

## **SUPPORTING INFORMATION**

**Supramolecular synthesis of selenazoles using selenourea in water in the presence of  
 $\beta$ -cyclodextrin under atmospheric pressure**

**M. Narender, M. Somi Reddy, V. Pavan Kumar, V. Prakash Reddy,  
Y. V. D. Nageswar and K. Rama Rao\***

*Organic Chemistry Division-I, Indian Institute of Chemical Technology, Uppal Road,  
Hyderabad 500-007, India*

*E-mail: [drkrrao@yahoo.com](mailto:drkrrao@yahoo.com)*

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**4-phenyl-1,3-selenazol-2-amine (Table 1, entry 1)**

mp: 132 °C.

IR (KBr): 707, 770, 1011, 1279, 1322, 1480, 1528, 1594, 3258, 3419  $\text{cm}^{-1}$

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200 MHz):  $\delta$  = 5.65 (br, s, 2H), 7.20-7.45 (m, 4H), 7.78 (d, 2H,  $J=6.59$  Hz).

Mass (EI):  $m/z$  = 224, 182, 155, 141, 102, 76, 51.

Anal calcd for  $\text{C}_9\text{H}_8\text{N}_2\text{Se}$  (223.14): C, 48.45; H, 3.61; N, 12.55

Found: C, 48.38; H, 3.70; N, 12.66.

**4-*p*-tolyl-1,3-selenazol-2-amine (Table 1, entry 2)**

mp: 167 °C.

IR (KBr): 725, 820, 1020, 1181, 1281, 1323, 1528, 1635, 2922, 3119, 3382  $\text{cm}^{-1}$

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200 MHz):  $\delta$  = 2.32 (s, 3H), 5.65 (br, s, 2H), 7.10-7.20 (m, 3H), 7.63 (d, 2H,  $J=8.08$  Hz).

Mass (EI):  $m/z$  = 237, 195, 115, 91, 63.

Anal calcd for  $\text{C}_{10}\text{H}_{10}\text{N}_2\text{Se}$  (237.16): C, 50.64; H, 4.25; N, 11.81

Found: C, 50.54; H, 4.18; N, 11.90.

**4-(4-methoxyphenyl)-1,3-selenazol-2-amine (Table 1, entry 3)**

mp: 173 °C.

IR (KBr): 720, 815, 1020, 1050, 1190, 1325, 1540, 1650, 3360  $\text{cm}^{-1}$

$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 200 MHz):  $\delta$  = 3.80 (s, 3H), 5.65 (br, s, 2H), 6.85-7.00 (m, 3H), 7.20-7.30 (d, 2H,  $J=6.89$ ).

Mass (EI):  $m/z$  = 253, 211, 155, 141, 102, 76, 51.

Anal calcd for  $\text{C}_{10}\text{H}_{10}\text{N}_2\text{OSe}$  (253.16): C, 47.44; H, 3.98; N, 11.06

Found: C, 47.38; H, 3.85; N, 11.12.

**4-(4-chlorophenyl)-1,3-selenazol-2-amine (Table 1, entry 4)**

mp: 157 °C.

IR (KBr): 688, 726, 831, 1020, 1089, 1187, 1324, 1397, 1476, 1540, 1633, 2925, 3143, 3289, 3452  $\text{cm}^{-1}$

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 200 MHz): δ = 5.25 (br, s, 2H), 7.22 (s, 1H), 7.35-7.45 (d, 2H, *J*=7.83 Hz), 7.60-7.70 (d, 2H, *J*=7.83 Hz).

Mass (EI): *m/z* = 258, 215, 168, 154, 141, 111, 101, 83, 75, 69, 57, 43

Anal calcd for C<sub>9</sub>H<sub>7</sub>ClN<sub>2</sub>Se (257.58): C, 41.97; H, 2.74; N, 10.88.

Found: C, 41.88; H, 2.60; N, 10.80.

**4-(4-bromophenyl)-1,3-selenazol-2-amine (Table 1, entry 5)**

mp: 132 °C.

IR (KBr): 652, 687, 723, 829, 1004, 1020, 1185, 1320, 1393, 1474, 1540, 1633, 3122, 3287, 3442 cm<sup>-1</sup>

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ = 5.27 (br, s, 2H), 7.25 (s, 1H), 7.42-7.52 (d, 2H, *J*=8.25 Hz), 7.60-7.70 (d, 2H, *J*=8.25 Hz).

Mass (EI): *m/z* = 303, 301, 262, 260, 182, 180, 101, 89, 75, 43.

Anal calcd for C<sub>9</sub>H<sub>7</sub>BrN<sub>2</sub>Se (302.03): C, 35.79; H, 2.34; N, 9.28

Found: C, 35.90; H, 2.25; N, 9.12.

**4-(4-iodophenyl)-1,3-selenazol-2-amine (Table 1, entry 6)**

mp: 190 °C.

IR (KBr): 654, 685, 721, 825, 1000, 1019, 1182, 1319, 1389, 1471, 1537, 1633, 3116, 3283, 3427 cm<sup>-1</sup>

<sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz): δ = 5.32 (br, s, 2H), 7.25 (s, 1H), 7.43-7.53 (d, 2H, *J*=8.49 Hz), 7.62-7.72 (d, 2H, *J*=8.49 Hz).

Mass (EI): *m/z* = 349, 304, 229, 179, 140, 101, 97, 68, 43.

Anal calcd for C<sub>9</sub>H<sub>7</sub>IN<sub>2</sub>Se (349.03): C, 30.97; H, 2.02; N, 8.03

Found: C, 30.88; H, 2.12; N, 7.92.

**4-(4-nitrophenyl)-1,3-selenazol-2-amine (Table 1, entry 7)**

mp: 250 °C.

IR (KBr): 707, 844, 1017, 1102, 1321, 1463, 1498, 1542, 1592, 1639, 1733, 2853, 2924, 3396 cm<sup>-1</sup>

<sup>1</sup>H NMR (DMSO-d<sub>6</sub>, 300 MHz): δ = 5.27 (br, s, 2H), 7.25 (s, 1H), 7.42-7.52 (d, 2H, *J*=8.25 Hz), 7.60-7.70 (d, 2H, *J*=8.25 Hz).

Mass (EI):  $m/z$  = 268, 226, 148, 135, 120, 97, 83, 71, 57, 41.

Anal calcd for  $C_9H_7N_3O_2Se$  (268.13): C, 40.32; H, 2.63; N, 15.67.

Found: C, 40.22; H, 2.75; N, 15.59.

**4,5-diphenyl-1,3-selenazol-2-amine (Table 1, entry 8)**

mp: 200 °C.

IR (KBr): 825, 1009, 1019, 1184, 1322, 1540, 1633, 3122, 3287, 3442  $cm^{-1}$

$^1H$  NMR ( $CDCl_3$ , 300 MHz):  $\delta$  = 5.25 (br, s, 2H), 7.22-7.42 (m, 10H).

Mass (EI):  $m/z$  = 300, 258, 220, 193, 178, 152, 128, 110, 89, 51.

Anal calcd for  $C_{15}H_{12}N_2Se$  (299.23): C, 60.21; H, 4.04; N, 9.36.

Found: C, 60.29; H, 4.15; N, 9.48.

**4-tert-butyl-1,3-selenazol-2-amine (Table 1, entry 9)**

mp: 60 °C.

IR (KBr): 685, 744, 932, 1020, 1054, 1119, 1212, 1312, 1467, 1536, 1629, 2962, 3119, 3286, 3434  $cm^{-1}$

$^1H$  NMR ( $CDCl_3$ , 300 MHz):  $\delta$  = 1.25 (s, 9H), 5.45 (br, s, 2H), 6.55 (s, 1H).

Mass (EI):  $m/z$  = 203, 161, 146, 130, 123, 57.

Anal calcd for  $C_7H_{12}N_2Se$  (203.14): C, 41.39; H, 5.95; N, 13.79

Found: C, 41.50; H, 5.80; N, 13.60.

**Ethyl-2-amino-4-methyl-1,3-selenazole-5-carboxylate (Table 1, entry 10)**

mp: 164 °C.

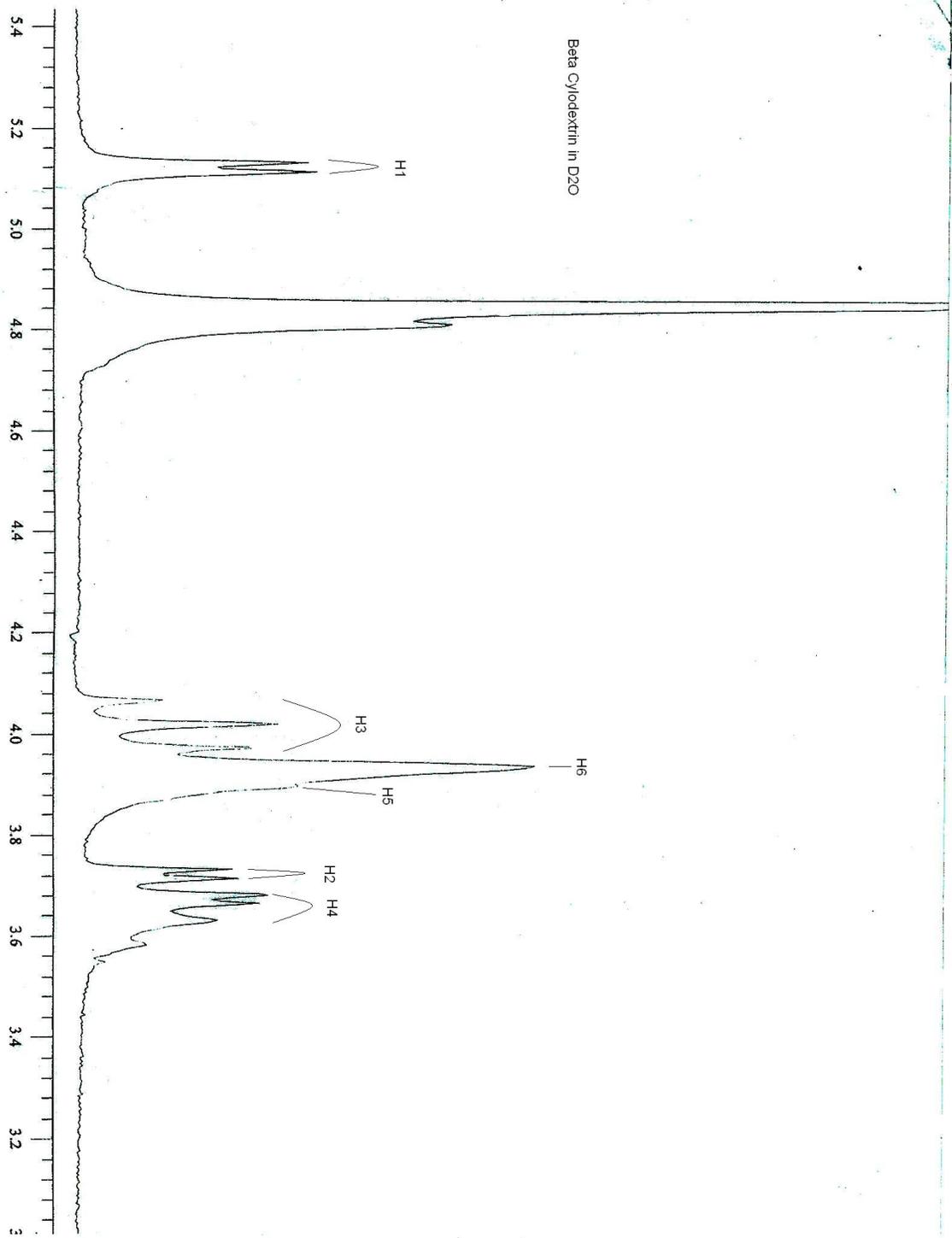
IR (KBr): 755, 1008, 1086, 1124, 1263, 1332, 1370, 1509, 1665, 2757, 2929, 3064, 3375  $cm^{-1}$

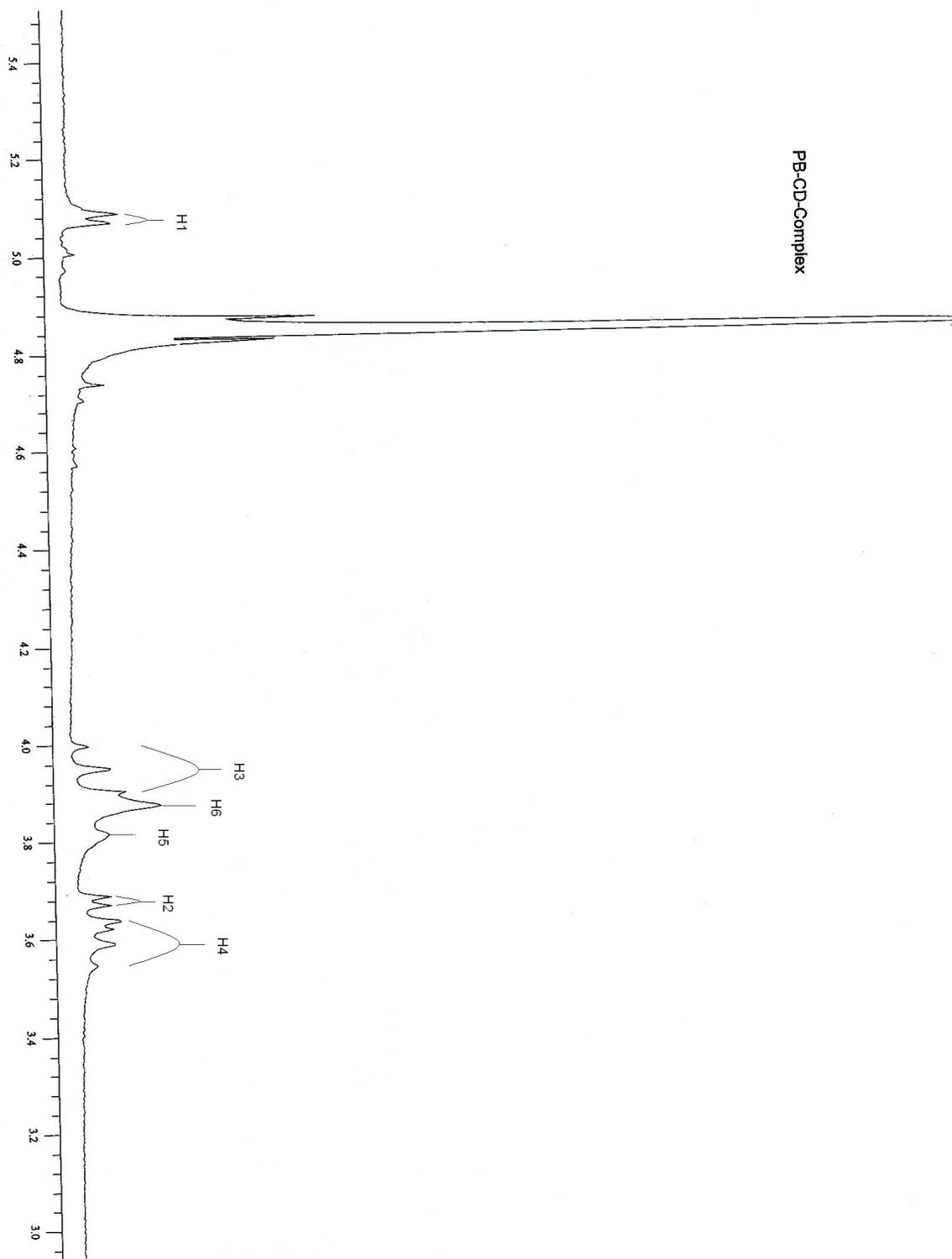
$^1H$  NMR ( $DMSO-d_6$ , 200 MHz):  $\delta$  = 1.30-1.40 (t, 3H,  $J=7.03$  Hz), 2.45 (s, 3H), 4.15-4.30 (q, 2H,  $J=7.03$  Hz) 7.73 (s, 2H).

Mass (EI):  $m/z$  = 233, 191, 188, 160, 153, 101, 87, 57.

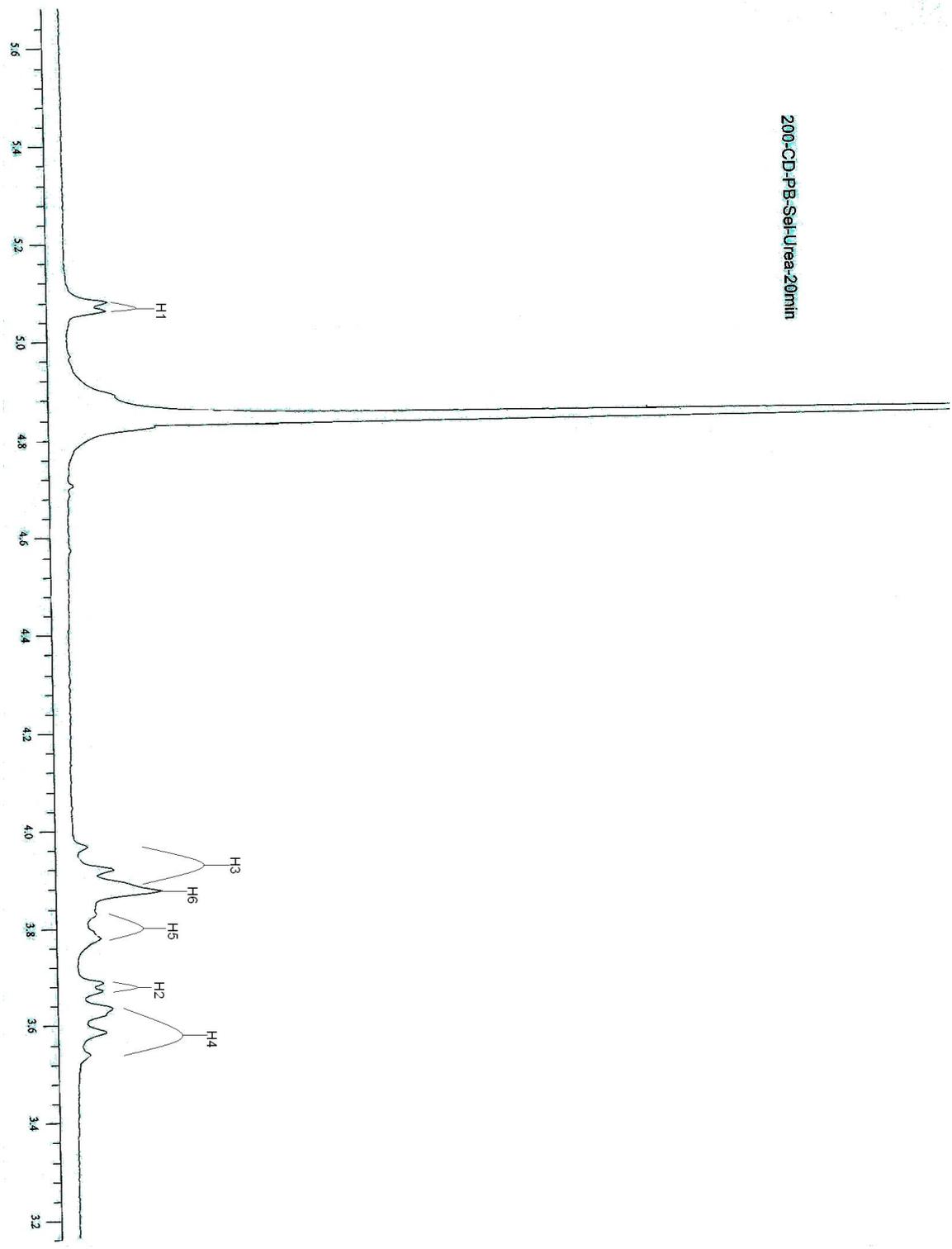
Anal calcd for  $C_7H_{10}N_2O_2Se$  (233.13): C, 36.06; H, 4.32; N, 12.02

Found: C, 35.90; H, 4.20; N, 12.15.

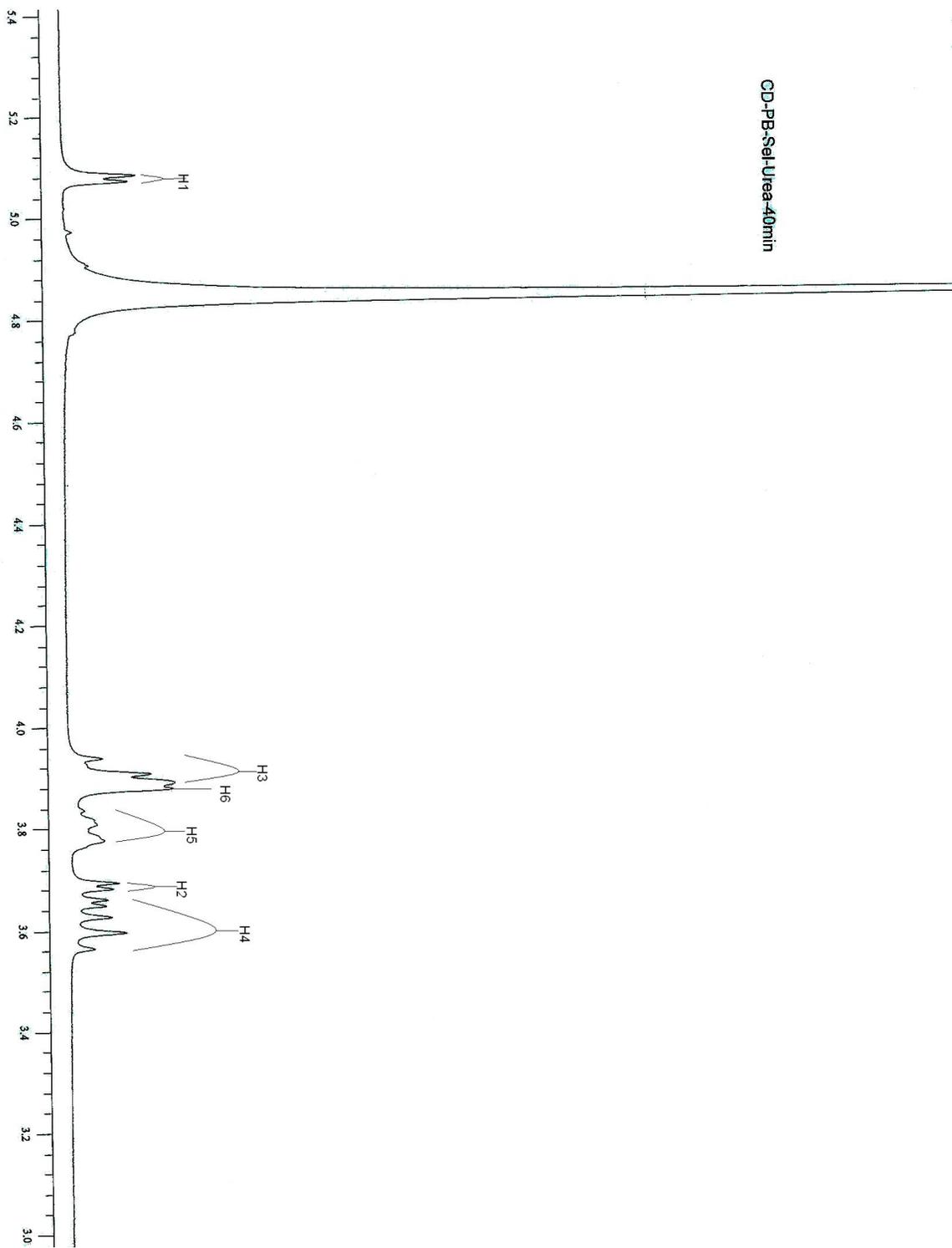


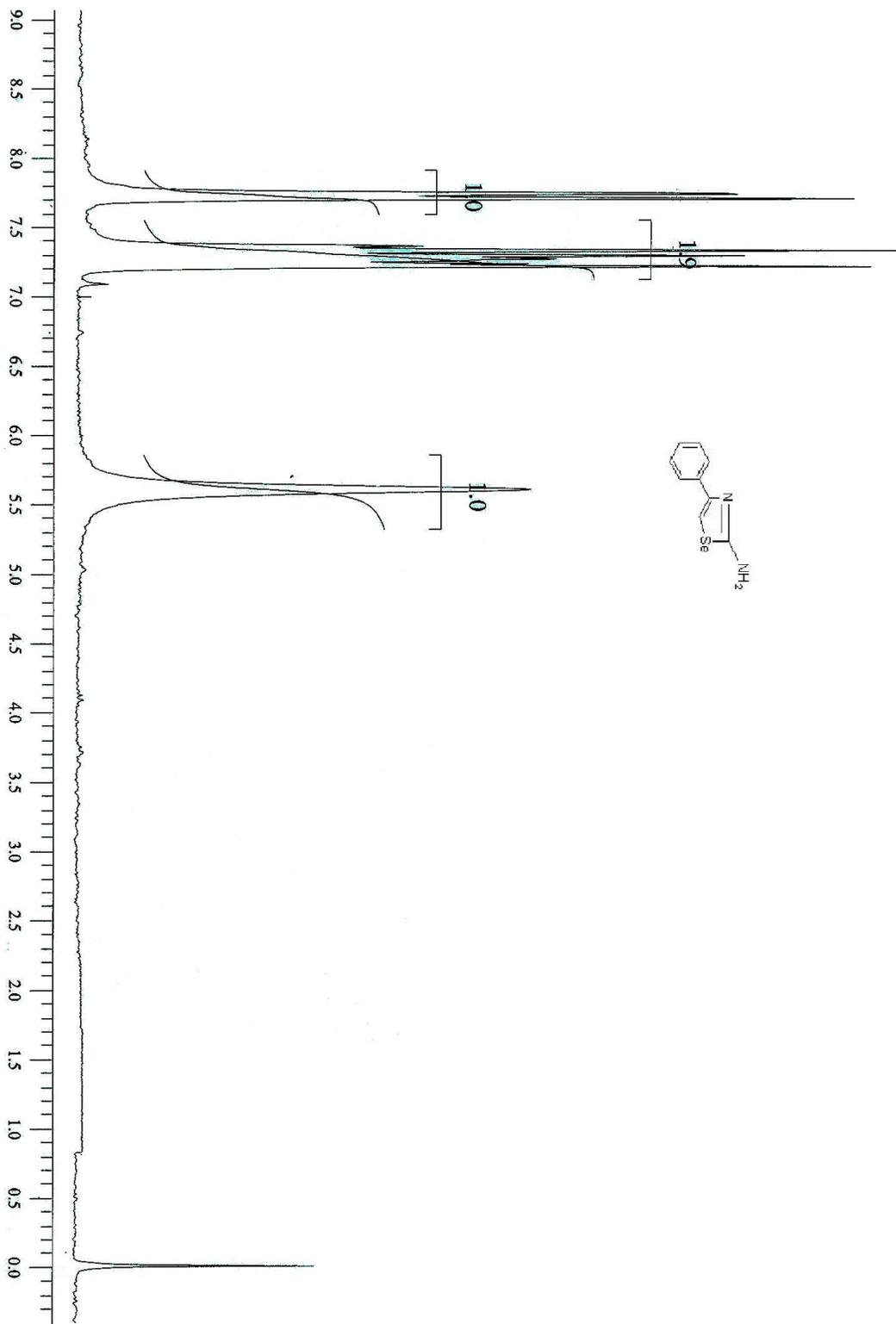


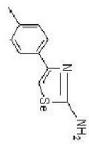
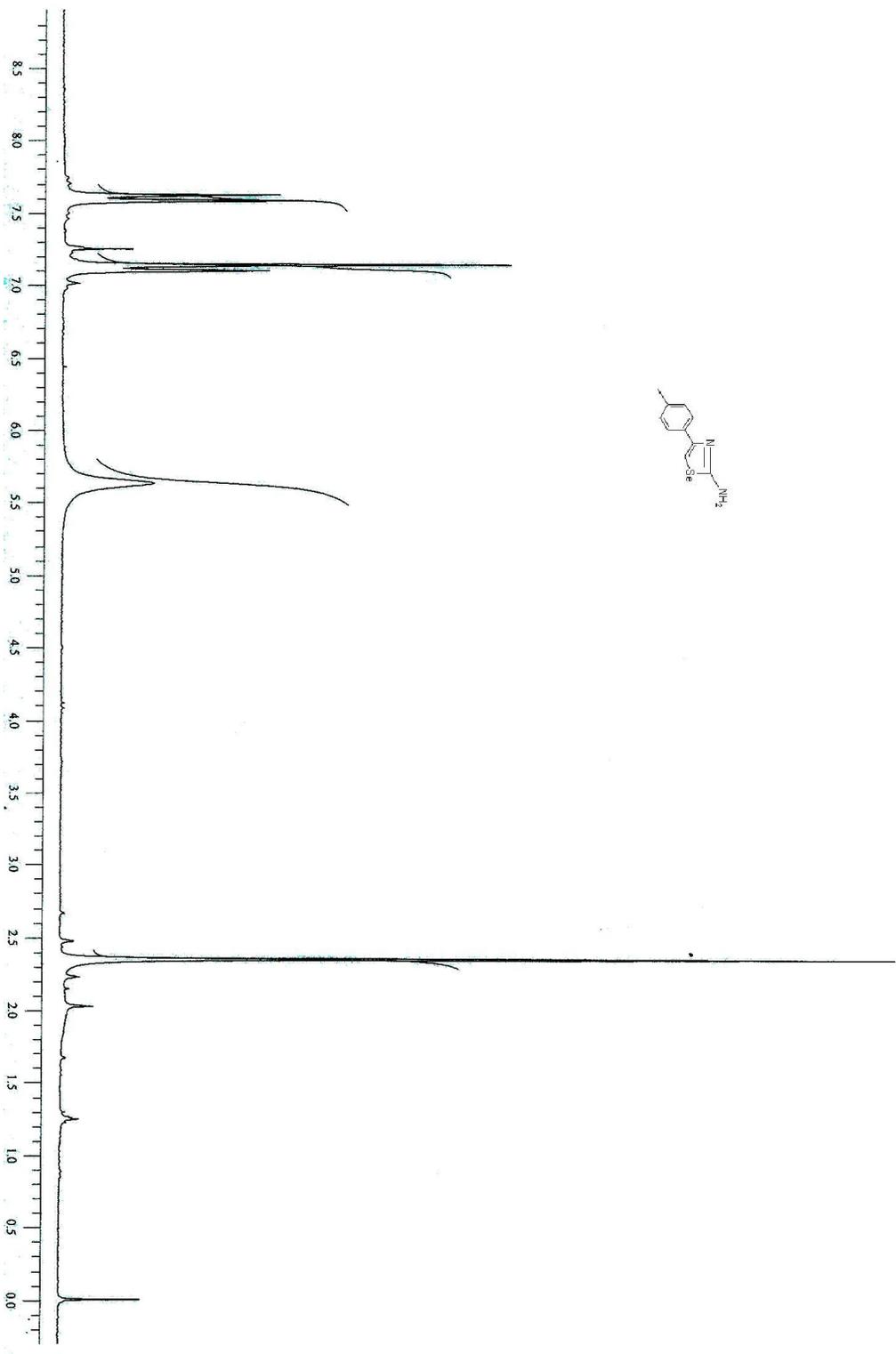
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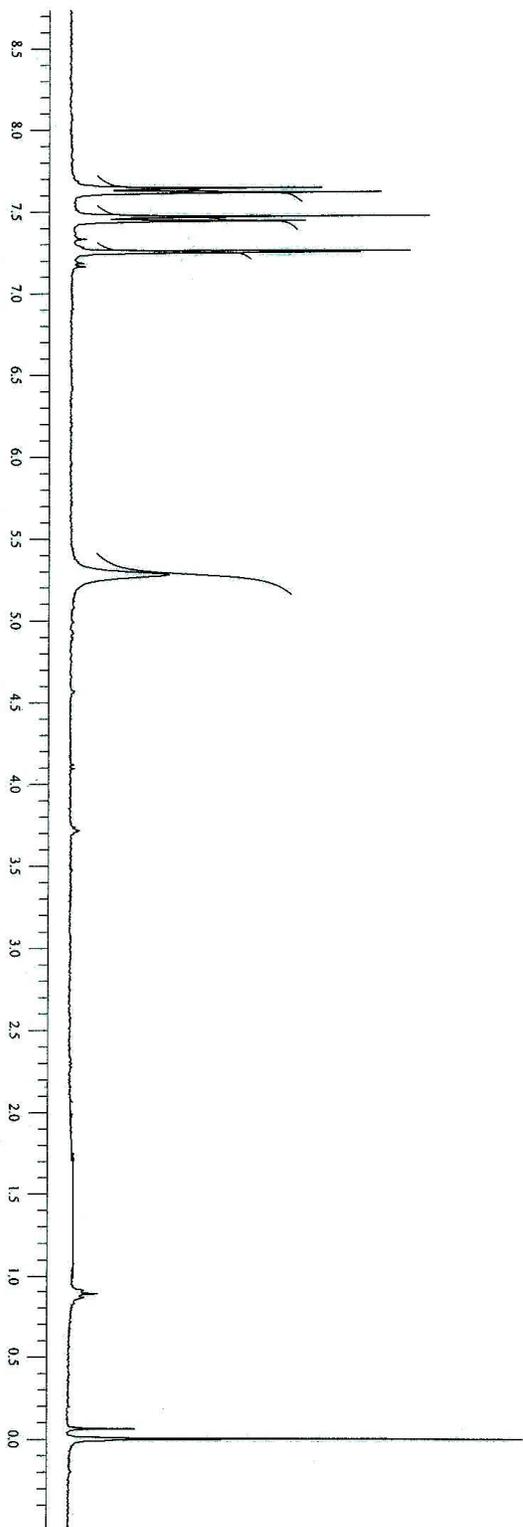
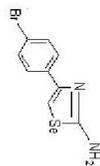


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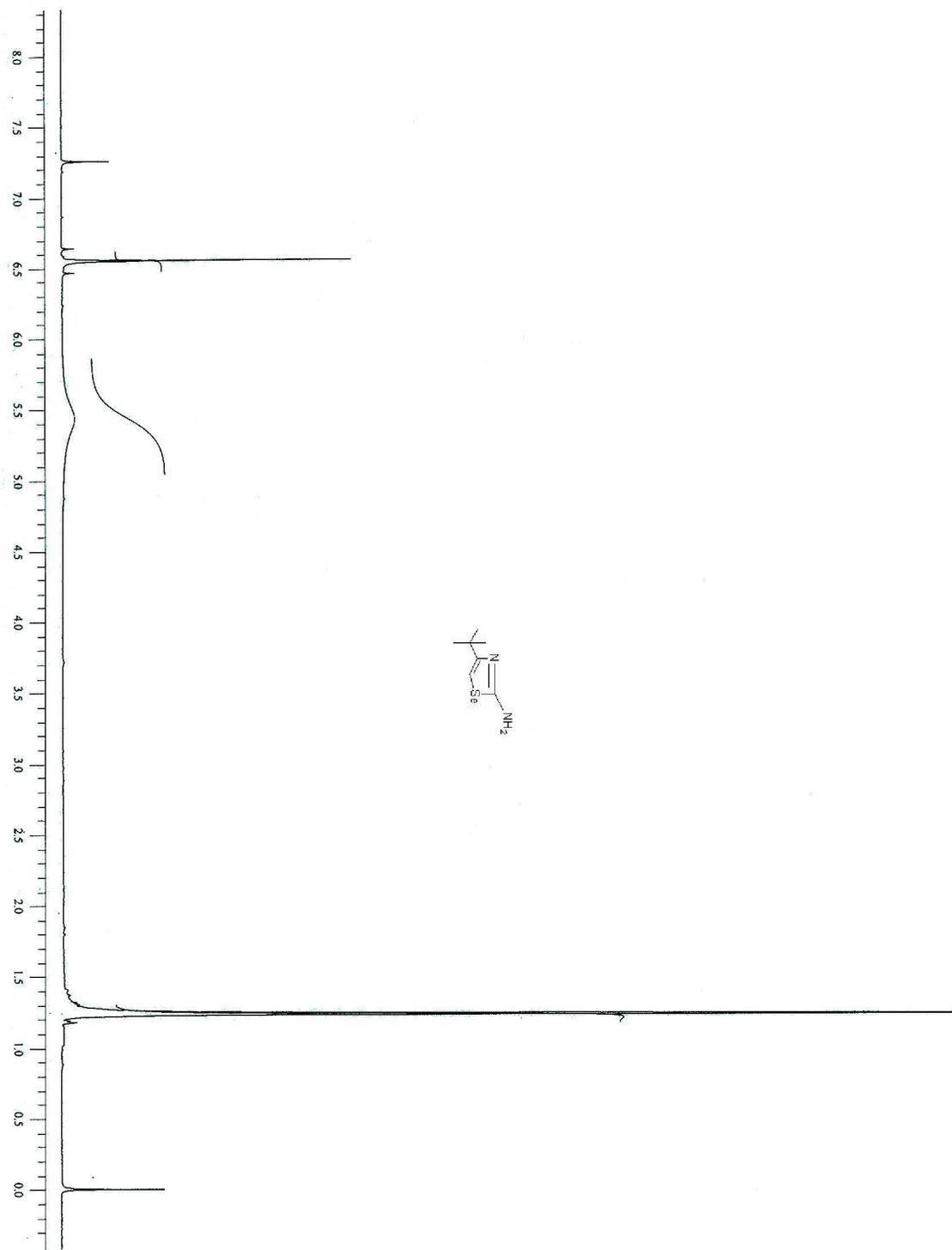


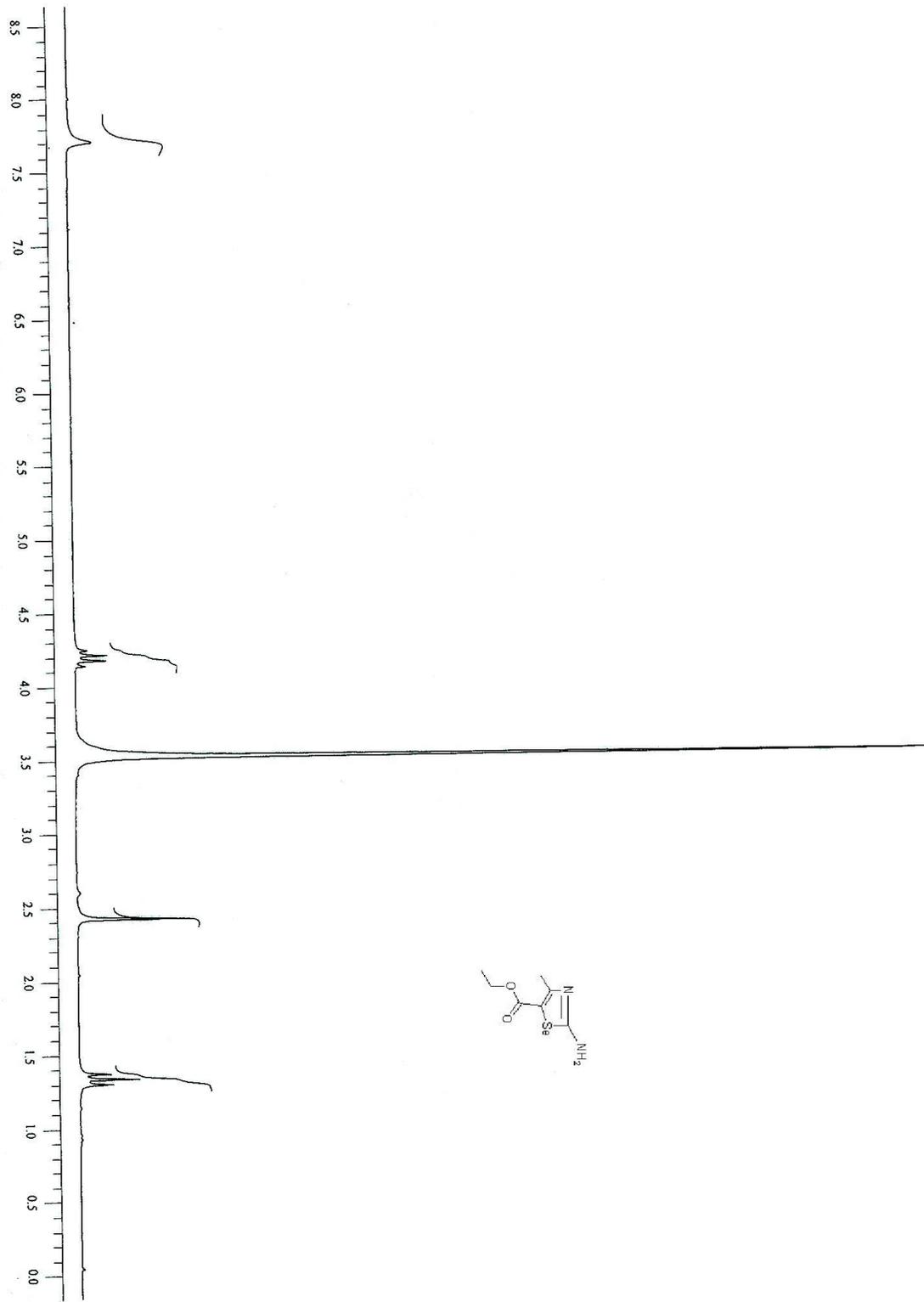




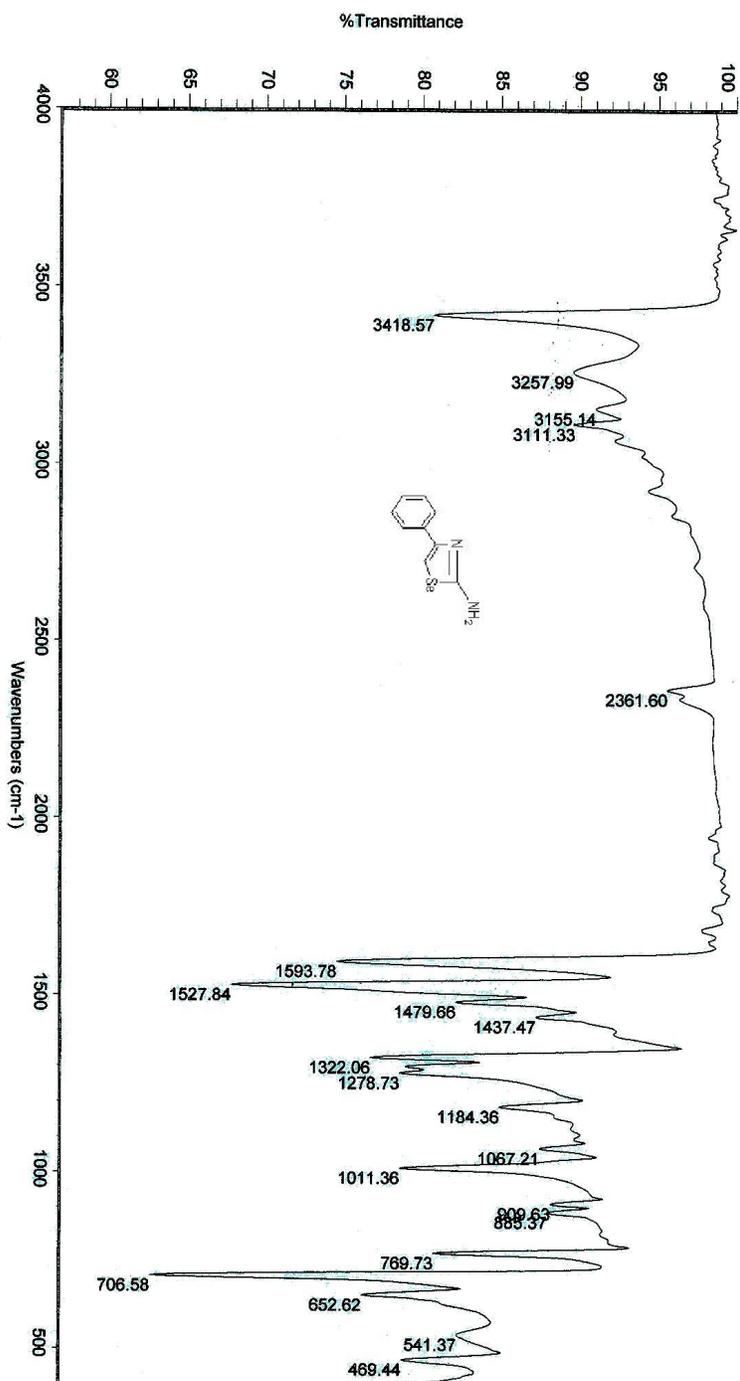


S11





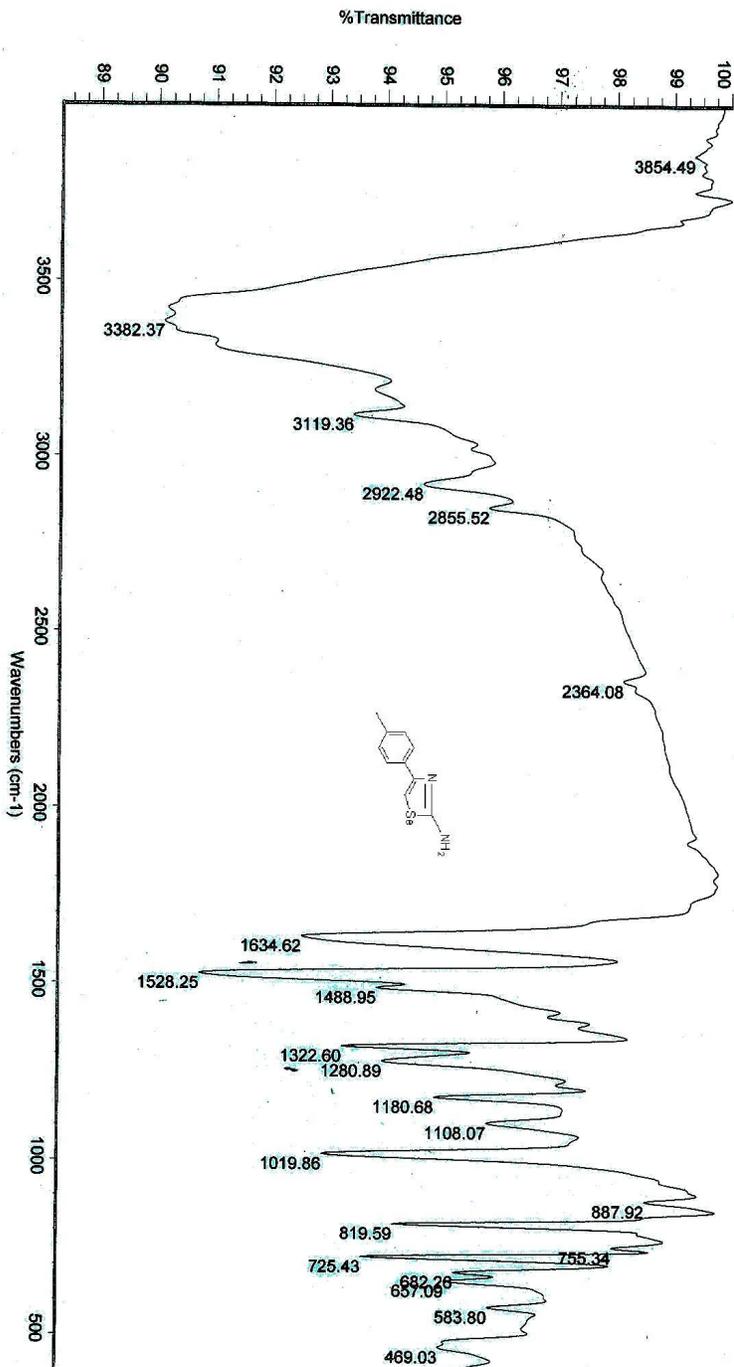
Indian Institute of Chemical Technology, Hyderabad  
FTIR Analysis Report



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Sample Preparation: KBR  
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Bench: Thermo Nicolet Nexus 670 Spectrometer.  
Resolution: 4 cm<sup>-1</sup>

Detector: DTGS KBr  
Beamsplitter: KBr  
Source: IR  
Analyst Name:

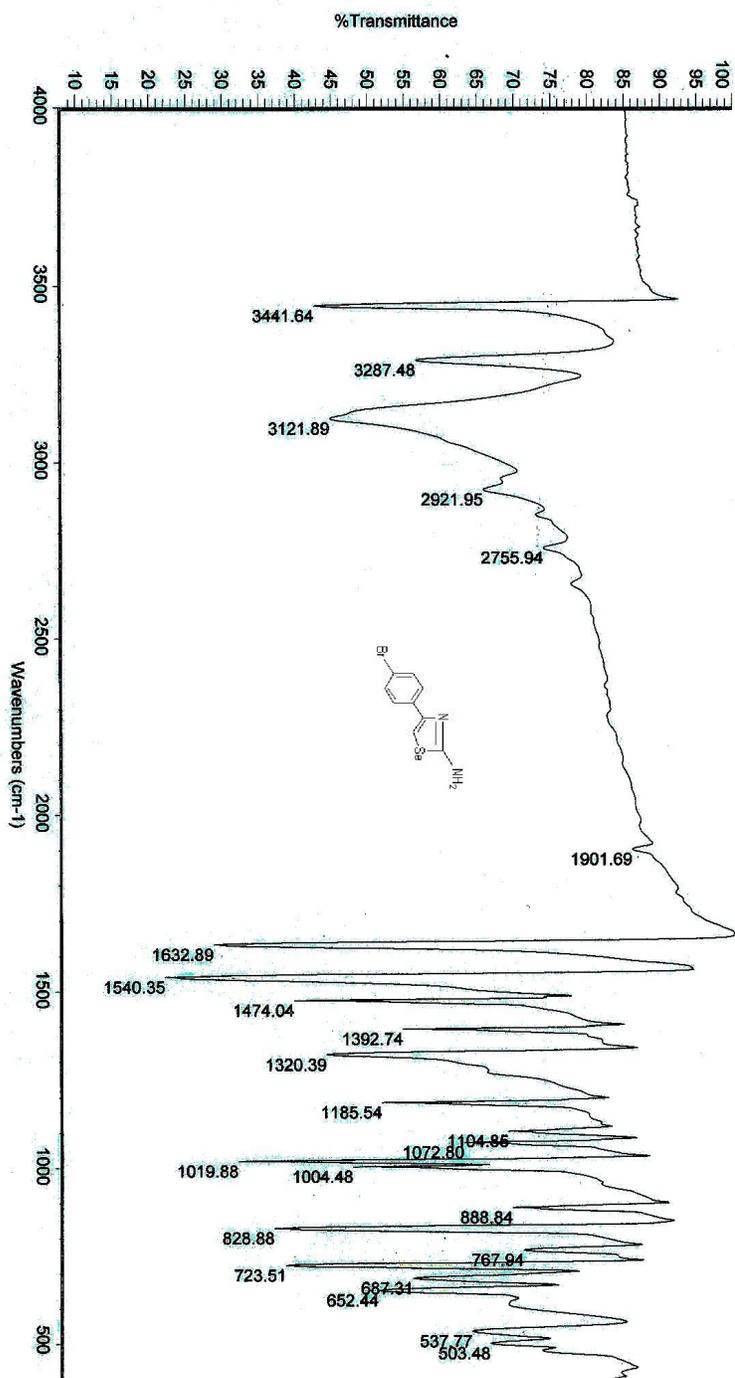
Indian Institute of Chemical Technology, Hyderabad  
FTIR Analysis Report



Sample Name: KRR-ME  
Sample Preparation: KBR  
Collection time: Wed Nov 01 16:23:17 2006 (GMT+05:30)  
Bench: Thermo Nicolet Nexus 670 Spectrometer  
Resolution: 4 cm-1

Detector: DTGS KBr  
Beamsplitter: KBr  
Source: IR  
Analyst Name:

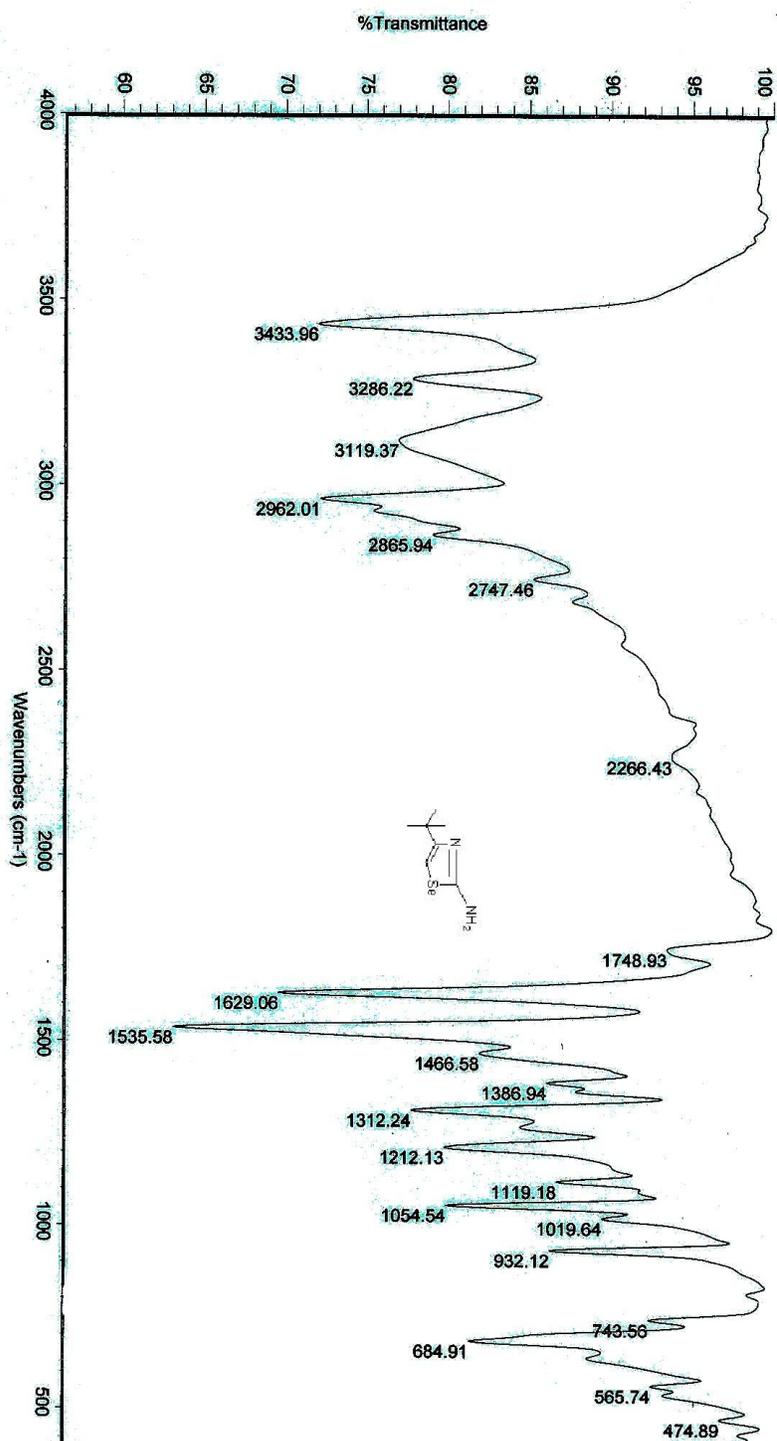
Indian Institute of Chemical Technology, Hyderabad  
FTIR Analysis Report



Sample Name: KRR-BR  
Sample Preparation: KBR  
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Resolution: 4 cm<sup>-1</sup>

Detector: DTGS KBr  
Beamsplitter: KBr  
Source: IR  
Analyst Name:

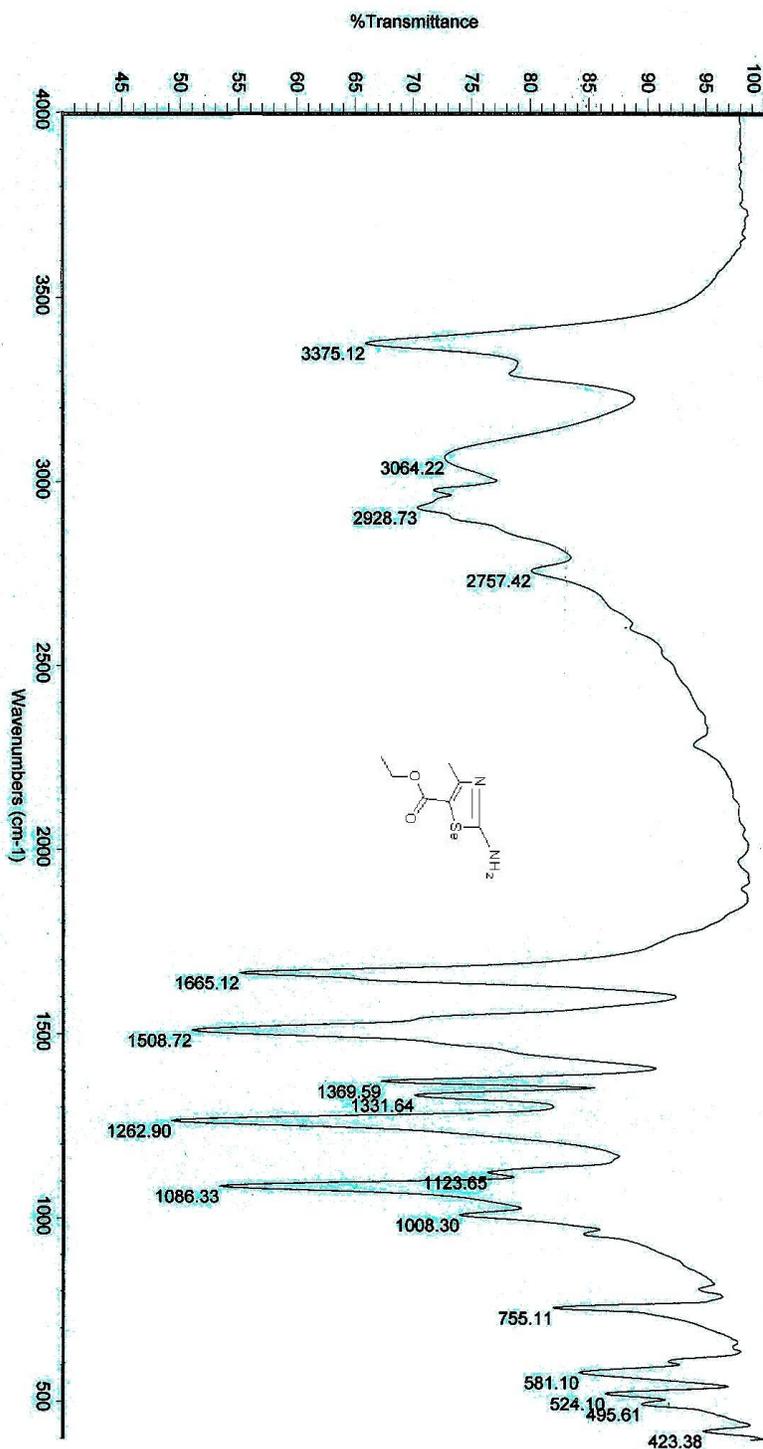
Indian Institute of Chemical Technology, Hyderabad  
FTIR Analysis Report



Sample Name: KRR-T-BU  
Sample Preparation: KBR  
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Bench: Thermo Nicolet Nexus 670 Spectrometer  
Resolution: 4 cm<sup>-1</sup>

Detector: DTGS KBr  
Beamsplitter: KBr  
Source: IR  
Analyst Name:

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FTIR Analysis Report



Sample Name: KRR-ET  
Sample Preparation: KBR  
Collection time: Tue Nov 21 12:25:37 2006 (GMT+05:30)  
Bench: Thermo Nicolet Nexus 670 Spectrometer  
Resolution: 4 cm-1

Detector: DTGS KBr  
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Analyst Name: