

Table S1. List of predicted LasR inhibitors subjected to wet-lab assay

Sr. No.	Lab ID	Manufacturer's Code	Compound Name	Compound Formula	Molecular Weight	PubChem ID
1	G1	Z30981775	N-(3-chloro-4-cyanophenyl)-2-[4-(2-chlorophenyl)piperazin-1-yl]acetamide	C ₁₉ H ₁₈ Cl ₂ N ₄ O	389.278	2100251
2	G2	Z65195564	2-[2-(3,4-dihydro-2H-1,5-benzodioxepin-7-yl)pyrrolidin-1-yl]-N-(4-fluorophenyl)acetamide	C ₂₁ H ₂₃ FN ₂ O ₃	370.417	17497500
3	G3	Z212728858	2-[[4-(4-propoxybenzoyl)piperazin-1-yl]methyl]-3,4-dihydroquinazolin-4-one	C ₂₃ H ₂₆ N ₂ O ₃	406.477	136019073
4	G4	Z221514312	2-[4-(4-phenylpiperazine-1-carbonyl)piperidin-1-yl]-1,3-benzoxazole	C ₂₃ H ₂₆ N ₄ O ₂	390.478	25333627
5	G5	Z354444420	2-[2-(1,2,3,4-tetrahydroisoquinolin-2-yl)ethyl]-2H,3H-[1,2,4]triazolo[4,3-a]pyridin-3-one	C ₁₇ H ₁₈ N ₄ O	294.351	42954882
6	G6	Z400859658	methyl 5-[[3-(1,3-benzoxazol-2-yl)piperidin-1-yl]methyl]-3-methylfuran-2-carboxylate	C ₂₀ H ₂₂ N ₂ O ₄	354.399	45886710
7	G7	Z299619614	3-(phenylamino)-1-[4-(1,3-thiazol-2-yl)piperazin-1-yl]propan-1-one	C ₁₆ H ₂₀ N ₄ OS	316.421	51076608
8	G8	Z926917134	N-[(1-benzyl-1H-pyrazol-4-yl)methyl]-3,4-dihydro-2H-1-benzopyran-4-amine hydrochloride	C ₂₀ H ₂₂ ClN ₃ O	355.861	47010164
9	G9	Z955949446	2-(4-[[1-(3-fluorophenyl)-1H-pyrazol-3-yl]methyl]-1,4-diazepan-1-yl)-1-(pyrrolidin-1-yl)ethan-1-one	C ₂₁ H ₂₈ FN ₃ O	385.478	71935069
10	G10	Z1426094174	[1-(3-bromo-4-methoxyphenyl)ethyl][(5-methylpyridin-2-yl)methyl]amine	C ₁₆ H ₁₉ BrN ₂ O	353.238	75539664
11	G11	Z1625994950	methyl 4-[[4-(4-methylbenzoyl)piperazin-1-yl]methyl]-1H-pyrrole-2-carboxylate	C ₁₉ H ₂₃ N ₃ O ₃	341.404	75518332
12	G12	Z1250668201	N-[[1-(1H-1,3-benzodiazol-2-yl)methyl]piperidin-4-yl]-3-(difluoromethoxy)benzamide	C ₂₁ H ₂₂ F ₂ N ₄ O ₂	400.421	86777812
13	G13	Z989721494	1-[[3-(4-chlorophenyl)-1,2-oxazol-5-yl]methyl]-4-(1-methyl-1H-pyrazol-5-yl)piperidine	C ₁₉ H ₂₁ ClN ₄ O	356.849	100667054
14	G14	Z104586200	1-[4-(2-methoxyphenyl)piperazin-1-yl]-2-[methyl(phenyl)amino]ethan-1-one	C ₂₀ H ₂₅ N ₃ O ₂	339.431	8241234
15	G15	Z1896945496	1-(4-fluorophenyl)-3-[[3-(3-methoxy-4-methylphenyl)methyl]piperidin-4-yl]urea	C ₂₁ H ₂₆ FN ₃ O ₂	371.448	119050072
16	G16	Z740067852	1-(6-chloroimidazo[1,2-a]pyridin-2-yl)methyl-4-(5-methylthiophene-2-carbonyl)piperazine	C ₁₈ H ₁₉ ClN ₄ OS	374.887	47064516
17	G17	Z1082829664	2-[4-(2,5-dimethylphenoxy)piperidin-1-yl]-N-(pyridin-3-yl)acetamide	C ₂₀ H ₂₈ N ₃ O ₂	339.431	51135865
18	G18	Z1084397894	2-(1-methyl-2,3,4,5-tetrahydro-1H-1,4-benzodiazepin-4-yl)-N-(1,3,5-trimethyl-1H-pyrazol-4-yl)acetamide	C ₁₈ H ₂₈ N ₃ O	327.424	53570170
19	G19	Z1212781307	N-[[2-(4-ethylphenyl)ethyl]piperidin-4-yl]-1-methyl-1H-pyrazole-4-carboxamide	C ₂₀ H ₂₈ N ₄ O	340.462	56791313
20	G20	Z241931598	1-[[4-(cyano-2-fluorophenyl)methyl]-N-(5-methyl-1,2-oxazol-3-yl)piperidine-4-carboxamide	C ₁₈ H ₁₉ FN ₃ O ₂	342.367	32743075
21	G21	Z1080685796	6-[[1-((2-hydroxyethyl)-3,5-dimethyl-1H-pyrazol-4-yl)methyl]amino]ethyl]-1,2,3,4-tetrahydroquinolin-2-one hydrochloride	C ₁₉ H ₂₇ ClN ₂ O ₂	378.896	47617575
22	G22	Z1262446645	methyl 1-[[1-((imidazo[1,2-a]pyridin-3-yl)methyl)piperidin-4-yl]-1H-pyrrole-2-carboxylate	C ₁₉ H ₂₂ N ₄ O ₂	338.403	71873709
23	G23	Z1415906953	N-(3-fluorophenyl)-2-[[4-[[1-(4-hydroxy-6-methylpyrimidin-2-yl)ethyl]piperazin-1-yl]propanamide	C ₂₀ H ₂₆ FN ₃ O ₂	387.451	136231938
24	G24	Z991005820	4-[[3-(3-oxo-3,4-dihydroquinoxalin-2-yl)methyl]propyl]amino)methyl]benzotrile	C ₂₀ H ₂₀ N ₄ O	332.399	86774534
25	G25	Z130191792	1-[[2-(4-acetyl-3,5-dimethyl-1H-pyrol-2-yl)-2-oxoethyl]piperidin-4-yl]-2,3-dihydro-1H-1,3-benzodiazol-2-one	C ₂₂ H ₂₆ N ₄ O ₃	394.466	9450455
26	G26	Z105310536	N-(3-bromo-4-methylphenyl)-2-[[1-methyl-1H,2H,3H,4H-pyrrolo[1,2-a]pyrazin-2-yl]acetamide	C ₁₇ H ₂₀ BrN ₃ O	362.264	17469264
27	G27	Z991009968	1-[4-(4-fluorophenyl)piperazin-1-yl]-2-[[5H,6H,7H,8H-imidazo[1,2-a]pyrazin-7-yl]ethan-1-one	C ₁₈ H ₂₂ FN ₅ O	343.398	86774596
28	G28	Z102814326	[2-(2-methoxy-5-methylphenyl)ethyl][(2-phenyl-2H-1,2,3-triazol-4-yl)methyl]amine	C ₁₉ H ₂₂ N ₄ O	322.404	8851263
29	G29	Z52740722	4-[[2-(4-(2-phenoxyethyl)piperazin-1-yl]propanamido]benzamide	C ₂₂ H ₂₈ N ₄ O ₃	396.482	16266558
30	G30	Z196076630	1-((7-chloro-4-oxo-4H-pyrido[1,2-a]pyrimidin-2-yl)methyl)-N-phenylpiperidine-3-carboxamide	C ₂₁ H ₂₁ ClN ₄ O ₂	396.870	18125294
31	G31	Z57052975	2-[[2-(dimethylamino)-2-phenylethyl]amino]-N-(3-fluoro-4-methylphenyl)acetamide; oxalic acid	C ₂₁ H ₂₆ FN ₃ O ₃	419.446	16246086
32	G32	Z2436905648	(2R)-2-methyl-4-(5-methyl-1H-pyrazole-3-carbonyl)-1-[2-(3-methylpyridin-4-yl)ethyl]piperazine	C ₁₈ H ₂₅ N ₅ O	327.424	138001282
33	G33	Z106911468	2-[[1-(3,4-dihydro-2H-1,5-benzodioxepin-7-yl)-2-methylpropyl]amino]-N-(5-methyl-1,2-oxazol-3-yl)acetamide	C ₁₉ H ₂₅ N ₃ O ₄	359.419	17506266
34	G34	Z1217399392	N-[[1-(1-phenylethyl)piperidin-4-yl]indolizine-2-carboxamide	C ₂₂ H ₂₅ N ₃ O	347.453	126779988
35	G35	Z729867922	N-[[2-[[5-methylimidazo[1,2-a]pyridin-2-yl)methyl]-1,2,3,4-tetrahydroisoquinolin-5-yl]acetamide	C ₂₀ H ₂₂ N ₄ O	334.414	71939672
36	G36	Z990493794	N-(5-chloropyridin-2-yl)-1-[[1-(ethyl-1H-imidazol-2-yl)methyl]piperidine-4-carboxamide	C ₁₇ H ₂₂ ClN ₅ O	347.842	51104657
37	G37	Z2036909608	2-[[3-methyl-4-oxo-3H,4H,5H,6H,7H,8H-pyrido[3,4-d]pyrimidin-7-yl]-N-(2,4,6-trimethylphenyl)acetamide	C ₁₉ H ₂₄ N ₄ O ₂	340.419	100765307
38	G38	Z89293640	6-chloro-2-[4-(diphenylmethyl)piperazine-1-carbonyl]-4H-chromen-4-one	C ₂₇ H ₂₃ ClN ₂ O ₃	458.936	23605545
39	G39	Z1332352764	2-[[4-[[1-(pyridin-2-yl)ethyl]piperazine-1-carbonyl]-1H-indole	C ₂₀ H ₂₂ N ₄ O	334.414	136512338
40	G40	Z3480644988	N-(2-[[2-(chloro-5-hydroxyphenyl)methyl]amino]propyl)-1-ethyl-1H-pyrrole-2-carboxamide	C ₁₈ H ₂₄ ClN ₃ O ₂	349.855	Not listed
41	G41	Z650877888	2-[[1-(2-chlorophenyl)ethyl](methyl)amino]methyl]-4H-pyrido[1,2-a]pyrimidin-4-one	C ₁₈ H ₁₈ ClN ₃ O	327.808	47057126
42	G42	Z961312656	N-[[1-[[2-(3-dihydro-1,4-benzodioxin-5-yl)methyl]piperidin-4-yl]-4-methyl-1,3-thiazole-5-carboxamide	C ₁₉ H ₂₃ N ₃ O ₃ S	373.469	49448407
43	G43	Z90623639	[(2-butyl-1-benzofuran-3-yl)methyl][(1,2,4)triazolo[4,3-a]pyridin-3-yl)methyl]amine	C ₂₀ H ₂₂ N ₄ O	334.414	47009098
44	G44	Z1169074483	3-[[4-[[1-methyl-1H-imidazol-2-yl)methyl]piperazin-1-yl]-1-phenylpyrrolidin-2-one	C ₁₉ H ₂₅ N ₃ O	339.434	121528088
45	G45	Z2208342824	(3S,4R)-1-[2-(4-oxo-3,4-dihydroquinazolin-2-yl)ethyl]-4-phenylpyrrolidine-3-carbonitrile	C ₂₁ H ₂₀ N ₄ O	344.409	137873383
46	G46	Z44599754	4-[[1,3-benzothiazol-2-yl)methyl]-N-(4-fluorophenyl)piperazine-1-carboxamide	C ₁₉ H ₁₉ FN ₃ O ₂	370.443	17416320
47	G47	Z2996734799	2-[[4-(2,3-dimethylphenyl)-1,2,3,6-tetrahydropyridin-1-yl)methyl]-1,3-oxazole-4-carboxylic acid	C ₁₈ H ₂₀ N ₂ O ₃	312.363	138021503
48	G48	Z147056328	7-[[4-(5-bromo-2-fluorobenzoylethyl)piperazin-1-yl]methyl]-5H-[1,3]thiazolo[3,2-a]pyrimidin-5-one	C ₁₈ H ₁₆ BrFN ₄ O ₂ S	451.312	42920622
49	G49	Z1171728251	N-[[1,4-dimethylpiperazin-2-yl)methyl]-5-methyl-2-phenyl-1,3-oxazole-4-carboxamide	C ₁₈ H ₂₄ N ₄ O ₂	328.408	53586427
50	G50	Z1139434605	2-[[3-methyl-5H,6H,7H,8H-[1,2,4]triazolo[4,3-a]pyrazin-7-yl]-1-(3-phenyl-4,5-dihydro-1H-pyrazol-1-yl)ethan-1-one	C ₁₇ H ₂₀ N ₆ O	324.380	53576067
51	G51	Z364541138	N-[[2-(1,2,3,4-tetrahydroisoquinolin-2-yl)butyl]pyridine-2-carboxamide	C ₁₉ H ₂₃ N ₃ O	309.405	45878695
52	G52	Z238829562	methyl 2-[[4-(1H-indol-3-yl)piperidin-1-yl]methyl]furan-3-carboxylate	C ₂₀ H ₂₂ N ₂ O ₃	338.400	40135547

53	G53	Z1139229674	1-(2,3-dihydro-1H-indol-1-yl)-2-{5H,6H,7H,8H-pyrido[3,4-d]pyrimidin-7-yl} ethan-1-one	C ₁₇ H ₁₈ N ₄ O	294.351	53570799
54	G54	Z52993934	2-({1-(2,3-dihydro-1,4-benzodioxin-6-yl)ethyl}amino)methyl-3,4-dihydroquinazolin-4-one	C ₁₉ H ₁₉ N ₃ O ₃	337.372	135775996
55	G55	Z394150106	1-(6-methylpyridine-2-carbonyl)-4-[(thiophen-2-yl)methyl]-1,4-diazepane	C ₁₇ H ₂₁ N ₃ OS	315.433	35384642
56	G56	Z1185918928	[2-(1H-1,3-benzodiazol-1-yl)ethyl][1-(4-bromophenyl)ethyl]amine	C ₁₇ H ₁₈ BrN ₃	344.248	71876443
57	G57	Z46420586	N-(2,3-dimethylphenyl)-2-{methyl[2-(pyridin-4-yl)ethyl]amino}acetamide	C ₁₈ H ₂₃ N ₃ O	297.394	17401544
58	G58	Z46476391	1-(2,3-dihydro-1,4-benzodioxine-2-carbonyl)-4-{{5-(furan-2-yl)-1,3,4-oxadiazol-2-yl}methyl}piperazine	C ₂₀ H ₂₀ N ₄ O ₅	396.396	42914177
59	G59	Z1760011829	1-(3-fluoro-4-methylbenzoyl)-N-methyl-N-[(pyrimidin-2-yl)methyl]pyrrolidin-3-amine	C ₁₈ H ₂₁ FN ₃ O	328.383	128999728
60	G60	Z1298837774	N,N-dimethyl-2-{{4-(pyrazine-2-carbonyl)piperazin-1-yl}methyl}aniline	C ₁₈ H ₂₃ N ₅ O	325.408	75375171
61	G61	Z1912460119	2-{3-bromo-5H,6H,7H,8H-imidazo[1,2-a]pyrazin-7-yl}-N-(2-phenylpropyl)propanamide	C ₁₈ H ₂₃ BrN ₄ O	391.305	119036481
62	G62	Z1757891890	N-({4-{{1-(6-methylimidazo[1,2-a]pyridin-3-yl)methyl}pyrrolidin-3-yl}oxy}pyridin-2-yl)methyl}acetamide	C ₂₁ H ₂₅ N ₅ O ₂	379.455	137866116
63	G63	Z324745286	2-{3-[methyl({4-(trifluoromethoxy)phenyl}methyl)amino]propyl}-2,3-dihydro-1H-isoindole-1,3-dione	C ₂₀ H ₁₉ F ₃ N ₃ O ₃	392.371	45872856
64	G64	Z2396502728	3-{4-[(1-cyclopropyl-1H-pyrazol-5-yl)methyl]piperazin-1-yl}oxolane-3-carboxylic acid	C ₁₈ H ₂₈ N ₄ O ₃	348.439	137866381
65	G65	Z2721873427	3-(2-{2-tert-butyl-5H,6H,7H,8H-pyrido[4,3-d]pyrimidin-6-yl}ethoxy)benzoic acid	C ₂₀ H ₂₅ N ₃ O ₃	355.430	136555481
66	G66	Z1994302045	2-methoxy-4-({1-(pyridine-4-carbonyl)pyrrolidin-3-yl}amino)methylbenzotrile	C ₁₉ H ₂₀ N ₄ O ₂	336.387	137850529
67	G67	Z1568338932	3-({3-[(morpholin-4-yl)methyl]piperidin-1-yl}methyl)quinolin-2-ol	C ₂₀ H ₂₇ N ₃ O ₂	341.447	Not listed
68	G68	Z1584184614	2-{2-[4-(2,2-difluoroethyl)-1,4-diazepan-1-yl]ethyl}-2,3-dihydro-1H-isoindole-1,3-dione	C ₁₇ H ₂₁ F ₂ N ₃ O ₂	337.364	122138587
69	G69	Z2215634871	6-({1-phenyl-1H,4H,5H,6H,7H-[1,2,3]triazolo[4,5-c]pyridin-5-yl)methyl}-5-oxaspiro[2.4]heptan-4-one	C ₁₈ H ₂₀ N ₄ O ₂	324.377	137864917
70	G70	Z2351626153	1-[2-{{1-(3-fluorophenyl)-3-methyl-1H-pyrazol-4-yl}methyl}amino]propylpyrrolidin-2-one	C ₁₈ H ₂₃ FN ₃ O	330.399	137997783
71	G71	Z90556724	[2-(dimethylamino)-2-(furan-2-yl)ethyl][3-(methyl-1-phenyl-1H-pyrazol-4-yl)methyl]amine	C ₁₉ H ₂₄ N ₄ O	324.420	Not listed
72	G72	Z2732441096	N-(1-benzyl-4-methylpiperidin-3-yl)-6-methyl-4-oxo-1,4-dihydropyridine-3-carboxamide	C ₂₀ H ₂₅ N ₃ O ₂	339.431	126830322
73	G73	Z2504626564	[2-(4-fluoro-2-methylphenyl)ethyl](1-{imidazo[1,2-a]pyridin-2-yl}ethyl)amine	C ₁₈ H ₂₀ FN ₃	297.369	136551322
74	G74	Z2936915390	dimethyl({1-[(5-phenyl-1,3-oxazol-2-yl)methyl]piperidin-4-yl}methyl)imino-?-sulfanone	C ₁₈ H ₂₅ N ₃ O ₂ S	347.475	136562060
75	G75	Z2047442057	1-(3-{1-[(5H,6H,7H,8H-imidazo[1,2-a]pyridin-3-yl)methyl]amino}ethyl)phenylpyrrolidin-2-one	C ₂₀ H ₂₆ N ₄ O	338.446	126808609
76	G76	Z1232726459	2-{2-[4-(3-methoxybenzoyl)-1,4-diazepan-1-yl]ethyl}-1-methyl-1H-1,3-benzodiazole	C ₂₃ H ₂₈ N ₄ O ₂	392.494	119041891
77	G77	Z125796648	N-(2,4-dimethylphenyl)-2-(4-{{1,2,4}triazolo[4,3-a]pyridin-3-yl}piperidin-1-yl)propanamide	C ₂₂ H ₂₇ N ₅ O	377.482	119040990
78	G78	Z1522173585	N-{1-[(3,5-dimethoxyphenyl)methyl]pyrrolidin-3-yl}-3-methyl-2-oxo-2,3-dihydro-1,3-benzoxazole-7-carboxamide	C ₂₂ H ₂₅ N ₃ O ₅	411.451	138994323
79	G79	Z1994314456	1-(4-{{(5-chloro-1-methyl-1H-imidazol-2-yl)methyl}amino}-1,2,3,4-tetrahydroquinolin-1-yl)ethan-1-one	C ₁₆ H ₁₉ ClN ₄ O	318.801	137865522
80	G80	Z2999234257	2-(4-{{4-(3,5-dimethylphenyl)piperidin-1-yl}methyl}-1H-1,2,3-triazol-1-yl)acetic acid	C ₁₈ H ₂₄ N ₄ O ₂	328.408	Not listed
81	G81	Z1272067625	[(2H-1,3-benzodioxol-4-yl)methyl]({1-[3-(3-fluorophenyl)-1,2,4-oxadiazol-5-yl]ethyl}amino)	C ₁₈ H ₁₆ FN ₃ O ₃	341.336	Not listed
82	G82	Z1119610673	1-[1-(3-methoxyphenyl)ethyl]-4-(3-methyl-1,2-oxazole-5-carbonyl)piperazine	C ₁₈ H ₂₃ N ₃ O ₃	329.393	146085811
83	G83	Z3826822203	3-(2-{{2-(4-methylphenyl)cyclopentyl}amino}ethyl)-3,4-dihydroquinazolin-4-one	C ₂₂ H ₂₅ N ₃ O	347.453	145901549
84	G84	Z1903319810	2-(6-methoxy-2,3,4,5-tetrahydro-1H-3-benzazepin-3-yl)-N-(pyrimidin-2-yl)propanamide	C ₁₈ H ₂₂ N ₄ O ₂	326.392	136537519
85	G85	Z2369149772	1-(2-aminoethyl)-N-(3,4-dichlorophenyl)piperidine-4-carboxamide	C ₁₄ H ₁₉ Cl ₂ N ₃ O	316.226	121831654
86	G86	Z1269285686	1-{3-methyl-4-{{(7-methylimidazo[1,2-a]pyridin-3-yl)methyl}amino}piperidin-1-yl}ethan-1-one	C ₁₇ H ₂₄ N ₄ O	300.398	71927566
87	G87	Z2900814427	3-({methyl[2-(methylnaphthalen-1-yl)methyl]amino}methyl)-5H,6H,7H,8H-[1,2,4]triazolo[4,3-a]pyrazin-8-one	C ₁₉ H ₂₁ N ₅ O	335.402	145879599
88	G88	Z85487734	N-[2-(4-benzylpiperazin-1-yl)ethyl]pyridine-4-carboxamide	C ₁₉ H ₂₄ N ₄ O	324.420	39303046
89	G89	Z1639535660	methyl[1-(phenyl-1H-pyrazol-4-yl)methyl](2-phenylethyl)amine	C ₁₉ H ₂₁ N ₃	291.390	53537284
90	G90	Z1420680671	4-{{(2,2-dimethyl-3,4-dihydro-2H-1-benzopyran-4-yl)amino}methyl}-1,5-dimethyl-2-phenyl-2,3-dihydro-1H-pyrazol-3-one	C ₂₃ H ₂₇ N ₃ O ₂	377.479	132291704
91	G91	Z2161442409	2-[2-(5-methyl-1H-1,3-benzodiazol-2-yl)pyrrolidin-1-yl]-N-(1-phenylethyl)acetamide	C ₂₂ H ₂₆ N ₄ O	362.468	121566850
92	G92	Z86141505	[(6-bromo-2H-1,3-benzodioxol-5-yl)methyl][2-(pyridin-2-yl)ethyl]amine	C ₁₅ H ₁₅ BrN ₂ O ₂	335.195	17460496
93	G93	Z1759864327	methyl[({1-(2-methyl-1H-pyrrole-3-carbonyl)pyrrolidin-3-yl}methyl)][(pyridin-3-yl)methyl]amine	C ₁₈ H ₂₄ N ₄ O	312.409	128970166
94	G94	Z2275232885	1-{{5-(propan-2-yl)-1,3,4-oxadiazol-2-yl}methyl}-1,2,5,6-tetrahydro-3,3'-bipyridine	C ₁₆ H ₂₀ N ₄ O	284.356	Not listed
95	G95	Z2755041952	2-{2-[methyl({2-[methyl(2-methylpyrimidin-4-yl)amino}ethyl)-2,3-dihydro-1H-isoindole-1,3-dione	C ₁₉ H ₂₃ N ₃ O ₂	353.418	126832823
96	G96	Z2483074855	2-{{4-(2-bromophenyl)piperidin-1-yl}methyl}pyridine-3-carboxylic acid	C ₁₈ H ₁₉ BrN ₂ O ₂	375.259	136550710