

Supporting Information

**Cationic Polycyclization of Ynamides:
Building up Molecular Complexity**

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Computational data

Computational details:

All molecular species were fully optimized by density functional theory at the B3LYP level.¹ The correlation-consistent double-zeta + polarization basis sets of Dunning, cc-pVDZ,² were used for all atoms. For each structure, the analytic Hessian was calculated to obtain the vibrational frequencies (zero and one imaginary frequency for local minima and transition structures, respectively). Unscaled frequencies were used to calculate the zero-point energy corrections (ZPE). Calculations were performed using the Gaussian 09 suite of programs.³

¹ (a) Becke's three parameters hybrid method using the LYP correlation functional of Lee and al. (b) A. D. Becke, *J. Phys. Chem.* **1993**, *98*, 5648-5652. (c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789.

² T. H. Dunning, *J. Chem. Phys.* **1989** *90* 1007-1023.

³ Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Calculated total electronic energies (E_e)^a, zero-point corrected energies (E_{ZPE}) and relative zero-point corrected energies (ΔE_{ZPE})^b for gas phase compounds at the B3LYP/cc-pVDZ level:

Compound	E_e	E_{ZPE}	ΔE_{ZPE}
ynamide 11_x	-900.15685	-899.87170	
H ₇ F ₆ ⁺	-603.01991	-602.94130	
(HF) ₆	-602.74012	-602.66689	
keteniminium (II_x)	-900.52454	-900.22767	0.0 (-51.2) ^c
TS(II_x-IV_x)	-900.50738	-900.21337	9.0
IV_x	-900.54334	-900.24456	-10.6
TS(IV_x-V_x)	-900.52498	-900.22728	+0.2
V_x	-900.55147	-900.25149	-15.0
TS(V_x-σ complex)	-900.53423	-900.23367	-3.8
σ complex	-900.53889	-900.23709	-5.9
polycyclic product 12_x	-900.22747	-899.93607	(+16.7) ^d

^a in atomic units (a.u.).

^b in kcal mol⁻¹ (1 a.u. = 627.51 kcal mol⁻¹).

^c relative ZPE corrected energy of [**II_x** + (HF)₆] with respect to [**11_x** + H₇F₆⁺].

^d relative ZPE corrected energy of [**12_x** + H₇F₆⁺] with respect to [σ complex + (HF)₆].

B3LYP/cc-pVDZ Cartesian coordinates:

Symbol, 0, x, y, z

ynamide **11_x**

Charge = 0 Multiplicity = 1

C, 0, -0.3583660194, -0.9302006297, -0.8447802368
 C, 0, 0.8469439757, -0.8821372837, -0.6798869485
 C, 0, -1.7641670195, -0.9693243111, -1.0953002481
 N, 0, 2.1772260513, -0.8111884333, -0.4910495375
 C, 0, 2.8932269401, -1.4295742027, 0.6402118834
 C, 0, 3.0504039654, -0.2807705084, -1.4513110693
 C, 0, -2.2900449417, -0.3290147224, -2.2489542664
 C, 0, -3.6715270751, -0.3914759665, -2.4653901335
 C, 0, -4.5256456566, -1.0579467364, -1.5813901567
 C, 0, -4.0001834144, -1.6844000048, -0.448092352
 C, 0, -2.6278876259, -1.6411981764, -0.2074960969
 C, 0, -1.3777346404, 0.3982106915, -3.2023449609
 C, 0, 2.830571525, -2.9464444858, 0.6421123616
 C, 0, 4.2998729011, -0.8248718847, 0.3997403014
 O, 0, 2.7638108911, 0.1914908792, -2.5157579611
 O, 0, 4.3230642651, -0.4026516672, -0.9734353207

C, 0, 3.3501292373, -3.6942106026, -0.4275173711
C, 0, 3.2881653278, -5.0879570798, -0.4104075065
C, 0, 2.7071434045, -5.753991663, 0.6749495265
C, 0, 2.1884959232, -5.0181009311, 1.7421580528
C, 0, 2.2494668198, -3.6207583702, 1.7226828737
H, 0, 2.4710733684, -1.0531383039, 1.5836842468
H, 0, -4.0863331132, 0.0965632355, -3.3513492729
H, 0, -5.5993952425, -1.0877504802, -1.7796967194
H, 0, -4.6578136921, -2.2091499464, 0.2484091613
H, 0, -2.2052278249, -2.130135863, 0.6722789862
H, 0, -0.567598329, -0.2548437808, -3.5653937338
H, 0, -0.8787456449, 1.2483396752, -2.7072752555
H, 0, -1.9335734688, 0.7826100714, -4.069724275
H, 0, 4.4746461878, 0.054736975, 1.0398830441
H, 0, 5.1048251154, -1.5547715895, 0.5507558543
H, 0, 3.8052390634, -3.1860159305, -1.2813762526
H, 0, 3.6939899765, -5.6582481695, -1.2488894752
H, 0, 2.6585341584, -6.8450922804, 0.6855763351
H, 0, 1.7308592059, -5.5300833787, 2.5915631664
H, 0, 1.8378064052, -3.0475891449, 2.5579303566

H₇F₆⁺

Charge = 1 Multiplicity = 1

F, 0, 2.6144545605, 1.6050706569, 0.1858396246
F, 0, 0.2092511436, 2.1213923214, -0.5901471295
F, 0, -1.4486590107, 0.8542190195, 0.5636318628
F, 0, -2.0841411591, -1.0821155287, -0.5006373269
F, 0, -0.3347051031, -2.5626958393, 0.0302811018
F, 0, 1.1189864405, -0.5403780568, 0.305236639
H, 0, 1.1194892964, 2.0339591385, -0.3165430979
H, 0, -0.7453259619, 1.3958860486, 0.0875526231
H, 0, -1.8076087697, -0.1217224075, -0.0013209667
H, 0, -1.3714372635, -1.7968747654, -0.288859758
H, 0, 0.4163474335, -1.987631482, 0.1830171985
H, 0, 2.020939203, -0.3034249866, 0.4236549233
H, 0, 3.3650885383, 2.1697520506, 0.2176651503

(HF)₆

Charge = 0 Multiplicity = 1

F, 0, 1.9320615572, 1.0925916262, 0.4880823307
F, 0, 0.0198186744, 2.2195102033, -0.4880823307
F, 0, -1.9122428828, 1.1269185772, 0.4880823307
F, 0, -1.9320615572, -1.0925916262, -0.4880823307
F, 0, -0.0198186744, -2.2195102033, 0.4880823307
F, 0, 1.9122428828, -1.1269185772, -0.4880823307
H, 0, 1.1908663467, 1.6078683396, 0.1074674923
H, 0, -0.7970216547, 1.8352546785, -0.1074674923
H, 0, -1.9878880014, 0.2273863389, 0.1074674923
H, 0, -1.1908663467, -1.6078683396, -0.1074674923
H, 0, 0.7970216547, -1.8352546785, 0.1074674923
H, 0, 1.9878880014, -0.2273863389, -0.1074674923

keteniminium II_x

Charge = 1 Multiplicity = 1

C,0,2.1114655436,-0.6700705641,0.2108138167
N,0,0.7596207083,-0.9066411831,0.8604279386
C,0,0.9715285139,-1.6591345977,2.1551227004
O,0,2.2402946473,-2.0323539609,2.1715965765
C,0,2.9157650673,-1.779729066,0.910059435
C,0,-0.3753614838,-0.5145553405,0.4812643511
C,0,-1.5943294115,-0.2612620644,0.067277944
C,0,-2.4930051522,0.8636133146,0.294662056
C,0,-2.1736633903,1.9313759003,1.1740115949
C,0,-3.113437153,2.9554660163,1.3228010857
C,0,-4.3297896494,2.9372329841,0.6324684195
C,0,-4.6392991973,1.8798844312,-0.2287848887
C,0,-3.7242355465,0.8462558205,-0.3942330815
C,0,-0.8765670125,1.9577475545,1.9334678893
O,0,0.1201947795,-1.815047592,2.9630412108
C,0,2.0929707912,-0.6860657092,-1.2925020217
C,0,2.4685576926,0.4684601318,-1.9945124956
C,0,2.4741349491,0.4733486178,-3.3918357502
C,0,2.0954749584,-0.6723098106,-4.0956827997
C,0,1.7127906416,-1.826185295,-3.4016989526
C,0,1.7141406349,-1.8369025944,-2.0065791826
H,0,2.4382441221,0.3138476731,0.579589396
H,0,3.9414088228,-1.4729913721,1.1428244265
H,0,2.9270746257,-2.7174575373,0.3376816488
H,0,-1.9689537669,-1.070596494,-0.5790654984
H,0,-2.8900858569,3.7847581976,1.9970817698
H,0,-5.0412444057,3.7533710944,0.772842062
H,0,-5.5893695895,1.8610842862,-0.7646294898
H,0,-3.9568795168,0.0134193636,-1.0617512366
H,0,-0.0098369636,1.9997831542,1.2480701258
H,0,-0.7684619399,1.0646750748,2.5745607936
H,0,-0.8124412936,2.838740282,2.5861841503
H,0,2.7669343336,1.3670867839,-1.4484307991
H,0,2.7755866029,1.3741011515,-3.9293946111
H,0,2.1005457404,-0.6695782494,-5.1873380801
H,0,1.4197870913,-2.7233652099,-3.9500920229
H,0,1.4173020626,-2.7491331918,-1.4817054808

TS(II_x-IV_x)

Charge = 1 Multiplicity = 1

C,0,3.5852009609,0.5963665867,-0.4136010005
N,0,2.3414516295,0.3742263851,0.3978035136
C,0,2.6786717324,-0.2821812323,1.6487531187
O,0,3.9553583606,-0.6598560533,1.5847681964
C,0,4.497428906,-0.4533042995,0.2583014423
C,0,1.140663295,0.880938813,0.2226456036
C,0,0.3289857328,1.2482028526,-0.799407712
C,0,-0.6746932221,2.2632604129,-0.6480152809
C,0,-0.7162293079,2.9363903578,0.6098613903

C, 0, -1.8426156334, 3.7108179425, 0.9372745531
C, 0, -2.8336275229, 3.9200789937, -0.0165836652
C, 0, -2.7522888824, 3.3187646826, -1.2888510485
C, 0, -1.6915013648, 2.4831335316, -1.6030482074
C, 0, 0.4077132962, 2.7094389417, 1.5112016615
O, 0, 1.9258331772, -0.3919711603, 2.5688152815
C, 0, 3.4011188804, 0.4461028345, -1.9019040683
C, 0, 3.7517445098, 1.5058336582, -2.7507609073
C, 0, 3.618774473, 1.3765409278, -4.1366279147
C, 0, 3.1240493026, 0.1901679541, -4.6831101063
C, 0, 2.7640551863, -0.870282962, -3.842148826
C, 0, 2.905124634, -0.7467964794, -2.4592264237
H, 0, 3.9475264274, 1.6107105178, -0.1832622276
H, 0, 5.5310290251, -0.1059740659, 0.3679359673
H, 0, 4.4831303997, -1.4152222615, -0.2736090356
H, 0, 0.3729432106, 0.6447339345, -1.7118353955
H, 0, -1.9072119332, 4.1920147304, 1.9146972549
H, 0, -3.682204671, 4.5640862479, 0.2217463698
H, 0, -3.5450828218, 3.4900637537, -2.0189579682
H, 0, -1.6497199595, 1.9754667834, -2.5685427471
H, 0, 1.3630261326, 3.1654920182, 1.2226605035
H, 0, 0.6562392896, 1.4474571297, 1.3512090052
H, 0, 0.2259295925, 2.7741613502, 2.5923123244
H, 0, 4.1418155334, 2.4357060102, -2.3285842422
H, 0, 3.9044395428, 2.2044116231, -4.7881828827
H, 0, 3.0216930602, 0.0870505475, -5.7651477234
H, 0, 2.3811376018, -1.8002644549, -4.2668795046
H, 0, 2.6255174268, -1.5859125523, -1.8163792984

IV_x

Charge = 1 Multiplicity = 1

C, 0, 2.2264461734, -0.5304409951, 0.094413602
N, 0, 1.1142983049, -0.6739767735, 1.0557310676
C, 0, 1.5068740507, -1.4628600221, 2.1960042821
O, 0, 2.7547831411, -1.8934065899, 2.0002889542
C, 0, 3.2222483698, -1.5723328221, 0.6732804067
C, 0, -0.0649559568, -0.0304499263, 1.097757946
C, 0, -0.5857163996, 0.8051144629, 0.1220266899
C, 0, -1.8220565295, 1.4834904969, 0.2531072142
C, 0, -2.4517109121, 1.7815945621, 1.5506095447
C, 0, -3.8680958251, 2.1074410084, 1.5797610728
C, 0, -4.5408652535, 2.3634771379, 0.420854851
C, 0, -3.8517416817, 2.2785206882, -0.8302150425
C, 0, -2.5371140088, 1.8683714311, -0.9128125958
C, 0, -1.7134413367, 1.9673463825, 2.6854320029
O, 0, 0.8196686342, -1.6572485332, 3.1558923928
C, 0, 1.8700841003, -0.7788030476, -1.3587334782
C, 0, 2.3237246475, 0.1123748148, -2.3410113027
C, 0, 2.0556675848, -0.1291009619, -3.6925820105
C, 0, 1.3254715176, -1.2587239651, -4.0693225448
C, 0, 0.8663513078, -2.1500884348, -3.0924088502

C,0,1.1401858096,-1.9152256883,-1.744058168
H,0,2.6344731096,0.488130899,0.1993129114
H,0,4.2428618831,-1.1805873463,0.7583591982
H,0,3.2293204241,-2.4976989833,0.0807783602
H,0,-0.0908903432,0.8522947582,-0.8498130692
H,0,-4.3515956935,2.2247225805,2.551655913
H,0,-5.5913058527,2.6570133321,0.438723151
H,0,-4.3961209944,2.5091350136,-1.7489550981
H,0,-2.0627019804,1.746785377,-1.8883213773
H,0,-0.6231897724,1.9830525282,2.6738386037
H,0,-0.6322358709,-0.2809368246,1.999470342
H,0,-2.2038559778,2.1866734142,3.6373720255
H,0,2.8975437953,0.9972164794,-2.0520416745
H,0,2.4213290737,0.5667347458,-4.4502110347
H,0,1.116498049,-1.4488691927,-5.1238842508
H,0,0.2978210156,-3.0357132522,-3.3830420604
H,0,0.7794173969,-2.6220587541,-0.9919819742

TS(IV_x-V_x)

Charge = 1 Multiplicity = 1

C,0,-0.7351672763,0.8535355789,0.1325368513
C,0,0.4450013161,0.8424615931,0.93507004
N,0,1.5418947268,0.0682797582,0.702501859
C,0,-1.5326766685,2.0012159197,0.1999102529
C,0,2.1053609123,-0.3772567015,-0.5902490505
C,0,-0.8510714108,3.1033646013,0.838995985
C,0,-1.6138812474,4.1574854818,1.3944942957
C,0,-2.9677043242,4.2044080593,1.1141365996
C,0,-3.6122405505,3.1949336955,0.3384978956
C,0,-2.9158281975,2.1014536179,-0.1250328008
C,0,0.5625765068,2.9727023197,0.859148711
C,0,2.524200308,-0.0056652584,1.7377691533
C,0,3.3661505383,-1.1182925571,-0.0765929939
O,0,3.6124874329,-0.6141539031,1.2537002665
O,0,2.3819607125,0.4415871276,2.8414741182
C,0,1.1913590771,-1.2341319498,-1.4410793673
C,0,0.5522467825,-2.3660734289,-0.905800796
C,0,-0.2662756953,-3.1584146343,-1.7125270588
C,0,-0.4473833445,-2.8357432704,-3.0632646571
C,0,0.1898180934,-1.7160711604,-3.6027648572
C,0,1.0028452134,-0.9157647098,-2.7930304232
H,0,-0.9860535325,-0.0023658367,-0.4983762218
H,0,0.3649180828,1.0851833799,2.0029117455
H,0,2.4016211099,0.5173474077,-1.1659022975
H,0,-1.126455811,4.9634907243,1.9453436783
H,0,-3.5591813999,5.0509995588,1.4690505262
H,0,-4.6822945806,3.2832933471,0.1422652863
H,0,-3.4155256689,1.2960090606,-0.6659424243
H,0,1.0864783837,2.8079384703,-0.0833316051
H,0,1.1568400476,3.4636743022,1.6371020892
H,0,4.2545205208,-0.9197109488,-0.6874597422

H,0,3.1980238627,-2.2026435706,-0.0091328218
H,0,0.6874501146,-2.6294311385,0.1467024375
H,0,-0.7594574102,-4.0353262785,-1.2883628841
H,0,-1.0824033194,-3.4612342504,-3.6936706245
H,0,0.0568565105,-1.4629136844,-4.6563446086
H,0,1.4996951847,-0.0409437224,-3.2213395561

V_x

Charge = 1 Multiplicity = 1

C,0,-0.7613723179,0.4426093348,0.928048253
C,0,0.5992114409,0.8983887359,1.3214439668
N,0,1.6668076093,0.0120516639,0.9585983089
C,0,-1.5651769213,1.505598742,0.5402362953
C,0,2.1422916437,-0.2268997045,-0.4092628844
C,0,-0.7810100284,2.71416499,0.5712229412
C,0,-1.40326051,3.9380182472,0.358096965
C,0,-2.7736769312,3.9409977795,0.0646959298
C,0,-3.5469751943,2.7530759863,-0.0022717408
C,0,-2.9587480693,1.5281946379,0.2344836616
C,0,0.6510532045,2.3915494676,0.8611844174
C,0,2.6943538812,-0.1792401078,1.8914884327
C,0,3.3753741162,-1.1065326618,-0.0812222969
O,0,3.7329341647,-0.7811890963,1.2784598081
O,0,2.6508508612,0.1449724764,3.0511536612
C,0,1.1158324518,-0.8680947765,-1.3202978885
C,0,0.4505654408,-2.0521109181,-0.9447321289
C,0,-0.4723487481,-2.6492103037,-1.8055815028
C,0,-0.7407471144,-2.0757464838,-3.0541008595
C,0,-0.0837099593,-0.9024196242,-3.4367985643
C,0,0.8377781646,-0.302291077,-2.5737466415
H,0,-1.0810126968,-0.5985049945,1.0057144949
H,0,0.6251307292,0.8876374433,2.438450115
H,0,2.4772382915,0.7220629297,-0.8693624912
H,0,-0.8455528378,4.8750268073,0.3972564746
H,0,-3.2692196706,4.8962719706,-0.126102567
H,0,-4.6107221684,2.8216846921,-0.2339395106
H,0,-3.5342653026,0.6013539456,0.2045347591
H,0,1.2472556356,2.471252776,-0.0642514861
H,0,1.1113173886,3.0644212992,1.5993006235
H,0,4.2364981898,-0.8928169303,-0.7255062247
H,0,3.1334870233,-2.1788744496,-0.1325510476
H,0,0.6655698915,-2.5146300422,0.0220888555
H,0,-0.9742647794,-3.5722041017,-1.5078605023
H,0,-1.455403336,-2.5484560894,-3.7308123748
H,0,-0.2838334237,-0.456021894,-4.4128818042
H,0,1.3564528812,0.6091343302,-2.8837704476

TS(V_x-σ complex)

Charge = 1 Multiplicity = 1

C,0,-0.3928424769,-0.2622661676,0.8853277094
C,0,0.7919742757,0.2460283335,1.7276190597

N,0,1.9796832186,-0.5502712976,1.626833589
C,0,-1.2640981159,0.9075012644,0.7200825989
C,0,2.5483759802,-1.0076436847,0.3647504462
C,0,-0.5376877018,2.0879575186,1.0107588539
C,0,-1.1771603579,3.3259870764,0.9690972655
C,0,-2.5331727456,3.373861136,0.6259492213
C,0,-3.2558647956,2.2011049931,0.3407204106
C,0,-2.6272544495,0.959082567,0.3836301721
C,0,0.8840768038,1.7562571523,1.3836929515
C,0,2.8438463044,-0.7574679136,2.6975120174
C,0,3.7010435773,-1.8925606354,0.893654219
O,0,3.9190315779,-1.4624123398,2.2442900519
O,0,2.6857612465,-0.3833778613,3.8266534681
C,0,1.4205696266,-1.637407789,-0.4197606895
C,0,1.2745738846,-2.9916569903,-0.6807350182
C,0,0.1410285732,-3.4574436962,-1.3682691928
C,0,-0.8744243942,-2.584853205,-1.8067114674
C,0,-0.7580021037,-1.2348249491,-1.547435334
C,0,0.3514556065,-0.7244744103,-0.7801607595
H,0,-0.8369671073,-1.218527433,1.1772374054
H,0,0.4647198557,0.1594633307,2.7787745667
H,0,2.9495450613,-0.159937774,-0.2268964987
H,0,-0.6362089905,4.2436354628,1.20833977
H,0,-3.0438652756,4.3383280407,0.5887213044
H,0,-4.3169664489,2.2673301001,0.0946706806
H,0,-3.1910074329,0.0459956368,0.1785500742
H,0,1.5731807081,1.929070126,0.5350179465
H,0,1.2701756466,2.3442925303,2.2284518823
H,0,4.6315825565,-1.75627761,0.3295134032
H,0,3.4414738501,-2.9620242509,0.9128096076
H,0,2.0383572271,-3.7084758399,-0.3792506507
H,0,0.0511679727,-4.5269985798,-1.5741889493
H,0,-1.7292506925,-2.976391952,-2.3599538688
H,0,-1.5228461622,-0.5346153774,-1.8893932544
H,0,0.6725006977,0.291517488,-1.0354019923

σ complex

Charge = 1 Multiplicity = 1

C,0,-0.840176848,-0.0007383209,0.1631022956
C,0,0.3534619338,0.5486500568,1.0007893879
N,0,1.5847856057,-0.1918654379,0.8979556569
C,0,-1.7341362561,1.1778854915,0.0198137926
C,0,2.10416782,-0.6384896081,-0.4016892125
C,0,-1.008015076,2.362459632,0.2753814359
C,0,-1.6489070393,3.5996876805,0.2232741606
C,0,-3.0127238802,3.6429306917,-0.0880978412
C,0,-3.7374475591,2.4646809029,-0.3307649845
C,0,-3.103143547,1.2230027878,-0.2788559863
C,0,0.4239008882,2.0469089314,0.6322391566
C,0,1.9154823706,-1.1476149033,1.8769779687
C,0,3.2885355932,-1.4857938497,0.0806145662

O,0,2.8850433865,-1.9634461912,1.3738226466
O,0,1.4363330626,-1.2433626117,2.9715530107
C,0,0.9487321938,-1.3483965798,-1.0698295288
C,0,0.8385437469,-2.7229474783,-1.2141912967
C,0,-0.3117329121,-3.2760147393,-1.8019306932
C,0,-1.3855599748,-2.4763010773,-2.2505493883
C,0,-1.322131775,-1.1132793838,-2.0777920152
C,0,-0.1988274635,-0.4944395301,-1.3870748374
H,0,-1.2919318556,-0.9154670839,0.5645538789
H,0,0.0412353571,0.447059038,2.0533481525
H,0,2.4366817861,0.2121702571,-1.017772539
H,0,-1.1025743407,4.5212906775,0.4344165705
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H,0,1.6434305254,-3.3881567928,-0.9005730004
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polycyclic product 12x

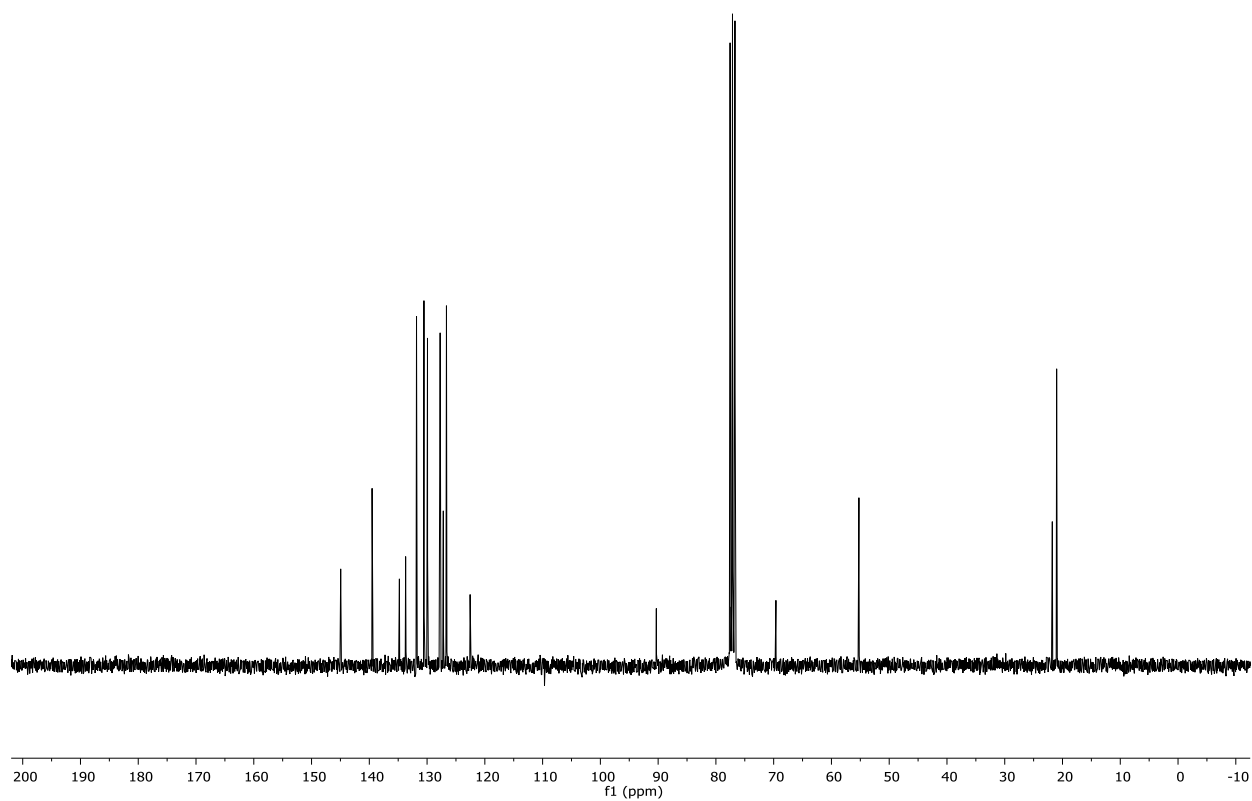
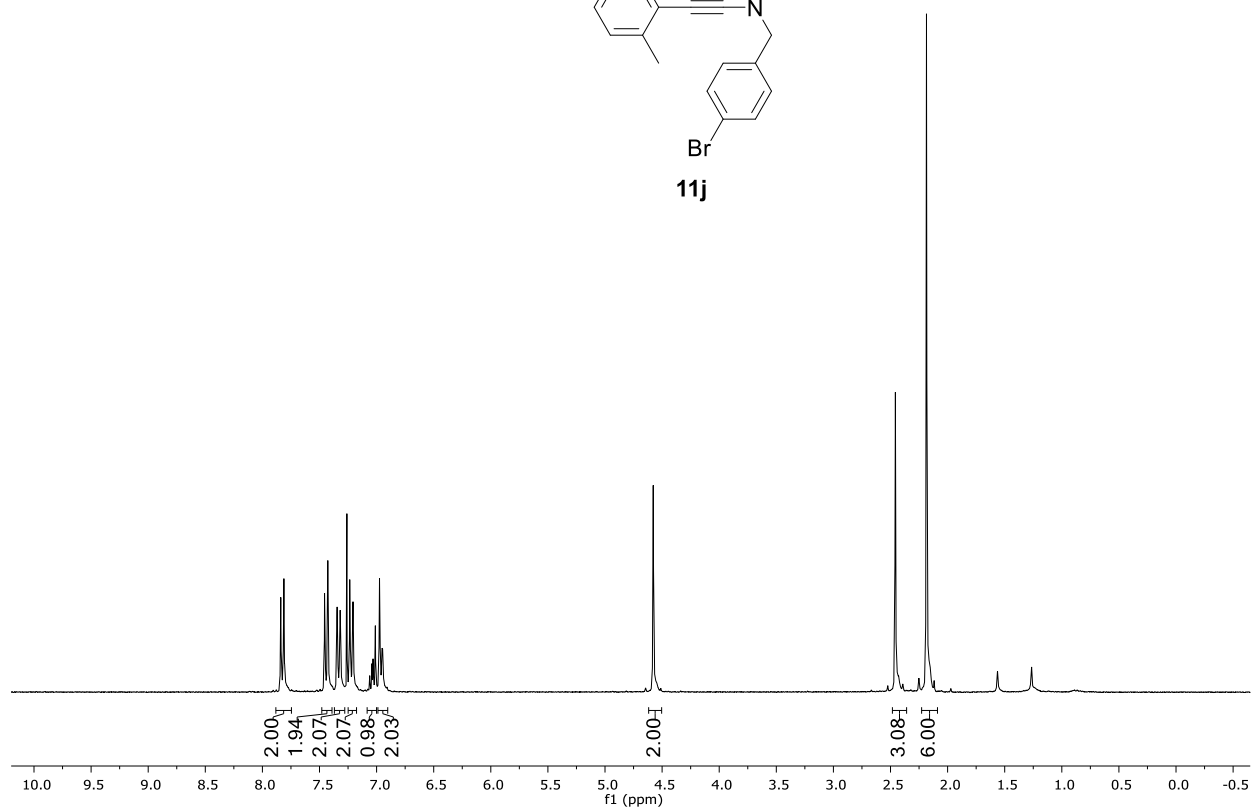
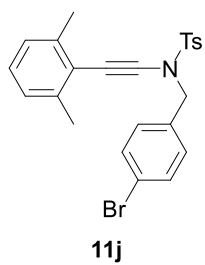
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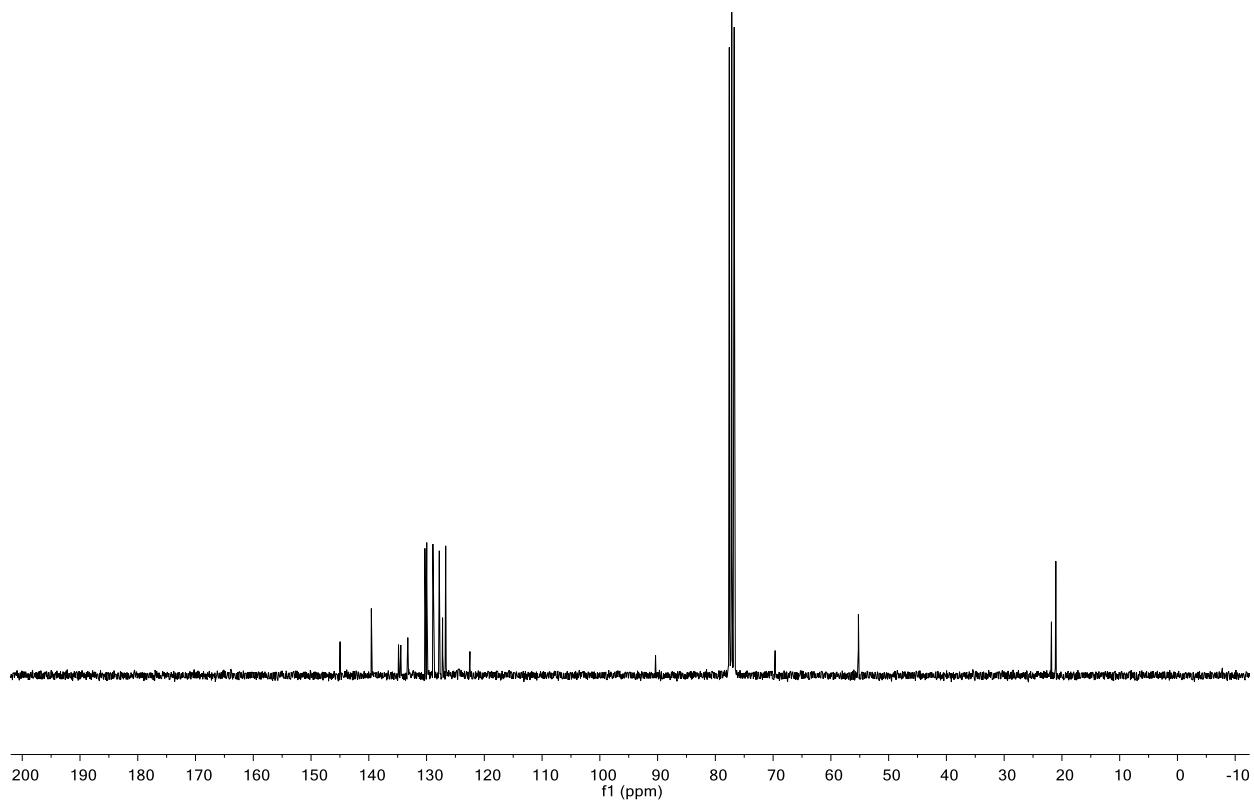
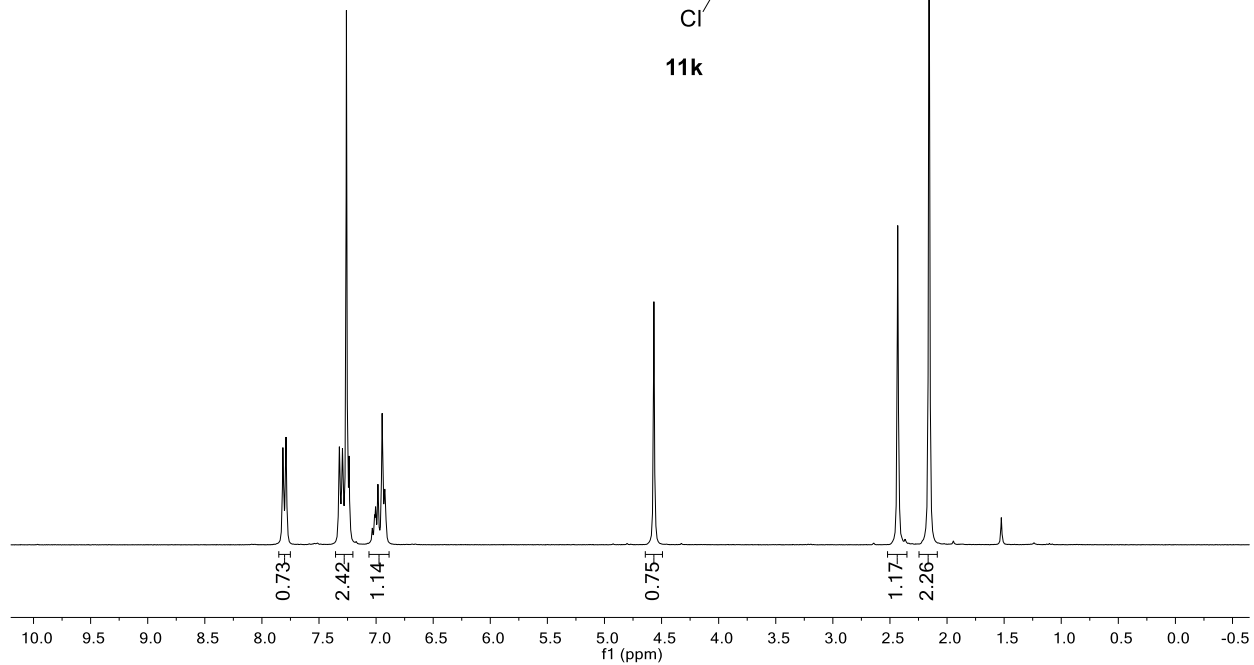
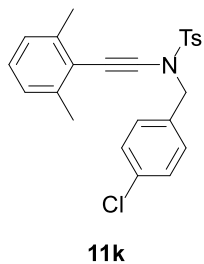
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C,0,0.8899822875,0.4427871669,1.8489045817
N,0,2.0831005604,-0.3782302112,1.8114218799
C,0,-1.2325177084,0.918163588,0.8774355135
C,0,2.482655996,-1.0090512265,0.5637820897
C,0,-0.4483145147,2.0786693936,0.7555837919
C,0,-1.0343478728,3.2966512191,0.409216126
C,0,-2.4163291693,3.3528280901,0.1918694048
C,0,-3.202125866,2.2038381244,0.3353206533
C,0,-2.6142185421,0.9815026079,0.6839149295
C,0,0.9977709141,1.7775164555,1.0729279154
C,0,2.3917236563,-1.1787197356,2.9015016402
C,0,3.5032188146,-2.0486990425,1.0972352248
O,0,3.2300211112,-2.1799801756,2.4981266072
O,0,2.0142998731,-1.0457511219,4.0392117762
C,0,1.2993558407,-1.5687991763,-0.2158568647
C,0,1.549194773,-2.4190593803,-1.3057972591
C,0,0.5083771484,-2.9503335805,-2.0633319493
C,0,-0.8111154381,-2.6237012893,-1.7350559232
C,0,-1.065439663,-1.7624104089,-0.669956711
C,0,-0.0263256579,-1.2111995875,0.0998623033
H,0,-0.8516966524,-0.8761568884,2.0512822277
H,0,0.7057080505,0.6555071517,2.9101031966
H,0,3.0111632747,-0.283895231,-0.0808468286

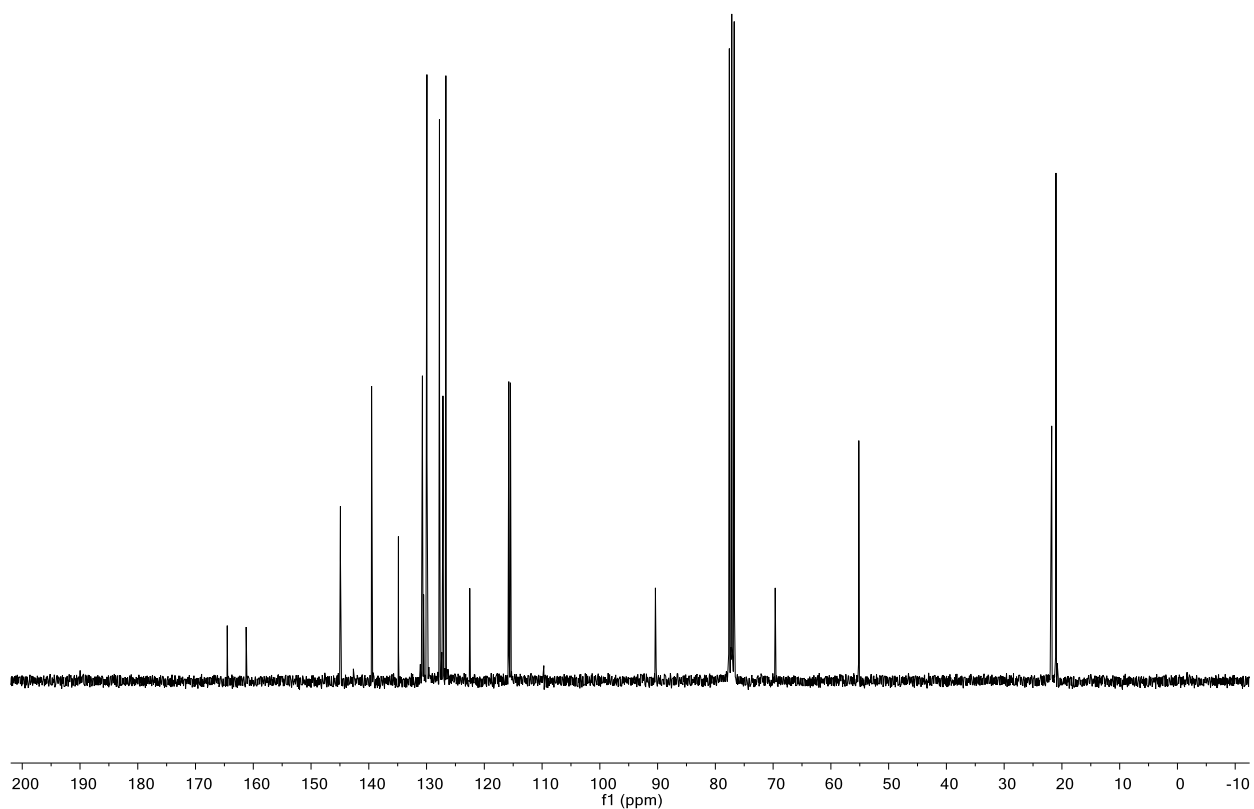
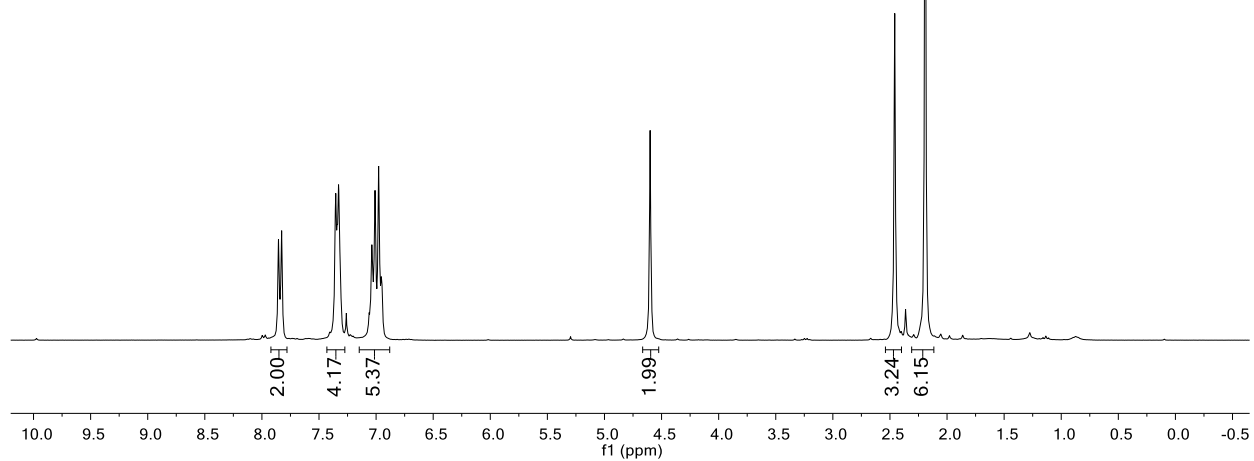
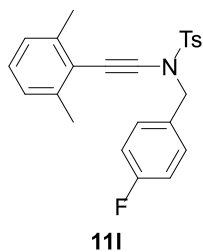
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H, 0, -4.2826994822, 2.2622389019, 0.1859451574
H, 0, -3.2401685289, 0.0961503619, 0.8196125737
H, 0, 1.5810630623, 1.6496399468, 0.1429885302
H, 0, 1.4943854307, 2.5633133409, 1.6615050102
H, 0, 4.5390976489, -1.6948632009, 0.9722050141
H, 0, 3.3965526398, -3.0362382192, 0.6290967851
H, 0, 2.5819314675, -2.6683616016, -1.5664874964
H, 0, 0.723633361, -3.6154378897, -2.9023625539
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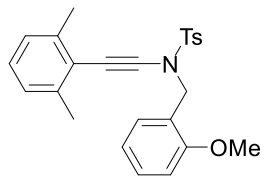
Supporting Information

^1H and ^{13}C NMR spectra

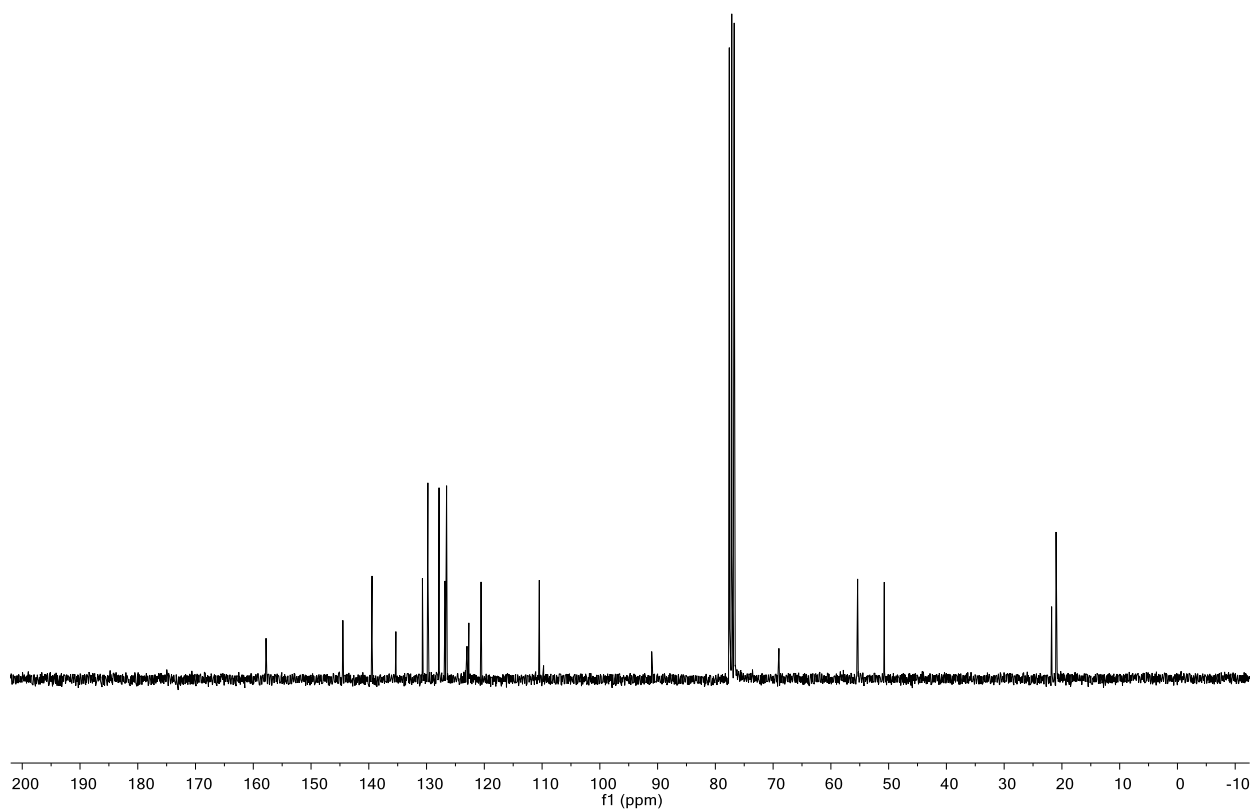
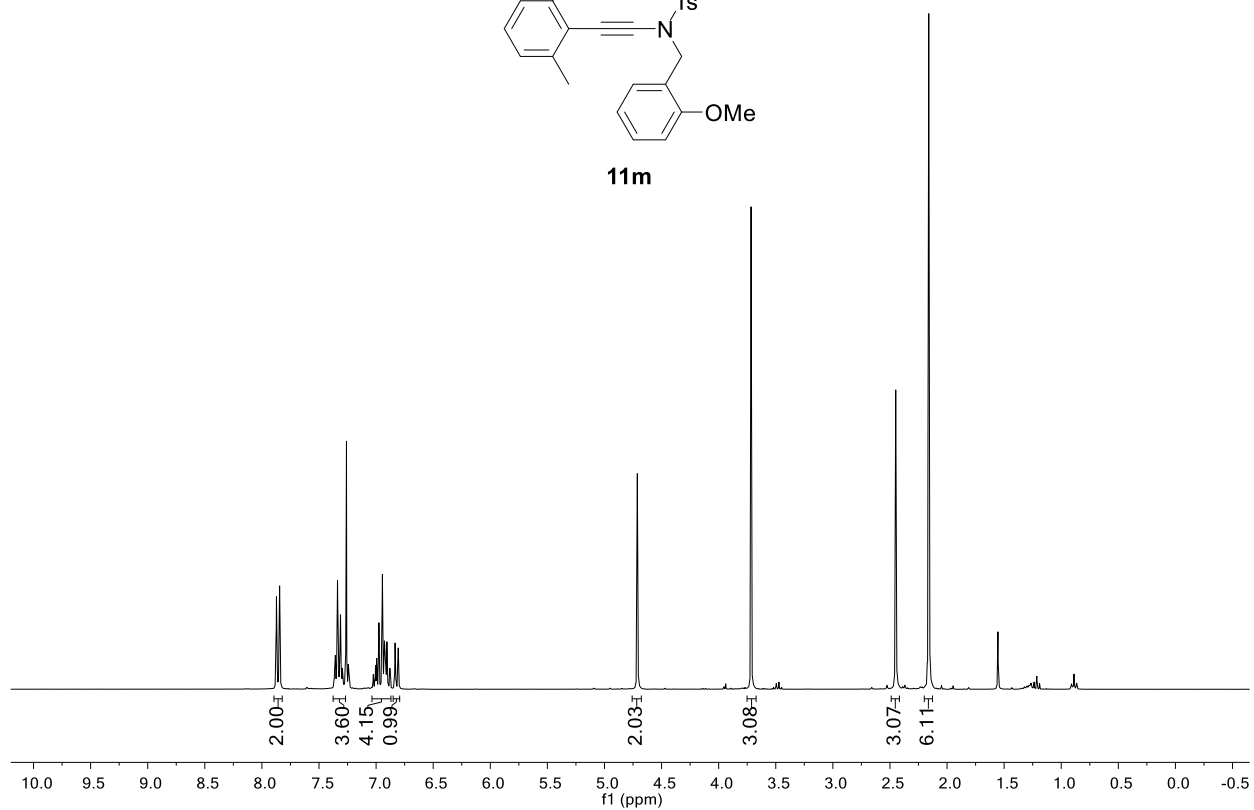


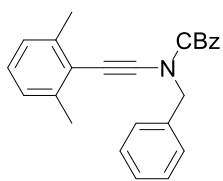




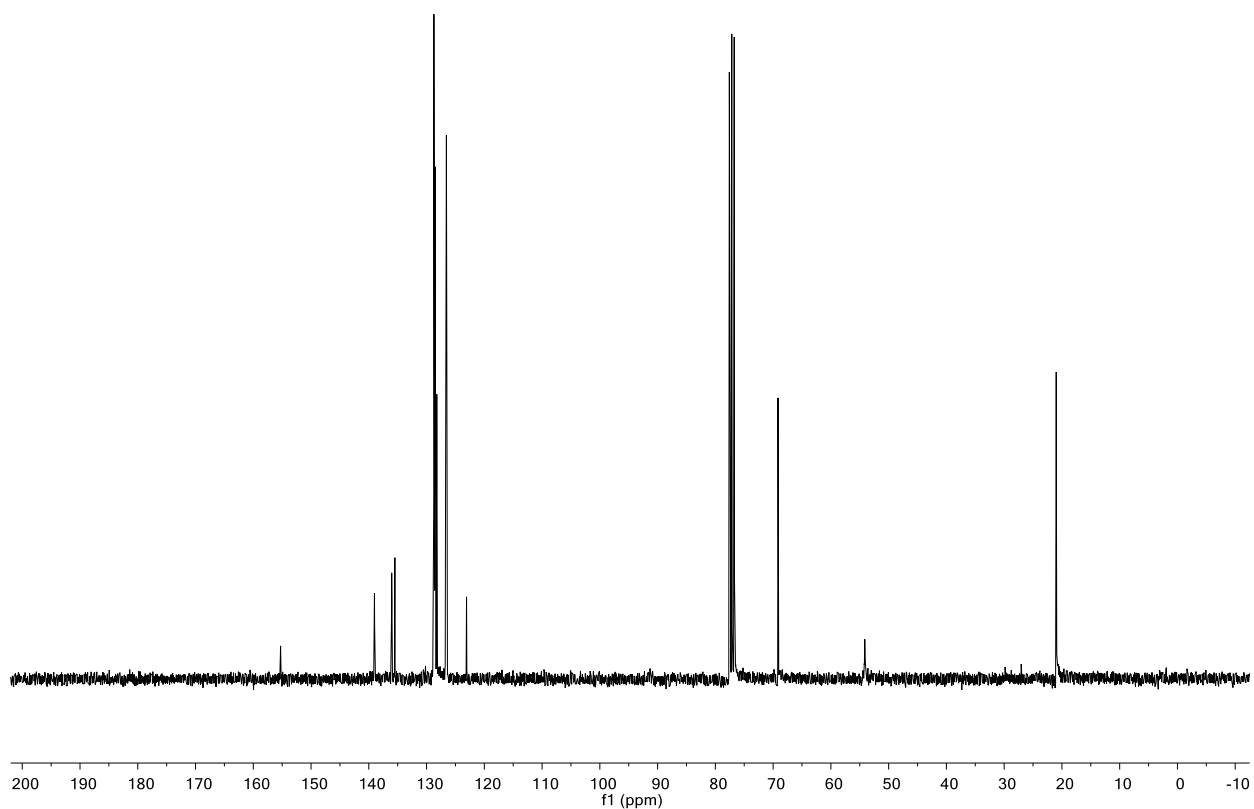
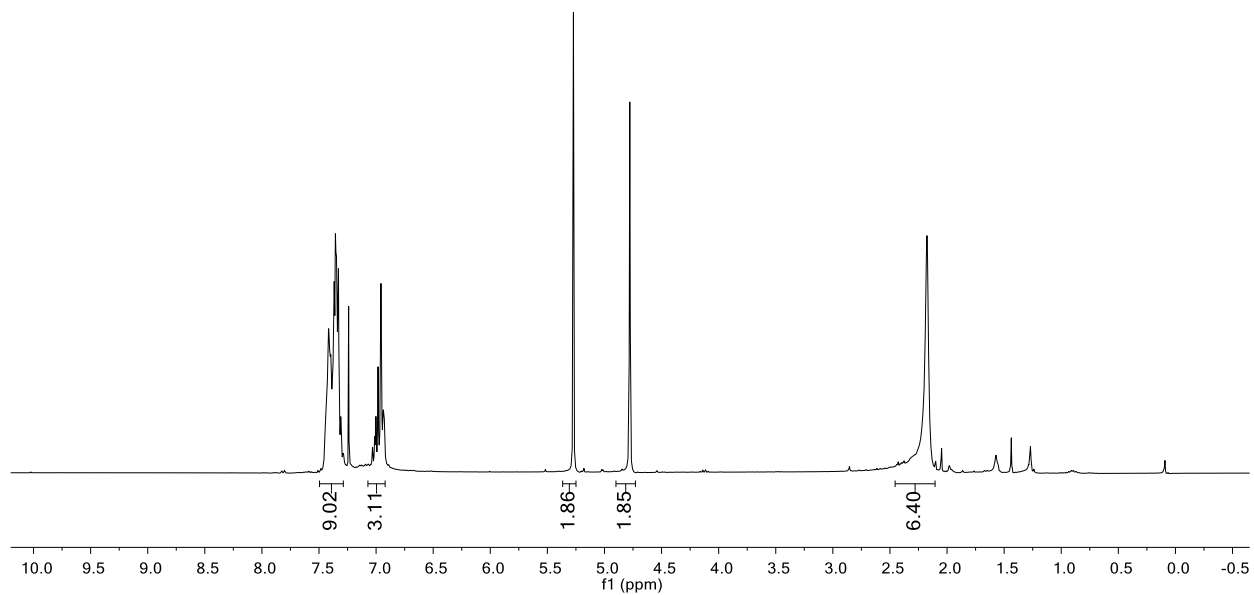


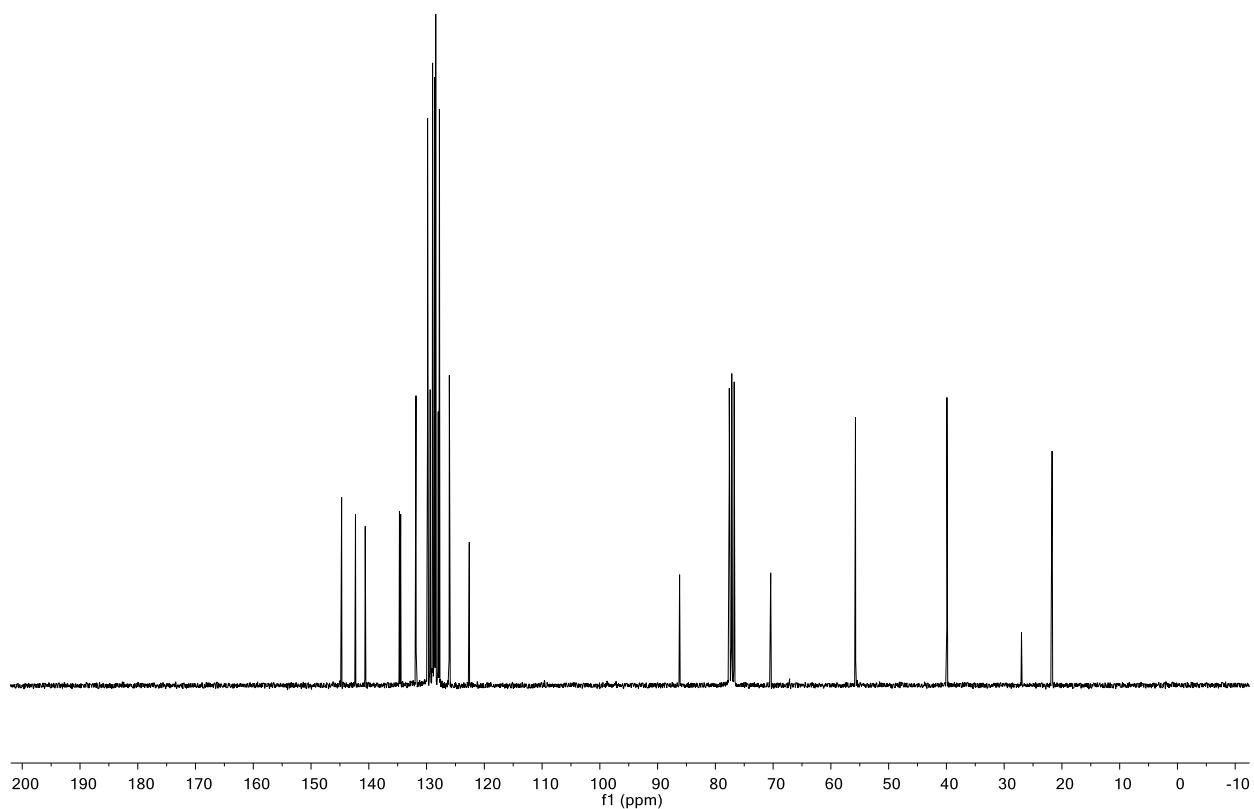
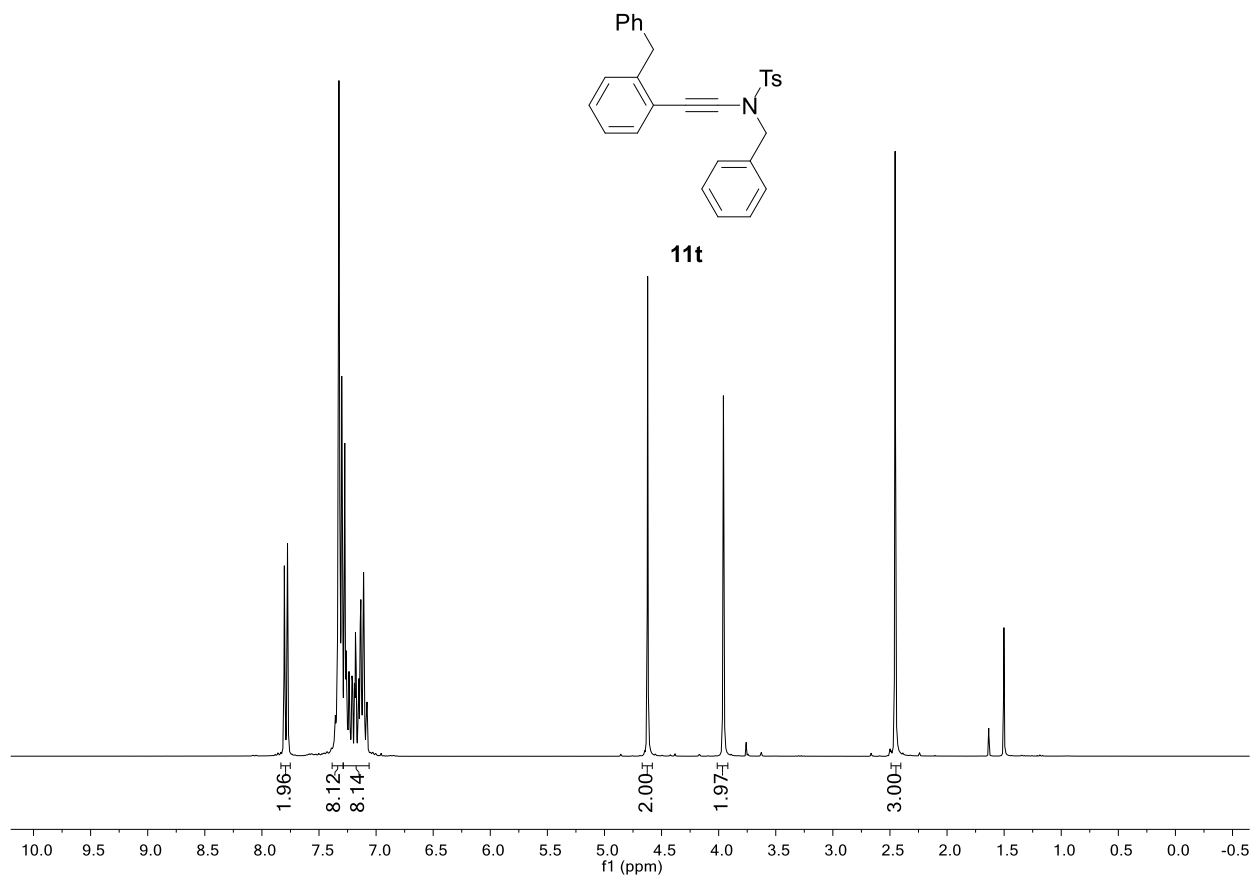
11m

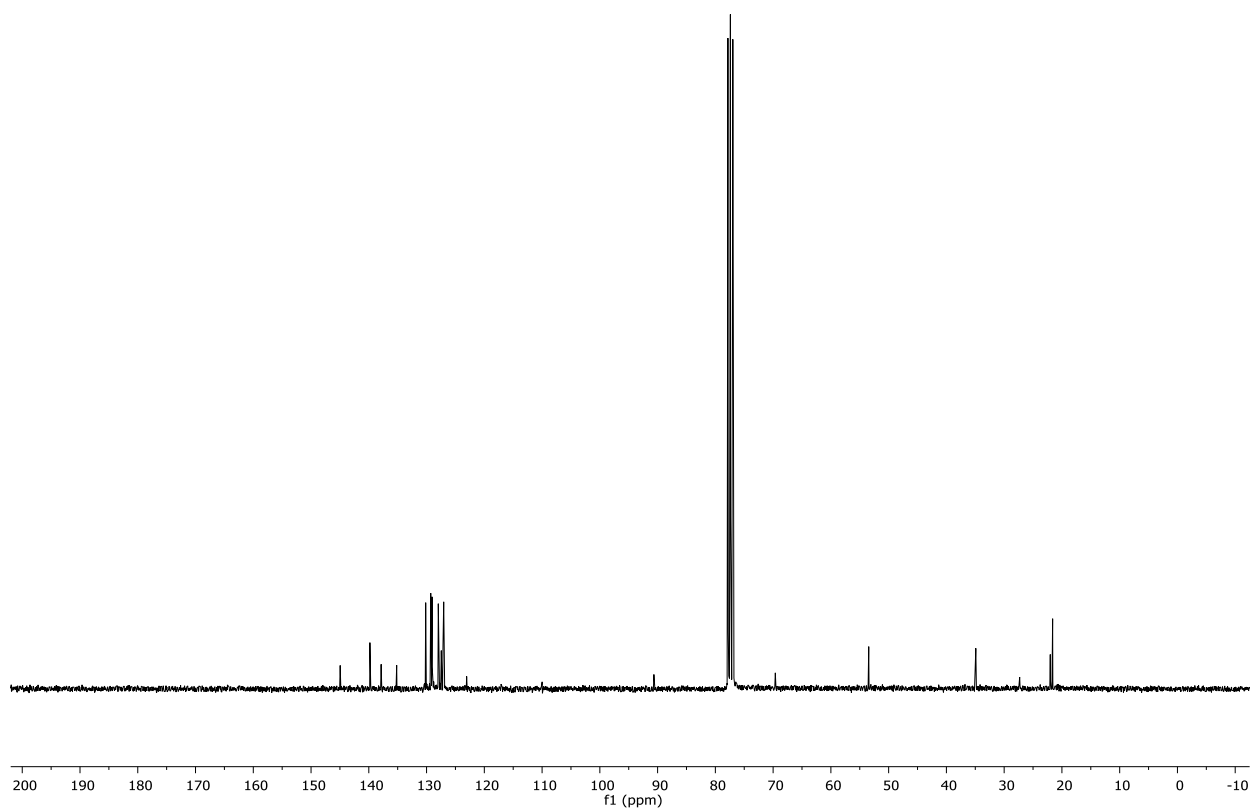
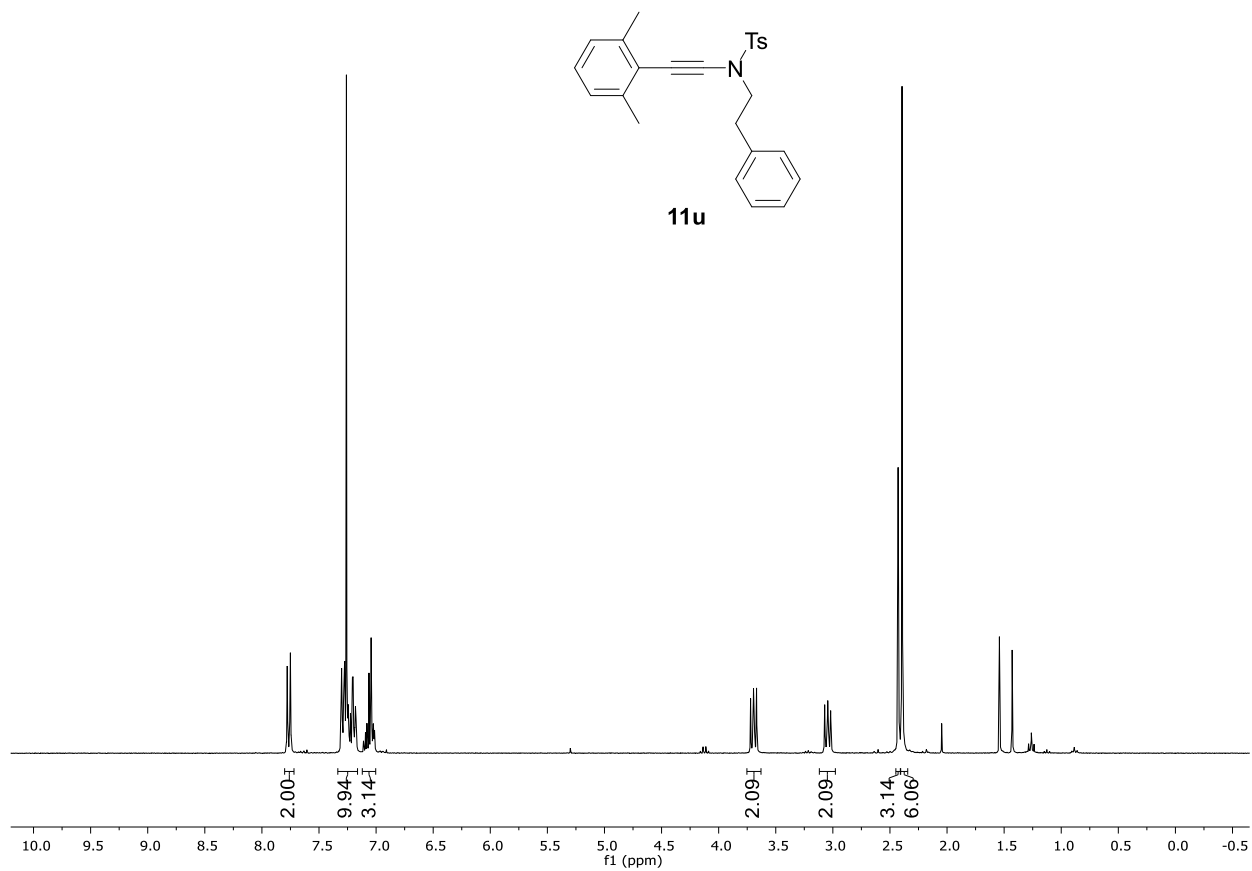


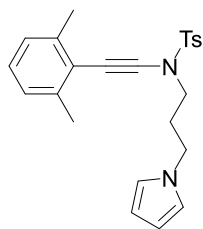


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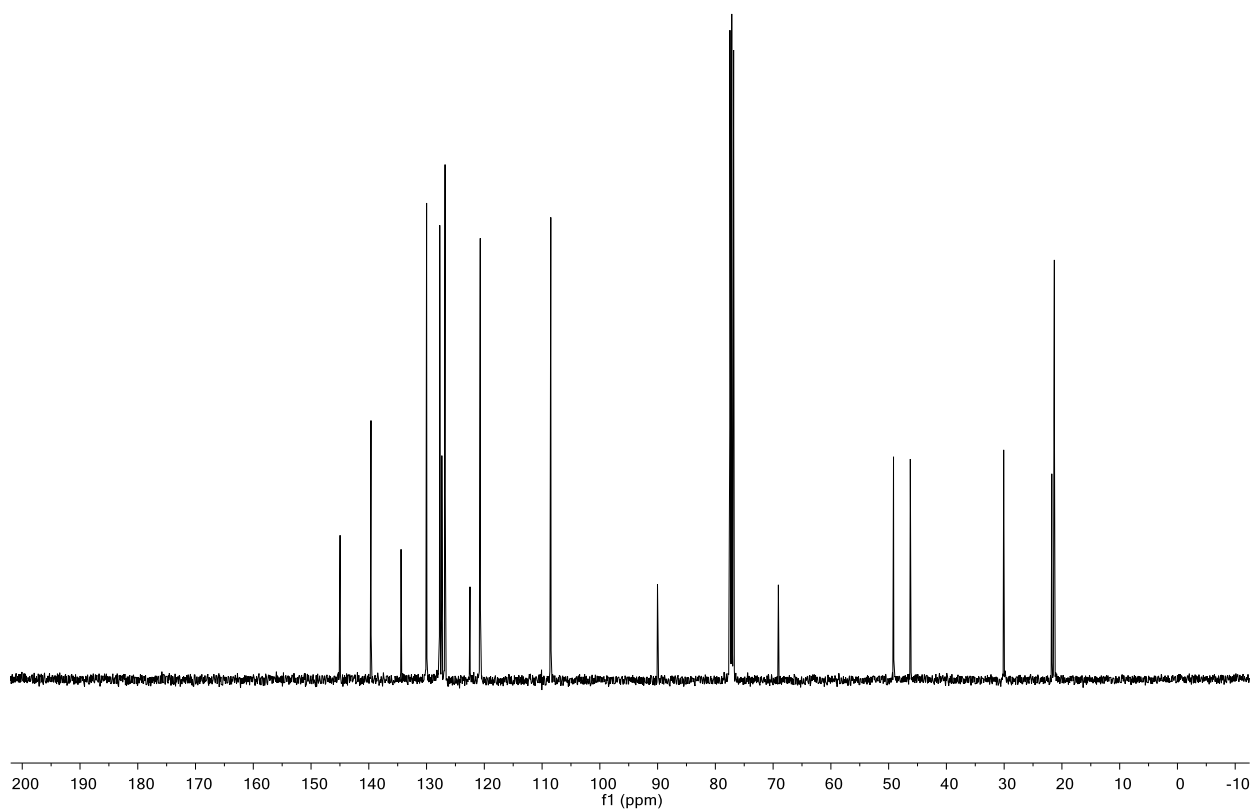
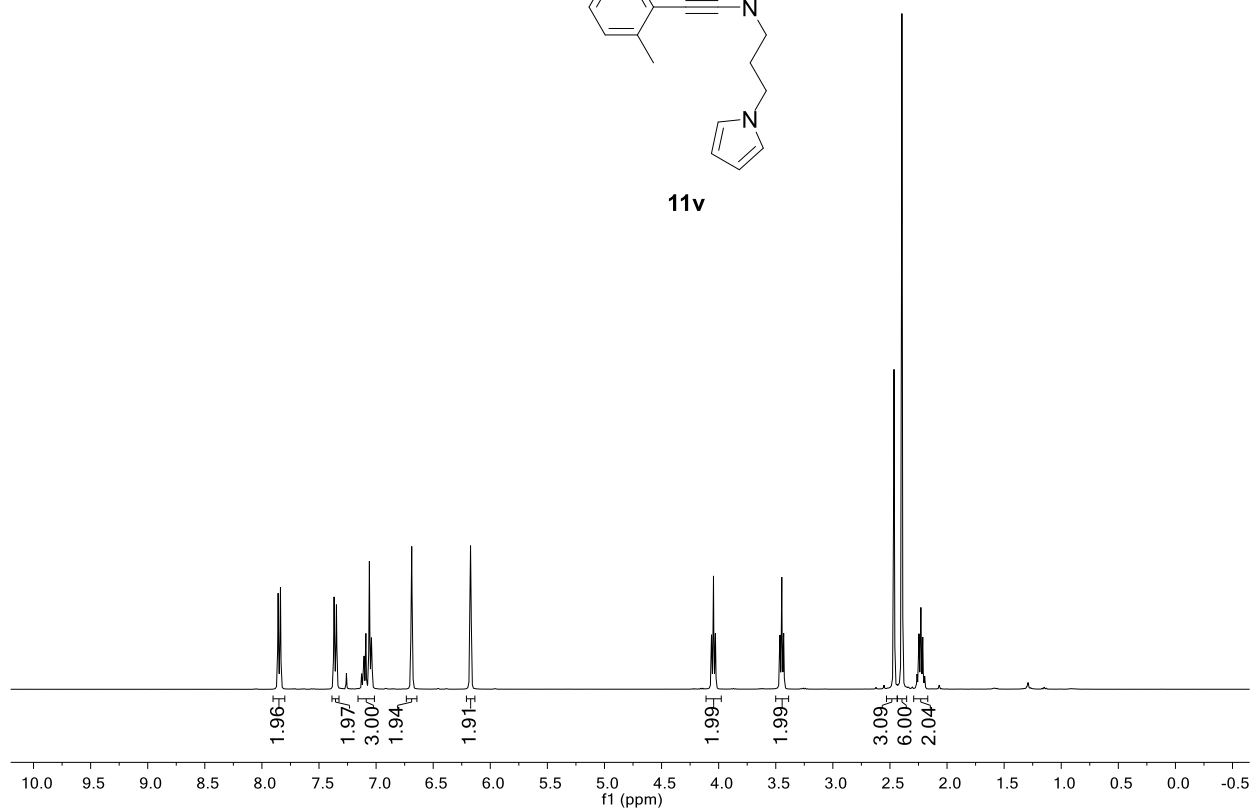


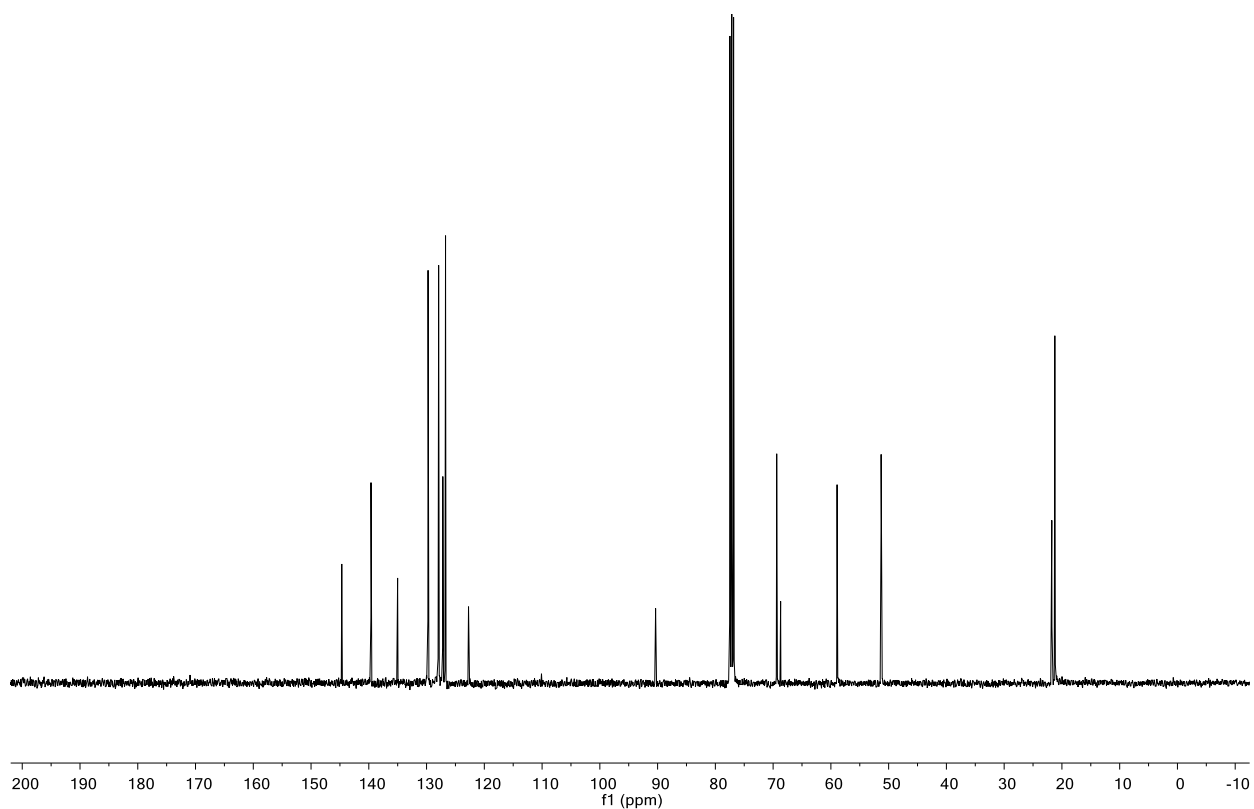
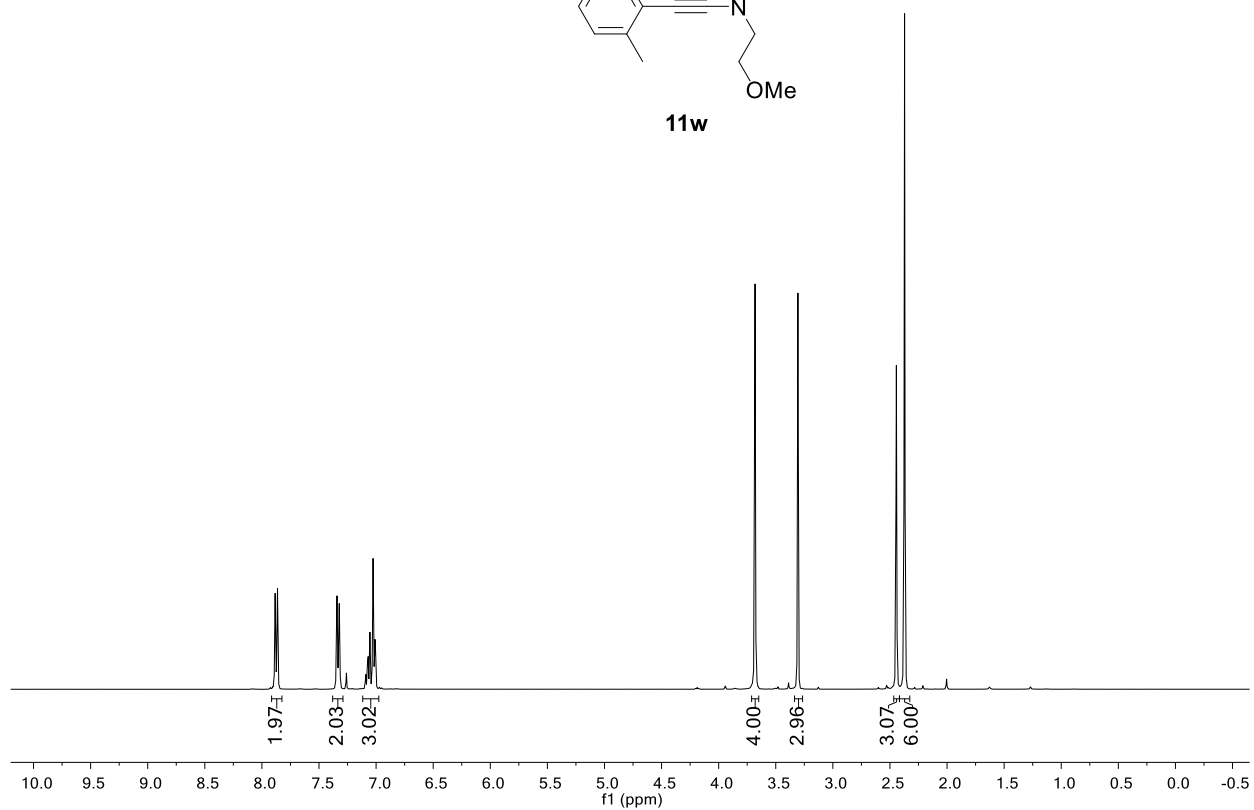
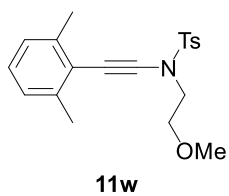


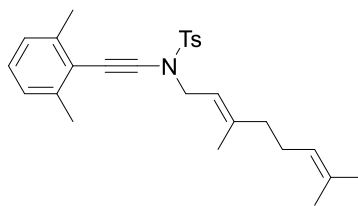




11v







27d

