Supporting Information

Design and Evaluation of New Quinazolin-4(3*H*)-one Derived PqsR Antagonists as Quorum Sensing Quenchers in *Pseudomonas aeruginosa*.

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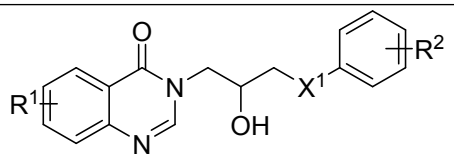
Table S1. Structures and activities of commercial analogues of **22**.



ID	R^1	R^2	X^1	Remaining activity in PAO1-L at 10 μM (RA%)	IC_{50} μM
Z197489918	7-F	*p*-$COCH_2CH_3$	O	NA	-
Z197489566	7-Cl	*p*-Br	O	NA	-
Z197486244	6-Br	*p*-Cl	O	NA	-
Z197490172	7-F	*p*-$COCH_2CH_3$	O	NA	-
Z197486158	6-Br	*o*-Cl	OCH_2	NA	-
Z197487796	6-Cl	*p*-Cl	OCH_2CH_2O	NA	-
Z281175654	6-Cl, 7-NO_2	*p*-Cl	O	NA	-
Z281933246	6,7-Cl	*p*-Cl	OCH_2	NA	-
ZZ281175446	6-NO_2,7-Cl	*O*-CH_3	O	NA	-
Z197486322	6-Br	*o*-OCH_3, *p*-CH_2CHCH_2	O	NA	-

Z281162800	6,7-OMe	*m*-$COCH_3$	O	NA	-
Z197489948	7-F	*p*-$CH_2CH_2COCH_3$	O	NA	-
Z197490034	7-F	*p*-CH_2CH_3	O	NA	-
Z197489906	7-F	*o*-F	OCH_2	NA	-
Z197487738	6-Cl	*p*-$COCH_2CH_3$	O	NA	-

* NA denotes no activity observed

Table S2. Crystallographic data collection and refinement statistics:

Data collection	PqsR – 61 Complex	PqsR – 40 Complex
Beamline	I04	I04
Wavelength (Å)	0.9159	0.9159
Space group	P 6_5 2 2	P 6_5 2 2
a ,b, c (Å)	119.79, 119.79, 116.5	120.43, 120.43 115.78
α, β, γ (°)	90, 90, 120	90, 90, 120
Resolution	77.47 – 2.65	104.3 – 3.00
No. of unique reflections	14874	10259
R_{merge} (%)	8.9 (99)	11.1 (225.2)
Mean I/Sig(I)	10.7 (2)	17.3 (1.2)
Completeness	99.9 (100)	99.1 (99.5)
Redundancy	9.3 (9.9)	18.6 (18)
CC½	0.806 (0.676)	1.000 (0.887)
Refinement		
Resolution range (Å)	77.59 – 2.65	77.61 - 3.00
R/Rfree	0.23 / 0.26	0.22 / 0.27
Mean B-Factor (Å)	108.3	120.8
r.m.s.d bond lengths (Å)	0.0038	0.0034
r.m.s.d bond angles (°)	1.32	1.300
Ramachandran plot statistics (%)		
Preferred regions	95.52	97.51
Outliers	0	0.5
PDB ID	7O2T	7O2U

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                    (1-60)
PAO1                MPIHNLNHVNMFLQVIASGSISSAARILRKSHTAVSSAVSNLEIDLCVELVRRDGYKVEP
LESB58              MPIHNLNHVNMFLQVIASGSISSAARILRKSHTAVSSAVSNLEIDLCVELVRRDGYKVEP
197S020911BSL_PA3   MPIHNLNHVNMFLQVIASGSISSAARILRKSHTAVSSAVSNLEIDLCVELVRRDGYKVEP
PA14                MPIHNLNHVNMFLQVIASGSISSAARILRKSHTAVSSAVSNLEIDLCVELVRRDGYKVEP
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                    (61-120)
PAO1                TEQALRLIPYMRSLLNYQQLIGDIAFNLNKGPRNLRVLLDTAIPPSFCDTVSSVLLDDFN
LESB58              TEQALRLIPYMRSLLNYQQLIGDIAFNLNKGPRNLRVLLDTAIPPSFCDTVSSVLLDDFN
197S020911BSL_PA3   TEQALRLIPYMRSLLNYQQLIGDIAFNLNKGPRNLRVLLDTAIPPSFCDTVSSVLLDDFN
PA14                TEQALRLIPYMRSLLNYQQLIGDIAFNLNKGPRNLRVLLDTAIPPSFCDTVSSVLLDDFN
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                    (121-180)
PAO1                MVSLIRTSPADSLATIKQDNAEIDIAITIDEELKISRFNQCVLGYTKAFVVAHPQHPLCN
LESB58              MVSLIRTSPADSLATIKQDNAEIDIAITIDEELKISRFNQCVLGYTKAFVVAHPQHPLCN
197S020911BSL_PA3   MVSLIRTSPADSLATIKQDNAEIDIAITIDEELKISRFNQCVLGYTKAFVVAHPQHPLCN
PA14                MVSLIRTSPADSLATIKQDNAEIDIAITIDEELKISRFNQCVLGYTKAFVVAHPQHPLCN
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                    (181-240)
PAO1                ASLHSIASLANYRQISLGSRSGQHSNLLRPVSDKVLFVENFDDMLRLVEAGVGWGIAPHY
LESB58              ASLHSIASLANYRQISLGSRSGQHSNLLRPVSDKVLFVENFDDMLRLVEAGVGWGIAPHY
197S020911BSL_PA3   ASLHSIASLANYRQISLGSRSGQHSNLLRPVSDKVLFVENFDDMLRLVEAGVGWGIAPHY
PA14                ASLHSIASLANYRQISLGSRSGQHSNLLRPVSDKVLFVENFDDMLRLVEAGVGWGIAPHY
                    ************************************************************

                    (241-300)
PAO1                FVEERLRNGTLAVLSELYEPGGIDTKVYCYYNTALESERSFLRFLESARQRLRELGRQRF
LESB58              FVEERLRNGTLAVLSELYEPGGIDTKVYCYYNTALESERSFLRFLESARQRLRELGRQRF
197S020911BSL_PA3   FVEERLRNGTLAVLSELYEPGGIDTKVYCYYNTALESERSFLRFLESARQRLRELGRQRF
PA14                FVEERLRNGTLAVLSELYEPGGIDTKVYCYYNTALESERSFLRFLESARQRLRELGRQRF
                    ************************************************************

                    (300-333)
PAO1                DDAPAWQPSIVETAQRRSGPKALAYRQRAAPEX
LESB58              DDAPAWQPSIVETAQRRSGPKALAYRQRAAPEX
197S020911BSL_PA3   DDAPAWQPSIVETAQRRSGPKALAYRQRAAPEX
PA14                DDAPAWQPSIVETVQRRSGPKALAYRQRAAPEX
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Figure S1. PqsR sequence alignment in tested strains.