

## **Supporting Information**

### **Role of surfactant and micelle promoted mild, green, highly efficient and sustainable approach for construction of novel fused pyrimidines at room temperature in water**

Pramod K. Sahu,<sup>\*a, b</sup>

<sup>a</sup>*School of Studies in Chemistry, Jiwaji University, Gwalior-474011, Madhya Pradesh, India*

<sup>b</sup>*Department of Industrial Chemistry, Jiwaji University, Gwalior-474011, Madhya Pradesh, India*

\*To whom correspondence should be addressed: Email: [sahu.chemistry@gmail.com](mailto:sahu.chemistry@gmail.com), [researchdata6@gmail.com](mailto:researchdata6@gmail.com) (Pramod Kumar Sahu)

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## Materials and methods

### Experimental

The  $^1\text{H}$  NMR spectra were measured using BRUKER AVANCE II 400 NMR spectrometer with tetramethylsilane as an internal standard at 20-25 °C; data for  $^1\text{H}$  NMR are reported as follows: chemical shift (ppm), integration, multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet, and br, broad), coupling constant (Hz). IR spectra were recorded by SHIMADZU; IR spectrometer of sample dispersed in KBr pellet or Nujol is reported in terms of frequency of absorption ( $\text{cm}^{-1}$ ). E-Merck pre-coated TLC plates and RANKEM silica gel G were used for preparative thin-layer chromatography. Melting points were determined in open capillaries and are uncorrected. AR grade of 4-hydroxy coumarin, aldehydes, SLS and other catalysts were purchased from Himedia Laboratory Ltd., Mumbai, India. 2-Amino benzothiazole was purchased from Sigma Aldrich and used without further purification.

### One-pot three-component reaction

*Typical procedure.* A mixture of substituted aromatic aldehydes (2 mmol), 4-hydroxy coumarin (2 mmol), and 2-amino benzothiazole (2 mmol) were stirred at room temperature in water (10 mL) using SLS as catalyst (10 mol%). The reaction was monitored by TLC. After completion of the reaction, the reaction mixture was cooled to room temperature and solid mass was filtered then washed with water. Collect the solid material as target compounds and recrystallized from ethanol (5 mL) to afford the pure product.

## Characterization Data

### 7-phenylchromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4a**)

White powder, mp 200-202 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2930, 2850, 1720, 1600, 1402, 1202, 1160, 1050;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  6.23 (s, 1H, -CH), 7.05-7.12 (m, 3H, Ar-H), 7.17 (t, 2H,  $J = 8.0$  Hz, Ar-H), 7.22-7.29 (m, 4H, Ar-H), 7.30-7.52 (m, 4H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 68, 103, 114, 115, 115, 119, 122, 122, 123, 123, 124, 126, 126, 127, 127, 131, 141, 152, 164, 167, 168; ESI-MS:  $m/z$  Calculated for  $\text{C}_{23}\text{H}_{14}\text{N}_2\text{O}_2\text{S}$  382.43 Found  $[\text{M}+\text{H}]^+$  382.

### 7-styrylchromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4b**)

Light brown crystal, mp 180-182; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2950, 2830, 1716, 1609, 1412, 1206, 1103, 1044;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  5.73 (s, 1H, -CH), 6.38 (d, 1H, =CH), 6.78 (d, 1H, =CH), 7.10-7.45 (m, 8H, Ar-H), 7.56 (t, 2H,  $J = 7.5$  Hz, Ar-H), 7.63 (m, 3H, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 65, 101, 102, 104, 111, 115, 116, 117, 123, 124, 126, 127, 128, 129, 131, 132, 137, 143, 152, 153, 160, 161, 163, 164, 165; ESI-MS:  $m/z$  Calculated for  $\text{C}_{25}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$  408.47 Found  $[\text{M}+\text{H}]^+$  409.

### 7-(4-chlorophenyl)chromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4c**)

Light yellow powder, mp 188-189; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2953, 2810, 1718, 1622, 1432, 1232, 1110, 1005;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  6.39 (s, 1H, -CH), 6.94-7.09 (m, 2H, Ar-H), 7.16 (d, 1H,  $J = 8.0$  Hz, Ar-H), 7.21 (t, 1H,  $J = 7.5$  Hz, Ar-H), 7.39-7.59 (m, 4H,  $J = 8.0$  Hz), 7.82 (d, 2H,  $J = 8.5$  Hz, Ar-H), 7.90 (d, 2H,  $J = 7.0$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 68, 106, 113, 118, 118, 121, 125, 125, 125, 126, 129, 130, 134, 146, 155, 163, 167, 170; ESI-MS:  $m/z$  Calculated for  $\text{C}_{23}\text{H}_{13}\text{ClN}_2\text{O}_2\text{S}$  416.88 Found  $[\text{M}+\text{H}]^+$  418.

7-(4-dimethylaminophenyl)chromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4d**)

Reddish brown powder, mp 160-162; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2943, 2809, 1718, 1604, 1415, 1202, 1106, 1022;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  3.08 (s, 6H,  $-\text{N}(\text{CH}_3)_2$ ), 6.26 (s, 1H,  $-\text{CH}$ ), 7.15-7.41 (m, 8H, Ar-H), 7.51 (t, 2H,  $J = 7.5$  Hz, Ar-H), 7.79 (d, 2H,  $J = 7.5$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 44, 65, 103, 111, 115, 115, 118, 119, 122, 122, 122, 124, 126, 128, 128, 128, 131, 141, 152, 164, 167; ESI-MS:  $m/z$  Calculated for  $\text{C}_{25}\text{H}_{19}\text{N}_3\text{O}_2\text{S}$  425.50 Found  $[\text{M}+\text{H}]^+$  426.

7-(3-hydroxyphenyl)chromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4e**)

Off white powder, mp 200-202 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2933, 2819, 1720, 1600, 1402, 1206, 1115, 1005;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  6.20 (s, 1H,  $-\text{CH}$ ), 6.45-6.56 (m, 3H, Ar-H), 6.94 (t, 1H,  $J = 7.5$  Hz, Ar-H), 7.22-7.31 (m, 4H, Ar-H), 7.38-7.51 (m, 4H, Ar-H), 9.26 (br, 1H, OH);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 65, 103, 112, 113, 114, 115, 117, 119, 122, 122, 123, 123, 124, 127, 128, 131, 141, 143, 152, 157, 164, 167, 168; ESI-MS:  $m/z$  Calculated for  $\text{C}_{23}\text{H}_{14}\text{N}_2\text{O}_3\text{S}$  398.43 Found  $[\text{M}+\text{H}]^+$  399.

7-(4-methoxyphenyl)chromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4f**)

Off white powder, mp 234-236 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2963, 2849, 1713, 1612, 1402, 1212, 1121, 1034;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  3.73 (s, 3H,  $\text{OCH}_3$ ), 6.24 (s, 1H,  $-\text{CH}$ ), 6.80 (d, 2H,  $J = 7.0$  Hz, Ar-H), 7.16-7.29 (m, 4H, Ar-H), 7.51 (t, 2H,  $J = 7.5$  Hz, Ar-H), 7.68 (d, 2H,  $J = 7.0$  Hz, Ar-H), 7.79 (d, 2H,  $J = 7.5$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 56, 66, 103, 118, 121, 125, 128, 133, 133, 133, 134, 138, 141, 142, 145, 150, 152, 164, 166; ESI-MS:  $m/z$  Calculated for  $\text{C}_{24}\text{H}_{16}\text{N}_2\text{O}_3\text{S}$  412.46 Found  $[\text{M}+\text{H}]^+$  413.

7-(4-methylphenyl)chromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4g**)

Yellow powder, mp >250 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2963, 2844, 1712, 1612, 1442, 1202, 1105, 1035;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  2.80 (s, 3H,  $\text{CH}_3$ ), 6.24 (s, 1H, -CH), 7.19-7.40 (m, 8H, Ar-H), 7.51 (t, 2H,  $J = 7.5$  Hz, Ar-H), 7.80 (d, 2H,  $J = 7.0$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 27, 65, 102, 111, 116, 119, 119, 123, 123, 124, 124, 128, 131, 140, 145, 152, 154, 164, 167; ESI-MS:  $m/z$  Calculated for  $\text{C}_{24}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$  396.46 Found  $[\text{M}]^+$  397.

7-(4-nitrophenyl)chromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4h**)

Off white powder, mp 200-202 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2952, 2822, 1715, 1602, 1412, 1217, 1125, 1021;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  6.34 (s, 1H, -CH), 7.22-7.31 (m, 5H, Ar-H), 7.36 (d, 2H,  $J = 7.0$  Hz, Ar-H), 7.53 (t, 2H,  $J = 7.5$  Hz, Ar-H), 7.81 (d, 2H,  $J = 7.5$  Hz, Ar-H), 8.08 (d, 2H,  $J = 7.5$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 67, 103, 111, 115, 118, 122, 123, 123, 124, 124, 126, 128, 128, 131, 144, 152, 161, 164, 167; ESI-MS:  $m/z$  Calculated for  $\text{C}_{23}\text{H}_{13}\text{N}_3\text{O}_4\text{S}$  427.43 Found  $[\text{M}+\text{H}]^+$  427.48.

7-(2-methylphenyl)chromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4i**)

Off white powder, mp >250 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2954, 2839, 1709, 1618, 1422, 1232, 1115, 1022;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  2.61 (s, 3H,  $\text{CH}_3$ ), 6.37 (s, 1H, -CH), 7.27 (t, 2H,  $J = 7.0$  Hz, Ar-H), 7.32 (d, 2H,  $J = 7.5$  Hz, Ar-H), 7.39 (d, 2H,  $J = 7.0$  Hz, Ar-H), 7.56 (t, 2H,  $J = 7.5$  Hz, Ar-H), 7.86 (d, 2H,  $J = 7.5$  Hz, Ar-H), 8.08 (d, 2H,  $J = 7.5$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 38, 67, 103, 115, 118, 123, 123, 124, 124, 128, 128, 130, 131, 140, 144, 150, 152, 164, 166; ESI-MS:  $m/z$  Calculated for  $\text{C}_{24}\text{H}_{16}\text{N}_2\text{O}_2\text{S}$  396.46 Found  $[\text{M}+\text{H}]^+$  397.

7-(2-methoxyphenyl)chromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4j**)

Off white powder, mp 234-236 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2953, 2824, 1716, 1615, 1415, 1209, 1119, 1018;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  3.73 (s, 3H,  $\text{OCH}_3$ ), 6.26 (s, 1H, -CH), 6.78 (d, 2H,  $J = 7.0$  Hz, Ar-H), 7.14-7.30 (m, 4H, Ar-H), 7.52 (t, 2H,  $J = 7.5$  Hz, Ar-H), 7.68 (d, 2H,  $J = 7.0$  Hz, Ar-H), 7.79 (d, 2H,  $J = 7.5$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 55, 66, 106, 115, 119, 122, 122, 123, 123, 126, 131, 134, 135, 143, 149, 152, 156, 167, 169; ESI-MS:  $m/z$  Calculated for  $\text{C}_{24}\text{H}_{16}\text{N}_2\text{O}_3\text{S}$  412.46 Found  $[\text{M}+\text{H}]^+$  413.

7-(4-hydroxyphenyl)chromeno[4,3-*d*]benzothiazolo[3,2-*a*]pyrimidin-6(7*H*)-one (**4k**)

Off white powder, mp 200-202 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2931, 2837, 1718, 1630, 1441, 1214, 1127, 1015;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  6.18 (s, 1H, -CH), 6.54 (d, 1H,  $J = 7.5$  Hz, Ar-H), 6.86 (t, 1H,  $J = 7.5$  Hz, Ar-H), 7.19-7.26 (m, 4H, Ar-H), 7.42- 7.51 (m, 4H, Ar-H), 7.60 (d, 2H,  $J = 7.5$  Hz, Ar-H), 8.91 (br, 1H, OH);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 65, 101, 109, 111, 112, 113, 115, 117, 120, 120, 120, 121, 124, 125, 128, 138, 141, 149, 159, 154, 162, 164, 166, 167; ESI-MS:  $m/z$  Calculated for  $\text{C}_{23}\text{H}_{14}\text{N}_2\text{O}_3\text{S}$  398.43 Found  $[\text{M}+\text{H}]^+$  399.

7-(4-chloroophenyl)-11-methylbenzo[4,5]thiazolo[3,2-*a*]chromeno[4,3-*d*]pyrimidin-6(7*H*)-one (**4l**)

Off white powder, mp 184-186 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2921, 2830, 1708, 1609, 1410, 1208, 1106, 1019;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  2.29 (s, 3H,  $\text{CH}_3$ ), 6.29 (s, 1H, -CH), 7.14 (d, 2H,  $J = 7.5$  Hz, Ar-H), 7.22-7.40 (m, 4H, Ar-H), 7.40-7.629 (m, 2H, Ar-H), 7.88 (d, 2H,  $J = 7.5$  Hz, Ar-H), 7.93 (d, 1H,  $J = 8.5$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 23, 67, 104, 116, 116, 117, 117, 123, 128, 129, 129, 129, 130, 131, 132, 138, 139, 152, 164, 166; ESI-MS:  $m/z$  Calculated for  $\text{C}_{24}\text{H}_{15}\text{ClN}_2\text{O}_2\text{S}$  430.91 Found  $[\text{M}]^+$  430.

11-nitro-7-phenyl-11-methylbenzo[4,5]thiazolo[3,2-*a*]chromeno[4,3-*d*]pyrimidin-6(7*H*)-one

**(4m)**

Off white powder, mp 215-217 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2970, 2834, 1720, 1615, 1411, 1201, 1104, 1019;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  6.42 (s, 1H, -CH), 7.21 (t, 2H,  $J = 8.0$  Hz, Ar-H), 7.28 (d, 2H,  $J = 8.5$  Hz, Ar-H), 7.36 (d, 2H,  $J = 8.5$  Hz, Ar-H), 7.53 (t, 2H,  $J = 8.0$  Hz, Ar-H), 7.81 (d, 2H,  $J = 8.0$  Hz, Ar-H), 8.04 (d, 2H,  $J = 9.0$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 69, 103, 111, 115, 118, 122, 122, 123, 127, 130, 131, 139, 145, 149, 151, 157, 164, 166; ESI-MS:  $m/z$  Calculated for  $\text{C}_{23}\text{H}_{13}\text{N}_3\text{O}_4\text{S}$  427.43 Found  $[\text{M}]^+$  427.08.

2-chloro-7-(*p*-tolyl)benzo[4,5]thiazolo[3,2-*a*]chromeno[4,3-*d*]pyrimidin-6(7*H*)-one **(4n)**

Off white powder, mp 225-227 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2962, 2844, 1709, 1618, 1419, 1222, 1118, 1022;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  2.39 (s, 3H,  $\text{CH}_3$ ), 6.30 (s, 1H, -CH), 6.89-6.94 (dd, 2H,  $J = 8.0, 8.5$  Hz, Ar-H), 7.06 (t, 2H,  $J = 8.0$  Hz), 7.40 (t, 1H,  $J = 7.0$  Hz, Ar-H), 7.32 (d, 2H,  $J = 7.5$  Hz, Ar-H), 7.36 (d, 1H,  $J = 7.5$  Hz, Ar-H), 7.70 (d, 1H,  $J = 7.5$  Hz, Ar-H), 8.10 (d, 2H,  $J = 8.5$  Hz, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 21, 69, 102, 117, 118, 121, 121, 121, 126, 127, 128, 129, 129, 129, 130, 1132, 134, 143, 150, 151, 161, 163, 167; ESI-MS:  $m/z$  Calculated for  $\text{C}_{24}\text{H}_{15}\text{ClN}_2\text{O}_2\text{S}$  430.90 Found  $[\text{M}]^+$  430.9.

7-(4-bromophenyl)-2-chloro-11-methylbenzo[4,5]thiazolo[3,2-*a*]chromeno[4,3-*d*]pyrimidin-6(7*H*)-one **(4o)**

Off white powder, mp >250 °C; IR ( $\nu_{\max}$ )  $\text{cm}^{-1}$  2956, 2833, 1710, 1602, 1412, 1202, 1105, 1015;  $^1\text{H}$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_{\text{H}}$  2.23 (s, 3H,  $\text{CH}_3$ ), 6.31 (s, 1H, -CH), 6.82-7.05 (m, 1H, Ar-H), 7.09-7.23 (m, 4H, Ar-H), 7.32 (d, 2H,  $J = 7.5$  Hz, Ar-H), 7.52 (d, 1H,  $J = 7.0$  Hz, Ar-H), 7.80-7.92 (m, 2H, Ar-H);  $^{13}\text{C}$  NMR (125 MHz, DMSO  $d_6$ ): 22, 70, 104, 109, 113, 125, 126, 126,

127, 128, 129,129, 129, 130, 130, 138, 143, 151, 153, 165, 170; ESI-MS: m/z Calculated for  $C_{24}H_{14}BrClN_2O_2S$  509.80 Found  $[M]^+$  509.8.

4-Pheny l-3,4-dihydro-2H-chromeno[4,3-d]pyrimidine-2,5(1H)-dione (**6a**)

Off white powder, mp 160-162 °C (Reported 160-162 °C)<sup>42</sup>;  $^1H$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_H$  6.36 (s, 3H, -CH), 7.09-7.39 (m, 9H, Ar-H), 7.60 (s, 1H, NH), 7.90 (s, 1H, NH);  $^{13}C$  NMR (125 MHz, DMSO  $d_6$ ): 36, 104, 116, 118, 123, 123, 125, 125, 126, 126, 127, 131, 140, 152, 164, 165; ESI-MS: m/z Calculated for  $C_{17}H_{12}N_2O_3$  292.29 Found  $[M]^+$  292.3.

4-(4-Chlorophenyl)-3,4-dihydro-2H-chromeno[4,3-d]pyrimidine-2,5(1H)-dione (**6b**)

4-Pheny Off white powder, mp 195-197 °C (Reported 197-198 °C)<sup>43</sup>;  $^1H$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_H$  6.28 (s, 1H), 7.13 (d, 2H, J = 8.5 Hz, Ar-H), 7.54-7.34 (m, 6H, Ar-H), 7.56 (s, 1H, NH), 7.87 (s, 1H, Ar-H);  $^{13}C$  NMR (125 MHz, DMSO  $d_6$ ): 35, 104, 116, 118, 123, 128, 128, 129, 130, 131, 132, 137, 139,152, 164, 165; ESI-MS: m/z Calculated for  $C_{17}H_{11}ClN_2O_3$  326.73 Found  $[M]^+$  326.73.

4-Phenyl-2-thioxo-1,2,3,4-tetrahydro-5H-chromeno[4,3-d]pyrimidine-5-one (**6c**)

Off white powder, mp 185-187 °C (Reported 188-190 °C)<sup>42</sup>;  $^1H$  NMR (500 MHz, DMSO  $d_6$ ):  $\delta_H$  6.34 (s, 1H, -CH), 7.24-7.39 (m, 9H, Ar-H), 7.82 (s, 1H, Ar-H), 8.09 (s, 1H, Ar-H);  $^{13}C$  NMR (125 MHz, DMSO  $d_6$ ): 36, 103, 115, 119, 123, 123, 124, 127, 131, 132, 145, 150, 152, 164, 166; ESI-MS: m/z Calculated for  $C_{17}H_{12}N_2O_2S$  308.35 Found  $[M]^+$  308.35.

4-(4-Dimethylaminophenyl)-2-thioxo-1,2,3,4-tetrahydro-5H-chromeno[4,3-d]pyrimidine-5-one (**6d**)



Off white powder, mp 232-234 °C (Reported 232-234 °C)<sup>42</sup>; <sup>1</sup>H NMR (500 MHz, DMSO d<sub>6</sub>): δ<sub>H</sub> 3.11 (s, 6H, N(CH<sub>3</sub>)<sub>2</sub>), 6.26 (s, 1H, -CH), 7.17-7.28 (m, 4H, Ar-H), 7.49-7.56 (m, 4H, Ar-H), 7.69 (s, 1H, NH), 7.80 (s, 1H, NH); <sup>13</sup>C NMR (125 MHz, DMSO d<sub>6</sub>): 36, 45, 103, 111, 115, 119, 123, 123, 124, 124, 128, 131, 153, 164, 167; ESI-MS: m/z Calculated for C<sub>19</sub>H<sub>17</sub>N<sub>3</sub>O<sub>2</sub>S 351.42 Found [M]<sup>+</sup> 351.42.

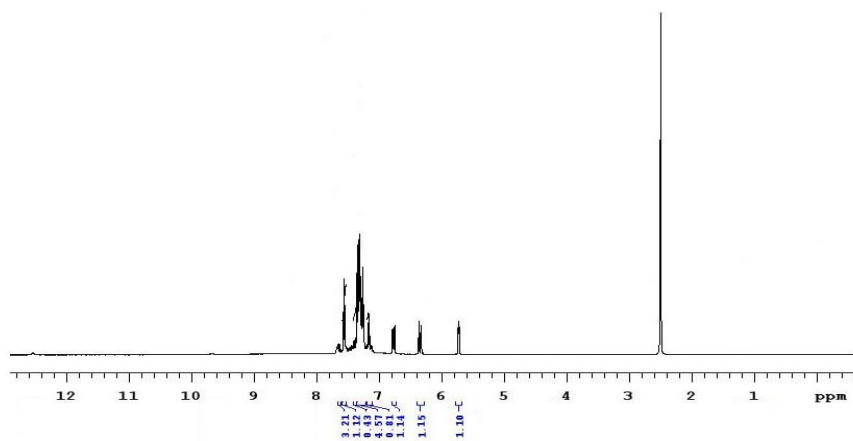
7-(2-hydroxyphenyl)-7,12-dihydro-6H-chromeno[4,3-d][1,2,4]triazolo[1,5-a]pyrimidin-6-one (**8**)

Off white powder, mp 210-212 °C; <sup>1</sup>H NMR (500 MHz, DMSO d<sub>6</sub>): δ<sub>H</sub> 6.26 (s, 1H, -CH), 6.89-6.69 (m, 2H, Ar-H), 7.40-7.51 (m, 4H, Ar-H), 7.69-7.75 (m, 2H, Ar-H), 7.88 (d, 1H, J = 7.5 Hz, Ar-H), 8.35 (s, 1H, =CH), 10.38 (s, 1H, OH); <sup>13</sup>C NMR (125 MHz, DMSO d<sub>6</sub>): 36, 102, 116, 116, 118, 119, 123, 125, 128, 129, 130, 133, 135, 143, 153, 158, 158; ESI-MS: m/z Calculated for C<sub>18</sub>H<sub>12</sub>N<sub>4</sub>O<sub>3</sub> 332.3 Found [M]<sup>+</sup> 332.3.

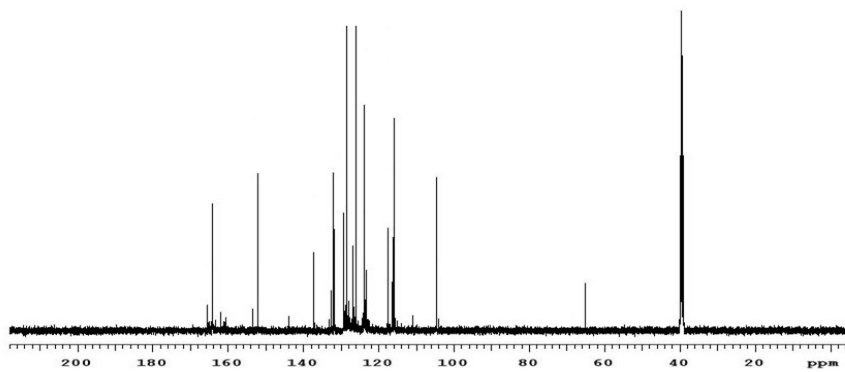


## Compound 4b

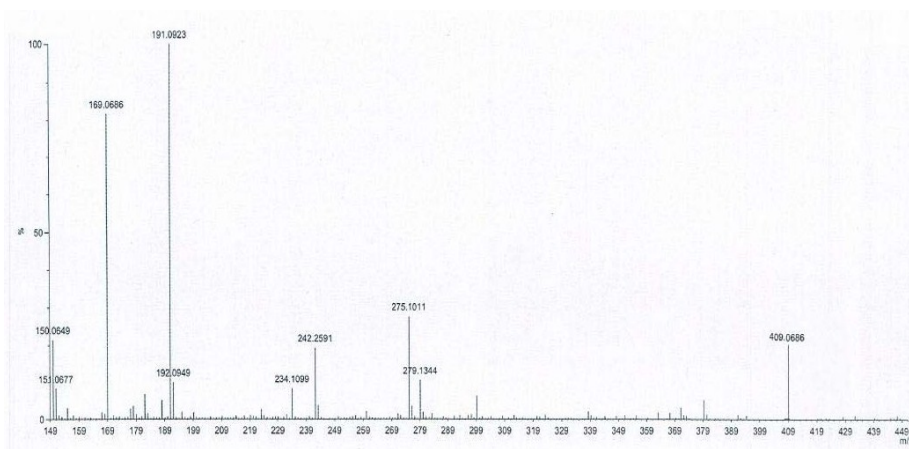
### <sup>1</sup>H NMR



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



### Mass spectra

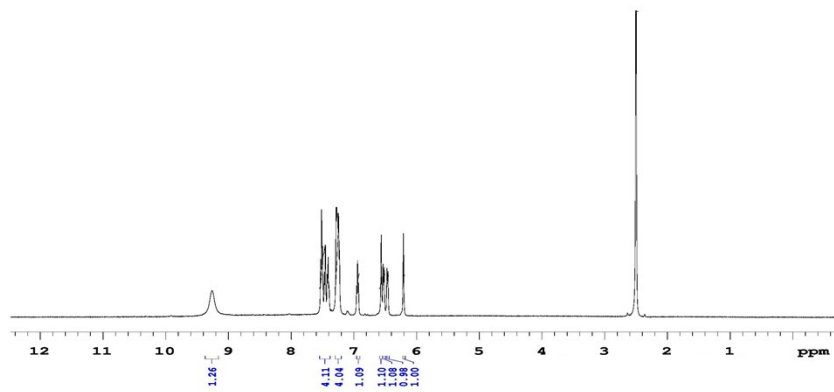




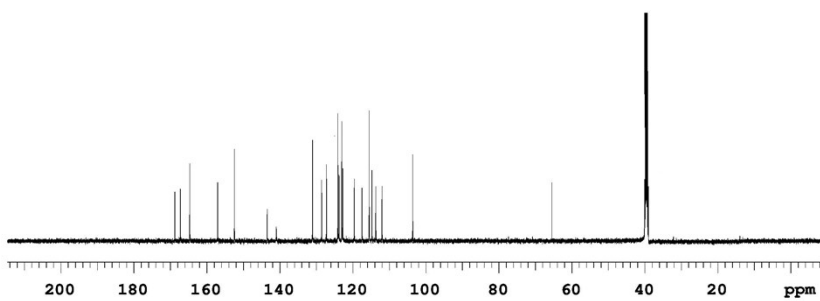


## Compound 4e

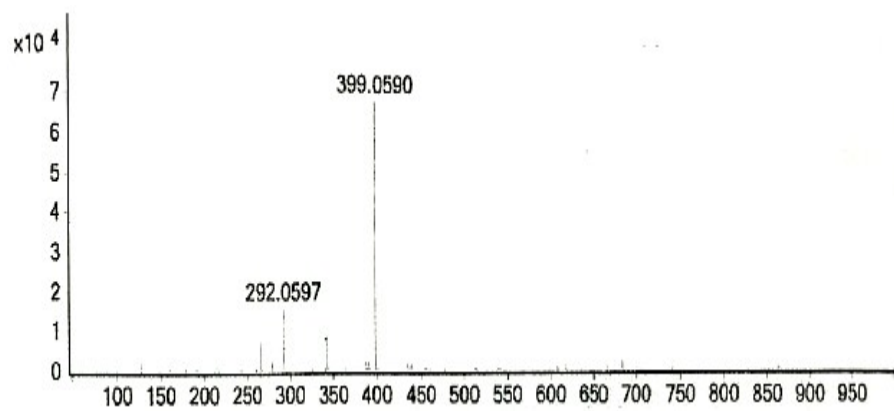
### <sup>1</sup>H NMR



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

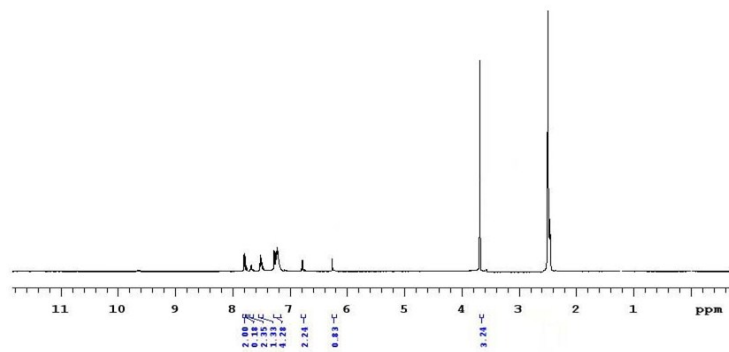


### Mass spectra

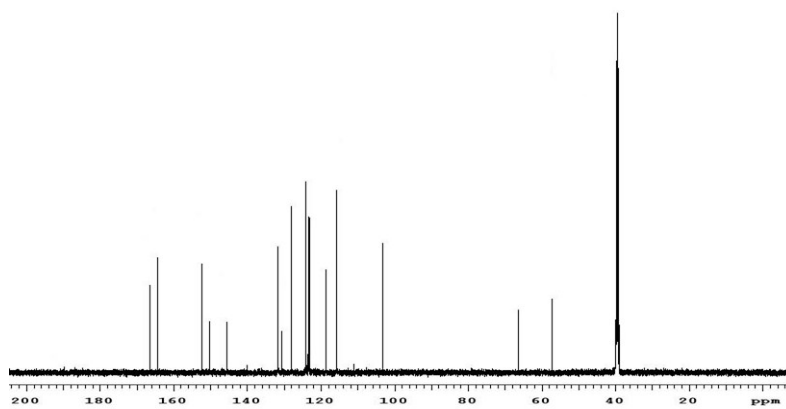


## Compound 4f

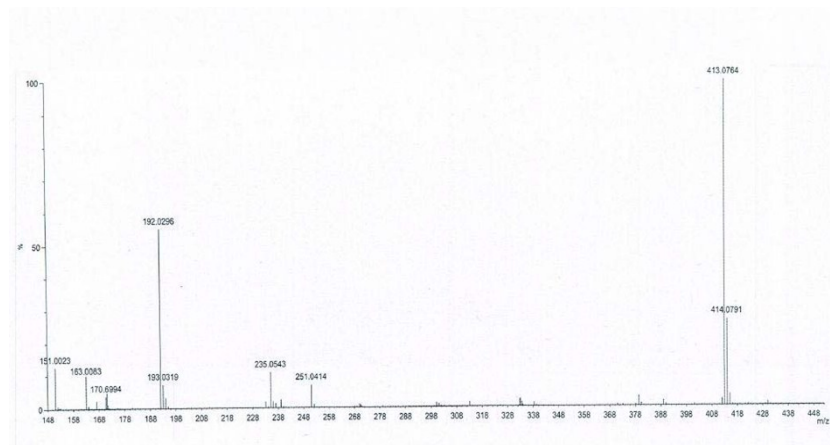
### <sup>1</sup>H NMR



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

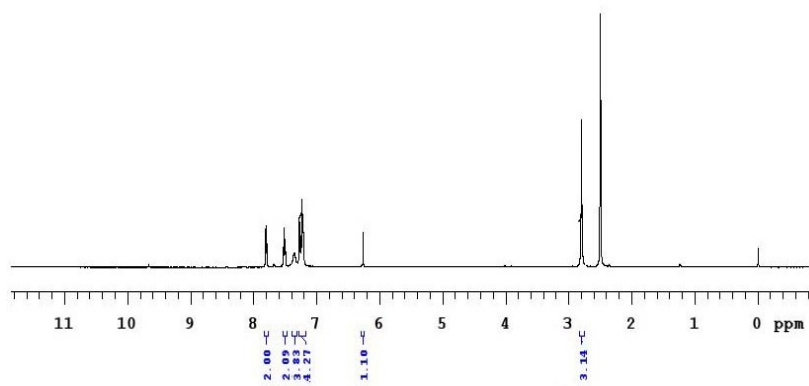


### Mass spectra

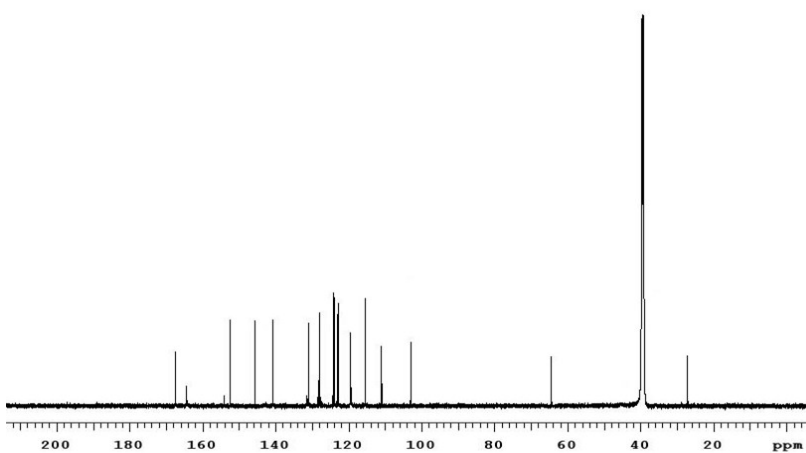


## Compound 4g

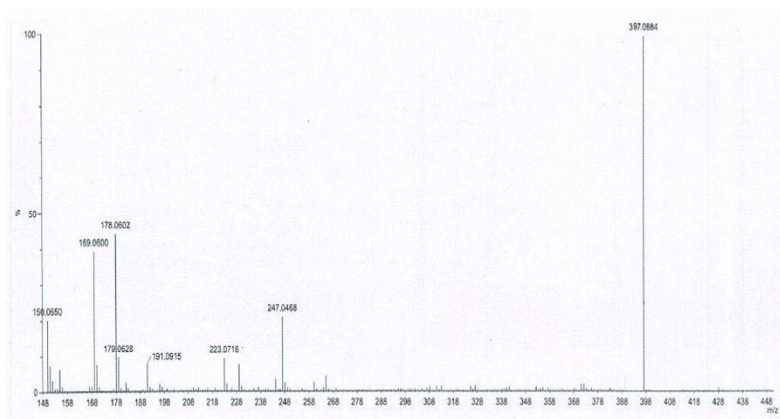
### <sup>1</sup>H NMR



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



### Mass spectra

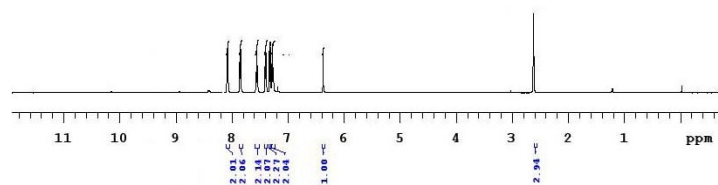




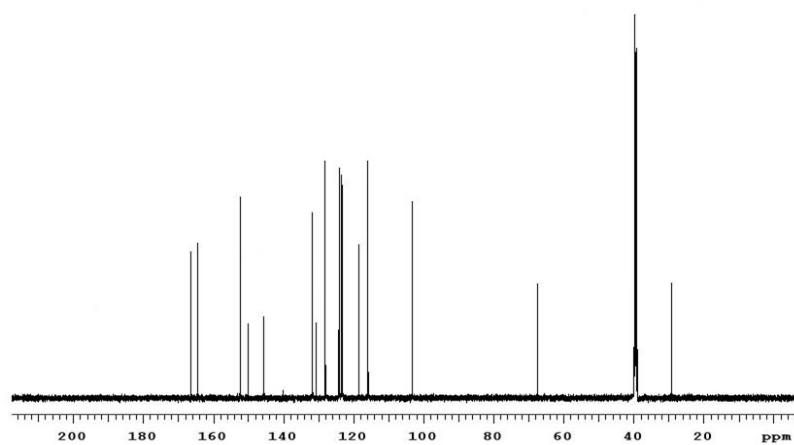


## Compound 4i

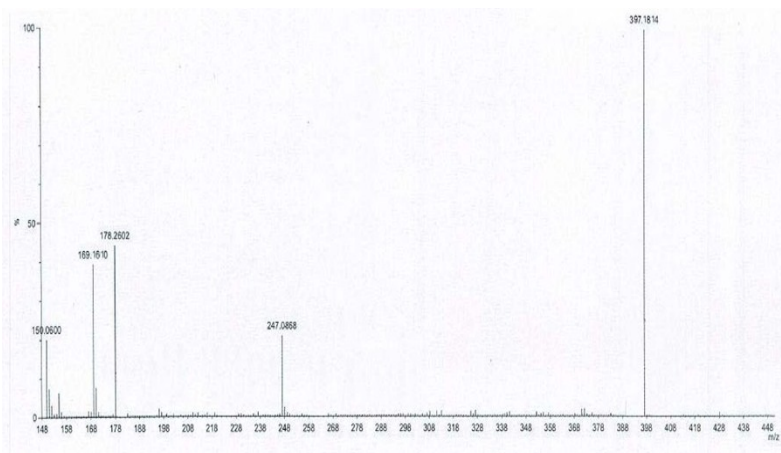
### <sup>1</sup>H NMR



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



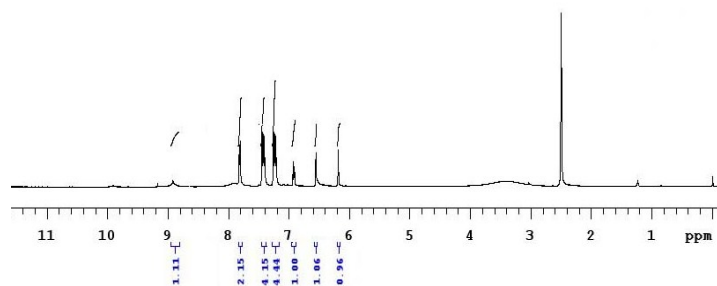
### Mass spectra



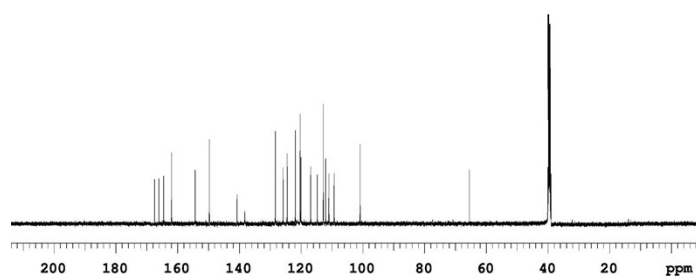


## Compound 4k

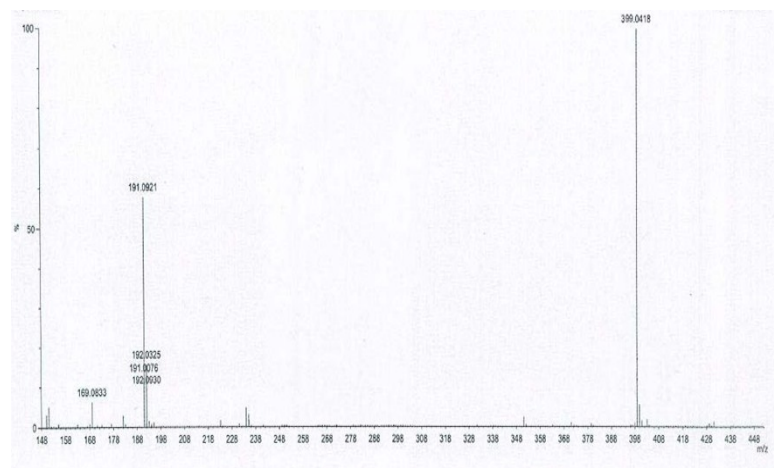
### <sup>1</sup>H NMR



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



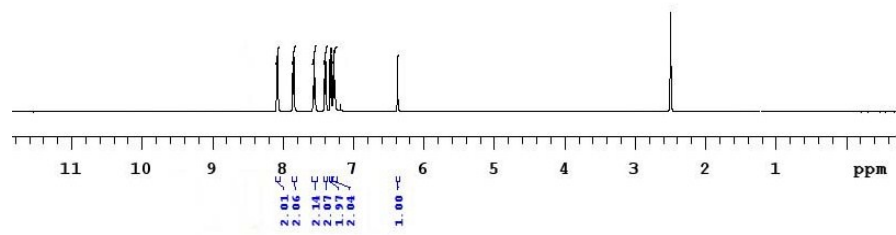
### Mass spectra



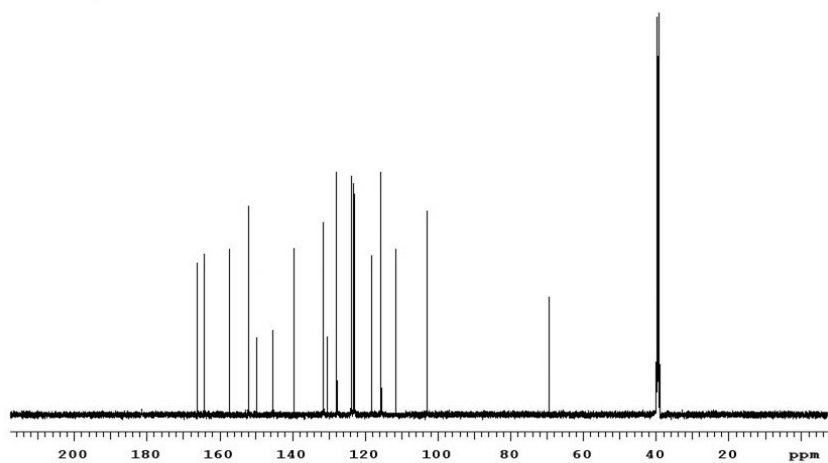


## Compound 4m

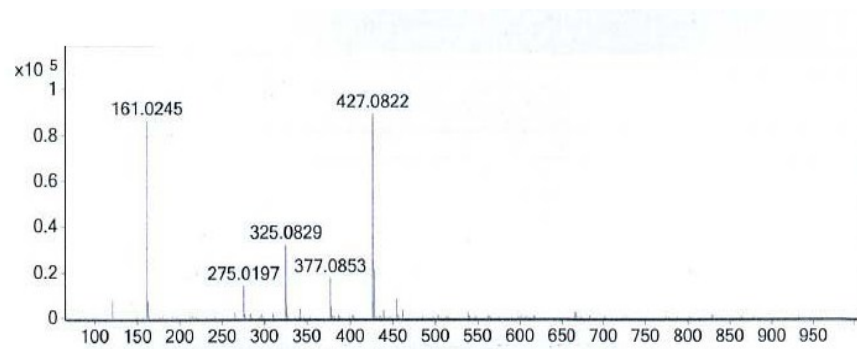
### <sup>1</sup>H NMR



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



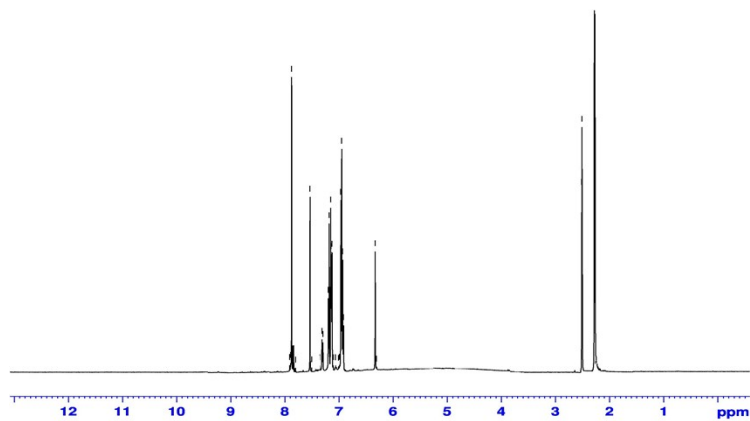
### Mass spectra



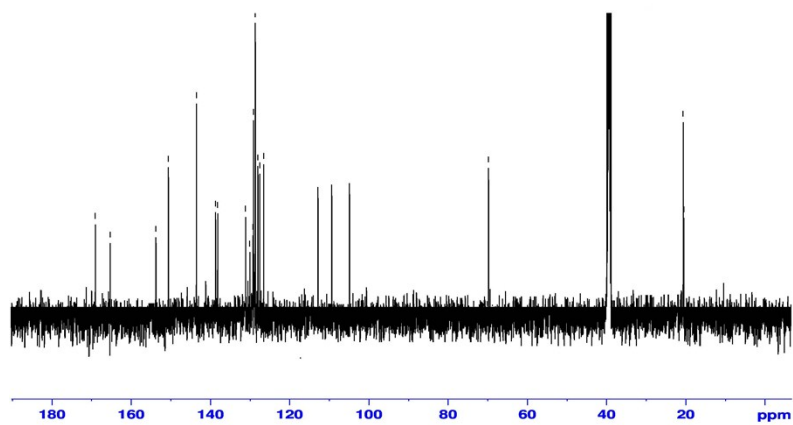


## Compound 4o

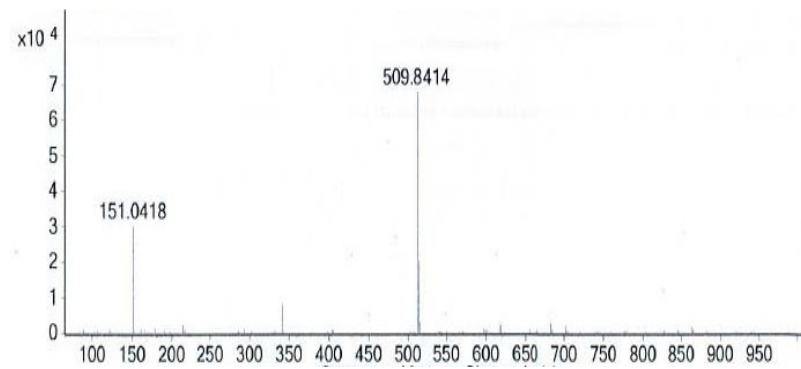
### <sup>1</sup>H NMR



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



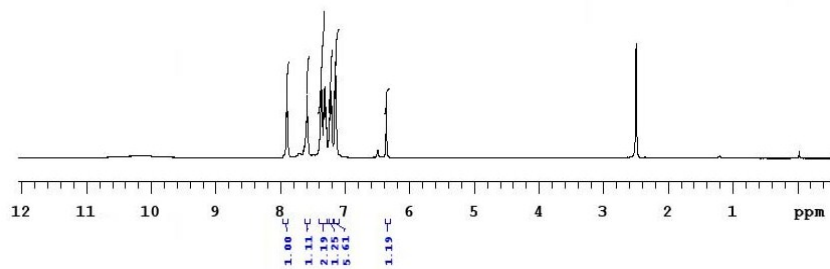
### Mass spectra



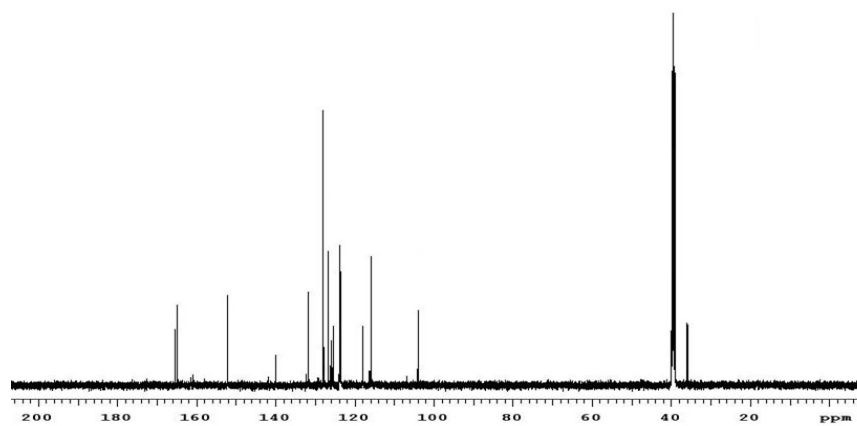


## Compound 6a

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

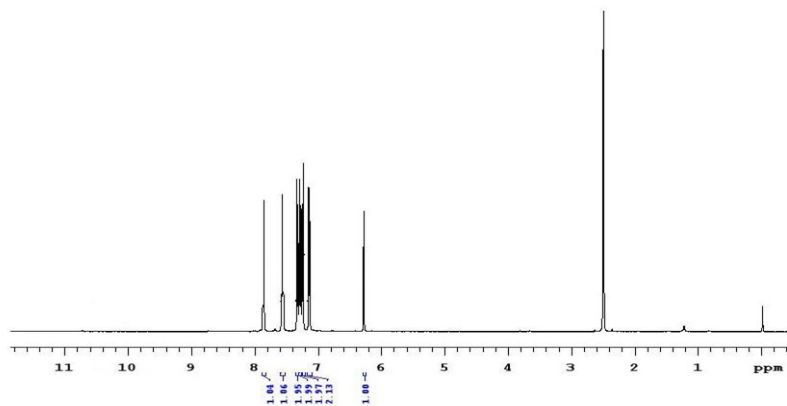


### <sup>13</sup>C NMR

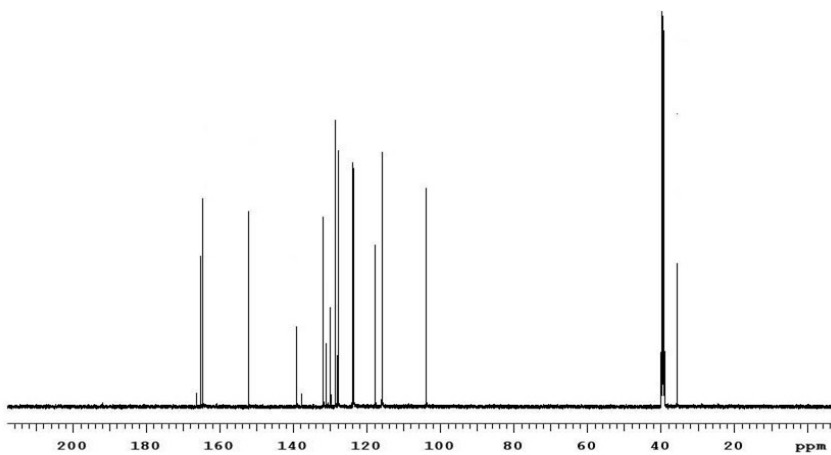


## Compound 6b

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

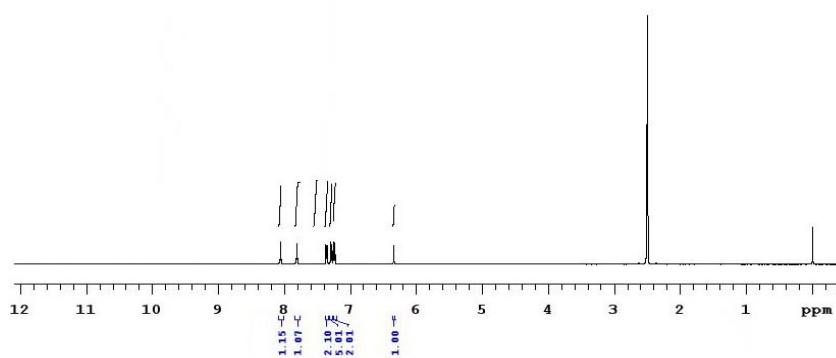


### <sup>13</sup>C NMR

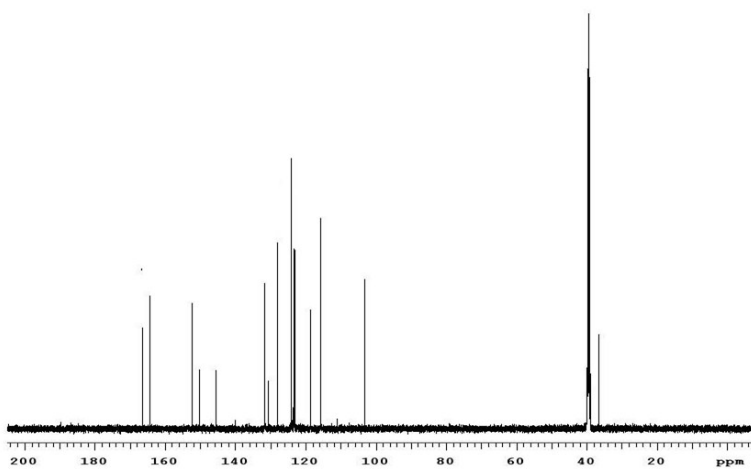


### Compound 6c

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

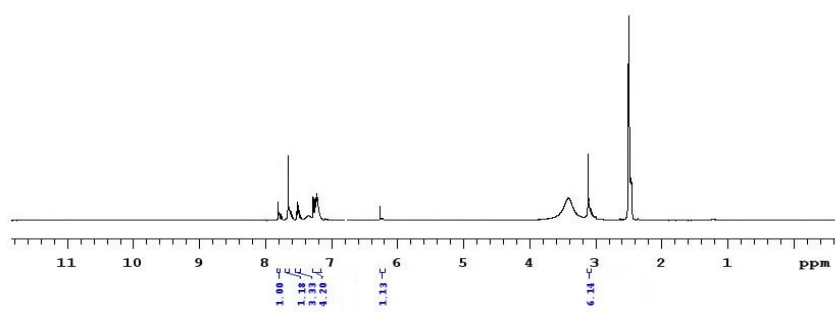


### <sup>13</sup>C NMR

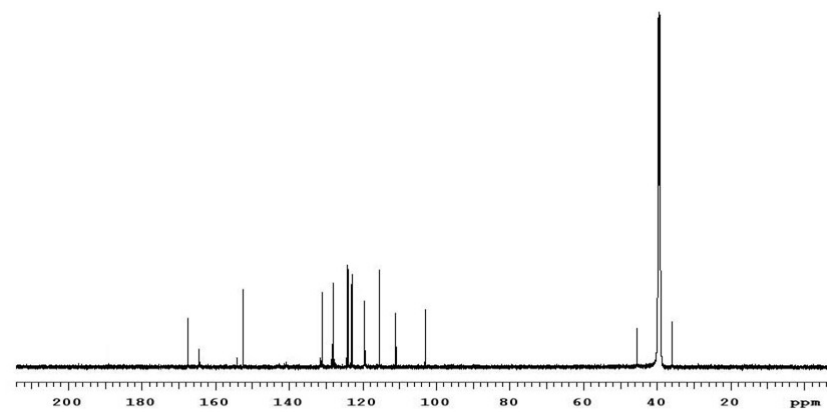


### Compound 6d

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

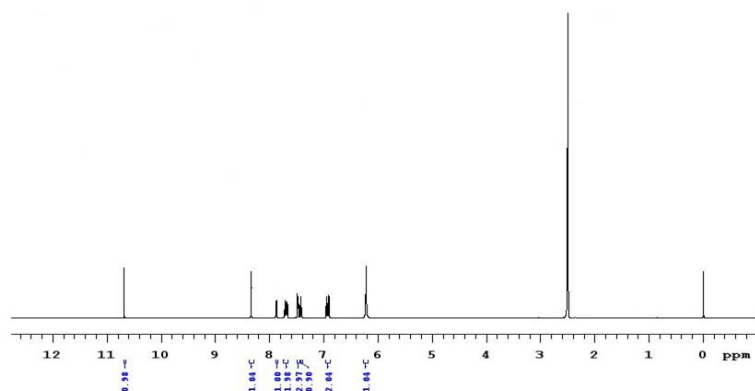


#### <sup>13</sup>C NMR

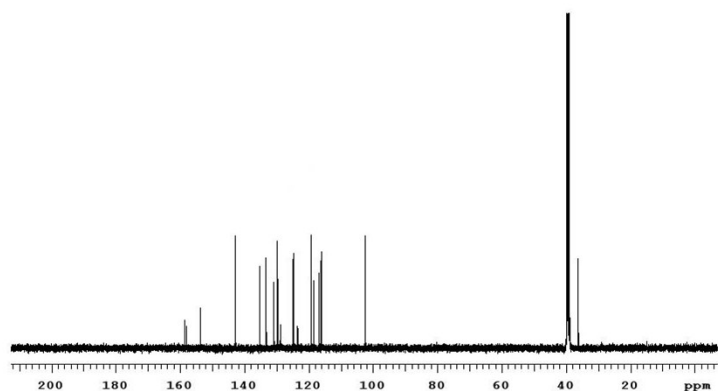


### Compound 8

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



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



## Mass spectra

