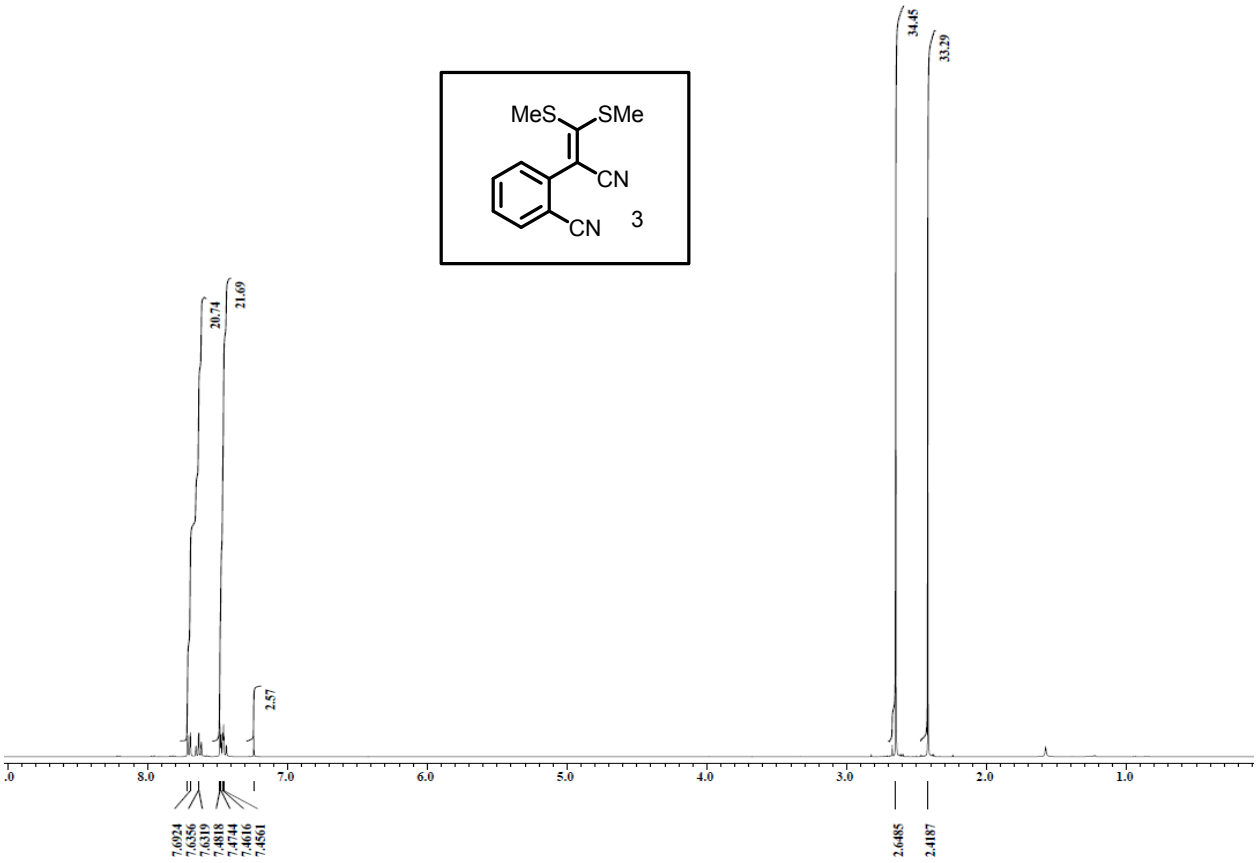
Synthesis of 1-amino-2-aroyl/acetylnaphthalenes through base mediated one pot inter and intramolecular C-C bond formation strategy

Surjeet Singh,[a] Pratik Yadav, [a] Satya Narayan Sahu,[a] Ismail Althagafi,[b] Abhinav Kumar, [c] Brijesh Kumar,[d] Vishnu Ji Ram[c] and Ramendra Pratap[a,] *

Supporting Information

Contents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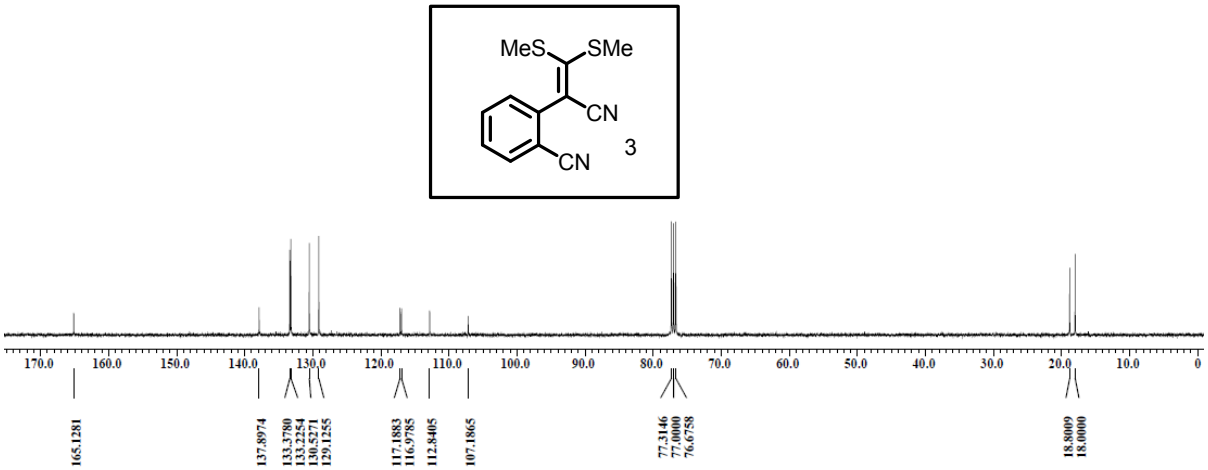
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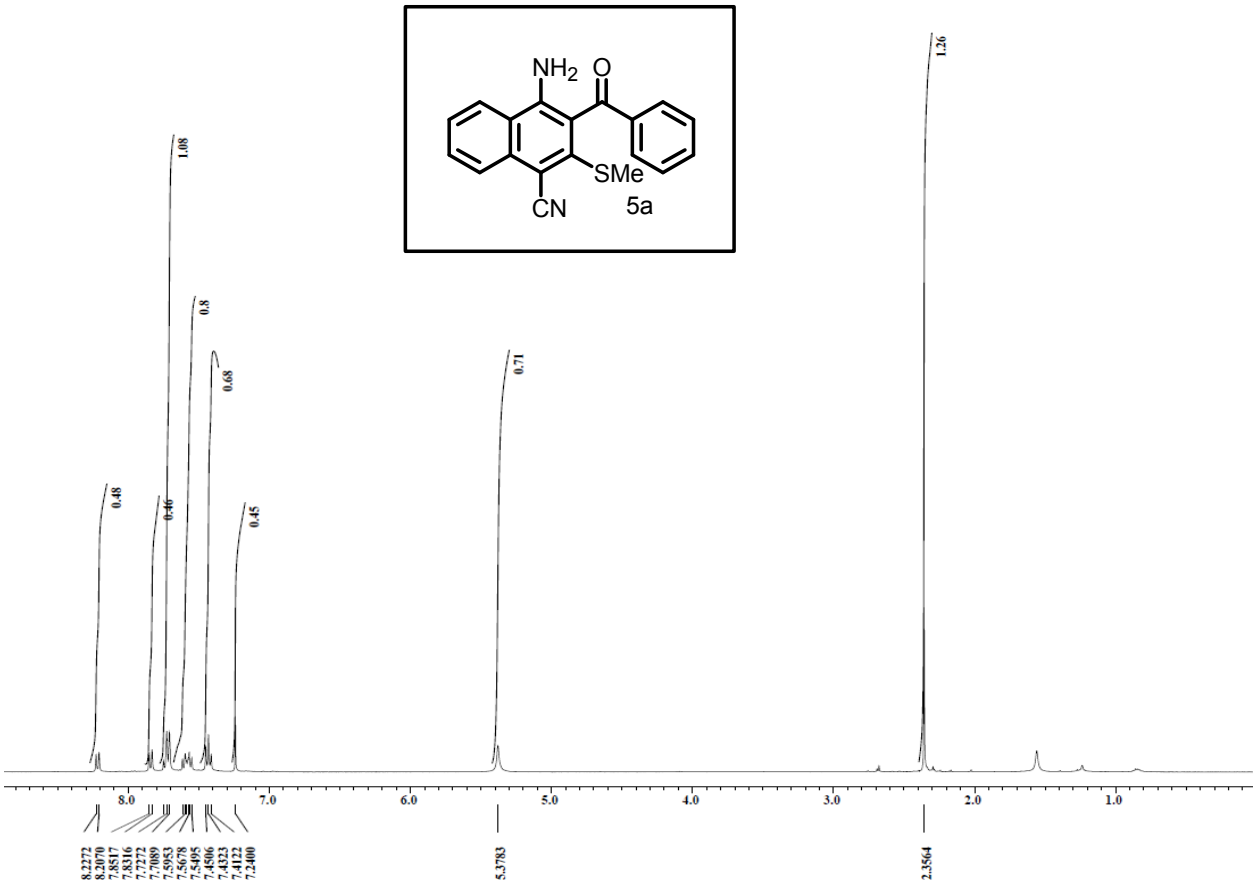
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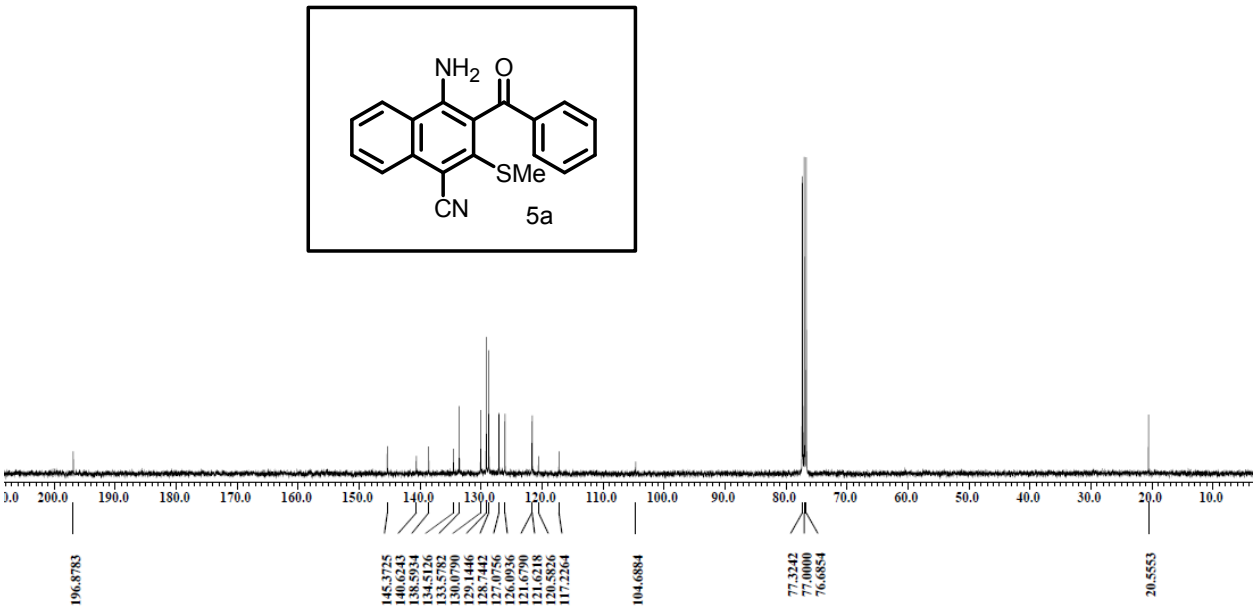
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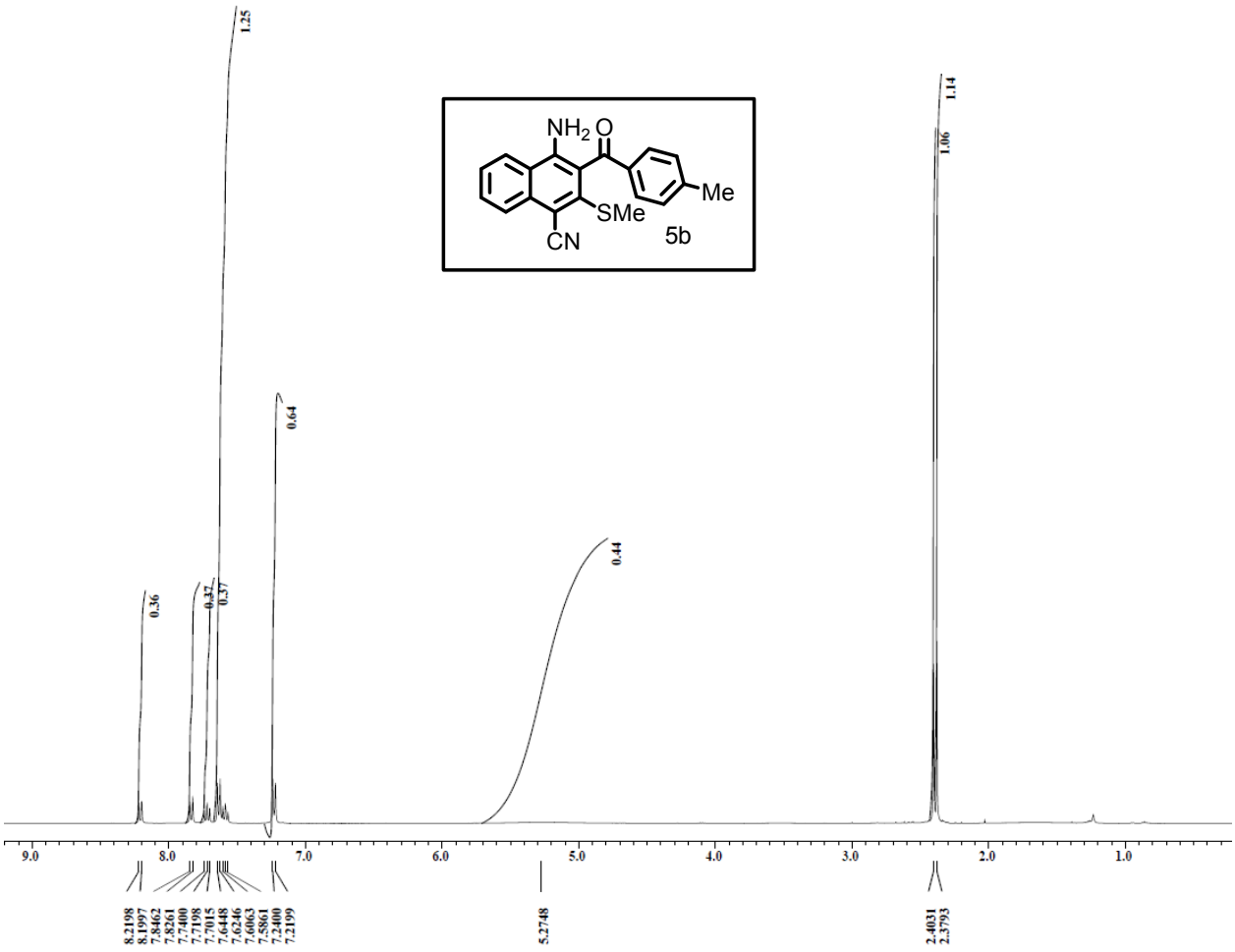
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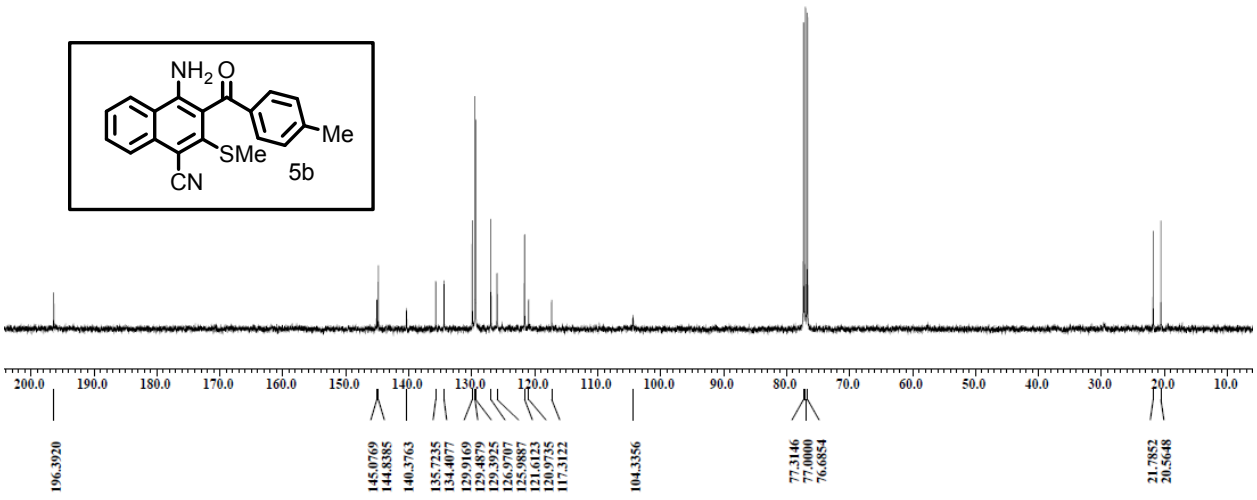
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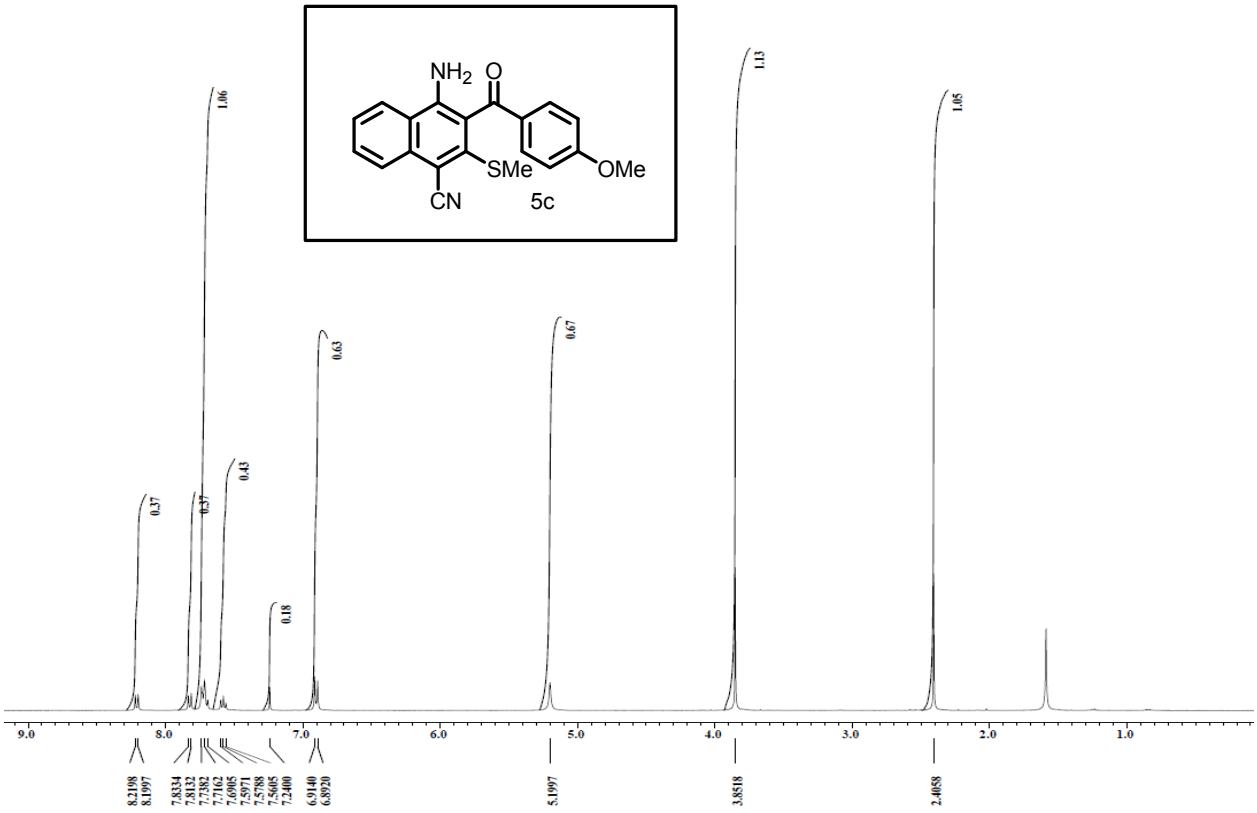
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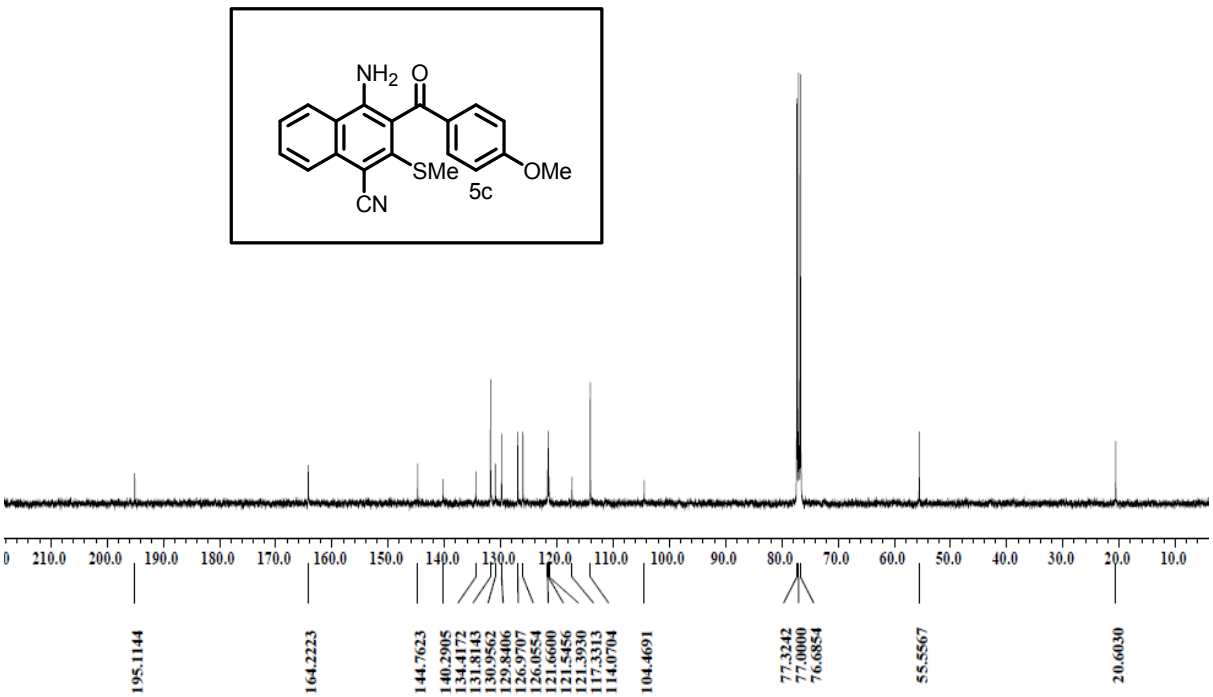
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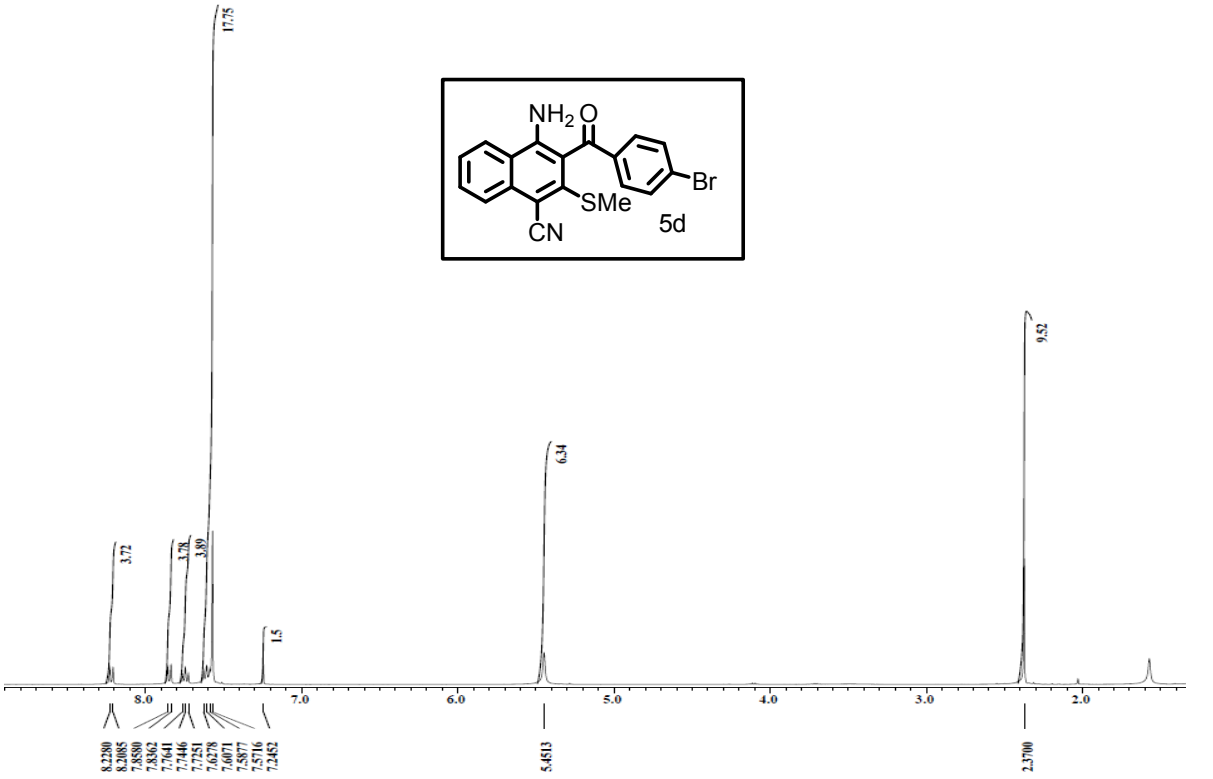
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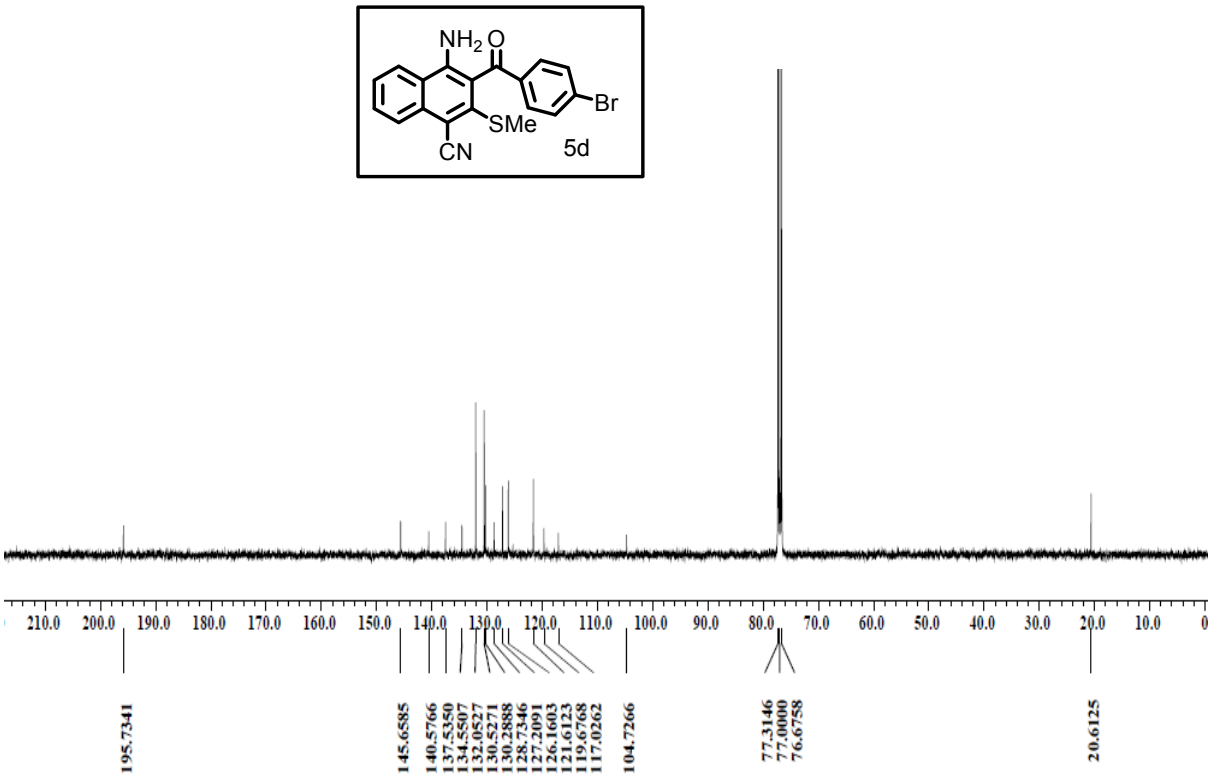
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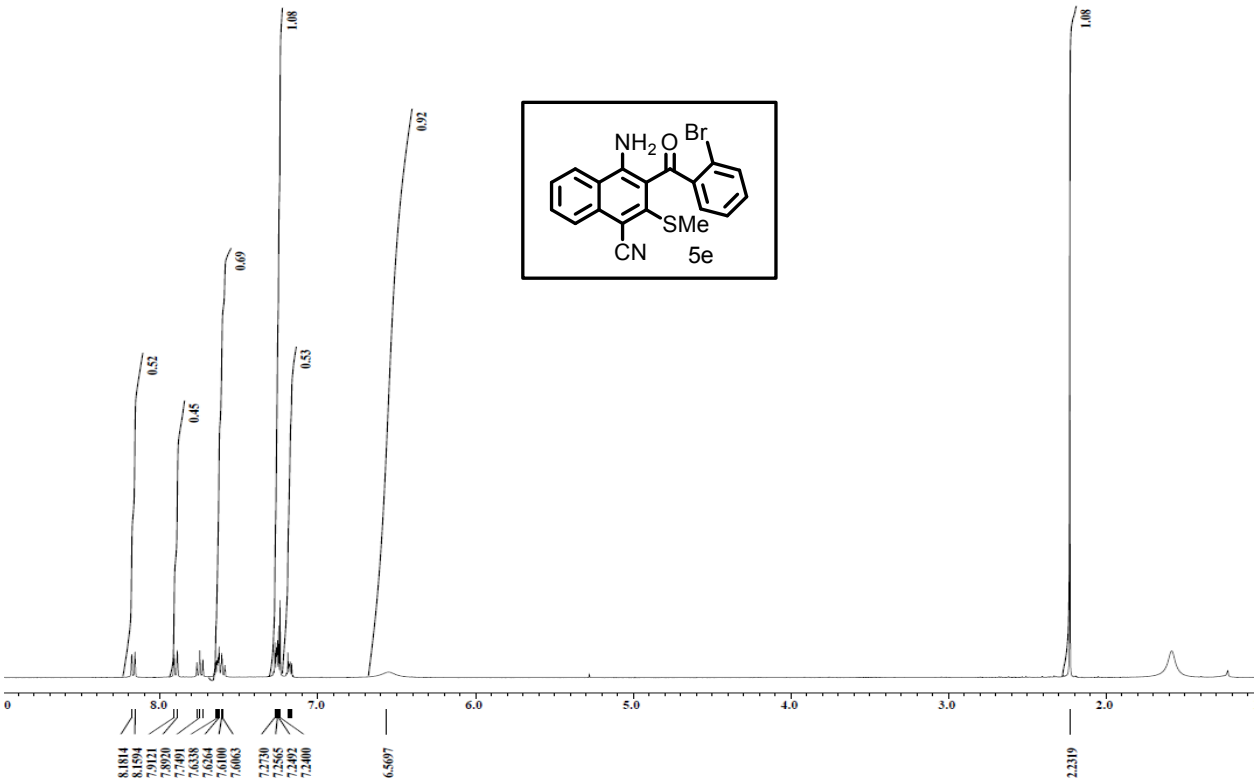
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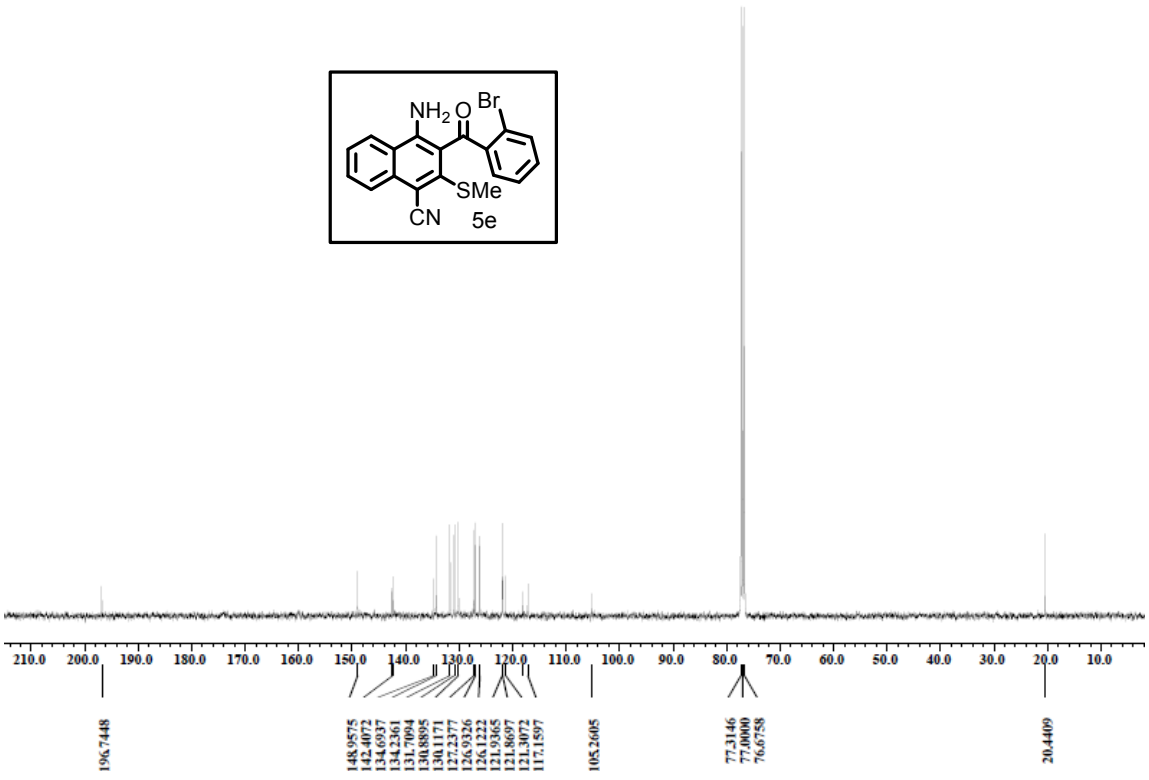
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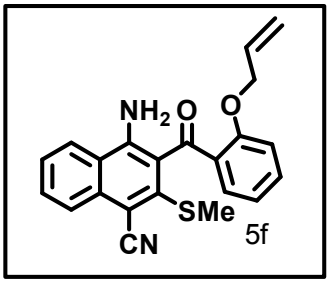
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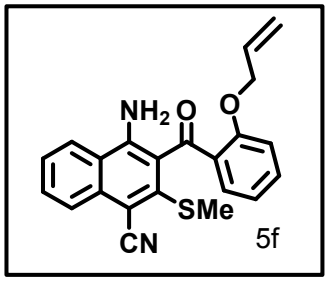
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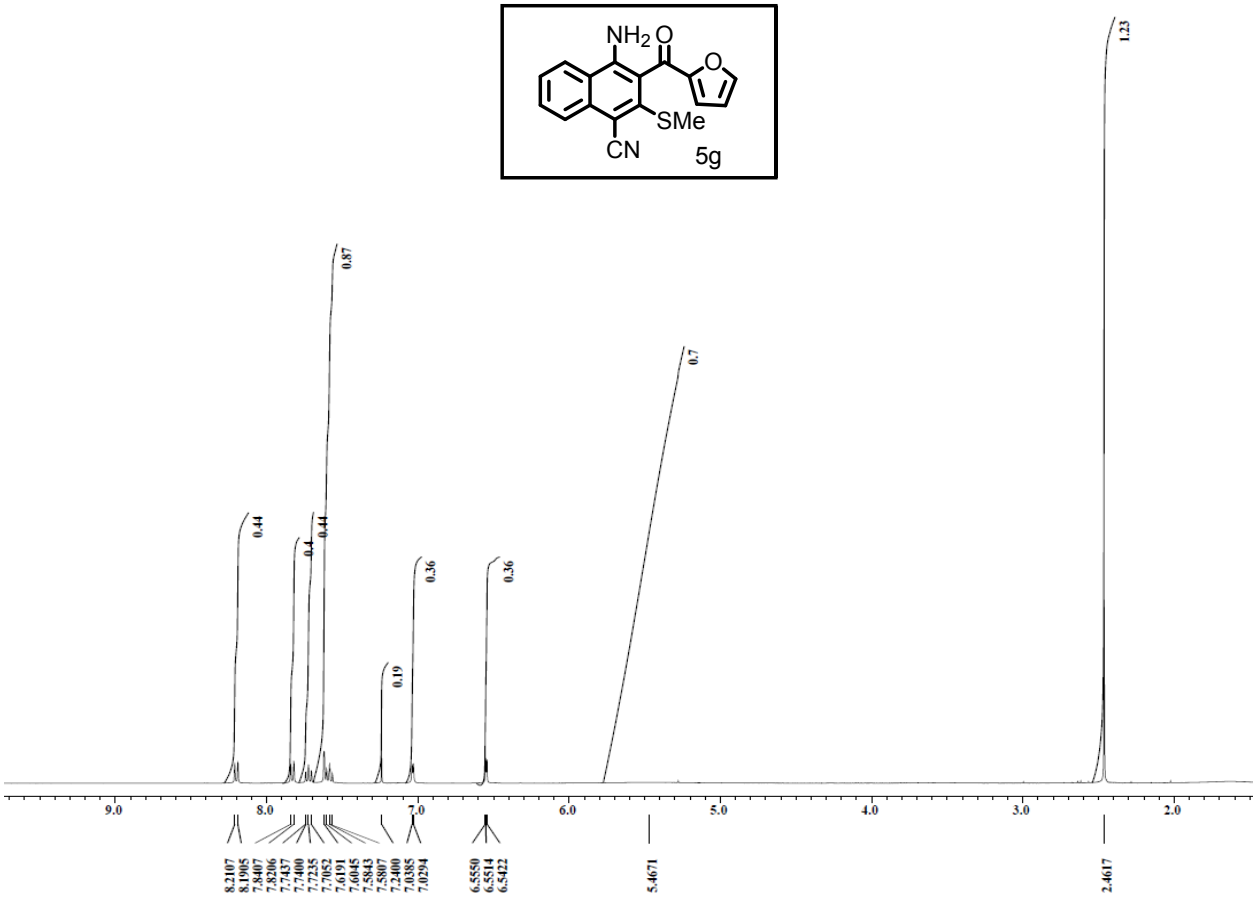
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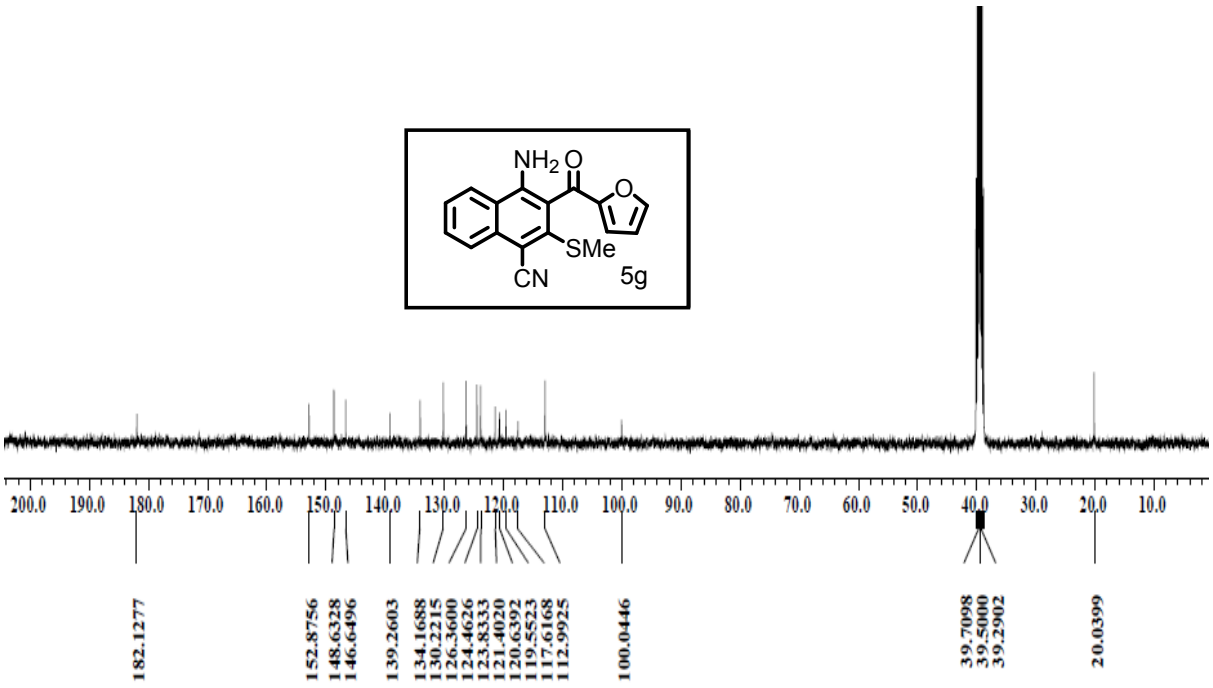
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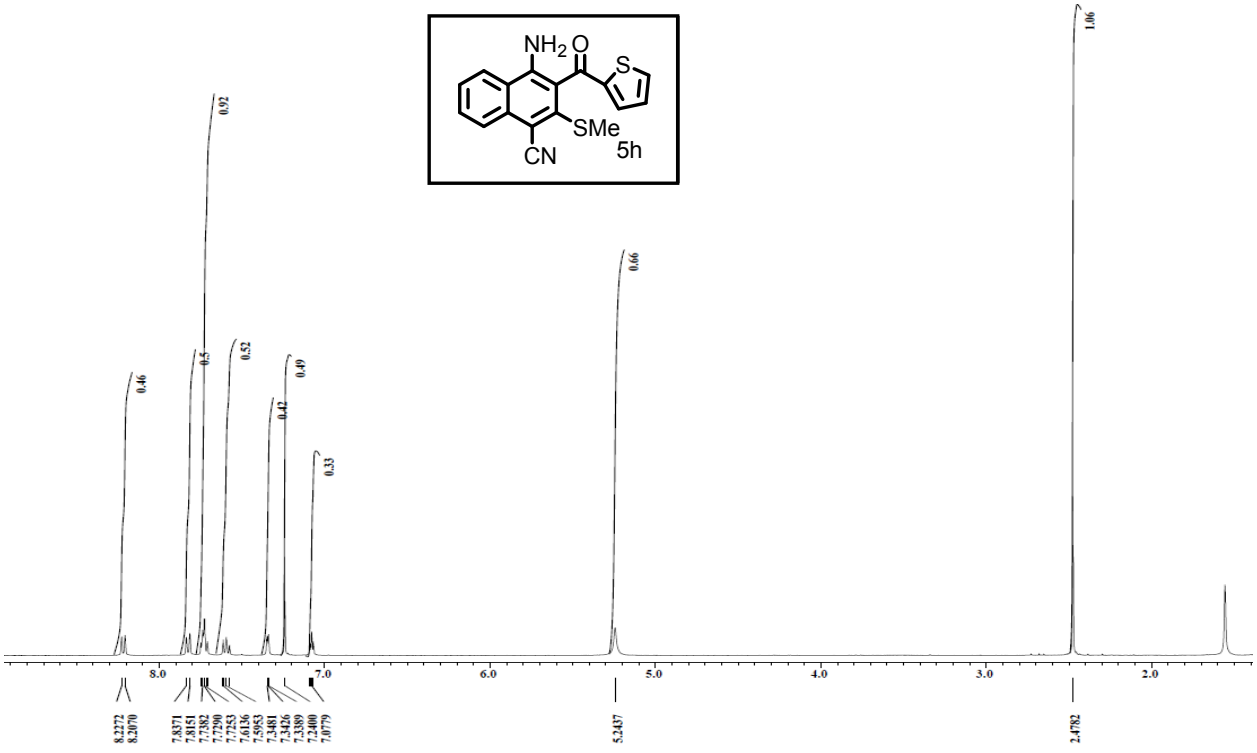
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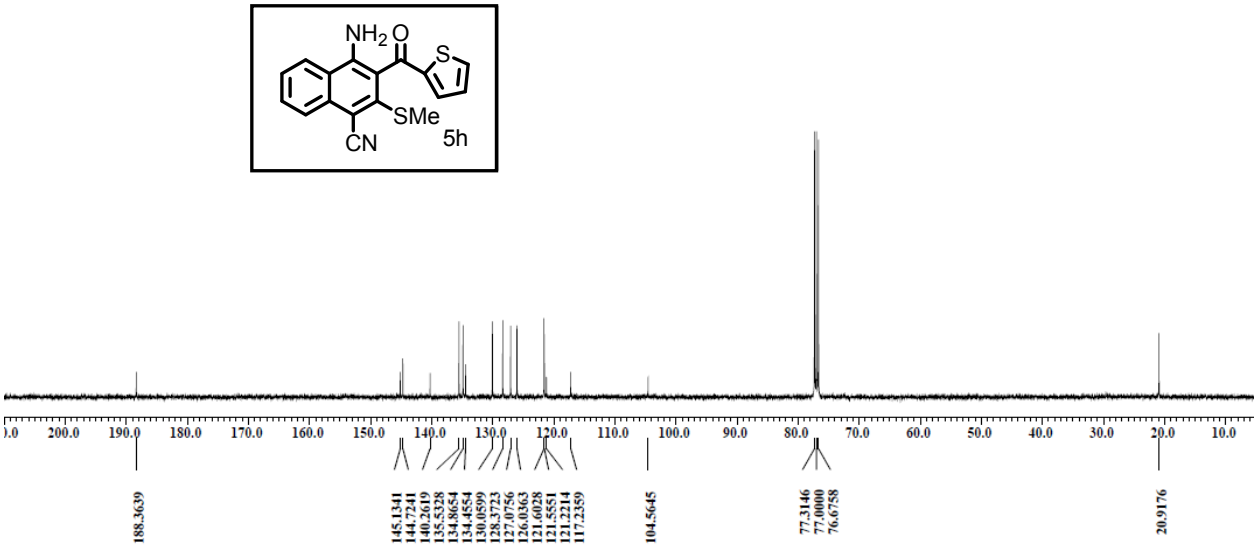
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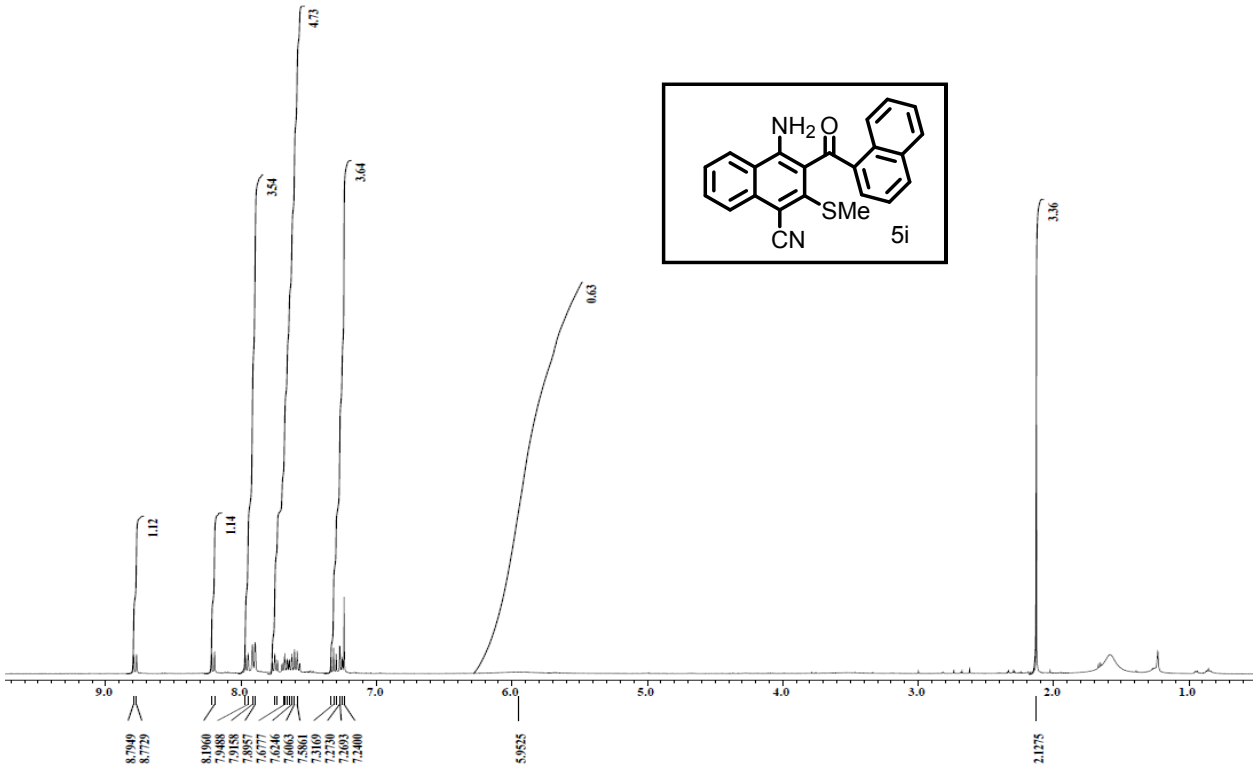
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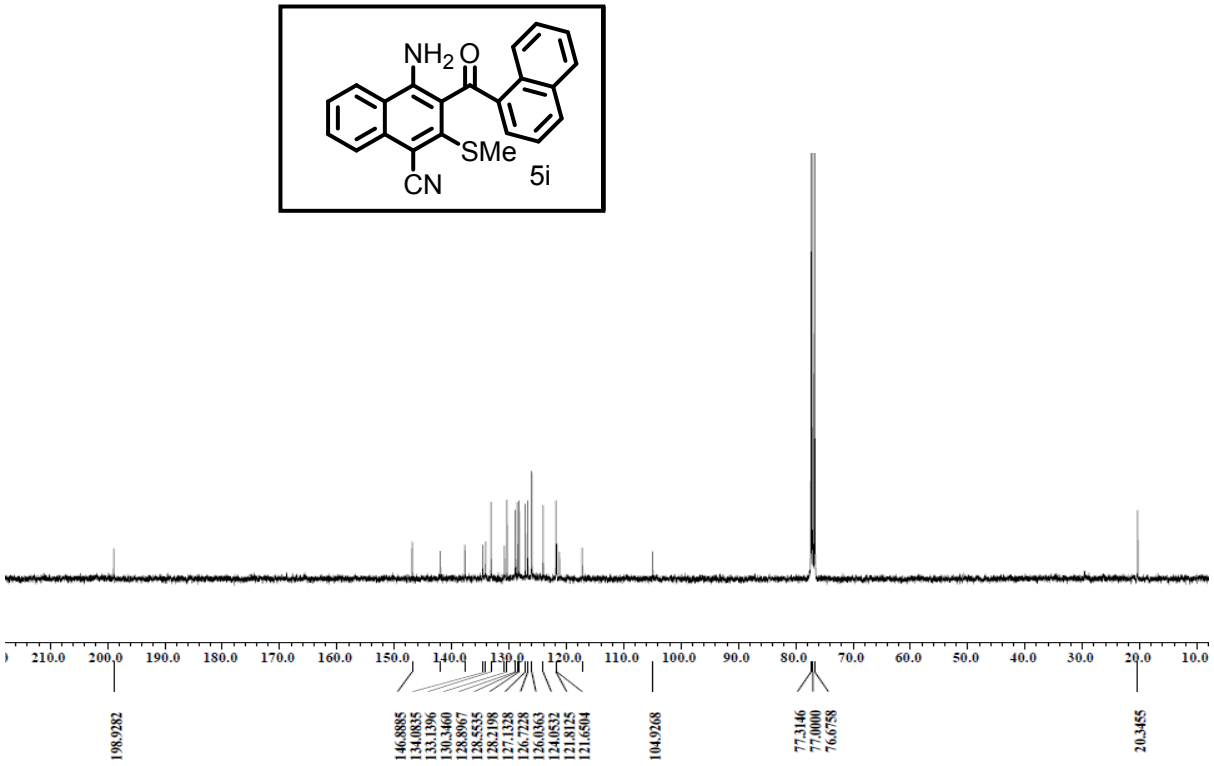
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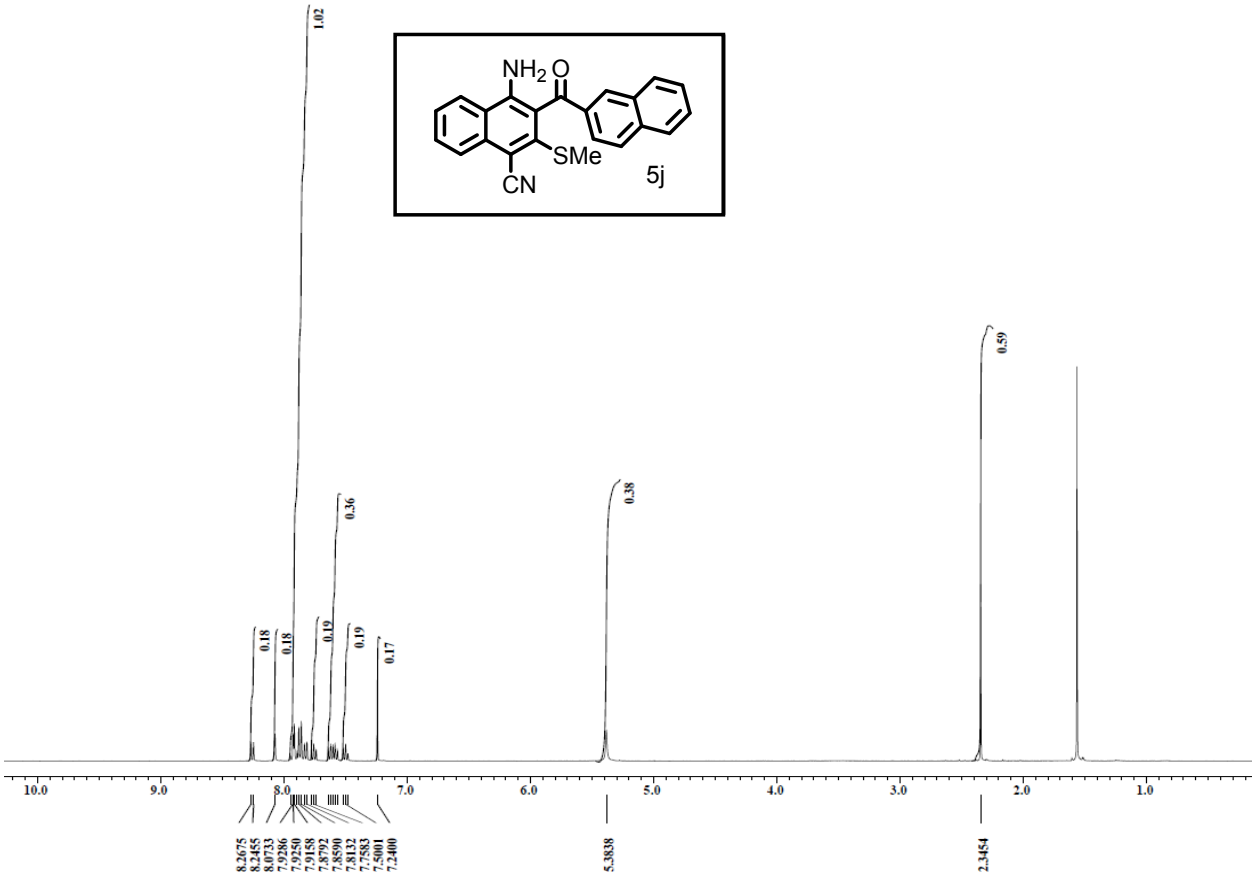
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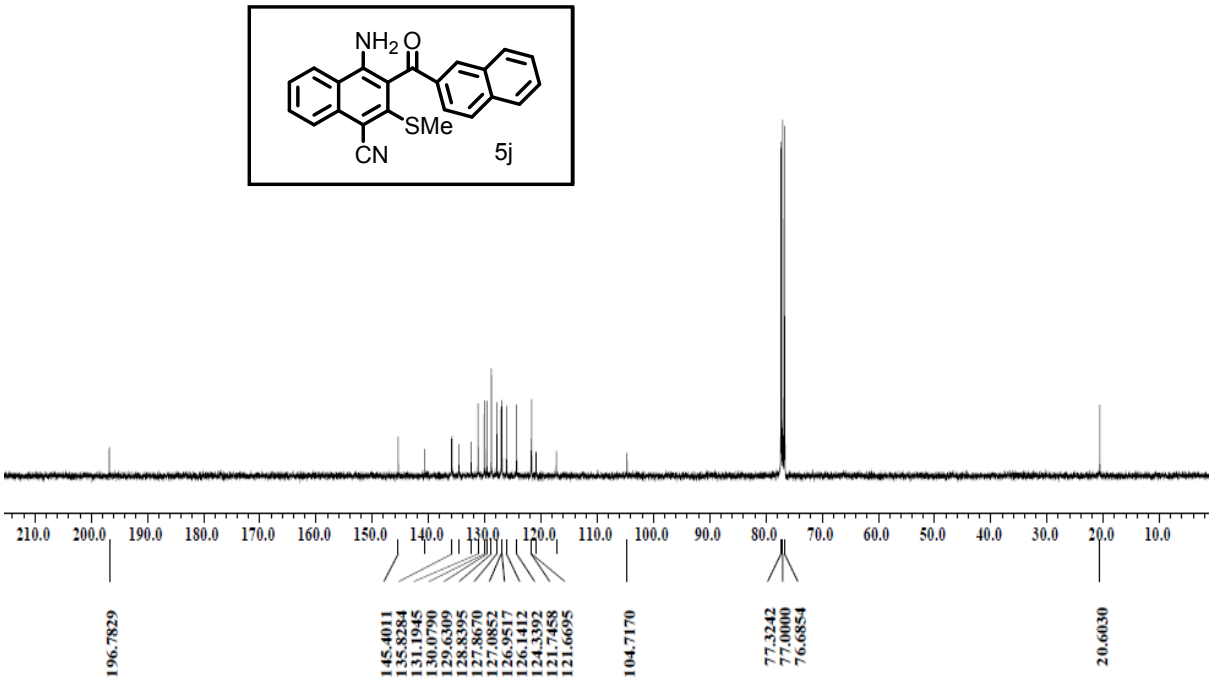
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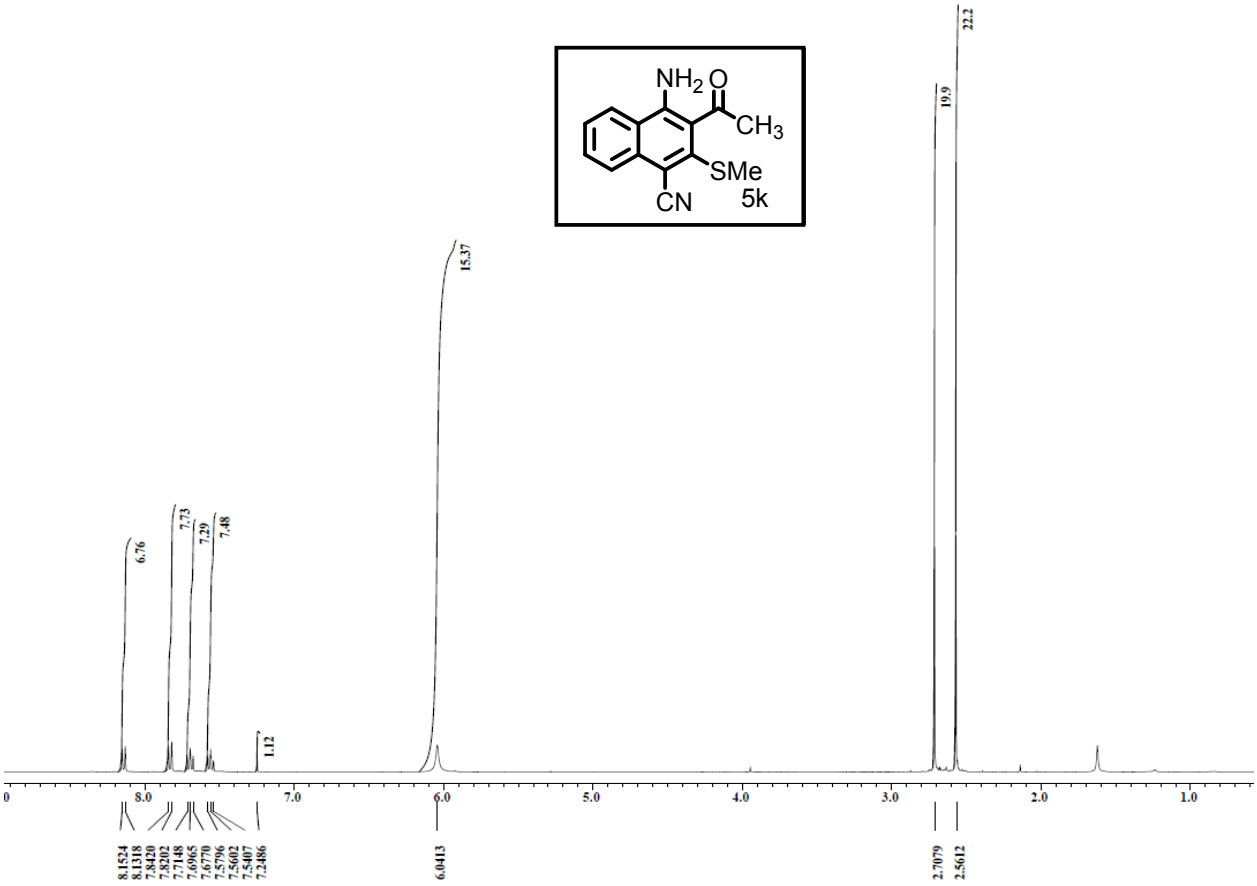
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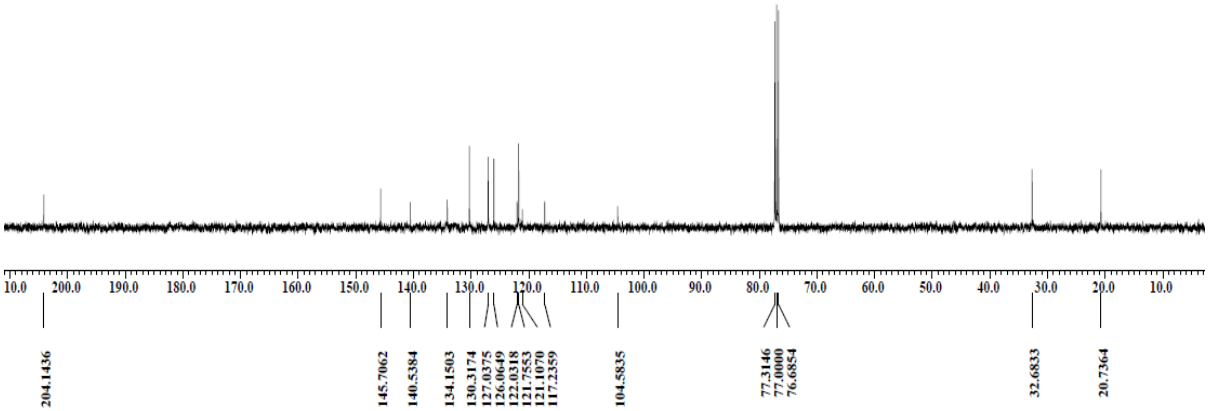
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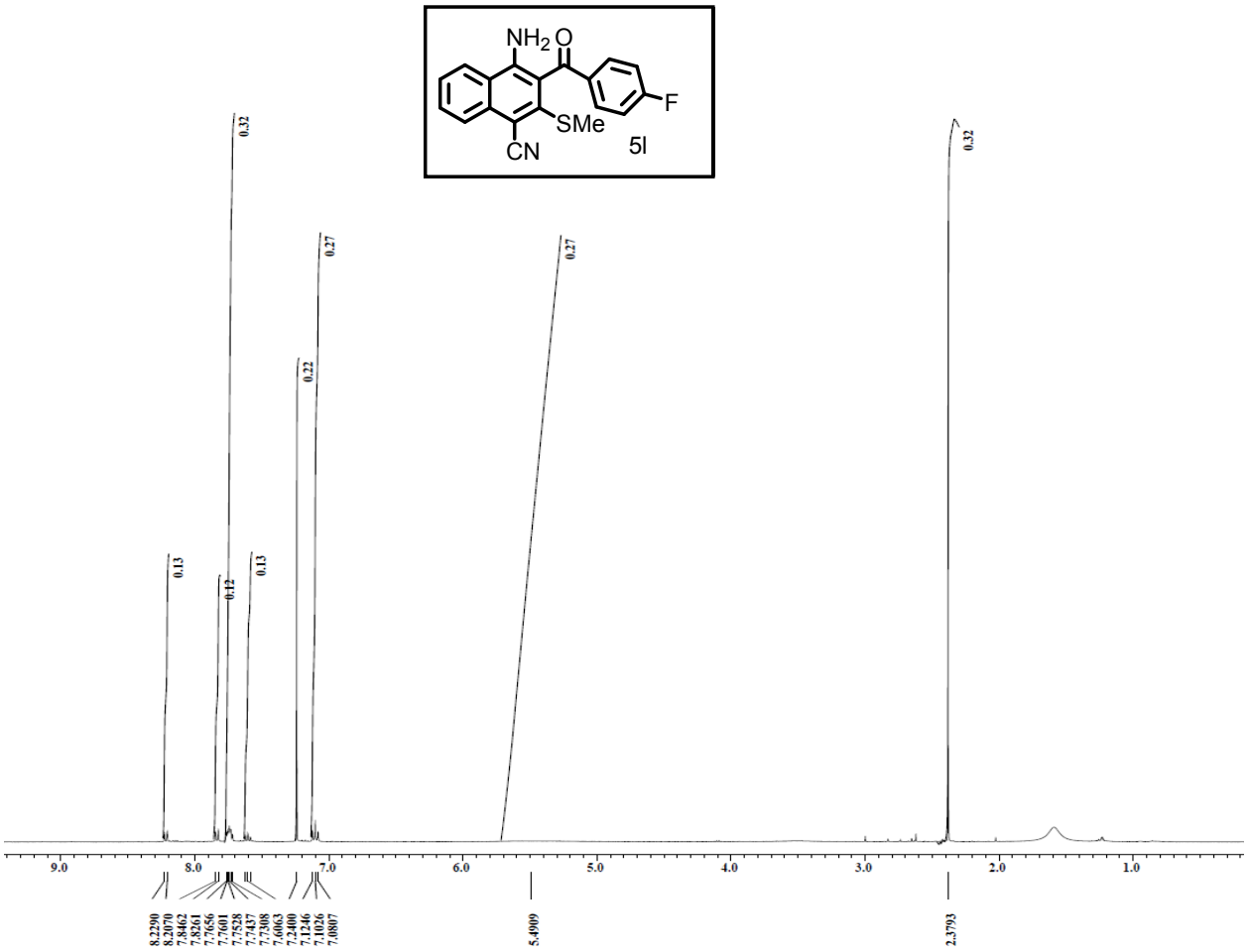
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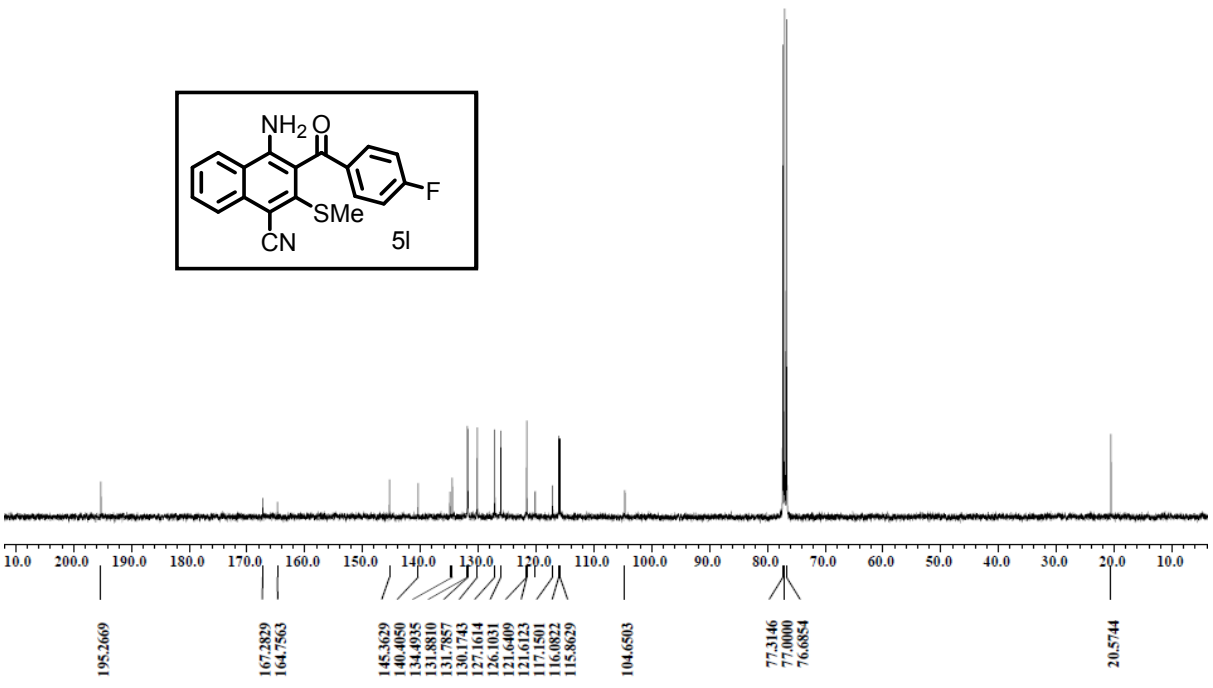
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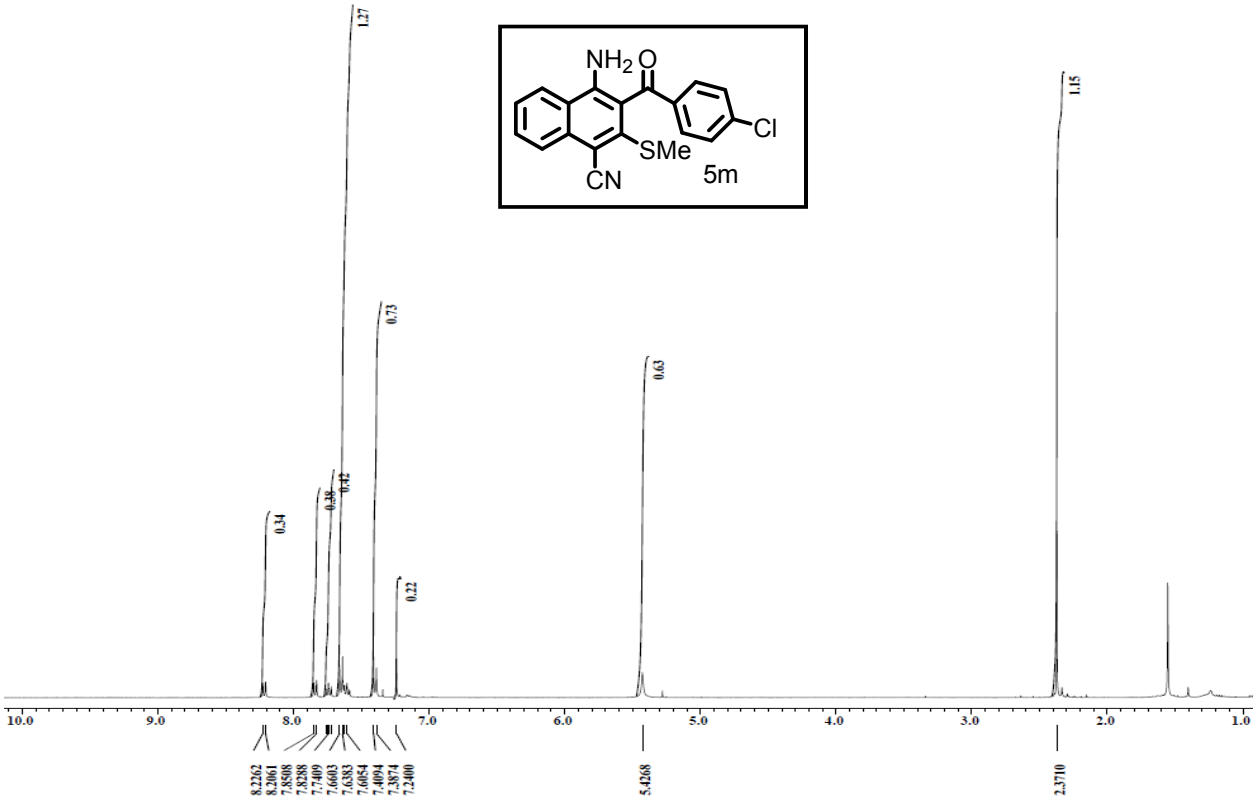
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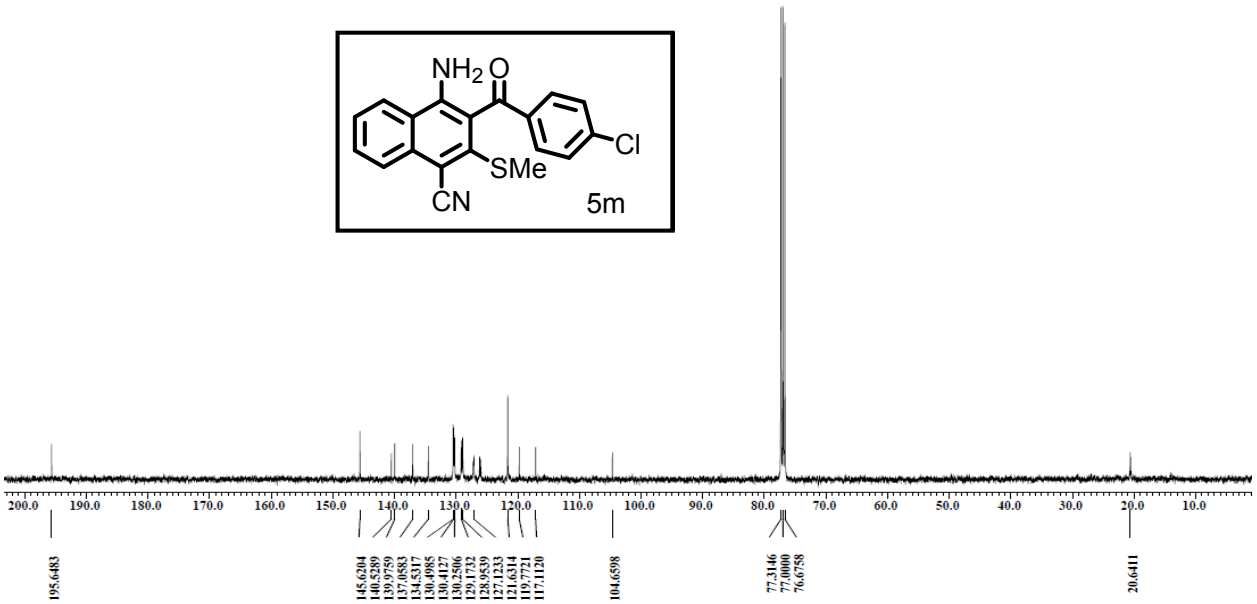
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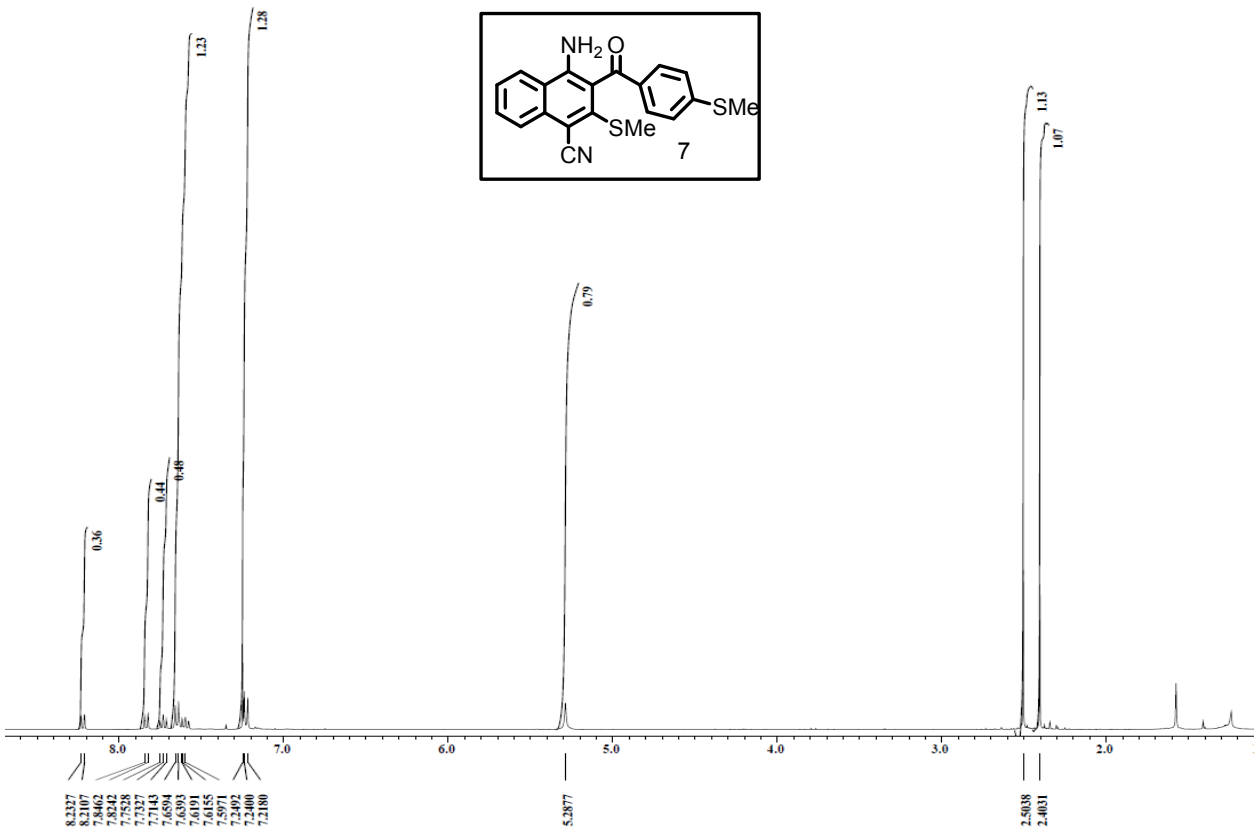
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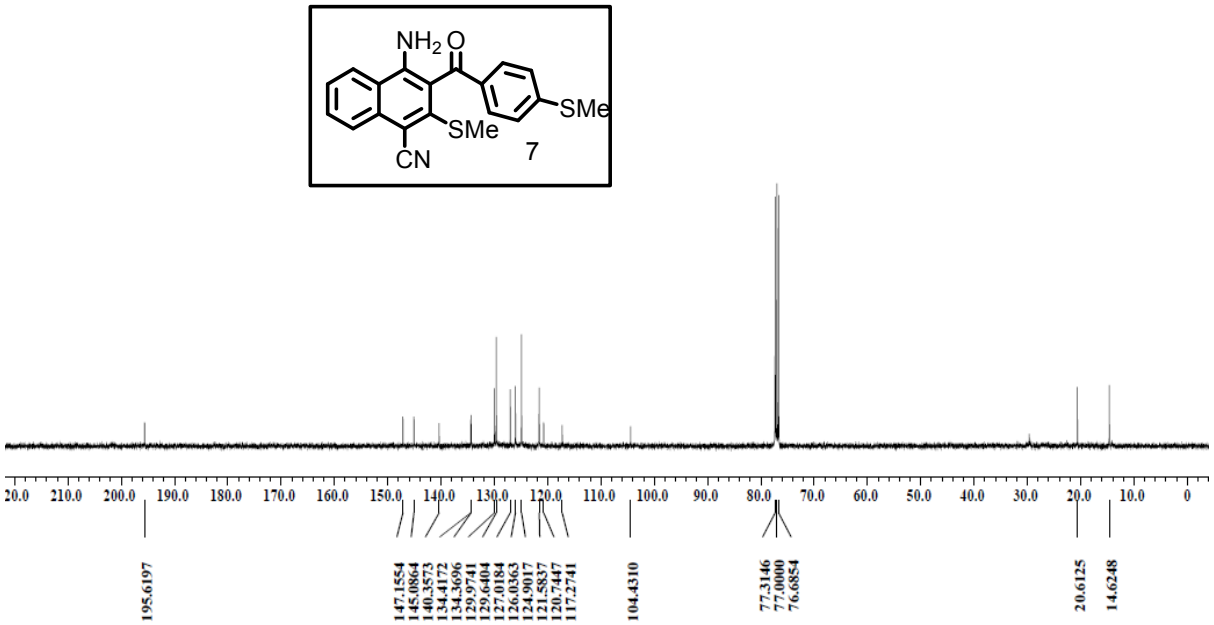
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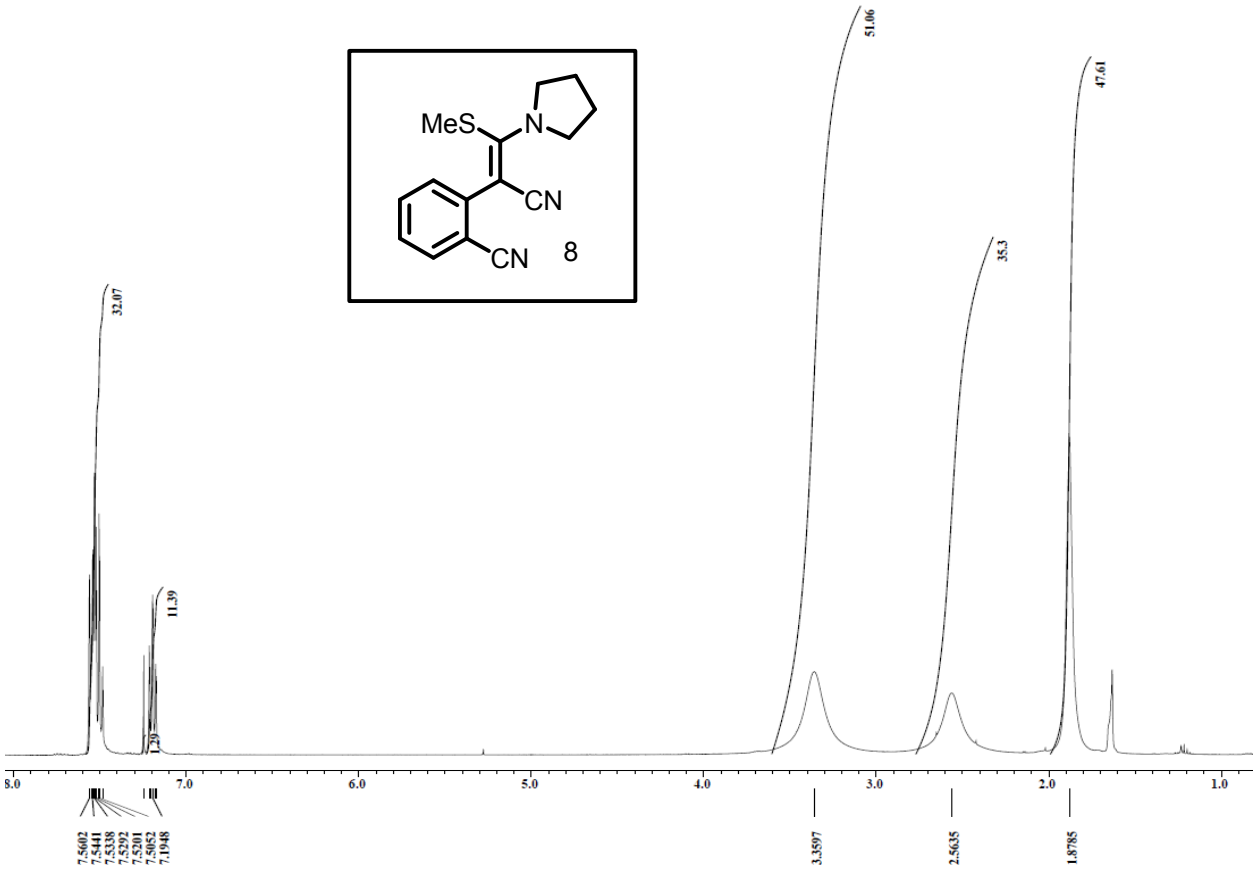
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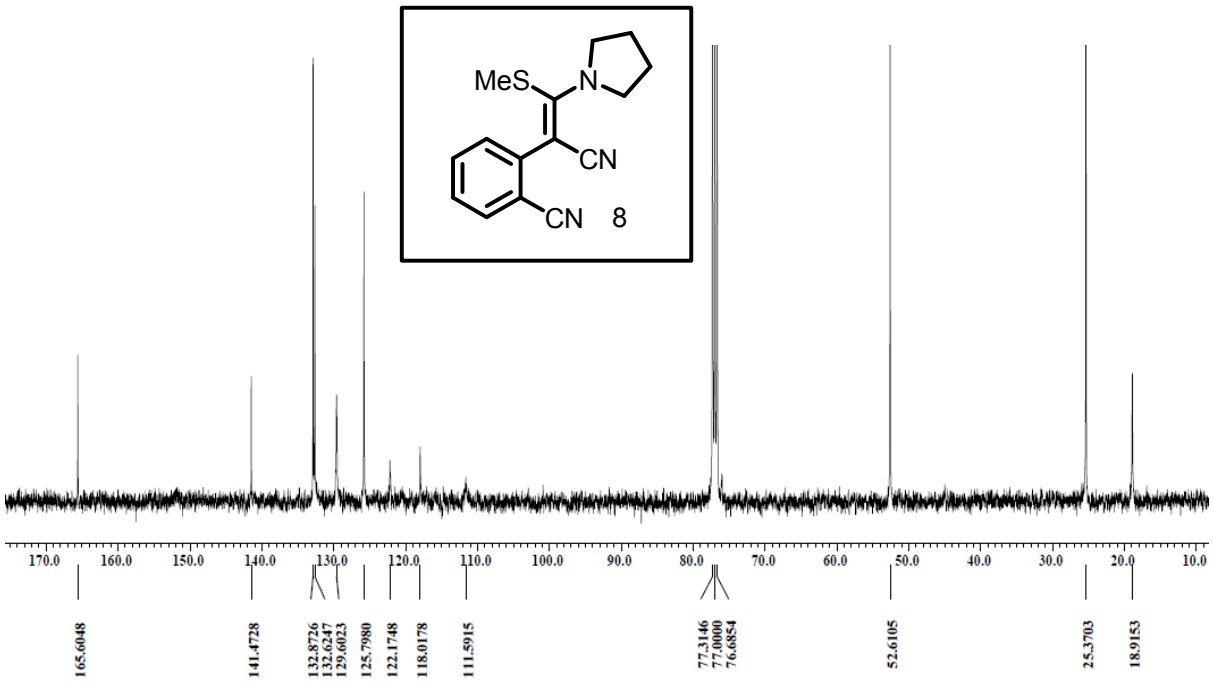
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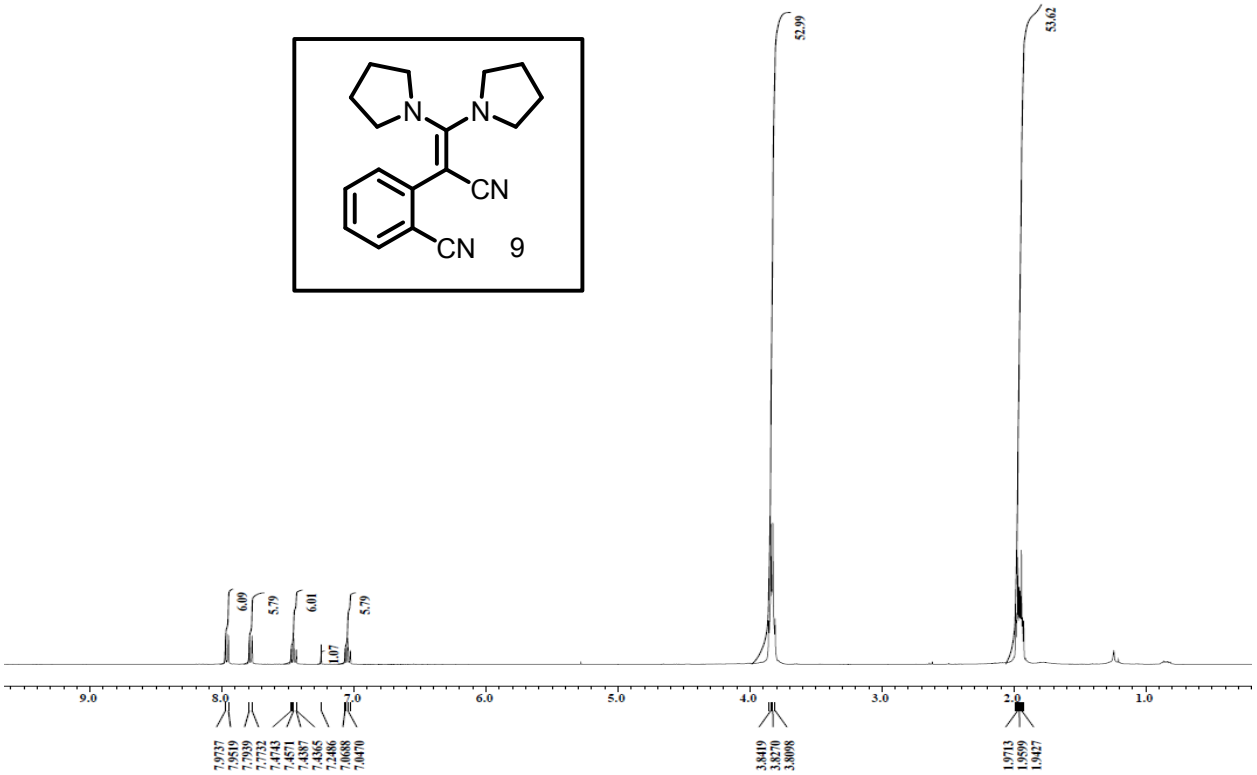
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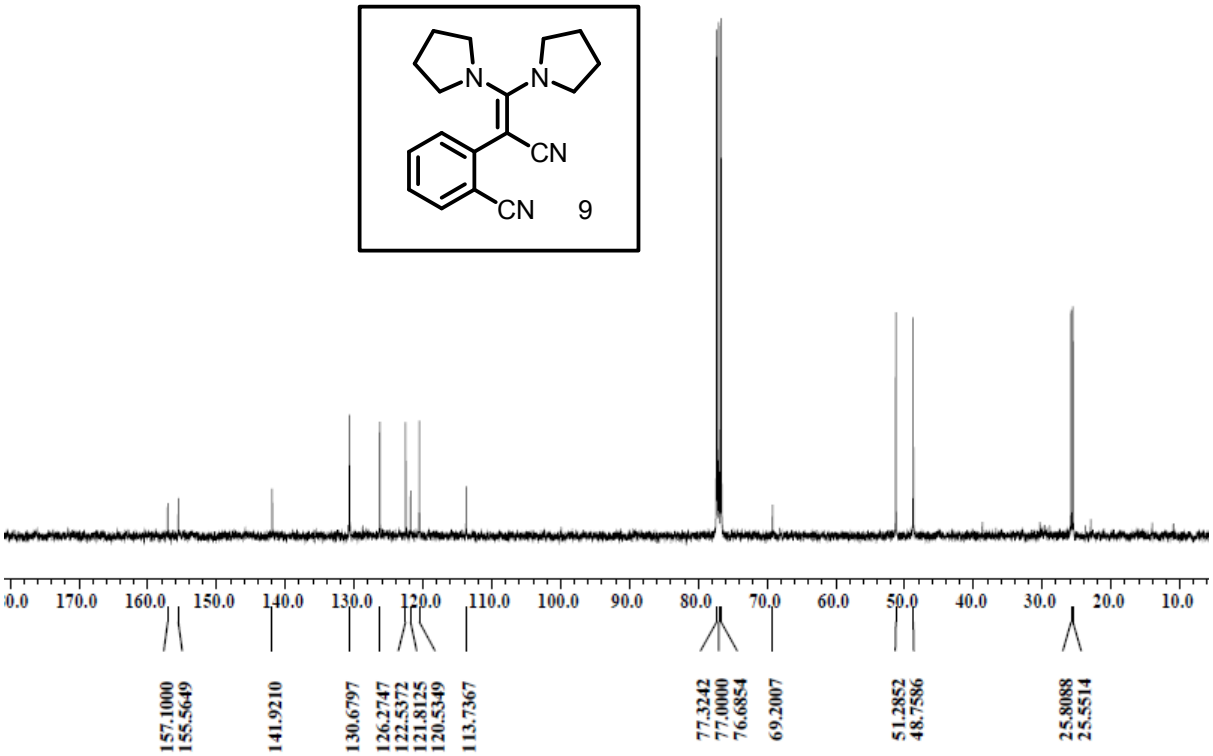
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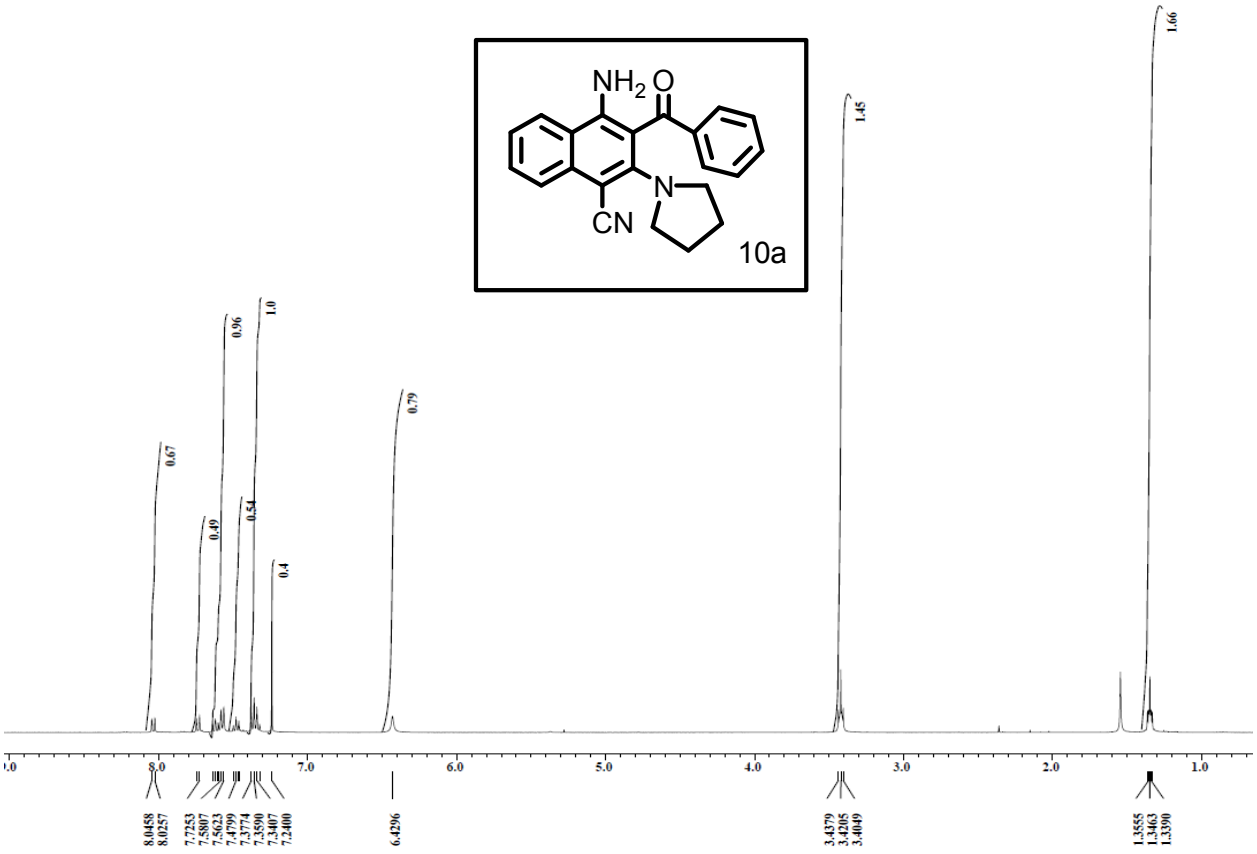
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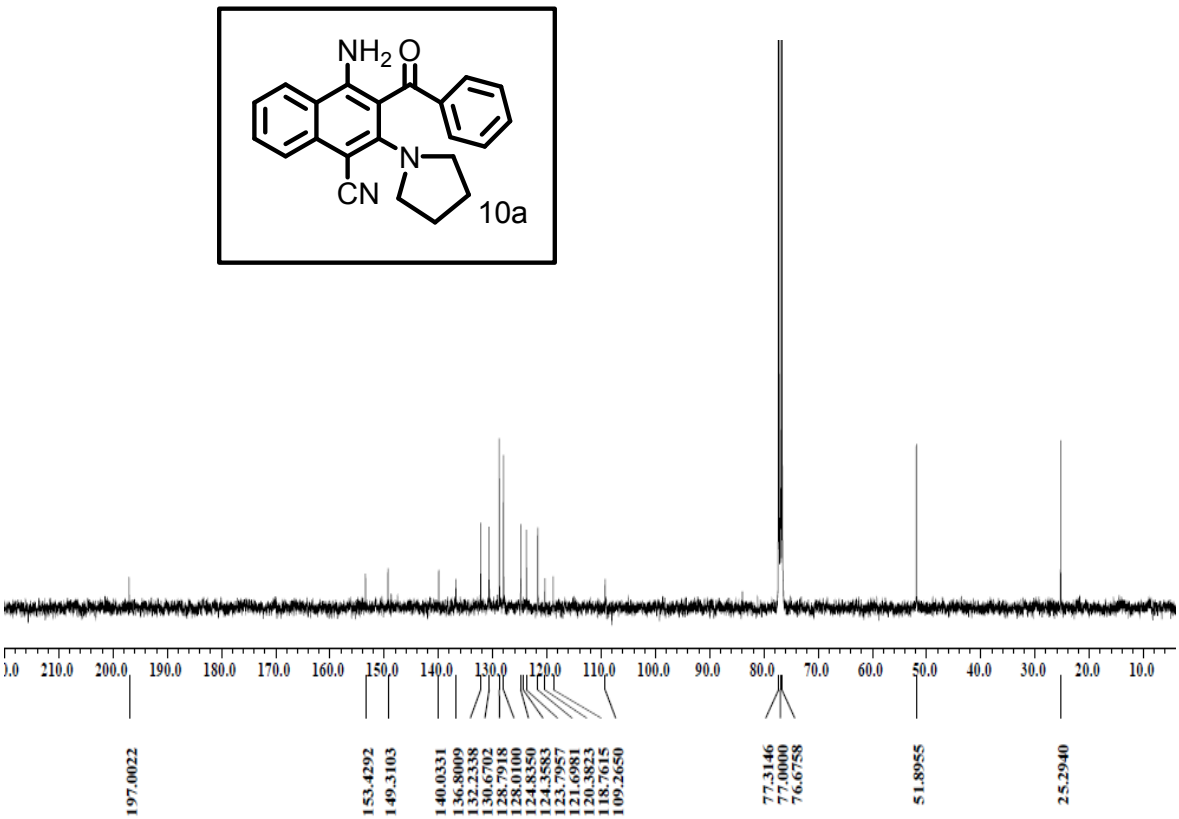
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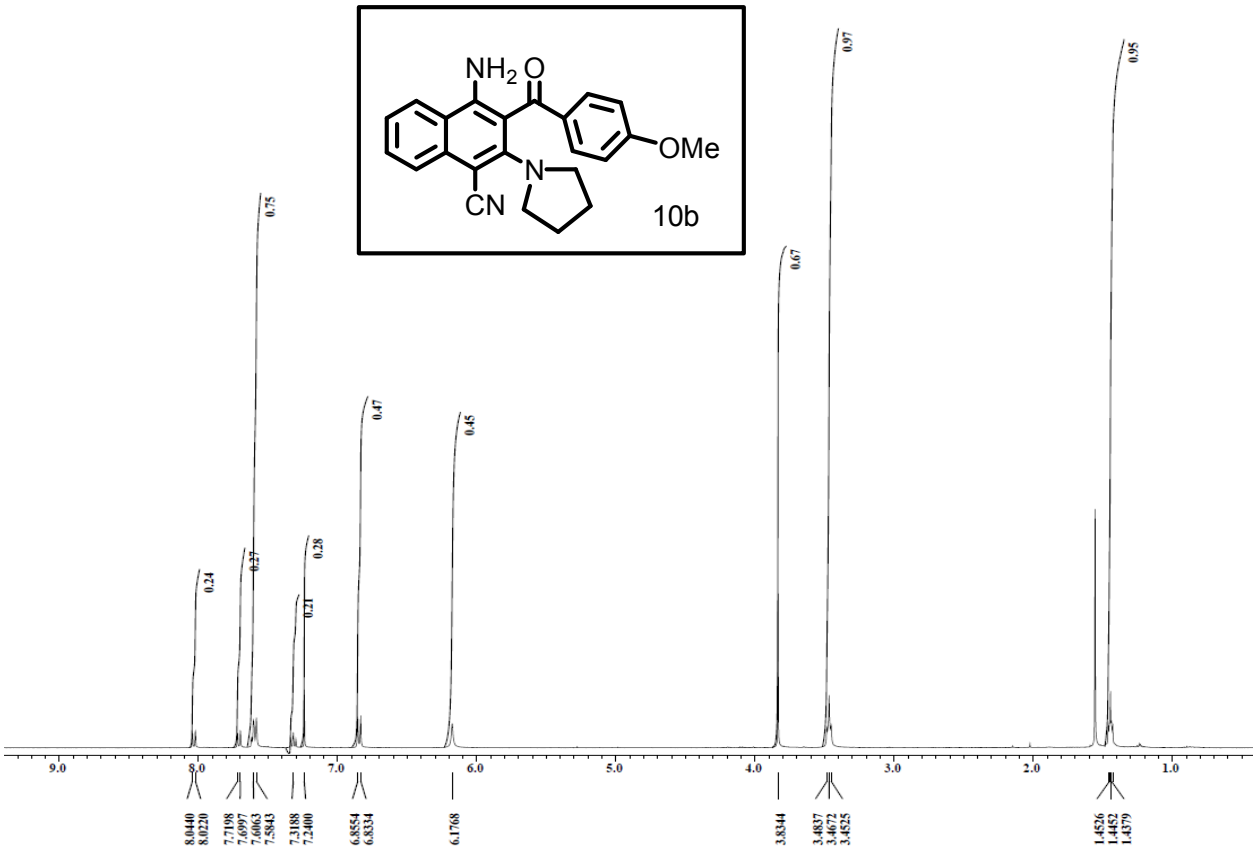
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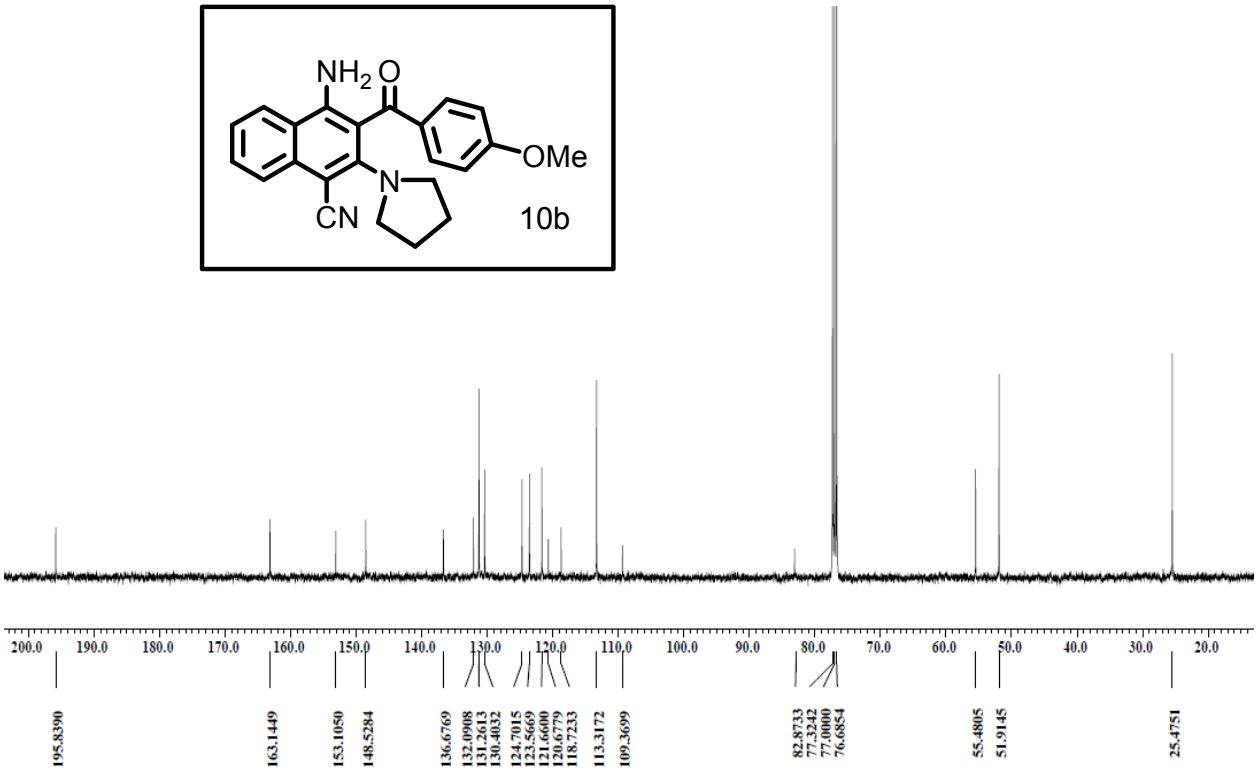
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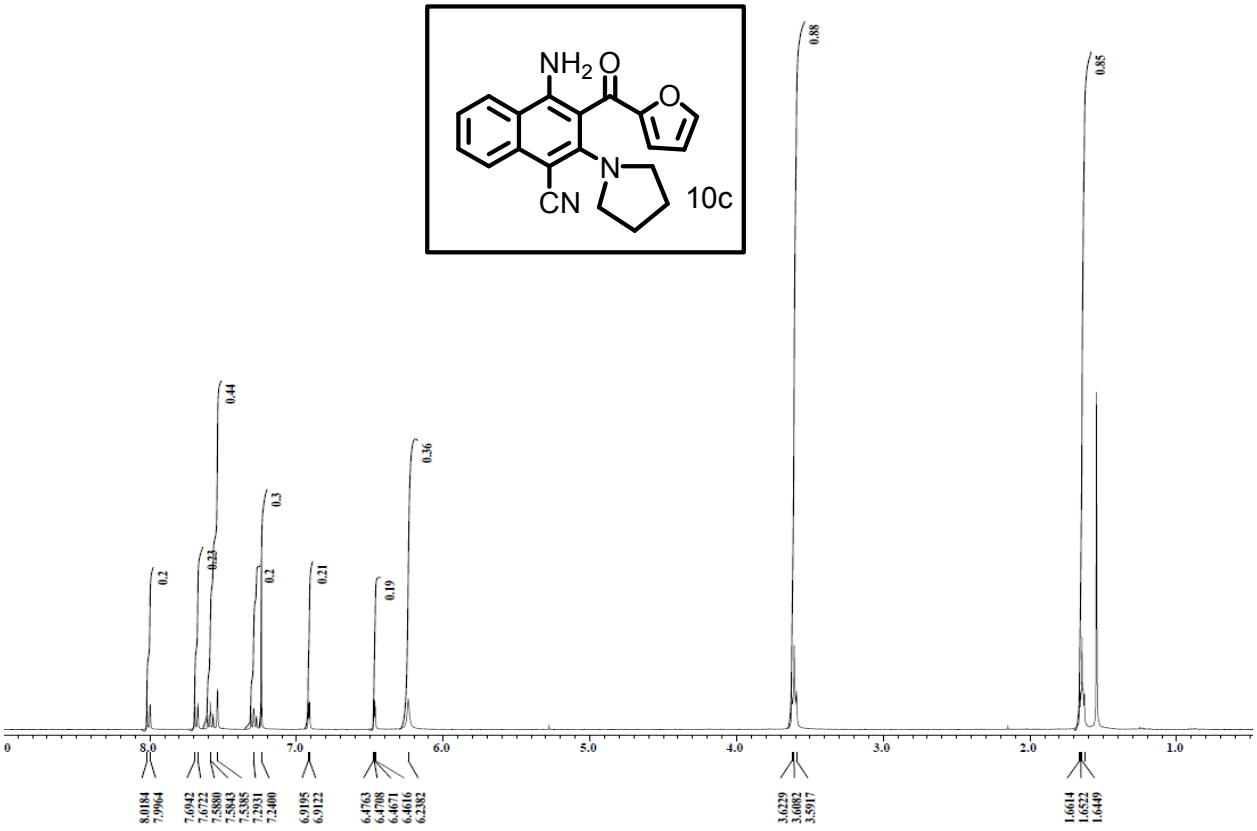
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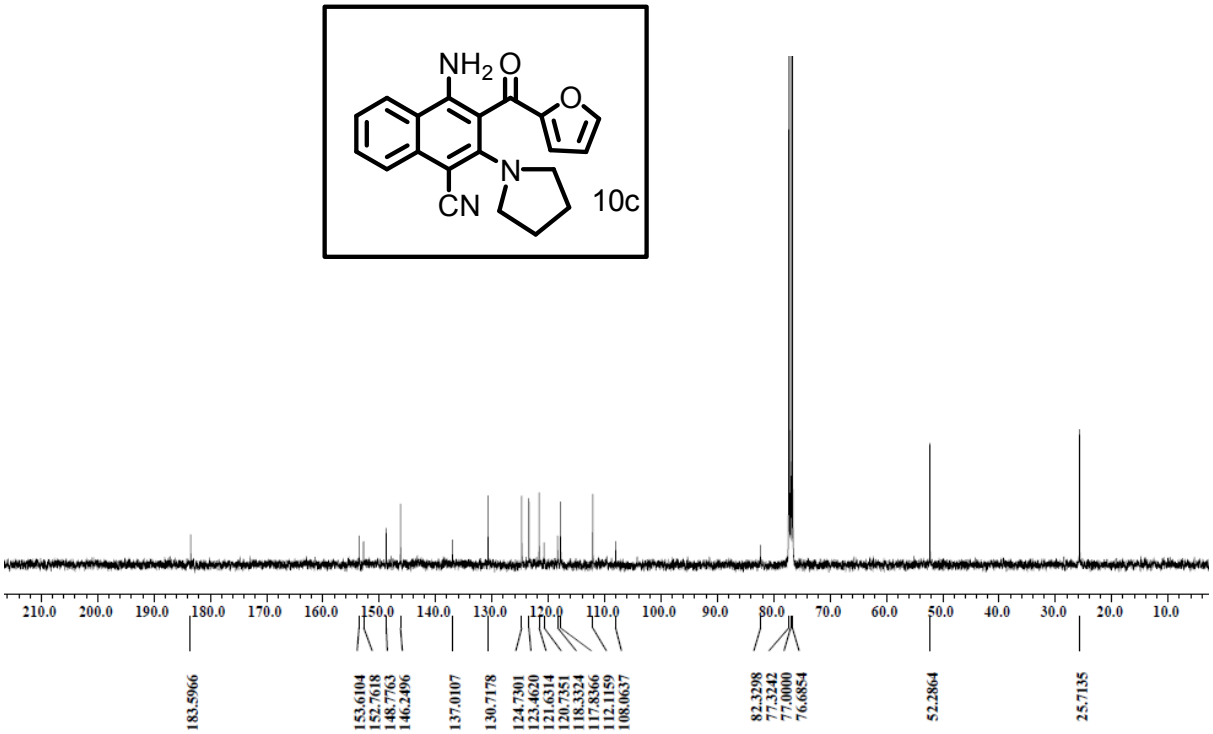
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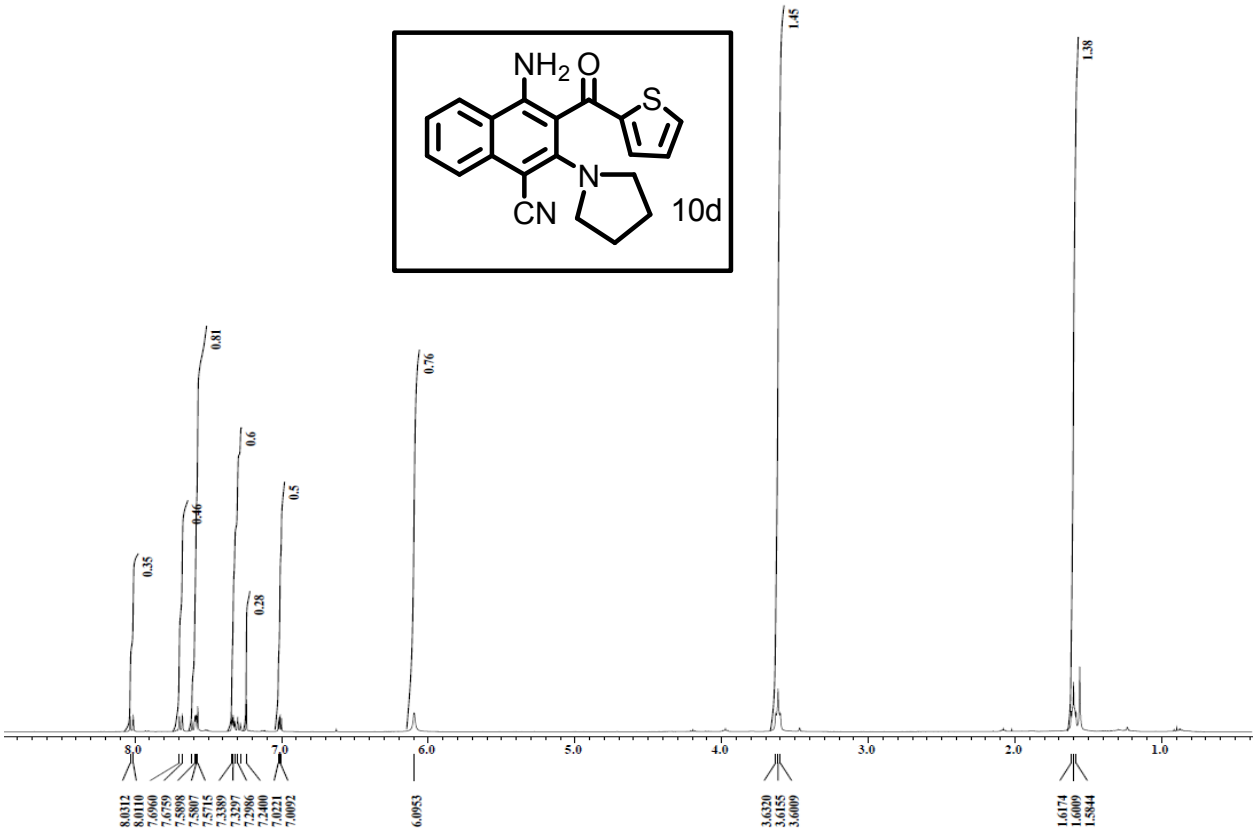
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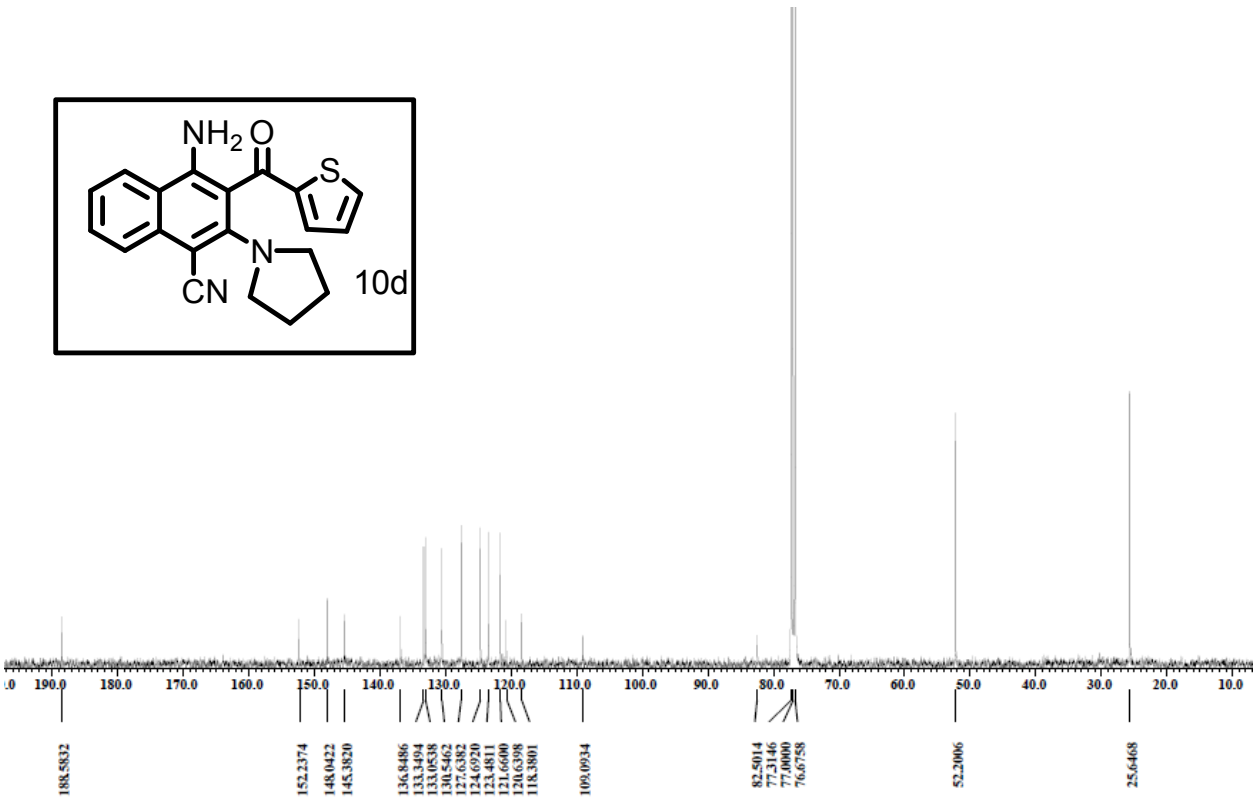
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NMR Study of reaction of 3 and acetone and acetone-d6

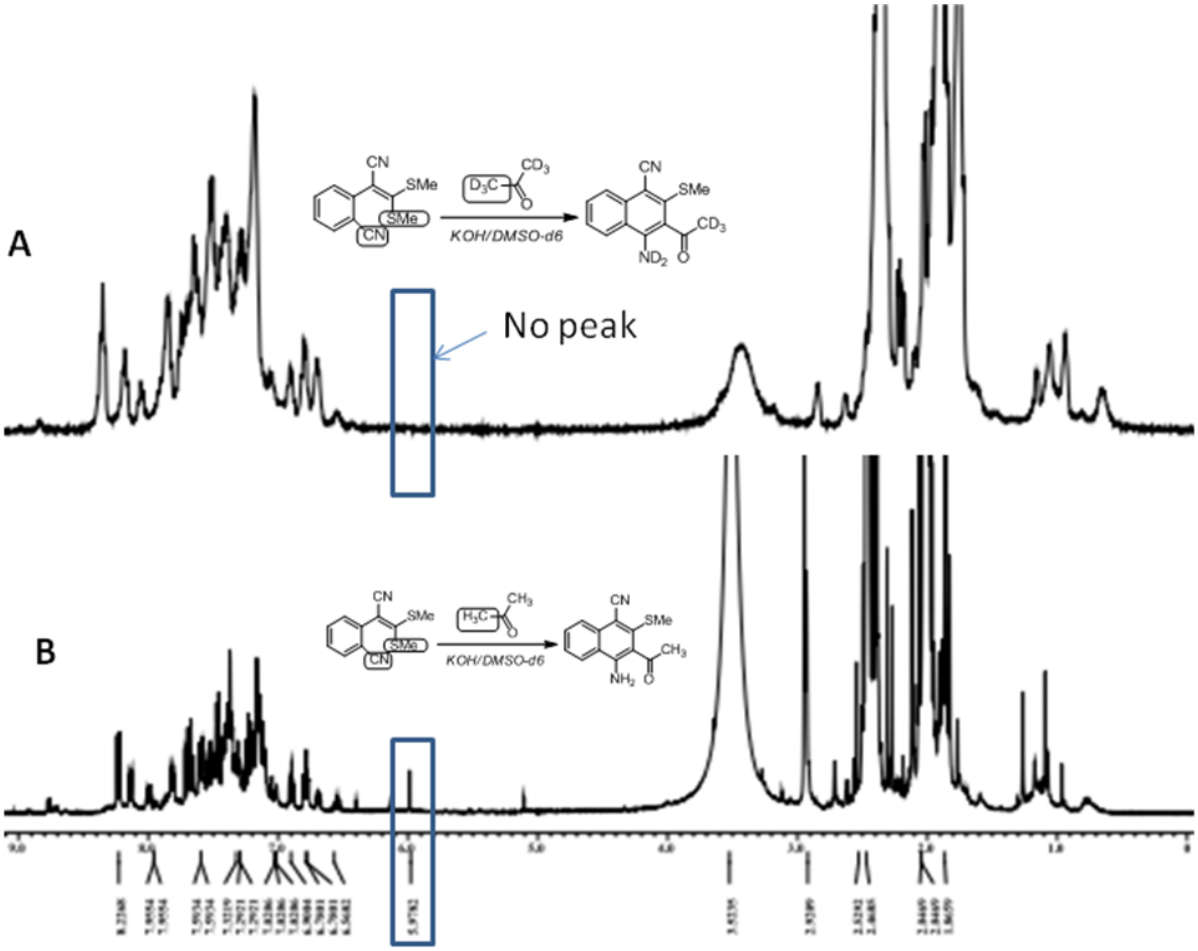

Figure 1: NMR showing the apperance of peak at ~5.98 (appear from NH_2) [A] NMR of reaction mixture containg **3** and acetone-d6; [B] NMR of reaction mixture containg **3** and acetone;

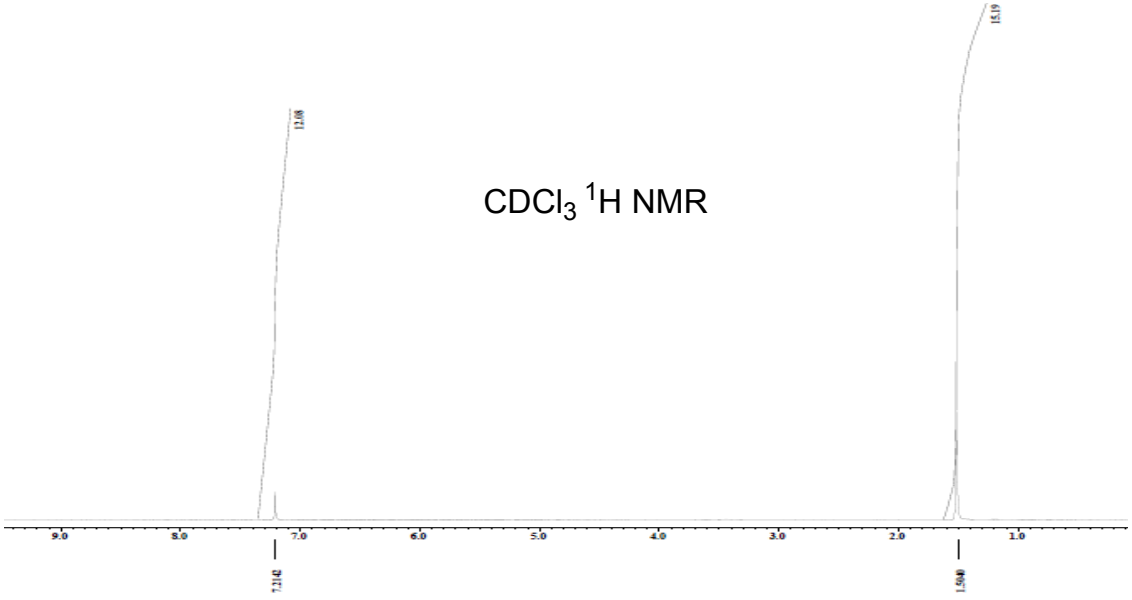

Figure 2: ^1H NMR of neat $CDCl_3$

Crystallography

Intensity data for the yellow coloured crystal of **10b** was collected at 298(2) K on a OXFORD CrysAlis diffractometer system equipped with graphite monochromated Mo Kα radiation λ = 0.71073 Å. The final unit cell determination, scaling of the data, and corrections for Lorentz and polarization effects were performed with CrysAlis RED [1]. The structures were solved by direct methods (SHELXS-97) [2] and refined by a full-matrix least-squares procedure based on F^2 [3]. All the calculations were carried out using WinGX system Ver-1.64 [4]. All non-hydrogen atoms were refined anisotropically; hydrogen atoms were located at calculated positions and refined using a riding model with isotropic thermal parameters fixed at 1.2 times the U_{eq} value of the appropriate carrier atom.

Computational Details

In order to understand the stability of various non-covalent interactions and π-stacking motifs, some quantum chemical calculations were carried out. All the calculations were performed using the Gaussian09 package.[5] Initial geometries of the π-stacked and non-covalentaly bonded dimers and trimers were taken from the respective crystal structures. Starting from these initial geometries all dimeric and trimeric motifs were optimized by keeping the interaction distances frozen. All calculations were performed at the density functional theory (DFT) level using B3LYP[6] functional and 6-31G** basis set for all the atoms. The stabilization energies for *n*-meric (dimeric [n = 2] and trimeric [n = 3]) motifs involving the n number of molecules ($\Delta E_{\text{n-mer}}$) was calculated from the formula $\Delta E_{\text{n-mer}} = E_{\text{n-mer}} - (n \times E_{\text{monomer}})$. E_{monomer} was calculated by optimizing a single molecule at the same level of theory. The intermolecular interaction strengths are significantly weaker than either ionic or covalent bonding, therefore it was essential to do basis set superposition error (BSSE) corrections. The BSSE corrections in the interaction energies were done using Boys-Bernardi scheme. In this paper all interaction energies have been reported after BSSE correction.[7]

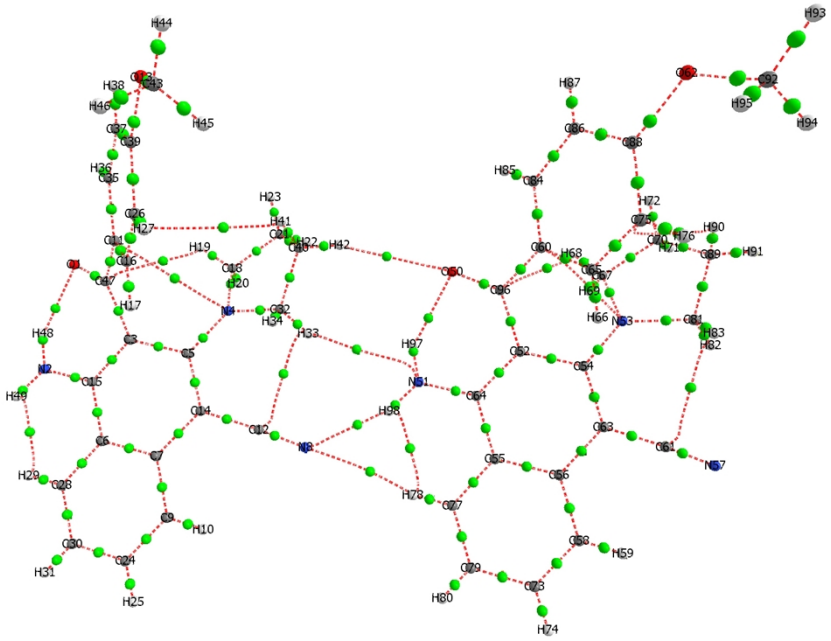

Fig. S1 Molecular graph of the dimer held by N−H···N≡C interaction calculated by AIM using B3LYP/6-31G** level of theory.

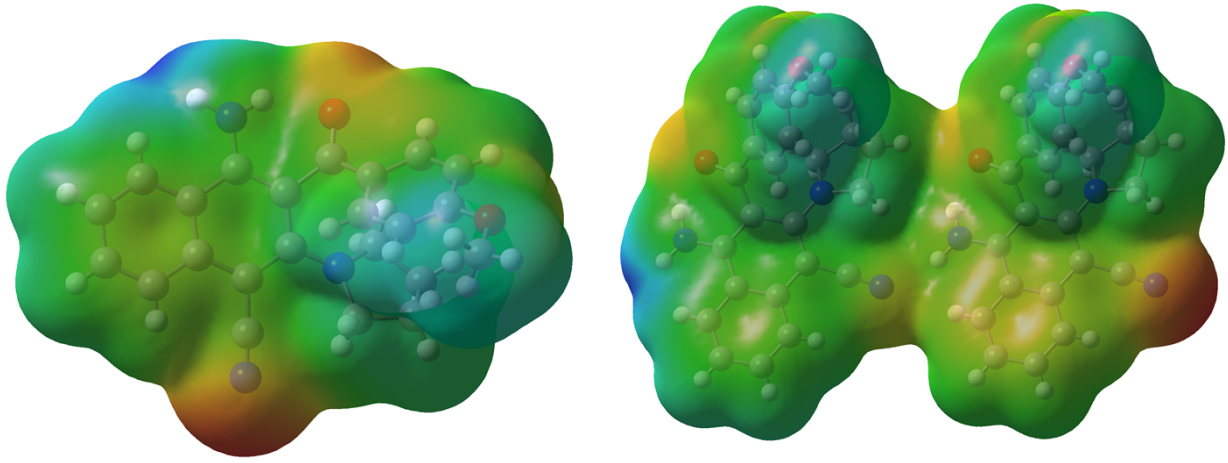

Fig. S2 Electrostatic potential surface for the monomer and dimer, red region indicates the electron rich while blue region is indicative of the electron deficient sites.

1. CrysAlis CCD, RED version 1.711.13, copyright 1995-2003, Oxford Diffraction Poland Sp.
2. Sheldrick, G. M. SHELXS97, Program for Crystal Structure Solution, University of Göttingen, Göttingen, **1997**.
3. Sheldrick, G. M. SHELXL97, Program for Crystal Structure Refinement, University of Göttingen, Göttingen, **1997**.

4. Farrugia, L. J.; WinGX-A Wnidow Program for Crystal Structure Analysis, *J. Appl. Crystallogr.,* **1999**, *32*, 837-838.
5. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, T. Vreven Jr., K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. D. Dapprich, A. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, W. M. Wong, C. Gonzalez and J. A. Pople, Gaussian 09 (Revision C. 01) Gaussian, Inc., Wallingford CT, 2009.
6. (a) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (b) C. T. Lee, W. T. Yang and R. G. Parr, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1998, **37**, 1133.
7. S. F. Boys and F. Bernardi, *Mol. Phys.*, 1970, **19**, 553.

Tables of atom coordinates

Monomer

E= -1203.4827225

Standard orientation:

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6	6	0	3.163980	-0.924611	0.191254
7	6	0	3.037445	0.432798	0.555382
8	7	0	2.106427	3.731045	0.457274
9	6	0	4.089071	1.020858	1.286104
10	1	0	4.020974	1.910113	1.549706
11	6	0	-1.577424	-1.280123	-0.294905
12	6	0	1.978383	2.600954	0.298538
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15	6	0	2.085643	-1.542468	-0.553110
16	6	0	-1.593476	-0.607614	0.916301
17	1	0	-0.789669	-0.321864	1.286628
18	6	0	-0.892357	1.021603	-2.333562
19	1	0	-1.242191	0.117736	-2.372681
20	1	0	-0.270514	1.150078	-3.066859
21	6	0	-2.004975	2.029214	-2.392488
22	1	0	-1.800993	2.718473	-3.043800
23	1	0	-2.835836	1.598909	-2.648238
24	6	0	5.206835	0.307275	1.613955
25	1	0	5.895493	0.719081	2.084133
26	6	0	-2.760961	-0.353336	1.581003
27	1	0	-2.747766	0.079255	2.404157
28	6	0	4.322621	-1.629374	0.548128
29	1	0	4.410841	-2.521814	0.301791

30	6	0	5.322737	-1.023204	1.252185
31	1	0	6.082376	-1.504715	1.488813
32	6	0	-0.764734	2.501353	-0.465260
33	1	0	-0.216722	3.263222	-0.710535
34	1	0	-0.807500	2.442082	0.501983
35	6	0	-2.782167	-1.702481	-0.823365
36	1	0	-2.793656	-2.180072	-1.621279
37	6	0	-3.955358	-1.424577	-0.184056
38	1	0	-4.761385	-1.695090	-0.560961
39	6	0	-3.955297	-0.743383	1.020769
40	6	0	-2.125847	2.614655	-1.051693
41	1	0	-2.772197	2.125253	-0.519124
42	1	0	-2.401837	3.543046	-1.104797
43	6	0	-5.207675	0.085825	2.870388
44	1	0	-6.119399	0.193811	3.150922
45	1	0	-4.777639	0.943680	2.842731
46	1	0	-4.747043	-0.483168	3.491410
47	6	0	-0.324944	-1.623391	-1.028740
48	1	0	1.482541	-3.141117	-1.424427
49	1	0	3.014221	-3.372723	-0.725050
