SUPPORTING INFORMATION FOR

Stereoselective Synthesis of New Pyran-dioxane based Polycycles from Glycal Derived Vinyl Epoxide

2-((tert-butyldimethylsilyl)oxy)ethan-1-ol (2).

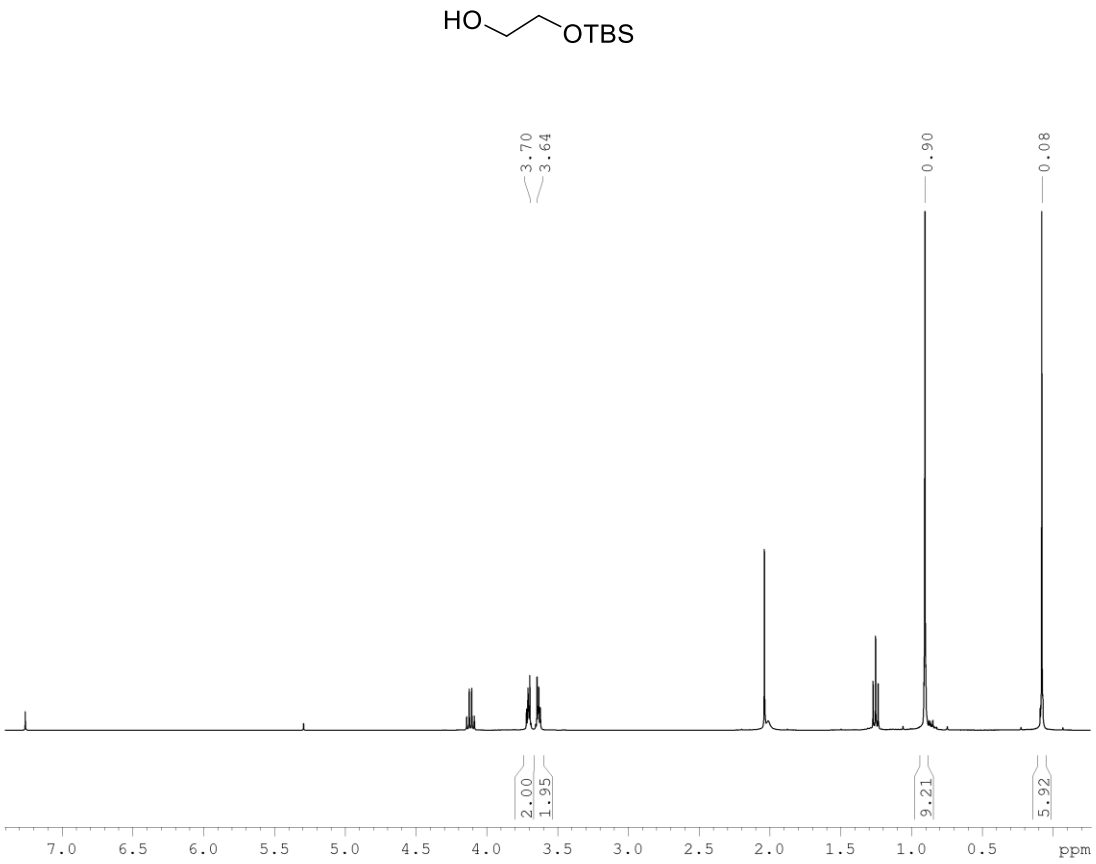
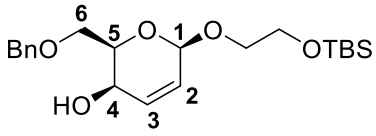


Figure 1. ^{1}H spectrum of compound 2.

(*1R,4R,5R*)-5-((benzyloxy)methyl)-1-(2-((tert-butyldimethylsilyl)oxy)ethoxy)-2,3-dihydro-2H-pyran-4-ol (3).



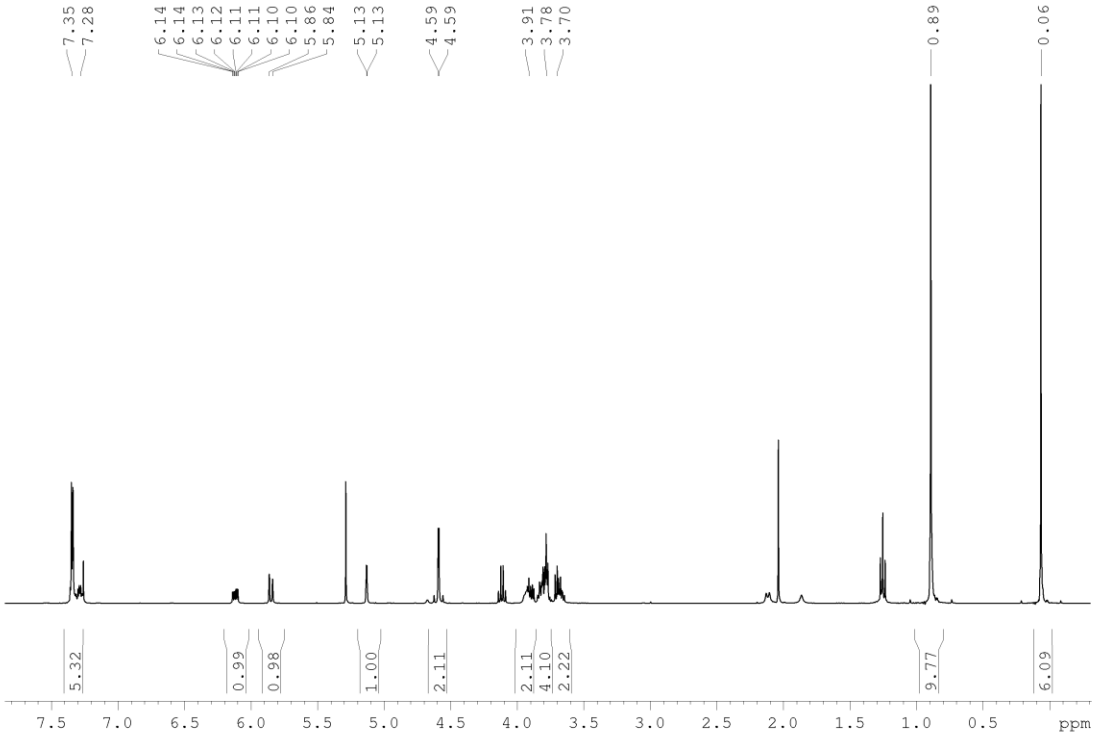


Figure 2. ^{1}H-NMR spectrum of compound 3.

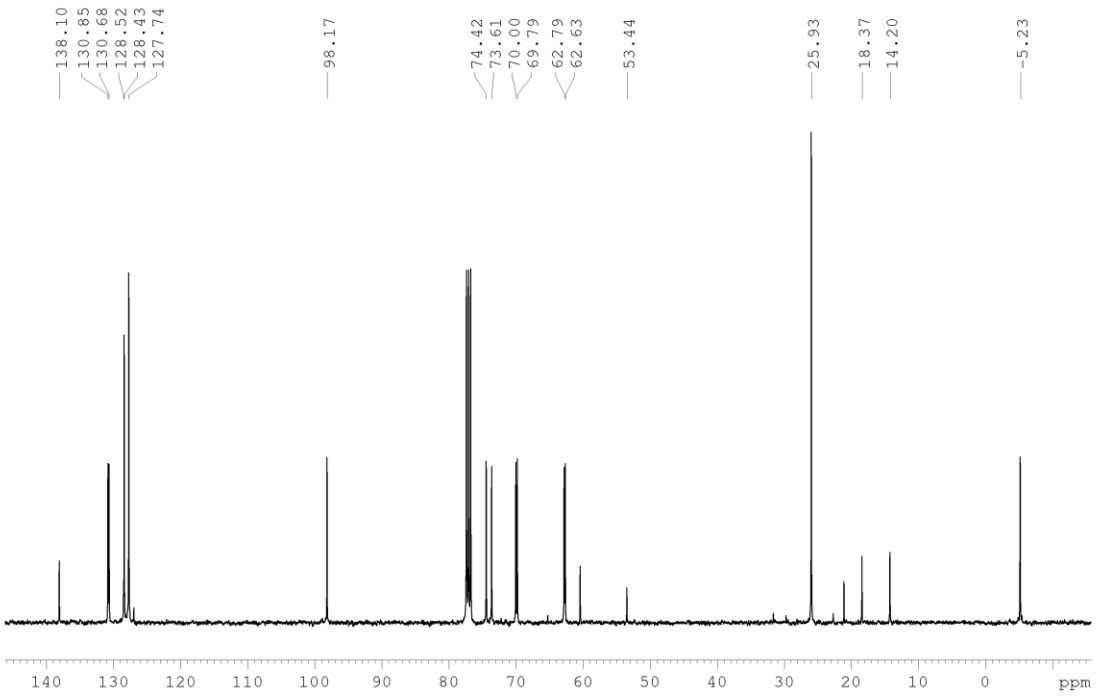


Figure 3.^{13}C-NMR spectrum of compound 3.

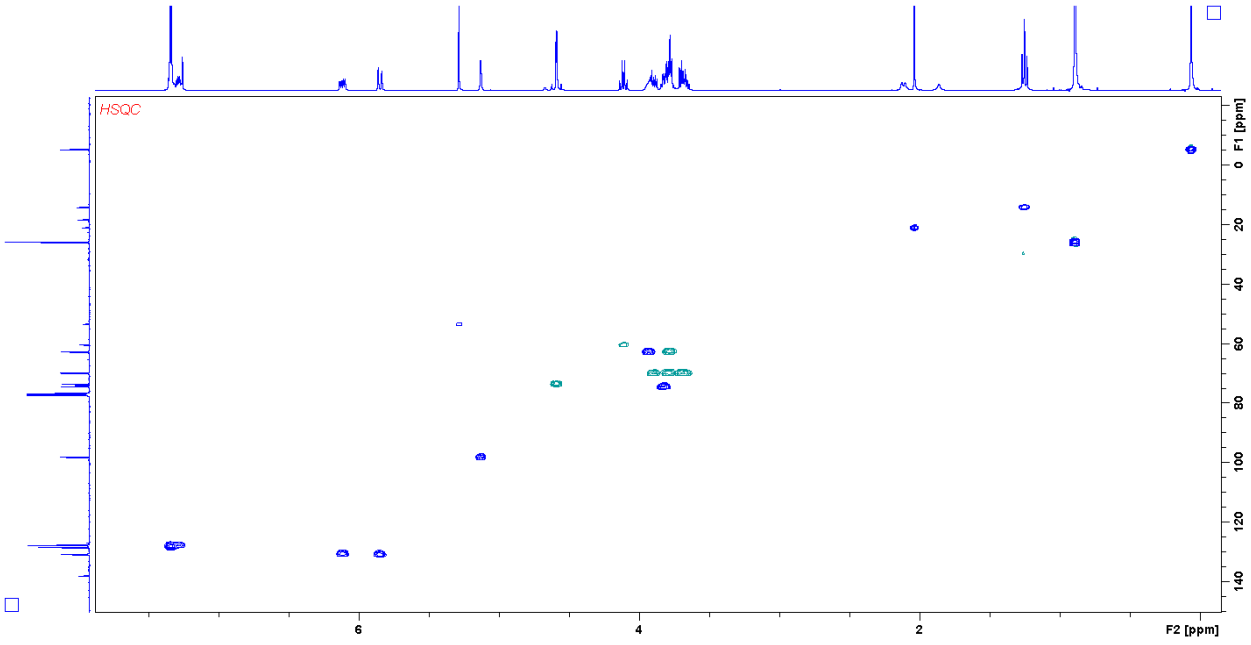


Figure 4. HSQC of compound 3.

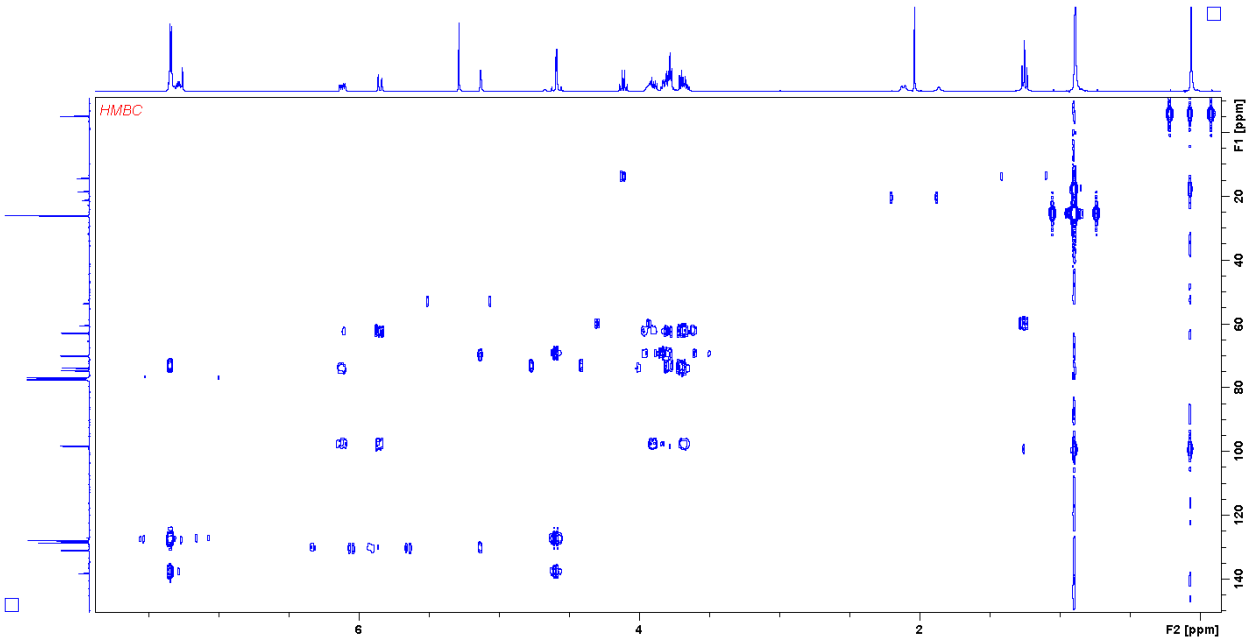


Figure 5. HMBC of compound 3.

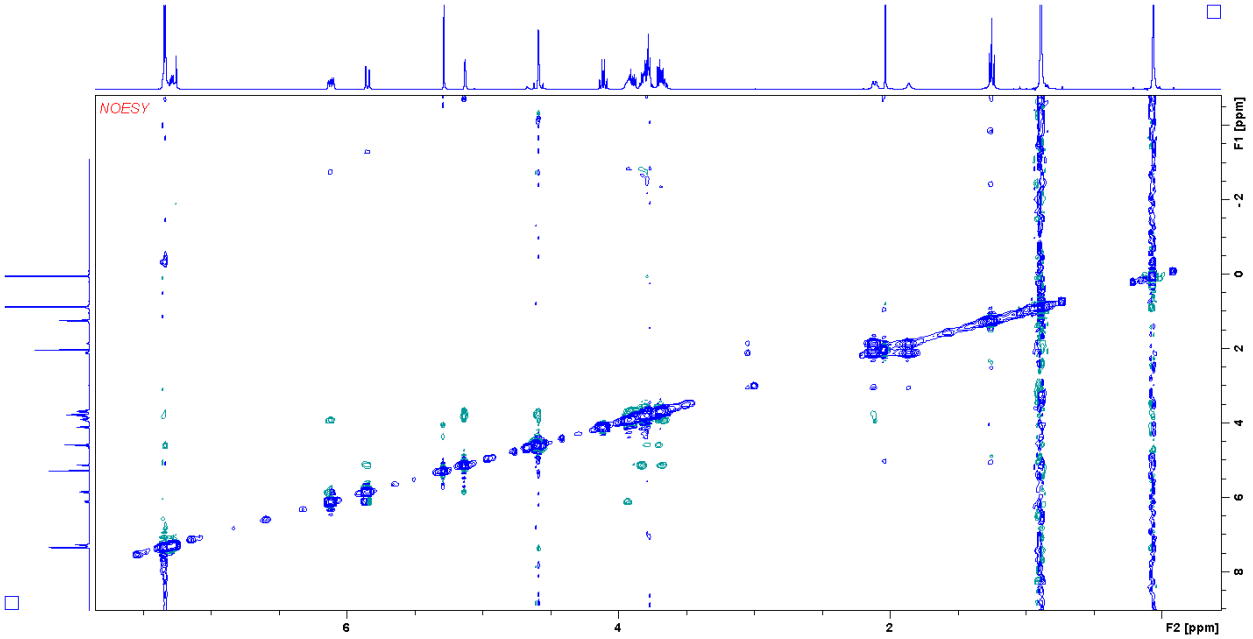
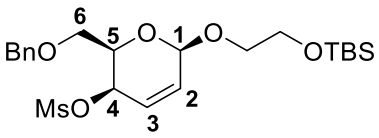


Figure 6. NOESY of compound 3.

(*1R,4R,5R*)-5-((benzyloxy)methyl)-1-(2-((tert-butyldimethylsilyl)oxy)ethoxy)-2,3-dihydro-2H-pyran-4-yl methanesulfonate (4).



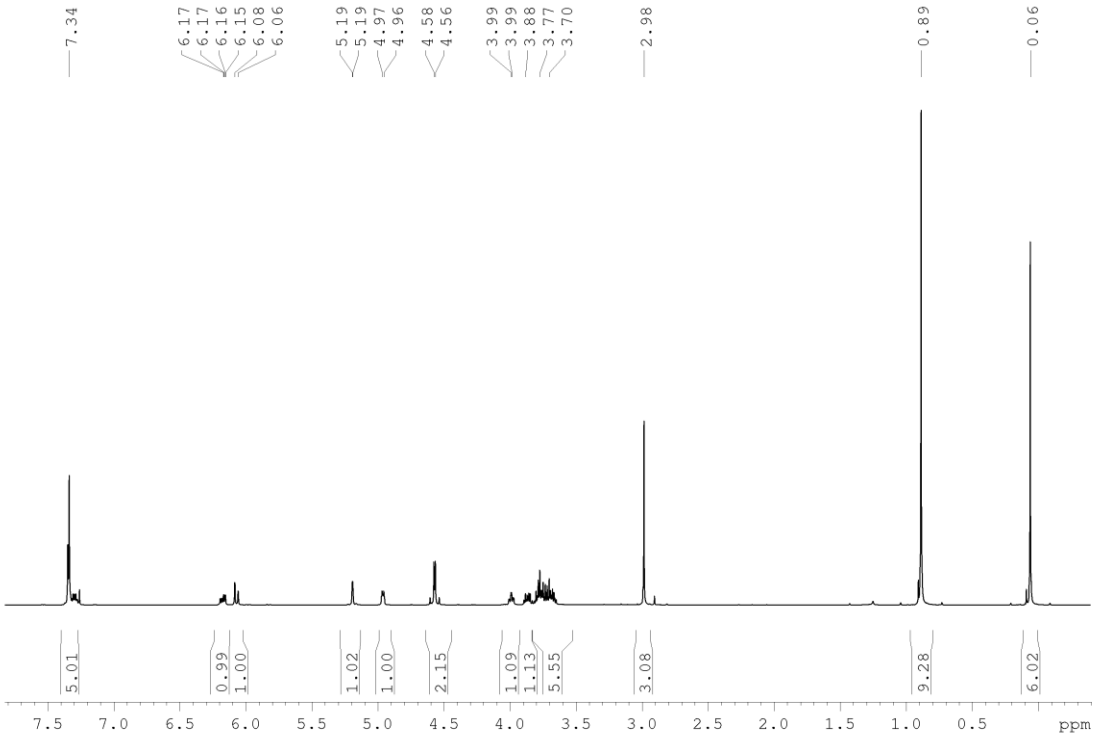


Figure 7. ^{1}H-NMR spectrum of compound 4.

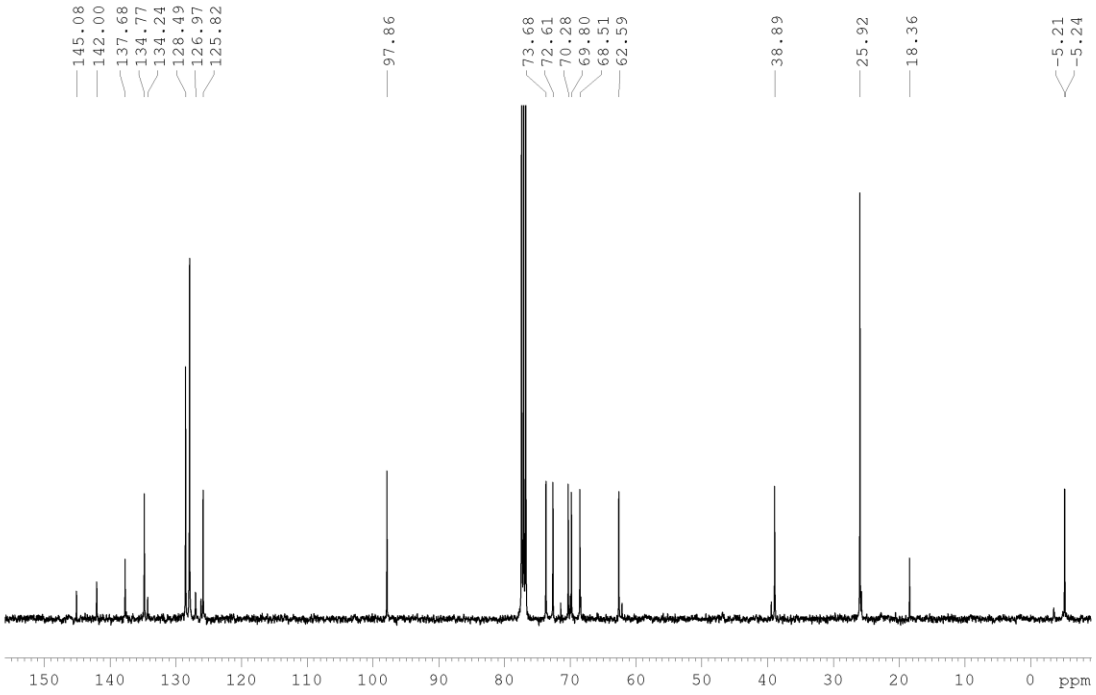
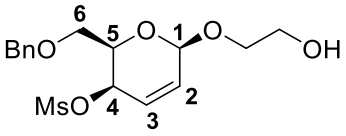


Figure 8. ^{13}C-NMR of compound 4.

(*1R,4R,5R*)-5-((benzyloxy)methyl)-1-(2-hydroxyethoxy)-2,3-dihydro-2H-pyran-4-yl methanesulfonate (5).



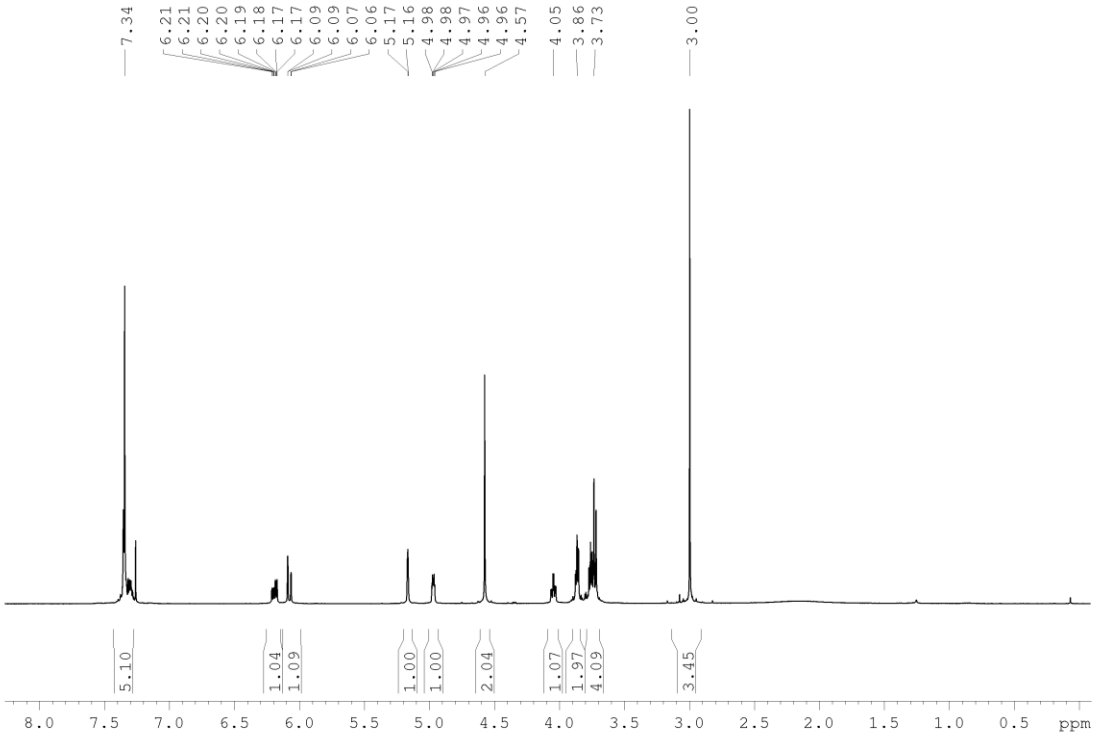


Figure 9. ^{1}H-NMR spectrum of compound 5.

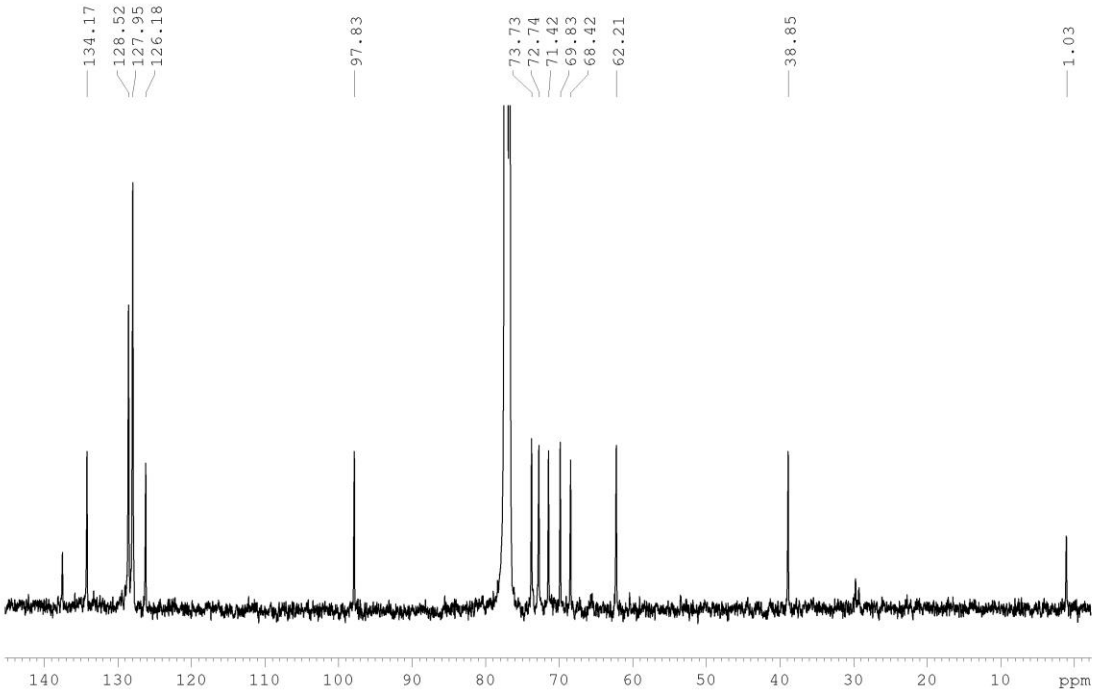


Figure 10. ^{13}C-NMR spectrum of compound 5.

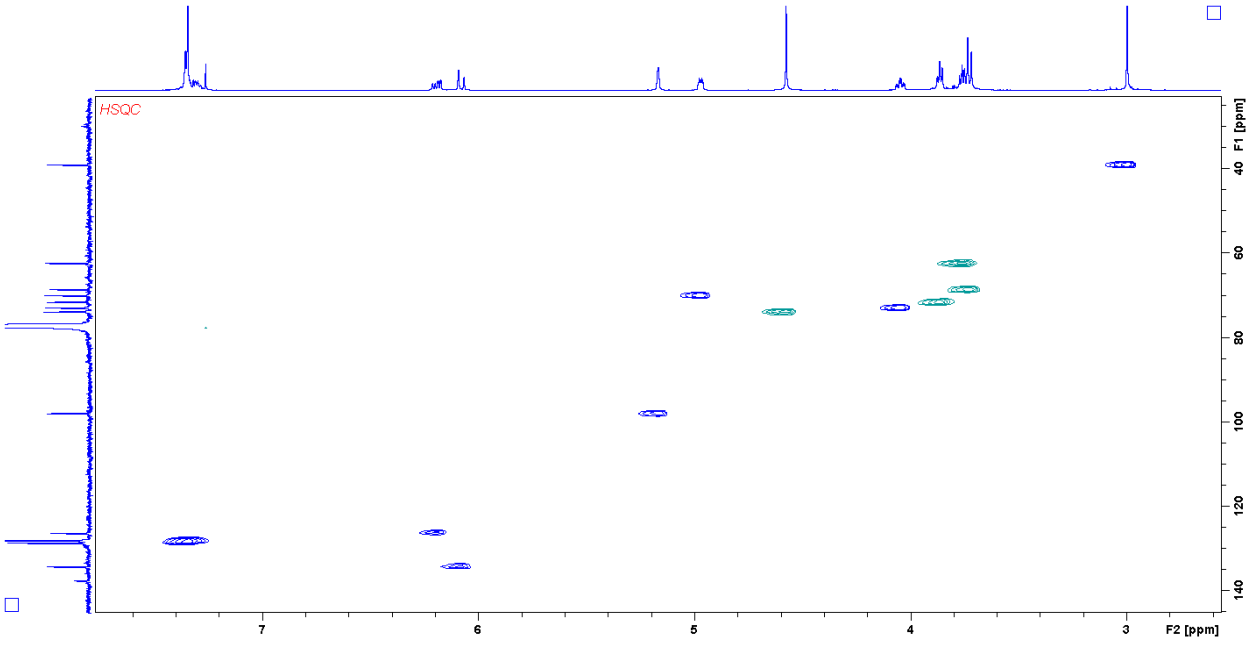


Figure 11. HSQC of compound 5.

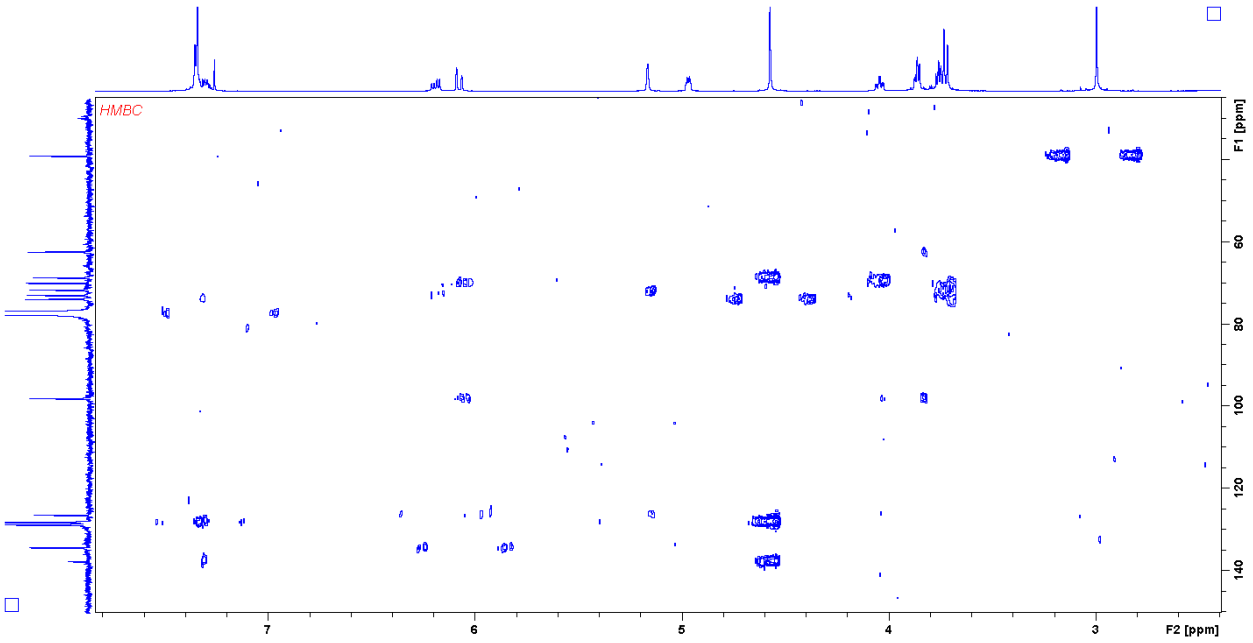


Figure 12. HMBC of compound 5.

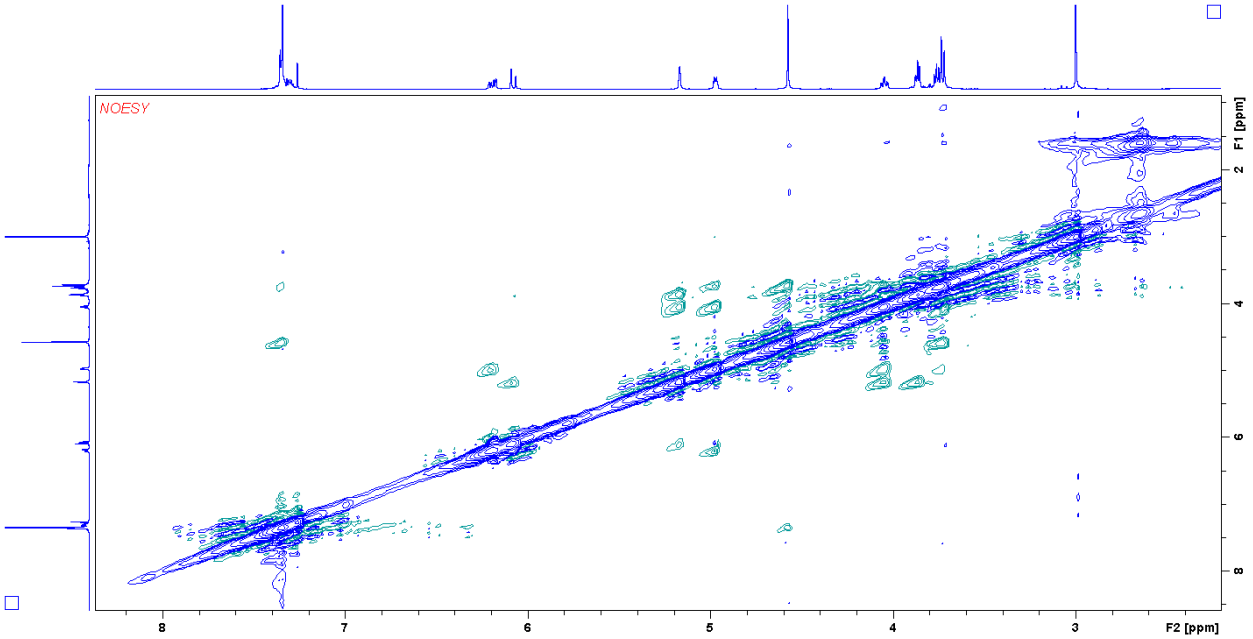
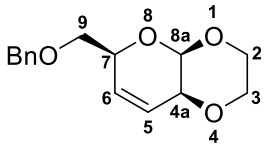


Figure 13. NOESY of compound 5.

(*4aS,7S,8aR*)-7-((benzyloxy)methyl)-2,3,4a,8a-tetrahydro-6H-pyrano[2,3-b][1,4]dioxine (6).



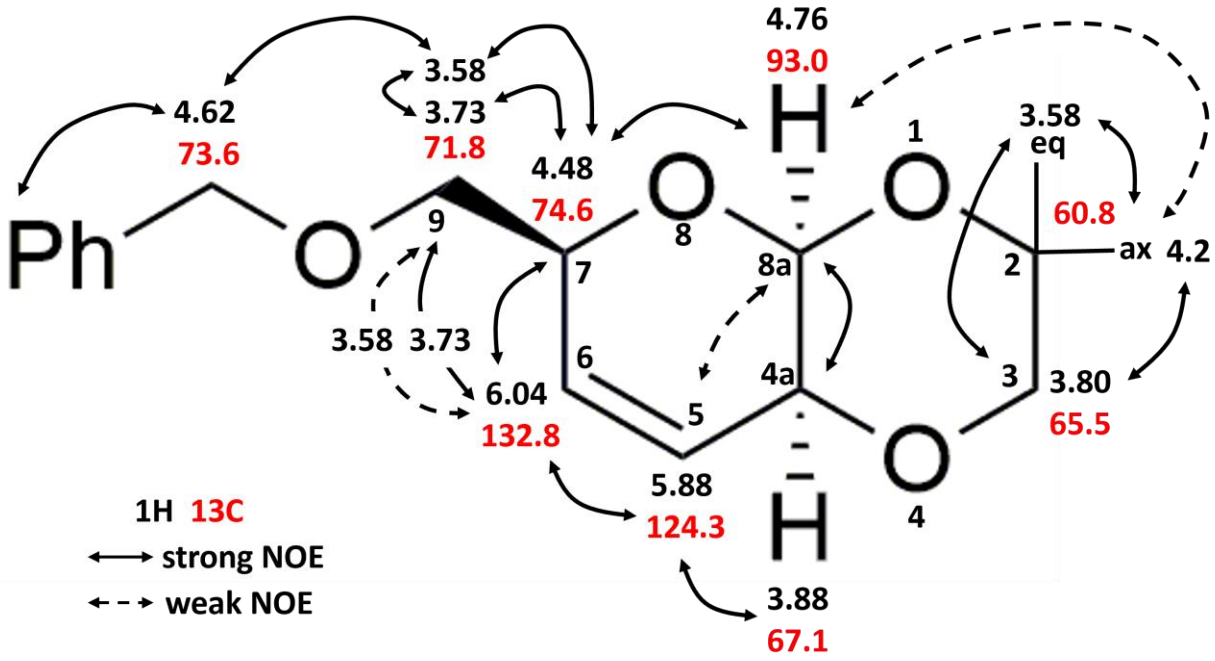


Figure 14. NMR detailed assignment of compound 6 with the NOE correlations.

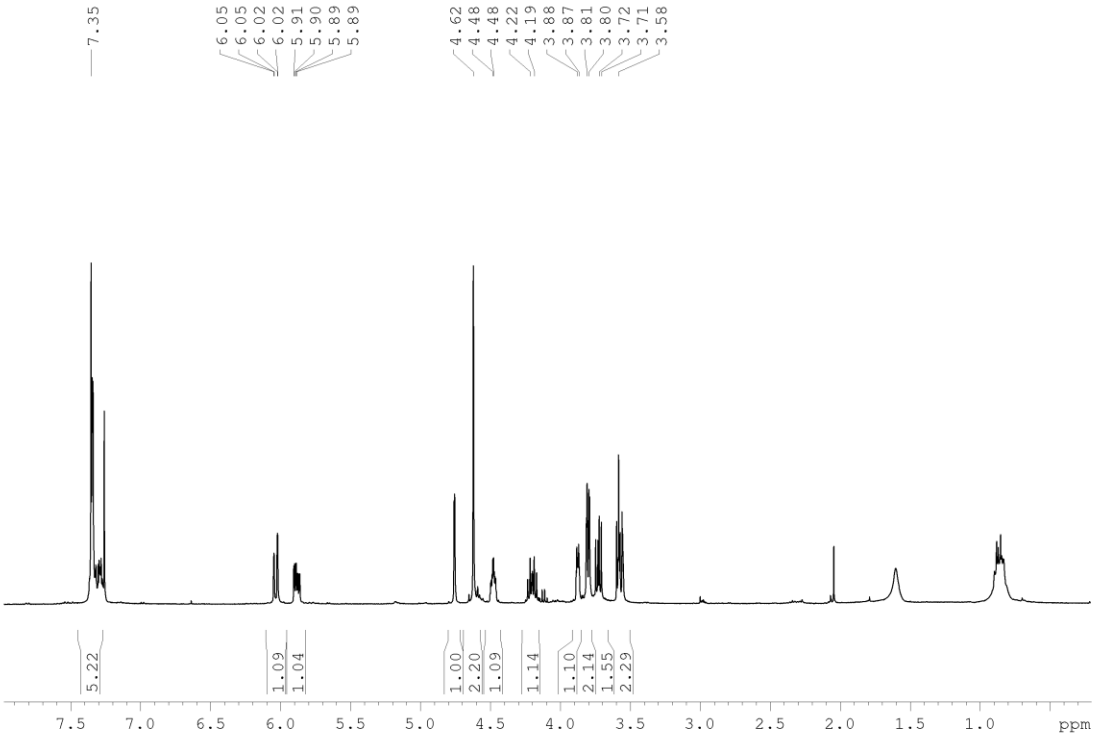


Figure 15. ^{1}H-NMR spectrum of compound 6.

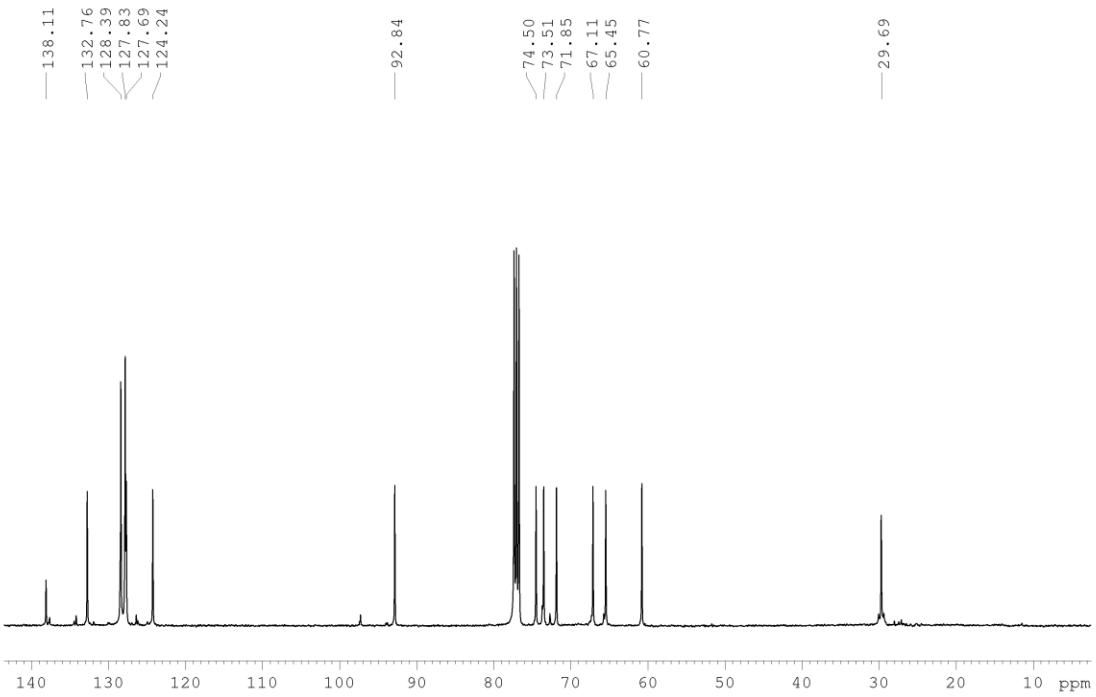


Figure 16. ^{13}C-NMR spectrum of compound 6.

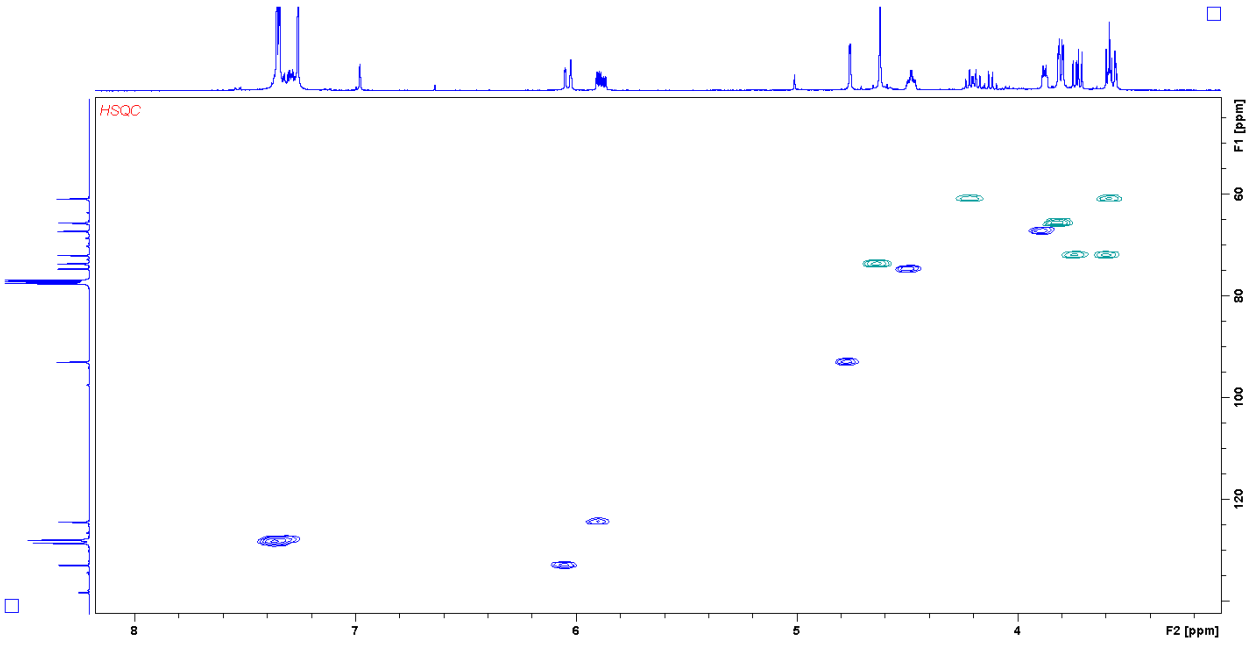


Figure 17. HSQC of compound 6.

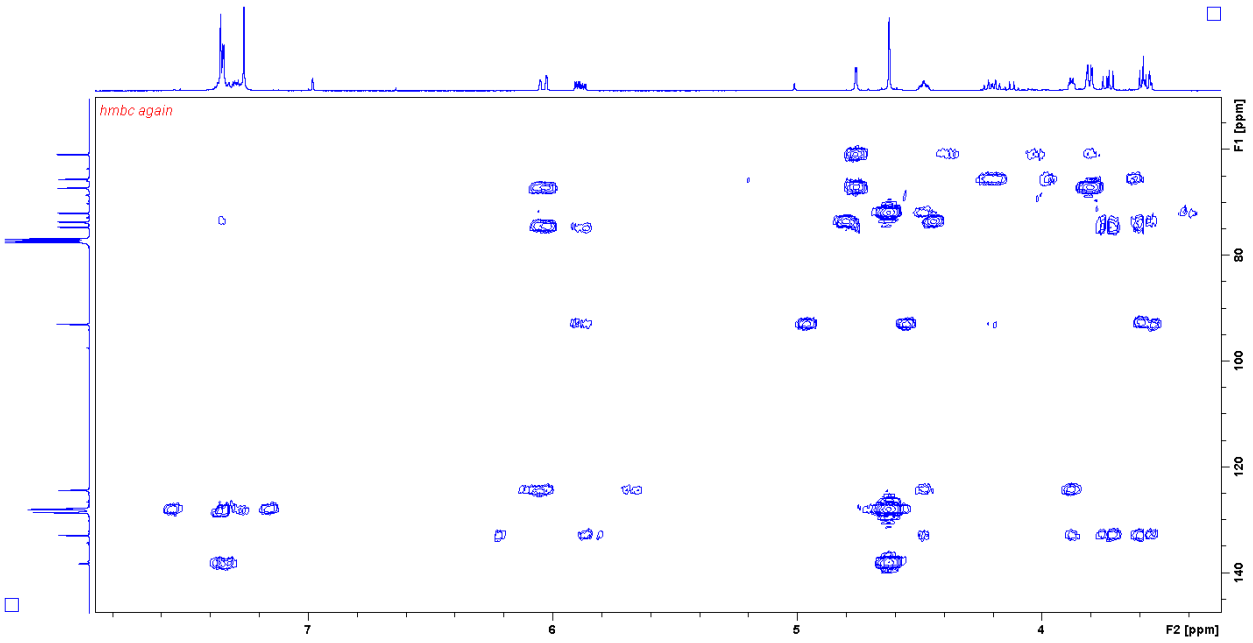


Figure 18. HMBC of compound 6.

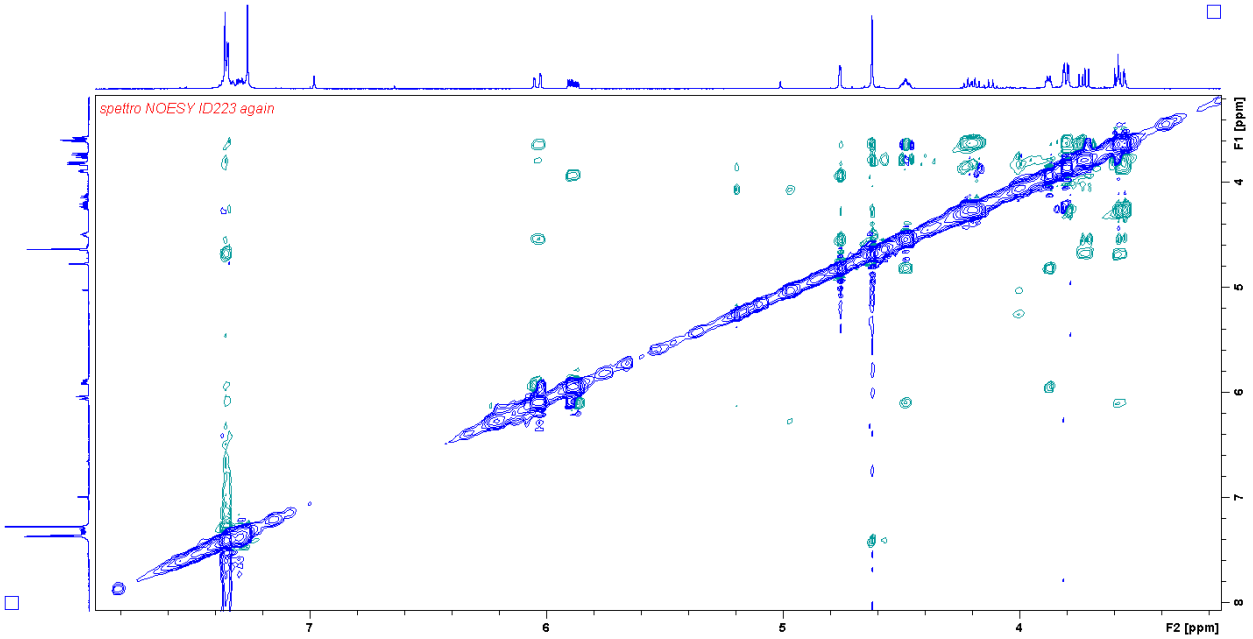


Figure 19. NOESY of compound 6.

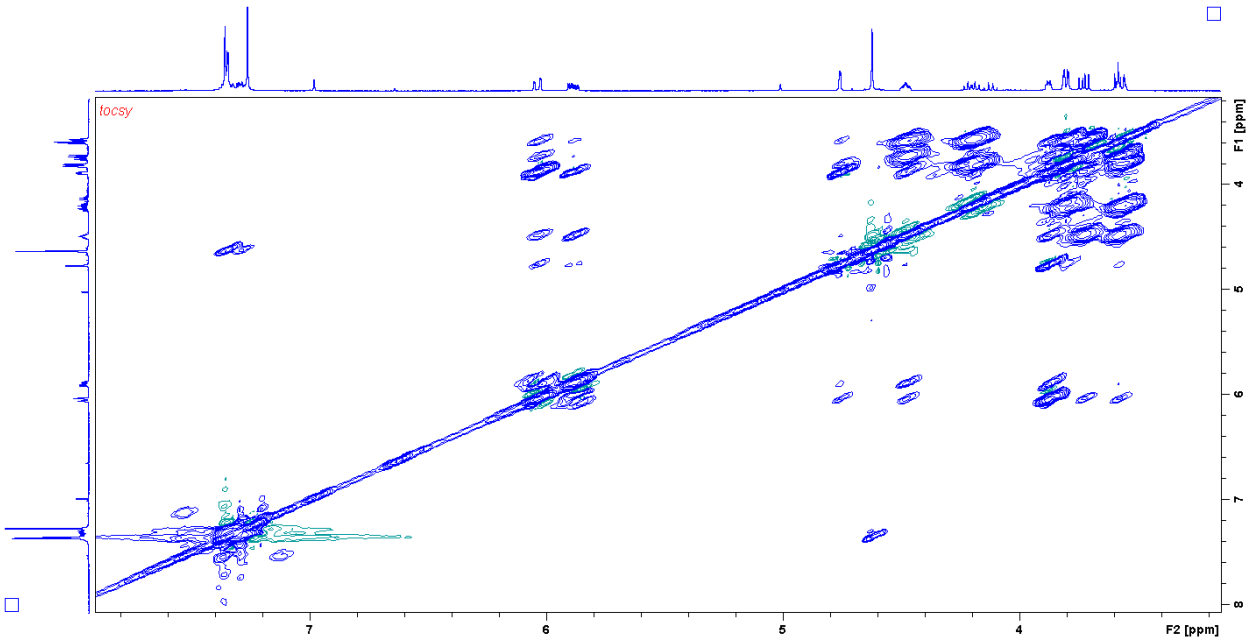


Figure 20. TOCSY of compound 6.

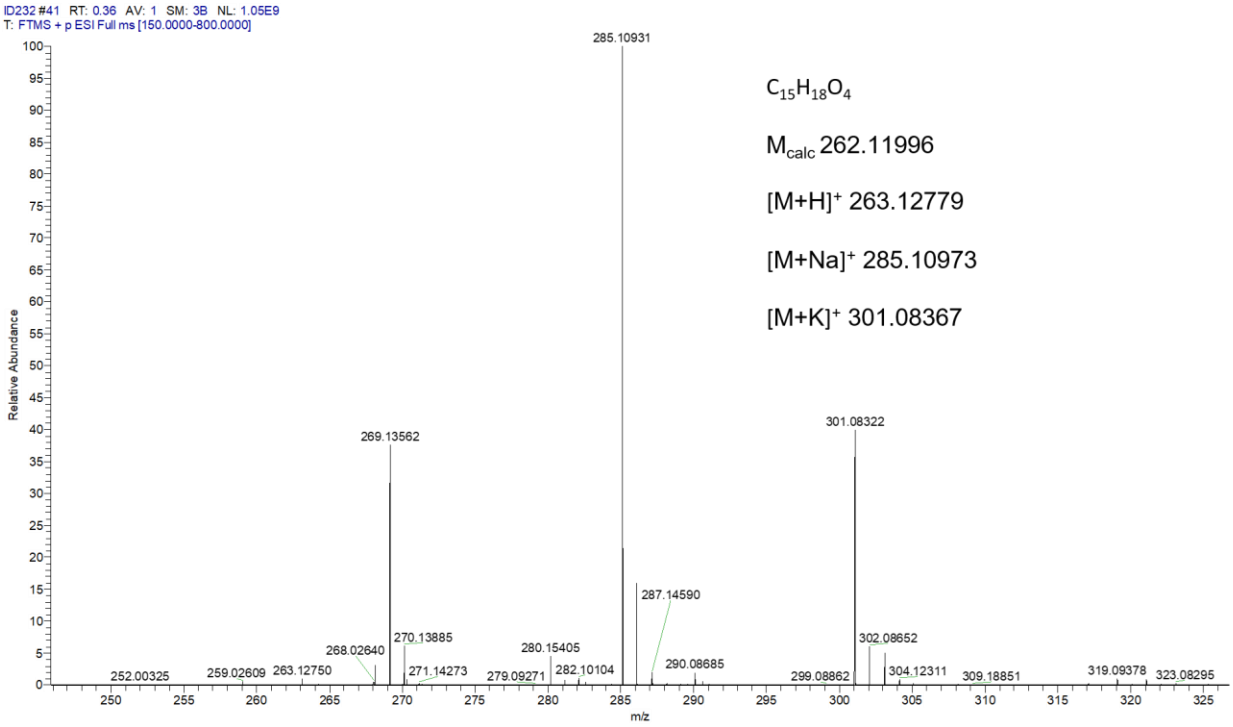


Figure 21. HRMS (ESI) of compound 6.

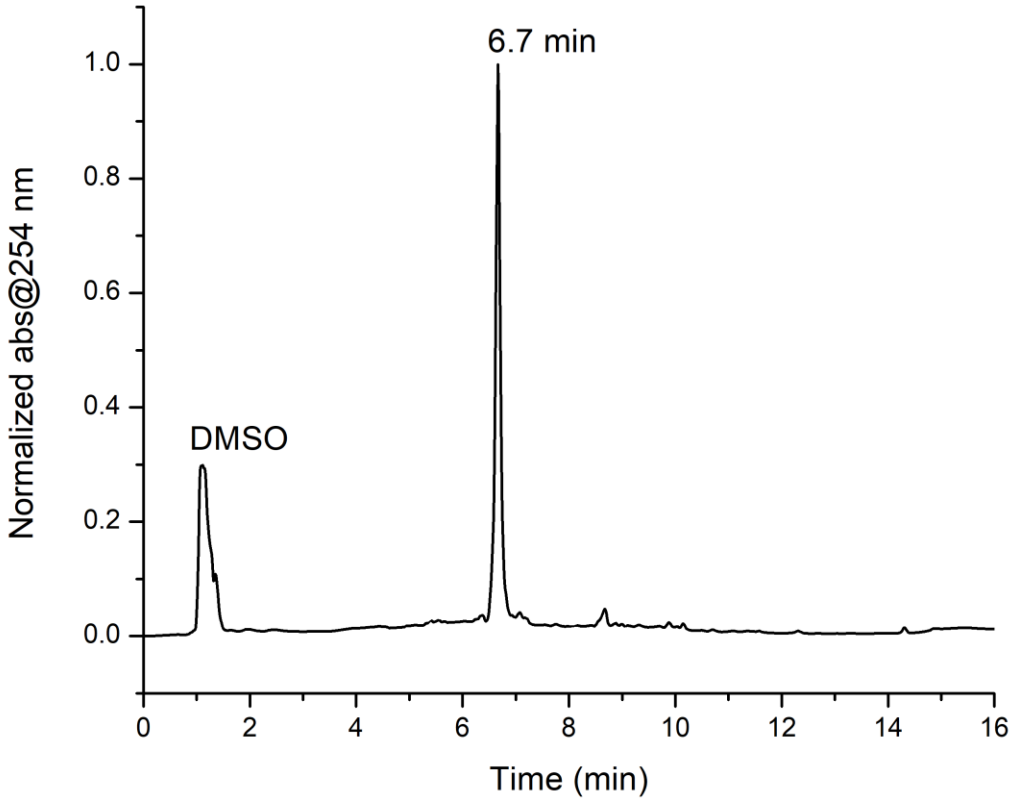
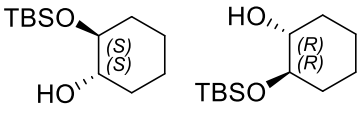


Figure 22. HPLC chromatogram at 254nm of bicycle 6.

Racemic mixture of (*1S,2S*) and (*1R,2R*)-2-((tert-butyldimethylsilyl)oxy)cyclohexan-1-ol (*rac*-7).



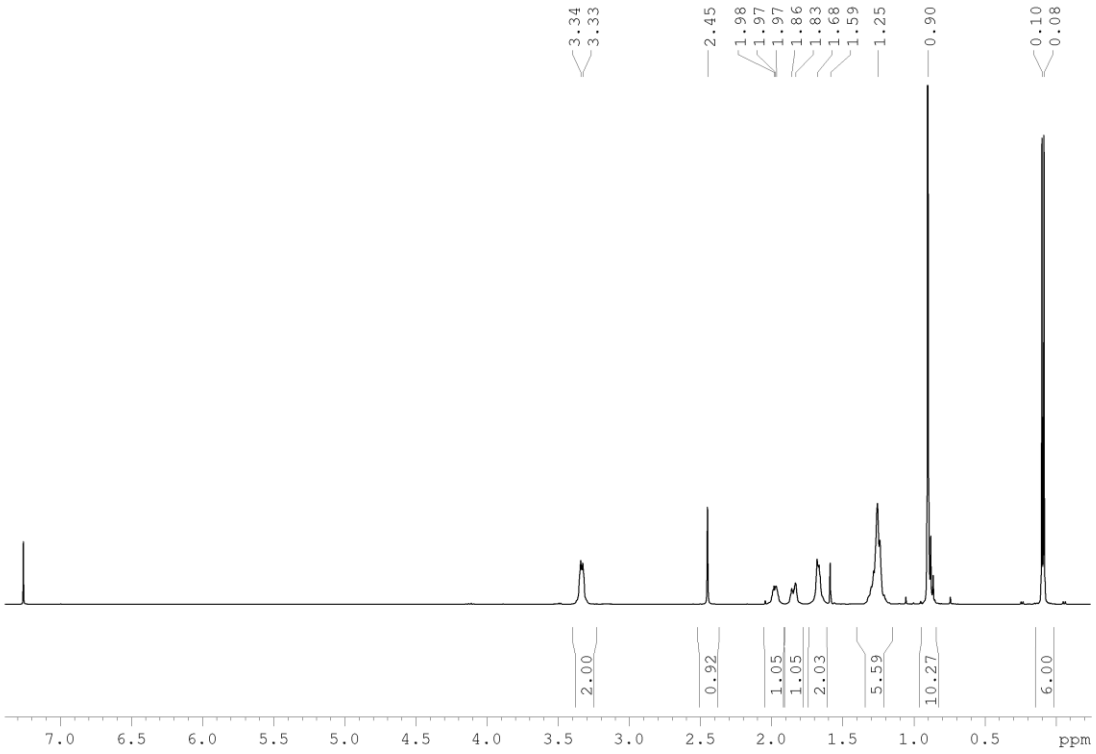
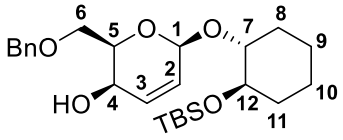


Figure 23. ^{1}H-NMR spectrum of *rac*-7.

(*1R,4R,5R*)-5-((benzyloxy)methyl)-1-(((*1R,2R*)-2-((tert-butyldimethylsilyl)oxy)cyclohexyl)oxy)-2,3-dihydro-2H-pyran-4-ol (8b).



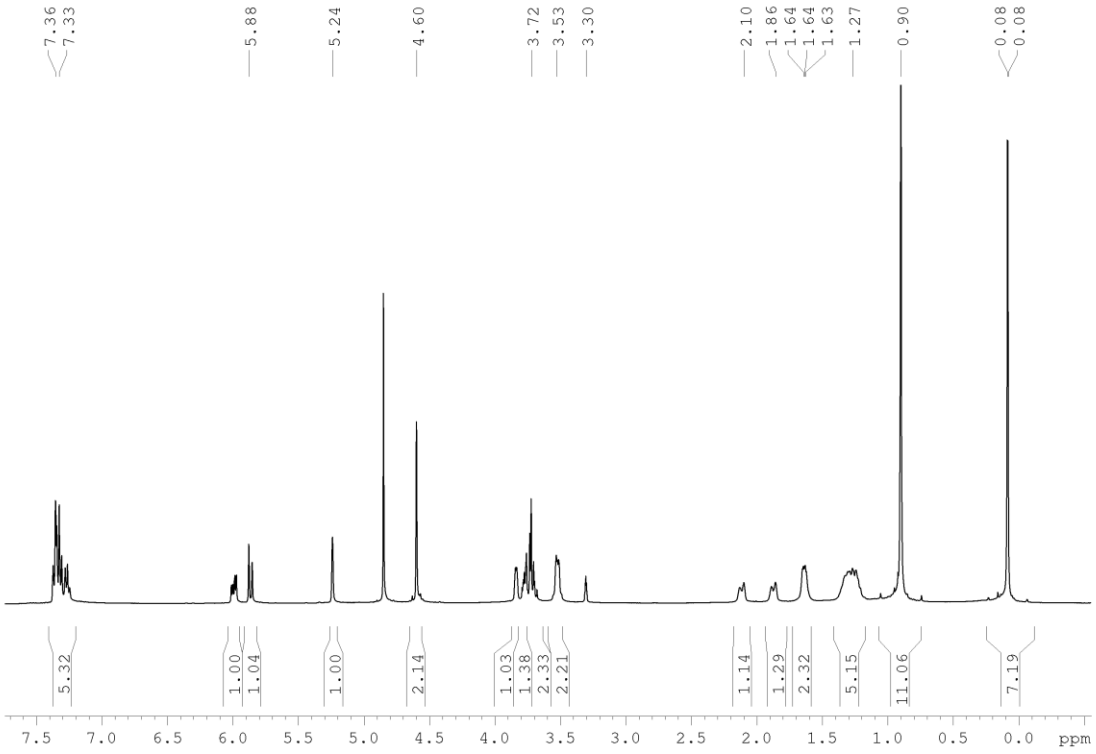


Figure 24. ^{1}H-NMR spectrum of compound 8b.

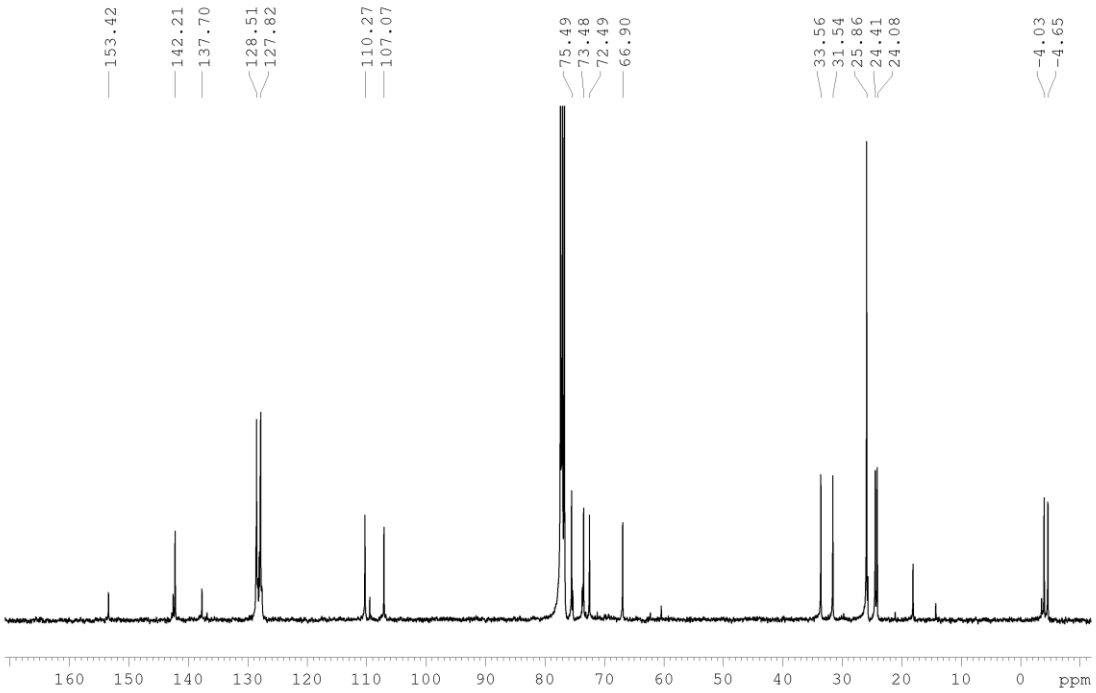


Figure 25. ^{13}C-NMR spectrum of compound 8b.

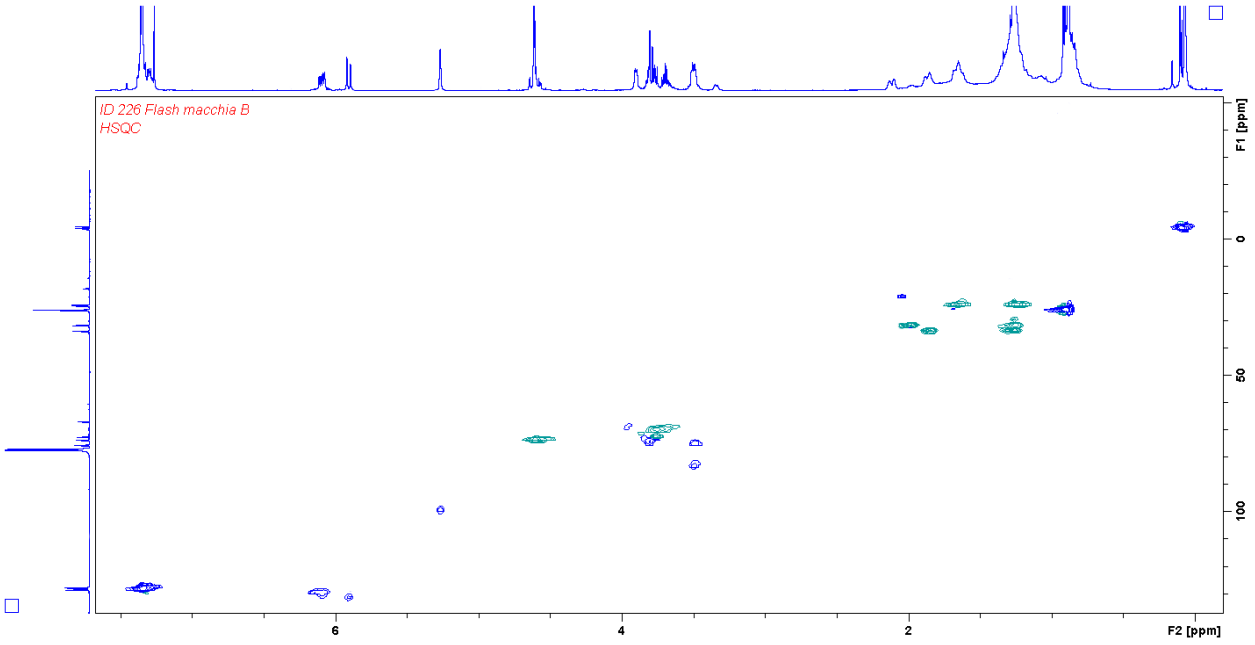


Figure 26. HSQC of compound 8b.

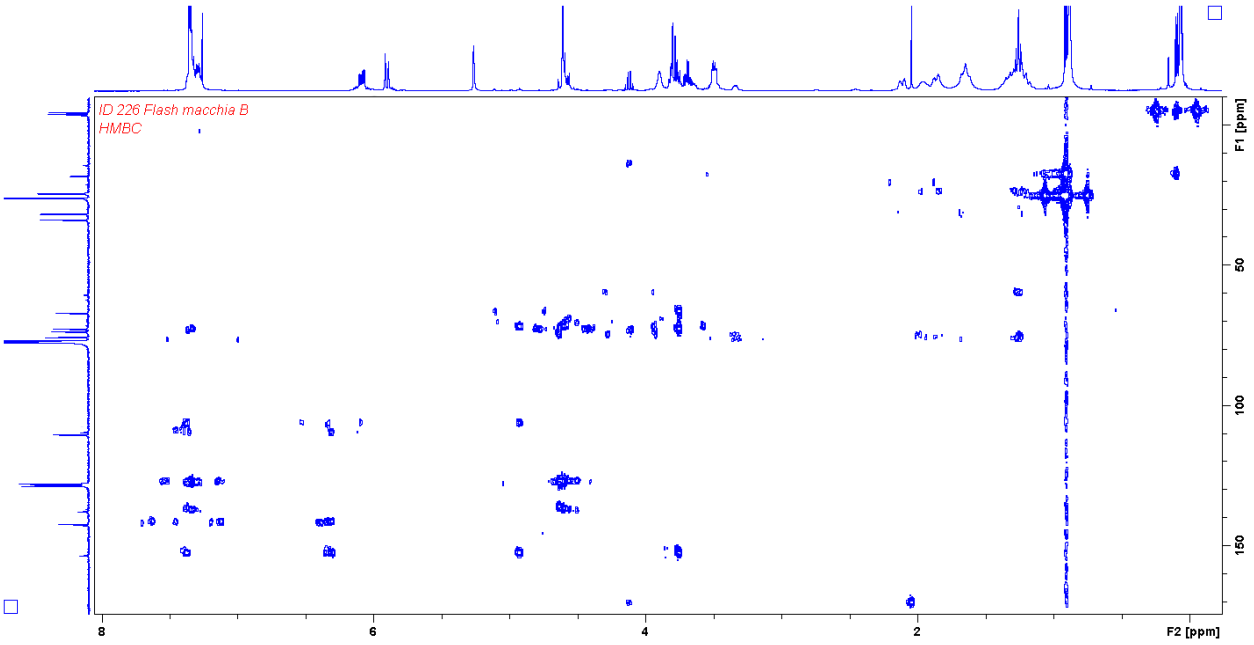


Figure 27. HMBC of compound 8b.

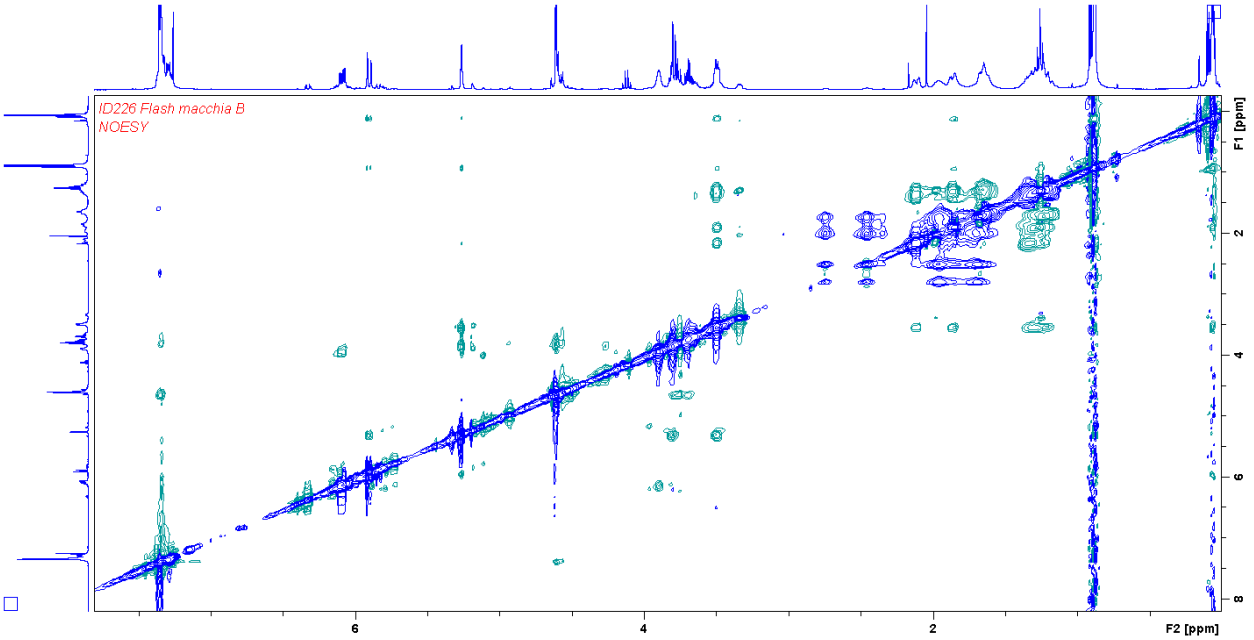


Figure 28. NOESY of compound 8b.

(*1R,4R,5R*)-5-((benzyloxy)methyl)-1-(((*1S,2S*)-2-((tert-butyldimethylsilyl)oxy)cyclohexyl)oxy)-2,3-dihydro-2H-pyran-4-ol (8a).

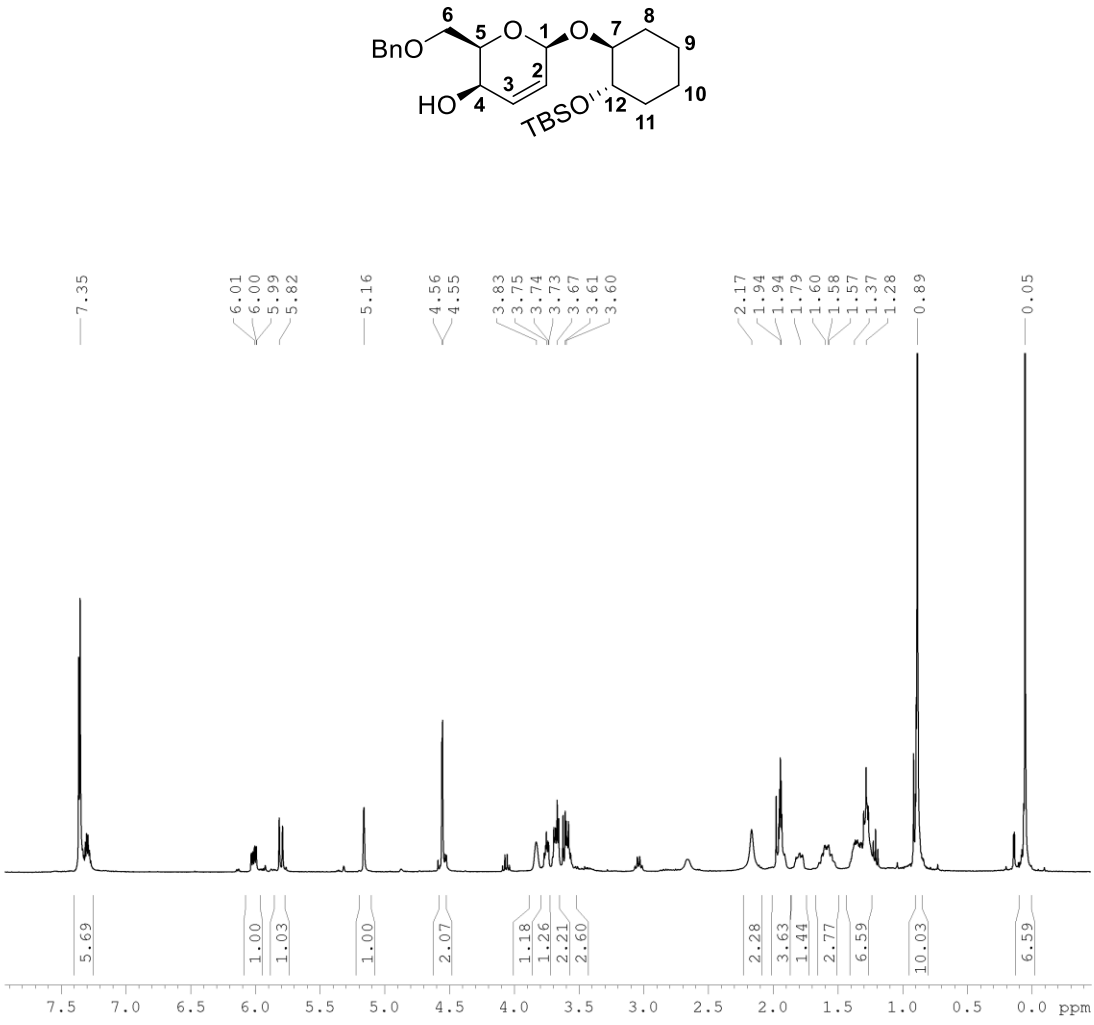


Figure 29. ^{1}H-NMR spectrum of compound 8a.

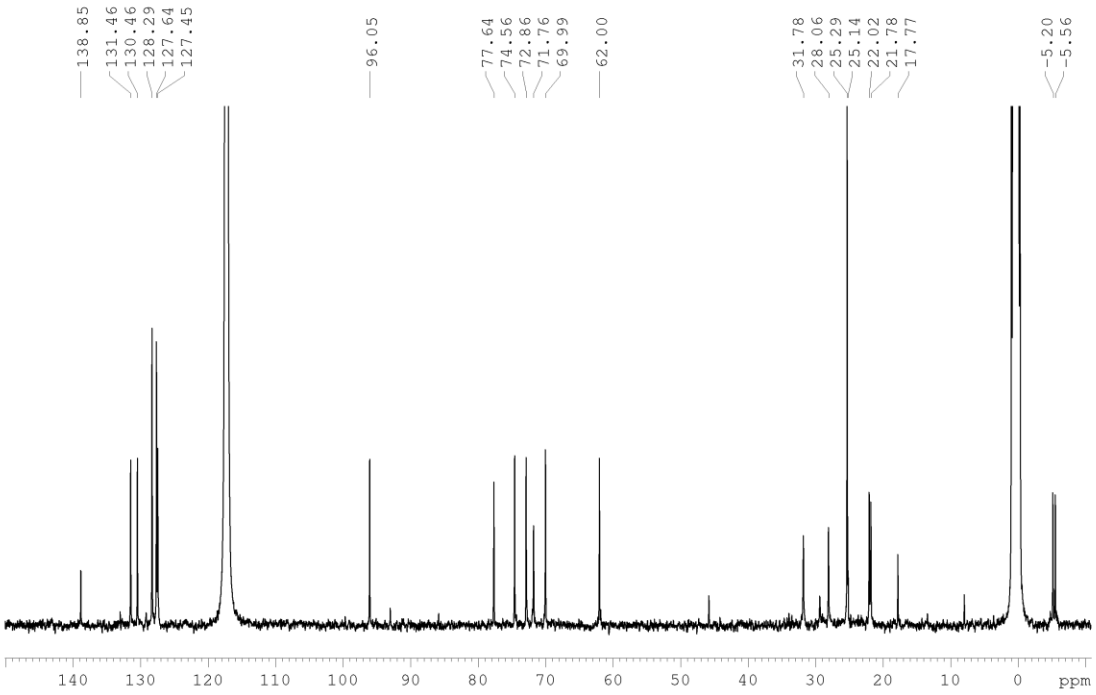


Figure 30. ^{13}C-NMR spectrum of compound 8a.

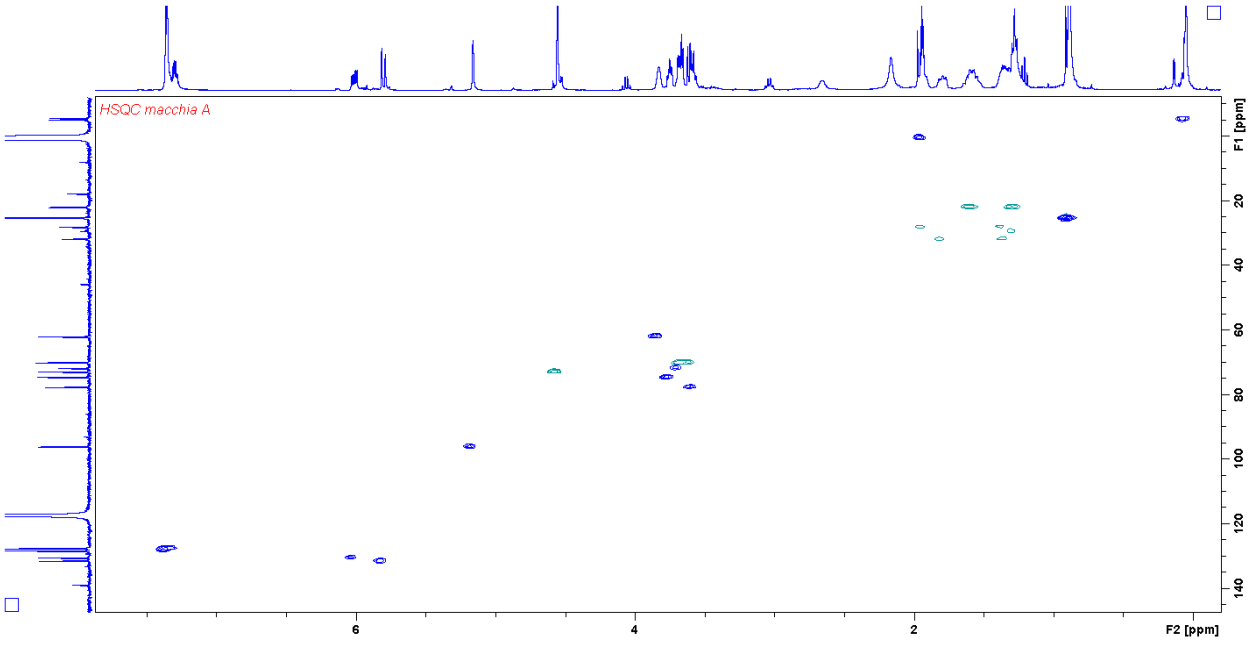


Figure 31. HSQC of compound 8a.

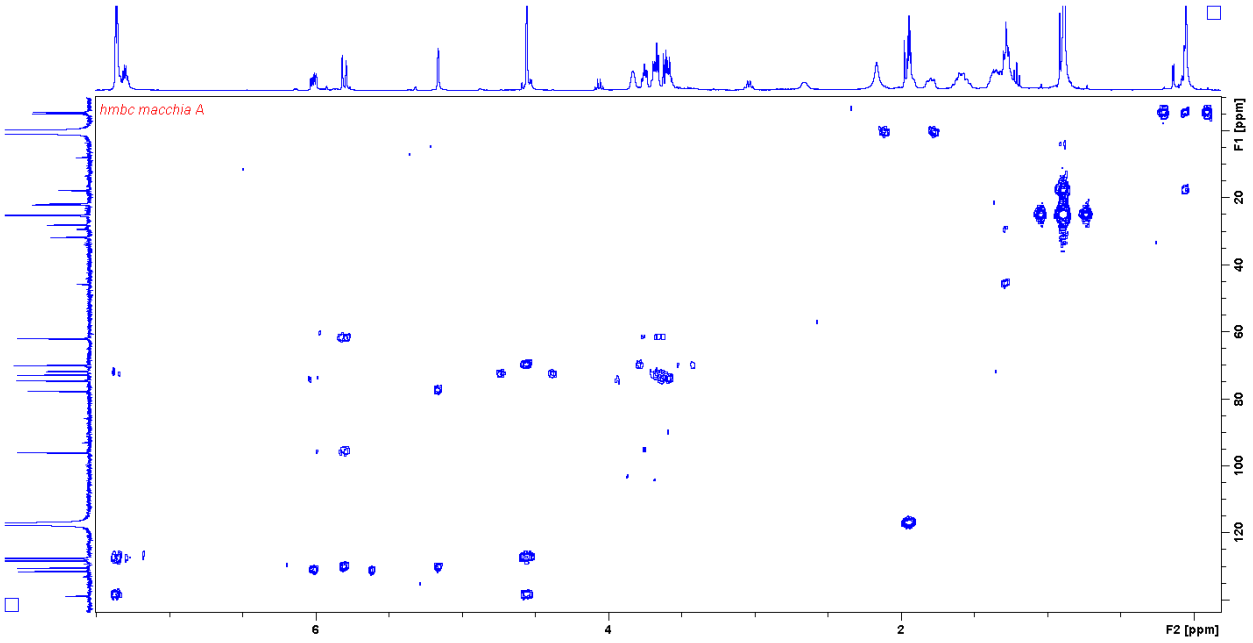


Figure 32. HMBC of compound 8a.

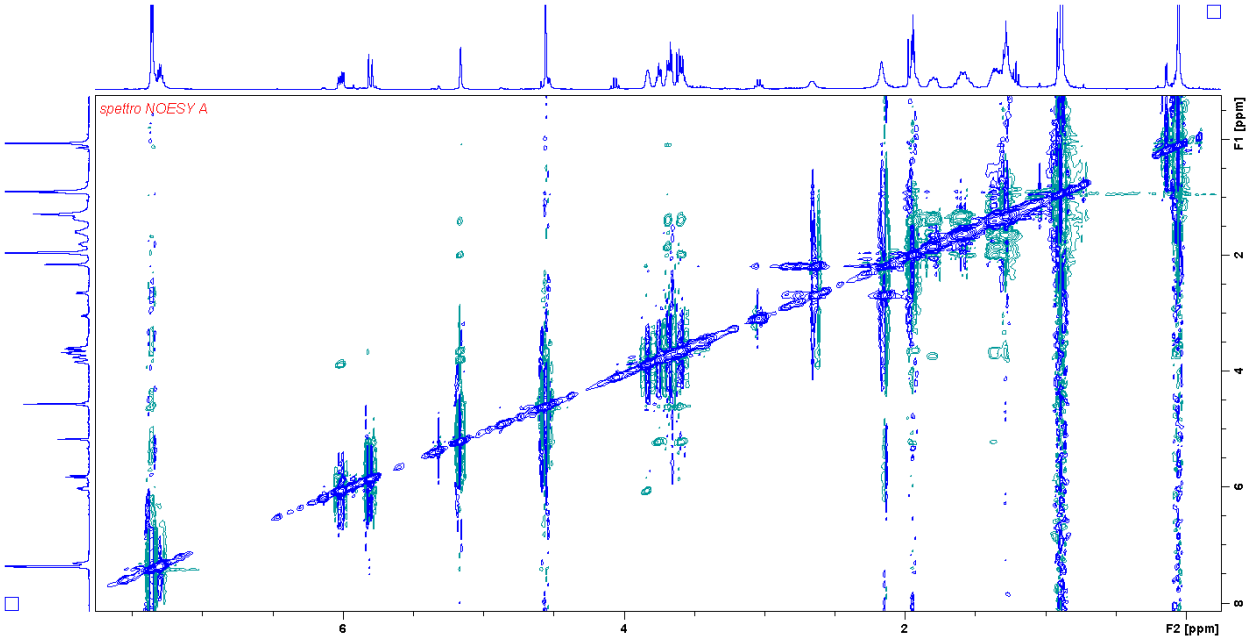


Figure 33. NOESY of compound 8a.

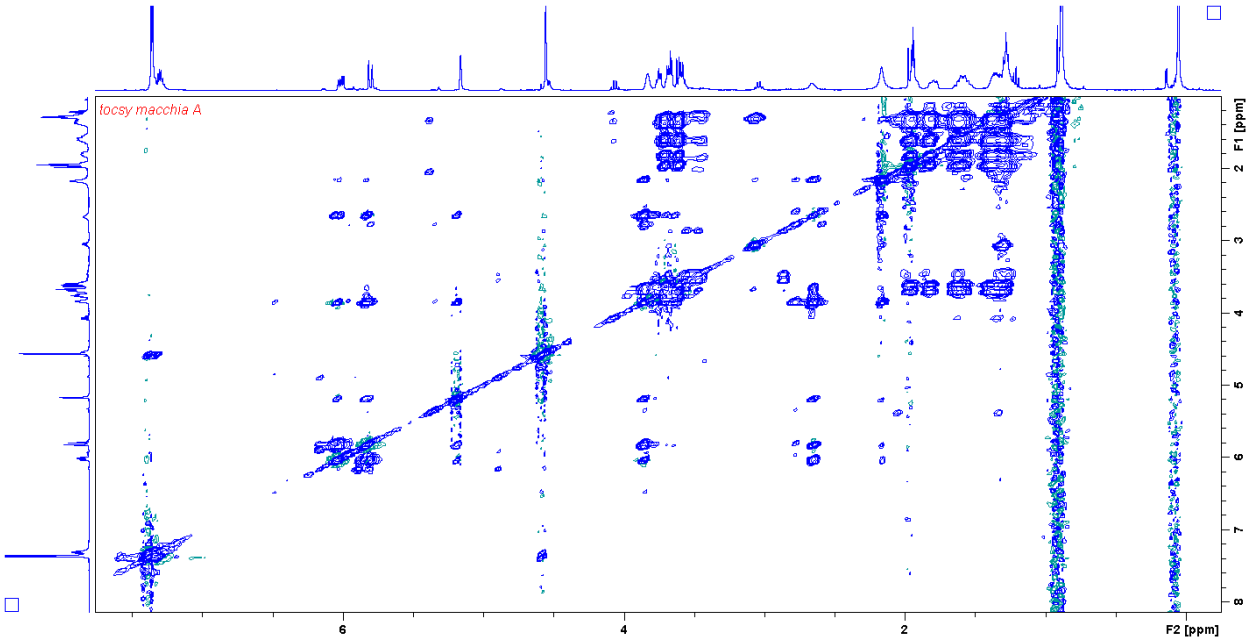
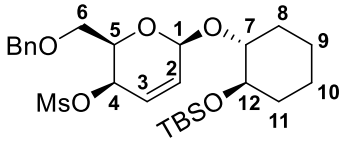


Figure 34. TOCSY of compound 8a.

(*1R,4R,5R*)-5-((benzyloxy)methyl)-1-(((*1R,2R*)-2-((tert-butyldimethylsilyl)oxy)cyclohexyl)oxy)-2,3-dihydro-2H-pyran-4-yl methanesulfonate (9b).



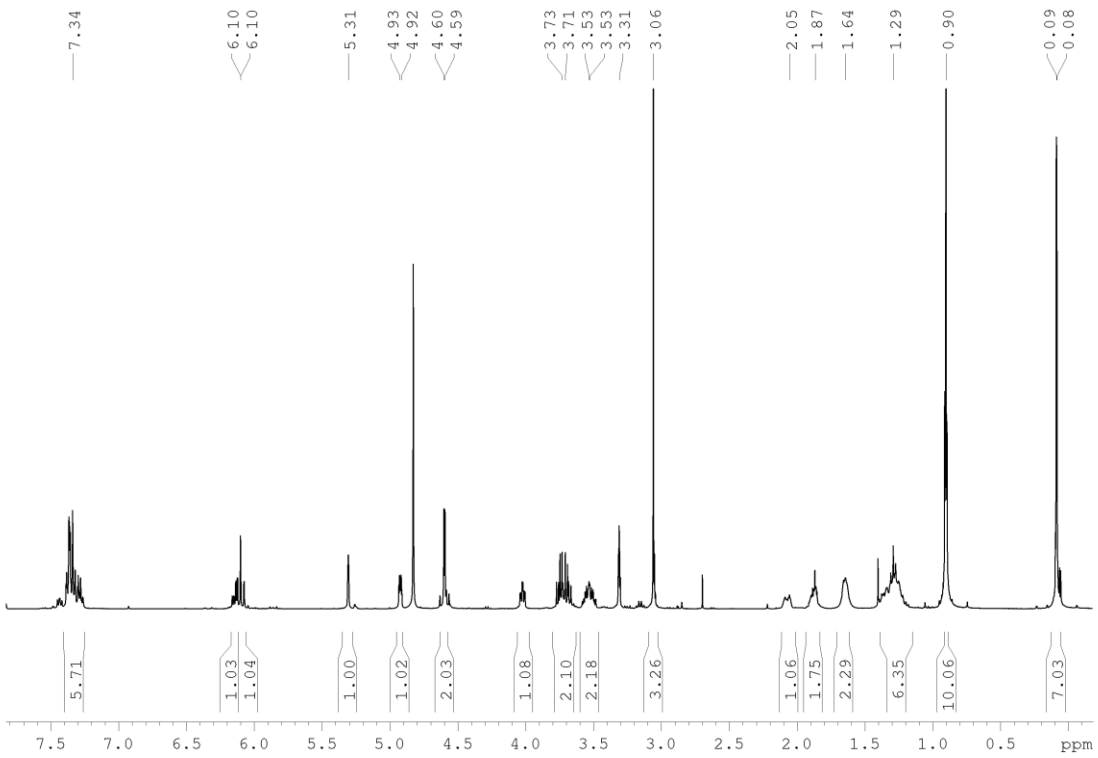


Figure 35. ^{1}H-NMR spectrum of compound 9b.

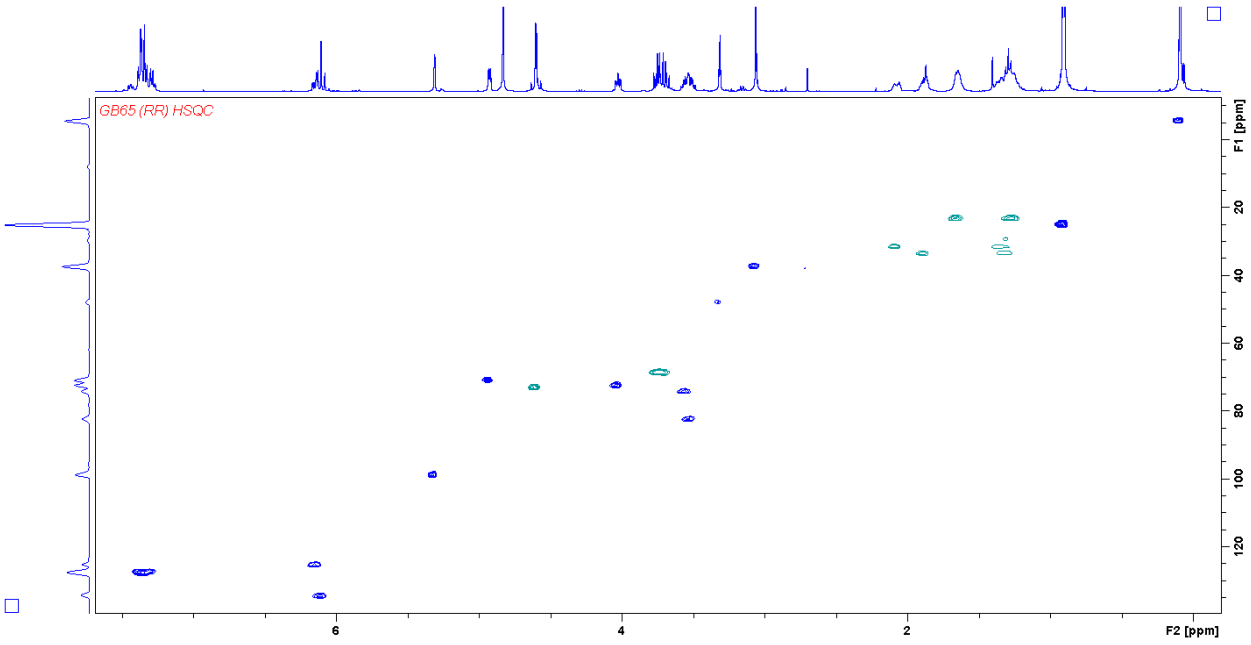


Figure 36. HSQC of compound 9b.

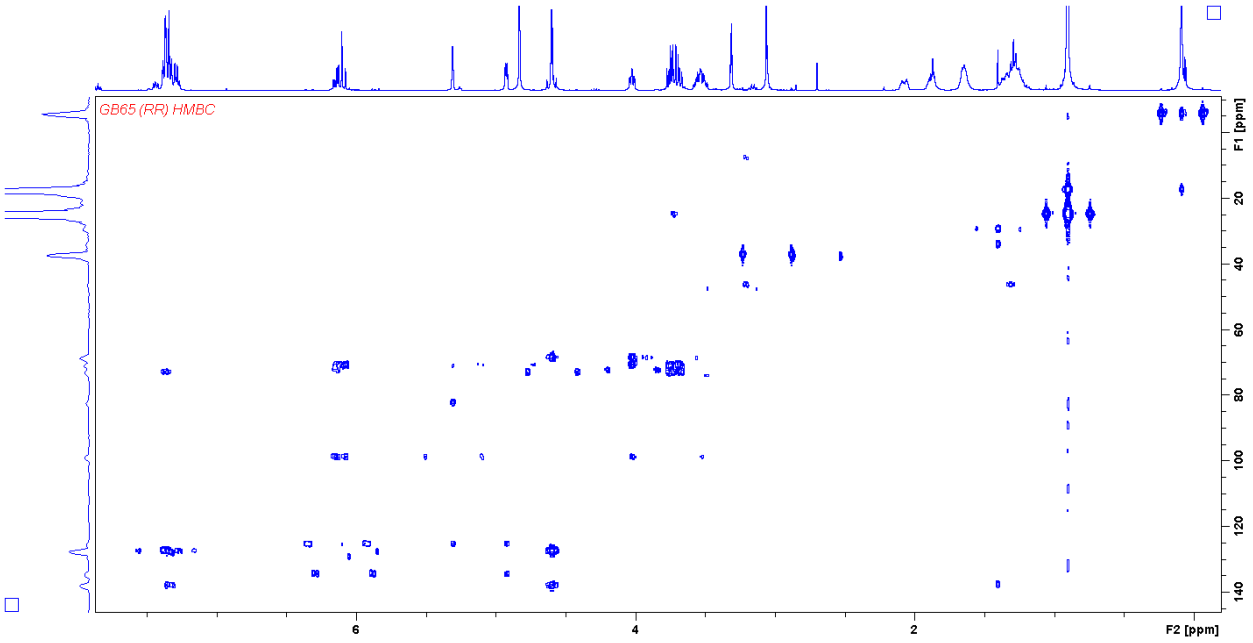


Figure 37. HMBC of compound 9b.

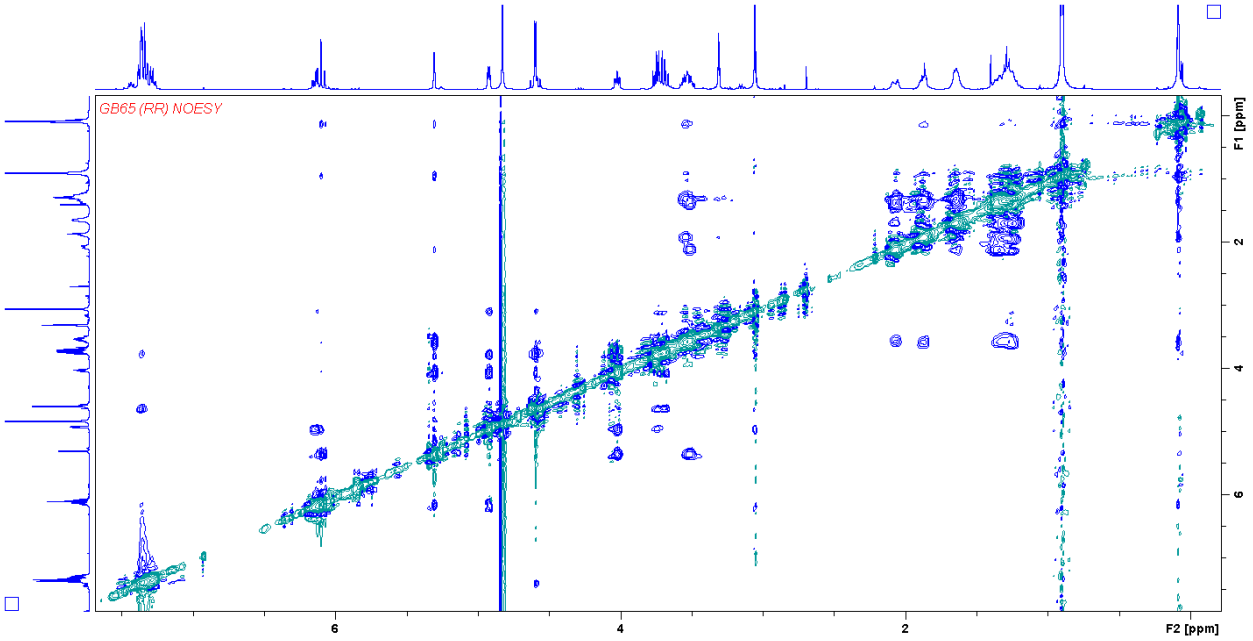


Figure 38. NOESY of compound 9b.

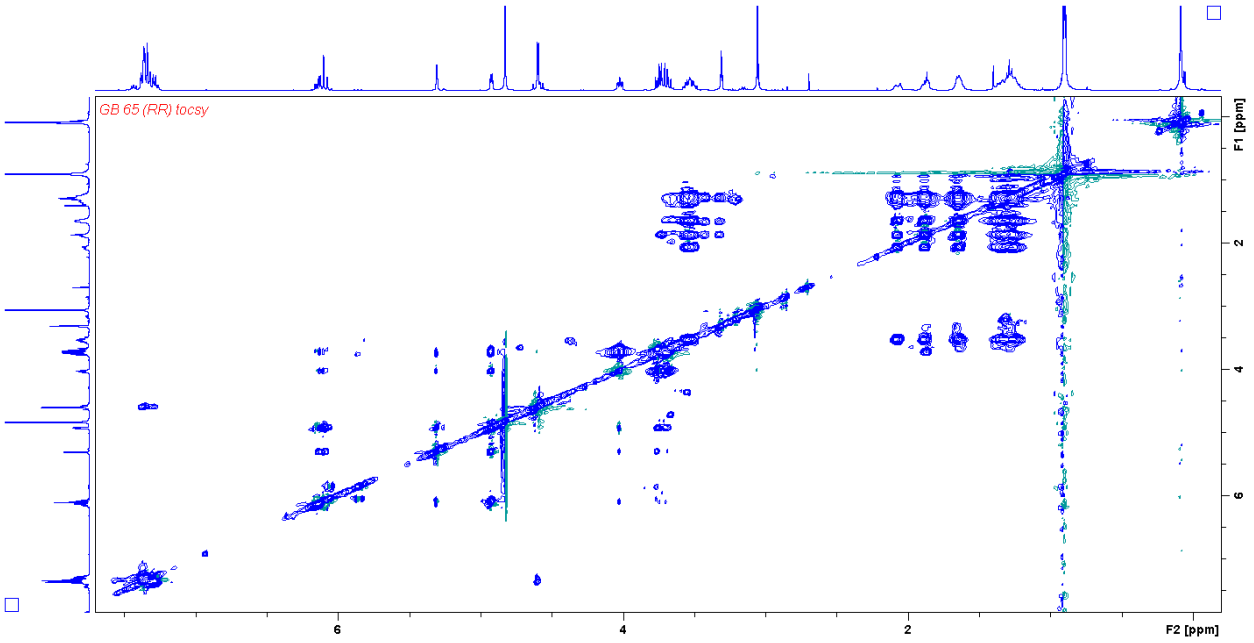
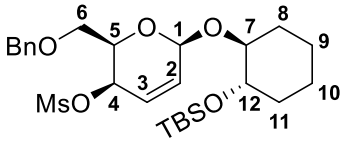


Figure 39. TOCSY of compound 9b.

(*1R,4R,5R*)-5-((benzyloxy)methyl)-1-(((*1S,2S*)-2-((tert-butyldimethylsilyl)oxy)cyclohexyl)oxy)-2,3-dihydro-2H-pyran-4-yl methanesulfonate (9a).



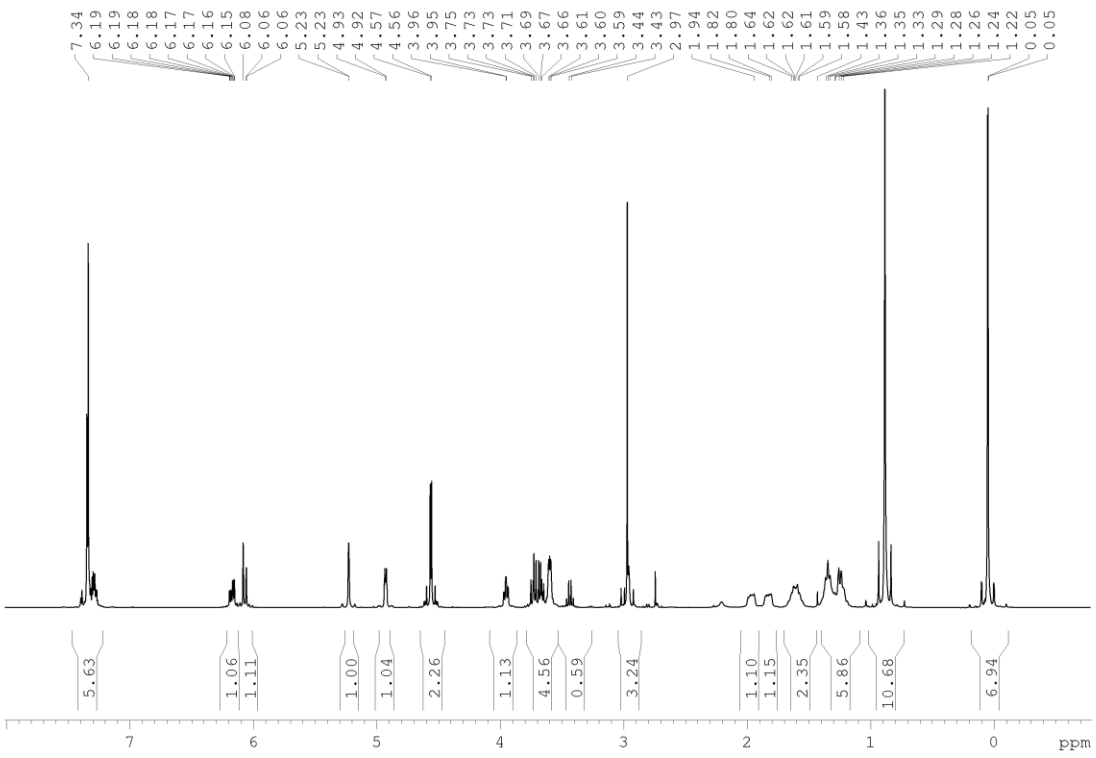


Figure 40. ^{1}H-NMR spectrum of compound 9a.

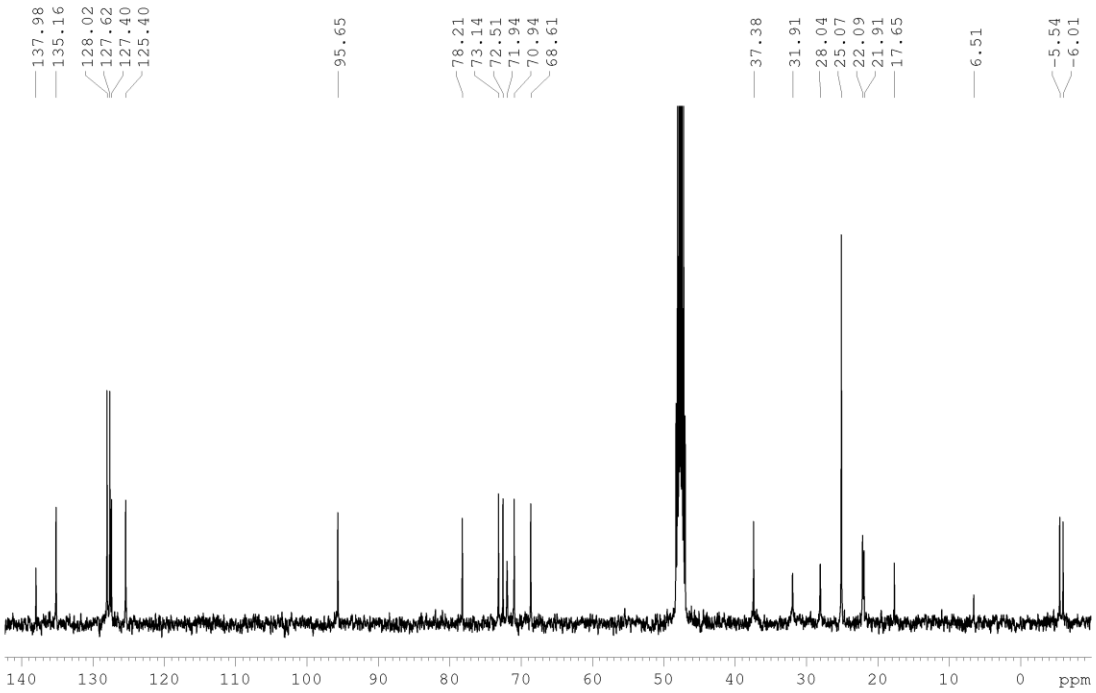


Figure 41. ^{13}C-NMR spectrum of compound 9a.

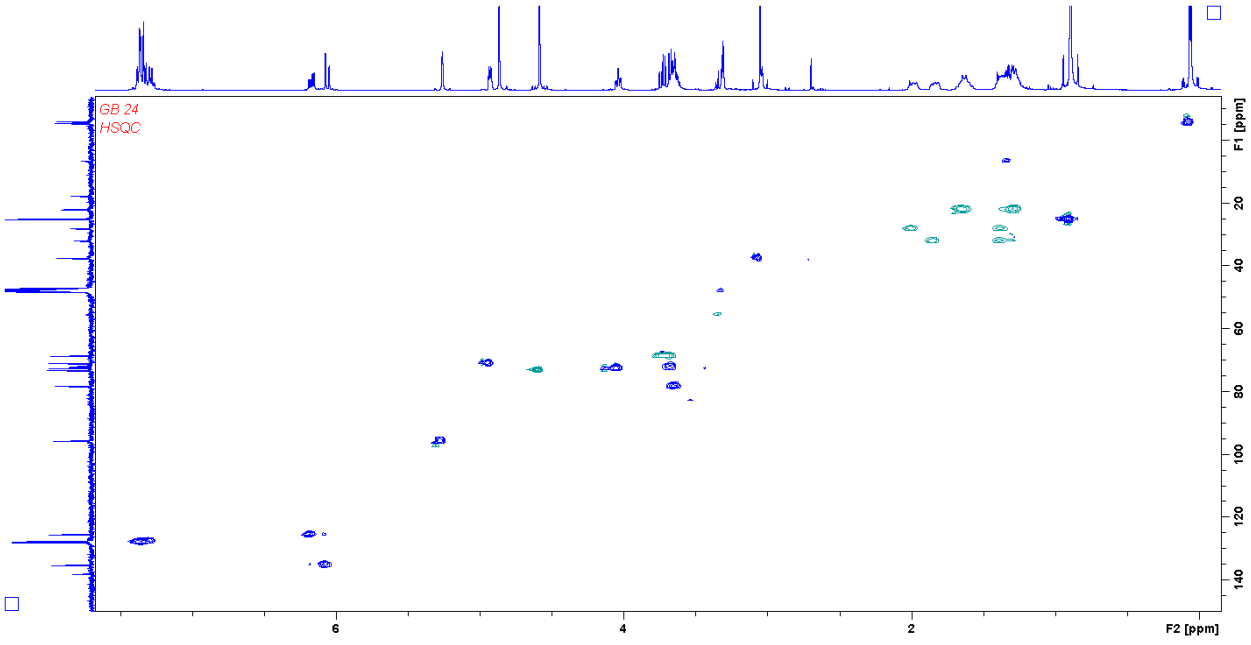


Figure 42. HSQC of compound 9a.

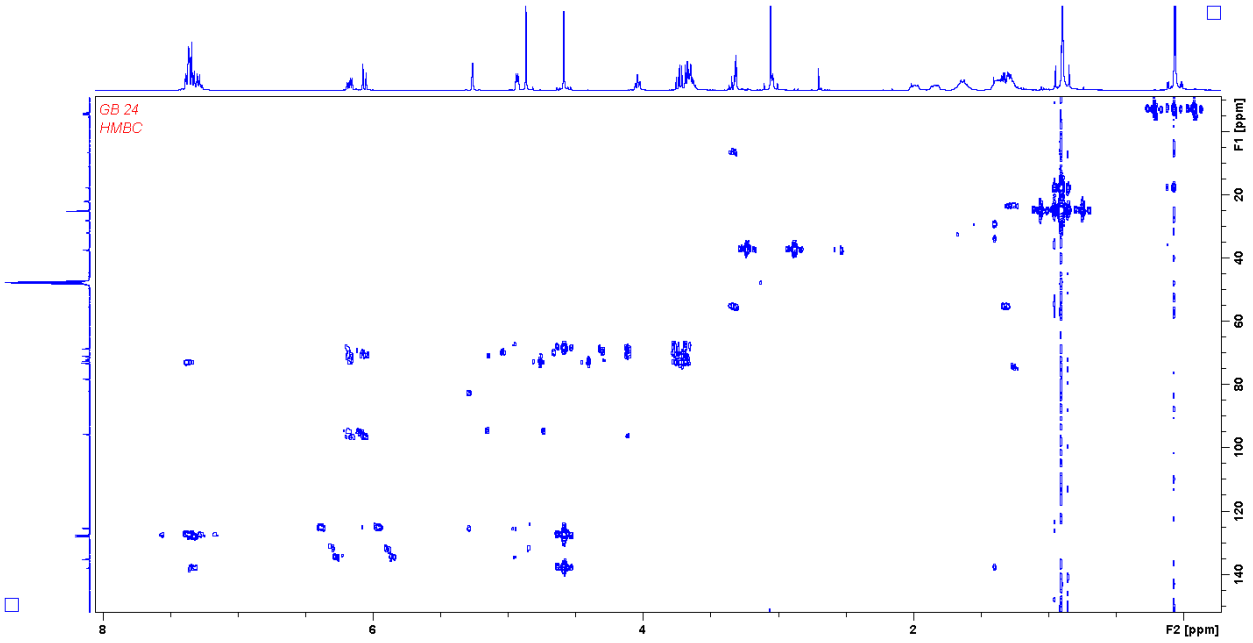


Figure 43. HMBC of compound 9a.

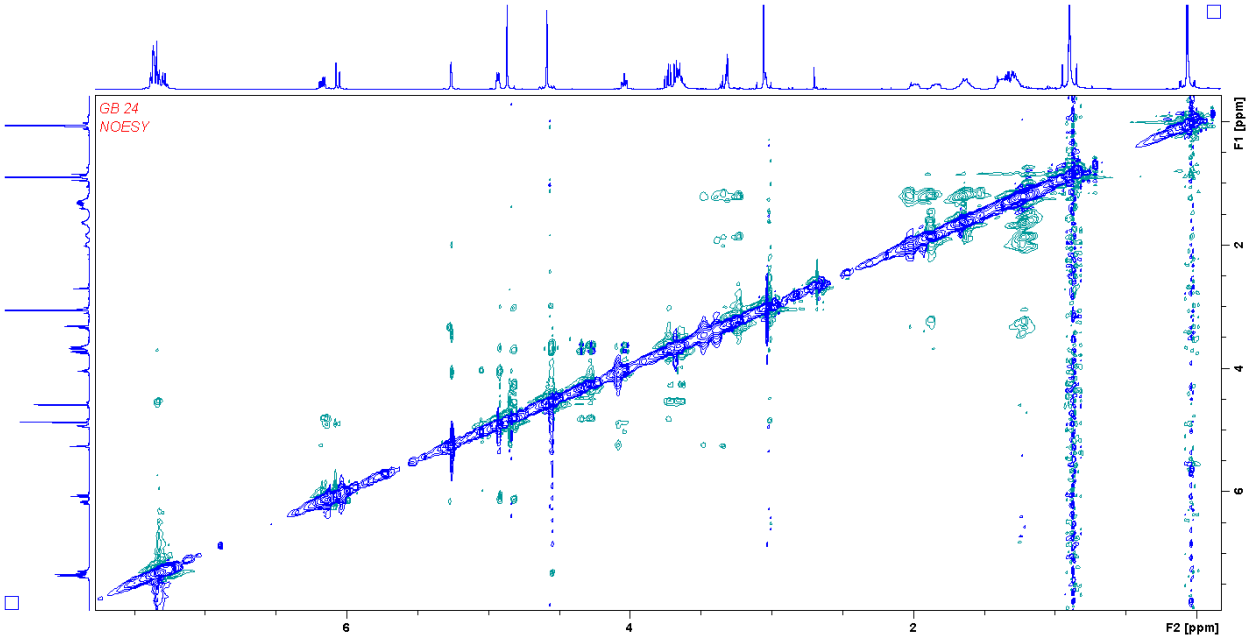


Figure 44. NOESY of compound 9a.

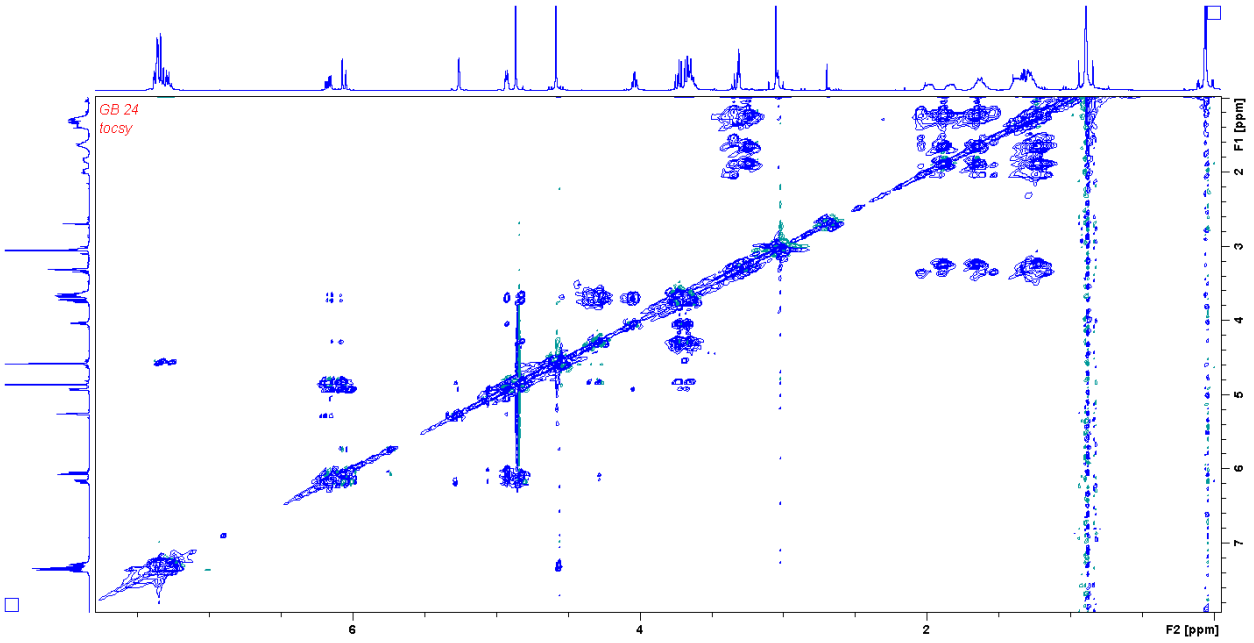
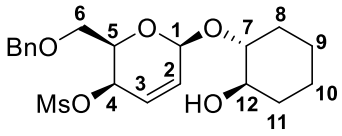


Figure 45. TOCSY of compound 9a.

(*1R,4R,5R*)-5-((benzyloxy)methyl)-1-(((*1R,2R*)-2-hydroxycyclohexyl)oxy)-2,3-dihydro-2H-pyran-4-yl methanesulfonate (10b).



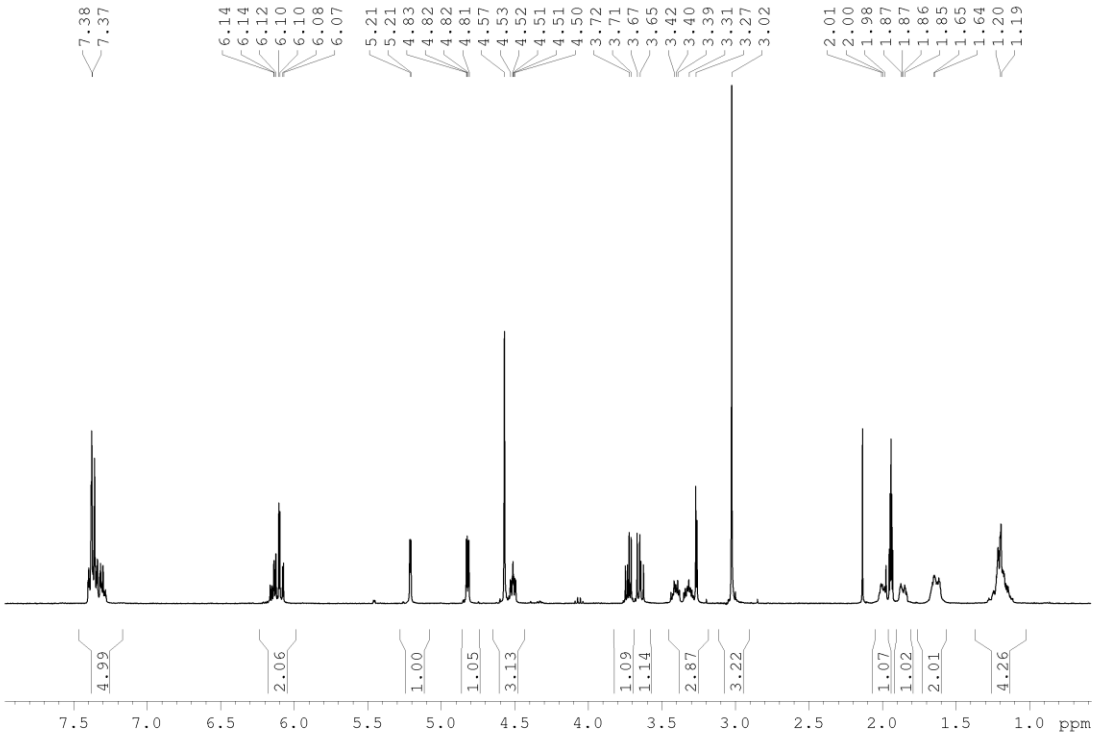


Figure 46. ^{1}H-NMR spectrum of compound 10b.

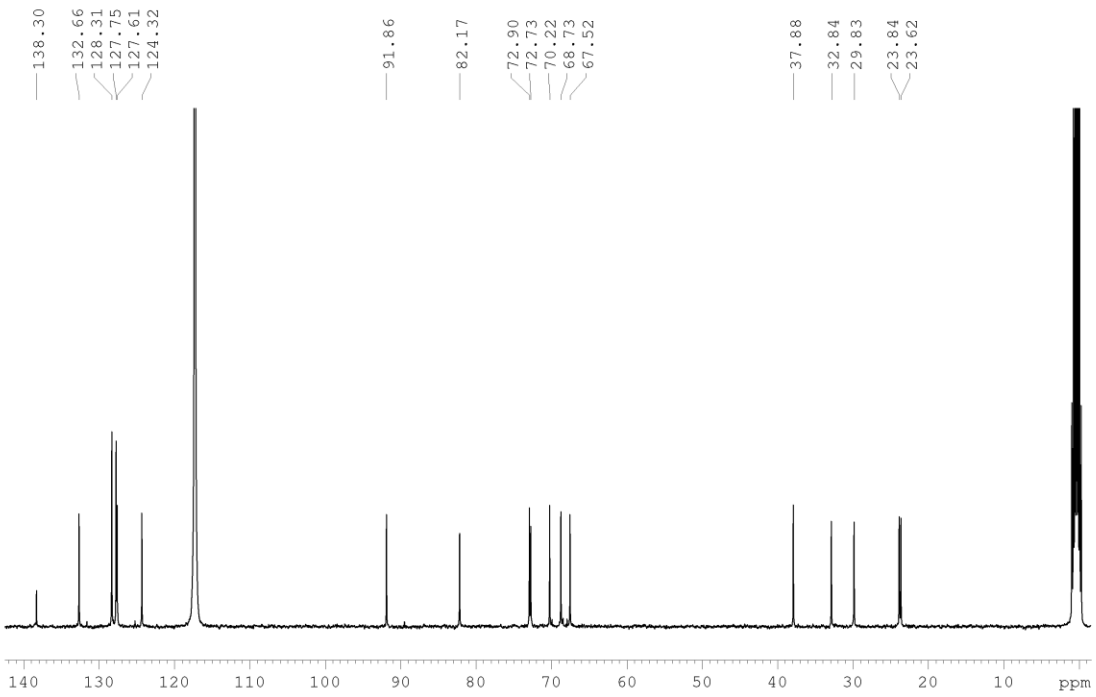


Figure 47. ^{13}C-NMR spectrum of compound 10b.

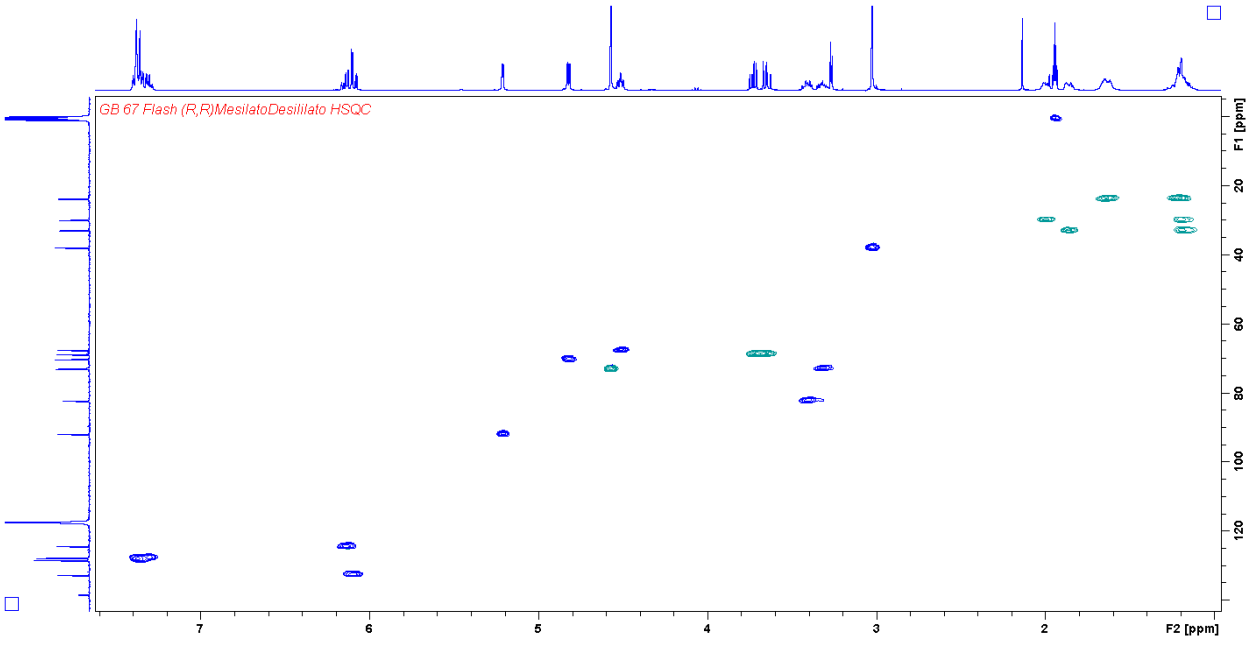


Figure 48. HSQC of compound 10b.

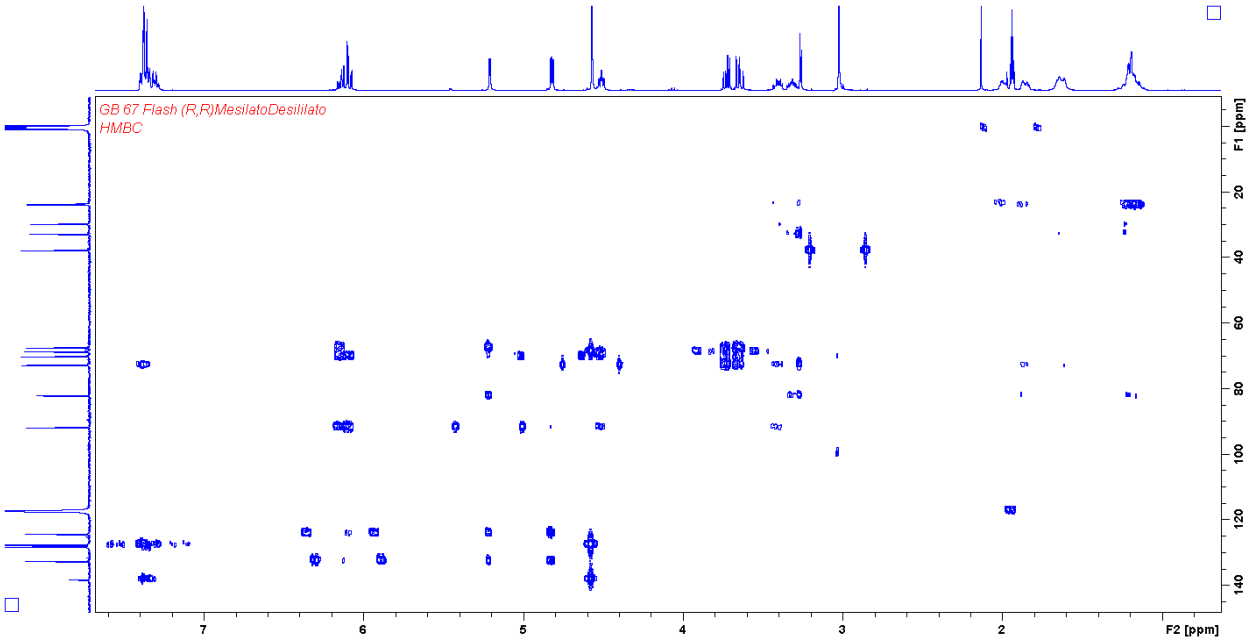


Figure 49. HMBC of compound 10b.

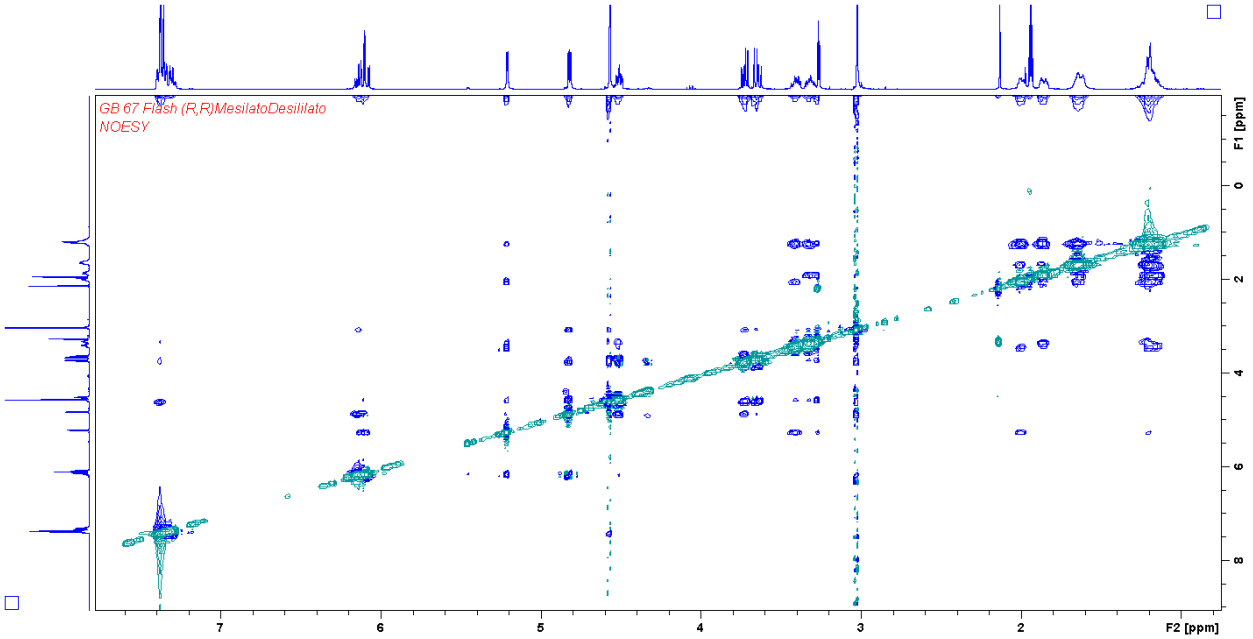


Figure 50. NOESY of compound 10b.

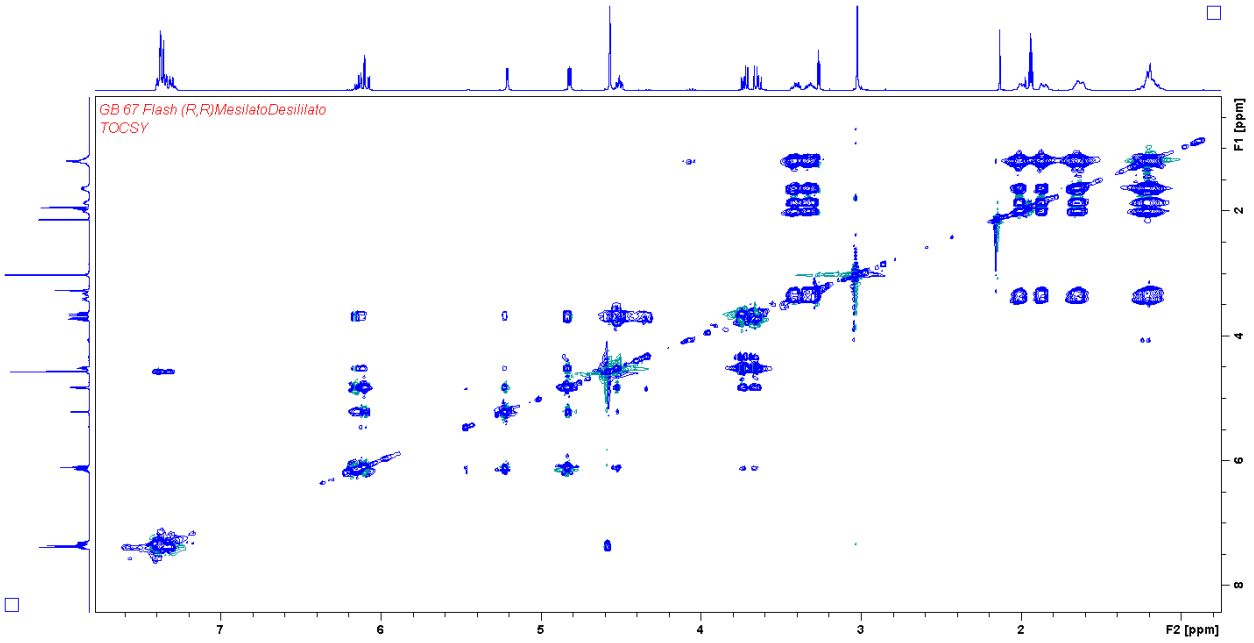
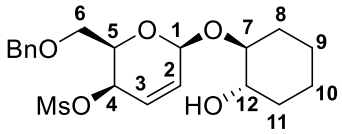


Figure 51. TOCSY of compound 10b.

(1*R,4R,5R*)-5-((benzyloxy)methyl)-1-(((*1S,2S*)-2-hydroxycyclohexyl)oxy)-2,3-dihydro-2H-pyran-4-yl methanesulfonate (10a).



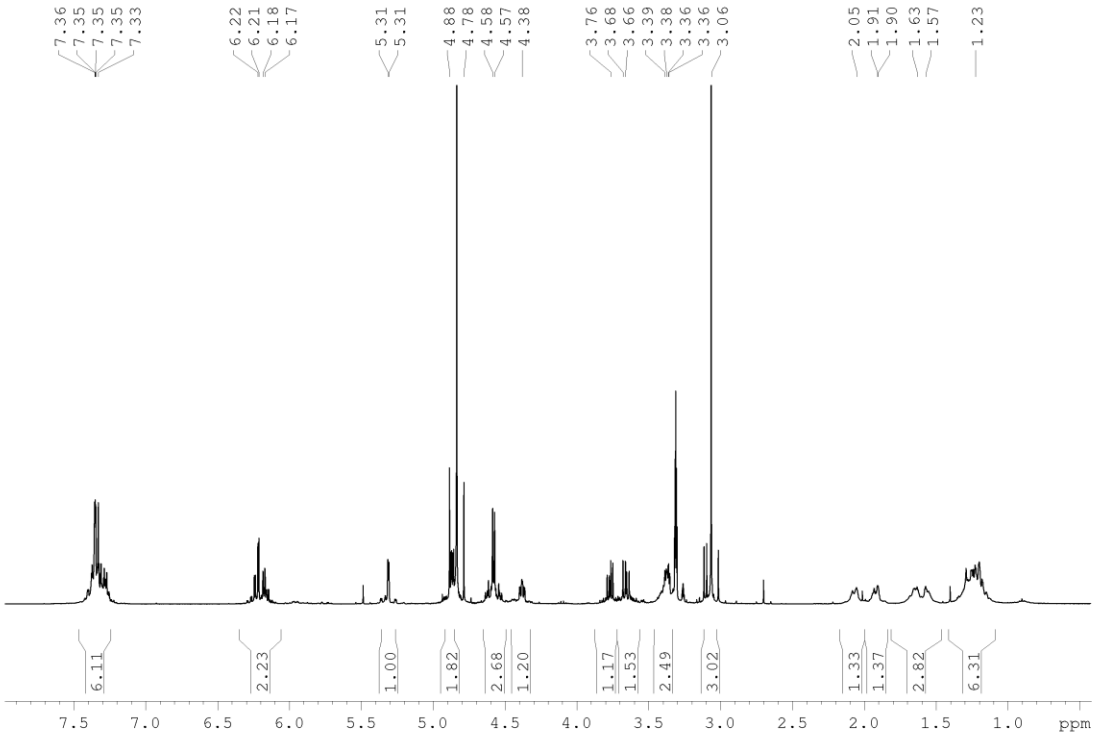


Figure 52. ^{1}H-NMR spectrum of compound 10a.

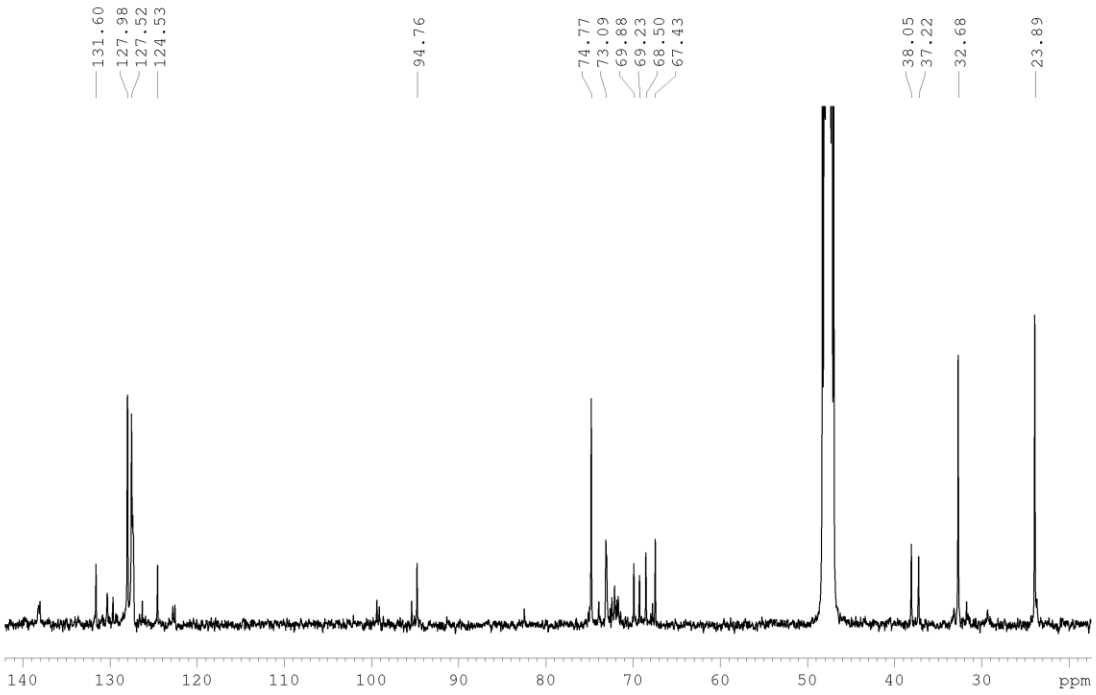


Figure 53. ^{13}C-NMR spectrum of compound 10a.

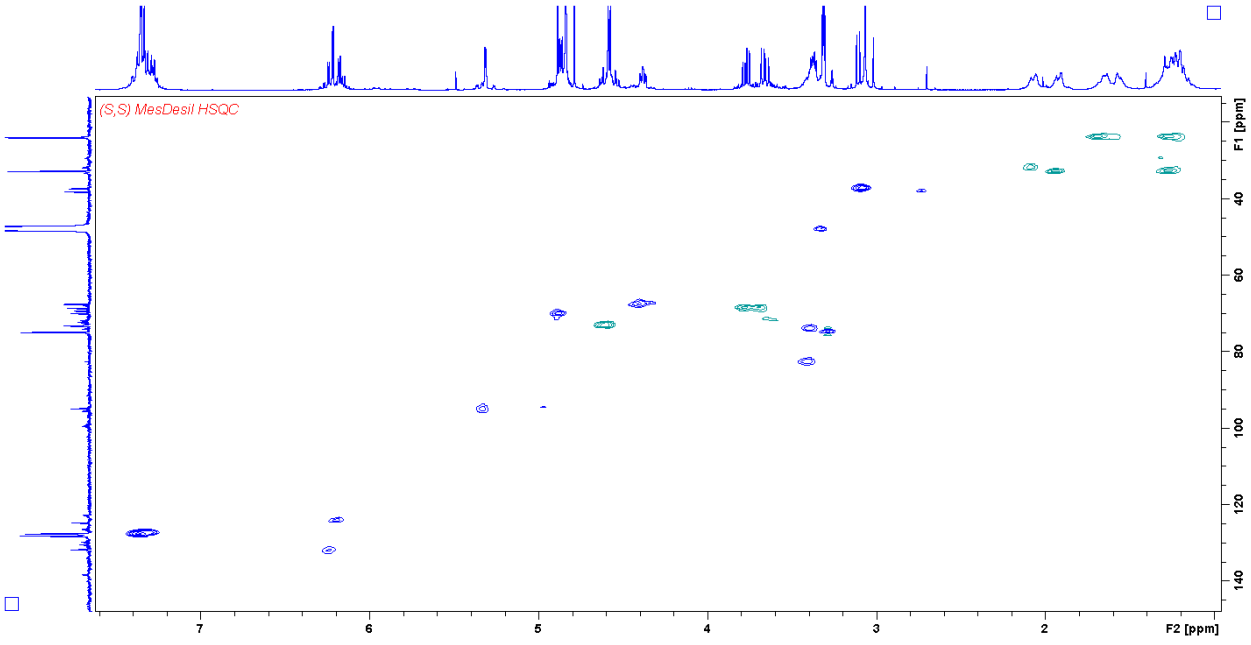


Figure 54. HSQC of compound 10a.

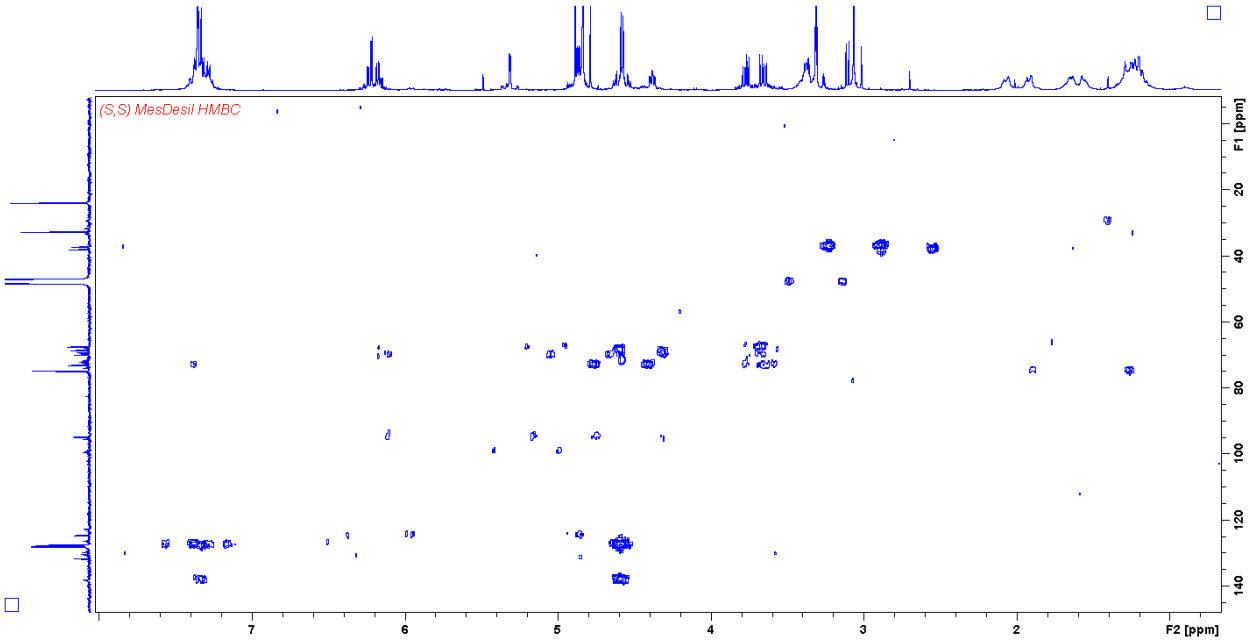


Figure 55. HMBC of compound 10a.

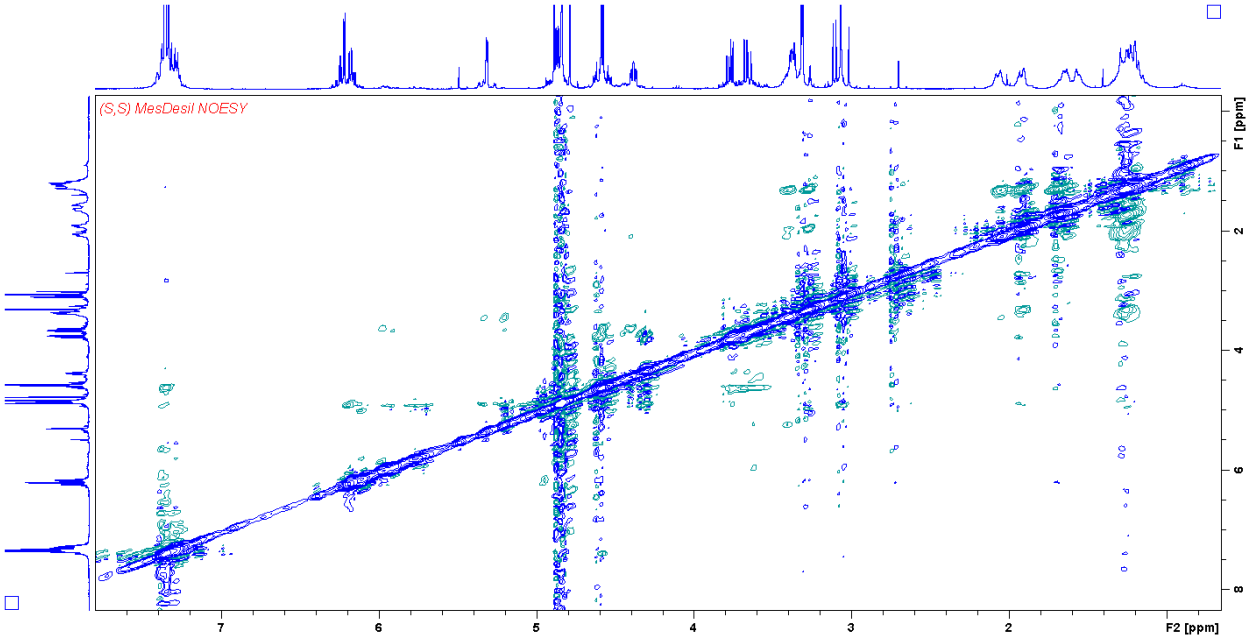


Figure 56. NOESY of compound 10a.

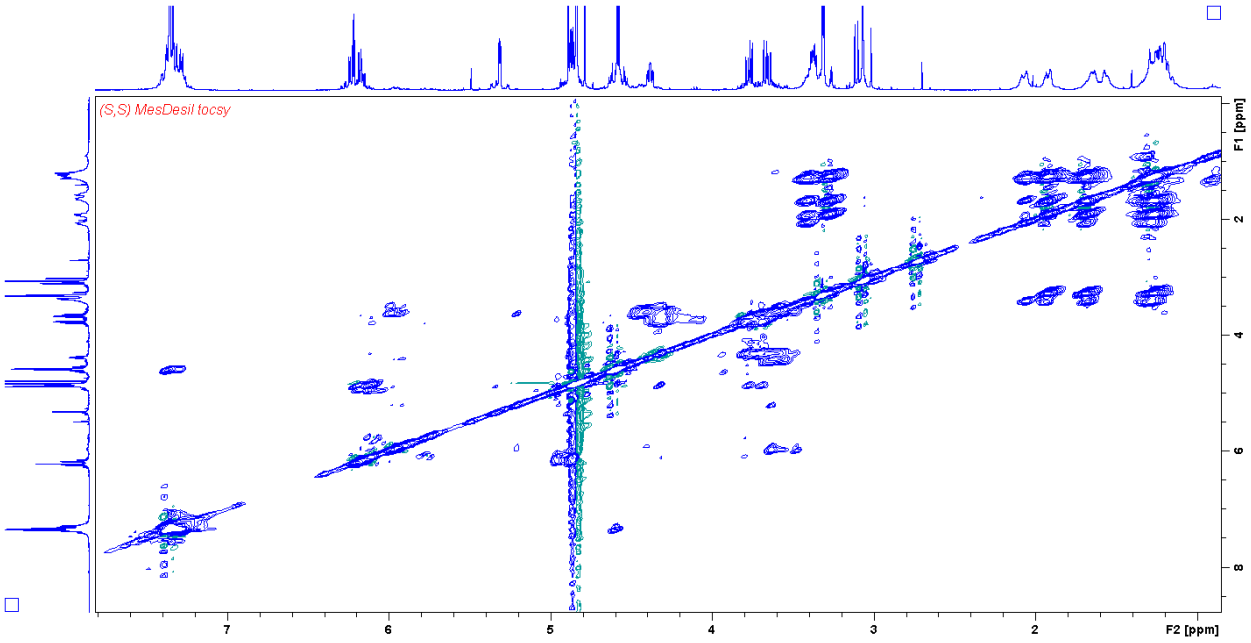
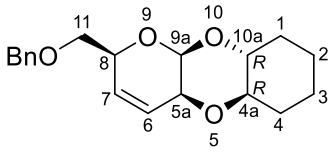


Figure 57. TOCSY of compound 10a.

(*4aR,5aS,8R,9aS,10aR*)-8-((benzyloxy)methyl)-1,2,3,4,4a,5a,9a,10a-octahydro-2H-benzo[b]pyrano[2,3-e][1,4]dioxine (11).



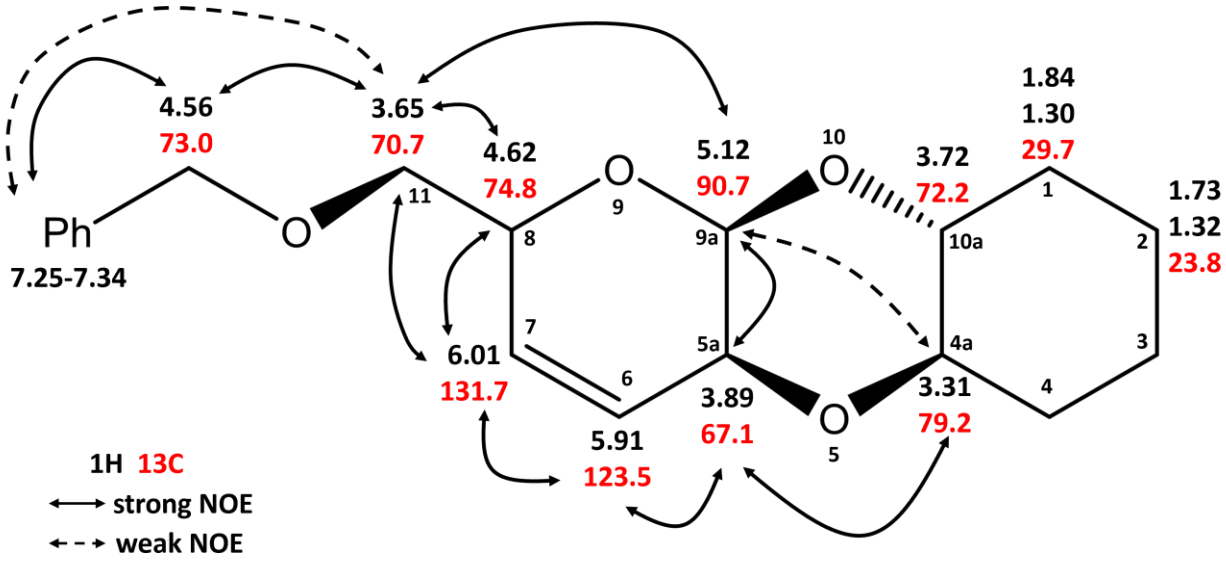


Figure 58. NMR detailed assignment of compound 11 with the NOE correlations.

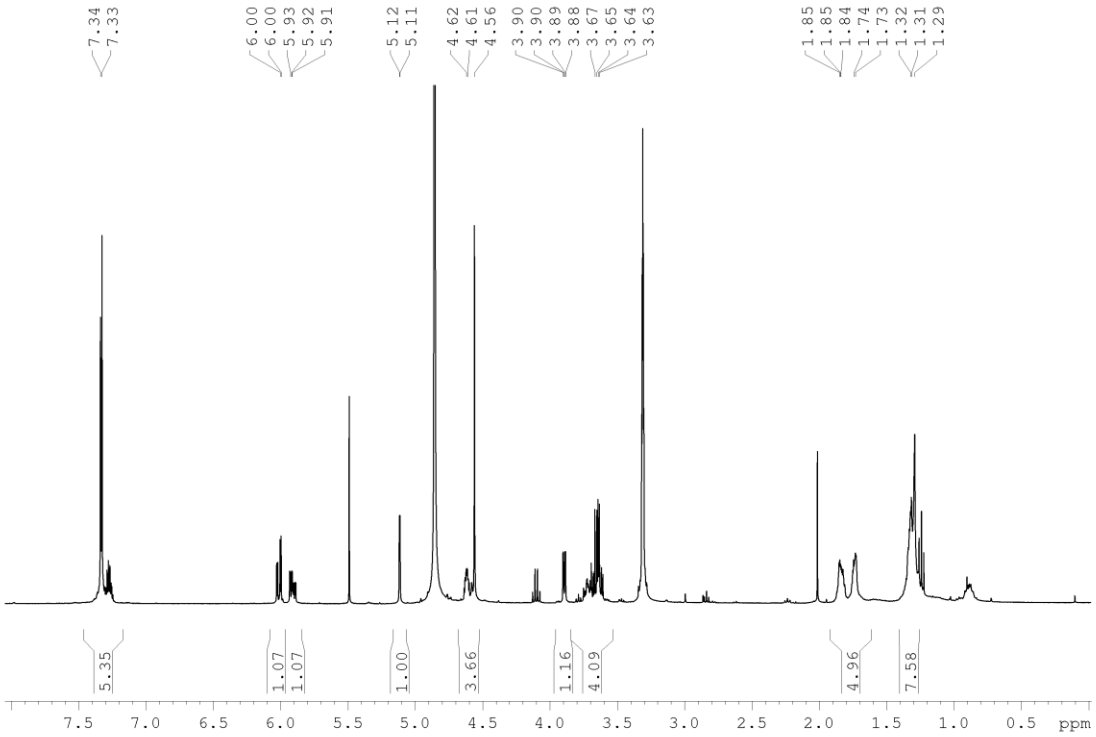


Figure 59. ^{1}H-NMR spectrum of compound 11.

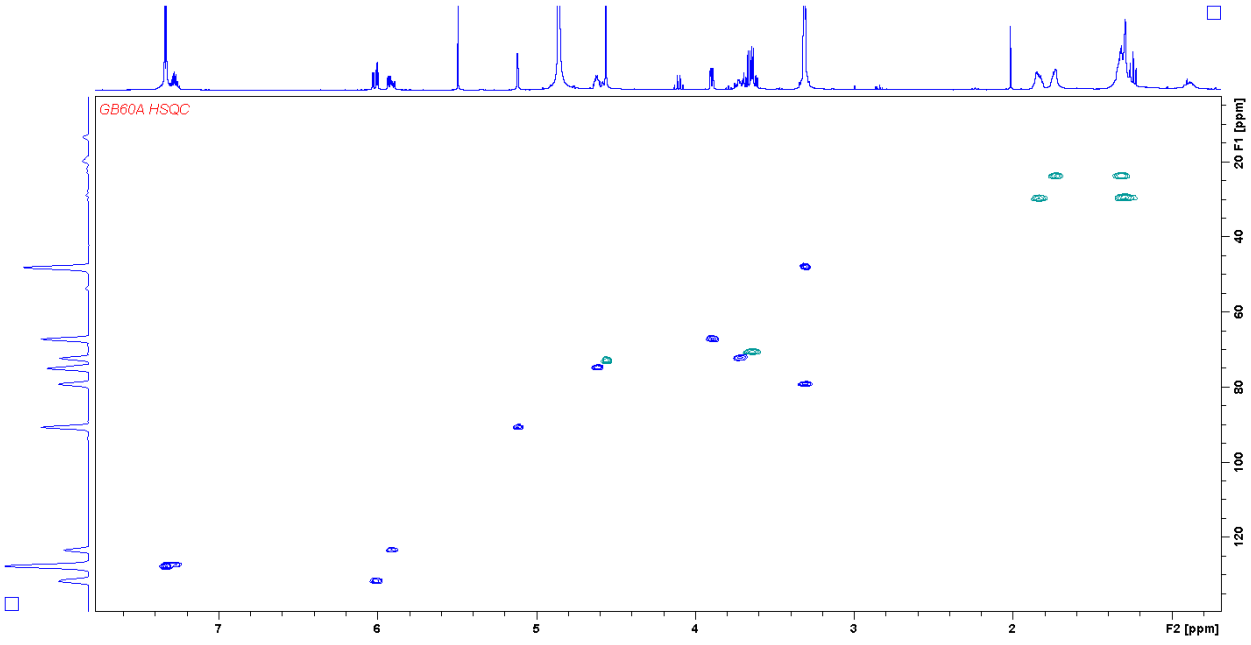


Figure 60. HSQC of compound 11.

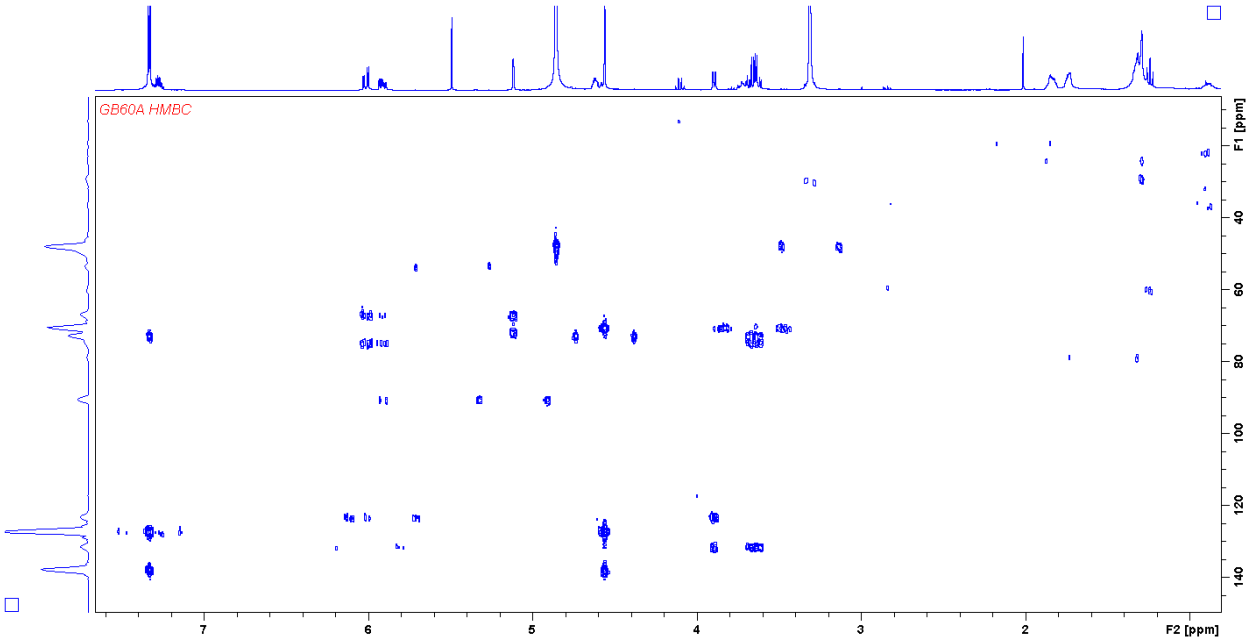


Figure 61. HMBC of compound 11.

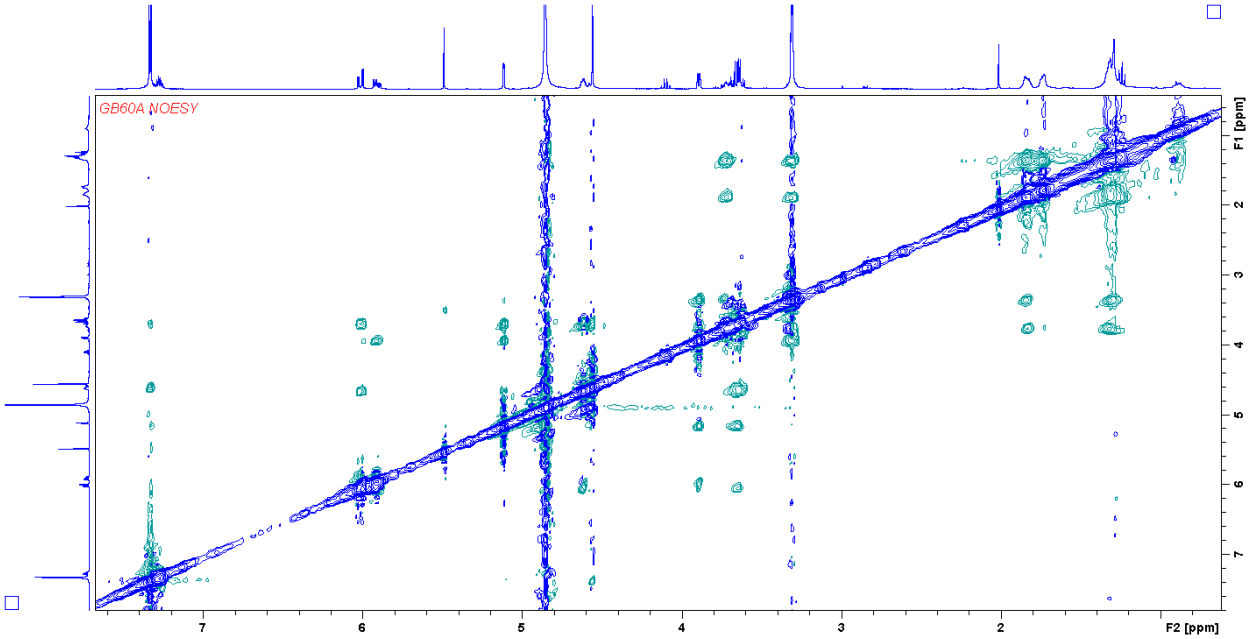


Figure 62. NOESY of compound 11.

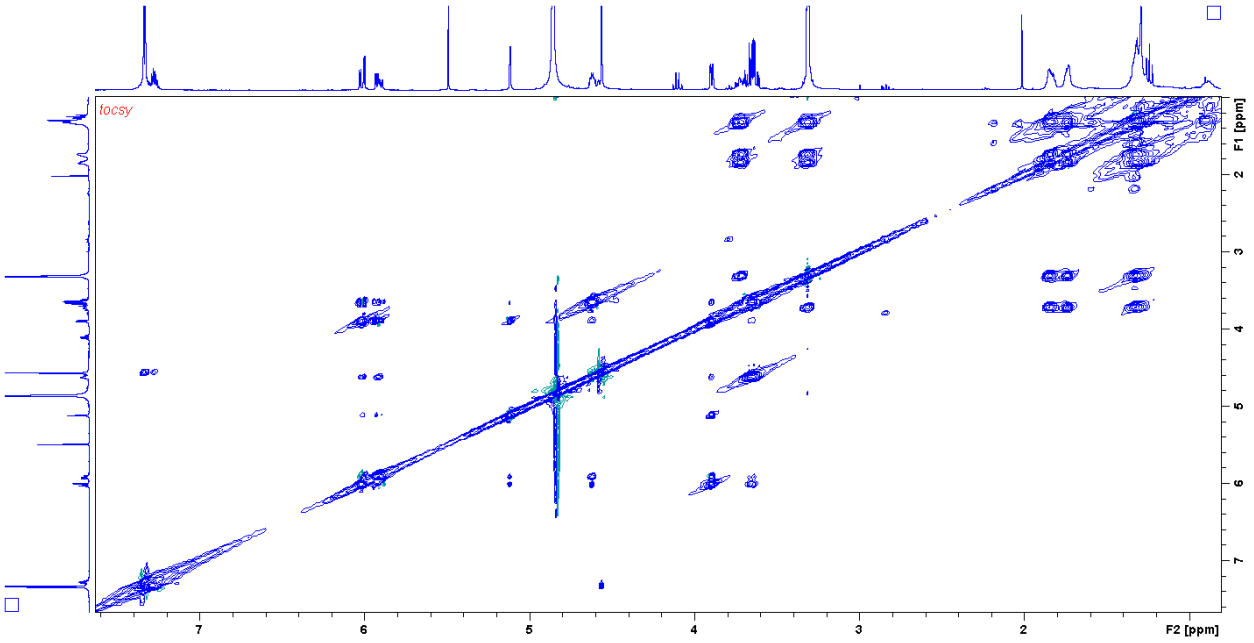


Figure 63. TOCSY of compound 11.

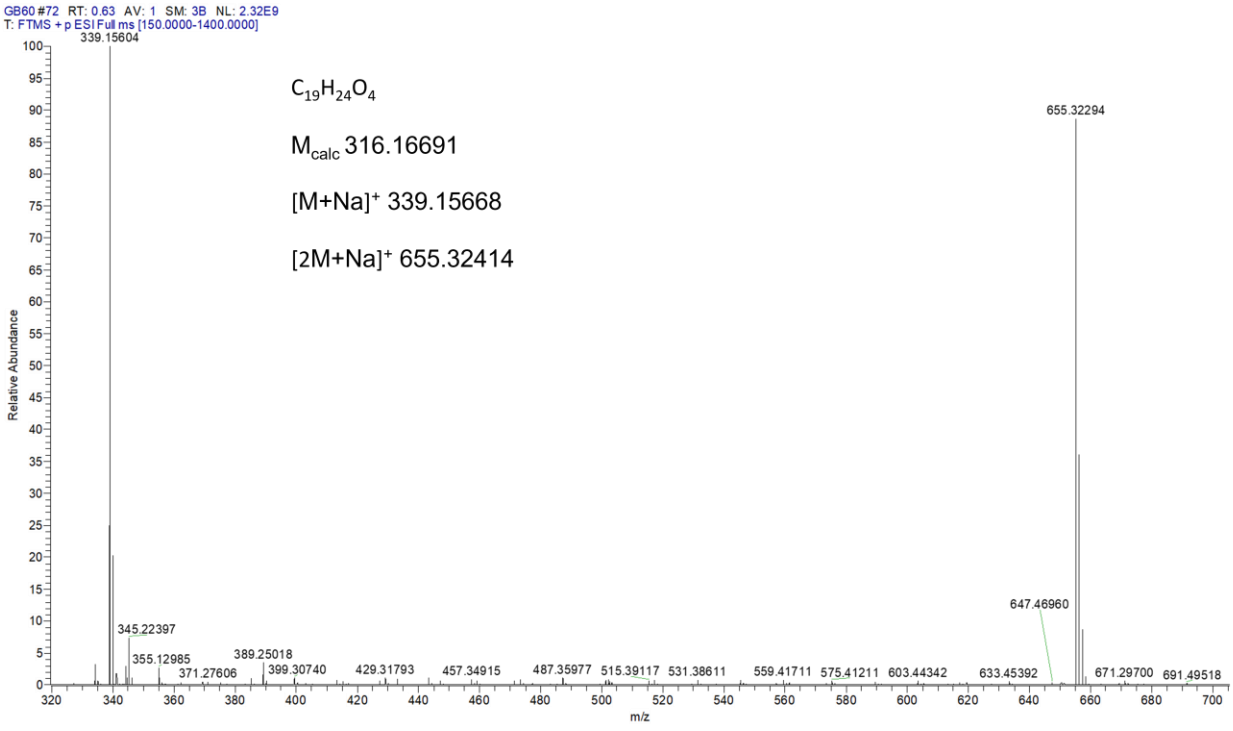


Figure 64. HRMS (ESI) of compound 11.

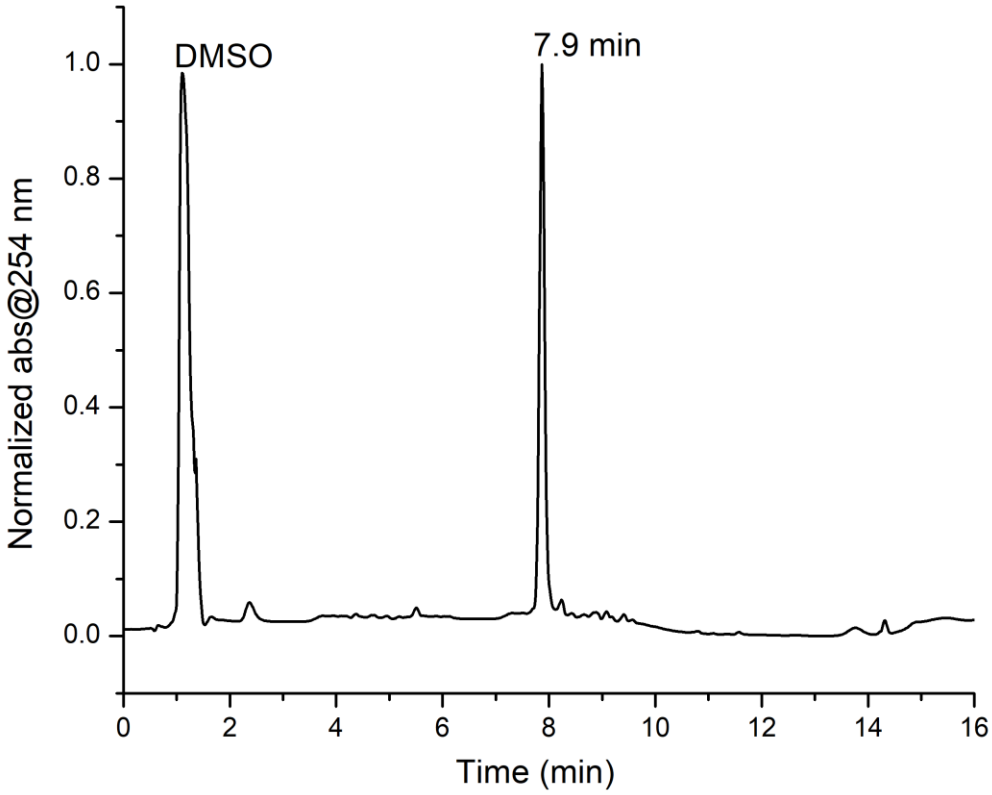


Figure 65. HPLC chromatogram at 254 nm of tricycle 11.

Cartesian Coordinates and Thermochemical data of the optimized structures

Bicycle 6 TS-trans-6311

CARTESIAN COORDINATES

C	0.169586	-0.760722	-0.732865
C	-0.506659	0.479580	-0.914832
C	0.253143	1.718910	-0.508840
O	1.089370	1.470563	0.602691
C	2.033106	0.498775	0.222630

C	1.374067	-0.811635	-0.092536
C	-0.590478	2.933172	-0.204907
O	2.975258	0.410731	1.241202
C	3.945104	-0.605721	0.968430
O	-1.866432	0.581181	0.185107
S	-2.972430	-0.469380	0.073916
O	-4.202041	0.087433	0.587319
C	-2.456586	-1.722843	1.219030
O	-2.993283	-1.063340	-1.245544
H	1.699327	-1.700344	0.410703
H	-0.336265	-1.659053	-1.045831
H	0.891045	1.938546	-1.377129
H	-1.111615	0.607613	-1.799936
H	2.504449	0.855043	-0.698347
H	3.616014	-1.545009	1.417676
H	0.051421	3.803416	-0.109407
H	-1.308156	3.103635	-1.001843
H	-1.137705	2.785708	0.716931
H	-2.411408	-1.274016	2.202552
H	-3.190619	-2.518557	1.188277
H	-1.478973	-2.072030	0.913483

C	4.187548	-0.823952	-0.524337
H	4.561031	0.141989	-0.925521
O	3.102682	-1.311139	-1.189973
H	4.856709	-0.285727	1.469622
H	5.056196	-1.507935	-0.580935

Electronic Energy = -1203.00380304 (Hartree/Particle)

Dipole Moment (Debye): 2.4624

index 1

Number of imaginary frequencies= 1

Negatives Eigenvalues: -389.014

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.245408 (Hartree/Particle)

Thermal correction to Energy= 0.261223

Thermal correction to Enthalpy= 0.262168

Thermal correction to Gibbs Free Energy= 0.201980

Sum of electronic and zero-point Energies= -1202.758395

Sum of electronic and thermal Energies= -1202.742580

Sum of electronic and thermal Enthalpies= -1202.741636

Sum of electronic and thermal Free Energies= -1202.801823

Bicycle 6 TS-cis-6311

CARTESIAN COORDINATES

C	-0.064394	0.115425	1.590830
C	0.619231	1.119305	0.778642
C	-0.356947	2.088454	0.139728
O	-1.456002	1.411025	-0.427346
C	-2.207887	0.718019	0.547190
C	-1.353572	-0.232077	1.335201
C	0.234383	2.971872	-0.932748
O	-3.348167	0.205316	-0.049603
C	-3.148744	-0.799849	-1.044672
C	-2.630112	-2.077697	-0.429229
O	1.429658	0.585034	-0.409059
S	2.522636	-0.508233	-0.146568
O	3.491874	-0.367622	-1.204177
C	1.644173	-2.016551	-0.388319
O	2.977434	-0.426243	1.221108
H	-1.896030	-0.832477	2.045410

H	0.519205	-0.430393	2.312104
H	-0.718903	2.712212	0.967465
H	1.368543	1.664639	1.342890
H	-2.594869	1.458894	1.261098
H	-4.128364	-0.930171	-1.503377
H	-2.442005	-0.435828	-1.788581
H	-3.393288	-2.418403	0.302777
H	-2.623442	-2.848748	-1.225945
H	-0.498540	3.708784	-1.247288
H	1.116501	3.483802	-0.558099
H	0.525993	2.372070	-1.786477
H	1.468535	-2.113201	-1.451664
H	2.283172	-2.813033	-0.025643
H	0.688246	-1.975425	0.127706
O	-1.401510	-1.881561	0.118197

Electronic Energy = -1203.02600050 (Hartree/Particle)

Dipole Moment (Debye): 2.6005

index 1

Number of imaginary frequencies= 1

Negatives Eigenvalues: -170.399

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.245806 (Hartree/Particle)

Thermal correction to Energy= 0.261245

Thermal correction to Enthalpy= 0.262190

Thermal correction to Gibbs Free Energy= 0.203359

Sum of electronic and zero-point Energies= -1202.780195

Sum of electronic and thermal Energies= -1202.764755

Sum of electronic and thermal Enthalpies= -1202.763811

Sum of electronic and thermal Free Energies= -1202.822642

10b

CARTESIAN COORDINATES

C	-1.126550	0.670521	-1.697048
C	-1.871960	1.208934	-0.536349
C	-1.069797	2.242358	0.238970
O	0.267238	1.823732	0.389338
C	0.938769	1.759634	-0.861498

C	0.208223	0.829039	-1.794607
C	-1.620836	2.565398	1.609661
O	2.283908	1.555464	-0.677503
C	2.753426	0.452351	0.121048
C	4.169886	0.821660	0.524410
O	-2.162919	0.092626	0.457680
S	-3.377034	-0.904965	0.164381
O	-4.276057	-0.343394	-0.824324
C	-4.166587	-0.947940	1.752571
O	-2.763114	-2.214507	-0.078451
H	0.755350	0.488334	-2.660882
H	-1.689841	0.133446	-2.453681
H	-1.094116	3.147973	-0.388702
H	-2.852792	1.599073	-0.804408
H	0.884155	2.761715	-1.320434
H	2.113761	0.371594	1.007298
H	4.157377	1.764474	1.077265
H	-1.057695	3.389650	2.045739
H	-2.671747	2.855557	1.544159
H	-1.533016	1.700145	2.265440
H	-4.561121	0.042183	1.965786

H	-4.970419	-1.678936	1.687445
H	-3.433235	-1.248852	2.496397
C	2.672702	-0.862849	-0.646390
H	3.296398	-0.727740	-1.556035
C	4.813045	-0.292188	1.344773
H	5.842372	-0.022844	1.597627
H	4.275401	-0.401314	2.294588
C	3.337341	-1.961552	0.195546
H	3.291083	-2.897057	-0.368890
H	2.728598	-2.105833	1.098990
C	4.769657	-1.618702	0.591404
H	5.387419	-1.539269	-0.310883
H	5.205310	-2.417185	1.199693
O	1.376931	-1.153990	-0.963012
H	4.753404	0.994176	-0.386625
Na	-0.495082	-1.728116	-0.376796

Electronic Energy = -1521.49352247 (Hartree/Particle)

Dipole Moment (Debye): 7.3903

index 0

Harmonic frequencies

Number of imaginary frequencies= 0

THERMOCHEMICAL DATA 6-31+g(D)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.344067 (Hartree/Particle)

Thermal correction to Energy= 0.365444

Thermal correction to Enthalpy= 0.366388

Thermal correction to Gibbs Free Energy= 0.293107

Sum of electronic and zero-point Energies= -1521.149455

Sum of electronic and thermal Energies= -1521.128079

Sum of electronic and thermal Enthalpies= -1521.127135

Sum of electronic and thermal Free Energies= -1521.200415

SP 6-311++G(2D,2P) Electronic Energy= -1521.82128101

Corrected Free Energy = -1521.200415+1521.49352247-1521.82128101= -1521.52817354

TS-CIS-01 10b

CARTESIAN COORDINATES

C	-0.994036	0.659685	-1.716722
C	-1.787268	1.200353	-0.618339

C	-1.050480	2.232413	0.215503
O	0.288034	1.841476	0.428586
C	1.011667	1.774470	-0.789347
C	0.368424	0.783636	-1.724057
C	-1.672225	2.537033	1.560047
O	2.356696	1.628804	-0.532728
C	2.799251	0.479116	0.201417
C	4.248921	0.738440	0.562728
O	-2.148285	0.053808	0.433482
S	-3.390730	-0.886048	0.155990
O	-4.282342	-0.304265	-0.830760
C	-4.189945	-0.904394	1.741943
O	-2.835638	-2.225853	-0.088673
H	0.929562	0.549013	-2.617118
H	-1.514157	0.161229	-2.527550
H	-1.060355	3.145033	-0.403200
H	-2.774692	1.548713	-0.911480
H	0.939643	2.758878	-1.280330
H	2.188865	0.390045	1.107940
H	4.319684	1.651201	1.159247
H	-1.158562	3.381490	2.018546

H	-2.728566	2.789709	1.445737
H	-1.584912	1.675577	2.220309
H	-4.537988	0.102109	1.960030
H	-5.027751	-1.595454	1.669700
H	-3.475665	-1.243201	2.487971
C	2.615551	-0.785241	-0.622649
H	3.206089	-0.646234	-1.551074
C	4.840229	-0.456308	1.305768
H	5.893789	-0.271517	1.531908
H	4.329373	-0.574465	2.268904
C	3.217738	-1.972842	0.133048
H	3.096107	-2.872194	-0.477259
H	2.630349	-2.124782	1.048394
C	4.681734	-1.740499	0.495168
H	5.274550	-1.661218	-0.423494
H	5.079529	-2.594016	1.051705
O	1.282118	-0.967155	-0.904110
H	4.809819	0.916230	-0.361301
Na	-0.582278	-1.709006	-0.402441

Electronic Energy = -1521.49283328 (Hartree/Particle)

Dipole Moment (Debye): 5.2228

index 1

Number of imaginary frequencies= 1

Negatives Eigenvalues: -151.257

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.343896 (Hartree/Particle)

Thermal correction to Energy= 0.364479

Thermal correction to Enthalpy= 0.365423

Thermal correction to Gibbs Free Energy= 0.294444

Sum of electronic and zero-point Energies= -1521.148937

Sum of electronic and thermal Energies= -1521.128355

Sum of electronic and thermal Enthalpies= -1521.127411

Sum of electronic and thermal Free Energies= -1521.198390

SP 6-311++G(2D,2P) Electronic Energy= -1521.82020776

Corrected Free Energy = -1521.198390+1521.49283328-1521.82020776= -1521.52576448

10a

CARTESIAN COORDINATES

C	1.294272	0.269716	1.653038
C	2.278334	1.124936	0.914800
C	1.571673	2.342886	0.335548
O	0.441026	1.910859	-0.395708
C	-0.567896	1.347683	0.400925
C	-0.015443	0.430586	1.460401
C	2.423989	3.178614	-0.591432
O	-1.359450	0.611592	-0.482026
C	-2.704535	0.353953	0.002908
C	-2.949477	-1.162503	-0.040670
O	2.896989	0.457610	-0.248444
S	3.221695	-1.106181	-0.180786
O	3.804536	-1.442038	1.104474
C	4.441254	-1.161000	-1.465611
O	2.050459	-1.856400	-0.636924
H	-0.753336	-0.172084	1.982497
H	1.677352	-0.448631	2.367764
H	1.253149	2.949381	1.195265
H	3.107462	1.416773	1.560897
H	-1.166194	2.153268	0.857264

H	-2.748416	0.648886	1.059379
H	1.864366	4.056990	-0.911086
H	3.333750	3.506959	-0.085391
H	2.698657	2.601942	-1.473458
H	5.294025	-0.561798	-1.158070
H	4.722304	-2.206021	-1.581194
H	3.995876	-0.779158	-2.380663
C	-3.695750	1.164955	-0.809001
H	-3.592114	0.882921	-1.862126
C	-4.389098	-1.404670	0.438293
H	-4.582204	-2.478793	0.388068
H	-4.438155	-1.128528	1.498941
C	-5.118205	0.881240	-0.329789
H	-5.835665	1.437418	-0.939677
H	-5.231580	1.246473	0.698177
C	-5.420144	-0.615548	-0.364062
H	-5.408032	-0.956591	-1.406440
H	-6.430208	-0.803106	0.012565
H	-2.949817	-1.416532	-1.135570
O	-2.010771	-1.843730	0.666623
H	-3.462792	2.232641	-0.741542

Na -0.215610 -1.608341 -0.431734

Electronic Energy = -1521.49565014 (Hartree/Particle)

Dipole Moment (Debye): 8.7844

index 0

Harmonic frequencies

Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.344328 (Hartree/Particle)

Thermal correction to Energy= 0.365622

Thermal correction to Enthalpy= 0.366567

Thermal correction to Gibbs Free Energy= 0.293915

Sum of electronic and zero-point Energies= -1521.151323

Sum of electronic and thermal Energies= -1521.130028

Sum of electronic and thermal Enthalpies= -1521.129083

Sum of electronic and thermal Free Energies= -1521.201735

SP 6-311++G(2D,2P) Electronic Energy= -1521.82319624

Corrected Free Energy = -1521.201735+1521.49565014-1521.82319624= -1521.52928110

TS-CIS-03 10a

CARTESIAN COORDINATES

C	0.757486	0.071355	1.688257
C	1.645472	0.954623	0.948072
C	0.949120	2.158287	0.341886
O	-0.304770	1.796167	-0.193645
C	-1.187821	1.326876	0.811268
C	-0.600146	0.127835	1.505452
C	1.728426	2.883120	-0.732553
O	-2.460070	1.199402	0.299275
C	-2.665086	0.329659	-0.828238
C	-2.487532	-1.125182	-0.406344
O	2.266523	0.196586	-0.333536
S	3.541949	-0.716064	-0.142142
O	4.238299	-0.399972	1.092231
C	4.544298	-0.234683	-1.527311
O	3.089689	-2.098036	-0.367104
H	-1.255642	-0.378885	2.198094

H	1.195736	-0.620936	2.398931
H	0.788381	2.839901	1.193689
H	2.548788	1.234623	1.483898
H	-1.283246	2.116627	1.574858
H	-1.916767	0.575339	-1.586749
H	-2.649536	-1.731651	-1.320099
H	1.213215	3.805266	-0.999852
H	2.730554	3.132097	-0.377034
H	1.814187	2.260707	-1.621805
H	4.821639	0.808785	-1.400839
H	5.426521	-0.872134	-1.520444
H	3.971674	-0.380998	-2.439578
O	-1.209124	-1.313045	0.077068
C	-3.570696	-1.524731	0.598798
H	-3.434971	-2.578694	0.855496
H	-3.421454	-0.947506	1.517607
C	-4.066210	0.628672	-1.334049
H	-4.145716	1.692595	-1.570888
H	-4.209901	0.076471	-2.269521
C	-4.972332	-1.258372	0.056772
H	-5.144778	-1.882782	-0.829268

H	-5.729035	-1.545809	0.792430
C	-5.132247	0.210525	-0.325029
H	-5.035631	0.830276	0.571546
H	-6.128205	0.395907	-0.737044
Na	0.777476	-1.791719	-0.274123

Electronic Energy = -1521.49102500 (Hartree/Particle)

Dipole Moment (Debye): 5.1126

index 1

Number of imaginary frequencies= 1

Negatives Eigenvalues: -200.803

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.343909 (Hartree/Particle)

Thermal correction to Energy= 0.364507

Thermal correction to Enthalpy= 0.365451

Thermal correction to Gibbs Free Energy= 0.294629

Sum of electronic and zero-point Energies= -1521.147116

Sum of electronic and thermal Energies= -1521.126518

Sum of electronic and thermal Enthalpies= -1521.125574

Sum of electronic and thermal Free Energies= -1521.196396

SP 6-311++G(2D,2P) Electronic Energy= -1521.81845131

Corrected Free Energy = -1521.196396+1521.49102500-1521.81845131= -1521.52382231

10b with PCM

CARTESIAN COORDINATES

C	-1.126550	0.670521	-1.697048
C	-1.871960	1.208934	-0.536349
C	-1.069797	2.242358	0.238970
O	0.267238	1.823732	0.389338
C	0.938769	1.759634	-0.861498
C	0.208223	0.829039	-1.794607
C	-1.620836	2.565398	1.609661
O	2.283908	1.555464	-0.677503
C	2.753426	0.452351	0.121048
C	4.169886	0.821660	0.524410

O	-2.162919	0.092626	0.457680
S	-3.377034	-0.904965	0.164381
O	-4.276057	-0.343394	-0.824324
C	-4.166587	-0.947940	1.752571
O	-2.763114	-2.214507	-0.078451
H	0.755350	0.488334	-2.660882
H	-1.689841	0.133446	-2.453681
H	-1.094116	3.147973	-0.388702
H	-2.852792	1.599073	-0.804408
H	0.884155	2.761715	-1.320434
H	2.113761	0.371594	1.007298
H	4.157377	1.764474	1.077265
H	-1.057695	3.389650	2.045739
H	-2.671747	2.855557	1.544159
H	-1.533016	1.700145	2.265440
H	-4.561121	0.042183	1.965786
H	-4.970419	-1.678936	1.687445
H	-3.433235	-1.248852	2.496397
C	2.672702	-0.862849	-0.646390
H	3.296398	-0.727740	-1.556035
C	4.813045	-0.292188	1.344773

H	5.842372	-0.022844	1.597627
H	4.275401	-0.401314	2.294588
C	3.337341	-1.961552	0.195546
H	3.291083	-2.897057	-0.368890
H	2.728598	-2.105833	1.098990
C	4.769657	-1.618702	0.591404
H	5.387419	-1.539269	-0.310883
H	5.205310	-2.417185	1.199693
O	1.376931	-1.153990	-0.963012
H	4.753404	0.994176	-0.386625
Na	-0.495082	-1.728116	-0.376796

Electronic Energy = -1521.49352247 (Hartree/Particle)

Dipole Moment (Debye): 7.3903

index 0

Harmonic frequencies

Number of imaginary frequencies= 0

THERMOCHEMICAL DATA 6-31+g(D)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.344067 (Hartree/Particle)

Thermal correction to Energy= 0.365444

Thermal correction to Enthalpy= 0.366388

Thermal correction to Gibbs Free Energy= 0.293107

Sum of electronic and zero-point Energies= -1521.149455

Sum of electronic and thermal Energies= -1521.128079

Sum of electronic and thermal Enthalpies= -1521.127135

Sum of electronic and thermal Free Energies= -1521.200415

SP 6-311++G(2D,2P) Electronic Energy= -1521.82128101

Corrected Free Energy = -1521.200415+1521.49352247-1521.82128101= -1521.52817354

SP 6-311++G(2D,2P) SCRF=PCM solvent=DMF Electronic Energy= -1521.85087352

Corrected Free Energy = -1521.200415+1521.49352247-1521.85087352 = -1521.55776605

TS-CIS-01 10b with PCM

CARTESIAN COORDINATES

C	-0.994036	0.659685	-1.716722
C	-1.787268	1.200353	-0.618339
C	-1.050480	2.232413	0.215503

O	0.288034	1.841476	0.428586
C	1.011667	1.774470	-0.789347
C	0.368424	0.783636	-1.724057
C	-1.672225	2.537033	1.560047
O	2.356696	1.628804	-0.532728
C	2.799251	0.479116	0.201417
C	4.248921	0.738440	0.562728
O	-2.148285	0.053808	0.433482
S	-3.390730	-0.886048	0.155990
O	-4.282342	-0.304265	-0.830760
C	-4.189945	-0.904394	1.741943
O	-2.835638	-2.225853	-0.088673
H	0.929562	0.549013	-2.617118
H	-1.514157	0.161229	-2.527550
H	-1.060355	3.145033	-0.403200
H	-2.774692	1.548713	-0.911480
H	0.939643	2.758878	-1.280330
H	2.188865	0.390045	1.107940
H	4.319684	1.651201	1.159247
H	-1.158562	3.381490	2.018546
H	-2.728566	2.789709	1.445737

H	-1.584912	1.675577	2.220309
H	-4.537988	0.102109	1.960030
H	-5.027751	-1.595454	1.669700
H	-3.475665	-1.243201	2.487971
C	2.615551	-0.785241	-0.622649
H	3.206089	-0.646234	-1.551074
C	4.840229	-0.456308	1.305768
H	5.893789	-0.271517	1.531908
H	4.329373	-0.574465	2.268904
C	3.217738	-1.972842	0.133048
H	3.096107	-2.872194	-0.477259
H	2.630349	-2.124782	1.048394
C	4.681734	-1.740499	0.495168
H	5.274550	-1.661218	-0.423494
H	5.079529	-2.594016	1.051705
O	1.282118	-0.967155	-0.904110
H	4.809819	0.916230	-0.361301
Na	-0.582278	-1.709006	-0.402441

Electronic Energy = -1521.49283328 (Hartree/Particle)

Dipole Moment (Debye): 5.2228

index 1

Number of imaginary frequencies= 1

Negatives Eigenvalues: -151.257

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.343896 (Hartree/Particle)

Thermal correction to Energy= 0.364479

Thermal correction to Enthalpy= 0.365423

Thermal correction to Gibbs Free Energy= 0.294444

Sum of electronic and zero-point Energies= -1521.148937

Sum of electronic and thermal Energies= -1521.128355

Sum of electronic and thermal Enthalpies= -1521.127411

Sum of electronic and thermal Free Energies= -1521.198390

SP 6-311++G(2D,2P) Electronic Energy= -1521.82020776

Corrected Free Energy = -1521.198390+1521.49283328-1521.82020776= -1521.52576448

SP 6-311++G(2D,2P) SCRF=PCM solvent=DMF Electronic Energy= -1521.84678094

Corrected Free Energy = -1521.198390+1521.49283328-1521.84678094= -1521.55233766

10a with PCM

CARTESIAN COORDINATES

C	1.294272	0.269716	1.653038
C	2.278334	1.124936	0.914800
C	1.571673	2.342886	0.335548
O	0.441026	1.910859	-0.395708
C	-0.567896	1.347683	0.400925
C	-0.015443	0.430586	1.460401
C	2.423989	3.178614	-0.591432
O	-1.359450	0.611592	-0.482026
C	-2.704535	0.353953	0.002908
C	-2.949477	-1.162503	-0.040670
O	2.896989	0.457610	-0.248444
S	3.221695	-1.106181	-0.180786
O	3.804536	-1.442038	1.104474
C	4.441254	-1.161000	-1.465611
O	2.050459	-1.856400	-0.636924
H	-0.753336	-0.172084	1.982497

H	1.677352	-0.448631	2.367764
H	1.253149	2.949381	1.195265
H	3.107462	1.416773	1.560897
H	-1.166194	2.153268	0.857264
H	-2.748416	0.648886	1.059379
H	1.864366	4.056990	-0.911086
H	3.333750	3.506959	-0.085391
H	2.698657	2.601942	-1.473458
H	5.294025	-0.561798	-1.158070
H	4.722304	-2.206021	-1.581194
H	3.995876	-0.779158	-2.380663
C	-3.695750	1.164955	-0.809001
H	-3.592114	0.882921	-1.862126
C	-4.389098	-1.404670	0.438293
H	-4.582204	-2.478793	0.388068
H	-4.438155	-1.128528	1.498941
C	-5.118205	0.881240	-0.329789
H	-5.835665	1.437418	-0.939677
H	-5.231580	1.246473	0.698177
C	-5.420144	-0.615548	-0.364062
H	-5.408032	-0.956591	-1.406440

H	-6.430208	-0.803106	0.012565
H	-2.949817	-1.416532	-1.135570
O	-2.010771	-1.843730	0.666623
H	-3.462792	2.232641	-0.741542
Na	-0.215610	-1.608341	-0.431734

Electronic Energy = -1521.49565014 (Hartree/Particle)

Dipole Moment (Debye): 8.7844

index 0

Harmonic frequencies

Number of imaginary frequencies= 0

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.344328 (Hartree/Particle)

Thermal correction to Energy= 0.365622

Thermal correction to Enthalpy= 0.366567

Thermal correction to Gibbs Free Energy= 0.293915

Sum of electronic and zero-point Energies= -1521.151323

Sum of electronic and thermal Energies= -1521.130028

Sum of electronic and thermal Enthalpies= -1521.129083

Sum of electronic and thermal Free Energies= -1521.201735

SP 6-311++G(2D,2P) Electronic Energy= -1521.82319624

Corrected Free Energy = -1521.201735+1521.49565014-1521.82319624= -1521.52928110

SP 6-311++G(2D,2P) SCRF=PCM solvent=DMF Electronic Energy= -1521.85805737

Corrected Free Energy = -1521.201735+1521.49565014-1521.85805737= -1521.56414223

TS-CIS-03 10a with PCM

CARTESIAN COORDINATES

C	0.757486	0.071355	1.688257
C	1.645472	0.954623	0.948072
C	0.949120	2.158287	0.341886
O	-0.304770	1.796167	-0.193645
C	-1.187821	1.326876	0.811268
C	-0.600146	0.127835	1.505452
C	1.728426	2.883120	-0.732553
O	-2.460070	1.199402	0.299275
C	-2.665086	0.329659	-0.828238

C	-2.487532	-1.125182	-0.406344
O	2.266523	0.196586	-0.333536
S	3.541949	-0.716064	-0.142142
O	4.238299	-0.399972	1.092231
C	4.544298	-0.234683	-1.527311
O	3.089689	-2.098036	-0.367104
H	-1.255642	-0.378885	2.198094
H	1.195736	-0.620936	2.398931
H	0.788381	2.839901	1.193689
H	2.548788	1.234623	1.483898
H	-1.283246	2.116627	1.574858
H	-1.916767	0.575339	-1.586749
H	-2.649536	-1.731651	-1.320099
H	1.213215	3.805266	-0.999852
H	2.730554	3.132097	-0.377034
H	1.814187	2.260707	-1.621805
H	4.821639	0.808785	-1.400839
H	5.426521	-0.872134	-1.520444
H	3.971674	-0.380998	-2.439578
O	-1.209124	-1.313045	0.077068
C	-3.570696	-1.524731	0.598798

H	-3.434971	-2.578694	0.855496
H	-3.421454	-0.947506	1.517607
C	-4.066210	0.628672	-1.334049
H	-4.145716	1.692595	-1.570888
H	-4.209901	0.076471	-2.269521
C	-4.972332	-1.258372	0.056772
H	-5.144778	-1.882782	-0.829268
H	-5.729035	-1.545809	0.792430
C	-5.132247	0.210525	-0.325029
H	-5.035631	0.830276	0.571546
H	-6.128205	0.395907	-0.737044
Na	0.777476	-1.791719	-0.274123

Electronic Energy = -1521.49102500 (Hartree/Particle)

Dipole Moment (Debye): 5.1126

index 1

Number of imaginary frequencies= 1

Negatives Eigenvalues: -200.803

THERMOCHEMICAL DATA

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.343909 (Hartree/Particle)

Thermal correction to Energy= 0.364507

Thermal correction to Enthalpy= 0.365451

Thermal correction to Gibbs Free Energy= 0.294629

Sum of electronic and zero-point Energies= -1521.147116

Sum of electronic and thermal Energies= -1521.126518

Sum of electronic and thermal Enthalpies= -1521.125574

Sum of electronic and thermal Free Energies= -1521.196396

SP 6-311++G(2D,2P) Electronic Energy= -1521.81845131

Corrected Free Energy = -1521.196396+1521.49102500-1521.81845131= -1521.52382231

SP 6-311++G(2D,2P) SCRF=PCM solvent=DMF Electronic Energy= -1521.84435760

Corrected Free Energy = -1521.196396+1521.49102500-1521.84435760= -1521.54972860