# Supplementary Data

## Pyridofuropyrrolo[1,2-*a*]pyrimidines and pyridofuropyrimido[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**.

***Ethyl [(1-butyl-4-cyano-6,7-dihydro-5H-cyclopenta[c]pyridin-3-yl)oxy]acetate (2b)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 0.93 (t, *J* = 7.3 Hz, 3H, $CH_2C\underline{H}_3$), 1.28 (t, *J* = 7.1 Hz, 3H, $OCH_2C\underline{H}_3$), 1.27–1.39 (m, 2H, $C\underline{H}_2CH_3$), 1.56–1.67 (m, 2H, $C\underline{H}_2C_2H_5$), 2.13–2.24 (m, 2H, 6-$CH_2$), 2.60 (t, *J* = 7.4 Hz, 2H, $C\underline{H}_2C_3H_7$), 2.86 (t, *J* = 7.5 Hz, 2H, 7-$CH_2$), 3.06 (t, *J* = 7.6 Hz, 2H, 5-$CH_2$), 4.17 (q, *J* = 7.1 Hz, 2H, $OC\underline{H}_2CH_3$), 4.89 (s, 2H, $OCH_2CO$).

***Ethyl [(5-cyano-3,3-dimethyl-8-ethyl-3,4-dihydro-1H-pyrano[3,4-c]pyridin-6-yl)oxy] acetate (2g)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.21 (t, *J* = 7.4 Hz, 3H, $CH_2C\underline{H}_3$), 1.26 (s, 6H, $C(CH_3)_2$), 1.30 (t, *J* = 7.1 Hz, 3H, $OCH_2C\underline{H}_3$), 2.58 (q, *J* = 7.4 Hz, 2H, $C\underline{H}_2CH_3$), 2.78 (s, 2H, $CH_2$), 4.18 (q, *J* = 7.1 Hz, 2H, $OC\underline{H}_2CH_3$), 4.61 (s, 2H, $OCH_2$), 4.92 (s, 2H, $OCH_2CO$).

***Ethyl [(8-butyl-5-cyano-3,3-dimethyl-3,4-dihydro-1H-pyrano[3,4-c]pyridin-6-yl)oxy] acetate (2h)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 0.93 (t, *J* = 7.3 Hz, 3H, $CH_2C\underline{H}_3$),1.27 (s, 6H, $C(CH_3)_2$), 1.27 (t, *J* = 7.1 Hz, 3H, $OCH_2C\underline{H}_3$), 1.30–1.41 (m, 2H, $C\underline{H}_2CH_3$), 1.57–1.68 (m, 2H, $C\underline{H}_2C_2H_5$), 2.50–2.55 (m, 2H, $C\underline{H}_2C_3H_7$), 2.78 (s, 2H, $CH_2$), 4.17 (q, *J* = 7.1 Hz, 2H, $OC\underline{H}_2CH_3$), 4.62 (s, 2H, $OCH_2$), 4.91 (s, 2H, $OCH_2CO$).

***Ethyl 1-amino-5-butyl-7,8-dihydro-6H-cyclopenta[d]furo[2,3-b]pyridine-2-carboxylate (3b)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 0.95 (t, *J* = 7.3 Hz, 3H, $CH_2C\underline{H}_3$), 1.32–1.45 (m, 2H, $C\underline{H}_2CH_3$), 1.40 (t, *J* = 7.1 Hz, 3H, $OCH_2C\underline{H}_3$), 1.63–1.75 (m, 2H, $C\underline{H}_2C_2H_5$), 2.15–2.27 (m, 2H, 7-$CH_2$), 2.68–2.74 (m, 2H, $C\underline{H}_2C_3H_7$), 2.89 (t, *J* = 7.5 Hz, 2H, 6-$CH_2$), 3.27 (t, *J* = 7.6 Hz, 2H, 8-$CH_2$), 4.32 (q, *J* = 7.1 Hz, 2H, $OC\underline{H}_2CH_3$), 5.70 (br s, 2H, $NH_2$).

***Ethyl 1-amino-8,8-dimethyl-5-ethyl-8,9-dihydro-6H-furo[2,3-b]pyrano[4,3-d]pyridine-2-carboxylate (3g)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.29 (t, *J* = 7.4 Hz, 3H, $CH_2C\underline{H}_3$), 1.30 (s, 6H, $C(CH_3)_2$), 1.41 (t, *J* = 7.1 Hz, 3H, $OCH_2C\underline{H}_3$), 2.65 (q, *J* = 7.4 Hz, 2H, $C\underline{H}_2CH_3$), 3.11 (s, 2H, $CH_2$), 4.33 (q, *J* = 7.1 Hz, 2H, $OC\underline{H}_2CH_3$), 4.71 (s, 2H, $OCH_2$), 5.74 (br s, 2H, $NH_2$).

***Ethyl 1-amino-8,8-dimethyl-5-butyl-8,9-dihydro-6H-furo[2,3-b]pyrano[4,3-d]pyridine-2-carboxylate (3h)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 0.97 (t, *J* = 7.3 Hz, 3H, $CH_2C\underline{H}_3$), 1.29 (s, 6H, $C(CH_3)_2$), 1.35–1.48 (m, 2H, $C\underline{H}_2CH_3$), 1.40 (t, *J* = 7.1 Hz, 3H, $OCH_2C\underline{H}_3$), 1.65–1.76 (m, 2H, $C\underline{H}_2C_2H_5$), 2.61 (t, *J* = 7.5 Hz, 2H, $C\underline{H}_2C_3H_7$), 3.11 (s, 2H, $CH_2$), 4.33 (q, *J* = 7.1 Hz, 2H, $OC\underline{H}_2CH_3$), 4.71 (s, 2H, $OCH_2$), 5.75 (br s, 2H, $NH_2$).

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

***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)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.31 (d, *J* = 6.6 Hz, 6H, $CH(C\underline{H}_3)_2$), 2.20–2.41 (m, 4H, 2-$CH_2$, 10-$CH_2$), 3.02 (t, *J* = 7.4 Hz, 2H, 3-$CH_2$), 3.19 (t, *J* = 7.8 Hz, 2H, 11-$CH_2$), 3.20 (sp, *J* = 6.7 Hz, 1H, $C\underline{H}(CH_3)_2$), 3.35 (t, *J* = 7.6 Hz, 2H, 1-$CH_2$), 4.18–4.24 (m, 2H, 9-$CH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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.

***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)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 0.98 (t, *J* = 7.3 Hz, 3H, $CH_2C\underline{H}_3$), 1.37–1.50 (m, 2H, $C\underline{H}_2CH_3$), 1.70–1.80 (m, 2H, $C\underline{H}_2C_2H_5$), 2.23–2.41 (m, 4H, 2-$CH_2$, 10-$CH_2$), 2.80 (t, *J* = 7.5 Hz, 2H, $C\underline{H}_2C_3H_7$), 2.99 (t, *J* = 7.4 Hz, 2H, 3-$CH_2$), 3.19 (t, *J* = 7.9 Hz, 2H, 11-$CH_2$), 3.34 (t, *J* = 7.6 Hz, 2H, 1-$CH_2$), 4.18–4.24 (m, 2H, 9-$CH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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.

***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)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.28 (d, *J* = 6.6 Hz, 6H, $CH(C\underline{H}_3)_2$), 1.83–1.98 (m, 4H, 2,3-$CH_2$), 2.29–2.40 (m, 2H, 11-$CH_2$), 2.82–2.88 (m, 2H, 4-$CH_2$), 3.18 (t, *J* = 7.9 Hz, 2H, 12-$CH_2$), 3.30–3.38 (m, 3H, 1-$CH_2$, $C\underline{H}(CH_3)_2$), 4.17–4.23 (m, 2H, 10-$CH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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.

***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)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.00 (d, *J* = 6.6 Hz, 6H, CH(C<u>H</u>$_3$)$_2$), 1.83–1.97 (m, 4H, 2,3-$CH_2$), 2.21–2.40 (m, 3H, C<u>H</u>$(CH_3)_2$, 11-$CH_2$), 2.68 (d, *J* = 7.0 Hz, 2H, CHC<u>H</u>$_2$), 2.76–2.82 (m, 2H, 4-$CH_2$), 3.18 (t, *J* = 7.9 Hz, 2H, 12-$CH_2$), 3.31–3.37 (m, 2H, 1-$CH_2$), 4.17–4.23 (m, 2H, 10-$CH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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.

***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)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.33 (s, 6H, C$(CH_3)_2$), 2.30–2.41 (m, 2H, 11-$CH_2$), 2.48 (s, 3H, $CH_3$), 3.19 (s, 2H, $CH_2$), 3.20 (t, *J* = 7.9 Hz, 2H, 12-$CH_2$), 4.20 (t, *J* = 7.3 Hz, 2H, 10-$CH_2$), 4.74 (s, 2H, $OCH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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.

***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)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.33 (s, 6H, C$(CH_3)_2$), 1.35 (t, *J* = 7.3 Hz, 3H, $CH_2$C<u>H</u>$_3$), 2.30–2.41 (m, 2H, 11-$CH_2$), 2.74 (t, *J* = 7.3 Hz, 2H, C<u>H</u>$_2$$CH_3$), 3.20 (t, *J* = 7.9 Hz, 2H, 12-$CH_2$), 3.22 (s, 2H, $CH_2$), 4.18–4.24 (t, *J* = 7.3 Hz, 2H, 10-$CH_2$), 4.79 (s, 2H, $OCH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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.

***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)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 0.99 (t, *J* = 7.3 Hz, 3H, $CH_2$C<u>H</u>$_3$), 1.33 (s, 6H, C$(CH_3)_2$), 1.39–1.52 (m, 2H, C<u>H</u>$_2$$CH_3$), 1.71–1.82 (m, 2H, C<u>H</u>$_2$$C_2H_5$), 2.30–2.41 (m, 2H, 11-$CH_2$), 2.66–2.73 (m, 2H, C<u>H</u>$_2$$C_3H_7$), 3.20 (t, *J* = 7.9 Hz, 2H, 12-$CH_2$), 3.22 (s, 2H, $CH_2$), 4.18–4.25 (t, *J* = 7.3 Hz, 2H, 10-$CH_2$), 4.80 (s, 2H, $OCH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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.

***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)***. IR *ν*/cm$^{-1}$: 1687 (C=O). $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.37 (s, 6H, C$(CH_3)_2$), 2.28–2.39 (m, 2H, 11-$CH_2$), 3.21 (t, *J* = 7.9 Hz, 2H, 12-$CH_2$), 3.30 (s, 2H, $CH_2$), 4.17–4.23 (t, *J* = 7.3 Hz, 2H, 10-$CH_2$), 5.14 (s, 2H, $OCH_2$), 6.67 (dd, *J* = 3.5, 1.7 Hz, 1H, 4-CH, furyl), 7.22 (dd, *J* = 3.5, 0.7 Hz, 1H, 3-CH, furyl), 7.83 (dd, *J* = 1.7, 0.7 Hz, 1H, 5-CH, furyl). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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 $C_{21}H_{19}N_3O_4$: C 66.83; H 5.07; N 11.13 %. Found: C 66.71; H 5.08; N 11.11 %.

**Table S3**. Spectroscopic data for compounds **5a**–**h**.

***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)***. $^1$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.31 (d, *J* = 6.7 Hz, 6H, CH(C<u>H</u>$_3$)$_2$), 1.76–1.93 (m, 6H, 10,11,12-$CH_2$), 2.23–2.34 (m, 2H, 2-$CH_2$), 3.02 (t, *J* = 7.4 Hz, 2H, 3-$CH_2$), 3.12–3.17 (m, 2H, 13-$CH_2$), 3.19 (sp, *J* = 6.7 Hz, 1H, C<u>H</u>$(CH_3)_2$), 3.36 (t, *J* = 7.6 Hz, 2H, 1-$CH_2$), 4.41–4.46 (m, 2H, 9-$CH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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.

***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)***. $^{1}$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 0.98 (t, *J* = 7.3 Hz, 3H, $CH_2C\underline{H}_3$), 1.36–1.49 (m, 2H, $C\underline{H}_2CH_3$), 1.69–1.93 (m, 8H, $C\underline{H}_2C_2H_5$, 10,11,12-$CH_2$), 2.23–2.33 (m, 2H, 2-$CH_2$), 2.80 (t, *J* = 7.6 Hz, 2H, $C\underline{H}_2C_3H_7$), 2.99 (t, *J* = 7.4 Hz, 2H, 3-$CH_2$), 3.11–3.16 (m, 2H, 13-$CH_2$), 3.34 (t, *J* = 7.6 Hz, 2H, 1-$CH_2$), 4.40–4.45 (m, 2H, 9-$CH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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)***. $^{1}$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.78–1.95 (m, 6H, $CH_2$, 10,11,12-$CH_2$), 2.23–2.35 (m, 2H, 2-$CH_2$), 3.13–3.20 (m, 2H, 13-$CH_2$), 3.24 (t, *J* = 7.3 Hz, 2H, 3-$CH_2$), 3.43 (t, *J* = 7.5 Hz, 2H, 1-$CH_2$), 4.41–4.49 (m, 2H, $NCH_2$), 7.38–7.51 and 7.83–7.88 (both m, 3H and 2H, Ph). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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)***. $^{1}$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.28 (d, *J* = 6.7 Hz, 6H, $CH(C\underline{H}_3)_2$), 1.75–1.98 (m, 10H, 2,3-$CH_2$ and 11,12,13-$CH_2$), 2.82–2.88 (m, 2H, 4-$CH_2$), 3.11–3.16 (m, 2H, 14-$CH_2$), 3.33 (sp, *J* = 6.7 Hz, 1H, $C\underline{H}(CH_3)_2$), 3.32–3.38 (m, 2H, 1-$CH_2$), 4.40–4.45 (m, 2H, 10-$CH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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)***. $^{1}$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 0.99 (d, *J* = 6.6 Hz, 6H, $CH(C\underline{H}_3)_2$), 1.75–1.97 (m, 10H, 2,3-$CH_2$ and 11,12,13-$CH_2$), 2.21–2.34 (m, 1H, $C\underline{H}(CH_3)_2$), 2.68 (d, *J* = 7.0 Hz, 2H, $CHC\underline{H}_2$), 2.76–2.82 (m, 2H, 4-$CH_2$), 3.11–3.17 (m, 2H, 14-$CH_2$), 3.32–3.38 (m, 2H, 1-$CH_2$), 4.40–4.45 (m, 2H, 10-$CH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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)***. $^{1}$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.34 (s, 6H, $C(CH_3)_2$), 1.76–1.94 (m, 6H, 11,12,13-$CH_2$), 2.49 (s, 3H, $CH_3$), 3.14–3.20 (m, 2H, 14-$CH_2$), 3.22 (s, 2H, $CH_2$), 4.41–4.46 (m, 2H, 10-$CH_2$), 4.75 (s, 2H, $OCH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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)***. $^{1}$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 1.34 (s, 6H, $C(CH_3)_2$), 1.35 (t, *J* = 7.4 Hz, 3H, $CH_2C\underline{H}_3$), 1.76–1.94 (m, 6H, 11,12,13-$CH_2$), 2.74 (q, *J* = 7.4 Hz, 2H, $C\underline{H}_2CH_3$), 3.14–3.20 (m, 2H, 14-$CH_2$), 3.23 (s, 2H, $CH_2$), 4.41–4.47 (m, 2H, 10-$CH_2$), 4.80 (s, 2H, $OCH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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.

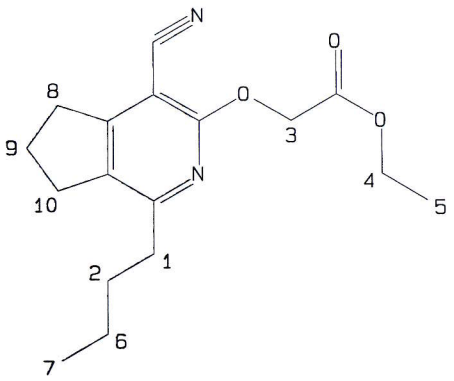
***5-Butyl-2,2-dimethyl-1,4,11,12,13,14-hexahydro-2H-pyrano[4''',3''':4'',5'']pyrido-[3'',2'':4',5']furo[3',2':4,5]pyrimido[1,2-a]azepin-8(10H)-one (5h)***. $^{1}$H NMR (300 MHz, DMSO/$CCl_4$, 1/3) δ 0.99 (t, *J* = 7.3 Hz, 3H, $CH_2C\underline{H}_3$), 1.33 (s, 6H, $C(CH_3)_2$), 1.38–1.51 (m, 2H, $C\underline{H}_2CH_3$), 1.71–1.94 (m, 8H, $C\underline{H}_2C_2H_5$, 11,12,13-$CH_2$), 2.69 (t, *J* = 7.6 Hz, 2H, $C\underline{H}_2C_3H_7$), 3.13–3.20 (m, 2H, 14-$CH_2$), 3.23 (s, 2H, $CH_2$), 4.40–4.47 (m, 2H, 10-$CH_2$), 4.80 (s, 2H, $OCH_2$). $^{13}$C NMR (75 MHz, DMSO/$CCl_4$, 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

*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/CCl4 1/3 Feb 29 2016

**HA-463**

SAMV_16 ha-463



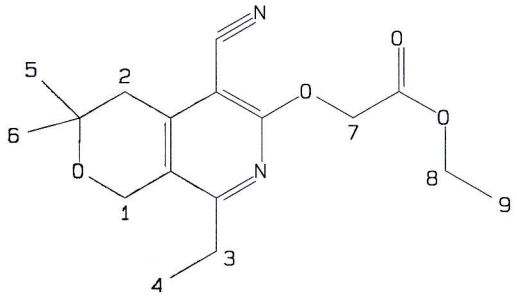

$C_{17}H_{22}N_2O_3$

2g

*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/CCl4 1/3 **Feb 29 2016**

**HA-137**

SAMV_16 ha-137




$C_{17}H_{22}N_2O_4$

2h

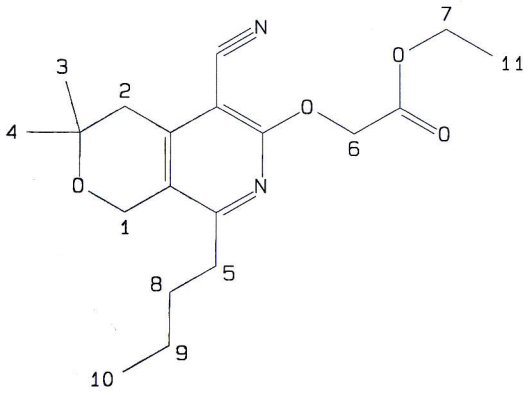
*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX*

H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Jun 29 2011

**HA-378**

SAMV_11 ha-378



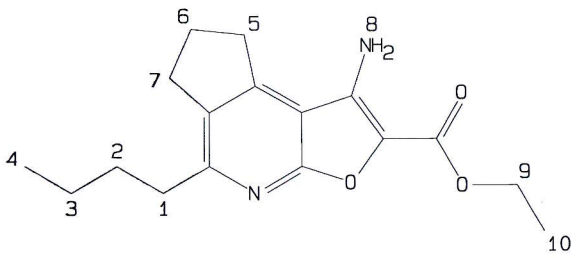

$C_{19}H_{26}N_2O_4$

36

*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/CCl4 1/3 **Oct 31 2011**

**HA-457**

SAMV_11 ha-457




$C_{17}H_{22}N_2O_3$

3g

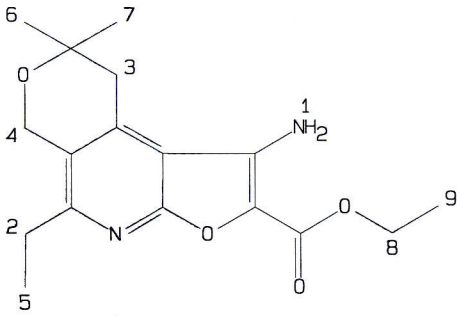
*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX*

H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

May 2 2013

**HA-138**

SAMV_13 ha-138



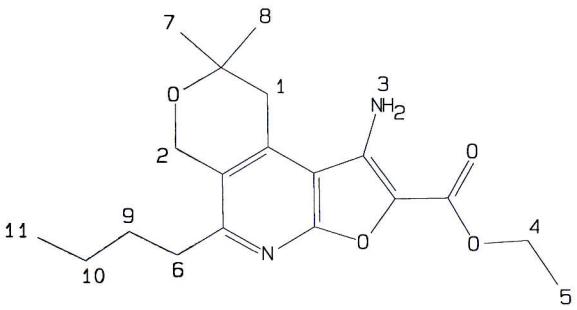

$C_{17}H_{22}N_2O_4$

3h

*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/CCl4 1/3 Jun 27 2011

**HA-379**

SAMV_11 ha-379



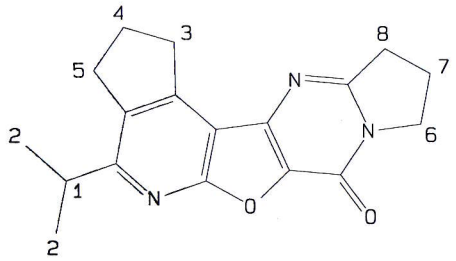

$C_{19}H_{26}N_2O_4$

4a

*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/CCl4 1/3 Feb 29 2016

**HA-317**

SAMV_16 ha-317



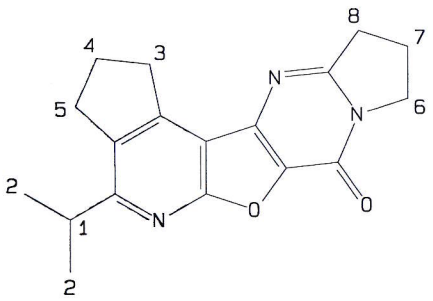

$C_{18}H_{19}N_3O_2$

4a

*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/CCl4 1/3 Oct 21 2014

**HA-317**

SAMV_14 ha-317



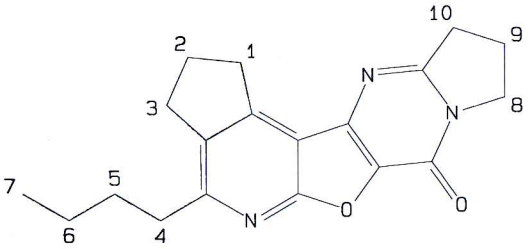

$C_{18}H_{19}N_3O_2$

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/CCl4 1/3 Nov 8 2011

**HA-459**

SAMV_11 ha-459




$C_{19}H_{21}N_3O_2$

46

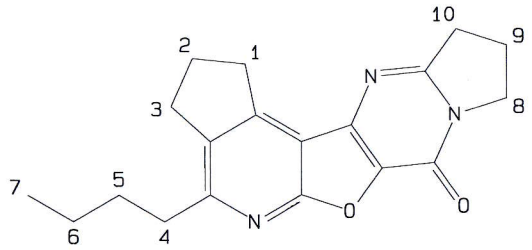
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.462 MHz, nt = 368, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Oct 22 2014

SAMV_11 ha-459

**HA-459**




$C_{19}H_{21}N_3O_2$

95.476

161.564
160.642
156.937
150.781
149.341
142.538
135.396
134.061
109.114
46.473
40.058
39.783
39.500
39.225
38.950
34.930
31.613
31.071
29.761
29.267
24.357
21.898
19.560
13.518

160 140 120 100 80 60 40 20 ppm

4c

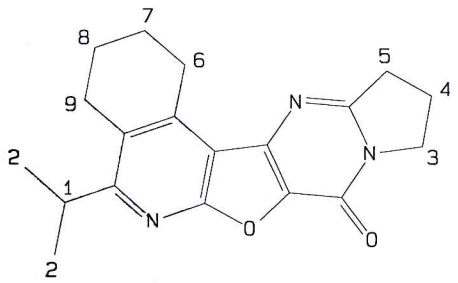
*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX*

H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Feb 29 2016

**HA-334**

SAMV_16 ha-334



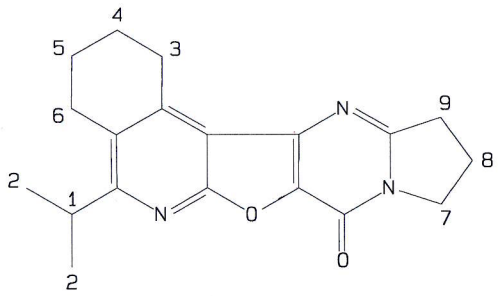

$C_{19}H_{21}N_3O_2$

4c

*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* C13 75.462 MHz, nt = 1600, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Oct 20 2014

SAMV_14 ha-334

**HA-334**




$C_{19}H_{21}N_3O_2$

95.476

164.929
160.261
160.3
150.789
143.970
143.5
135.07
125.050
109.964
46.448
40.333
40.058
39.783
39.500
39.225
38.950
38.675
31.735
30.424
26.533
24.705
22.400
21.300
20.758
19.560

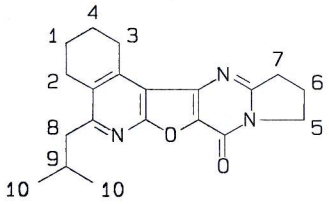
160 140 120 100 80 60 40 20 ppm

4d

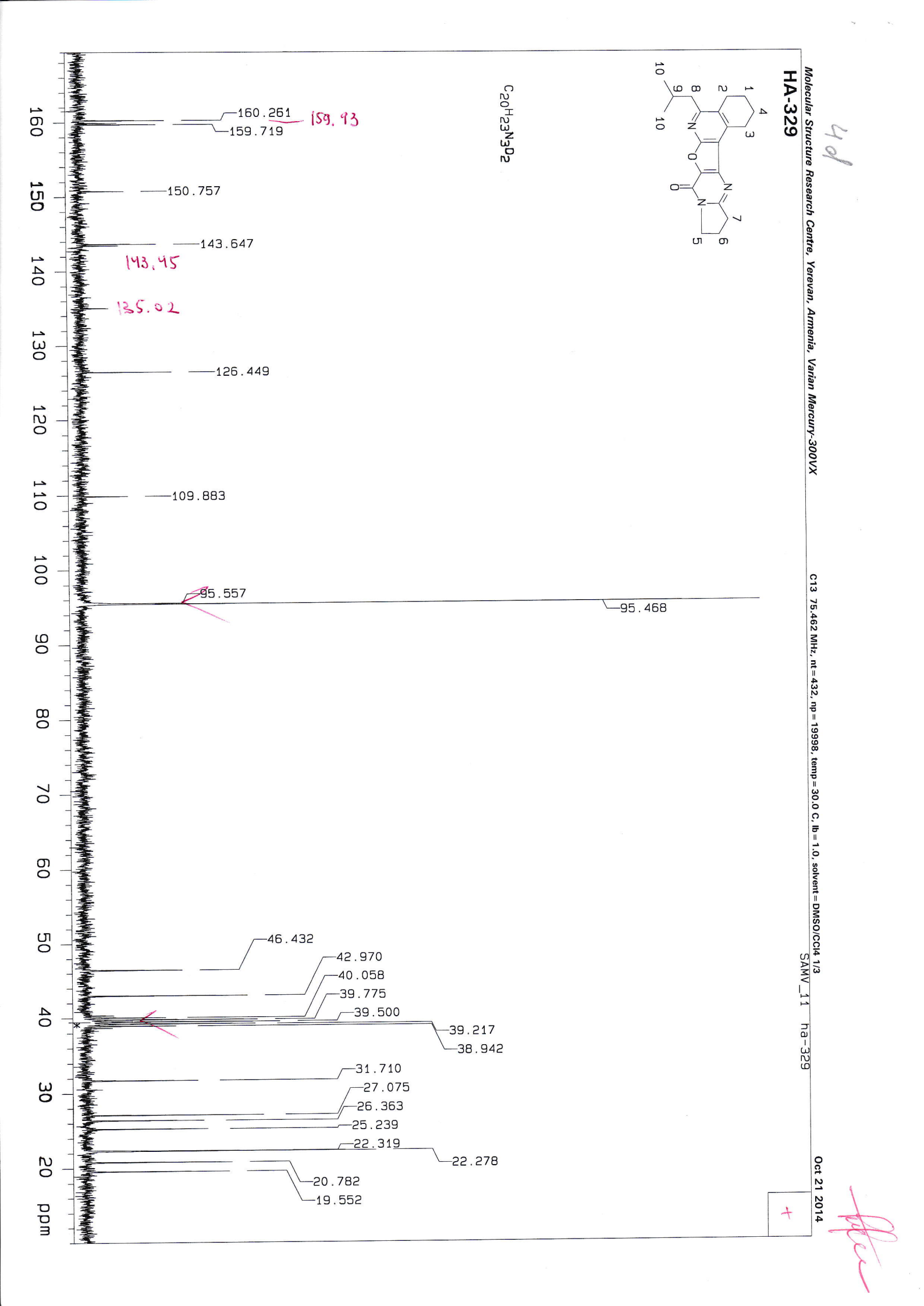
*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3 Oct 19 2011

**HA-329**

SAMV_11 ha-329




$C_{20}H_{23}N_3O_2$

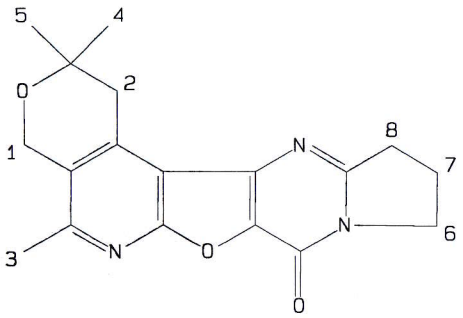

HA-329
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX
C13 75.462 MHz, nt = 432, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3
SAMV_11 ha-329
Oct 21 2014
$C_{20}H_{23}N_3O_2$
160.261
159.719
159.93
150.757
143.647
143.95
135.02
126.449
109.883
95.557
95.468
46.432
42.970
40.058
39.775
39.500
39.217
38.942
31.710
27.075
26.363
25.239
22.319
22.278
20.782
19.552
ppm

4e

*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.3, solvent = DMSO/CCl4 1/3 Feb 8 2012

**HA-588**

SAMV_12 ha-588



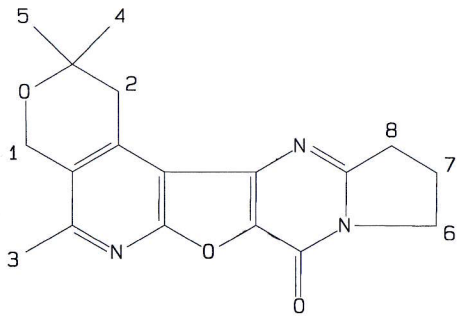

$C_{18}H_{19}N_3O_3$

4e

*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* C13 75.462 MHz, nt = 448, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Oct 22 2014

SAMV_12 ha-588

**HA-588**




$C_{18}H_{19}N_3O_3$

Me2
2C

95.476
95.371
68.645
60.022
59.973
46.497
40.333
40.058
39.775
39.500
39.225
39.152
38.942
38.667
36.297
31.710
25.813
20.830
19.617
160.714
160.342
153.572
150.708
143.007
139.570
135.121
123.699
110.134

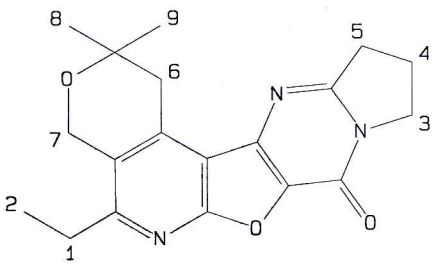
160 140 120 100 80 60 40 20 ppm

4f

*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, fb = -0.2, solvent = DMSO/CCl4 1/3 May 4 2011

**HA-318**

SAMV_11 ha-318




$C_{19}H_{21}N_3O_3$

4f

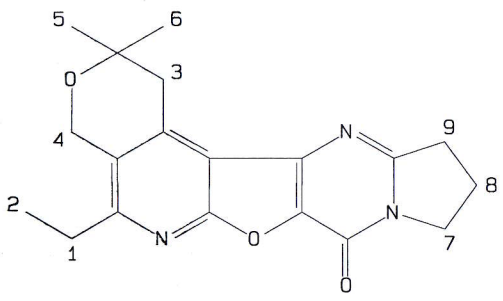
*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX*

C13 75.462 MHz, nt = 464, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Oct 21 2014

SAMV_14 ha-318

**HA-318**



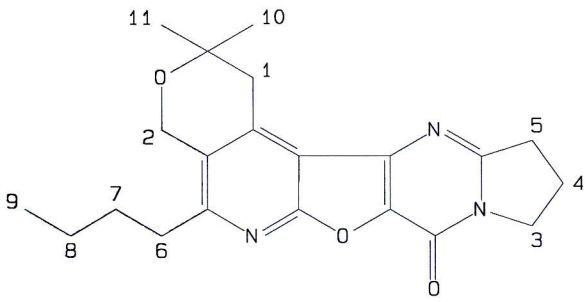

$C_{19}H_{21}N_3O_3$

4g

*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/CCl4 1/3 Nov 30 2011

**HA-455**

SAMV_11 ha-455



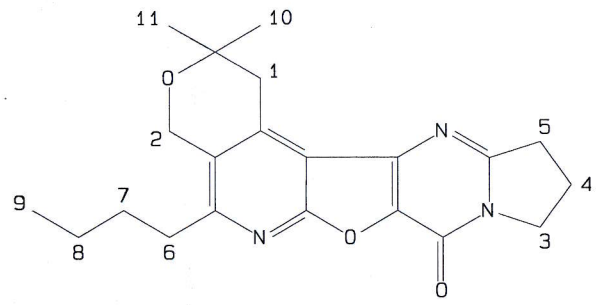

$C_{21}H_{25}N_3O_3$

4g

*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* C13 75.462 MHz, nt = 1008, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Oct 21 2014

**HA-455**

SAMV_14 ha-455




95.476
68.572
59.828
59.787
59.731
46.497
40.333
40.058
39.783
39.500
39.225
38.950
38.667
36.467
33.013
31.710
29.389
25.821
21.947
19.609
13.542
160.682
160.593
157.268
150.724
143.080
139.869
135.234
123.254
110.061

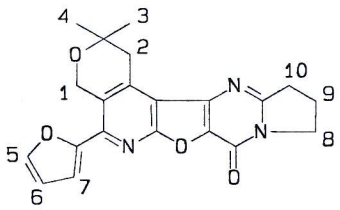
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

4h

*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/CCl4 1/3 Oct 20 2011

**HA-450**

SAMV_11 ha-450



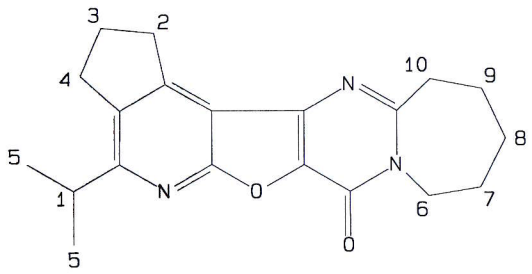

$C_{21}H_{19}N_3O_4$

5a

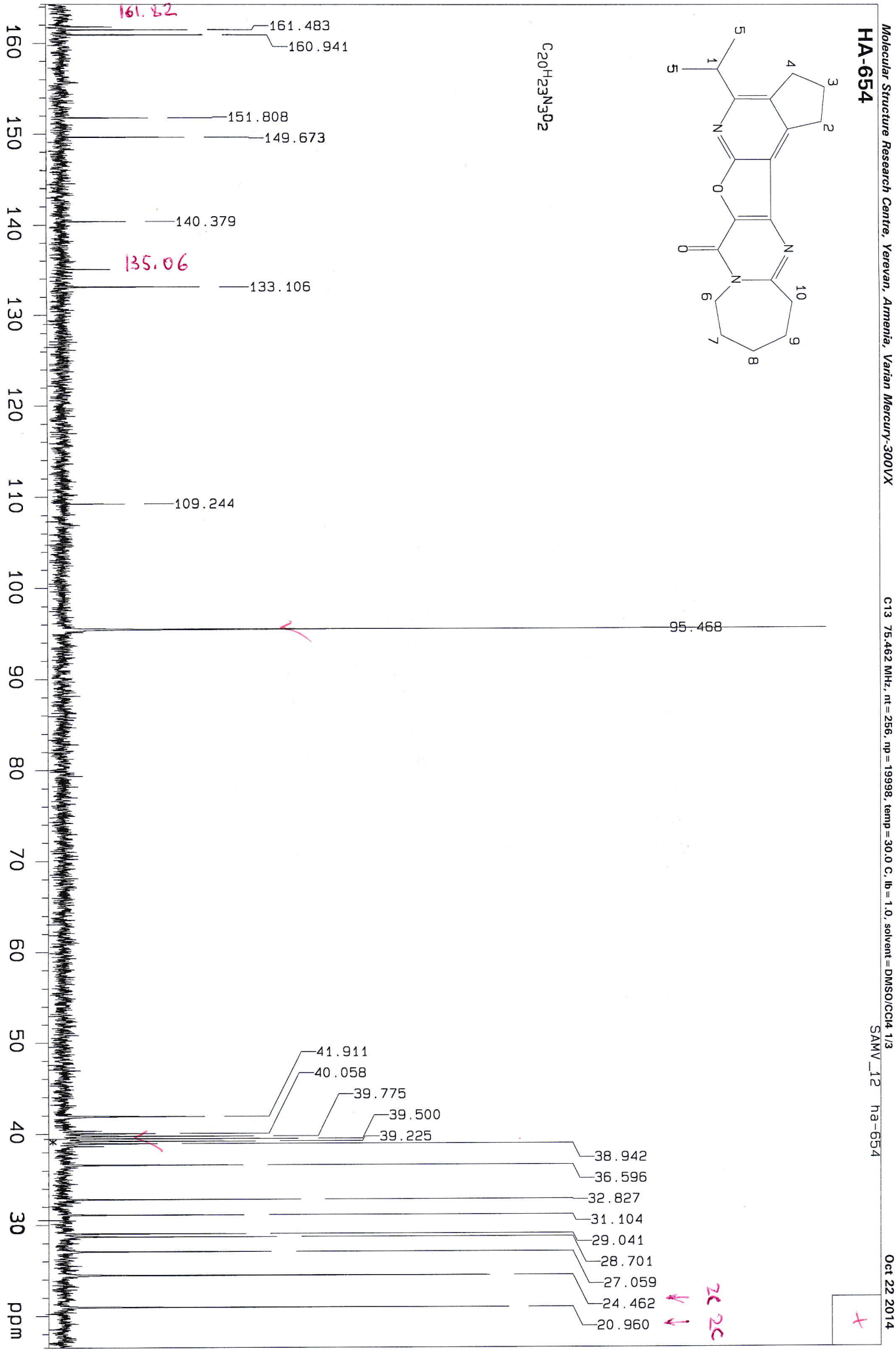
*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* H1 300.077 MHz, nt=16, np=16000, temp=30.0 C, lb=-0.2, solvent=DMSO/CCl4 1/3 Apr 6 2012

**HA-654**

SAMV_12 ha-654




$C_{20}H_{23}N_3O_2$

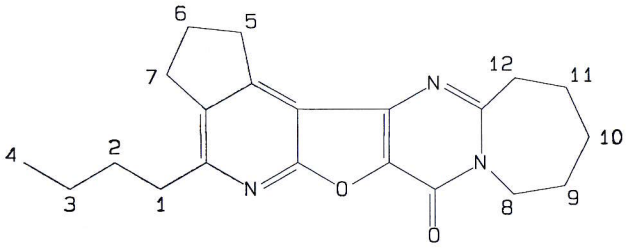

HA-654
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX
C13 75.462 MHz, nt = 256, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3
SAMV_12 ha-654
Oct 22 2014
$C_{20}H_{23}N_3O_2$
161.82
161.483
160.941
151.808
149.673
140.379
135.06
133.106
109.244
95.468
41.911
40.058
39.775
39.500
39.225
38.942
36.596
32.827
31.104
29.041
28.701
27.059
24.462
20.960
ppm

56

*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/CCl4 1/3 Jan 17 2012

**HA-554**

NOCI_12 ha-554



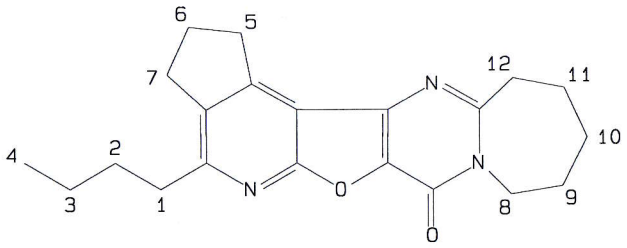

$C_{21}H_{25}N_3O_2$

56

*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* C13 75.462 MHz, nt = 192, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Oct 21 2014

**HA-554**

SAMV_14 ha-554



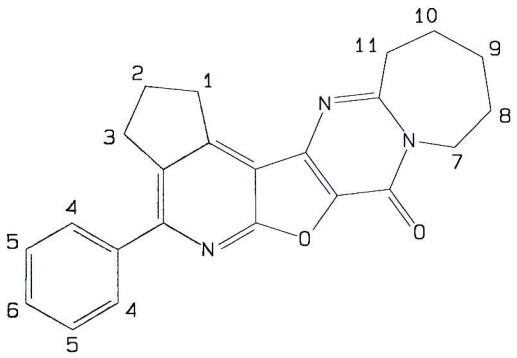

$C_{21}H_{25}N_3O_2$

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/CCl4 1/3 Dec 26 2011

**HA-553**

SAMV_11 ha-553




$C_{23}H_{21}N_3O_2$

5c

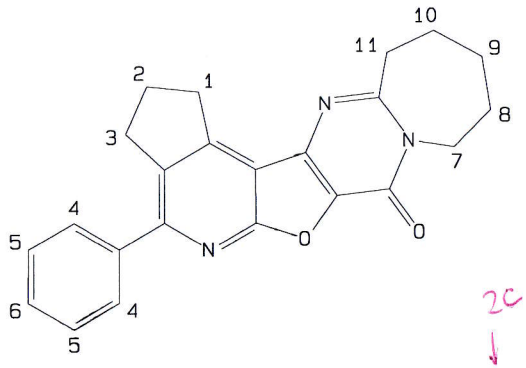
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.462 MHz, nt=720, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO/CCl4 1/3

Oct 22 2014

SAMV_11 ha-553

**HA-553**




$C_{23}H_{21}N_3O_2$

2c

2c

128.366
127.889
95.436
39.783
39.500
39.225
38.950
38.667
36.620
31.783
31.152
28.596
26.954
40.058
42.113
40.341
25.692
24.414
161.766
152.302
152.043
151.816
140.330
138.631
135.873
134.215
128.480
110.239
161, 52

160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

5 of

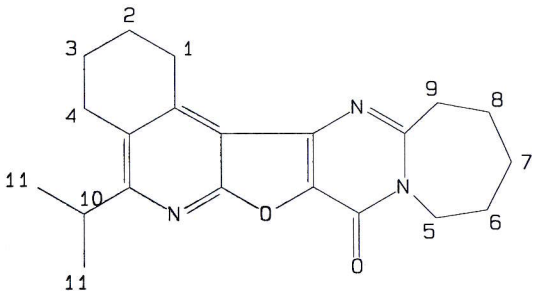
*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX*

H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Feb 1 2012

**HA-583**

SAMV_12 ha-583



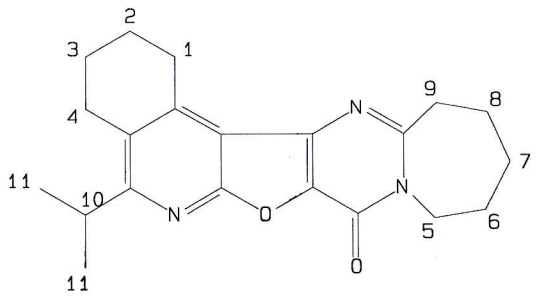

$C_{21}H_{25}N_3O_2$

5d

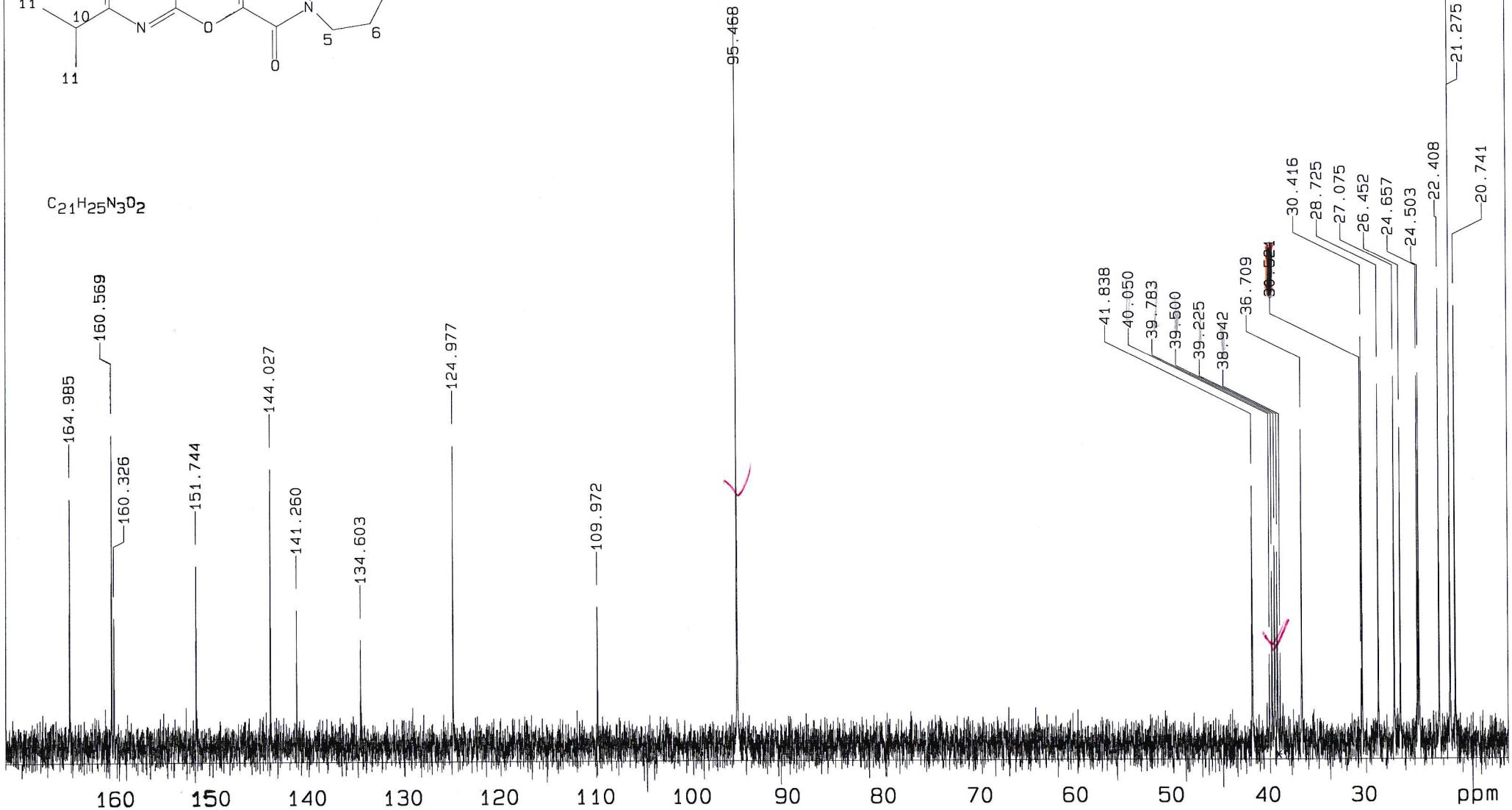
*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* C13 75.462 MHz, nt = 240, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Oct 22 2014

**HA-583**

SAMV_12 ha-583




$C_{21}H_{25}N_3O_2$

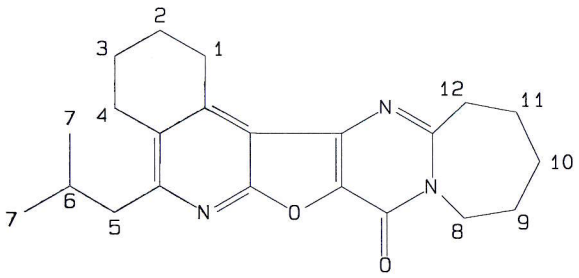


5e

*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/CCl4 1/3 Dec 20 2011

**HA-547**

SAMV_11 ha-547



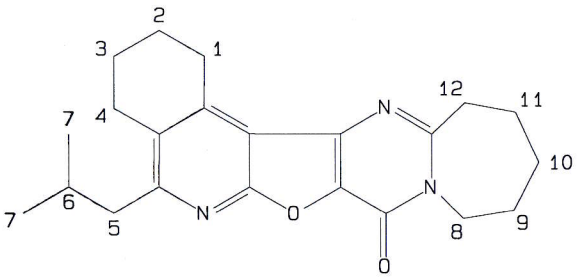

$C_{22}H_{27}N_3O_2$

5e

*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* C13 75.462 MHz, nt = 256, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3 Oct 22 2014

**HA-547**

SAMV_14 ha-547




95.468

160.601
159.986
159.800
151.784
143.760
141.301
134.611
126.433
109.964

42.954
41.846
40.341
40.325
40.050
39.775
39.500
39.217
38.942
36.717
28.725
27.091
26.347
25.223
24.527
22.367
22.246
20.798

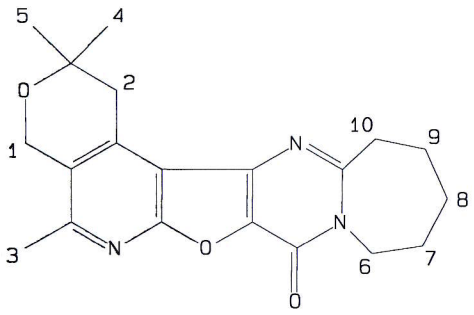
160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

5f

*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/CCl4 1/3 Feb 8 2012

**HA-587**

SAMV_12 ha-587




$C_{20}H_{23}N_3O_3$

5f

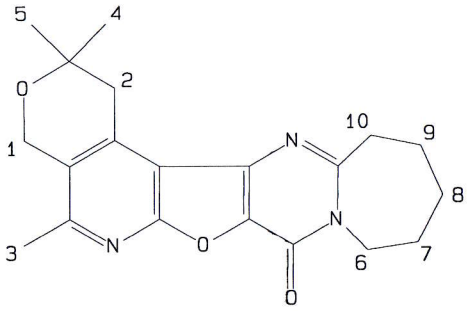
Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX

C13 75.462 MHz, nt = 480, np = 19998, temp = 30.0 C, lb = 1.0, solvent = DMSO/CCl4 1/3

Oct 22 2014

SAMV_12 ha-587

**HA-587**




$C_{20}H_{23}N_3O_3$

(CH3)2

95.468
68.637
60.022
59.981
41.935
40.050
39.775
39.500
39.217
38.942
36.620
36.264
28.717
27.035
25.789
24.462
20.839
161.046
160.391
153.620
151.736
140.840
139.651
134.69
123.683
110.198

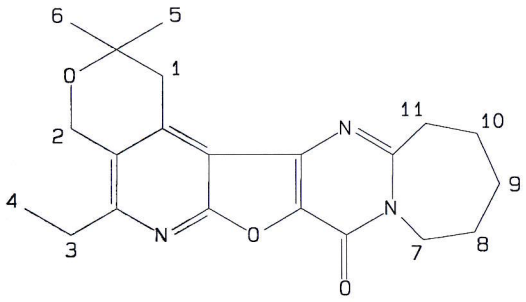
160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

5g

*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/CCl4 1/3 Dec 9 2011

**HA-538**

SAMV_11 ha-538



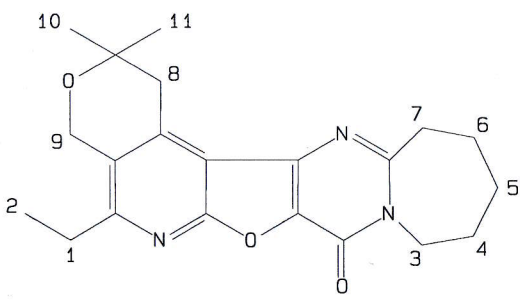

$C_{21}H_{25}N_3O_3$

5g

*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/CCl4 1/3 Oct 21 2014

**HA-538**

SAMV_14 ha-538




$C_{21}H_{25}N_3O_3$

5h

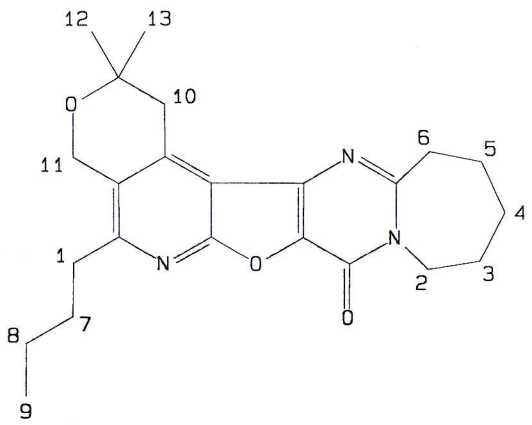
*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX*

H1 300.077 MHz, nt = 16, np = 16000, temp = 30.0 C, lb = -0.2, solvent = DMSO/CCl4 1/3

Dec 13 2011

**HA-542**

SAMV_11 ha-542



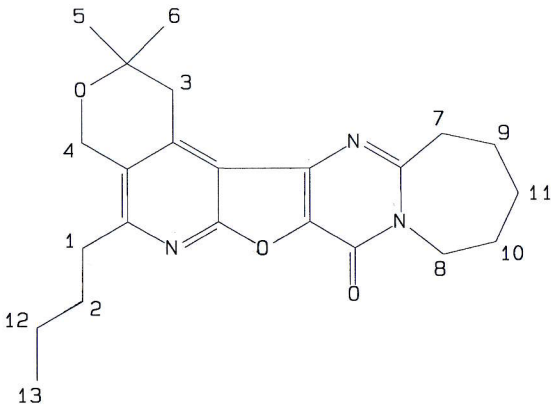

$C_{23}H_{29}N_3O_3$

5h

*Molecular Structure Research Centre, Yerevan, Armenia, Varian Mercury-300VX* C13 75.462 MHz, nt=656, np=19998, temp=30.0 C, lb=1.0, solvent=DMSO/CCl4 1/3 Oct 21 2014

SAMV_14 ha-542

**HA-542**




$C_{23}H_{29}N_3O_3$

Me2

25

95.468

39.775
39.500
39.217
38.942
38.667
36.612
36.459
32.996
29.389
28.709
27.075
25.805
24.511
21.914
13.526
40.050
68.564
59.804
41.927
40.333
161.022
160.658
157.349
151.760
140.921
139.966
134.82
123.254
110.150

160 140 120 100 80 60 40 20 ppm