

Supplementary Material

Efficient synthesis of 2-substituted 1-phenylchromen[3,4-*d*]imidazol-4(1*H*)-ones with possible anti-inflammatory activity

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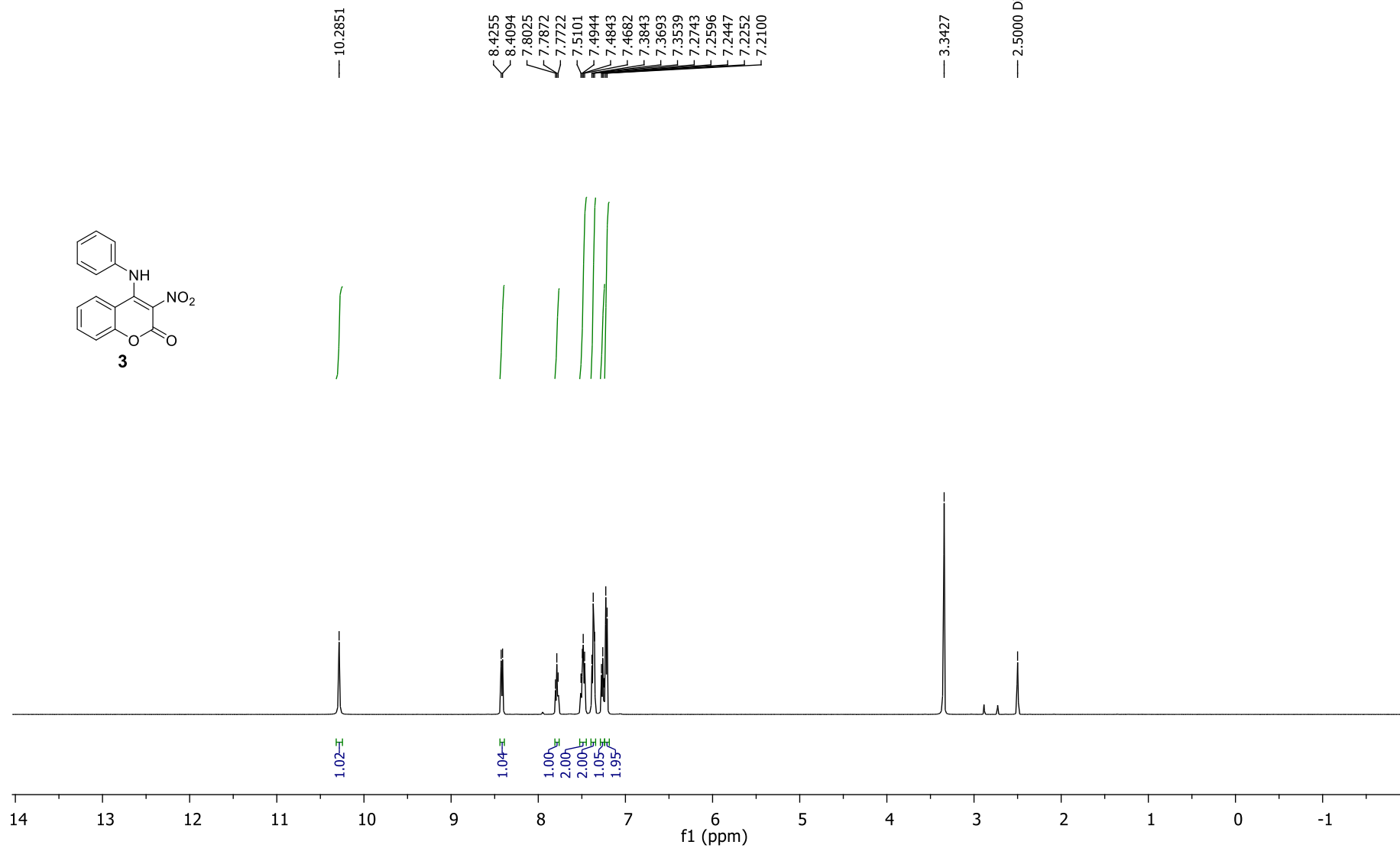
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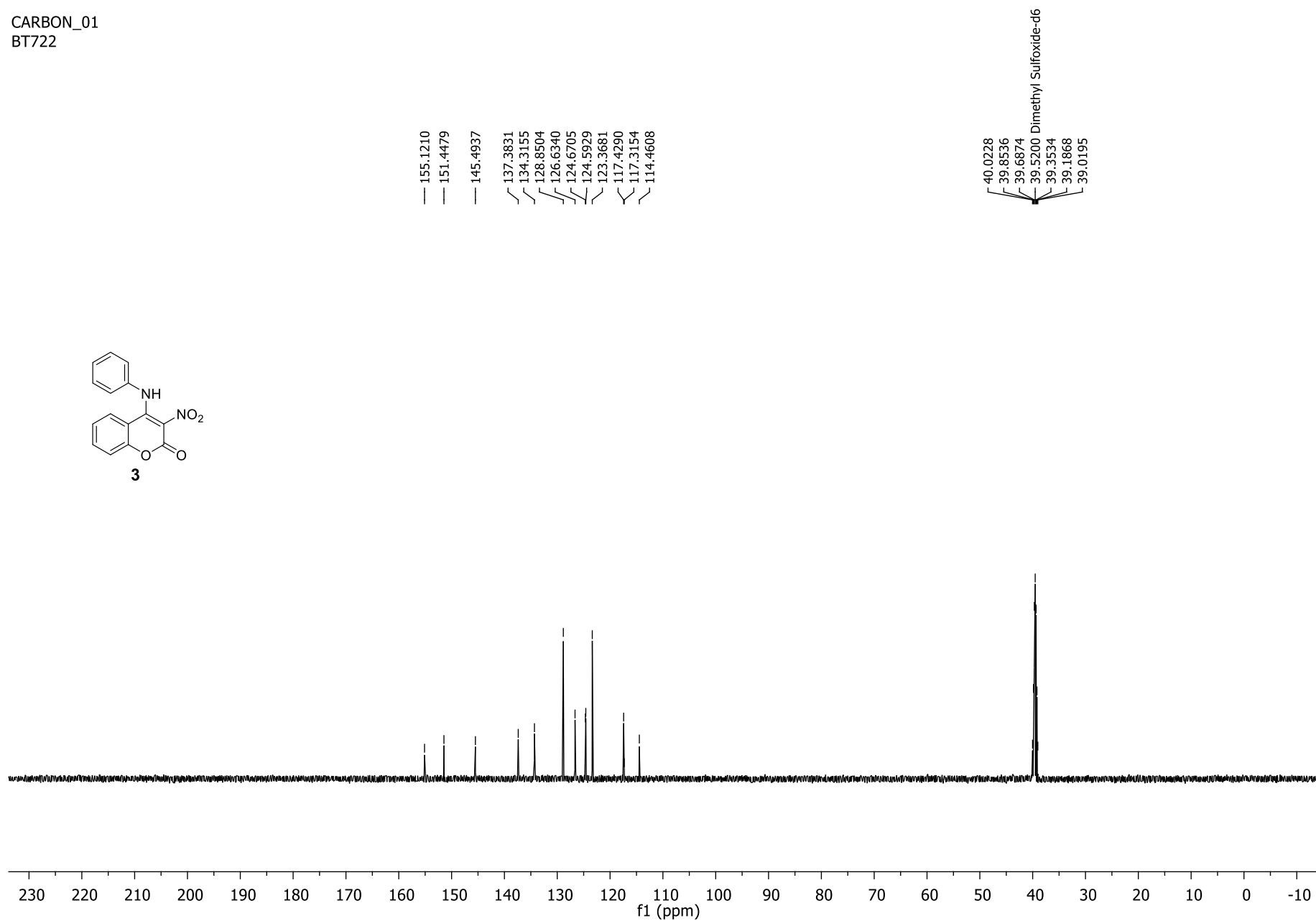
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BT722

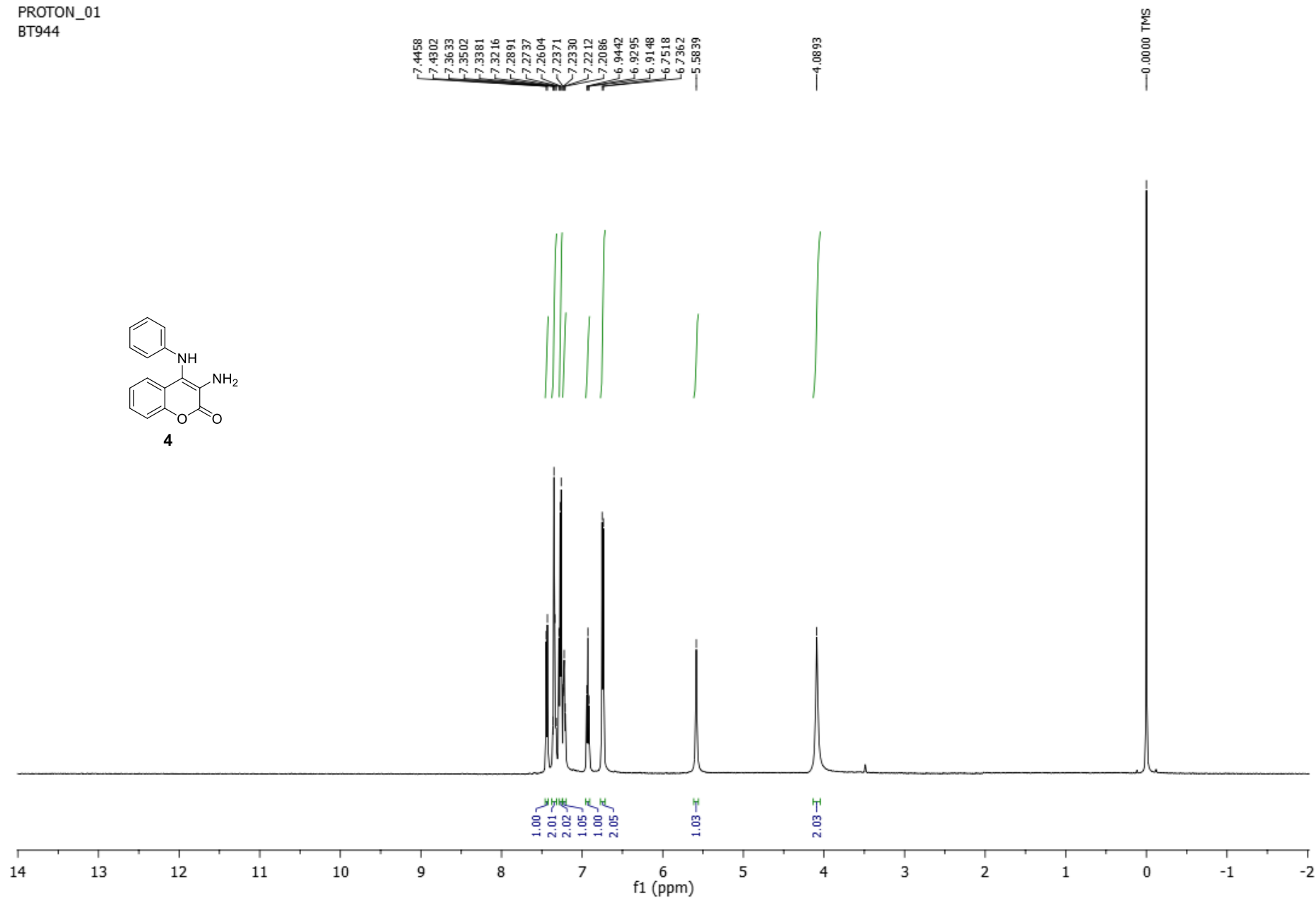
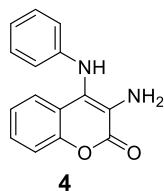
— 2.5000 Dimethyl Sulfoxide-d6



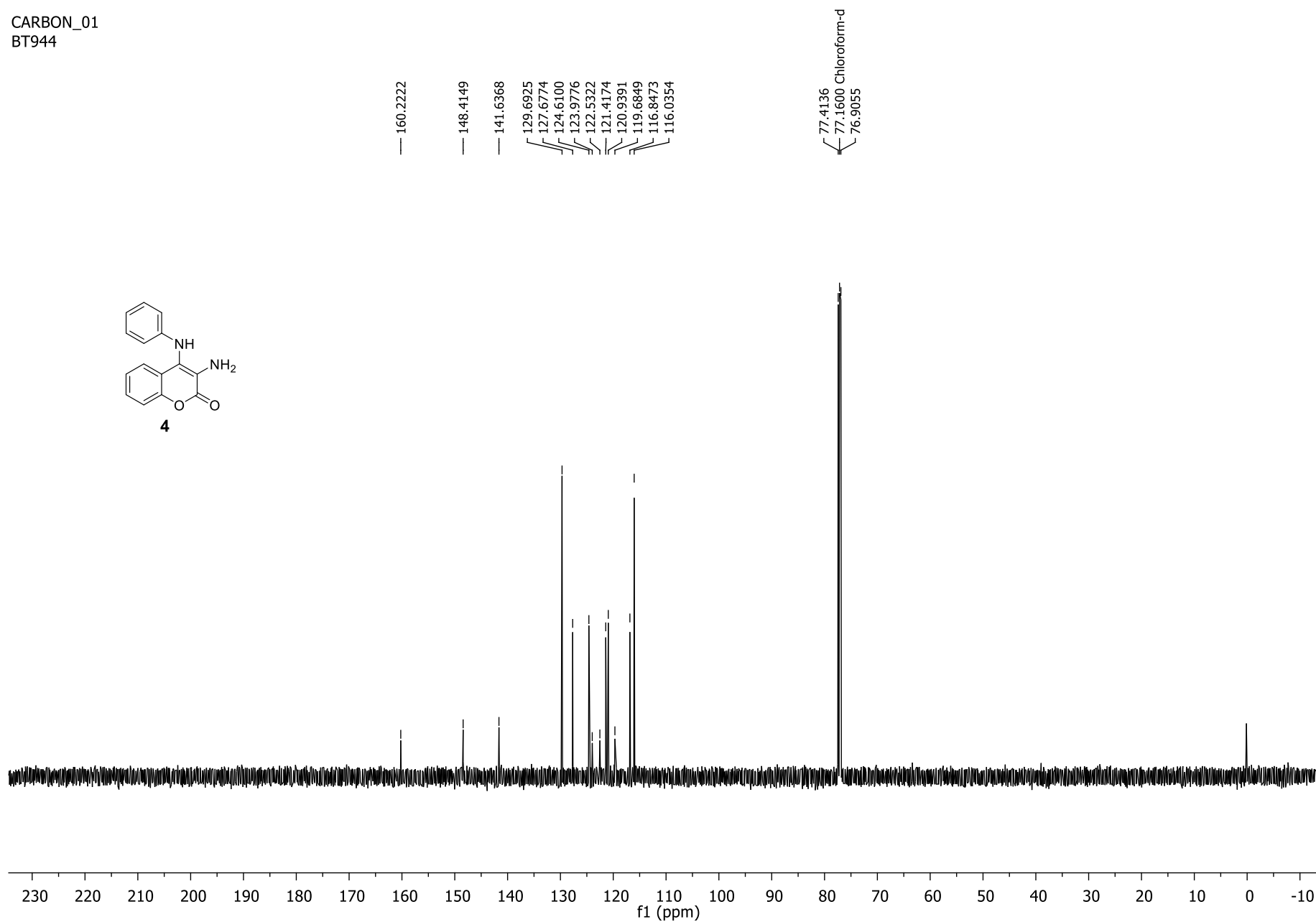
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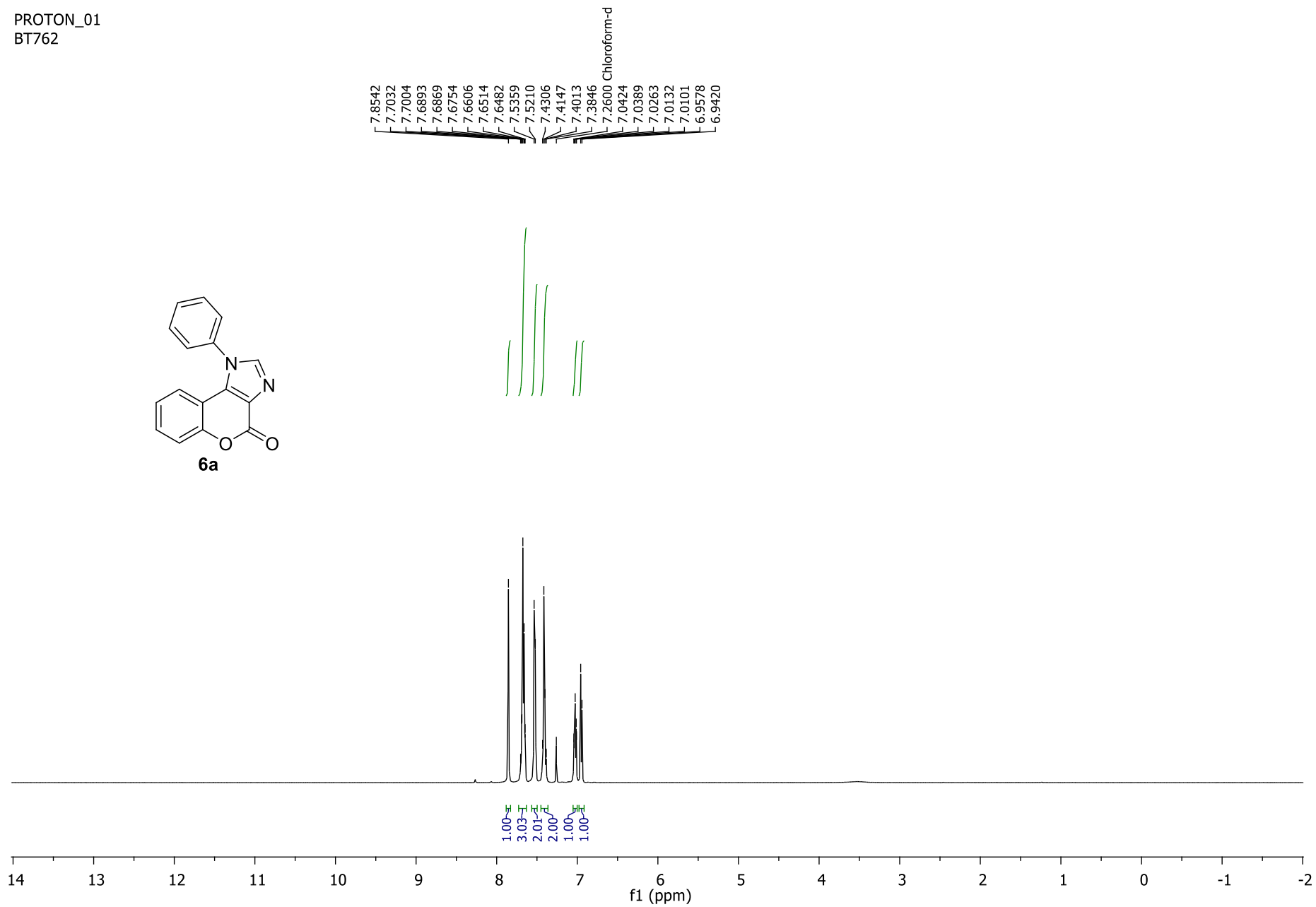
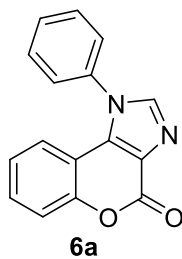


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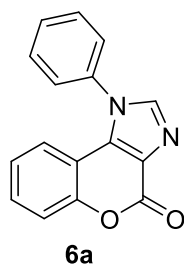
PROTON_01
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CARBON_01
BT944



1-phenylchromeno[3,4-*d*]imidazol-4(1*H*)-one (6a)PROTON_01
BT762

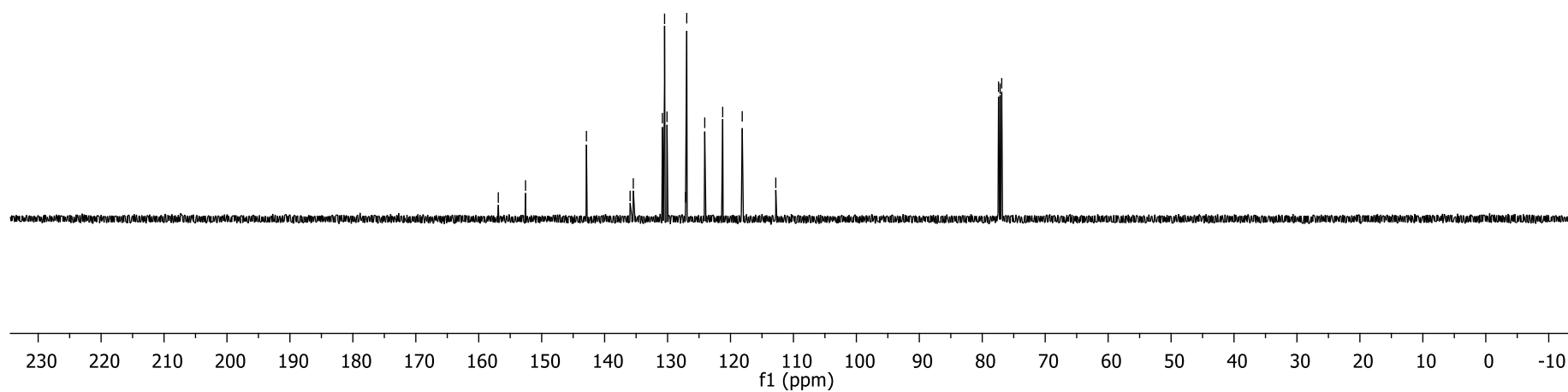
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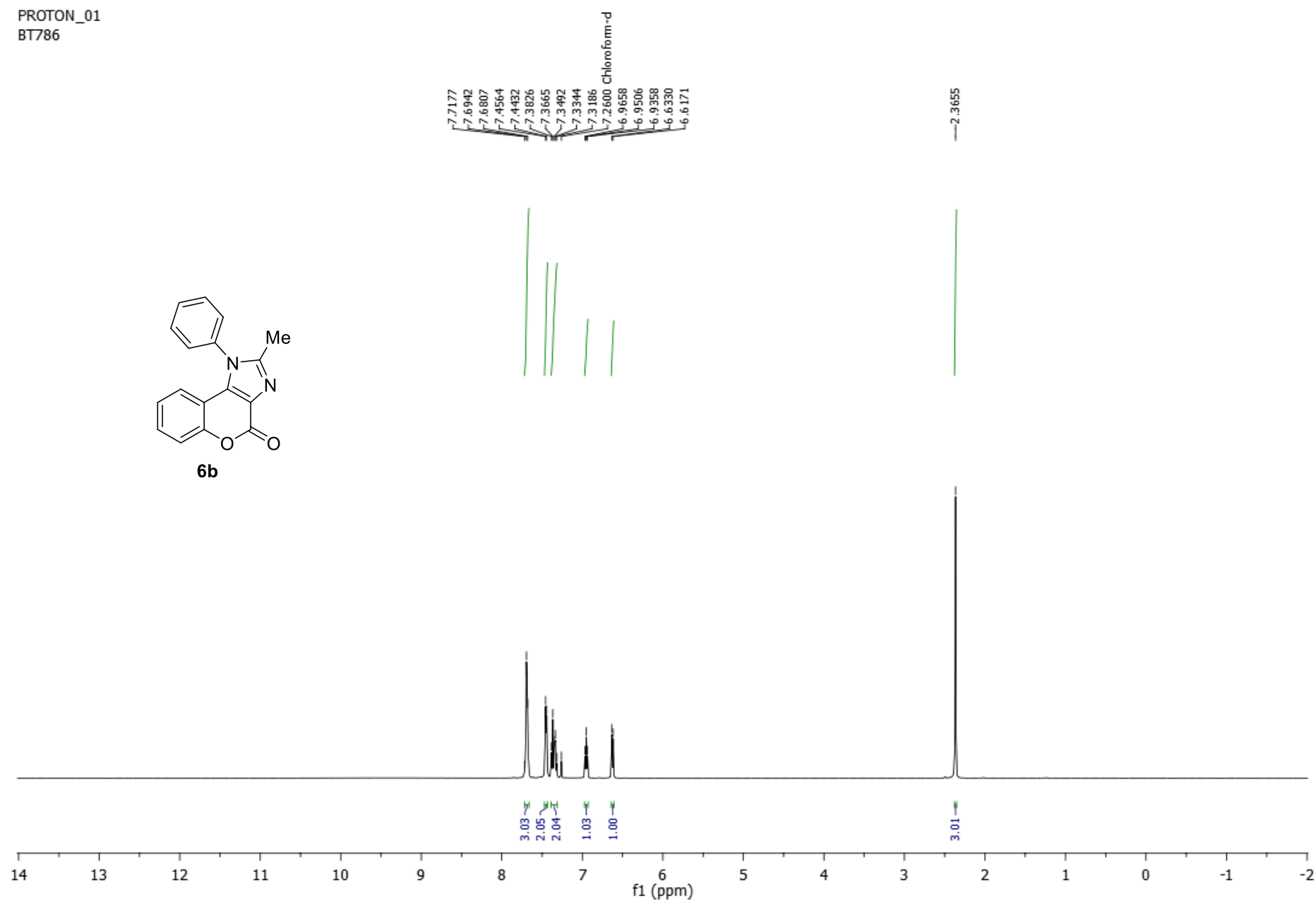


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— 152.5689

— 142.8893
/ 135.9471
/ 135.4430
/ 130.8213
/ 130.4772
/ 130.0858
/ 127.1449
/ 126.9522
/ 124.0924
/ 121.2410
/ 118.1365
/ 112.8051

/ 77.4146
/ 77.1600 Chloroform-d
/ 76.9057



2-methyl-1-phenylchromeno[3,4-*d*]imidazol-4(1*H*)-one (6b)PROTON_01
BT786

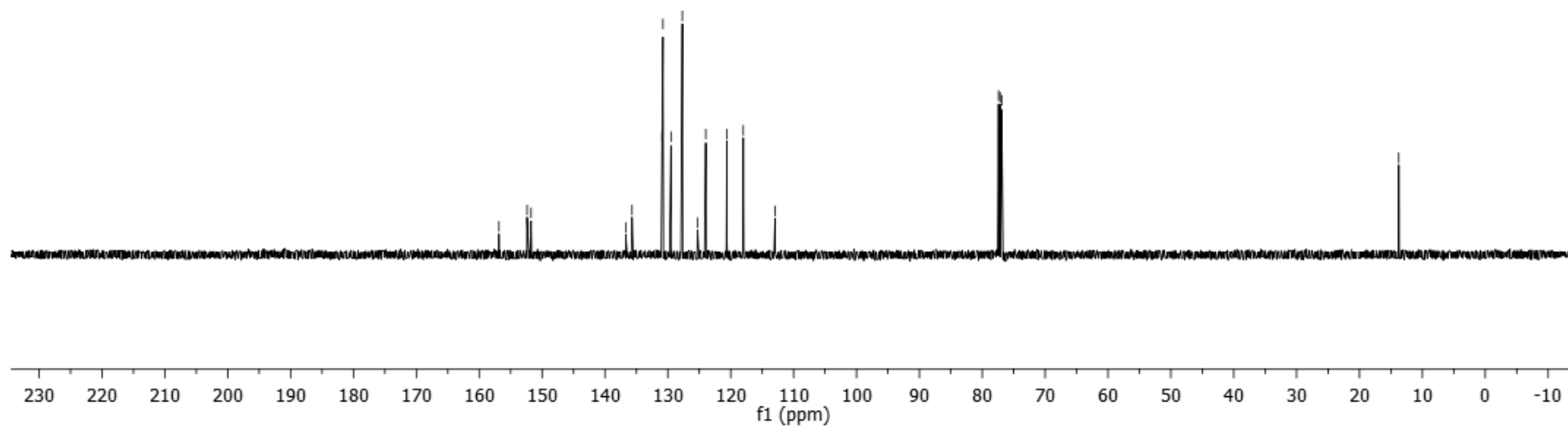
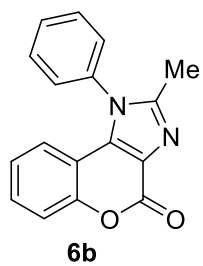
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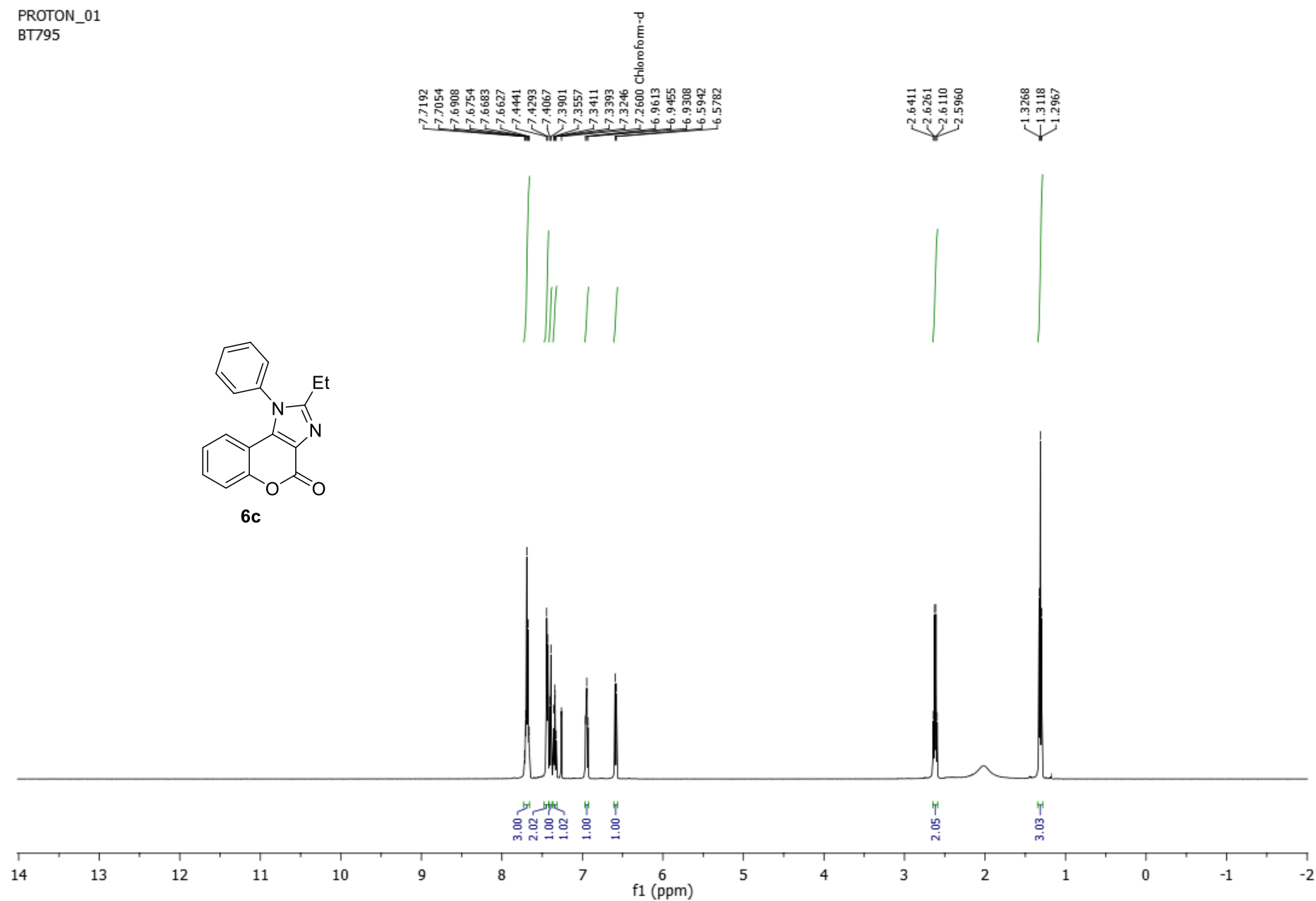
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120.6149
118.0018
112.9379

77.4147
77.1600 Chloroform-d
76.9062

13.7499



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BT795

CARBON_01
BT795

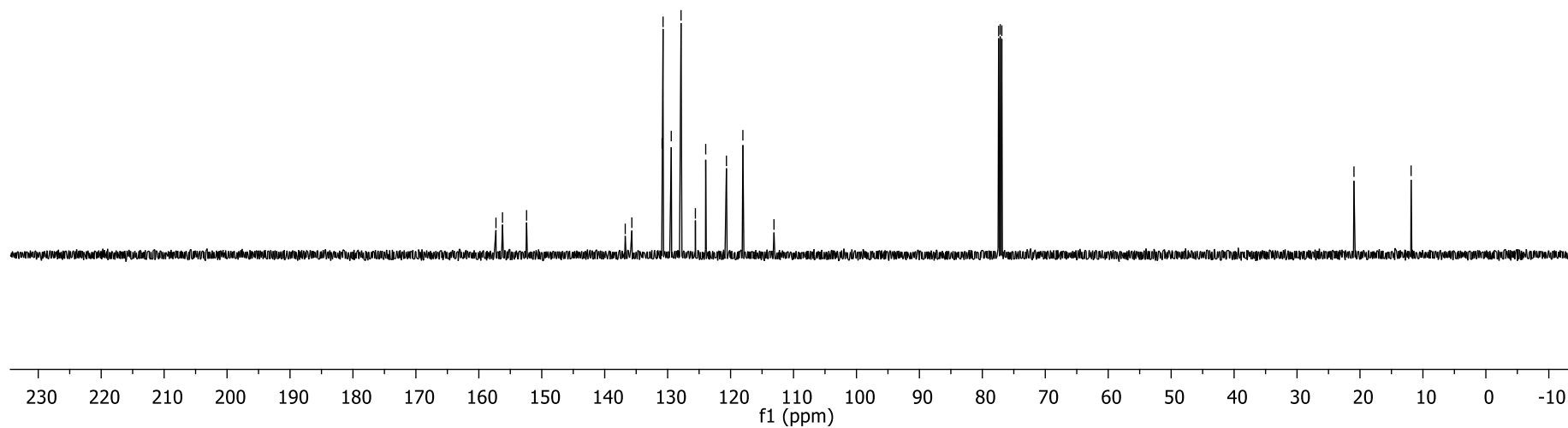
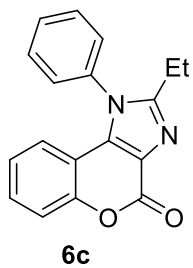
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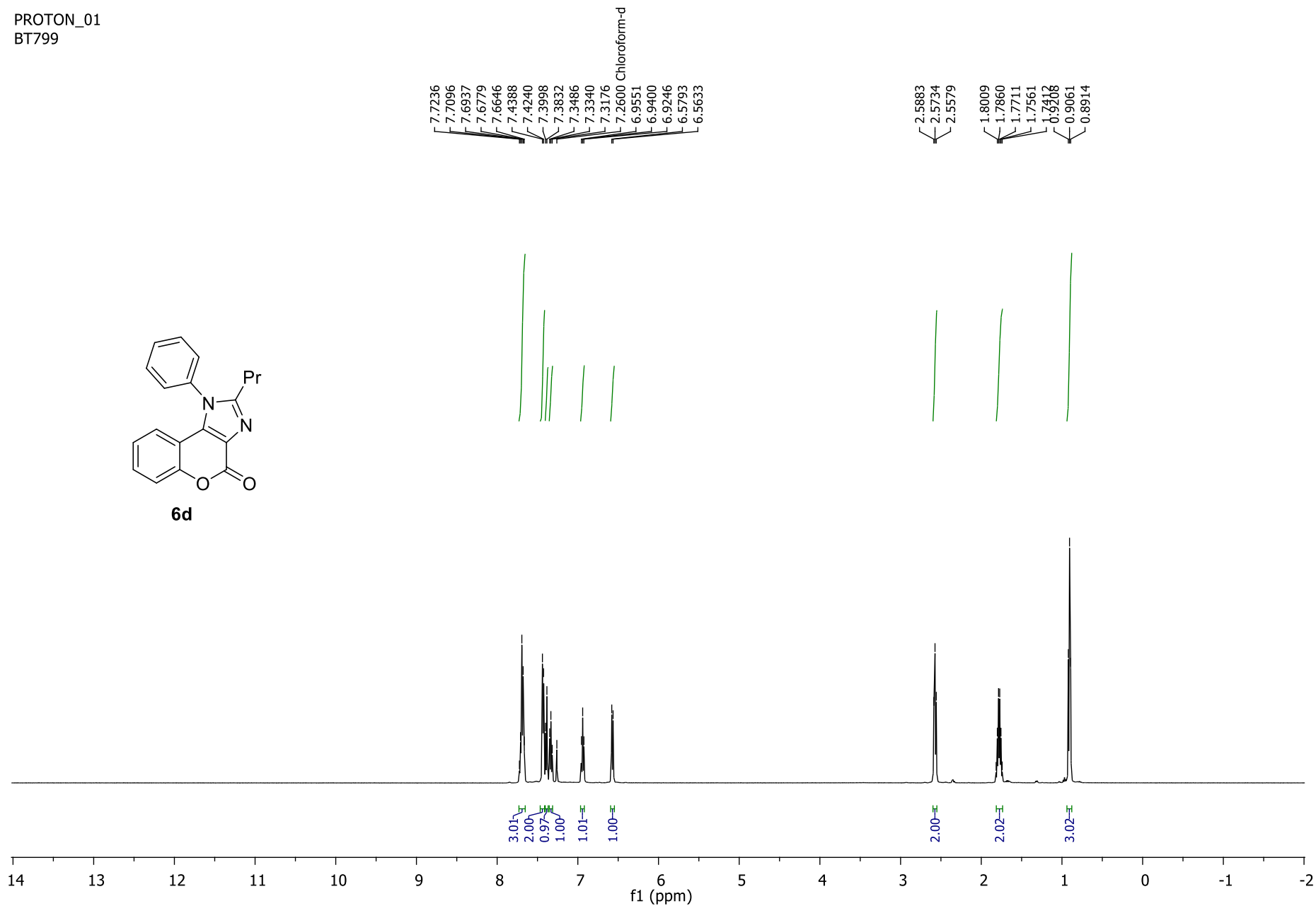
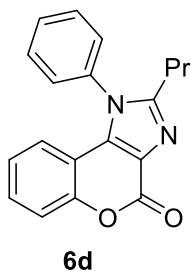
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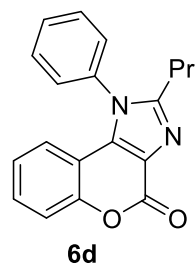
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11.8794



1-phenyl-2-propylchromeno[3,4-*d*]imidazol-4(1*H*)-one (6d)PROTON_01
BT799

CARBON_01
BT799

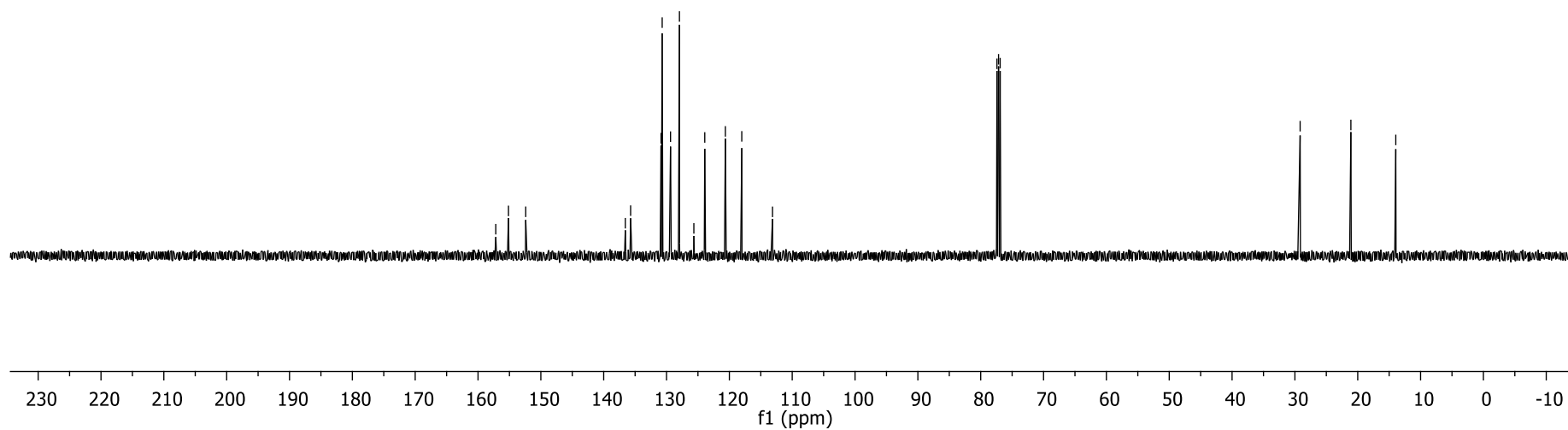


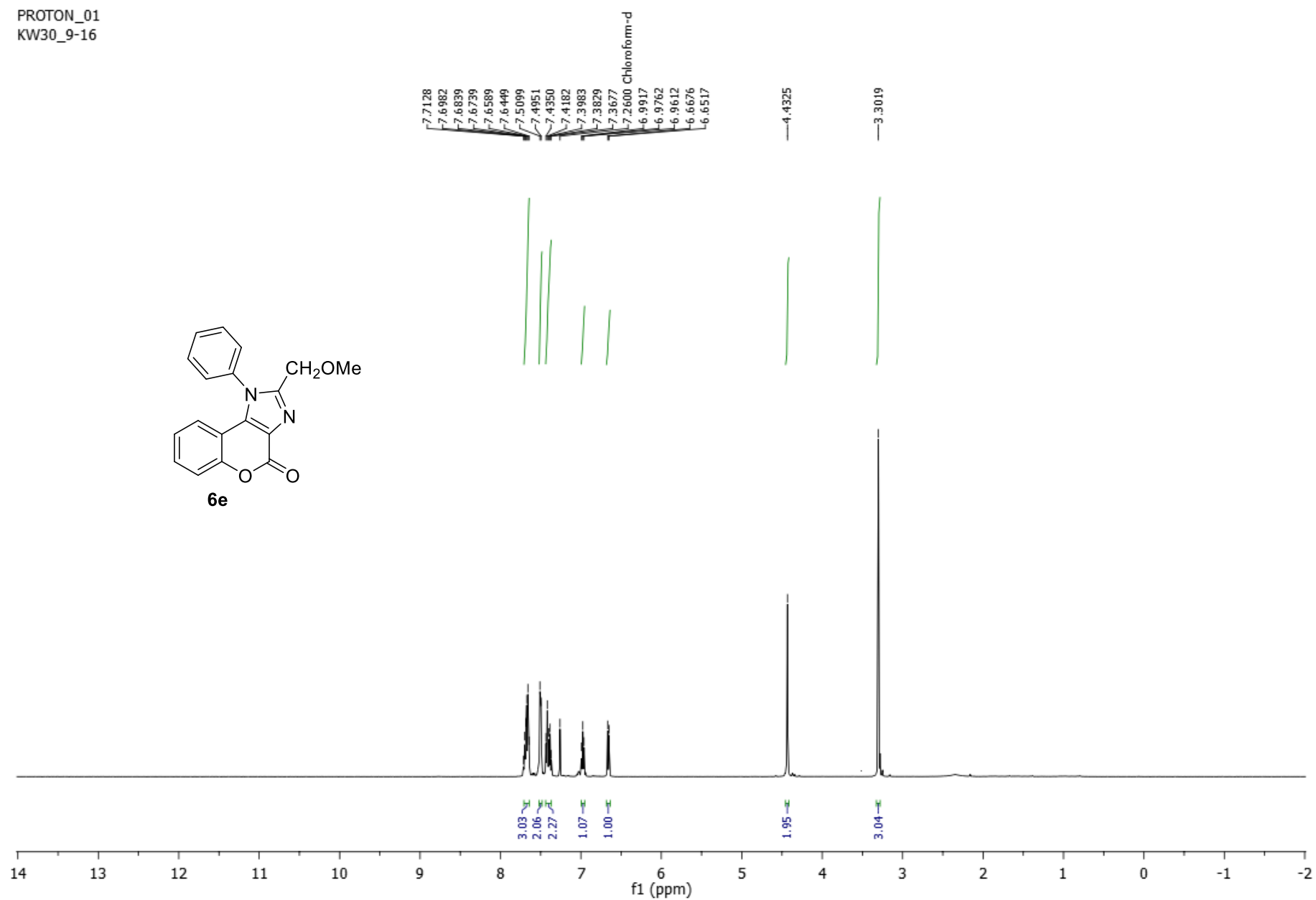
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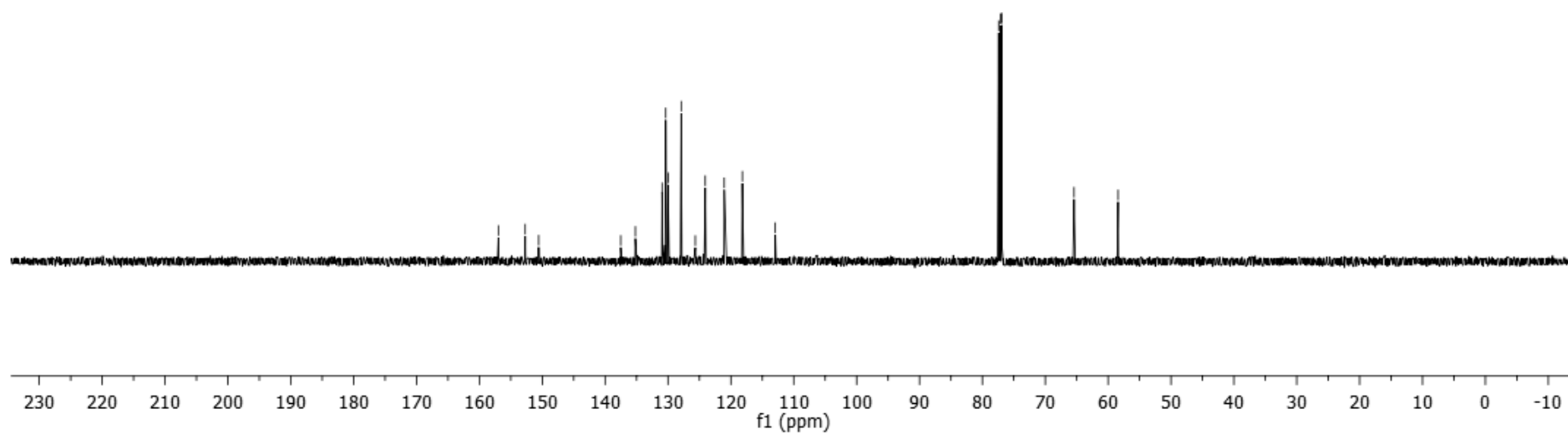
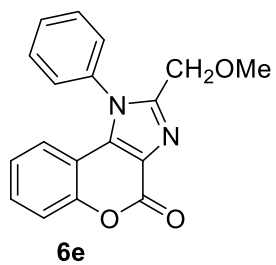
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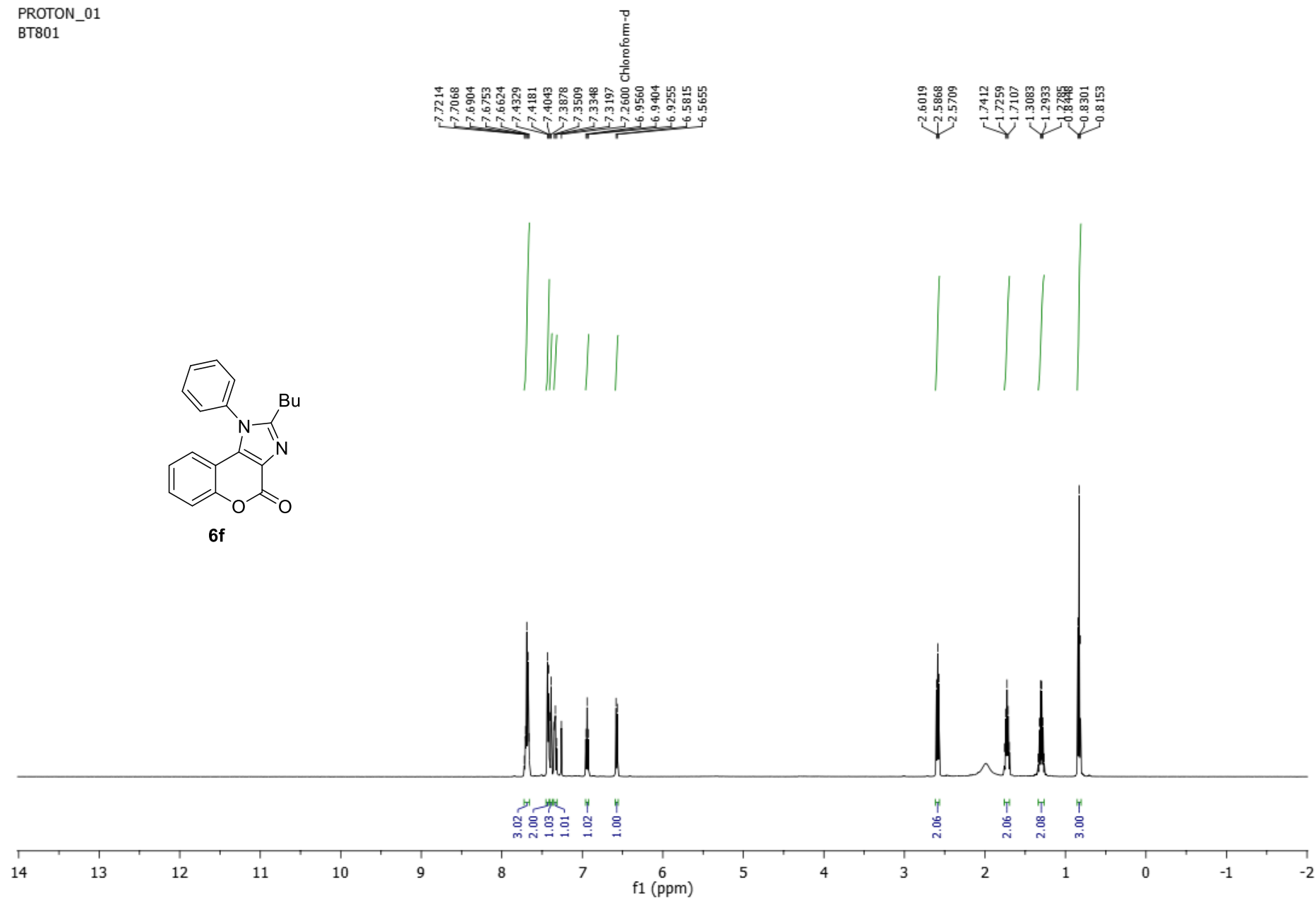
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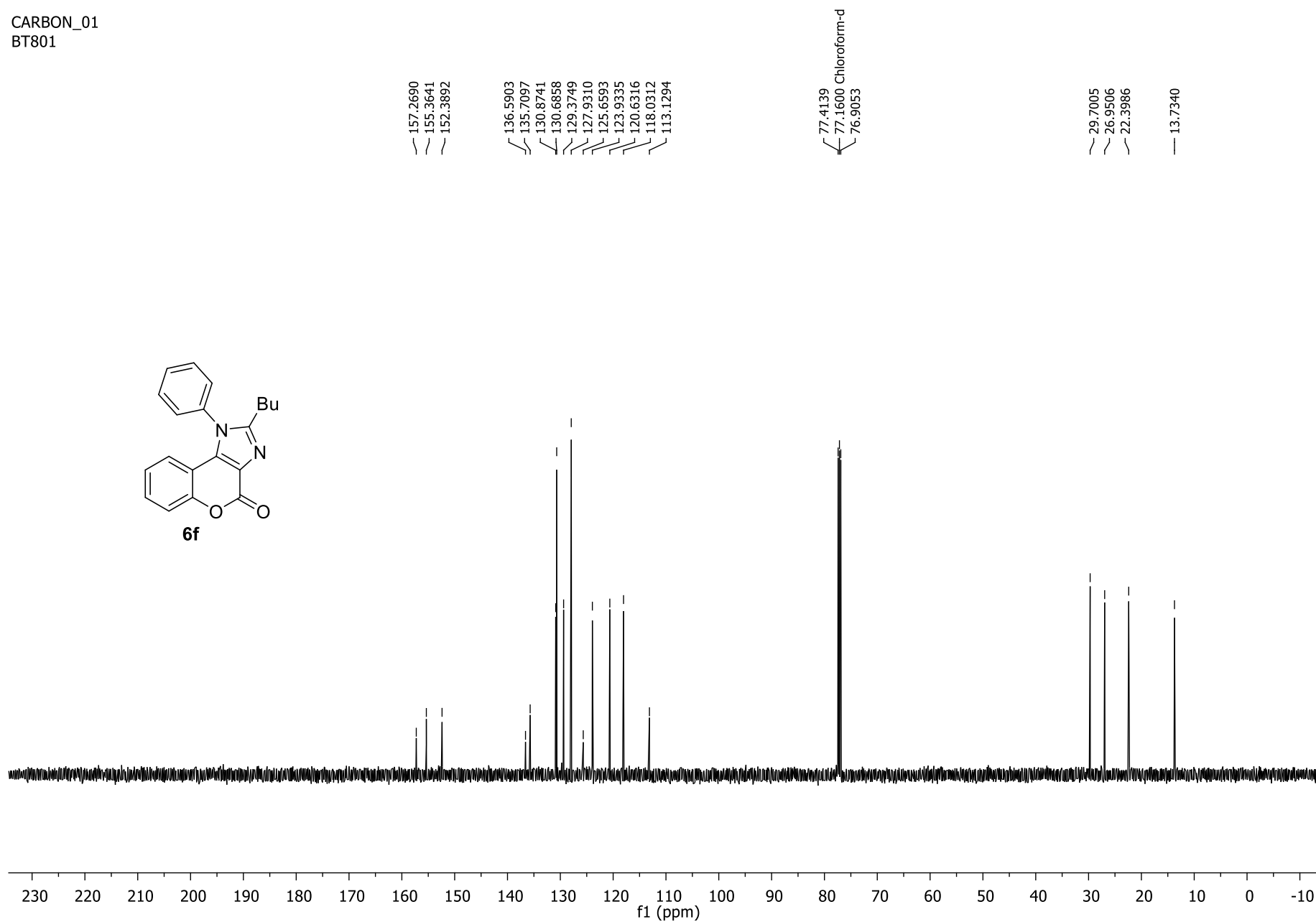


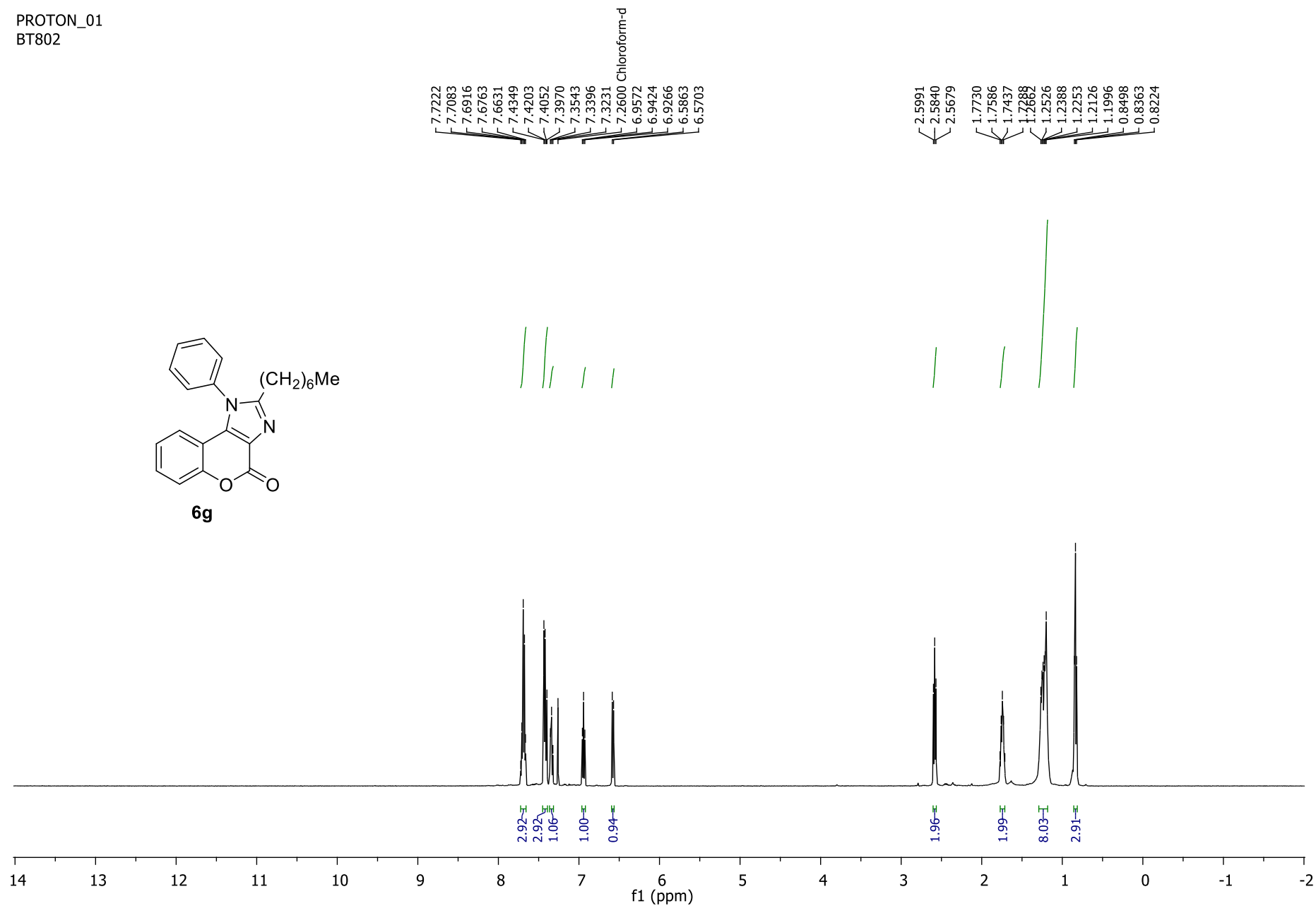
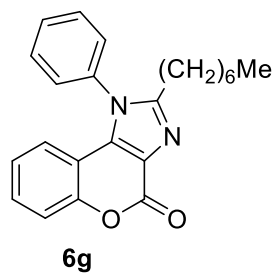
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KW30_9-16

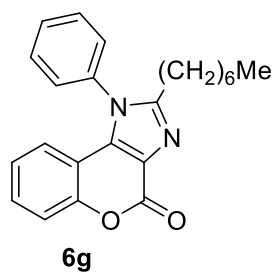
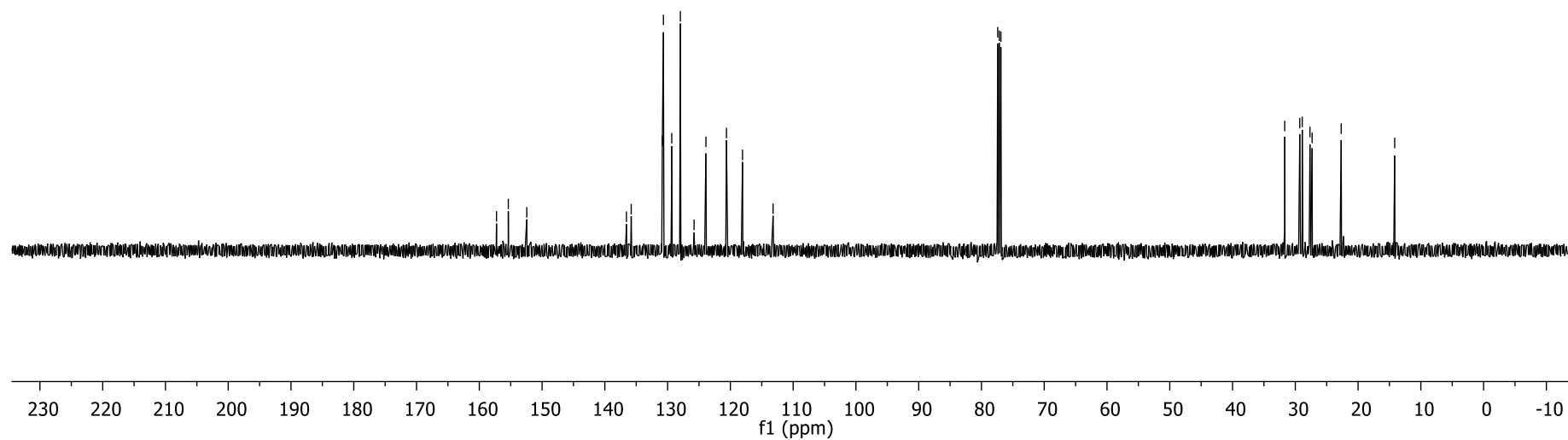
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KW30_9-16

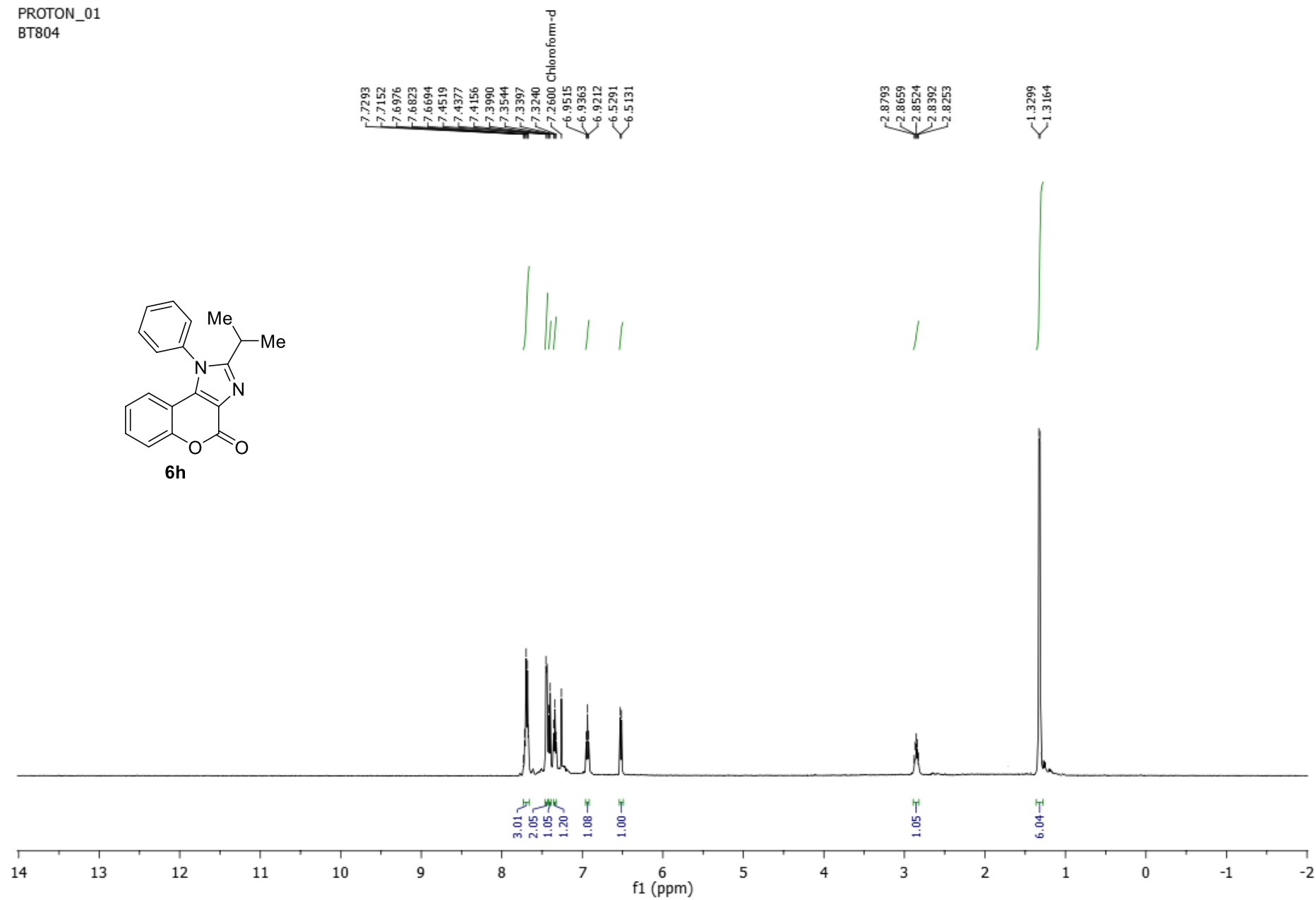


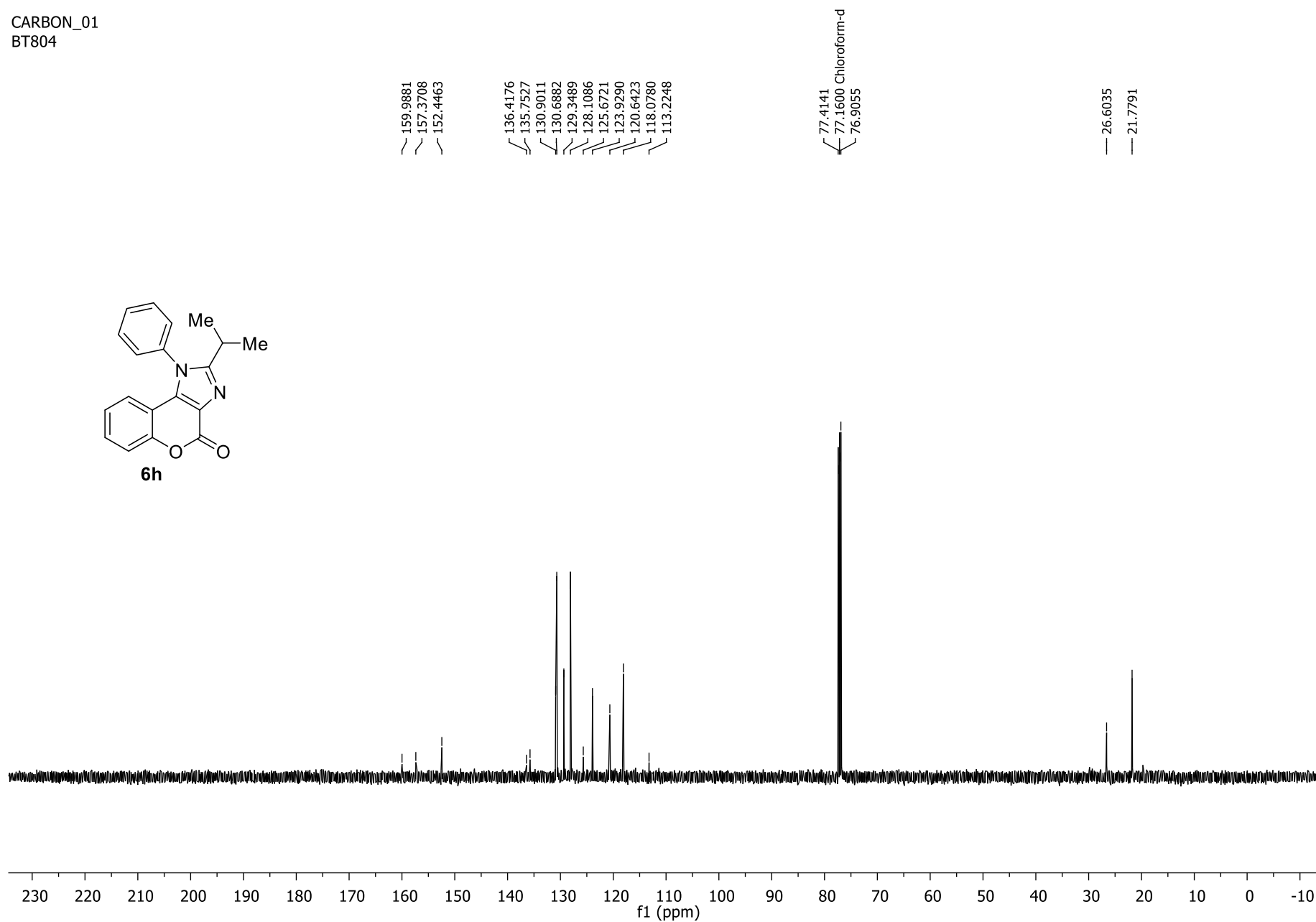
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BT801

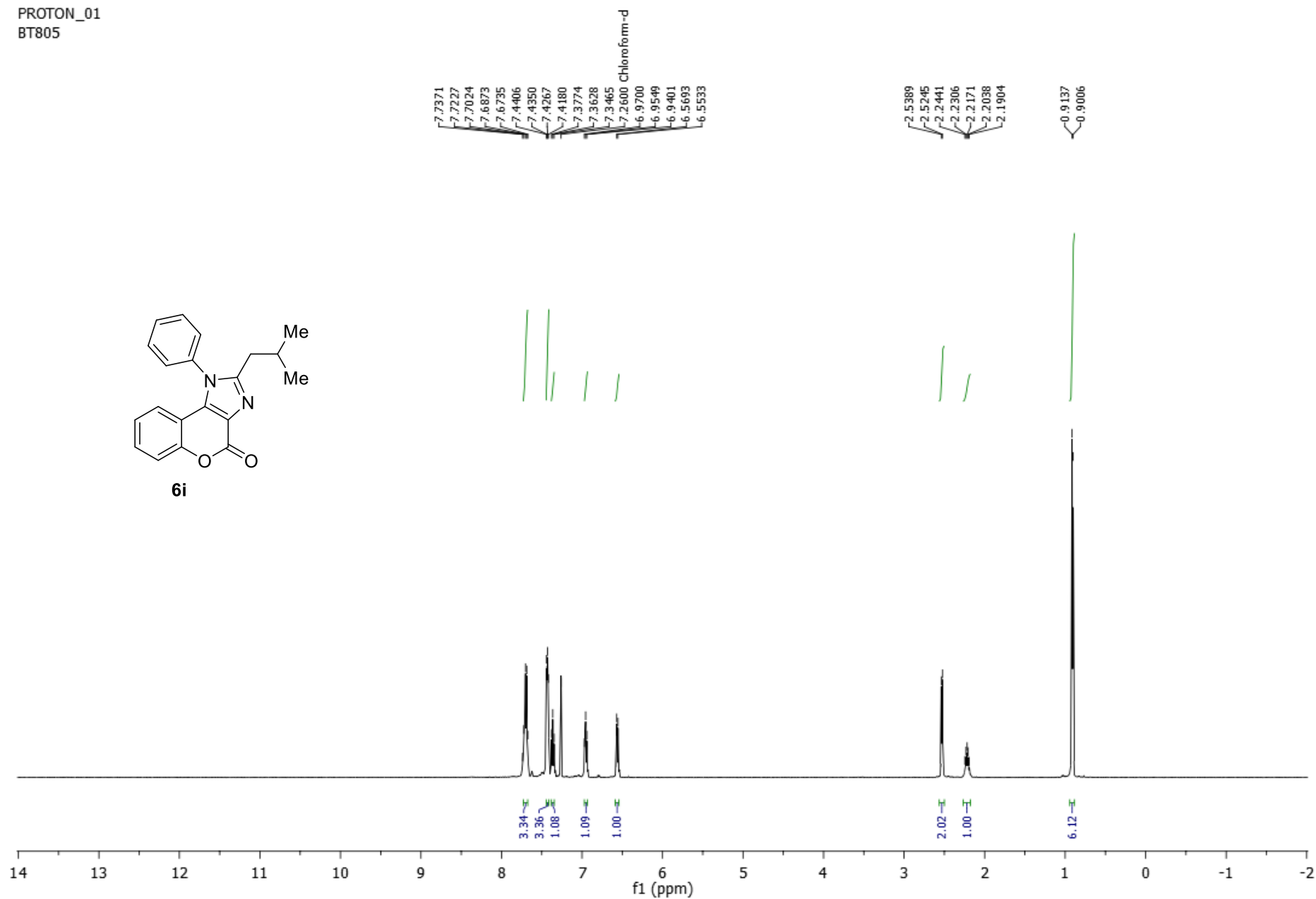
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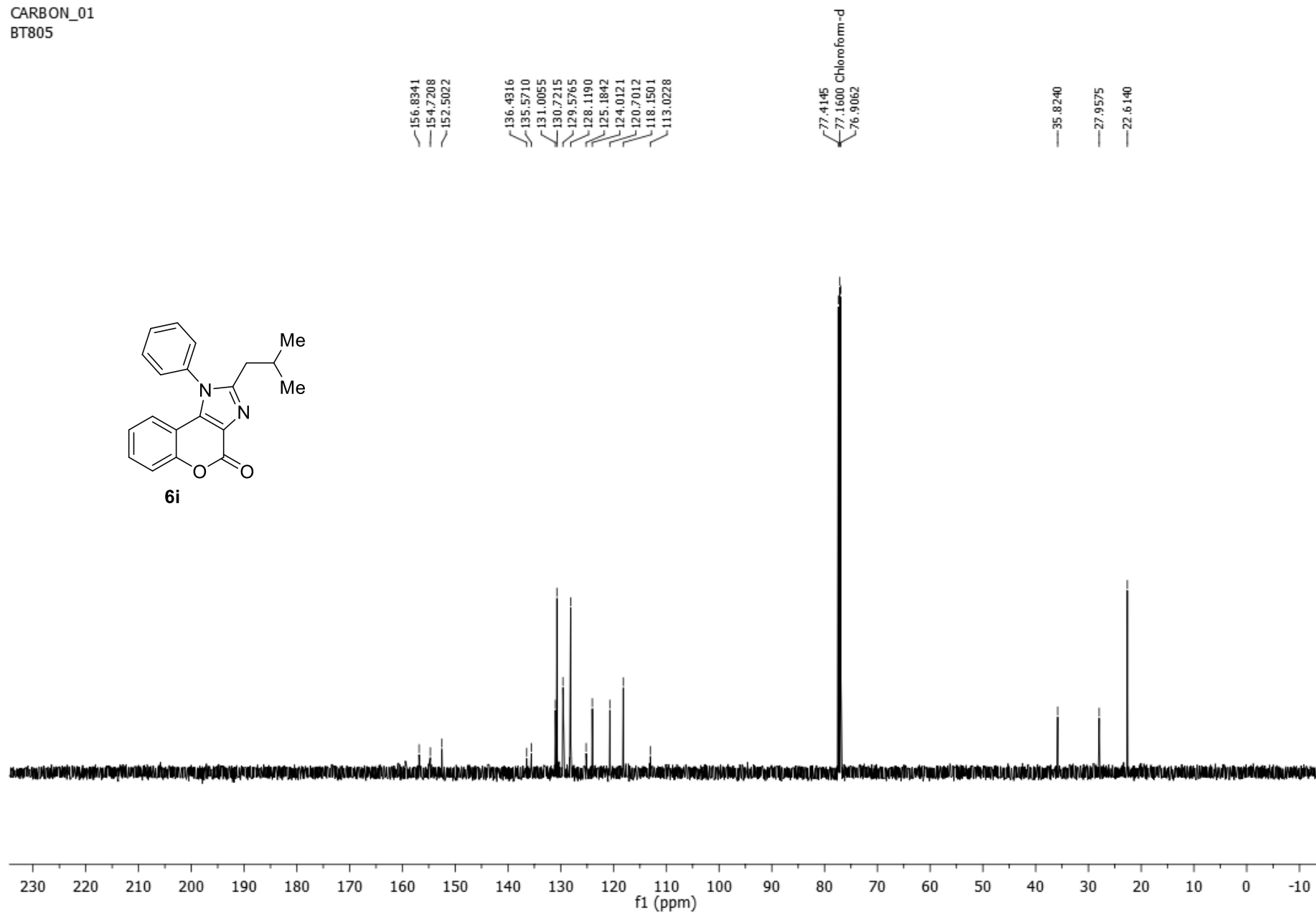
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BT802

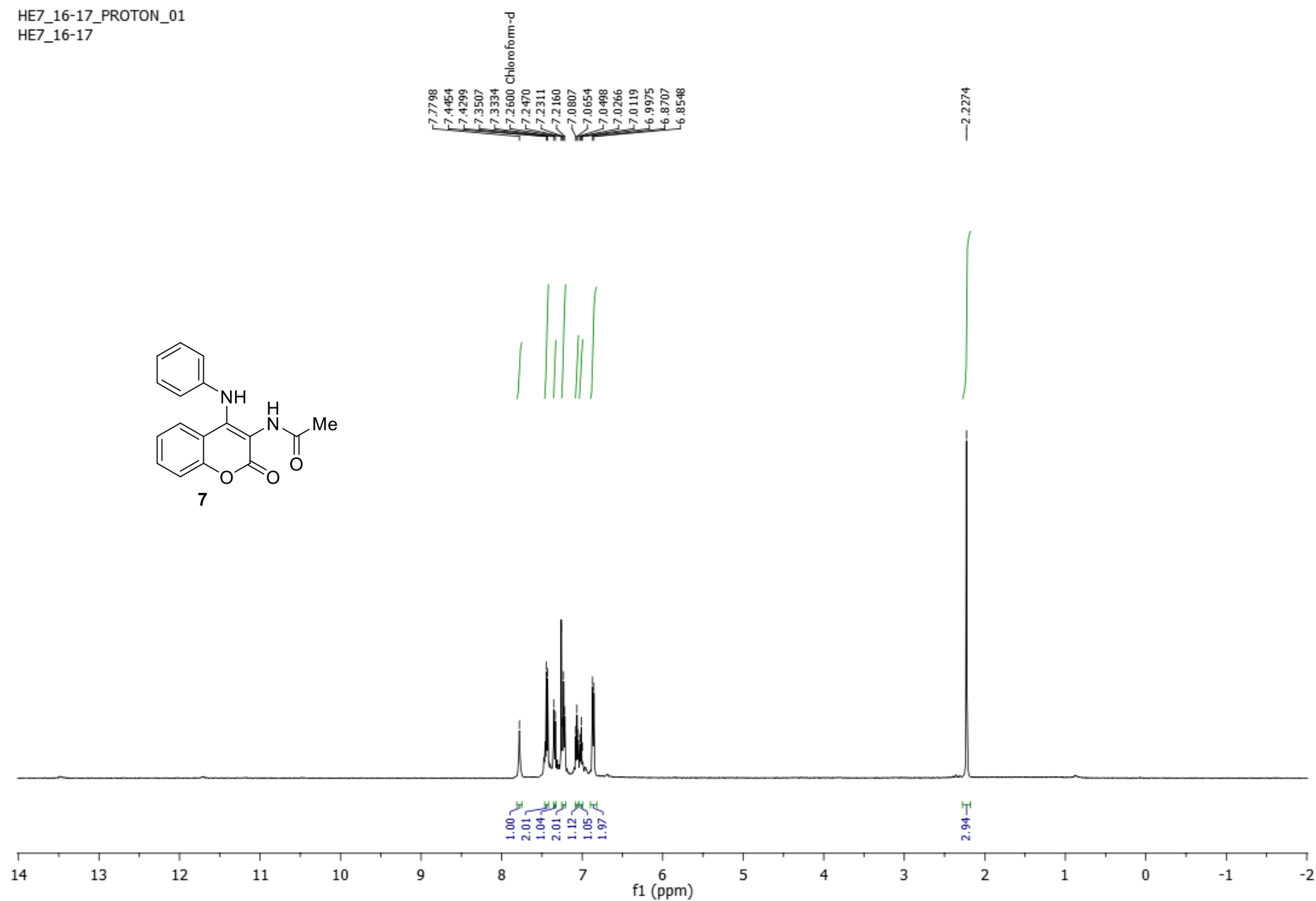
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77.1600 Chloroform-d
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2-isopropyl-1-phenylchromeno[3,4-*d*]imidazol-4(1*H*)-one (6h)PROTON_01
BT804

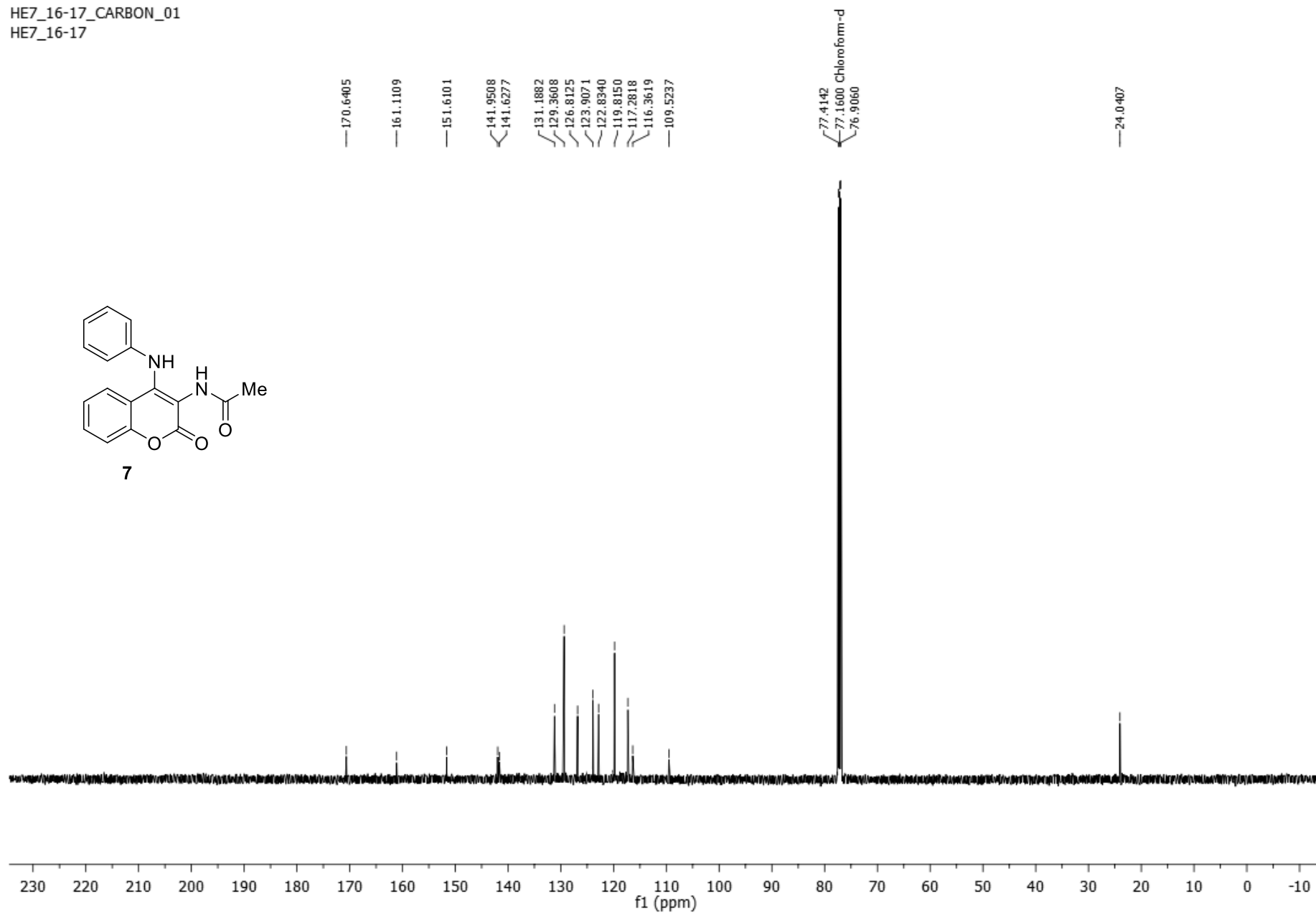
CARBON_01
BT804

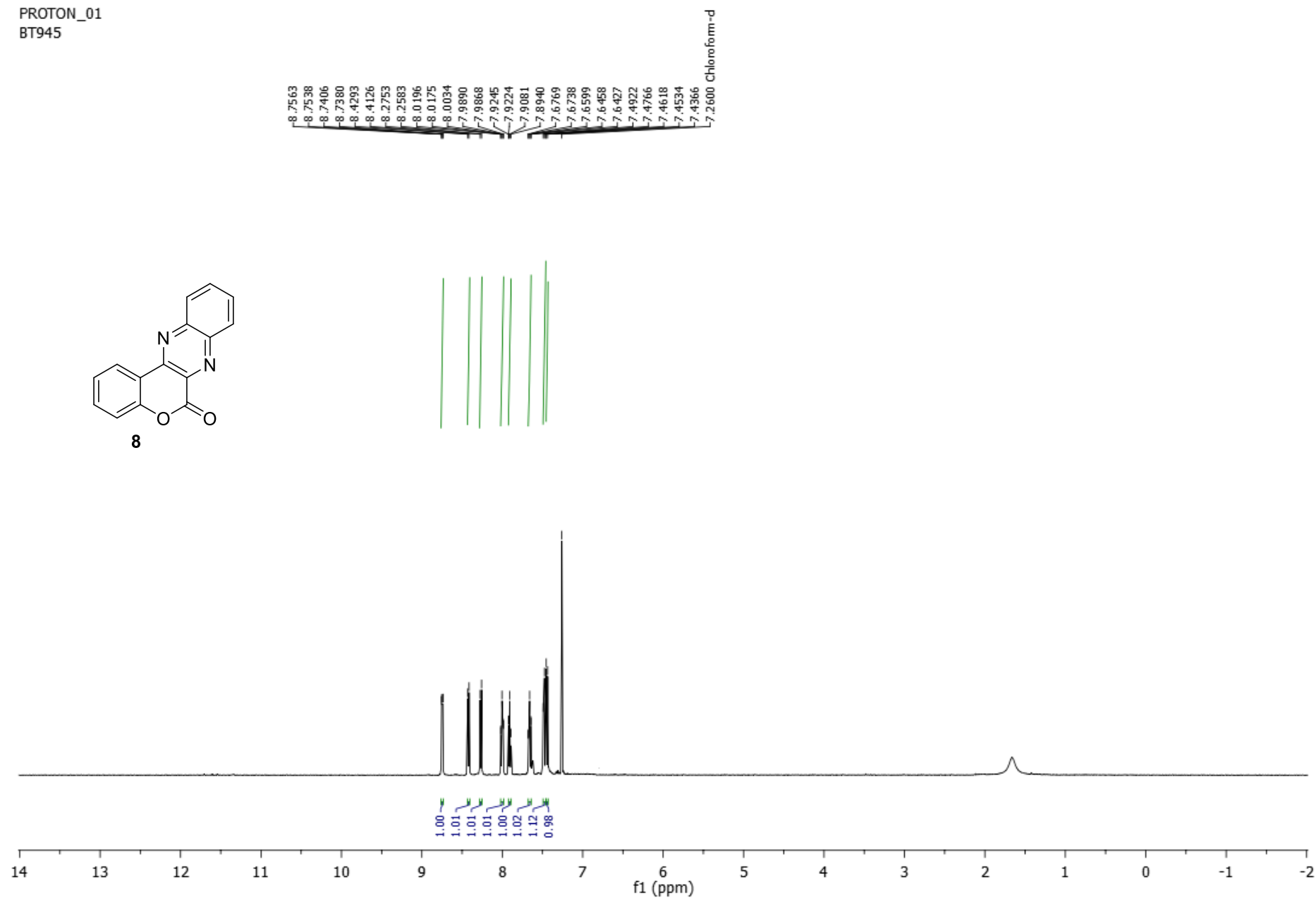
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BT805

CARBON_01
BT805

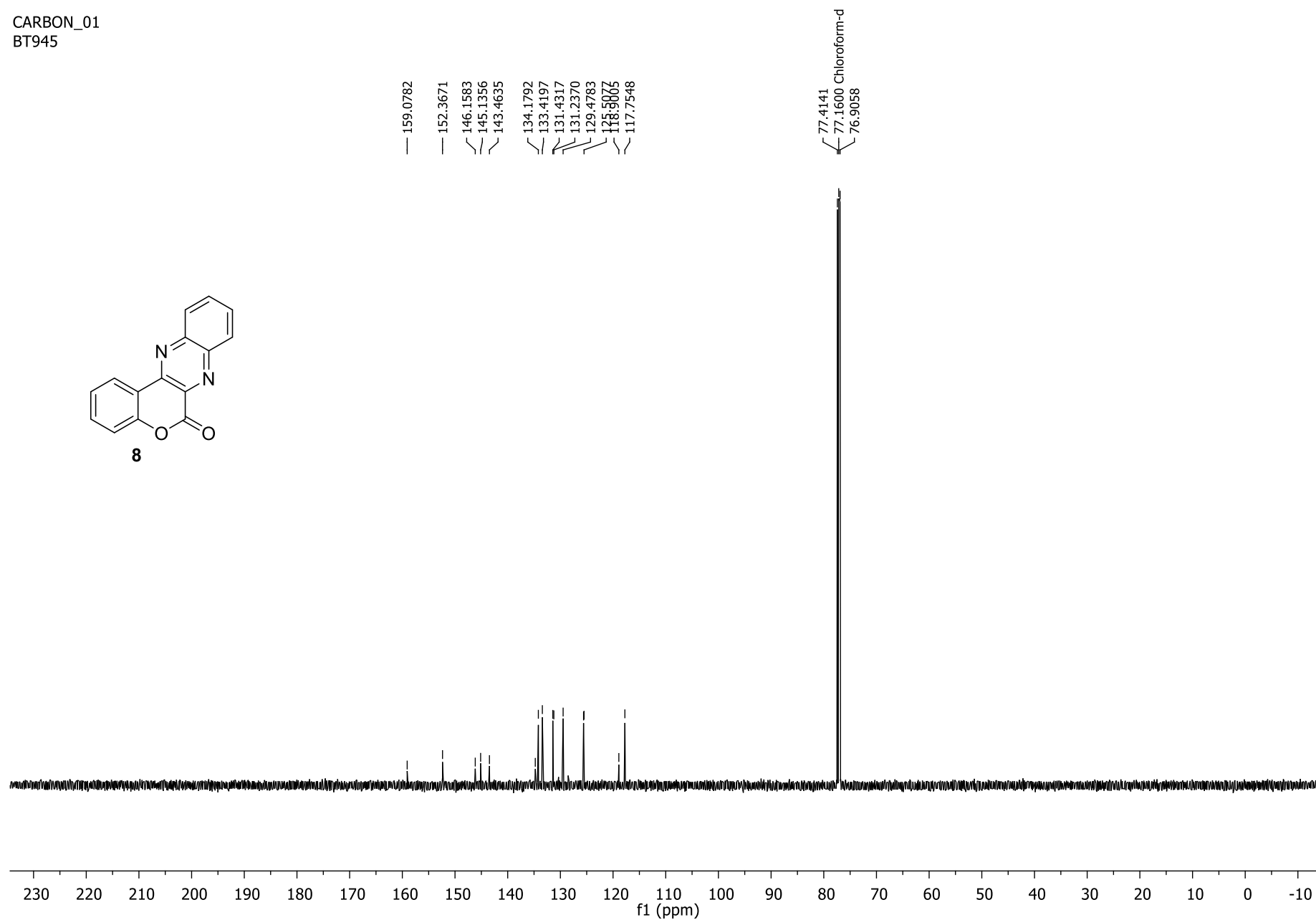
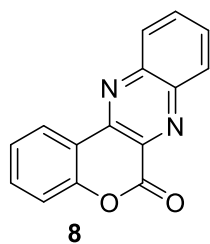
***N*-(2-oxo-4-(phenylamino)-2*H*-chromen-3-yl)acetamide (7)**HE7_16-17_PROTON_01
HE7_16-17

HE7_16-17_CARBON_01
HE7_16-17

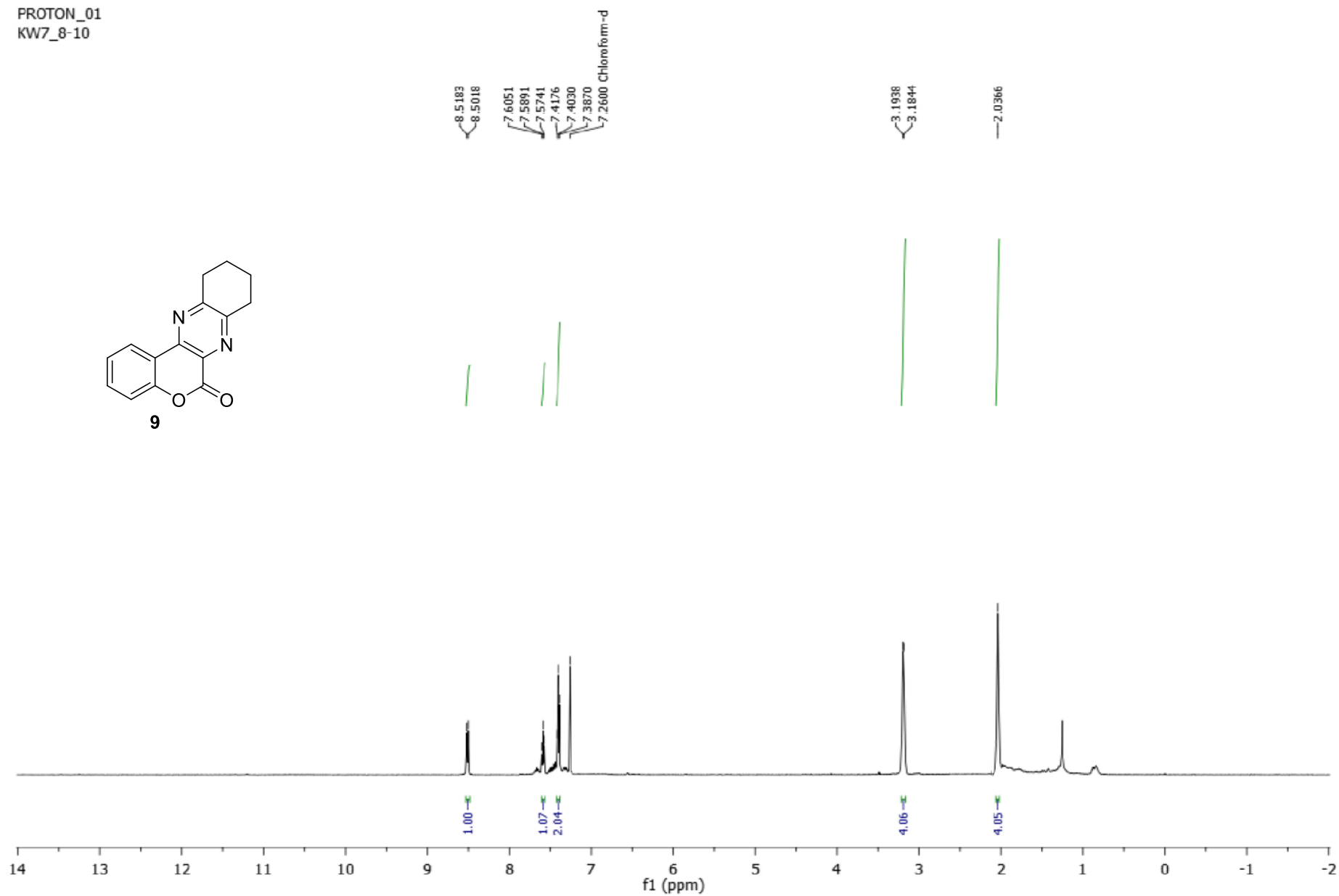
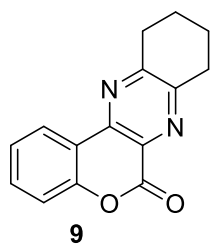


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BT945

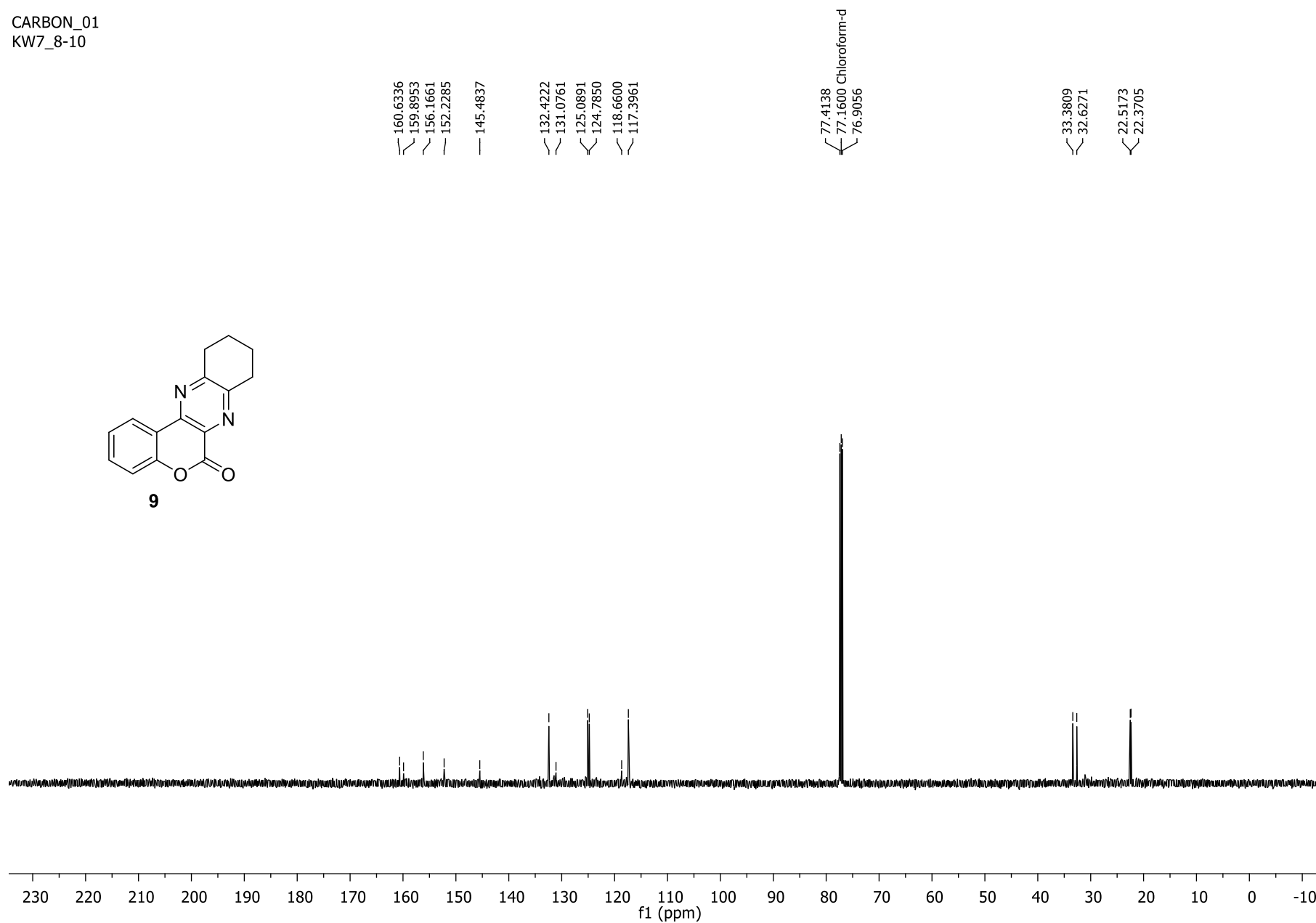
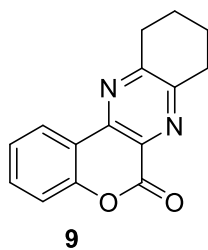
CARBON_01
BT945



8,9,10,11-tetrahydro-6H-chromeno[3,4-b]quinoxalin-6-one (9)

PROTON_01
KW7_8-10

CARBON_01
KW7_8-10



Visualization of the protein (PDB code: 3PZW) was performed using UCSF Chimera.¹ Water molecules were removed, missing residues were added with Modeller,² hydrogen atoms and AMBER99SB-ILDN charges were added and the charge on iron was set to +2.0, with no restraint applied to the iron atom and the ligands. Ligand 3D coordinates were generated and minimised with OpenBabel³ using the MMFF94 force field.⁴ ACPYPE (AnteChamber PYthon Parser interface)⁵ was used to generate ligand topologies and parameters using Antechamber.⁶ Energy minimizations were carried out using the AMBER99SB-ILDN force field⁷ with GROMACS 4.6.5 as the molecular dynamics simulation toolkit.⁸ Docking was performed with AutoDock Vina (1.1.2)⁹ using a grid box of size 25 Å in X, Y, Z dimensions, centred on iron atom. UCSF-Chimera was used to generate docking input files and to analyze docking results. Docking was carried out with an exhaustiveness value of 10 and a maximum output of 20 docking modes.

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