## P. aeruginosa MurD inhibition data

Data in blue, the compound did not impact upon the coupling system sufficiently to invalidate the assay with respect to estimation of MurD inhibition.
Data in light green, the compound was sufficiently active against the coupling system employed to invalidate the assay.
Will require re-assay in spectrophotometric methyl thioguanosine variant of the MurD assay.

| Original Hit | Structure | Compound | Average \% Inhibition | SD |
| :---: | :---: | :---: | :---: | :---: |
|  <br> AW17 <br> MurC (Pa) + MurD (Ec) + MurE (Pa + Ec) |  | OSA_001145 | 108.87 | 15.09 |
|  <br> AW53 <br> MurC (Pa) + MurD (Ec) + |  <br> Made by Yiwei Wang | OSA_001170 | 98.61 | 18.36 |
| MurE (Ec) |  | OSA_001165 | 95.01 | 9.05 |
|  |  | ADPCP | 92.35 | 4.29 |
|  <br> AW53 <br> MurC (Pa) + MurD (Ec) + MurE (Ec) |  | OSA_001164 | 89.39 | 9.79 |
|  <br> AW17 <br> MurC ( Pa ) $+\mathrm{MurD}(\mathrm{Ec})+$ MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) |  <br> Bought from Enamine | OSA_001143 | 89.25 | 0.66 |
|  <br> Compound 4 (Finlay MacLean) |  | OSA_001155 | 87.91 | 4.32 |
|  |  | ADPCP | 81.86 | 1.74 |
|  <br> AW53 <br> MurC ( Pa ) + MurD (Ec) + MurE (Ec) |  | OSA_001171 | 81.66 | 4.70 |


|  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> Made by Eve Carter | OSA_001160 | 81.11 | 12.73 |
| :---: | :---: | :---: | :---: | :---: |
|  |  | ADPCP | 79.46 | 1.48 |
|  <br> Compound 4 (Finlay MacLean) |  | OSA_001154 | 79.27 | 12.43 |
|  |  | ADPCP | 78.28 | 4.97 |
|  <br> Compound 4 (Finlay MacLean) |  | OSA_001153 | 74.98 | 3.07 |
|  |  | OSA_001172 | 72.69 | 6.22 |
| AW53 <br> MurC (Pa) + MurD (Ec) + <br> MurE (Ec) |  | OSA_001168 | 70.79 | 7.08 |
|  |  | OSA_001156 | 69.57 | 9.48 |
|  |  | OSA_001162 | 68.88 | 8.06 |
| AW53 <br> MurC (Pa) + MurD (Ec) + MurE (Ec) |  | OSA_001173 | 65.77 | 15.05 |
|  <br> AW5 <br> MurC + MurE (Pa + Ec) |  | OSA_001140 | 65.64 | 5.29 |
|  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> AW9 <br> Made by Eve Carter | OSA_001167 | 64.39 | 11.95 |
|  <br> AW17 <br> MurC ( Pa ) $+\mathrm{MurD}(\mathrm{Ec})+$ MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) |  <br> Bought from Enamine | OSA_001147 | 60.43 | 2.60 |
|  <br> AW53 <br> MurC (Pa) + MurD (Ec) + MurE (Ec) |  | OSA_001169 | 54.74 | 6.51 |


|  <br> AW8 MurC (Pa) + MurE (Ec) |  <br> Bought from Enamine | OSA_001134 | 49.07 | 2.18 |
| :---: | :---: | :---: | :---: | :---: |
|  <br> AW17 <br> MurC ( Pa ) $+\mathrm{MurD}(\mathrm{Ec})+$ MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) |  | OSA_001150 | 48.25 | 8.67 |
|  <br> AW17 <br> MurC ( Pa ) $+\mathrm{MurD}(\mathrm{Ec})+$ MurE $(\mathrm{Pa}+\mathrm{Ec})$ | Bought from Enamine | OSA_001148 | 47.26 | 3.72 |
|  |  | OSA_001133 | 46.87 | 5.54 |
|  <br> AW77 <br> MurC (Pa) + MurE (Ec) | Bought from Enamine | OSA_001137 | 39.47 | 4.91 |
|  <br> AW5 <br> MurC + MurE (Pa + Ec) |  | OSA_001144 | 38.85 | 8.03 |
|  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> Made by Eve Carter | OSA_001159 | 38.16 | 1.09 |
|  <br> AW5 <br> MurC + MurE (Pa + Ec) |  | OSA_001142 | 36.92 | 3.40 |
|  <br> AW8 <br> MurC (Pa) + MurE (Ec) |  <br> Bought from Enamine | OSA_001135 | 34.88 | 8.50 |


|  <br> AW17 <br> MurC ( Pa ) $+\mathrm{MurD}(\mathrm{Ec})+$ MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) |  | OSA_001151 | 30.88 | 4.02 |
| :---: | :---: | :---: | :---: | :---: |
|  <br> AW8 MurC ( Pa ) $+\mathrm{MurE}(\mathrm{Ec})$ |  <br> Bought from Enamine | OSA_001136 | 30.48 | 3.94 |
|  <br> AW9 <br> MurC + MurE (Pa+Ec) |  | OSA_001141 | 30.23 | 13.03 |
|  <br> Compound 4 (Finlay MacLean) |  | OSA_001149 | 28.87 | 5.02 |
|  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> Made by Eve Carter | OSA_001161 | 28.09 | 0.63 |
|  <br> AW49 <br> MurC ( Pa ) $+\mathrm{MurD}(\mathrm{Ec})+$ MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) |  | OSA_001152 | 27.78 | 5.11 |
|  <br> AW9 <br> MurC + MurE (Pa+Ec) |  | OSA_001157 | 24.11 | 2.41 |
|  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> Made by Eve Carter | OSA_001158 | 23.46 | 5.01 |
|  <br> M02 <br> MurC + MurE |  <br> Bought from Enamine | OSA_001132 | 22.67 | 2.11 |
|  <br> AW77 <br> MurC (Pa) + MurE (Ec) |  <br> Bought from Enamine | OSA_001138 | 21.75 | 8.64 |


|  <br> AW53 <br> MurC (Pa) + MurD (Ec) + MurE (Ec) |  <br> Made by Yiwei Wang | OSA_001166 | 10.83 | 0.60 |
| :---: | :---: | :---: | :---: | :---: |
|  <br> AW77 <br> MurC (Pa) + MurE (Ec) |  <br> Bought from Enamine | OSA_001139 | 8.48 | 6.43 |
|  <br> L06 MurD + MurE + MurC |  <br> Bought from Enamine | OSA_001131 | 5.04 | 0.98 |
|  <br> AW17 <br> MurC ( Pa ) + MurD (Ec) + MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) |  | OSA_001146 | 3.92 | 6.54 |
|  <br> Made by Ed Tse |  | OSA_001113 | 2.17 | 3.36 |
|  |  | DMSO | 0.00 | 4.45 |
|  |  | DMSO | 0.00 | 6.21 |
|  |  | DMSO | -0.05 | 3.37 |
|  <br> L06 MurD + MurE + MurC |  <br> Bought from Enamine | OSA_001130 | -0.58 | 1.75 |
|  |  | OSA_001114 | -0.80 | 5.03 |
|  |  | DMSO | -4.36 | 2.74 |

