

## Supporting Information

### **Green synthesis of a benzothiazole based ‘turn-on’ type fluorimetric probe and its use for the selective detection of thiophenols in environmental samples and living cells**

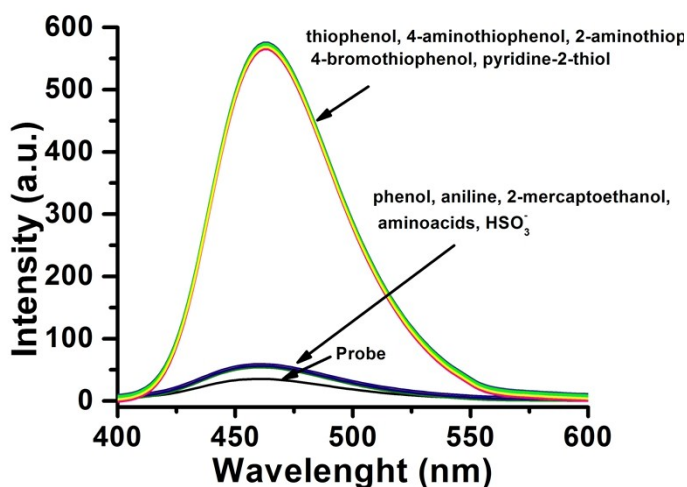
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## Synthesis of 2-(benzo[d]thiazol-2-yl)phenol (**2**):

In a 10 mL of round-bottomed flask was taken *o*-aminothiophenol (53  $\mu$ L, 0.5 mmol) and salicylaldehyde (53  $\mu$ L, 0.5 mmol) in 1 mL of water followed by addition of CTAB (18.5 mg, 0.05 mmol). The reaction mixture was stirred at room temperature for 1 h. The reaction mixture was diluted with water (5 mL) and extracted with ethyl acetate (3 x 5 mL). The combined organic layer was collected, washed with brine, dried over anhydrous sodium sulphate and concentrated to afford the crude product, which was purified over silica gel (60-120 mesh) with 5:95 EtOAc:Petroleum ether to afford pure 2-(2-hydroxyphenyl)benzothiazole (**2**) (93 mg, 82%).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) 6.96 (1H, t,  $J = 7.6$  Hz), 7.10 (1H, d,  $J = 8.4$  Hz), 7.36-7.43 (2H, m), 7.51 (1H, t,  $J = 7.6$  Hz), 7.69 (1H, d,  $J = 7.6$  Hz), 7.90 (1H, d,  $J = 8.0$  Hz), 7.99 (1H, d,  $J = 8.0$  Hz);  $^{13}\text{C}$  NMR (100 MHz):  $\delta$  (ppm) 111.53, 112.62, 114.27, 116.24, 116.90, 120.28, 121.42, 123.42, 123.17, 127.33, 127.50, 127.53, 146.55, 152.71, 164.12; HR-MS (ESI):  $m/z$  calcd for  $\text{C}_{13}\text{H}_9\text{NOS}$   $[\text{M}+\text{H}]^+$  228.0438, found 228.0445.

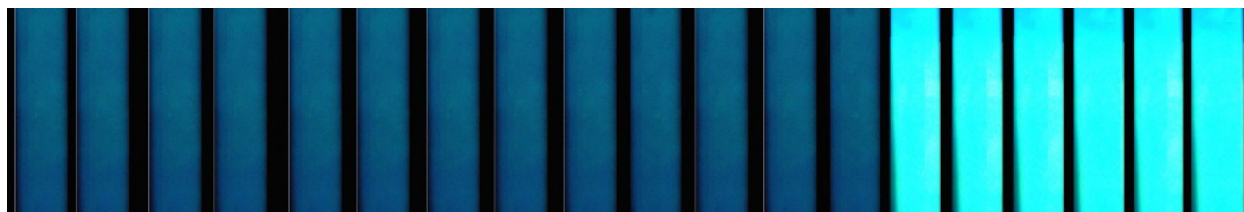
## Selectivity studies with different analytes



**Figure S1.** Maximum fluorescence response of probe **1** in 45% DMF-PBS (pH = 7.2) upon addition of different analytes (presence of other nucleophiles) in presence of a fixed concentration of probe **1** (30  $\mu$ M) [ $\lambda_{\text{ex}} = 365$  nm].

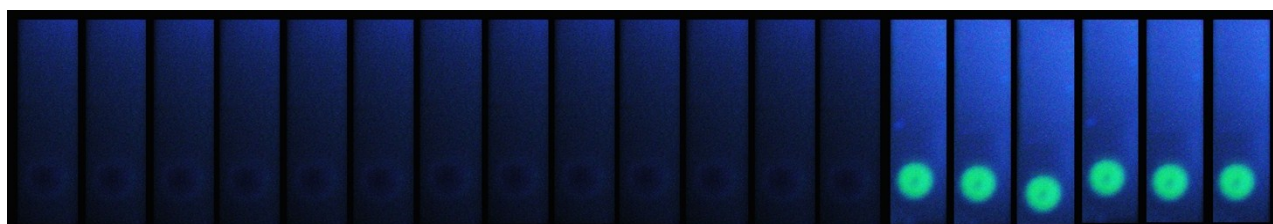
## Selective Detection of thiophenols by paper strips (A) and TLC plates (B).

(A)



(i) (ii) (iii) (iv) (v) (vi) (vii) (viii) (ix) (x) (xi) (xii) (xiii) (xiv) (xv) (xvi) (xvii) (xviii)  
(xx)

(B)



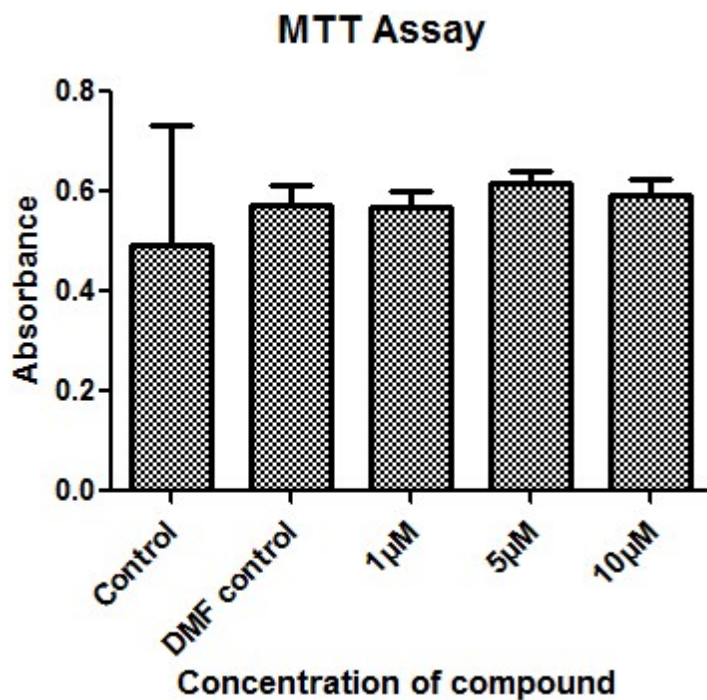
**Figure S2.** Response of amino acids, aliphatic thiols, other nucleophiles in the presence of probe **1** soaked on paper strips (A) and TLC plates (B): (i) = probe 1; (ii) = Cysteine, (iii) = Arginine, (iv) = Leucine, (v) = L-Proline, (vi) = Alanine, (vii) = Glycine, (viii) = Histidine, (ix) = Glutathione, (x) = phenol, (xi) = aniline, (xii) = 2-Mercaptoethanol, (xiii) =  $\text{HSO}_3^-$ , (xiv) = Thiophenol, (xv) = Pyridine-2-thiol, (xvi) = 2-Aminothiophenol, (xvii) = 4-Aminothiophenol, (xviii) = 4-Bromothiophenol and (xx) = thiophenol in the presence of other nucleophiles.

**Table S1.** Real sample analysis

Sl. no.	Sample	Concentration found from graph ( $\mu\text{M}$ )	Actual concentration ( $\mu\text{M}$ )	Recovery %
1.	Soil sample	1.164	1.2	97%
2.	Water sample 1 (Tap water)	1.503	1.5	100.2%
3	Water sample 2 (Zuari river water)	2.928	3.00	97.6%

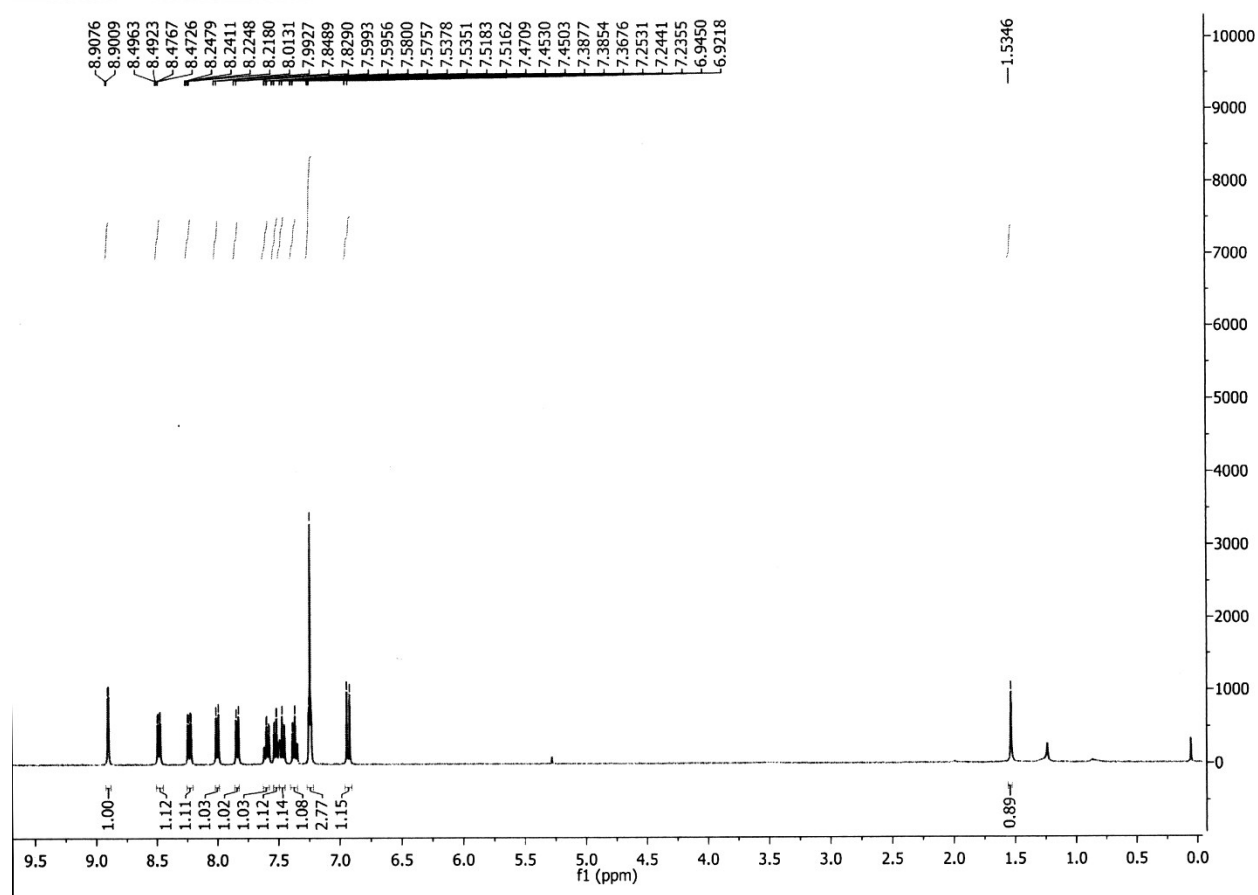
**MTT assay**

As a part of the standard protocol the cytotoxicity of probe **1** were assessed on HeLa cell line using MTT assay before fluorescence cell imaging studies. In the concentration range 1-20  $\mu\text{M}$  of probe **1** with 24 h incubation, hardly any cell death was seen (ESI) indicating the probe molecule is non-toxic even at much higher concentration than that required for the detection studies.

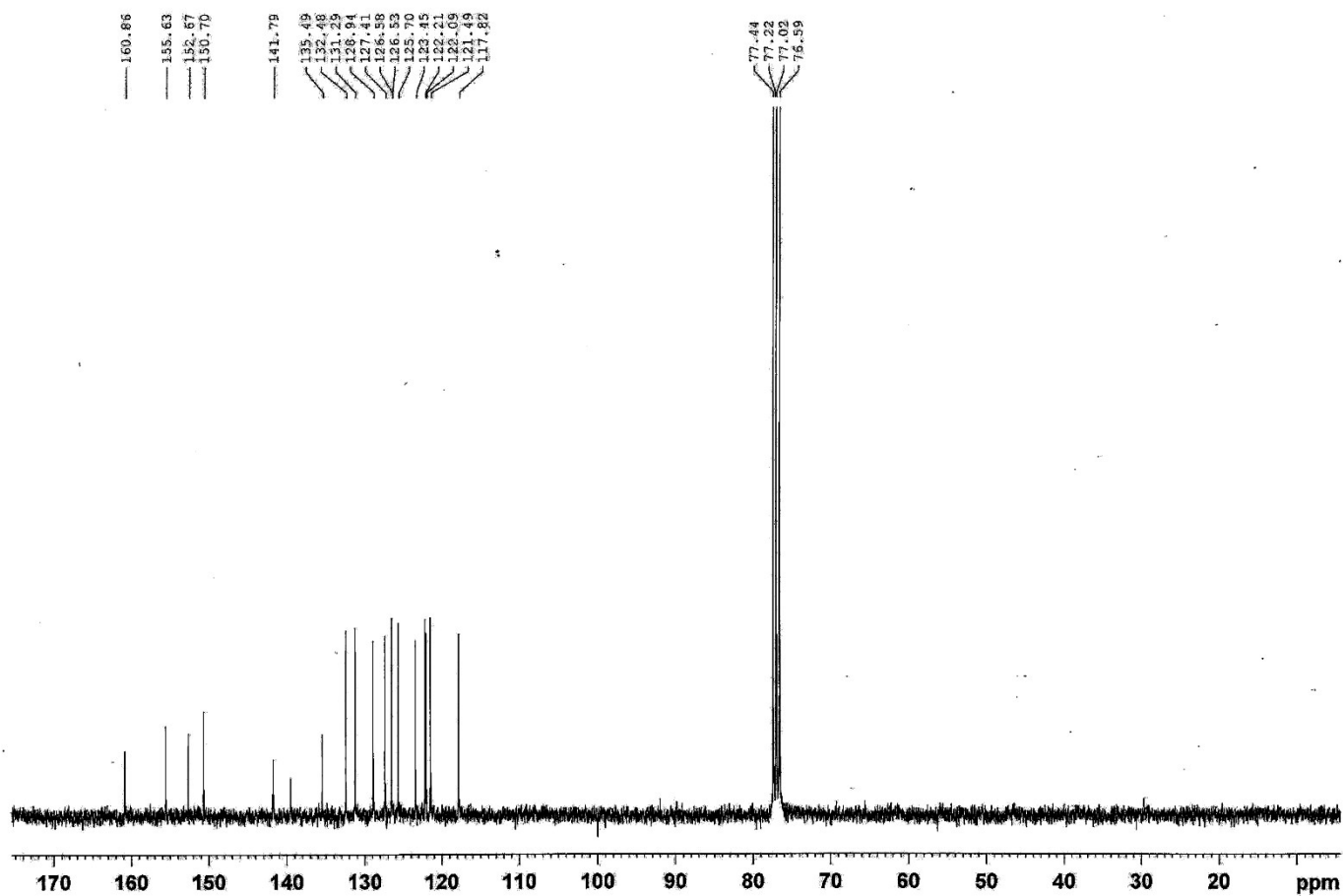


**Figure S3.** Cytotoxic assay of the probe **1** at different concentrations. The percentage of cell survival was monitored after different time intervals.

# <sup>1</sup>H NMR probe 1



# <sup>13</sup>C NMR probe 1



# HRMS of Probe 1

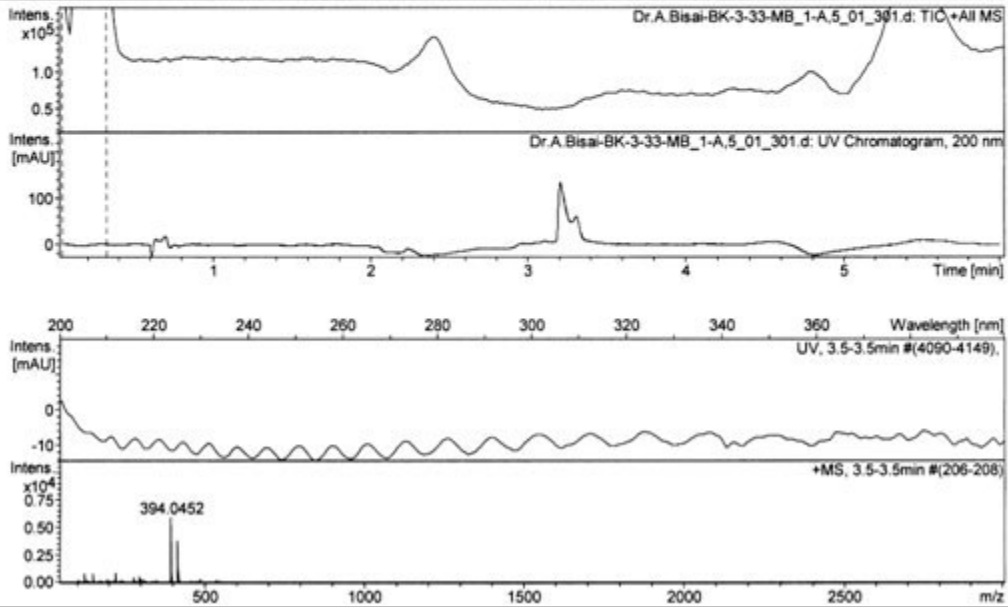
## Display Report

### Analysis Info

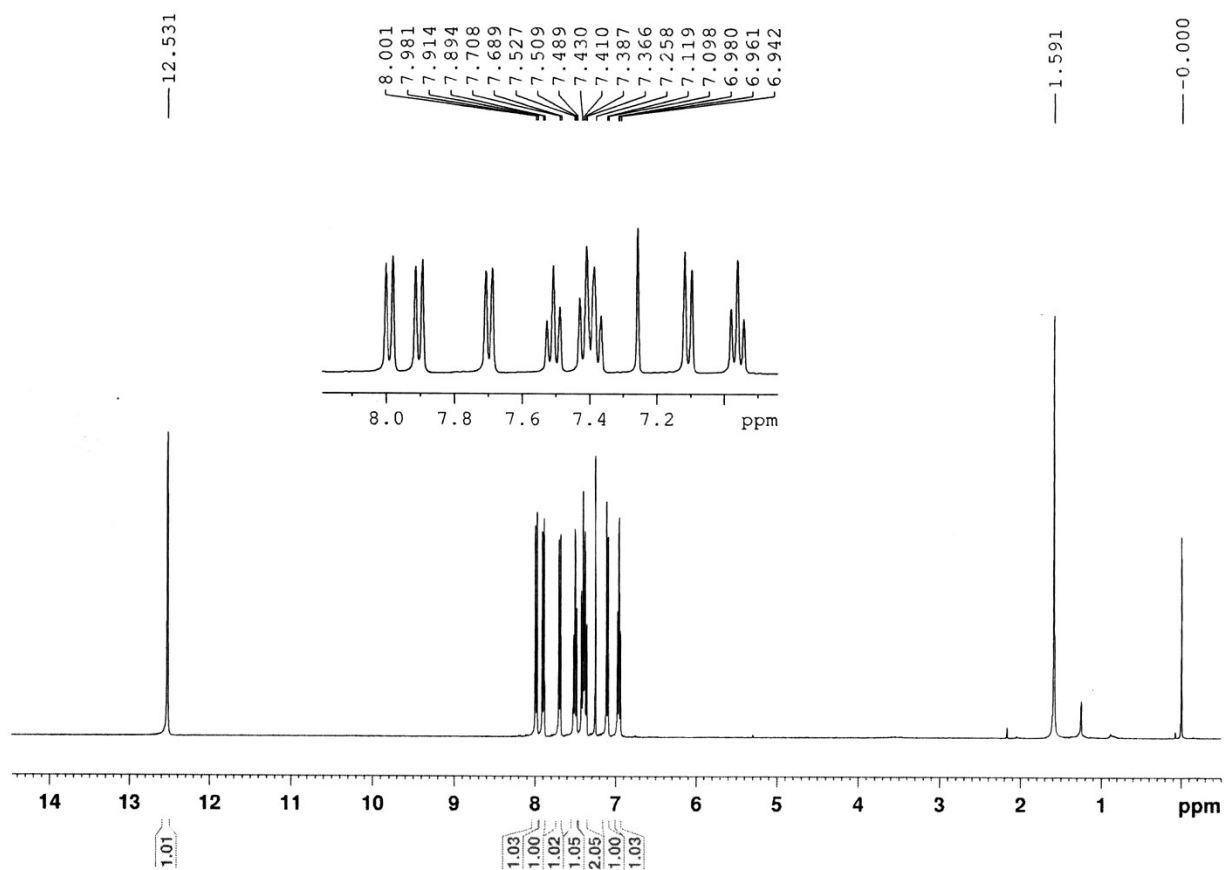
Analysis Name D:\Data\user data\2013\MAY\27 MAY\Dr.A.Bisai-BK-3-33-MB\_1-A,5\_01\_301.d Acquisition Date 5/27/2013 1:54:31 PM  
Method HRLCMS-14 may2013.m Operator Amit  
Sample Name Dr.A.Bisai-BK-3-33-MB Instrument micrOTOF-Q II 10330  
Comment

### Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

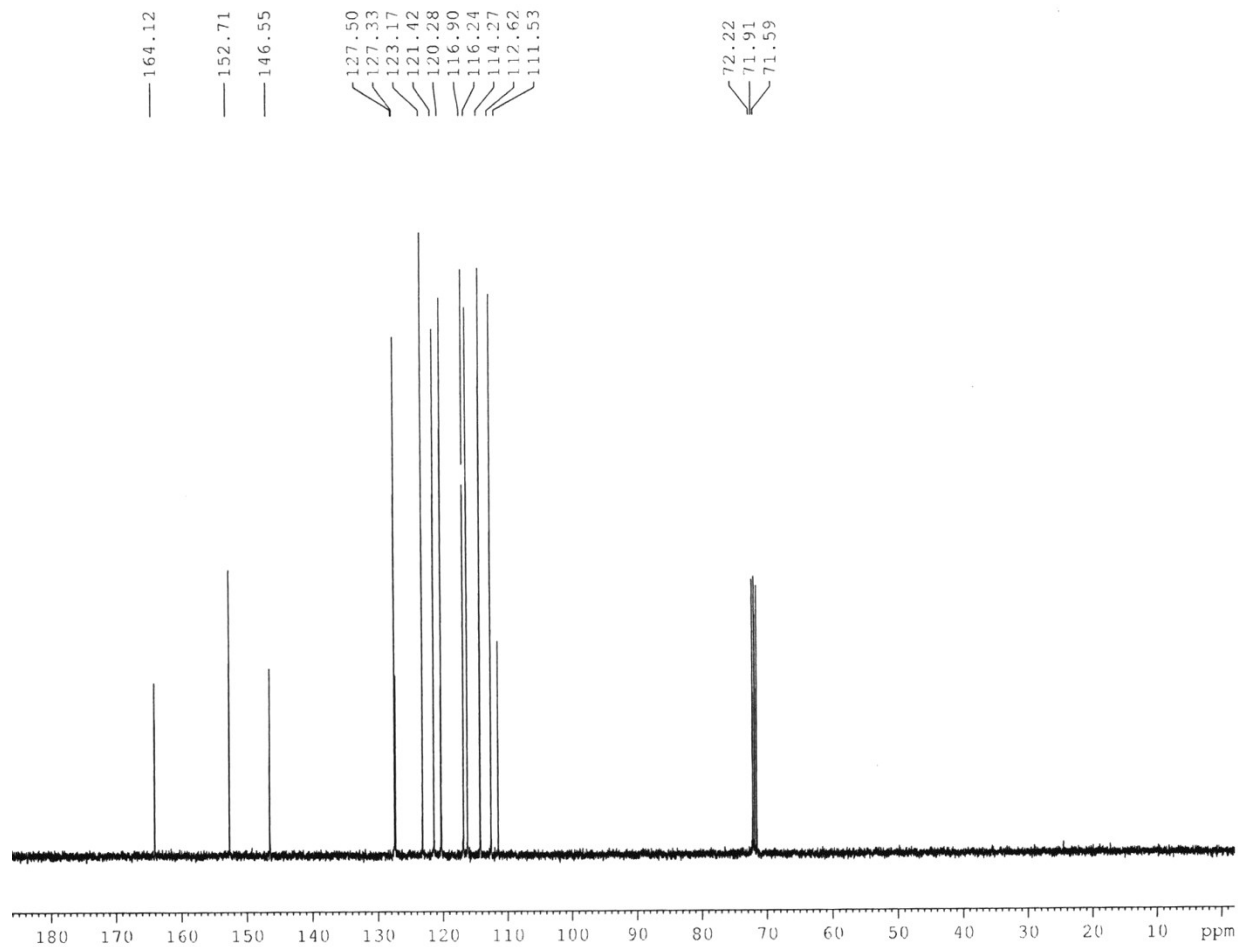


# <sup>1</sup>H spectra compound 2





# <sup>13</sup>C NMR of compound 2



## HRMS of compound 2

