***Supporting Information***

# Photoredox-Catalyzed Intermolecular Radical Arylthiocyanation/Arylselenocyanation of Alkenes: Access to Aryl substituted Alkylthiocyanates/Alkylselenocyanates

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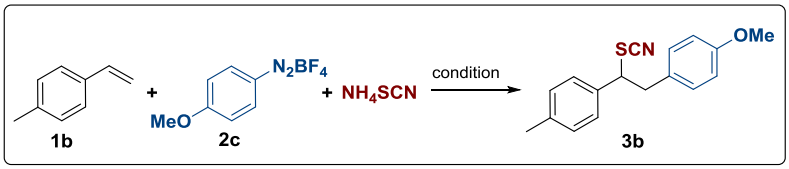
## 1. Optimization of the reaction condition:

***Table S1.*** Optimization of the reaction condition: [a]



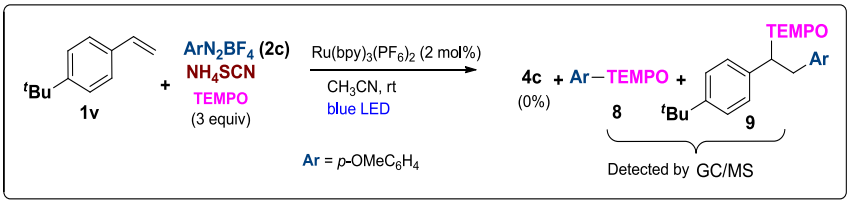

| entry | Photocatalyst | solvent | yield (%) |
|---|---|---|---|
| 1.[b] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 31 |
| **2.** | **$Ru(bpy)_3(PF_6)_2$** | **$CH_3CN$** | **76** |
| 3. | $Ru(bpy)_3(PF_6)_2$ | DCE | 51 |
| 4. | $Ru(bpy)_3(PF_6)_2$ | THF | 32 |
| 5. | $Ru(bpy)_3(PF_6)_2$ | Dioxane | 17 |
| 6. | $Ru(bpy)_3(PF_6)_2$ | Toluene | 24 |
| 7. | $Ru(bpy)_3(PF_6)_2$ | DMF | 0 |
| 8. | $Ru(bpy)_3(PF_6)_2$ | DMSO | 0 |
| 9. | Eosin Y | $CH_3CN$ | 28 |
| 10. | Rose Bengal | $CH_3CN$ | 33 |
| 11. | Methylene Blue | $CH_3CN$ | 18 |
| 12. | Rhodamine B | $CH_3CN$ | 23 |
| 13.[c] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 57 |
| 14.[d] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 52 |
| 15. | - | $CH_3CN$ | trace |
| 16.[e] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | trace |
| 17.[f] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 46 |
| 18.[g] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 67 |
| 19.[h] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 72 |
| 20.[i] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 31 |
| 21.[j] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 61 |
| 22.[k] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 65 |
| 23.[l] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 53 |
| 24.[m] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 48 |
| 25.[n] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 44 |

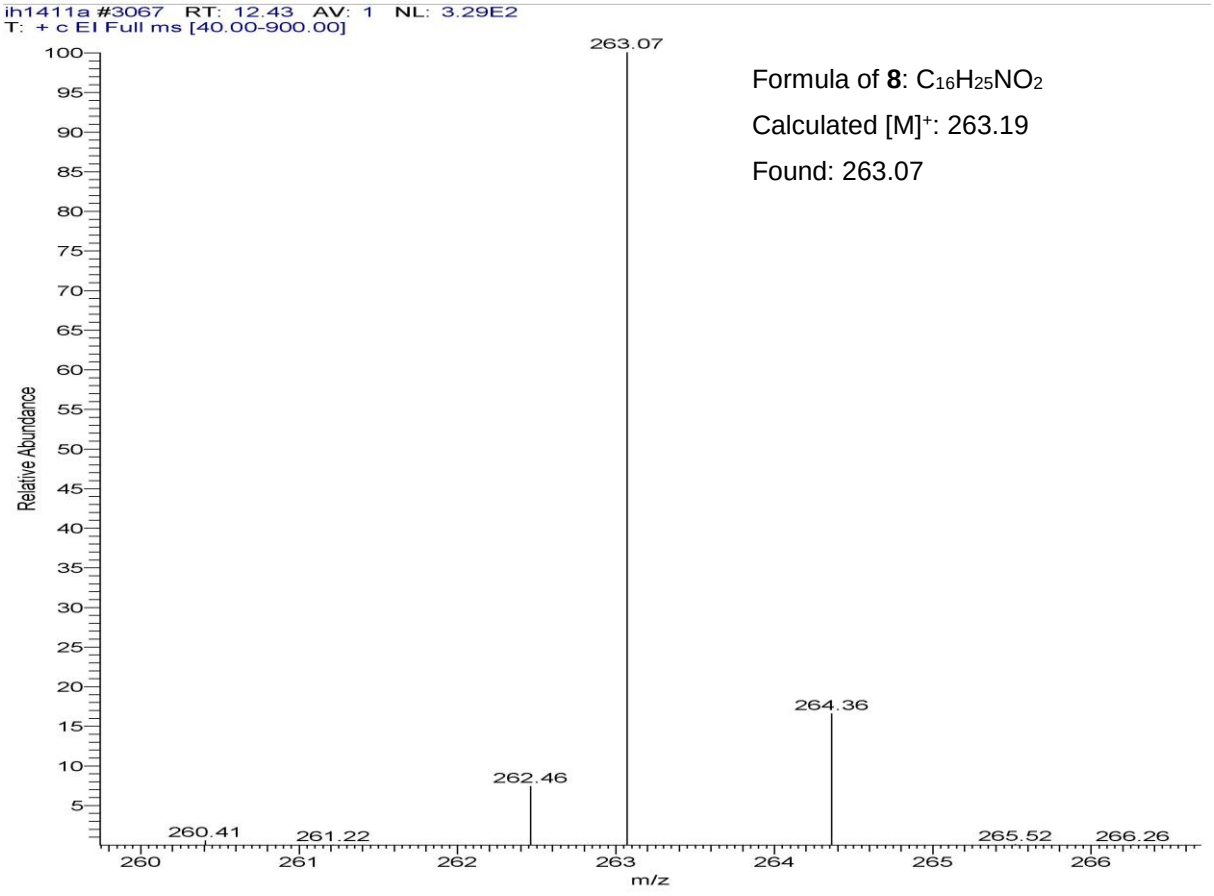
| | | | |
|---|---|---|---|
| 26.[o] | $Ru(bpy)_3(PF_6)_2$ | $CH_3CN$ | 37 |

[a]Unless otherwise noted, all reactions were carried out with: **1b** (0.4 mmol), **2c** (0.2 mmol), $NH_4SCN$ (0.6 mmol), photocatalyst (2 mol%), and degassed solvent (2 mL) in a culture tube under argon at rt irradiated with 12W blue LED for 6 h. [b]in air, [c]KSCN instead of $NH_4SCN$, [d]NaSCN instead of $NH_4SCN$,[e]in dark. [f]**1b** (0.2 mmol), [g]**1b** (0.3 mmol), [h]**1b** (0.5 mmol), [i]$NH_4SCN$ (0.2 mmol), [j]$NH_4SCN$ (0.4 mmol), [k]$NH_4SCN$ (0.7 mmol), [l]$CH_3CN$ (1 ml), [m]$CH_3CN$ (3 ml), [n]in 50 °C, [o]using house hold white CFL bulb.

## 2. Mechanistic Studies and Control Experiments:

***A. Radical trapping experiment:*** To investigation of the reaction mechanism for the present protocol, a radical trapping experiment was performed under the standard reaction condition. In presence of TEMPO free radical, the three-component reaction of 4-tert butyl styrene **1v**, 4-methoxybenzene diazonium tetrafluoroborate **2c** and ammonium thiocyanate was fully suppressed and no desired product **4c** was formed. A trace amount of the TEMPO adducts **8** and **9** were detected in GC/MS analysis from the crude reaction mixture. These results suggested that the reaction passes through radical pathway and aryl radical from **2c** and benzylic radical from adduct of **1v** and **2c** were involve as reaction intermediate.

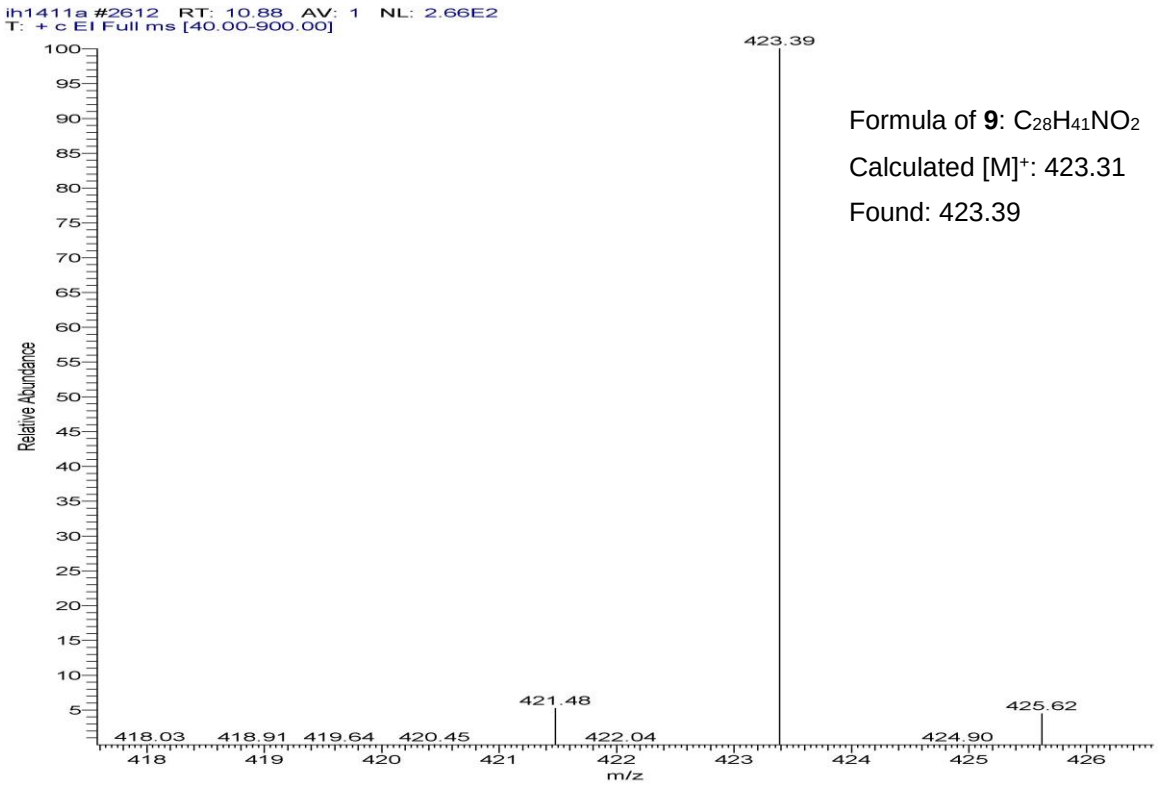


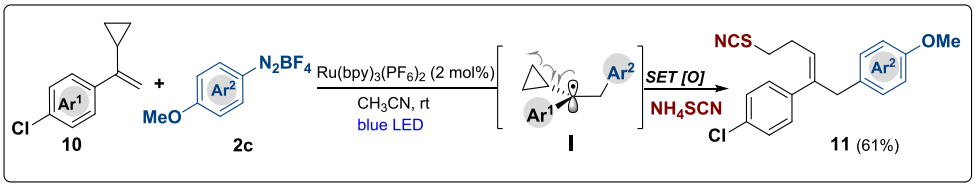

Formula of **8**: $C_{16}H_{25}NO_2$

Calculated $[M]^+$: 263.19

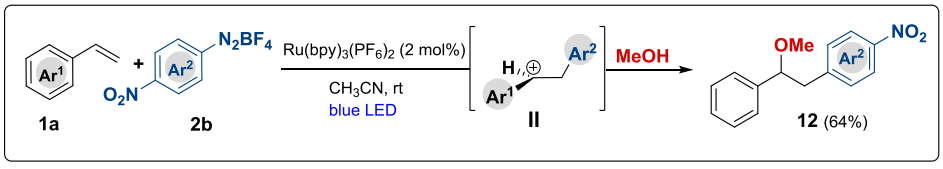
Found: 263.07




***B. Radical clock experiment:*** After the above Radical trapping experiments we have done radical clock experiment to prove the reaction mechanism. Here $\alpha$-cyclopropyl-4-chlorostyrene **10** react with 4-methoxybenzene diazonium tetrafluoroborate **2c** and ammonium thiocyanate under standard reaction conditions produces rearrangement product **11** in good yield. The rearrangement product **11** was resulted from oxidative addition with thiocyanate, which is generated from the rapid ring opening process of cyclopropylmethyl radical **I**, itself generated upon addition of the aryl radical to the alkene **10**. This experiment discloses strong support for the participation of aryl radical in this protocol via SET-type mechanism.




***C. Nucleophilic trapping experiment:*** When we carried out the reaction between styrene **1a** and 4-nitroybenzene diazonium tetrafluoroborate **2b** in presence of MeOH under the standard condition, we found to nucleophilic trapping adduct **12** in good yield. The methoxy product **12** was resulted from nucleophile trapping to the intermediate **II**, which is generated from the oxidative transformation of radical to cation, itself generated upon addition of the aryl radical to the alkene **1a**. This reveals strong support for the participation of the thiocyanate as anionic nucleophile in our protocol.



## 3. Stern-Volmer Study: Fluorescence Quenching Experiments:

Fluorescence quenching experiments were performed using a PerkinElmer LS 55 Fluorescence Spectrometer. In each experiment, measurement was carried out mixing a 2.33 x $10^{-4}$ M solution of $Ru(bpy)_3(PF_6)_2$ in MeCN (2 mL) with appropriate amount of quencher in quartz cuvette. The sample solutions were previously degassed with argon. The solution was irradiated at 450 nm, and the emission intensity was overserved at 611 nm. Plots were derived according to the Stern-Volmer equation and $K_{sv}$ calculated.

Stern-Volmer equation

$$I_0/I = 1 + K_{sv}[Q]$$

Where $I_0$ is the luminescence intensity without the quencher, I is the intensity with the quencher, [Q] is the concentration of added quencher and $K_{sv}$ is the Stern-Volmer quenching constant.

**Stern-Volmer Quenching Studies with Diazonium salt:**

Increasing amounts of 4-methoxybenzene diazonium tetrafluoroborate were added to the solution of $Ru(bpy)_3(PF_6)_2$ in acetonitrile. Emission spectrum were recorded after each addition. The results in Figure S1 (a) shows a huge change in the emission intensity of $Ru(bpy)_3(PF_6)_2$ with a calculated $K_{sv}$ of 12 $mM^{-1}$ [Figure S1 (b)].

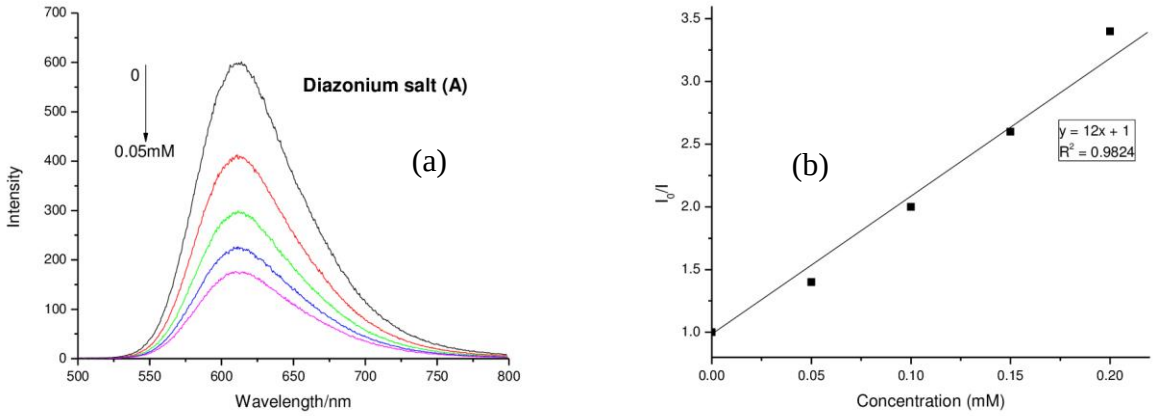



**Figure S1. (a)** Emission spectrum of $Ru(bpy)_3(PF_6)_2$ with varying concentration of 4-Methoxybenzene diazonium tetrafluoroborate & **(b)** Stern-Volmer plots of $Ru(bpy)_3(PF_6)_2$ quenching with 4-Methoxybenzene diazonium tetrafluoroborate.

**Stern-Volmer Quenching Studies with $NH_4SCN$:**

Increasing amounts of ammonium thiocyanate were added to the solution of $Ru(bpy)_3(PF_6)_2$ in acetonitrile. Emission spectrum were recorded after each addition. The results in Figure S2 (a) shows a slight change in the emission intensity of $Ru(bpy)_3(PF_6)_2$ with a calculated $K_{sv}$ of 0.72 $mM^{-1}$ [Figure S2 (b)].

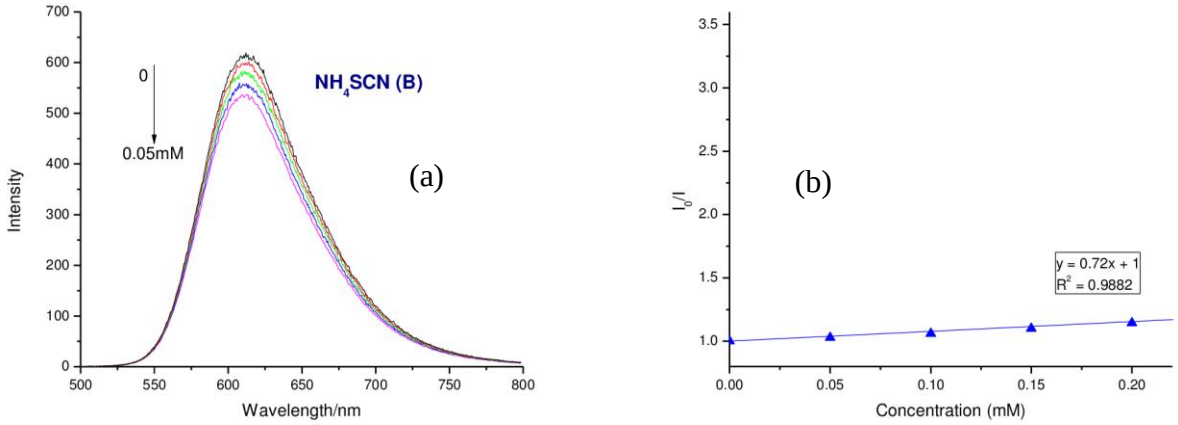



**Figure S2. (a)** Emission spectrum of $Ru(bpy)_3(PF_6)_2$ with varying concentration of Ammonium thiocyanate & **(b)** Stern-Volmer plots of $Ru(bpy)_3(PF_6)_2$ quenching with Ammonium thiocyanate.

**Stern-Volmer Quenching Studies with Styrene:**

Increasing amounts of 4-Methyl styrene were added to the solution of $Ru(bpy)_3(PF_6)_2$ in acetonitrile. Emission spectrum were recorded after each addition. The results in Figure S3 (a) shows a negligible change in the emission intensity of $Ru(bpy)_3(PF_6)_2$ with a calculated $K_{sv}$ of 0.4 $mM^{-1}$ [Figure S3 (b)].

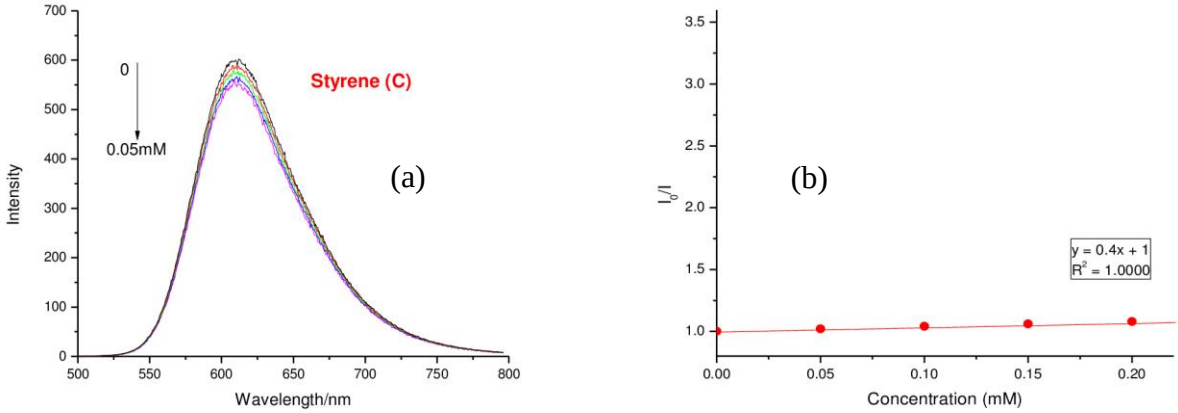



**Figure S3. (a)** Emission spectrum of $Ru(bpy)_3(PF_6)_2$ with varying concentration of 4-Methyl styrene & **(b)** Stern-Volmer plots of $Ru(bpy)_3(PF_6)_2$ quenching with 4-Methyl styrene.

## 4. X-ray Crystal Data with ORTEP Plot for Compound 3k:

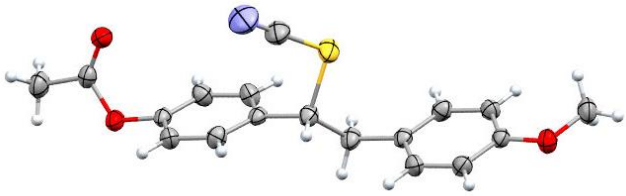


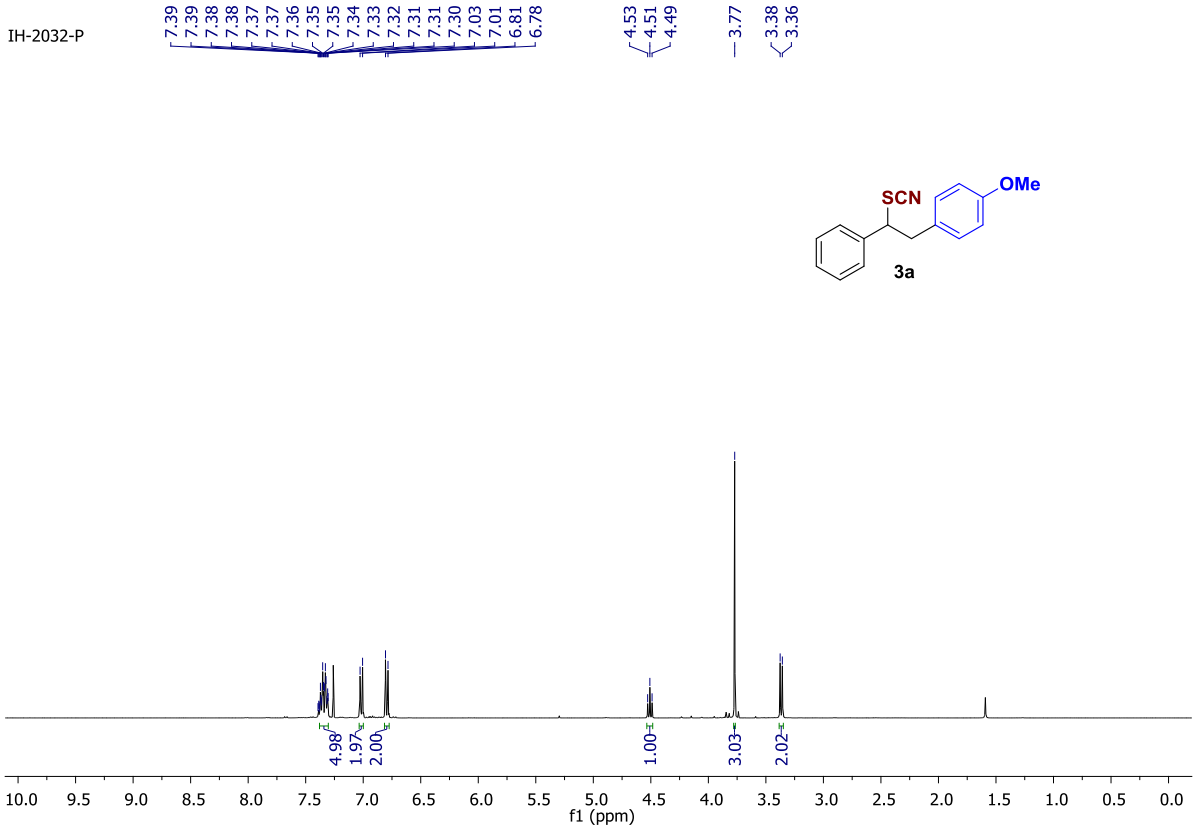
**Figure S4**. ORTEP plot of compound **3k** with 30% ellipsoid probability.

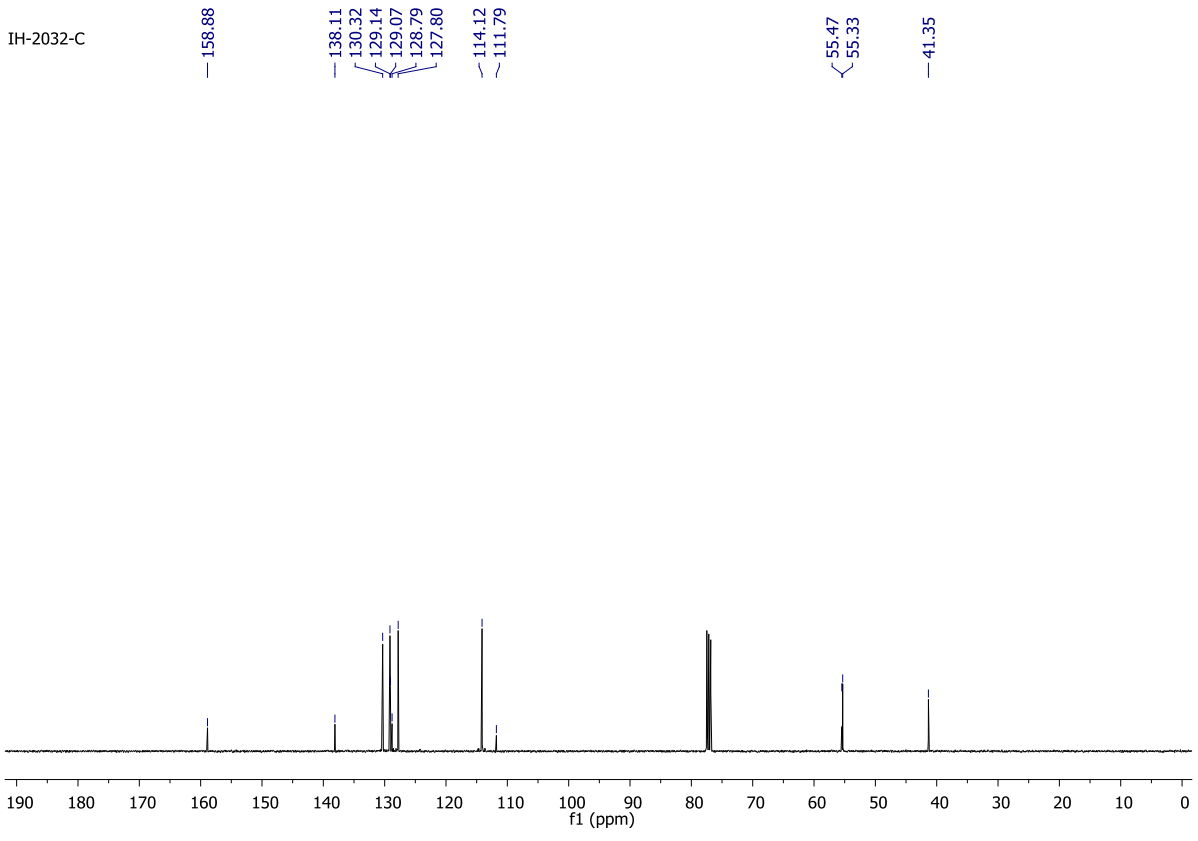
**Crystal data for 3k**: X-ray single crystal data were collected using MoKα (λ = 0.71073 Å) radiation on a Rigaku SuperNova diffractometer equipped with an Eos S2 detector. Structure solution/refinement were carried out using Shelx-2013. The structure was solved by direct method and refined in a routine manner. Non-hydrogen atoms were treated anisotropically. All hydrogen atoms were geometrically fixed. CCDC (CCDC No: 1813182) contains the supplementary crystallographic data of **3k**. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

**Table S2: Crystal data and structure refinement for compound 3k.**

| | |
|---|---|
| Identification code | CCDC 1813182 |
| Empirical formula | $C_{18}H_{17}NO_3S$ |
| Formula weight | 327.38 |
| Temperature/K | 293(2) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 11.3799(10) |
| b/Å | 7.7646(8) |
| c/Å | 20.862(2) |
| α/° | 90 |
| β/° | 113.081(8) |
| γ/° | 90 |
| Volume/Å$^3$ | 1695.8(3) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.282 |
| μ/mm$^{-1}$ | 0.204 |
| F(000) | 688.0 |
| Crystal size/mm$^3$ | 0.16 × 0.14 × 0.11 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.89 to 53.986 |
| Index ranges | -12 ≤ h ≤ 14, -8 ≤ k ≤ 9, -22 ≤ l ≤ 26 |
| Reflections collected | 7298 |
| Independent reflections | 3650 [$R_{int}$ = 0.0327, $R_{sigma}$ = 0.0777] |
| Data/restraints/parameters | 3650/0/208 |
| Goodness-of-fit on F$^2$ | 1.036 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0739, $wR_2$ = 0.1674 |
| Final R indexes [all data] | $R_1$ = 0.1298, $wR_2$ = 0.1932 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.63/-0.28 |

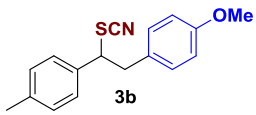
## 5. NMR Spectra:



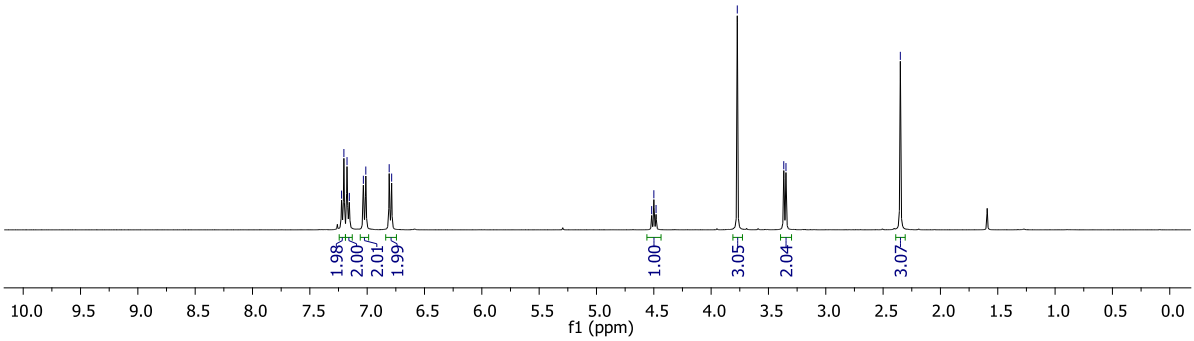



IH-1070P-1H-(ND)-400

7.22 7.20 7.18 7.16 7.03 7.01 6.81 6.79 4.52 4.50 4.48 3.77 3.37 3.35 2.35

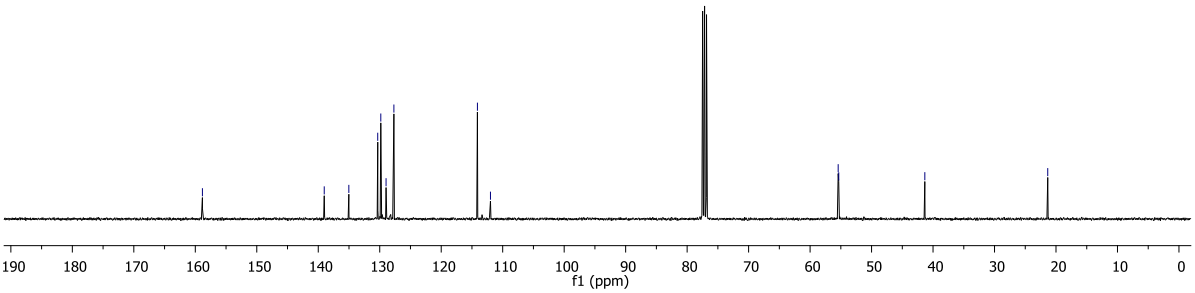



3b




IH-1070-C

158.84 139.03 135.03 130.33 129.83 128.97 127.70 114.11 111.99 55.43 55.34 41.34 21.34



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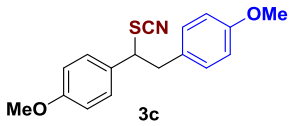
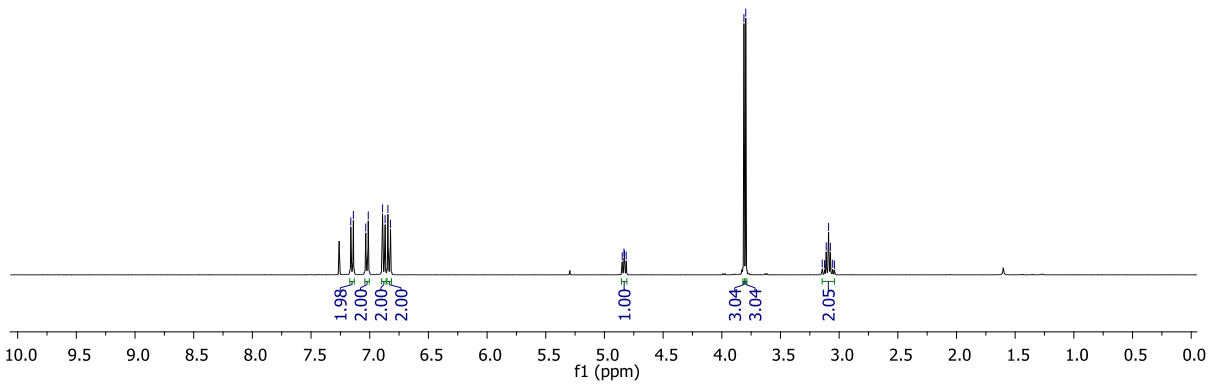



3c

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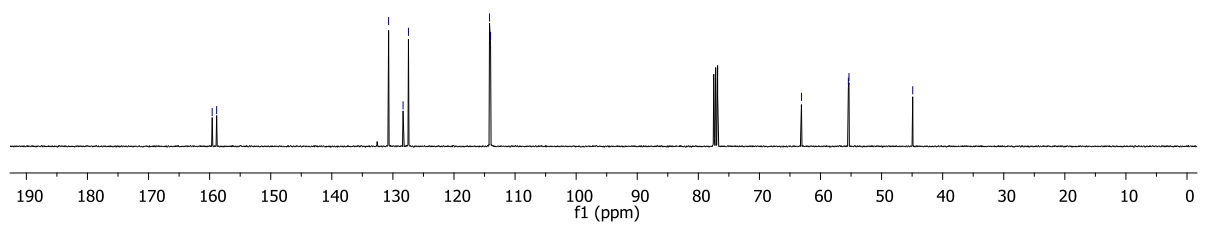

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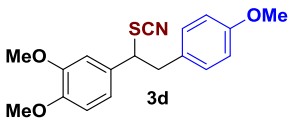
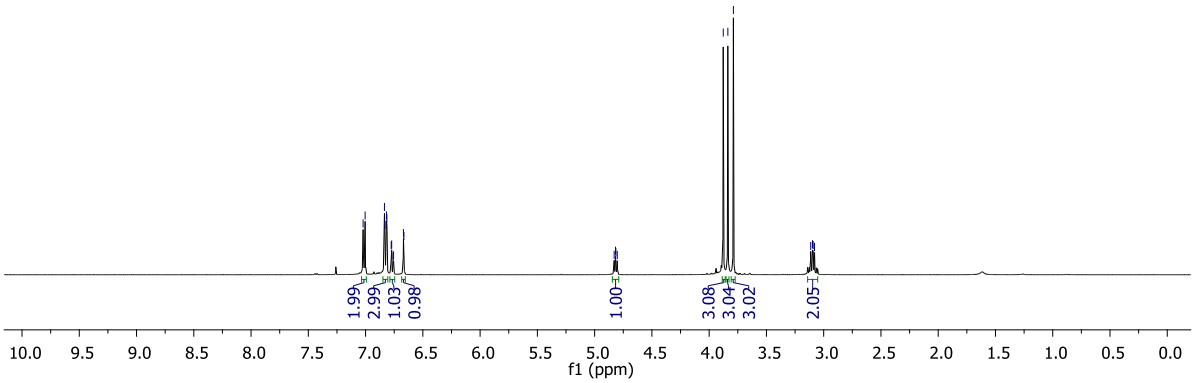
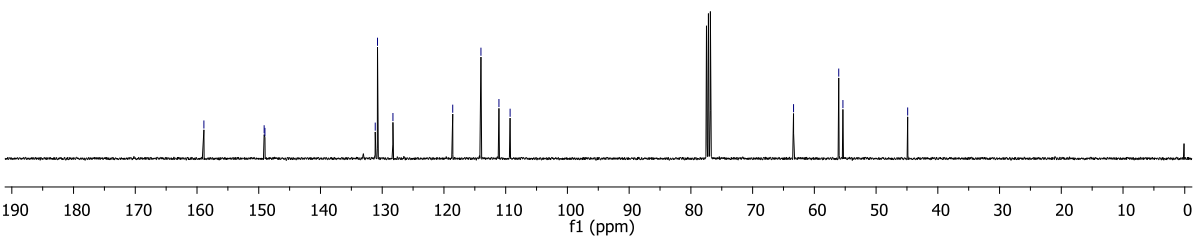
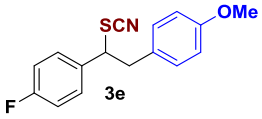


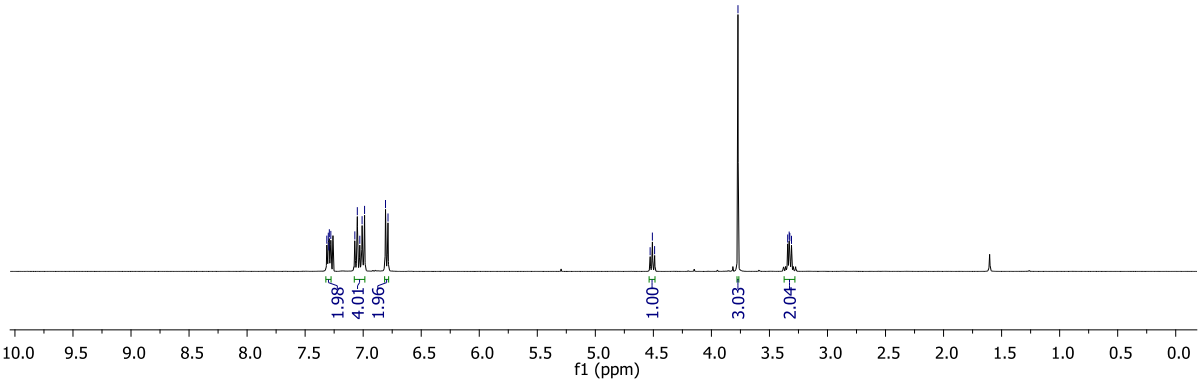




IH-2044

IH-2031-P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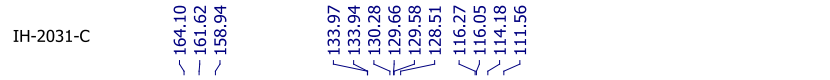


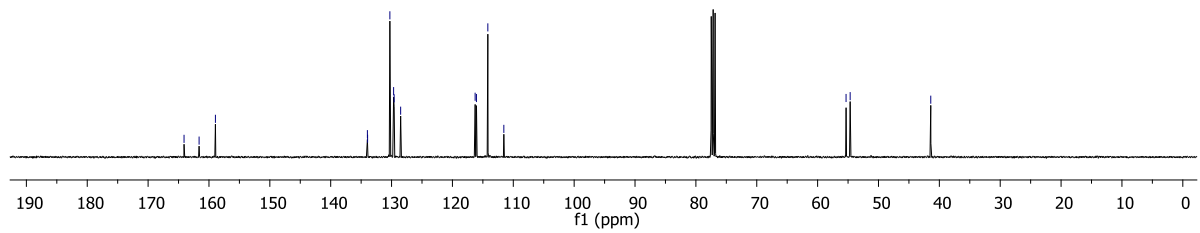

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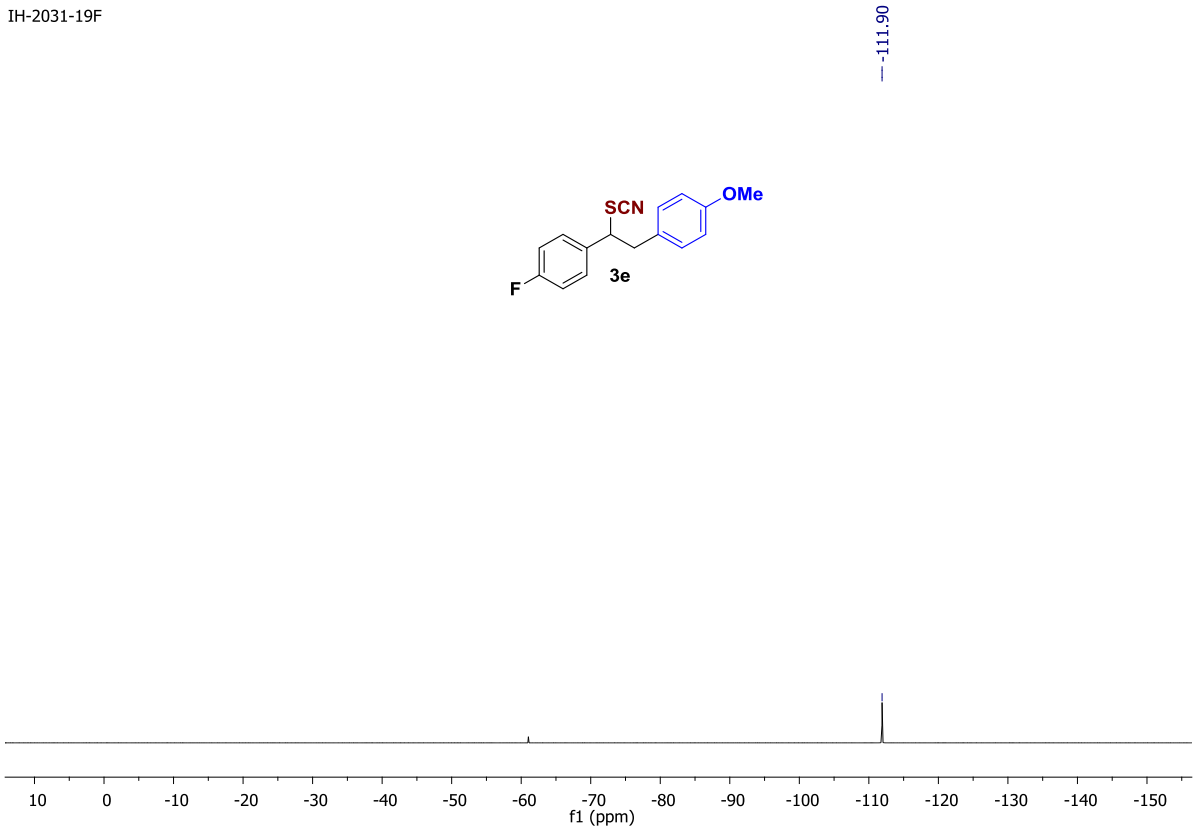
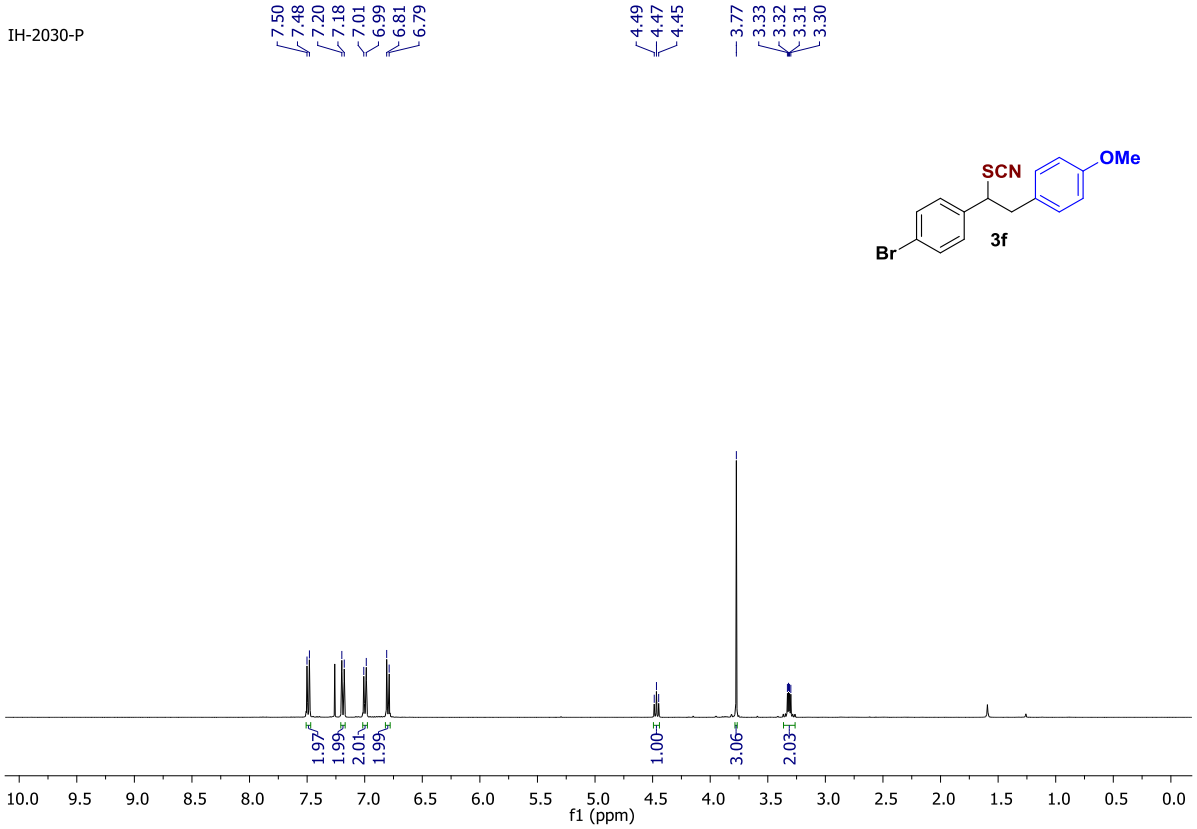

-111.90
SCN
OMe
F
3e
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

IH-2030-P

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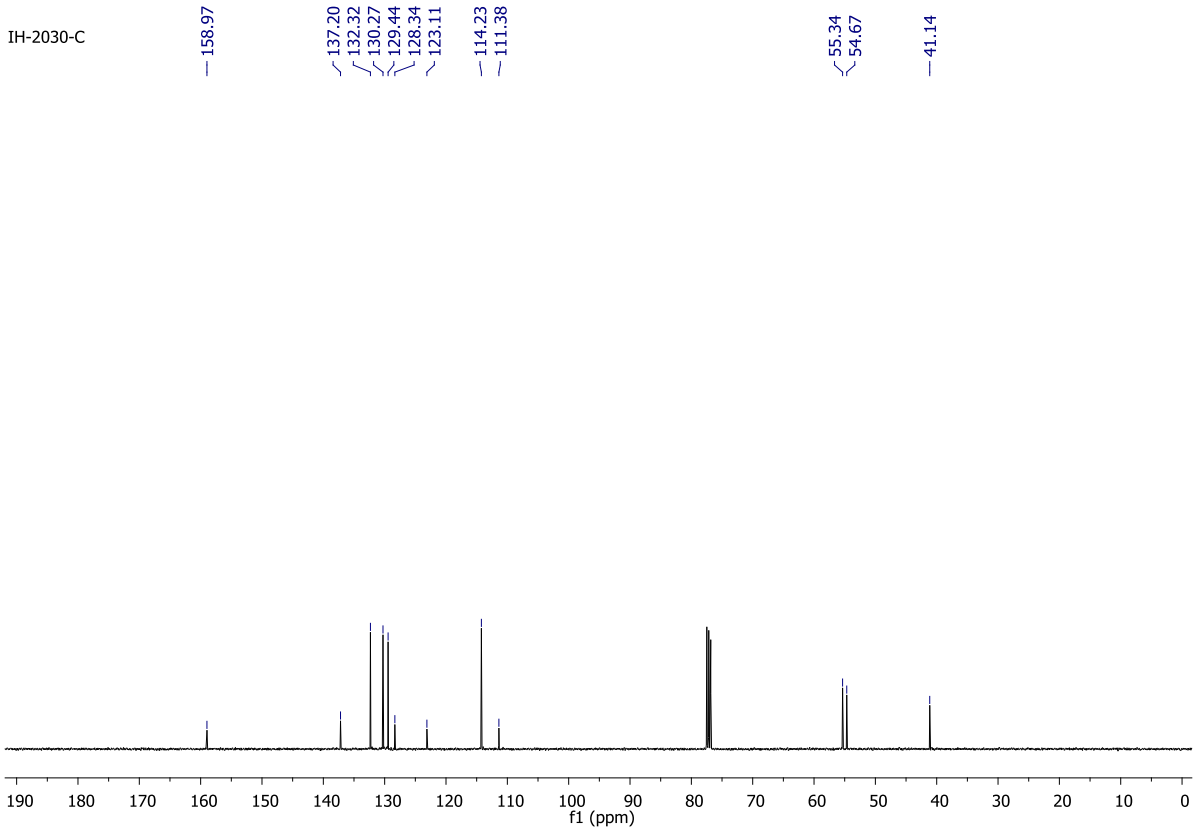

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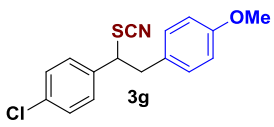


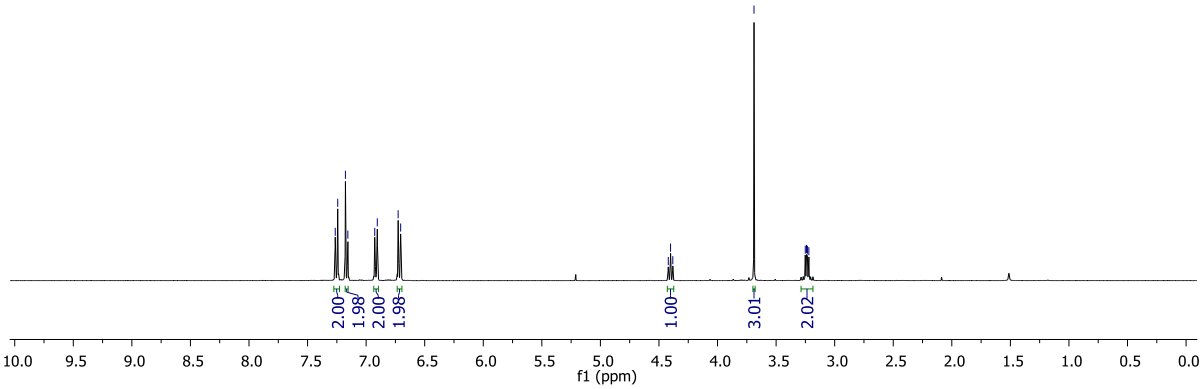


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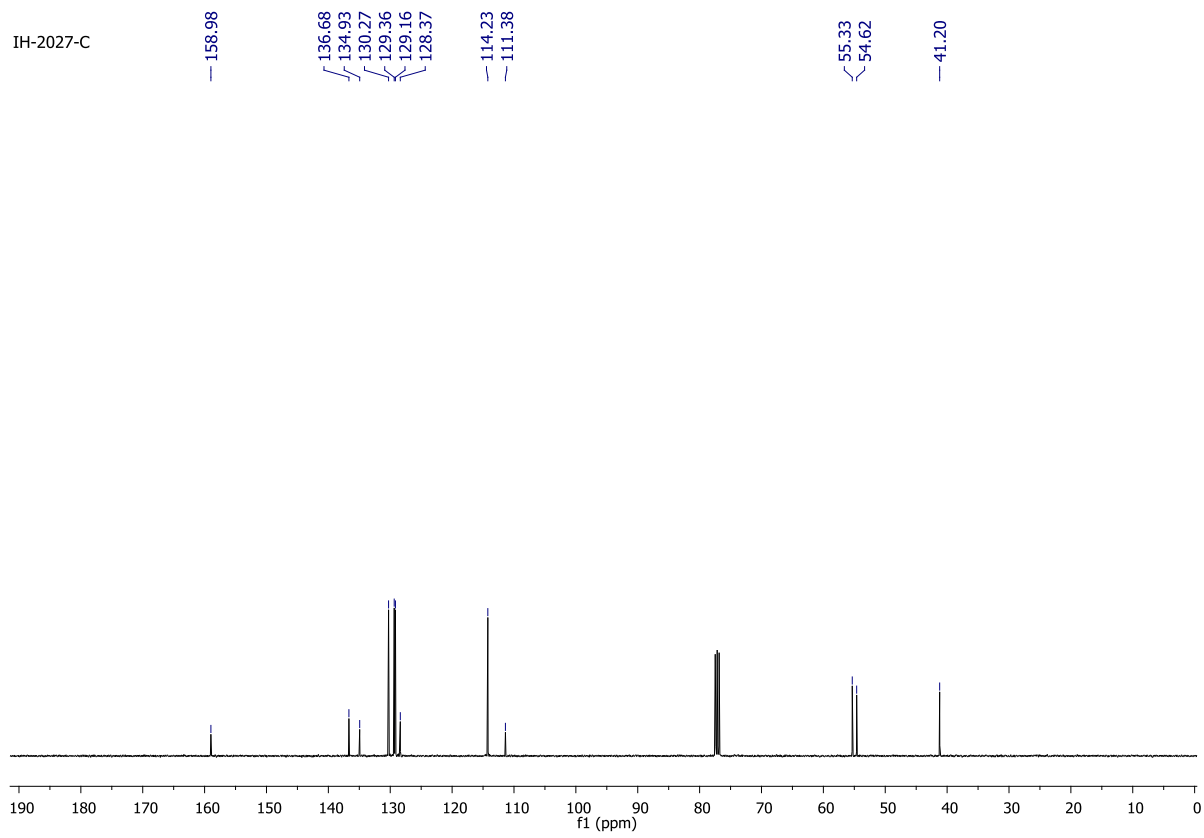

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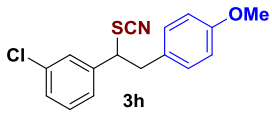


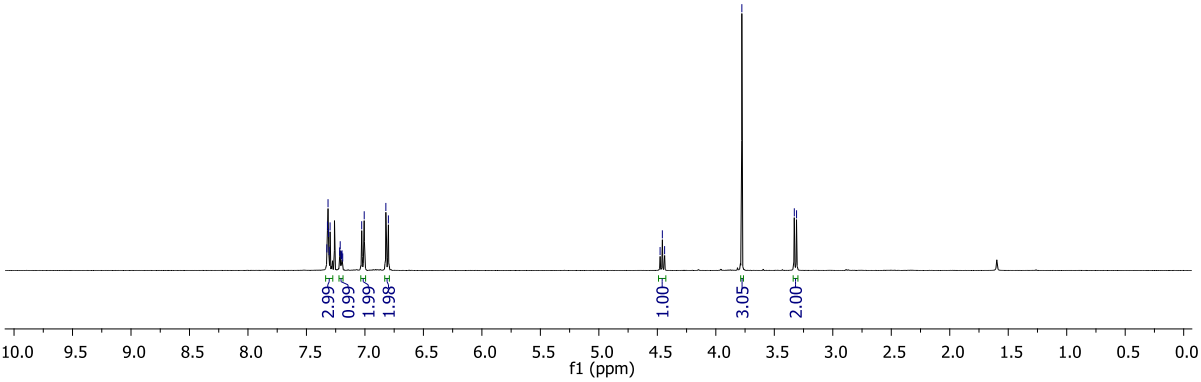


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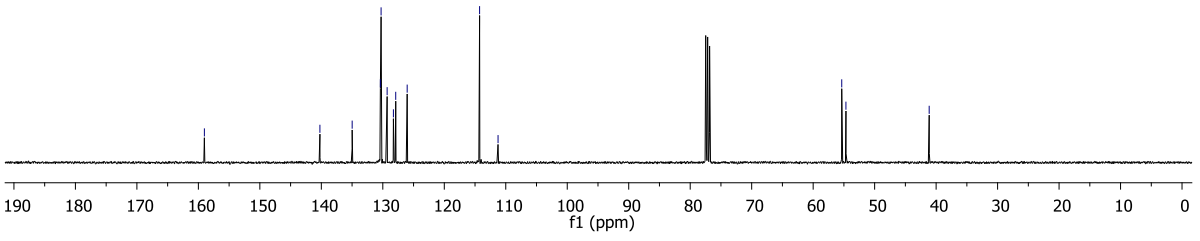
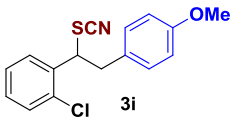
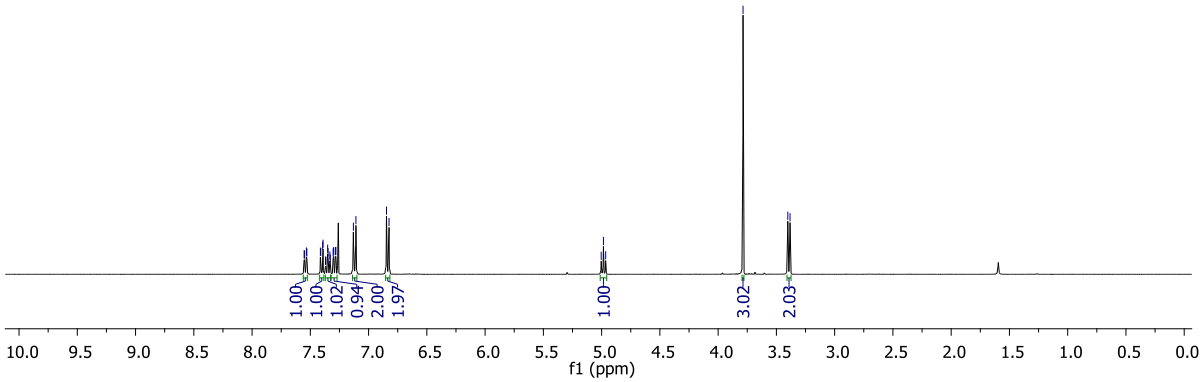
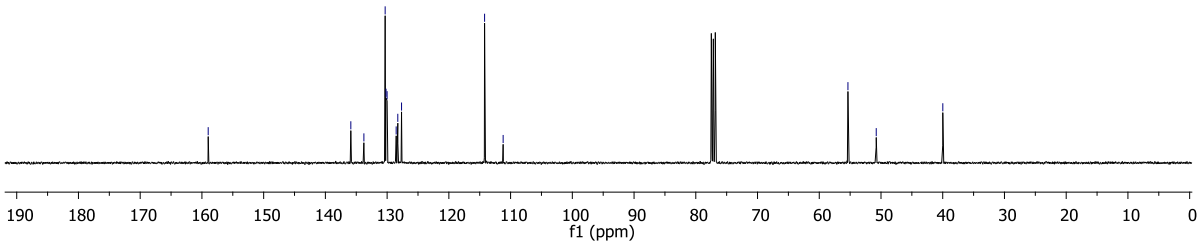


IH-2029-P

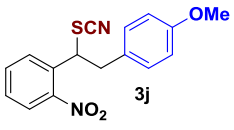



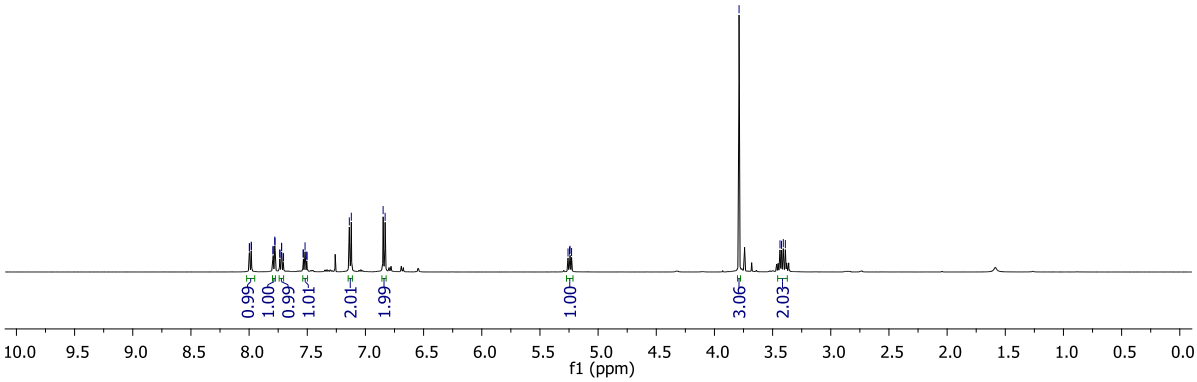




IH-2029-C

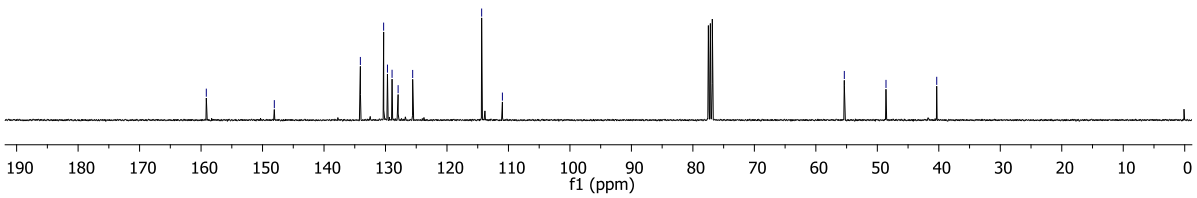




IH-2045-P-1H-(ND)-500
8.00
8.00
7.98
7.98
7.80
7.79
7.78
7.78
7.74
7.73
7.72
7.72
7.54
7.53
7.52
7.14
7.12
6.85
6.83
5.26
5.25
5.24
5.23
3.79
3.44
3.42
3.41
3.39

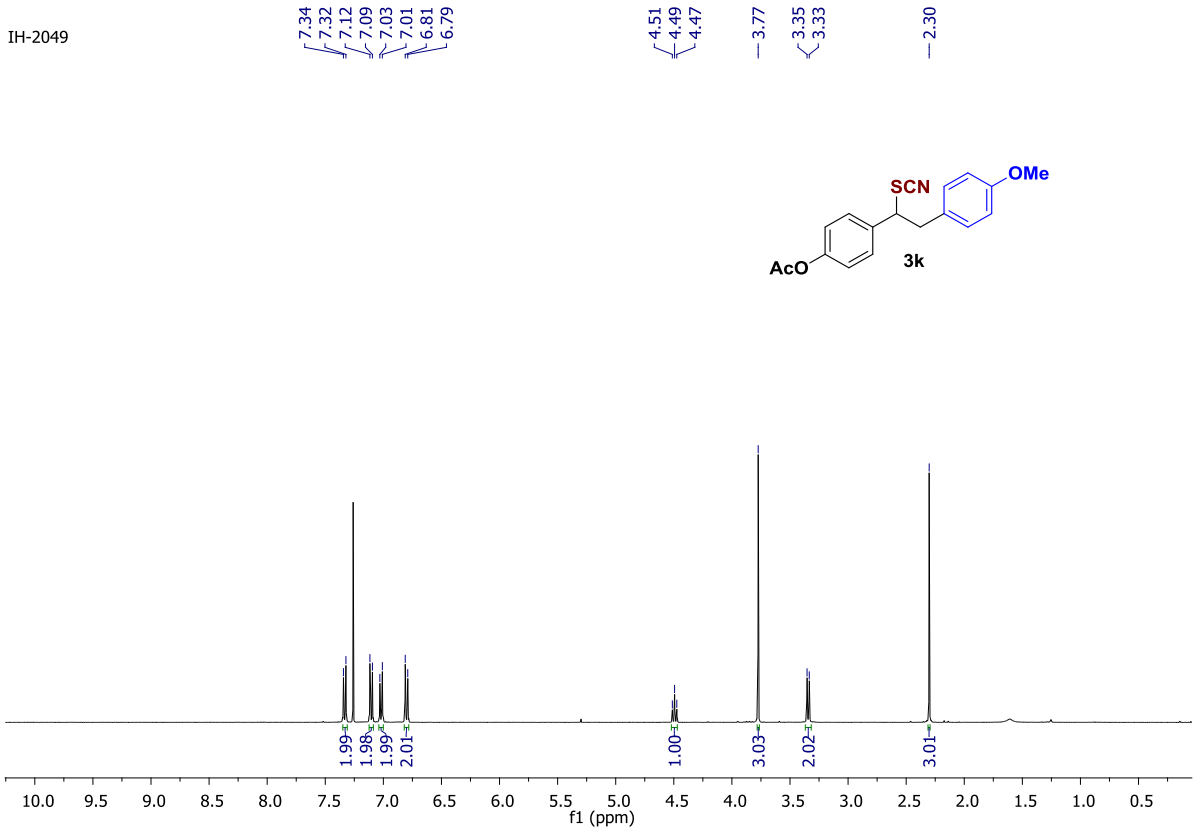

SCN
OMe
NO2
3j


0.99
1.00
0.99
1.01
2.01
1.99
1.00
3.06
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

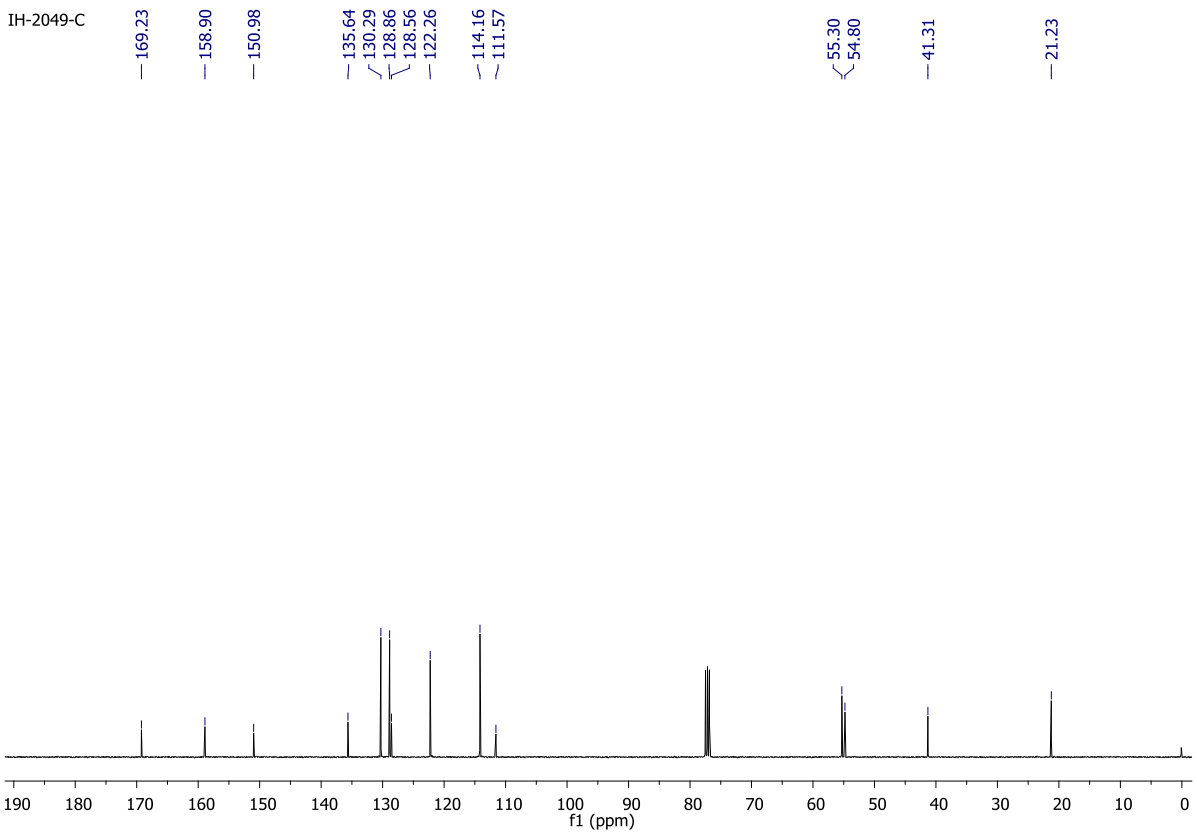

IH-2045
159.15
148.08
134.09
130.30
129.68
128.93
127.95
125.58
114.36
110.98
55.37
48.59
40.34


190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

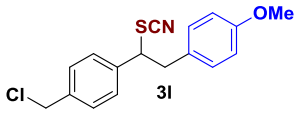
IH-2049

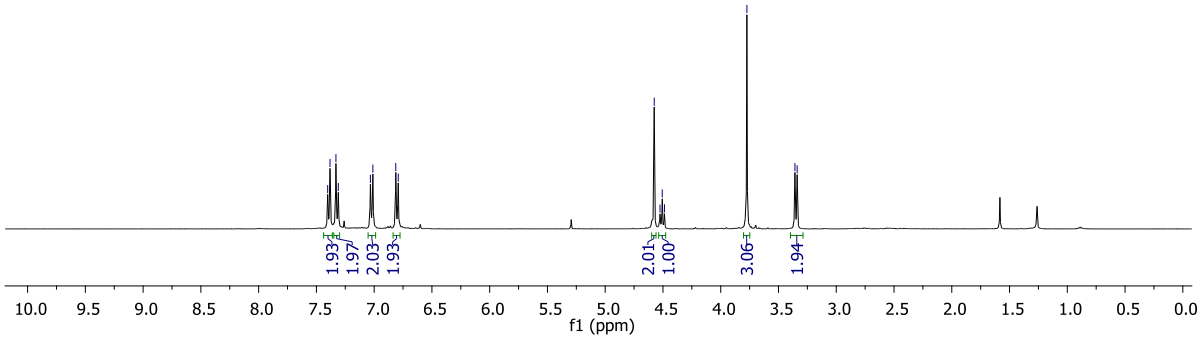



IH-2049-C

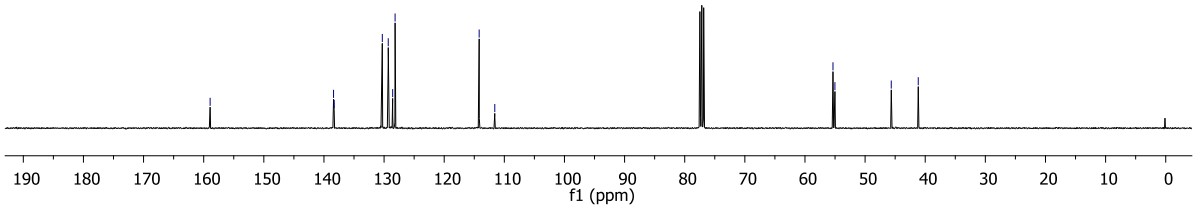


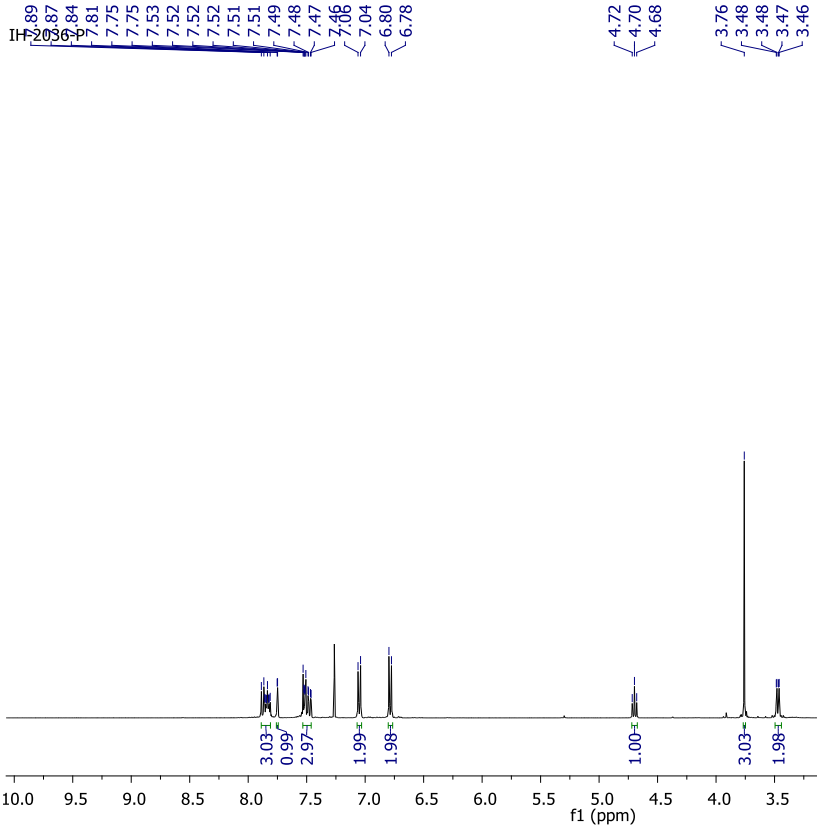
IH-2042-W-1H-(ND)-400

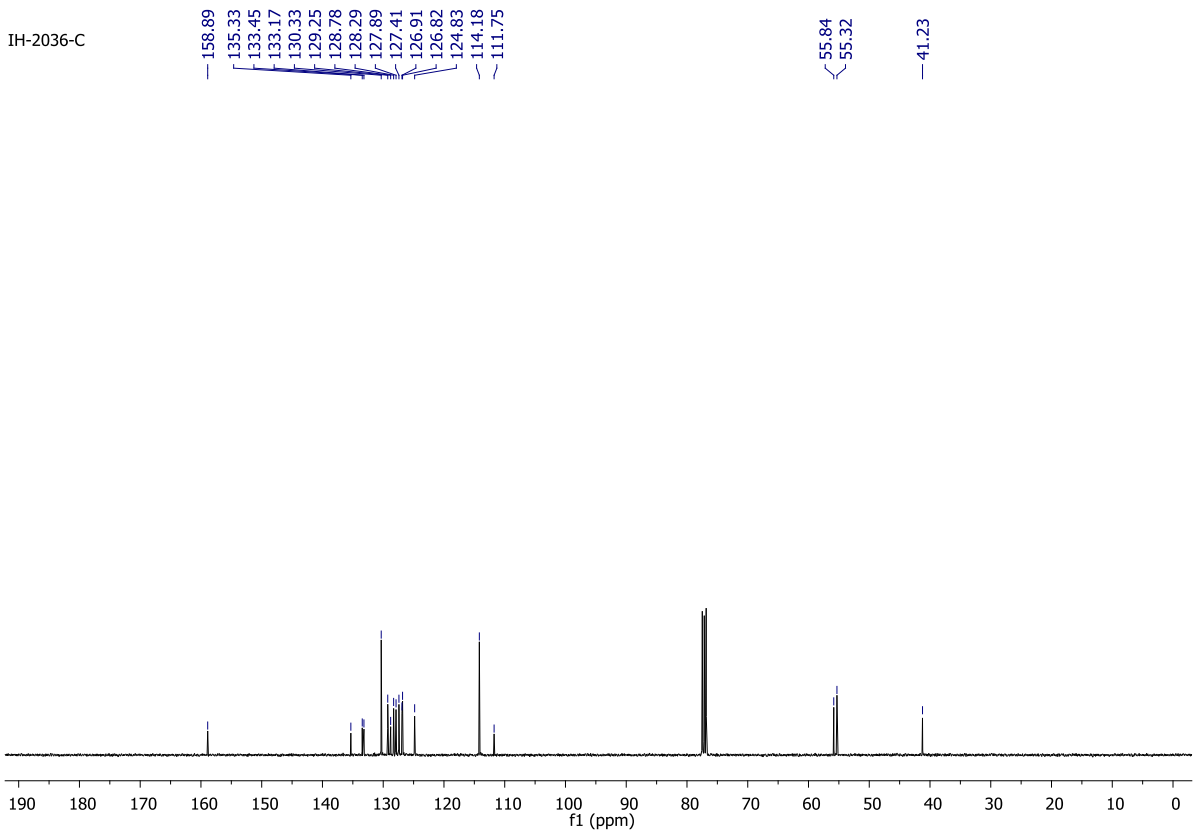




IH-2042-L

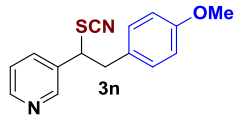




IH-2036-P
7.89
7.87
7.84
7.81
7.75
7.75
7.53
7.52
7.52
7.52
7.51
7.51
7.49
7.48
7.47
7.46
7.08
7.04
6.80
6.78
4.72
4.70
4.68
3.76
3.48
3.48
3.47
3.46
SCN
OMe
3m
3.03
0.99
2.97
1.99
1.98
1.00
3.03
1.98
f1 (ppm)

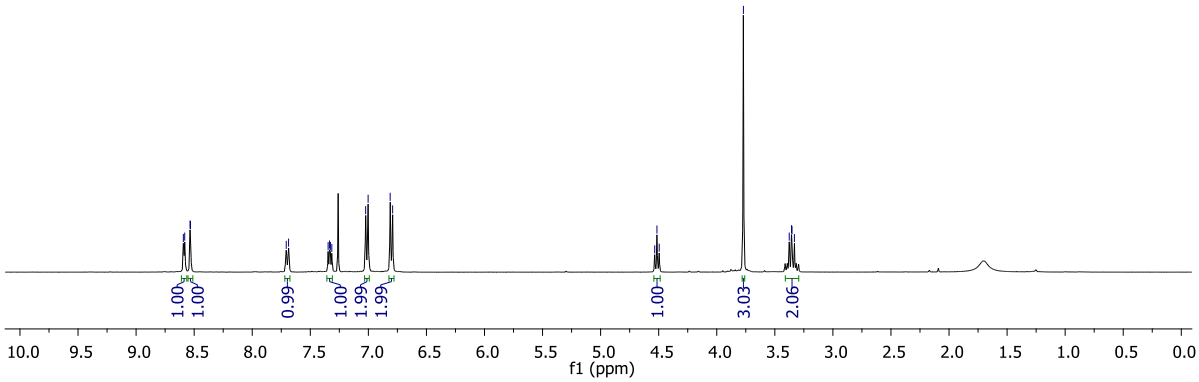

IH-2036-C
158.89
135.33
133.45
133.17
130.33
129.25
128.78
128.29
127.89
127.41
126.91
126.82
124.83
114.18
111.75
55.84
55.32
41.23
f1 (ppm)

IH-2039-1H(ND) 400MHz

8.59 8.58 8.54 8.53 7.71 7.69 7.35 7.33 7.33 7.31 7.02 7.00 6.81 6.79 4.53 4.51 4.50 3.77 3.38 3.36 3.35 3.33

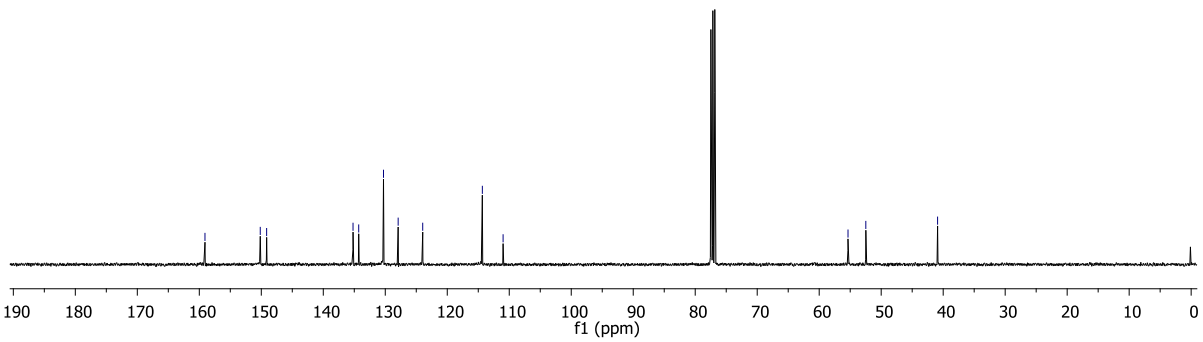


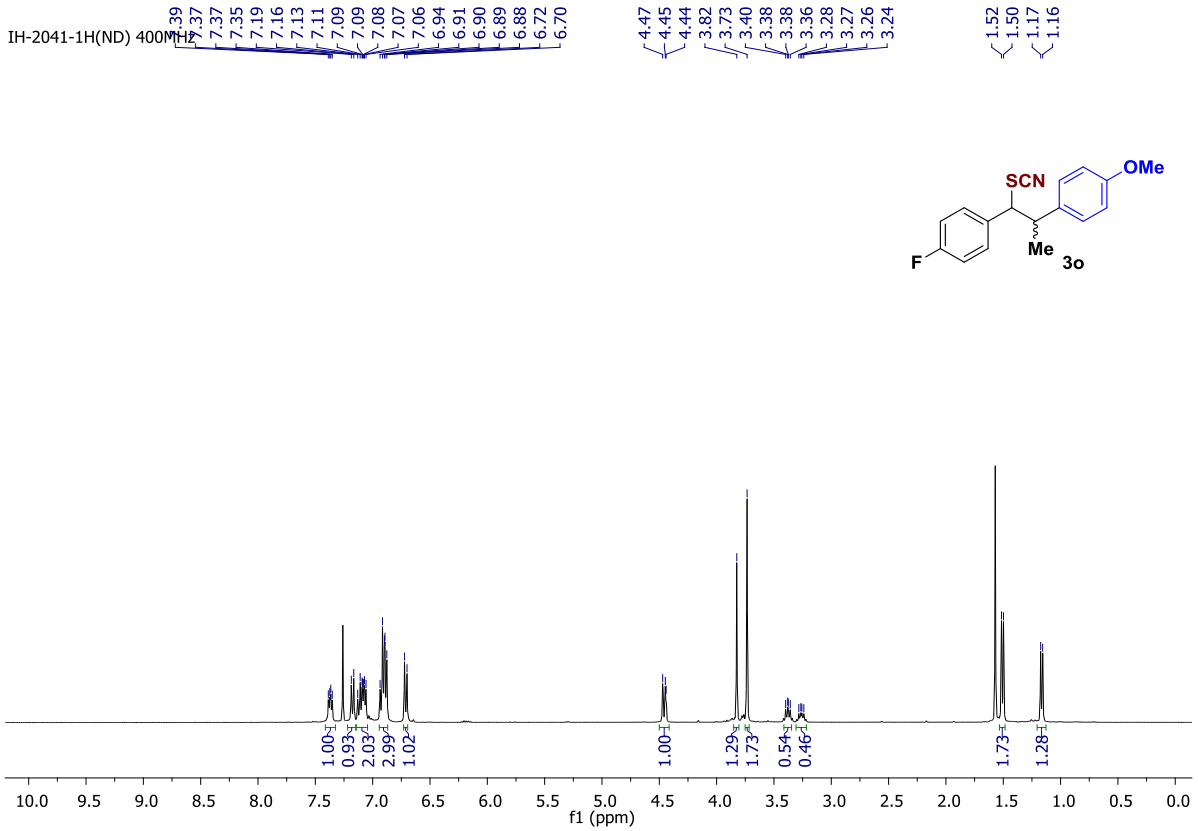

3n

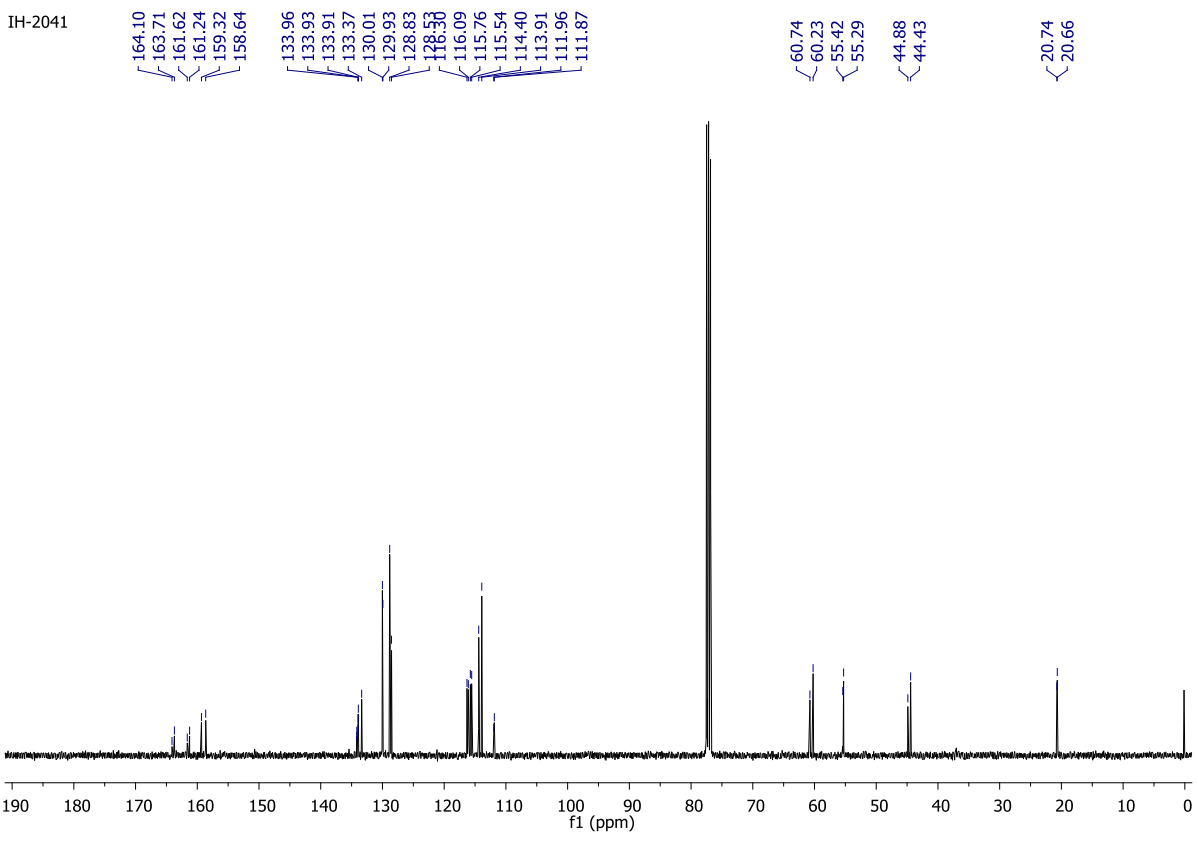



IH-2039

159.09 150.17 149.14 135.20 134.29 130.29 127.92 123.96 114.34 110.99 55.35 52.48 40.90

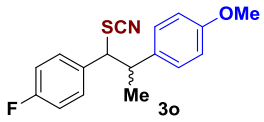



IH-2041-1H(ND) 400MHz
7.39 7.37 7.37 7.35 7.19 7.16 7.13 7.11 7.09 7.09 7.08 7.07 7.06 6.94 6.91 6.90 6.89 6.88 6.72 6.70
4.47 4.45 4.44 3.82 3.73 3.40 3.38 3.38 3.36 3.28 3.27 3.26 3.24
1.52 1.50 1.17 1.16
SCN
OMe
Me
F
3o
1.00 0.93 2.03 2.99 1.02 1.00 1.29 1.73 0.54 0.46 1.73 1.28
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

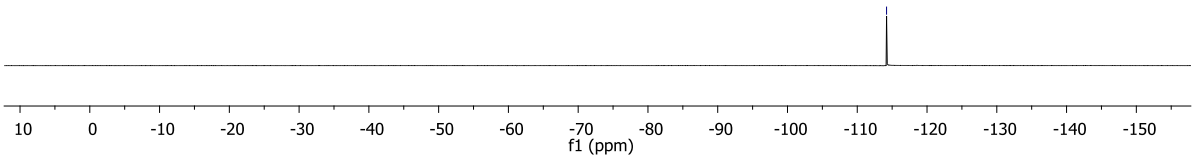

IH-2041
164.10 163.71 161.62 161.24 159.32 158.64
133.96 133.93 133.91 133.37 130.01 129.93 128.83 128.53 116.30 116.09 115.76 115.54 114.40 113.91 111.96 111.87
60.74 60.23 55.42 55.29
44.88 44.43
20.74 20.66
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

IH-2041-19F

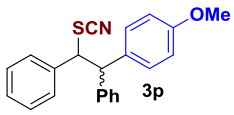
-114.20

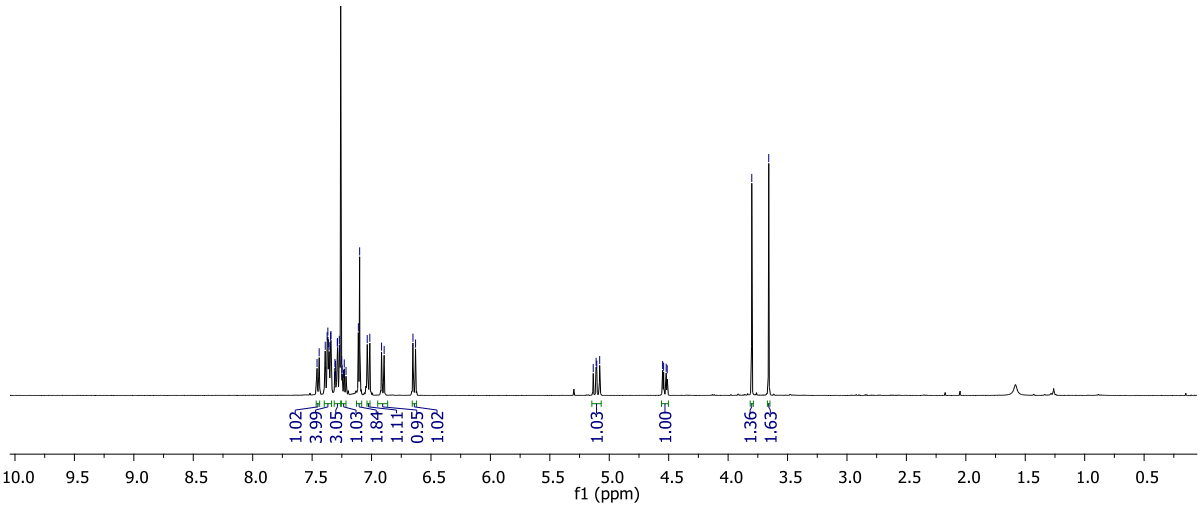



3o

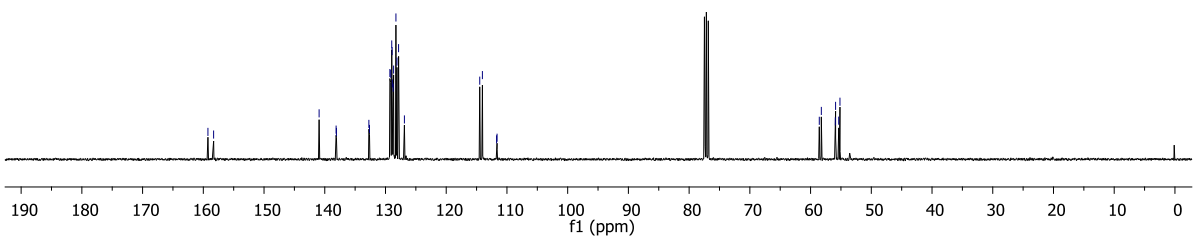


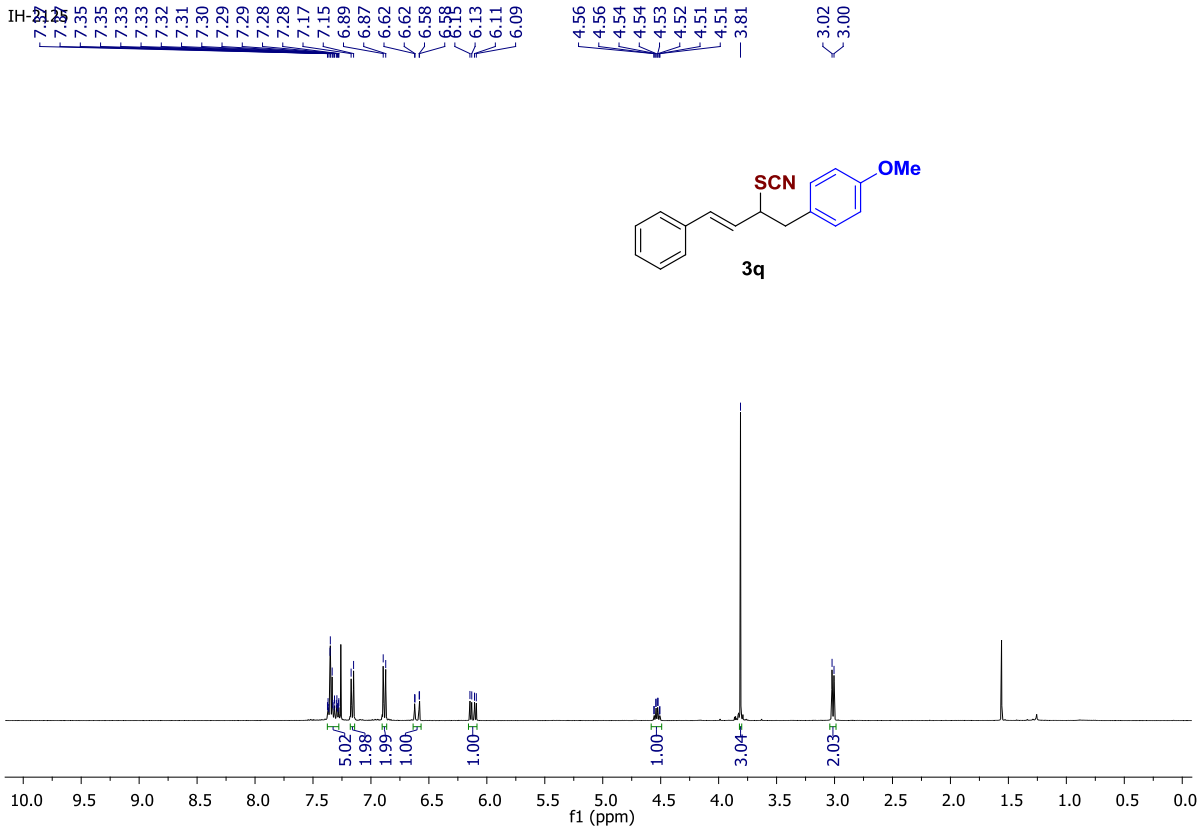
IH-2048

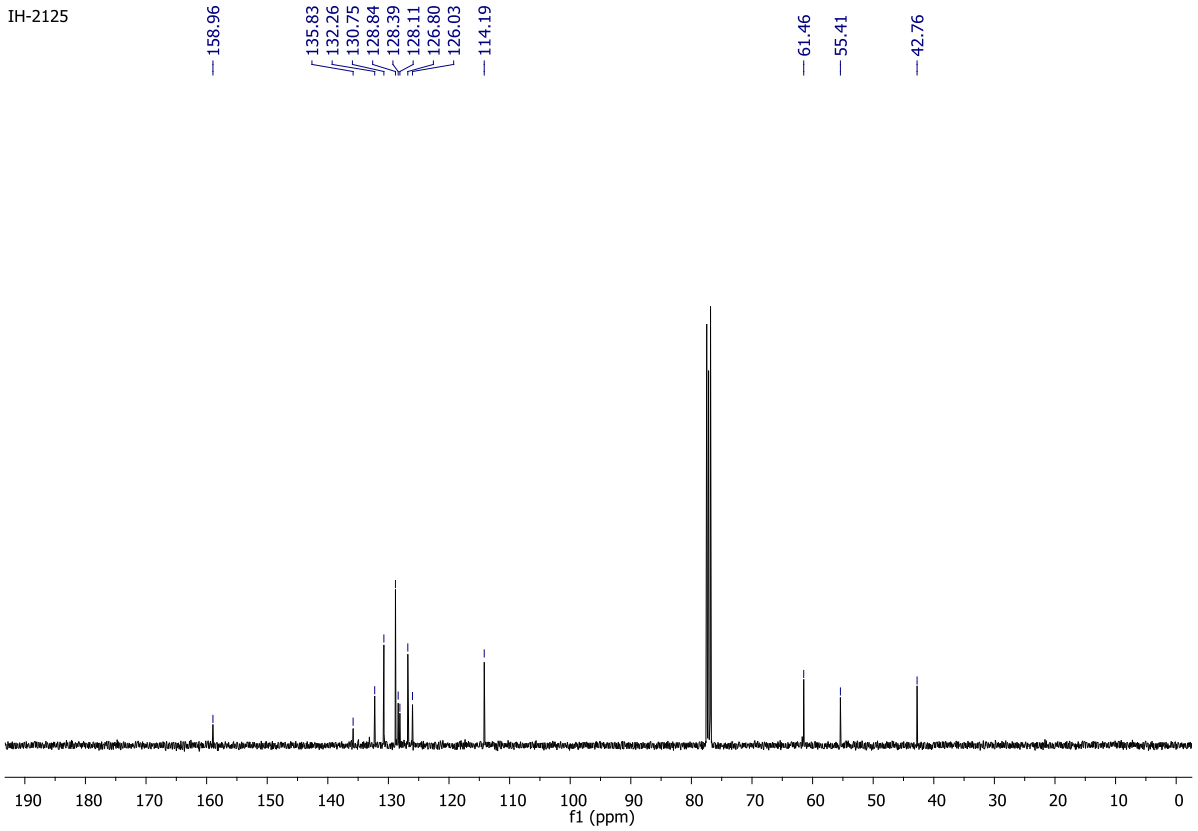



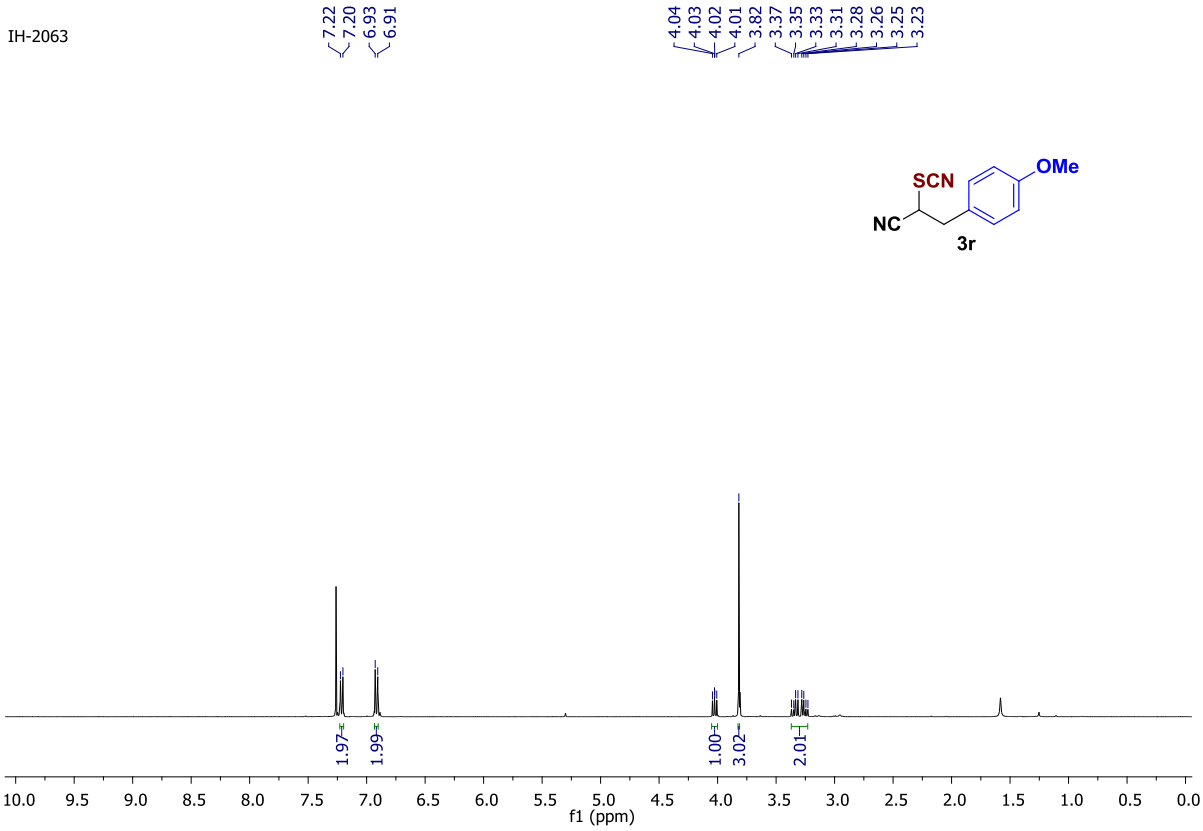

IH-2048

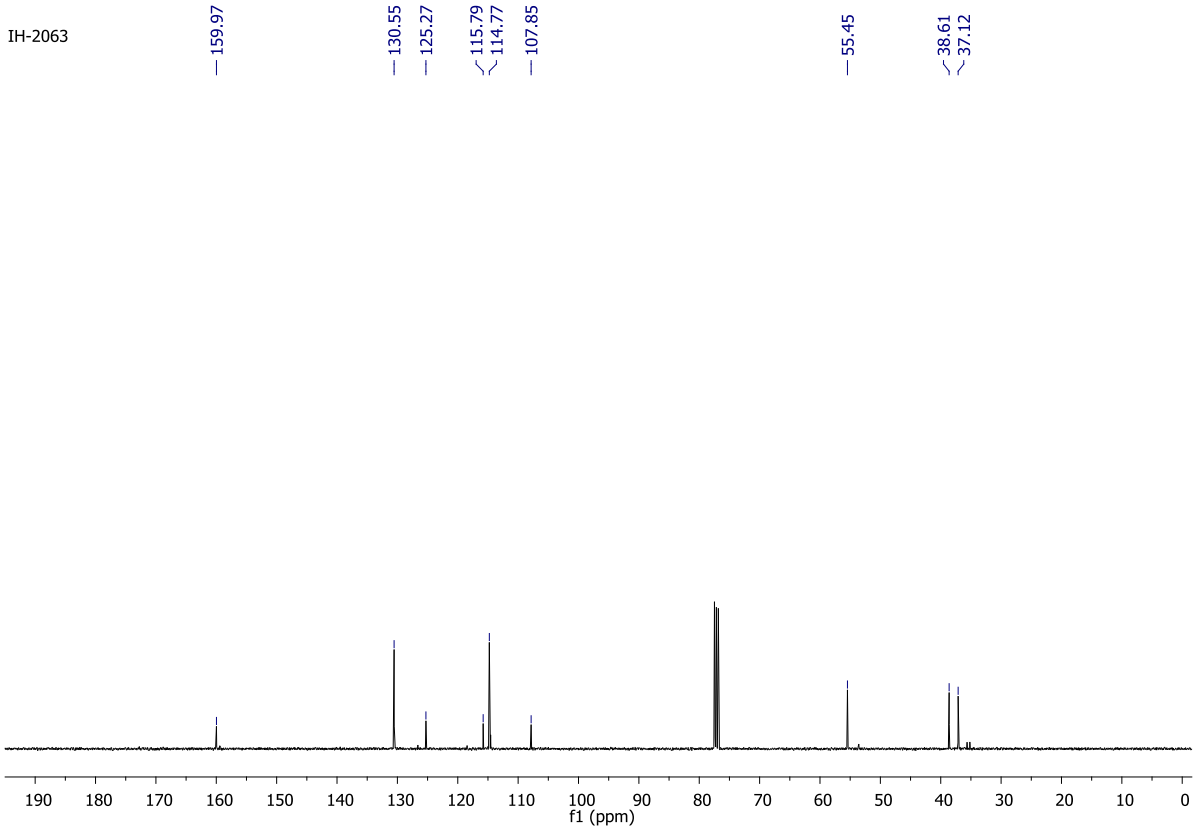

IH-2125
7.37
7.35
7.35
7.33
7.33
7.32
7.31
7.30
7.29
7.29
7.28
7.28
7.17
7.15
6.89
6.87
6.62
6.62
6.58
6.58
6.15
6.13
6.11
6.09
4.56
4.56
4.54
4.54
4.53
4.52
4.51
4.51
3.81
3.02
3.00
SCN
OMe
3q
5.02
1.98
1.99
1.00
1.00
1.00
3.04
2.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


IH-2125
158.96
135.83
132.26
130.75
128.84
128.39
128.11
126.80
126.03
114.19
61.46
55.41
42.76
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

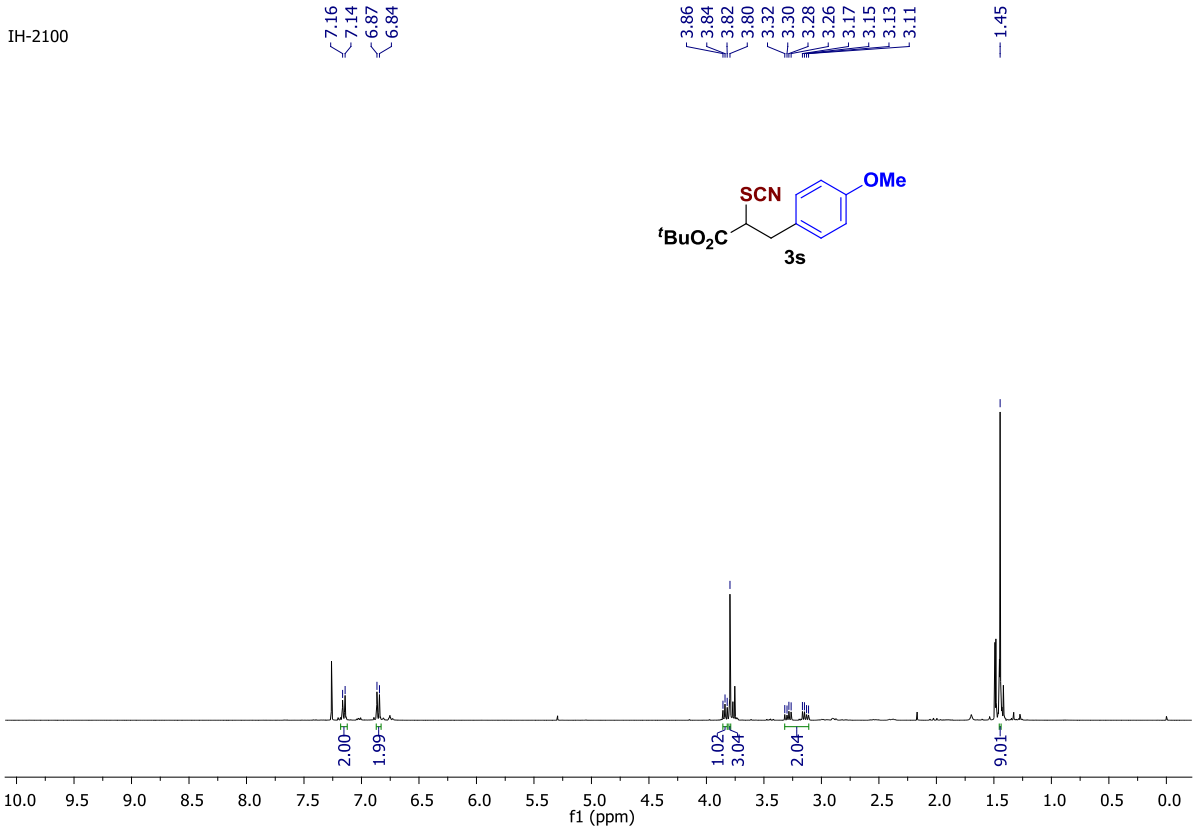
IH-2063



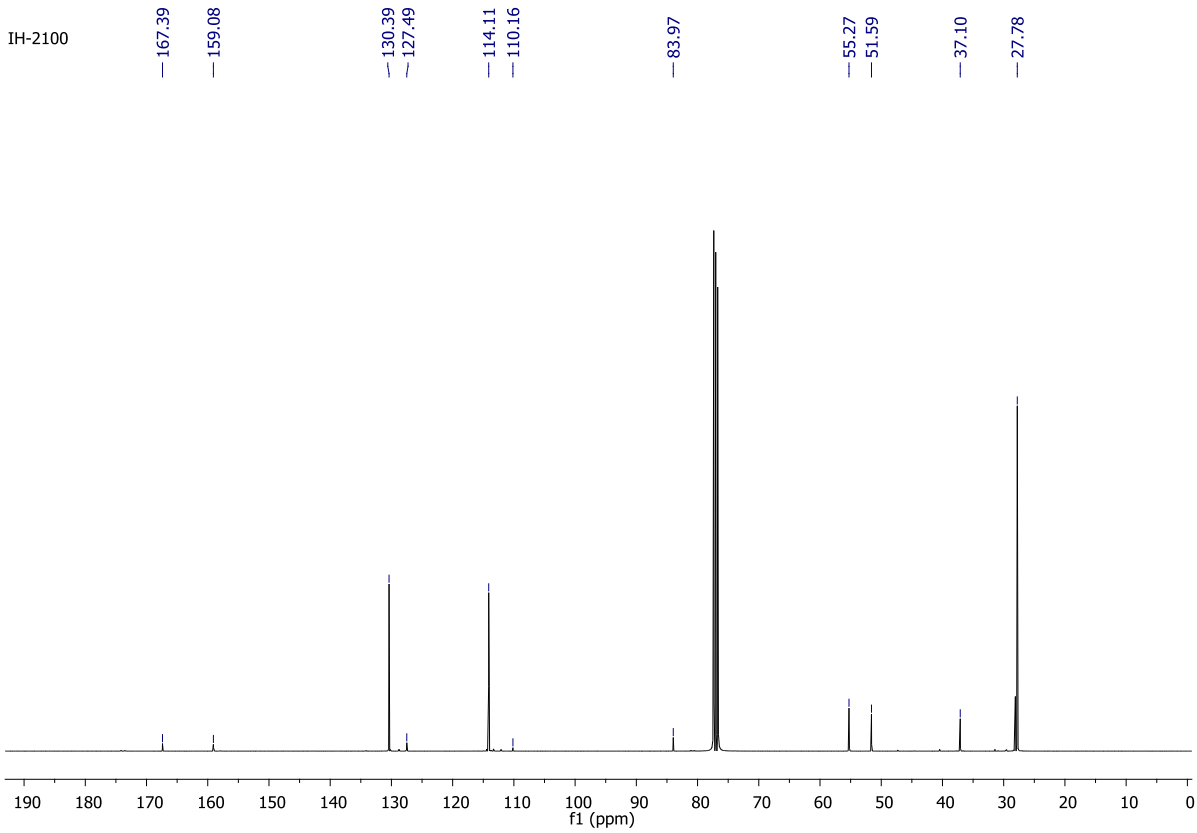

IH-2063



IH-2100

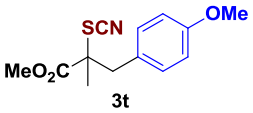



IH-2100

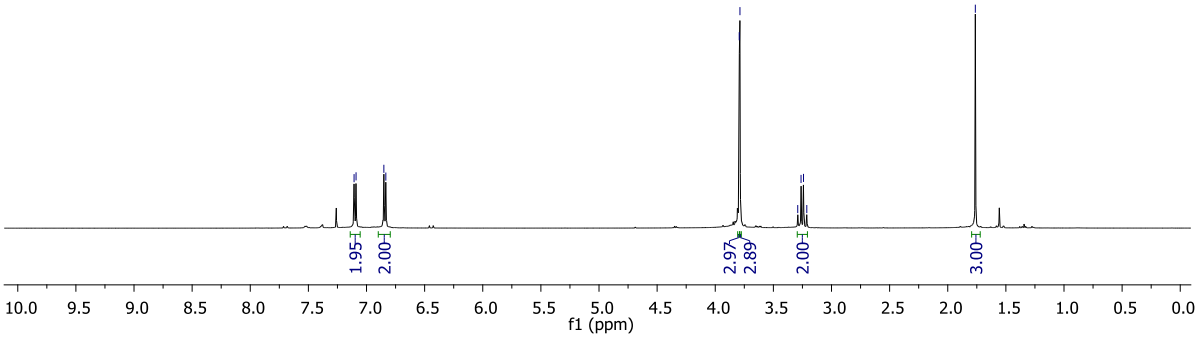


IH-2082-1H(ND) 500MHz.

7.11 7.09 6.85 6.83 3.79 3.79 3.29 3.26 3.24 3.21 1.76

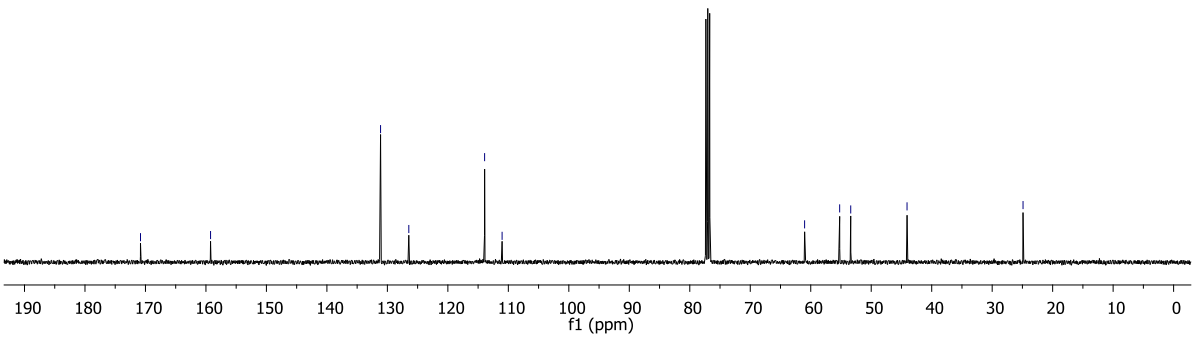



3t



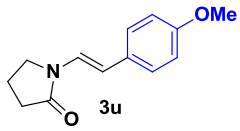

IH-2082

170.82 159.24 131.13 126.46 113.92 111.03 61.01 55.22 53.39 44.08 24.90

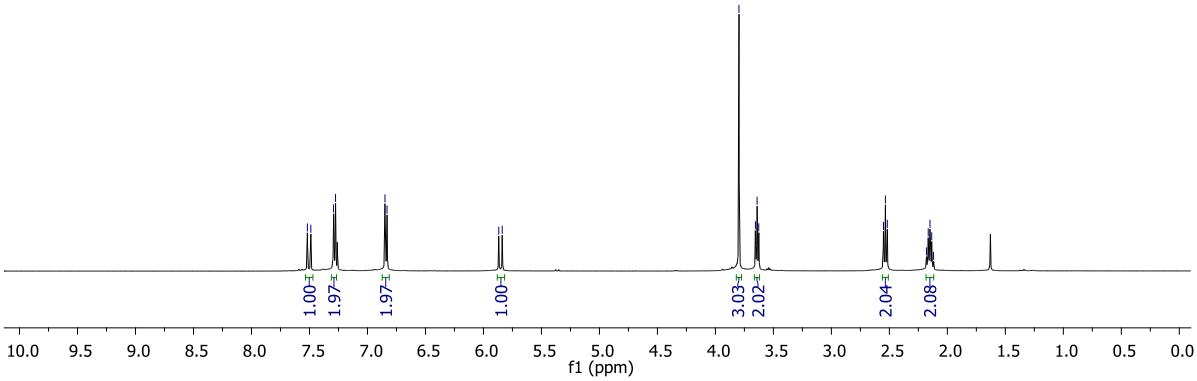


IH-2081-1H(ND) 500MHz.

7.52 7.49 7.29 7.28 6.85 6.83 5.87 5.84 3.80 3.66 3.64 3.63 2.55 2.53 2.52 2.18 2.16 2.15 2.13 2.12

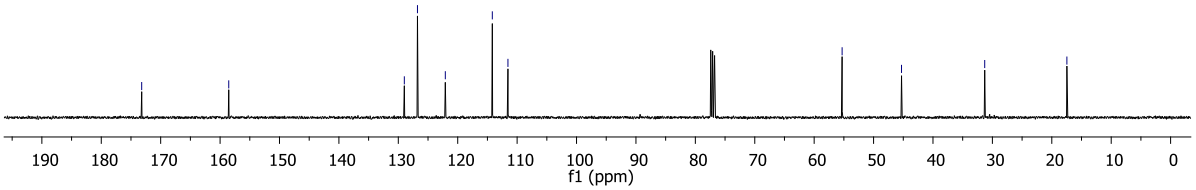



3u



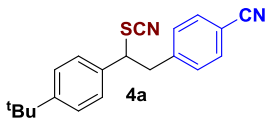

IH-2081

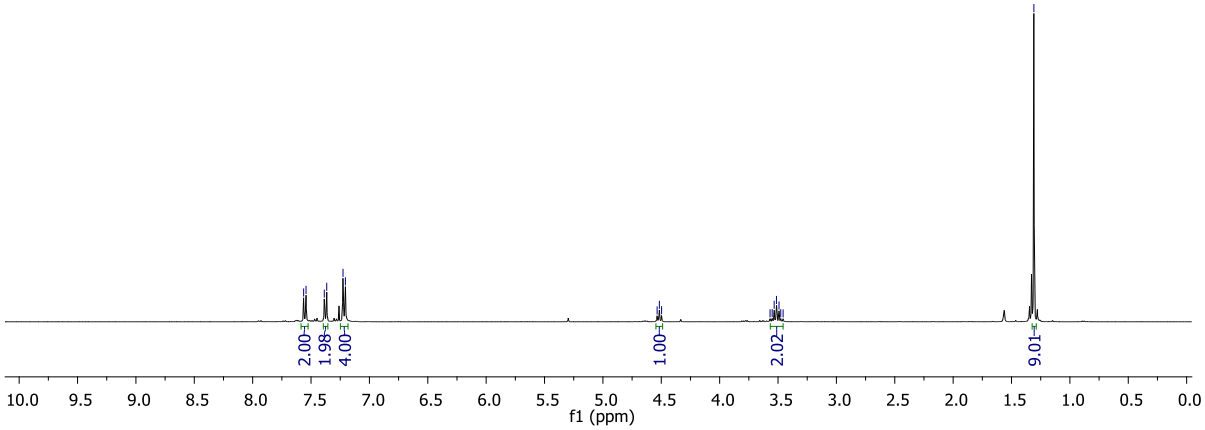
173.20 158.54 128.99 126.77 122.09 114.18 111.54 55.30 45.30 31.29 17.46



IH-2002-1H- 400MHz-(ND)

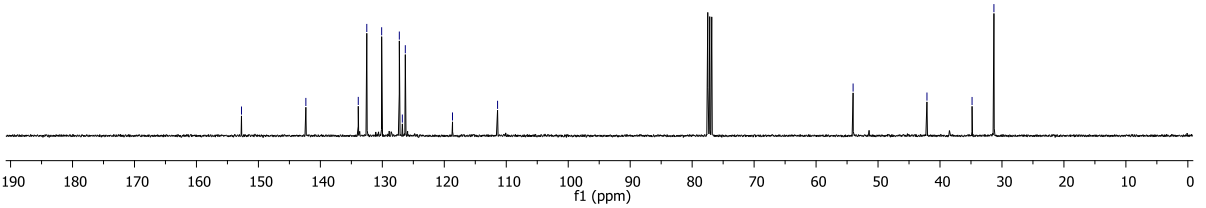
7.56 7.54 7.39 7.37 7.23 7.21 4.54 4.52 4.50 3.57 3.55 3.53 3.51 3.49 3.48 3.46 1.31



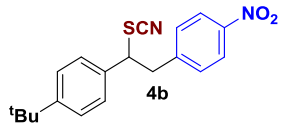

IH-2002

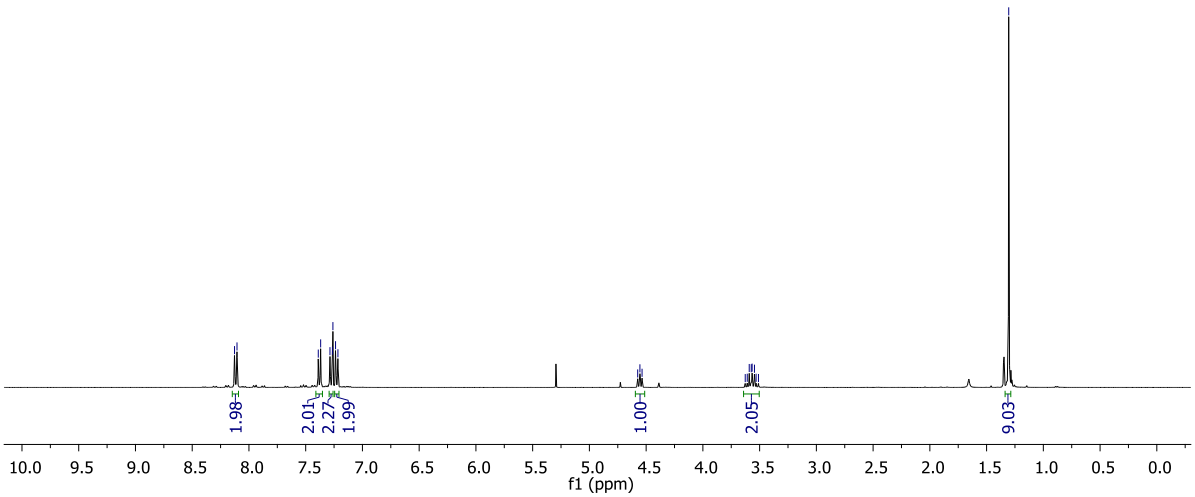
152.73 142.34 133.88 132.51 130.11 127.26 126.77 126.29 118.68 111.40 54.03 42.11 34.83 31.30



IH-2006-PC

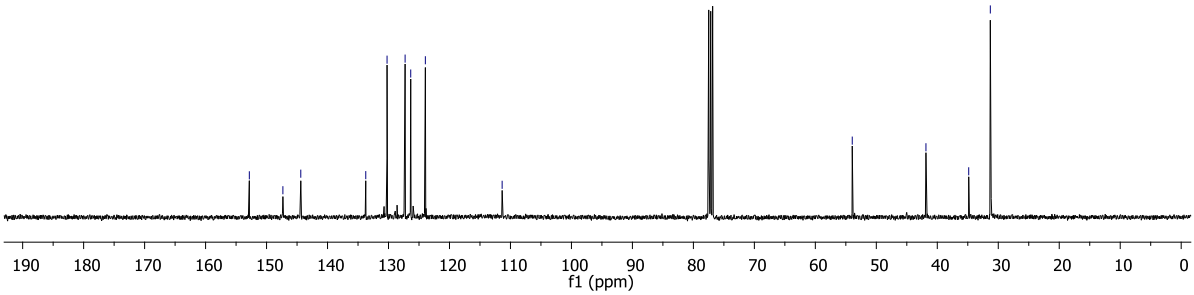
8.13 8.11 7.39 7.37 7.29 7.26 7.26 7.24 7.22 4.57 4.55 4.54 3.63 3.61 3.59 3.57 3.57 3.55 3.53 3.51 1.30



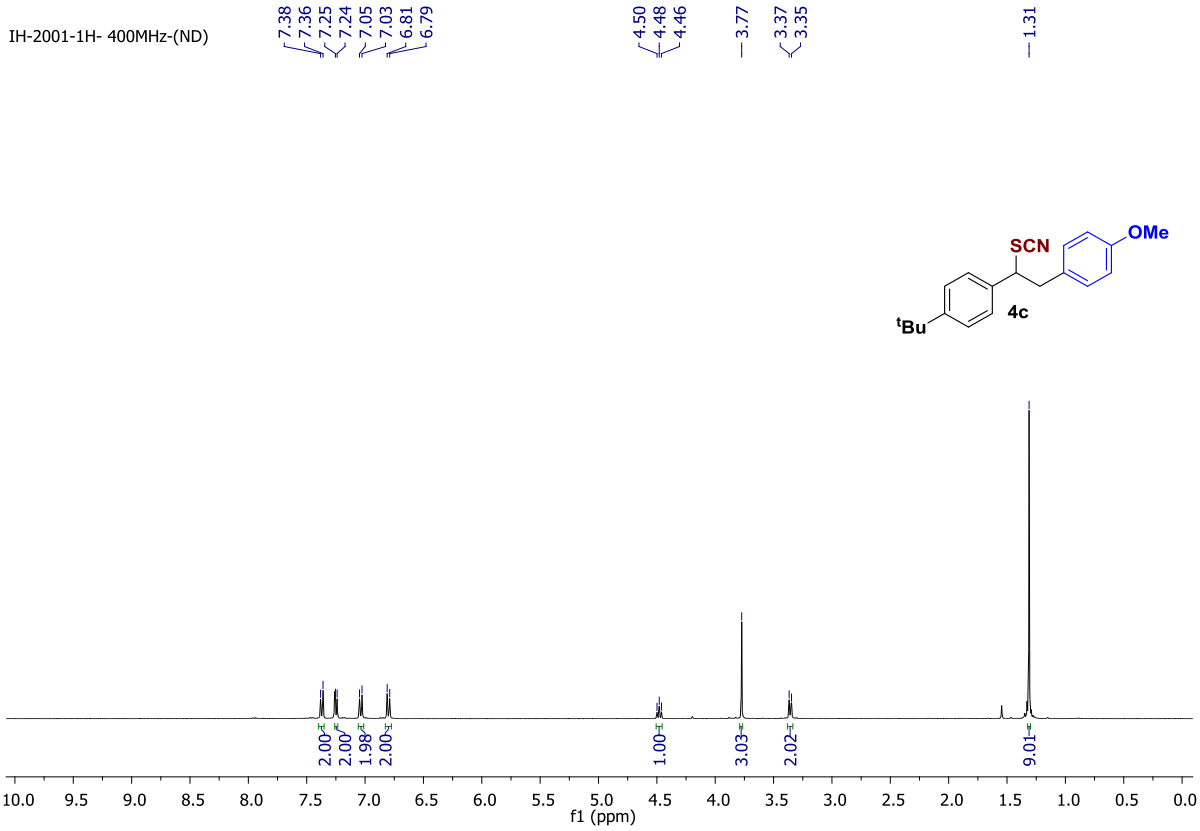




IH-2006-PC

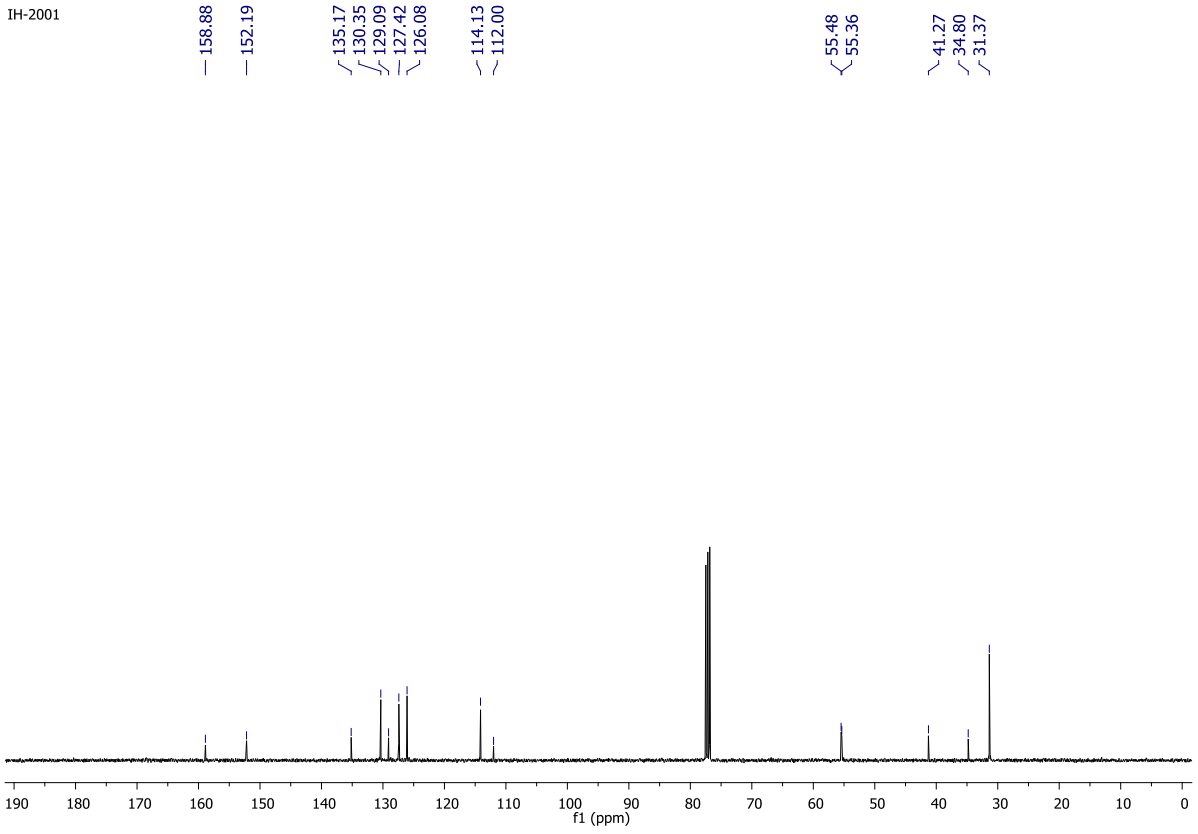
152.83 147.32 144.39 133.73 130.24 127.28 126.36 123.96 111.36 53.95 41.86 34.85 31.30



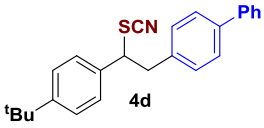
IH-2001-1H- 400MHz-(ND)

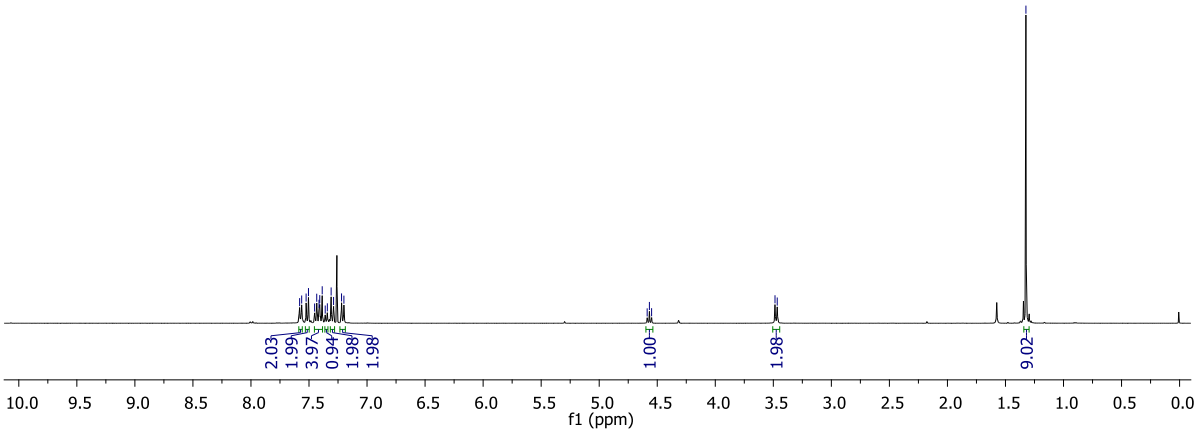



IH-2001

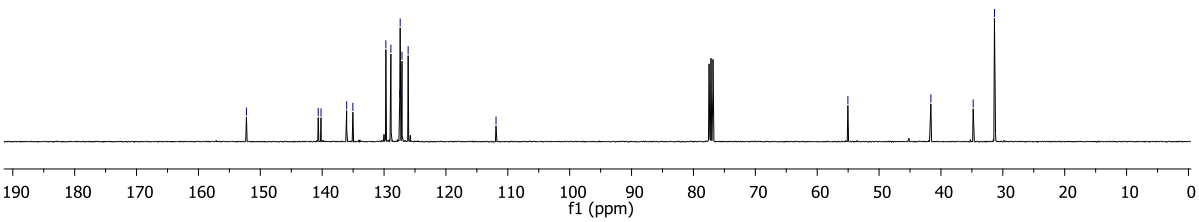


IH-2056

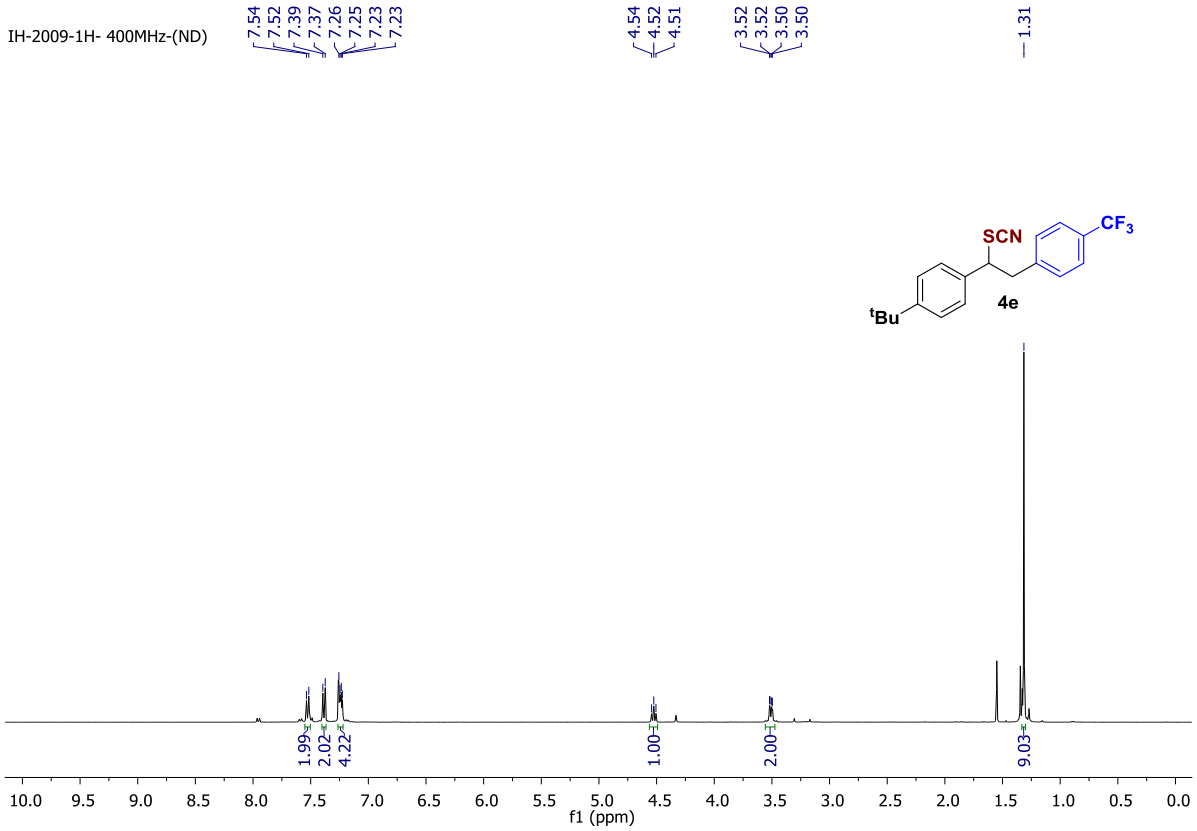



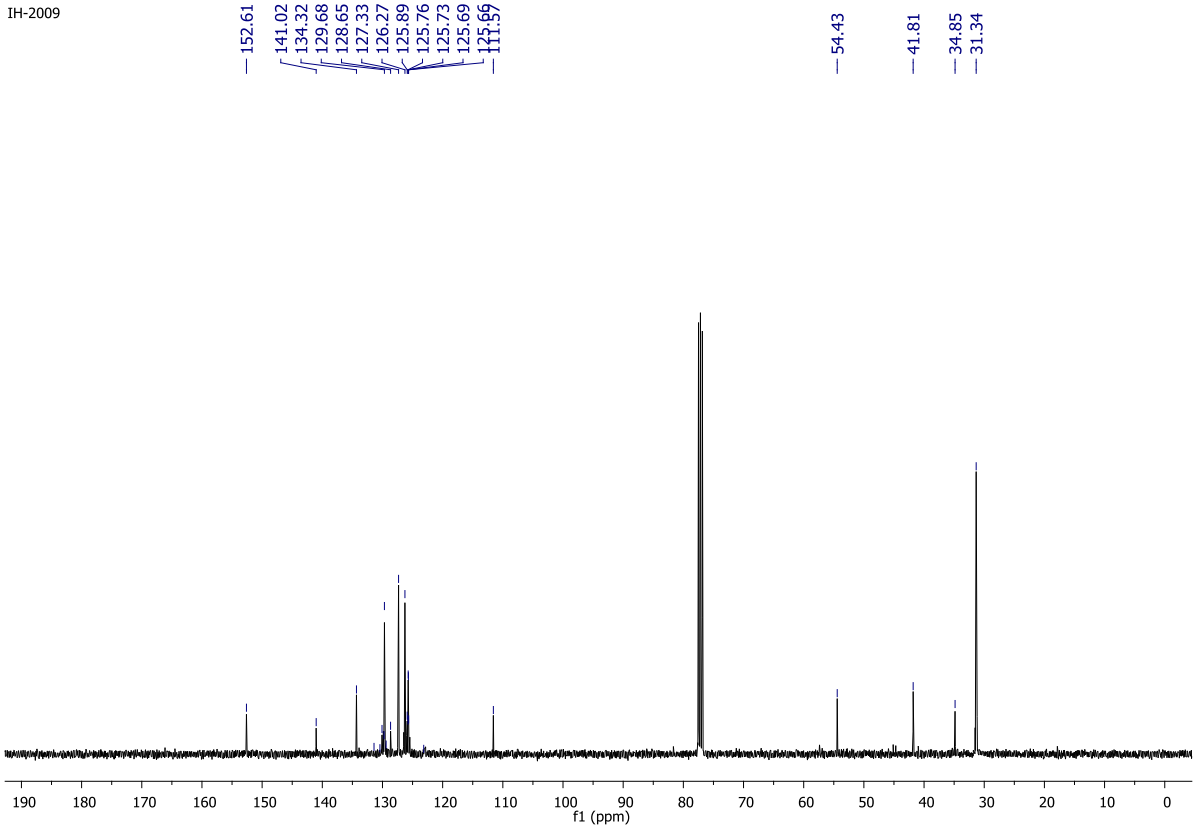

IH-2056-C

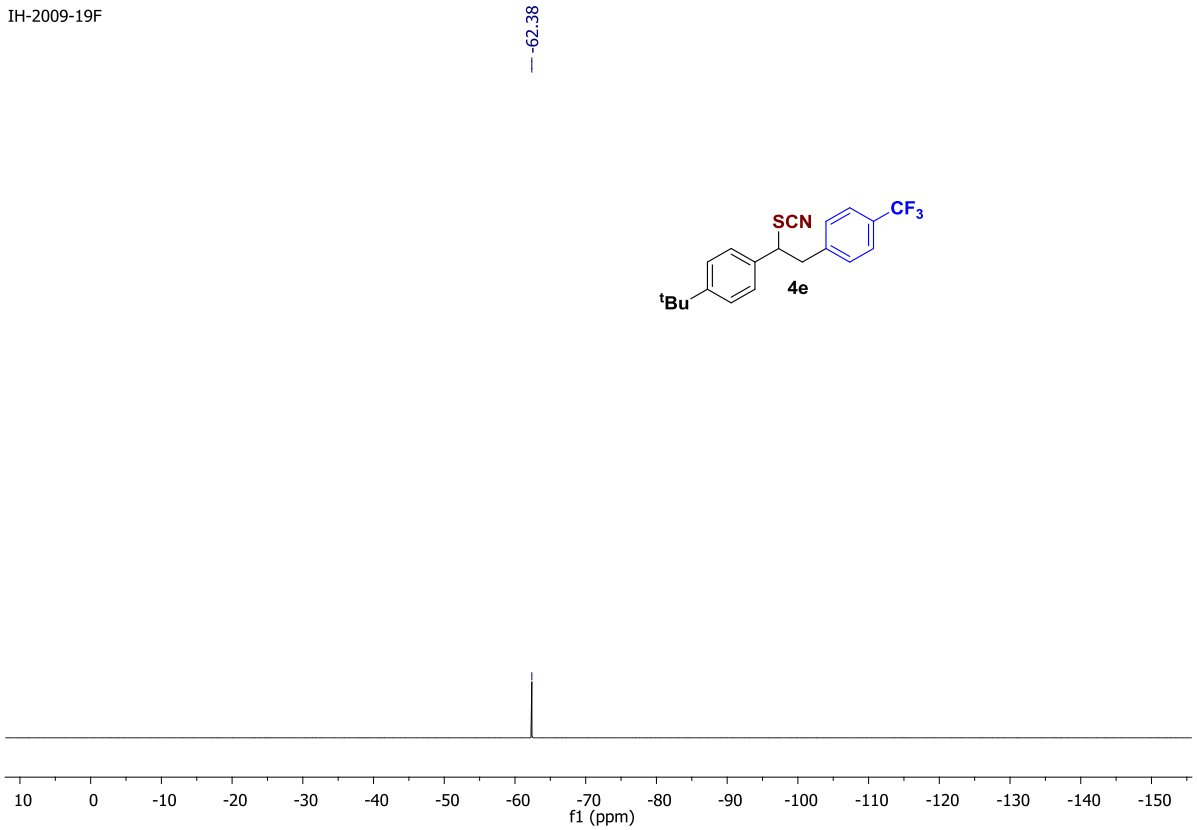
IH-2009-1H- 400MHz-(ND)



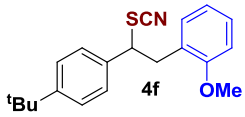

IH-2009

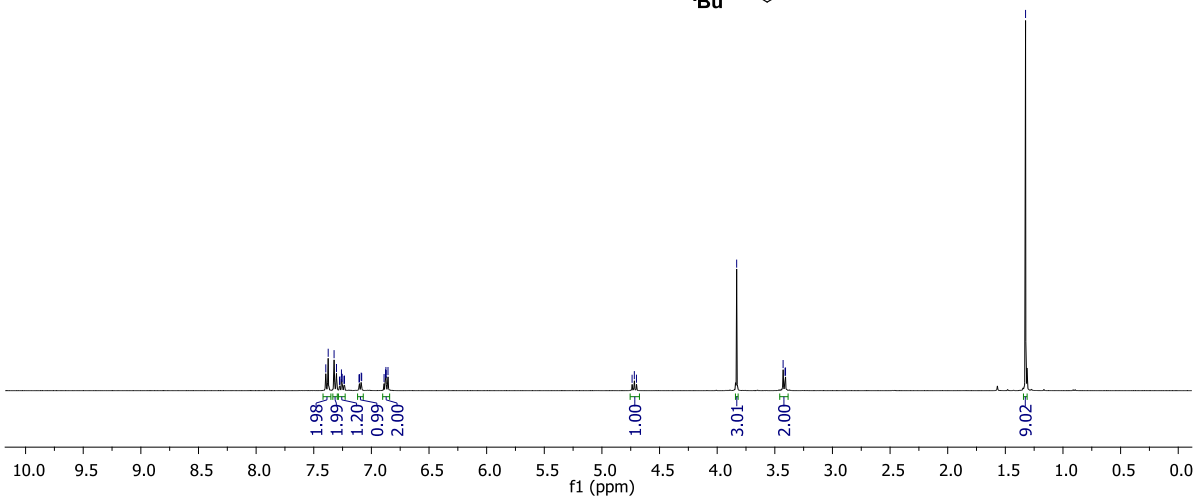


IH-2009-19F

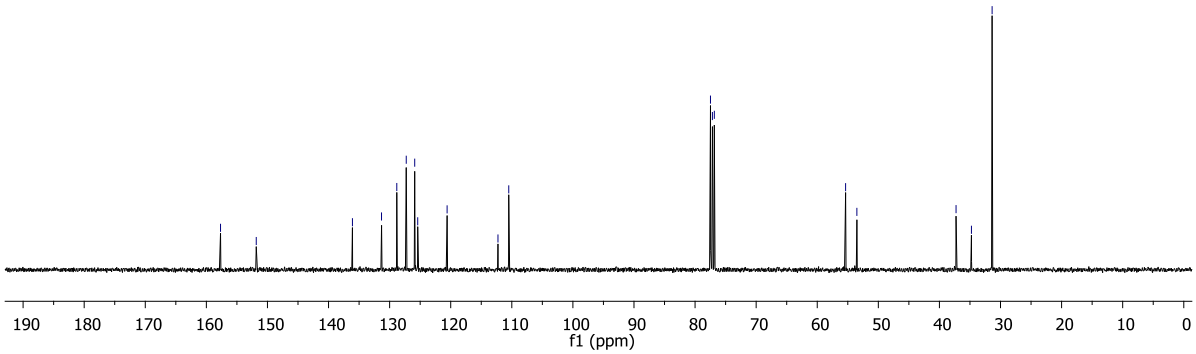

-62.38
SCN
CF3
tBu
4e
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

IH-2124

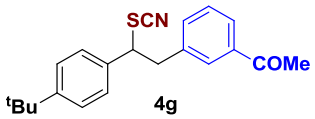




IH-2124

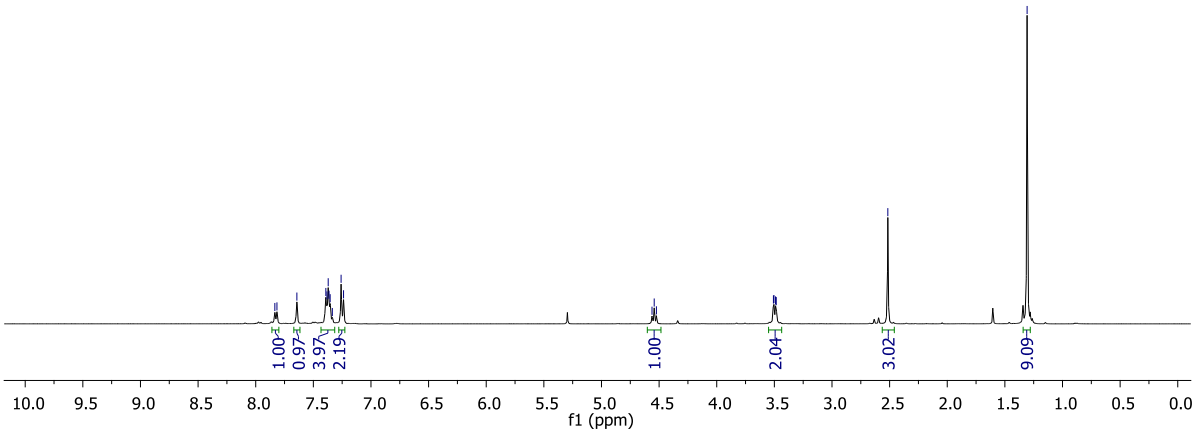



IH-2077-1H-(ND)-400

7.83 7.82 7.64 7.39 7.38 7.37 7.36 7.35 7.34 7.26 7.24 4.56 4.54 4.52 3.51 3.50 3.49 3.48 2.52 1.31

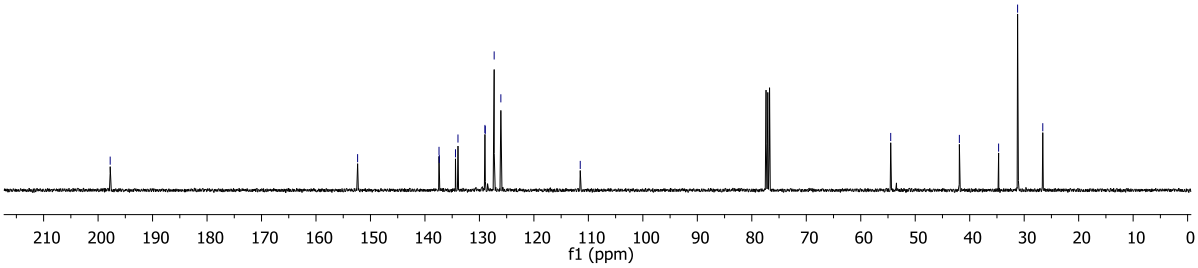



4g



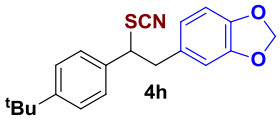

IH-2077

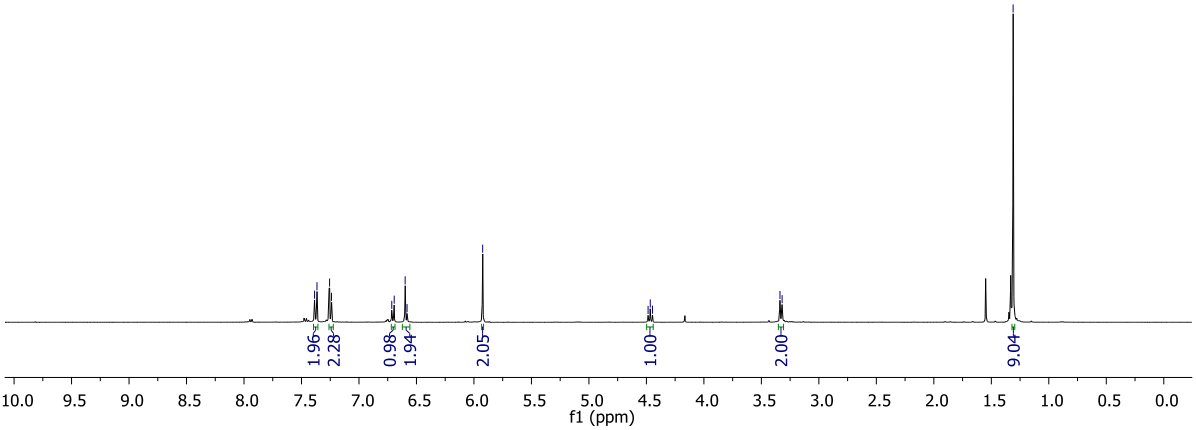
197.78 152.36 137.42 137.37 134.40 133.94 128.99 128.93 127.29 126.07 111.49 54.50 41.90 34.69 31.21 26.59



IH-2017-1H- 400MHz-(ND)

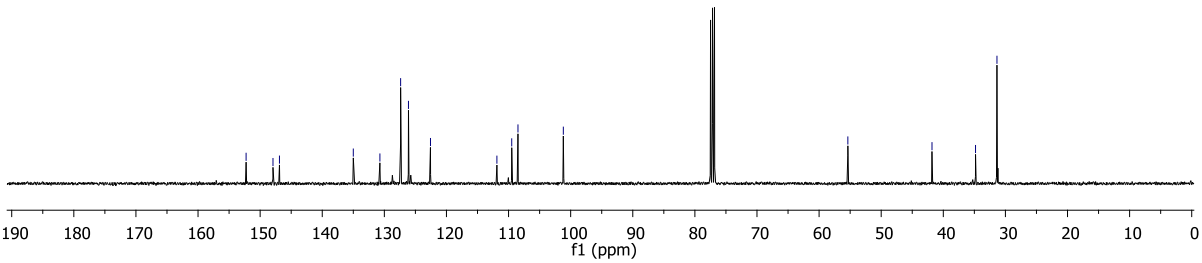
7.39
7.37
7.26
7.24
6.71
6.69
6.60
6.58
5.92
4.49
4.47
4.45
3.34
3.32
1.31



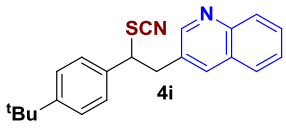



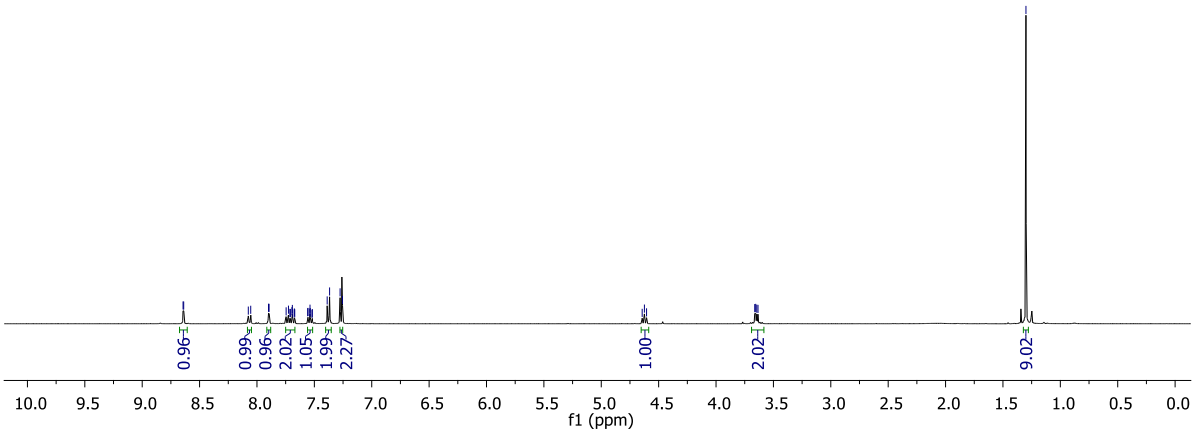

IH-2017

152.26
147.93
146.89
135.00
130.72
127.38
126.12
122.57
111.88
109.49
108.48
101.18
55.37
41.82
34.81
31.36

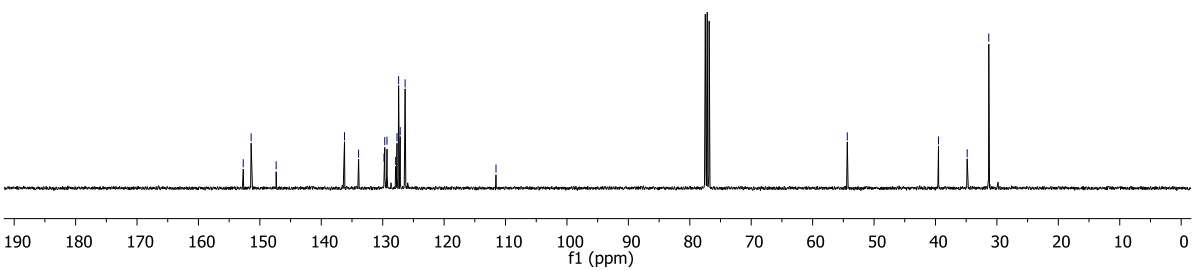


IH-2026-P

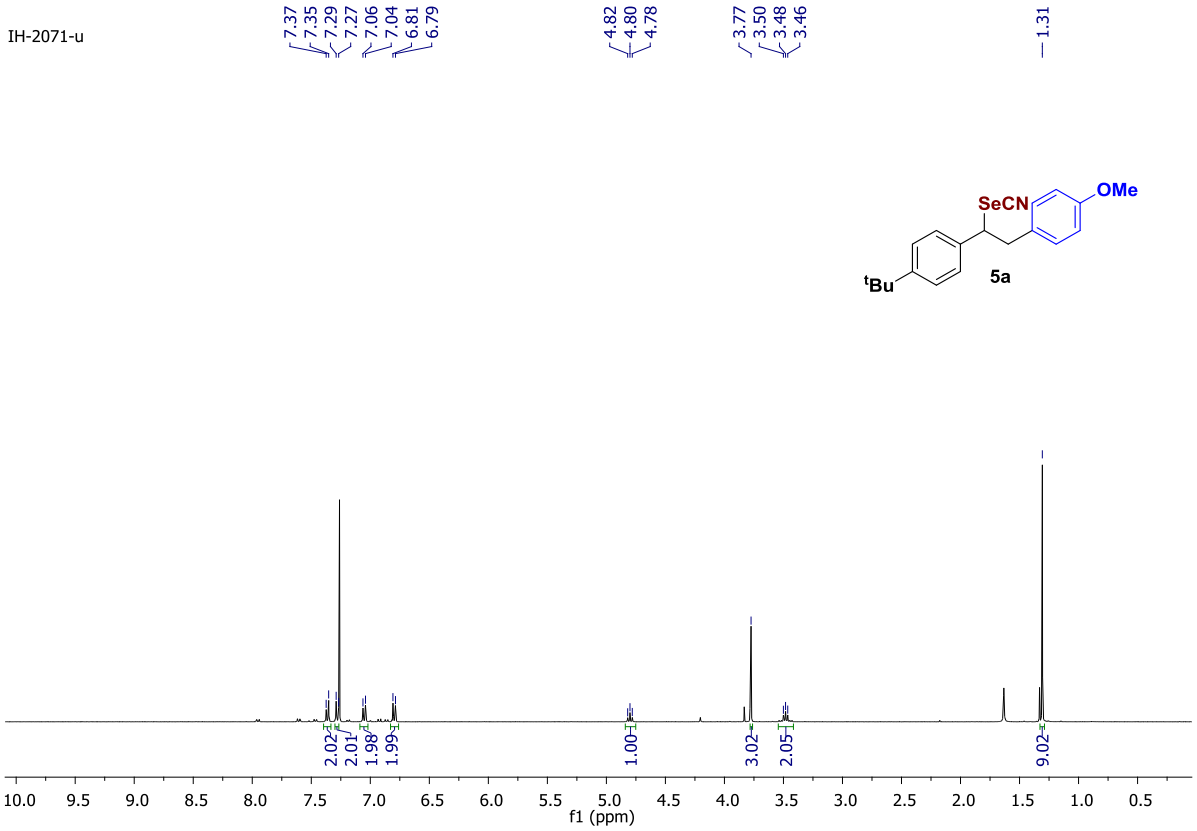



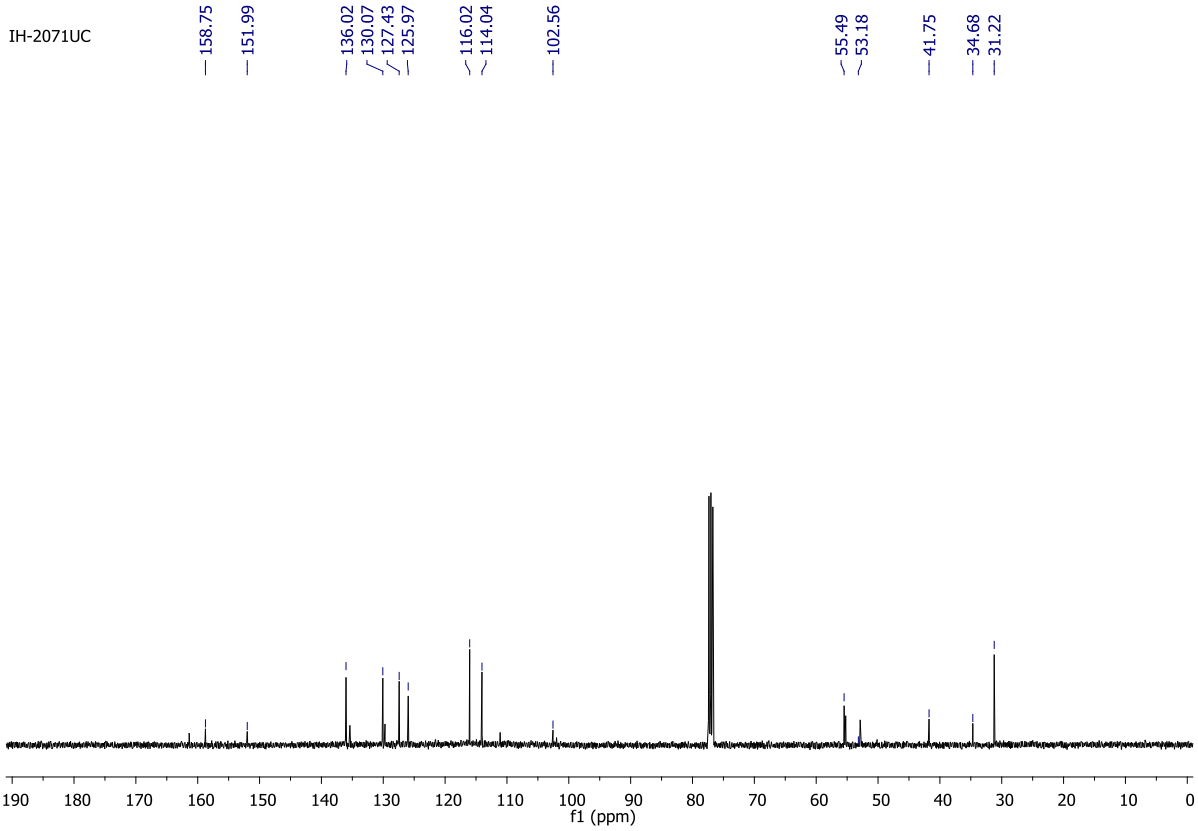

IH-2026-C

IH-2071-u




IH-2071UC

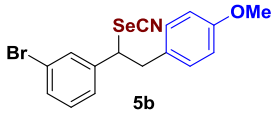


IH-2086-P-1H-(ND)-500

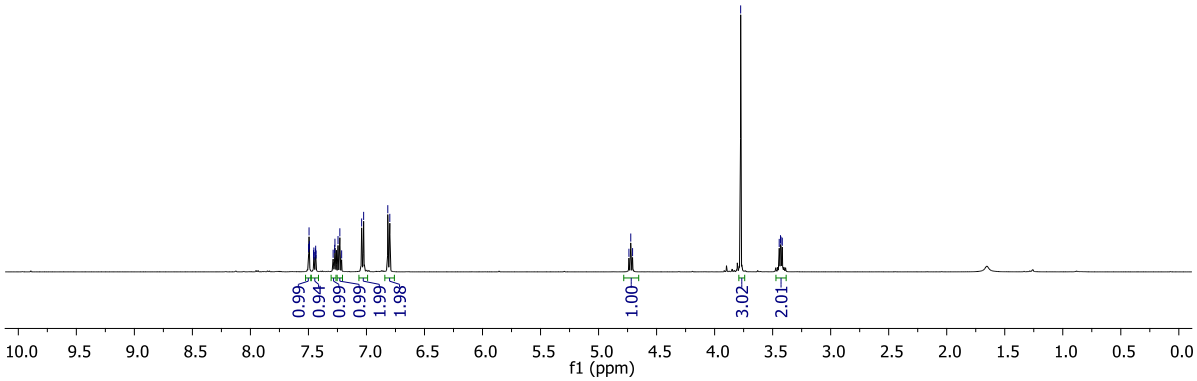
7.50 7.49 7.49 7.46 7.45 7.45 7.44 7.44 7.43 7.29 7.27 7.27 7.25 7.23 7.21 7.04 7.02 6.82 6.80

4.74 4.72 4.71

3.78 3.44 3.43 3.43 3.42

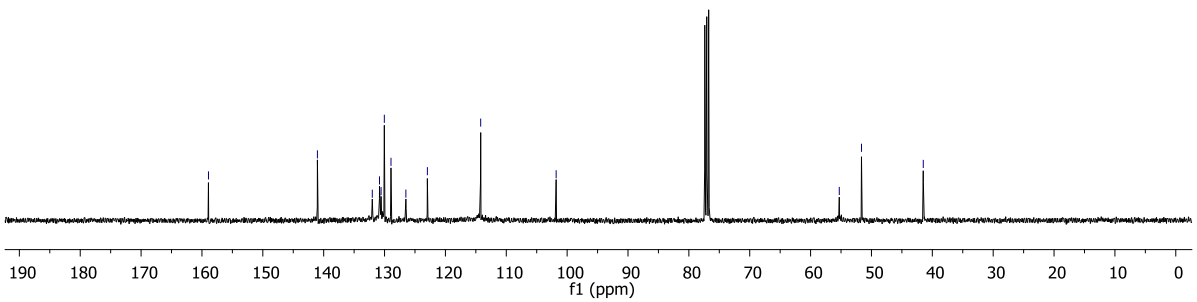



5b

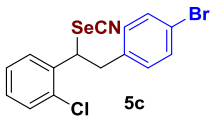


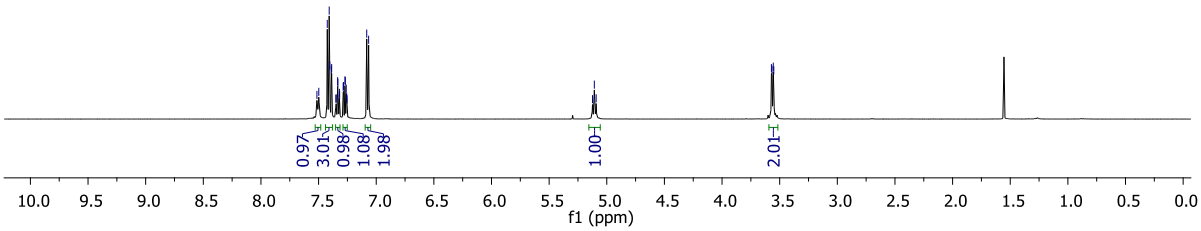

IH-2086

158.93 141.03 132.01 130.83 130.57 130.04 128.94 126.49 122.96 114.20 101.81 55.29 51.64 41.49

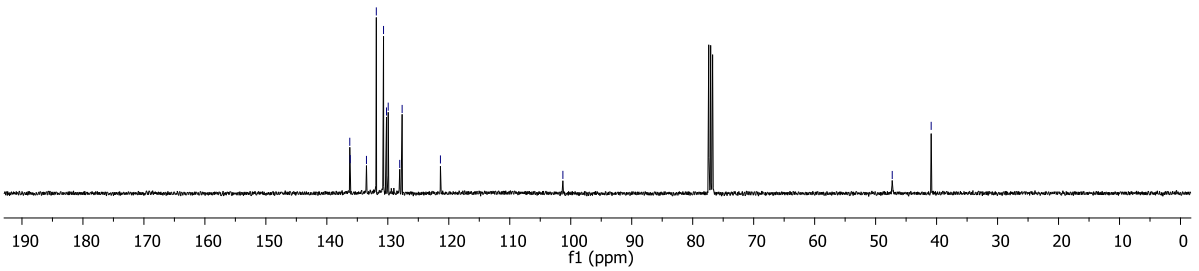


IH-2093-1H-(ND)-500

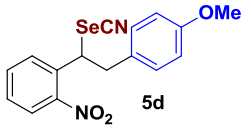




IH-2093C

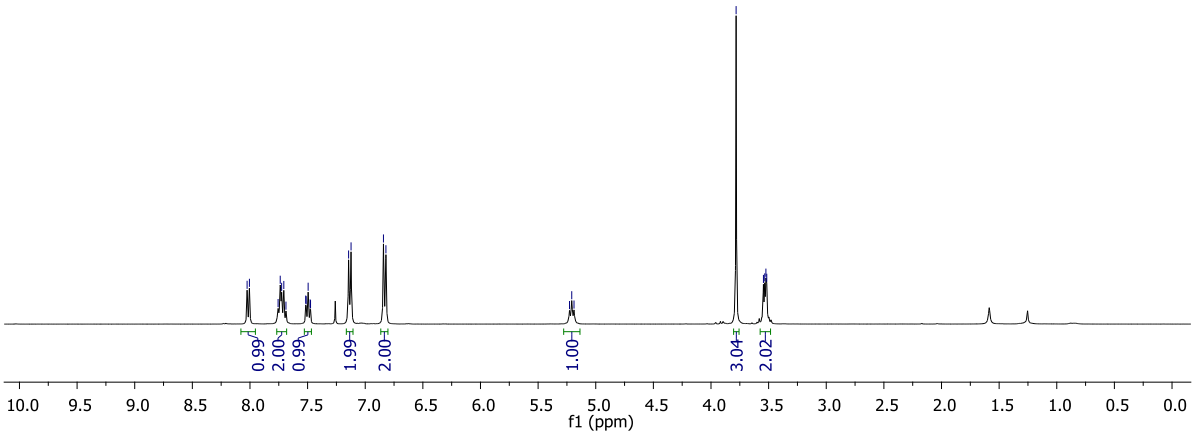



IH-2117

8.02 8.00 7.76 7.74 7.73 7.71 7.69 7.52 7.51 7.50 7.48 7.47 7.14 7.12 6.84 6.82 5.23 5.21 5.19 3.78 3.55 3.53 3.52 3.52

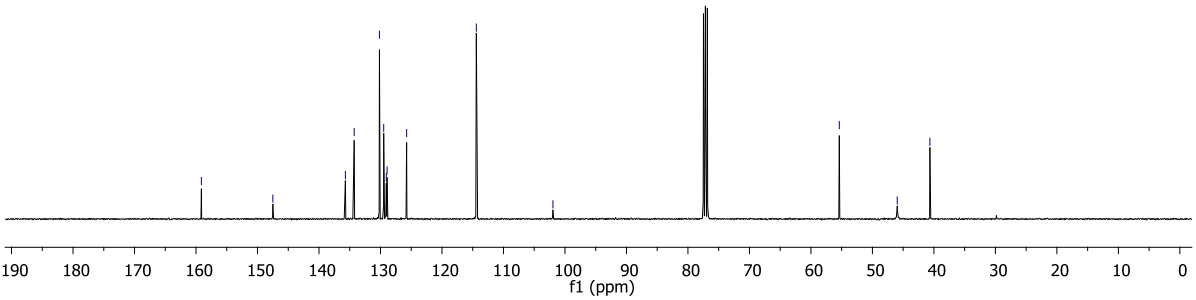



5d

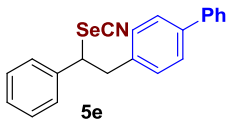



IH-2117

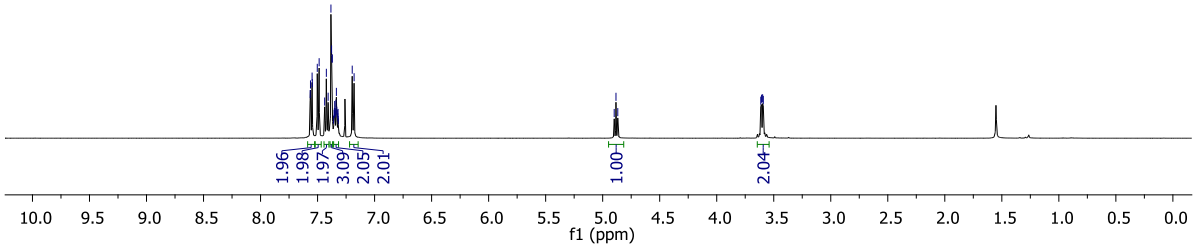
159.13 147.50 135.71 134.28 130.17 129.48 129.06 128.93 125.75 114.41 101.95 55.38 45.96 40.65



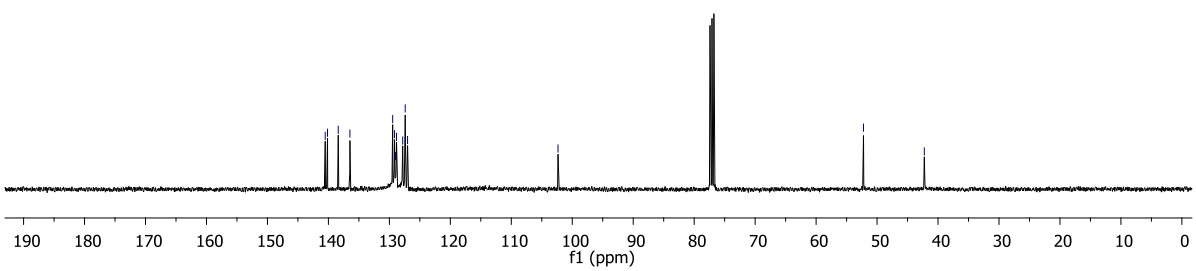

IH-2092-P-1H-(ND)-500
7.56
7.56
7.55
7.55
7.50
7.49
7.44
7.42
7.41
7.38
7.38
7.37
7.37
7.36
7.35
7.35
7.35
7.35
7.34
7.34
7.34
7.33
7.33
7.32
7.32
7.32
7.20
7.18
4.90
4.88
4.87
3.61
3.61
3.60
3.59


SeCN
Ph

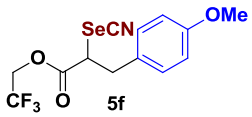
5e

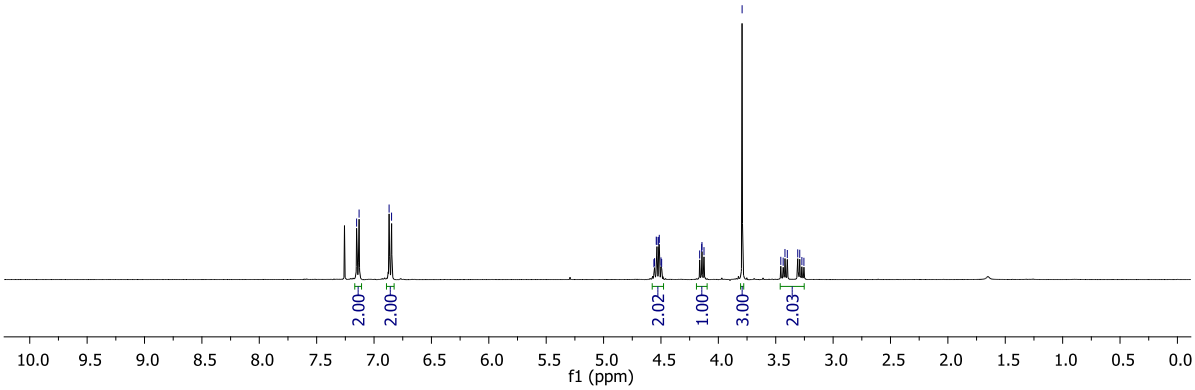

1.96
1.98
1.97
3.09
2.05
2.01
1.00
2.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


IH-2092
140.52
140.15
138.39
136.47
129.46
129.15
128.99
128.82
127.81
127.40
127.01
102.34
52.23
42.25

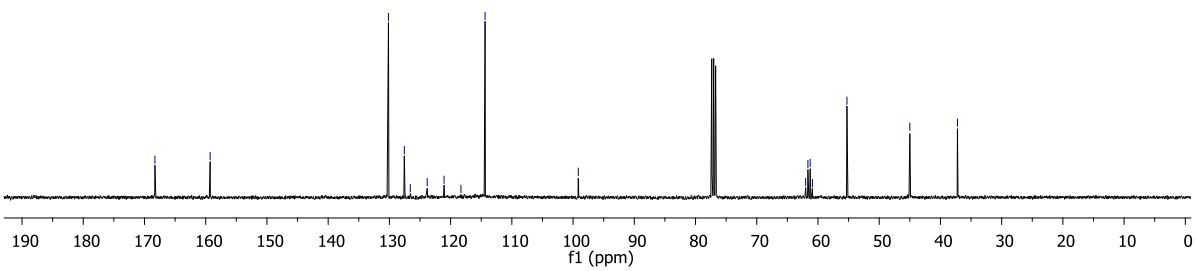

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

IH-2096

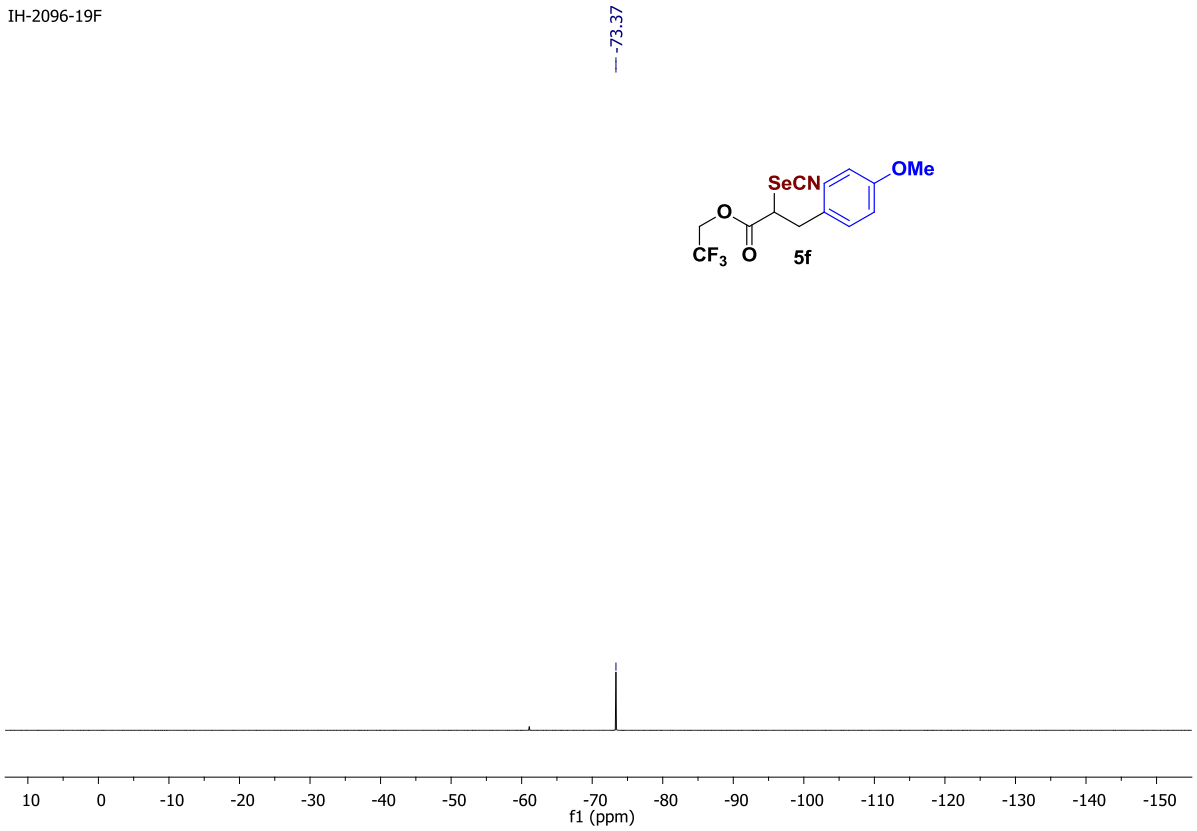



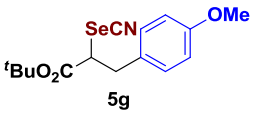

IH-2096

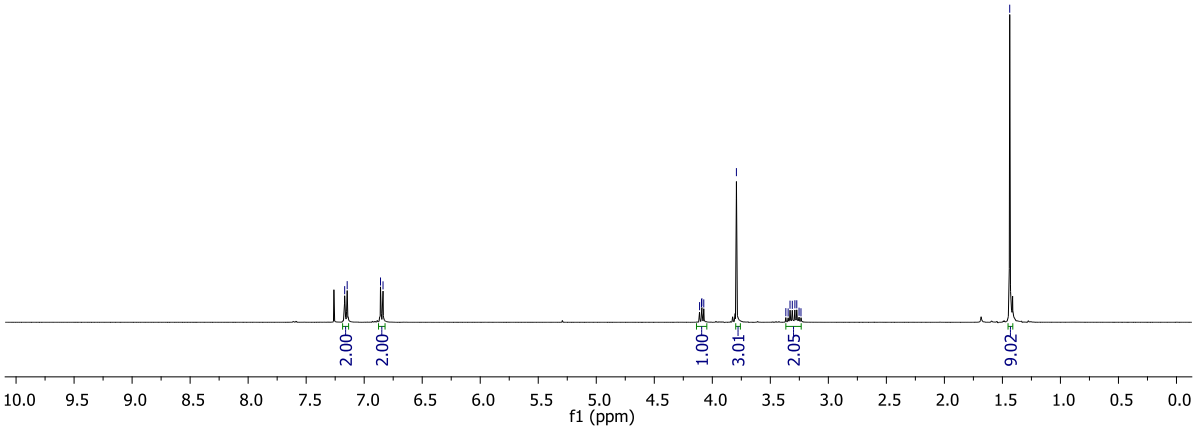
IH-2096-19F


-73.37
SeCN
OMe
O
CF3
O
5f
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

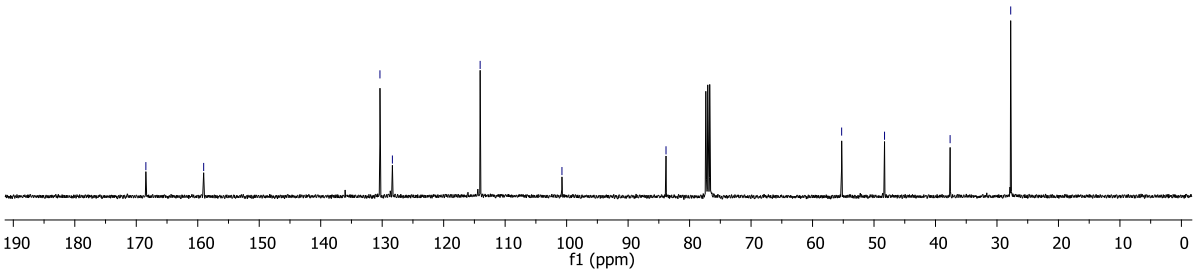
IH-2098

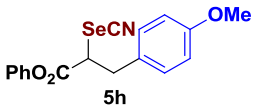

5g



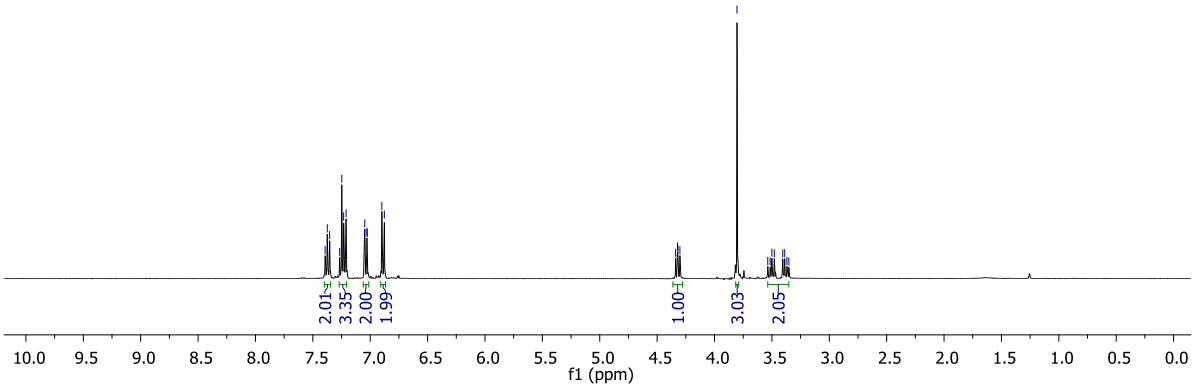

IH-2098

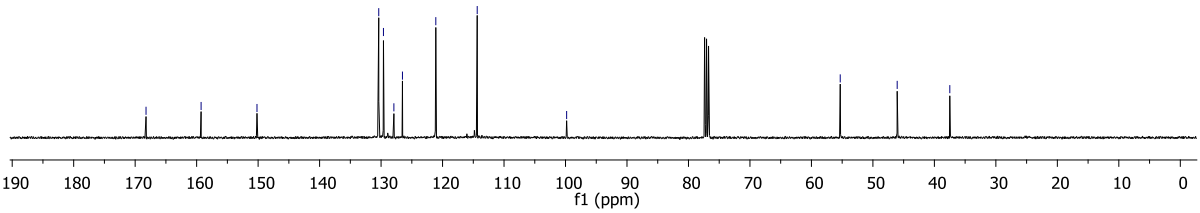
IH-2097

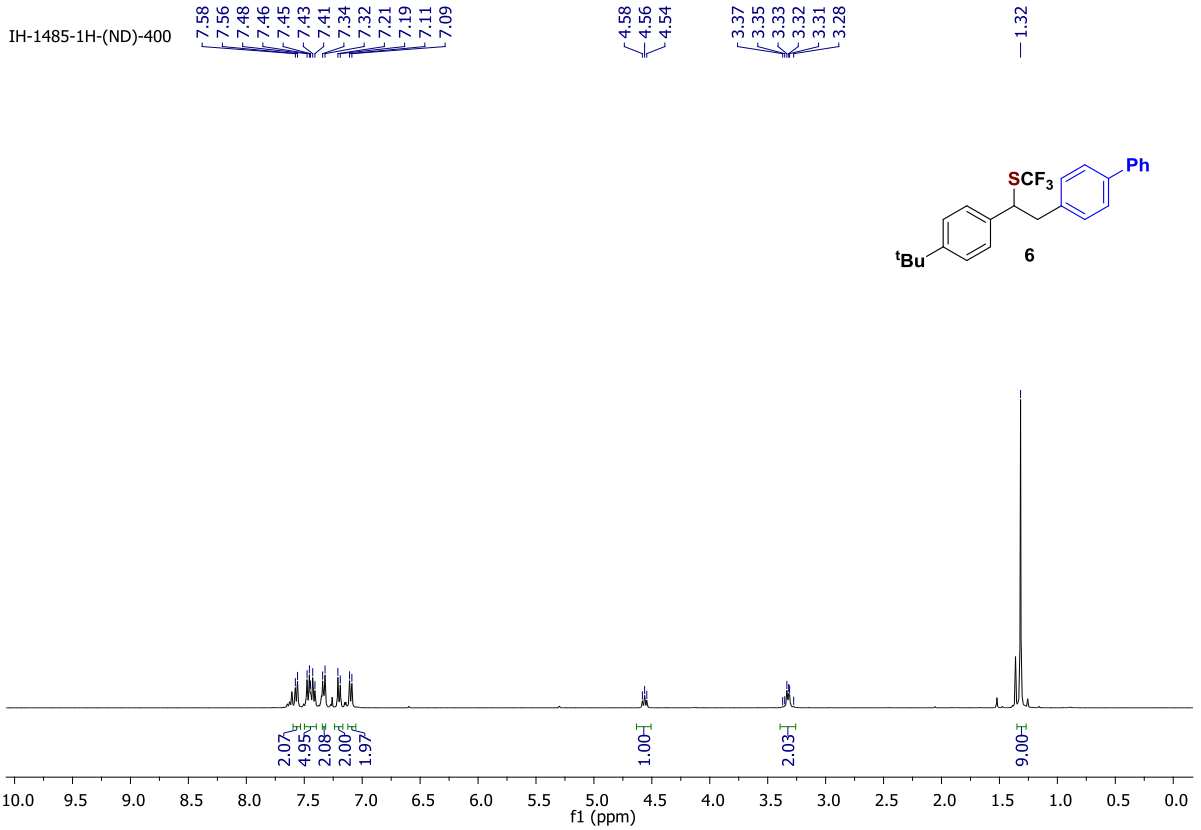



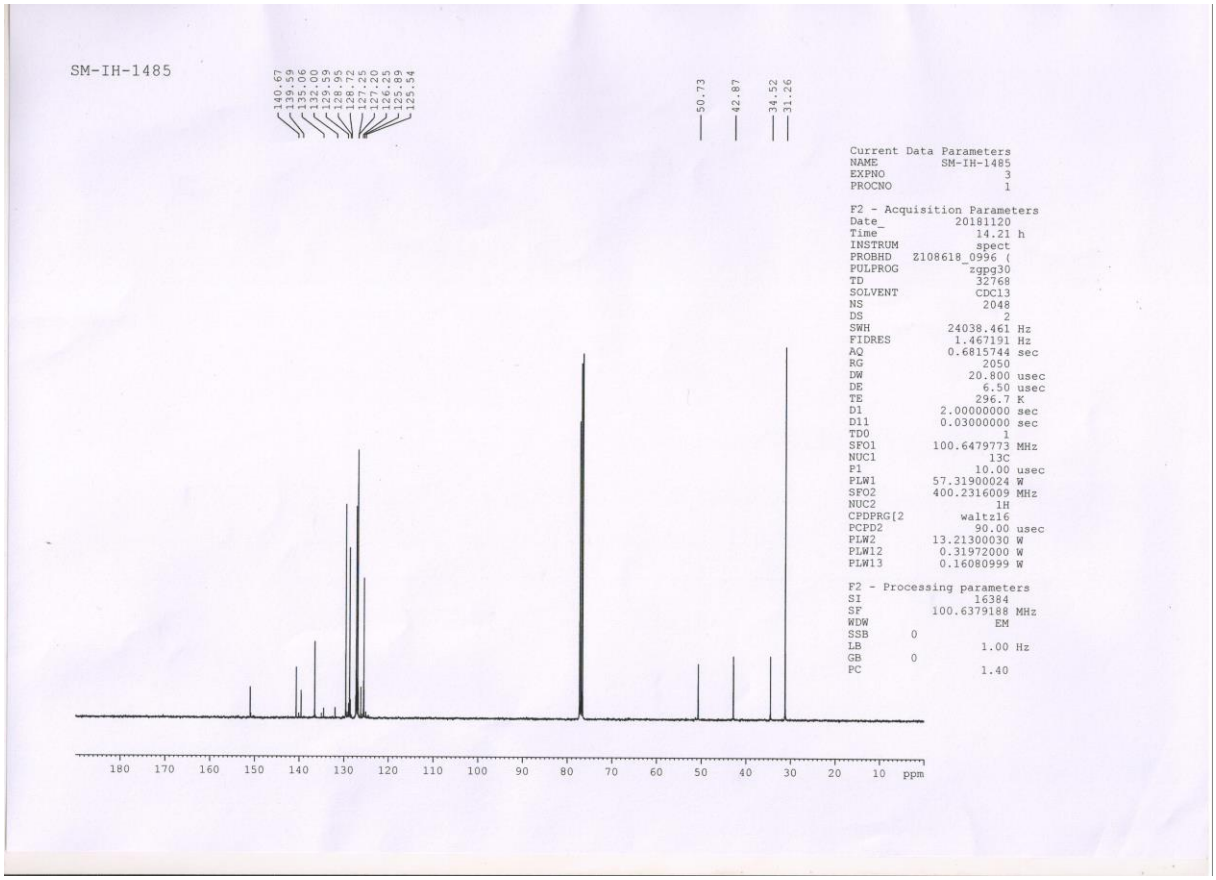

5h

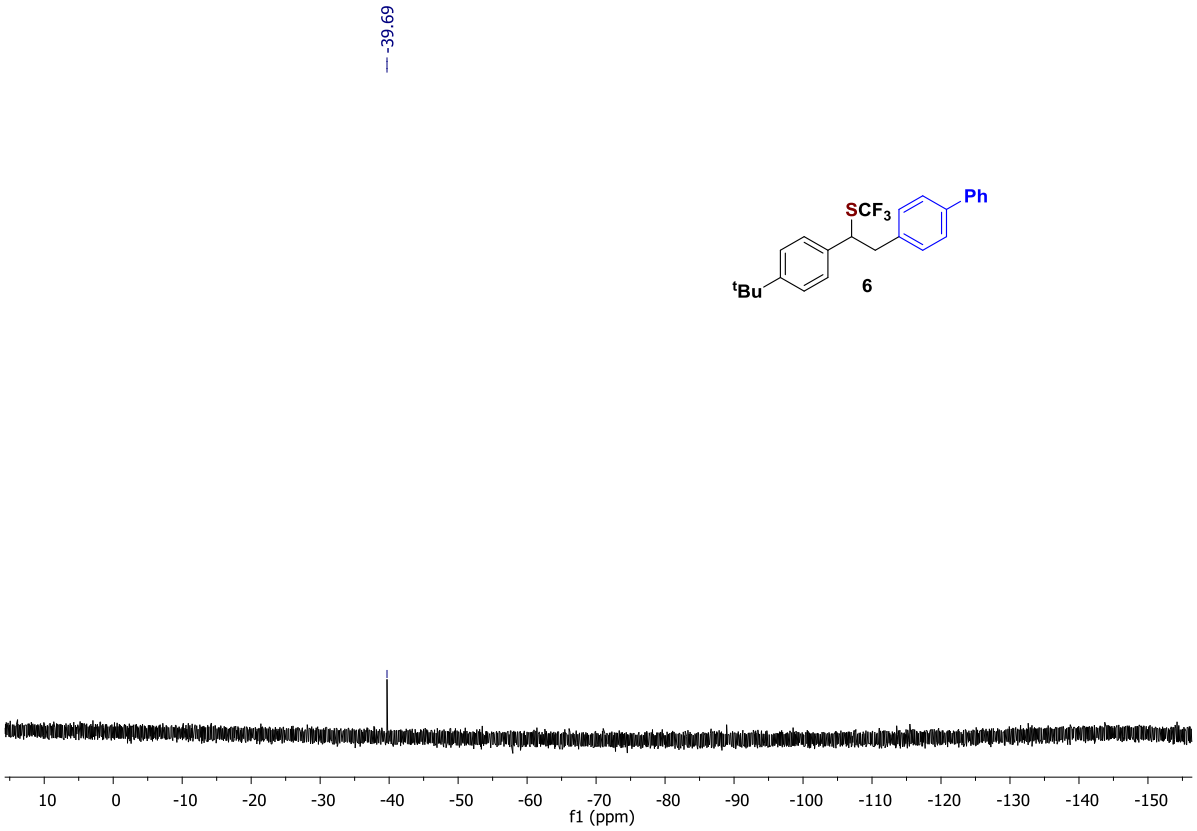



IH-2097

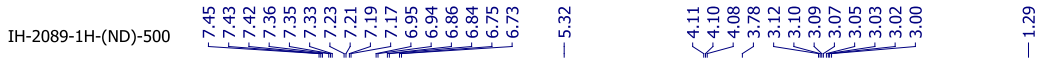



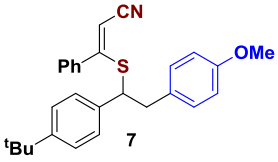

IH-1485-1H-(ND)-400
7.58
7.56
7.48
7.46
7.45
7.43
7.41
7.34
7.32
7.21
7.19
7.11
7.09
4.58
4.56
4.54
3.37
3.35
3.33
3.32
3.31
3.28
1.32
SCF3
Ph
tBu
6
2.07
4.95
2.08
2.00
1.97
1.00
2.03
9.00
f1 (ppm)

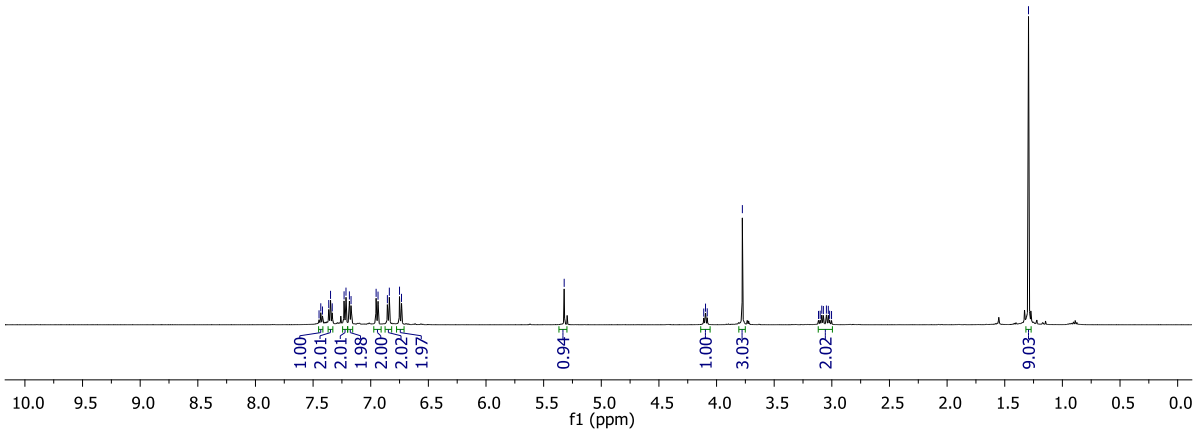

SM-IH-1485
140.67
139.69
135.06
132.00
129.59
128.95
128.72
127.25
127.20
126.25
125.89
125.54
50.73
42.87
34.52
31.26
Current Data Parameters
NAME SM-IH-1485
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20181120
Time 14.21 h
INSTRUM spect
PROBHD Z108618_0996 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2048
DS 2
SWH 24038.461 Hz
FIDRES 1.467191 Hz
AQ 0.6815744 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6479773 MHz
NUC1 13C
P1 10.00 usec
PLW1 57.31900024 W
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.21300030 W
PLW12 0.31972000 W
PLW13 0.16080999 W
F2 - Processing parameters
SI 16384
SF 100.6379188 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm


-39.69
SCF3
Ph
tBu
6
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
f1 (ppm)

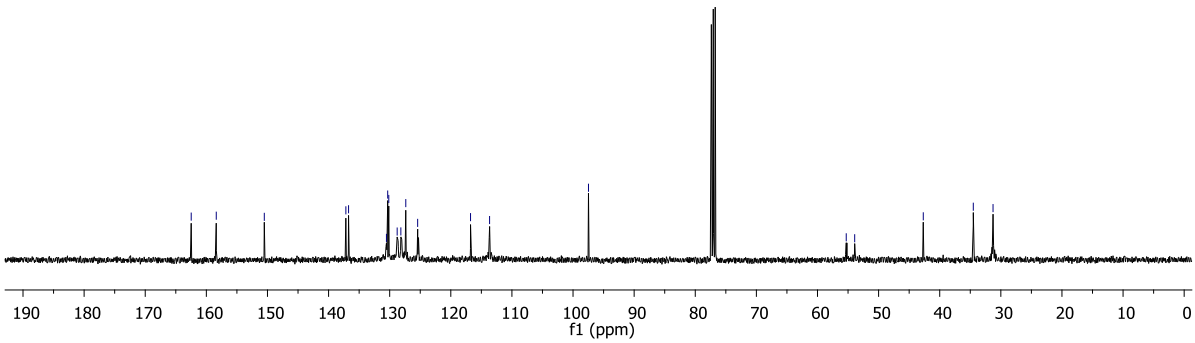
IH-2089-1H-(ND)-500



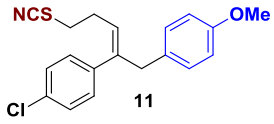



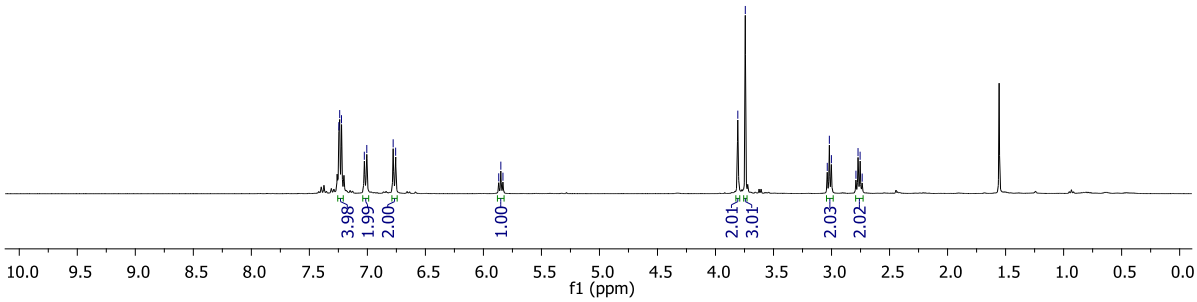

IH-2089

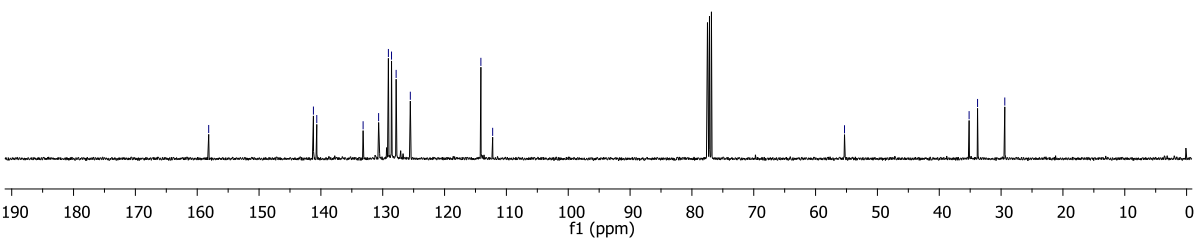
IH-2046-L-1H(ND) 400MHz

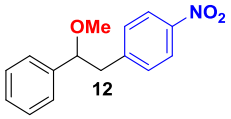

11

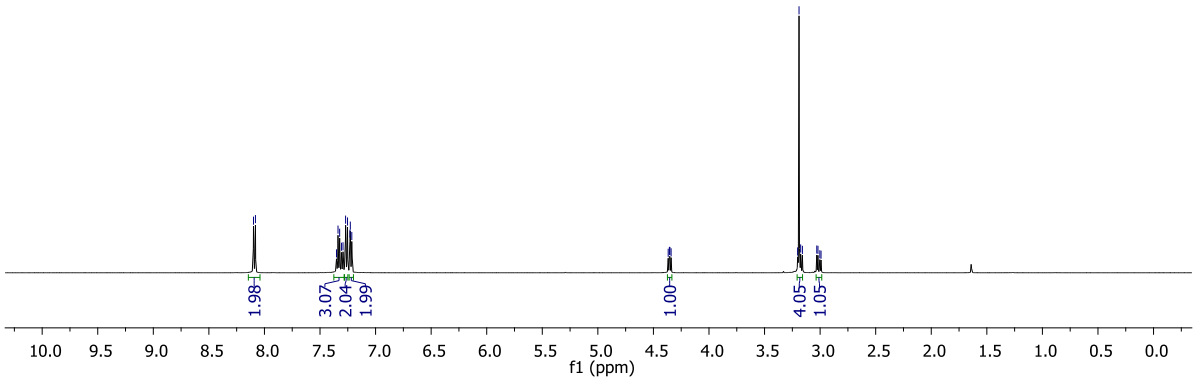



IH-2046-L

IH-2064-P-1H-(ND)-500


IH-2064