

Supporting Information

Boron Carboxylate Catalysis of Homoallylboration

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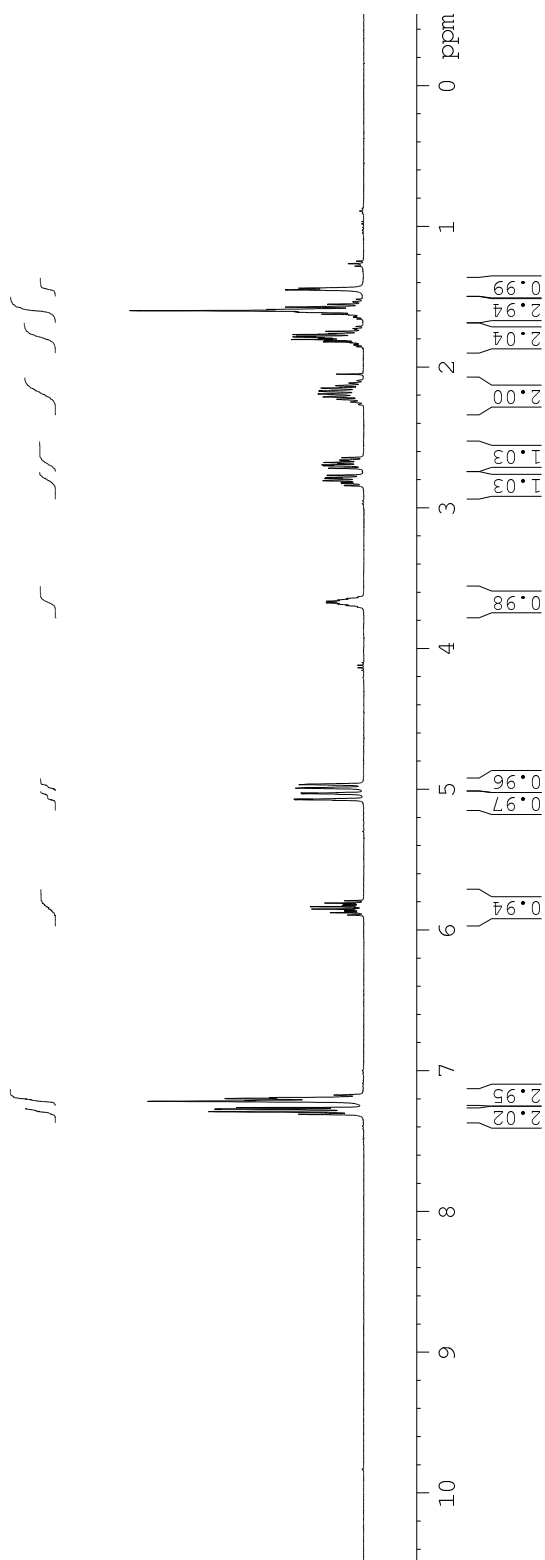
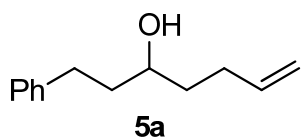
[‡] Department of Chemistry and Biochemistry, University of California, Los Angeles, California 90095-1569, United States

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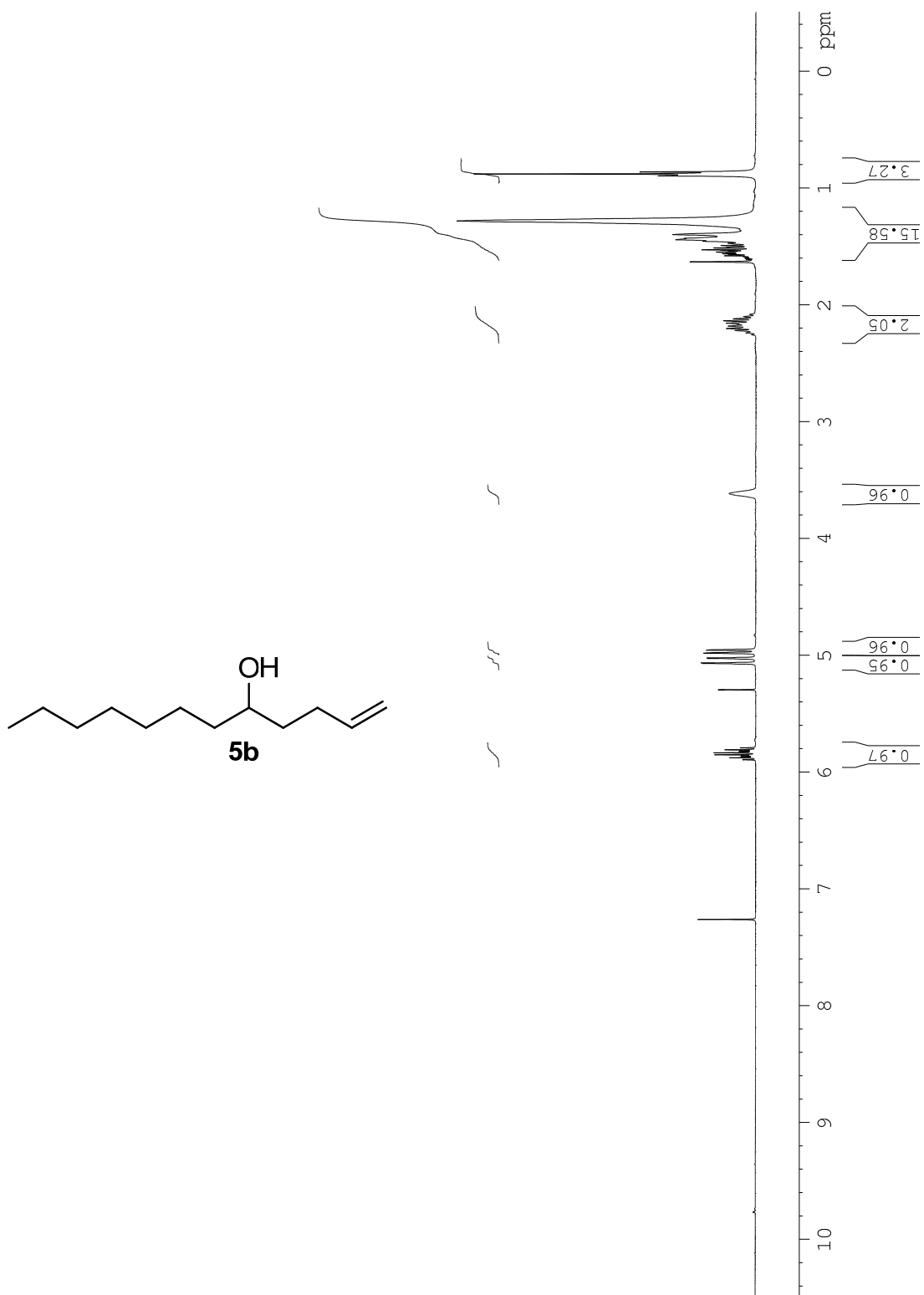
Page S2: Spectra

Page S46: Computational Section

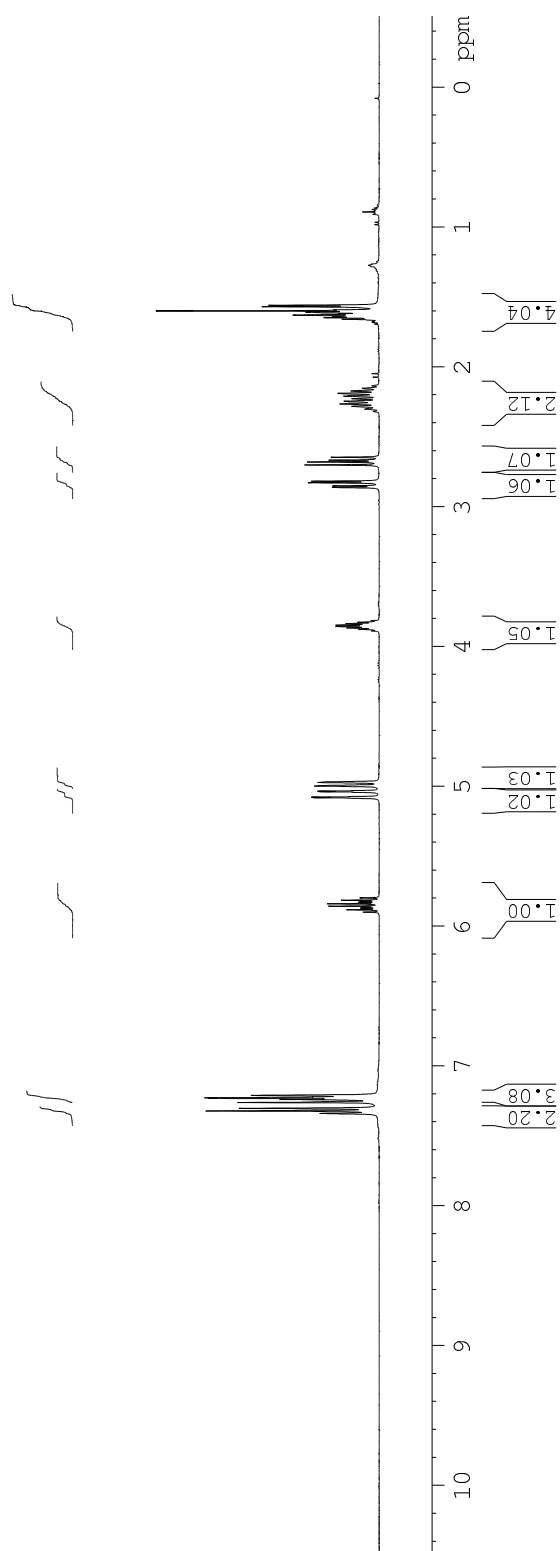
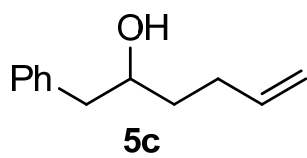
400 MHz ^1H NMR spectrum of **5a** (CDCl_3)



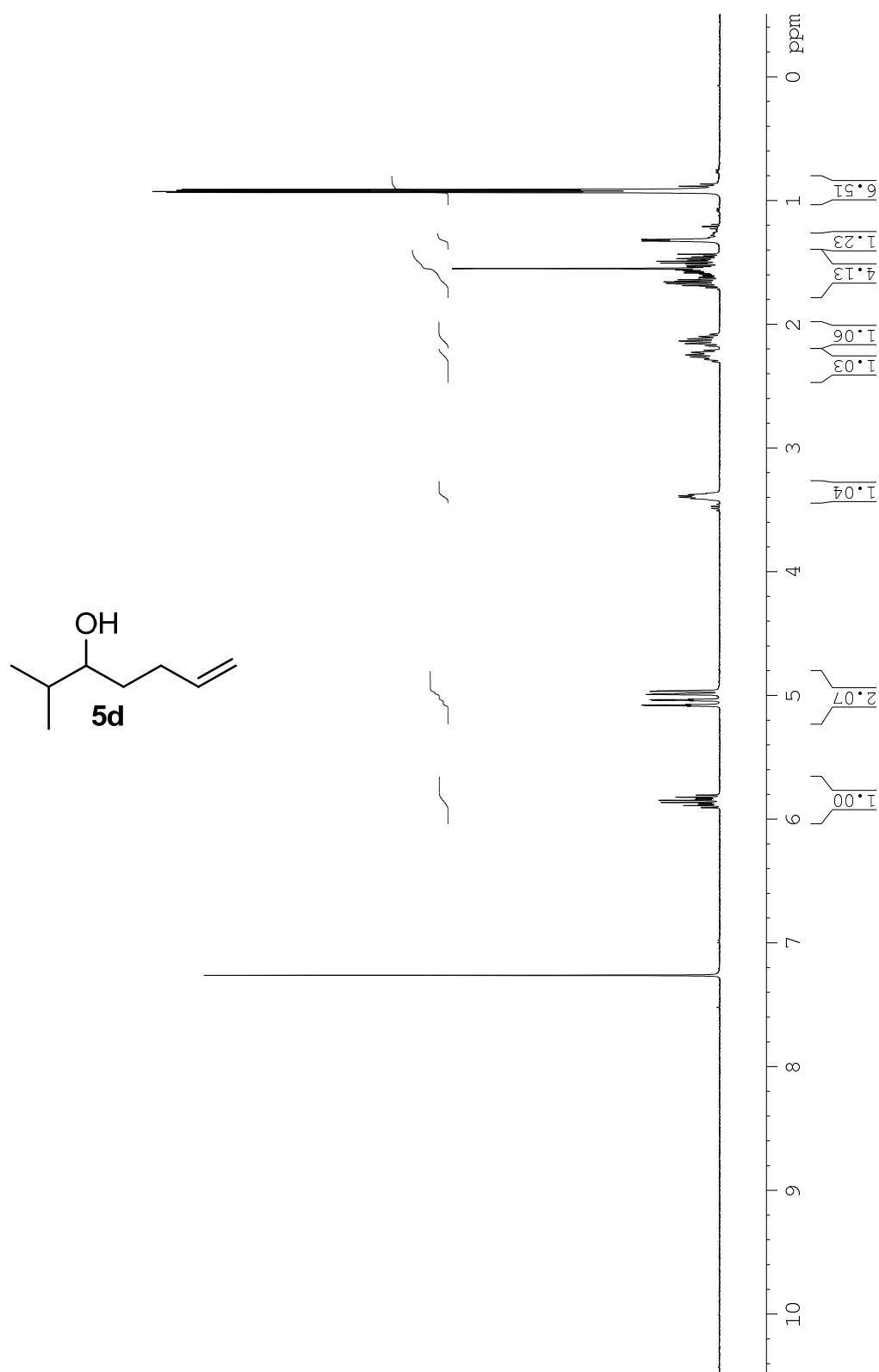
400 MHz ^1H NMR spectrum of **5b** (CDCl_3)



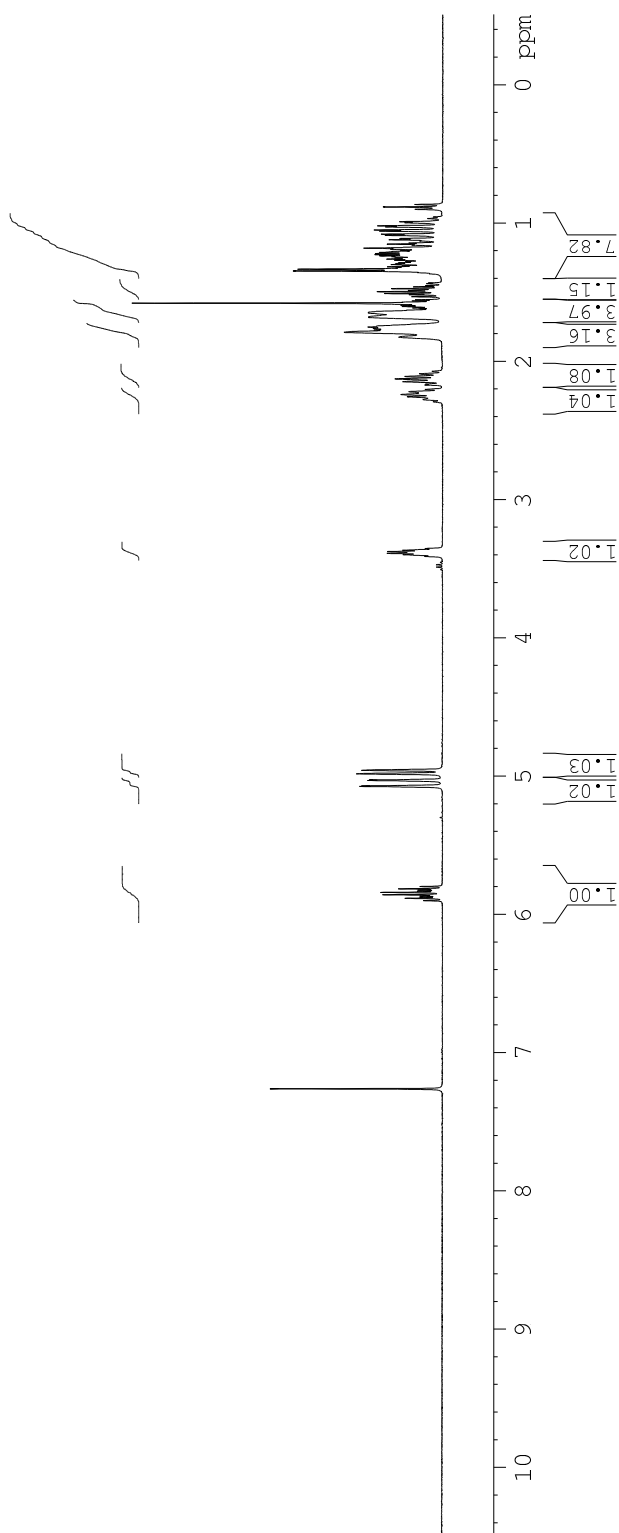
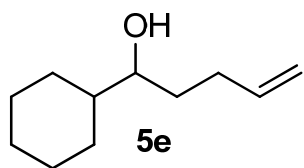
400 MHz ^1H NMR spectrum of **5c** (CDCl_3)



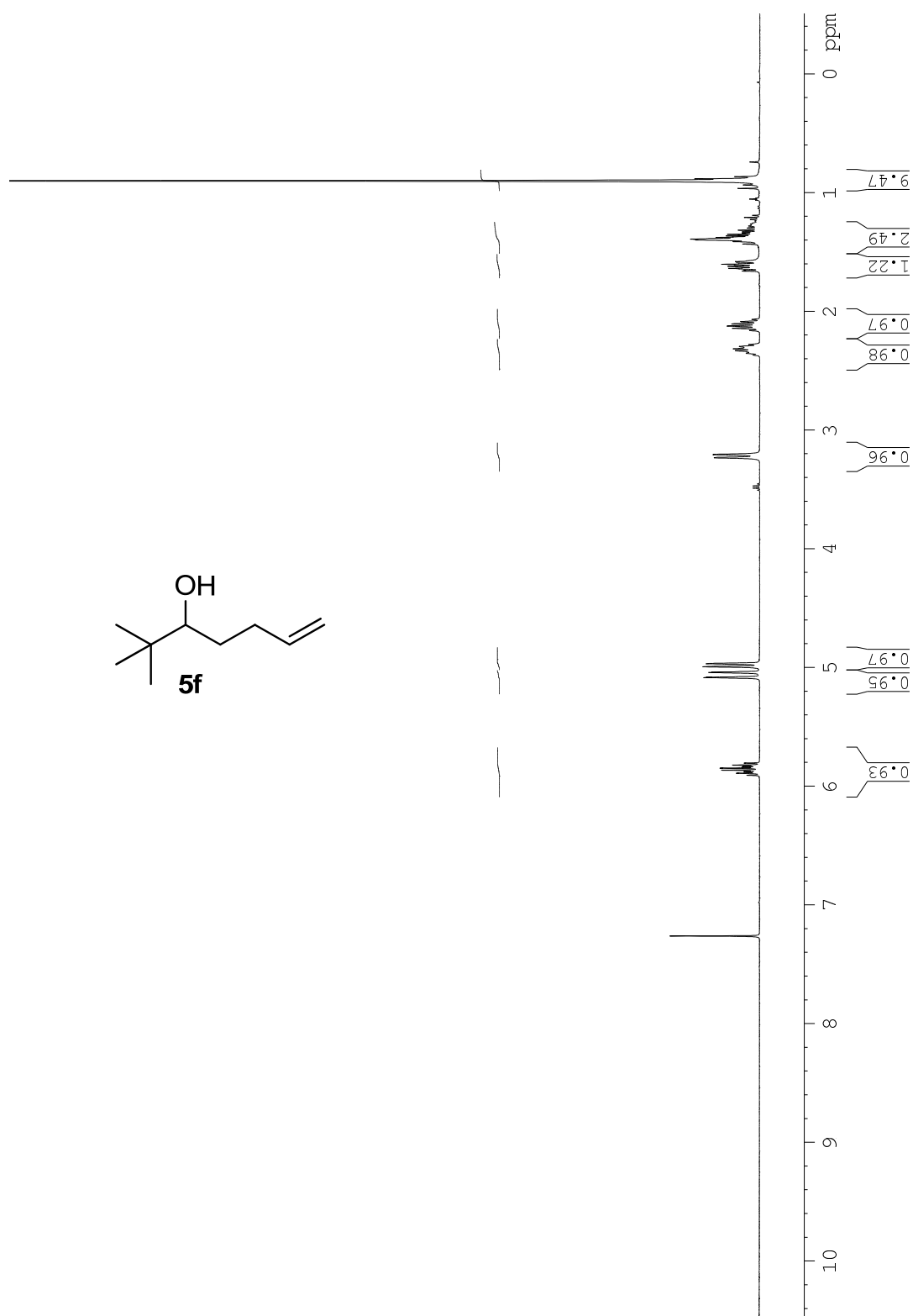
400 MHz ^1H NMR spectrum of **5d** (CDCl_3)



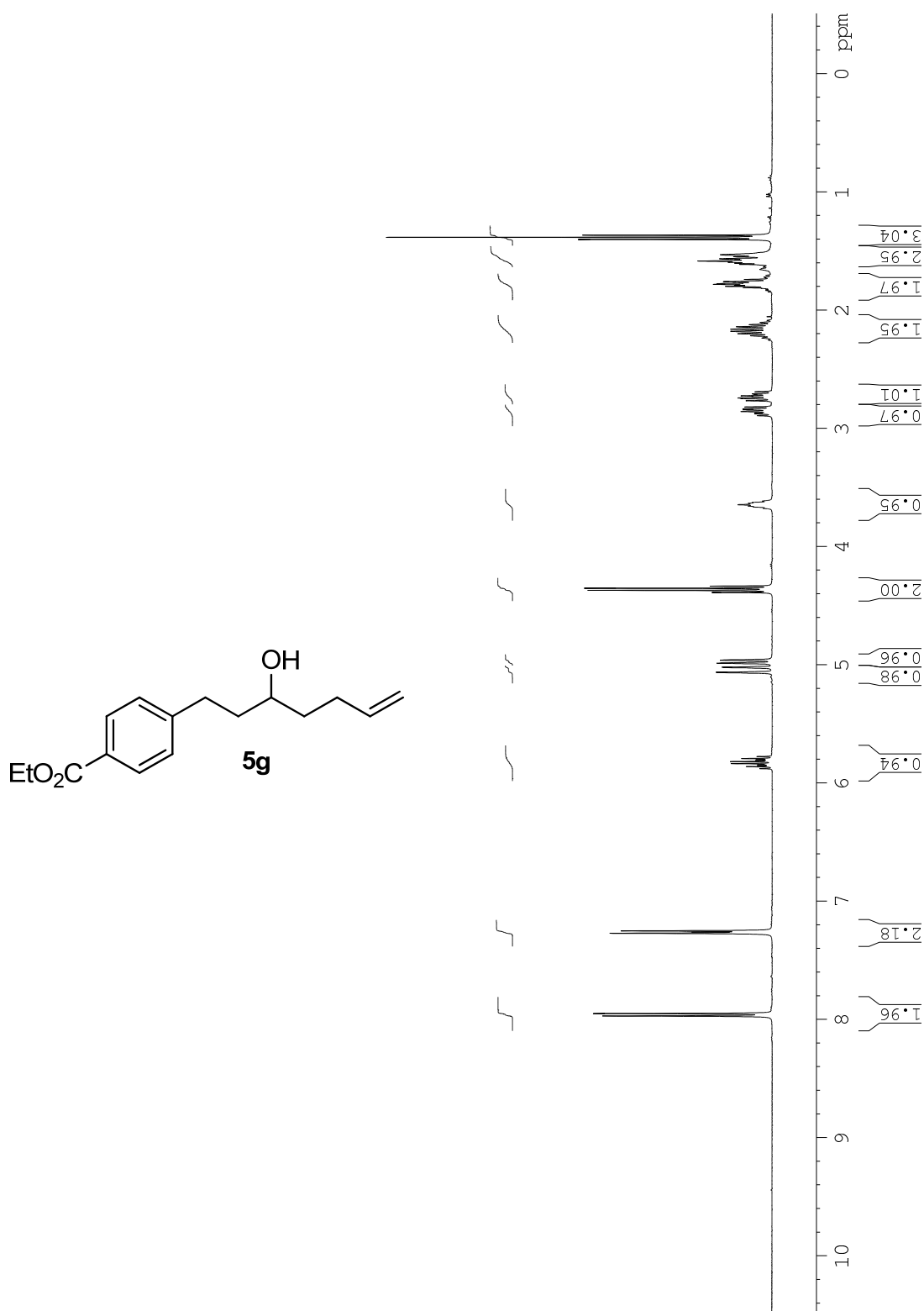
400 MHz ^1H NMR spectrum of **5e** (CDCl_3)



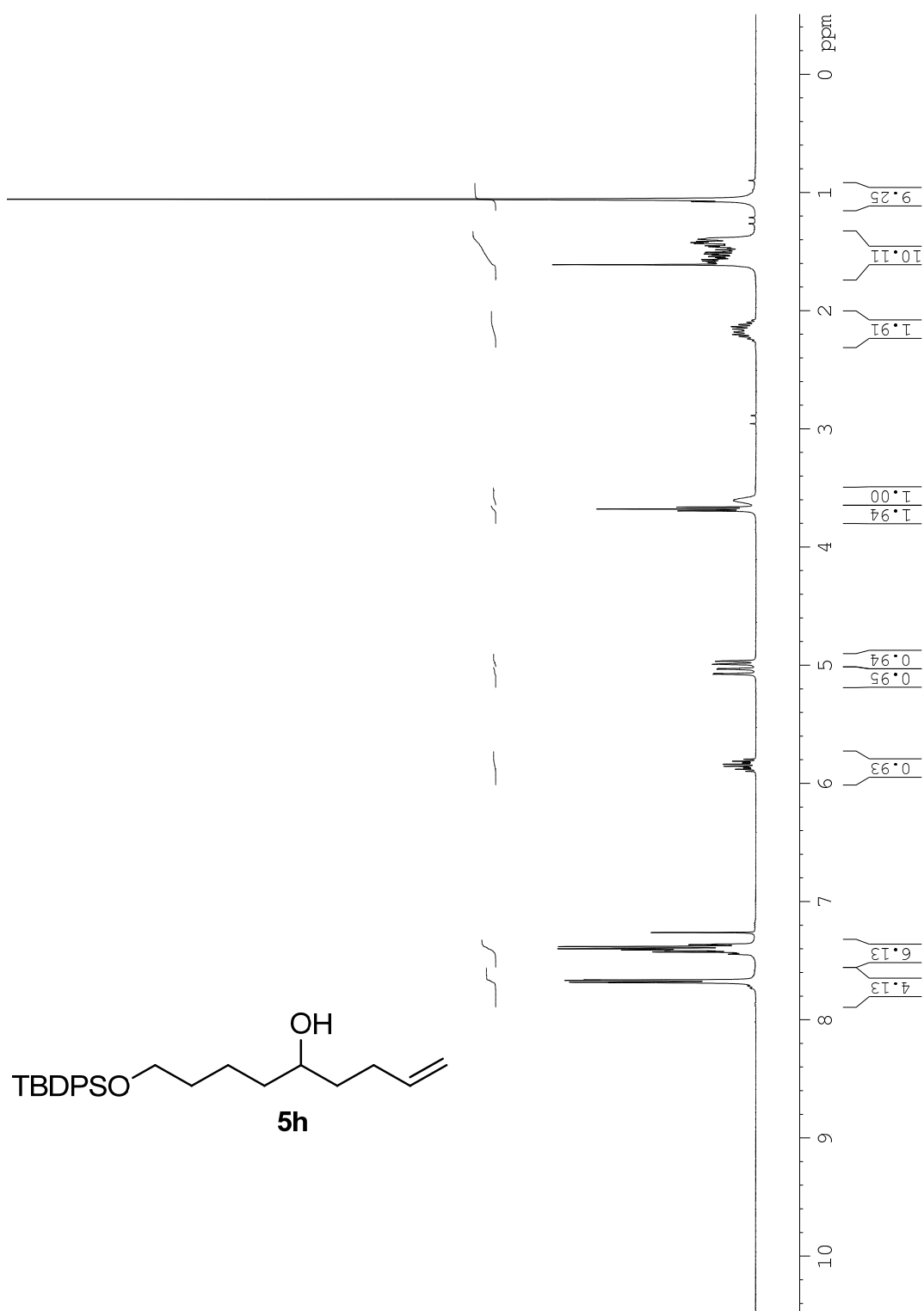
400 MHz ^1H NMR spectrum of **5f** (CDCl_3)



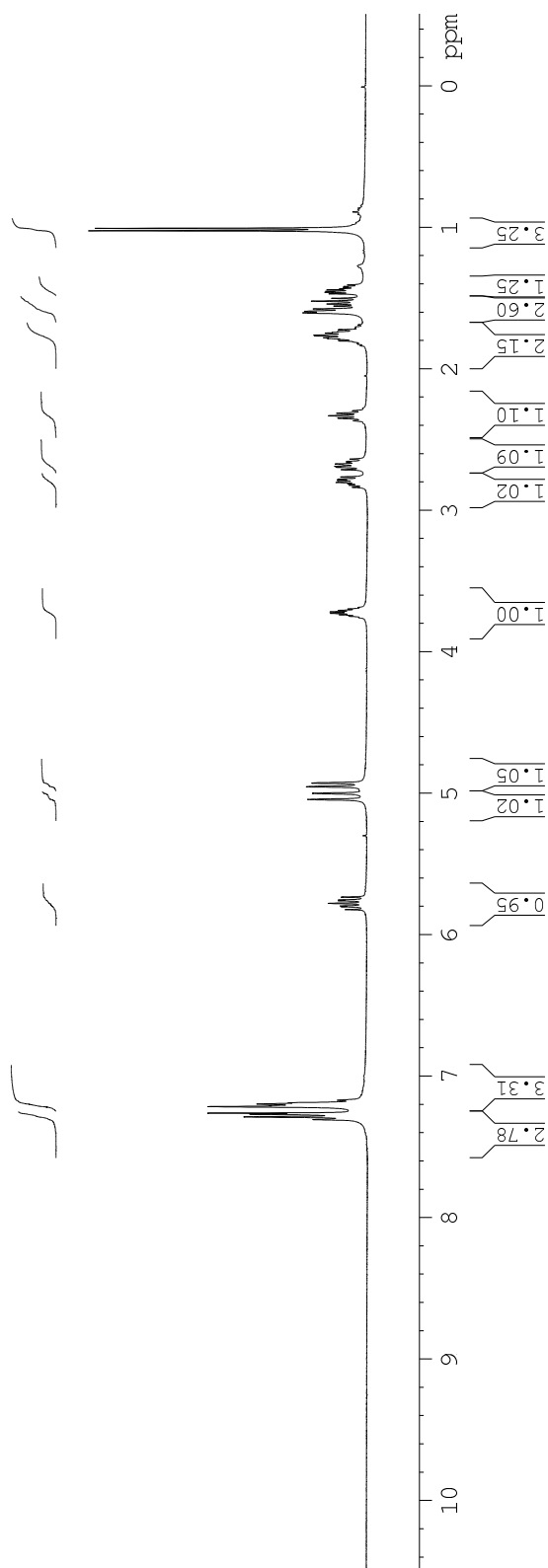
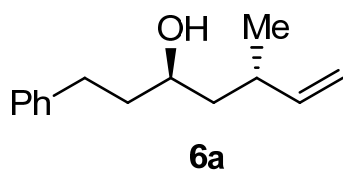
400 MHz ^1H NMR spectrum of **5g** (CDCl_3)



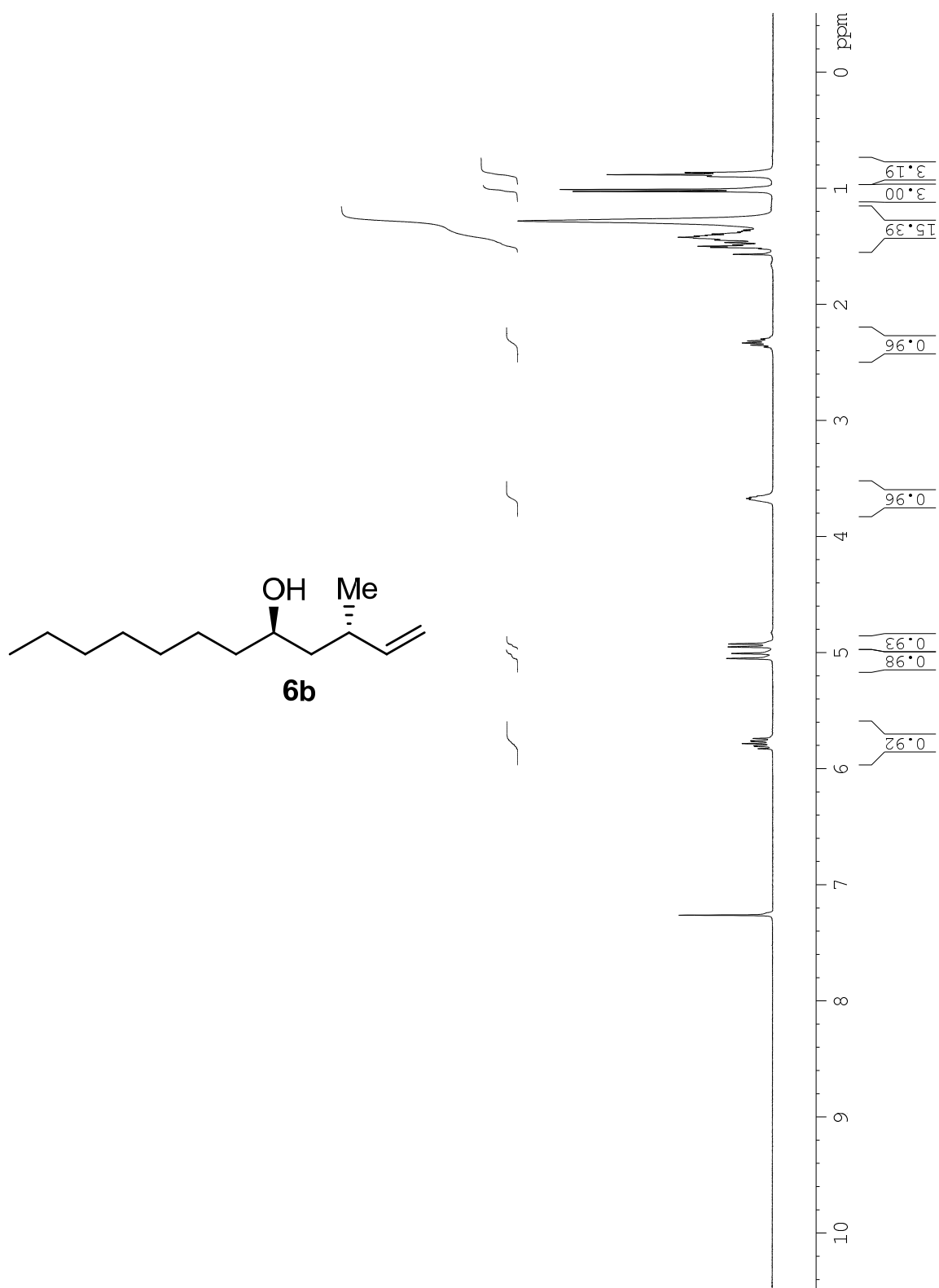
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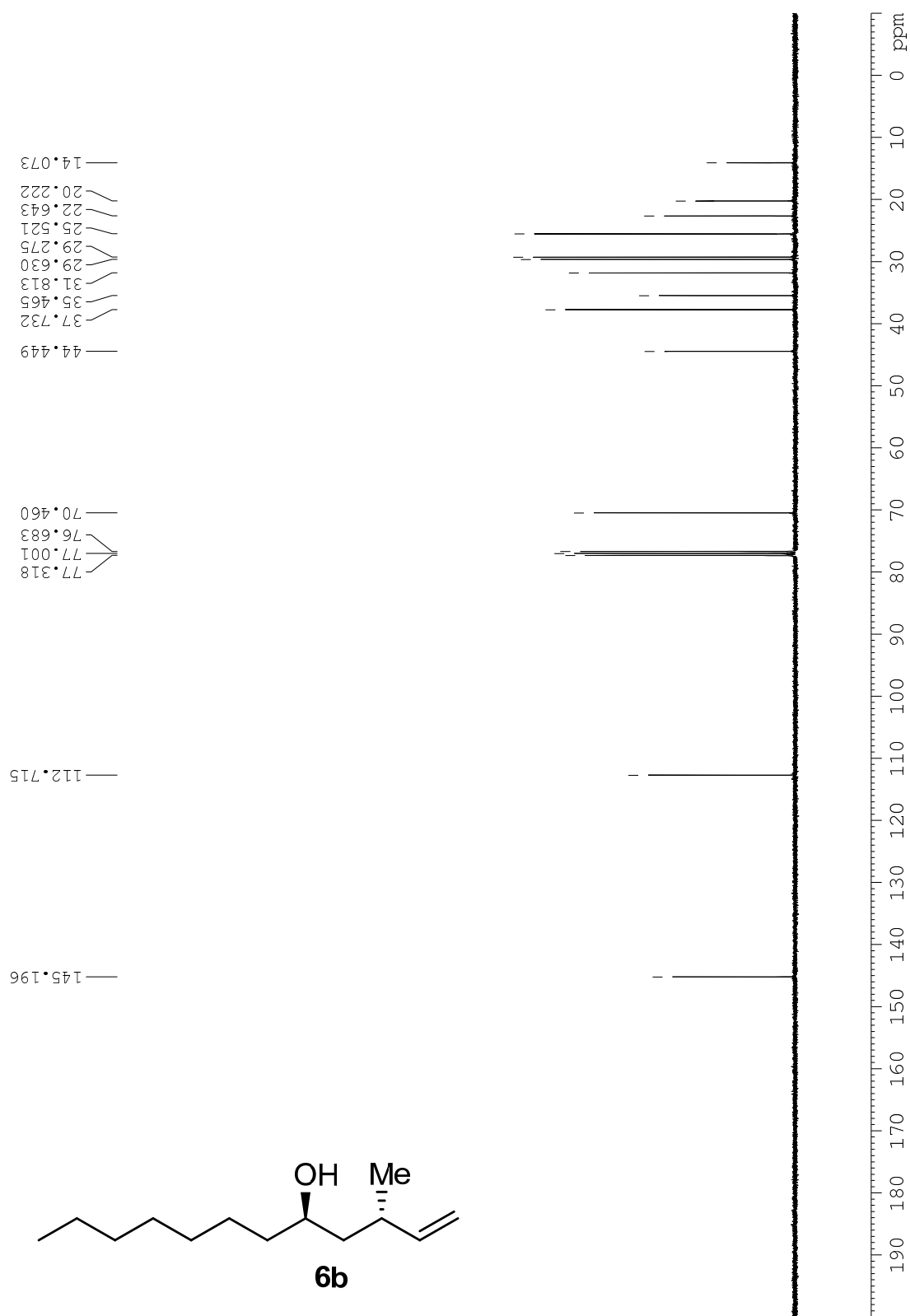
400 MHz ^1H NMR spectrum of **6a** (CDCl_3)



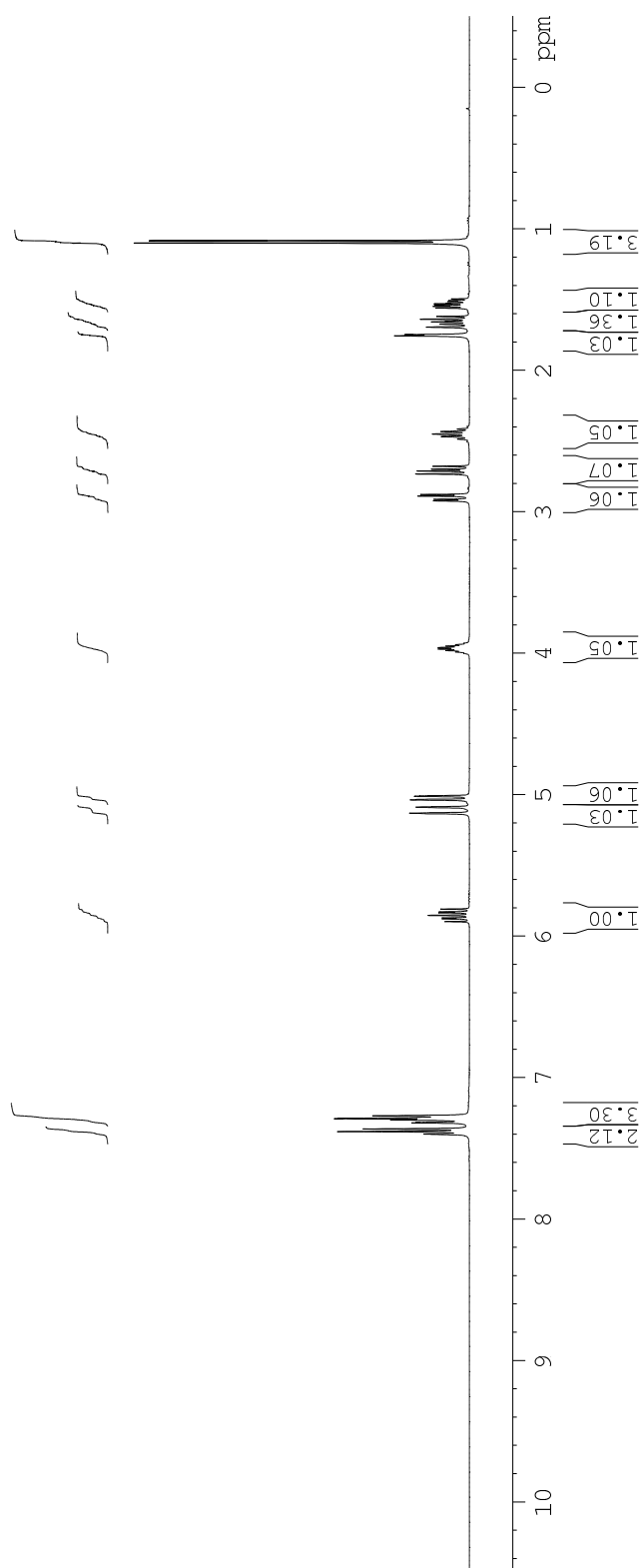
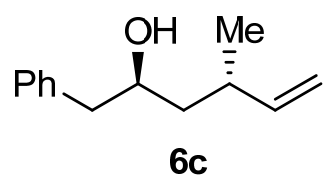
400 MHz ^1H NMR spectrum of **6b** (CDCl_3)



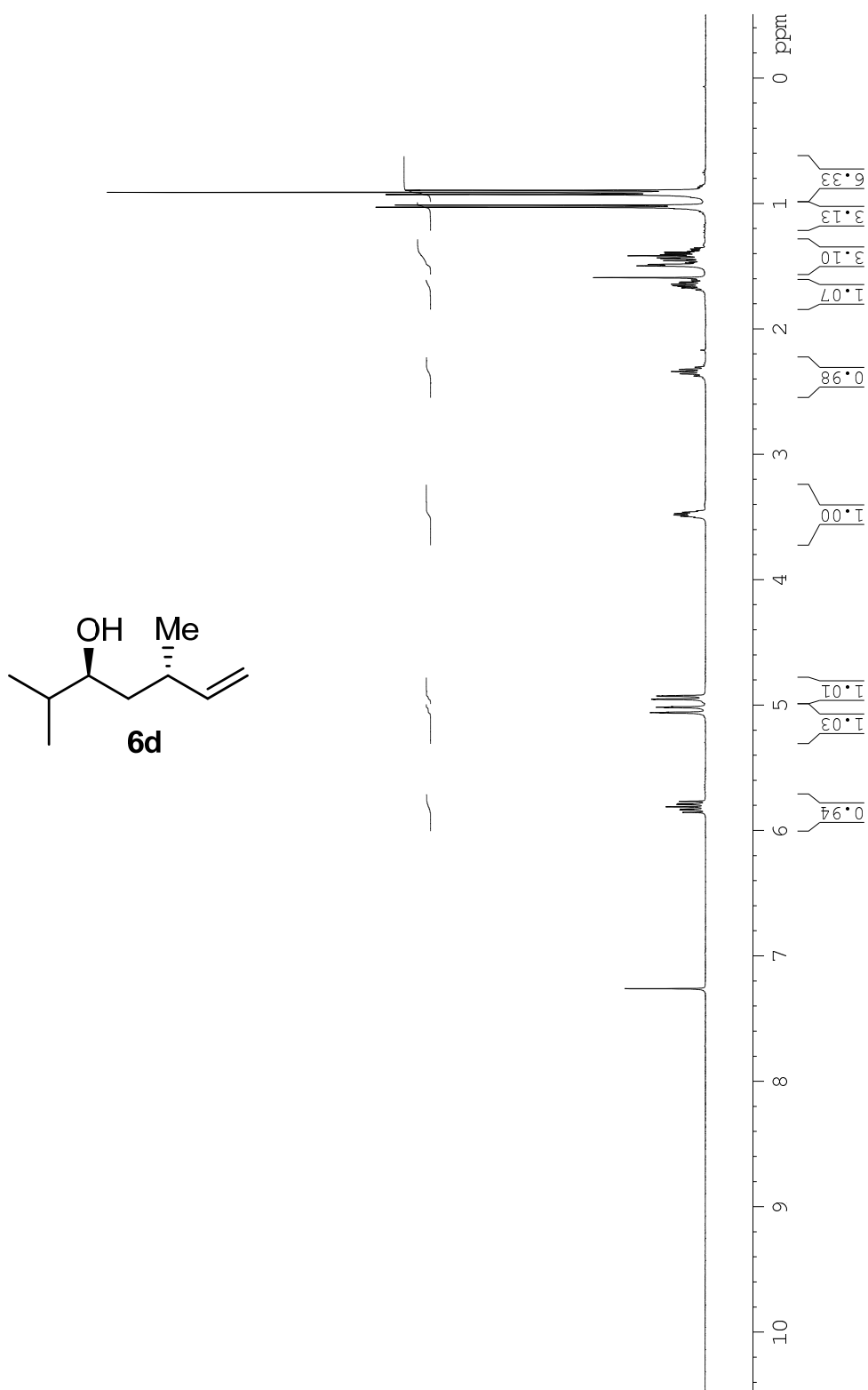
100 MHz ^{13}C NMR spectrum of **6b** (CDCl_3)



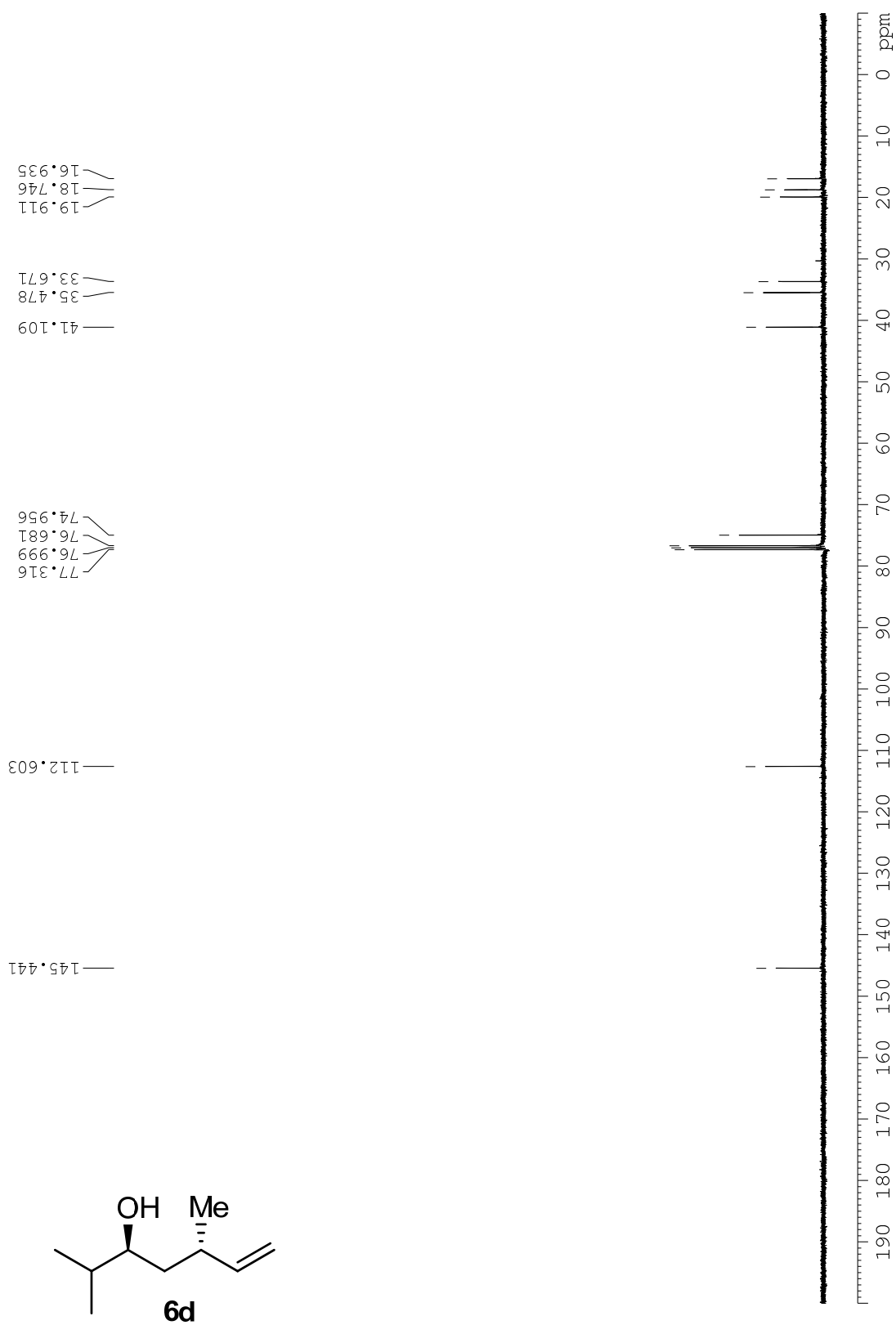
400 MHz ^1H NMR spectrum of **6c** (CDCl_3)



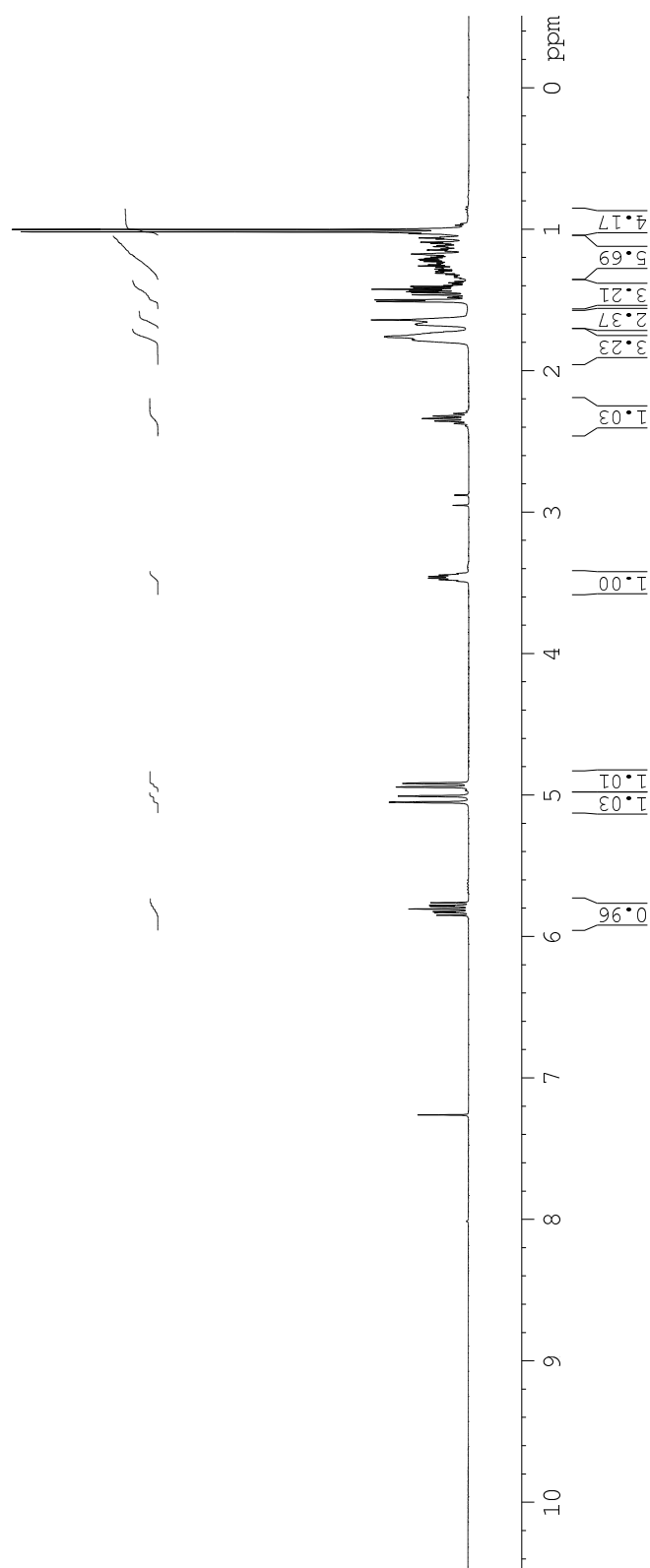
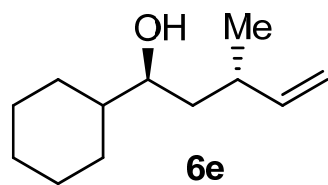
400 MHz ^1H NMR spectrum of **6d** (CDCl_3)



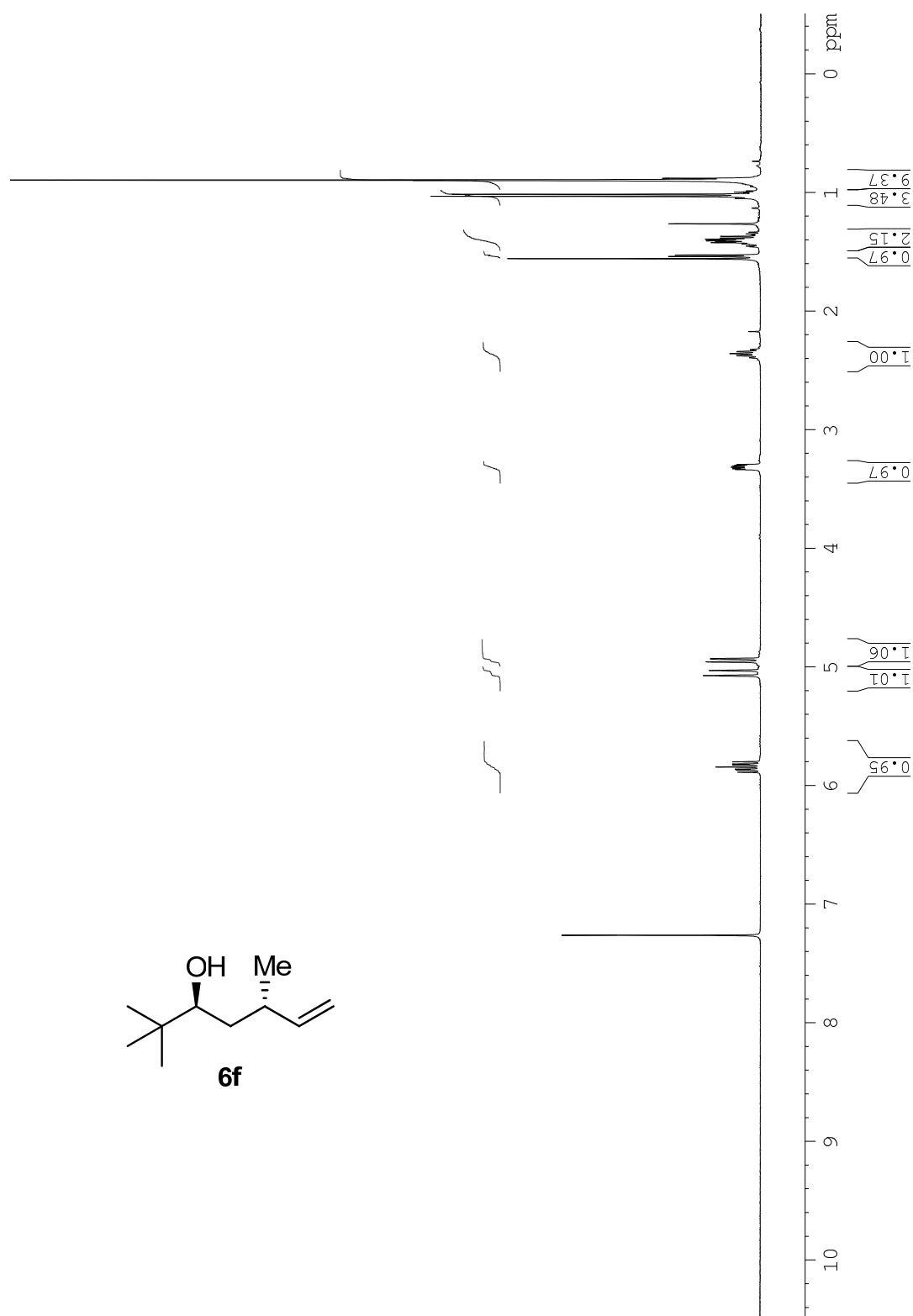
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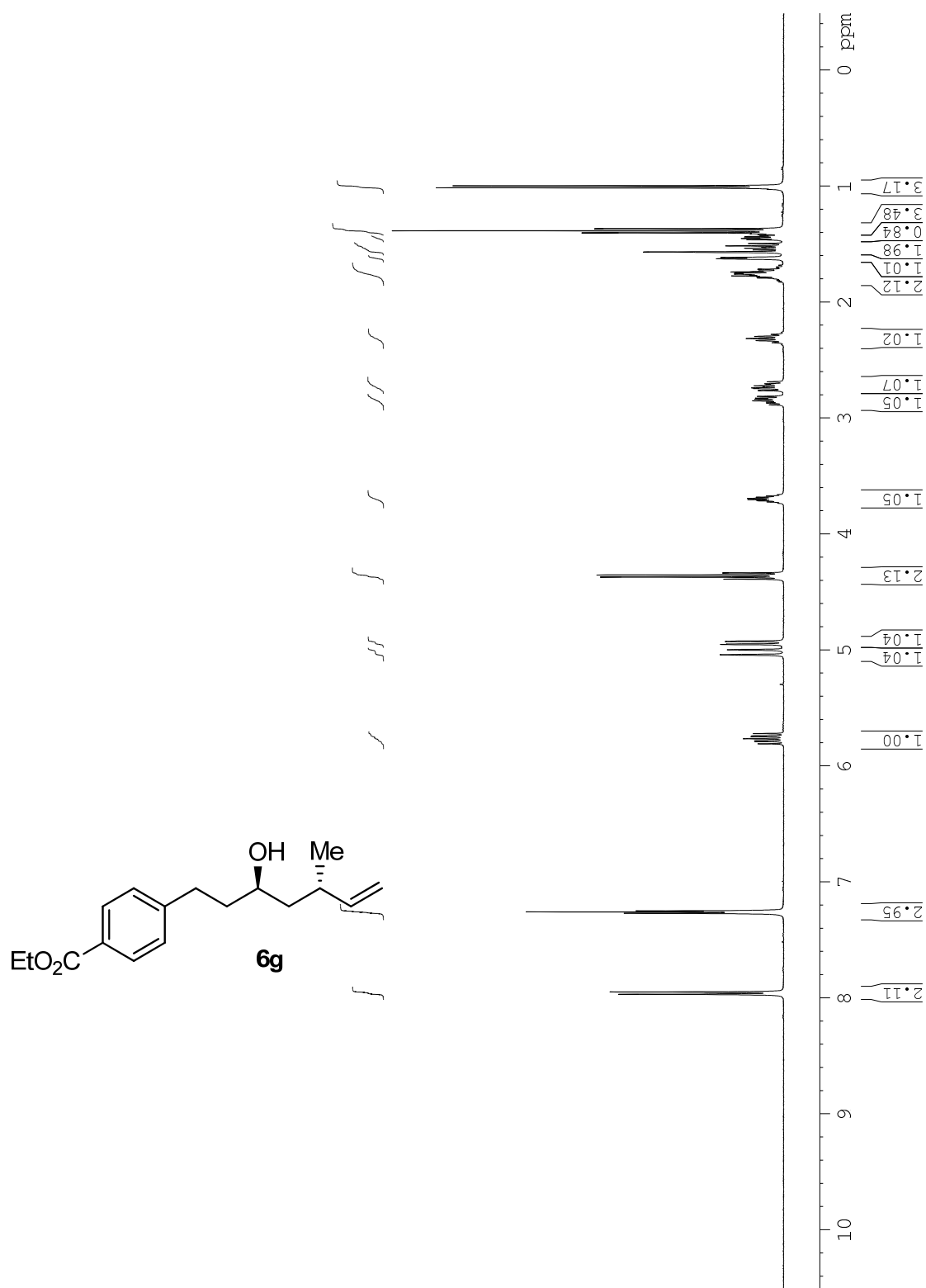
400 MHz ^1H NMR spectrum of **6e** (CDCl_3)



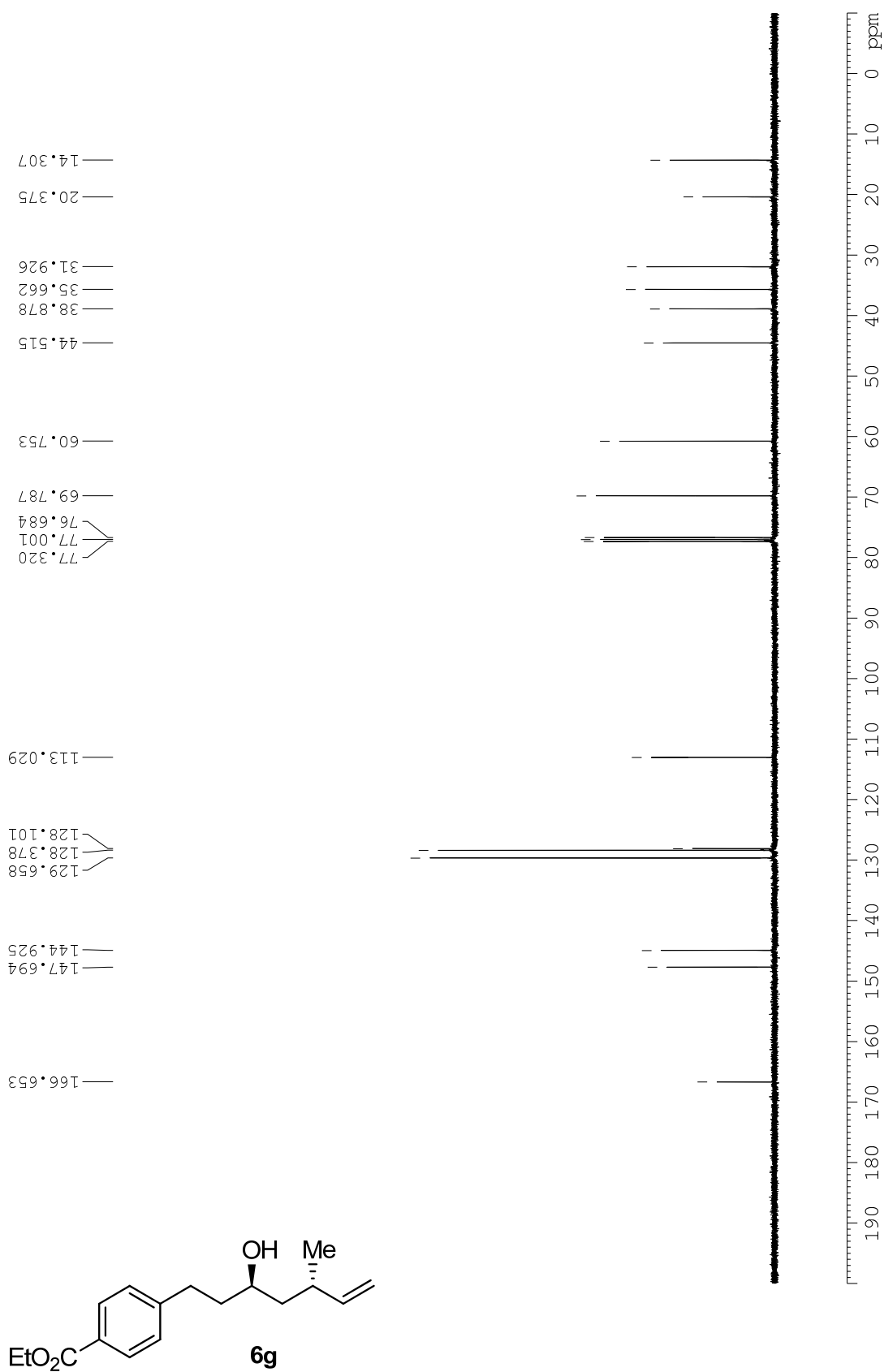
400 MHz ^1H NMR spectrum of **6f** (CDCl_3)



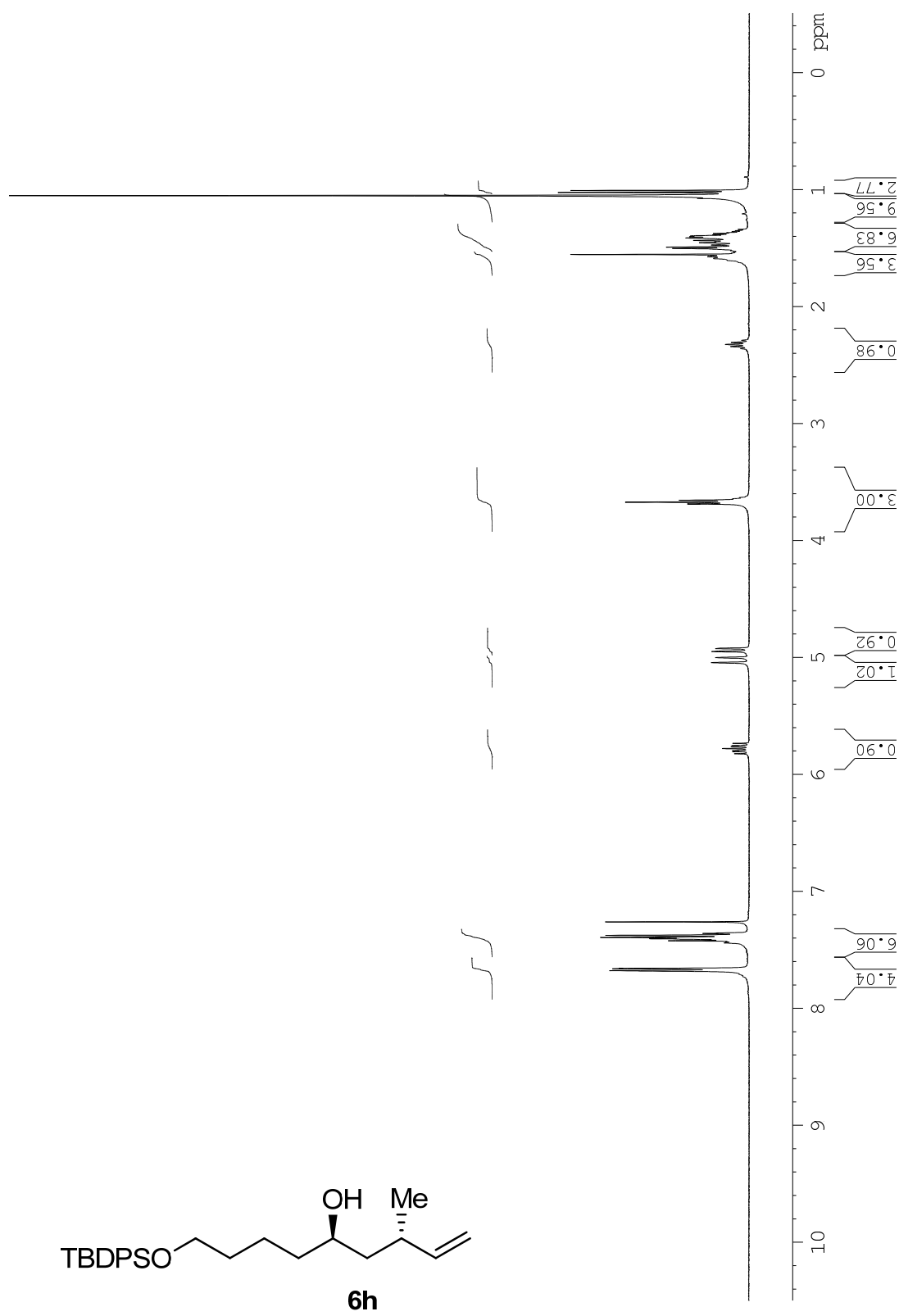
400 MHz ^1H NMR spectrum of **6g** (CDCl_3)



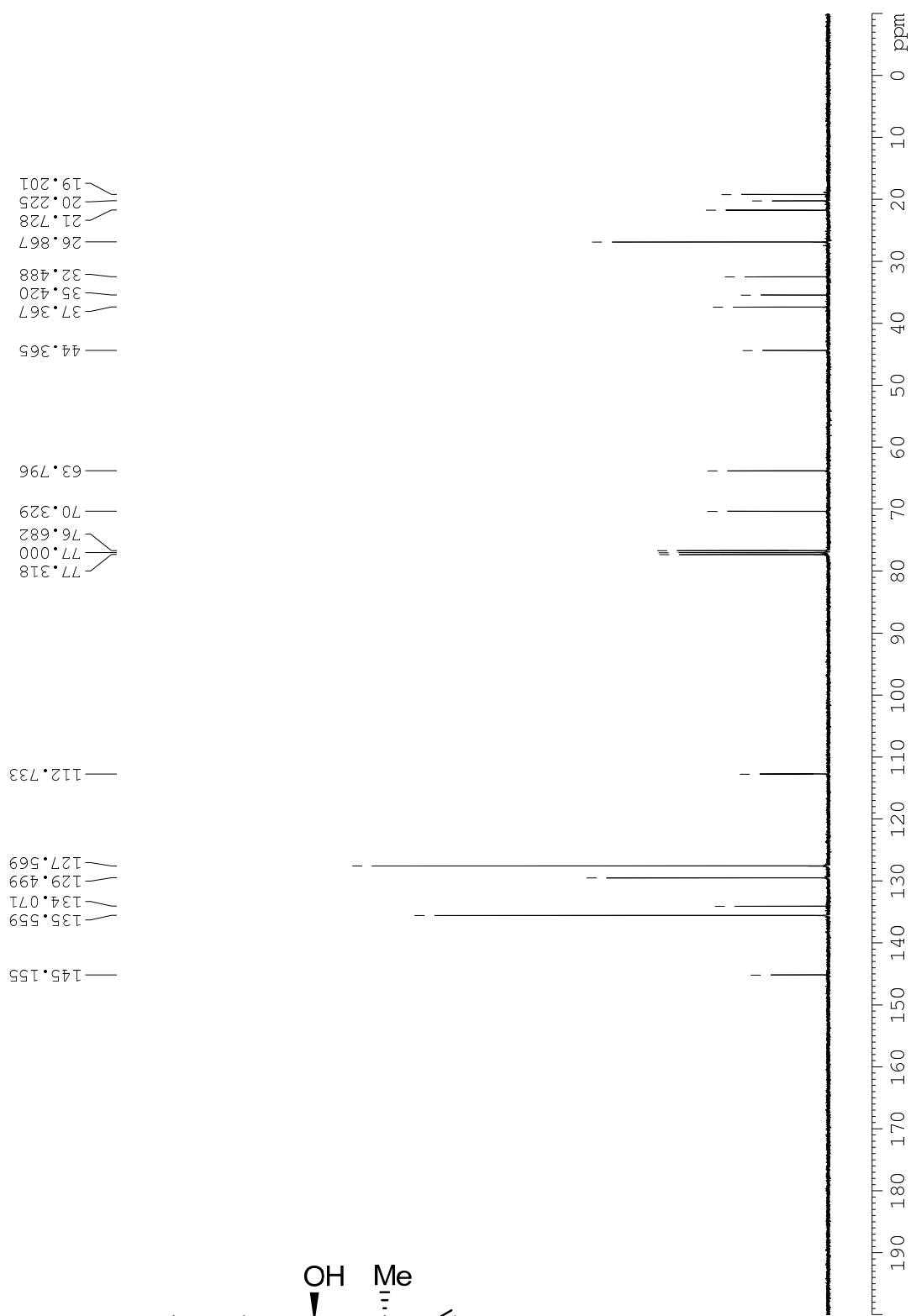
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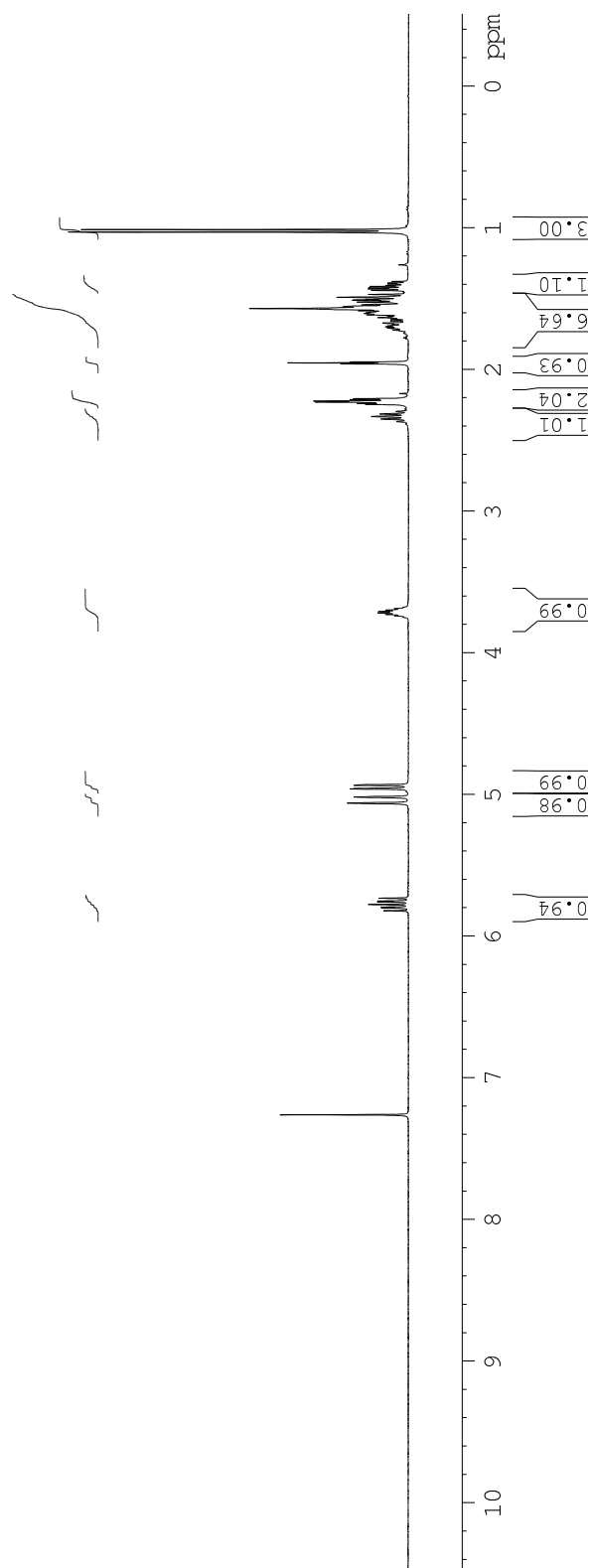
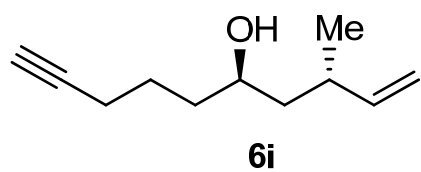
400 MHz ^1H NMR spectrum of **6h** (CDCl_3)



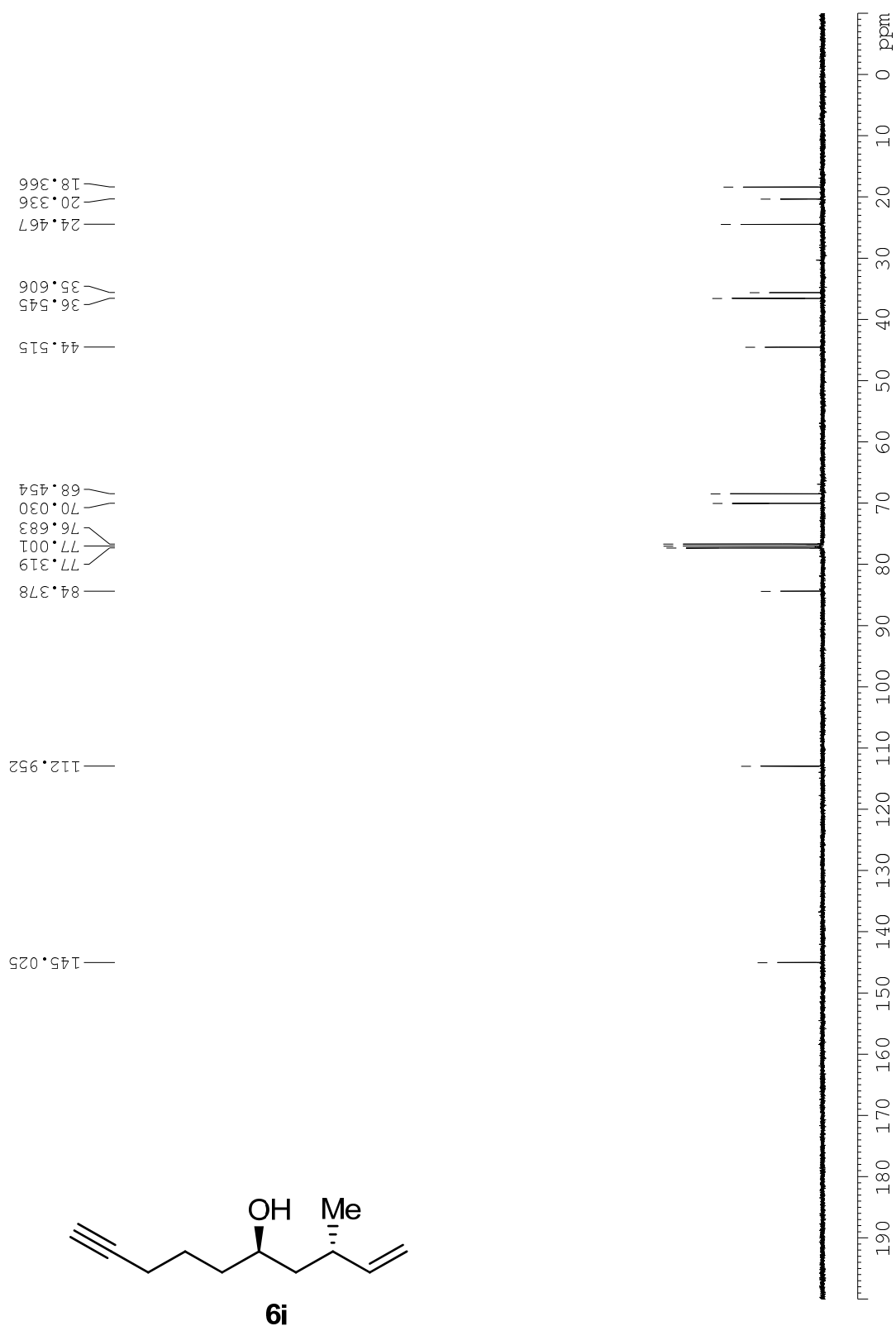
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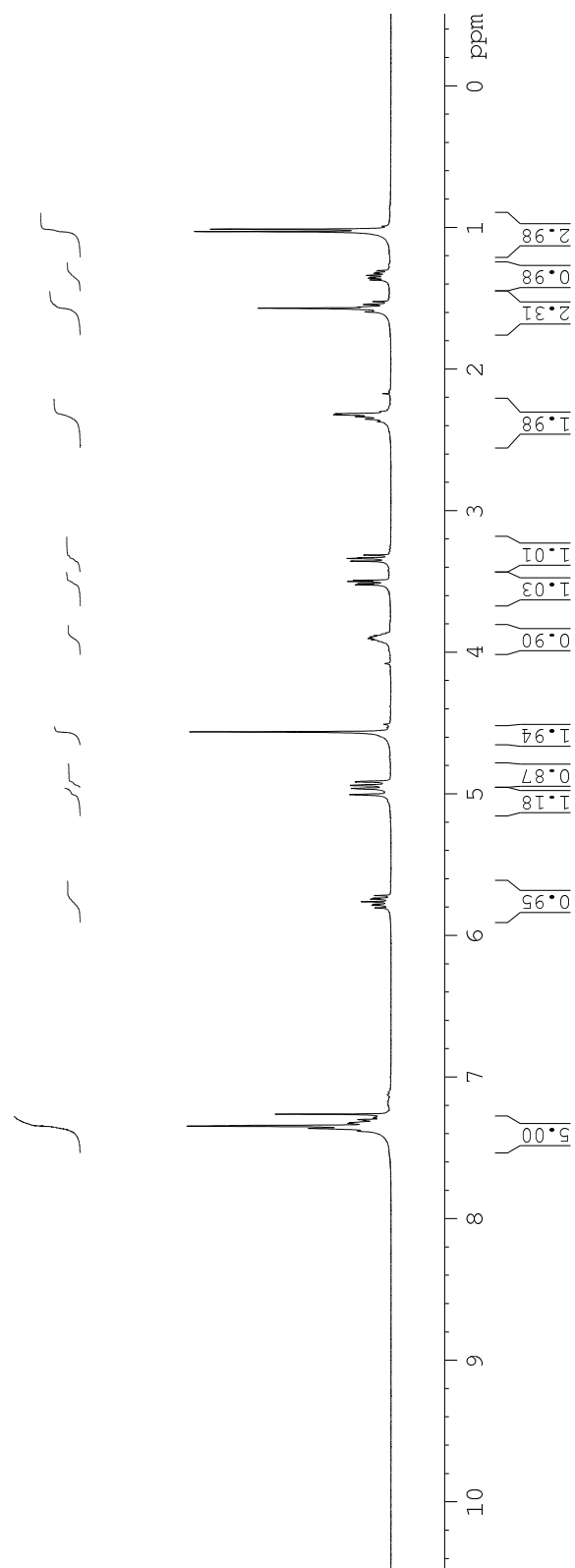
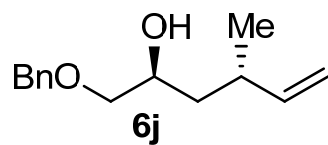
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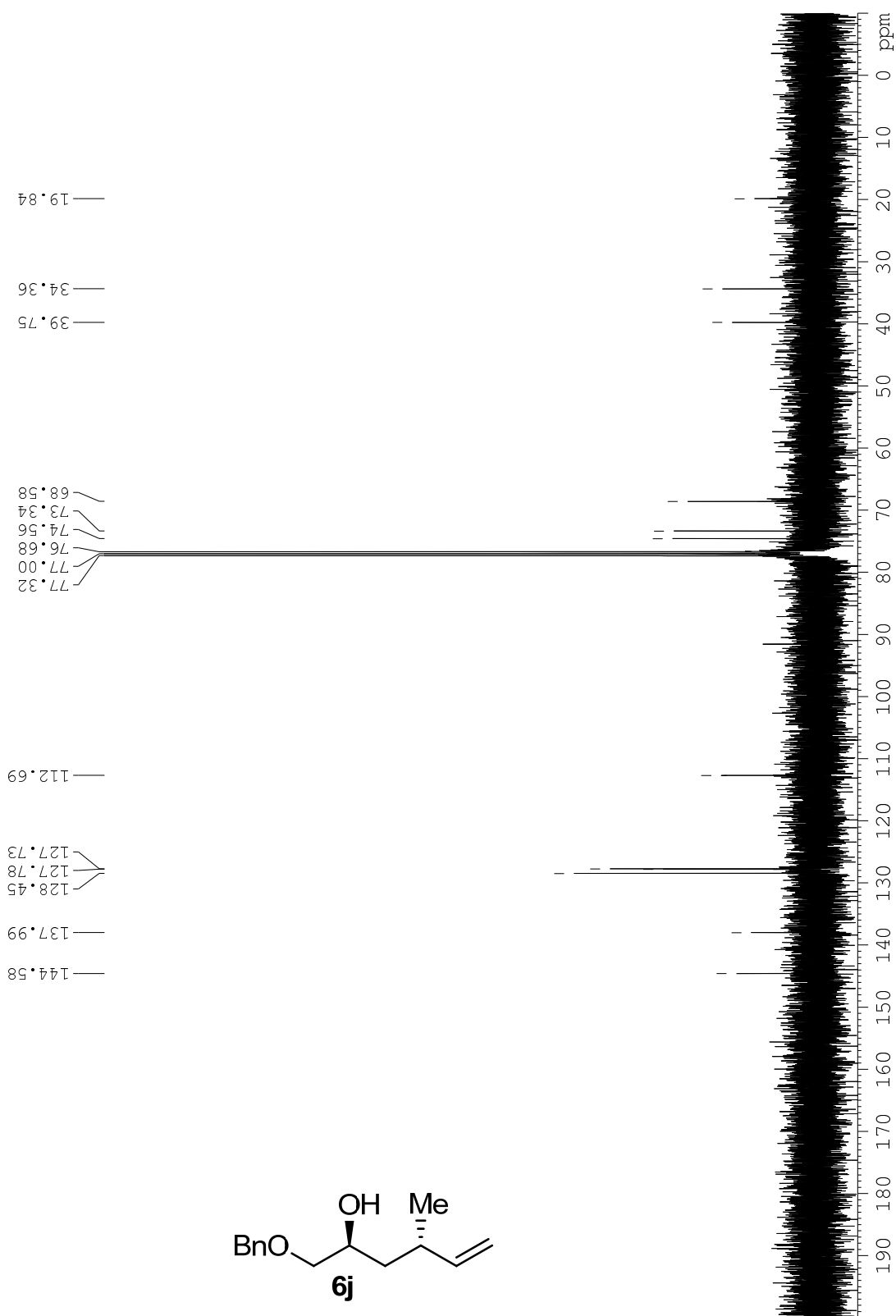
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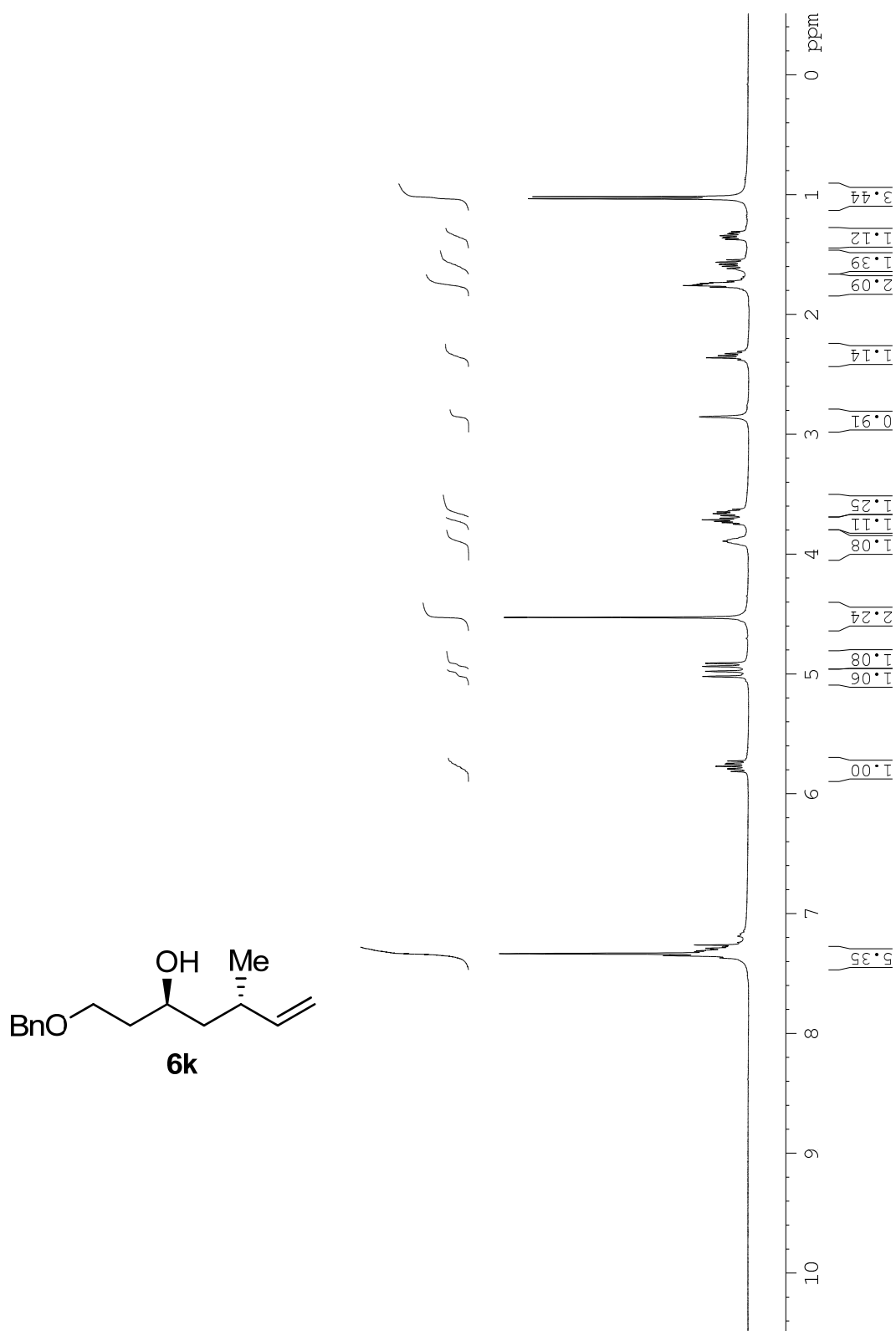
400 MHz ^1H NMR spectrum of **6j** (CDCl_3)



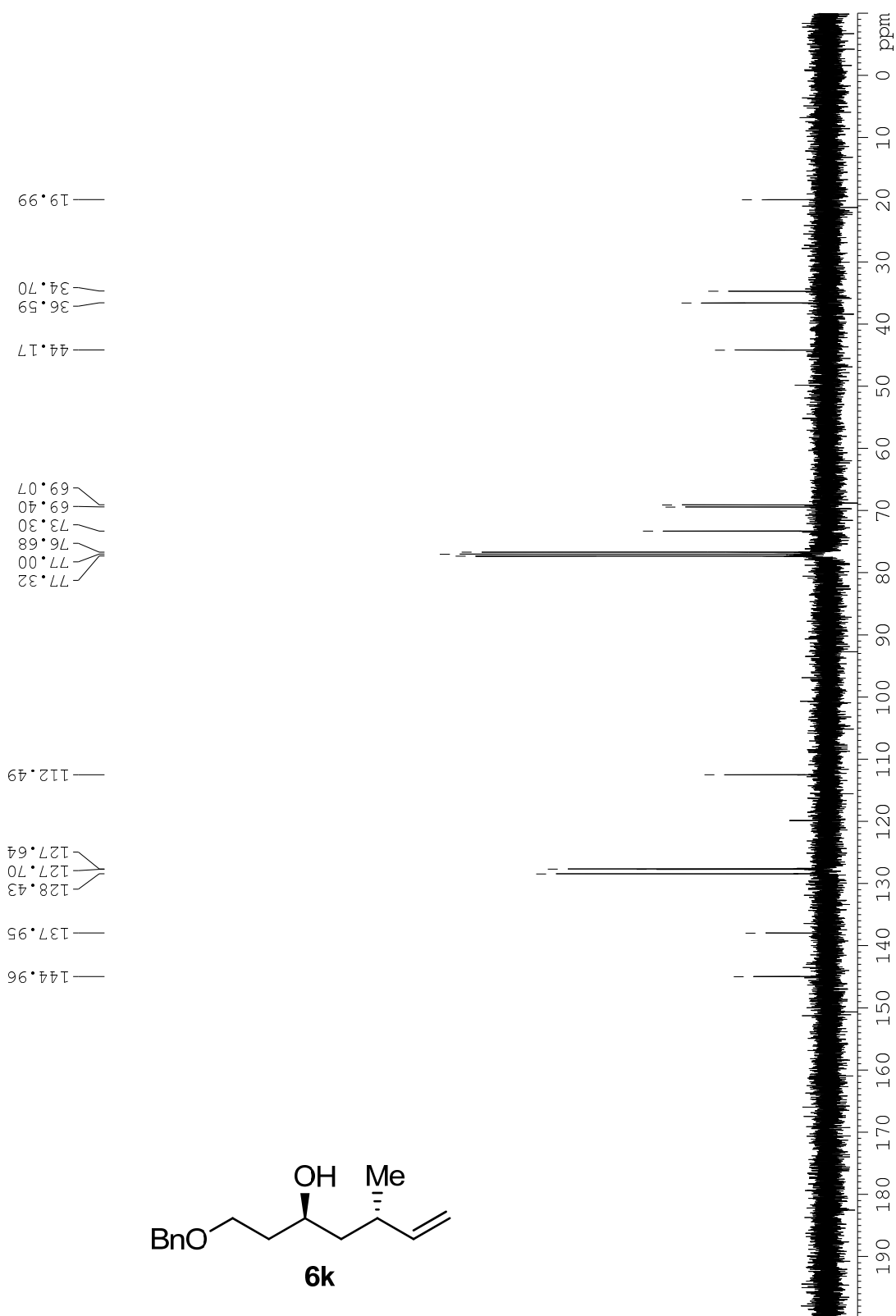
100 MHz ^{13}C NMR spectrum of **6j** (CDCl_3)



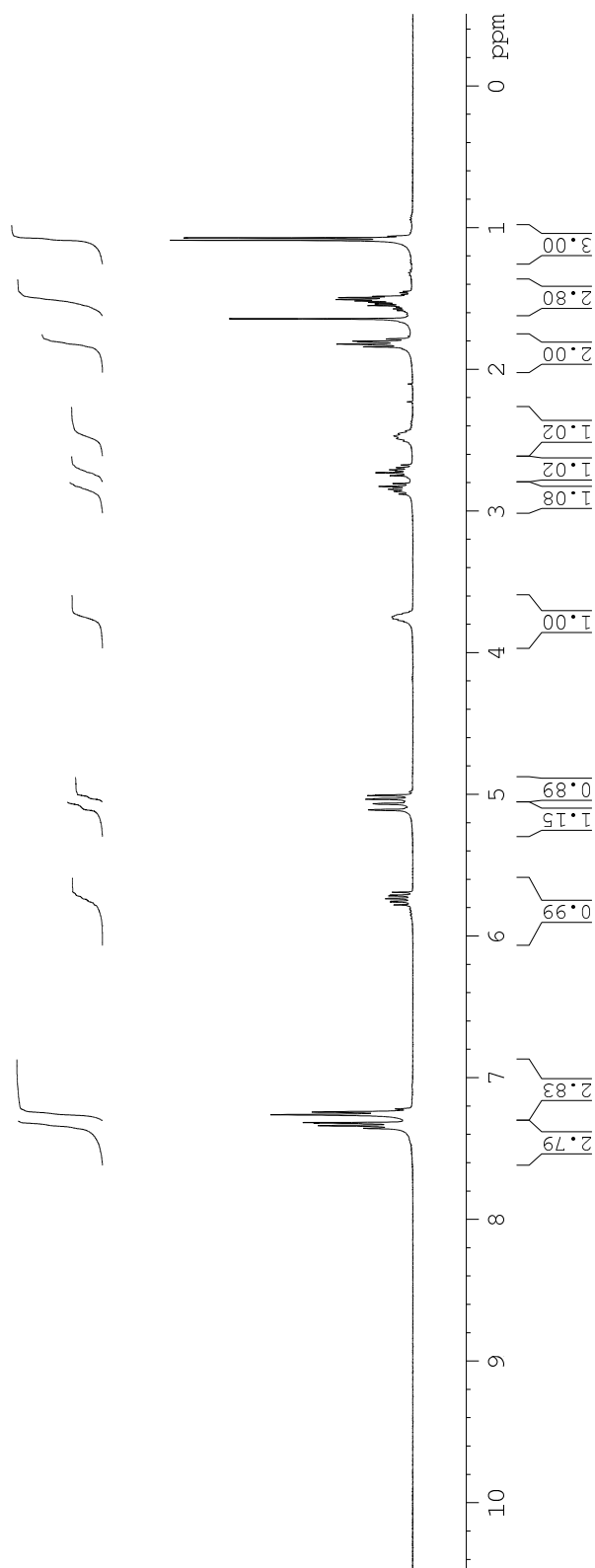
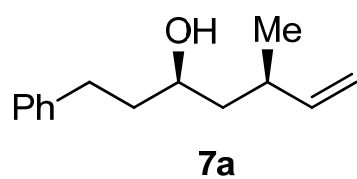
400 MHz ^1H NMR spectrum of **6k** (CDCl_3)



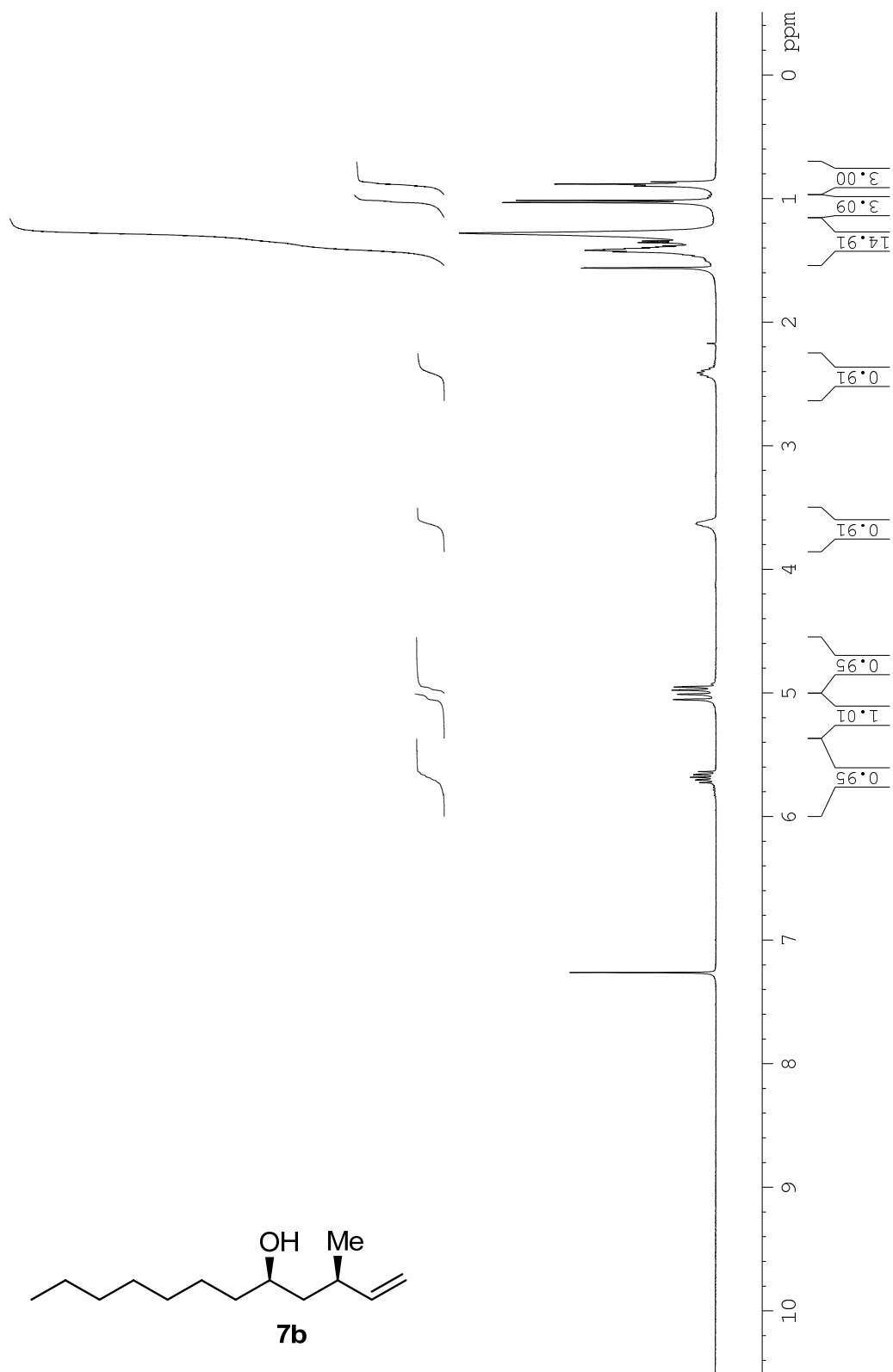
100 MHz ^{13}C NMR spectrum of **6k** (CDCl_3)



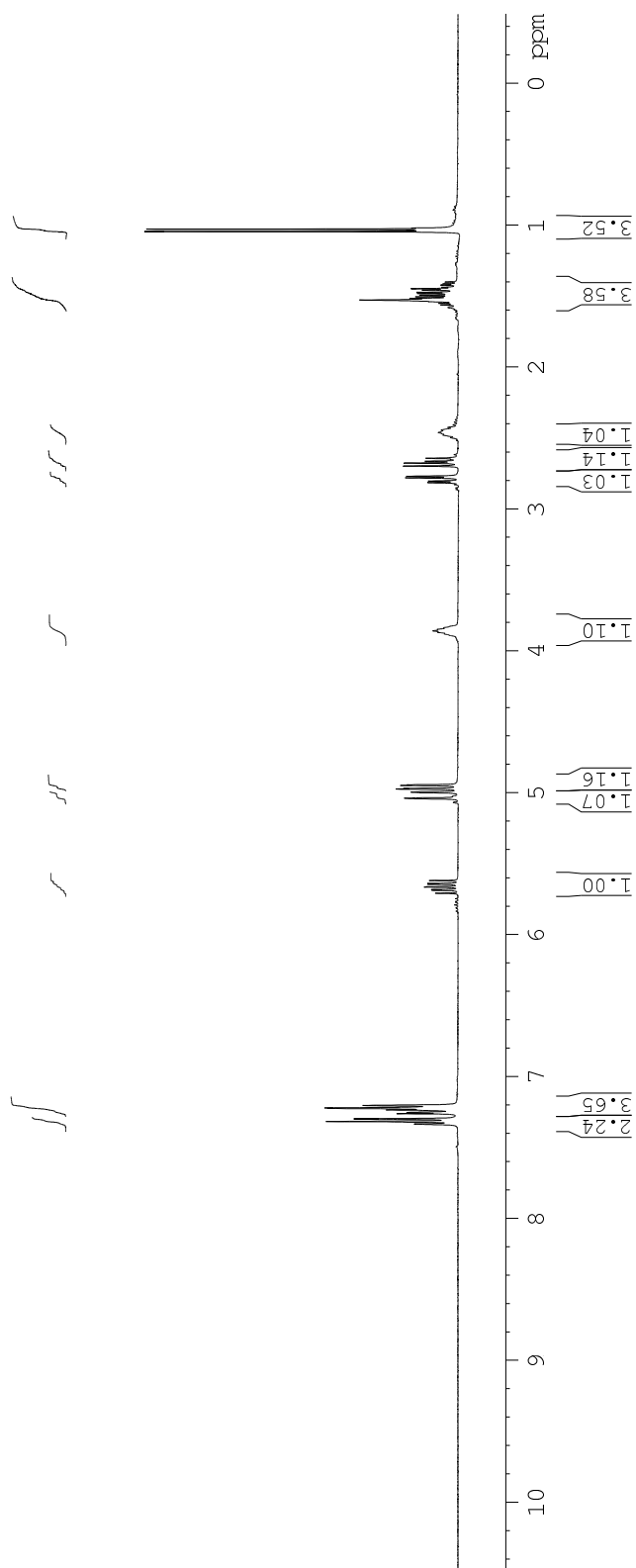
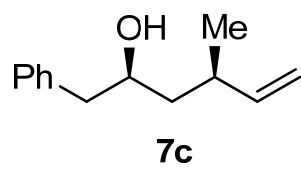
400 MHz ^1H NMR spectrum of **7a** (CDCl_3)



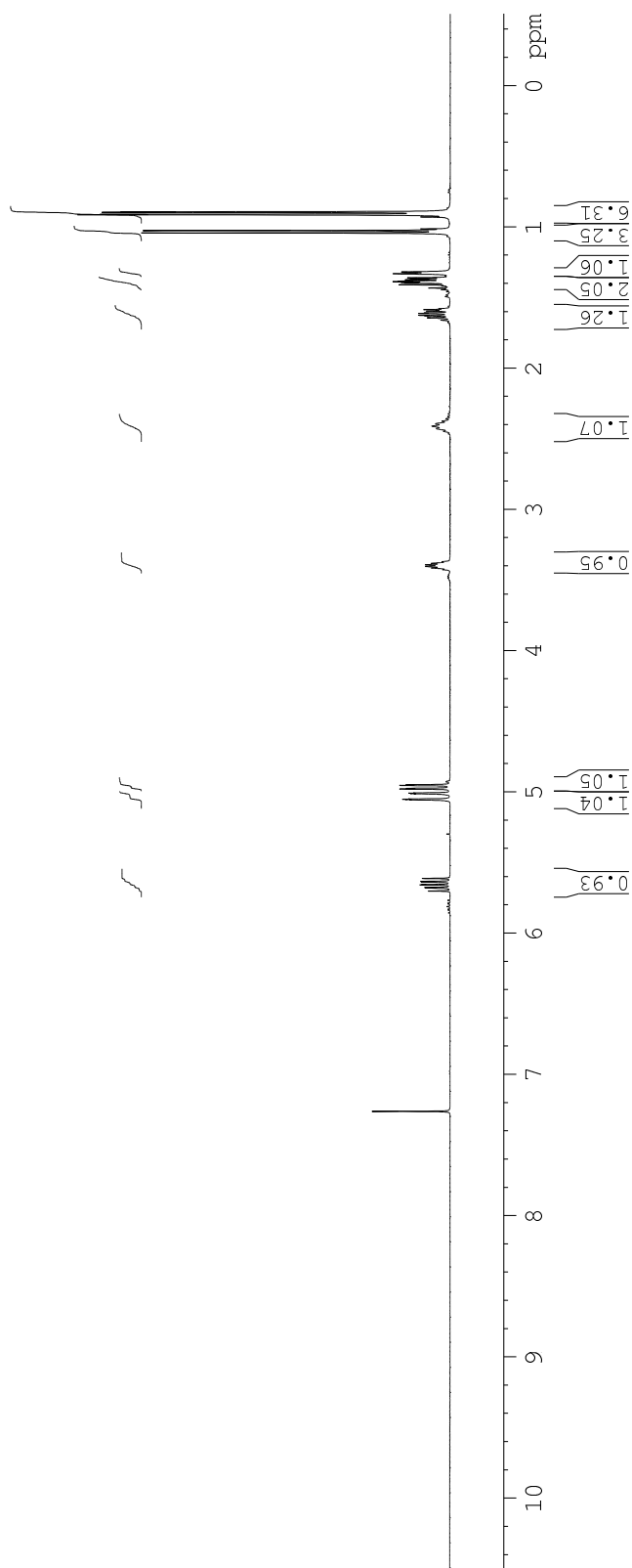
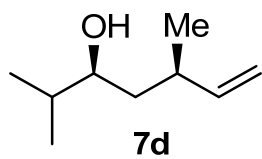
400 MHz ^1H NMR spectrum of **7b** (CDCl_3)



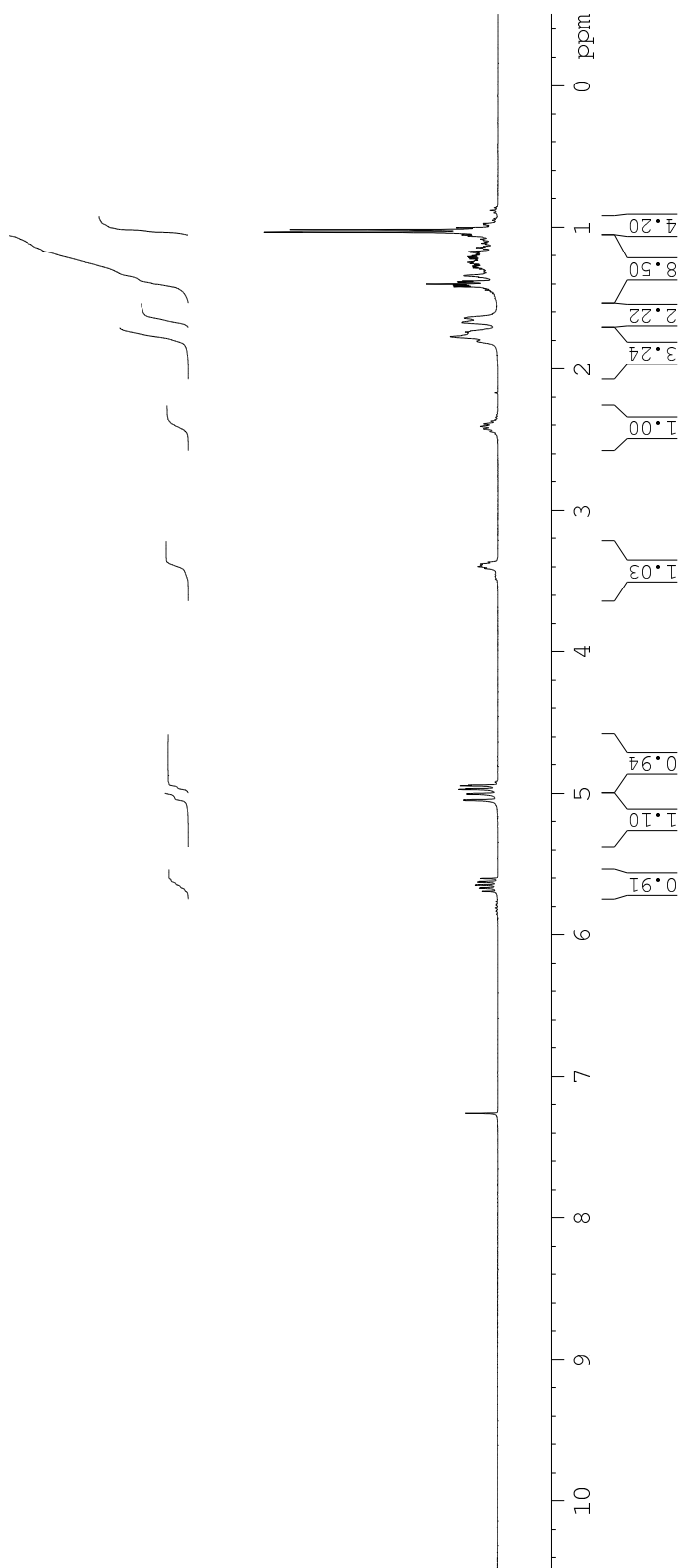
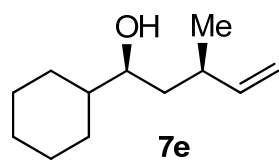
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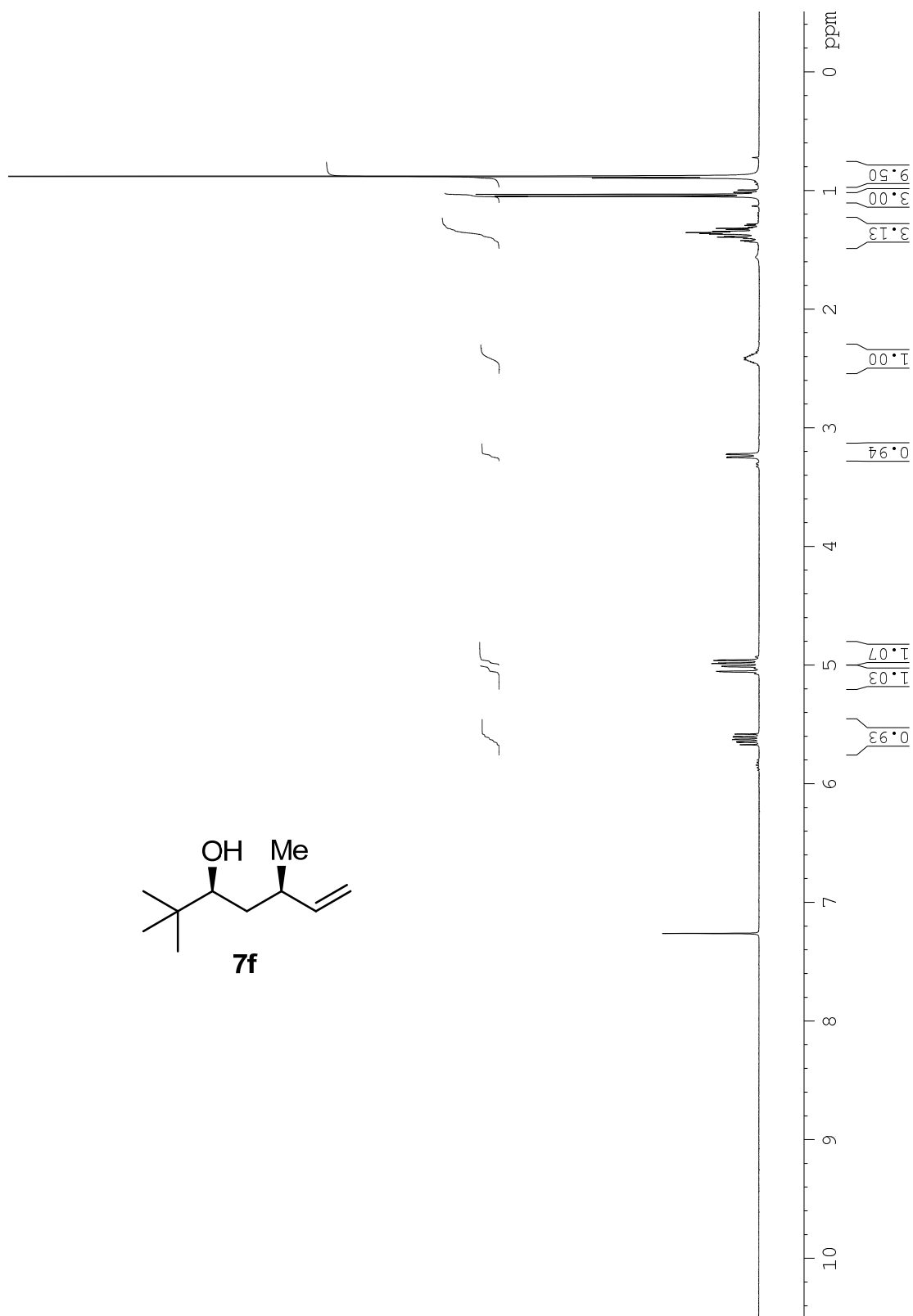
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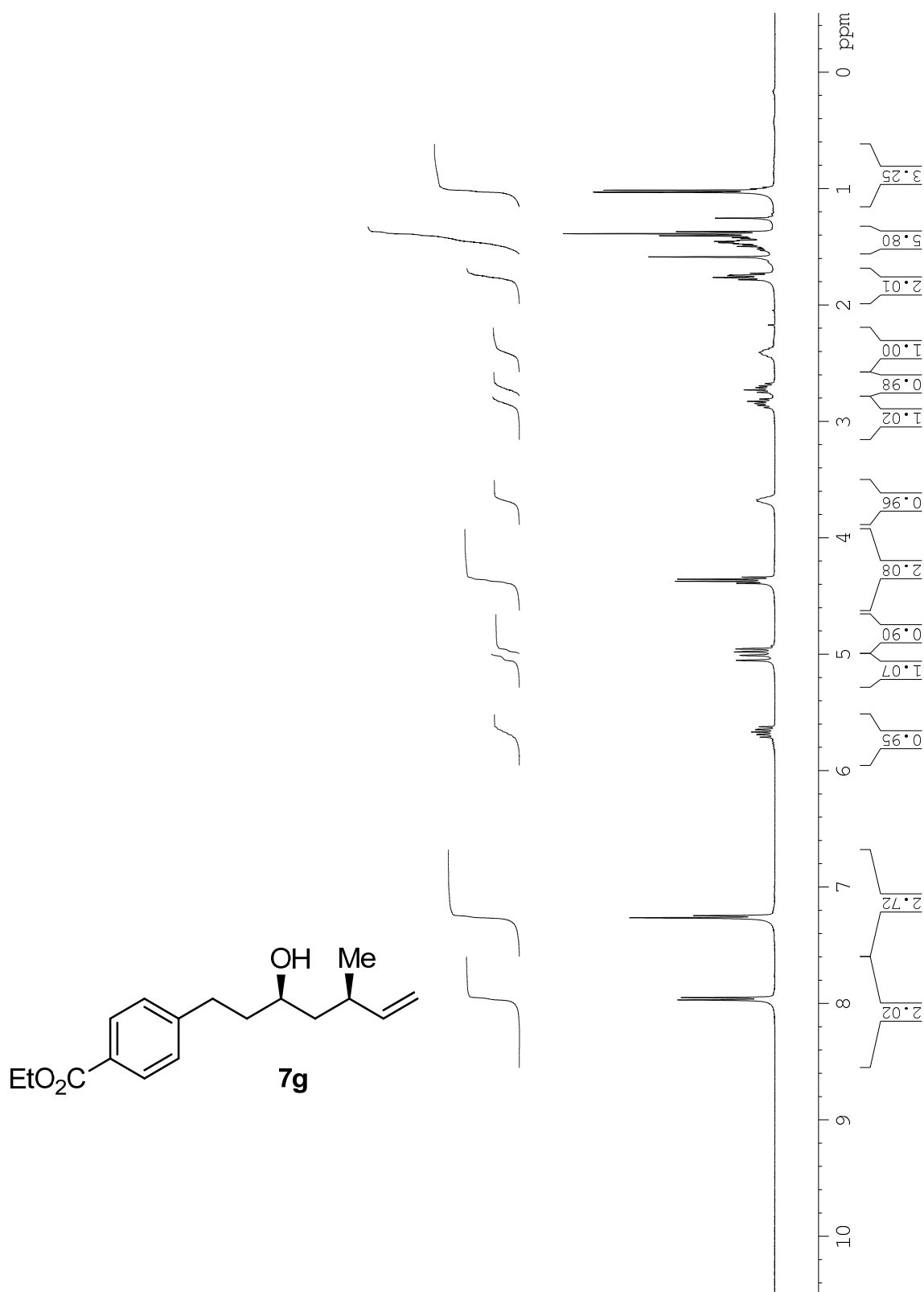
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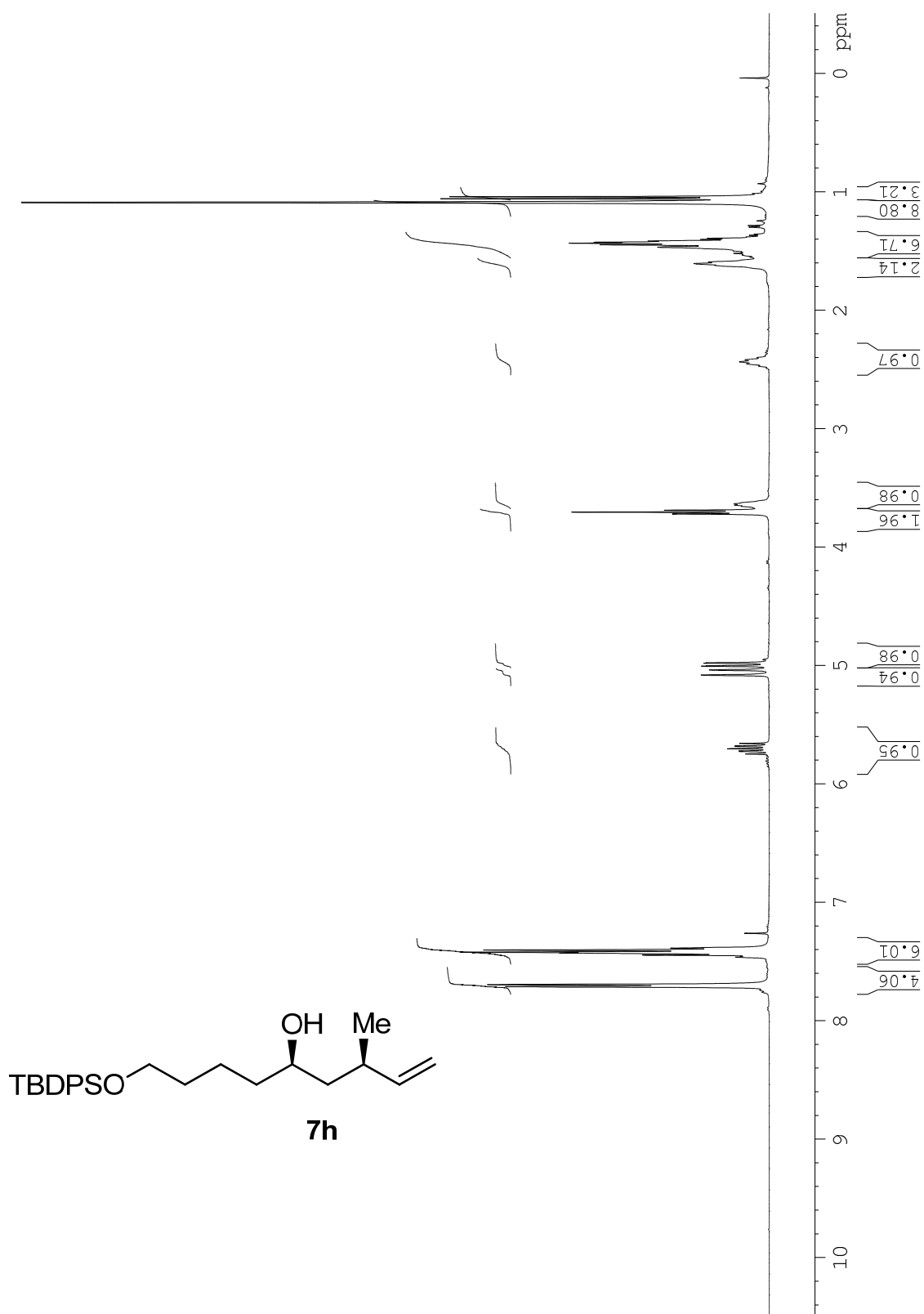
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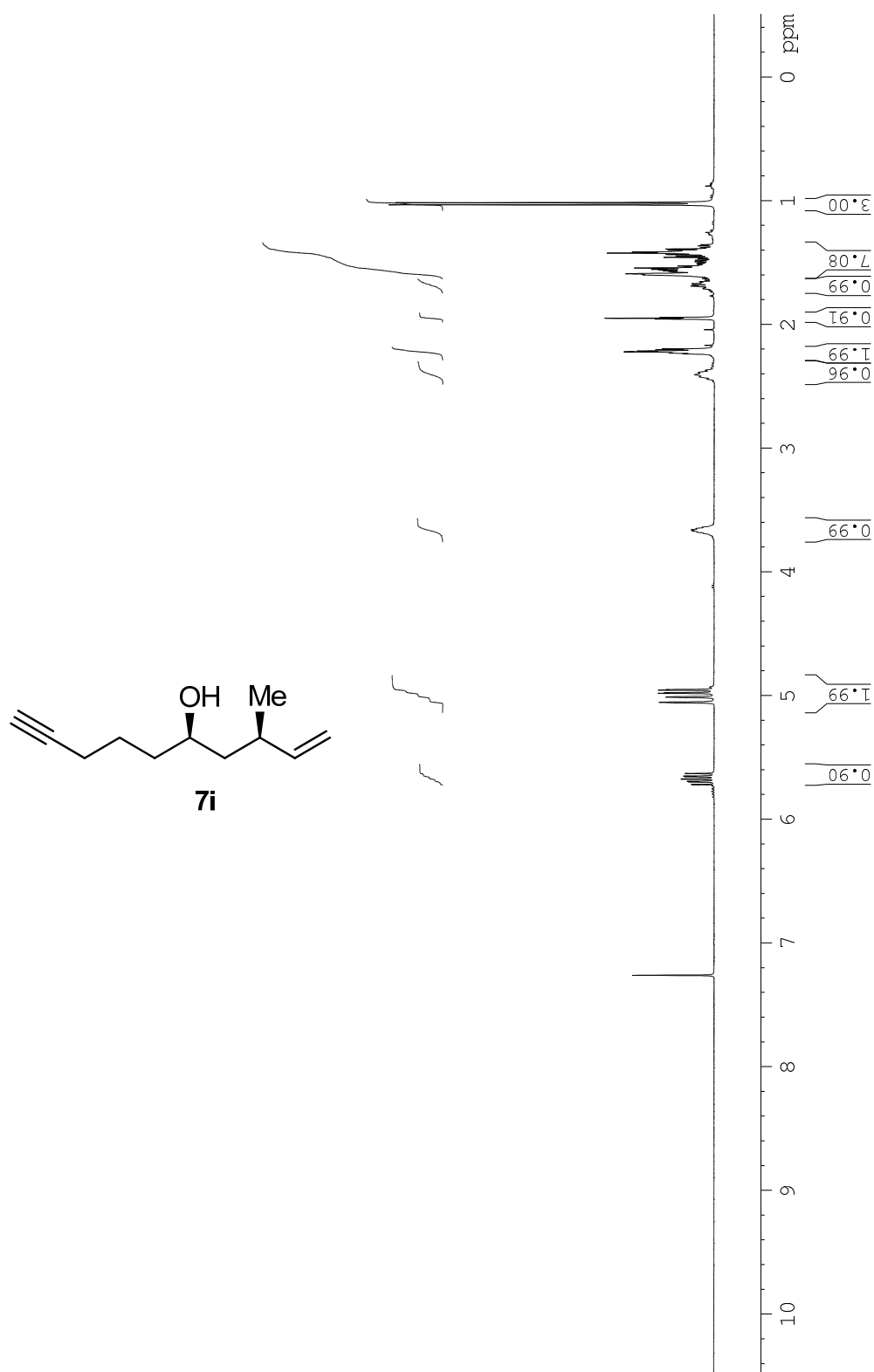
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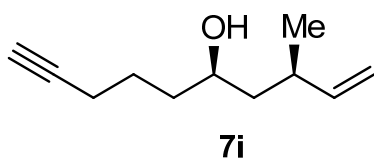
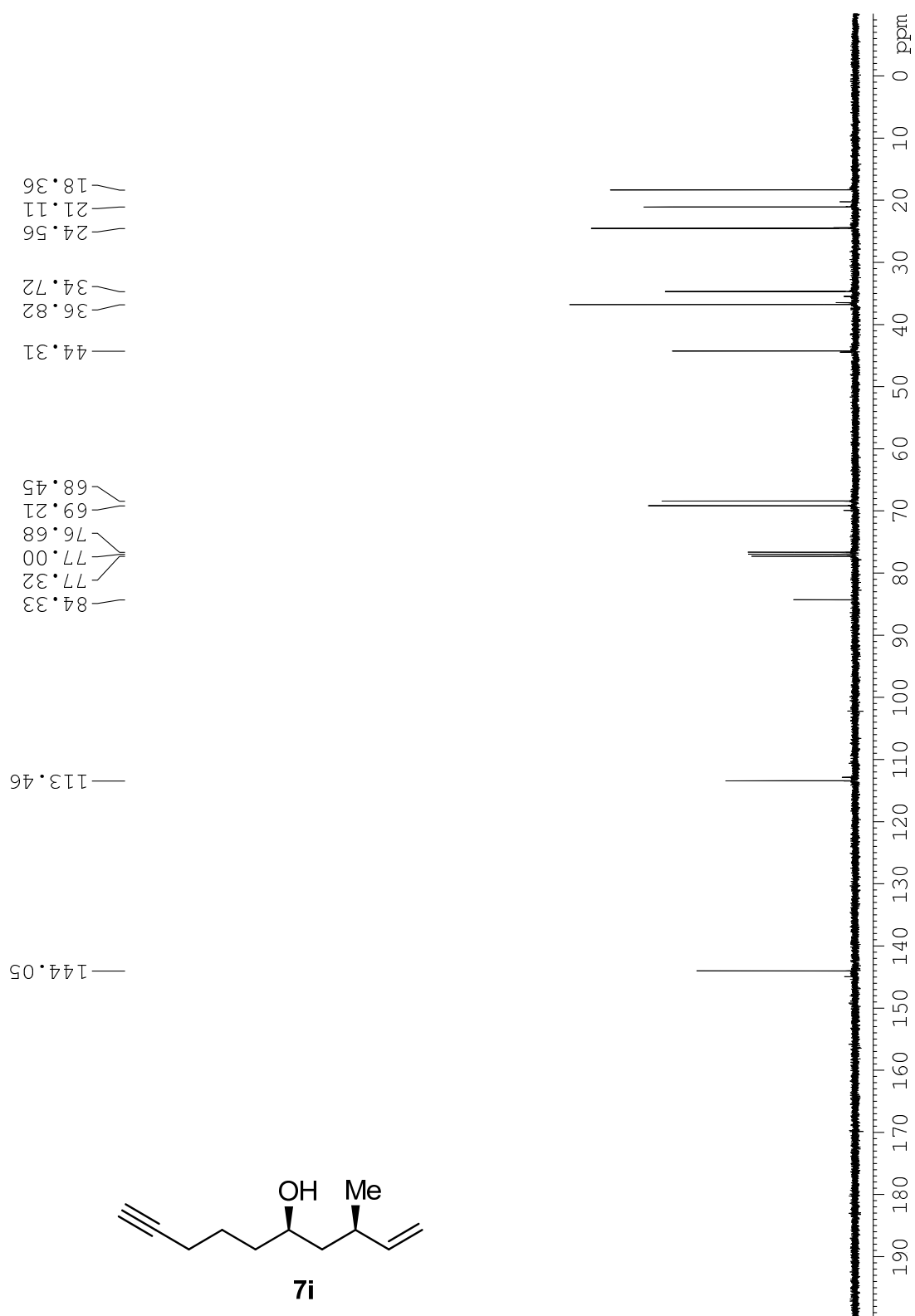
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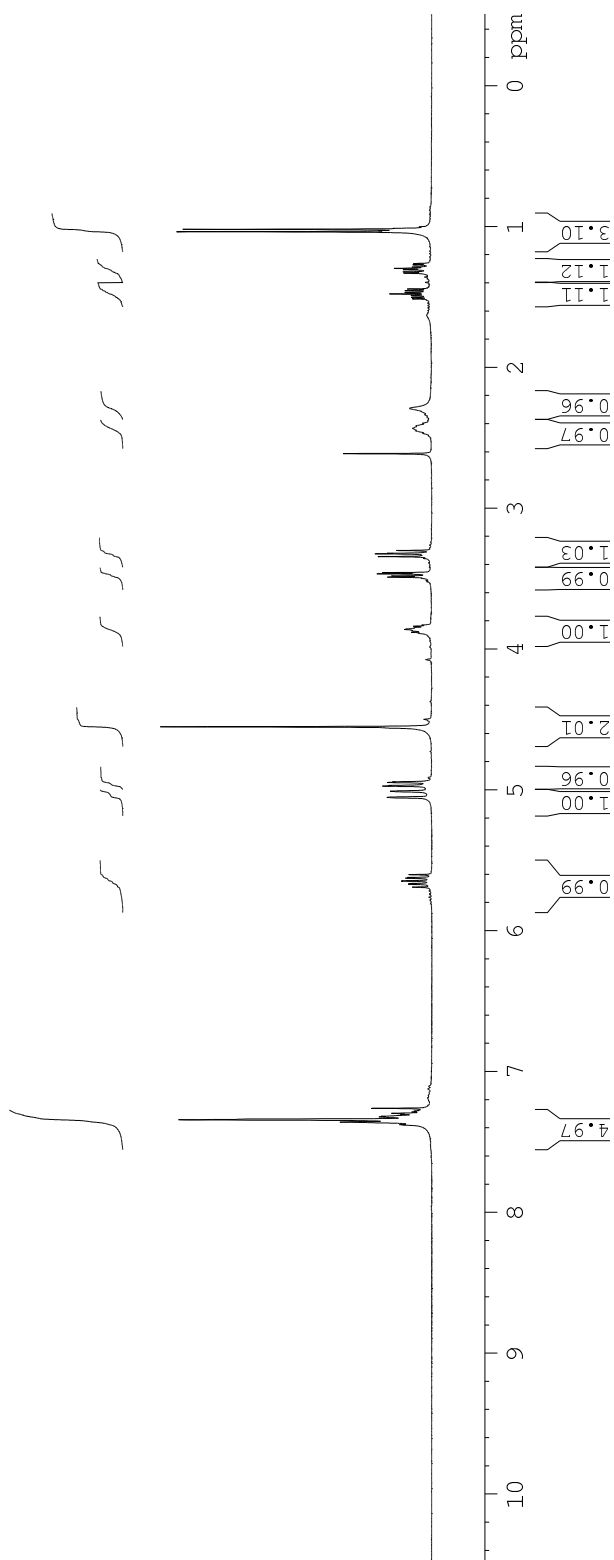
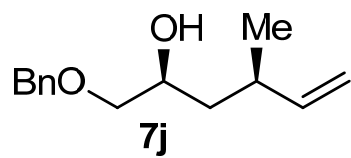
400 MHz ^1H NMR spectrum of **7i** (CDCl_3)



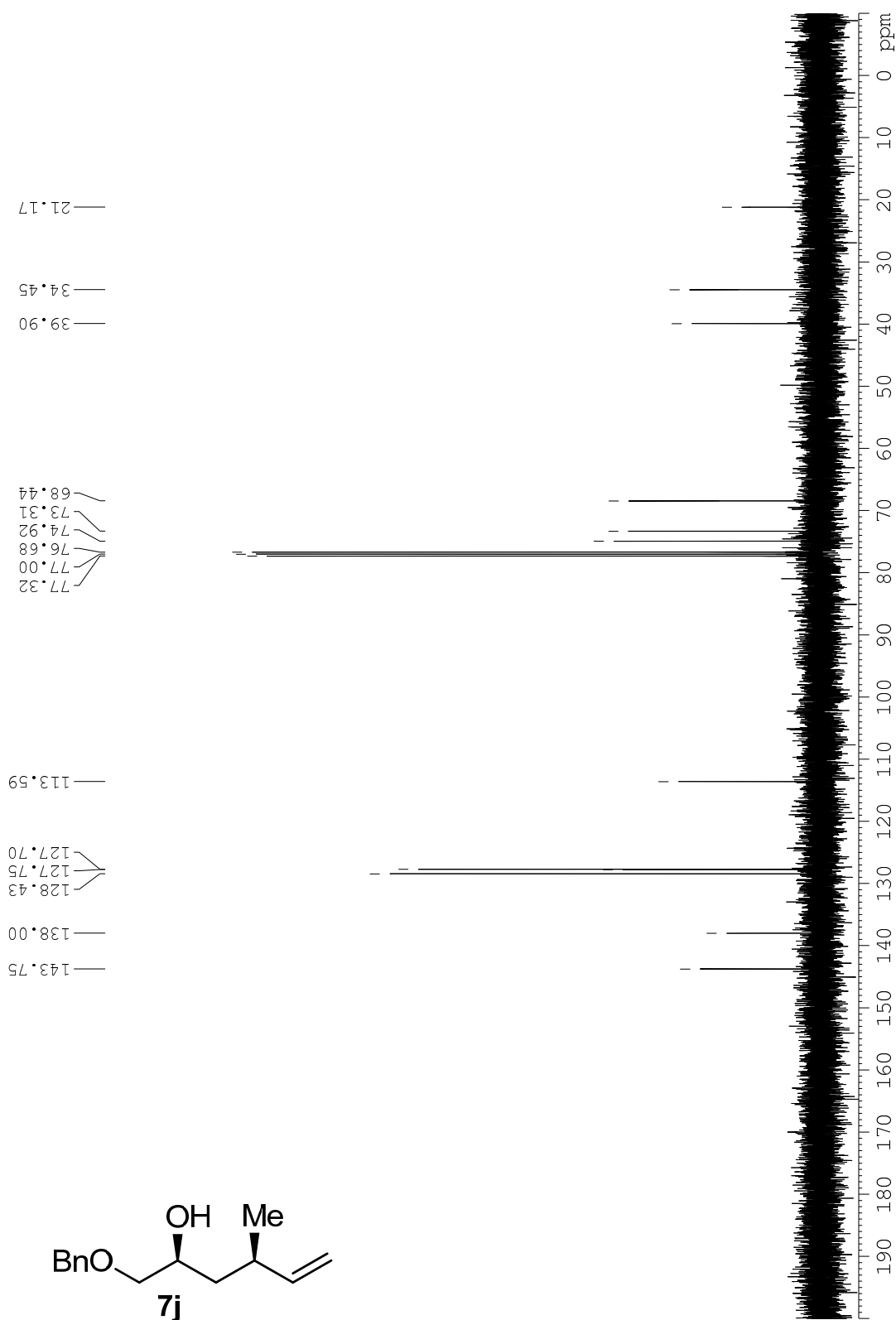
100 MHz ^{13}C NMR spectrum of **7i** (CDCl_3)



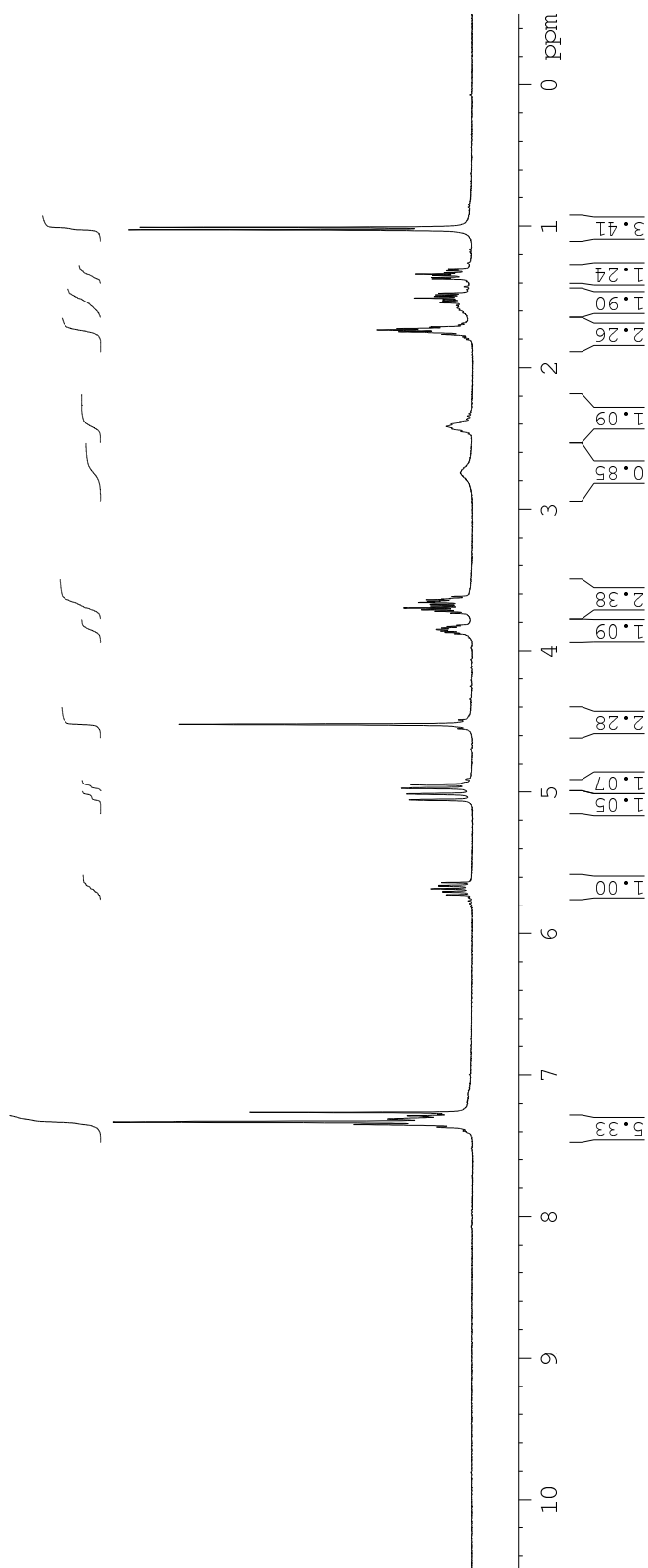
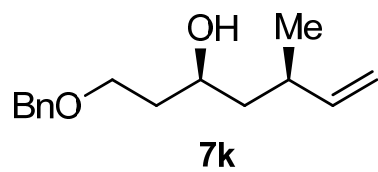
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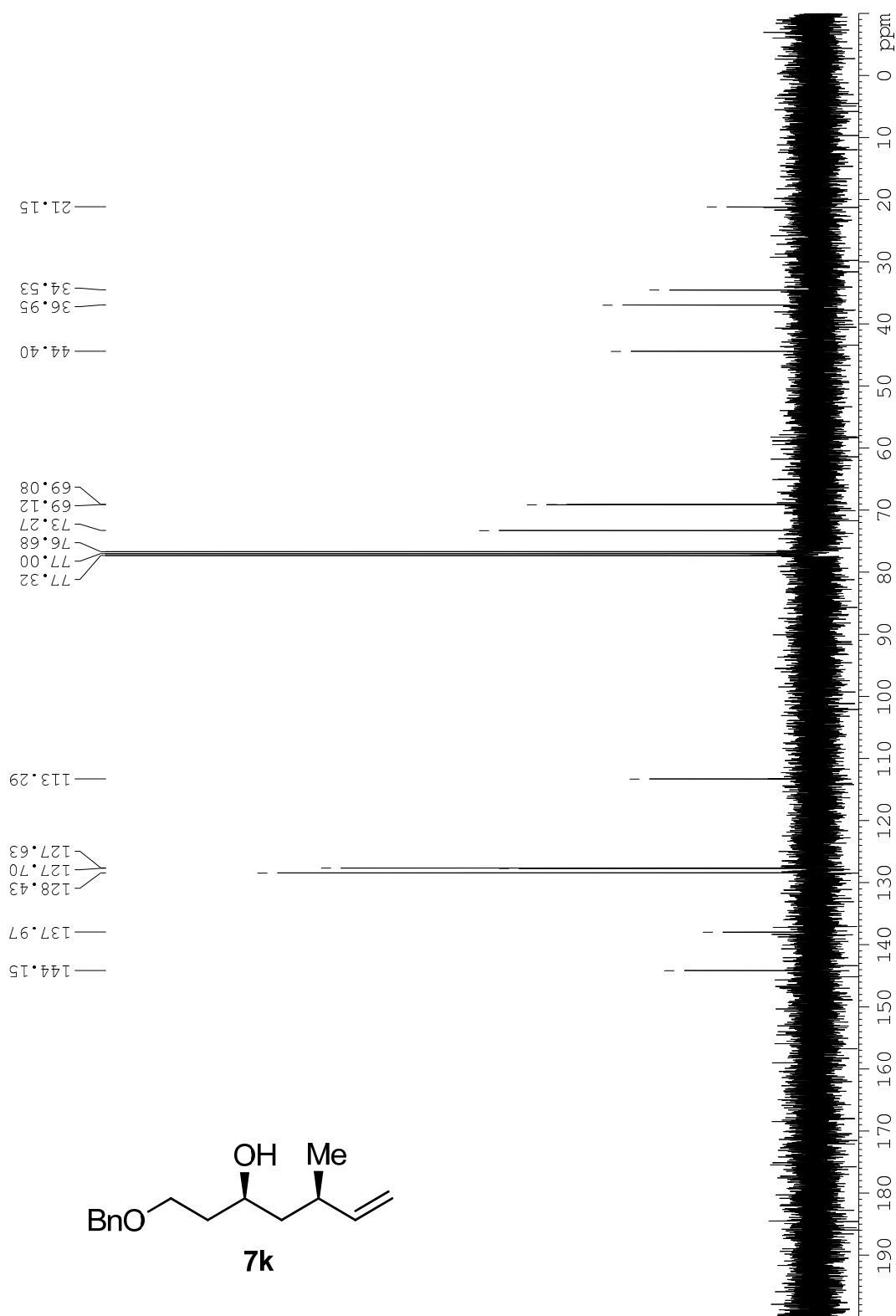
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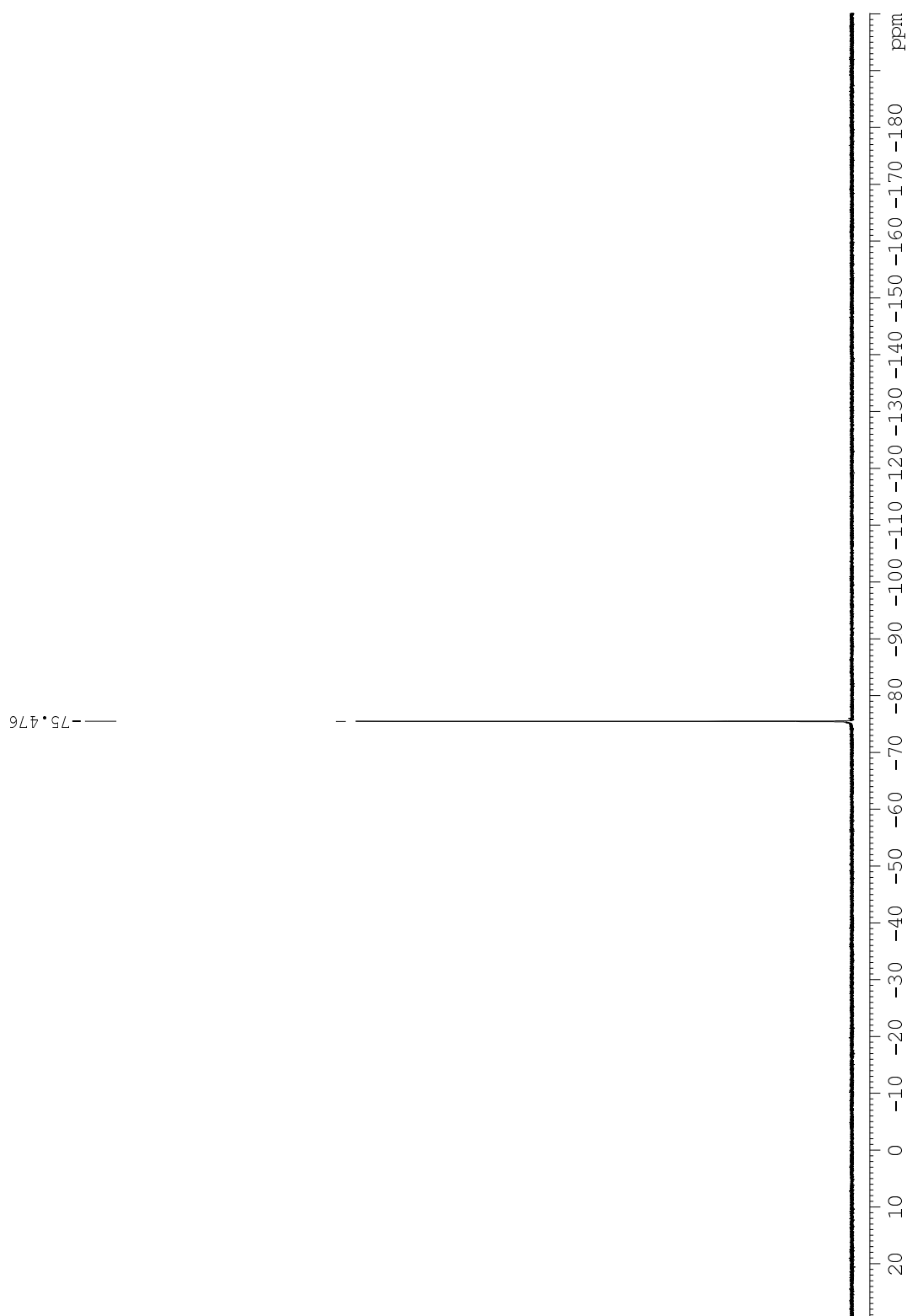
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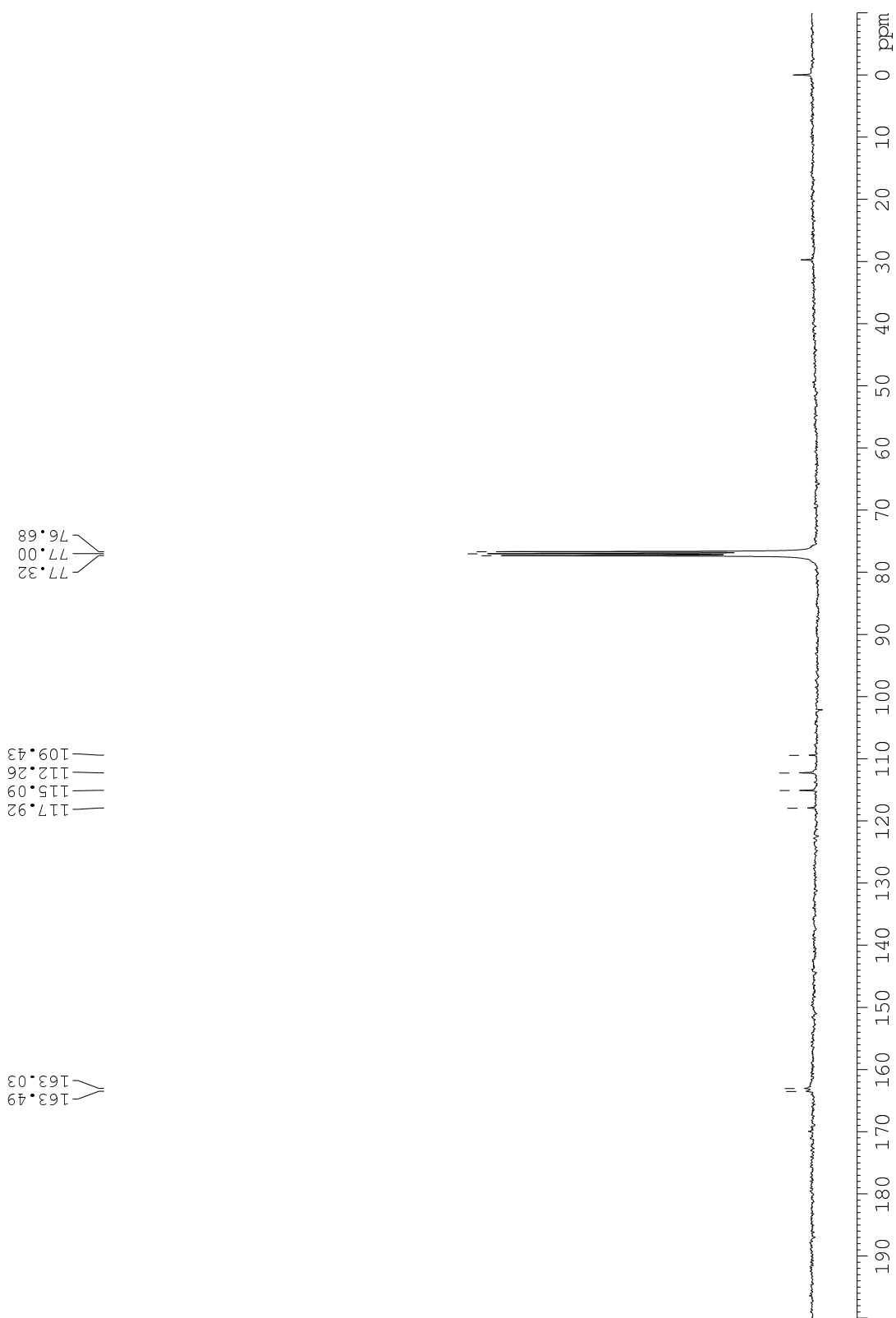
100 MHz ^{13}C NMR spectrum of **7k** (CDCl_3)



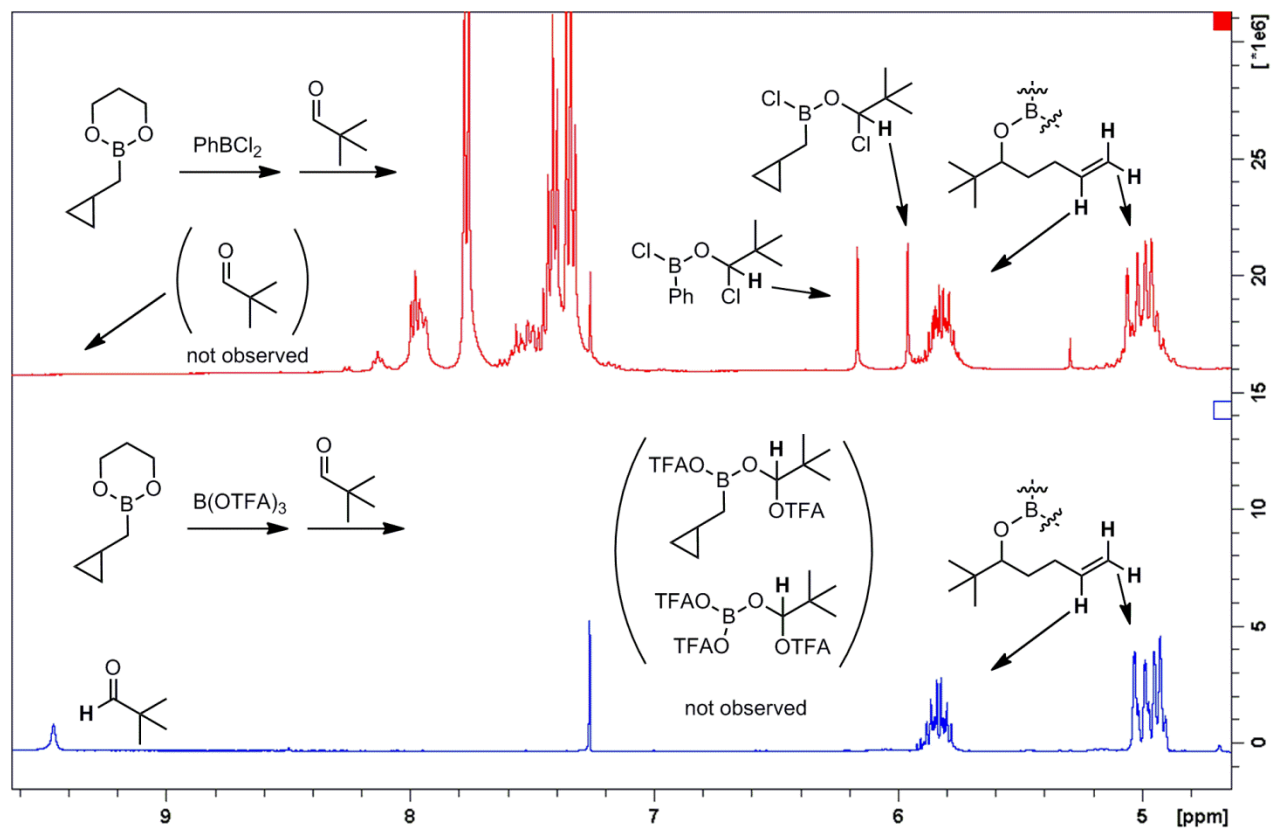
376 MHz ^{19}F spectrum of $\text{B}(\text{OTFA})_3$



100 MHz ^{13}C spectrum of $\text{B}(\text{OTFA})_3$



400 MHz ^1H NMR (CDCl_3) observation of homoallylation at partial conversion (PhBCl_2 promoter vs $\text{B}(\text{TFA})_3$), supporting Scheme 2 of the main text.



Complete citation for ref. 33:

a) *Gaussian 09*, Rev. D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, C.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian, Inc. Wallingford CT, 2013.* b) *Gaussian 09*, Rev. B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian, Inc. Wallingford CT, 2010.*

Cartesian coordinates and energies

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Compound 1      C7H13B1O2
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C, 3.667244693, 0.0251049746, -0.2117498982
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Thermal energy = -449.926325
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Zero-point electronic energy = -1604.128250
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Free energy = -1604.186687
Free energy (quasiharmonic approximation) = -1604.175566

Compound 9 C5H6B1F3O4
B,-1.1120273147,0.2200970148,0.0151903184
O,-1.5527703887,-1.0227144778,0.3182628515
O,-1.8855469319,1.2738871573,-0.3334119774
C,-3.310618356,1.0913734248,-0.4143647862
C,-2.9611861093,-1.296752295,0.2201212624
C,-3.7741805604,-0.0401428193,0.4909854886
H,-3.765116813,2.0404865802,-0.1337936825
H,-3.5637845632,0.8851584155,-1.4576578283
H,-4.8348208936,-0.2383054715,0.321051165
H,-3.6550344212,0.2532200001,1.5374332086
H,-3.1629649599,-1.6884512458,-0.7804266898
H,-3.1791973544,-2.0799566357,0.9445040424
O,0.2717440749,0.4828460102,0.1446864252
C,1.2043796672,-0.2503863653,-0.454070586
O,1.0526007669,-1.0319701539,-1.3446357925
C,2.5967549941,0.0728805234,0.1508745534
F,2.6206934615,-0.2343013709,1.4606557586
F,3.551008124,-0.6267420895,-0.4621670574
F,2.8800975775,1.3804737984,0.0227333263
Electronic energy = -819.9071
Zero-point electronic energy = -819.778631
Thermal energy = -819.766721
Enthalpy = -819.765777
Free energy = -819.820137
Free energy (quasiharmonic approximation) = -819.816163

Compound 17 C13H13B2F9O8
B,1.9522296274,0.364338269,1.6040169582
C,2.7411424366,0.8951737091,0.3650696711
H,2.3102771746,0.5463105121,-0.5726469489
H,2.631966728,1.9865185258,0.3398843817
O,0.5797397941,-0.0908121103,1.4968774407
O,2.5452582896,0.3088695229,2.8089975315
B,-0.2972561688,0.1396598767,0.1884747863
C,1.9468566297,-0.2589606279,3.9817005017
C,-0.0900797974,-0.7582444118,2.6550601703
C,0.9541249059,-1.3282154234,3.5795299032
H,2.7601259451,-0.6627088138,4.5821284374
H,1.4646954889,0.5428230093,4.5465371348
H,0.4437404164,-1.7295237673,4.4577754794
H,1.4700911556,-2.1568775282,3.0891384042
H,-0.7055606386,0.0050553979,3.125633821
H,-0.7090882802,-1.5326348683,2.2237640186
O,0.229511833,-0.6870113508,-0.8761893899
C,0.3156521275,-1.9996551637,-0.771598078
O,0.1219392335,-2.6646688814,0.2091553566

O, -1.6535323349, -0.1073946765, 0.6105397239
C, -2.607153907, -0.7681723013, -0.0419566149
O, -2.5042637418, -1.4753687565, -0.9960958788
O, -0.0697729277, 1.5395195181, -0.1090543896
C, -0.7928269058, 2.1824666086, -1.0157575007
O, -1.6971704024, 1.7532372242, -1.6689481537
C, 0.7969632861, -2.6167555959, -2.110387571
F, 2.0839077449, -2.253708185, -2.3215639188
F, 0.7433398928, -3.9466352149, -2.0619428714
F, 0.0695547443, -2.1909412967, -3.1444751294
C, -3.9604889174, -0.5208713872, 0.6770561315
C, -0.2990415285, 3.6498776314, -1.125343754
F, -0.4306932695, 4.2789550888, 0.0585624945
F, 1.0027365416, 3.6846096812, -1.468929555
F, -0.9947718493, 4.3199785131, -2.039026474
F, -4.2600824534, 0.7865081087, 0.7061793026
F, -3.8826860007, -0.9567865967, 1.9555885758
F, -4.9485487107, -1.1729192797, 0.0731927548
C, 4.2115200545, 0.5221445469, 0.422147832
C, 4.6645683701, -0.8040459521, -0.128865428
C, 5.0205707435, 0.4773411697, -0.8418321215
H, 4.730945223, 0.8646046945, 1.3086701247
H, 3.9222731559, -1.4403340177, -0.5943885505
H, 5.450746167, -1.3382689511, 0.3882821906
H, 6.0487483573, 0.8130684508, -0.8082791962
H, 4.5107717674, 0.6911250993, -1.772871603
Electronic energy = -2054.3934447
Zero-point electronic energy = -2054.100202
Thermal energy = -2054.068782
Enthalpy = -2054.067838
Free energy = -2054.170530
Free energy (quasiharmonic approximation) = -2054.156703

TS-11 C10H11B1F6O5
B, -0.0712829745, -0.6786805715, -0.2350614452
C, -0.7774611998, -1.2725200083, -1.5889857462
C, -2.1653261133, -1.6595684715, -1.3375897427
C, -2.3505954445, -2.9985050371, -0.1285956055
H, -0.7817326422, -0.4388610867, -2.2990651299
H, -0.1966330726, -2.0897748379, -2.0186444881
C, -2.7549360282, -2.9120972222, -1.6734895595
H, 3.8262554131, -2.9595392581, -1.8169490476
H, -2.1822382418, -3.5883571485, -2.295354813
H, -2.8435135441, -0.8769155436, -1.0135939148
H, -3.2674211865, -3.159463288, 0.4199943799
H, -1.6109408424, -3.7826047806, -0.0507863128
C, -1.5325807996, -1.9186422199, 1.1811502141
H, -2.1968990596, -1.0562551598, 1.2207777904
C, -1.6286439045, -2.8121911636, 2.3902498339
H, -1.2246754114, -2.2535391351, 3.2368811165
H, -2.6589364509, -3.0844591295, 2.6161487204
H, -1.0260602396, -3.7111532183, 2.2620988699
O, -0.2842864541, -1.6511012406, 0.8408216438
O, -0.7737721781, 0.5752753659, 0.2030327785
C, -0.8209070516, 1.6761332923, -0.5008441114
O, -0.2900775096, 1.9206736621, -1.5517218673
O, 1.3625034812, -0.5136237187, -0.4724834942
C, 2.1814051706, 0.0023805484, 0.4206130421
O, 1.9245775788, 0.4555445316, 1.5002544009
C, -1.7620914499, 2.7006626611, 0.1927570953
C, 3.6388732638, -0.0514268071, -0.1183537717
F, -3.0310756042, 2.2124190532, 0.1863821924
F, -1.4176319905, 2.9188543024, 1.4690529048
F, -1.7714080602, 3.8676958263, -0.449187188
F, 3.7475915472, 0.5835826688, -1.2980683379
F, 4.4882145559, 0.5159582322, 0.7408086731
F, 4.0240072693, -1.3324610979, -0.3008790806
Electronic energy = -1388.3549952
Zero-point electronic energy = -1388.133037
Thermal energy = -1388.111503
Enthalpy = -1388.110559
Free energy = -1388.188039
Free energy (quasiharmonic approximation) = -1388.179877

TS-17 C15H17B2F9O9
B, 1.7792589002, -1.1237168287, 0.9292412785
C, 2.1792486931, -1.3075735633, -0.639341777
C, 3.6413983748, -1.2284081409, -0.8054547282
C, 4.3200710779, 0.3397782543, -0.3878895946
H, 1.8899620266, -2.3311758799, -0.89640967
H, 1.6832840005, -0.6296405971, -1.3261422425

C,4.295955527,-0.4543992444,-1.7995925448
H,5.2916645355,-0.7299727838,-2.1185293778
H,3.6886644082,0.052959202,-2.5371885159
H,4.2345928793,-1.972244261,-0.2852770191
H,5.3682522665,0.4768079561,-0.1661300727
H,3.7455373155,1.2387804118,-0.5543499305
C,3.7814371657,0.1151331094,1.3901761163
H,4.2848639615,-0.8156393024,1.6574456668
C,4.3773291356,1.3424726953,2.0326081196
H,4.1485982799,1.2986173745,3.0995758023
H,5.459504048,1.3818394661,1.914626109
H,3.9259055964,2.2477717969,1.6279346632
O,2.4654442378,0.0858854391,1.471036198
O,0.2734173414,-0.7754388528,1.137250024
O,2.1320519085,-2.3190468153,1.6203867221
B,-0.5415477976,0.0142871024,0.1297021804
C,1.7137471899,-2.4531187516,2.9702610206
C,-0.2110277745,-0.9258197131,2.520828262
C,0.2074965034,-2.2758303889,3.0581686282
H,2.0137140719,-3.4453116407,3.3091694664
H,2.2177678344,-1.7123955188,3.6070722638
H,-0.1293032336,-2.3441325377,4.0963415741
H,-0.2940193236,-3.0592912712,2.4871240069
H,0.214437095,-0.1007205664,3.0938016432
H,-1.2872184401,-0.8275536491,2.4868810849
O,-0.8605140444,-0.8628185955,-0.9982367556
C,-1.5366376155,-1.9772425168,-0.8175892047
O,-1.9810994053,-2.4132275676,0.2085538881
O,-1.6639381083,0.601132072,0.8350645493
C,-2.914409896,0.7359649026,0.417450321
O,-3.4460030955,0.2579125163,-0.5379952875
O,0.3612693346,1.0615989473,-0.3796773725
C,-0.0314141509,2.11630123,-1.0548091448
O,-1.1377363439,2.4628731331,-1.3528226155
C,-1.6477554284,-2.7545979116,-2.1554646398
F,-0.4220657301,-3.2269223915,-2.4950753345
F,-2.4707334507,-3.7961501488,-2.0382104391
F,-2.0789265443,-1.9787250044,-3.1561769971
C,-3.6787813903,1.6332964022,1.4289795233
C,1.2224637418,2.9394873433,-1.4664189908
F,1.9486204331,3.2995624179,-0.3863960517
F,2.0376648024,2.191570114,-2.2563818596
F,0.8961072413,4.0372962586,-2.1362546627
F,-3.1066562624,2.8445887906,1.5336695351
F,-3.664113839,1.064200624,2.6558423059
F,-4.9481980532,1.7961068836,1.0626438762
Electronic energy = -2208.2789521
Zero-point electronic energy = -2207.926462
Thermal energy = -2207.892254
Enthalpy = -2207.891310
Free energy = -2207.998615
Free energy (quasiharmonic approximation) = -2207.984939

BC12(OMe) C1H3B1Cl2O1
B,0.1278918863,-0.1502484357,0.0407759762
Cl,1.8315039344,-0.5303989002,-0.2265532571
Cl,-0.3113049481,1.4446550232,0.6961775549
O,-0.7863874842,-1.0759278804,-0.258452755
C,-2.1995366327,-0.8961052022,-0.0893025902
H,-2.6723432488,-1.8179590299,-0.4176140184
H,-2.4373108105,-0.7090803201,0.9577349844
H,-2.5526726964,-0.0614752547,-0.6947058949
Electronic energy = -1060.6260636
Zero-point electronic energy = -1060.576715
Thermal energy = -1060.570569
Enthalpy = -1060.569625
Free energy = -1060.607945
Free energy (quasiharmonic approximation) = -1060.607610

Compound 8 C4H7B1Cl2
B,-0.7995360565,0.0106531621,-0.2932441734
C,0.5665180473,0.2213984046,-1.014705828
H,0.8606884896,-0.6808305753,-1.5557761338
H,0.5074966403,1.0413526724,-1.7361018092
C,1.6292754614,0.5487749833,0.0330902707
C,2.2544709877,-0.5545158568,0.8438639359
C,3.0653730716,0.1687285143,-0.20064758
H,1.4643896682,1.4850311258,0.5535267919
H,1.9462886207,-1.5697905134,0.628767593
H,2.4740368132,-0.3668240614,1.8864560621
H,3.835903873,0.8527482821,0.1303762649

H, 3.3000945413, -0.3619853604, -1.1146890881
Cl, -1.7700372591, 1.3947733842, 0.2219248691
Cl, -1.3829228988, -1.6043341614, 0.1174788247
Electronic energy = -1102.0826893
Zero-point electronic energy = -1101.976056
Thermal energy = -1101.968143
Enthalpy = -1101.967199
Free energy = -1102.010808
Free energy (quasiharmonic approximation) = -1102.009211

B(OMe)(OCH₂CH₂CH₂O) C₄H₉B₁O₃
C, -1.7804128233, -1.0242111215, -0.1601913912
C, -1.1808964071, 1.3892955336, -0.2007476047
C, -2.0851242625, 0.3435497132, 0.432382452
H, -2.0696053508, -1.0537395043, -1.2166964715
H, -2.3288705898, -1.8112411419, 0.3584412311
H, -1.2811568421, 2.3558567521, 0.2941755298
H, -1.4336948337, 1.523801061, -1.2578542774
H, -1.9182282382, 0.3198525289, 1.5130067107
H, -3.13317342, 0.6023236173, 0.2624197851
O, 0.1950803141, 1.0082380486, -0.1058111337
O, -0.3918798164, -1.3391692824, -0.0537936889
B, 0.5322502626, -0.3254848883, -0.0425643544
O, 1.8433093645, -0.6849736623, 0.0461000822
C, 2.8620370586, 0.3083955098, 0.0808231192
H, 3.8176674625, -0.2117581492, 0.1255303928
H, 2.8356053083, 0.937463168, -0.8118564404
H, 2.7607328133, 0.9498018174, 0.9594960593
Electronic energy = -408.6744642
Zero-point electronic energy = -408.532429
Thermal energy = -408.524236
Enthalpy = -408.523292
Free energy = -408.565663
Free energy (quasiharmonic approximation) = -408.565314

B(O₂COCF₃)₂(OMe) C₅H₃B₁F₆O₅
B, -0.0025968074, 1.1114680808, -0.11247415
O, 0.3156874171, 2.3963100066, -0.2453153102
C, -0.636865102, 3.4570221446, -0.4068295343
H, -0.5450507905, 4.1237618386, 0.4488125469
H, -0.3822980114, 3.9972688943, -1.3166998895
H, -1.6540654882, 3.0733076407, -0.4722764835
O, 0.9709263272, 0.1287092497, 0.0258690656
C, 2.2195337482, 0.3166873192, 0.4967165349
O, 2.5890147668, 1.1752996058, 1.2302034234
O, -1.3380783919, 0.6959605647, -0.0970782895
C, -1.8114568054, -0.5119450026, -0.4567919414
O, -1.2974584136, -1.2956402314, -1.1870722055
C, 3.1391490125, -0.8174734455, -0.0293158549
C, -3.2003245038, -0.7321628708, 0.1991515873
F, 3.1767015792, -0.7968036023, -1.3721362002
F, 4.3779758236, -0.663829332, 0.4329682752
F, 2.6791981701, -2.0152127944, 0.3638946945
F, -3.0869436618, -0.7174149283, 1.5383396953
F, -4.0485959737, 0.2468832873, -0.1616210706
F, -3.7144828947, -1.8996864251, -0.1731348935
Electronic energy = -1193.0009657
Zero-point electronic energy = -1192.896111
Thermal energy = -1192.878915
Enthalpy = -1192.877971
Free energy = -1192.947491
Free energy (quasiharmonic approximation) = -1192.939660

Compound 11 C₈H₇B₁F₆O₄
B, -0.0081278078, 0.7021005805, 0.4685060488
O, 0.9662112772, -0.2286901485, 0.1152044438
C, 2.2606782506, 0.0321170033, -0.1293477861
O, 2.7306879401, 1.0744206262, -0.4606184699
O, -1.3134003599, 0.2340351736, 0.3507289813
C, -1.7508755967, -0.7089055793, -0.507626745
O, -1.2906908867, -0.9739133474, -1.5711689205
C, 3.0961084894, -1.2617515131, 0.0589040435
C, -3.0231917153, -1.3838729796, 0.0685026642
F, 2.641539286, -2.2410030345, -0.734333215
F, 4.3753394992, -1.0359583699, -0.2269023747
F, 3.0076042751, -1.6749731547, 1.3368464981
F, -2.7435987749, -1.9683907911, 1.2462886544
F, -3.9863652012, -0.4691478984, 0.2703389961
F, -3.4827705483, -2.3094284959, -0.7682062539
C, 0.2258018535, 2.1367267675, 1.015054437
H, 1.1924488522, 2.2509076033, 1.5093498687

H, -0.5538521463, 2.3620197273, 1.7482268547
C, 0.1215274749, 3.1300779765, -0.1421171689
C, -1.2284756581, 3.5087374627, -0.6931047815
C, -0.4246951983, 4.5106372657, 0.0943830608
H, 0.9289321262, 3.0548004793, -0.8594306506
H, -2.1035388585, 3.0835079223, -0.2178249741
H, -1.3263434948, 3.6520234661, -1.7609244587
H, 0.029745094, 5.3362833833, -0.4370455982
H, -0.7608081718, 4.7518098748, 1.0949468458
Electronic energy = -1234.4609787
Zero-point electronic energy = -1234.298574
Thermal energy = -1234.279836
Enthalpy = -1234.278892
Free energy = -1234.351621
Free energy (quasiharmonic approximation) = -1234.343484