

Supplementary Information

**Protein-ligand interaction study of signal transducer
smoothened protein with different drugs: Molecular docking and
QM/MM calculations**

Hossein Farrokhpour*, Vahid Pakatchian, Abdolreza Hajipour*, Fatemeh

Abyar, Alireza Najafi Chermahini and Farzaneh Fakhari

Chemistry Department, Isfahan University of Technology, Isfahan, 84156-83111, Iran

E-mail: farrokhphossein@gmail.com ; h-farrokh@cc.iut.ac.ir (H. Farrokhpour)

haji@cc.iut.ac.ir (Abdolreza Hajipour)

Tel : +98 311 3912343

Fax: +98 311 3912350

Table S1: List of ligands considered in virtual screening in this work.

Table S1

Name of the ligand	No
1-benzyl-4-(4-phenylpiperazin-1-yl)phthalazine	1
1-benzyl-4-(4-(pyridin-2-yl)piperazin-1-yl)phthalazine	2
1-benzyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)phthalazine	3
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinonitrile	4
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinamide	5
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridine-3-sulfonamide	6
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)-N,N-dimethylmethanamine	7
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)acetamide	8
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-amine	9
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinic acid	10
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methanol	11
1-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)ethanol	12
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-ol	13
2-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)cyclopropanol	14
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propane-1,2-diol	15
1-(4-(pyridin-2-yl)piperazin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	16
6-(4-(4-(4-fluorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	17
6-(4-(4-(3-chlorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	18
6-(4-(4-(4-chlorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	19
6-(4-(4-(4-cyanobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	20
6-(4-(4-(4-trifluoromethyl)benzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	21
methyl 4-((4-(4-(5-cyanopyridin-2-yl)piperazin-1-yl)phthalazin-1-yl)methyl)benzoate	22
4-((4-(4-(5-cyanopyridin-2-yl)piperazin-1-yl)phthalazin-1-yl)methyl)benzoic acid	23
6-(4-(4-benzylphthalazin-1-yl)-1,4-diazepan-1-yl)nicotinonitrile	24
(S)-6-(4-(4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl)nicotinonitrile	25

(R)-6-(4-(4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl)nicotinonitrile	26
(R)-6-(4-(4-benzylphthalazin-1-yl)-3-methylpiperazin-1-yl)nicotinonitrile	27
(S)-6-(4-(4-benzylphthalazin-1-yl)-3-methylpiperazin-1-yl)nicotinonitrile	28
4-(1-(4-benzylphthalazin-1-yl)piperidin-4-yl)benzonitrile	29
6-(4-(1-benzylisoquinolin-4-yl)piperazin-1-yl)nicotinonitrile	30
6-(4-(1-benzyl-1H-indol-3-yl)piperidin-1-yl)nicotinonitrile	31
7-benzyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)furo[3,2-d]pyridazine	32
4-benzyl-7-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)furo[2,3-d]pyridazine	33
7-benzyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)-1H-imidazo[4,5-d]pyridazine	34
N-(4-methoxy-3-(pyridin-4-yl)benzyl)-3-chloro-4,7-difluoro-N-(4-(methylamino)cyclohexyl)benzo[b]thiophene-2-carboxamide	35
N-(4-chloro-3-(6-(dimethylamino)-1H-benzo[d]imidazol-2-yl)phenyl)-3,5-dimethoxybenzamide	36
2-chloro-N-(4-chloro-3-(pyridin-2-yl)phenyl)-4-(methylsulfonyl)benzamide	37
6-hydroxy-9'-methoxystaurosporinone	38
Arcyriaflavin B	39
6-hydroxystaurosporinone	40
6,9'-dihydroxystaurosporinone	41
9'-hydroxystaurosporinone	42
-(-)Cyclopamine	43
(3R,5S)-5-methyl-2-((S)-1-((3S,6aS,11bR)-3,10,11b-trimethyl-2,3,4,6,6a,11,11a,11b-octahydro-1H-benzo[a]fluoren-9-yl)ethyl)piperidin-3-ol	44
Germine	45
IPI-926	46
1-(3-benzamidophenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	47
1-(3-benzamidophenyl)-3-(3,4,5-trimethoxybenzoyl)urea	48
1-(3-benzamidophenyl)-3-(3,5-dimethoxybenzoyl)thiourea	49
1-(3-benzamidophenyl)-3-(4-ethoxy-3,5-dimethoxybenzoyl)thiourea	50
1-(3-benzamidophenyl)-3-(3,4-diethoxy-5-methoxybenzoyl)thiourea	51
1-(3-benzamidophenyl)-3-(4-methoxybenzo[d][1,3]dioxole-6-carbonyl)thiourea	52
1-(3-benzamido-4-methoxyphenyl)-3-(4-methoxybenzoyl)thiourea	53

1-(3-benzamidophenyl)-3-(3,4,5-triethoxybenzoyl)thiourea	54
1-(3-benzamidophenyl)-3-(2,3-dihydrobenzo[b][1,4]dioxine-6-carbonyl)thiourea	55
1-(3-benzamidophenyl)-3-(3,4-dimethoxybenzoyl)thiourea	56
1-(3-(2-methoxybenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	57
1-(3-(3-methoxybenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	58
1-(3-(4-methoxybenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	59
1-(3-(2-chlorobenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	60
1-(3-(4-chlorobenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	61
1-(3-(4-phenylbenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	62
1-(3-(3,4,5-trimethoxybenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	63
1-(3-(4-fluorobenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	64
1-(3-(isonicotinamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	65
1-(3-(cyclohexanecarboxamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	66
1-(3-(thiophene-2-carboxamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	67
1-(3-isobutyramidophenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	68
1-(3-(1-naphthamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	69
1-(3-(2-naphthamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	70
1-(3-(furan-2-carboxamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	71
1-(3-(4-morpholinobenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	72
1-phenyl-3-(3-(3,4,5-trimethoxybenzoyl)thioureido)phenyl)urea	73
1-diphenyl-3-(3-(3,4,5-trimethoxybenzoyl)thioureido)phenyl)urea	74
1-(3-(1-H-indole-2-carboxamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	75
1-(3-(H-imidazo[1,2-a]pyridine-2-carboxamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	76
1-(3-(1-H-benzo[d]imidazole-1-carboxamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	77
1-(3-(imidazo[2,1-b]thiazole-6-carboxamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	78
1-(3-(1-H-indole-1-carboxamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	79
1-(3-benzamido-4-chlorophenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	80
1-(3-benzamido-4-fluorophenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	81

1-(3-benzamido-4-methoxyphenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	82
1-(3-benzamido-4-methylphenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	83
1-(5-benzamido-2-fluorophenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	84
1-(3-fluorobenzamido-4-methylphenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	85
1-(3-benzamido-4-methylphenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	86
1-(3-phenylbenzamido-4-methylphenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	87
1-(4-methyl-3-(4-phenoxybenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	88
1-(3-(4-phenylbenzamido)2-chlorophenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	89
1-(3-(4-phenylbenzamido)2-methylphenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	90
1-(4-methyl-3-(4-phenylbenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	91
1-(4-chloro-3-(phenylcarbamoyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	92
1-(4-chloro-3-((4-chlorophenyl)carbamoyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	93
1-(4-chloro-3-((4-(dimethylamino)phenyl)carbamoyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	94
1-(4-chloro-3-((4-methoxyphenyl)carbamoyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	95
1-(4-methyl-3-(phenylcarbamoyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	96
1-(3-benzamidophenyl)-3-(4-methoxybenzo[d][1,3]dioxole-6-carbonyl)urea	97
1-(3-benzamidophenyl)-3-(3,4,5-triethoxybenzoyl)urea	98
1-(3-(4-methoxybenzamido)phenyl)-3-(3,4,5-trimethoxybenzoyl)urea	99
1-(3-isobutyramidophenyl)-3-(3,4,5-trimethoxybenzoyl)urea	100
1-(4-diphenylamidophenyl)-3-(3,4,5-trimethoxybenzoyl)urea	101
1-(3-(1-H-indol-2-yl)phenyl)-3-(3,4,5-trimethoxybenzoyl)urea	102
2-chloro-1-(3-(4-diphenylamidophenyl)-3-(3,4,5-trimethoxybenzoyl)urea	103
N-(3-(3,4,5-trimethoxybenzoyl)guanidino)phenyl)benzamide	104
1-(3-(1-H-indol-2-yl)phenyl)-3-(3,4,5-trimethoxybenzoyl)guanidine	105
4-morpholino-N-(3-(3,4,5-trimethoxybenzoyl)guanidino)phenyl)benzamide	106
1-(3-(imidazo[2,1-b]thiazol-6-yl)phenyl)-3-(3,4,5-trimethoxybenzoyl)guanidine	107
1-(3-(1-H-indol-1-yl)phenyl)-3-(3,4,5-trimethoxybenzoyl)guanidine	108
1-(2-methyl-3-(4-fluorophenyl-4phenyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)guanidine	109

1-(2-chloro-3-(4-fluorophenyl-4phenyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)guanidine	110
1-(3-(4-diphenyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)guanidine	111
1-(2-methyl-3-(4-diphenyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)guanidine	112
1-(2-methyl-3-(3-phenyl)phenyl)-3-(3,4,5-trimethoxybenzoyl)guanidine	113
N-(2-chloro-5-(3-(3,4,5-trimethoxybenzoyl)guanidino)phenyl)benzamide	114
N-(2-methyl-5-(3-(3,4,5-trimethoxybenzoyl)guanidino)phenyl)benzamide	115
2-methyl-N-phenyl-5-(3-(3,4,5-trimethoxybenzoyl)guanidino)benzamide	116
2-chloro-N-phenyl-5-(3-(3,4,5-trimethoxybenzoyl)guanidino)benzamide	117
2-chloro-N-(4-chloro-3-(pyridin-2-yl)phenyl)-4-(methylsulfonyl)benzamide	118
1-(3-benzamidophenyl)-3-(3,4,5-trimethoxybenzoyl)thiourea	119
(13R,13aS)-11-Oxo-13-hydroxyantofine	120
(13S,13aS)-11-Oxo-13-hydroxyantofine	121
(13S,13aS)-13-Hydroxyantofine	122
(13R,13aS)-13-Hydroxyantofine	123
(S)-11-Oxo-12-methoxy-antofine-12-ene	124
N(S)-12-Methoxyantofine-12-ene	125
(S)-12-Oxo-antofine	126
(12R,13aS)-12-Hydroxyantofine	127
(12S,13aS)-12-hydroxyantofine	128
(S)-13-Oxo-cryptopleurine	129
(13S,14aS)-13-Hydroxycryptopleurine	130
(13R,14aS)-13-Hydroxy-cryptopleurine	131
(R)-11-Oxo-12-methoxycryptopleurine-12-ene	132
(R)-12-Methoxycryptopleurine-12-ene	133
(R)-12-Oxo-cryptopleurine	134
(12R,14aR)-12-Hydroxy-cryptopleurine	135
(12S,14aR)-12-Hydroxy-cryptopleurine	136
(14R,14aS)-11-Oxo-14-hydroxyl-cryptopleurine	137

(14S,14aS)-11-Oxo-14-hydroxyl-cryptopleurine	138
(14S,14aS)-11-Oxo-14-hydroxycryptopleurine	139
(14R,14aS)-11-Oxo-14-hydroxycryptopleurine	140
(12S,12R,14aS)-11-Oxo-12,13-dihydroxycryptopleurine	141
(13S, 13R,14aS)-11-Oxo-12,13-dihydroxycryptopleurine	142
(12S,13S,14aS)-12,13-Dihydroxycryptopleurine	143
(12R,13R,14aS)-12,13-Dihydroxycryptopleurine	144
(13R,14aS)-13-Ethyl-13-hydroxycryptopleurine	145
(13S,14aS)-13-Methoxycryptopleurine (26a)	146
(13R,14aS)-13-Methoxy-cryptopleurine	147
R-antofine	148
R-cryptopleurine	149
R-tylocrebrine	150
R-tylophorine	151
Hh-Ag 1	152
N-(2-methyl-5-((methylamino)methyl)phenyl)-4-(4-phenylquinazolin-2-ylamino)benzamide	153
LDE225 (Novartis)	154
1-((2R,4R)-2-(1H-benzo[d]imidazol-2-yl)-1-methylpiperidin-4-yl)-3-(4-cyanophenyl)urea	155
Cholesterol	156
Cyclopamine	157
Cycloposine	158
Dehydroepiandrosterone	159
Dehydroepiandrosterone	160
Dormantinone	161
Epirubijervine	162
Etioline	163
Hosukinidine	164
Jervine	165

KAAD-cyclopamine	166
Solanidine	167
Teinamine	168
US 7,230,004 IPI-269609	169
Veratramine	170
Verazine	171
WO2008083248 IPI-926	172
WO2008109184	173
WO2008109829	174
2-fluoro-N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-3-(trifluoromethyl)benzamide	175
N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-4-(trifluoromethoxy)benzamide	176
N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(trifluoromethoxy)benzamide	177
5-fluoro-N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(trifluoromethyl)benzamide	178
3,5-dichloro-N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)benzamide	179
4-cyano-N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)benzamide	180
N-(1-(4-(1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-4-fluoro-N-methyl-2-(trifluoromethyl)benzamide	181
N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-4-(trifluoromethoxy)benzamide	182
N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(trifluoromethoxy)benzamide	183
5-fluoro-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(trifluoromethyl)benzamide	184
4-fluoro-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(trifluoromethyl)benzamide	185
4-cyano-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)benzamide	186
N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(methylsulfonyl)benzamide	187
5-fluoro-N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(methylsulfonyl)benzamide	188
2-chloro-4-fluoro-N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)benzamide	189
2-cyano-N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)benzamide	190
4-(difluoromethoxy)-N-methyl-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)benzamide	191
N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(methylsulfonyl)benzamide	192
4-chloro-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(methylsulfonyl)benzamide	193

N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)-2-(trifluoromethylsulfonyl)benzamide	194
2-chloro-4-fluoro-N-(1-(4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl)piperidin-4-yl)benzamide	195
N-(2-chloro-6-methylphenyl)-2-(6-(4-(2-hydroxyethyl)piperazin-1-yl)-2-methylpyrimidin-4-ylamino)thiazole-5-carboxamide	196
Etoposide	197
N-(3-chloro-4-fluorophenyl)-7-methoxy-6-(3-morpholinopropoxy)quinazolin-4-amine	198
Ixabepilone	199
4-(3-(1-(cyclopropanecarbonyl)piperazine-4-carbonyl)-4-fluorobenzyl)phthalazin-1(2H)-one	200
(R)-2-(2-methylpyrrolidin-2-yl)-1H-benzo[d]imidazole-4-carboxamide	201
1-methyl-1-((4-oxo-3,4-dihydroquinazolin-2-yl)methyl)-3-(3-(trifluoromethyl)phenyl)urea	202
1-(1-(3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)ethyl)-1-methyl-3-(3-(trifluoromethyl)phenyl)urea	203
1-(1-(3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)ethyl)-3-(3-(trifluoromethyl)phenyl)urea	204
1-((3-isopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)methyl)-3-(3-(trifluoromethyl)phenyl)urea	205
1-((3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)methyl)-3-(3-(trifluoromethyl)phenyl)urea	206
1-((3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)methyl)-3-(3-methoxy-5-(trifluoromethyl)phenyl)urea	207
1-(2,6-dichloropyridin-4-yl)-3-((3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)methyl)urea	208
1-(4-chloro-3-(trifluoromethyl)phenyl)-3-((3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)methyl)urea	209
1-(1-(1-(4-fluorophenyl)-6-oxo-1,6-dihydropyrimidin-2-yl)ethyl)-1-methyl-3-(3-(trifluoromethyl)phenyl)urea	210
Robotnikinin derivative	211
Robotnikinin	212
Tetrahydrojervine	213
Cyclopamine-4-en-3-one	214
Solasodine	215
Tomatidine	216
3-carbamate cyclopamine-1	217
3-carbamate cyclopamine-2	218
Cyclopamine analogue-1	219
Cyclopamine analogue-2	220
Cyclopamine analogue-3	221

IPI-611	222
IPI-269609-IPI-609	223
Cyclopamine analogue-4	224
Cyclopamine analogue-5	225
Cyclopamine analogue-6	226
Cyclopamine analogue-7	227
Cyclopamine analogue-8	228
Cyclopamine analogue-9	229
Cyclopamine analogue-10	230
Cyclopamine analogue-11	231
Cyclopamine analogue-12	232
Cyclopamine analogue-13	233
Cyclopamine analogue-14	234
Cyclopamine analogue-15	235
Cyclopamine analogue-16	236
Cyclopamine analogue-17	237
Cyclopamine analogue-18	238
Cyclopamine analogue-19	239
Cyclopamine analogue-20	240
Cyclopamine analogue-21	241
Cyclopamine analogue-22	242
Cyclopamine analogue-23	243
Cyclopamine analogue-24	244
Cyclopamine analogue-25	245
Cyclopamine analogue-26	246
Cyclopamine analogue-27	247
Cyclopamine analogue-28	248
Cyclopamine analogue-29	249

Cyclopamine analogue-30	250
Cyclopamine analogue-31	251
Mu-HSSKLQ-NCyclopamine	252
Mu-SSKYQ-Cyclopamine	253
SANT-1	254
SANT-2	255
SANT-3	256
SANT-4	257
CUR-61414	258
N-(3-methoxybenzyl)-N-(1-(benzo[d][1,3]dioxol-5-ylmethyl)-5-(piperazine-1-carbonyl)pyrrolidin-3-yl)cyclopropanecarboxamide	259
N-(3-methoxybenzyl)-N-(1-(benzo[d][1,3]dioxol-5-ylmethyl)-5-(piperazine-1-carbonyl)pyrrolidin-3-yl)isobutyramide	260
N-(3-methoxybenzyl)-N-(1-(benzo[d][1,3]dioxol-5-ylmethyl)-5-(piperazine-1-carbonyl)pyrrolidin-3-yl)-2-cyclopentylacetamide	261
N-(3-methoxybenzyl)-N-(1-(benzo[d][1,3]dioxol-5-ylmethyl)-5-(piperazine-1-carbonyl)pyrrolidin-3-yl)-4,4,4-trifluoro-3-methylbutanamide	262
1-(3-methoxybenzyl)-1-(1-(benzo[d][1,3]dioxol-5-ylmethyl)-5-(piperazine-1-carbonyl)pyrrolidin-3-yl)-3-tert-butylurea	263
1-(3-methoxybenzyl)-1-(1-(3-methoxybenzyl)-5-(piperazine-1-carbonyl)pyrrolidin-3-yl)-3-tert-butylurea	264
1-(1-(2,3,4-trimethoxybenzyl)-5-(piperazine-1-carbonyl)pyrrolidin-3-yl)-1-(3-methoxybenzyl)-3-tert-butylurea	265
1-(3-methoxybenzyl)-3-tert-butyl-1-(1-((2,3-dihydrobenzo[b][1,4]dioxin-6-yl)methyl)-5-(piperazine-1-carbonyl)pyrrolidin-3-yl)urea	266
1-(3-methoxybenzyl)-1-(1-(4-fluorobenzyl)-5-(piperazine-1-carbonyl)pyrrolidin-3-yl)-3-tert-butylurea	267
1-(3-methoxybenzyl)-1-((3R,5S)-1-(benzo[d][1,3]dioxol-5-ylmethyl)-5-(1-methylpiperazine-4-carbonyl)pyrrolidin-3-yl)-3-tert-butylurea	268
1-(3-methoxybenzyl)-1-((3R,5S)-1-(benzo[d][1,3]dioxol-5-ylmethyl)-5-(piperidine-1-carbonyl)pyrrolidin-3-yl)-3-tert-butylurea	269
1-((3R,5S)-5-((4-aminobutyl)carbamoyl)-1-(benzo[d][1,3]dioxol-5-ylmethyl)pyrrolidin-3-yl)-1-(3-methoxybenzyl)-3-tert-butylurea	270
1-(1-(3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)ethyl)-1-methyl-3-(3-(trifluoromethyl)phenyl)urea	271
1-((3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)methyl)-3-(3-(trifluoromethyl)phenyl)urea	272
1-((3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)methyl)-1-methyl-3-(3-(trifluoromethyl)phenyl)urea	273
1-(4-chloro-3-(trifluoromethyl)phenyl)-3-((3-(4-fluorophenyl)-4-oxo-3,4-dihydroquinazolin-2-yl)methyl)urea	274
1-((3-isopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)methyl)-3-(3-(trifluoromethyl)phenyl)urea	275
N-(1-methyl-1,2,3,4-tetrahydroquinolin-7-yl)-4-(4-phenylquinazolin-2-ylamino)benzamide	276
3-fluoro-N-(2-methyl-5-(morpholinomethyl)phenyl)-4-(4-phenylquinazolin-2-ylamino)benzamide	277

4-(4-cyclopropylquinazolin-2-ylamino)-N-(2,6-dimethylphenyl)benzamide	278
N-(5-((benzyl(methyl)amino)methyl)-2-methylphenyl)-4-(4-methylquinazolin-2-ylamino)benzamide	279
N-(2,6-dimethylphenyl)-4-(4-phenylpyrido[2,3-d]pyrimidin-2-ylamino)benzamide	280
R-Biaryl(methoxamide)	281
S-Biaryl(2-phenyl)methoxamide	282
R-Biaryl(2-pyridyl)methoxamide	283
S-Biaryl(2-pyridyl)methoxamide	284
S-Biaryl(4-pyridyl)methoxamide	285
R-Biaryl(2-thiazolyl)methoxamide	286
S-Biaryl(2-thiazolyl)methoxamide	287
S-Biaryl(2-thienyl)methoxamide	288
S-Biaryl(2-furanyl)methoxamide	289
4-chloro-3-(4- N,N-dimethylbenzenamine)-N-(6-morpholinopyridin-3-yl)benzamide	290
N-(3-benzamido-4-chlorophenyl)-6-(4-methylpiperazin-1-yl)nicotinamide	291
N-(4-chloro-3-(4-methylbenzamido)phenyl)-6-((3S,5R)-3,5-dimethylpiperazin-1-yl)nicotinamide	292
N-(3-benzamido-4-chlorophenyl)-6-morpholinonicotinamide	293
N-(3-benzamido-4-chlorophenyl)-4-methyl-6-(trifluoromethyl)nicotinamide	294
N-(3-(1H-benzo[d]imidazol-2-yl)phenyl)-2,3-dihydrobenzo[b][1,4]dioxine-6-carboxamide	295
N-(3-(5-methyl-1H-benzo[d]imidazol-2-yl)phenyl)-2,3-dihydrobenzo[b][1,4]dioxine-6-carboxamide	296
N-(3-(5-chloro-1H-benzo[d]imidazol-2-yl)phenyl)-2,3-dihydrobenzo[b][1,4]dioxine-6-carboxamide	297
N-(3-(5-(dimethylamino)-1H-benzo[d]imidazol-2-yl)phenyl)-2,3-dihydrobenzo[b][1,4]dioxine-6-carboxamide	298
N-(3-(5-(dimethylamino)-1H-benzo[d]imidazol-2-yl)phenyl)-3,5-dimethoxybenzamide	299
2,5-dichloro-N-(3-fluoro-5-(trifluoromethyl)phenyl)thiophene-3-sulfonamide	300
4-isopropyl-N-(2-(trifluoromethyl)-1H-benzo[d]imidazol-5-yl)benzenesulfonamide	301
2,4-dichloro-5-methyl-N-(3,4,5-trifluorophenyl)benzenesulfonamide	302
5-(dimethylamino)-N-(3-(oxazol-5-yl)phenyl)naphthalene-1-sulfonamide	303
2-chloro-N-(4-chloro-3-(pyridin-2-yl)phenyl)-4-(1-methylpiperazine-4-carbonyl)benzamide	304
N-(4-chloro-3-(pyridin-2-yl)phenyl)-5-(methylsulfonyl)thiophene-2-carboxamide	305

2-chloro-N-(4-chloro-3-(quinoxalin-2-yl)phenyl)-4-(methylsulfonyl)benzamide	306
2,5-dichloro-N-(4-chloro-3-(quinoxalin-2-yl)phenyl)thiophene-3-carboxamide	307
N-(4-chloro-3-(quinoxalin-2-yl)phenyl)-2-methyl-6-(trifluoromethyl)nicotinamide	308
N-(3-(3-nitro-4-methoxy)benzamido)phenyl)-4-chlorobenzamide	309
2-(6-(4-ethoxyphenyl)-7-oxo-2-thioxo-3-o-tolyl-2,3,6,7-tetrahydrothiazolo[4,5-d]pyrimidin-5-ylthio)acetonitrile	310
2-(3-(2,4-dimethylphenyl)-7-oxo-2-thioxo-6-o-tolyl-2,3,6,7-tetrahydrothiazolo[4,5-d]pyrimidin-5-ylthio)acetonitrile	311
3-(2-fluorobenzyl)-N-(3-(4-chloro-3-methylphenoxy)-5-nitrophenyl)-5-methyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidine-6-carboxamide	312
3-(2-fluorobenzyl)-N-(3-(4-fluorophenylthio)-5-nitrophenyl)-5-methyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidine-6-carboxamide	313
5-methyl-N-(3-nitro-5-phenoxyphenyl)-4-oxo-3-propyl-3,4-dihydrothieno[2,3-d]pyrimidine-6-carboxamide	314
N-(4-chlorophenyl)-3-(6-methyl-4-phenylquinazolin-2-ylamino)benzamide	315
3-(2-phenylquinazolin-4-yl)benzenamine	316
N-(2-ethoxyphenyl)-4-(pyridin-3-yl)thiazol-2-amine	317
4-(2,4-dimethylthiazol-5-yl)-N-(2-ethoxyphenyl)thiazol-2-amine	318
4-(4-methyl-3-(4-methylpiperazin-1-ylsulfonyl)phenyl)-N-o-tolylphthalazin-1-amine	319
N-(benzo[d][1,3]dioxol-5-yl)-4-(4-methyl-3-(4-methylpiperazin-1-ylsulfonyl)phenyl)phthalazin-1-amine	320
ethyl 3-(5-(4-(4-chlorophenylamino)phthalazin-1-yl)-2-methylphenylsulfonamido)propanoate	321
N-(benzo[d][1,3]dioxol-5-yl)-4-(4-chlorophenyl)phthalazin-1-amine	322
4-benzyl-N-p-tolylphthalazin-1-amine	323
N-(benzo[d][1,3]dioxol-5-yl)-4-p-tolylphthalazin-1-amine	324
4-(4-chlorophenyl)-N-(1-o-tolyl-1H-benzo[d]imidazol-5-yl)phthalazin-1-amine	325
3-(2-chlorophenyl)-4-oxo-4H-chromen-7-yl 2,6-dimethoxybenzoate	326
3-(4-methoxyphenoxy)-4-oxo-4H-chromen-7-yl 2,6-dimethoxybenzoate	327
4-(5-ethylpyridin-2-yl)-N-(2-iodophenyl)benzamide	328
4-(5-butylpyridin-2-yl)-N-(2,4-dichlorophenyl)benzamide	329
4-(5-pentylpyridin-2-yl)-N-(3-(trifluoromethyl)phenyl)benzamide	330
N-(2,4-dimethylphenyl)-4-(5-pentylpyridin-2-yl)benzamide	331
N-(2,6-dichlorophenyl)-4-(5-pentylpyridin-2-yl)benzamide	332
N-(4-methoxy-2-nitrophenyl)-4-(5-propylpyridin-2-yl)benzamide	333

N-(4-acetylphenyl)-4-(5-propylpyridin-2-yl)benzamide	334
4-(2-methyl-1H-imidazo[1,2-a]pyridin-3-yl)-N-p-tolylthiazol-2-amine	335
N-(4-methoxyphenyl)-4-(2-methyl-1H-imidazo[1,2-a]pyridin-3-yl)thiazol-2-amine	336
4-(2,7-dimethyl-1H-imidazo[1,2-a]pyridin-3-yl)-N-(4-ethoxyphenyl)thiazol-2-amine	337
(Z)-N'-(1-benzyl-2-oxoindolin-3-ylidene)-2-(4-tert-butylbenzamido)acetohydrazide	338
2-(5-(4-aminophenyl)-4-methyl-4H-pyrazol-3-ylthio)acetamide- 2-(benzo[d]thiazol-2-ylthio)-1-(4-chlorophenyl)ethanone	339
N-(4-(thieno[2,3-d]pyrimidin-4-yloxy)phenyl)benzamide	340
2-(3-cyano-5-oxo-4-(4,5,6,7-tetrahydrobenzo[b]thiophene-2-yl)-1,4,5,6,7,8-hexahydroquinolin-2-ylthio)-N-(2,5-dimethylphenyl)acetamide	341
1-benzyl-4-(4-(pyrimidin-2-yl)-1,4-diazepan-1-yl)phthalazine	342
N-(3-(benzo[d]thiazol-2-yl)-4-chlorophenyl)-1H-1,2,4-triazole-3-carboxamide	343
(E)-5-(2-(4-fluorobenzyloxy)benzylidene)imidazolidine-2,4-dione	344
N-(4-(5,7-dimethylbenzo[d]oxazol-2-yl)phenyl)-4-ethoxybenzamide	345
5-(2-methyl-1,3-dioxolan-2-yl)-3-phenyl-3,3a-dihydrobenzo[c]isoxazole	346
N-((2,3-dihydrobenzo[b][1,4]dioxin-2-yl)methyl)-1-(4-(pyridin-2-yl)piperazin-1-yl)isoquinoline-4-carboxamide	347
ethyl 4-(4-((4-(2,4-dimethylphenyl)thiazol-2-yl)carbamoyl)phenylsulfonyl)piperazine-1-carboxylate	348
(E)-ethyl 2-(3-(ethylamino)-6-(ethylimino)-2,7-dimethyl-6H-xanthen-9-yl)benzoate	349
1-benzyl-4-(4-(2,5-difluoropyridin-3-yl)piperazin-1-yl)phthalazine	350
2-amino-4-(3-chloro-4-hydroxy-5-methoxyphenyl)-4H-benzo[h]chromene-3-carbonitrile	351
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinamide	352
N-(4-(benzo[d]thiazol-2-yl)phenyl)-4-methoxybenzamide	353
(E)-N'-(4-nitrobenzylidene)-5-chloro-3-phenyl-1H-indole-2-carbohydrazide	354
(Z)-6,6,7,7,8,8,8-heptafluoro-2,2-dimethyl-4-(2-(4-nitrophenyl)hydrazono)octane-3,5-dione	355
(4-(dimethylamino)naphthalen-1-yl)(4-(dimethylamino)phenyl)methanone	356
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinonitrile	357
1-benzyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)phthalazine	358
1-benzyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)-1,4-diazepan-1-yl)phthalazine	359
6-(4-(4-(pyridin-4-ylmethyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	360
ethyl 4-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)benzoate	361

1-(4-phenylpiperazin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	362
1-benzyl-4-(4-(4-tert-butylphenyl)piperazin-1-yl)phthalazine	363
1-(4-(4-tert-butylphenyl)piperazin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	364
1-(3,5-dichlorobenzyl)-4-(4-(4-tert-butylphenyl)piperazin-1-yl)phthalazine	365
4-(4-(4-tert-butylphenyl)piperazin-1-yl)-6-methyl-1-(pyridin-4-ylmethyl)phthalazine	366
1-((2-methylpyridin-4-yl)methyl)-4-(4-phenylpiperazin-1-yl)phthalazine	367
1-benzyl-4-(4-phenylpiperidin-1-yl)phthalazine	368
1-(4-phenylpiperidin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	369
1-((2-methylpyridin-4-yl)methyl)-4-(4-phenylpiperidin-1-yl)phthalazine	370
1-(pyridin-4-ylmethyl)-4-(4-(3-(trifluoromethyl)phenyl)piperazin-1-yl)phthalazine	371
4-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)benzoic acid	372
1-benzyl-4-(4-(3-chloro-5-(trifluoromethyl)pyridin-2-yl)-1,4-diazepan-1-yl)phthalazine	373
1-benzyl-4-(4-(quinolin-2-yl)piperazin-1-yl)phthalazine	374
6-(4-(4-benzylphthalazin-1-yl)-1,4-diazepan-1-yl)nicotinonitrile	375
1-(4-(pyrazin-2-yl)piperazin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	376
1-benzyl-4-(4-(pyrazin-2-yl)piperazin-1-yl)phthalazine	377
1-((2-methylpyridin-4-yl)methyl)-4-(4-(pyridin-2-yl)piperazin-1-yl)phthalazine	378
1-(4-(pyridin-2-yl)piperazin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	379
1-benzyl-4-(4-(pyridin-2-yl)piperazin-1-yl)phthalazine	380
1-benzyl-4-(4-(pyrimidin-2-yl)piperazin-1-yl)phthalazine	381
1-(4-(pyridin-4-yl)piperazin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	382
1-benzyl-4-(3-methyl-4-p-tolylpiperazin-1-yl)phthalazine	383
1-(3-methyl-4-p-tolylpiperazin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	384
1-(3-methyl-4-p-tolylpiperazin-1-yl)-4-((2-methylpyridin-4-yl)methyl)phthalazine	385
1-benzyl-4-(4-(3,4-dichlorophenyl)piperazin-1-yl)phthalazine	386
1-benzyl-4-(4-(naphthalen-2-yl)piperazin-1-yl)phthalazine	387
1-(4-(naphthalen-2-yl)piperazin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	388
1-((2-methylpyridin-4-yl)methyl)-4-(4-(naphthalen-2-yl)piperazin-1-yl)phthalazine	389

1-benzyl-4-(4-(naphthalen-1-yl)piperazin-1-yl)phthalazine	390
1-((2-methylpyridin-4-yl)methyl)-4-(4-(naphthalen-1-yl)piperazin-1-yl)phthalazine	391
1-(4-(naphthalen-1-yl)piperazin-1-yl)-4-(pyridin-4-ylmethyl)phthalazine	392
1-benzyl-4-(4-(pyridin-4-yl)piperazin-1-yl)phthalazine	393
1-benzyl-4-(4-o-tolylpiperazin-1-yl)phthalazine	394
2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrimidine-5-carbonitrile	395
1-benzyl-4-(4-(pyrimidin-2-yl)-1,4-diazepan-1-yl)phthalazine	396
1-benzyl-4-(4-(4-methylpyrimidin-2-yl)-1,4-diazepan-1-yl)phthalazine	397
1-benzyl-4-(4-(5-propylpyrimidin-2-yl)piperazin-1-yl)phthalazine	398
1-benzyl-4-(4-(5-ethylpyrimidin-2-yl)piperazin-1-yl)phthalazine	399
1-benzyl-4-(4-(5-propylpyrimidin-2-yl)-1,4-diazepan-1-yl)phthalazine	400
1-benzyl-4-(4-(5-ethylpyrimidin-2-yl)-1,4-diazepan-1-yl)phthalazine	401
2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-6-methoxypyrimidin-4(3H)-one	402
1-benzyl-4-(4-(4-methylpyrimidin-2-yl)piperazin-1-yl)phthalazine	403
1-benzyl-4-(4-(4,6-dimethylpyrimidin-2-yl)piperazin-1-yl)phthalazine	404
1-benzyl-4-(4-(5-chloro-3-fluoropyridin-2-yl)piperazin-1-yl)phthalazine	405
1-benzyl-4-(4-(4-(trifluoromethyl)pyrimidin-2-yl)piperazin-1-yl)phthalazine	406
1-benzyl-4-(4-(2,5-difluoropyridin-3-yl)piperazin-1-yl)phthalazine	407
1-benzyl-4-(4-(3,5-difluoropyridin-2-yl)piperazin-1-yl)phthalazine	408
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinamide	409
ethyl 6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinate	410
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-ol	411
2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N,N-dimethylpyrimidine-5-carboxamide	412
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinic acid	413
(2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrimidin-5-yl)(morpholino)methanone	414
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-(2-hydroxyethyl)-N-methylnicotinamide	415
2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-(2-hydroxyethyl)-N-methylpyrimidine-5-carboxamide	416
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-(2-hydroxyethyl)nicotinamide	417

6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-(2-methoxyethyl)nicotinamide	418
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-(2-methoxyethyl)-N-methylnicotinamide	419
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-(2-(dimethylamino)ethyl)nicotinamide	420
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)(4-methylpiperazin-1-yl)methanone	421
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)(piperazin-1-yl)methanone	422
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)(morpholino)methanone	423
N-benzyl-6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinamide	424
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-(cyclohexylmethyl)nicotinamide	425
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-propylnicotinamide	426
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)(3-hydroxypyrrolidin-1-yl)methanone	427
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)(thiazolidin-3-yl)methanone	428
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)(thioxazolidin-3-yl)methanone	429
methyl 2-(2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinamido)acetate	430
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-(3-hydroxypropyl)-N-methylnicotinamide	431
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-N-(2-hydroxy-2-methylpropyl)nicotinamide	432
tert-butyl 1-(2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinoyl)azetidin-3-ylcarbamate	433
(3-aminoazetidin-1-yl)(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methanone	434
benzyl 3-(2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinamido)azetidine-1-carboxylate	435
N-(azetidin-3-yl)-6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinamide	436
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)(3-hydroxyazetidin-1-yl)methanone	437
1-benzyl-4-(4-(4-(trifluoromethyl)phenyl)piperazin-1-yl)phthalazine	438
6-(4-(4-(3-(trifluoromethyl)benzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	439
6-(4-(4-(4-cyanobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	440
6-(4-(4-(3,4-dimethoxybenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	441
6-(4-(4-(4-chlorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	442
6-(4-(4-(3-chlorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	443
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinonitrile	444
6-(4-(4-(naphthalen-2-ylmethyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	445

6-(4-(4-(4-(trifluoromethyl)benzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	446
6-(4-(4-(4-methoxybenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	447
6-(4-(4-(3-cyanobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	448
6-(4-(4-(1-phenylethyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	449
6-(4-(4-(3-methylbenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	450
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)acetamide	451
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methanamine	452
(4-(4-(4-(pyridin-4-ylmethyl)phthalazin-1-yl)piperazin-1-yl)phenyl)methanamine	453
(4-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)phenyl)methanamine	454
No Name Available	455
N-(4-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)benzyl)acetamide	456
N-(4-(4-(4-(pyridin-4-ylmethyl)phthalazin-1-yl)piperazin-1-yl)benzyl)acetamide	457
benzyl 4-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)benzylcarbamate	458
benzyl 4-(4-(4-(pyridin-4-ylmethyl)phthalazin-1-yl)piperazin-1-yl)benzylcarbamate	459
N-(4-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)benzyl)propionamide	460
N-(4-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)benzyl)-2-methoxyacetamide	461
N-(4-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)benzyl)-3-methylbutanamide	462
6-(4-(1-(3-cyanobenzyl)isoquinolin-4-yl)piperazin-1-yl)nicotinonitrile	463
6-(4-(1-(3-chlorobenzyl)isoquinolin-4-yl)piperazin-1-yl)nicotinonitrile	464
6-(4-(1-(3-(trifluoromethyl)benzyl)isoquinolin-4-yl)piperazin-1-yl)nicotinonitrile	465
6-(4-(4-benzylisoquinolin-1-yl)piperazin-1-yl)nicotinonitrile	466
6-(4-(6-(4-fluorobenzyl)-4-methylpyridazin-3-yl)piperazin-1-yl)nicotinonitrile	467
6-(4-(6-(4-fluorobenzyl)-5-methylpyridazin-3-yl)piperazin-1-yl)nicotinonitrile	468
6-(4-(6-benzyl-4-methylpyridazin-3-yl)piperazin-1-yl)nicotinonitrile	469
6-(4-(6-benzyl-5-methylpyridazin-3-yl)piperazin-1-yl)nicotinonitrile	470
6-benzyl-4-methyl-3-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)pyridazine	471
3-benzyl-4-methyl-6-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)pyridazine	472
6-(4-fluorobenzyl)-4-methyl-3-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)pyridazine	473

3-(4-fluorobenzyl)-4-methyl-6-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)pyridazine	474
6-(4-(6-(4-chlorobenzyl)-4-methylpyridazin-3-yl)piperazin-1-yl)nicotinonitrile	475
6-(4-(6-(4-chlorobenzyl)-5-methylpyridazin-3-yl)piperazin-1-yl)nicotinonitrile	476
6-(4-(6-(4-fluorobenzyl)-4,5-dimethylpyridazin-3-yl)piperazin-1-yl)nicotinonitrile	477
6-(4-(4-(4-fluorobenzyl)-5,6,7,8-tetrahydrophthalazin-1-yl)piperazin-1-yl)nicotinonitrile	478
6-(4-(4-(4-fluorobenzyl)-6,7-dihydro-5H-cyclopenta[d]pyridazin-1-yl)piperazin-1-yl)nicotinonitrile	479
3-(4-(1-(4-fluorobenzyl)-1H-indol-3-yl)piperidine-1-carbonyl)benzonitrile	480
1-(4-fluorobenzyl)-3-(1-(5-(trifluoromethyl)pyridin-2-yl)piperidin-4-yl)-1H-indole	481
4-((3-(1-(5-(trifluoromethyl)pyridin-2-yl)piperidin-4-yl)-1H-indol-1-yl)methyl)benzonitrile	482
1-benzyl-3-(1-(5-(trifluoromethyl)pyridin-2-yl)piperidin-4-yl)-1H-indole	483
6-(4-(1-(4-fluorobenzyl)-1H-indol-3-yl)piperidin-1-yl)nicotinonitrile	484
6-(4-(1-benzyl-1H-indol-3-yl)piperidin-1-yl)nicotinonitrile	485
(4-(1-(4-fluorobenzyl)-1H-indol-3-yl)piperidin-1-yl)(3-fluorophenyl)methanone	486
4-(4-(1-(4-fluorobenzyl)-1H-indol-3-yl)piperidine-1-carbonyl)benzonitrile	487
3-(4-(1-benzyl-1H-indol-3-yl)piperidine-1-carbonyl)benzonitrile	488
(4-(1-(4-fluorobenzyl)-1H-indol-3-yl)piperidin-1-yl)(4-(trifluoromethyl)phenyl)methanone	489
(4-(1-benzyl-1H-indol-3-yl)piperidin-1-yl)(4-(trifluoromethyl)phenyl)methanone	490
1-benzyl-4-(4-phenylpiperazin-1-yl)phthalazine	491
1-benzyl-4-(4-(5-(dimethylphosphoryl)pyridin-2-yl)piperazin-1-yl)phthalazine	492
4-(4-benzylphthalazin-1-yl)-1-phenylpiperazin-2-one	493
1-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)-2,2,2-trifluoroethanol	494
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)-1,1,1,3,3,3-hexafluoropropan-2-ol	495
3-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)oxetan-3-ol	496
1-benzyl-4-(4-(4-(trifluoromethyl)-1H-imidazol-2-yl)piperidin-1-yl)phthalazine	497
1-(4-(1H-indol-3-yl)piperidin-1-yl)-4-benzylphthalazine	498
1-(4-(1H-benzo[d]imidazol-2-yl)piperidin-1-yl)-4-benzylphthalazine	499
methyl 4-(1-(4-benzylphthalazin-1-yl)piperidin-4-yl)benzoate	500
4-(1-(4-benzylphthalazin-1-yl)piperidin-4-yl)benzonitrile	501

(S)-6-(4-(4-benzylphthalazin-1-yl)-3-methylpiperazin-1-yl)nicotinonitrile	502
(R)-6-(4-(4-benzylphthalazin-1-yl)-3-methylpiperazin-1-yl)nicotinonitrile	503
6-((2R,5S)-4-(4-benzylphthalazin-1-yl)-2,5-dimethylpiperazin-1-yl)nicotinonitrile	504
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-amine	505
N-(2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-yl)-2-methoxyacetamide	506
N-(2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-yl)-3-methoxypropanamide	507
benzyl 2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-ylcarbamate	508
2-(4-(1-(4-benzylphthalazin-1-yl)piperidin-4-yl)phenyl)propan-2-ol	509
(4-(1-(4-benzylphthalazin-1-yl)piperidin-4-yl)phenyl)methanamine	510
N-(4-(1-(4-benzylphthalazin-1-yl)piperidin-4-yl)benzyl)acetamide	511
1-benzyl-4-(4-(4-nitrophenyl)piperidin-1-yl)phthalazine	512
4-(1-(4-benzylphthalazin-1-yl)piperidin-4-yl)benzenamine	513
N-(4-(1-(4-benzylphthalazin-1-yl)piperidin-4-yl)phenyl)acetamide	514
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-2-methylnicotinonitrile	515
1-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)pyrrolidin-2-one	516
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridine-3-sulfonamide	517
1-benzyl-4-(4-(5-(pyrrolidin-1-ylsulfonyl)pyridin-2-yl)piperazin-1-yl)phthalazine	518
1-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)ethanone	519
1-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)cyclopropanol	520
methyl 6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-4-(trifluoromethyl)nicotinate	521
ethyl 2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-4-(trifluoromethyl)pyrimidine-5-carboxylate	522
methyl 5-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrazine-2-carboxylate	523
methyl 6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridazine-3-carboxylate	524
methyl 2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrimidine-5-carboxylate	525
methyl 6-((4-(4-benzylphthalazin-1-yl)piperazin-1-yl)methyl)nicotinate	526
(R)-6-(4-(4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl)nicotinonitrile	527
(S)-6-(4-(4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl)nicotinonitrile	528
(R)-ethyl 6-(4-(4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl)nicotinate	529

(R)-methyl 5-(4-(4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl)pyrazine-2-carboxylate	530
(S)-methyl 6-(4-(4-benzylphthalazin-1-yl)-3-methylpiperazin-1-yl)nicotinate	531
(S)-ethyl 2-(4-(4-benzylphthalazin-1-yl)-2-(methoxycarbonyl)piperazin-1-yl)-4-(trifluoromethyl)pyrimidine-5-carboxylate	532
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-4-(trifluoromethyl)pyridin-3-yl)propan-2-ol	533
2-(2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)-4-(trifluoromethyl)pyrimidin-5-yl)propan-2-ol	534
2-(5-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrazin-2-yl)propan-2-ol	535
2-(2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrimidin-5-yl)propan-2-ol	536
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridazin-3-yl)propan-2-ol	537
1-(5-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrazin-2-yl)ethanone	538
(R)-2-(6-(4-(4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl)pyridin-3-yl)propan-2-ol	539
(S)-2-(6-(4-(4-benzylphthalazin-1-yl)-3-methylpiperazin-1-yl)pyridin-3-yl)propan-2-ol	540
(R)-2-(5-(4-(4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl)pyrazin-2-yl)propan-2-ol	541
(R)-1-(5-(4-(4-benzylphthalazin-1-yl)-2-methylpiperazin-1-yl)pyrazin-2-yl)ethanone	542
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methanol	543
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl 2-methoxyacetate	544
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl dimethylcarbamate	545
1-benzyl-4-(4-(5-(2-methoxypropan-2-yl)pyridin-2-yl)piperazin-1-yl)phthalazine	546
N-(2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-yl)acetamide	547
1-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)ethanol	548
1-benzyl-4-(4-(5-(2-methyl-1,3-dioxolan-2-yl)pyridin-2-yl)piperazin-1-yl)phthalazine	549
1-benzyl-4-(4-(5-isopropylpyrazin-2-yl)piperazin-1-yl)phthalazine	550
2-(5-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrazin-2-yl)propane-1,2-diol	551
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propane-1,2-diol	552
2-(5-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrazin-2-yl)-2-hydroxypropyl methanesulfonate	553
2-(5-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrazin-2-yl)-1-(dimethylamino)propan-2-ol	554
1-(2-(5-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrazin-2-yl)-2-hydroxypropyl)piperidin-4-ol	555
2-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)-1-(pyrrolidin-1-yl)ethanone	556
1-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)-2-methylpropan-2-ol	557

6-(4-(4-(4-methylbenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	558
6-(4-(4-(2-chlorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	559
6-(4-(4-(2-methoxybenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	560
6-(4-(4-(3,4-dichlorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	561
6-(4-(4-(2,4-dichlorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	562
6-(4-(4-(4-chloro-3-(trifluoromethyl)benzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	563
methyl 4-((4-(4-(5-cyanopyridin-2-yl)piperazin-1-yl)phthalazin-1-yl)methyl)benzoate	564
4-((4-(4-(5-cyanopyridin-2-yl)piperazin-1-yl)phthalazin-1-yl)methyl)benzoic acid	565
6-(4-(4-(4-fluorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	566
6-(4-(4-(3-fluorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinonitrile	567
ethyl 6-(4-(4-(4-fluorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinate	568
ethyl 6-(4-(4-(2-fluorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinate	569
ethyl 6-(4-(4-(3-fluorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinate	570
ethyl 6-(4-(4-(2,4-dichlorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinate	571
(S)-ethyl 6-(4-(4-(2,4-difluorobenzyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)nicotinate	572
(S)-ethyl 6-(4-(4-(2-chlorobenzyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)nicotinate	573
6-(4-(4-(4-fluorobenzyl)-7-chlorophthalazin-1-yl)piperazin-1-yl)nicotinonitrile	574
6-(4-(4-(4-fluorobenzyl)-6-chlorophthalazin-1-yl)piperazin-1-yl)nicotinonitrile	575
1-(4-fluorobenzyl)-4-(4-(5-cyanopyridin-2-yl)piperazin-1-yl)phthalazine-6-carbonitrile	576
4-(4-fluorobenzyl)-1-(4-(5-cyanopyridin-2-yl)piperazin-1-yl)phthalazine-6-carbonitrile	577
2-(6-(4-(4-(4-fluorobenzyl)phthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-ol	578
2-(6-(4-(4-(2-chlorobenzyl)phthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-ol	579
2-(6-(4-(4-(2,4-difluorobenzyl)phthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-ol	580
2-(6-(4-(4-(2-methylbenzyl)phthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)propan-2-ol	581
(S)-2-(6-(4-(4-(2,4-difluorobenzyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)pyridin-3-yl)propan-2-ol	582
(S)-2-(6-(4-(4-(2-chlorobenzyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)pyridin-3-yl)propan-2-ol	583
6-(4-(4-(4-fluorobenzyl)phthalazin-1-yl)piperazin-1-yl)nicotinic acid	584
6-(4-(4-(4-fluorobenzyl)phthalazin-1-yl)piperazin-1-yl)-N-(2-hydroxyethyl)-N-methylnicotinamide	585

6-(4-(4-(2,4-difluorobenzyl)phthalazin-1-yl)piperazin-1-yl)-N-(2-hydroxyethyl)-N-methylnicotinamide	586
6-(4-(4-(2-chlorobenzyl)phthalazin-1-yl)piperazin-1-yl)-N-(2-hydroxyethyl)-N-methylnicotinamide	587
6-(4-(4-(3,4-dichlorobenzyl)phthalazin-1-yl)piperazin-1-yl)-N-(2-hydroxyethyl)-N-methylnicotinamide	588
6-(4-(4-(2,4-difluorobenzyl)phthalazin-1-yl)piperazin-1-yl)-N,N-dimethylnicotinamide	589
ethyl 6-(4-(4-(morpholinomethyl)phthalazin-1-yl)piperazin-1-yl)nicotinate	590
tert-butyl (6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methylcarbamate	591
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)methanesulfonamide	592
1-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)-3-methylurea	593
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)propionamide	594
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)-2-methoxyacetamide	595
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)morpholine-4-carboxamide	596
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)-3-methylbutanamide	597
isopropyl (6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methylcarbamate	598
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)-2-(dimethylamino)acetamide	599
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)-3-hydroxybutanamide	600
2-(2-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methylamino)-2-oxoethylthio)succinic acid	601
dimethyl 2-(2-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methylamino)-2-oxoethylthio)succinate	602
(S)-N-((6-(4-(4-benzylphthalazin-1-yl)-3-methylpiperazin-1-yl)pyridin-3-yl)methyl)acetamide	603
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)-N,N-dimethylmethanamine	604
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)nicotinaldehyde	605
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)(cyclopropyl)methanol	606
1-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)-2-methylpropan-1-ol	607
(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)(cyclopentyl)methanol	608
1-benzyl-4-(4-(5-(morpholinomethyl)pyridin-2-yl)piperazin-1-yl)phthalazine	609
1-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)pyrrolidin-3-ol	610
1-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)azetidin-3-ol	611
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)-tetrahydro-2H-pyran-4-amine	612
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)-N-methyl-tetrahydro-2H-pyran-4-amine	613

1-benzyl-4-(4-(5-((4-fluoropiperidin-1-yl)methyl)pyridin-2-yl)piperazin-1-yl)phthalazine	614
1-benzyl-4-(4-(5-((4,4-difluoropiperidin-1-yl)methyl)pyridin-2-yl)piperazin-1-yl)phthalazine	615
1-benzyl-4-(4-(5-((3,3-difluoroazetidin-1-yl)methyl)pyridin-2-yl)piperazin-1-yl)phthalazine	616
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)oxetan-3-amine	617
N-((6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)methyl)-N-(oxetan-3-yl)oxetan-3-amine	618
1-benzyl-4-(4-(5-nitropyridin-2-yl)piperazin-1-yl)phthalazine	619
1-benzyl-4-(4-(5-nitropyrimidin-2-yl)piperazin-1-yl)phthalazine	620
6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-amine	621
1-benzyl-4-(4-(5-iodopyrimidin-2-yl)piperazin-1-yl)phthalazine	622
N-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)acetamide	623
N-(2-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyrimidin-5-yl)acetamide	624
3-(6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-yl)-1,1-dimethylurea	625
methyl 6-(4-(4-benzylphthalazin-1-yl)piperazin-1-yl)pyridin-3-ylcarbamate	626
1-benzyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)-5,6,7,8-tetrahydrophthalazine	627
N-((6-benzyl-5-methyl-3-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)pyridazin-4-yl)methyl)(phenyl)methanamine	628
N-((3-benzyl-5-methyl-6-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)pyridazin-4-yl)methyl)(phenyl)methanamine	629
6-(4-methoxybenzyl)-1-benzyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)-6,7-dihydro-5H-pyrrolo[3,4-d]pyridazine	630
1-benzyl-6-isopropyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)-6H-pyrrolo[3,4-d]pyridazine	631
7-benzyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)furo[3,2-d]pyridazine	632
4-benzyl-7-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)furo[2,3-d]pyridazine	633
7-benzyl-4-(4-(5-(trifluoromethyl)pyridin-2-yl)piperazin-1-yl)-1H-imidazo[4,5-d]pyridazine	634
(2-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(thiophen-2-yl)methanone	635
(2-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	636
phenyl((1S,4S)-5-(4-phenylphthalazin-1-yl)-2,5-diaza-bicyclo[2.2.1]heptan-2-yl)methanone	637
(R)-(3-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	638
(S)-(2-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	639
(R)-(2-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	640
(S)-(4-(4-(4-chlorophenyl)phthalazin-1-yl)-2-methylpiperazin-1-yl)(phenyl)methanone	641

(S)-(2-methyl-4-(4-p-tolylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	642
((S)-4-(4-(3,4-dichlorophenyl)phthalazin-1-yl)-2-methylpiperazin-1-yl)(phenyl)methanone	643
(S)-(3-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	644
((2S,6R)-2,6-dimethyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	645
(S)-(2-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(pyridin-3-yl)methanone	646
(S)-(2-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(pyridin-4-yl)methanone	647
(S)-(2-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(thiazol-2-yl)methanone	648
(R)-cyclopentyl(3-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)methanone	649
(R)-cyclopropyl(3-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)methanone	650
(R)-cyclohexyl(3-methyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)methanone	651
((R)-3-methyl-4-(4-(pyridin-2-yl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	652
((S)-2-methyl-4-(4-(pyridin-2-yl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	653
(R)-(3-methyl-4-(4-p-tolylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	654
(R)-(4-(4-(4-chlorophenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	655
(R)-(4-(4-(4-tert-butylphenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	656
(R)-(3-methyl-4-(4-(4-(trifluoromethyl)phenyl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	657
(R)-(4-(4-(4-isopropylphenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	658
((R)-4-(4-(benzofuran-2-yl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	659
((2S,5R)-2,5-dimethyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	660
((2R,5S)-2,5-dimethyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	661
(S)-(2-methyl-4-(4-(4-(trifluoromethyl)phenyl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	662
(S)-(2-methyl-4-(4-(4-vinylphenyl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	663
((S)-4-(4-(2-fluoro-4-methylphenyl)phthalazin-1-yl)-2-methylpiperazin-1-yl)(phenyl)methanone	664
((S)-4-(4-(3-fluoro-4-methylphenyl)phthalazin-1-yl)-2-methylpiperazin-1-yl)(phenyl)methanone	665
((S)-4-(4-(2-fluorophenyl)phthalazin-1-yl)-2-methylpiperazin-1-yl)(phenyl)methanone	666
((R)-4-(4-(2-fluoro-4-methylphenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	667
((R)-4-(4-(3-fluoro-4-methylphenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	668
((R)-4-(4-(4-chloro-2-fluorophenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	669

((S)-4-(4-(4-chloro-2-fluorophenyl)phthalazin-1-yl)-2-methylpiperazin-1-yl)(phenyl)methanone	670
((R)-4-(4-(2-fluorophenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	671
1-benzyl-4-(4-(4-(trifluoromethyl)phenyl)phthalazin-1-yl)piperazin-2-one	672
(R)-(4-(4-(4-fluorophenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	673
(R)-methyl 4-(4-(4-benzoyl-2-methylpiperazin-1-yl)phthalazin-1-yl)benzoate	674
(R)-(4-(4-(4-(dimethylamino)phenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	675
methyl 1-benzoyl-4-(4-phenylphthalazin-1-yl)piperazine-2-carboxylate	676
((2S,5S)-2,5-dimethyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	677
(R)-4-(4-(4-benzoyl-2-methylpiperazin-1-yl)phthalazin-1-yl)benzonitrile	678
(R)-(4-(4-(4-(hydroxymethyl)phenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	679
(R)-(3-methyl-4-(4-(4-morpholinophenyl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	680
(R)-(4-(4-(4-hydroxyphenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	681
(R)-cyclohexyl(4-(4-(4-fluorophenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)methanone	682
(R)-(3-methyl-4-(7-nitro-4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	683
(R)-(3-methyl-4-(6-nitro-4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	684
(R)-cyclohexyl(4-(4-(4-(hydroxymethyl)phenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)methanone	685
(R)-cyclohexyl(4-(7-fluoro-4-phenylphthalazin-1-yl)-3-methylpiperazin-1-yl)methanone	686
(R)-(4-(6-fluoro-4-phenylphthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	687
(S)-(4-(6-fluoro-4-phenylphthalazin-1-yl)-2-methylpiperazin-1-yl)(phenyl)methanone	688
(S)-(4-(4-(4-cyclopropylphenyl)phthalazin-1-yl)-2-methylpiperazin-1-yl)(phenyl)methanone	689
(S)-(2-methyl-4-(4-(pyridin-4-yl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	690
(R)-(3-methyl-4-(4-(pyridin-4-yl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	691
((2S,5R)-4-(4-(4-(hydroxymethyl)phenyl)phthalazin-1-yl)-2,5-dimethylpiperazin-1-yl)(phenyl)methanone	692
((2R,5S)-4-(4-(4-(hydroxymethyl)phenyl)phthalazin-1-yl)-2,5-dimethylpiperazin-1-yl)(phenyl)methanone	693
((2S,5R)-4-(4-(4-chloro-2-fluorophenyl)phthalazin-1-yl)-2,5-dimethylpiperazin-1-yl)(phenyl)methanone	694
((2R,5S)-4-(4-(4-chloro-2-fluorophenyl)phthalazin-1-yl)-2,5-dimethylpiperazin-1-yl)(phenyl)methanone	695
(2,2-dimethyl-4-(4-phenylphthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	696
(R)-4-(4-(4-(4,4-difluorocyclohexanecarbonyl)-2-methylpiperazin-1-yl)phthalazin-1-yl)benzonitrile	697

(R)-(3-methyl-4-(4-morpholinophthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	698
(S)-1-(3-methyl-4-(phenylsulfonyl)piperazin-1-yl)-4-phenylphthalazine	699
(R)-1-(2-methyl-4-(phenylsulfonyl)piperazin-1-yl)-4-phenylphthalazine	700
(R)-4-(2-methyl-1-(4-phenylphthalazin-1-yl)piperazine-4-carbonyl)cyclohexanone	701
3-((R)-2-methyl-1-(4-phenylphthalazin-1-yl)piperazine-4-carbonyl)cyclohexanone	702
(R)-4-(4-(4-benzoyl-2-methylpiperazin-1-yl)phthalazin-1-yl)benzamide	703
(R)-4-(4-(4-(cyclohexanecarbonyl)-2-methylpiperazin-1-yl)phthalazin-1-yl)benzonitrile	704
((S)-2-methyl-4-(4-(pyridin-3-yl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	705
((R)-3-methyl-4-(4-(pyridin-3-yl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	706
4-(4-((2R,5S)-4-benzoyl-2,5-dimethylpiperazin-1-yl)phthalazin-1-yl)benzonitrile	707
4-(4-((2S,5R)-4-benzoyl-2,5-dimethylpiperazin-1-yl)phthalazin-1-yl)benzonitrile	708
((S)-4-(4-(1H-imidazol-1-yl)phthalazin-1-yl)-2-methylpiperazin-1-yl)(phenyl)methanone	709
((R)-4-(4-(1H-pyrazol-1-yl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	710
((R)-4-(4-(1H-indol-1-yl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	711
(R)-(4-(4-(1H-pyrrol-1-yl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	712
(R)-(4-(4-benzoyl-2-methylpiperazin-1-yl)phthalazin-1-yl)methyl carbamate	713
(R)-(4-(4-(4-(cyclohexanecarbonyl)-2-methylpiperazin-1-yl)phthalazin-1-yl)phenyl)methyl carbamate	714
((R)-3-methyl-4-(4-(4-(2-(tetrahydro-2H-pyran-2-yloxy)ethyl)phenyl)phthalazin-1-yl)piperazin-1-yl)(phenyl)methanone	715
(R)-(4-(4-(4-(2-hydroxyethyl)phenyl)phthalazin-1-yl)-3-methylpiperazin-1-yl)(phenyl)methanone	716