

## Supporting Information

### Synthesis of energy transfer cassettes via click and Suzuki-Miyaura cross coupling reactions

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Experimental details for new compounds	S1-S19
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#### Instrumentations and chemicals:

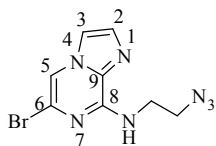
All commercially available compounds (Avra, Spectrochem, Aldrich, Merck etc.) were used without further purification. Final reactions were carried out in an oil bath using Microwave Vials (10-15 ml). Melting points were determined in open capillaries and were uncorrected. <sup>1</sup>H and <sup>13</sup>C NMR spectra were performed on Jeol ECS 400 NMR spectrometer, which was operated at 400 MHz for <sup>1</sup>H nuclei and 100 MHz for <sup>13</sup>C nuclei, using CDCl<sub>3</sub>, DMSO-*d*<sub>6</sub> and trifluoroacetic acid (TFA) as solvents. Chemical shifts are reported in parts per million (ppm) with TMS as internal reference and *J* values are given in hertz. 2D NOE studies were performed on same instrument. Mass Spectra of the synthesized compounds were recorded at Water Micromass-Q-T of Micro. Reactions were monitored by thin layer chromatography (TLC) with silica plate coated with silica gel HF-254 and column chromatography was performed with silica gel 60-120/100-200 mesh. Ethylacetate and methanol were adopted solvent systems.

**Procedure for synthesis of 2-azidoethanamine (2):** 2-Bromoethanamine hydrobromide **1** (1 g, 4.90 mmol) was dissolved in distilled water with stirring. Sodium azide was added (0.90 g, 13.84 mmol) carefully to this solution in succession with continuous stirring. The reaction mixture was refluxed for 12 h. After completion of reaction, reaction mixture was cooled to room temperature

and was quenched by addition of sodium hydroxide (0.7 g, 17.5 mmol) and further stirred for 30 min at room temperature. Thereafter, mixture was extracted with diethyl ether and dried over sodium sulphate to obtain ether extract and stored at low temperature. The ether extract being volatile in nature, was used as such for next reaction.

**Procedure for synthesis of *N*-(2-azidoethyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine (4):** To the ether extract containing 2-azidoethanamine **2** was added solution of 6,8-dibromoimidazo[1,2-*a*]pyrazine **3** (0.5 g, 1.80 mmol) in acetonitrile in the presence of diisopropylethylamine (DIPEA). The reaction mixture was refluxed for 24 h. After completion of reaction, the mixture was extracted with chloroform and water. Organic layer was separated, dried over sodium sulphate, filtered and concentrated under vacuum. The crude mixture was then purified by silica gel chromatography 60-120 mesh using hexane : ethyl acetate (8:2) as eluents.

**Spectral data of *N*-(2-azidoethyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine (4):** light orange

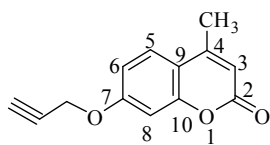


solid; yield: 72%; mp 66-68 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 3.59 (t, *J* = 5.74 Hz, 2H, NCH<sub>2</sub>), 3.74 (q, *J* = 5.81 Hz, 2H, NHCH<sub>2</sub>), 7.29 (t, *J* = 5.04 Hz, 1H, NH), 7.47 (d, *J* = 0.92 Hz, 1H, H-2), 7.54 (d, *J* = 0.92 Hz,

1H, H-3), 7.60 (s, 1H, H-5); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 39.9 (NHCH<sub>2</sub>), 50.0 (NCH<sub>2</sub>), 109.3 (C-5), 114.7 (C-3), 122.5 (C-6), 131.9 (C-2), 132.3 (C-9), 147.2 (C-8); MS (ESI): *m/z* 284.1 (M<sup>+</sup>+2); Anal. Calcd for C<sub>8</sub>H<sub>8</sub>BrN<sub>7</sub>: C, 34.06; H, 2.86; N, 34.76. Found: C, 34.10; H, 2.81; N, 34.70.

**Procedure for synthesis of 4-methyl-7-(prop-2-ynyloxy)-2*H*-chromen-2-one (6):** To 7-hydroxy-4-methyl-2*H*-chromen-2-one **5** (1 g, 5.15 mmol) was added 80% solution of propargyl bromide in toluene (1.33 g, 11.30 mmol) in the presence of potassium carbonate (0.7 g, 5.15 mmol) and acetone. The mixture was stirred at room temperature for 12 h. Completion of reaction was monitored by TLC. Reaction was quenched by addition of ice cold water. The solid product was filtered on vacuum pump to obtain off white solid.

**Spectral data of 4-methyl-7-(prop-2-ynyloxy)-2*H*-chromen-2-one (6):** Off white solid; yield:

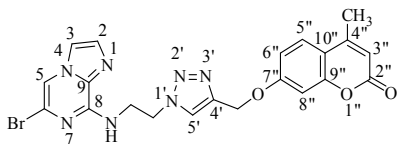


81%; mp 102-104 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 2.41 (d, *J* = 1.36 Hz, 3H, CH<sub>3</sub>), 2.59 (t, *J* = 2.52 Hz, 1H, CH), 4.77 (d, *J* = 2.32 Hz, 2H, OCH<sub>2</sub>), 6.16 (d, *J* = 1.36 Hz, 1H, H-3), 6.92-6.95 (m, 2H, H-5, H-8),

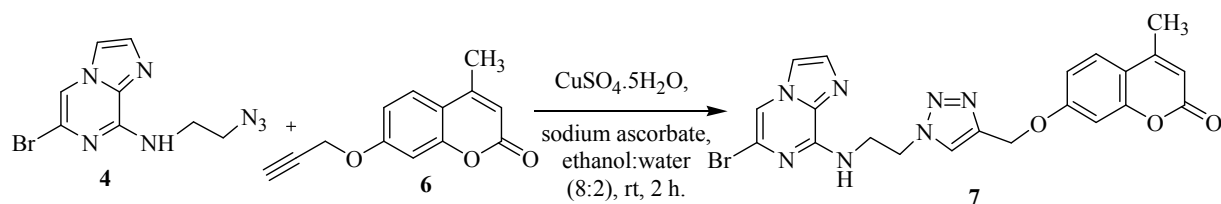
7.53 (d,  $J = 9.16$  Hz, 1H, H-6);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  18.6 ( $\text{CH}_3$ ), 56.0 ( $\text{OCH}_2$ ), 76.4 (alkyne CH, C), 102.0 (C-8), 112.3 (C-6), 112.6 (C-9), 114.1 (C-3), 125.5 (C-5), 152.4 (C-4), 154.9 (C-10), 160.2 (C-7), 161.1 (C=O); MS (ESI):  $m/z$  216.2 ( $\text{M}^++2$ ).

**Procedure for synthesis of 7-((1-(2-(6-bromoimidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (7):** To the stirred solution of 4-methyl-7-(prop-2-ynyloxy)-2*H*-chromen-2-one **6** (1g, 4.67 mmol) and *N*-(2-azidoethyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine **4** (1.31 g, 4.67 mmol) in ethanol:water (8:2), copper sulphate pentahydrate (5 mol%) and sodium ascorbate (10 mol%) was added and stirred at room temperature for 2 h. After completion of reaction, water was added and extracted with chloroform. Organic layer was dried over sodium sulphate, filtered and concentrated in vacuum to obtain off white solid.

**Spectral data of 7-((1-(2-(6-bromoimidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (7):** off white solid; yield: 91%; mp 156-158 °C;



$^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  2.40 (d,  $J = 1.36$  Hz, 3H,  $\text{CH}_3$ ), 4.13 (q,  $J = 5.80$  Hz, 2H,  $\text{NHCH}_2$ ), 4.73 (t,  $J = 5.94$  Hz, 2H,  $\text{NCH}_2$ ), 5.24 (s, 2H,  $\text{OCH}_2$ ), 6.15 (d,  $J = 0.92$  Hz, 1H, H-3''), 6.82 (t,  $J = 5.72$  Hz, 1H, NH), 6.90 (d,  $J = 2.76$  Hz, 1H, H-8''), 6.93-6.96 (dd,  $^2J = 9.16$  Hz,  $^3J = 2.52$  Hz, 1H, H-5''), 7.47 (s, 2H, H-2, H-3), 7.50 (d,  $J = 9.16$  Hz, 1H, H-6''), 7.62 (s, 1H, H-5'), 7.73 (s, 1H, H-5);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  18.7 ( $\text{CH}_3$ ), 40.8 ( $\text{NHCH}_2$ ), 49.3 ( $\text{NCH}_2$ ), 62.1 ( $\text{OCH}_2$ ), 102.0 (C-8''), 110.1 (C-5), 112.2 (C-3), 112.3 (C-6''), 114.9 (C-3''), 122.3 (C-9''), 123.7 (C-6), 125.6 (C-5''), 131.8 (C-2), 132.8 (C-9), 143.0 (C-4', C-5'), 147.1 (C-8), 152.5 (C-4''), 155.0 (C-10''), 161.0 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  498.3 ( $\text{M}^++2$ ); Anal. Calcd for  $\text{C}_{21}\text{H}_{18}\text{BrN}_7\text{O}_3$ : C, 50.82; H, 3.66; N, 19.75. Found: C, 50.79; H, 3.60; N, 19.81.

**Table S1** Optimization of click reactions

Entry	Cu (5 mol%)	Sodium ascorbate	Solvent	Temp.	Yield (%)
1	CuBr	10 mol%	Butanol:H <sub>2</sub> O	rt	50
2	CuI	10 mol%	Butanol:H <sub>2</sub> O	rt	52
3	CuCl <sub>2</sub>	10 mol%	Butanol:H <sub>2</sub> O	rt	52
4	CuSO <sub>4</sub> .5H <sub>2</sub> O	10 mol%	Butanol:H <sub>2</sub> O	rt	61
5	CuBr	10 mol%	Ethanol:H <sub>2</sub> O	rt	20
6	CuI	10 mol%	Ethanol:H <sub>2</sub> O	rt	60
7	CuCl <sub>2</sub>	10 mol%	Ethanol:H <sub>2</sub> O	rt	30
<b>8</b>	<b>CuSO<sub>4</sub>.5H<sub>2</sub>O</b>	<b>10 mol%</b>	<b>Ethanol:H<sub>2</sub>O</b>	rt	<b>91</b>
9	CuBr	10 mol%	H <sub>2</sub> O	rt	< 5
10	CuI	10 mol%	H <sub>2</sub> O	rt	15
11	CuCl <sub>2</sub>	10 mol%	H <sub>2</sub> O	rt	20
12	CuSO <sub>4</sub> .5H <sub>2</sub> O	10 mol%	H <sub>2</sub> O	rt	49
13	CuSO <sub>4</sub> .5H <sub>2</sub> O	10 mol%	Ethanol:H <sub>2</sub> O	60 °C	79
14	CuSO <sub>4</sub> .5H <sub>2</sub> O	10 mol%	Ethanol:H <sub>2</sub> O	80 °C	78
15	CuSO <sub>4</sub> .5H <sub>2</sub> O (10 mol%)	10 mol%	Ethanol:H <sub>2</sub> O	rt	81
16	CuSO <sub>4</sub> .5H <sub>2</sub> O (15 mol%)	10 mol%	Ethanol:H <sub>2</sub> O	rt	83

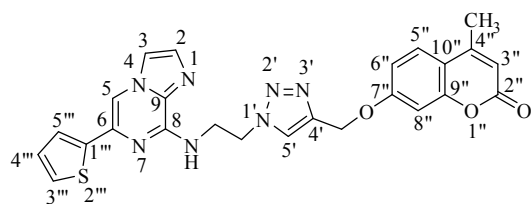
**General procedure for synthesis of 6-arylated-7-((1-(2-(6-bromoimidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (9-24):** To a solution of **7** (0.10 g, 0.201 mmol) in 1,4-dioxane: water (9:1) in a sealed tube, boronic acid (0.201 mmol) and K<sub>2</sub>CO<sub>3</sub> (0.027 g, 0.201 mmol) were added under inert atmosphere. Pd(PPh<sub>3</sub>)<sub>4</sub> (5mol%) was added with continued nitrogen purging and refluxed the reaction mixture for 6-8 hrs. Completion of reaction was determined by TLC. The mixture was extracted with chloroform and water. Organic layer was dried over sodium sulphate to obtain crude product which was further purified by column chromatography using ethylacetate : methanol as eluents.

**Table S2** Optimization of Suzuki-Miyaura cross coupling reaction

Entry	Time (h)	Catalyst	Base	Solvent	Yield (%)
1	12	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	Cs <sub>2</sub> CO <sub>3</sub>	MeCN:H <sub>2</sub> O	38
2	12	Pd <sub>2</sub> (dba) <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub>	MeCN:H <sub>2</sub> O	19
3	8	Pd(PPh <sub>3</sub> ) <sub>4</sub>	Cs <sub>2</sub> CO <sub>3</sub>	MeCN:H <sub>2</sub> O	33
4	8	[PdCl <sub>2</sub> ( <i>dppf</i> )]DCM	Cs <sub>2</sub> CO <sub>3</sub>	MeCN:H <sub>2</sub> O	35
5	10	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	K <sub>2</sub> CO <sub>3</sub>	MeCN:H <sub>2</sub> O	28
6	12	Pd <sub>2</sub> (dba) <sub>3</sub>	K <sub>2</sub> CO <sub>3</sub>	MeCN:H <sub>2</sub> O	25
7	12	Pd(PPh <sub>3</sub> ) <sub>4</sub>	K <sub>2</sub> CO <sub>3</sub>	MeCN:H <sub>2</sub> O	27
8	18	[PdCl <sub>2</sub> ( <i>dppf</i> )]DCM	K <sub>2</sub> CO <sub>3</sub>	MeCN:H <sub>2</sub> O	27
9	19	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	DIPEA	MeCN:H <sub>2</sub> O	15
10	18	Pd <sub>2</sub> (dba) <sub>3</sub>	DIPEA	MeCN:H <sub>2</sub> O	15
11	12	Pd(PPh <sub>3</sub> ) <sub>4</sub>	DIPEA	MeCN:H <sub>2</sub> O	20
12	19	[PdCl <sub>2</sub> ( <i>dppf</i> )]DCM	DIPEA	MeCN:H <sub>2</sub> O	15
13	10	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	Cs <sub>2</sub> CO <sub>3</sub>	Dioxane:H <sub>2</sub> O	51
14	10	Pd <sub>2</sub> (dba) <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub>	Dioxane:H <sub>2</sub> O	32
15	15	Pd(PPh <sub>3</sub> ) <sub>4</sub>	Cs <sub>2</sub> CO <sub>3</sub>	Dioxane:H <sub>2</sub> O	55
16	14	[PdCl <sub>2</sub> ( <i>dppf</i> )]DCM	Cs <sub>2</sub> CO <sub>3</sub>	Dioxane:H <sub>2</sub> O	55
17	14	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	K <sub>2</sub> CO <sub>3</sub>	Dioxane:H <sub>2</sub> O	58
18	15	Pd <sub>2</sub> (dba) <sub>3</sub>	K <sub>2</sub> CO <sub>3</sub>	Dioxane:H <sub>2</sub> O	53
<b>19</b>	<b>12</b>	<b>Pd(PPh<sub>3</sub>)<sub>4</sub></b>	<b>K<sub>2</sub>CO<sub>3</sub></b>	<b>Dioxane:H<sub>2</sub>O</b>	<b>73</b>
20	12	[PdCl <sub>2</sub> ( <i>dppf</i> )]DCM	K <sub>2</sub> CO <sub>3</sub>	Dioxane:H <sub>2</sub> O	70
21	12	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	DIPEA	Dioxane:H <sub>2</sub> O	42
22	20	Pd <sub>2</sub> (dba) <sub>3</sub>	DIPEA	Dioxane:H <sub>2</sub> O	12
23	12	Pd(PPh <sub>3</sub> ) <sub>4</sub>	DIPEA	Dioxane:H <sub>2</sub> O	22
24	12	[PdCl <sub>2</sub> ( <i>dppf</i> )]DCM	DIPEA	Dioxane:H <sub>2</sub> O	27
25	8	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	Cs <sub>2</sub> CO <sub>3</sub>	DME:H <sub>2</sub> O	45
26	12	Pd <sub>2</sub> (dba) <sub>3</sub>	Cs <sub>2</sub> CO <sub>3</sub>	DME:H <sub>2</sub> O	10
27	11	Pd(PPh <sub>3</sub> ) <sub>4</sub>	Cs <sub>2</sub> CO <sub>3</sub>	DME:H <sub>2</sub> O	32
28	10	[PdCl <sub>2</sub> ( <i>dppf</i> )]DCM	Cs <sub>2</sub> CO <sub>3</sub>	DME:H <sub>2</sub> O	33

29	10	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	K <sub>2</sub> CO <sub>3</sub>	DME:H <sub>2</sub> O	41
30	9	Pd <sub>2</sub> (dba) <sub>3</sub>	K <sub>2</sub> CO <sub>3</sub>	DME:H <sub>2</sub> O	9
31	12	Pd(PPh <sub>3</sub> ) <sub>4</sub>	K <sub>2</sub> CO <sub>3</sub>	DME:H <sub>2</sub> O	68
32	12	[PdCl <sub>2</sub> ( <i>dppf</i> )]DCM	K <sub>2</sub> CO <sub>3</sub>	DME:H <sub>2</sub> O	65
33	12	Pd(PPh <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub>	DIPEA	DME:H <sub>2</sub> O	15
34	12	Pd <sub>2</sub> (dba) <sub>3</sub>	DIPEA	DME:H <sub>2</sub> O	<5
35	12	Pd(PPh <sub>3</sub> ) <sub>4</sub>	DIPEA	DME:H <sub>2</sub> O	12
36	12	[PdCl <sub>2</sub> ( <i>dppf</i> )]DCM	DIPEA	DME:H <sub>2</sub> O	15

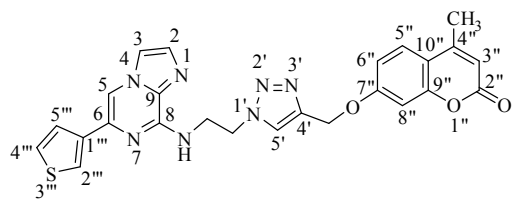
**Spectral data of 4-methyl-7-((1-(2-(6-(thiophen-2-yl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (9):** greenish solid; yield:



73%; mp 180-182 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 2.38 (s, 3H, CH<sub>3</sub>), 4.17 (q, *J* = 5.96 Hz, 2H, NHCH<sub>2</sub>), 4.82 (t, *J* = 5.74 Hz, 2H, NCH<sub>2</sub>), 5.15 (s, 2H, OCH<sub>2</sub>), 6.13 (d, *J* = 0.68 Hz, 1H, H-3''), 6.74 (t, *J* = 5.16 Hz,

1H, NH), 6.83 (d, *J* = 2.28 Hz, 1H, H-8''), 6.88-6.90 (dd, <sup>2</sup>*J* = 8.72 Hz, <sup>3</sup>*J* = 2.30 Hz, 1H, H-5''), 7.09-7.11 (m, 1H, H-4'''), 7.34 (d, *J* = 5.04 Hz, 1H, H-5'''), 7.43-7.47 (m, 2H, H-2, H-3), 7.48 (s, 1H, H-6''), 7.54 (s, 1H, H-5'), 7.74 (s, 1H, H-3'''), 7.88 (s, 1H, H-5); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 18.6 (CH<sub>3</sub>), 41.1 (NHCH<sub>2</sub>), 49.2 (NCH<sub>2</sub>), 62.1 (OCH<sub>2</sub>), 102.0 (C-8''), 105.3 (C-5), 112.1 (C-6''), 112.3 (C-9''), 113.9 (C-3), 115.3 (C-3''), 122.5 (C-4'''), 123.8 (C-6), 125.6 (C-5''), 126.0 (C-5'''), 127.9 (C-3'''), 131.9 (C-2), 132.1 (C-9), 134.1 (C-5'), 142.2 (C-1'''), 142.8 (C-4'), 147.2 (C-8), 152.4 (C-4''), 155.0 (C-10''), 161.0 (C-7''), 161.2 (C=O); MS (ESI): *m/z* 500.4 (M<sup>+</sup>+1); Anal. Calcd for C<sub>25</sub>H<sub>21</sub>N<sub>7</sub>O<sub>3</sub>S: C, 60.11; H, 4.24; N, 19.63; S, 6.42. Found: C, 60.38; H, 4.09; N, 19.75; S, 6.33.

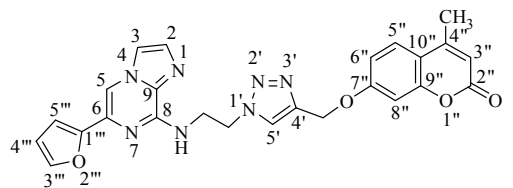
**Spectral data of 4-methyl-7-((1-(2-(6-(thiophen-3-yl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (10):** off white solid; yield



: 75%; mp 182-184 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 2.38 (d, *J* = 0.68 Hz, 3H, CH<sub>3</sub>), 4.19 (q, *J* = 5.80 Hz, 2H, NHCH<sub>2</sub>), 4.81 (t, *J* = 5.72 Hz, 2H, NCH<sub>2</sub>), 5.14 (s, 2H, OCH<sub>2</sub>), 6.13 (d, *J* = 1.36 Hz, 1H, H-3''), 6.64 (t, *J*

= 5.96 Hz, 1H, NH), 6.82 (d, *J* = 2.76 Hz, 1H, H-8''), 6.87-6.89 (dd, <sup>2</sup>*J* = 8.72 Hz, <sup>3</sup>*J* = 2.28 Hz, 1H, H-5''), 7.39-7.41 (dd, <sup>2</sup>*J* = 5.04 Hz, <sup>3</sup>*J* = 3.24 Hz, 1H, H-5'''), 7.44-7.47 (m, 3H, H-2, H-2''', H-6''), 7.54 (d, *J* = 0.88 Hz, 1H, H-3), 7.68 (s, 1H, H-5'), 7.80-7.81 (dd, <sup>2</sup>*J* = 3.20 Hz, <sup>3</sup>*J* = 1.14 Hz, 1H, H-4'''), 7.82 (s, 1H, H-5); <sup>13</sup>C (CDCl<sub>3</sub>, 100 MHz): δ 18.6 (CH<sub>3</sub>), 40.9 (NHCH<sub>2</sub>), 49.5 (NCH<sub>2</sub>), 62.0 (OCH<sub>2</sub>), 102.0 (C-8''), 106.7 (C-5), 112.1 (C-6''), 112.2 (C-9''), 113.9 (C-3), 115.2 (C-3'''), 122.3 (C-5'''), 123.7 (C-6), 124.7 (C-4'''), 125.6 (C-5''), 126.5 (C-2'''), 128.5 (C-2), 132.3 (C-9), 134.7 (C-5'), 139.2 (C-1'''), 142.8 (C-4'), 147.4 (C-8), 152.4 (C-4''), 155.0 (C-10''), 161.0 (C-7''), 161.2 (C=O); MS (ESI): *m/z* 500.4 (M<sup>+</sup>+1); Anal. Calcd for C<sub>25</sub>H<sub>21</sub>N<sub>7</sub>O<sub>3</sub>S: C, 60.11; H, 4.24; N, 19.63; S, 6.42. Found: C, 59.99; H, 4.11; N, 19.50; S, 6.53.

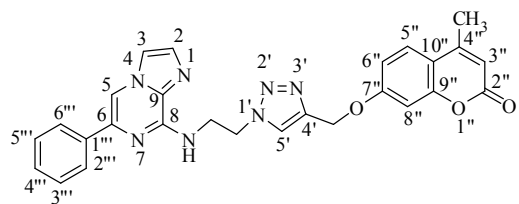
**Spectral data of 7-((1-(2-(6-(furan-2-yl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (11):** light pink solid; yield: 58%; mp 99-



101 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 2.38 (d, *J* = 0.72 Hz, 3H, CH<sub>3</sub>), 4.16 (q, *J* = 5.84 Hz, 2H, NHCH<sub>2</sub>), 4.78 (t, *J* = 5.72 Hz, 2H, NCH<sub>2</sub>), 5.15 (s, 2H, OCH<sub>2</sub>), 6.13 (d, *J* = 0.68 Hz, 1H, H-3''), 6.51-6.52 (dd, <sup>2</sup>*J* = 3.20

Hz, <sup>3</sup>*J* = 1.84 Hz, 1H, H-4'''), 6.70 (t, *J* = 5.72 Hz, 1H, NH), 6.84 (d, *J* = 2.72 Hz, 1H, H-8''), 6.87-6.90 (m, 2H, H-5'', H-6''), 7.45-7.47 (m, 3H, H-2, H-3''', H-5'''), 7.54 (d, *J* = 1.36 Hz, 1H, H-3), 7.69 (s, 1H, H-5'), 7.89 (s, 1H, H-5); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 18.6 (CH<sub>3</sub>), 40.9 (NHCH<sub>2</sub>), 49.4 (NCH<sub>2</sub>), 62.0 (OCH<sub>2</sub>), 101.9 (C-8''), 105.6 (C-5'''), 107.8 (C-4'''), 111.7 (C-5), 112.1 (C-6''), 112.2 (C-9''), 113.9 (C-3), 115.5 (C-3'''), 123.7 (C-6), 125.6 (C-5''), 131.0 (C-3'''), 132.1 (C-2), 132.3 (C-9), 142.3 (C-5'), 142.8 (C-4'), 147.5 (C-8), 152.0 (C-1'''), 152.4 (C-4''), 155.0 (C-10''), 161.0 (C-7''), 161.2 (C=O); MS (ESI): *m/z* 484.4 (M<sup>+</sup>+1); Anal. Calcd for C<sub>25</sub>H<sub>21</sub>N<sub>7</sub>O<sub>4</sub>: C, 62.11; H, 4.38; N, 20.28. Found: C, 61.90; H, 4.44; N, 20.12.

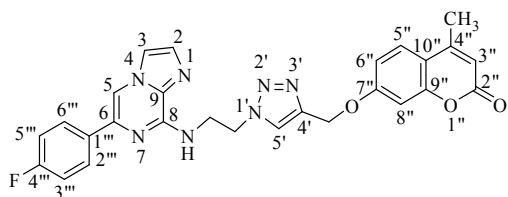
**Spectral data of 4-methyl-7-((1-(2-(6-phenylimidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (12):** light orange solid; yield: 71%; mp 176-



178 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 2.36 (s, 3H, CH<sub>3</sub>), 4.20 (q, *J* = 5.81 Hz, 2H, NHCH<sub>2</sub>), 4.80 (t, *J* = 5.72 Hz, 2H, NCH<sub>2</sub>), 5.10 (s, 2H, OCH<sub>2</sub>), 6.12 (s, 1H, H-3''), 6.80 (d, *J* = 2.28 Hz, 1H, H-8''), 6.84-6.87

(dd, <sup>2</sup>*J* = 8.72 Hz, <sup>3</sup>*J* = 2.28 Hz, 1H, H-5''), 6.91 (t, *J* = 4.88 Hz, 1H, NH), 7.36-7.47 (m, 5H, H-3''', H-4''', H-5''', H-2, H-3), 7.56 (s, 1H, H-5'), 7.69 (s, 1H, H-6'''), 7.88 (s, 1H, H-2'''), 7.90 (s, 2H, H-5, H-6''); <sup>13</sup>C (CDCl<sub>3</sub>, 100 MHz): δ 18.6 (CH<sub>3</sub>), 40.9 (NHCH<sub>2</sub>), 49.5 (NCH<sub>2</sub>), 62.0 (OCH<sub>2</sub>), 101.9 (C-8''), 107.0 (C-5), 112.1 (C-6''), 112.2 (C-9''), 113.8 (C-3), 115.3 (C-3'''), 123.8 (C-6), 125.5 (C-5''), 125.8 (C-2''', C-6''', C-3''', C-5'''), 128.4 (C-2), 128.7 (C-9), 132.3 (C-4'''), 136.9 (C-5'), 138.1 (C-1'''), 142.8 (C-4'), 147.3 (C-8), 152.4 (C-4''), 154.9 (C-10''), 160.9 (C-7''), 161.2 (C=O); MS (ESI): *m/z* 494.5 (M<sup>+</sup>+1); Anal. Calcd for C<sub>27</sub>H<sub>23</sub>N<sub>7</sub>O<sub>3</sub>: C, 65.71; H, 4.70; N, 19.87. Found: C, 65.82; H, 4.76; N, 19.77.

**Spectral data of 7-((1-(2-(6-(4-fluorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (13):** white solid; yield: 80%; mp

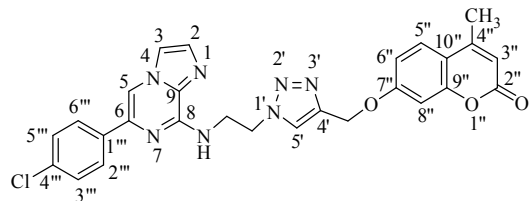


250-252 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>+ TFA, 400 MHz): δ 2.47 (d, *J* = 0.92 Hz, 3H, CH<sub>3</sub>), 4.37 (t, *J* = 5.04 Hz, 2H, NHCH<sub>2</sub>), 4.89 (t, *J* = 5.50 Hz, 2H, NCH<sub>2</sub>), 5.14 (s, 2H, OCH<sub>2</sub>), 6.31 (d, *J* = 1.36 Hz, 1H, H-3''), 6.76 (d, *J*

= 2.28 Hz, 1H, H-8''), 6.94-6.97 (dd, <sup>2</sup>*J* = 9.16 Hz, <sup>3</sup>*J* = 2.50 Hz, 1H, H-5''), 7.17 (t, *J* = 8.48 Hz, 2H, H-2''', H-6'''), 7.59 (d, *J* = 8.72 Hz, 1H, H-6''), 7.79-7.83 (m, 3H, H-3''', H-5''', H-2), 7.95 (d, *J* = 1.84 Hz, 1H, H-3), 7.99 (s, 1H, H-5'), 8.06 (s, 1H, H-5); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz): δ 18.1 (CH<sub>3</sub>), 40.8 (NHCH<sub>2</sub>), 48.7 (NCH<sub>2</sub>), 61.6 (OCH<sub>2</sub>), 101.5 (C-8''), 111.3 (C-6''), 112.5 (C-10''), 113.3 (C-3''), 115.2 (C-3'''), 115.4 (C-5'''), 116.0 (C-3), 125.2 (C-5''), 126.4 (C-5''), 127.5 (C-2'''), 127.6 (C-6'''), 131.8 (C-1'''), 132.2 (C-9), 133.6 (C-5), 133.7 (C-5'), 135.4 (C-2), 141.8 (C-4'), 147.4 (C-8), 153.4 (C-6), 154.6 (C-4''), 160.2 (C-9''), 160.8 (C-7''), 161.0 (C=O), 163.3 (C-4'''); MS (ESI): *m/z* 512.5 (M<sup>+</sup>+1); Anal. Calcd for C<sub>27</sub>H<sub>22</sub>FN<sub>7</sub>O<sub>3</sub>: C, 63.40; H, 4.34; N, 19.17. Found: C, 63.18; H, 4.28; N, 19.02.

**Spectral data of 7-((1-(2-(6-(4-chlorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (14):** creamish solid; yield: 82%; mp

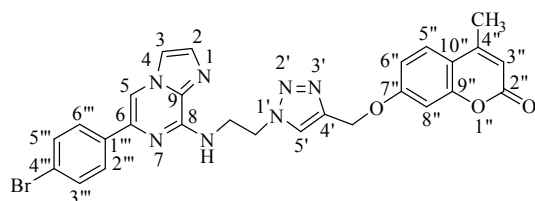




127-129 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  2.37 (d, 3H,  $\text{CH}_3$ ), 4.22 (q,  $J = 5.18$  Hz, 2H,  $\text{NHCH}_2$ ), 4.81 (t,  $J = 5.74$  Hz, 2H,  $\text{NCH}_2$ ), 5.13 (s, 2H,  $\text{OCH}_2$ ), 6.13 (d,  $J = 0.92$  Hz, 1H, H-3''), 6.81-6.83 (m, 1H, H-8''),

6.87-6.89 (dd,  $^2J = 8.68$  Hz,  $^3J = 2.30$  Hz, 1H, H-5''), 7.39-7.42 (m, 1H, H-2), 7.45 (d,  $J = 8.24$  Hz, 2H, H-3''', H-5'''), 7.46 (s, 1H, H-3), 7.50 (s, 1H, H-5'), 7.57 (s, 1H, NH), 7.70 (s, 1H, H-5), 7.81 (d,  $J = 8.72$  Hz, 1H, H-6''), 7.89 (d,  $J = 8.24$  Hz, 2H, H-2'', H-6''');  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  18.6 ( $\text{CH}_3$ ), 40.9 ( $\text{NHCH}_2$ ), 49.6 ( $\text{NCH}_2$ ), 62.0 ( $\text{OCH}_2$ ), 102.0 (C-8''), 107.0 (C-5), 112.2 (C-6''), 113.9 (C-9''), 123.8 (C-3), 125.6 (C-3''), 125.9 (C-6), 127.1 (C-5''), 128.7 (C-2''), C-6'''), 132.2 (C-3''', C-5'''), 134.2 (C-2), 135.4 (C-9), 136.9 (C-5'), 137.2 (C-1'''), 138.2 (C-4''), 142.9 (C-4'), 147.3 (C-8), 152.5 (C-4''), 154.9 (C-10''), 160.9 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  528.9 ( $\text{M}^++1$ ); Anal. Calcd for  $\text{C}_{27}\text{H}_{22}\text{ClN}_7\text{O}_3$ : C, 61.42; H, 4.20; N, 18.57. Found: C, 61.55; H, 4.04; N, 18.66.

**Spectral data of 7-((1-(2-(6-(4-bromophenyl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (15):** off white solid; yield: 64%; mp

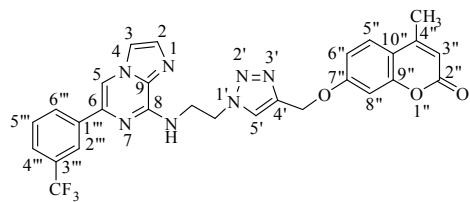


138-140 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  2.37 (d,  $J = 0.92$  Hz, 3H,  $\text{CH}_3$ ), 4.21 (q,  $J = 5.80$  Hz, 2H,  $\text{NHCH}_2$ ), 4.79 (t,  $J = 5.72$  Hz, 2H,  $\text{NCH}_2$ ), 5.12 (s, 2H,  $\text{OCH}_2$ ), 6.13 (d,  $J = 0.68$  Hz, 1H, H-3''), 6.71 (t,

$J = 5.72$  Hz, 1H, NH), 6.81 (d,  $J = 2.28$  Hz, 1H, H-8''), 6.85-6.88 (dd,  $^2J = 8.72$  Hz,  $^3J = 2.76$  Hz, 1H, H-5''), 7.40-7.45 (m, 3H, H-2''', H-6''', H-6''), 7.54-7.58 (m, 2H, H-2, H-3), 7.67 (s, 1H, H-5'), 7.75 (d,  $J = 8.00$  Hz, 2H, H-3''', H-5'''), 7.90-7.97 (s, 1H, H-5);  $^{13}\text{C}$  ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  18.6 ( $\text{CH}_3$ ), 40.9 ( $\text{NHCH}_2$ ), 49.5 ( $\text{NCH}_2$ ), 62.0 ( $\text{OCH}_2$ ), 101.9 (C-8''), 107.0 (C-5), 112.1 (C-6''), 113.9 (C-9''), 115.4 (C-3), 122.4 (C-3''), 123.7 (C-6), 125.6 (C-5''), 126.3 (C-1'''), 127.4 (C-2''), C-6'''), 128.4 (C-2), 131.7 (C-3''', C-5'''), 132.5 (C-9), 135.9 (C-5'), 137.0 (C-4'''), 142.8 (C-4'), 147.3 (C-8), 152.4 (C-4''), 154.9 (C-10''), 160.9 (C-7''), 161.1 (C=O); MS (ESI):  $m/z$  573.4 ( $\text{M}^++1$ ); Anal. Calcd for  $\text{C}_{27}\text{H}_{22}\text{BrN}_7\text{O}_3$ : C, 56.65; H, 3.87; N, 17.13. Found: C, 56.92; H, 3.71; N, 17.09.

**Spectral data of 4-methyl-7-((1-(2-(6-(3-(trifluoromethyl)phenyl)imidazo[1,2-a]pyrazin-8-**

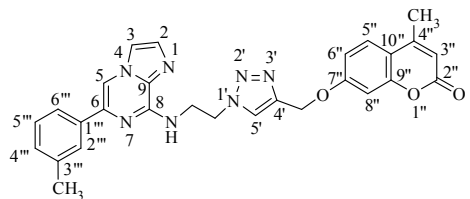
**ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (16):** white solid; yield:



71%; mp 220-122 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>+ TFA, 400 MHz): δ 2.41 (d, *J* = 1.36 Hz, 3H, CH<sub>3</sub>), 4.35 (d, *J* = 3.64 Hz, 2H, NHCH<sub>2</sub>), 4.86 (t, *J* = 5.72 Hz, 2H, NCH<sub>2</sub>), 5.09 (s, 2H, OCH<sub>2</sub>), 6.21 (d, *J* = 1.36 Hz, 1H, H-3''), 6.70 (d, *J* = 2.28

Hz, 1H, H-8''), 6.88-6.91 (dd, <sup>2</sup>*J* = 8.72 Hz, <sup>3</sup>*J* = 2.30 Hz, 1H, H-5''), 7.51 (d, *J* = 9.48 Hz, 1H, H-6''), 7.63 (t, *J* = 7.80 Hz, 1H, H-5'''), 7.71 (d, *J* = 7.76 Hz, 1H, H-6'''), 7.85 (d, *J* = 1.84 Hz, 1H, H-2), 7.96 (s, 2H, H-5', H-3), 8.06 (d, *J* = 9.6 Hz, 2H, H-2''', H-4'''), 8.10 (s, 1H, H-5), 8.89 (s, 1H, NH); <sup>13</sup>C NMR (CDCl<sub>3</sub>+ TFA, 100 MHz): δ 18.7 (CH<sub>3</sub>), 40.8 (NHCH<sub>2</sub>), 49.8 (NCH<sub>2</sub>), 60.8 (OCH<sub>2</sub>), 101.8 (C-8''), 106.3 (C-5), 111.6 (C-6''), 112.9 (C-9''), 114.2 (C-3), 122.4 (C-3''), 123.0 (C-6), 124.2 (C-5'''), 124.4 (C-6'''), 125.1 (C-5''), 125.9, 126.0, 126.6 (CF<sub>3</sub>), 126.7 (C-2'''), 129.6 (C-4'''), 129.7 (C-1'''), 131.3 (C-2), 131.6 (C-9), 135.2 (C-5'), 142.1 (C-3'''), 142.5 (C-4'), 144.1 (C-4''), 154.3 (C-8), 154.5 (C-10''), 160.8 (C-7''), 163.0 (C=O); MS (ESI): *m/z* 562.5 (M<sup>+</sup>+1); Anal. Calcd for C<sub>28</sub>H<sub>22</sub>F<sub>3</sub>N<sub>7</sub>O<sub>3</sub>: C, 59.89; H, 3.95; N, 17.46. Found: C, 60.10; H, 4.01; N, 17.39.

**Spectral data of 4-methyl-7-((1-(2-(6-*m*-tolylimidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (17):** creamish solid; yield: 65%; mp 122-124

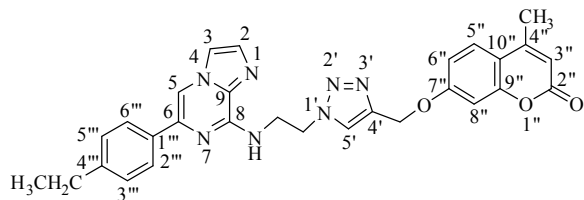


°C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 2.37 (d, *J* = 1.40 Hz, 3H, CH<sub>3</sub>), 2.44 (s, 3H, CH<sub>3</sub>), 4.22 (q, *J* = 5.80 Hz, 2H, NHCH<sub>2</sub>), 4.81 (t, *J* = 5.74 Hz, 2H, NCH<sub>2</sub>), 5.13 (s, 2H, OCH<sub>2</sub>), 6.13 (d, *J* = 0.92 Hz, 1H, H-3''), 6.73 (s, 1H, NH),

6.82 (d, *J* = 2.28 Hz, 1H, H-8''), 6.86-6.89 (dd, <sup>2</sup>*J* = 8.68 Hz, <sup>3</sup>*J* = 2.76 Hz, 1H, H-5''), 7.20 (d, *J* = 7.32 Hz, 1H, H-4'''), 7.35 (t, *J* = 7.76 Hz, 1H, H-5'''), 7.45 (d, *J* = 8.72 Hz, 1H, H-6''), 7.49 (d, *J* = 0.92 Hz, 1H, H-2), 7.56 (d, *J* = 0.92 Hz, 1H, H-3), 7.68-7.70 (m, 3H, H-5', H-2''', H-6'''), 7.89 (s, 1H, H-5); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 18.6 (CH<sub>3</sub>), 21.6 (CH<sub>3</sub>), 40.9 (NHCH<sub>2</sub>), 49.5 (NCH<sub>2</sub>), 62.0 (OCH<sub>2</sub>), 102.0 (C-8''), 107.0 (C-5), 112.1 (C-6''), 112.2 (C-9''), 113.9 (C-3), 115.2 (C-3''), 123.1 (C-4''', C-5'''), 123.8 (C-6), 125.6 (C-5''), 126.6 (C-6'''), 128.6 (C-2'''), 129.2 (C-2), 132.2 (C-9), 136.9 (C-5'), 138.3 (C-3'''), 138.3 (C-1'''), 142.8 (C-4'), 147.2 (C-8), 152.5 (C-4''), 154.9 (C-10''), 161.0 (C-7''), 161.2 (C=O); MS (ESI): *m/z* 508.5 (M<sup>+</sup>+1); Anal. Calcd for

C<sub>28</sub>H<sub>25</sub>N<sub>7</sub>O<sub>3</sub>: C, 66.26; H, 4.96; N, 19.32. Found: C, 66.42; H, 4.85; N, 19.39.

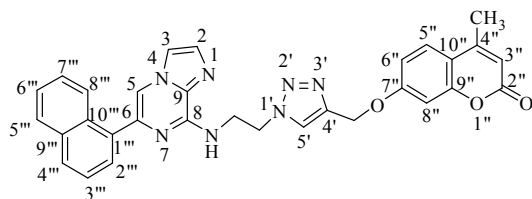
**Spectral data of 7-((1-(2-(6-(4-ethylphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (18):** creamish solid; yield: 66%;



mp 155-157 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 1.27 (t, *J* = 7.56 Hz, 3H, CH<sub>3</sub>), 2.38 (d, *J* = 1.36 Hz, 3H, CH<sub>3</sub>), 2.70 (q, *J* = 7.64 Hz, 2H, CH<sub>2</sub>), 4.21 (q, *J* = 5.81 Hz, 2H, NHCH<sub>2</sub>), 4.81 (t, *J* =

5.72 Hz, 2H, NCH<sub>2</sub>), 5.14 (s, 2H, OCH<sub>2</sub>), 6.14 (d, *J* = 0.72 Hz, 1H, H-3''), 6.77 (t, *J* = 5.72 Hz, 1H, NH), 6.83 (d, *J* = 2.52 Hz, 1H, H-8''), 6.88-6.91 (dd, <sup>2</sup>*J* = 9.16 Hz, <sup>3</sup>*J* = 2.54 Hz, 1H, H-5''), 7.29 (d, *J* = 8.24 Hz, 2H, H-3''', H-5'''), 7.46 (d, *J* = 9.16 Hz, 1H, H-6''), 7.49 (d, *J* = 1.40 Hz, 1H, H-2), 7.55 (d, *J* = 0.92 Hz, 1H, H-3), 7.70 (s, 1H, H-5'), 7.81 (d, *J* = 8.24 Hz, 2H, H-2''', H-6'''), 7.87 (s, 1H, H-5); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 15.5 (CH<sub>3</sub>), 18.6 (CH<sub>3</sub>), 28.6 (CH<sub>2</sub>), 40.9 (NHCH<sub>2</sub>), 49.5 (NCH<sub>2</sub>), 62.0 (OCH<sub>2</sub>), 102.0 (C-8''), 106.5 (C-5), 112.1 (C-6''), 112.9 (C-9''), 113.9 (C-3), 115.2 (C-3'''), 123.8 (C-6), 125.6 (C-5'''), 125.9 (C-3''', C-5'''), 128.2 (C-2''', C-6'''), 132.0 (C-2), 134.4 (C-9), 138.4 (C-5'), 142.8 (C-4'), 144.8 (C-1''', C-4'''), 147.2 (C-8), 152.4 (C-4''), 155.0 (C-10''), 161.0 (C-7''), 161.2 (C=O); MS (ESI): *m/z* 522.5 (M<sup>+</sup>+1); Anal. Calcd for C<sub>29</sub>H<sub>27</sub>N<sub>7</sub>O<sub>3</sub>: C, 66.78; H, 5.22; N, 18.80. Found: C, 66.91; H, 5.28; N, 18.91.

**Spectral data of 4-methyl-7-((1-(2-(6-(naphthalen-1-yl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (19):** light orange solid; yield: 74%;

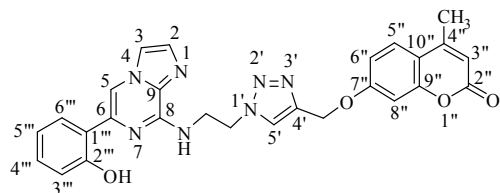


mp 165-167 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 2.34 (d, *J* = 1.36 Hz, 3H, CH<sub>3</sub>), 4.09 (q, *J* = 5.80 Hz, 2H, NHCH<sub>2</sub>), 4.69 (t, *J* = 5.74 Hz, 2H, NCH<sub>2</sub>), 5.05 (s, 2H, OCH<sub>2</sub>), 6.12 (d, *J* = 0.68 Hz, 1H, H-3'')

, 6.80 (d, *J* = 2.28 Hz, 1H, H-8''), 6.84-6.87 (dd, <sup>2</sup>*J* = 9.16 Hz, <sup>3</sup>*J* = 2.54 Hz, 1H, H-5''), 6.97 (t, *J* = 5.26 Hz, 1H, NH), 7.42 (d, *J* = 8.72 Hz, 1H, H-6''), 7.45-7.60 (m, 6H, H-2''', H-3''', H-4''', H-5''', H-6''', H-7'''), 7.61 (s, 1H, H-5'), 7.71 (s, 1H, H-8''), 7.90 (s, 1H, H-2), 7.92 (d, *J* = 1.36 Hz, 1H, H-3), 8.18-8.20 (m, 1H, H-5); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 18.6 (CH<sub>3</sub>), 40.9 (NHCH<sub>2</sub>), 49.5 (NCH<sub>2</sub>), 61.9 (OCH<sub>2</sub>), 101.9 (C-8''), 110.4 (C-5), 112.0 (C-6''), 112.2 (C-9''), 113.8 (C-3), 115.1 (C-3'''), 123.7 (C-6), 125.2 (C-5'''), 125.5 (C-4'''), 125.8 (C-6'''), 125.9 (C-5''), 126.1 (C-7'''),

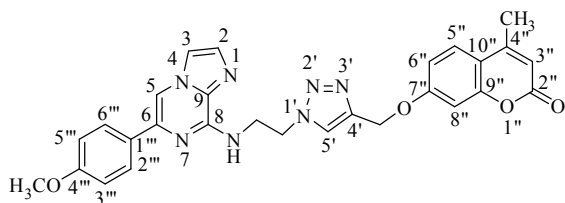
127.1 (C-3'''), 128.4 (C-8'''), 128.9 (C-2'''), 131.5 (C-9'''), 131.9 (C-2), 132.2 (C-9), 133.8 (C-10'''), 135.6 (C-5'), 139.5 (C-1'''), 142.7 (C-4'), 147.2 (C-8), 152.5 (C-4''), 154.9 (C-10''), 160.9 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  544.5 ( $M^++1$ ); Anal. Calcd for  $C_{31}H_{25}N_7O_3$ : C, 68.50; H, 4.64; N, 18.04. Found: C, 68.19; H, 4.72; N, 17.98.

**Spectral data of 7-((1-(2-(6-(2-hydroxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (20):** off white solid; yield: 53%; mp



249-251 °C;  $^1H$  NMR (DMSO- $d_6$ , 400 MHz):  $\delta$  2.38 (d,  $J = 0.88$  Hz, 3H, CH<sub>3</sub>), 3.94 (d,  $J = 5.52$  Hz, 2H, NHCH<sub>2</sub>), 4.74 (t,  $J = 5.74$  Hz, 2H, NCH<sub>2</sub>), 5.18 (s, 2H, OCH<sub>2</sub>), 6.21 (d,  $J = 0.92$  Hz, 1H, H-3''), 6.86-6.90 (m, 2H, H-6''', H-5'''), 6.96-6.99 (dd,  $^2J = 8.68$  Hz,  $^3J = 2.76$  Hz, 1H, H-5''), 7.09 (d,  $J = 2.32$  Hz, 1H, H-8''), 7.17-7.21 (m, 1H, H-4'''), 7.56 (d,  $J = 0.92$  Hz, 1H, H-2), 7.66 (d,  $J = 8.72$  Hz, 1H, H-6''), 7.81-7.84 (dd,  $^2J = 8.24$  Hz,  $^3J = 1.62$  Hz, 1H, H-3'''), 7.96 (s, 1H, H-3), 8.11 (t,  $J = 5.72$  Hz, 1H, NH), 8.29 (s, 1H, H-5'), 8.56 (s, 1H, H-5), 12.23 (s, 1H, OH);  $^{13}C$  NMR (DMSO- $d_6$ , 100 MHz):  $\delta$  18.1 (CH<sub>3</sub>), 40.8 (NHCH<sub>2</sub>), 48.27 (NCH<sub>2</sub>), 61.6 (OCH<sub>2</sub>), 101.5 (C-8''), 107.9 (C-5), 111.3 (C-6''), 112.5 (C-9''), 113.5 (C-3), 116.5 (C-3'''), 117.2 (C-5'''), 119.1 (C-4'''), 119.8 (C-6'''), 125.2 (C-6), 126.4 (C-5''), 126.6 (C-3'''), 129.4 (C-1'''), 131.1 (C-2), 132.5 (C-9), 135.3 (C-5'), 141.8 (C-4'), 146.5 (C-8), 153.4 (C-4''), 154.6 (C-10''), 156.7 (C-2'''), 160.1 (C-7''), 161.0 (C=O); MS (ESI):  $m/z$  510.5 ( $M^++1$ ); Anal. Calcd for  $C_{27}H_{23}N_7O_4$ : C, 63.65; H, 4.55; N, 19.24. Found: C, 63.53; H, 4.44; N, 19.30.

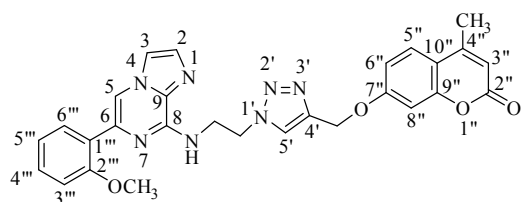
**Spectral data of 7-((1-(2-(6-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (21):** off white solid; yield: 90%; mp



172-174 °C;  $^1H$  NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  2.37 (d,  $J = 0.88$  Hz, 3H, CH<sub>3</sub>), 3.86 (s, 3H, OCH<sub>3</sub>), 4.20 (q,  $J = 5.28$  Hz, 2H, NHCH<sub>2</sub>), 4.80 (t,  $J = 5.50$  Hz, 2H, NCH<sub>2</sub>), 5.10 (s, 2H, OCH<sub>2</sub>), 6.17 (d,  $J = 0.88$  Hz, 1H, H-3''), 6.81 (m, 2H, H-8'', NH), 6.85-6.88 (dd,  $^2J = 8.72$  Hz,  $^3J = 2.28$  Hz, 1H, H-5''), 6.98 (d,  $J = 9.16$  Hz, 2H, H-2''', H-6'''), 7.44 (d,  $J = 8.68$  Hz, 2H, H-3''', H-5'''), 7.54 (s, 1H, H-5'), 7.69 (s, 1H, H-6''), 7.81 (s, 1H, H-2), 7.82 (s, 1H, H-3), 7.83 (s, 1H, H-5);  $^{13}C$  NMR

(CDCl<sub>3</sub>, 100 MHz):  $\delta$  18.6 (CH<sub>3</sub>), 40.9 (NHCH<sub>2</sub>), 49.6 (NCH<sub>2</sub>), 52.3 (OCH<sub>3</sub>), 62.0 (OCH<sub>2</sub>), 101.9 (C-8''), 106.0 (C-5), 112.1 (C-6''), 112.2 (C-9''), 113.9 (C-3), 114.0 (C-2'''), C-6'''), 115.1 (C-3'''), 123.8 (C-6), 125.6 (C-5'''), 127.1 (C-3''', C-5'''), 129.5 (C-2), 132.1 (C-9), 138.0 (C-5'), 142.8 (C-4'), 147.2 (C-8), 152.4 (C-4'''), 154.9 (C-10'''), 159.9 (C-1''', C-4'''), 161.0 (C-7'''), 161.2 (C=O); MS (ESI): m/z 524.5 (M<sup>+</sup>+1); Anal. Calcd for C<sub>28</sub>H<sub>25</sub>N<sub>7</sub>O<sub>4</sub>: C, 64.24; H, 4.81; N, 18.73. Found: C, 64.56; H, 4.92; N, 18.90.

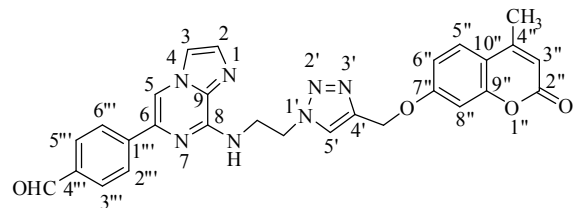
**Spectral data of 7-((1-(2-(6-(2-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (22):** creamish solid; yield: 91%; mp



120-122 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz):  $\delta$  2.36 (d, *J* = 0.68 Hz, 3H, CH<sub>3</sub>), 3.95 (s, 3H, OCH<sub>3</sub>), 4.16 (q, *J* = 5.65 Hz, 2H, NHCH<sub>2</sub>), 4.80 (t, *J* = 5.50 Hz, 2H, NCH<sub>2</sub>), 5.09 (s, 2H, OCH<sub>2</sub>), 6.12 (d, *J* = 1.36 Hz, 1H,

H-3''), 6.80 (d, *J* = 2.32 Hz, 1H, H-8''), 6.84 (d, *J* = 2.28 Hz, 1H, H-6''), 6.86 (d, *J* = 2.32 Hz, 1H, H-3'''), 7.02 (d, *J* = 8.24 Hz, 1H, H-5''), 7.08-7.12 (m, 1H, H-5''), 7.33-7.37 (m, 1H, H-2), 7.42 (d, *J* = 8.72 Hz, 1H, H-6''), 7.45 (s, 1H, NH), 7.55 (s, 1H, H-3), 7.67 (s, 1H, H-5'), 8.10-8.12 (dd, <sup>2</sup>*J* = 7.80 Hz, <sup>3</sup>*J* = 1.84 Hz, 1H, H-4'''), 8.35 (s, 1H, H-5); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz):  $\delta$  18.6 (CH<sub>3</sub>), 41.0 (NHCH<sub>2</sub>), 49.4 (NCH<sub>2</sub>), 55.5 (OCH<sub>3</sub>), 62.0 (OCH<sub>2</sub>), 101.9 (C-8''), 111.2 (C-5), 111.7 (C-6''), 112.0 (C-9''), 112.1 (C-3), 113.8 (C-3''), 115.3 (C-5'''), 120.9 (C-6), 123.8 (C-5''), 125.4 (C-4'''), 125.5 (C-2''), 129.2 (C-9), 130.2 (C-6'''), 132.2 (C-3'''), 134.2 (C-5'), 142.7 (C-1''', C-4'), 146.8 (C-8), 152.4 (C-4''), 154.9 (C-10''), 156.7 (C-2'''), 161.0 (C-7''), 161.2 (C=O); MS (ESI): m/z 524.5 (M<sup>+</sup>+1); Anal. Calcd for C<sub>28</sub>H<sub>25</sub>N<sub>7</sub>O<sub>4</sub>: C, 64.24; H, 4.81; N, 18.73. Found: C, 64.11; H, 4.79; N, 18.86.

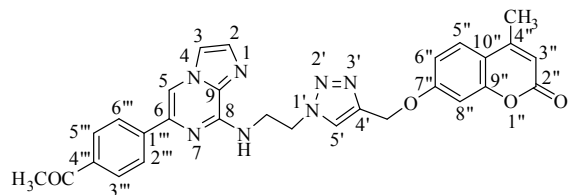
**Spectral data of 4-(8-(2-(4-((4-methyl-2-oxo-2*H*-chromen-7-yl)oxy)methyl)-1*H*-1,2,3-triazol-1-yl)ethylamino)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde (23):** yellowish solid; yield: 92%;



mp 212-214 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>+ DMSO-*d*<sub>6</sub>, 400 MHz):  $\delta$  2.37 (s, 3H, CH<sub>3</sub>), 4.04 (q, *J* = 5.96 Hz, 2H, NHCH<sub>2</sub>), 4.76 (t, *J* = 6.18 Hz, 2H, NCH<sub>2</sub>), 5.12 (s, 2H, OCH<sub>2</sub>), 6.19 (d, *J* = 1.36 Hz,

1H, H-3''), 6.90-6.92 (dd,  $^2J = 8.72$  Hz,  $^3J = 3.20$  Hz, 1H, H-5''), 7.02 (d,  $J = 2.28$  Hz, 1H, H-8''), 7.54 (s, 1H, H-5'), 7.62 (d,  $J = 8.72$  Hz, 1H, H-6''), 7.88-7.90 (m, 2H, H-2, H-3), 7.95 (d,  $J = 8.24$  Hz, 2H, H-3''', H-5'''), 8.17 (d,  $J = 8.68$  Hz, 2H, H-2''', H-6'''), 8.30 (bs, 1H, NH), 8.59 (s, 1H, H-5), 9.99 (s, 1H, CHO);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3 + \text{DMSO-}d_6$ , 100 MHz):  $\delta$  18.1 ( $\text{CH}_3$ ), 40.4 ( $\text{NHCH}_2$ ), 48.8 ( $\text{NCH}_2$ ), 61.6 ( $\text{OCH}_2$ ), 101.4 (C-8''), 108.9 (C-5), 111.3 (C-6''), 112.5 (C-9''), 113.3 (C-3), 116.4 (C-3'''), 125.2 (C-6), 126.0 (C-2''', C-6'''), 126.4 (C-5'''), 129.8 (C-3''', C-5'''), 132.0 (C-2), 132.4 (C-9), 134.9 (C-5'), 135.4 (C-1'''), 141.8 (C-4'''), 143.0 (C-4'), 147.5 (C-8), 153.4 (C-4''), 154.6 (C-10''), 160.2 (C-7''), 160.9 (C=O), 192.6 (CHO); MS (ESI):  $m/z$  522.5 ( $\text{M}^++1$ ); Anal. Calcd for  $\text{C}_{28}\text{H}_{23}\text{N}_7\text{O}_4$ : C, 64.48; H, 4.45; N, 18.80. Found: C, 64.56; H, 4.40; N, 18.73.

**Spectral data of 7-((1-(2-(6-(4-acetylphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (24):** creamish solid; yield: 90%; mp



235-237 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3 + \text{DMSO-}d_6$ , 400 MHz):  $\delta$  2.41 (s, 3H,  $\text{CH}_3$ ), 2.64 (s, 3H,  $\text{COCH}_3$ ), 4.24 (q,  $J = 5.65$  Hz, 2H,  $\text{NHCH}_2$ ), 4.84 (t,  $J = 5.72$  Hz, 2H,  $\text{NCH}_2$ ), 5.14 (s, 2H,  $\text{OCH}_2$ ), 6.12 (s,

1H, H-3''), 6.85-6.92 (m, 2H, H-5'', H-8''), 7.52 (m, 2H, H-2, H-3), 7.84-8.05 (m, 7H, H-6'', H-5', NH, H-2''', H-6''', H-3''', H-5'''), 8.27 (s, 1H, H-5);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3 + \text{DMSO-}d_6$ , 100 MHz):  $\delta$  17.2 ( $\text{CH}_3$ ), 25.3 ( $\text{CH}_3$ ), 41.0 ( $\text{NHCH}_2$ ), 47.8 ( $\text{NCH}_2$ ), 60.4 ( $\text{OCH}_2$ ), 100.2 (C-8''), 106.9 (C-5), 110.3 (C-6''), 111.0 (C-9''), 112.2 (C-3), 114.8 (C-3'''), 123.3 (C-8), 124.4 (C-2''', C-6'''), 124.5 (C-5'''), 127.1 (C-3''', C-5'''), 129.6 (C-2), 130.0 (C-9), 134.8 (C-1'''), 135.2 (C-5'), 140.1 (C-4'''), 140.8 (C-4'), 145.7 (C-4''), 151.5 (C-8), 153.4 (C-10''), 159.3 (C-7''), 159.7 (C=O), 195.9 (C=O); MS (ESI):  $m/z$  536.5 ( $\text{M}^++1$ ); Anal. Calcd for  $\text{C}_{29}\text{H}_{25}\text{N}_7\text{O}_4$ : C, 65.04; H, 4.71; N, 18.31. Found: C, 64.90; H, 4.56; N, 18.28.

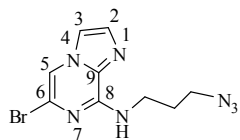
**Procedure for the synthesis of 3-azidopropanamine (26):** 3-Bromopropylamine hydrobromide **25** (1 g, 4.56 mmol) was dissolved in distilled water with stirring. Sodium azide was added (0.95 g, 14.61 mmol) carefully in succession with continuous stirring. The reaction mixture was refluxed for 12 h. After completion of reaction, reaction mixture was cooled to room temperature and was quenched by addition of sodium hydroxide (0.7 g, 17.5 mmol) and further stirred for 30

min at room temperature. Thereafter, mixture was extracted with diethyl ether and dried over sodium sulphate, filtered to obtain ether extract and stored at low temperature. The ether extract being volatile in nature, was used as such for next reaction.

**Procedure for synthesis of *N*-(3-azidopropyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine (27):**

To the ether extract containing 3-azidopropanamine **26**, was added mixture of 6,8-dibromoimidazo[1,2-*a*]pyrazine **3** (0.5 g, 1.80 mmol) in acetonitrile in the presence of diisopropylethylamine. The reaction mixture was refluxed for 24 h. After completion of reaction, the mixture was extracted with chloroform and water. Organic layer was dried over anhydrous sodium sulphate, filtered and concentrated over vacuum. The crude mixture was then purified by silica gel chromatography 60-120 mesh using hexane : ethyl acetate (6:1) as eluents.

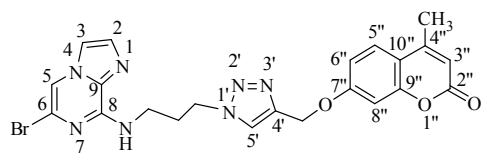
**Spectral data of *N*-(3-azidopropyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine (27):** red solid;



yield: 65%; mp 62-64 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 1.97 (m, 2H, CH<sub>2</sub>), 3.44 (t, *J* = 6.64 Hz, 2H, NCH<sub>2</sub>), 3.69 (q, *J* = 6.56 Hz, 2H, NHCH<sub>2</sub>), 6.64 (bs, 1H, NH), 7.45 (d, *J* = 0.92 Hz, 1H, H-2), 7.48 (d, *J* = 1.36 Hz, 1H, H-3), 7.58 (s, 1H, H-5); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 28.3 (CH<sub>2</sub>), 38.1 (NHCH<sub>2</sub>), 49.0 (NCH<sub>2</sub>), 109.1 (C-5), 114.7 (C-3), 122.9 (C-6), 132.0 (C-2), 132.2 (C-9), 147.5 (C-8); MS (ESI): *m/z* 297.0 (M<sup>+</sup>+1); Anal. Calcd for C<sub>9</sub>H<sub>10</sub>BrN<sub>7</sub>: C, 36.50; H, 3.40; N, 33.11. Found: C, 36.54; H, 3.41; N, 33.13.

**Procedure for synthesis of 7-((1-(3-(6-bromoimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (28):** To the stirred solution of 4-methyl-7-(prop-2-ynyloxy)-2*H*-chromen-2-one **6** (1g, 4.67 mmol) and *N*-(2-azidopropyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine **27** (1.31 g, 4.67 mmol) in ethanol:water (8:2), copper sulphate pentahydrate (5 mol%) and sodium ascorbate (10 mol%) was added and stirred at room temperature for 2 h. After completion of reaction, water was added and extracted with chloroform. Organic layer was dried over sodium sulphate, filtered and concentrated in vacuum to obtain off white solid.

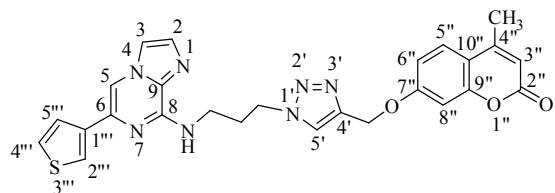
**Spectral data of 7-((1-(3-(6-bromoimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (28):** white solid; yield: 82%; mp 155-157



°C; <sup>1</sup>H NMR (DMSO-*d*<sub>6</sub>, 400 MHz): δ 2.18 (m, 2H, CH<sub>2</sub>), 2.35 (s, 3H, CH<sub>3</sub>), 3.43 (m, 2H, NHCH<sub>2</sub>), 4.45 (t, *J* = 6.88 Hz, 2H, NCH<sub>2</sub>), 5.24 (s, 2H, OCH<sub>2</sub>), 6.17 (d, *J* = 0.92 Hz, 1H, H-3''), 6.98-7.00 (dd, <sup>2</sup>*J* = 8.72 Hz, <sup>3</sup>*J* = 2.52 Hz, 1H, H-5''), 7.10 (d, *J* = 2.28 Hz, 1H, H-8''), 7.49 (d, *J* = 0.68 Hz, 1H, H-2), 7.63 (d, *J* = 8.72 Hz, 1H, H-6''), 7.81 (d, *J* = 0.92 Hz, 1H, H-3), 7.98 (s, 1H, H-5'), 8.13 (t, *J* = 5.50 Hz, 1H, NH), 8.35 (s, 1H, H-5); <sup>13</sup>C NMR (DMSO-*d*<sub>6</sub>, 100 MHz): δ 18.1 (CH<sub>3</sub>), 29.2 (CH<sub>2</sub>), 37.3 (NHCH<sub>2</sub>), 47.4 (NCH<sub>2</sub>), 61.7 (OCH<sub>2</sub>), 101.5 (C-8''), 109.1 (C-5), 111.2 (C-6''), 112.6 (C-9''), 113.3 (C-3''), 115.9 (C-3), 121.8 (C-6), 124.9 (C-5'), 126.4 (C-5''), 131.5 (C-2), 132.1 (C-9), 141.8 (C-4'), 147.5 (C-8), 153.4 (C-4''), 154.6 (C-10''), 160.1 (C-7''), 161.0 (C=O); MS (ESI): *m/z* 512.3 (M<sup>+</sup>+2); Anal. Calcd for C<sub>22</sub>H<sub>20</sub>BrN<sub>7</sub>O<sub>3</sub>: C, 51.78; H, 3.95; N, 19.21. Found: C, 51.91; H, 3.88; N, 19.07.

**General procedure for synthesis of 6-arylated-7-((1-(2-(6-bromoimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (29-38):** To a solution of 6-bromotriazole bridged imidazo[1,2-*a*]pyrazine-coumarin conjugate **28** (0.10 g, 0.196 mmol) in 1,4-dioxane: water (9:1) in a sealed tube, boronic acid (0.196 mmol) and K<sub>2</sub>CO<sub>3</sub> (0.027 g, 0.196 mmol) were added under inert atmosphere. Pd(PPh<sub>3</sub>)<sub>4</sub> (5mol%) was added with continued nitrogen purging and refluxed the reaction mixture for 6-8 h. Completion of reaction was determined by TLC. The mixture was extracted with chloroform and water. Organic layer was dried using sodium sulphate to obtain crude product which was further purified by column chromatography using ethylacetate : methanol as eluents.

**Spectral data of 4-methyl-7-((1-(3-(6-(thiophen-3-yl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (29):** reddish brown

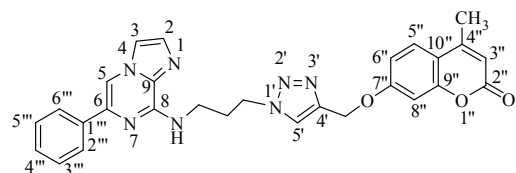


solid; yield: 72%; mp 170-172 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 2.37-2.43 (m, 5H, CH<sub>3</sub>, CH<sub>2</sub>), 3.79 (q, *J* = 6.41 Hz, 2H, NHCH<sub>2</sub>), 4.54 (t, *J* = 6.64 Hz, 2H, NCH<sub>2</sub>), 5.18 (s, 2H, OCH<sub>2</sub>), 6.15 (d, *J* = 1.36 Hz, 1H, H-3''), 6.40 (s, 1H, NH), 6.86 (d, *J* = 2.32 Hz, 1H, H-8''), 6.91-6.94 (dd, <sup>2</sup>*J* = 8.72 Hz, <sup>3</sup>*J* = 2.28 Hz, 1H, H-5''), 7.35-7.37 (m, 1H, H-6''), 7.44-7.45 (dd, <sup>2</sup>*J* = 5.04 Hz, <sup>3</sup>*J* = 1.36 Hz,



1H, H-5'''), 7.48 (s, 1H, H-5'), 7.51 (d,  $J = 0.92$  Hz, 1H, H-2), 7.54 (d,  $J = 0.88$  Hz, 1H, H-3), 7.77-7.78 (m, 2H, H-2''', H-4'''), 7.81 (s, 1H, H-5);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  18.6 ( $\text{CH}_3$ ), 30.2 ( $\text{CH}_2$ ), 37.0 ( $\text{NHCH}_2$ ), 47.7 ( $\text{NCH}_2$ ), 62.1 ( $\text{OCH}_2$ ), 101.9 (C-8''), 106.2 (C-5), 112.1 (C-6''), 112.4 (C-9''), 113.9 (C-3), 115.2 (C-3''), 122.4 (C-5'''), 123.7 (C-6), 124.8 (C-4'''), 125.6 (C-5''), 126.5 (C-2'''), 131.9 (C-2), 133.2 (C-9), 135.0 (C-5'), 139.3 (C-1'''), 142.7 (C-4'), 147.8 (C-8), 152.4 (C-4''), 155.0 (C-10''), 161.1 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  514.5 ( $\text{M}^++1$ ); Anal. Calcd for  $\text{C}_{26}\text{H}_{23}\text{N}_7\text{O}_3\text{S}$ : C, 60.81; H, 4.51; N, 19.09; S, 6.24. Found: C, 60.76; H, 4.43; N, 19.28; S, 6.08.

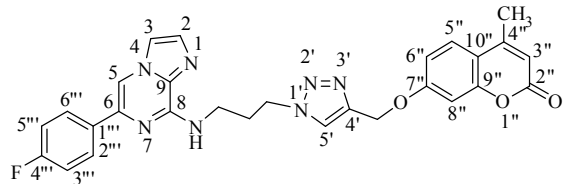
**Spectral data of 4-methyl-7-((1-(3-(6-phenylimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (30):** creamish solid; yield: 70%; mp 154-156



$^{\circ}\text{C}$ ;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  2.37-2.43 (m, 5H,  $\text{CH}_3$ ,  $\text{CH}_2$ ), 3.82 (q,  $J = 6.27$  Hz, 2H,  $\text{NHCH}_2$ ), 4.54 (t,  $J = 6.88$  Hz, 2H,  $\text{NCH}_2$ ), 5.09 (s, 2H,  $\text{OCH}_2$ ), 6.14 (d,

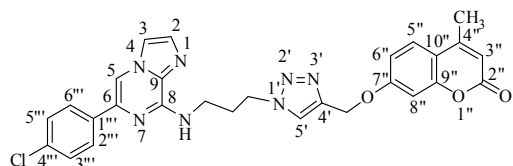
$J = 1.40$  Hz, 1H, H-3''), 6.40 (t,  $J = 5.96$  Hz, 1H, NH), 6.83 (d,  $J = 2.32$  Hz, 1H, H-8''), 6.89-6.91 (dd,  $^2J = 8.72$  Hz,  $^3J = 2.28$  Hz, 1H, H-5''), 7.32-7.36 (m, 1H, H-3'''), 7.43 (t,  $J = 7.22$  Hz, 2H, H-4''', H-5'''), 7.48 (d,  $J = 8.72$  Hz, 1H, H-6''), 7.52 (s, 1H, H-5'), 7.57 (d,  $J = 0.92$  Hz, 1H, H-2), 7.78 (s, 1H, H-3), 7.87 (s, 1H, H-5), 7.89 (d,  $J = 1.40$  Hz, 2H, H-2''', H-6''');  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  18.6 ( $\text{CH}_3$ ), 30.3 ( $\text{CH}_2$ ), 37.1 ( $\text{NHCH}_2$ ), 47.7 ( $\text{NCH}_2$ ), 61.9 ( $\text{OCH}_2$ ), 101.9 (C-8''), 106.6 (C-5), 112.1 (C-6''), 112.4 (C-9''), 113.9 (C-3''), 115.2 (C-3), 123.8 (C-6), 125.6 (C-5''), 126.0 (C-2''', C-6'''), 128.3 (C-4'''), 128.6 (C-3''', C-5'''), 132.1 (C-2), 132.4 (C-9), 137.1 (C-5'), 138.3 (C-1'''), 142.6 (C-4'), 147.8 (C-8), 152.5 (C-4''), 155.0 (C-10''), 161.0 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  508.5 ( $\text{M}^++1$ ); Anal. Calcd for  $\text{C}_{28}\text{H}_{25}\text{N}_7\text{O}_3$ : C, 66.26; H, 4.96; N, 19.32. Found: C, 66.41; H, 5.03; N, 19.19.

**Spectral data of 7-((1-(3-(6-(4-fluorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (31):** brown solid; yield: 76%; mp



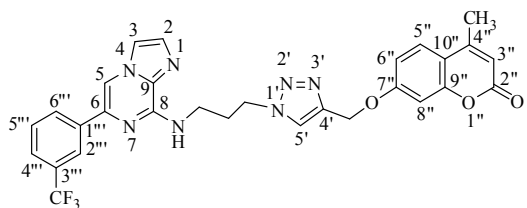
185-187 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3 + \text{TFA}$ , 400 MHz):  $\delta$  2.39 (d,  $J = 1.40$  Hz, 3H,  $\text{CH}_3$ ), 2.47 (m, 2H,  $\text{CH}_2$ ), 3.80 (d,  $J = 4.12$  Hz, 2H,  $\text{NHCH}_2$ ), 4.59 (t,  $J = 6.88$  Hz, 2H,  $\text{NCH}_2$ ), 5.21 (s, 2H,  $\text{OCH}_2$ ), 6.13 (d,  $J = 1.36$  Hz, 1H, H-3''), 6.87 (d,  $J = 2.76$  Hz, 1H, H-8''), 6.94-6.96 (dd,  $^2J = 8.72$  Hz,  $^3J = 2.30$  Hz, 1H, H-5''), 7.16 (t,  $J = 8.70$  Hz, 2H, H-2''', H-6'''), 7.50 (d,  $J = 8.68$  Hz, 1H, H-6''), 7.77 (d,  $J = 1.84$  Hz, 1H, H-2), 7.78 (d,  $J = 1.84$  Hz, 1H, H-3), 7.86-7.90 (m, 2H, H-3''', H-5'''), 7.96 (s, 1H, H-5'), 8.04 (s, 1H, H-5), 9.25 (s, 1H, NH);  $^{13}\text{C}$  NMR ( $\text{DMSO}-d_6$ , 100 MHz):  $\delta$  18.1 ( $\text{CH}_3$ ), 29.5 ( $\text{CH}_2$ ), 37.2 ( $\text{NHCH}_2$ ), 47.6 ( $\text{NCH}_2$ ), 61.7 ( $\text{OCH}_2$ ), 101.5 (C-8''), 106.4 (C-F), 111.3 (C-6''), 112.5 (C-10''), 113.3 (C-3''), 115.2 (C-3'''), 115.4 (C-5'''), 115.9 (C-3), 125.0 (C-5''), 126.4 (C-5'''), 127.4 (C-2'''), 127.5 (C-6'''), 131.9 (C-1'''), 132.0 (C-9), 133.7 (C-5), 133.7 (C-5'), 135.5 (C-2), 141.8 (C-4'), 147.6 (C-8), 153.3 (C-6), 154.6 (C-4''), 160.1 (C-9''), 160.8 (C-7''), 161.0 (C=O), 163.2 (C-4'''); MS (ESI):  $m/z$  526.5 ( $\text{M}^++1$ ); Anal. Calcd for  $\text{C}_{28}\text{H}_{24}\text{FN}_7\text{O}_3$ : C, 63.99; H, 4.60; N, 18.66. Found: C, 63.71; H, 4.52; N, 18.79.

**Spectral data of 7-((1-(3-(6-(4-chlorophenyl)imidazo[1,2-a]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (32):** creamish solid; yield: 70%; mp



188-190 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  2.43-2.44 (m, 5H,  $\text{CH}_3$ ,  $\text{CH}_2$ ), 3.80 (q,  $J = 6.25$  Hz, 2H,  $\text{NHCH}_2$ ), 4.54 (t,  $J = 6.66$  Hz, 2H,  $\text{NCH}_2$ ), 5.15 (s, 2H,  $\text{OCH}_2$ ), 6.15 (d,  $J = 0.92$  Hz, 1H, H-3''), 6.35 (t,  $J = 5.28$  Hz, 1H, NH), 6.85 (d,  $J = 2.76$  Hz, 1H, H-8''), 6.90-6.93 (dd,  $^2J = 8.68$  Hz,  $^3J = 2.74$  Hz, 1H, H-5''), 7.38 (d,  $J = 8.68$  Hz, 2H, H-2''', H-6'''), 7.50 (d,  $J = 9.16$  Hz, 1H, H-6''), 7.53 (s, 1H, H-5'), 7.57 (s, 1H, H-2), 7.74 (s, 1H, H-3), 7.82 (d,  $J = 8.72$  Hz, 2H, H-3''', H-5'''), 7.88 (s, 1H, H-5);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  18.6 ( $\text{CH}_3$ ), 30.2 ( $\text{CH}_2$ ), 37.1 ( $\text{NHCH}_2$ ), 47.8 ( $\text{NCH}_2$ ), 62.0 ( $\text{OCH}_2$ ), 102.0 (C-8''), 106.6 (C-5), 112.1 (C-6''), 112.2 (C-9''), 113.9 (C-3), 115.3 (C-3''), 123.5 (C-6), 125.6 (C-5''), 127.1 (C-2''', C-6'''), 128.8 (C-3''', C-5'''), 132.3 (C-2), 132.4 (C-9), 134.1 (C-5'), 135.6 (C-1'''), 137.2 (C-4'''), 142.8 (C-4'), 147.8 (C-8), 152.5 (C-4''), 155.0 (C-10''), 161.0 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  542.9 ( $\text{M}^++1$ ); Anal. Calcd for  $\text{C}_{28}\text{H}_{24}\text{ClN}_7\text{O}_3$ : C, 62.05; H, 4.46; N, 18.09. Found: C, 61.91; H, 4.32; N, 18.23.

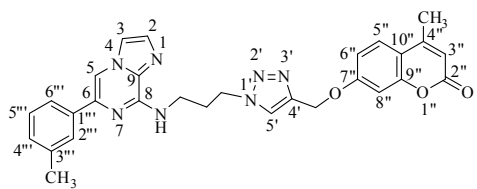
**Spectral data of 4-methyl-7-((1-(3-(6-(3-(trifluoromethyl)phenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (33):** creamish solid;



yield: 80%; mp 181-183 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub> + TFA, 400 MHz): δ 2.40 (d, *J* = 0.92 Hz, 3H, CH<sub>3</sub>), 2.51 (m, 2H, CH<sub>2</sub>), 3.84 (bs, 2H, NHCH<sub>2</sub>), 4.63 (t, *J* = 6.64 Hz, 2H, NCH<sub>2</sub>), 5.23 (s, 2H, OCH<sub>2</sub>), 6.13 (d, *J* = 1.36

Hz, 1H, H-3''), 6.83 (d, *J* = 2.28 Hz, 1H, H-8''), 6.92-6.95 (dd, <sup>2</sup>*J* = 8.68 Hz, <sup>3</sup>*J* = 2.52 Hz, 1H, H-5''), 7.52 (d, *J* = 8.68 Hz, 1H, H-6''), 7.63 (t, *J* = 7.80 Hz, 1H, H-5'''), 7.71 (d, *J* = 7.80 Hz, 1H, H-6'''), 7.85 (d, *J* = 1.80 Hz, 1H, H-2), 7.90 (d, *J* = 1.80 Hz, 1H, H-3), 8.07 (s, 1H, H-5), 8.11-8.12 (m, 3H, H-2''', H-4''', H-5), 8.97 (s, 1H, NH); <sup>13</sup>C NMR (CDCl<sub>3</sub> + TFA, 100 MHz): δ 18.6 (CH<sub>3</sub>), 28.6 (CH<sub>2</sub>), 38.2 (NHCH<sub>2</sub>), 48.6 (NCH<sub>2</sub>), 61.3 (OCH<sub>2</sub>), 101.9 (C-8''), 105.6 (C-5), 111.9 (C-6''), 112.6 (C-9''), 114.1 (C-3), 116.2 (C-3''), 119.7 (C-6), 122.4, 122.9, 124.0, 124.5 (CF<sub>3</sub>), 125.1 (C-6'''), 125.8 (C-5''), 126.2 (C-2'''), 126.5 (C-4'''), 129.6 (C-2), 129.7 (C-9), 131.2 (C-5'''), 131.5 (C-1'''), 135.7 (C-5'), 142.2 (C-4'), 142.4 (C-3'''), 144.4 (C-8), 153.3 (C-4''), 154.7 (C-10''), 160.9 (C-7''), 162.0 (C=O); MS (ESI): *m/z* 576.5 (M<sup>+</sup>+1); Anal. Calcd for C<sub>29</sub>H<sub>24</sub>F<sub>3</sub>N<sub>7</sub>O<sub>3</sub>: C, 60.52; H, 4.20; N, 17.04. Found: C, 60.88; H, 4.05; N, 17.19.

**Spectral data of 4-methyl-7-((1-(3-(6-*m*-tolylimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (34):** brown solid; yield: 81%; mp 95-97 °C;

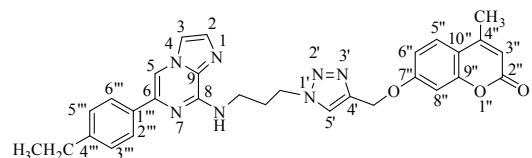


<sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 2.37-2.44 (m, 7H, CH<sub>3</sub>, CH<sub>3</sub>, CH<sub>2</sub>), 3.83 (q, *J* = 6.25 Hz, 2H, NHCH<sub>2</sub>), 4.54 (t, *J* = 6.64 Hz, 2H, NCH<sub>2</sub>), 5.09 (s, 2H, OCH<sub>2</sub>), 6.15 (d, *J*

= 0.92 Hz, 1H, H-3''), 6.36 (t, *J* = 5.72 Hz, 1H, NH), 6.83 (d, *J* = 2.28 Hz, 1H, H-8''), 6.88-6.91 (dd, <sup>2</sup>*J* = 8.68 Hz, <sup>3</sup>*J* = 2.30 Hz, 1H, H-5''), 7.17 (d, *J* = 7.36 Hz, 1H, H-6''), 7.32 (d, *J* = 7.56 Hz, 1H, H-4''), 7.49 (d, *J* = 8.72 Hz, 1H, H-6''), 7.53 (d, *J* = 0.88 Hz, 1H, H-2), 7.56 (d, *J* = 1.36 Hz, 1H, H-3), 7.67-7.69 (m, 2H, H-5', H-5'''), 7.78 (s, 1H, H-2'''), 7.88 (s, 1H, H-5); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 18.6 (CH<sub>3</sub>), 21.6 (CH<sub>3</sub>), 30.3 (CH<sub>2</sub>), 37.1 (NHCH<sub>2</sub>), 47.7 (NCH<sub>2</sub>), 61.9 (OCH<sub>2</sub>), 101.9 (C-8''), 106.6 (C-5), 112.1 (C-6''), 112.4 (C-9''), 113.9 (C-3), 115.2 (C-3''), 123.2 (C-5'''), 123.8 (C-6), 125.6 (C-5''), 126.6 (C-2'''), 128.6 (C-4'''), 129.1 (C-6'''), 132.1 (C-2),

132.4 (C-9), 137.1 (C-5'), 138.3 (C-1'''), 138.5 (C-3'''), 142.6 (C-4'), 147.8 (C-8), 152.5 (C-4''), 155.0 (C-10''), 161.1 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  522.6 ( $M^++1$ ); Anal. Calcd for  $C_{29}H_{27}N_7O_3$ : C, 66.78; H, 5.22; N, 18.80. Found: C, 66.62; H, 5.34; N, 18.91.

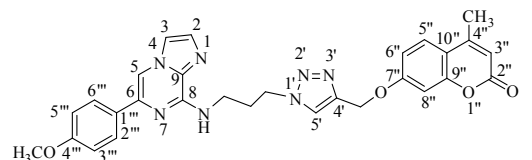
**Spectral data of 7-((1-(3-(6-(4-ethylphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (35):** creamish solid; yield: 56%; mp



100-102 °C;  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  1.23 (t,  $J$  = 7.56 Hz, 3H,  $CH_3$ ), 2.35-2.42 (m, 5H,  $CH_3$ ,  $CH_2$ ), 2.65 (q,  $J$  = 7.64 Hz, 2H,  $CH_2$ ), 3.81 (q,  $J$  = 6.10 Hz,

2H,  $NHCH_2$ ), 4.54 (t,  $J$  = 6.64 Hz, 2H,  $NCH_2$ ), 5.15 (s, 2H,  $OCH_2$ ), 6.14 (d,  $J$  = 1.36 Hz, 1H, H-3''), 6.41 (s, 1H, NH), 6.84 (d,  $J$  = 2.76 Hz, 1H, H-8''), 6.89-6.92 (dd,  $^2J$  = 9.16 Hz,  $^3J$  = 2.52 Hz, 1H, H-5''), 7.25 (m, 2H, H-3''', H-5'''), 7.48 (d,  $J$  = 8.68 Hz, 1H, H-6''), 7.52 (s, 1H, H-5'), 7.56 (s, 1H, H-2), 7.79 (d,  $J$  = 2.76 Hz, 2H, H-2''', H-6'''), 7.81 (s, 1H, H-3), 7.86 (s, 1H, H-5);  $^{13}C$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  15.5 ( $CH_3$ ), 18.6 ( $CH_3$ ), 28.5 ( $CH_2$ ), 30.3 ( $CH_2$ ), 37.1 ( $NHCH_2$ ), 47.8 ( $NCH_2$ ), 62.0 ( $OCH_2$ ), 101.9 (C-8''), 106.2 (C-5), 112.1 (C-6''), 112.4 (C-9''), 113.9 (C-3), 115.2 (C-3'''), 123.8 (C-6), 125.6 (C-5''), 125.9 (C-3''', C-5'''), 128.2 (C-2''', C-6'''), 131.9 (C-2), 132.3 (C-9), 134.5 (C-5'), 138.5 (C-1'''), 142.6 (C-4'), 144.7 (C-4''), 147.7 (C-8), 152.4 (C-4''), 155.0 (C-10''), 161.1 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  536.5 ( $M^++1$ ); Anal. Calcd for  $C_{30}H_{29}N_7O_3$ : C, 67.27; H, 5.46; N, 18.31. Found: C, 67.10; H, 5.51; N, 18.19.

**Spectral data of 7-((1-(3-(6-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (36):** brownish solid; yield:

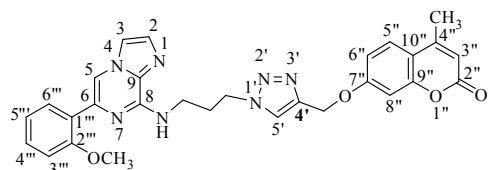


76%; mp 118-120 °C;  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  2.37-2.44 (m, 5H,  $CH_3$ ,  $CH_2$ ), 3.79-3.83 (m, 5H,  $NHCH_2$ ,  $OCH_3$ ), 4.54 (t,  $J$  = 6.64 Hz, 2H,  $NCH_2$ ), 5.12

(s, 2H,  $OCH_2$ ), 6.14 (d,  $J$  = 1.40 Hz, 1H, H-3''), 6.64 (t,  $J$  = 5.96 Hz, 1H, NH), 6.84 (d,  $J$  = 2.76 Hz, 1H, H-8''), 6.89-6.92 (dd,  $^2J$  = 9.20 Hz,  $^3J$  = 2.52 Hz, 1H, H-5''), 6.95 (d,  $J$  = 8.72 Hz, 2H, H-2''', H-6'''), 7.47 (s, 1H, H-5'), 7.50 (d,  $J$  = 1.36 Hz, 1H, H-2), 7.54 (d,  $J$  = 1.36 Hz, 1H, H-3), 7.80 (d,  $J$  = 1.40 Hz, 2H, H-3''', H-5'''), 7.81 (s, 1H, H-5), 7.83 (s, 1H, H-6'');  $^{13}C$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  18.6 ( $CH_3$ ), 30.2 ( $CH_2$ ), 37.0 ( $NHCH_2$ ), 47.7 ( $NCH_2$ ), 55.3 ( $OCH_3$ ), 62.0 ( $OCH_2$ ),

101.9 (C-8''), 105.5 (C-5), 112.1 (C-6''), 112.4 (C-9''), 113.9 (C-3), 114.0 (C-2''', C-6'''), 115.1 (C-3''), 123.8 (C-6), 125.6 (C-5''), 127.2 (C-3''', C-5'''), 129.6 (C-1'''), 131.7 (C-2), 132.1 (C-9), 138.3 (C-5'), 142.6 (C-4'), 147.7 (C-8), 152.4 (C-4''), 155.0 (C-10''), 159.8 (C-4'''), 161.1 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  538.5 ( $M^++1$ ); Anal. Calcd for  $C_{29}H_{27}N_7O_4$ : C, 64.79; H, 5.06; N, 18.24. Found: C, 64.63; H, 4.91; N, 18.36.

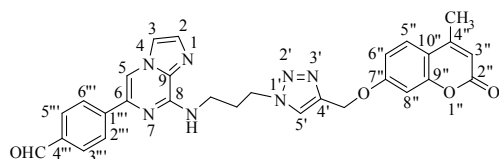
**Spectral data of 7-((1-(3-(6-(2-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (37):** brown solid; yield: 68%;



mp 162-164 °C;  $^1H$  NMR ( $CDCl_3$ , 400 MHz):  $\delta$  2.35-2.42 (m, 5H,  $CH_3$ ,  $CH_2$ ), 3.79 (q,  $J = 6.12$  Hz, 2H,  $NHCH_2$ ), 3.92 (s, 3H,  $OCH_3$ ), 4.54 (t,  $J = 6.64$  Hz, 2H,

$NCH_2$ ), 5.05 (s, 2H,  $OCH_2$ ), 6.14 (d,  $J = 0.92$  Hz, 1H, H-3''), 6.55 (bs, 1H, NH), 6.84 (d,  $J = 2.28$  Hz, 1H, H-8''), 6.89-6.92 (dd,  $^2J = 8.72$  Hz,  $^3J = 2.54$  Hz, 1H, H-5''), 6.99 (d,  $J = 8.24$  Hz, 1H, H-6''), 7.04-7.08 (m, 1H, H-5'''), 7.28-7.33 (m, 1H, H-4'''), 7.49 (d,  $J = 8.72$  Hz, 1H, H-6''), 7.53 (d,  $J = 0.92$  Hz, 1H, H-2), 7.56 (d,  $J = 1.40$  Hz, 1H, H-3), 7.87 (s, 1H, H-5'), 8.04-8.06 (dd,  $^2J = 7.80$  Hz,  $^3J = 1.84$  Hz, 1H, H-3'''), 8.28 (s, 1H, H-5);  $^{13}C$  NMR ( $CDCl_3$ , 100 MHz):  $\delta$  18.6 ( $CH_3$ ), 30.4 ( $CH_2$ ), 37.1 ( $NHCH_2$ ), 47.7 ( $NCH_2$ ), 55.5 ( $OCH_3$ ), 61.9 ( $OCH_2$ ), 101.9 (C-8''), 111.1 (C-5), 111.2 (C-6''), 112.1 (C-9''), 112.4 (C-5'''), 113.8 (C-3), 115.3 (C-3''), 120.9 (C-4'''), 124.1 (C-6), 125.4 (C-6'''), 125.5 (C-5''), 129.3 (C-3'''), 130.4 (C-1'''), 131.4 (C-2), 131.8 (C-9), 134.8 (C-5'), 142.4 (C-4'), 147.2 (C-8), 152.5 (C-4''), 155.0 (C-10''), 156.8 (C-2'''), 161.1 (C-7''), 161.2 (C=O); MS (ESI):  $m/z$  538.5 ( $M^++1$ ); Anal. Calcd for  $C_{29}H_{27}N_7O_4$ : C, 64.79; H, 5.06; N, 18.24. Found: C, 64.52; H, 4.92; N, 18.08.

**Spectral data of 4-(8-(3-(4-((4-methyl-2-oxo-2*H*-chromen-7-yl)oxy)methyl)-1*H*-1,2,3-triazol-1-yl)propylamino)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde (38):** brownish solid; yield: 90%



; mp 194-196 °C;  $^1H$  NMR ( $CDCl_3 + DMSO-d_6$ , 400 MHz):  $\delta$  2.40-2.45 (m, 5H,  $CH_3$ ,  $CH_2$ ), 3.80 (q,  $J = 6.10$  Hz, 2H,  $NHCH_2$ ), 4.58 (t,  $J = 6.64$  Hz, 2H,  $NCH_2$ ),

5.17 (s, 2H,  $OCH_2$ ), 6.12 (s, 1H, H-3''), 6.86 (d,  $J = 2.28$  Hz, 1H, H-8''), 6.90-6.93 (dd,  $^2J = 8.72$  Hz,  $^3J = 2.28$  Hz, 1H, H-5''), 7.05 (t,  $J = 5.04$  Hz, 1H, NH), 7.52 (d,  $J = 6.40$  Hz, 2H, H-2, H-3),

7.67 (s, 1H, H-5'), 7.92 (d,  $J = 8.24$  Hz, 2H, H-2''', H-6'''), 7.94 (s, 1H, H-6''), 8.10 (d,  $J = 8.28$  Hz, 2H, H-3''', H-5'''), 8.14 (s, 1H, H-5), 9.98 (s, 1H, CHO);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3 + \text{DMSO-}d_6$ , 100 MHz): 18.0 ( $\text{CH}_3$ ), 29.3 ( $\text{CH}_2$ ), 36.4 ( $\text{NHCH}_2$ ), 47.2 ( $\text{NCH}_2$ ), 61.4 ( $\text{OCH}_2$ ), 101.2 (C-8''), 107.5 (C-5), 111.3 (C-6''), 111.7 (C-9''), 113.2 (C-3), 115.1 (C-3''), 123.4 (C-6), 125.2 (C-5''), 125.6 (C-2''', C-6'''), 129.3 (C-3''', C-5'''), 131.7 (C-2), 132.0 (C-9), 135.0 (C-5'), 135.8 (C-1'''), 141.9 (C-4'''), 142.7 (C-4'), 147.4 (C-8), 152.1 (C-4''), 154.3 (C-10''), 160.4 (C-7''), 160.5 (C=O), 191.2 (CHO); MS (ESI):  $m/z$  536.5 ( $\text{M}^+ + 1$ ); Anal. Calcd for  $\text{C}_{29}\text{H}_{25}\text{N}_7\text{O}_4$ : C, 65.04; H, 4.71; N, 18.31. Found: C, 64.89; H, 4.58; N, 18.25.

### $^1\text{H}$ NMR and $^{13}\text{C}$ NMR spectra

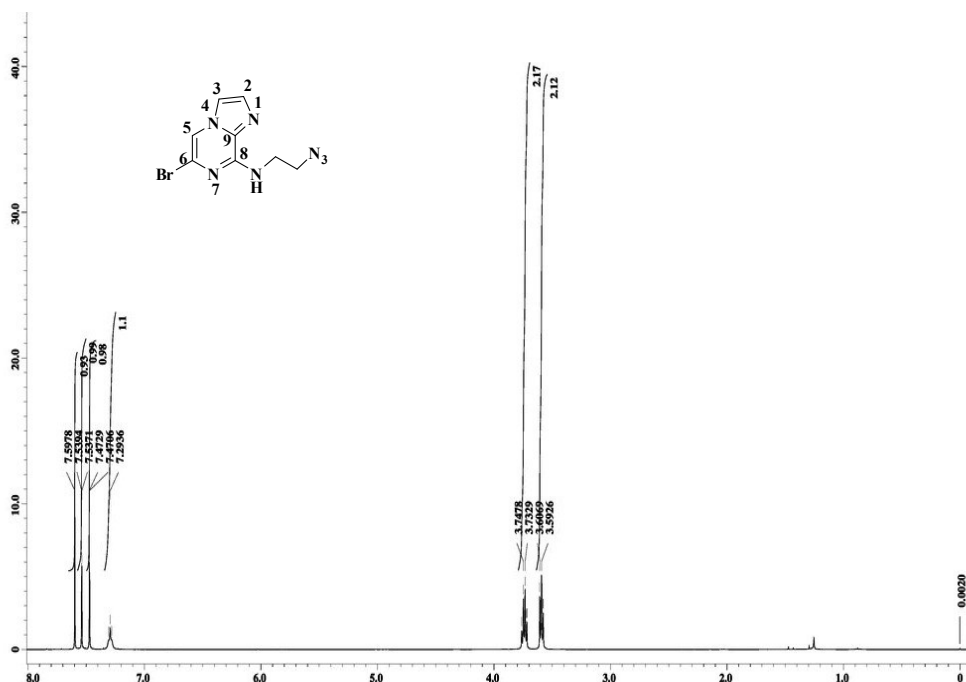


Fig S1:  $^1\text{H}$  NMR Spectrum of *N*-(2-azidoethyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine (4)

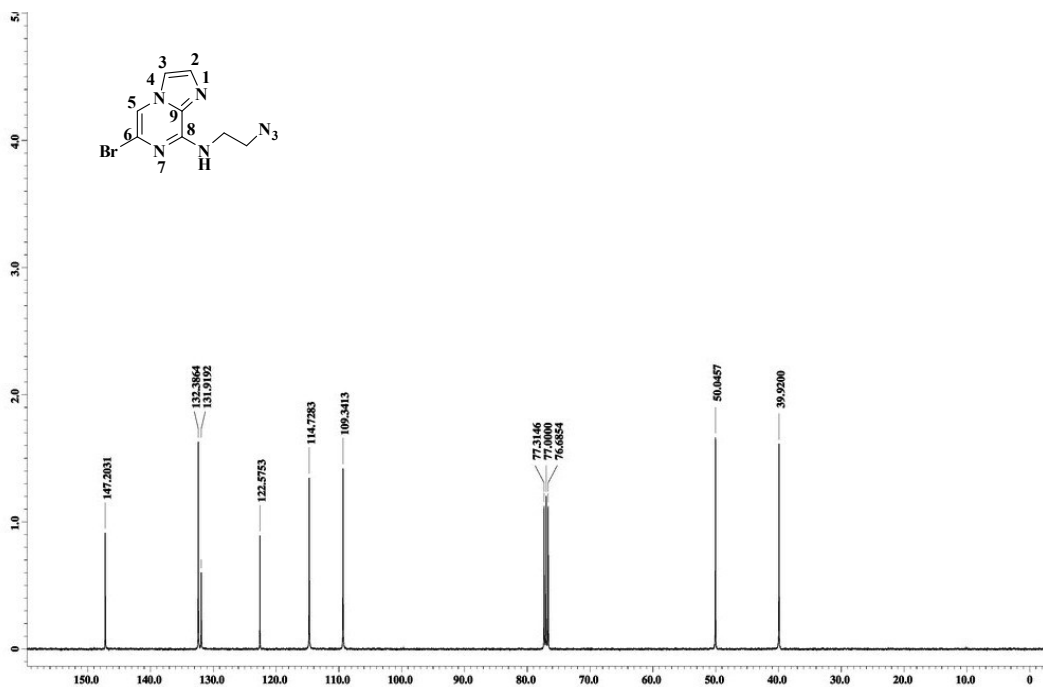


Fig S2: <sup>13</sup>C NMR Spectrum of *N*-(2-azidoethyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine (4)

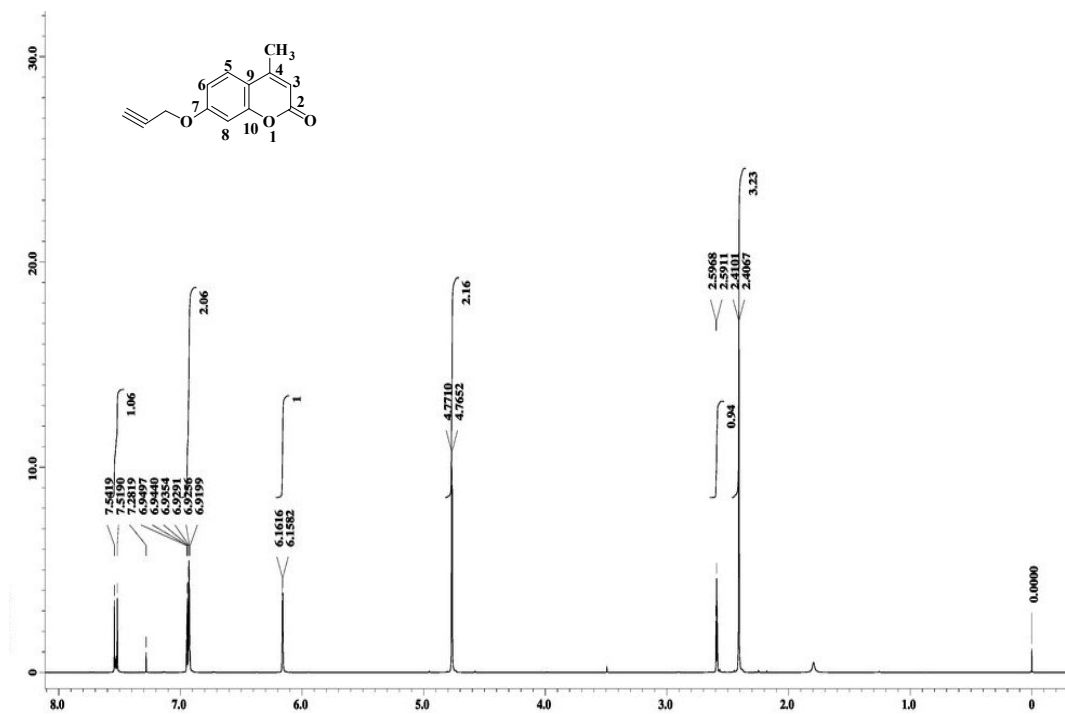


Fig S3: <sup>1</sup>H NMR spectrum of 4-methyl-7-(prop-2-ynyloxy)-2H-chromen-2-one (6)

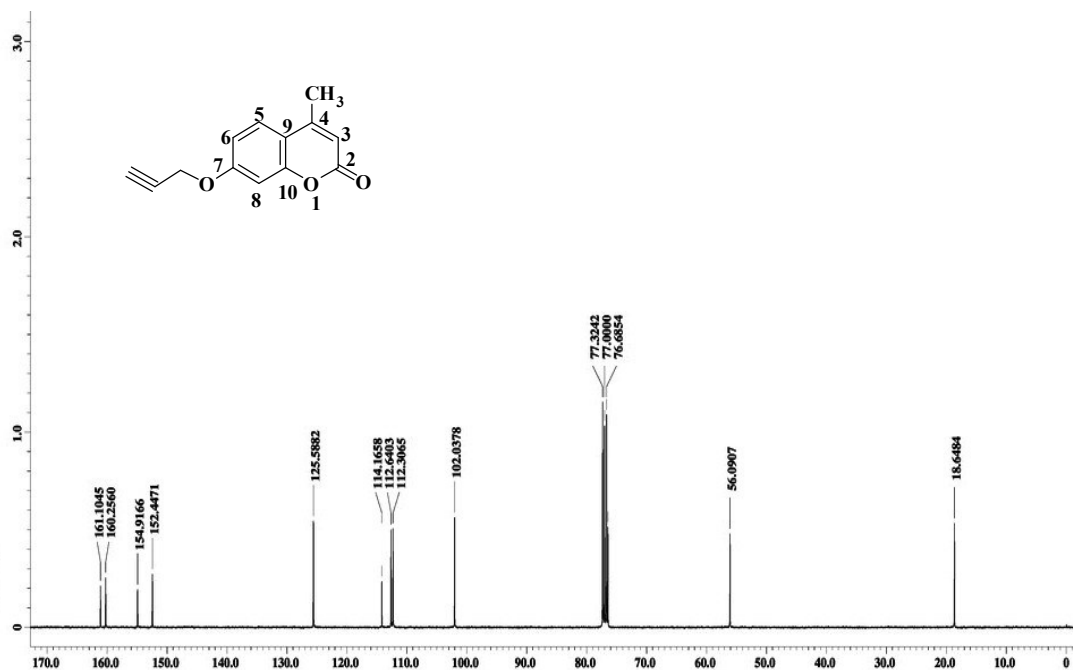


Fig S4:  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-(prop-2-ynyloxy)-2H-chromen-2-one (6)

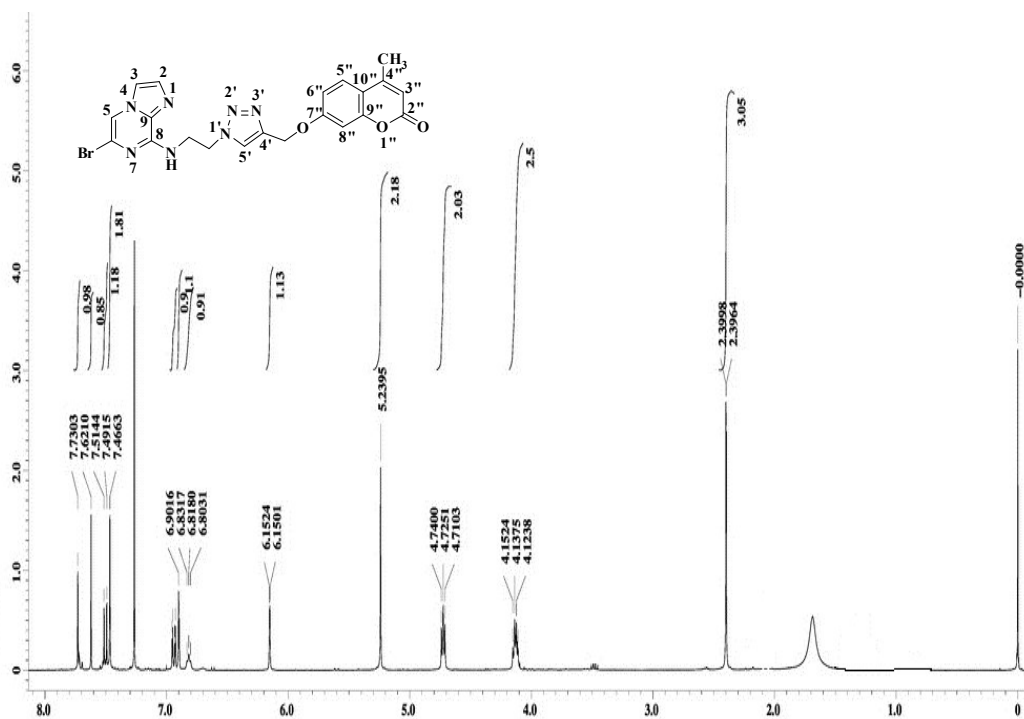


Fig S5:  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-bromoimidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (7)



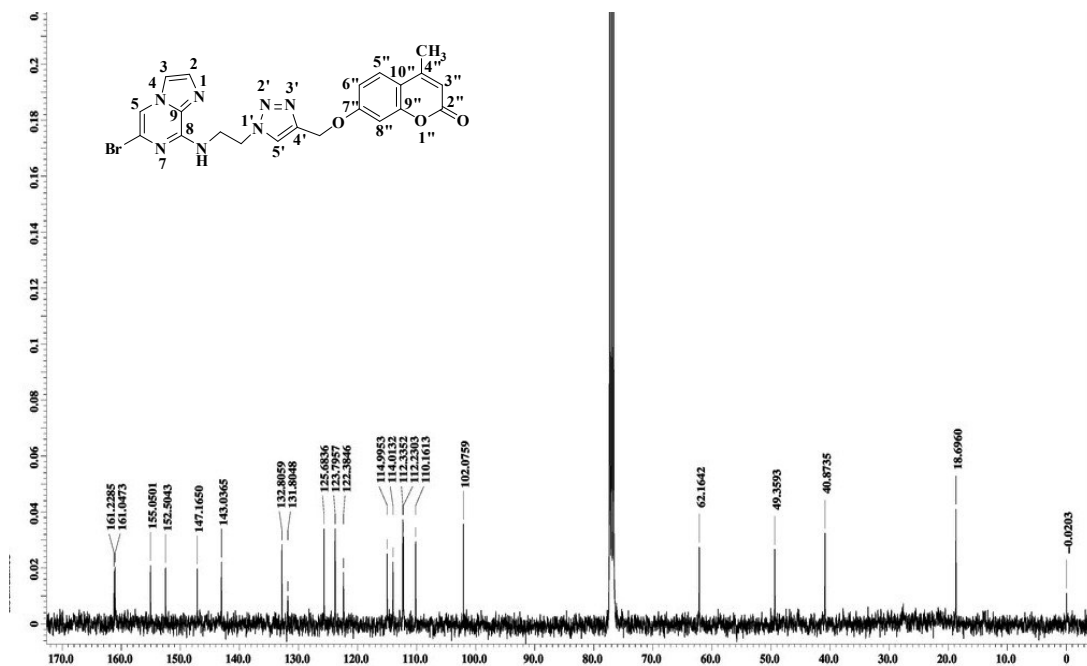


Fig S6: <sup>13</sup>C NMR spectrum of 7-((1-(2-(6-bromoimidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (7)

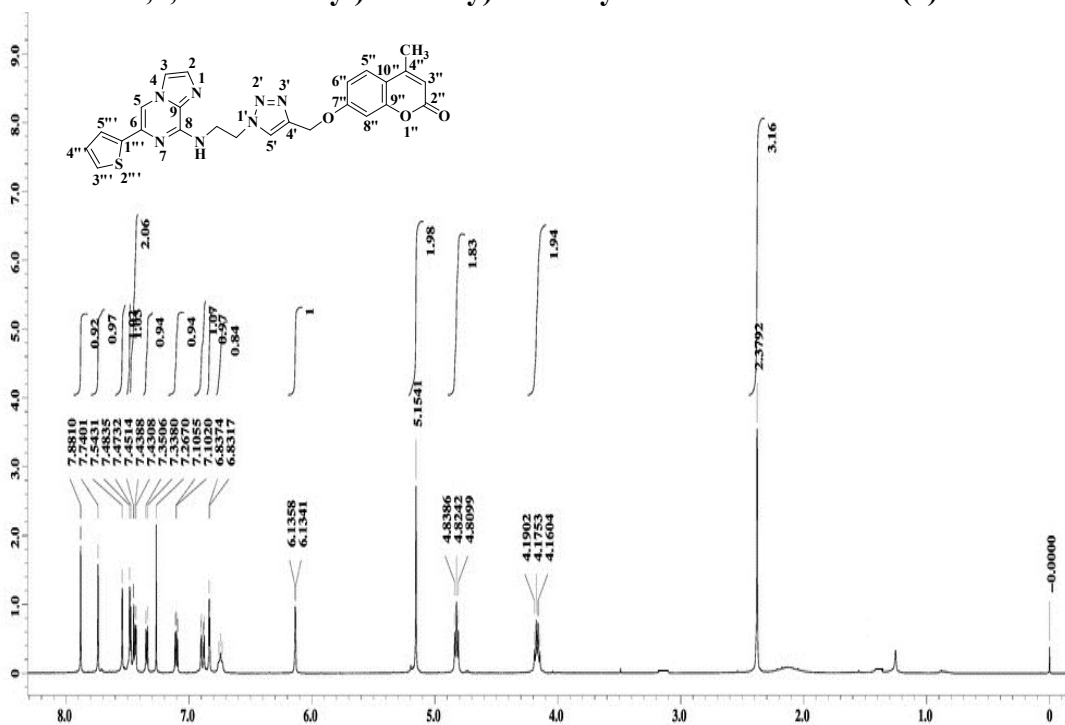


Fig S7: <sup>1</sup>H NMR spectrum of 4-methyl-7-((1-(2-(6-(thiophen-2-yl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (9)

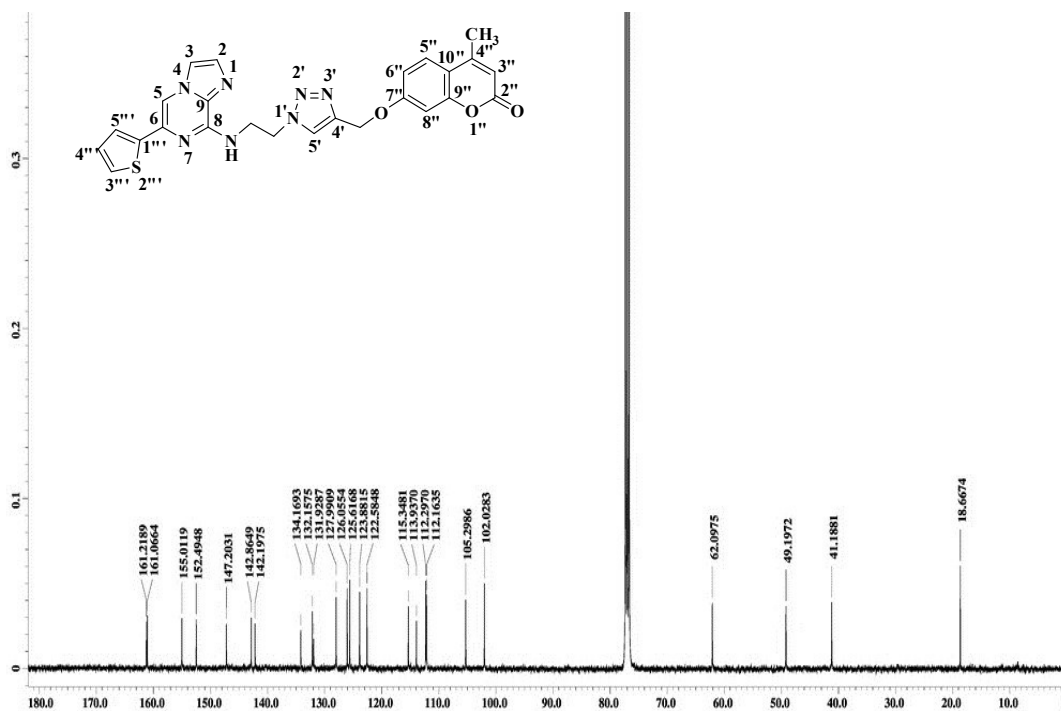


Fig S8:  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(2-(6-(thiophen-2-yl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (9)

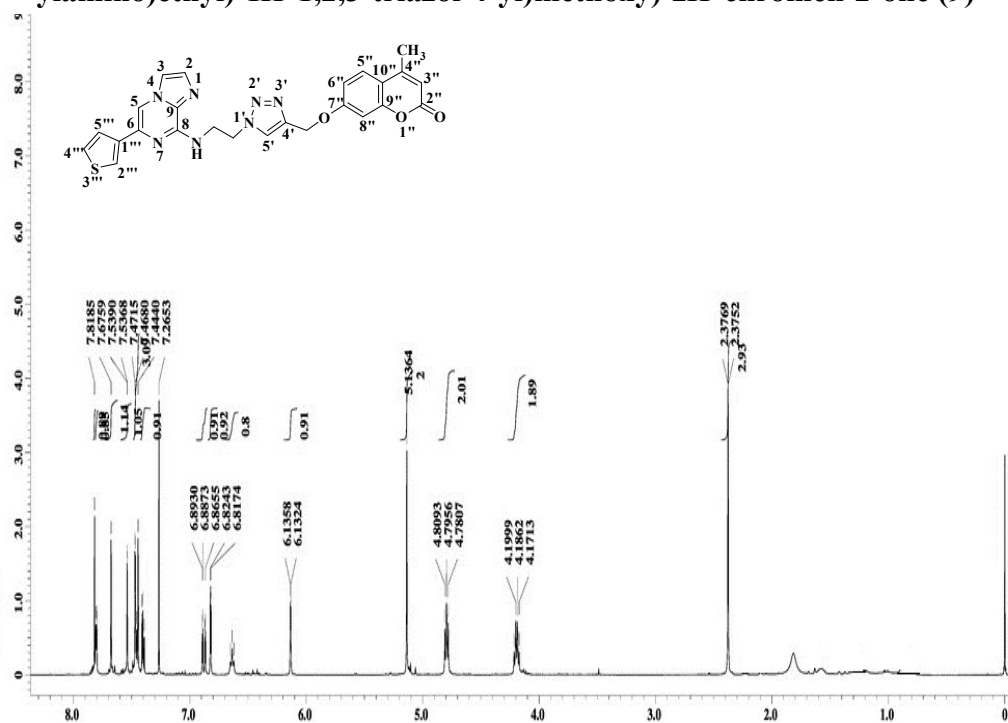


Fig S9:  $^1\text{H}$  NMR spectrum of 4-methyl-7-((1-(2-(6-(thiophen-3-yl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (10)

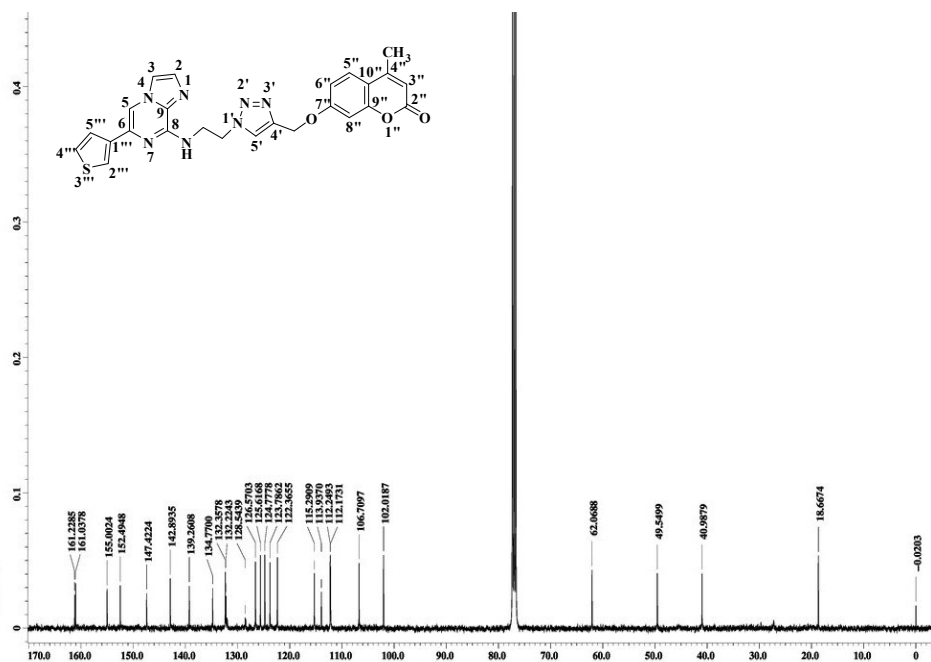


Fig S10:  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(2-(6-(thiophen-3-yl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (10)

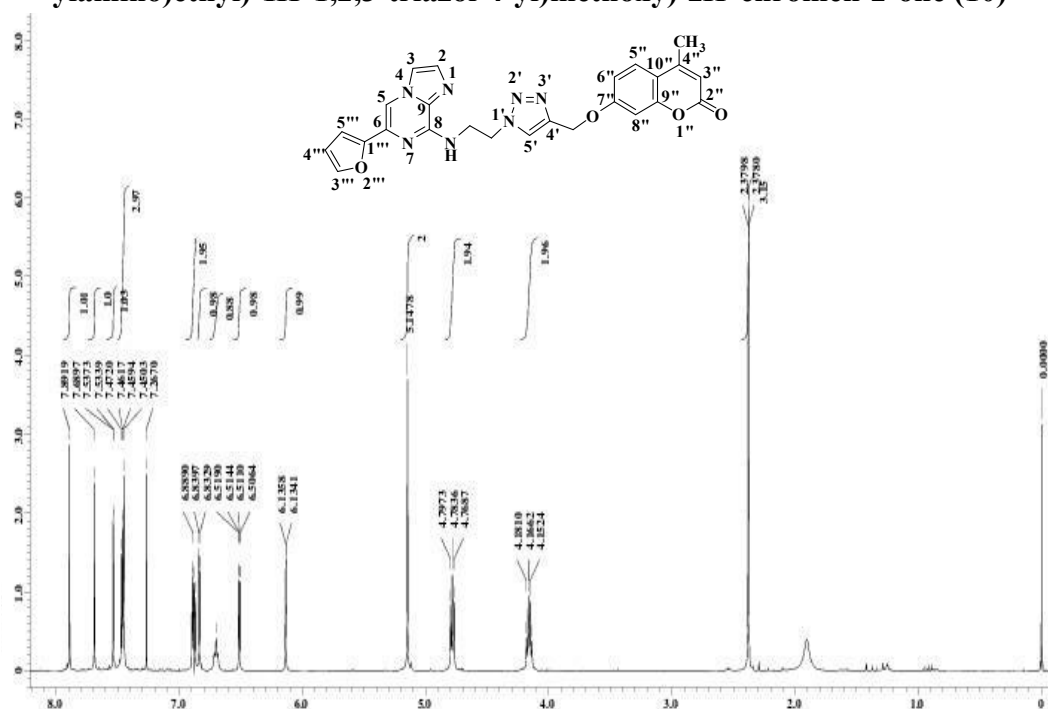
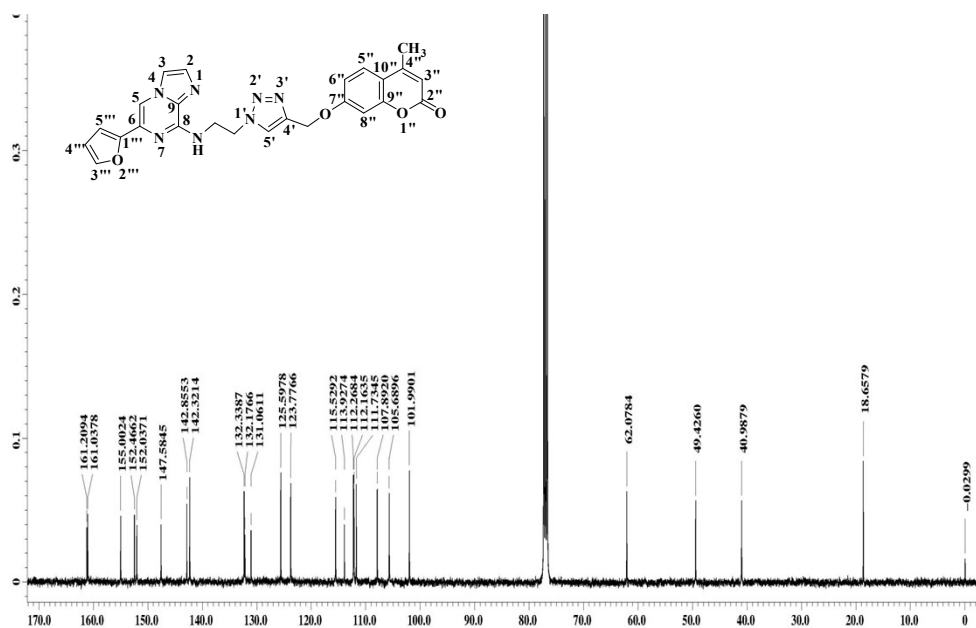
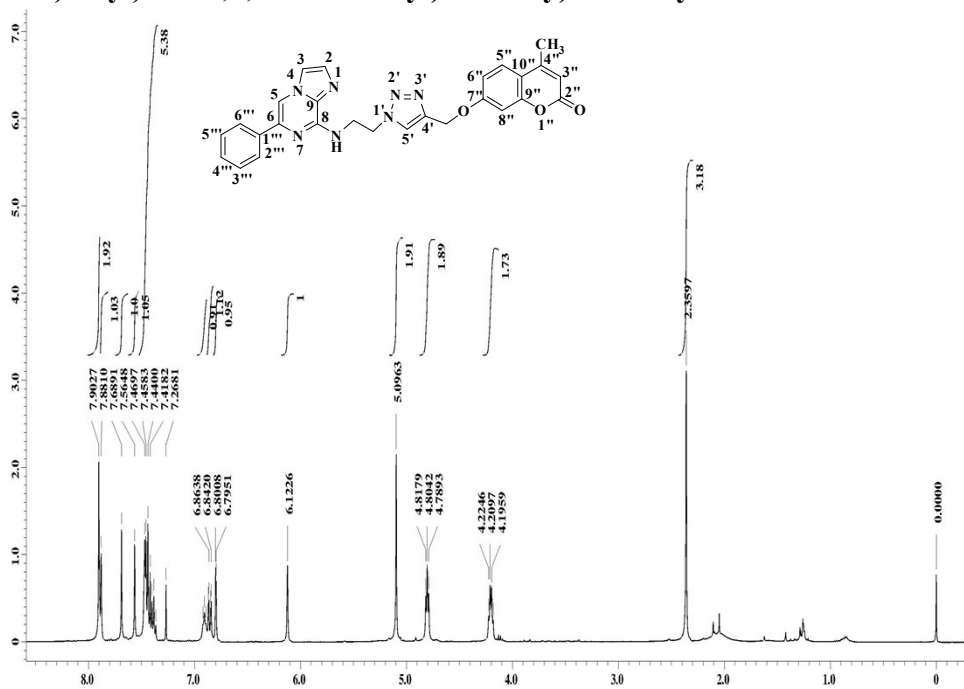


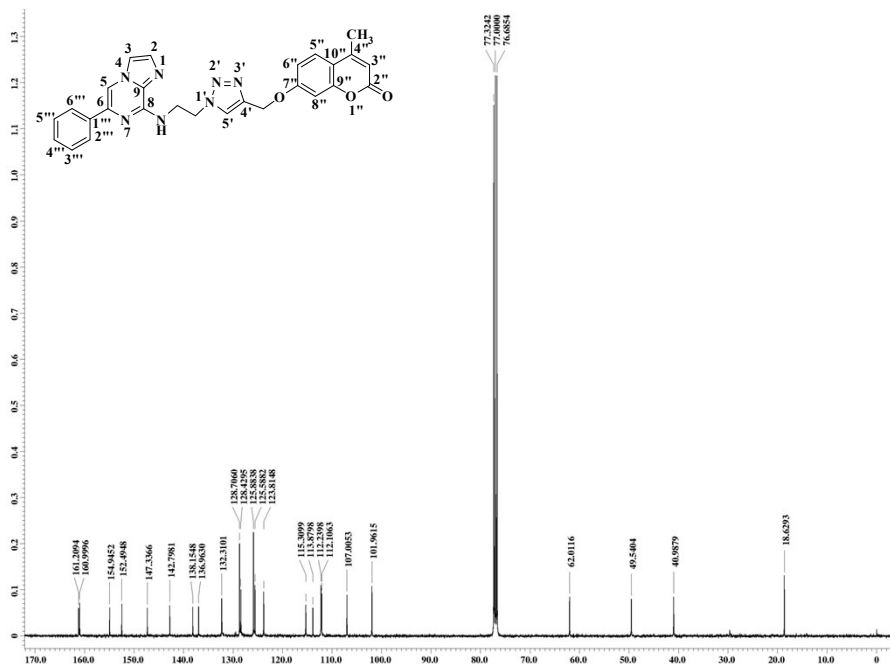
Fig S11:  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-(furan-2-yl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (11)



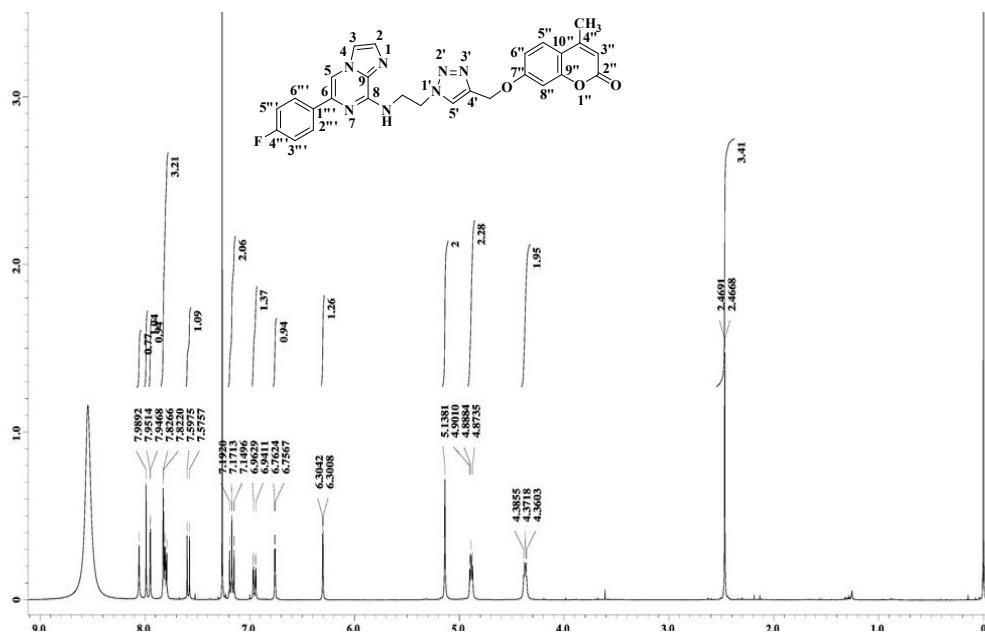
**Fig S12:**  $^{13}\text{C}$  NMR spectrum of 7-((1-(2-(6-(furan-2-yl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (11)



**Fig S13:**  $^1\text{H}$  NMR spectrum of 4-methyl-7-((1-(2-(6-phenylimidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (12)



**Fig S14:**  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(2-(6-phenylimidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (12)



**Fig S15:**  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-(4-fluorophenyl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (13)

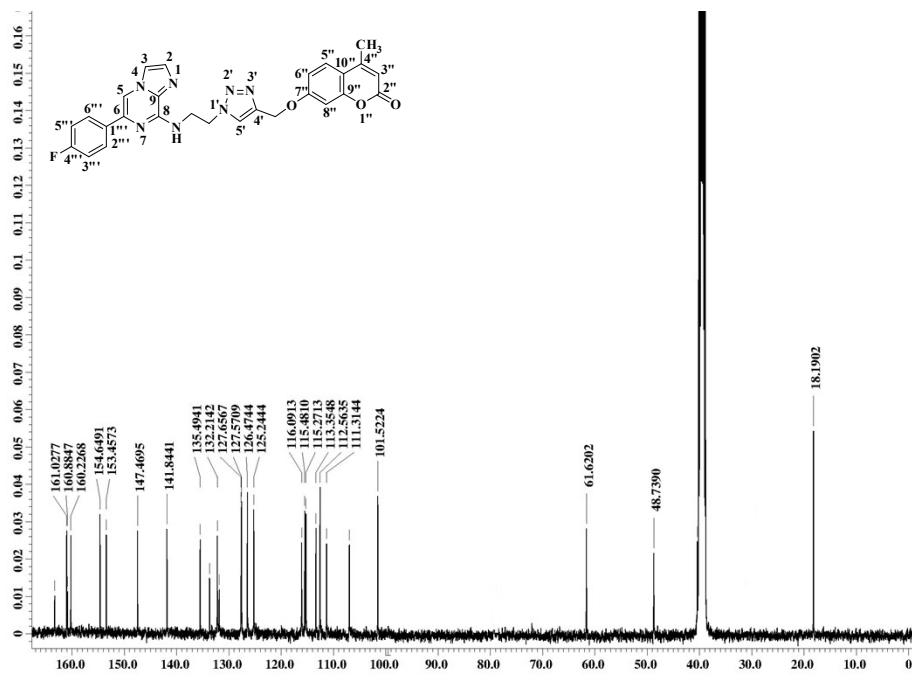


Fig S16:  $^{13}\text{C}$  NMR spectrum of 7-((1-(2-(6-(4-fluorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (13)

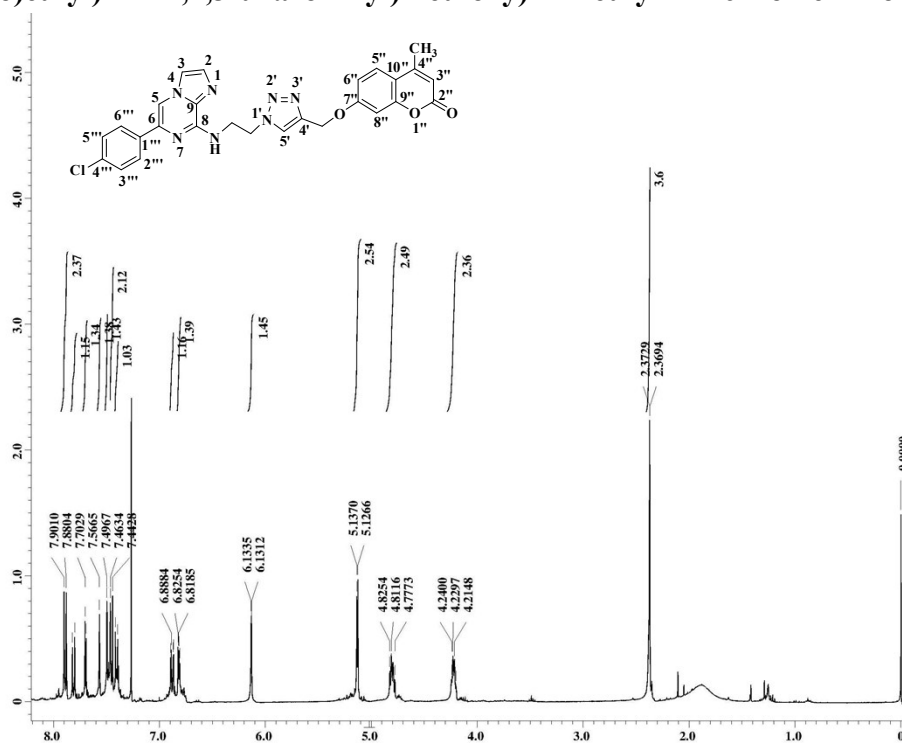


Fig S17:  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-(4-chlorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (14)

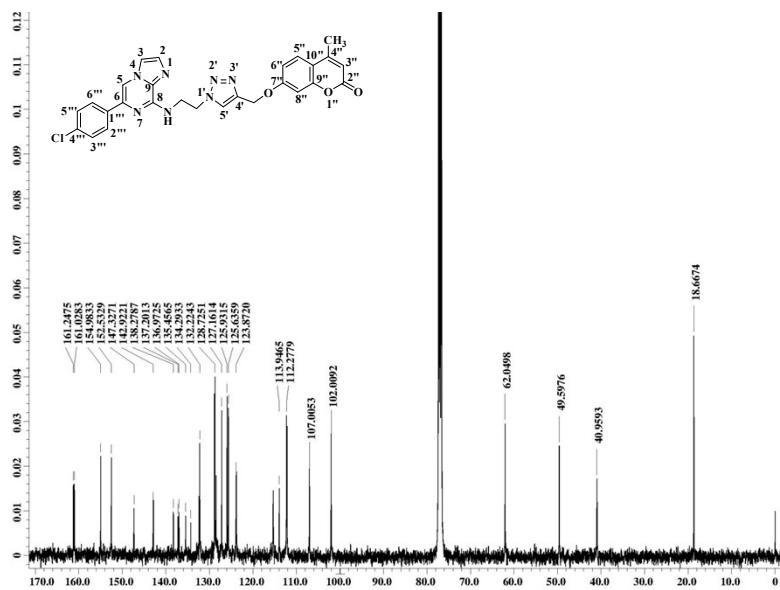


Fig S18:  $^{13}\text{C}$  NMR spectrum of 7-((1-(2-(6-(4-chlorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (14)

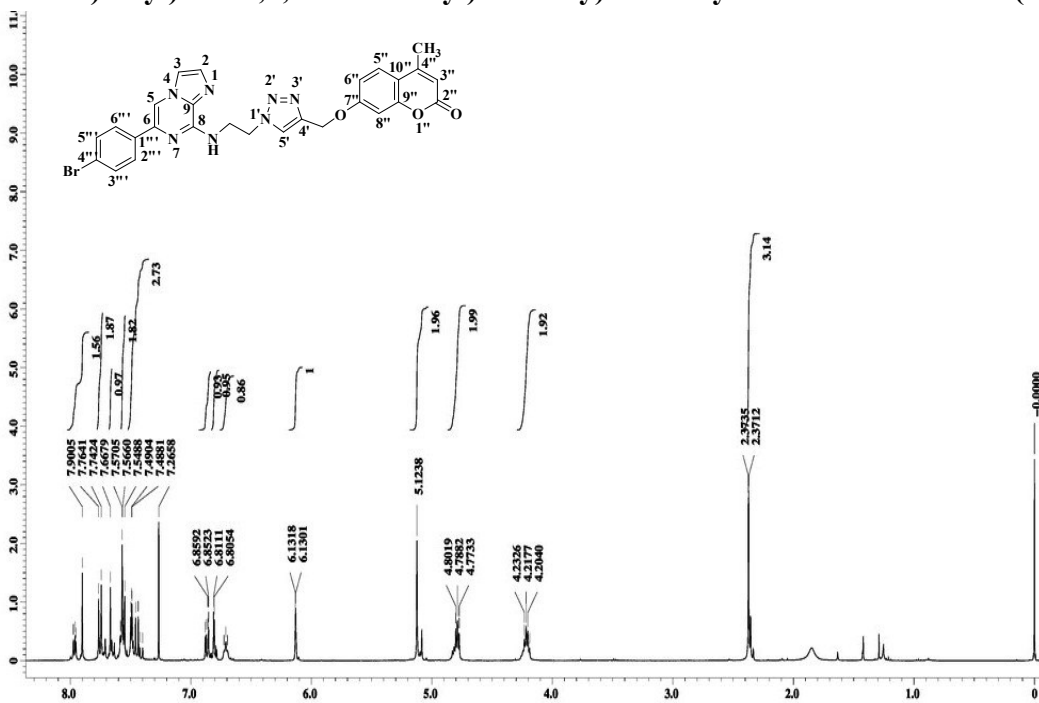


Fig S19:  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-(4-bromophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (15)

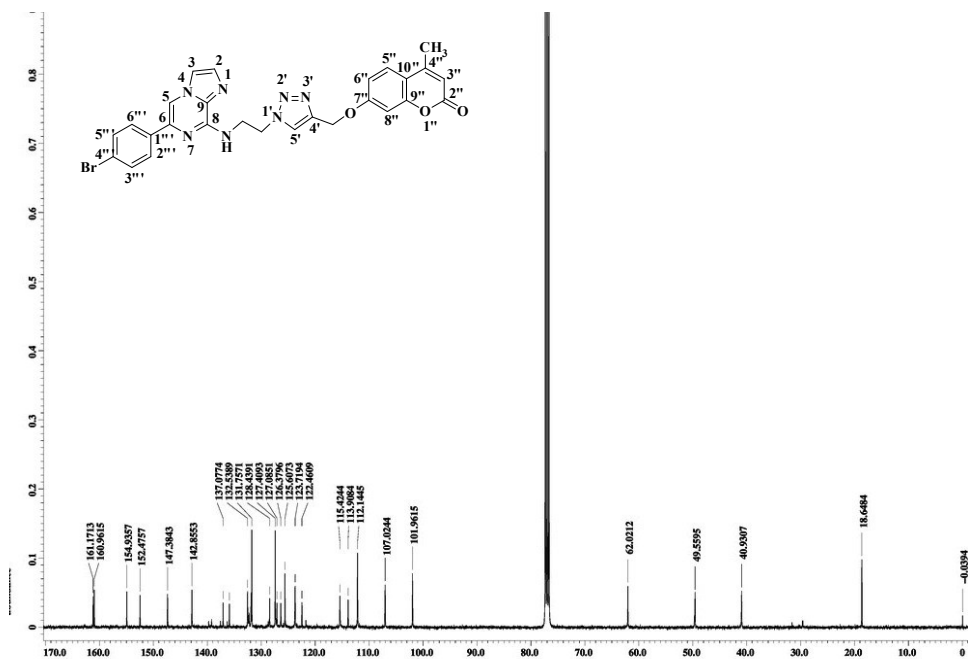


Fig S20:  $^{13}\text{C}$  NMR spectrum of 7-((1-(2-(6-(4-bromophenyl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (15)

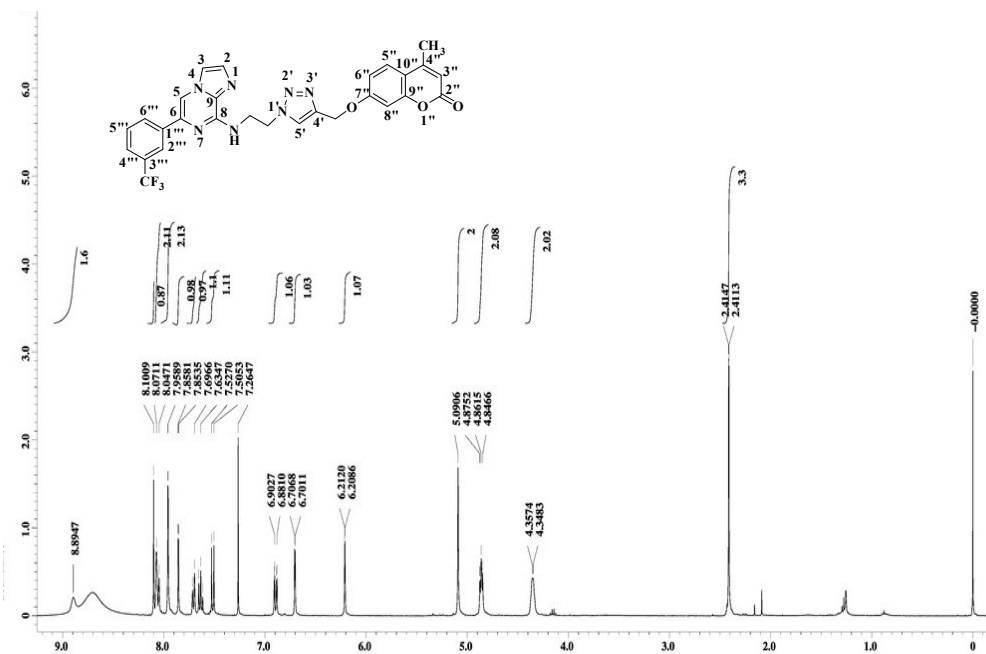


Fig S21:  $^1\text{H}$  NMR spectrum of 4-methyl-7-((1-(2-(6-(3-(trifluoromethyl)phenyl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (16)



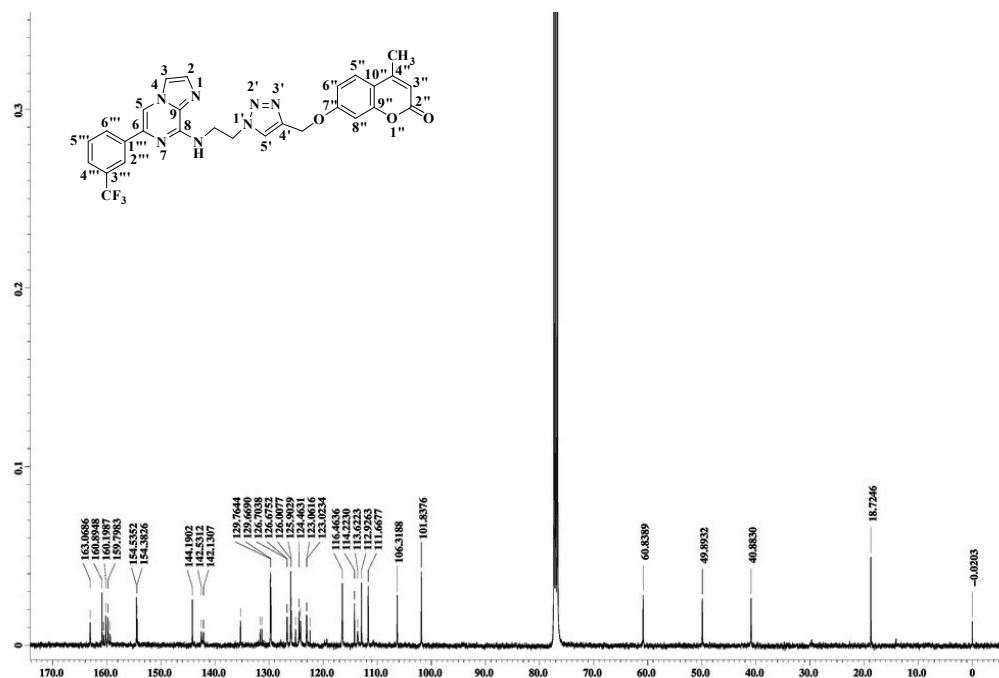


Fig S22:  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(2-(6-(3-(trifluoromethyl)phenyl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (16)

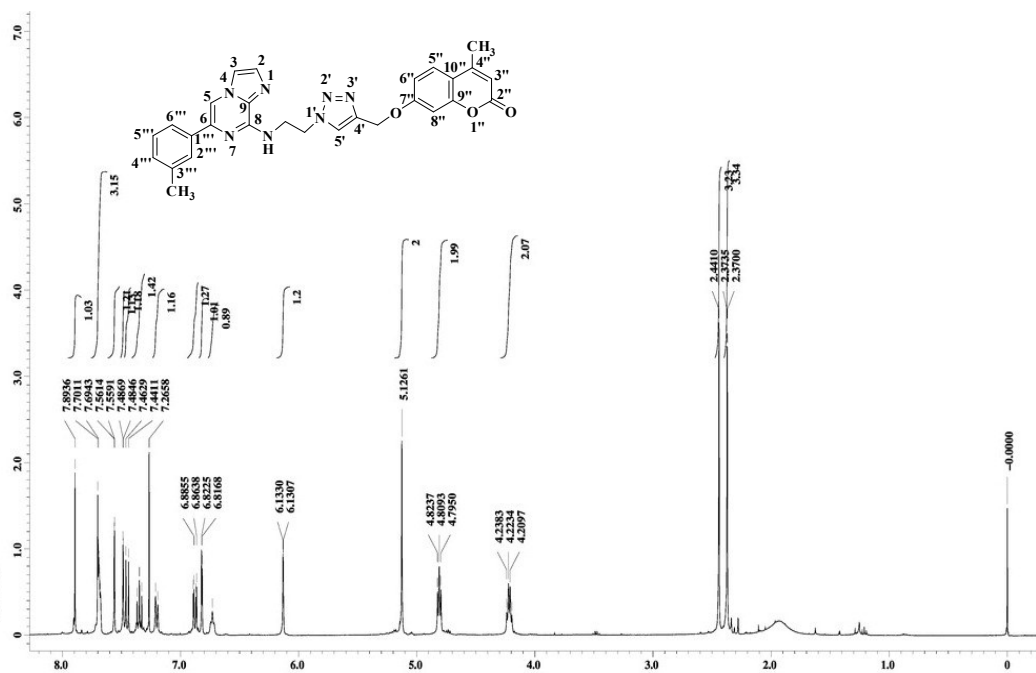


Fig S23:  $^1\text{H}$  NMR spectrum of 4-methyl-7-((1-(2-(6-m-tolylimidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (17)

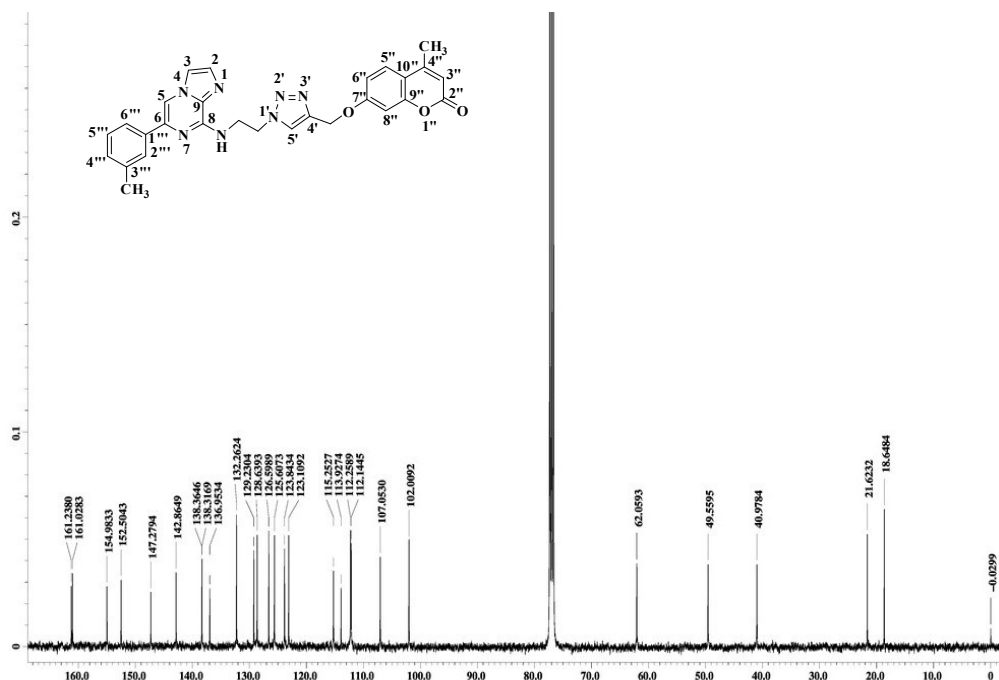


Fig S24:  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(2-(6-*m*-tolylimidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (17)

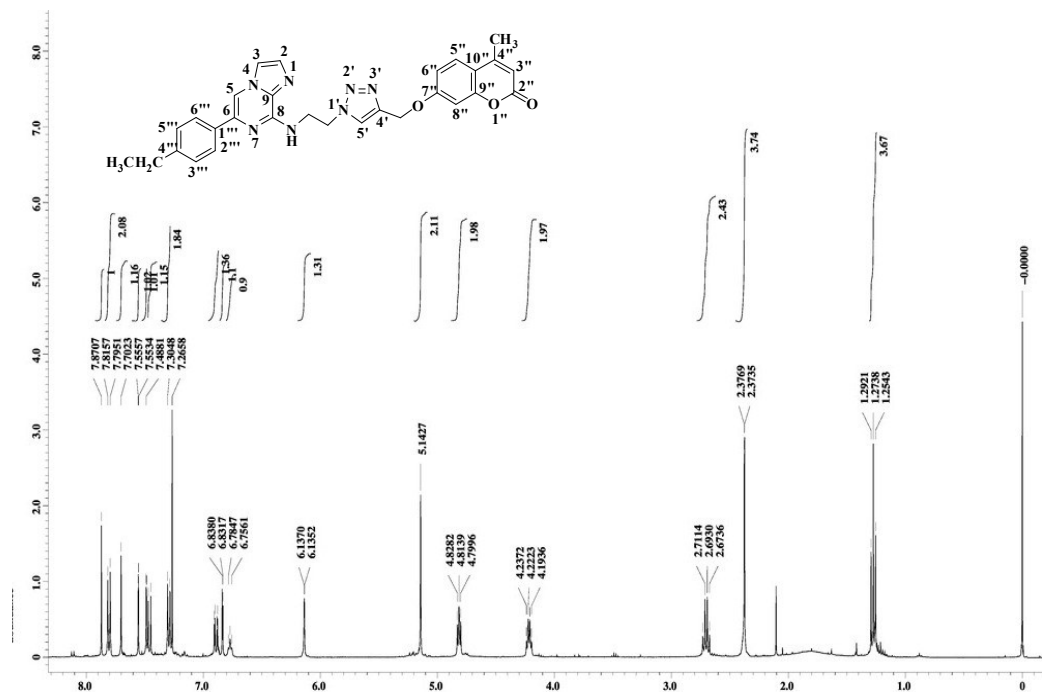


Fig S25:  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-(4-ethylphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (18)

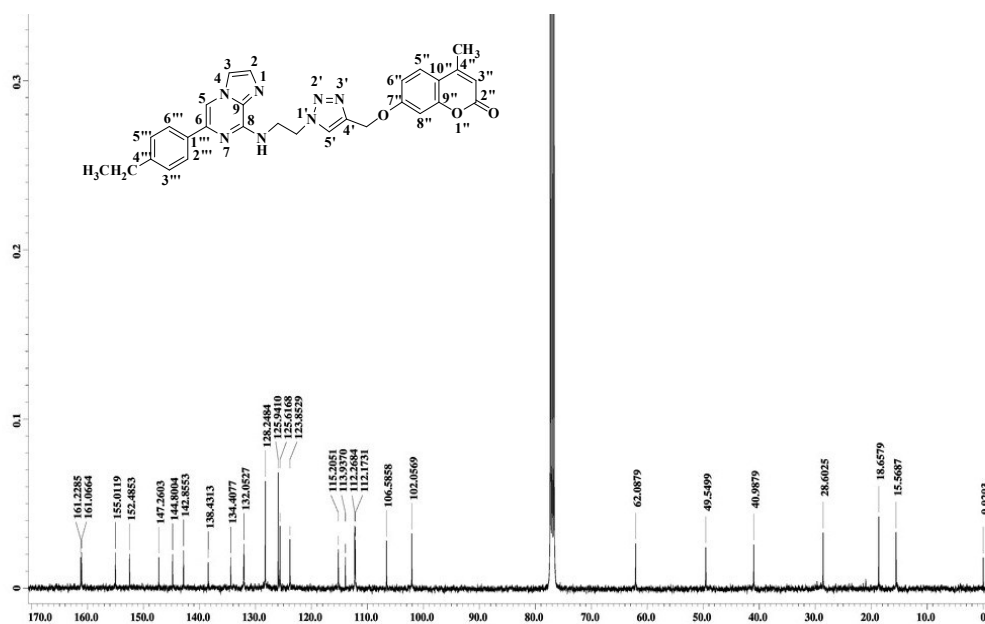


Fig S26:  $^{13}\text{C}$  NMR spectrum of 7-((1-(2-(6-(4-ethylphenyl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (18)

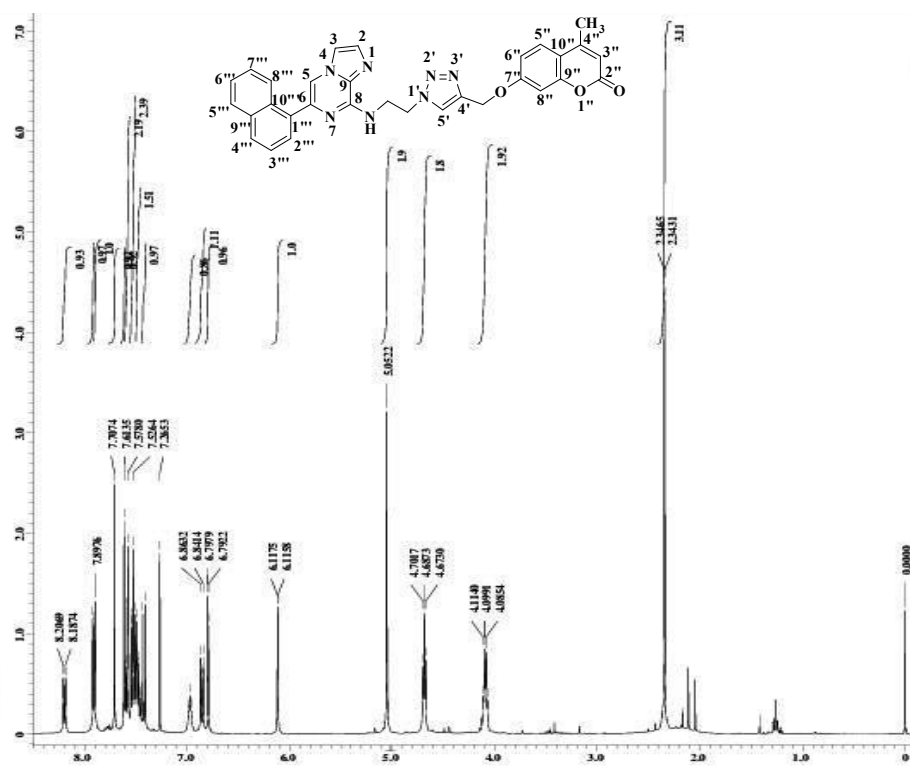
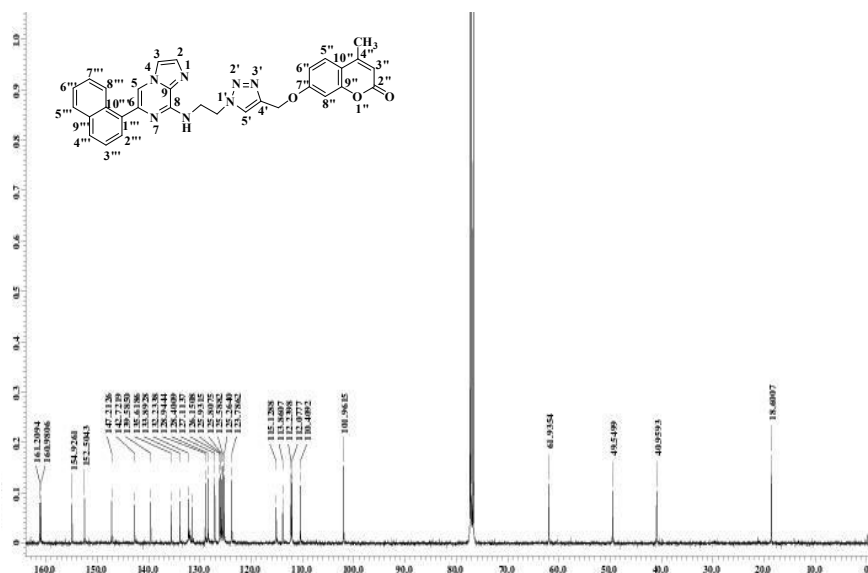
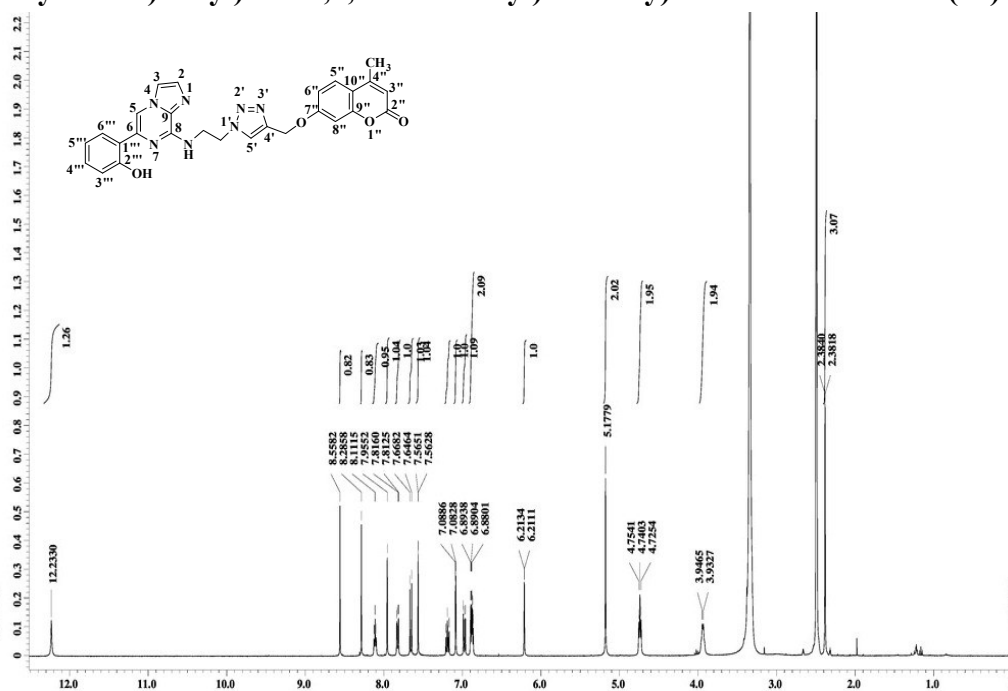


Fig S27:  $^1\text{H}$  NMR spectrum of 4-methyl-7-((1-(2-(6-(naphthalen-1-yl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (19)



**Fig S28:**  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(2-(6-(naphthalen-1-yl)imidazo[1,2-*a*]pyrazin-8-ylamino) ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (19)



**Fig S29:**  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-(2-hydroxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino) ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (20)

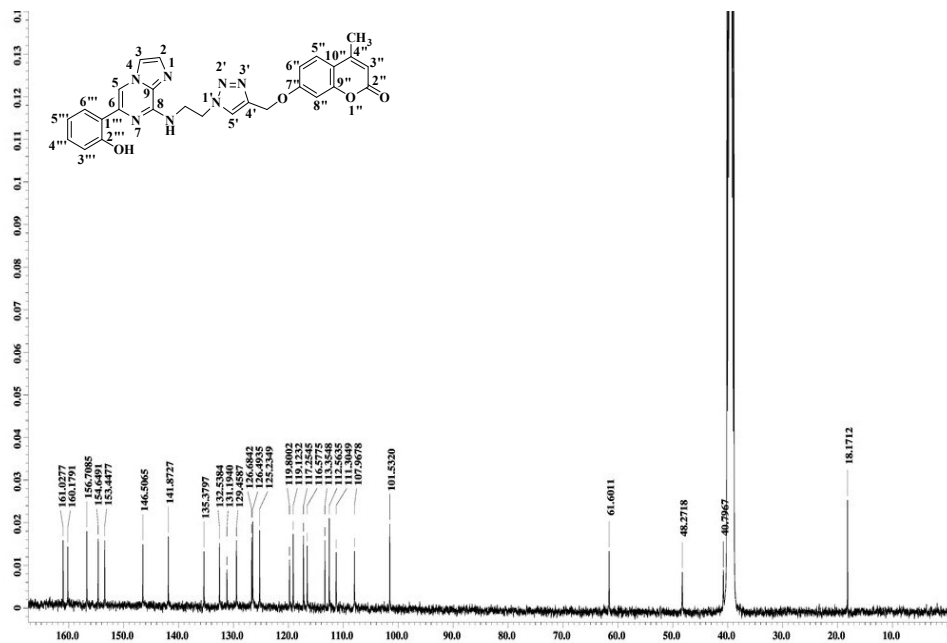


Fig S30:  $^{13}\text{C}$  NMR spectrum of 7-((1-(2-(6-(2-hydroxyphenyl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (20)

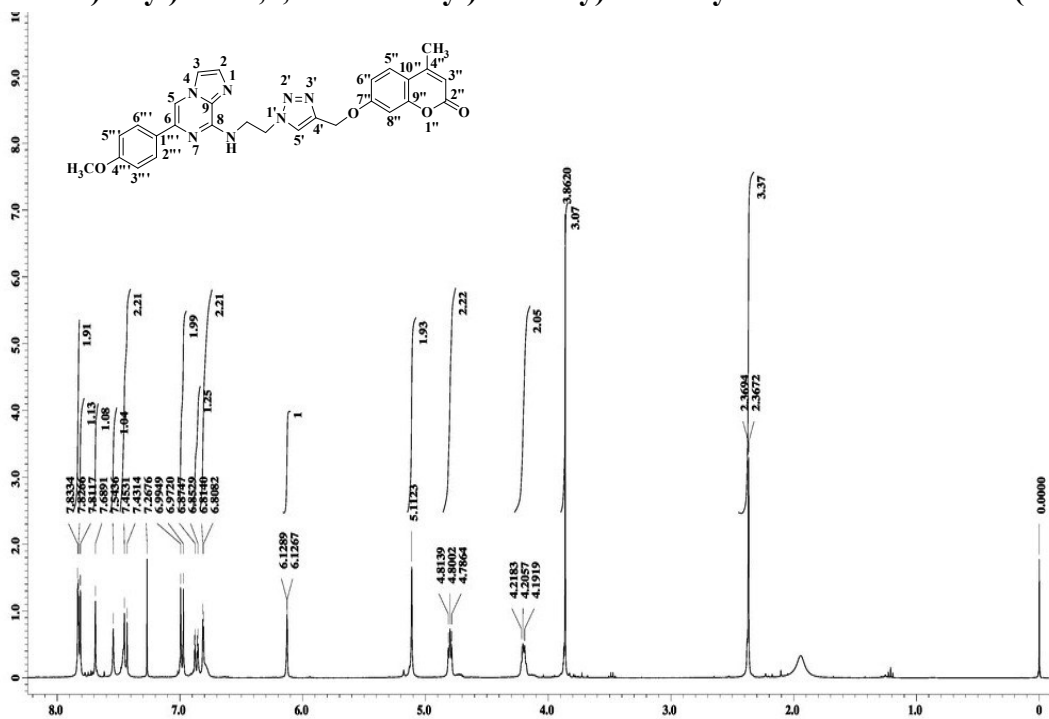


Fig S31:  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-(4-methoxyphenyl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (21)

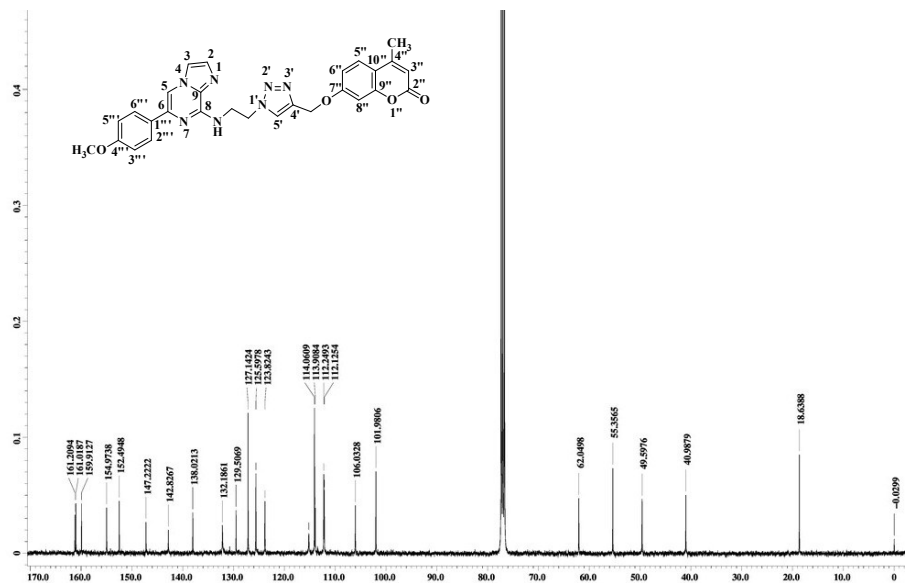


Fig S32:  $^{13}\text{C}$  NMR spectrum of 7-((1-(2-(6-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (21)

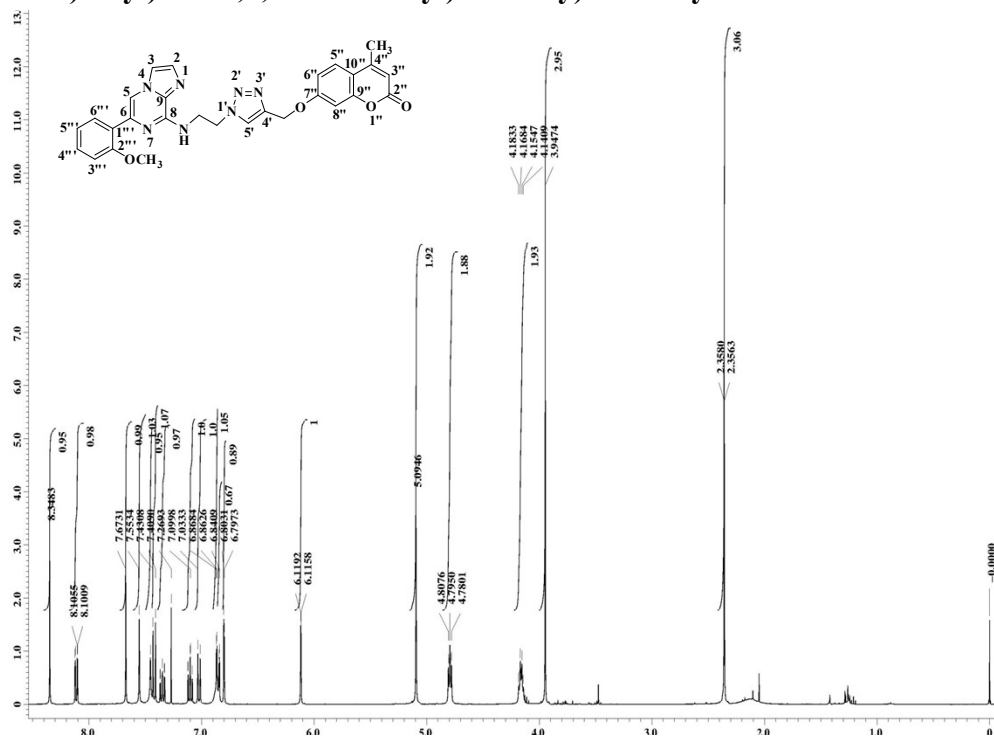


Fig S33:  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-(2-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (22)

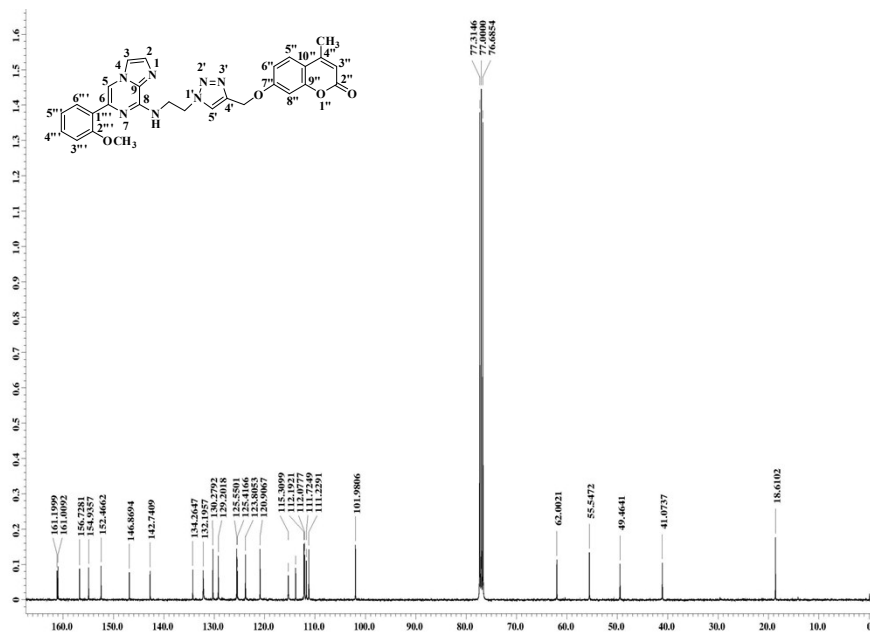


Fig S34:  $^{13}\text{C}$  NMR spectrum of 7-((1-(2-(6-(2-methoxyphenyl)imidazo[1,2-a]pyrazin-8-ylamino)ethyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (22)

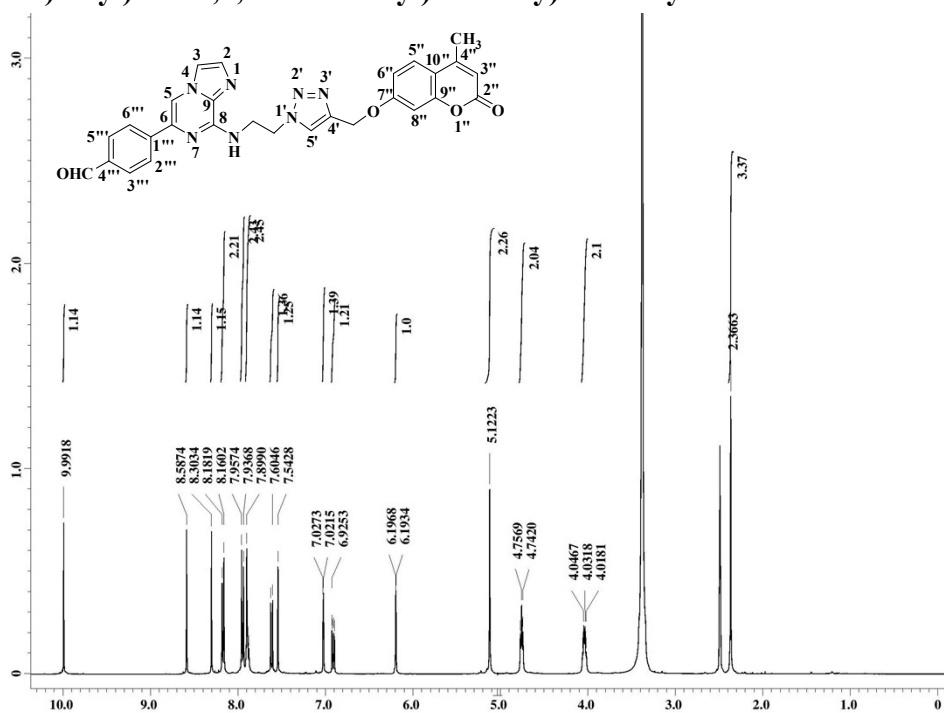


Fig S35:  $^1\text{H}$  NMR spectrum of 4-(8-(2-(4-((4-methyl-2-oxo-2H-chromen-7-yloxy)methyl)-1H-1,2,3-triazol-1-yl)ethylamino)imidazo[1,2-a]pyrazin-6-yl)benzaldehyde (23)

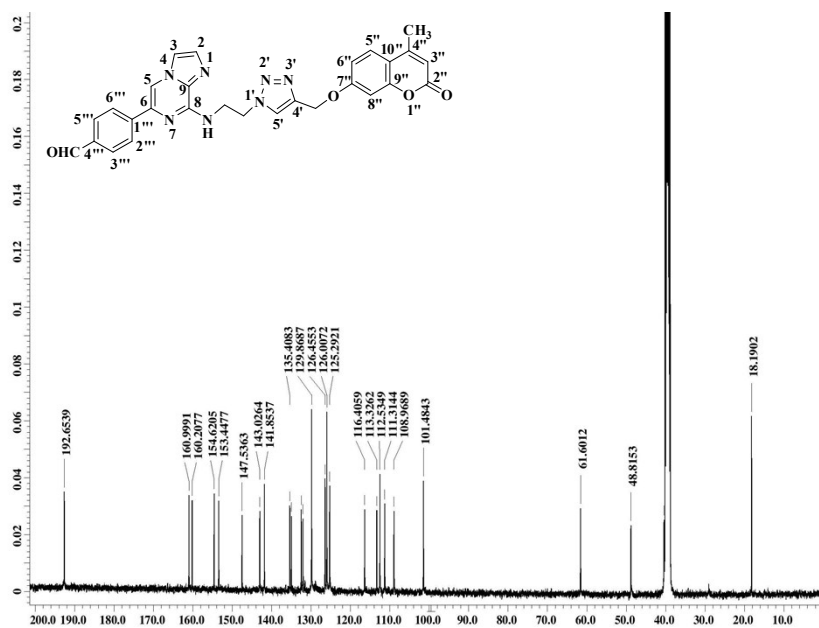


Fig S36:  $^{13}\text{C}$  NMR spectrum of 4-(8-(2-(4-((4-methyl-2-oxo-2*H*-chromen-7-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)ethylamino)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde (23)

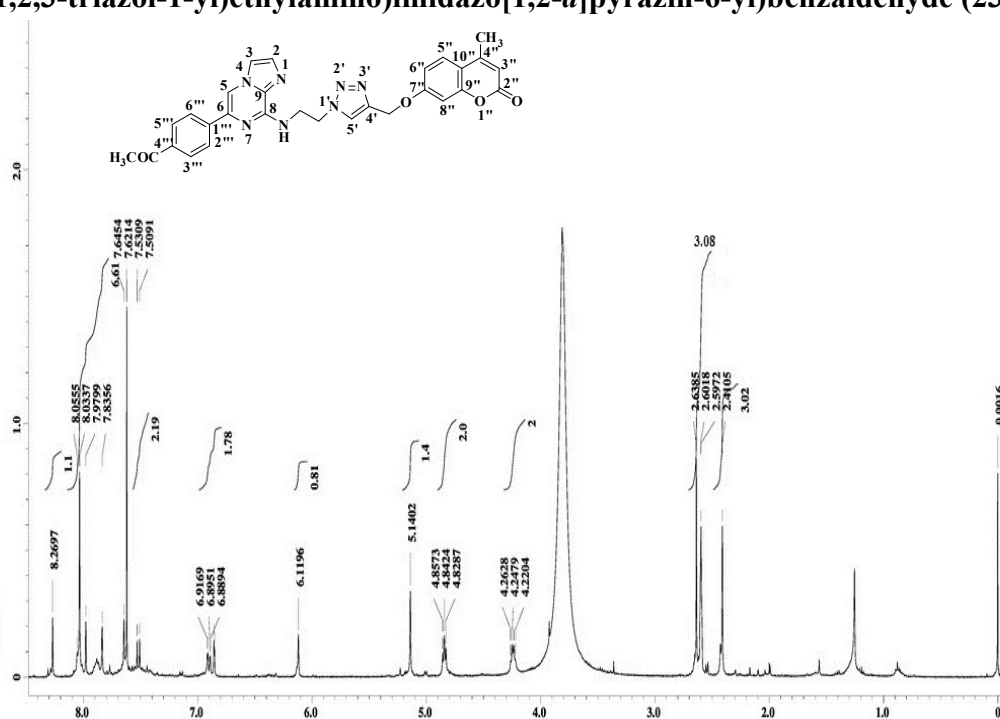


Fig S37:  $^1\text{H}$  NMR spectrum of 7-((1-(2-(6-(4-acetylphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (24)



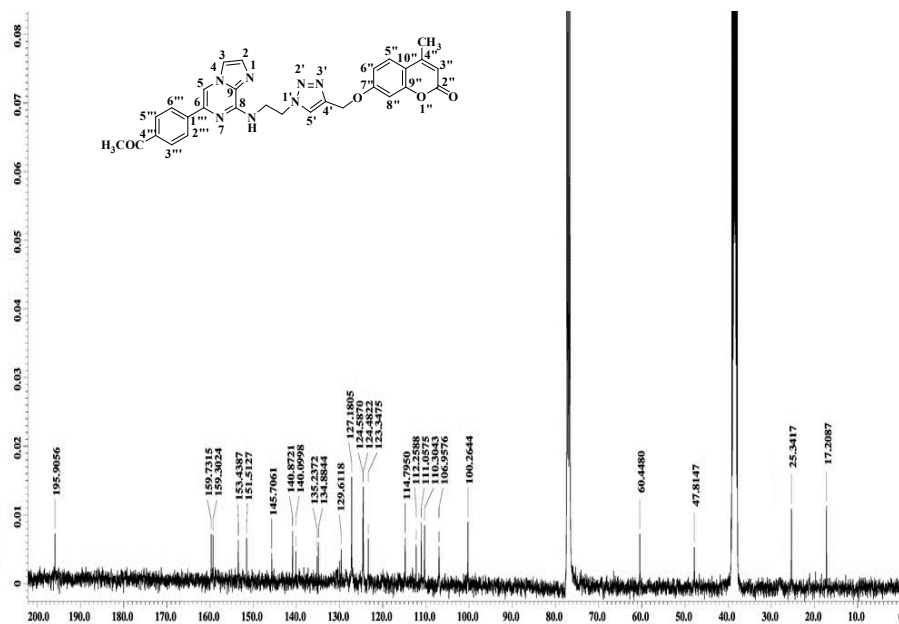


Fig S38:  $^{13}\text{C}$  NMR spectrum of 7-((1-(2-(6-(4-acetylphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)ethyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (24)

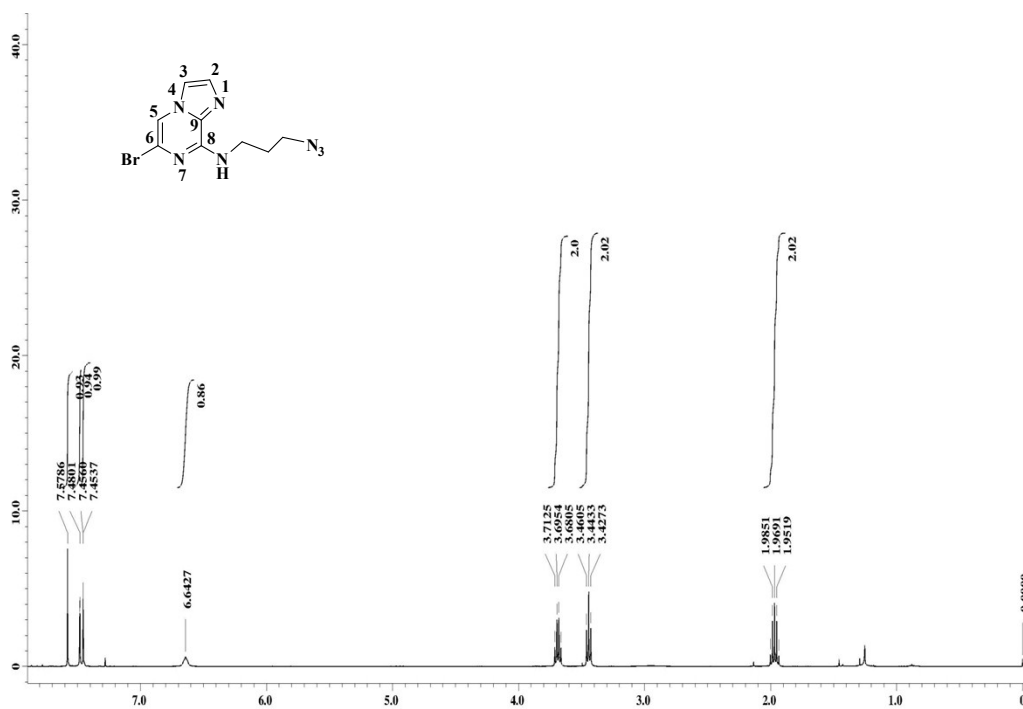


Fig S39:  $^1\text{H}$  NMR spectrum of *N*-(3-azidopropyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine (27)

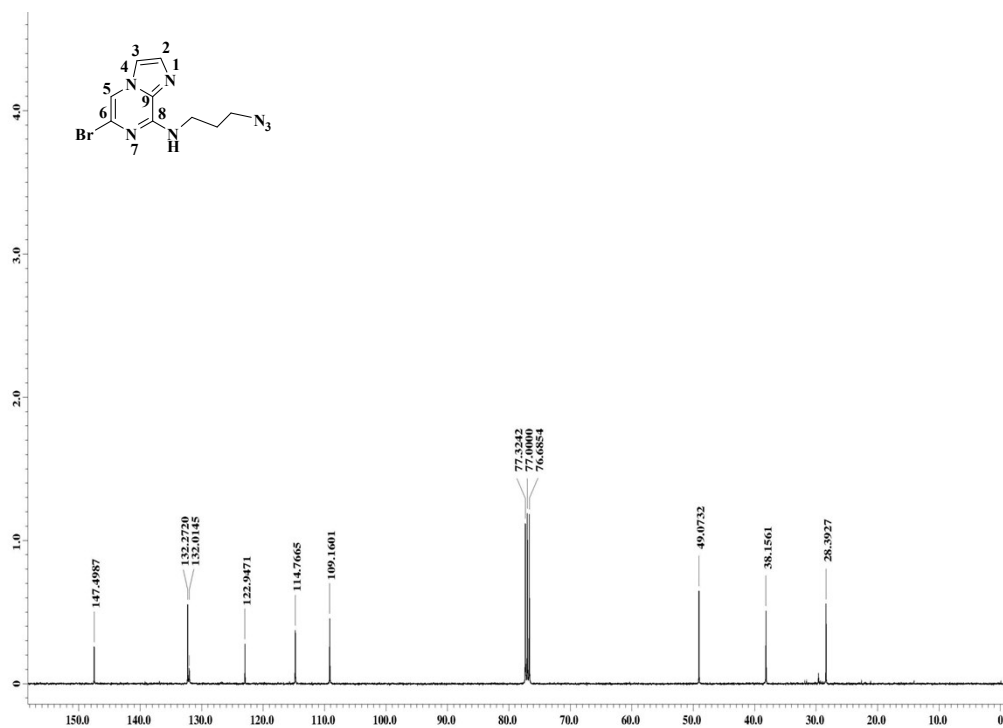


Fig S40: <sup>13</sup>C NMR spectrum of *N*-(3-azidopropyl)-6-bromoimidazo[1,2-*a*]pyrazin-8-amine (27)

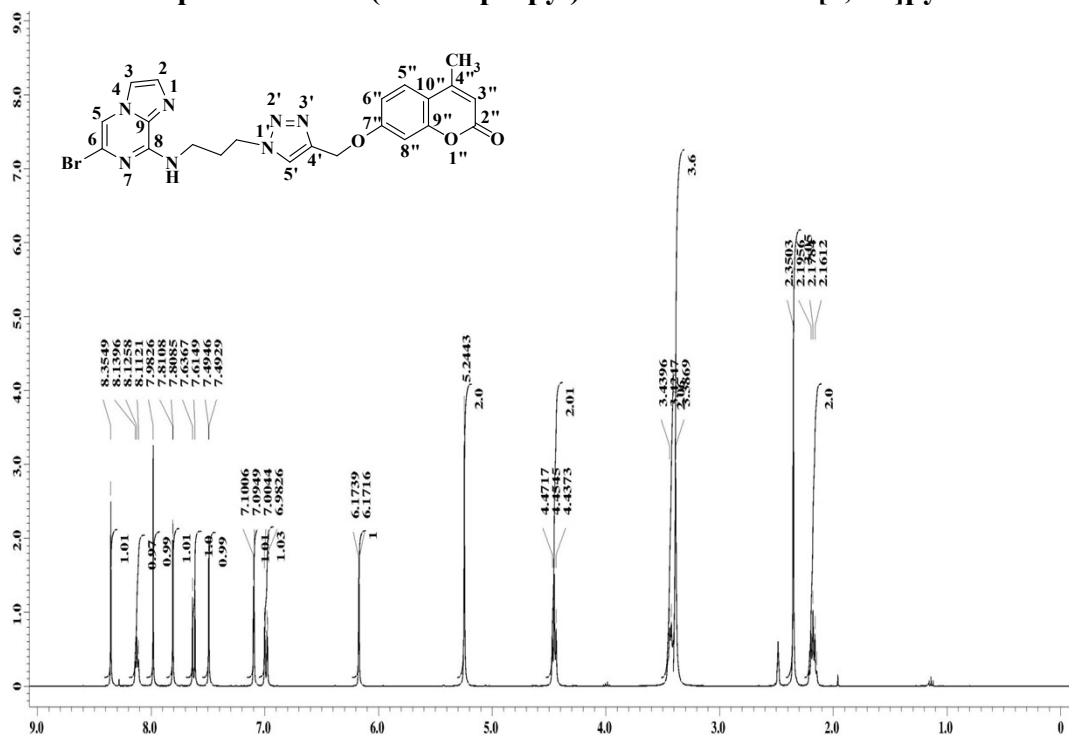


Fig S41: <sup>1</sup>H NMR spectrum of 7-((1-(3-(6-bromoimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (28)

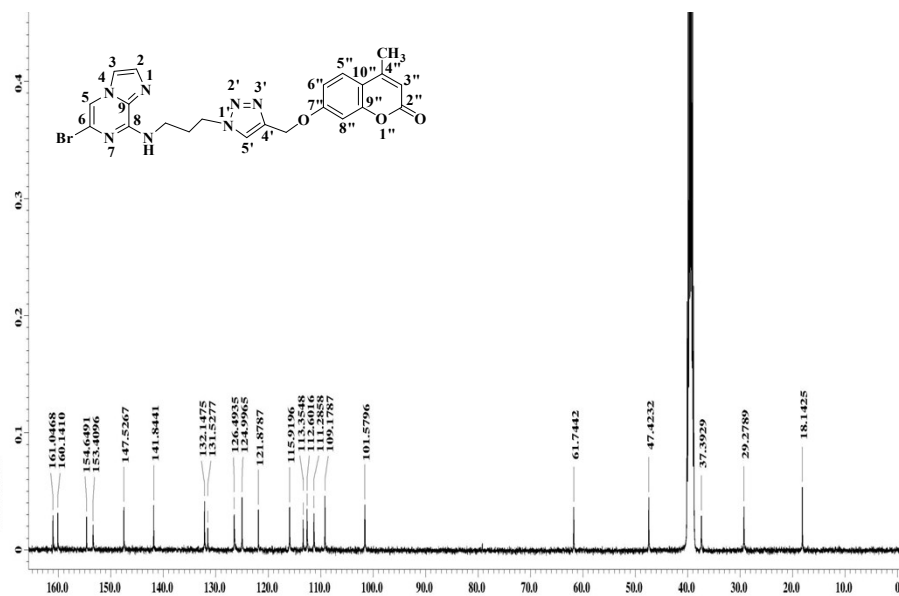


Fig S42:  $^{13}\text{C}$  NMR spectrum of 7-((1-(3-(6-bromoimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (28)

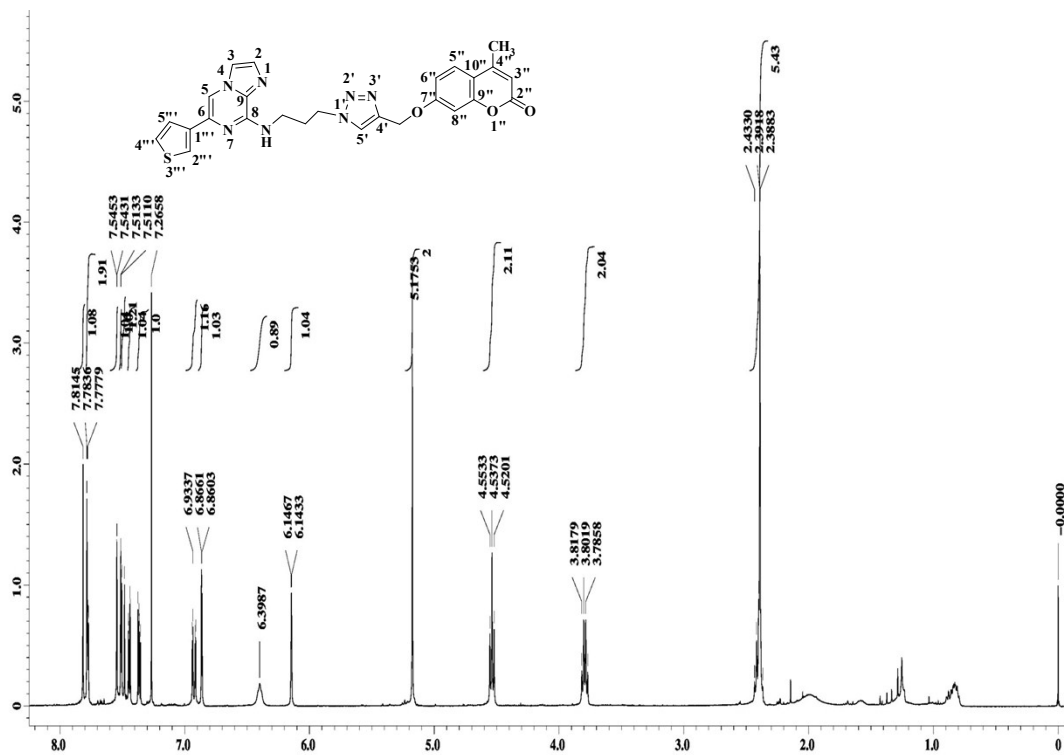


Fig S43:  $^1\text{H}$  NMR spectrum of 4-methyl-7-((1-(3-(6-(thiophen-3-yl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (29)

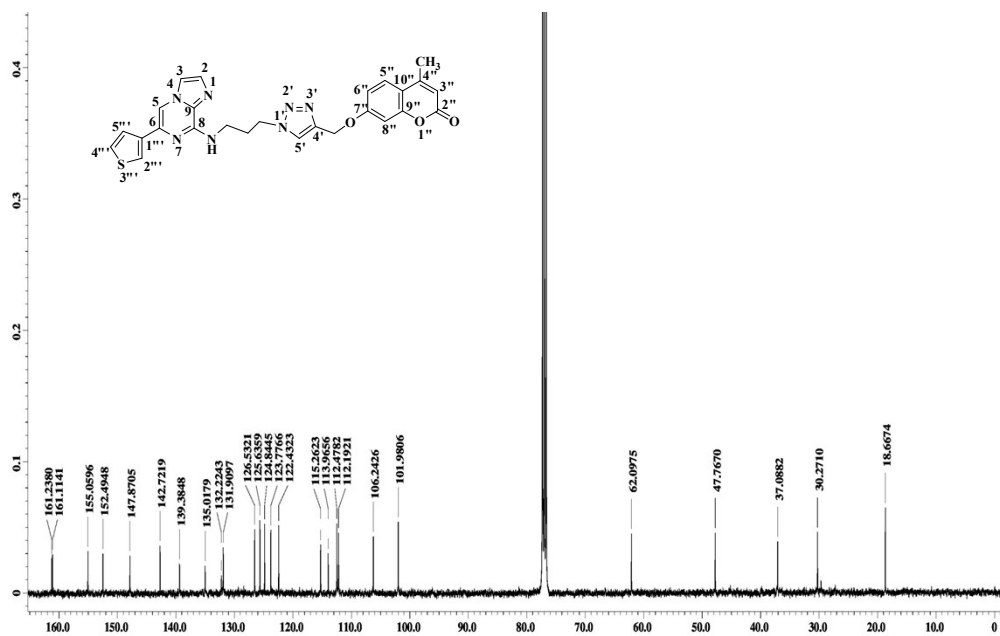


Fig S44:  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(3-(6-(thiophen-3-yl)imidazo[1,2-a]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (29)

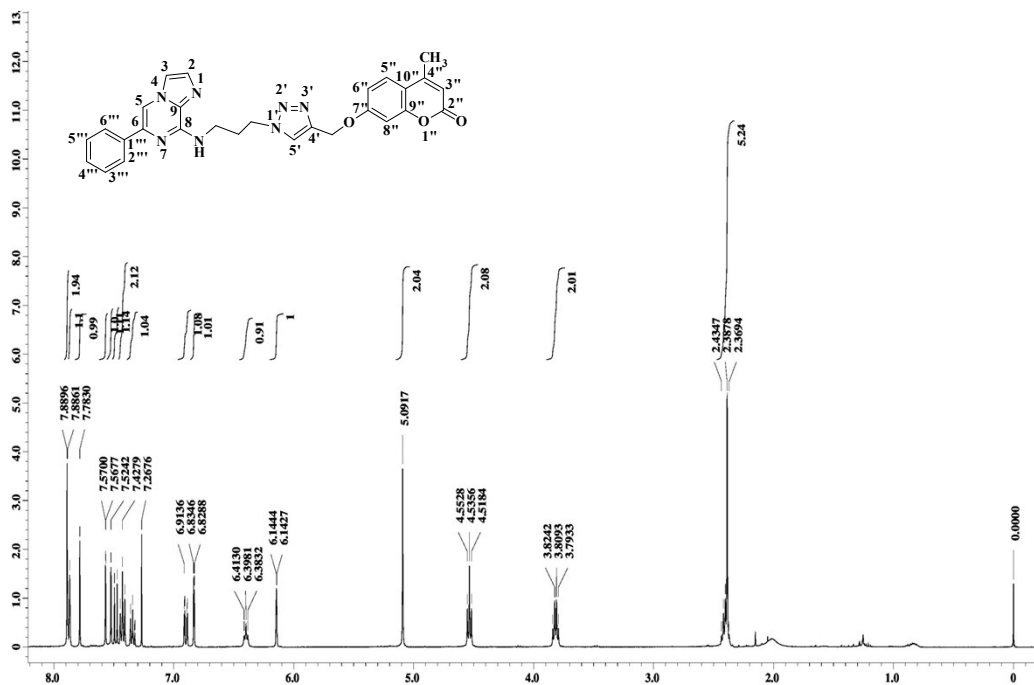
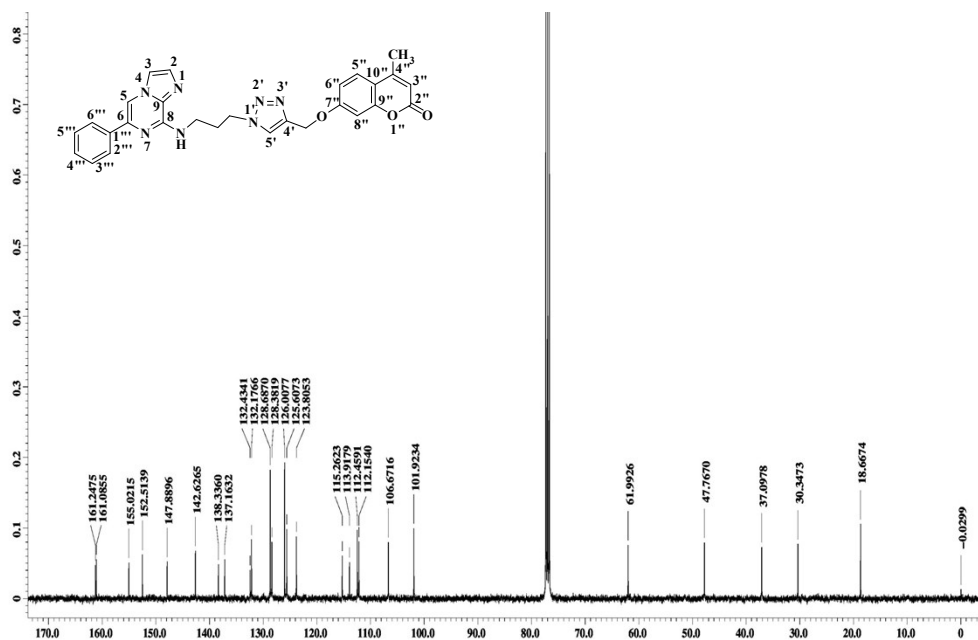
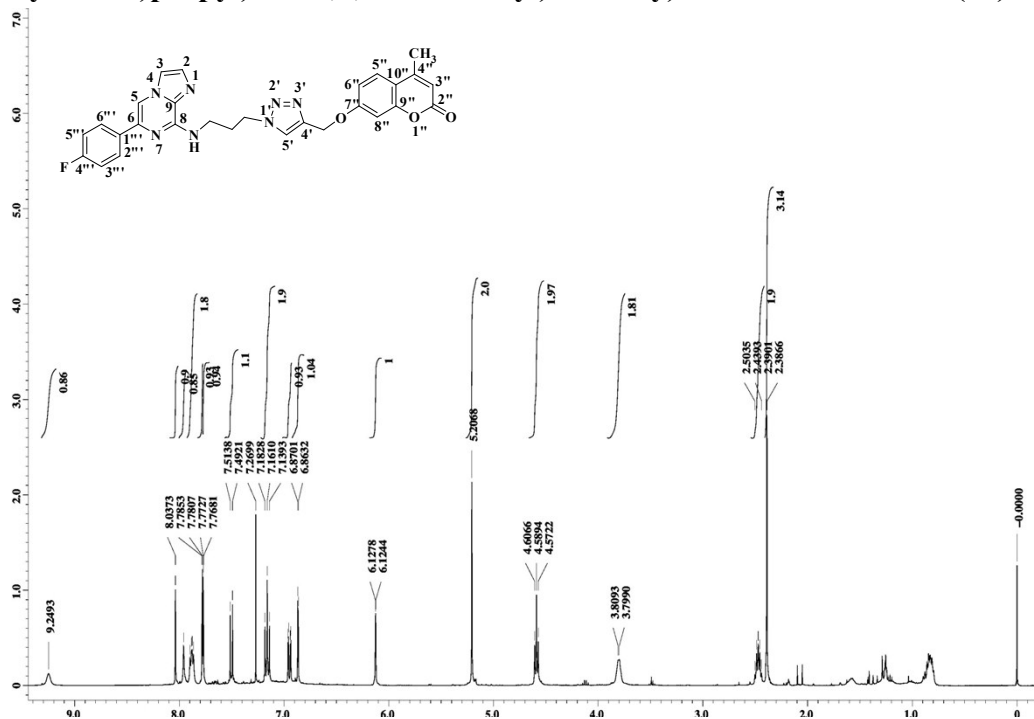


Fig S45:  $^1\text{H}$  NMR spectrum of 4-methyl-7-((1-(3-(6-phenylimidazo[1,2-a]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (30)



**Fig S46:**  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(3-(6-phenylimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (30)



**Fig S47:**  $^1\text{H}$  NMR spectrum of 7-((1-(3-(6-(4-fluorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (31)

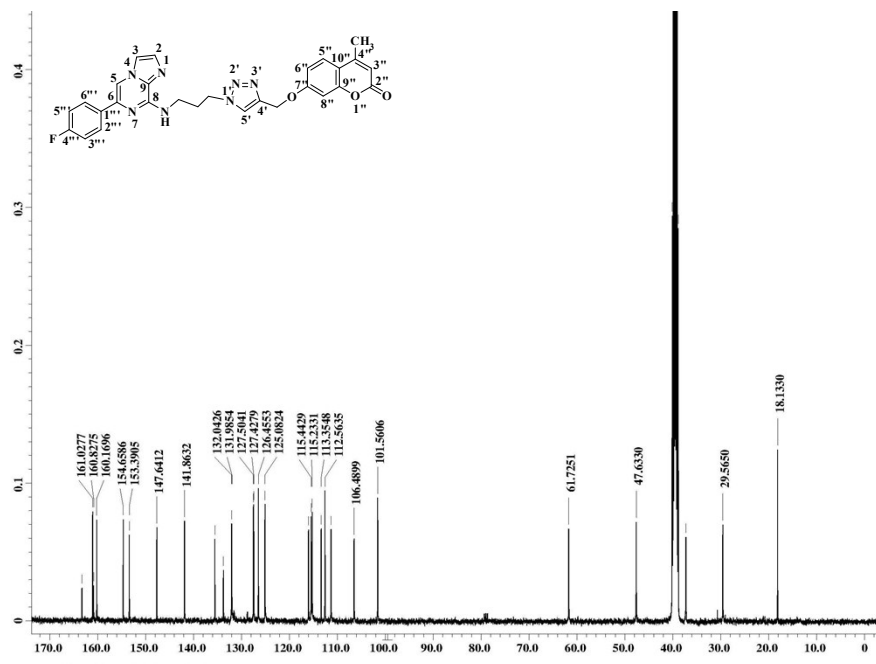


Fig S48: <sup>13</sup>C NMR spectrum of 7-((1-(3-(6-(4-fluorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (31)

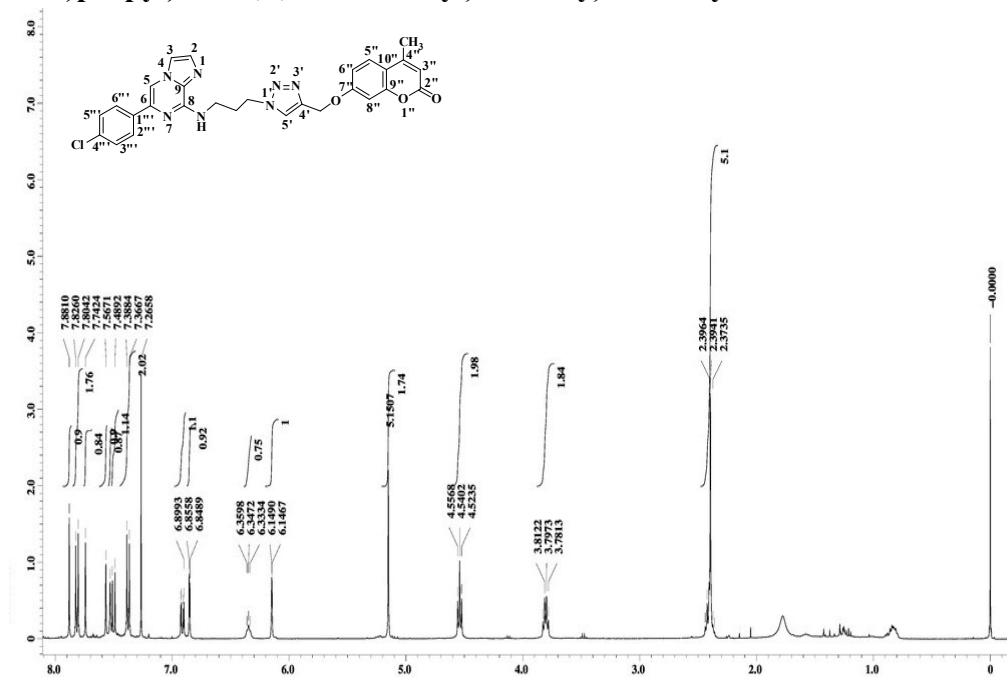


Fig S49: <sup>1</sup>H NMR spectrum of 7-((1-(3-(6-(4-chlorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (32)

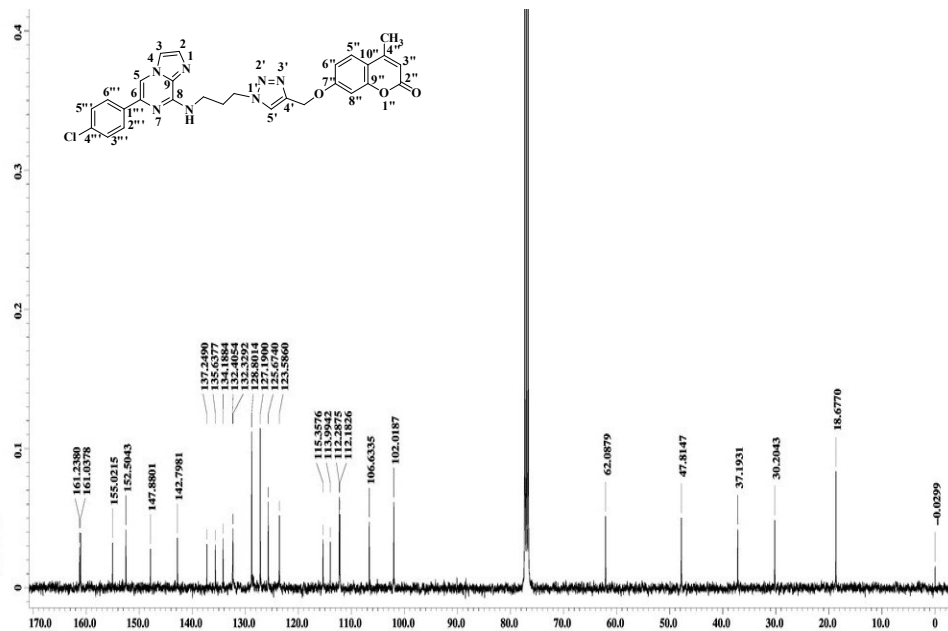


Fig S50:  $^{13}\text{C}$  NMR spectrum of 7-((1-(3-(6-(4-chlorophenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-4-methyl-2*H*-chromen-2-one (32)

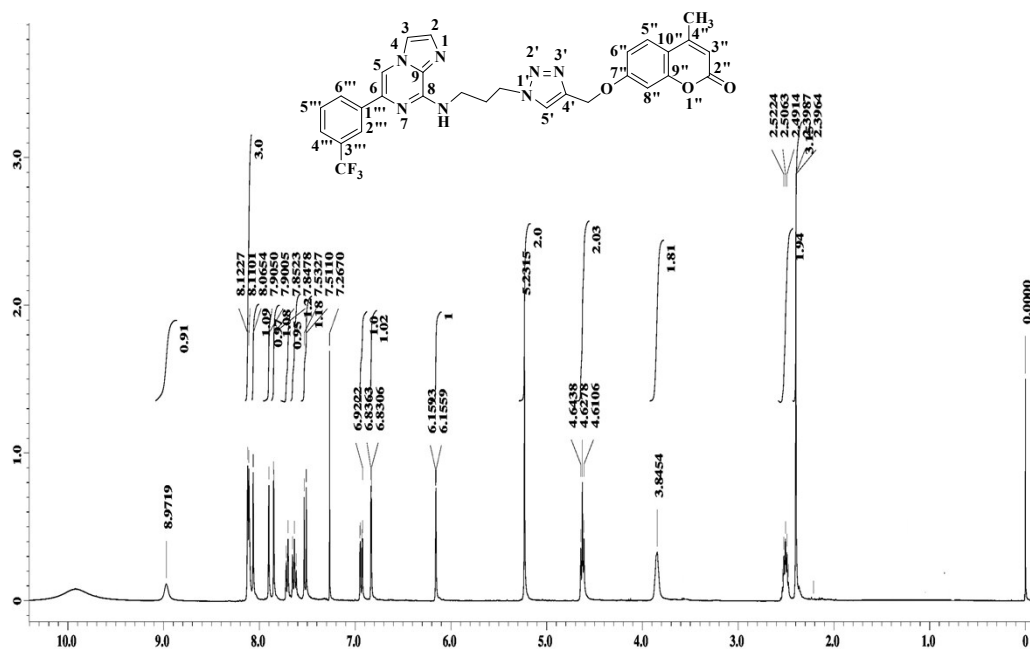


Fig S51:  $^1\text{H}$  NMR spectrum of 4-methyl-7-((1-(3-(6-(3-(trifluoromethyl)phenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (33)

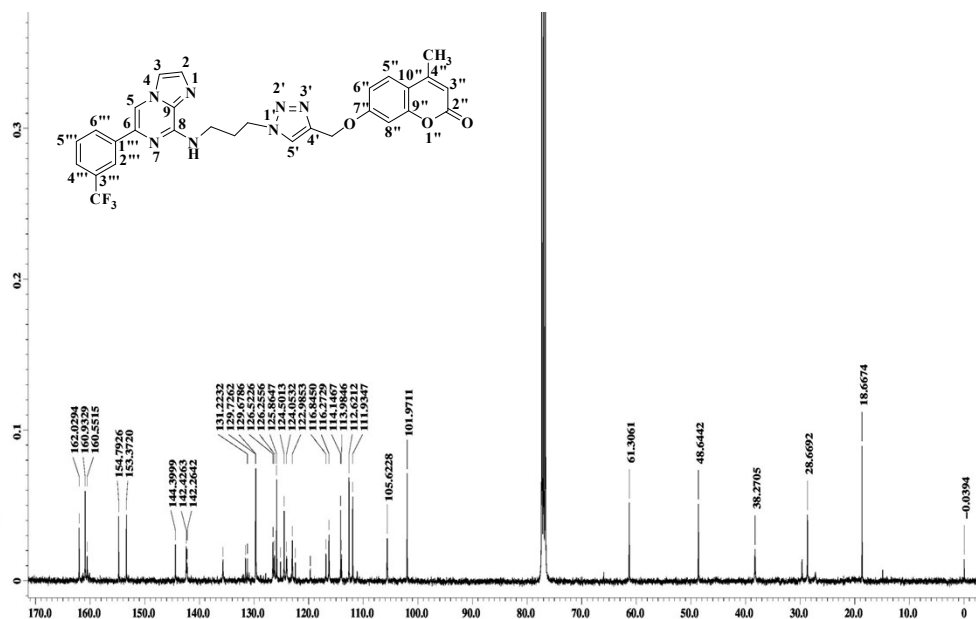


Fig S52:  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(3-(6-(3-(trifluoromethyl)phenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (33)

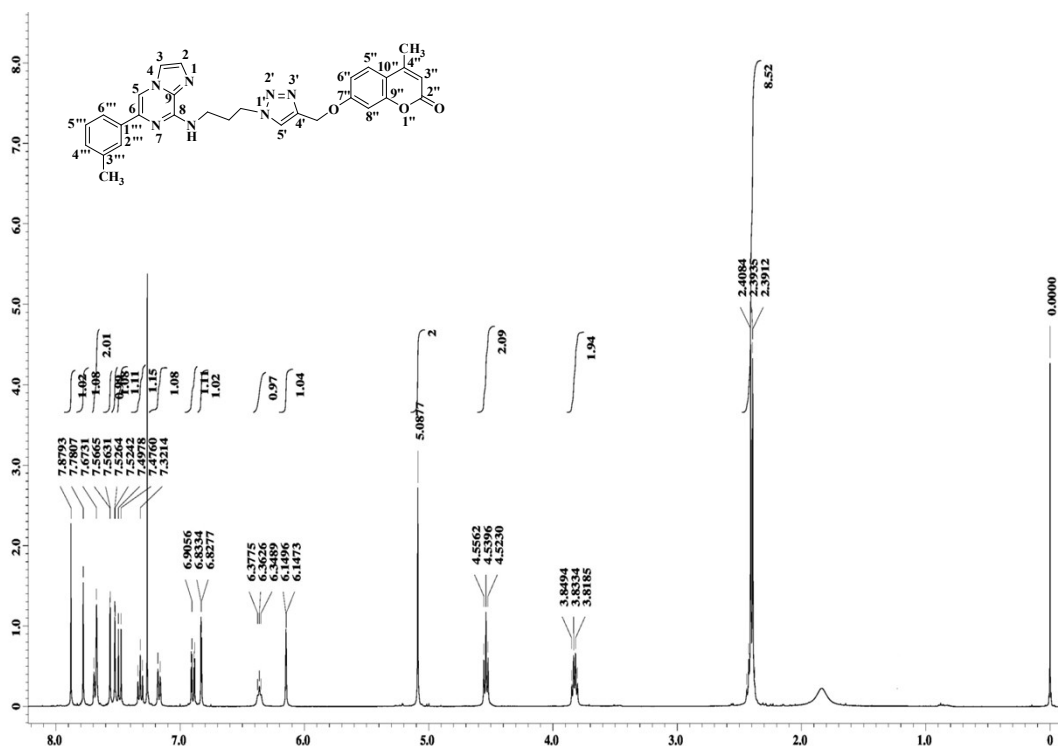


Fig S53:  $^1\text{H}$  NMR spectrum of 4-methyl-7-((1-(3-(6-*m*-tolylimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (34)



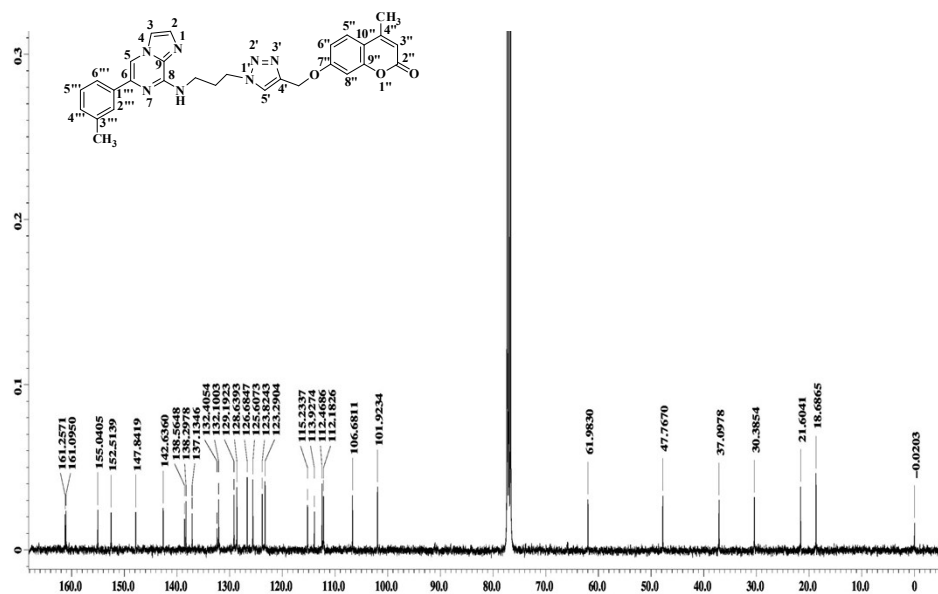


Fig S54:  $^{13}\text{C}$  NMR spectrum of 4-methyl-7-((1-(3-(6-*m*-tolylimidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-2H-chromen-2-one (34)

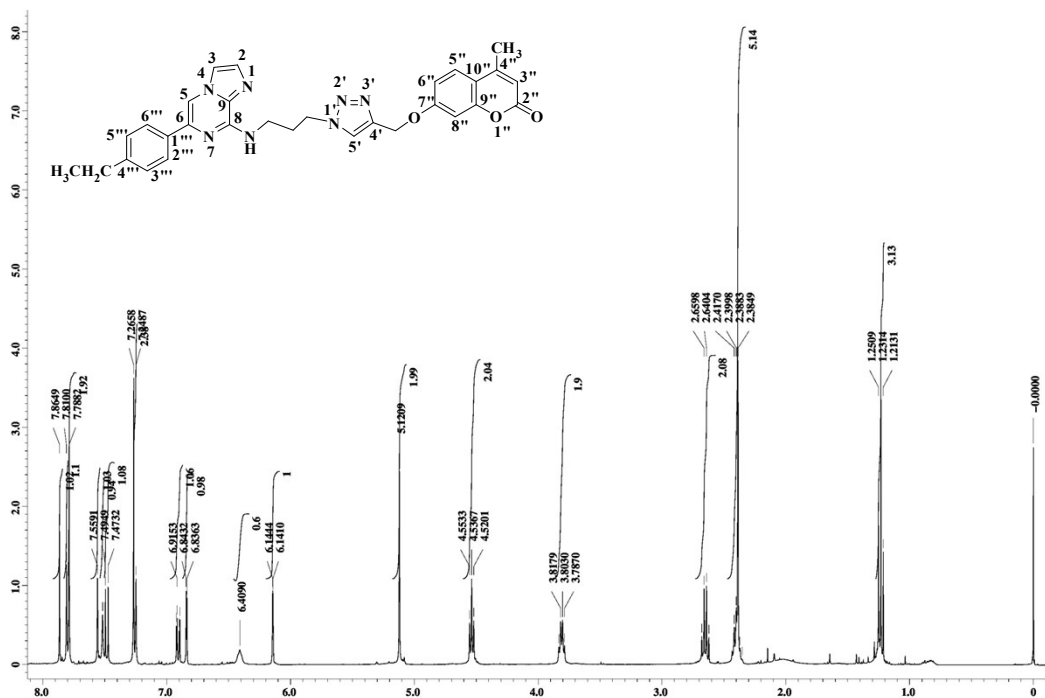


Fig S55:  $^1\text{H}$  NMR spectrum of 7-((1-(3-(4-ethylphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (35)

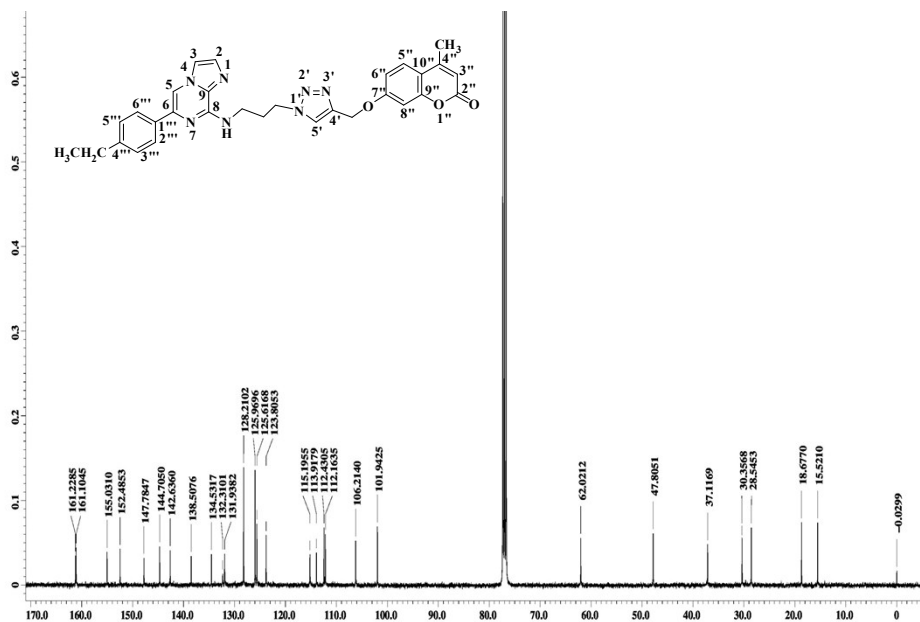


Fig S56:  $^{13}\text{C}$  NMR spectrum of 7-((1-(3-(6-(4-ethylphenyl)imidazo[1,2-a]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (35)

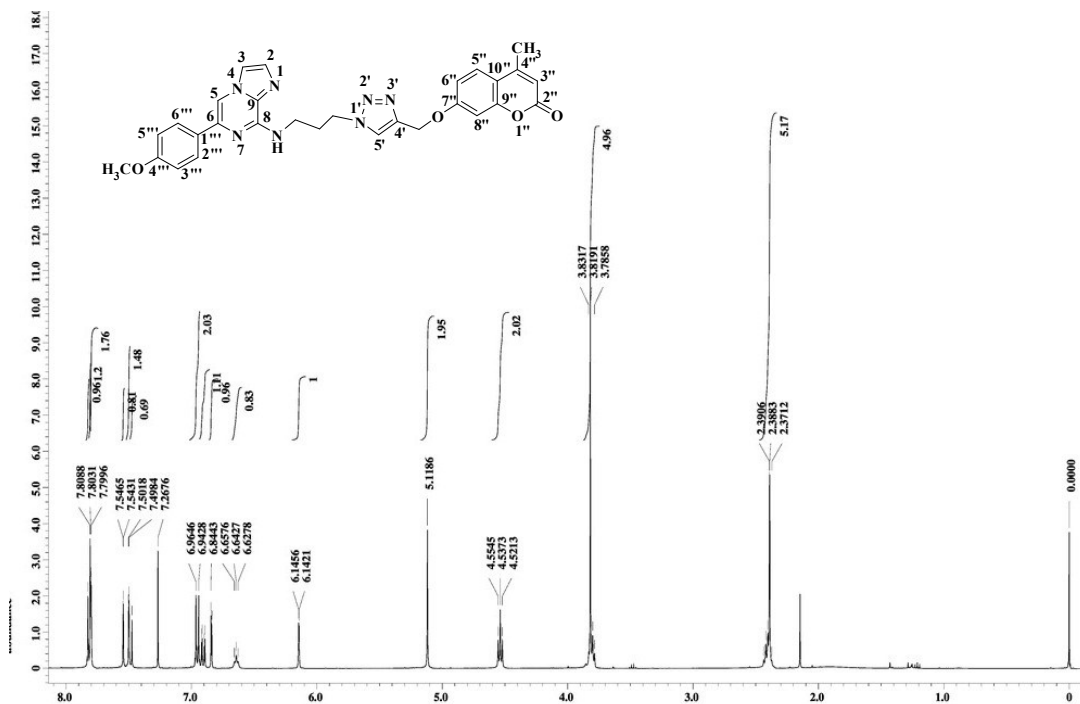


Fig S57:  $^1\text{H}$  NMR spectrum of 7-((1-(3-(6-(4-methoxyphenyl)imidazo[1,2-a]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (36)

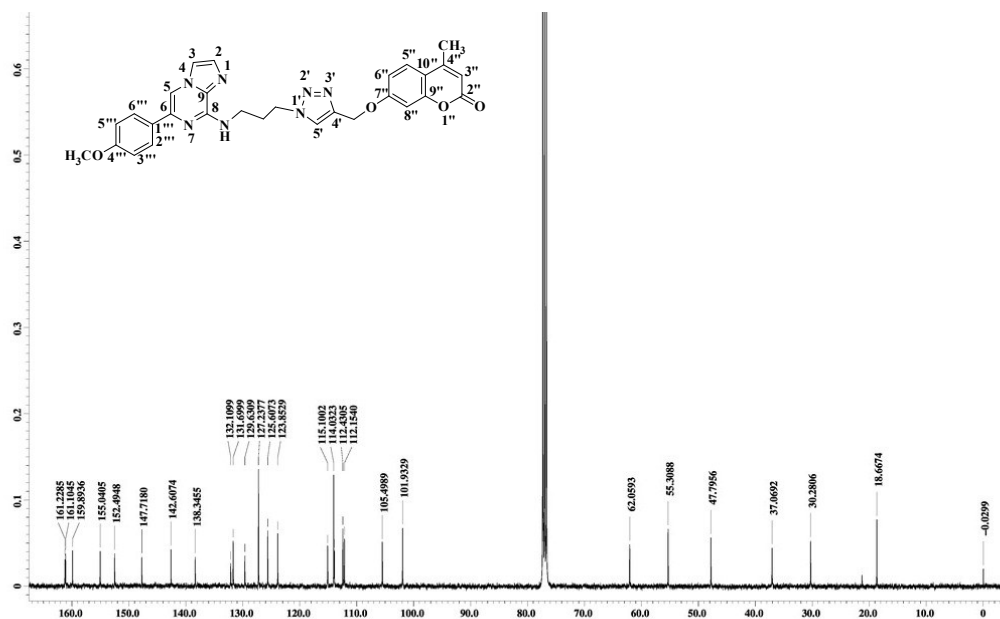


Fig S58:  $^{13}\text{C}$  NMR spectrum of 7-((1-(3-(6-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (36)

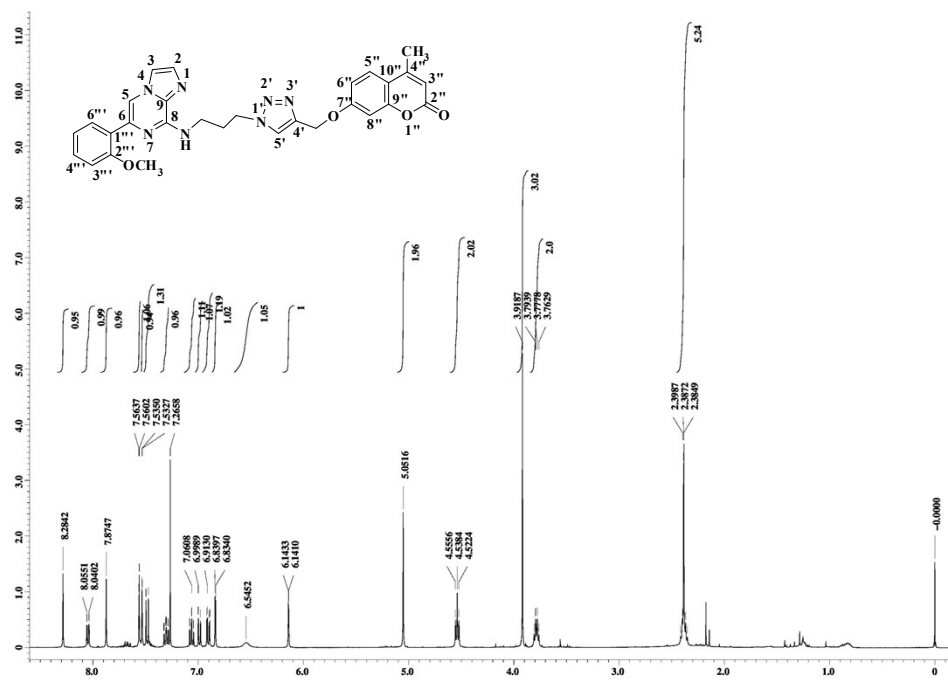


Fig S59:  $^1\text{H}$  NMR spectrum of 7-((1-(3-(6-(2-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (37)

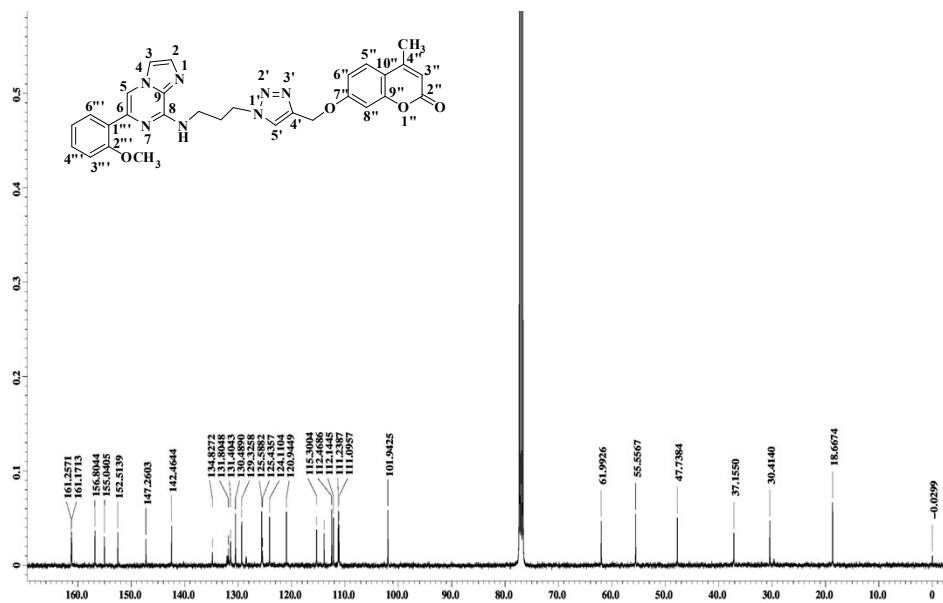


Fig S60:  $^{13}\text{C}$  NMR spectrum of 7-((1-(3-(6-(2-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-ylamino)propyl)-1H-1,2,3-triazol-4-yl)methoxy)-4-methyl-2H-chromen-2-one (37)

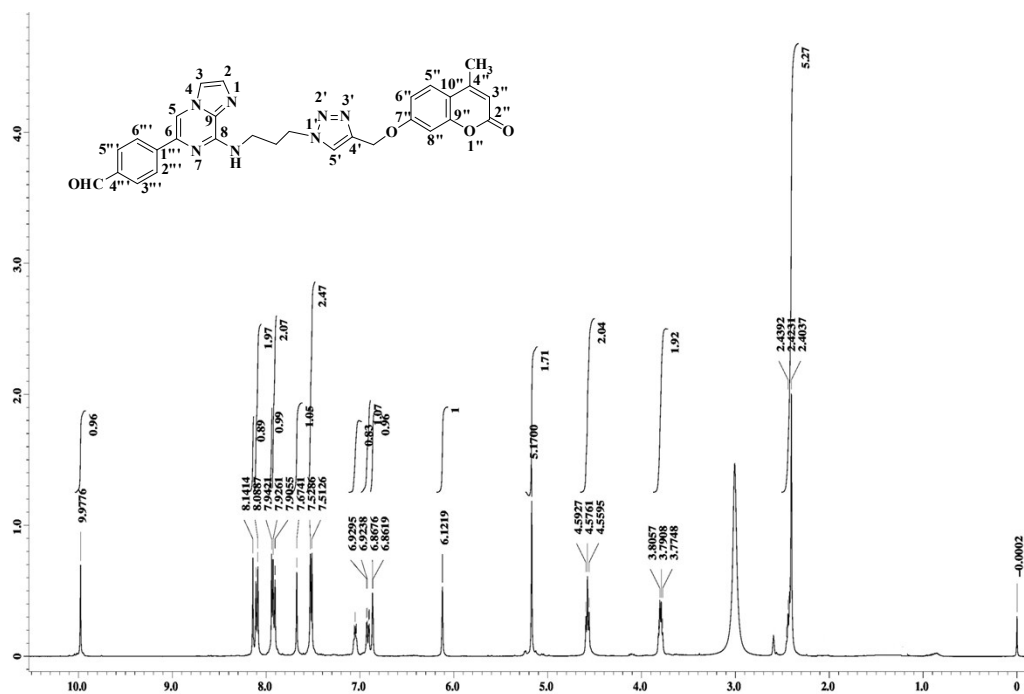
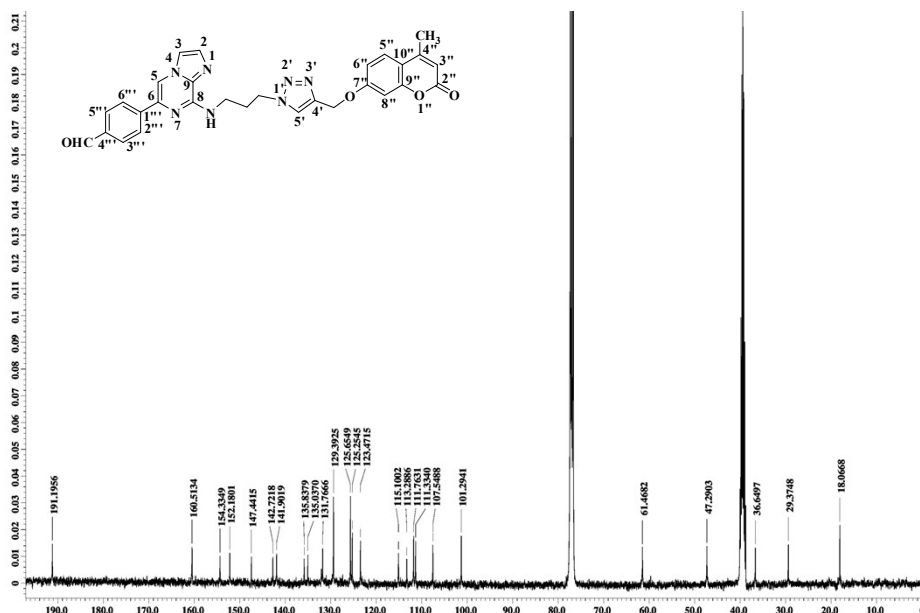


Fig S61:  $^1\text{H}$  NMR spectrum of 4-(8-(3-(4-((4-methyl-2-oxo-2H-chromen-7-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)propylamino)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde (38)



**Fig S62:**  $^{13}\text{C}$  NMR spectrum of 4-(8-(3-(4-((4-methyl-2-oxo-2*H*-chromen-7-yloxy)methyl)-1*H*-1,2,3-triazol-1-yl)propylamino)imidazo[1,2-*a*]pyrazin-6-yl)benzaldehyde (**38**)

### Photophysical measurements

All photophysical measurements were performed in acetonitrile. Absorption spectra were measured with a UV-2500, Shimadzu spectrophotometer. Fluorescent measurements were performed with a Carry Eclipse spectrophotometer. The quantum yields of the imidazo[1,2-*a*]pyrazine analogues were determined relative to anthracene.

### Fluorescence quantum yield

The fluorescence quantum yield  $\Phi_{\text{fs}}$  for all compounds was determined at room temperature in analytical grade  $\text{CH}_3\text{CN}$  using anthracene ( $\Phi_{\text{fr}} = 0.22$ ) in acetonitrile as the standard. The quantum yield was calculated by using eqn--1, in which  $\Phi_{\text{fs}}$  is the radiative quantum yield of the sample,  $\Phi_{\text{fr}}$  is the radiative quantum yield of reference,  $A_{\text{s}}$  and  $A_{\text{r}}$  are the absorbance of the sample and the reference, respectively,  $D_{\text{s}}$  and  $D_{\text{r}}$  are the areas of emission for the sample and reference respectively,  $L_{\text{s}}$  and  $L_{\text{r}}$  are the lengths of the absorption cells, and  $N_{\text{s}}$  and  $N_{\text{r}}$  are the refractive indices of the respective sample and reference solutions (pure solvents were assumed).

$$\Phi_{fs} = \Phi_{fr} \times \frac{1 - 10^{-A_r L_r}}{1 - 10^{-A_s L_s}} \times \frac{N_s^2}{N_r^2} \times \frac{D_s}{D_r} \quad \text{-----1}$$

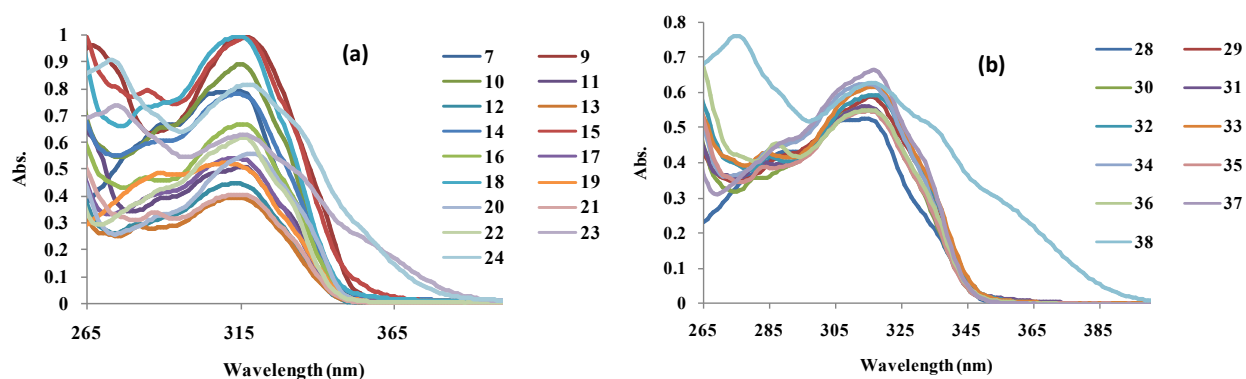


Fig. S63 Absorption spectra of (a) compounds 7-24 and (b) compounds 28-38

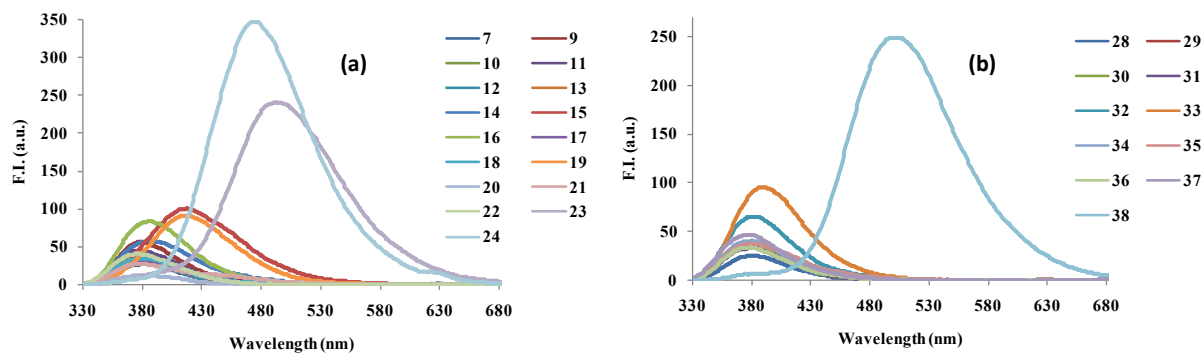


Fig. S64 Emission spectra of (a) compounds 7-24 and (b) compounds 28-38