

## Supporting Information

### The first potent Inhibitors for Human Glutaminyl Cyclase (QC), Synthesis and SAR

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#### Contents:

- MS data, ESI-FTICR-MS data, HPLC-purity data and retention times, routine <sup>1</sup>H NMR data
- a zip-file containing a molecular database with the 192 suggestions and their respective values for strain energy (U) and configuration score (S) in sdf-format is provided. The file is readable as a MOE<sup>®</sup>-database (Version: 2003.02 or higher) with the chemical structures provided in 3-D-format. A 2-D-visualization is possible after importing into ChemFinder (7.0 or higher) or any other software accepting the sdf-file format.

Compound	MS [m/z]	ESI-FTICR-MS [m/z]	Purity [%] (HPLC, 214 nm)	rt [min]	<sup>1</sup> H NMR δ
<b>6</b>	242.2 (M+H) <sup>+</sup> , 174.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup> .				
<b>7</b>	270.3 (M+H) <sup>+</sup> , 202.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup> , 160.1 ([M- C <sub>9</sub> H <sub>6</sub> NO <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup>				
<b>8</b>	112.1 (M+H) <sup>+</sup>				
<b>10</b>	140.3 (M+H) <sup>+</sup>				
<b>13</b>	304.3 (M+H) <sup>+</sup> , 321.3 (M+NH <sub>4</sub> ) <sup>+</sup> , 220.3 ([M- C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup>				
<b>14</b>	304.3 (M+H) <sup>+</sup> , 321.3 (M+NH <sub>4</sub> ) <sup>+</sup> , 220.4 ([M- C <sub>5</sub> H <sub>9</sub> O <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup> .				
<b>15</b>	298.2 (M+H) <sup>+</sup>				
<b>16</b>	298.1 (M+H) <sup>+</sup> .				
<b>17</b>	140.2 (M+H) <sup>+</sup> .				
<b>18</b>	140.4 (M+H) <sup>+</sup>				
<b>19a</b>	102.15 (M+H) <sup>+</sup>				

20	202.2 (M+H) <sup>+</sup> , 128.1 ([M- C <sub>4</sub> H <sub>9</sub> O] <sup>+</sup> ), 101.1 ([M- C <sub>5</sub> H <sub>10</sub> NO] <sup>+</sup> )				0.38–0.50 (m, 4H), 1.42 (s, 9H), 3.09 (s, 2H), 3.36 (s, 2H), 4.85 (br s, 1H)
21	252.1 (M+H) <sup>+</sup> , 196.2 ([M- C <sub>4</sub> H <sub>9</sub> ] <sup>+</sup> ), 128.1 ([M- C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> ] <sup>+</sup> )				0.38–0.50 (m, 4H), 1.42 (s, 9H), 3.09 (s, 2H), 3.56 (s, 2H), 7.32–7.51 (m, 2H), 7.65 (s, 1H)
22	152.2 (M+H) <sup>+</sup> , 84.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> )				
24	208.2 (M+H) <sup>+</sup> , 230.3 (M+Na) <sup>+</sup> , 150.2 ([M- C <sub>4</sub> H <sub>9</sub> ] <sup>+</sup> )				
25	140.3 (M+H) <sup>+</sup>				
26	199.1 (M+H) <sup>+</sup> , 221.3 (M+Na) <sup>+</sup>	221.08304 [M+Na] <sup>+</sup>	100	1.89	1.85–1.95 (m, 2H), 2.84 (s, 3H), 3.31–3.35 (m, 2H), 3.95–3.97 (m, 2H), 6.85 (d, <i>J</i> = 1.0 Hz, 1H), 7.15 (s, 1H), 7.42 (br s, 2H), 7.65 (s, 1H)
27	241.1 (M+H) <sup>+</sup> , 173.1 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> )	241.14805 [M+H] <sup>+</sup>	98.6	15.15	0.82–0.90 (m, 3H), 1.21–1.51 (m, 4H), 1.84–1.98 (m, 2H), 3.17–3.33 (m, 4H), 3.92–3.99 (m, 2H), 6.87 (s, 1H), 7.15 (s, 1H), 7.36–7.38 (m, 2H), 7.65 (s, 1H)
28	241.1 (M+H) <sup>+</sup> , 173.1 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> )	263.13002 [M+Na] <sup>+</sup>	97.8	14.21	1.36 (s, 9H), 1.85–1.95 (m, 2H), 3.22–3.32 (m, 2H), 3.88–3.95 (m, 2H), 6.85 (s, 1H), 7.11–7.13 (m, 1H), 7.21–7.29 (m, 2H), 7.65 (s, 1H)

29	227.3 (M+H) <sup>+</sup> , 159.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup>	249.11429 [M+Na] <sup>+</sup>	96.4	4.57	1.00–1.06 (m, 6H), 1.85–1.89 (m, 2H), 3.28–3.41 (m, 3H), 3.90–3.94 (m, 2H), 6.85 (s, 1H), 7.15 (s, 1H), 7.16–7.25 (m, 2H), 7.65 (s, 1H)
30	277.0 (M+H) <sup>+</sup> , 299.3 (M+Na) <sup>+</sup> , 209.9 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup>	299.12991 [M+Na] <sup>+</sup>	98.3	21.04	1.22–1.25 (m, 1H), 1.40–1.45 (m, 1H), 1.52–1.56 (m, 1H), 1.91–1.95 (m, 2H), 2.74 (s, 1H), 2.80 (s, 1H), 3.29–3.35 (m, 3H), 3.94–3.97 (m, 2H), 6.04–6.06 (m, 1H), 6.13–6.15 (m, 1H), 6.85 (s, 1H), 7.15 (s, 1H), 7.26 (br s, 1H), 7.53 (br s, 1H), 7.65 (s, 1H)
31	267.2 (M+H) <sup>+</sup> , 199.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup> ,	267.16389 [M+H] <sup>+</sup>	98.5	18.78	0.97–1.27 (m, 5H), 1.48–1.91 (m, 6H), 3.33–3.41 (m, 4H) 3.87–3.94 (m, 2H), 6.85 (s, 1H), 7.15 (s, 1H), 7.27–7.53 (m, 2H), 7.65 (s, 1H)
32	275.3 (M+H) <sup>+</sup> , 207.1 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup> ,	297.11456 [M+Na] <sup>+</sup>	97.5	20.61	1.85–1.95 (m, 2H), 3.28–3.40 (m, 2H), 3.92–3.93 (m, 2H), 4.61 (s, 2H), 6.85 (s, 1H), 7.15 (s, 1H), 7.19–7.35 (m, 5H), 7.52–7.57 (m, 2H), 7.85 (s, 1H)
33	261.1 (M+H) <sup>+</sup> , 193.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup> ,	283.09865 [M+Na] <sup>+</sup>	97.4	14.00	1.95–2.05 (m, 2H), 3.39–3.44 (m, 2H), 3.92–4.01 (m, 2H), 6.85 (s, 1H), 7.04–7.09 (m, 1H) 7.15 (s, 1H), 7.25–7.30 (m, 2H), 7.31–7.35 (m, 2H), 7.61 (s, 1H), 7.77 (br s, 1H), 9.46 (br s, 1H)

34	311.3 (M+H) <sup>+</sup> , 243.4 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	333.11410 [M+Na] <sup>+</sup>	98.6	22.07	1.95–2.05 (m, 2H), 3.40–3.45 (m, 2H), 3.92–4.01 (m, 2H), 6.86 (s, 1H), 7.13 (s, 1H), 7.44–7.64 (m, 6H), 7.84–7.88 (m, 2H), 7.94–7.97 (m, 1H), 9.63 (br s, 1H)
35	275.2 (M+H) <sup>+</sup> , 207.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	297.11419 [M+Na] <sup>+</sup>	97.4	19.72	1.95–2.05 (m, 2H), 3.40–3.45 (m, 2H), 2.23 (s, 3H), 3.92–4.01 (m, 2H), 6.86 (s, 1H), 7.07–7.09 (m, 2H), 7.13 (s, 1H), 7.17–7.19 (m, 2H), 7.59 (s, 1H), 7.64 (br s, 1H), 9.35 (br s, 1H)
36	289.3 (M+H) <sup>+</sup> , 221.1 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	311.12976 [M+Na] <sup>+</sup>	99.1	22.62	1.16–1.18 (m, 3H), 1.95–2.02 (m, 2H), 2.55–2.59 (m, 2H), 3.41–3.45 (m, 2H), 3.97–4.00 (m, 2H), 6.85 (s, 1H), 7.14–7.17 (m, 3H), 7.23–7.25 (m, 2H), 7.63 (s, 1H), 7.70 (br s, 1H), 9.40 (br s, 1H)
37	279.3 (M+H) <sup>+</sup> , 211.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> )	301.08915 [M+Na] <sup>+</sup>	97.3	16.76	1.95–2.05 (m, 2H), 3.39–3.40 (m, 2H), 3.90–4.05 (m, 2H), 6.85 (s, 1H), 7.05–7.15 (m, 3H), 7.32–7.41 (m, 2H), 7.60 (s, 1H), 7.76 (br s, 1H), 9.41 (br s, 1H)
38	304.2 (M+H) <sup>+</sup> , 236.0 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	326.14070 [M+Na] <sup>+</sup>	98.2	9.15	1.91–2.02 (m, 2H), 2.93 (s, 6H), 3.39–3.42 (m, 2H), 3.93–4.01 (m, 2H), 6.67–6.70 (m, 2H), 6.92 (s, 1H), 7.05–7.10 (m, 2H), 7.15 (s, 1H), 7.40 (br s, 1H), 7.66 (s, 1H), 9.22 (s, 1H)

39	306.2 (M+H) <sup>+</sup> , 237.9 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	328.08369 [M+Na] <sup>+</sup>	100	22.30	1.91–2.05 (m, 2H), 3.30–3.51 (m, 2H), 3.95–4.05 (m, 2H), 6.85 (s, 1H), 7.15 (s, 1H), 7.62 (s, 1H), 7.73–7.76 (m, 2H), 8.12– 8.13 (m, 2H), 8.31 (br s, 1H), 10.12 (br s, 1H)
40	303.2 (M+H) <sup>+</sup> , 235.1 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	325.10906 [M+Na] <sup>+</sup>	99.8	18.58	1.91–2.12 (m, 2H), 2.48 (s, 3H), 3.20–3.52 (m, 2H), 3.92–4.11 (m, 2H), 6.85 (s, 1H), 7.15 (s, 1H), 7.51–7.65 (m, 3H), 7.81–7.92 (m, 2H), 8.02–8.09 (m, 1H), 9.81 (br s, 1H)
41	307.2 (M+H) <sup>+</sup> , 239.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	329.08653 [M+Na] <sup>+</sup>	97.8	22.18	1.98–2.05 (m, 2H), 2.48 (s, 3H), 3.22–3.52 (m, 2H), 3.95–4.05 (m, 2H), 6.85 (s, 1H), 7.16–7.33 (m, 5H), 7.63 (s, 1H), 7.76 (br s, 1H), 9.44 (br s, 1H)
42	367.2 (M+H) <sup>+</sup> , 299.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	389.14028 [M+Na] <sup>+</sup>	98.2	23.73	2.03–2.10 (m, 2H), 3.58–3.63 (m, 2H), 3.94–3.97 (m, 2H), 5.04 (s, 2H), 6.01 (s, 1H), 6.81 (br s, 1H), 6.90–6.96 (m, 4H), 7.11–7.19 (m, 2H), 7.31–7.40 (m, 5H), 7.92 (s, 1H)
43	305.2 (M+H) <sup>+</sup> , 237.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	327.12504 [M+Na] <sup>+</sup>	98.4	20.64	1.28–1.32 (m, 3H), 1.94–2.01 (m, 2H), 3.41–3.45 (m, 2H), 3.93–4.02 (m, 4H), 6.85 (s, 1H), 7.16–7.33 (m, 5H), 7.63 (s, 1H), 7.76 (br s, 1H), 9.44 (br s, 1H)
44	291.1 (M+H) <sup>+</sup> , 223.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	313.10913 [M+Na] <sup>+</sup>	97.3	22.83	1.87–2.00 (m, 2H), 3.29–3.44 (m, 2H), 3.70 (s, 3H), 3.91–4.02 (m, 2H), 6.72–6.93 (m, 3H), 7.11–7.21 (m, 3H), 7.50 (s, 1H), 7.61 (s, 1H), 9.21 (s, 1H)

45	305.2 (M+H) <sup>+</sup> , 237.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	305.10642 [M+H] <sup>+</sup>	96.6	13.71	1.99–2.03 (m, 2H), 3.42–3.44 (m, 2H), 4.08–4.15 (m, 2H), 6.01 (s, 2H), 6.66–6.69 (d, <i>J</i> = 6.6 Hz, 1H), 6.90 (d, <i>J</i> = 8.3 Hz, 1H), 6.95 (s, 1H), 7.25 (s, 1H), 7.45 (s, 1H), 7.68 (br s, 1H), 8.32 (br s, 1H), 9.38 (br s, 1H)
46	291.1 (M+H) <sup>+</sup> , 223.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	313.10922 [M+Na] <sup>+</sup>	98.5	16.40	1.99–2.05 (m, 2H), 3.42–3.46 (m, 2H), 3.71 (s, 3H), 3.97–4.01 (m, 2H), 6.67 (dd, <i>J</i> = 5.8 Hz, 2.5 Hz, 1H), 6.85–6.90 (m, 2H), 6.99–7.07 (m, 1H), 7.15–7.25 (m, 2H), 7.62 (s, 1H), 7.86 (br s, 1H), 9.51 (s, 1H)
47	335.3 (M+H) <sup>+</sup> , 267.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	357.113546 [M+Na] <sup>+</sup>	97.3	19.41	1.93–1.99 (m, 2H), 3.42–3.46 (m, 2H), 3.71 (s, 3H), 3.72 (s, 3H), 3.96–3.99 (m, 2H), 4.72 (s, 2H), 6.75–6.77 (m, 1H), 6.89–6.90 (m, 2H), 6.95 (s, 1H), 7.16 (s, 1H), 7.59 (br s, 1H), 7.62 (s, 1H), 9.33 (s, 1H)
48	319.3 (M+H) <sup>+</sup> , 251.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	341.10400 [M+Na] <sup>+</sup>	97.1	16.03	1.94–1.99 (m, 2H), 3.33–3.41 (m, 2H), 3.95–3.98 (m, 2H), 4.19–4.26 (m, 4H), 6.68–6.71 (m, 1H), 6.78–6.80 (m, 1H), 6.86–6.87 (m, 2H), 7.16 (s, 1H), 7.63 (s, 2H), 9.28 (s, 1H)
49	321.2 (M+H) <sup>+</sup> , 253.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	343.12010 [M+Na] <sup>+</sup>	97.2	21.12	1.95–2.01 (m, 2H), 3.42–3.49 (m, 2H), 3.61 (s, 6H), 3.97–4.00 (m, 2H), 6.25 (s, 1H), 6.59 (s, 2H), 6.87 (s, 1H), 7.17 (s, 1H), 7.62 (s, 1H), 7.83 (s, 1H), 9.47 (s, 1H)

50	321.2 (M+H) <sup>+</sup> , 253.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	343.12011 [M+Na] <sup>+</sup>	99.0	17.71	1.95–2.01 (m, 2H), 3.42–3.49 (m, 2H), 3.74 (s, 3H), 3.75 (s, 3H), 3.97–3.99 (m, 2H), 6.48 (dd, <i>J</i> = 6.1 Hz, 2.4 Hz, 1H), 6.60 (s, 1H), 6.87 (s, 1H), 7.15 (s, 1H), 7.31 (d, <i>J</i> = 6.1 Hz, 1H), 7.47 (br s, 1H), 7.61 (s, 1H), 8.73 (s, 1H)
51	305.0 (M+H) <sup>+</sup> , 237.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	327.14255 [M+Na] <sup>+</sup>	97.1	11.73	1.81–1.86 (m, 2H), 3.00–3.05 (m, 2H), 3.66 (s, 3H), 3.69 (s, 3H), 3.95–3.98 (m, 2H), 6.09–6.12 (m, 1H), 6.79 (s, 2H), 6.88 (s, 1H), 7.14 (s, 1H), 7.17 (s, 1H), 7.62 (s, 1H), 8.24 (s, 1H)
52	351.3 (M+H) <sup>+</sup> , 283.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	373.12977 [M+Na] <sup>+</sup>	98.6	16.85	1.94–2.01 (m, 2H), 3.41–3.52 (m, 2H), 3.62 (s, 3H), 3.73 (s, 6H), 3.97–4.00 (m, 2H), 6.65 (s, 2H), 6.87 (s, 1H), 7.17 (s, 1H), 7.63 (s, 1H), 7.73 (br s, 1H), 9.41 (s, 1H)
53	321.2 (M+H) <sup>+</sup> , 253.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	343.12009 [M+Na] <sup>+</sup>	99.8	14.00	1.93–1.99 (m, 2H), 3.42–3.46 (m, 2H), 3.71 (s, 3H), 3.72 (s, 3H), 3.96–3.99 (m, 2H), 6.75–6.77 (m, 1H), 6.89–6.90 (m, 2H), 6.95 (s, 1H), 7.16 (s, 1H), 7.59 (br s, 1H), 7.62 (s, 1H), 9.33 (s, 1H)
54	307.2 (M+H) <sup>+</sup> , 239.1 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	329.10398 [M+Na] <sup>+</sup>	99.4	11.12	3.69 (s, 3H), 3.72 (s, 3H), 3.74–3.78 (m, 2H), 4.16–4.19 (m, 2H), 6.68–6.70 (m, 1H), 6.85–6.89 (m, 1H), 6.85–6.89 (m, 2H), 7.13 (s, 1H), 7.47 (br s, 1H), 7.59 (s, 1H), 9.48 (s, 1H)

55	335.3 (M+H) <sup>+</sup> , 267.1 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	357.13563 [M+Na] <sup>+</sup>	99.1	16.47	1.42–1.51 (m, 2H), 1.63–1.71 (m, 2H), 3.42–3.51 (m, 2H), 3.69 (s, 3H), 3.72 (s, 3H), 3.95–4.01 (m, 2H), 6.68–6.70 (m, 1H), 6.85–6.89 (m, 1H), 6.91–6.98 (m, 2H), 7.13 (s, 1H), 7.47 (br s, 1H), 7.59 (s, 1H), 9.48 (s, 1H)
56	335.3 (M+H) <sup>+</sup> , 267.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	335.15345 [M+H] <sup>+</sup>	97.9	19.13	0.83 (d, <i>J</i> = 6.6 Hz, 3H), 2.31–2.39 (m, 1H), 3.37–3.43 (m, 2H), 3.71 (s, 3H), 3.72 (s, 3H), 4.04–4.08 (m, 1H), 4.16–4.18 (m, 1H), 6.78 (d, <i>J</i> = 8.5 Hz, 1H), 6.89 (d, <i>J</i> = 8.5 Hz, 1H), 6.99 (s, 1H), 7.67 (s, 1 H), 7.75 (s, 2H), 9.11 (s, 1H), 9.50 (s, 1H)
57	335.4 (M+H) <sup>+</sup> , 267.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	335.15344 [M+H] <sup>+</sup>	98.1	17.93	0.83 (d, <i>J</i> = 6.6 Hz, 3H), 2.36–2.41 (m, 1H), 3.37–3.43 (m, 2H), 3.71 (s, 3H), 3.72 (s, 3H), 4.04–4.08 (m, 1H), 4.16–4.18 (m, 1H), 6.77 (d, <i>J</i> = 8.5 Hz, 1H), 6.89 (d, <i>J</i> = 8.5 Hz, 1H), 6.99 (s, 1H), 7.67 (s, 1 H), 7.75 (s, 2H), 9.11 (s, 1H), 9.50 (s, 1H)

58	347.2 (M+H) <sup>+</sup> , 279.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>•</sup> ) <sup>+</sup> , 137.5 ([M- C <sub>9</sub> H <sub>13</sub> N <sub>4</sub> S] <sup>•</sup> ) <sup>+</sup> ,	347.15352 [M+H] <sup>+</sup>	97.8	19.85	0.69–0.73 (m, 4H), 1.85–1.86 (m, 1.3H), 2.11–2.21 (m, 2.7H), 3.35–3.40 (m, 2H), 3.43–3.44 (m, 2H), 3.68–3.71 (4 × s, 12H), 4.13 (s, 2H), 4.94 (s, 2H), 6.75–6.78 (m, 2H), 6.84–6.89 (m, 2H), 6.98 (s, 2H), 7.48–7.49 (m, 2H), 7.60–7.61 (m, 2H), 7.65 (s, 1H), 7.78 (s, 1H), 8.82 (s, 1H), 9.07 (s, 1H), 9.36 (s, 1H), 9.43 (s, 1H)
59	335.4 (M+H) <sup>+</sup> , 267.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>•</sup> ) <sup>+</sup>	357.13522 [M+Na] <sup>+</sup>	97.5	15.05	2.17–2.21 (m, 2H), 3.08 (s, 3H), 3.83 (s, 3H), 3.84 (s, 3H), 3.94–3.98 (m, 2H), 4.03–4.07 (m, 2H), 6.76–6.81 (m, 2H), 6.81 (s, 1H), 6.89 (s, 1H), 7.04 (s, 1H), 7.14 (s, 1H), 7.52 (s, 1H)
66	259.4 (M+H) <sup>+</sup> , 191.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>•</sup> ) <sup>+</sup>	281.08301 [M+Na] <sup>+</sup>	99.1	9.71	1.98–2.02, (m, 2H), 3.27–3.34 (m, 2H), 4.03–4.06 (m, 2H), 6.89 (s, 1H), 6.98–7.00 (m, 1H), 7.18–7.21 (m, 2H), 7.35–7.37 (m, 1H), 7.65 (s, 2H), 8.06 (s, 1H)
67	293.3 (M+H) <sup>+</sup>	293.06204 [M+H] <sup>+</sup>	98.2	21.29	1.98–2.02, (m, 2H), 3.27–3.34 (m, 2H), 4.03–4.06 (m, 2H), 6.90 (s, 1H), 7.20–7.22 (m, 2H), 7.32–7.37 (m, 1H), 7.65 (s, 1H), 7.77 (s, 1H), 8.20 (s, 1H)
68	289.1 (M+H) <sup>+</sup> , 221.4 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>•</sup> ) <sup>+</sup>	289.11150 ([M+H] <sup>+</sup> )	97.7	14.77	1.98–2.02, (m, 2H), 3.27–3.34 (m, 2H), 3.69 (s, 3H), 4.03–4.06 (m, 2H), 6.77–6.78 (m, 1H), 6.87 (s, 1H), 7.17 (s, 1H), 7.23–7.26 (m, 2H), 7.63 (s, 1H), 7.81 (s, 1H)

69	319.2 (M+H) <sup>+</sup> , 251.4 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup>	319.12219 [M+H] <sup>+</sup>	99.7	13.09	1.98–2.02, (m, 2H), 3.27–3.34 (m, 2H), 3.84 (s, 3H), 3.86 (s, 3H), 4.03–4.06 (m, 2H), 6.91 (s, 1H), 7.02 (s, 1H), 7.05 (s, 1H), 7.10 (s, 1H), 7.24 (s, 1H), 7.48 (s, 1H)
70	320.2 (M+H) <sup>+</sup> , 252.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup>	342.12408 [M+Na] <sup>+</sup>	100	21.25	2.06–2.09 (m, 2H), 3.45–3.47 (m, 2H), 3.70 (s, 6H), 3.77 (s, 2H), 4.11–4.15 (m, 2H), 6.80–6.86 (m, 3H), 7.66 (s, 1H), 7.72 (s, 1H), 8.92 (s, 1H), 9.09 (s, 1H)
71	274.4 (M+H) <sup>+</sup> , 206.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup>	296.11895 [M+Na] <sup>+</sup>	99.2	23.01	1.48 (d, <i>J</i> = 7.3 Hz, 3H), 1.94–1.99 (m, 2H), 3.40–3.45 (m, 2H), 3.89–3.93 (m, 2H), 4.05 (q, <i>J</i> = 7.3 Hz, 1H), 6.88 (s, 1H), 7.12 (s, 1H), 7.15–7.23 (m, 1H), 7.24–7.35 (m, 2H), 7.35–7.41 (m, 2H), 7.55 (s, 1H), 10.09 (s, 1H)
72	274.4 (M+H) <sup>+</sup> , 206.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup>	296.11918 [M+Na] <sup>+</sup>	98.7	22.72	1.48 (d, <i>J</i> = 7.3 Hz, 3H), 1.94–1.99 (m, 2H), 3.40–3.45 (m, 2H), 3.89–3.93 (m, 2H), 4.05 (q, <i>J</i> = 7.3 Hz, 1H), 6.88 (s, 1H), 7.12 (s, 1H), 7.15–7.23 (m, 1H), 7.24–7.35 (m, 2H), 7.35–7.41 (m, 2H), 7.55 (s, 1H), 10.09 (s, 1H)
73	336.3 (M+H) <sup>+</sup> , 268.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ) <sup>+</sup>	336.15246 [M+H] <sup>+</sup>	97.9	23.93	1.94–1.99 (m, 2H), 3.40–3.45 (m, 2H), 3.89–3.93 (m, 2H), 4.73 (s, 1H), 6.88 (s, 1H), 6.91 (s, 1H), 7.09 (s, 1H), 7.15–7.23 (m, 4H), 7.24–7.35 (m, 2H), 7.35–7.45 (m, 4H), 10.13 (s, 1H)

74	316.0 (M+H) <sup>+</sup> , 248.4 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> ),	338.12952 [M+Na] <sup>+</sup>	98.2	14.96	1.06–1.08 (m, 2H), 1.54–1.56 (m, 2H), 1.90–1.97 (m, 2H), 3.44–3.48 (m, 2H), 3.73 (s, 3H), 3.82–3.89 (m, 2H), 6.87–6.88 (m, 3H), 7.10 (s, 1H), 7.25–7.26 (m, 2H), 7.58 (s, 1H), 8.96 (br s, 1H)
75	334.3 (M+H) <sup>+</sup> , 266.1 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> )	338.12952 [M+H] <sup>+</sup>	100	14.67	1.55–1.75 (m, 2H), 1.85–1.95 (m, 2H), 2.48–2.53 (m, 2H), 2.77–2.83 (m, 2H), 3.41–3.45 (m, 2H), 3.79–3.81 (m, 2H), 6.85 (s, 1H), 7.03 (s, 1H), 7.37–7.39 (m, 2H), 7.48 (s, 1H), 7.52–7.54 (m, 2H), 9.62 (s, 1H)
76	348.2 (M+H) <sup>+</sup> , 280.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> )	348.12930 [M+H] <sup>+</sup>	99.3	15.67	1.51–1.63 (m, 4H), 1.86–1.92 (m, 2H), 2.00–2.05 (m, 2H), 2.57–2.62 (m, 2H), 3.44–3.48 (m, 2H), 3.76–3.79 (m, 2H), 6.85 (s, 1H), 7.03 (s, 1H), 7.34–7.37 (m, 2H), 7.40–7.42 (m, 2H), 7.48 (s, 1H), 9.34 (s, 1H)
77	358.3 (M+H) <sup>+</sup> , 290.3 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>+</sup> )	358.19456 [M+H] <sup>+</sup>	99.2	12.61	1.26–1.29 (m, 1H), 1.39–1.49 (m, 5H), 1.86–1.96 (m, 4H), 2.46–2.49 (m, 2H), 3.46–3.53 (m, 2H), 3.68 (s, 3H), 3.74–3.77 (m, 2H), 6.82–6.85 (m, 3H), 7.02 (s, 1H), 7.30–7.33 (m, 2H), 7.49 (s, 1H), 9.17 (s, 1H)
79	(anion mode) m/z 221.2 (M-H) <sup>-</sup> .				1.11 (dd, <i>J</i> = 3.7 Hz, 2.9 Hz, 2H), 1.58 (dd, <i>J</i> = 3.7 Hz, 2.9 Hz, 2H), 6.88–6.90 (m, 3H);

80	MS m/z 330.1 (M+H) <sup>+</sup> , 262.1 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>•</sup> ) <sup>+</sup>				1.11 (dd, <i>J</i> = 3.7 Hz, 2.9 Hz, 2H), 1.57 (dd, <i>J</i> = 3.7 Hz, 2.9 Hz, 2H), 2.02–2.05 (m, 2H), 3.48–3.55 (m, 2H), 3.73 (s, 6H), 4.09–4.23 (m, 2H), 6.88–6.90 (m, 3H), 7.65 (s, 1H), 7.75 (s, 1H), 8.15–8.27 (m, 1H), 9.09 (s, 1H);
81	346.0 (M+H) <sup>+</sup> , 278.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>•</sup> ) <sup>+</sup> , 177.1 ([M- C <sub>6</sub> H <sub>8</sub> N <sub>3</sub> S] <sup>•</sup> ) <sup>+</sup>	346.15810 [M+H] <sup>+</sup>	98.5	22.90	1.12 (dd, <i>J</i> = 3.7 Hz, 2.9 Hz, 2H), 1.57 (dd, <i>J</i> = 3.7 Hz, 2.9 Hz, 2H), 2.02–2.05 (m, 2H), 3.48–3.55 (m, 2H), 3.73 (s, 6H), 4.09–4.23 (m, 2H), 6.88–6.90 (m, 3H), 7.65 (s, 1H), 7.75 (s, 1H), 8.92 9.05(m, 1H), 9.09 (s, 1H)
83	251.1 (M+H) <sup>+</sup>				
85	320.2 (M+H) <sup>+</sup> , 252.2 ([M- C <sub>3</sub> H <sub>3</sub> N <sub>2</sub> ] <sup>•</sup> ) <sup>+</sup>	320.13550 [M+H] <sup>+</sup>	99.2	24.35	1.65–1.70 (m, 2H), 1.75–1.80 (m, 2H), 2.71–2.72 (m, 2H), 3.71 (s, 3H), 3.74 (s, 3H), 4.02–4.05 (m, 2H), 6.87–7.13 (m, 2H), 7.19 (s, 1H), 7.28–7.29 (m, 1H), 7.52 (s, 1H), 7.72 (s, 1H), 11.40 (s, 1H)