Electronic Supporting Information:

Studies on acedan-based mononuclear zinc complexes toward selective fluorescent probes for pyrophosphate

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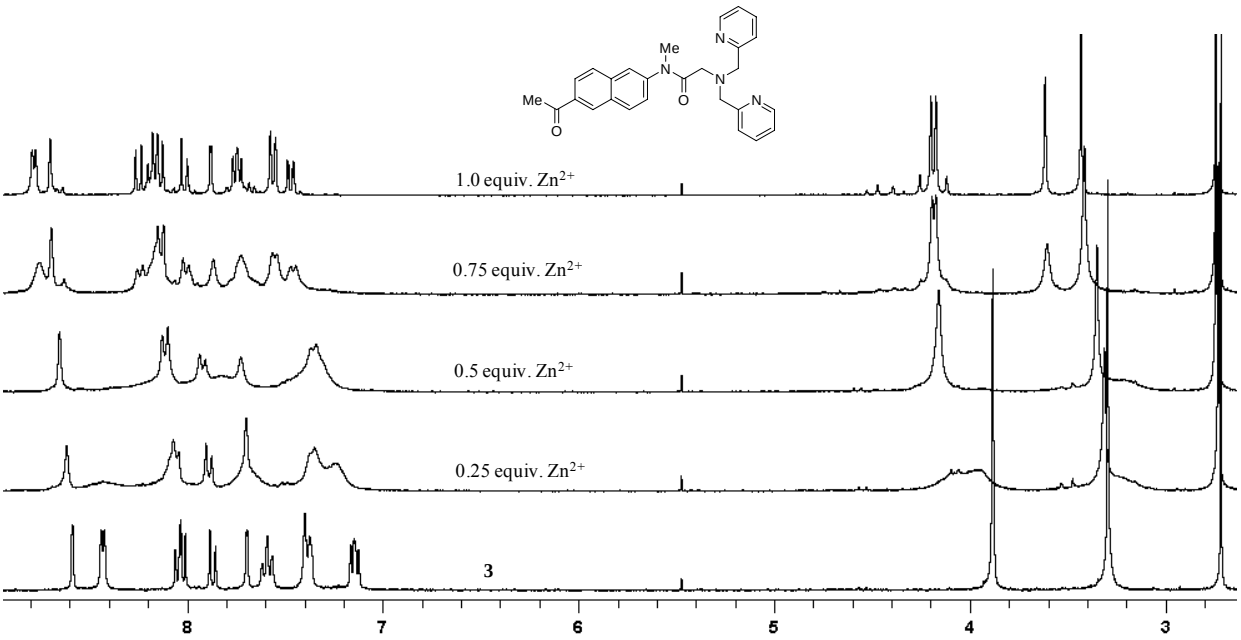


Fig. S1 ^{1}H NMR (300 MHz) spectral change of **3** (10 mM) upon addition of Zn^{2+} (4 × 2.5 mM) in CD_3CN.

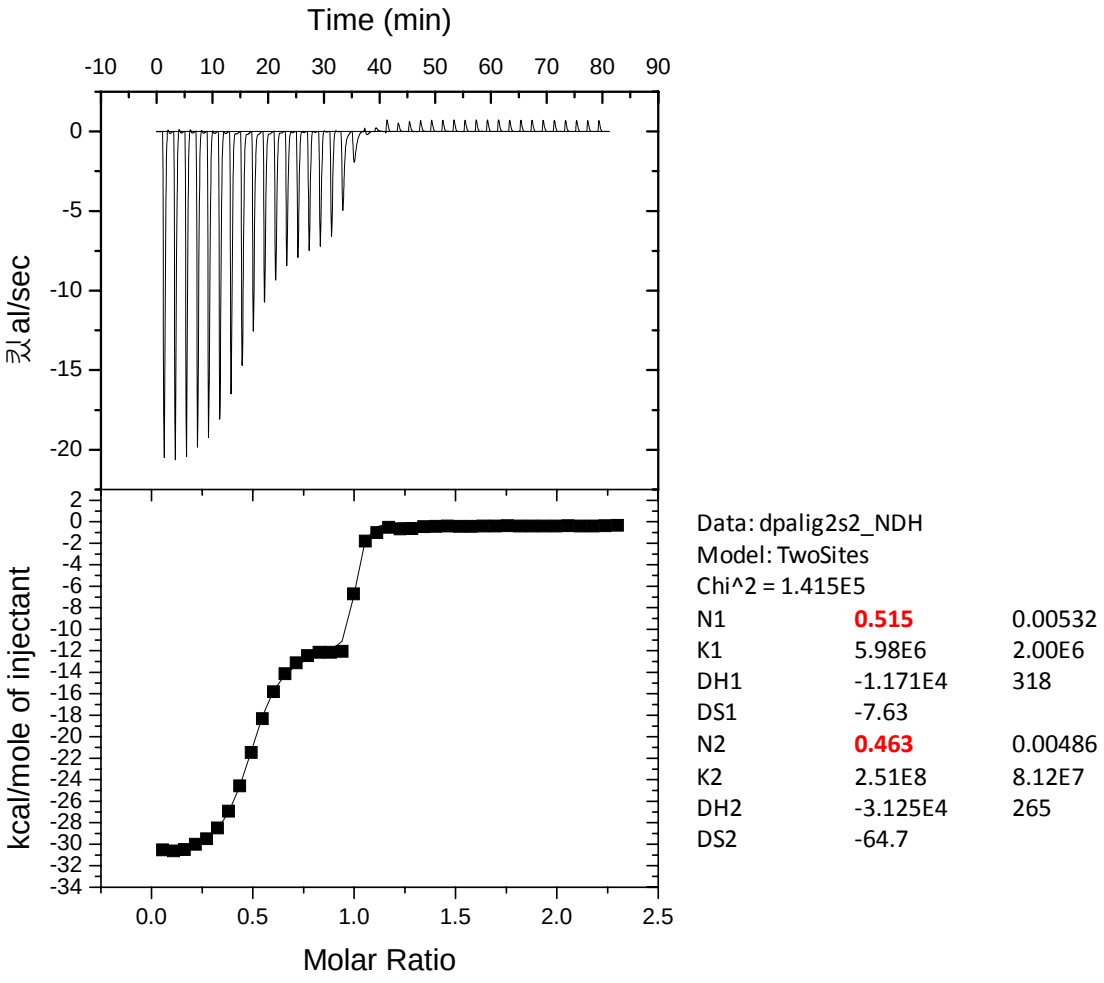


Fig. S2 Isothermal Titration Calorimetry (ITC) data: (a) **3** (0.2 mM) with $Zn(ClO_4)_2$ (3.0 mM); measured in CH_3CN at 30 °C.

Procedure: To a solution of **3** in the calorimeter cell, 5.0 µL of zinc perchlorate was injected 40 times at 30 °C. The dilution effects were corrected by carrying out a separate blank titration. The titration data was analyzed by the built-in curve-fitting Origin software: the "two sets of sites" model was used, which applies to a receptor system that has non-identical and independent sites for binding (support@microcalorimetry.com).

Conditions:

Cell: **3** (0.2 mM) in acetonitrile

Syringe: zinc perchlorate hexahydrate solution (3.0 mM) in acetonitrile

Reference power: 26

Temperature: 30 °C

Stirring rate: 220 rpm.

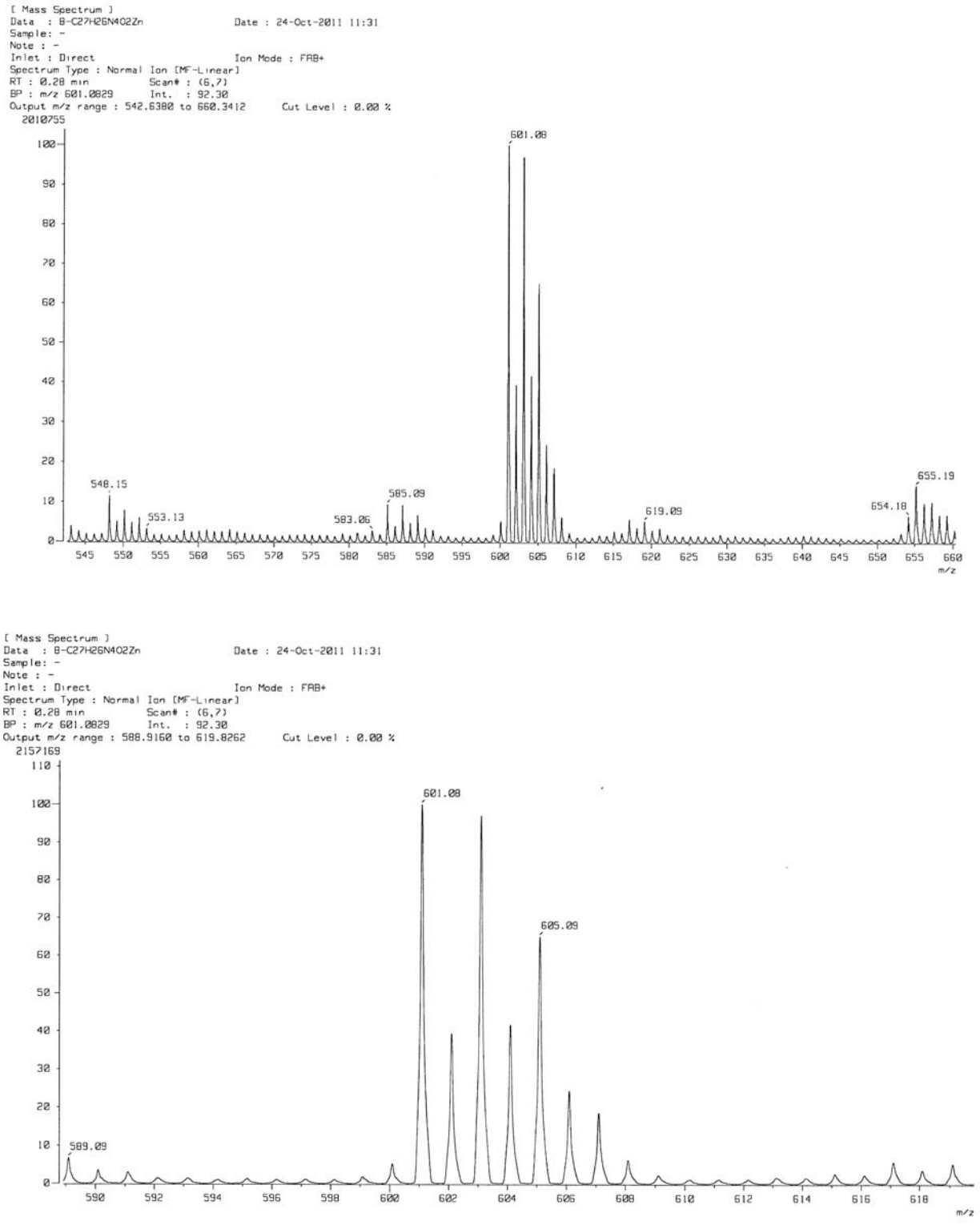


Fig. S3 HRMS (FAB+) of **3**-Zn(II) as perchlorate salt.

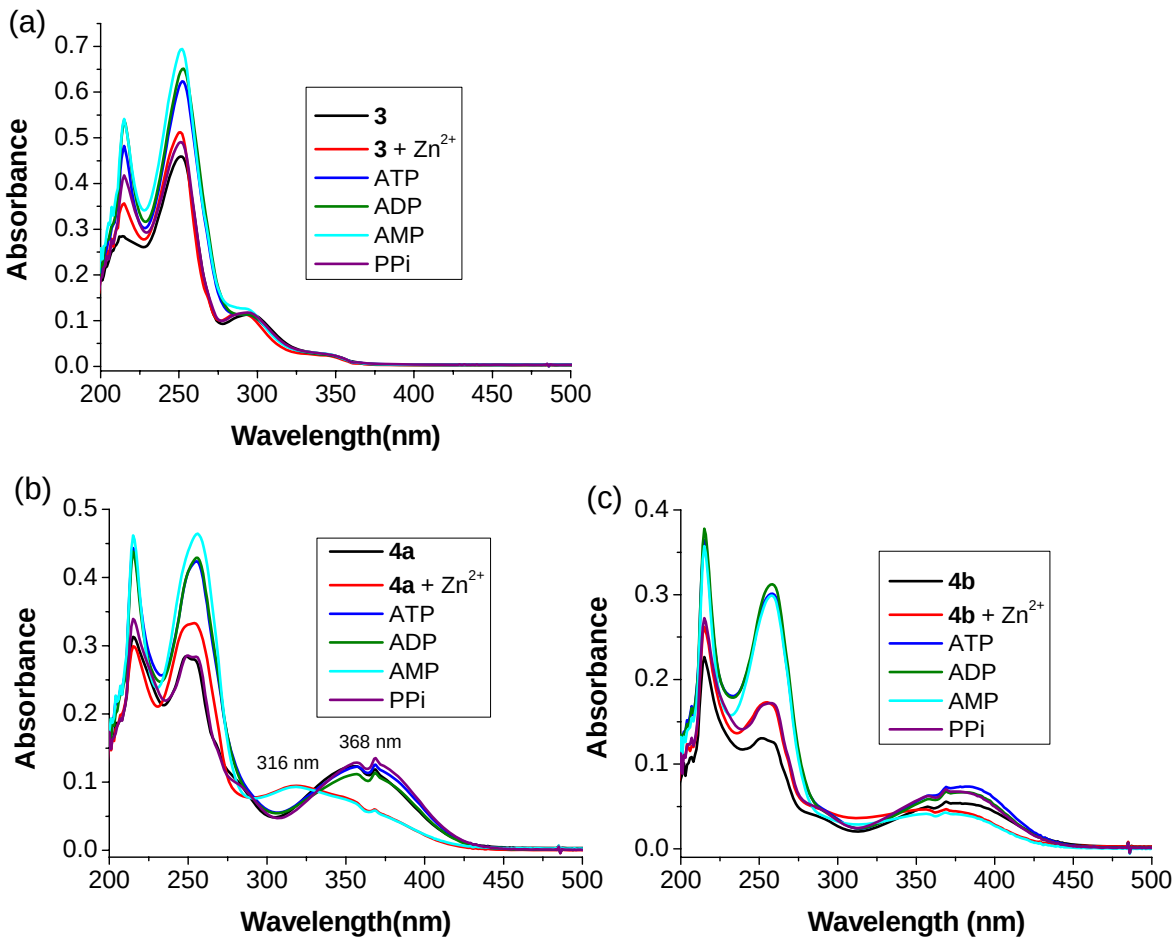


Fig. S4 UV absorption changes of (a) **3**, (b) **4a** and (c) **4b** (10 μM each) with addition of Zn^{2+} (1 equiv.) in HEPES buffer (10 mM, pH 7.4; containing 1% CH_3CN) followed by anion (1 equiv.) addition. PPi, ATP, ADP, and AMP were used as corresponding sodium salts.

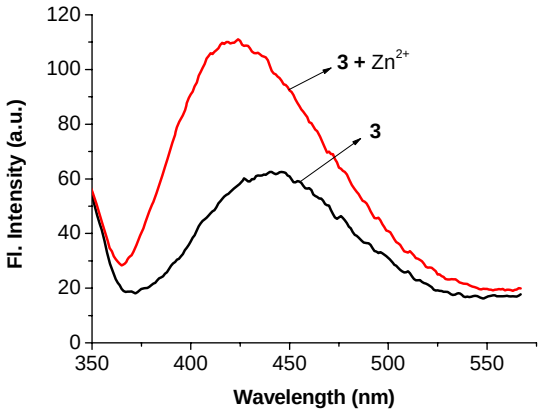


Fig. S5 Fluorescence spectral change of **3** (10 μM) upon addition of Zn^{2+} (1 equiv.) in pH 7.4 buffer (10 mM HEPES containing 1% CH_3CN). λ_{ex} = 295 nm. Due to second-order diffraction interference fluorescence data were cut down at 570 nm.

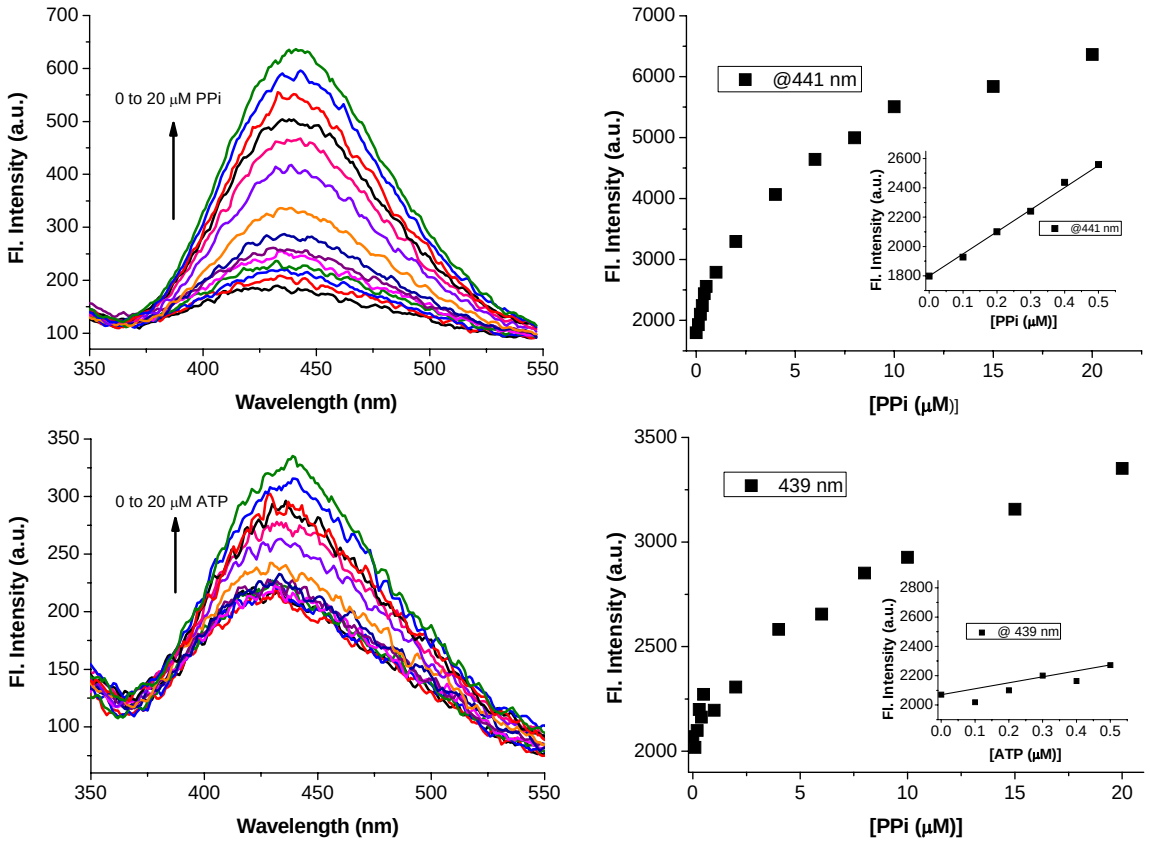
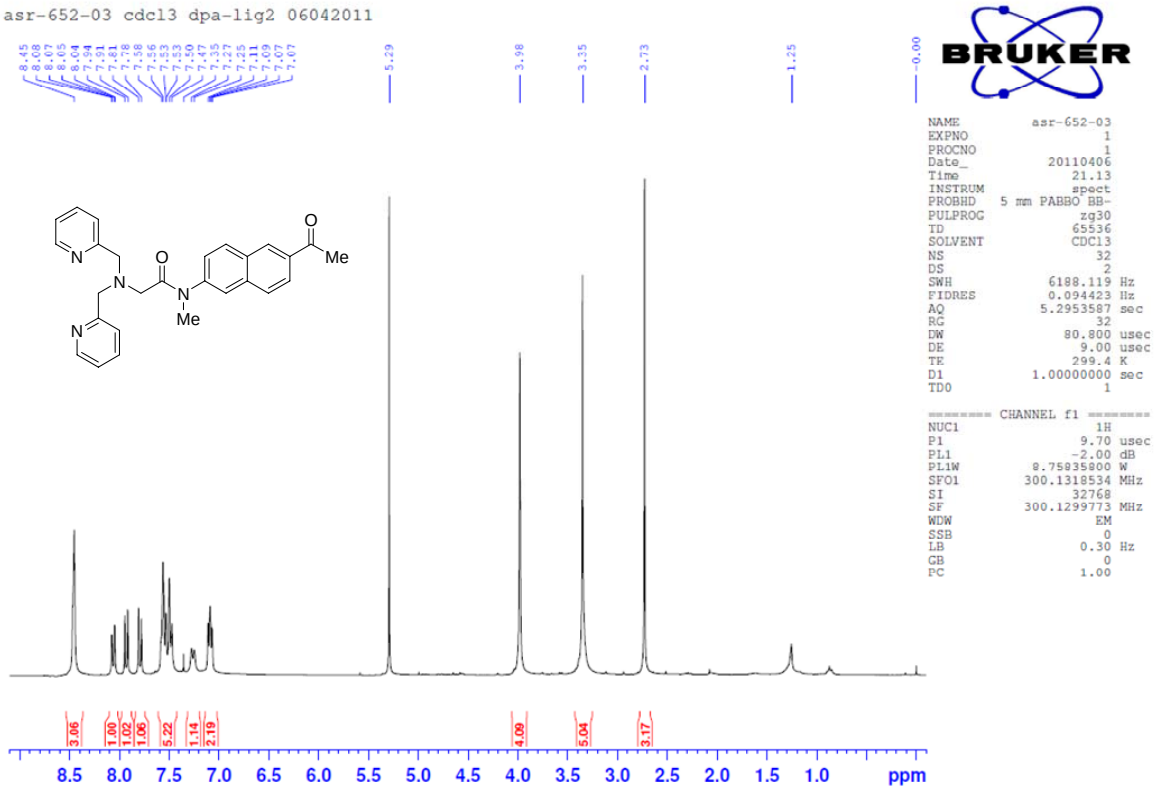


Fig. S6 Fluorescence spectral change of **3**-Zn (10 μM) upon addition of PPi (top) and ATP (bottom) up to 20 μM in pH 7.4 buffer (10 mM HEPES containing 1% CH_3CN). λ_{ex} = 295 nm. Inset is a part of the plot in the range from 0 to 0.5 μM. Due to second-order diffraction interference fluorescence data were cut down at 550 nm.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7.25
7.11
7.09
7.07
7.07
5.29
3.98
3.35
2.73
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0.00
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Me
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1.02
1.06
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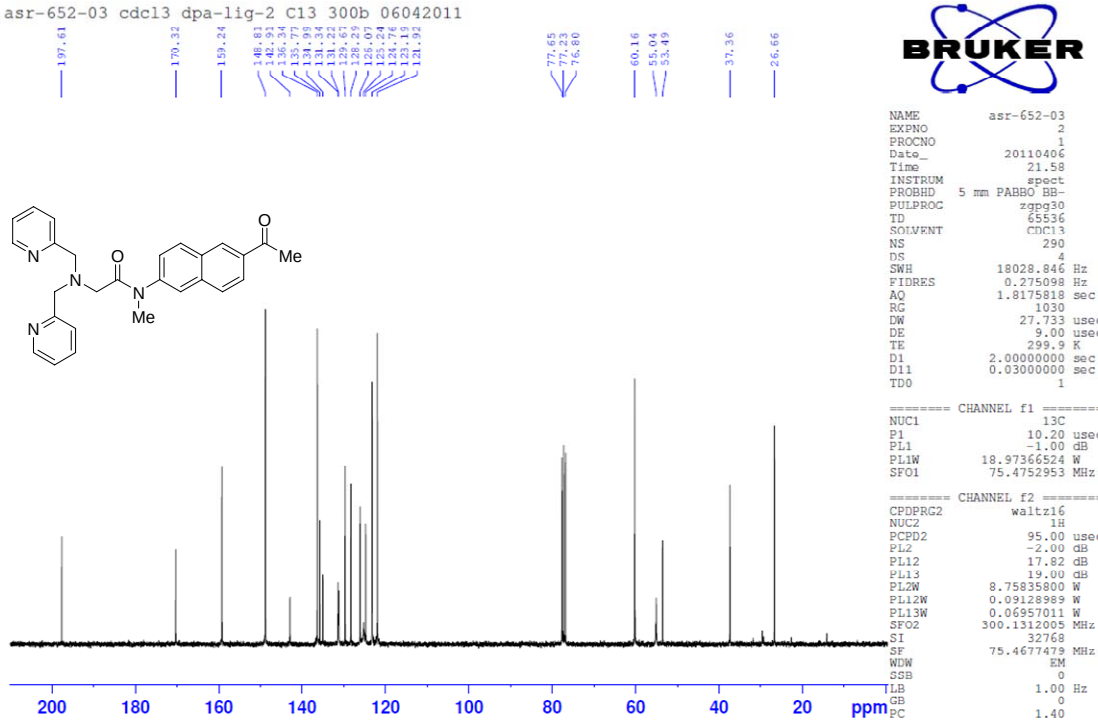
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PCPD2 95.00 usec
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PL12 17.82 dB
PL13 19.00 dB
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PL12W 0.09128989 W
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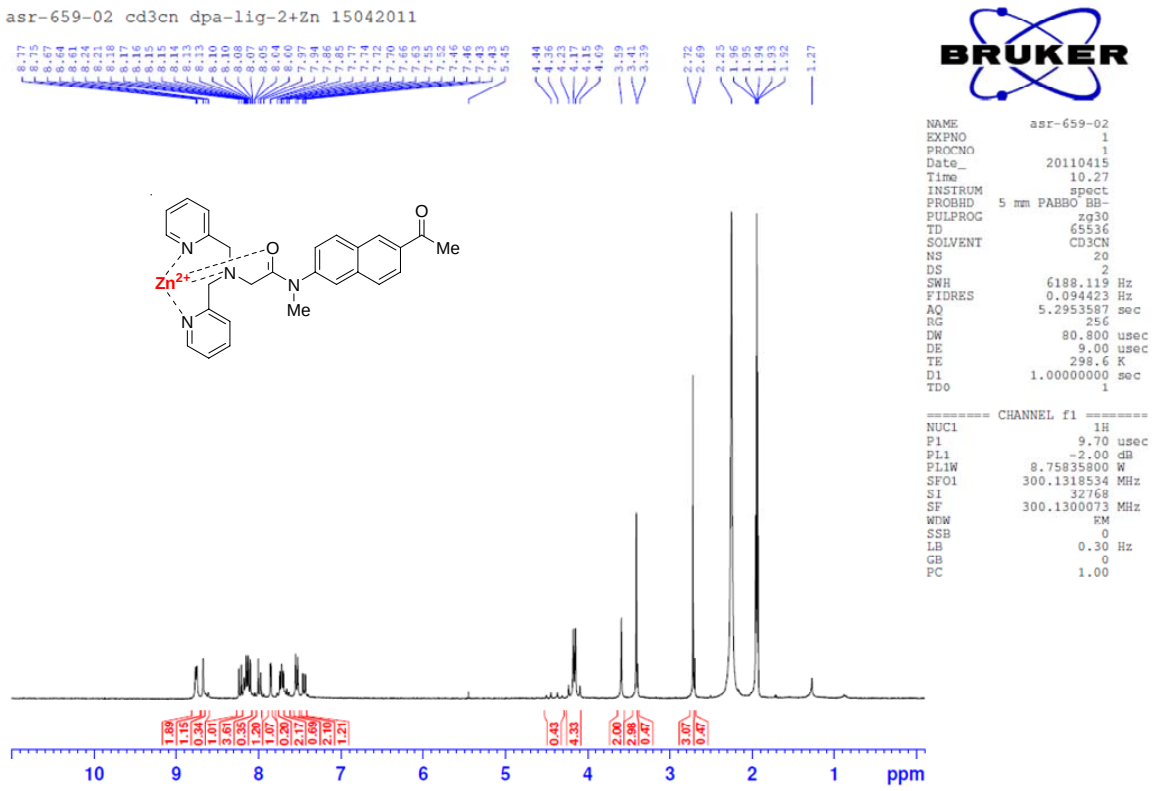

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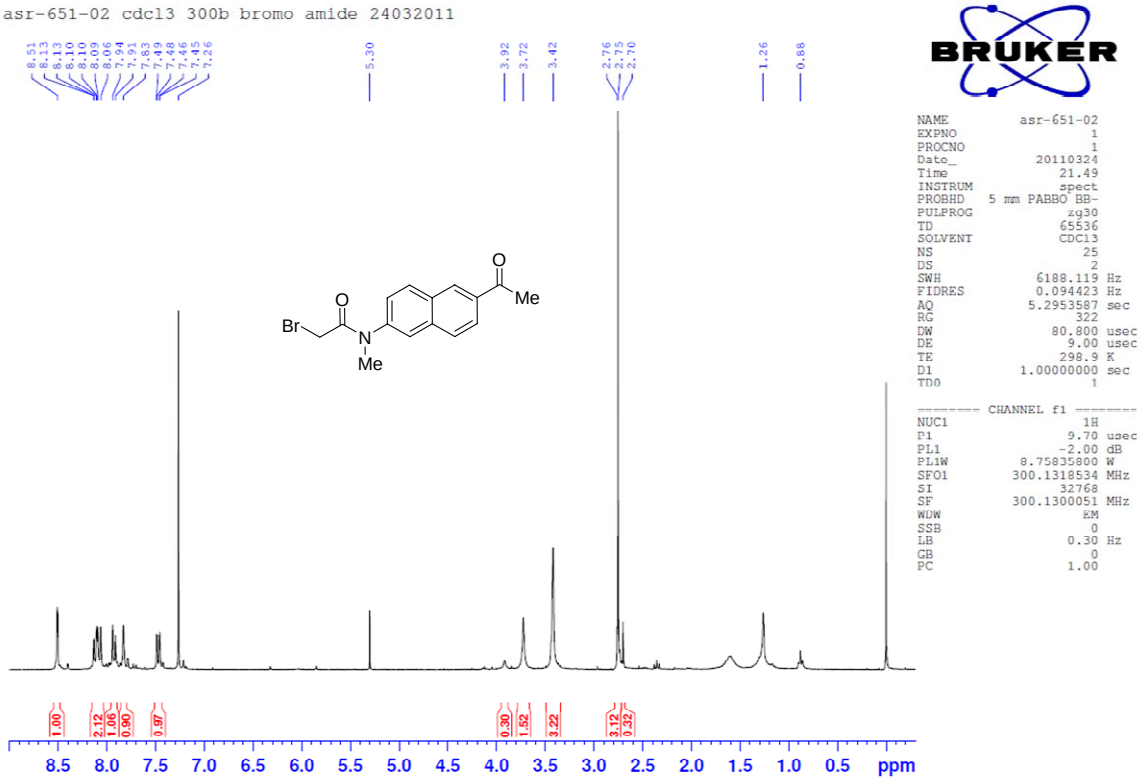

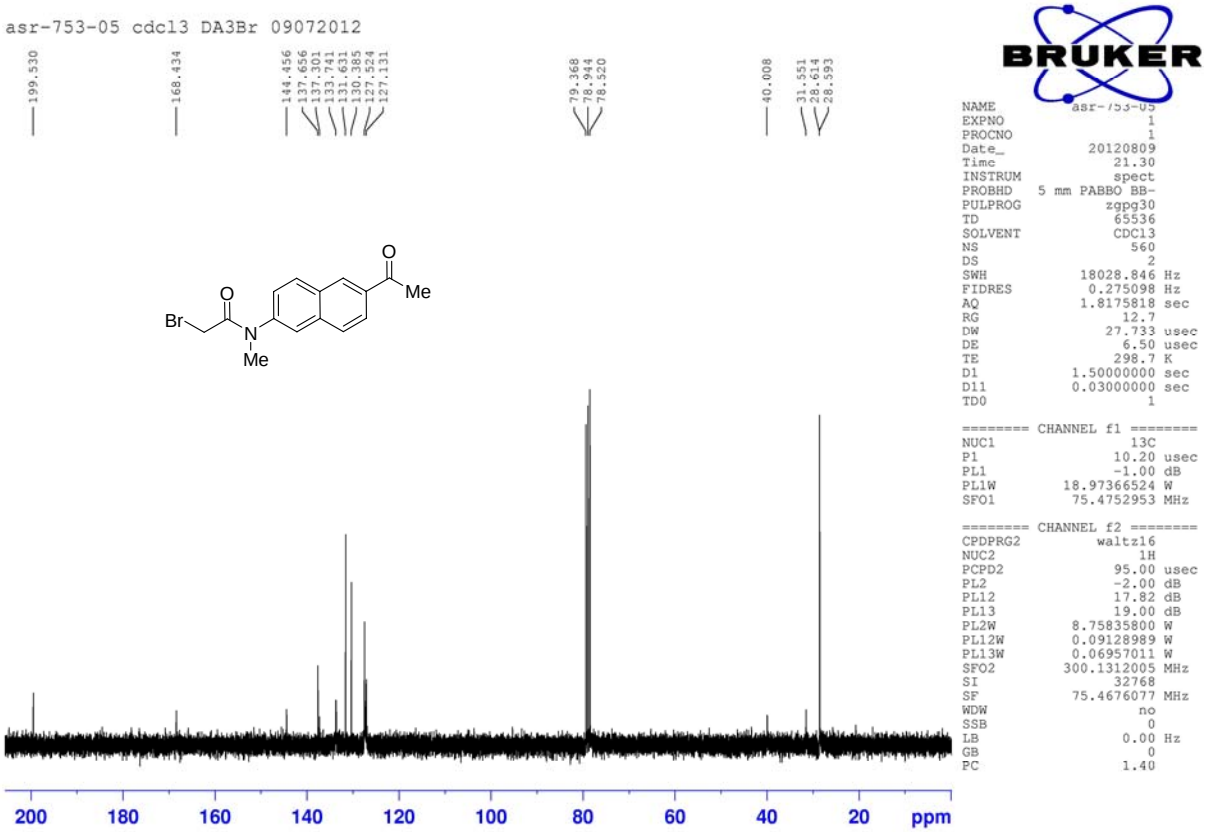

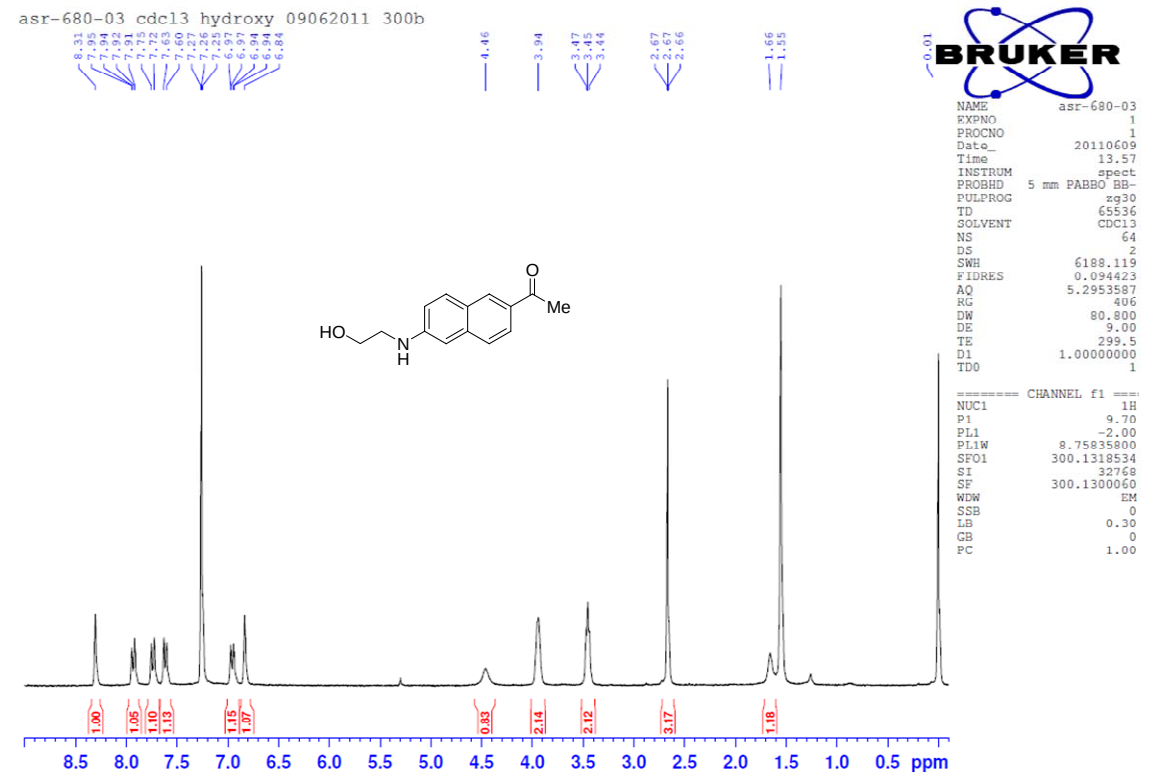

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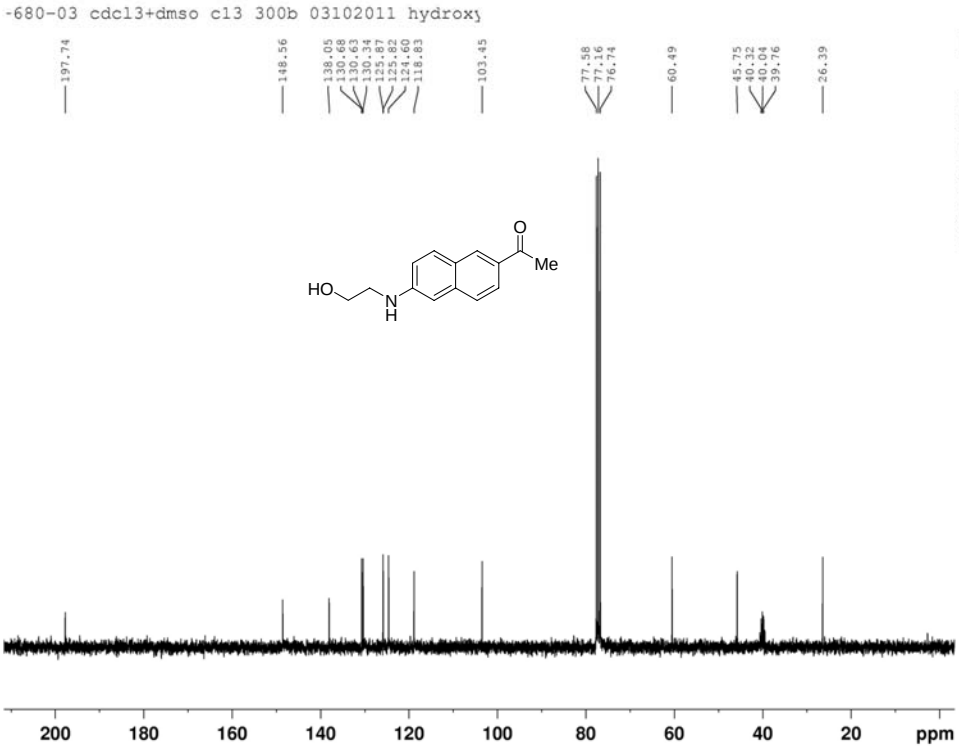

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PL2W	8.75835800
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PL13W	0.06957011
SFO2	300.1312005
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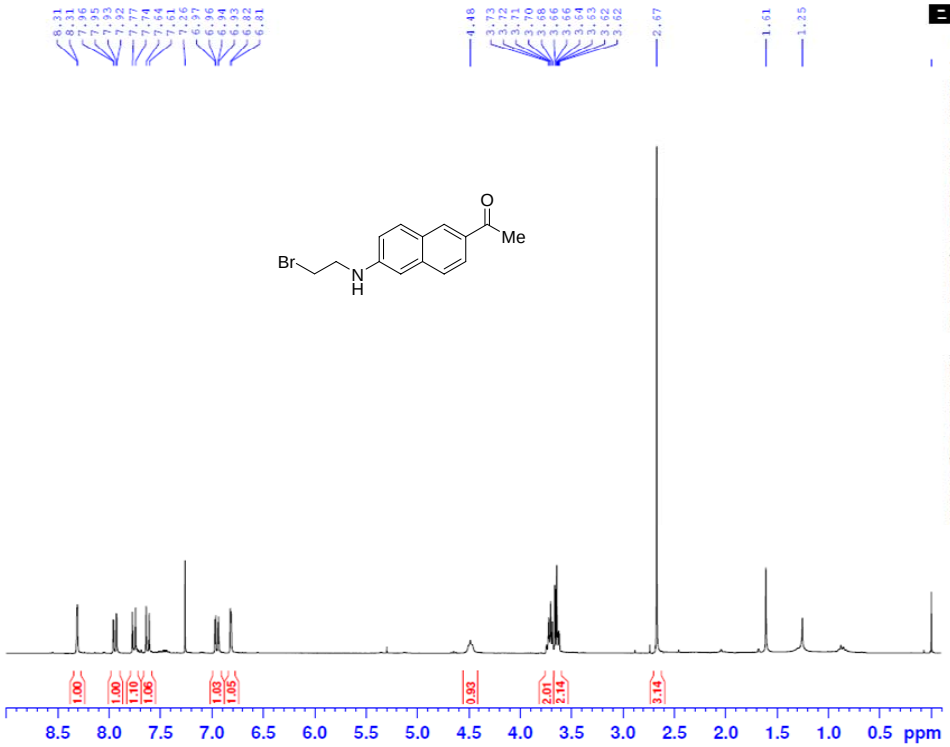

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AQ	5.2953587
RG	228
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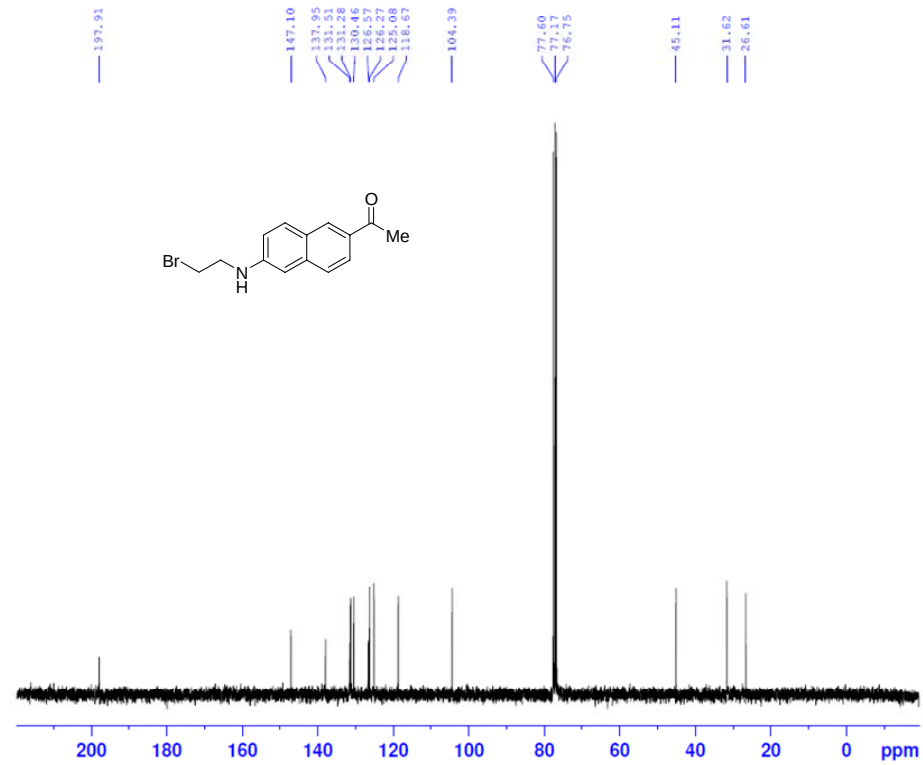

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RG	575
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DE	9.00 usec
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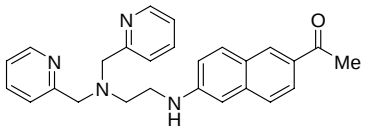

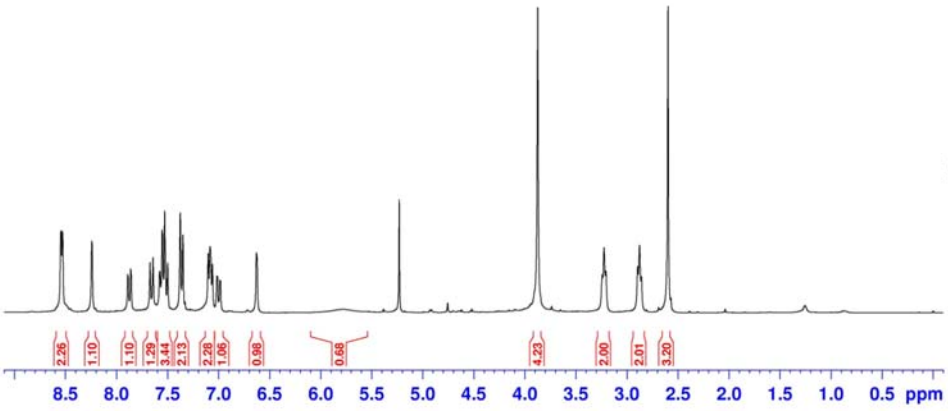

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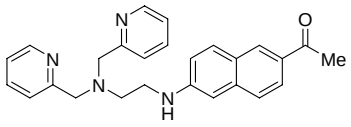

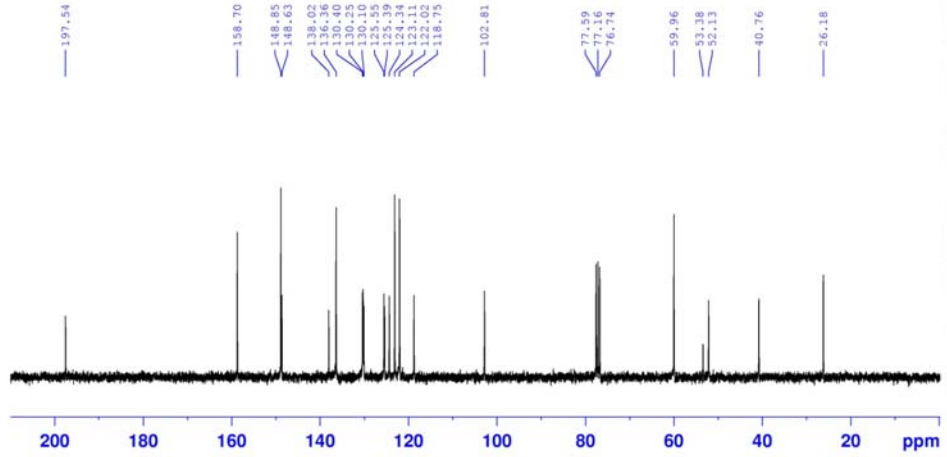

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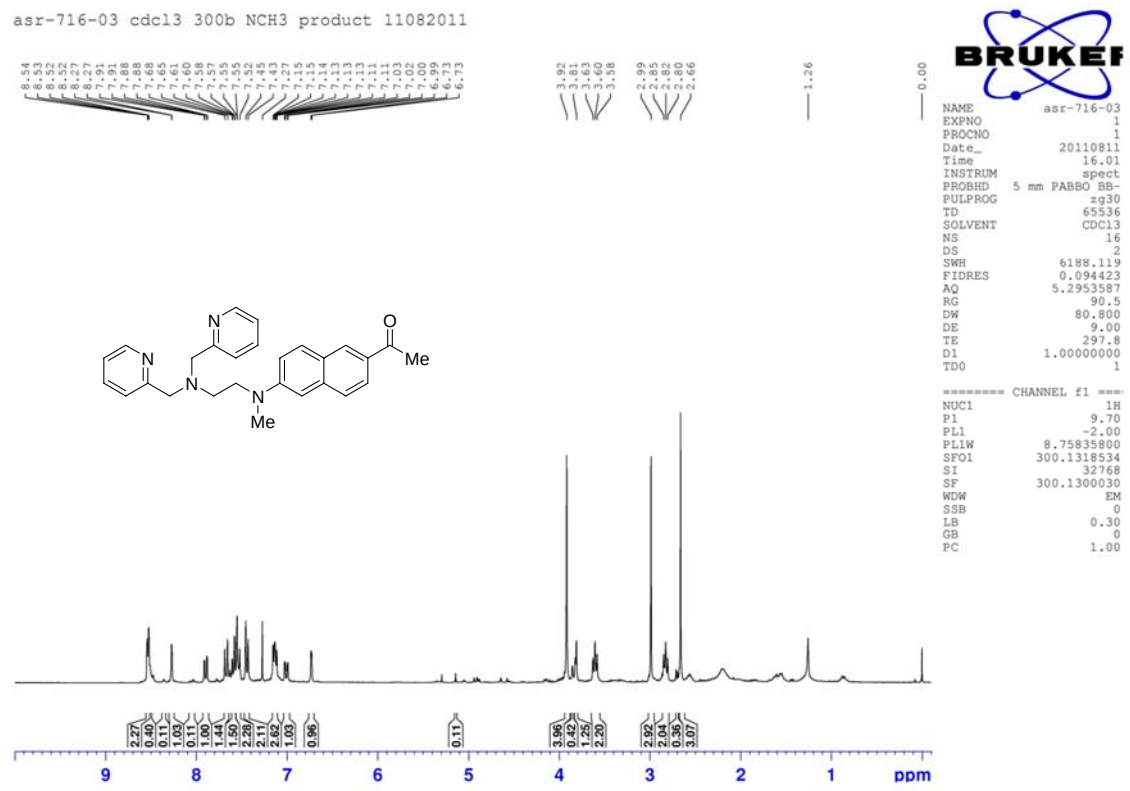
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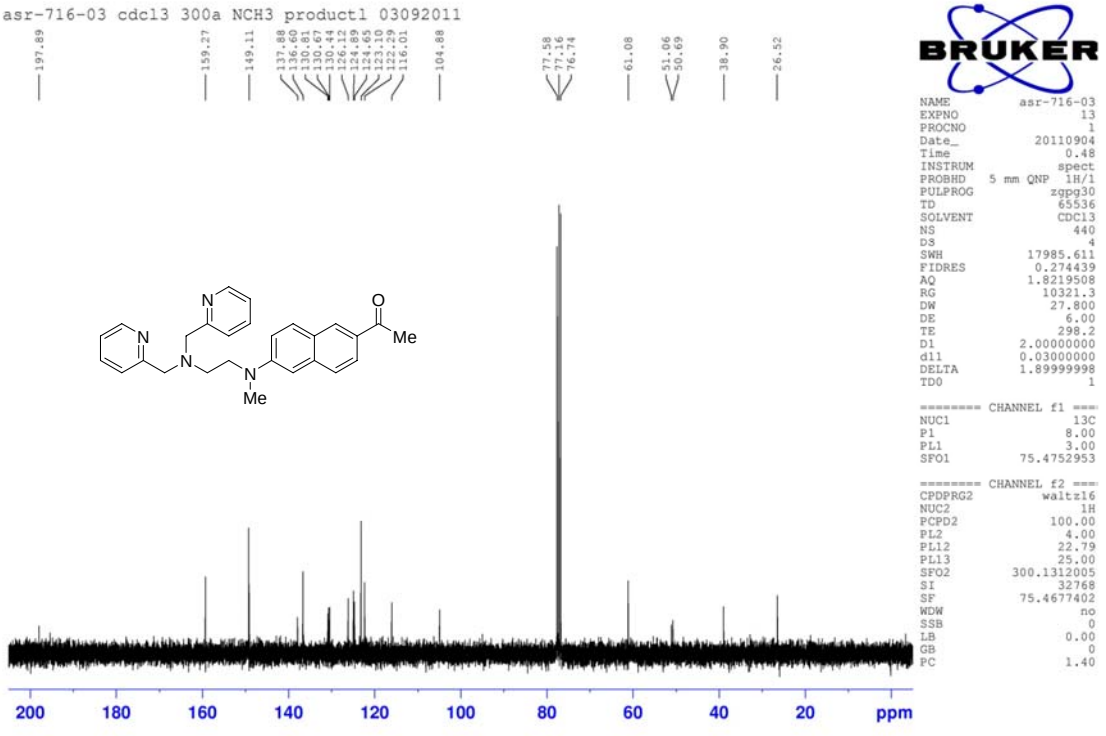
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