**Supplemental Material**

# Discovery of Novel Bacterial Elongation Condensing Enzyme Inhibitors by Virtual Screening

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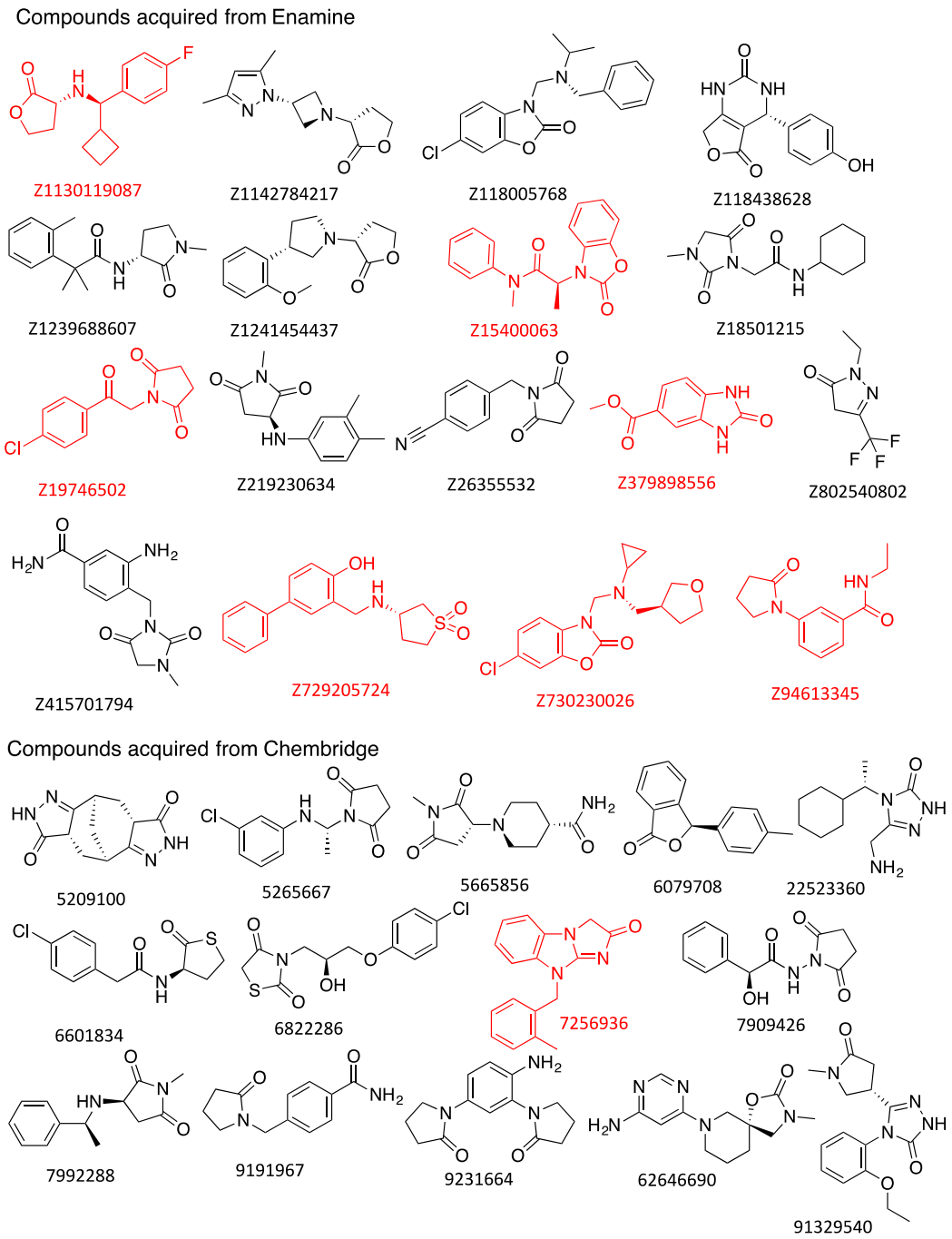
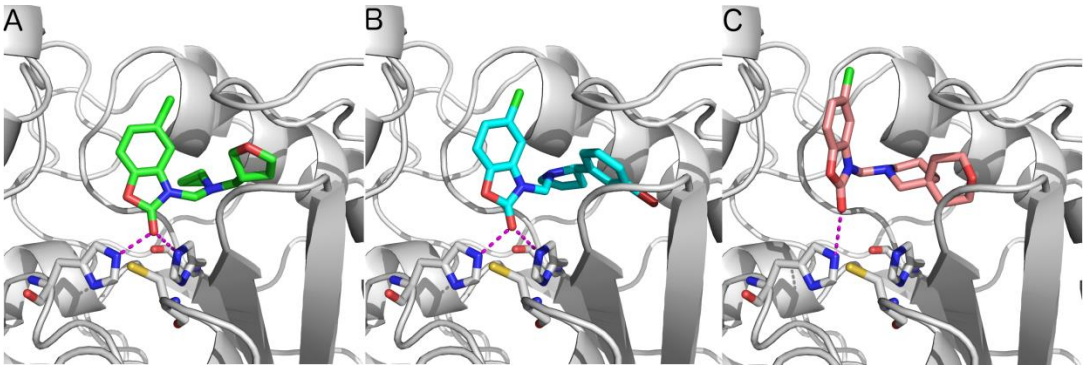
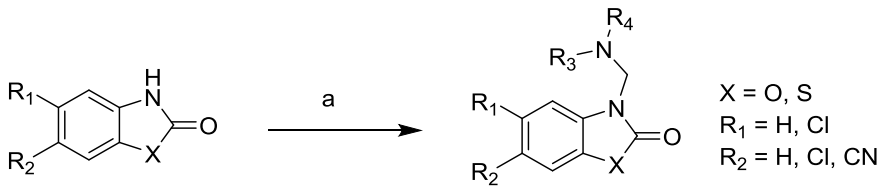



Figure S1 Cherry-picked commercial compounds with catalog numbers from virtual screen acquired from Enamine and Chembridge. Compounds highlighted in red were hits in NMR wLOGSY.




Supplemental Figure S2: Binding modes of compound **6 (A)**, **27 (B)** and **11 (C)**. Dashed lines are hydrogen bonds.

Scheme-S1




Reagents: a) $R_3R_4NH$, $H_2CO$, MeOH, Reflux, 1h

**$^1$H NMR spectra for synthesis compounds:**

Compound **7**, 6-chloro-3-((methyl((tetrahydro-2H-pyran-4-yl)methyl)amino)methyl) benzo[d]oxazol-2(3H)-one

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.26 (d, *J* = 1.9 Hz, 1H), 7.19 (dd, *J* = 8.4, 1.9 Hz, 1H), 7.03 (d, *J* = 8.3 Hz, 1H), 4.63 (s, 2H), 3.97 (ddd, *J* = 11.7, 4.6, 2.1 Hz, 2H), 3.39 (td, *J* = 11.8, 2.1 Hz, 2H), 2.45 (d, *J* = 7.3 Hz, 2H), 2.40 (s, 3H), 1.87 – 1.72 (m, 1H), 1.69 – 1.58 (m, 2H), 1.30 – 1.15 (m, 2H).

Compound **8**, 6-chloro-3-((methyl(2-morpholinopropyl)amino)methyl) benzo[d]oxazol-2(3H)-one

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.16 (t, *J* = 1.5 Hz, 1H), 7.10 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.04 (d, *J* = 8.4 Hz, 1H), 4.71 – 4.42 (m, 2H), 3.76 – 3.45 (m, 4H), 2.86 – 2.61 (m, 2H), 2.61 – 2.22 (m, 8H), 0.92 (d, *J* = 6.2 Hz, 3H).

Compound **10**, 3-((9-oxa-2-azaspiro[5.5]undecan-2-yl)methyl)-6-chlorobenzo[d]oxazol-2(3H)-one

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.13 (m, 2H), 7.02 (dd, *J* = 8.98, 11.49 Hz, 1H), 4.61 (s, 2H), 3.88 – 3.35 (m, 4H), 2.63 (s, 2H), 2.49 (s, 2H), 1.80 – 1.22 (m, 8H).

Compound **11**, 3-((9-oxa-2-azaspiro[5.5]undecan-2-yl)methyl)-5-chlorobenzo[d]oxazol-2(3H)-one

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.14 – 6.95 (m, 3H), 4.49 (s, 2H), 3.67 – 3.40 (m, 4H), 2.54 (t, *J* = 5.3 Hz, 2H), 2.40 (s, 2H), 1.59 – 1.50 (m, 2H), 1.50 – 1.36 (m, 4H), 1.35 – 1.27 (m, 2H).

Compound **12**, 6-chloro-3-((methyl(2-(pyrrolidin-1-yl)ethyl)amino)methyl) benzo[d]oxazol-2(3H)-one

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.15 (d, *J* = 1.9 Hz, 1H), 7.08 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.04 (d, *J* = 8.3 Hz, 1H), 4.61 (s, 2H), 2.72 (t, *J* = 7.0 Hz, 2H), 2.67 – 2.56 (m, 2H), 2.56 – 2.43 (m, 4H), 2.35 (s, 3H), 1.86 – 1.61 (m, 4H).

Compound **13**, 6-chloro-3-((methyl((1-methylpyrrolidin-3-yl)methyl)amino)methyl) benzo[d]oxazol-2(3H)-one

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.15 (d, *J* = 1.93 Hz, 1H), 7.12 – 7.06 (m, 1H), 6.98 (d, *J* = 8.37 Hz, 1H), 4.55 (s, 2H), 2.65 – 2.33 (m, 6H), 2.34 – 2.11 (m, 7H), 1.92 (dddd, *J* = 5.42, 7.55, 8.94, 12.92 Hz, 1H), 1.50 – 1.29 (m, 1H).

Compound **17**, 6-chloro-3-((cyclopropyl(3-methoxybenzyl)amino)methyl) benzo[d]oxazol-2(3H)-one

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.14 (t, *J* = 7.83 Hz, 1H), 7.10 (d, *J* = 1.96 Hz, 1H), 7.02 (dd, *J* = 1.92, 8.39 Hz, 1H), 6.84 – 6.75 (m, 3H), 6.72 (ddd, *J* = 0.99, 2.67, 8.26 Hz, 1H), 4.63 (s, 2H), 3.81 (s, 2H), 3.72 (s, 3H), 2.01 (tt, *J* = 3.13, 6.53 Hz, 1H), 0.64 – 0.48 (m, 2H), 0.39 (qt, *J* = 2.21, 4.91 Hz, 2H).

Compound **18**, 5-chloro-3-(((3-hydroxybenzyl)(methyl)amino)methyl)benzo[d]oxazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.17 – 7.10 (m, 1H), 7.07 – 6.98 (m, 2H), 6.89 (t, *J* = 1.3 Hz, 1H), 6.82 – 6.66 (m, 3H), 4.55 (d, *J* = 1.1 Hz, 2H), 3.60 (s, 2H), 2.32 (d, *J* = 1.2 Hz, 3H).

Compound **19**, 6-chloro-3-((cyclopropyl(pyridin-3-ylmethyl)amino)methyl) benzo[d]oxazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 8.60 – 8.33 (m, 2H), 7.59 (ddd, *J* = 1.48, 2.25, 7.87 Hz, 1H), 7.19 – 7.11 (m, 2H), 7.07 (dd, *J* = 1.94, 8.38 Hz, 1H), 6.90 (d, *J* = 8.35 Hz, 1H), 4.65 (s, 2H), 3.87 (s, 2H), 2.01 (tt, *J* = 3.65, 6.41 Hz, 1H), 0.64 – 0.48 (m, 2H), 0.41 (td, *J* = 2.61, 3.80 Hz, 2H).

Compound **20**, 6-chloro-3-((cyclopropyl(pyridin-2-ylmethyl)amino)methyl) benzo[d]oxazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 8.48 (ddd, *J* = 0.94, 1.86, 4.97 Hz, 1H), 7.57 (td, *J* = 1.81, 7.66 Hz, 1H), 7.24 (dt, *J* = 1.06, 7.81 Hz, 1H), 7.15 – 7.08 (m, 2H), 7.05 (dd, *J* = 1.91, 8.36 Hz, 1H), 6.98 (d, *J* = 8.37 Hz, 1H), 4.80 (s, 2H), 4.03 (s, 2H), 2.07 (tt, *J* = 3.69, 6.50 Hz, 1H), 0.58 – 0.25 (m, 4H).

Compound **23**, 6-chloro-3-((2-phenylpiperidin-1-yl)methyl)benzo[d]oxazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.28 – 7.04 (m, 8H), 6.96 (d, *J* = 8.4 Hz, 1H), 4.70 – 4.47 (m, 2H), 3.15 – 2.86 (m, 2H), 2.72 (t, *J* = 11.4 Hz, 1H), 2.31 (dt, *J* = 15.3, 11.4 Hz, 2H), 1.84 (ddd, *J* = 12.2, 4.7, 2.7 Hz, 1H), 1.79 – 1.48 (m, 2H), 1.35 (qd, *J* = 12.5, 4.0 Hz, 1H).

Compound **24**, 5-chloro-3-((2-phenylpiperidin-1-yl)methyl)benzo[d]oxazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.27 (m, 2H), 7.23 (td, *J* = 6.4, 5.9, 2.6 Hz, 3H), 7.19 – 7.08 (m, 3H), 4.66 (s, 2H), 3.27 – 2.99 (m, 2H), 2.82 (dq, *J* = 11.8, 5.9, 3.9 Hz, 1H), 2.55 – 2.30 (m, 2H), 1.95 (ddd, *J* = 12.2, 4.6, 2.6 Hz, 1H), 1.85 (dt, *J* = 13.4, 3.4 Hz, 1H), 1.80 – 1.56 (m, 2H), 1.46 (qd, *J* = 12.4, 4.0 Hz, 1H).

Compound **25**, 6-chloro-3-((2-(3-methoxyphenyl)pyrrolidin-1-yl)methyl)benzo[d]oxazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.18 (d, *J* = 9.3 Hz, 1H), 7.06 (d, *J* = 1.9 Hz, 1H), 6.99 (dd, *J* = 8.4, 2.0 Hz, 1H), 6.86 (dt, *J* = 7.4, 1.4 Hz, 2H), 6.77 – 6.69 (m, 1H), 6.58 (d, *J* = 8.4 Hz,

1H), 4.63 – 4.46 (m, 2H), 3.72 (s, 3H), 3.57 (t, *J* = 8.0 Hz, 1H), 3.23 (t, *J* = 8.9 Hz, 1H), 2.70 (q, *J* = 8.6 Hz, 1H), 2.20 – 2.05 (m, 1H), 1.99 – 1.57 (m, 3H).

Compound **26**, 5-chloro-3-((2-(3-methoxyphenyl)pyrrolidin-1-yl)methyl)benzo[d]oxazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.23 – 7.16 (m, 1H), 6.95 (d, *J* = 1.3 Hz, 2H), 6.88 (dd, *J* = 7.1, 1.5 Hz, 2H), 6.79 – 6.71 (m, 1H), 6.62 (s, 1H), 4.52 (q, *J* = 13.1 Hz, 2H), 3.74 (s, 3H), 3.56 (t, *J* = 7.9 Hz, 1H), 3.30 – 3.16 (m, 1H), 2.69 (q, *J* = 8.6 Hz, 1H), 2.23 – 2.06 (m, 1H), 2.02 – 1.60 (m, 3H)

Compound **27**, 3-((2-(3-bromophenyl)pyrrolidin-1-yl)methyl)-5-chlorobenzo[d]oxazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.45 (q, *J* = 1.7 Hz, 1H), 7.30 (ddt, *J* = 7.9, 2.8, 1.3 Hz, 1H), 7.25 – 7.17 (m, 1H), 7.12 (td, *J* = 7.7, 1.4 Hz, 1H), 7.00 – 6.91 (m, 2H), 6.67 (s, 1H), 4.53 (qd, *J* = 13.2, 1.5 Hz, 2H), 3.60 (t, *J* = 7.9 Hz, 1H), 3.36 – 3.12 (m, 1H), 2.72 (q, *J* = 8.6, 8.1 Hz, 1H), 2.27 – 2.04 (m, 1H), 2.00 – 1.83 (m, 1H), 1.83 – 1.71 (m, 1H), 1.71 – 1.59 (m, 1H).

Compound **28**, 5-chloro-3-((2-phenylazetidin-1-yl)methyl)benzo[d]oxazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.30 (m, 2H), 7.25 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 2H), 7.22 – 7.16 (m, 1H), 6.97 (dd, *J* = 1.8, 1.2 Hz, 2H), 6.81 (dd, *J* = 1.7, 0.8 Hz, 1H), 4.46 (s, 2H), 4.27 (t, *J* = 8.1 Hz, 1H), 3.49 – 3.11 (m, 2H), 2.26 – 2.16 (m, 1H), 2.14 – 2.01 (m, 2H).

Compound **29**, 3-((2-(3-bromophenyl)pyrrolidin-1-yl)methyl)-2-oxo-2,3-dihydrobenzo[d]oxazole-5-carbonitrile
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.43 (m, 1H), 7.41 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.37 – 7.31 (m, 1H), 7.22 (dt, *J* = 7.7, 1.5 Hz, 1H), 7.19 – 7.13 (m, 2H), 6.99 (dd, *J* = 1.7, 0.5 Hz, 1H), 4.65 (d, *J* = 3.1 Hz, 2H), 3.64 (t, *J* = 7.9 Hz, 1H), 3.34 (ddd, *J* = 9.0, 7.6, 3.1 Hz, 1H), 2.78 (td, *J* = 8.8, 7.9 Hz, 1H), 2.37 – 2.15 (m, 1H), 2.11 – 1.93 (m, 1H), 1.93 – 1.81 (m, 1H), 1.81 – 1.67 (m, 1H).

Compound **30**, 3-((2-(3-bromophenyl)pyrrolidin-1-yl)methyl)-5-chlorobenzo[d]thiazol-2(3H)-one
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.46 (t, *J* = 1.8 Hz, 1H), 7.38 – 7.33 (m, 1H), 7.29 – 7.20 (m, 2H), 7.17 (t, *J* = 7.8 Hz, 1H), 7.09 (dd, *J* = 8.3, 2.0 Hz, 1H), 6.85 (d, *J* = 2.0 Hz, 1H), 4.79 – 4.55 (m, 2H), 3.63 (t, *J* = 7.9 Hz, 1H), 3.37 – 3.20 (m, 1H), 2.74 (td, *J* = 9.1, 7.9 Hz, 1H), 2.33 – 2.12 (m, 1H), 2.02 – 1.77 (m, 2H), 1.77 – 1.65 (m, 1H).