

# Supporting Information

for

## **A general and facile one-pot process of isothiocyanates from amines under aqueous conditions**

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Xinquan Hu\*<sup>1,2</sup>

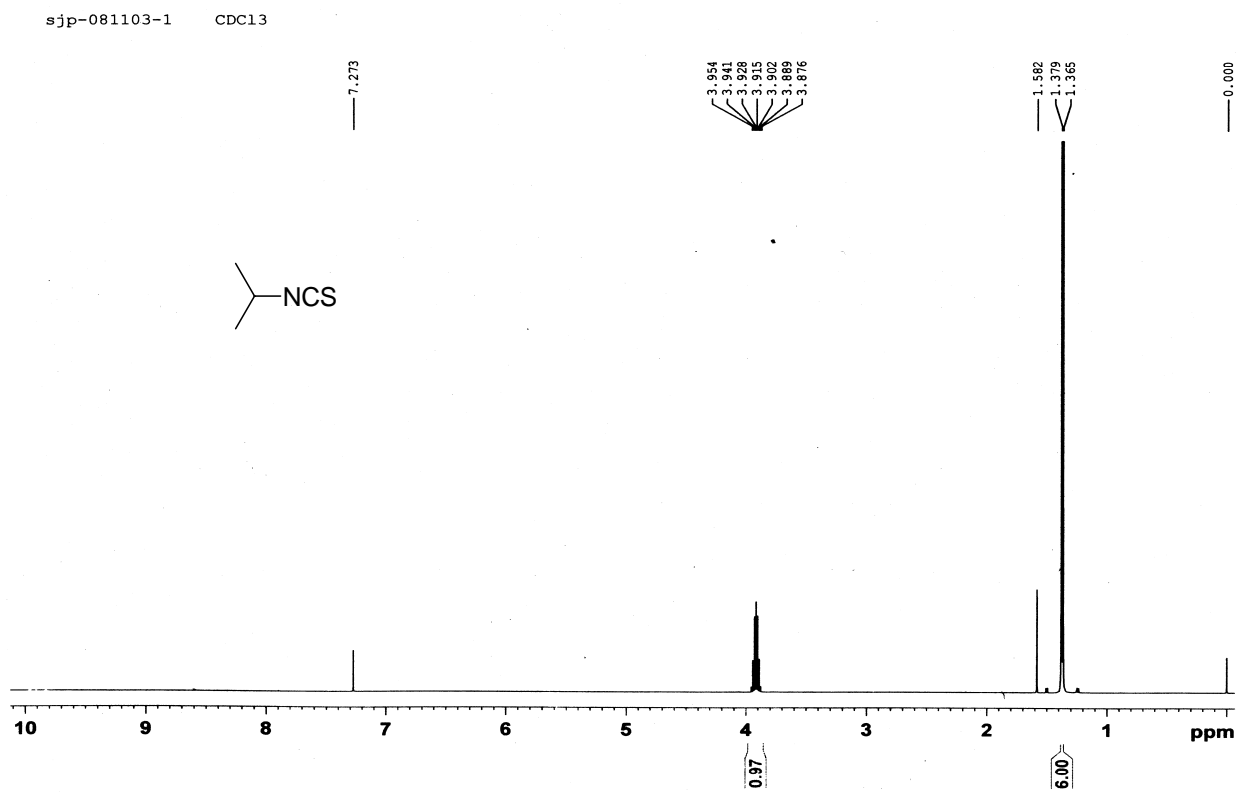
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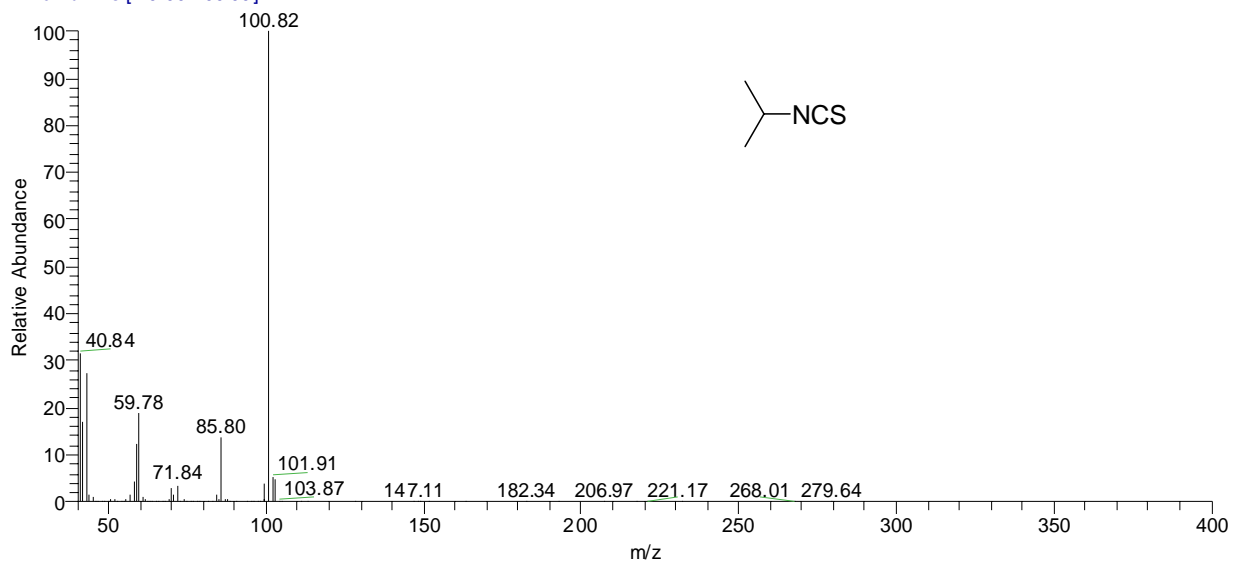
\* Corresponding author

## **Proton NMR and GC–MS spectra**

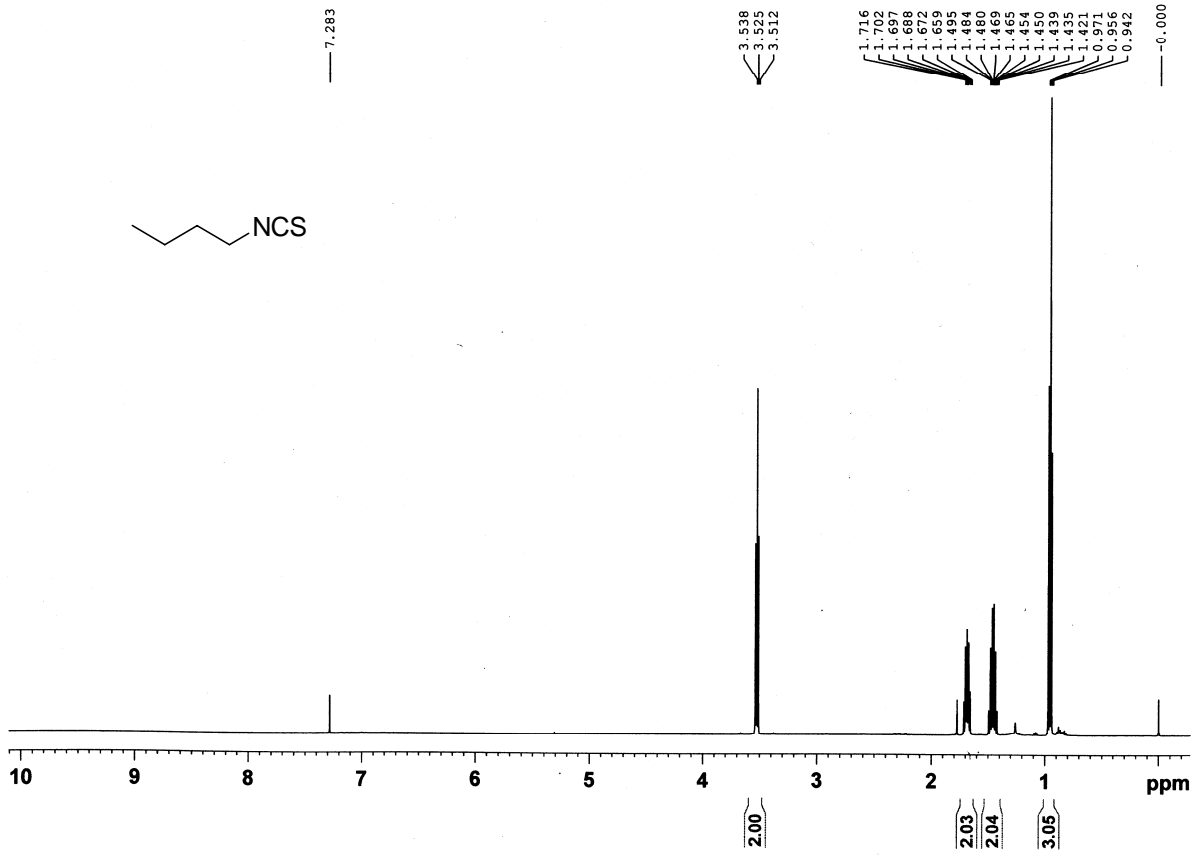
# Proton NMR and GC-MS spectra for isothiocyanates



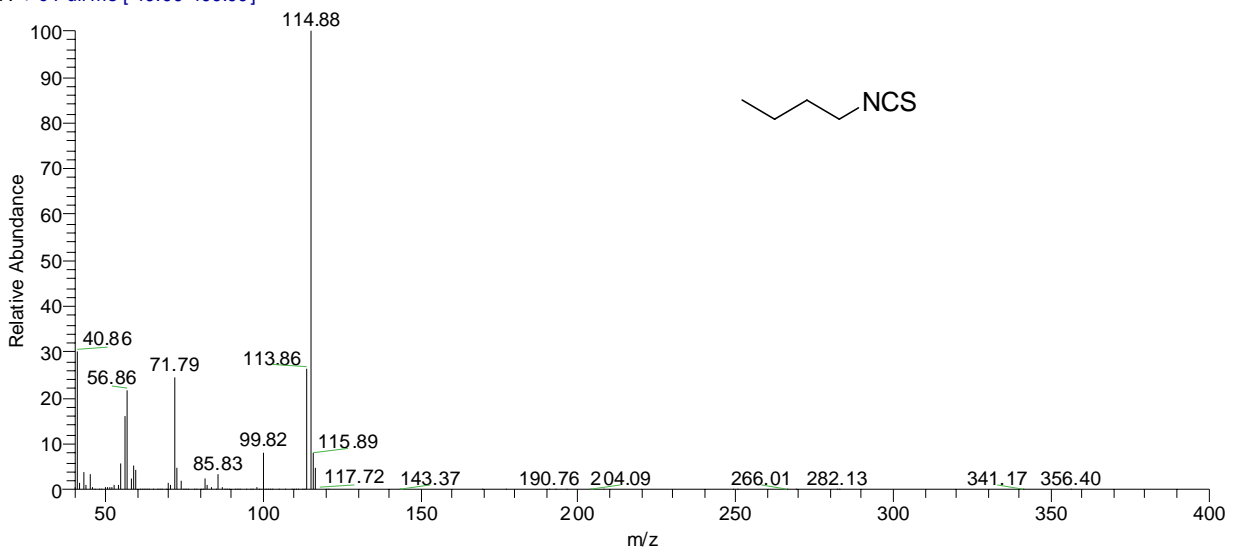
090311005 #46 RT: 3.20 AV: 1 SB: 37 3.09-3.12, 3.40-3.52 NL: 4.68E6  
T: + c Full ms [ 40.00-400.00]

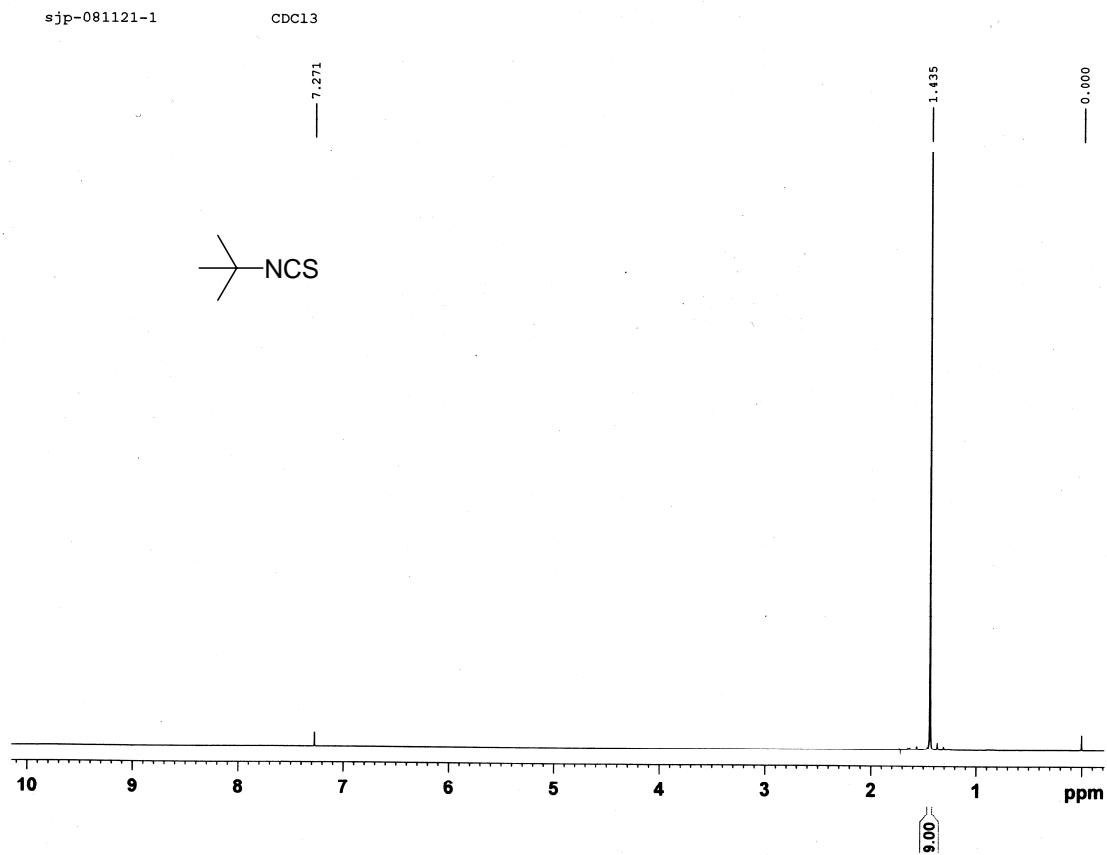


sjp081208 CDC13

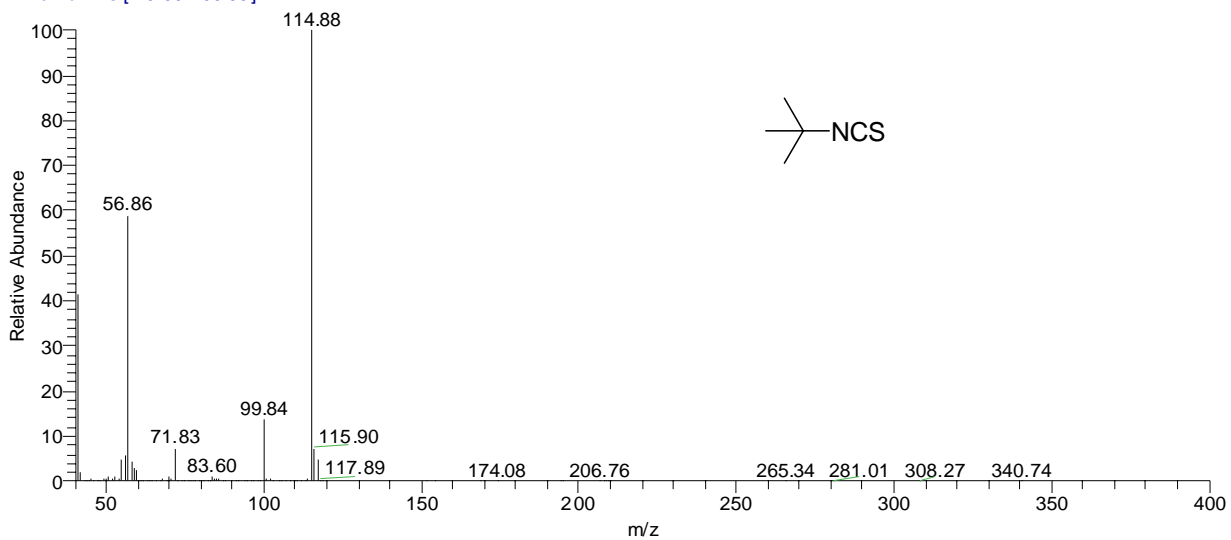


090312006 #489 RT: 5.12 AV: 1 SB: 25 5.02-5.08, 5.28-5.33 NL: 4.43E6  
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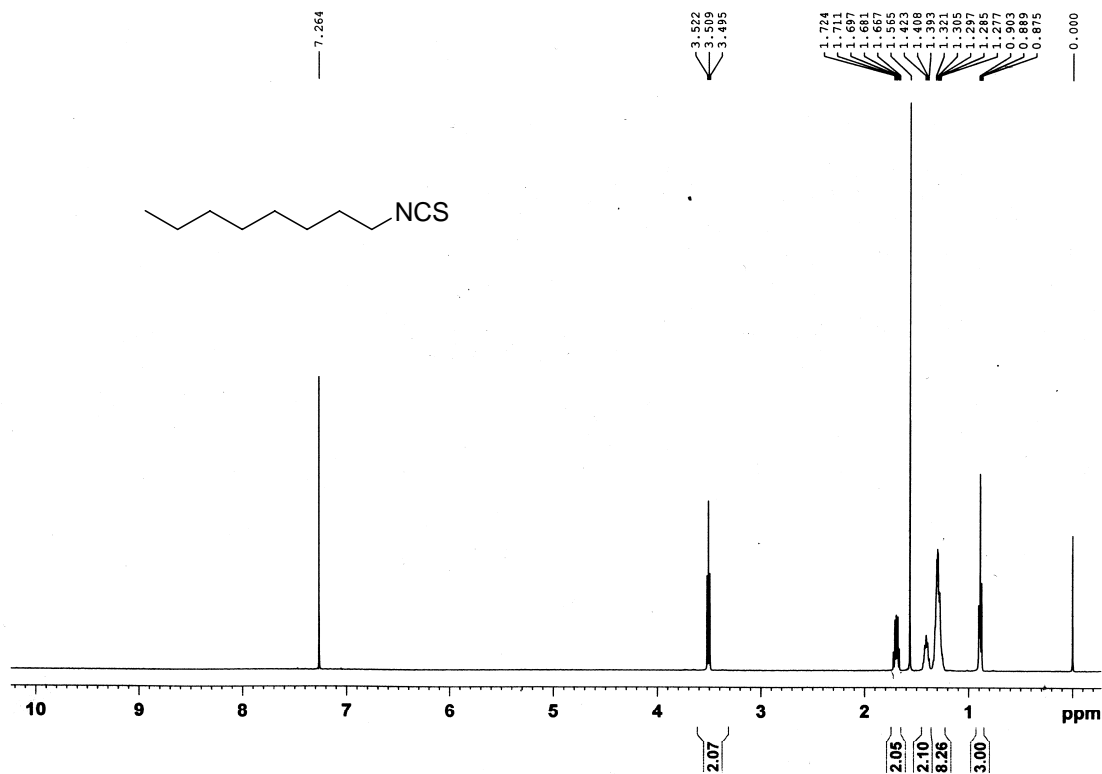




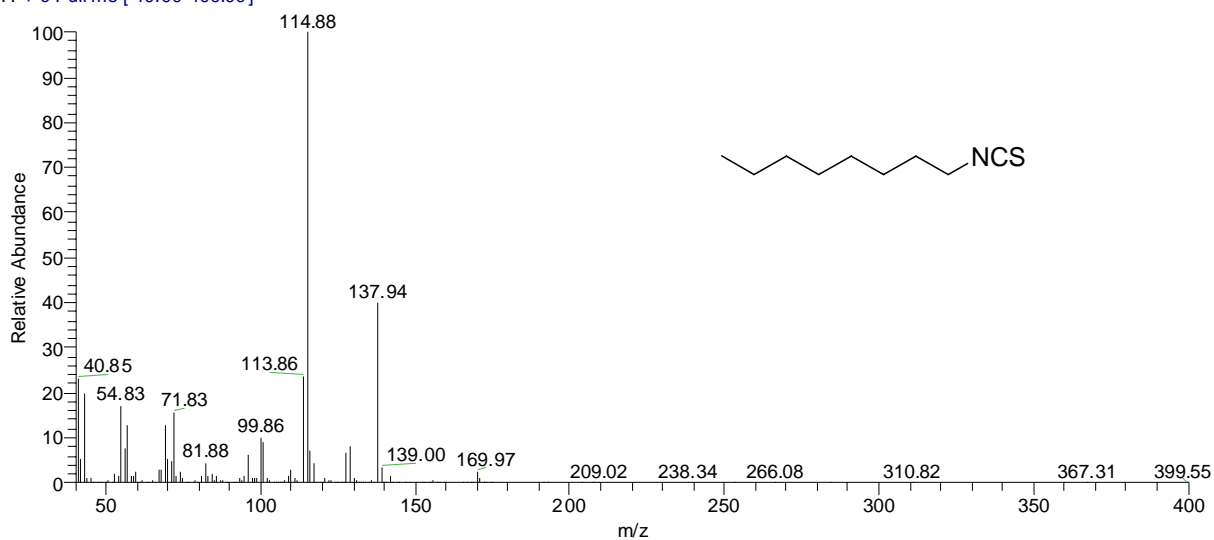
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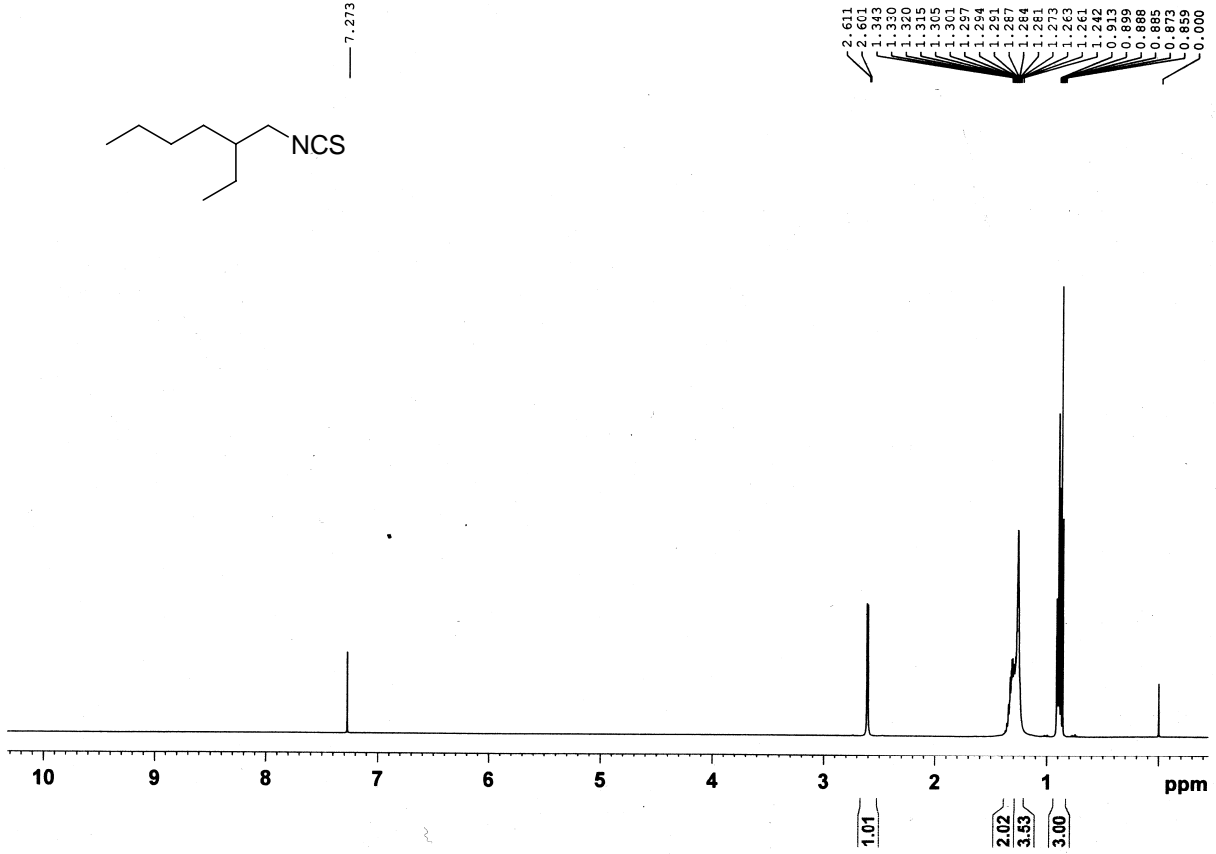
sn091215-2 CDC13



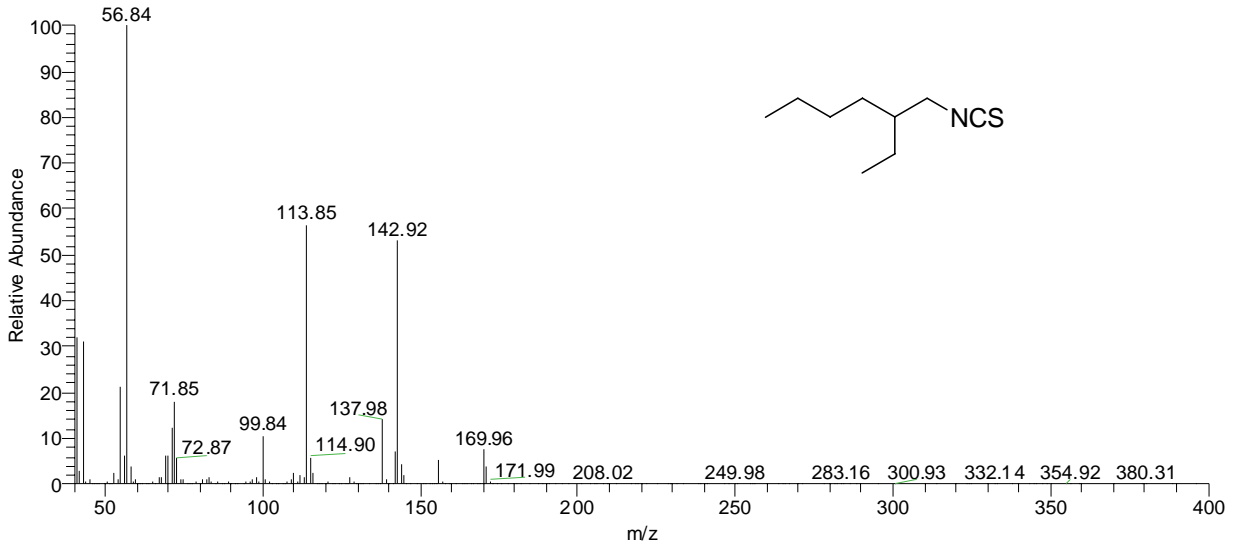
090311008 #1801 RT: 10.82 AV: 1 SB: 109 10.50-10.65, 11.09-11.41 NL: 1.65E7  
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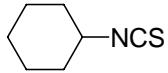
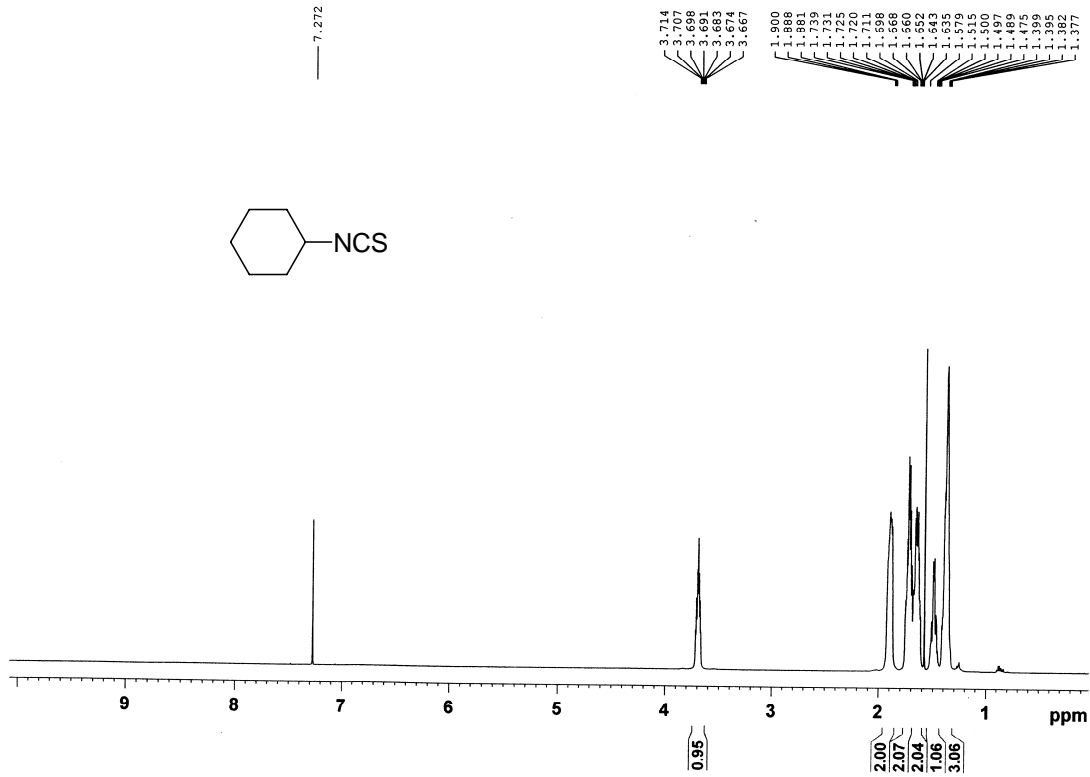
LB20091221 CDC13



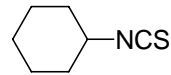
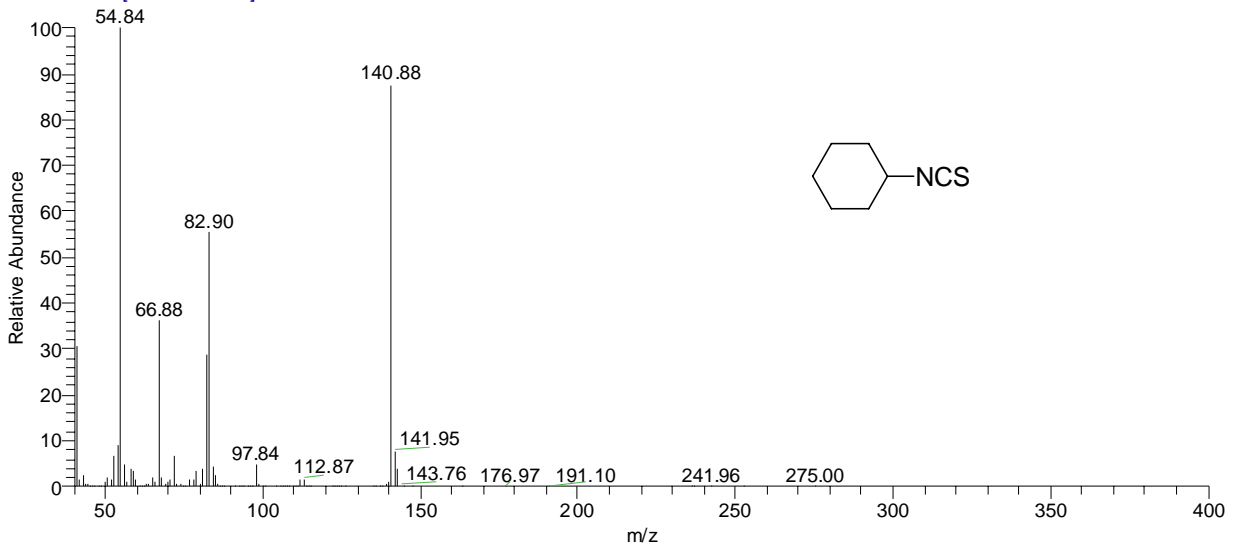
090312005 #1576-1667 RT: 9.84-10.23 AV: 92 SB: 46 9.73-9.78, 10.05-10.20 NL: 1.45E5  
T: + c Full ms [ 40.00-400.00]



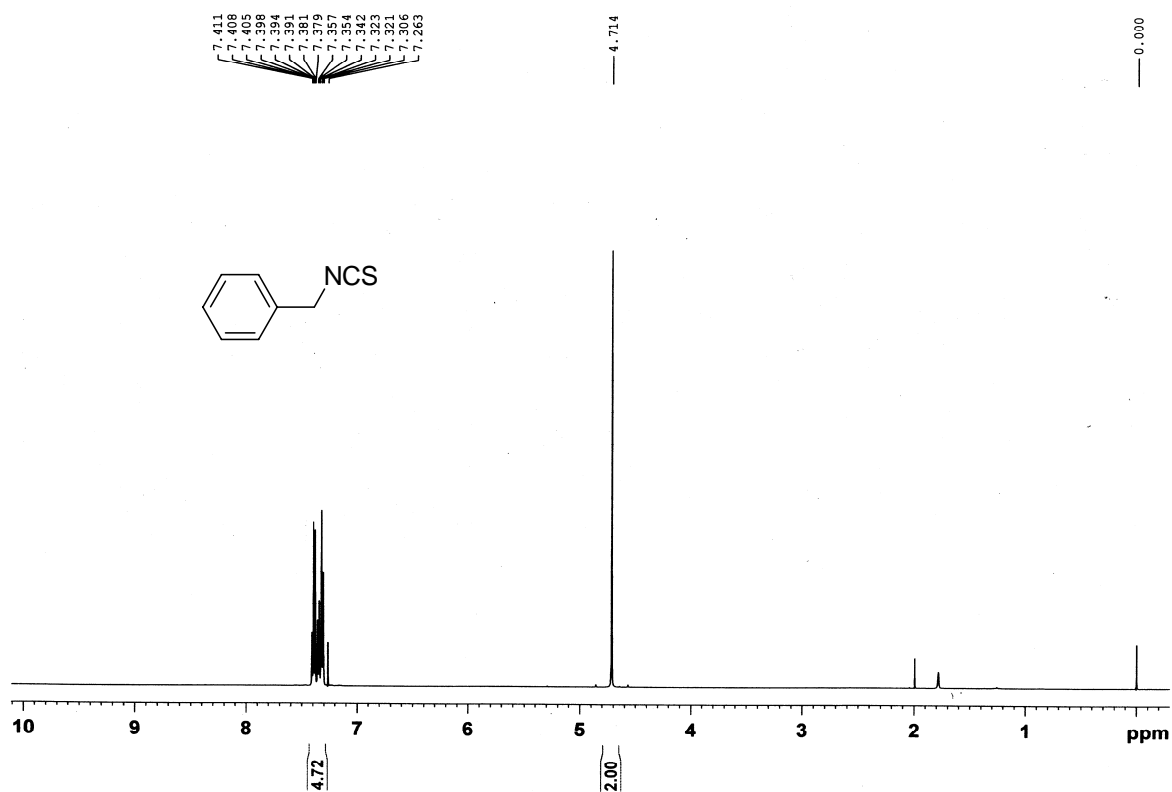
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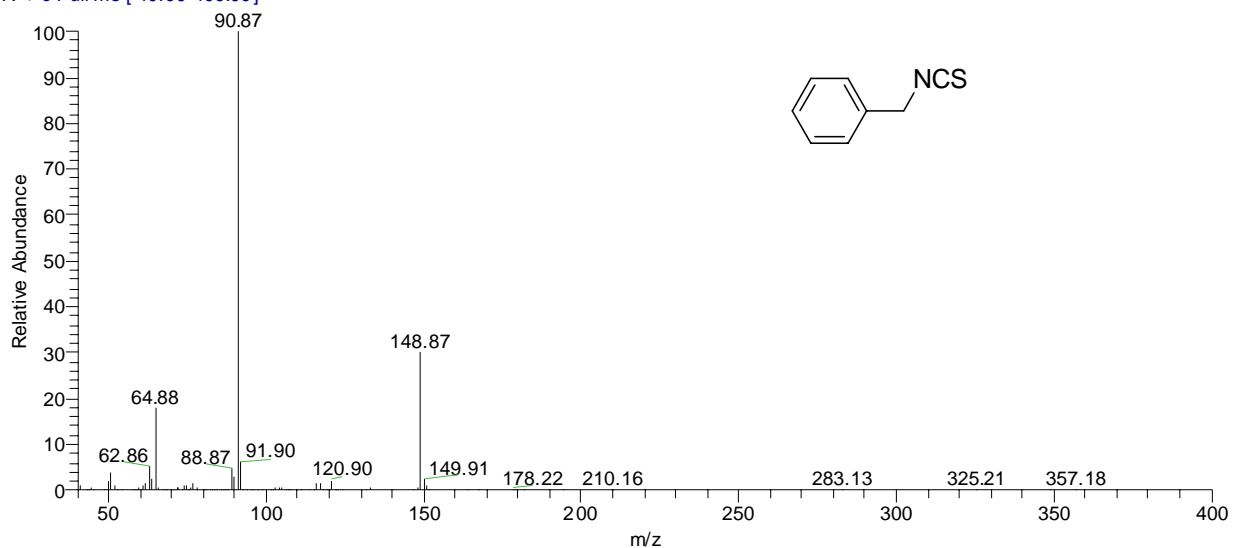
090312003#1264 RT: 8.48 AV: 1 SB: 36 8.32-8.36, 8.68-8.79 NL: 4.01E6  
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sjp081222-1 CDC13

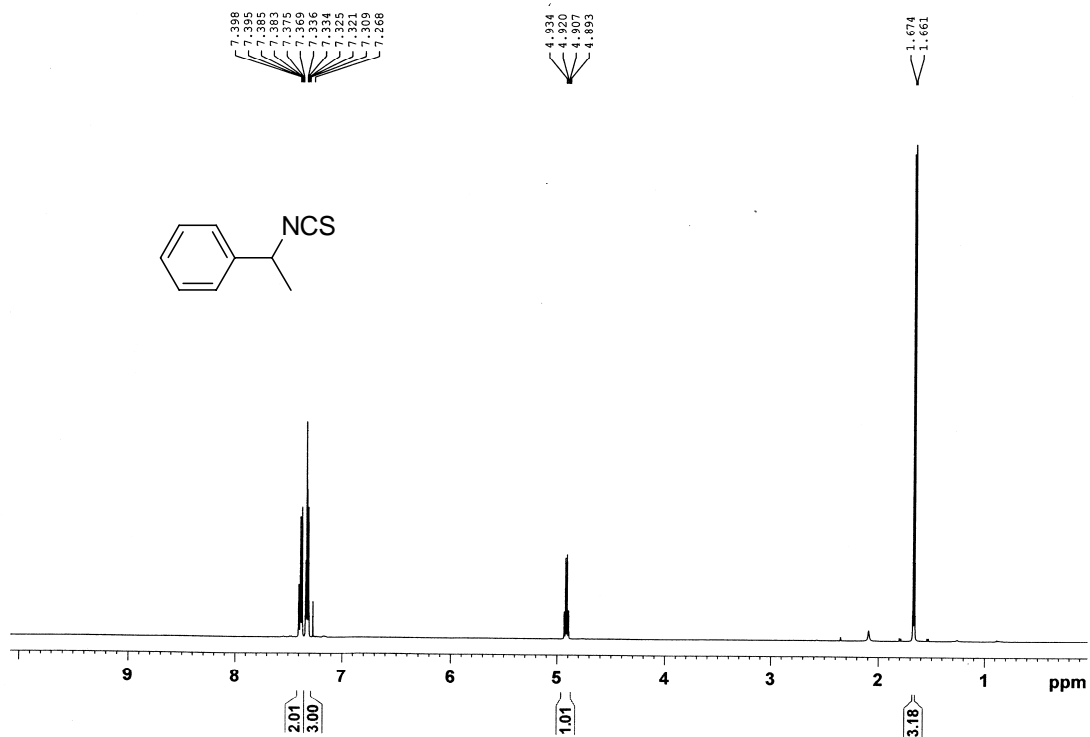


090312002#1700 RT: 10.38 AV: 1 SB: 99 9.98-10.09, 11.34-11.65 NL: 1.39E6  
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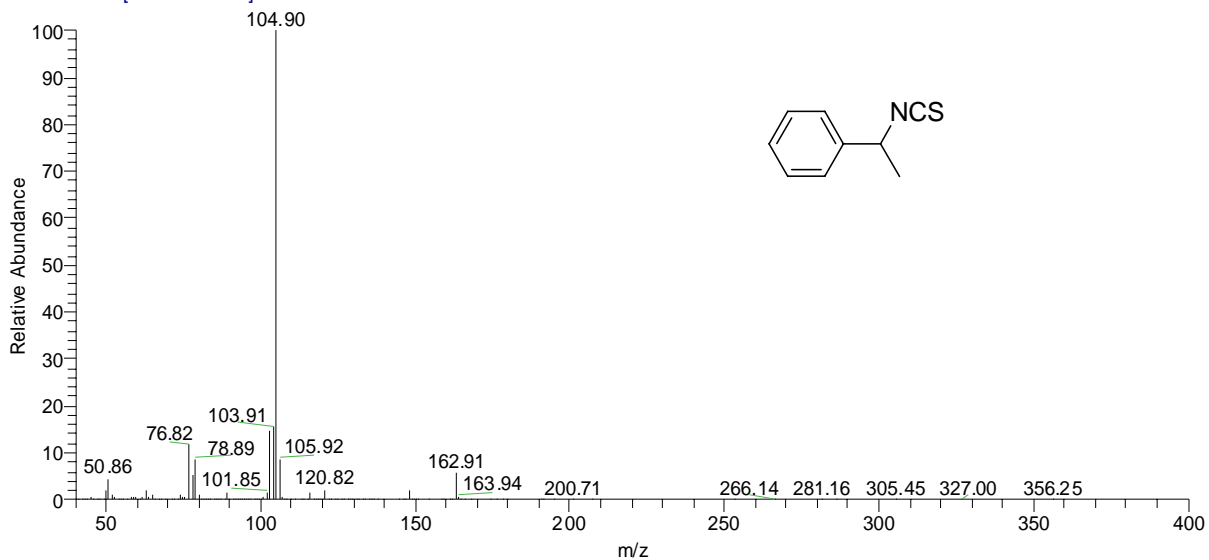




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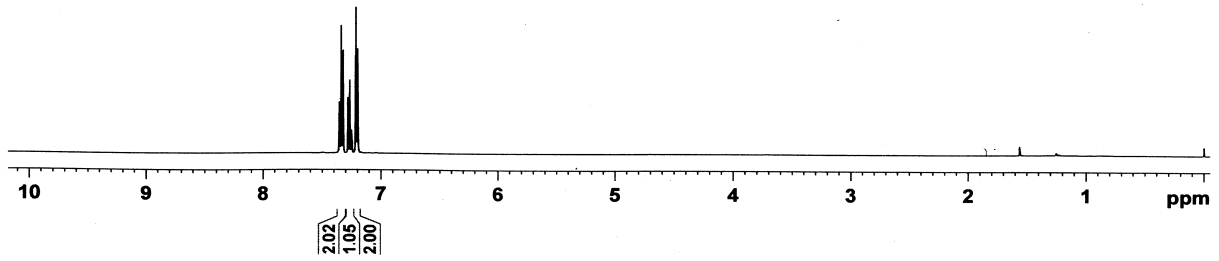
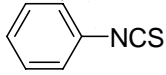
090311006 #1724 RT: 10.48 AV: 1 SB: 49 10.27-10.36, 10.73-10.85 NL: 1.26E7  
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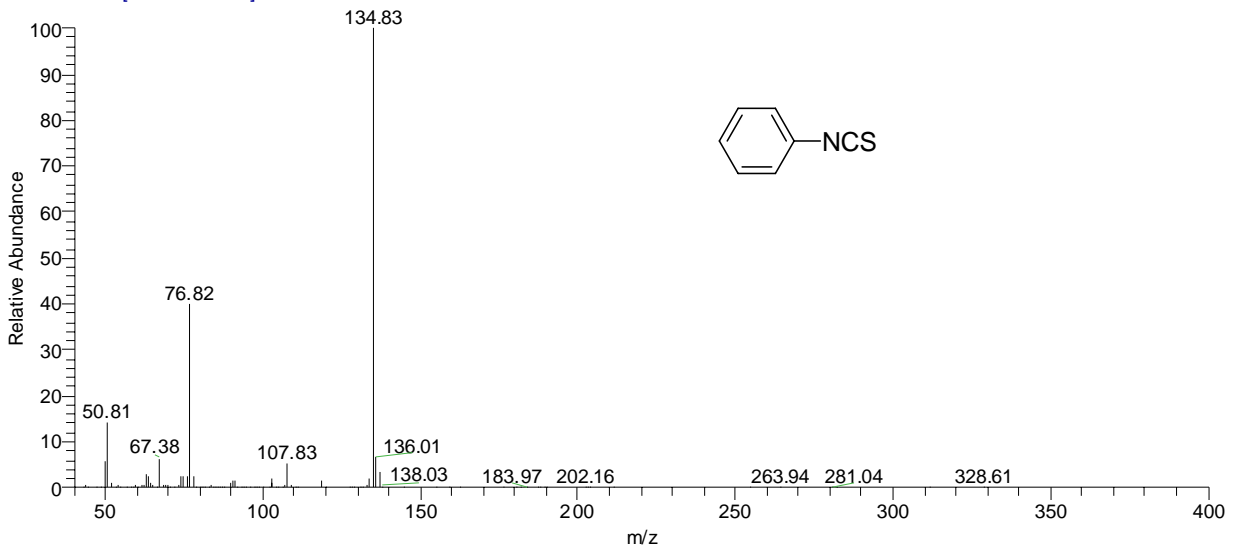
cwrbtnan CDCL3

7.351  
7.351  
7.338  
7.326  
7.322  
7.281  
7.278  
7.270  
7.266  
7.262  
7.253  
7.246  
7.217  
7.214  
7.198

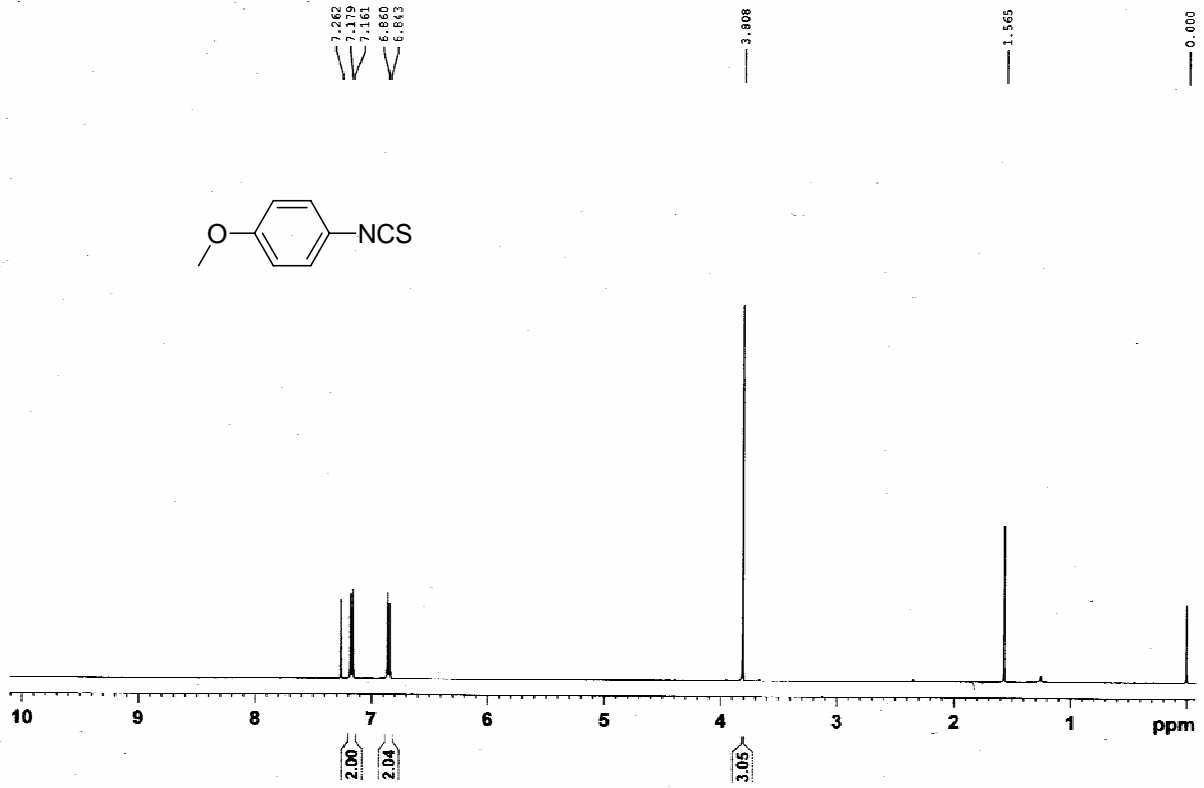
1.561



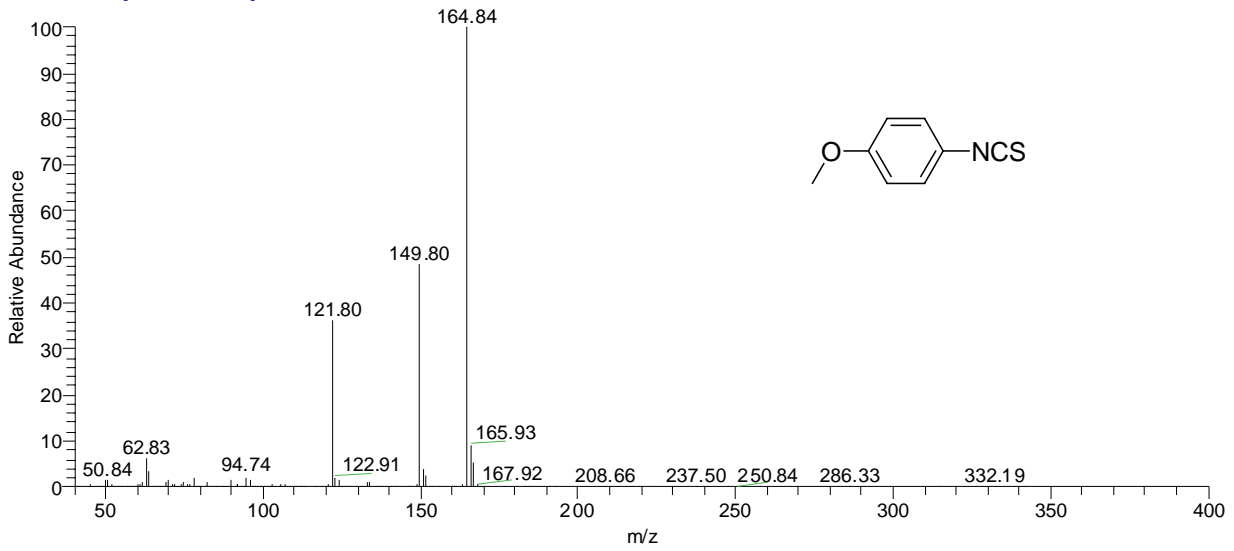
090309004 #1181 RT: 8.12 AV: 1 SB: 492 7.04-7.73, 10.30-11.73 NL: 1.81E6  
T: + c Full ms [ 40.00-400.00]



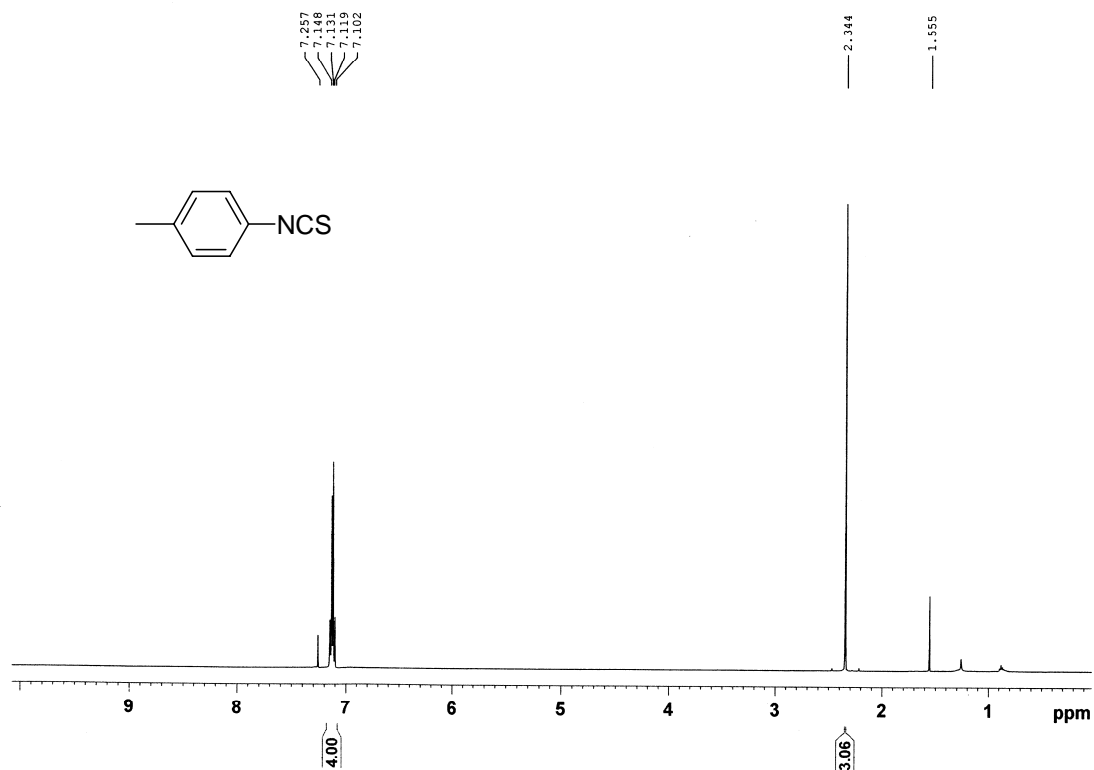
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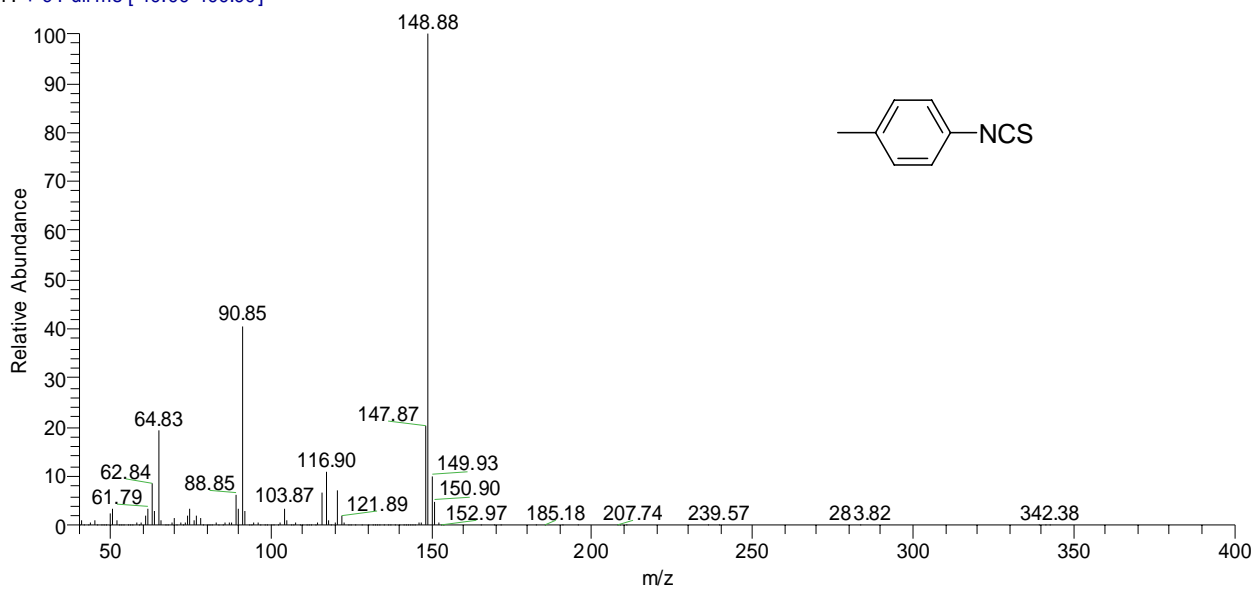
090310007 #2043 RT: 11.87 AV: 1 SB: 160 11.23-11.48, 12.46-12.90 NL: 9.36E6  
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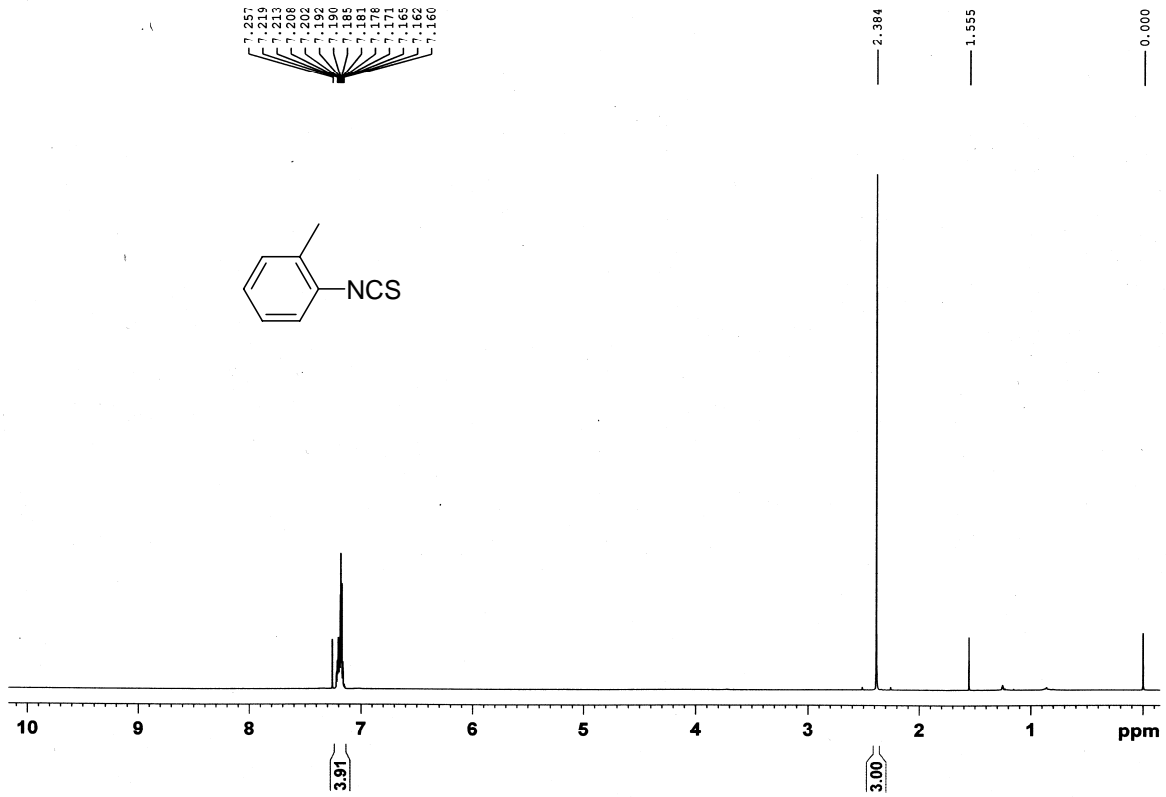
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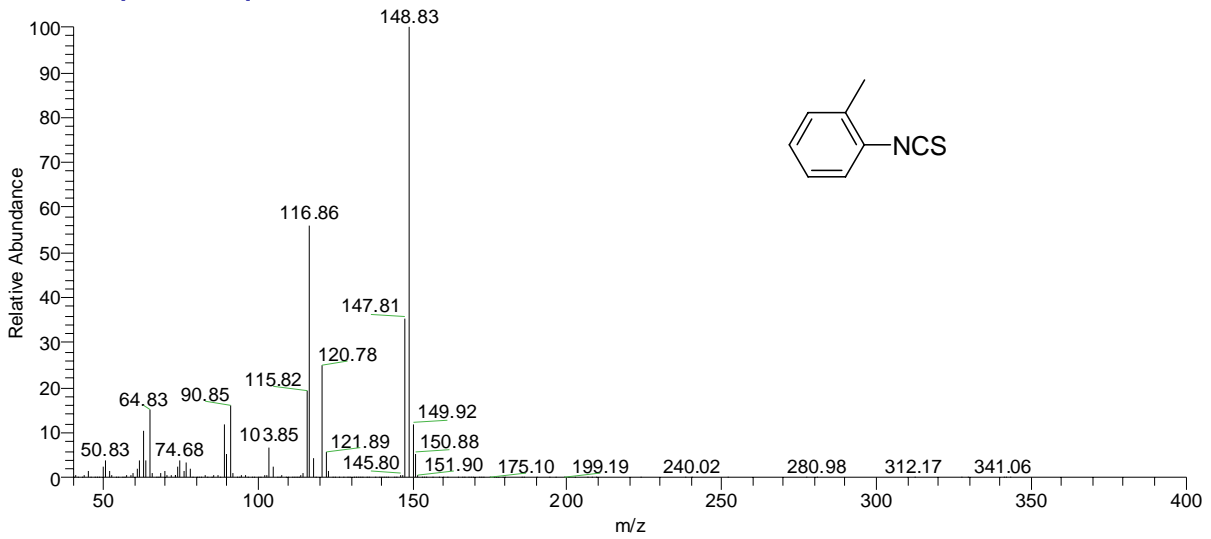
090311002 #1516 RT: 9.58 AV: 1 SB: 21 9.44-9.48, 9.74-9.79 NL: 2.64E7  
T: + c Full ms [ 40.00-400.00]



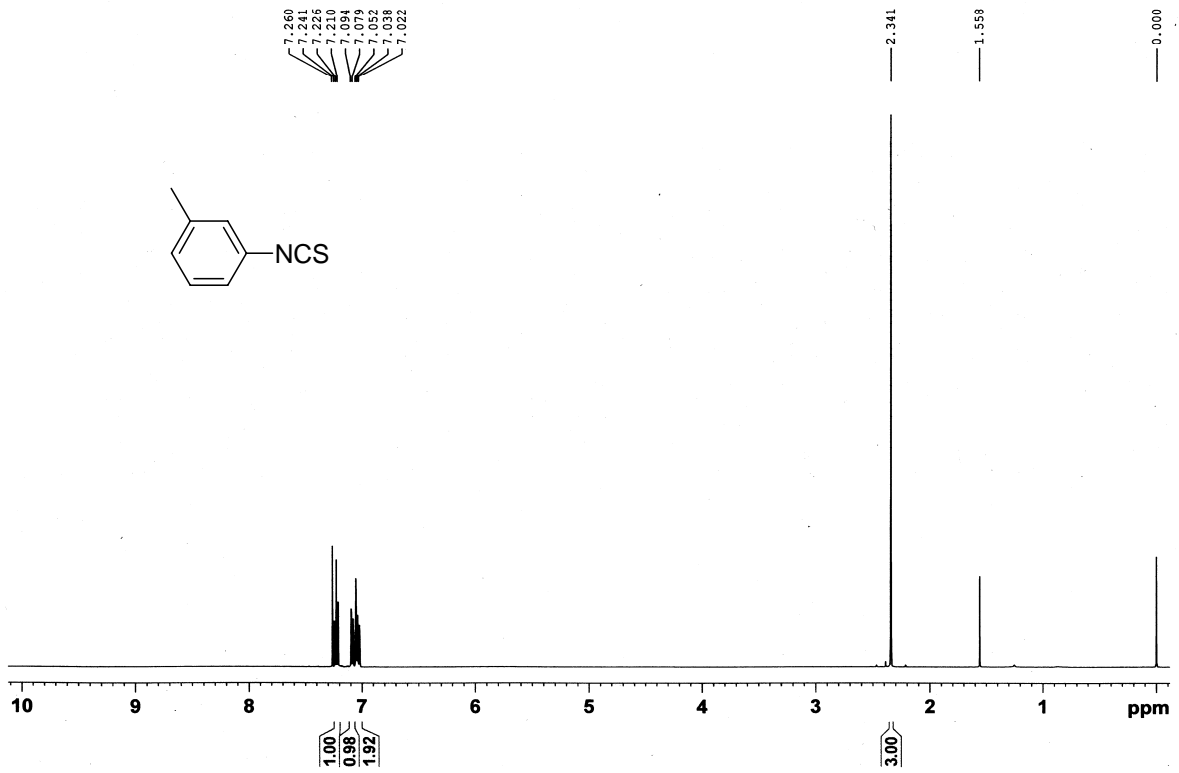
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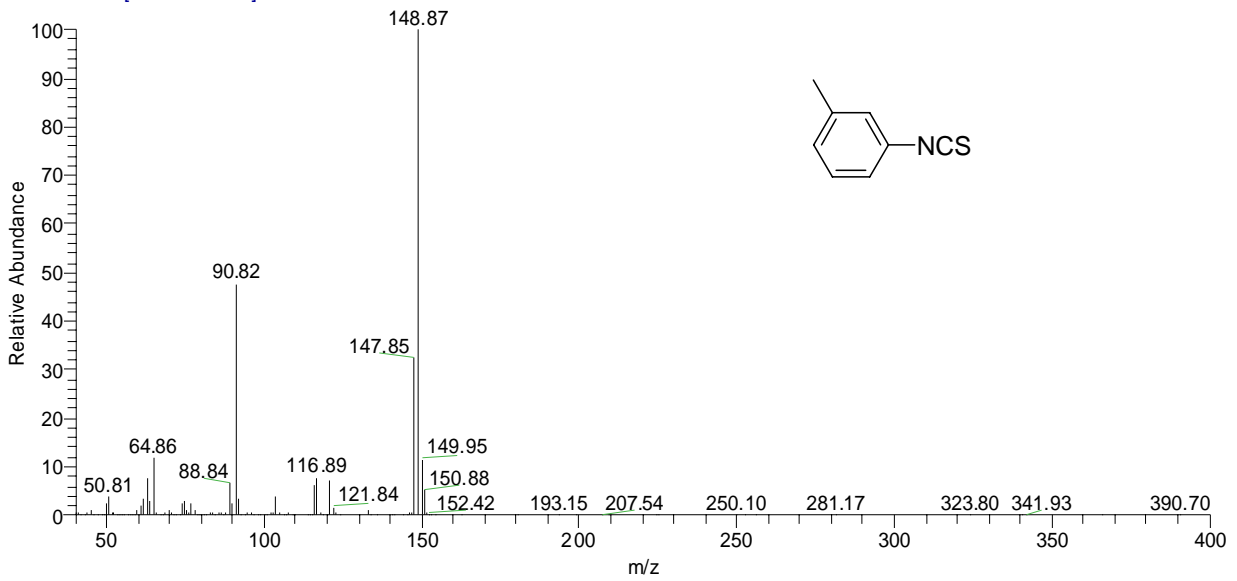
090310004 #1486 RT: 9.45 AV: 1 SB: 28 9.30-9.35, 9.55-9.61 NL: 5.68E7  
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cwr090112-2 CDC13



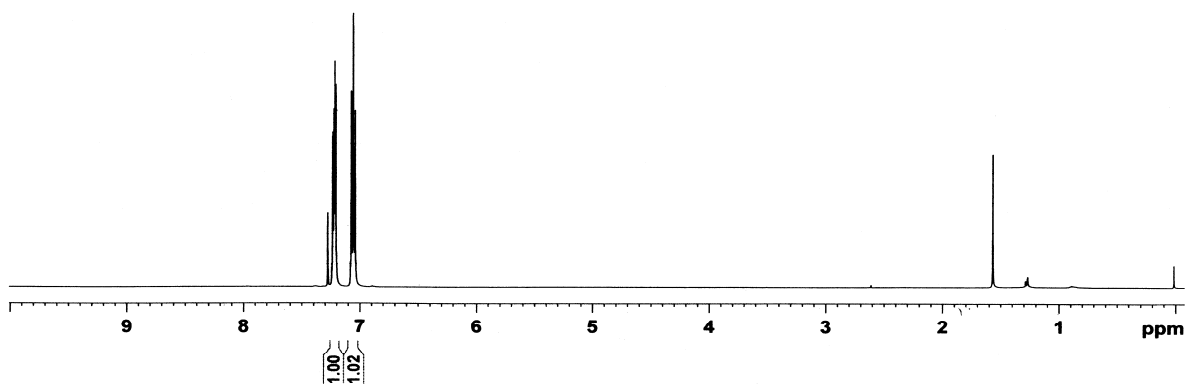
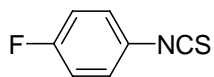
090310011#1556 RT: 9.75 AV: 1 SB: 281 9.05-9.40, 11.03-11.88 NL: 3.69E6  
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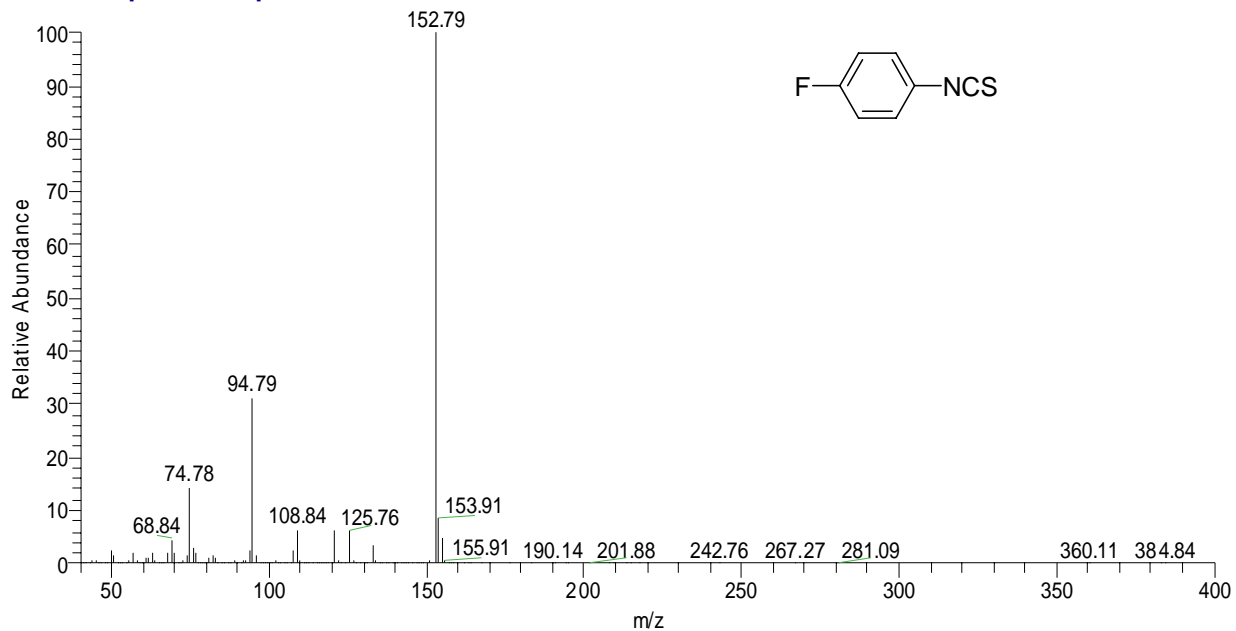
PF-1 CDCl3

7.276  
7.235  
7.235  
7.225  
7.221  
7.217  
7.212  
7.208  
7.075  
7.058  
7.045  
7.040

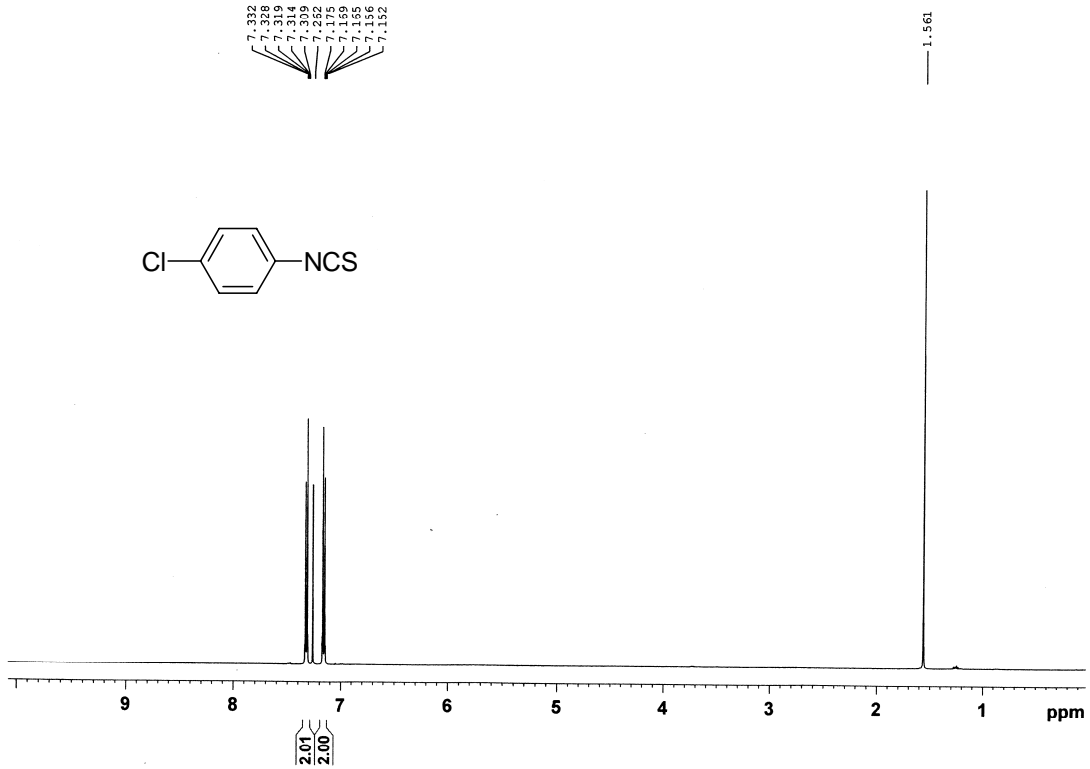
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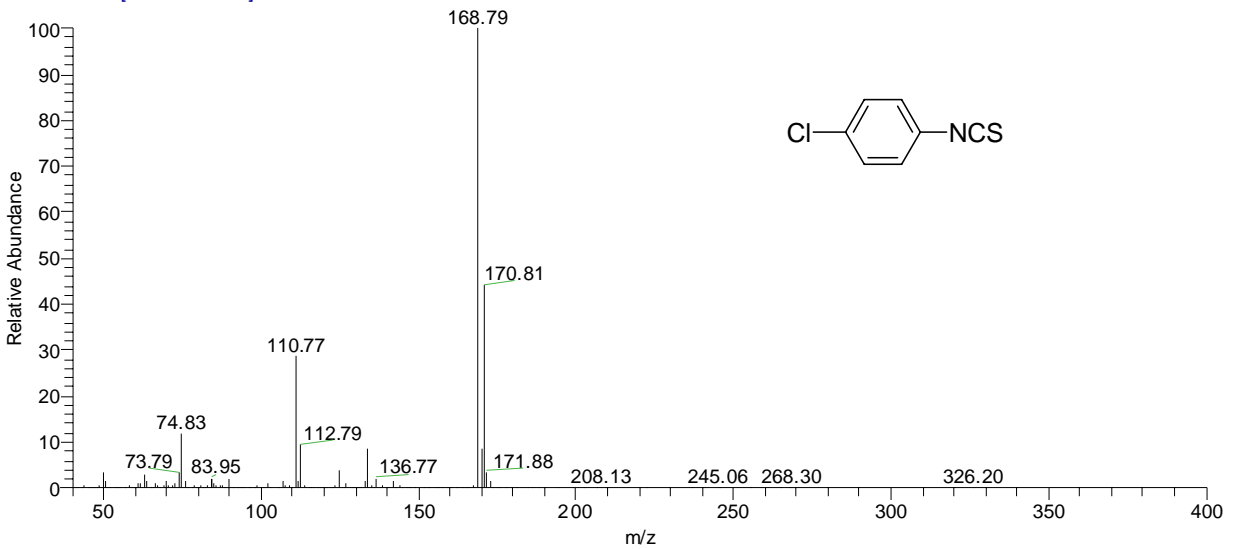
090310005#1140 RT: 7.95 AV: 1 SB: 105 7.60-7.81, 8.14-8.38 NL: 5.08E7  
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LB2009120801 CDCl3

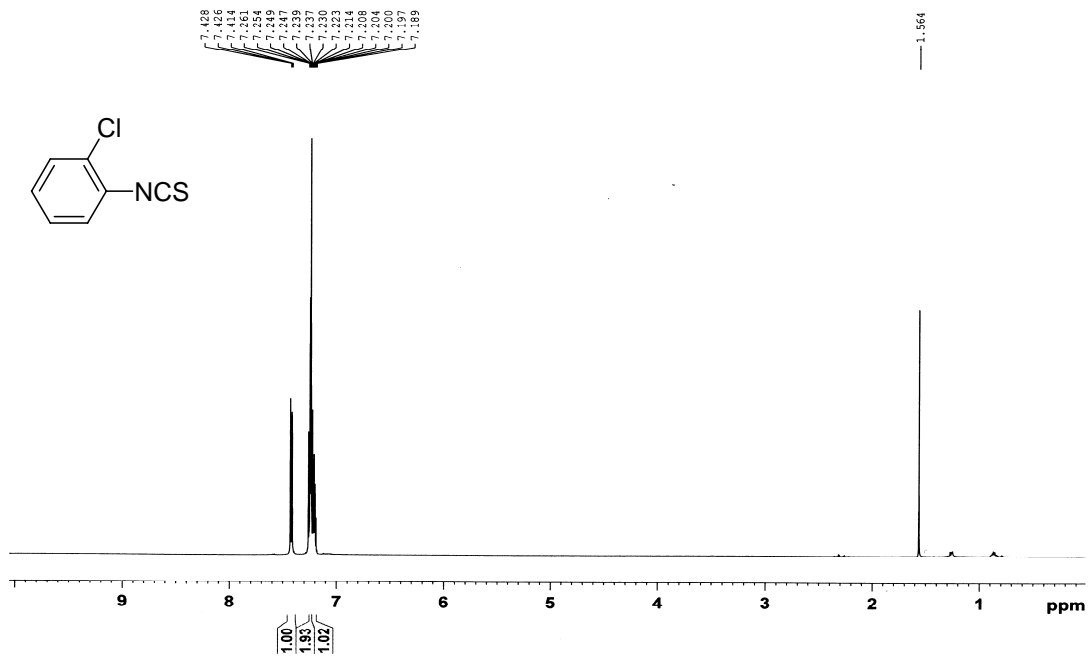


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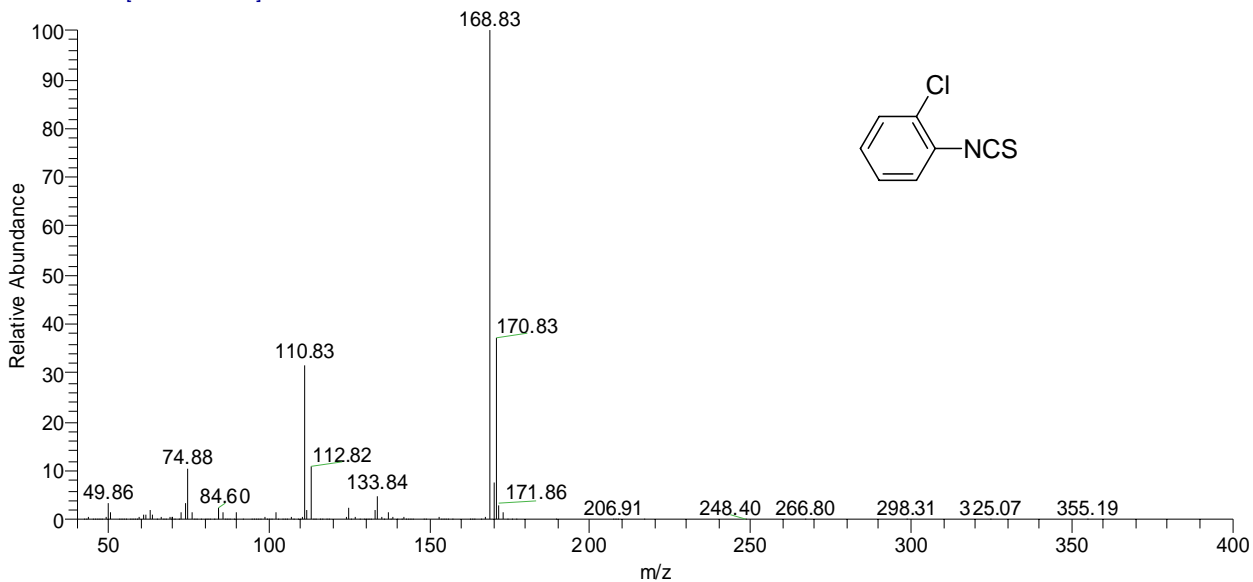




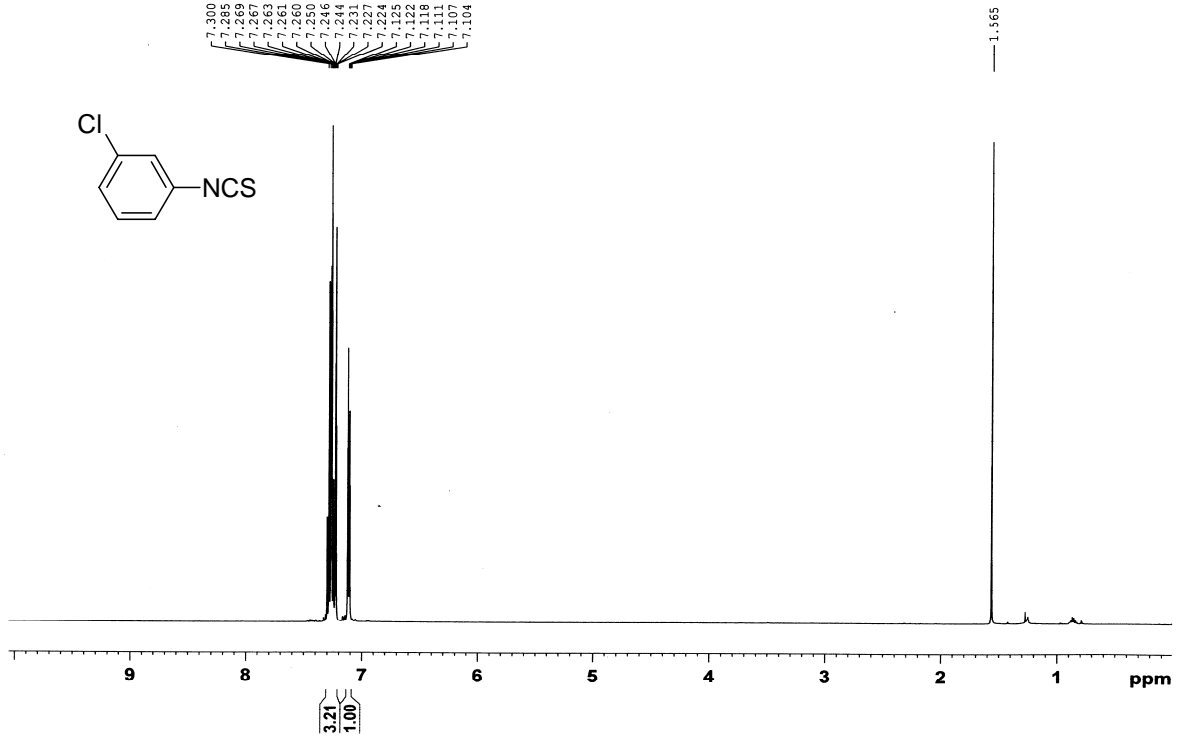
OCL20100324 CDC13



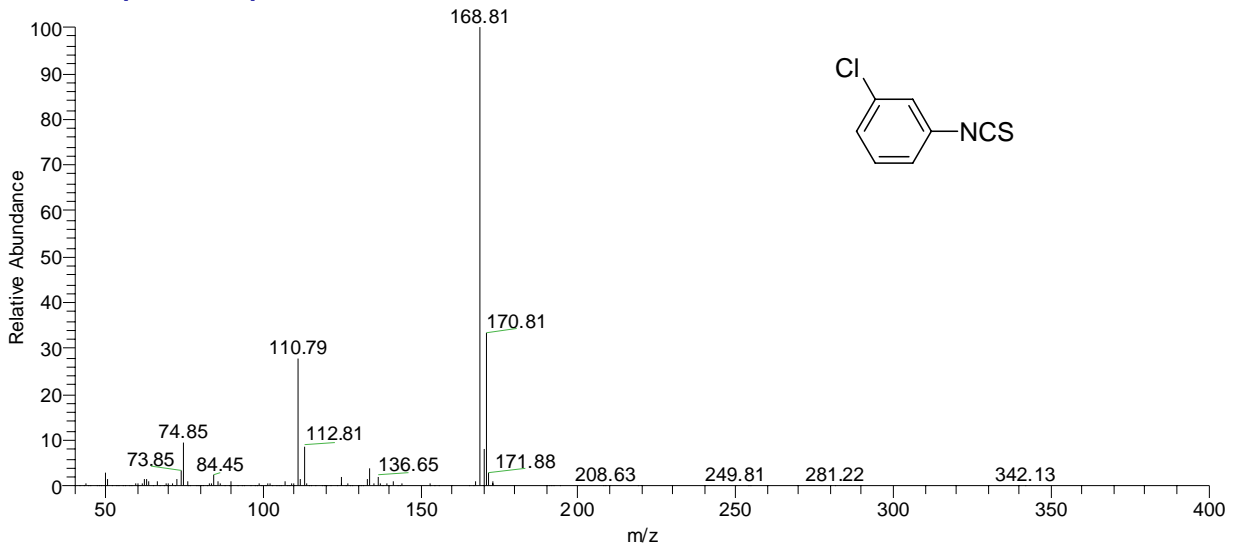
090311003#1693 RT: 10.35 AV: 1 SB: 252 9.57-9.98, 12.30-12.97 NL: 2.21E6  
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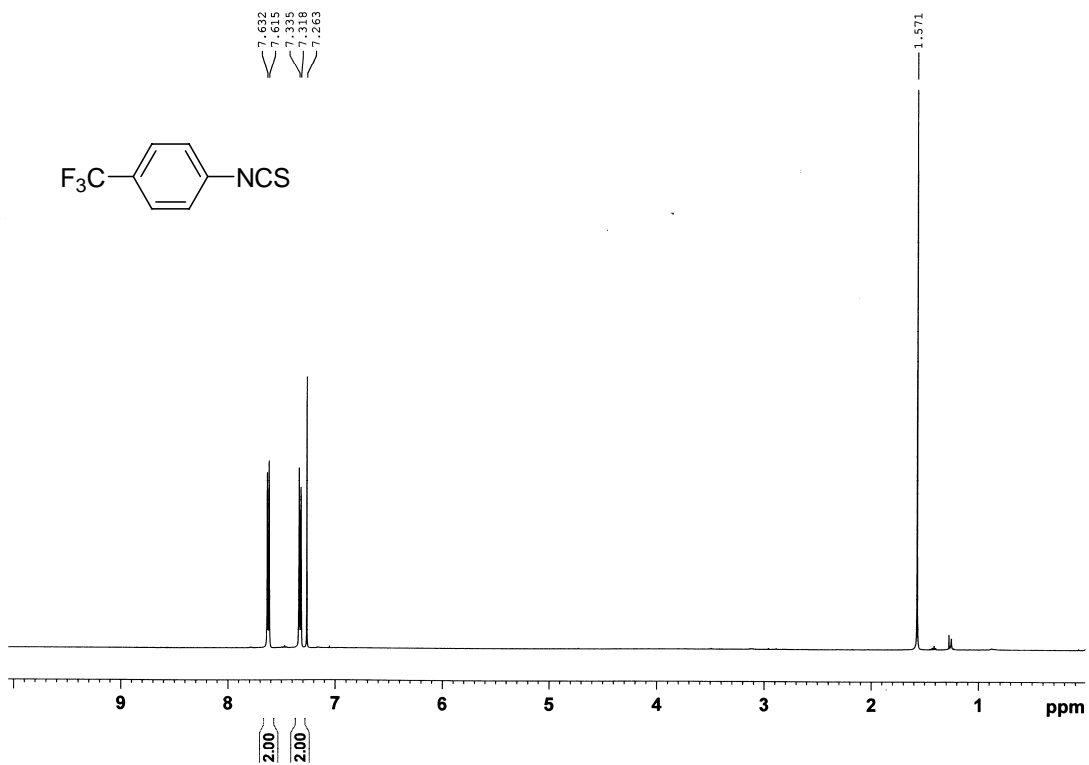
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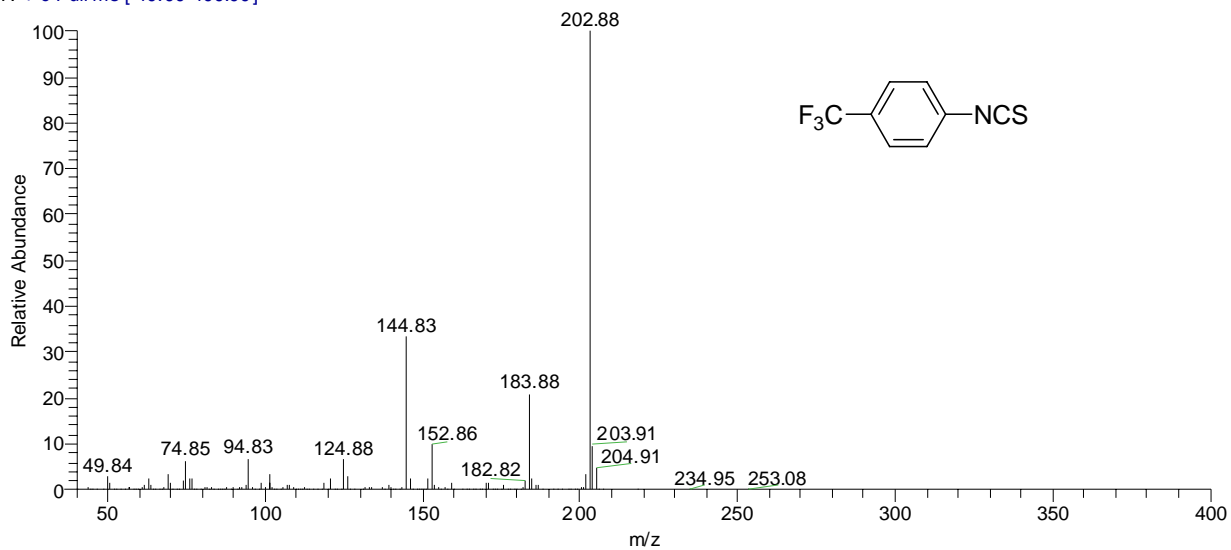
090310010 #1756 RT: 10.62 AV: 1 SB: 583 7.22-8.51, 13.55-14.78 NL: 1.79E6  
T: + c Full ms [40.00-400.00]



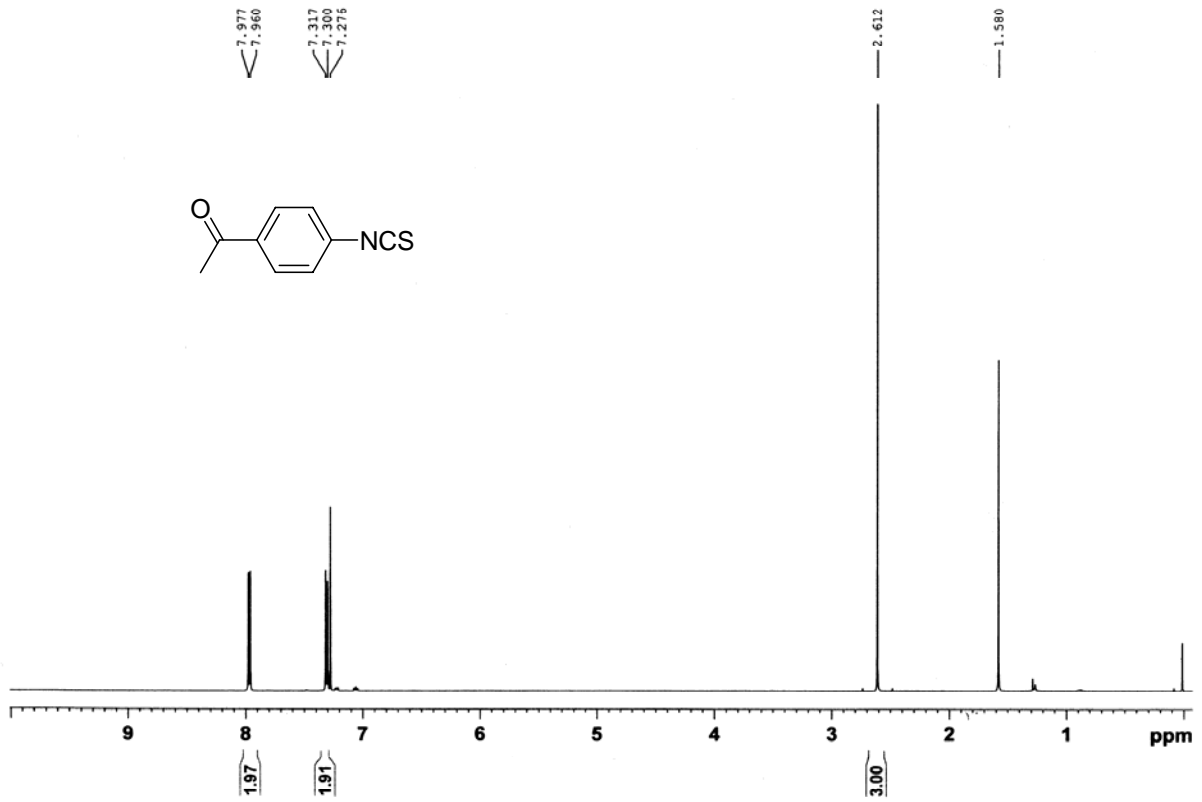
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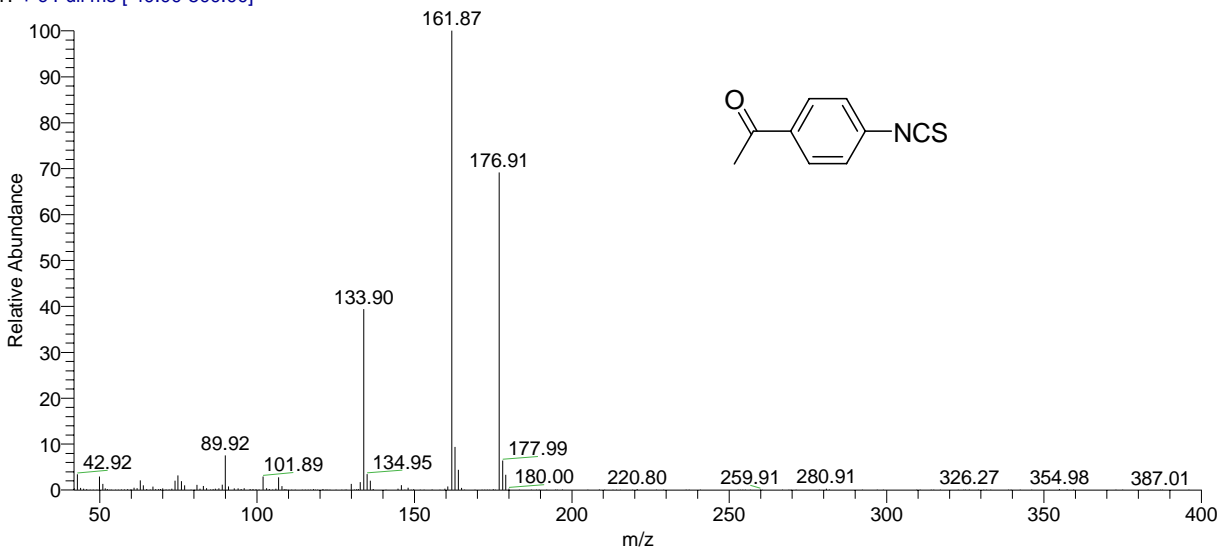
090311004#1126 RT: 7.89 AV: 1 SB: 70 7.72-7.79, 8.28-8.50 NL: 3.81E6  
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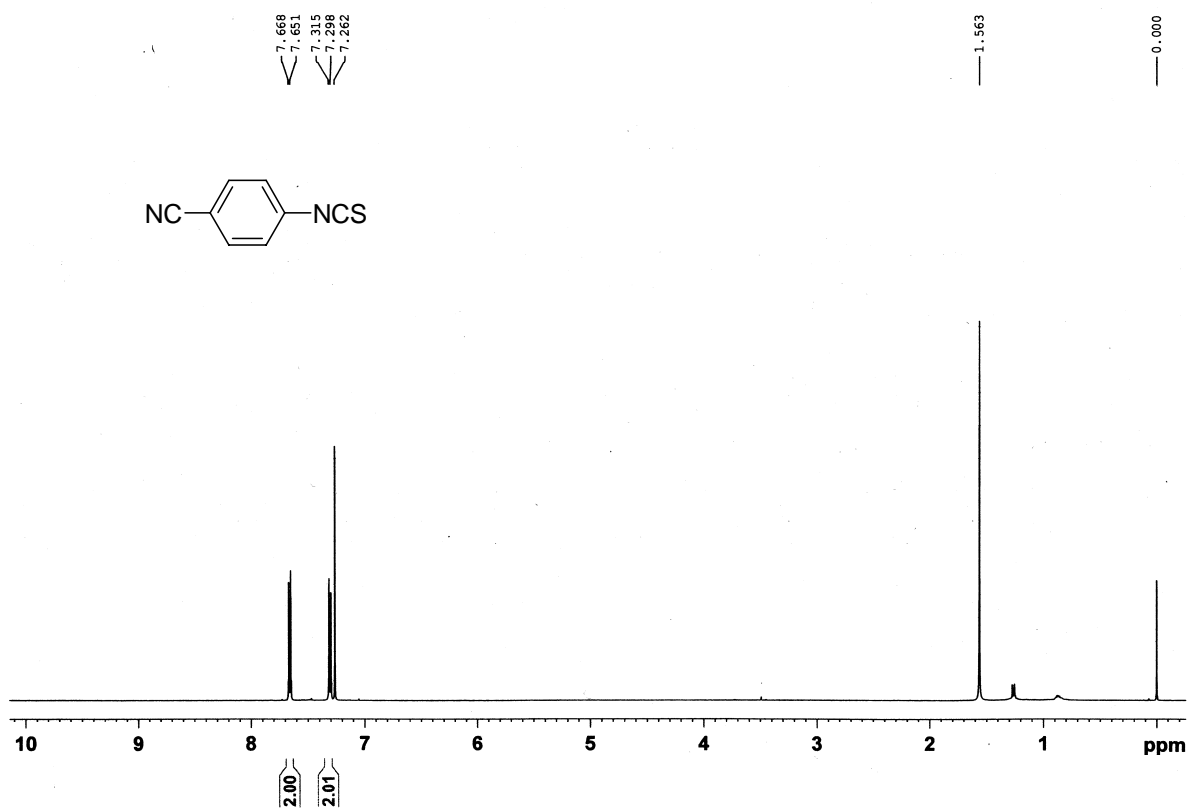
PCO-1 CDC13



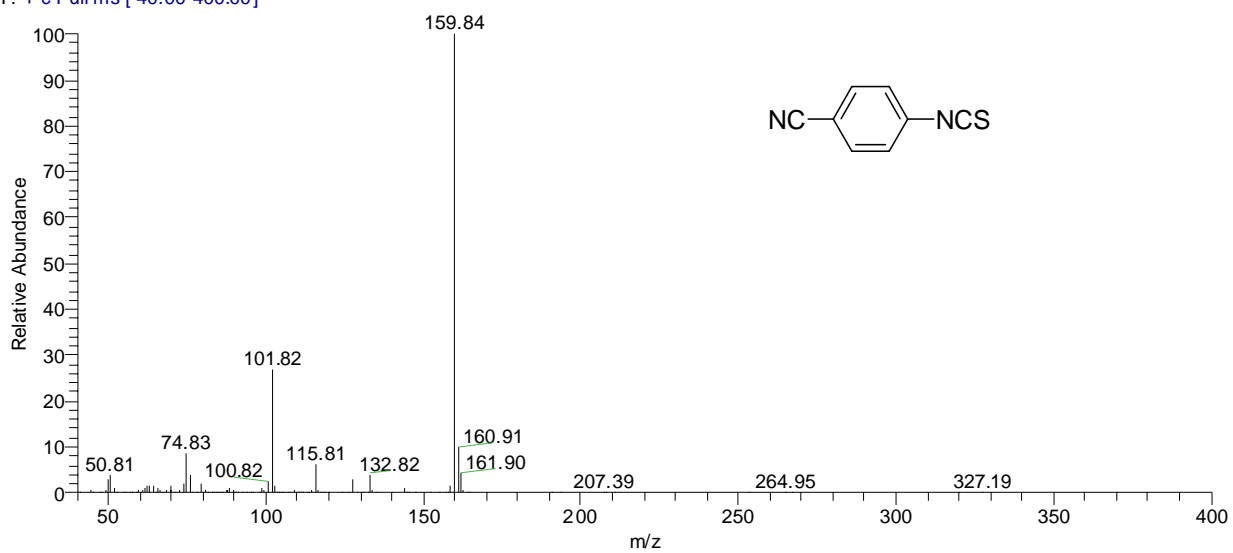
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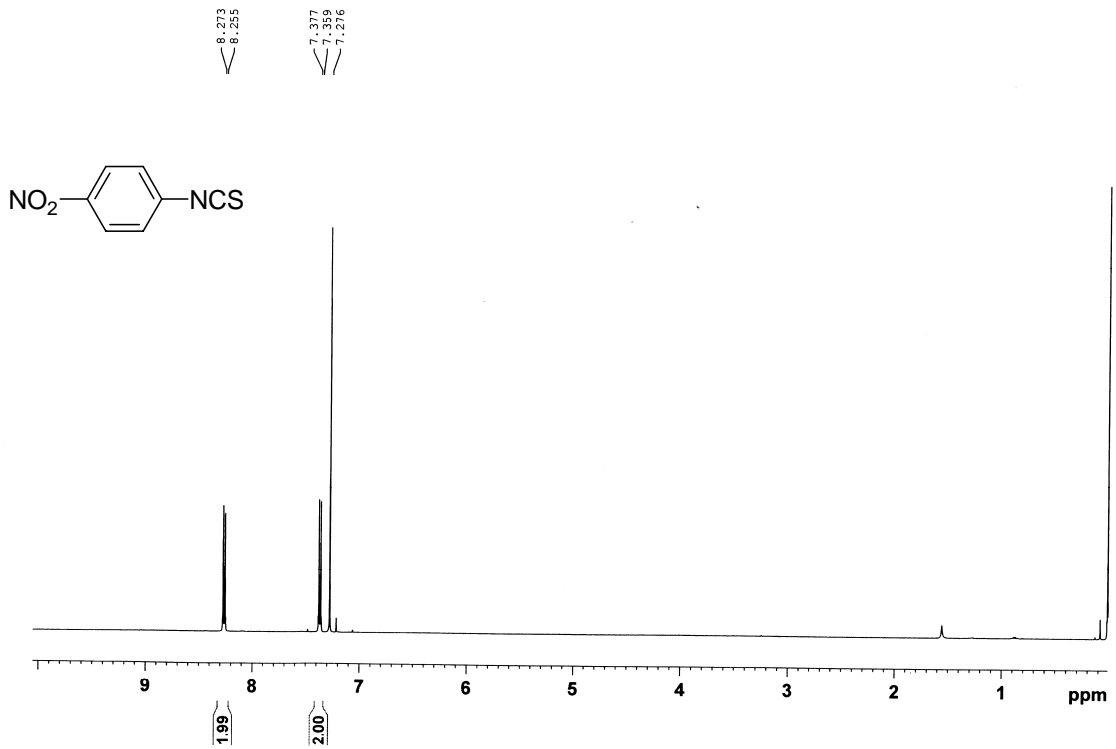
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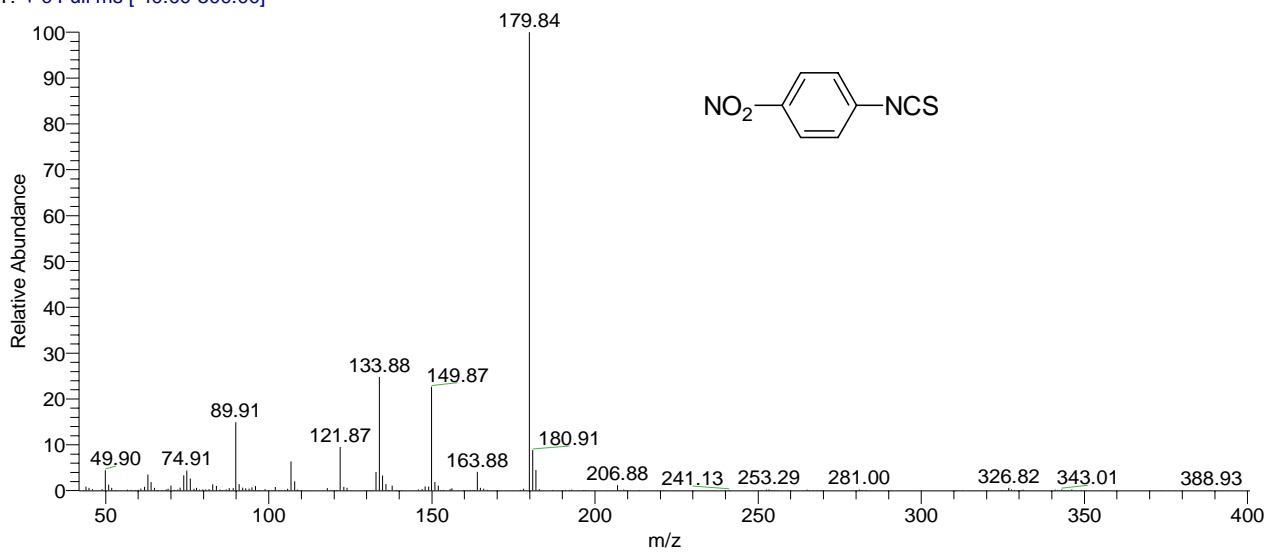
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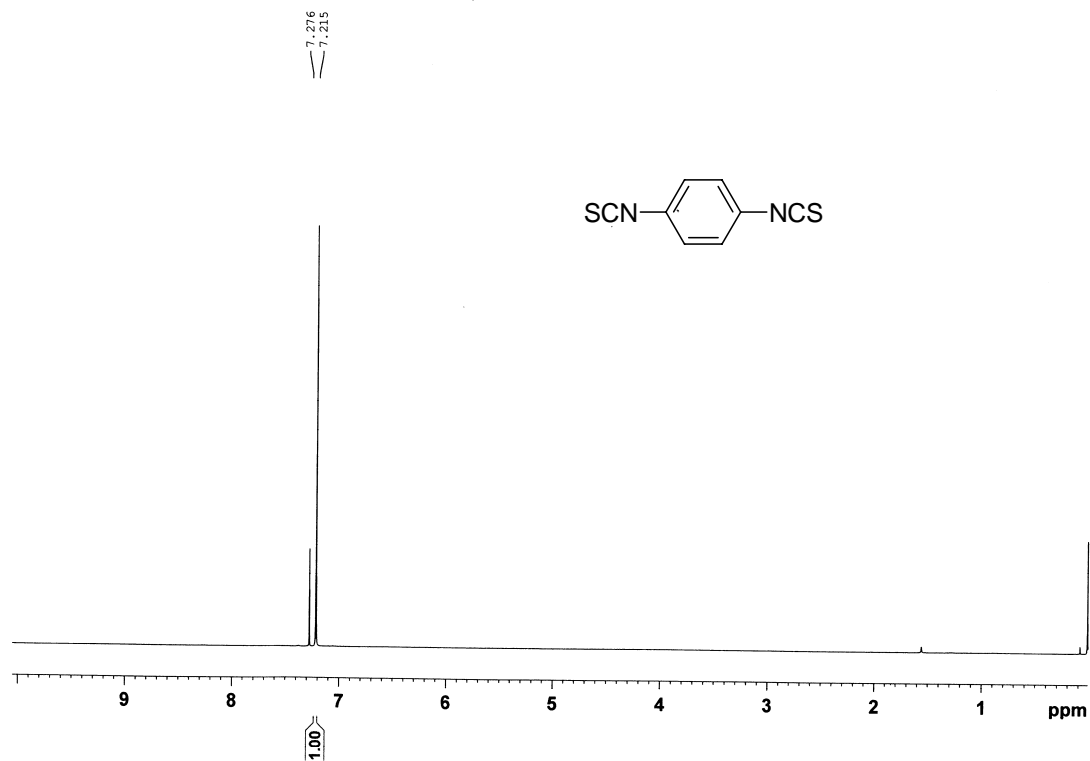
1 CDC13



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T: + c Full ms [ 40.00-500.00]



2 CDC13



lsp20110220004 #725 RT: 3.89 AV: 1 NL: 3.45E7  
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