**Supplementary file 2.2.** **The summary of dose response assays (xL3 motility and L4 development) for 32 active compounds and cytotoxicity assessment.** The ‘half of the maximum inhibitory concentration’ (IC50) values of compounds and monepantel or moxidectin, expressed as mean IC50 ± standard error of mean for xL3 motility and toxicity on MCF10A cells, and IC50 ± standard deviation for L4 development. The seven candidate compounds are highlighted.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Compound(analogue)  | Chemical structure  | xL3 motility (IC50; µM) a  | L4development (IC50; µM) a | Cytotoxicity on MCF10A cells   |
| 24 h | 48 h | 72 h | 7 days | % cell density (at 50 µM) | IC50; µM |
| mqq 3-O-1 |   | 127.7 b | 13.79 ± 1.31 | 19.57 ± 5.27 | 1.81 ± 0.07 | 14.14± 0.64 | 4.87± 1.78 |
| mqq 3-O-9 |   | 35.30 ± 0.20 | 24.46 ± 4.54 | 18.62 ± 6.27 | 10.50 ± 1.78 | 4.32 ± 0.32 | 2.92 ± 0.62 |
| mqq 3-O-11 |   | 15.11 ± 4.25 | 4.921 ± 0.08 | 5.05 ± 0.67 | 2.49 ± 0.53 | 1.91 ± 0.30 | 2.18 ± 0.01 |
| mqq 3-O-13 |   | 20.70 ± 1.74 | 11.11 ± 3.72 | 7.27 ± 0.61 | 5.09 ± 0.32 | 1.86 ± 0.14 | 2.16 ± 0.03 |
| mqq 3-O-14 |   | nd | 19.53 ± 5.48 | 6.64 ± 4.64 | 3.32 ± 1.91 | 1.29 ± 0.01 | 2.16 ± 0.03 |
| mqq 3-S-1 |   | 22.80 ± 3.38 | 22.92 ± 5.47 | 10.58 ± 3.68 | 8.43 ± 0.36 | 4.81 ± 0.64 | 2.20 ± 0.03 |
| Zpx012 |   | 47.14 ± 3.09 | 33.1 b | 23.21 ± 4.43 | 18.18 ± 1.34 | 15.00 ± 0.56 | 5.25 ± 1.82 |
| Zpx016 |   | 41.5 b | 18.70 ± 1.02 | 17.67 ± 0.37 | 22.86 ± 0.65 | 14.89 ± 0.99 | 10.21 ± 1.76 |
| Zpx019 |   | nd | 11.18 ± 0.19 | 7.40 ± 1.22 | 4.28 ± 0.75 | 54.98 ± 19.88 | >50 |
| Zpx020 |   | nd | nd | 3.86 ± 0.28 | 7.24 ± 1.57 | 37.61 ± 17.25 | >50 |
| Zpx021 |   | nd | nd | nd | nd | 40.24 ± 9.05 | >50 |
| Zpx022 |   | nd | 10.62 ± 4.07 | 9.14 ± 3.33 | 13.98 ± 1.96 | 31.88 ± 9.69 | >50 |
| Zpx023 |   | nd | > 100 | 31.6 b | 13.89 ± 1.13 | 15.24 ± 0.96 | 23.54 ± 7.11 |
| Zpx024 |   | 25.26 ± 8.50 | 9.17 ± 2.60 | 3.2 b | 1.99 ± 0.04 | 31.84 ± 12.43 | 26.11 ± 3.92 |
| Zpx026 |   | 63.5 b | 22.35 ± 2.58 | 7.12 ± 1.46 | 5.72 ± 0.16 | 17.88 ± 0.49 | 24 ± 12.04 |
| Zpx027 |   | 9.79 ± 2.54 | 3.1 ± 0.01 | 1.22 ± 0.09 | 1.18 ± 0.30 | 15.53 ± 0.18 | 6.38 ± 3.29 |
| Zpx028 |   | 8.63 ± 0.90 | 2.9 b | 1.25 ± 0.36 | 0.57 ± 0.08 | 16.63 ± 4.21 | 16.50 ± 2.58 |
| Zpx029 |   | 26.93 ± 5.05 | 13.79 ± 5.21 | 6.10 ± 1.72 | 3.04 ± 1.26 | 16.57 ± 1.32 | 10.61 ± 2.48 |
| Zpx030 |   | nd | nd | 11.87 ± 5.91 | 16.80 ± 0.26 | 19.57 ± 0.45 | 23.35 ± 1.61 |
| Zpx031 |   | nd | 8.22 ± 1.80 | 8.75 ± 0.05 | 8.20 ± 1.15 | 11.87 ± 2.02 | 5.18 ± 1.06 |
| Zpx035 |   | nd | 5.80 ± 2.66 | 3.34 ± 0.27 | 3.51 ± 1.16 | 10.72 ± 1.18 | 2.89 ± 0.47 |
| Zpx040 |   | nd | 3.1 b  | 1.675 ± 0.66 | 1.58 ± 0.17 | 21.92 ± 4.97 | 35.7 b |
| Zpx050 |   | 51.52 ± 6.69 | 14.16 ± 1.78 | 4.82 ± 0.47 | 3.20 ± 0.01 | 14.20 ± 2.16 | 7.12 ± 0.09 |
| Zpx052 |   | nd | 22.55 ± 0.65 | 5.86 ± 3.71 | 4.73 ± 0.19 | 4.53 ± 0.17 | 2.95 ± 0.66 |
| Zpx054 |   | 40.6 b | 9.21 ± 2.76 | 11.43 ± 5.47 | 7.52 ± 1.01 | 9.99 ± 0.55 | 5.94 ± 1.28 |
| Zpx062 |   | 22.71 ± 0.84 | 18.71 ± 1.60 | 12.79 ± 1.22 | 8.44 ± 0.73 | 11.96 ± 0.38 | 3.38 ± 0.76 |
| Zpx063 |   | 48.13 ± 2.71 | 23.4 b | 5.20 ± 2.15  | 7.89 ± 0.99 | 14.46 ± 0.89 | 11.72 ± 4.78 |
| Zpx065 |   | 33.8 b | 24.52 ± 0.53 | 8.64 ± 4.15 | 10.31 ± 1.53 | 9.78 ± 0.49 | 2.96 ± 0.24 |
| Zpx079 |   | nd | nd | nd | 14.77 ± 9.08 | 16.35 ± 2.15 | 7.20 ± 1.59 |
| Zpx090 |   | nd | nd | nd | nd | 26.88 ± 9.49 | 45.0 b |
| zqq1726 |   | nd | 2.40 ± 0.08 | 1.37 ± 0.40 | 1.21 ± 0.05 | 13.48 ± 2.13 | 8.83 ± 3.44 |
| zqq1341 |   | nd | 13.49 ± 6.88 | 9.86 ± 4.77 | 3.27 ± 0.12 | 12.94 ± 0.85 | 18.2 b |
| Monepantel |  | 2.12 ± 0.55 | 0.76 ± 0.32 | 0.59 ± 0.01 | 0.43 ± 0.03 | 18.22 ± 2.93 | 32.8 b |
| Moxidectin c |  | 0.49 ± 0.31 | 0.19 ± 0.04 | 0.08 ± 0.02 | na | na | na |
| Doxorubicin c |  | na | na | na | na | 0.50 ± 0.30 | 2.17± 0.02 |

a IC50 values that could not be accurately determined using the log (inhibitor) *vs.* response-variable slope four parameters model are indicated as not determined (nd)

b Estimated from the relevant dose response graphs

c Not applicable