

Controlling *cis/trans*-selectivity in intramolecular Diels–Alder reactions of benzo-tethered, ester linked 1,3,9-decatrienes

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1. Computation details

All calculations were carried out using the B3LYP/6-31G(d) theoretical model and Gaussian 03:

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, *Gaussian 2003*, Revision D.01, Gaussian, Inc., Pittsburgh, PA, 2003.

The Cartesian coordinates, imaginary frequencies, energies, enthalpies and free energies of the *cis* and *trans* IMDA TSs for **2–7** are listed below.

Trans-2 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 462i cm⁻¹ ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -880.8453852 au; Energy+zpe (0K) = -880.5860532 au

Enthalpy (298K) = -880.5687382 au; Gibbs free energy (298K) = -880.6301852 au

O,-1.772672,1.850580,0.129478

O,0.033238,2.905621,0.864259

C,2.671339,-0.022999,-0.740474

C,1.992469,-0.473188,1.956749

C,1.416304,-1.670245,1.547333

C,1.775521,0.776415,0.123721

C,0.096341,-1.747635,1.083324

C,0.416285,0.802039,-0.198354

C,-4.410230,-0.327131,-1.128060

C,-4.011029,-1.574335,-0.644692

C,-3.629023,0.800990,-0.879051

C,-2.829668,-1.689603,0.086774

C,-2.453873,0.675107,-0.143006

C,-2.029005,-0.571069,0.358091

C,-0.401389,1.928839,0.300380

C,-0.745119,-0.639438,1.080433

O,2.307331,-0.891035,-1.512032

O,3.970083,0.318687,-0.558821

C,4.911000,-0.408099,-1.362683

H,3.054815,-0.435049,2.180263

H,1.402216,0.295284,2.444590

H,2.067805,-2.518251,1.349491

H,2.207182,1.622829,0.645265

H,-0.186330,-2.624833,0.505630

H,0.074598,0.243545,-1.061155

H,-5.328934,-0.228427,-1.699029

H,-4.618458,-2.454889,-0.831693

H,-3.914004,1.782937,-1.242393

H,-2.527555,-2.657557,0.475911

H,-0.614713,0.089191,1.876759

H,4.704569,-0.260746,-2.426214

H,4.864925,-1.477928,-1.139884

H,5.890510,-0.004819,-1.103509

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Cis-2 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 451i cm⁻¹ ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -880.8437101 au; Energy+zpe (0K) = -880.5846721 au

Enthalpy (298K) = -880.5672211 au; Gibbs free energy (298K) = -880.6291641 au

O,1.690467,1.290661,-1.178401
O,-0.124625,2.562158,-1.248271
C,-2.728807,-0.709145,-0.470304
C,-2.033517,0.668385,1.903035
C,-1.838052,0.465687,-0.407430
C,-0.938407,1.459150,2.205508
C,-0.483086,0.273506,-0.679325
C,4.416500,-1.062525,-0.644574
C,4.003704,-1.738143,0.506086
C,3.611227,-0.070895,-1.199904
C,2.784053,-1.412661,1.096783
C,2.396088,0.252388,-0.595167
C,1.965282,-0.403463,0.571079
C,0.641835,-0.081391,1.161672
C,0.324065,1.458374,-1.051389
C,0.374720,1.089201,1.870595
O,-2.363137,-1.869060,-0.374008
O,-4.024439,-0.346989,-0.617243
C,-4.961372,-1.433223,-0.679098
H,-3.039397,1.049772,2.053498
H,-1.950366,-0.412220,1.881702
H,-2.273283,1.446691,-0.544505
H,-1.105923,2.483975,2.530268
H,-0.151393,-0.707029,-1.003788
H,5.362860,-1.311198,-1.116351
H,4.624597,-2.517379,0.938006
H,3.903717,0.463850,-2.097676
H,2.453376,-1.939981,1.987880
H,-0.010872,-0.937600,1.316245
H,1.161918,1.834684,1.960968
H,-4.921283,-2.030711,0.235931
H,-4.744399,-2.080663,-1.532993
H,-5.941083,-0.967814,-0.791199

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Cis-3 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 450i cm⁻¹ ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -3451.9479473 au; Energy+zpe (0K) = -3451.6991463 au

Enthalpy (298K) = -3451.6802163 au; Gibbs free energy (298K) = -3451.7464523 au

Br,-1.912322,2.193798,-0.150225
O,0.338240,0.688485,2.621357
O,-1.214138,-0.659289,1.789131
C,3.322553,-0.747519,-0.043559
C,2.067269,1.551472,-1.139712
C,2.242389,-0.000547,0.626599
C,0.833407,2.114068,-0.880953
C,0.990312,-0.608295,0.725288
C,-0.335609,1.337175,-0.807597
C,0.057710,-0.124955,1.776045
C,-0.308788,-0.054533,-0.908027
C,-3.512653,-2.785391,-0.066299
C,-3.168764,-2.508353,-1.391153
C,-2.826570,-2.170348,0.978491
C,-2.138485,-1.610018,-1.662683
C,-1.802593,-1.267222,0.695534
C,-1.447981,-0.962954,-0.629601

O,3.151471,-1.667993,-0.826623
O,4.543250,-0.267582,0.287060
C,5.653990,-0.938342,-0.328541
H,2.961130,2.163711,-1.064334
H,2.168438,0.657887,-1.743682
H,2.511191,0.785319,1.320173
H,0.775880,3.144093,-0.541852
H,0.893957,-1.635136,0.386822
H,0.443017,-0.459725,-1.582005
H,-4.310986,-3.487302,0.157025
H,-3.696372,-2.990973,-2.208290
H,-3.069475,-2.372026,2.016579
H,-1.861428,-1.394439,-2.691200
H,5.591830,-0.868475,-1.418062
H,5.672456,-1.993470,-0.042834
H,6.543907,-0.426770,0.039140

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Trans-3 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 474i cm⁻¹ ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -3451.9454175 au; Energy+zpe (0K) = -3451.6962595 au

Enthalpy (298K) = -3451.6774385 au; Gibbs free energy (298K) = -3451.7436845 au

Br,0.118052,2.685913,-0.001950
O,-0.130538,-3.535229,0.859468
O,1.688398,-2.528117,0.100060
C,-2.738393,-0.588731,-0.723686
C,-1.967270,-0.262078,1.974135
C,-1.833535,-1.412680,0.111280
C,-1.456284,0.964482,1.566568
C,-0.478512,-1.444068,-0.232543
C,-0.165058,1.094366,1.034612
C,0.322753,-2.576569,0.277485
C,0.725007,0.022390,0.995971
C,4.469729,-0.496882,-1.056778
C,4.128676,0.767563,-0.576851
C,3.609056,-1.572356,-0.847777
C,2.921148,0.958254,0.092702
C,2.410632,-1.375908,-0.166326
C,2.024872,-0.102013,0.302040
O,-2.379173,0.309508,-1.460453
O,-4.032563,-0.944869,-0.549024
C,-4.982559,-0.193465,-1.321077
H,-3.012572,-0.321817,2.264352
H,-1.337718,-1.027986,2.414169
H,-2.260468,-2.275197,0.610369
H,-2.141229,1.793164,1.418984
H,-0.137812,-0.891062,-1.099782
H,0.598690,-0.668011,1.827959
H,5.405904,-0.651780,-1.585343
H,4.801352,1.608240,-0.717805
H,3.851893,-2.572997,-1.189747
H,2.667543,1.941761,0.466602
H,-4.785299,-0.307845,-2.390275
H,-4.933771,0.868531,-1.064906
H,-5.958884,-0.606129,-1.065279

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Cis-4 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 450i cm⁻¹ ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -1289.5169245 au; Energy+zpe (0K) = -1289.1555915 au

Enthalpy (298K) = -1289.1303805 au; Gibbs free energy (298K) = -1289.2096535 au

Si,2.060097,-2.048849,-0.145319
 O,-0.425526,-0.478291,2.604637
 O,0.907773,1.091834,1.777649
 C,-3.561808,0.461178,-0.106328
 C,-1.964667,-1.586894,-1.139676
 C,-2.380606,-0.112921,0.571905
 C,-0.683321,-2.023122,-0.848780
 C,-1.242889,0.684264,0.689532
 C,0.450478,-1.176828,-0.719095
 C,-0.270704,0.366636,1.752880
 C,2.463438,-3.297976,-1.516193
 C,1.733534,-2.967551,1.475475
 C,0.232458,0.194837,-0.908352
 C,2.832881,3.530676,-0.123931
 C,2.612741,3.115031,-1.438862
 C,2.225352,2.854994,0.932354
 C,1.784426,2.021513,-1.688049
 C,3.543217,-0.899244,0.070619
 C,1.409096,1.755191,0.669884
 C,1.182414,1.307179,-0.642416
 O,-3.535276,1.397337,-0.886726
 O,-4.694625,-0.201343,0.224316
 C,-5.894025,0.289944,-0.393604
 H,-2.794188,-2.287284,-1.092172
 H,-2.135659,-0.720797,-1.768987
 H,-2.543746,-0.910958,1.284472
 H,-0.579803,-3.056797,-0.519905
 H,-1.270170,1.691582,0.288853
 H,1.634262,-3.991346,-1.698822
 H,2.687992,-2.793980,-2.463696
 H,3.340773,-3.897159,-1.242124
 H,0.968839,-3.744991,1.361413
 H,1.391287,-2.281791,2.257788
 H,2.650865,-3.458421,1.824342
 H,-0.566191,0.483424,-1.590808
 H,3.470370,4.385816,0.081694
 H,3.075803,3.643935,-2.266655
 H,2.371681,3.160889,1.963231
 H,1.598203,1.703390,-2.710764
 H,4.434054,-1.513329,0.256347
 H,3.739108,-0.289350,-0.817216
 H,3.424928,-0.224177,0.923484
 H,-5.821015,0.226874,-1.482885
 H,-6.073695,1.330892,-0.111626
 H,-6.695906,-0.350281,-0.024681

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Trans-4 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 474 cm⁻¹ ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -1289.5140834 au; Energy+zpe (0K) = -1289.1519894 au

Enthalpy (298K) = -1289.1270384 au; Gibbs free energy (298K) = -1289.2046374 au

Si,-0.118819,2.567053,0.072055
 O,0.092005,-3.757452,0.826708
 O,1.844266,-2.658444,0.034063
 C,-2.682393,-0.917567,-0.669823
 C,-1.855126,-0.637783,2.046352
 C,-1.722814,-1.719501,0.115635
 C,-1.426346,0.626332,1.659551
 C,-0.374247,-1.679292,-0.245431
 C,-0.175392,0.906787,1.050251
 C,0.485249,-2.772543,0.243929
 C,0.745792,-0.154034,1.021280

C,4.560730,-0.466597,-0.964844
 C,4.163062,0.759016,-0.430723
 C,3.735369,-1.580127,-0.825962
 C,2.931699,0.865526,0.214274
 C,2.513874,-1.463702,-0.164817
 C,2.062939,-0.227655,0.346616
 O,-2.385927,0.000960,-1.415942
 O,-3.957204,-1.315266,-0.453781
 C,-4.961412,-0.589451,-1.178491
 C,0.887542,3.882165,1.008393
 C,-1.877153,3.264431,-0.052570
 C,0.494021,2.326503,-1.700335
 H,-2.884062,-0.768711,2.371354
 H,-1.173745,-1.397421,2.414710
 H,-2.104055,-2.605747,0.608861
 H,-2.194865,1.391767,1.607431
 H,-0.064454,-1.101577,-1.106802
 H,0.648676,-0.884185,1.824307
 H,5.514664,-0.563011,-1.475219
 H,4.808155,1.629248,-0.507869
 H,4.024971,-2.554534,-1.205526
 H,2.641431,1.811873,0.652248
 H,-4.780742,-0.651117,-2.254857
 H,-4.967708,0.462991,-0.880496
 H,-5.908380,-1.064493,-0.920465
 H,0.768562,4.850086,0.504596
 H,1.961750,3.683360,1.076424
 H,0.509619,3.998974,2.031412
 H,-1.849659,4.178744,-0.658998
 H,-2.309240,3.537166,0.917463
 H,-2.548360,2.556019,-0.549161
 H,0.410797,3.275857,-2.244746
 H,-0.147217,1.596324,-2.207202
 H,1.529849,1.986211,-1.774328

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Cis-5 Transition structure B3LYP/6-31g(d)

Imaginary frequency = $448i\text{ cm}^{-1}$; SCF Energy (no zpe) ; SCF Energy (no zpe) = -3451.9475801 au; Energy+zpe (0K) = -3451.6987151 au

Enthalpy (298K) = -3451.6797451 au; Gibbs free energy (298K) = -3451.7462511 au

Br,2.604128,-2.133025,0.162474
 O,-1.570907,3.054938,0.913042
 O,0.426244,2.709257,0.012358
 C,-3.216654,-0.458825,-0.838821
 C,-2.288558,-0.908234,1.795984
 C,-2.591318,0.559835,0.028786
 C,-1.347212,-0.238756,2.559302
 C,-1.326566,1.030377,-0.324635
 C,-0.883133,2.318116,0.249401
 C,-0.094138,0.137862,2.048861
 C,0.245132,-0.100426,0.718774
 C,3.618734,1.612484,-1.331268
 C,3.646266,0.261655,-0.984017
 C,2.519677,2.402972,-1.007690
 C,2.558368,-0.278131,-0.303869
 C,1.443429,1.838910,-0.322733
 C,1.437086,0.482331,0.057027
 O,-2.612689,-1.180838,-1.613866
 O,-4.554750,-0.521321,-0.649696
 C,-5.242322,-1.494680,-1.451359
 H,-3.292171,-1.063226,2.181319
 H,-1.982483,-1.599398,1.018931

H,-3.236768,1.179361,0.637252
H,-1.650669,0.184354,3.514521
H,-0.882140,0.687411,-1.252766
H,0.521305,0.818634,2.632648
H,-0.155984,-0.983903,0.229469
H,4.459246,2.047783,-1.863587
H,4.493871,-0.365036,-1.235908
H,2.474203,3.453481,-1.273557
H,-4.864214,-2.500033,-1.246429
H,-5.111759,-1.278288,-2.515040
H,-6.292861,-1.414464,-1.170604

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Trans-5 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 461i cm^{-1} ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -3451.9444814 au; Energy+zpe (0K) = -3451.6952834 au

Enthalpy (298K) = -3451.6764624 au; Gibbs free energy (298K) = -3451.7424874 au

Br,-2.967119,-1.936129,0.146409
O,1.641886,2.976048,1.382931
O,-0.334632,2.724786,0.411164
C,2.337530,-0.859117,1.829494
C,3.325369,-0.315039,-0.737643
C,1.456106,-1.751862,1.224646
C,2.673226,0.581496,0.246333
C,1.427942,1.117498,-0.096017
C,0.210593,-1.357597,0.720176
C,0.976018,2.322057,0.614353
C,-0.282724,-0.069306,0.901659
C,-1.423023,0.540876,0.181834
C,-3.418118,1.908577,-1.310329
C,-3.567992,0.555986,-1.018353
C,-2.302294,2.599903,-0.847977
C,-2.585477,-0.104452,-0.280255
C,-1.335781,1.926137,-0.108027
O,2.755614,-0.878804,-1.652519
O,4.647916,-0.450637,-0.481733
C,5.361936,-1.305371,-1.388187
H,3.337984,-1.192139,2.091971
H,1.971617,-0.033154,2.431322
H,1.838620,-2.717874,0.903888
H,3.321071,1.157956,0.897326
H,0.975677,0.849188,-1.042299
H,-0.270830,-2.015190,0.005699
H,0.010025,0.454694,1.807953
H,-4.178921,2.424765,-1.887961
H,-4.443755,0.009149,-1.347410
H,-2.165099,3.659029,-1.036596
H,5.290932,-0.926261,-2.411164
H,4.958329,-2.321367,-1.359513
H,6.397371,-1.294137,-1.046502

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Cis-6 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 454i cm^{-1} ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -1289.5172363 au; Energy+zpe (0K) = -1289.1559773 au

Enthalpy (298K) = -1289.1306593 au; Gibbs free energy (298K) = -1289.2096153 au

O,-0.028942,2.939590,-0.105344
O,-2.127586,3.120252,0.580763
C,-3.154917,-0.774727,-0.807566
C,-2.351100,-0.760152,1.920453
C,-2.747711,0.428757,-0.060465

C,-1.512382,0.108225,2.597095
 C,-1.536337,1.029635,-0.404418
 C,3.286111,2.153338,-1.360756
 C,3.436511,0.822332,-0.966425
 C,2.105733,2.831473,-1.079754
 C,2.425420,0.134970,-0.272997
 C,1.094126,2.172343,-0.383024
 C,1.240165,0.842626,0.050427
 C,0.096429,0.212750,0.761733
 C,-1.296467,2.419043,0.054980
 C,-0.300141,0.564676,2.053501
 Si,2.690131,-1.711580,0.139552
 C,4.475793,-2.182798,-0.283810
 C,1.537678,-2.774941,-0.928232
 C,2.422575,-2.059842,1.982136
 O,-2.392715,-1.509012,-1.417434
 O,-4.485143,-1.000936,-0.712203
 C,-4.960946,-2.167046,-1.401735
 H,-3.340749,-0.978271,2.311529
 H,-1.951633,-1.502669,1.239553
 H,-3.511114,1.010785,0.438289
 H,-1.885022,0.608703,3.488441
 H,-1.006760,0.668885,-1.279498
 H,4.084184,2.657940,-1.898579
 H,4.361636,0.310177,-1.212821
 H,1.944960,3.859680,-1.387129
 H,-0.205470,-0.759891,0.384940
 H,0.219277,1.378321,2.554979
 H,5.205618,-1.589549,0.279485
 H,4.698711,-2.067471,-1.350809
 H,4.645632,-3.236415,-0.029663
 H,1.805652,-2.676265,-1.987173
 H,0.476657,-2.515434,-0.841318
 H,1.641951,-3.834224,-0.660762
 H,1.403821,-1.842255,2.316977
 H,3.106370,-1.460341,2.595136
 H,2.627585,-3.116336,2.196659
 H,-4.476066,-3.068412,-1.016646
 H,-4.760510,-2.089071,-2.473701
 H,-6.034723,-2.198876,-1.214737

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Trans-6 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 463i cm^{-1} ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -1289.5116328 au; Energy+zpe (0K) = -1289.1500378 au

Enthalpy (298K) = -1289.1248388 au; Gibbs free energy (298K) = -1289.2036778 au

O,0.187497,2.860010,0.473936
 O,2.135231,2.828333,1.533690
 C,3.515864,-0.516174,-0.707893
 C,2.357012,-1.131332,1.759658
 C,1.394780,-1.849394,1.053874
 C,2.920919,0.381367,0.309905
 C,0.233390,-1.247864,0.554096
 C,1.759387,1.076978,-0.041344
 C,-2.867246,2.460703,-1.432489
 C,-3.204787,1.139584,-1.145051
 C,-1.703959,3.003689,-0.899745
 C,-2.386844,0.299436,-0.363111
 C,-0.877854,2.199602,-0.121802
 C,-1.162323,0.836050,0.122273
 C,1.424808,2.296609,0.710847
 C,-0.110462,0.070563,0.833055

Si,-3.179020,-1.392465,0.085402
 C,-5.062734,-1.182581,-0.031185
 C,-2.815574,-1.913197,1.869811
 C,-2.722842,-2.766882,-1.143139
 O,2.929935,-0.960445,-1.677111
 O,4.806683,-0.806256,-0.416891
 C,5.464775,-1.672692,-1.353326
 H,3.298318,-1.608540,2.018227
 H,2.073160,-0.318400,2.420382
 H,1.665555,-2.823556,0.653743
 H,3.597882,0.838455,1.023127
 H,-0.285443,-1.759139,-0.250186
 H,1.320215,0.916105,-1.017888
 H,-3.521720,3.072697,-2.046960
 H,-4.146306,0.759832,-1.528613
 H,-1.422010,4.038851,-1.061916
 H,0.214050,0.484746,1.784903
 H,-5.418782,-1.043401,-1.058302
 H,-5.421452,-0.336430,0.565835
 H,-5.547084,-2.088022,0.355606
 H,-3.063183,-1.104773,2.568421
 H,-1.774636,-2.196913,2.043298
 H,-3.446390,-2.773205,2.128300
 H,-1.679751,-3.094107,-1.087093
 H,-2.912366,-2.444730,-2.174025
 H,-3.350804,-3.646937,-0.953914
 H,5.473607,-1.225849,-2.351122
 H,4.959067,-2.641053,-1.405203
 H,6.481712,-1.791038,-0.977846

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Trans-7 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 483i cm⁻¹ ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -1068.2076325 au; Energy+zpe (0K) = -1067.9554665 au

Enthalpy (298K) = -1067.9367145 au; Gibbs free energy (298K) = -1068.0011965 au

O,1.567662,-2.435727,0.364998
 O,-0.342996,-3.347810,1.033335
 C,4.130382,-0.358158,-1.233816
 C,3.650050,0.926816,-0.984159
 C,3.443707,-1.497403,-0.790933
 C,2.481668,1.068771,-0.234004
 O,1.951136,2.325258,-0.072863
 C,2.291786,-1.324581,-0.036607
 C,1.849250,-0.044198,0.324960
 C,-2.098143,0.426203,1.890557
 C,-2.715872,-0.304607,-0.791586
 C,-1.912792,-1.097960,0.168504
 C,-1.367645,1.503268,1.418098
 C,-0.552133,-1.252734,-0.106017
 C,-0.025590,1.374033,1.021218
 C,0.180215,-2.423458,0.463823
 C,0.614556,0.127848,1.060414
 C,0.660750,2.533338,0.404994
 O,0.217437,3.654163,0.358417
 O,-2.248751,0.421601,-1.648443
 O,-4.041075,-0.484745,-0.596013
 C,-4.896107,0.245516,-1.491508
 H,5.034727,-0.481196,-1.822006
 H,4.140470,1.808439,-1.381614
 H,3.776664,-2.497536,-1.045219
 H,-3.165963,0.526539,2.058718
 H,-1.620672,-0.372325,2.448635

H,-2.428618,-1.826744,0.782575
H,-1.863444,2.438298,1.172973
H,-0.180936,-0.809360,-1.022938
H,0.424502,-0.523689,1.907822
H,-4.702174,-0.043015,-2.527849
H,-4.732622,1.321541,-1.386812
H,-5.913739,-0.019031,-1.203350

#####

Cis-7 Transition structure B3LYP/6-31g(d)

Imaginary frequency= 461i cm⁻¹ ; SCF Energy (no zpe) ; SCF Energy (no zpe) = -1068.1855997 au; Energy+zpe (0K)
= -1067.9340677 au

Enthalpy (298K) = -1067.9152007 au; Gibbs free energy (298K) = -1067.9801037 au

O,-0.070052,-1.744575,1.649191
O,-0.798017,-2.333508,-0.450067
C,1.931116,1.595382,-0.646400
C,3.573054,-0.344439,-0.158330
C,2.150480,-0.186706,0.302164
C,0.755574,2.227599,-0.206639
C,1.225313,-1.088047,-0.254590
C,-0.524205,1.680968,-0.361043
C,0.135178,-1.713578,0.461669
C,-0.750496,0.415090,-0.905753
C,-1.684150,2.433123,0.200459
C,-4.338554,-1.532718,0.143750
C,-4.271555,-0.138964,0.197617
C,-3.200918,-2.315877,-0.103140
C,-3.054299,0.477429,-0.085154
C,-2.008705,-1.674530,-0.401789
O,-2.931248,1.834402,0.099786
C,-1.959253,-0.270777,-0.534509
O,-1.623533,3.554661,0.639836
O,3.910039,-0.666762,-1.278590
O,4.430922,-0.068039,0.842577
C,5.826163,-0.210271,0.515035
H,2.863716,2.110797,-0.427329
H,1.938524,1.101439,-1.613928
H,2.032789,0.064247,1.352288
H,0.824503,3.107585,0.427504
H,1.414213,-1.453257,-1.259943
H,-0.131976,0.019960,-1.698218
H,-5.277398,-2.024457,0.380677
H,-5.122750,0.463211,0.495204
H,-3.222075,-3.394978,0.000246
H,6.097007,0.460937,-0.303984
H,6.044748,-1.239696,0.220586
H,6.365345,0.052673,1.424951

#####

2. Anisotropic Displacement Ellipsoid Plots for *cis*-3P, *cis*-4P, *cis*-5P, *cis*-6P and *trans*-7P

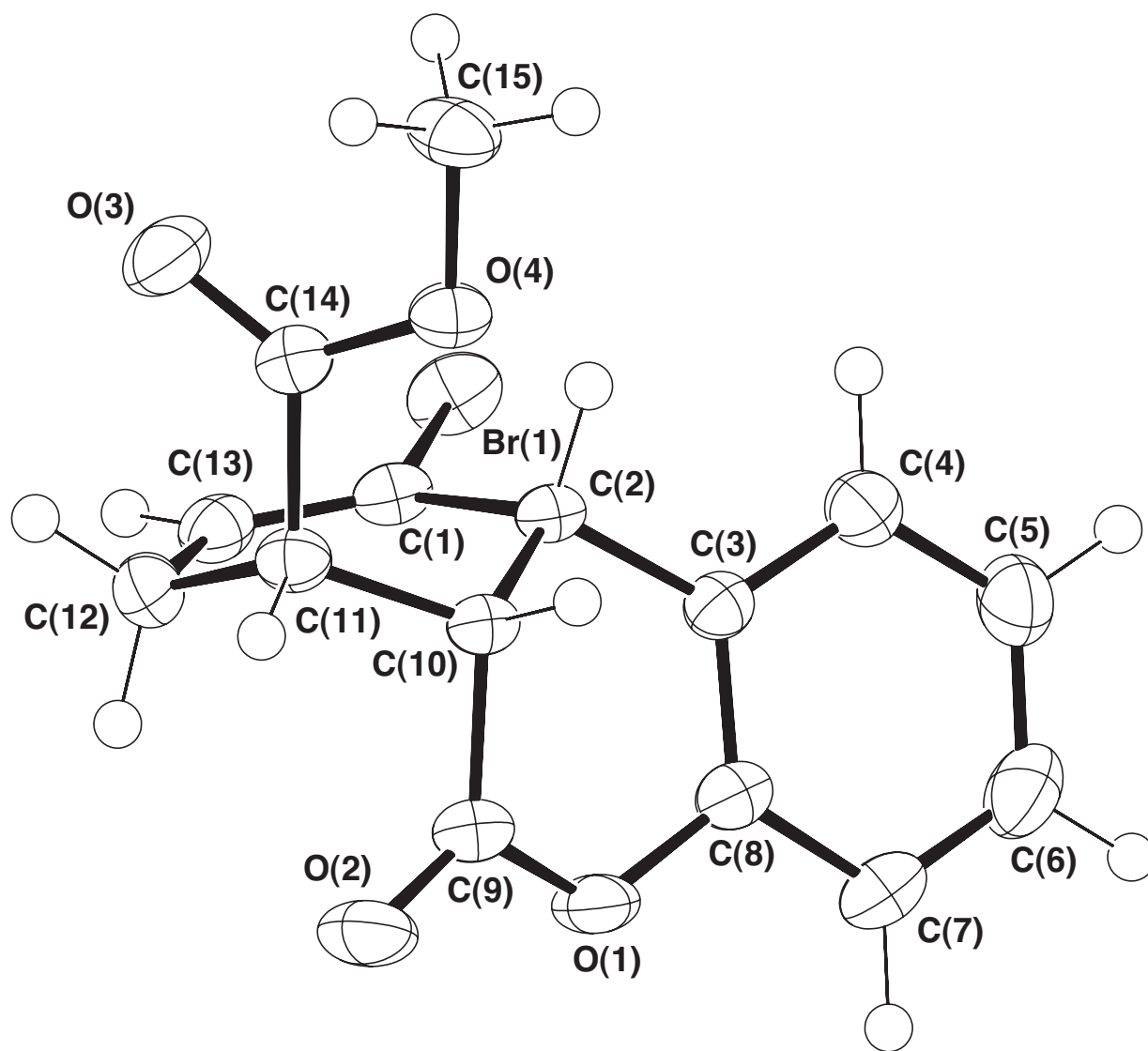


FIGURE S1. Anisotropic displacement ellipsoid plot of compound *cis*-3P (CCDC 664829) with labeling of selected atoms. Ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii.

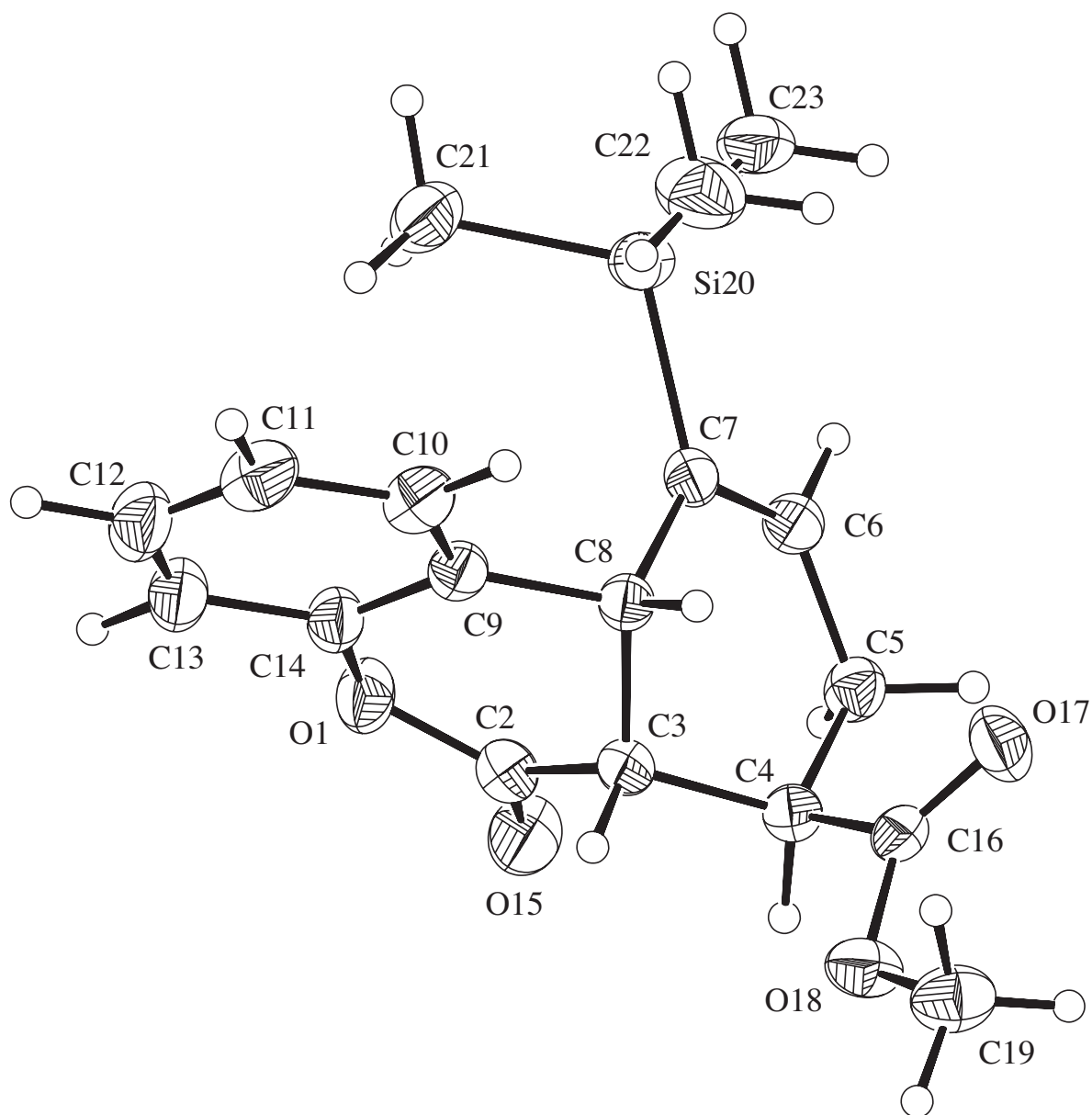


FIGURE S2. Anisotropic displacement ellipsoid plot of molecule one of compound *cis*-4P (CCDC 664830) with labeling of selected atoms. Ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

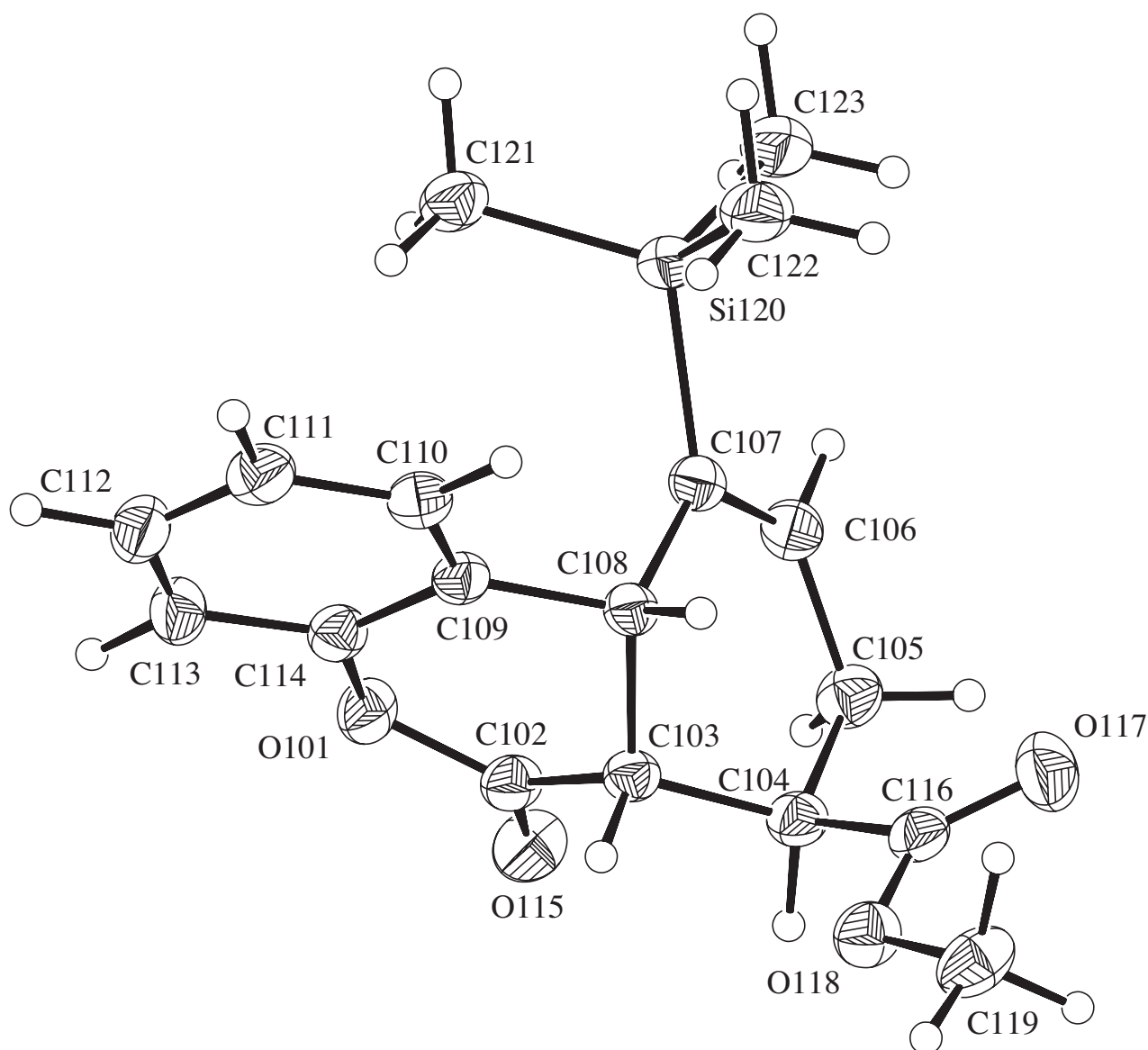


FIGURE S3. Anisotropic displacement ellipsoid plot of molecule two of compound *cis*-4P (CCDC 664830) with labeling of selected atoms. Ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

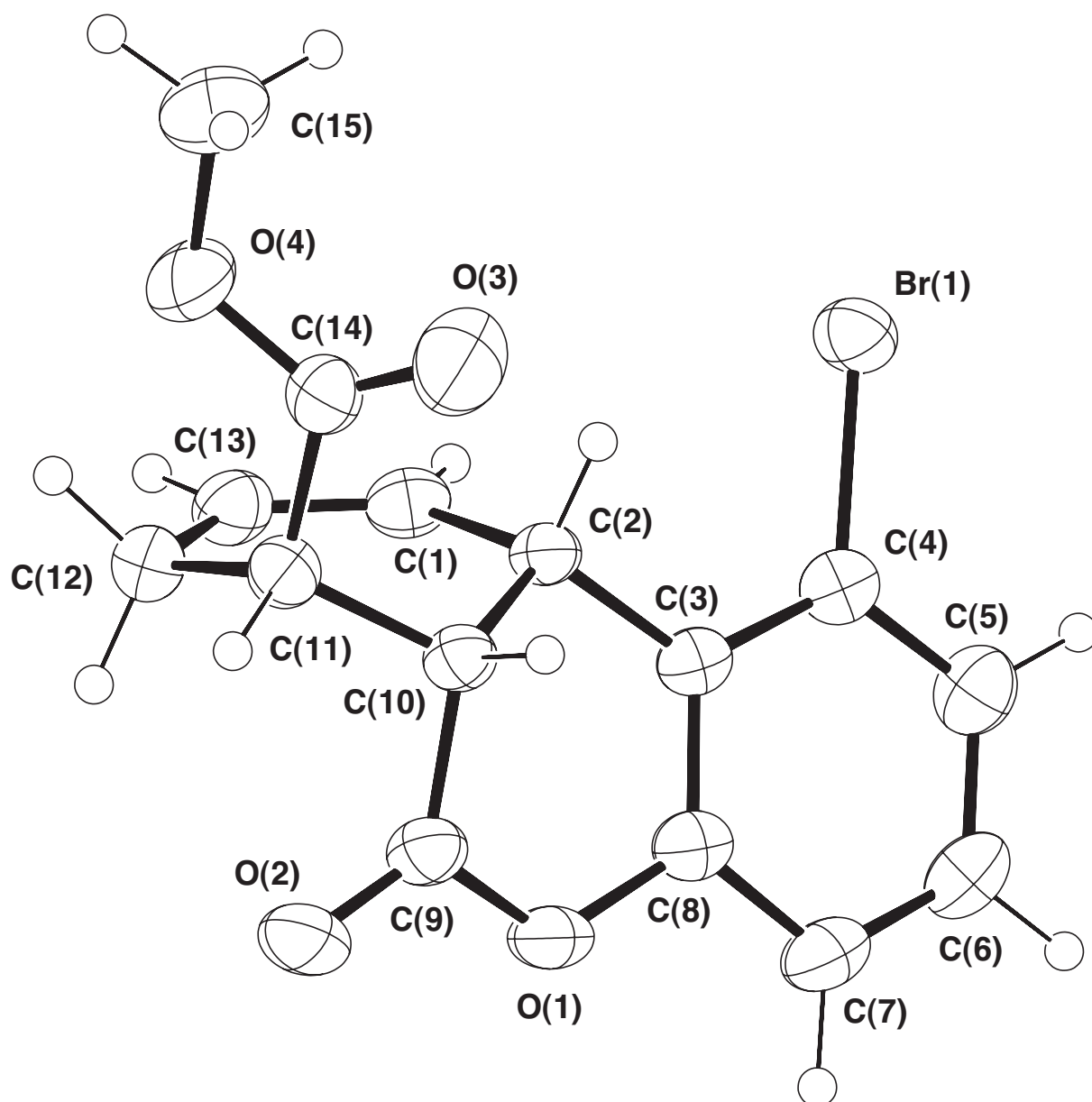


FIGURE S4. Anisotropic displacement ellipsoid plot of compound *cis*-**5P** (CCDC 664831) with labeling of selected atoms. Ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii.

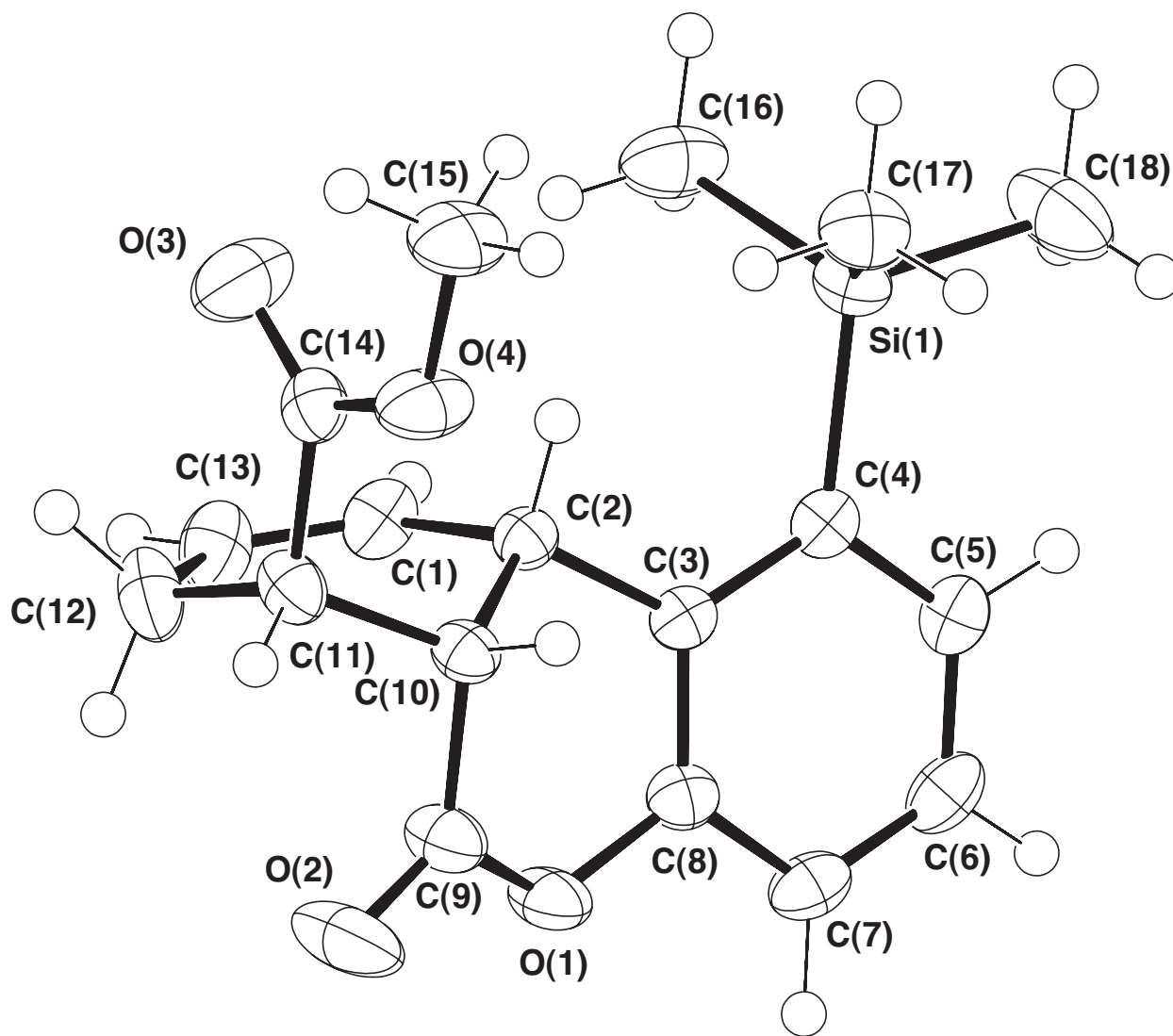


FIGURE S5. Anisotropic displacement ellipsoid plot of compound *cis*-6P (CCDC 664832) with labeling of selected atoms. Ellipsoids show 50% probability levels. Hydrogen atoms are drawn as circles with small radii.

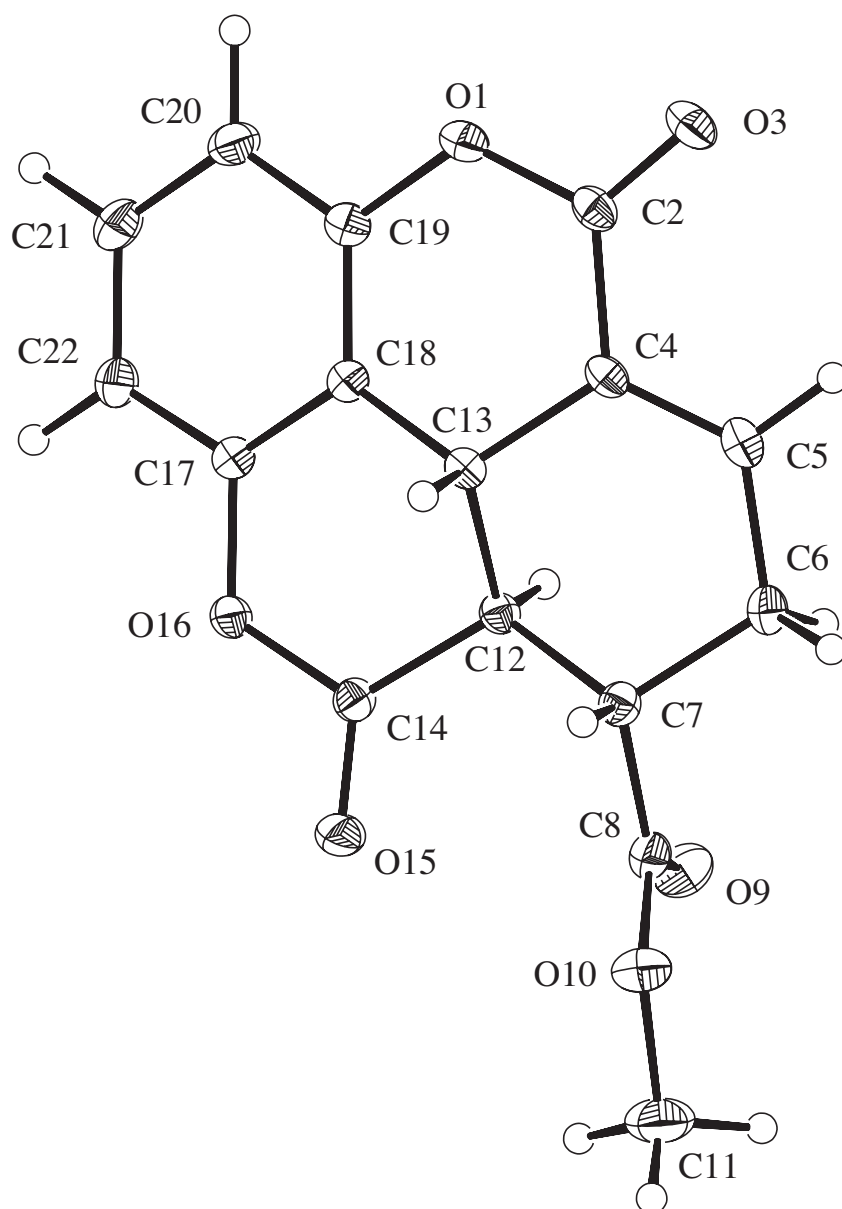
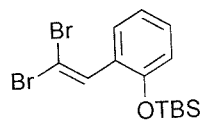
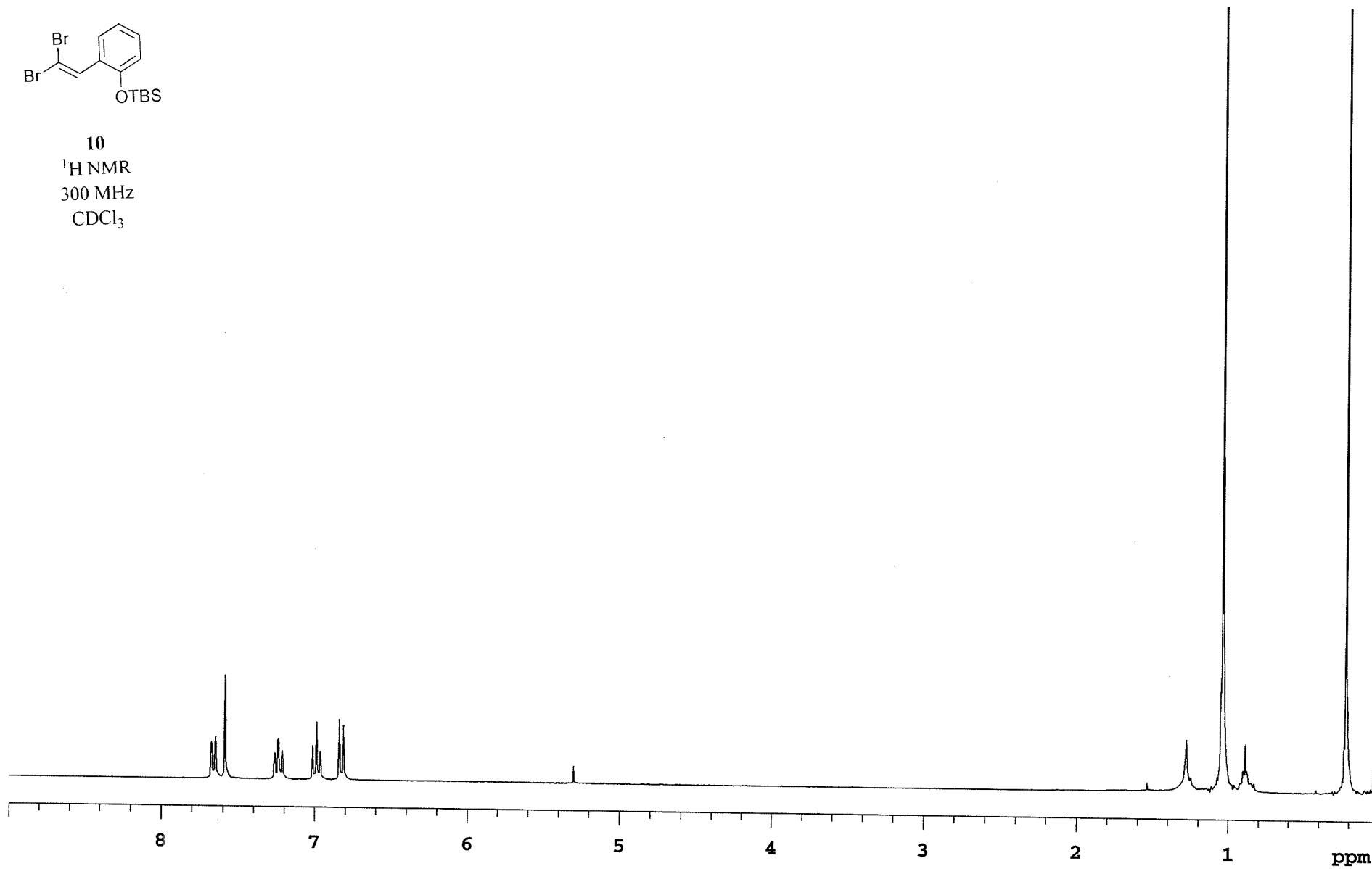
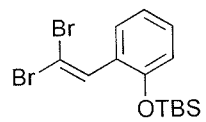


FIGURE S6. Anisotropic displacement ellipsoid plot of compound *trans*-**7P** (CCDC 664833) with labeling of selected atoms. Ellipsoids show 30% probability levels. Hydrogen atoms are drawn as circles with small radii.

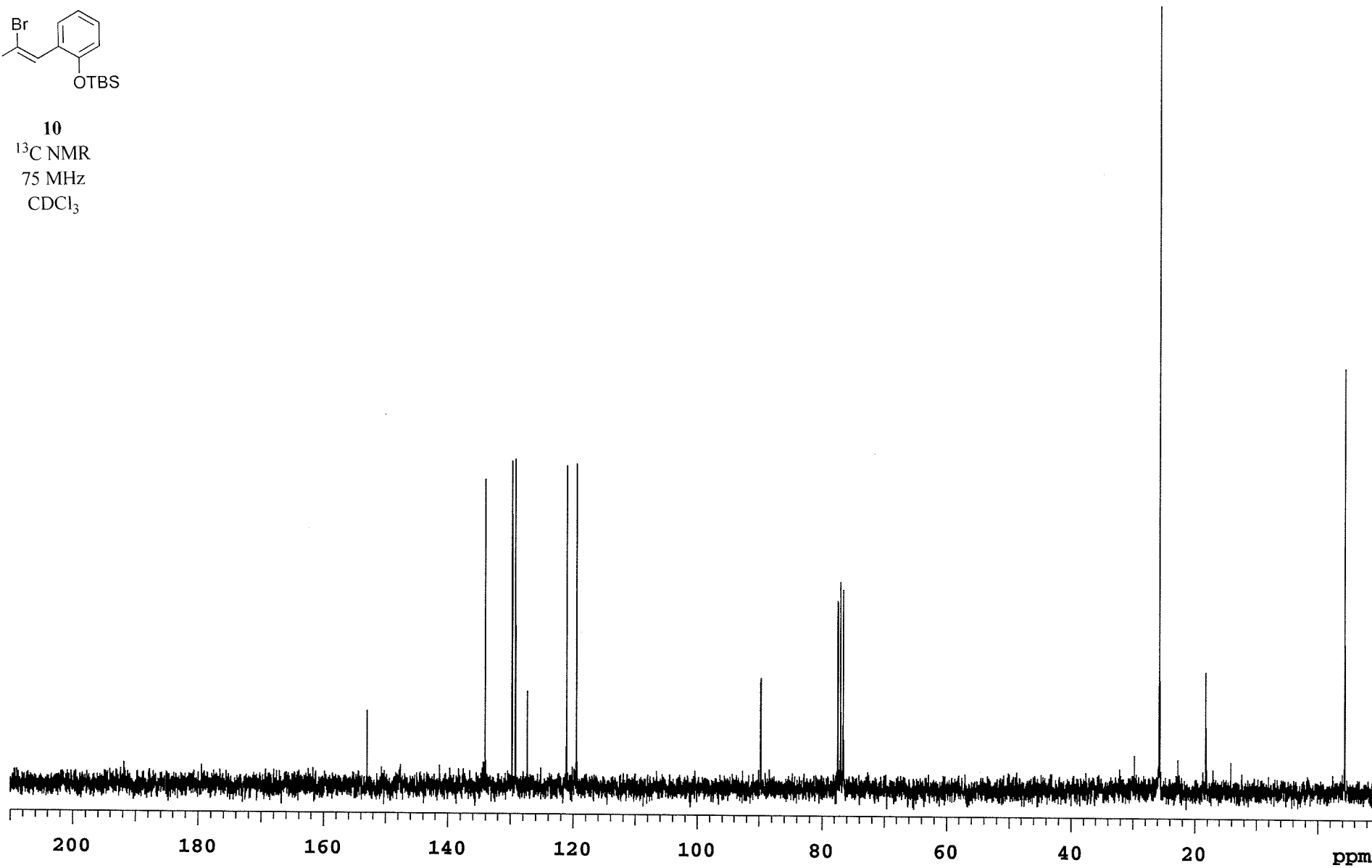


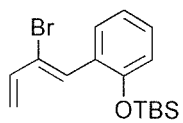
10
 ^1H NMR
300 MHz
 CDCl_3





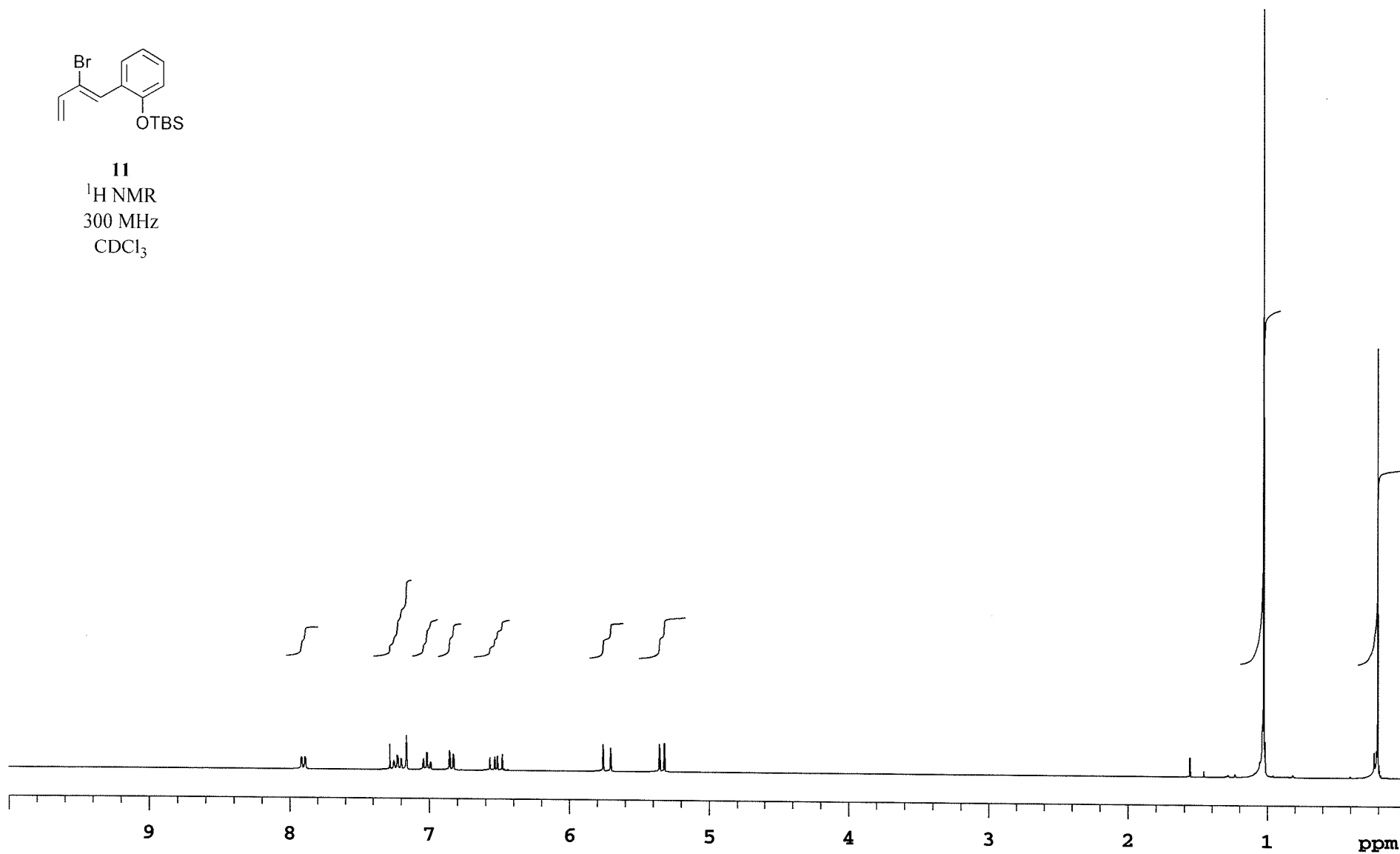
10
 ^{13}C NMR
75 MHz
 CDCl_3

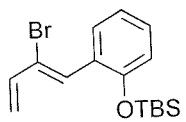




11

^1H NMR
300 MHz
 CDCl_3



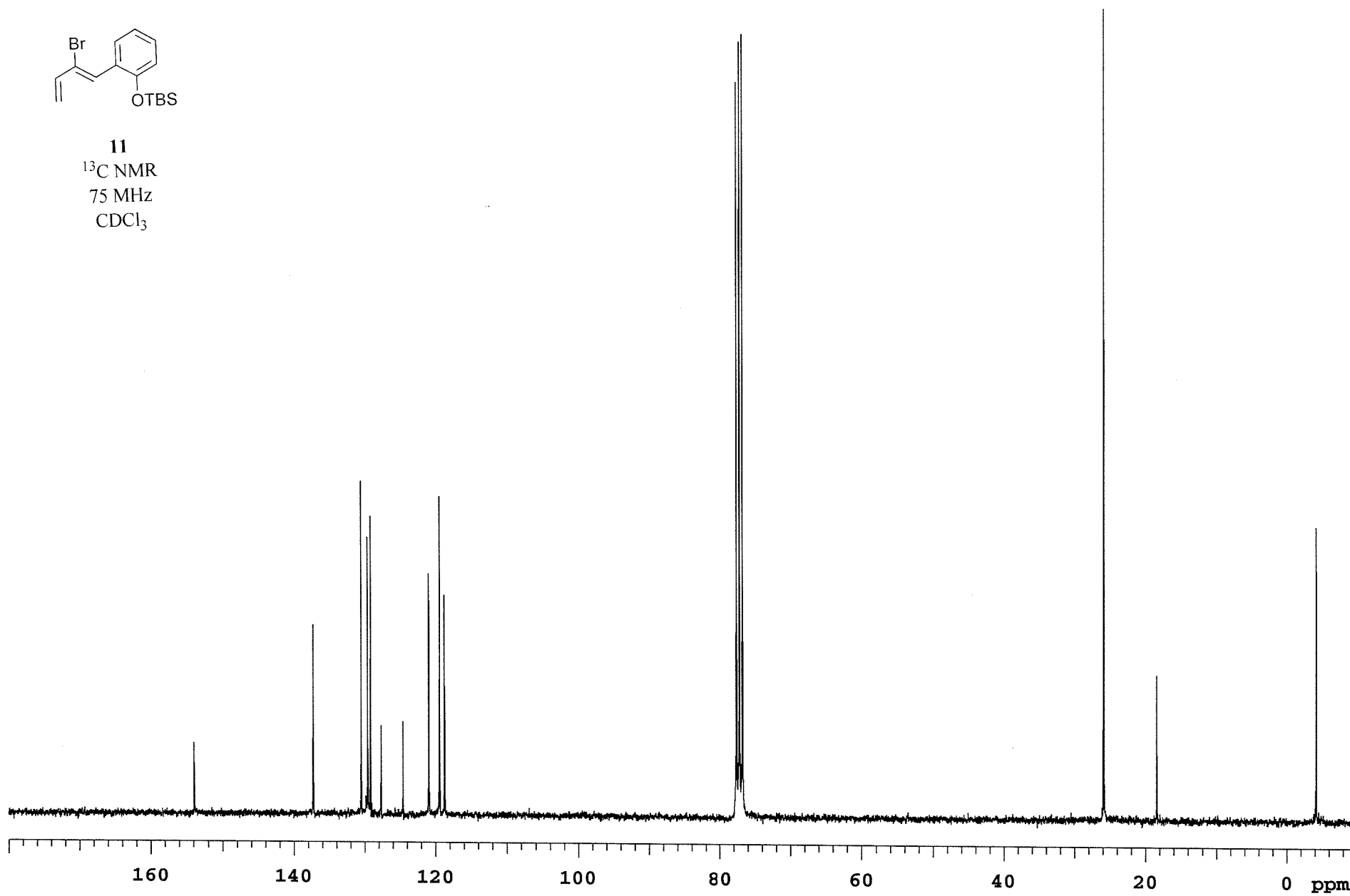


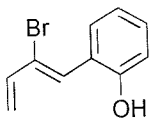
11

^{13}C NMR

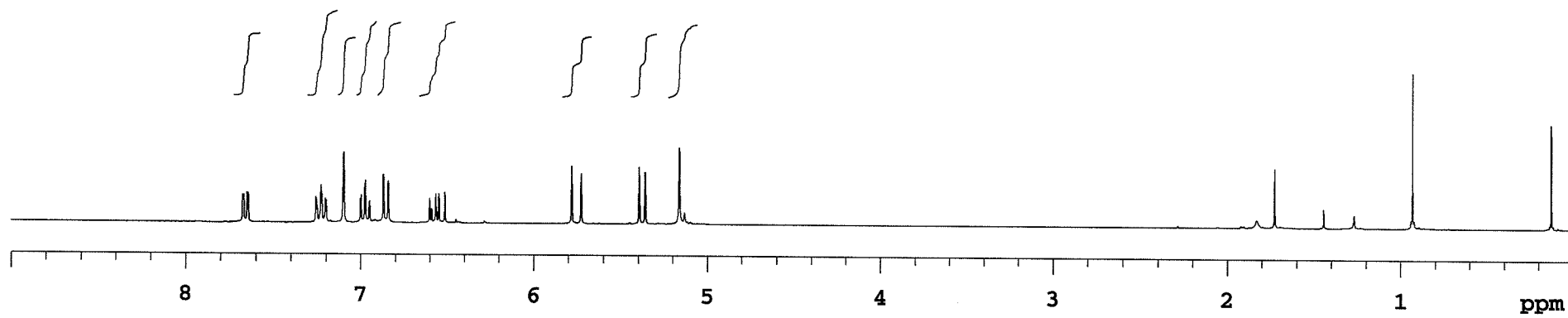
75 MHz

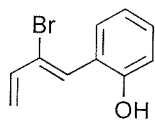
CDCl_3



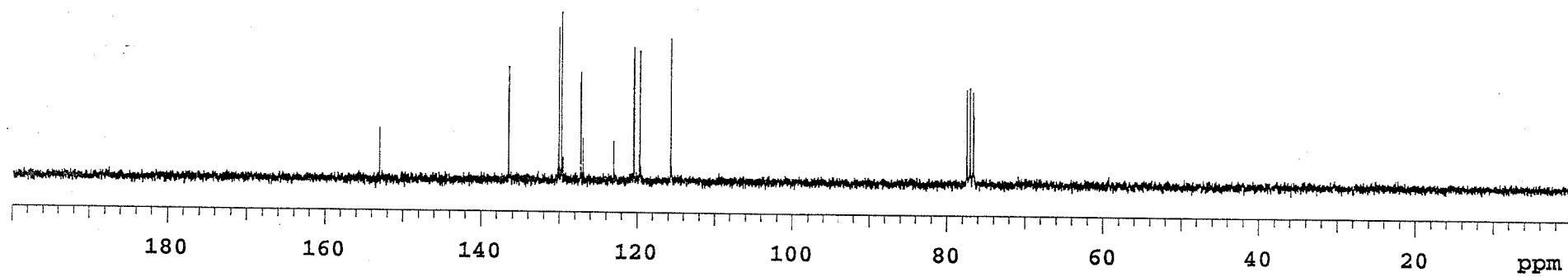


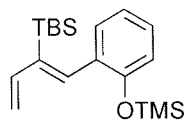
12
 ^1H NMR
300 MHz
 CDCl_3





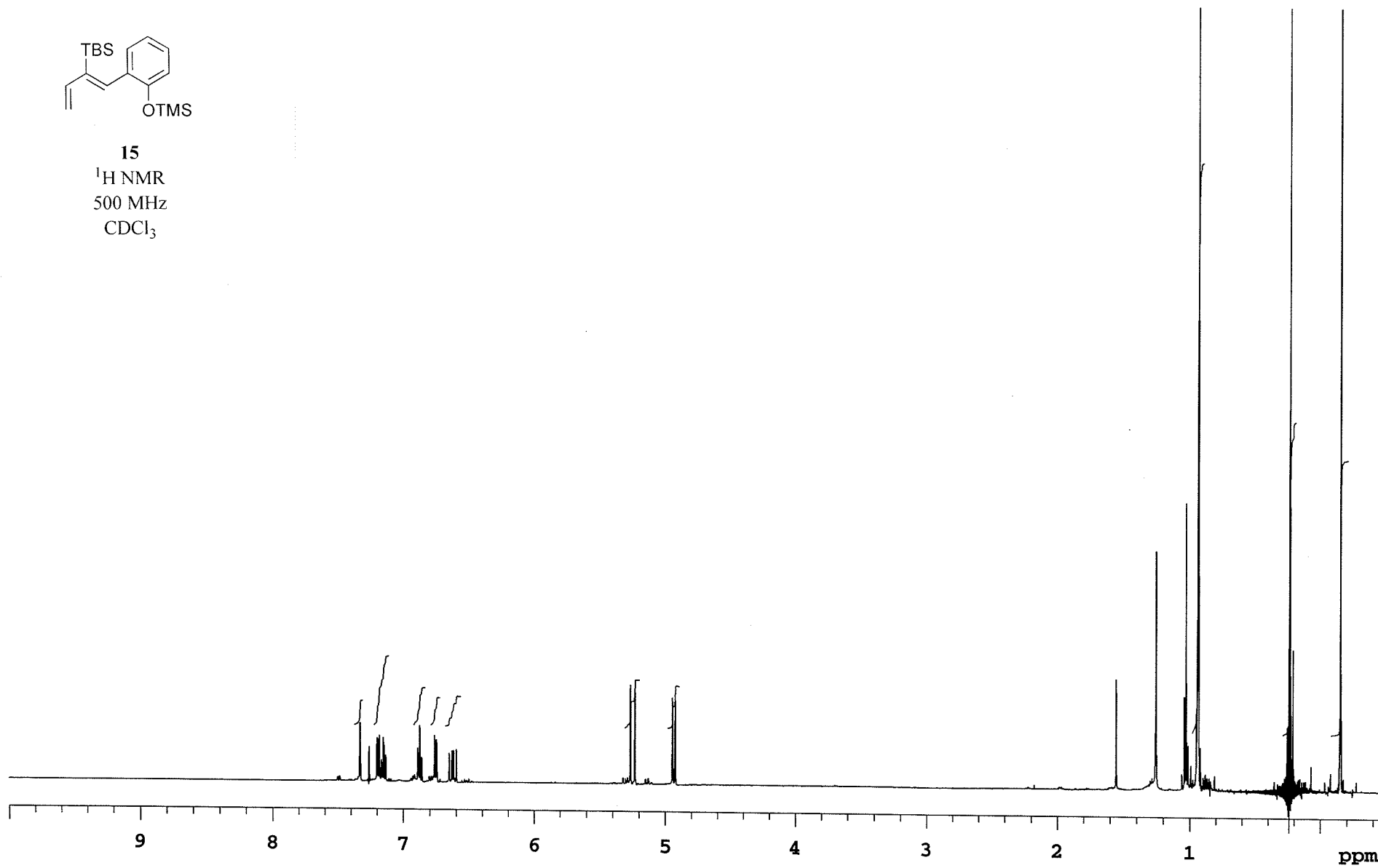
12
 ^{13}C NMR
75 MHz
 CDCl_3

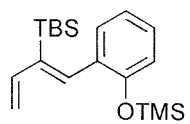




15

¹H NMR
500 MHz
CDCl₃



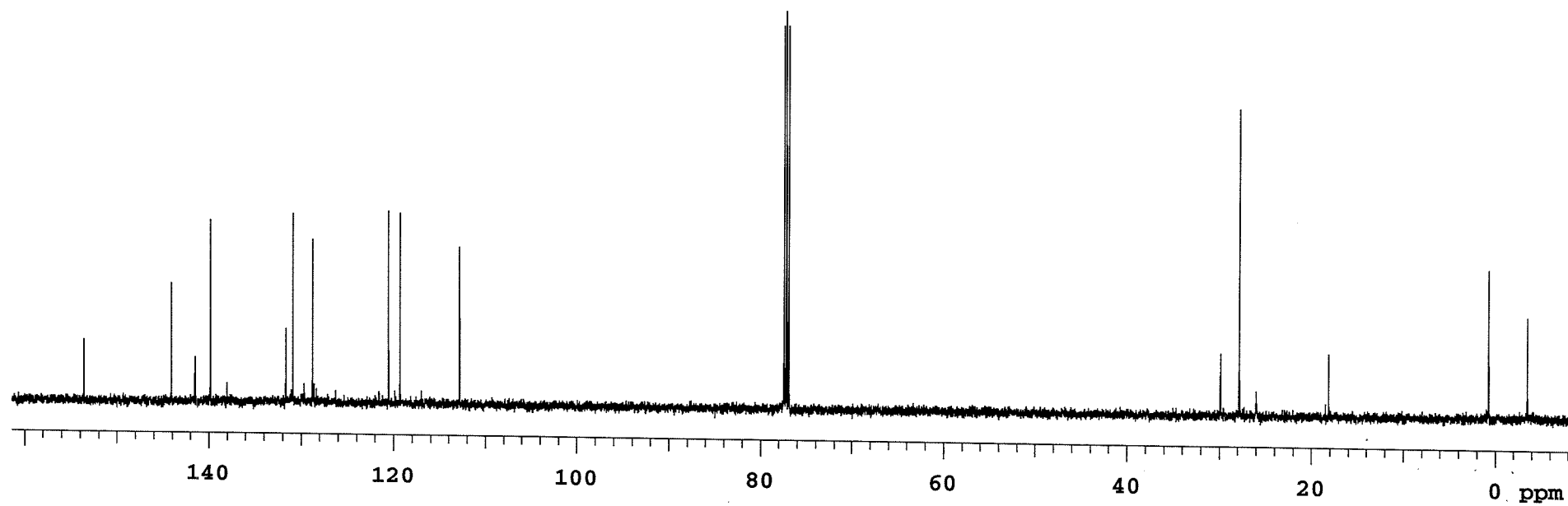


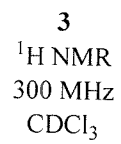
15

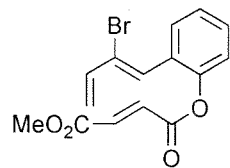
^{13}C NMR

125 MHz

CDCl_3





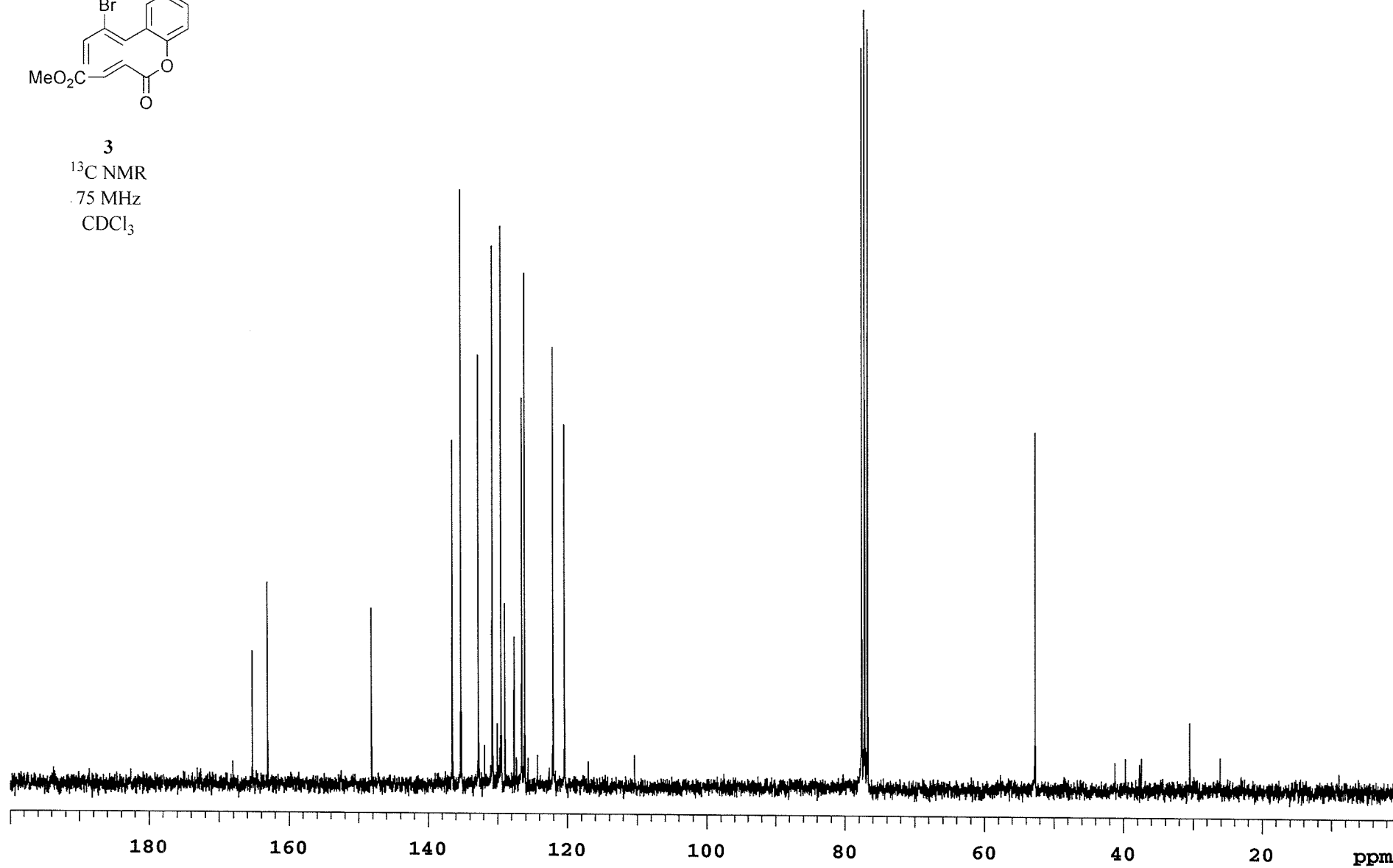


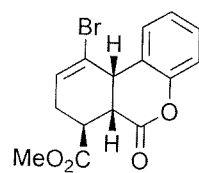
3

^{13}C NMR

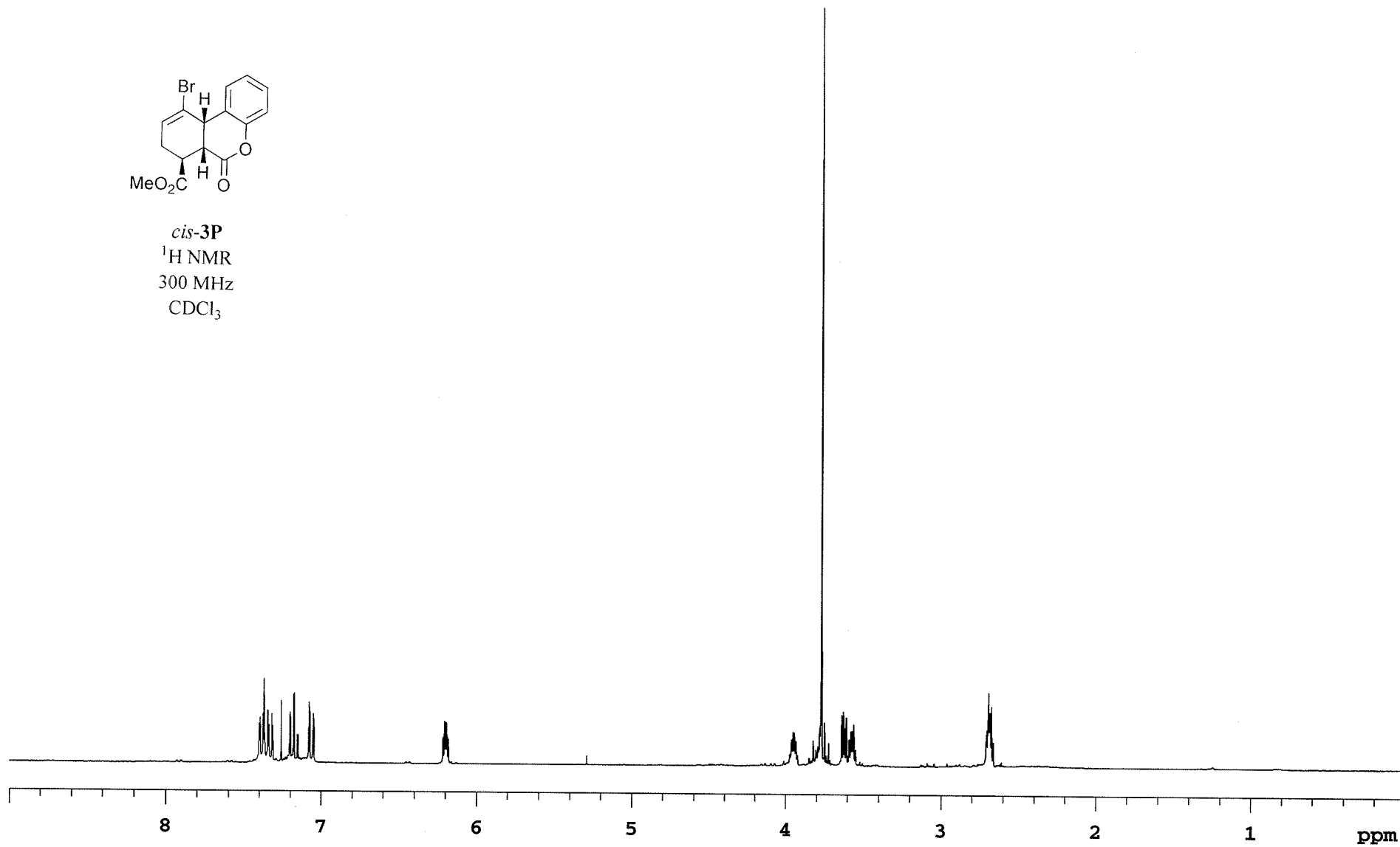
75 MHz

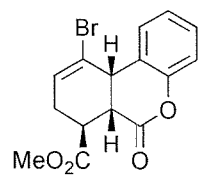
CDCl_3





cis-3P
 ^1H NMR
300 MHz
 CDCl_3



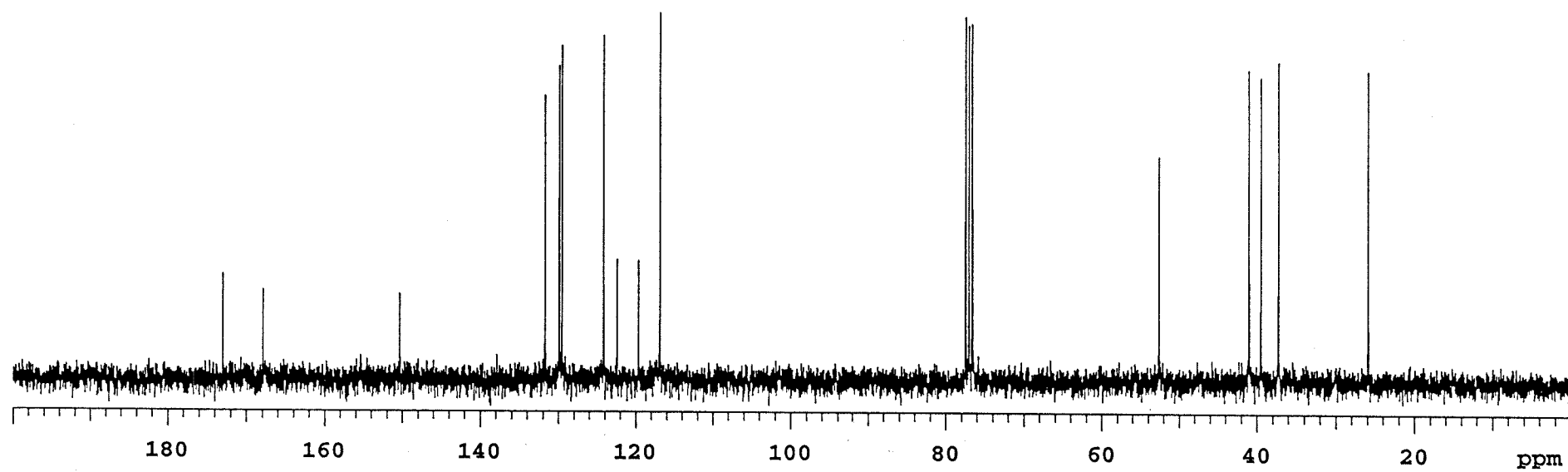


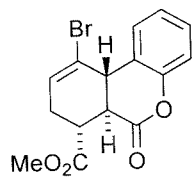
cis-3P

¹³C NMR

75 MHz

CDCl₃



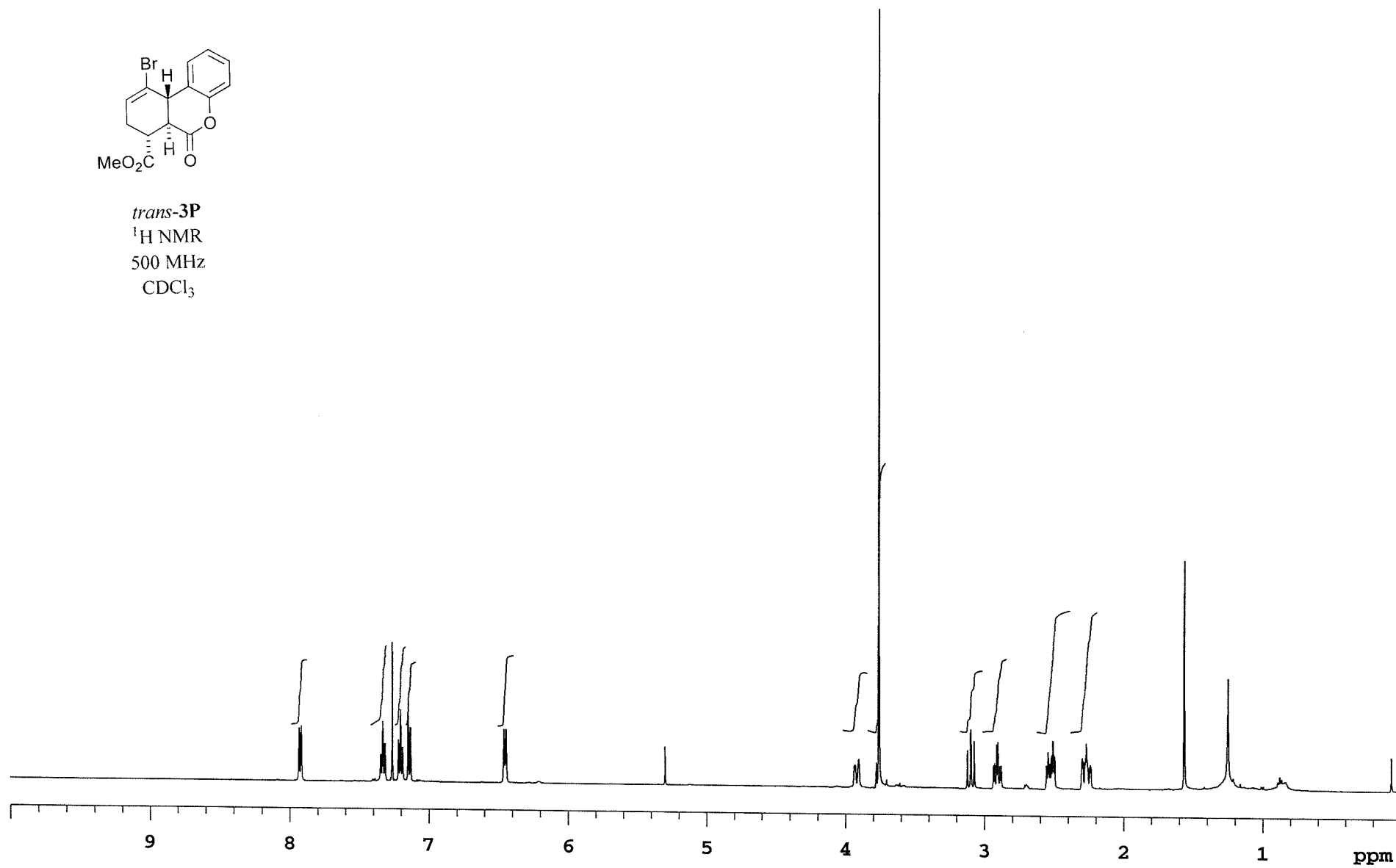


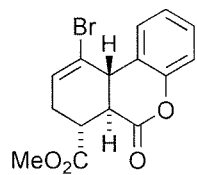
trans-**3P**

^1H NMR

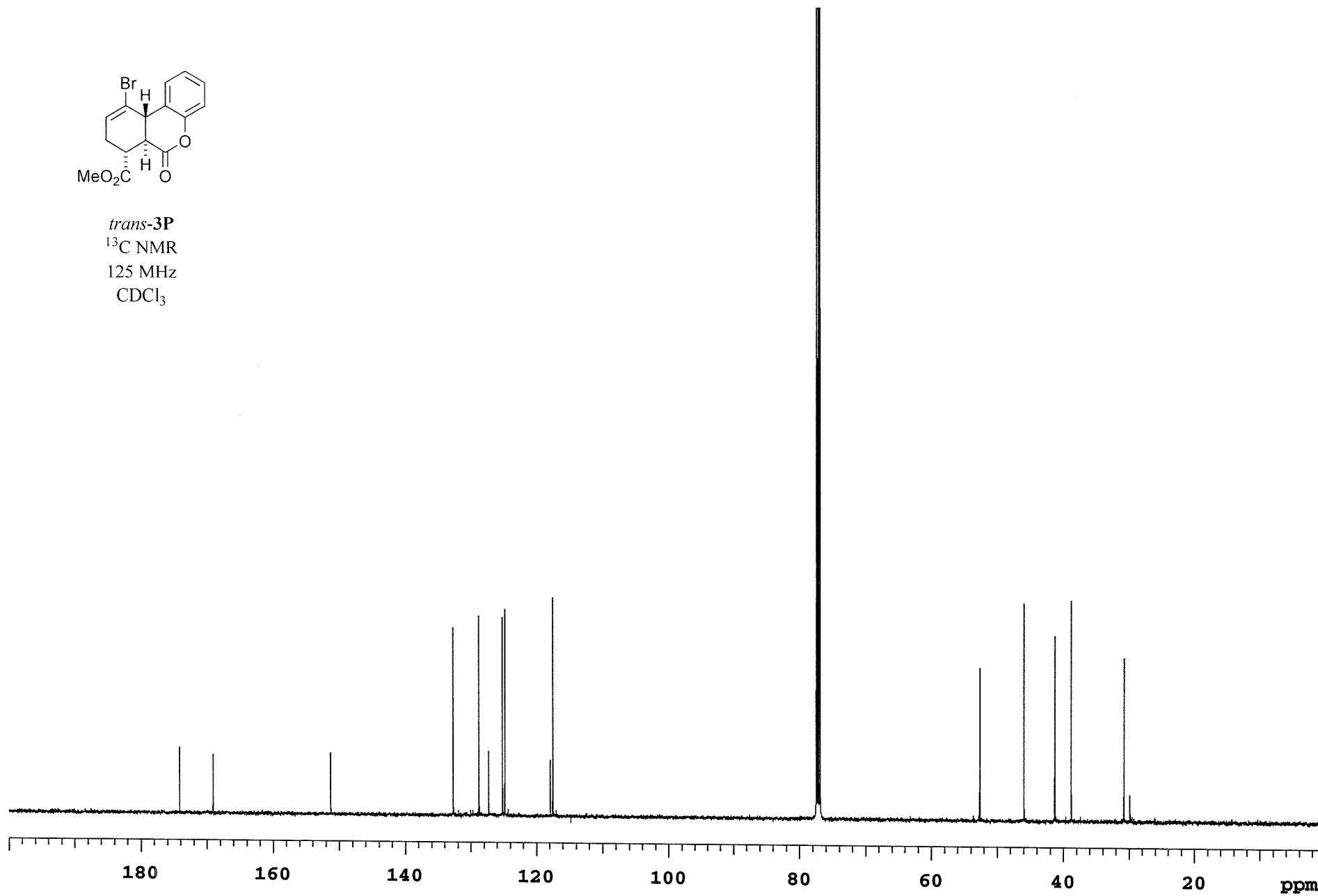
500 MHz

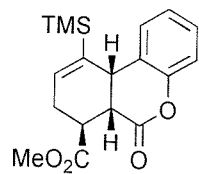
CDCl_3



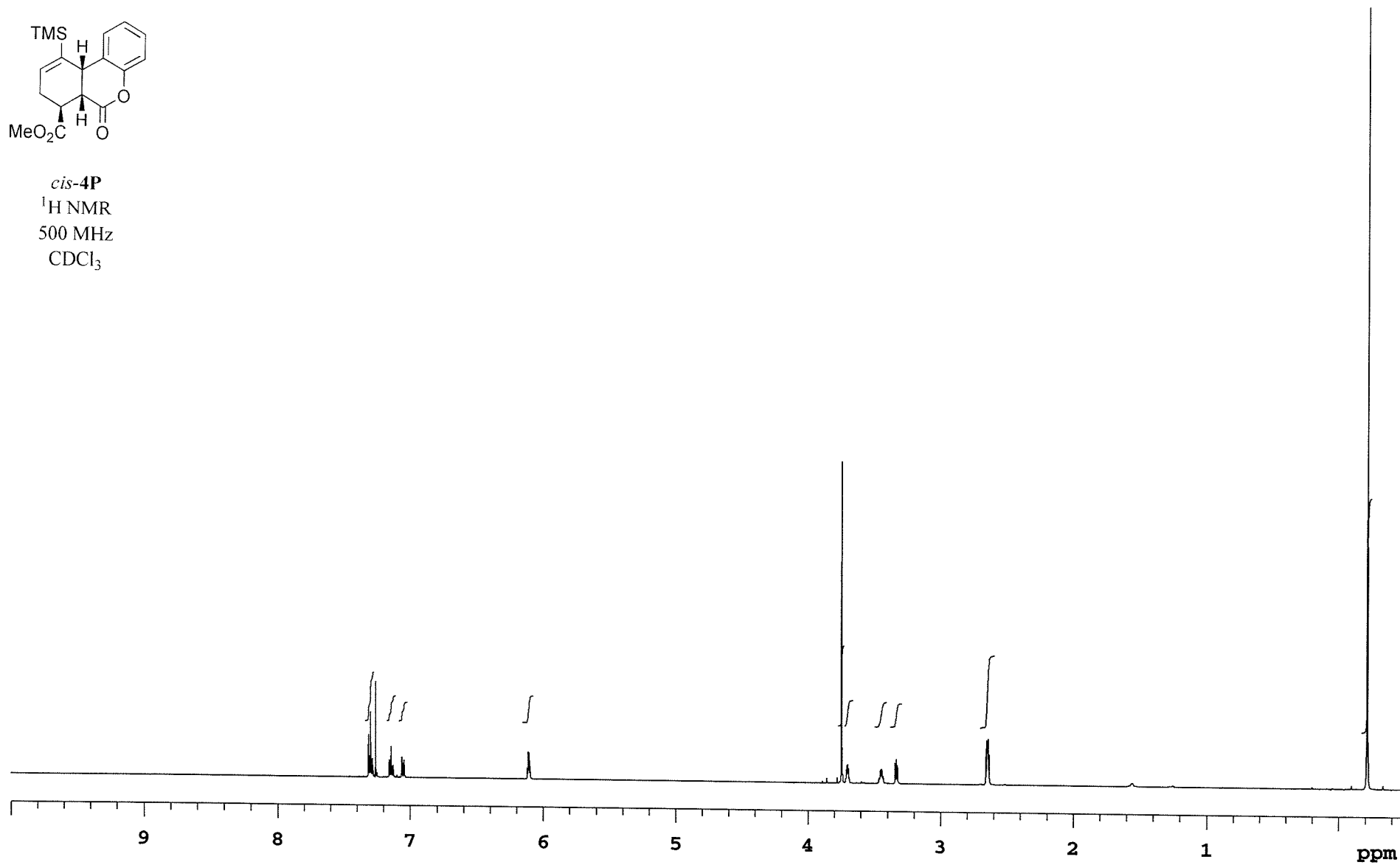


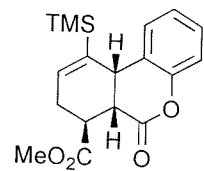
trans-3P
¹³C NMR
 125 MHz
 CDCl₃





cis-4P
 ^1H NMR
 500 MHz
 CDCl_3



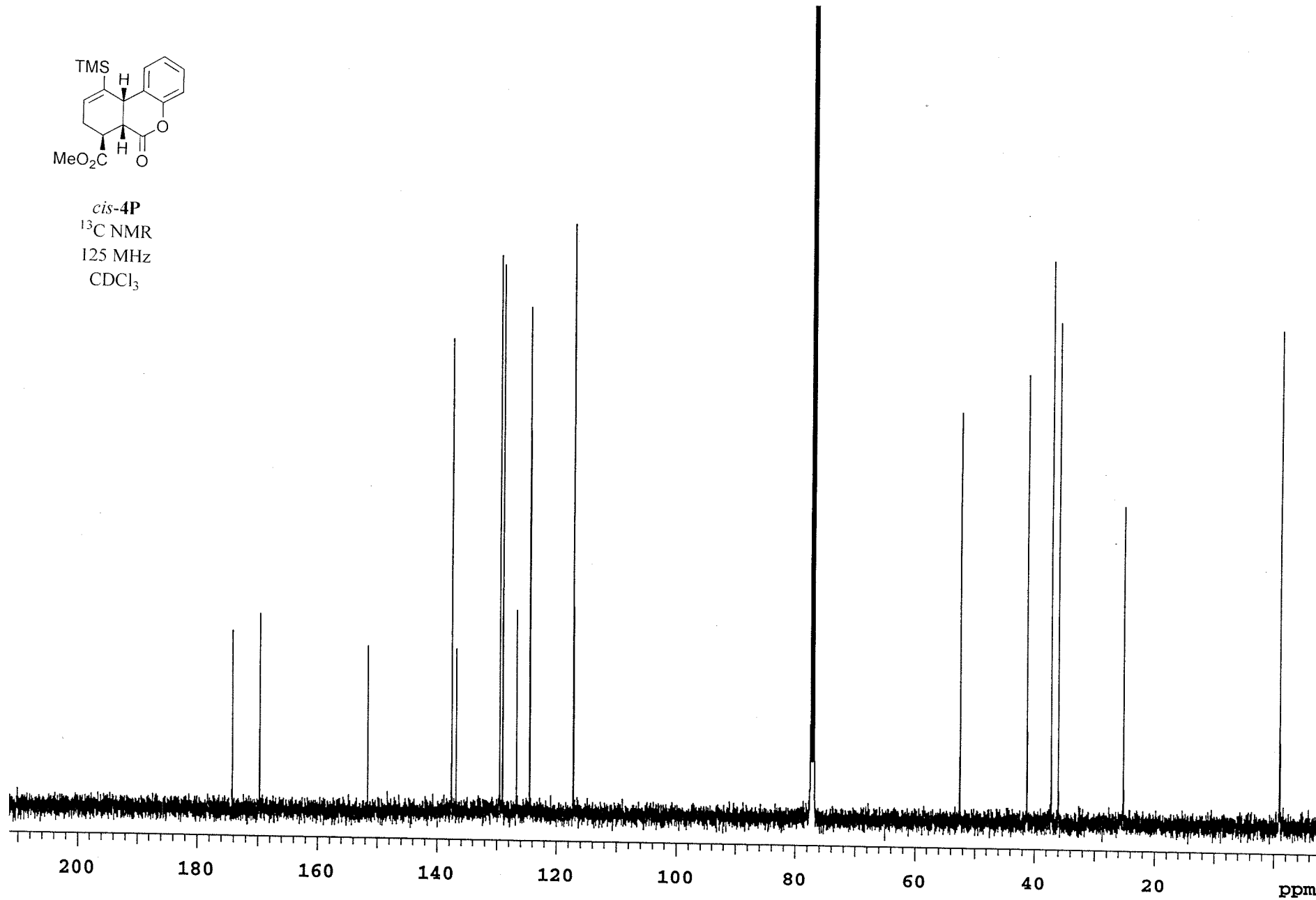


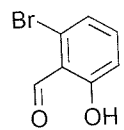
cis-4P

^{13}C NMR

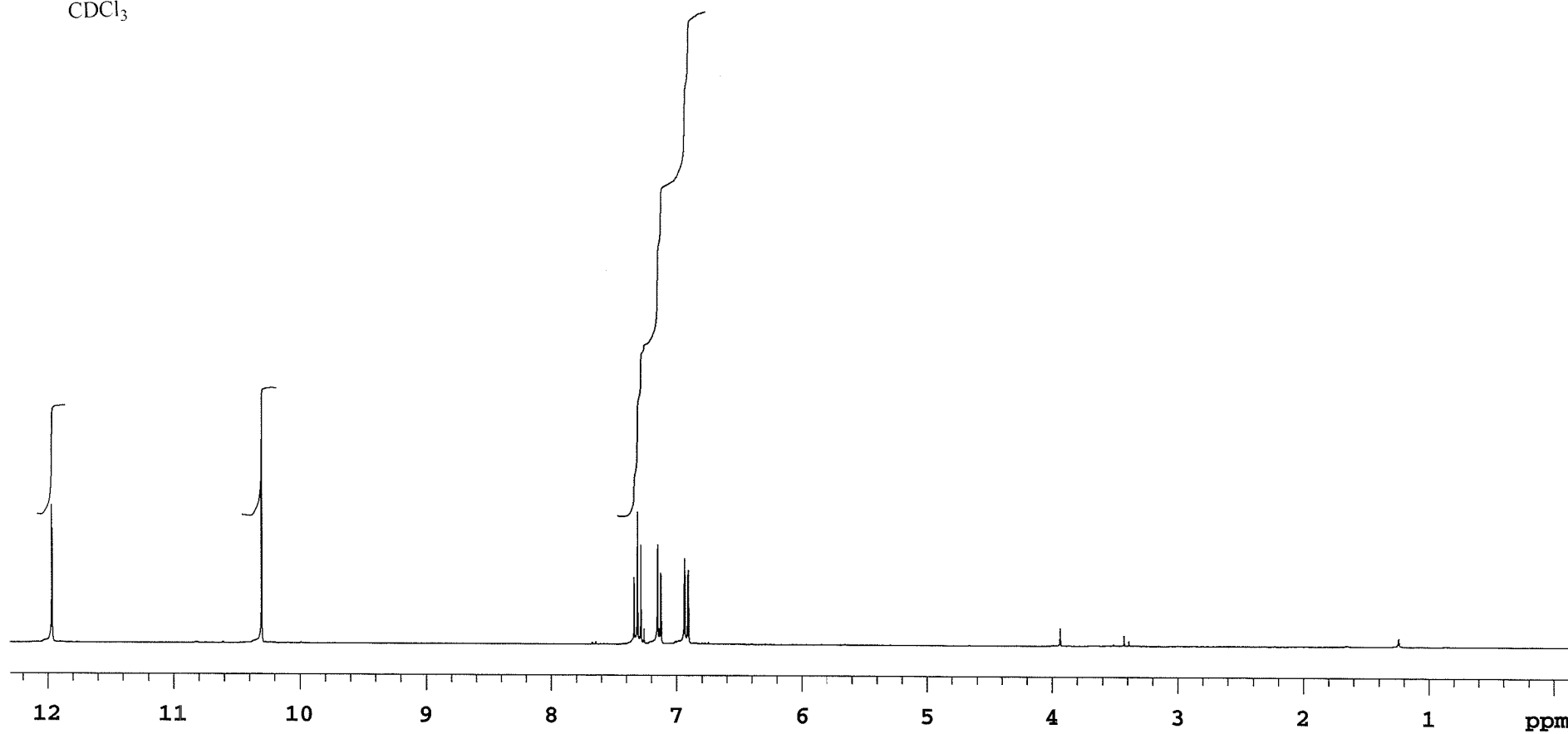
125 MHz

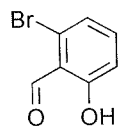
CDCl_3





17
 ^1H NMR
300 MHz
 CDCl_3



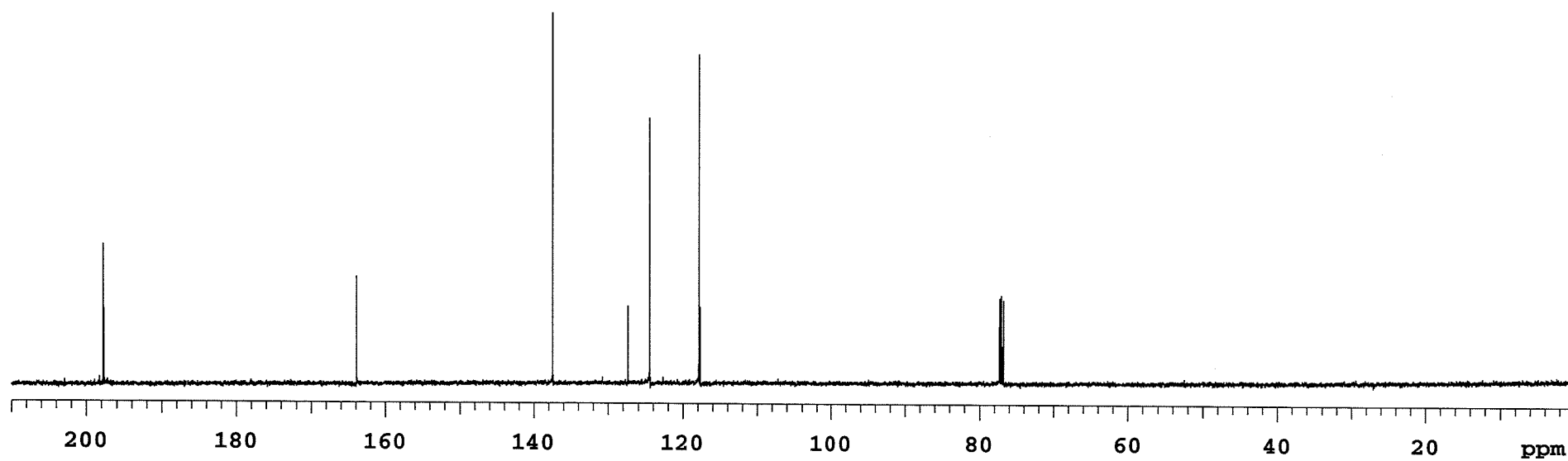


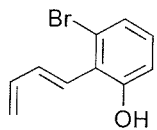
17

^{13}C NMR

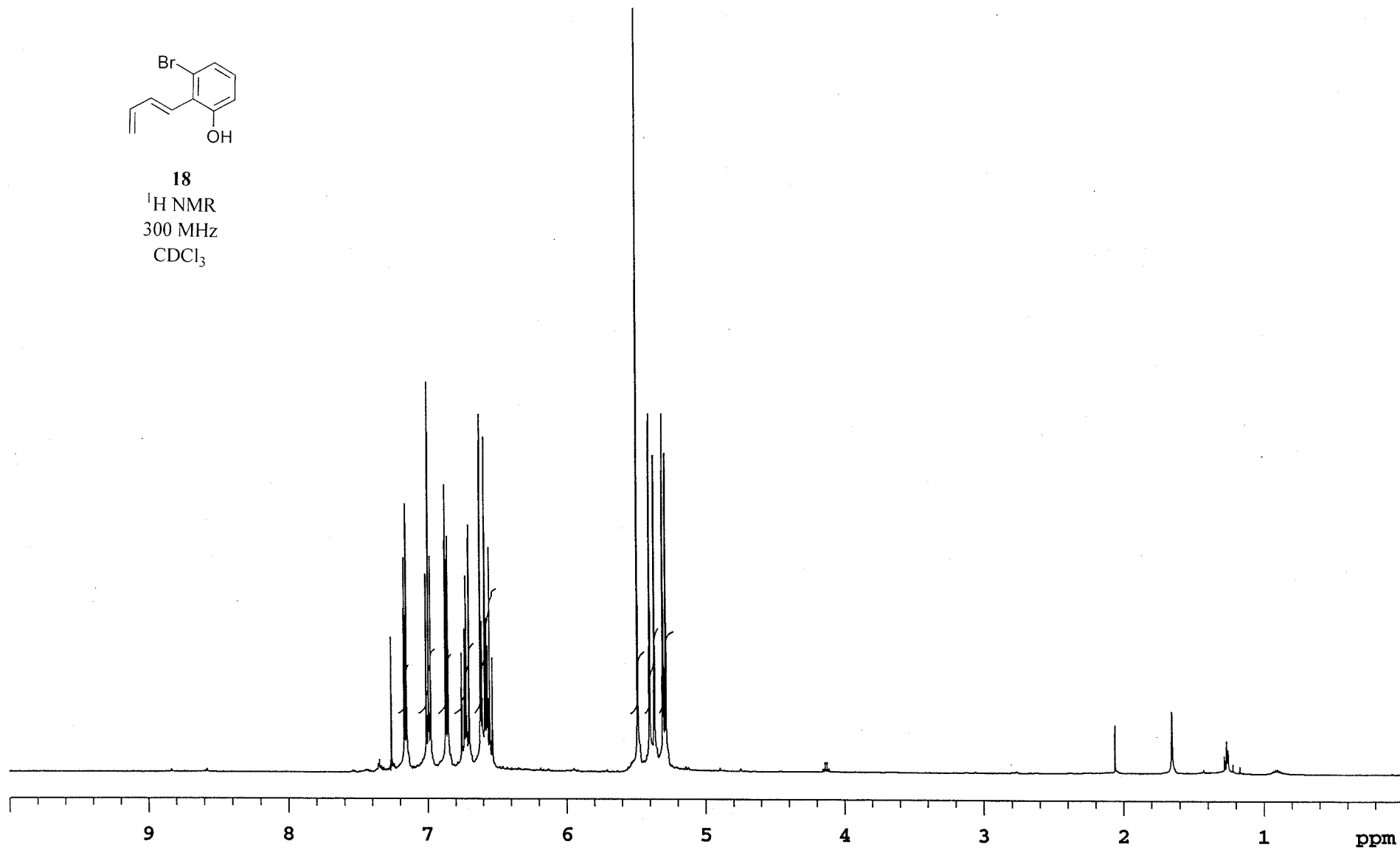
75 MHz

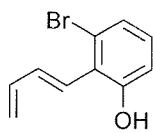
CDCl_3





18
 ^1H NMR
300 MHz
 CDCl_3



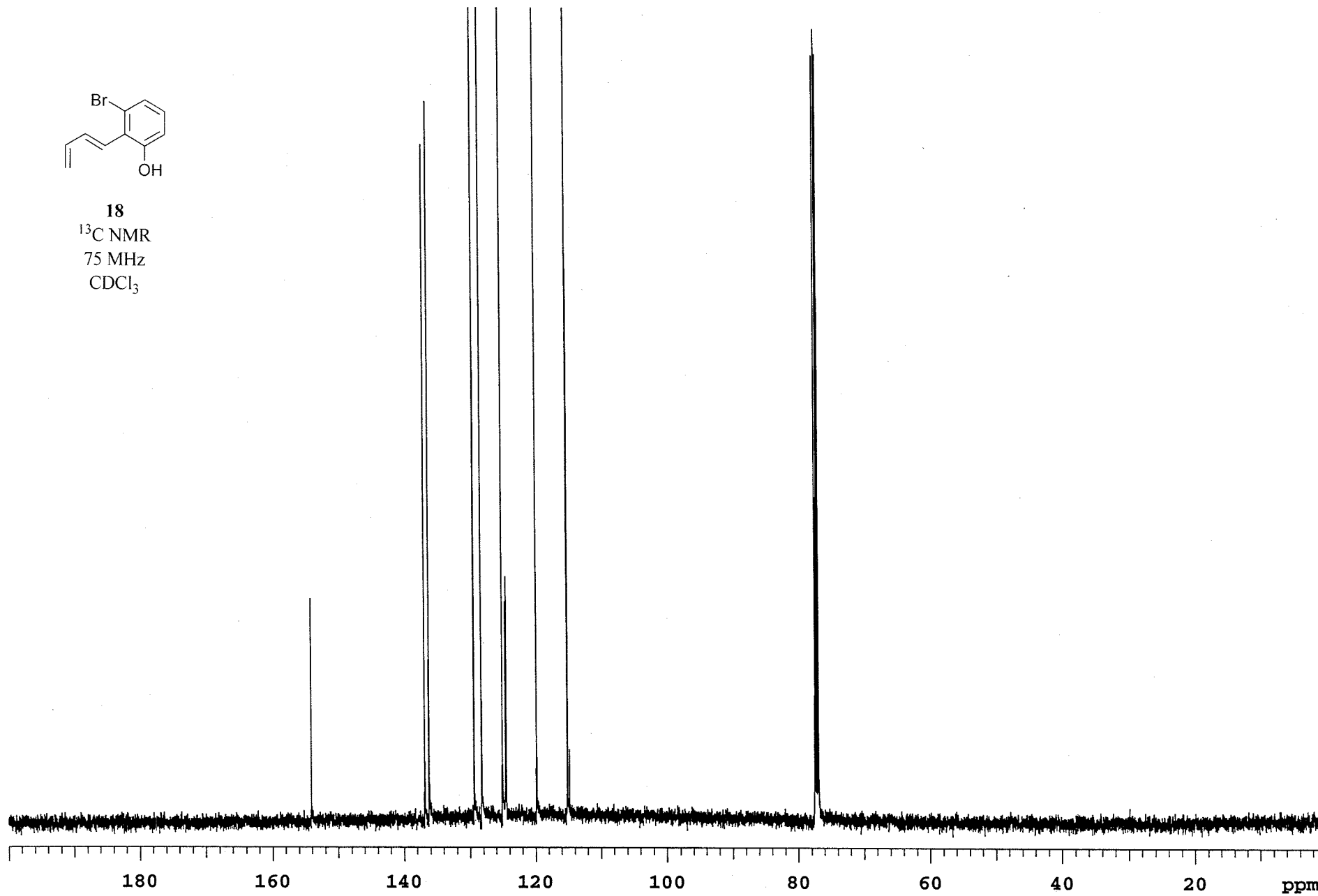


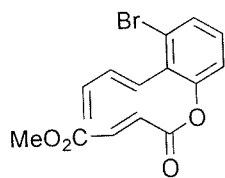
18

^{13}C NMR

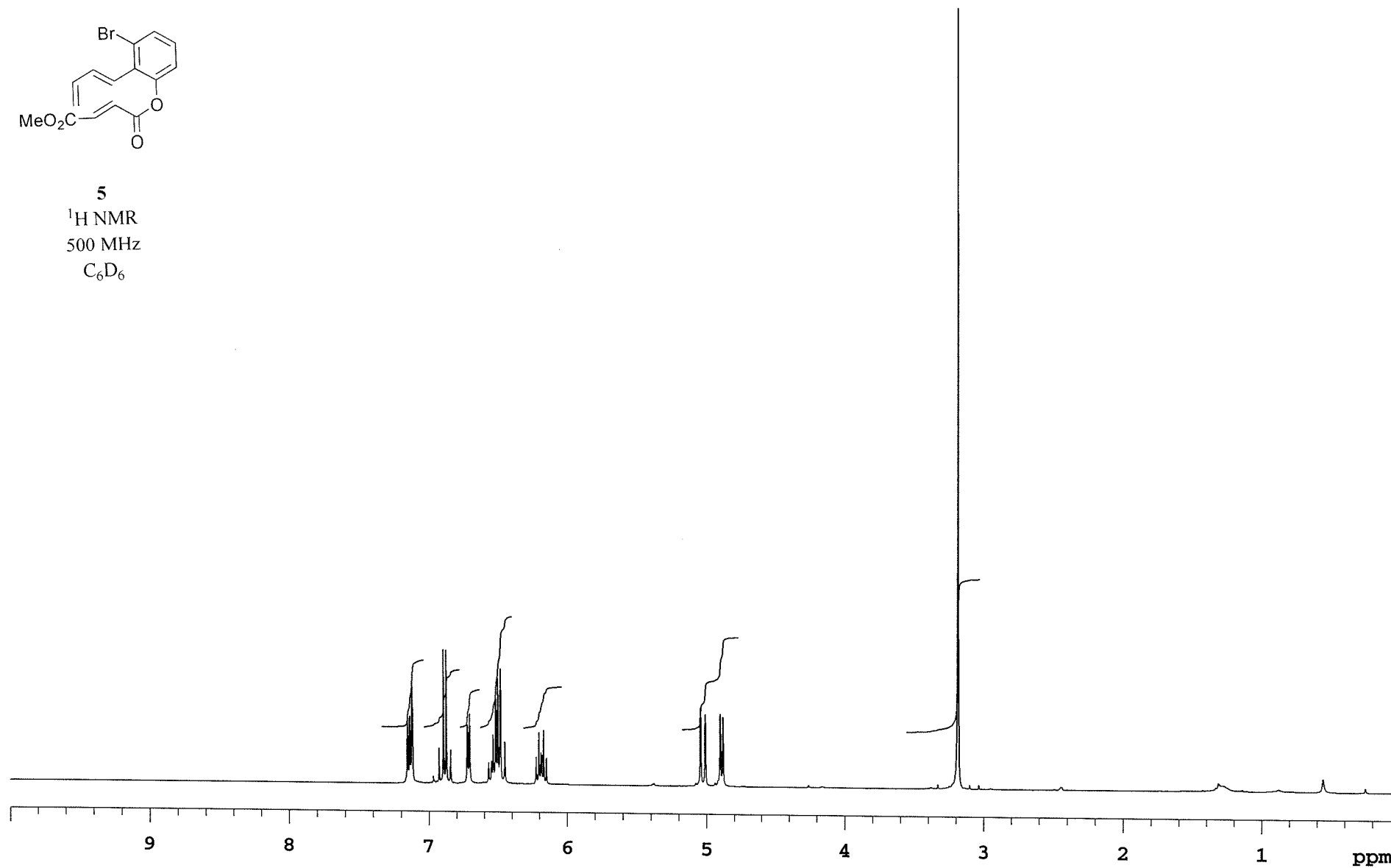
75 MHz

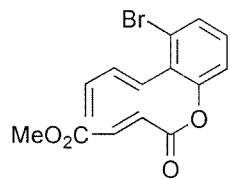
CDCl_3



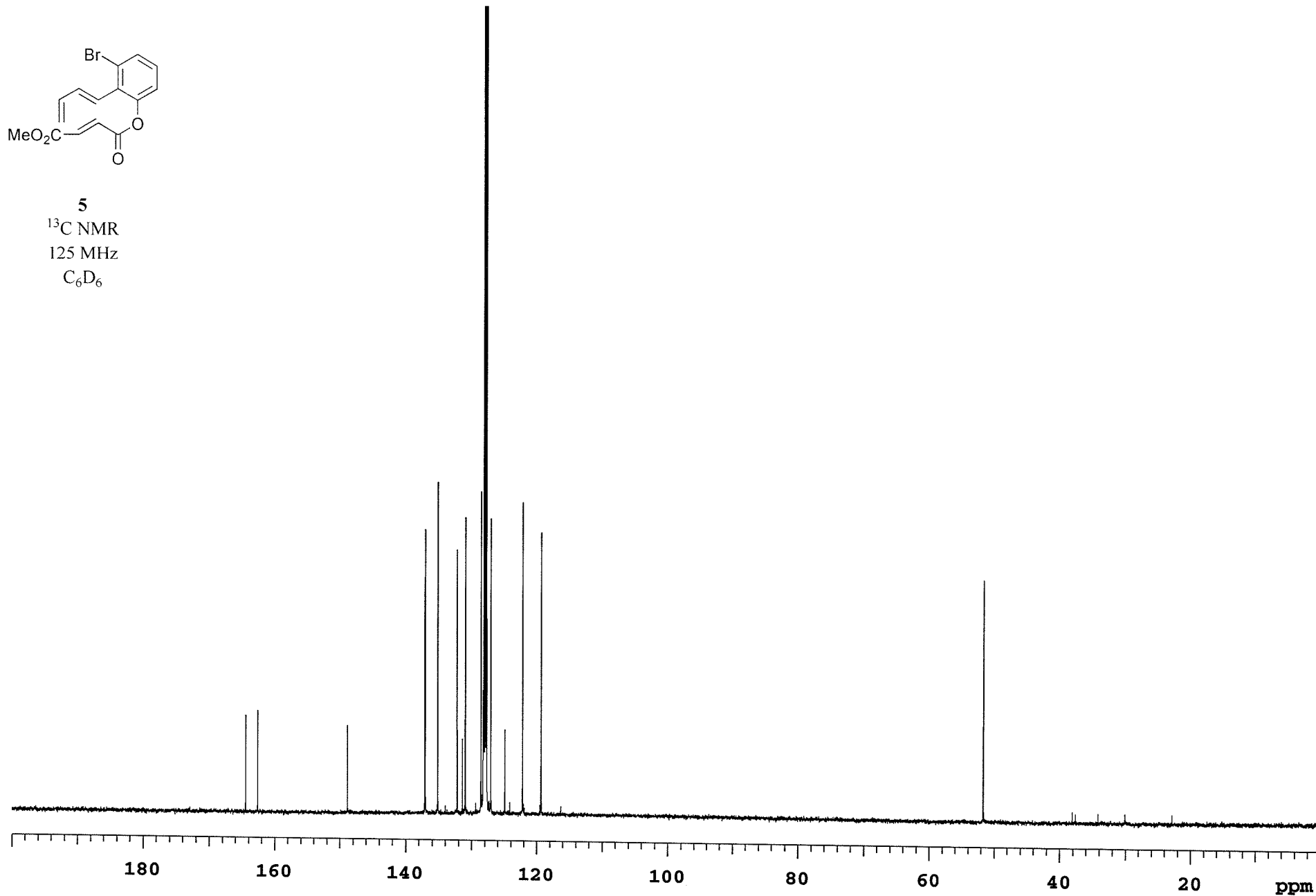


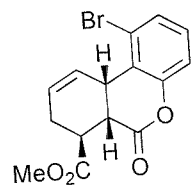
5
 ^1H NMR
500 MHz
 C_6D_6



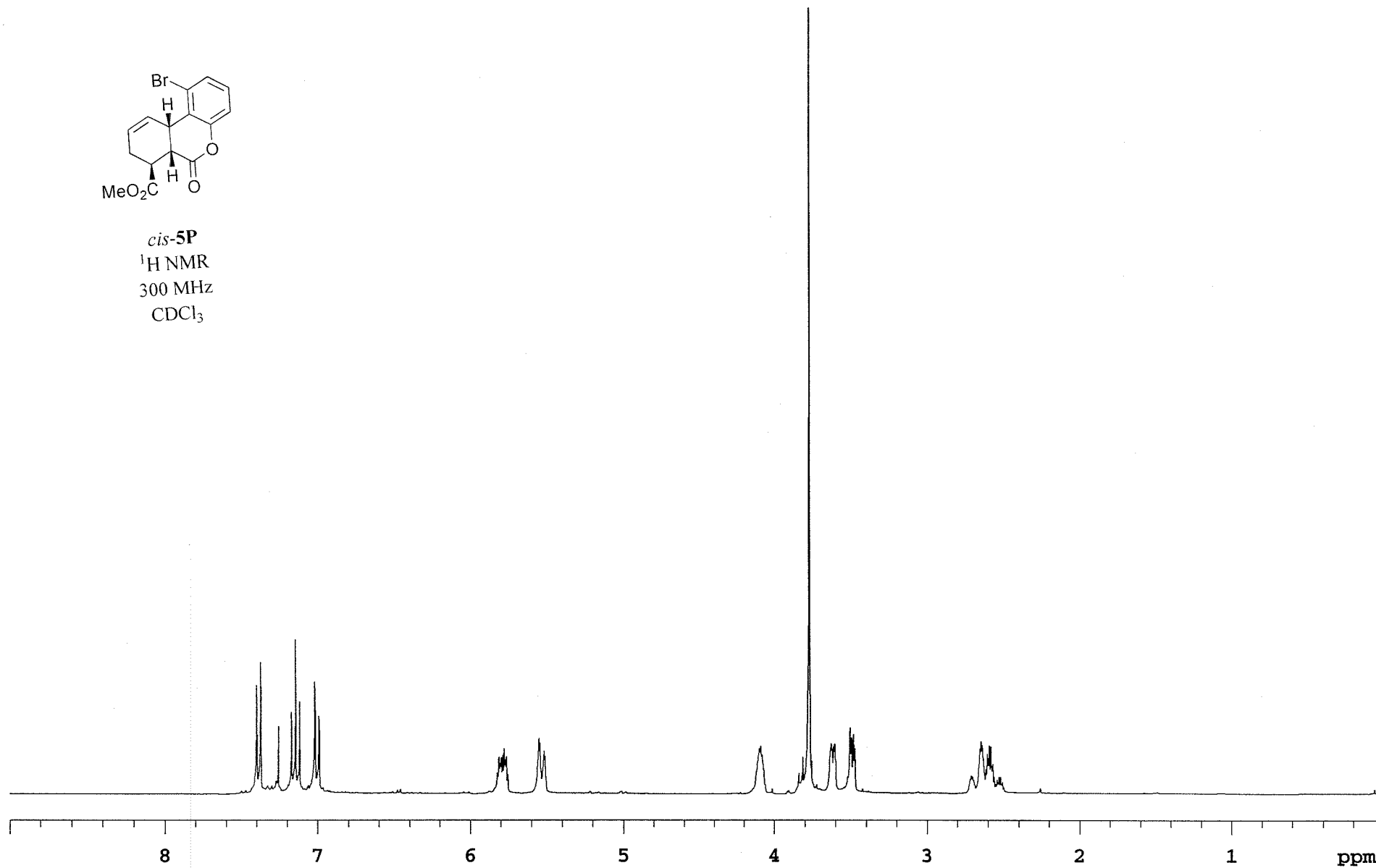


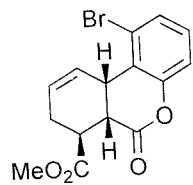
5
 ^{13}C NMR
 125 MHz
 C_6D_6





cis-**5P**
 ^1H NMR
 300 MHz
 CDCl_3



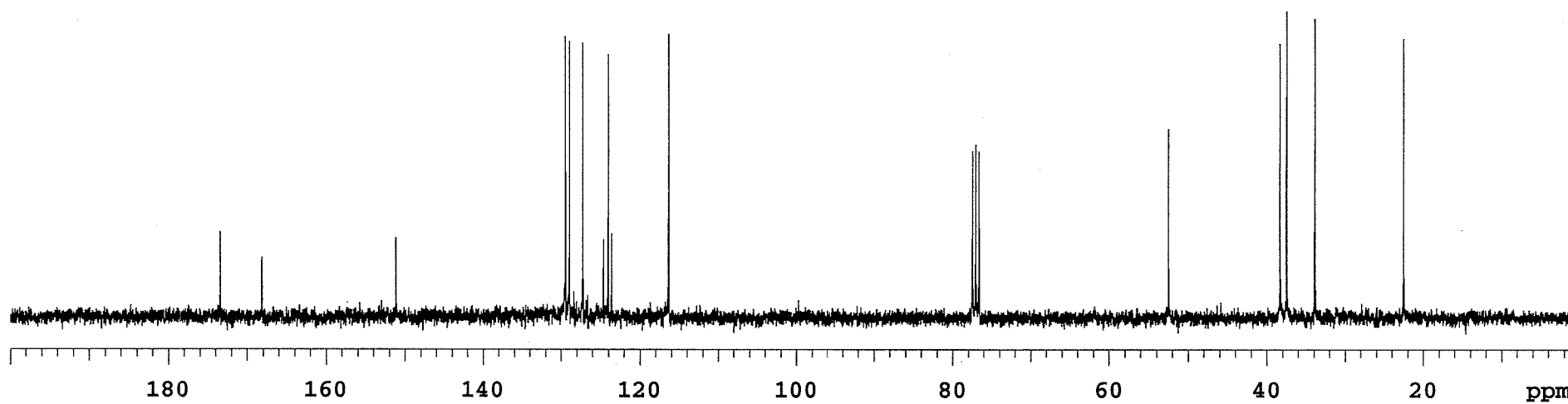


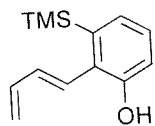
cis-**5P**

^{13}C NMR

75 MHz

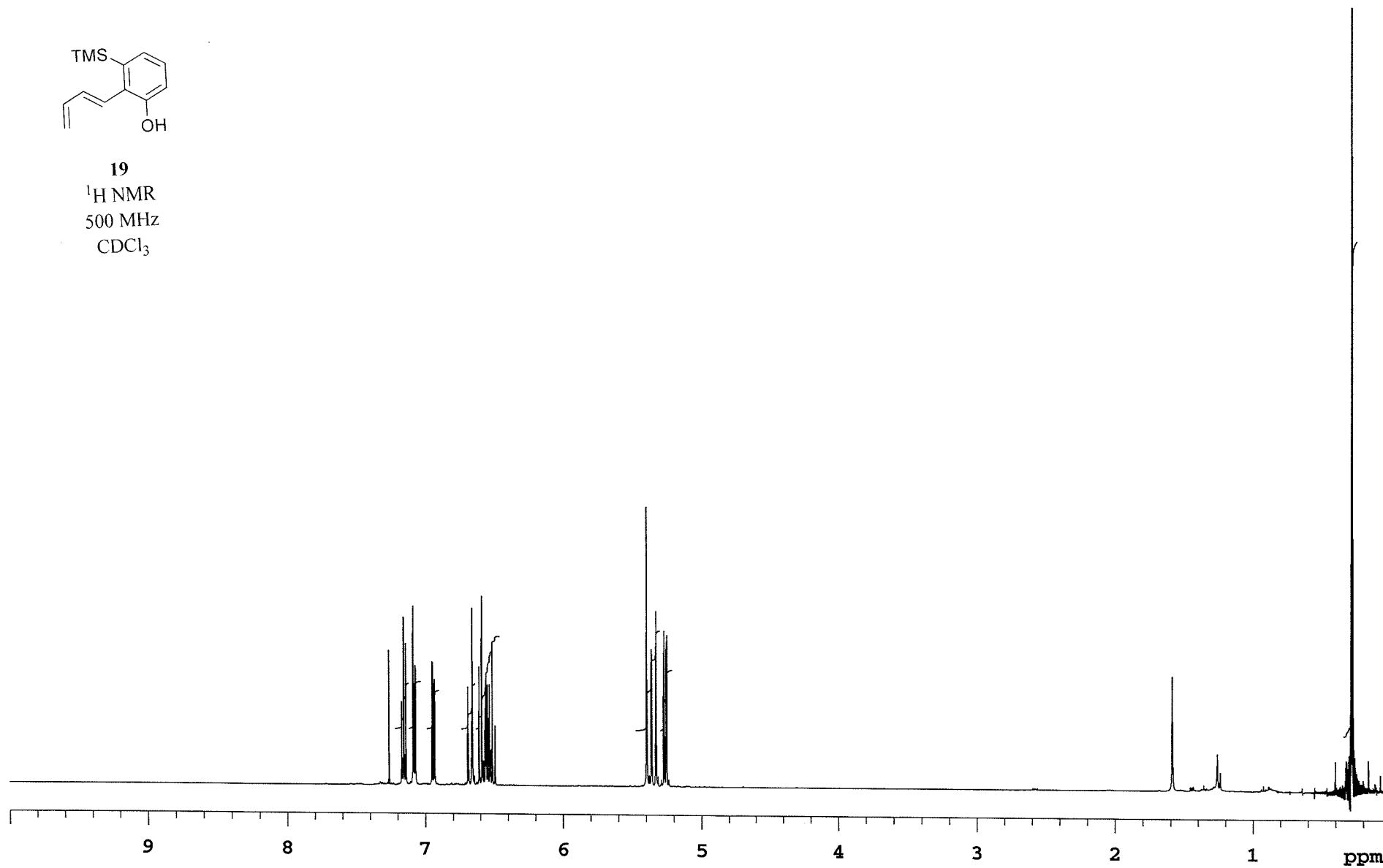
CDCl_3

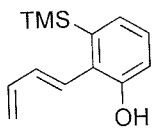




19

^1H NMR
500 MHz
 CDCl_3



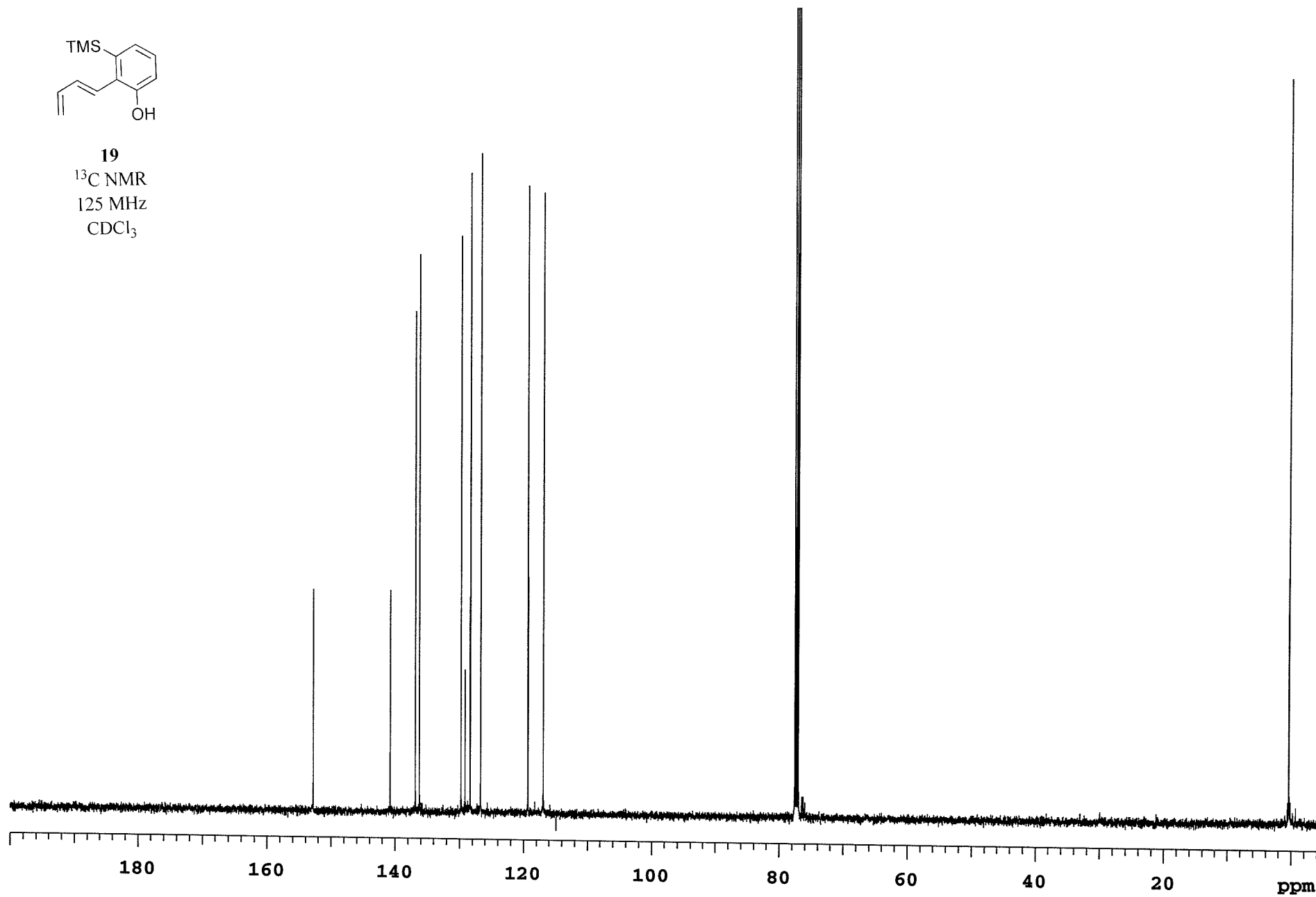


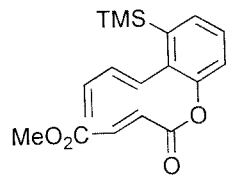
19

^{13}C NMR

125 MHz

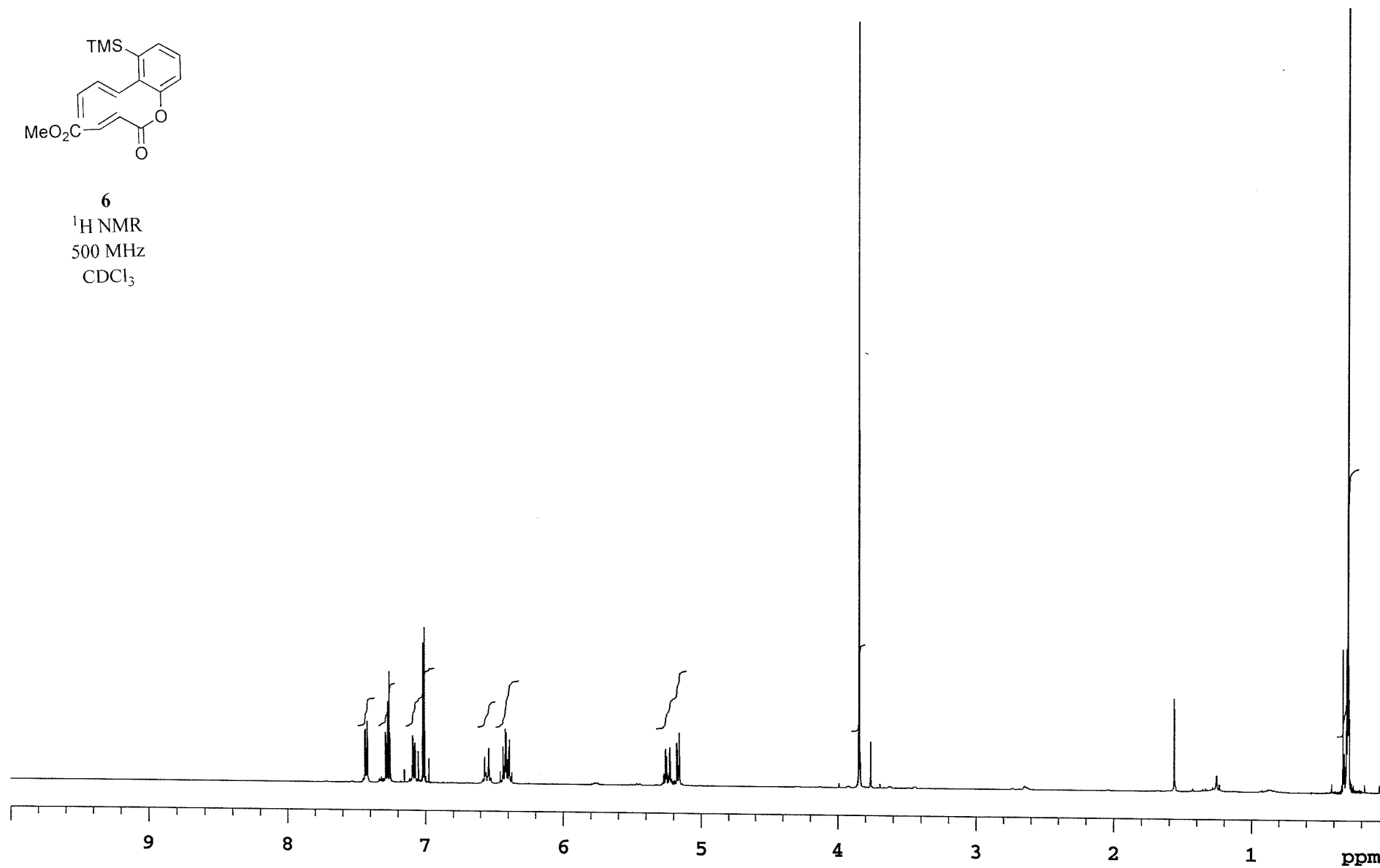
CDCl_3

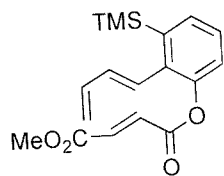




6

¹H NMR
500 MHz
CDCl₃



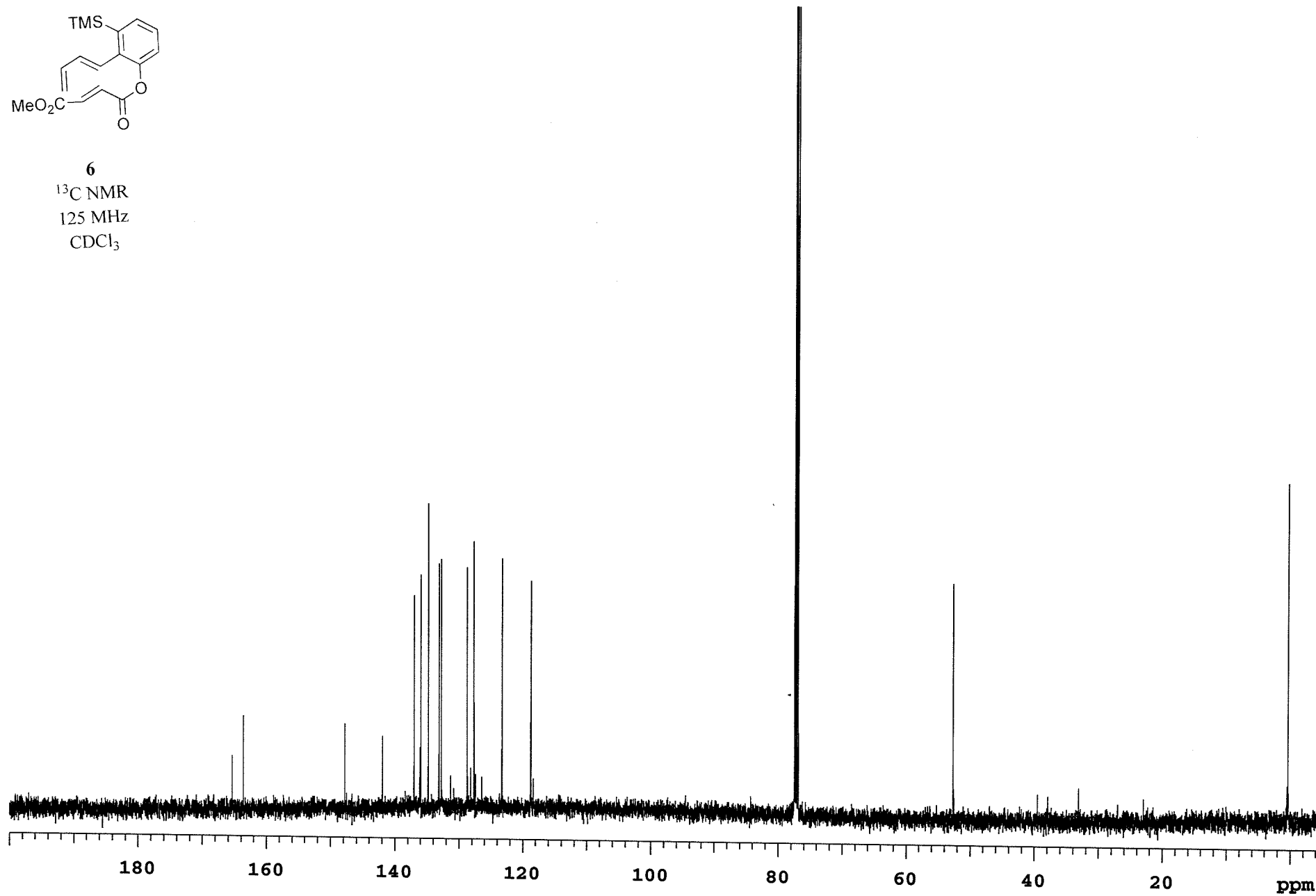


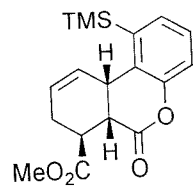
6

^{13}C NMR

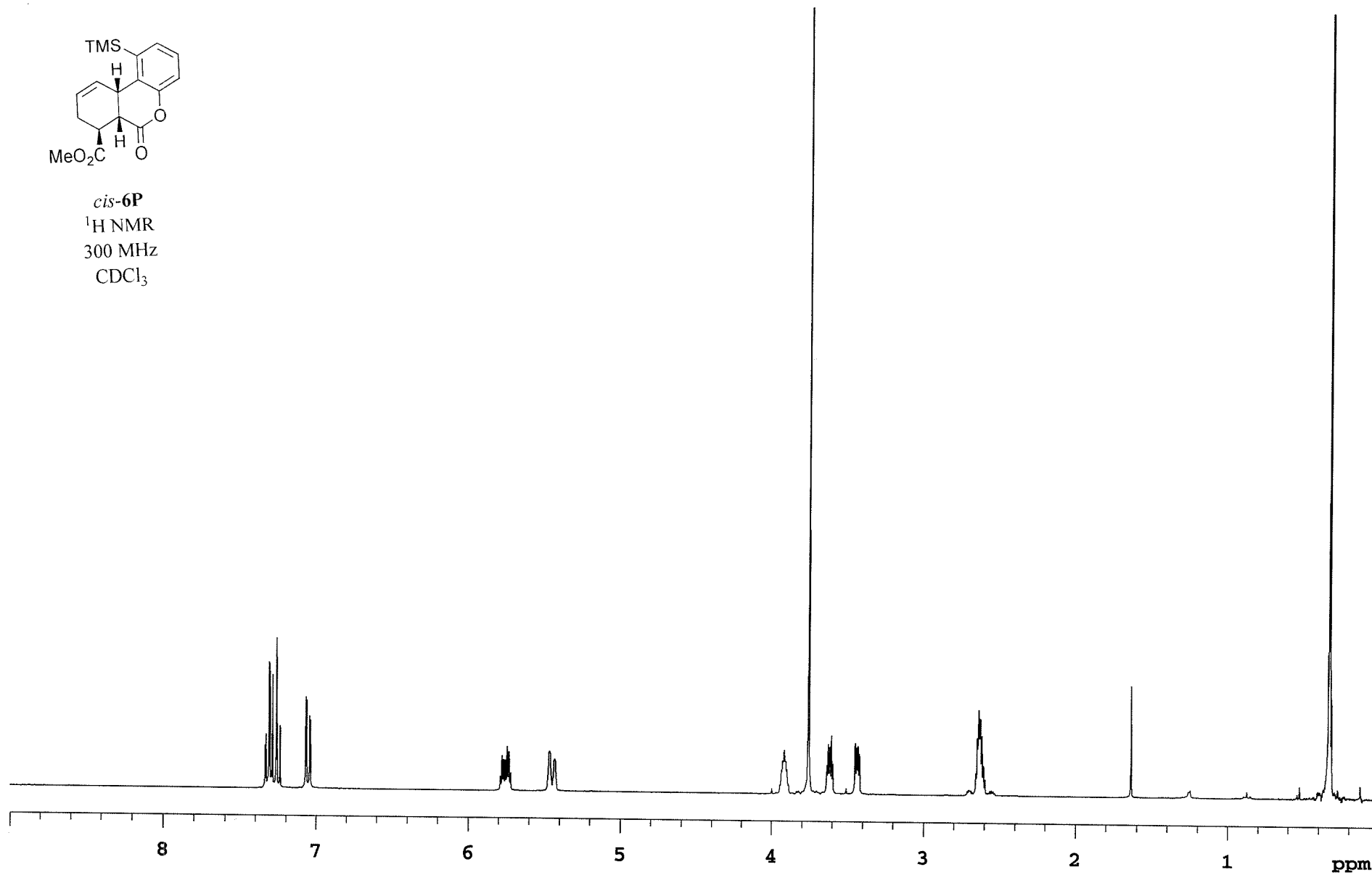
125 MHz

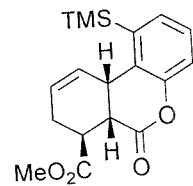
CDCl_3



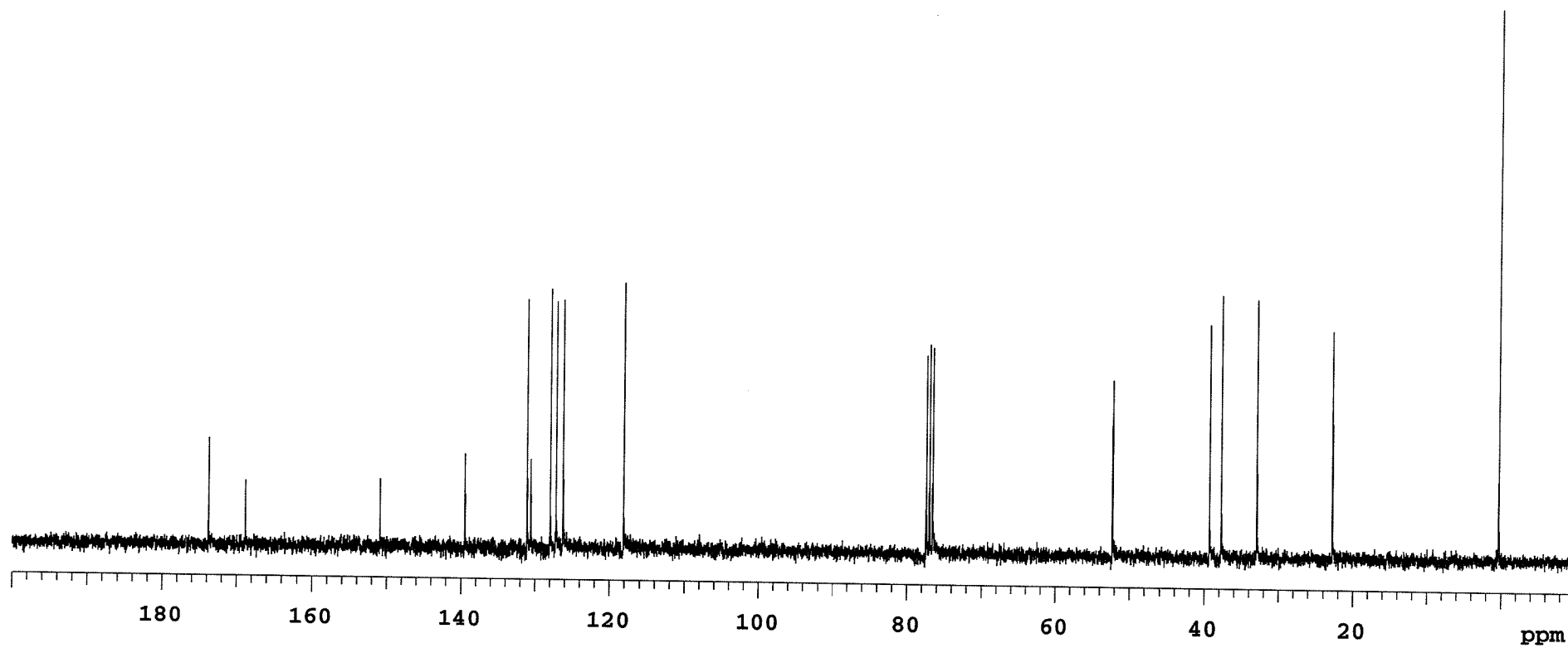


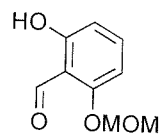
cis-**6P**
 ^1H NMR
 300 MHz
 CDCl_3





cis-6P
 ^{13}C NMR
 75 MHz
 CDCl_3



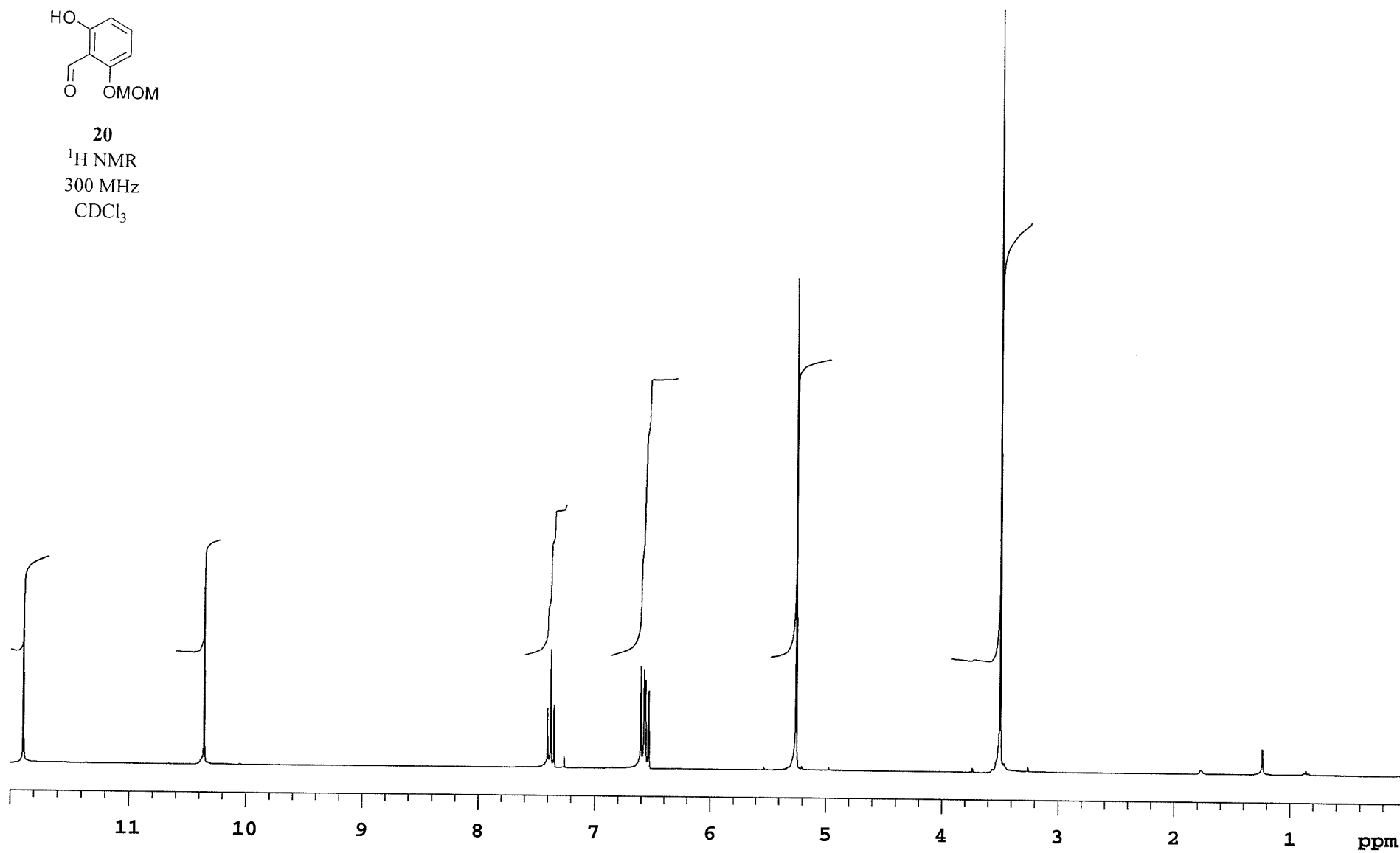


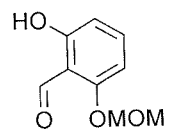
20

^1H NMR

300 MHz

CDCl_3



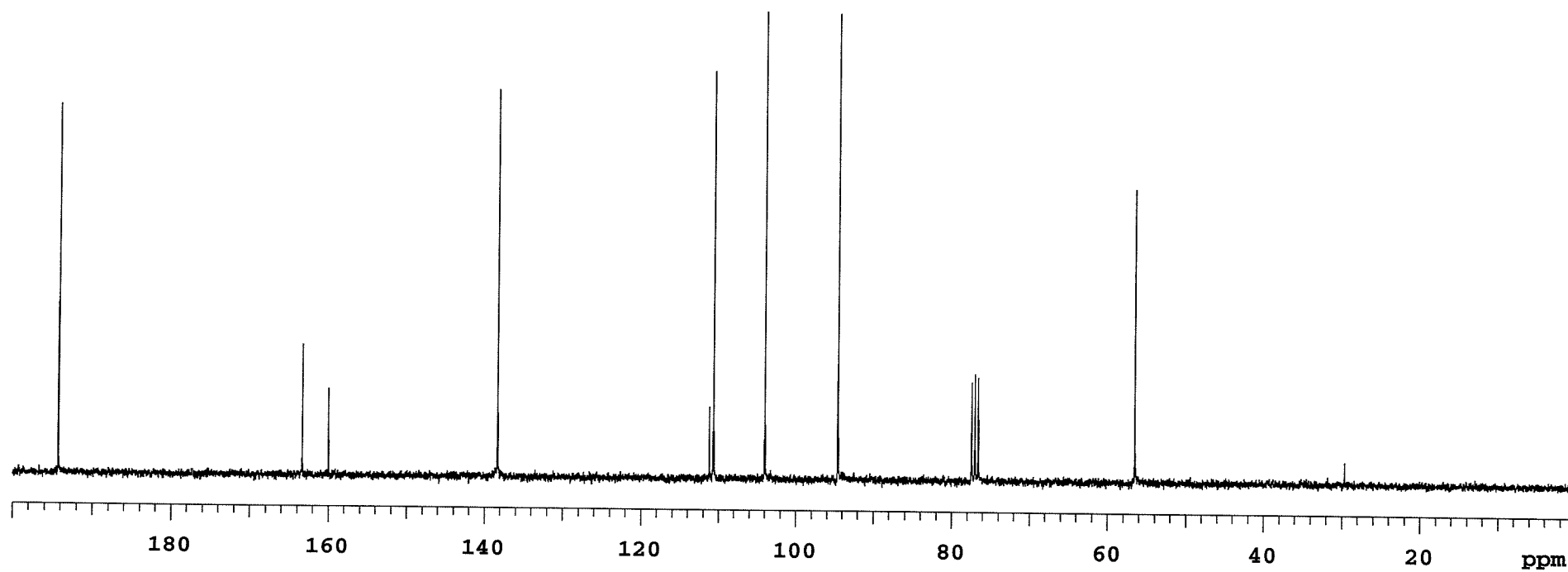


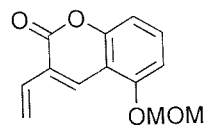
20

^{13}C NMR

75 MHz

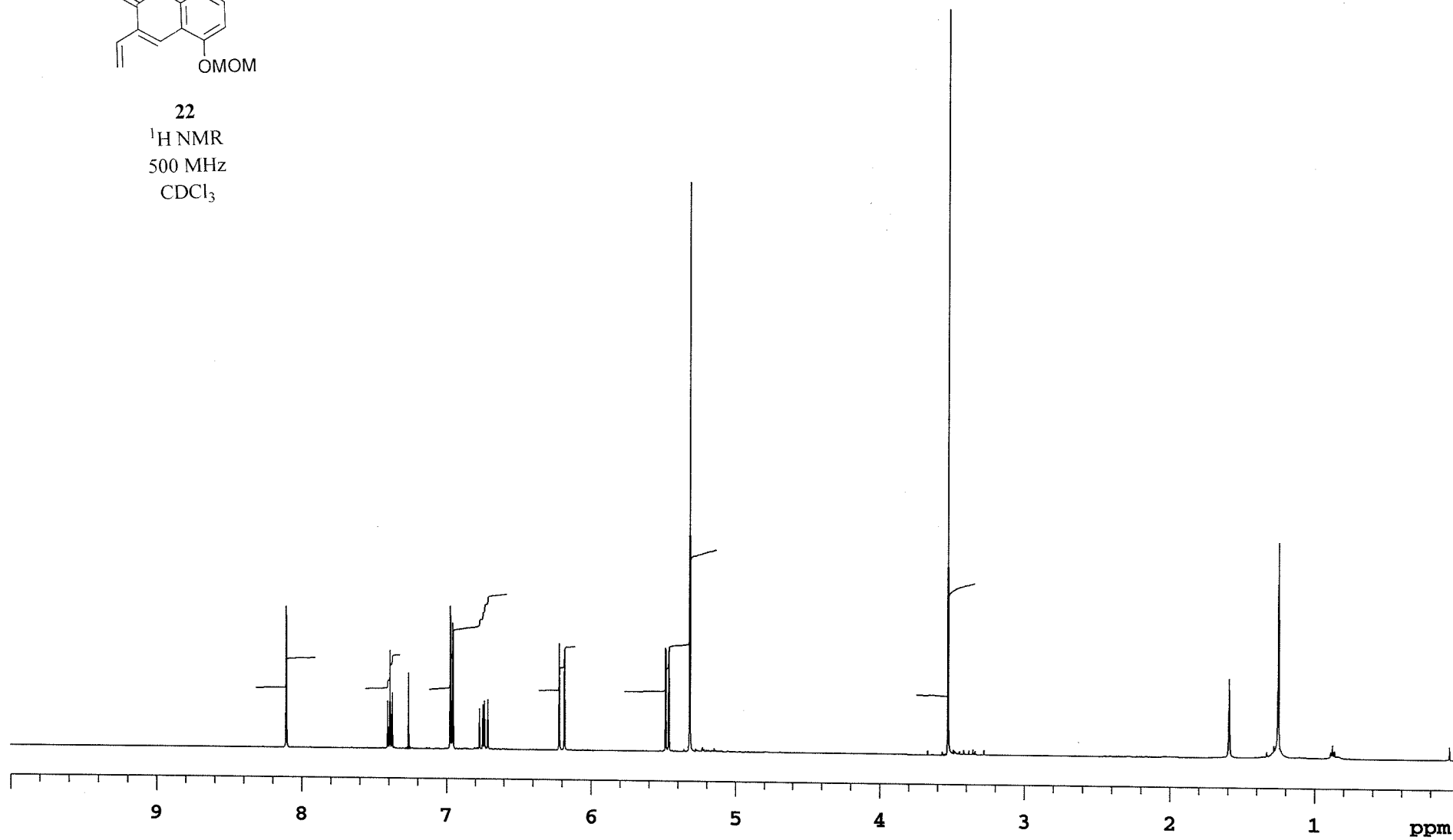
CDCl_3

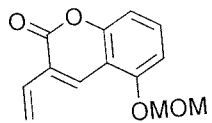




22

^1H NMR
500 MHz
 CDCl_3



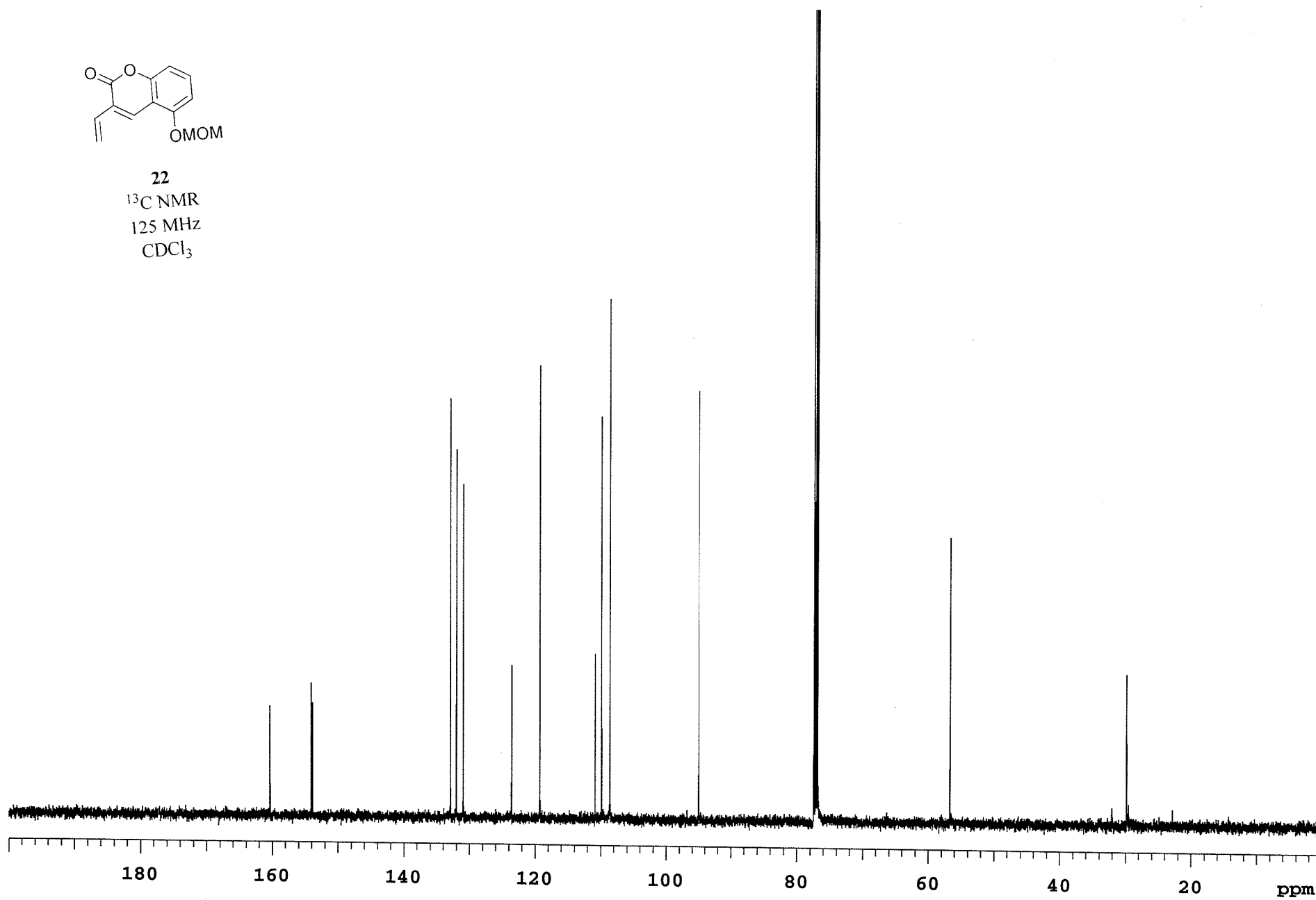


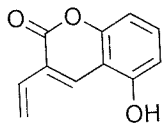
22

^{13}C NMR

125 MHz

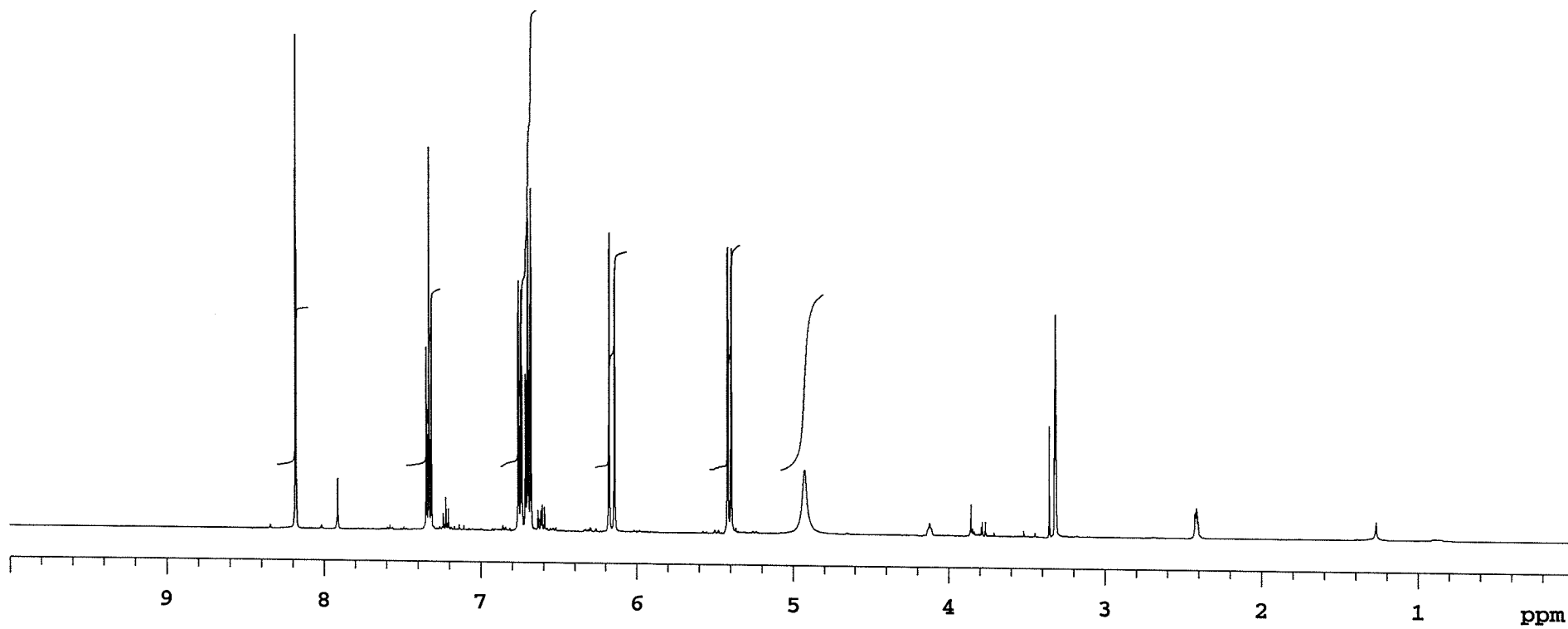
CDCl_3

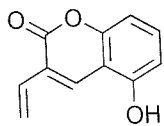




23

^1H NMR
500 MHz
 CD_3OD



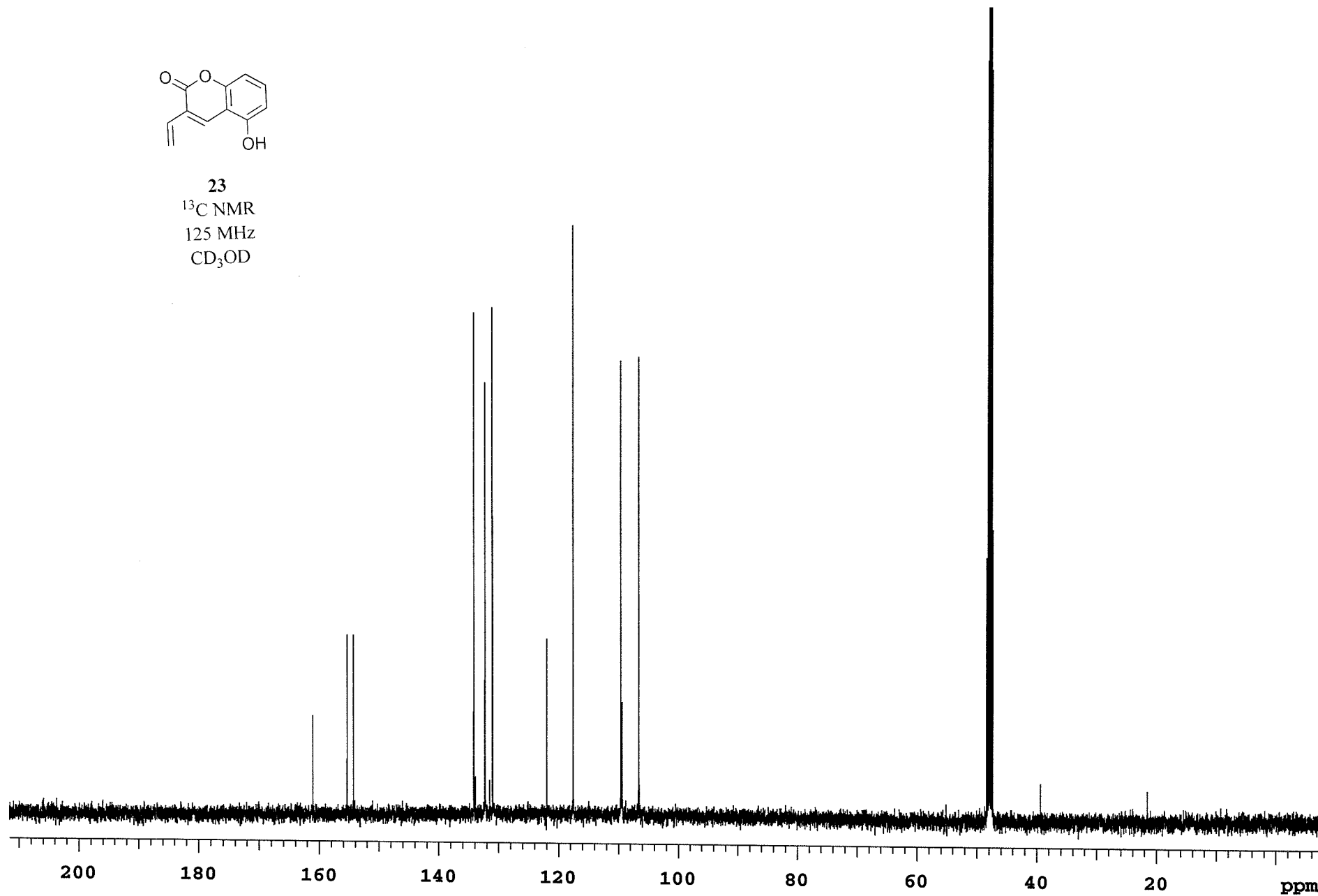


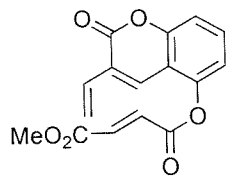
23

^{13}C NMR

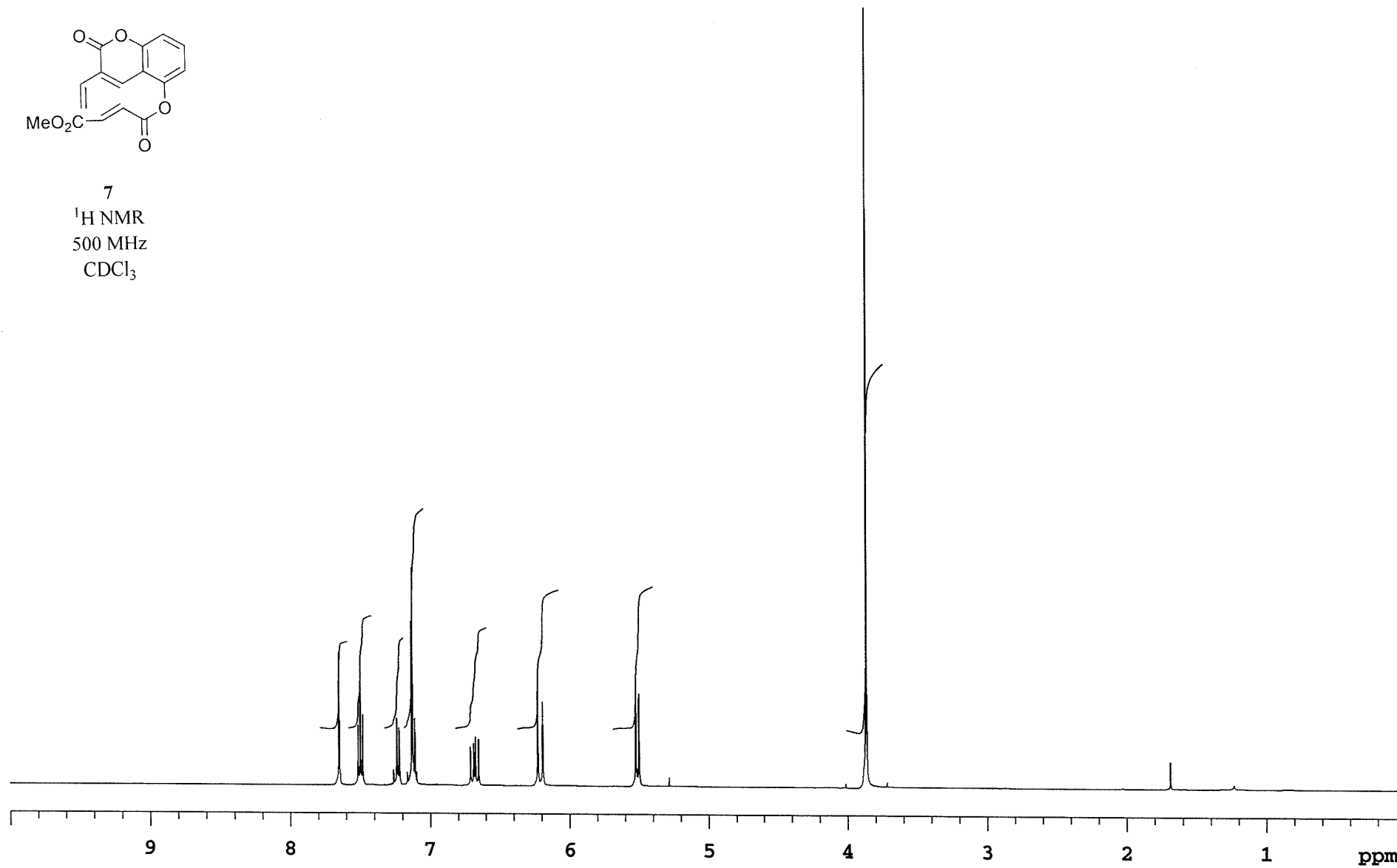
125 MHz

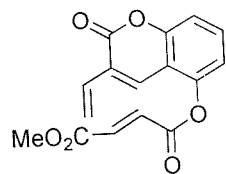
CD_3OD





7
 ^1H NMR
500 MHz
 CDCl_3



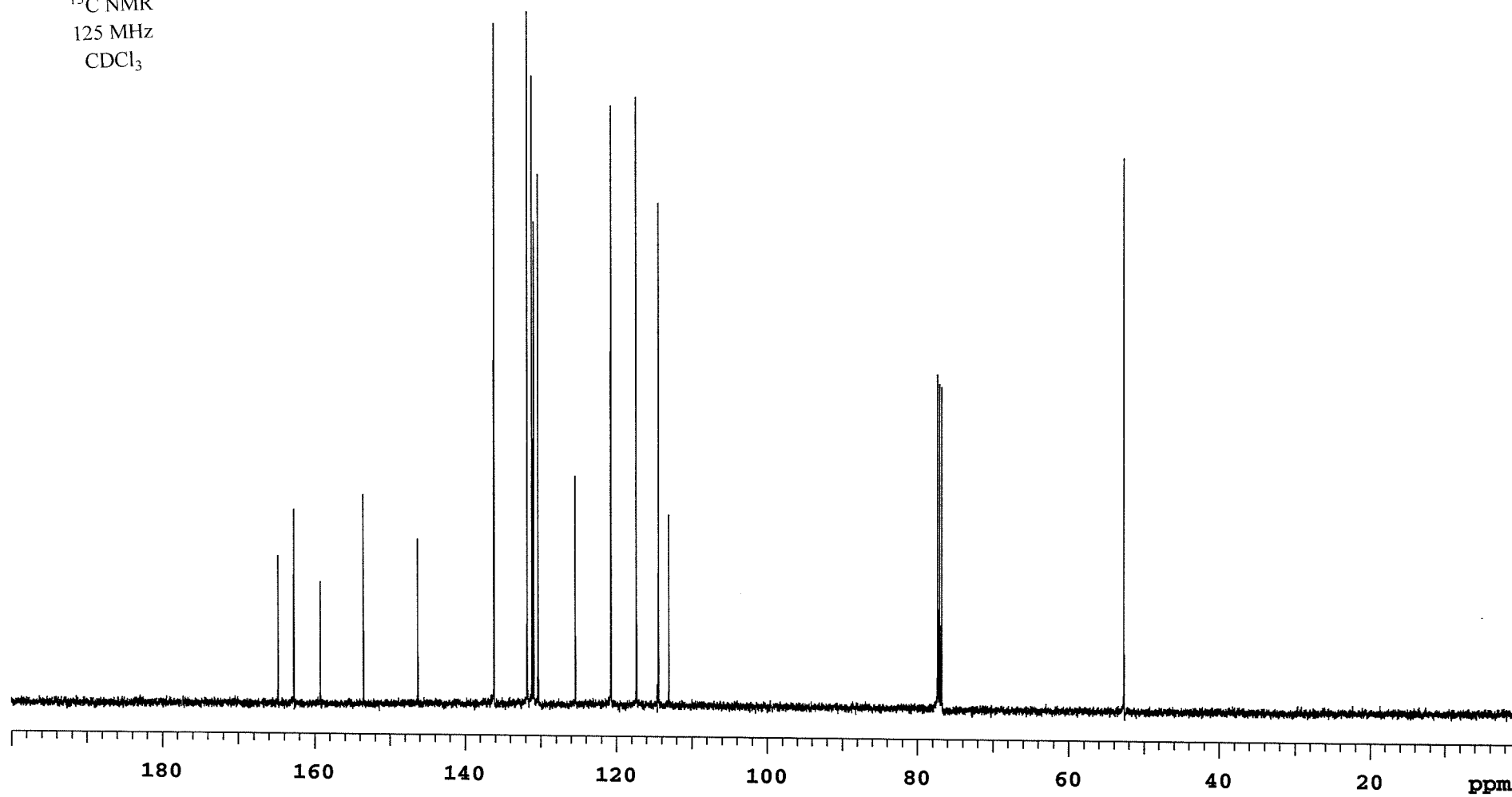


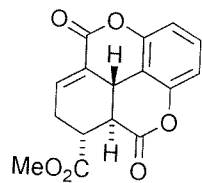
7

^{13}C NMR

125 MHz

CDCl_3



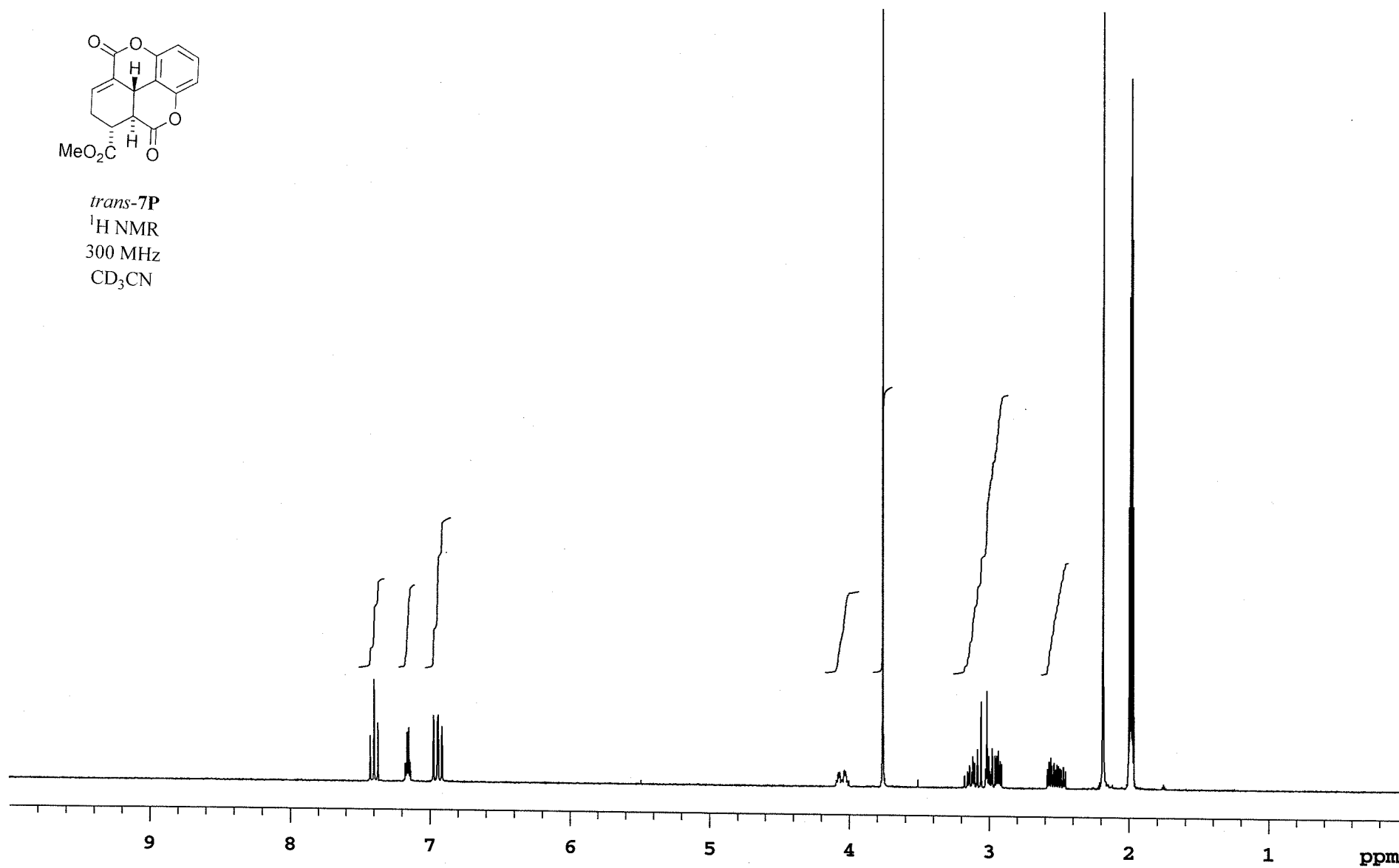


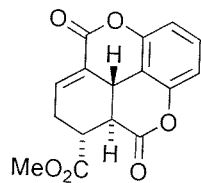
trans-7P

^1H NMR

300 MHz

CD_3CN





trans-7P
 ^{13}C NMR
 125 MHz
 $\text{CDCl}_3/\text{CD}_3\text{OD}$

