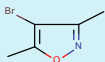
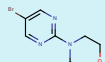
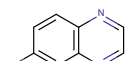
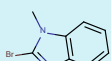


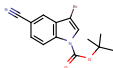
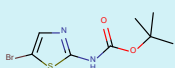
BOEHRINGER INGELHEIM B-SMART Kit

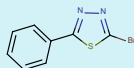
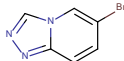
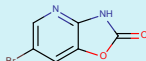
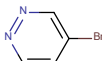
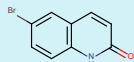
Building block appendix*

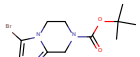
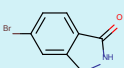
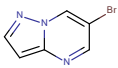
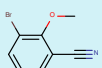
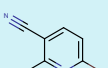
List of building blocks that your methodology will be screened against.

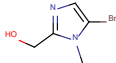
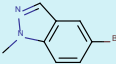
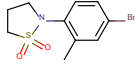
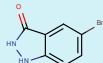
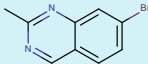
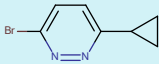
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1	5-bromopyrimidine	MFCD00006117	4595-59-9	
2	4-bromo-3,5-dimethylisoxazole	MFCD00068187	10558-25-5	
3	1-bromoisquinoline	MFCD00234478	1532-71-4	
4	4-(5-bromopyrimidin-2-yl)morpholine	MFCD00483251	84539-22-0	
5	6-bromoquinoxaline	MFCD00837757	50998-17-9	
6	2-bromo-1-methyl-1h-benzo[d]imidazole	MFCD00839528	49572-60-3	
7	4-bromo-2-(piperidin-1-yl)pyridine	MFCD01646272	24255-98-9	
8	5-bromo-7h-pyrrolo[2,3-d]pyrimidine	MFCD01877574	175791-49-8	

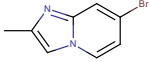
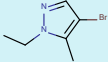
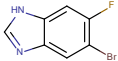
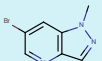
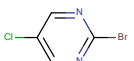
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10	3-bromo-2-methyl-6-nitro-2h-indazole	MFCD02666041	74209-41-9	
11	6-bromo-1h-indazole	MFCD03265457	79762-54-2	
12	2-acetylamino-5-bromo-6-methylpyridine	MFCD03909755	142404-84-0	
13	2-bromo-4-methylpyrimidine	MFCD04037883	130645-48-6	
14	4-(4-bromophenyl)morpholine	MFCD04112483	30483-75-1	
15	4-bromo-1,5-dimethyl-3-(trifluoromethyl)-1h-pyrazole	MFCD04972688	721402-02-4	
16	2-bromo-5-(trifluoromethyl)phenylacetonitrile	MFCD04973763	732306-26-2 875664-34-9	

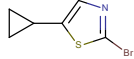
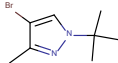
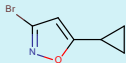
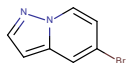
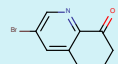
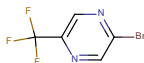
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18	2-bromo-4-methoxypyridine	MFCD06254613	89488-29-9	
19	2-bromo-1,5-dimethyl-1H-imidazole	MFCD06659902	235426-31-0	
20	N-boc-2-amino-5-bromothiazole	MFCD07368614	405939-39-1	
21	4-bromo-3,5-dimethylbenzonitrile	MFCD07369910	75344-77-3	
22	4-bromoquinoline	MFCD07644514	3964-04-3	
23	4-bromo-2-(trifluoromethyl)pyridine	MFCD07774089	887583-90-6	
24	1-(5-bromopyridin-2-yl)ethanol	MFCD07776421	159533-68-3	

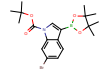
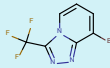
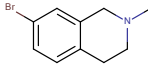
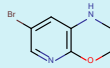
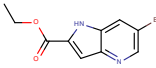
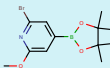
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26	2-bromo-5-phenyl-1,3,4-thiadiazole	MFCD08436697	53645-95-7	
27	6-bromo-[1,2,4]triazolo[4,3-a]pyridine	MFCD08689506	108281-79-4	
28	6-bromo-3h-oxazolo[4,5-b]pyridin-2-one	MFCD08689590	21594-52-5	
29	4-bromopyridazine	MFCD08690718	115514-66-4	
30	6-bromoquinolin-2(1h)-one	MFCD08703169	1810-66-8	
31	2-bromo-3-methylpyrazine	MFCD08705769	120984-76-1	
32	1-tert-butyl 2-ethyl 5-bromo-1h-indole-1,2-dicarboxylate	MFCD09027164	937602-51-2	

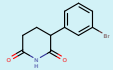
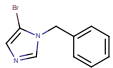
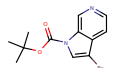
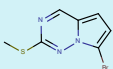
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33	4-bromobenzo[d]isoxazole	MFCD09027766	1126848-34-7	
34	5-bromo-6-methylisoquinoline	MFCD09264577	1146298-61-4	
35	Tert-butyl 3-bromo-5,6-dihydroimidazo[1,2-a]pyrazine-7(8h)-carboxylate	MFCD09701262	949922-61-6	
36	5-bromoisindolin-1-one	MFCD09701292	552330-86-6	
37	6-bromopyrazolo[1,5-a]pyrimidine	MFCD09832894	705263-10-1	
38	3-bromo-2-methoxybenzonitrile	MFCD09834773	874472-98-7	
39	6-bromo-8-methoxyimidazo[1,2-a]pyrazine	MFCD09835036	63744-25-2	
40	6-bromo-2-methylnicotinonitrile	MFCD09839266	1003711-39-4	

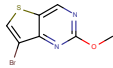
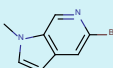
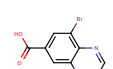
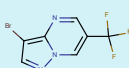
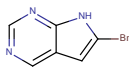
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42	5-bromo-1-methyl-1h-indazole	MFCD09878568	465529-57-1	
43	2-(4-bromo-2-methylphenyl)-1lambda6,2-thiazolidine-1,1-dione	MFCD09937072	1016816-88-8	
44	5-bromo-1,2-dihydro-3h-indazol-3-one	MFCD10697926	7364-27-4	
45	6-bromo-1-methyl-1h-imidazo[4,5-b]pyrazine	MFCD11043997	55635-64-8	
46	7-bromo-2-methylquinazoline	MFCD11044811	552331-87-0	
47	4-bromo-2-cyclopropylpyrimidine	MFCD11223249	1086381-83-0	
48	3-bromo-6-cyclopropylpyridazine	MFCD11223464	1046816-40-3	

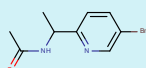
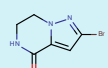
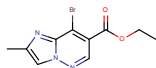
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49	7-bromo-2-methylimidazo[1,2-a]pyridine	MFCD11226901	1194375-40-0	
50	4-bromo-1-ethyl-5-methyl-1h-pyrazole	MFCD11500994	1171667-09-6	
51	5-bromo-6-fluoro-1h-benzo[d]imidazole	MFCD11846341	1008360-84-6	
52	8-bromoquinazoline	MFCD11858521	1123169-41-4	
53	3-bromo-1-methyl-1h-pyrazolo[3,4-b]pyridine	MFCD11878034	116855-03-9	
54	6-bromo-1-methyl-1h-pyrazolo[4,3-b]pyridine	MFCD12024535	1150617-56-3	
55	2-bromo-5-chloropyrimidine	MFCD12026299	124405-67-0	
56	6-bromo-8-methylimidazo[1,2-a]pyrazine	MFCD12033249	1159815-50-5	

#	Name	MFCD No.	CAS No.	Structure
57	2-bromo-5-cyclopropylthiazole	MFCD12033477	1159815-90-3	
58	3-bromo-4-methyl-1h-pyrazole	MFCD12755927	5932-20-7	
59	4-bromo-1-(tert-butyl)-3-methyl-1h-pyrazole	MFCD12756448	1187385-83-6	
60	3-bromo-5-cyclopropylisoxazole	MFCD12913765	1187933-05-6	
61	5-bromopyrazolo[1,5-a]pyridine	MFCD13189494	1060812-84-1	
62	3-bromo-6,7-dihydroquinolin-8(5h)-one	MFCD13189704	904929-24-4	
63	2-bromo-5-(trifluoromethyl)pyrazine	MFCD13190007	1196152-38-1	
64	8-bromo-6-fluoroquinazolin-4(3h)-one	MFCD14706747	1204101-90-5	

#	Name	MFCD No.	CAS No.	Structure
65	Tert-butyl 6-bromo-3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1h-indole-1-carboxylate	MFCD15143608	1218790-27-2	
66	8-bromo-3-(trifluoromethyl)-[1,2,4]triazolo[4,3-a]pyridine	MFCD15144597	1379344-24-7	
67	7-bromo-2-methyl-1,2,3,4-tetrahydroisoquinoline	MFCD15474923	258515-54-7	
68	7-bromo-2,3-dihydro-1h-pyrido[2,3-b][1,4]oxazine	MFCD15527041	946121-78-4	
69	Ethyl 6-bromo-1h-pyrrolo[3,2-b]pyridine-2-carboxylate	MFCD16657717	1234616-09-1	
70	2-bromo-6-methoxy-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine	MFCD16995251	2096340-13-3	
71	3-bromo-5,6,7,8-tetrahydro-[1,2,4]triazolo[4,3-a]pyridine	MFCD17215706	1378861-55-2	
72	3-bromo-5-fluoro-4-methylpyridine	MFCD18257616	1211517-76-8	

#	Name	MFCD No.	CAS No.	Structure
73	4-bromo-1-methyl-1h-benzo[d]imidazole	MFCD18378523	1353679-63-6	
74	3-(3-bromophenyl)piperidine-2,6-dione	MFCD19372738	1268142-04-6	
75	5-bromo-4-methoxy-6-methylpyrimidine	MFCD19382397	4319-87-3	
76	7-bromo-5h-pyrrolo[3,2-d]pyrimidine	MFCD19687341	1378816-68-2	
77	1-benzyl-5-bromo-1h-imidazole	MFCD19688638	132430-59-2	
78	5-bromo-4-cyclopropylpyrimidine	MFCD19688785	1346697-39-9	
79	Tert-butyl 3-bromo-1h-pyrrolo[2,3-c]pyridine-1-carboxylate	MFCD20277906	192189-17-6	
80	7-bromo-2-(methylthio)pyrrolo[2,1-f][1,2,4]triazine	MFCD20922038	1233094-95-5	

#	Name	MFCD No.	CAS No.	Structure
81	7-bromo-2-methoxythieno[3,2-d]pyrimidine	MFCD21099549	1259978-35-2	
82	5-bromo-1-methyl-1h-pyrrolo[2,3-c]pyridine	MFCD22039249	1369356-14-8	
83	8-bromoquinoxaline-6-carboxylic acid	MFCD22371614	1378260-89-9	
84	3-bromo-6-(trifluoromethyl)pyrazolo[1,5-a]pyrimidine	MFCD22628132	1314893-94-1	
85	8-bromo-7-methyl-imidazo[1,2-a]pyridine	MFCD23708218	1427418-46-9	
86	5-bromo-8-(trifluoromethyl)quinoline	MFCD25542357	1239460-75-3	
87	6-bromo-7h-pyrrolo[2,3-d]pyrimidine	MFCD27923777	89280-82-0	
88	3-bromo-1,4-dimethyl-1h-pyrazole	MFCD28099396	13745-59-0	

#	Name	MFCD No.	CAS No.	Structure
89	5-bromo-7-fluoroquinoxaline	MFCD28101617	1628908-19-9	
90	7-bromo-1-methyl-1h-pyrazolo[4,3-b]pyridine	MFCD28347006	1823268-58-1	
91	5-bromo-3-methylquinazolin-4-one	MFCD30182429	1410973-83-9	
92	N-[1-(5-bromopyridin-2-yl)ethyl]acetamide	MFCD30246511		
93	3-bromo-2-methyl-6,7-dihydro-5h-pyrazolo[1,5-a]pyridin-4-one	MFCD32642527	2408429-61-6	
94	2-bromo-5h,6h,7h-pyrazolo[1,5-a]pyrazin-4-one	MFCD34576675	2468022-89-9	
95	Ethyl 8-bromo-2-methylimidazo[1,2-b]pyridazine-7-carboxylate	MFCD35093868	2748771-09-5	
96	6-bromo-4-fluoro-1,2-dimethyl-1,3-benzodiazole	MFCD35316039	2189739-26-0	

*The final selection of shared building blocks may differ slightly.