

## Supplementary Data

### Pyridofuopyrrolo[1,2-*a*]pyrimidines and pyridofuopyrimido[1,2-*a*]azepines: New Chemical Entities (NCE) with anticonvulsive and psychotropic properties

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**Table S1.** Spectroscopic data for compounds **2b**, **g**, **h** and **3b**, **g**, **h**.

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
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| <b>Ethyl [(1-butyl-4-cyano-6,7-dihydro-5H-cyclopenta[c]pyridin-3-yl)oxy]acetate (2b).</b> <sup>1</sup> H NMR (300 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ 0.93 (t, <i>J</i> = 7.3 Hz, 3H, CH <sub>2</sub> CH <sub>3</sub> ), 1.28 (t, <i>J</i> = 7.1 Hz, 3H, OCH <sub>2</sub> CH <sub>3</sub> ), 1.27–1.39 (m, 2H, CH <sub>2</sub> CH <sub>3</sub> ), 1.56–1.67 (m, 2H, CH <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ), 2.13–2.24 (m, 2H, 6-CH <sub>2</sub> ), 2.60 (t, <i>J</i> = 7.4 Hz, 2H, CH <sub>2</sub> C <sub>3</sub> H <sub>7</sub> ), 2.86 (t, <i>J</i> = 7.5 Hz, 2H, 7-CH <sub>2</sub> ), 3.06 (t, <i>J</i> = 7.6 Hz, 2H, 5-CH <sub>2</sub> ), 4.17 (q, <i>J</i> = 7.1 Hz, 2H, OCH <sub>2</sub> CH <sub>3</sub> ), 4.89 (s, 2H, OCH <sub>2</sub> CO). |
| <b>Ethyl [(5-cyano-3,3-dimethyl-8-ethyl-3,4-dihydro-1H-pyrano[3,4-c]pyridin-6-yl)oxy] acetate (2g).</b> <sup>1</sup> H NMR (300 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ 1.21 (t, <i>J</i> = 7.4 Hz, 3H, CH <sub>2</sub> CH <sub>3</sub> ), 1.26 (s, 6H, C(CH <sub>3</sub> ) <sub>2</sub> ), 1.30 (t, <i>J</i> = 7.1 Hz, 3H, OCH <sub>2</sub> CH <sub>3</sub> ), 2.58 (q, <i>J</i> = 7.4 Hz, 2H, CH <sub>2</sub> CH <sub>3</sub> ), 2.78 (s, 2H, CH <sub>2</sub> ), 4.18 (q, <i>J</i> = 7.1 Hz, 2H, OCH <sub>2</sub> CH <sub>3</sub> ), 4.61 (s, 2H, OCH <sub>2</sub> ), 4.92 (s, 2H, OCH <sub>2</sub> CO).                                                                                                                                                        |
| <b>Ethyl [(8-butyl-5-cyano-3,3-dimethyl-3,4-dihydro-1H-pyrano[3,4-c]pyridin-6-yl)oxy] acetate (2h).</b> <sup>1</sup> H NMR (300 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ 0.93 (t, <i>J</i> = 7.3 Hz, 3H, CH <sub>2</sub> CH <sub>3</sub> ), 1.27 (s, 6H, C(CH <sub>3</sub> ) <sub>2</sub> ), 1.27 (t, <i>J</i> = 7.1 Hz, 3H, OCH <sub>2</sub> CH <sub>3</sub> ), 1.30–1.41 (m, 2H, CH <sub>2</sub> CH <sub>3</sub> ), 1.57–1.68 (m, 2H, CH <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ), 2.50–2.55 (m, 2H, CH <sub>2</sub> C <sub>3</sub> H <sub>7</sub> ), 2.78 (s, 2H, CH <sub>2</sub> ), 4.17 (q, <i>J</i> = 7.1 Hz, 2H, OCH <sub>2</sub> CH <sub>3</sub> ), 4.62 (s, 2H, OCH <sub>2</sub> ), 4.91 (s, 2H, OCH <sub>2</sub> CO).                                |
| <b>Ethyl 1-amino-5-butyl-7,8-dihydro-6H-cyclopenta[d]furo[2,3-b]pyridine-2-carboxylate (3b).</b> <sup>1</sup> H NMR (300 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ 0.95 (t, <i>J</i> = 7.3 Hz, 3H, CH <sub>2</sub> CH <sub>3</sub> ), 1.32–1.45 (m, 2H, CH <sub>2</sub> CH <sub>3</sub> ), 1.40 (t, <i>J</i> = 7.1 Hz, 3H, OCH <sub>2</sub> CH <sub>3</sub> ), 1.63–1.75 (m, 2H, CH <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ), 2.15–2.27 (m, 2H, 7-CH <sub>2</sub> ), 2.68–2.74 (m, 2H, CH <sub>2</sub> C <sub>3</sub> H <sub>7</sub> ), 2.89 (t, <i>J</i> = 7.5 Hz, 2H, 6-CH <sub>2</sub> ), 3.27 (t, <i>J</i> = 7.6 Hz, 2H, 8-CH <sub>2</sub> ), 4.32 (q, <i>J</i> = 7.1 Hz, 2H, OCH <sub>2</sub> CH <sub>3</sub> ), 5.70 (br s, 2H, NH <sub>2</sub> ).        |
| <b>Ethyl 1-amino-8,8-dimethyl-5-ethyl-8,9-dihydro-6H-furo[2,3-b]pyrano[4,3-d]pyridine-2-carboxylate (3g).</b> <sup>1</sup> H NMR (300 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ 1.29 (t, <i>J</i> = 7.4 Hz, 3H, CH <sub>2</sub> CH <sub>3</sub> ), 1.30 (s, 6H, C(CH <sub>3</sub> ) <sub>2</sub> ), 1.41 (t, <i>J</i> = 7.1 Hz, 3H, OCH <sub>2</sub> CH <sub>3</sub> ), 2.65 (q, <i>J</i> = 7.4 Hz, 2H, CH <sub>2</sub> CH <sub>3</sub> ), 3.11 (s, 2H, CH <sub>2</sub> ), 4.33 (q, <i>J</i> = 7.1 Hz, 2H, OCH <sub>2</sub> CH <sub>3</sub> ), 4.71 (s, 2H, OCH <sub>2</sub> ), 5.74 (br s, 2H, NH <sub>2</sub> ).                                                                                                                                                  |
| <b>Ethyl 1-amino-8,8-dimethyl-5-butyl-8,9-dihydro-6H-furo[2,3-b]pyrano[4,3-d]pyridine-2-carboxylate (3h).</b> <sup>1</sup> H NMR (300 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ 0.97 (t, <i>J</i> = 7.3 Hz, 3H, CH <sub>2</sub> CH <sub>3</sub> ), 1.29 (s, 6H, C(CH <sub>3</sub> ) <sub>2</sub> ), 1.35–1.48 (m, 2H, CH <sub>2</sub> CH <sub>3</sub> ), 1.40 (t, <i>J</i> = 7.1 Hz, 3H, OCH <sub>2</sub> CH <sub>3</sub> ), 1.65–1.76 (m, 2H, CH <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ), 2.61 (t, <i>J</i> = 7.5 Hz, 2H, CH <sub>2</sub> C <sub>3</sub> H <sub>7</sub> ), 3.11 (s, 2H, CH <sub>2</sub> ), 4.33 (q, <i>J</i> = 7.1 Hz, 2H, OCH <sub>2</sub> CH <sub>3</sub> ), 4.71 (s, 2H, OCH <sub>2</sub> ), 5.75 (br s, 2H, NH <sub>2</sub> ).            |

**Table S2.** Spectroscopic data for compounds **4a–h**.

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| <b>4-Isopropyl-2,3,10,11-tetrahydro-1H-cyclopenta[4',5']pyrido[3',2':4,5]furo[3,2-d]pyrrolo[1,2-a]pyrimidin-7(9H)-one (4a).</b> <sup>1</sup> H NMR (300 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ 1.31 (d, <i>J</i> = 6.6 Hz, 6H, CH(CH <sub>3</sub> ) <sub>2</sub> ), 2.20–2.41 (m, 4H, 2-CH <sub>2</sub> , 10-CH <sub>2</sub> ), 3.02 (t, <i>J</i> = 7.4 Hz, 2H, 3-CH <sub>2</sub> ), 3.19 (t, <i>J</i> = 7.8 Hz, 2H, 11-CH <sub>2</sub> ), 3.20 (sp, <i>J</i> = 6.7 Hz, 1H, CH(CH <sub>3</sub> ) <sub>2</sub> ), 3.35 (t, <i>J</i> = 7.6 Hz, 2H, 1-CH <sub>2</sub> ), 4.18–4.24 (m, 2H, 9-CH <sub>2</sub> ). <sup>13</sup> C NMR (75 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ: 19.6, 21.0, 24.5, 29.1, 31.1, 31.6, 32.8, 46.5, 109.2, 133.2, 135.5, 142.6, 149.6, 150.8, 160.7, 161.4, 161.8.                                                                                                                                          |
| <b>4-Butyl-2,3,10,11-tetrahydro-1H-cyclopenta[4',5']pyrido[3',2':4,5]furo[3,2-d]pyrrolo[1,2-a]pyrimidin-7(9H)-one (4b).</b> <sup>1</sup> H NMR (300 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ 0.98 (t, <i>J</i> = 7.3 Hz, 3H, CH <sub>2</sub> CH <sub>3</sub> ), 1.37–1.50 (m, 2H, CH <sub>2</sub> CH <sub>3</sub> ), 1.70–1.80 (m, 2H, CH <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ), 2.23–2.41 (m, 4H, 2-CH <sub>2</sub> , 10-CH <sub>2</sub> ), 2.80 (t, <i>J</i> = 7.5 Hz, 2H, CH <sub>2</sub> C <sub>3</sub> H <sub>7</sub> ), 2.99 (t, <i>J</i> = 7.4 Hz, 2H, 3-CH <sub>2</sub> ), 3.19 (t, <i>J</i> = 7.9 Hz, 2H, 11-CH <sub>2</sub> ), 3.34 (t, <i>J</i> = 7.6 Hz, 2H, 1-CH <sub>2</sub> ), 4.18–4.24 (m, 2H, 9-CH <sub>2</sub> ). <sup>13</sup> C NMR (75 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ: 13.5, 19.6, 21.9, 24.4, 29.3, 29.8, 31.1, 31.6, 34.9, 46.5, 109.1, 134.1, 135.4, 142.5, 149.3, 150.8, 156.9, 160.6, 161.6. |
| <b>5-Isopropyl-1,2,3,4,11,12-hexahydropyrrolo[1'',2'':1',2']pyrimido[4',5':4,5]furo[2,3-c]-isoquinolin-8(10H)-one (4c).</b> <sup>1</sup> H NMR (300 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ 1.28 (d, <i>J</i> = 6.6 Hz, 6H, CH(CH <sub>3</sub> ) <sub>2</sub> ), 1.83–1.98 (m, 4H, 2,3-CH <sub>2</sub> ), 2.29–2.40 (m, 2H, 11-CH <sub>2</sub> ), 2.82–2.88 (m, 2H, 4-CH <sub>2</sub> ), 3.18 (t, <i>J</i> = 7.9 Hz, 2H, 12-CH <sub>2</sub> ), 3.30–3.38 (m, 3H, 1-CH <sub>2</sub> , CH(CH <sub>3</sub> ) <sub>2</sub> ), 4.17–4.23 (m, 2H, 10-CH <sub>2</sub> ). <sup>13</sup> C NMR (75 MHz, DMSO/CCl <sub>4</sub> , 1/3) δ: 19.5, 20.8, 21.3, 22.4, 24.7, 26.5, 30.4, 31.7, 46.4, 109.9, 125.1, 135.1, 143.5, 143.9, 150.8, 160.2, 160.3, 164.9.                                                                                                                                                                                |

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| <p><b>5-Isobutyl-1,2,3,4,11,12-hexahydropyrrolo[1'',2'':1',2']pyrimido[4',5':4,5]furo[2,3-c]isoquinolin-8(10H)-one (4d).</b> <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 1.00 (d, <i>J</i> = 6.6 Hz, 6H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.83–1.97 (m, 4H, 2,3-CH<sub>2</sub>), 2.21–2.40 (m, 3H, CH(CH<sub>3</sub>)<sub>2</sub>, 11-CH<sub>2</sub>), 2.68 (d, <i>J</i> = 7.0 Hz, 2H, CHCH<sub>2</sub>), 2.76–2.82 (m, 2H, 4-CH<sub>2</sub>), 3.18 (t, <i>J</i> = 7.9 Hz, 2H, 12-CH<sub>2</sub>), 3.31–3.37 (m, 2H, 1-CH<sub>2</sub>), 4.17–4.23 (m, 2H, 10-CH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 19.6, 20.8, 22.2, 22.3, 25.2, 26.4, 27.1, 31.7, 42.9, 46.4, 109.9, 126.4, 135.0, 143.4, 143.6, 150.8, 159.7, 159.9, 160.3.</p> <p><b>2,2,5-Trimethyl-1,4,11,12-tetrahydro-2H-pyrano[4'',3'':4',5']pyrido[3',2':4,5]furo[3,2-d]pyrrolo[1,2-a]pyrimidin-8(10H)-one (4e).</b> <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 1.33 (s, 6H, C(CH<sub>3</sub>)<sub>2</sub>), 2.30–2.41 (m, 2H, 11-CH<sub>2</sub>), 2.48 (s, 3H, CH<sub>3</sub>), 3.19 (s, 2H, CH<sub>2</sub>), 3.20 (t, <i>J</i> = 7.9 Hz, 2H, 12-CH<sub>2</sub>), 4.20 (t, <i>J</i> = 7.3 Hz, 2H, 10-CH<sub>2</sub>), 4.74 (s, 2H, OCH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 19.6, 20.8, 25.8, 31.7, 36.3, 46.5, 60.0, 68.6, 110.1, 123.7, 135.1, 139.6, 143.0, 150.7, 153.5, 160.3, 160.7.</p> <p><b>2,2-Dimethyl-5-ethyl-1,4,11,12-tetrahydro-2H-pyrano[4'',3'':4',5']pyrido[3',2':4,5]furo[3,2-d]pyrrolo[1,2-a]pyrimidin-8(10H)-one (4f).</b> <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 1.33 (s, 6H, C(CH<sub>3</sub>)<sub>2</sub>), 1.35 (t, <i>J</i> = 7.3 Hz, 3H, CH<sub>2</sub>CH<sub>3</sub>), 2.30–2.41 (m, 2H, 11-CH<sub>2</sub>), 2.74 (t, <i>J</i> = 7.3 Hz, 2H, CH<sub>2</sub>CH<sub>3</sub>), 3.20 (t, <i>J</i> = 7.9 Hz, 2H, 12-CH<sub>2</sub>), 3.22 (s, 2H, CH<sub>2</sub>), 4.18–4.24 (t, <i>J</i> = 7.3 Hz, 2H, 10-CH<sub>2</sub>), 4.79 (s, 2H, OCH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 11.3, 19.6, 25.8, 26.4, 31.7, 36.4, 46.5, 59.7, 68.5, 109.9, 123.1, 135.2, 139.7, 143.0, 150.7, 157.9, 160.6, 160.7.</p> <p><b>5-Butyl-2,2-dimethyl-1,4,11,12-tetrahydro-2H-pyrano[4'',3'':4',5']pyrido[3',2':4,5]furo[3,2-d]pyrrolo[1,2-a]pyrimidin-8(10H)-one (4g).</b> <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 0.99 (t, <i>J</i> = 7.3 Hz, 3H, CH<sub>2</sub>CH<sub>3</sub>), 1.33 (s, 6H, C(CH<sub>3</sub>)<sub>2</sub>), 1.39–1.52 (m, 2H, CH<sub>2</sub>CH<sub>3</sub>), 1.71–1.82 (m, 2H, CH<sub>2</sub>C<sub>2</sub>H<sub>5</sub>), 2.30–2.41 (m, 2H, 11-CH<sub>2</sub>), 2.66–2.73 (m, 2H, CH<sub>2</sub>C<sub>3</sub>H<sub>7</sub>), 3.20 (t, <i>J</i> = 7.9 Hz, 2H, 12-CH<sub>2</sub>), 3.22 (s, 2H, CH<sub>2</sub>), 4.18–4.25 (t, <i>J</i> = 7.3 Hz, 2H, 10-CH<sub>2</sub>), 4.80 (s, 2H, OCH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 13.5, 19.6, 21.9, 25.8, 29.4, 31.7, 33.0, 36.5, 46.5, 59.8, 68.6, 110.1, 123.3, 135.2, 139.9, 143.1, 150.7, 157.3, 160.6, 160.7.</p> <p><b>2,2-Dimethyl-5-(2-furyl)-1,4,11,12-tetrahydro-2H-pyrano[4'',3'':4',5']pyrido[3',2':4,5]furo[3,2-d]pyrrolo[1,2-a]pyrimidin-8(10H)-one (4h).</b> IR ν/cm<sup>-1</sup>: 1687 (C=O). <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 1.37 (s, 6H, C(CH<sub>3</sub>)<sub>2</sub>), 2.28–2.39 (m, 2H, 11-CH<sub>2</sub>), 3.21 (t, <i>J</i> = 7.9 Hz, 2H, 12-CH<sub>2</sub>), 3.30 (s, 2H, CH<sub>2</sub>), 4.17–4.23 (t, <i>J</i> = 7.3 Hz, 2H, 10-CH<sub>2</sub>), 5.14 (s, 2H, OCH<sub>2</sub>), 6.67 (dd, <i>J</i> = 3.5, 1.7 Hz, 1H, 4-CH, furyl), 7.22 (dd, <i>J</i> = 3.5, 0.7 Hz, 1H, 3-CH, furyl), 7.83 (dd, <i>J</i> = 1.7, 0.7 Hz, 1H, 5-CH, furyl). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 21.7, 25.8, 31.6, 36.5, 46.5, 60.0, 68.7, 107.8, 109.7, 110.1, 123.8, 135.0, 139.8, 140.9, 144.2, 152.7, 153.5, 155.7, 160.7, 161.9. Anal. Calcd. for C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O<sub>4</sub>: C 66.83; H 5.07; N 11.13 %. Found: C 66.71; H 5.08; N 11.11 %.</p> |
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Table S3. Spectroscopic data for compounds 5a–h.

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| <p><b>4-Isopropyl-2,3,10,11,12,13-hexahydro-1H-cyclopenta[4'',5'']pyrido[3'',2'':4',5']furo[3',2':4,5]pyrimido[1,2-a]azepin-7(9H)-one (5a).</b> <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 1.31 (d, <i>J</i> = 6.7 Hz, 6H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.76–1.93 (m, 6H, 10,11,12-CH<sub>2</sub>), 2.23–2.34 (m, 2H, 2-CH<sub>2</sub>), 3.02 (t, <i>J</i> = 7.4 Hz, 2H, 3-CH<sub>2</sub>), 3.12–3.17 (m, 2H, 13-CH<sub>2</sub>), 3.19 (sp, <i>J</i> = 6.7 Hz, 1H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.36 (t, <i>J</i> = 7.6 Hz, 2H, 1-CH<sub>2</sub>), 4.41–4.46 (m, 2H, 9-CH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 20.9, 24.5, 27.1, 28.7, 29.0, 31.1, 32.8, 36.6, 41.9, 109.2, 133.1, 135.1, 140.4, 149.7, 151.8, 160.9, 161.5, 161.8.</p> |
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**4-Butyl-2,3,10,11,12,13-hexahydro-1H-cyclopenta[4'',5'']pyrido[3'',2'':4',5']furo[3',2':4,5]-pyrimido[1,2-a]azepin-7(9H)-one (5b).** <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 0.98 (t, *J* = 7.3 Hz, 3H, CH<sub>2</sub>CH<sub>3</sub>), 1.36–1.49 (m, 2H, CH<sub>2</sub>CH<sub>3</sub>), 1.69–1.93 (m, 8H, CH<sub>2</sub>C<sub>2</sub>H<sub>5</sub>, 10,11,12-CH<sub>2</sub>), 2.23–2.33 (m, 2H, 2-CH<sub>2</sub>), 2.80 (t, *J* = 7.6 Hz, 2H, CH<sub>2</sub>C<sub>3</sub>H<sub>7</sub>), 2.99 (t, *J* = 7.4 Hz, 2H, 3-CH<sub>2</sub>), 3.11–3.16 (m, 2H, 13-CH<sub>2</sub>), 3.34 (t, *J* = 7.6 Hz, 2H, 1-CH<sub>2</sub>), 4.40–4.45 (m, 2H, 9-CH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 13.5, 21.9, 24.4, 24.5, 27.1, 28.7, 29.2, 29.7, 31.1, 34.9, 36.6, 41.9, 109.2, 134.1, 134.9, 140.4, 149.4, 151.8, 156.9, 160.9, 161.6.

**4-Phenyl-2,3,10,11,12,13-hexahydro-1H-cyclopenta[4'',5'']pyrido[3'',2'':4',5']furo[3',2':4,5]pyrimido[1,2-a]azepin-7(9H)-one (5c).** <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 1.78–1.95 (m, 6H, CH<sub>2</sub>, 10,11,12-CH<sub>2</sub>), 2.23–2.35 (m, 2H, 2-CH<sub>2</sub>), 3.13–3.20 (m, 2H, 13-CH<sub>2</sub>), 3.24 (t, *J* = 7.3 Hz, 2H, 3-CH<sub>2</sub>), 3.43 (t, *J* = 7.5 Hz, 2H, 1-CH<sub>2</sub>), 4.41–4.49 (m, 2H, NCH<sub>2</sub>), 7.38–7.51 and 7.83–7.88 (both m, 3H and 2H, Ph). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 24.4, 25.7, 26.9, 28.6, 31.2, 31.8, 36.6, 42.1, 110.2, 127.9, 128.4, 128.5, 134.2, 135.9, 138.6, 140.3, 151.8, 152.0, 152.3, 161.5, 161.8.

**5-Isopropyl-1,2,3,4,11,12,13,14-octahydroazepino[1'',2'':1',2']pyrimido[4',5':4,5]furo[2,3-c]isoquinolin-8(10H)-one (5d).** <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 1.28 (d, *J* = 6.7 Hz, 6H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.75–1.98 (m, 10H, 2,3-CH<sub>2</sub> and 11,12,13-CH<sub>2</sub>), 2.82–2.88 (m, 2H, 4-CH<sub>2</sub>), 3.11–3.16 (m, 2H, 14-CH<sub>2</sub>), 3.33 (sp, *J* = 6.7 Hz, 1H, CH(CH<sub>3</sub>)<sub>2</sub>), 3.32–3.38 (m, 2H, 1-CH<sub>2</sub>), 4.40–4.45 (m, 2H, 10-CH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 20.7, 21.3, 22.4, 24.5, 24.7, 26.5, 27.1, 28.7, 30.4, 36.7, 41.8, 109.9, 124.9, 134.6, 141.3, 144.0, 151.7, 160.3, 160.6, 164.9.

**5-Isobutyl-1,2,3,4,11,12,13,14-octahydroazepino[1'',2'':1',2']pyrimido[4',5':4,5]furo[2,3-c]isoquinolin-8(10H)-one (5e).** <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 0.99 (d, *J* = 6.6 Hz, 6H, CH(CH<sub>3</sub>)<sub>2</sub>), 1.75–1.97 (m, 10H, 2,3-CH<sub>2</sub> and 11,12,13-CH<sub>2</sub>), 2.21–2.34 (m, 1H, CH(CH<sub>3</sub>)<sub>2</sub>), 2.68 (d, *J* = 7.0 Hz, 2H, CHCH<sub>2</sub>), 2.76–2.82 (m, 2H, 4-CH<sub>2</sub>), 3.11–3.17 (m, 2H, 14-CH<sub>2</sub>), 3.32–3.38 (m, 2H, 1-CH<sub>2</sub>), 4.40–4.45 (m, 2H, 10-CH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 20.8, 22.2, 22.4, 24.5, 25.2, 26.3, 27.1, 28.7, 36.7, 41.8, 42.9, 109.9, 126.4, 134.6, 141.3, 143.8, 151.8, 159.8, 159.9, 160.6.

**2,2,5-Trimethyl-1,4,11,12,13,14-hexahydro-2H-pyrano[4''',3''':4'',5'']pyrido[3'',2'':4',5']furo[3',2':4,5]pyrimido[1,2-a]azepin-8(10H)-one (5f).** <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 1.34 (s, 6H, C(CH<sub>3</sub>)<sub>2</sub>), 1.76–1.94 (m, 6H, 11,12,13-CH<sub>2</sub>), 2.49 (s, 3H, CH<sub>3</sub>), 3.14–3.20 (m, 2H, 14-CH<sub>2</sub>), 3.22 (s, 2H, CH<sub>2</sub>), 4.41–4.46 (m, 2H, 10-CH<sub>2</sub>), 4.75 (s, 2H, OCH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 20.8, 24.5, 25.8, 27.0, 28.7, 36.3, 36.6, 41.9, 60.0, 68.6, 110.2, 123.7, 134.7, 139.7, 140.8, 151.7, 153.6, 160.4, 161.0.

**2,2-Dimethyl-5-ethyl-1,4,11,12,13,14-hexahydro-2H-pyrano[4''',3''':4'',5'']pyrido[3'',2'':4',5']furo[3',2':4,5]pyrimido[1,2-a]azepin-8(10H)-one (5g).** <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 1.34 (s, 6H, C(CH<sub>3</sub>)<sub>2</sub>), 1.35 (t, *J* = 7.4 Hz, 3H, CH<sub>2</sub>CH<sub>3</sub>), 1.76–1.94 (m, 6H, 11,12,13-CH<sub>2</sub>), 2.74 (q, *J* = 7.4 Hz, 2H, CH<sub>2</sub>CH<sub>3</sub>), 3.14–3.20 (m, 2H, 14-CH<sub>2</sub>), 3.23 (s, 2H, CH<sub>2</sub>), 4.41–4.47 (m, 2H, 10-CH<sub>2</sub>), 4.80 (s, 2H, OCH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 11.3, 24.5, 25.8, 26.4, 27.1, 28.7, 36.4, 36.6, 41.9, 59.7, 68.6, 110.1, 123.1, 134.8, 139.8, 140.9, 151.7, 158.0, 160.7, 161.0.

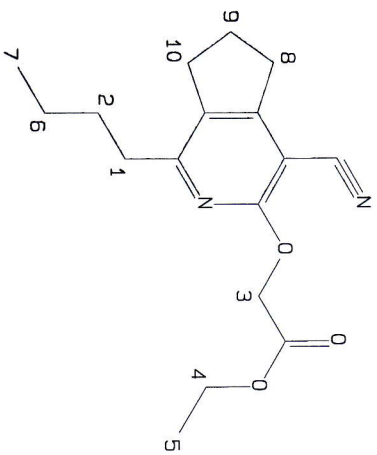
**5-Butyl-2,2-dimethyl-1,4,11,12,13,14-hexahydro-2H-pyrano[4''',3''':4'',5'']pyrido[3'',2'':4',5']furo[3',2':4,5]pyrimido[1,2-a]azepin-8(10H)-one (5h).** <sup>1</sup>H NMR (300 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ 0.99 (t, *J* = 7.3 Hz, 3H, CH<sub>2</sub>CH<sub>3</sub>), 1.33 (s, 6H, C(CH<sub>3</sub>)<sub>2</sub>), 1.38–1.51 (m, 2H, CH<sub>2</sub>CH<sub>3</sub>), 1.71–1.94 (m, 8H, CH<sub>2</sub>C<sub>2</sub>H<sub>5</sub>, 11,12,13-CH<sub>2</sub>), 2.69 (t, *J* = 7.6 Hz, 2H, CH<sub>2</sub>C<sub>3</sub>H<sub>7</sub>), 3.13–3.20 (m, 2H, 14-CH<sub>2</sub>), 3.23 (s, 2H, CH<sub>2</sub>), 4.40–4.47 (m, 2H, 10-CH<sub>2</sub>), 4.80 (s, 2H, OCH<sub>2</sub>). <sup>13</sup>C NMR (75 MHz, DMSO/CCl<sub>4</sub>, 1/3) δ: 13.5, 21.9, 24.5, 25.8, 27.1, 28.7, 29.4, 32.9, 36.5, 36.6, 41.9, 59.8, 68.6, 110.2, 123.3, 134.8, 139.9, 140.9, 151.8, 157.3, 160.7, 161.0.

2b

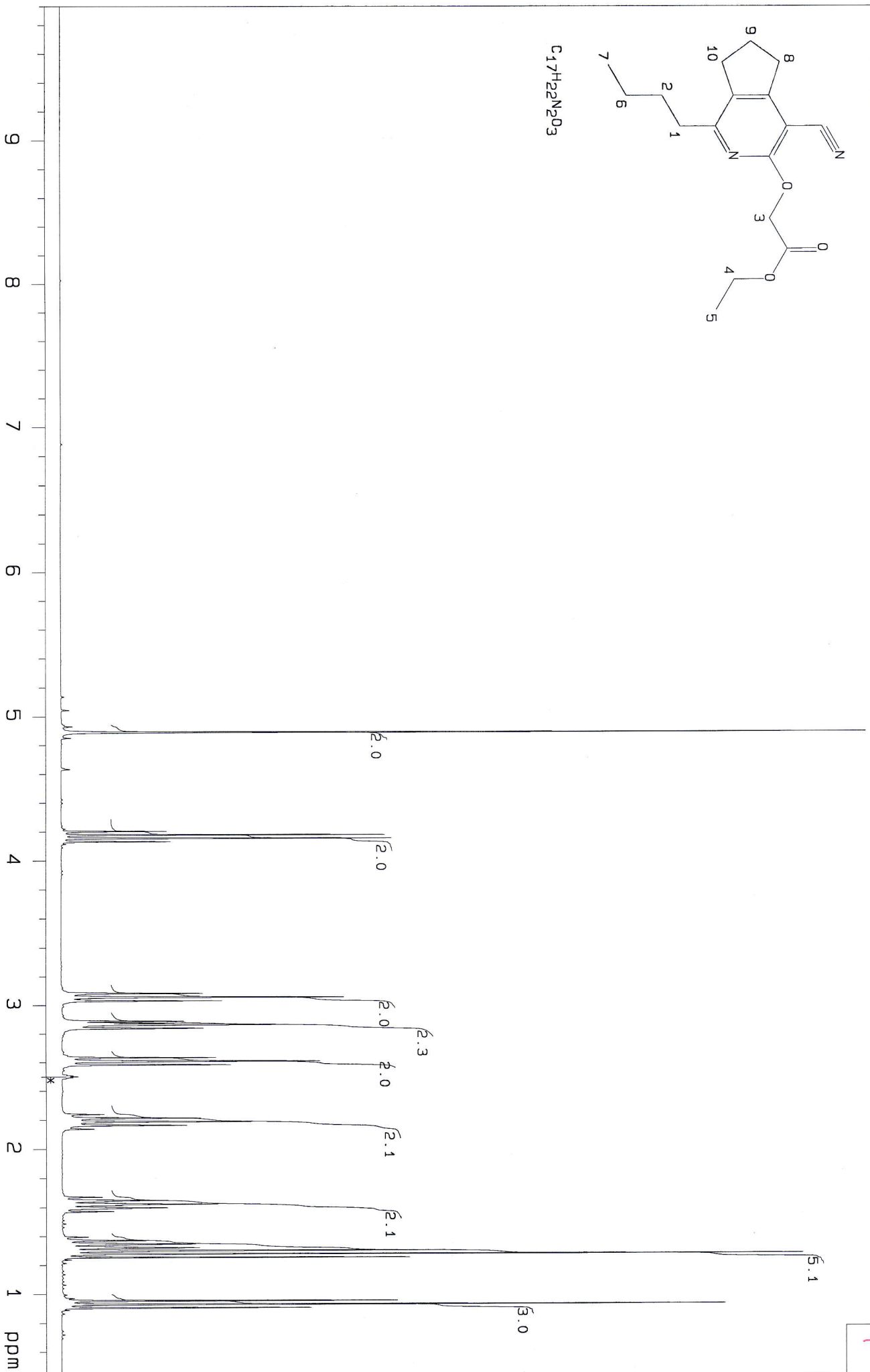
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HA-463

SAMV\_16 ha-463



C<sub>17</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>

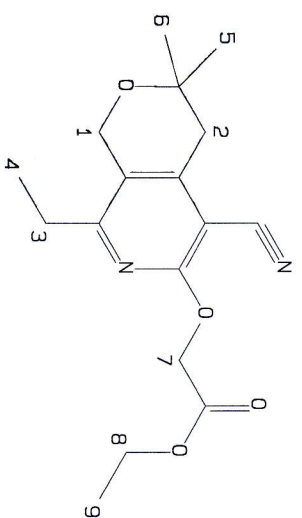


29

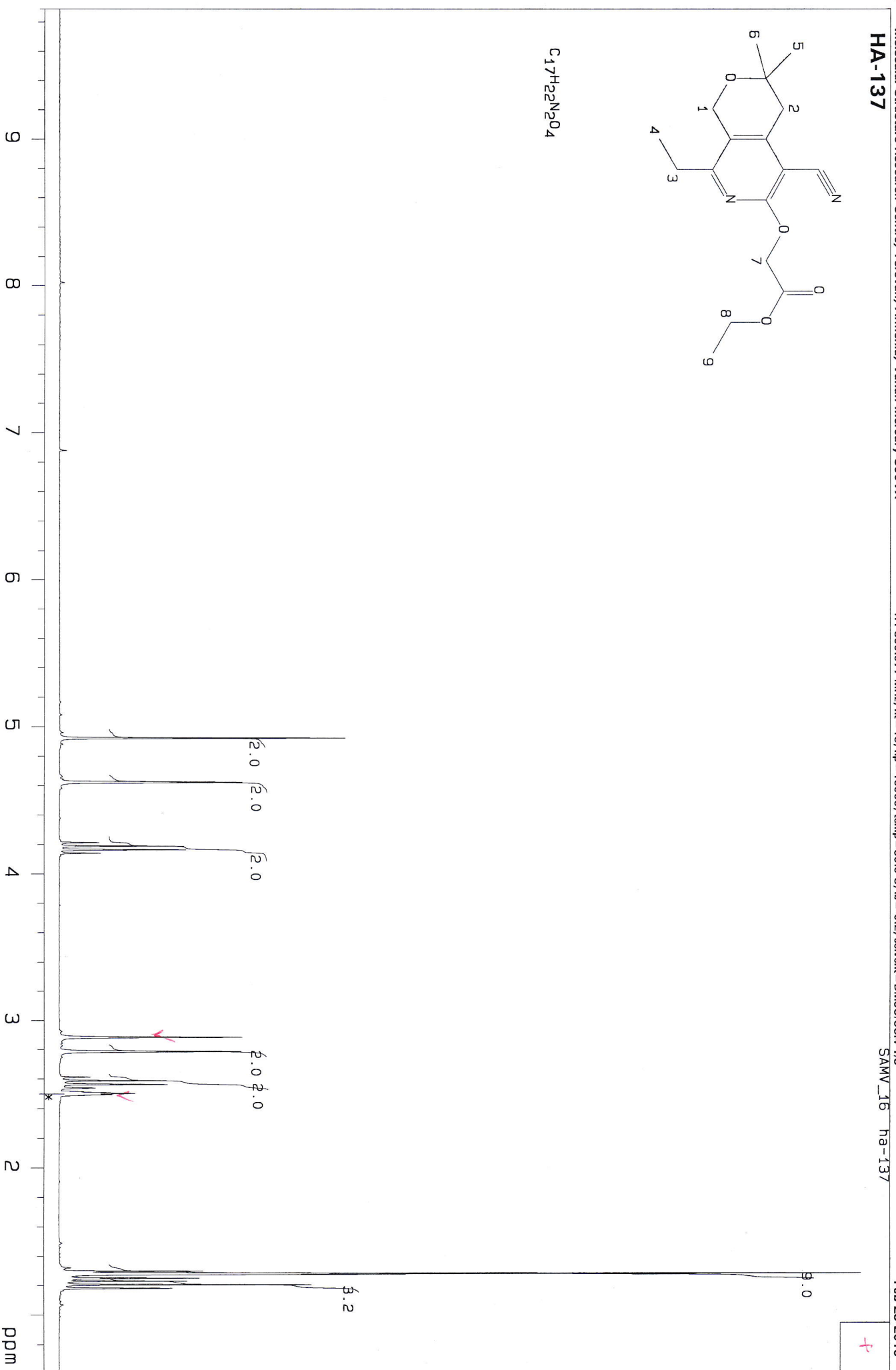
HA-137

SAMV\_16 ha-137

Feb 29 2016



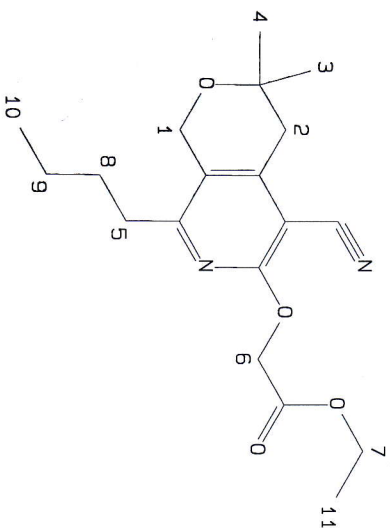
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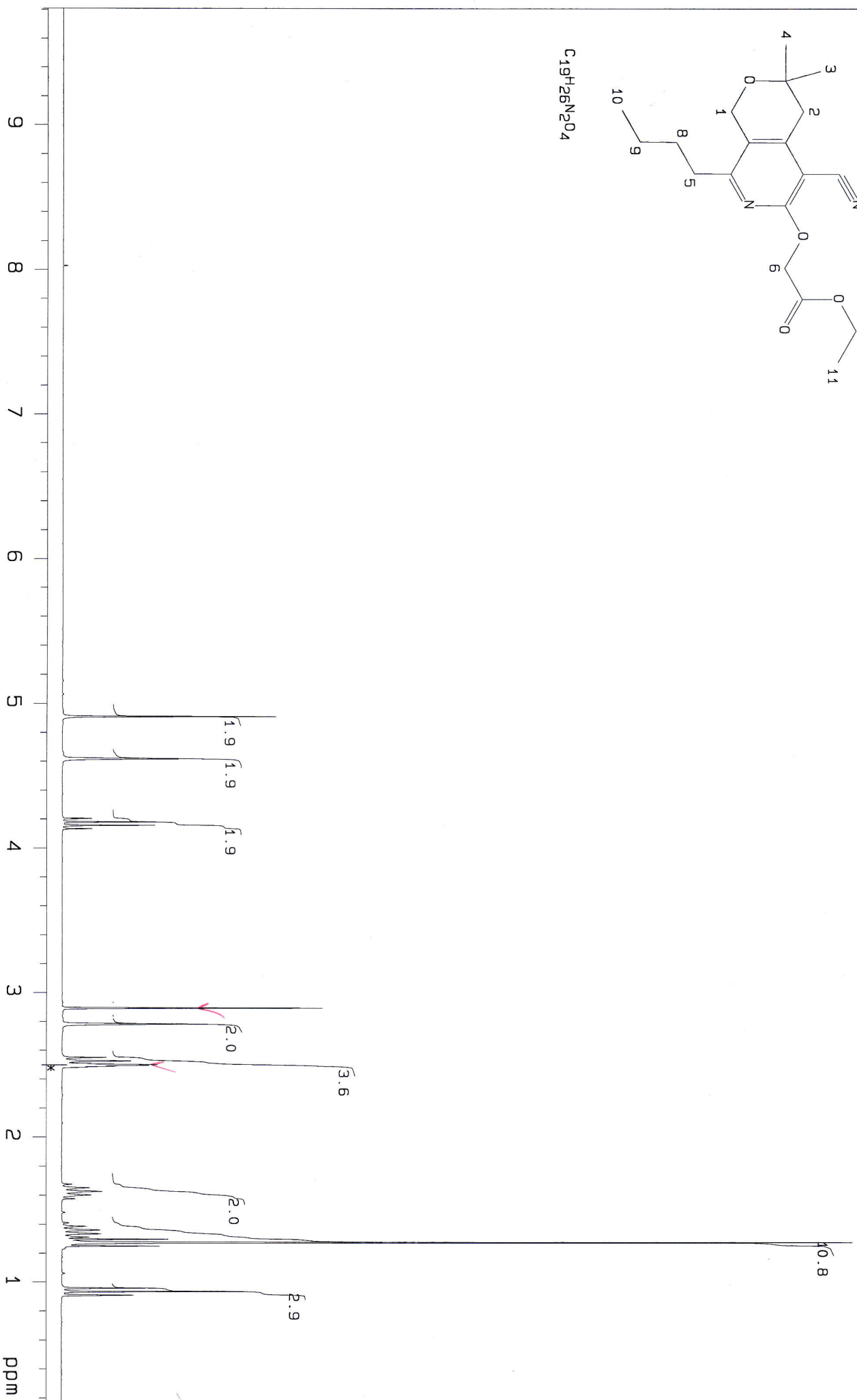
226

HA-378

SAMV\_11 ha-378



C<sub>19</sub>H<sub>12</sub>N<sub>2</sub>O<sub>4</sub>

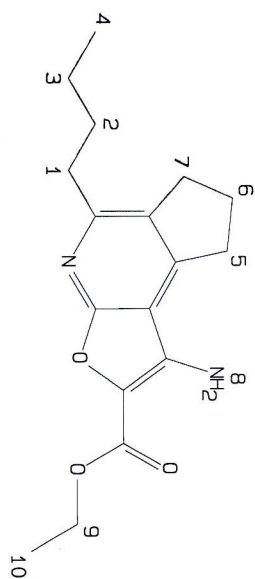
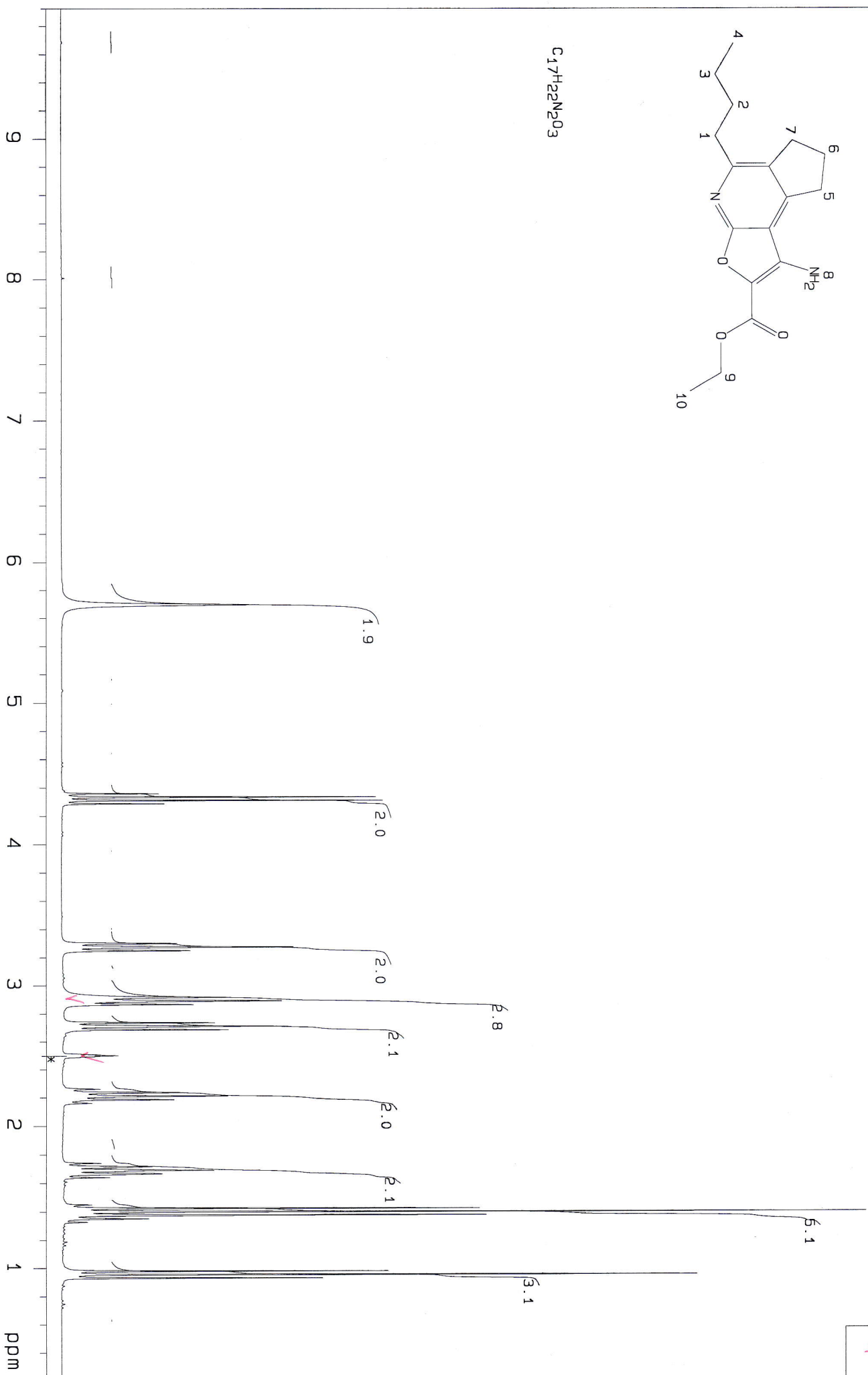


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36

HA-457

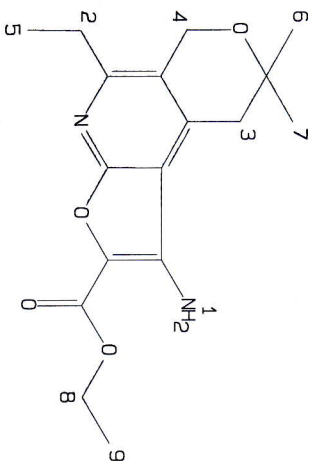
SAMV\_11 na-457

 $C_{17}H_{22}N_2O_3$ 

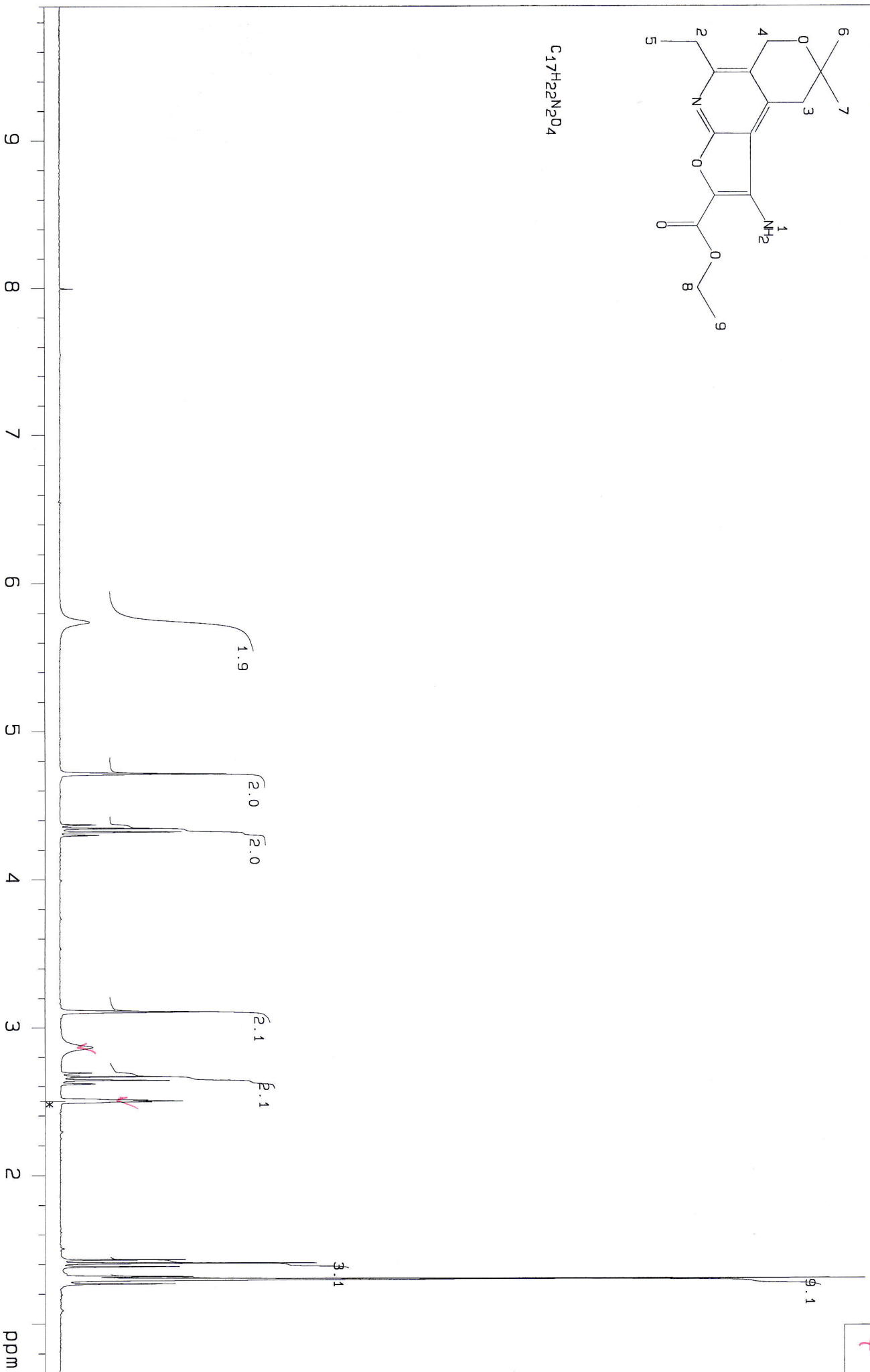
38

HA-138

SAMV\_13 ha-138



C<sub>17</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub>

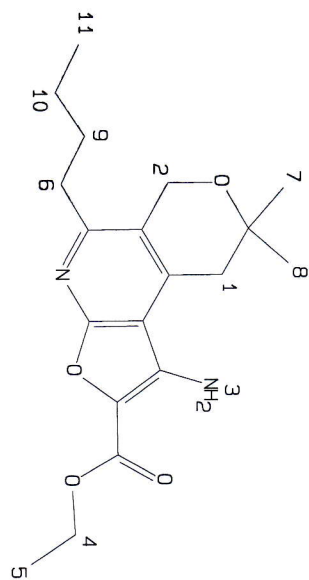


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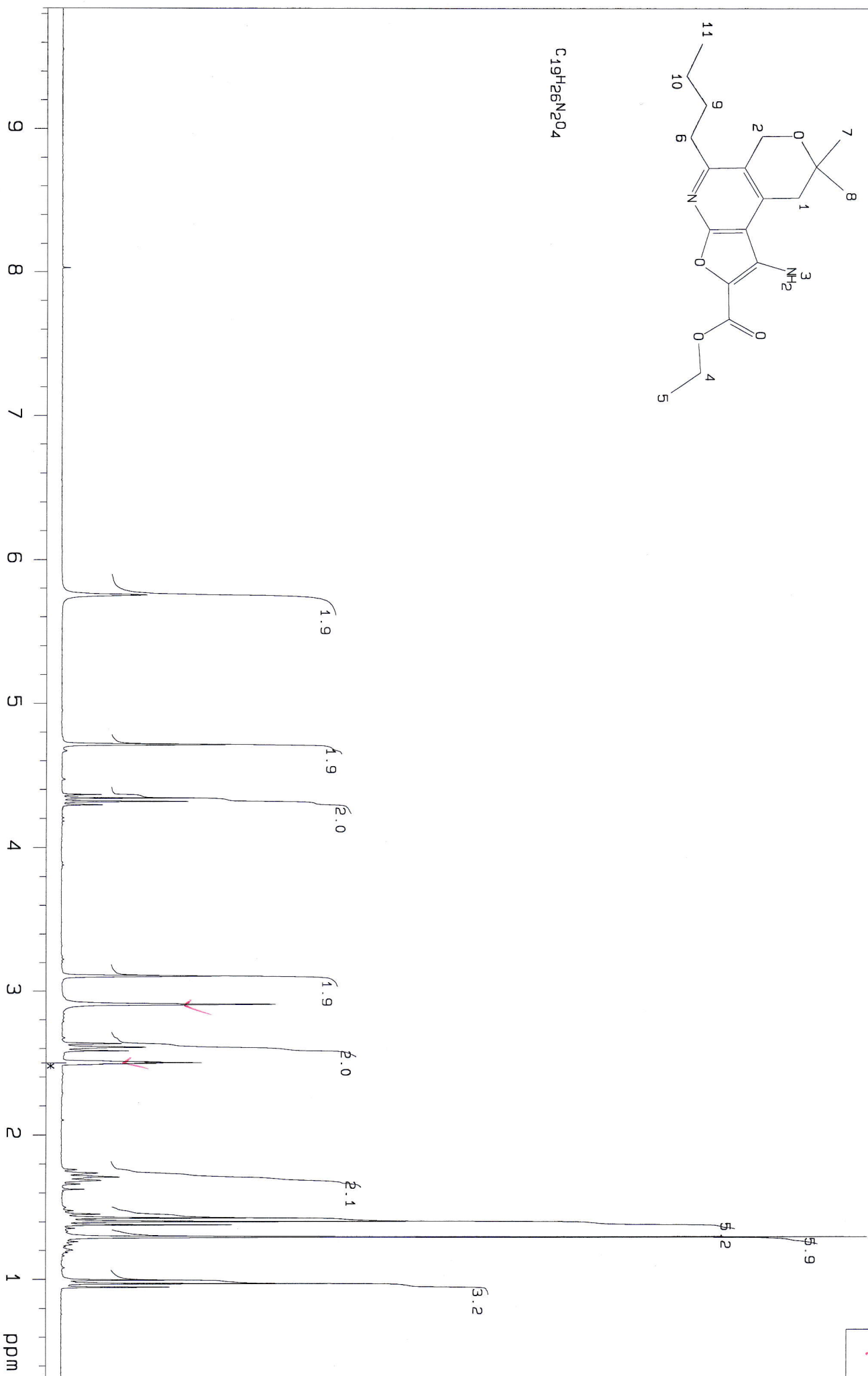
3h

HA-379

SAMV\_11 ha-379



C<sub>19</sub>H<sub>26</sub>N<sub>2</sub>O<sub>4</sub>



*[Handwritten signature]*

4a

4a

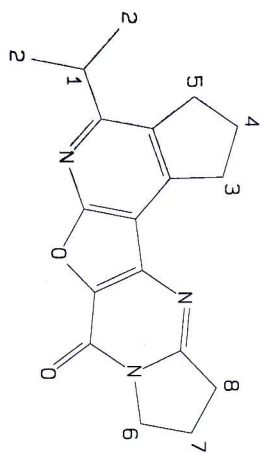
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

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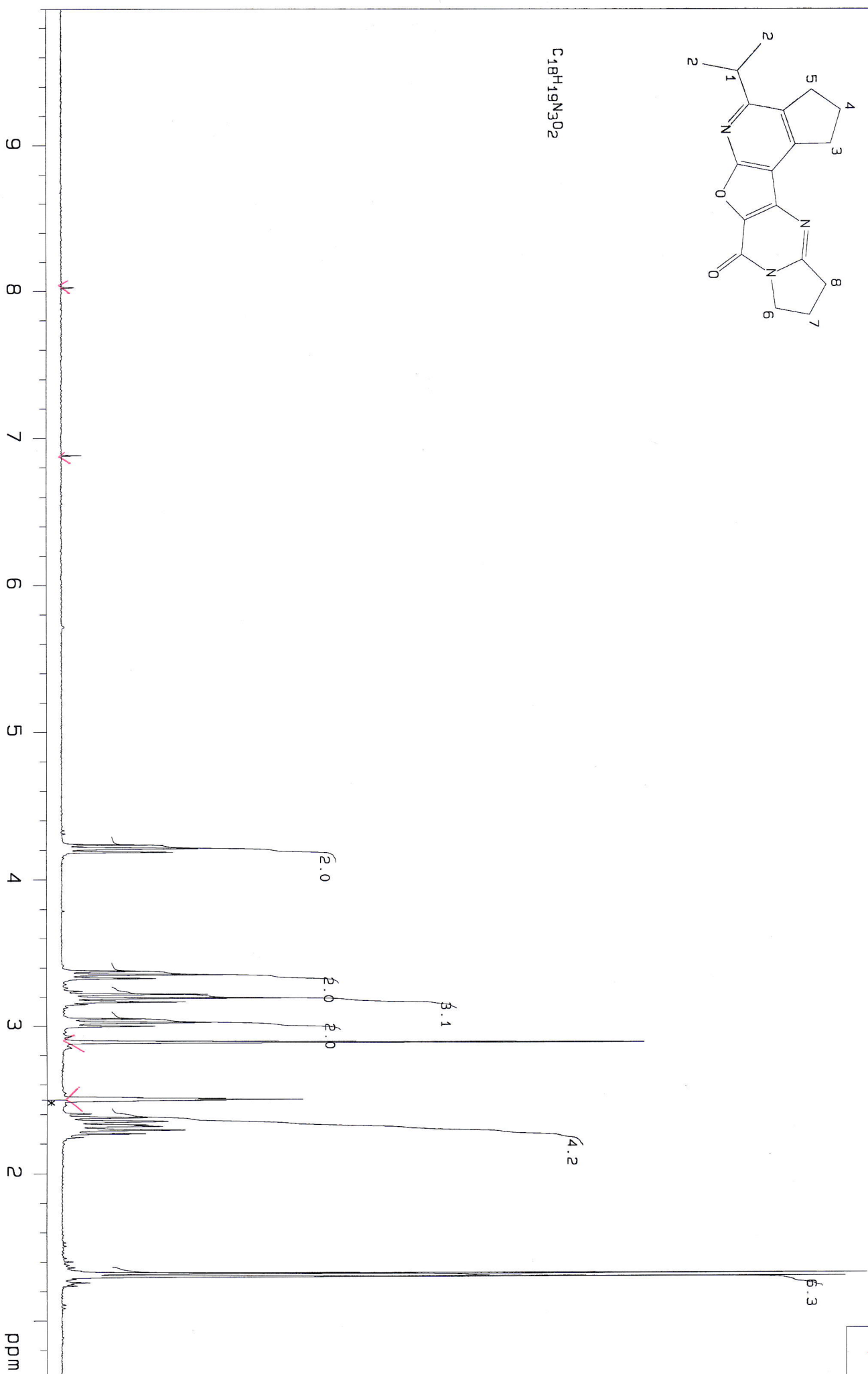
Feb 29 2016

HA-317

SAMV\_16 ha-317



C<sub>18</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>



4a

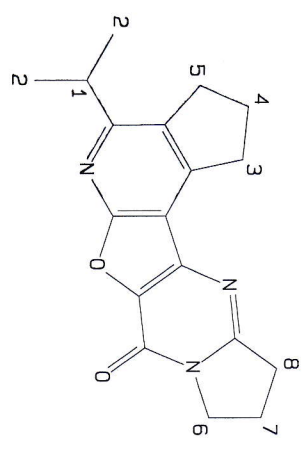
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

HA-317

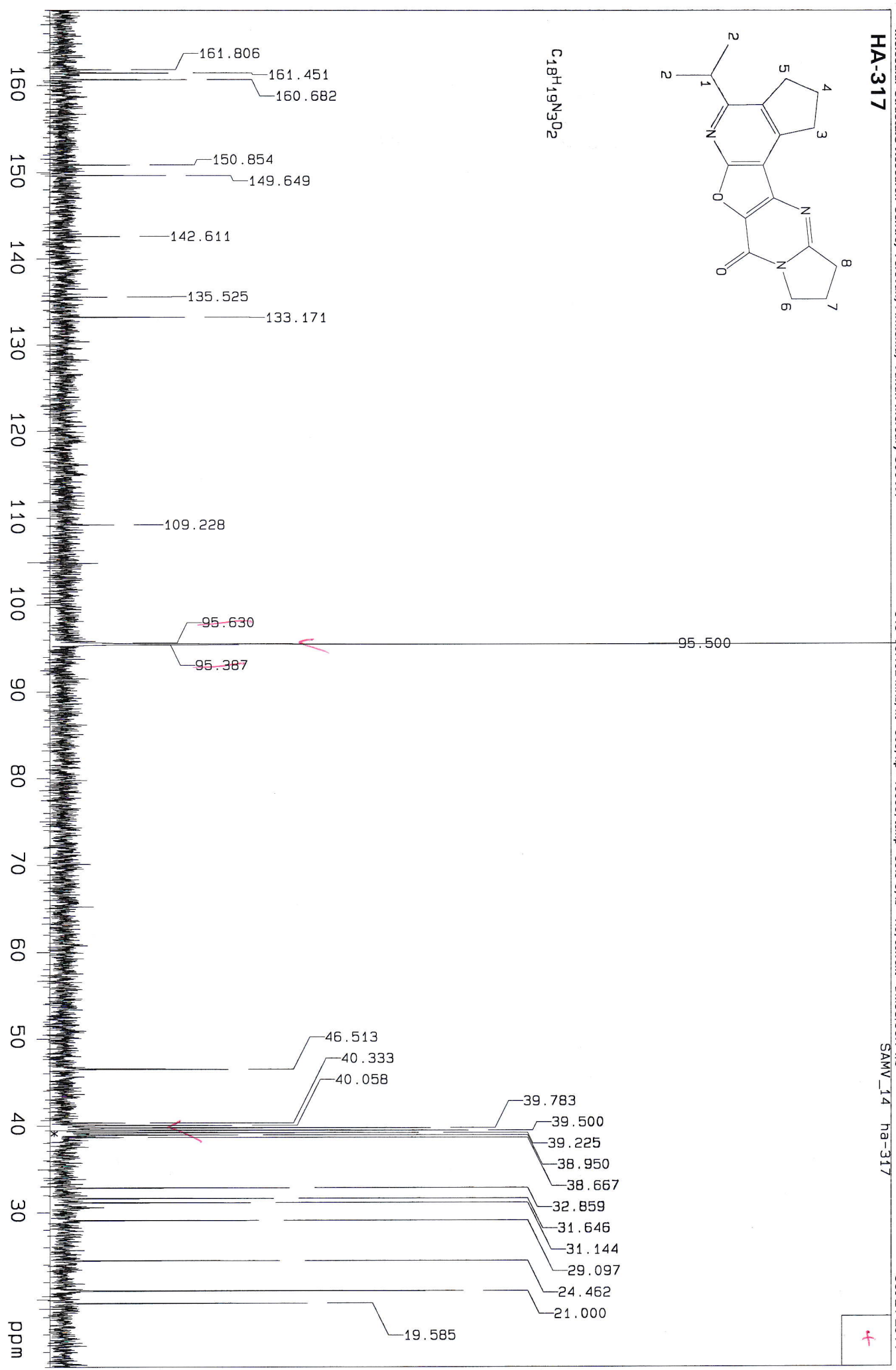
C13 75.462 MHz, nt = 368, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CD4 1/3

SAMV\_14 ha-317

Oct 21 2014



C<sub>18</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>



*[Handwritten signature]*

46

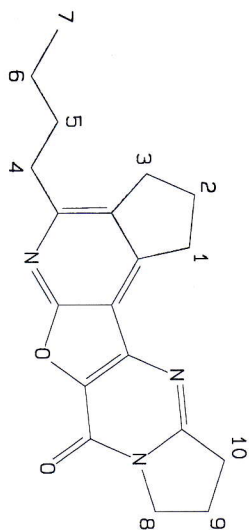
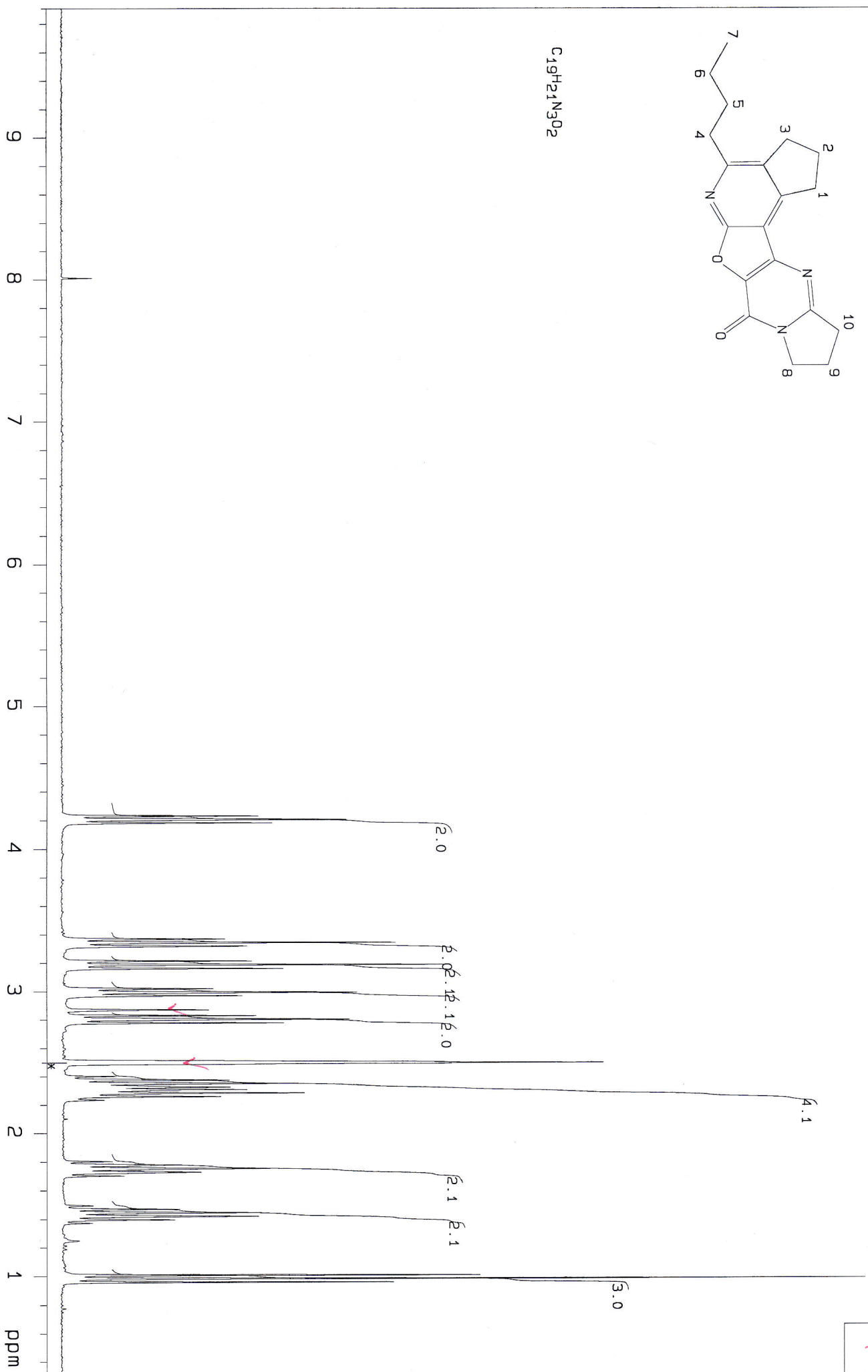
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.2, solvent = DMSO/Cd4 1/3

Nov 8 2011

HA-459

SAMV\_11 na-459

 $C_{19}H_{21}N_3O_2$ 

46

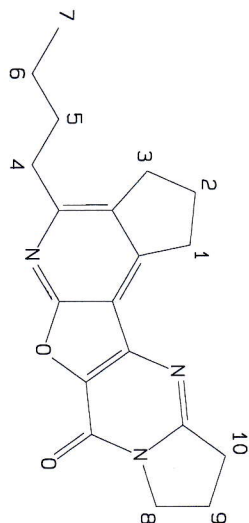
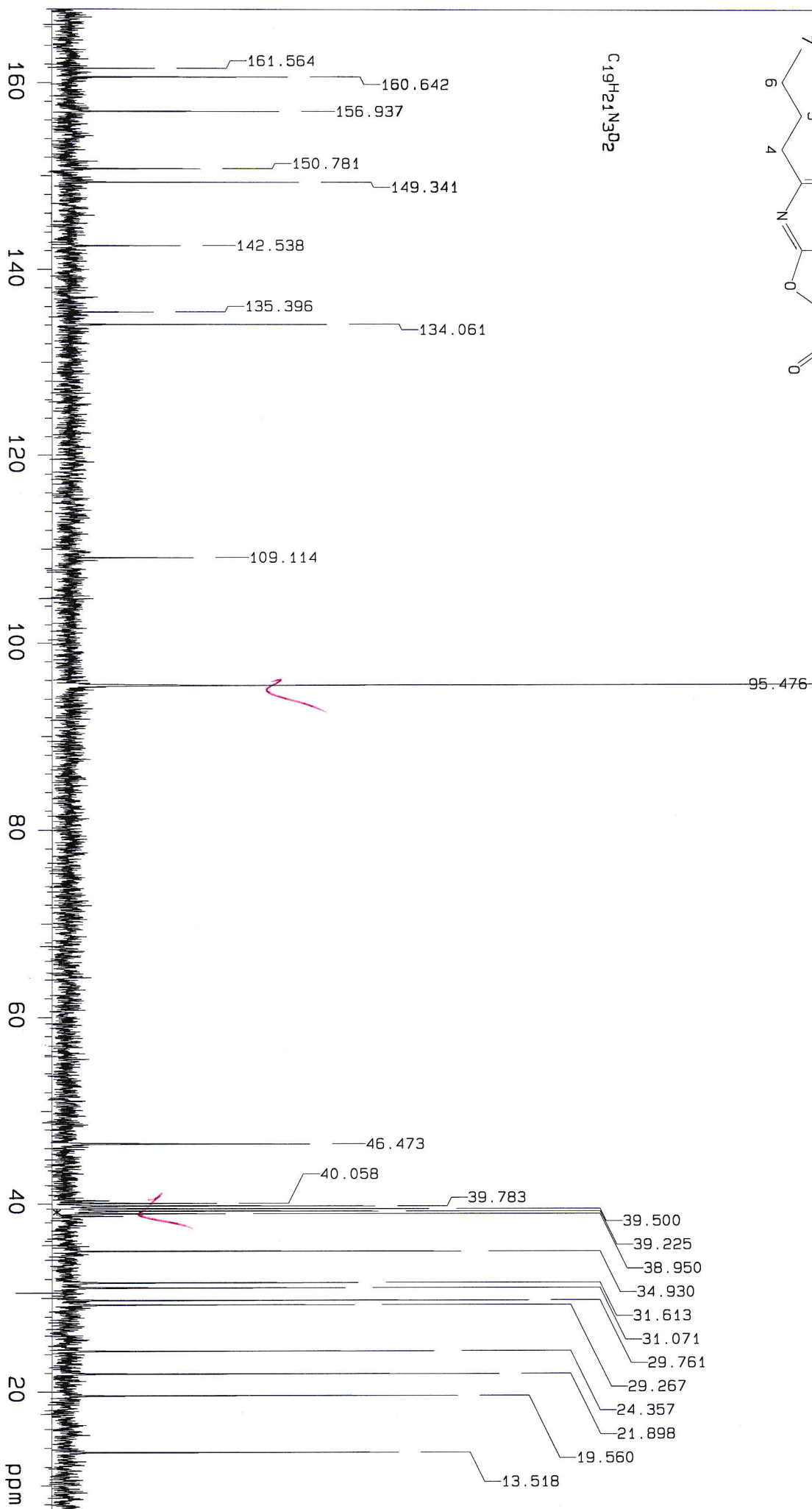
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.462 MHz, nt=368, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO-CD4 1/3

Oct 22 2014

HA-459

SAMV\_11 ha-459

C<sub>13</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>

4c

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

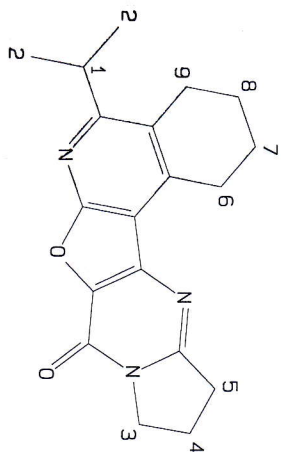
H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CDCl4 1/3

Feb 29 2016

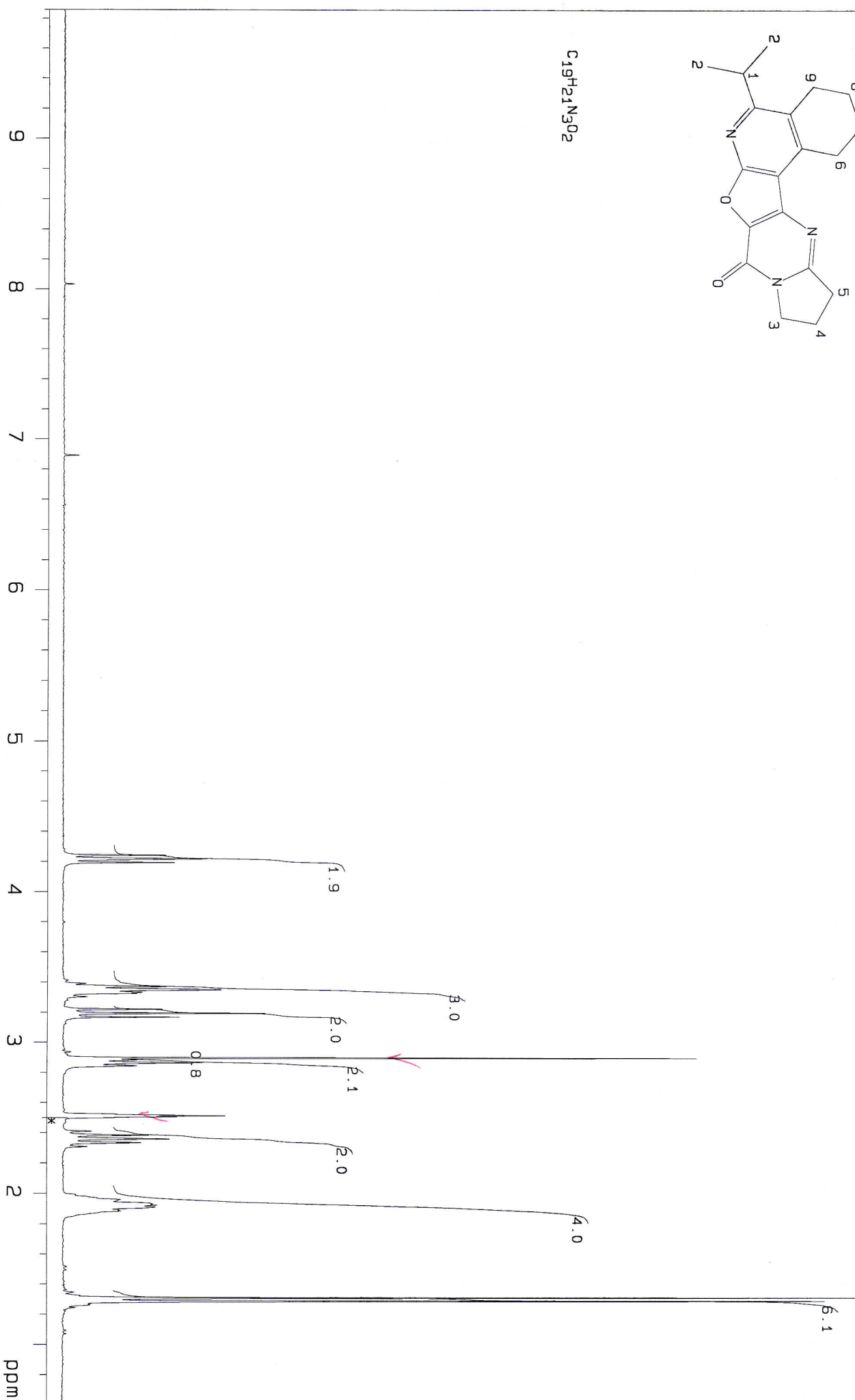
HA-334

SAMV\_16 ha-334

+



C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>



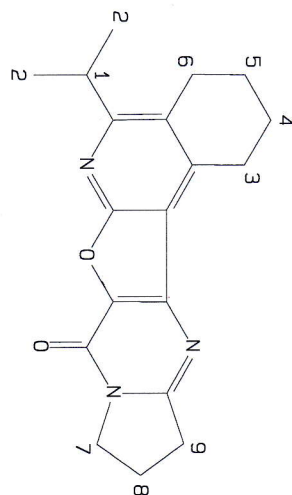
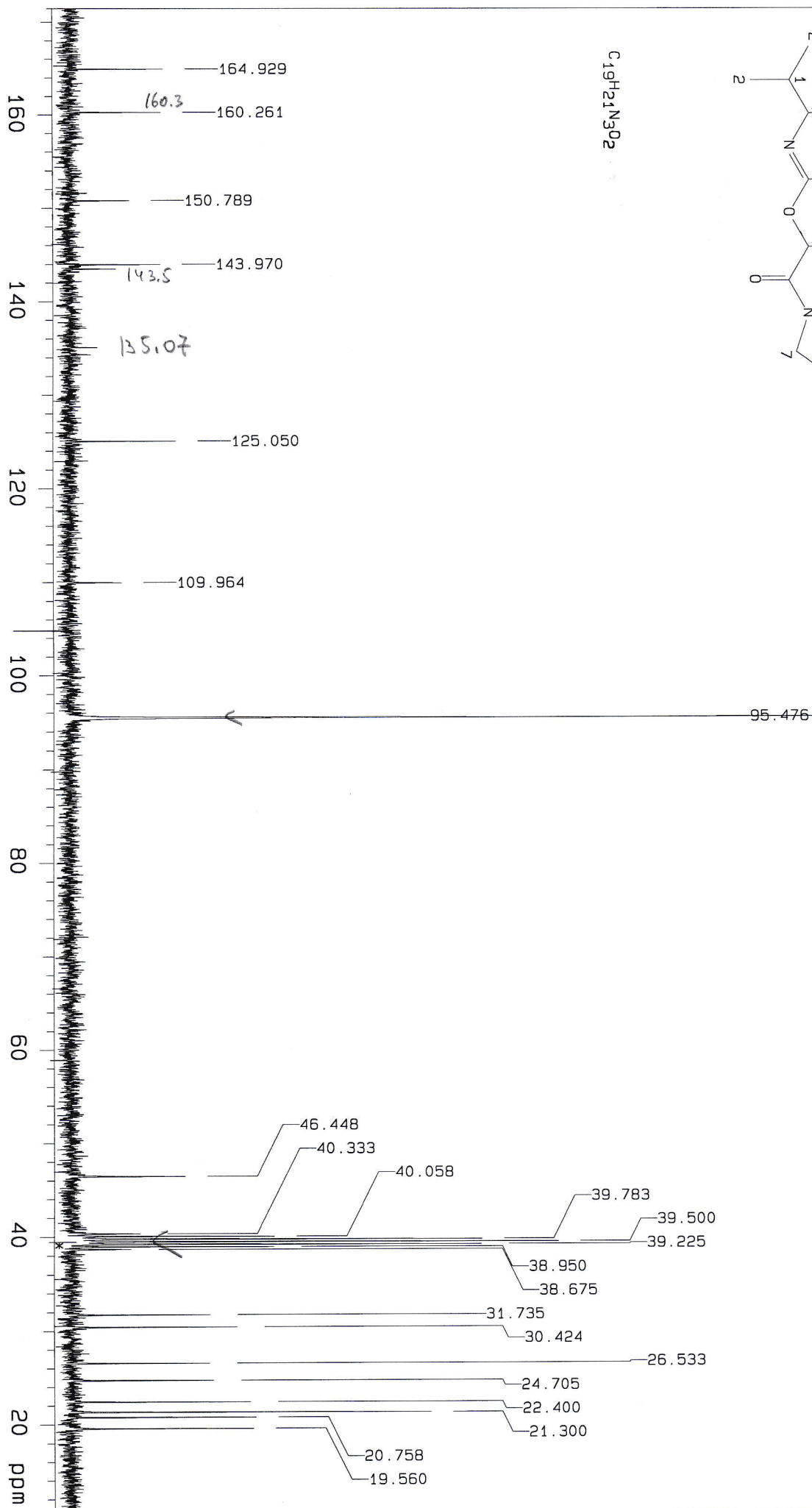
4c

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX  
HA-334

C13 75.462 MHz, nt = 1600, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO-CCl4 1/3

SAMV\_14 ha-334

Oct 20 2014

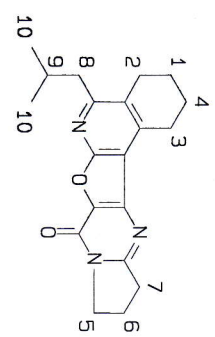
C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>

4d

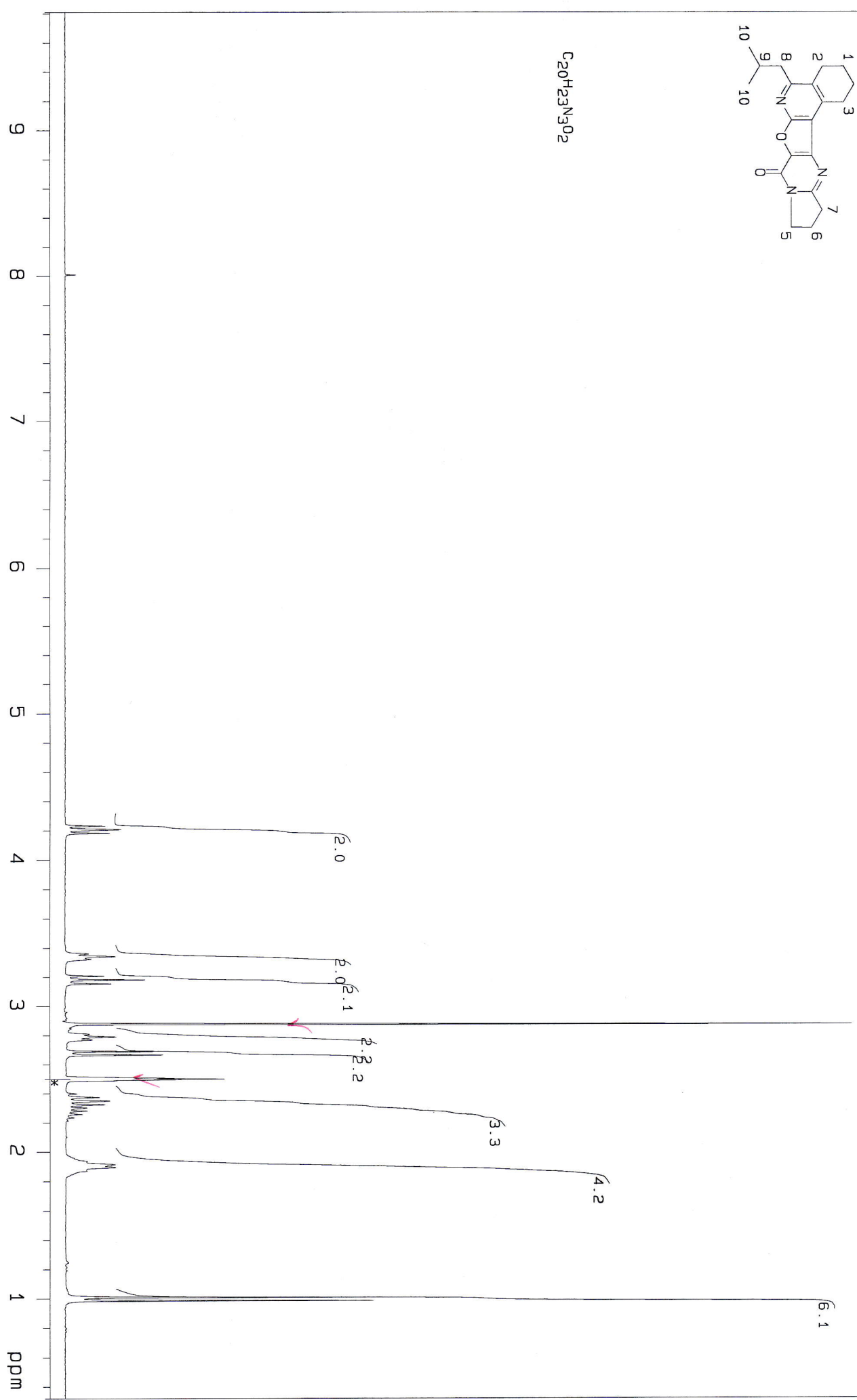
*[Signature]*

HA-329

SAMV\_11 ha-329



C<sub>20</sub>H<sub>23</sub>N<sub>3</sub>O<sub>2</sub>



4d

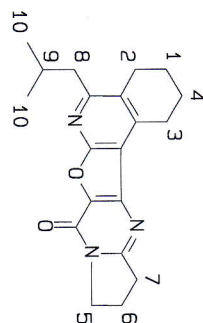
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX  
HA-329

C13 75.462 MHz, nt=432, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO/CDCl4 1/3

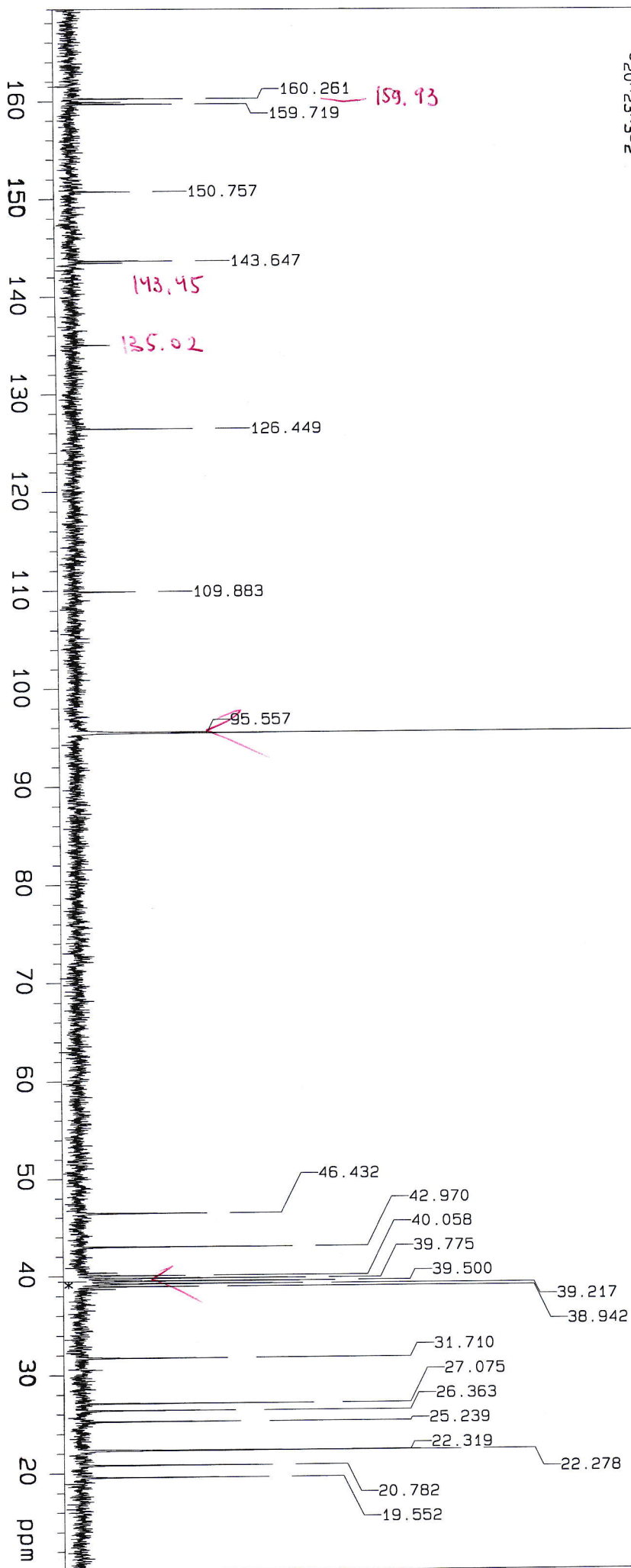
SAWV\_11 ha-329

Oct 21 2014

+



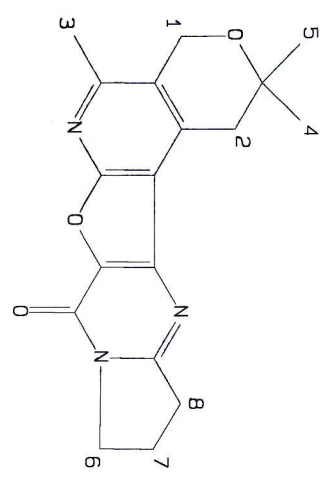
C<sub>20</sub>H<sub>12</sub>N<sub>3</sub>O<sub>2</sub>



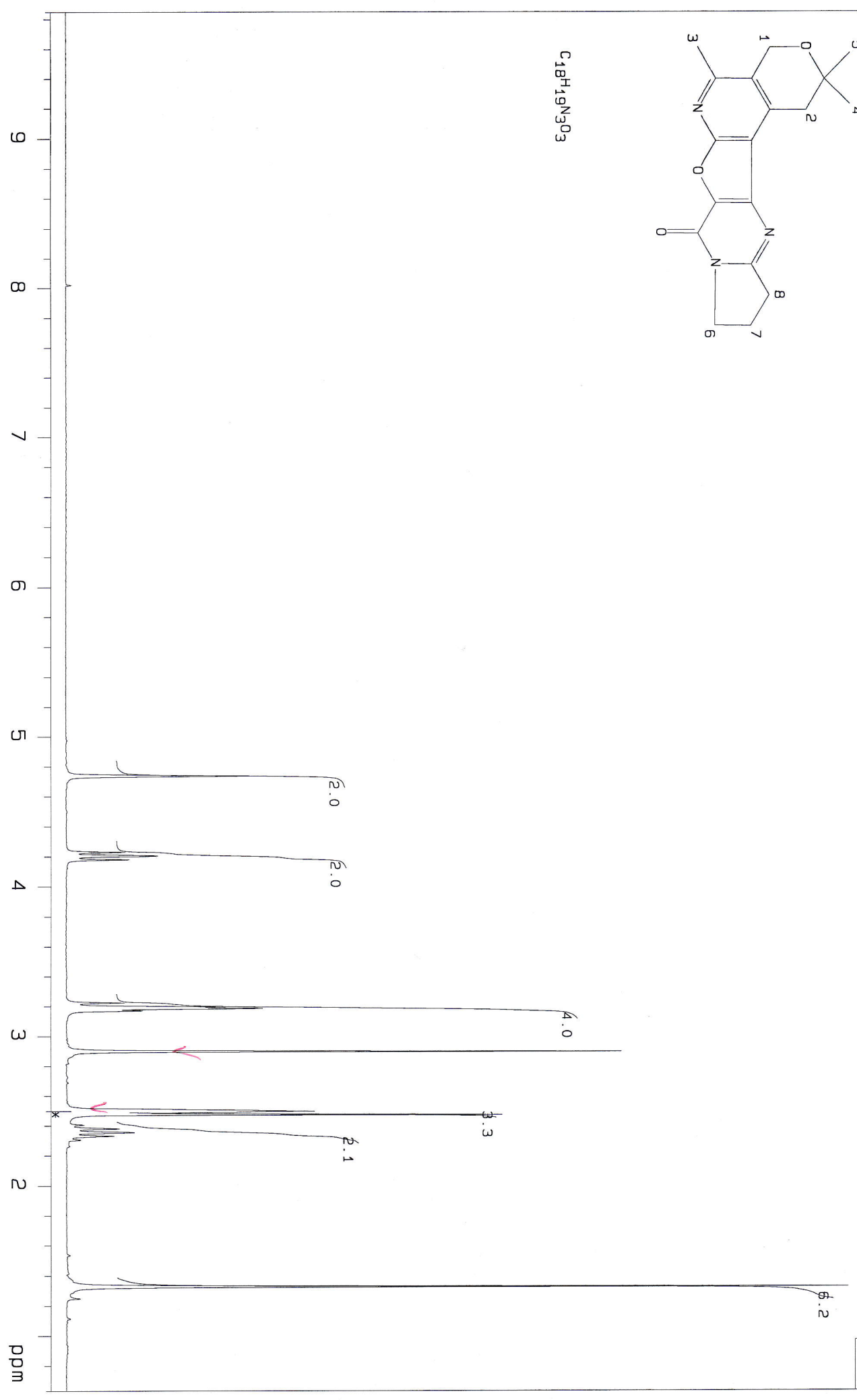
4e

HA-588

SAMV\_12 ha-588



C<sub>1</sub>B<sub>1</sub>H<sub>1</sub>9N<sub>3</sub>O<sub>3</sub>



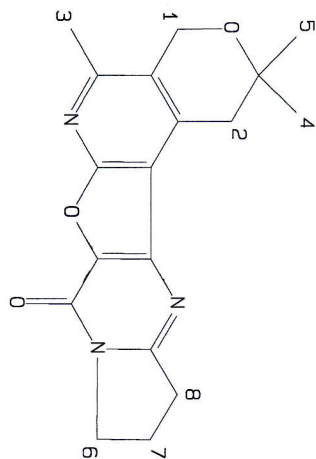
HA-588

4c

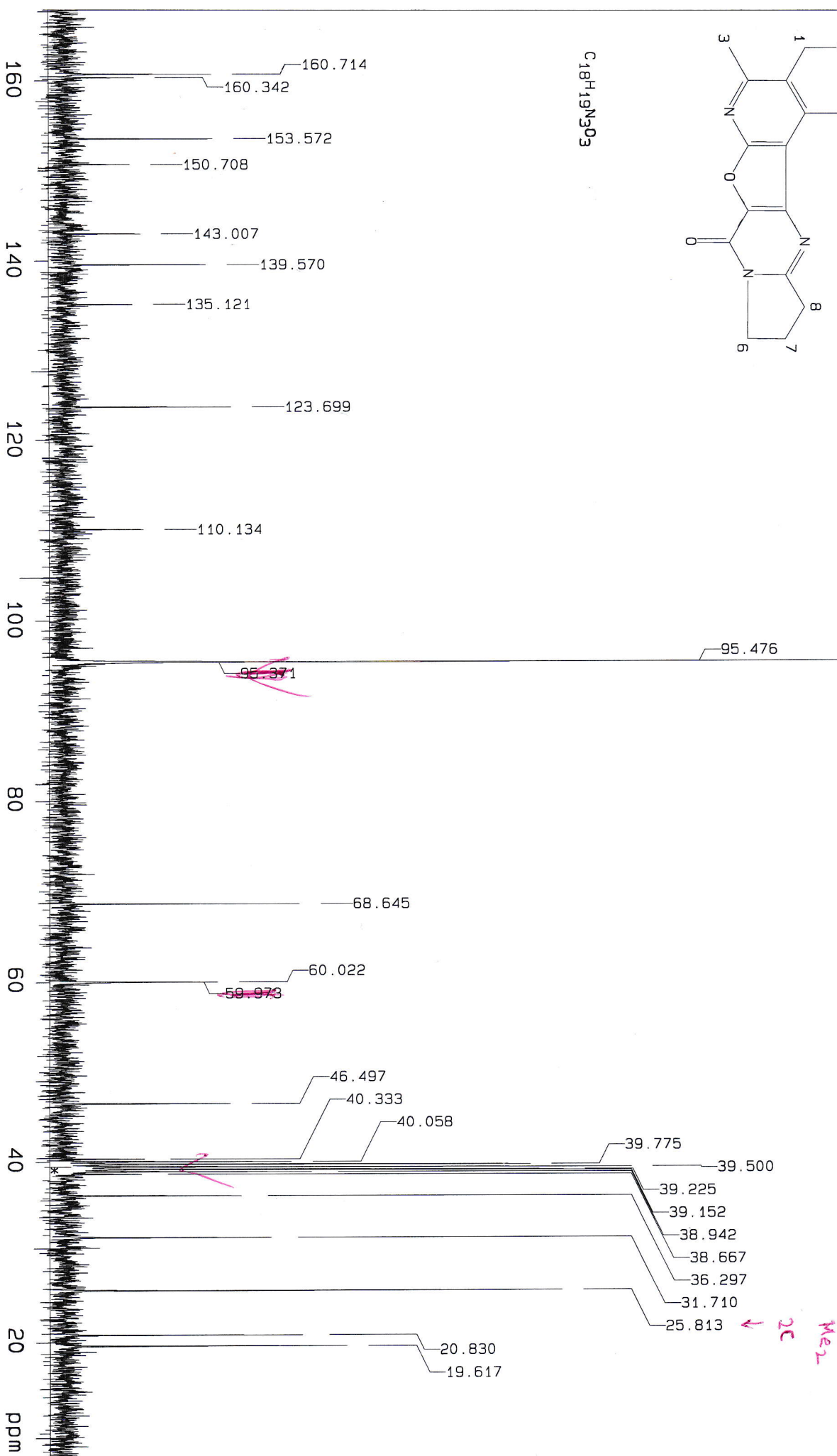
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX  
HA-588

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SAMV\_12 ha-588

Oct 22 2014



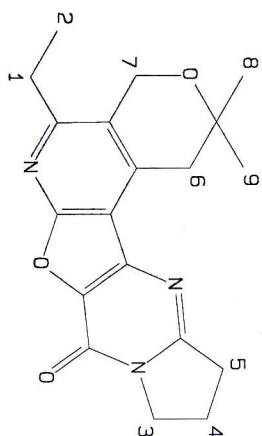
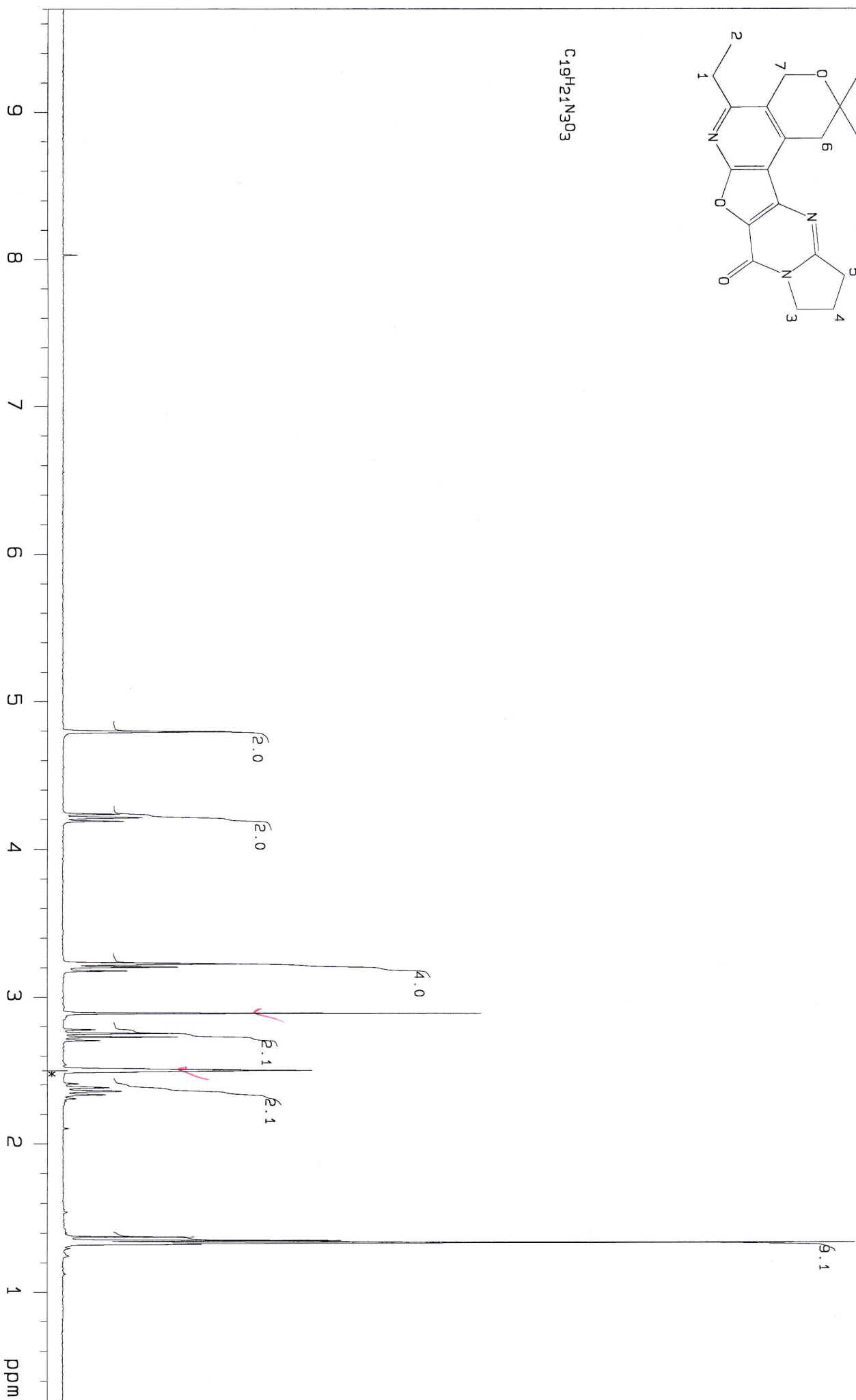
C<sub>18</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>



41p

HA-318

SAMV\_11 ha-318

 $C_{19}H_{21}N_3O_3$ 

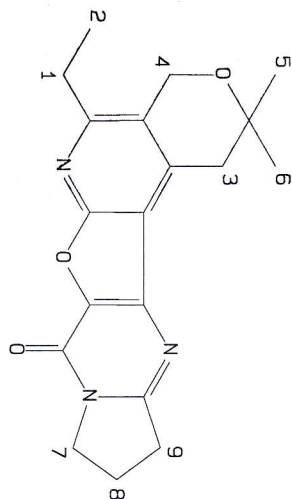
4f

HA-318

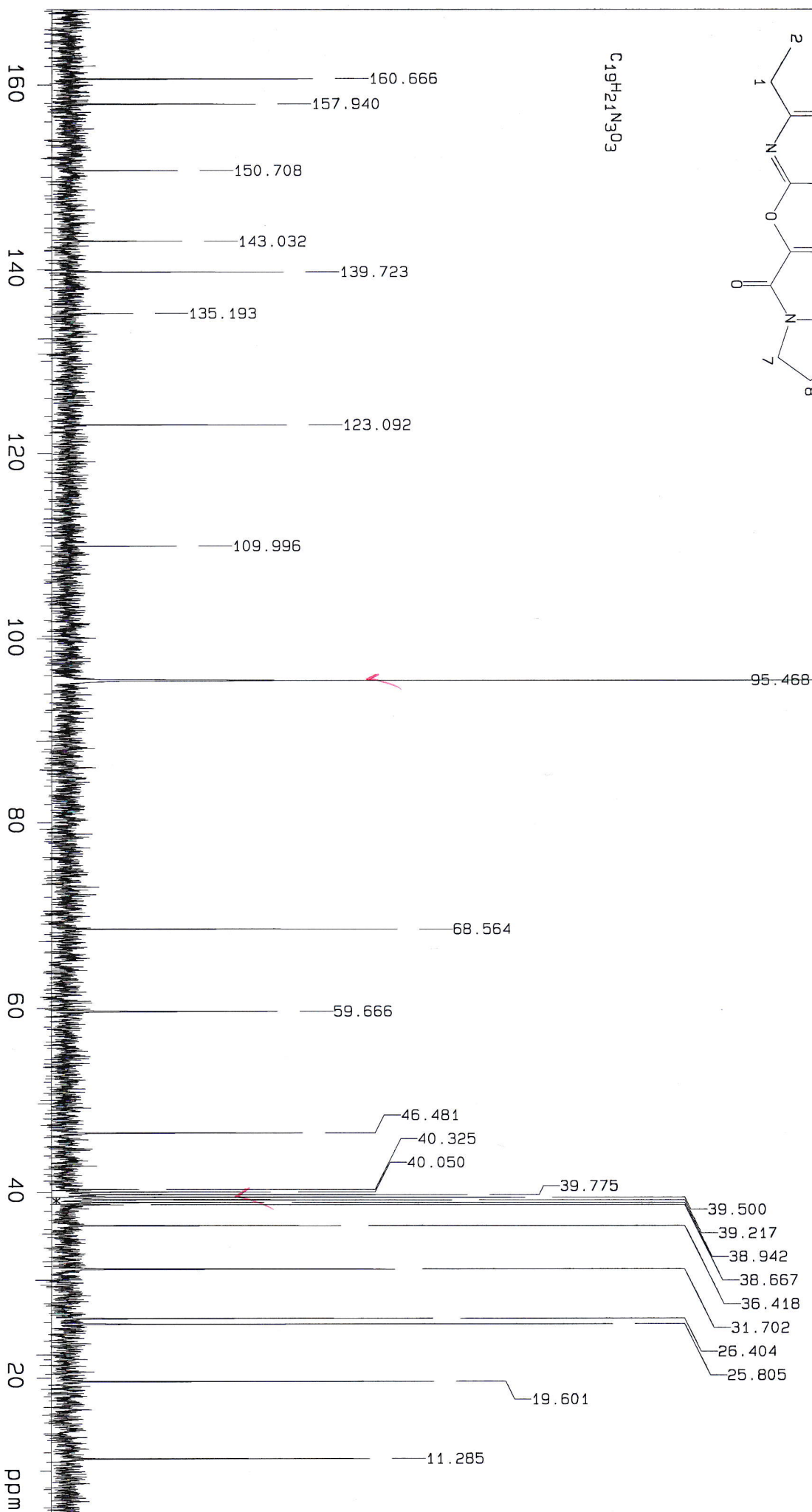
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SAMV\_14 ha-318

Oct 21 2014



C<sub>19</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>

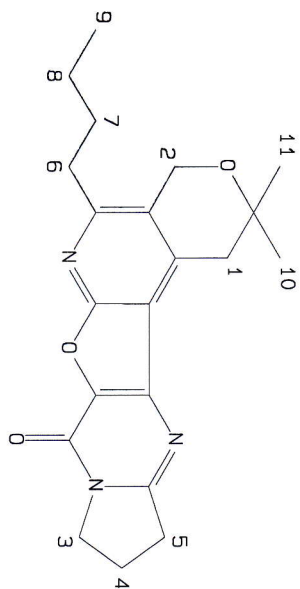
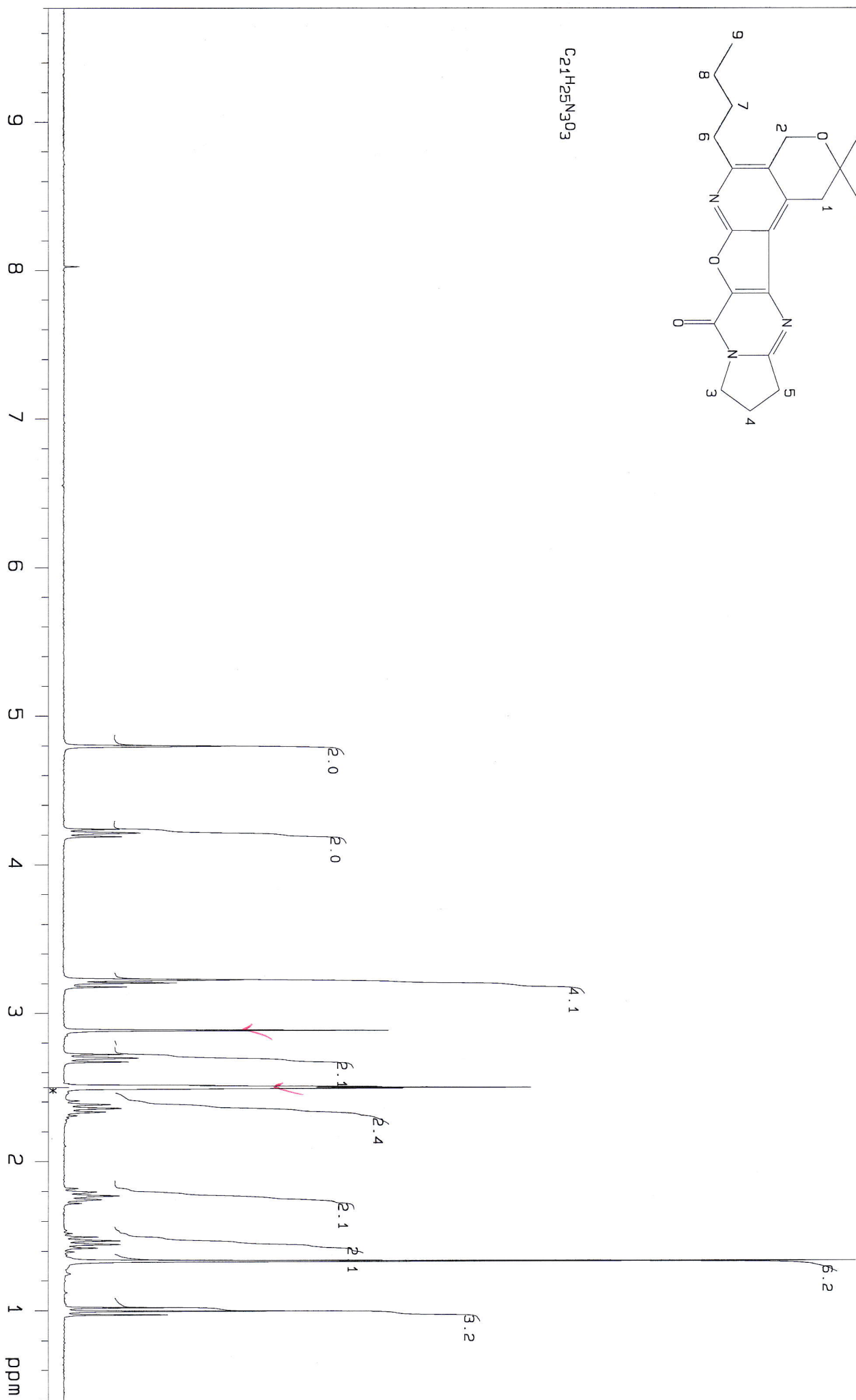


*[Handwritten signature]*

49

HA-455

SAMV\_11 ha-455

 $C_{21}H_{25}N_3O_3$ 

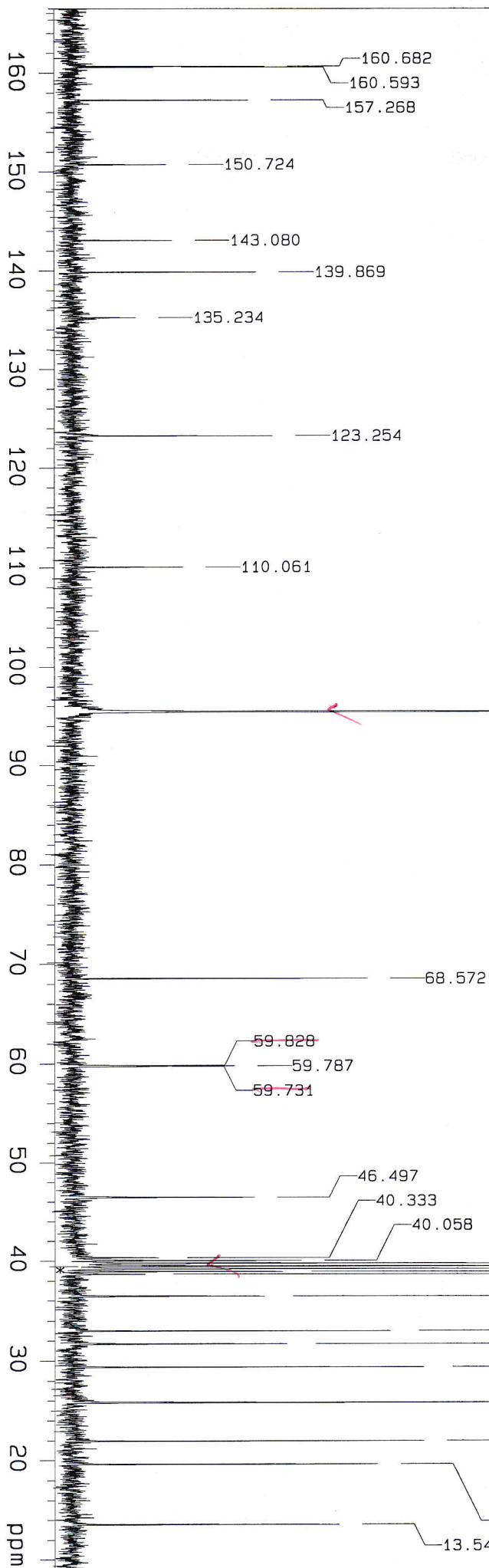
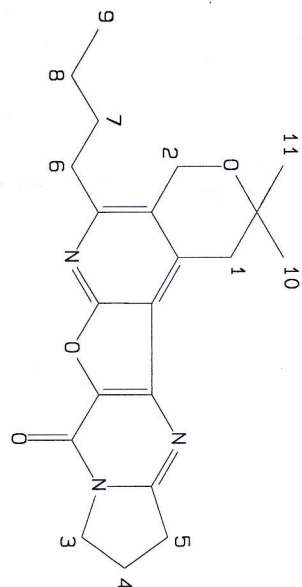
49

HA-455

C13 75.462 MHz, nt = 1008, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO-CCl4 1/3

SAMV\_14 ha-455

Oct 21 2014

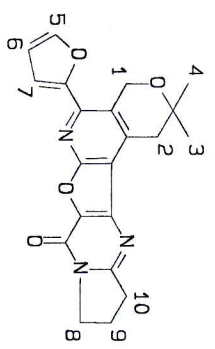


*[Handwritten signature]*

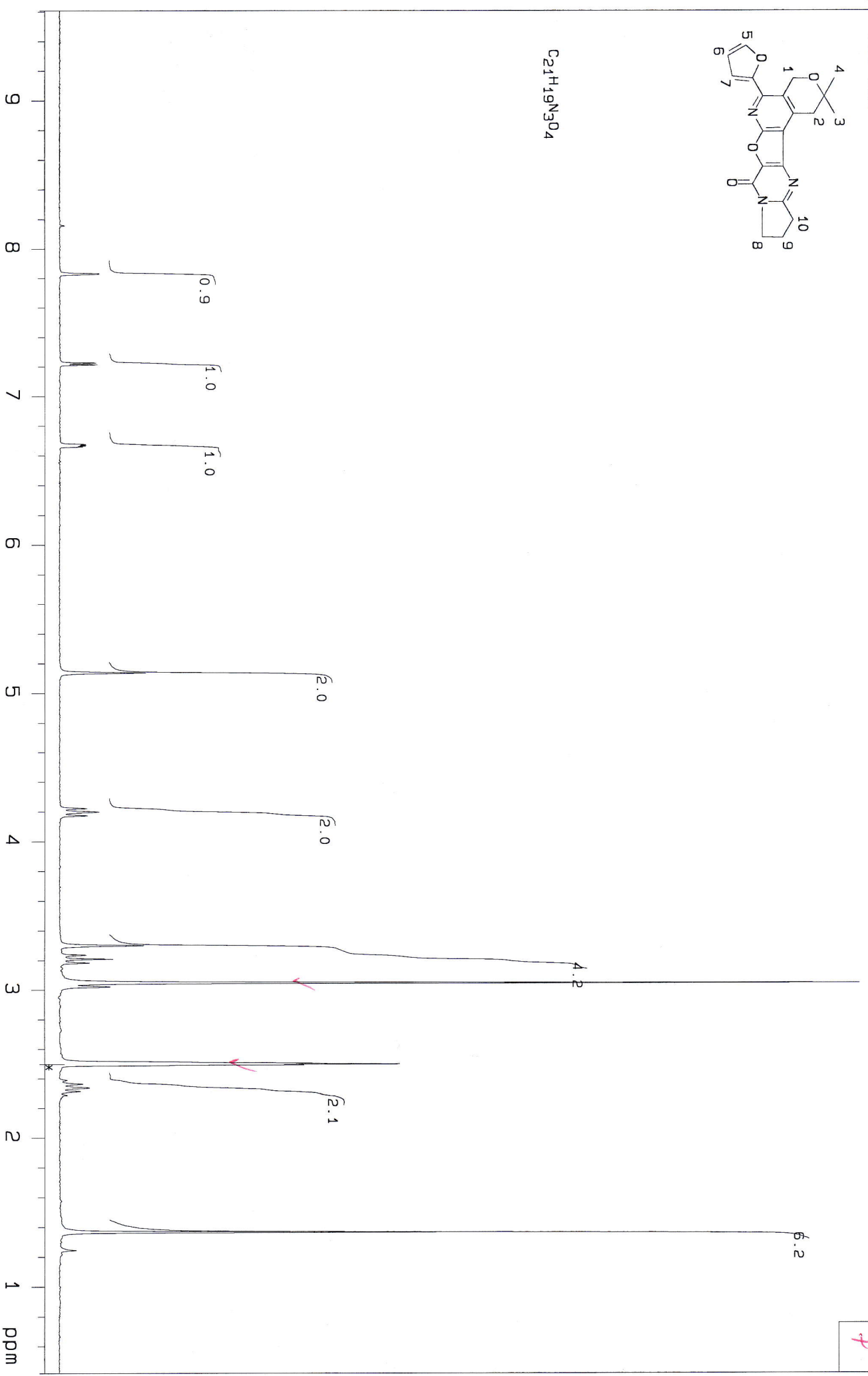
4h

HA-450

SAMV\_11 na-450



C<sub>21</sub>H<sub>19</sub>N<sub>3</sub>O<sub>4</sub>



+

*[Handwritten signature]*

5a

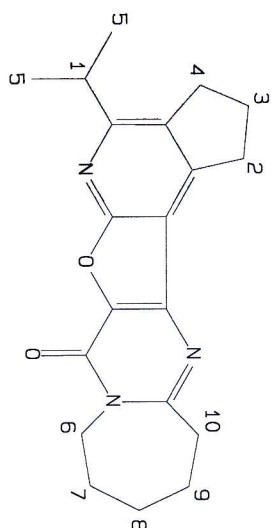
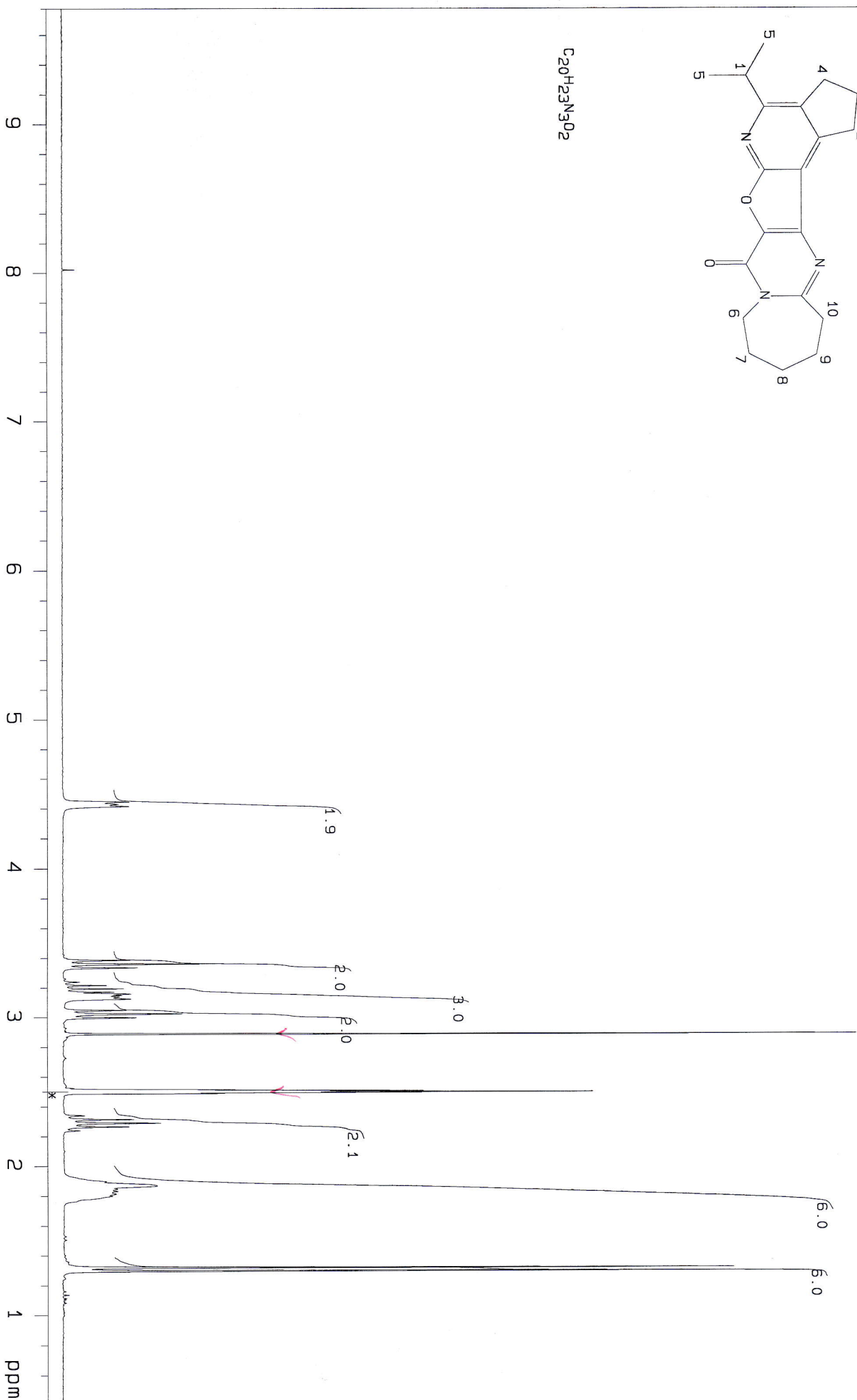
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.077 MHz, nt=16, np=16000, temp=30.0 C, lb=-0.2, solvent=DMSO-CD4 1/3

HA-654

SAMV\_12 ha-654

Apr 6 2012

 $C_{20}H_{23}N_3O_2$ 

5a

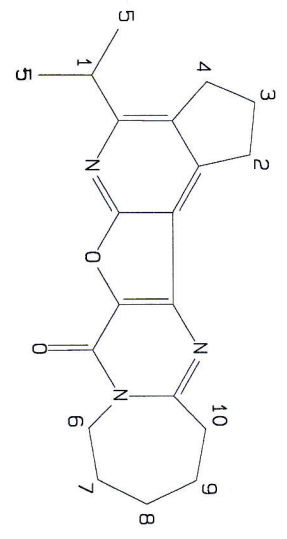
*Handwritten signature*

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX  
**HA-654**

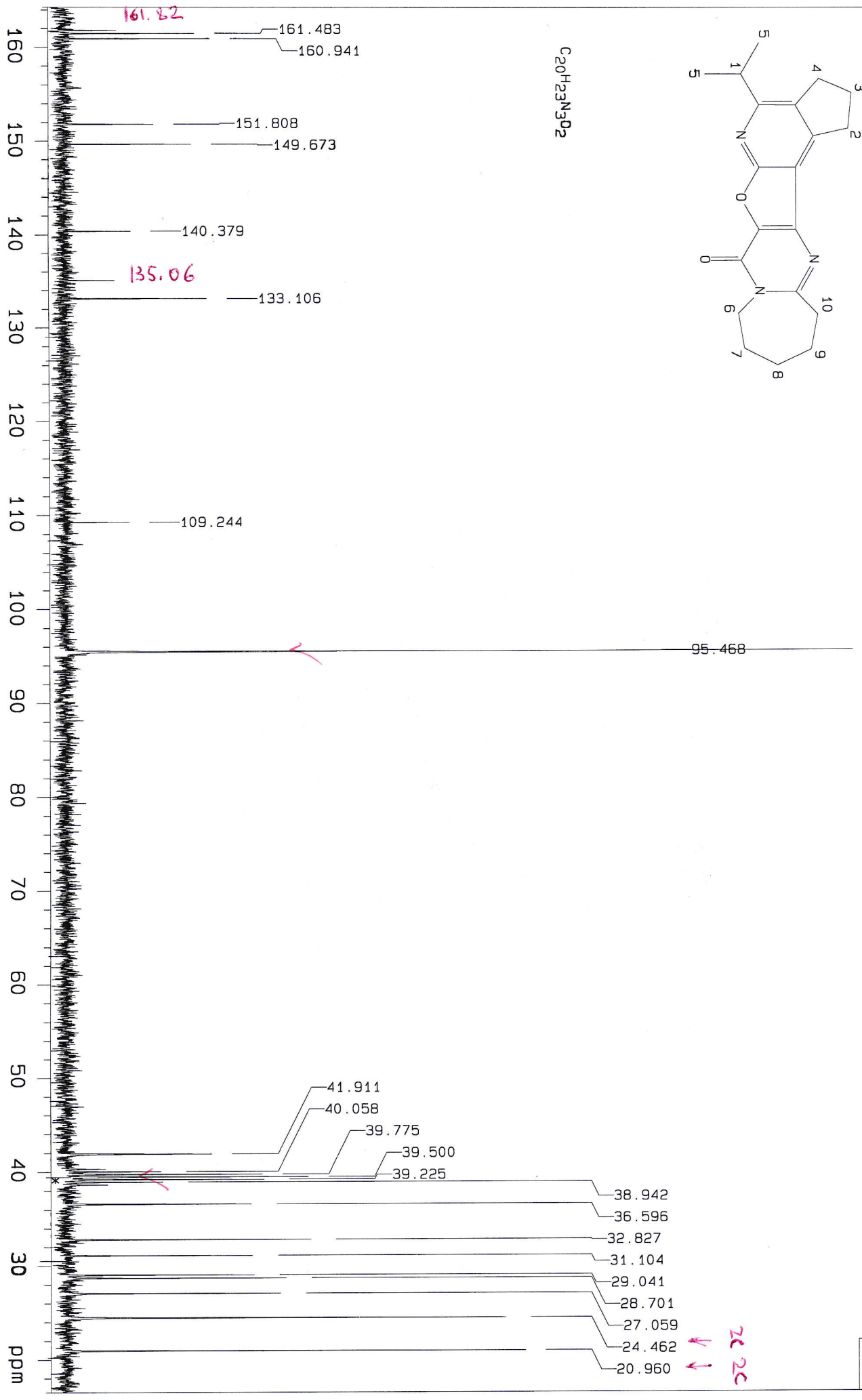
C13 75.462 MHz, nt=256, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO-CD4 1/3

SAMV\_12 ha-654

Oct 22 2014



C<sub>20</sub>H<sub>23</sub>N<sub>3</sub>O<sub>2</sub>



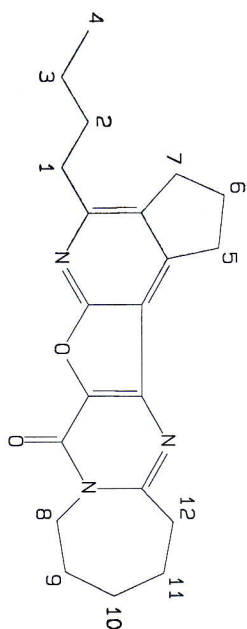
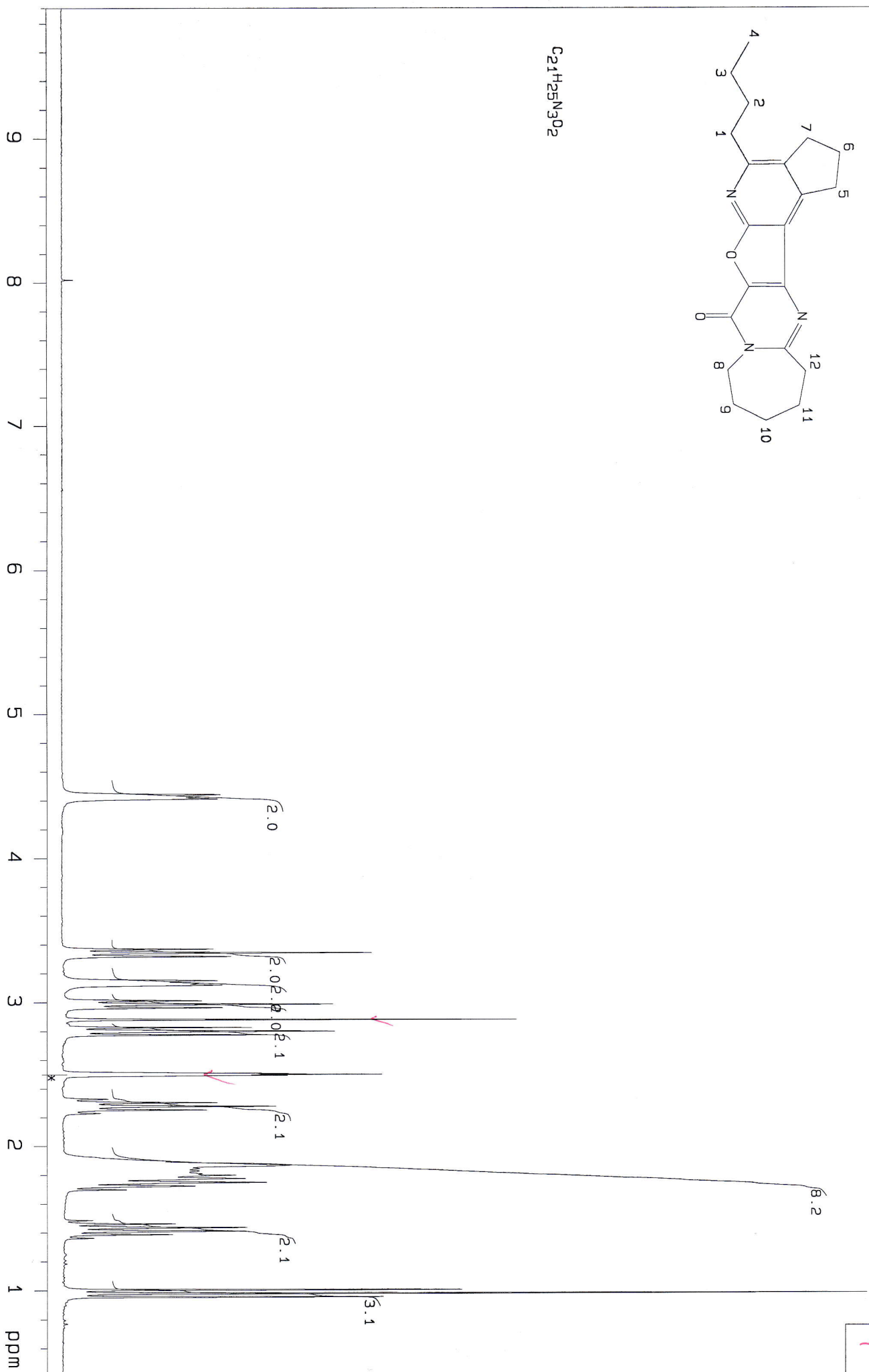
2c 2c

+

56

HA-554

NOCT\_12 ha-554

 $C_{21}H_{25}N_3O_2$ 

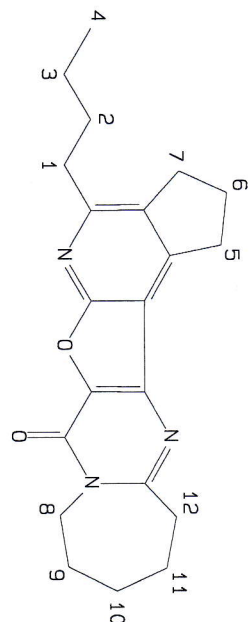
56

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX  
HA-554

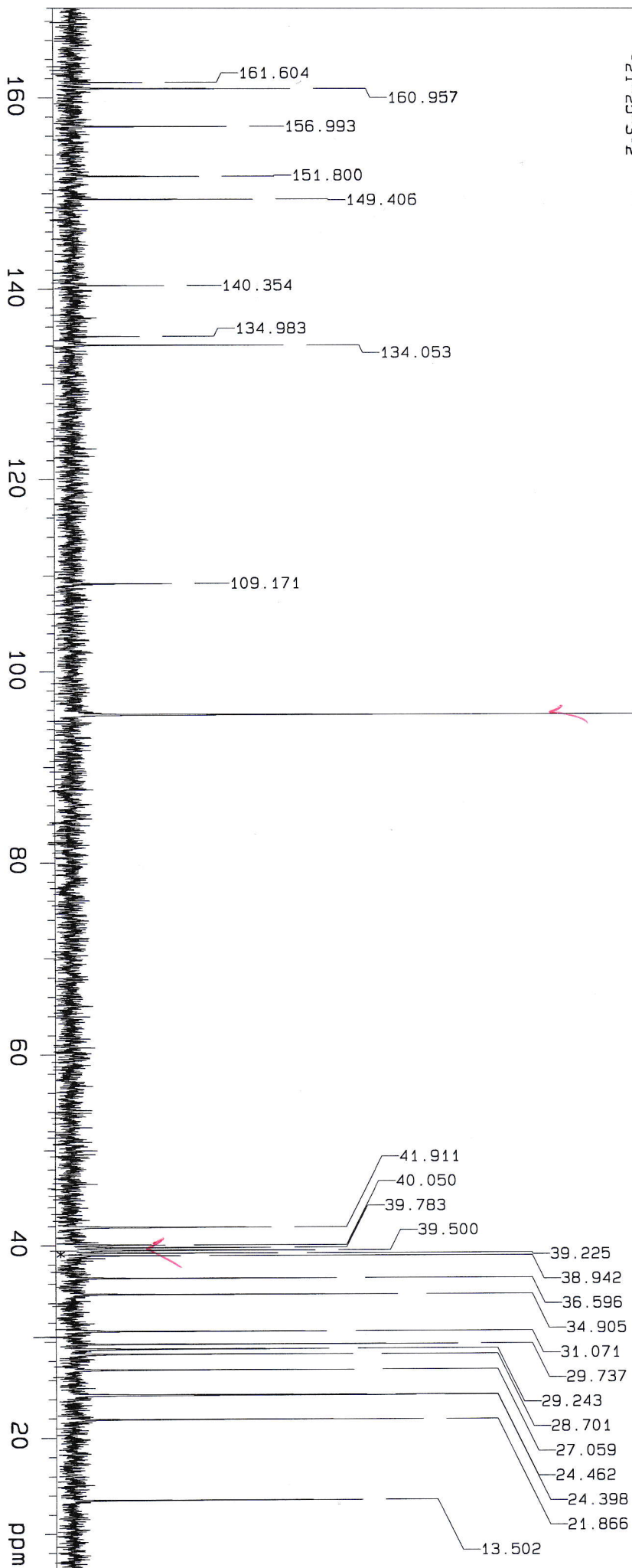
C13 75.462 MHz, nt = 192, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/C4 1/3

SAMV\_14 ha-554

Oct 21 2014



C<sub>21</sub>H<sub>25</sub>N<sub>3</sub>O<sub>2</sub>



5c

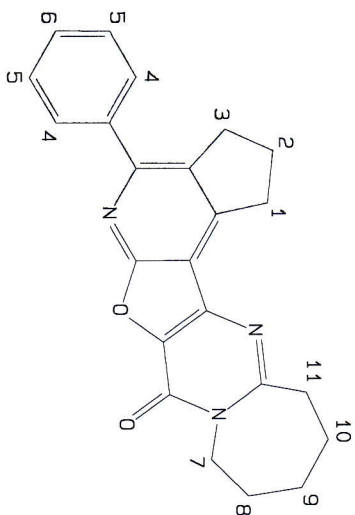
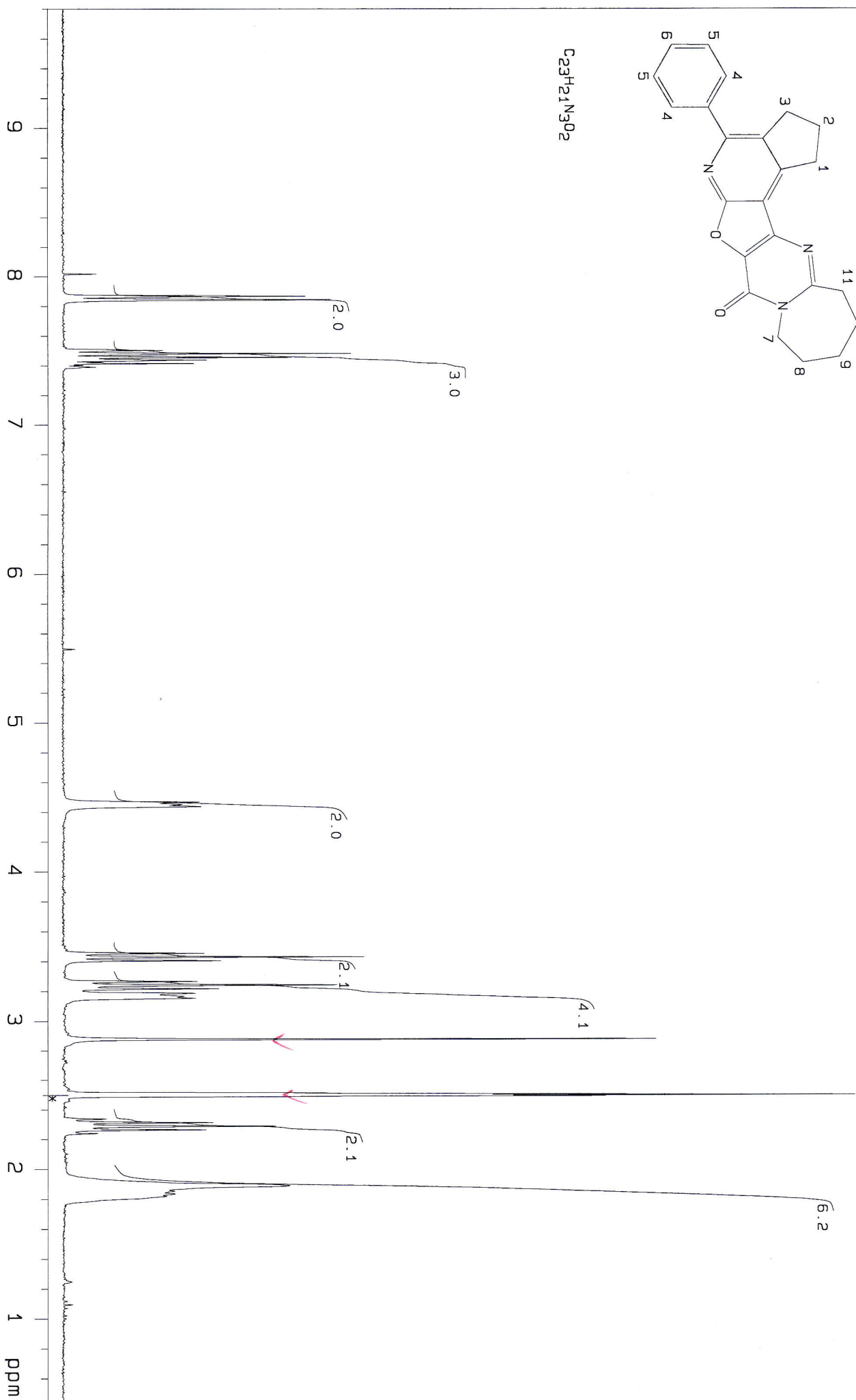
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.2, solvent = DMSO-CD<sub>3</sub> 1/3

Dec 26 2011

HA-553

SAMV\_11 ha-553

C<sub>23</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>

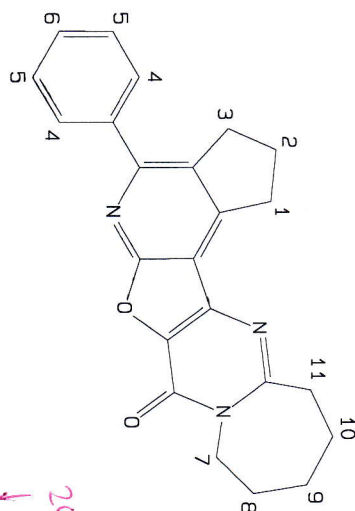
5c

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX  
HA-553

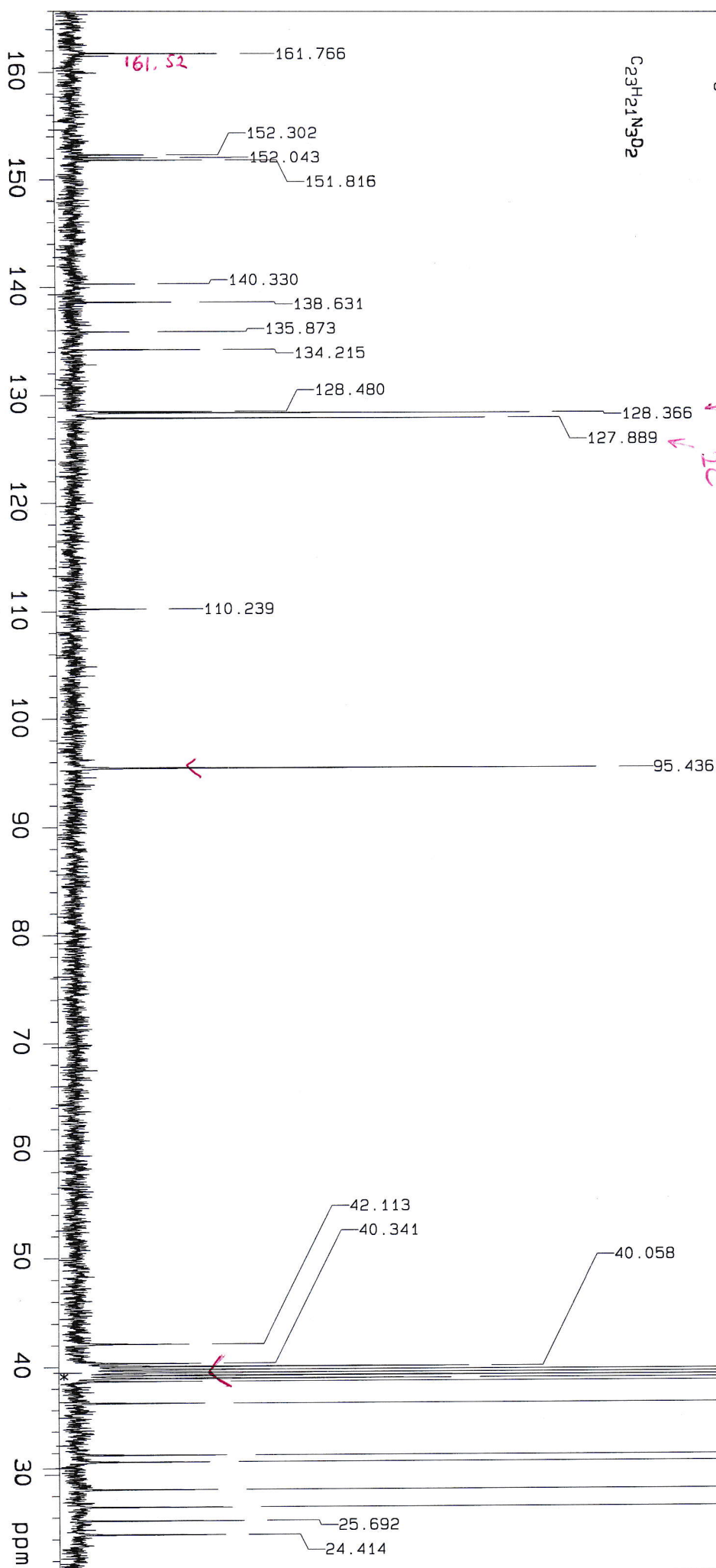
C13 75.462 MHz, nt=720, mp=19998, temp=30.0 C, lb=1.0, solvent=DMSO-CD4 1/3

SAMV\_11 ha-553

Oct 22 2014



C<sub>23</sub>H<sub>21</sub>N<sub>3</sub>O<sub>2</sub>



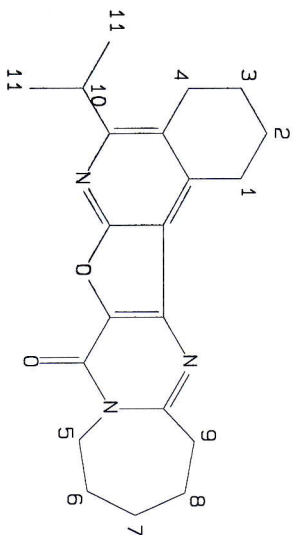
+

hpc

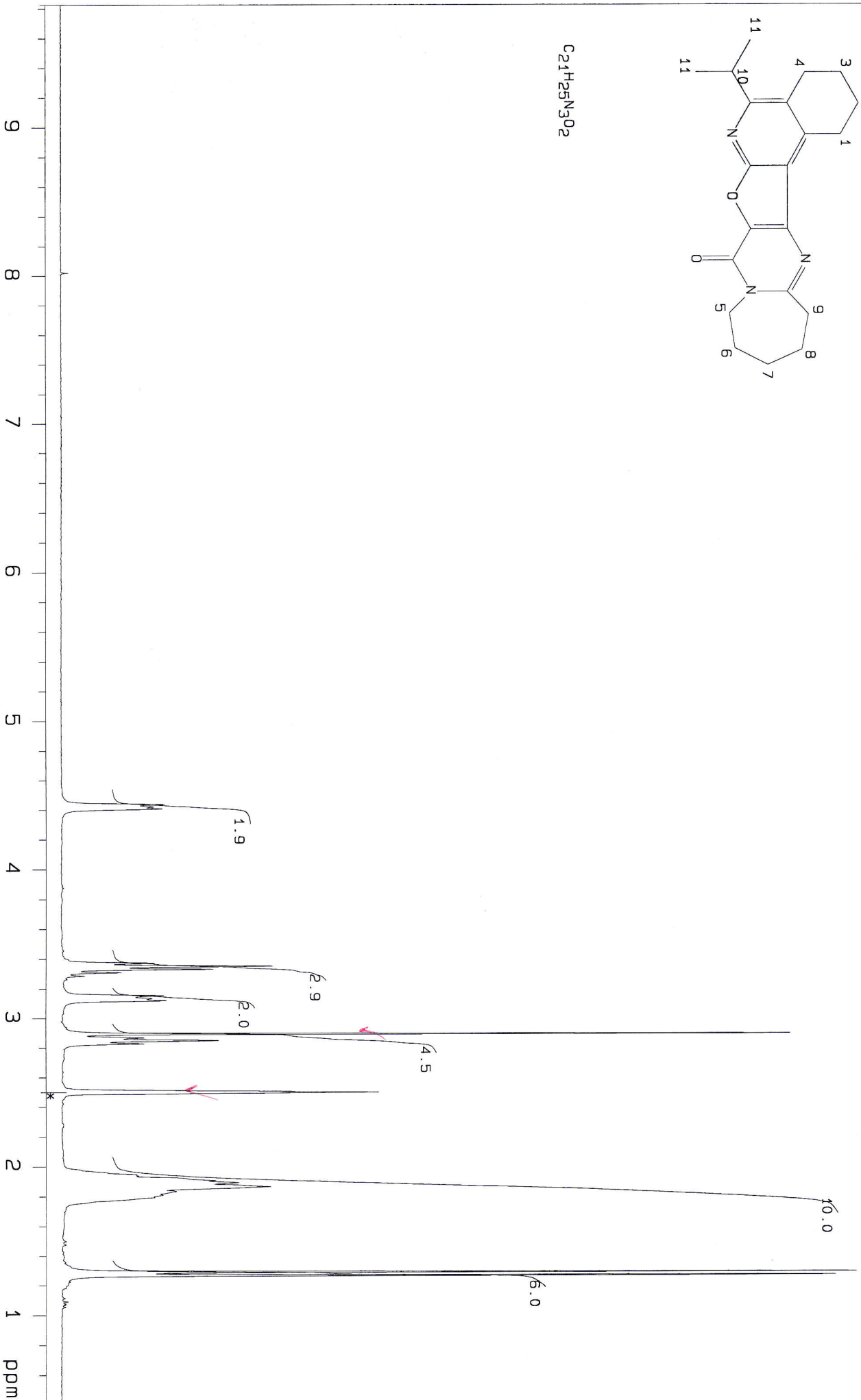
5d

HA-583

SAMV\_12 ha-583



C<sub>21</sub>H<sub>25</sub>N<sub>3</sub>O<sub>2</sub>



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5d

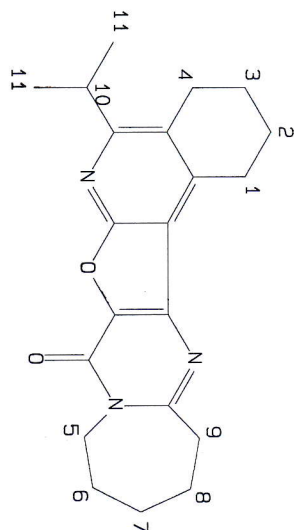
HA-583

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

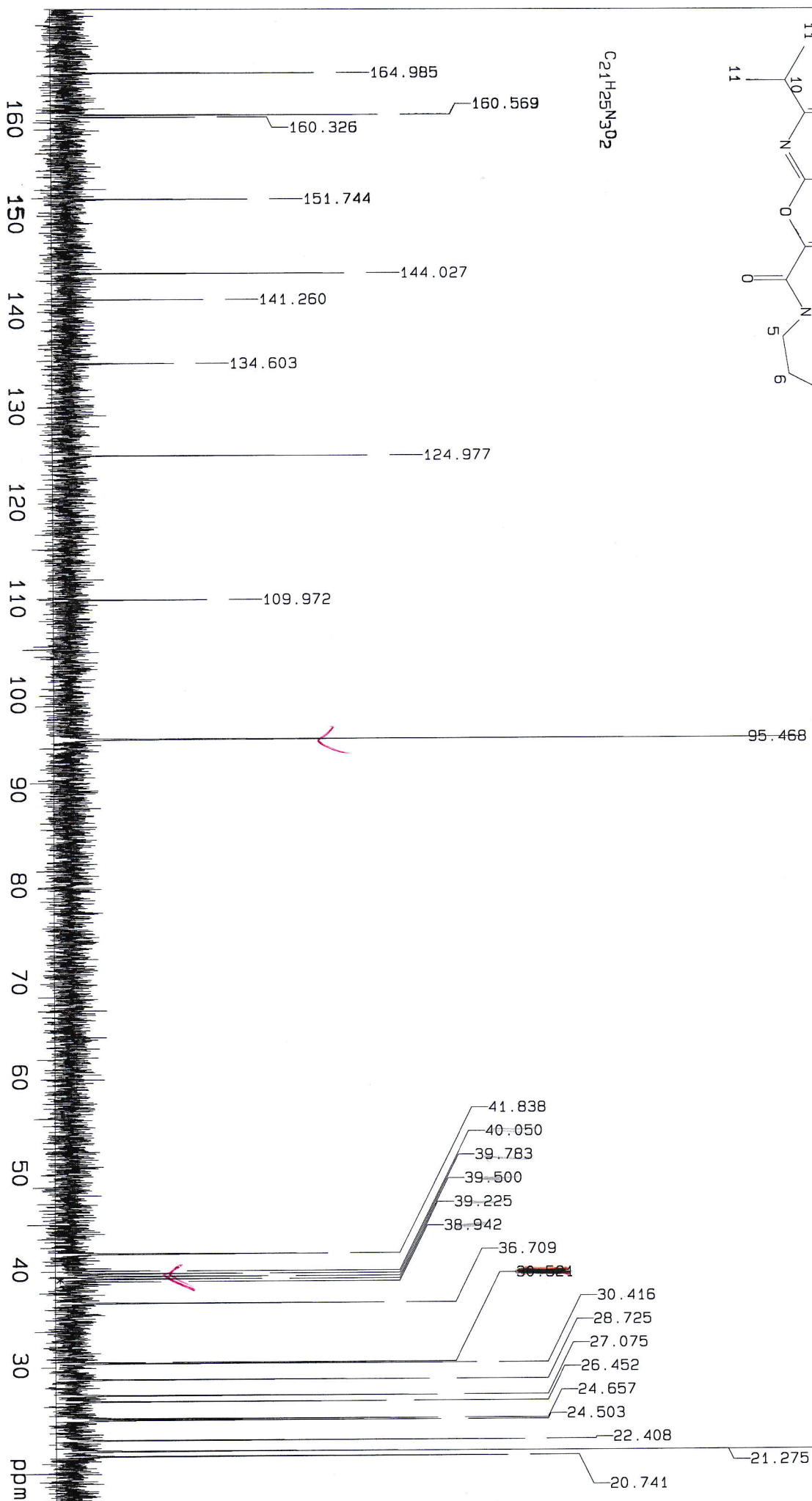
C13 75.462 MHz, nt=240, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO-CD4 1/3

SAMV\_12 ha-583

Oct 22 2014



C<sub>21</sub>H<sub>25</sub>N<sub>3</sub>O<sub>2</sub>

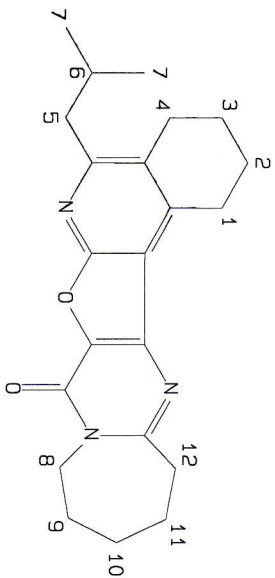


*[Handwritten signature]*

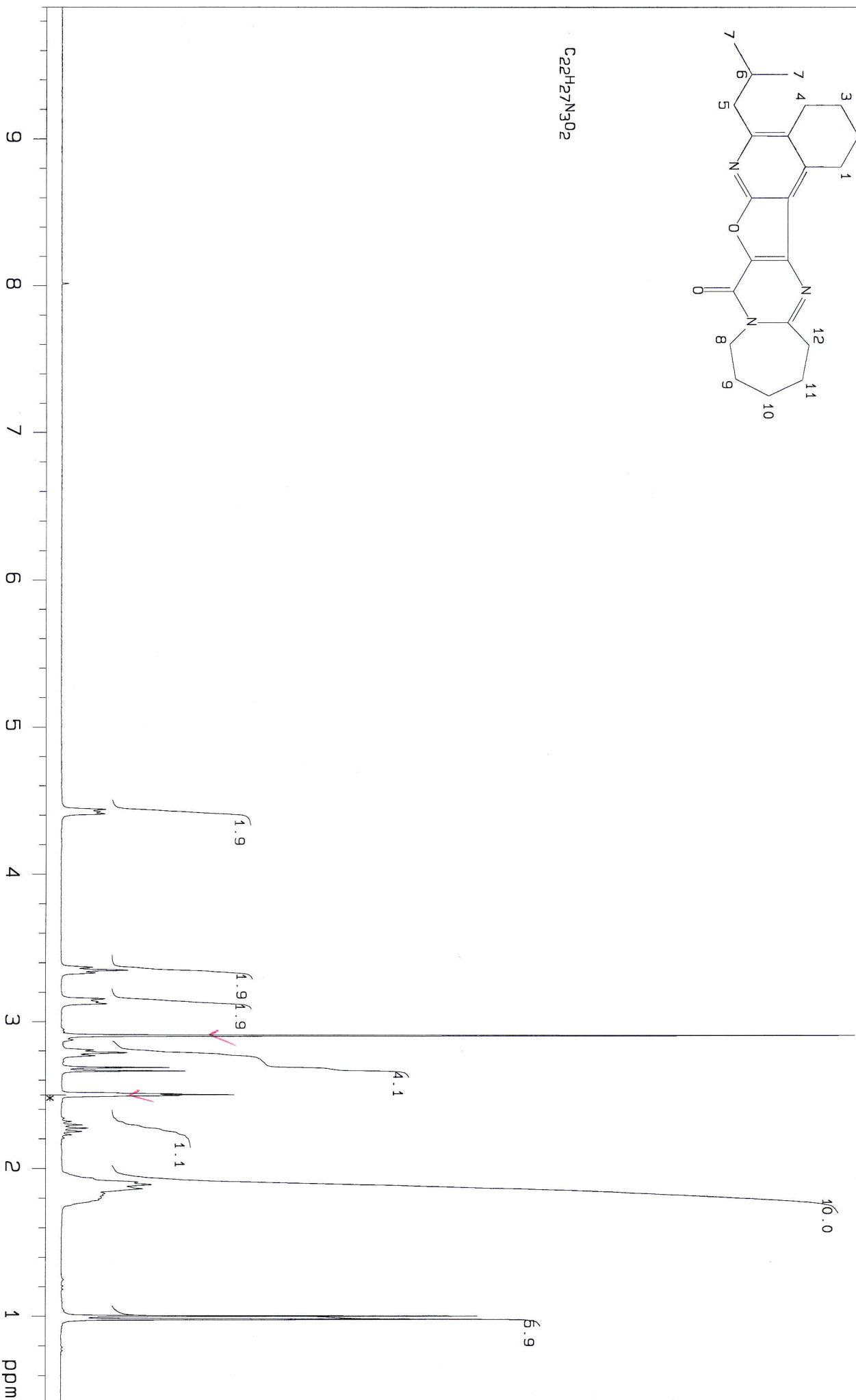
5e

HA-547

SAMV\_11 ha-547



C<sub>22</sub>H<sub>27</sub>N<sub>3</sub>O<sub>2</sub>



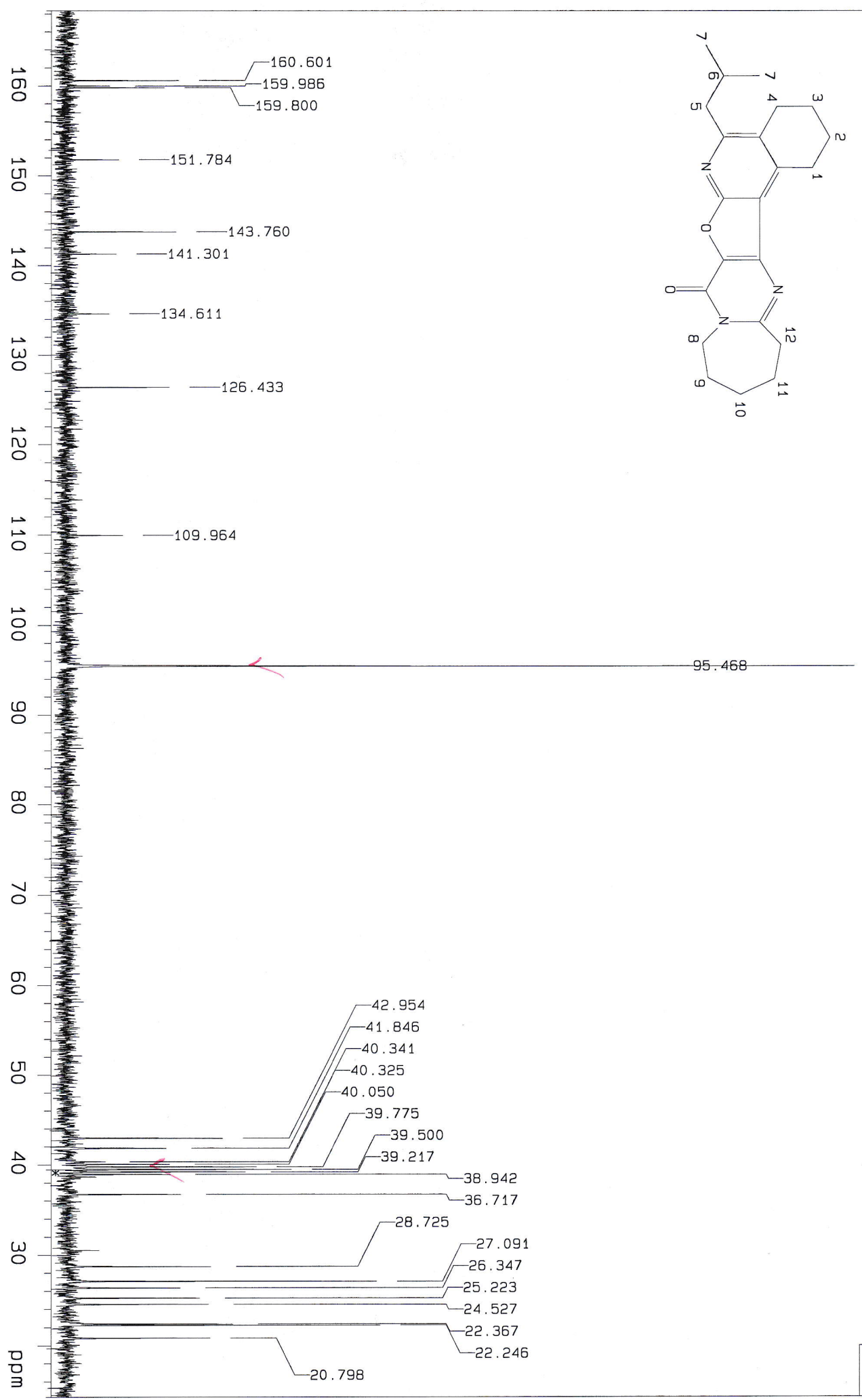
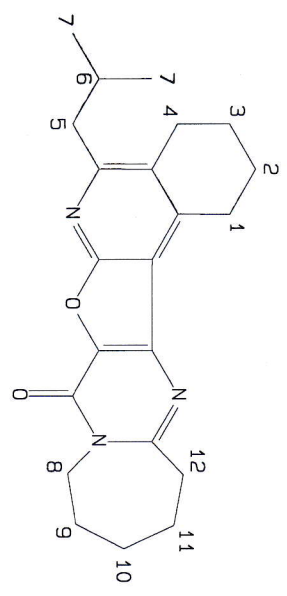
*[Handwritten signature]*

5e

HA-547

SAMV\_14 na-547

Oct 22 2014



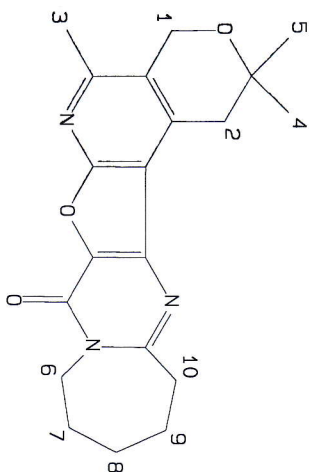
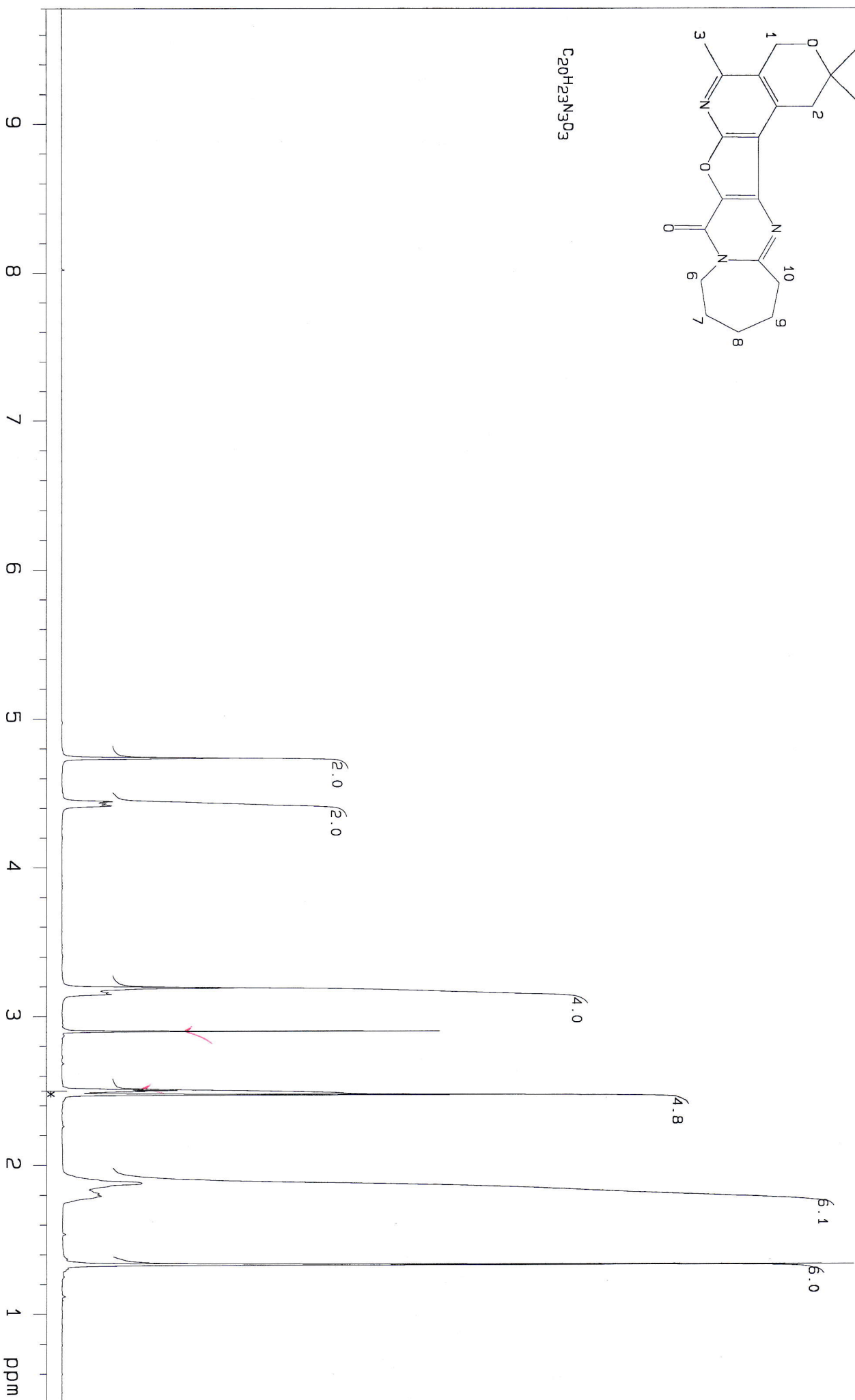
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*[Handwritten signature]*

52

HA-587

SAMV\_12 ha-587

 $C_{20}H_{23}N_3O_3$ 

5f

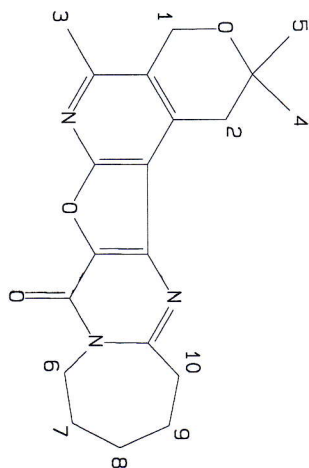
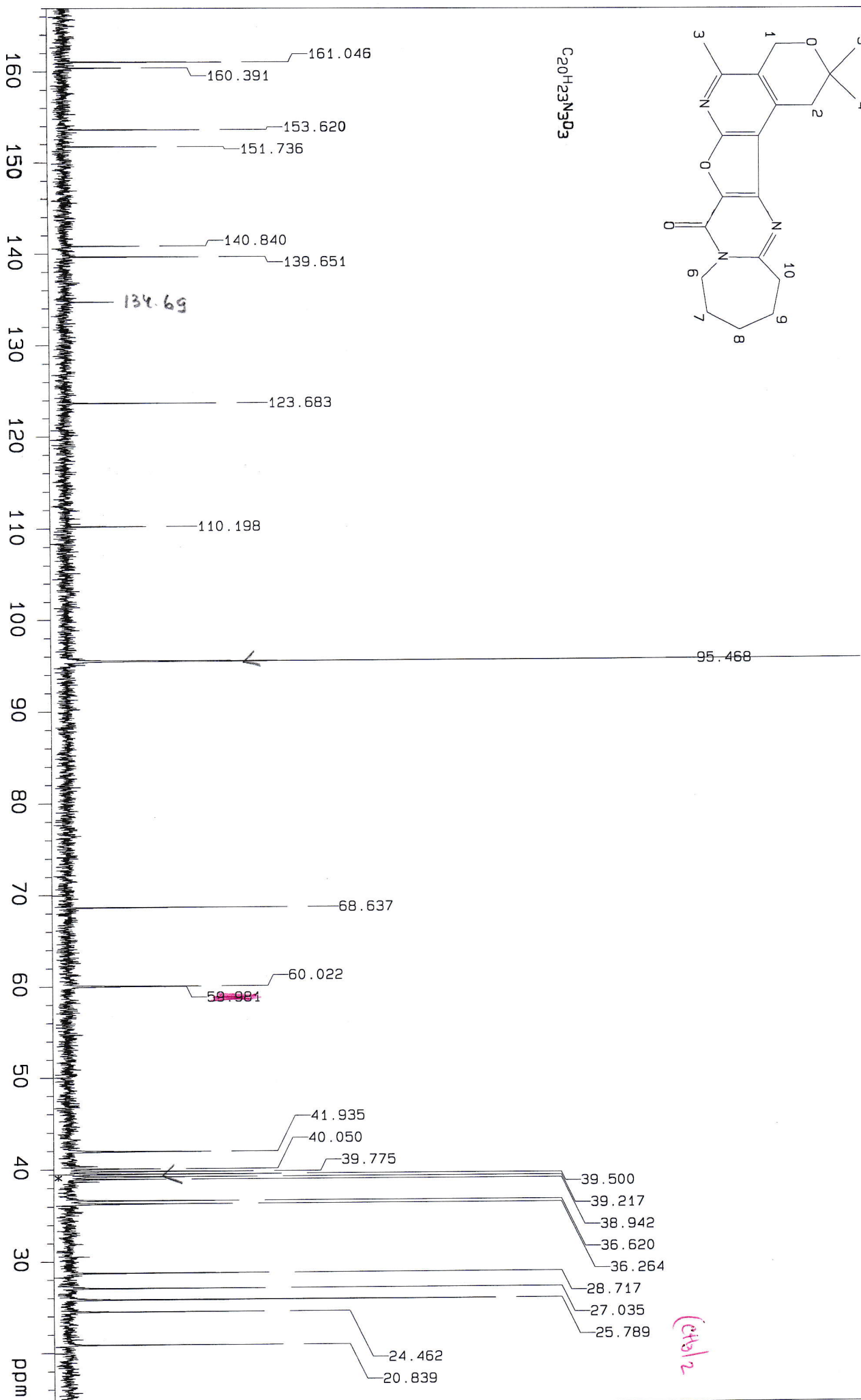
HA-587

Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.462 MHz, nt = 480, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CDCl4 1/3

SAMV\_12 ha-587

Oct 22 2014

C<sub>20</sub>H<sub>23</sub>N<sub>3</sub>O<sub>3</sub>(CH<sub>2</sub>)<sub>2</sub>

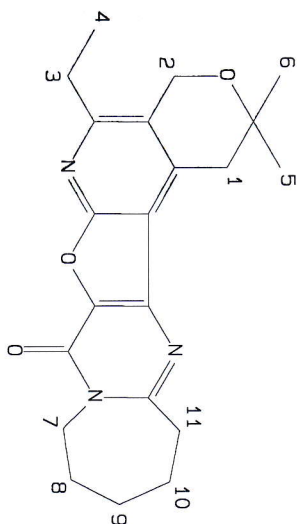
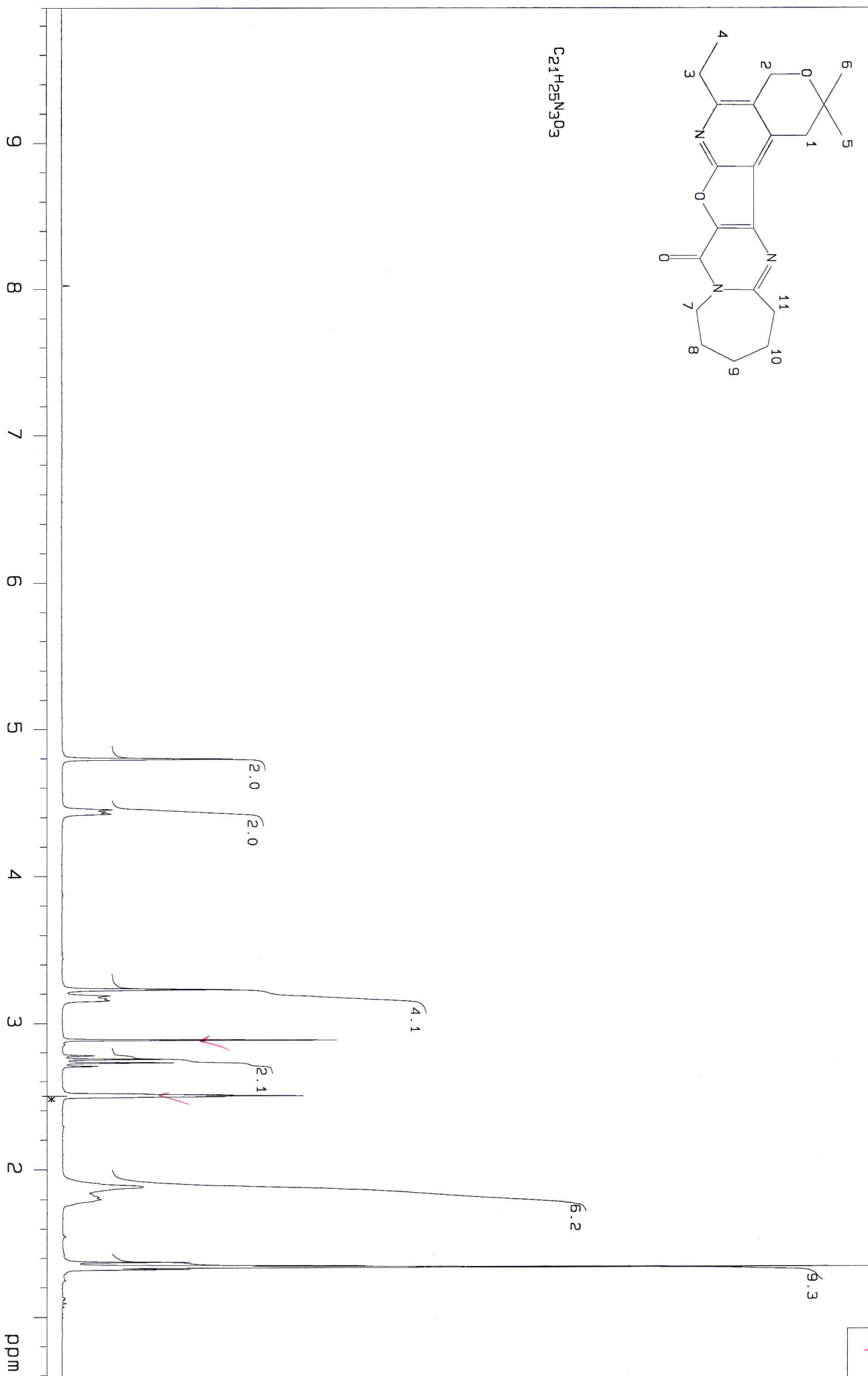
+

fjw

59

HA-538

SAMV\_11 ha-538

 $C_{21}H_{25}N_3O_3$ 

5g

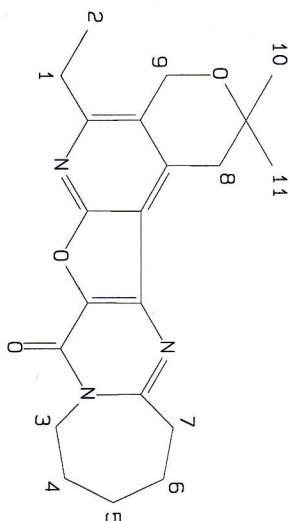
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX  
HA-538

C13 75.462 MHz, nt = 240, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/C14 1/3

SAMV\_14 na-538

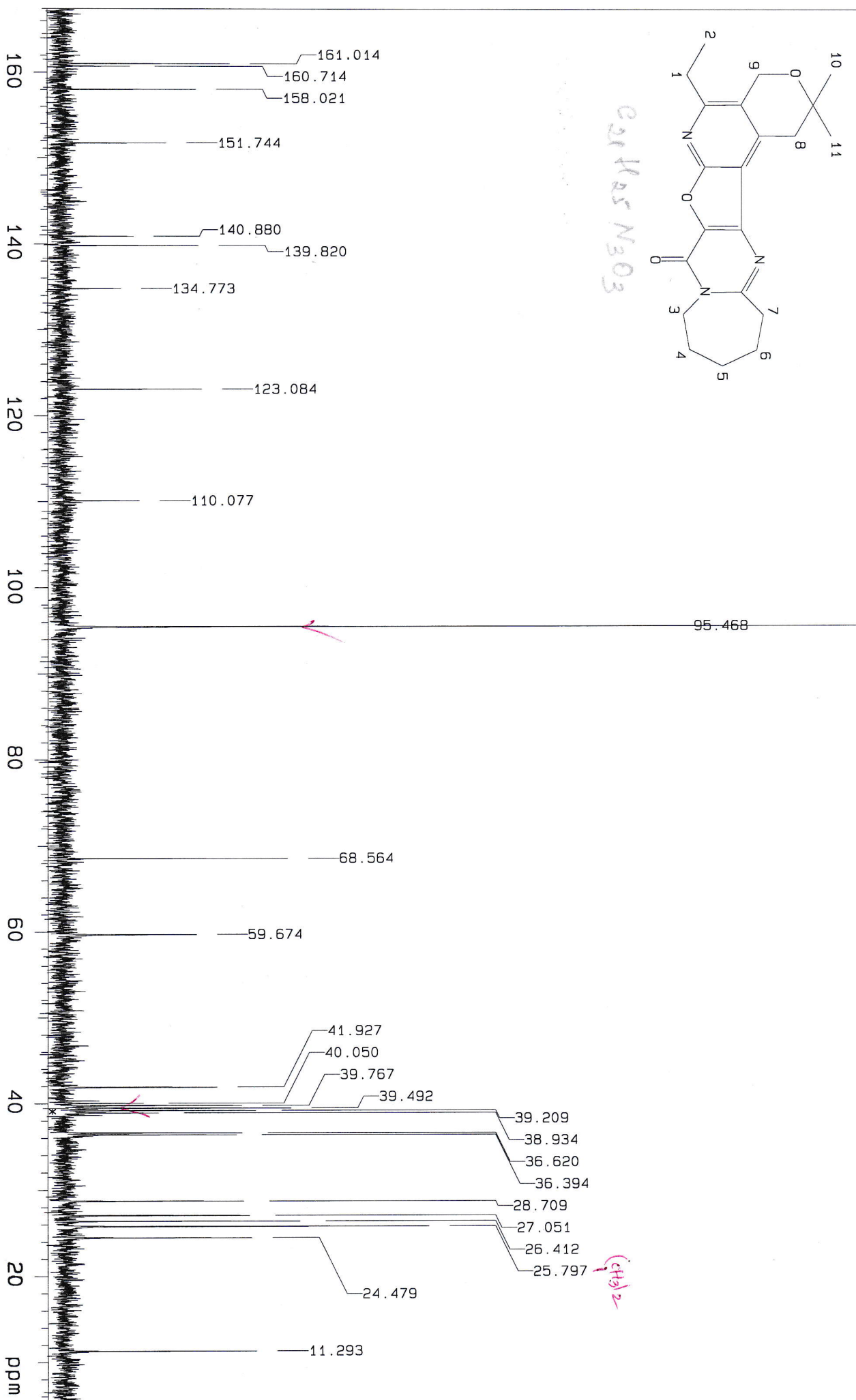
Oct 21 2014

+



C2H4.5N3O3

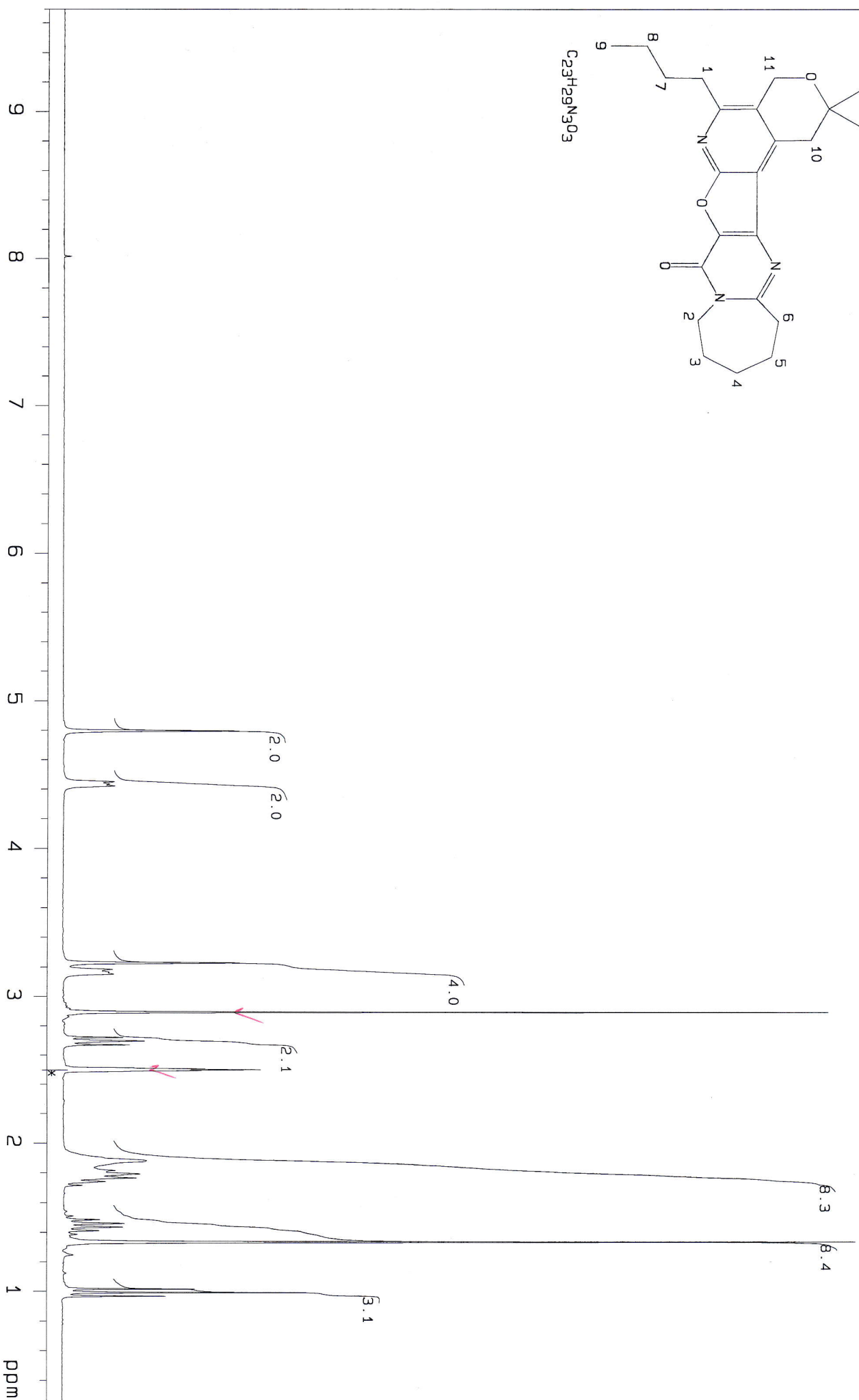
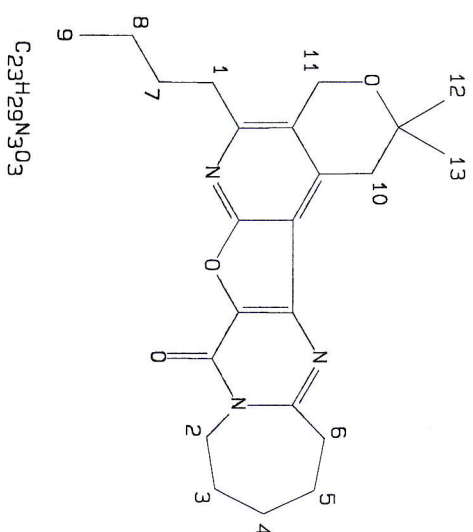
(CH<sub>3</sub>)<sub>2</sub>



5h

HA-542

SAMV\_11 ha-542

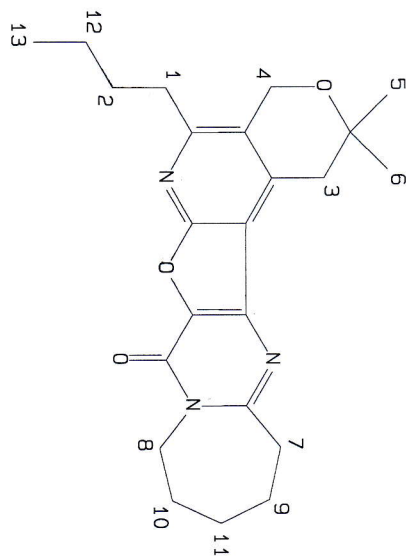


5h

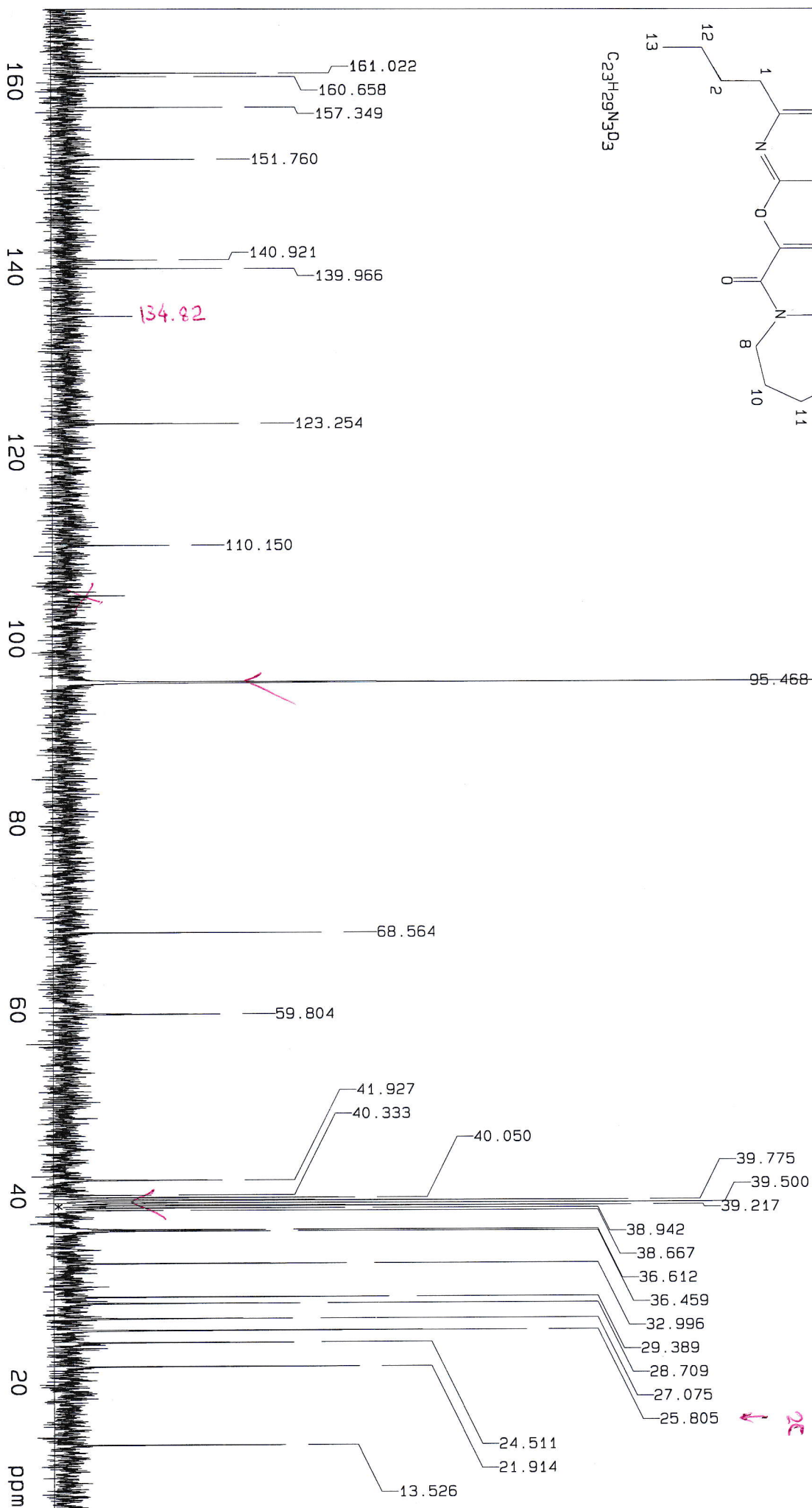
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX  
HA-542

C13 75.462 MHz, nt=656, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO-CCl4 1/3  
SAMV\_14 ha-542

Oct 21 2014



C<sub>23</sub>H<sub>29</sub>N<sub>3</sub>O<sub>3</sub>



Me<sub>2</sub>  
N

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