Electronic Supplementary Material (ESI) for ChemComm.

Multicomponent decarboxylative allylations

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Supporting information

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General experimental:

All reactions were run in flame-dried glassware under Argon atmosphere. Commercially available pyrrole was distilled to a colorless liquid prior to use. Compound purification was effected by flash chromatography using 230x400 mesh, 60Å porosity, silica obtained from Sorbent Technologies. The ^{1}H and ^{13}C NMR spectra were obtained on a Bruker Avance 400 or Bruker Avance 500 DRX spectrometer in $CDCl_3$ unless otherwise indicated and are referenced to the residual solvent peak $CDCl_3$ at δ 7.26 and δ 77.16 in ^{1}H and ^{13}C NMR respectively. Multiplicities are reported as follows: singlet (s), doublet (d), broad singlet (bs), doublet of doublets (dd), doublet of triplets (dt), triplet (t), quartet (q), multiplet (m). Structural assignments are based on ^{1}H, ^{13}C, DEPT-135, COSY, HSQC, and FT-IR spectroscopies. Mass spectrometry was run using ESI techniques. Lithium pyrrolide, substituted Meldrum's acid and allyl methyl carbonates[1] were synthesized according to the literature procedures.

1. Trost, M. B.; Miller, J. R.; Hoffman. Jr, C. M. *J. Am. Chem. Soc*. **2011**, *133,* 8165.

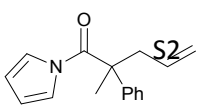
Representative procedure for 3-component palladium-catalyzed decarboxylative allylation

Synthesis of **2a**;

In a flame-dried Schlenk tube, Meldrum's acid (0.5 mmol, 117 mg, 1.0 eq.) in anhydrous 1,4-dioxane (2.5 ml, 0.2 M) was treated with lithium pyrrolide (0.6 mmol, 44 mg, 1.2 eq.). The reaction mixture was stirred for about a minute. $Pd(PPh_3)_4$ (0.05 mmol, 58 mg, 10 mol%) and allyl methyl carbonate (0.6 mmol, 70 mg, 1.2 eq.) were added and then the Schlenk tube was sealed and stirred overnight at room temperature. Next, the reaction mixture was concentrated *in vacuo* and purified via flash chromatography using 2% - 5% EtOAc/Hexane to obtain colorless oil (85% yield).

Note- freshly prepared lithium pyrrolide and highly anhydrous conditions are required.

Spectral Characterization of **2a**;



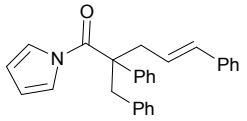
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (dt, *J* = 9.7, 1.9 Hz, 2H), 7.23 – 7.15 (m, 3H), 6.92 – 6.87 (m, 2H), 5.97 (d, *J* = 2.4 Hz, 2H), 5.48 (m, 1H), 4.99 – 4.94 (m, 1H), 4.88 (m, 1H), 2.81 (dd, *J* = 13.7, 8.0 Hz, 1H), 2.71 (dd, *J* = 13.7, 6.6 Hz, 1H), 1.60 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.7, 142.3, 132.1, 128.1, 126.2, 124.8, 119.6, 118.1, 110.8, 51.0, 44.0, 23.6

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3020, 1704, 1494, 1465, 1213, 1155, 700, 503

Calcd. HRMS for $C_{16}H_{17}NO$ (M+) – 239.1310, found 239.1245

Spectral Characterization of **2b**;



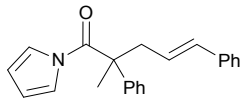
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 – 7.28 (4 H, m), 7.28 – 7.20 (9 H, m), 7.20 – 7.08 (6 H, m), 6.98 (2 H, s), 6.63 (2 H, dd, *J* = 7.8, 1.3), 6.21 (1 H, d, *J* = 15.8), 6.09 – 6.06 (2 H, m), 6.06 – 5.97 (1 H, m), 3.52 (1 H, d, *J* =13.5), 3.40 (1 H, d, *J* = 13.5), 2.94 (2 H, d, *J* = 7.1)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.8, 142.1, 137.4, 136.3, 134.8, 130.8, 129.3, 128.7, 128.1, 127.8, 127.6, 126.9, 126.4, 124.5, 120.8, 112.3, 57.6, 42.3, 38.8

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3024, 2354, 1704, 1465, 1290, 1078, 744, 696

Calcd. HRMS for $C_{28}H_{26}NO$ (M+H) – 392.2014, found 392.2013

Spectral Characterization of **2c**;



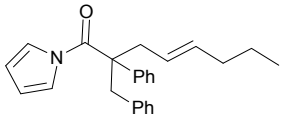
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 – 7.34 (m, 2H), 7.31 – 7.20 (m, 7H), 7.19 – 7.15 (m, 1H), 6.99 – 6.95 (m, 2H), 6.24 (d, *J* = 15.8 Hz, 1H), 6.06 – 6.03 (m, 2H), 5.96 – 5.88 (m, 1H), 3.03 – 2.96 (m, 1H), 2.90 (m, 1H), 1.72 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.8, 143.3, 137.3, 134.1, 129.2, 128.5, 127.3, 126.2, 125.9, 124.9, 120.7, 111.9, 52.5, 44.6, 24.5

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3020, 2364, 1703, 1467, 1290, 1099, 970, 744, 696, 597

Calcd. HRMS for $C_{22}H_{22}NO$ (M+H) – 316.1701, found 316.1681

Spectral Characterization of **2d**;



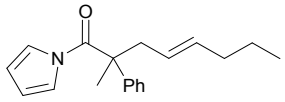
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.25 (3 H, m), 7.15 – 7.10 (1 H, m), 7.10 – 7.04 (4 H, m), 6.95 (2 H, s), 6.58 – 6.53 (2 H, m), 6.06 – 6.01 (2 H, m), 5.39 – 5.30 (1 H, m), 5.30 – 5.20 (1 H, m), 3.44 (1 H, d, *J* = 13.5), 3.31 (1 H, d, *J* = 13.4), 2.74 (2 H, d, *J* = 6.8), 1.91 (2 H, q, *J* = 6.8), 1.33 – 1.23 (2 H, m), 0.83 (3 H, t, *J* = 7.4)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.0, 142.3, 136.5, 136.2, 130.9, 129.1, 127.9, 127.6, 127.0, 126.7, 123.8, 120.8, 112.1, 57.5, 42.5, 37.8, 35.1, 22.8, 13.8

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 2962, 2360, 1703, 1460, 1286, 1108, 970, 744, 692

Calcd. HRMS for $C_{25}H_{28}NO$ (M+H) – 358.2171, found 358.2160

Spectral Characterization of **2e**;



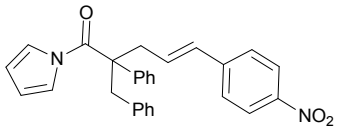
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.30 (2 H, m), 7.28 – 7.18 (9 H, m), 6.99 – 6.89 (2 H, m), 6.04 – 5.96 (2 H, m), 5.33 – 5.07 (2 H, m), 2.83 (1 H, dd, *J* = 13.6, 7.8), 2.70 (1 H, dd, *J* = 13.0, 6.1), 1.86 (2 H, dt, *J* = 7.4, 3.8), 1.62 (3 H, s), 1.26 (2 H, dt, *J* = 14.6, 7.4), 0.80 (3 H, t, *J* = 7.4)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.9, 144.0, 135.6, 129.3, 127.3, 125.9, 124.4, 120.8, 111.9, 52.7, 43.7, 34.9, 25.4, 22.7, 13.8

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 2948, 2366, 1704, 1463, 1286, 1093, 964, 742, 700

Calcd. HRMS for $C_{19}H_{23}NO$ (M+) – 281.1780, found 281.1741

Spectral Characterization of **2f**;



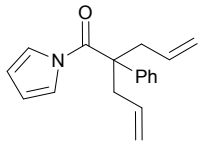
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 – 8.08 (2 H, m), 7.35 (5 H, dd, *J* = 16.4, 8.1), 7.15 (5 H, dd, *J* =15.6, 7.6), 6.98 (2 H, s), 6.62 (2 H, d, *J* = 6.7), 6.22 (2 H, s), 6.10 (2 H, d, *J* = 1.9), 3.55 (1 H, d, *J* = 13.5), 3.41 (1 H, d, *J* = 13.6), 3.11 – 2.98 (1 H, m), 2.98 – 2.87 (1 H, m)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.5, 147.0, 143.7, 141.7, 135.9, 132.8, 130.6, 130.1, 129.4, 128.3, 128.0, 127.2, 126.9, 126.8, 124.2, 120.8, 112.6, 57.7, 42.6, 39.4

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3072, 2351, 3062, 2360, 1778, 1739, 1706, 1598, 1514, 1340, 1280, 1076, 1035, 948, 744, 700

Calcd. HRMS for $C_{28}H_{25}N_2O_3$ (M+H) – 437.1865, found 437.1827

Spectral Characterization of **2g**;



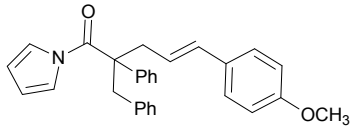
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (2 H, t, *J* = 7.5), 7.27 (1 H, dd, *J* = 10.5, 4.3), 7.21 (2 H, dd, *J* = 8.3, 1.1), 6.93 (2 H, s), 6.06 – 5.99 (2 H, m), 5.55 – 5.39 (2 H, m), 5.08 – 4.99 (2 H, m), 4.91 (2 H, dd, *J* = 17.0, 1.2), 2.86 (4 H, d, *J* = 7.3)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.9, 142.0, 132.7, 129.3, 127.7, 126.5, 120.6, 119.7, 112.1, 55.8, 40.3

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3072, 2351, 1703, 1463, 1325, 1282, 1101, 921, 740, 696

Calcd. HRMS for $C_{18}H_{20}NO$ (M+H) – 266.1545, found 266.1500

Spectral Characterization of **2h**;



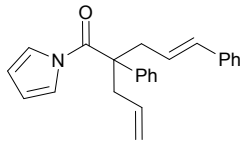
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.26 (3 H, m), 7.22 – 7.09 (7 H, m), 6.98 (2 H, s), 6.87 – 6.77 (2 H, m), 6.65 – 6.59 (2 H, m), 6.15 (1 H, d, *J* = 15.8), 6.10 – 6.05 (2 H, m), 5.94 – 5.82 (1 H, m), 3.78 (3 H, s), 3.51 (1 H, d, *J* = 13.5), 3.40 (1 H, d, *J* = 13.5), 2.93 (2 H, d, *J* = 7.2)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.9, 159.3, 142.2, 136.3, 134.1, 130.8, 130.3, 129.2, 128.0, 127.8, 127.5, 126.9, 122.1, 120.8, 114.1, 112.2, 57.6, 55.5, 42.4, 38.7

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3037, 2354, 1703, 1604, 1512, 1471, 1290, 1249, 1176, 1035, 966, 744, 702

Calcd. HRMS for $C_{29}H_{28}NO_2$ (M+H) – 422.2120, found 422.2118

Spectral Characterization of **2i**;



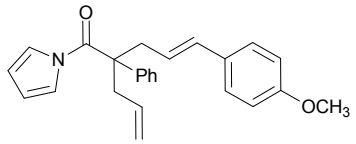
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (2 H, dd, *J* = 10.3, 4.7), 7.33 – 7.28 (1 H, m), 7.27 – 7.22 (4 H, m), 7.22 – 7.16 (3 H, m), 6.95 (2 H, s), 6.22 (1 H, d, *J* = 15.8), 6.07 – 6.02 (2 H, m), 5.85 – 5.76 (1 H, m), 5.54 (1 H, m), 5.09 – 5.05 (1 H, m), 4.95 (1 H, dd, *J* = 17.0, 1.7), 3.04 – 2.98 (2 H, m), 2.92 (2 H, d, *J* = 7.7)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.9, 142.1, 137.4, 134.5, 132.7, 129.4, 128.7, 127.7, 127.5, 126.5, 126.4, 124.3, 120.7, 119.7, 112.1, 56.2, 40.4, 39.8

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3028, 1706, 1460, 1294, 1097, 970, 748, 694

Calcd. HRMS for $C_{24}H_{24}NO$ (M+H) – 342.1858, found 342.1837

Spectral Characterization of **2j**;



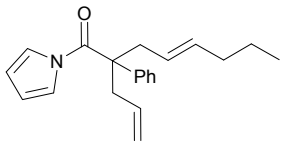
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (2 H, t, *J* = 7.5), 7.29 (1 H, dd, *J* = 8.4, 6.2), 7.24 (2 H, dd, *J* = 5.5, 3.1), 7.16 – 7.11 (2 H, m), 6.95 (2 H, s), 6.83 – 6.74 (2 H, m), 6.15 (1 H, d, *J* = 15.8), 6.06 – 6.00 (2 H, m), 5.66 (1 H, dt, *J* = 15.4, 7.5), 5.53 (1 H, m), 5.06 (1 H, dd, *J* = 10.2, 1.4), 4.94 (1 H, dd, *J* = 17.0, 1.4), 3.77 (3 H, s), 3.04 – 2.94 (2 H, m), 2.94 – 2.85 (2 H, m)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.9, 159.2, 142.2, 133.9, 132.8, 130.3, 129.3, 127.7, 127.5, 126.6, 121.9, 120.7, 119.7, 114.1, 112.1, 56.3, 55.5, 40.4, 39.8

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 2945, 2354, 1701, 1606, 1512, 1463, 1290, 1249, 1170, 1101, 1031, 966, 740, 703

Calcd. HRMS for $C_{25}H_{26}NO_2$ (M+H) – 372.1964, found 372.1952

Spectral Characterization of **2k**;



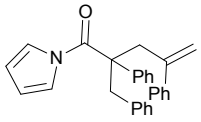
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.24 (2 H, m), 7.22 – 7.17 (1 H, m), 7.13 (2 H, dt, *J* = 8.4, 1.8), 6.87 (2 H, s), 5.97 – 5.92 (2 H, m), 5.37 (1 H, m), 5.19 (1 H, dt, *J* = 15.0, 6.8), 5.03 (1 H, m), 4.97 – 4.93 (1 H, m), 4.85 (1 H, m), 2.77 (3 H, dd, *J* = 17.0, 7.4), 1.81 (2 H, q, *J* = 7.1), 1.28 – 1.14 (2 H, m), 0.75 (3 H, t, *J* = 7.4)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.0, 142.3, 135.9, 132.9, 129.2, 127.5, 126.5, 123.6, 120.6, 119.4, 111.9, 56.0, 40.7, 38.8, 34.9, 22.7, 13.8

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 2958, 1704, 1461, 1292, 1101, 970, 746, 700

Calcd. HRMS for $C_{21}H_{26}NO$ (M+H) – 308.2014, found 308.2000

Spectral Characterization of **2l**;



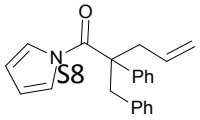
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 – 7.12 (8 H, m), 7.09 – 7.01 (3 H, m), 6.98 (2 H, t, *J* = 7.5), 6.84 (2 H, s), 6.43 (2 H, d, *J* = 7.4), 6.00 – 5.95 (2 H, m), 5.19 (1 H, d, *J* = 1.3), 4.89 (1 H, d, *J* = 0.9), 3.44 (1 H, d, *J* = 13.6), 3.41 – 3.33 (2 H, m), 3.23 (1 H, d, *J* =13.6)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.4, 145.3, 143.1, 141.9, 136.4, 130.9, 128.7, 128.0, 127.4, 127.0, 126.8, 126.4, 120.7, 119.2, 111.9, 57.7, 40.8

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3058, 2368, 1703, 1596, 1463, 1290, 1101, 898, 742, 696

Calcd. HRMS for $C_{28}H_{26}NO$ (M+H) – 392.2014, found 392.2013

Spectral Characterization of **2m**;



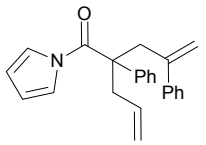
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 – 7.26 (3 H, m), 7.16 – 7.06 (5 H, m), 6.97 (2 H, s), 6.60 – 6.54 (2 H, m), 6.07 – 6.04 (2 H, m), 5.69 (1 H, m), 5.15 – 5.08 (1 H, m), 4.95 (1 H, dd, *J* = 17.0, 1.8), 3.47 (1 H, d, *J* = 13.5), 3.35 (1 H, d, *J* = 13.5), 2.81 (2 H, d, *J* = 7.1)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.8, 142.1, 136.3, 132.9, 130.8, 129.2, 128.0, 127.7, 126.9, 126.9, 120.8, 119.9, 112.2, 57.2, 42.2, 39.3

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3028, 2364, 1701, 1463, 1284, 1101, 1074, 887, 734, 694

Calcd. HRMS for $C_{22}H_{22}NO$ (M+H) – 316.1701, found 316.1697

Spectral Characterization of **2n**;



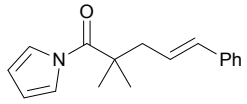
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 (3 H, d, *J* = 14.8), 7.20 – 7.15 (1 H, m), 7.15 – 7.08 (6 H, m), 6.80 (2 H, s), 5.97 – 5.92 (2 H, m), 5.48 – 5.29 (1 H, m), 5.10 (1 H, d, *J* = 1.6), 4.93 – 4.86 (1 H, m), 4.67 (1 H, d, *J* = 0.8), 4.55 (1 H, m), 3.35 (2 H, dt, *J* = 43.4, 10.6), 2.84 – 2.66 (2 H, m)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.7, 145.2, 142.6, 142.2, 132.7, 129.0, 128.1, 127.5, 127.2, 126.8, 120.6, 119.6, 112.0, 56.7, 40.7, 40.1

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3089, 2372, 1697, 1471, 1288, 1101, 904, 742, 698

Calcd. HRMS for $C_{24}H_{23}NONa$ (M+Na) –364.1677, found 364.1697

Spectral Characterization of **2o**;



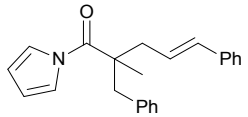
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (2 H, d, *J* = 4.3), 7.21 (1 H, s), 7.19 – 7.11 (1 H, m), 6.30 (1 H, d, *J* = 15.7), 6.26 – 6.24 (2 H, m), 6.24 – 6.22 (2 H, m), 6.08 (1 H, dd, *J* =15.4, 7.8), 2.65 (2 H, dd, *J* =7.5, 1.2), 1.44 (6 H, s)

^{13}C NMR (126 MHz, $CDCl_3$) δ 175.1, 137.3, 133.9, 129.2, 128.6, 128.4, 128.2, 127.5, 127.2, 126.5, 125.1, 120.8, 118.4, 112.2, 56.9, 44.8, 26.5, 24.1

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3075, 3069, 2360, 1735, 1702, 1645, 1070, 1020, 945, 746, 690

Calcd. HRMS for $C_{17}H_{18}NO$ (M-H) – 252.1388 found 252.1325

Spectral Characterization of **2p**;



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.49 (2 H, m), 7.27 – 7.24 (5 H + $CDCl_3$, m), 7.22 – 7.15 (5 H, m), 6.97 – 6.90 (2 H, m), 6.38 – 6.23 (3 H, m), 6.15 – 6.05 (1 H, m), 3.38 – 3.27 (1 H + byproduct-α-H, m), 3.17 (byproduct-benzylic H, dd, *J* =13.8, 6.7), 3.06 (1 H, d, *J* =13.8), 2.97 (1 H, dd, *J* =14.2, 6.8), 2.76 (byproduct-benzylic H, dd, *J* =13.6, 7.6), 2.50 (1 H, dd, *J* = 14.2, 8.1), 1.40 (3 H, s), 1.29 (byproduct-methyl, d, *J* = 6.9)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.9, 139.1, 137.3, 136.7, 134.3, 130.2, 129.2, 128.7, 128.6, 128.5, 127.6, 127.1, 126.8, 126.4, 124.8, 120.7, 119.2, 113.4, 112.6, 50.1, 45.8, 43.3, 40.7, 39.9, 23.8, 17.9

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3070, 3060, 2358, 1729, 1706, 1639, 1076, 1035, 940, 740, 688

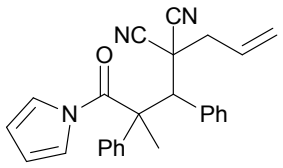
Calcd. HRMS for $C_{23}H_{24}NO$ (M+H) – 330.1858 found 330.1865

Representative procedure for 4-component palladium-catalyzed decarboxylative interceptive allylation

Synthesis of **4a**;

In a flame-dried Schlenk tube, Meldrum's acid (0.43 mmol, 100 mg, 1.0 eq.) in anhydrous 1,4-dioxane (4.3 mL, 0.1 M) was treated with lithium pyrrolide (0.51 mmol, 37.5 mg, 1.2 eq.). The reaction mixture was stirred for a minute. Then Pd_2dba_3 (0.021 mmol, 19.7 mg, 5 mol%), dppe (0.056 mmol, 22.3 mg, 13 mol%) followed by benzylidene malononitrile (0.43 mmol, 66.3 mg, 1.0 eq.) were added. Next, allyl methyl carbonate (0.51 mmol, 59.2 mg, 1.2 eq.) was added to the reaction mixture. The Schlenk tube was sealed and the reaction mixture was stirred overnight at room temperature. After overnight reaction, ^{1}H NMR spectroscopic analysis of the crude reaction mixture was done. During the next two days, 2 more portions of lithium pyrrolide were added (0.21 mmol, 15.7 mg, 0.5 eq. / 0.13 mmol, 9.4 mg, 0.3 eq.) while examining the ^{1}H NMR spectra of the crude reaction mixture. After a complete consumption of Meldrum's acid was observed, the reaction mixture was concentrated *in vacuo* and purified via flash chromatography using 5% EtOAc/Hexane to obtain **4a** as a white solid (76% yield). The solid was then recrystallized using EtOAc and Hexane to obtain the minor diastereomer as white crystals (28% yield).

Spectral Characterization of **4a**;



mixture of diastereomers

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.58 (s, 2H), 7.49 (s, 5H), 7.41 – 7.33 (m, 3H), 7.12 – 7.02 (m, 4H), 7.02 – 6.96 (m, 1H), 6.95 – 6.89 (m, 2H), 6.84 (d, *J* = 2.0, 2H), 6.66 (s, 1H), 6.08 – 6.05 (m, 2H), 6.05 – 5.97 (m, 3H), 5.89 (m, 1H), 5.44 (d, *J* = 10.1, 1H), 5.34 (dd, *J* = 20.5, 13.6, 2H), 5.19 (dd, *J* = 16.9, 1.0, 1H), 4.59 (s, 1H), 4.57 (s, 1H), 2.70 (dd, *J* = 13.8, 8.0, 1H), 2.61 (dd, *J* = 13.9, 6.4, 1H), 2.52 (s, 3H), 2.44 – 2.34 (m, 2H), 1.60 (s, 3H)

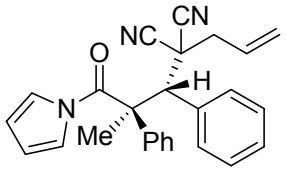
^{13}C NMR (126 MHz, $CDCl_3$) δ 173.6, 173.5, 139.1, 137.3, 134.6, 134.1, 133.5, 129.9, 129.7, 129.3, 129.1, 129.0, 128.96, 128.9, 128.8, 128.6, 128.4, 127.95, 127.9, 126.8, 123.6, 123.2,

121.6, 121.4, 116.6, 115.92, 115.9, 114.9, 112.6, 112.5, 56.5, 55.9, 55.8, 55.7, 44.3, 43.4, 39.8, 39.2, 26.2, 19.2

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3058, 2368, 1703, 1596, 1463, 1290, 1101, 898, 742, 696

Calcd. HRMS for $C_{26}H_{24}N_3O$ (M+H) – 394.1919, found 394.1906

Spectral Characterization of **4a**;

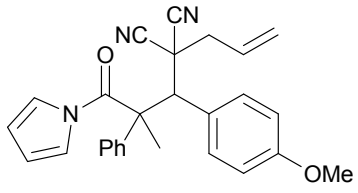


one diastereomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.17 (dd, *J* = 8.8, 2.9 Hz, 1H), 7.13 – 6.94 (m, 7H), 6.94 – 6.89 (m, 2H), 6.66 (s, 1H), 6.09 – 6.04 (m, 2H), 5.99 (dd, *J* = 17.3, 7.3 Hz, 1H), 5.38 (dd, *J* = 49.1, 13.6 Hz, 2H), 4.59 (s, 1H), 2.65 (m, 2H), 2.51 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.4, 138.9, 133.3, 128.8, 128.7, 128.5, 128.3, 127.7, 126.6, 123.3, 121.2, 116.4, 115.7, 112.4, 56.3, 55.6, 43.2, 39.6, 19.0

Spectral Characterization of **4b**;



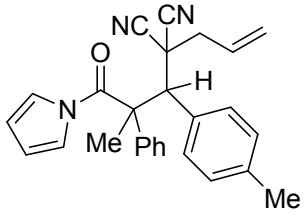
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (s, 3H), 7.49 (s, 3H), 7.40 (t, *J* = 7.8, 1H), 7.16 (d, *J* = 7.6, 1H), 7.12 – 6.98 (m, 4H), 6.91 (d, *J* = 1.8, 2H), 6.90 – 6.85 (m, 2H), 6.83 (s, 2H), 6.77 – 6.40 (m, 2H), 6.06 (d, *J* = 1.8, 1H), 6.02 (dd, *J* = 3.5, 2.4, 2H), 5.98 (d, *J* = 6.6, 1H), 5.89 (m, 1H), 5.43 (d, *J* = 10.2, 1H), 5.34 (dd, *J* = 21.1, 13.6, 2H), 5.20 (d, *J* = 16.9, 1H), 4.53 (s, 1H), 4.50 (s, 1H), 3.82 (d, *J* = 1.3, 3H), 3.67 (d, *J* = 1.3, 2H), 2.70 (dd, *J* = 13.8, 7.9, 1H), 2.62 (dd, *J* = 13.4, 5.9, 1H), 2.49 (s, 2H), 2.41 (d, *J* = 7.1, 2H), 1.59 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.7, 173.5, 160.1, 159.5, 139.2, 137.3, 135.8, 129.8, 129.7, 129.1, 129.0, 128.9, 128.8, 127.9, 126.7, 125.8, 125.3, 123.35, 123.3, 121.5, 121.4, 116.6, 116.0, 115.9, 115.0, 114.4, 114.1, 113.6, 112.5, 112.4, 55.95, 55.9, 55.8, 55.4, 55.34, 55.3, 44.3, 43.3, 39.9, 39.2, 26.2, 19.1

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3020, 2933, 1703, 1612, 1583, 1512, 1467, 1297, 1280, 1182, 1095, 902, 744

Calcd. HRMS for $C_{27}H_{25}N_3O_2Na$ (M+Na) – 446.1844, found 446.1883

Spectral Characterization of **4c**;



mixture of 2 diastereomers

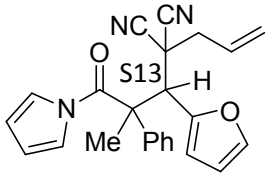
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (s, 3H), 7.49 (s, 3H), 7.37 (d, *J* = 5.0 Hz, 1H), 7.15 (t, *J* = 9.1 Hz, 3H), 7.02 (dt, *J* = 6.5, 5.7 Hz, 4H), 6.91 (d, *J* = 1.7 Hz, 2H), 6.83 (s, 2H), 6.06 (s, 2H), 6.01 (d, *J* = 1.8 Hz, 2H), 5.94 – 5.84 (m, 1H), 5.47 – 5.25 (m, 3H), 5.19 (d, *J* = 15.7 Hz, 1H), 4.54 (d, *J* = 2.6 Hz, 1H), 4.52 (d, *J* = 2.8 Hz, 1H), 2.65 (m, 2H), 2.50 (d, *J* = 2.7 Hz, 2H), 2.39 (d, *J* = 7.2 Hz, 2H), 2.36 (d, *J* = 2.4 Hz, 3H), 2.16 (d, *J* = 2.3 Hz, 2H), 1.59 (d, *J* = 2.7 Hz, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.7, 173.6, 139.3, 139.2, 138.5, 137.4, 134.5, 130.9, 130.3, 129.8, 129.7, 129.1, 129.0, 128.9, 127.9, 127.8, 126.8, 123.4, 123.2, 121.6, 121.4, 116.6, 116.0, 115.9, 114.9, 112.5, 112.4, 56.3, 55.9, 55.8, 55.7, 44.3, 43.4, 41.0, 39.9, 39.2, 26.2, 21.3, 21.1, 19.2

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 2923, 1701, 1514, 1467, 1298, 1091, 1076, 902, 736, 702

Calcd. HRMS for $C_{27}H_{25}N_3ONa$ (M+Na) – 430.1895, found 430.1906

Spectral Characterization of **4d**;



mixture of 2 diastereomers

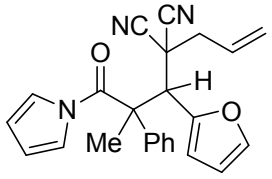
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 – 7.51 (m, 2H), 7.51 – 7.43 (m, 4H), 7.22 – 7.08 (m, 7H), 6.94 – 6.90 (m, 2H), 6.87 (s, 2H), 6.51 – 6.47 (m, 1H), 6.42 (dd, *J* = 3.3, 1.8 Hz, 1H), 6.10 – 5.96 (m, 8H), 5.91 – 5.79 (m, 1H), 5.46 (dd, *J* = 10.2, 1.0 Hz, 1H), 5.41 – 5.34 (m, 2H), 5.23 (dd, *J* = 16.9, 1.3 Hz, 1H), 4.74 (s, 1H), 4.57 (s, 1H), 2.79 – 2.73 (m, 2H), 2.50 (s, 3H), 2.37 (d, *J* = 7.3 Hz, 2H), 1.72 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.2, 172.8, 148.4, 146.9, 143.3, 142.8, 138.9, 136.6, 130.0, 129.8, 129.1, 128.9, 128.5, 128.2, 126.0, 123.8, 123.6, 121.5, 121.2, 115.9, 115.4, 114.7, 114.4, 113.1, 112.7, 112.6, 112.3, 111.2, 110.4, 56.4, 55.6, 51.9, 50.6, 43.7, 43.4, 38.6, 38.4, 24.0, 18.6

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3153, 2954, 1699, 1498, 1467, 1307, 1149, 1091, 1080, 900, 736, 702

Calcd. HRMS for $C_{24}H_{22}N_3O_2$ (M+H) – 384.1712, found 384.1697

Spectral Characterization of **4d**;

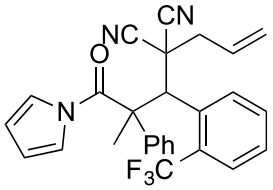


one diastereomer

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 – 7.10 (m, 6H), 6.94 – 6.90 (m, 2H), 6.09 – 6.06 (m, 2H), 6.05 – 5.97 (m, 3H), 5.42 (m, 2H), 4.57 (s, 1H), 2.81 – 2.74 (m, 2H), 2.50 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.2, 146.9, 143.3, 138.9, 129.1, 128.9, 128.2, 126.0, 123.6, 121.2, 115.9, 115.4, 113.1, 112.7, 110.4, 55.6, 51.9, 43.4, 38.6, 18.6

Spectral Characterization of **4e**;



mixture of diastereomers

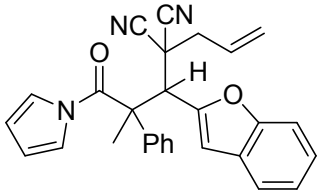
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 – 7.81 (m, 3H), 7.66 – 7.62 (m, 1H), 7.61 – 7.53 (m, 3H), 7.45 (s, 2H), 6.86 (s, 1H), 6.04 (t, *J* = 2.5 Hz, 2H), 5.78 (m, 1H), 5.54 (s, 1H), 5.35 – 5.17 (m, 2H), 2.78 (dd, *J* = 13.6, 7.6 Hz, 1H), 1.99 (m, 1H), 1.50 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.7, 137.5, 133.8, 132.7, 130.1, 129.5, 129.3, 128.7, 123.4, 121.7, 115.7, 113.8, 112.4, 56.1, 49.3, 43.6, 41.1, 25.7

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3060, 2265, 1701, 1585, 1415, 1190, 1101, 880, 7352, 687

Calcd. HRMS for $C_{27}H_{23}F_3N_3O$ (M+H) – 462.1715, found 462.1702

Spectral Characterization of **4f**;



Major diastereomer

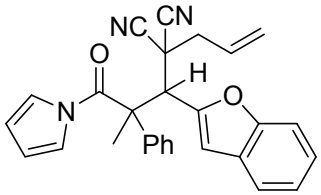
1H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.5, 3H), 7.52 (d, *J* = 7.2, 4H), 7.38 – 7.31 (m, 1H), 7.28 (d, *J* = 7.4, 1H), 6.91 (s, 1H), 6.87 (s, 2H), 6.08 – 5.97 (m, 2H), 5.86 (m, 1H), 5.36 (d, *J* = 10.1, 1H), 5.22 (d, *J* = 16.8, 1H), 4.87 (s, 1H), 2.45 (d, *J* = 7.0, 2H), 1.82 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 172.7, 154.3, 151.0, 136.5, 130.2, 129.9, 128.3, 127.7, 125.3, 124.0, 123.7, 121.7, 121.4, 114.4, 114.3, 112.6, 111.7, 109.3, 56.3, 50.9, 43.7, 38.2, 23.9

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3163, 1701, 1475, 1454, 1299, 1097, 1076, 991, 937, 904, 746, 707

Calcd. HRMS for $C_{28}H_{23}N_3O_2Na$ (M+Na) – 456.1688, found 456.1694

Spectral Characterization of **4f**;

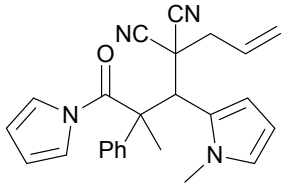


Minor diastereomer

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.2, 1H), 7.32 (d, *J* = 7.5, 1H), 7.22 (dd, *J* = 7.3, 1.0, 1H), 7.18 (dd, *J* = 9.4, 4.4, 2H), 7.11 (t, *J* = 7.5, 1H), 7.04 (t, *J* = 7.8, 2H), 7.01 – 6.96 (m, 1H), 6.94 (d, *J* = 2.2, 2H), 6.40 (s, 1H), 6.14 – 6.07 (m, 2H), 6.07 – 5.99 (m, 1H), 5.48 (d, *J* = 10.1, 1H), 5.39 (d, *J* = 16.9, 1H), 4.72 (s, 1H), 2.83 (d, *J* = 7.3, 2H), 2.60 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 173.0, 154.7, 149.6, 138.5, 129.1, 128.7, 128.3, 126.9, 126.0, 125.1, 123.8, 123.2, 121.3, 121.1, 115.8, 115.3, 112.8, 111.3, 110.0, 55.6, 52.4, 43.4, 38.4, 18.8.

Spectral Characterization of **4g**;



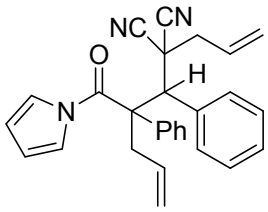
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 23.7, 17.5, 5H), 7.12 (q, *J* = 6.7, 2H), 7.03 (d, *J* = 8.0, 1H), 6.92 – 6.85 (m, 4H), 6.67 (d, *J* = 1.4, 2H), 6.33 – 6.28 (m, 1H), 6.19 – 6.12 (m, 2H), 6.09 (d, *J* = 1.7, 1H), 6.04 (d, *J* = 1.6, 2H), 6.04 – 5.92 (m, 2H), 5.84 (m, 1H), 5.46 – 5.29 (m, 3H), 5.20 (d, *J* = 16.9, 1H), 4.75 (s, 1H), 4.59 (s, 1H), 3.67 (s, 3H), 3.08 (s, 2H), 2.71 (dd, *J* = 13.5, 7.7, 1H), 2.57 (dd, *J* = 13.3, 6.1, 1H), 2.48 – 2.36 (m, 3H), 2.28 (dd, *J* = 13.2, 5.9, 1H), 1.62 (s, 3H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 174.0, 173.8, 138.7, 137.1, 129.9, 129.5, 129.0, 128.9, 128.6, 128.2, 126.3, 124.9, 123.4, 123.3, 123.2, 123.1, 123.0, 121.6, 121.3, 116.6, 115.7, 115.6, 114.0, 112.7, 112.6, 110.8, 110.2, 108.2, 107.8, 56.7, 56.1, 43.5, 42.9, 41.2, 40.8, 34.6, 33.9, 24.9, 18.7

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3159, 1699, 1465, 1290, 1091, 989, 902, 740

Calcd. HRMS for $C_{25}H_{24}N_4ONa$ (M+Na) – 419.1848, found 419.1859

Spectral Characterization of **4h**;



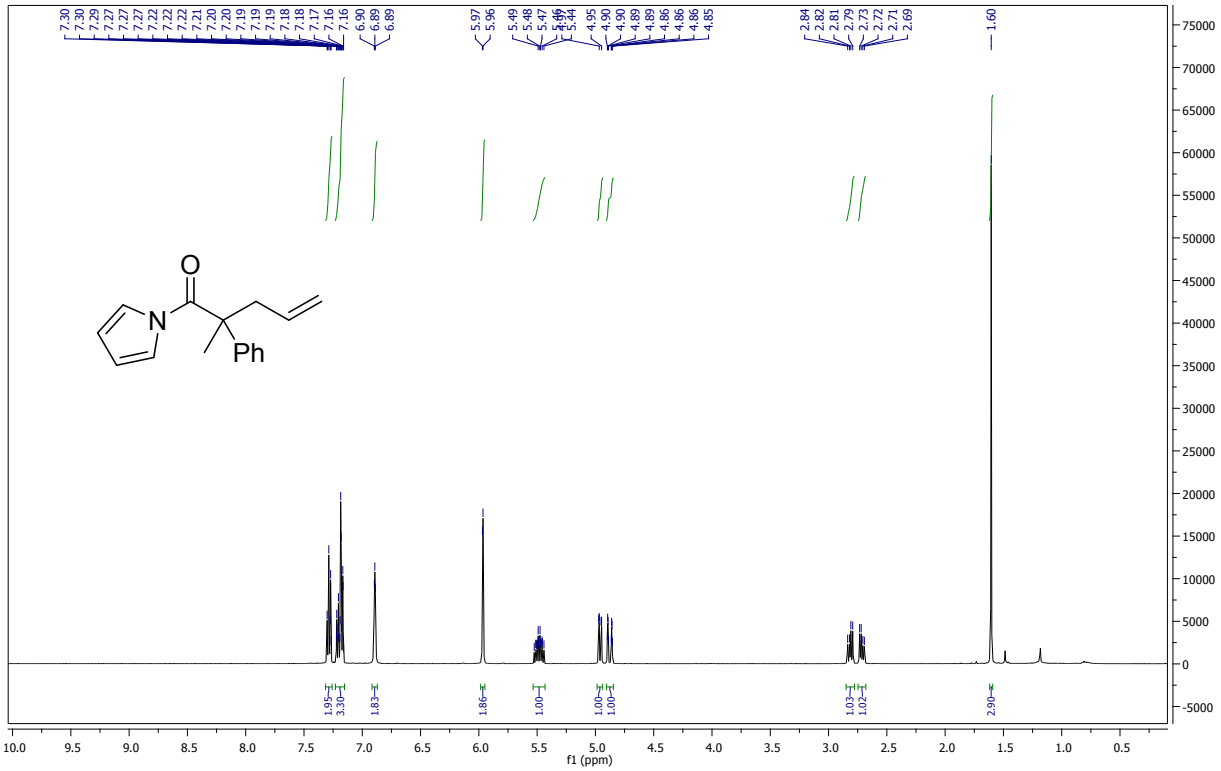
one diastereomer

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.59 (s, 1H), 7.53 (t, *J* = 6.9 Hz, 3H), 7.39 (m, 5H), 7.23 (t, *J* = 5.7 Hz, 3H), 6.02 (s, 2H), 5.99 – 5.87 (m, 1H), 5.54 (m, 1H), 5.38 (d, *J* = 10.1 Hz, 1H), 5.22 (d, *J* = 16.9 Hz, 1H), 4.93 (d, *J* = 10.2 Hz, 1H), 4.59 (s, 1H), 4.46 (d, *J* = 16.9 Hz, 1H), 2.68 (d, *J* = 7.2 Hz, 2H), 2.40 (m, 2H)

^{13}C NMR (126 MHz, $CDCl_3$) δ 171.3, 137.7, 134.5, 133.5, 132.4, 130.9, 130.0, 129.7, 129.6, 129.5, 129.4, 128.9, 128.8, 128.2, 127.6, 123.4, 121.5, 120.8, 116.3, 114.6, 112.5, 60.1, 54.1, 44.52, 42.6, 39.9

FT-IR (CH_2Cl_2) υ_{max} cm^{-1} 3089, 2923, 1733, 1641, 1440, 1276, 1166, 1124, 993, 937, 702

Calcd. HRMS for $C_{28}H_{29}N_4O$ ($M+NH_4$) – 437.2341, found 437.2217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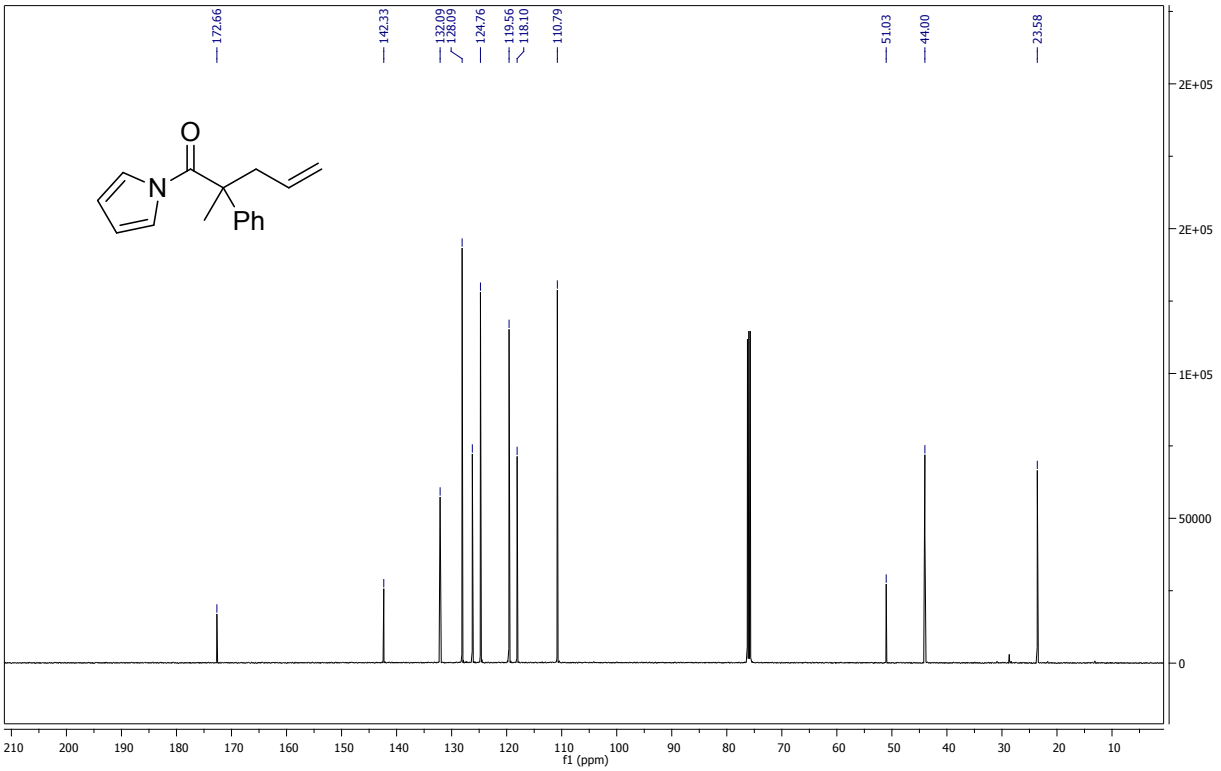
1.86
1.00
1.00
1.00
1.03
1.02
2.90
f1 (ppm)


172.66
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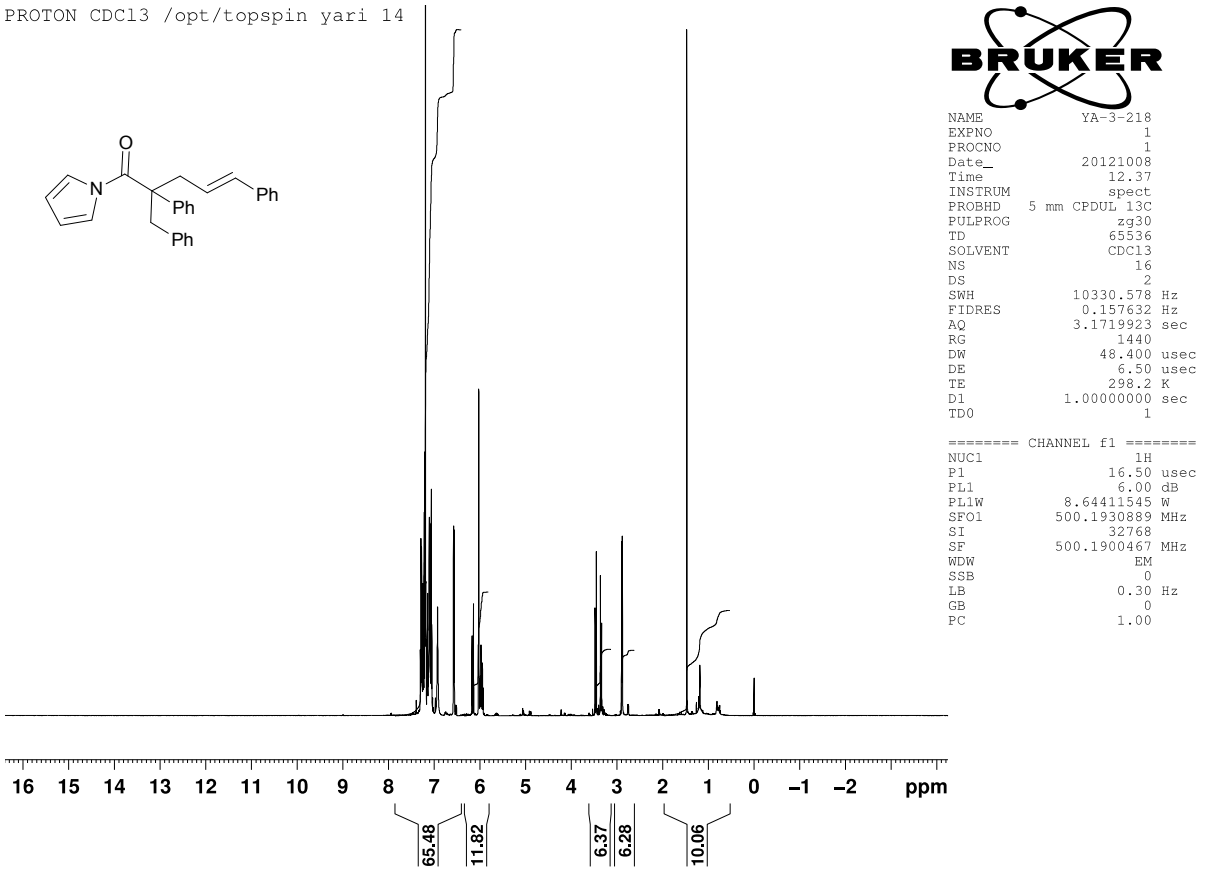
110.79
51.03
44.00
23.58
O
N
Ph
f1 (ppm)


PROTON CDCl3 /opt/topspin yari 14
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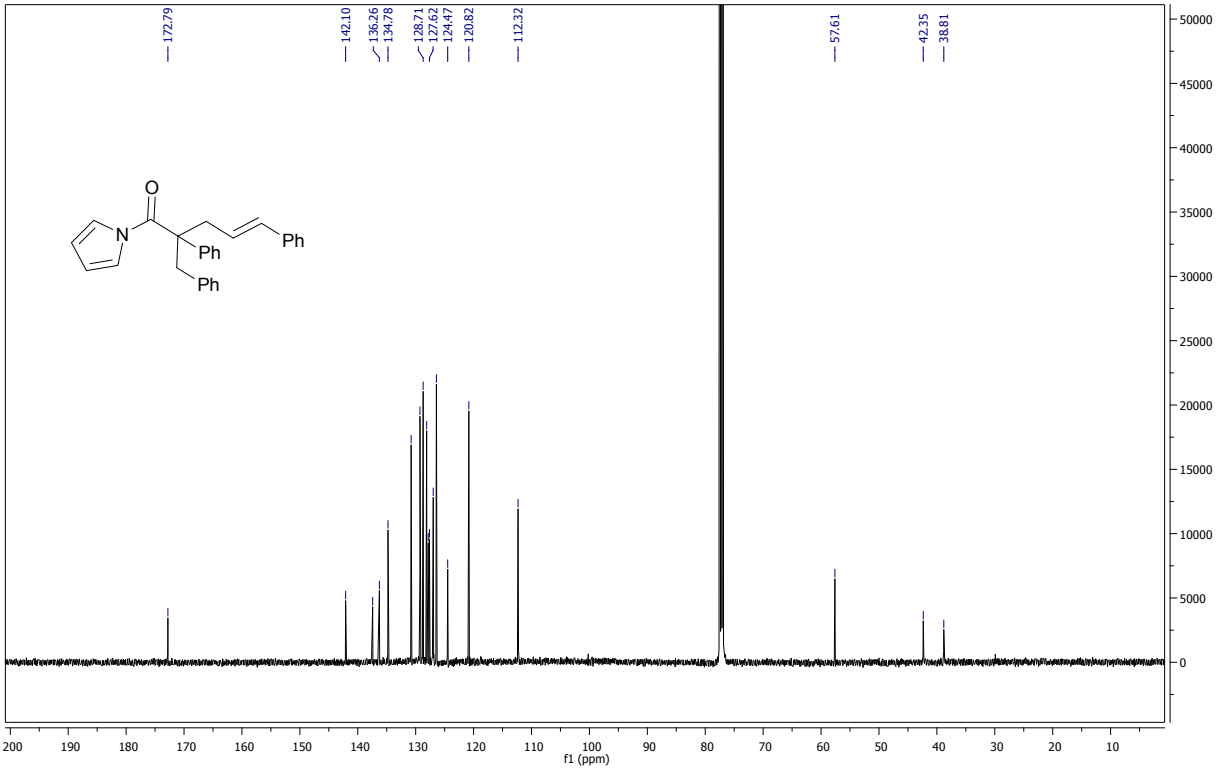
Ph
Ph
Ph
NAME YA-3-218
EXPNO 1
PROCNO 1
Date_ 20121008
Time 12.37
INSTRUM spect
PROBHD 5 mm CPDUL 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 1440
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 6.00 dB
PL1W 8.64411545 W
SFO1 500.1930889 MHz
SI 32768
SF 500.1900467 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
65.48
11.82
6.37
6.28
10.06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142.10
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134.78
128.71
127.62
124.47
120.82
112.32
57.61
42.35
38.81
O
N
Ph
Ph
Ph
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
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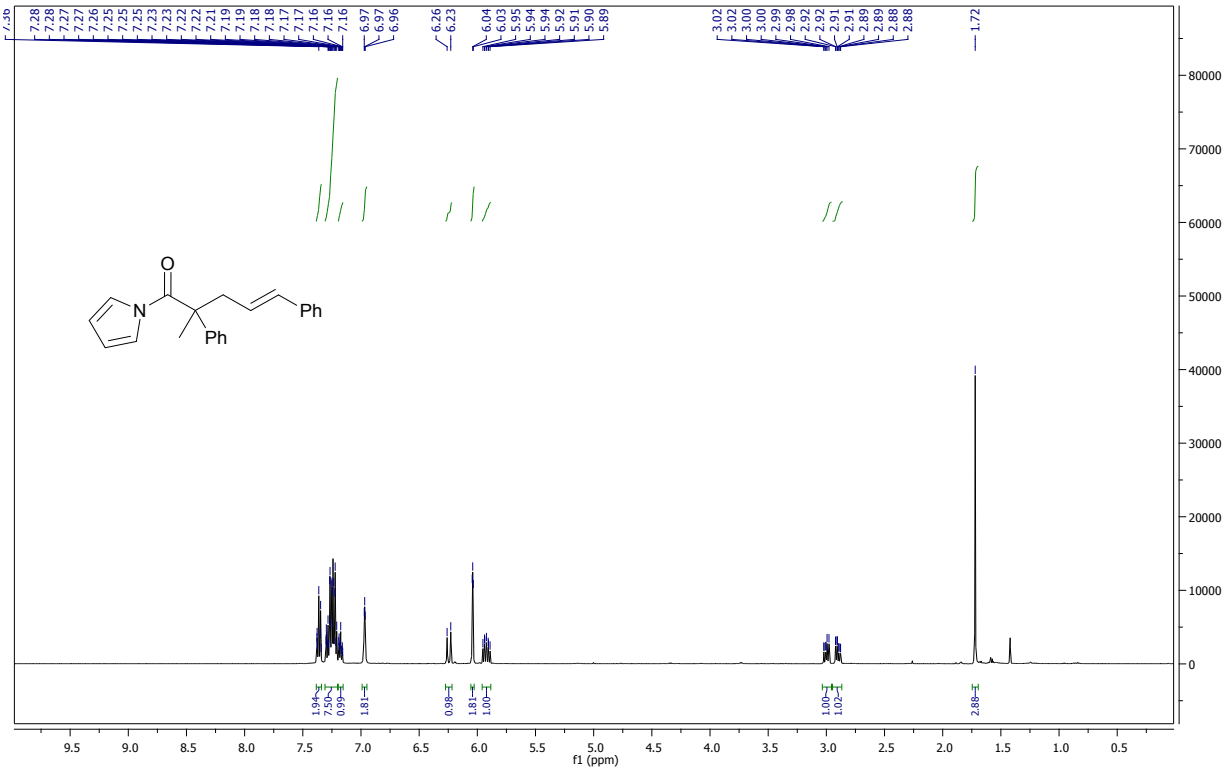
f1 (ppm)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7.19
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7.17
7.17
7.16
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7.16
6.97
6.97
6.96
6.26
6.23
6.04
6.03
5.95
5.94
5.94
5.92
5.91
5.90
5.89
3.02
3.02
3.00
3.00
2.99
2.98
2.92
2.92
2.91
2.91
2.89
2.89
2.88
2.88
1.72
O
N
Ph
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0.99
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0.98
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1.00
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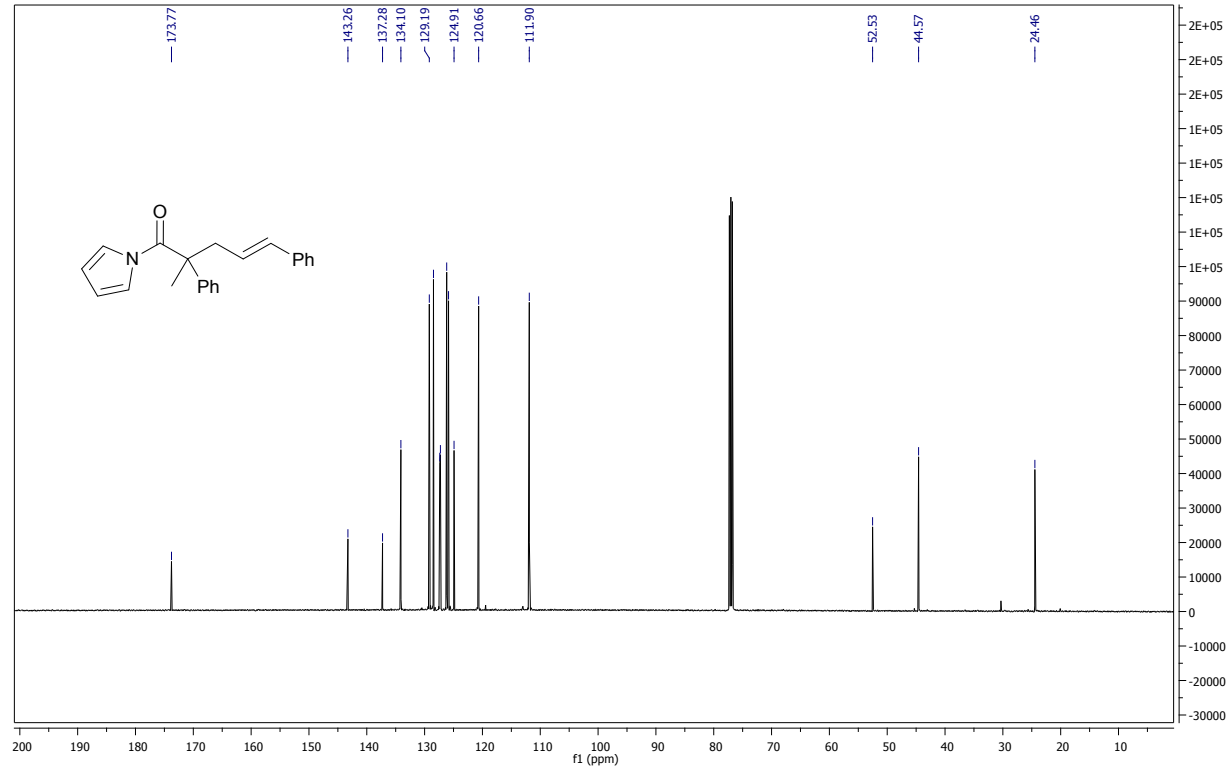
2.88
f1 (ppm)


173.77
143.26
137.28
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124.91
120.66
111.90
52.53
44.57
24.46
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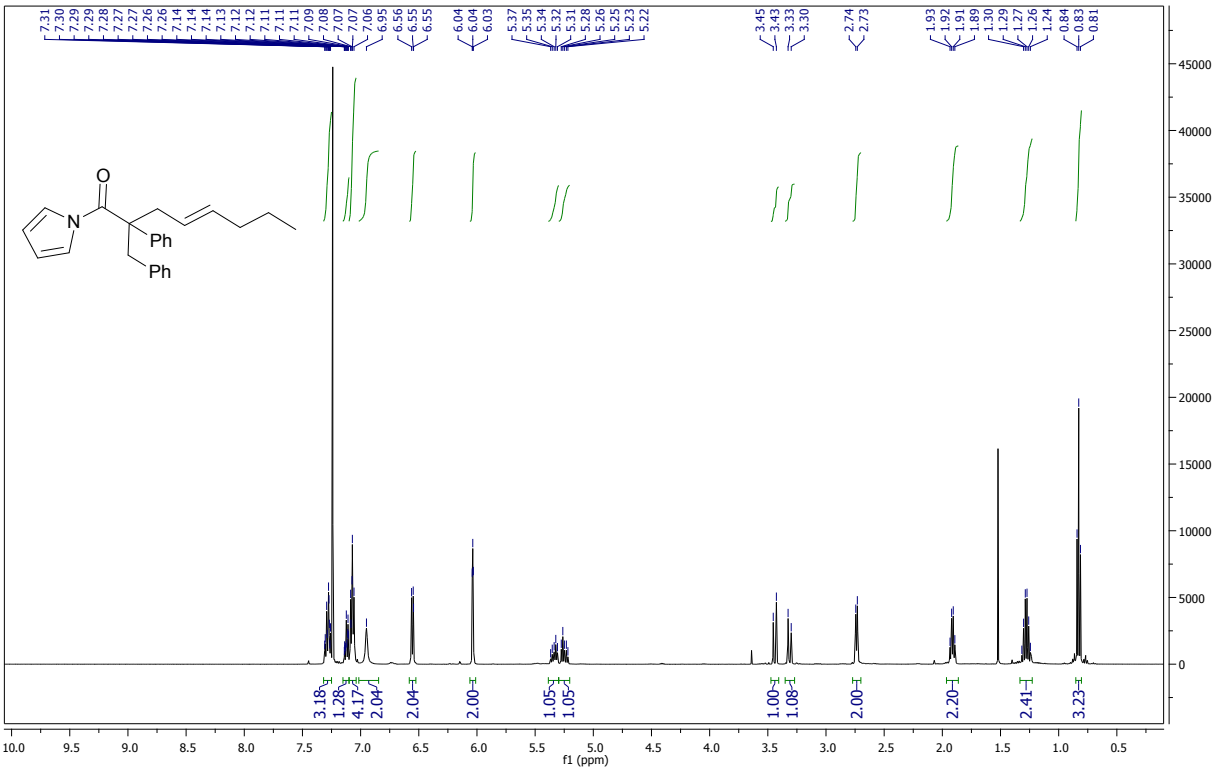
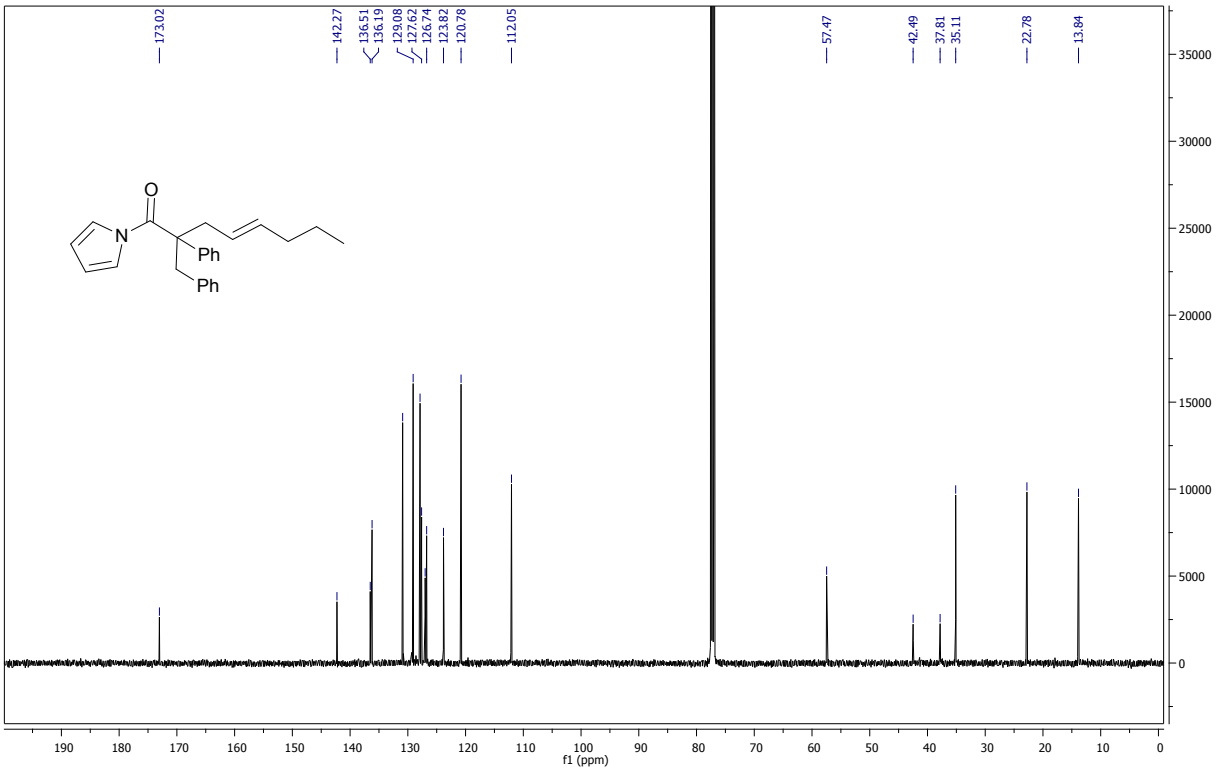
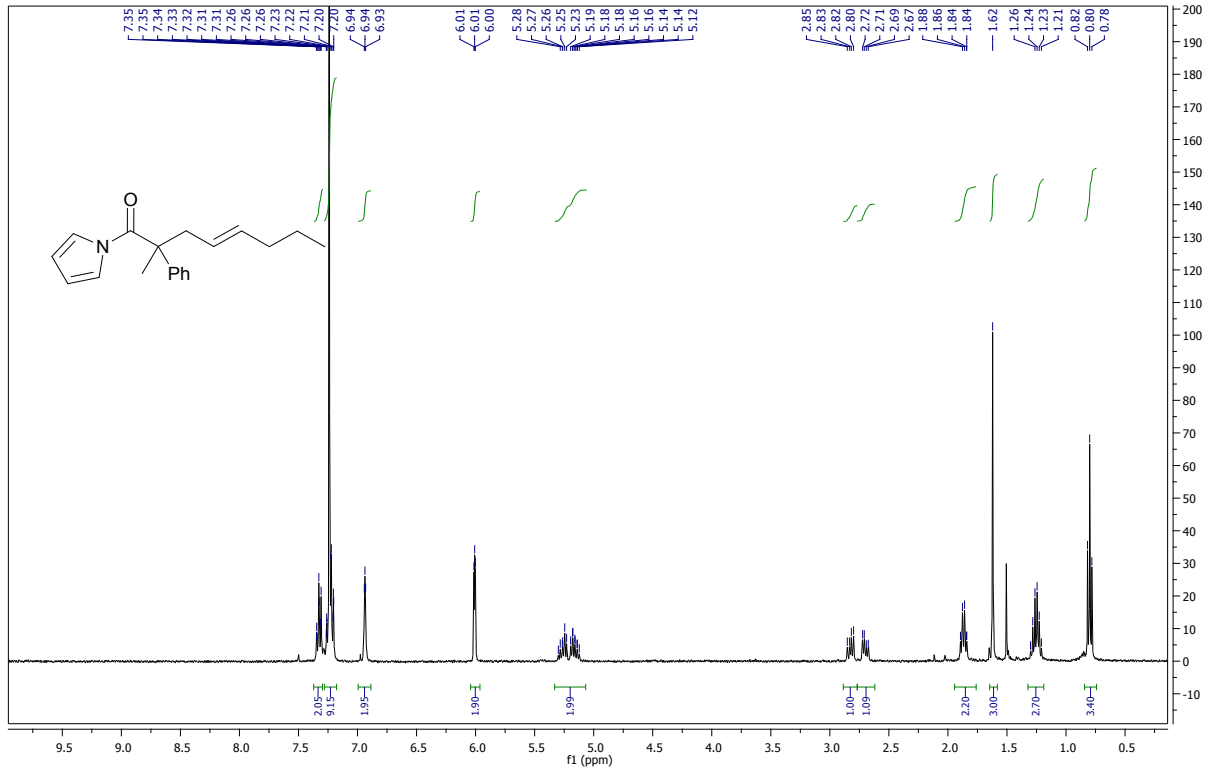
N
Ph
Ph
f1 (ppm)


7.31 7.30 7.29 7.29 7.28 7.27 7.27 7.26 7.26 7.14 7.14 7.13 7.12 7.12 7.11 7.11 7.11 7.09 7.08 7.07 7.07 7.06 6.95 6.56 6.55 6.55 6.04 6.04 6.03 5.37 5.35 5.34 5.32 5.31 5.28 5.26 5.25 5.23 5.22 3.45 3.43 3.33 3.30 2.74 2.73 1.93 1.92 1.91 1.89 1.30 1.29 1.27 1.26 1.24 0.84 0.83 0.81
O
N
Ph
Ph
3.18 1.28 4.17 2.04 2.04 2.00 1.05 1.05 1.00 1.08 2.00 2.20 2.41 3.23
f1 (ppm)


173.02 142.27 136.51 136.19 129.08 127.62 126.74 123.82 120.78 112.05 57.47 42.49 37.81 35.11 22.78 13.84
O
N
Ph
Ph
f1 (ppm)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7.31
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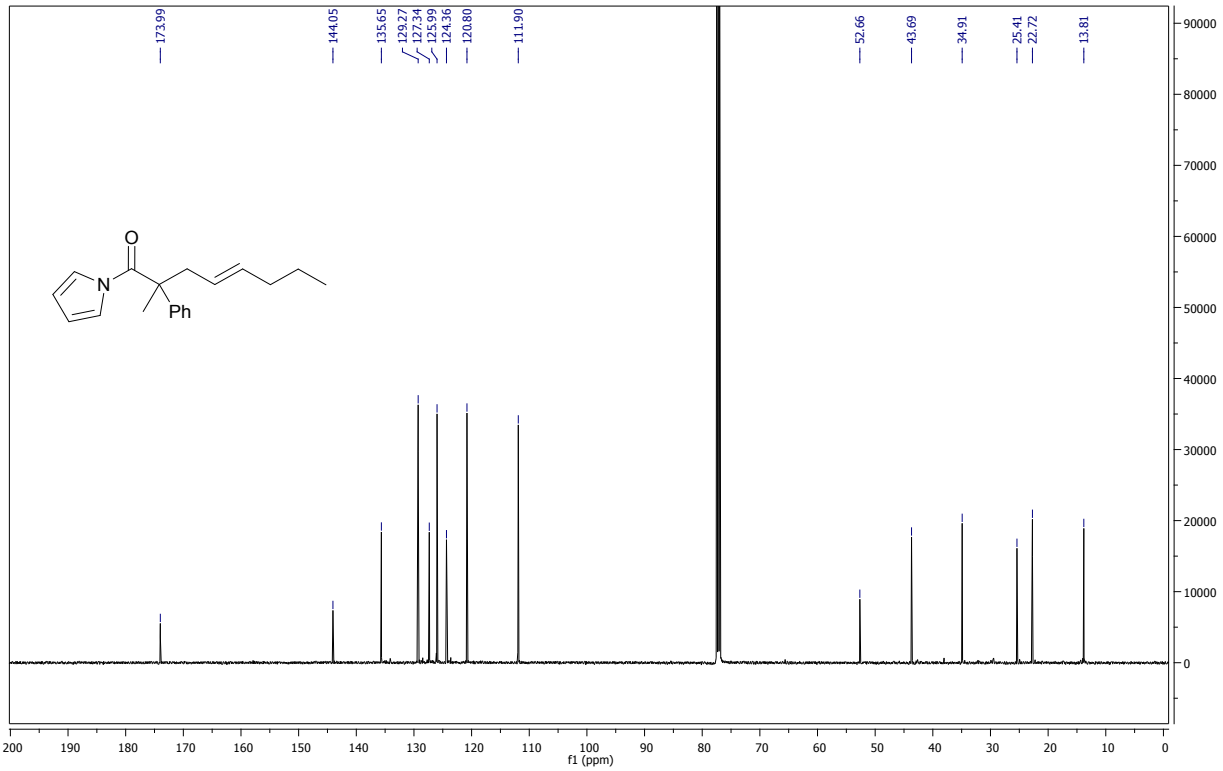
7.26
7.23
7.22
7.21
7.20
7.20
6.94
6.94
6.93
6.01
6.01
6.00
5.28
5.27
5.26
5.25
5.23
5.19
5.18
5.16
5.16
5.14
5.14
5.12
2.85
2.83
2.82
2.80
2.72
2.71
2.69
2.67
1.88
1.86
1.84
1.84
1.62
1.26
1.24
1.23
1.21
0.82
0.80
0.78
O
N
Ph
2.05
9.15
1.95
1.90
1.99
1.00
1.09
2.20
3.00
2.70
3.40
f1 (ppm)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135.65
129.27
127.34
125.99
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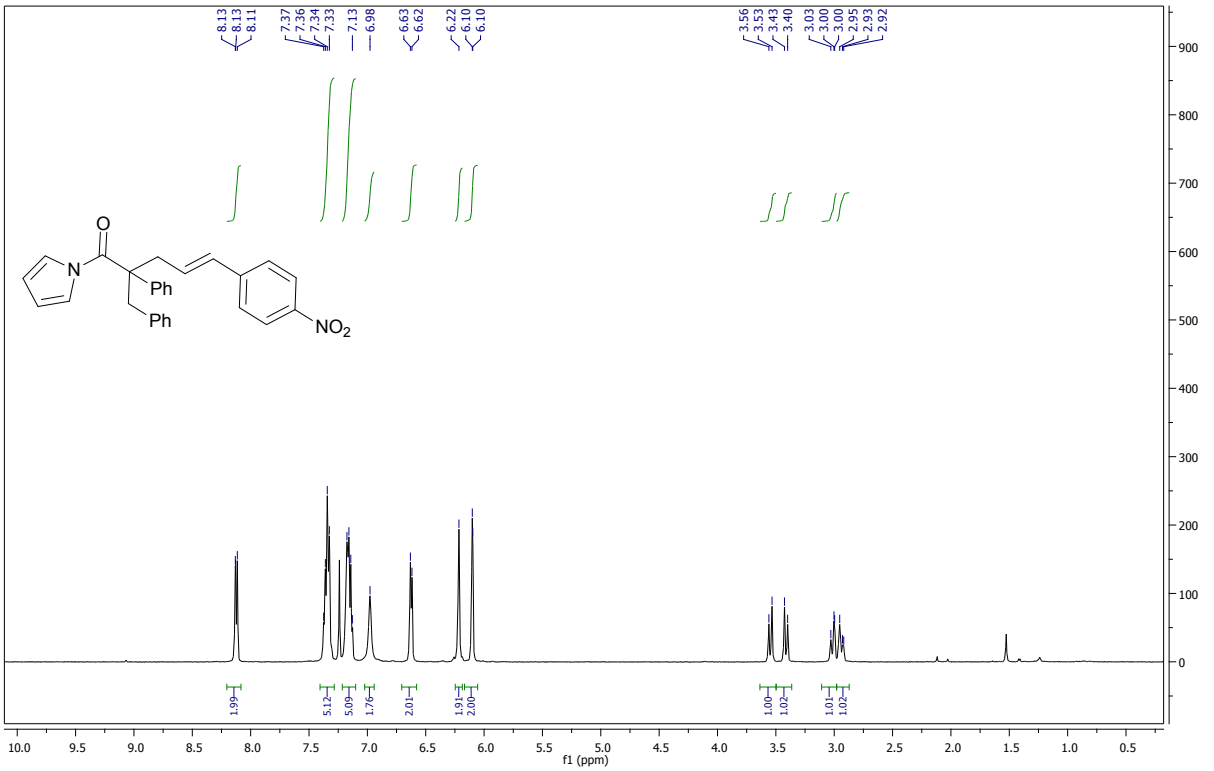
25.41
22.72
13.81
O
N
Ph
f1 (ppm)


8.13
8.13
8.11
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7.36
7.34
7.33
7.13
6.98
6.63
6.62
6.22
6.10
6.10
3.56
3.53
3.43
3.40
3.03
3.00
3.00
2.95
2.93
2.92
O
N
Ph
Ph
NO2
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5.12
5.09
1.76
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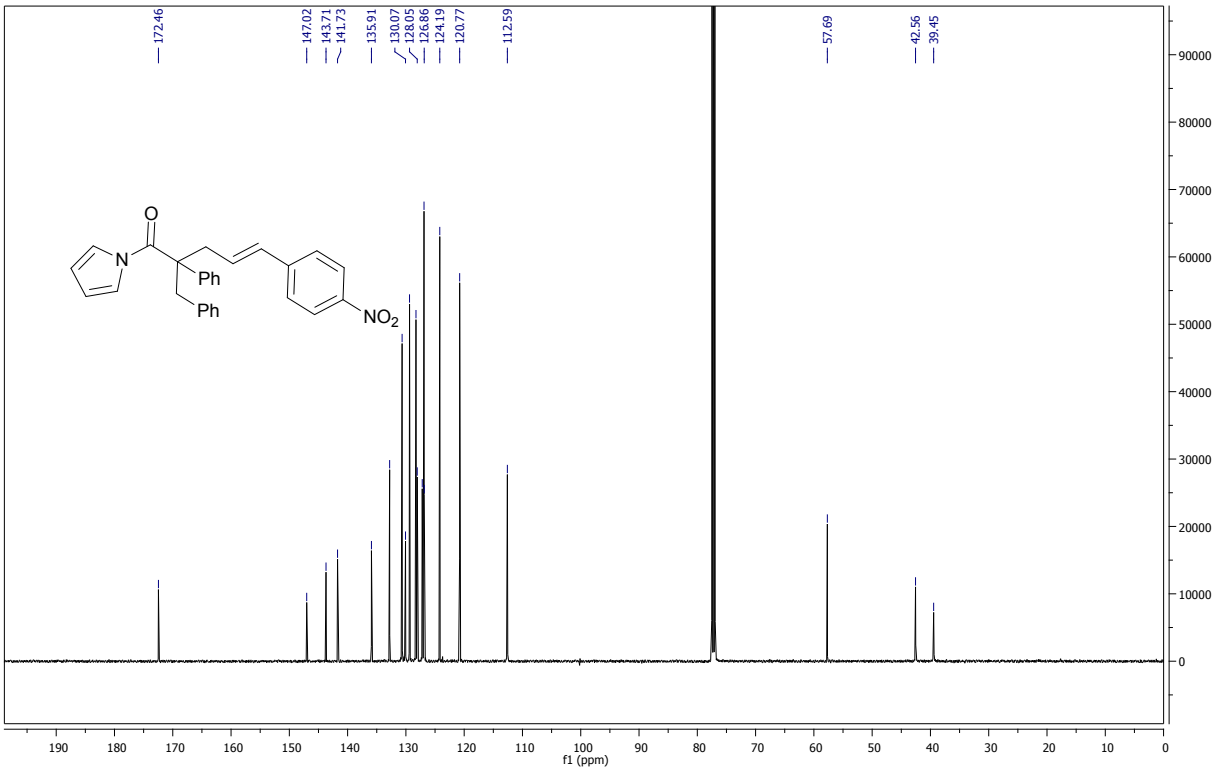
1.91
2.00
1.00
1.02
1.01
1.02
f1 (ppm)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147.02
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120.77
112.59
57.69
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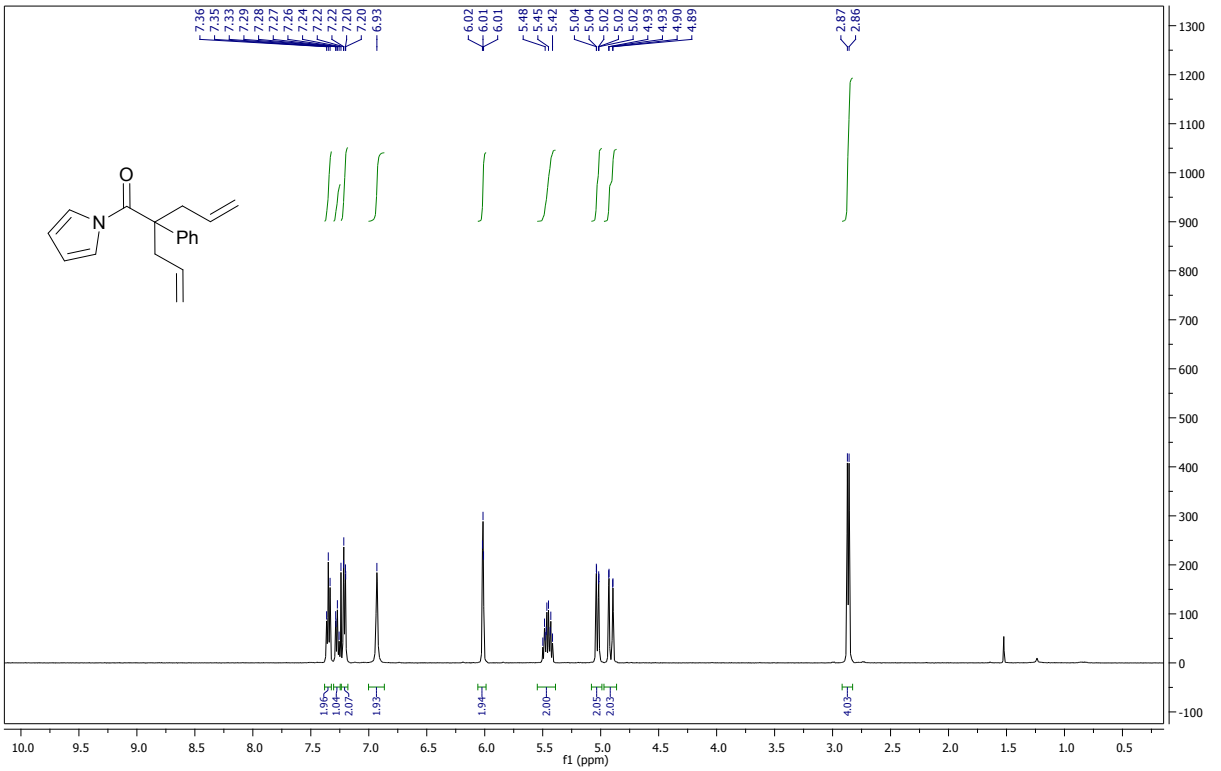
O
N
Ph
Ph
NO2
f1 (ppm)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6.93
6.02
6.01
6.01
5.48
5.45
5.42
5.04
5.04
5.02
5.02
5.02
4.93
4.93
4.90
4.89
2.87
2.86
O
N
Ph
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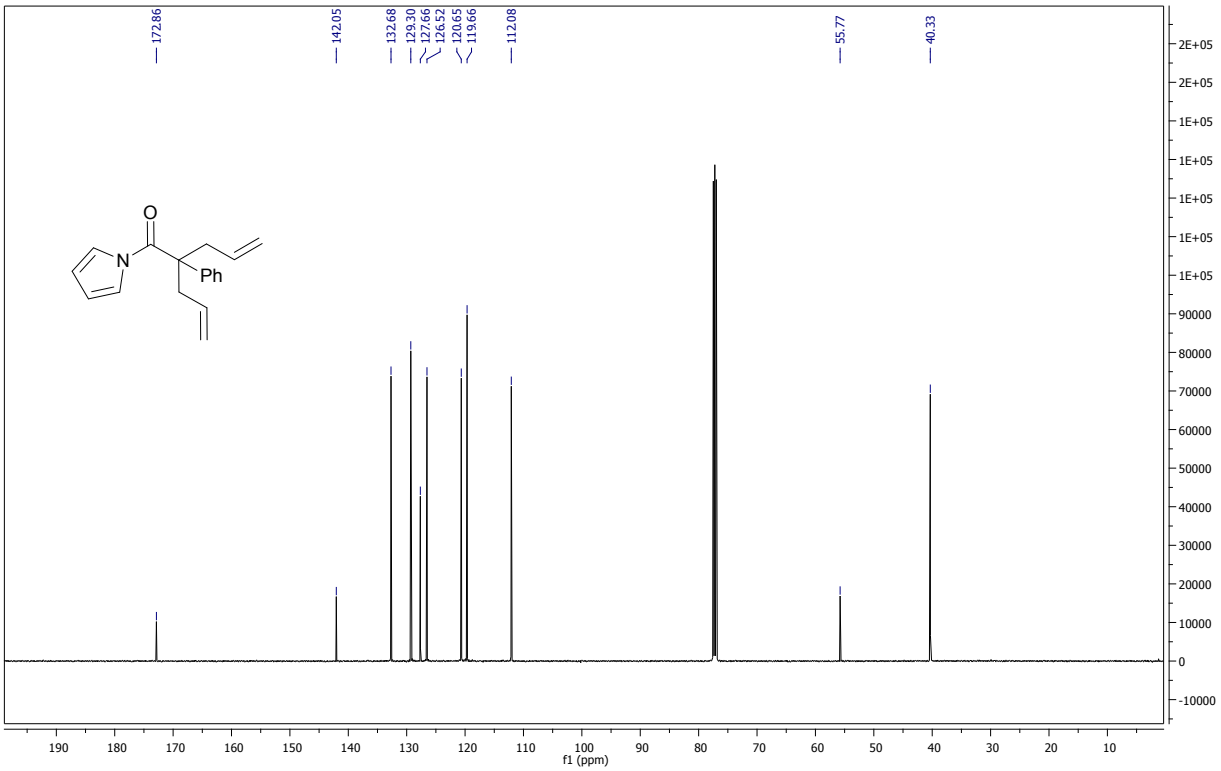
1.04
2.07
1.93
1.94
2.00
2.05
2.03
4.03
f1 (ppm)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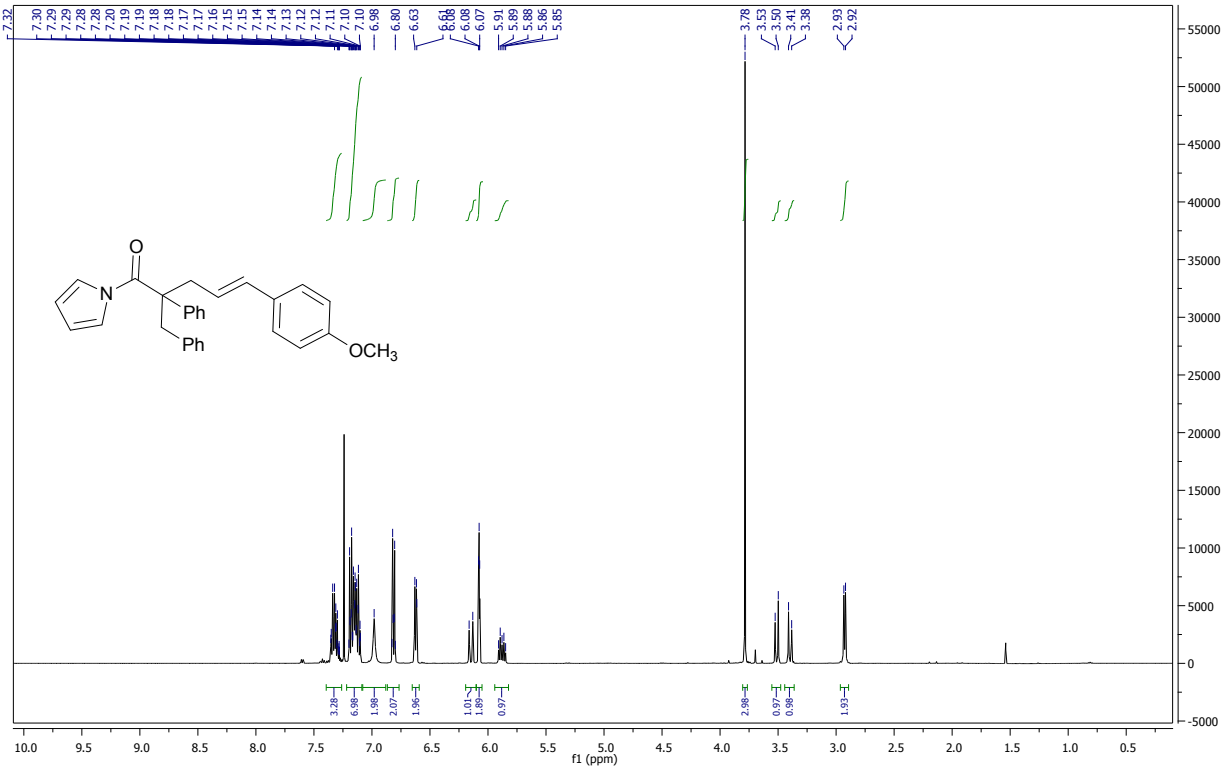
N
Ph
f1 (ppm)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7.14
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7.12
7.12
7.11
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7.10
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6.80
6.63
6.61
6.08
6.07
5.91
5.89
5.88
5.86
5.85
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3.53
3.50
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2.92
O
N
Ph
Ph
OCH3
3.28
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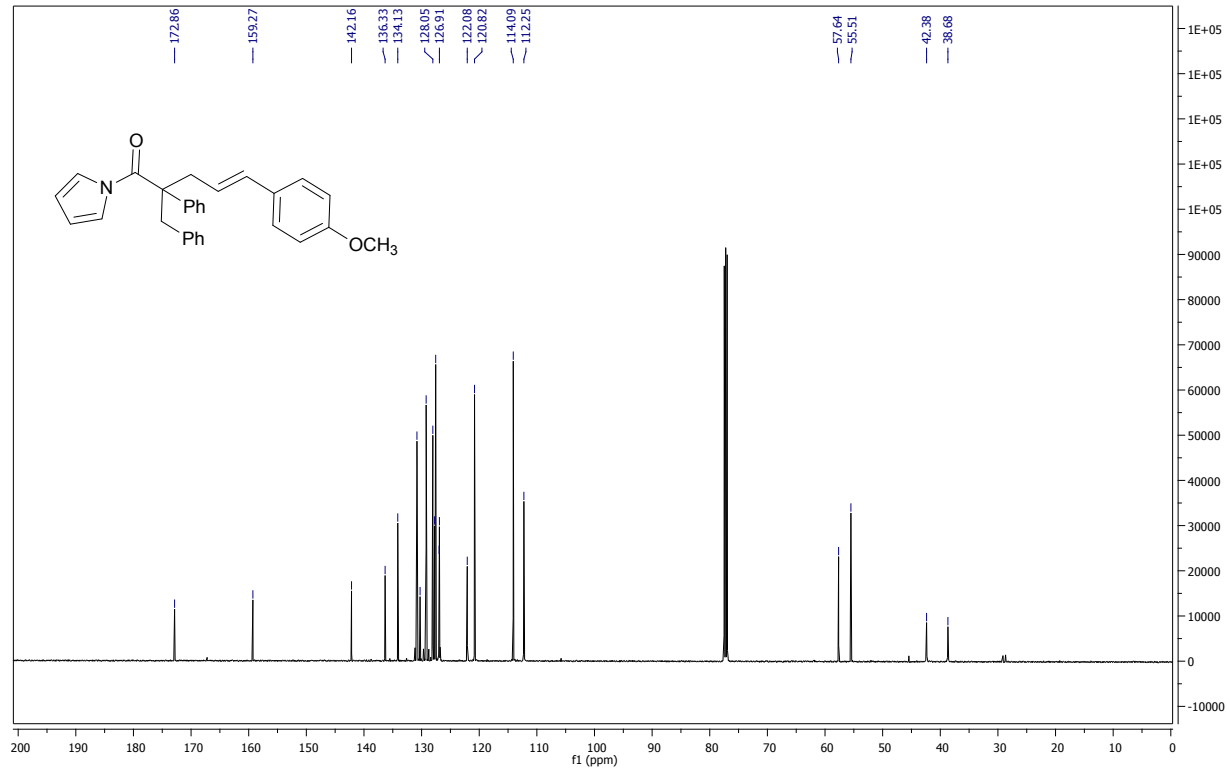
1.98
2.07
1.96
1.01
1.89
0.97
2.98
0.97
0.98
1.93
f1 (ppm)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122.08
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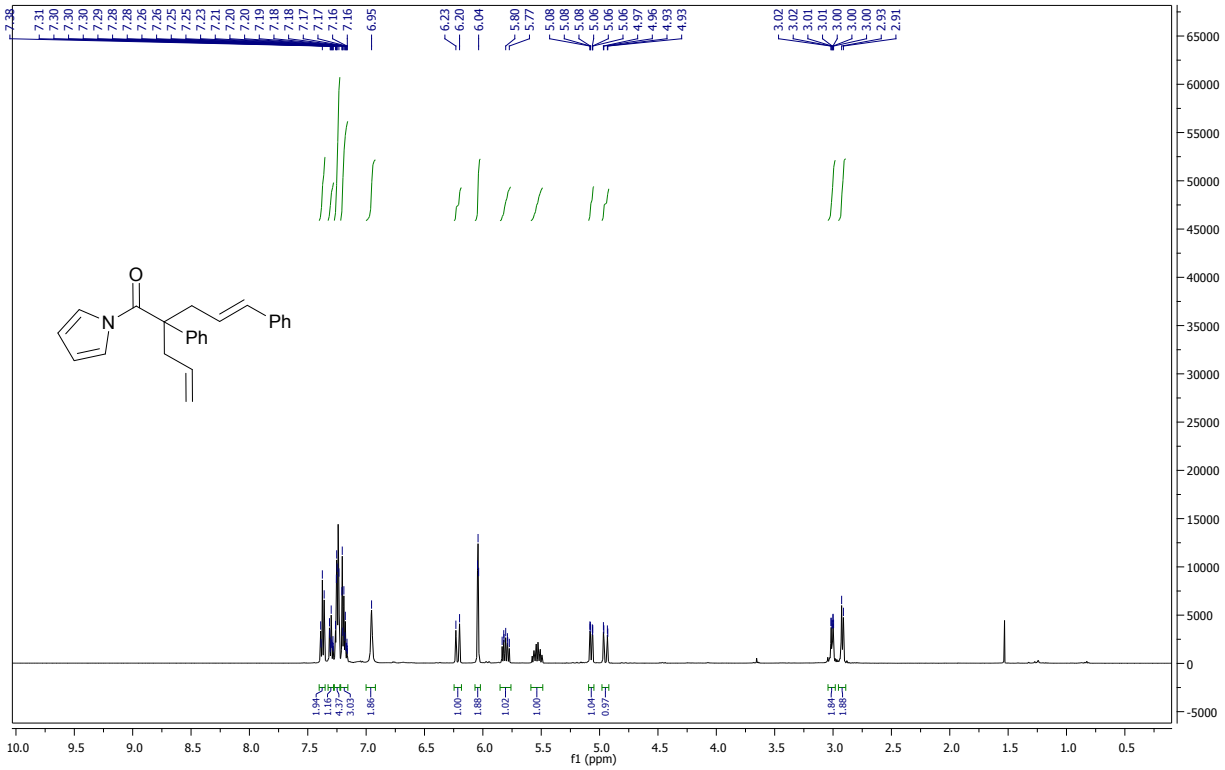
112.25
57.64
55.51
42.38
38.68
O
N
Ph
Ph
OCH3
f1 (ppm)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7.21
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7.20
7.19
7.18
7.18
7.17
7.17
7.16
7.16
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6.23
6.20
6.04
5.80
5.77
5.08
5.08
5.08
5.06
5.06
5.06
4.97
4.96
4.93
4.93
3.02
3.02
3.01
3.01
3.00
3.00
3.00
2.93
2.91
O
N
Ph
Ph
1.94
1.16
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3.03
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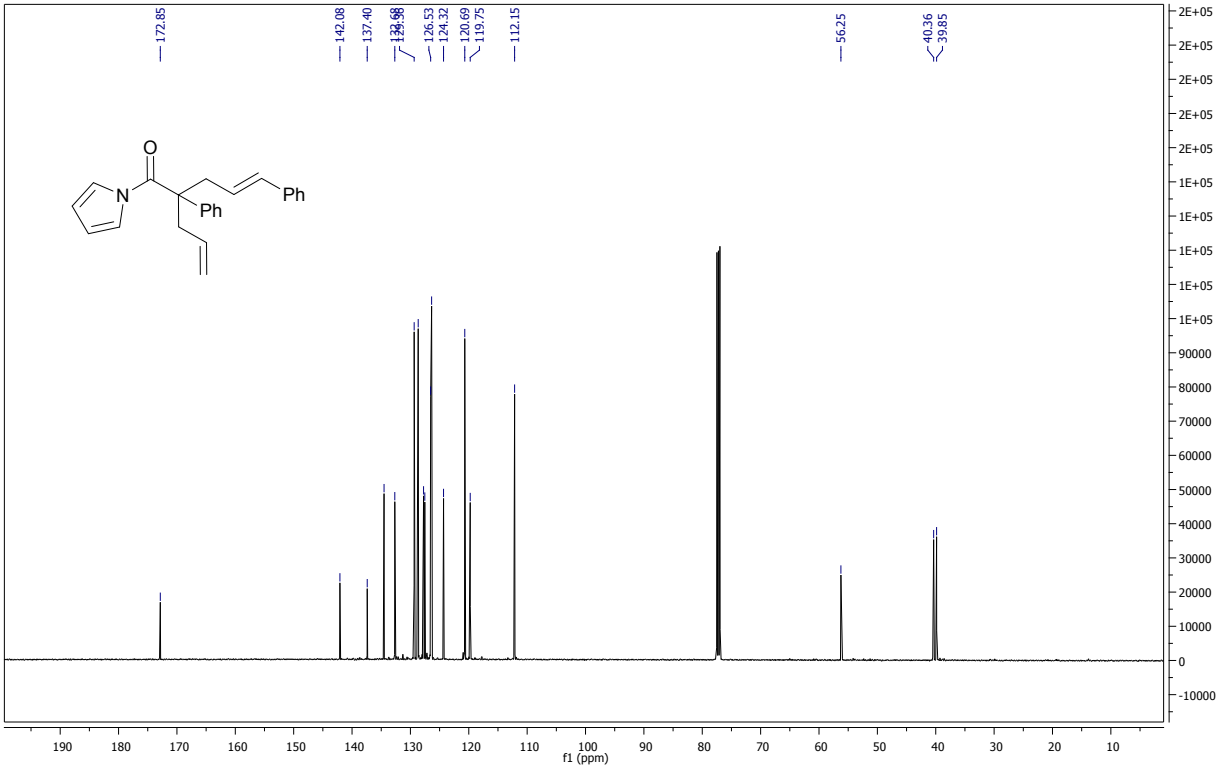
1.00
1.04
0.97
1.84
1.88
f1 (ppm)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39.85
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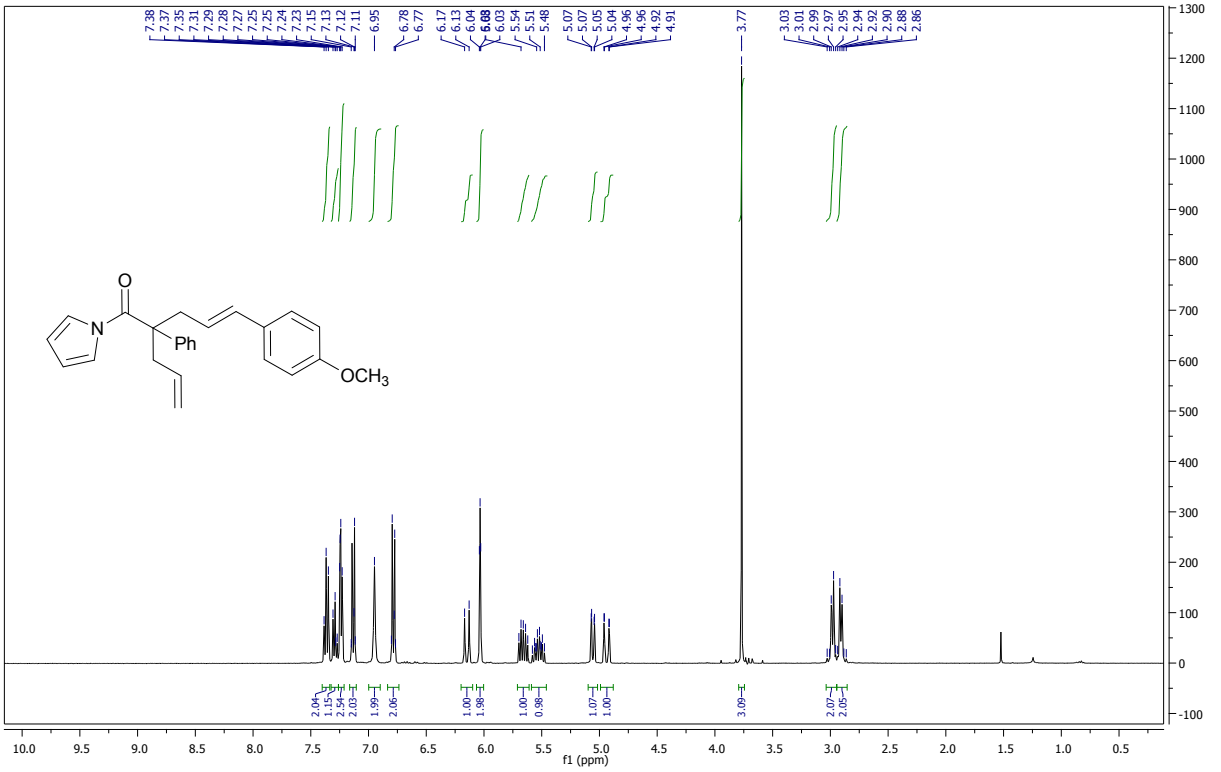
N
Ph
Ph
f1 (ppm)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7.24
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7.15
7.13
7.12
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5.07
5.05
5.04
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4.91
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3.03
3.01
2.99
2.97
2.95
2.94
2.92
2.90
2.88
2.86
O
N
Ph
OCH3
2.04
1.15
2.54
2.03
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2.06
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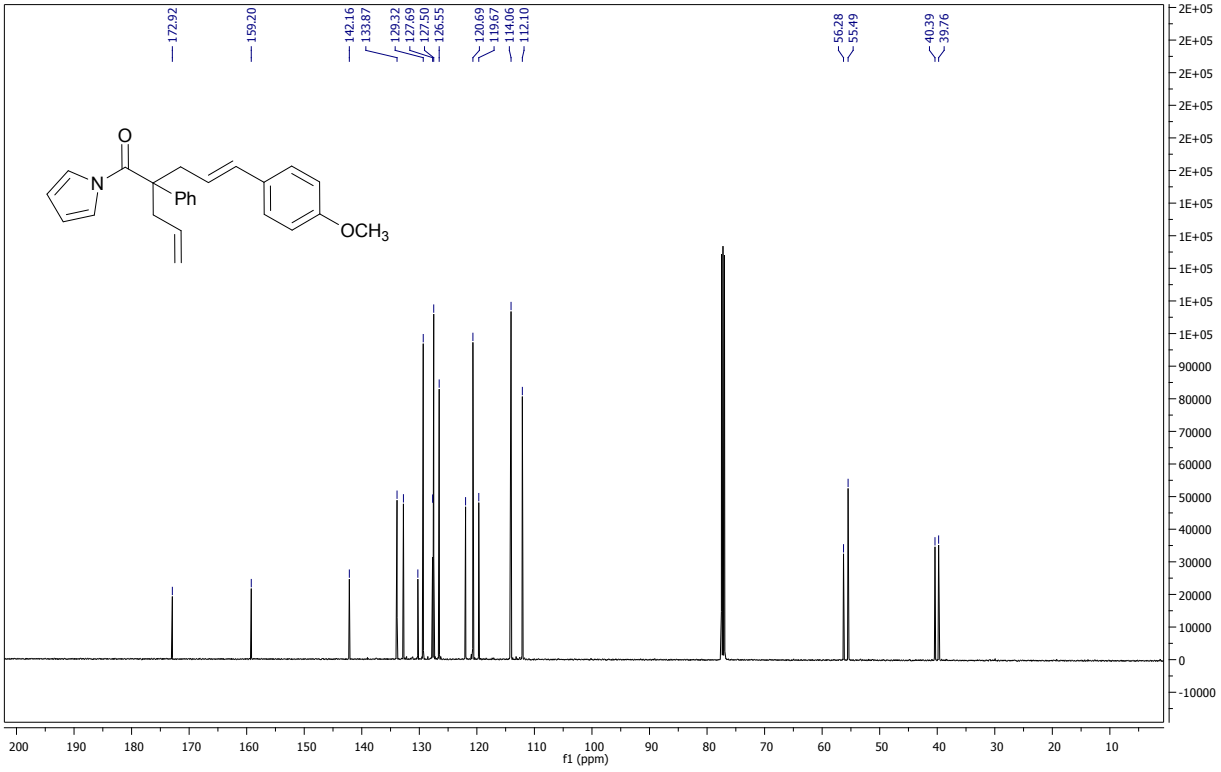
1.98
1.00
0.98
1.07
1.00
3.09
2.07
2.05
f1 (ppm)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126.55
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119.67
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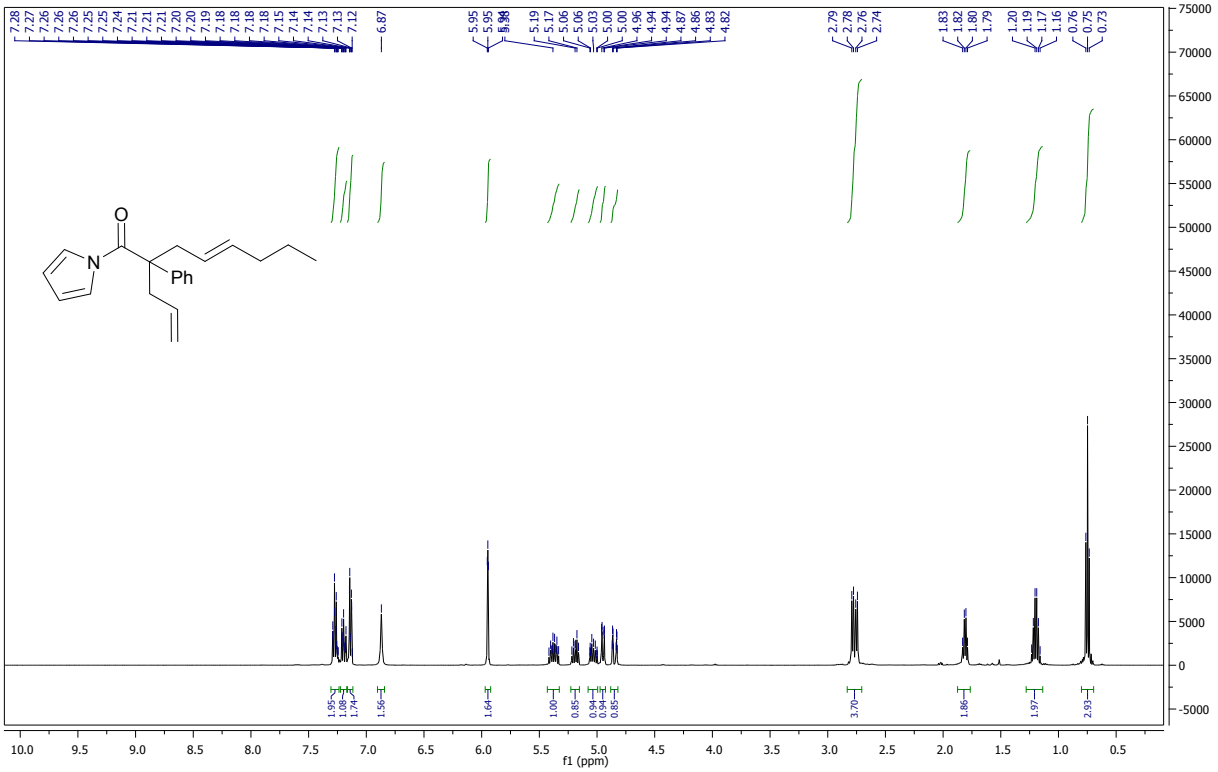
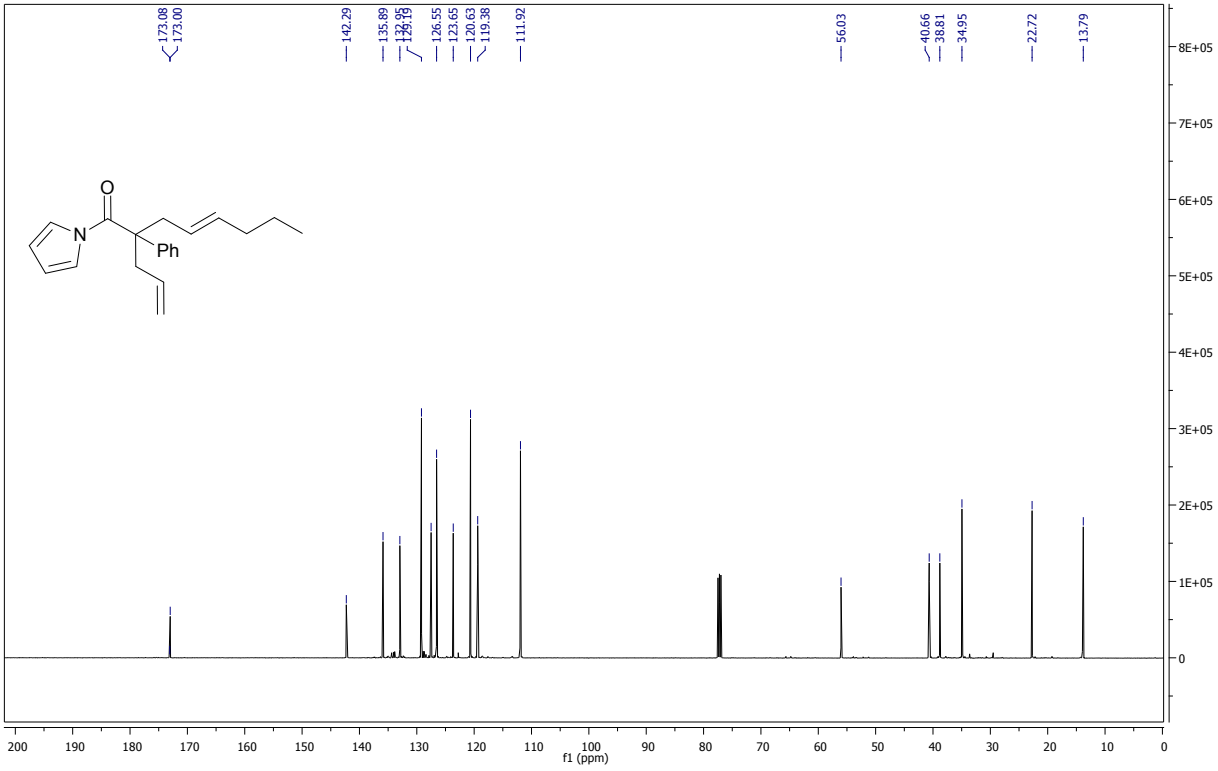
112.10
56.28
55.49
40.39
39.76
O
N
Ph
OCH3
f1 (ppm)


O
N
Ph
f1 (ppm)


O
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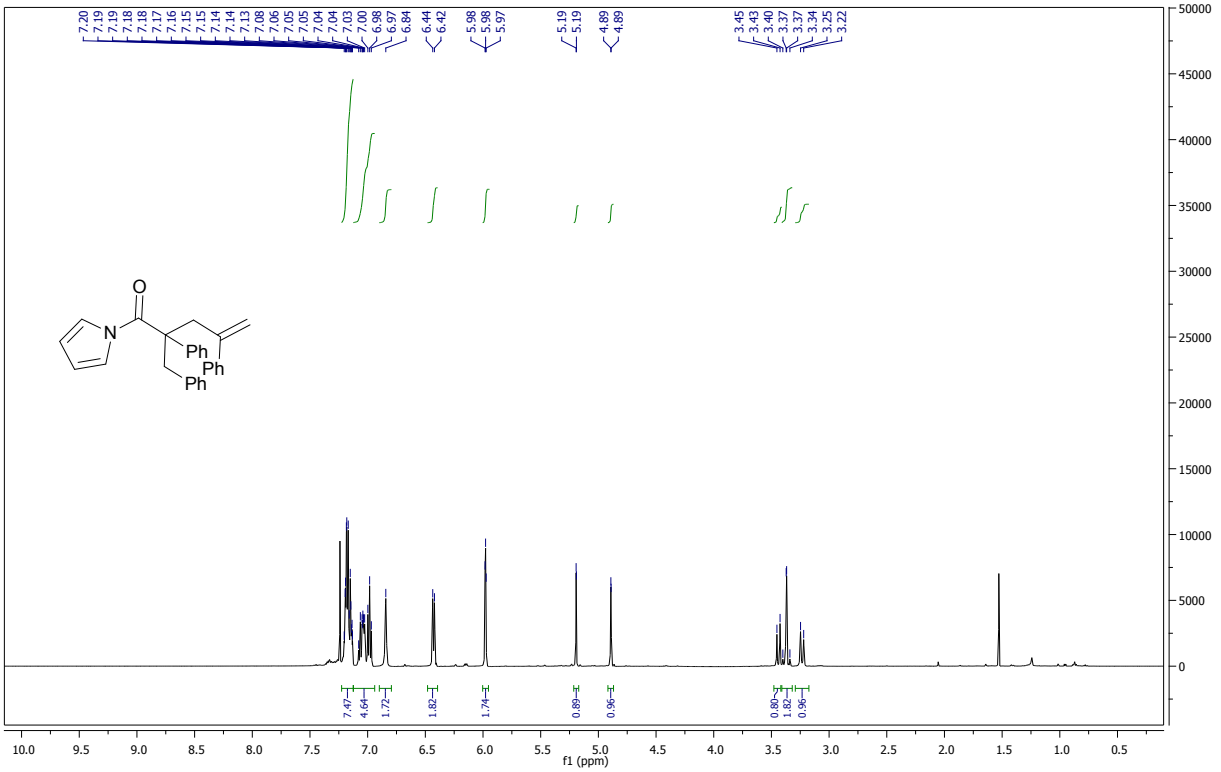
Ph
f1 (ppm)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7.05
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7.04
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7.03
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3.37
3.34
3.25
3.22
O
N
Ph
Ph
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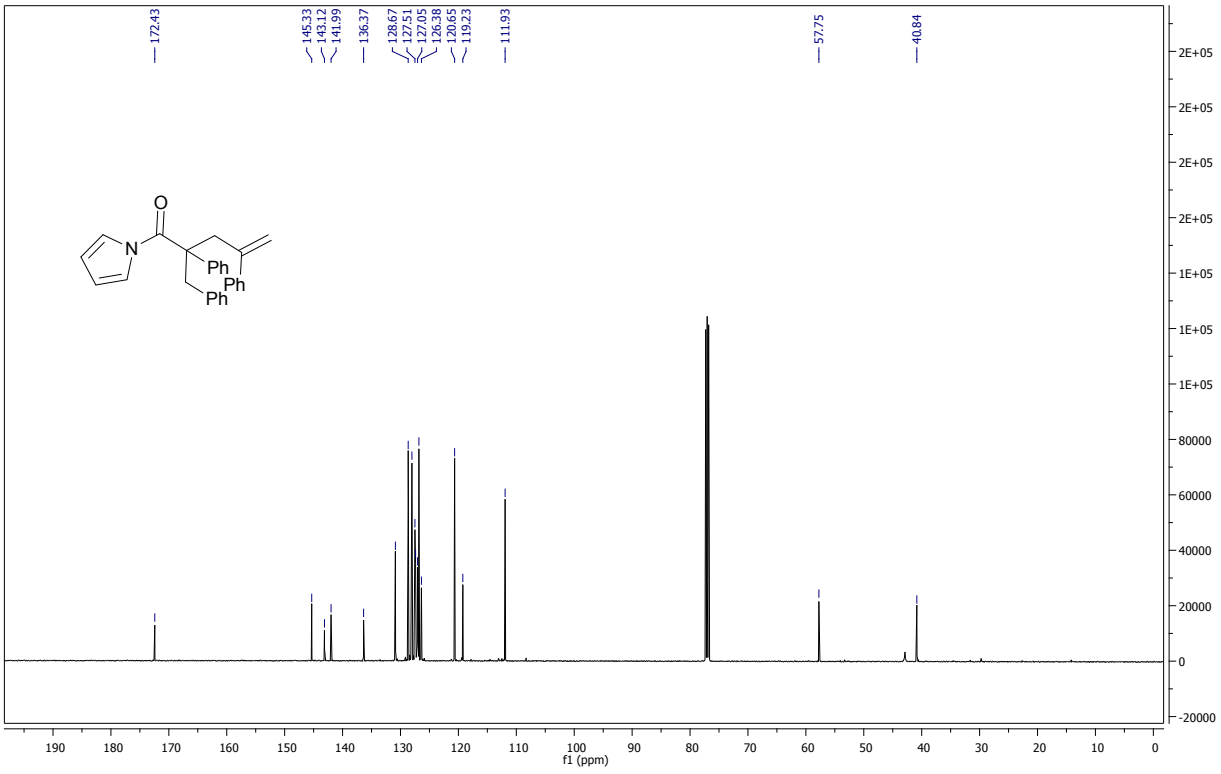
1.72
1.82
1.74
0.89
0.96
0.80
1.82
0.96
f1 (ppm)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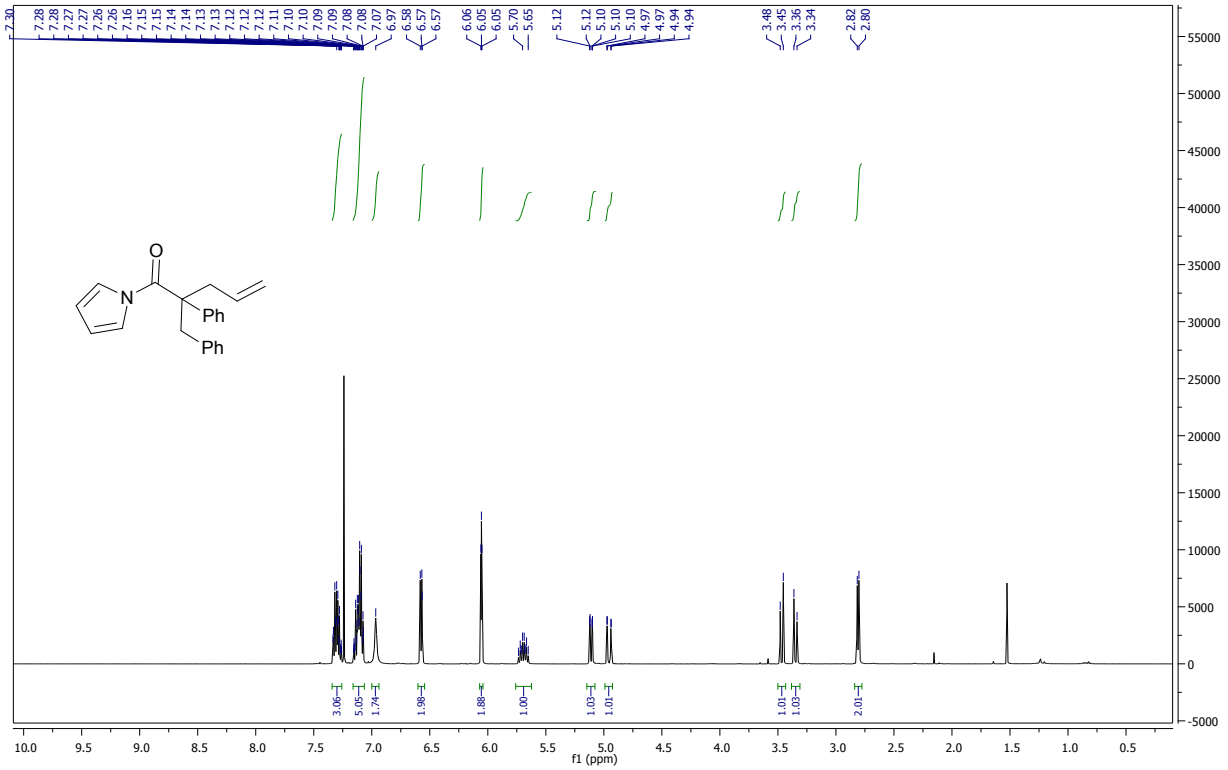
O
N
Ph
Ph
Ph
f1 (ppm)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6.06
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5.70
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5.12
5.10
5.10
5.10
4.97
4.97
4.94
4.94
3.48
3.45
3.36
3.34
2.82
2.80
O
N
Ph
Ph
3.06
5.05
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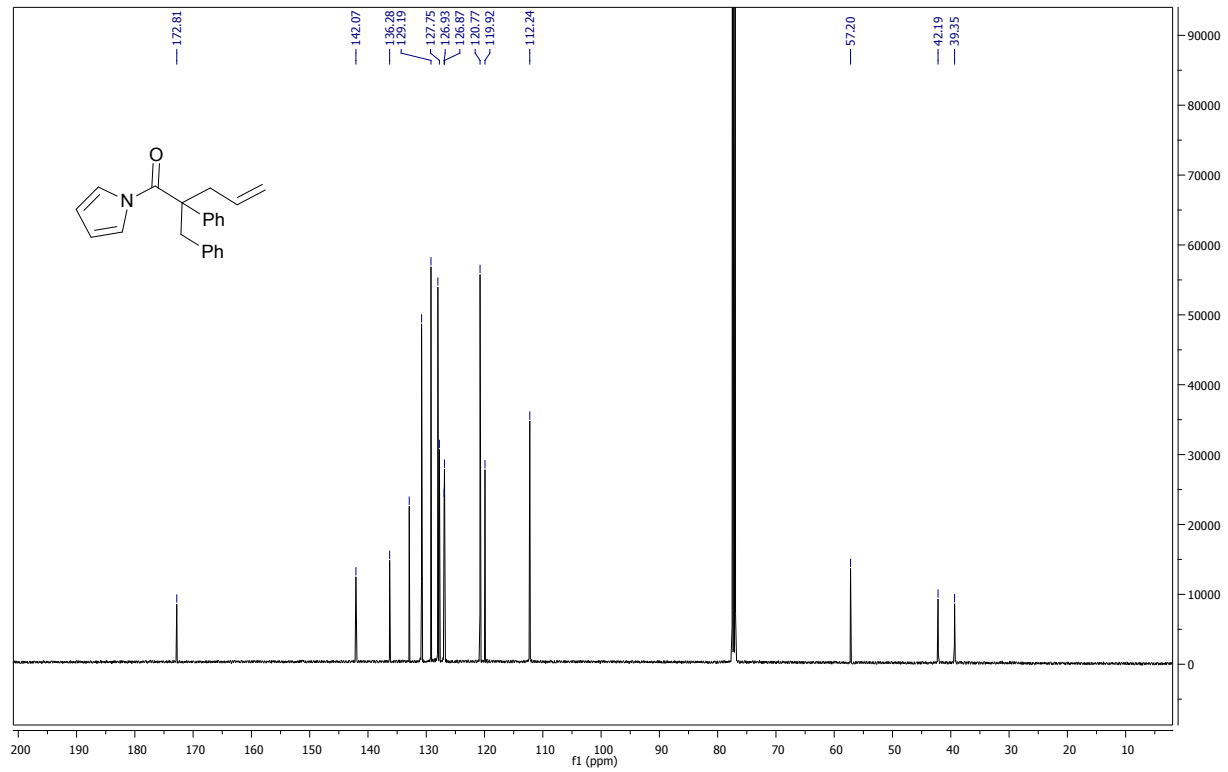
1.98
1.88
1.00
1.03
1.01
1.01
1.03
2.01
f1 (ppm)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112.24
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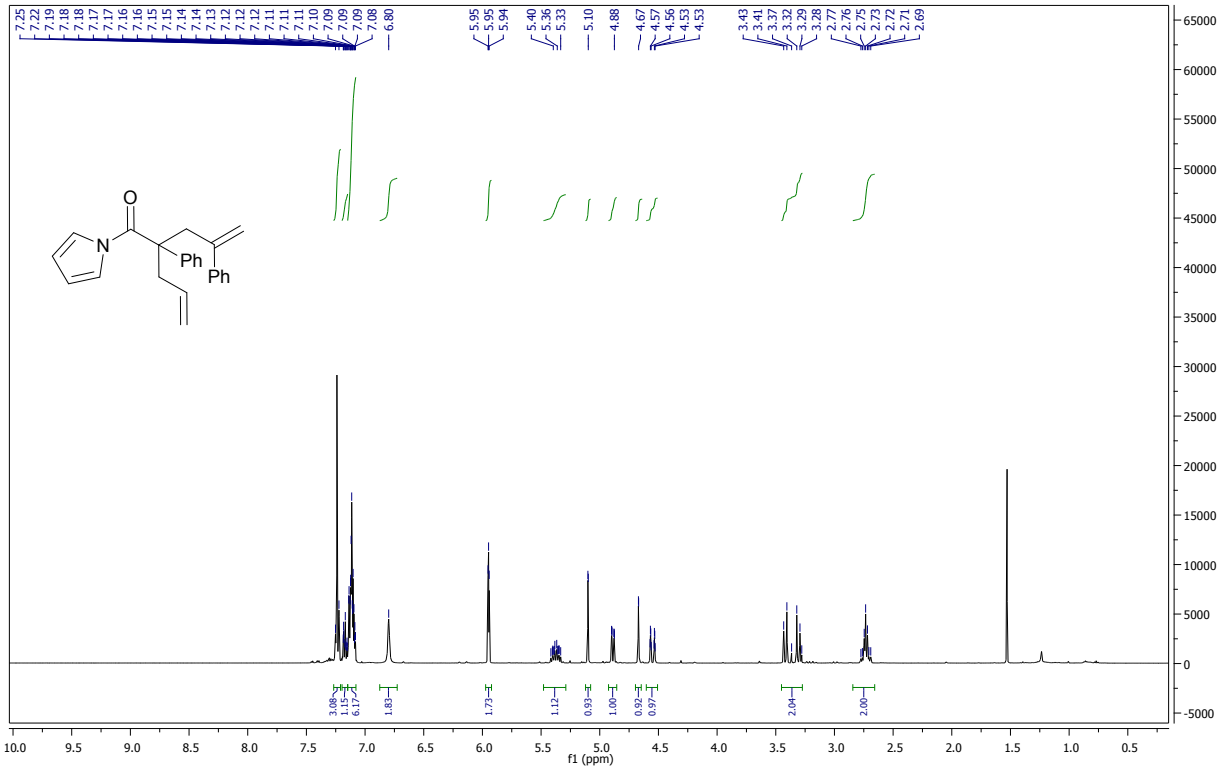
39.35
O
N
Ph
Ph
f1 (ppm)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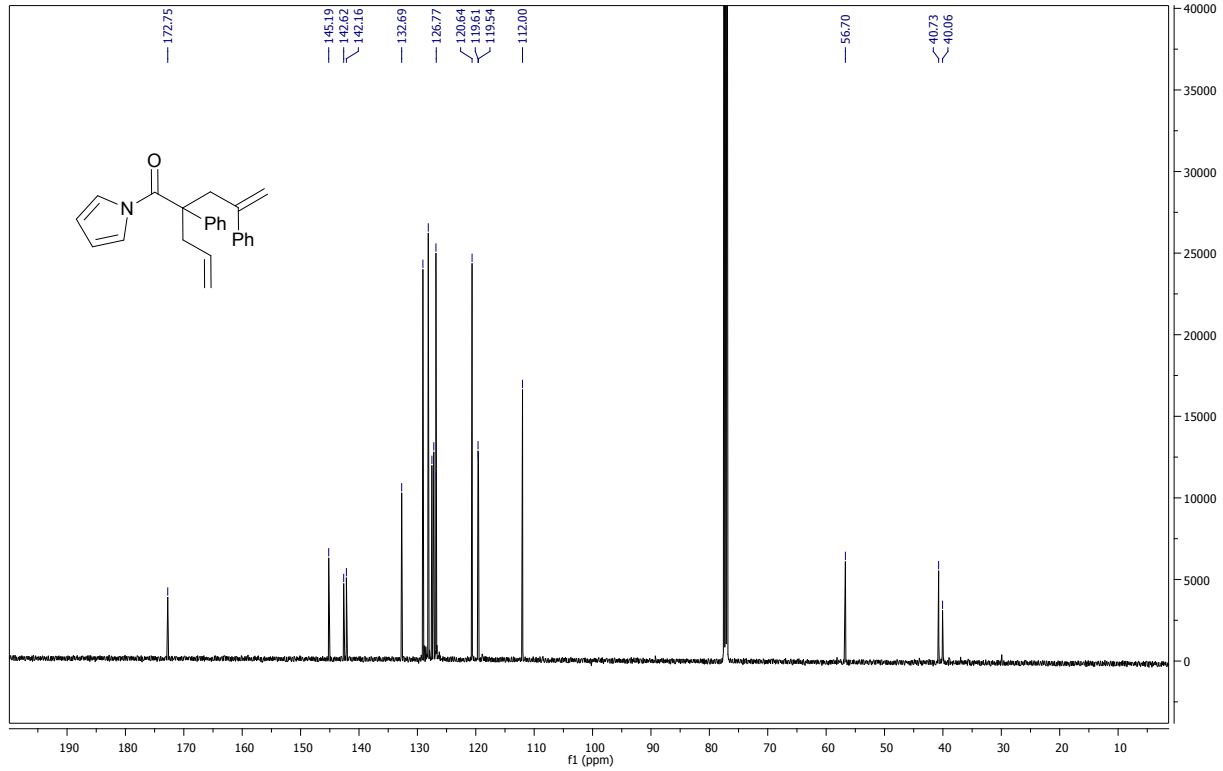
5.95 5.95 5.94 5.40 5.36 5.33 5.10 4.88 4.67 4.57 4.56 4.53 4.53
3.43 3.41 3.37 3.32 3.29 3.28 2.77 2.76 2.75 2.73 2.72 2.71 2.69
O
N
Ph
Ph
3.08 1.15 6.17 1.83 1.73 1.12 0.93 1.00 0.92 0.97 2.04 2.00
f1 (ppm)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56.70 40.73 40.06
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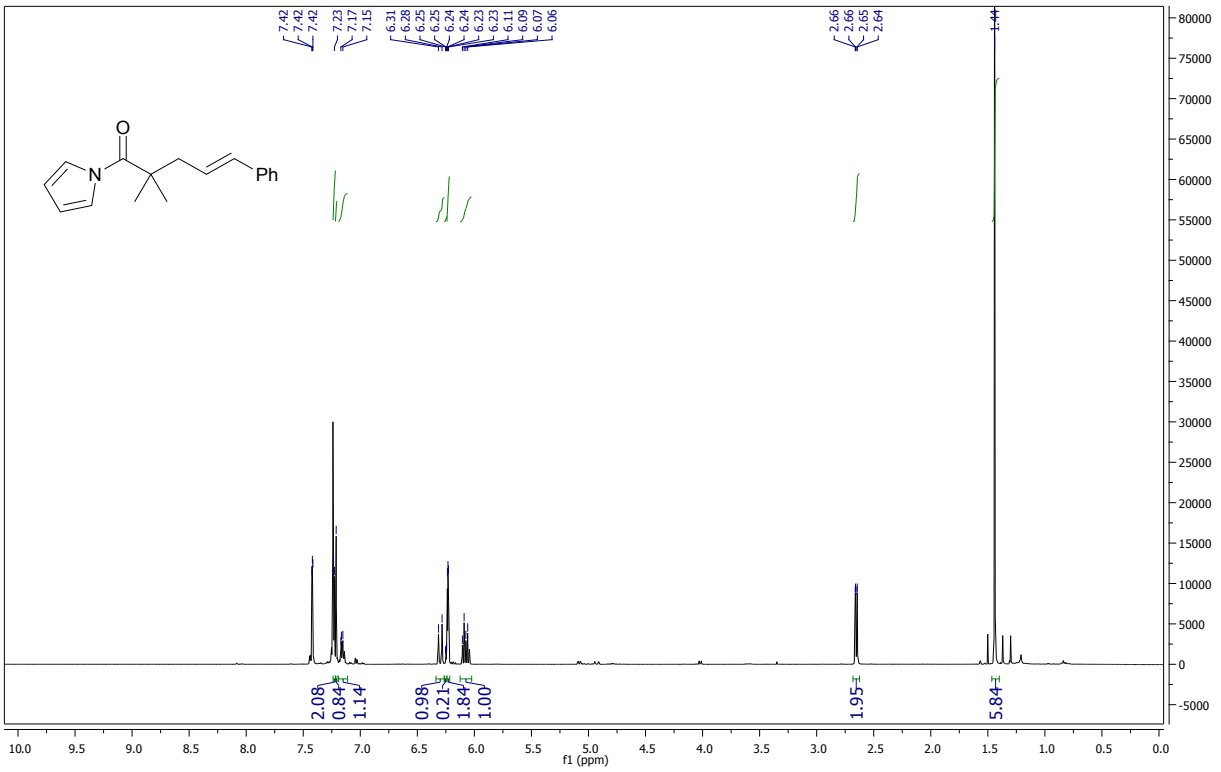
N
Ph
Ph
f1 (ppm)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7.42
7.42
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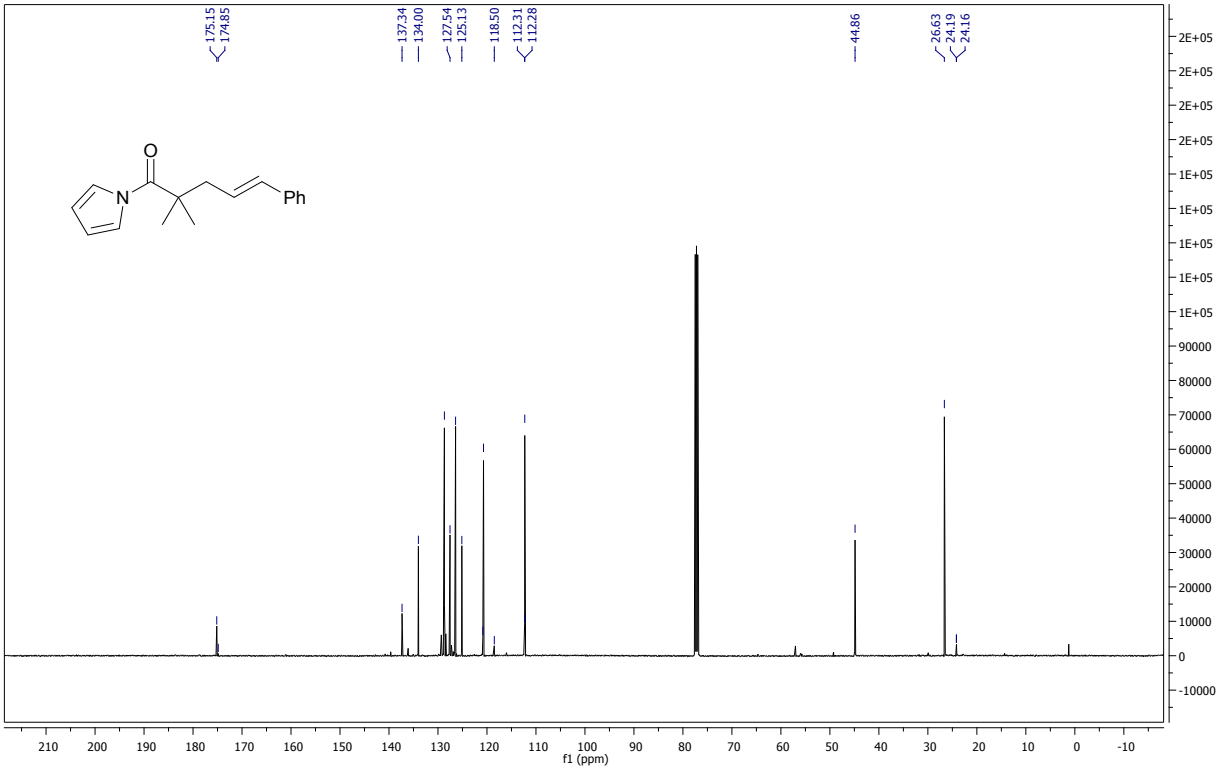
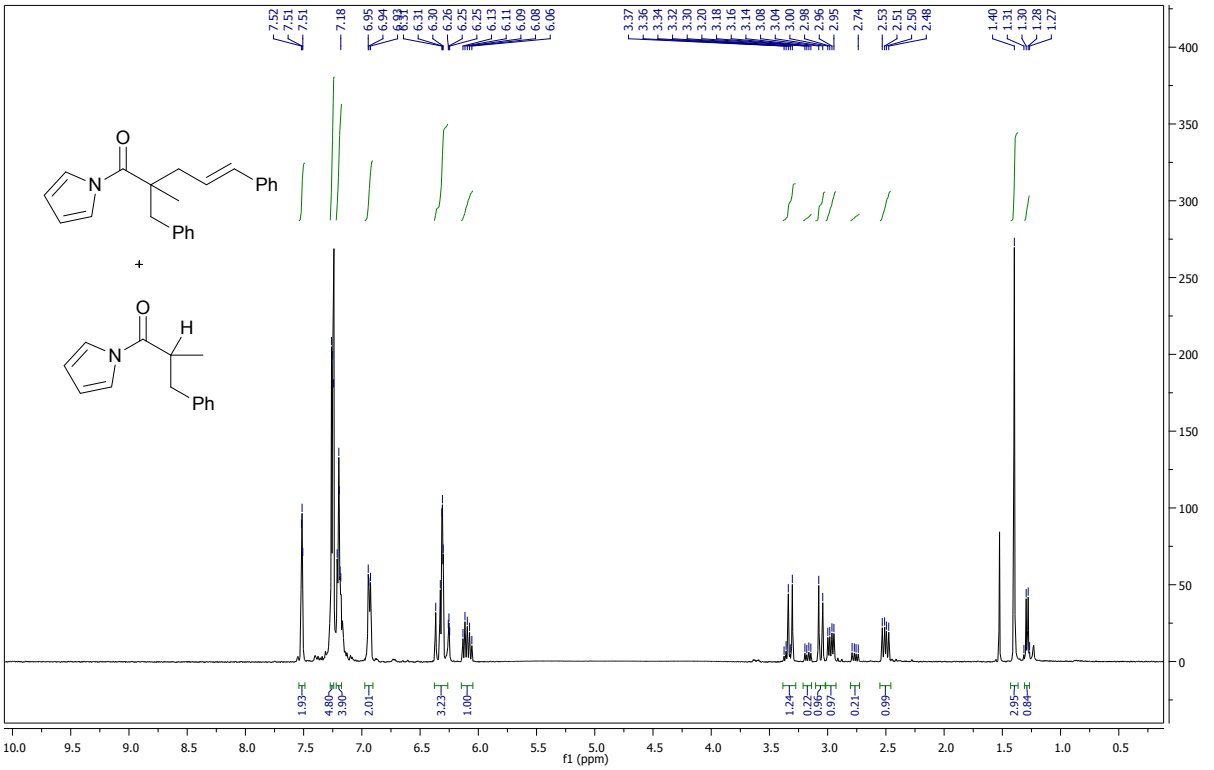
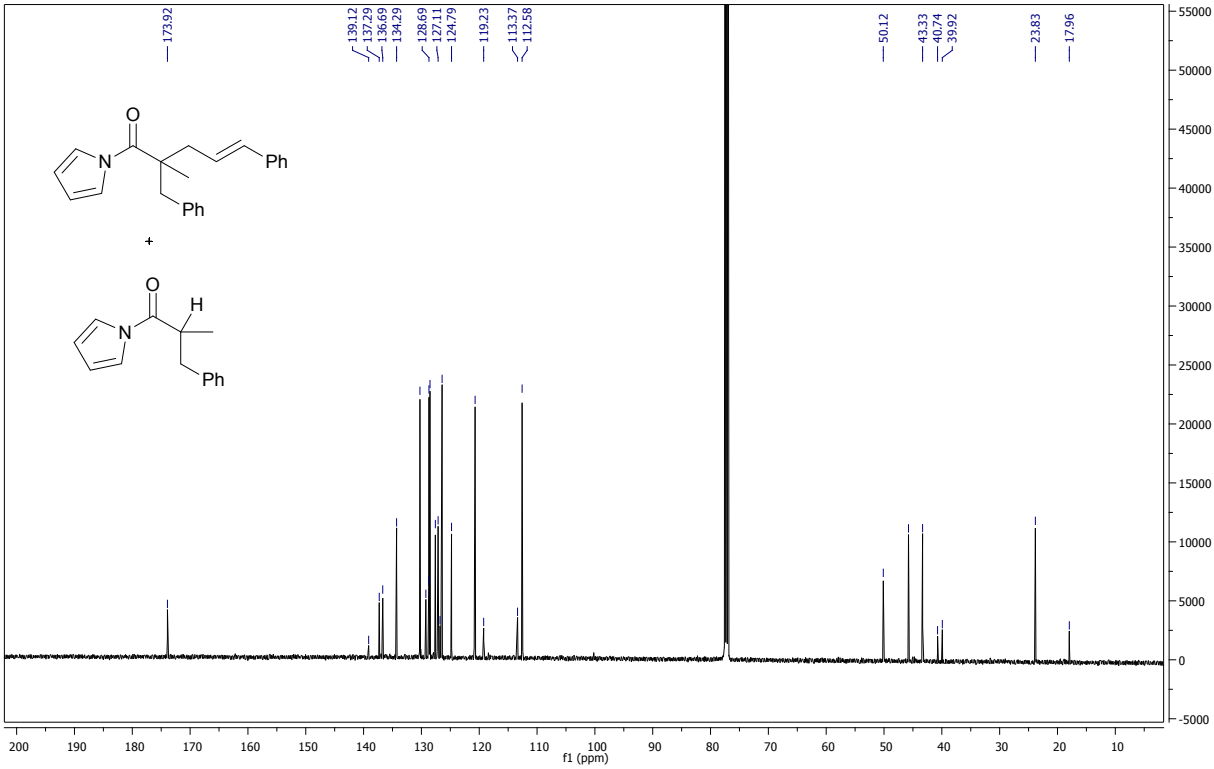
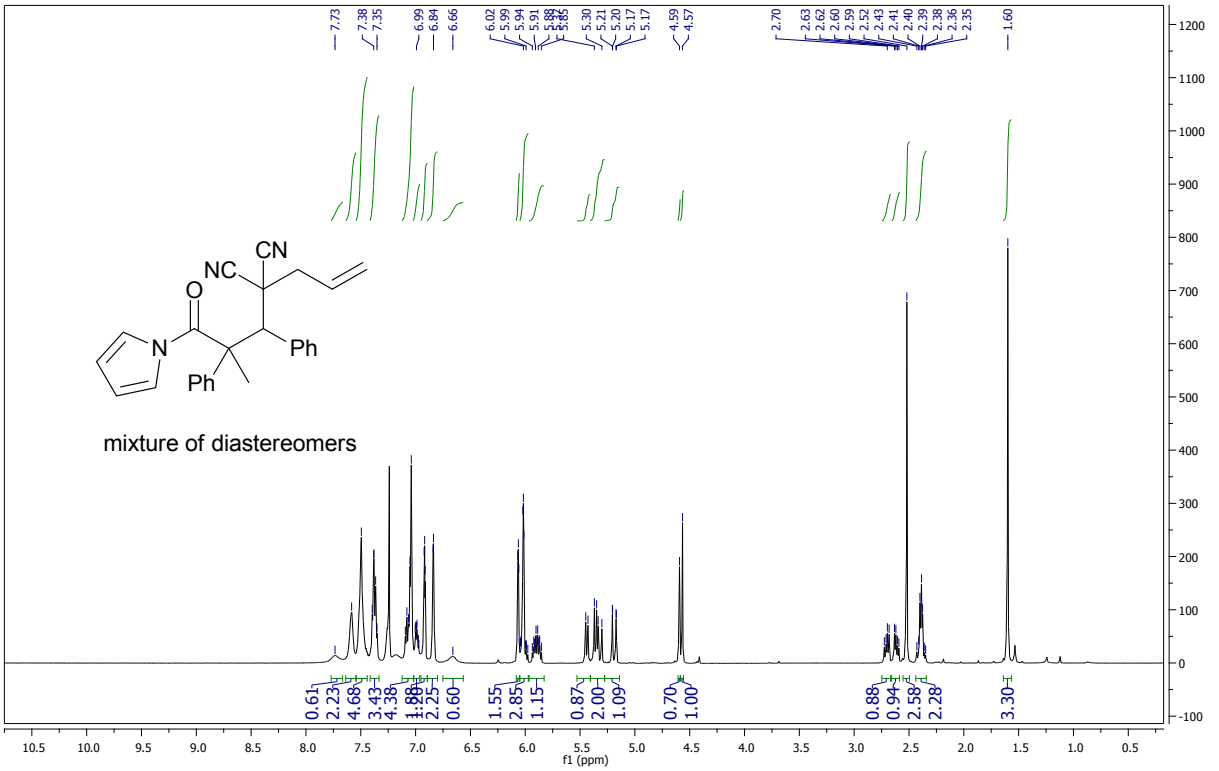
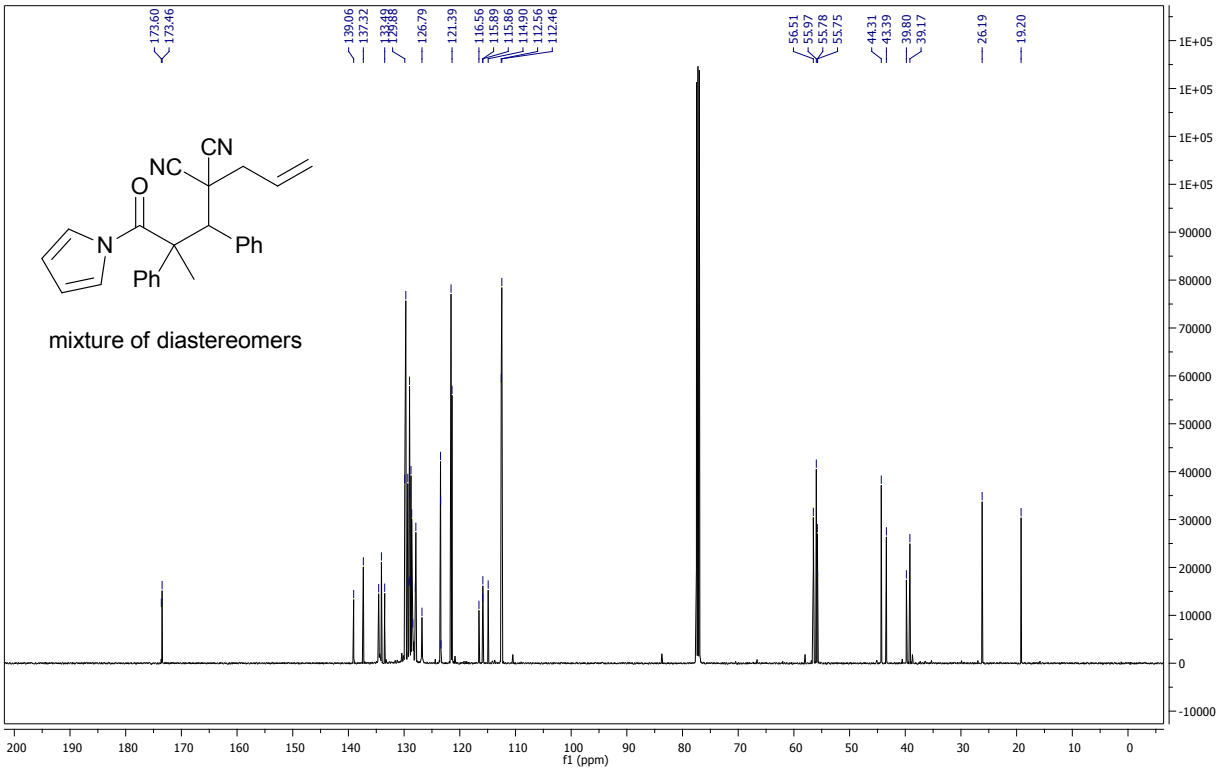
7.15
6.31
6.28
6.25
6.25
6.24
6.24
6.23
6.23
6.11
6.09
6.07
6.06
2.66
2.66
2.65
2.64
1.44
O
N
Ph
2.08
0.84
1.14
0.98
0.21
1.84
1.00
1.95
5.84
f1 (ppm)

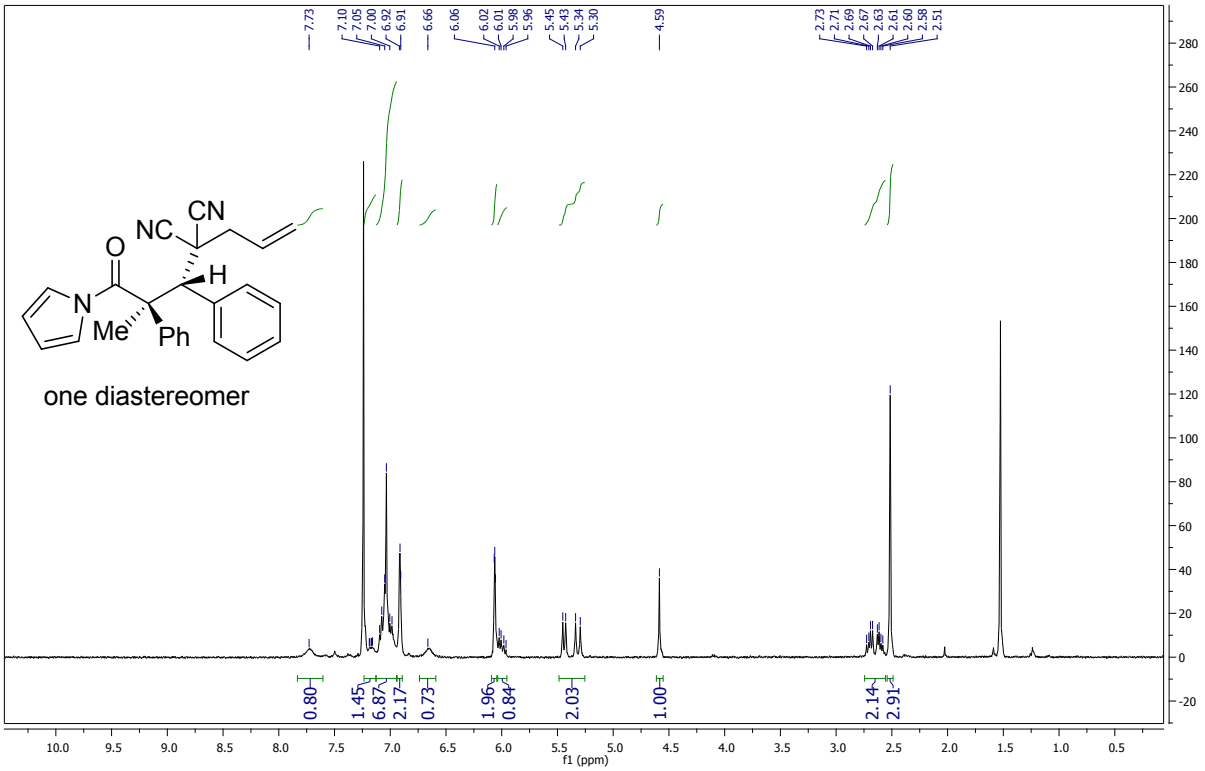

175.15
174.85
137.34
134.00
127.54
125.13
118.50
112.31
112.28
44.86
26.63
24.19
24.16
O
N
Ph
f1 (ppm)

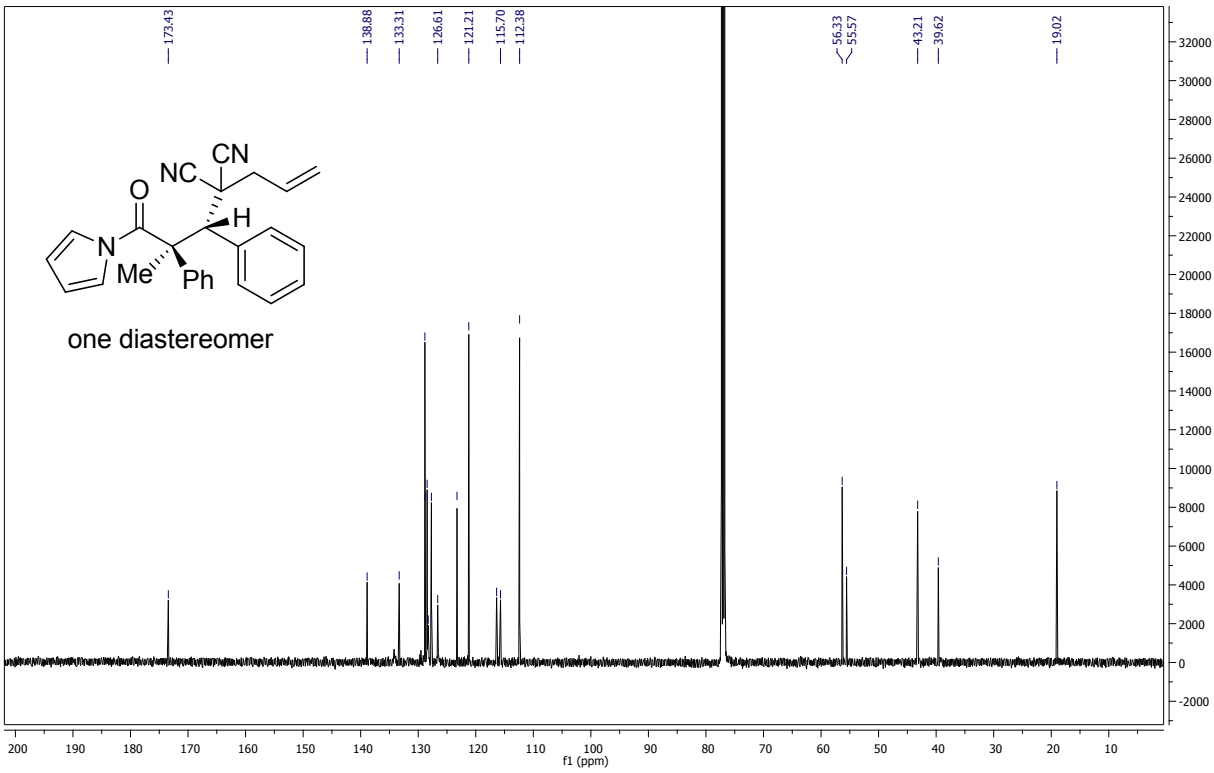

7.52
7.51
7.51
7.18
6.95
6.94
6.93
6.31
6.30
6.26
6.25
6.13
6.11
6.09
6.08
6.06
3.37
3.36
3.34
3.32
3.30
3.20
3.18
3.16
3.14
3.08
3.04
3.00
2.98
2.96
2.95
2.74
2.53
2.51
2.50
2.48
1.40
1.31
1.30
1.28
1.27
O
N
Ph
Ph
+
O
H
N
Ph
1.93
4.80
3.90
2.01
3.23
1.00
1.24
0.22
0.96
0.97
0.21
0.99
2.95
0.84
f1 (ppm)

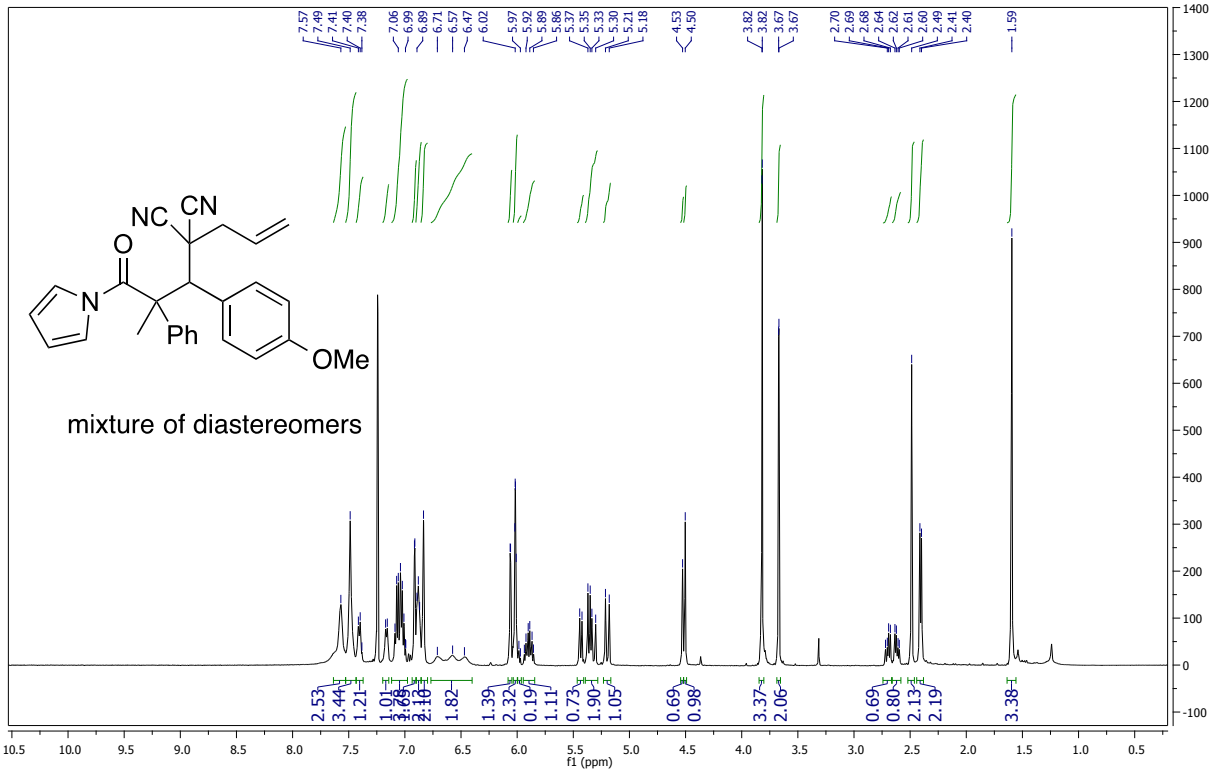

173.92
139.12
137.29
136.69
134.29
128.69
127.11
124.79
119.23
113.37
112.58
50.12
43.33
40.74
39.92
23.83
17.96
O
N
Ph
Ph
+
O
H
N
Ph
f1 (ppm)

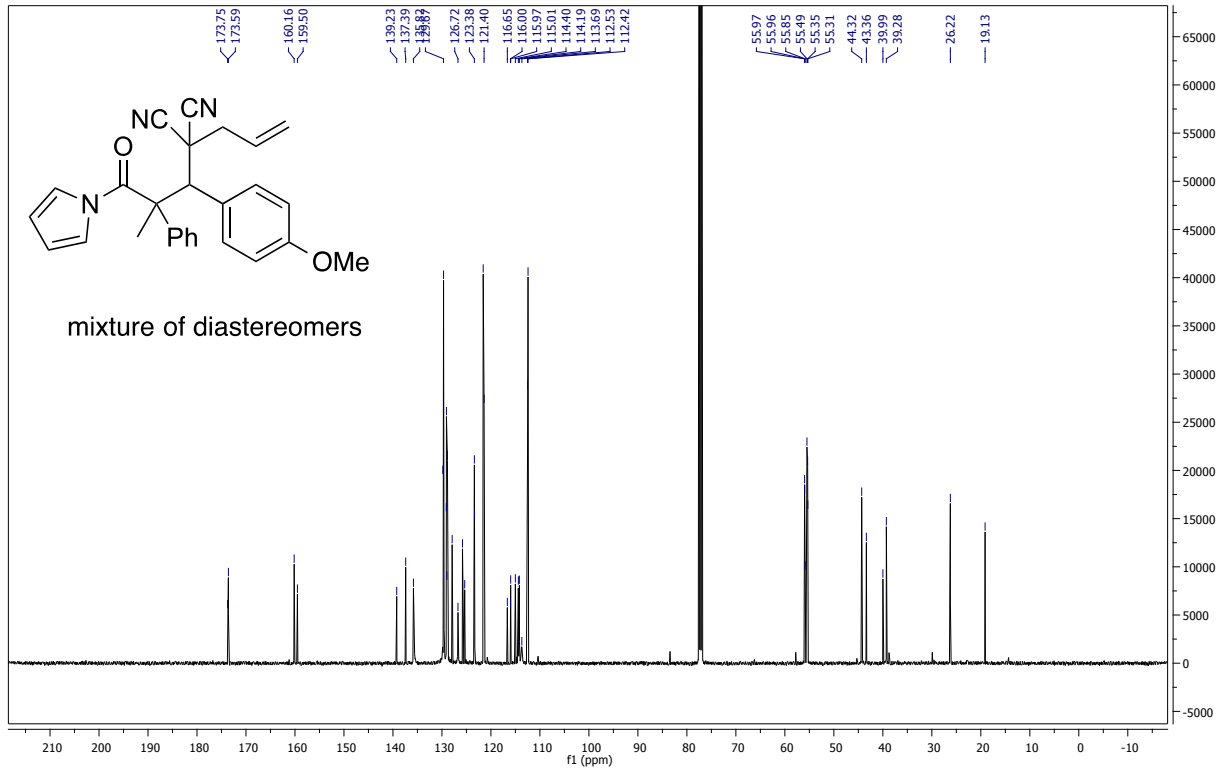

CN
NC
O
N
Ph
Ph
mixture of diastereomers
f1 (ppm)

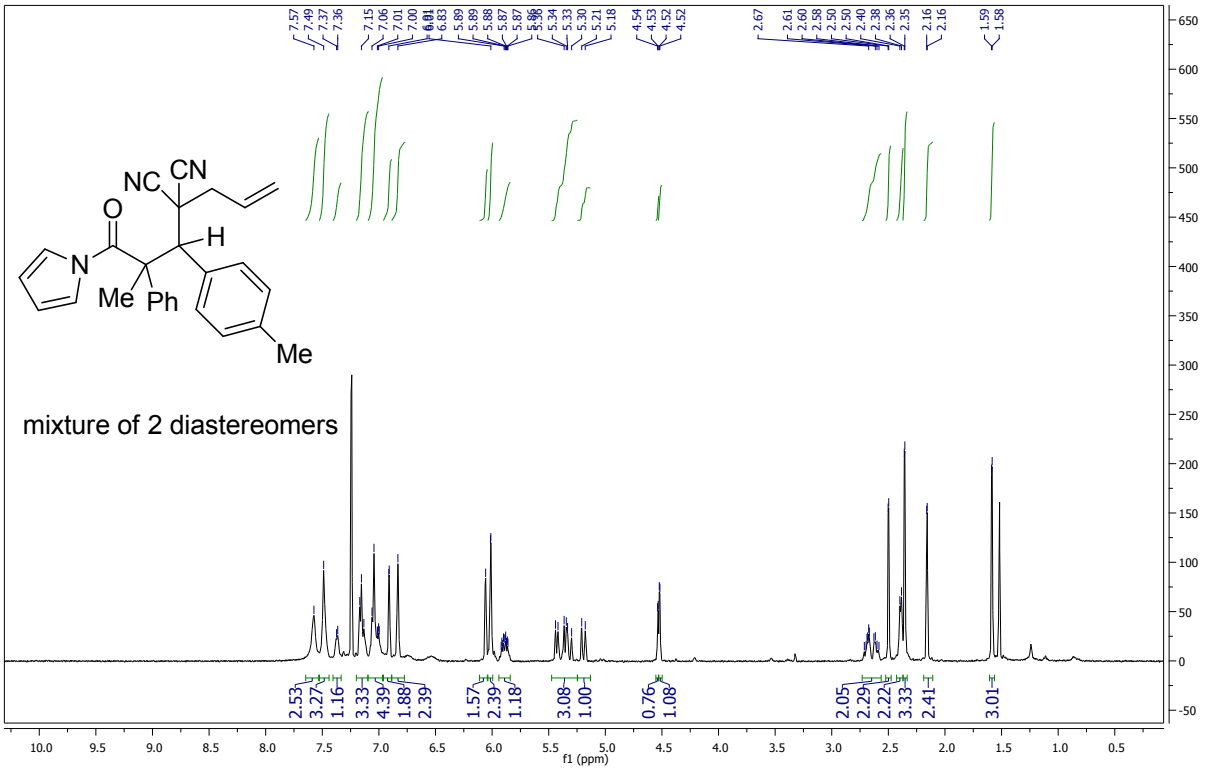

CN
NC
O
N
Ph
Ph
mixture of diastereomers
f1 (ppm)

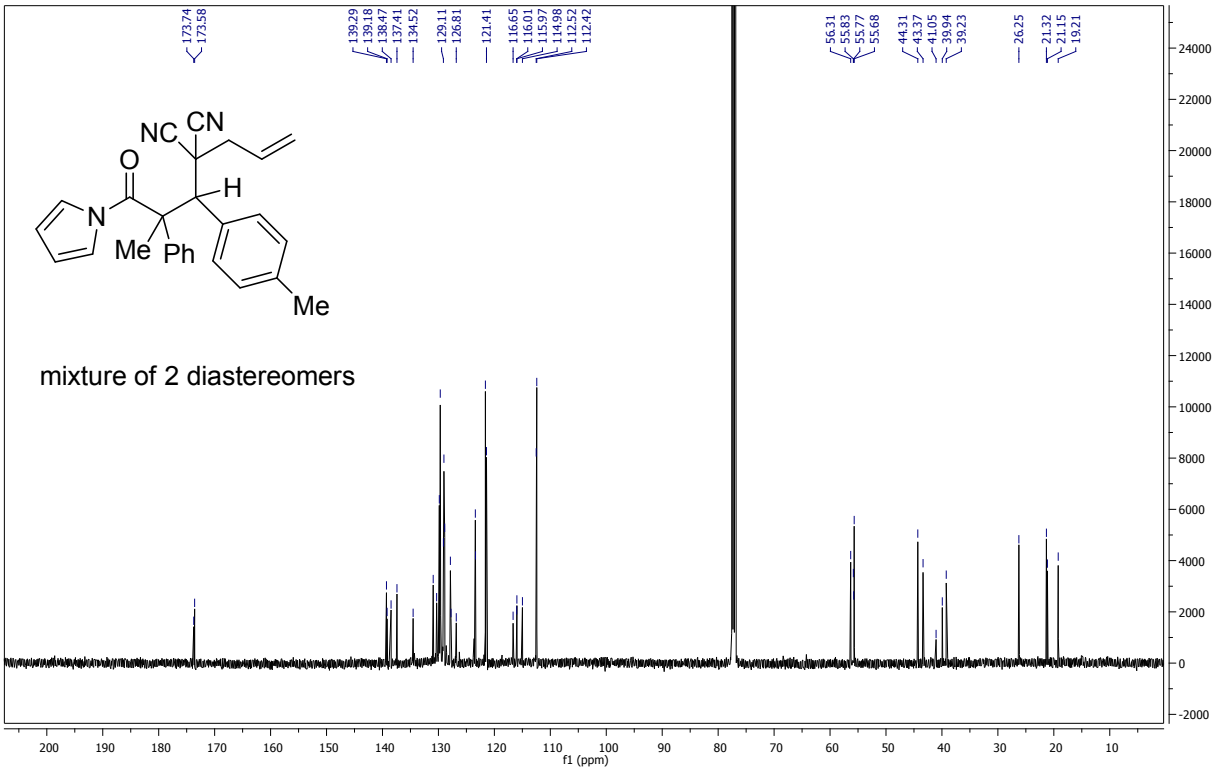

7.73
7.10
7.05
7.00
6.92
6.91
6.66
6.06
6.02
6.01
5.98
5.96
5.45
5.43
5.34
5.30
4.59
2.73
2.71
2.69
2.67
2.63
2.61
2.60
2.58
2.51
CN
NC
O
H
N
Me
Ph
one diastereomer
0.80
1.45
6.87
2.17
0.73
1.96
0.84
2.03
1.00
2.14
2.91
f1 (ppm)

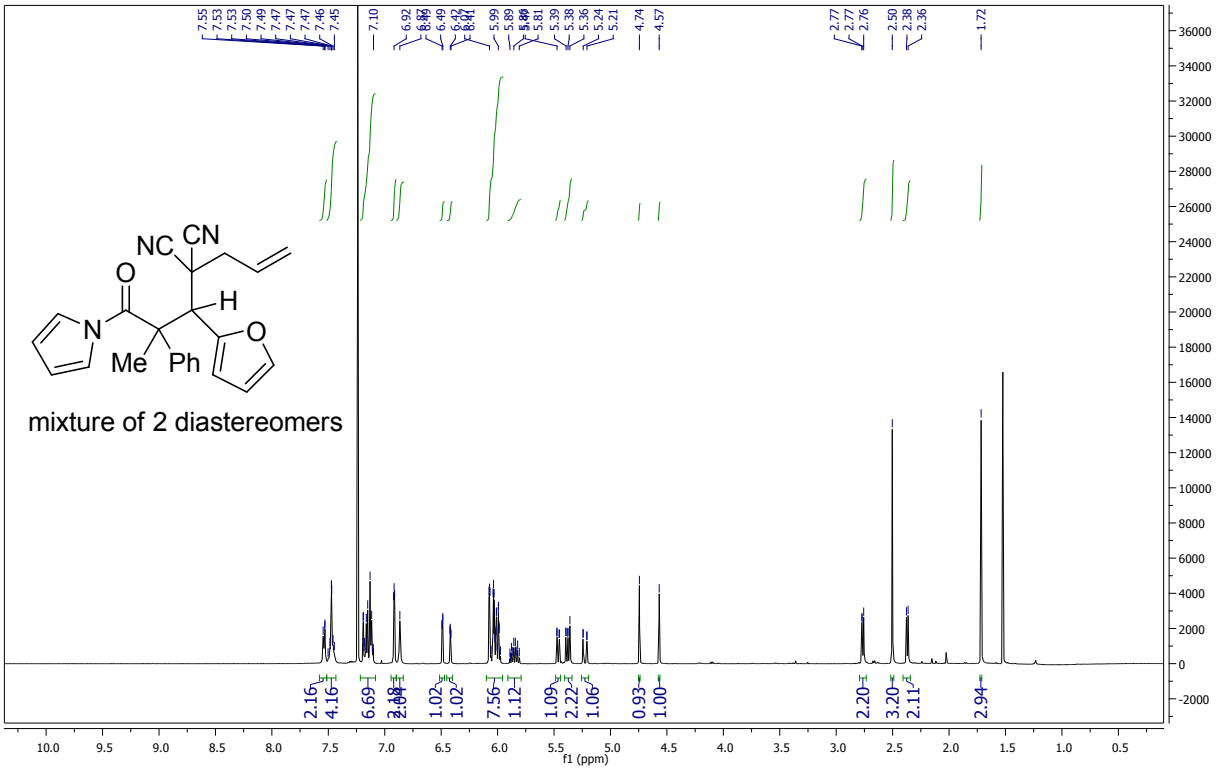

173.43
138.88
133.31
126.61
121.21
115.70
112.38
56.33
55.57
43.21
39.62
19.02
CN
NC
O
H
N
Me
Ph
one diastereomer
f1 (ppm)

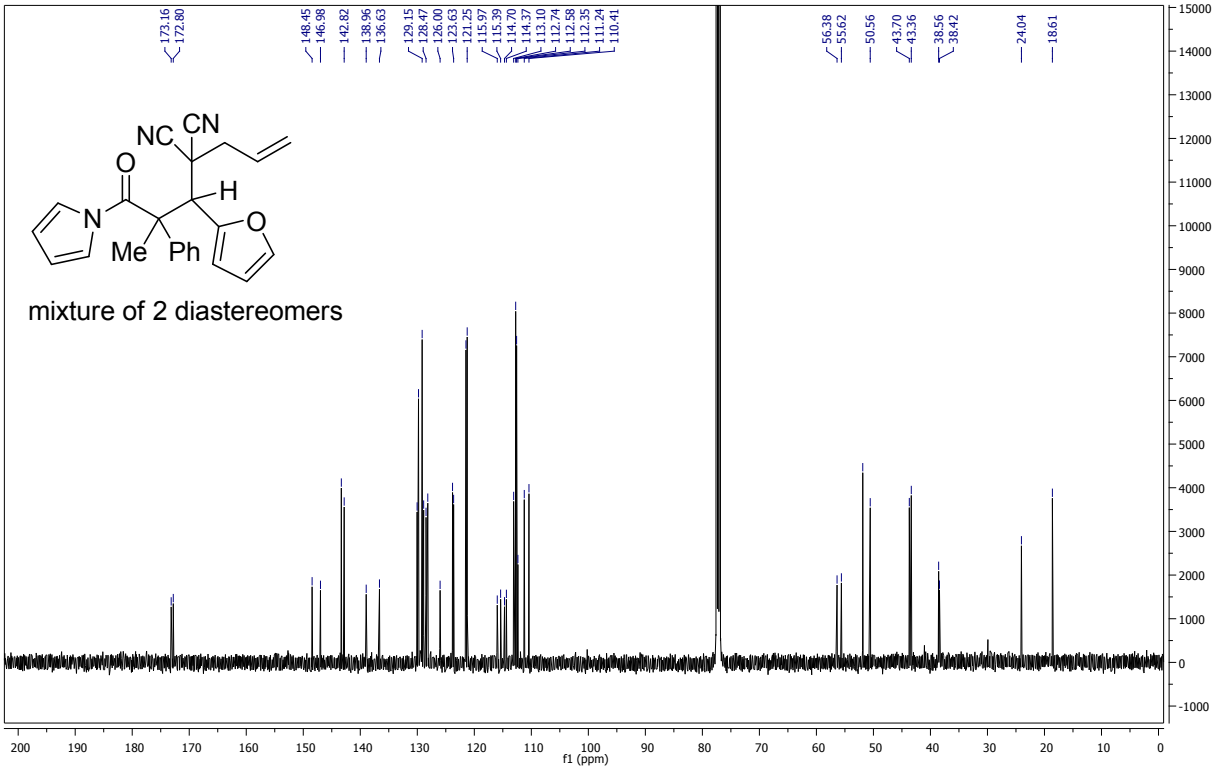

NC
CN
O
N
Ph
OMe
mixture of diastereomers
f1 (ppm)

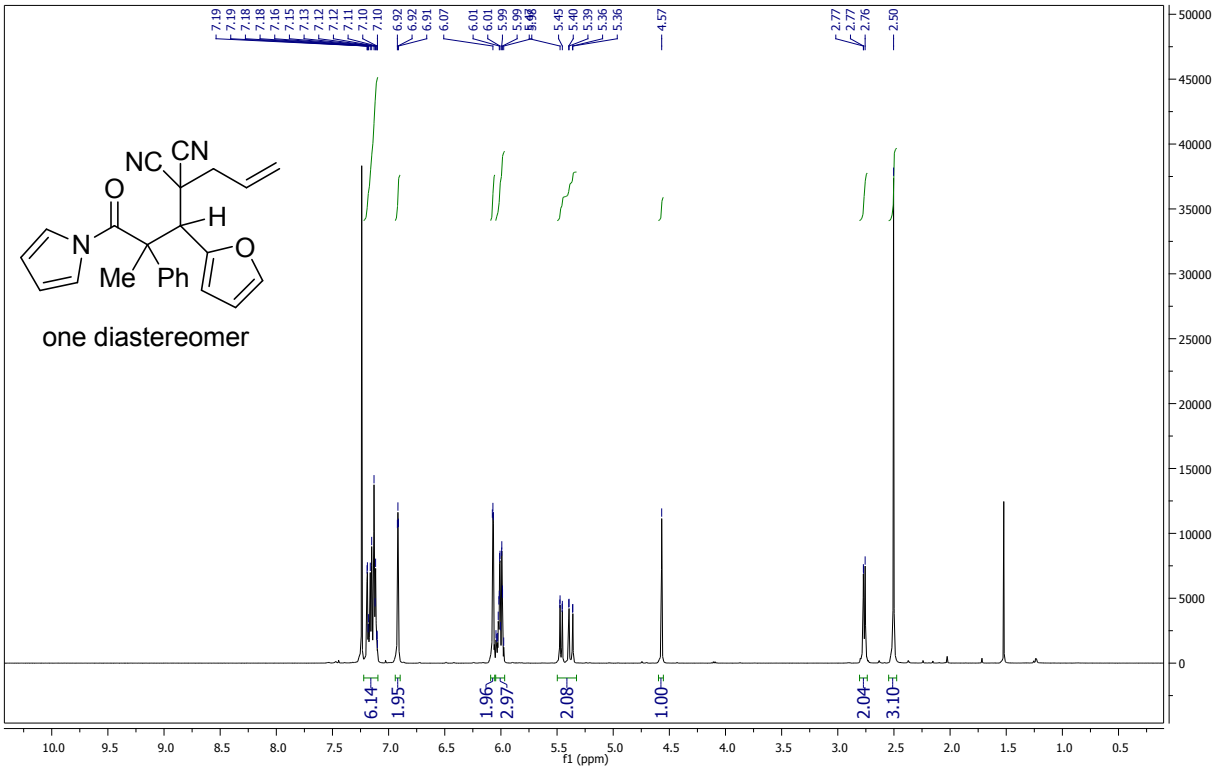

NC
CN
O
N
Ph
OMe
mixture of diastereomers
f1 (ppm)

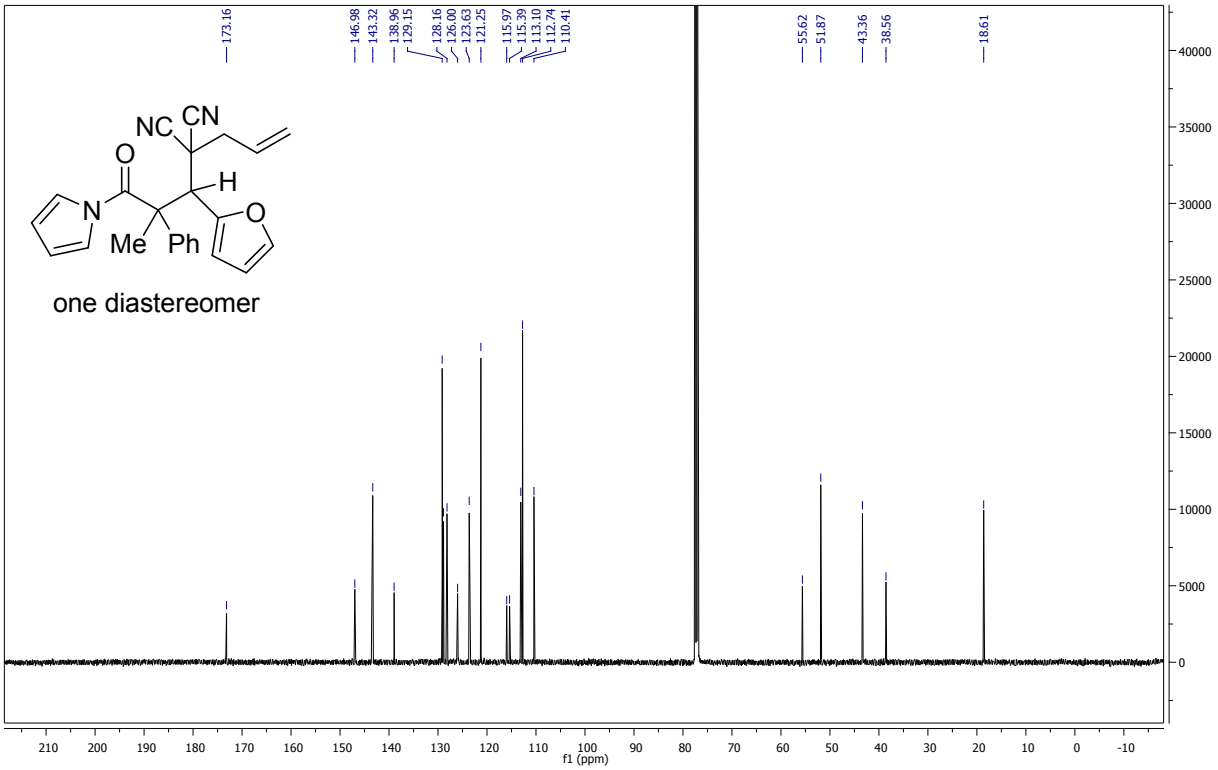

NC
CN
O
H
N
Me
Ph
Me
mixture of 2 diastereomers
f1 (ppm)


NC
CN
O
H
N
Me
Ph
Me
mixture of 2 diastereomers
f1 (ppm)

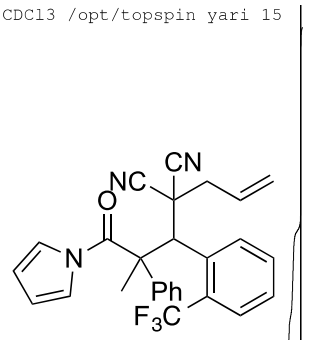

NC
CN
O
H
N
O
Me
Ph
mixture of 2 diastereomers
f1 (ppm)


NC
CN
O
H
N
O
Me
Ph
mixture of 2 diastereomers
f1 (ppm)


NC
CN
O
H
N
O
Me
Ph
one diastereomer
f1 (ppm)


NC
CN
O
H
N
O
Me
Ph
one diastereomer
f1 (ppm)

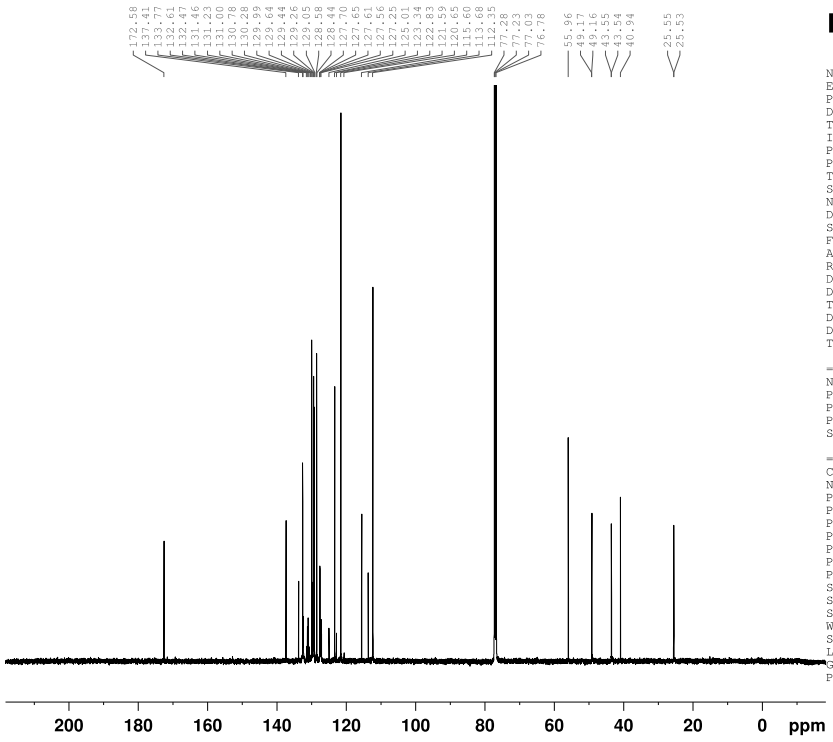
PROTON CDCl3 /opt/topspin yari 15



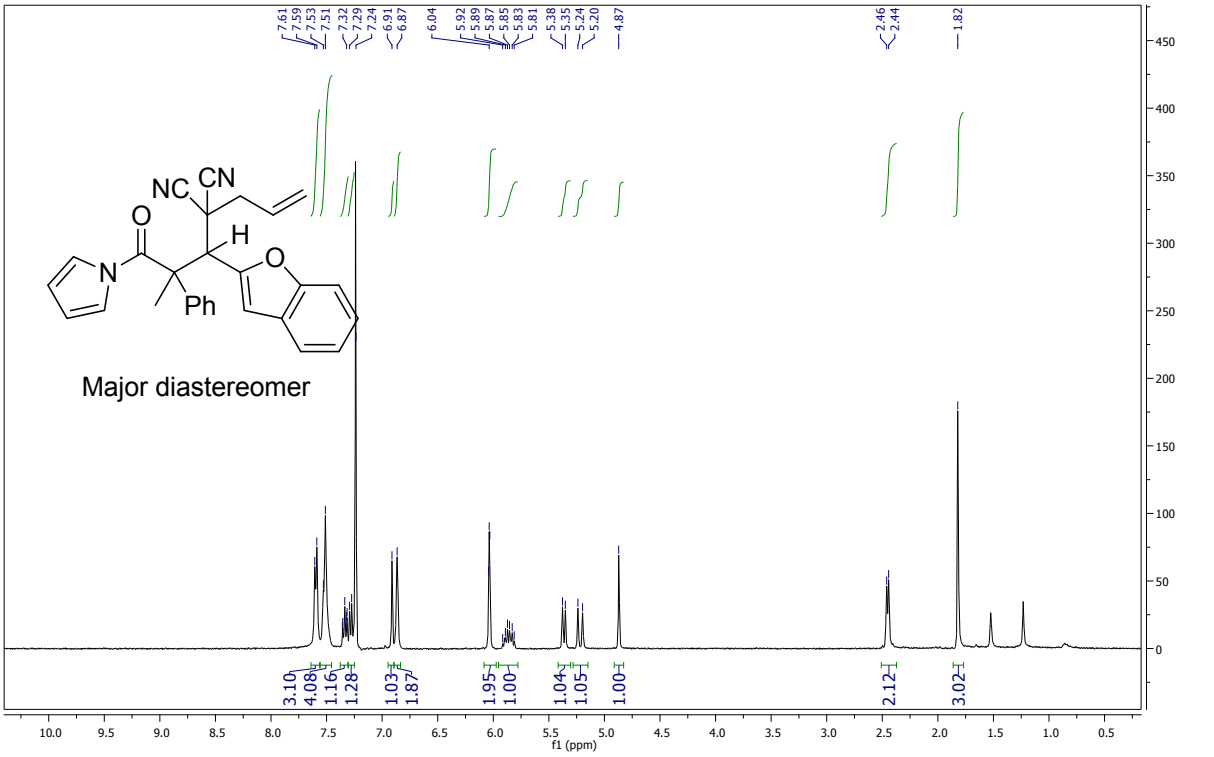
mixture of diastereomers

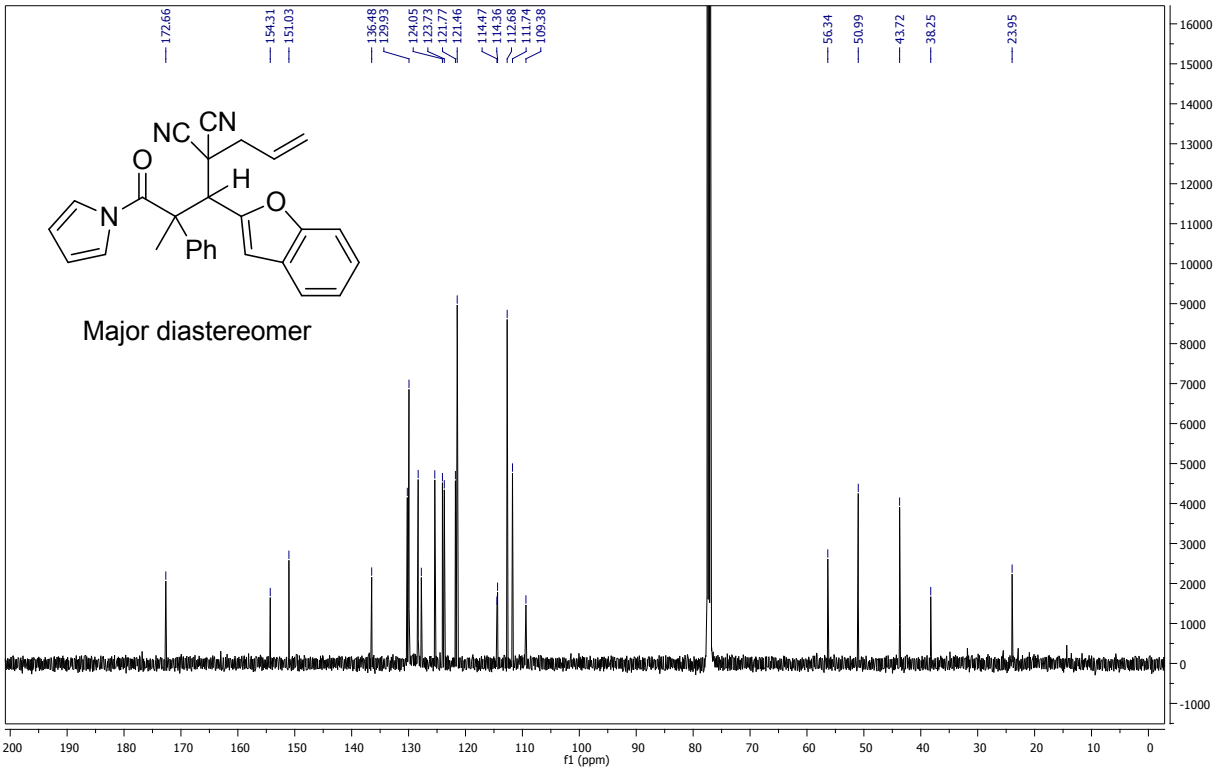

```
NAME            YA-04-214p
EXPNO                    1
PROCNO                   1
Date_             20140514
Time                 19.33
INSTRUM              spect
PROBHD   5 mm CPDUL 13C
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH             10330.578 Hz
FIDRES              0.157632 Hz
AQ                3.1719923 sec
RG                     322
DW                  48.400 usec
DE                   6.50 usec
TE                  298.2 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.70 usec
PL1                   6.00 dB
PL1W           8.64411545 W
SFO1          500.1930889 MHz
SI                   32768
SF            500.1900461 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

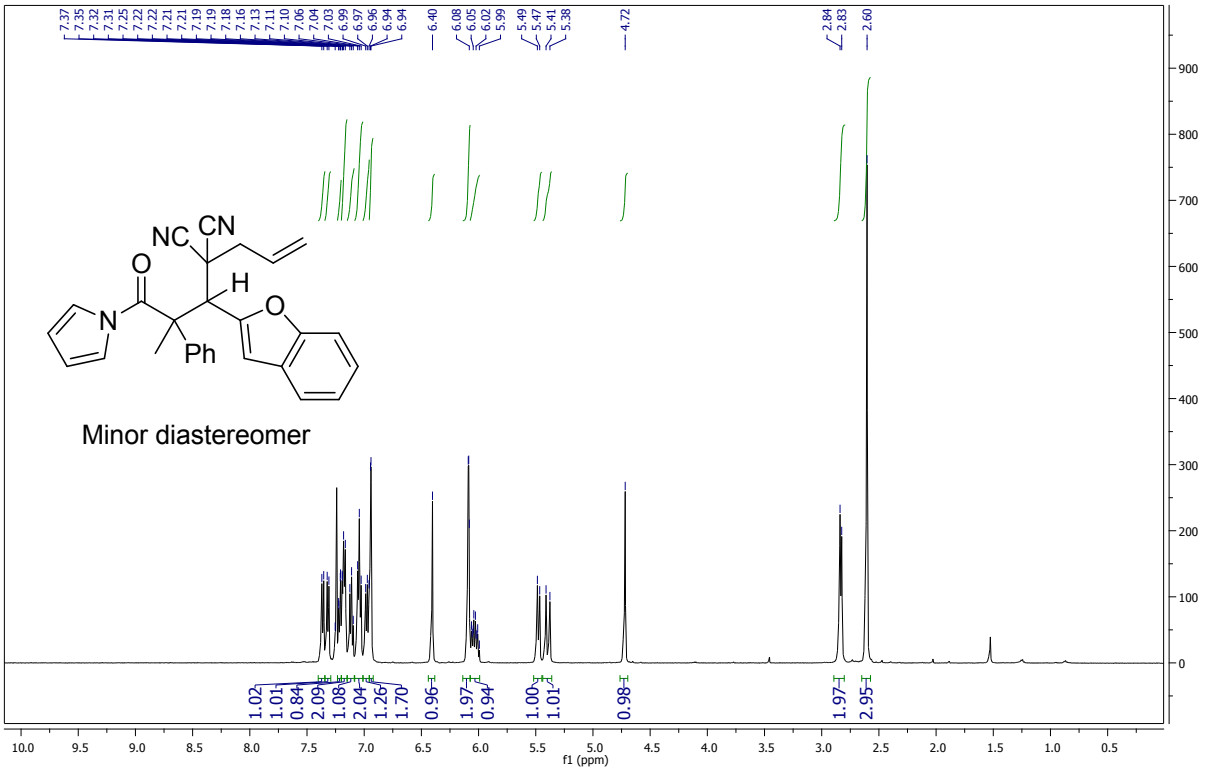
C13CPD CDCl3 /opt/topspin yari 15

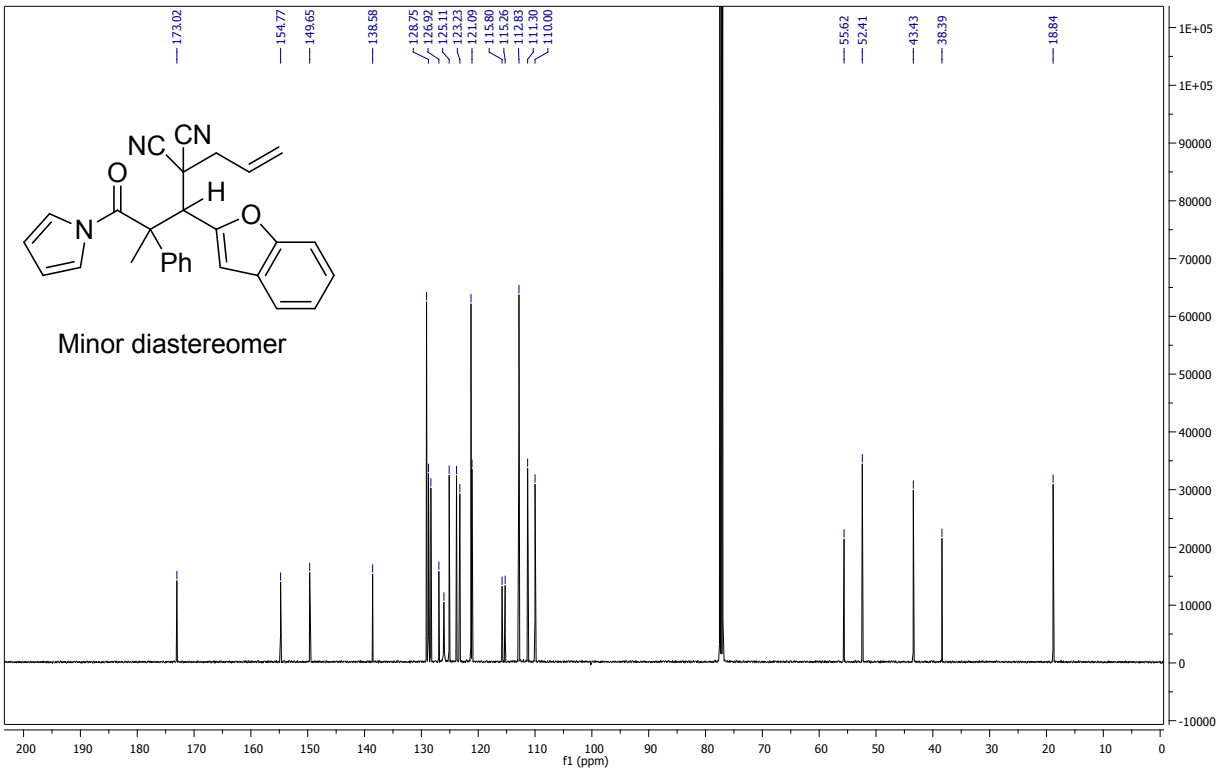


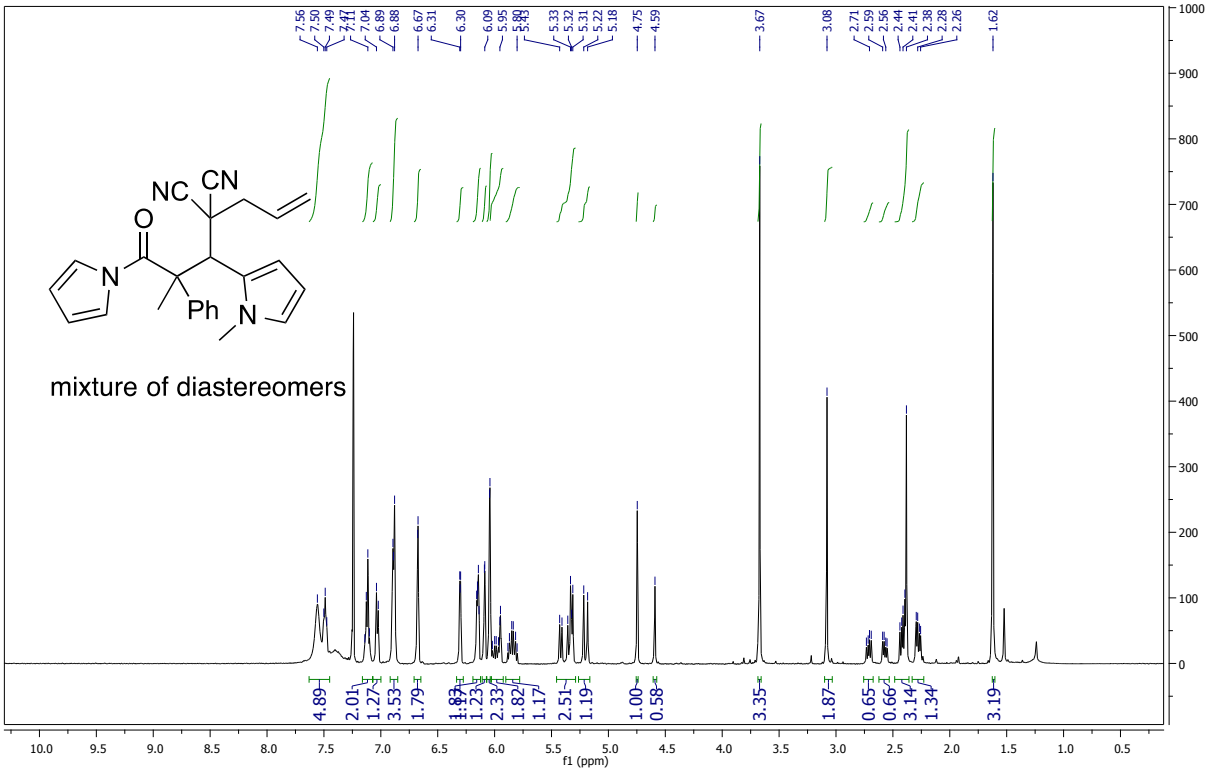

```
NAME            YA-04-214p
EXPNO                    2
PROCNO                   1
Date_             20140514
Time                 19.56
INSTRUM              spect
PROBHD   5 mm CPDUL 13C
PULPROG           zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH             29761.904 Hz
FIDRES              0.454131 Hz
AQ                1.1010548 sec
RG                    2050
DW                  16.800 usec
DE                   6.50 usec
TE                  298.2 K
D1             0.15000001 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.70 usec
PL1                   3.00 dB
PL1W          53.00075912 W
SFO1         125.7854528 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   6.00 dB
PL12                 20.14 dB
PL13                 25.00 dB
PL2W           8.64411545 W
PL12W          0.33321199 W
PL13W          0.10882297 W
SFO2          500.1920008 MHz
SI                   32768
SF            125.7728760 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

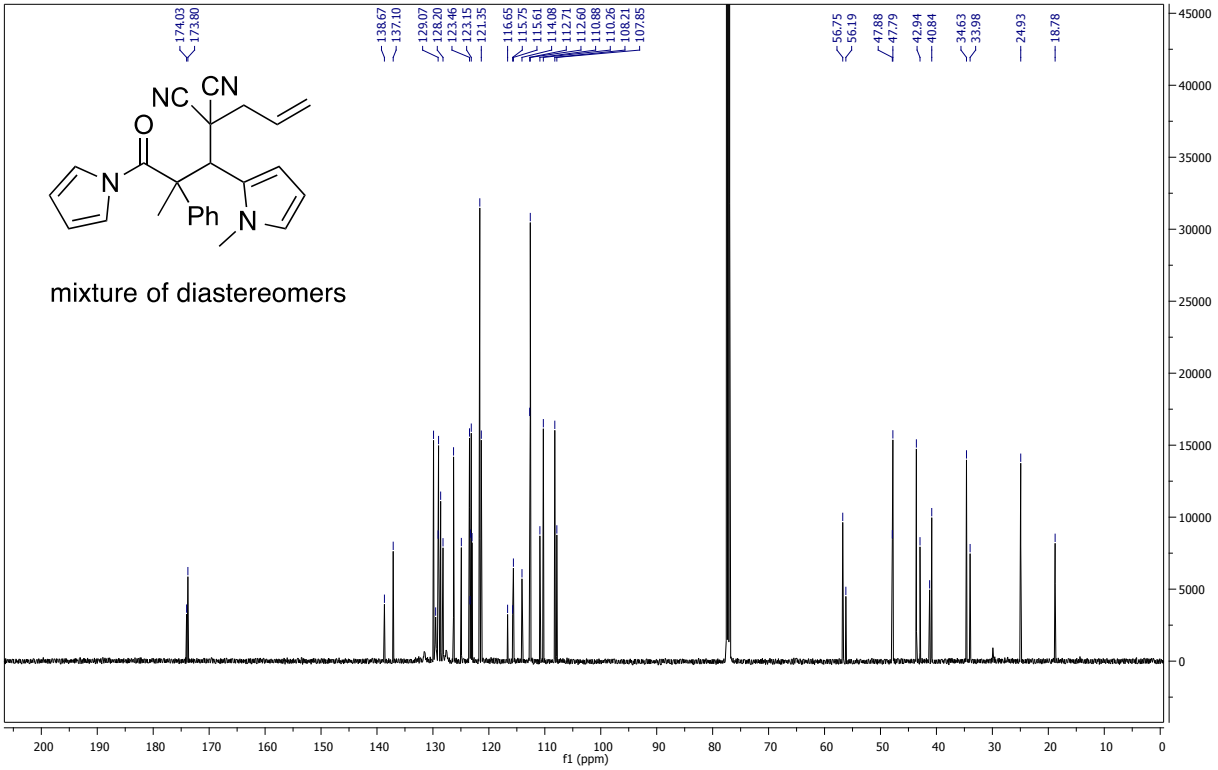

7.61
7.59
7.53
7.51
7.32
7.29
7.24
6.91
6.87
6.04
5.92
5.89
5.87
5.85
5.83
5.81
5.38
5.35
5.24
5.20
4.87
2.46
2.44
1.82
NC
CN
O
H
N
O
Ph
Major diastereomer
3.10
4.08
1.16
1.28
1.03
1.87
1.95
1.00
1.04
1.05
1.00
2.12
3.02
f1 (ppm)

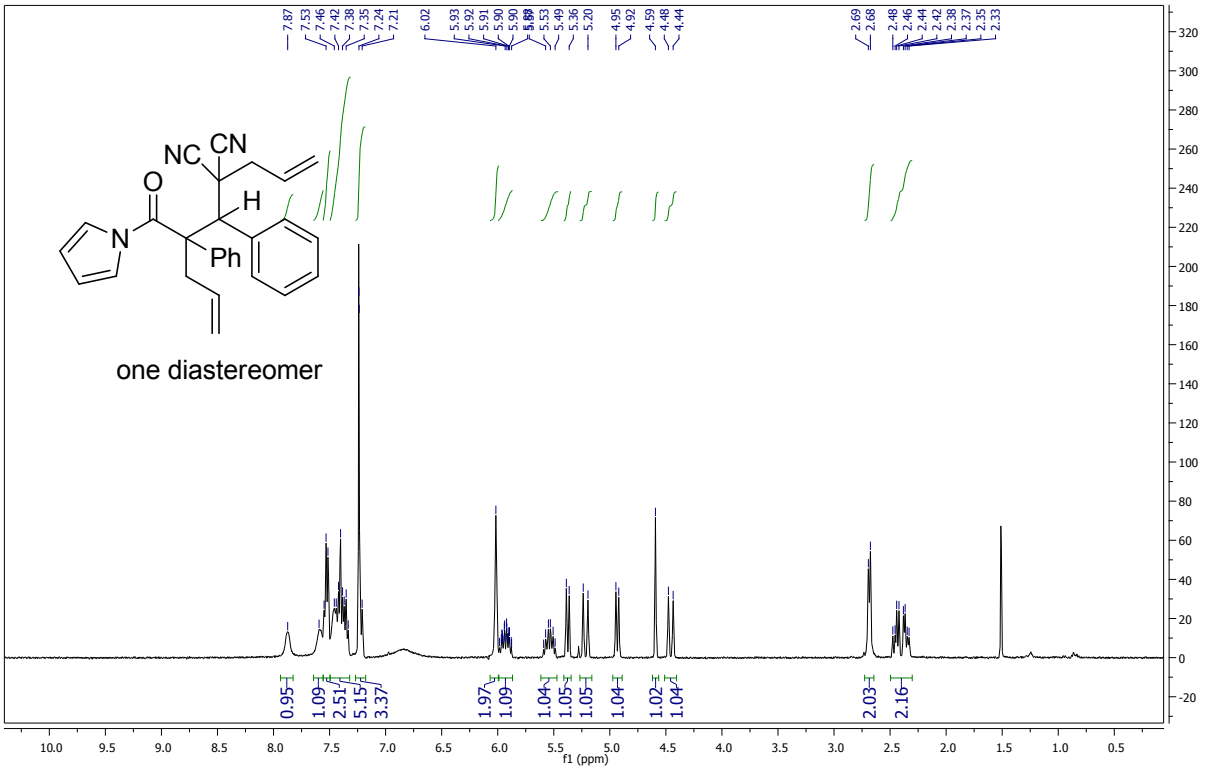

172.66
154.31
151.03
136.48
129.93
124.05
123.73
121.77
121.46
114.47
114.36
112.68
111.74
109.38
56.34
50.99
43.72
38.25
23.95
NC
CN
O
H
N
O
Ph
Major diastereomer
f1 (ppm)

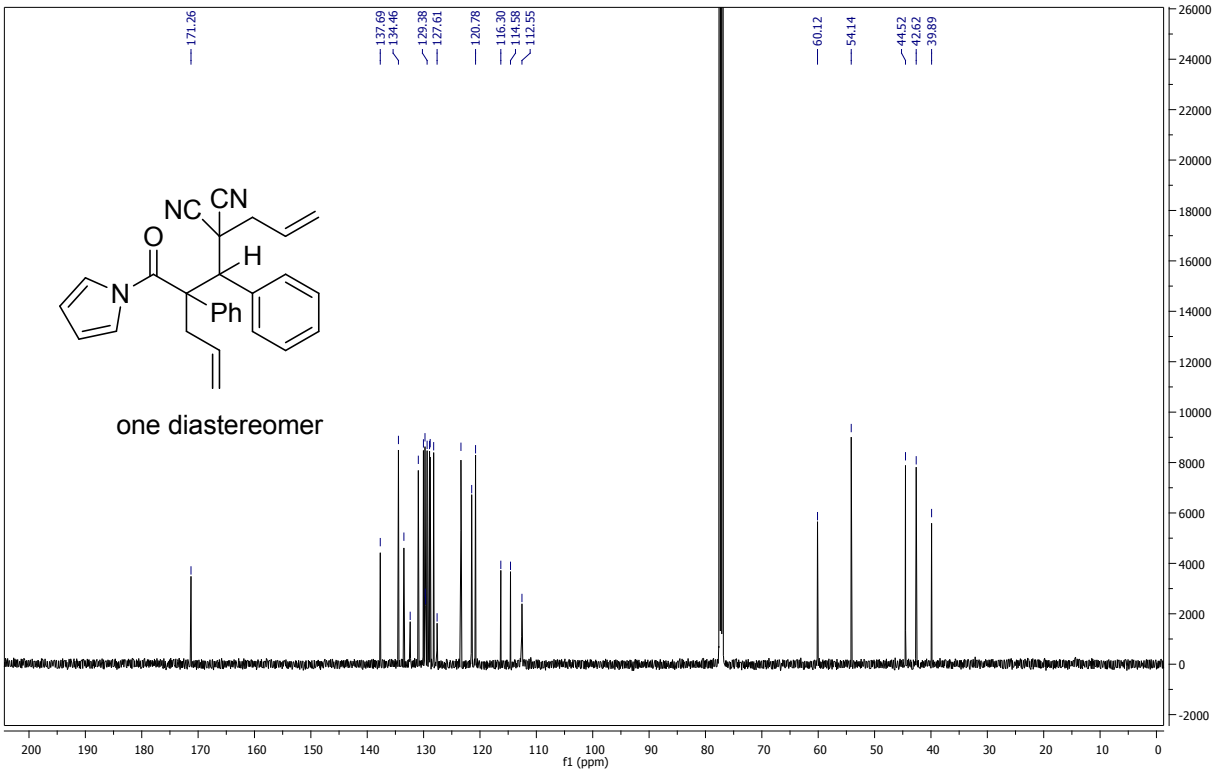

NC
CN
O
H
N
O
Ph
Minor diastereomer
f1 (ppm)


NC
CN
O
H
N
O
Ph
Minor diastereomer
f1 (ppm)


NC
CN
O
N
Ph
N
mixture of diastereomers
f1 (ppm)


NC
CN
O
N
Ph
N
mixture of diastereomers
f1 (ppm)


NC
CN
O
H
N
Ph
one diastereomer
f1 (ppm)


NC
CN
O
H
N
Ph
one diastereomer
f1 (ppm)

Crystal structure of the minor diastereomer of **4a**;