# The influence of ionic liquids on the Knoevenagel condensation of pyrrole with phenyl acetonitriles

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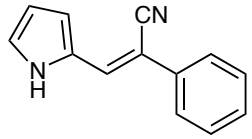
## Supplementary Data

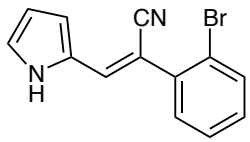
**Material**

All starting materials were purchased from Aldrich Chemical Co. and Lancaster Synthesis. Solvents were bulk, and distilled from glass prior to use. TLC monitored reaction progress, on aluminium plates coated with silica gel with fluorescent indicator (Merck 60 $F_{254}$) and flash chromatography was conducted utilising SNAP Biotage KP-SIL columns.

**General method for synthesis of (*Z*)-2-phenyl-3-(1*H*-pyrrol-2-yl)acrylonitrile (3).**

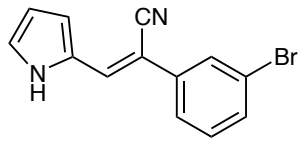



1*H*-Pyrrole-2-carbaldehyde (165 mg, 1.74 mmol) was added to vigorously stirred $H_2O$ (10 mL) and heated to 50 °C upon which it dissolved. Phenylacetonitrile (193 mg, 1.65 mmol) was then slowly added forming a suspension. Heating was continued at 50 °C and once a clear solution was evident, typically 5–10 min, added room temperature ionic liquid (7 mL) was added dropwise. The reaction vessel was sealed and the mixture stirred at 50 °C for 5 h, the solution filtered hot, washed with warm $H_2O$ and dried under suction and recrystallised from EtOH to afford compound (3) as a brown solid. MP 93–94 °C; IR υR($CM^{-1}$): 3396, 2206, 1600, 1588, 1129, 753, 729, 681, 588, 484; $^1$H NMR (400 MHz, $CDCl_3$) δ 9.80 (brs, 1H), 7.61 – 7.55 (m, 2H), 7.44 – 7.38 (m, 3H), 7.36 – 7.29 (m, 2H), 7.10 – 7.04 (m, 1H), 6.74 – 6.66 (m, 1H), 6.37 – 6.32 (m, 1H);$^{13}$C NMR (101 MHz, $CDCl_3$) δ 134.0, 131.4, 129.2, 128.3, 127.9, 125.1, 124.1, 120.8, 119.3, 110.9, 101.5.



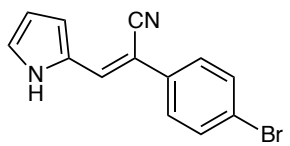

*(Z)-2-(2-Bromophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**4**).*

Synthesised using the general procedure as described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 2-bromophenylacetonitrile to afford **4** as a light yellow solid. MP 122–123 °C; IR υR($CM^{-1}$): 3309, 2205, 1596, 1139,731, 596, 444; $^1$H NMR: (400 MHz, Chloroform-*d*) δ 9.99 (brs, 1H), 7.79 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.57 – 7.45 (m, 2H), 7.40 (s, 1H), 7.41 – 7.32 (m, 1H), 7.27 – 7.20 (m, 1H), 6.84 – 6.77 (m, 1H), 6.53 – 6.46 (m, 1H);$^{13}$C NMR: (101 MHz, $CDCl_3$) δ 137.5, 135.7, 133.8, 131.0, 130.1, 128.1, 127.4, 124.5, 123.0, 120.1, 119.6, 110.9, 100.7.




*(Z)-2-(3-Bromophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**5**).*

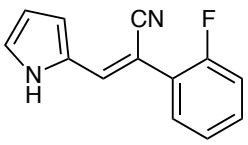
Synthesised using the general procedure as for the synthesis of (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 3-bromophenylacetonitrile to afford **5** as a brown solid. MP 121– 22 °C. IR υR($CM^{-1}$): 3309, 2205, 1597, 1430, 1139, 731, 596,444; $^1$H NMR (400 MHz, Chloroform-*d*) δ 9.79 (brs, 1H), 7.71 (t, *J* = 1.9 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.47 – 7.42 (m, 1H), 7.39 (s, 1H), 7.31 – 7.27 (m, 1H), 7.09 (q, *J* = 2.6 Hz, 1H), 6.73 (t, *J* = 3.7 Hz, 1H), 6.40 – 6.33 (m, 1H); $^{13}$C NMR: (101 MHz, $CDCl_3$) δ 136.2, 132.2, 131.2, 130.7, 127.9, 127.6, 124.8, 123.8, 123.4, 120.4, 120.1, 111.2, 99.8.




*(Z)-2-(4-Bromophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**6**)*

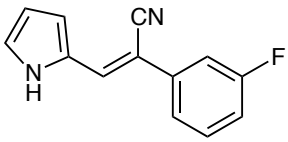
Synthesised using the general procedure as for the synthesis of (**3**) from 1*H*-

pyrrole-2-carbaldehyde (**1**) and 4-bromophenylacetonitrile to afford **6** as a yellow solid. MP 123–124 °C; IR υR($CM^{-1}$): 3374, 2213, 1487, 1131, 817, 739,594, 489; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 9.77 (brs, 1H), 7.53 (d, *J* = 8.6 Hz, 2H), 7.44 (d, *J* = 8.6 Hz, 2H), 7.38 (s, 1H), 7.11 – 7.06 (m, 1H), 6.74 – 6.66 (m, 1H), 6.40 – 6.32 (m, 1H);$^{13}$C NMR (101 MHz, $CDCl_3$) δ 133.1, 132.3, 131.6, 127.7, 126.6, 124.6, 122.2, 120.4, 119.8, 111.2, 100.3.



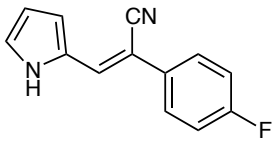

*(Z)-2-(2-Fluorophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (7)*

Synthesised using the general procedure as for the synthesis of (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 2-fluorophenylacetonitrile to afford **7** as a brown solid. MP 100–102 °C; IR υR($CM^{-1}$): 3409, 2205, 1603, 1125, 740, 677. $^{1}$H NMR: (400 MHz, Chloroform-*d*) δ 9.83 (brs, 1H), 7.57 – 7.47 (m, 2H), 7.35 – 7.06 (m, 4H), 6.75 – 6.65 (m, 1H), 6.40 – 6.31 (m, 1H);$^{13}$C NMR: (101 MHz, $CDCl_3$) δ 159.7 (d, *J* = 248.7 Hz), 135.9 (d, *J* = 9.35 Hz),129.7 (d, *J* = 8.55 Hz),, 129.1 (d, *J* = 2.5 Hz), 127.8, 124.8 (d, *J* = 3.69 Hz), 124.6, 122.4 (d, *J* = 10.7 Hz), 120.6, 119.9, 116.6 (d, *J* = 22.2 Hz), 111.0, 95.9 (d, *J* = 2.2 Hz).



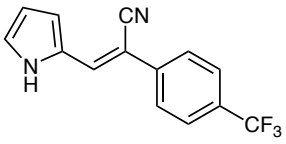

*(Z)-2-(3-Fluorophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**8**)*

Synthesised using the general procedure described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 3-fluorophenylacetonitrile to afford **8** as a green solid. MP 104–107 °C; IR υR($CM^{-1}$): 3396, 2208, 1583, 1407, 1121, 745, 594, 522; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ δ 9.79 (brs, 1H), 7.41 – 7.34 (m, 3H), 7.30 – 7.27 (m, 1H), 7.09 (td, *J* = 2.8, 1.4 Hz, 1H), 7.04 – 6.98 (m, 1H), 6.73 (dd, *J* = 3.7, 1.6 Hz, 1H), 6.37 (dt, *J* = 3.7, 2.4 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 163.3 (d, *J* = 245.2 Hz), 136.3 (d, *J* = 8.1 Hz), 132.1, 130.8 (d, *J* = 8.5 Hz), 127.6, 124.7, 120.9 (d, *J* = 2.9 Hz), 120.4, 120.0, 115.1 (d, *J* = 21.2 Hz), 111.9 (d, *J* = 23.4 Hz), 111.2, 100.2 (d, *J* = 2.9 Hz).




*(Z)-2-(4-Fluorophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**9**)*

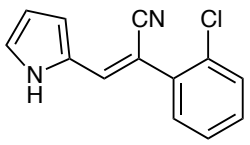
Synthesised using the general procedure as described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 4-fluorophenylacetonitrile to afford **9** as a light yellow solid. MP 10–103 °C; IR υ($CM^{-1}$): 3393, 2208, 1593, 1122, 857, 745, 687; $^{1}$H NMR ($CDCl_3$) δ 9.76 (s, 1H), 7.54 (dd, *J* = 8.7, 5.2 Hz, 2H), 7.32 (s, 1H), 7.16 – 7.04 (m, 3H), 6.69 (s, 1H), 6.35 (q, *J* = 2.8 Hz, 1H); $^{13}$C NMR (101 MHz, $CDCl_3$) δ 162.7 (d, *J* = 246.7 Hz) , 131.3 (d, *J* = 22.1 Hz), 130.3 (d, *J* = 3.4 Hz), 127.7, 126.9 (d, *J* = 8.2 Hz), 124.2, 120.6, 119.3, 116.2 (d, *J* = 21.9 Hz), 111.0, 100.4.




*(Z)-3-(1H-Pyrrol-2-yl)-2-(4-rifluoromethyl)phenyl)acrylonitrile (**10**).*

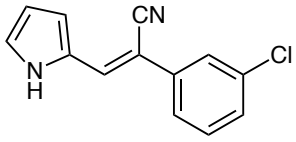
Synthesised using the general procedure as described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 4-trifluoromethylphenylacetonitrile to afford **10** as a yellow solid. MP 149–150 °C; IR υ($CM^{-1}$): 3389, 2205, 1590, 1167, 1111, 833, 752, 583; $^{1}$H NMR: ($CDCl_3$) δ 9.83 (brs, 1H), 7.72 – 7.62 (m, 4H), 7.48 (s, 1H), 7.16 – 7.09 (m, 1H), 6.80 – 6.73 (m, 1H), 6.42 – 6.35 (m, 1H); $^{13}$C NMR: ($CDCl_3$) δ 137.6 (q, *J* = 1.4 Hz), 132.8, 130.0 (q, *J* = 32.6 Hz), 127.6,

126.2 (q, *J* = 3.8 Hz), 125.2, 124.0 (q, *J* = 270.3 Hz), 120.6, 120.3, 111.4, 99.7.



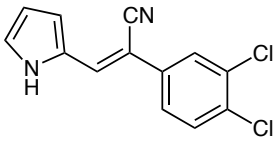
*(Z)-2-(2-Chlorophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**11**)*

Synthesised using the general procedure as described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 2-chlorophenylacetonitrile to afford **11** as a brown solid. MP 110–112 °C. IR υ($CM^{-1}$): 3309, 2207, 1595, 1141, 730, 595. $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 9.87 (brs, 1H), 7.47 – 7.43 (m, 1H), 7.42 – 7.38 (m, 1H), 7.34 – 7.29 (m, 2H), 7.18 (s, 1H), 7.12 – 7.06 (m, 1H), 6.72 – 6.65 (m, 1H), 6.40 – 6.32 (m, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 137.5, 133.8, 133.1, 130.6, 130.5, 129.9, 127.5, 124.5, 120.2, 119.6, 110.9, 98.9.

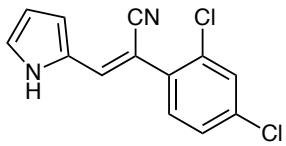


*(Z)-2-(3-Chlorophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**12**)*

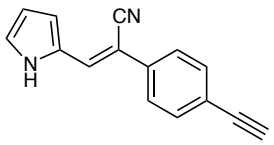
Synthesised using the general procedure as described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 3-chlorophenylacetonitrile to afford **12** as a yellow solid. MP 111–112 °C; IR υR($CM^{-1}$): 3386, 2212, 1605, 1528, 1398, 1132, 1039, 732, 681, 590. $^{1}$H NMR: (400 MHz, Chloroform-*d*) δ 9.79 (brs, 1H), 7.62 – 7.51 (m, 1H), 7.50 – 7.42 (m, 2H), 7.40 (s, 1H), 7.34 (t, *J* = 7.8 Hz, 1H), 7.13 – 7.06 (m, 1H), 6.76 – 6.69 (m, 1H), 6.40 – 6.33 (m, 1H); $^{13}$C NMR: (101 MHz, $CDCl_3$) δ 135.9, 135.3, 132.1, 130.4, 128.2, 127.6, 125.0, 124.8, 123.3, 120.4, 120.1, 111.2, 100.0.



*(Z)-2-(3,4-Dichlorophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**13**).* Synthesised using the general procedure as described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 3,4-dichlorophenylacetonitrile to afford **13** as a yellow solid. MP 140–141 °C; IR υ($CM^{-1}$): 3416, 2200, 1604, 1125, 748, 590, 492; $^{1}$H NMR ($CDCl_3$): δ 9.77 (brs, 1H), 7.65 (d, *J* = 2.2 Hz, 1H), 7.47 (d, *J* = 8.5 Hz, 1H), 7.41 (d, *J* = 2.3 Hz, 1H), 7.38 (s, 1H), 7.15 – 7.07 (m, 1H), 6.77 – 6.72 (m, 1H), 6.40 – 6.34 (m, 1H); $^{13}$C NMR ($CDCl_3$): δ 134.2, 133.6, 132.2, 131.1, 130.1, 127.5, 126.7, 125.1, 124.2, 120.4, 120.1, 111.4, 98.9.



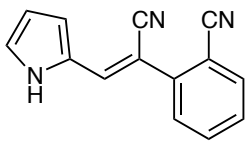
*(Z)-2-(2,4-dichlorophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile.* (**14**).Synthesised using the general procedure as described for (**3**) from 1H-pyrrole-2-carbaldehyde (**1**) and 2,4-dichlorophenylacetonitrile to afford **14** as a light yellow solid. MP 148–156.6 °C; IR υ($CM^{-1}$): 3381, 2208, 1593, 1141,742, 594; $^{1}$H NMR ($CDCl_3$) δ 9.83 (brs, 1H), 7.47 (d, J = 2.0 Hz, 1H), 7.36 – 7.27 (m, 2H), 7.16 (s, 1H), 7.12 – 7.08 (m, 1H), 6.71 – 6.66 (m, 1H), 6.39 – 6.33 (m, 1H). $^{13}$C NMR ($CDCl_3$) δ 137.7, 135.2, 133.8, 132.4, 131.3, 130.4, 127.9, 127.3, 124.9, 120.2, 120.0, 111.1, 97.7.



*(Z)-2-(4-Ethynylphenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**15**)*

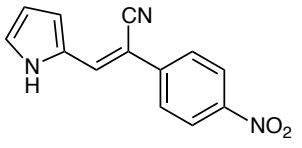
Synthesised using the general procedure as described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 4-ethynylphenylacetonitrile to afford **15** as a brown solid. MP 100 – 102 °C; IR υR($CM^{-1}$): 3446, 3268, 2194, 1588, 1037, 831, 720, 520, 435. $^{1}$H NMR: (400 MHz,

Chloroform-*d*) δ 9.79 (brs, 1H), 7.60 – 7.47 (m, 4H), 7.41 (s, 1H), 7.12 – 7.05 (m, 1H), 6.75 – 6.68 (m, 1H), 6.40 – 6.32 (m, 1H), 3.16 (s, 1H);$^{13}$C NMR: (101 MHz, $CDCl_3$) δ 134.4, 132.9, 131.7, 127.8, 124.8, 124.7, 121.9, 120.4, 119.9, 111.2, 100.6, 83.2, 78.8.




*(Z)-2-(1-Cyano-2-(1H-pyrrol-2-yl)vinyl)benzonitrile (**16**)*

Synthesised using the general procedure as described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 2-cyanophenylacetonitrile to afford (**16**) as a green solid. MP 148–149 °C; IR υR($CM^{-1}$): 3420, 2218, 2199, 1605, 1403, 1333, 740, 572. $^1$H NMR: (400 MHz, Chloroform-*d*) δ 9.79 (brs, 1H), 7.75 (d, *J* = 7.7 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.56 (s, 1H), 7.43 (ddd, *J* = 7.7, 5.9, 2.7 Hz, 1H), 7.14 (q, *J* = 2.7 Hz, 1H), 6.85 – 6.81 (m, 1H), 6.41 – 6.37 (m, 1H);$^{13}$C NMR: (101 MHz, $CDCl_3$) δ 138.2, 137.3, 134.7, 133.4, 129.2, 128.5, 127.2, 125.6, 121.1, 120.0, 117.9, 111.6, 110.0, 97.2.




*(Z)-2-(4-Nitrophenyl)-3-(1H-pyrrol-2-yl)acrylonitrile (**17**)*

Synthesised using the general procedure as described for (**3**) from 1*H*-pyrrole-2-carbaldehyde (**1**) and 4-nitrophenylacetonitrile to afford **16** as a brown solid. MP 130–133 °C; IR υR($CM^{-1}$): 3368, 2208, 1507, 1576, 1327, 1034, 757, 683, 482.$^1$H NMR: $^1$H NMR (400 MHz, Chloroform-*d*) δ 9.87 (brs, 1H), 8.27 (d, *J* = 8.9 Hz, 2H), 7.72 (d, *J* = 8.9 Hz, 2H), 7.55 (s, 1H), 7.22 – 7.10 (m, 1H), 6.88 – 6.73 (m, 1H), 6.47 – 6.29 (m, 1H).$^{13}$C NMR: .(101 MHz, $CDCl_3$) δ 147.1, 140.5, 133.8, 127.6, 126.2, 125.4, 124.6, 121.8, 120.0, 111.8, 98.8.

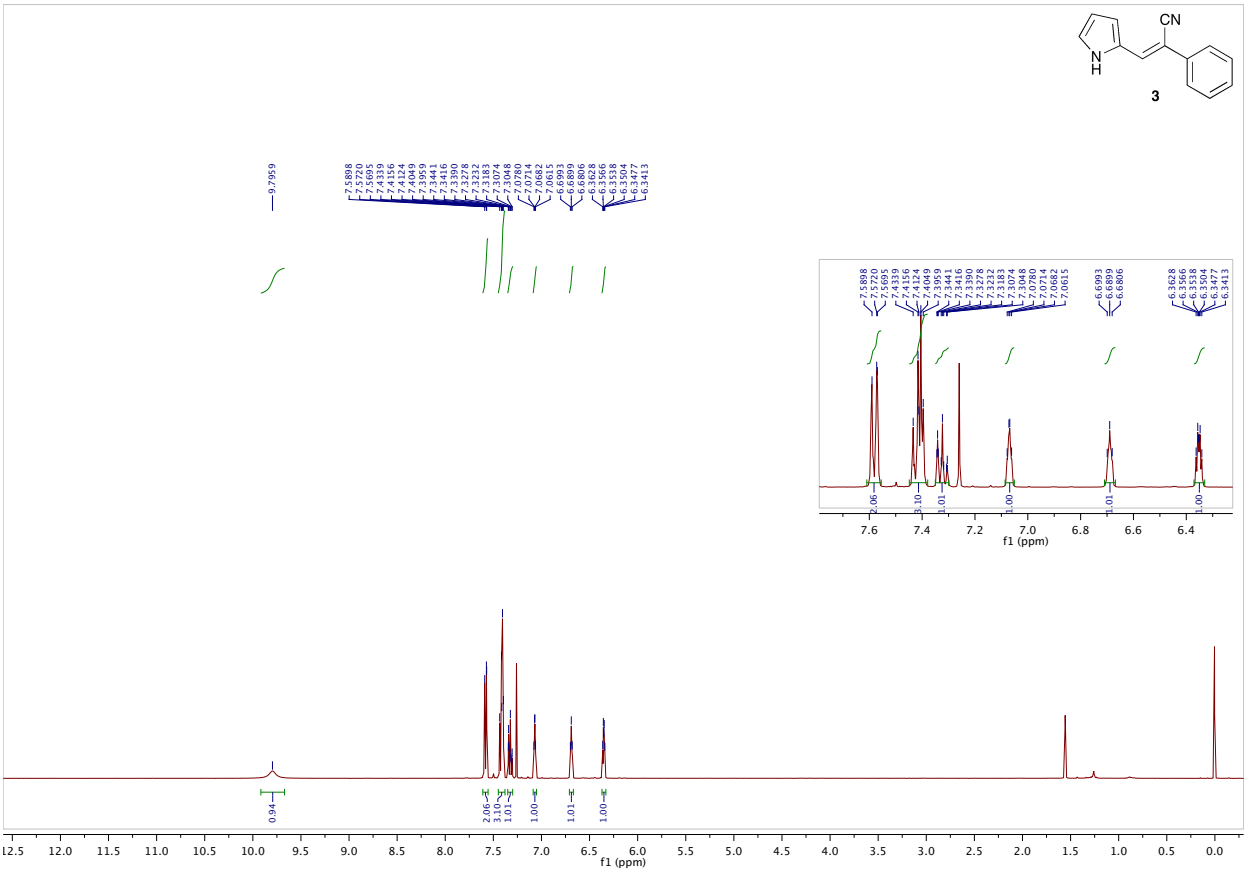
**General method for recycling of ionic liquid:**

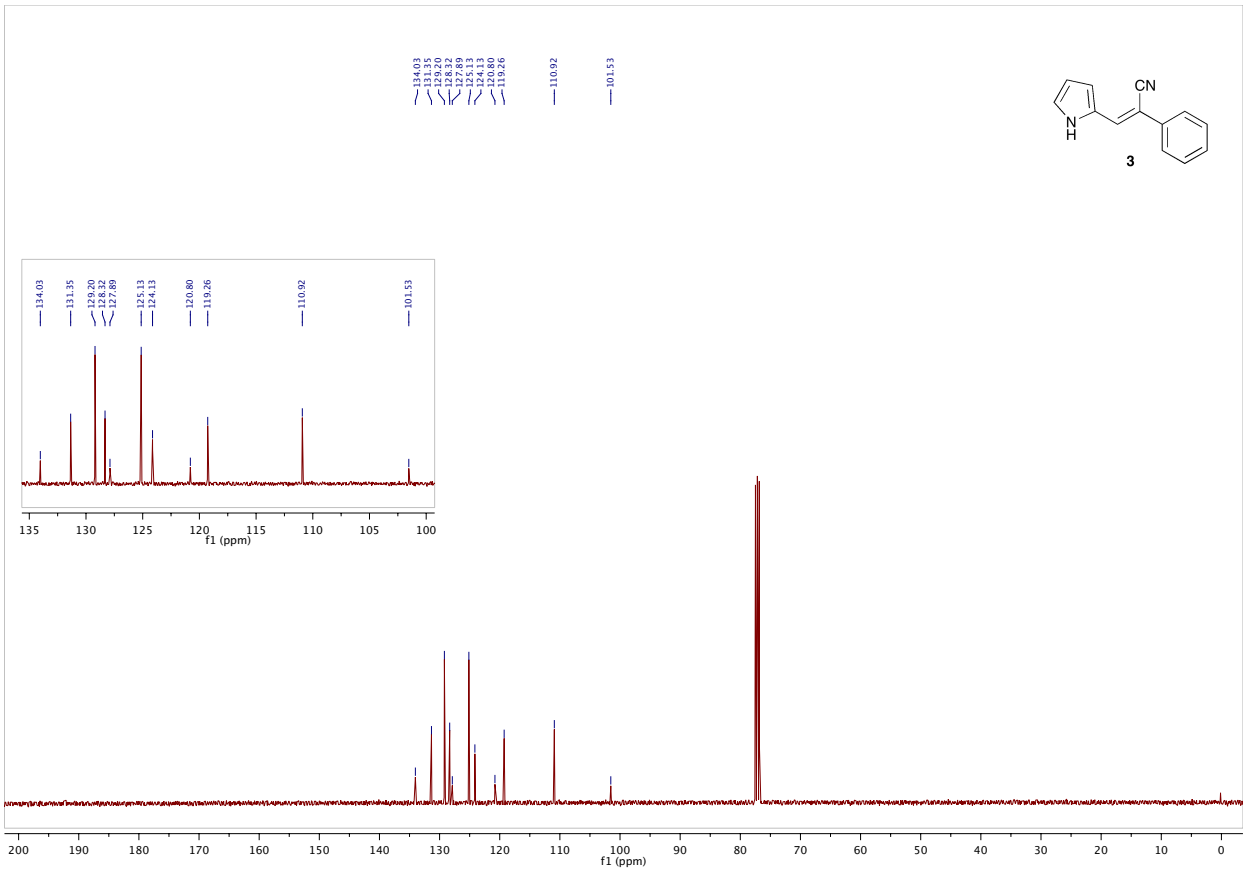
The procedure generally employed was to dissolve the ionic liquid in the EtOAc (10 mL), and wash it with $H_2O$ (3 × 5 mL) and saturated brine solution (5 mL). The second step is added of $Et_2O$ (20 mL), so that form two layers. The lower being essentially pure ionic liquid.

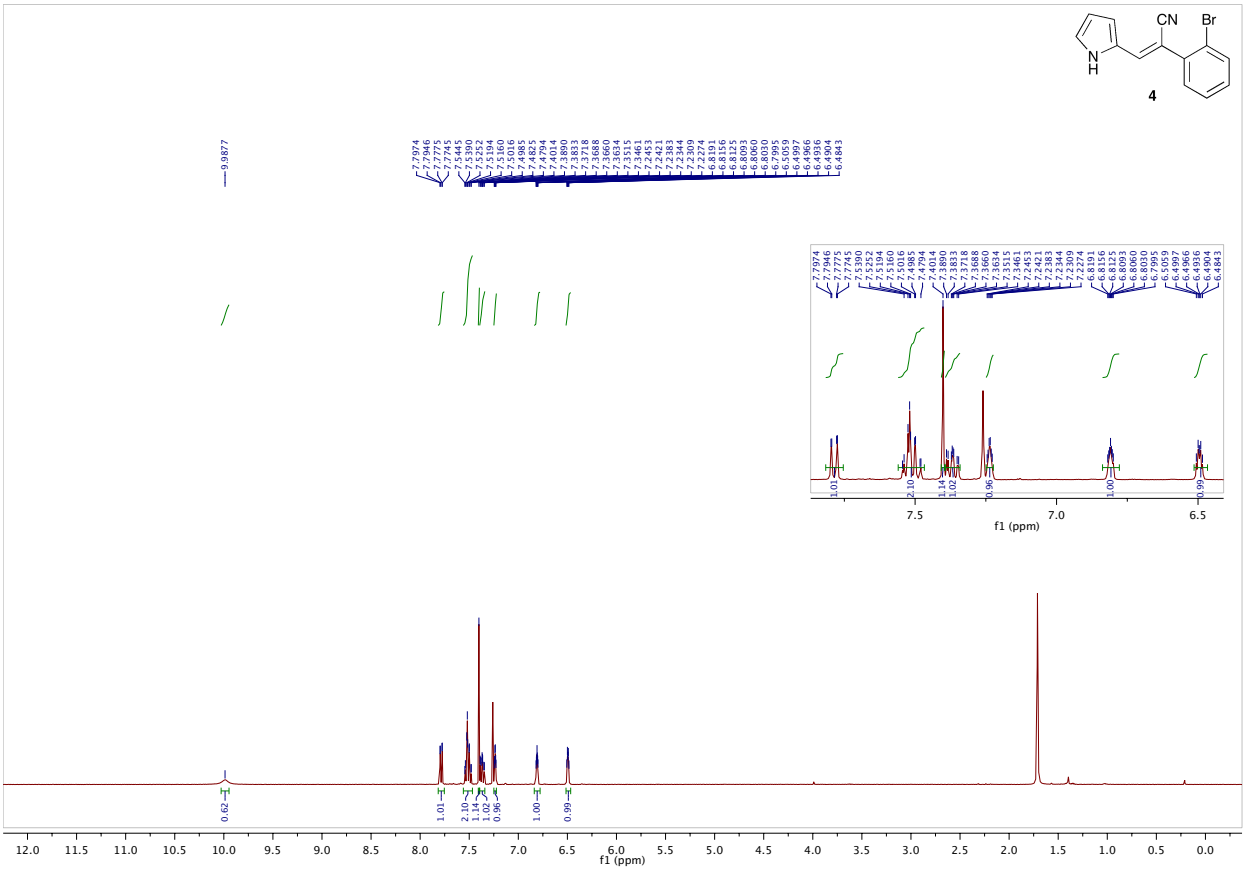
**Table 6.** Model reaction of pyrrole 2-carboxaldehyde with phenyl acetonitrile and recycling of [BMIM][Br] in recycled ILs.

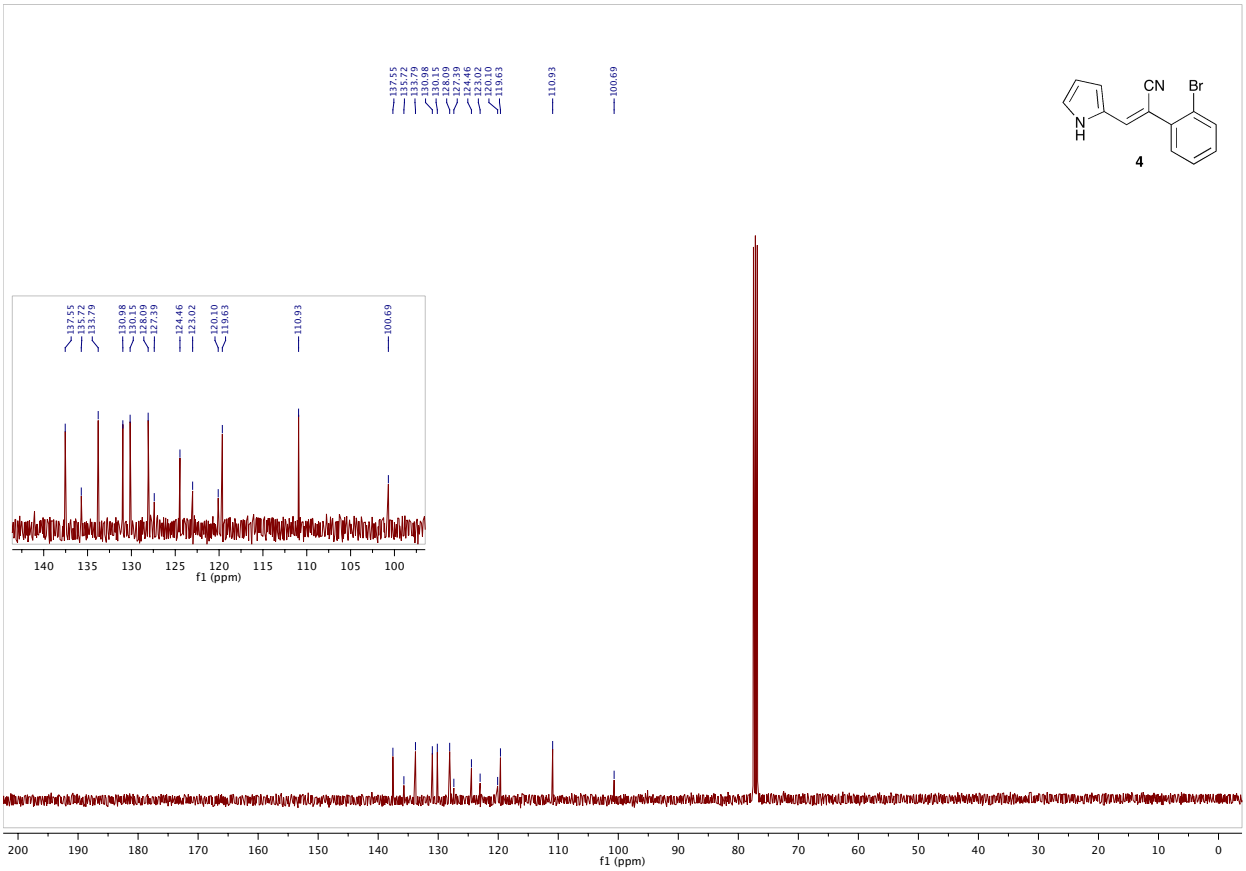
| Entry | Run [a] | Yield % |
|---|---|---|
| 1 | 1 | 56 |
| 2 | 2 | 53 |
| 3 | 3 | 49 |

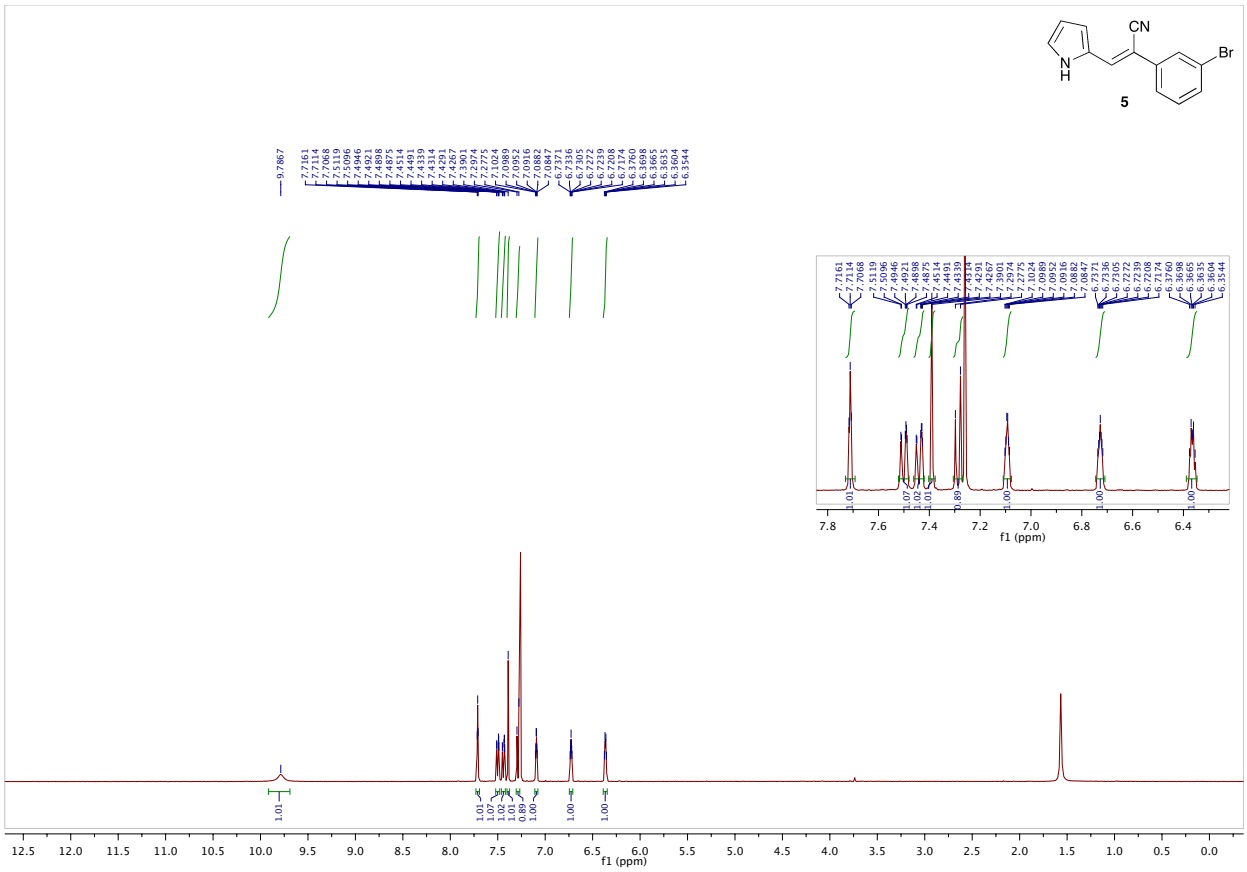
[a] Reaction conditions: Pyrrole-2-carboxaldehyde (165 mg, 1.74 mmol), phenylacetonitrile (193 mL, 1.65 mmol), piperidine (2 drops, catalytic), $H_2O$ (10 mL) and room temperature ionic liquid (7 mL) heated at 50 ºC for 5 h.

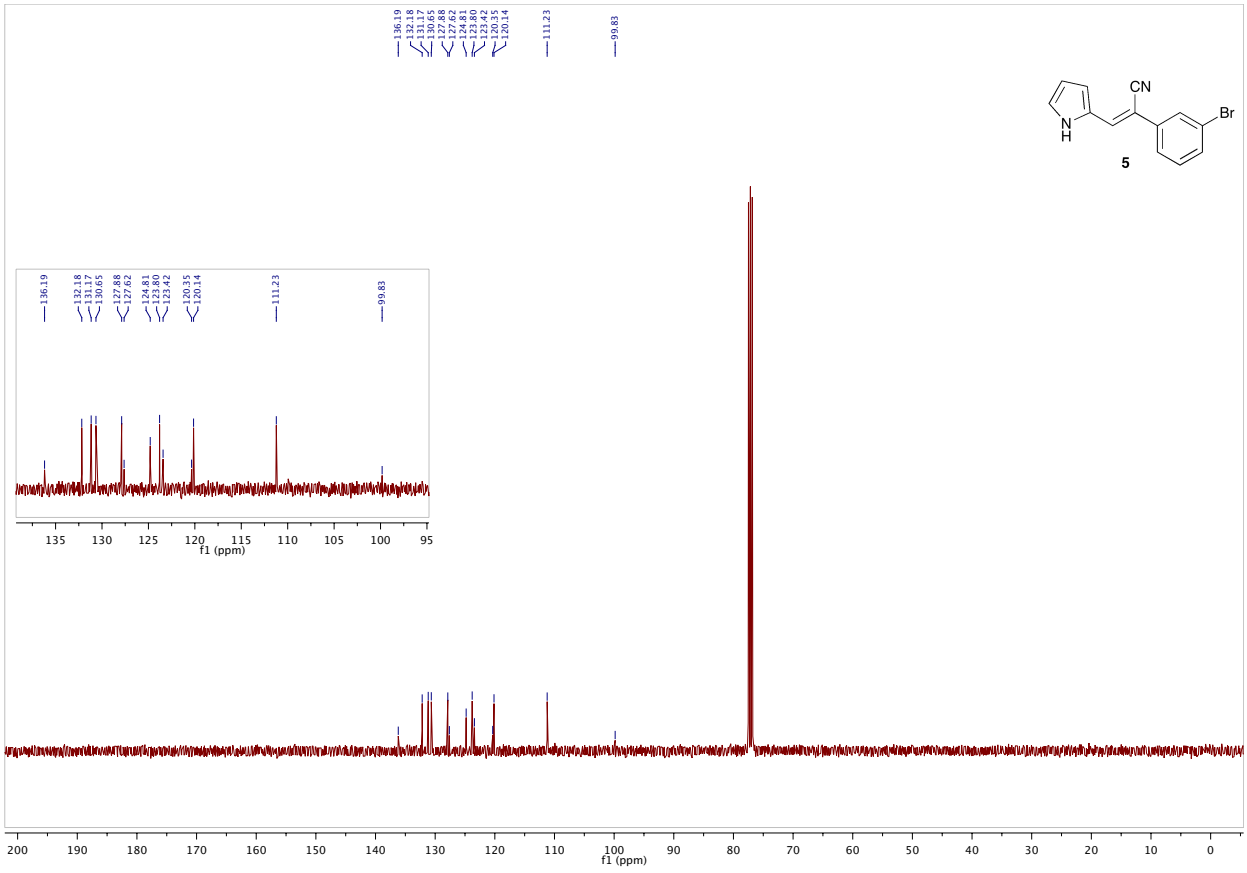

CN
N
H
3
f1 (ppm)

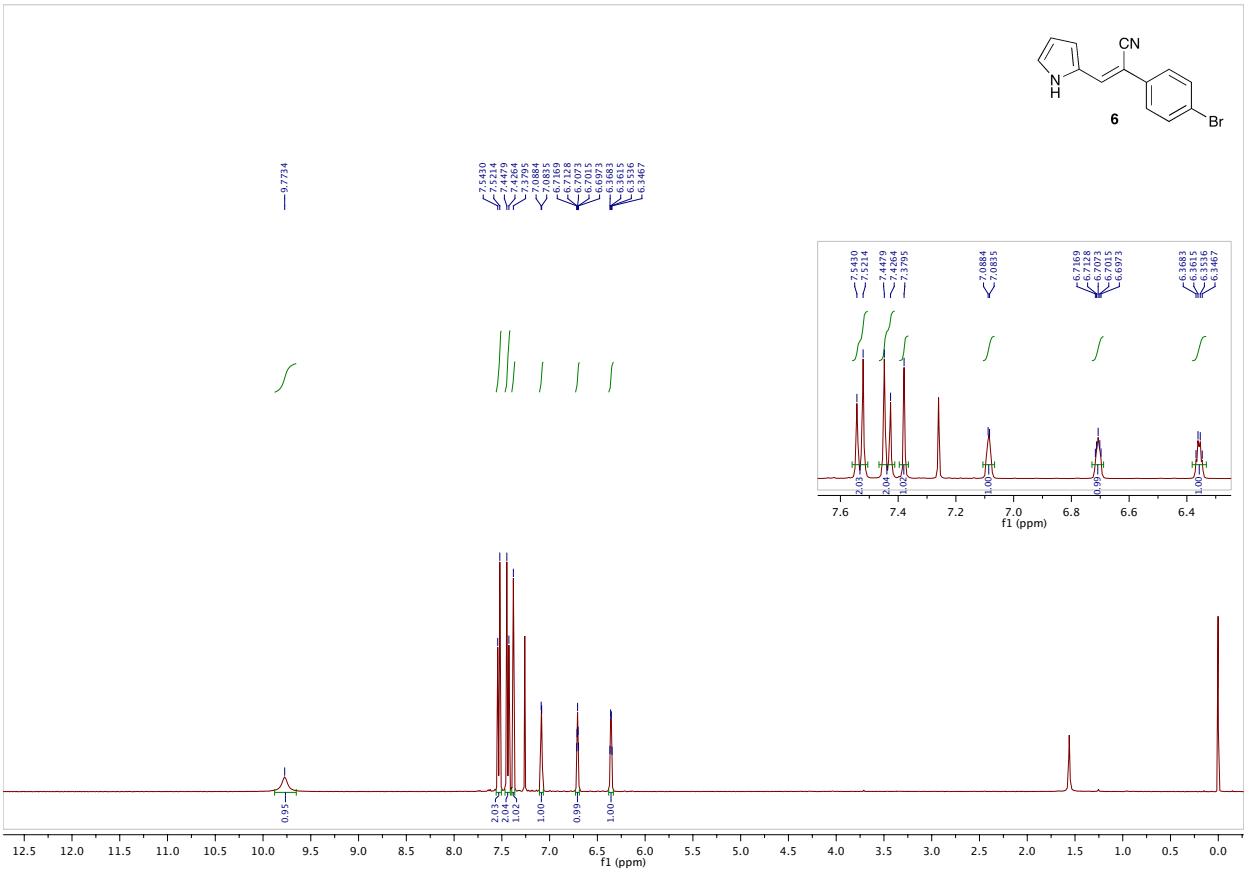

CN
N
H
3
f1 (ppm)


CN
Br
N
H
4
f1 (ppm)


CN
Br
N
H
4
f1 (ppm)


CN
Br
N
H
5
f1 (ppm)


CN
Br
N
H
5
f1 (ppm)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H
Br
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7.5214
7.4479
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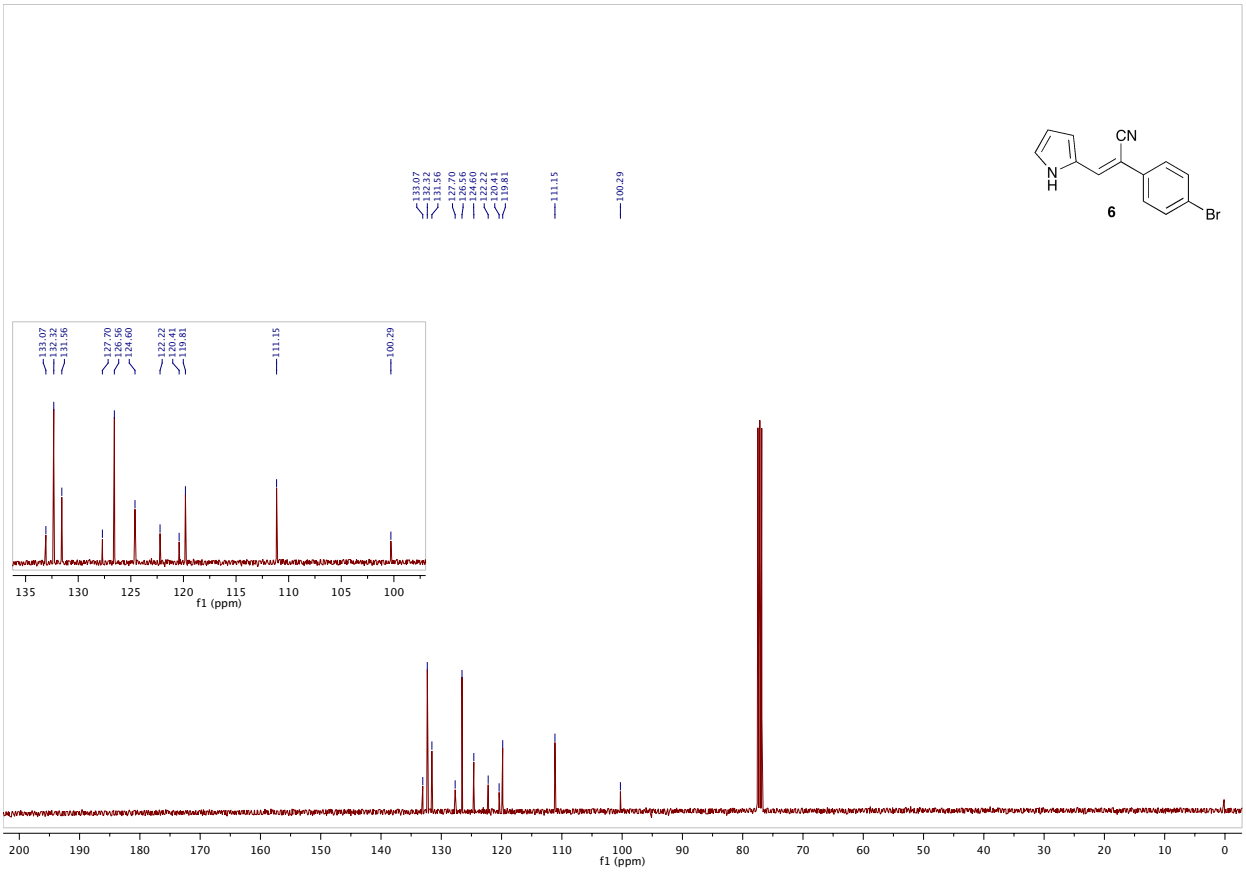
7.3795
7.0884
7.0835
6.7128
6.7073
6.7015
6.6973
6.3683
6.3615
6.3536
6.3467
0.95
2.03
2.04
1.02
1.00
0.99
1.00
f1 (ppm)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H
Br
6
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126.56
124.60
122.22
120.41
119.81
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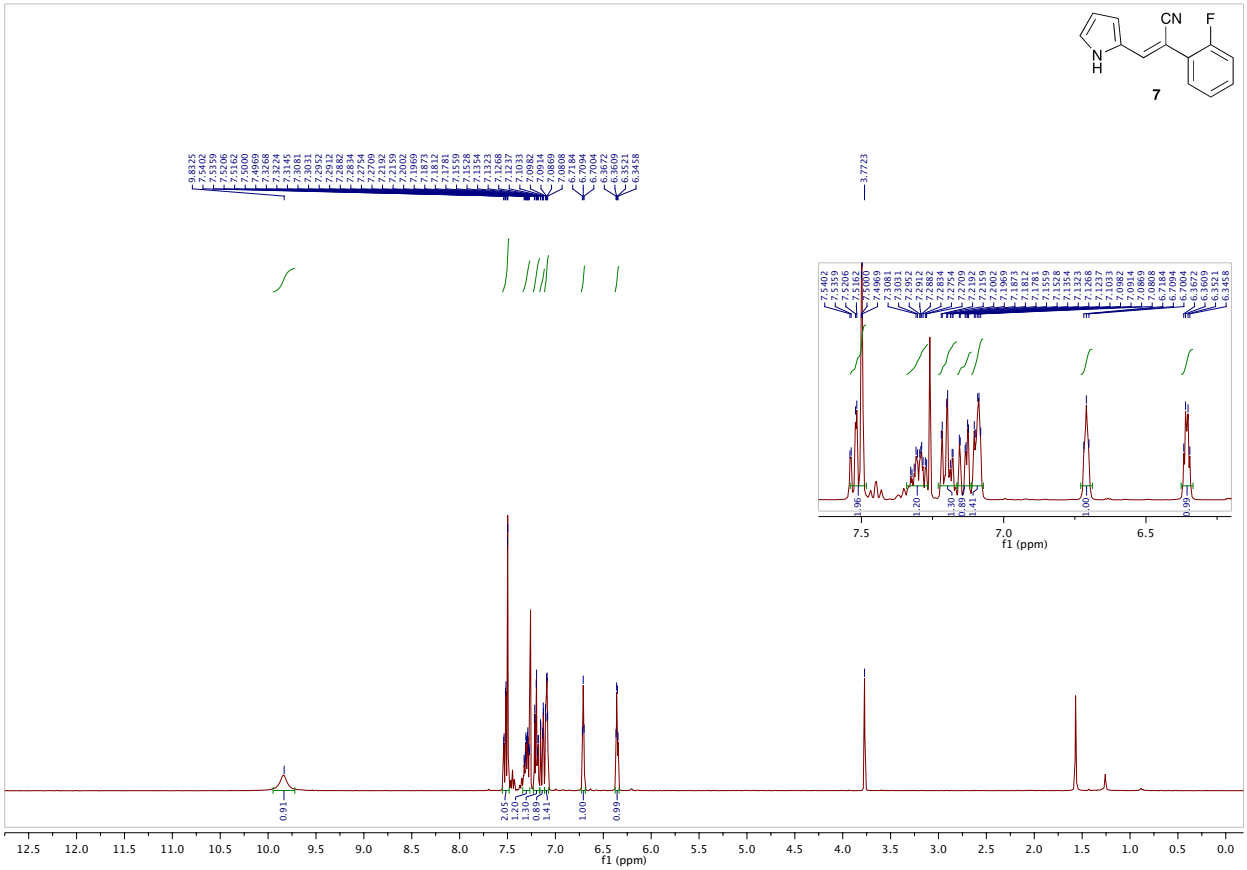
100.29
f1 (ppm)


CN
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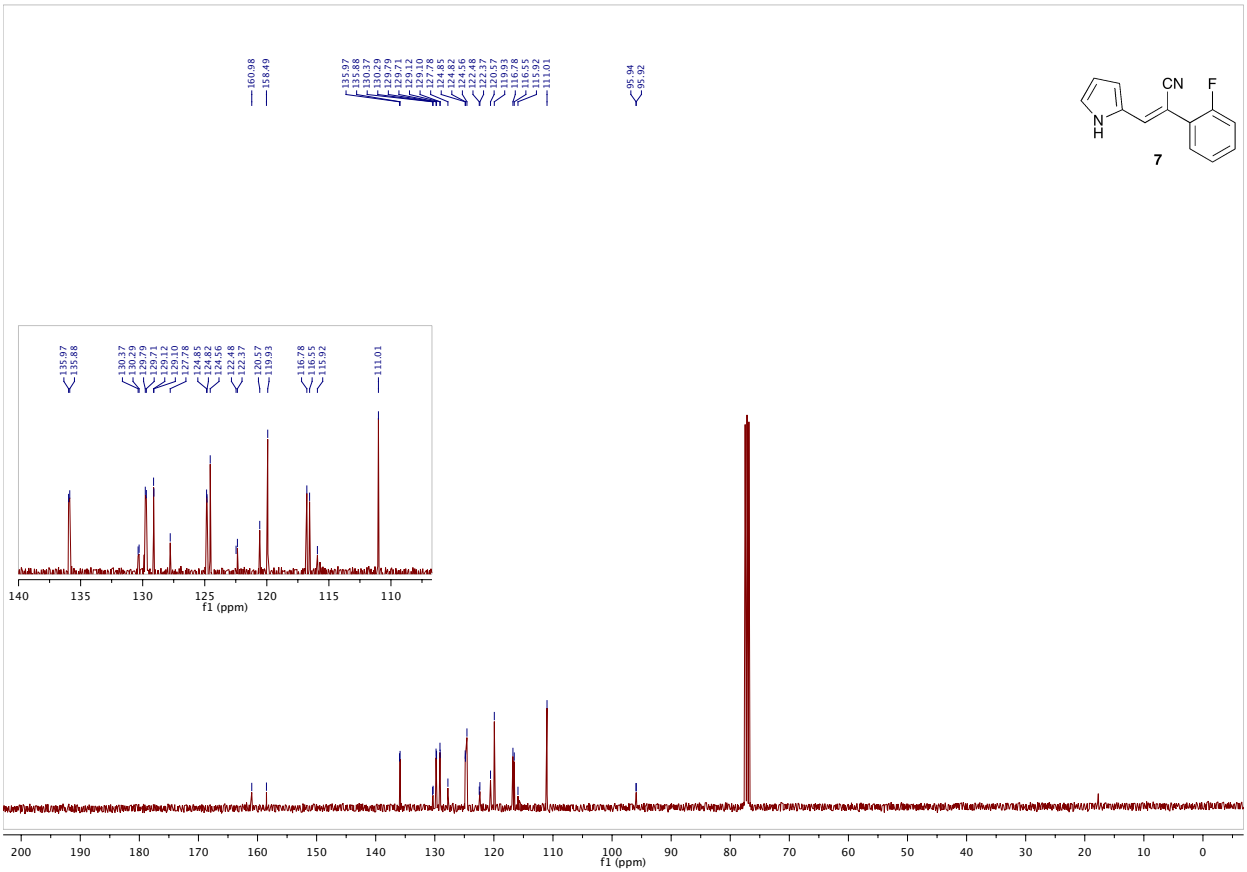
N
H
7
f1 (ppm)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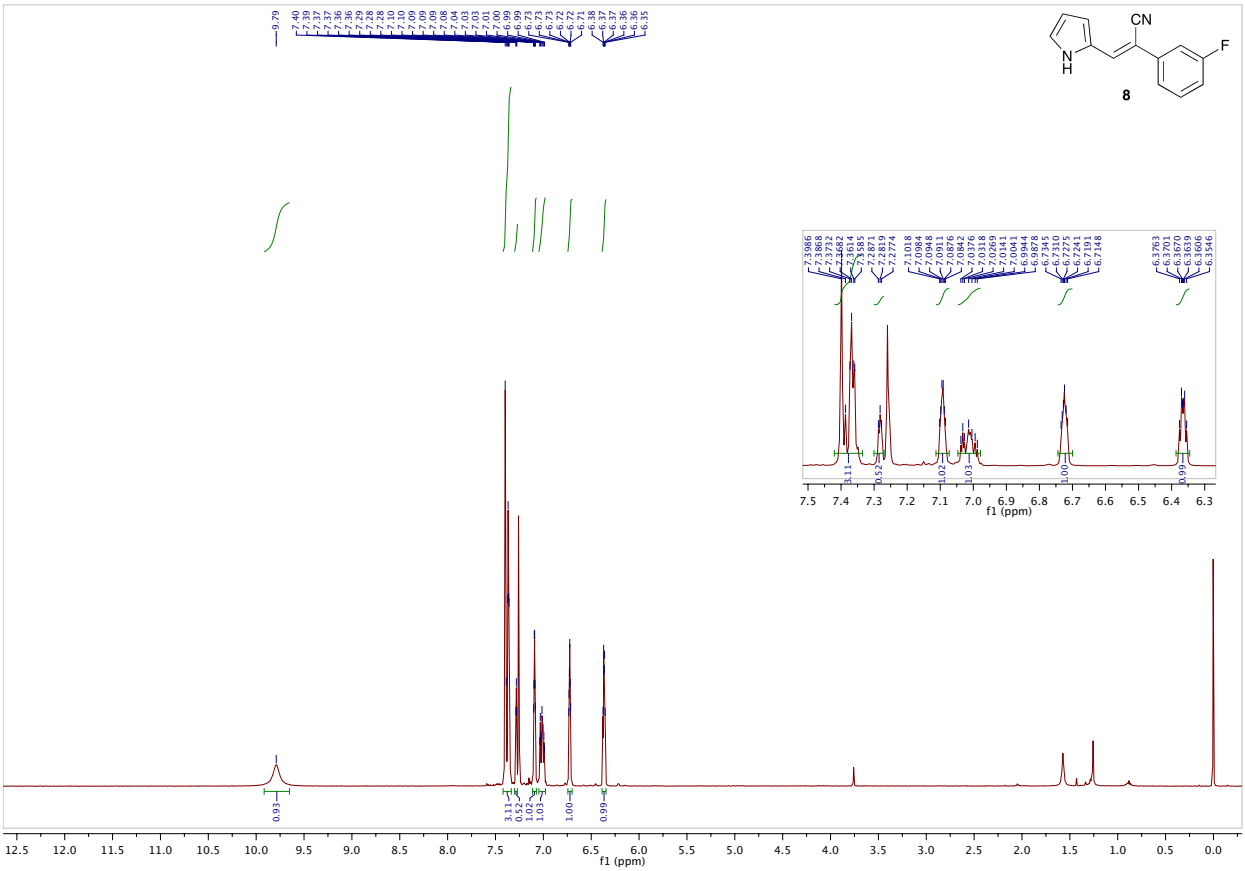
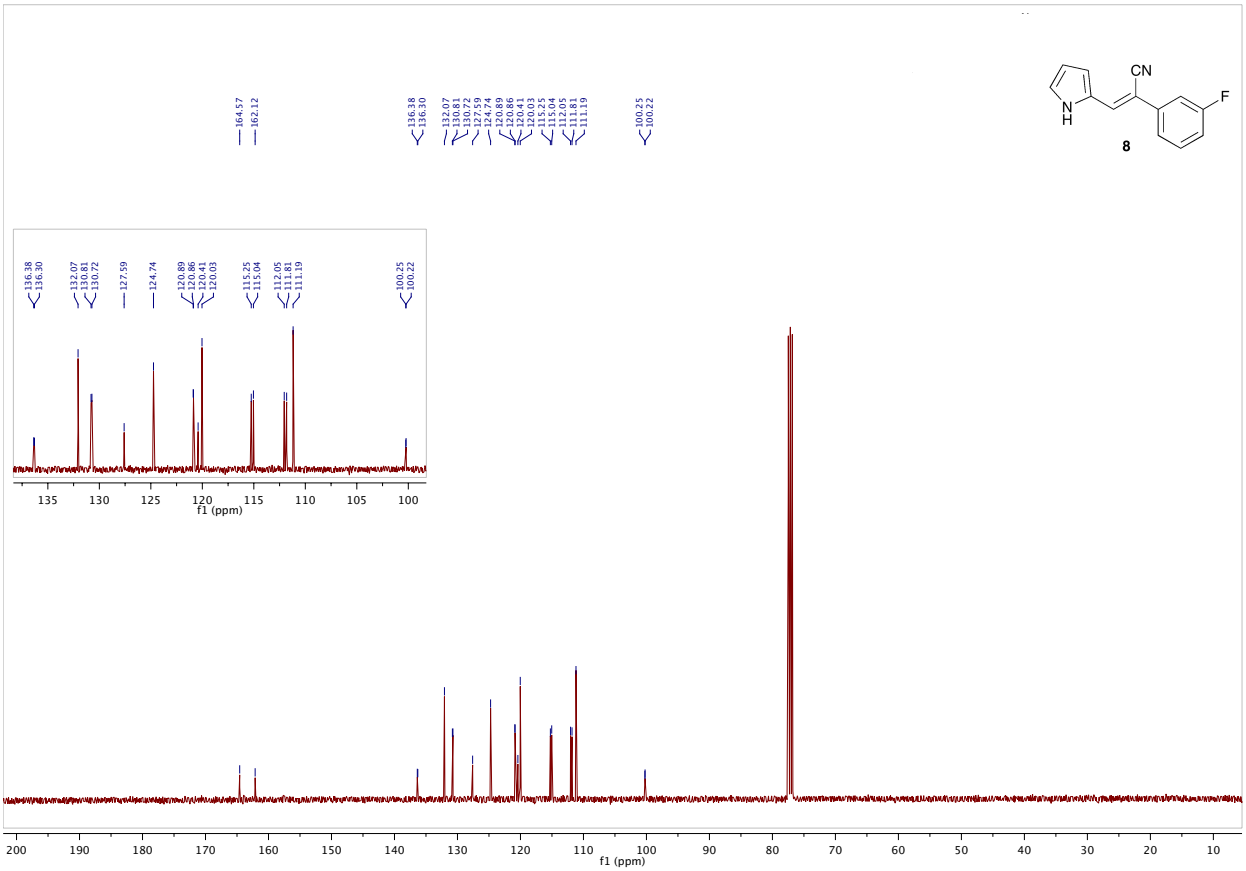
F
N
H
7
f1 (ppm)


CN
F
N
H
8
f1 (ppm)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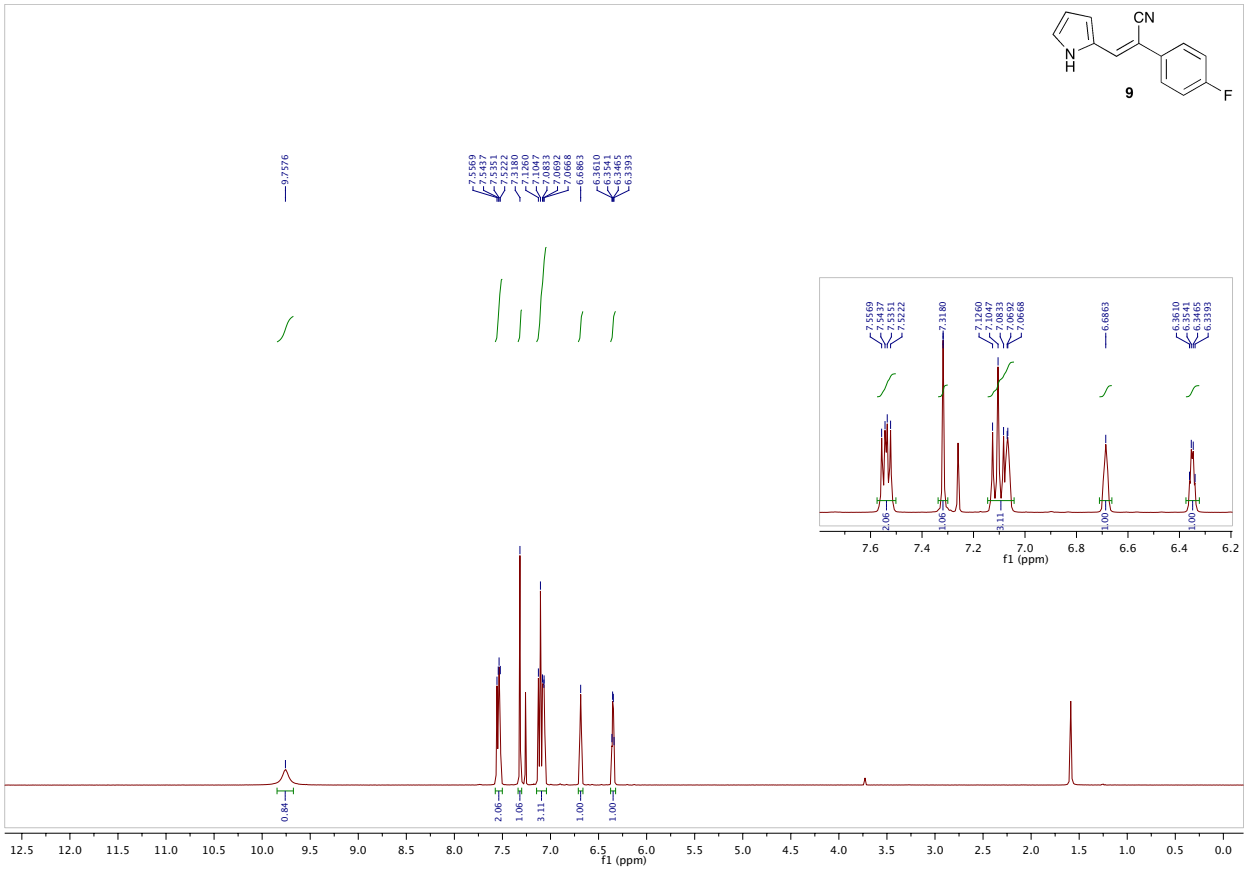
F
N
H
8
f1 (ppm)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N
H
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7.5351
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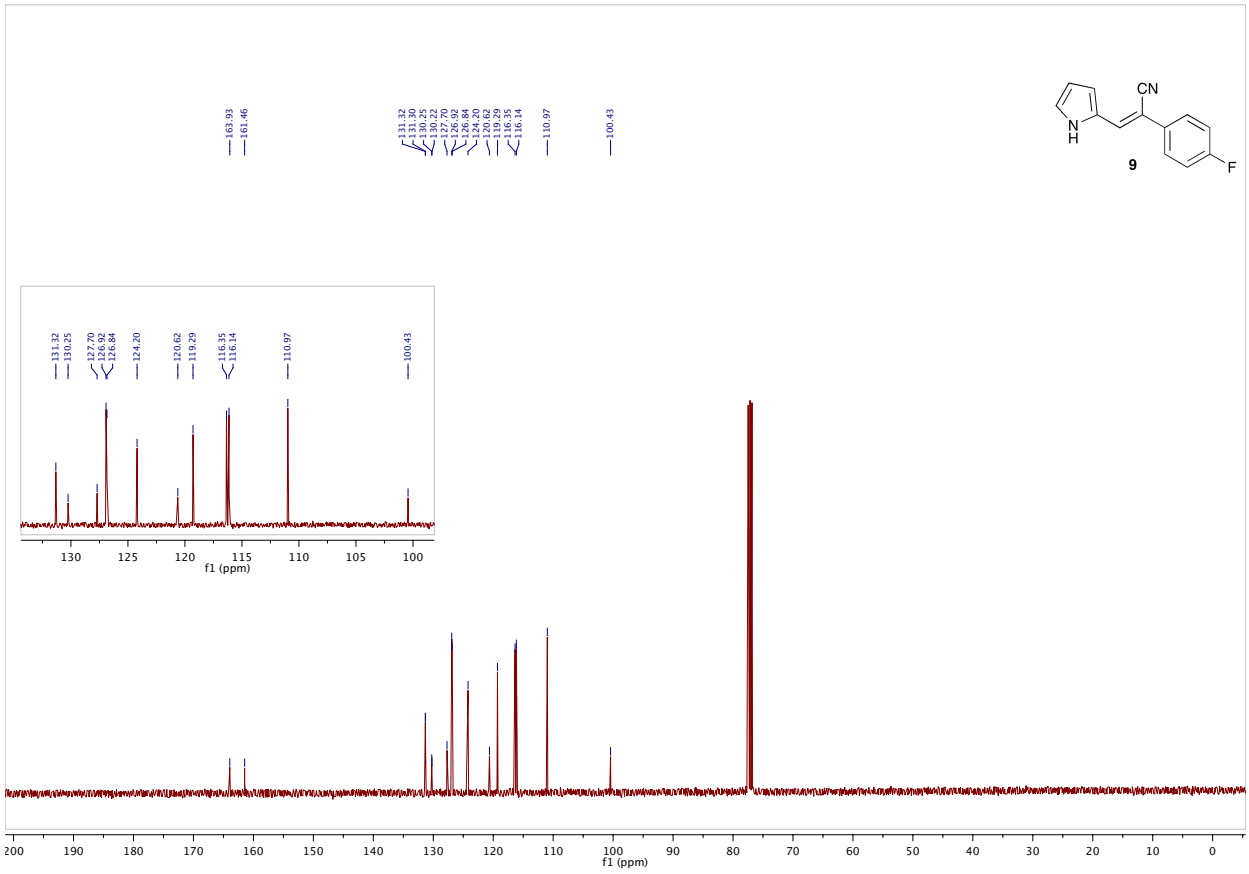
7.3180
7.1260
7.1047
7.0833
7.0692
7.0668
6.6863
6.3610
6.3541
6.3465
6.3393
0.84
2.06
1.06
3.11
1.00
1.00
f1 (ppm)


CN
N
H
F
9
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161.46
131.32
131.30
130.25
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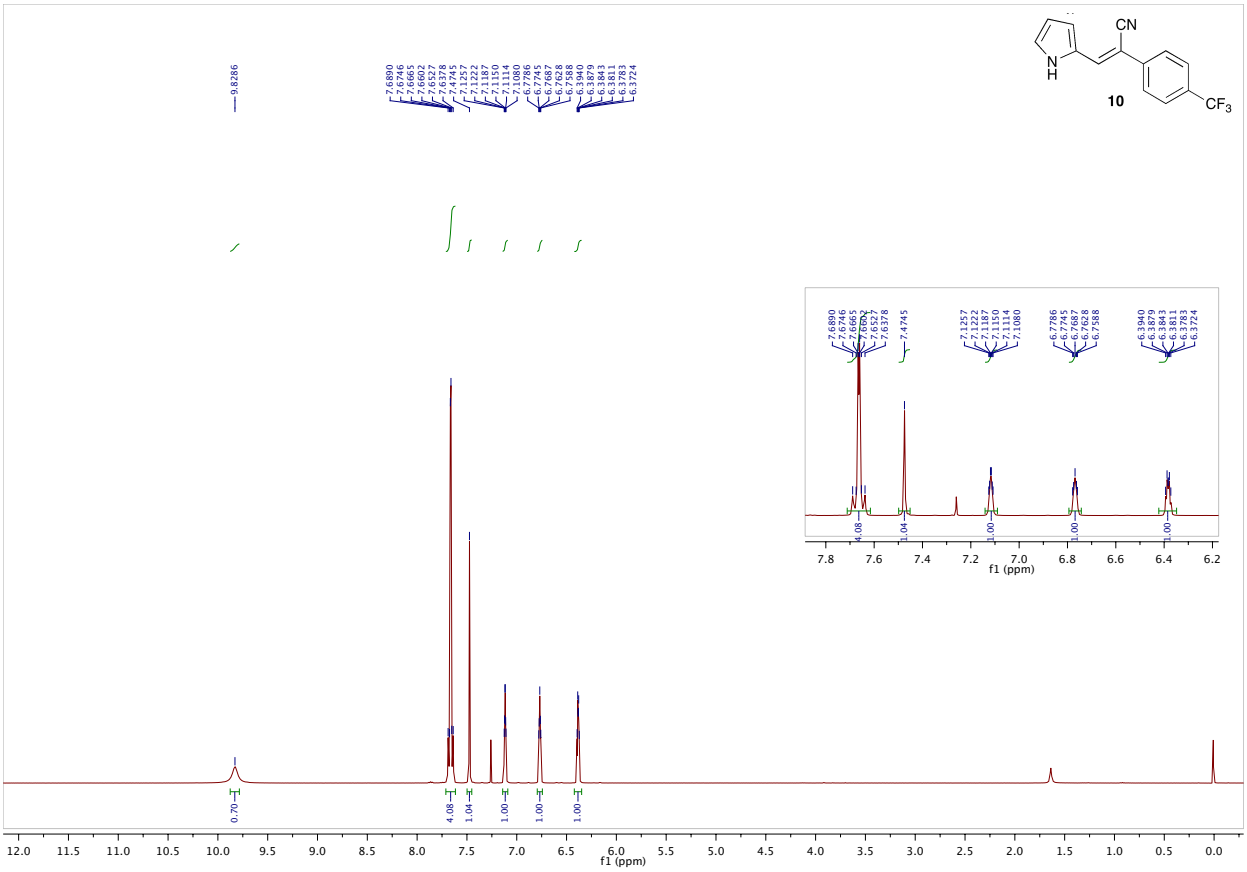
127.70
126.92
126.84
124.20
120.62
119.29
116.35
116.14
110.97
100.43
f1 (ppm)


CN
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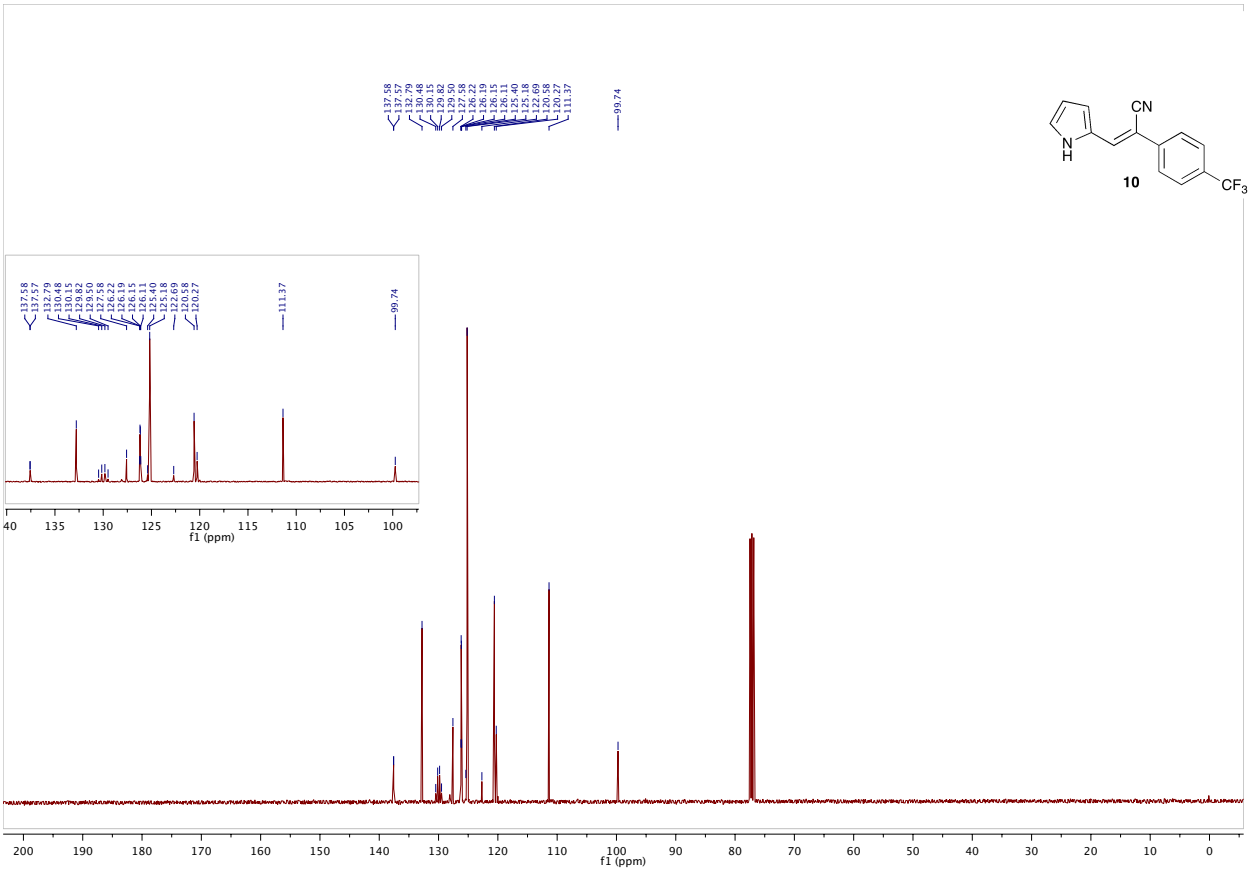
H
10
CF3
f1 (ppm)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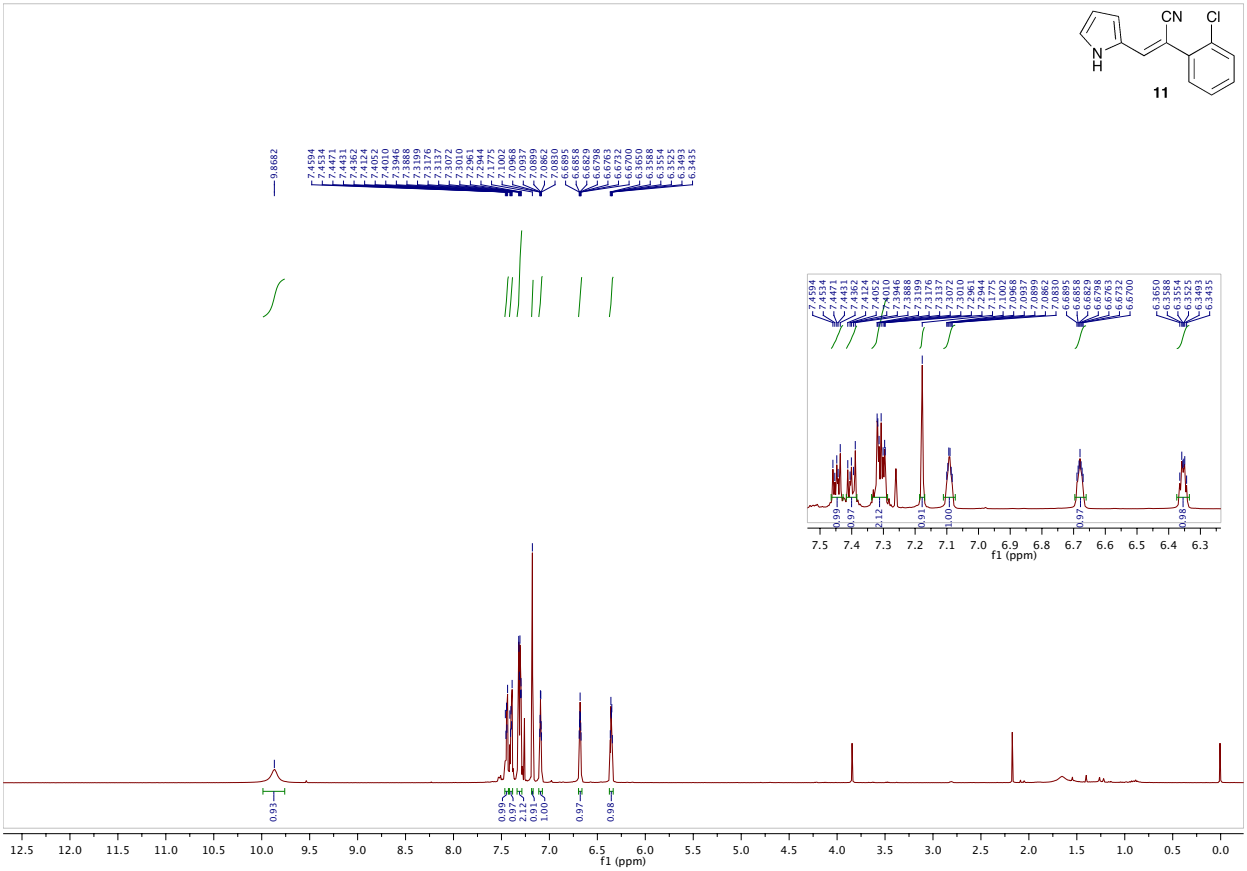
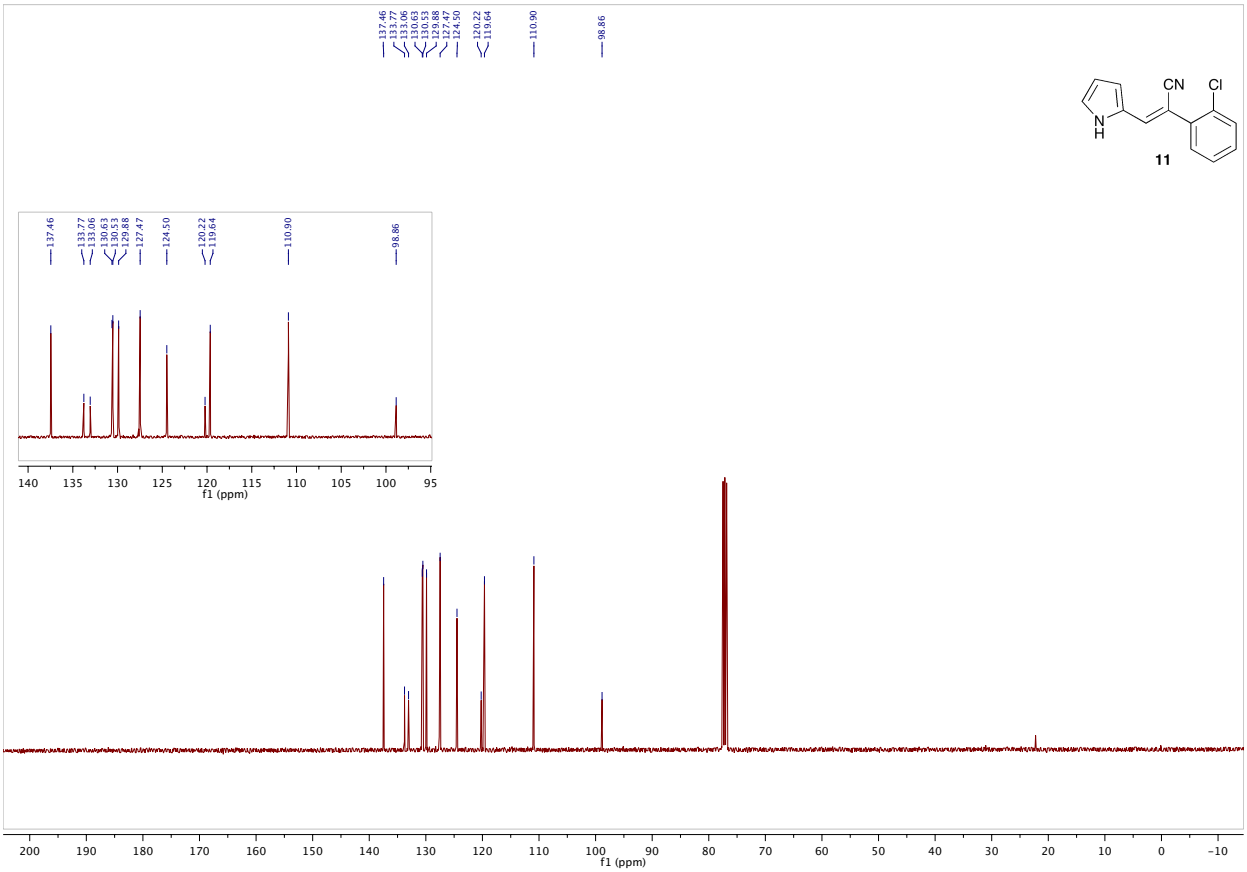
N
H
10
CF3
f1 (ppm)


CN
Cl
N
H
11
f1 (ppm)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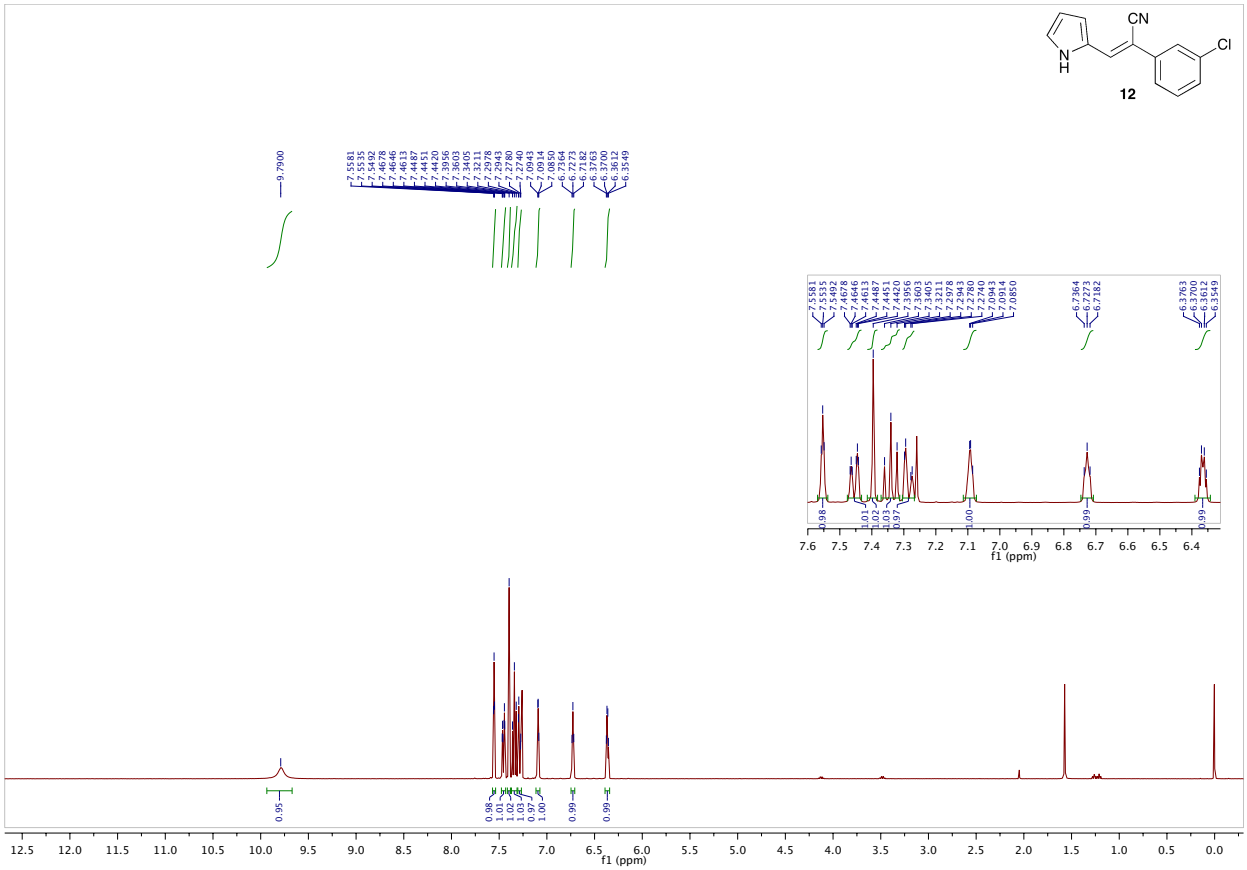
Cl
N
H
11
f1 (ppm)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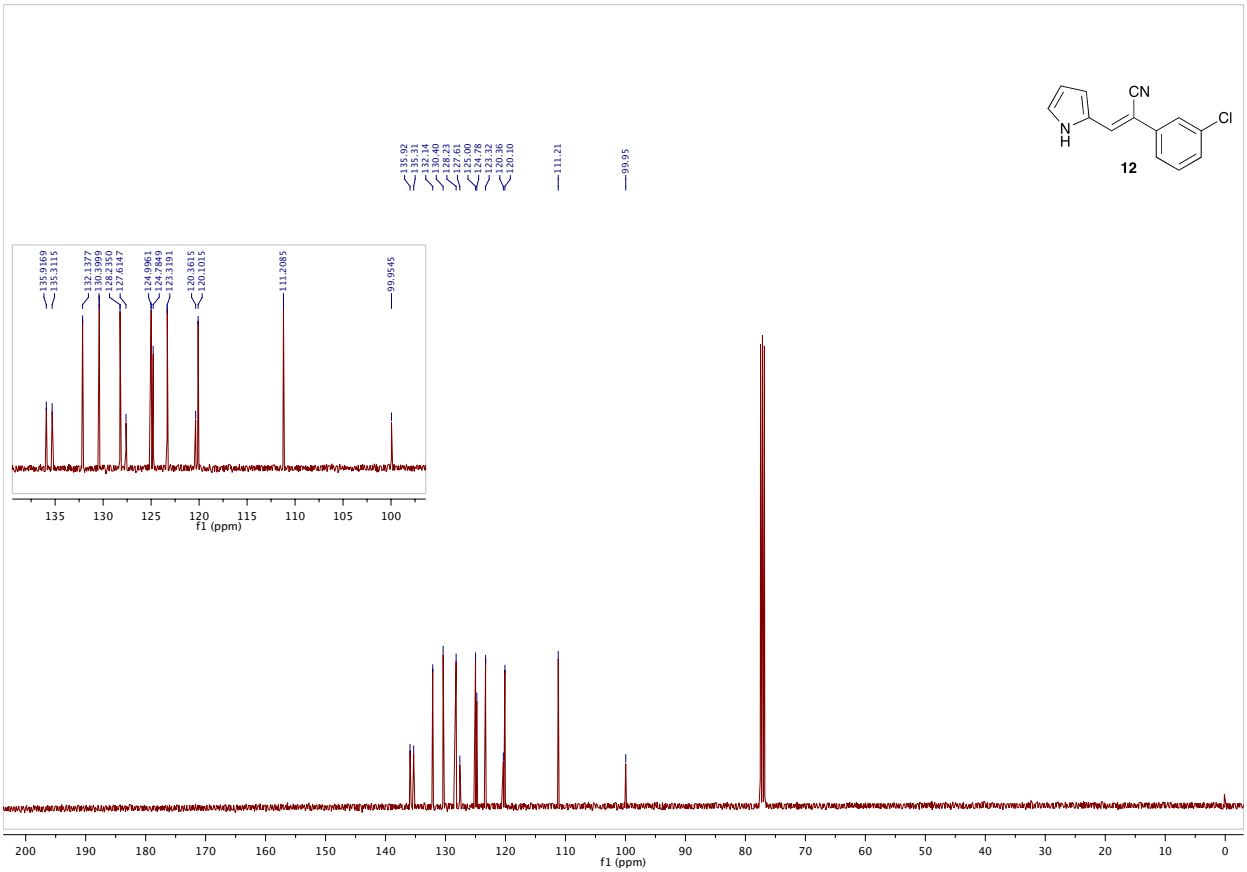
Cl
N
H
12
f1 (ppm)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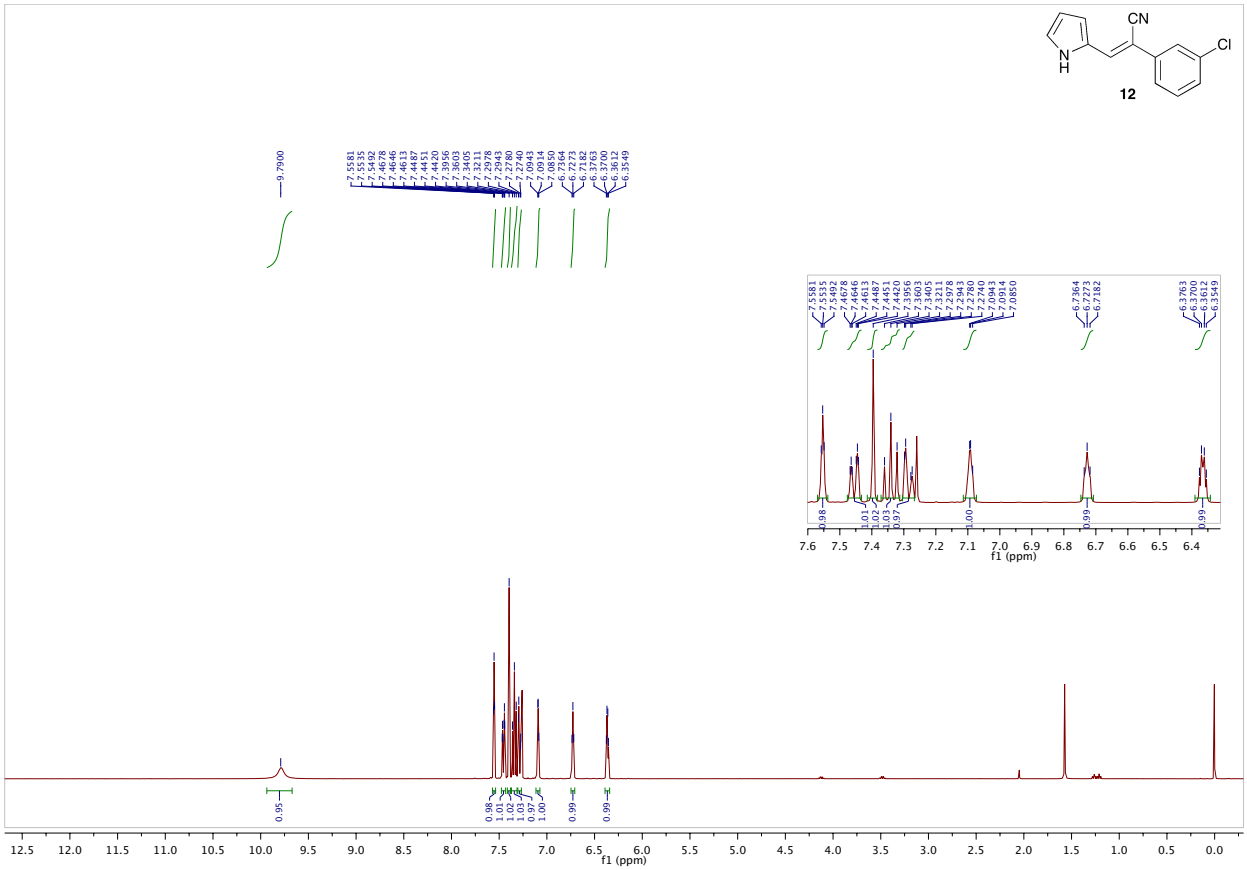
Cl
N
H
12
f1 (ppm)


CN
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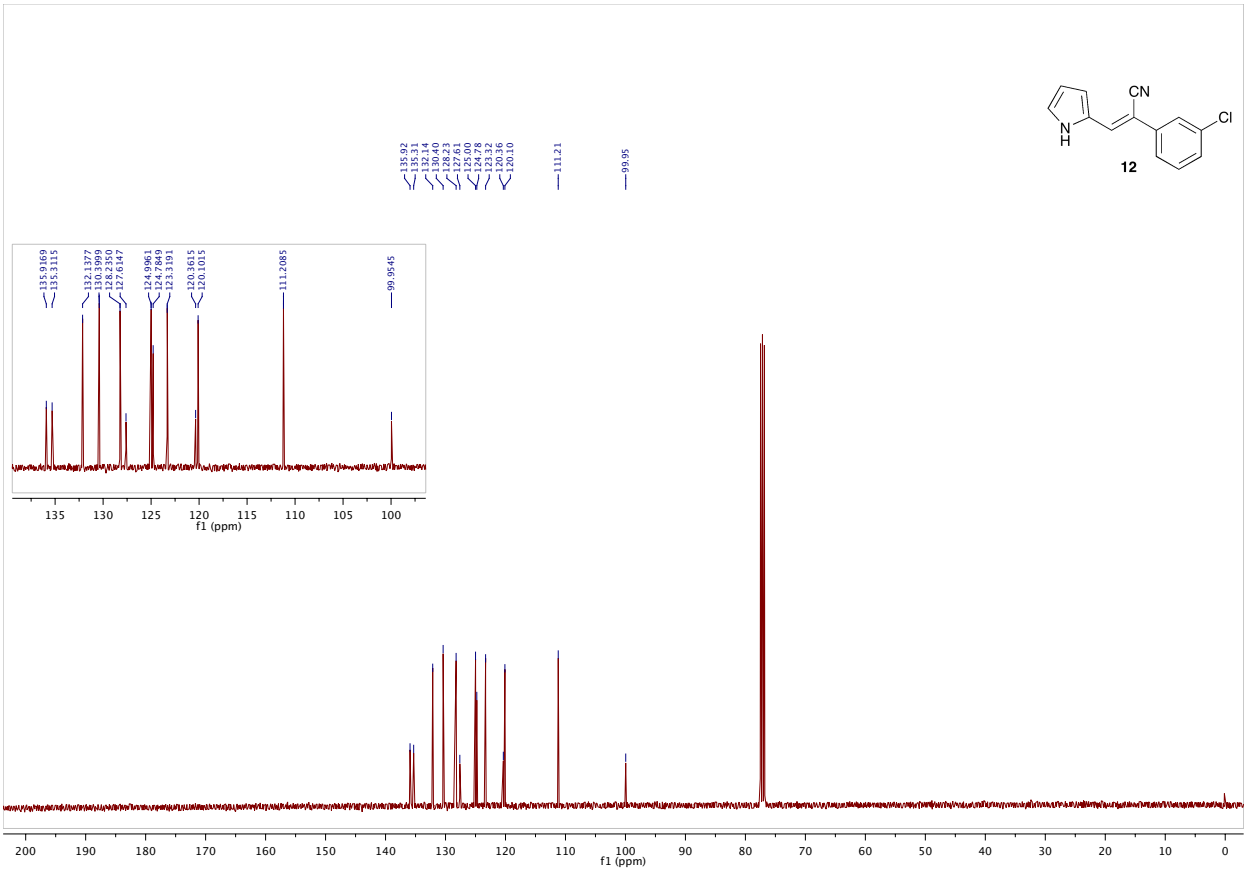
7.4646
7.4613
7.4487
7.4451
7.4420
7.3856
7.3805
7.3405
7.3211
7.2978
7.2943
7.2780
7.2740
7.0943
7.0914
7.0850
6.7364
6.7273
6.7182
6.3763
6.3700
6.3612
6.3549
0.95
0.98
1.01
1.02
1.03
0.97
1.00
0.99
0.99
f1 (ppm)


CN
Cl
N
H
12
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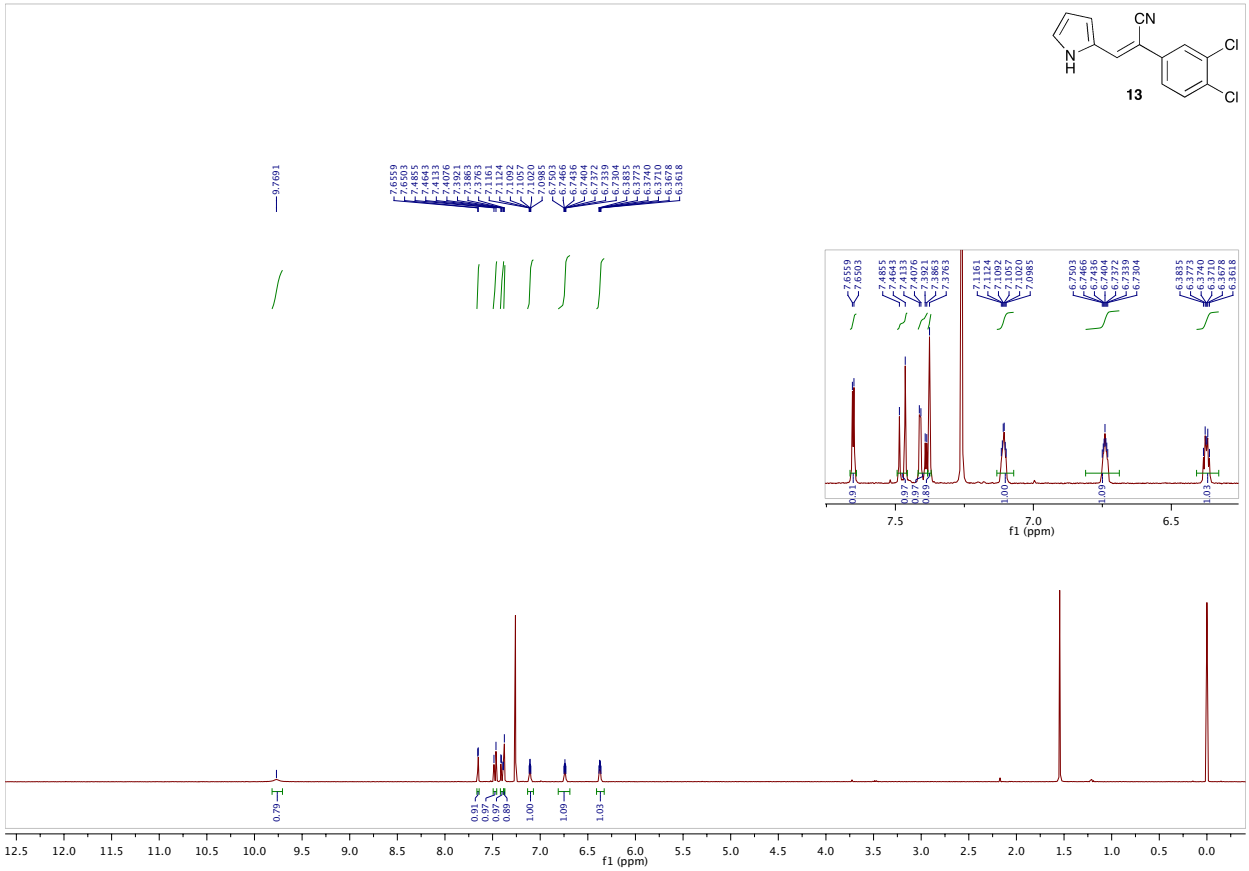
135.31
132.14
130.40
128.23
127.61
125.00
124.78
123.32
120.36
120.10
111.21
99.95
135.9169
135.3115
132.1377
130.3999
128.2350
127.6147
124.9961
124.7849
123.3191
120.3615
120.1015
111.2085
99.9545
f1 (ppm)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Cl
Cl
N
H
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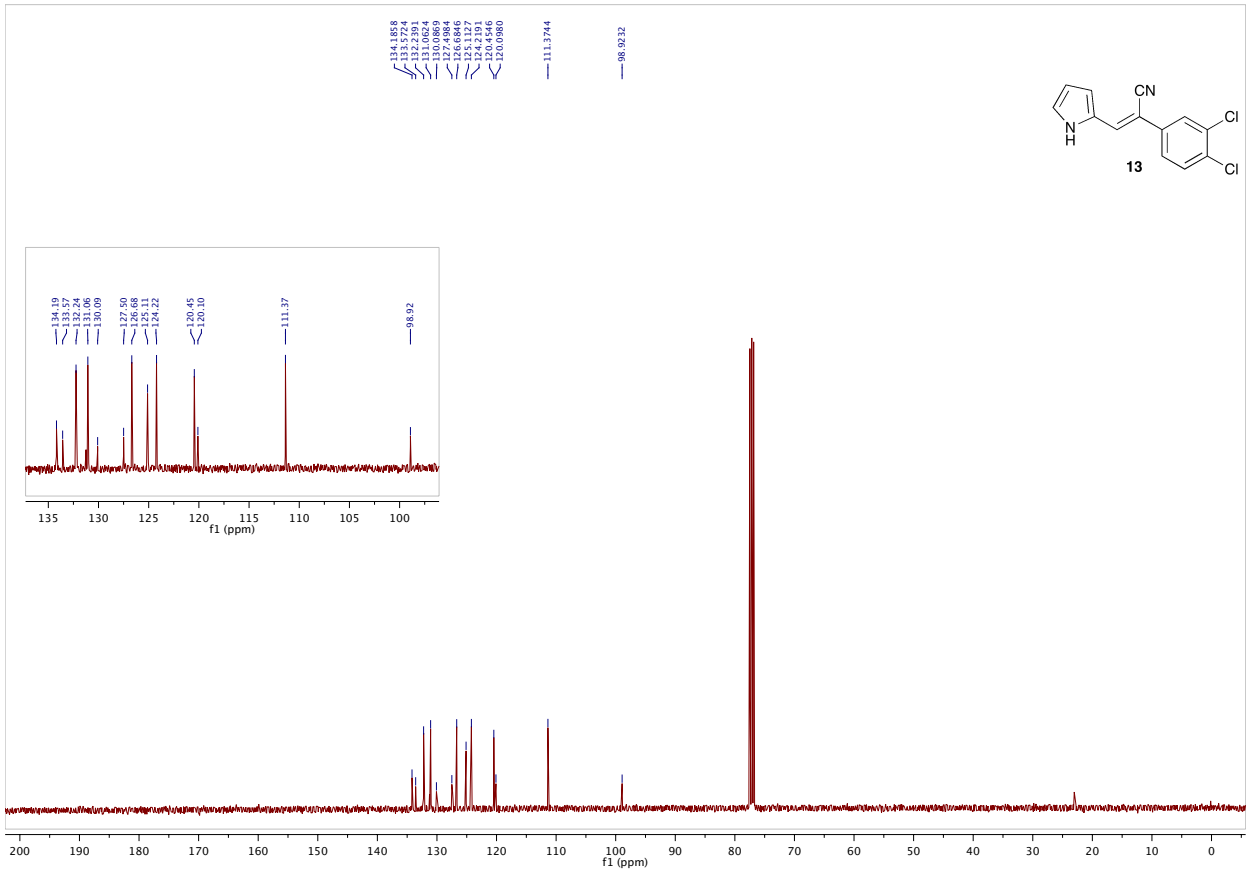
7.4133
7.4076
7.3921
7.3863
7.3763
7.3655
7.1124
7.1092
7.1057
7.1000
7.0985
6.7503
6.7466
6.7436
6.7404
6.7372
6.7339
6.7304
6.3835
6.3773
6.3740
6.3710
6.3678
6.3618
0.79
0.91
0.97
0.97
0.89
1.00
1.09
1.03
f1 (ppm)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Cl
Cl
N
H
13
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127.4984
126.6846
125.1127
124.2191
120.4546
120.0980
111.3744
98.9232
134.19
133.57
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127.50
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125.11
124.22
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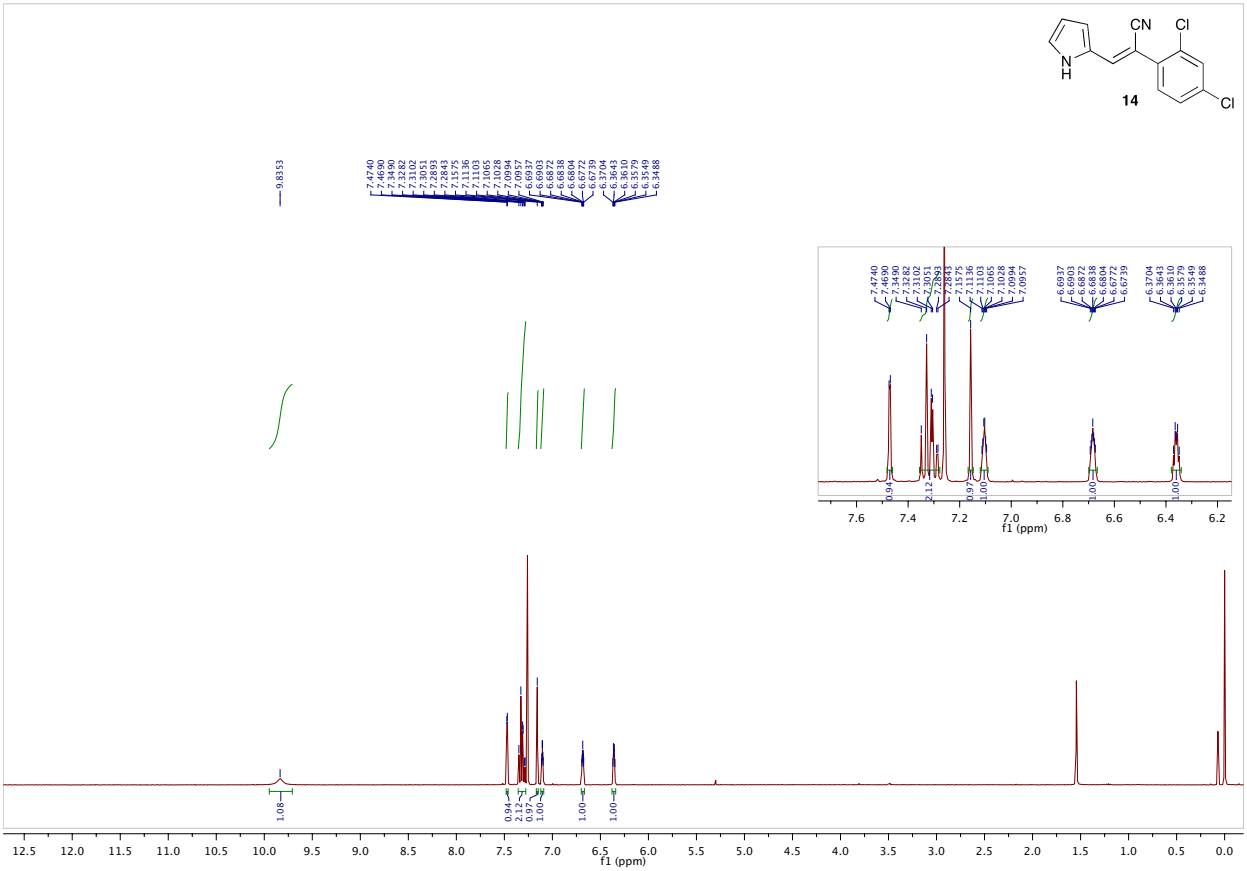
120.10
111.37
98.92
f1 (ppm)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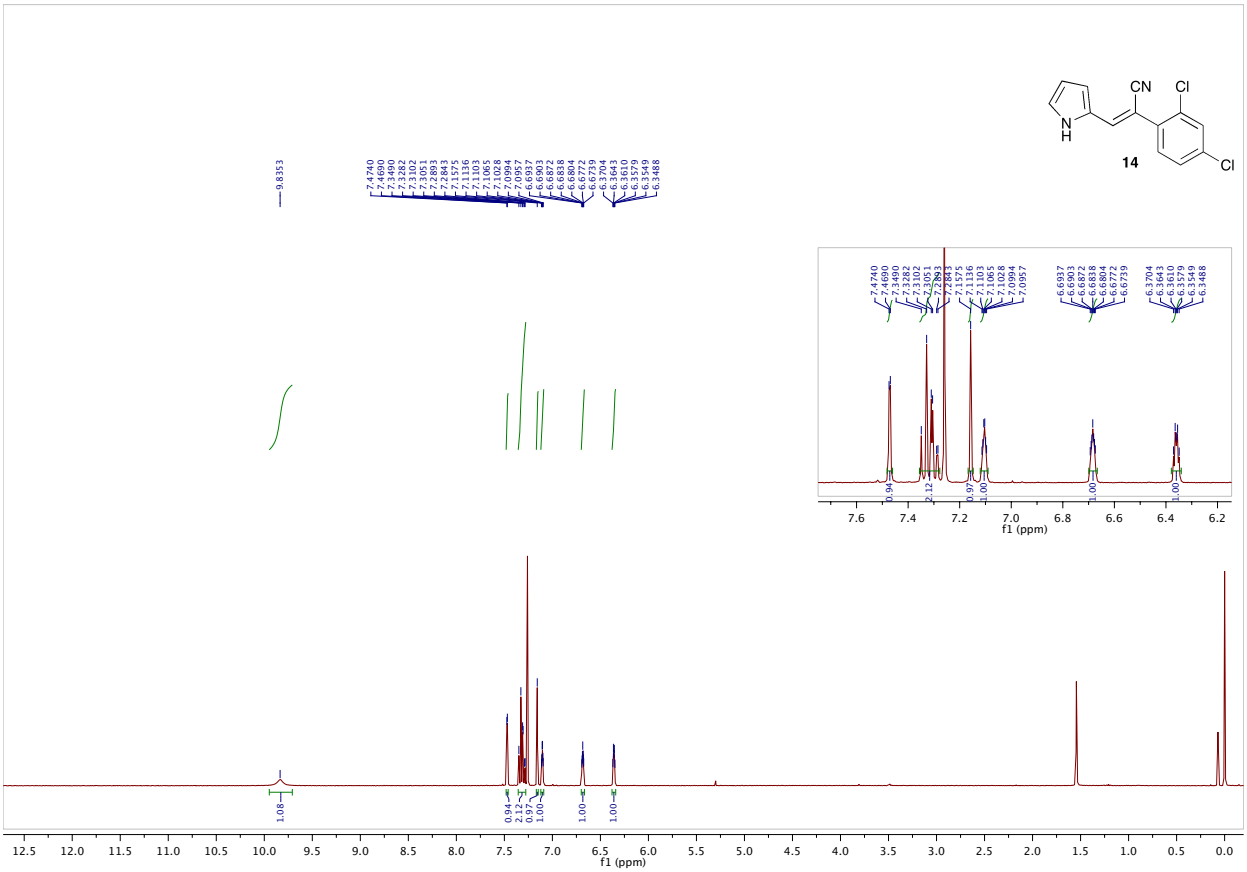
H
Cl
14
f1 (ppm)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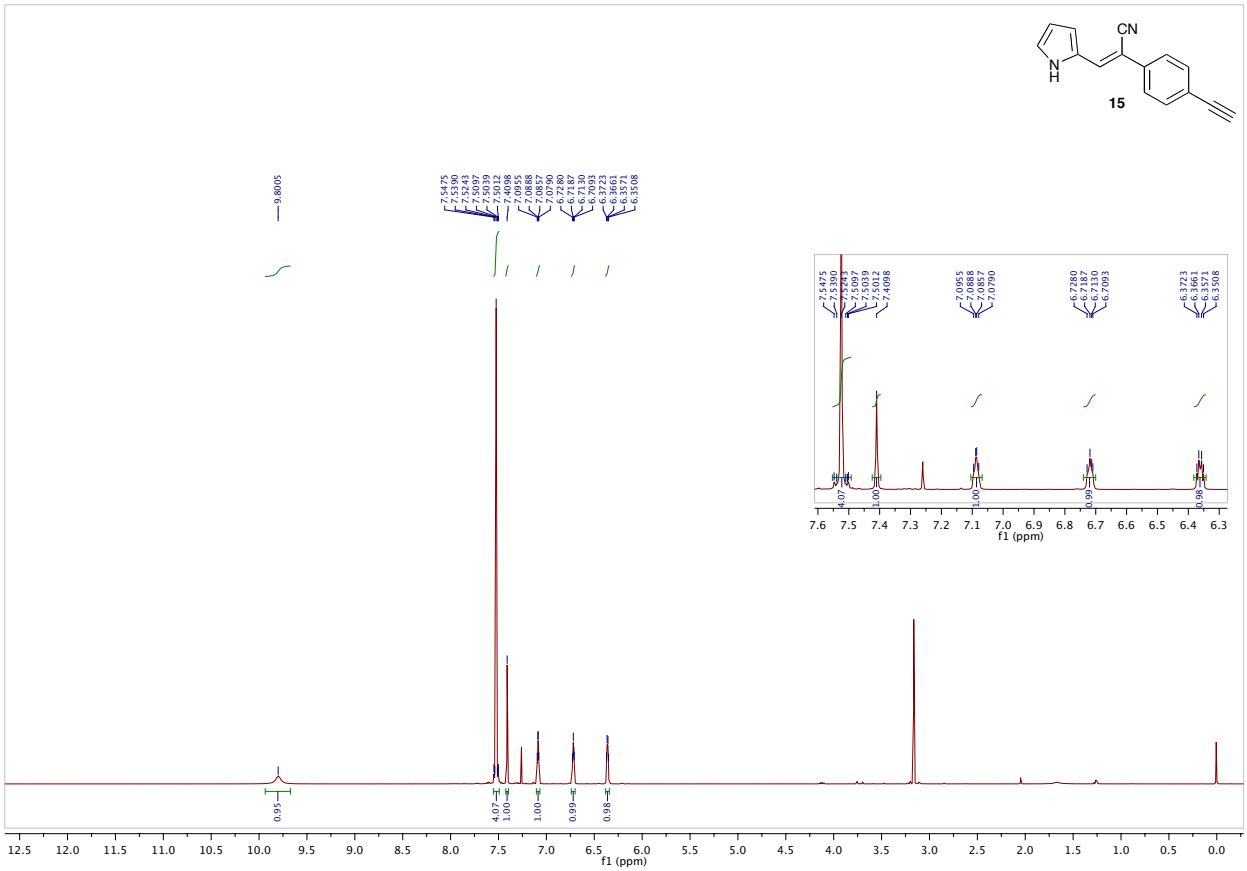
Cl
N
H
Cl
14
f1 (ppm)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N
H
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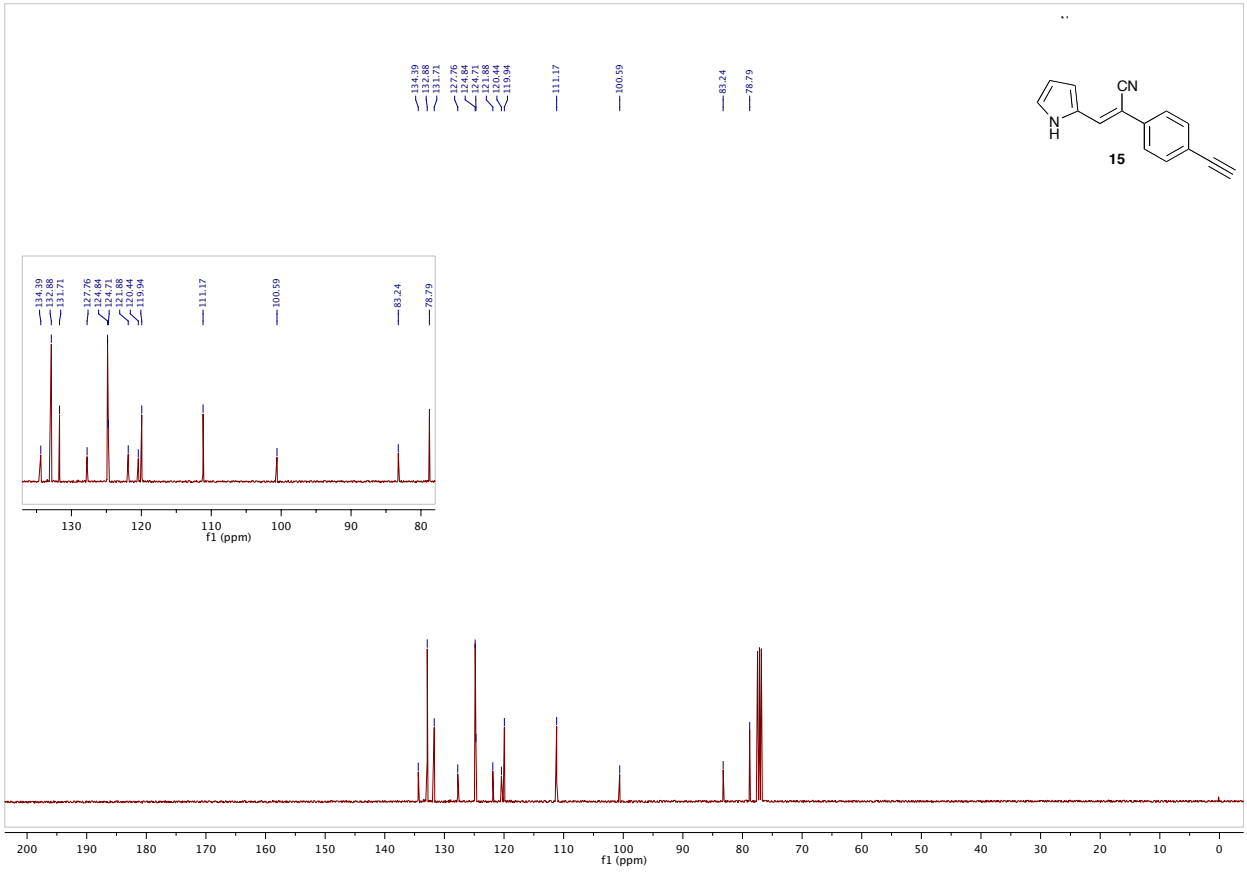
7.5390
7.5243
7.5097
7.5059
7.5012
7.4098
7.0955
7.0888
7.0857
7.0790
6.7280
6.7187
6.7130
6.7093
6.3723
6.3661
6.3571
6.3508
0.95
4.07
1.00
1.00
0.99
0.98
f1 (ppm)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H
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124.71
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119.94
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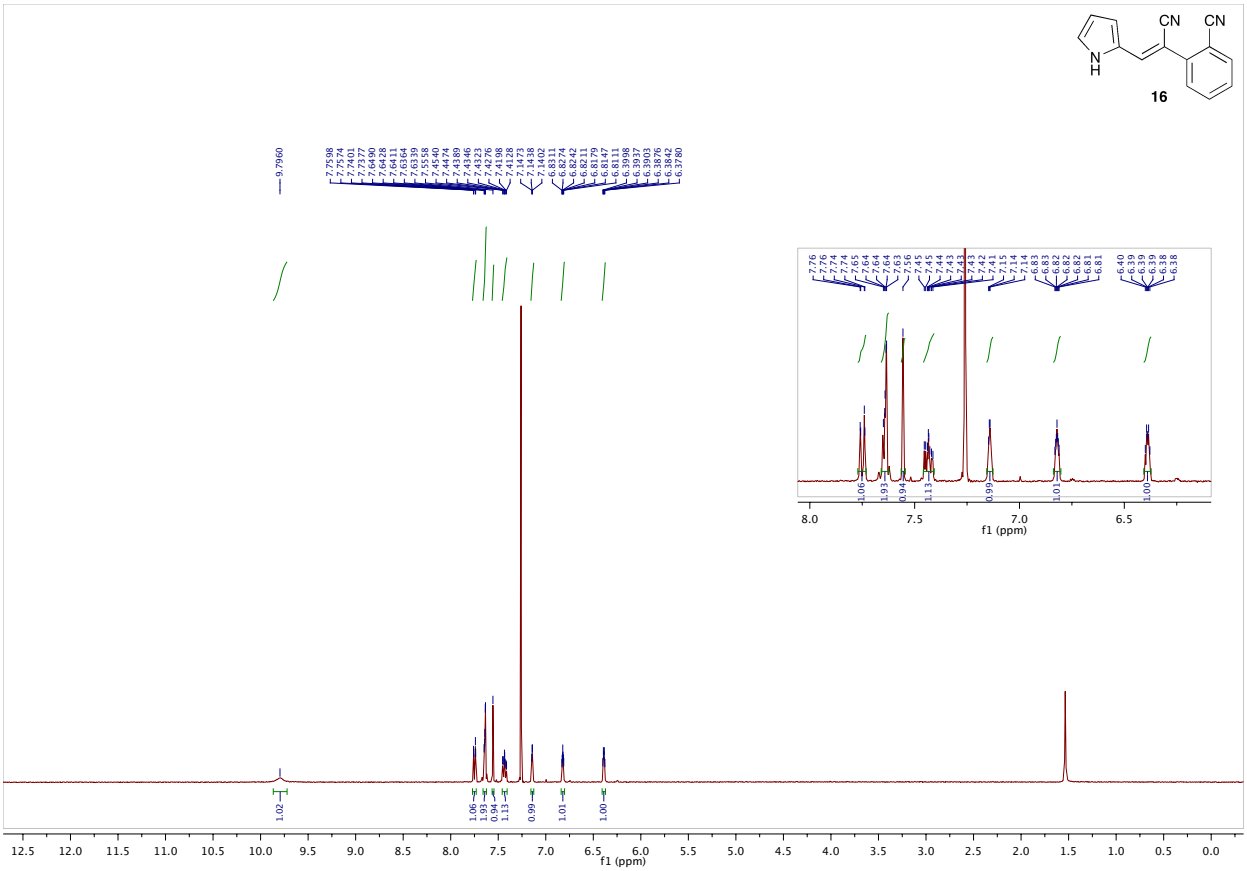
78.79
f1 (ppm)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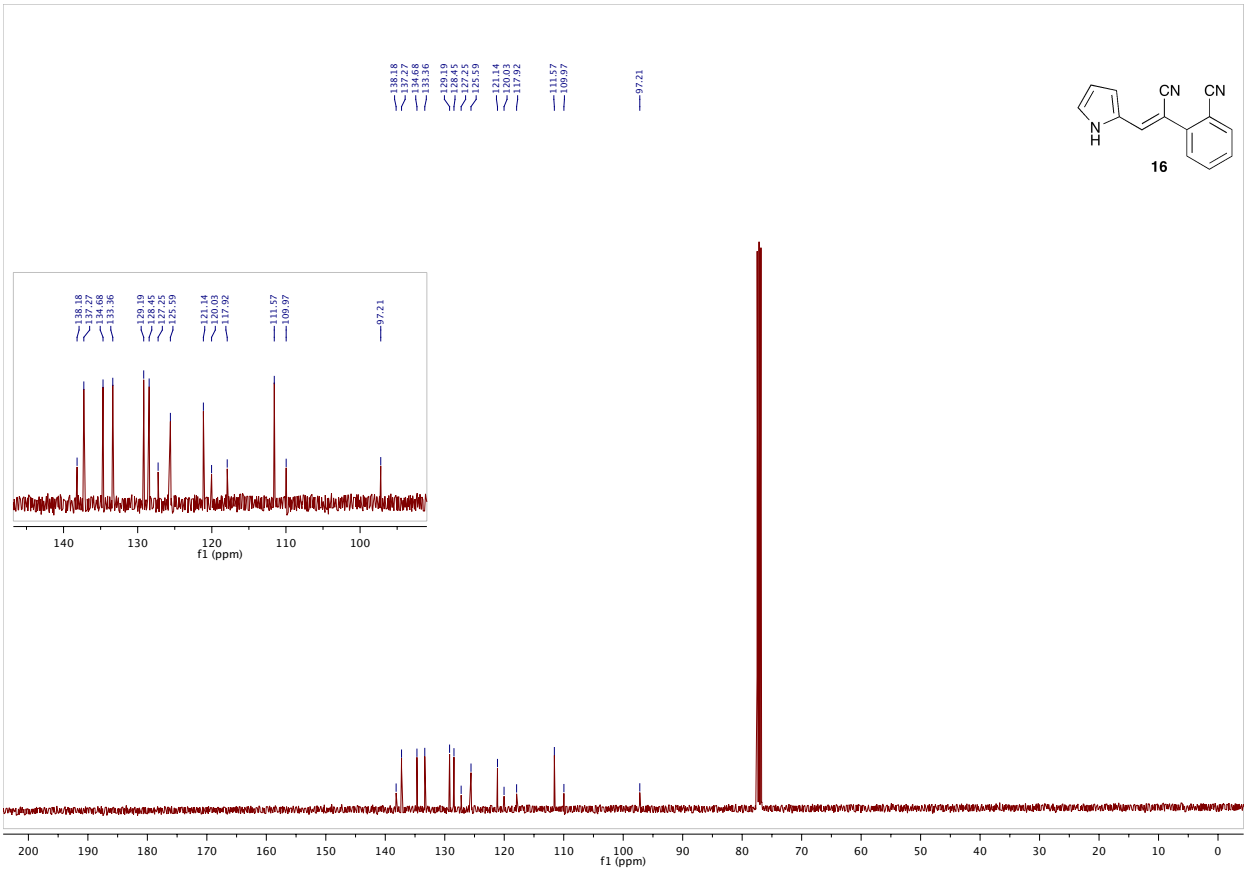
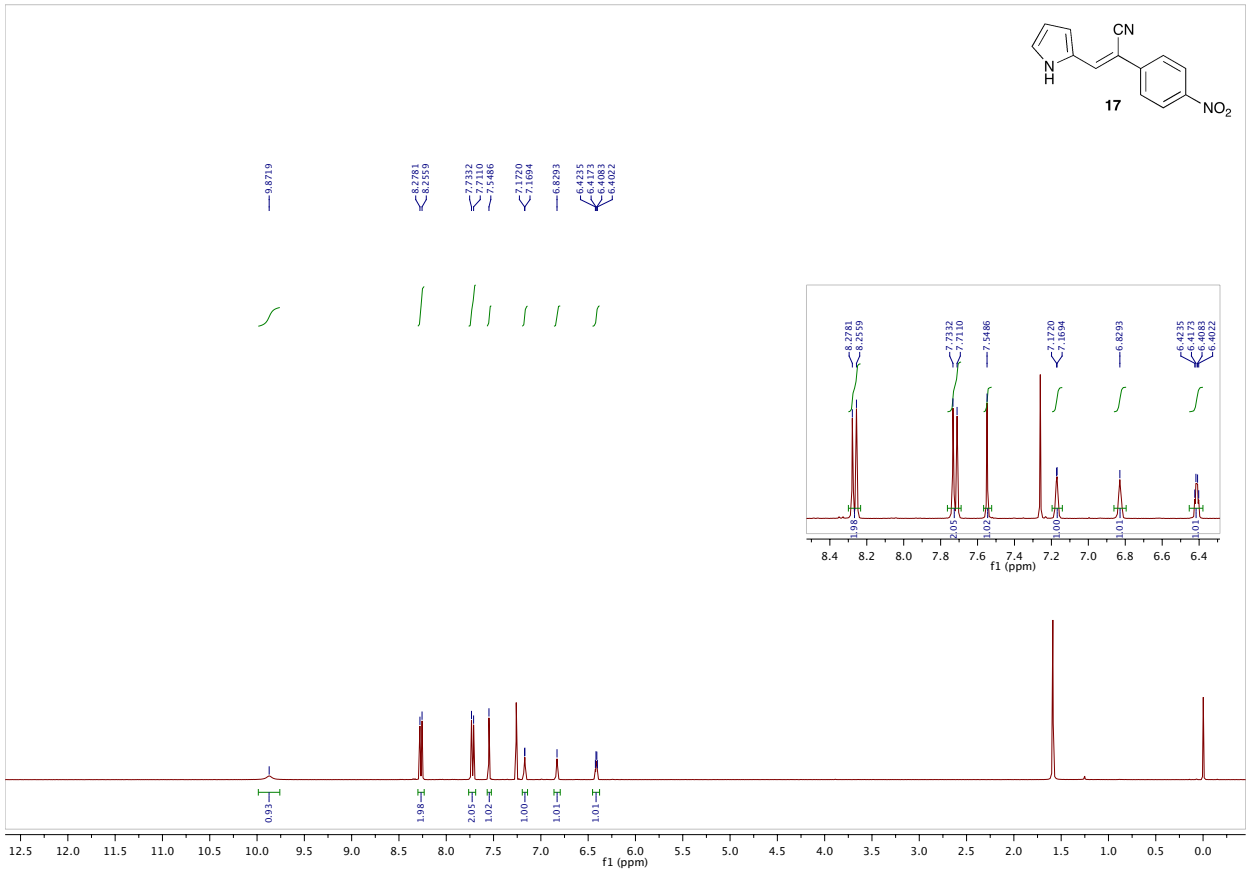
CN
N
H
16
f1 (ppm)


CN
CN
N
H
16
f1 (ppm)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H
NO2
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8.2559
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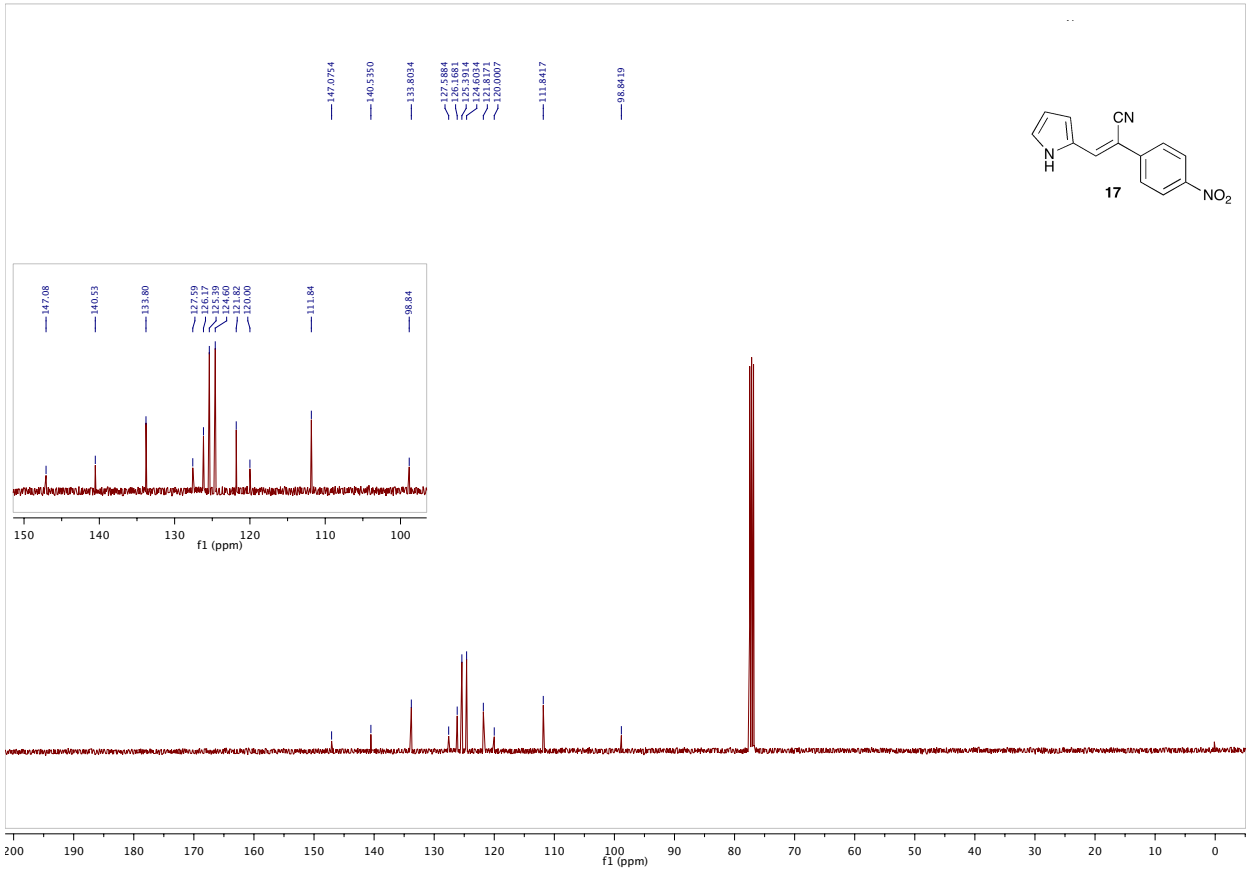
7.7110
7.5486
7.1720
7.1694
6.8293
6.4235
6.4173
6.4085
6.4022
0.93
1.98
2.05
1.02
1.00
1.01
1.01
f1 (ppm)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H
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126.1681
125.3914
124.6034
123.8731
120.0007
111.8417
98.8419
f1 (ppm)