

Table S2. List of predicted NOR inhibitors subjected to wet-lab assay

Sr. No.	Lab ID	Manufacturer's Code	Compound Name	Compound Formula	Molecular Weight	PubChem ID
1	N1	Z1526792053	5-bromo-N,4-dimethyl-N-[(1-methyl-1H-pyrazol-4-yl)methyl]pyridin-2-amine	C <sub>12</sub> H <sub>15</sub> BrN <sub>4</sub>	295.178	75514219
2	N2	Z802764748	6-[[3,5-dimethylphenyl(ethyl)amino]methyl]-1-methyl-1H,4H,5H-pyrazolo[3,4-d]pyrimidin-4-one	C <sub>17</sub> H <sub>21</sub> N <sub>5</sub> O	311.381	136051817
3	N3	Z1511548068	1-[(4,5-dimethyl-4H-1,2,4-triazol-3-yl)methyl]-6-methoxy-2,3,4,5-tetrahydro-1H-1-benzazepine	C <sub>16</sub> H <sub>22</sub> N <sub>4</sub> O	286.372	75432145
4	N4	Z954454636	4-({imidazo[2,1-b][1,3]thiazol-6-yl)methyl}-N-methyl-3,4-dihydro-2H-1,4-benzoxazine-2-carboxamide	C <sub>16</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub> S	328.388	51100444
5	N5	Z972752888	N-[2-(3,5-dimethylphenoxy)ethyl]-N-methylpyrido[2,3-b]pyrazin-6-amine	C <sub>18</sub> H <sub>20</sub> N <sub>4</sub> O	308.377	75418827
6	N6	Z1537369455	2-(3-methyl-1H-pyrazol-1-yl)-N-[(5-methylpyridin-2-yl)methyl]aniline	C <sub>17</sub> H <sub>18</sub> N <sub>4</sub>	278.351	84592296
7	N7	Z56864401	5-chloro-8-({5-methylimidazo[1,2-a]pyridin-2-yl)methoxy}quinoline	C <sub>18</sub> H <sub>14</sub> ClN <sub>3</sub> O	323.776	722284
8	N8	Z1626099769	6-[3-(4-phenyl-1H-1,2,3-triazol-1-yl)azetidin-1-yl]pyridine-3-carbonitrile	C <sub>17</sub> H <sub>14</sub> N <sub>6</sub>	302.333	75474147
9	N9	Z1166113790	3-{5-[4-(4-bromophenyl)oxan-4-yl]-1,2,4-oxadiazol-3-yl}pyridine	C <sub>18</sub> H <sub>16</sub> BrN <sub>3</sub> O <sub>2</sub>	386.242	53625623
10	N10	Z56944153	4-phenyl-1,5,6,10-tetraazatetracyclo[7.7.0.0 <sup>2,6</sup> .0 <sup>11,16</sup> ]hexadeca-2,4,9,11,13,15-hexaene	C <sub>18</sub> H <sub>14</sub> N <sub>4</sub>	286.330	3302076
11	N11	Z1165357648	2-[1-(5-phenyl-1,3,4-oxadiazol-2-yl)-6-azaspiro[2.5]octan-6-yl]-1,3-benzoxazole	C <sub>22</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>	372.419	56803870
12	N12	Z354334736	N-cyclopropyl-N-[(4-methylphenyl)methyl]thieno[3,2-d]pyrimidin-4-amine	C <sub>17</sub> H <sub>17</sub> N <sub>3</sub> S	295.401	122136271
13	N13	Z2177121342	1-{{1-(4-fluorophenyl)-1H-pyrazol-4-yl)methyl}-1,2,3,5-tetrahydro-4,1-benzoxazepine	C <sub>19</sub> H <sub>18</sub> FN <sub>3</sub> O	323.364	126808560
14	N14	Z1765101069	2-[1-(2,6-dimethylpyrimidin-4-yl)pyrrolidin-2-yl]-1-(thiophen-2-yl)ethan-1-ol	C <sub>16</sub> H <sub>21</sub> N <sub>3</sub> OS	303.422	121533222
15	N15	Z2094351482	2-methyl-6-{3-phenyl-octahydroprano[4,3-b]pyrrol-1-yl}pyrazine	C <sub>18</sub> H <sub>21</sub> N <sub>3</sub> O	295.378	121561731
16	N16	Z1414604660	5-({imidazo[1,2-a]pyridin-3-yl)methyl}-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one	C <sub>17</sub> H <sub>16</sub> N <sub>4</sub> O	292.335	71919705
17	N17	Z1052607496	1-[3-(3,4-dimethylphenoxy)propyl]-3-methyl-5-phenyl-1H-1,2,4-triazole	C <sub>20</sub> H <sub>23</sub> N <sub>3</sub> O	321.416	52878166
18	N18	Z110018576	N,5-dimethyl-N-{{2-(pyrrolidin-1-yl)phenyl)methyl}imidazo[1,2-a]pyridine-2-carboxamide	C <sub>21</sub> H <sub>24</sub> N <sub>4</sub> O	348.441	17411699
19	N19	Z161956388	4-methyl-5-({9-methyl-4-oxo-4H-pyrido[1,2-a]pyrimidin-2-yl)methyl}-2,3,4,5-tetrahydro-1H-1,5-benzodiazepin-2-one	C <sub>20</sub> H <sub>20</sub> N <sub>4</sub> O <sub>2</sub>	348.398	45799055
20	N20	Z1765033426	4-{4-[(1H-imidazol-2-yl)methyl]piperidin-1-yl}-2,6-dimethylpyrimidine		271.360	Not listed
21	N21	Z1462003105	2-cyclopropyl-5-[3-(4-methoxyphenyl)pyrrolidin-1-yl]-1,3,4-thiadiazole	C <sub>16</sub> H <sub>19</sub> N <sub>3</sub> OS	301.406	75384942
22	N22	Z1900851573	6-methoxy-3-(pyrazin-2-yl)-2,3,4,5-tetrahydro-1H-3-benzazepine	C <sub>15</sub> H <sub>17</sub> N <sub>3</sub> O	255.314	122139489
23	N23	Z1742733381	{1-[2-(2-methyl-1H-1,3-benzodiazol-1-yl)ethyl]-1H-imidazol-2-yl}(phenyl)methanol	C <sub>20</sub> H <sub>20</sub> N <sub>4</sub> O	332.399	86817095
24	N24	Z1632828351	4-(4-[[2,4-dimethylphenyl(methyl)amino]methyl]-1-methyl-1H-pyrazol-3-yl)benzoxazole	C <sub>21</sub> H <sub>22</sub> N <sub>4</sub>	330.426	86785822
25	N25	Z734239720	N-[3-[3-(3-fluorophenyl)-1H-pyrazol-5-yl]propyl]-N-methyl-1,3-benzoxazol-2-amine	C <sub>20</sub> H <sub>19</sub> FN <sub>3</sub> O	350.389	56797418
26	N26	Z1084021514	4-{6-ethylthieno[2,3-d]pyrimidin-4-yl}-1-methyl-2,3,4,5-tetrahydro-1H-1,4-benzodiazepine	C <sub>18</sub> H <sub>20</sub> N <sub>4</sub> S	324.443	71879598
27	N27	Z1611882500	1-benzyl-N-[1-(thiophen-3-yl)propan-2-yl]-1H-pyrazol-5-amine	C <sub>17</sub> H <sub>19</sub> N <sub>3</sub> S	297.417	86782955
28	N28	Z1681952610	N-({imidazo[1,2-a]pyrimidin-3-yl)methyl}-N-methyl-3-(methylsulfanyl)aniline	C <sub>15</sub> H <sub>16</sub> N <sub>4</sub> S	284.379	75506927
29	N29	Z1832204971	2-[[{5,7-dimethylimidazo[1,2-a]pyrimidin-3-yl)methyl}(phenyl)amino]ethan-1-ol	C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> O	296.366	99835018
30	N30	Z2034493837	5-fluoro-2-{4-[(1H-1,2,3-triazol-1-yl)methyl]piperidin-1-yl}pyridine	C <sub>13</sub> H <sub>16</sub> FN <sub>5</sub>	261.298	121557943
31	N31	Z1037455082	3-(1-{5H,6H,7H-cyclopenta[d]pyrimidin-4-yl}pyrrolidin-2-yl)-5-methyl-1,2-oxazole	C <sub>15</sub> H <sub>18</sub> N <sub>4</sub> O	270.329	51108330
32	N32	Z1863847680	2-chloro-4-[4-(6-methylpyridazin-3-yl)-1,4-diazepan-1-yl]benzoxazole	C <sub>17</sub> H <sub>18</sub> ClN <sub>5</sub>	327.811	121546160
33	N33	Z940779984	3-chloro-5-[4-(1H-pyrrol-1-yl)piperidin-1-yl]-1,2-thiazole-4-carbonitrile	C <sub>13</sub> H <sub>13</sub> ClN <sub>4</sub> S	292.787	71882290
34	N34	Z328694138	N-[1-(1-benzofuran-2-yl)ethyl]-N,5-dimethyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-amine	C <sub>17</sub> H <sub>17</sub> N <sub>5</sub> O	307.349	42951295
35	N35	Z57684918	3-[3-(2-bromo-4,6-dimethylphenoxy)propyl]-3,4-dihydroquinazolin-4-one	C <sub>19</sub> H <sub>19</sub> BrN <sub>2</sub> O <sub>2</sub>	387.270	16614100
36	N36	Z39775956	4,6-dimethyl-2-[4-(4-methyl-1,3-thiazol-2-yl)piperazin-1-yl]pyrimidine	C <sub>14</sub> H <sub>19</sub> N <sub>5</sub> S	289.399	36785635
37	N37	Z1190350270	4-fluoro-2-[[1-(pyridin-2-yl)methyl]-1H-imidazol-2-yl]sulfanyl)methyl]-1H-1,3-benzodiazole	C <sub>17</sub> H <sub>14</sub> FN <sub>3</sub> S	339.389	56789186
38	N38	Z1272396589	3-(3-methyl-1,2,4-oxadiazol-5-yl)-2-(3-methyl-3-phenylpiperidin-1-yl)pyridine	C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> O	334.414	75422650
39	N39	Z1939154930	N,3-dimethyl-N-(2-phenoxyethyl)-[1,2]oxazolo[5,4-d]pyrimidin-4-amine	C <sub>15</sub> H <sub>16</sub> N <sub>4</sub> O <sub>2</sub>	284.313	126773809
40	N40	Z1320214890	2-[[4-(2,2,2-trifluoroethyl)-1,2,3,4-tetrahydroquinoxalin-1-yl)methyl]-3,4-dihydroquinazolin-4-one	C <sub>19</sub> H <sub>17</sub> F <sub>3</sub> N <sub>4</sub> O	374.359	136266461
41	N41	Z2370587222	1-[3-(difluoromethyl)-[1,2,4]triazolo[4,3-b]pyridazin-6-yl]-2,2-dimethyl-3-phenylpyrrolidine	C <sub>18</sub> H <sub>19</sub> F <sub>2</sub> N <sub>5</sub>	343.373	126819088
42	N42	Z244394766	N-[(4-ethyl-3,4-dihydro-2H-1,4-benzoxazin-2-yl)methyl]-N-methyl-1,3-benzoxazol-2-amine	C <sub>19</sub> H <sub>21</sub> N <sub>3</sub> O <sub>2</sub>	323.388	56807427
43	N43	Z425071952	1-(1,3-benzothiazol-2-yl)-N-methyl-N-[(1-phenyl-1H-pyrazol-4-yl)methyl]piperidine-3-carboxamide	C <sub>24</sub> H <sub>25</sub> N <sub>3</sub> OS	431.553	42962010
44	N44	Z1461940284	3-cyclopropyl-N-methyl-N-[(5-methylfuran-2-yl)methyl]-[1,2,4]triazolo[4,3-b]pyridazin-6-amine	C <sub>15</sub> H <sub>17</sub> N <sub>5</sub> O	283.328	75384895
45	N45	Z228055694	N-[2-phenyl-2-(2-phenyl-1H-indol-3-yl)ethyl]-3-(1H-1,2,4-triazol-1-yl)propanamide	C <sub>27</sub> H <sub>25</sub> N <sub>3</sub> O	435.520	47017924
46	N46	Z1498697342	N-[1-(6-ethylpyrimidin-4-yl)piperidin-4-yl]-2,5-dimethyl-1,3-thiazole-4-carboxamide	C <sub>17</sub> H <sub>23</sub> N <sub>3</sub> OS	345.462	121543105
47	N47	Z2017205408	8-(5-bromopyrimidin-2-yl)-3-(1-methyl-1H-pyrazol-5-yl)-8-azabicyclo[3.2.1]oct-2-ene	C <sub>15</sub> H <sub>16</sub> BrN <sub>5</sub>	346.225	121537717

48	N48	Z1367326602	4-[(2-phenylethyl)[2-(1H-1,2,4-triazol-1-yl)ethyl]amino]phenol	C <sub>18</sub> H <sub>20</sub> N <sub>4</sub> O	308.377	75377685
49	N49	Z805387830	2-(6-chloropyrazin-2-yl)-5,8-dimethoxy-1,2,3,4-tetrahydroisoquinolin-4-ol	C <sub>15</sub> H <sub>16</sub> ClN <sub>3</sub> O <sub>3</sub>	321.758	51112814
50	N50	Z1557056875	1-[6-ethyl-2-(pyridin-4-yl)pyrimidin-4-yl]-1,2,3,6-tetrahydropyridine-4-carbonitrile	C <sub>17</sub> H <sub>17</sub> N <sub>5</sub>	291.350	75396075
51	N51	Z1139214749	2-{2-[(1H-1,2,4-triazol-1-yl)methyl]piperidin-1-yl}-1,3-benzothiazole	C <sub>15</sub> H <sub>17</sub> N <sub>3</sub> S	299.393	72144394
52	N52	Z1607106826	1-cyclopropyl-3-[[2-(3-fluorophenoxy)ethyl](methyl)amino]-1,2-dihydropyrazin-2-one	C <sub>16</sub> H <sub>18</sub> FN <sub>3</sub> O <sub>2</sub>	303.331	75400991
53	N53	Z1911018298	3-chloro-2-[1-(2-phenylethyl)-1H,4H,5H,6H,7H-imidazo[4,5-c]pyridin-5-yl]pyridine-4-carbonitrile	C <sub>20</sub> H <sub>18</sub> ClN <sub>5</sub>	363.843	100711917
54	N54	Z1661482535	4-[2-(1-methyl-1H-pyrazol-4-yl)morpholin-4-yl]-3-(methylsulfanyl)quinoline	C <sub>18</sub> H <sub>20</sub> N <sub>4</sub> OS	340.442	86771371
55	N55	Z1823998167	7-fluoro-4-[(6-methylimidazo[1,2-a]pyridin-3-yl)methyl]-3,4-dihydro-2H-1,4-benzoxazine	C <sub>17</sub> H <sub>16</sub> FN <sub>3</sub> O	297.326	86806784
56	N56	Z1654777250	2-[2-(3-{[3-(pyridin-4-yl)propyl]sulfanyl}-4H-1,2,4-triazol-4-yl)ethyl]pyridine	C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> S	325.431	75454915
57	N57	Z1408657444	5-bromo-2-[4-(thiophen-2-yl)piperazin-1-yl]pyrimidine	C <sub>12</sub> H <sub>13</sub> BrN <sub>4</sub> S	325.227	122134624
58	N58	Z1343415755	3-chloro-N-methyl-N-[(1-phenyl-1H-pyrazol-4-yl)methyl]pyridin-4-amine	C <sub>16</sub> H <sub>15</sub> ClN <sub>4</sub>	298.770	72104974
59	N59	Z1247221759	N-(5-bromopyridin-2-yl)-2-methyl-5,6,7,8-tetrahydroquinazolin-5-amine	C <sub>14</sub> H <sub>13</sub> BrN <sub>4</sub>	319.199	75372891
60	N60	Z1576911624	4-(3-ethyl-1,2,4-thiadiazol-5-yl)-5-methyl-2-phenylmorpholine	C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> OS	289.395	121545281
61	N61	Z2740017161	5-cyclopropyl-2-[1-[6-(propan-2-yl)pyrimidin-4-yl]azetidin-3-yl]pyrimidine	C <sub>17</sub> H <sub>21</sub> N <sub>5</sub>	295.382	126834698
62	N62	Z235529402	4-(1-[5-methyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl]piperidin-4-yl)phenol	C <sub>17</sub> H <sub>19</sub> N <sub>5</sub> O	309.365	36730055
63	N63	Z1999535238	N,4-dimethyl-5-(5-methylthiophen-2-yl)-N-(1-phenylethyl)-4H-1,2,4-triazol-3-amine	C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> S	312.432	119037850
64	N64	Z354282258	N-{3-[ethyl(phenyl)amino]propyl}-6-methylimidazo[2,1-b][1,3,4]thiadiazol-2-amine	C <sub>16</sub> H <sub>21</sub> N <sub>5</sub> S	315.436	33979059
65	N65	Z1874308288	4-(2-chlorophenyl)-1-(4-methylpyrimidin-2-yl)piperidin-4-ol	C <sub>16</sub> H <sub>18</sub> ClN <sub>3</sub> O	303.786	122139392
66	N66	Z1217940981	7-bromo-4-(1-cyclopropyl-1H,4H,5H,6H,7H-imidazo[4,5-c]pyridin-5-yl)quinoline	C <sub>18</sub> H <sub>17</sub> BrN <sub>4</sub>	369.258	75371951
67	N67	Z643773316	N-[(2,4-difluorophenyl)methyl]-N,2-dimethylpyrazolo[1,5-a]quinazolin-5-amine	C <sub>19</sub> H <sub>16</sub> F <sub>2</sub> N <sub>4</sub>	338.353	53537529
68	N68	Z56842761	2-(1,3-diphenyl-1H-pyrazol-4-yl)-3-[(pyridin-2-yl)methyl]-1,3-thiazolidin-4-one	C <sub>24</sub> H <sub>20</sub> N <sub>4</sub> OS	412.506	3588672
69	N69	Z1127125074	1-(4-fluorophenyl)-2-[methyl({5-propyl-[1,2,4]triazolo[1,5-a]pyrimidin-7-yl})amino]ethan-1-ol	C <sub>17</sub> H <sub>20</sub> FN <sub>3</sub> O	329.372	53546182
70	N70	Z1165357090	7-methyl-1-[10-methyl-7-thia-9,11-diazatricyclo[6.4.0.0 <sup>2,6</sup> ]{2,6}]dodeca-1(12),2(6),8,10-tetraen-12-yl]-1,4-diazepan-5-one	C <sub>16</sub> H <sub>20</sub> N <sub>4</sub> OS	316.421	56784721
71	N71	Z1348401895	2-(3-cyclopropyl-1,2,4-thiadiazol-5-yl)-4-(1H-pyrazol-1-yl)-1,2,3,4-tetrahydroisoquinoline	C <sub>17</sub> H <sub>17</sub> N <sub>5</sub> S	323.415	75494681
72	N72	Z1979753549	3,5-dimethyl-1-propyl-4-((2H,4H,5H,6H,7H-pyrazolo[4,3-b]pyridin-4-yl)methyl)-1H-pyrazole	C <sub>15</sub> H <sub>23</sub> N <sub>5</sub>	273.376	100660838
73	N73	Z1908535836	2-[[4-(4-bromo-3-methylphenyl)methyl]amino]-1-methyl-1H-1,3-benzodiazole-4-carbonitrile	C <sub>17</sub> H <sub>13</sub> BrN <sub>4</sub>	355.231	100708786
74	N74	Z56811872	9-(3-methylthiophen-2-yl)-8,10,17-triazatetracyclo[8.7.0.0 <sup>2,7</sup> .0 <sup>4,11</sup> .1,6]heptadeca-1(17),2(7),3,5,11(16),12,14-heptaene	C <sub>19</sub> H <sub>15</sub> N <sub>3</sub> S	317.407	3462048
75	N75	Z2142877672	2-methyl-4-{3-[(2-methyl-1,3-thiazol-4-yl)methoxy]pyrrolidin-1-yl}pyridine	C <sub>15</sub> H <sub>19</sub> N <sub>3</sub> OS	289.395	126796649
76	N76	Z1270081935	4-methoxy-N-methyl-N-(1-phenylbutan-2-yl)pyrimidin-2-amine	C <sub>16</sub> H <sub>21</sub> N <sub>3</sub> O	271.357	71871514
77	N77	Z1661426674	2-cyclopentyl-N-methyl-N-[(pyridin-2-yl)methyl]pyrimidin-4-amine	C <sub>16</sub> H <sub>20</sub> N <sub>4</sub>	268.356	75455284
78	N78	Z2020722999	4-[4,5-bis(2-phenylethyl)-4H-1,2,4-triazol-3-yl]piperazin-2-one	C <sub>22</sub> H <sub>25</sub> N <sub>5</sub> O	375.466	119052049
79	N79	Z2582963692	4-[4-(5-fluoropyridin-3-yl)piperazin-1-yl]-2-(methoxymethyl)-6-methylpyrimidine	C <sub>16</sub> H <sub>20</sub> FN <sub>5</sub> O	317.361	125423946
80	N80	Z1139220275	1-(1-{5H,6H,7H-cyclopenta[d]pyrimidin-4-yl}azetidin-3-yl)-1H-pyrazole	C <sub>13</sub> H <sub>15</sub> N <sub>5</sub>	241.291	53565584
81	N81	Z1478308313	2-[benzyl(pyridin-2-yl)pyrazin-6-yl]amino-1-(furan-2-yl)ethan-1-ol	C <sub>20</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>	346.382	75430738
82	N82	Z994882256	7-chloro-2-[[2-(2-hydroxypropyl)(phenyl)amino]methyl]-4H-pyrido[1,2-a]pyrimidin-4-one	C <sub>18</sub> H <sub>18</sub> ClN <sub>3</sub> O <sub>2</sub>	343.807	51106365
83	N83	Z1818000755	9-[(2-methylphenyl)methyl]-3,4,5,9-tetraazatricyclo[8.4.0.0 <sup>2,7</sup> .0 <sup>4,11</sup> .1,6]tetradeca-1(10),4,6,11,13-pentaene	C <sub>18</sub> H <sub>18</sub> N <sub>4</sub>	290.362	121569223
84	N84	Z955940262	1-[[1-(3-fluorophenyl)-1H-pyrazol-3-yl]methyl]-2,3-dihydro-1H-indole	C <sub>18</sub> H <sub>16</sub> FN <sub>3</sub>	293.338	71881467
85	N85	Z1188807506	N-ethyl-1-methyl-N-[(4-methylphenyl)(pyridin-3-yl)methyl]-1H-pyrazole-4-carboxamide	C <sub>20</sub> H <sub>22</sub> N <sub>4</sub> O	334.414	122137146