

**Supporting Information for**  
**Iodine catalyzed one-pot multi-component synthesis of a library of**  
**compounds containing tetrazolo[1,5-*a*]pyrimidine core**

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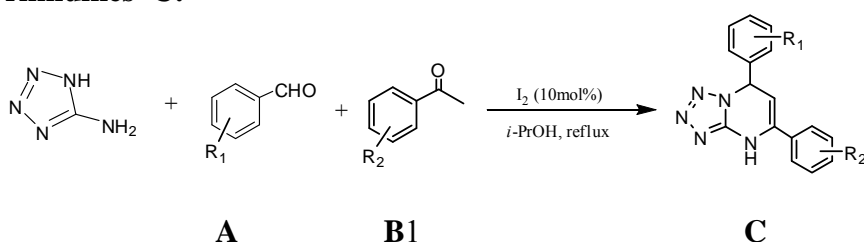
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## General Consideration and Procedures

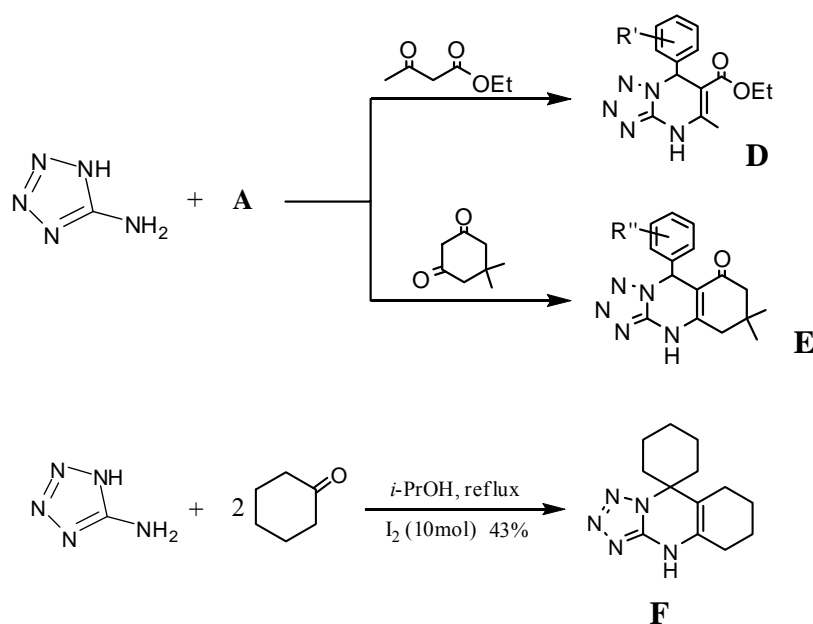
Starting material 5-AT was prepared according to literature procedure,<sup>1</sup> others were obtained from commercial suppliers and used without further purification. Analytical thin-layer chromatography were performed on glass plates precoated with silica gel impregnated with a fluorescent indicator (254 nm), and the plates were visualized by exposure to ultraviolet light. All melting points are uncorrected. Mass spectra were taken on a Agilent LC-MS 1100 series instrument in the electrospray ionization (positive ESI) mode. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded at 300 MHz and 75 MHz, respectively, in DMSO-*d*<sub>6</sub>, and chemical shifts were reported in ppm from internal TMS (δ). Elemental analyses were performed on a Yanagimoto MT3CHN recorder.

### General Procedure for the Synthesis of 5,7-Diaryl-4,7-dihydro-tetrazolo[1,5-*a*]pyrimidines **C**:



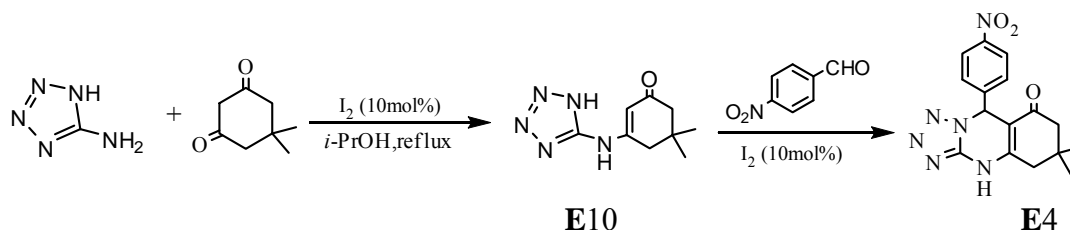
Iodine (0.127g, 0.5mmol) was added into a stirred mixture containing 5-AT (0.425g, 5mmol), chalcone (1.04g, 5mmol), or **A** (5mmol) and **B1** (5mmol) in AcOEt (5mL) or *i*-PrOH (5mL) at refluxing temperature. After several hours, the mixture was cooled to room temperature and added with cold MeOH (1mL), the solid precipitated was filtrated and washed with a solution of sodium thiosulfate followed by water, and dried to afford the crude product.

### General Procedure for the Synthesis of Ethyl 5-Methyl-7-aryl-4,7-dihydro-tetrazolo[1,5-*a*]pyrimidine-6-carboxylates **D**, 6,6-Dimethyl-9-aryl-5,6,7,9-tetrahydro-tetrazolo[1,5-*a*]quinazolin-8(4H)-ones **E** and 5',6',7',8'-Tetrahydro-4'H-spiro[cyclohexane-1,9'-tetrazolo[5,1-*b*]quinazoline] **F**:



Iodine (0.127g, 0.5mmol) was added into a stirred mixture containing 5-AT (0.425g, 5mmol), **A** (5mmol) and **B2** (0.65g, 5mmol) or **B3** (0.70g, 5mmol) in *i*-PrOH (5mL) at refluxing temperature. After a period of time, the mixture was cooled to room temperature and added with a solution of sodium thiosulfate (10M, 2mL), the solid precipitated was filtrated and washed with cold MeOH (2mL) followed by water, and dried to afford the crude product.

**Two-step for Synthesis of 6,6-Dimethyl-9-aryl-5,6,7,9-tetrahydro-1,5-a-quinazolin-8(4H)-ones E:**



Iodine (0.127g, 0.5mmol) was added into a stirred mixture containing 5-AT (0.425g, 5mmol) and **B3** (0.70g, 5mmol) in *i*-PrOH (5mL) at refluxing temperature. After 5 minutes, the reaction was quenched with solution of sodium thiosulfate and cooled to room temperature, the solid precipitated was filtrated and washed with cold MeOH (2mL), and dried to afford the crude product. Further purification from EtOH afford compound **E10**.

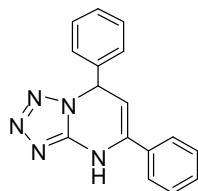
The product **E10** (0.2g, 2.5mmol) obtained above and 4-nitrobenzaldehyde (0.302g, 2mmol) were stirred in refluxing *i*-PrOH (5mL) in the present of iodine (0.508g, 0.2mmol) for about 12 minutes, the solid was precipitated, and the reaction was terminated. After cooling the mixture to room temperature, the solid precipitated was filtrated and washed with solution of sodium thiosulfate followed by cold MeOH (2mL), and dried to afford the crude product. And the purification was similar with the one-pot method.

**Reference:**

(1) Murotani, M.; Mura, H.; Takeda, M.; Shibafuchi, H. U. S. Patent 5 594 146, **1997**.

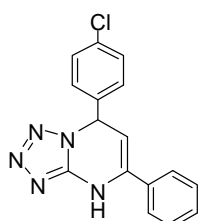
## Characterization Data

### Compound C1 (Entry 1, Table2)



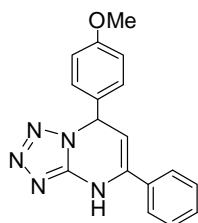
recrystallized from EtOH. Yield 0.73g (57%) of colorless prisms, 99% pure by LC-MS. Mp 236-240°C ([3c], 232-233°C); <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 5.32 (d, 6-CH, *J*=3.03Hz), 6.61 (d, 5-CH, *J*=3.03Hz), 7.35-7.67 (m, 10H, aromatic), 10.56 (s, 1H, NH); MS (ES<sup>+</sup>) *m/z* 276(M + H); Anal. Calcd for C<sub>16</sub>H<sub>13</sub>N<sub>5</sub>: C, 59.67; H, 5.44; N, 21.68. Found: C, 59.61; H, 5.53; N, 21.70.

### Compound C2 (Entry 2, Table2)



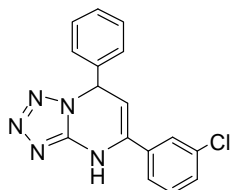
recrystallized from benzene-dimethylformamine (5:1). Yield 0.84g (54%) of white prisms, 99% pure by LC-MS. Mp 238-240°C; <sup>1</sup>H NMR(500MHz, DMSO-*d*<sub>6</sub>) δ 5.30-5.31 (m, 6-CH), 6.65 (d, 5-CH, *J*=3.5Hz), 7.40-7.67 (m, 10H, aromatic), 10.58 (s, 1H, NH); MS (ES<sup>+</sup>) *m/z* 310(M + H); Anal. Calcd for C<sub>16</sub>H<sub>12</sub>N<sub>5</sub>Cl: C, 62.04; H, 3.90; N, 22.61. Found: C, 61.97; H, 3.95; N, 22.67.

### Compound C3 (Entry 4, Table2)



recrystallized from benzene-dimethylformamine (5:1). Yield 0.85g (56%) of white prisms, 99% pure by LC-MS. Mp 226-228°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 3.73 (s, OCH<sub>3</sub>), 5.25 (d, 6-CH, *J*=3.6Hz), 6.53 (d, 5-CH, *J*=3.9Hz), 6.93-7.65 (m, 9H, aromatic), 10.46 (s, 1H, NH); MS (ES<sup>+</sup>) *m/z* 306(M + H); Anal. Calcd for C<sub>17</sub>H<sub>15</sub>N<sub>5</sub>O: C, 66.87; H, 4.95; N, 22.94. Found: C, 66.83; H, 4.99; N, 22.95.

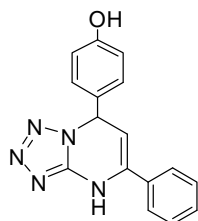
### Compound C4 (Entry 5, Table 2)



recrystallized from benzene-dimethylformamine (5:1). Yield 0.96g (61%) of white floc, 98% pure by LC-MS. Mp 218-220°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 5.42 (d, 6-CH, *J*=3.6Hz), 6.59 (d, 5-CH, *J*=3.9Hz), 7.33-7.72 (m, 9H, aromatic), 10.57 (s, 1H, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>)

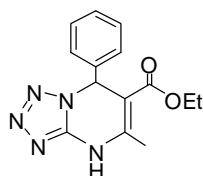
$\delta$  58.91, 98.39, 124.92, 126.08, 127.34, 128.79, 129.07, 129.23, 130.60, 133.57, 133.99, 135.73, 140.55, 150.72; MS (ES<sup>+</sup>)  $m/z$  310(M + H); Anal. Calcd for C<sub>16</sub>H<sub>13</sub>N<sub>5</sub>: C, 59.67; H, 5.44; N, 21.68. Found: C, 59.57; H, 5.59; N, 21.61.

**Compound C5 (Entry 6, Table 2)**



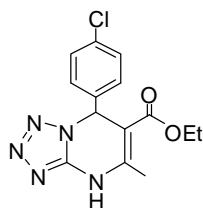
recrystallized from MeOH. Yield 0.46g (33%) of colorless prisms, 97% pure by LC-MS. Mp 241-244°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>)  $\delta$  5.25 (s, 6-CH), 6.48 (d, 5-CH,  $J=1.5$ Hz), 6.77-7.66 (m, 9H, aromatic), 9.61 (s, OH), 10.46 (s, 1H, NH); MS (ES<sup>+</sup>)  $m/z$  292(M + H); Anal. Calcd for C<sub>17</sub>H<sub>15</sub>N<sub>5</sub>O: C, 65.97; H, 4.50; N, 24.04. Found: C, 65.91; H, 4.63; N, 24.01.

**Compound D1 (Entry 1, Table 3)**



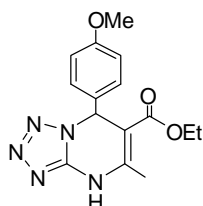
recrystallized from EtOH. Yield 1.07g (72%) of colorless prisms, 96% pure by LC-MS. Mp 203-205°C; <sup>1</sup>H NMR(500MHz, DMSO-*d*<sub>6</sub>)  $\delta$  1.01-1.16 and 3.91-4.02 (m, CH<sub>2</sub>CH<sub>3</sub>), 2.47-2.51 (m, 5-CH<sub>3</sub>), 6.63 (s, 7-CH), 7.29-7.37 (m, 5H, aromatic), 11.29 (s, 1H, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>)  $\delta$  13.94, 18.57, 58.97, 59.82, 97.92, 127.34, 128.64, 128.82, 141.12, 146.81, 148.65, 164.74; MS (ES<sup>+</sup>)  $m/z$  286(M + H); Anal. Calcd for C<sub>14</sub>H<sub>15</sub>N<sub>5</sub>O<sub>2</sub>: C, 58.94; H, 5.30; N, 24.55. Found: C, 58.90; H, 5.21; N, 24.43.

**Compound D2 (Entry 2, Table 3)**



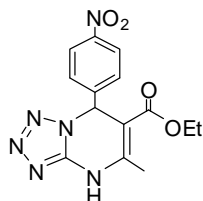
recrystallized from EtOH. Yield 1.11g (69%) of white flocc, 99% pure by LC-MS. Mp 234-236°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>)  $\delta$  1.00-1.05 and 3.34-3.99 (m, CH<sub>2</sub>CH<sub>3</sub>), 2.46-2.50 (m, 5-CH<sub>3</sub>), 6.69 (s, 5-CH), 7.34-7.44 (m, 4H, aromatic), 11.33 (s, 1H, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>)  $\delta$  13.96, 18.63, 58.26, 59.88, 97.43, 128.85, 129.99, 133.32, 140.07, 147.15, 148.52, 164.61; MS (ES<sup>+</sup>)  $m/z$  320(M + H); Anal. Calcd for C<sub>16</sub>H<sub>12</sub>ClN<sub>5</sub>: C, 52.59; H, 4.41; N, 21.90. Found: C, 52.61; H, 4.46; N, 21.93.

**Compound D3 (Entry 3, Table 3)**



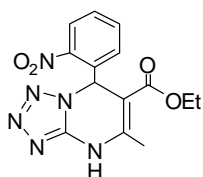
recrystallized from EtOH-H<sub>2</sub>O (2:1). Yield 0.63g (39%) of white prisms, 98% pure by LC-MS. Mp 194-197°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 1.02-1.07 and 3.94-3.99 (m, CH<sub>2</sub>CH<sub>3</sub>), 2.45-2.52 (m, 5-CH<sub>3</sub>), 3.72 (d, OCH<sub>3</sub>, *J*=1.5Hz), 6.61 (s, 7-CH), 6.88-7.24 (m, 4H, aromatic), 11.23 (s, 1H, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>) δ 14.03, 18.57, 55.29, 58.42, 59.83, 98.15, 114.15, 128.62, 133.34, 146.46, 148.60, 159.45, 164.83; MS (ES<sup>+</sup>) *m/z* 316(M + H); Anal. Calcd for C<sub>15</sub>H<sub>17</sub>N<sub>5</sub>O<sub>3</sub>: C, 51.13; H, 5.43; N, 22.21. Found: C, 51.09; H, 5.46; N, 22.25.

**Compound D4 (Entry 4, Table 3)**



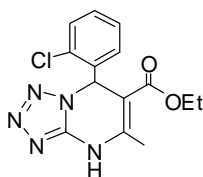
recrystallized from MeOH. Yield 1.28g (77%) of brown prisms, 99% pure by LC-MS. Mp 218-220°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 1.00-1.05 and 3.92-3.98 (m, CH<sub>2</sub>CH<sub>3</sub>), 2.48-2.52 (m, 5-CH<sub>3</sub>), 6.85 (s, 7-CH), 7.62-7.66 and 8.20-8.23 (m, 4H, aromatic), 11.44 (s, 1H, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>) δ 13.96, 18.75, 58.23, 60.01, 96.91, 124.08, 128.99, 147.60, 147.79, 148.54, 164.49; MS (ES<sup>+</sup>) *m/z* 331(M + H); Anal. Calcd for C<sub>14</sub>H<sub>14</sub>N<sub>6</sub>O<sub>4</sub>: C, 50.91; H, 4.27; N, 25.44. Found: C, 50.94; H, 4.21; N, 25.48.

**Compound D5 (Entry 5, Table 3)**



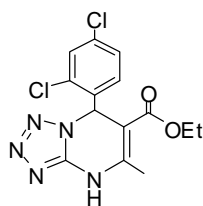
recrystallized from EtOH. Yield 1.23g (74%) of bright yellow flocs, 99% pure by LC-MS. Mp 239-241°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 0.89-0.93 and 3.86-3.95 (m, CH<sub>2</sub>CH<sub>3</sub>), 2.46-2.52 (m, 5-CH<sub>3</sub>), 7.28 (s, 7-CH), 7.47-7.99 (m, 4H, aromatic), 11.03 (d, NH, *J*=4.8Hz); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>) δ 13.81, 18.74, 53.81, 59.93, 96.85, 124.49, 129.99, 130.14, 134.21, 134.92, 148.22, 148.29, 148.56, 164.32; MS (ES<sup>+</sup>) *m/z* 331(M + H); Anal. Calcd for C<sub>14</sub>H<sub>14</sub>N<sub>6</sub>O<sub>4</sub>: C, 50.91; H, 4.27; N, 25.44. Found: C, 50.97; H, 4.23; N, 25.51.

**Compound D6 (Entry 6, Table 3)**



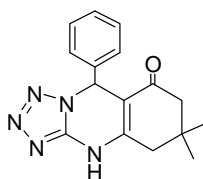
recrystallized from EtOH. Yield 0.97g (67%) of brown prisms, 98% pure by LC-MS. Mp 209-211°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 0.93-0.98 and 3.89-3.93 (m, CH<sub>2</sub>CH<sub>3</sub>), 2.46-2.50 (m, 5-CH<sub>3</sub>), 7.03(s, 7-CH), 7.32-7.48 (m, 4H, aromatic), 11.41 (s, 1H, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>) δ 13.82, 18.55, 56.23, 59.77, 96.66, 127.99, 129.85, 130.11, 130.41, 132.47, 138.16, 147.72, 148.48, 164.46; MS (ES<sup>+</sup>) *m/z* 320(M + H); Anal. Calcd for C<sub>16</sub>H<sub>12</sub>ClN<sub>5</sub>: C, 52.59; H, 4.41; N, 21.90. Found: C, 52.62; H, 4.45; N, 21.93.

**Compound D7 (Entry 7, Table 3)**



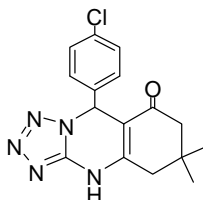
recrystallized from EtOH. Yield 1.03g (64%) of white prisms, 98% pure by LC-MS. Mp 256-258°C; <sup>1</sup>H NMR (300MHz, DMSO-*d*<sub>6</sub>) δ 0.97-1.02 and 3.92-3.96 (m, CH<sub>2</sub>CH<sub>3</sub>), 2.46-2.52 (m, 5-CH<sub>3</sub>), 7.02 (s, 7-CH), 7.43-7.44 and 7.67 (m, 3H, aromatic), 11.41 (s, 1H, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>) δ 13.90, 18.62, 55.79, 59.86, 96.25, 128.23, 129.31, 131.58, 133.46, 134.13, 137.31, 148.06, 148.45, 164.38; MS (ES<sup>+</sup>) *m/z* 354 (M + H); Anal. Calcd for C<sub>14</sub>H<sub>13</sub>Cl<sub>2</sub>N<sub>5</sub>O<sub>2</sub>: C, 47.47; H, 3.70; N, 19.77. Found: C, 47.41; H, 3.76; N, 19.72.

**Compound E1 (Entry 8, Table 3)**



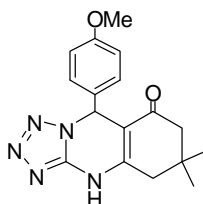
recrystallized from EtOH. Yield 1.23g (83%) of white floccs, 99% pure by LC-MS. Mp > 270°C; <sup>1</sup>H NMR (500MHz, DMSO-*d*<sub>6</sub>) δ 1.01 and 1.07 (s, 2CH<sub>3</sub>), 2.13-2.26 and 2.51-2.61 (m, 2CH<sub>2</sub>), 6.60 (s, 9-CH), 7.27-7.35 (m, 5H, aromatic), 11.61 (s, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>) δ 27.20, 28.48, 32.47, 50.04, 57.67, 105.87, 127.33, 128.50, 128.77, 140.66, 148.74, 150.76, 193.74; MS (ES<sup>+</sup>) *m/z* 296 (M + H); Anal. Calcd for C<sub>16</sub>H<sub>17</sub>N<sub>5</sub>O: C, 65.07; H, 5.80; N, 23.71. Found: C, 65.09; H, 5.76; N, 23.75.

**Compound E2 (Entry 9, Table 3)**



recrystallized from EtOH. Yield 1.52g (92%) of white floccs, 99% pure by LC-MS. Mp 254-256°C; <sup>1</sup>H NMR (300MHz, DMSO-*d*<sub>6</sub>) δ 0.97 and 1.03 (s, 2CH<sub>3</sub>), 2.14-2.18 and 2.47-2.49 (m, 2CH<sub>2</sub>), 6.60 (s, 9-CH), 7.29-7.39 (m, 4H, aromatic), 11.63 (s, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>) δ 27.25, 28.32, 32.44, 49.97, 57.03, 105.48, 128.74, 129.29, 133.14, 139.51, 148.58, 150.83, 193.17; MS (ES<sup>+</sup>) *m/z* 330 (M + H); Anal. Calcd for C<sub>16</sub>H<sub>16</sub>ClN<sub>5</sub>O: C, 58.27; H, 4.89; N, 21.24. Found: C, 58.21; H, 4.94; N, 21.29.

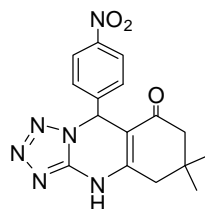
**Compound E3 (Entry 10, Table 3)**



recrystallized from EtOH. Yield 1.32g (81%) of white floccs, 99% pure by LC-MS. Mp 226-228°C; <sup>1</sup>H NMR (300MHz, DMSO-*d*<sub>6</sub>) δ 0.98 and 1.04 (s, 2CH<sub>3</sub>), 2.08-2.24 and 2.47-2.57 (m, 2CH<sub>2</sub>), 3.69 (s, OMe), 6.53 (s, 9-CH), 6.83-6.86 and 7.16-7.19 (m, 4H, aromatic), 11.53 (s, NH); <sup>13</sup>C

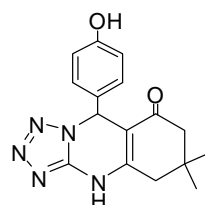
NMR (75MHz, DMSO-*d*<sub>6</sub>)  $\delta$  27.15, 28.47, 32.40, 50.03, 55.25, 57.08, 106.00, 114.06, 128.53, 132.87, 148.57, 150.38, 159.29, 193.11; MS (ES<sup>+</sup>) *m/z* 326 (M + H); Anal. Calcd for C<sub>17</sub>H<sub>19</sub>N<sub>5</sub>O<sub>2</sub>: C, 62.75; H, 5.89; N, 21.52. Found: C, 62.70; H, 5.83; N, 21.58.

**Compound E4 (Entry 11, Table 3)**



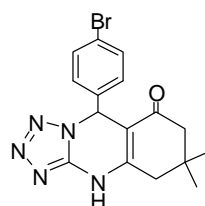
recrystallized from EtOH. 70% pure of reaction mixture by LC-MS, white floccs. Mp 220-225°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>)  $\delta$  0.97 and 1.03 (s, 2CH<sub>3</sub>), 2.13-2.18 and 2.47-2.58 (m, 2CH<sub>2</sub>), 6.75 (s, 9-CH), 7.56-7.60 and 8.15-8.18 (m, 4H, aromatic); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>)  $\delta$  27.31, 28.24, 32.51, 49.90, 59.11, 105.10, 123.95, 129.00, 147.21, 147.48, 148.60, 151.28, 193.25; MS (ES<sup>+</sup>) *m/z* 341 (M + H); Anal. Calcd for C<sub>16</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>: C, 56.47; H, 4.74; N, 24.69. Found: C, 56.70; H, 4.83; N, 24.78.

**Compound E5 (Entry 12, Table 3)**



recrystallized from EtOH. Yield 1.21g (76%) of white prisms, 98% pure by LC-MS, Mp > 270°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>)  $\delta$  0.98 and 1.03 (s, 2CH<sub>3</sub>), 2.08-2.24 and 2.48-2.56 (m, 2CH<sub>2</sub>), 6.46 (s, 9-CH), 6.65-6.67 and 7.04-7.07 (m, 4H, aromatic), 9.49 (s, OH), 11.49 (s, 1H, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>)  $\delta$  27.18, 28.55, 32.43, 50.10, 57.18, 106.18, 115.42, 148.61, 150.32, 157.61, 193.17; MS (ES<sup>+</sup>) *m/z* 312 (M + H); Anal. Calcd for C<sub>16</sub>H<sub>17</sub>N<sub>5</sub>O<sub>2</sub>: C, 61.72; H, 5.50; N, 22.49. Found: C, 61.70; H, 5.59; N, 22.51.

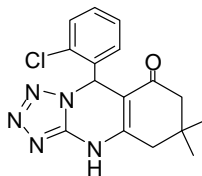
**Compound E6 (Entry 13, Table 3)**



recrystallized from EtOH. Yield 1.67g (89%) of white prisms, 99% pure by LC-MS. Mp 246-249°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>)  $\delta$  0.96 and 1.02 (s, 2CH<sub>3</sub>), 2.13-2.17 and 2.46-2.56 (m, 2CH<sub>2</sub>), 6.57 (s, 9-CH), 7.22-7.25 and 7.49-7.51 (m, 4H, aromatic), 11.63 (s, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>)  $\delta$  27.31, 28.36, 32.49, 50.01, 57.16, 105.48, 121.76, 129.66, 131.71, 139.97, 148.60, 150.88, 193.22; MS (ES<sup>+</sup>) *m/z* 374 (M + H); Anal. Calcd for C<sub>16</sub>H<sub>16</sub>BrN<sub>5</sub>O: C, 51.35; H, 4.31; N, 21.35. Found: C, 51.29; H, 4.42; N, 21.29.

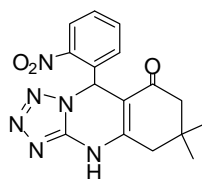
**Compound E7 (Entry 14, Table 3)**





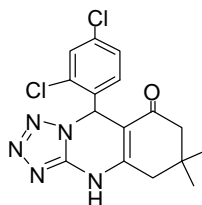
recrystallized from EtOH. Yield 1.52g (92%) of white floccs, 99% pure by LC-MS. Mp > 270 °C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 1.00 and 1.04 (s, 2CH<sub>3</sub>), 2.06-2.23 and 2.47-2.56 (m, 2CH<sub>2</sub>), 6.88 (s, 9-CH), 7.28-7.42 (m, 4H, aromatic), 11.67 (s, NH); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>) δ 27.22, 28.46, 32.41, 50.03, 56.04, 104.83, 127.64, 130.07, 130.29, 131.01, 132.40, 137.15, 148.78, 151.34, 193.11; MS (ES<sup>+</sup>) *m/z* 330 (M + H); Anal. Calcd for C<sub>16</sub>H<sub>16</sub>ClN<sub>5</sub>O: C, 58.27; H, 4.89; N, 21.24. Found: C, 58.26; H, 4.87; N, 21.28.

**Compound E8 (Entry 15, Table 3)**



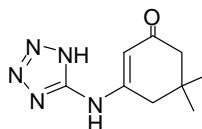
recrystallized from EtOH. Yield 1.07g (63%) of green prisms, 92% pure by LC-MS. Mp 261-263°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 0.92 and 1.01 (s, 2CH<sub>3</sub>), 2.02-2.17 and 2.47-2.53 (m, 2CH<sub>2</sub>), 7.18 (s, 9-CH), 7.31-7.91 (m, 4H, aromatic); <sup>13</sup>C NMR (75MHz, DMSO-*d*<sub>6</sub>) δ 27.33, 28.16, 32.52, 49.70, 53.08, 105.41, 124.44, 129.82, 130.00, 133.84, 134.15, 148.55, 148.86, 151.27, 193.37; MS (ES<sup>+</sup>) *m/z* 341 (M + H); Anal. Calcd for C<sub>16</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>: C, 56.47; H, 4.74; N, 24.69. Found: C, 56.48; H, 4.69; N, 24.75.

**Compound E9 (Entry 16, Table 3)**



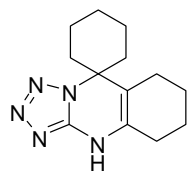
recrystallized from EtOH. Yield 1.58g (92%) of white floccs, 92% pure by LC-MS. Mp >270°C; <sup>1</sup>H NMR(300MHz, DMSO-*d*<sub>6</sub>) δ 1.01 and 1.06 (s, 2CH<sub>3</sub>), 2.10-2.23 and 2.50-2.58 (m, 2CH<sub>2</sub>), 6.89 (s, 9-CH), 7.41-7.61 (m, 4H, aromatic), 11.74 (s, NH); MS (ES<sup>+</sup>) *m/z* 364 (M + H); Anal. Calcd for C<sub>16</sub>H<sub>15</sub>Cl<sub>2</sub>N<sub>5</sub>O: C, 52.76; H, 4.15; N, 19.23. Found: C, 52.71; H, 4.10; N, 19.24.

**Compound E10 (Entry 17, Table 4)**



recrystallized from EtOH. White floccs, 99% pure by LC-MS. Mp 256-258°C; <sup>1</sup>H NMR(400MHz, DMSO-*d*<sub>6</sub>) δ 0.99 (s, 2CH<sub>3</sub>), 2.08 and 2.42-2.49 (m, 2CH<sub>2</sub>), 6.28 (s, 2-CH), 10.12 (s, NH); MS (ES<sup>+</sup>) *m/z* 208 (M + H); Anal. Calcd for C<sub>9</sub>H<sub>13</sub>N<sub>5</sub>: C, 52.16; H, 6.32; N, 33.79. Found: C, 52.15; H, 6.35; N, 33.73.

**Compound F**



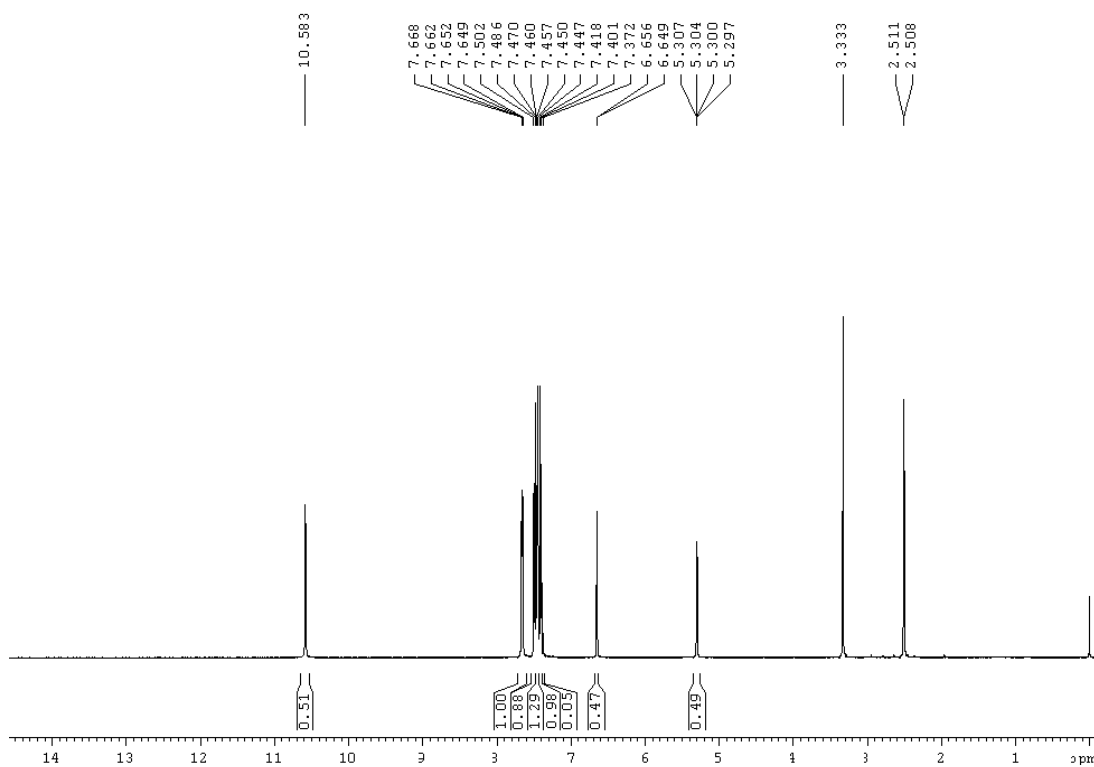
recrystallized from EtOH. 76% pure of reaction mixture by LC-MS. Mp 226-230°C ([8], 224-226°C);  $^1\text{H}$  NMR(300MHz, DMSO-*d*6)  $\delta$  1.23 and 2.12 (m, 18H), 9.60 (s, NH); MS ( $\text{ES}^+$ )  $m/z$  246 (M + H); Anal. Calcd for  $\text{C}_{13}\text{H}_{19}\text{N}_5$ : C, 63.65; H, 7.81; N, 28.55. Found: C, 63.61; H, 7.87; N, 28.51.

# Copies of $^1\text{H}$ NMR, $^{13}\text{C}$ NMR Spectra

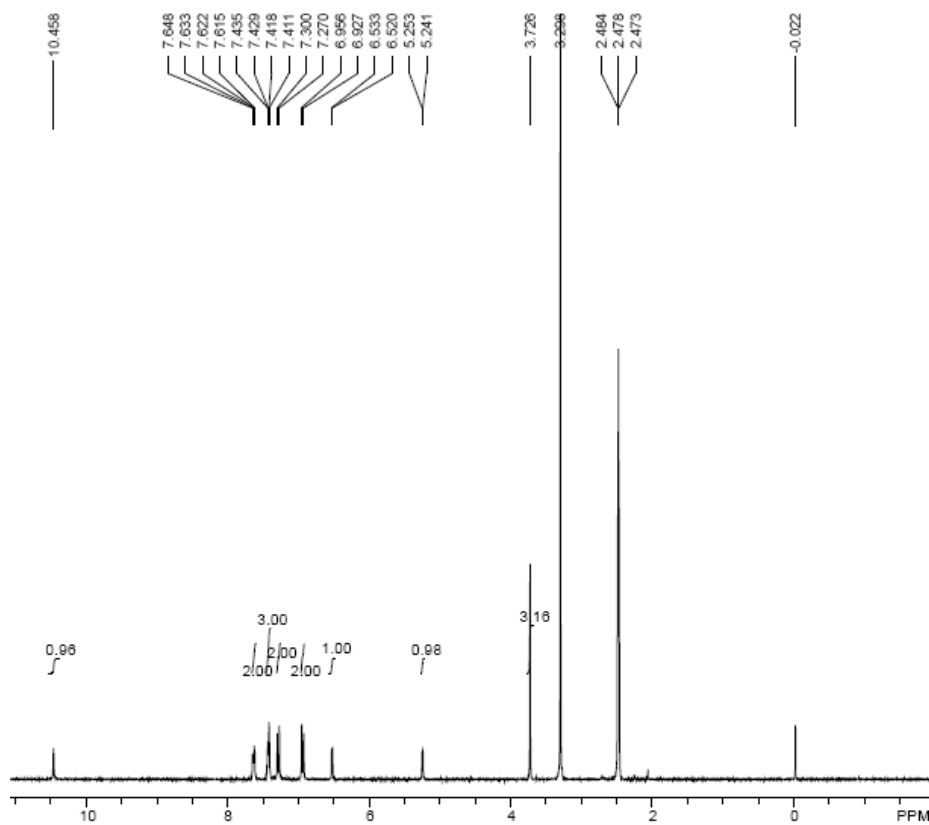


$^1\text{H}$  NMR Spectrum (300 MHz, DMSO- $d_6$ ) of Compound C1

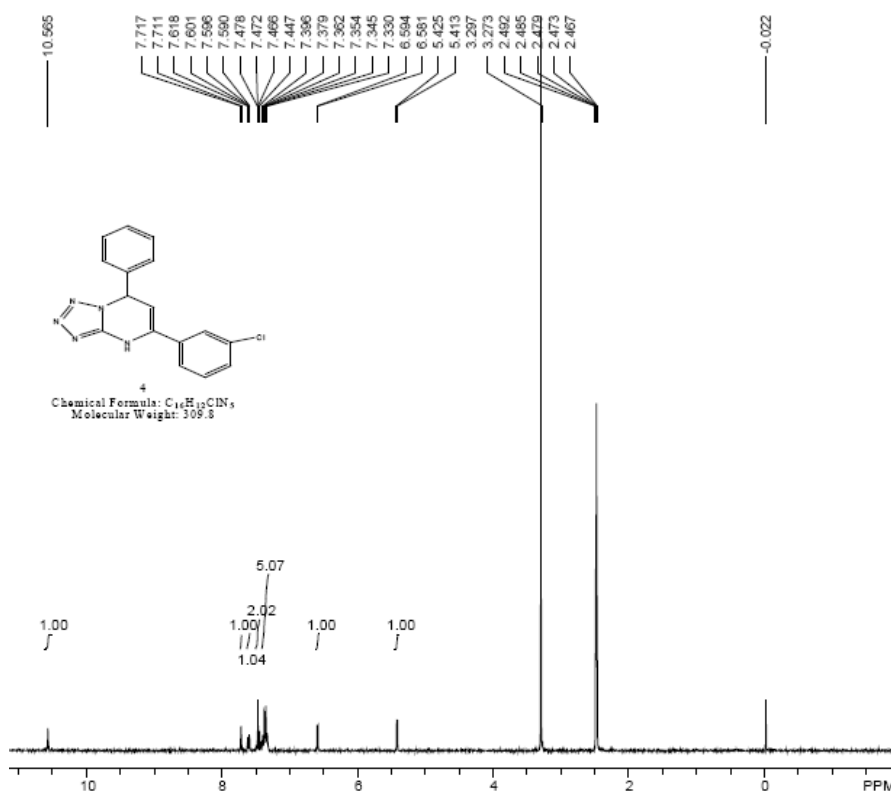
DMSO  $^1\text{H}$  Bruker DRX 500



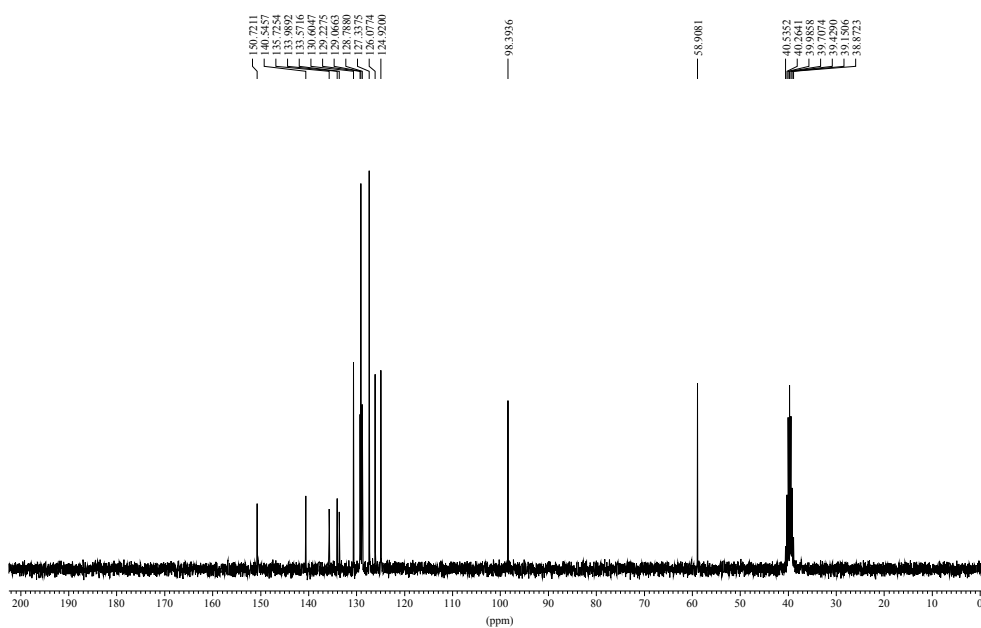
$^1\text{H}$  NMR Spectrum (500 MHz, DMSO- $d_6$ ) of Compound C2



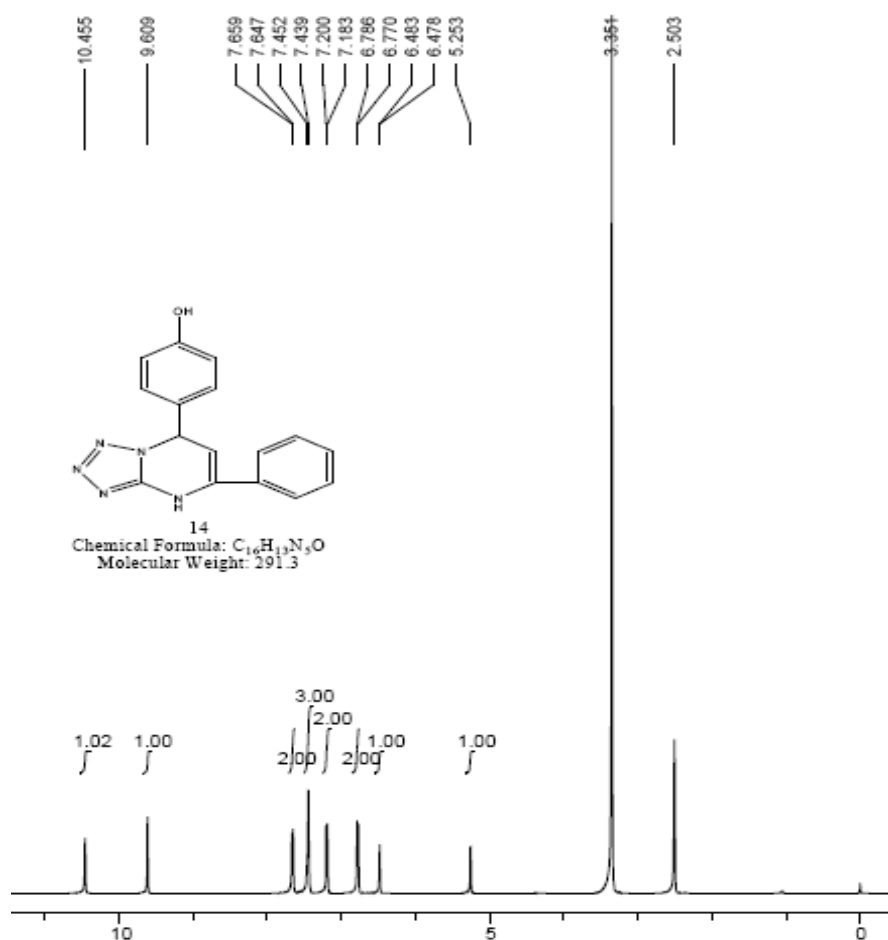
**<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound C3**



**<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound C4**

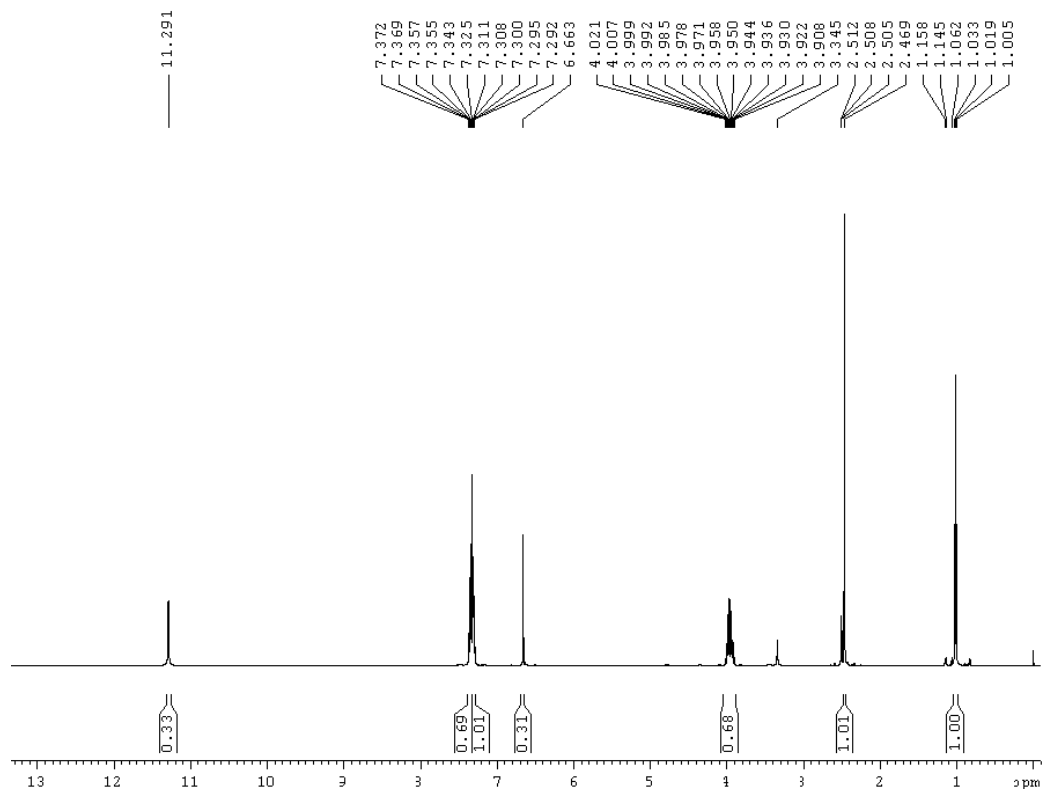


<sup>13</sup>C NMR Spectrum (75 MHz, DMSO-*d*<sub>6</sub>) of Compound C4



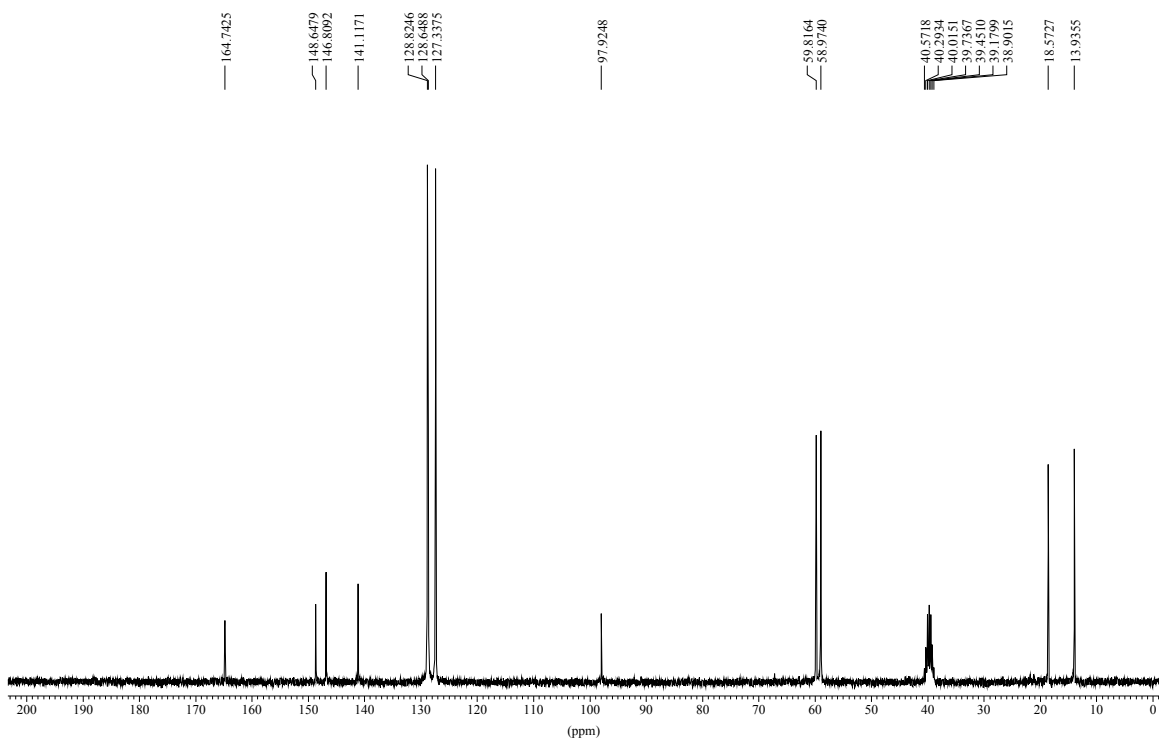
<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound C5

DMSO 1H Bruker DRX 500

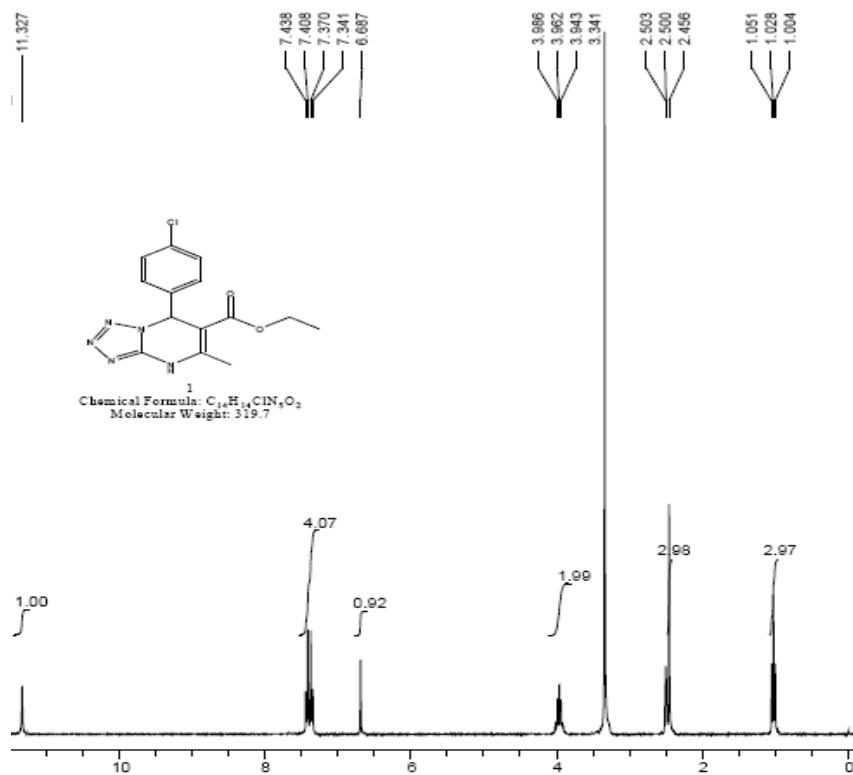


<sup>1</sup>H NMR Spectrum (500 MHz, DMSO-*d*<sub>6</sub>) of Compound D1

5# 13C-NMR DMSO-D6 303K AV-300

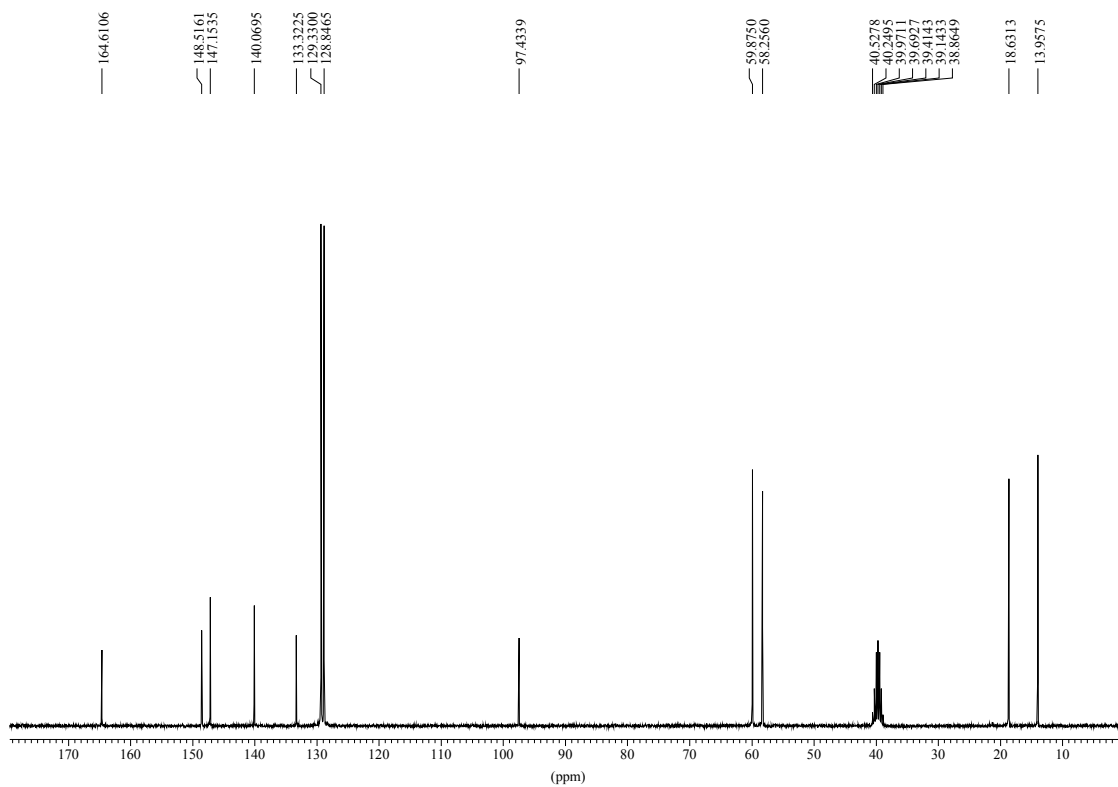


<sup>13</sup>C NMR Spectrum (75 MHz, DMSO-*d*<sub>6</sub>) of Compound D1

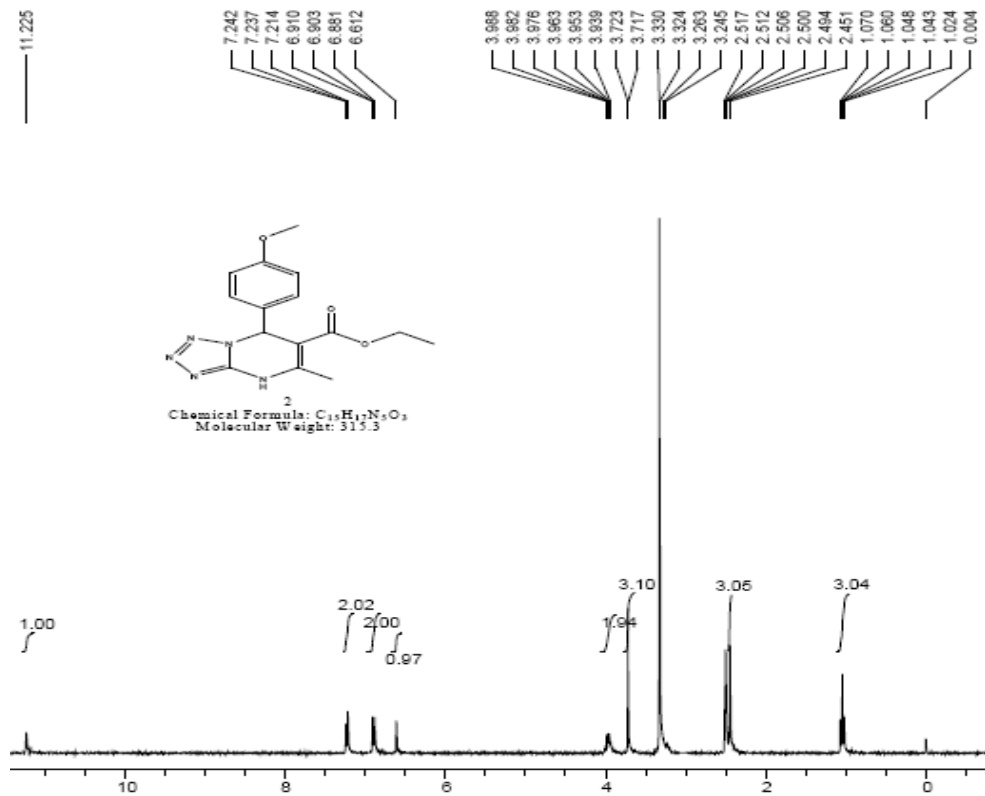


$^1H$  NMR Spectrum (300 MHz, DMSO- $d_6$ ) of Compound D2

1# 1H-NMR DMSO-D6 303K AV-300

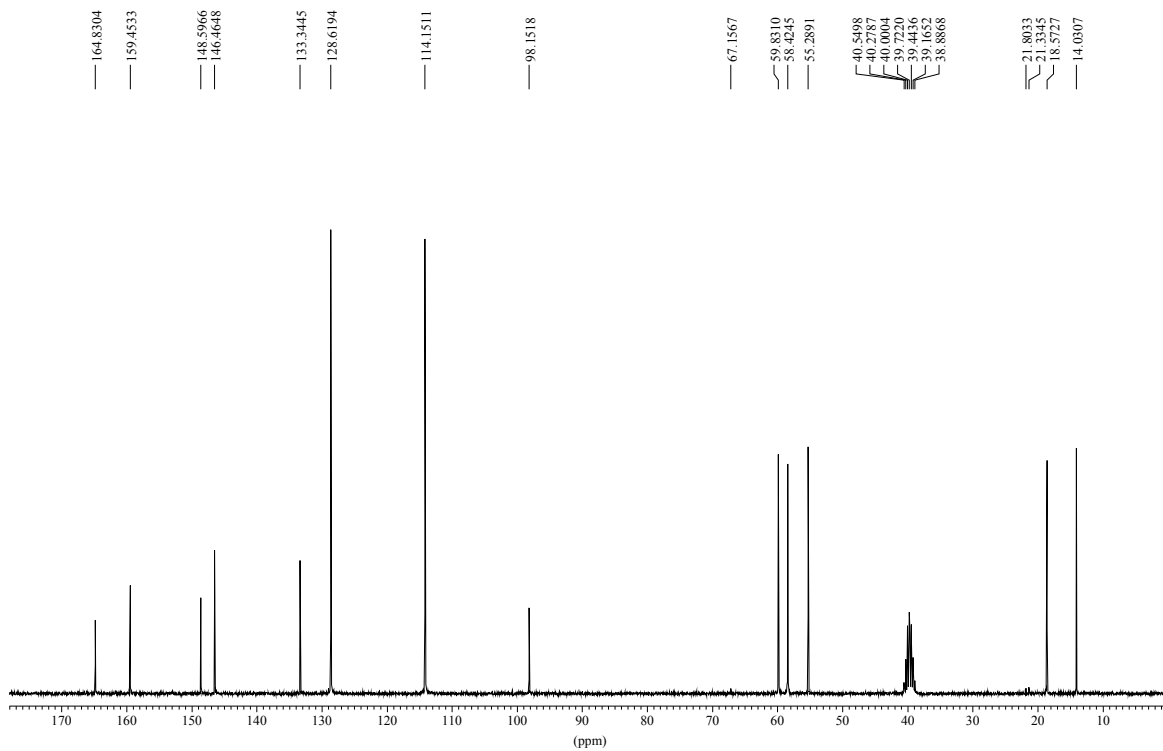


$^{13}C$  NMR Spectrum (75 MHz, DMSO- $d_6$ ) of Compound D2



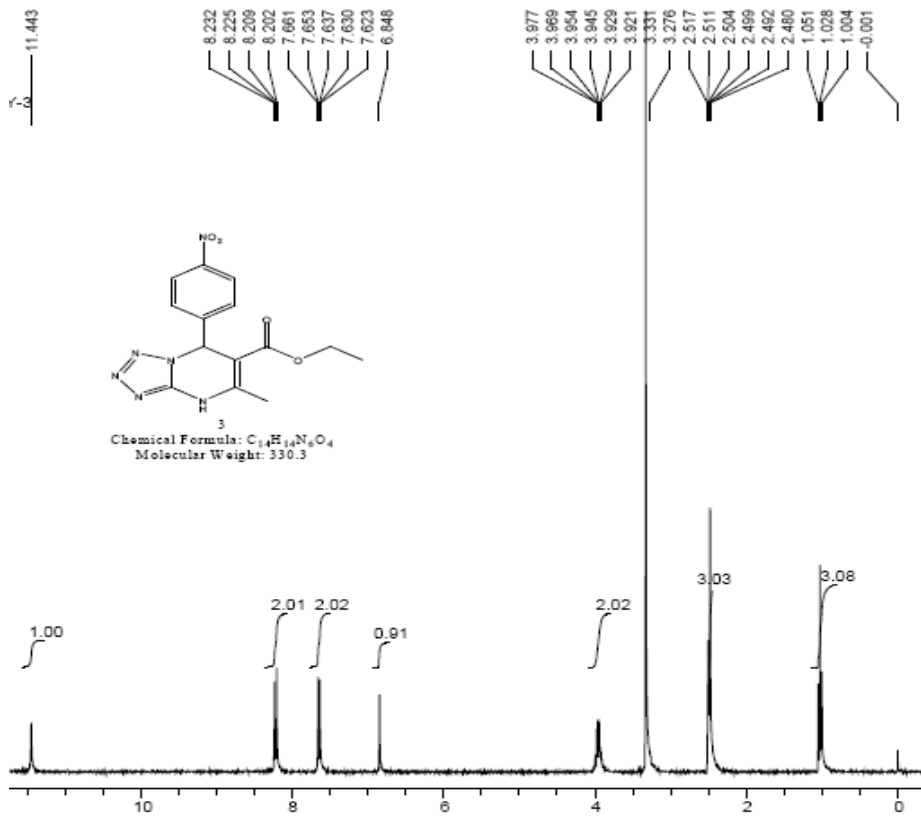
**$^1H$  NMR Spectrum (300 MHz, DMSO- $d_6$ ) of Compound D3**

2# 1H-NMR DMSO-D6 300 AV-300



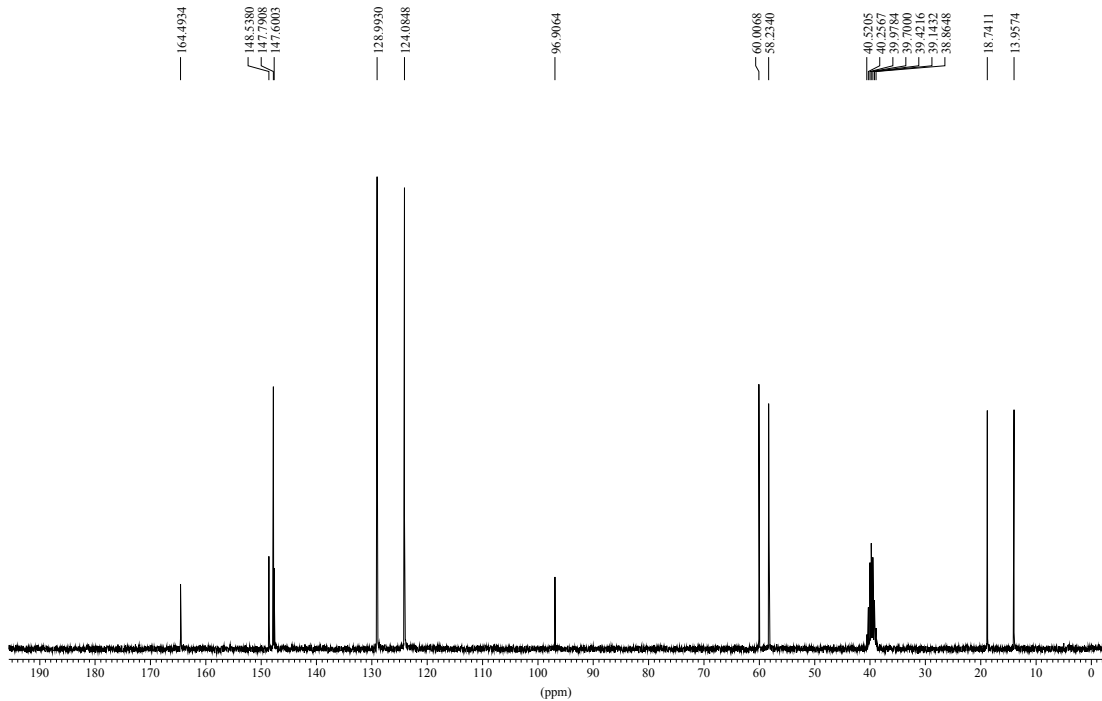
**$^{13}C$  NMR Spectrum (75 MHz, DMSO- $d_6$ ) of Compound D3**



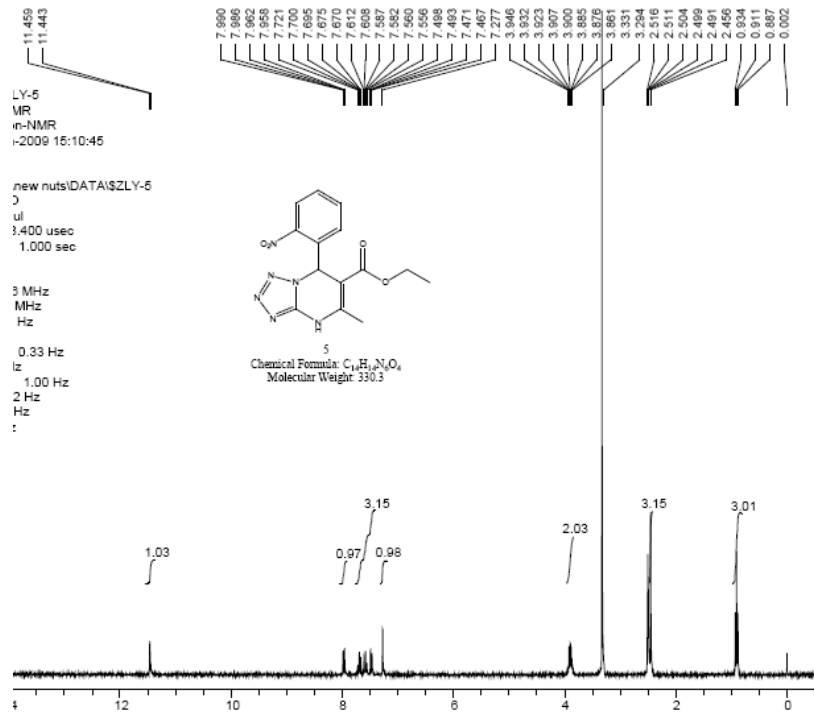


**$^1\text{H}$  NMR Spectrum (300 MHz, DMSO-*d*6) of Compound D4**

3# 13C-NMR DMSO-D6 300 AV-300

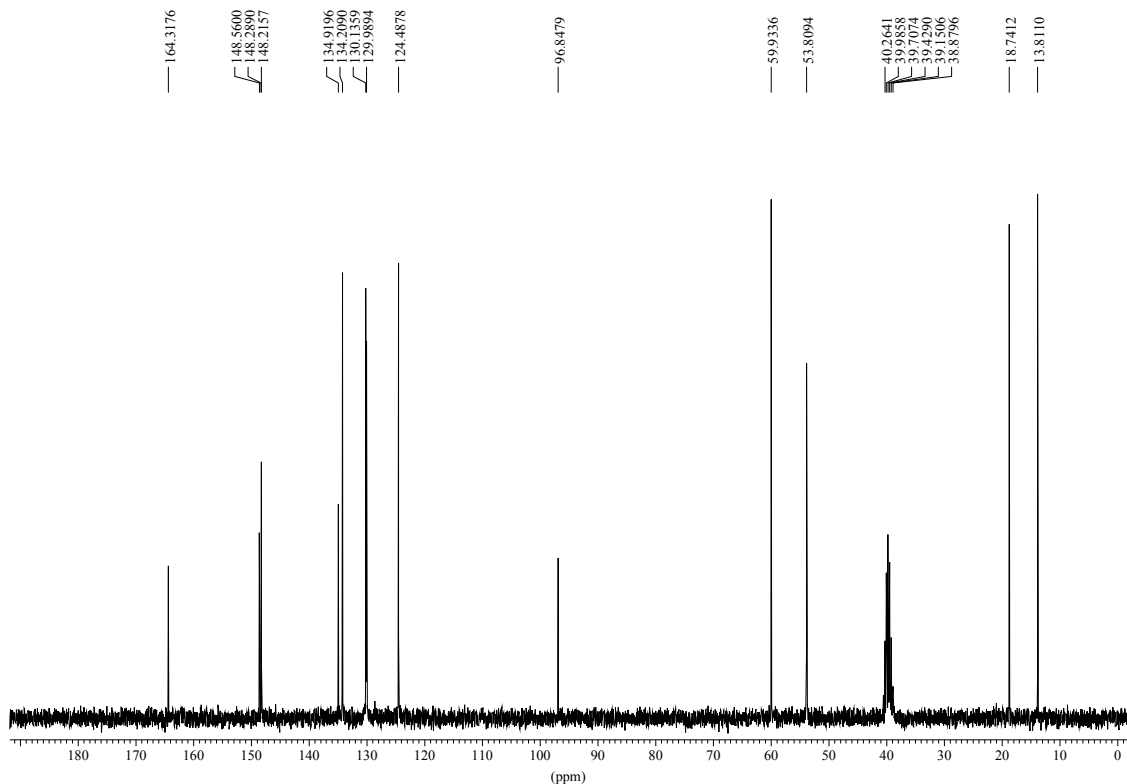


**$^{13}\text{C}$  NMR Spectrum (75 MHz, DMSO-*d*6) of Compound D4**

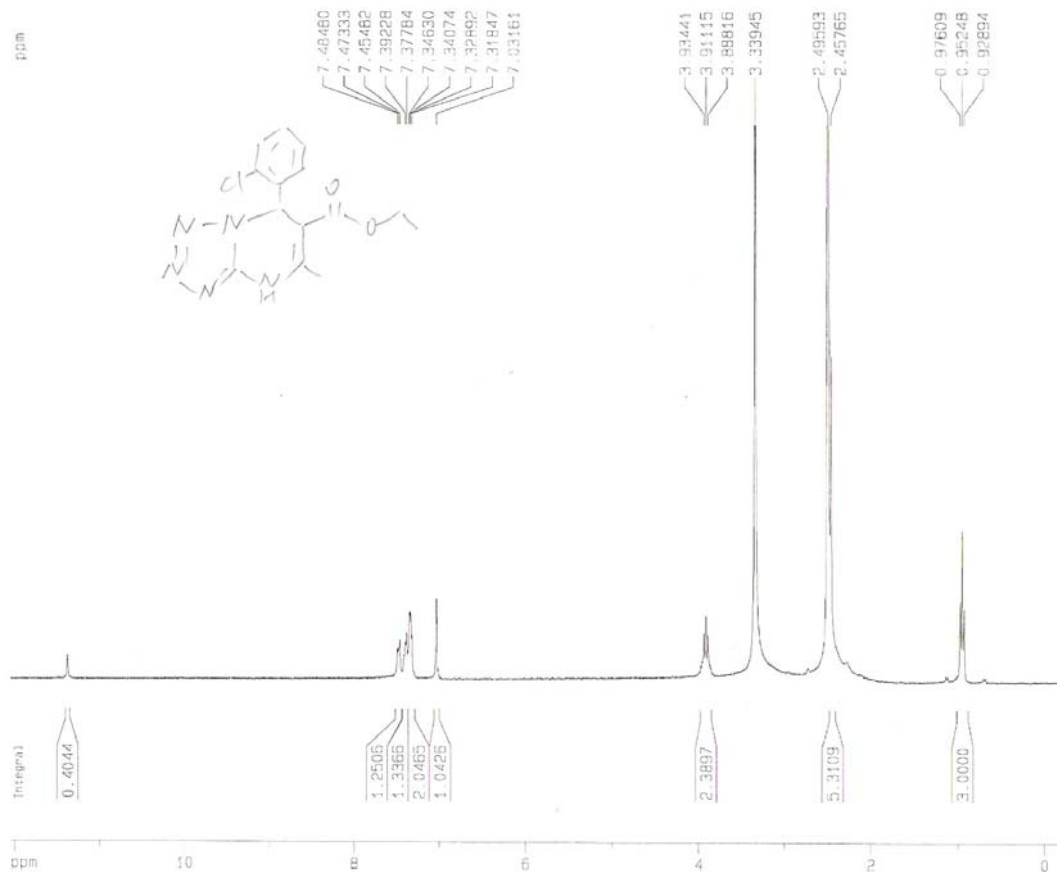


**$^1\text{H}$  NMR Spectrum (300 MHz,  $\text{DMSO-}d_6$ ) of Compound D5**

5# 13C-NMR DMSO-D6 300 AV-300

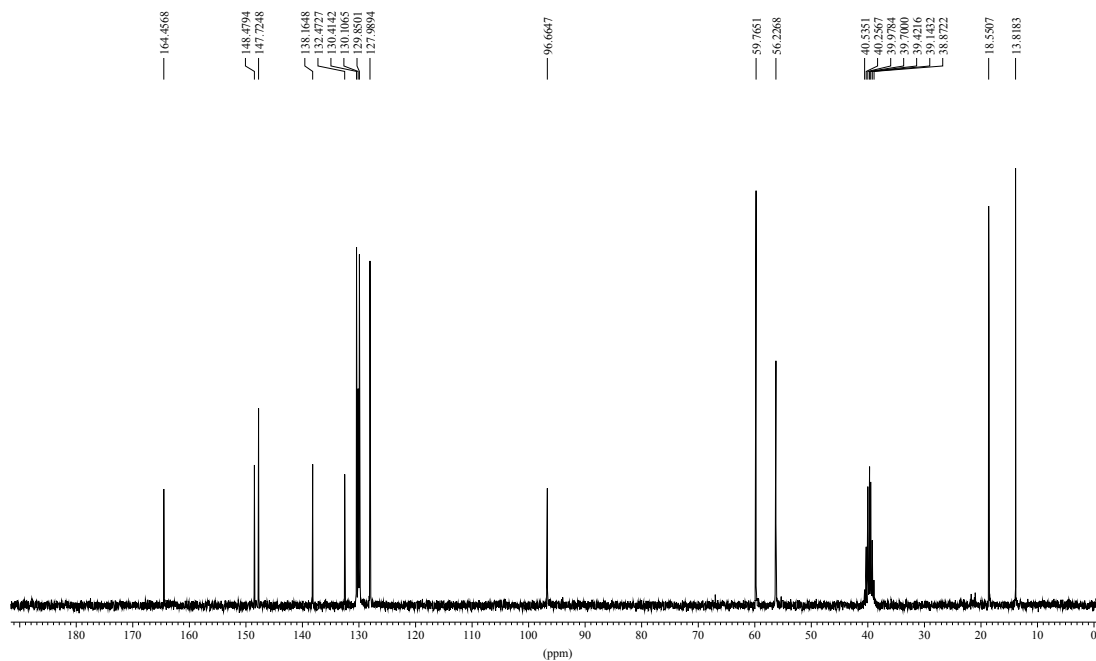


**$^{13}\text{C}$  NMR Spectrum (75 MHz,  $\text{DMSO-}d_6$ ) of Compound D5**

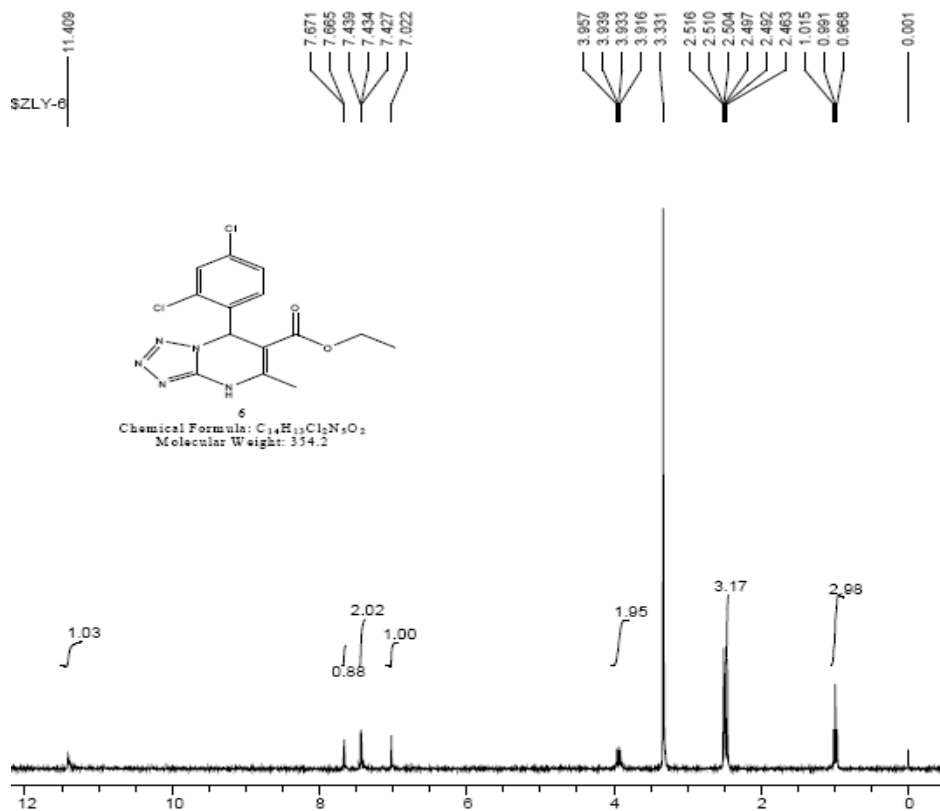


**<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound D6**

4# 13C-NMR DMSO-D6 300 AV-300

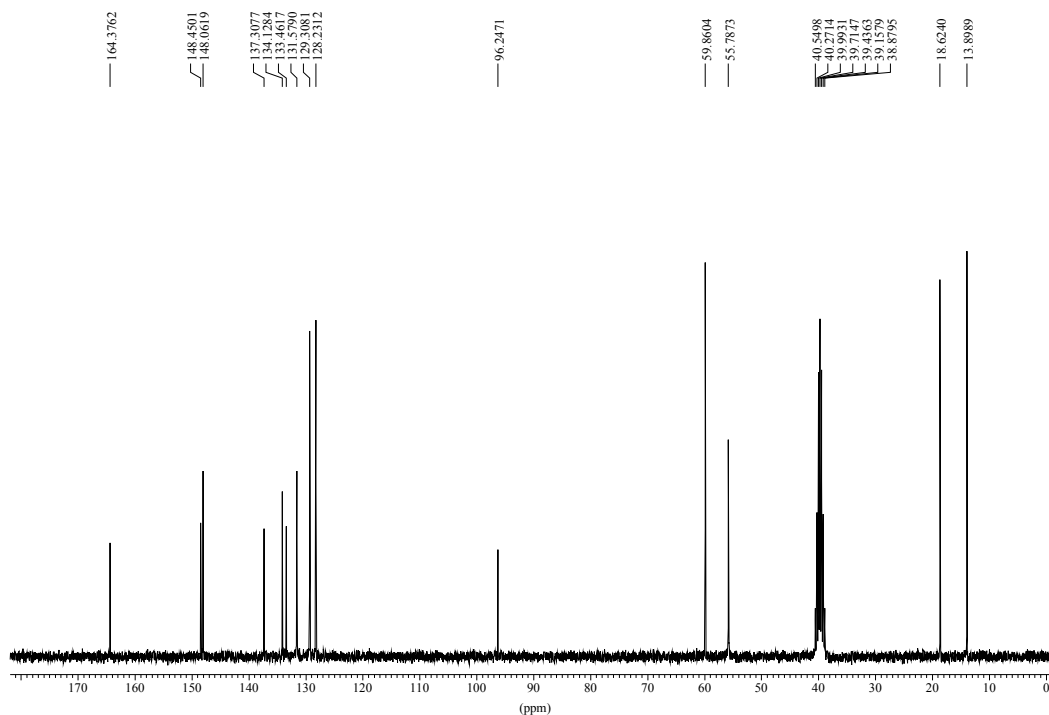


**<sup>13</sup>C NMR Spectrum (75 MHz, DMSO-*d*<sub>6</sub>) of Compound D6**



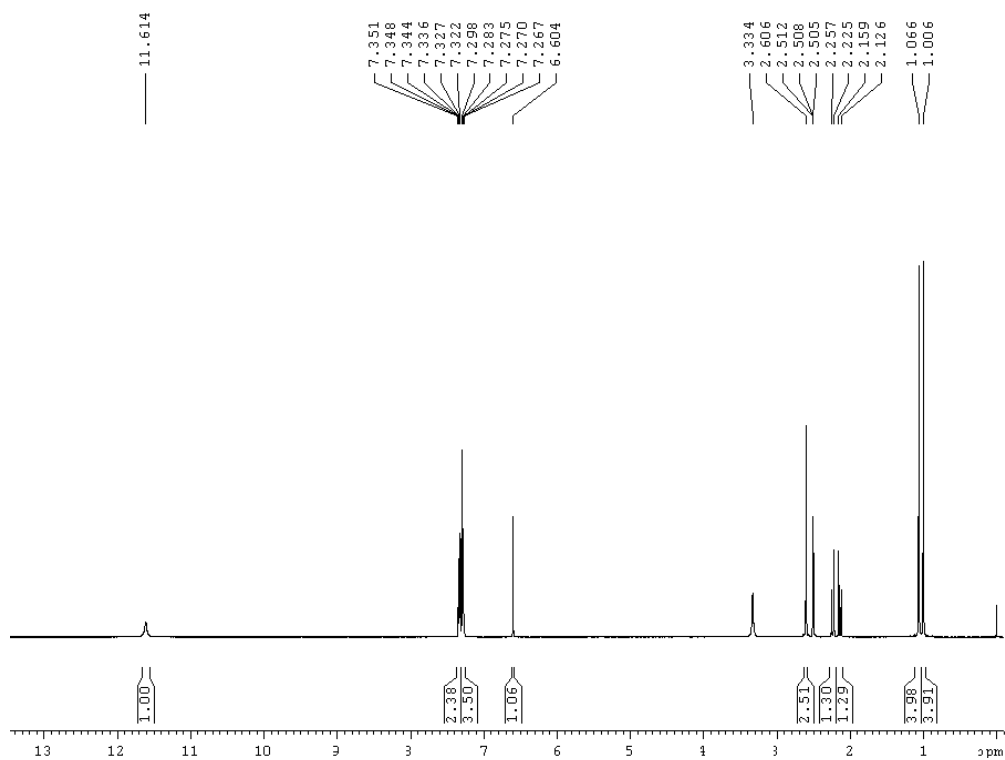
**$^1\text{H}$  NMR Spectrum (300 MHz, DMSO- $d_6$ ) of Compound D7**

6# 13C-NMR DMSO-D6 300 AV-300



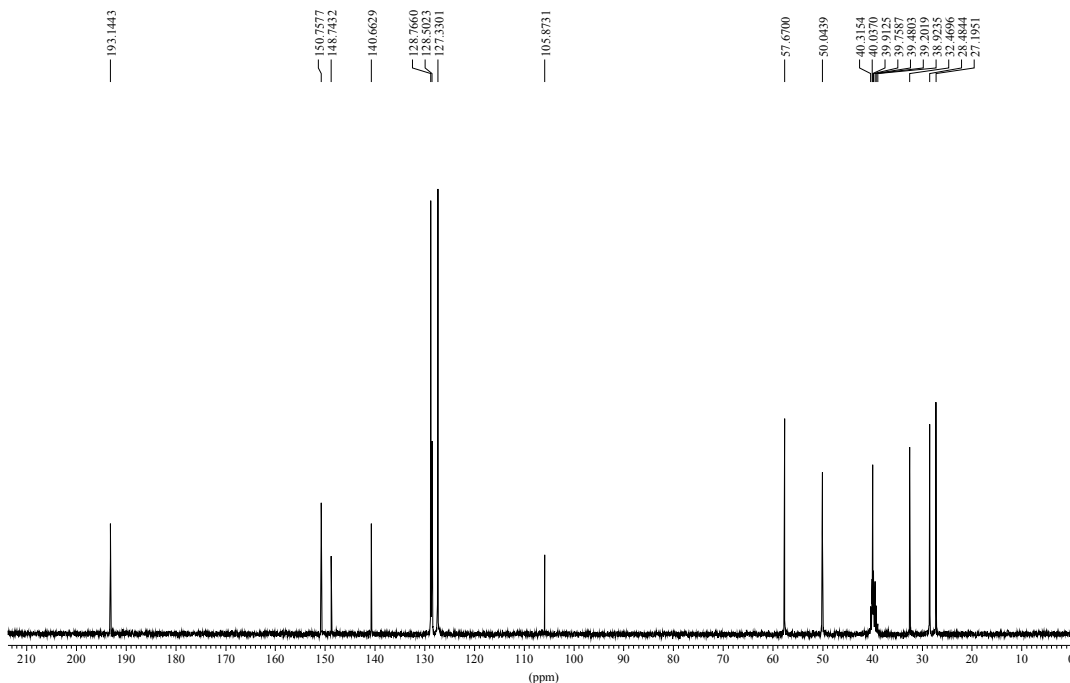
**$^{13}\text{C}$  NMR Spectrum (75 MHz, DMSO- $d_6$ ) of Compound D7**

DMSO 1H Bruker DRX 500

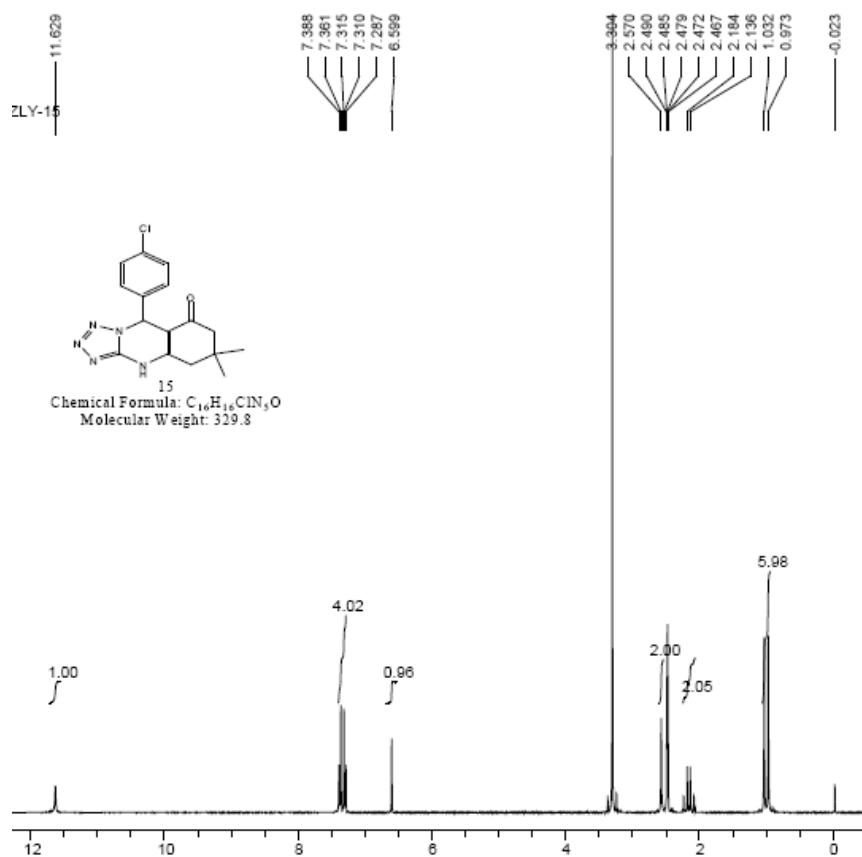


**<sup>1</sup>H NMR Spectrum (500 MHz, DMSO-*d*<sub>6</sub>) of Compound E1**

6# 13C-NMR DMSO-*d*<sub>6</sub> 303K AV-300

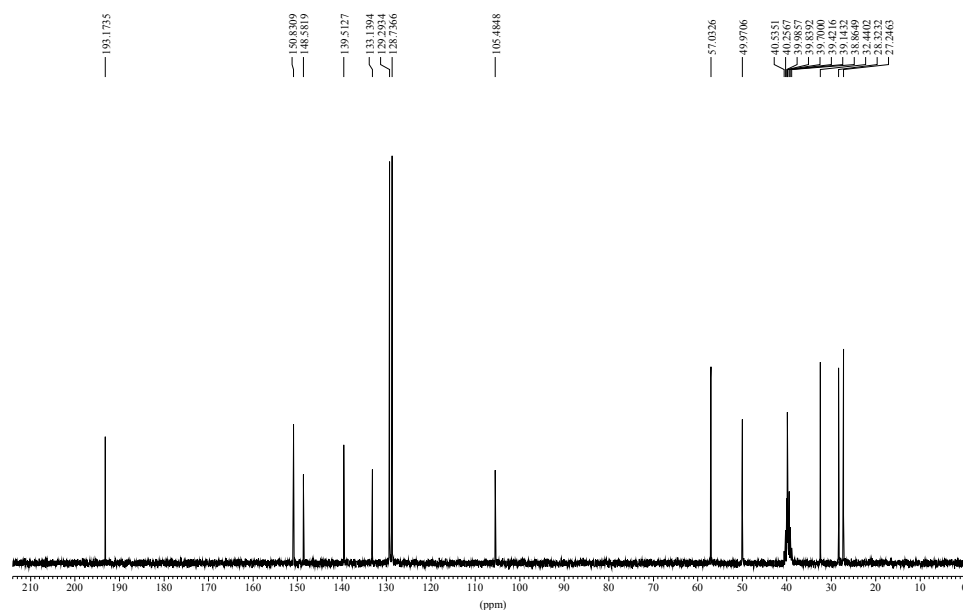


**<sup>13</sup>C NMR Spectrum (75 MHz, DMSO-*d*<sub>6</sub>) of Compound E1**

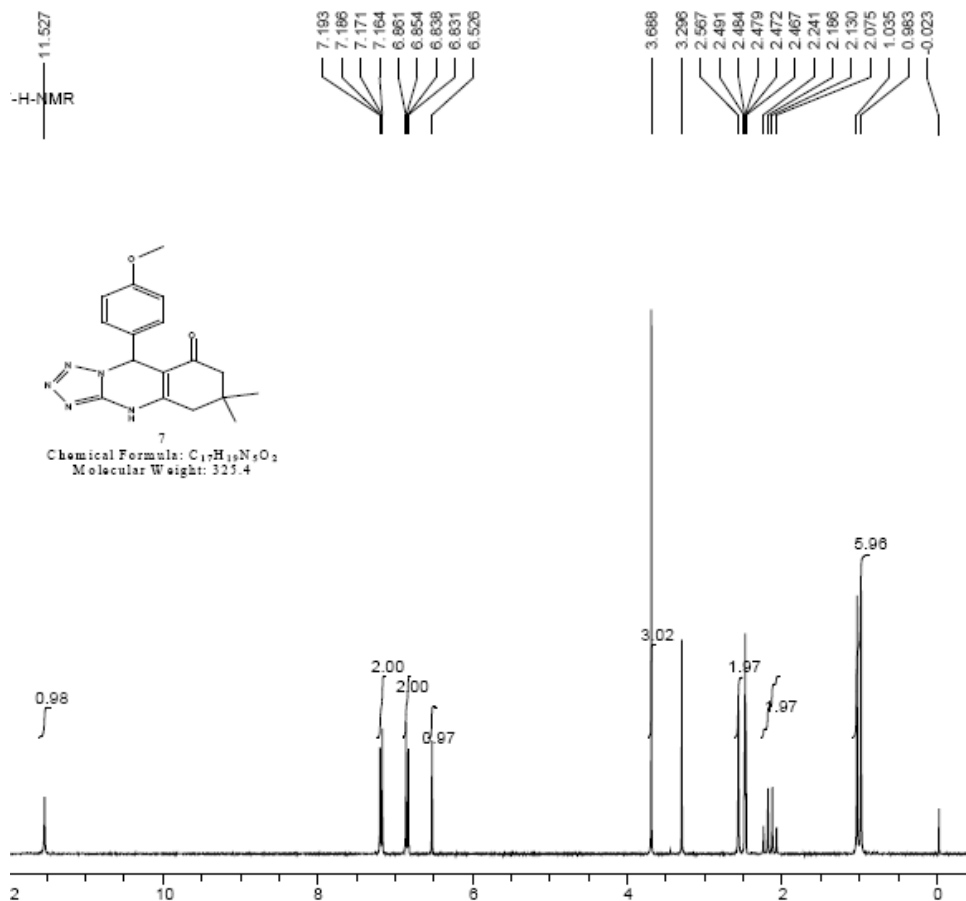


**<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound E2**

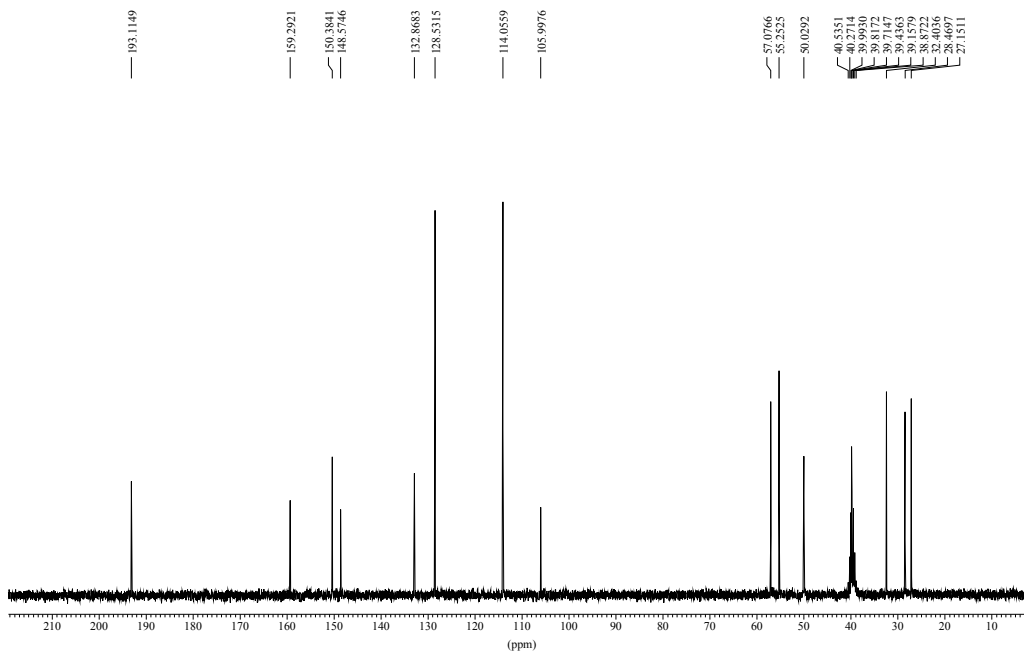
15# 13C-NMR DMSO-D6 303K AV-300



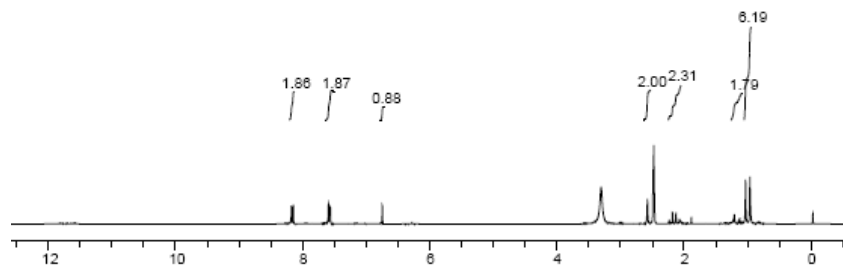
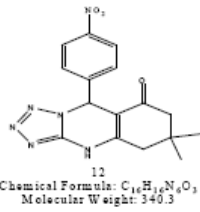
**<sup>13</sup>C NMR Spectrum (75 MHz, DMSO-*d*<sub>6</sub>) of Compound E2**



7# 13C-NMR DMSO-D6 303K AV-300

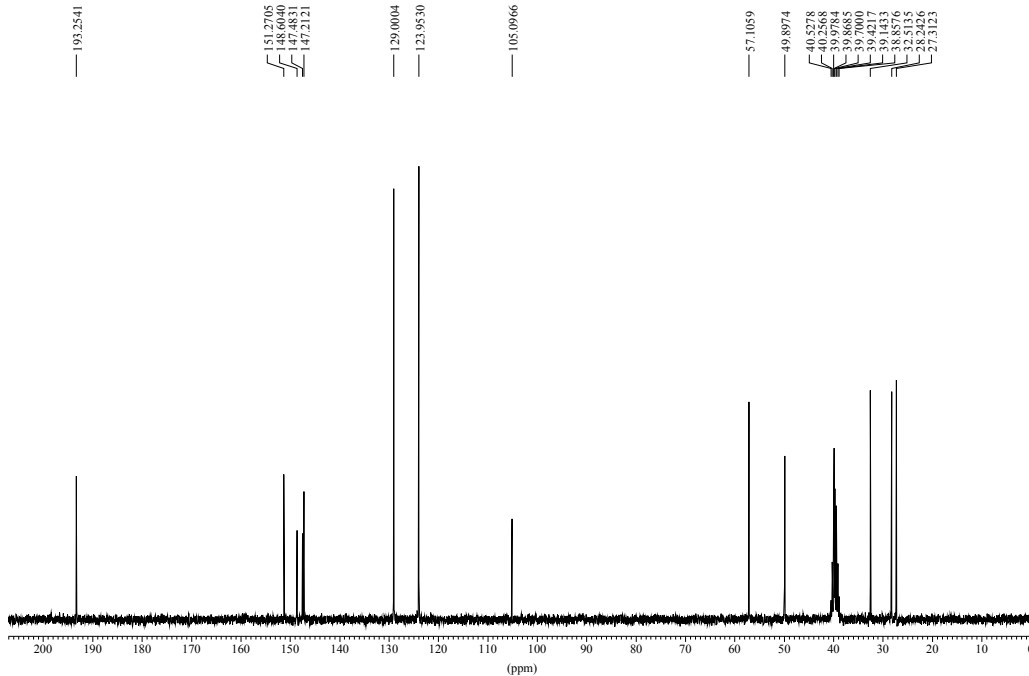


<sup>1</sup>H-NMR  
MSZLY-12



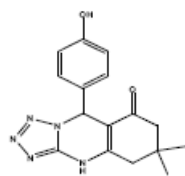
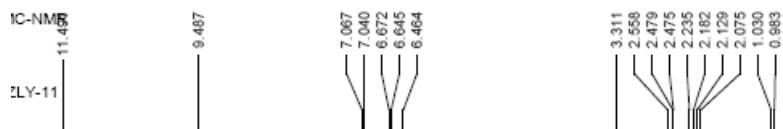
<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-d<sub>6</sub>) of Compound E4

7# <sup>13</sup>C-NMR DMSO-D6 300 AV-300

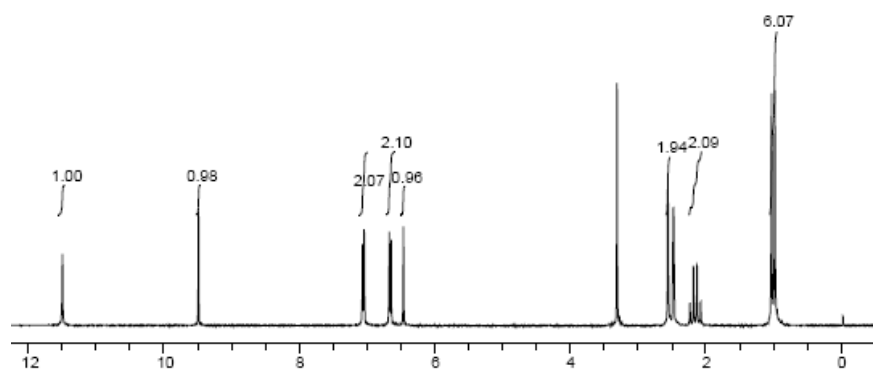


<sup>13</sup>C NMR Spectrum (75 MHz, DMSO-d<sub>6</sub>) of Compound E4



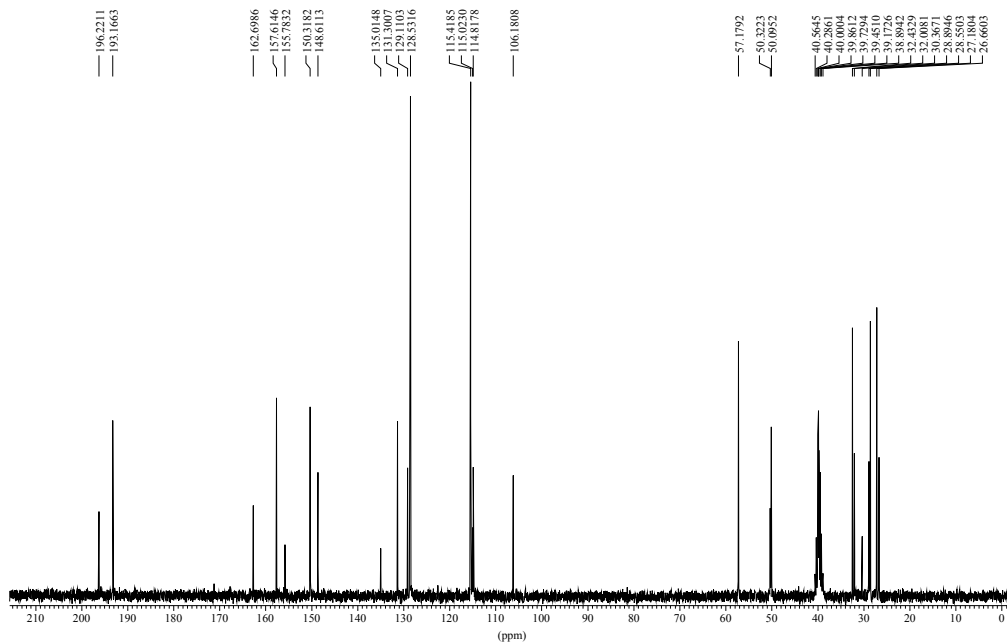


11  
 Chemical Formula:  $C_{18}H_{19}N_4O_2$   
 Molecular Weight: 311.3

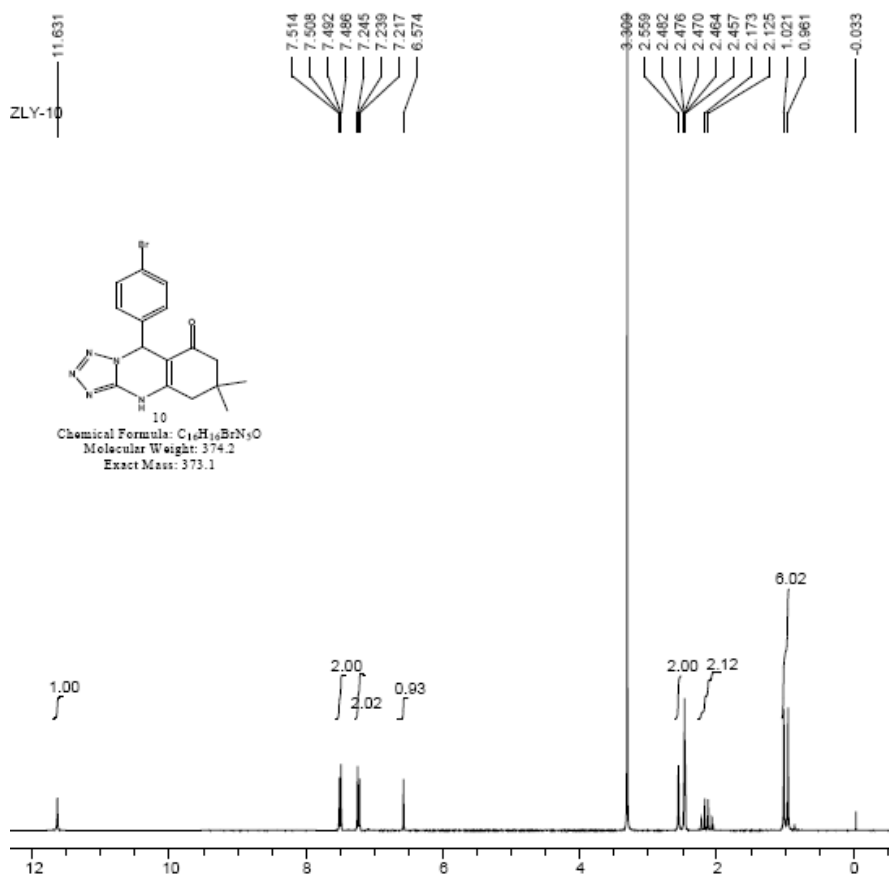


<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound E5

11# 13C-NMR DMSO-D6 303K AV-300

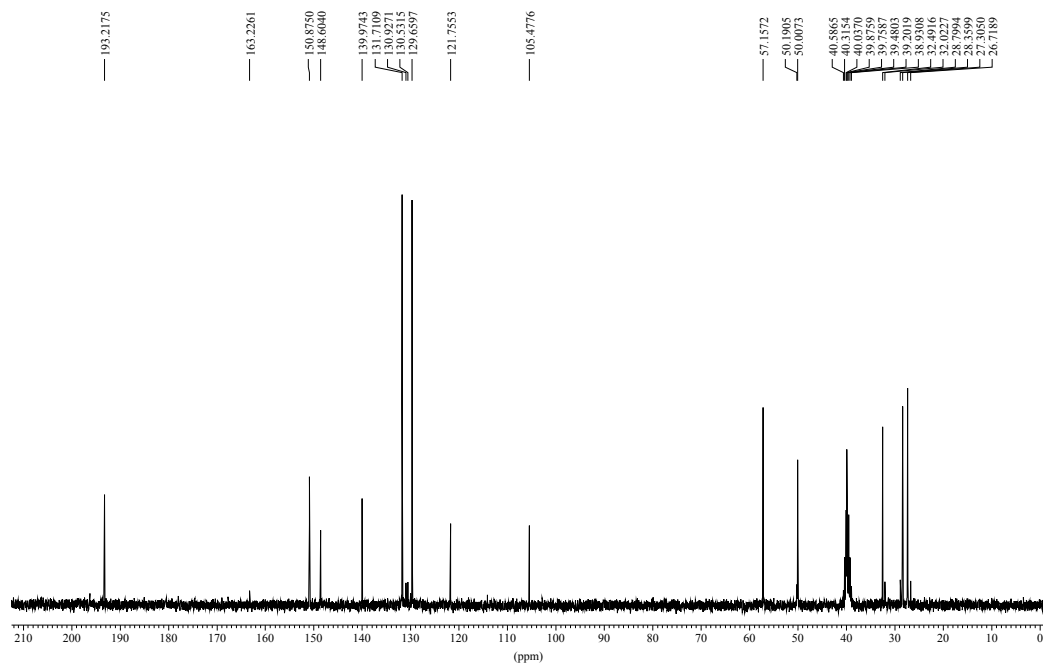


<sup>13</sup>C NMR Spectrum (75 MHz, DMSO-*d*<sub>6</sub>) of Compound E5

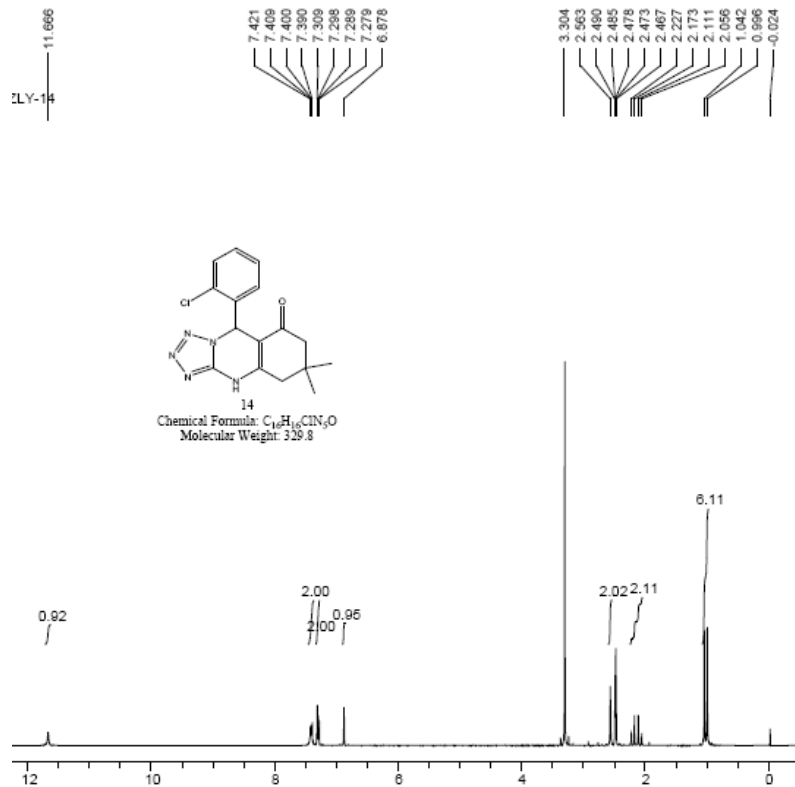


**$^1H$  NMR Spectrum (300 MHz, DMSO- $d_6$ ) of Compound E6**

10# 13C-NMR DMSO-D6 303K AV-300

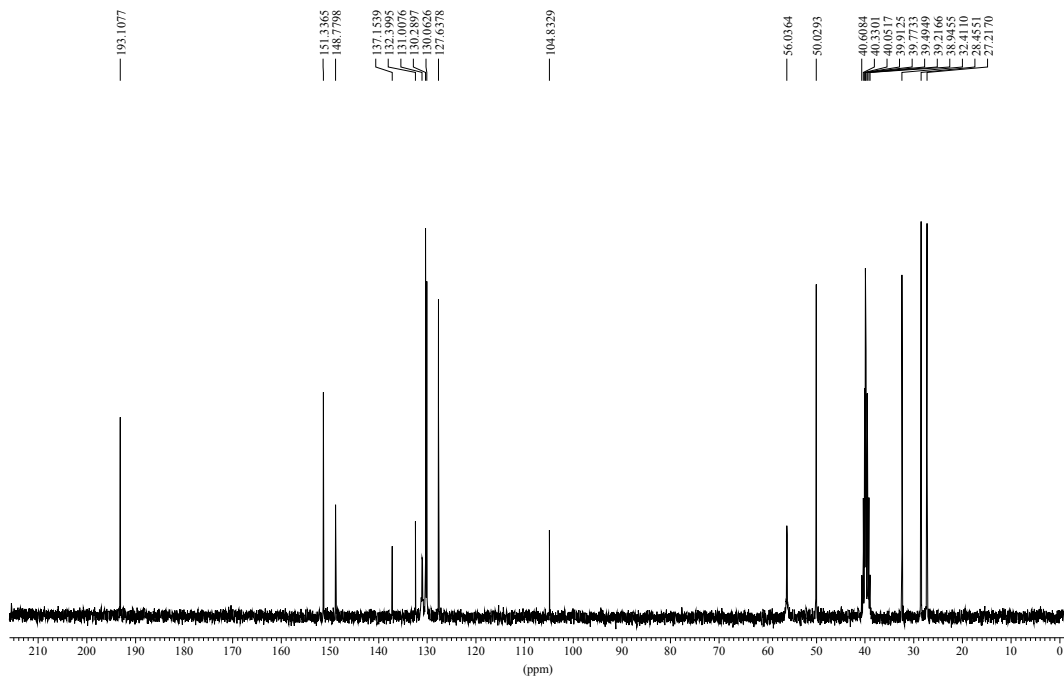


**$^{13}C$  NMR Spectrum (75 MHz, DMSO- $d_6$ ) of Compound E6**

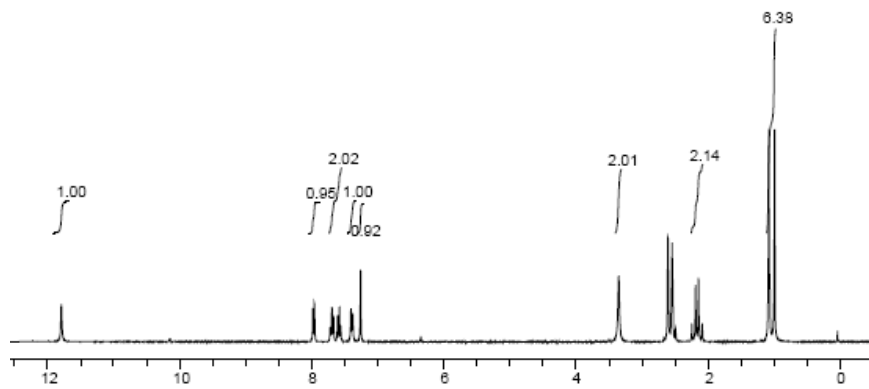
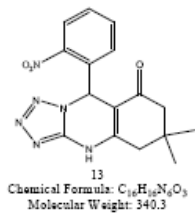
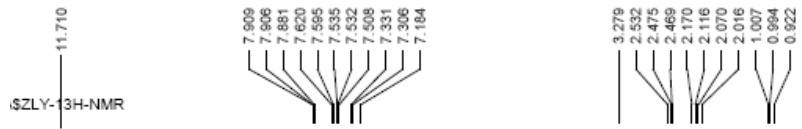


**<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound E7**

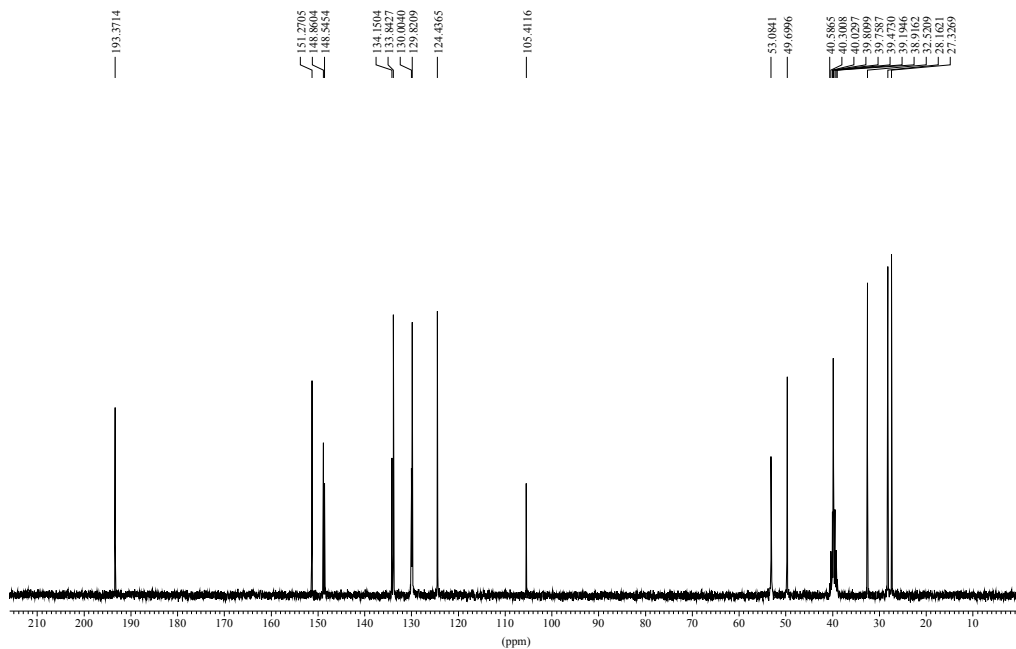
14# 13C-NMR DMSO-D6 303K AV-300



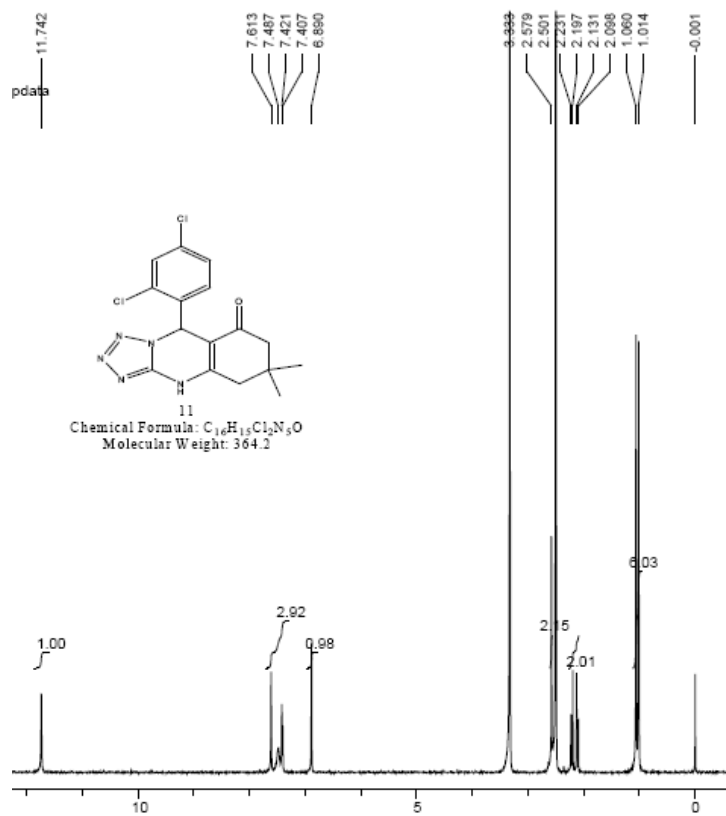
**<sup>13</sup>C NMR Spectrum (75 MHz, DMSO-*d*<sub>6</sub>) of Compound E7**



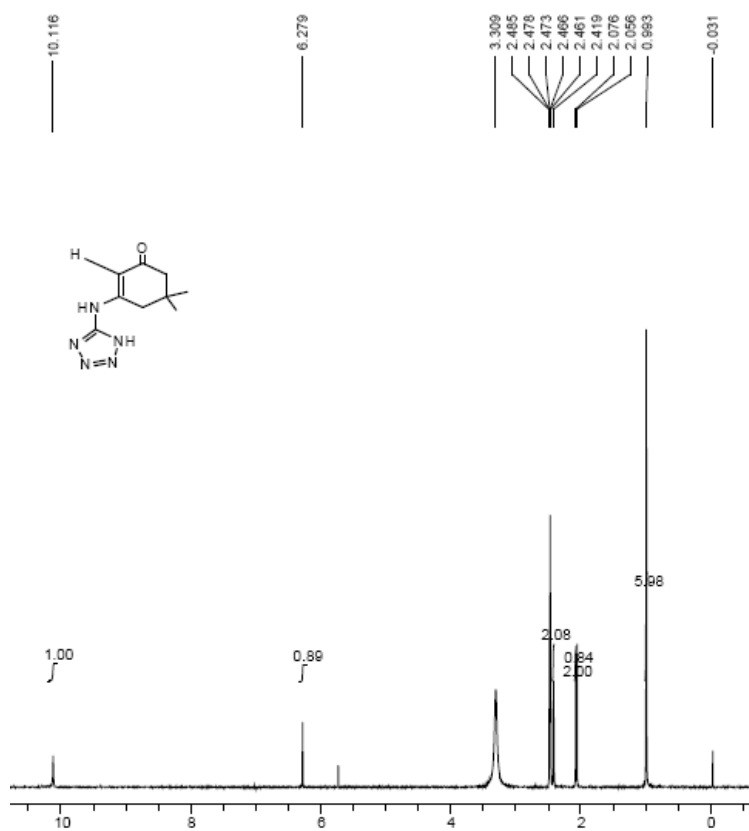
13# 13C-NMR DMSO-D6 303K AV-300



$^{13}C$  NMR Spectrum (75 MHz, DMSO- $d_6$ ) of Compound E8



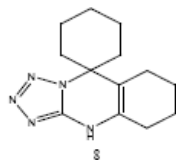
**<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound E9**



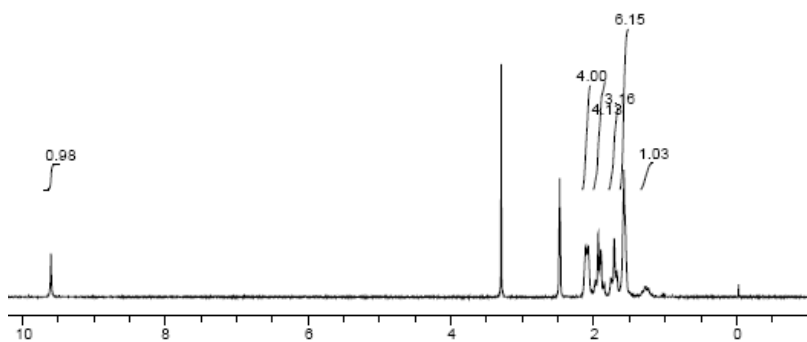
**<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound E10**

9.597

2.485  
2.478  
3.297  
2.473  
2.118  
2.080  
1.960  
1.940  
1.904  
1.851  
1.757  
1.720  
1.683  
1.580  
1.282  
1.269  
1.238  
1.229  
-0.025



Chemical Formula: C<sub>13</sub>H<sub>19</sub>N<sub>3</sub>  
Molecular Weight: 245.3



**<sup>1</sup>H NMR Spectrum (300 MHz, DMSO-*d*<sub>6</sub>) of Compound F**