 = 0.0661
R indices (all data)	R1 = 0.1072, wR2 = 0.0744
Absolute structure parameter	0.18(8)
Largest diff. peak and hole	0.178 and -0.177 e.$Å^{-3}$

Table S2. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$x 10^3) for **11c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	9076(1)	5228(4)	2800(2)	53(1)
S(1)	6533(1)	7857(1)	4505(1)	59(1)
O(1)	8379(1)	9423(3)	1086(2)	64(1)
O(2)	5842(1)	7784(4)	4171(2)	84(1)
O(3)	6821(1)	9798(3)	4748(2)	73(1)
O(4)	8231(1)	7401(3)	2819(1)	48(1)
O(5)	8162(1)	4814(3)	1661(2)	64(1)
C(1)	8470(2)	10495(5)	148(2)	80(1)
C(2)	7761(2)	9418(4)	1401(2)	48(1)
C(3)	7225(2)	10418(5)	893(2)	58(1)
C(4)	6618(2)	10246(5)	1272(2)	61(1)
C(5)	6540(2)	9086(5)	2129(2)	56(1)
C(6)	7070(1)	8059(5)	2649(2)	45(1)
C(7)	7672(1)	8281(4)	2279(2)	43(1)
C(8)	6993(1)	6671(4)	3559(2)	50(1)
C(9)	6685(2)	4663(5)	3188(2)	83(1)
C(10)	6681(2)	6342(5)	5631(2)	84(1)
C(11)	8475(2)	5714(5)	2357(2)	48(1)
C(12)	9415(2)	3547(5)	2342(2)	77(1)
C(13)	9713(2)	4113(7)	1358(3)	104(1)
C(14)	9430(2)	6394(5)	3652(3)	74(1)
C(15)	9842(2)	8019(7)	3292(3)	123(2)

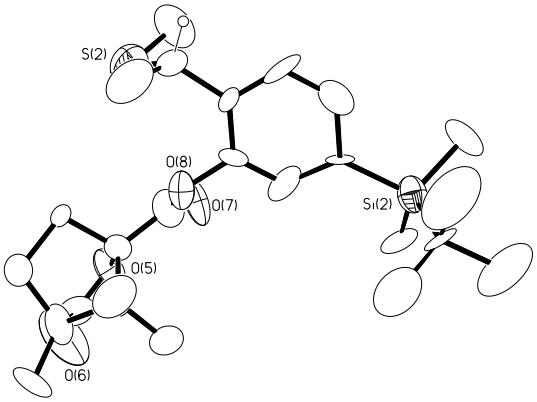


Figure S2. Molecular Structure of **19**.

X-Ray Diffraction Analysis Report for Compound 19

The crystal of the compound was mounted on a glass fiber with epoxy glue. The data for the compound were collected on a CCD-detector-equipped SMART system with graphite monochromated Mo Kα radiation (λ=0.71073 Å) operated at 50 kV and 35 mA at 23 °C over the 2θ range of 4-56°. No significant decay was observed for the crystal.

The data were processed on a Pentium PC using Siemens SHELXTL (version 5.0) software package. The data were corrected for Lorentz-polarization effects. Neutral atoms scattering factors were taken from Cromer and Waber. The structure was solved by direct method. Full-matrix least-square refinements minimizing the function $\sum w(F_o^2 - F_c^2)^2$ were applied to the compound. The positions of hydrogen were calculated and refined successfully.

Enantiomer I (correct one): Final R1 = 0.0868, wR2 = 0.1846, Flack x parameter = 0.0492 with esd 0.1821.

Enantiomer II (for comparing purpose): Final R1 = 0.0870, wR2 = 0.1848, Flack x parameter = 0.9186 with esd 0.1823.

Table S3. Crystal Data and Structure Refinement for **19**.

Identification code	016w	
Empirical formula	C25 H38 O4 S Si	
Formula weight	462.70	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 6.4850(12) Å	α= 90°.
	b = 11.608(2) Å	β= 92.732(4)°.
	c = 35.604(7) Å	γ = 90°.
Volume	2677.3(9) $Å^3$	
Z	4	
Density (calculated)	1.148 Mg/m^3	
Absorption coefficient	0.192 mm^{-1}	
F(000)	1000	
Crystal size	0.4 x 0.3 x 0.2 mm^3	
Theta range for data collection	1.72 to 28.34°.	
Index ranges	-7<=h<=8, -14<=k<=15, -46<=l<=47	
Reflections collected	19877	
Independent reflections	11856 [R(int) = 0.1656]	
Completeness to theta = 28.34°	96.1 %	
Absorption correction	Empirical(Bruker SADABS)	
Max. and min. transmission	1.0000 and 0.8002	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11856 / 1 / 554	
Goodness-of-fit on F^2	0.670	
Final R indices [I>2sigma(I)]	R1 = 0.0868, wR2 = 0.1273	
R indices (all data)	R1 = 0.4334, wR2 = 0.1846	
Absolute structure parameter	0.05(18)	
Largest diff. peak and hole	0.698 and -0.759 $e.Å^{-3}$	

Table S4. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$x 10^3) for **19**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	9531(12)	7403(8)	5134(2)	73(3)
O(2)	9658(13)	8435(10)	4598(2)	105(4)
O(3)	7891(11)	6942(8)	5797(2)	79(3)
O(4)	10872(9)	6436(7)	6074(3)	66(3)
O(5)	3557(11)	495(7)	9456(3)	67(3)
O(6)	3617(14)	-253(11)	10025(3)	149(6)
O(7)	4871(11)	1731(7)	8872(2)	79(3)
O(8)	1832(11)	2553(7)	8766(3)	58(3)
C(1)	13328(18)	9597(9)	4921(3)	81(5)
C(2)	12388(17)	8553(12)	5079(4)	60(4)
C(3)	11775(16)	8581(10)	5493(3)	37(3)
C(4)	10922(17)	7330(12)	5469(3)	51(4)
C(5)	13592(15)	8728(10)	5779(3)	91(5)
C(6)	10143(17)	9484(9)	5572(3)	80(4)
C(7)	10400(19)	8149(14)	4920(4)	67(5)
C(8)	13801(17)	7422(11)	5084(3)	78(5)
C(9)	12701(15)	6647(9)	5348(3)	61(4)
C(10)	9675(18)	6924(11)	5767(3)	49(4)
C(11)	10046(18)	5950(12)	6380(4)	45(4)
C(12)	8580(20)	5037(12)	6306(4)	77(5)
C(13)	7912(19)	4437(12)	6607(4)	71(5)
C(14)	8513(18)	4788(11)	6973(4)	82(5)
C(15)	9851(16)	5764(11)	7027(3)	57(4)
C(16)	10567(16)	6309(11)	6725(4)	44(3)
C(17)	12017(17)	7301(11)	6761(3)	61(4)
C(18)	9390(20)	8547(14)	7194(4)	150(7)
C(19)	14150(20)	6996(16)	6789(4)	193(9)
C(20)	4492(18)	3518(13)	6089(3)	133(6)
C(21)	3989(16)	3383(12)	6932(3)	119(6)
C(22)	7240(20)	1968(13)	6565(5)	94(5)
C(23)	5430(20)	899(13)	6494(4)	188(9)

C(24)	8190(20)	1688(13)	6912(4)	148(7)
C(25)	8810(20)	1830(14)	6265(5)	173(8)
C(26)	-198(15)	1076(11)	10187(3)	75(4)
C(27)	693(18)	926(12)	9815(4)	61(4)
C(28)	1238(16)	2003(12)	9564(3)	52(4)
C(29)	2056(16)	1262(10)	9255(3)	36(3)
C(30)	2823(16)	2732(9)	9751(3)	71(4)
C(31)	-653(16)	2725(8)	9465(3)	74(5)
C(32)	-642(15)	186(9)	9521(3)	52(4)
C(33)	262(15)	450(10)	9124(3)	67(4)
C(34)	2770(20)	289(13)	9783(4)	69(5)
C(35)	3060(20)	1818(12)	8929(4)	69(4)
C(36)	2508(18)	3288(12)	8482(3)	37(3)
C(37)	3790(16)	4128(12)	8571(4)	61(4)
C(38)	4494(15)	4977(9)	8337(3)	31(3)
C(39)	3648(19)	4814(12)	7962(4)	72(4)
C(40)	2236(18)	3960(11)	7867(4)	58(4)
C(41)	1711(19)	3148(13)	8131(4)	66(5)
C(42)	151(16)	2248(10)	7990(3)	55(4)
C(43)	-1938(15)	2348(12)	8158(3)	104(5)
C(44)	3066(16)	753(12)	7739(3)	102(5)
C(45)	8327(14)	5560(10)	8791(3)	77(4)
C(46)	7607(14)	6574(10)	8017(3)	84(5)
C(47)	5150(17)	7338(10)	8661(3)	46(3)
C(48)	4123(15)	7058(11)	9022(4)	105(5)
C(49)	3303(18)	7842(11)	8383(4)	143(7)
C(50)	6490(20)	8429(12)	8748(4)	155(7)
S(1)	11875(15)	8159(7)	7106(3)	485(9)
S(2)	1076(6)	790(3)	8065(1)	99(2)
Si(1)	5847(6)	3272(4)	6528(1)	86(1)
Si(2)	6396(5)	6142(3)	8449(1)	58(1)

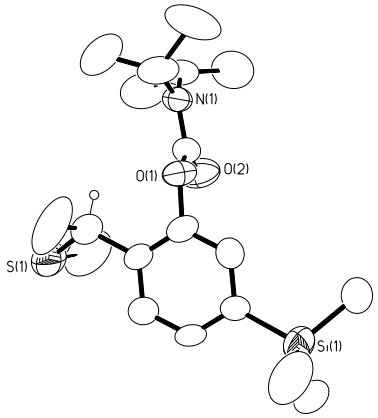


Figure S3. Molecular Structure of **21a**.

X-Ray Diffraction Analysis Report for Compound 21a

The crystal of the compound was mounted on a glass fiber with epoxy glue. The data for the compound were collected on a CCD-detector-equipped SMART system with graphite monochromated Mo Kα radiation (λ=0.71073 Å) operated at 50 kV and 35 mA at 23°C over the 2θ range of 4-56°. No significant decay was observed for the crystal.

The data were processed on a Pentium PC using Siemens SHELXTL (version 5.0) software package. An empirical absorption correction was applied for the crystal. The data were corrected for Lorentz-polarization effects. Neutral atoms scattering factors were taken from Cromer and Waber. The structure was solved by direct method. Full-matrix least-square refinements minimizing the function $\sum w(F_o^2 - F_c^2)^2$ were applied to the compound. The positions of hydrogen were calculated and refined successfully.

Enantiomer I (correct one): Final R1 = 0.0387, wR2 = 0.0705, Flack x parameter = 0.0680 with esd 0.0257.

Enantiomer II (mirror): Final R1 = 0.0445, wR2 = 0.1171, Flack x parameter = 0.9214 with esd 0.0285.

Table S5. Crystal Data and Structure Refinement for **21a**.

Identification code	0152	
Empirical formula	C19 H33 N O2 S Si	
Formula weight	367.61	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 7.8570(16) Å	α= 70.095(4)°.
	b = 11.876(3) Å	β= 77.111(4)°.
	c = 13.396(3) Å	γ = 79.851(4)°.
Volume	1138.8(4) $Å^3$	
Z	2	
Density (calculated)	1.072 Mg/m^3	
Absorption coefficient	0.205 mm^{-1}	
F(000)	400	
Crystal size	0.2 x0.3 x 0.4 mm^3	
Theta range for data collection	1.64 to 28.29°.	
Index ranges	-9<=h<=10, -15<=k<=14, -17<=l<=16	
Reflections collected	8419	
Independent reflections	7214 [R(int) = 0.0261]	
Completeness to theta = 28.29°	93.1 %	
Absorption correction	Empirical (Bruker SADABS)	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7214 / 3 / 433	
Goodness-of-fit on F^2	0.744	
Final R indices [I>2sigma(I)]	R1 = 0.0437, wR2 = 0.0791	
R indices (all data)	R1 = 0.1223, wR2 = 0.0920	
Absolute structure parameter	0.08(8)	
Largest diff. peak and hole	0.227 and -0.235 $e.Å^{-3}$	

Table S6. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$x 10^3) for **21a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Si(1)	4360(2)	8123(1)	3222(1)	75(1)
Si(2)	5699(3)	879(2)	5399(1)	110(1)
S(1)	2478(2)	2948(1)	2117(2)	110(1)
S(2)	8515(2)	5984(1)	5943(1)	106(1)
O(1)	324(4)	6845(3)	1249(3)	63(1)
O(2)	2440(4)	6881(4)	-225(3)	93(1)
O(3)	9325(4)	2293(3)	7523(3)	67(1)
O(4)	7293(4)	2075(3)	9031(3)	83(1)
N(1)	-465(5)	7212(3)	-361(4)	59(1)
N(2)	10211(5)	1754(4)	9114(4)	59(1)
C(1)	4047(7)	3480(7)	975(7)	154(3)
C(2)	1151(6)	4324(4)	2159(4)	79(2)
C(3)	-442(7)	3991(6)	3086(6)	144(3)
C(4)	2124(6)	5239(5)	2314(4)	55(1)
C(5)	3370(6)	4913(5)	2985(4)	70(2)
C(6)	4087(6)	5778(5)	3193(4)	61(1)
C(7)	3581(6)	6989(5)	2794(4)	54(1)
C(8)	2332(6)	7312(4)	2132(4)	60(1)
C(9)	1636(5)	6456(5)	1897(4)	57(1)
C(10)	3242(8)	7967(6)	4642(5)	129(3)
C(11)	6754(6)	7795(5)	3215(4)	96(2)
C(12)	3860(8)	9675(5)	2316(5)	120(2)
C(13)	899(7)	6971(4)	173(5)	59(1)
C(14)	-83(7)	7315(6)	-1514(5)	76(2)
C(15)	792(7)	6141(6)	-1694(5)	120(2)
C(16)	788(8)	8434(6)	-2186(5)	138(3)
C(17)	-2345(6)	7257(5)	207(4)	77(2)
C(18)	-3166(6)	6183(6)	271(5)	114(2)
C(19)	-3386(7)	8419(6)	-319(5)	138(3)
C(20)	10429(9)	5190(7)	5431(6)	174(4)
C(21)	6051(8)	5237(6)	7697(5)	120(2)

C(22)	7661(6)	4755(4)	7015(4)	64(1)
C(23)	7196(6)	3803(5)	6627(4)	58(1)
C(24)	5968(6)	4058(5)	5963(4)	72(2)
C(25)	5515(7)	3199(6)	5620(4)	81(2)
C(26)	6340(7)	2021(5)	5904(4)	79(2)
C(27)	7563(6)	1764(5)	6577(4)	71(2)
C(28)	7984(5)	2632(5)	6914(4)	57(1)
C(29)	6739(11)	1085(7)	4039(5)	192(4)
C(30)	3215(8)	1153(7)	5405(7)	190(4)
C(31)	6205(10)	-623(6)	6296(6)	152(3)
C(32)	8831(7)	2034(5)	8607(5)	61(2)
C(33)	12005(6)	1730(5)	8559(4)	74(2)
C(34)	13066(7)	549(6)	8975(6)	149(3)
C(35)	12851(7)	2761(7)	8567(6)	157(3)
C(36)	9903(7)	1534(6)	10279(5)	82(2)
C(37)	8960(8)	458(6)	10924(5)	144(3)
C(38)	8989(6)	2656(6)	10583(5)	114(2)