Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Supplementary Information

# Synthesis and Fluorosolvatochromic Properties of 1,7-Annulated Indoles

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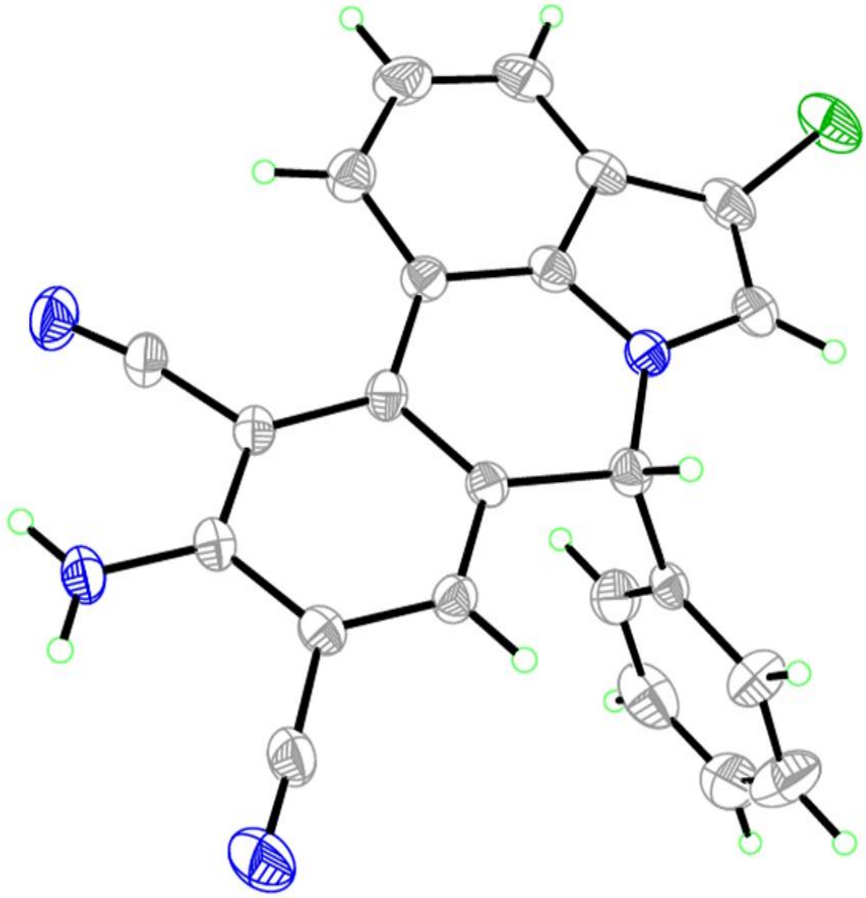
1. X-ray data for **3**

Crystals suitable for X-ray analysis were grown by slow evaporation at room temperature of a solution of **3** in dichloromethane. $C_{23}H_{13}ClN_4$, $M_w$ = 380.82, monoclinic, space group $P2_1$; dimensions: a = 13.9521(8) Å, b = 10.5005(5) Å, c = 14.1217(8) Å, $\beta$ = 117.346(3)°, V = 1837.68(18) $Å^3$; Z = 4; μ = 0.22 $mm^{-1}$; 86494 reflections measured at room temperature; independent reflections: 6476 [5069 Fo > 4s(Fo)]; data were collected up to a 2Θ max value of 50.07° (99.6 % coverage). Number of variables: 505; $R_1$ = 0.053, $wR_2$ = 0.140, S = 1.11; absolute structure parameter: 0.03(4); highest residual electron density 0.26 e.$Å^{-3}$; CCDC = 1528334.



## 2. UV and fluorescence data

For each compound and each solvent, a mother solution with a concentration of $2.10^{-4}$ mol.L$^{-1}$ was prepared. This solution was further diluted to obtain 4 solutions at $1.10^{-6}$, $2.10^{-6}$, $5.10^{-6}$ and $1.10^{-5}$ mol.L$^{-1}$. Spectra were recorded in order of increasing concentrations. Between each solution, the cuvette was rinsed two times with the next solution. When solvent changed, the cuvette was first rinsed three times with pure new solvent, then two times with the first solution in this solvent.

UV-Visible spectra were first recorded. Excitation wavelength for each compound was obtained from the rounded maximum absorption wavelengths. Fluorescence spectra were then recorded using this excitation wavelength. All other properties, e.g. ε, Δν and ϕ, were determined using these experimental values.

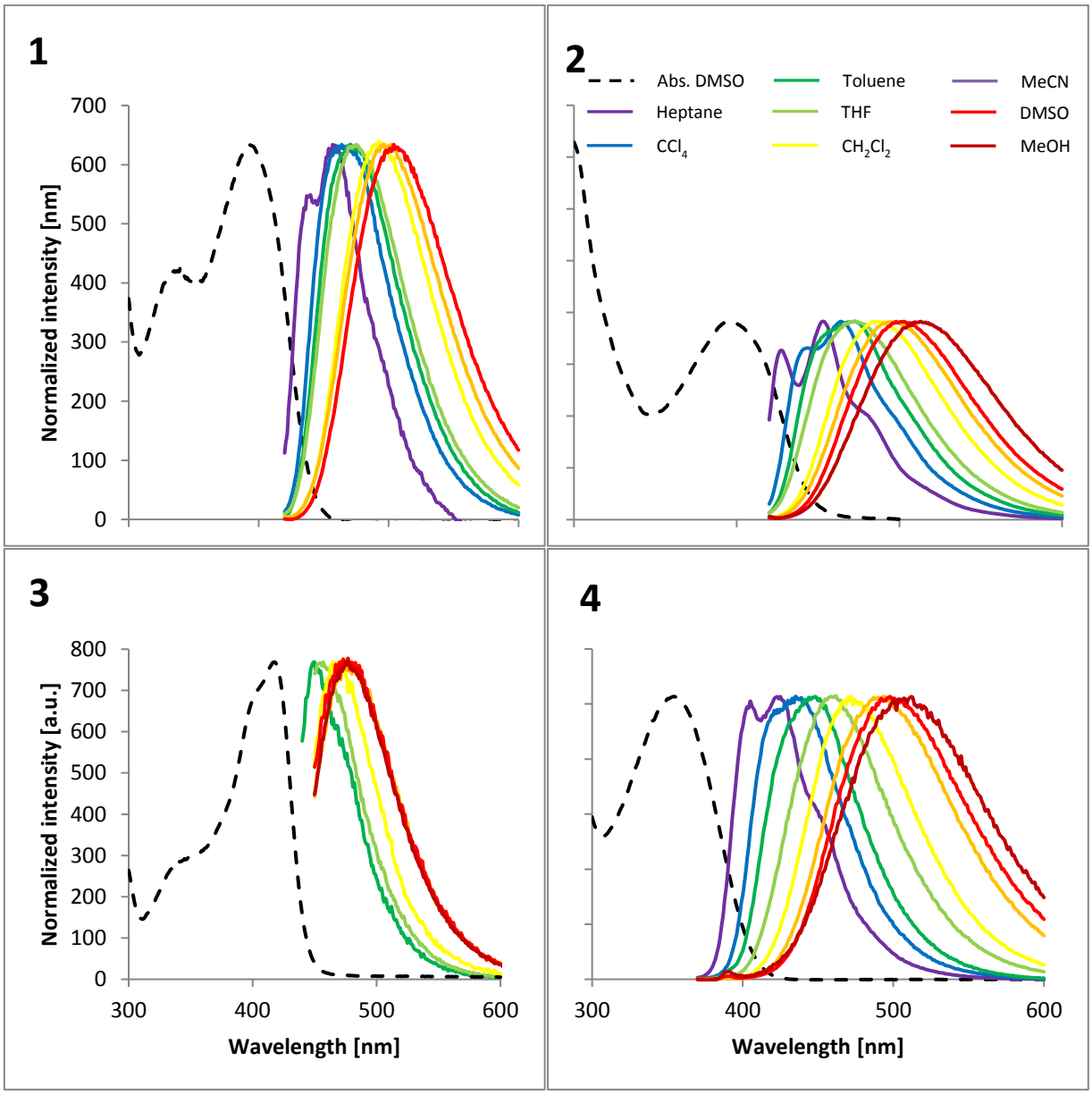
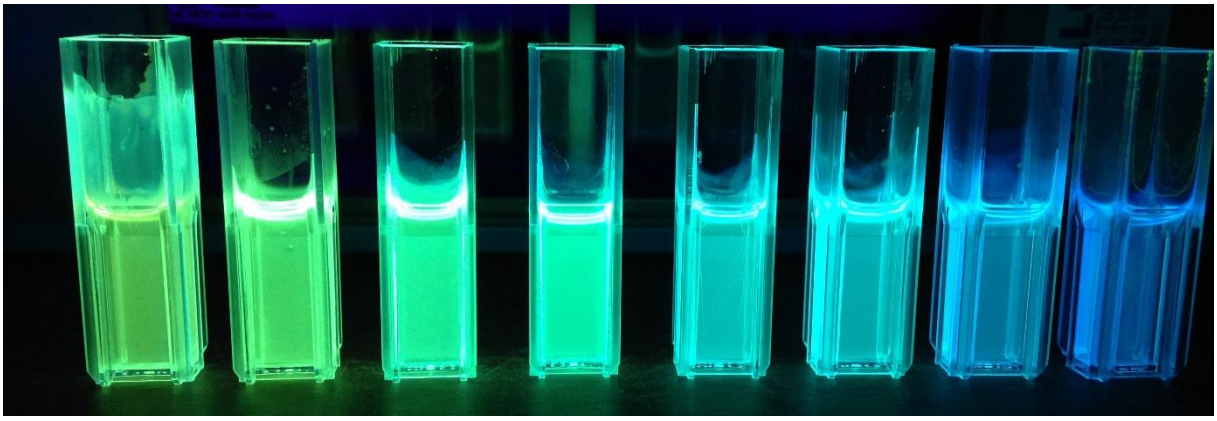


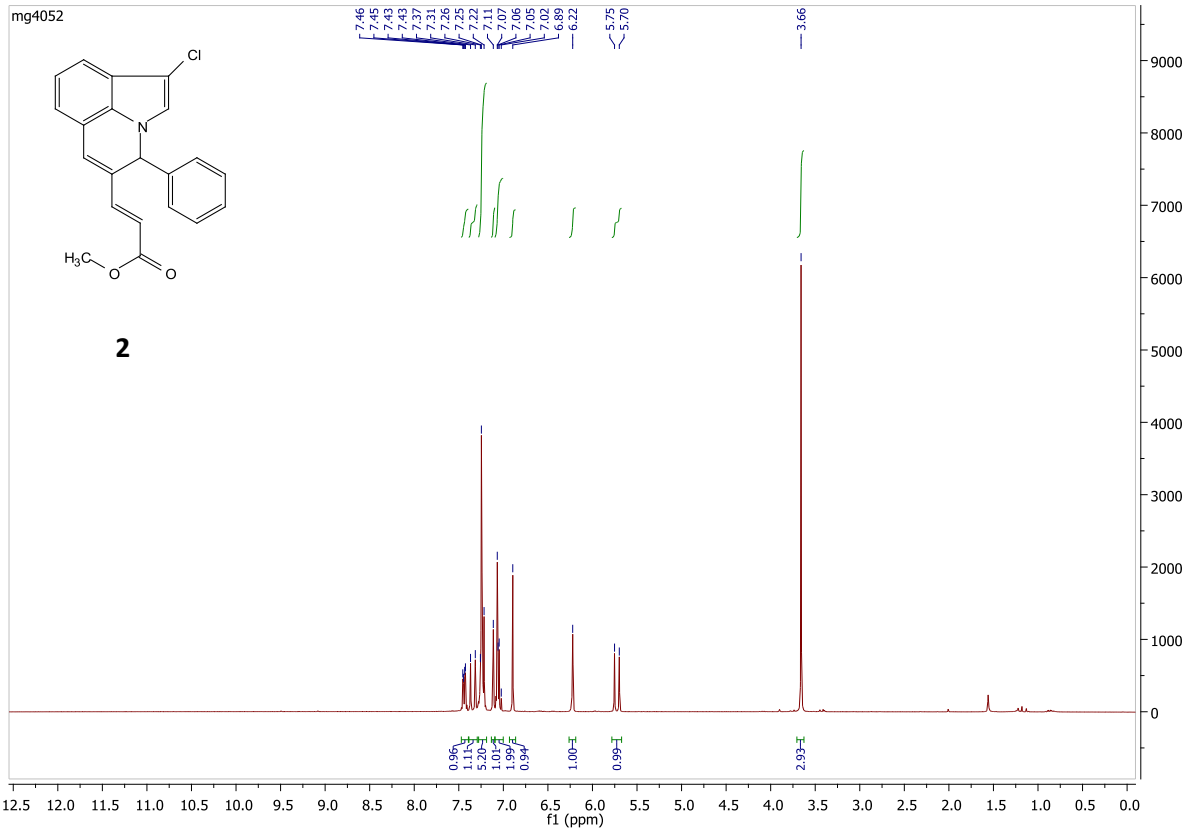

**Figure S1** Normalized absorption and fluorescence spectra for compounds **1-4** in various solvents. Dashed lines are used for absorption spectra, when plain lines are for fluorescence spectra.

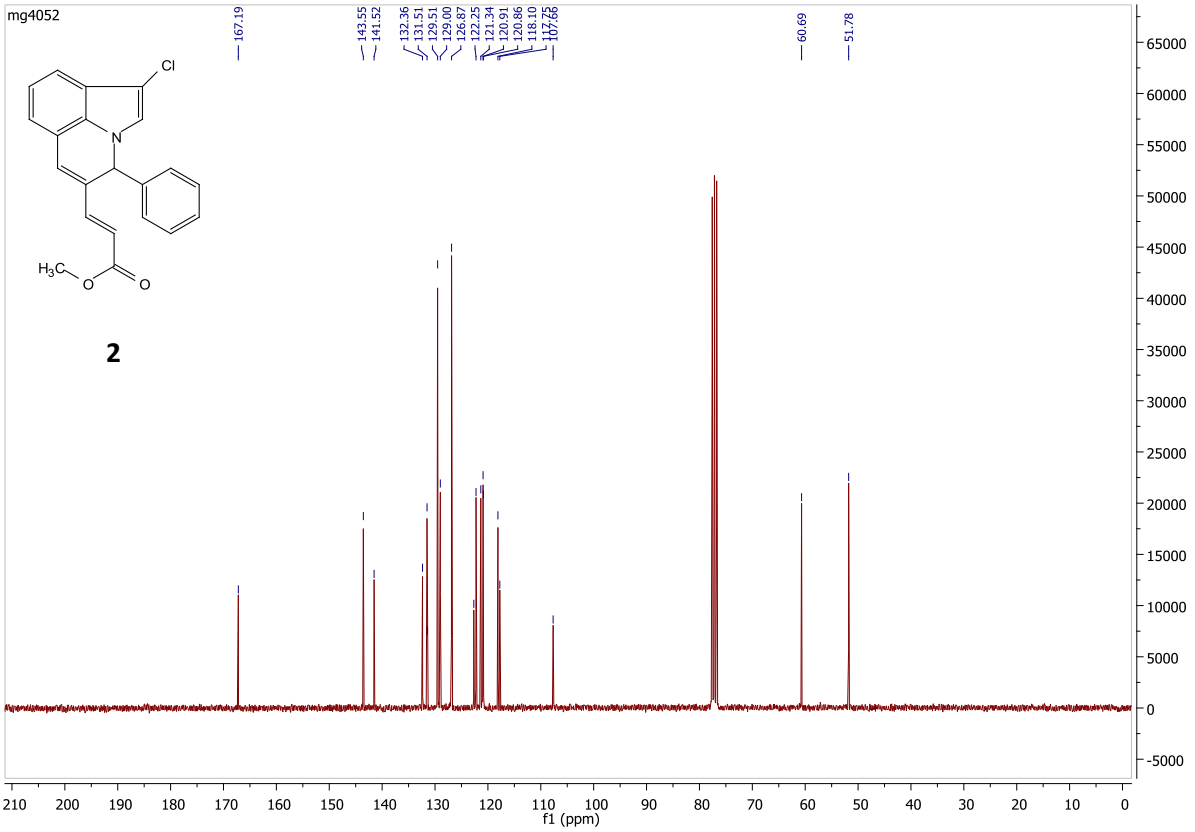
3. Fluorescence colors of **2** in various solvents

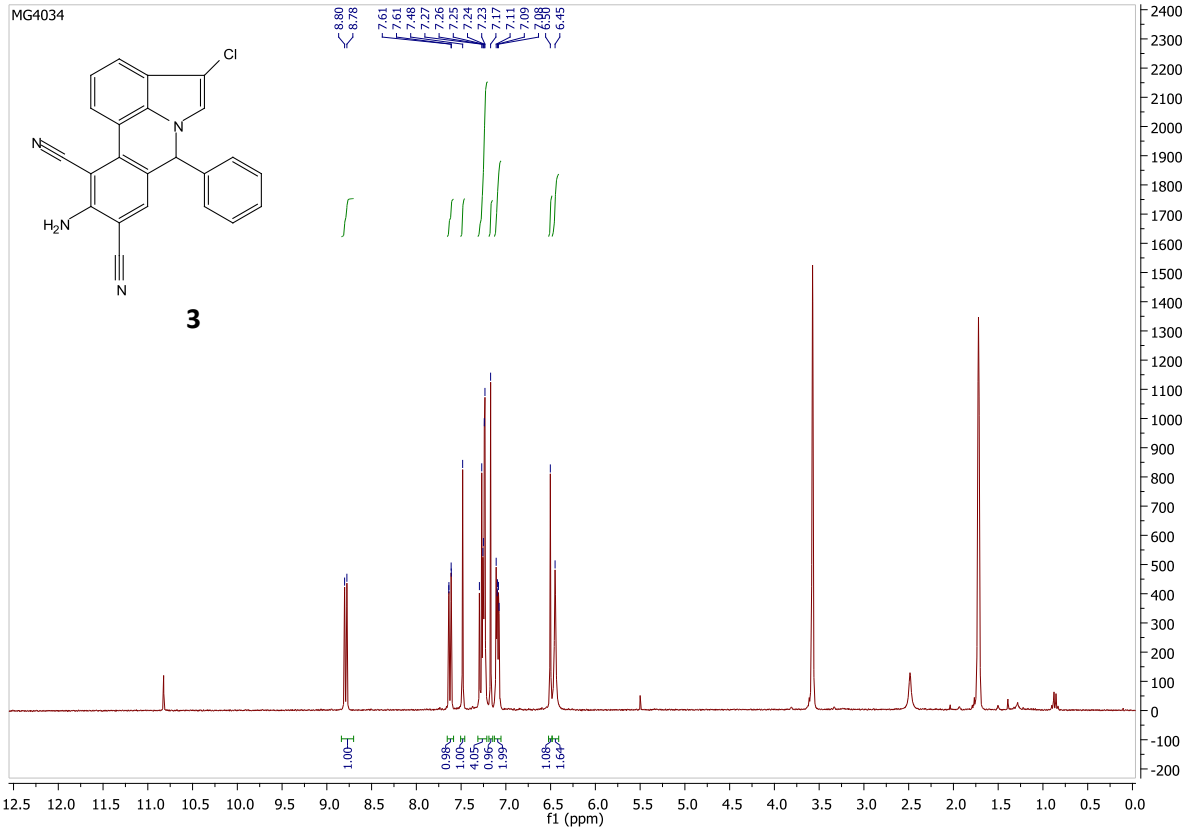
Fluorescence color changes of **2** in various solvents (from left to right: MeOH, DMSO, MeCN, $CH_2Cl_2$, THF, Toluene, $CCl_4$ and heptane). The picture was taken in the dark upon irradiation with a hand-held UV lamp (excitation: 366 nm).



4. NMR spectra

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N
N
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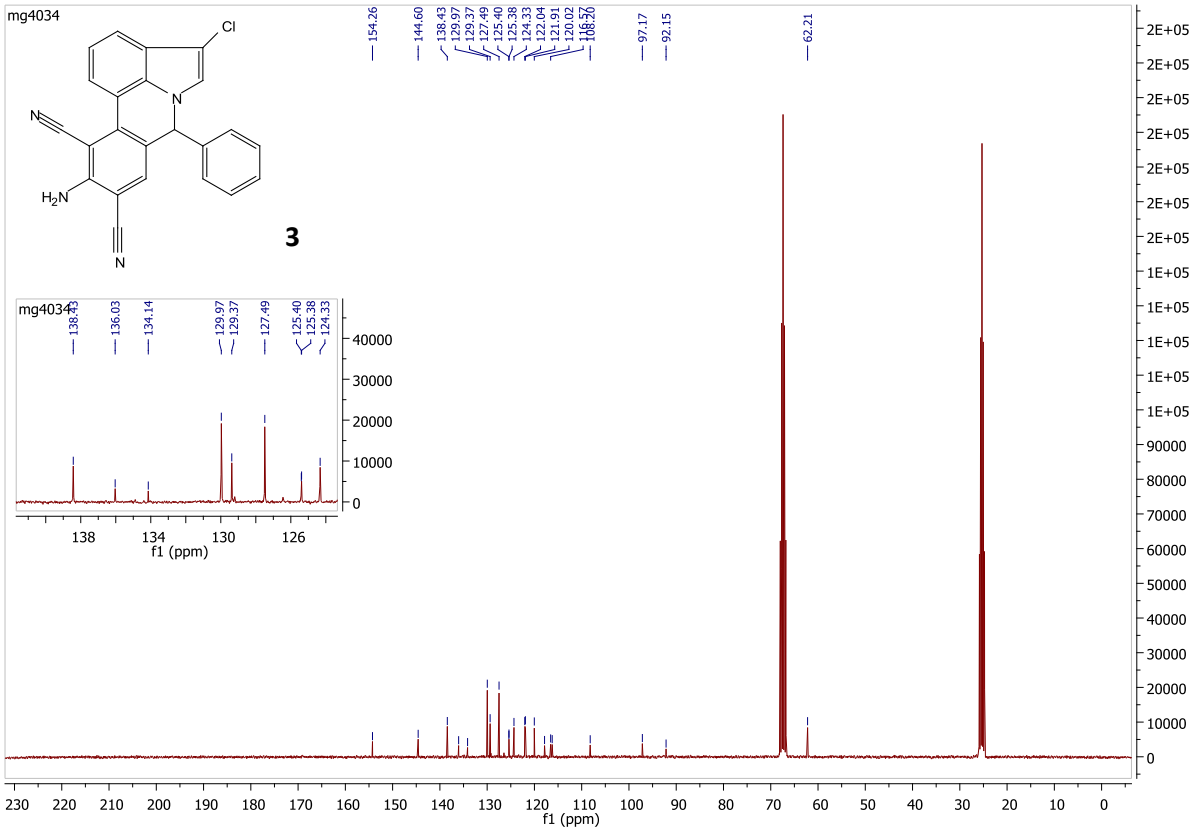
N
3
8.80
8.78
7.61
7.61
7.48
7.27
7.26
7.25
7.24
7.23
7.17
7.11
7.09
6.98
6.45
1.00
0.98
1.00
4.05
0.96
1.99
1.08
1.64
f1 (ppm)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N
N
$H_2N$
N
3
154.26
144.60
138.43
129.97
129.37
127.49
125.40
125.38
124.33
122.04
121.91
120.02
97.17
92.15
62.21
mg4034
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129.97
129.37
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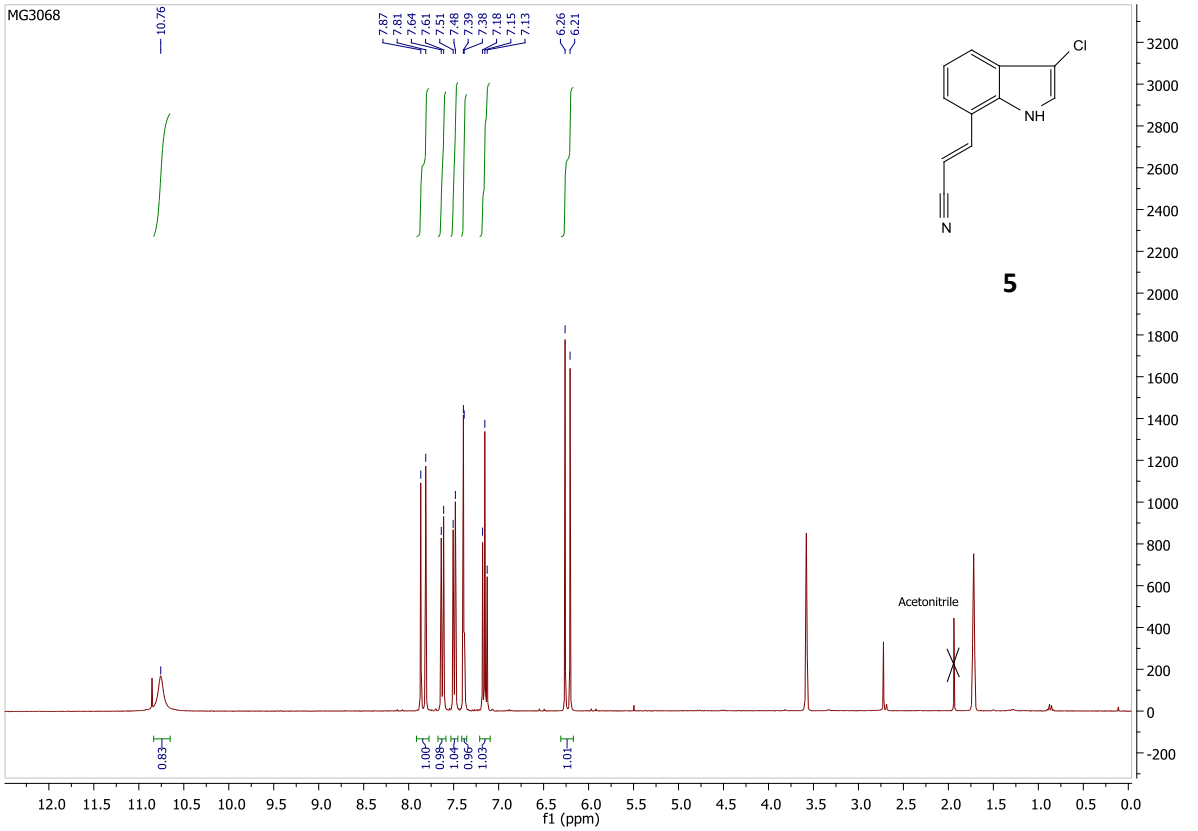
125.38
124.33
f1 (ppm)
f1 (ppm)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7.13
6.26
6.21
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N
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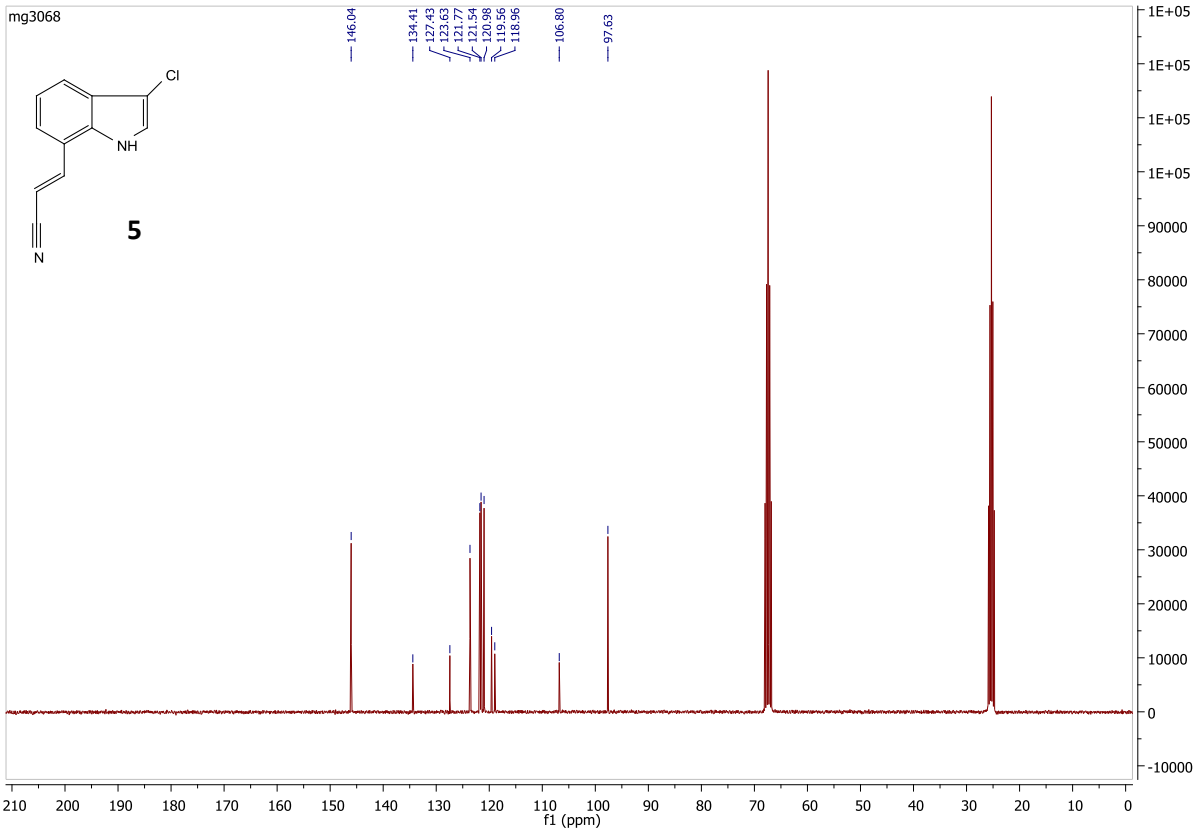
1.03
1.01
f1 (ppm)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134.41
127.43
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120.98
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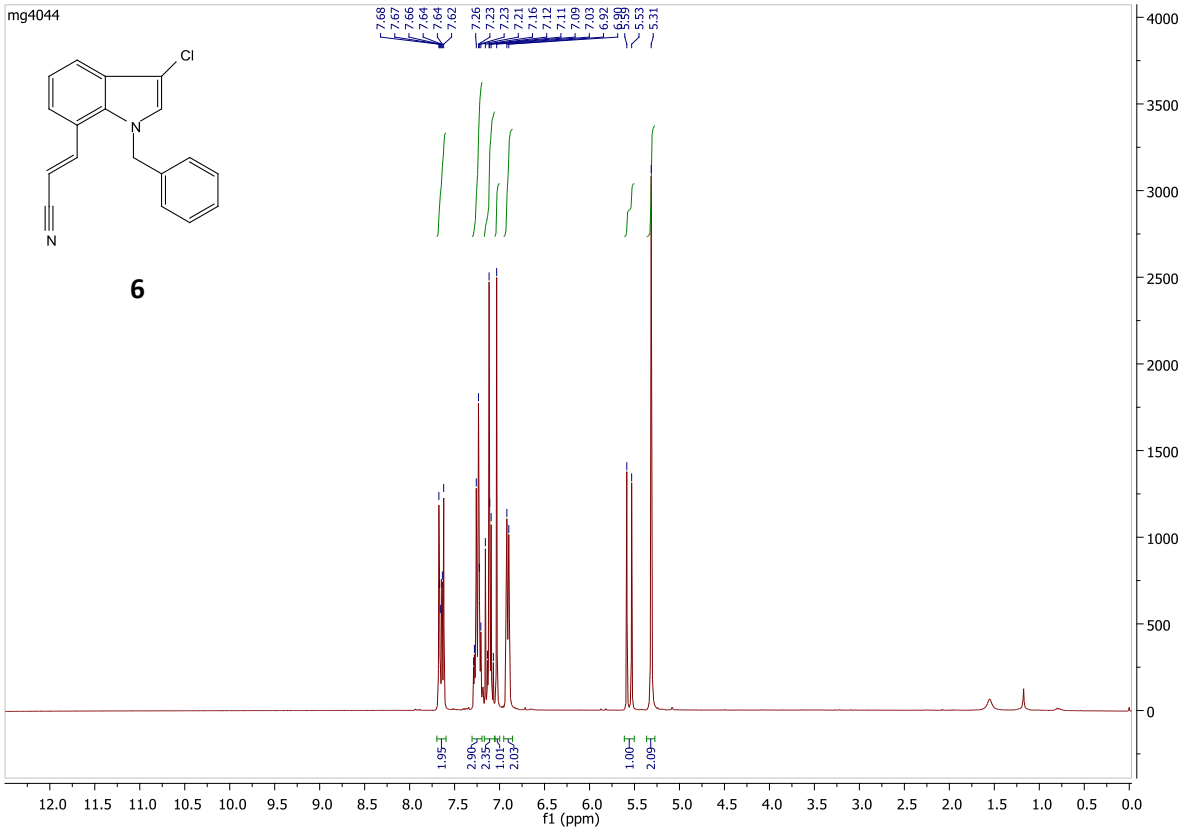
Cl
NH
N
5
f1 (ppm)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7.23
7.21
7.16
7.12
7.11
7.09
7.03
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5.31
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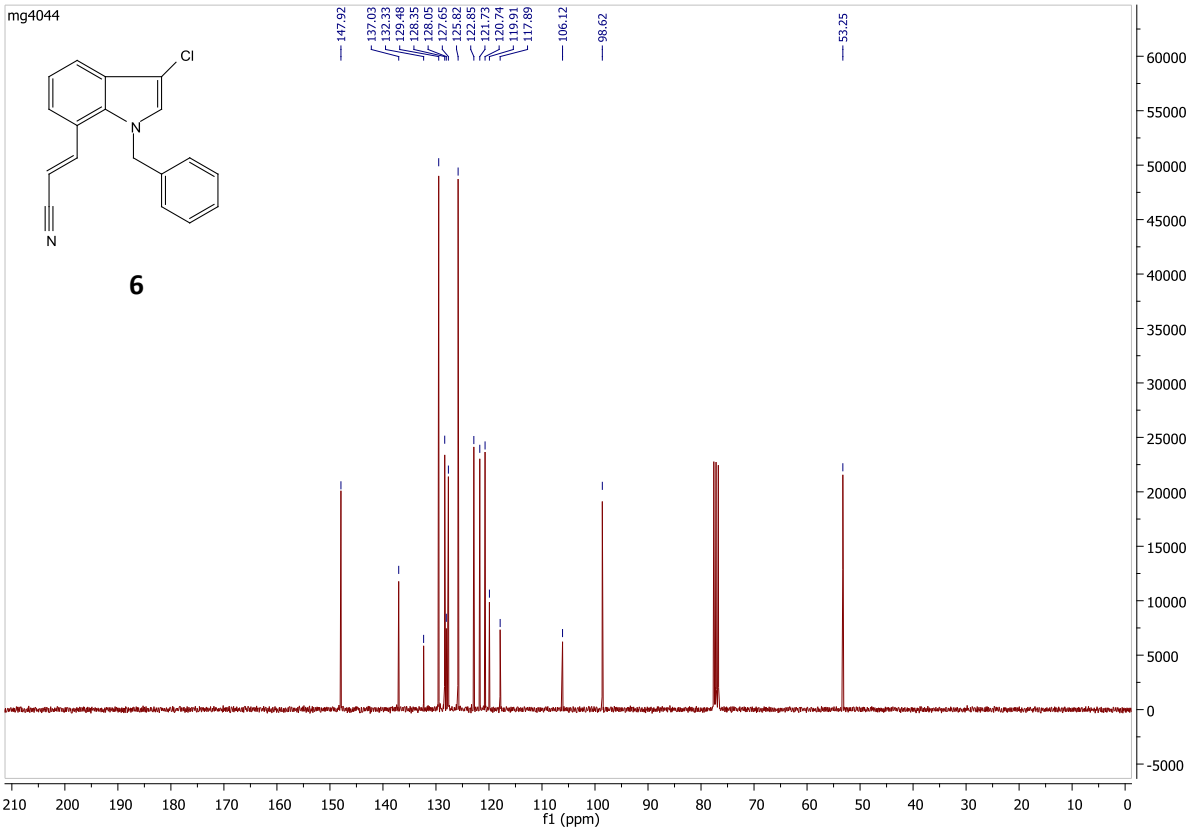
2.35
1.01
2.03
1.00
2.09
f1 (ppm)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N
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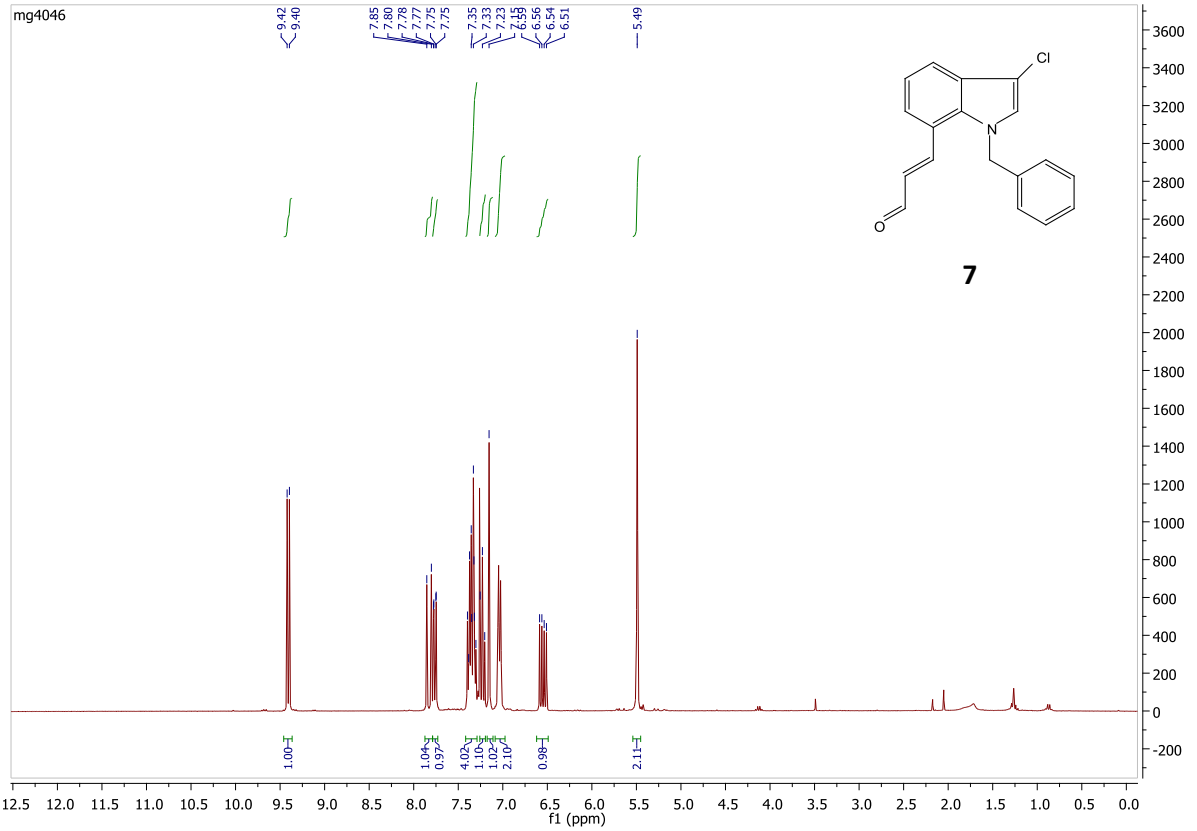
f1 (ppm)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7.75
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6.58
6.56
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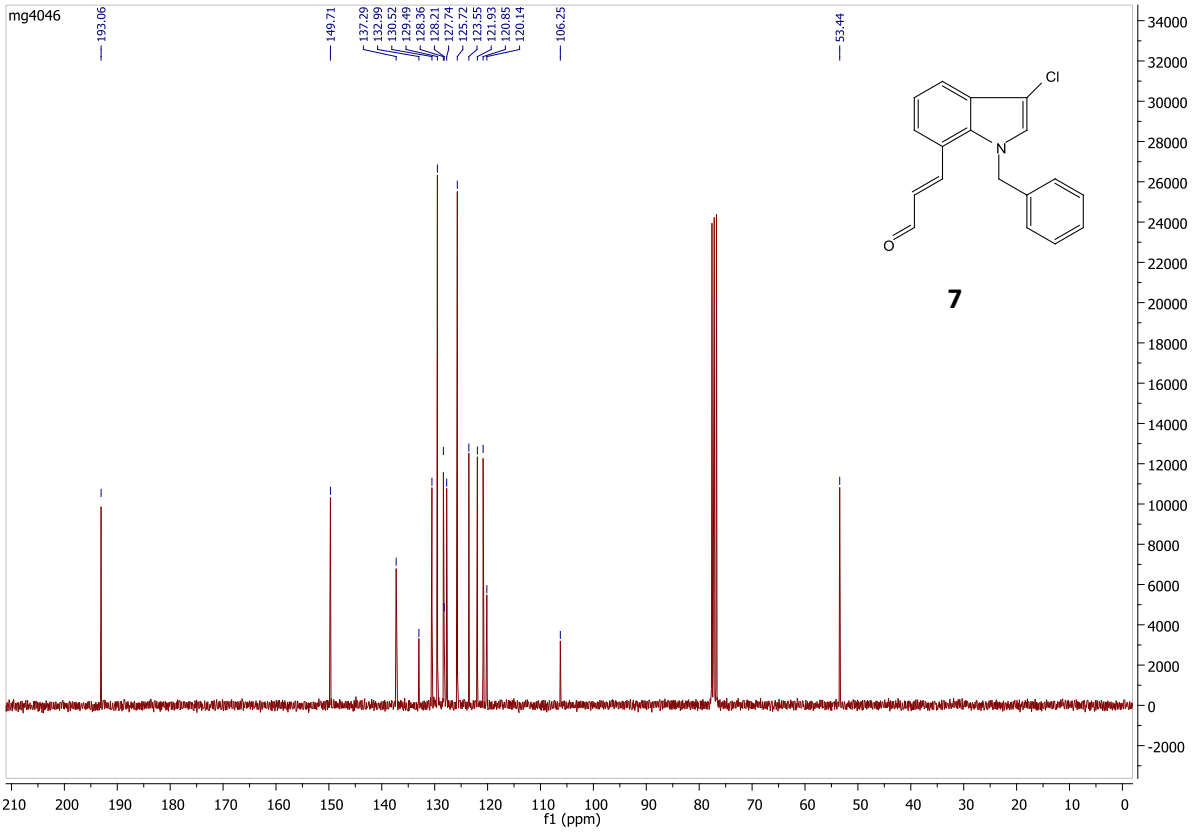
6.51
5.49
Cl
N
O
7
f1 (ppm)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129.49
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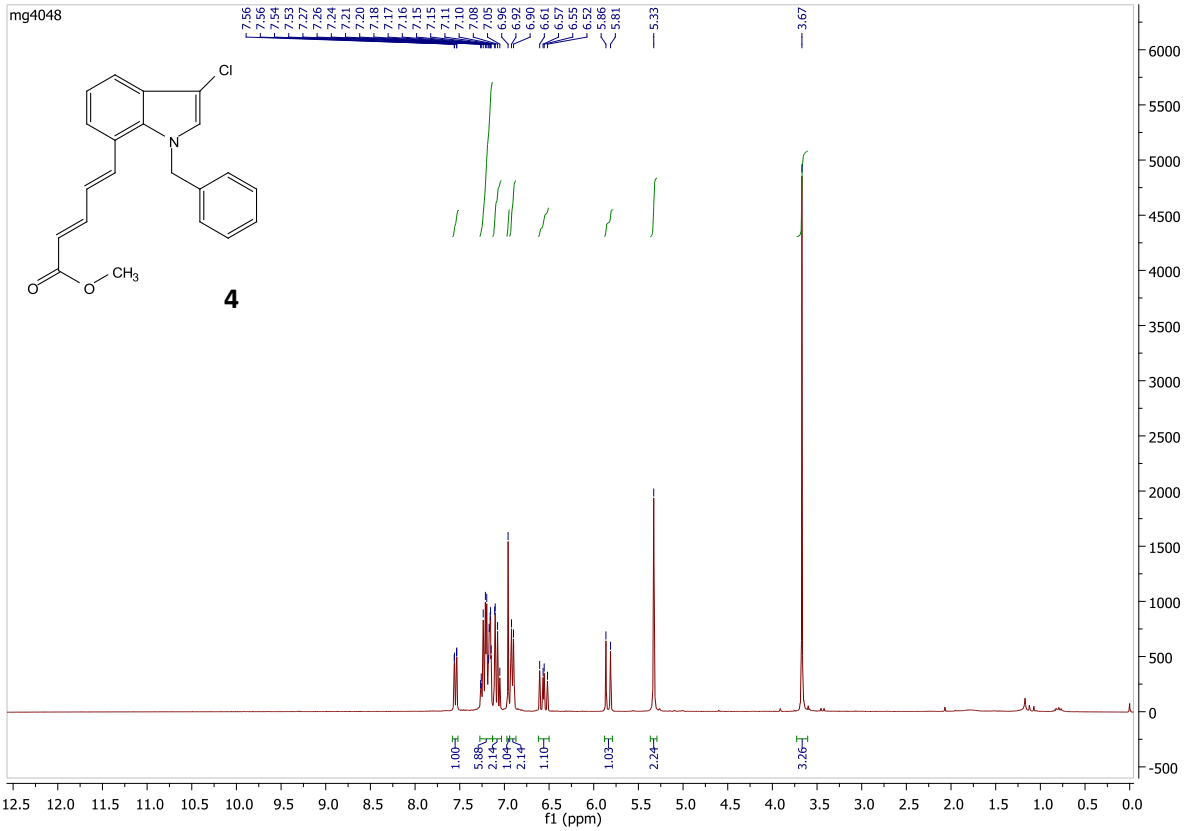
53.44
Cl
N
O
7
f1 (ppm)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O
O
CH3
4
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7.56
7.54
7.53
7.27
7.26
7.24
7.21
7.20
7.18
7.17
7.16
7.15
7.15
7.11
7.10
7.08
7.05
6.96
6.92
6.90
6.61
6.57
6.55
6.52
5.86
5.81
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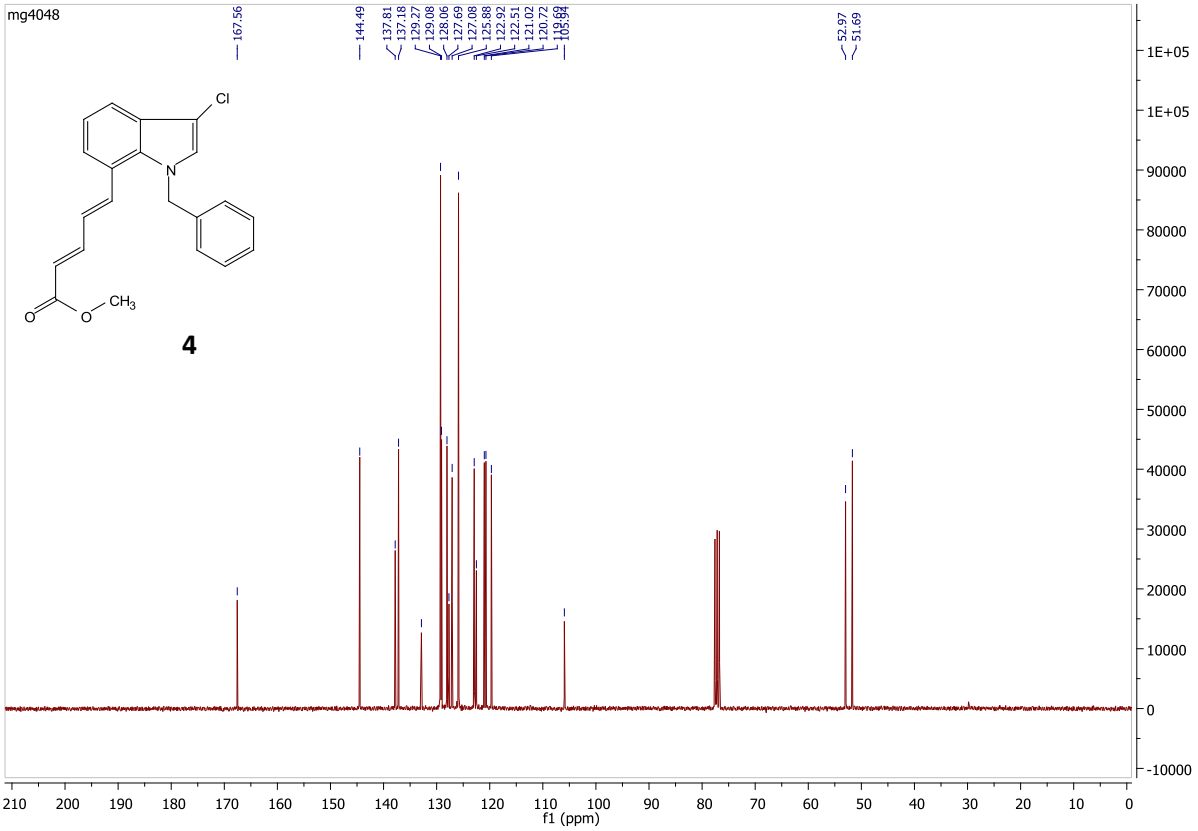
1.10
1.03
2.24
3.26
f1 (ppm)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O
O
CH3
4
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144.49
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137.18
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129.08
128.06
127.69
127.08
125.88
122.92
122.51
121.02
120.72
119.69
105.94
52.97
51.69
f1 (ppm)