P. aeruginosa MurE Inhibition Data

|  | Original Hit | Derivative's Structure | Compound | Average\% Inhibition |
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| All compounds exert >50\% inhibition of MurE. <br> Compounds in green exert >50\% Activity against MurD. |  <br> AW53 <br> MurC ( Pa ) +MurD ( Ec ) + MurE (Ec) |  | OSA_001172 | $78.0 \pm 8.4$ |
|  |  |  | OSA_001164 | $76.0 \pm 9.0$ |
|  |  <br> Compound 4 (Finlay MacLean) |  | OSA_001155 | $69.3 \pm 4.0$ |
|  |  <br> AW17 <br> MurC (Pa) + MurD (Ec) + MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) |  | OSA_001145 | $67.3 \pm 0.8$ |
|  |  <br> Compound 4 (Finlay MacLean) |  | OSA_001156 | $56.1 \pm 5.8$ |
|  |  <br> AW17 <br> MurC (Pa) + MurD (Ec) + MurE (Pa + Ec) |  | OSA_001147 | $55.9 \pm 6.3$ |
|  |  <br> Compound 4 (Finlay MacLean) |  | OSA_001153 | $55.0 \pm 5.6$ |
|  |  <br> M02 <br> MurC + MurE |  | OSA_001133 | $55.0 \pm 1.7$ |
|  |  <br> Compound 4 (Finlay MacLean) |  | OSA_001149 | $53.8 \pm 1.8$ |
|  |  |  | OSA_001169 | $52.8 \pm 0.3$ |


|  |  <br> AW17 <br> MurC (Pa) + MurD (Ec) + MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) | Bought from Enamine | OSA_001148 | $51.5 \pm 3.4$ |
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|  |  <br> AW53 <br> MurC (Pa) + MurD (Ec) + MurE (Ec) |  | OSA_001168 | $47.8 \pm 8.8$ |
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|  |  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> Made by Eve Carter | OSA_001160 | $47.2 \pm 9.7$ |
|  |  <br> AW8 <br> MurC (Pa) + MurE (Ec) |  <br> Bought from Enamine | OSA_001134 | $46.7 \pm 1.2$ |
|  |  <br> AW5 <br> MurC + MurE (Pa + Ec) |  | OSA_001144 | $44.8 \pm 4.1$ |
|  |  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> AW9 <br> Made by Eve Carter | OSA_001167 | $43.8 \pm 3.1$ |
|  |  <br> AW9 <br> MurC + MurE (Pa+Ec) |  | OSA_001141 | $43.2 \pm 4.2$ |
|  |  <br> AW49 <br> MurC (Pa) + MurD (Ec) + MurE (Pa + Ec) |  | OSA_001152 | $40.3 \pm 1.4$ |
|  |  <br> AW8 <br> $\operatorname{MurC}(\mathrm{Pa})+\mathrm{MurE}(\mathrm{Ec})$ |  <br> Bought from Enamine | OSA_001135 | $39.5 \pm 5.8$ |


|  |  <br> AW17 <br> MurC (Pa) + MurD (Ec) + MurE (Pa + Ec) |  | OSA_001150 | $38.1 \pm 3.4$ |
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|  |  <br> M02 <br> MurC + MurE |  <br> Bought from Enamine | OSA_001132 | $31.8 \pm 4.1$ |
|  |  |  <br> Bought from Enamine | OSA_001131 | $30.8 \pm 5.0$ |
|  |  <br> AW77 <br> MurC (Pa) + MurE (Ec) |  <br> Bought from Enamine | OSA_001137 | $28.2 \pm 6.7$ |
|  |  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> Made by Eve Carter | OSA_001158 | $27.3 \pm 11.0$ |
|  |  <br> AW8 <br> MurC ( Pa ) $+\mathrm{MurE}(\mathrm{Ec})$ |  <br> Bought from Enamine | OSA_001136 | $27.0 \pm 3.7$ |
|  |  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> Made by Eve Carter | OSA_001159 | $26.1 \pm 7.8$ |
|  |  <br> AW77 <br> MurC (Pa) + MurE (Ec) |  <br> Bought from Enamine | OSA_001138 | $24.0 \pm 5.6$ |
|  |  <br> AW17 <br> MurC ( Pa ) $+\mathrm{MurD}(\mathrm{Ec})+$ MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) |  | OSA_001151 | $22.2 \pm 3.4$ |
|  |  <br> AW9 <br> MurC + MurE (Pa+Ec) |  | OSA_001157 | $20.4 \pm 2.2$ |


|  |  <br> AW9 <br> MurC + MurE (Pa+Ec) |  <br> Made by Eve Carter | OSA_001161 | $15.2 \pm 14.6$ |
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|  |  <br> AW77 <br> $\operatorname{MurC}(\mathrm{Pa})+\mathrm{MurE}(\mathrm{Ec})$ |  <br> Bought from Enamine | OSA_001139 | $14.2 \pm 3.0$ |
|  |  <br> AW5 <br> MurC + MurE (Pa + Ec) |  | OSA_001142 | $12.6 \pm 12.3$ |
|  |  <br> AW17 <br> MurC ( Pa ) + MurD (Ec) + MurE ( $\mathrm{Pa}+\mathrm{Ec}$ ) |  | OSA_001146 | $7.9 \pm 5.2$ |


|  |  <br> MurD + MurE + MurC |  <br> Bought from Enamine | OSA_001130 | $-8.1 \pm 9.5$ |
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|  |  <br> AW53 <br> MurC ( Pa ) +MurD ( Ec ) + MurE (Ec) |  <br> Bought from Enamine | OSA_001166 | $-11.8 \pm 4.8$ |
|  | Competition Compounds |  <br> Made by Ed Tse | OSA_001113 | $-23.5 \pm 17.0$ |
|  |  |  | OSA_001114 | $-25.0 \pm 18.5$ |

