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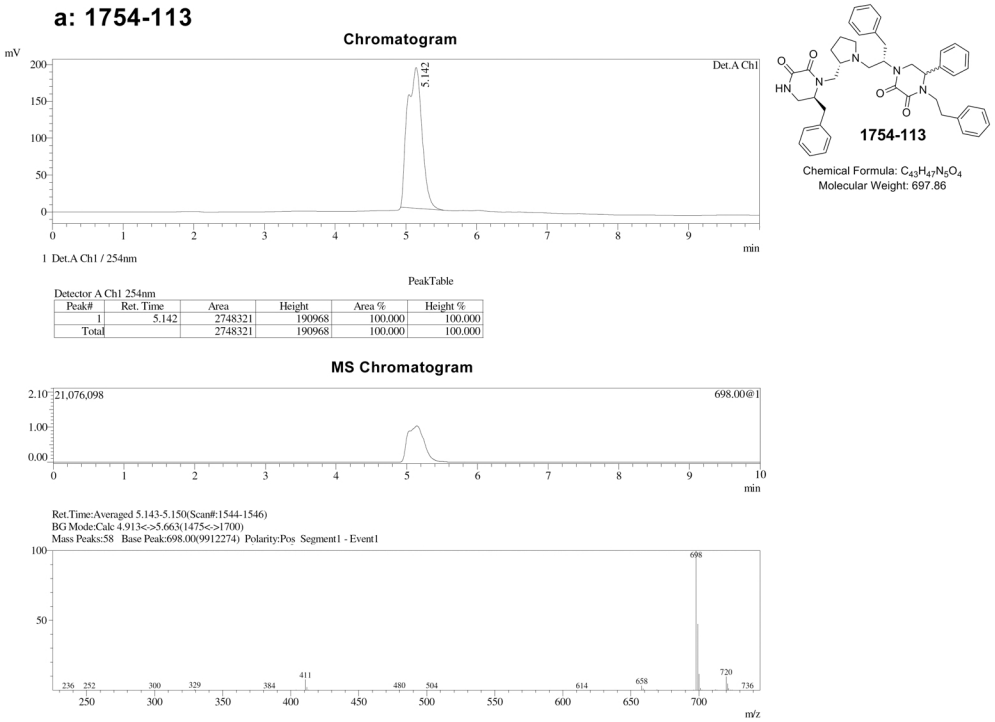
Selective agonists and antagonists of formylpeptide receptors:
duplex flow cytometry and mixture-based positional scanning libraries

Molecular Pharmacology



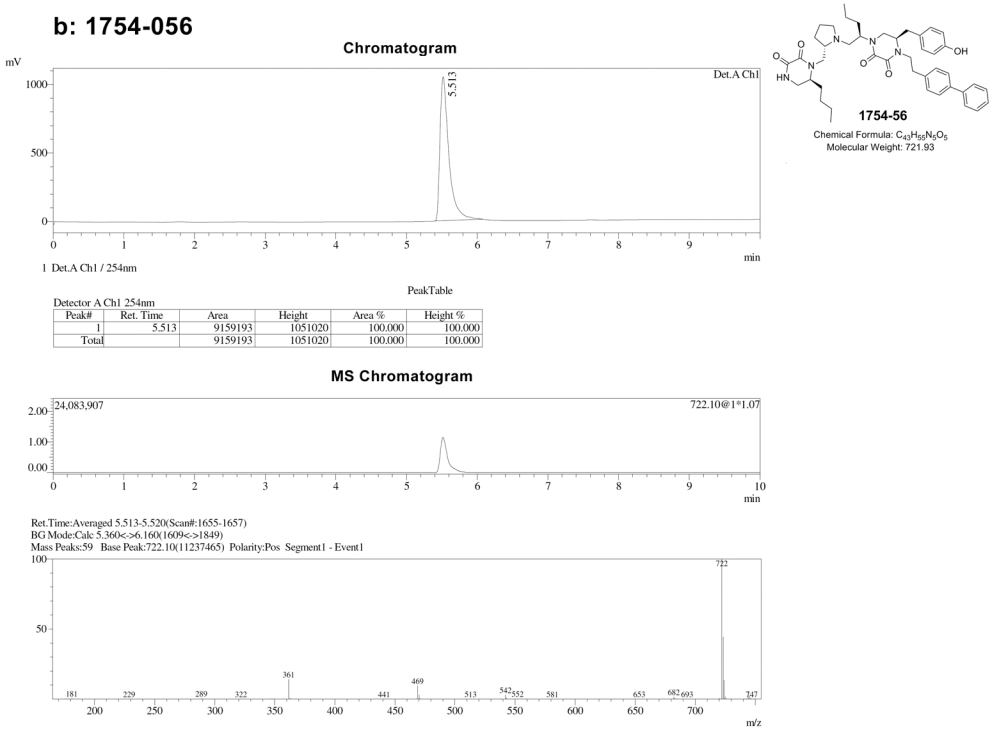


Figure S1. Analytical data for individual compounds shown in Table 2. The analytical data was obtained using a Shimadzu LCMS 2010 in ESI positive mode. The samples were run using a Phenomenex Luna C18 100A 50x4.60 5micron column. The two solvents used for the column runs were solvent A (water with 0.01% Formic acid) and solvent B (acetonitrile with 0.01% Formic acid). The gradient used is 5% to 95% over 6 minutes with an additional 2 minute clean time at 95% and another 3 minute equilibration at 5%. Sample 1753-103 used a gradient of 5% to 95% over 6 minutes with an additional 22 minute clean time at 95% and another 2 minute equilibration at 5%. Shown is the 254 nm UV trace, integrated UV peak table, total ion count trace for the desired product, and associated MW spectrum for each compound. The summary of these results is shown in Table S3.

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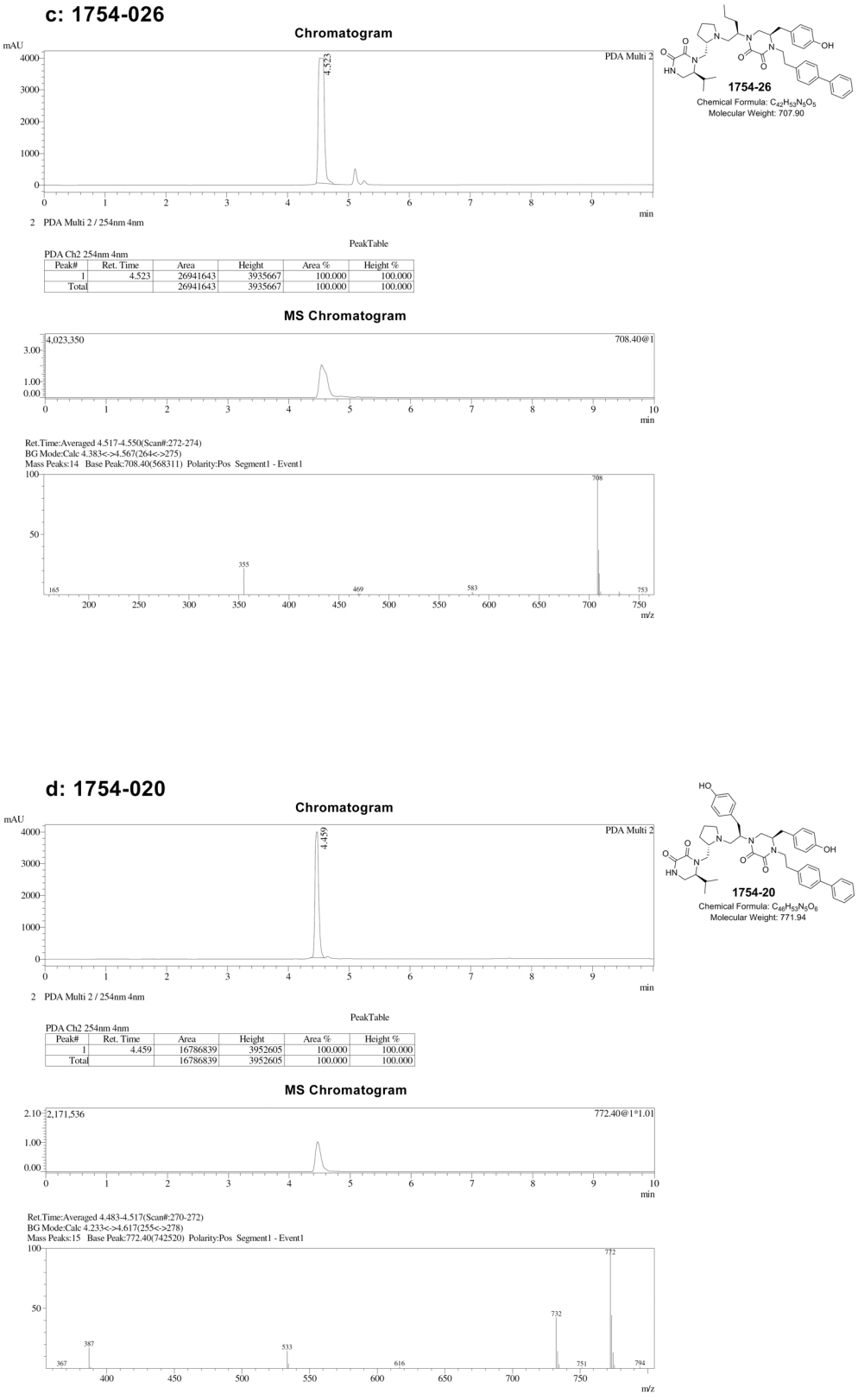

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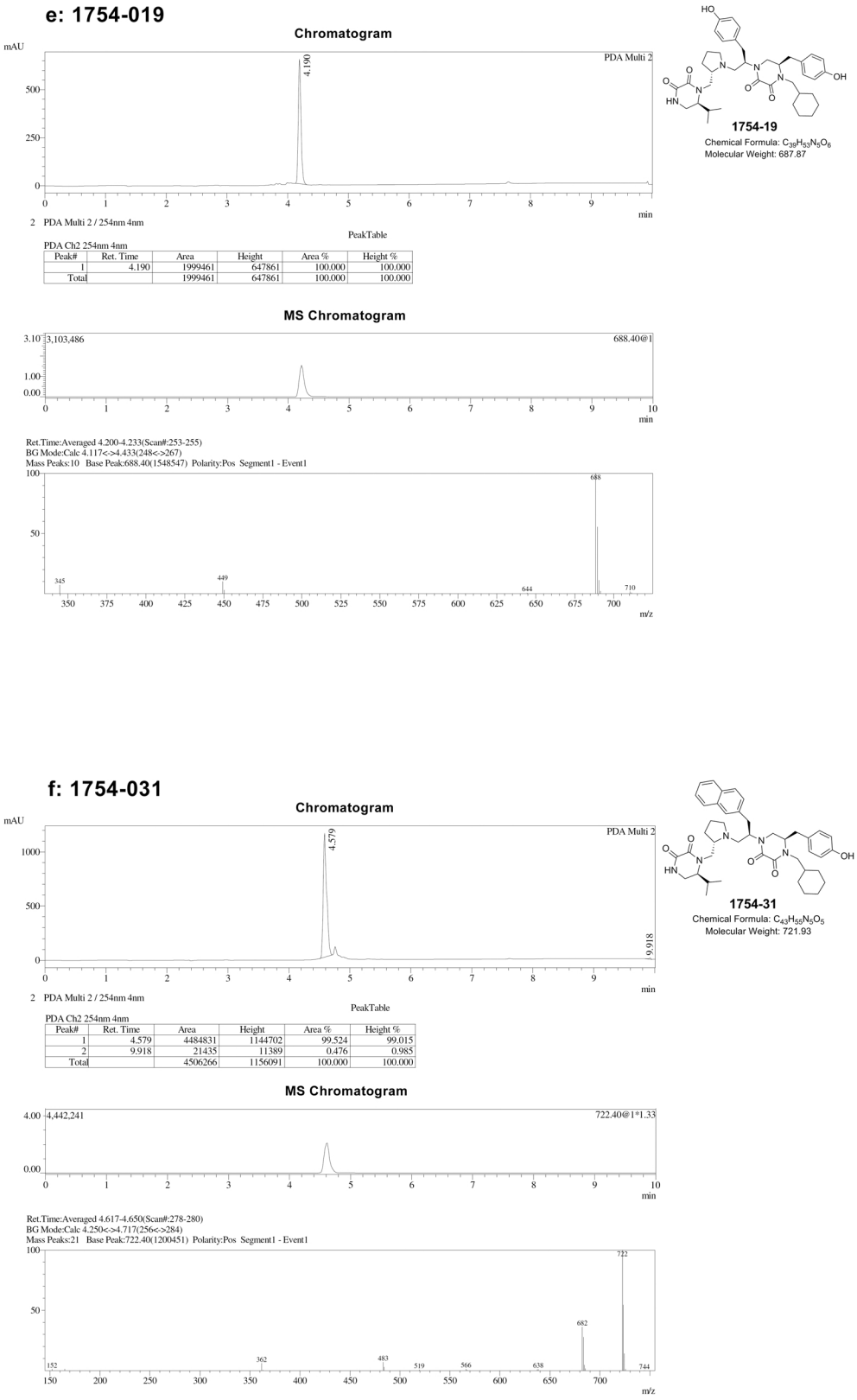

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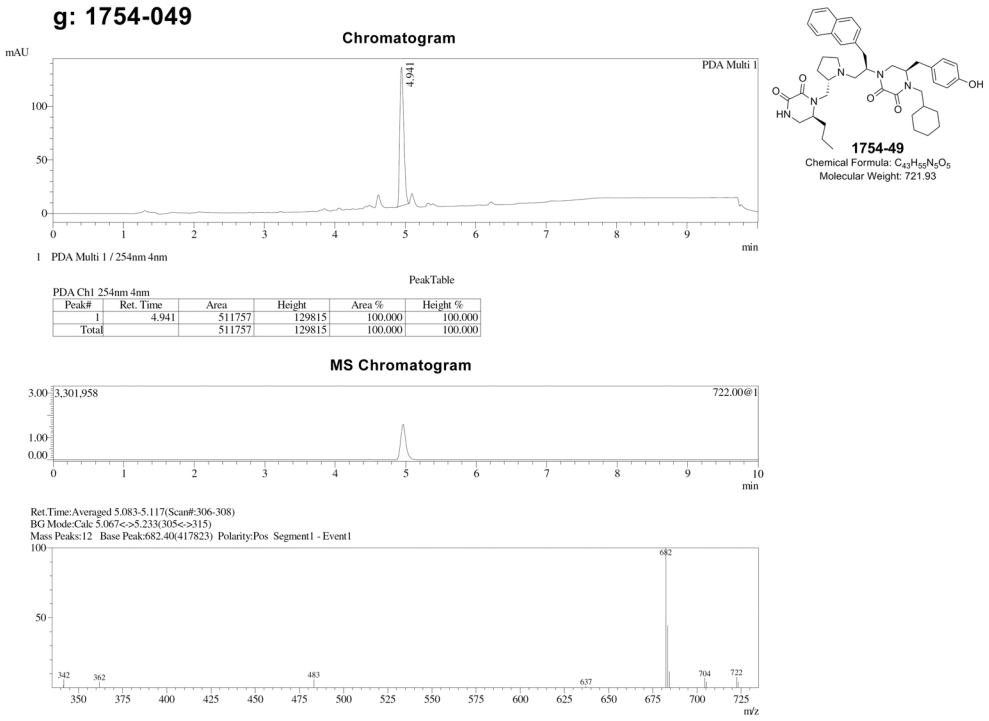

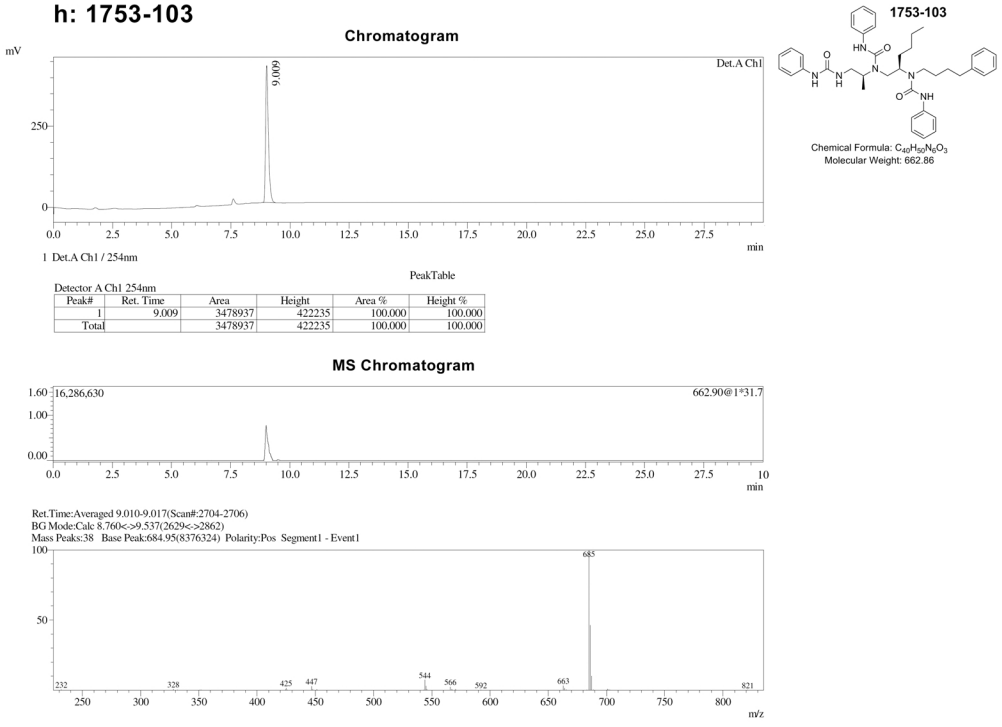

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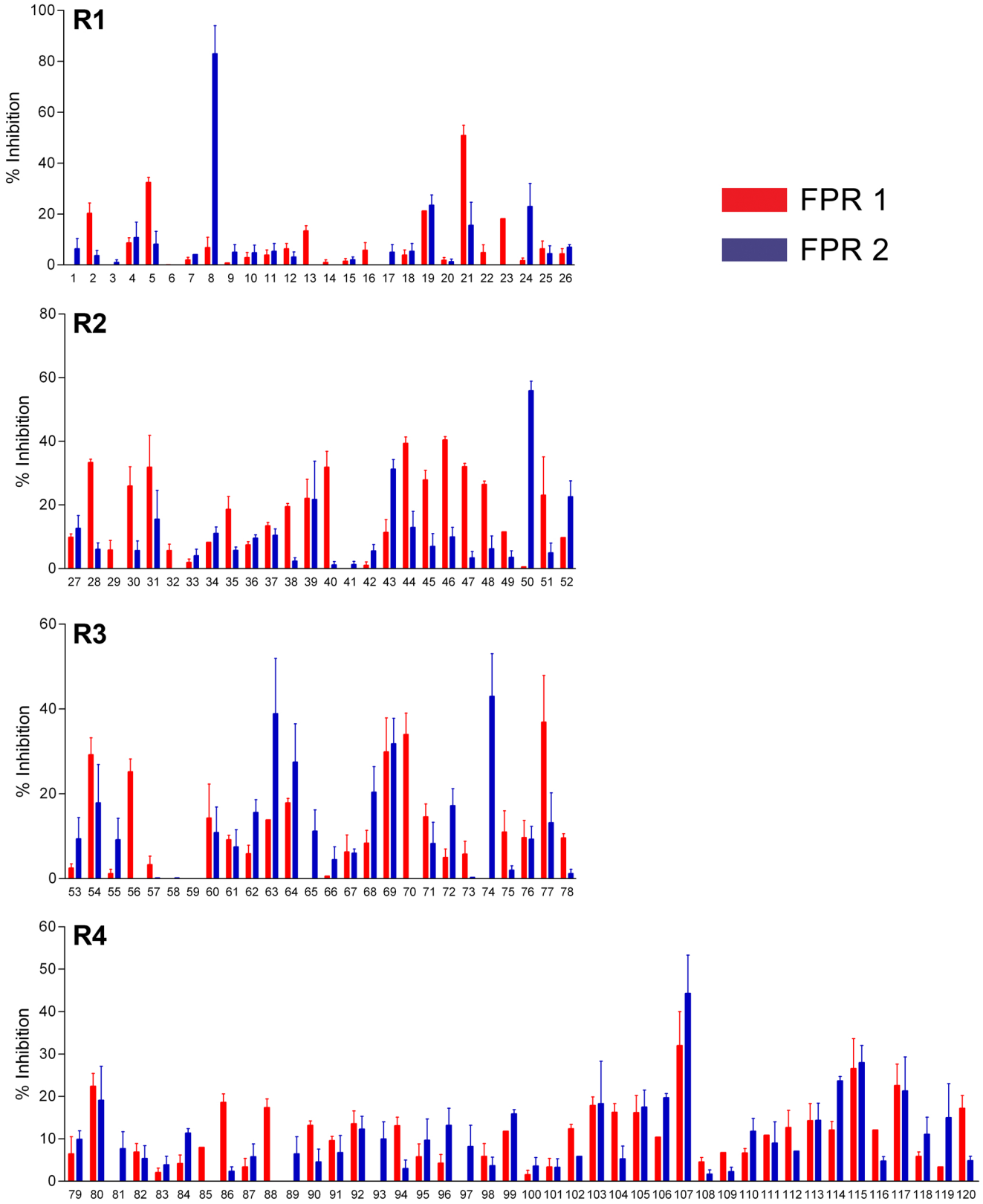

Figure S2. Activity profiles for FPR1 and FPR2 screened against pyrrolidine bis-diketopiperazine positional scanning library (library 21 in Figure 1, library 1344 in Table S1). Each bar represents the activity (% inhibition of labeled ligand binding to receptor) for a given mixture at each of the 4 positions of diversity (R1-R4). See Table S2 for library 1344 details.

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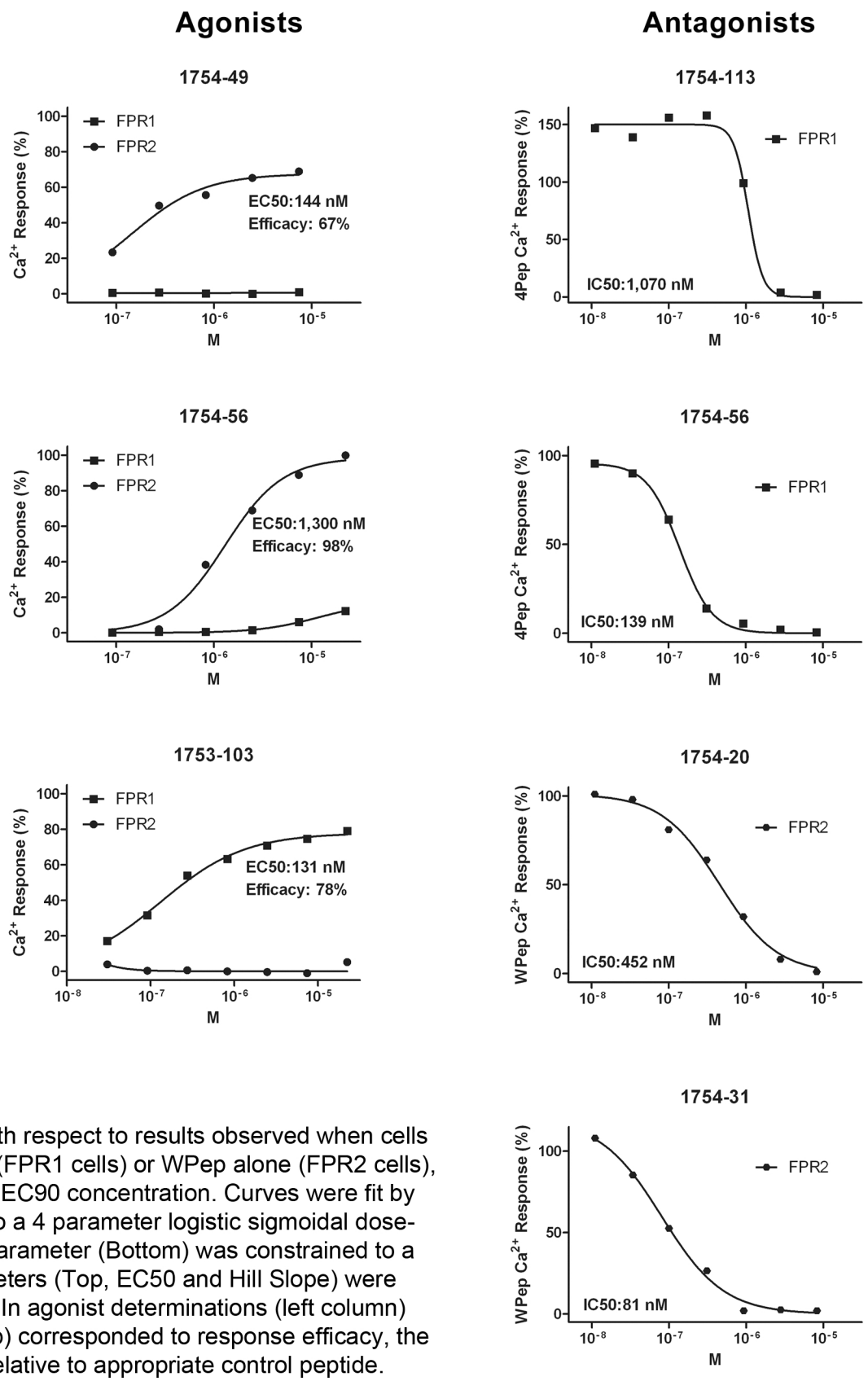

Figure S3. Agonist and antagonist concentration dependent activity of selected compounds. Test compounds with agonist activity (left column) were added to mixtures of FPR1 and FPR2 cells at the indicated final concentrations to determine changes in Fluo4 fluorescence intensity in FPR1 cells (squares) and FPR2 cells (circles), indicative of mobilization of intracellular calcium. Responses were normalized to results observed with control peptides (4pep for FPR1 and Wpep for FPR2) as described in the methods section. Test compounds with antagonist activity (right column) were pre-incubated 5 min with mixtures of differentially labeled FPR1 and FPR2 cells after which control peptides were added and Fluo4 fluorescence intensity changes in FPR1 cells (top two figures) or FPR2 cells (bottom two figures) were recorded.

Responses were normalized with respect to results observed when cells were treated with fMLFF alone (FPR1 cells) or WPep alone (FPR2 cells), each used at its predetermined EC90 concentration. Curves were fit by GraphPad Prism 5.0 software to a 4 parameter logistic sigmoidal dose-response model in which one parameter (Bottom) was constrained to a value of 0%. The other parameters (Top, EC50 and Hill Slope) were determined by the fitted curve. In agonist determinations (left column) the fitted response plateau (Top) corresponded to response efficacy, the maximum response achieved relative to appropriate control peptide. Response efficacies of 1754-49, 1754-56 and 1753-103 were 67, 98 and 78%, respectively.

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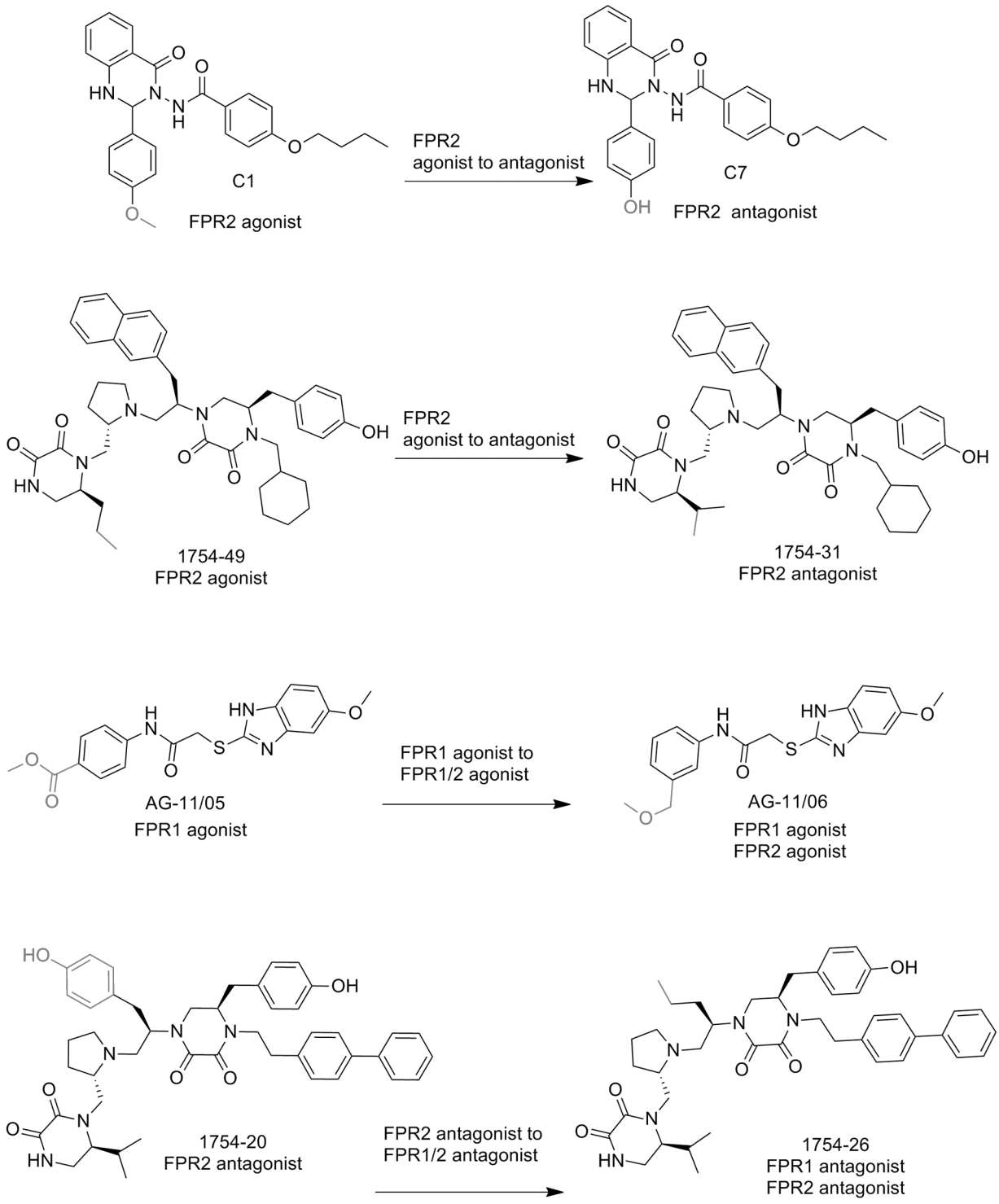
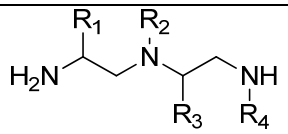
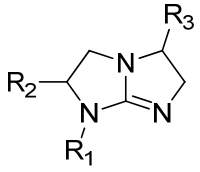
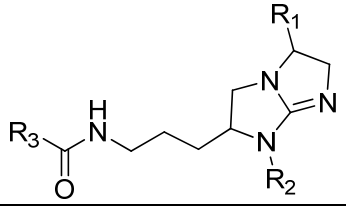
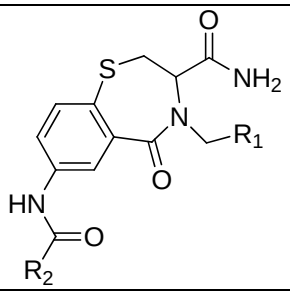
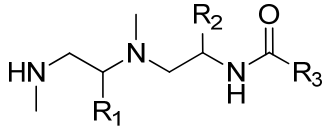
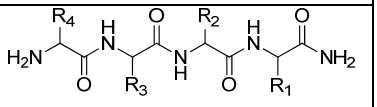
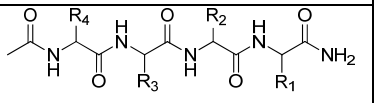
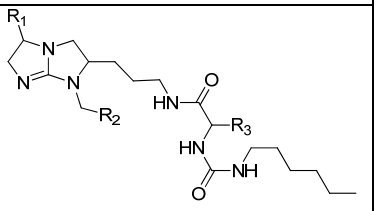


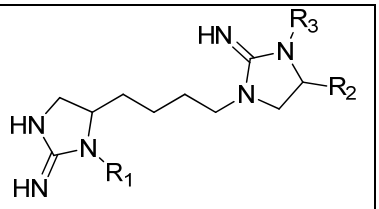
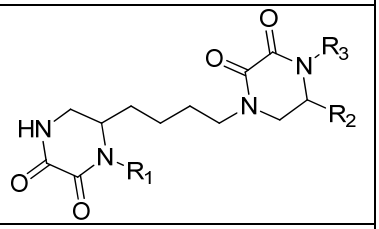
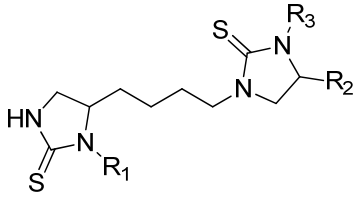
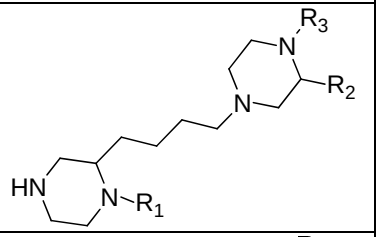
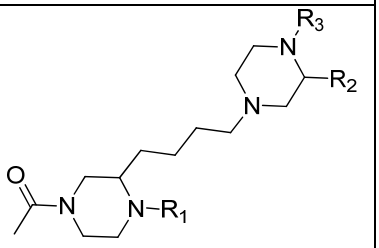
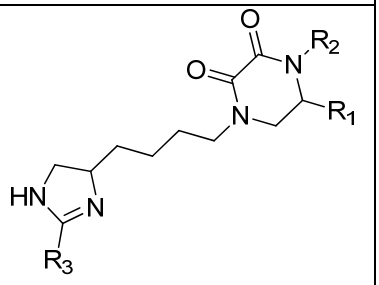
Figure S4. Structural differences result in shift of receptor functionality or specificity. Previously reported C1 to C7 (1) and AG-11/05 to AG-11/06 (2) as well as examples shown in this work [1754-49 to 1754-31 and 1754-20 to 1754-26] where slight structural modifications to a ligand produced a shift in receptor functionality.

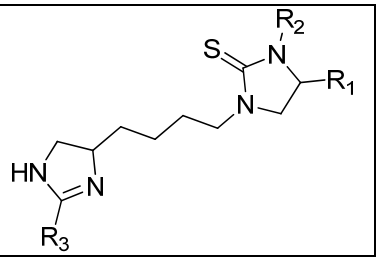
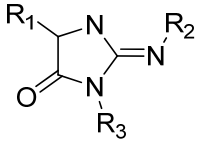
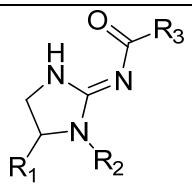
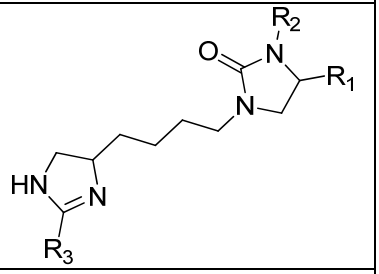
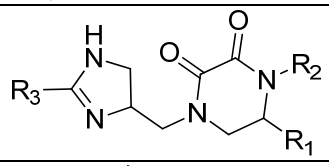
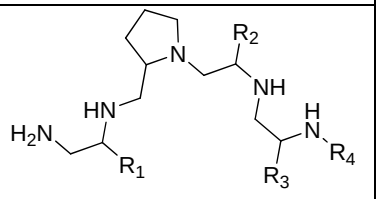
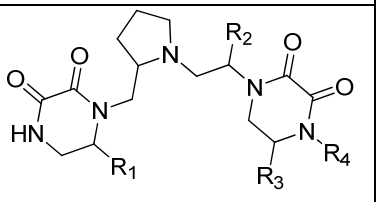
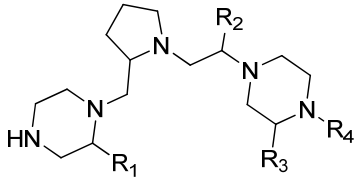
1. Zhou C et al. (2007) Pharmacological characterization of a novel nonpeptide antagonist for formyl peptide receptor-like 1. Mol Pharmacol 72:976-983.

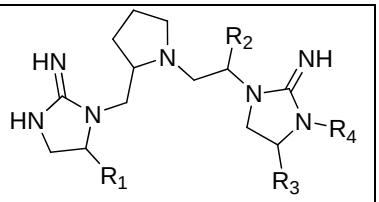
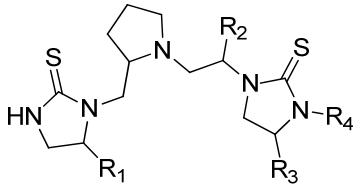
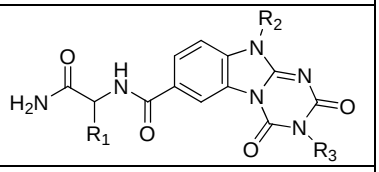
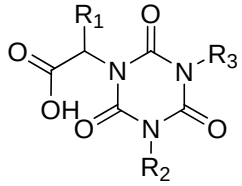
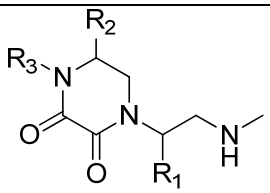
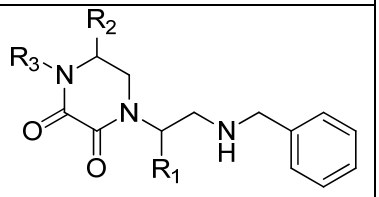
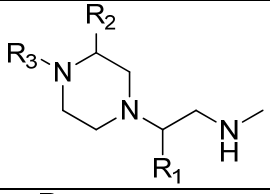
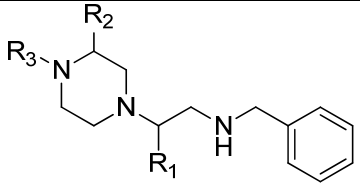
2. Kirpotina LN et al. (2010) Identification of novel small-molecule agonists for human formyl peptide receptors and pharmacophore models of their recognition. Mol Pharmacol 77:159-170.

Table S1. 37 small-molecule libraries tested against FPR1 and FPR2.

Number	Library	Samples	Compounds/mix	Total	Name	Structure
1	506	364	230	42,320	Alkylated triamine	
2	531	141	2,009 -2,499	102,459	Bicyclic guanidine	
3	882	125	1,681 – 1,763	72,283	C-6-acylamino bicyclic guanidine	
4	886	95	48	4,560	Benzothiazepene	
5	914	150	2,500	125,000	N-acyl triamine	
6	923	240	216,000	12,960,000	L-, D-, unnatural Tetrapeptide	
7	924	240	216,000	12,960,000	L-, D-, unnatural Tetrapeptide	
8	1002	109	1,190 – 1,400	47,600	Urea-linked bicyclic guanidine	

9	1169	110	1,092 -1,764	45,864	Bis-cyclic guanidine	
10	1170	110	1,092 -1,764	45,864	Bis-diketopiperazine	
11	1171	110	1,092 -1,764	45,864	Bis-cyclic thiourea	
12	1172	110	1,092 -1,764	45,864	Bis-piperazine	
13	1174	110	1,092 -1,764	45,864	N-acylated Bis-piperazine	
14	1275	116	1,258 – 1,665	56,610	Dihydroimidazolyl-butyl-diketopiperazine	

15	1276	116	1,258 – 1,665	56,610	Dihydroimidazolyl-butyl-cyclic thiourea	
16	1277	400	41	16,400	Guanidino hydantoin	
17	1295	107	1,224 – 1,332	45,288	Acylated cyclic guanidine	
18	1319	116	1,258 – 1,665	56,610	Dihydroimidazolyl-butyl-cyclic urea	
19	1324	116	1,258 – 1,665	56,610	Dihydroimidazolyl-methyl-diketopiperazine	
20	1343	120	17,576 - 28,392	738,192	Pyrrolidine pentamine	
21	1344	120	17,576 - 28,392	738,192	Pyrrolidine Bis-diketopiperazine	
22	1345	120	17,576 - 28,392	738,192	Pyrrolidine Bis-piperazine	

23	1346	120	17,576 - 28,392	738,192	Pyrrolidine Bis-cyclic guanidine	
24	1347	120	17,576 - 28,392	738,192	Pyrrolidine Bis-cyclic thiourea	
25	1387	400	40	16,000	Trisubstituted triazinobenzimidazolediones	
26	1409	400	27	10,800	Triazinetrione	
27	1418	96	783 -1,160	31,320	N-Methyl-1,4,5-trisubstituted-2,3-diketopiperazine	
28	1419	96	783 -1,160	31,320	N-Benzyl-1,4,5-trisubstited-2,3-diketopiperazine	
29	1420	96	783 -1,160	31,320	N-methylated 1,3,4-trisubstituted piperazine	
30	1421	96	783 -1,160	31,320	N-benzylated 1,3,4-trisubstituted piperazine	

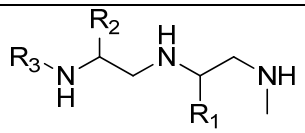
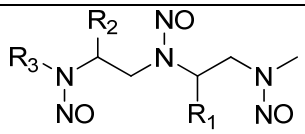
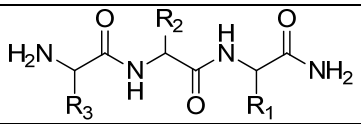
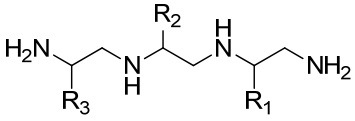
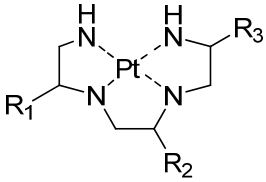
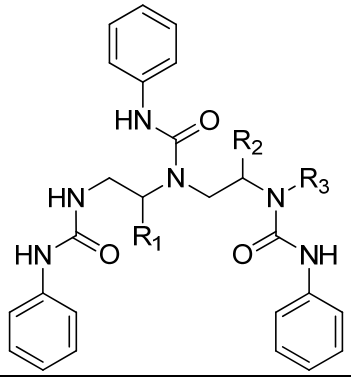
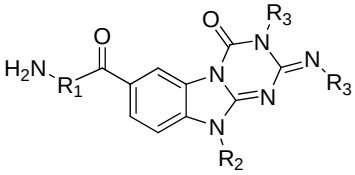
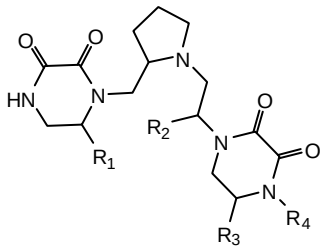
31	1422	96	783 -1,160	31,320	N-Methyltriamine	
32	1433	74	361 - 684	12,996	Nitrosamine	
33	1455	174	3,364	195,112	L-, D-, unnatural Tripeptide	
34	1456	174	3,364	195,112	Tetramine	
35	1477	174	3,364	195,112	Platinum tetramine	
36	1481	135	1,872 – 2,304	89,856	Poly-phenylurea	
37	1509	319	42	13,398	2-imino-1,3,5-triazino [1,2-a] benzimidazoles	

Table S2. Pyrrolidine bis-diketopiperazine positional scanning library (1344, library 21 in Figure 1) and resulting functionalities at the four positions of diversity.



Number			Building block	Functionality
1	27	53	Boc-L-Ala	*S*-methyl
2	28	54	Boc-L-Phe	*S*-benzyl
3	29	55	Boc-Gly	Hydrogen
4	30	56	Boc-L-Ile	*S*-2-butyl
5	31	57	Boc-L-Leu	*S*-isobutyl
6	32	58	Boc-L-Ser(Bzl)	*R*-hydroxymethyl
7	33	59	Boc-L-Thr(Bzl)	(*R*,*R*)-1-hydroxyethyl
8	34	60	Boc-L-Val	*S*-isopropyl
9	35	61	Boc-L-Tyr(BrZ)	*S*-4-hydroxybenzyl
10	36	62	Boc-D-Ala	*R*-methyl
11	37	63	Boc-D-Phe	*R*-benzyl
12	38	64	Boc-D-Ile	*R*-2-butyl
13	39	65	Boc-D-Leu	*R*-isobutyl
14	40	66	Boc-D-Ser(Bzl)	*S*-hydroxymethyl
15	41	67	Boc-D-Thr(Bzl)	(*S*,*S*)-1-hydroxyethyl
16	42	68	Boc-D-Val	*R*-isopropyl
17	43	69	Boc-D-Tyr(BrZ)	*R*-4-hydroxybenzyl
18	44	70	Boc-L-Phenylglycine	*S*-phenyl
19	45	71	Boc-L-Norvaline	*S*-propyl
20	46	72	Boc-D-Norvaline	*R*-propyl
21	47	73	Boc-L-Norleucine	*S*-butyl
22	48	74	Boc-D-Norleucine	*R*-butyl
23	49	75	Boc-L-Naphthylalanine	*S*-2-naphthylmethyl
24	50	76	Boc-D-Naphthylalanine	*R*-2-naphthylmethyl
25	51	77	Boc-L-Cyclohexylalanine	*S*-cyclohexyl
26	52	78	Boc-D-Cyclohexylalanine	*R*-cyclohexyl
		79	1-Phenyl-1-cyclopropanecarboxylic acid	(1-Phenyl-cyclopropyl)-methyl
		80	2-Phenylbutyric acid	2-Phenylbutyl
		81	3-Phenylbutyric acid	3-Phenylbutyl
		82	*m*-Tolylacetic acid	*m*-tolylethyl
		83	3-Fluorophenylacetic acid	2-(3-Fluoro-phenyl)-ethyl
		84	3-Bromophenylacetic acid	2-(3-Bromo-phenyl)-ethyl
		85	α,α,α-Trifluoro-m-Tolyl) acetic acid	2-(3-Trifluoromethyl-phenyl)-ethyl
		86	*p*-Tolylacetic acid	*p*-tolylethyl
		87	4-Fluorophenylacetic acid	2-(4-Fluoro-phenyl)-ethyl

88	3-Methoxyphenylacetic acid	2-(3-Methoxy-phenyl)-ethyl
89	4-Bromophenylacetic acid	2-(4-Bromo-phenyl)-ethyl
90	4-Methoxyphenylacetic acid	2-(4-Methoxy-phenyl)-ethyl
91	4-Ethoxyphenylacetic acid	2-(4-Ethoxy-phenyl)-ethyl
92	4-Isobutyl-alpha-Methylphenylacetic acid	2-(4-Isobutyl-phenyl)-propyl
93	3,4-Dichlorophenylacetic acid	3,4-Dichlorophenethyl
94	3,5-Bis(Trifluoromethyl)-Phenylacetic acid	2-(3,5-bis-trifluoromethyl-phenyl)-ethyl
95	3-(3,4-Dimethoxyphenyl)-Propionic acid	3-(3,4-Dimethoxy-phenyl)-propyl
96	Phenylacetic acid	Phenethyl
97	3,4,5-Trimethoxybenzoic acid	3,4,5-Trimethoxy-benzyl
98	Butyric acid	Butyl
99	Heptanoic acid	Heptyl
100	Isobutyric acid	Isobutyl
101	2-Methylbutyric acid	2-Methylbutyl
102	Isovaleric acid	3-Methylbutyl
103	3-Methylvaleric acid	3-Methylpentyl
104	4-Methylvaleric acid	4-Methylpentyl
105	p-Toluic acid	4-Methyl-benzyl
106	Cyclopentanecarboxylic acid	Cyclopentyl-methyl
107	Cyclohexanecarboxylic acid	Cyclohexyl-methyl
108	Cyclohexylacetic acid	Cyclohexyl-ethyl
109	Cyclohexanebutyric acid	Cyclohexyl-butyl
110	Cycloheptanecarboxylic acid	Cycloheptyl-methyl
111	2-Methylcyclopropanecarboxylic acid	(2-Methyl-cyclopropyl)-methyl
112	Cyclobutanecarboxylic acid	Cyclobutyl-methyl
113	3-Cyclopentylpropionic acid	3-Cyclopentyl-propyl
114	Cyclohexanepropionic acid	Cyclohexyl-propyl
115	4-Methyl-1-Cyclohexanecarboxylic acid	4-Methyl-1-cyclohexyl-methyl
116	4-tert-Butyl-Cyclohexanecarboxylic acid	4-*tert*-butyl-cyclohexyl-methyl
117	4-Biphenylacetic acid	2-Biphenyl-4-yl-ethyl
118	1-Adamantanecarboxylic acid	Adamantan-1-yl-methyl
119	1-Adamantaneacetic acid	2-Adamantan-1-yl-ethyl
120	2-Norbornaneacetic acid	2-Bicyclo[2.2.1]hept-2-yl-ethyl

Sublibrary 1: R_1 defined for samples 1-26 (28,392 compounds each). Sublibrary 2: R_2 defined for samples 27-52 (28,392 compounds each). Sublibrary 3: R_3 defined for samples 53-78 (28,392 compounds each). Sublibrary 4: R_4 defined for samples 79-120 (17,576 compounds each).

Table S3. Analytical information for compounds shown in Table 2.

Compund	Molecular weight	Molecular weight found	% Peak area at 254nm
a: 1754-113	697.86	698	35:65 [a]
b: 1754-56	721.93	722	99
c: 1754-26	707.9	708	99
d: 1754-20	771.94	772	99
e: 1754-19	687.87	688	99
f: 1754-31	721.93	722	99
g: 1754-49	721.93	722	99
h: 1753-103	662.86	663	99

[a] Compound 1754-113 contains a racemic mixture at the R3 position with a ratio of 35:65.

Dataset S1. Structure and activity information for 106 individual compounds derived from library 21:1344

All compounds were analyzed by LCMS. In all cases the LCMS data identified the desired compound as the major product; the MW found for the major product is reported in the table. 55 of the 106 compounds were tested in the duplex assay as crude material, while the remaining 51 compounds underwent RP-HPLC purification prior to obtaining their reported activity values. It should be noted that all "Pure" compounds were initially screened as "Crude" and the values reported for purified compounds did not deviate significantly from their activity levels when tested as crude. We therefore consider the activity values reported for the 56 "Crude" compounds to be accurate.

Compound #	R1 Functionality	R2 Functionality	R3 Functionality	R4 Functionality	FPR1 Ki, nM	FPR2 Ki, nM
1754-1	R-2-naphthylmethyl	R-4-hydroxybenzyl	R-benzyl	4-methyl-1-cyclohexyl-methyl	>10,000	>10,000
1754-2	R-2-naphthylmethyl	R-4-hydroxybenzyl	R-4-hydroxybenzyl	cyclohexyl-propyl	>10,000	>10,000
1754-3	R-2-naphthylmethyl	R-4-hydroxybenzyl	R-butyl	4-methyl-1-cyclohexyl-methyl	4,078	>10,000
1754-4	R-2-naphthylmethyl	R-2-naphthylmethyl	R-benzyl	cyclohexyl-methyl	>10,000	>10,000
1754-5	R-2-naphthylmethyl	R-2-naphthylmethyl	R-benzyl	4-methyl-1-cyclohexyl-methyl	>10,000	>10,000
1754-6	R-2-naphthylmethyl	R-2-naphthylmethyl	R-4-hydroxybenzyl	cyclohexyl-methyl	>10,000	>10,000
1754-7	R-2-naphthylmethyl	R-2-naphthylmethyl	R-4-hydroxybenzyl	cyclohexyl-propyl	>10,000	>10,000
1754-8	R-2-naphthylmethyl	R-2-naphthylmethyl	R-butyl	cyclohexyl-methyl	>10,000	>10,000
1754-10	S-propyl	R-2-naphthylmethyl	R-butyl	4-methyl-1-cyclohexyl-methyl	>10,000	135
1754-11	S-isopropyl	R-2-naphthylmethyl	R-propyl	cyclopently-methyl	>10,000	9
1754-12	S-isopropyl	R-2-naphthylmethyl	R-butyl	cycloheptyl-methyl	2,667	12
1754-13	S-isopropyl	R-2-naphthylmethyl	R-butyl	cyclobutyl-methyl	1,438	6
1754-14	S-isopropyl	R-cyclohexyl	R-4-hydroxybenzyl	3-methylpentyl	>10,000	505
1754-15	S-isopropyl	R-cyclohexyl	R-4-hydroxybenzyl	cyclopently-methyl	>10,000	183
1754-16	S-isopropyl	R-cyclohexyl	R-4-hydroxybenzyl	cyclohexyl-methyl	>10,000	69
1754-17	S-isopropyl	R-4-hydroxybenzyl	R-benzyl	cyclohexyl-methyl	753	10
1754-18	S-isopropyl	R-4-hydroxybenzyl	R-benzyl	2-Biphenyl-4-yl-ethyl	355	21
1754-19	S-isopropyl	R-4-hydroxybenzyl	R-4-hydroxybenzyl	cyclohexyl-methyl	3,368	6
1754-20	S-isopropyl	R-4-hydroxybenzyl	R-4-hydroxybenzyl	2-Biphenyl-4-yl-ethyl	>10,000	15
1754-21	S-isopropyl	R-4-hydroxybenzyl	R-butyl	cyclohexyl-methyl	951	5
1754-22	S-isopropyl	R-4-hydroxybenzyl	R-butyl	2-Biphenyl-4-yl-ethyl	>10,000	31
1754-23	S-isopropyl	R-propyl	R-benzyl	cyclohexyl-methyl	1,053	1,500
1754-24	S-isopropyl	R-propyl	R-benzyl	2-Biphenyl-4-yl-ethyl	330	229
1754-25	S-isopropyl	R-propyl	R-4-hydroxybenzyl	cyclohexyl-methyl	721	2,400
1754-26	S-isopropyl	R-propyl	R-4-hydroxybenzyl	2-Biphenyl-4-yl-ethyl	46	70
1754-27	S-isopropyl	R-propyl	R-butyl	cyclohexyl-methyl	758	602
1754-28	S-isopropyl	R-propyl	R-butyl	2-Biphenyl-4-yl-ethyl	279	58
1754-29	S-isopropyl	R-2-naphthylmethyl	R-benzyl	cyclohexyl-methyl	754	8
1754-30	S-isopropyl	R-2-naphthylmethyl	R-benzyl	2-Biphenyl-4-yl-ethyl	>10,000	51
1754-31	S-isopropyl	R-2-naphthylmethyl	R-4-hydroxybenzyl	cyclohexyl-methyl	>10,000	1
1754-32	S-isopropyl	R-2-naphthylmethyl	R-4-hydroxybenzyl	2-Biphenyl-4-yl-ethyl	>10,000	21
1754-33	S-isopropyl	R-2-naphthylmethyl	R-butyl	cyclohexyl-methyl	260	1
1754-34	S-isopropyl	R-2-naphthylmethyl	R-butyl	2-Biphenyl-4-yl-ethyl	664	11
1754-35	S-propyl	R-4-hydroxybenzyl	R-benzyl	cyclohexyl-methyl	385	98
1754-36	S-propyl	R-4-hydroxybenzyl	R-benzyl	2-Biphenyl-4-yl-ethyl	1,123	175
1754-37	S-propyl	R-4-hydroxybenzyl	R-4-hydroxybenzyl	cyclohexyl-methyl	436	105
1754-38	S-propyl	R-4-hydroxybenzyl	R-4-hydroxybenzyl	2-Biphenyl-4-yl-ethyl	1,792	98
1754-39	S-propyl	R-4-hydroxybenzyl	R-butyl	cyclohexyl-methyl	1,336	163
1754-40	S-propyl	R-4-hydroxybenzyl	R-butyl	2-Biphenyl-4-yl-ethyl	877	265
1754-41	S-propyl	R-propyl	R-benzyl	cyclohexyl-methyl	228	>10,000
1754-42	S-propyl	R-propyl	R-benzyl	2-Biphenyl-4-yl-ethyl	63	591
1754-43	S-propyl	R-propyl	R-4-hydroxybenzyl	cyclohexyl-methyl	90	>10,000
1754-44	S-propyl	R-propyl	R-4-hydroxybenzyl	2-Biphenyl-4-yl-ethyl	2	162
1754-45	S-propyl	R-propyl	R-butyl	cyclohexyl-methyl	966	5,997
1754-46	S-propyl	R-propyl	R-butyl	2-Biphenyl-4-yl-ethyl	473	410
1754-47	S-propyl	R-2-naphthylmethyl	R-benzyl	cyclohexyl-methyl	1,373	74
1754-48	S-propyl	R-2-naphthylmethyl	R-benzyl	2-Biphenyl-4-yl-ethyl	>10,000	512
1754-49	S-propyl	R-2-naphthylmethyl	R-4-hydroxybenzyl	cyclohexyl-methyl	2,322	33
1754-50	S-propyl	R-2-naphthylmethyl	R-4-hydroxybenzyl	2-Biphenyl-4-yl-ethyl	>10,000	445
1754-51	S-propyl	R-2-naphthylmethyl	R-butyl	cyclohexyl-methyl	3,492	44
1754-52	S-propyl	R-2-naphthylmethyl	R-butyl	2-Biphenyl-4-yl-ethyl	>10,000	454
1754-56	S-butyl	R-propyl	R-4-hydroxybenzyl	2-Biphenyl-4-yl-ethyl	2	1,321
1754-57	S-benzyl	S-hydroxymethyl	R,S-phenyl	4-methyl-1-cyclohexyl-methyl	2,964	>10,000
1754-59	S-butyl	S-hydroxymethyl	S-2-butyl	4-methyl-1-cyclohexyl-methyl	>10,000	>10,000
1754-60	S-butyl	S-hydroxymethyl	S-cyclohexyl	4-methyl-1-cyclohexyl-methyl	>10,000	>10,000
1754-61	S-butyl	R-propyl	S-cyclohexyl	4-methyl-1-cyclohexyl-methyl	411	8,519
1754-64	S-butyl	S-hydroxymethyl	S-2-butyl	cyclohexyl-methyl	>10,000	>10,000
1754-65	S-butyl	S-hydroxymethyl	S-2-butyl	4-tert-butyl-cyclohexyl-methyl	1,847	>10,000
1754-67	S-butyl	R-propyl	S-cyclohexyl	cyclobutyl-methyl	773	>10,000
1754-68	S-butyl	R-butyl	S-cyclohexyl	cyclohexyl-methyl	2,336	>10,000
1754-69	S-propyl	S-hydroxymethyl	R,S-phenyl	cyclohexyl-methyl	1,953	>10,000
1754-70	S-propyl	S-hydroxymethyl	R,S-phenyl	4-methyl-1-cyclohexyl-methyl	2,232	>10,000
1754-71	S-propyl	S-hydroxymethyl	R,S-phenyl	2-Biphenyl-4-yl-ethyl	1,265	3,799
1754-75	S-butyl	S-hydroxymethyl	R,S-phenyl	cyclohexyl-methyl	5,493	>10,000
1754-76	S-butyl	S-hydroxymethyl	R,S-phenyl	4-methyl-1-cyclohexyl-methyl	3,192	>10,000
1754-77	S-butyl	S-hydroxymethyl	R,S-phenyl	2-Biphenyl-4-yl-ethyl	1,504	>10,000
1754-78	S-butyl	S-hydroxymethyl	S-cyclohexyl	2-Biphenyl-4-yl-ethyl	797	>10,000
1754-79	S-propyl	S-benzyl	R,S-phenyl	cyclohexyl-methyl	872	>10,000
1754-80	S-propyl	S-benzyl	R,S-phenyl	4-methyl-1-cyclohexyl-methyl	583	>10,000
1754-81	S-propyl	S-benzyl	R,S-phenyl	2-Biphenyl-4-yl-ethyl	121	>10,000
1754-82	S-propyl	S-benzyl	S-cyclohexyl	cyclohexyl-methyl	560	>10,000
1754-83	S-propyl	S-benzyl	S-cyclohexyl	4-methyl-1-cyclohexyl-methyl	410	>10,000
1754-84	S-propyl	S-benzyl	S-cyclohexyl	2-Biphenyl-4-yl-ethyl	2,019	>10,000
1754-85	S-propyl	S-isobutyl	R,S-phenyl	cyclohexyl-methyl	6,139	3,262
1754-86	S-propyl	S-isobutyl	R,S-phenyl	4-methyl-1-cyclohexyl-methyl	3,641	5,861
1754-87	S-propyl	S-isobutyl	R,S-phenyl	2-Biphenyl-4-yl-ethyl	663	>10,000
1754-88	S-propyl	S-isobutyl	S-cyclohexyl	cyclohexyl-methyl	145	>10,000
1754-89	S-propyl	S-isobutyl	S-cyclohexyl	4-methyl-1-cyclohexyl-methyl	463	>10,000
1754-90	S-propyl	S-isobutyl	S-cyclohexyl	2-Biphenyl-4-yl-ethyl	1,133	>10,000
1754-91	S-butyl	S-benzyl	R,S-phenyl	cyclohexyl-methyl	470	>10,000
1754-93	S-butyl	S-benzyl	R,S-phenyl	2-Biphenyl-4-yl-ethyl	52	>10,000
1754-94	S-butyl	S-benzyl	S-cyclohexyl	cyclohexyl-methyl	375	>10,000
1754-95	S-butyl	S-benzyl	S-cyclohexyl	4-methyl-1-cyclohexyl-methyl	217	>10,000
1754-96	S-butyl	S-benzyl	S-cyclohexyl	2-Biphenyl-4-yl-ethyl	595	>10,000

Compound #	R1 Functionality	R2 Functionality	R3 Functionality	R4 Functionality	FPR1 Ki, nM	FPR2 Ki, nM
1754-97	S-butyl	S-isobutyl	R,S-phenyl	cyclohexyl-methyl	>10,000	2,569
1754-98	S-butyl	S-isobutyl	R,S-phenyl	4-methyl-1-cyclohexyl-methyl	1,684	>10,000
1754-99	S-butyl	S-isobutyl	R,S-phenyl	2-Biphenyl-4-yl-ethyl	592	>10,000
1754-100	S-butyl	S-isobutyl	S-cyclohexyl	cyclohexyl-methyl	173	>10,000
1754-101	S-butyl	S-isobutyl	S-cyclohexyl	4-methyl-1-cyclohexyl-methyl	511	>10,000
1754-102	S-butyl	S-isobutyl	S-cyclohexyl	2-Biphenyl-4-yl-ethyl	677	>10,000
1754-103	S-benzyl	S-benzyl	R,S-phenyl	2-(3-methoxy-phenyl)-ethyl	15	>10,000
1754-104	S-benzyl	S-benzyl	R,S-phenyl	2-(4-Isobutyl-phenyl)-propyl	7	>10,000
1754-105	S-benzyl	S-benzyl	R,S-phenyl	2-Biphenyl-4-yl-ethyl	12	>10,000
1754-106	S-butyl	S-benzyl	S-2-butyl	2-(3-methoxy-phenyl)-ethyl	84	3,863
1754-107	S-butyl	S-benzyl	R,S-phenyl	m-tolylethyl	20	>10,000
1754-108	S-butyl	S-benzyl	R,S-phenyl	p-tolylethyl	37	>10,000
1754-109	S-butyl	S-benzyl	R,S-phenyl	2-(3-methoxy-phenyl)-ethyl	16	>10,000
1754-110	S-butyl	S-benzyl	R,S-phenyl	2-(4-methoxy-phenyl)-ethyl	14	>10,000
1754-111	S-butyl	S-benzyl	R,S-phenyl	2-(4-ethoxy-phenyl)-ethyl	73	>10,000
1754-113	S-benzyl	S-benzyl	R,S-phenyl	phenethyl	3	>10,000
1754-114	S-benzyl	S-benzyl	S-benzyl	3-(3 4-dimethoxy-phenyl)-propyl	491	>10,000
1754-115	S-benzyl	S-benzyl	S-propyl	phenethyl	9	>10,000
1754-116	S-benzyl	S-benzyl	S-2-butyl	phenethyl	77	>10,000
1858-480	S-butyl	R-propyl	R-4-hydroxybenzyl	4-methyl-1-cyclohexyl-methyl	>10,000	>10,000
1858-482	S-butyl	R-propyl	R-4-hydroxybenzyl	cyclohexyl-methyl	28	>10,000
1858-483	S-propyl	R-propyl	R-4-hydroxybenzyl	4-methyl-1-cyclohexyl-methyl	>10,000	>10,000

Compound #	Molecular Weight	Molecular Weight Found	Compound grade
1754-1	784	784	Pure
1754-2	814	814	Pure
1754-3	750	750	Pure
1754-4	804	804	Pure
1754-5	818	818	Pure
1754-6	820	820	Pure
1754-7	848	848	Pure
1754-8	770	771	Pure
1754-10	686	686	Pure
1754-11	644	644	Pure
1754-12	686	686	Pure
1754-13	644	644	Pure
1754-14	666	666	Pure
1754-15	664	664	Pure
1754-16	678	678	Pure
1754-17	672	673	Pure
1754-18	756	757	Pure
1754-19	688	688	Pure
1754-20	772	772	Pure
1754-21	638	638	Pure
1754-22	722	722	Pure
1754-23	608	608	Crude
1754-24	692	692	Crude
1754-25	624	624	Crude
1754-26	708	708	Pure
1754-27	574	574	Pure
1754-28	658	658	Crude
1754-29	706	706	Pure
1754-30	790	790	Pure
1754-31	722	722	Pure
1754-32	806	806	Pure
1754-33	672	672	Pure
1754-34	756	756	Pure
1754-35	672	672	Crude
1754-36	756	756	Crude
1754-37	688	688	Crude
1754-38	772	772	Crude
1754-39	638	638	Crude
1754-40	722	722	Crude
1754-41	608	608	Crude
1754-42	692	695	Crude
1754-43	624	624	Pure
1754-44	708	708	Pure
1754-45	574	574	Crude
1754-46	658	658	Crude
1754-47	706	706	Crude
1754-48	790	790	Crude
1754-49	722	722	Crude
1754-50	806	806	Crude
1754-51	672	672	Crude
1754-52	756	756	Crude
1754-56	722	722	Pure
1754-57	644	644	Pure
1754-59	590	590	Pure
1754-60	630	630	Pure
1754-61	642	642	Pure
1754-64	576	576	Crude
1754-65	632	632	Crude
1754-67	600	600	Crude
1754-68	642	642	Crude
1754-69	582	582	Crude
1754-70	596	596	Crude
1754-71	666	666	Crude
1754-75	596	596	Crude
1754-76	610	610	Crude
1754-77	680	680	Crude
1754-78	700	700	Crude
1754-79	642	642	Crude
1754-80	656	656	Crude
1754-81	726	726	Crude
1754-82	662	662	Crude
1754-83	676	676	Crude
1754-84	746	746	Crude
1754-85	608	608	Crude
1754-86	622	622	Crude
1754-87	692	692	Crude
1754-88	628	628	Crude
1754-89	642	642	Crude
1754-90	712	712	Crude
1754-91	656	656	Crude
1754-93	740	740	Pure
1754-94	676	676	Crude
1754-95	690	690	Crude
1754-96	760	760	Crude
1754-97	622	622	Crude
1754-98	636	636	Crude

Compound #	Molecular Weight	Molecular Weight Found	Compound grade
1754-99	706	706	Crude
1754-100	642	642	Crude
1754-101	656	656	Pure
1754-102	726	726	Crude
1754-103	728	728	Crude
1754-104	768	768	Pure
1754-105	774	774	Pure
1754-106	674	674	Pure
1754-107	678	678	Pure
1754-108	678	678	Crude
1754-109	694	694	Pure
1754-110	694	694	Pure
1754-111	708	708	Pure
1754-113	698	698	Pure
1754-114	786	786	Crude
1754-115	664	664	Pure
1754-116	678	678	Pure
1858-480	652	652	Pure
1858-482	638	638	Pure
1858-483	638	638	Pure

Compound #	SMILES
1754-1	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CC2CCC(CC2)C(=O)C1=O)Cc1ccccc1)CN1CCC[C@H]1CN1[C@@H](CNC(=O)C1=O)Cc1cc2c(cc1)cccc2
1754-2	Oc1ccc(cc1)C[C@H]1N(CCCC2CCCCC2)C(=O)C(=O)N(C1)[C@H](Cc1ccc(O)cc1)CN1CCC[C@H]1CN1[C@@H](CNC(=O)C1=O)Cc1cc2c(cc1)cccc2
1754-3	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CC2CCC(CC2)C(=O)C1=O)CCCC)CN1CCC[C@H]1CN1[C@@H](CNC(=O)C1=O)Cc1cc2c(cc1)cccc2
1754-4	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@@H](CNC(=O)C2=O)Cc2cc3c(cc2)cccc3)C1=O)Cc1ccccc1
1754-5	O=C1N(CC2CCC(CC2)C)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@@H](CNC(=O)C2=O)Cc2cc3c(cc2)cccc3)C1=O)Cc1ccccc1
1754-6	Oc1ccc(cc1)C[C@H]1N(CC2CCCCC2)C(=O)C(=O)N(C1)[C@H](Cc1cc2c(cc1)cccc2)CN1CCC[C@H]1CN1[C@@H](CNC(=O)C1=O)Cc1cc2c(cc1)cccc2
1754-7	Oc1ccc(cc1)C[C@H]1N(CCCC2CCCCC2)C(=O)C(=O)N(C1)[C@H](Cc1cc2c(cc1)cccc2)CN1CCC[C@H]1CN1[C@@H](CNC(=O)C1=O)Cc1cc2c(cc1)cccc2
1754-8	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@@H](CNC(=O)C2=O)Cc2cc3c(cc2)cccc3)C1=O)CCCC
1754-10	O=C1N(CC2CCC(CC2)C)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CCCC
1754-11	O=C1N(CC2CCCC2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)CCC
1754-12	O=C1N(CC2CCCCCC2)[C@@H](CN([C@H](Cc2cc3c(cc2)ccccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)CCCC
1754-13	O=C1N(CC2CCC2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)CCCC
1754-14	Oc1ccc(cc1)C[C@H]1N(CCC(CC)C)C(=O)C(=O)N(C1)[C@H](CC1CCCCC1)CN1CCC[C@H]1CN1C(=O)C(=O)NCC1C(C)C
1754-15	Oc1ccc(cc1)C[C@H]1N(CC2CCCC2)C(=O)C(=O)N(C1)[C@H](CC1CCCCC1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-16	Oc1ccc(cc1)C[C@H]1N(CC2CCCCC2)C(=O)C(=O)N(C1)[C@H](CC1CCCCC1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-17	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CC2CCCCC2)C(=O)C1=O)Cc1ccccc1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-18	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CCc2ccc(cc2)-c2ccccc2)C(=O)C1=O)Cc1ccccc1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-19	Oc1ccc(cc1)C[C@H]1N(CC2CCCCC2)C(=O)C(=O)N(C1)[C@H](Cc1ccc(O)cc1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-20	Oc1ccc(cc1)C[C@H]1N(CCc2ccc(cc2)-c2ccccc2)C(=O)C(=O)N(C1)[C@H](Cc1ccc(O)cc1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-21	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CC2CCCCC2)C(=O)C1=O)CCCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-22	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CCc2ccc(cc2)-c2ccccc2)C(=O)C1=O)CCCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-23	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)Cc1ccccc1
1754-24	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)Cc1ccccc1
1754-25	Oc1ccc(cc1)C[C@H]1N(CC2CCCCC2)C(=O)C(=O)N(C1)[C@H](CCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-26	Oc1ccc(cc1)C[C@H]1N(CCc2ccc(cc2)-c2ccccc2)C(=O)C(=O)N(C1)[C@H](CCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-27	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)CCCC
1754-28	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)CCCC
1754-29	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)Cc1ccccc1
1754-30	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)Cc1ccccc1
1754-31	Oc1ccc(cc1)C[C@H]1N(CC2CCCCC2)C(=O)C(=O)N(C1)[C@H](Cc1cc2c(cc1)cccc2)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-32	Oc1ccc(cc1)C[C@H]1N(CCc2ccc(cc2)-c2ccccc2)C(=O)C(=O)N(C1)[C@H](Cc1cc2c(cc1)cccc2)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)C(C)C
1754-33	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)CCCC
1754-34	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)C(C)C)C1=O)CCCC
1754-35	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CC2CCCCC2)C(=O)C1=O)Cc1ccccc1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-36	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CCc2ccc(cc2)-c2ccccc2)C(=O)C1=O)Cc1ccccc1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-37	Oc1ccc(cc1)C[C@H]1N(CC2CCCCC2)C(=O)C(=O)N(C1)[C@H](Cc1ccc(O)cc1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-38	Oc1ccc(cc1)C[C@H]1N(CCc2ccc(cc2)-c2ccccc2)C(=O)C(=O)N(C1)[C@H](Cc1ccc(O)cc1)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-39	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CC2CCCCC2)C(=O)C1=O)CCCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-40	Oc1ccc(cc1)C[C@@H](N1C[C@H](N(CCc2ccc(cc2)-c2ccccc2)C(=O)C1=O)CCCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-41	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)Cc1ccccc1
1754-42	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)Cc1ccccc1
1754-43	Oc1ccc(cc1)C[C@H]1N(CC2CCCCC2)C(=O)C(=O)N(C1)[C@H](CCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-44	Oc1ccc(cc1)C[C@H]1N(CCc2ccc(cc2)-c2ccccc2)C(=O)C(=O)N(C1)[C@H](CCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-45	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CCCC
1754-46	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CCCC
1754-47	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)Cc1ccccc1
1754-48	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)Cc1ccccc1
1754-49	Oc1ccc(cc1)C[C@H]1N(CC2CCCCC2)C(=O)C(=O)N(C1)[C@H](Cc1cc2c(cc1)cccc2)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-50	Oc1ccc(cc1)C[C@H]1N(CCc2ccc(cc2)-c2ccccc2)C(=O)C(=O)N(C1)[C@H](Cc1cc2c(cc1)cccc2)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC
1754-51	O=C1N(CC2CCCCC2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CCCC
1754-52	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@@H](CN([C@H](Cc2cc3c(cc2)cccc3)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CCCC
1754-56	Oc1ccc(cc1)C[C@H]1N(CCc2ccc(cc2)-c2ccccc2)C(=O)C(=O)N(C1)[C@H](CCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCCC
1754-57	O=C1N(CC2CCC(CC2)C)C(CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)Cc2ccccc2)CO)C1=O)c1ccccc1
1754-59	O=C1N(CC2CCC(CC2)C)[C@H](CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)CO)C1=O)C(CC)C
1754-60	O=C1N(CC2CCC(CC2)C)[C@H](CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)CO)C1=O)CC1CCCCC1
1754-61	O=C1N(CC2CCC(CC2)C)[C@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)CC1CCCCC1
1754-64	O=C1N(CC2CCCCC2)[C@H](CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)CO)C1=O)C(CC)C
1754-65	O=C1N(CC2CCC(CC2)C(C)(C)C)[C@H](CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)CO)C1=O)C(CC)C
1754-67	O=C1N(CC2CCC2)[C@H](CN([C@H](CCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)CC1CCCCC1
1754-68	O=C1N(CC2CCCCC2)[C@H](CN([C@H](CCCC)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)CC1CCCCC1
1754-69	O=C1N(CC2CCCCC2)C(CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)CO)C1=O)c1ccccc1
1754-70	O=C1N(CC2CCC(CC2)C)C(CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)CO)C1=O)c1ccccc1
1754-71	O=C1N(CCc2ccc(cc2)-c2ccccc2)C(CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)CO)C1=O)c1ccccc1
1754-75	O=C1N(CC2CCCCC2)C(CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)CO)C1=O)c1ccccc1
1754-76	O=C1N(CC2CCC(CC2)C)C(CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)CO)C1=O)c1ccccc1
1754-77	O=C1N(CCc2ccc(cc2)-c2ccccc2)C(CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)CO)C1=O)c1ccccc1
1754-78	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@H](CN([C@@H](CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)CO)C1=O)CC1CCCCC1
1754-79	O=C1N(CC2CCCCC2)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)c1ccccc1
1754-80	O=C1N(CC2CCC(CC2)C)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)c1ccccc1
1754-81	O=C1N(CCc2ccc(cc2)-c2ccccc2)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)c1ccccc1
1754-82	O=C1N(CC2CCCCC2)[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CC1CCCCC1
1754-83	O=C1N(CC2CCC(CC2)C)[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CC1CCCCC1
1754-84	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CC1CCCCC1
1754-85	O=C1N(CC2CCCCC2)C(CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)c1ccccc1
1754-86	O=C1N(CC2CCC(CC2)C)C(CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)c1ccccc1
1754-87	O=C1N(CCc2ccc(cc2)-c2ccccc2)C(CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)c1ccccc1
1754-88	O=C1N(CC2CCCCC2)[C@H](CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CC1CCCCC1
1754-89	O=C1N(CC2CCC(CC2)C)[C@H](CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CC1CCCCC1
1754-90	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@H](CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCC)C1=O)CC1CCCCC1
1754-91	O=C1N(CC2CCCCC2)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)c1ccccc1
1754-93	O=C1N(CCc2ccc(cc2)-c2ccccc2)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)c1ccccc1
1754-94	O=C1N(CC2CCCCC2)[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)CC1CCCCC1

Compound #	SMILES
1754-95	O=C1N(CC2CCC(CC2)C)[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)CC1CCCCC1
1754-96	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)CC1CCCCC1
1754-97	O=C1N(CC2CCCCC2)C(CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)c1ccccc1
1754-98	O=C1N(CC2CCC(CC2)C)C(CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)c1ccccc1
1754-99	O=C1N(CCc2ccc(cc2)-c2ccccc2)C(CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)c1ccccc1
1754-100	O=C1N(CC2CCCCC2)[C@H](CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)CC1CCCCC1
1754-101	O=C1N(CC2CCC(CC2)C)[C@H](CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)CC1CCCCC1
1754-102	O=C1N(CCc2ccc(cc2)-c2ccccc2)[C@H](CN([C@@H](CC(C)C)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)CC1CCCCC1
1754-103	O(C)c1cc(ccc1)CCN1C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)Cc2ccccc2)C(=O)C1=O)c1ccccc1
1754-104	O=C1N(CC(C)c2ccc(cc2)CC(C)C)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)Cc2ccccc2)C1=O)c1ccccc1
1754-105	O=C1N(CCc2ccc(cc2)-c2ccccc2)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)Cc2ccccc2)C1=O)c1ccccc1
1754-106	O(C)c1cc(ccc1)CCN1[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C(=O)C1=O)[C@H](CC)C
1754-107	O=C1N(CCc2cc(ccc2)C)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)c1ccccc1
1754-108	O=C1N(CCc2ccc(cc2)C)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C1=O)c1ccccc1
1754-109	O(C)c1cc(ccc1)CCN1C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C(=O)C1=O)c1ccccc1
1754-110	O(C)c1ccc(cc1)CCN1C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C(=O)C1=O)c1ccccc1
1754-111	O(CC)c1ccc(cc1)CCN1C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)CCCC)C(=O)C1=O)c1ccccc1
1754-113	O=C1N(CCc2ccccc2)C(CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)Cc2ccccc2)C1=O)c1ccccc1
1754-114	O(C)c1cc(ccc1OC)CCCN1[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)Cc2ccccc2)C(=O)C1=O)Cc1ccccc1
1754-115	O=C1N(CCc2ccccc2)[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)Cc2ccccc2)C1=O)CCC
1754-116	O=C1N(CCc2ccccc2)[C@H](CN([C@@H](Cc2ccccc2)CN2CCC[C@H]2CN2[C@H](CNC(=O)C2=O)Cc2ccccc2)C1=O)[C@H](CC)C
1858-480	Oc1ccc(cc1)C[C@H]1N(CC2CCC(CC2)C)C(=O)C(=O)N(C1)[C@H](CCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCCC
1858-482	Oc1ccc(cc1)C[C@H]1N(CC2CCCCC2)C(=O)C(=O)N(C1)[C@H](CCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCCC
1858-483	Oc1ccc(cc1)C[C@H]1N(CC2CCC(CC2)C)C(=O)C(=O)N(C1)[C@H](CCC)CN1CCC[C@H]1CN1[C@H](CNC(=O)C1=O)CCC

Dataset S2. Structure and activity information for 4 individual compounds derived from library 36:1481

All compounds were analyzed by LCMS. In all cases the LCMS data identified the desired compound as the major product; the MW found for the major product is reported in the table. All 4 compounds were tested in the duplex assay as pure material, as they underwent RP-HPLC purification prior to obtaining their reported activity values.

Compound #	R1 functionality	R2 functionality	R3 functionality	FPR1 Ki, nM	FPR2 Ki, nM
1753-101	S-methyl	R-4-(1-methyl-3-phenyl urea) butyl	4-phenylbutyl	1	>10,000
1753-102	S-methyl	R-4-(1-methyl-3-phenyl urea) butyl	4-methyl-1-cyclohexylmethyl	6	>10,000
1753-103	S-methyl	R-butyl	4-phenylbutyl	4	>10,000
1753-104	S-methyl	R-butyl	4-methyl-1-cyclohexylmethyl	21	>10,000

Compound #	Molecular Weight	Molecular Weight Found	Compound grade
1753-101	811	811	Pure
1753-102	789	789	Pure
1753-103	663	663	Pure
1753-104	641	641	Pure

Compound #	SMILES
1753-101	O=C(Nc1ccccc1)N(CCCC[C@@H](N(CCCCc1ccccc1)C(=O)Nc1ccccc1)CN([C@H](CNC(=O)Nc1ccccc1)C)C(=O)Nc1ccccc1)C
1753-102	O=C(Nc1ccccc1)N(CCCC[C@@H](N(CC1CCC(CC1)C)C(=O)Nc1ccccc1)CN([C@H](CNC(=O)Nc1ccccc1)C)C(=O)Nc1ccccc1)C
1753-103	O=C(Nc1ccccc1)N([C@H](CCCC)CN([C@H](CNC(=O)Nc1ccccc1)C)C(=O)Nc1ccccc1)CCCCc1ccccc1
1753-104	O=C(Nc1ccccc1)N([C@H](CCCC)CN([C@H](CNC(=O)Nc1ccccc1)C)C(=O)Nc1ccccc1)CC1CCC(CC1)C