

Supplementary Information

One-pot, Two-step Synthesis and Photophysical Properties of 2-(5-Phenylindol-3-yl) benzoimidazole Derivatives

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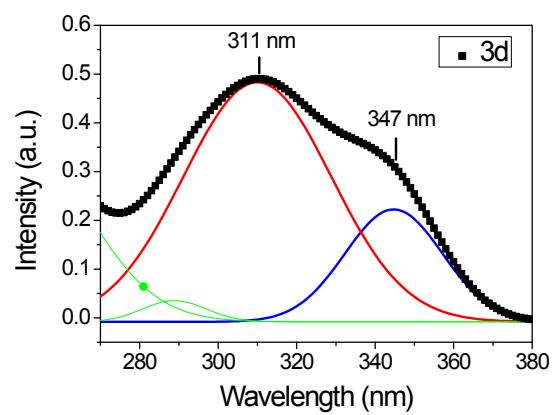


Figure S1 Fitted curve for the absorption spectrum of 3d in ethanol solution.

Table S1 UV-Vis absorption and fluorescence emission spectra of compounds **3b and **3d** in different solvents.**

| Compound ^a | Solvent | UV-visible Absorption | | | Emission | Stoke's shift(cm ⁻¹) |
|-----------------------|------------------|-------------------------|-------------------------|-------------------------|---|----------------------------------|
| | | λ_{\max}^1 (nm) | λ_{\max}^2 (nm) | λ_{\max}^3 (nm) | λ_{em} (nm) ^b | |
| 3b | Ethanol | 262 | 325 | | 375 | 4103 |
| 3b | Dichloroethane | 264 | 328 | | 379 | 4103 |
| 3b | <i>n</i> -Hexane | 325 | | | 373 | 3960 |
| 3d | Ethanol | 248 | 311 | 347 | 398 | 3693 |
| 3d | Dichloroethane | 256 | 312 | 352 | 410 | 4019 |
| 3d | <i>n</i> -Hexane | 309 | 344 | | 378 | 2615 |

a: $c = 1.0 \times 10^{-5}$ mol/L, at 25 °C; *b*: The excitation wavelength of compound **3b** and **3d** were 330 nm and 350 nm respectively

Spectra of selective samples of compounds 3 in ethanol solution

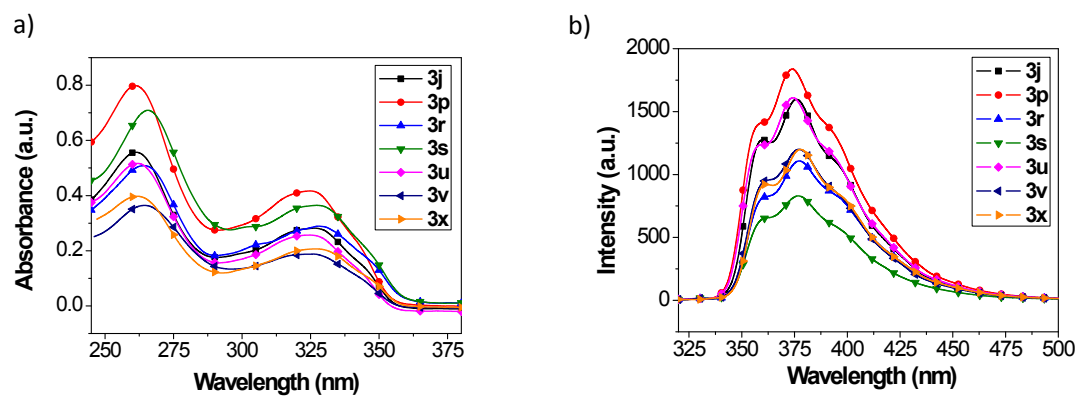


Figure S2. (a) UV-visible and (b) fluorescence spectra of selective samples of compounds 3 in ethanol solution.

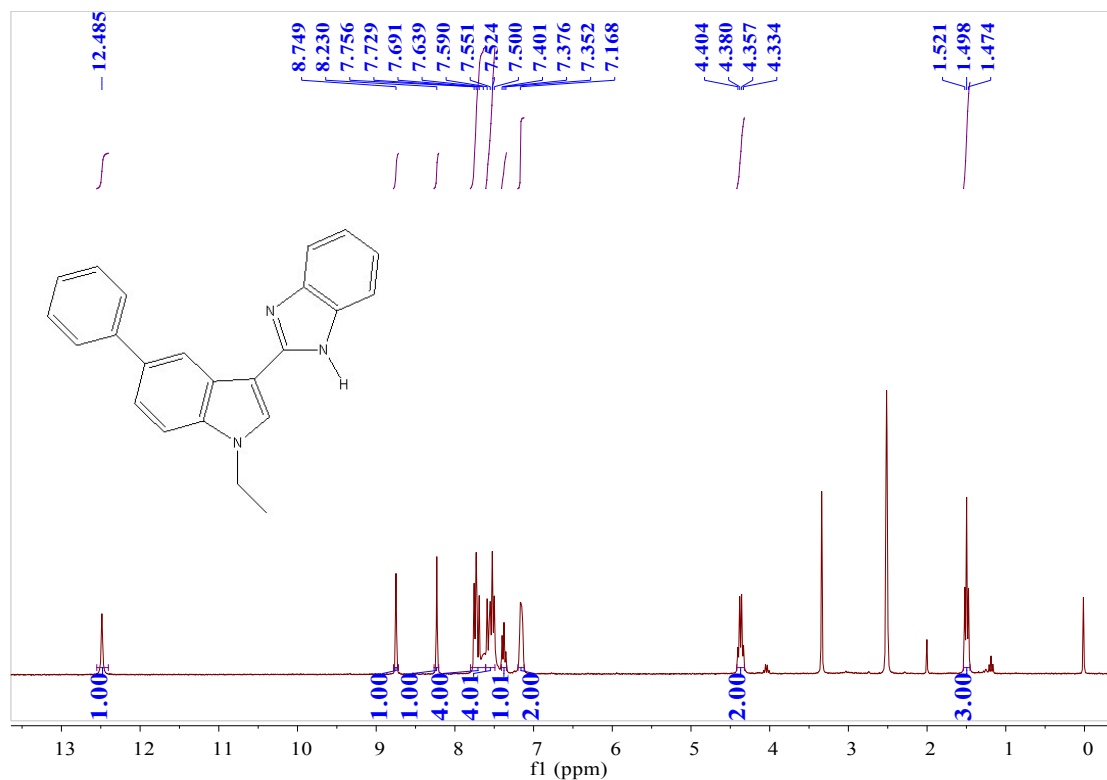
Table S2. Photoluminescence quantum yields of selective sample compounds

| sample | Integrated emission intensity (I) | Abs. at 330 nm (A) | Refractive index of solvent | Quantum yield at 330 nm (Φ) |
|-----------------|-----------------------------------|--------------------|-----------------------------|------------------------------------|
| Quinine sulfate | 113969.8 | 0.0147 | 1.33 | 0.54 |
| 3b | 255398.6 | 0.0514 | 1.36 | 0.36 |
| 3i | 198298.9 | 0.0404 | 1.36 | 0.35 |
| 3o | 203325.1 | 0.043 | 1.36 | 0.34 |
| 3t | 241497.8 | 0.0557 | 1.36 | 0.31 |

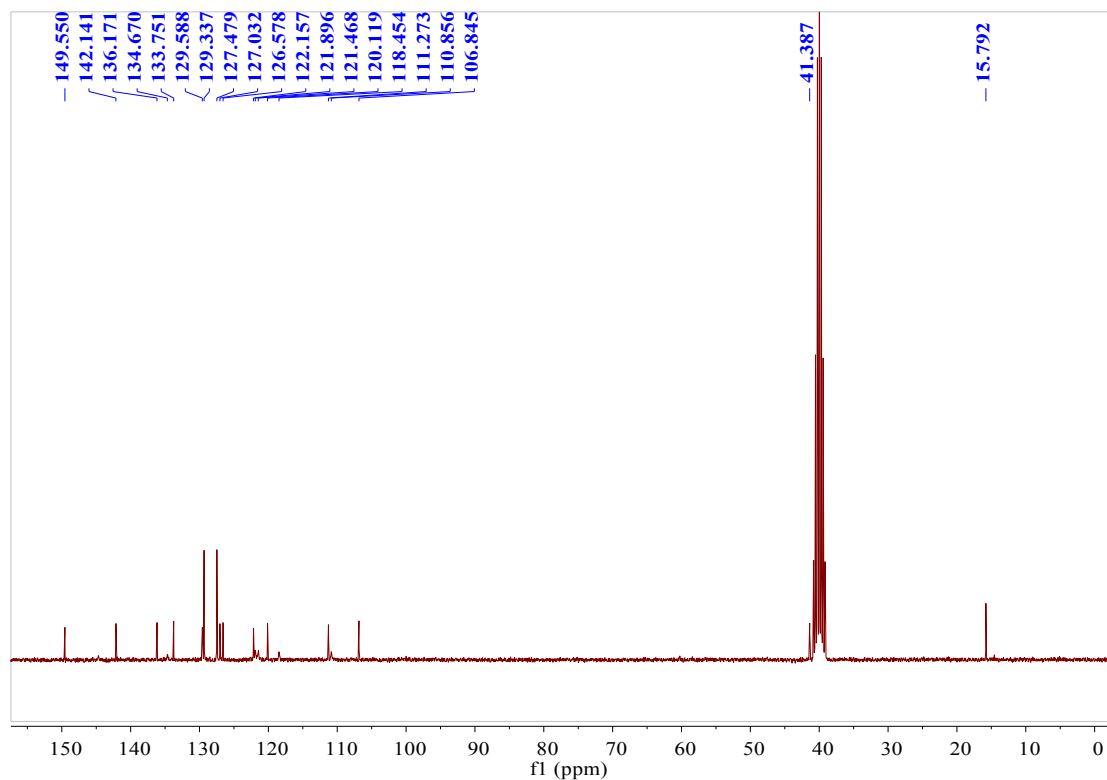
Quinolone sulfate (referenced dye) as a function of optical absorbance at 330 nm and relevant data

¹H and ¹³C NMR Spectra of compounds 3a - 3x

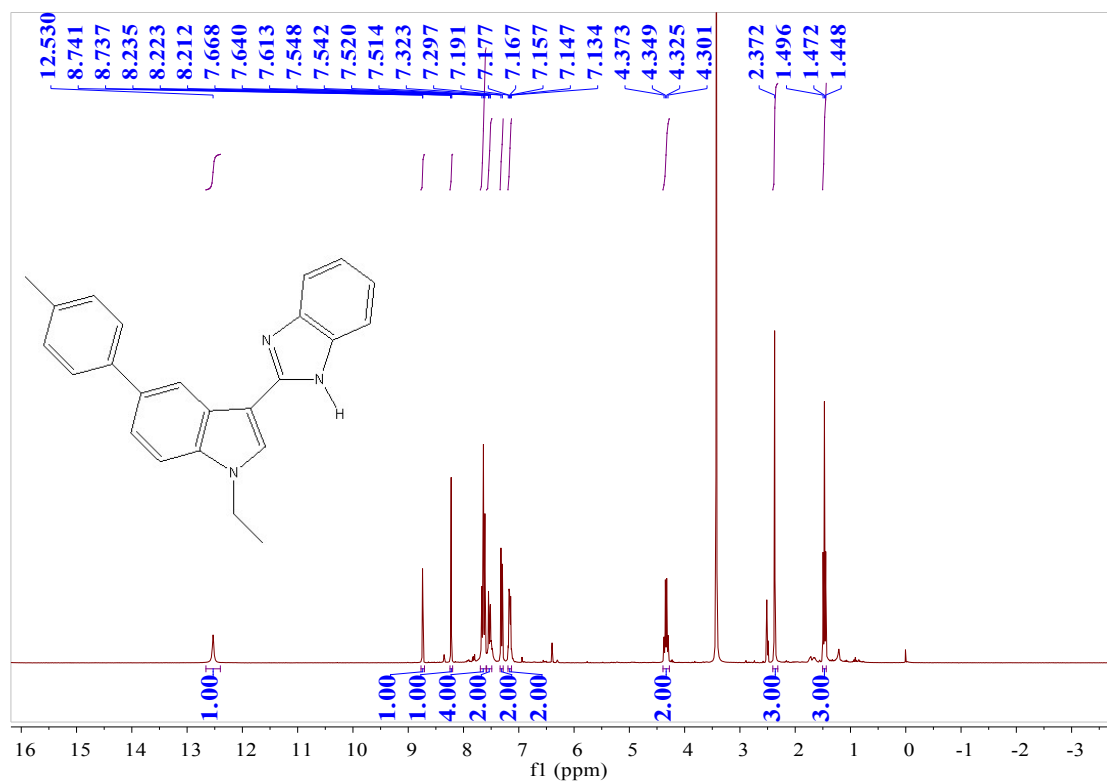
¹H NMR Spectra of 2-(1-ethyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3a)



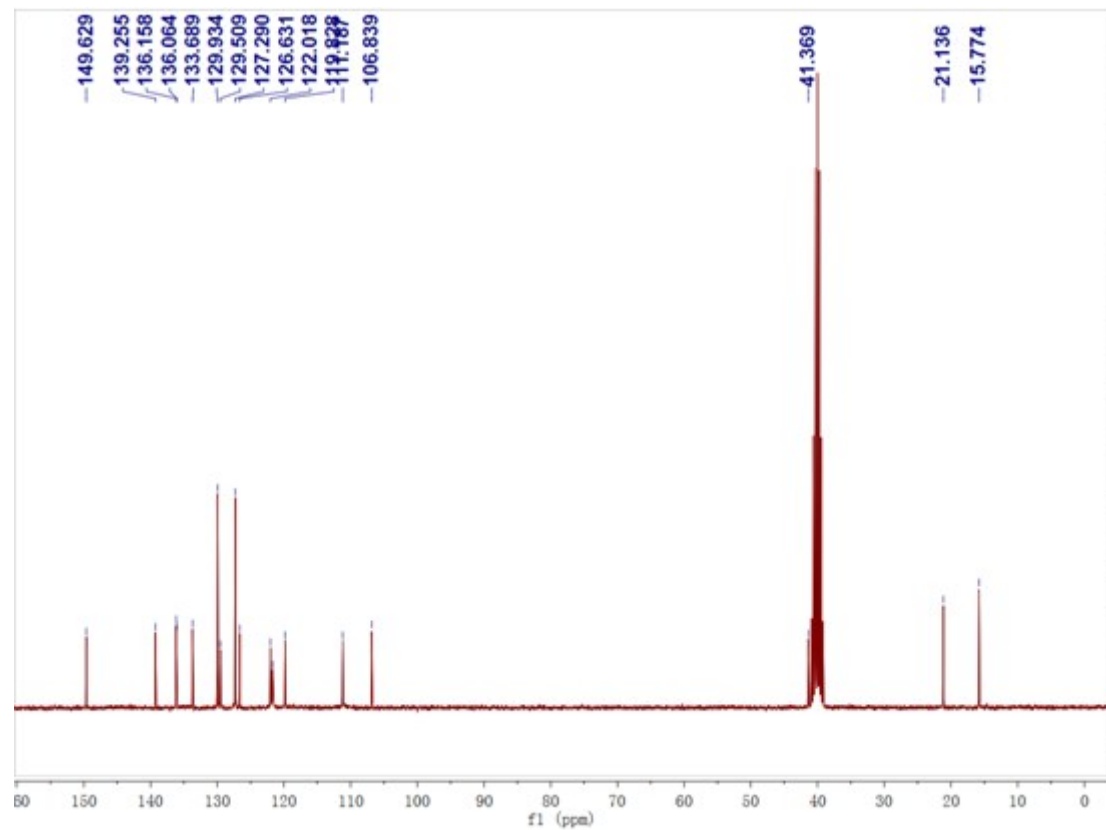
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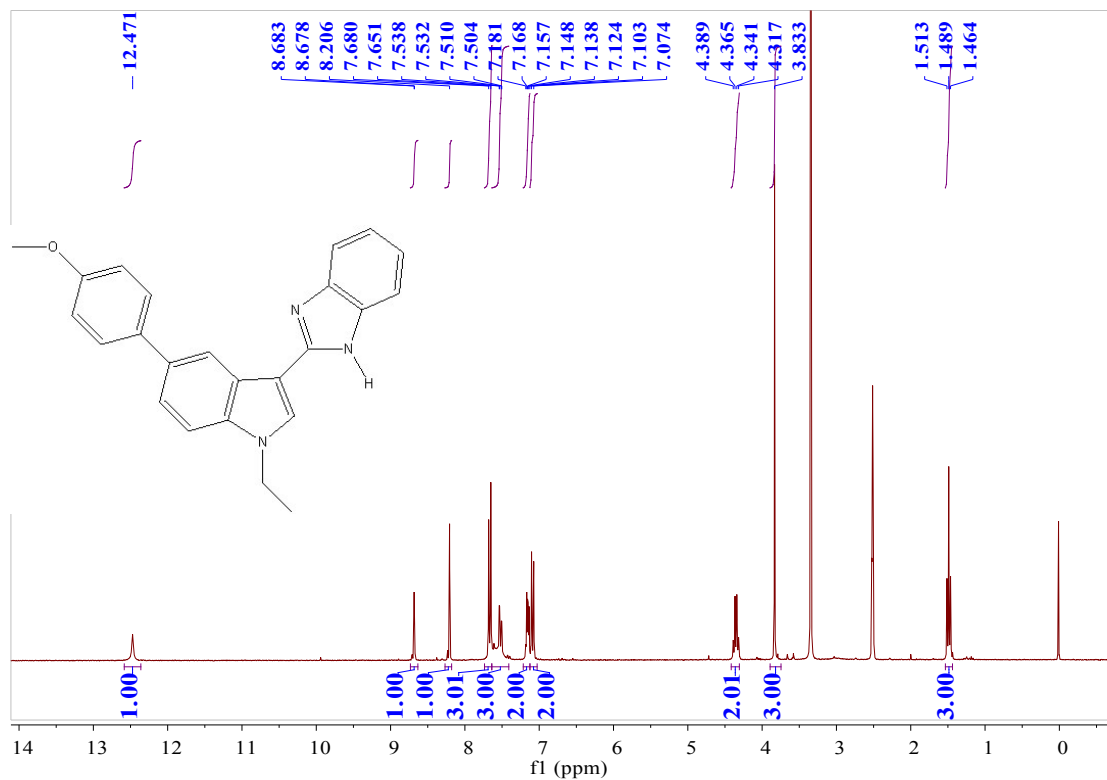
¹H NMR Spectra of 2-(1-ethyl-5-(*p*-tolyl)-1*H*-indol-3-yl)-1*H*-benzo[*d*]imidazole (3b)



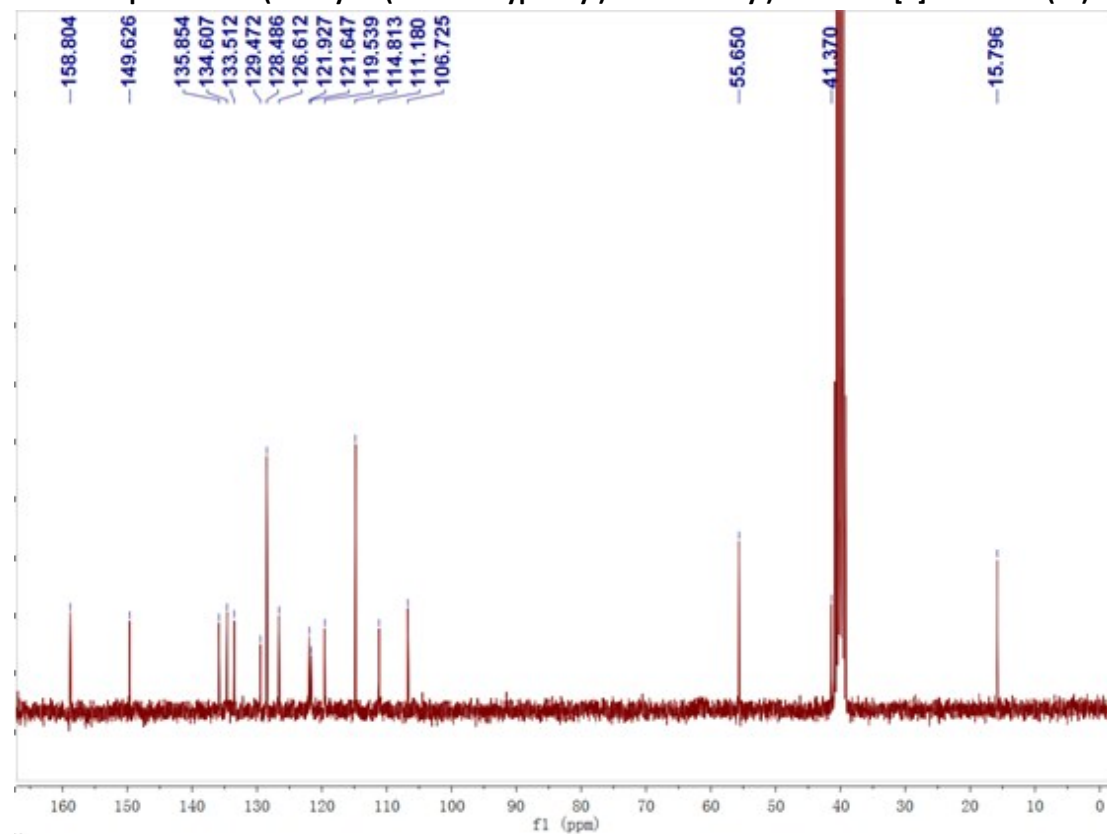
¹³C NMR Spectra of 2-(1-ethyl-5-(*p*-tolyl)-1*H*-indol-3-yl)-1*H*-benzo[*d*]imidazole (3b)



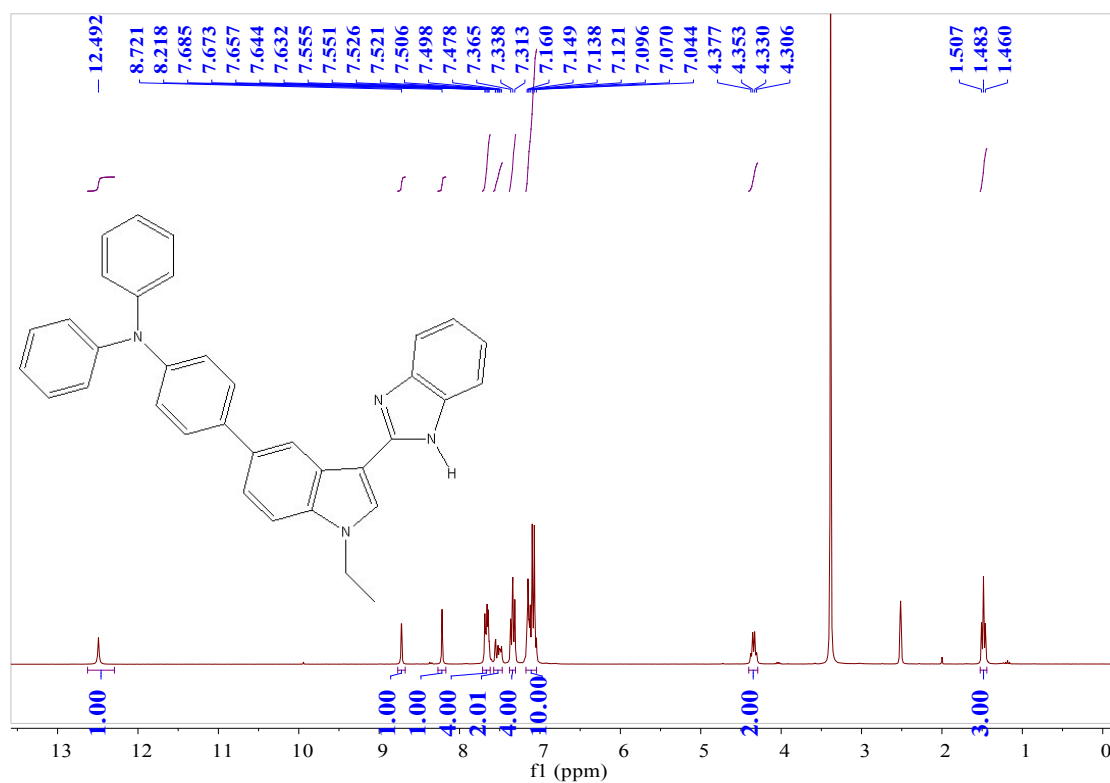
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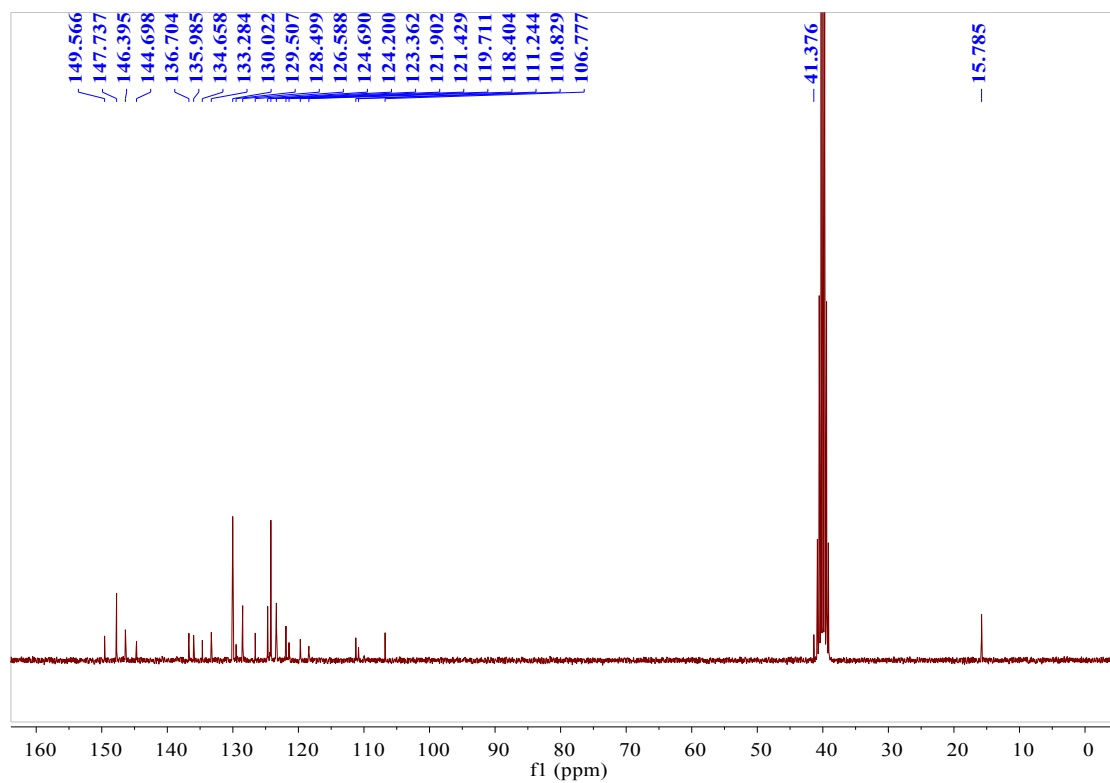
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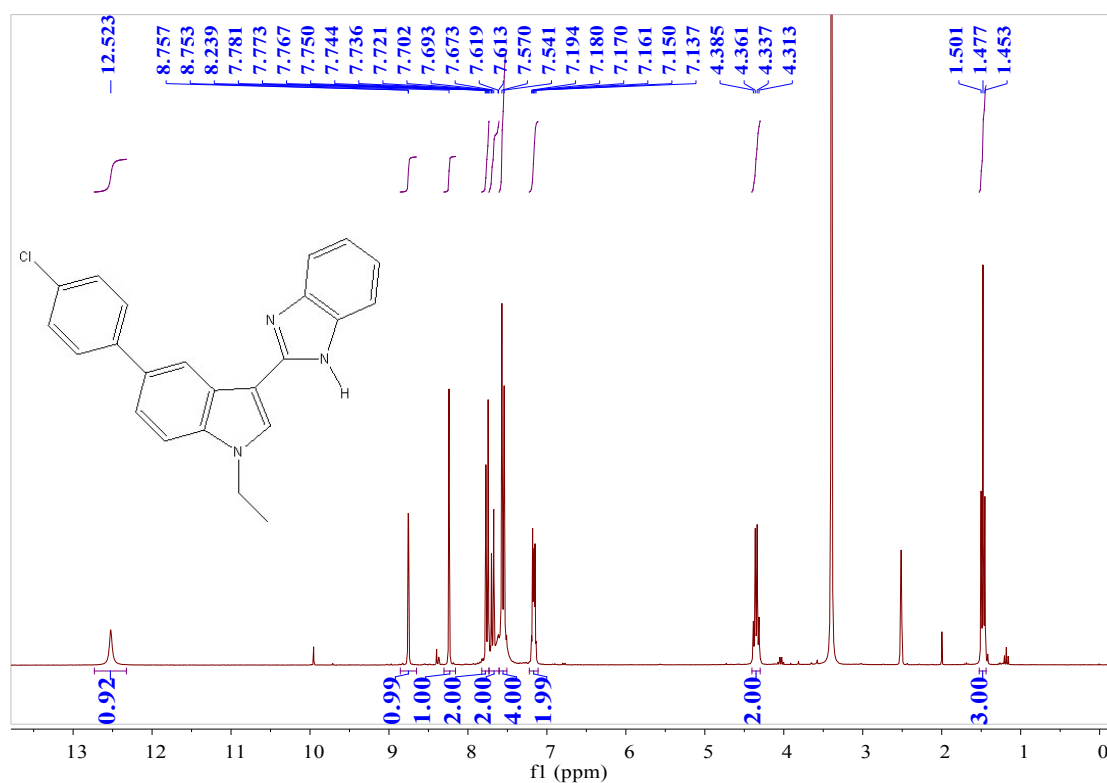
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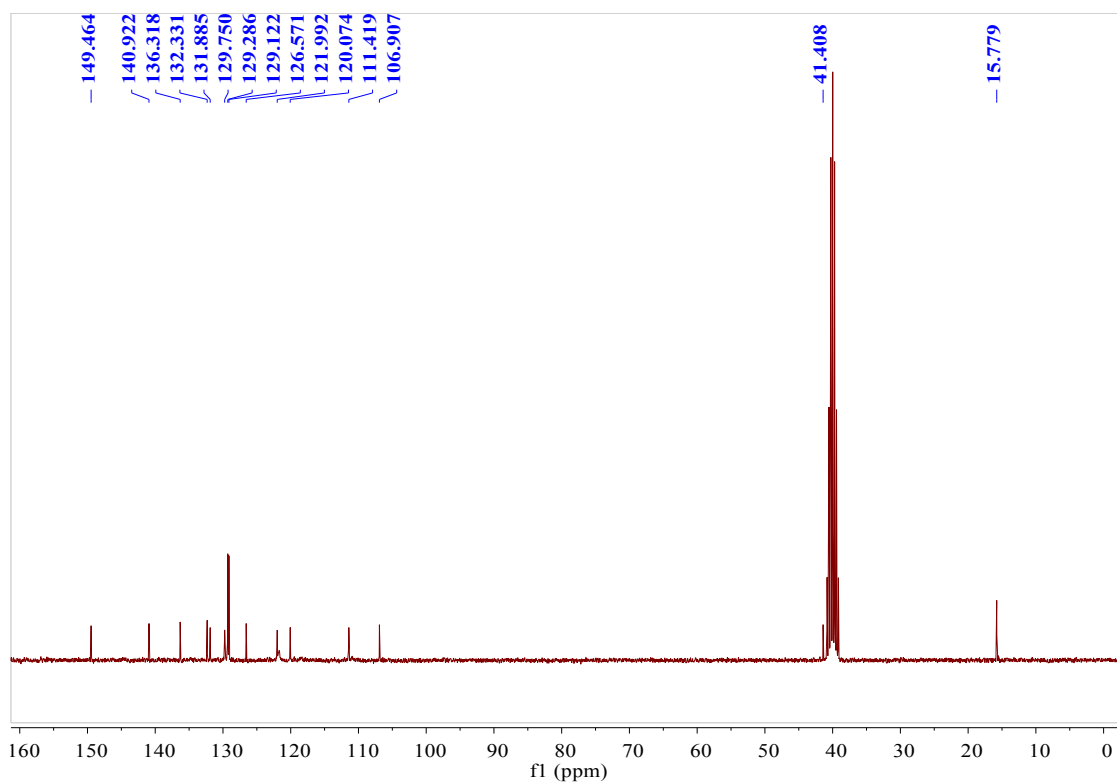
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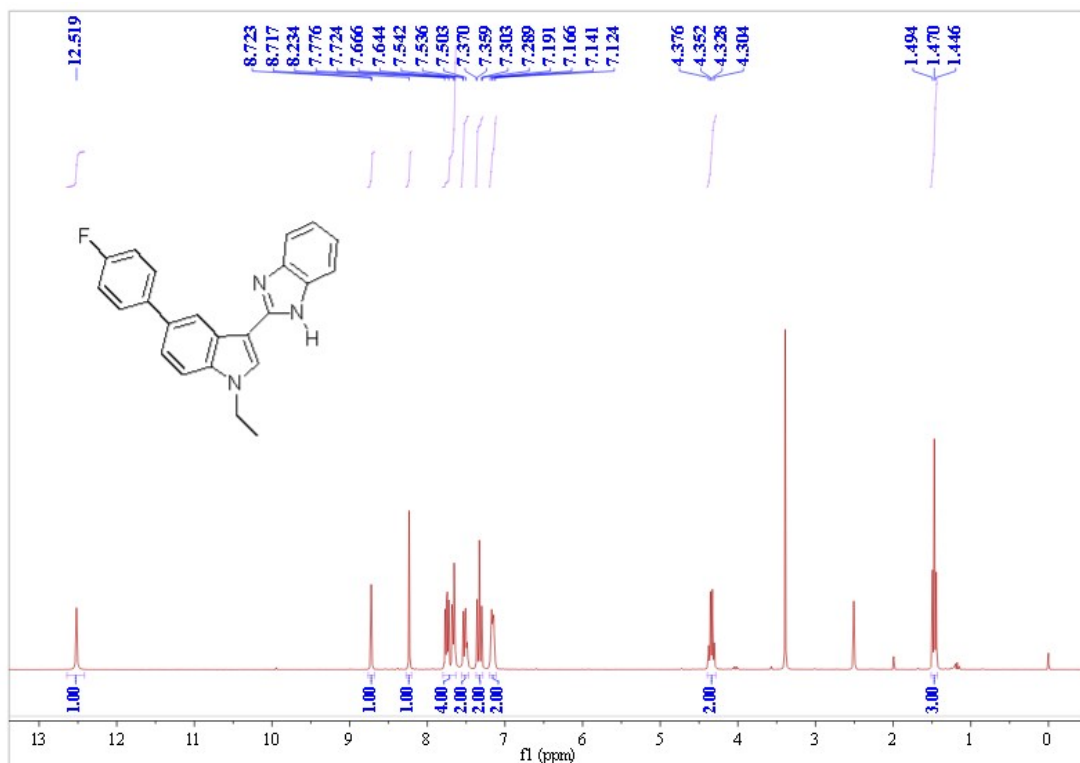
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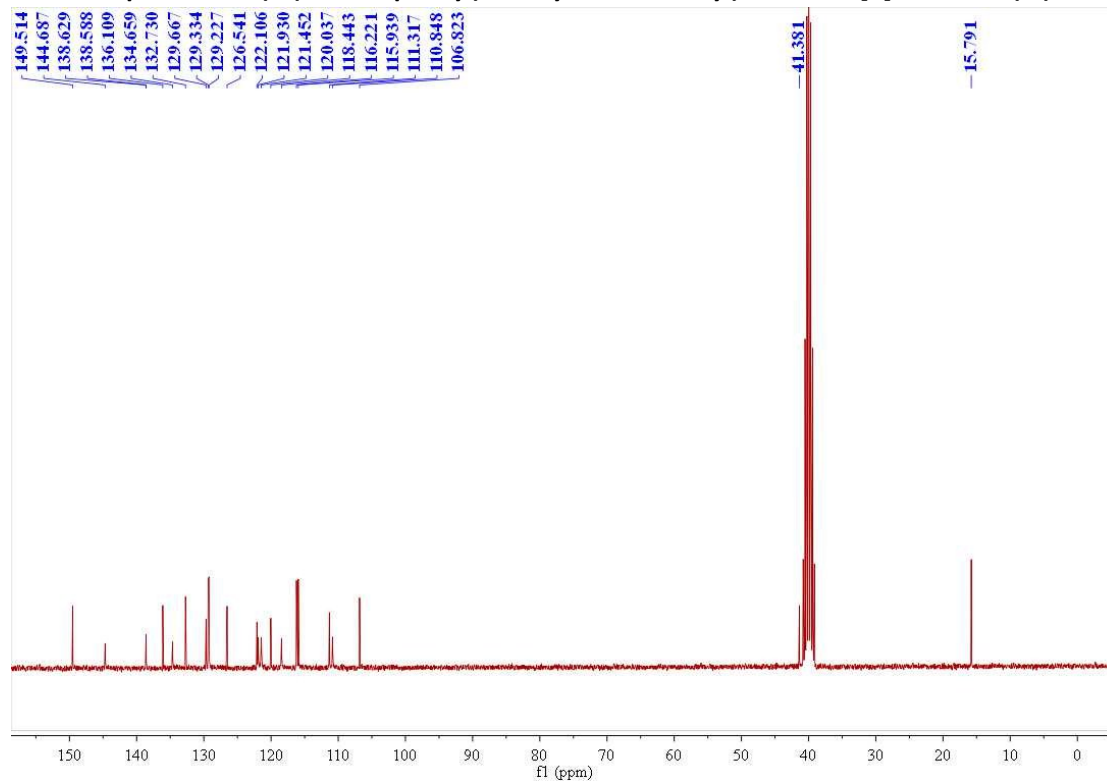
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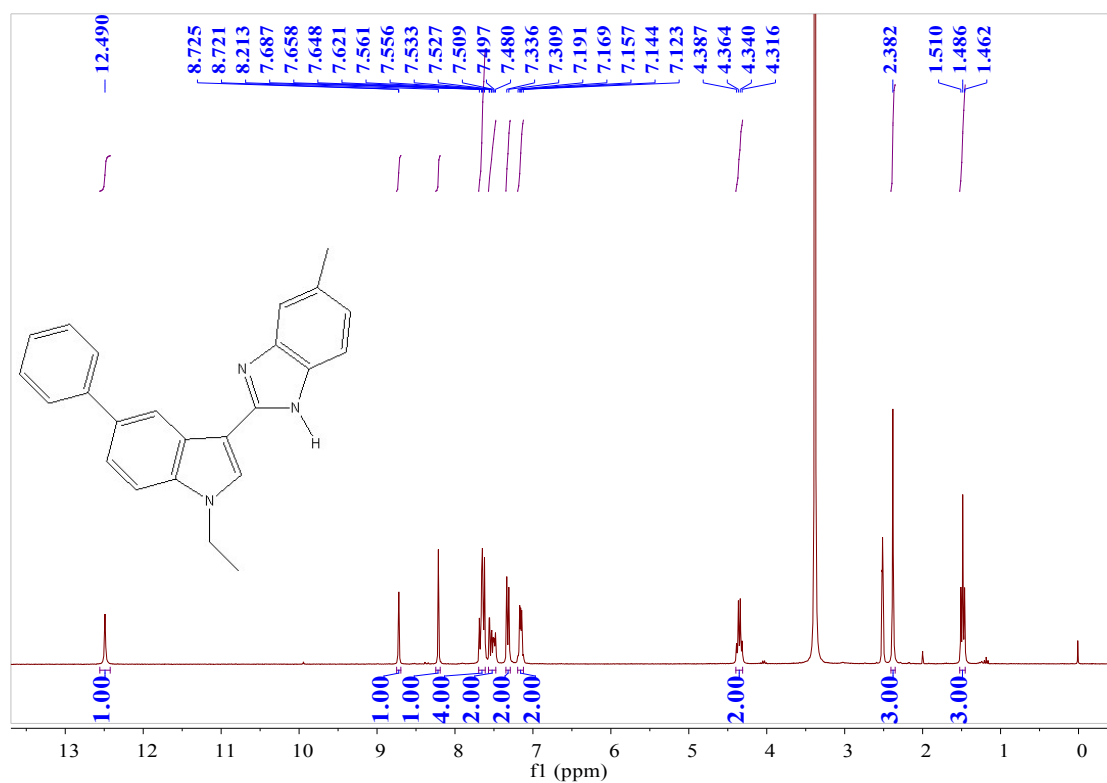
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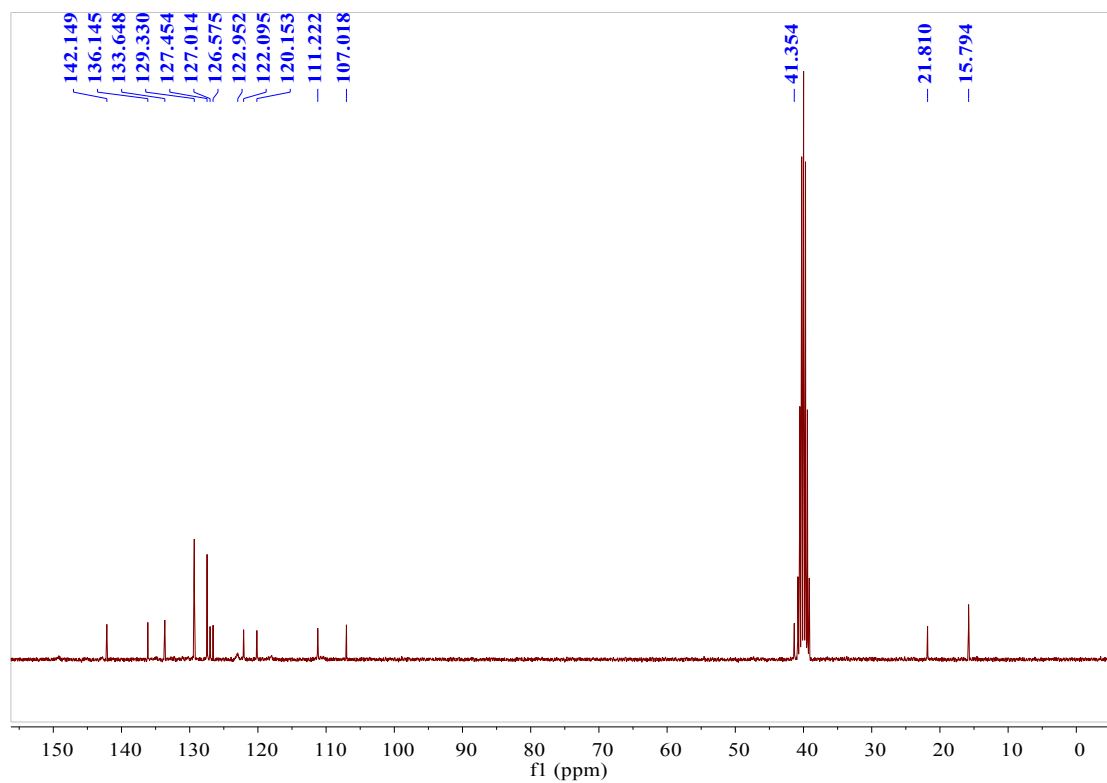
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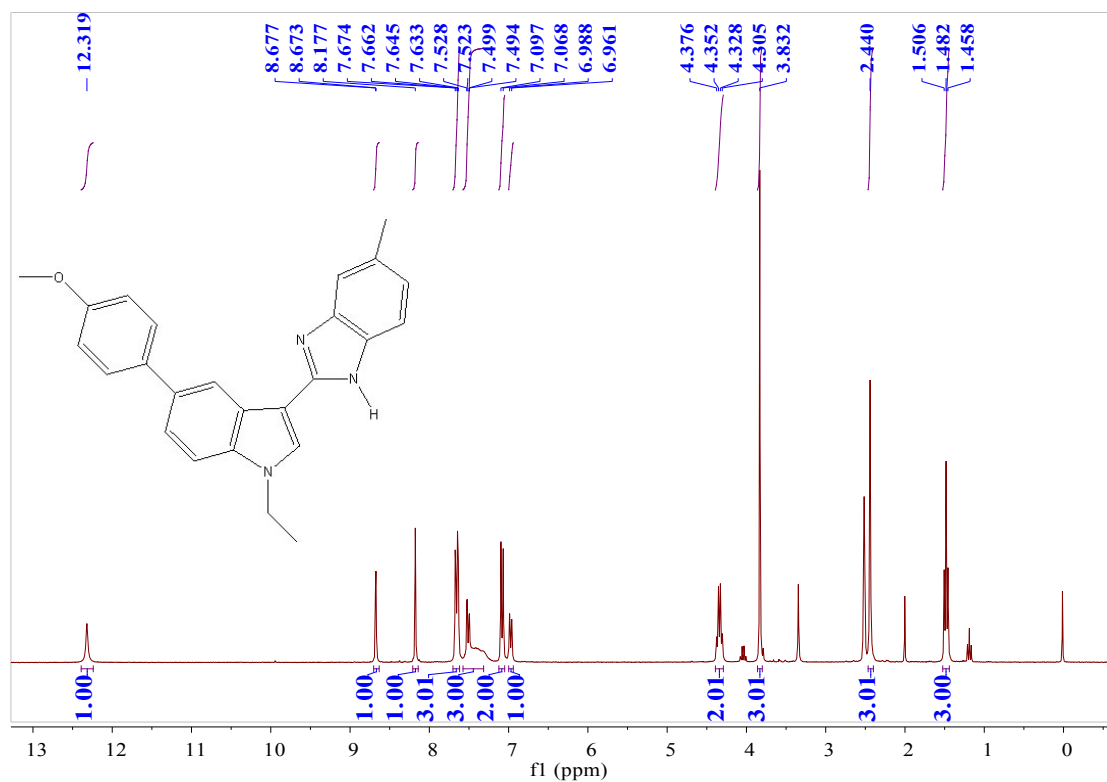
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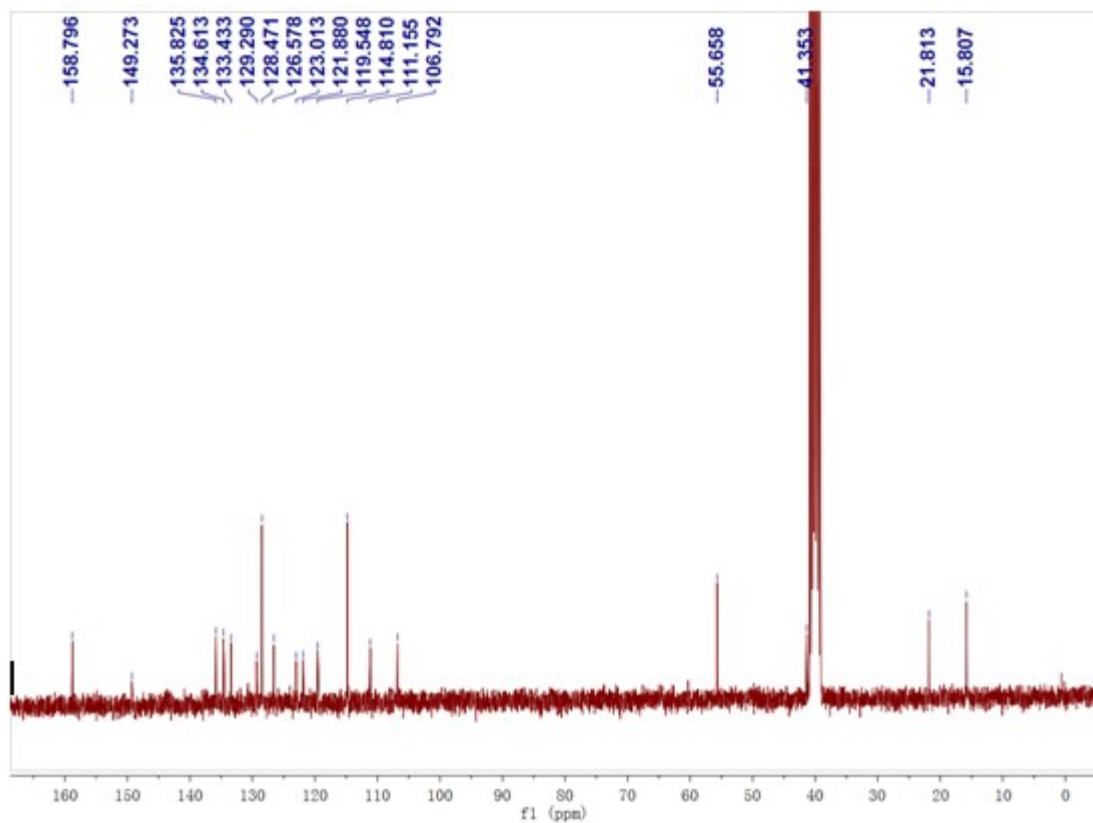
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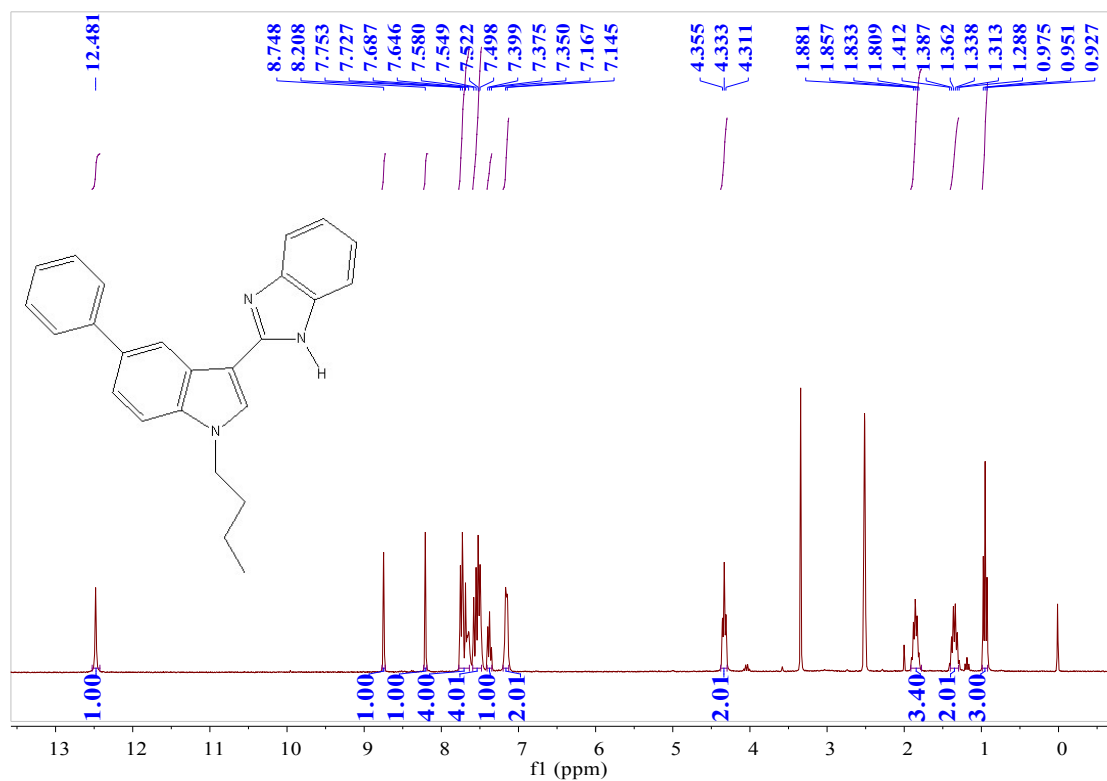
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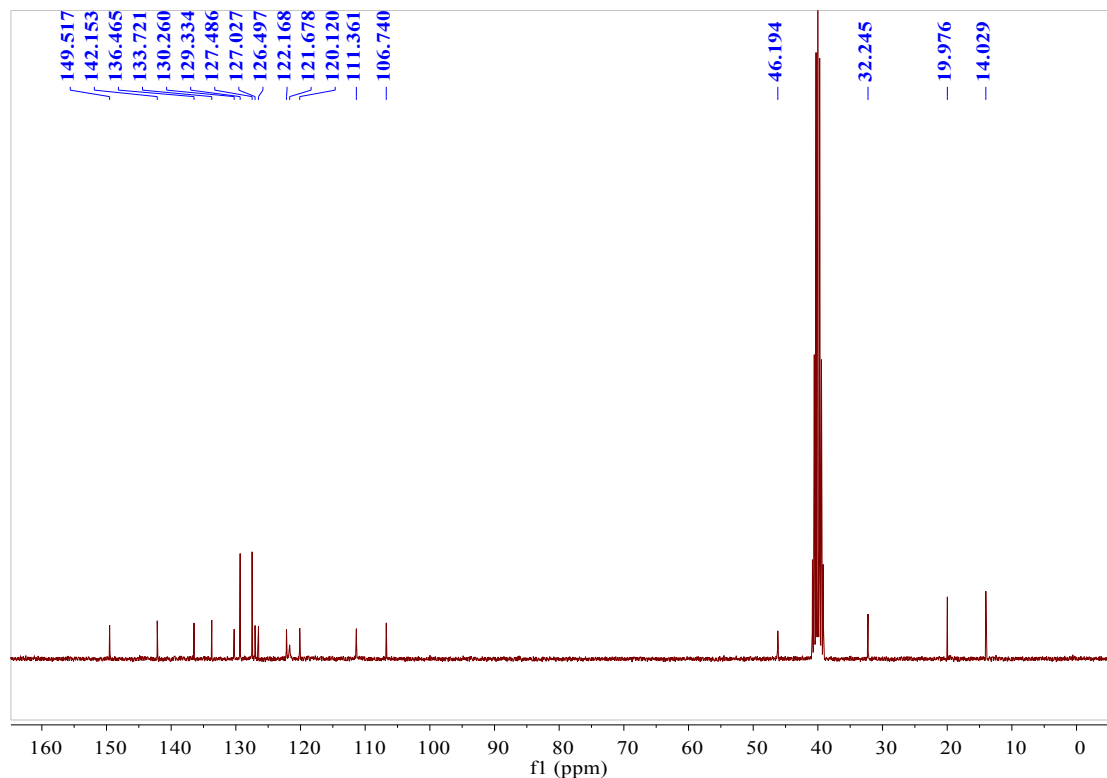
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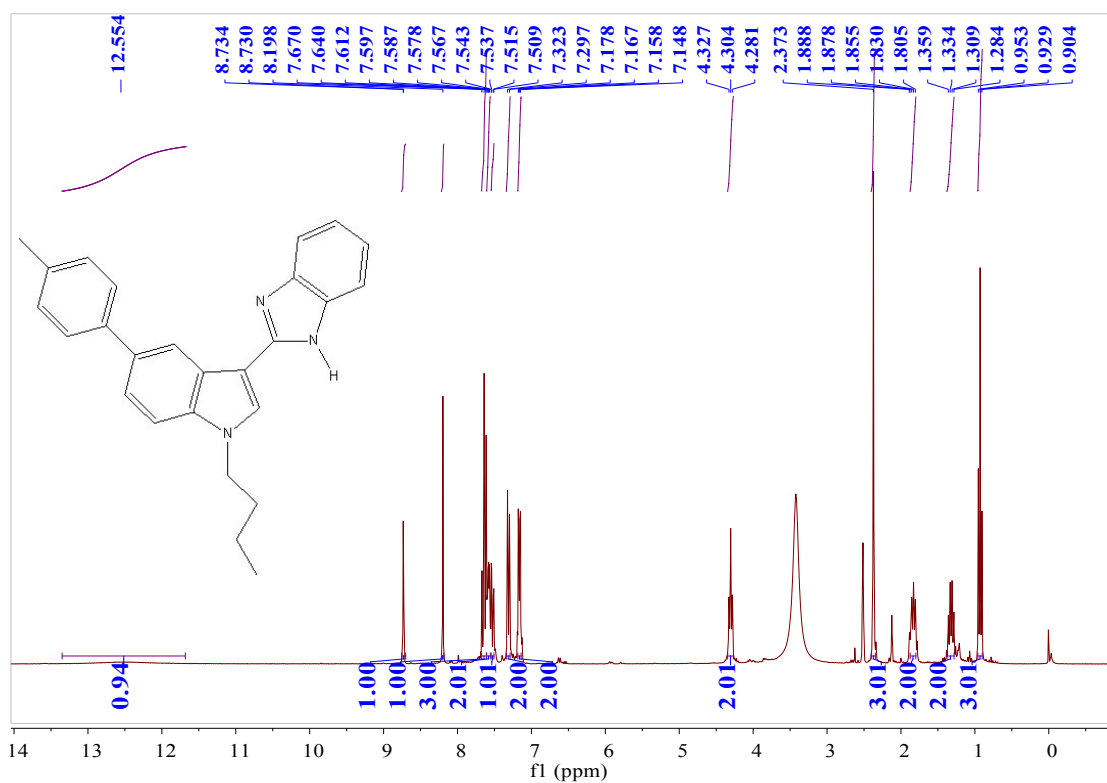
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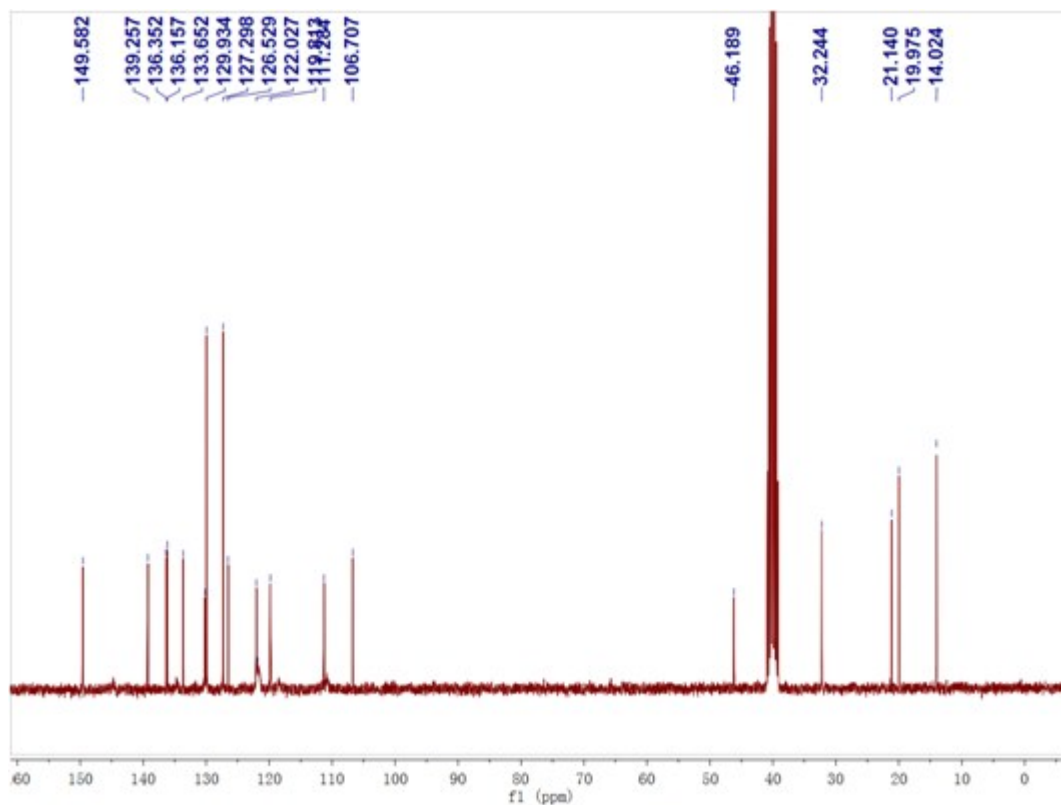
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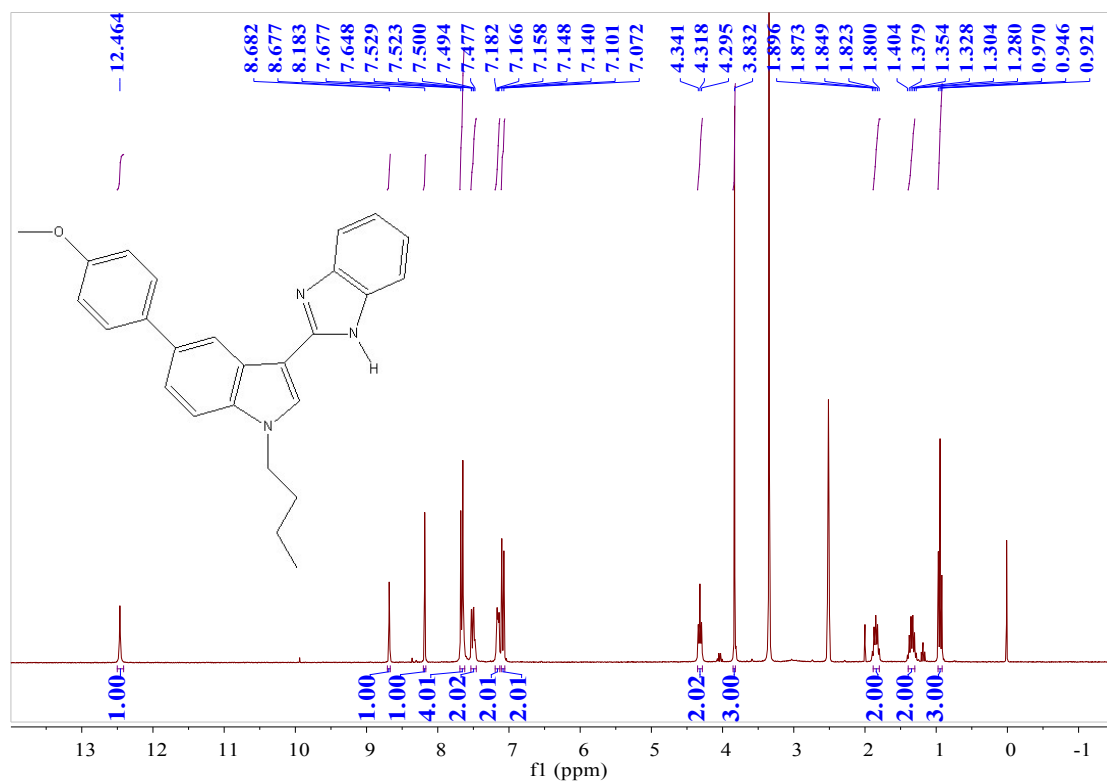
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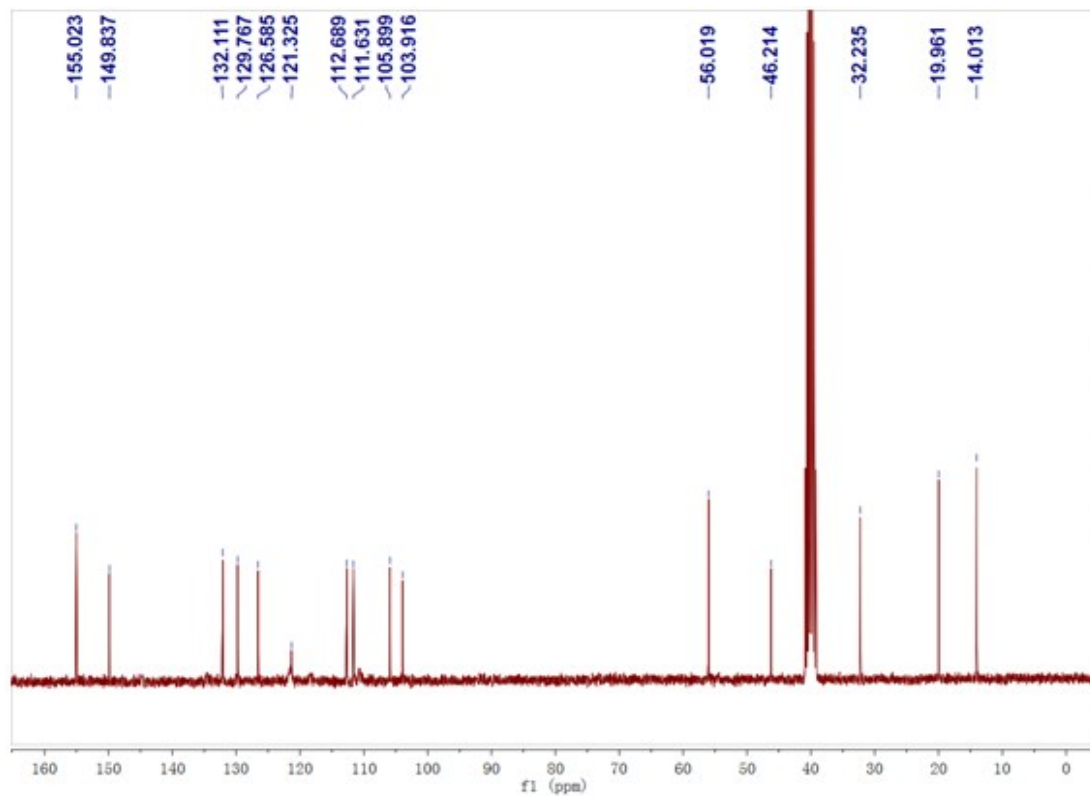
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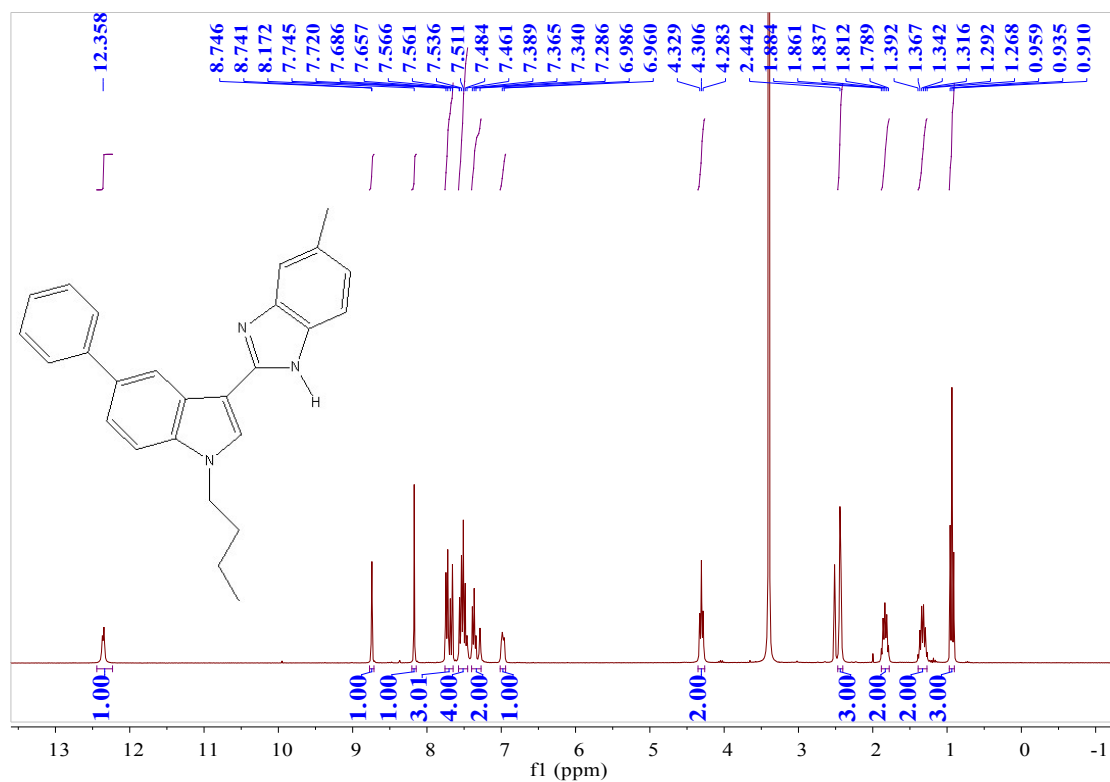
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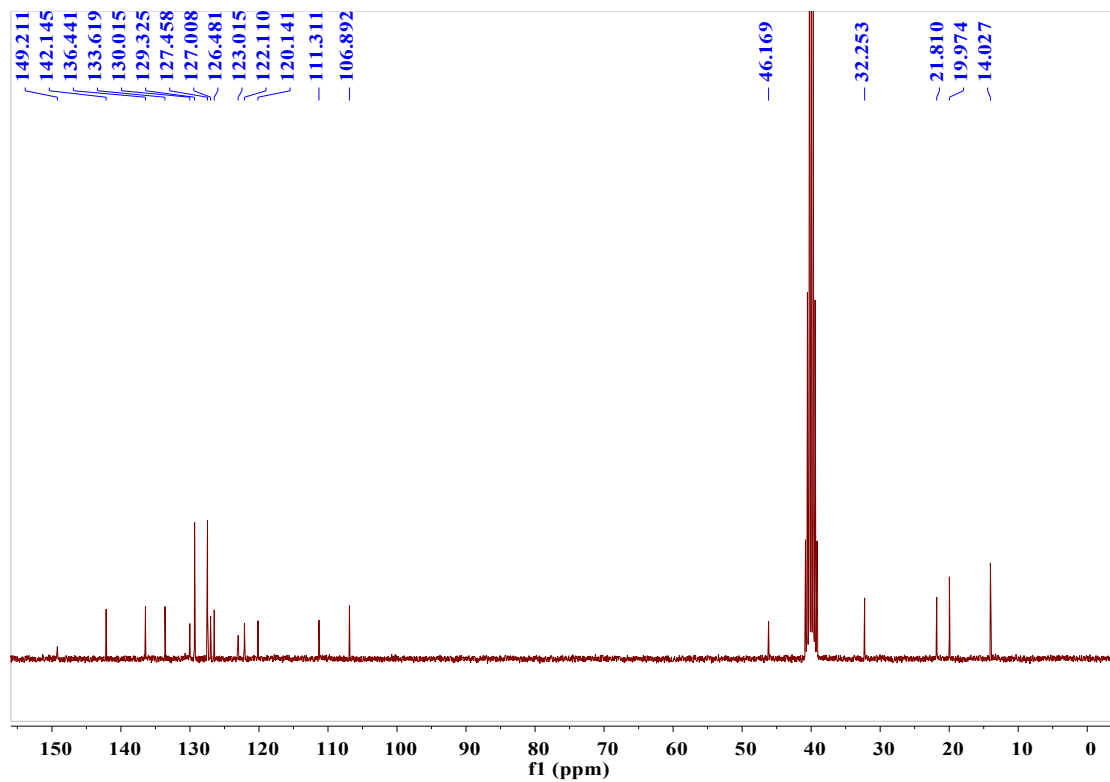
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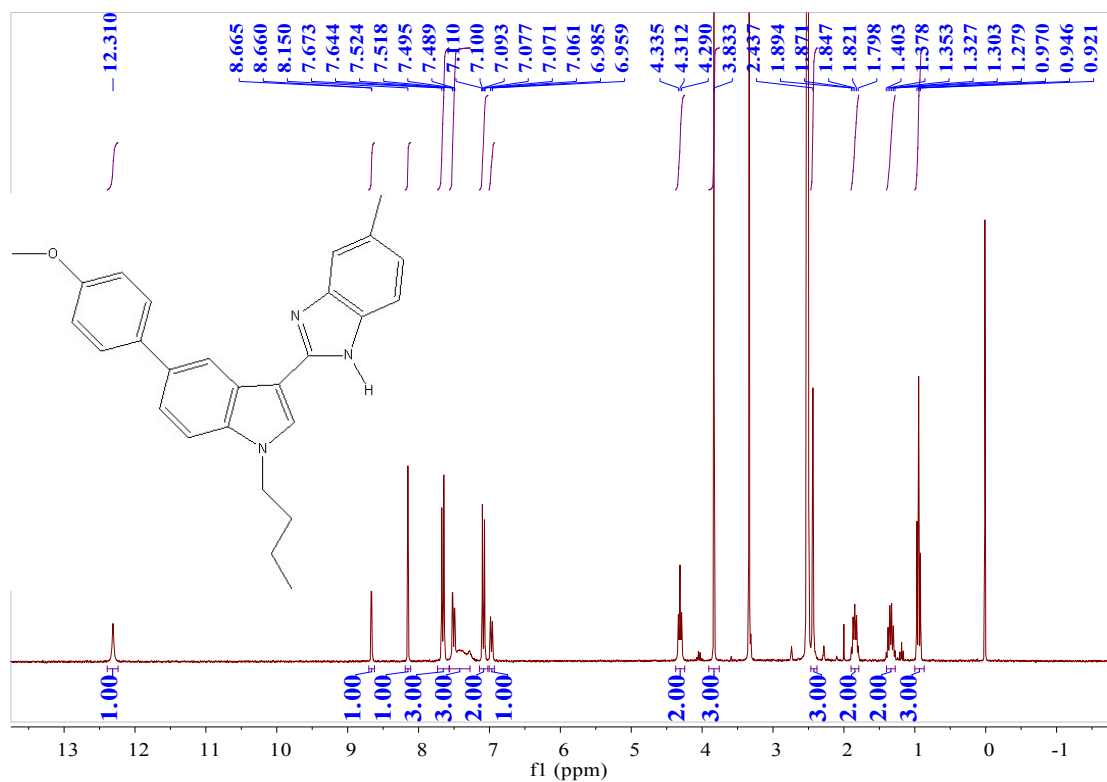
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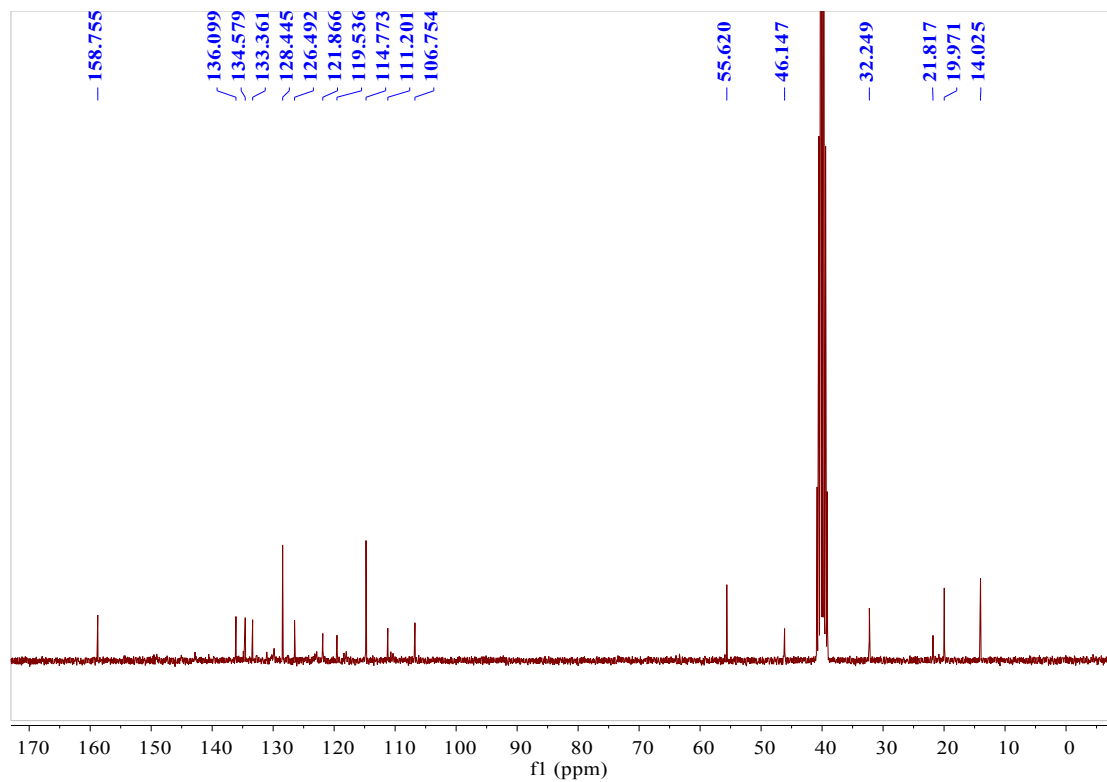
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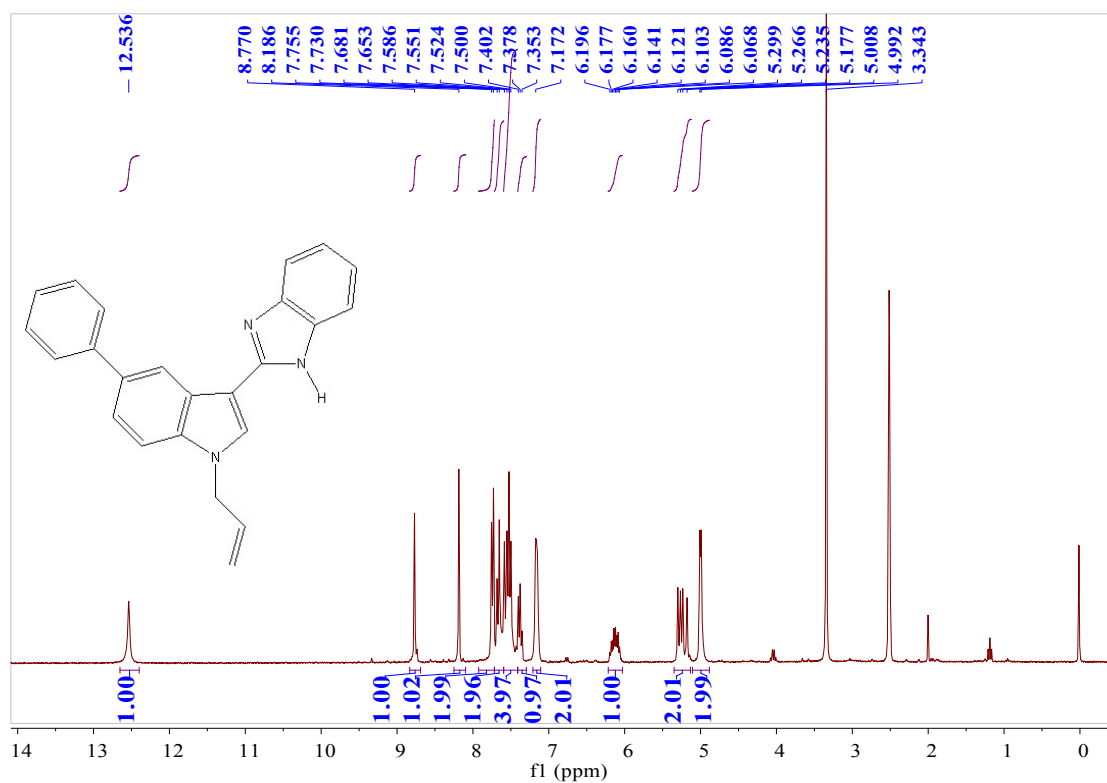
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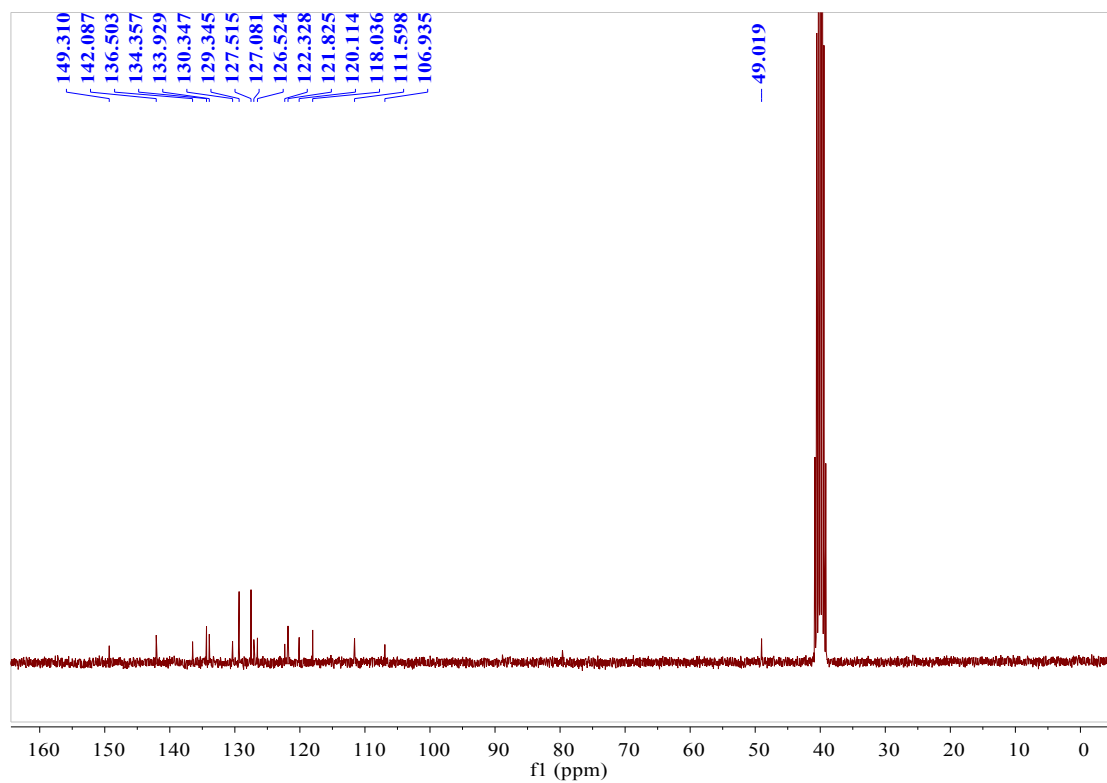
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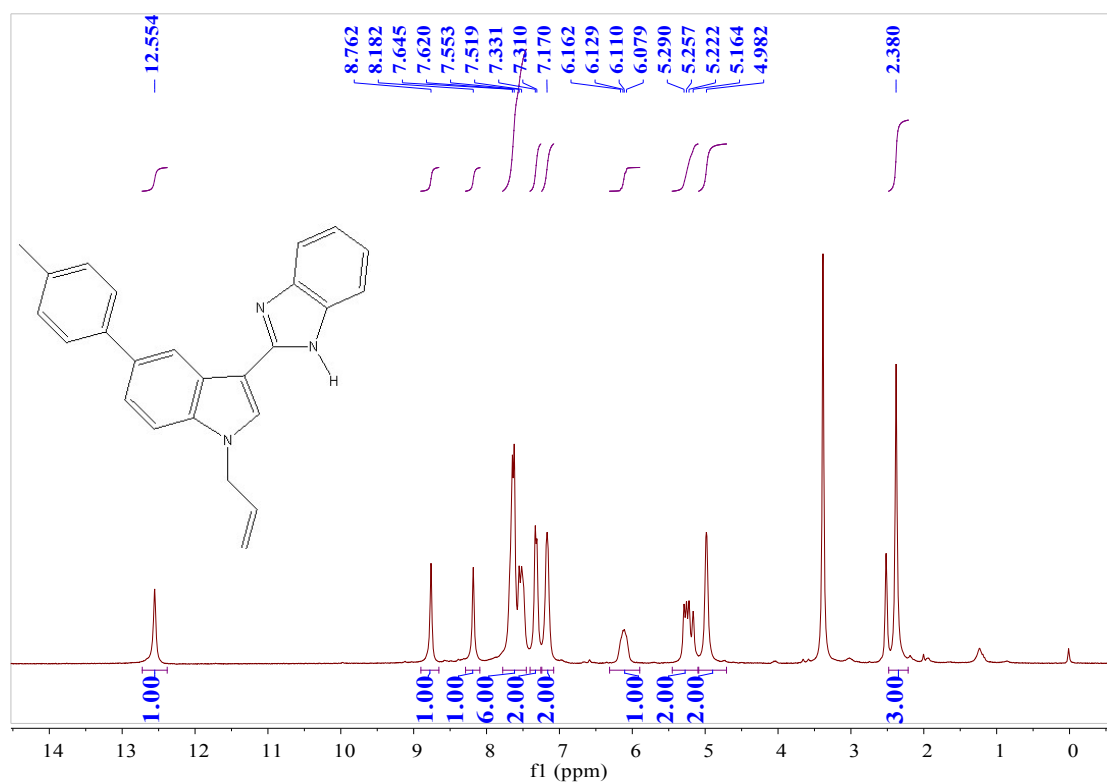
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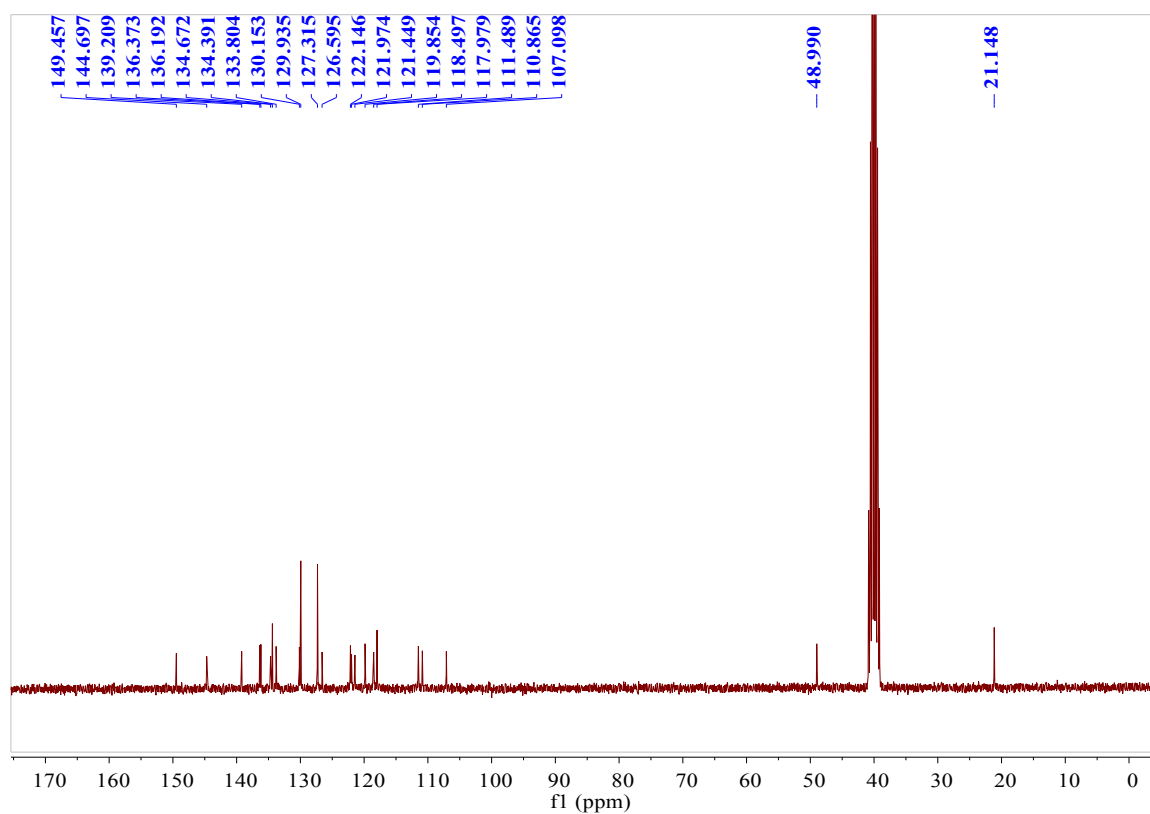
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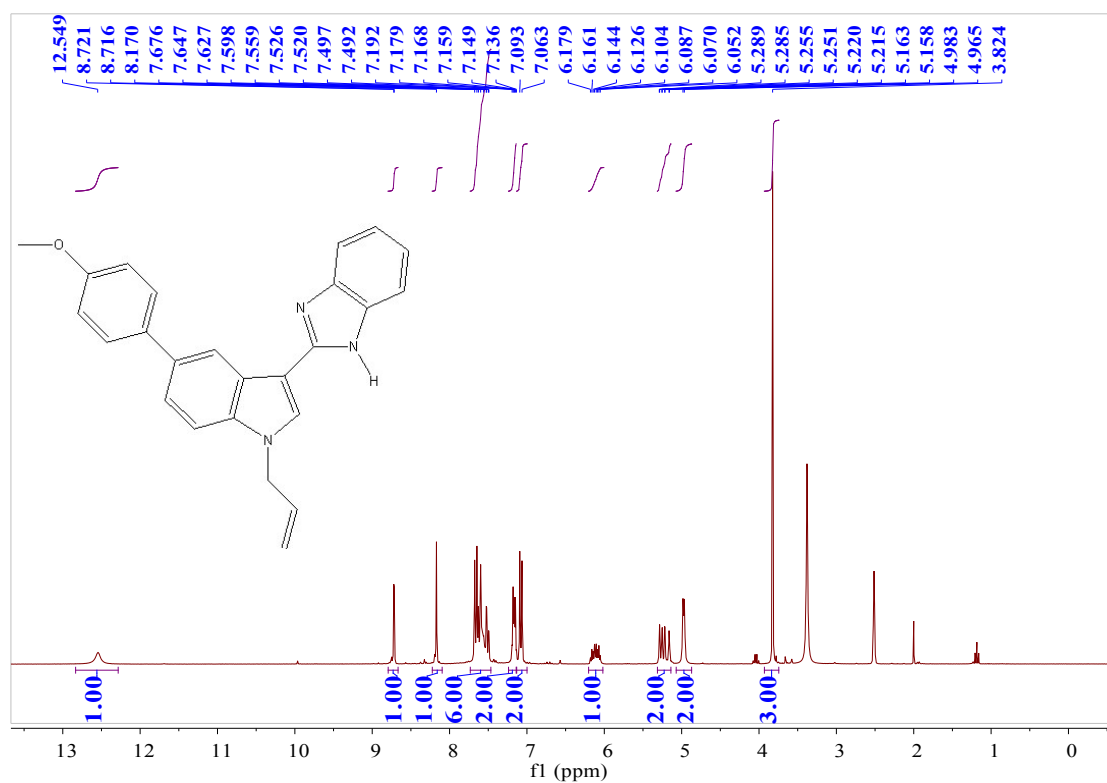
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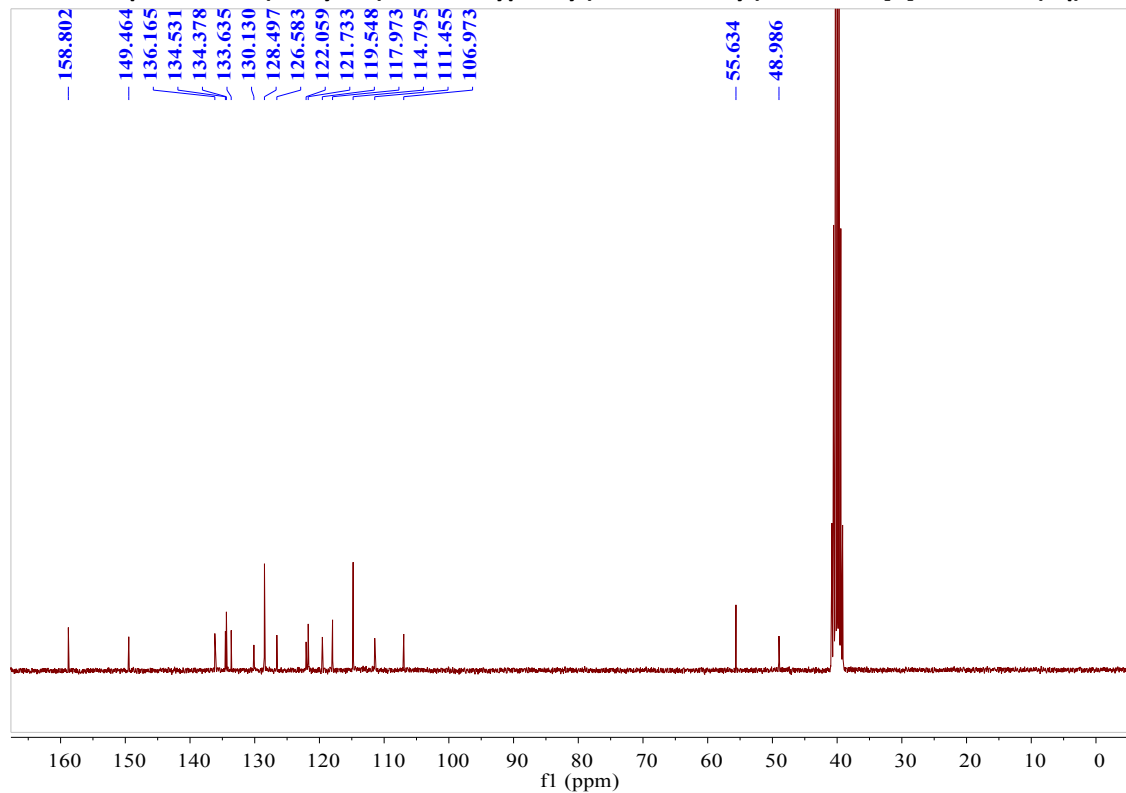
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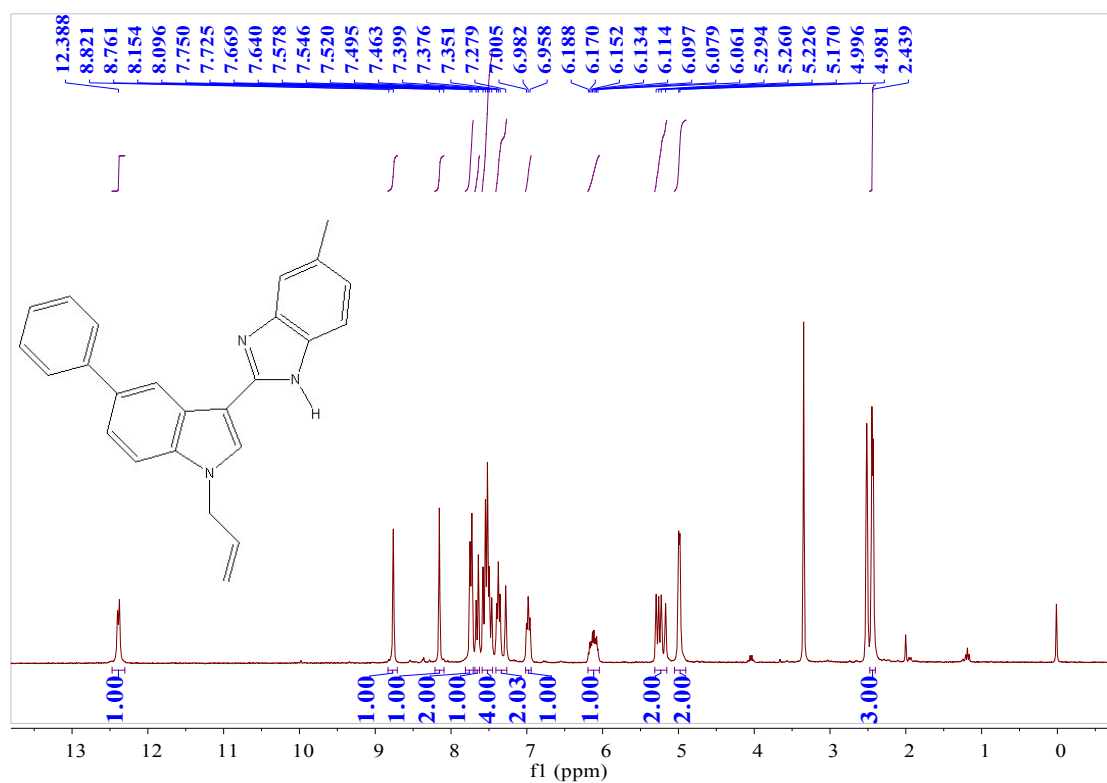
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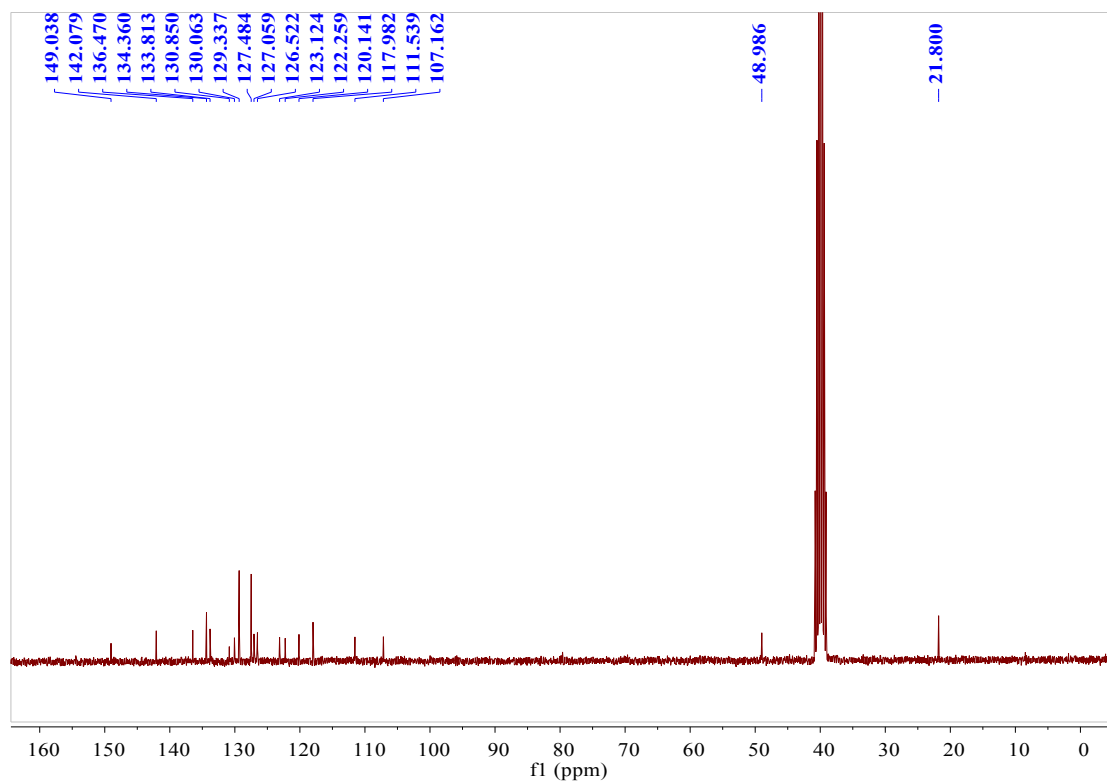
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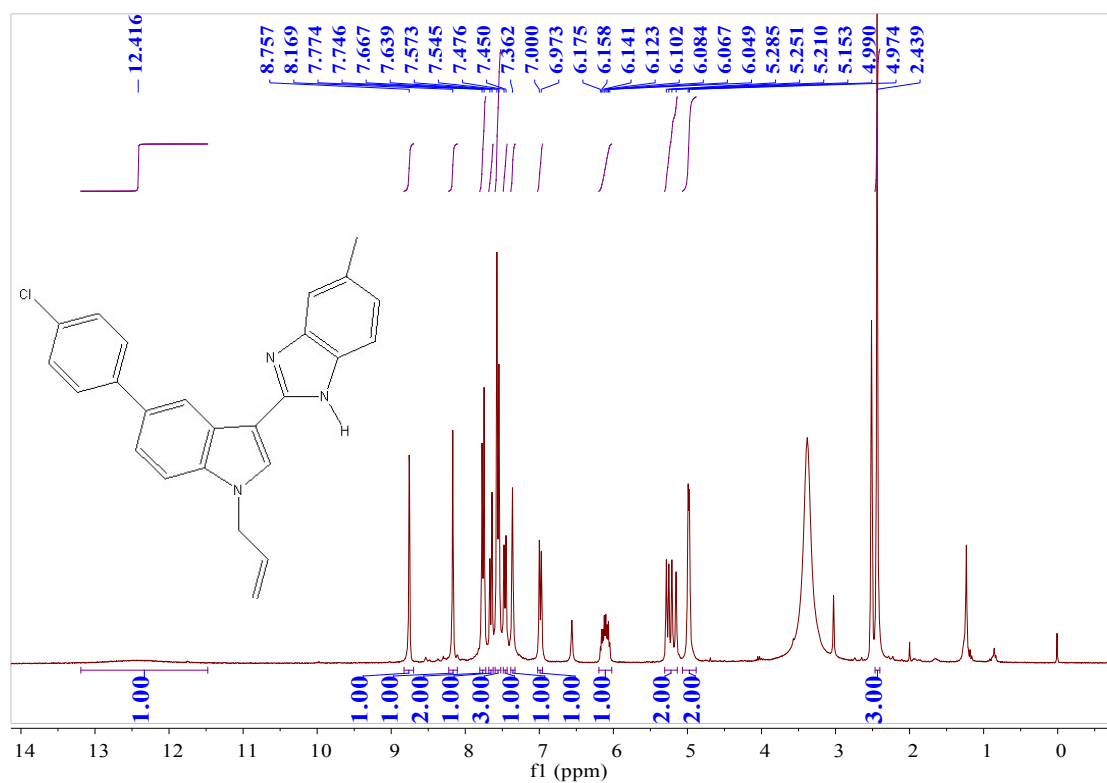
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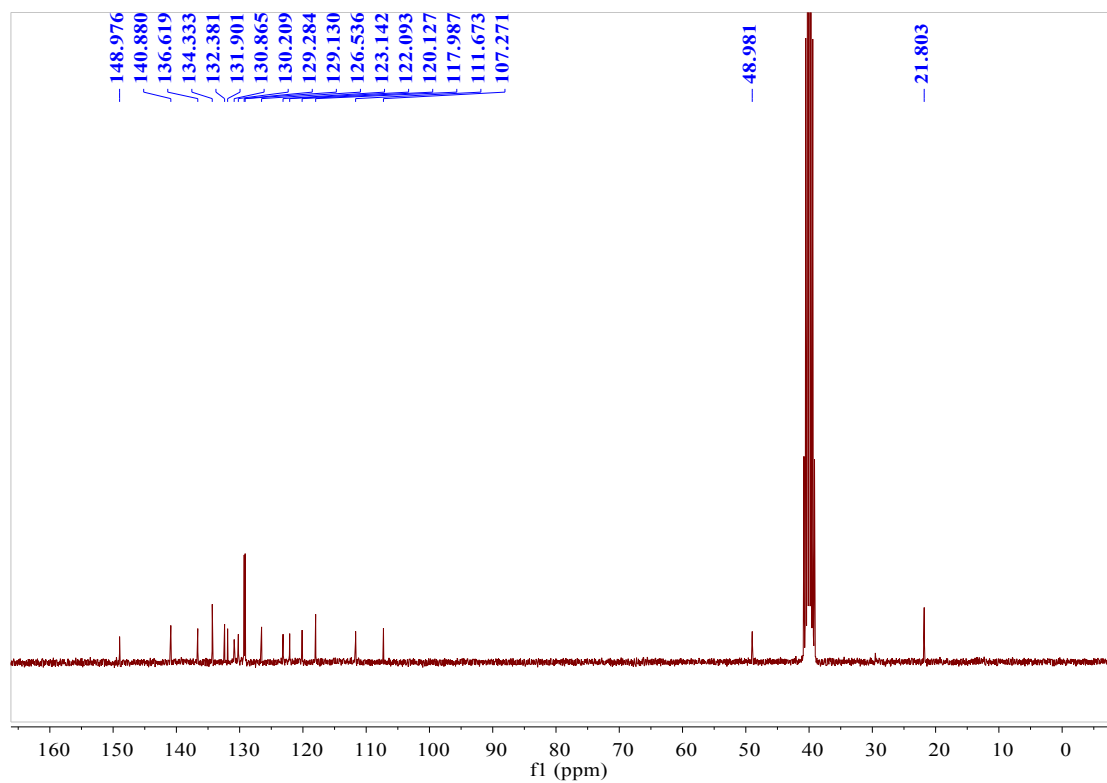
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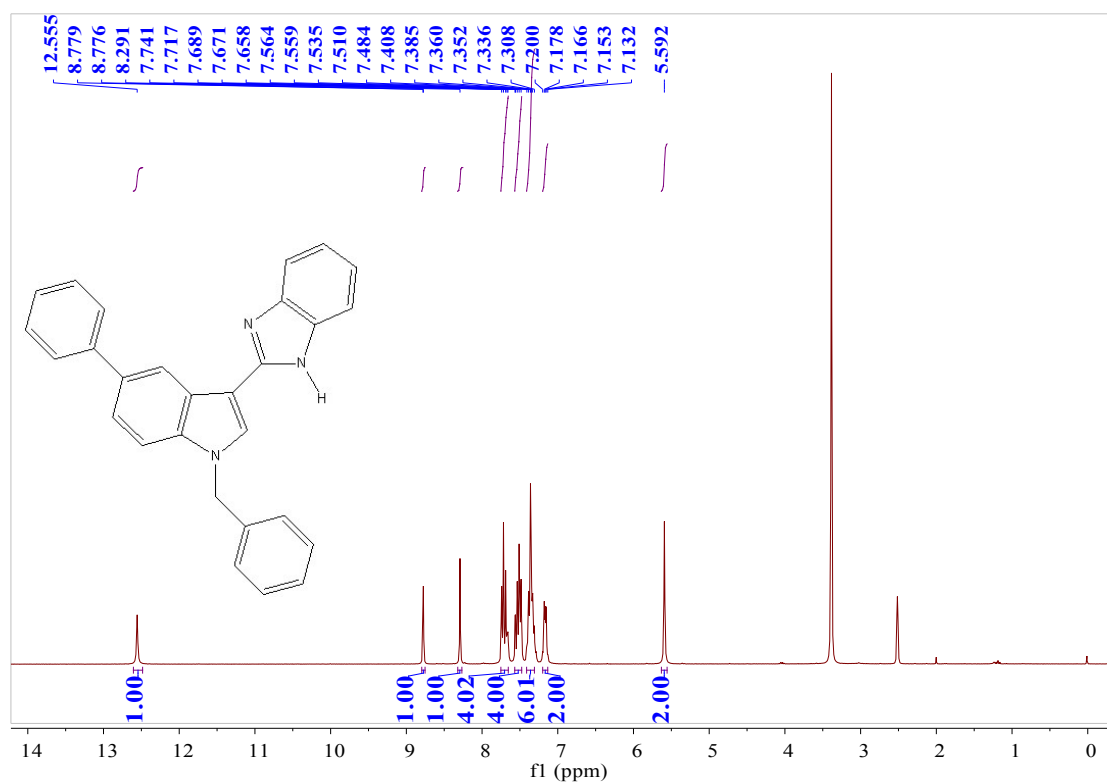
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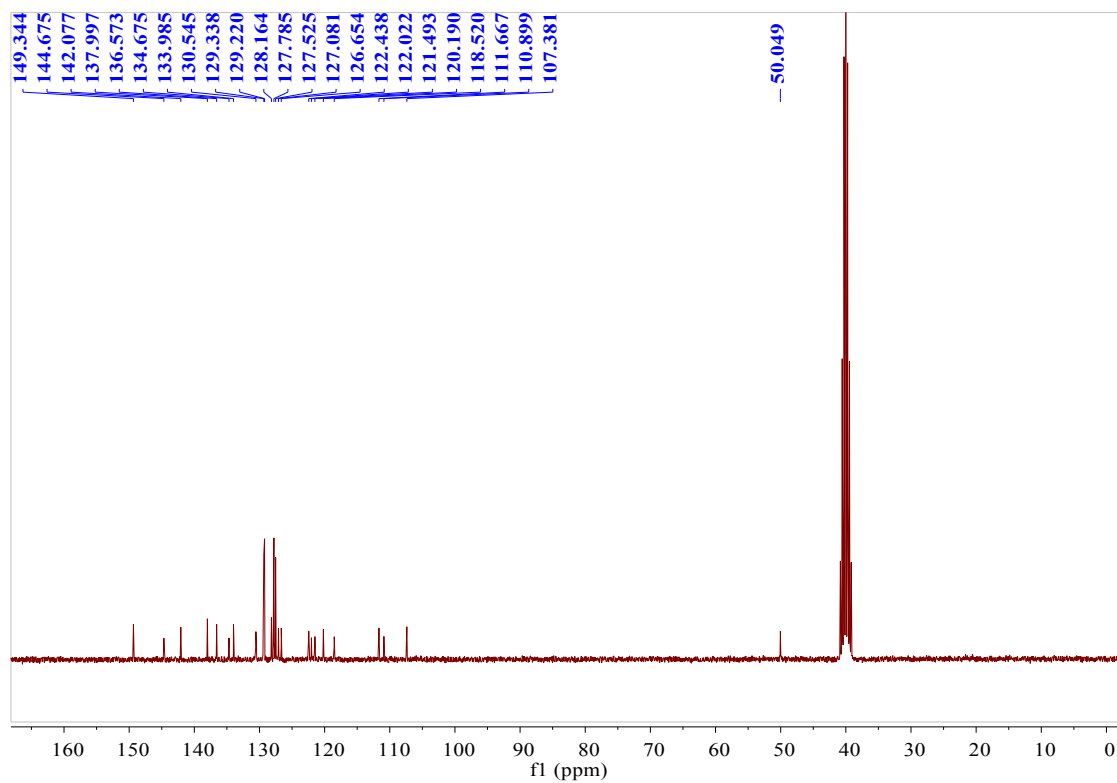
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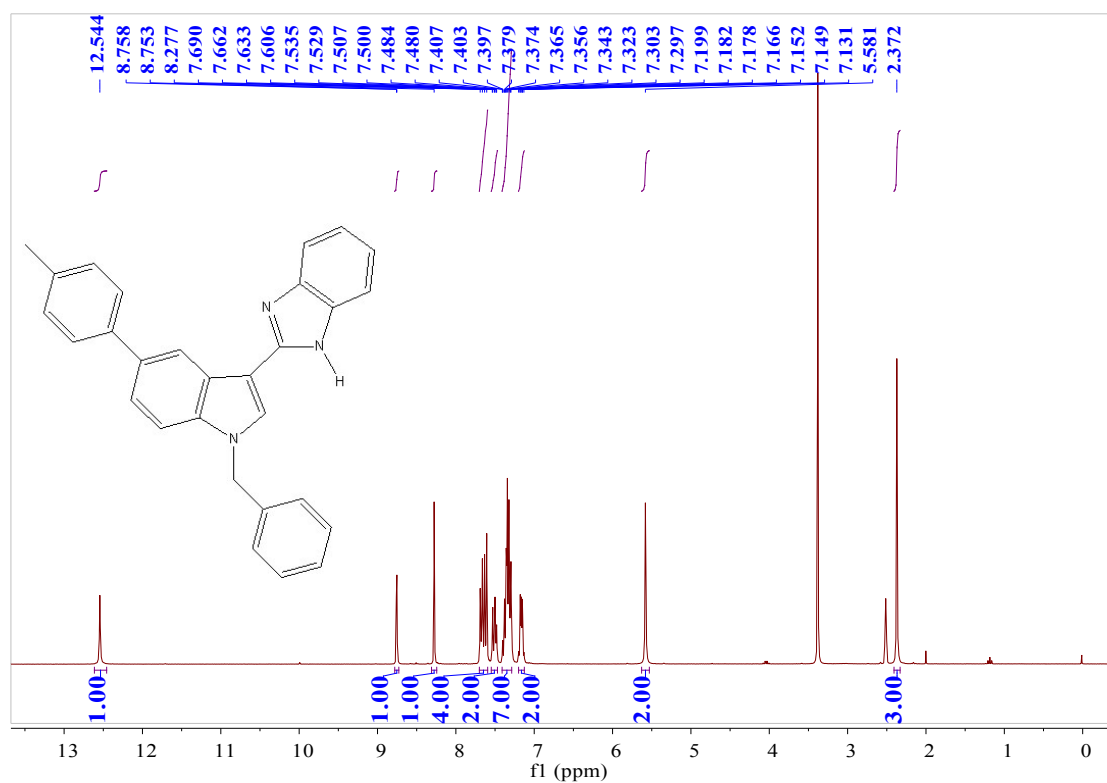
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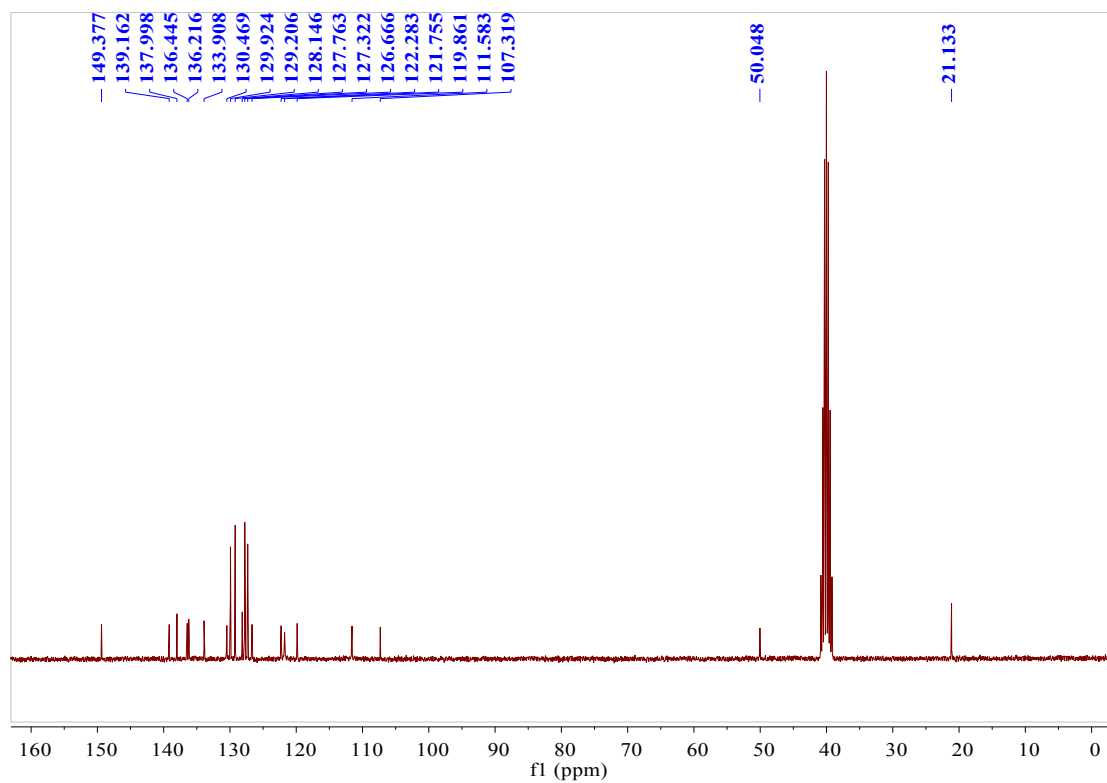
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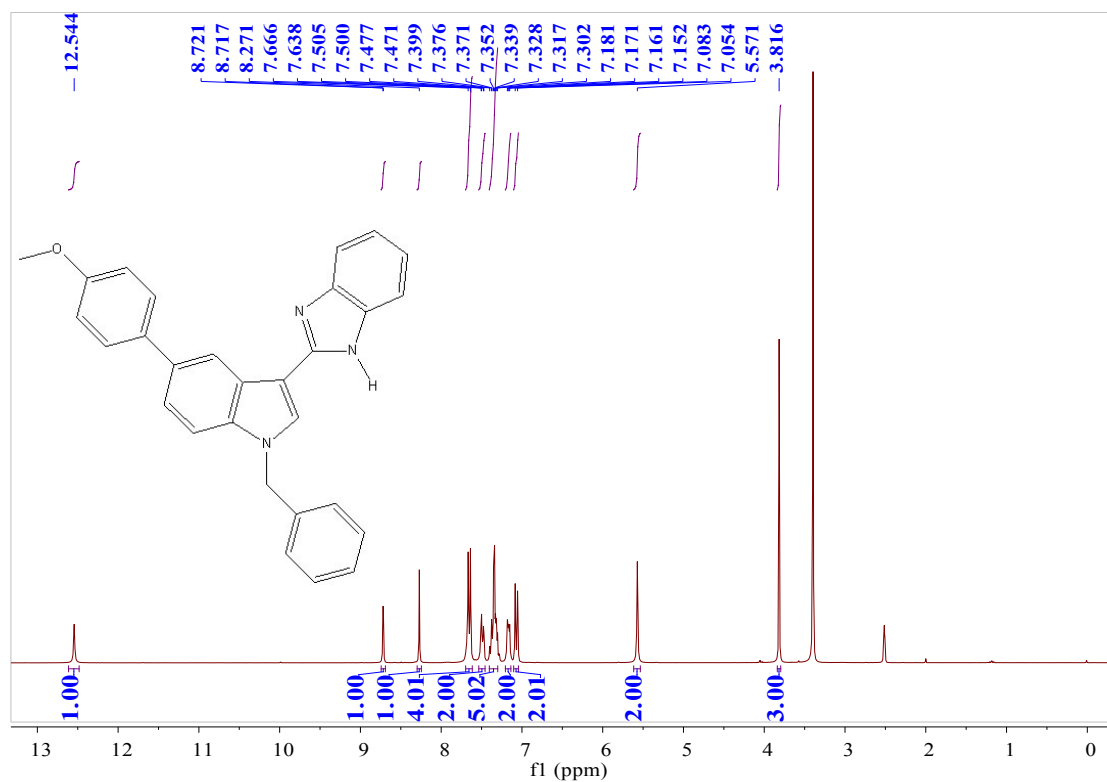
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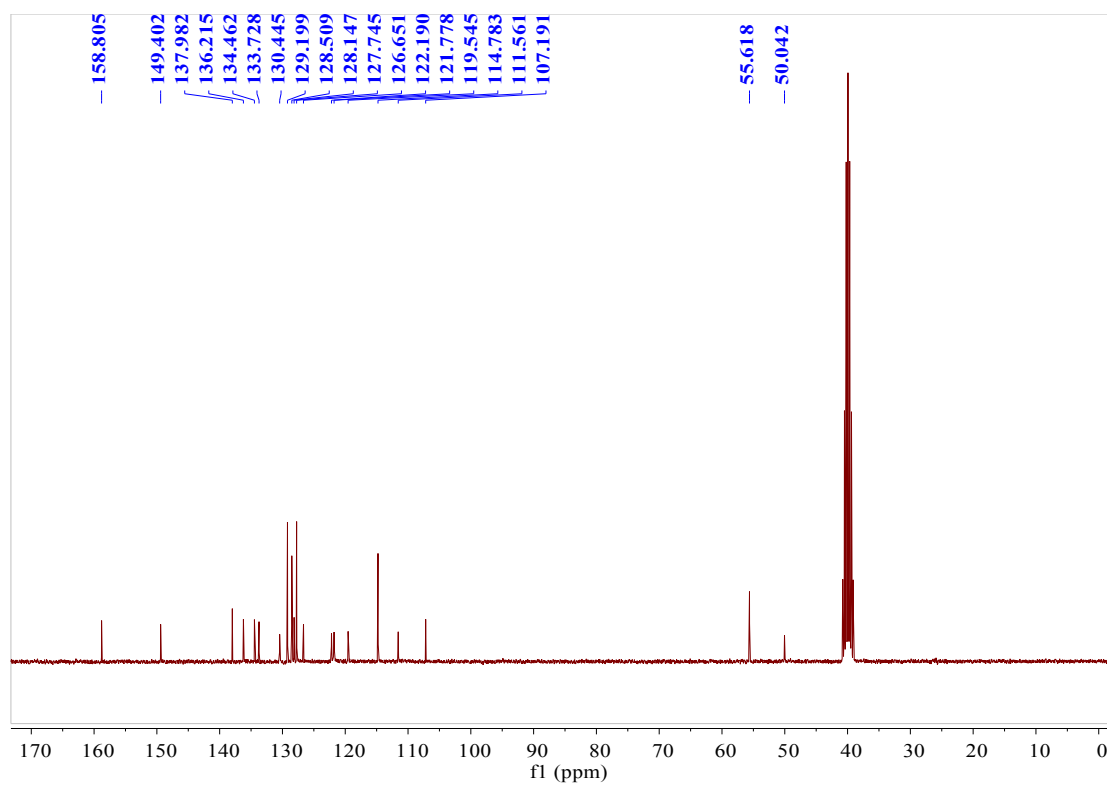
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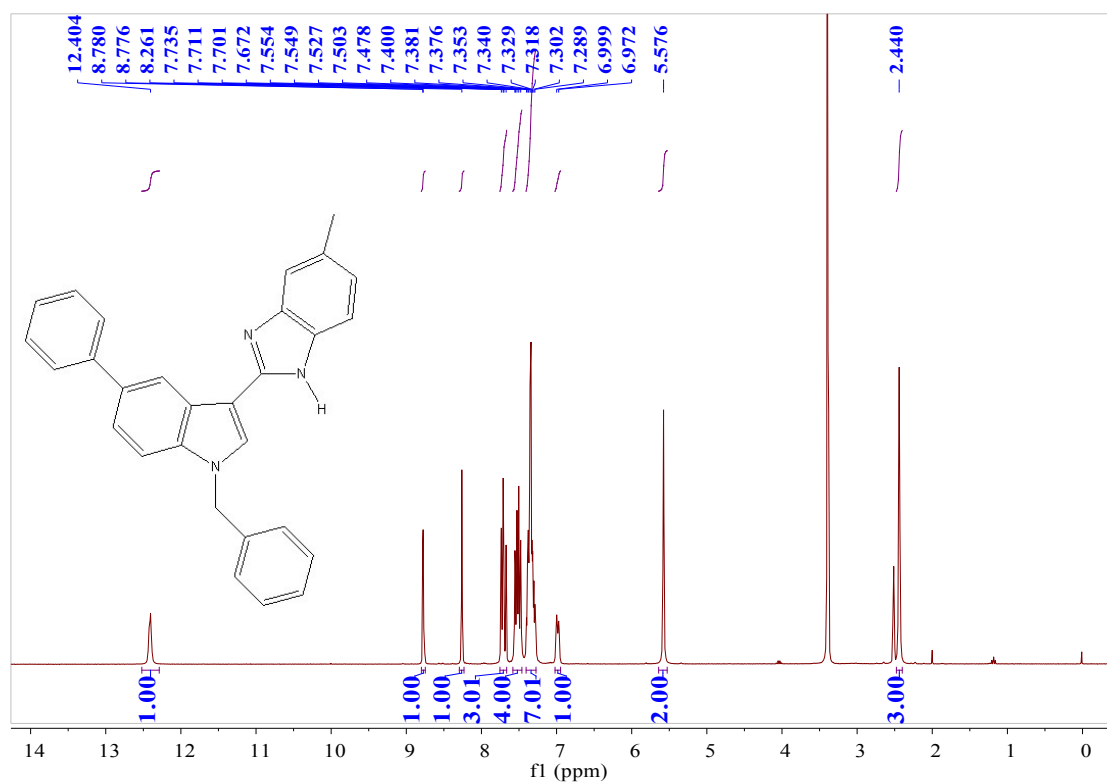
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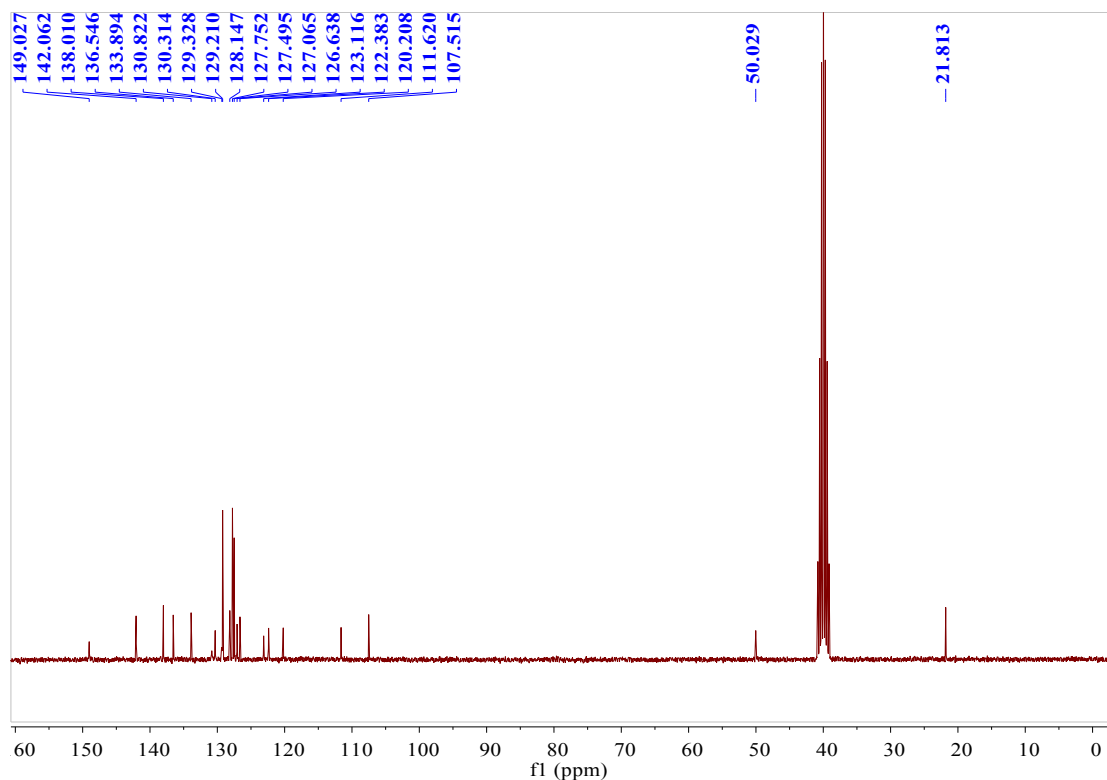
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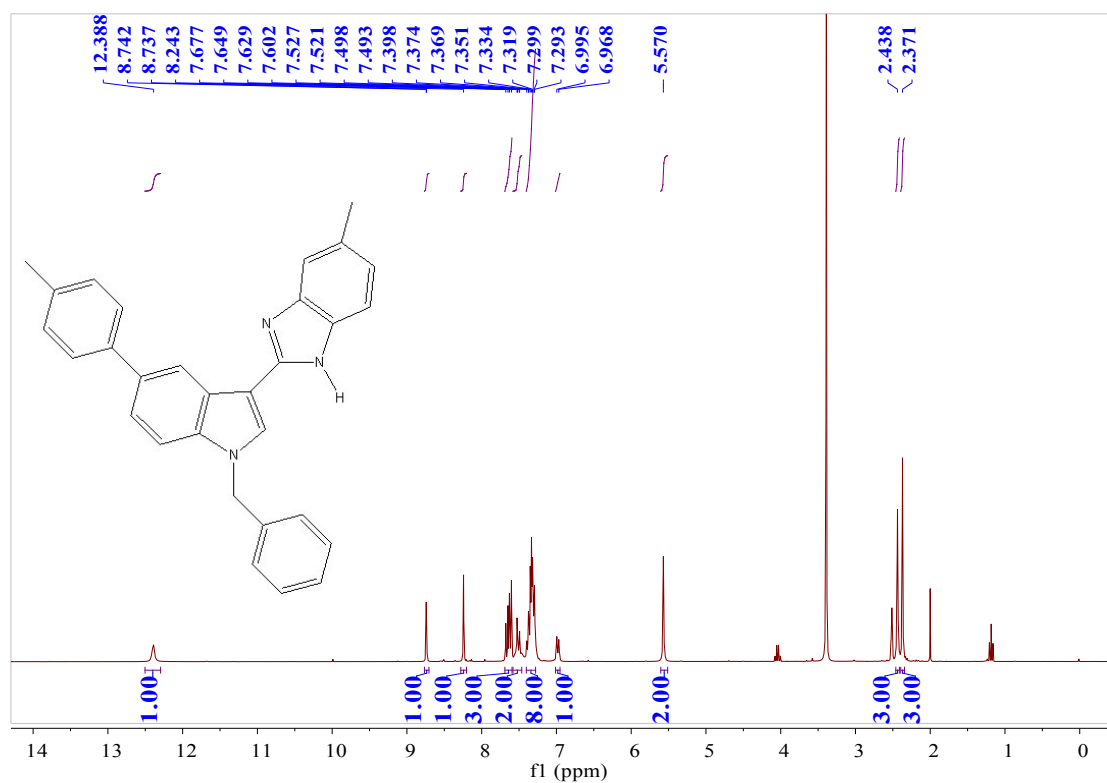
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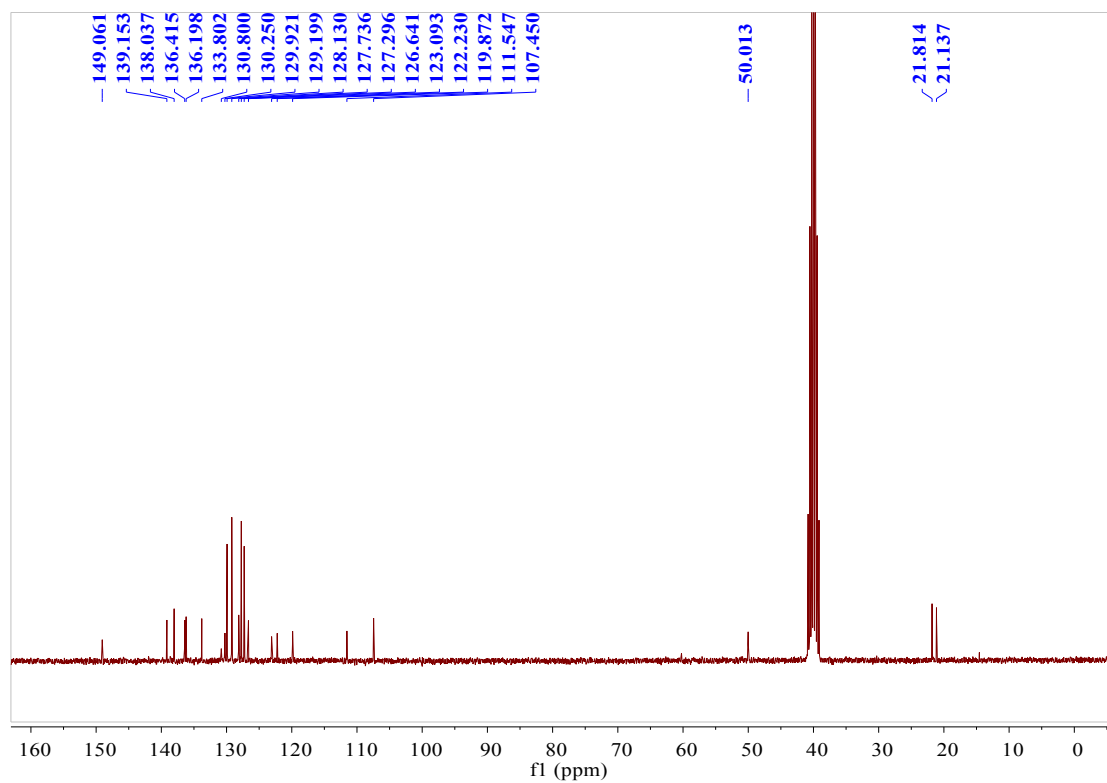
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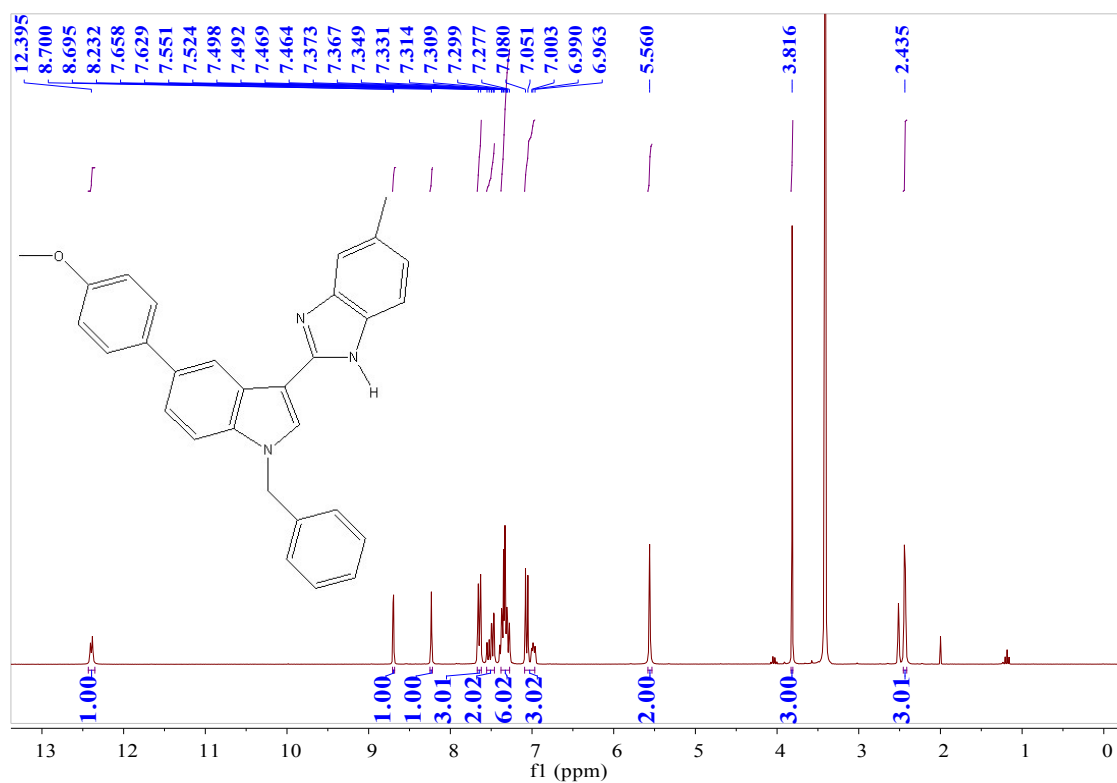
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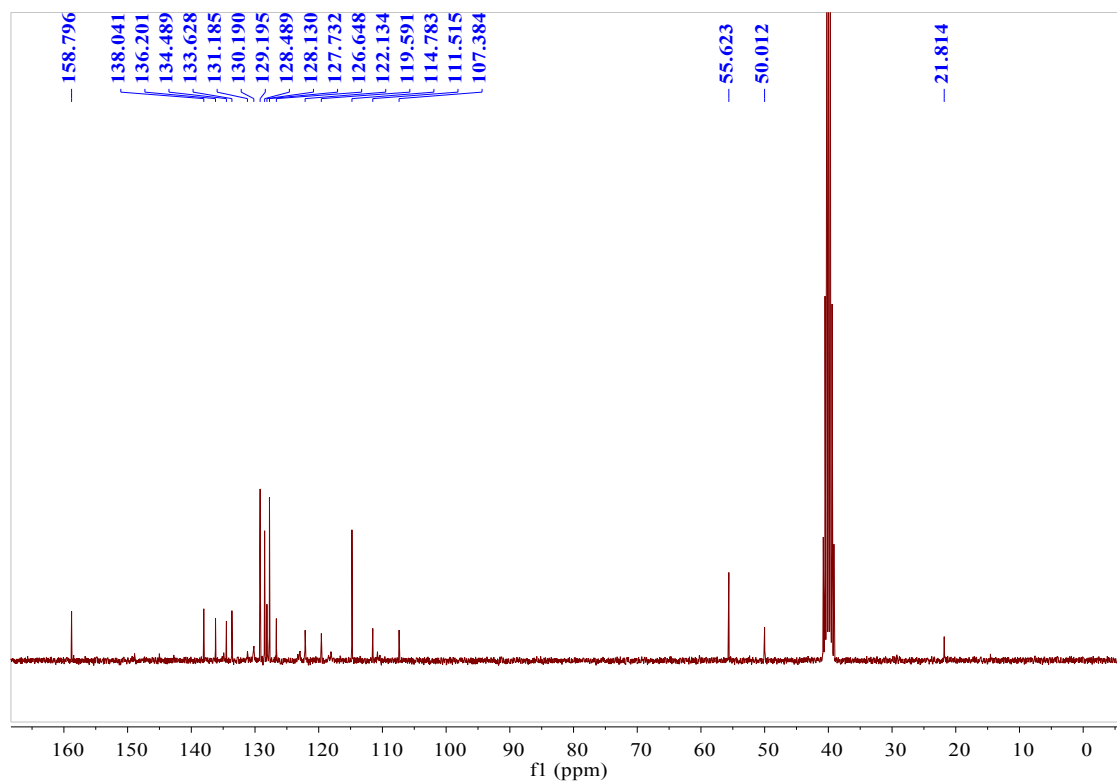
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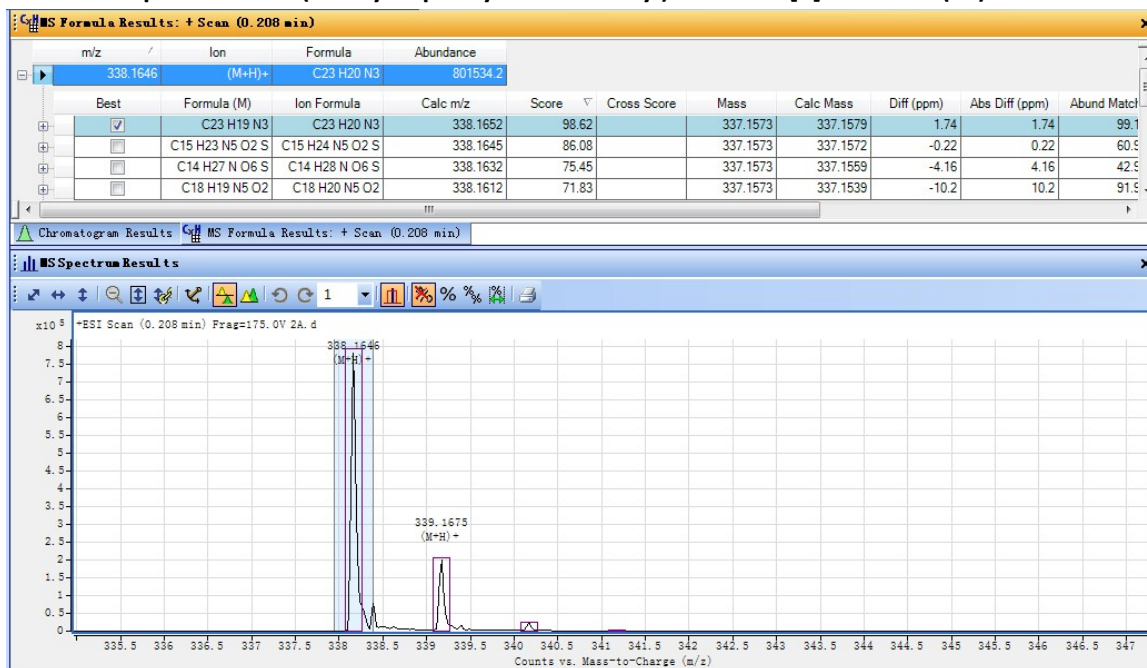


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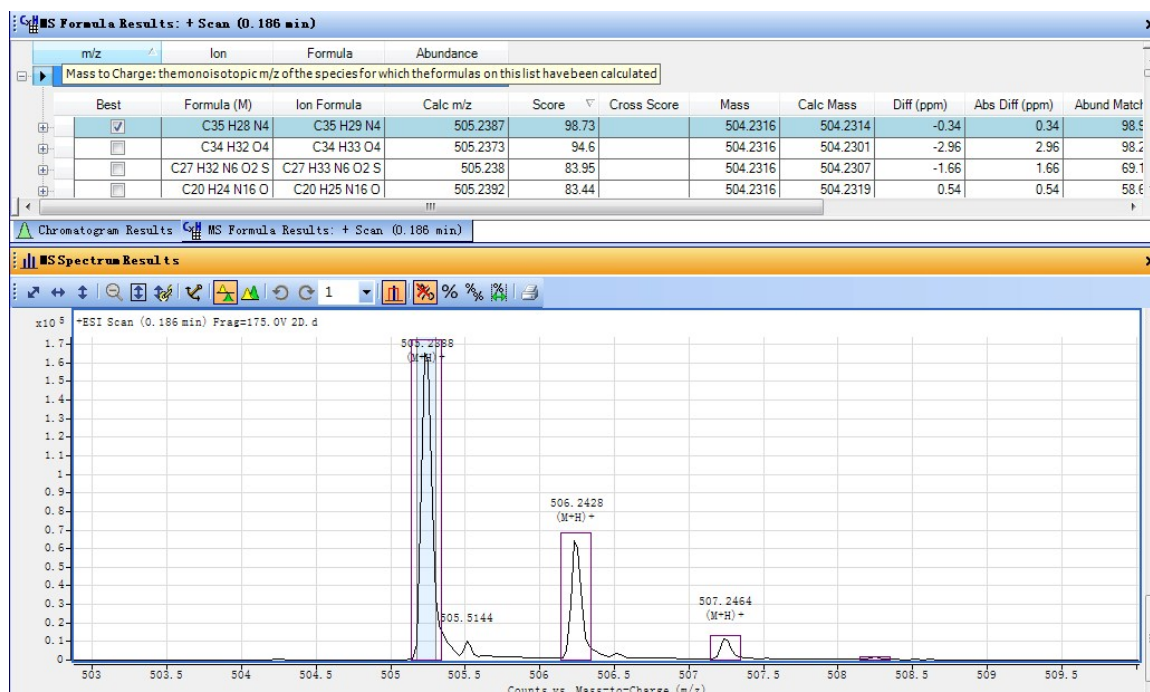


HR-ESI-MS Spectra of compounds 3

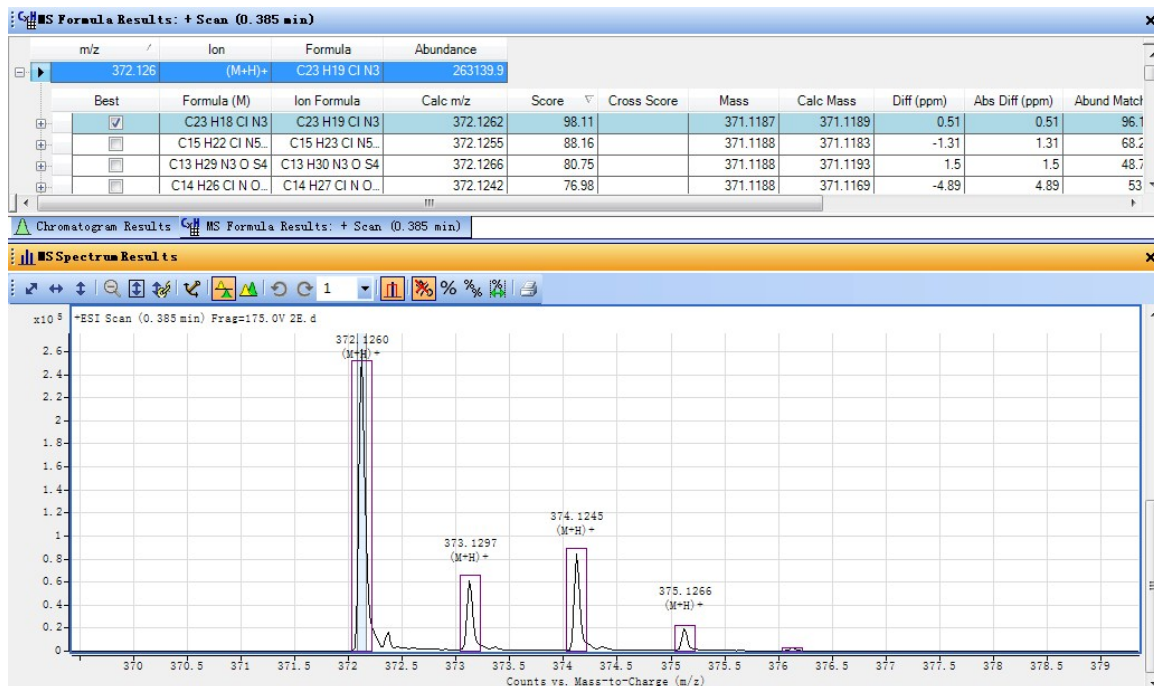
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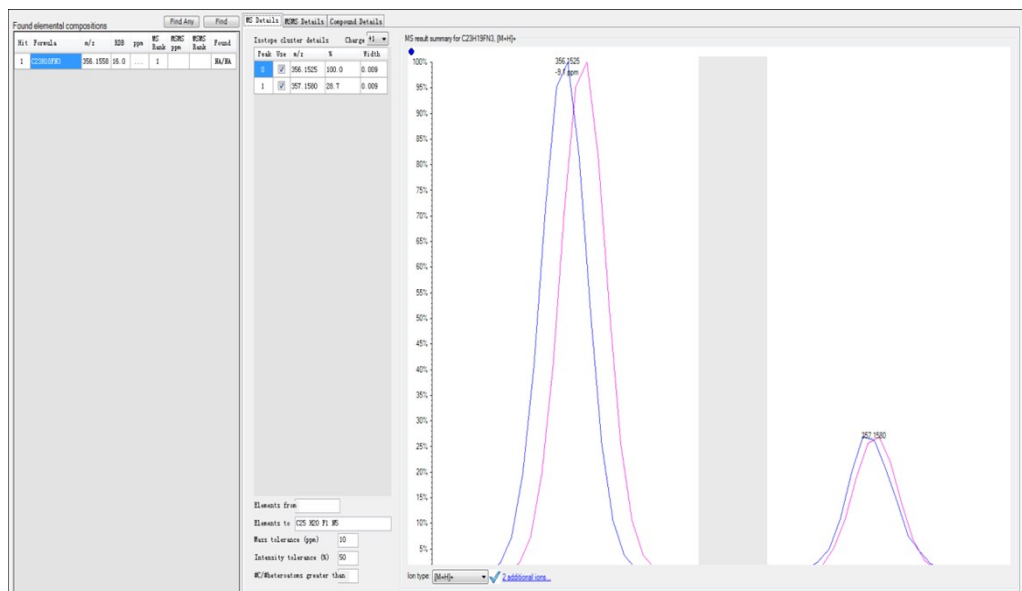
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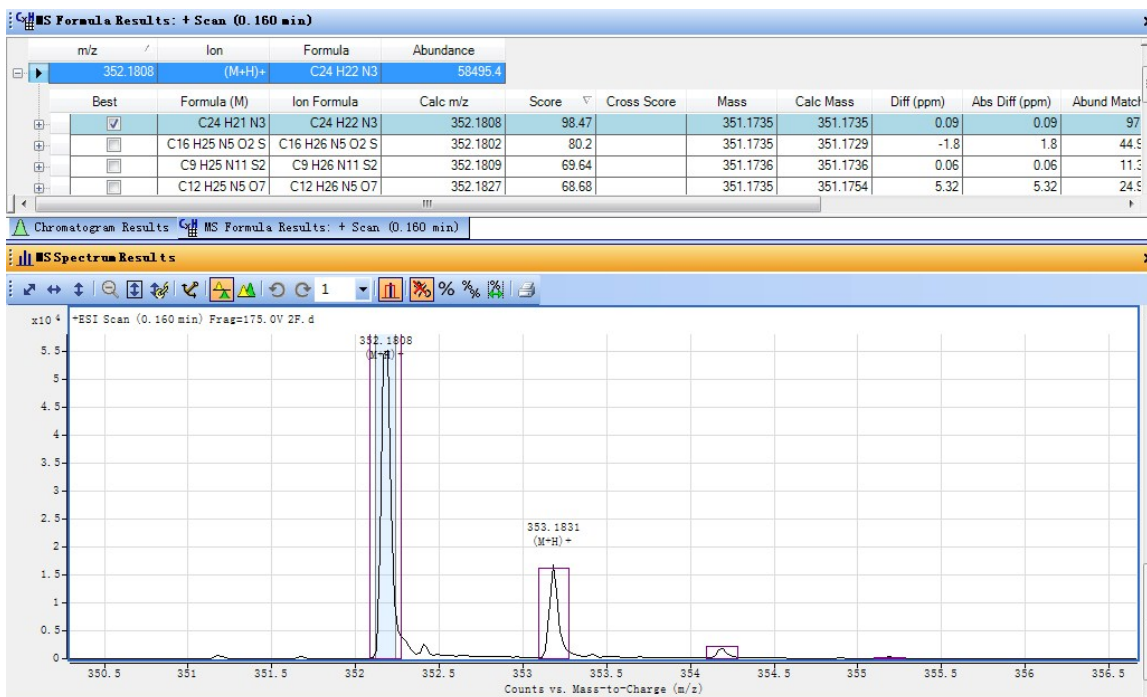
HR-ESI-MS spectrum of 2-(5-(4-chlorophenyl)-1-ethyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3e)



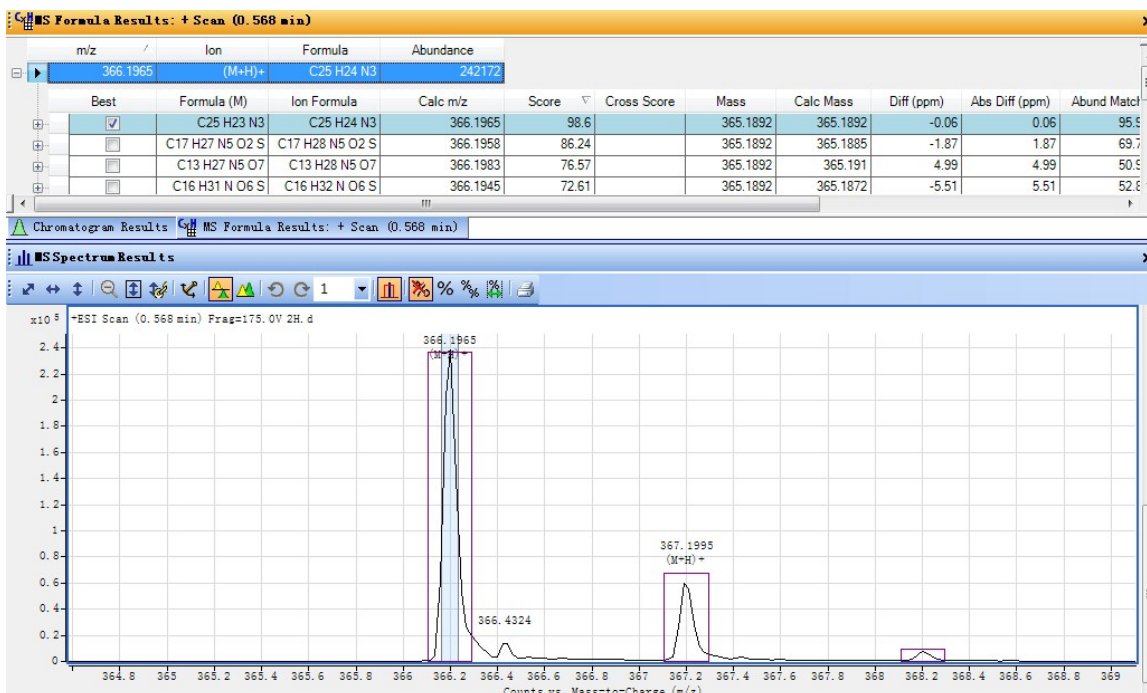
HR-ESI-MS spectrum of 2-(5-(4-fluorophenyl)-1-ethyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3f)



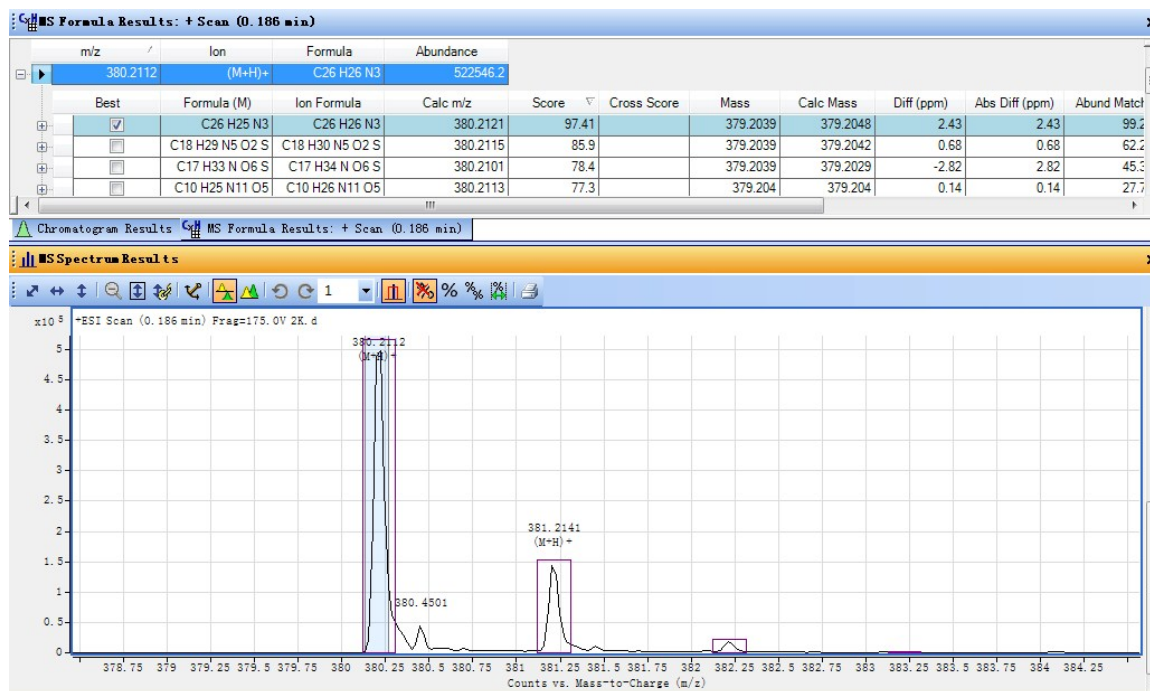
HR-ESI-MS spectrum of 2-(1-ethyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3g)



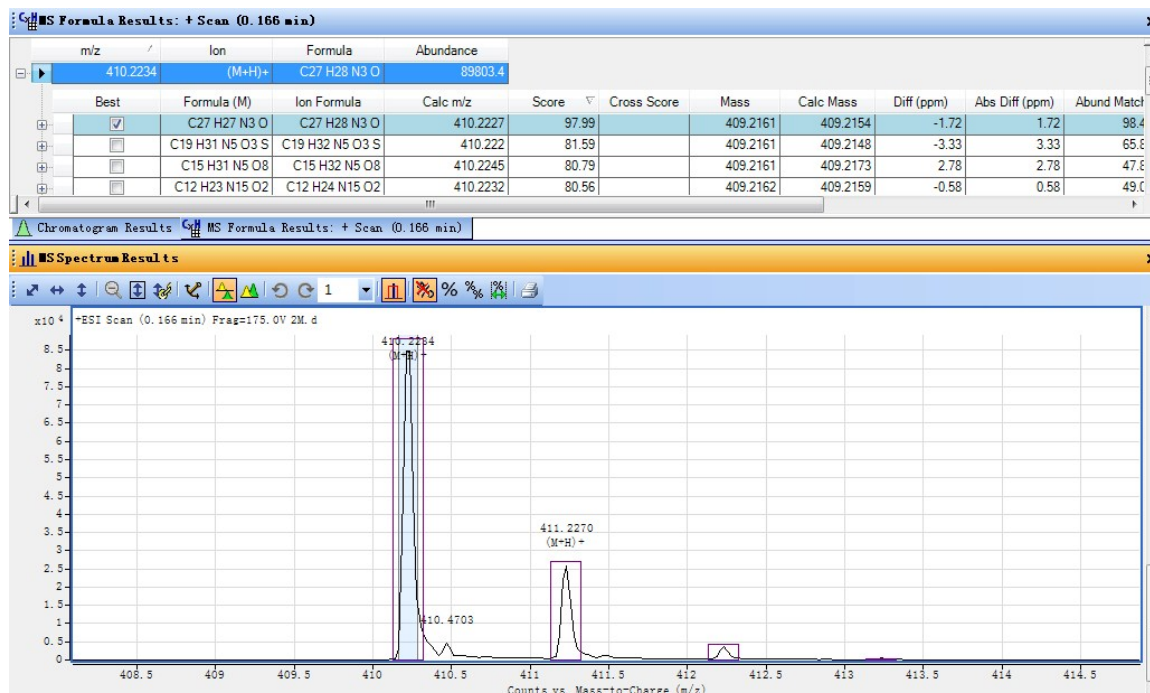
HR-ESI-MS spectrum of 2-(1-butyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3i)



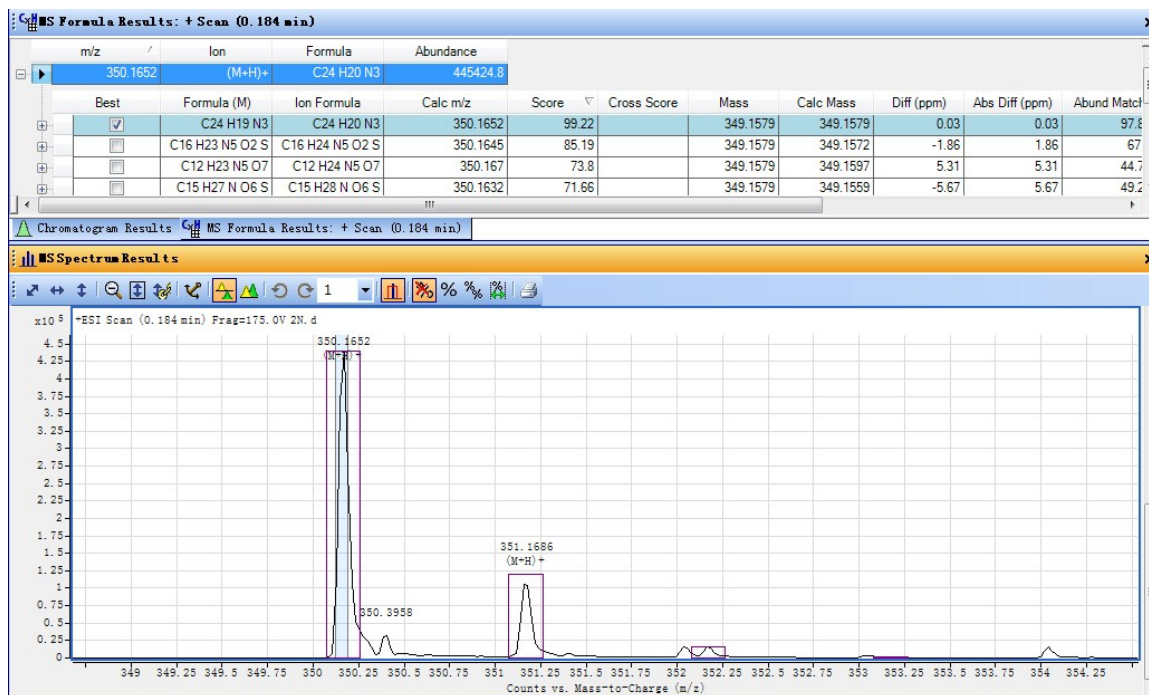
HR-ESI-MS spectrum of 2-(1-butyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3m)



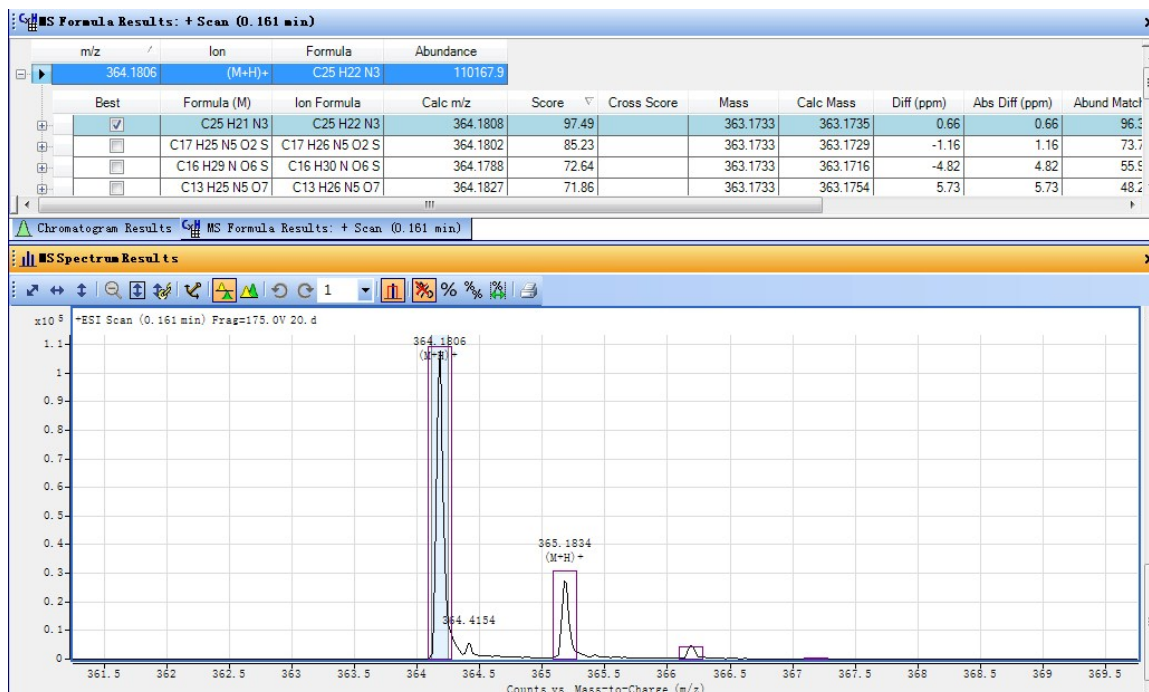
HR-ESI-MS spectrum of 2-(1-butyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3n)



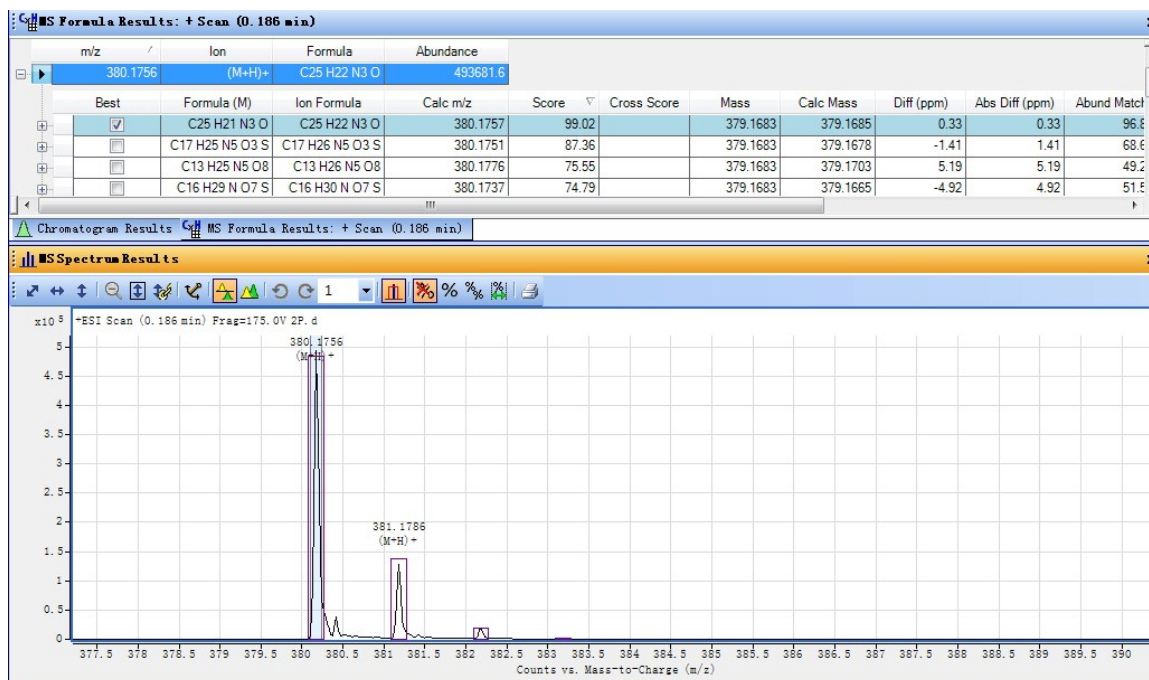
HR-ESI-MS spectrum of 2-(1-allyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3o)



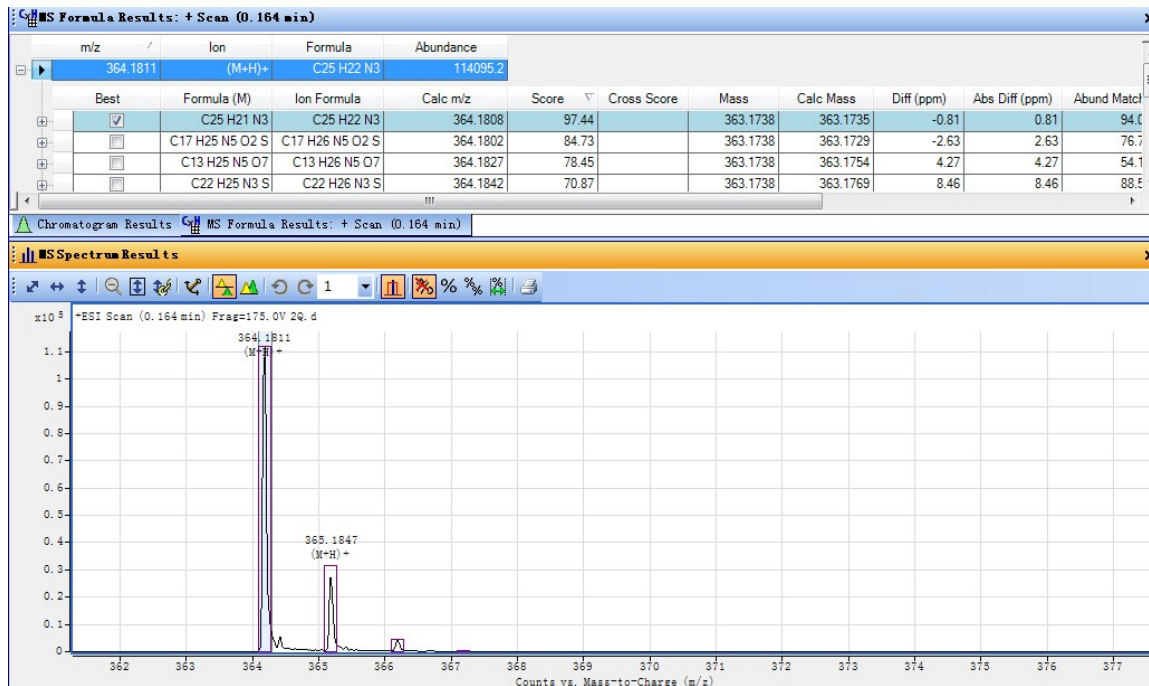
HR-ESI-MS spectrum of 2-(1-allyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3p)



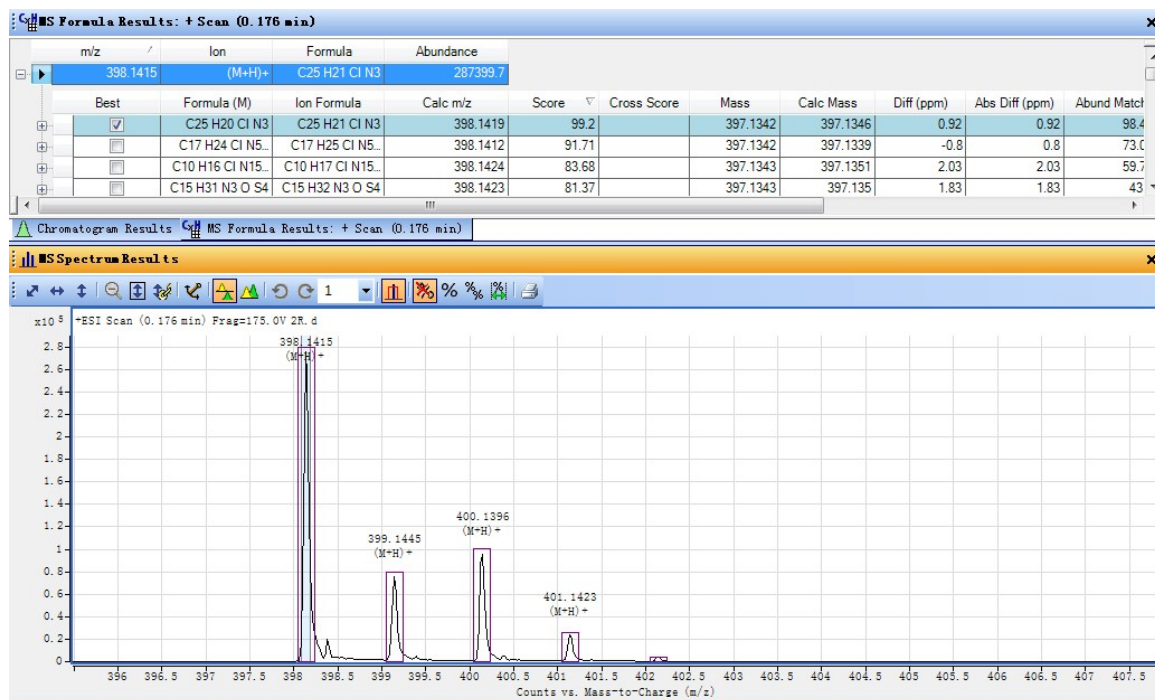
HR-ESI-MS spectrum of 2-(1-allyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3q)



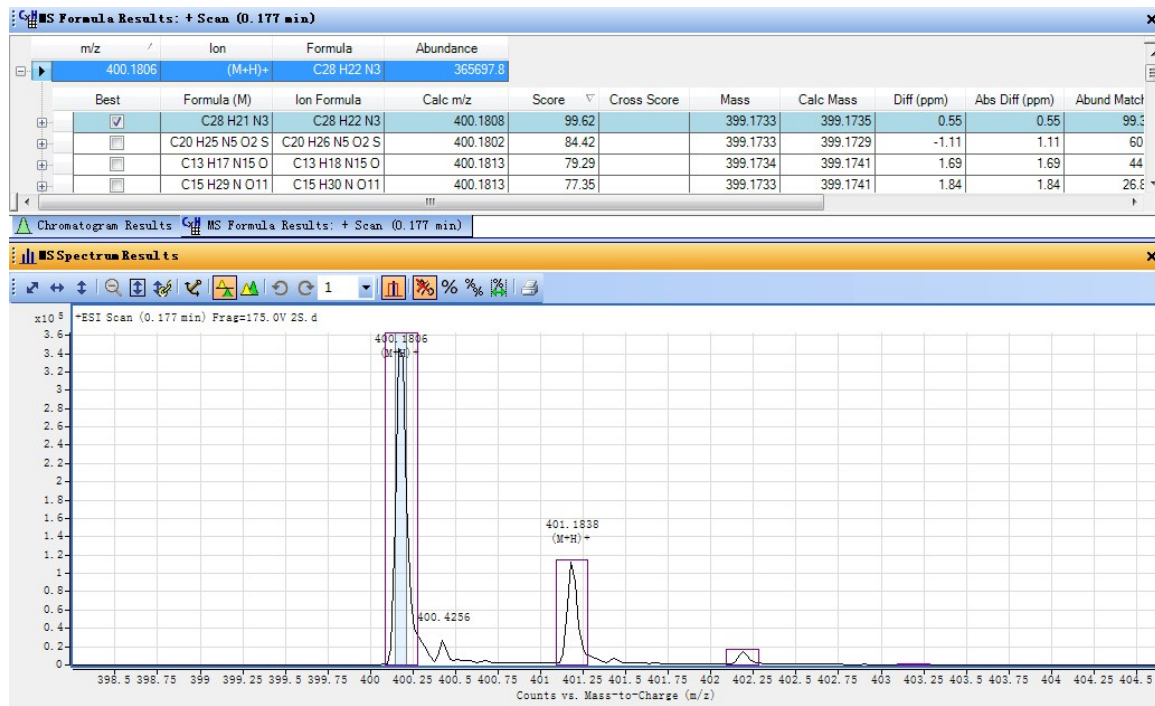
HR-ESI-MS spectrum of 2-(1-allyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3r)



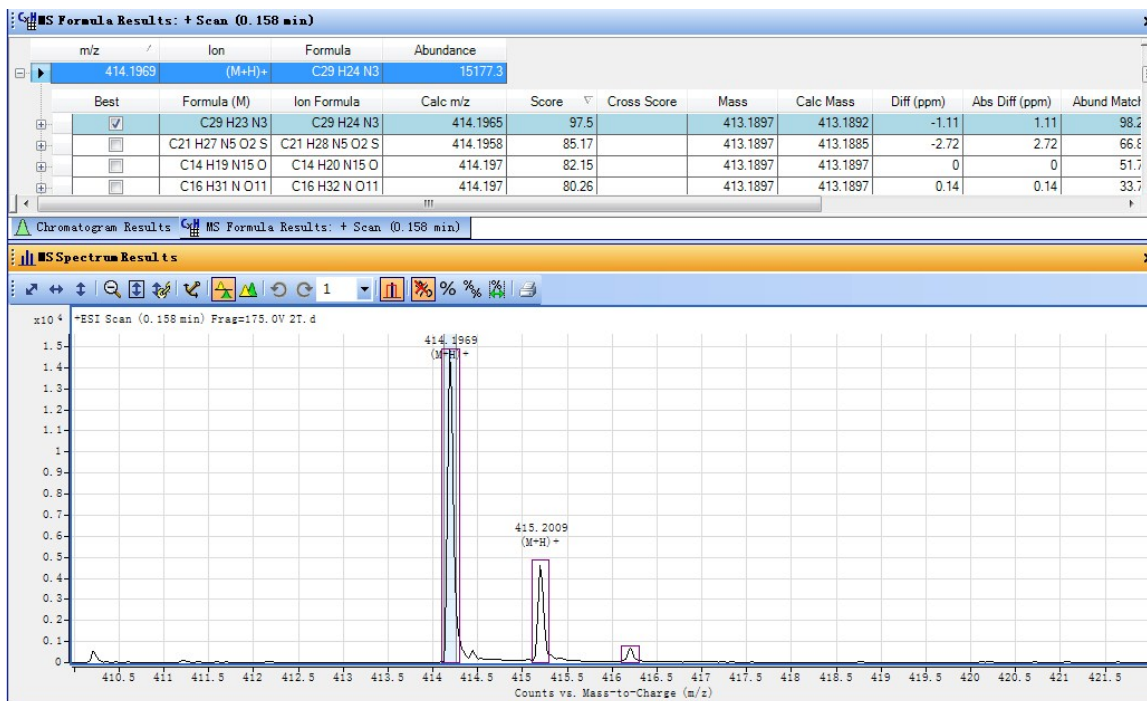
HR-ESI-MS spectrum of 2-(1-allyl-5-(4-chlorophenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3s)



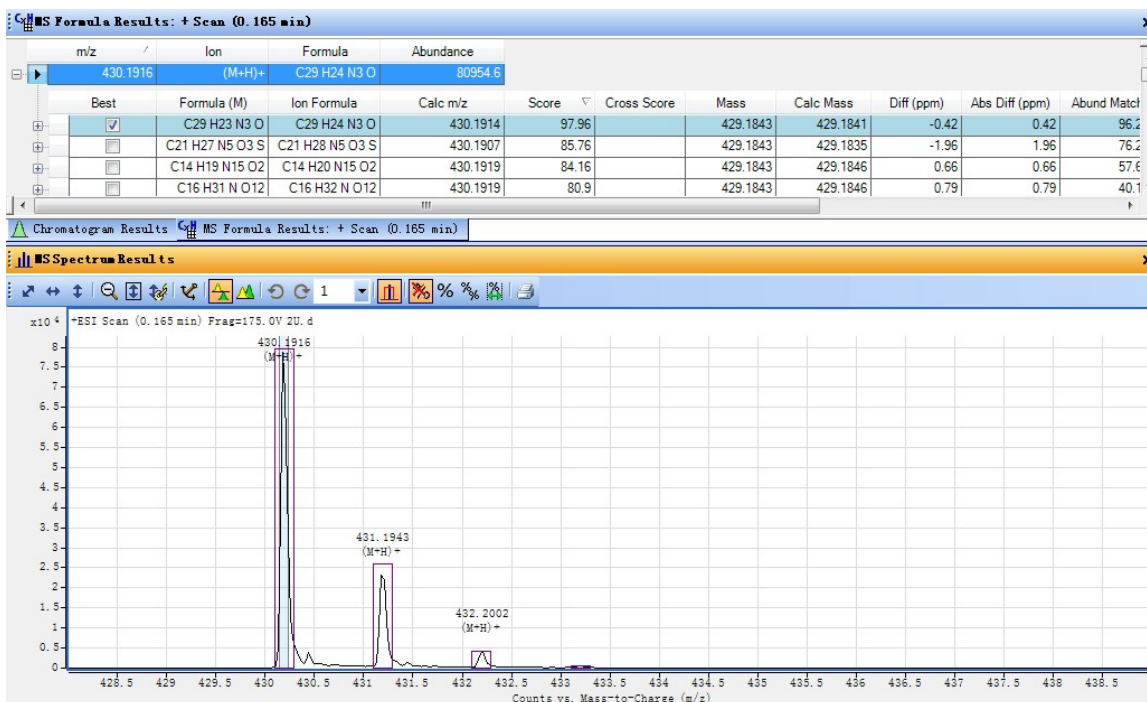
HR-ESI-MS spectrum of 2-(1-benzyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3t)



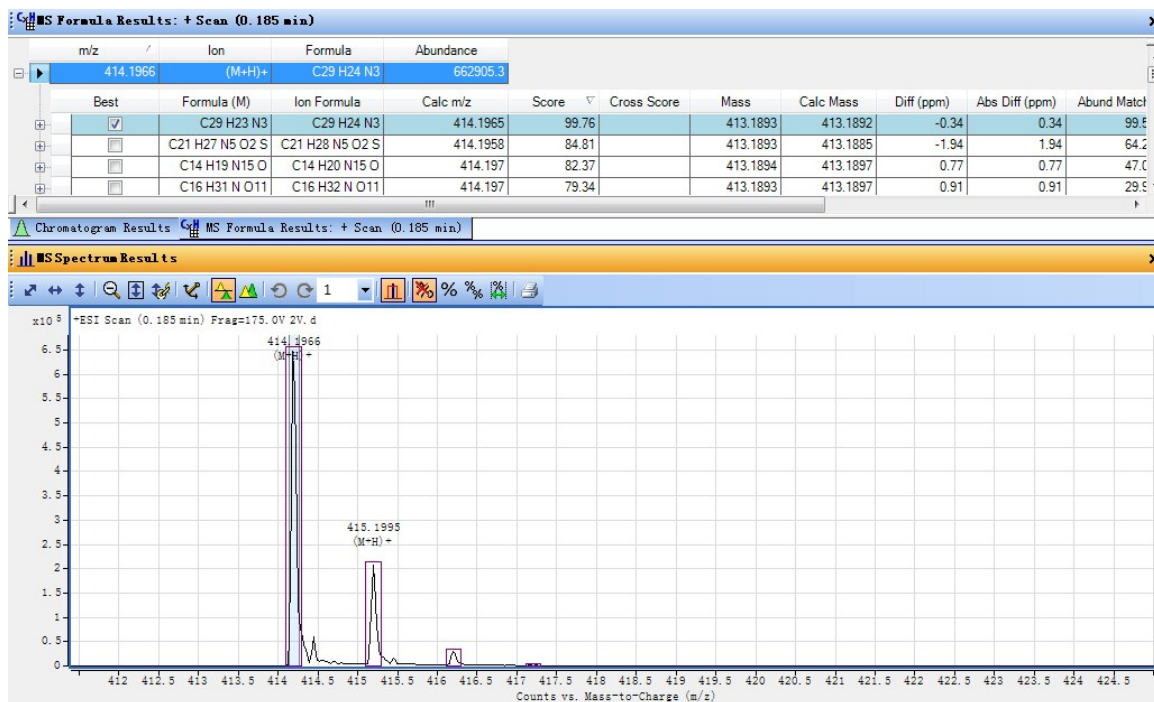
HR-ESI-MS spectrum of 2-(1-benzyl-5-(*p*-tolyl)-1*H*-indol-3-yl)-1*H*-benzo[*d*]imidazole (3u)



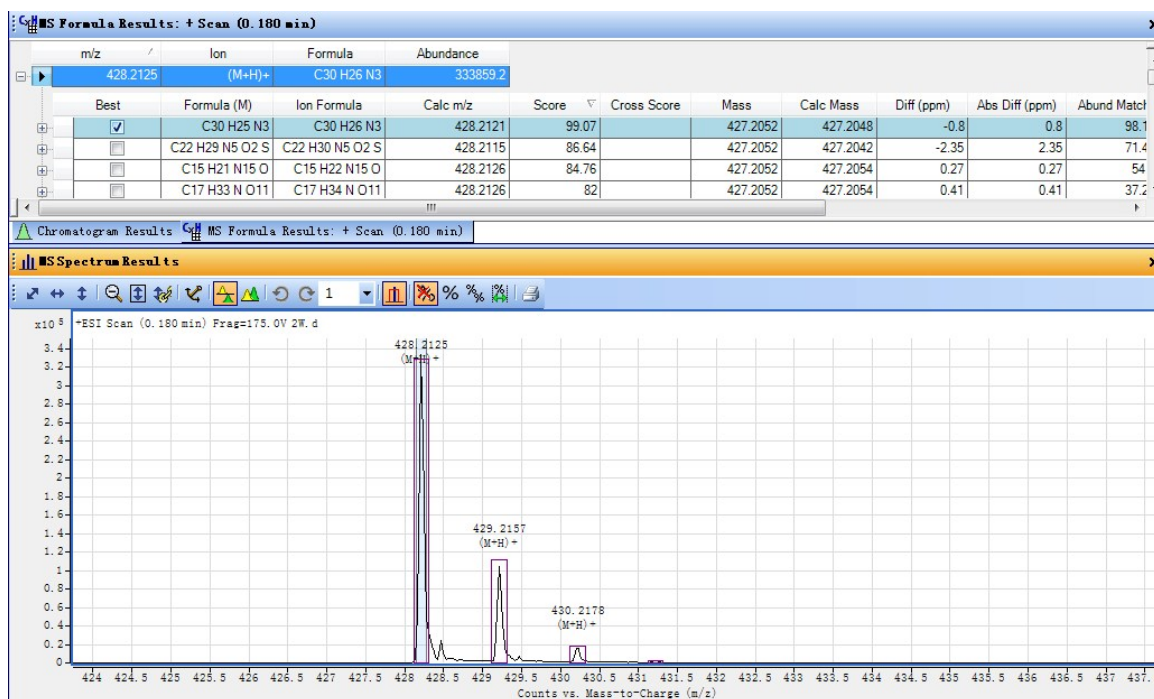
HR-ESI-MS spectrum of 2-(1-benzyl-5-(4-methoxyphenyl)-1*H*-indol-3-yl)-1*H*-benzo[*d*]imidazole (3v)



HR-ESI-MS spectrum of 2-(1-benzyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3w)



HR-ESI-MS spectrum of 2-(1-benzyl-5-(p-tolyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3x)



HR-ESI-MS spectrum of 2-(1-benzyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3y)

