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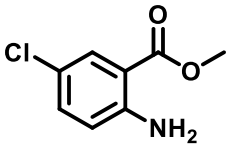
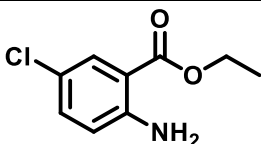
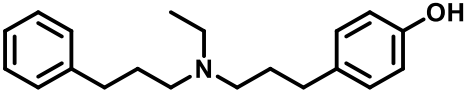
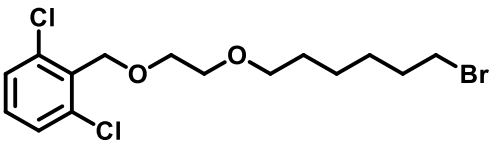
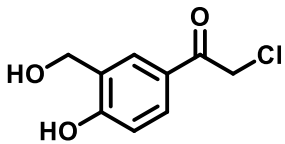
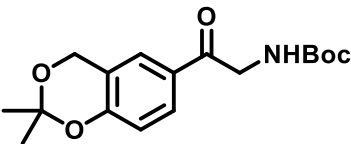
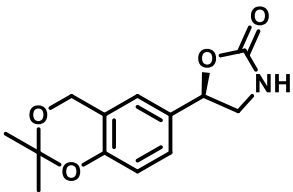
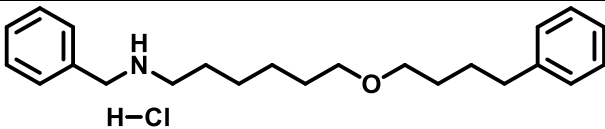
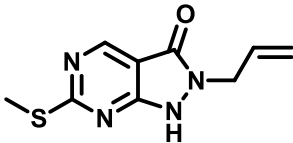
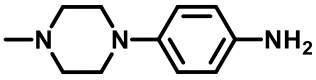
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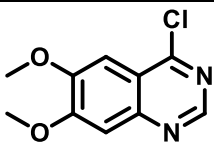
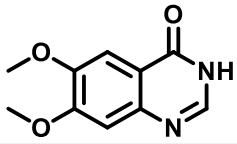
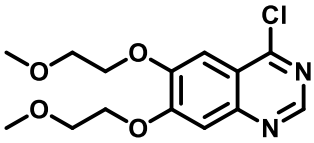
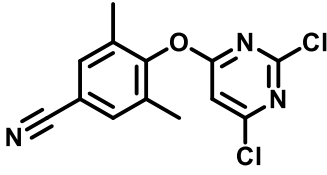
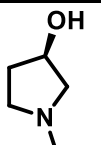
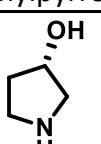
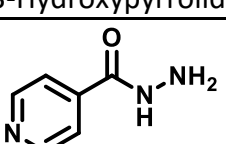
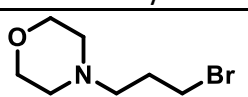
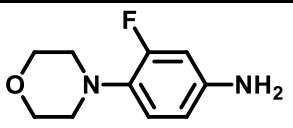
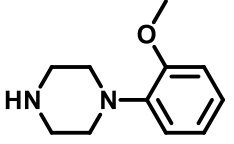
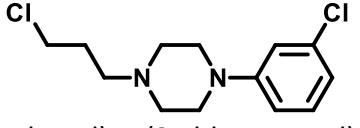
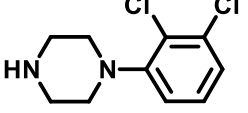
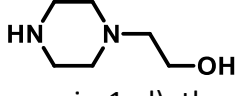
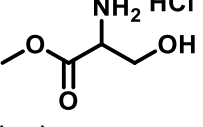
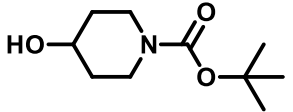
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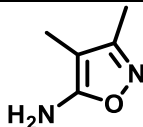
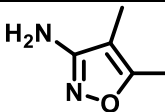
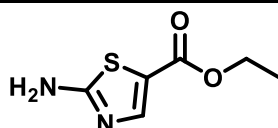
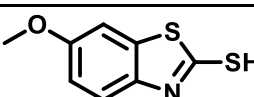
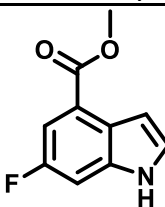
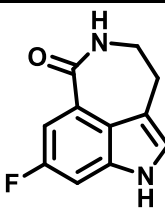
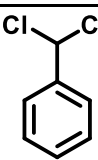
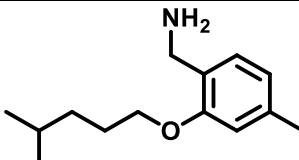
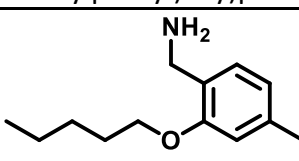
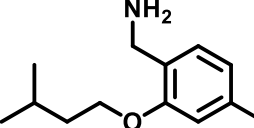
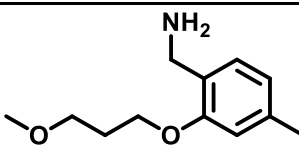
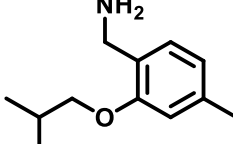
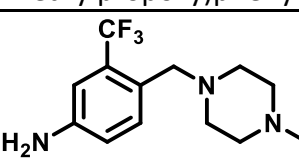
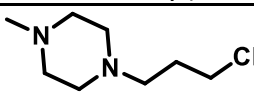
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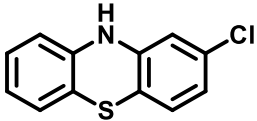
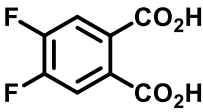
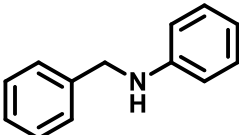
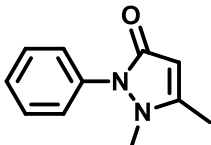
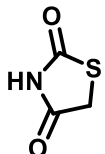
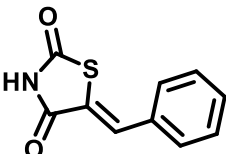
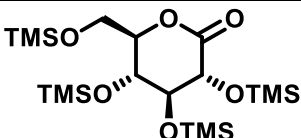
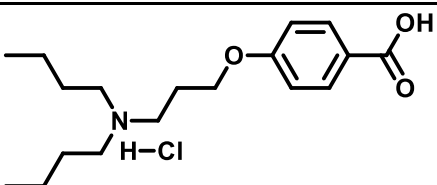
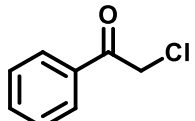
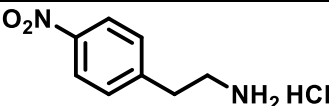
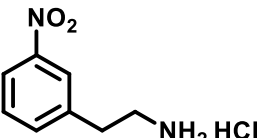
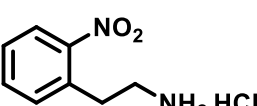
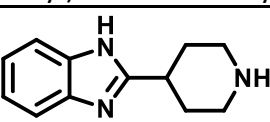
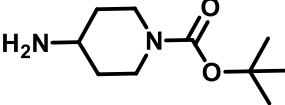


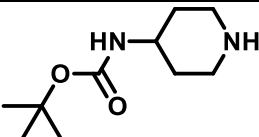
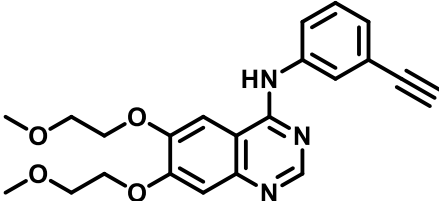
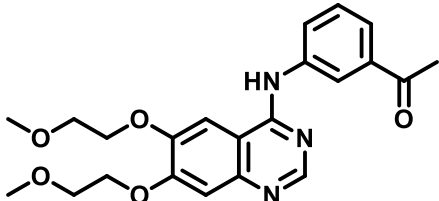
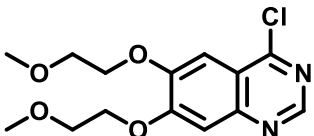
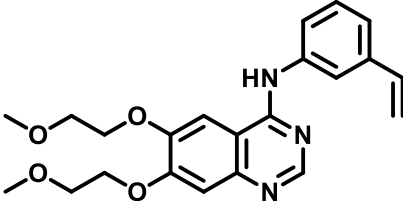
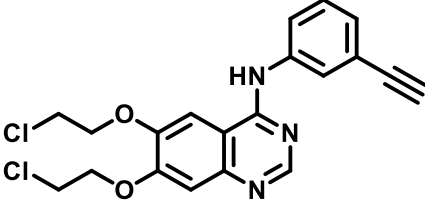
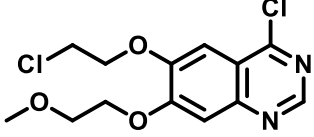
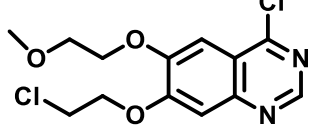
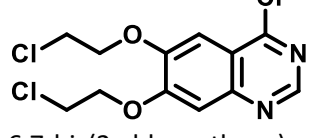
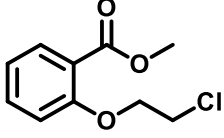
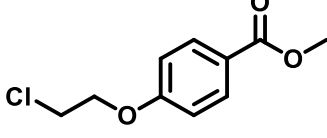
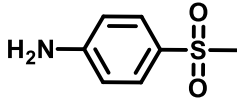
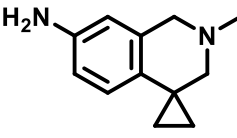
List of available products

S.No	CAS	Chemical structure and name	M.F. & M.Wt.	End use	Status
1	5202-89-1	 Methyl 2-amino-5-chlorobenzoate	M.F.: C ₈ H ₈ ClNO ₂ M.Wt.: 185.02	Chlorantraniliprole	Developed
2	63243-75-4	 Ethyl 2-amino-5-chlorobenzoate	M.F.: C ₉ H ₁₀ ClNO ₂ M.Wt.: 199.04	Chlorantraniliprole	Developed
3	142047-94-7	 4-Hydroxy alverine	M.F.: C ₂₀ H ₂₇ NO M.Wt.: 297.44	Alverine	Developed
4	503070-57-3	 2-((2-((6-Bromohexyl)oxy)ethoxy)methyl)-1,3-dichlorobenzene	M.F.: C ₁₅ H ₂₁ BrCl ₂ O ₂ M.Wt.: 382.01	Vilanterol	Developed
5	62932-94-9	 2-Chloro-1-(4-hydroxy-3-(hydroxymethyl)phenyl)ethan-1-one	M.F.: C ₉ H ₉ ClO ₃ M.Wt.: 200.02	Vilanterol	Developed
6	452339-71-8	 Tert-butyl (2-(2,2-dimethyl-4H-benzo[d][1,3]dioxin-6-yl)-2-oxoethyl)carbamate	M.F.: C ₁₇ H ₂₃ NO ₅ M.Wt.: 321.16	Vilanterol	Developed
7	208925-08-0	 (R)-5-(2,2-dimethyl-4H-benzo[d][1,3]dioxin-6-yl)oxazolidin-2-one	M.F.: C ₁₃ H ₁₅ NO ₄ M.Wt.: 249.10	Vilanterol	Developed
8	163923-18-0	 N-Benzyl-6-(4-phenyl-butoxy)hexan-1-amine hydrochloride	M.F.: C ₂₃ H ₃₄ ClNO M.Wt.: 375.23	Salmeterol	Developed
9	955368-90-8	 2-Allyl-6-(methylthio)-1,2-dihydro-3H-pyrazolo[3,4-d]pyrimidin-3-one	M.F.: C ₉ H ₁₀ N ₄ OS M.Wt.: 222.06	Adavosertib	Developed
10	16153-81-4	 4-(4-Methylpiperazin-1-yl)aniline	M.F.: C ₁₁ H ₁₇ N ₃ M.Wt.: 191.14	Adavosertib	Developed

11	13790-39-1	 4-Chloro-6,7-dimethoxyquinazoline	M.F.: C ₁₄ H ₁₆ N ₁₀ O ₄ M.Wt.: 224.04	Fruquintinib	Developed
12	13794-72-4	 6,7-Dimethoxy-3H-quinazolin-4-one	M.F.: C ₁₀ H ₁₀ N ₂ O ₃ M.Wt.: 206.07	Fruquintinib	Developed
13	183322-18-1	 4-Chloro-6,7-bis(2-methoxyethoxy)-quinazoline	M.F.: C ₁₄ H ₁₈ N ₂ O ₅ M.Wt.: 294.12	Erlotinib	Developed
14	1225383-63-0	 4-[(2,6-Dichloro)-4-pyrimidinyl]-3,5-dimethylbenzonitrile	M.F.: C ₁₃ H ₉ Cl ₂ N ₃ O M.Wt.: 293.01	Etravirine	Developed
15	104641-60-3	 (R)-1-Methylpyrrolidin-3-ol	M.F.: C ₅ H ₁₁ NO M.Wt.: 101.08	Sofpironium bromide	Developed
16	100243-39-8	 (S)-3-Hydroxypyrrolidine;	M.F.: C ₄ H ₉ NO M.Wt.: 87.07	Larotrectinib	Developed
17	54-85-3	 Isonicotinohydrazide	M.F.: C ₆ H ₇ N ₃ O M.Wt.: 137.06	Isoniazid	Developed
18	125422-83-5	 4-(3-Bromopropyl)morpholine	M.F.: C ₇ H ₁₄ BrNO M.Wt.: 207.03	Gefitinib	Developed
19	93246-53-8	 3-Fluoro-4-morpholinoaniline	M.F.: C ₁₀ H ₁₃ FN ₂ O M.Wt.: 196.10	Linezolid	Developed
20	35386-24-4	 1-(2-Methoxyphenyl) piperazine	M.F.: C ₁₁ H ₁₆ N ₂ O M.Wt.: 192.13	Nesapidil	Developed
21	39577-43-0	 1-(3-Chlorophenyl)-4-(3-chloropropyl)piperazine	M.F.: C ₁₃ H ₁₈ Cl ₂ N ₂ M.Wt.: 273.20	Trazodone	Developed
22	41202-77-1	 1-(2,3-Dichlorophenyl) piperazine	M.F.: C ₁₀ H ₁₂ Cl ₂ N ₂ M.Wt.: 230.04	Aripiperazole	Developed
23	103-76-4	 2-(Piperazin-1-yl)ethan-1-ol	M.F.: C ₆ H ₁₄ N ₂ O M.Wt.: 130.11	Dasatinib	Developed
24	5619-04-5	 Methyl 2-amino-3-hydroxypropanoate hydrochloride (DL-Serine methyl ester hydrochloride)	M.F.: C ₄ H ₁₀ ClNO ₃ M.Wt.: 155.03	Benserazide	Developed
25	10984-19-2	 N-BOC-4-hydroxypiperidine	M.F.: C ₁₀ H ₁₉ NO ₃ M.Wt.: 201.14	Lonafarnib Crizotinib, Sapitinib	Developed

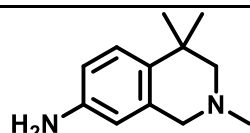
26	19947-75-2	 3,4-Dimethylisoxazol-5-amine	M.F.: C ₅ H ₈ N ₂ O M.Wt.: 112.06	Truxazole (Sulfisoxazole)	Developed
27	13999-39-8	 4,5-Dimethylisoxazol-3-amine	M.F.: C ₅ H ₈ N ₂ O M.Wt.: 112.06	Truxazole (Sulfisoxazole)	Developed
28	32955-21-8	 Ethyl 2-aminothiazole-5-carboxylate	M.F.: C ₆ H ₈ N ₂ O ₂ S M.Wt.: 172.03	Dasatinib	Developed
29	2182-73-2	 2-Mercapto-6-methoxybenzothiazole	M.F.: C ₈ H ₇ NOS ₂ M.Wt.: 197.00	Omeprazole Esomeprazole	Developed
30	1082040-43-4	 Methyl 6-fluoro-1 <i>H</i> -indole-4-carboxylate	M.F.: C ₁₀ H ₈ FNO ₂ M.Wt.: 193.05	Rucaparib	Developed
31	1408282-26-7	 8-Fluoro-2,3,4,6-tetrahydro-1 <i>H</i> -azepino[5,4,3- <i>cd</i>]indol-1-one	M.F.: C ₁₁ H ₉ FN ₂ O M.Wt.: 204.07	Rucaparib	Developed
32	98-87-3	 (Dichloromethyl)benzene	M.F.: C ₇ H ₆ Cl ₂ M.Wt.: 159.98	DCTCB	Developed
33	1249171-23-0	 (4-Methyl-2-((4-methylpentyl)oxy)phenyl)methanamine	M.F.: C ₁₄ H ₂₃ NO M.Wt.: 221.18	Advanced building block	Developed
34	1250130-58-5	 (4-Methyl-2-(pentyloxy)phenyl)methanamine	M.F.: C ₁₃ H ₂₁ NO M.Wt.: 207.16	Advanced building block	Developed
35	1249299-60-2	 (2-(isopentyloxy)-4-methylphenyl)methanamine	M.F.: C ₁₃ H ₂₁ NO M.Wt.: 207.16	Advanced building block	Developed
36	1247807-01-7	 2-(3-Methoxypropoxy)-4-methylphenyl]methanamine	M.F.: C ₁₂ H ₁₉ NO ₂ M.Wt.: 209.14	Advanced building block	Developed
37	1250934-67-8	 4-Methyl-2-(2-methylpropoxy)phenyl]methanamine	M.F.: C ₁₂ H ₁₉ NO M.Wt.: 193.15	Advanced building block	Developed
38	694499-26-8	 4-((4-Methylpiperazin-1-yl)methyl)-3-(trifluoromethyl)aniline	M.F.: C ₁₃ H ₁₈ F ₃ N ₃ M.Wt.: 273.30	Ponatinib	Developed
39	104-16-5	 1-(3-Chloropropyl)-4-methylpiperazine	M.F.: C ₈ H ₁₇ ClN ₂ M.Wt.: 176.11	Prochlorperazine	Developed

40	92-39-7	 2-Chloro-10H-phenothiazine	M.F.: C ₁₂ H ₈ ClNS M.Wt.: 233.01	Chlorpromazine	Developed
41	18959-31-4	 4,5-Difluorophthalic acid	M.F.: C ₈ H ₄ F ₂ O ₄ M.Wt.: 202.01	Building block	Developed
42	103-32-2	 N-Phenylbenzylamine	M.F.: C ₁₃ H ₁₃ N M.Wt.: 183.25	Antazoline	Developed
43	60-80-0	 1,5-Dimethyl-2-phenyl-1,2-dihydro-3H-pyrazol-3-one	M.F.: C ₁₁ H ₁₂ N ₂ O M.Wt.: 188.09	Antipyrine	Developed
44	2295-31-0	 2,4-Thiazolidinedione	M.F.: C ₃ H ₃ NO ₂ S M.Wt.: 116.99	Pioglitazone	Developed
45	103788-60-9	 5-Benzylidenethiazolidine-2,4-dione	M.F.: C ₁₀ H ₇ NO ₂ S M.Wt.: 205.02	Pioglitazone	Developed
46	32384-65-9	 (3R,4S,5R,6R)-3,4,5-tris((trimethylsilyl)oxy)-6- (((trimethylsilyl)oxy)methyl)tetrahydro-2H-pyran-2-one	M.F.: C ₁₈ H ₄₂ O ₆ Si ₄ M.Wt.: 466.21	Dapagliflozin	Developed
47	437651-44-0	 4-(3-(Dibutylamino)propoxy)benzoic acid hydrochloride	M.F.: C ₁₈ H ₃₀ ClNO ₃ M.Wt.: 343.1	Dronedarone	Developed
48	532-27-4	 Phenacyl chloride	M.F.: C ₈ H ₇ ClO M.Wt.: 154.02	KSM	Developed
49	29968-78-3	 2-(4-nitrophenyl)ethan-1-aminehydrochloride	M.F.: C ₈ H ₁₁ ClN ₂ O ₂ M.Wt.: 202.05	Mirabegron	Developed
50	190082-62-9	 2-(3-nitrophenyl)ethan-1-amine hydrochloride	M.F.: C ₈ H ₁₁ ClN ₂ O ₂ M.Wt.: 202.05	Meta-Mirabegron	Developed
51	861337-74-8	 2-(2-Nitrophenyl)ethanamine Hydrochloride	M.F.: C ₈ H ₁₁ ClN ₂ O ₂ M.Wt.: 202.05	Mirabegron	Developed
52	38385-95-4	 2-(piperidin-4-yl)-1H-benzo[d]imidazole	M.F.: C ₁₂ H ₁₅ N ₃ M.Wt.: 201.13	Bilastine	Developed
53	87120-72-7	 4-Amino-1-Boc-piperidine	M.F.: C ₁₀ H ₂₀ N ₂ O ₂ M.Wt.: 200.15	Relebactam Prucalopride Succinate	Under developing

54	73874-95-0		M.F.: C ₁₀ H ₂₀ N ₂ O ₂ M.Wt.: 200.15	Astemizole Prucalopride Succinate	Under developing
55	183321-74-6		M.F.: C ₂₂ H ₂₃ N ₃ O ₄ M.Wt.: 393.44	Erlotinib	Developed
56	1354727-63-1		M.F.: C ₂₂ H ₂₅ N ₃ O ₅ M.Wt.: 411.46	Erlotinib Impurity C	Developed
57	183322-18-1		M.F.: C ₁₄ H ₁₇ ClN ₂ O ₄ M.Wt.: 312.75	Erlotinib Impurity D	Developed
58	1058132-82-3		M.F.: C ₂₂ H ₂₅ N ₃ O ₄ M.Wt.: 395.46	Erlotinib Impurity E	Developed
59	183321-82-6		M.F.: C ₂₀ H ₁₇ Cl ₂ N ₃ O ₂ M.Wt.: 402.28	Erlotinib Impurity L	Developed
60	183322-19-2		M.F.: C ₁₃ H ₁₄ Cl ₂ N ₂ O ₃ M.Wt.: 317.17	Erlotinib Impurity G	Developed
61	183322-20-5		M.F.: C ₁₃ H ₁₄ Cl ₂ N ₂ O ₃ M.Wt.: 317.17	Erlotinib Impurity I	Developed
62	183322-21-6		M.F.: C ₁₂ H ₁₁ Cl ₃ N ₂ O ₂ M.Wt.: 321.58	Erlotinib Impurity M	Developed
63	312631-02-0		M.F.: C ₁₀ H ₁₁ ClO ₃ M.Wt.: 214.04	KSM	Developed
64	38567-00-9		M.F.: C ₁₀ H ₁₁ ClO ₃ M.Wt.: 214.04	KSM	Developed
65	5470-49-5		M.F.: C ₉ H ₉ NO ₂ S M.Wt.: 171.21	Esaxerenone	Developed
66	1092794-11-0		M.F.: C ₁₂ H ₁₆ N ₂ M.Wt.: 188.27	Advanced building block	Developed

67

745778-71-6



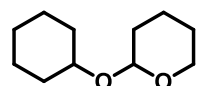
2,4,4-Trimethyl-1,2,3,4-tetrahydroisoquinolin-7-amine

M.F.: C₁₂H₁₈N₂

M.Wt.: 190.29

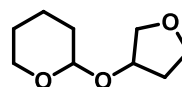
Advanced building
block

Developed

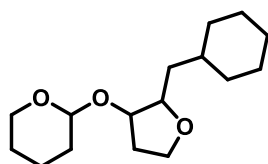
Multi-target antitubercular scaffold in mycobacterium tuberculosis

CAS # 709-83-1

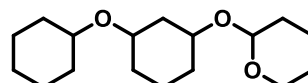
2-(cyclohexyloxy)tetrahydro-2H-pyran



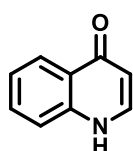
2-((tetrahydrofuran-3-yl)oxy)tetrahydro-2H-pyran



2-((2-(cyclohexylmethyl)tetrahydrofuran-3-yl)oxy)tetrahydro-2H-pyran

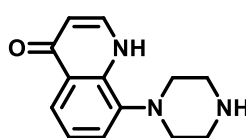


2-((3-(cyclohexyloxy)cyclohexyl)oxy)tetrahydro-2H-pyran

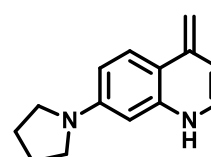


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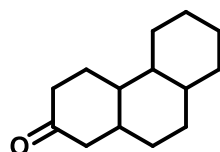
quinolin-4(1H)-one



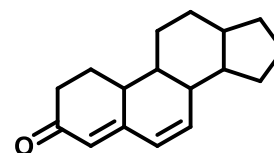
8-(piperazin-1-yl)quinolin-4(1H)-one



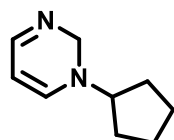
4-methylene-7-(pyrrolidin-1-yl)-1,4-dihydroquinoline

Top repurposable scaffolds with anticancer properties

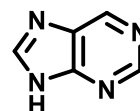
dodecahydrophenanthren-2(1H)-one



1,2,8,9,10,11,12,13,14,15,16,17-dodecahydro-3H-cyclopenta[a]phenanthren-3-one



1-cyclopentyl-1,2-dihydropyrimidine

CAS # 120-73-0
9H-purine