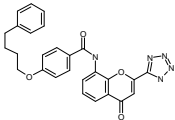
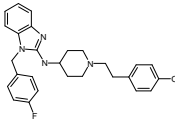
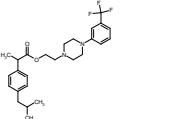
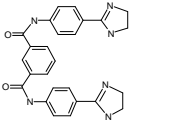
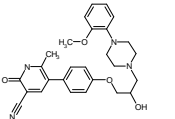
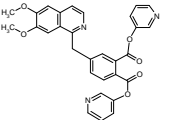
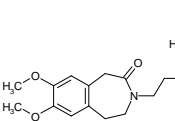
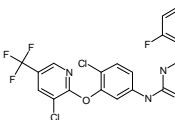
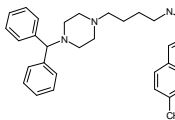
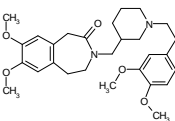
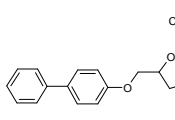
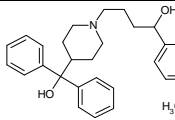
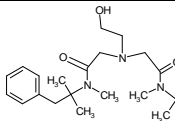
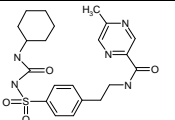
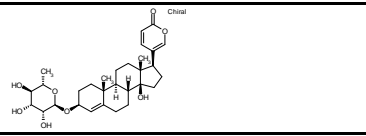
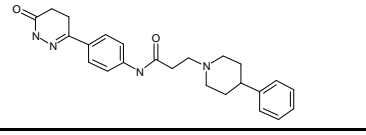
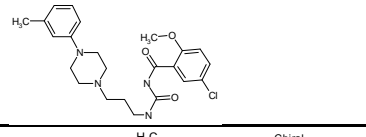
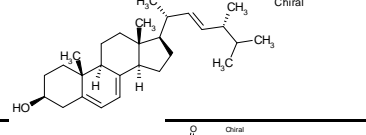
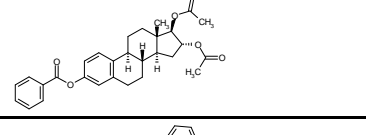
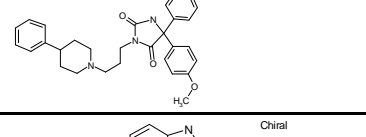
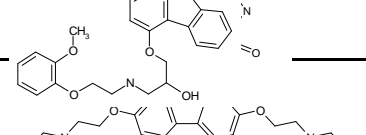
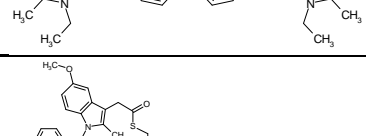
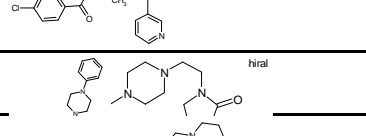
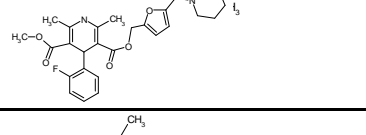
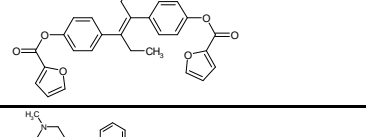
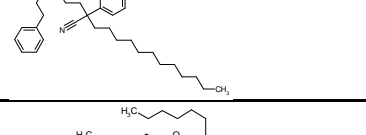
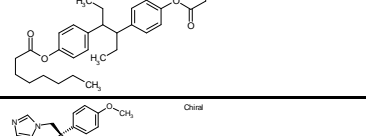
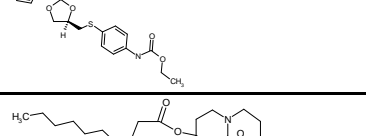
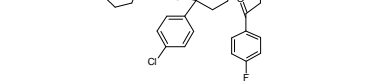

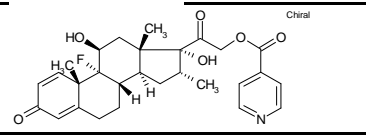
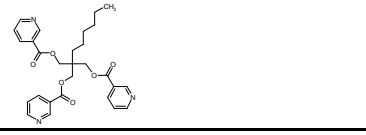
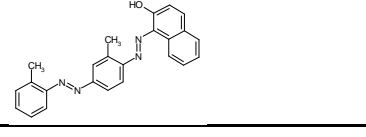
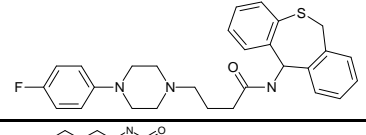
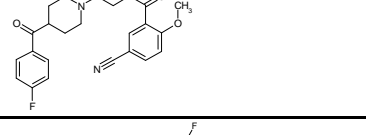
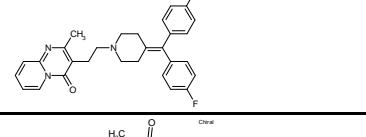
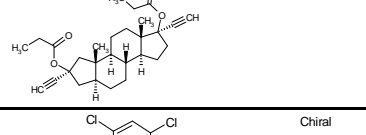
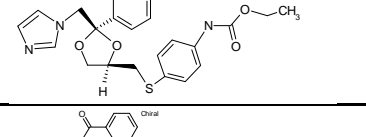
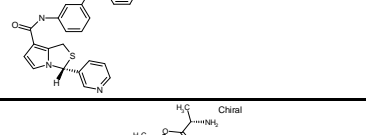
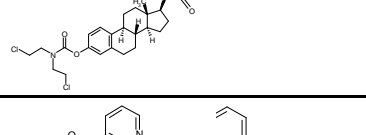
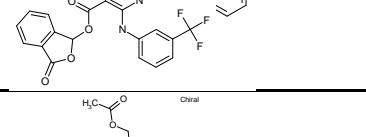
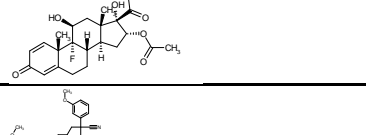
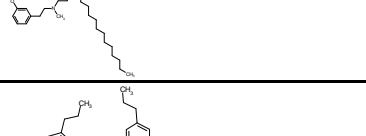
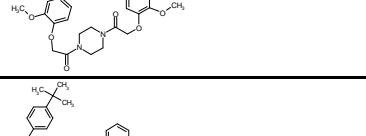
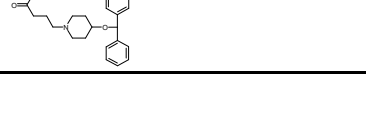
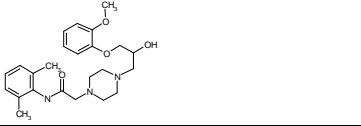
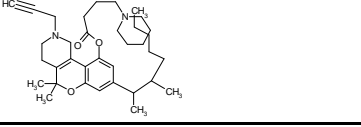
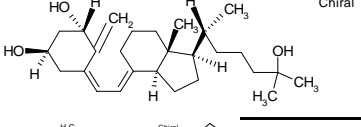
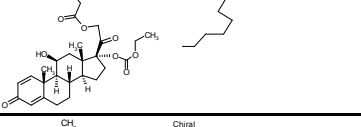
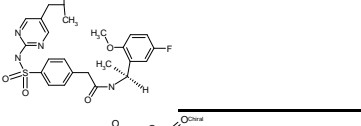
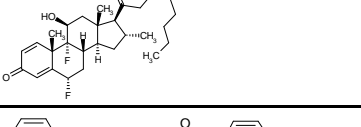
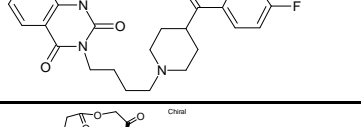
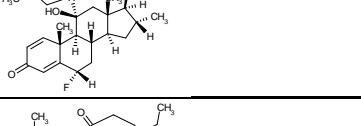
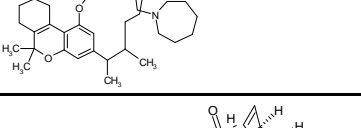
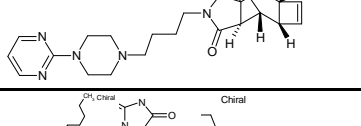
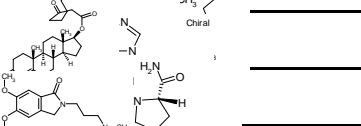
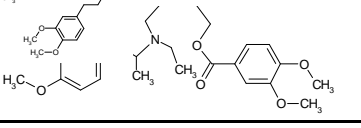
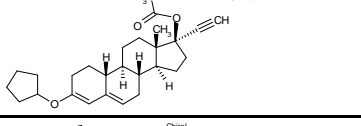
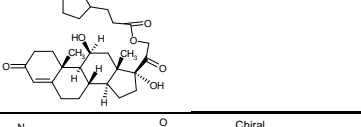
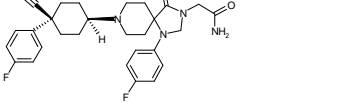



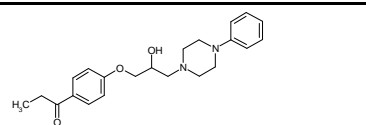
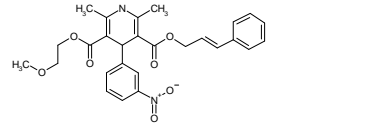
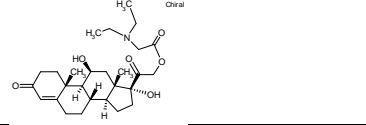
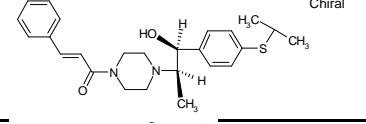
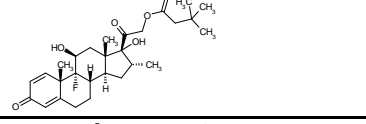
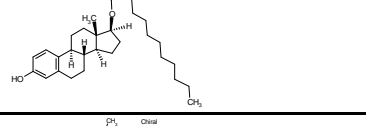
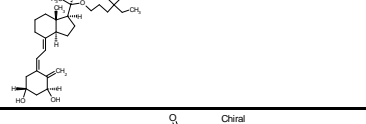
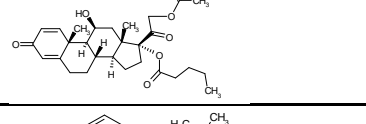
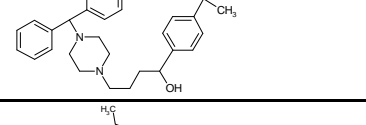
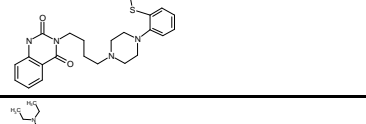
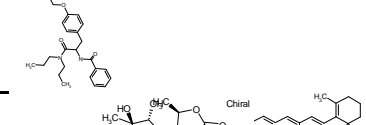
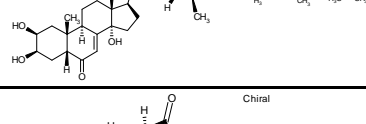
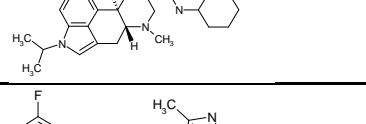
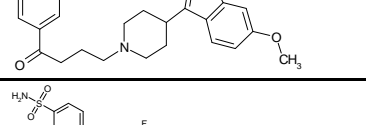

Appendix A: The top 173 compounds of GEMDOCK by screening the CMC database

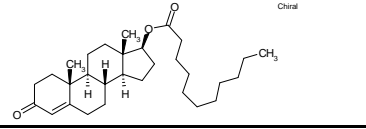
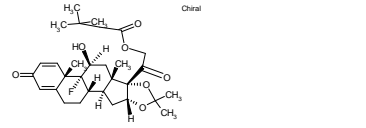
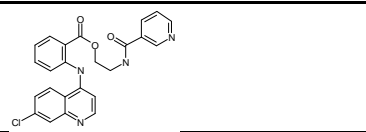
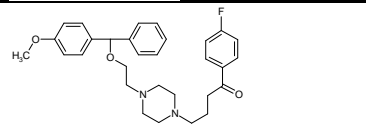
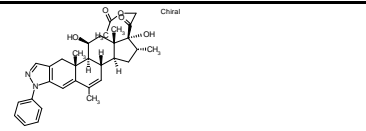
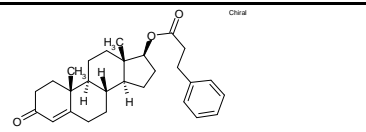
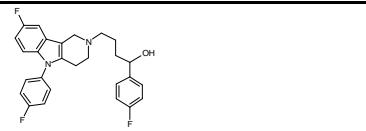
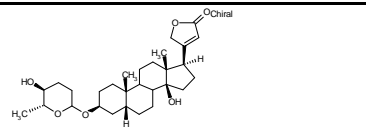
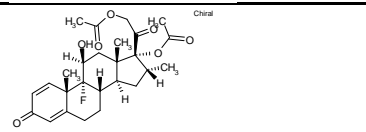
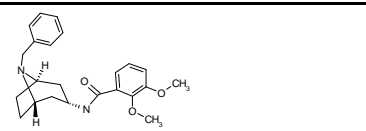
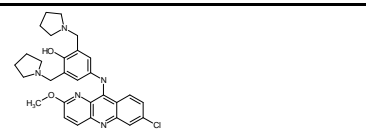
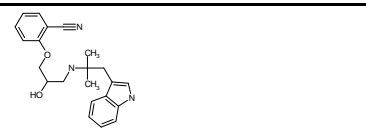
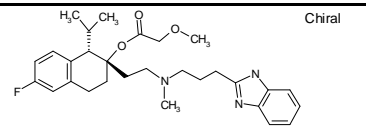
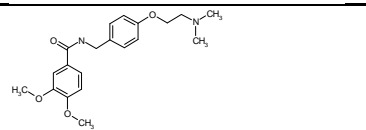
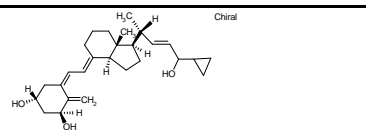
Molecular structure	MDL number	molecular weight	Molecular Name	Rank	Energy
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	MCMC00004876	458.584	ASTEMIZOLE	2	-125.721
	MCMC00005482	462.56	FRABUPROFEN	3	-124.395
	MCMC00002249	452.52	ISOTIC	4	-123.209
	MCMC00005714	474.565	SATERINONE	5	-121.472
	MCMC00001853	521.5341	NICEVERINE	6	-121.194
	MCMC00005922	456.587	ZATEBRADINE	7	-120.367
	MCMC00006275	506.219	FLUAZURON	8	-119.333
	MCMC00007477	468.648	TAGORIZINE	9	-119.226
	MCMC00006040	482.625	CILOBRADINE	10	-118.452
	MCMC00004528	481.377	DOCONAZOLE	11	-118.317
	MCMC00004032	471.689	TERFENADINE	12	-112.280
	MCMC00000751	467.657	OXETHAZINE	13	-111.531
	MCMC00003498	445.544	GLIPIZIDE	14	-109.651

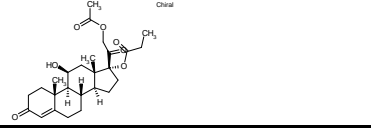
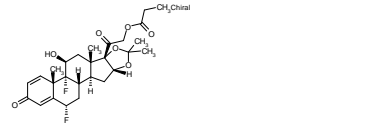
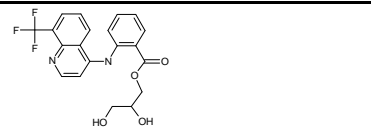
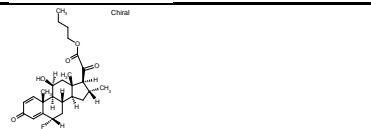
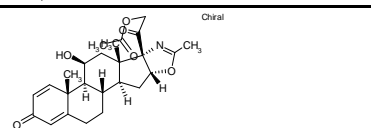
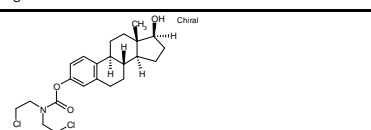
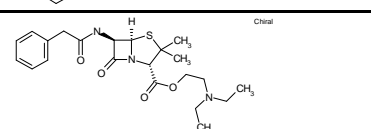
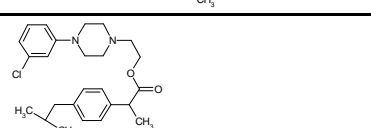
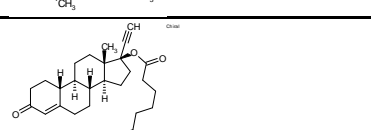
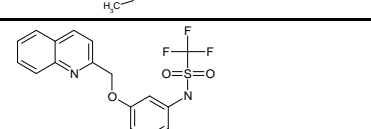
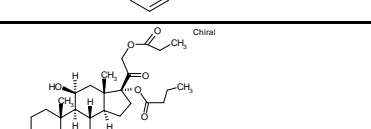
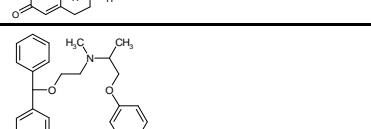
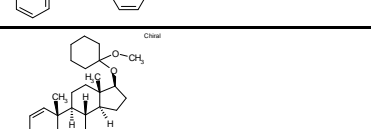
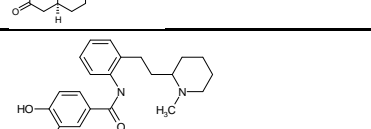
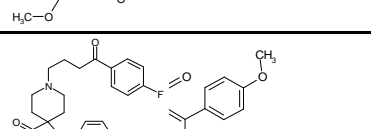
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	MCMC00006947	396.662	ERGOSTEROL	18	-96.032
	MCMC00010202	476.566	HOLIN-DEPOT	19	-95.330
	MCMC00004342	483.616	ROPITOIN	20	-95.185
	MCMC00007319	470.696	TRICAPRILIN	21	-94.863
	MCMC00003454	410.561	TILORONE	22	-94.706
	MCMC00005257	464.975	PIMETACIN	23	-94.512
	MCMC00003427	437.544	ALPERTINE	24	-94.142
	MCMC00006442	482.557	SAGANDIPINE	25	-93.803
	MCMC00001304	456.5	FUROSTILBESTROL	26	-93.700
	MCMC00005430	460.753	RONIPAMIL	27	-93.567
	MCMC00010262	522.765	HEXESTROL DICAPRYLATE	28	-93.513
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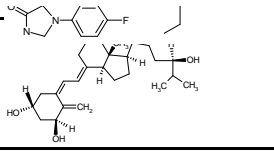
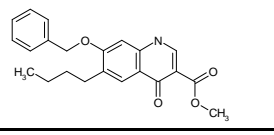
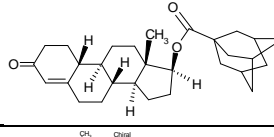
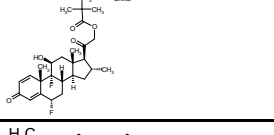
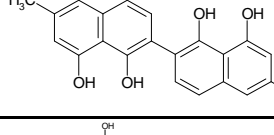
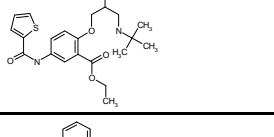
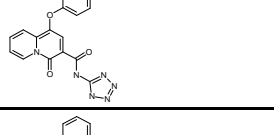
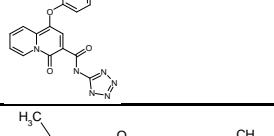
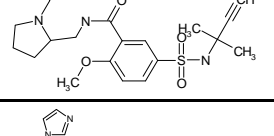
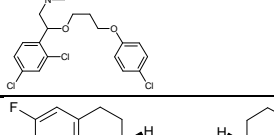
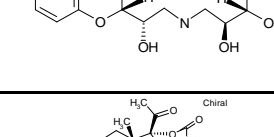
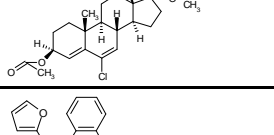
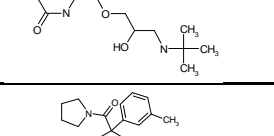
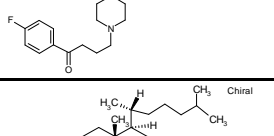
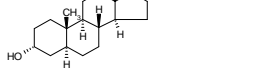
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	MCMC00006472	475.633	MONATEPIL	34	-92.543
	MCMC00005627	409.464	PRIDEPERONE	35	-92.288
	MCMC00005508	471.555	SEGANSERIN	36	-91.554
	MCMC00010192	438.604	ANORDRIN	37	-91.336
	MCMC00005412	508.424	TUBULOZOLE	38	-91.198
	MCMC00006389	425.513	TULOPAFANT	39	-91.188
	MCMC00007524	511.494	ALESTRAMUSTINE	40	-90.837
	MCMC00005219	399.494	ANSOXETINE	41	-90.581
	MCMC00006975	478.519	TRIAMCINOLONE DIACETATE	42	-90.375
	MCMC00005367	520.806	ANIPAMIL	43	-90.314
	MCMC00000901	498.625	SIMETRIDE	44	-90.120
	MCMC00005577	469.673	EBASTINE	45	-89.341

	MCMC00005630	427.548	RANOLAZINE	46	-89.207
	MCMC00004792	548.816	NABITAN	47	-89.134
 Chiral	MCMC00003603	416.642	CALCITRIOL	48	-88.780
 Chiral	MCMC00005044	488.573	PREDNICARBATE	49	-88.760
 Chiral	MCMC00003720	500.592	GLIFLUMIDE	50	-88.262
	MCMC00010176	478.572	DIFLUCORTOLONE VALERATE	51	-87.957
	MCMC00005490	423.492	BUTANSERIN	52	-87.587
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	MCMC00004449	537.834	NABAZENIL	54	-86.942
	MCMC00006380	419.526	ZALOSPIRONE	55	-86.847
 Chiral	MCMC00006119	464.56	TRELNARIZINE	56	-86.544
 Chiral	MCMC00006369	421.903	MOSAPRIDE	57	-86.497
	MCMC00005183	428.533	FALIPAMIL	58	-86.480
	MCMC00002025	429.561	MEBEVERINE	59	-86.422
 Chiral	MCMC00001905	408.578	QUINGESTANOL ACETATE	60	-86.383
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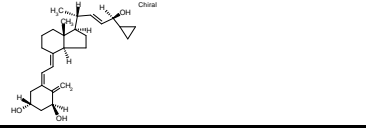
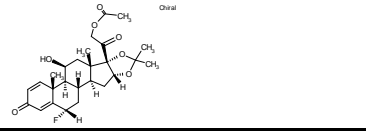
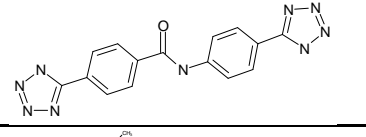
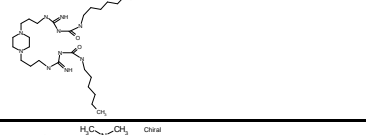
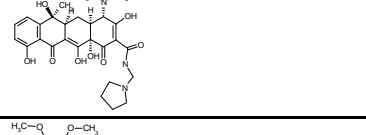
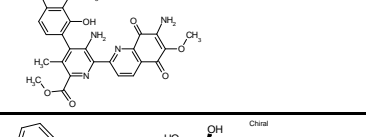
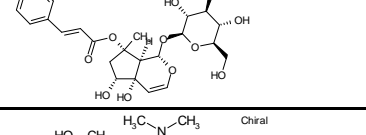
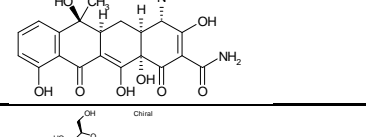
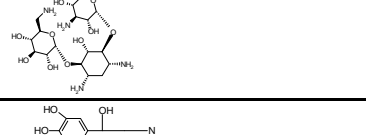
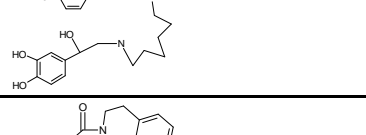
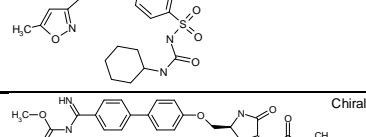
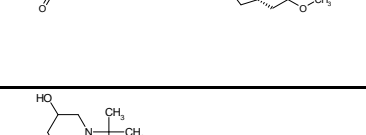
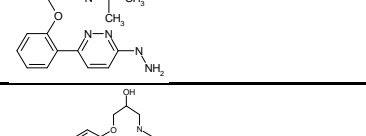
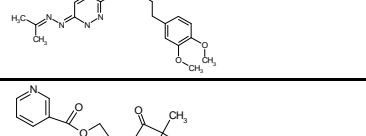
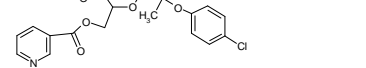
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	MCMC00005434	424.606	SUNAGREL	66	-85.252
	MCMC00010194	490.608	DEXAMETHASONE TERT.- BUTYLACETATE	67	-85.216
	MCMC00002001	440.664	ESTRADIOL UNDECYLATE	68	-85.121
	MCMC00007647	460.694	LEXACALCITOL	69	-85.021
	MCMC00006751	486.601	PREDNISOLONE VALERATE ACETATE	70	-84.715
	MCMC00005340	456.677	TRENIZINE	71	-84.591
	MCMC00004119	452.623	TIOPERIDONE	72	-84.396
	MCMC00004404	481.684	SEVOPRAMIDE	73	-84.342
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	MCMC00006419	393.577	AMESERGIDE	75	-84.195
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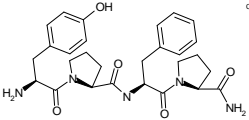
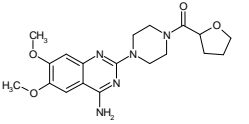
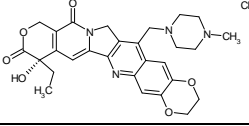
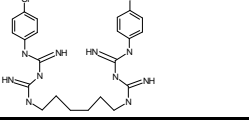
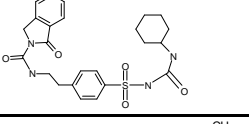
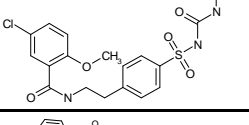
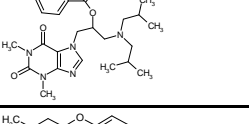
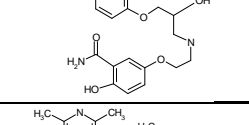
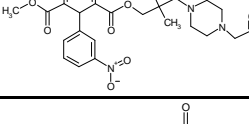
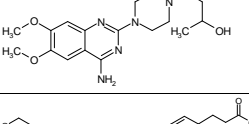
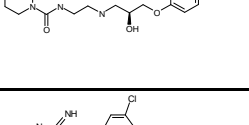
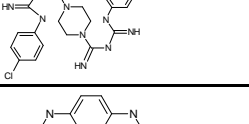
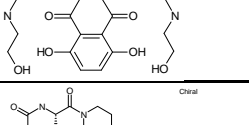
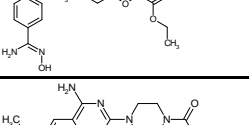

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	MCMC00004679	446.897	NICAFENINE	80	-82.912
	MCMC00004737	490.623	MOBENZOXAMINE	81	-82.904
 Chiral	MCMC00001576	530.6609	CORTIVAZOL	82	-82.756
 Chiral	MCMC00010189	420.589	TESTOSTERONE PHENYLPROPIONATE	83	-82.657
	MCMC00004941	450.508	FLUTROLINE	84	-82.602
 Chiral	MCMC00003632	488.661	RAMNODIGIN	85	-82.503
 Chiral	MCMC00006567	476.538	DEXAMETHASONE ACETATE	86	-82.145
	MCMC00005125	380.485	TROPAPRIDE	87	-81.839
	MCMC00010201	518.058	BENZONAPHTHYRIDINE 7351	88	-81.678
	MCMC00004956	363.463	BUCINDOLOL	89	-81.493
 Chiral	MCMC00007471	495.643	MIBEFRADIL	90	-80.946
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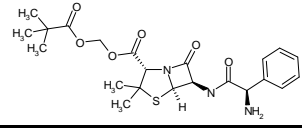
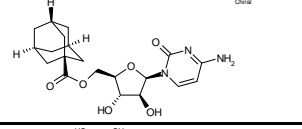
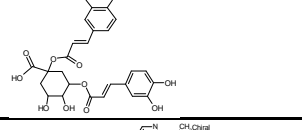
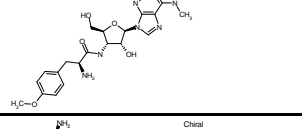
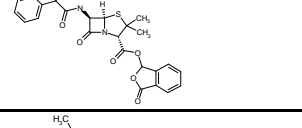
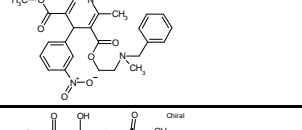
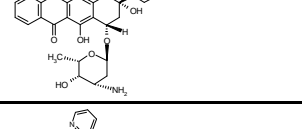
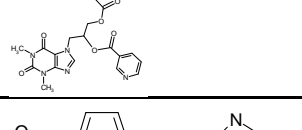
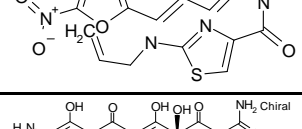
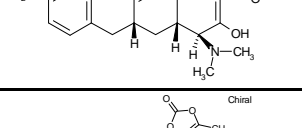
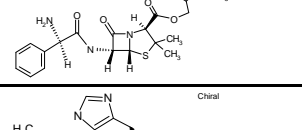
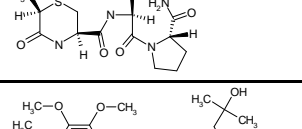
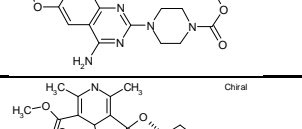
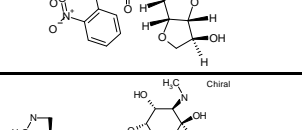
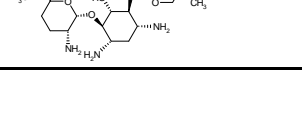
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	MCMC00007244	508.565	PROCINONIDE	94	-80.766
	MCMC00003287	406.365	FLOCTAFENINE	95	-80.625
	MCMC00003935	446.555	FLUOCORTIN BUTYL	96	-79.919
	MCMC00002786	441.521	DEFLAZACORT	97	-79.318
	MCMC00001904	440.408	ESTRAMUSTINE	98	-77.901
	MCMC00010073	433.57	PENETHAMATE HYDROIODIDE	99	-77.861
	MCMC00005635	429.007	LOBUPROFEN	100	-77.750
	MCMC00010178	410.594	NORETHINDRONE ENANTHATE	101	-77.706
	MCMC00006056	382.364	RITOLUKAST	102	-77.603
	MCMC00005892	488.617	HYDROCORTISONE BUTEPRATE	103	-76.851
	MCMC00004732	375.515	PRENOVERINE	104	-76.602
	MCMC00002535	400.599	MESABOLONE	105	-75.995
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	MCMC00004265	413.471	FLUSPIPERONE	107	-75.470

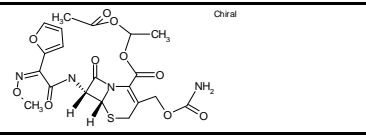
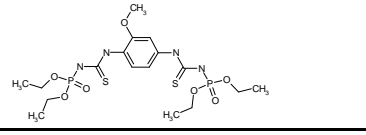
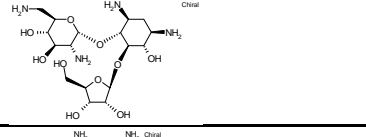
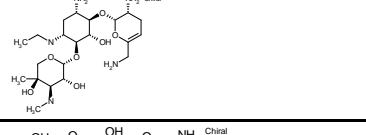
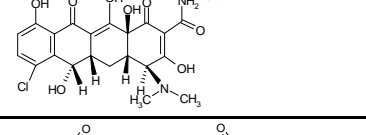
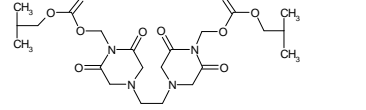
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	MCMC00007170	478.582	DIFLUCORTOLONE PIVALATE	111	-74.482
	MCMC00010046	346.38	DIOSPYROL	112	-74.459
	MCMC00005556	420.532	TIENOXOLOL	113	-74.035
	MCMC00006202	348.321	QUINOTOLAST	114	-73.874
	MCMC00006202	348.321	QUINOTOLAST	115	-73.874
	MCMC00004894	407.536	TINISULPRIDE	116	-73.656
	MCMC00004952	425.746	ZOFICONAZOLE	117	-73.571
	MCMC00005680	405.439	NEBIVOLOL	118	-73.196
	MCMC00001911	448.984	CLOGESTONE ACETATE	119	-73.124
	MCMC00005103	332.403	ANCAROLOL	120	-72.912
	MCMC00010171	436.568	MEPERIDIDE	121	-72.613
	MCMC00006715	388.675	EPIDIHYDROCHOLE STERIN	122	-72.199



	MCMC00006371	412.618	CALCIPOTRIENE	123	-72.013
	MCMC00002169	476.538	FLUNISOLIDE ACETATE	124	-71.378
	MCMC00006478	333.315	ANDOLAST	125	-70.674
	MCMC00004882	538.786	IPEXIDINE	126	-69.594
	MCMC00007079	527.579	ROLITETRACYCLINE	127	-69.574
	MCMC00001958	520.503	METHYLSTREPTONIGRIN	128	-66.946
	MCMC00010126	494.49	HARPAGOSIDE	129	-66.708
	MCMC00006963	444.445	TETRACYCLINE	130	-60.419
	MCMC00006958	484.508	KANAMYCIN	131	-53.576
	MCMC00001935	420.51	HEXOPRENALINE	132	-52.259
	MCMC00003320	434.518	GLISOLAMIDE	133	-51.420
	MCMC00007873	439.465	LEFRADAFIBAN	134	-50.403
	MCMC00004492	331.421	PRIZIDILOL	135	-50.205
	MCMC00005150	403.485	DRAMEDILOL	136	-47.967
	MCMC00004883	498.924	BINIFIBRATE	137	-46.008

 Chiral	MCMC00010188	521.615	MORPHICEPTIN	138	-45.856
	MCMC00004658	387.442	TERAZOSIN	139	-45.411
 Chiral	MCMC00007618	518.567	GI147211	140	-44.963
	MCMC00000120	505.457	CHLORHEXIDINE	141	-44.314
	MCMC00004946	484.579	GLISINDAMIDE	142	-43.950
	MCMC00004132	425.894	GLICONDAMIDE	143	-43.451
	MCMC00007448	469.589	DIISOBUTYLAMINO BENZOXYPROP YL THEOPHYLLINE	144	-43.293
	MCMC00005147	420.467	TRIGEVOLOL	145	-42.905
	MCMC00006786	526.638	IGANIDIPINE	146	-42.714
	MCMC00006353	375.431	NELDAZOSIN	147	-41.933
 Chiral	MCMC00007871	509.596	LANDIOLOL	148	-41.717
	MCMC00002335	475.387	PICLOXYDINE	149	-40.938
	MCMC00004733	444.492	MITOXANTRONE	150	-40.259
 Chiral	MCMC00007926	420.463	SIBRAFIBAN	151	-38.854
	MCMC00005060	451.486	DOXAZOSIN	152	-38.541

 Chiral	MCMC00003657	463.552	PIVAMPICILLIN	153	-37.287
 Chiral	MCMC00009952	405.448	ADAMANTOYL CYTARABINE	154	-37.025
	MCMC00001729	516.463	CYNARINE	155	-36.837
 Chiral	MCMC00006935	471.52	PUROMYCIN	156	-34.527
 Chiral	MCMC00003999	481.527	TAMAMPICILLIN	157	-34.508
	MCMC00004336	479.538	NICARDIPINE	158	-33.459
 Chiral	MCMC00004696	513.496	MEDORUBICIN	159	-31.643
	MCMC00003023	464.441	DINIPROPHYLLINE	160	-30.049
	MCMC00004250	347.355	NIFURALIDE	161	-29.937
 Chiral	MCMC00002374	429.427	AMICYCLINE	162	-29.299
 Chiral	MCMC00005462	461.493	LENAMPICILLIN	163	-29.040
 Chiral	MCMC00005563	408.481	MONTIRELIN	164	-28.311
	MCMC00003746	435.484	TRIMAZOSIN	165	-28.153
 Chiral	MCMC00005624	460.437	SORNIDIPINE	166	-26.193
 Chiral	MCMC00004092	463.572	MICRONOMICIN	167	-25.181

 <p>Chiral</p>	MCMC00004703	510.478	CEFUROXIME AXETIL	168	-21.350
	MCMC00004798	528.527	IMCARBOFOS	169	-19.970
 <p>Chiral</p>	MCMC00003356	454.474	RIBOSTAMYCIN	170	-18.811
 <p>Chiral</p>	MCMC00004361	475.583	NETILMICIN	171	-18.155
 <p>Chiral</p>	MCMC00000758	464.856	DEMECLOCYCLINE	172	-17.077
	MCMC00005987	514.537	SOBUZOXANE	173	-11.418