A Systematic Study of Thermochromic Aromatic Donor-Acceptor Materials

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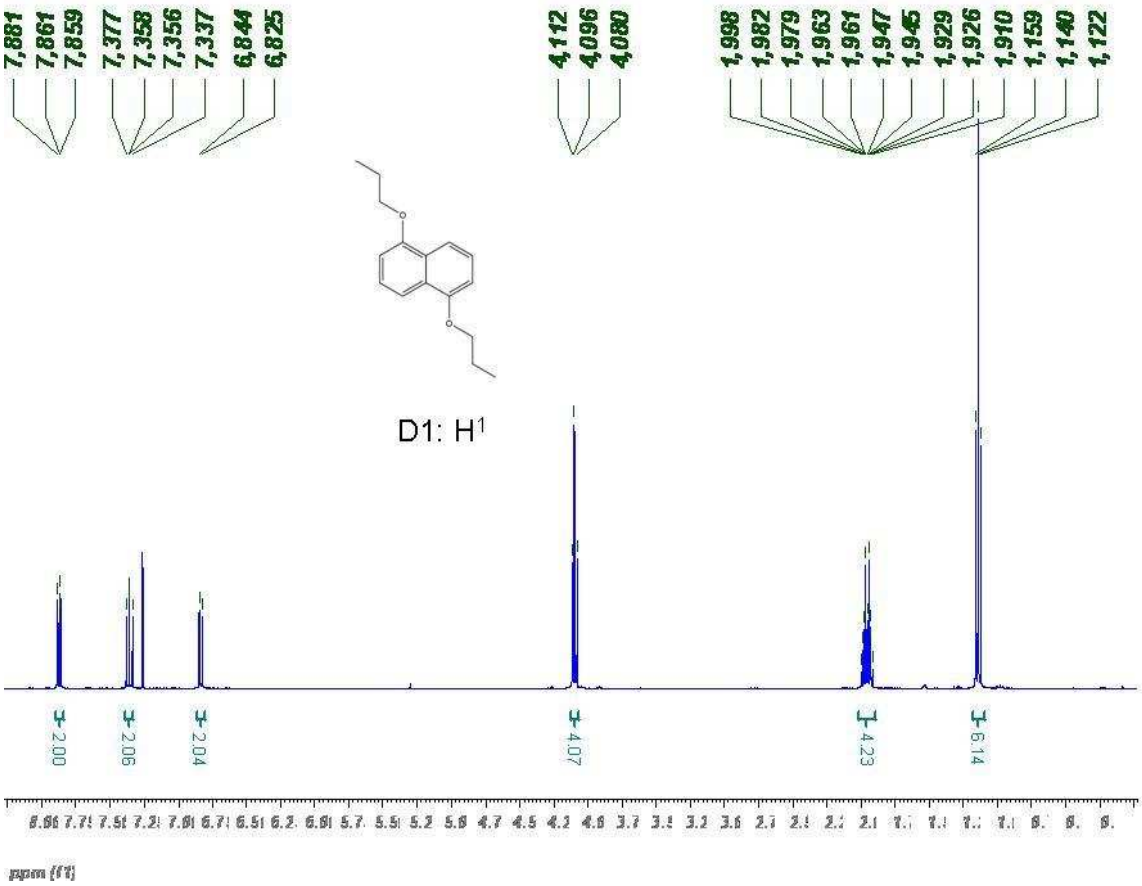
Supporting Information

Contents

Materials and Methods

All starting materials and solvents were commercially available and used without further purification. NMR spectra were taken on a 400 MHz spectrometer in $CDCl_3$. TLC was performed on silica gel plates and column chromatography was carried out using silica gel. Optical microscopy was carried out using standard glass microscope cover slips on a microscope equipped with a hot stage and digital camera. Experimental melting points of the individual components were obtained using DSC and recorded as a temperature range on the second heating cycle at 5ºC/min. UV-Vis spectra were taken of equimolar Dan:Ndi mixtures using glass microscope. All compounds were synthesized in a 60-80% yield using modifications of previously reported methods.[1,2] A CEM Microwave Accelerated Reaction System (model MARS®) was used to synthesize the Ndi derivatives.

NMR Spectra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1,929
1,926
1,910
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1,140
1,122
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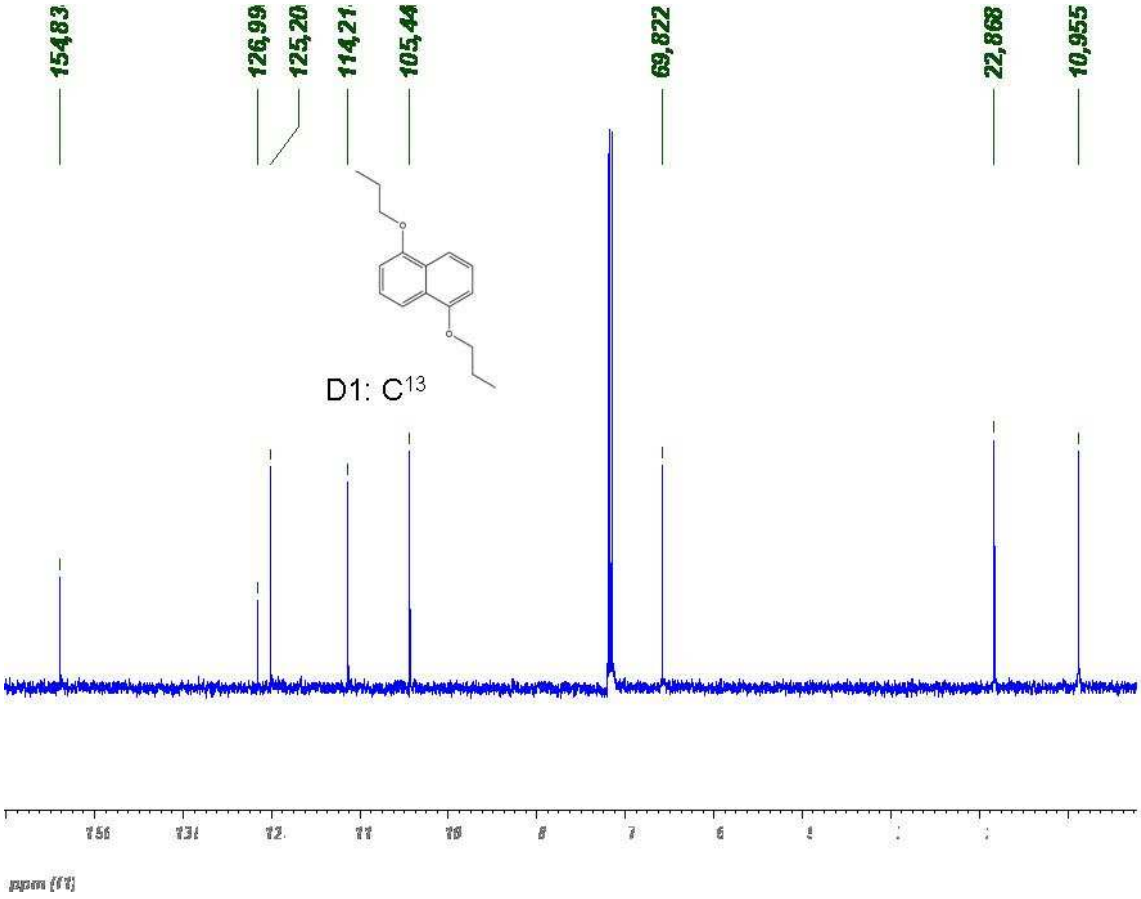
2,04
4,07
4,23
6,14
ppm (f1)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5
4
3
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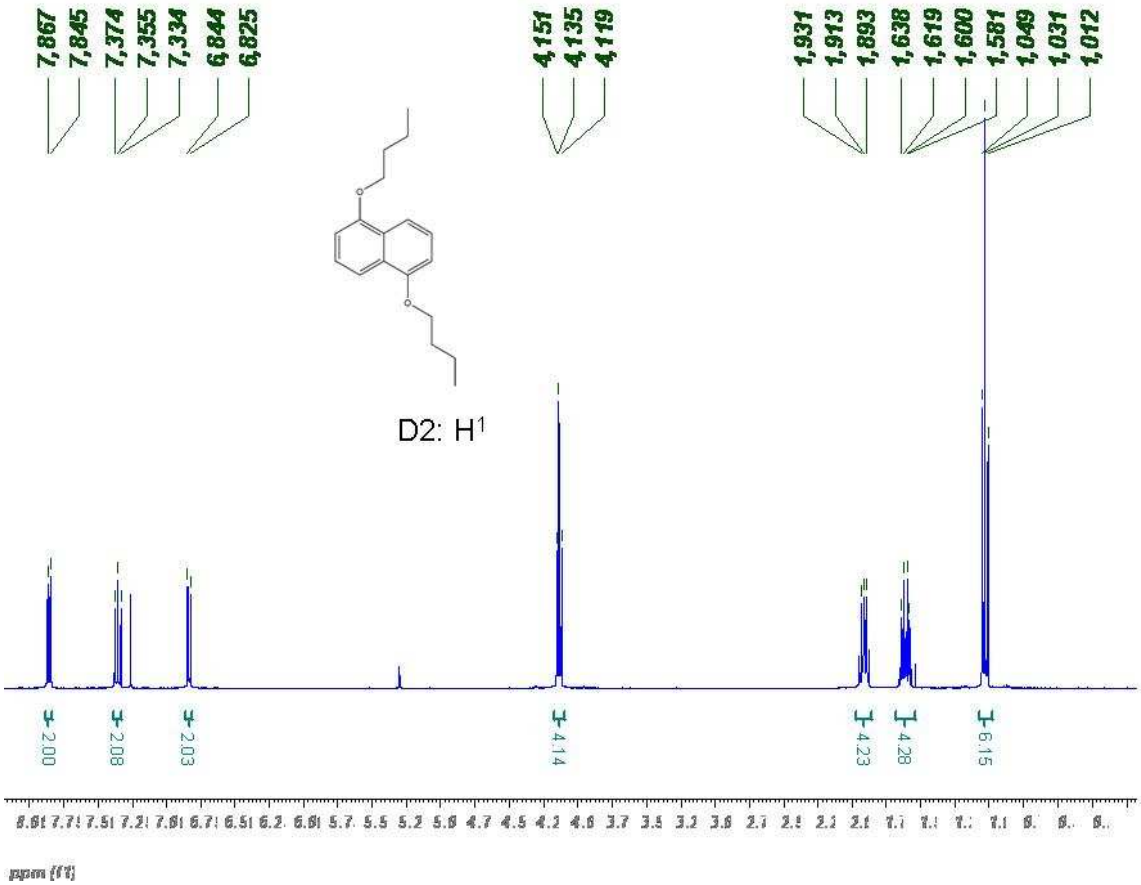
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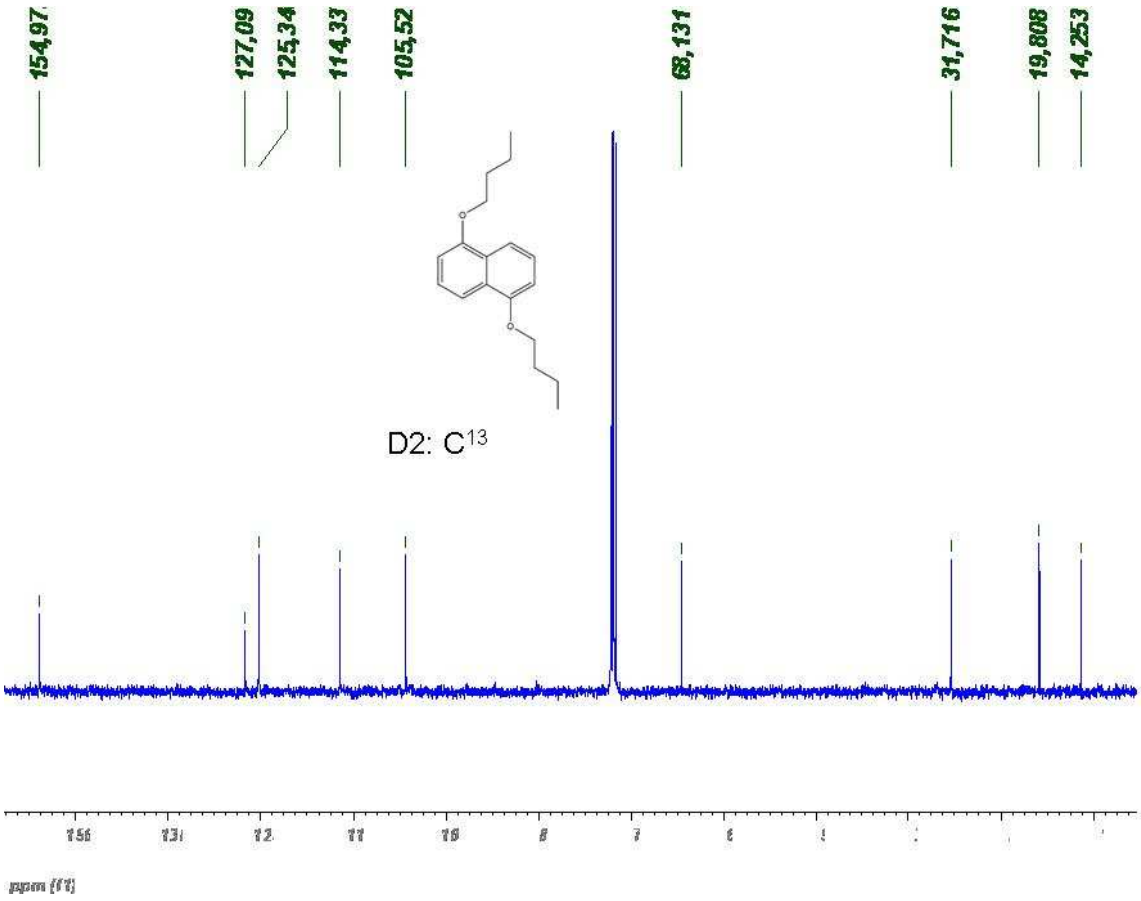
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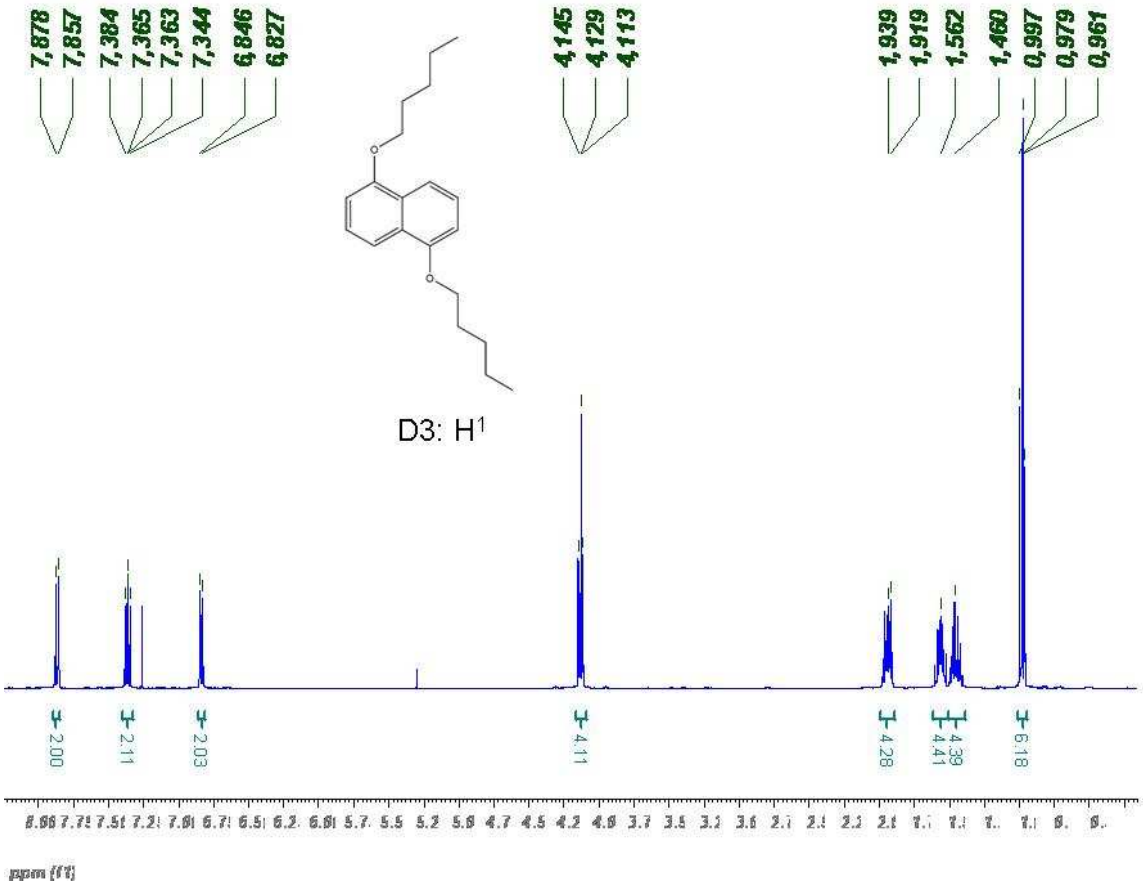
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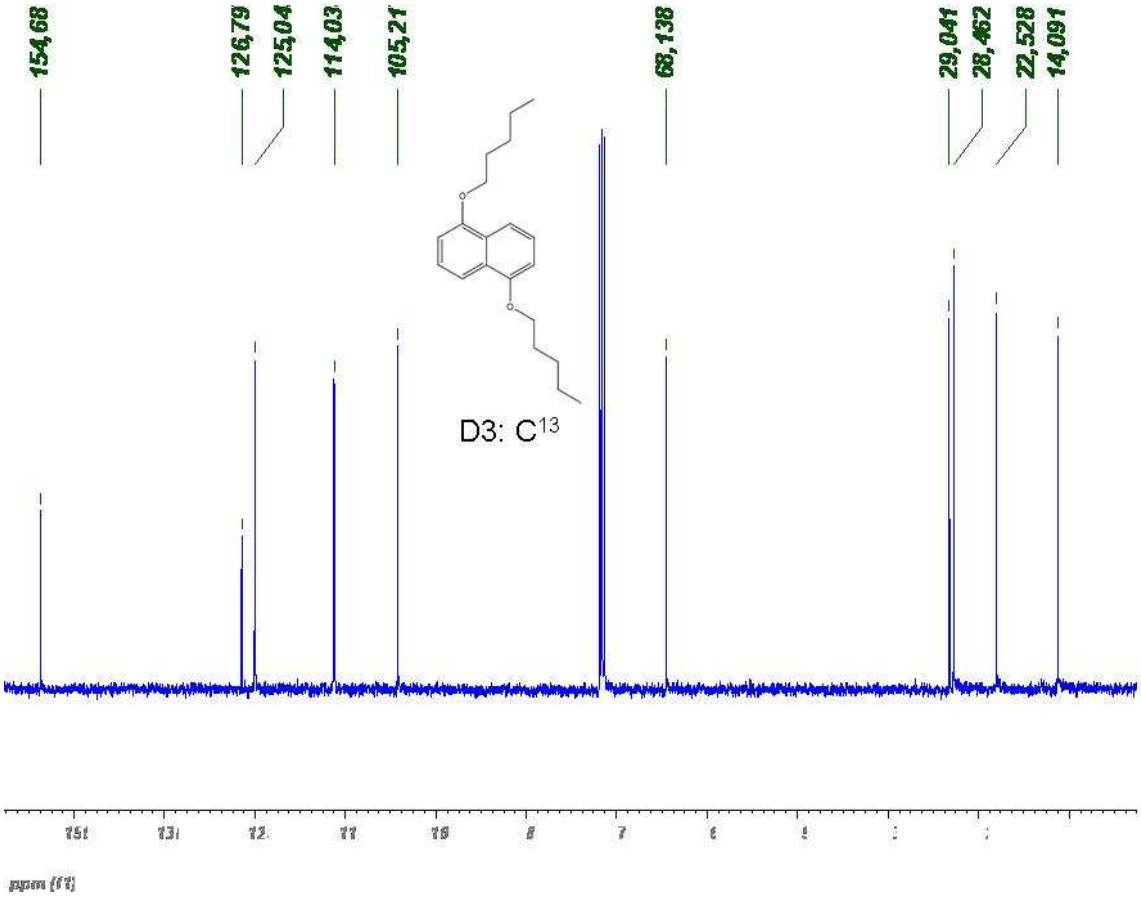
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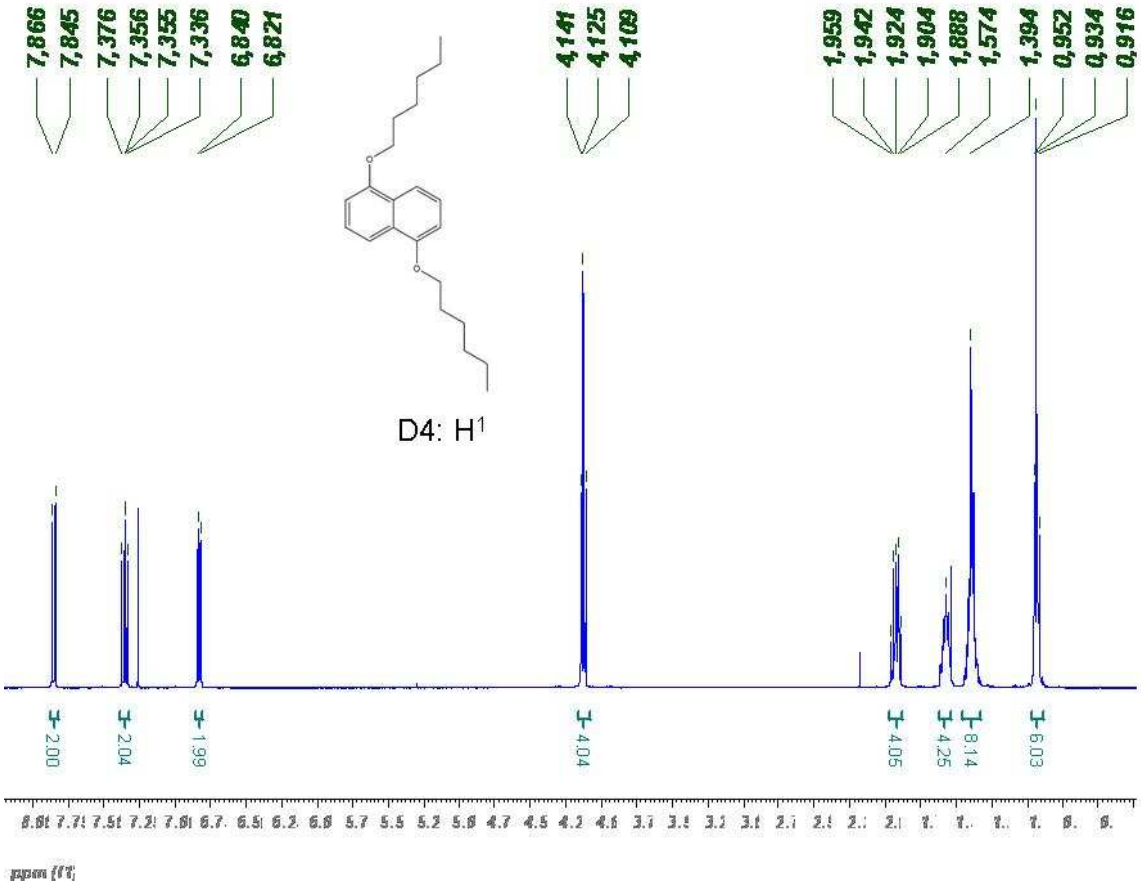
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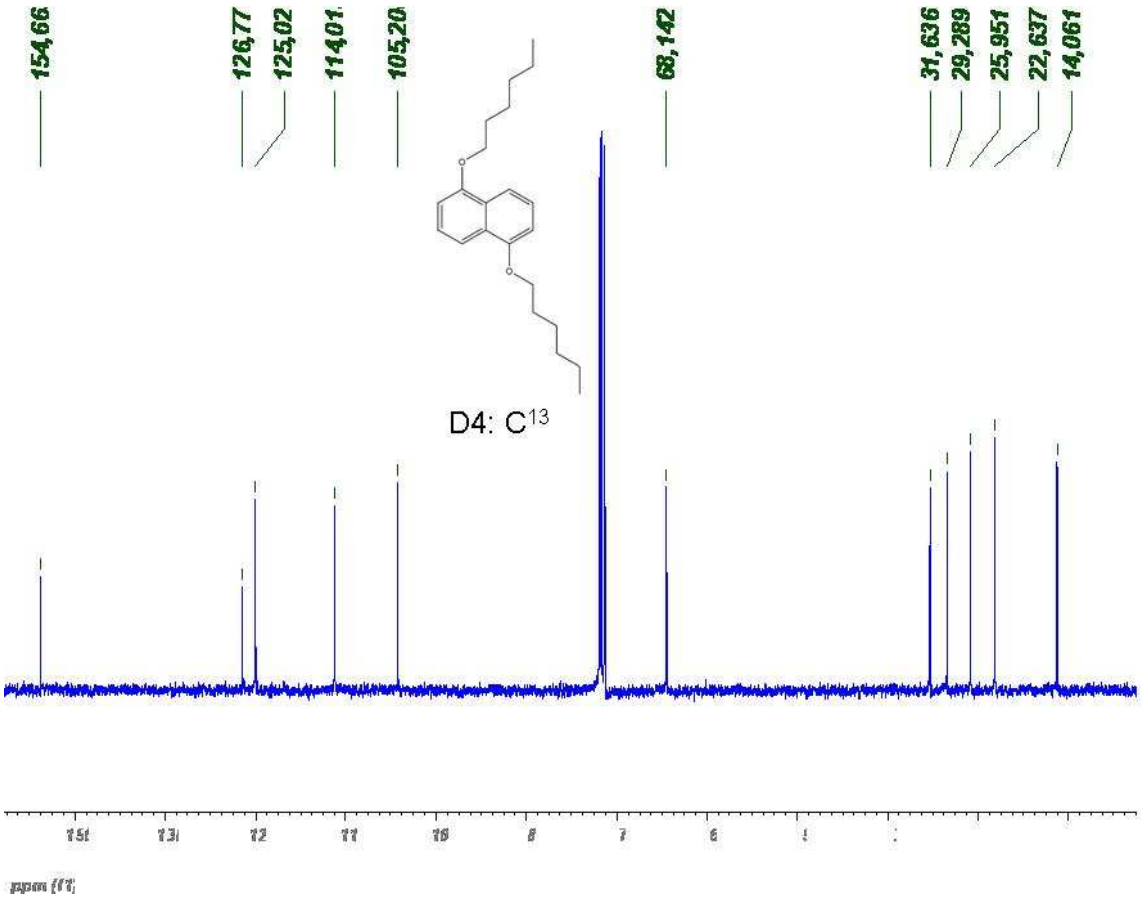
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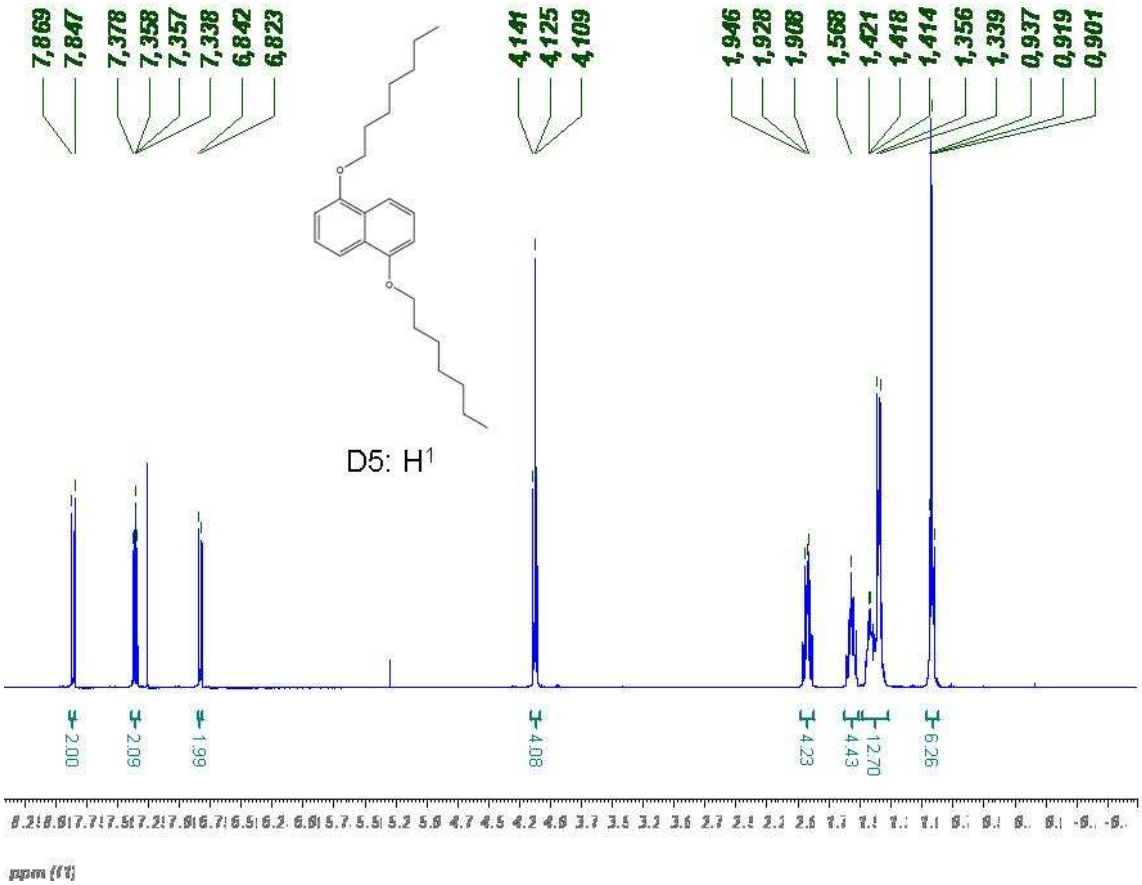
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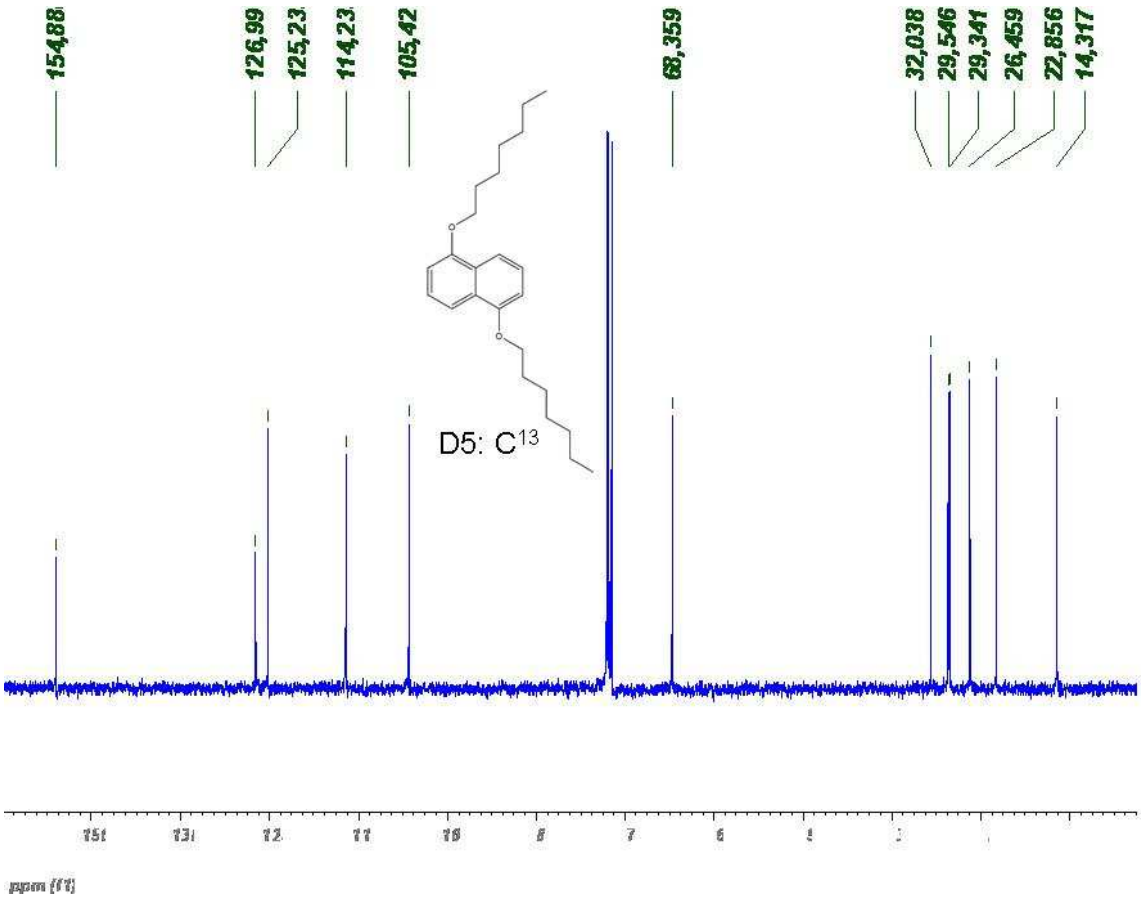
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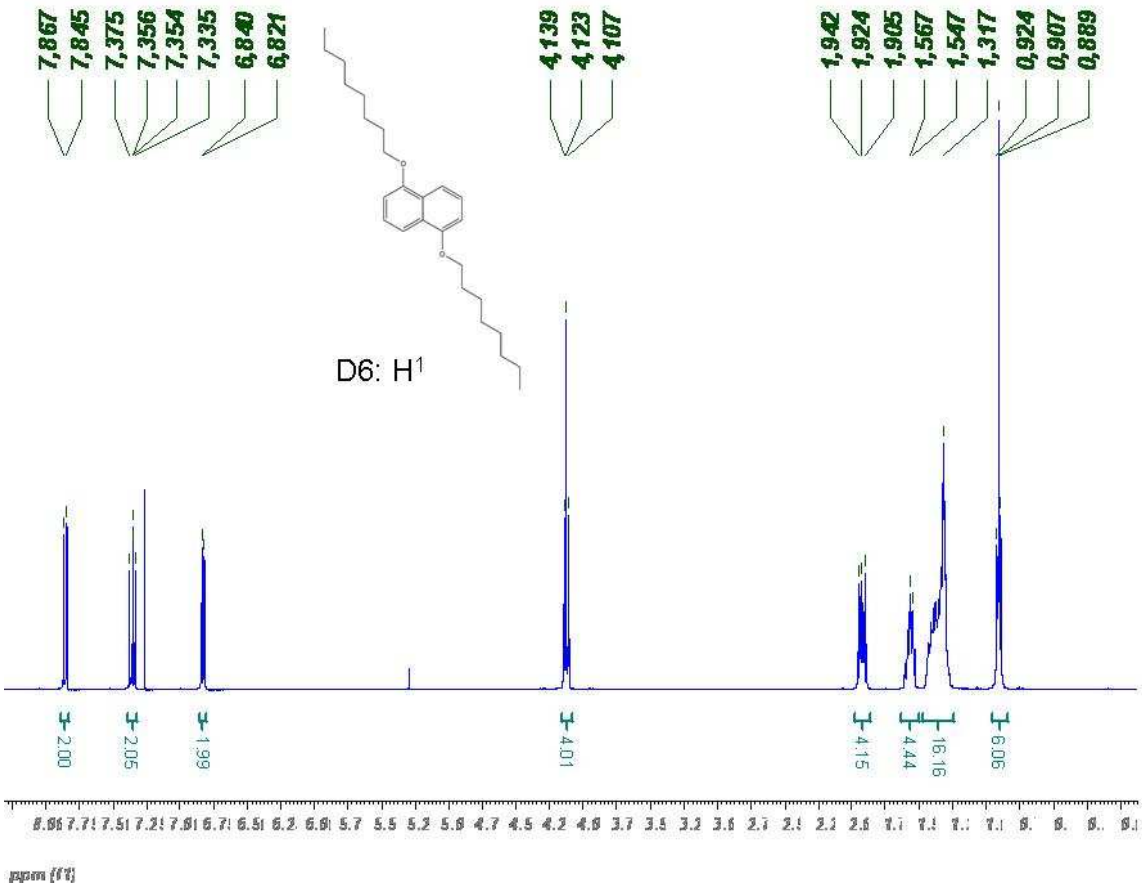
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0,907
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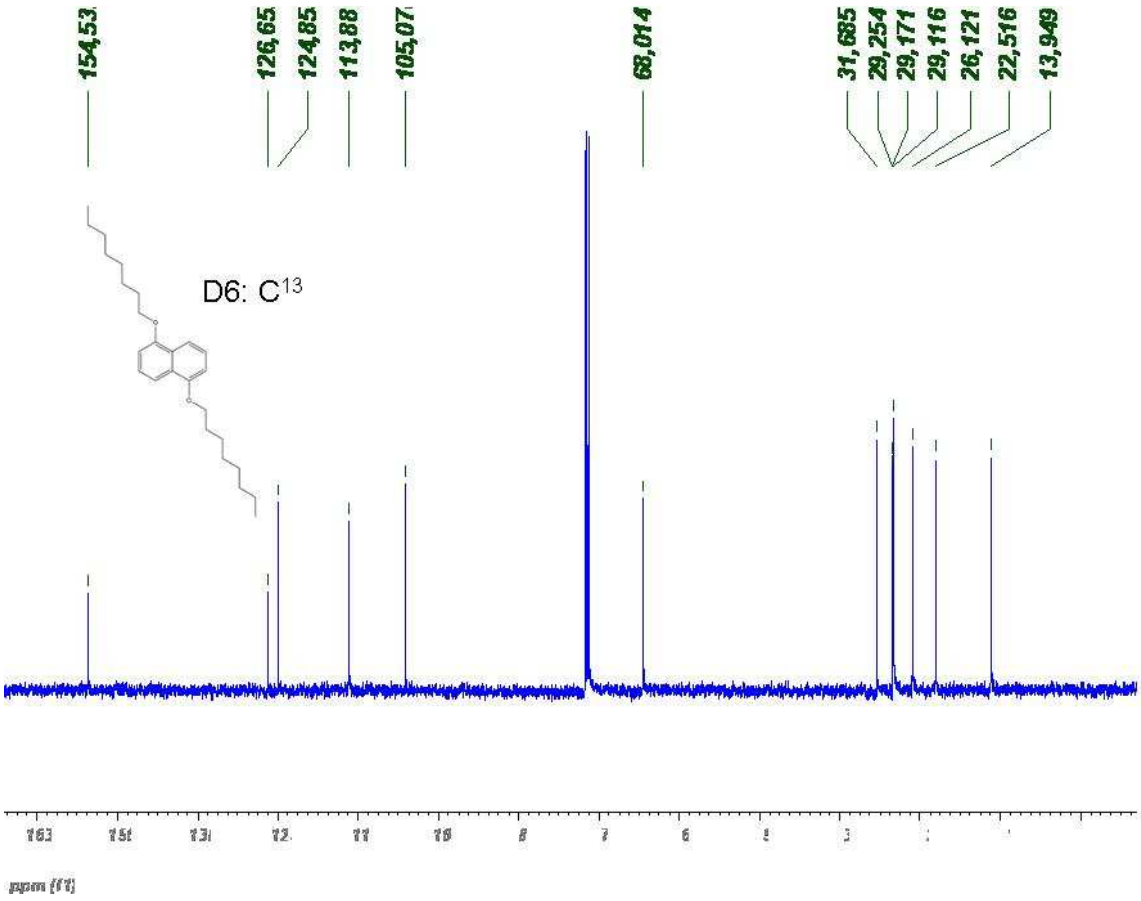
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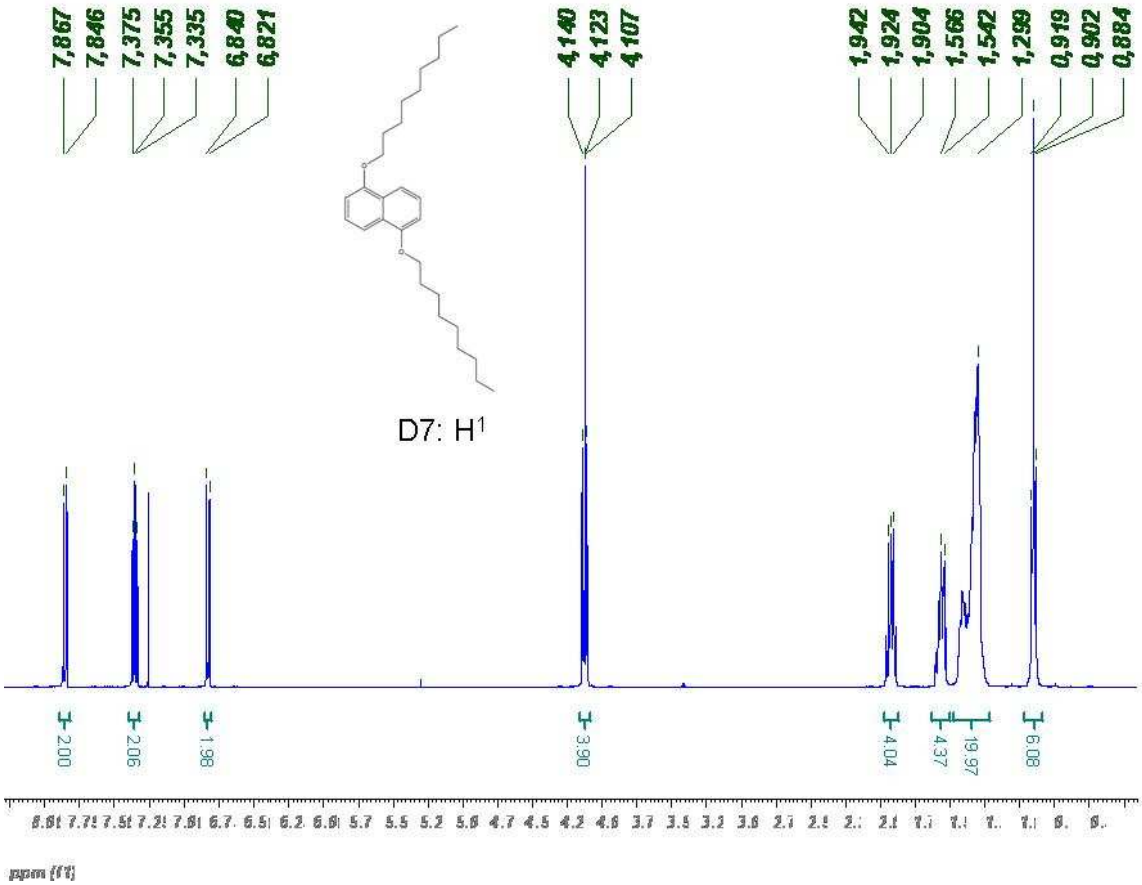
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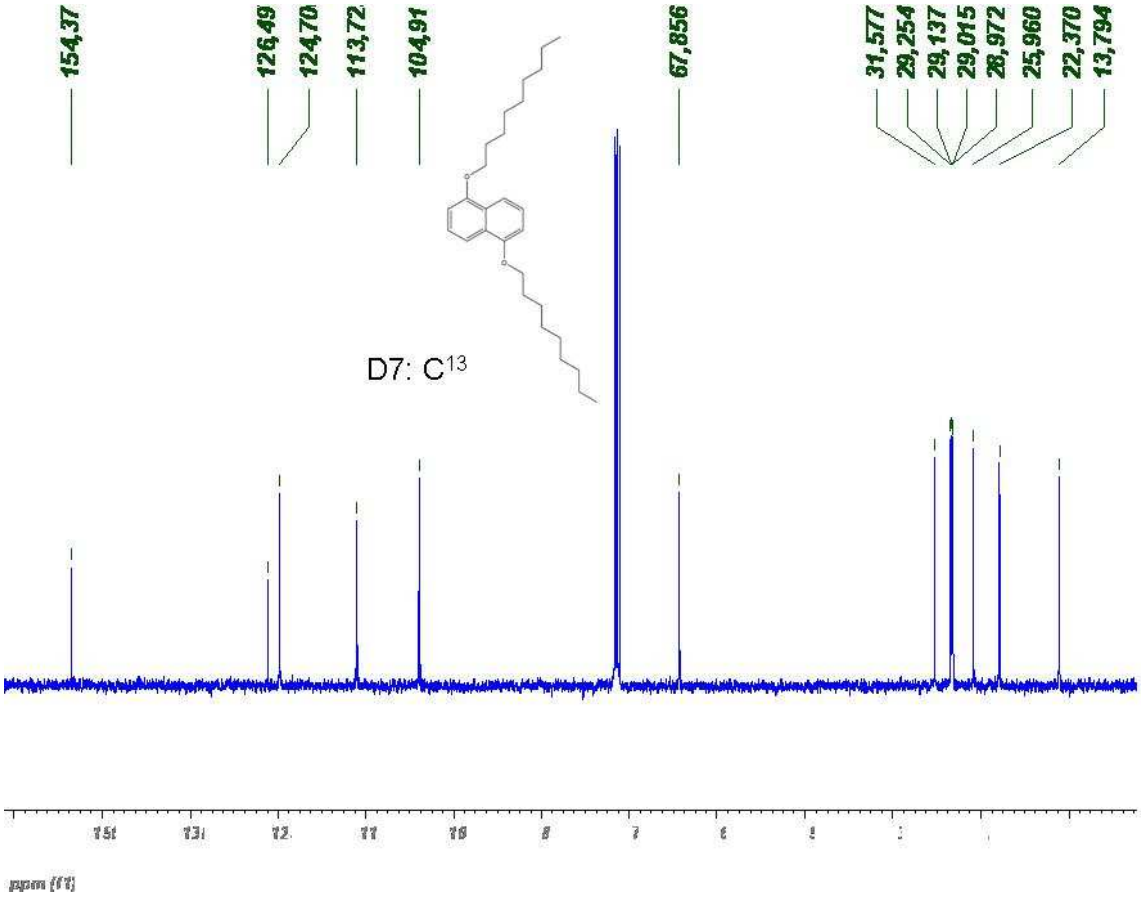
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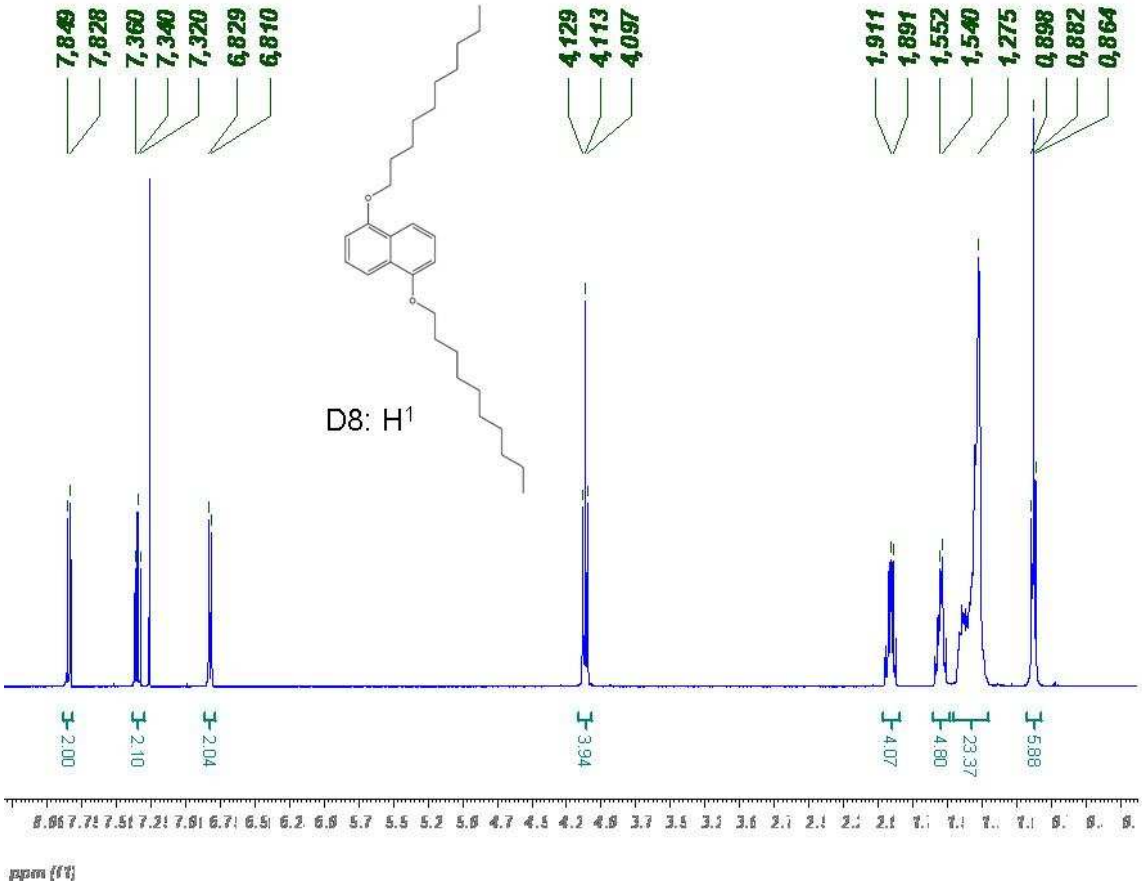
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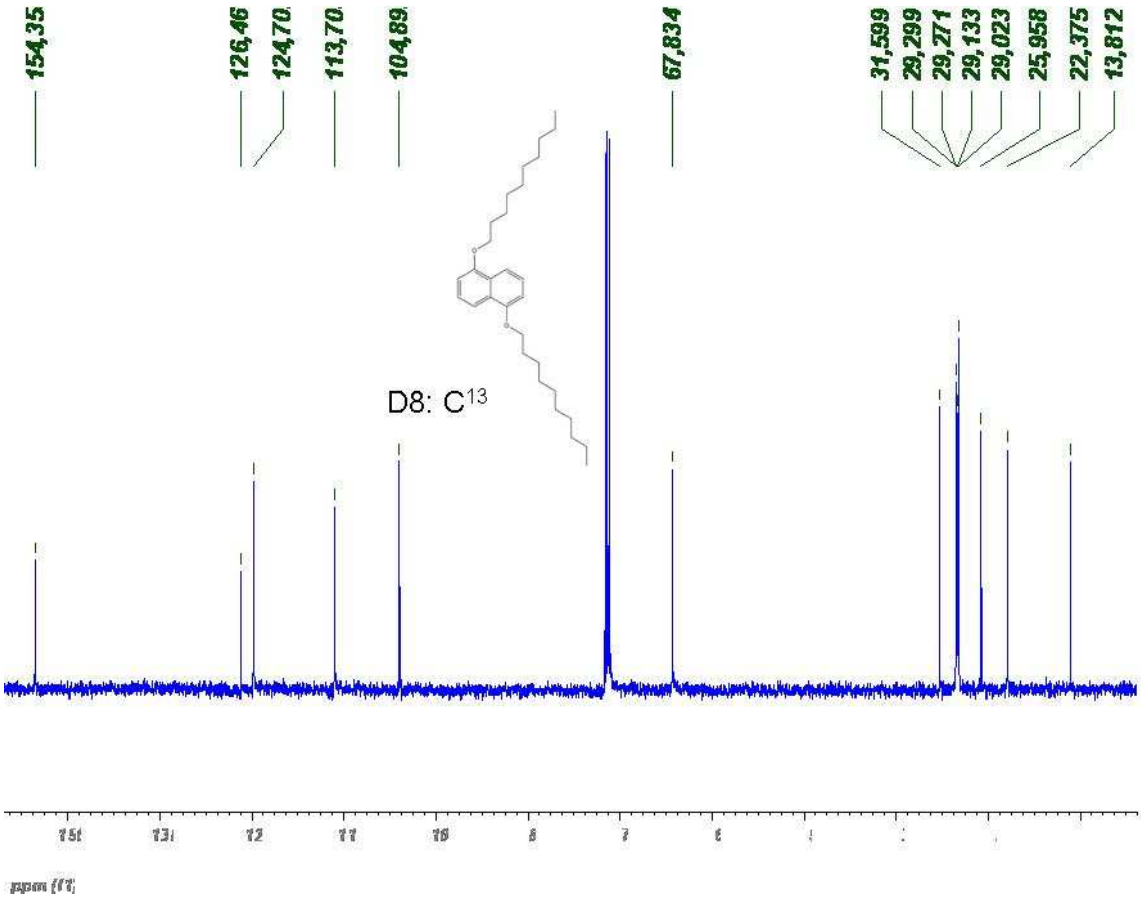
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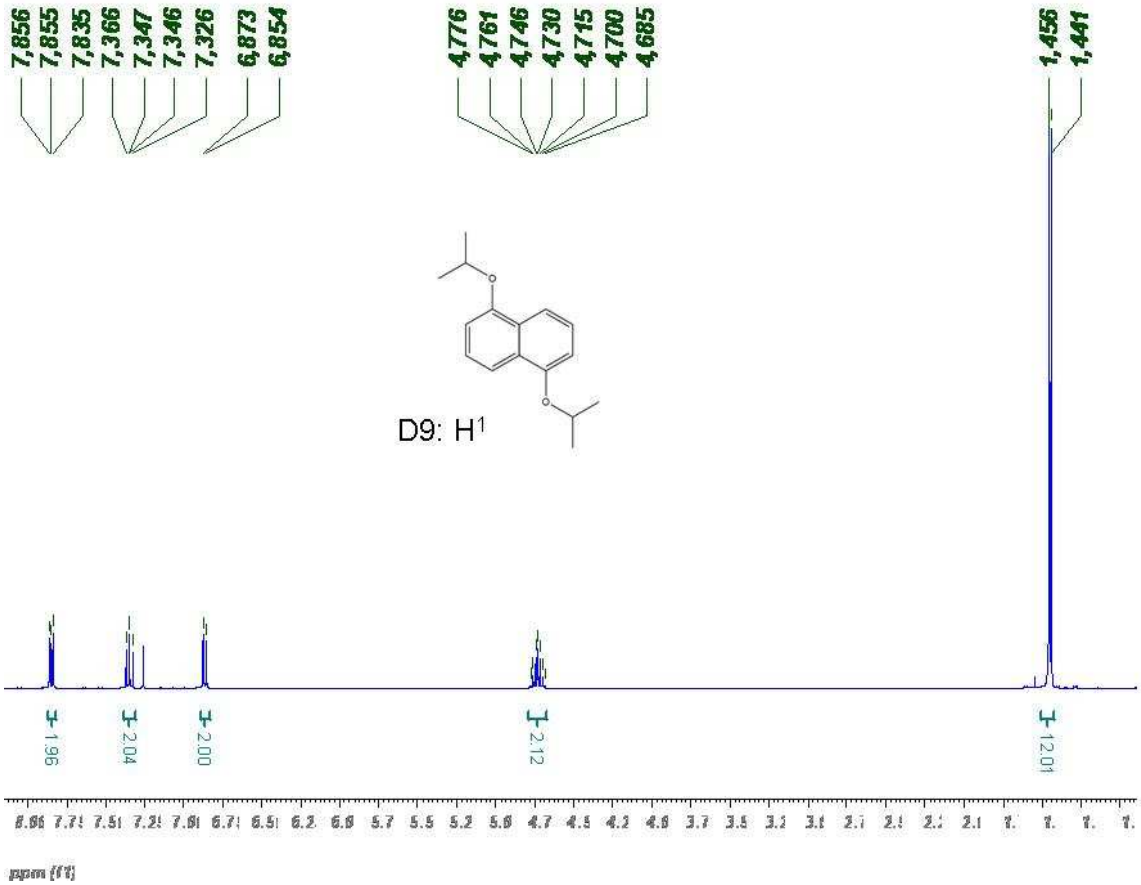
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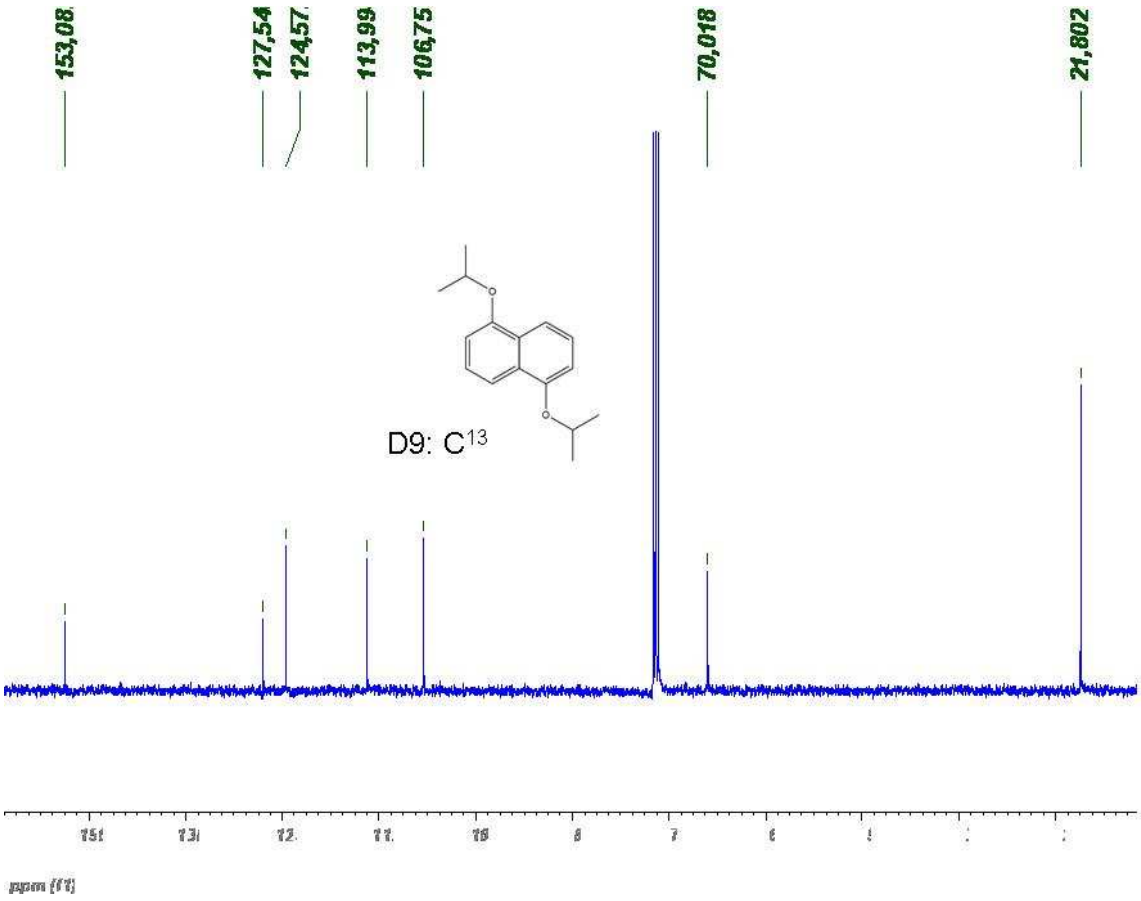
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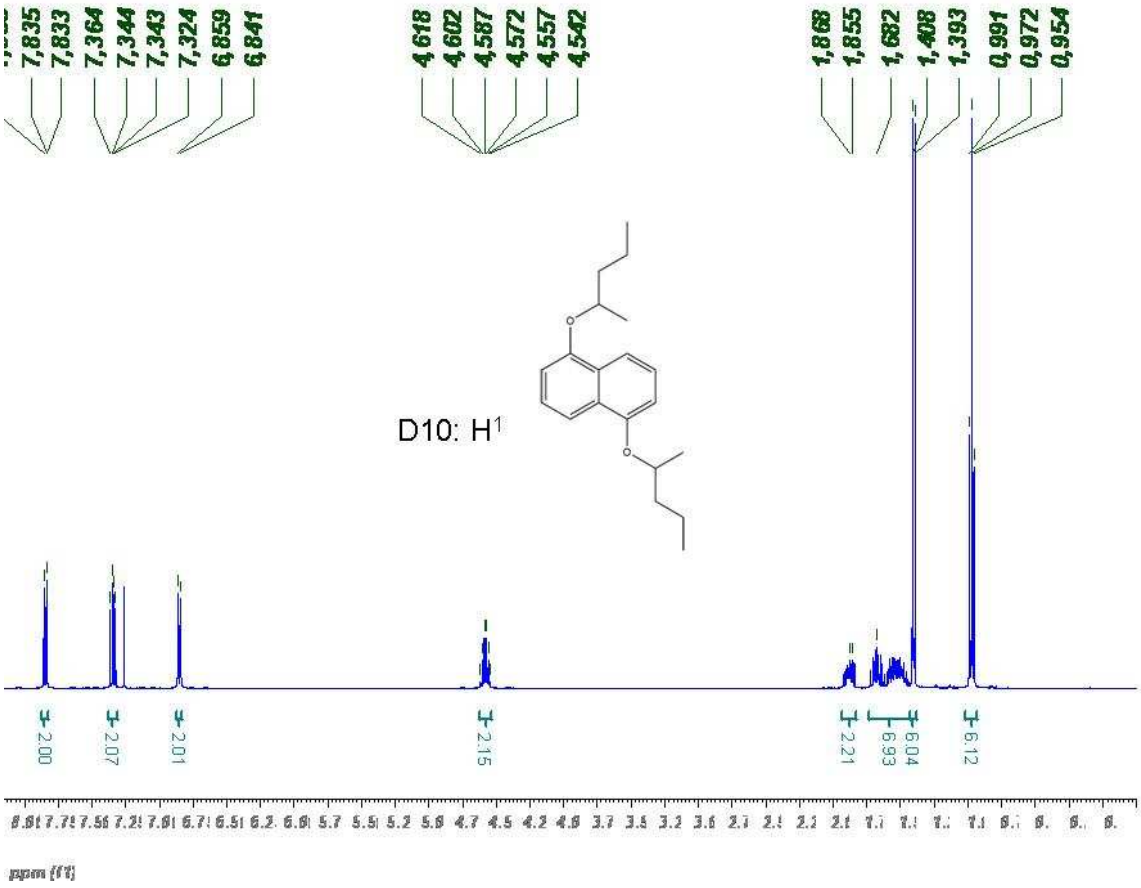
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1,855
1,682
1,408
1,393
0,991
0,972
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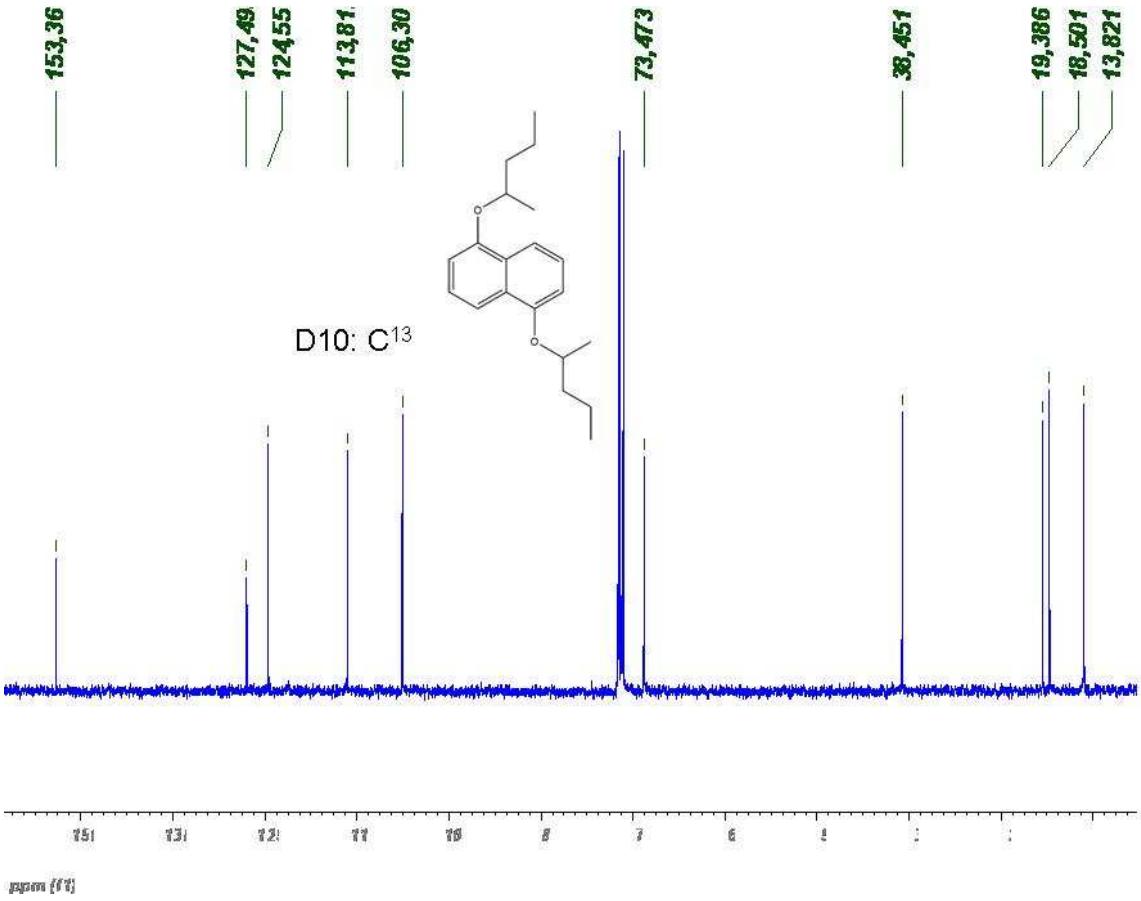
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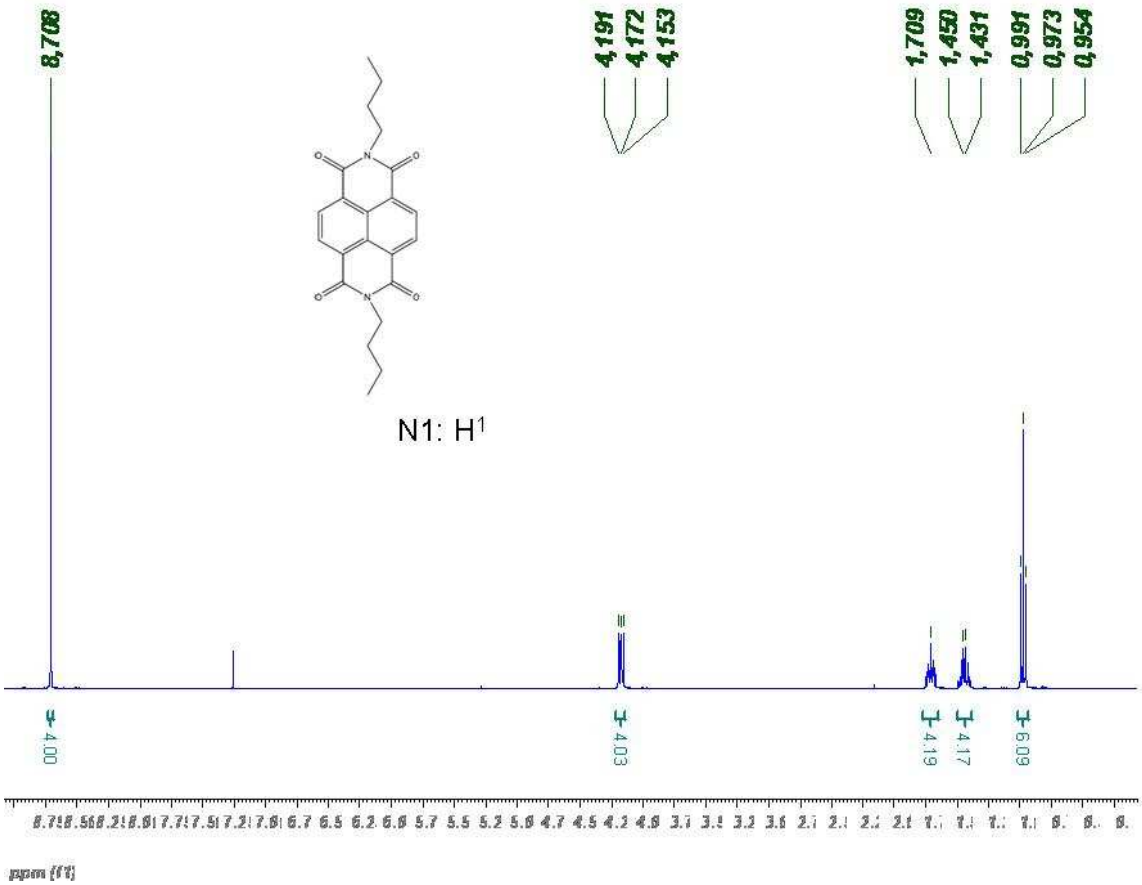
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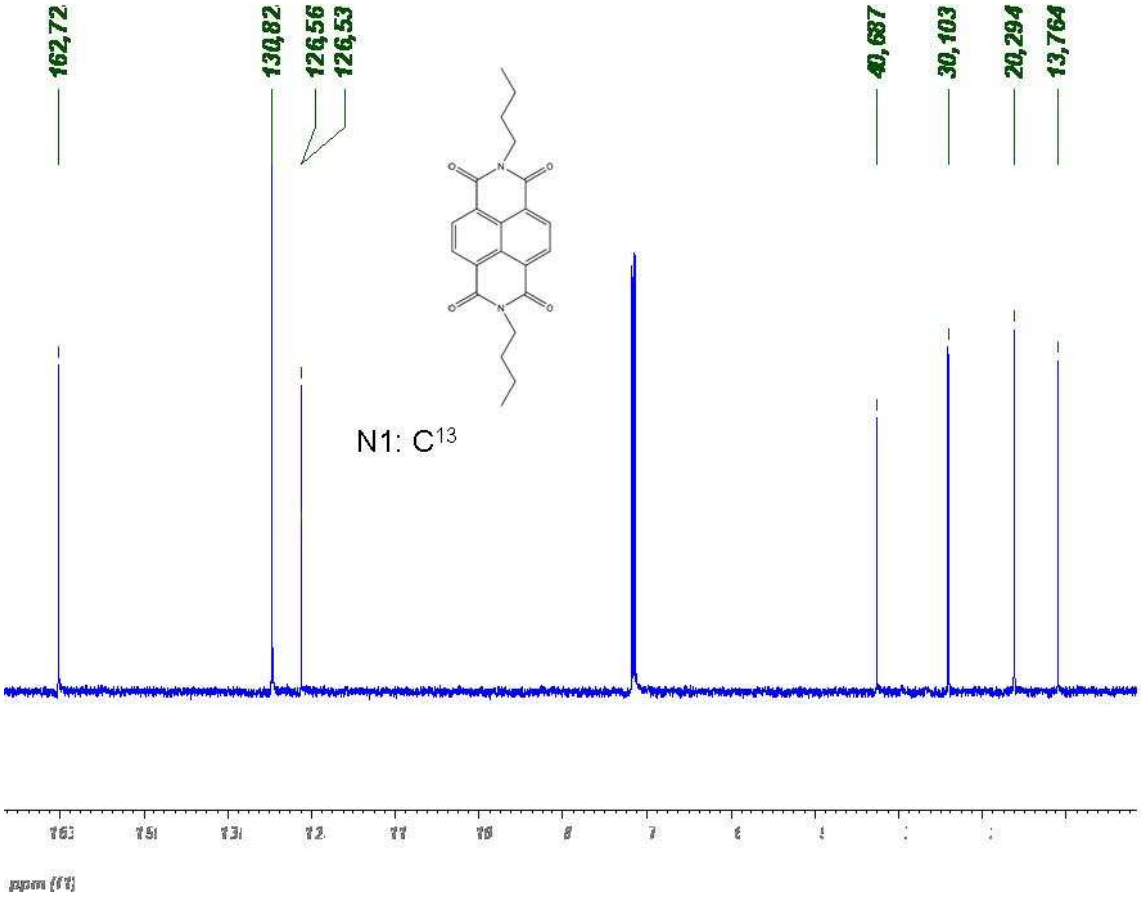
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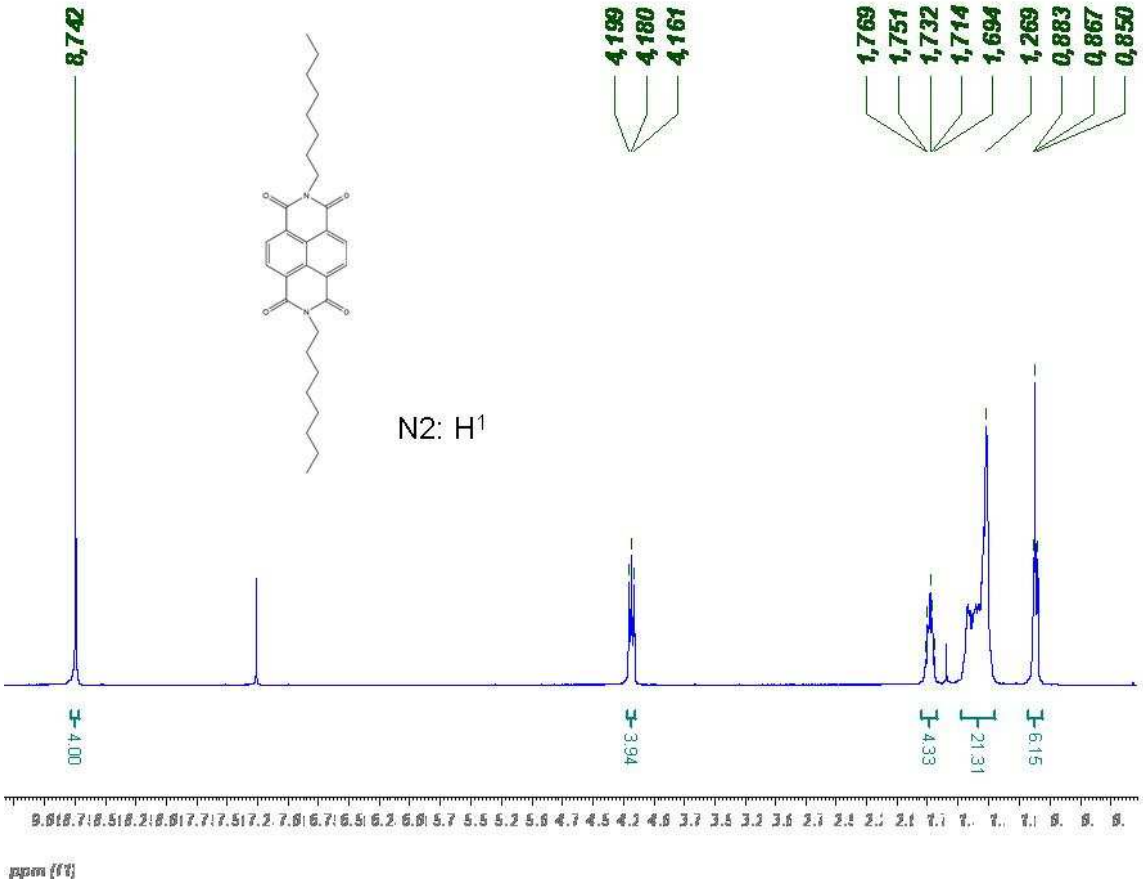
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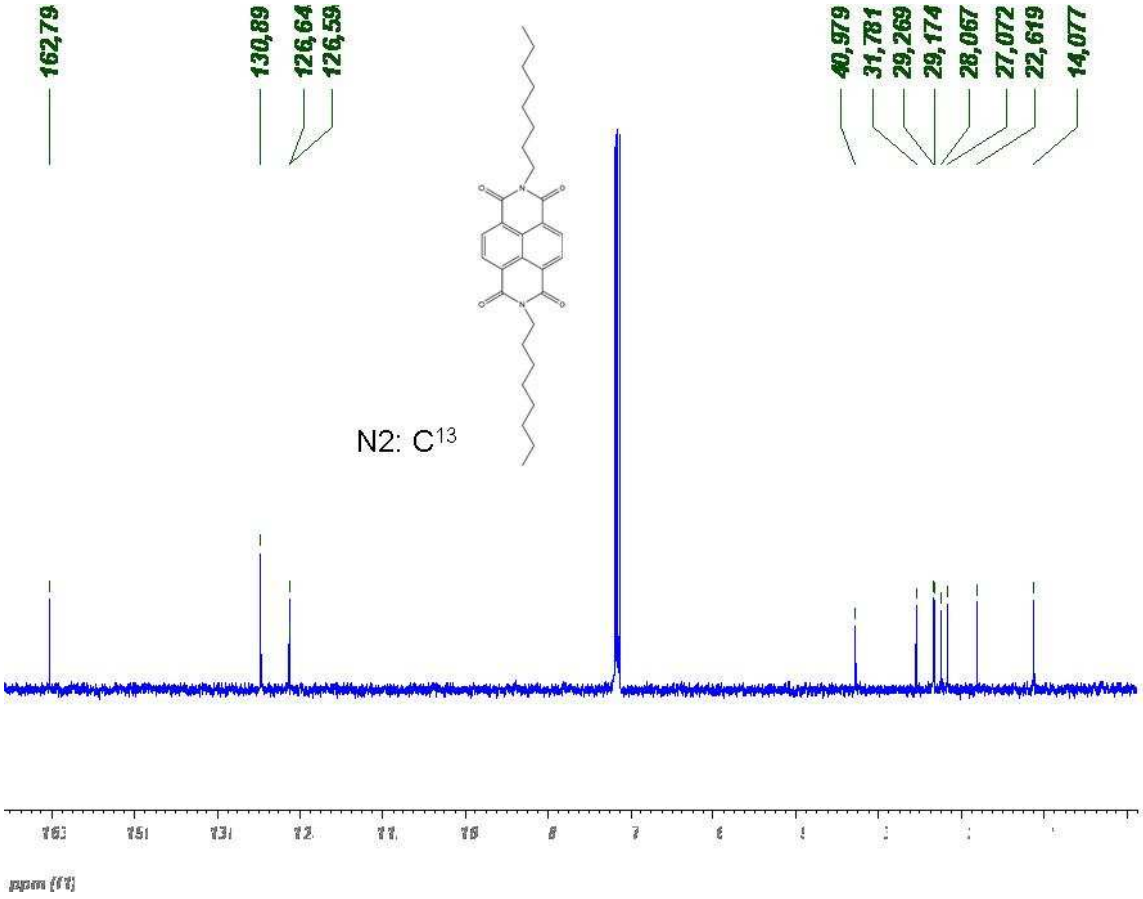
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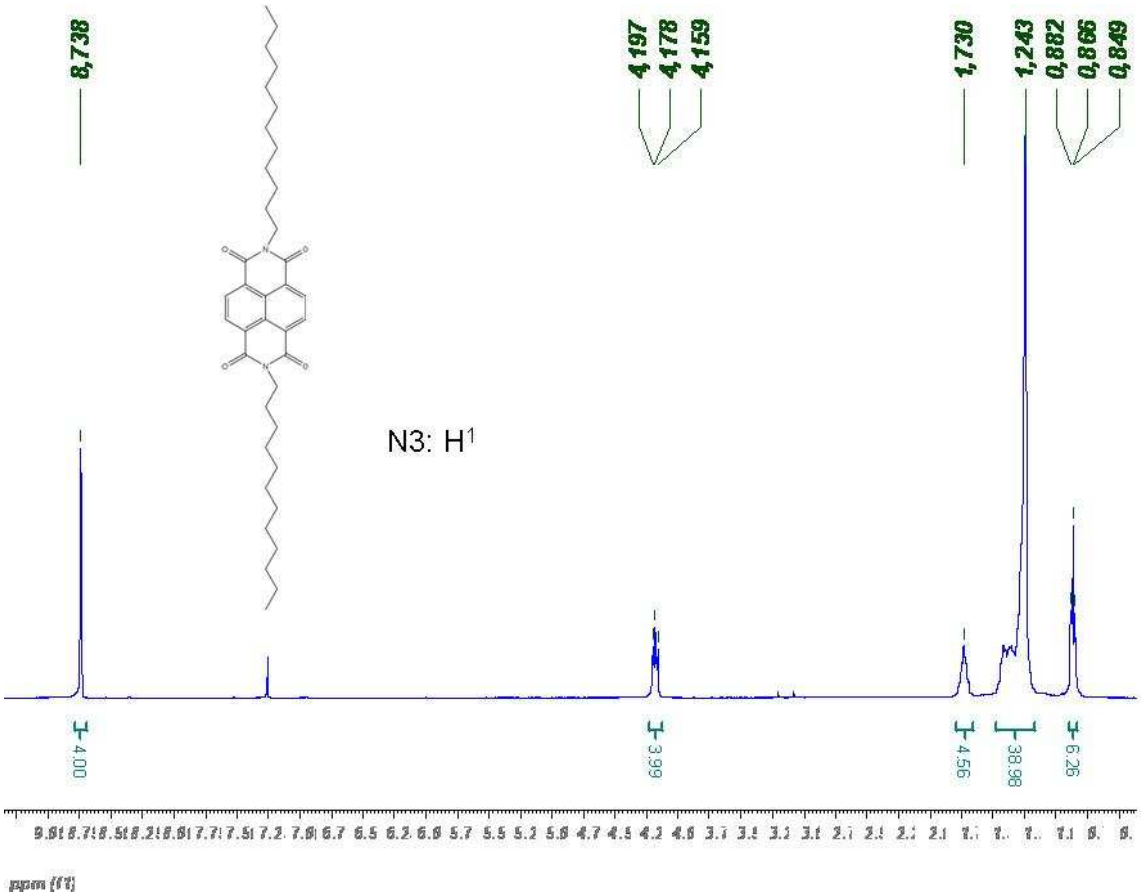
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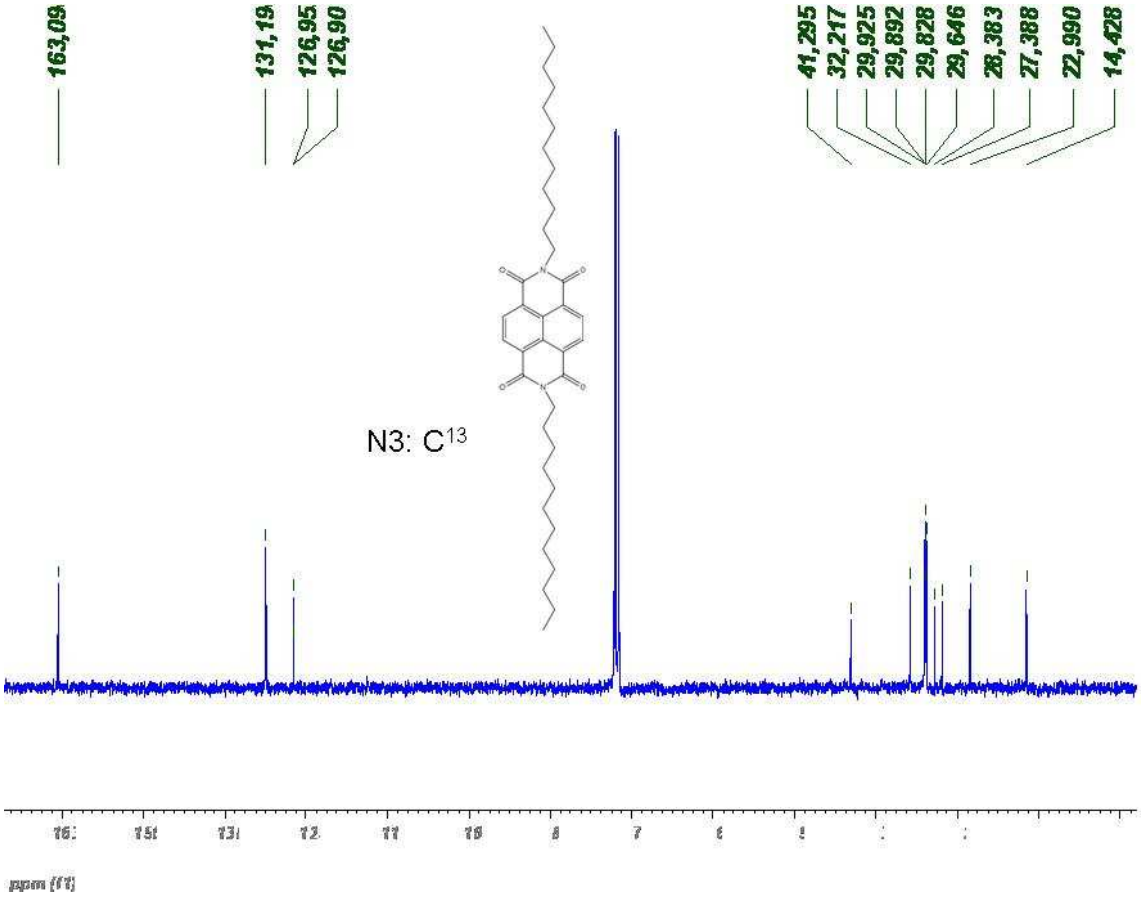
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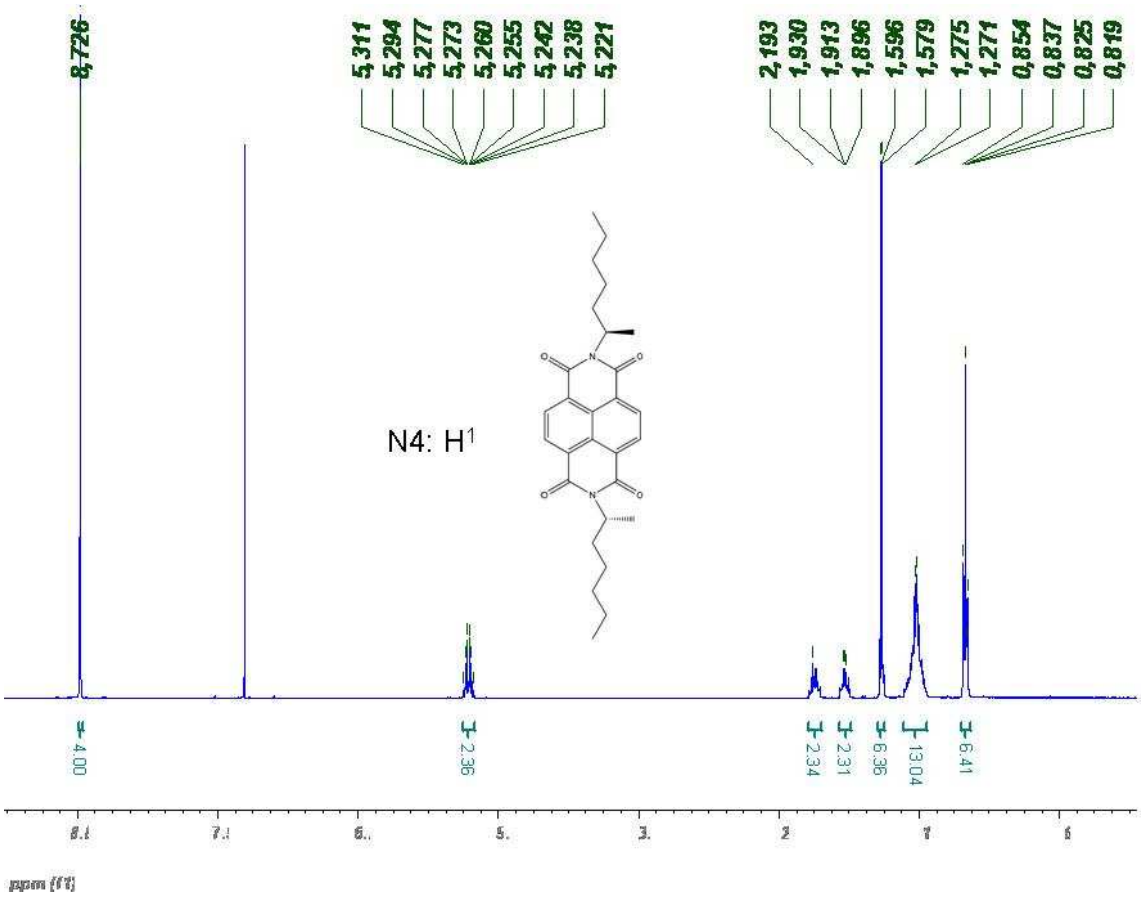
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1,579
1,275
1,271
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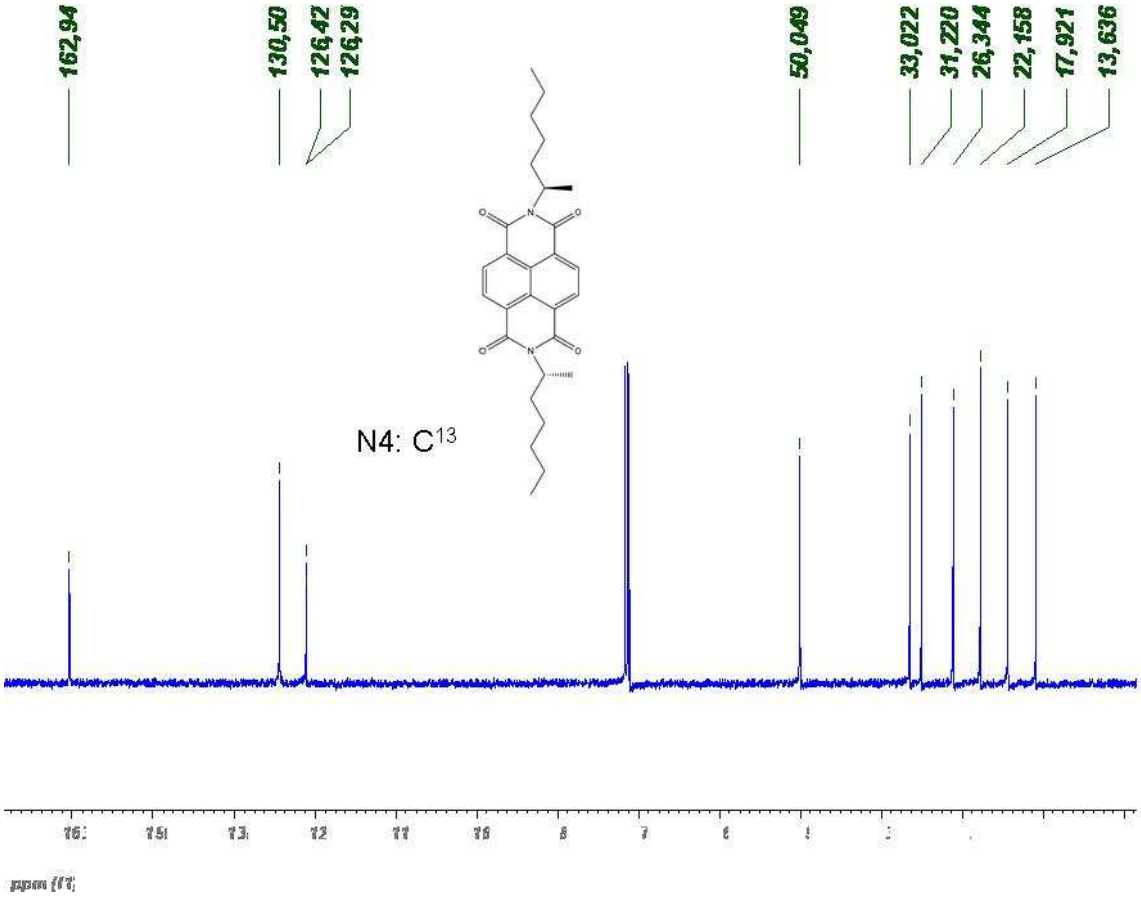
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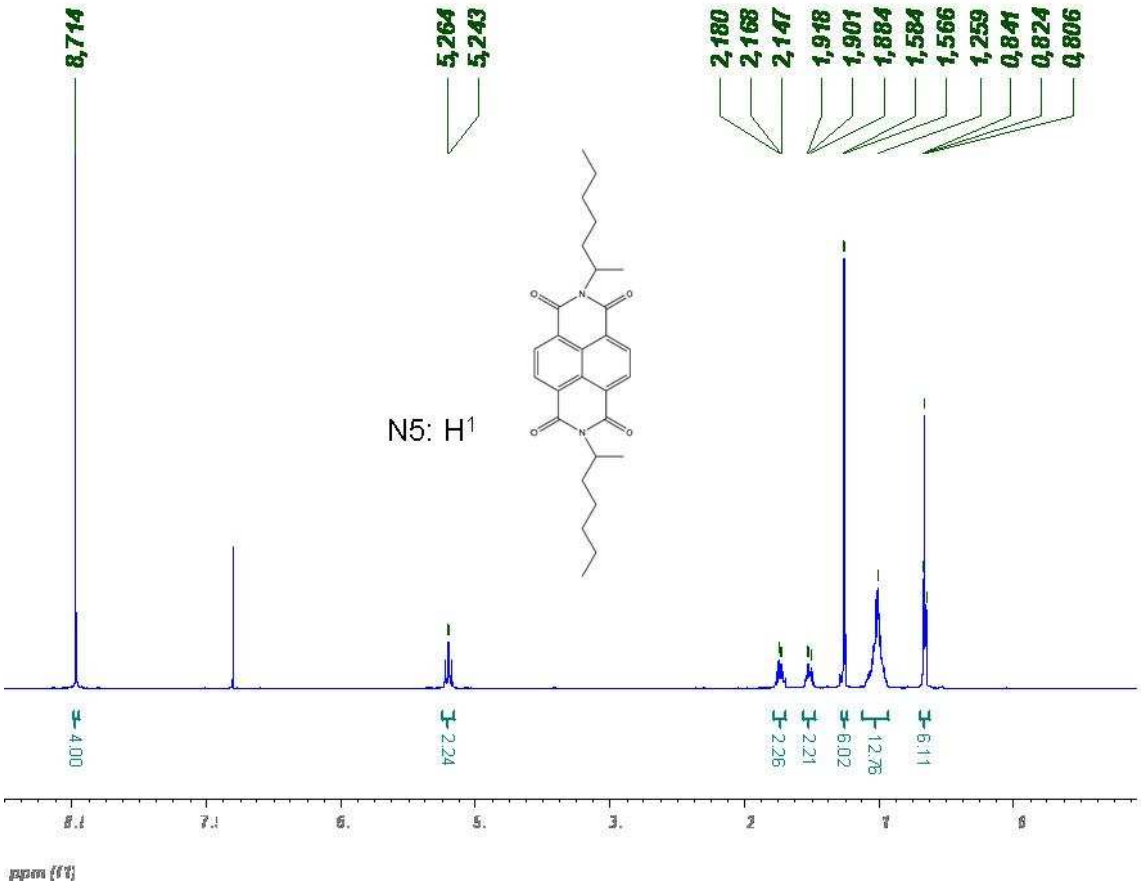
ppm (f1)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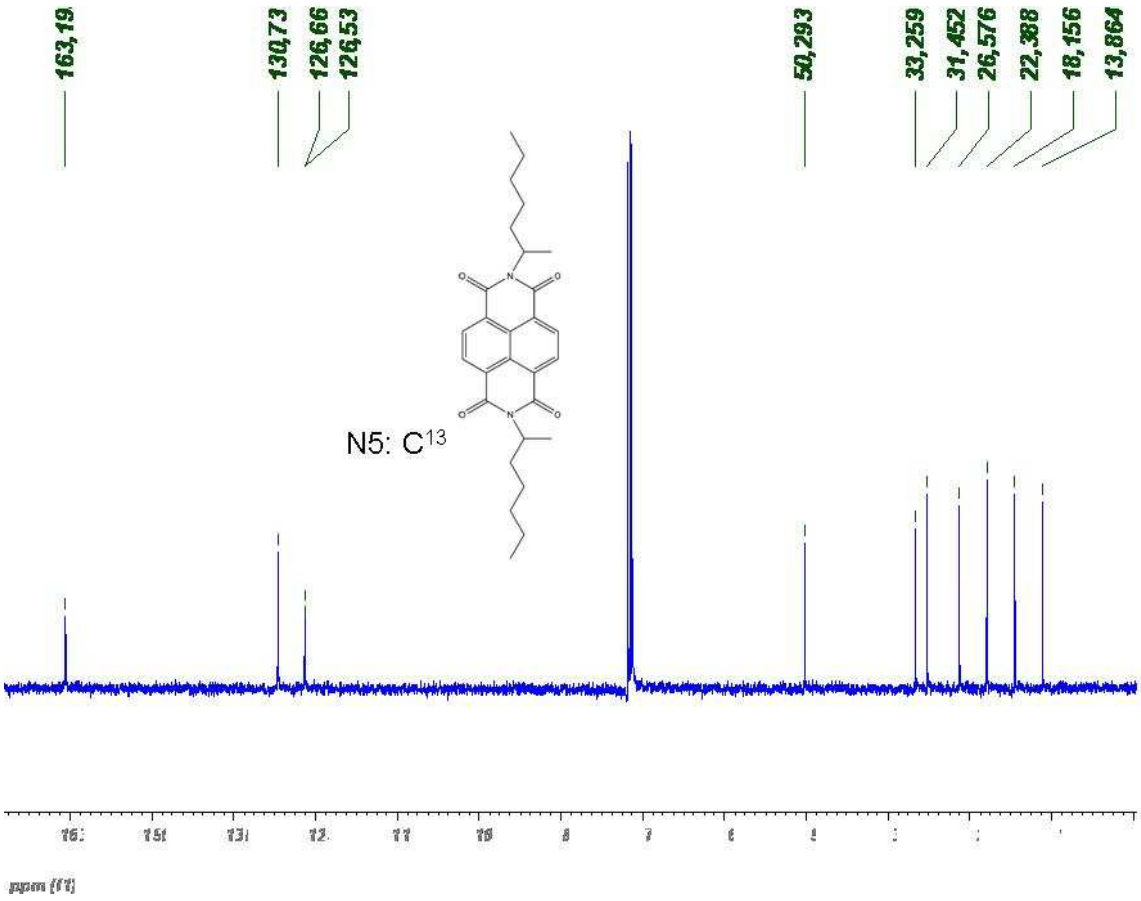
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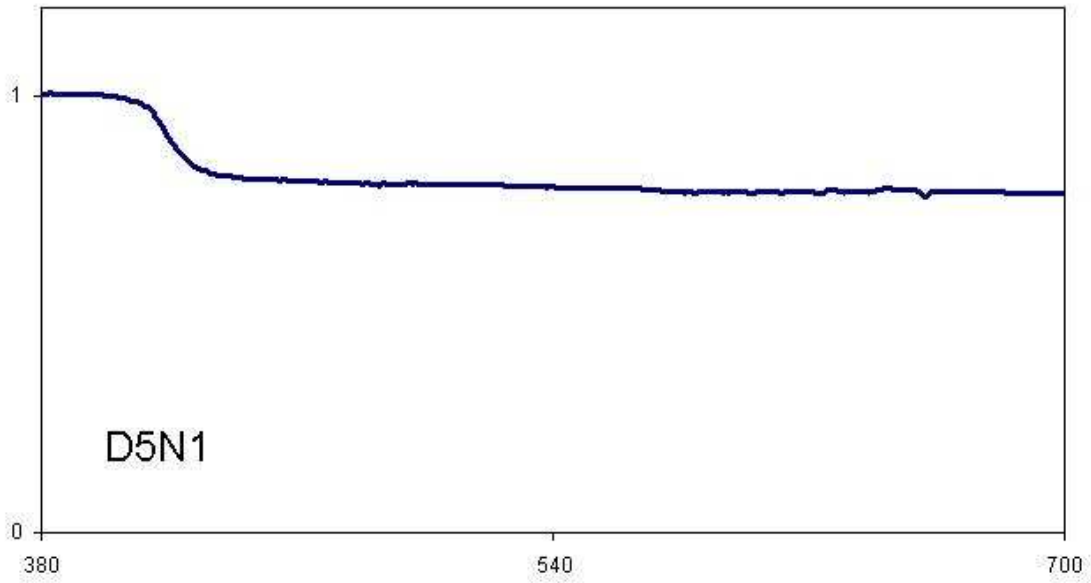
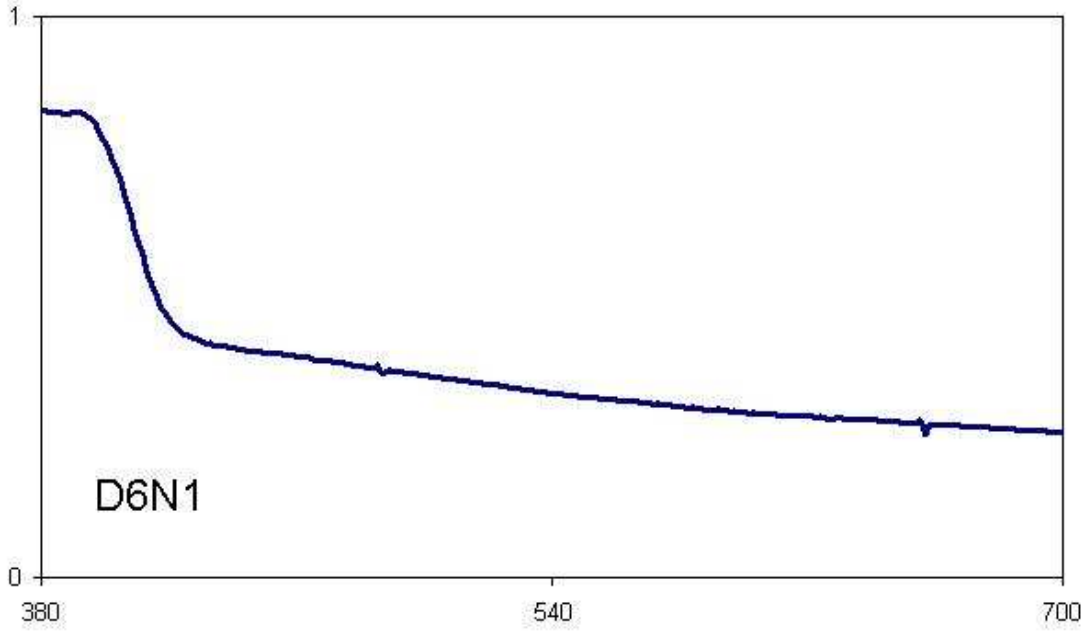
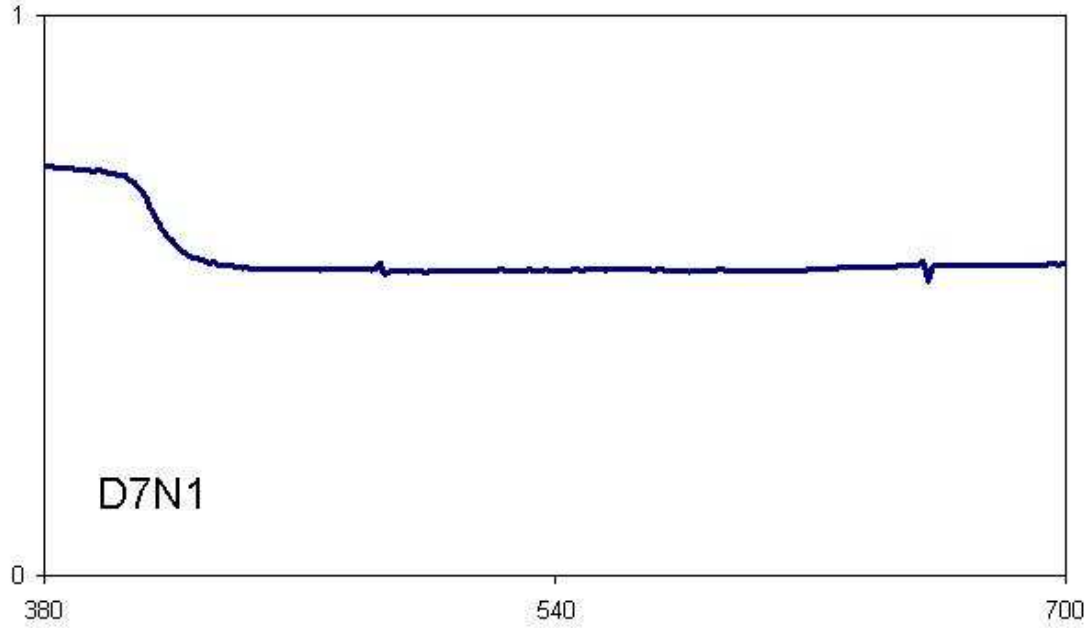
13,864
N5: C13
ppm (f1)

UV-Vis Spectra. Y-axis is absorbance and X-axis is wavelength (nm). 1:1 molar Dan:Ndi mixtures were placed between two glass slides and heated to the isotropic state. Spectra were collected at least 5 min after reaching the mixture crystallization temperature.



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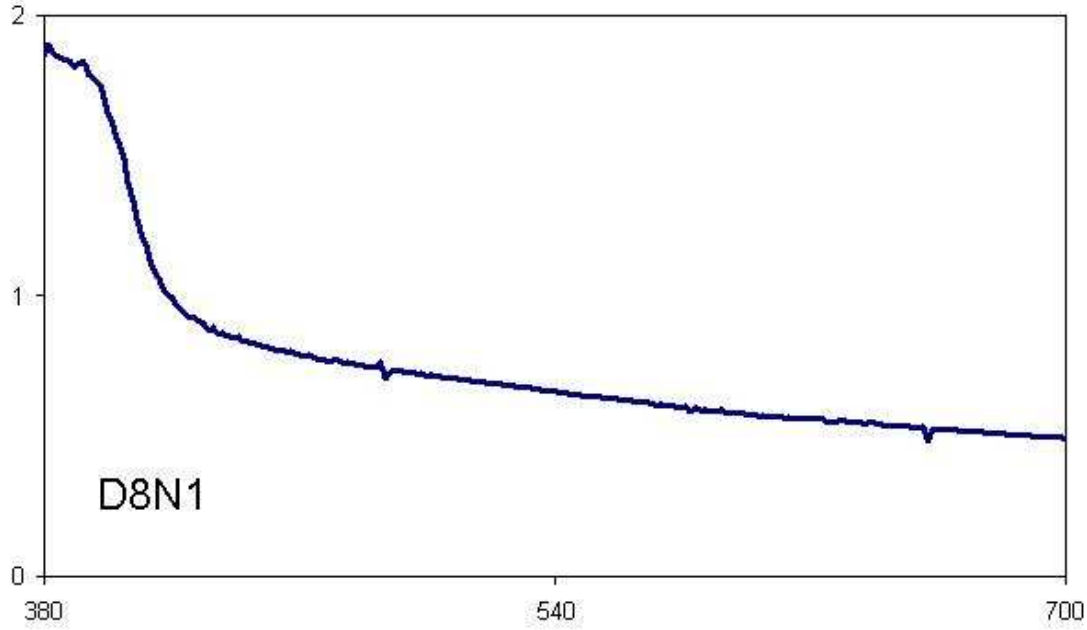
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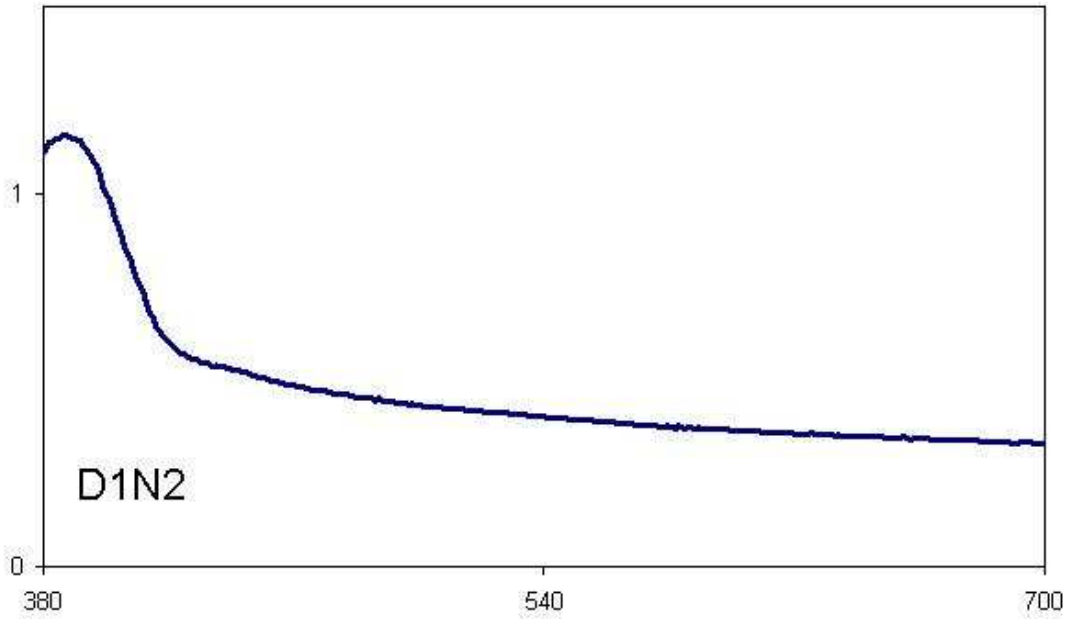
D8N1
380
540
700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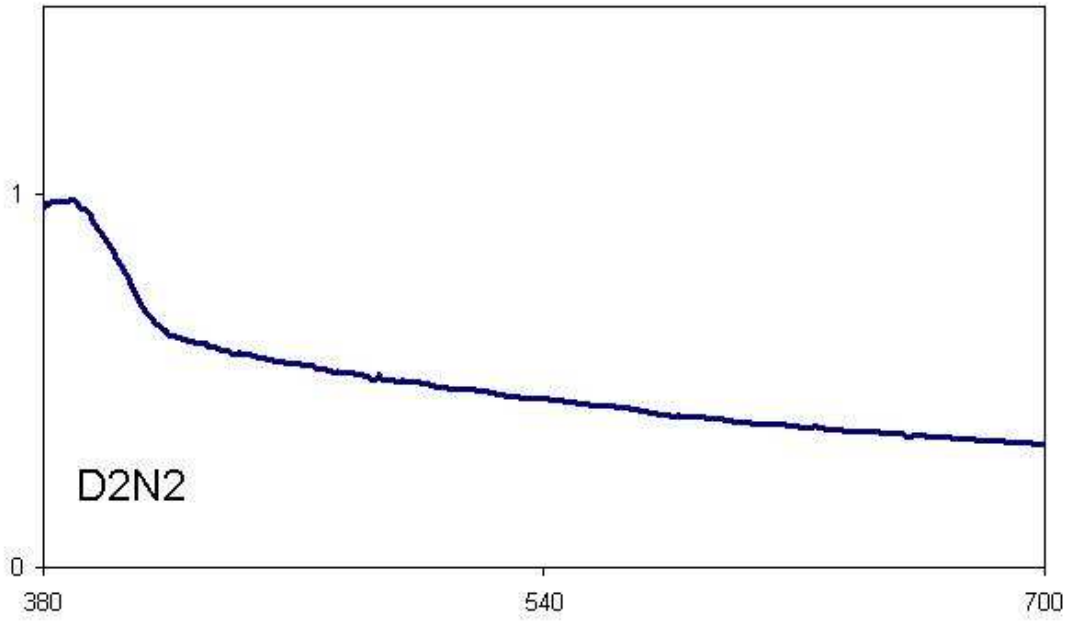
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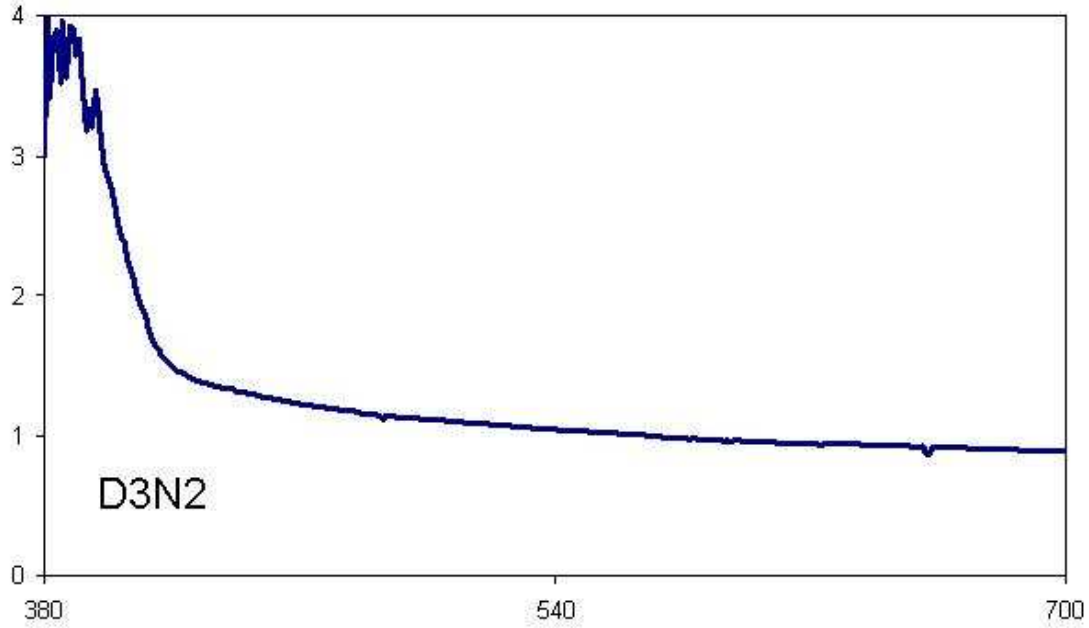
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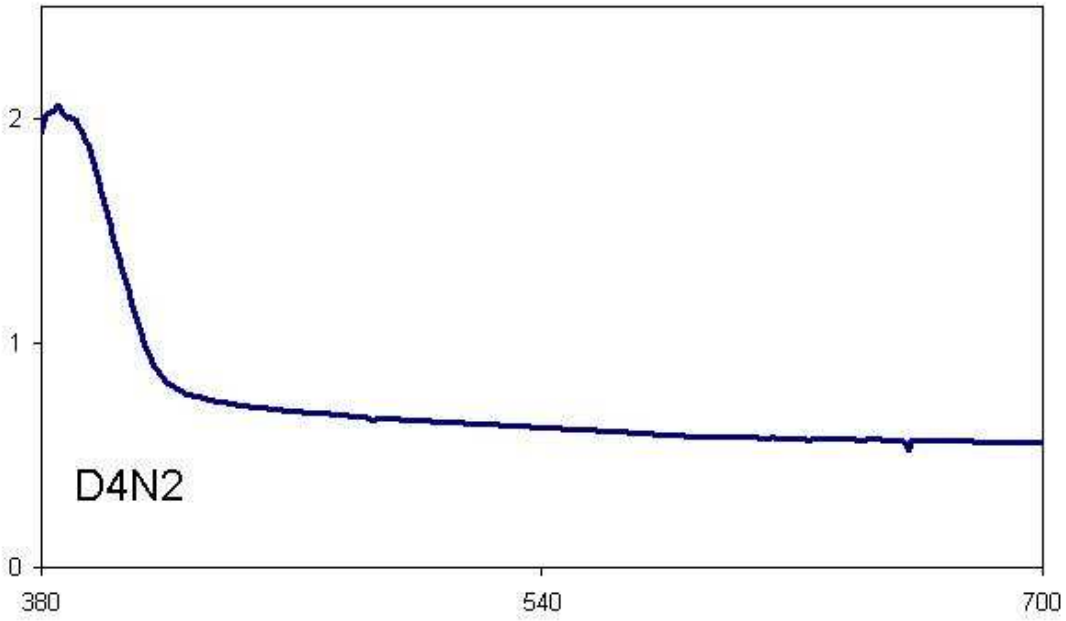
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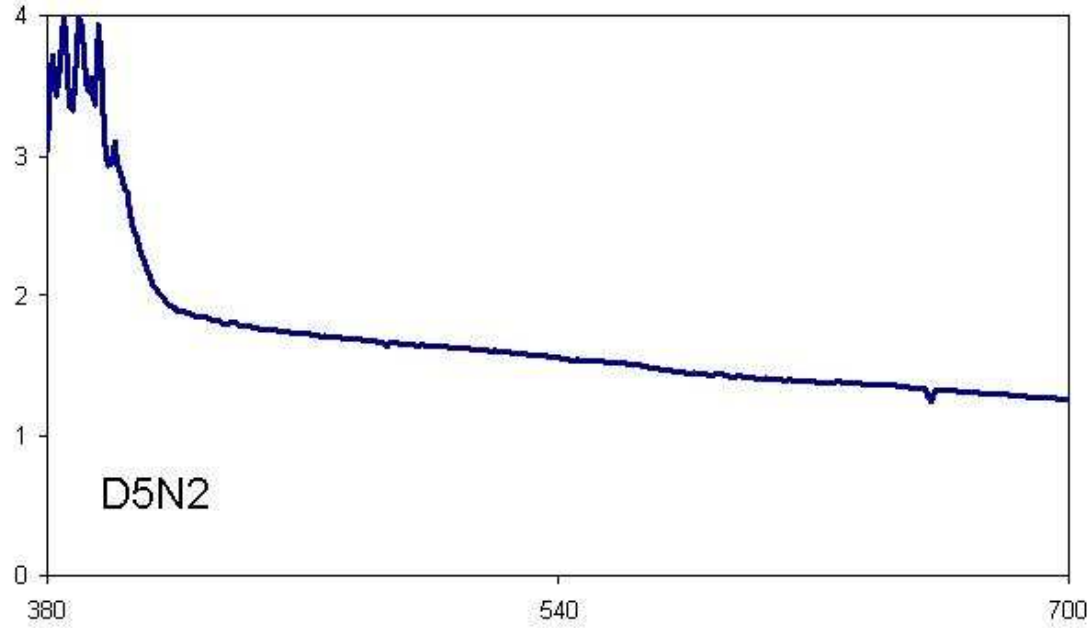
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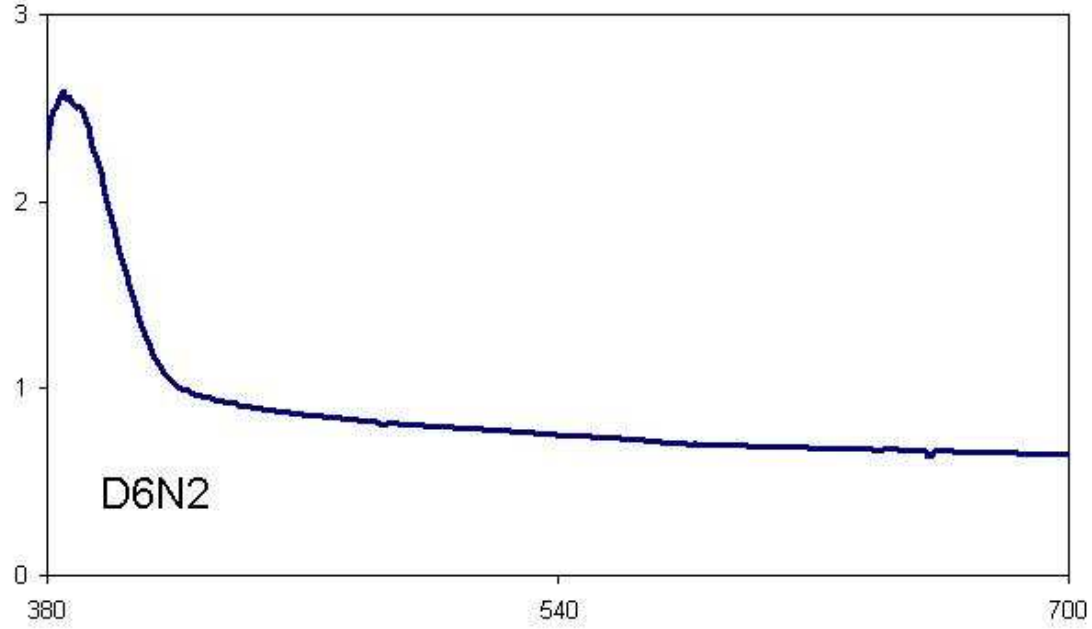
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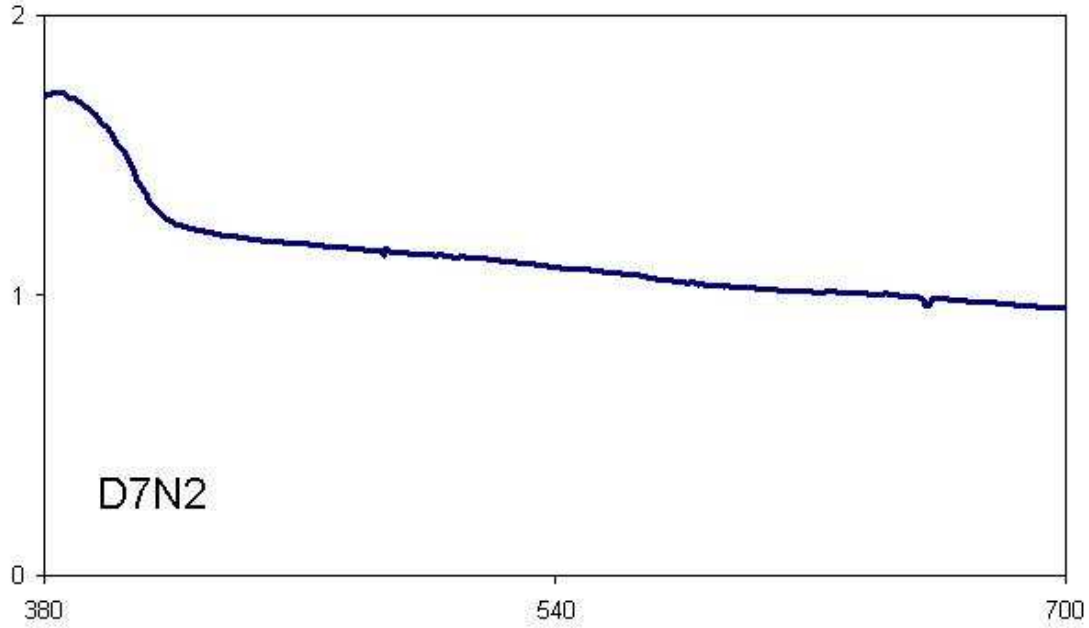
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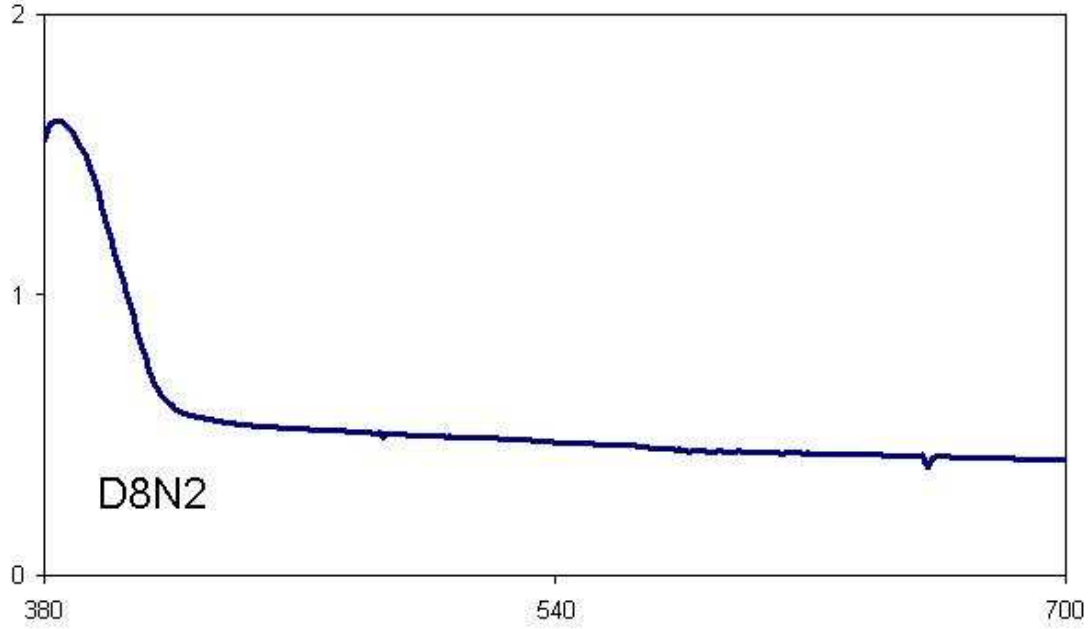
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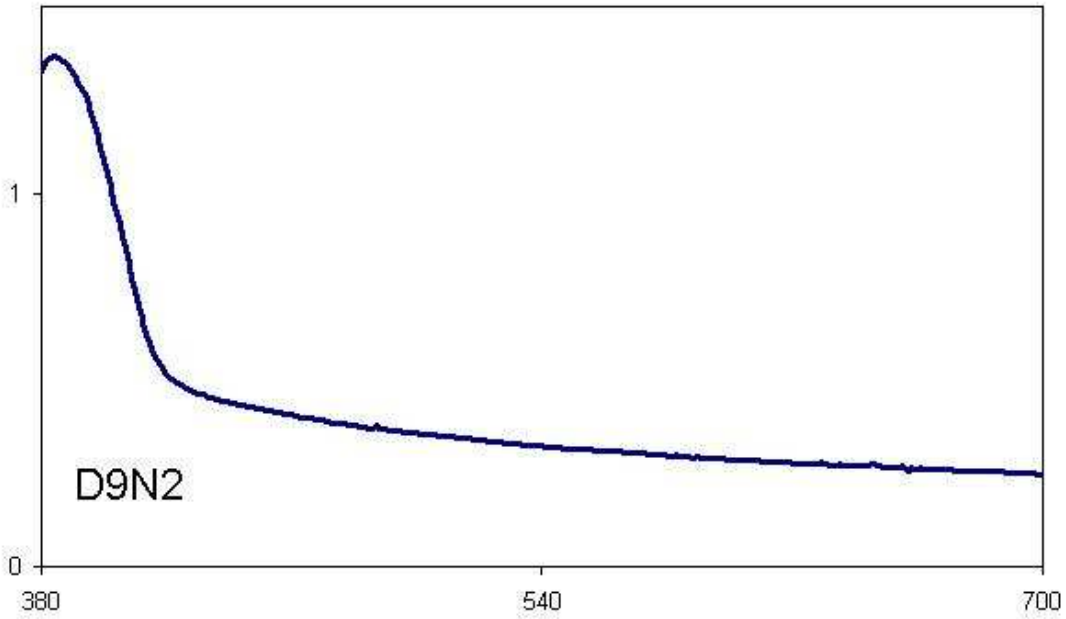
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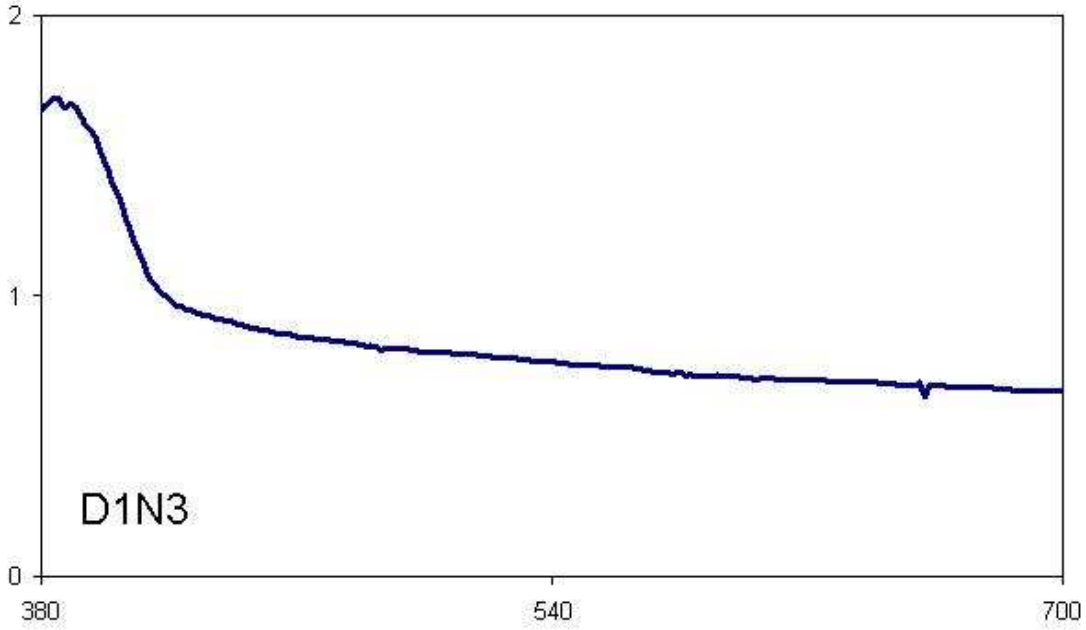
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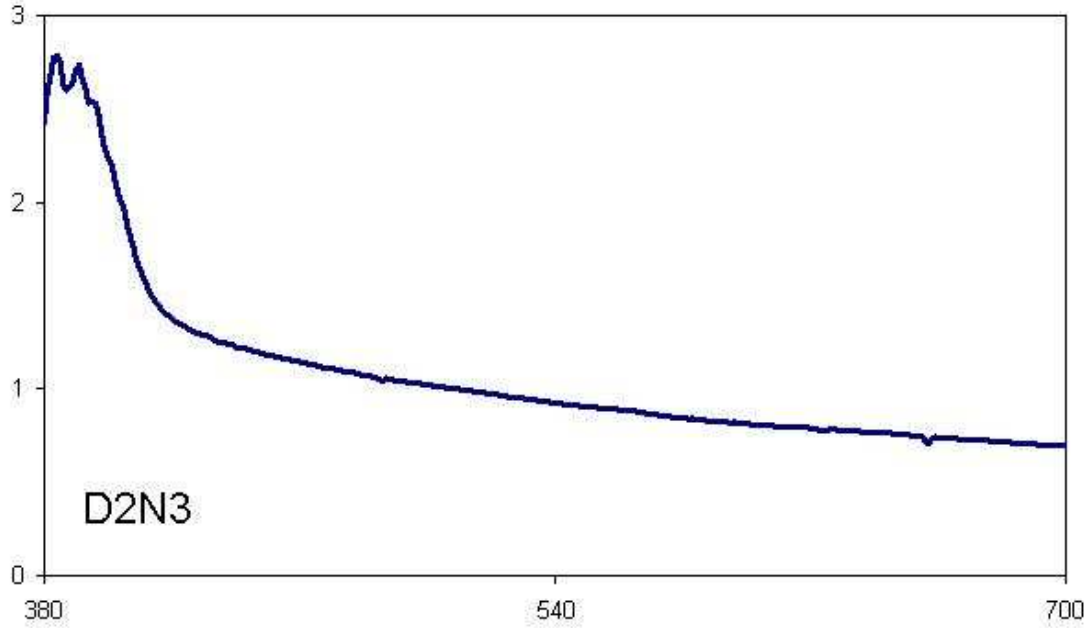
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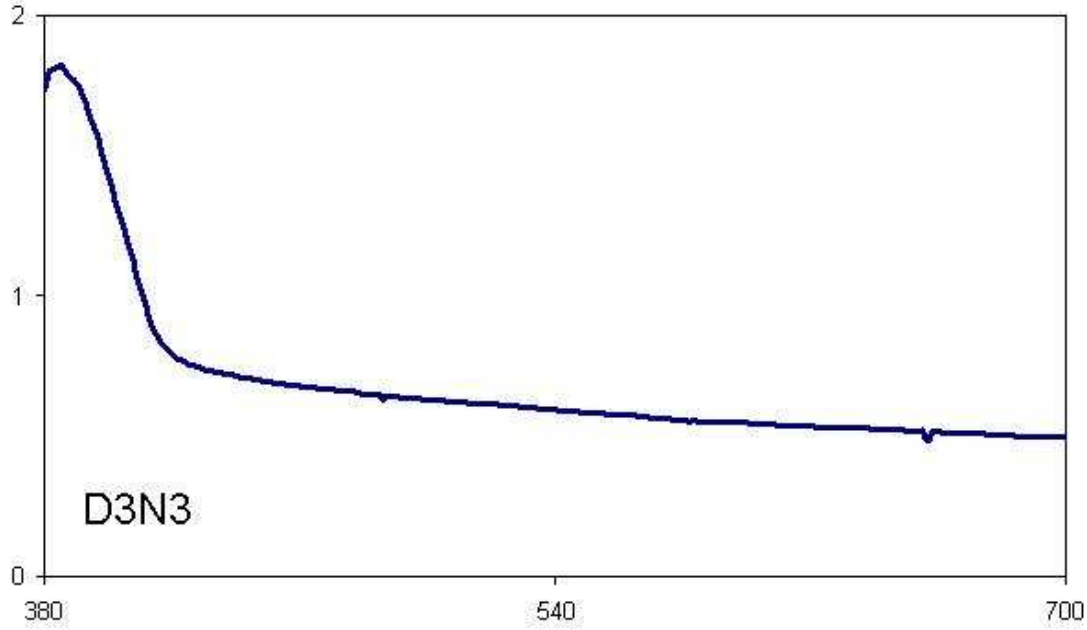
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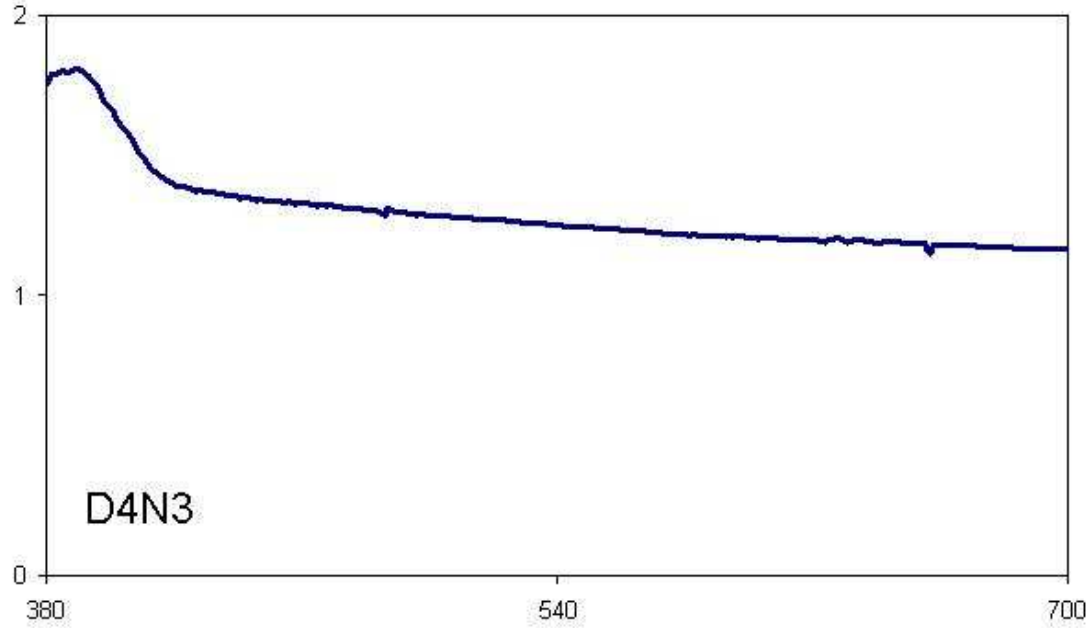
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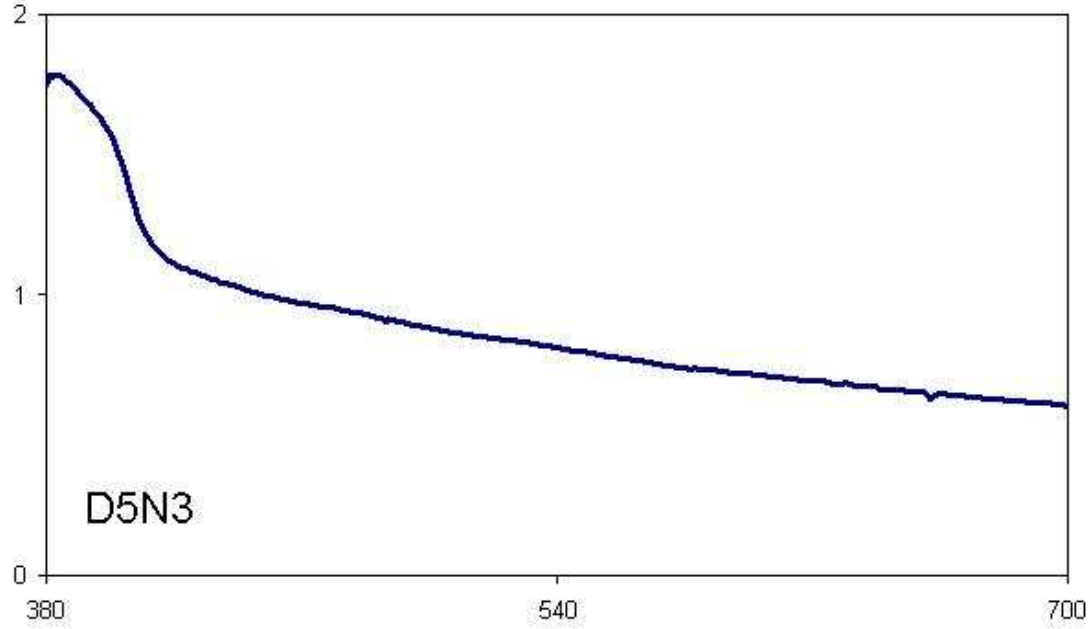
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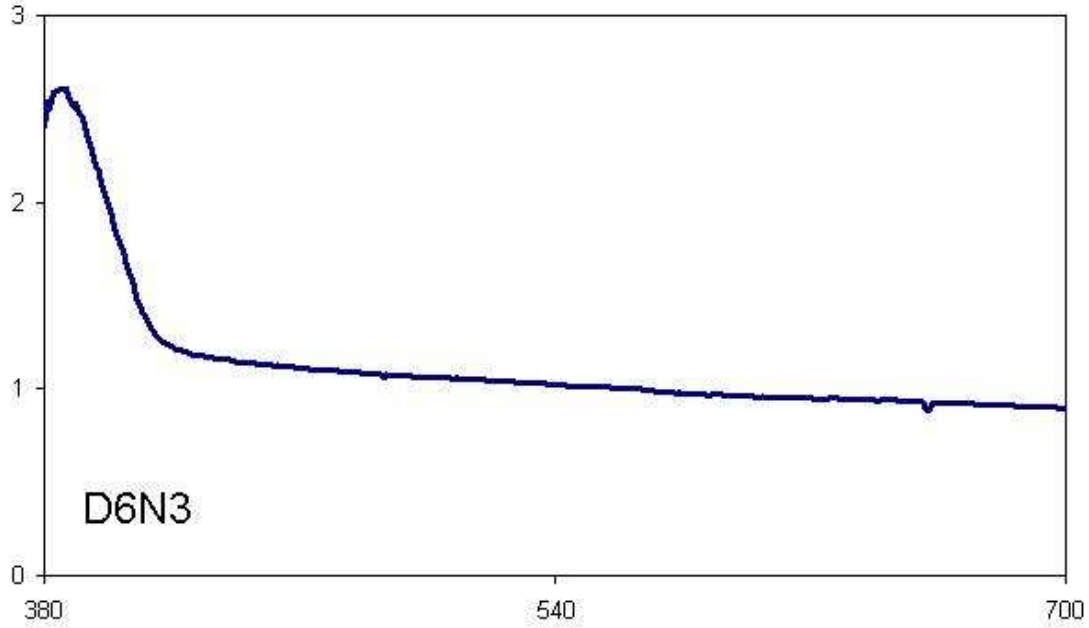
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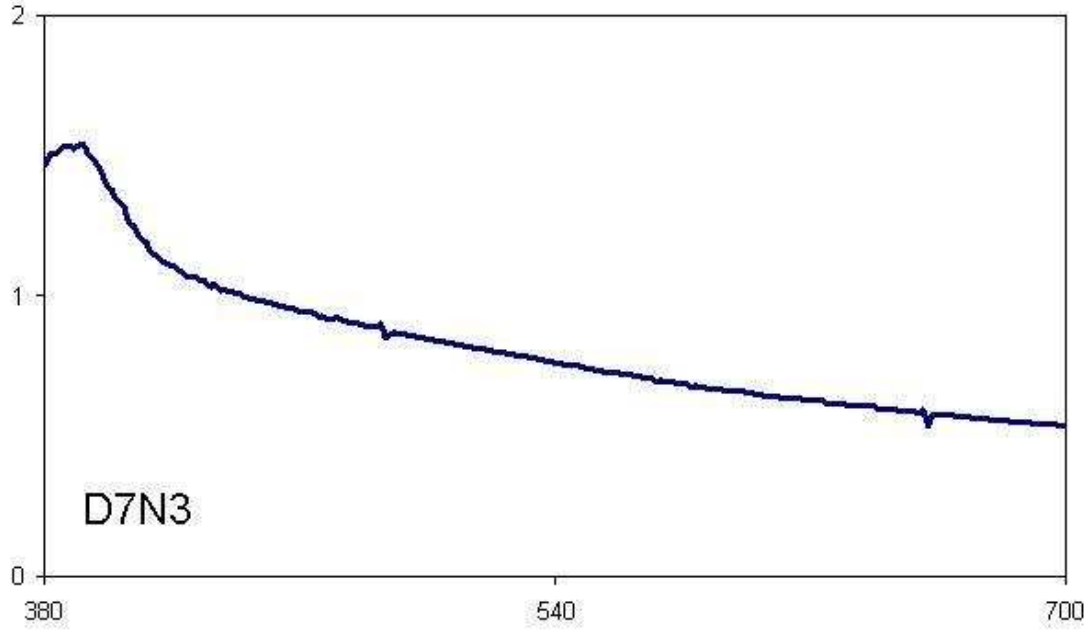
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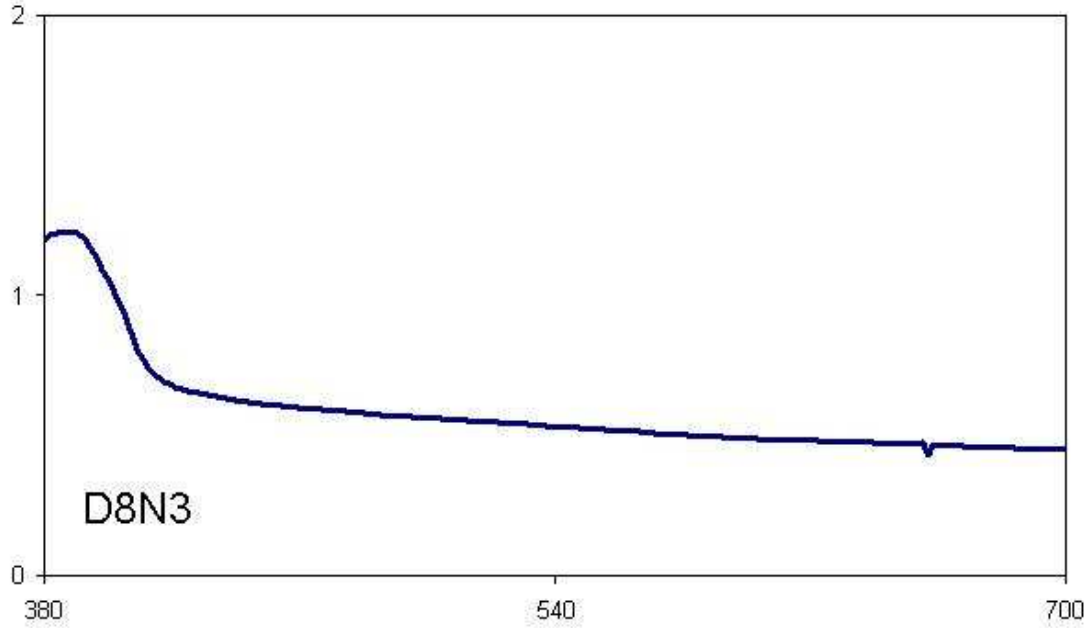
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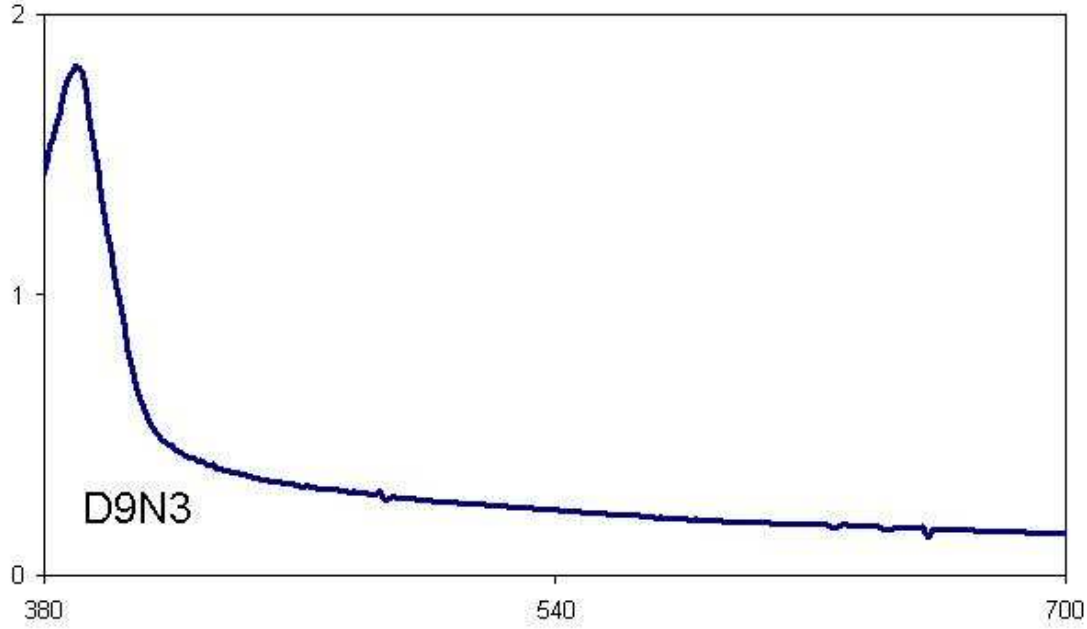
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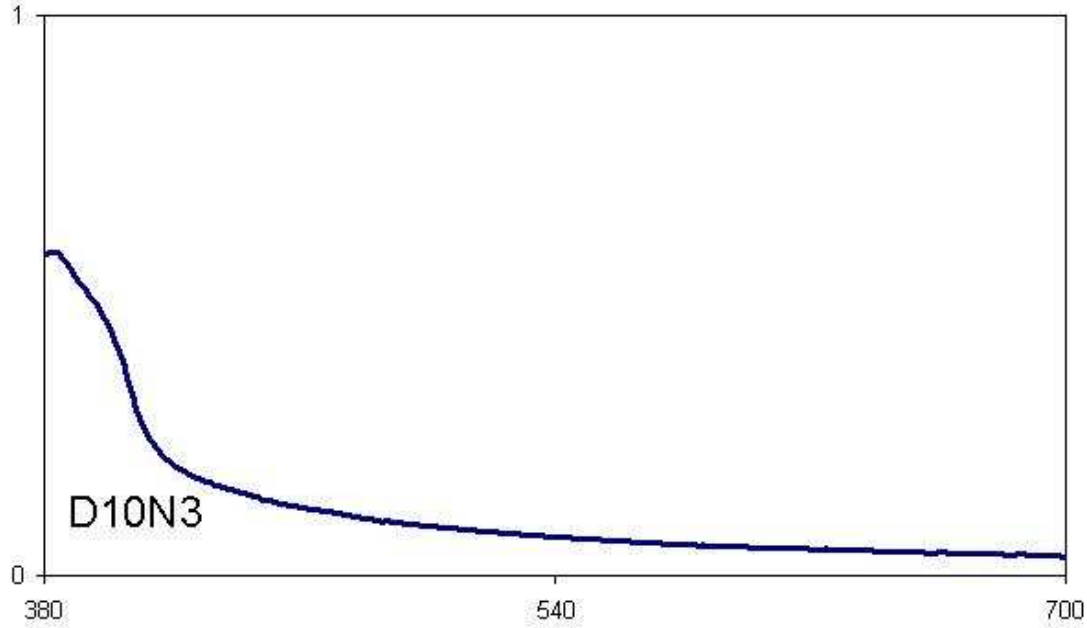
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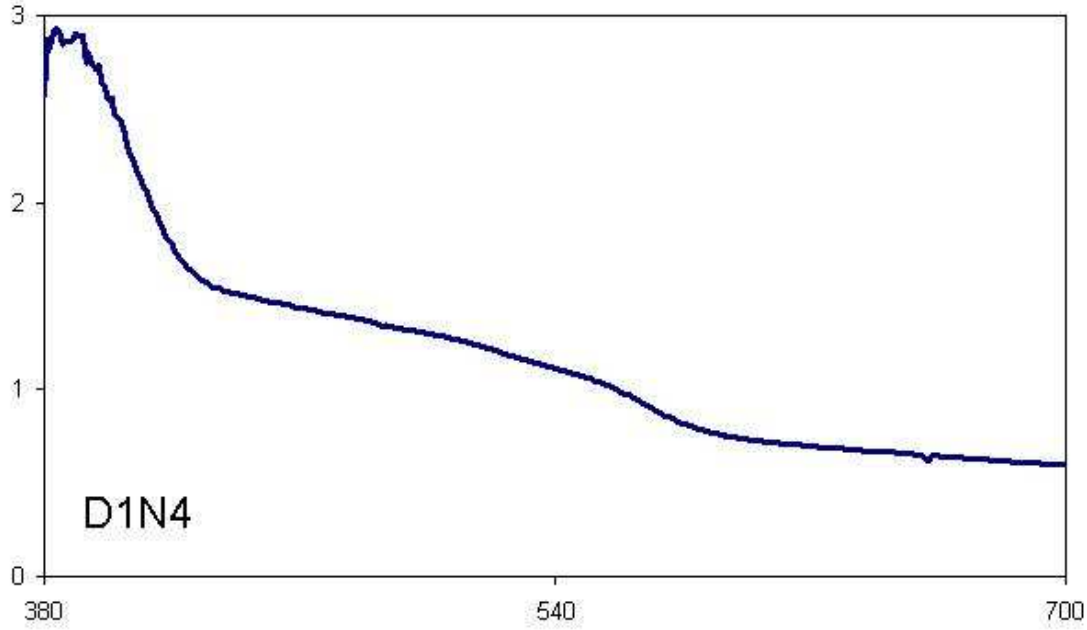
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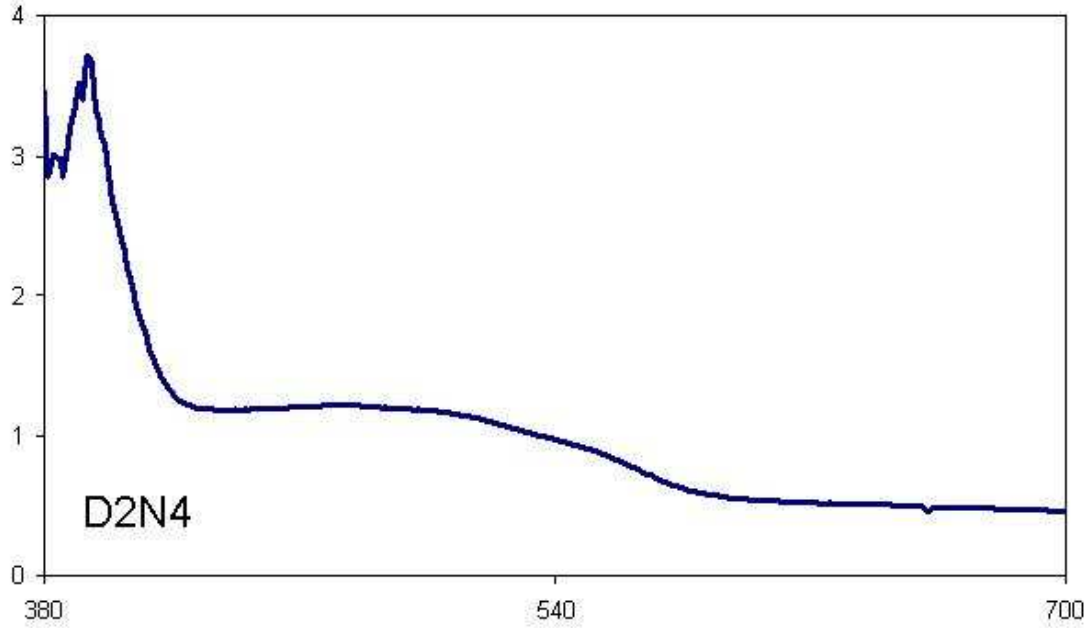
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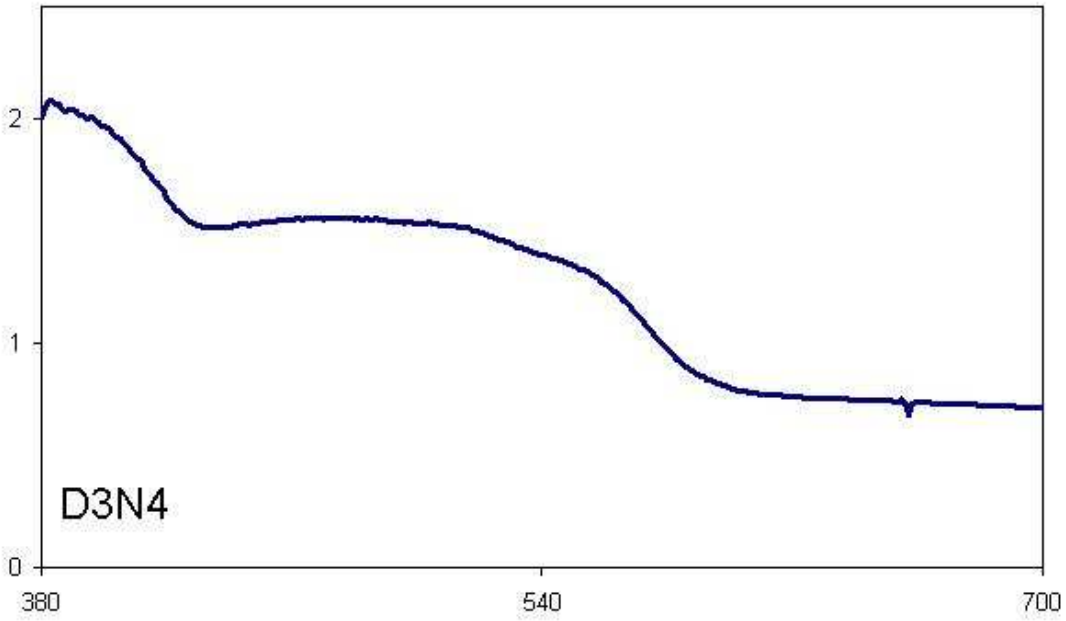
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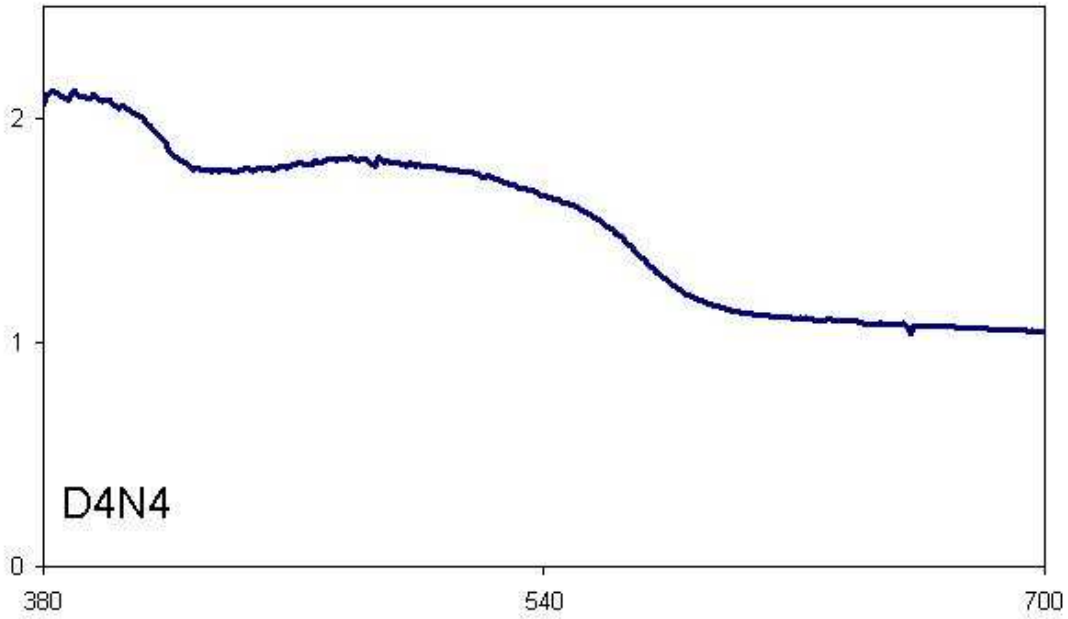
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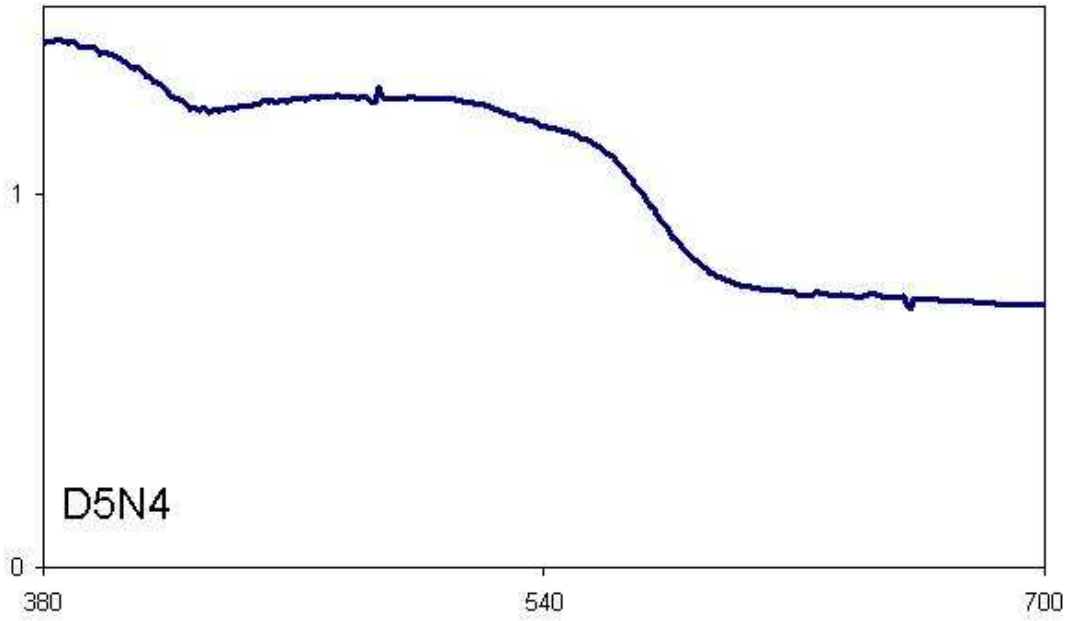
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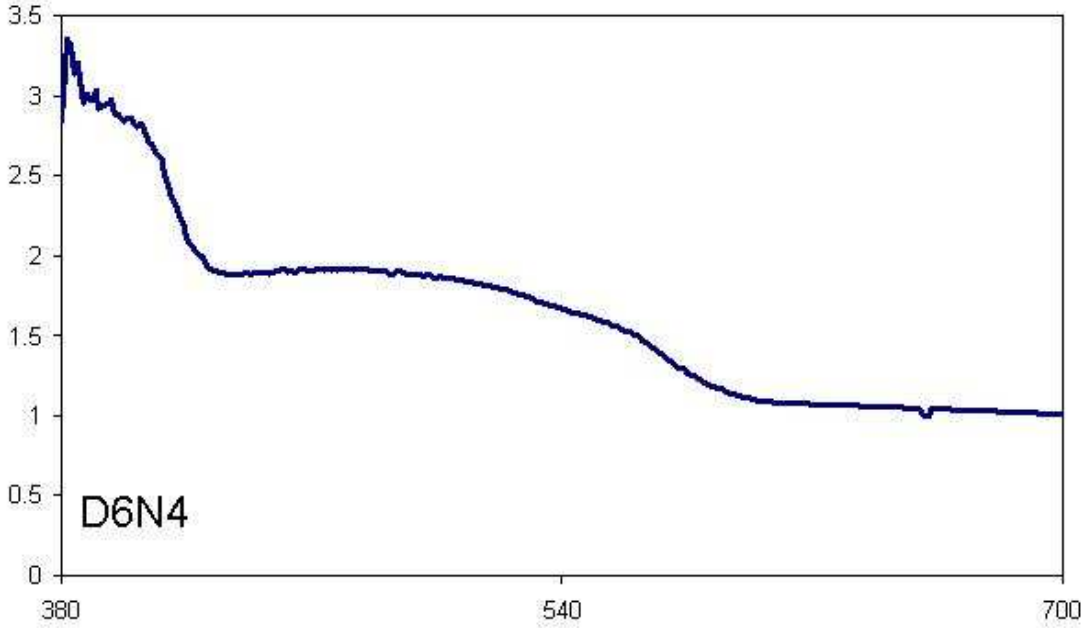
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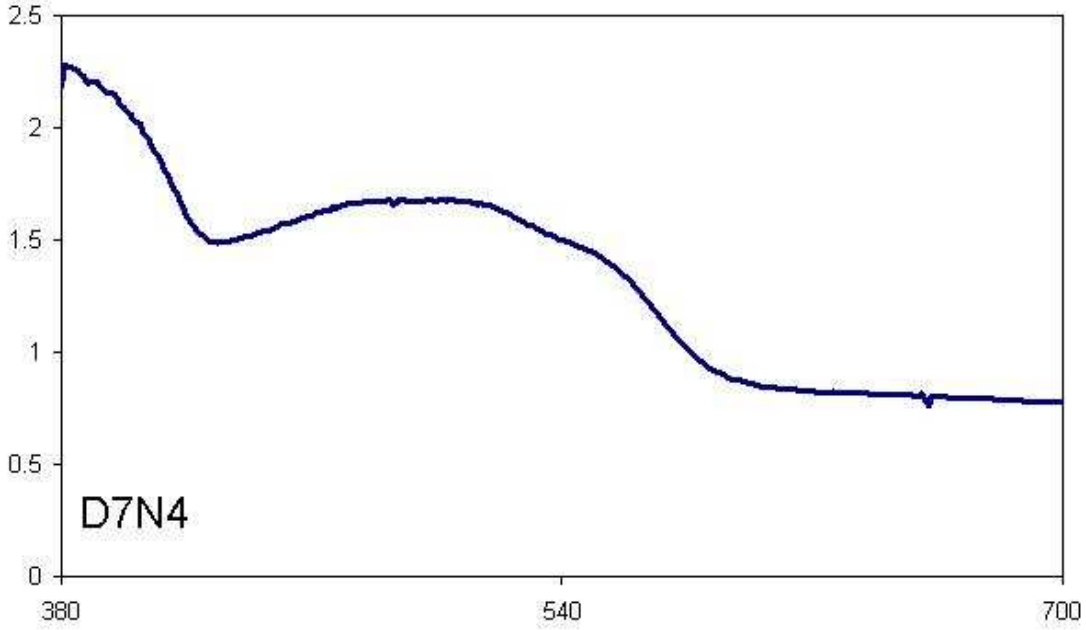
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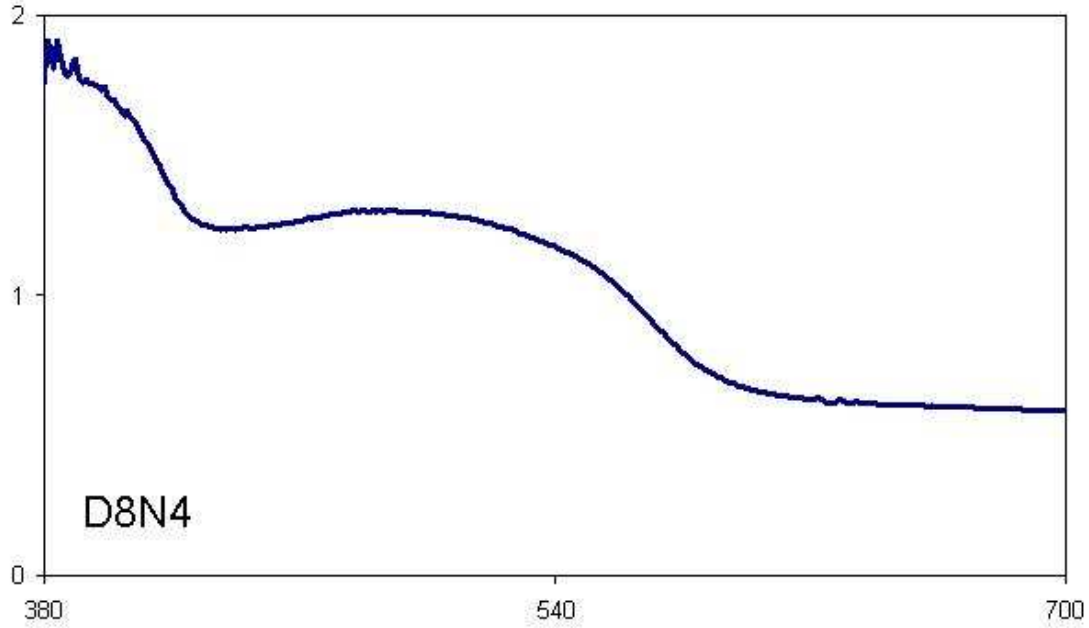
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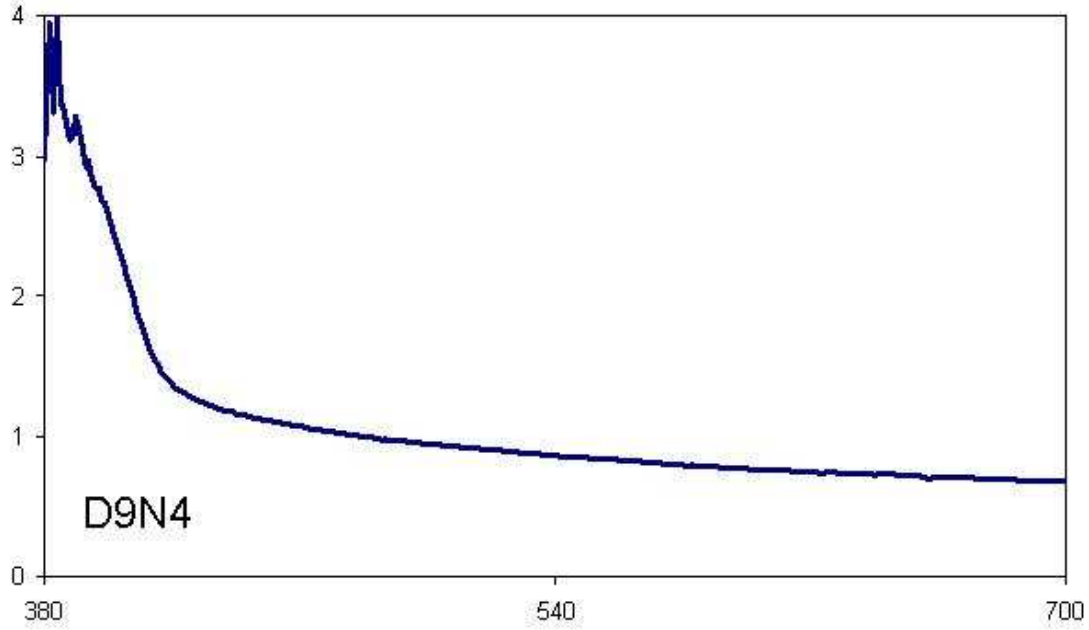
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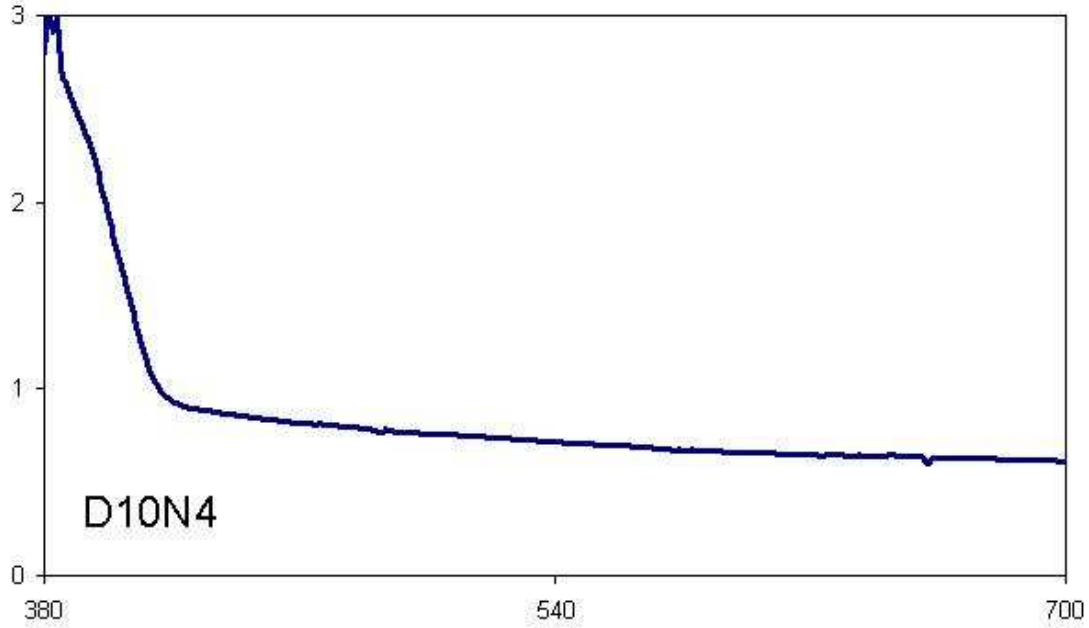
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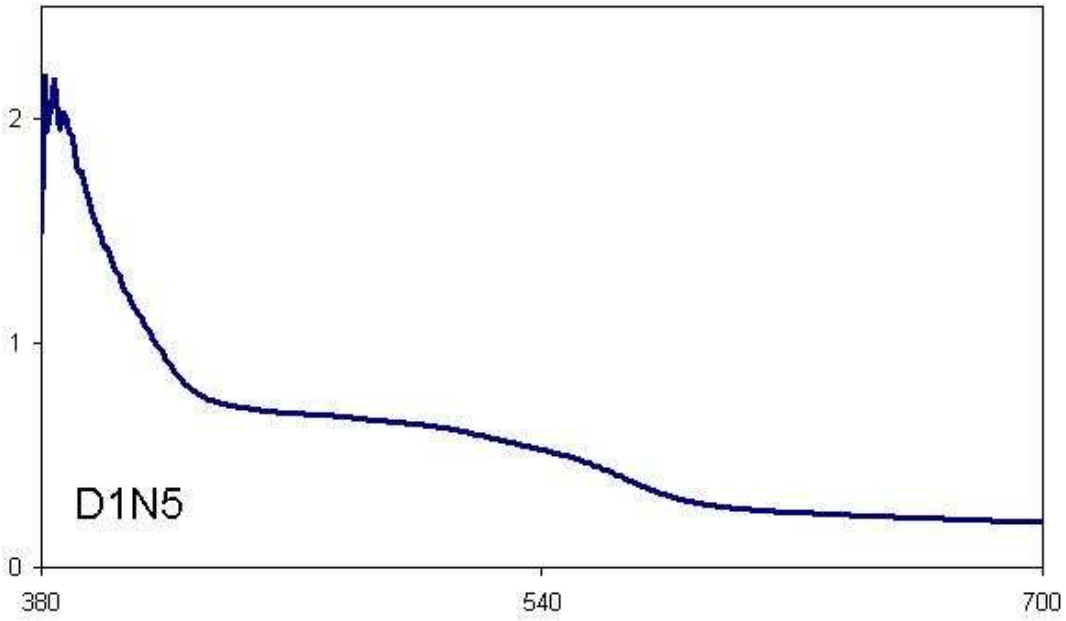
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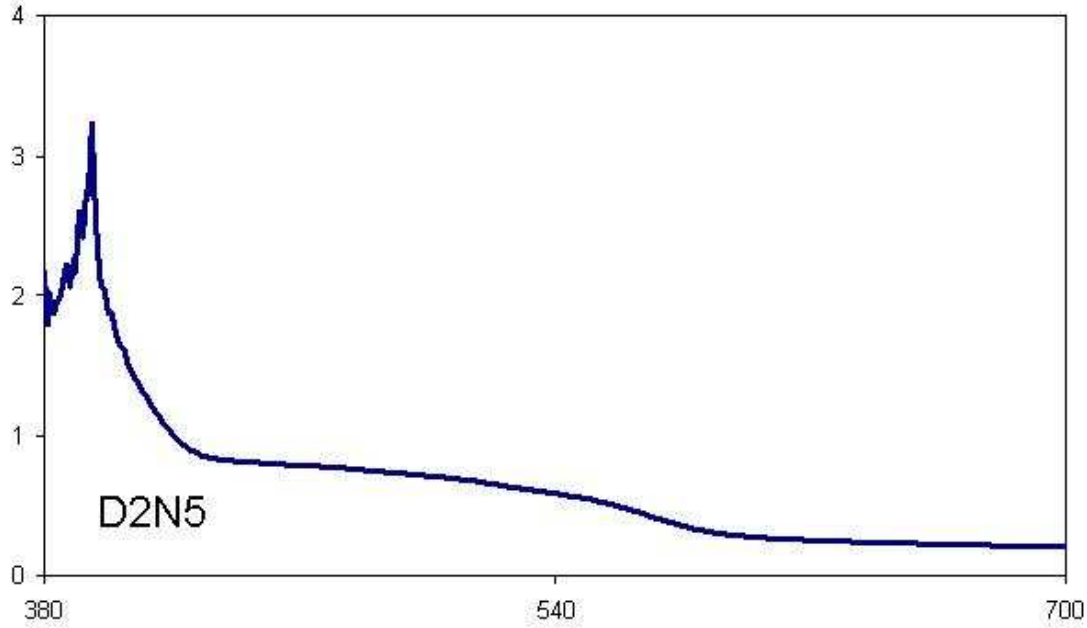
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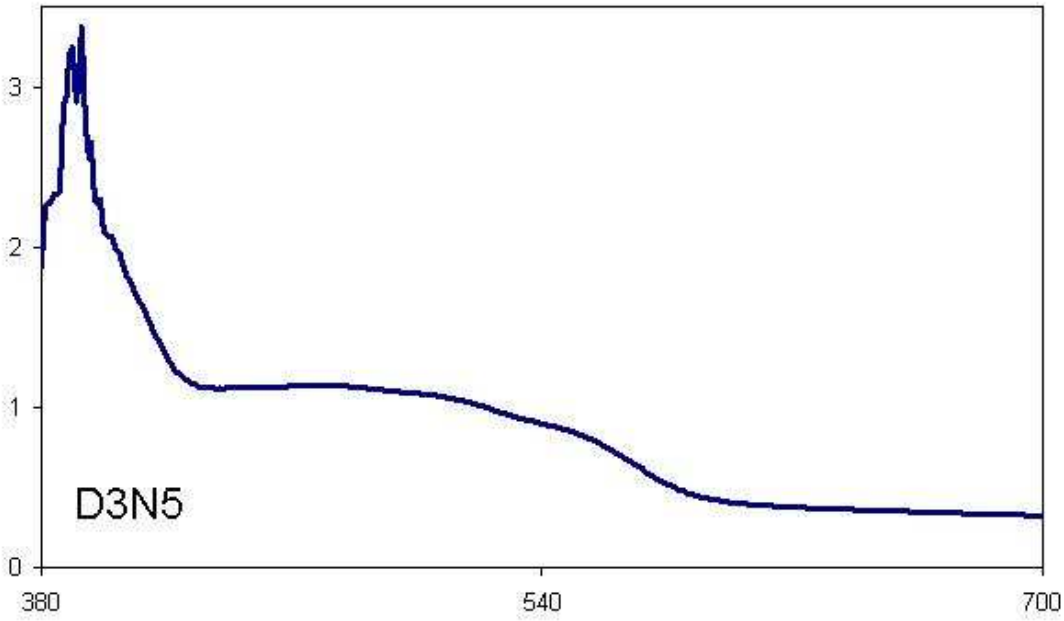
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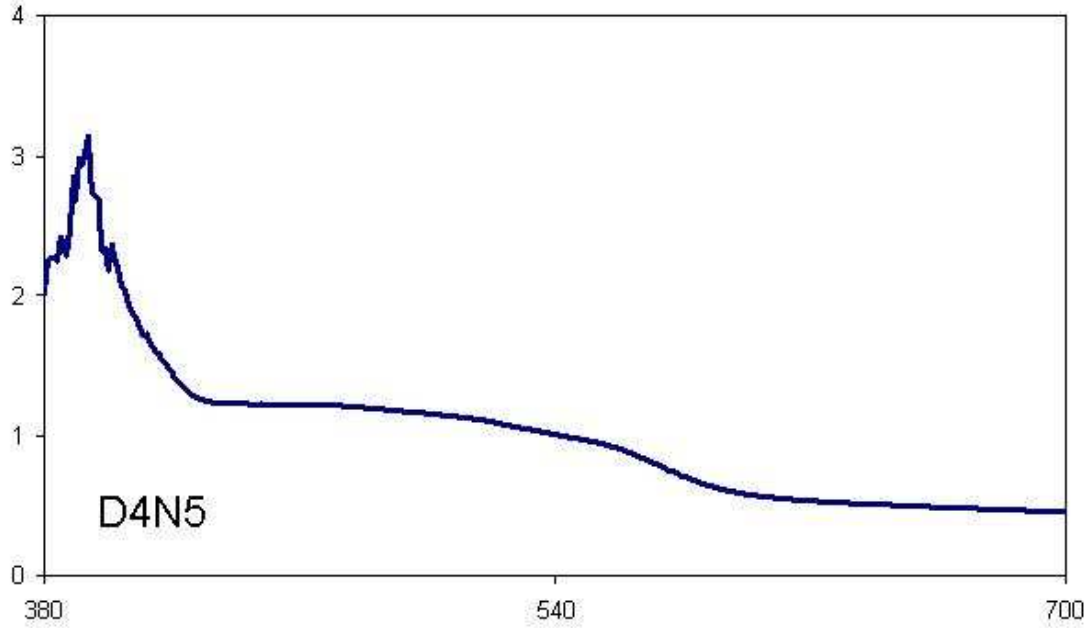
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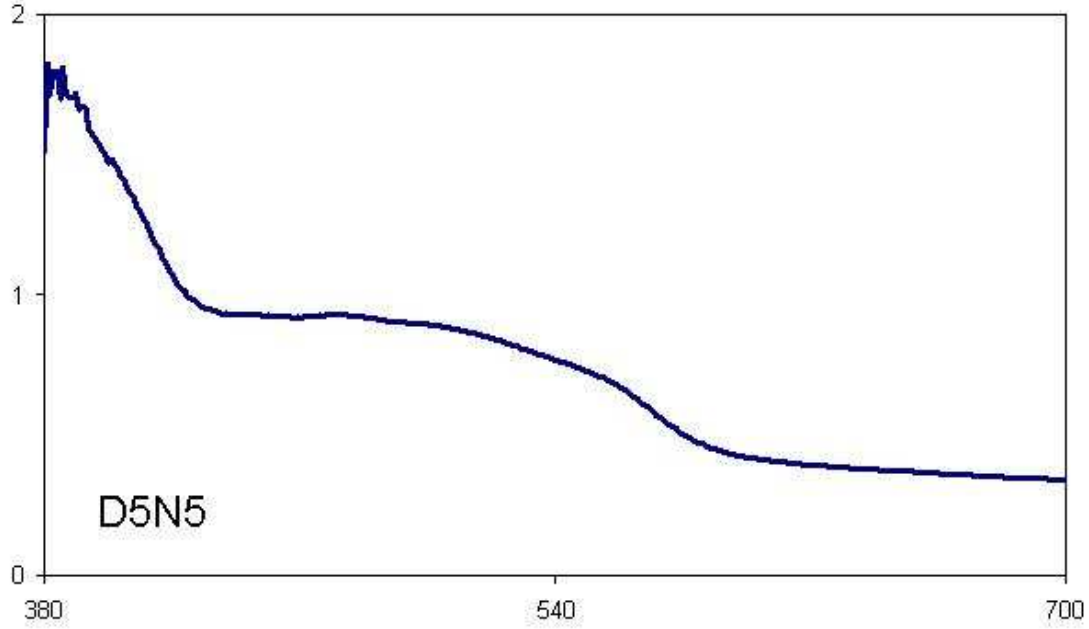
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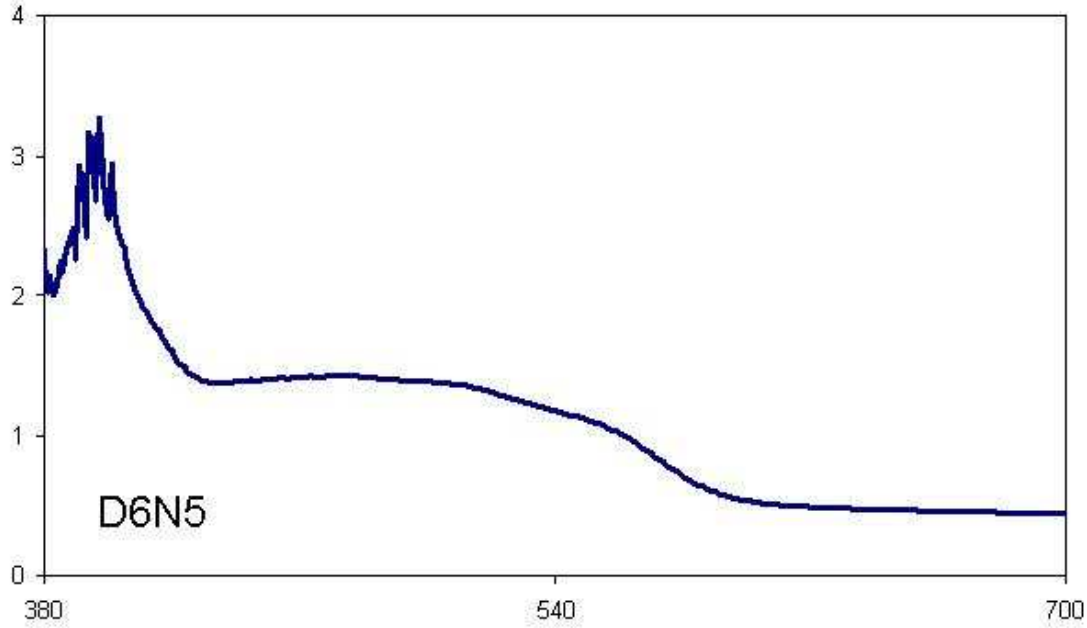
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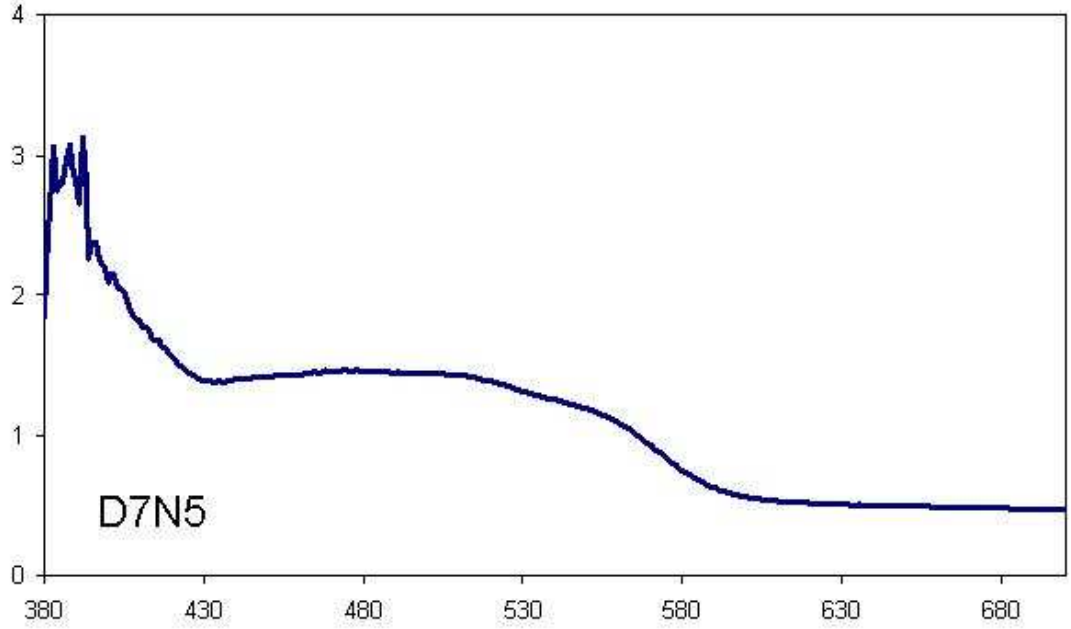
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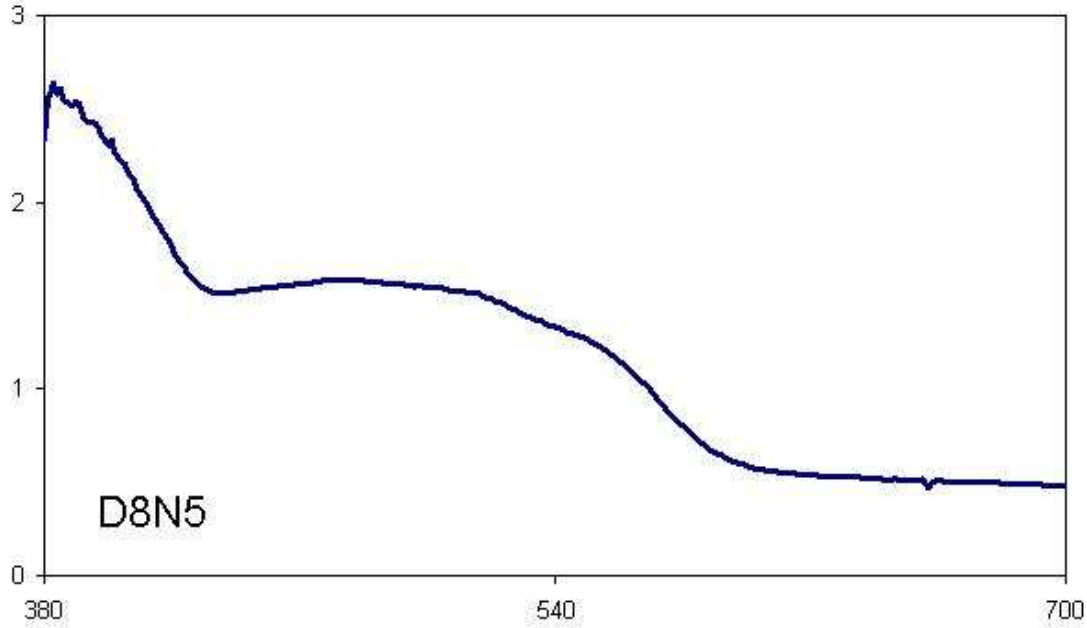
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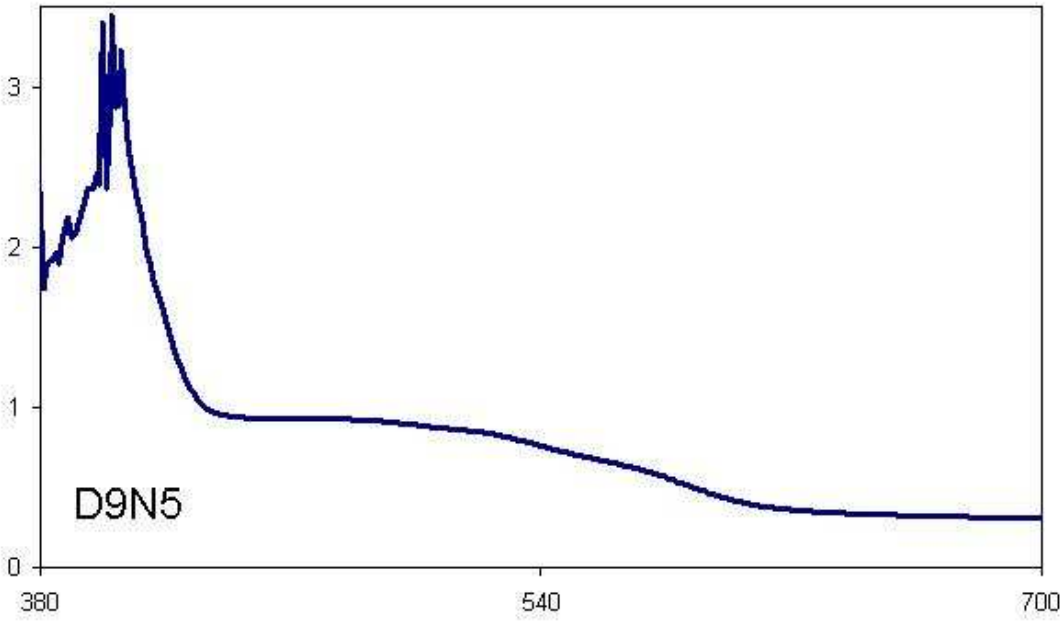
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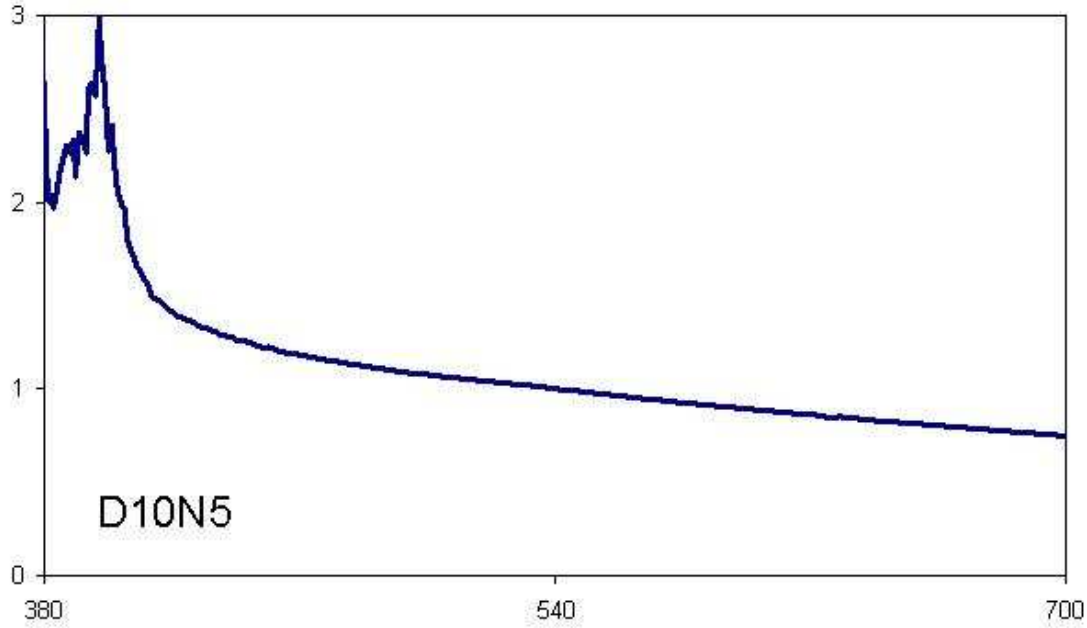
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References

1. Reczek, J. J.; Villazor, K. R.; Lynch, V.; Swager, T. M.; Iverson, B. L. *J. Am. Chem. Soc*. **2006**, *128* (24), 7995.

2. Pengo, P.; Pantos, G. D.; Otto, S.; Sanders, J. K. M. *J. Org. Chem.* **2006**, *71* (18), 7063.