

WFS scores of compounds predicted as active by at least one of the SARS-CoV-2 BABM models

Compound ID	Structure	Sample Name	CM-M	CM-S
AGJBLWCLQCKRJP	Cl.CCN(CC)CCOC(=O)C(c1ccc	Drofenine hydrochl	0.238834	0.263079
VZTUIEROBZXUFA	COC1=C(OC)C2=C(CC3N(CCC	(d,l)-Tetrahydroberb	0.239483	0.272581
DZAUSKKPHXFGNN	COC1=CC(C2=NN=C3SCC(=N	ML030	0.256866	0.231271
UKMHVECLTZDSBD	[O-][N+](=O)C1=CC=C(CN2CC	ML111	0.312066	0.299525
XECQQDXTQRYVBH	CNCCC=C1C2=C(C=CC=C2)\C	Norcyclobenzaprine	0.264062	0.294532
IOMRUVGLZCUFRT	COC1=CC=C(CN2CCC(CC2)N(C	CCC3=CC=CC=C3)CC4	0.240461	0.245893
DMJWENQHWZZWDF	Oc3cc4[C@@H]1[C@H](CCc	Ecopipam	0.258394	0.263402
CBVFRUULJLOTQ	CCOC1=NC=CC=C1C(=O)N2CC	N(CCC2)C3=CC(Cl)=CC	0.243912	0.23287
ILNSWVUXAPSPEH	COC1=CC=C2C[C@H]3NCC[C	3-Methoxy-morphar	0.271975	0.251911
LXKCKCXTVCHHDJ	COC1=C(C=CC=C1)N2CCN(CC	C=C4C=CC=NC4=C(O)	0.249166	0.224476
HEYCRCGXZANZHI	CCOC1=C(C=CC=C1)N2CCN(CC	2)[S+](O)C3=C	0.259488	0.245568
JCTSLWVNRLJSRO	COC1=C(C=CC=C1)N2CCN(CC	2)C3=NC4=C(C=CC=C	0.26128	0.239822
GKQHRWNQTMNPNU	[O-][S+](=O)(CC1=CC=C(F)C	=C1)C2=NC(=C(N2CC#C)	0.275773	0.244099
OECZVBJQWUDON	CN1C(C)=NC2=C1C=CC(NCC3	=CC=C(Cl)C=C3)=C2	0.252857	0.223762
OYQJNUZLJJABAF	CN(C)C1=CC=C(CNCCC(CC2=CC	=CC=C2)C3=CC=CO	0.255629	0.244876
NUUYLSYEZFKFHN	CCCCCN1\C2=C(CCC2)/C(=N)	JF5 hydrochloride	0.269157	0.240794
GUILGOKXFRKEOS	CC1=CC=C(C=C1)[S+](O)N2C	(COC3=CC=CC=C	0.267198	0.236697
ANGFJDSIPQARK	COC1=C2C=C3C=CC=C(C(=O)N	CCN(C)C)C3=NC2=C	0.258197	0.236291
RLJFTICUTYVZDG	CSC1=CC2=C(SC3=C(CC2N4C	Methiothepin malea	0.273299	0.279054
XSXWINNAABRHDK	CCOC1=C(C=CC=C1)N2CCN(CC	2)C(=O)C3=C4C=CC	0.250735	0.231134
MHPIVQZZFBEHAM	CCOC(=O)C1=CC=C(NC2=CC(=N	C(=N2)C3=CC=CC=C	0.310473	0.287954
BYZBNLVKTLXVTR	O=C(NC1=CC=CC=C1)C2=CC=C	(CN3CCC4=C(C3)C=C	0.246844	0.228727
UFLCBIIQTOCIHZ	ClC1=CC=C(C[N]2C=NC3=C2C	=CC=C3)C=C1	0.245046	0.22704
OYPPVKRFBWMSX	Cl.Cl.O.Br1ccc(cc1)C(=C\CN	Zimeldine dihydrocl	0.274294	0.231696
ZZUZEMRHCMTVB	NS(=O)(=O)C#CC1=CC=CC=C1	Pifithrin-mu	0.238882	0.223362
DTRXURJDKOYCCD	ClC1=CC=C(C=C1)N2CCN(CC	2)FAUC 213	0.23899	0.248023
GHCCBWMZKJQGLS	ClC1=C(Cl)C=C(CC(=O)N2CCC	BRL 52537 hydrochl	0.263804	0.263417
WVZSEUPGUDIELE	C[C@@H](CN1CCC(CC1)CC2	Ro 25-6981 hydrocl	0.239753	0.240649
ITJNARMNRKSWTA	COc2ccccc2OC(CCNC)c1ccc	Nisoxetine	0.283356	0.296124
QJPPMXOOWNICQ	C1COC2=C(O1)C=CC=C2N3C	S15535	0.29727	0.277681
ALFGDCNSEBJYSP	CC(N)CC1=C[NH]C2=C1C=C(O	BW 723C86	0.244655	0.229329
MLDCBJPLHBPJET	C(N1CCC2(CCCC3=CC=CC=C2	L-687,384 hydrochl	0.299603	0.310166
QONNLUMTBIZJFP	FC1=CC=C(CN(C2=N\CCN2)C	IMID-4F hydrochlori	0.260044	0.308534
YMWVDVNGNLXSKR	CNCCC1=C[NH]C(=N1)CCC(C	2)N-Methylhistaprodii	0.290597	0.239345
GGUSQTSTQSHJAH	OC(CN1CCC(CC1)CC2=CC=C(F	Eliprodil	0.242312	0.269948
GYSZUJHYXCZAKI	Cl.COC1=CC=CC(=C1OCCNCC	2-(2,6-DIMETHOXY	0.253573	0.258831
BFNCJMURTMZBTE	Cl.CN(C(=N)Nc2cccc1cccc1	Aptiganel hydrochl	0.251866	0.252774
QAUVAHYHKLJRJCQ	Cl.COC1=CC=CC(OC)=C1OCC	Benoxathian hydroc	0.251056	0.303572
KZFDKINRISJFCO	CN1C2CCC1CC(C2)OC(C3=CC	AMINOBENZTROPINI	0.265034	0.259224
NNAIYOXJNVGUOM	CCNC(=O)N1CCN(CCCC(C2=C	Amperozide hydrocl	0.256516	0.246424
NGIFHAUKQGDVSR	CCOc1cc(cc(OCC)c1OCC)c3n	Octaverine	0.272203	0.288211
AFIHDGJQHWYCEI	CCC1=C(C)SC2=C1CCN(CC3=CC	=CC=C3)C2C4=CC=C	0.250273	0.22293
ZERLIHBKGPVVDX	COC1=CC=C(CN2CCC3=NC(=N	C=C3C2)N4CCN(CC4	0.269439	0.23179
BDKJNOPSOSKJIR	CCN1CCN(CC1)C2=C(N=C(O2)C	3=CC=C(COC4=C(C)	0.245546	0.230974
XZQQJDIBXKJVJF	CC1=C(CN2CCCC(C2)C(=O)N	3CCN(CC3)C4=CC=C(F	0.246241	0.225444

CIRKDOSLJLFKPN	CCOC(=O)C/1=C(CN(CC)CC2=CC=CC=C2)/NC(=O)NC	0.241342	0.224373
STCBAYQPVGPEJH	CCOC(=O)C1=CC=C(NC(=O)NC2=C(C=C3N(CC)C(=O)	0.24435	0.222754
LOGLBGSTNVTMEV	COC1=C(NC(=O)NCC2CCN(CC2)CC3=CC=CC=C3F)C:	0.270036	0.230708
VPVBRPZCLWKVIY	CC1=CC=C(C)C(=C1)CN2CCC(CC2)CNC(=O)NC3=C(F	0.283516	0.226523
ZKSQEVKHZNUREQ	CC1=CC=C(NC(=O)NCC2CCN(CC2)CC3=CC=CC(=C3)	0.261845	0.260004
IPDSTPSTHDVIDQ	CC1=CC=C(C=C1)[S+](=[O-])(=O)C2=C(OC(=N2)C3=C(f	0.250261	0.228122
WVQXUNBZLOXIIU	CCOC(=O)C1=C(C2=CC=CC=C2)C(=NN=C1NC3=CC=	0.245124	0.232116
ZMLWJWJTUFOMM	CC1=CC=C(NS(=O)(=O)C2=CC=C(C=C2)C(=O)NC3CC1	0.259456	0.235133
PAPMAGPVCPSSEQ	[Br-].COC1=CC=C(C=C1)C2=CN3CCCCC3=[N+]2C4	0.309639	0.295221
HHXJDHWPPPOVQFY	S=C(NCCCC1CCOCC1)N2CCN(CC2)C3=NC(=CS3)C4	0.282327	0.276722
GZFBOMZAQBAFPC	COC1=C(OCC2=C(Cl)C=C(Cl)C=C2)C(Cl)=CC(CNCCO,	0.252537	0.242298
BVNTYTGKKBBARC	ClC1=C(NC(=O)NC2=CC=C(CN3CCCC3)C=C2)C=CC	0.273893	0.273441
GQOMALJFAKJXAC	CC1=CC=C(CS(=O)(=O)C2=NC(=C(N2CC#C)C3=CC=C	0.272629	0.279836
WPSYTTKBGAZSCX	CCCCCCC[N+](CC)(CC)CCCC1 Clofilium tosylate		0.241723
SUIZRDJCBVPASY	CN1CCN(CC1)CCC2=CC(=C(Cl	BD 1063	0.264357
PKCYPHSCUSQDK	CC1=CC=C(C=C1)/C=C/2CNCC DUBInhibitor, NSC-6		0.245124
WHLUQAYNVOGZST	CCN(CC)CCSC(=O)C(c1cccc1 Thiphenamil		0.251491
UBAJTZKNDCEGKL	O=C(CN3CCN(Cc1ccc2OCoc2 Fenoverine		0.245379
LUYOZJXKSDIJJL	CN1CCN(CC1)C2=NC=NC3=C2C=NN3C4=CC=C(Cl)C		0.244958
JGDKHNHZZKSRBJ	CC(=C)CN1C(=NC2=C1C=CC=C2)C3=CC=CC=C3		0.243936
HQGDZPNAXRCSA	C(CCC1=CC=CC=C1)CN2CCC(4 4-PHENYL-1-(4-PHEN		0.251432
QXJOXLIOUDNDFH	O=C(N1CCN(CC1)C(C2=CC=C(MLS002586357-01	0.236355
LNOBZXNCABUBKK	C1=CC=C(C=C1)N2N=C(N=[N+ Chem Div, 0325-0423, NSC-261		0.332881
GWEHVDNNLFDJLR	O=C(NC1=CC=CC=C1)NC2=CC DIPHENYLUREA		0.23895
UUSFBNCIOFXBPP	OC(CCN1CCCC1)C2=CC=C(C=C2)C3=CC=CC=C3		0.23264
YMHOBZXQZVXHBM	Cl.COCc1cc(CCN)c(cc1Br)OC 4-Bromo-2,5-dimethoxyamphet		0.298582
ZQTOZLYOIRKCP	Clc1cc2N(c3cccc3Sc2cc1)C Azaclorzine		0.241673
CVHGCWVMTZWGAY	C(CCN1CCOCC1)c3ccc(COC2c Fomocaine		0.256329
PCFAAKWHZFXLIF	C[N]1N=NN=C1SCCCNCC2=C(OCC3=CC=C(F)C=C3)C=CC(=C2)Cl		0.226744
KBUOPNFNTRQMRH	CC1=C(CN2CCC(CC2)C(=O)NCCCN3CCN(CC3)C4=C		0.242191
KNJVRIMSFZQGE	CCN1CCN(CC1)C(=O)C2=CC3=C(C=C2)[S+](=[O-])(=O)C4=C(C=CC=		0.225264
UPLHUDRMLWWFRE	O=C(NC1=CC=CN=C1)C2=CC=CS2		0.228773
QUHHQVGVNSURGF	CN1CCN(CC1)C(=O)C2=CC=CC(=C2)COC3=CC(=CC=C3Cl)Cl		0.23717
ODKPRIUYEYROGE	CC1=CC=CC=C1N2CCN(CC2)C3=NC=NC4=C3C=N[N]4CC5=CC(=		0.229812
BFBGBTBYZIOWOF	COC1=CC=C(C(=O)N2CCN(CC2)C3=CC=CC(Cl)=C3)C(OC)=C1		0.251032
HYGDONULCUPJME	FC1=CC=CC(=C1)C(=O)N2CCN(CC2)C3=CC=CC(Cl)=C3		0.227876
FBZLYFODKQKGIQ	FC1=CC=CC(=C1)C(=O)N2CCN(CC2)C3=CC=CC(=C3)C(F)(F)F		0.223008
NYPQKNLHCFKMRM	ClC1=CC=C(OCCN2CCN(CC2)C3=NC=NC4=C3C=CS4)C=C1		0.23024
YQSPRFLNKVCSBN	COC1=CC=C(C=C1)C2=NN=C(4 MLS000588015-01		0.227784
INOKJENDVYITMZ	FC1=CC(=CC=C1)C(=O)N\N=C\ MLS000576932-01		0.229905
ZOAQYHQNVPIKDS	ClC1=C(Cl)C=C(CC(=O)NC2=C(C=CC=C2)N3CCCC3)C=C1		0.226163
LYLQJTSZYGWBO	O=C(NC1=NC2=C(N1)C=CC=C2)C3=CC=CC=C3		0.234202
NYYDXVOEUPUAPL	ClC1=CC=C(CNC(=O)N2CCN(CC3=CC=CC=C3)CC2)C=C1		0.231594
RSPWWPVPVHMZZPT	[O-][S+](=O)(N1CCN(CCC2=CC=CC=C2)CC1)C3=C(F)C=CC=C3		0.240089
IDYSNGDPYWXNRL	CN(C)C(=O)OC1=CC=C2C=CC=CC2=C1Cl		0.240211
HODZVUNFLGXUQV	O=C(NC1=CC=C(CSC2=CC=CC=C2)C=C1)C3=CC=C(CN4CCOCC4)		0.242556
UHGCEAWGKVKSQP	CC1=CC=C(CN2CCN(CC3CC4CC3C=C4)CC2)C=C1		0.252453
DXPSEJAAAVTTGJ	ClC1=CC=C(OCC2=NC(=NO2)C3=CC=NC=C3)C=C1		0.243136

KUYBIRBICYKWAX	CN1CCN(CC1)C2=C(N=C(O2)C3=C(F)C=CC=C3)[S+](O-)(=O)C4=	0.250255
JFIRKCGRMORWHA	CCOC1=CC2=C(C=C1)N=C(C)C=C2NC3=CC(=CC=C3)	0.2402
NEFIMYJEACGIMX	CC1=C(SC=C1)C(=O)C2CCCN(C2)CC3=CC(=CC=C3[N]4C=CC=N4	0.244693
QBXNQOWQGUPAEO	[O-][N+](=O)C1=C/C=C\N=C\1S(=O)(=O)C2=C/C=C\C	0.250607
XNRPWZMOVUAHLY	CCN(CC)CCN1\N=C/2C3=CC=CC=C3C4=CC=CC(=C24)C1=O	0.228109
NUWFSHWNAZZTED	COC1=CC=C(OCCN2CCN(CC2)C(=O)C3=CC=C(OC)C=C3)C=C1	0.251943
LOGTTZLPQLRADV	C1CN(CCO1)C2=NC(=NC3=CC=CC=C23)C4=CC=NC=C4	0.23402
KTTMEOWBIWLMSE	O1[As]2O[As]3O[As]1O[As](O2 Arsenic oxide (As2O3	0.30626
IAYKDNJLSYQHS	CCCCNCCOCCSC1=CC=C(Cl)C=C1	0.252335
NOSIYYJFMPDDSA	OC(=O)\C=C/C(O)=O.CN(C)CC(Acepromazine maleate	0.243708
VNICFCQJUVFULD	C1CN(CCN1)C2=C3C=CC=CC3 1-(1-Naphthyl) piperazine (hydr	0.291237
GAAKALASJNGQKD	NC1=CC=C(CCN2CCN(CC2)C3 LY-165,163	0.244893
VNZLQLYBRIOLFZ	Cl.COC1=C(C=CC=C1)N2CCN(1-(2-METHOXYPHENYL)PIERAZIN	0.229339
FCBRFERWWOBAJC	COC1=CC=C(CCCOC2=CC(CCN SKF 96365	0.226692
JXMYTVOBSFOHAF	CN1CCC2=C(C=C(O)C(=C2Cl)C SKF 83959 hydrobromide	0.247237
DEYFWGXTPWNADC	Cl.CCCN(CCC1=CC=CC=C1)C2 ()-PPHT hydrochloride	0.254643
ZHVWWEYETMPAMX	OC1=C2O[C@H]3C4=C(C[C@ NALTRIBEN	0.246656
WIYUZYBFCWCCQJ	OC1=CC=C2CC3N(CC4CC4)CC NALTRINDOLE	0.227155
YJZYDPRMWWYWYCG	COC1=C(C=CC=C1)N2CCN(CC p-MPPF	0.224174
GFIPROCAVXFHHK	CC1=CC=CC=C1/C=C/C2=N/C Metrazoline	0.239855
SNICMGDUOVKOPQ	FC1=CC=C(C=C1)C(OCCCC2=C 3-(1H-Imidazol-4-yl)propyl di(p-	0.229325
BDVFCVCGFMNCYPV	CC1CNCCN1[S+](O-)(=O)C2= 1-(5-Isoquinolinylsulfonyl)-2-m	0.223632
HPMRFMKYPGXPEP	C1C\N=C(/N1)C2COC3=C(O2) Idazoxan	0.255238
GOTMKOSCLKVOGG	CN1CCC2=C(C=C(O)C(=C2Cl) R(+)-SCH-23390 HCl	0.222381
HJWHHQIVUHOBQN	OC1=C(O)C(Cl)=C2CCN(CC=C) ()-Chloro-APB hydrobromide	0.223462
DIHXJZHAIHGSAAW	NC(=N)NC(=N)NC1=CC=CC(=C 1-(3-Chlorophenyl)biguanide hy	0.248549
DQVARXSGNFBPMB	COC1=CC(=CC=C1)C(=O)NCC N-(2-[4-(4-Chlorophenyl)piperaz	0.234699
RGSVXQJPSWZXOP	C1CCN(CC1)C2(CCCCC2)C3=(1-[1-(2-BENZO[b]THIENYL)CYCLO	0.255541
SPHRJZBOFIKMC	CN1CC\C=C(/C1)C(=O)OCC# ARECAIDINE PROPARGYL ESTER	0.262307
MKIKWCVTTNYSRM	C(N(CC1=CC=CC=C1)C2=CC=C Antozoline hydrochloride	0.24073
HSIBGVUMFOSJPD	Cl.COc4ccc5nc1c(CC[N@]3C Ibogaine hydrochloride	0.277103
BOOQTIHIKDDPRW	Cl.CCCN(CCC)CCc2cnc1cccc N,N-Dipropyltryptamine hydroc	0.343042
SRARDYUHGVMQEI	Cl.CCC(=O)N(c1cccc1)C2CC cis-N-[1-[2-(2-Thienyl)ethyl]-3-m	0.276151
HXJKWPGVENNMCC	Cl.COc1cc(CC)c(cc1C[C@H] (-)-2,5-Dimethoxy-4-ethylamph	0.273506
MLQRZXNZHAOCHQ	Cl.CCC(=O)N([C@H]2CCN(CC(dl)-trans-3-Methylfentanyl hyd	0.267412
QIRAYNIFEOXSPW	Cl.O[C@@H](CC)C(C[C@H])(C (-)-alpha-Methadol hydrochloric	0.268433
MOBGNTAHTMVGRR	COC1=C(C=C(Cl)C=C1)N=C(S)N2CCN(CC2)C3=NC=CC=C3	0.232718
YQGHHYKQSWMLODW	COC1=CC=C(C=C1)C(CC(=O)NC2=CC=C(F)C=C2)C3=	0.255879
HDDNYFLPWFSBLN	CN3[C@H]1CC[C@@H]3CC(Tropanyl 3,5-dimet	0.26114
KLOHYVOVXOUKQI	CN1CCC(CC1)N(Cc2cccc2)c3(Thenalidine	0.31913
DWGNPBBEALVNIR	CCOC1=CC=C(C=C1)C2=NC(=NO2)C3=CC=CN=C3	0.244372
UKMDHFPPBAQTFG	FC1=CC(NC2=NC(NC3CCCC3)=NC(Cl)=N2)=CC(F)=C	0.251922
IJJBBDVJOWKDH	COC1=CC=C(NC2=NC(NC3=CC=C(OC)C=C3)=NC(NCCN4CCOCC4	0.260326
BDILTGVTEOHPIK	C[C@H]1C=CC(=O)O[C@H]1C2=CC=CC=C2	0.224933
DFWLUVUOEZMWQPV	CCOC(=O)C1=C(N2CCN(CC2)C3=C(F)C=CC=C3)C4=C(C=CC(OCC)	0.227071
ZZKWNLZUYAGVOT	CCN(CC)CCC(=O)N1c3cccc3! Chloracizine	0.271526
VHEOUJNDDFHPGJ	CCN(CC)CCC(=O)N1c3cccc3! Fluacizine	0.223734
PXCGUZNRBAQKAB	CN1N=CC2=C1N=CN=C2N3CCN(CC3)C4=C(F)C=CC=C4	0.238083

APGOOCWNIINFPJ	CN1CCN(CC1)C2=NC=NC3=C2C=N[N]3C4=CC(=CC=C4)Cl	0.246938
DQQMGLDIAJRKW	COC(=O)C1=CC=C(OCC2N(CCC3=C2C=C(OC)C(=C3)OC)C(=O)C4=	0.22375
VETBVAKKYZIKRK	CC1=CC=C(C=C1Cl)N2C(=O)N(CC3=C\C(=O)N\4\C=C/C=C\C4=	0.235047
GPJVSQZGAOXHIW	CC\1=C\C/2=N/C(=C(NC(=O)C3=CC=CC(=C3C)[N+](O))\C(=C	0.327342
CEPGWKKGZRBHG	COC1=CC(=CC(=C1)OC)NC2=NC=C3CN(CCC3=N2)C	0.245695
JLHGCVVZJNGSQH	FC1=CC(=C(C=C1)C(N2CCN(CC2)C3=CC=CC=C3)C4=NN=C(O4)C	0.23493
DICMBJJRKNWXTG	COC1=CC=CC=C1N2CCN(CC2)C(C3=NN=C(O3)C4=CC=CC=C4Cl	0.23492
TXFUVYDUOHOUDL	CCC1CCCCN1CCCNC(=O)C2=CC=C3[N](CC)C(=C(C)C	0.245756
SXCRMWLOJMWHPG	CC1=CC=C(CNCC2=CC=C[N]2C3=NN=C(S3)N4CCCC4)C=C1	0.229774
MEGZOGVQYGEFBX	CCC1=C(C)SC=C1CN2CCN(CC: Chem Div, E534-0253	0.228431
PAQFEHWKTBIHQI	CC1=C(C)C(CN2CCN(CC2)C3= Chem Div, E534-0094	0.233827
HHUHTYPDNPXLCS	ClC1=CC=C(SC2=C([NH]C3=CC=CC=C23)C(=O)NCCC4CCCC4)	0.225248
VVZWQHYQWYYBDE	CCC1=NOC(=N1)C2=CC=C(N(C)CC3=CC=C(OC)C=C3)C(=C2)[N+](0.24165
XUVOEKZZGXXJJI	CCOC(=O)N1CCN(CC2=NC3=C Chem Div, D305-295	0.240706
JHCWGQKLJOGGAR	C[N]1N=NN=C1SCCCNCC2=C(OCC3=C(F)C=CC=C3)C=CC(=C2)Cl	0.239888
OSHCHHSOIGAPML	C[N]1N=NN=C1SCCCNCC2=C(OCC3=CC=CC=C3)C=CC(=C2)Cl	0.252126
TVGHFPDPQWJAGF	C[N]1N=NN=C1SCCCNCC2=CC(=CC=C2OCC3=CC=CC=C3F)Br	0.236409
UCEMOVOKNXCDUO	CC1CCN(CC1)C2=C(N=C(O2)C3=CC=C(COC4=CC=CC=C4)O3)C#	0.2268
NWEDWOABKQWTDU	C[N]1N=NN=C1SCCCNCC2=CC=CC(=C2)OCC3=CC=CC=C3	0.227293
QPGOBLUKOSGNHM	C[N]1N=NN=C1SCCCNCC2=C(OCC3=C(F)C=CC=C3)C=CC=C2	0.228976
FNZNPRYSUBBQJ	CC1=CC=C(CN2CCC(CNC(=O)NC3=C(C)C(=CC=C3)Cl)C2)C=C1	0.244336
QYCDHOMGRPUYGX	CC1=CC=C(CN2CCC(CNC(=O)NC3=C(C)C(=CC=C3)C)C2)C=C1	0.246675
VQQBZTNRGPPYFN	CCOC1=CC=C(C=C1)C2=NOC(=N2)CSC3=NN=C(CC4	0.250146
UVEIXJDMRJJAMC	COC1=CC(=C(C=C1)C2=NOC(=N2)CSC3=NN=C([N]3C4=CC=C(F)C	0.227963
DBTSMXDVKNLBP	CCOC1=CC=C(C=C1)[N]2C(=NN=C2SCC3=NC(=NO3)C4=C(OC)C=	0.231026
BUVXGEZANDRKKB	COC1=CC=C(C=C1)C2=NOC(=N2)CSC3=NN=C(CC4=CC=CC=C4)[0.265961
RYLMHLDCUKZUSS	COC1=CC=C(C=C1)C2=NOC(=N2)CSC3=NN=C(CC4=CC=CC=C4)[0.230362
QVNQLKRLMYARFB	CCCC[N]1C2=CC=CC=C2N=C1C3=CC(=CC=C3)C	0.240034
SEPNIPIXTZMOGZ	CC1=N[N](C2=CC=CC=C2)C(=C1C(=O)NCCC3CCN(CC3)C4=C(F)	0.233654
BWCSBZZQPYAWEW	CCN(CC)CCNC(=O)NC1=CC=C(SC3=C(C=CC=C3)C(=O)N2CC4=C	0.232125
NQZCPBKSHZHIDA	CCN1CCN(CC1)C2=C(C=NC3=CC=C(F)C=C23)[S+](O)(=O)C4=C	0.231722
DTATUEFDBHWISO	CCN1CCN(CC1)C2=C(C=NC3=CC(=C(OC)C=C23)OC)[S+](O)(=O	0.235165
JQWLNIKOJZUWLS	COC1=CC=C(C=C1)[S+](O)(=O)C2=C(N3CCCC3C)	0.242826
NNKVUACOWDPTOS	COC1=C(OC)C(=CC(=C1)C2=NOC(=N2)CN3CCN(CC3)C4=CC(=CC	0.23651
ZKASZIKRZDGTGO	CCN1C(=O)C2=C(SC(=C2)C(=O)NCCC3CCC(C)CC3)	0.250769
DNBSWMXOBBPNKG	CC1=CC=CC(=C1)C2=NC(=C(C)O2)CN3CCCC(C3)C(=	0.24314
IZGZVVFFWOPDG	CCC1=CC=C(C=C1)C2=NC(=C(C)O2)CN3CCCC(C3)C(0.24113
CRQMYNFFVQYLNBN	CCN(CC)CCCNC(=O)C1=CC=C(SC3=C(C=CC=C3)C(=	0.255032
UEGSWOARNYEWYSY	CC1=CC=C(CCNC(C2=NN=C(O2)C3=C(Cl)C=CC=C3)C4=CC=C(F)C	0.234111
OKPDBTJLFYBXNP	COC1=CC=C(CCNC(C2=NN=C(O2)C3=C(Cl)C=CC=C3)C4=CC=C(F)	0.253269
GXQRIOYHWKCKEE	CC\1=N\N=C2N1C3=C\C=C/C=C/3/N=C\2NCCC4=	0.252873
DDPHSKFUSLMYGE	COC1=C(C=CC=C1)N2CCN(CC2)C(C3=CC=C(Cl)C=C3)C4=NN=C(0.2695
WJYADGBJCBQJIT	CC1=CC=CC(=C1)N2CCN(CC2)C(C3=NN=C(O3)C4=	0.254785
CQNXXVWIPTIHWMO	FC1=CC=C(C=C1)N2CCN(CCCNC(=O)NC3=C(Cl)C=CC=C3)CC2	0.25768
SZWCDFDONZOYIQM	CCOC1=CC=C(NC(=O)NCCC2CCN(CC2)C3=CC=C(OC)C=C3)C=C	0.235476
HGBDQMVPLSVOPA	FC1=CC=C(NC(=O)NCC2CCN(CC2)CC3=CC=CC=C3F)C=C1Cl	0.230767
RUGYNWMSERWJIV	FC1=CC=C(NC(=O)NCC2CCN(CC2)CC3=CC=CC(=C3)	0.257308
UQBQZQCCEDCSSI	CCN1CCN(CC1)C2=NC3=CC=C(NC(=O)C4=CC(=CC=C	0.246823

PQFNWDHABGBCHB	C(NC(C1=CC=CC=C1))(C2=CC=UCL 2077	0.270768	0.265043
MDESCHUXWOWHQJ	CN(C)CC\C=C/1C2=C(SC3=C1 Chlorprothixene hyc	0.24483	0.271933
MNHDKMDLOJSCGN	COC1=C(C=CC=C1)N2CCN(CC BP 897	0.254893	0.246755
IBQMHBGFMHLHLE	CCN(CC)CCCCCCCCOC(=O)C1: TMB-8	0.266883	0.292467
INYHMKFEIYIEMI	CN1CCN(CC1)C2=CC(=CC=N2)C3=CC4=CC=CN=C4C	0.2656	0.226409
MKXUVDRBPODBNG	CN(C)CCCN1C2=C(CCC3=C1C=CC(=C3)[N+](O-)=O	0.244357	0.234317
CBHCDHNUZWWAPP	CN1CCCC(CN2C3=CC=CC=C3! Asinex Ltd.,BAS 011	0.347333	0.320256
HTHNSEMKEHCSTM	CN(C)CCN(CC1=CC=CO1)C(=O)C2=C(NC(=O)C3=CC=	0.240309	0.227063
BZKSQQXINBVDCB	COC1=CC=CC(=C1)CNCC2=CC=C[N]2C3=NN=C(S3)N	0.253486	0.230133
XYCGAHJDVGYNKA	C[N]1N=NN=C1SCCCNCC2=CC=CC(=C2)OCC3=C(Cl	0.287601	0.252479
SYOKJUFJPXSYSF	BrC1=CC(=CC=C1)NC(=O)NCCN2CCN(CC2)C3=CC=C	0.249429	0.230087
UZLVWFBDXMRGC	CCN(CC)C1=CC=C(C=C1)C(=O)NC2=CC=C3N=C(C=C	0.246475	0.224084
RCNQBNUIYIJXKA	CC1=CC(=CC=C1)NC2=NC(=NC(=N2)N3CCOCC3)NC	0.247441	0.225433
HCZJUQSPQYTBZ	CC1=CC=CC(\C=N\NC2=CC(=NC(=N2)N3CCOCC3)N	0.238906	0.229137
MWAUQHNLXGQFJC	Cl.C1C1=CC=C(CN2C3=CC=CC=C3N4CCCN=C24)C=	0.273576	0.261708
CZGWXYLLXFDSEJ	C1CN(CCO1)C2=CC(N\N=C\C3=CC=CC=C3)=NC(=N	0.239328	0.243454
HAFZKOVMNKGNKS	CN(C)C1=NC(=NN=C1C2=CC=CC=C2)C3=CC=CC=N3	0.267566	0.266358
FJUKDAZEABGEIH	FC1=CC=C(OCCCN2CCC3(CC2 AMI-193		0.230611
SDYYIRPAZHJOLM	CN1CCN(CC1)C2=CC3=C(OC4 Azaphen		0.222694
UNAHYJYOSSSJHH	CCCN(CCC)C1=C(C=C(C=C1[N Oryzalin	0.256952	
BDTGZELZUBXECI	C1CCN(C1)C2=NC(N3CCCC3 Enamine,T5241771		0.247205
FBMYKMYQHCBIGU	N#Cc3ccccc3OCC(O)CNC(C)(C Bucindolol		0.241779
HKGJEZIGDHFJFL	CC(NC1=NC(=NC2=CC=CC=C1 Importazole		0.258093
MHNSOBBJZCWUGS	CN1C2CCC1CC(C2)OC(C3=CC 3alpha-Bis-(4-fluoro	0.244653	
ASGIQUHBAVIOTI	CN(CCN1CCCC1)CCC2=CC=C BD 1008	0.238577	
MZRNPVMMFFYDMP	OC(COC(C1=CC=C(Cl)C=C1)C2 MLS000536652-01		0.29137
GZIZSEZACLKNGZ	Cl.OC(COCCCCCCCC)CN Decominol hydrochloride		0.225721
SASASNHHBSXROE	COC1=CC(=C(NC2=NC3=CC=CC=C3C(=C2)C(=O)NCC	0.241858	
SKEYWVHTUBBHY	CCCCN1C(=N)N(CCO2=C(OC)C=CC=C2)C3=C1C=CC=C3		0.230907
LBMRVOOUBNQXAX	COC1=CC=C(CNCCC(C2=CC=C3OCOC3=C2)C4=C(O	0.24729	
YLKDCSKJNOKCGZ	OC(COC1=CC=CC=C1)CN2C(= BEPP monohydrochloride		0.235306
UPBDZILZTPVMPX	CN(CCN1CCCCC1)CCC2=CC(N-[-(3,4-DICHLOROP	0.25028	
REQHIGZKPANFBN	CC(C)NCC(O)CN1CCN2C3=C(C=C(C)C=C3)C4=C2C1	0.255814	
HOFDPCCJQDBINI	CC1=CC=C(OC2=CC=C(NC(=O)CN3C=CSC3=N)C=C2	0.247549	
YCOOGVUXVXEMJG	FC1=CC=C(C=C1)C2=CSC3=C2C(=NC=N3)N4CCC5=C(C4)C=CC(=	0.227454	
CGRZMNFYFYXES	CC1=C(C)C2=C(S1)N=CN=C2NC3CCN(CC4=CC=CC=C4)CC3		0.222785
IFFPICMESYHZPQ	CC(CC1=CC=CC=C1)NCCC(C2: Prenylamine		0.246508
GNCXAVSTKVWZCH	CCN1CCN(CC1)C(=S)NC2=CC(Cl)=C(Cl)C=C2		0.24609
HFBNIJOVWGRREA	CCOC1=CC=C(NC2=NC(=NC(=N2)N3CCOCC3)N4CCOCC4)C=C1	0.265152	
IVHLLANKSUTQN	CC(NC1=C2C=CC=CC2=NC(=N1)N3CCCC3)C4=CC=CC=C4		0.232656
ISMDJEWLVHMDGS	ClC1=CC(=CC=C1)NC2=NC(=NC3=CC=CC=C23)C4=CC=NC=C4		0.2719
RAQPOZGWANIDQT	C=1C=CC(=CC1)CCCN2CCN(C GBR 12935		0.233512
RKXSQHTWNMDLJM	CCN1CC[C@@H](CNC(=O)C2: S-(-)-Eticlopride hydrochloride		0.226083
LXFHSCDLMBZYKY	CN1CCN(CC1)C=2C3=CC=CN CGS 12066B		0.225078
AMEKQAFGQBKLKX	CC=1OCCS(=O)(=O)C=1C(=O)N Oxycarboxin		0.226435
ZQHYKVKNPWDQSL	Br.Oc3ccc4C[C@@H]2[C@H](-)-Phenazocine hydrobromide		0.248728
BVURVTVDNWSNFN	CC(=O)OC2(CCN(CCCc1ccccc1 1-(2-Phenylethyl)-4-phenyl-4-ac	0.31054	
VWCUGCYZZGRKEE	Cl.C[C@@H](NC)CC(c1ccccc L-alpha-Acetyl-N-normethadol h		0.254403

MEZAVJNOAZTJPC	COC1=CC=C(C=C1)C2C3=C(OC4=CC=C5C=CC=CC5=	0.255373	
XBDPCQXFTHAEHE	CC1=NOC(\C=C\C2=CC(C)=CC=C2)=C1S(=O)(=O)N3(0.259232	
OPYDXMHWHHPGNV	CN(C)CCN(CC1=CC=CO1)C(=O)C2=C(NC(=O)C3=CC=CC=C3)C4=C	0.226729	
ADBFCSPXCVYNDU	CCN1CCC(CC1)N(CC2=CC=C(F)C=C2)C(=O)NC3=CC=CC(=C3)C(F	0.226412	
FKNPUTFWVWCFQZ	CN1CCN(CC1)C2(CCCCC2)CNC(=O)COC3=CC(=C(Cl)C(=C3)C)C	0.240241	
NKXGFAHVHMZMBQ	CN1CCN(CC1)C2(CCCCC2)CNC(=O)C3=CC=C(C=C3)C(C)C	0.236529	
NXRHQNINGABYRC	C[N]1N=NN=C1SCCNCC2=CC=CC=C2OCC3=CC=C(Cl)C=C3	0.226216	
KPOMOQCZFUZOEG	CC1=CC=C(CN2CCC(CNC(=O)NC3=CC=C(Cl)C=C3)C2)C=C1	0.23962	
YBEQARLMYVDZPS	CC1=CC=C(CN2CCC(CNC(=O)NC3=CC(=C(C)C=C3)C)C2)C=C1	0.269957	
CEBQGAWALVBGDD	ClC1=CC=C(CN2CCC(CC2)CNC3=NC=NC4=C3C(=NO4)C5=CC=C	0.22421	
YZNZQGRVSPBRCS	CCN(CC)CCOC(=O)C1=CC=C(NC2=C3CCCC3=NC4=CC=CC=C24)	0.251375	
SOPGMAUDVXIZMJ	CN1C(=O)\C=C(SCC(=O)N2CCN(CC2)C3=CC(=CC=C3)	0.238641	
VPLGPTNWXVJMBQ	CCCN(CCC)CCNC(=O)C1=CC2=C(S1)[N](C)N=C2C3=	0.25491	
WDEVVLOWARINKQ	CCC1=C(NC2=NC3=CC=CC=C3C(=C2)C(=O)NCCCN(0.246748	
GLWYWFYFMOQZWFQ	CN(C)CCNC(=O)C1=CC2=C(SC3=C(C=CC=C3)C(=O)N	0.24037	
HXUNRLYGWQEZF	CCCC/1=N/C2=C(SC3=C1C=CC=C3)C=CC(=C2)C(=O)NCCCN(CC)	0.23122	
JPZVQEUBNKRFL	FC1=CC=C(C=C1)N2CCN(CCCNC(=O)NC3=CC=C(Cl)C=C3)CC2	0.284918	
WEBXDMFWYIQYOX	CCN(CC)C1=NC2=CC=C(NC(=C Chem Div, C126-0067, NSC-261	0.231445	
OSEXCKTQMLTCE	FC1=CC=C(C=C1)C2N(CC(=O)NC3=C2C=C(Br)C=C3)C(=O)COC4=	0.224934	
VHJPMBFXS FVNMMW	CCOC1=C(CN(CCC2=CC3=C(OCO3)C=C2)CC4=CC=C	0.245177	
IPNLKYHAOUKDJV	CCN(CC)CCN\1/C(S\C=C1C2=CC=CC=C2)=N/C3=CC=CC=C3	0.245149	
SYEJOEKBJARQNW	CC[N]1C2=C(C=CC=C2)C3=C1C=CC(=C3)CN4CCN(C	0.247528	
WSLTYZVXORBBLB	IC1=CC=CC=C1CNC2C3CCN(C L-703,606 oxalate	0.239825	0.231216
HILYPTQJNFXLCJ	CCCN1N=CC(CN2CCC(CC2)C(=O)NC3=CC(=CC=C3)C	0.271927	0.251526
GUDVQJXODNRIJ	C[C@H]1CN(CCC[N]2C3=C(Rimcazole		0.237513
QPQKUYVJSJWQSDY	NC1=CC=C(C=C1)\N=N\C2=CC 4-amino azobenzene		0.222481
BGNXMDRDUPEAQZ	OC(CN1C(=N)N(CCN2CCCC2 InterBioScreen, STO	0.247433	0.23945
GBWZKWXAMNEFFC	CCCCSC1=C(OC)C=C(C(CNC)C(C)C)C(O)=C1	0.250342	0.244845
YITAORWEHMMACD	ClC1=CC=C2SC3=CC=CC=C3CC(N4CCNCC4)C2=C1	0.298102	0.277371
NGZXDRGWBULKFA	COC1=C(O)C2=C3[C@H](CC4=CC(OC5=C(OC)C=C	0.281002	0.253835
QEJWNTNYCWDNQTO	ClC1=CC(NC(=O)OCCN2CCN(CC3=CC=CC=C3)CCC2	0.238991	0.241263
AUPFODUFUNPAOB	CCN1CC\C=C(C1)C2=C[NH]C3=CC=CC=C23	0.255156	0.251044
WKLILWHYTVQKO	CCCCCN\1/C2=C(/CCC2)C(=N)\C3=C1CCC3	0.27052	0.288349
OZJZAHYJFKHRHA	ClC1=CC=C(CN/2\C3=C(CCCC3)/C(=N)C/4=C2CCC4	0.257234	0.252581
OJGAAQMNLKYWSQ	CCN(CC)CCN1=C2C=CC(Cl)=CC2=NC=C1	0.252913	0.271597
VAKMKOXCESUTKU	CN(C)CCNC(=O)C12CC3(C)CC(C)(CC(C)(C3)C1)C2	0.243472	0.254653
MKXZASYAUGDDCJ	COC1=CC2=C(C[C@H]3[C@H Dextromethorphan	0.263274	0.283705
SFALRUMUWIIQMK	CC(N1CCN(CC1)C(=O)CC)C2=CC=CC=C2	0.264278	0.224769
DVBSBxBABNLMIS	CC1=CC(CN2CCN(CC2)C(=O)CC)=CC=C1	0.255553	0.229207
IGSLPFRVZBFLCQ	CC(NC(=O)CC)C1=CC(Cl)=C(Cl)C=C1	0.245219	0.232732
XKNMHYBWPOWHGN	COC1=C(C\C(N)=N\OC(=O)C2=CC(=C(C)C=C2)[N+](0.273096	0.244716
JCTRJRHLGOKMCF	COC1=CC(=NC=C1)C2=CC=CC Caerulomycin A	0.273651	0.234422
AEQDJSLRWYMAQI	COC1=C(OC)C=C2[C@H]3C Asinex Ltd.,BAS 004	0.252843	0.275725
DTIOIVMYVABWOA	COC1=CC=CC(=C1)NC(=O)C2=CC(=C(NCCCN3CCC(C	0.246241	0.226254
TVEGJOPFJFHLHL	CCCCCCCCN1C=CC(=N)C=C1	0.280722	0.260172
ZVECUHIVPCIEDV	ClC1=CC=CC(=C1)CN\2\C3=C(CCCC3)\C(=N)C\4=C2	0.311502	0.287249
UDTBCHLPTINKIU	COC1=CC=CC(=C1O)CN2CCN(CC2)C(C3=CC=CC=C3	0.299565	0.281626
IMBPMAAMRHSTEU	ClC1=CC2=NC=CC(=C2C=C1)NCC3=CC=CC=C3	0.2785	0.240224

TYMAQOZPKMPEEI	[Cl]C1=NC=NC2=C1C(=CS2)C3=CC=C([Br])C=C3	0.253167	0.230683
HYNDEBBGYDBODO	CC1=CN=C(CCNCC2=C[N](N=C2C3=CC=C(F)C=C3)C	0.271427	0.256006
RCEPLTQHRCQLIM	CC(C)[N]1C=C(CN2CCCC(C2)C(=O)NC3=CC=CC(=C3	0.262347	0.22939
OFCFGAWKLIJWMU	CCCN1CCC(CC1)NCC2=C[N](C)N=C2C3=CC=C(OC4=	0.269558	0.250783
DIAIPLSVPPGLTG	CC(=NNC(=S)NC1=CC=CC=C1Cl)C2=CC=CC=N2	0.277022	0.240567
FCIINDKJSDJDMO	COC1=CC2=C(NN=CC3=CC=C(F)C=C3)C=C(C)N=C2C	0.252376	0.234881
WTCHDUNWZHYYS	ClC1=CC2=C(C=C1)C(N\N=C\C3=CN=CC=C3)=CC=N	0.24054	0.241441
DQGSSSLXBXDNFM	CC1(C)N=C(N)N=C(N)N1C2=C Chem Div, 0075-005	0.325842	0.310293
LSDJYKNINCJROA	CN(C)CC\C=C1\C2=C(SC3=C1C=C(Cl)C=C3O)C=CC=	0.272377	0.270472
TYKXLUMYKFFSJE	C(N1CCC(=CC1)C2=CNC3=CC Chem Div, C800-01C	0.253472	0.236226
TVZWPUCJIAREL	COC1=CC=C(C=C1)C2C3=C(OC4=C2C(=N)N(CCCN(C	0.261124	0.230841
KEUFFISILHOPIT	CCCC\C1=C(/CCC)C(=N)C2=C(C=CC=C2)N1C	0.260138	0.236403
BKARIVRTTVHMED	COC1=CC=C(C=C1)C(O)(CCC(C Chem Div, D163-00:	0.266826	0.226706
CYDRXTMLKJDRQH	CCCCCCCCCCCC[N+](C)(C)CC1 Alkyl* dimethyl ben:	0.265266	0.22571
SYKLCRHFGLITIY	CN1CCN(CCCC(=O)C2=CC=C(C=C2)C3CCCC3)CC1	0.265559	0.228372
KQKIJSXRQLKDCH	O=C1CC2=CC=CC=C2SC3=C(OCCN4CCCCC4)C=CC=	0.23934	0.232283
JXPQMHI XNPWEEK	NCCC1=CC(OCC2=CC=CC=C2)=C(OCC3=CC=CC=C3)	0.310731	0.26888
OFQDDTLVBDRDIE	COC1=CC=C(C=C1)\N=C2N(C(=S)N(C\2=N\C3=CC=C	0.254419	0.242925
UUPAPYGETUCQQY	CCCCCCCSC1=CC(=C(CCN(C)C)C=C1OC)OC	0.269895	0.26834
SPHRAOZAEYDNOD	CCCCCSC1=CC(=C(CCN)C=C1OC)OC	0.262074	0.231757
VYUFRDMGURKYMP	CCCCCSC1=CC(=C(CCN)C=C1OC)OC	0.292748	0.253168
NXIDBHKWPOTQRS	CCN\1CCSC1=C\C=C\C2=[N+](CC)\CCS2	0.238761	0.229115
LSMFRNHKRLJLH	CC1=CC2=C(C(=N1)C)C3=CC=CC=C3[NH]2	0.25232	0.244555
QHYGSNAGFBDJNF	CCCCCCCSC1=C(OC)C=C(CCN)C(=C1)OC	0.257646	0.232537
UAFVYCBWJBEHFW	CN(C)CCC1SC2=C(OC3=C1C=CC=C3)C=CC=C2	0.283065	0.290852
BJWIODCFNLUSQT	CN(C)CC\C=C1\C2=CC=CC=C2SC3=CC=C(F)C=C13	0.351761	0.348372
BMELRMVLLCJZEK	COCCCN1CCN(CC1)C2CC3=C(SC4=C2C=C(Cl)C=C4)	0.284025	0.288841
KKWBALVHTAINIA	CN1CCN(CC1)\C2=C\C3=CC=CC=C3SC4=CC(=CC=C:	0.300795	0.288834
KXECCBGQPJGJGD	COC1=CC(=CC2=C1SC3=CC=CC=C3/C2=C/CCN(C)C	0.284967	0.266838
XAFCDVVTUZRLTJ	COC1=CC2=C(C=C1Cl)C(=C/CCN(C)C)\C3=CC=CC=C	0.273576	0.255232
IJPYWKZIRIFQGO	CN1CCN(CC1)\C2=C\C3=CC=CC=C3SC4=CC(=C(Cl)C	0.250493	0.268361
CBOFLGIANBSBCN	CN1CCN(CC1)C2=CC3=C(SC4=C2C=C(F)C(F)=C4)C=	0.28091	0.30667
LXXWKTMDVBORIZ	CN1CCN(CC1)\C2=C\C3=CC(=CC=C3SC4=CC(=CC=C	0.267763	0.275218
OKHWNJARAFKRRE	CNCCCC1SC2=CC=CC=C2OC3=CC=CC=C13	0.292288	0.270041
DECPXWOQZCMYMS	CN(C)CC1=CC(SC2=CC=C(Cl)C=C2)=CC=C1	0.277699	0.267545
FTELXJYVTOFJAI	CNCC\C=C1\C2=CC=CC=C2CSC3=CC=CC=C13	0.323103	0.291664
UYUKSGQLYHPHCQ	CN1CCN(CC1)C(C2=CC=CC(=C2)Cl)C3=CC=CC=C3Cl	0.320103	0.337795
FGNRFYZVFTXMK	CCCCCSC1=C(OC)C=C(CCN(C)C)C(=C1)OC	0.290751	0.261087
SLSXXOCGDJFZGQ	CC1=C(NC(S)=NC2=C(C)C=CC=N2)N=CC=C1	0.242746	0.237437
SAIFDQQEXJWFQD	CC1=CC=CC(=N1)NC(=S)NC2=CC=CC(=N2)C	0.25839	0.259044
IENXZUWRUBNESG	ClC1=CC=C(C=C1)C(=O)NNC/2=N/C3=CC=CC=C3SC	0.24069	0.241574
RPSOLZRELOLSFM	COC1=CC=C2N(CC3=CC=CC=C3)C(C)=C(CC[NH3+])C	0.297249	0.258218
MPBJZRJBGUVTBE	COC1=CC=C(C=C1)N2CCN(CC2)C3=NC=CC=N3	0.253559	0.235383
WLTSTDGGFCQWTK	NC(=N)NN=CC1=CC=CC(Cl)=C Enamine,T0510-361	0.287371	0.287286
QPSNWMWKJWYOMD	CN(C)C1=CC=C(C=C1)\N=N\C2=CC=CC(=C2)F	0.240945	0.224368
MAMUGDCJLAKCPT	C(NC1CCCCC1)C2=CNC3=C2C=CC=C3	0.288402	0.237948
ONHBRYWYNVUGHT	NC(=N)NN=CC1=CC=C(Br)C=C Chem Div,0589-000	0.285636	0.244488
UJVPVNYJQYVQSO	CNCCCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.307366	0.279899

RDLIBCPWPNCFBW	NC(=N)NC(=N)NC1=CC=C2C=CC=CC2=C1	0.258906	0.234777
JYULRDHEGXZIJL	C1CCN(CC1)CCOCCOC2=CC=CC=C2C3=CC=CC=C3	0.312687	0.290109
MQOBLGHESXFRAZ	S=C(NCCC1=CC=CC=C1)NC2=CC=CC=C2	0.253062	0.233176
NUUUPPWZYJRJGI	CCN(CC)CC#CCOC(C1=CC=CC=C1)C2=CC=CC=C2	0.278414	0.245823
GMSJLIWEQRALHY	CN(C)CC1=C(C)[N](CC2=CC=CC=C2)C3=C1C4=C(C=C(0.260331	0.222787
KGFKMQPKZITFIV	CN1CCC(CC1)C2OC3=CC(=CC=C3SC4=CC=CC=C24)	0.3017	0.323234
DJBLGERXKWAXLD	CN1CCC(CC1)C2OC3=C(SC4=C2C=C(CI)C=C4)C=CC:	0.28818	0.294346
AMJLPOOQDHBZPR	COC1=CC=C2SC3=CC=CC=C3OC(C4CCN(C)CC4)C2=	0.32378	0.320216
YYKVLQRQUTRJDZ	COC1=CC(=CC(=C1OC)OC)C2=NOC(=C2C3=CC=C(N:	0.284721	0.267136
XQSLNGSRJSYIBL	CN(C)C1=CC=C(C=C1)C2=[N+](C)C3=C(C=CC=C3)N2	0.285322	0.276195
CBCFXXYRVWKHQC	CC1=CC2=C(C=C1)N=C(C)C3=C2N(CC3)C4=CC=CC=	0.270824	0.245063
OQOOPJFBMWZREC	CCNC(=S)N1N=C2C(CCC3=C2C=CC=C3)C1C4=CC=C	0.252733	0.235942
WILZNSGPHFGHJX	CCOC(=O)C1=C(CN(C)C)N(C2=C1C=C(OC)C(Br)=C2)(0.287419	0.259964
GGOXYHMFSLXAN	CCOC1=CC=C(C=C1)[N+] ₂ =C3CCCN3C=C2C4=CC=C	0.254825	0.248466
SUHSDBYPTUCXHW	CCOC1=CC=C(C=C1)[N+] ₂ =C3CCCCN3C=C2C4=CC	0.285423	0.272482
GBOMJGJESBMUBL	CS(O)(=O)=O.O[C@H](C1CCCCN1)C2=C3C=C(CI)C=C	0.266194	0.297212
RYQOGSFEJBUZBX	CN(C)CCCN3c1ccccc1C(C)(C) Dimetacrine	0.261877	0.282269
FFWJGCZSJMMGEI	CC1(C)N=C(N)N=C(N)N1CCCC2=CC=CC=C2	0.246413	0.283205
VGMOECBHITYGPM	CN(C)CCCN1C2=C(SC3=C1C4=C(C=CC=C4)C=C3)C=	0.238614	0.281319
LKIZLUUZCMZBLW	COC1=CC(=CC=C1)N2CCN(CC2C)C3=C4[NH]C5=C(C	0.287757	0.254118
BJMFBYNATMSQTP	CC1=CC=CC(CNCCC2=CNC3=C(Vitas-M Laboratory,!	0.26961	0.247251
CZKHLIOQQPRGJK	CCCCCCCC[N+](C)(C)CC#CC Vitas-M Laboratory,!	0.251676	0.255793
HQQKWRPQQKVXRB	CC1=CC=CC=[N+] ₁ CCCCCCCC Vitas-M Laboratory,!	0.254228	0.222447
LIJXCAFRPKFKCP	C(C#CCN1CCCC1)C(C2=CC=C(Vitas-M Laboratory,!	0.33135	0.335301
WDPPSRUIMSQVFX	NC(=N)N\N=C\1=CC=C(CI)C= Vitas-M Laboratory,!	0.319876	0.297283
STPQBRUWBPEJCN	OCCN(CCO)CC(O)COC1=CC=C Enamine,T5909565	0.262176	0.228533
SYJINUQHFMETCP	COC1=CC=C(OC)C(CN2CCC(C(Vitas-M Laboratory,!	0.279076	0.260116
FPDWKSDUHWBCL	CC1=CC=CC=C1C(O)(CC2=CC= Vitas-M Laboratory,!	0.3075	0.289571
CESGBQSBLXNVKX	OC(CNCC1=CC=C(C=C1)C2=C(Vitas-M Laboratory,!	0.263324	0.229641
USIDXIDZIUJEKU	CCC[N+] ₃ (CC#CCC(C1=CC=CC Vitas-M Laboratory,!	0.26382	0.244699
NIWNHZODVYNBFS	CC(C)C1=CC=C(NC(=N)NC2=N Chem Div,4477-289	0.249639	0.223979
FNEZJMQBSHKMIA	CC1=CC=CC(NC2=C3CCCC3=† Chem Div,C660-083	0.262994	0.228349
NVICAXRWBNEKMT	COC(=O)C1=CC=C2N=C(C)C=C Chem Div,4593-273	0.24047	0.226926
FGIVPSPMBRNHEY	COC(=O)C1=CC=C(NC2=CC(C): Chem Div,4491-097	0.268121	0.239245
UVVUMMGAJMWWVFM	CC1CCN(CC(=O)NC2=CC=CC(= Enamine,T5290474	0.270404	0.246545
KOMRTHWJNSSNLB	CN1CCN(CCNC(=O)C2=CC=C3 Chem Div,K216-768	0.274347	0.238955
REFRNPWWMHBHCL	O=C(NCCN1CCCC1)C2=CC=C‡ Chem Div,K216-789	0.254577	0.226584
YVKYTTQUAYMNOQ	C1CCCN(CC1)C2=NC(=NC3=C Vitas-M Laboratory,!	0.288818	0.241153
QOAKTPEJLHCBO	CC1CCN(CC1)C2=NC3=NON=† Vitas-M Laboratory,!	0.260071	0.243049
WYXTXIDBBBUKIV	CC1=CC(=NC(NCC2=CC=CC=C Vitas-M Laboratory,!	0.25461	0.241066
BZOHAWADDWQPIT	CN(C)CCCN(C(=O)COC1=CC=C Chem Div,E677-062	0.265708	0.262206
JAQENPDJAEDSC	CCOC1=CC=C(C=C1)N(C)[S+](† Chem Div,G008-480	0.278697	0.23539
FWCBUVFNUHGVBB	CC1=CC=CC=C1OC2=NC(=NC: Vitas-M Laboratory,!	0.250687	0.232835
ZXDFNGUSZJCZPH	CC1CCN(CC1)C2=CC(C)=NC(N Vitas-M Laboratory,!	0.244233	0.240309
PAKPPURFMNDWCG	CC1=CC=CC(OCC(=O)NC2=CC: Asinex Ltd.,BAS 072	0.257303	0.227814
FAYBXLDJSJPFDR	CC(C)C(=O)N1CCN(CC1)C2=C(ChemBridge,772314	0.257458	0.243442
QXIZHCZGPHGTBW	[O-][S+](=O)(N1CCN(CC1)C2=† Enamine,T5234320	0.283187	0.242025
DNZVGXSDOODGHQ	COC1=CC=C(C=C1[S+](†[O-])(=C Chem Div,G008-348	0.246499	0.236241

KIXWJXQGZKHFMX	CCOC(=O)C1=C(C)C(C(=O)OCC Enamine,T0501-114	0.29226	0.283935
MKAUGKLCXEBZIA	C1CN(CCO1)C2=NC(=NC(NC3 ChemBridge,52244:	0.255017	0.248909
OVYALIXIJXEDH	COC1=CC=CC=C1NC(=O)NCCCN2CCN(CC2)C3=CC=	0.246915	0.258963
WMC0BGJXXFYVRA	CCCCCOC1=CC=C(CN2CCN(C)CC2)C=C1	0.262366	0.270962
VHYFECUKHCCEAK	COC1=CC=C(C=C1)N2CCN(CCCN)CC2	0.24705	0.277661
PBZVAJFSCGGMOF	COC1=CC=C(CI)C=C1N2CCN(CCNC(=O)NC3=CC=CC	0.252792	0.253094
RJYPWYYZMZYMIR	CN(CCCNC(=O)CS(=O)CC1=C(C)OC(=N1)C2=CC=C(CI	0.252585	0.258507
BEZDSETXCGGGJR	CC(C)(C)NC1=N\C(=N/C(C)(C)C)C2=C1C=CC=C2	0.263024	0.259752
QLECRJJRHFSNEX	COC1=CC=C(C=C1)[N]2N=NN=C2C3=CC=CC(=C3)O(0.238504	0.310774
LFTMKYWQWYEXEN	COC1=CC=CC(=C1)NC2=CC(=NC3=CC=CC=C23)C	0.255843	0.29324
AUTUDPBMJAOGQU	CN1CC[C@H]2[C@@H](C1)C3=C(C=CC(C)=C3)N2C	0.262359	0.237461
QDEGMPXTGWEAPT	COC1=CC=C(NC2=CC(=NC(=N2)[N]3N=C(C)C=C3C)C	0.253169	0.250902
VZJMOBOCJKRZFP	CC(C(=O)C1=CC=C(C=C1)C2=C Chem Div, 0986-002	0.261824	0.249727
NWEBNKIPPLMNS	CN(C)C1=CC=[N+](CC2=C(CI)C Specs, AI-204/3171(0.298651	0.277554
PZLSVBQHOMDHF	CCOC1=CC=C(C=C1)C2=C(C)[N InterBioScreen,STOC	0.23886	0.226514
XSOOUJWKXLJQDS	CCN1CCN(CC1)C2=NC3=C(C= Chem Div,C267-010	0.284675	0.268429
TXIMTUQQVCEGL	C(C1CCCN(CC2=CN(N=C2C3= ChemBridge,89594:	0.241621	0.226868
NRCPSSPRJLREJB	C(CNC1[C@@H]2[C@H]3C[Vitas-M Laboratory,'	0.313088	0.304927
WLSZYJYDVSBLTI	CC1=CC=C(C=C1)C2=[N+](C3= Florida Center for Hc	0.26957	0.236143
NNJRYSTVBBMUKZ	CN1CCC(CC1)N(C)[S](=O)(=O)C2=CC=C(NC(=O)C3=C	0.263533	0.234697
NDBWIVOTAIDHPM	CC(C)(OCCOC(C1=CC=CC=C1)C2=CC=CC=C2)C#CCN	0.272185	0.254793
LNVXTFBKJKJARDM	CCOC(=O)C1=C(C)[N](CCC(=O)NCCN(C)C)C(=C1)C2=	0.292061	0.243317
ILJTXKNIYLUOKP	COC1=CC2=C(CN(CC3=C(OC)C(C)=C(OC)C=C3)CC2)	0.274061	0.270244
VEJZPHVTWOPCRO	C1CCN(CC1)C2=NC(=NC(=N2)N3CCNCC3)NC4=CC=	0.345024	0.315681
UXRRIDYXTYCVLB	CC[N]1C(=CC2=C1C=CS2)C(=O)NCCCN3CCC4=CC=C	0.260476	0.227834
WNZBBTJFOIOEMP	OC(CCCN1CCC(O)(CC1)C2=CC=C(CI)C=C2)C3=CC=C	0.2773	0.267416
OYPLCWQTVBUWTM	COC1=CC=C(NC(=O)NCCCN2CCN(CC2)C3=C(C)C=C(C	0.242868	0.253599
YYNYGLXURQQEQG	CC(C)(C)C1=NC(=CC(=C1O)CN2CCCC2)CN3CCCC	0.248203	0.253852
WFOUJWQZTHAZJG	OC(COC1=CC=CC=C1CI)CN2CCN(CC2)CC(O)COC3=	0.270486	0.280067
BCKIDIWAYYOCIW	CC(C)C1=CC=C(OCCN2CCCC2)C=C1C	0.248108	0.266694
CQVLIEXZVXLFLG	CN1CCN(CC2=CC=C(O2)C3=CC=C(CI)C=C3)CC1	0.279124	0.279137
AUBXBUBULXKDT	COC1=CC(OC)=C(CC(C)N2CCN(CC3=CC=CC=C3)CC2	0.301871	0.323638
FCBIYBXBWZVPBD	CCCN1CCC(CC1)N2CCN(CC2)C3=CC=CC(=C3)C(F)(F	0.244997	0.241441
HYKNYFJFLPXZRE	CN1CCCN(CC1)C2=CC(=C3C=CC(=CC3=N2)CI)C	0.255553	0.280873
ISKKHUSIKPRBKI	CC1=NC2=C(C=CC=C2)C(=C1)N3CCN(CC3)S(=O)(=O	0.244968	0.243099
BYFGRYLYFBKQEZ	CCN(CC)S(=O)(=O)C1=CC(=CC=C1)S(=O)(=O)C2=CC(=	0.24133	0.303796
CPCLOFLASZPHDE	CC1=CC(=CC(=C1CI)C)OCCCCNCCO	0.250397	0.246443
ZPERRVVQFXNOJR	FC1=CC=CC=C1N2CCN(CC2)C3CCN(CC3)CC4=C[NH	0.255999	0.250653
XQZHFUGHTZTKPS	COC1=CC=CC=C1N2CCN(CC2)C\C(C)=C\C3=CC=CC:	0.254175	0.233398
NKJPGWVVBAMXKV	COC1=CC=C(CC(C)N2CCN(CC2)C3=CC=CC=C3OC)C:	0.256038	0.237853
NYXWNDQIERERNF	ClC1=CC(CN2C=CC(=N)C=C2)=CC=C1	0.247573	0.292915
SSALKHAQQLSWJX	CC(C)COC1=CC=C(C=C1)C(=O)OC2CC(C)(C)OCC2CN	0.245272	0.239728
GINHCWKIPFCPGO	CCN(CC)CCNCC1=CC=C(O1)C2=CC=C(CI)C=C2	0.290588	0.282436
OYOPDPNOZYCMMQ	ClC1=CC=C(CN\2/C3=C(/CCC3)C(=N)\C4=C2CCC4)	0.252367	0.249941
WBUOONNMVHIUJT	COC1=C(OCC(O)CN2C(=N)N(CCN3CCCC3)C4=C2C	0.246184	0.236789
OFFPNKGMYSJLJY	CCCCCN1C=CC(=N)C=C1	0.247561	0.272177
VQTGKBAJYPPULX	CCCCN\1/C2=C(/CCC2)C(=N)\C3=C1CCC3	0.241008	0.263097
JALPLGVFZRCLGE	COC1=CC2=NC(=NC(=C2C=C1OC)N)N(C)C	0.240426	0.224816

QFVMLXCCDCNYCS	C1C1=CC=C(CN\2\C3=C(CCCC3)/C(=N)C/4=C2CCC4	0.280997	0.247862
UHWJVPVZFBUSSSG	CC(C)(C)NCC(O)COC1=C(C=CC=C1)C(C)(C)C	0.271044	0.244266
PZWBEOLGVSPLN	COC1=C(C=CC=C1)N2CCN(CC(O)COC3=C(CC=C)C=C	0.250155	0.237037
FLUSUHIOAMEDSO	COC1=CC(C(N2CCC3=C(C2)C=CC=C3)C4=NN=NN4(0.238729	0.259421
GVHBAMOZUBPHBK	CCC(C)(C)[N]1N=NN=C1C(N2CCN(C)CC2)C3=CC=C(0.24658	0.280337
JRXYNZLQRFULFO	Cl.CC(C)CCN1N=NN=C1C(N2CCN(C)CC2)C3=CC=C(0.260557	0.27278
YBVAHNMGJMBORJ	COC1=CC=C(C[N]2N=NN=C2C(N3CCN(CC3)C4CCCC	0.285907	0.280871
PBSQZIRUKNBOCE	COC1=CC=C(C=C1)C2=CSC(=N2)N(CCCN(C)C)C(=O)	0.247212	0.226466
KQLGOMMTFREDOH	FC1=CC=C(C=C1)C(N2CCN(CC2)C3CCCC3)C4=NN=	0.239895	0.242097
UZAKPJWEDZHORJ	CC(COC1=CC=CC2=CC=CC=C12)CN3CCN(C)CC3	0.303634	0.32356
HNGOLBWFANUTTN	CC1=C(CN2CCC(CC2)C(=O)NCC3=CC=CO3)N=C(O1)	0.244	0.232425
XIDPKWNHTMGYLI	CCN1CCCC1CNC(=O)C2CCN(CC2)CC3=C(C)OC(=N3	0.252213	0.258677
DJAFUYUUNCOPL	CCCN(CCC)CCNC(=O)C1CCN(CC2=C(C)OC(=N2)C3=	0.239844	0.250011
ZKSJDJCDPAHDEZ	CC1=CC(C)=NC(NC2=NCN(CC3=CC=CC=C3)CN2CC4	0.246962	0.260729
FDZVUOCOEGXCBN	COC(=O)C1=C(NC(=O)CCN2CCN(CC2)C3CCCC3)C4	0.247652	0.243597
RYMXUUSZSNQCDEU	CN1CCN(CC1)CC#CC[N]2C3=CC=CC=C3C4=CC=CC=	0.316952	0.302759
NUXNRDBZVAEAIN	COC1=CC=C(C=C1)N2CCN(CC2)CC3=NC(=NC(=N3)N	0.240402	0.255918
SXXXSTPMDGKCOCH	COC1=CC(CNC2=NC3=C(C=CC=C3)N2CCN4CCCC4	0.24205	0.246247
MXUQNKSYQMNLKF	CC1CC(C)CN(CC2=NC(N)=NC(NC3=CC=C4C=CC=CC	0.244239	0.260287
BYPSWJMJCJBEHG	CN1CCN(CC1)C2=C(NC(=O)C3=CC=C(C=C3)C4=CC=	0.24128	0.244371
SUWUZUZIVDBESQ	CN1CCC(CC1)N(C)C2=NC(=NC3=CC=CC=C23)C4=C(0.255853	0.270877
DTQFEZKWSNPMLU	OC1=C(CN2CCCN(CC3=C(O)C=CC=C3)C2)C=CC=C1	0.259455	0.269899
CPDQMHWCVLERNY	CC(OC1=C(Cl)C=C(Cl)C=C1)C(=O)NC2=CC=C(C=C2)N	0.247005	0.261109
BCEAOWDUQRYWIV	CN1CCC(CC1)OC(=O)C2=CC(=C(C)C(=C2)C)Br	0.252275	0.252163
IXIFGHGIRITVND	OC(=O)C(O)=O.COC1=CC=C(Br)C=C1CN2CCCC(C2)C	0.266826	0.229588
OZPGNDYAYQWBWDW	CC1=CC(=CC=C1)C2=NC(=C(C)O2)CN3CCCC(C3)C(=	0.25267	0.264437
RDLHLPXIDOQCOT	CCN(CC)CCCN(C=O)C1=NOC(=C1)C2=CC(Cl)=C(Cl)C	0.250524	0.247238
ZGXCULSRUGPOMX	OC(CN(CC=C)CC=C)C[N]1C2=CC=CC=C2C3=CC=CC=	0.243005	0.235857
IQADDSWPWJZCIDP	COC1=CC=C(C=C1)C2=CC(=NC(=N2)N3CCN(C)CC3)	0.259895	0.260842
JQTJFTYSSQMFNE	COC1=CC(NC(=O)NCCCN2CCN(CC2)C3=CC=C(F)C=C	0.288716	0.2855
FDDDVYRBXUWWGA	N#CC1=CN(N=C1C2=CC=CC=C2)C3=CC=CC=C3	0.242927	0.260122
XJARCBWQBOGRIF	OC(COCC1=CC=CO1)CN2CCN(CC2)C(C3=CC=CC=C3	0.244388	0.256156
QQIMTPNEIOSTBG	CN1CCN(CC1)C(C2=CC=CC(=C2)C(F)(F)F)C3=NN=N[0.241746	0.247099
JQKXCAKYDCGFPQ	COC1=CC=C(C=C1)C(N2CCN(CC2)C3=CC=C(OC)C=C	0.247332	0.267695
GTYGHNLEDSNBW	COC1=CC(C(N2CCN(CC2)C3=CC=CC=C3)C4=NN=NN	0.240679	0.261655
KKJLKEDWERCNBT	CC1=C(C=C(Cl)C=C1)N2CCN(CC3=NN=NN3C4CCCC	0.250939	0.285635
NQAWQTUJTNDVDCW	NC1=NC2=C(CCCC2)C3(CCCCC3)S1	0.281105	0.28076
NXUFLCBISRVMAG	COC1=CC=C(C[N]2N=NN=C2C(N3CCN(CC3)C4CCCC	0.239847	0.270564
GWPBJZLYMUVMV	CC1=CC=C(C=C1)C(N(CC2=CC=CO2)CC3=CC=CS3)C	0.249884	0.281768
QUFMFZUZPVSFQX	CCN(CC)CCCN(C(=O)C1=CC=CS1)C2=NC(=CS2)C3=C	0.239684	0.244021
XAFFCERJMHIDRK	COC1=CC(NC2=C3C=CC=CC3=NC(C)=C2)=C(OC)C=C	0.259026	0.262179
JAASKQSZJDOJLJ	CC(C)(C1=CC=C(C=C1)OCC(CN(C)C)O)C2=CC=C(C=C	0.254877	0.271054
NRRHFICIUBUJLNZ	CCOC1=CC(CN2CCCC2C3=CN=CC=C3)=CC=C1	0.248269	0.263586
LBTYJJUTDNCITA	COC1=CC=CC=C1N2CCN(CCCCOCC3=CC=C(F)C=C3)C	0.247223	0.258953
MODPIKSCMXTCPZ	CCOC(=O)C1=C(CNCCN(CC)CC)N(C)C2=C1C=C(OC)C	0.245612	0.231951
POTWBOICYBGNOO	CN1CCN(CC1)CCC(=O)N2C3=CC=CC=C3SC4=CC=C(0.24187	0.245958
HVGXTVMBLACNG	O=C1N(C2CCCC2)C(=O)C(=CNCCN3CCNCC3)C(=O	0.26531	0.238642
UQUXFXRMNTUFQA	C1C1=CC=C2N=C(N=C(C3=CC=CC=C3)C2=C1)N4CCI	0.243013	0.24409

GLVKFPUFWVMVQL	CCOC(=O)C1=C(CN2CCN(C)CC2)N(C)C3=CC(Br)=C(C	0.279788	0.266454
HNDWHMKTONQBSA	COC1=CC=C(NC(=S)N(CCC(C)C)C2CCN(CC2)C(C)C	0.250689	0.248527
VJUCHMDKYBGFJT	CCN(CC)CCNC(=O)C1=CC=C(NC(=O)C2=CC=CC=C2C	0.29126	0.271058
OBXAQYFZXPBRKV	O=C(C1CCCN(C1)C2CCN(CCC3=CC=CC=C3)CC2)C4:	0.254376	0.230901
OIWVPWJASBFTOV	CCN(CC)CCN=C(S)NC1=CC=C2N=C(C=C(C)C2=C1)N:	0.26556	0.248932
FAXASVFSGHQOHP	COC1=CC=C(C=C1)C2=CC(=NN2)C3=C(O)C=CC(C)=C	0.244006	0.230845
ZOXQYFLPDQGM DX	CN1CCCC(CC2OC3=CC=CC=C3SC4=CC=CC=C24)C1	0.310309	0.293957
OUCFZPJFLDVIFR	OC=O.C1C\C(CCN1)=C2\C3=C(SC=C3)SCC4=CC=CC	0.259587	0.241073
PZORWDLQCQBHBL	CCN(CC)CCNC1=NCCN2C1=CC3=CC(OC)=CC=C23	0.303628	0.285332
WSCOEDVASNROQD	ClC1=CC=C(NC(=S)NC2CCN(CC3=CC=CC=C3)CC2)C:	0.322649	0.291657
TYDPCFOMBQFAFW	CCCN(CC(=O)NC1=CC(Cl)=CC(Cl)=C1)CC(=O)NC2=Ci	0.250017	0.254446
XWEGKKKIRHQVSS	CC(C)N(CCNCC(COC1=CC=C(C=C1)C(C)C)C2=CC=Ci	0.258558	0.261663
PBDMGERAAPHHJC	CN(C)CCNS(=O)(=O)C1=CC=C(C=C1)N2CCN(CC2)C:	0.291947	0.255667
QYTLGHWFFIOPDG	CCOC(=O)C1=C(NC(=O)CNCCN(C)C)SC=C1C2=CC=Ci	0.251506	0.22623
MBHQKSKQJQNXFY	COC1=CC=C(C=C1)C2=C[N+](=C3CCC4=C(C=CC=C4)	0.247002	0.24646
BFHPGTOGFCEAS	CCOC1=CC=C(OC2=C(\C=N\NC(=O)COC3=C(OC)C=C	0.255086	0.253014
GJCKFQOJOGUGHY	CC(C)(C)N1N=NN=C1C(N(CC2=CC=CO2)CC3=CC=CC	0.24776	0.252943
WCVSEYBAUIPDKB	CC1=CC=C(C=C1)C2=NN=C(CSC3=NN=C(COC4=C5C	0.241337	0.236438
XOKVAQCOFZYPAN	FC(F)C1=C/C(=N\C2=C(\C=N\N\12)C(=O)N3CCN(CC	0.302867	0.290517
NWPWWINMTQWHBL	CCOC1=C(OCC2=C(Cl)C=CC=C2)C(Br)=CC(CNCCCNC	0.26155	0.249079
YBTUSMAEWFIBV	COC1=C(OCC2=CC=C(Cl)C=C2)C(Br)=CC(CNCCCNC3C	0.275566	0.264386
JZHIXFGGSZLEKB	CCC(C)NCCOC1=CC=C(C=C1)C(C)(C)C2=CC=CC=C2	0.252739	0.227286
KUNYYZPPEZEDAG	CC1=C(C)C=C(C=C1)N=C(S)N(CCCN2CCCC2)CC3=CC	0.276562	0.255465
NIHDZBOENNWHCN	COC1=C(C=CC=C1)C2=NC(SCC(=O)N3CCCCC3)=C4C	0.266332	0.252856
UHQWWMFSPGPEU	CCCCN(CC)CCCNC(S)=NC1=CC2=C(C=C1)N=C(C=C2	0.294866	0.282564
YDPZMUWTVKPGBB	CCN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)NCCCN	0.247559	0.231998
YDJIFKISSQNAIS	CN(C)CCCNC1=NC=C(C=C1)C2=NC=NC(NC3=CC(Cl)	0.270092	0.250211
WSYSDMJVVVJKIH	[O-][N+](=O)C1=CC=C(OC2=CN=CC=C2)C=C1)[N+](0.28269	0.235532
UBMWIWOZOGGSGI	O=C(\C(CN1CCCC1)=C\C2=CC=CC=C2)C3=CC=CC=C	0.25506	0.224271
BDTAOSJTPSFQD	C1CC2CC3=C(CN2C1)C4=CC=CC=C4C5=C3C=CC=C	0.245401	0.223677
POCHMWHMPRYMTC	COC1=CC2=C(C=C1)C=C(CNCCOCCOCCNCC3=CC4=	0.259311	0.233996
AEEZWHXVXFVAD	SC(=N\N=C\C1=NC=CC=C1)N(CC2=NC=CC=C2)CC3:	0.287555	0.239087
BTFYMPJMYCNLRM	SC(NCC1=NC=CC=C1)=N\N=C\C2=NC=CC=C2	0.282726	0.249059
FQWITMQQUMTMRE	NC(S)=N\N=C\C1=C2C=CC=CC2=CC=N1	0.279837	0.246458
TUHFYDGLBUXMEC	CC(=C)C1=NC(OC2=CC=CC=C2)=NC(OC3=CC=CC=C:	0.318574	0.273908
KKURDNASMPVGKT	C\C(=N/N=C(S)N1CCCCC1)C2=C3N=CC=CC3=CC=C	0.254948	0.227328
KLYOLLLMOLFUSQ	CC(NN=C(S)N1CCN(CC1)C2=NC=CC=C2)C3=C4C=C	0.268482	0.228347
VKRQERUBXPLFCD	CN(C)C(S)=NC(S)=NC1=CC2=C(C=CC=C2)C=C1	0.322749	0.27482
ZSMIAGRBYIUJAJ	CSC(\N=C(\SCC1=CC=CC=C1)N(C)C)=N/C2=CC=CC=C	0.319266	0.281876
FBWSJSWNFLJJJB	CSC(S)=N\N=C(/C)C1=NC(C)=CC=C1	0.276433	0.234662
GHIMMECAKCIHTG	C=C1CC2(OC1=O)C3=C(CCC4=C2C=CC=C4)C=CC=C	0.268211	0.224513
ZQRFGIQOJKEYBU	CCN(CC)CCC=C(C1=CC=CS1)C2=CC=CS2	0.279117	0.235644
SKDKPMWRWWHHRD	COC1=C(\C=N\NC(N\N=C\C2=C(OC)C=CC=C2)=N\N	0.281639	0.255748
QDSXVYQCPUYEZ	N(\N=C\C1=CC=CS1)C(N\N=C\C2=CC=CS2)=N\N=C\	0.250808	0.227884
WXMFLZGDXLEMN	OC1=C2N=CC=CC2=CC=C1CN3CCCCC3	0.272038	0.236253
ZYFVGABFAJUTDB	CN(CC1=C(O)C(C)=CC(C)=C1)CC2=C(O)C(Cl)=CC(Cl):	0.262857	0.230329
KJPKPBMWHKBKHG	O=C(C(CN1CCCCC1)C2=CC=CC=C2)C3=CC=CC=C3	0.263941	0.225233
VYVDPFREHHCGMM	CC(=O)OC1=CC=C(C=C1)C23C4=C(C=CC=C4)C2(OC	0.295103	0.266265

FAPPLTQTFIVGDU	OC1=C(C=CC=C1)C2SC(SC(S2)C3=C(O)C=CC=C3)C4:	0.297957	0.249339
ZHPDKZWRWNETEN	COC1=C(NS(=O)(=O)C2=C(Cl)C=CC(N\C(=N)\S(=O)=C	0.254276	0.25622
FMGRGIOUUGFHJP	CC1=CC(C)=C(C=C1)[N+]2=C3CCC4=C(C=CC=C4)N3	0.248609	0.22686
XHPUYICJDOILJN	CN(C)C1=CC=C(C=C1)[N+]2=C(=CC(=CC2C3=CC=CC:	0.247747	0.262023
LLCHPKABGFRGHB	COC1=CC=C(C=C1)[N+]2=C3CCC4=C(C=CC=C4)N3C	0.239064	0.229258
YFYTWDJVYRDONY	CCOC1=CC=C(C=C1)[N+]2=C3CCCCCN3C=C2C4=CC	0.265502	0.269271
KMZJWZKHQPPHCT	COC1=CC=C(C=C1)[N+]2=C3CCC4=C(C=CC=C4)N3C	0.242011	0.233558
JVPKVEYRQGOPSJ	CC1=NN(C(C)=C1NS(=O)(=O)C2=CC3=C(C=CC=C3)C:	0.279681	0.249951
VKOGOVIJXOGKGCJ	CCOC1=C(C=CC=C1)N2CCN(CC2)C(S)=NC(=O)C34C	0.263906	0.240339
UFAZASYMNCMYTC	CN1C=NC(=C1S(=O)(=O)OC2=CC=CC=C2)[N+](O-)=	0.268915	0.232912
OHUYUZQKKZNYPY	COC1=CC2=C(SC(=C2C3=CC=C(OCCN(C)C)C=C3)C4:	0.304434	0.301066
SOVQSFQUOYHQMZ	FC1=CC=C(C=C1)N2CCN(CCCNC(=O)CN3CCN(CC4=	0.238517	0.227538
JIOZLNOPICWVHE	CC1CCN(CCCNC(=O)C2=CC=C(CSCC3=CC(Cl)=CC=C:	0.281381	0.237617
NFTHRRMLFWIHQO	CC1=C(C)C=C(NC(=O)CSC2=NC3=C(C=CC=C3)C(=O)I	0.252901	0.244882
ZHPGEAXFYDMERE	COC1=CC(NC(=O)C2CCN(CC3=C(N4C=CC=C4)N(N=C	0.275065	0.237566
WNCALWIAHXATTF	COC1=CC(NC(=O)C2CCN(CC3=C(N4C=CC=C4)N(N=C	0.250651	0.23897
UFMJAGNPIYFMFZ	O=C(N1CCN(CC2=CC=CC=C2)CC1)C3=CC=C(CNS(=C	0.24445	0.232992
VOGUHDWNNRBEF	CC1=C(CN2C=CC=C2C3=NC(CO3)C4=CC=CC=C4)N=	0.245446	0.222908
BUCHHVOLSDDWQM	CN(CC1=CC=CC=C1)C(=O)C2CCN(CC3=CC=C(Cl)C=	0.253126	0.230069
LCCSPYUGQUDIOH	COC1=CC=C(C=C1)C2N(C)CCC3=C2C4=C(CCN(C)C4	0.326852	0.298524
HHFTZXSANTTSL	COC1=CC=C(CN2CN=C(NC3=NC(C)=CC(C)=N3)N(CC	0.312181	0.269586
KABGULJJPRGKSF	NC1=NON=C1C(=O)NCCNCC2=C3C=CC=CC3=CC=C:	0.285449	0.233275
TZFAMUNSQMIJVV	C1S2=NN=C(N2N=C1C3=CC=C(C=C3)C4=CC=CC=C	0.259765	0.232875
CDJWSJVYCFGVKO	[O-][N+](=O)C1=C(Cl)C=CC(=C1)C(=O)N(CC2=CC=C(C	0.246616	0.24538
RWUIVHVVFWEECH	O=C(CCN1CCN(CC2=CC=CC=C2)CC1)NC3=CC=C(OC	0.261332	0.232451
STFNAPXAWAEXNC	CCN(CC)CCNC(=O)C1=C(C)N(C2=C1C=C(OC)C(Br)=C	0.255659	0.261938
RFIYUELTRBMMNL	COC1=CC2=C(NC(C)=C2C(=O)CN3CCN(C\C=C\C4=C	0.255639	0.238185
GUEZCQOOEUTMJF	CCOC1=C(OC)C=C2C(NCCC3CCOCC3)=NC(=NC2=	0.247902	0.232933
NKZYFXVHBRNDO	CN1CCN(CC1)S(=O)(=O)C2=C(C)C=CC(=C2)C3=C4C=	0.242133	0.226224
GMVQRRVCNWDLLT	CCCOC1=CC=C(C=C1)C(=O)C(CN2CCCC2)C3=CC=CC	0.243618	0.228015
MEPXQVRXJLIKQB	COC1=C(OCC2=C(F)C=CC=C2)C=CC(CNCCC3=CNC4	0.273988	0.254527
UNOAJOUPOZILR	COC1=C(OCC2=C(Cl)C=CC=C2Cl)C=CC(CNCCC3=NC=	0.283663	0.250773
XLXROIVENNXDG	CC(C)C(=O)N1CCN(CC1)C2=C(Cl)C=C(NC(=O)C3=CC	0.238835	0.22294
ALDVIBYUEOPTBH	CC1=CC=C(C=C1)C2=NOC(CSC3=NN=C(N3C4=CC=C	0.264636	0.243165
XWNIJANSHVBAPT	CC1=CC=C(C=C1)C2=NOC(CSC3=NN=C(CCC4=CC=C	0.286341	0.273207
ZMVOSXWFIBSYRX	COC1=C(C=C(C=C1)S(=O)(=O)NC2=CC=C(C)C=C2)N(0.258807	0.236602
VDOIXPOUDOFLHO	COC1=C(C=C(C=C1)S(=O)(=O)N2CCCCC2)N(C)S(=O	0.248284	0.256118
LIGUMGRSVBLBKG	CCC(=O)C1=CC=C(OCC(O)CN2CCN(CC2)C(C3=CC=C	0.256523	0.247423
SOEYUDFSHJCWTE	Cl.CCOC1=CC(CNCCC2=CC=C(C=C2)S(N)(=O)=O)=CC	0.310624	0.273608
UDOZJWJRQUAFRO	Cl.CCOC1=CC(CNCC2=CC=NC=C2)=CC(Br)=C1OCC3	0.249491	0.228148
UTTIUDCHDUGGQB	COC1=C(OCC2=CC=C(Cl)C=C2)C=CC(CNCCC3=CC=C	0.274209	0.236019
CNGCLFKQUQPLB	COC1=C(OCC2=C(F)C=CC=C2)C(Br)=CC(CNCCC3=CC=	0.268126	0.246512
UKWQQECMOSVMNZ	COC1=C(OCC(=O)NC2=CC(=CC=C2)C(F)(F)C=CC(Cl	0.275889	0.225594
FVSMZXPZIKTWEG	CCOC1=C(OCC2=C(Cl)C=C(Cl)C=C2)C(Br)=CC(CNC(C	0.252049	0.230189
POWVYVDIGCYLAJ	CC1=C(C)C2=C(S1)N=CN=C2N3CCN(CCO4=CC=C(C	0.252601	0.25909
JCFWLXAYFIGFDY	COC1=CC(OCCCN2CCN(CC2)S(=O)(=O)C3=CC=C(NC	0.270821	0.236135
VTSCIKMVAOYQJV	SC(NC1CCN(CC2=CC=CC=C2)CC1)=NC3=CC(Cl)=C(C	0.263864	0.248681
CEGLMXXCTGCEDH	ClC1=C(C=C(Br)C=C1)C(=O)NC2=C(C=CC=C2)N3CC	0.278651	0.283627

ACGFRFTVPHBAR	OCCNCC1=C(OCC2=C(CI)C=C(CI)C=C2)C=CC(Br)=C1	0.289463	0.284052
SQLAYJLTBKSAB	FC1=CC=C(NC(=O)C2=CN(N=C2C3=CC=NC=C3)C4=C	0.249412	0.240691
GPUYCFVMTDOTMG	CC1CCCN(CCOCCOC2=C(Br)C=C(CI)C=C2)C1	0.282103	0.23456
CRHCUAOLDLBHMX	CN(CCCCOC1=C(CI)C=CC(C)=C1)CC2=CC=CC=C2	0.336733	0.295621
KATIPTFKORCOF	COC1=CC=C(C=C1)N2CCN(CC2)C(=O)CCCN3C(=O)C	0.247366	0.224626
NXCCEAXDSDHMQI	OC(=O)C(O)=O.CC1CCN(CCCOC2=CC=C(OCC3=CC=C	0.250045	0.222633
VQSUVBKRLYSTOA	COC1=C(OCCCCN2CCN(CC2)C3=C(OC)C=CC=C3)C=	0.285972	0.269084
DXKJLDCDDBTGGS	COC1=C(C=CC=C1)N2CCN(CC(O)COC3=CC4=C(CCC	0.239046	0.222784
VXGJTMACCOZJHX	COC1=CC(OC)=CC(NC(=S)N2CCN(CC2)C(C3=CC=CC	0.249859	0.280489
KGYWRBHKJVRKEV	CC1CC(N(C=O)C2=CC=C(CI)C=C2)C3=CC=CC=C3)C4	0.261146	0.228601
REIDSGGUBCVQW	FC(F)(F)C1=C(NC(=O)C2=CC=C(CN3CCC(CC4=CC=CC	0.283463	0.253921
DALKRTJBJKPL	CCC1=C(NC(=O)C2=CC=C(CN3CCC(CC4=CC=CC=C4)	0.27166	0.247455
POXGDUMCZNRN	COC1=C(OCC(O)CN2CCC(CC3=CC=CC=C3)CC2)C=C	0.264637	0.232873
MYNSQDLETAOVJE	OC1(CCCCC1)C#CC2=CC=C(C=C2)C(=O)N3CCN(CC3	0.246534	0.225768
MKGLHEFJSNUHSC	COC1=CC(CN(C)C(C2=NN=NN2C3=C(C)C=CC=C3)C4	0.284039	0.283493
WFWWTRNJTQDJW	[O-][N+](=O)C1=CC2=C(O\C=C/COC3=C(CI)C=C(CI)C	0.251122	0.238898
AWZHEICVGLZBJ	CCN(CC)CCN1C(NCC2=NC3=C(C=CC=C3)N2CC4=CC	0.270905	0.241023
KLRQIRDBMCPSPR	CC(C)(C)N1N=NN=C1C(N(CC2=CC=CO2)CC3=CN=C	0.267492	0.24343
BXJYYWCZOQPVNC	COC1=CC(=CC=C1)C2=CSC(=N2)N3CCN(CC3)C(\S)=	0.244818	0.236905
GYLLOWIYVUZCT	COC1=C(C=CC=C1)C(N2CCN(CC2)C3=C(C)C(C)=CC=	0.290895	0.268461
BHRDJGZWRNNORC	CC(C)(C)N1N=NN=C1C(N(CC2=CN=CC=C2)CC3=C(C	0.268238	0.268824
ASAIKGBIRKCLLU	CC(C)(C)N1N=NN=C1C(N(CC2=CC=CC=C2)CC3=CC=	0.268207	0.266058
PKDQPZHGBXEAQY	CC(C)(C)N1N=NN=C1C(N(CC2CCCO2)CC3=CC=C(CI)	0.251745	0.240796
KFNUXOPRMHDEF	CCC(C)(C)N1N=NN=C1C(N(CC2=CC=CO2)CC3=CC=C	0.273363	0.262021
MMFQCCJFVLDKCI	CC(C)(C)C1=CC=C(CN2C3=NC3C4=C2C=CC=C4	0.245869	0.23924
HWNCNYMVSQNVOB	CCC(C)(C)N1N=NN=C1CN2CCN(CC2)C(C3=CC=CC=C	0.268214	0.24954
LPXYGVAQIOTYKW	CN(\C=C\C1=[N+](C)C2=C(C=CC=C2)C1(C)C)C3=CC=	0.296228	0.262073
JZRHAPUVZGGWOG	CC1=CC=C(C=C1)CN2CCN(CC2)CC=3C=C(C=CC3[N	0.25805	0.22921
DMYSGPNXOWSMGP	CC1CCN(CC1)C(C2=NN=NN2CCC3=CC=CC=C3)C4=C	0.26786	0.269977
MKHUUMRWZZFAQU	CCOC1=CC=C(C=C1)C(O)CN2C(=N)N(CCN3CCCC3)	0.279893	0.223999
DUWSOQYQDUYMDE	CCN(CC)CCOC(=O)C(OC(C)C)(C1=CC=CC=C1)C2=C	0.334821	0.303677
JRPWIKCYHWOKAZ	CC(C)(C)N1N=NN=C1CN2CCN(CC2)C(C3=CC=CC=C	0.283754	0.284923
AWUBMIIAJHGFQS	CCCC1=C(N=C(N\N=C\C2=NC=CC=C2)S1)C3=CC=C	0.253002	0.225299
AEESOEJLSASDMP	CCN(CC)S(=O)(=O)C1=CC=C2C(=C1)C(=NO)C=3C2=C	0.247014	0.246197
ALJGMAYETVKWCM	CCCCN(C)C(=O)C1CCN(CC2=CC=C(OCC3=CC=CC=C	0.256689	0.243233
WFWSSBLAKXMSHT	CCCCNC(=O)C1CCN(CC2=CC=C(OCC3=CC=CC=C3)C	0.243114	0.231765
WDORARNTCODBGU	COC1=CC=CC=C1N2CCN(CC2)C(C3=CC=CC=C3)C4=C	0.284236	0.258942
IHTIAVMXLQAPNF	COC1=C(C)C=C(C=C1)S(=O)(=O)N2CCN(CC2)S(=O)	0.275313	0.264527
IHDTVQWTNDELLP	COC1=CC=C(C=C1)C2=C(C3=C(S2)C=CC=C3)C4=CC=	0.292588	0.274861
GLBKTSMZCIBQGM	COC1=CC(=CC=C1)C2=C(C3=C(S2)C=CC=C3)C4=CC=	0.262615	0.237985
HQDXGLXETMQWFK	CN(C)CCOC1=CC=C(C=C1)C2=C(SC3=C2C=CC=C3)C	0.261521	0.237251
ZLJCFEHKTHXYOP	C(CN1CCCC1)OC2=CC=C(C=C2)C3=C(SC4=C3C=CC	0.295545	0.27211
GQKRYQCHDLPPRE	COC1=CC2=C(C=C1OC)C(=C(S2)C3=C(OC)C=CC=C3)	0.278824	0.248626
GSFVSUDIBTYRBH	COC1=CC2=C(SC=C2C3=CC=C(OCCN(C)C)C=C3)C4=	0.255238	0.224249
JHFZIOXMCPUGLO	COC1=C(C=CC=C1)C2=C(C#CC3=CN=CN3C)C4=C(S2	0.241954	0.223182
GGIYASBPSGCVHI	COC1=CC=C(C=C1)C2=C(C#CC3=CN=CN3C)C4=C(S2	0.255087	0.244944
TXINADOSPSEZFG	COC1=CC2=C(C=C1)C=C(N=C2)C3=CC(OC)=CC(OC)=	0.256892	0.23107
UIICMRMNONXVGY	CN1CCN(CC1)C(=O)CCN2C(=S)S\C=C\C3=CC=C(F)C	0.267655	0.235357

SLEZRUPRYHGPTI	COC1=CC=C(C=C1)C(CNC(=O)C2=CC=C(C=C2)S(=O)(0.246032	0.222452
WKPNCXXQVJSLT	COC1=CC=C(C=C1)C(CNC(=O)C2=CC3=C(CCC(C)C3)	0.261677	0.225574
YAWMZCKLDJDBHO	CN(C)C(CNC(=O)C1=CC(=CC=C1)S(=O)(=O)N2CCN(C	0.256145	0.223428
PAPGWSJQNKUAIP	COC1=C(OC)C(CN(C)C(=O)C2=CC(=CC=C2)S(=O)(=O)	0.259225	0.23123
YNRKHUHPBRXTSE	O=C(NC1=CC(=CS1)C2=CC=CC=C2)C3=CC=CO3	0.251831	0.228109
XSFQETONKAKIRH	CN1CCN(CC1)C2=C(NC(=O)C3=C(C)C4=C(O3)C=CC(0.275511	0.229104
UVDMCAVZGBWMOW	CCN1CCN(CC1)C2=C(C)C=C(NC(=O)C3=C(OC)C=C4(0.27093	0.234377
MGOXGEYNAGHIIG	COC1=CC(=CC=C1)N2CCN(CC2)C3=C(C=C(C=C3)S(=	0.262989	0.243059
YPTLBORUSUHUOA	COC1=C(OC)C=C(CN(C)C2=C(C=C(C=C2)S(=O)(=O)N:	0.292414	0.256415
GGEDFXAKTRZLPC	CC(C)C[C@H]1CN=C(NC2=CC=CC=C2)N1CCCC3CC(0.243869	0.234065
OFUMMVWXZVSCDV	CCN1CCN(CC1)C2=CC=C(NC3=C4C=CC=CC4=NC=C	0.307023	0.266577
DUCMTCXRNAFIQO	CCC1=CC=C(OCCNC2=C(C=CC(=C2)N3CCNC(C)C3)]I	0.280153	0.263361
SKNIMWACWJQXID	CCOC(=O)C1(CCN(CCC(=O)NC2=CC(Br)=CC=C2)CC1	0.290397	0.255034
LTHBJHFXNJBMTQ	COC1=CC2=C(NC(C)=C2CCNCC3=CN(C)C4=C3C=CC	0.330624	0.286088
QAECBDXCFKOMLD	FC1=CC=C(C=C1)C(=O)C(CCCCC(CN2CCOCC2)C(=C	0.270169	0.228778
SZWDKYLRLWWCXMV	COC1=C(OCC2=CC=C(F)C=C2)C(Br)=CC(CNCCSC3=N	0.264112	0.236438
BYVGHTJAPCUMAU	CCOC1=C(OCC2=CC=CC=C2)C(Br)=CC(CNCCSC3=NI	0.258371	0.243265
DUBXCYUMCWFEIA	CN(C)CCOC1=CC=C(NC2C3=C(CSC4=C2C=CC=C4)C:	0.256799	0.235922
HXOBKEJHWPCMOX	OCl(=O)(=O)=O.[O-][N+](=O)C1=C(C=CC=C1)C2=[N+	0.254603	0.236647
KCMOVBPDRGDKSU	OCl(=O)(=O)=O.COC1=CC=C(C=C1)[N+] ₂ =C(C=C(C=C	0.285444	0.260996
ROIQDQJQRXREPV	OCl(=O)(=O)=O.FC1=CC=C(C[N+] ₂ =C(C=C(C=C2C3=C	0.260495	0.230712
JNGBTISOFZDKDB	OCl(=O)(=O)=O.ClC1=CC=C(C[N+] ₂ =C(C=C(C=C2C3=	0.269991	0.246466
WQWNQUNQRPJPC	CN(C)CCN(C(=O)C1=C2C=CC=CC2=CC=C1)C3=NC4=	0.241567	0.236129
AVOROEGEYAGDGQ	Cl.CN(C)CCCN(C(=O)C1=C/C=C(\C=C\1)S(=O)(=O)N2	0.287397	0.274232
OKTMFRKTDSCKQO	Cl.CN(C)CCCN(C(=O)C1=C/C=C(\C=C\1)S(=O)(=O)N2	0.276798	0.266508
LTYWSFWKTFEVPP	CCOC1=CC=CC2=C1N=C(S2)N(CCCN(C)C)C(=O)C3=(0.245024	0.224146
FKTZJXIWJXXAPE	CN(C)CCCN(C(=O)C1=CC=C(C=C1)S(=O)(=O)N2CCCC	0.248061	0.227532
UJRUBNLOVCQMRB	CN(C)CCCN(C(=O)C1=C2C=CC=CC2=NC(=C1)C3=CC	0.258798	0.231616
IWWLICALWBJNSIU	CCOC1=CC=CC2=C1N=C(S2)N(CCCN(C)C)C(=O)C3=(0.24751	0.230713
IXBJJZUFXKRYAE	CN(C)CCCN(C(=O)C1=CC=C(C=C1)S(=O)(=O)N2CCCC	0.264334	0.232719
TXUFZZUOCTZYJH	Cl.CN(C)CCCN(C(=O)C1=C/C=C(\C=C\1)S(=O)(=O)N2	0.267407	0.26175
KAEOSBXRKKEEV	CN(C)CCCN(C(=O)C1=CC=C(C=C1)S(=O)(=O)N2CCCC	0.265124	0.236978
SBLDHEVXEWMANF	CN(C)CCCN(C(=O)COC1=CC=C(Cl)C=C1)C2=NC3=C(0.264015	0.235167
UOTCPKSPHQQ	CCN(CC1=CC=CC=C1)S(=O)(=O)C2=CC=C(C=C2)C(=C	0.260522	0.230616
FVOFQSYXVYDDB	CN(C)CCCN(C(=O)C1=CC2=C(CCCC2)C=C1)C3=NC4:	0.280487	0.249136
FZJNTEQDWSFMNL	CN(C)CCCN(C(=O)C1=COCCO1)C2=NC3=C(S2)C=C(E	0.275734	0.250734
CLRFIEWSDSOYIS	CCN(C1=CC=CC=C1)S(=O)(=O)C2=CC=C(C=C2)C(=O)	0.252298	0.227519
DYXQUXUYUXXNO	CN(C)CCCN(C(=O)C1=CC=C(C=C1)S(=O)(=O)N(C)C2C	0.275904	0.252726
QJOVEDKWCJOBQV	CN(C)CCCN(C(=O)C1=CC2=C(OCCO2)C=C1)C3=NC4	0.261444	0.226782
DJZHAASERPCFC	CN1CCN(CC1)C2=NN=C(C=C2)C3=CC(NC(=O)COC4:	0.258871	0.241287
HOVUEWSGLRURJL	CN1CCN(CC1)C2=NN=C(C=C2)C3=CC(NC(=O)COC4:	0.253686	0.223462
HJUVJMSPHVGNCJ	CCC1=CC2=C(C=C1)N=C(S2)N(CCCN(C)C)C(=O)C3=C	0.246333	0.226814
YJTSNDABJLKQKP	COC1=C(NC(=O)NC2=NC(CC(=O)NC3=C(OC)C=C(C)C	0.283102	0.238241
RUJSHAUPVUAXDM	COC1=C(NC(=O)NC2=NC(CC(=O)N3CCN(CC3)C4=C(0.246165	0.223266
GRTDCVKGLAJLB	COC1=C(NC(=O)NC2=NC(CC(=O)N3CCN(CC3)C4=CC	0.271285	0.242654
YORRTVYDYMZFM	CCN(CC)CCNC(=O)C1=CC=C(NC(=O)C2=CN(N=C2C3	0.265489	0.255911
DONIJVVJKXUIR	CC(NC(S)=NC1CCCC1)C2=C(C)C=CC(C)=C2	0.305547	0.265596
DDOYOGJJZUJWSQ	COC(=O)C1=CN(C=C(C1C2=CC(OC)=CC=C2)C(=O)OC	0.283392	0.252152

DTEWCMYGXOZQX	[O-][N+](=O)C1=CC(NC(=O)NC2=CC3=C(CCC3)C=C2)	0.239262	0.226951
KQBMETCMIIYQPE	FC1=CC(NC(=O)NC2CCCCC2)=CC=C1	0.239539	0.237794
MFLNRTKARSUFLO	SC(NC1CCN(CC2=CC=CC=C2)CC1)=NC3=CC(Cl)=CC	0.282174	0.249414
RMLDFBSTXJIBGG	ClC1=C2N=C(C=C(C(=O)N\N=C\C3=CN=CC=C3)C2=(0.271496	0.258917
DZKPHHMCPRGNLD	ClC1=CC=C(C=C1)N2CCN(CC2)C(=O)NC3CCCC3	0.240041	0.232808
VGNBTOMRNPGLG	OC1=CC=C(NC(=O)C2=CC=C(NC(=O)C3=CC=CS3)C=(0.239731	0.228038
DOBZEONUJACQKA	CC(C)(C)C1=CC=C(C=C1)C(=O)ON=C(N)C2=NC=CC=C	0.241333	0.245259
GAOFHEWOWSMUCM	FC(F)(F)C1=C(NC(=O)CN2C3CCCC2CC(C3)NC(=O)C4	0.255302	0.223817
GXFAQSFFENFHCG	COC1=CC(=CC=C1)C(=O)NC2CC3CCCC(C2)N3CC(=C	0.244336	0.235289
MDXBSQDWOQSRFD	CN1CCN(CC1)C2=C(Cl)C=C(NC(=O)C3=CC=C(O3))[N-	0.252693	0.2331
ZTRXFNYQKYIUPF	CC(NC(S)=NC1CCCC1)C2=CC=C(C=C2)C(C)(C)C	0.242923	0.227013
BGTNQCWYXQNPV	CCOC1=CC=C(C=C1)C(C)\N=C(/S)NCC2=CC=C(F)C=C	0.276061	0.27168
AJMAIBOMZGOQKJ	CCC1=CC=C(C=C1)C(C)\N=C(/S)NCC2=CC=C(F)C=C2	0.261415	0.23879
KADBDPLNZVMZIZ	SC(NC1CCN(CC2=CC=CC=C2)CC1)=NC3=CC=C(Br)C	0.307648	0.265786
MNIXWTWZNOKBKZ	CCC1=CC(=C(OC)C=C1)S(=O)(=O)NC2=CC=C(CC3=C	0.252977	0.233234
RNJSIRHZODXFS	CCOC1=CC(NC(=O)C2CC2)=C(OCC)C=C1NC(=O)C3=	0.269918	0.228587
JXLNILKAXGFVFB	CN1CCN(CC1)C(=O)CCN2C(=S)S\C(=C/C3=CC(Br)=C	0.265355	0.228804
AAQDANSDDLBBNH	COC1=C/C=C\C=C\1)N(C(C(=O)NC2CCCC2)C3=C/C	0.247975	0.235887
CWXFBBLKWFGUOA	CC1=C(N=C(NC(=O)CN2CCCC2)S1)C3=CC4=C(C=C3	0.242275	0.23064
ROXSVTHVYLYGQN	COC1=CC=C\C=C2\SC(=S)N(CCC(=O)N3CCN(C)CC3	0.252287	0.230937
KYPNRQRUJSJAIR	FC1=C/C=C\C=C\1C(=O)N2CCC3=C\C(=C/C=C2/3)\(0.372312	0.379318
CTHUZLIUSZTHMB	COC1=C(OC)C=C2CN(CCC2=C1)C3=C(C=CC=N3)[N+	0.248728	0.22311
SQLSTWVWXOCLOD	COC1=CC=C(C=C1)C2C3=C(OC4=C2C(=N)N(CCN(C)	0.281696	0.245119
KOUSBZMTRLNIFB	CN(C)CCCNC1=NC=NC2=C1C(=C(O2)C3=CC=CC=C3	0.264123	0.235826
CSKLCXHKHIKWDL	COC1=C(C=CC=C1)C2C3=C(OC4=C2C(=N)N(CCN(C)	0.272383	0.243021
VGJCPUJNUJHWDU	CC(C)C(CCN1CCN(C)CC1)C2=CC=C(Cl)C=C2	0.271519	0.244809
CPGFYXCUVMTLJF	CC(C)CCC(CCNCC1=NC=CC=C1)C2=CC=C(Cl)C=C2	0.247754	0.222811
WIUJOZTZDSBSCB	CC(C)C(CCNCC1=NC=CC=C1)C2=CC=C(Cl)C=C2	0.275418	0.229765
LRIJTMWZNPBCOZ	CN1CCC(CC1)NCCC(C2=CC=C(F)C=C2)C3=CC=C(Cl)	0.293413	0.276454
PFBMOEVTKCJYLV	CN(C)CCCNC(=O)C\C1=C(C)\C2=C3O/C=C\C\3=C(C	0.301684	0.31253
HXIGEHHGZVUBWJV	FC1=CC=C(C=C1)C(CCN2CCOCC2)C3=CC=C(Cl)C=C:	0.271557	0.260916
VZPVYMYKXNRNSK	COC1=CC=C(C=C1)C2=NOC(CCCC(=O)NC3CCCC3)=	0.261932	0.228433
SMWXXNBPZMKFOS	COC1=C/C=C\C=C\1)C2C3=C/C=C4/C=C\C=C\C4=	0.359221	0.41072
FYTBEHAACLDCSC	BrC1=CC(=CC=C1)C2N3[C@@H](CC4=C2NC5=C4C	0.254398	0.230457
CVFDUSPRRDVDAK	ClC1=CC=C(C=C1)C(CCN2CCCC2)CC3=CC=CC=C3	0.290511	0.263901
WHNXQKIPNNLBQD	OCCNCC1=C2C=CC=CC2=CC=C1OCC3=CC=C(Cl)C=(0.28761	0.304266
TXCOIOMQKZPPQM	COC1=CC=C\C=C\N\NC2=C3C=C(Br)C=CC3=NC(C)=C:	0.240993	0.241353
ZHKSHBSAJCOKAP	OC1=CC(NC2=NC(=NC(=N2)N3CCOCC3)N4CCOCC4	0.257277	0.230776
PKCIQDZGRVGTGO	COC1=C(OC)C(CNCC2=C3C=CC=CC3=C(OC)C=C2)=(0.241838	0.240706
NDAPSSVOIVJURB	FC1=CC\C=C\N\NC2=NC=NC(=C2)N3CCOCC3)=CC=C	0.24379	0.222437
ZLRIKJMGXXQLFB	CCOC1=CC=C(CN2CCN(CC3=CNC4=C3C=CC=C4)CC	0.256913	0.237432
ZHPZSHVMZHNSBW	COC1=CC=C(C=C1)C2=CSC(=N2)N(CCCN(C)C)C(=O)	0.272016	0.283163
ZBJVJAVXHLRPPY	CSC1=CC=C(CN2CCN(CC2)C3=C(C)C=CC=C3)C=C1	0.258721	0.234011
OFUOEGQNHFUNKF	COC1=C(C=CC=C1)N2N=C(CC2C3=CC=CC=C3)C4=C	0.243111	0.243451
ACCMGQIBJRYVMD	[O-][N+](=O)C1=CC=C(C=C1)N2CCN(CC3=CC(=CC=C	0.313462	0.260897
CNOVTKOJJHFXXG	COC1=CC=C(C=C1)C2=CSC(=N2)N(CCCN(C)C)C(=O)	0.295609	0.257954
JFMVGTZHMZMOEEU	CN(C)CCCNC1(=O)C2=CC=CC3=CC=CC(C1=O)=C23	0.255108	0.232045
ITNTXIROIJKNAX	BrC1=CC(NC(=O)C2=CC=C(CN3CCC4=C(C3)C=CC=C	0.245546	0.239459

JPFBRBOZKXOCNQ	CC1CN(CC(C)N1)C2=CC(NCCOC3=CC=C(Cl)C=C3)=C	0.242815	0.230031
OWUUZSMCTWKDQE	CN1C2=C(C=C(C=C2))[N+](O)N(C)C1(C)C3=CC=	0.243938	0.239409
YTBVBKJJZHNJFF	CC(C)CCNC(=O)C1CCN(CC2=CC(OCC3=CC=CC=C3)=	0.264955	0.230456
CXXRTSRZMBHJJR	COC1=C(C=CC=C1)N2CCN(CC2)\N=C\3=CC(Cl)=CC	0.265669	0.229968
KFJQYKWOBSTTA	CC\N=C(/S)N1CCN(CC1)C2=NC(CC)=NC3=C2C4=C(C	0.243886	0.227567
VKBQZSAOIDUDJG	[O-][N+](=O)C1=C(\C=N\N2CCN(CC3=CC=CC=C3)CC	0.247747	0.231705
NMOLJCFDAQVRFO	CCOC1=C(OC)C=CC(CNCC2=CC(OC)=CC(OC)=C2)=C	0.272902	0.271138
CVUOPNNMCJKVDV	CC(=O)OC1=C2C=CC=CC2=C(C=C1)N(C(C)=O)S(=O)(0.247363	0.234027
ZHTRWWCLHQXSRF	C(CN1CCOCC1)NC2=NC(NC3=CC=CC=C3)=NC(NC4=	0.27563	0.24245
DDUHHVSVZVKCPO	OC1=C(\C=N\NC(=O)CN2CCOCC2)C3=C(C=CC=C3)C	0.256681	0.229338
ROTPPERZHFRPH	COC1=C(OC)C=C(CN2CCN(CC3=CC4=C(C=CC=C4)C=	0.305103	0.270265
LYIBOGKIVCZEPH	CCN(CC)CCCN(C(=O)C1=CC=C(F)C=C1)C2=NC(=CS2	0.312641	0.29527
AOKXQURIGCNUKW	CCN(CC)C1=C2C=CC=CC2=NC(=N1)C3=CC=CC=C3	0.262014	0.23703
ZBCKEYDGRZTDT	CC1=CC(NC2=NC(=NC(=N2)N3CCOCC3)N4CCOCC4	0.262762	0.246976
ZRWBLXCLXQYXAH	COC1=C(C=CC=C1)N2CCN(CC3=CC=C(SC)C=C3)CC2	0.283411	0.256725
DHKXDKGYBXRQV	CCN(CC)CCCN(C(=O)C1=CC=C(OC)C=C1)C2=NC(=CS	0.321394	0.297017
WCGNEUNDEPMGTB	BrC1=CC=C(CN2CCN(CC3=CNC4=C3C=CC=C4)CC2)	0.264469	0.244928
PFNLTXPEWXUGPM	CCOC(=O)C1=CC=C(NC(=O)C2=CC=C(CN3CCC4=C(C	0.248925	0.227722
BNEVHZDJSBDRX	CC1=CC=C(NC2=C3C=C(C)C=CC3=NC(C)=C2)C=C1	0.265256	0.246169
NSPFQFRJDFLOGQ	COC1=CC=C(NC2=C3C=C(OC)C=CC3=NC(C)=C2)C=C	0.279839	0.254512
DJTKIILFRBLODT	[O-][N+](=O)C1=CC(=CC=C1)C2CC(=NN2C3=CC=CC=	0.253243	0.238519
ANYPJMIYSNMPB	C\C(=N/NC1=NC(C)=NC(=C1)N2CCCC2)C3=CC=C(f	0.2503	0.237766
RHOPKNAPSLGREM	FC1=CC(NC(=O)NC2=CC(Cl)=CC=C2)=CC=C1	0.243988	0.247151
OHNJUBVCPYDMTK	C1CN(CCO1)C2=CC=C(NC3=C4C=CC=CC4=NC(=N3)	0.279165	0.249215
ZZLSURCVZHTTQF	ClC1=CC2=C(NC(COC3=CC=CC=C3)=N2)C=C1	0.264009	0.246112
JMYLZKXFAKCSQR	CNC1=NC2=C(C=CC=C2)C(NCC3=CC=CC=C3)=N1	0.289783	0.263494
DAIKYBWCCHUQB	[O-]Cl(=O)(=O)=O.COC1=C/C=C(\C=C\1)/[N+]2=C/C	0.278911	0.304751
WTWQIRJUUIBKBL	BrC1=CC=C(C=C1)C(=O)NC2=CC3=C(OCCO3)C=C2	0.243561	0.227154
SBWIYNYNJAKRHN	CC1=CC(NC2=NC(=CS2)C3=CC=C(Cl)C=C3)=NC=C1	0.242974	0.226794
MZJMUFHIELJBQT	COC1=CC=C(C=C1)C2=CSC(=N2)N(CCCN(C)C)C(=O)(0.246853	0.223785
JMWXUYGKQRTIM	COC1=CC(OC)=C(CNCC2=CC3=C(C=CC=C3)C=C2)C=	0.25738	0.254915
PCUVKQPOGOOBGR	O=S(=O)(CCN1CCOCC1)C2=CC=C(OC3=CC=C(C=C3)	0.260815	0.241463
QCNHHYSOAGAKW	COC1=CC=C(CN2CCN(CC3=CC=C(C=C3)C(F)(F)F)CC	0.252662	0.225642
PFYOKZAFMIWTQL	CC1=CC(C(C2=CC=C(O)C=C2)C3=CC(C)=C(O)C=C3C)	0.260619	0.233066
XUGVAQQYXUOUNN	CCOC1=C(Cl)C=C(CNC(S)=NC2=CC=CC=C2)C=C1	0.254128	0.229408
GNAOYSCNQZGVBP	FC1=CC=C(CNCCC2=CNC3=C2C=CC=C3)C=C1	0.276638	0.261634
OAOXDMSWICFKHW	COC1=CC(OC)=C(CN2CCN(CC3=CC=C(C=C3)C(F)(F)F	0.245846	0.235279
KSUUNRFHOPONSZ	C\C(=N/N=C(\N)S)C1=CC(=C(S1)C2=CC=CC=C2)C3=	0.289136	0.273566
XUXFFVQPCZGDK	CCN(CC)CCN1C(=N)N(CC(=O)C2=CC=C(C)C=C2)C3=	0.255332	0.223136
VNGZFJXEGLRVGO	CC1CN(CC(C)N1)C2=CC(NCCOC3=CC=CC=C3)=C(C=	0.299824	0.266885
KVNONDCPTRPNHC	[O-][N+](=O)C1=CC=C(CN2CCN(CC2)C3=CC=C(C=C3	0.291474	0.268684
CTZRVLWWCNVIHZ	CCN(CC)CCCN(C(=O)C1=CC=CO1)C2=NC(=CS2)C3=(0.276061	0.239755
KGUZRVWUOOZVMN	Cl.CN(C)CCCN(C(=O)C1=C/C=C\O\1)C2=N/C(=C\S\2	0.300779	0.31749
CBBLVOCYASNUSU	CN(C)CCC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC	0.32316	0.298162
MKFGMSIDXGIITI	CCN(CC)CCC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=	0.321864	0.295104
UEAVAZMVBWUWQR	CCN(CC)CCCN(C(=O)C1=CC=C(Br)C=C1)C2=NC(=CS	0.28295	0.26128
DVJDXLQARYGDAZ	CN(C1=CC(NC(=O)C2=CC=C(CN3CCC4=C(C3)C=CC=	0.249458	0.222466
LWUDFYXDCVQEFW	CCOC1=CC=C(NC(=O)NC2=NC(SCC)=NS2)C=C1	0.241107	0.235989

QPQSTQFEFGCFFU	CCN(CC)CCCN(C(=O)C1=C(F)C=CC=C1)C2=NC(=CS2)	0.291803	0.267314
XPGJDFWJFAUJKV	CCC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC=C(C)	0.267258	0.241836
CRWPLZXAAQIQKO	CN(C)CCC\N=C(/S)N1CCCN(CC1)C2=C(C=C3C=CC(C	0.267901	0.229224
ITOFQOOZDWVBAP	COC1=CC=C(C=C1)C2=CSC(=N2)N(CCCN(C)C(=O)(0.244953	0.241229
GJXFDRBSVMOVST	CCN1C2=C(C=CC=C2)C3=C1C=CC(CNCCCN4CCOCC	0.262394	0.225849
WXUSHHJQSJVXEJ	C\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC=C(Cl)C=	0.283617	0.280039
RQJOQECENSPTND	CC(C)C\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC=C(Cl	0.259028	0.267274
FPOFNQBKOEIEEA	COC1=CC(=CC=C1)C2=CSC(=N2)N3CCN(CC3)C(\S)=	0.268633	0.233444
FJVVYRIPCWAORAE	COC1=C(C=CC=C1)N2CCN(CC3=CC=C(Br)C=C3)CC2	0.2649	0.230953
XEMBTCUNACMZFD	C\C(=N/NC1=NC(C)=NC(=C1)N2CCOCC2)C3=CC=C(Cl	0.269162	0.281963
MFQPUFGHYQLDRC	C\C(=N/NC1=NC(C)=CC(C)=N1)C2=CC=C(Br)C=C2	0.256096	0.261139
ISEWSVBZRATECX	CC(C)(C1=CC=CC=C1)C2=CC=C(OCC(O)CN3CCCC3)(0.288373	0.255589
FABUNCRPUMHTPR	COC1=C(OC)C(CN2CCN(CC3=CC(Br)=CC=C3)CC2)=C	0.28326	0.279423
DZGJTWCDDKZSYKY	CN(C)CCC\N=C(/S)N1CCCN(CC1)C2=C(C=C3C(C)=C(Cl	0.257193	0.236726
YXMIIEYJAFIPM	O=C(CN1CCCCC1)NC(C2=CC=CC=C2)C3=CC=CC=C	0.261121	0.226038
LJSIXDJBHLLWHD	CN1CCN(CC1)C2=CC=C(NC3=C4C=CC(Cl)=CC4=NC=C	0.303473	0.271857
LICYPTOKHVLFLU	COC1=C(C=CC=C1)N2CCN(CC2)C(=O)C3=CC(=CC=C	0.243237	0.241719
AHRVABCWBXYVJE	COC1=C(C=CC=C1)\N=C(/S)N2CCN(CC2)C3=C(C)C(C	0.306042	0.260334
SGBITSSLZOCNAP	CCOCCC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC=C	0.275544	0.241787
FSKSDDYTVAGMMN	CCN(CC)CCC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=C	0.30875	0.285098
LFQZRGHJOLHCGV	[O-][N+](=O)C1=CC(=C(NC2=NC=C(Cl)C=C2)N=C1)[N	0.248934	0.240099
BWLWFTYUJPBAPC	CC1=C(Cl)C=C(NC2=NC=C(C=C2)[N+](O)=O)C=C1	0.242943	0.241708
RIVIXGROZDPFNF	COC1=CC=CC(OC)=C1C(=O)NC2=C(C=CC=C2)N3CC(C	0.242268	0.223825
UGHDYUBXCXCMFR	CCOC(=O)C1=C(NCCCN(C)C)C2=C(N=C1)C3=C(C=CC	0.251059	0.241319
VGBJXXVKWAWGRC	CCCC(=O)NC(C1=CC=C(OC)C=C1)C2=C3C=CC=CC3=	0.248125	0.222648
BITFYXYDSVPGFA	FC1=CC=C(C=C1)C2=NN(CC3=C(Cl)C=CC=C3)N=N2	0.289046	0.252435
RHMNEXKZSZPUMG	CN(C)CCCNC1=NC=NC2=C1C(C)=C(C)N2CCC3=CC=C	0.26258	0.238023
DLLSGBLSMPVTAR	CCN(CC)CCCNC(=O)C1=CC=C(S1)N2CCCC2)C3=C(Cl	0.269329	0.238105
MMXGXIVVWSANMS	CN(C)C1=CC=C(\C=N\NC2=NC3=C(O2)C=CC=C3)C=C	0.270965	0.26515
NPKZNTOZHCKVOH	SC(NCCN(C1CCCC1)C2CCCC2)=NC3=CC=CC(Cl)=C	0.334905	0.314792
OCVGPQWRSPURJS	CCCC(O)(C(CN1CCOCC1)C2=CC=C(Cl)C=C2)C3=CC=C	0.267496	0.241784
FGDPYKGIUAGQEH	CCCC1=NC(=CC(C)=N1)N2CCN(CC2)C3=CC=CC=C3	0.295107	0.266207
BKYIVNQKSIGXRM	CC1=CC(CN2CCC(CNC(=O)NC3=CC(Cl)=C(F)C=C3)C	0.281294	0.248541
VUDCRIRVGLIINY	CC1=C(C=C(N1)C2=CC=C(F)C=C2)C(=O)N3CCN(CC3	0.300976	0.269561
XPWPEKTXJVXIX	COC1=C(NC(=O)NCC2CCN(CC3=CC=C(Cl)C=C3)CC2	0.241063	0.224497
NNRMUSLLIKBBTF	FC1=C(CN2CCC(CNC(=O)NC3=CC(Br)=CC=C3)CC2)C	0.26263	0.226011
MBSXRUSJFAEHRG	CCCCN(C)CCNC(=O)C1=CC2=C(S1)N(C)N=C2C3=CC=C	0.267007	0.244239
YFGMDFJJYXETSM	COC1=CC(=CC=C1)C2=NN(C)C3=C2C=C(S3)C(=O)NC	0.274756	0.234538
KHRRAJSWMKPZAS	CCN(CCCNC(=O)C1=CC2=C(S1)N(C)N=C2C3=CC(OC	0.285433	0.264325
HXOVPCUOUQBBIK	COC1=CC(NC2=C3C=CC=CC3=NC4=C2CCC4)=CC(O	0.248682	0.222891
BQRLKZANJNANMD	CCCN(CCC)CCCNC(=O)C1=CC2=C(S1)C3=C(C=CC=C	0.269952	0.234701
XEVLACCZPZZGJT	CCCCN(CC)CCNC(=O)C1=CC2=C(C=C1)C(Cl)=C3CCC	0.253847	0.2363
AWLAVUPHQVCYJT	CCN1C(=O)C2=C(SC(=C2)C(=O)NCCN(C)C)C3=C1C=C	0.286126	0.243151
ZDJMLRLONVLBBO	CCCCN(CC)CCCNC(=O)C1=C/C2=C(S\1)/C3=C/C=C\	0.349234	0.310505
WDDVXGNECLUTE	CCN(CC)CCCNC1=NC2=C(C=CC=C2)C3=NC(=NN13)	0.257128	0.225153
YNYCCCCIGYKPGZ	CCN(CC)CCCNC(=O)C1=C(SC2=CC=C(Cl)C=C2)C3=C(Cl	0.267899	0.237876
SSZPKFQNZNKWCD	CCOC1=C(OCC2=CC=C(Cl)C=C2)C=CC(CNCC3=CC=C	0.290462	0.274933
IEBHUWAFPRHWNL	CC1=CC2=C(C=C1)N(CC(O)CN3CCCCC3)C4=C2CC	0.279333	0.238948

USPZQLNIMWQTEE	COC1=CC(NC2=C3C=CC=CC3=NC4=CC=CC=C24)=C	0.251094	0.238691
DAMPPXDFGMIGTC	CN1C(CNC2=CC=C(Br)C=C2)=NC3=C1C=CC=C3	0.252015	0.225225
UXDGHROWHOPKIL	CCN(CC)CCNC(S)=NC1=CC2=C(C=C1)N=C(C=C2C)N:	0.279293	0.237463
HDLNBEFFMKMYDP	CCCCN(CC)CCNC(S)=NC1=CC2=C(C=C1)N=C(C=C2C	0.242266	0.230409
CDPAADHJCKLJNH	CCN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)N(C)CC	0.283961	0.266213
ODOVHNYXEOQRDQ	CCCCN(C)CCNC(S)=NC1=CC2=C(C=C1)N=C(C=C2C)N	0.293734	0.252972
LGMULVZWLGRMPF	SC1=NC2=C(C=CC=C2)C(=O)N1CCCN3CCN(CC3)C4:	0.265665	0.230822
MQHUFUXBAXMQAM	Cl.CCOC(=O)C1=C(CN(C)C)/N(C)C2=C(O)\C(N=NC(N	0.260783	0.22417
VXJWCJHMLDRQIN	OC1=CC=C(C=C1)C2=CC(=NC(=N2)C3=CC=CC=C3)C	0.255147	0.231907
IXGFDLKNLSPKQB	COC1=C(OC)C(OC)=C(CN2CCN(CC3=CC(OC4=CC=C(C	0.258036	0.227316
SZXONIJERUCDDL	COC1=CC=C(NC2=C3C=CC=CC3=NC4=C2CCC4)C=C	0.271697	0.236232
RJXSUDNVAHALJK	CCOC(=O)C1=C(CSC2=CC=C(CC)C=C2)OC3=C1C(CN	0.246145	0.224565
BHRJLUKNGZIPRN	COC1=CC=C(C=C1)C(=O)ON=C(N)C2=CC=C(Br)C=C2	0.258284	0.245506
GYKXPGJPKYFFTF	COC1=C(CN2CCN(CC3=CNC4=C3C=CC=C4)CC2)C=C	0.291019	0.258203
GZNLWQYOQRHZNH	COC1=CC(OC)=CC(CNCCC2=CNC3=C2C=CC=C3)=C1	0.264446	0.246735
FQAMOSMBTRUACZ	CCN(CC)CCCCN1C2=C(SC3=C1C=CC=C3)C=CC=C2	0.347432	0.29707
GCJYJDOVBMBSCE	COC1=C\C=C(/C=C/1C)\C2=C\S/C(NC3=C/C=C\C(C)	0.262995	0.247234
BOLSJMUPEQCJLH	CCN(CC)CC(O)CN1C(C)=C(C2=C1C=CC(=C2)[N+][O-	0.307398	0.258852
FNYAPDXDSVIDFZ	CCOC(=O)C1=C(C)N(C2=C1C=C(OCCN(C)C)C=C2)C3	0.249572	0.252713
ZJFOKJSDQHKEQ	CN1CCN(CC1)C2=NC(NC3=CC=C(F)C=C3)=NC(NC4=	0.314444	0.281759
OWNLMVNSQNECB	CSC1=CC(NC(=O)C2=CC=C(CN3CCC4=C(C3)C=CC=C	0.270942	0.258924
UEJXPSAODFFJD	COC1=C(OC)C=C(C=C1)C(=O)ON=C(N)C2=CC=CC=C:	0.332315	0.315959
HGXVDDVKAGBVNC	COC1=CC=C(C=C1)C(CCNCC2=CC=C(C=C2)N(C)C)C3	0.324605	0.287457
ZSDFFIMGQOYQT	CC1CCN(CCCCOC2=CC=C(C=C2)C(C)C)CC1	0.243676	0.232134
GWIGKMUIRGDAEF	COC(\C(=N/O)C1=CC=C(Cl)C=C1)C2=CC=CC=C2	0.250606	0.23321
BQRGVCUSYIEHMO	CCCOC1=CC2=C(C=C1)C3=C(C=C(OCCC)C=C3)C2=N	0.260339	0.230681
XDYSRIVVDQDQIV	COC(=O)N1C2=C(CCC3=C1C=CC=C3)C=CC=C2	0.268464	0.230238
FIXJAWHYMVGEC	CN1CCN(CC1)C2=CC=C(NC(=O)C3=CC=C(OC4=CC=C	0.289519	0.255646
ONKKDYJXTGAGJI	FC1=C(CNC2=C3C=CC=CC3=NC(=N2)C4=CN=CC=C4	0.247664	0.235813
ZACALRGLMFHCPU	COC1=C(CN2CCN(CC2)C(C3=CC=CC=C3)C4=CC=CC	0.280904	0.255299
KUAIKNGLESWEFE	C(N1CCN(CC1)C(C2=CC=CC=C2)C3=CC=CC=C3)C4=	0.310114	0.275417
DAJYCBWDMVKA EZ	CCOC1=CC=C(CNCCN2CCCC2)C=C1	0.296464	0.274543
NTONURKZJLUF AV	CC1=CC(C)=C(C=C1)\N=C(/S)NCCC2=CC=C(Cl)C=C2	0.258772	0.228325
SXHRGEIXIVPHSL	N\C(=N/OC(=O)C1=C(C=C(Cl)C=C1)[N+][O-])=O)C2=	0.270797	0.261743
DFKUDGSHKQMFLA	Cl.ON=C1C2=C/C(OCCN3CCCC3)=C\C=C\2\C4=C\	0.293451	0.253346
OFZLIRIVOWNZBZ	FC1=C(NC(=O)C2=CC=C(CN3CCN(CC3)C4=CC=CC=C	0.258982	0.226497
NXKAANUEZJOF LD	BrC1=CC=C(C=C1)N=NNC2=CC=CC=C2	0.242323	0.236329
UDHPCSKJAVK OOC	COC1=C(OC)C=C(\C=N\NC2=NC(=CC(C)=N2)C3=CC=	0.245012	0.240536
DFBFIMGLDFNRJX	CC1=C(C=CC=C1Cl)\N=C(/S)NCCC2=CC=C(Cl)C=C2	0.254808	0.238297
JWJAVRXS B WYMIN	COC1=CC2=C(C=C1)C=C(C=C2)C3=NNC=C3	0.297934	0.308036
ZLNCFBWKFOHGP	CN(C1=CC=CC=C1)C2=C(Cl)C(C)=NC(=N2)C3=NC=C1	0.259798	0.239162
SGXGHCIPPADGCD	C(CN1CCCC1)NC2=C3C=CC=CC3=NC(=C2)C4=CC=	0.283139	0.266572
SFLCOJSXUPYSML	CC(C)N(C)C(C)C(=O)N1CCN(CC1)C2=C3C=CC(Cl)=C	0.266207	0.23671
BDPUNHHPOHJBAE	COC1=CC(\C=N\N=C(/S)NCCC2=CC=CC=C2)=CC(OC	0.279382	0.279879
CCROLCXCZVRR LJ	COC1=CC(=CC=C1)N2CCC3=C(C)N=C4C=CC(Cl)=CC	0.257403	0.224199
GWQBMMQQR FARIX	COC1=C(C=CC=C1)C2CCN(CC3=CC4=C(C=CC=C4)C:	0.260162	0.225976
XAGQUXXKPOLDOJ	CCOC1=CC=C(C=C1)C2=CN=C(NCC3=C4C=CC=CC4:	0.24713	0.235009
NXJHVBQTAW EKDP	COC1=C(CNC(C)CCC2=CC=CC=C2)C3=C(C=CC=C3)C	0.277862	0.266484

GTWXBYHHAIEPAP	CN(C)CCNC(=O)C1=CSC(NC2=C3C=CC=CC3=CC=C2)	0.262711	0.231908
JVFRFFOOSNRDIS	OC1=C(CN2CCN(CC2)C(O)(C3=CC=CC=C3)C4=CC=C	0.267078	0.238809
BTBCZXLAEONYQQ	COC1=CC(CN2CCN(CC2)C(C3=CC=CC=C3)C4=CC=C	0.269471	0.259361
FXOVIBPVLJUBH	CN(CCC1=CC=CC=C1)CC2=CNC3=C2C=CC=C3	0.256659	0.222555
JQQLPEVHIXSHCN	COC1=C(OCC2=CC=CC=C2)C=CC(CN(CCN(C)C)CC3=	0.32119	0.29487
MMRZDJRHCVDJCD	CC(C)N(CC(O)COC1=C(C=CC=C1)C(C)C)CC(O)COC2=	0.281974	0.259217
OWSNUUWZYRMBCB	CN(C)CCNC1=NC=NC2=C1C=C(S2)C3=CC=CC=C3	0.2808	0.25657
GHKCUYOQOJIXEZ	CC1=C2C=CC=CC2=NC(NCC3CCCC3)=C1	0.244754	0.227507
AGGRIJMWXCXMZIX	COC1=CC=C(CNC2=C3C=C(OC)C=CC3=NC(C)=C2)C=	0.2446	0.232475
LLAONCZFIOOLBA	ClC1=CC=C(CNC2=CC=C(C=C2)N3CCN(CC4=CC=CC	0.271471	0.245125
FAPGOSVHYQLFEO	CN1CCN(CC1)C2CC3=C(SC4=C2C=C(Cl)C(F)=C4)C=C	0.353638	0.316682
GPRZDPJGSSBXME	CN1CCN(CC1)C2CC3=C(SC4=C2C=C(F)C=C4)C=C(Cl	0.399864	0.349709
SCFLHZZHVEZKS	NS(=O)(=O)C1=CC=C(CCNCC2=C(OCC3=CC=C(Cl)C=C	0.298097	0.279203
AQGYXBXZRINPFW	CC(C)C1=CC2=C(SC3=C(CC2N4CCNCC4)C=CC(F)=C:	0.299594	0.265079
CQFNMVZADWUPL	[O-][N+](=O)C1=CC=C(C2=CN(N=C2)C3=CC=CC=C3)	0.288925	0.230312
LSQRYZDRBPWXTJ	CCOC1=CC=C(CNC2=CC=C(C=C2)N3CCN(CC4=CC=C	0.269269	0.235078
DYJAZHBRHRTIQO	FC1=CC=C(CNC2=CC=C(C=C2)N3CCN(CC4=CC=CC=	0.255243	0.237051
DMEJWDPKCIUKQG	COC1=C(OCC2=CC=CC=C2)C(Br)=CC(CNC(C)C3=CC=	0.275211	0.303427
HCGKUKCQPZDMJD	OC1=C(C=C(Br)C=C1)C2=CC=NN2C3=CC=CC=C3	0.268739	0.239903
LOGJTUFUBPRCNQ	COC1=C(OCC2=CC=C(F)C=C2)C(Br)=CC(CNC(C)C3=C	0.256258	0.261425
VJXKDSOBCYQHN	CC(C)(CO)NCC1=C2C=CC=CC2=CC=C1OCC3=CC=C(I	0.259879	0.234271
WADIXOUBCHKQIQ	BrC1=C(CN2CCN(CC3=CNC4=C3C=CC=C4)CC2)C=C	0.281891	0.240279
LSLZRFFCASZXC	CN(C)C1=CC(C)=C(C=C1)\N=N\C2=CC=C(N)C=C2	0.288329	0.251106
OAFFJWURAXUAAK	COC1=CC(=CC(OC)=C1OC)C2=CSC(NC3CCCC3)=N:	0.264493	0.242634
FAGWHYGBKPHGSL	CC1CN(CC(O)COC2=C(C)C=CC=C2)CCN1CC(O)COC:	0.270432	0.233705
IWELQSHVPPXCIO	CN(C)C2(CNC(=O)NC1=CC(Cl)=C(Cl)C=C1)CCCC2	0.320725	0.305035
CJYOGNCIFBDUBX	NS(=O)(=O)C1=CN=C(C=C1)N2CCN(CCOC3=CC=C(Cl	0.241089	0.222903
WQSJKFKDKTGKSBV	CC1CCCN(CC(O)COC2=CC=C(C=C2)C3=CC=CC=C3)(0.337028	0.282569
ITCUNKYUOLFRFB	OC(COC1=CC=C(C=C1)C#N)CN2CCN(CC2)C3=C(Cl)C	0.267257	0.238622
VYPZWWWVRCGDIMK	NC(N)=N\N=C\C1=CC(OCC2=CC=CC=C2)=C(OCC3=C	0.269251	0.237413
WIMVUYIMFDPRIH	SC(=NCCCN1CCOCC1)N2CCN(CC2)C3=CC=CC(Cl)=C	0.272001	0.259033
IMVTXWGTGSCGQI	COC1=CC=C(CN(C)CC(O)COC(C2=CC=C(OC)C=C2)C:	0.3157	0.295609
CMUPNGQUIBIZOF	COC1=C(C=CC=C1)N2CCN(CC2)C3=C4C=CC(Cl)=CC	0.31675	0.296756
WTRMIJZSVOYJC	CN(C)\C=N\C1=NC(=CS1)C2=CC3=C(C=CC=C3)C=C2	0.241473	0.230631
XECCJSKVKMPDOS	CCOC(=O)C1=C(C)NC(C(=O)OCC2=C(F)C=CC=C2)=C1	0.259761	0.238005
YJVPHQFVPIMSIN	C1CN(CCN1C2=NC3=C(C=CC=C3)C=C2)C4=NC=CC=	0.25588	0.245451
RYOMGTNXPFHBB	CN(C)CCCNC(S)=NCC(C1=CNC2=C1C=CC=C2)C3=C(0.265949	0.247633
ABROOOZQBGVEKG	COC(=O)C1=CC=C(OCC(O)CN2CCC3=C(C=C(OC)C(O	0.260255	0.235948
SYIBKYWIXGVQPD	COC1=CC=C(C=C1)C(NC(=O)C2=C(OC)C=CC(OC)=C2	0.254309	0.22319
JUHKKAOQMHXTRE	COC1=C(OC)C=C(CCN(C)CC(O)COC(C2=CC=C(F)C=C:	0.315742	0.290537
RDKIYQXDMXFMCP	COC1=CC(CN(C)CC(O)COC(C2=CC=CC=C2)C3=C(C)C	0.272633	0.24423
BVENFMNYIOTMEI	CCOC1=CC=C(CN(C)CC(O)COC(C2=CC=C(OC)C=C2)C	0.300889	0.285562
UINVHAHNSNAZSP	CC1=CN=C(NC(=O)NCC2CCCC(CNC(=O)NC3=NC=C(I	0.239986	0.223535
PHDGPLDNPCUCGA	COC1=C(OC)C(OC)=C(CN(C)CC(O)COC(C2=CC=CC=C	0.297088	0.264962
IFTXFDVOSCKHCK	COC1=C(OC)C=C(CN(C)CC(O)COC2=CC=C(C=C2)C3=	0.299978	0.25648
GRILGNVIUNFCMS	COC1=CC=C(C=C1)C(OCC(O)CNCCC2=CC=CC=C2)C:	0.253033	0.248936
IOTJPQOUWORJET	CN1CCN(CC1)C2=CC(C)=C(NS(=O)(=O)C3=CC4=C(C:	0.305859	0.291788
SZRWUQVACAZGHO	COC1=CC=C(\C=C\C(=O)NC2=C(C=CC=C2)C(=O)NCC	0.255797	0.25382

FFZANWWIWPKASH	CN(C)CCCNS(=O)(=O)C1=CC=C(C=C1)N2CCN(CC3=	0.265825	0.239189
VKDMQKVSBOCZIQ	CCCCNC(S)=NCC(C1=CNC2=C1C=CC=C2)C3=CC=CC	0.255725	0.230828
AOHPZXYMKDSMLT	CCOC(=O)C1=C(C)C(C(=O)OCC2=C(F)C=CC=C2)=C(C	0.258615	0.260148
UQZPLFLUUGHBOA	CN1CCN(CC(O)COC(C2=CC=C(Cl)C=C2)C3=CC=C(Cl	0.258891	0.240347
YVJFWWZNCXDTNS	CC(N(C)CCOC1=CC=C(Cl)C=C1)C(=O)NC2=C(C)C=CC	0.251341	0.226823
ZSDPRZMPVINHHO	BrC1=CC=C(C=C1)N2C=NC(=C2)C3=CC=CC=C3	0.251624	0.230423
CEOHLJLDAZQMNT	ClC1=C(Cl)C=C(NC(=O)NCC2CC2(Cl)Cl)C=C1	0.240818	0.227274
ZJODBUNAXOHTHH	COC1=C(CN(C)CC(O)COC2=CC=C(Br)C=C2)C=C(Br)C	0.32022	0.28266
BQQIGHILYUCELW	OC(CNC1CCCCC1)COC2=C3C=CC=CC3=CC=C2	0.288645	0.290629
JBKKGKCIZZUFNE	OC1=C(C=CC=C1)N2CCN(CC2)C3=NC=NC4=C3C(=C	0.273542	0.245264
LHUOLVDDERDQNF	COC1=C(C=CC(SC)=C1)C(=O)NC2=CC3=C(CCC3)C=C	0.245107	0.237331
YOHYDILJABSZKI	CC1=NC(N\N=C\C2=CC=CC=C2)=NC(=C1)C3=CC=CC	0.268847	0.263003
QIZKKBWPVZSWAD	COC1=CC=C(C=C1)N2CCN(CC2)C3=C4C=C(OC)C=C(0.315937	0.273654
SGDQPSJNELHSAJ	COC1=CC2=C(C=C1)N=C(C)C=C2NCC3=CC(=CC=C3)	0.267778	0.225
JGPZOOUILAFLSU	COC1=CC2=C(C=C1)N=C(C)C=C2N3CCN(CC3)C4=C(0.294979	0.244884
GSIQYCKOUGIZQC	COC1=CC(NC2=C3C=CC=CC3=NC(=N2)C4=CC=CC(=	0.263504	0.258078
UVNVEKUILAKEEW	CCN(CC)CCNC(=O)C1=CC=C(NC(=O)C2=CC(OC3=CC	0.266935	0.26273
KFEZGJFTVICLIJ	CN(C)CC(CCC(CN(C)C)C(O)(C1=CC=CC=C1)C2=CC=C	0.316038	0.299546
UOMQOXZSEIQJNP	OCl(=O)(=O)=O.CCOC1=CC=C(C=C1)C2=CC(C3=CC=	0.247025	0.246645
AWHOUECFNVCQJN	COC1=C(OC)C(OC)=C(CN(C)C2=NC=NC3=C2C=CS3)	0.296817	0.24913
ZIBPFPDJVNOBOW	COC1=CC=C(C=C1)C2=C(N=C(S2)N3CCN(C)CC3)C4=	0.288785	0.282861
XQVFAYFYLYUCUM	COC1=CC=C(CCNCC2=CC=C(OCC3=CC=CC=C3)C=C:	0.279679	0.251392
AXZKBTZTOYIHSX	CN(C)CCNS(=O)(=O)C1=CC=C(C=C1)N2CCC3=C2C=	0.283178	0.252628
XDBUTLHMCHHUGS	OCCCNCC1=CC=C(C=C1)N(C2=CC=CC=C2)C3=CC=C	0.262936	0.249505
UJRNCRJRODDDSH	COC1=CC=C(OCCN2CCN(CC2)C(=O)C3=CC(OC)=C(C	0.255843	0.242394
CCQDRGSVHATBMH	COC1=CC=C(C=C1)N2CCN(CC2)C3=NC=NC4=C3C(=	0.260606	0.228048
ANHZFWMMEHONEN	SC(=NCCN1CCOCC1)N2CCN(CC2)C3=CC=CC(Cl)=C3	0.245683	0.235059
VGXUBWBZIFNJAK	COC1=CC=C(C=C1)N2CCN(CC2)C3=NC=NC4=C3C(=	0.26222	0.225279
JVCNICMRHFNHMP	CC(C)C1=CC=C(C=C1)C2=CSC3=C2C(=NC=N3)N4CC	0.27493	0.246342
WIQVPSDSSXAQHC	CN(C)CCSC1=NC2=C(C=C(C)S2)C3=CC=C(F)C=C3)Cl	0.276434	0.241403
HYVZDOGMSWPIJR	CN(C)CCCNS(=O)(=O)C1=CC=C(NC2CCCCC2)C=C1	0.272361	0.235184
RXMRVUXDYLSHTD	CN(CC1=CC(=O)OC2=C1C=CC(C)=C2)CC3=C(C)C=C	0.249331	0.238378
NXVPKVZFHONGSO	CCS(=O)(=O)C1=CC2=C(OC(NC3=C(Cl)C=CC=C3)=N2	0.250667	0.23679
XORTWRWOUJPGVIK	CN(C)C1=CC=C(C=C1)\N=C\C2=CC=CN2C	0.253738	0.225513
VJTTVMHLSVNJCE	BrC1=C(C=CC=C1)C2=NN=C(COC3=C(C=CC=C3)C#N	0.243439	0.236647
YZFDYAPPWGHIE	CCC1=CC=C(CN(C)CC(O)COC2=C3C=CC=CC3=CC=C:	0.25561	0.229082
BXUKOIPKEOHXAA	CN(CC1=C(F)C=CC=C1)C2=C3C=CC=CC3=NC(=N2)C	0.248172	0.234137
OLUMAWOALAGELM	OC(COC1=C(Cl)C=C(F)C=C1)CN2CCC(CC3=CC=CC=C	0.244192	0.223077
JHLQDOPYNDWWEY	CCN(CC)S(=O)(=O)C1=CC(N)=C(C=C1)N2CCN(CC2)C	0.269021	0.240211
GRUMPROWLYTPSY	CN(C)C1=CC=C(C=C1)\N=N\C2=C(Br)C=CC=C2	0.246904	0.24601
GUMHGLZFULHKGGS	COC1=CC=C(OCC(O)CN(CC(O)COC2=CC=C(OC)C=C2	0.260188	0.23108
XECGRNUQFTZTKC	CC1=CC=C(C=C1)C2=CSC3=C2C(=NC=N3)N4CCN(C	0.264285	0.232479
XQHROMJMEVGBIZ	CCOC1=CC=CC2=C1N=C(S2)N(CCN(C)C)C(=O)\C=C\	0.264764	0.23229
DSDAMEGZKXSORM	CCOC1=CC=CC2=C1N=C(S2)N(CCN(C)C)C(=O)C3=C(0.265375	0.230586
ZMUKEKXXBRHBML	COC1=C(C=C2C=CC=CC2=C1)C(=O)N(CCN(C)C)C3=N	0.263903	0.23394
YJLYTSUDDPXUPO	CCOC(=O)C1=C(OC2=C1C=C(OCC(O)CN(C)C)C=C2)C	0.258821	0.223847
SIKHDKPKYMOGJ	ClC1=CC2=C(NC(=N2)C3=CN=C(Cl)C=C3)C=C1	0.239834	0.225844
NNULEIYGHDBJHH	COC1=CC=C(C=C1)C2=CSC(=N2)N3CCSCC3	0.272476	0.269237

FLLGZHLDRRHIKJ	COC1=C(N=C(N=C1)C2=NC=CC=C2)N(C)C3=CC=CC=	0.26659	0.257718
ZLXVPWOJUYRELC	CCCCNC(NCC1=CC(=CC=C1)C(F)(F)F)=NC2=CC=CC=	0.294055	0.253455
HMDIJVAOPRALJU	CSCC1=NC(=NC(=C1)N(C)C2=CC=CC=C2)C3=NC=CC	0.246916	0.23037
RSYCVESFMFLJAO	CC1=CC=C(CN2CCC(CC2)C3=CC(=NN3)C4=CC=C(Cl	0.333794	0.295448
DUQIPPKZDHSFNV	OCCN1CCN(CC1)C2=C3C=CC=CC3=NC(=N2)C4=C(C	0.267316	0.237186
HJQQHUQIDZOELS	COC1=CC=C(C=C1)C(C)NCCC(C2=CC=C(OC(C)C)C=C	0.2646	0.245885
RINUGOJBPTXRGQ	CC(C)CCCC(C)NCC1[C@H]2CC3C(=C)CCC[C@]3(C)(C	0.247997	0.222562
PDYBCZFHAOLDH	CN(C)C1=CC=C(C=C1)\C=N\N2C(S)=NN=C2C3CCCC	0.249306	0.222914
SEMBABNNFURFAZ	CC1=CC(C)=C(OCCCCN2CCC3=C(C2)C=CC=C3)C=C1	0.25782	0.251481
NGPSAIVNGUIZQR	CC(C)C1=C(OCCCCN2CCNCC2)C=C(C)C=C1	0.264875	0.239649
CKNCIEDFYBKWED	CCOC(=O)C1=C(N2CCN(CC)CC2)C3=C(N=C1)C(C)=C	0.246649	0.244552
VFCNYGFBZKCIW	COC1=CC=C(C=C1)C2=CSC3=C2C(=NC=N3)N4CCN(0.258856	0.237024
JFUUICKSJOTRHS	CC1=CC(Cl)=CC(C)=C1OCCCCN2C=CN=C2	0.243233	0.224225
PBFYXGZMUFFNNM	COC1=C2N=C(C=C(C)C2=C(OC)C=C1)N3CCCCC3	0.250272	0.224585
UJDWHTUENPHQKB	CCCN1C(=N)N(CC(=O)C2=CC=C(Cl)C=C2)C3=C1C=C	0.238775	0.223044
GZMRVEFNKBOYQH	CC(C)OC1=CC=C(C=C1)C(CCNCC2=CC=C(O)C=C2)C	0.263918	0.233468
JPEXNVDDTWRGBR	COC1=CC=C(CN2CCN(CC2)C3=NC=NC4=C3C(=CS4)	0.29089	0.268207
UISSSYMXXNFAVAB	COC1=CC=C(C=C1)C(CCNCC2=CC=C(C=C2)N(C)C)C	0.273225	0.241504
QBEPQNSUAFPEK	CC1=NC(=NC(NC2=CC(Cl)=CC=C2)=C1)C3=C(O)C=C	0.250378	0.232196
MSYMTZURVQYITF	COC1=C(C=CC=C1)C(CCNCC2=CC=CC=C2)C3=CC=C	0.275208	0.243135
NIOBXJAUQMLYQK	COC1=C(OC)C=C(CNCCC(C2=CC=C(OC(C)C)C=C2)C3	0.2811	0.267078
GHCVIPZFNLGPE	COC1=CC=C(CNCCC(C2=CC=C(OC(C)C)C=C2)C3=C(C	0.283517	0.26699
ZWAQPQWYVAMZOD	COC1=C(OC)C=C(CNCCC(C2=CC=CC=C2)C3=CC=C(C	0.276467	0.25612
ZMBOEIGIAUJKY	CC1=CC(CN2CCC3=C(C2)NC4=C3C=CC=C4)=CC=C1	0.267761	0.229524
TYPGOIVFIGRRQL	CN1C(=N)N(CC(=O)C2=CC=C(F)C=C2)C3=C1C=CC=C	0.26701	0.252406
NWNMBTJQRYWWPQ	OC(CN1C2=C(C=CC=C2)C3=C1C=CC(Br)=C3)CN4CC	0.278612	0.251331
WCVBRQCZDPBUIL	Cl.CC(C)CC1=C/C=C\C=C\1)C(C)C(=N)NCCC2=C/C=C	0.28829	0.268562
FLWNDNXNAFAHLN	COC1=CC=CC(OC)=C1OCCN2CCN(CC2)C(C3=CC=CC	0.29075	0.285319
OUIDHMRCLSZNME	CC(C)(C1=CC=CC=C1)C2=CC=C(OCCN3CCCC3)C=C2	0.297164	0.267947
RAEBDRHINKPDEM	ClC1=CC(OCCCCN2CCNCC2)=C(Cl)C=C1	0.323579	0.281272
AETVFPDBNPBKCG	CC(C)(C)C1=C(OCCOCCN2CCCC2)C=CC(Cl)=C1	0.282953	0.263072
QAHFCUQWQJAXMZ	COC1=C(OC)C=C(C=C1)C2=NC(NN)=NC(=C2)C3=CC	0.292801	0.281221
SOSROGHMSDAWKN	[O-][N+](=O)C1=CN=C(C=C1)N2CCN(CC3=CC4=C(OC	0.252441	0.223915
XRVVLMFVYFIAP	CN1C(=NC2=C1C=CC=C2)N3CCN(CC3)C(C4=CC=CC	0.293959	0.274911
SESXXNVJLXTYNC	COC(=O)\C=C1/N=C(NC2=N/C(C)=C3/C=C(OC)\C=C,	0.251368	0.308166
PBCZNIHRKHYSO	CC1=NC(=CS1)C2=CC=C(C=C2)C(=O)NC3=CC(F)=CC	0.250712	0.243673
ASTRBBDWJBPONC	COC1=CC=C(OCC(=O)NC2=C(C=CC=C2)N3CCCCC3)	0.25887	0.241745
XNPJVJWSJESDM	COC1=CC=C(OCC(=O)NC2=CC(Cl)=C(C=C2)N3CCN(C	0.241193	0.224531
BNWICQIQHOIRBP	CCOC1=CC=C(C=C1)S(=O)(=O)N2CCCC(C2)C(=O)N3	0.243312	0.224846
VUAJRKGGPPHDMSA	COC1=C(OC)C(CN(C)C(=O)C2=CC(=CC=C2)S(=O)(=O)	0.259903	0.227571
MDLXVKUVUOTCHM	CC(NC(=O)C1=CC(=CC=C1)S(=O)(=O)N2CCN(CC3=C	0.248316	0.232157
YRENCYSKNXJWAW	CCN1CCN(CC1)C2=C(NC(=O)CC3=CC(Cl)=C(Cl)C=C3	0.257365	0.222666
ULTXJTNKVGFMZJ	CCOC1=C(C=CC=C1)N2CCN(CC2)C3=NC=NC4=C3C	0.282172	0.245601
XAKSZJOYEUDHOK	ClC1=C(COC2=C(C=CC=C2)C(=O)NC3CCN(CC4=CC=	0.258826	0.240336
JUXUSGAZQWXVOV	CN(C)C1=NC=NC2=C1C=C(S2)C3=CC=CC=C3	0.251736	0.228045
ONEWYKJLXUUHJT	COC1=C\C=C(/C=C/1)\C2=C\SC3=N\C=N\C(N4CCN	0.368732	0.313066
CQVBKWSQOMDHSP	COC1=CC=C(C=C1)C2=CSC3=C2C(=NC=N3)N4CCN(0.256245	0.238341
VRUKLCFOWMVSAO	CN(C)C1=NC=C(C=C1)C2=C(ON=C2C3=CC=CO3)C4	0.283738	0.24376

GQIURKFIXVCNMB	COC1=C(F)C=C(COC(=O)C2=C(C=CC(=C2)[N+])([O-])=	0.260576	0.224659
KWRWXYSVOUTWAY	CC1CCN(CCC2=NC3=C(C=CC(NC(=O)COC4=CC=C(C	0.264599	0.239983
WNSYZUCOWVUFAM	CN1CCN(CC1)C2=CC=C(NC(=O)C3=CC4=C(C=CC=C4	0.263568	0.261459
SJIYBYGJOSWZBE	CCC1CCC2=C(C1)C=C(S2)C(=O)NC3CCN(CC4=CC=C	0.276769	0.23828
KCEMYSVFROXCSP	COC1=C(OC)C=C(NC(=O)COC2=CC=C(C=C2)N(C)S(=	0.257639	0.224826
FNZIQFHZOIRQGG	CCN1C=C(CN2CCC(CC2)C(=O)NC3=CC(=CC=C3)C4=	0.275932	0.256732
OGTZWHHAPGLLFZ	CC1=C(C(=O)N2CCN(CC2)C3=C(C)C(C)=CC=C3)C(=N	0.250795	0.223994
PWMIWEPTWWAQOX	BrC1=CC(NC(=O)C2=CC(OC(=S)N3CCOCC3)=CC=C2,	0.260474	0.235812
QONRQALSXOAUARD	CN1CCN(CC1)C2=CC=C(NC(=O)C3=CC=C(O3)C4=CC	0.260375	0.245352
ZHSXNWKLLXOUNW	CN(C)CCCNC1=C(N=C(O1)C2=C(CI)C=CC=C2)S(=O)(=	0.277188	0.258175
ICWQOMBLDBHQHC	CN1CCN(CC1)C2=C(NC(=O)C3=CC=C(O3)[N+])([O-])=	0.26262	0.226193
GOKLUMFHFBABDS	FC1=C(C=CC=C1)C(=O)NC(S)=NC2=C(C=CC=C2)N3C	0.243563	0.227292
GURGIAHFVKHWTL	CN(C)C1=C(N=C(O1)C2=CC=C(C)C=C2)S(=O)(=O)C3=	0.244946	0.229236
NWCRVUNKPIKMNQ	CC1CN(CCCNC(=O)C2=CC=C(NC(=O)C3=CSCCO3)C=	0.253803	0.239079
RJERXRUALHYQQU	[O-][N+](=O)C1=CC2=C(NC=C2S(=O)(=O)N3CCN(CC3	0.285299	0.257496
DARLBPMWSYXKLJ	CC(C)(C)OC(=O)N1CCC(CC1)C2=C(C=NN2C3=CC(CI)	0.270086	0.250664
KQWMLSKVICKNJX	ClC1=CC2=C(OCCN2C(=O)CCC(=O)NCCCN3CCC(CC	0.246696	0.22344
QRFXWUZQZNSJDZ	CC1CN(C(=O)CCC(=O)NCCCN2CCC(CC3=CC=CC=C3	0.286757	0.249795
OUCPPRBAYBUPGC	[O-][N+](=O)C1=CC(N2C=CC=C2)=C(C=C1)N3CCN(C	0.239632	0.237103
GYQNXYYQGNUDXME	CC1=CSC2=C1C(NC3CCN(CC4=CC=CC=C4)CC3)=NC	0.265606	0.24214
CFHYAXQWEYGRM	COC(=O)C1=C(N)C=C(S1)C2=CC=CS2	0.245111	0.229451
DAKBXCCNKUPXRY	COC1=C(OCC2=CC(=NO2)C(=O)N3CCN(C)C(C3)C4=	0.244454	0.226592
QYJVOLSFWOOVIO	CCC(C)N(CCNC(=O)C1=CC2=C(SC3=C(C=CC=C3)C(=	0.271395	0.234149
YPFSAMLWHLOEKP	CCN1CCN(CC1)C2=C(N=C(S2)S(C)(=O)=O)S(=O)(=O)(0.266639	0.245298
RKEKVGQXQNBGLM	COC1=C(C=CC=C1)N2CCN(CC2)C(CNS(=O)(=O)C3=C	0.267346	0.224918
ROIWSBGTSPIVISQ	CC(C)N1C=C(CN2CCC(CC2)C(=O)NC3=CC=C(OC4=C	0.276842	0.237068
WCOQTOBKVVBPZ	CCOC1=C(CI)C=C(CN2CCC(CC2)C(=O)NC3=CC(=CC=	0.273281	0.239337
YTBFIKLEWMMBR	CCN1C=C(CN2CCC(CC2)C(=O)NC3=CC(=CC=C3)C4=	0.295756	0.273155
JPHQP MJPTFSEGS	CN1C(CN2CCCC(C2)C(=O)NC3=CC=C(C=C3)C4=CC(I	0.286552	0.255164
GFFPMKFJDMVYCW	COC1=CC(=CC=C1)C2=CC=C(NC(=O)C3CCN(CCCN	0.268116	0.232567
GMHPZRMQJRBMJ	COC1=C(F)C=C(CN2CCC(CC2)C(=O)NC3=CN=C(OC4	0.252572	0.230882
OQMACQSNNKBGBJ	CC1=CC(OCC2=CC(=NO2)C(=O)NCCN3CCCCC3CO)=	0.255723	0.233516
AXBLXKUXVCHEBL	CC(C)C1=C(C=C(C=C1)C2=CC(C)=NO2)S(=O)(=O)N3C	0.261413	0.234503
APXUNOXFZGEJOZ	CCC1=C(C=C(C=C1)C2=CC(C)=NO2)S(=O)(=O)N3CC	0.241433	0.225005
WQVDJDGTAMSLE	CC1=C(C)C2=C(C=CC(=C2)C(=O)NCCCN3CCOCC3)N	0.25843	0.237658
MVJDCERCEUYUJL	COC1=C(C=C(C)C=C1)S(=O)(=O)NC2=CC(=CC=C2)C3	0.258292	0.226991
DBUXPKRXRIUEDD	CC1=C(C)C(=CC=C1)N2CCN(CC2)C(=O)CCC(=O)N3C	0.249329	0.225458
MNTSZSWLQUKGCT	COC1=CC(CCN2CCC(CNS(=O)(=O)C3=C(C)C=CC(=C3	0.285195	0.241452
UZDHAKOABAIRTB	COC1=C(C=C(C=C1)C2=CC(C)=NO2)S(=O)(=O)N3CC	0.241982	0.222972
FXEYUBCEWXHJAV	CC1=NOC(=C1)C2=CC(=C(C)C=C2)S(=O)(=O)NCC3C	0.280945	0.242747
RBYQLIMJHILDLF	CC1=NOC(=C1)C2=CC(=C(C)C=C2)S(=O)(=O)NCC3C	0.3029	0.268549
HQCBHCQGBWTZLG	CN1C(C)=C(C)C2=C1C=CC(=C2)C(=O)NCCCN3CCN(C	0.250963	0.232185
MNLJQFJILWSOQS	CN1C(C)=C(C)C2=C1C=CC(=C2)C(=O)NCCCN3CCN(C	0.25561	0.235455
PZHQTEVQGUAXTM	CCN1N=CC(CN2CCCC(C2)C(=O)NC3=CC(=CC=C3)C4	0.256679	0.238404
XQXZJYVDFJINN	CCOC1=C(CN2CCCC(C2)C(=O)NC3=CC(=CC=C3)N4C	0.29219	0.259501
WQVWVOQQWVSDKX	CC(C)N1C=C(CN2CCC(CC2)C(=O)NC3=CC(=CC=C3)C	0.271597	0.240104
WRBVNQAJRKFPO	CC1=CC(=NO1)C(=O)NC2CCCC3=C2C=NN3C4=C(C)	0.260763	0.223377
SNLRHQHRYPTMF	ClC1=CC(=CC=C1)C2=CC(NC(=O)C3CCN(CC4=NC=C	0.266686	0.26847

VZHPQIXNLKUDII	COC1=CC(=CC=C1)C2=CC=C(NC(=O)C3CCCN(CC4=C	0.268242	0.235303
VTGKECSOVZGDFJ	FC1=CC(=CC=C1)C2=CC=C(NC(=O)C3CCCN(CC4=NC	0.253536	0.231503
BCYNSARSDGREIL	CCN1C=C(CN2CCCC(C2)C(=O)NC3=CC(=CC=C3)C4=	0.276897	0.256473
RTFURTSIKJGZHS	CCN1C=C(CN2CCCC(C2)C(=O)NC3=CC(=CC=C3)C4=	0.276515	0.245546
QOBPFWGFVDFD	CN(C1CCN(C)CC1)S(=O)(=O)C2=CC=C(NC(=O)COC3=	0.265281	0.228808
PKMGMNUTKUDDHG	CN1CCN(CC1)C2=CC(C)=C(NC(=O)C3=CC=C(O3)C4=	0.251086	0.222579
NHCILWCCBOHEKL	COC1=CC=C(NS(=O)(=O)C2=CC(=CC=C2)C(=O)NC3C	0.266214	0.236759
DEMRCDDXWGUKEH	CN(C)C(CNC(=O)CCC1=NC2=C(C=CC(CI)=C2)N(CC3=	0.258137	0.227737
XUBMWKYFGUSFCT	CCOC(=O)C1=C(C)NC(C(=O)OCC(=O)C2=CC=CC=C2):	0.277382	0.250195
VOYVDQIPUWRVSF	COC1=C(C=CC=C1)C(CNC(=O)C2=CC=C(O2)C3=C(CI	0.298533	0.267317
UIIYWPIRVFKBBM	CC(OC1=CC=C(Br)C=C1)C(=O)NC2=C(C=CC(CI)=C2)N	0.325593	0.288986
UKTSXBGQGMWYDJ	COC1=C/C(NC2=N/C3=C/C=C\C=C/3\N=C\2NS(=O)I	0.295167	0.282005
PVOMHWQKAKFWDU	CCCC1=NC=C(CN2CCCC(C2)C(=O)NC3=CC=C(C=C3)	0.265879	0.232662
FACJLGXUVVXWOR	CC(OC1=CC=C(Br)C=C1)C(=O)NC2=CC=C(C=C2)S(=C	0.271397	0.234845
FLHNXQCEOOJUGR	COC1=CC=C(OC)C2=C1SC(=N2)N(CCN(C)C)C(=O)\C:	0.256595	0.23666
NWCMEBYXDVYBII	CCN(CC)CCN(C(=O)C1=C(OC)C=C2C=CC=CC=C1)C:	0.26087	0.232354
VVZZSLWVHYPDP	COC1=C(C=C2C=CC=CC2=C1)C(=O)N(CCN(C)C)C3=N	0.25017	0.227626
HGQLWRCILKLOMM	ClC1=CC=CC(CI)=C1CN2C=CC(=N)C=C2	0.2797	0.238828
AWNLVKPHFGNVQD	CCCN1C2=C(CCC2)C(=N)C3=C1CCC3	0.264624	0.241656
MPVBHEQNIQZVJXP	CCCCCCCCCN1C=CC(=N)C=C1	0.252573	0.238657
OKCJSJRJQAGPQL	CCCCCCCCCN1C=CC(=N)C=C1	0.269885	0.256066
YKTGLPHPYRTGRT	CN1CCN(CC1)\N=C\C2=CC=C(OCC3=CC=CC=C3)C=I	0.255406	0.242863
UOFDUGZZJBYOJI	COC1=C(C=CC=C1)C(=O)ON=C(N)C2=NC=CC=C2	0.260643	0.264105
POANTKOHXPOYEB	CCN(CC)CCN1C(=N)N(CC(=O)C2=CC=C(Br)S2)C3=C1	0.26626	0.222658
REJSIUIKZYMFQW	[O-][N+](=O)C1=CC=C(C=C1)C2=NC3=C(C=CC=C3)C(0.270165	0.24438
USHNXZAJLJZIKS	COC1=C(OC)C=C(C=C1)C(N)=NOC(=O)C2=C(C)ON=C	0.283756	0.282629
HUCFCNNWKPUVBP	ClC1=C(OCC(=O)NC2=CC=C(C=C2)N3CCN(CC3)C(=C	0.241326	0.227834
VYNPOQSODVQHKP	COC1=C(C=CC=C1)C(=O)NC2=C(C=CC=C2)N3CCN(C	0.250976	0.226619
FJVJXNJFZGWPCD	CN1CCN(CC1)C2=C(NC(=O)C3=CC=C(O3)C4=C(C=C	0.248365	0.222326
IDBAMXHGGSWDOD	CN1CCN(CC1)C2=C(NC(=O)\C=C\C3=CC(F)=CC=C3)I	0.247653	0.243796
BAHWXLHTUVXXKN	CN(CC1=CC=CC=C1)C2=CC(CC(C)C)C2)=[N+]3CCCC	0.257886	0.230681
QUMDSKWDUIUZNB	CCN1CCN(CC1)C2=C(NC(=O)COC3=C(CI)C=C(F)C=C:	0.259902	0.225475
QZDNACUTXRZZHL	CCC1=CC=C(C=C1)C2=NC(CS(=O)CC(=O)NCCN3CCC	0.241077	0.233448
XZGTYZZQPLODGY	CC1=C(CS(=O)CC(=O)NCCCN2CCN(CC3=CC=CC=C3)	0.252239	0.234081
DMUBBYXIJZVCFD	CC1=C(CSCC(=O)NC2CCN(CC3=CC=CC=C3)CC2)N=C	0.261086	0.238502
XHMJOWSQIAUPAK	CC1=NC(NCC2=CC=CC=C2)=NC(N\N=C\C3=CC(F)=C	0.238658	0.226886
OFVWSWOGBFORDU	CC1=NC(NCC2=CC=CC=C2)=NC(N\N=C\C3=CC=C(F)	0.255495	0.254231
YIOUNHISXQMMEG	CC1=CC(C)=NN1C2=NC(N\N=C\C3=CC(CI)=CC=C3)=	0.263625	0.252844
HZCUSYUUMGSVCS	CC1=CC(C)=NN1C2=NC(N\N=C\C3=CC=C(Br)C=C3):	0.273162	0.249876
IONZMLSFEITLRK	CCCCOC1=C(CI)C=C(CSC(N)=N)C=C1	0.268619	0.246176
NPCBUTBQJRWYEU	CCN(CC)C(=O)C1=NN(C2=C1C3CCC2(C)C3(C)C)C4=	0.240676	0.234756
IAEAEBWWPMMKPU	CC1(C)C2C\C(=N/O)C(C)(CC12)[N+][([O-])=CC3=CC(=	0.259442	0.244116
SHTBCPUEULZIOI	OCl(=O)(=O)=O.C[N+]1=C(C=C(C=C1)C2=CC=CC=C2)(0.250067	0.2545
IEOBQTYHOHTUKL	COC1=CC2=C(C=C1)C(C)=CC(=N2)N3CCCCC3	0.249602	0.243357
KCELIRRYXRQITP	COC1=CC=C(C=C1)[N+]2=C3CCCCN3C(=C2)C4=CC	0.317155	0.311301
NIBYEUDXSSPXDT	COC1=CC=C(C=C1)[N+]2=C3CCCCN3C=C2C4=CC=C(I	0.296639	0.257865
SMHKYGNXTZSHHS	COC1=CC=C(C=C1)[N+]2=C3CCCCN3C=C2C4=CC=	0.258736	0.237287
KGGXBIFSHPETL	OCl(=O)(=O)=O.COC1=CC=C(C=C1)C2=CC(C3=CC=C	0.245538	0.256793

BQQZIJQIMNHCD0	CCC1=CC=C(C=C1)[N+]2=C3SCCCN3C(=C2)C4=CC=	0.247501	0.233716
LYNNCZMXICEEU	CN1CCN(CC1)NC(=O)C2=CN(N=C2C3=CC(Br)=CC=C	0.258817	0.229052
DVXAOTCGCJNNQD	COC1=CC=C(CCNC(S)=NC2CCN(CC3=CC=CC=C3)CC	0.278463	0.282083
ORONCDNHWTZLKC	CCN1CCCC(C1)OC(=O)C2=C3C=CC=CC3=NC(=C2)C4	0.244175	0.240997
CSEAICBGUWNOFL	CCOC(=O)C1=C(NC(=O)CN2CCN(C)CC2)SC(C(=O)NC	0.25759	0.251896
IWKLXNHIGJNDLO	COC1=CC=C(C=C1)C2CC(C)(NC3=C(N2)C=CC=C3)C4	0.266343	0.255723
HBZLTUAXQJAGCL	NC(=NOC(=O)C1=C2C=CC=CC2=CC=C1)C3=NC=CC=	0.251277	0.257188
BQGZWZUJISIWKHU	CC1(C)CC(=CC(C1)=[N+]2CCCC2)N3CCCC3	0.260823	0.251162
SZWJOMFGHPFQSN	CC1(C)CC(=CC(C1)=[N+]2CCCC2)N3CCCC3	0.267365	0.245986
LNUAAHAFAERZTED	CC1CC2(C)OC3=C(CC2C(C)C1CNCCN(C)C)C=CC=C	0.27376	0.28643
WYYJSVREMNIWIRS	COC1=C(C=CC=C1)N2C(=C[N+]3=C2CCC4=C3C=CC=	0.256884	0.235959
RZKJWHNLYVYZMI	[O-][N+](=O)C1=CC(CN2CCN(CC2)C3=NC=CC=N3)=C	0.239685	0.223352
AAMIRUAPNCAFAU	COC1=CC(OC)=C(Br)C=C1CN2CCC(CC3=CC=CC=C3)	0.27038	0.255461
FPYHIYCBCNOEIP	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC(OC)=	0.306374	0.283046
LYGAAHYMZHBKOM	CC(NCCCCOC1=C(C)C=C(C)C=C1)C2=CC=CC=C2	0.308465	0.275022
KFGUBVRIRRHLYD	C(CNCCC1=CC=CC=C1)COC2=C3C=CC=CC3=CC=C2	0.291241	0.283656
YXGRRKZZDIPOLM	CSC1=CC=C(\C=N\N2CCN(CC3=CC=C(CI)C=C3)CC2)	0.245691	0.240867
KQOGHJUNYNFRNT	CC1(C)CC(=CC(C1)=[N+]2CCCC2)N3CCCC3	0.271367	0.246667
FBLYJVKTJDEHJQ	COC1=CC=C(C=C1)C2CC(=NN2C(=O)CN3CCN(CC4=	0.264527	0.267831
XNBNJFWYXXSJGT	COC1=C(OCCCCN2CCC(C)CC2)C=CC(\C=C\C)=C1	0.27998	0.261477
GTXVYQKWOMIUNX	COC1=C(\C=N\N=C(S)NCCN2CCOCC2)C3=C(C=CC=	0.247877	0.240788
VDGSGEDIQNWBAS	CC1CCCCN1CC(O)COCCC2CC4CC(CC(C4)C2)C3	0.283765	0.250472
VCERLNGTLWEWPR	COC1=C(OC)C=C2CN(CCC2=C1)C3=NC(CN4CCCC4)	0.245055	0.242692
JEPORSKVSUFAPU	CC1CCN(CCCOC2=C(Br)C=C(CI)C=C2)CC1	0.260382	0.266579
PDSHQZBTONOLJP	CC1CCN(CCCOC2=C(CI)C=C(Br)C=C2)CC1	0.264173	0.258083
PWZLITFPKRHCIF	CN1CCN(CC1)\N=C\C2=CC=C(C=C2)N(C3=CC=CC=C	0.276293	0.291095
MRNDYULFWGWPRO	C(N1CCC(CC1)NC2=NN=C(CS2)C3=CC4=C(OCCO4)(0.25421	0.230616
LFQHTMSWDYZADE	CCN(\C(S)=N\C1=CC=CC=C1)C2=C3C=CC=CC3=CC	0.249802	0.244326
RMPUCWLQCSXYGC	CN(CC1=CC=CC=C1)C(=O)CN2CCN(CC2)C(C3=CC=C	0.260797	0.24958
RGFWHRXRCDUWIP	COC1=C(NC(=O)C2=C(CI)N=NC(CI)=C2)C=CC=C1	0.240209	0.24503
KZIWZOOEBFXZHH	CC1=C2C=CC=CC2=[N+](C=C1)C3=CC=CC=C3	0.239188	0.249605
ZYTZKHQYGJASAI	CC1=[N+](C)C(=CC(=C1)C2=CC=CC=C2)C3=CC=CC=C	0.290735	0.278364
NUIMACVJXPXSLA	CC1=CC=C(NP(=O)(NC2=CC=C(C)C=C2)NC3=CC=C(C	0.266626	0.255672
HQUYMWZHIKIES	CCOC1=CC=C(C=C1)N2C(=C[N+]3=C2SCC3)C4=CC=	0.245511	0.227234
ZMYLPJFGIDIKKI	COC1=C(C=CC=C1)C(\C)=N\N=C(S)NCC2=CC=CC=C	0.248499	0.235126
HTTXEKZUKHDEX	C\C(=N/N=C(N)N)C1=C(CI)C=C(CI)C=C1	0.303911	0.308711
VRNFMFWOARQBIL	CCN(CC)CCOCCOC1=C2C=CC=CC2=C(CI)C=C1	0.319134	0.306436
DSRUNNBBZOHHPD	CC1CCN(CCCOC2=C(Br)C=C(C)C=C2)CC1	0.293018	0.298585
AICNPCABIMNBQK	CN(C)CC(O)COC(C1=CC=C(CI)C=C1)C2=CC=C(CI)C=C	0.32596	0.291798
WYHUOAPUTIPIK	N\C(S)=N/N=C/C1=CN(CCC#N)N=C1C2=CC=C(Br)C=	0.243448	0.236165
YNOOKMFOMDSECL	CC1=C(\N=N\C2=CC=C(Br)C=C2)C(C)=NN1	0.258102	0.257247
VVNQQPUZUFMHKJ	CN(C)CCCN(CC1=CC=CC=C1)C(\S)=N\C2=CC(CI)=C(f	0.336826	0.31797
GUXRNCAQTWASOC	CC(C)C1=CC=C(C=C1)N2C(=C[N+]3=C2CCC4=C3C=C	0.242177	0.233145
MCNLXNKNZVFOEA	OC(CNCCC(C1=CC=CC=C1)C2=CC=CC=C2)COC3=CC	0.274304	0.280019
ZEFBGBNUVPLUCI	CCCN1CCC(CC1)=NNC2=C(C=C(C=C2)S(=O)(=O)N(CI	0.242158	0.222456
FMBVMBZAESFWFX	CC1=C(C=CC(OCCN2CCC(CC3=CC=CC=C3)CC2)=C1	0.24449	0.243843
MCLUGZKXPXGFEFR	CCC(=O)C1=C(OCCCN2CCC(CC3=CC=CC=C3)CC2)C=	0.284016	0.254773
AGIJYYOJJDOYET	N#CC1=C(OCCCN2CCC(CC3=CC=CC=C3)CC2)C=CC=	0.259126	0.228648

KAZDJDMKBIJSQB	[O-][N+](=O)C1=CC=C(OC2=CC=C(C=C2)C(=O)N3CC(0.252257	0.243925
JKXQZIHAEQBKON	COC1=CC=CC(OC)=C1OCCCN2CCC(CC3=CC=CC=C3	0.295212	0.273198
IKQRUNJCNLAWLM	COC1=CC(OC)=C(C=C1)S(=O)(=O)N2CCN(CCC3=CC=	0.271468	0.270142
CAIOAFRWOLEVOM	C\C(=N/NC1=NC(=CC(C)=N1)C2=CC=CC=C2)C3=CC=	0.297539	0.256866
JDFXORKCCZHUNF	CCOC1=C(O)C(CN2CCCC(C2)N3CCN(CC3)C4=CC(Cl	0.257504	0.238642
HGNOQQFCBMFMNQ	COC1=C(CN2CCC(CC2)C(=O)NC3=CC=C(C=C3)C4=C	0.255187	0.23514
AVLVKMUKWOULKR	COC1=CC(OC)=C(C=C1)C(=O)NC2=CC3=C(C=CC=C3	0.243967	0.233761
GNODRDHUYWDQJH	OCC2(CC1=CC=C(F)C=C1)CCCN(CC3=C(Cl)C=C(F)C=	0.251702	0.230161
COXBRPPASOVKAC	COC1=C(C)C=CC(=C1)C(=O)N(C)CC2CCN(CCC3=CC(0.260092	0.226456
HRTJDFZRPAYGEZ	NNC1=NC(=CC(=N1)C2=CC=CC=C2)C3=CC=C(Br)C=	0.261278	0.226674
SRWOANFVXCQHMS	CC1=CC=C(SCCSC2=NC=CC=N2)C=C1	0.241198	0.226183
MIEQTGGXHMZWBB	OC(COC1=CC=CC=C1)CN2CCN(CC2)C(C3=CC=CC=C	0.258394	0.236287
AHLCHIOKZHMFPB	CCN1CCN(CCOC2=CC=C(C=C2)C(C)(C)C3=CC=CC=C	0.270916	0.244708
CWCNWWYUPYPWGJA	O[C@@H]1CN(CC2=CC=C(C=C2)N3C=CC=N3)CC[C	0.265197	0.231768
FHTNWUJIGFCNA	COC1=C(C)C(C)=C(CN2CCN(CC3=NC4=C(C=C3)C=C(0.258173	0.235067
AZCDBPOTZGGHKF	CCN1CCN(CC#CCOC2=C(OC)C=CC=C2)CC1	0.241265	0.228396
ARUKTMULLAAOLS	ClC1=CC(C=O)=C(OCCN2CCC(CC3=CC=CC=C3)CC2)	0.244576	0.226595
DGUPKONDRZCVTL	COC1=CC(OC)=C(Br)C=C1CN2CCC3=C(C2)NC4=C3(0.265486	0.250586
QHMQAJKQNLVLL	CC(C)CC1N(CC2=NC(C)=CC=C2)CCC3=C1NC4=C3C=	0.262052	0.265522
VAFJZYVAGXXYFP	CCOC(=O)C2(CCC1=CC=CC=C1)CCN(CC3=C(OC)C=C	0.276201	0.250896
FNDDWFQDOPSAJL	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC(COC	0.265353	0.231998
GIZKJVMWCIFXCM	COCCN(CC1=C(C)OC(=N1)C2=CC=C(C=C2)C3=CC=C	0.254549	0.230487
DBMWZIWBWJMKMHC	COC1=CC(OC)=C(CN2CCCC(C2)C(=O)C3=CC=C(Cl)C	0.271969	0.253142
KJBVBKOUWYLTN	COC1=CC(OC)=C(C=C1)C(=O)NC2CCCN(CC3=CC=C(I	0.264513	0.2466
SKSCJXHJCNFGIP	COC1=CC(OC)=C(C=C1)C(=O)C2CCCN(CC3=C(O)C=C	0.274696	0.24233
FLGUEQLEOWFNPG	CC1=NN(C(C)=C1Cl)C2=CC=C(NC(=O)C3=CC=NC=C3	0.247597	0.230821
NBRUKEFADYTPPM	CN1CCN(CCCOC2=CC=C(C=C2)C3=CC=CC=C3)CC1	0.272872	0.264731
JEXKWZVWRFGTKD	COC1=CC(CN(C)CC2CCCN(CCC3=CC=C(F)C=C3)C2)=	0.376319	0.335049
JGNZDNGRHHYTMK	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=C(OC)C(0.285881	0.284463
GLWDHFPSJNICSX	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC(OCC	0.284803	0.238619
OXNNXZXOFWUOLX	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=C(O)C(O	0.282446	0.258756
WCIOXRVBDMJIRY	CC1CN(CCCOC2=C3C=CC=CC3=C(Cl)C=C2)CC(C)O	0.272017	0.257558
VKZUXKFTDPLPAS	CCC(C)C1=C(OCCCN(C)CC2=CC=CC=C2)C=CC=C1	0.254549	0.246462
WZBJENIOBSYDSR	CC1=CC(Cl)=CC(C)=C1OCCOCCNCC2=CC=CC=C2	0.24524	0.226695
PYSQGUGELWTMPU	CC(CCC1=CC=C(O)C=C1)NCCC(C2=CC=CC=C2)C3=C	0.342739	0.296925
GJRPTEZZYDDVJF	COC1=CC=C(CCC(C)NCCC2=C(Cl)C=C(Cl)C=C2)C=C1	0.283635	0.244573
JPXZWXZAHSVNB	CCCN1CCC(CC1)NC2=CC(OC)=CC(OC)=C2	0.270852	0.259889
QLPAJZWONBXDTG	CC(CCC1=CC=C(O)C=C1)NC(C2=CC=CC=C2)C3=CC=	0.265569	0.249118
JBDNRLFNOXESPO	COC1=CC=C(CC(C)NCCC(C2=CC=CC=C2)C3=CC=CC=	0.286529	0.247276
AOLFEVCPUHDWDH	NC(N\N=C\C1=CC=C(F)C=C1)=N\N=C\C2=CC=C(F)C	0.241145	0.226062
GBBGYHUYLONBJ	CC(C)C1=C(OCC(O)CN2CCC3=C(C2)C=CC=C3)C=C(C	0.302154	0.269815
FEHSPDGIMNPGSF	CC(C)C1=C(C)C=C(OCC(O)CNC(C)C2=CC=CC=C2)C=C	0.251009	0.229326
YHNQYEQBWINYML	CC1=CC(Br)=C(OCCCN2CCCC2)C(Cl)=C1	0.268236	0.258003
MAXODDXKVCZCAU	COC1=C(OC)C(OC)=C(CN2CCN(CC3C=CC=C(C)C=C	0.250698	0.245954
UOMUQAJKVVYJKR	CC1=CC(Br)=C(OCCCN2CCCC2)C(C)=C1	0.261186	0.238766
KYLDCBUDNVECC	COC1=CC=C(C=C1)C2=NC(CN3CCN(CC4=CC(Cl)=CC	0.250468	0.231972
CHVWMSPMCIYOG	CC(C)N(CCO)CC1=C(C)OC(=N1)C2=CC=C(C=C2)C3=(0.28657	0.290963
PCIPRUBBZSOJFK	COCCNC(=O)C1=CC(OC2CCN(CC3=CC=C(C=C3)C(C)	0.249815	0.230928

QKBQBZRKMWCREJ	FC1=CC=C(C=C1)N2CCN(CC2)C(=O)C3CCC(CNS(=O)	0.251826	0.232606
WMLYDIBRHRFUSH	CC1CCCN(CCCNC(=O)C2=CC3=C(S2)C4=C(OC3)C=C	0.253594	0.23085
CKKMJZYUHLRHM	CCOC(=O)N1CCN(CC1)C(=O)C2=CC3=C(SCCN3CC4=	0.253708	0.222643
JGZSGXTUCLJOMX	CN1CCN(CCCNC(=O)C2=CC3=C(SCCN3CC4=CC=C(F	0.241274	0.222733
QFGJRYXCULDYHZ	CN1CCN(CCCNC(=O)C2=CC3=C(SCCN3CC4=CC=C(C	0.254326	0.227512
BABGDNDVMSPQPZ	CCN1CCN(CCCNC(=O)C2=CC3=C(C=C2)C(Cl)=C4CC	0.286767	0.261154
SKRXFKGFKFOOKW	CCC1CCCCN1CCCNC(=O)C2=CC3=C(C=C2)S(=O)C4=	0.244499	0.225204
SQKDINORIMCUSU	CC1CCCN(CCCNC(=O)C2=CC3=C(C=C2)S(=O)C4=C(C	0.268601	0.25378
HVFPVNVZGVJZOV	CC1CC(C)CN(CCCNC(=O)CS(=O)CC2=C(C)OC(=N2)C:	0.280688	0.238846
QOMBVOFZPURYGG	CCOC(=O)N1CCC(CC1)NC(=O)C2CCCN(CC3=C(C)OC	0.247185	0.24
NBVQTGYWYLPEDO	CCOC(=O)N1CCC(CC1)NC(=O)C2CCCN(CC3=C(C)OC	0.26507	0.251153
WNQCXXKOTZBYGA	CC1=C(C)C(=CC=C1)N2CCN(CC2)C(=O)C3=CC(=CC=	0.285979	0.249725
LFOBRSPYTQPWCV	FC(F)(F)C1=CC(=CC(CCN2CCNC[C@H]2)CC3=C4C=C	0.259324	0.227879
WJJYRAQTLJJCNF	OC1=CC=C(C[C@H]2)CNCCN2CCC3=C4C=CC=C4=	0.274042	0.231893
FKUGFZNBSPHYHT	OC1=CC=C(C[C@H]2)CNCCN2CCC34CC5CC(CC(C5)	0.290954	0.243456
DIFKFIKRWZMOHH	ClC1=NC2=C(C=CC=C2)C3=C1C=C(S3)C(=O)NCCCN	0.239535	0.232218
PALAORSVCXZEFA	COC1=C(CN2CCCC(C2)C(=O)C3=C(SC)C=CC=C3)C(O	0.256329	0.250995
ZRTSDOXTEQTCCP	CCOC(=O)C2(CC1=CC(OC)=CC=C1)CCN(CC3=C(O)C(0.252741	0.225065
RQGVRIYROYVBIW	COC1=CC=C(NC(=O)C2=C(C)N(CC3=CC=CS3)C(C)=C:	0.244366	0.223618
VBNTYDSJLTWWID	FC(F)(F)C1=CC(Cl)=C(N=C1)N2CCN(CC2)C(\S)=N\CC	0.250198	0.228862
QCWZYJPDPROWAC	ClC1=CC(NC(=O)OC2CN3CCC2CC3)=CC=C1	0.238762	0.235773
YHONNHGZTNLOQR	CC1=C(CNC(=O)NC2=CC(Cl)=CC=C2)C(=NO1)C3=CC	0.294081	0.264296
WFLVKCLJXXUYGU	COC1=CC=C(CN2CSC(=S)N(CC3=CC=C(OC)C=C3)C2,	0.252967	0.2297
OWWCVXXHBITLBA	S=C1SCN(CC2CC2)CN1CC3CC3	0.25923	0.238014
NRQUAVYOAZGFFD	ClC1=CC=CC(Cl)=C1\C=N\NC2=C(Cl)C=NC=C2Cl	0.253793	0.263286
NFOGCEURFJXCRE	CC1=NC(=NC(OC2=CC=C(Cl)C=C2)=C1)C3=NC=CC(=	0.291144	0.257891
NWPLPOACXICHEB	ClC1=CC2=C(C=C1)C(=CC=N2)N3CCN(CC3)C(=O)C4	0.244981	0.232624
VCRGBXUBYNLNRI	CN1C(CSC2=C(C)NC3=C2C=CC=C3)=NN=C1SCC4=C	0.252302	0.256089
RYVDNKBIXSRLKF	CCOC(=O)N1CCN(CC(=O)NC2=C(C=C(CC)S2)C(=O)C:	0.250075	0.229737
BBQJERVLZYDMBV	C(N1CCSCC1)C2=CSC(=N2)C3=CC=CS3	0.27046	0.249558
UZZHGEWFVOTYDT	CC1=CC(C)=NC(\N=C(/N)NC2=CC=C(OC3=CC=CC=	0.27249	0.243643
ARMSHPQLBWTDEC	CCCCCCCCN1C2=C(CCC2)C(=N)C3=C1C=CC=C3	0.265322	0.22784
MRXPVZNUMFKYQT	COC1=CC=C(NS(=O)(=O)C2=CC=C(OC3=C(C=CC=C3)	0.267813	0.26917
CLCZTVMOKLEKO	CC(C)(C)C1=CC=C(C=C1)C(=O)NC2=CC=C(CN3CCS(=	0.243838	0.227962
JACFQTMRYXXVCX	COC1=CC=C(C=C1)C2=NNC=C2CN3CCC(O)(CC3)C4	0.291155	0.282903
VDYRINLHVJBFDA	CC1CN(CC2=CSC(=N2)C3=CC=C(Cl)C=C3)CC(C)O1	0.245287	0.23645
FSMVIBBHLWPBMC	CCOC1=C(OC2=C(F)C=NC(Cl)=N2)C=CC(\C=N\NC3=	0.240704	0.229467
LQJPHZXMKIKHMK	CCN(CC)C1=CC=C(C=C1)\C=N\NC2=NC(C)=CC(C)=N	0.272524	0.225564
BWYOTOAMUYEMBT	ClC1=CC=C(C=C1)C2=NC3=C(C=CC=C3)C(NCCCN4C	0.275294	0.237932
NFOJBMIMTCWPBX	COC1=CC=C(C=C1)[N+]2=C3CCCN3C=C2C4=CC=CC	0.282391	0.251367
ZPMLWCNMSTVVDE	CCC1(C)CC(CCNCC2=CC=C(C=C2)N(C)C)(CCO1)C3=	0.251506	0.233403
VSMBPTAACRCDOF	CN(C)CC(CCCCC(CN(C)C)C(=O)C1=CC=CC=C1)C(=O)	0.27641	0.244114
MTAUNVGSPWPEJS	COC1=C(O)C(=CC=C1)C2=NC3=C(C=CC=C3)C(=N2)N	0.266349	0.257434
LAMMKLVPNOMHMX	CCOC(=O)C1=C(CN2CCN(CCO)CC2)N(C3=C1C=C(O)	0.286902	0.251909
CLZSZXFWIQZEED	CCOC(=O)C1=C(CSCC2=CC=CC=C2)OC3=C1C(CN(C)	0.250397	0.245633
HXVLXVBIEVNEAI	FC1=CC=C(NS(=O)(=O)C2=CC=C(C=C2)C(=O)N3CCN	0.251077	0.232258
LPGPLBXMFLZLNY	CN(CC(=O)NC1=CC(=CC=C1)S(=O)(=O)NC2=NCCCC	0.265744	0.247572
NSBIQDPNYPJSLY	CN(C)S(=O)(=O)C1=CC(NC(=O)CN2CCC3=C(C2)C=CC	0.241224	0.223781

DTPXOPHEXZTIJV	CC1=CC=C(C=C1)S(=O)(=O)NC(C)(C)CN2CCC(CC3=C	0.267347	0.258843
PHSKGWBKURXITR	COC1=CC(O)=C(C=C1)C2=C(C3=CN(N=C3)C4=CC=C1	0.271078	0.240959
AIUYBISEZVZGCT	CC1=CC=C(C=C1)N2C=C(CN3CCC(O)(CC3)C4=NC=C	0.278107	0.259731
GQYOFTMNGJXJKO	CN1C=CN=C1CN2CCN(CC3=CN(N=C3C4=CC(C)=CC	0.297937	0.26921
ZRGMBGUBVCLYQ	CCN1CCC(CNCC2=CN(N=C2C3=C(CI)C=CC=C3)C4=(0.33463	0.324295
QFFCLOOUBDASLM	CC1=C(CN2CCC(CO)(CCOC3=CC=CC=C3)CC2)NC4=	0.240687	0.237114
LNEWQDFILQEPQS	C(CNCC1=CN=C1C2=C3C=CC=CC3=CC=C2)CN4N=	0.293704	0.281922
BWXVQCRKPHRWF	CN(CC1=CC=C(OCC(O)CN2CCCC2)C=C1)CC3=C4C	0.251128	0.226063
ZVVQHARLDKPBTD	CCC(CC)NCC(O)COC1=CC=C(Br)C=C1	0.247657	0.232807
LKSAYGICQRLOOE	COCC(C)\N=C(/S)NCCC1=C(CI)C=C(CI)C=C1	0.259951	0.229262
DWXSWTXNVTTWDK	COC1=CC=C(C=C1)C(CNC(S)=NCC2=CC=CC=C2)N3C	0.256302	0.241166
WMFATYUZVIJFRF	CC(C)C1=CC=C(C=C1)N=C2N=C(N)C3=C2C=CC=C3	0.252981	0.238443
OORGOYKNVOPPRY	ClC1=C2C=CC=NC2=C(OC(=O)C3=CC=CC=C3)C(CN4	0.243563	0.247567
OASGMNNTQISCE	OC(CNCC1(CCCCC1)N2CCCC2)COC3=C(CI)C=C(CI	0.258295	0.25376
CCJWRQJDAJKRW	CC1=C(CI)C=CC(OCCCCN2CCCC2)=C1	0.264688	0.246068
AYVPLULUJAHKKX	COC1=CC(OC)=C(NC(=O)C2=C3C=CC=CC3=NC4=C2	0.245782	0.239618
PNGOQSXNWXMLT	CN(C1=CC=CC=C1)C2=NC(N3CCCCC3)=C(C(N)=N2	0.244985	0.222736
QNFHCWXWQLNHQX	C\C(=N/N1CCN(CC2=CC=C(CI)C=C2)CC1)C3=CC=C(I	0.240014	0.253609
QTADTPSSBBVBQA	[O-][N+](=O)C1=CC(\C=N\N2CCN(CC3=CC=C(CI)C=C	0.26739	0.283421
CJMNNPHUGBJINN	COC1=C(C=CC=C1)N2CCN(CC2)\N=C\C(CI)=C\C3=C	0.28034	0.252085
GKDCYDHTHCBRLI	C\C(=N/N1CCN(CC2=C(CI)C=CC=C2)CC1)C3=CC=C(I	0.320304	0.328814
SWTMHBFDSGLJKE	NC1=C(C(NC2=CC(CI)=CC=C2)=NC(NCCCN3CCOCC:	0.265369	0.228365
TXSMRDKQYDZAO	OCl(=O)(=O)=O.CCOC1=CC=C(C=C1)C2=CC(C3=CC=	0.252279	0.268221
GGHVOBZSGLNUTN	OC(CNCCC1=CC=CC=C1)COC2=CC=C(OCC(O)CNCC(0.283613	0.251395
XITSNPPPOFRDTN	OCl(=O)(=O)=O.CCOC1=CC=C(C=C1)C2=CC(C3=CC=	0.250594	0.24352
FYKSUAVLSLEKNU	COC1=CC=C(OCC(=O)ON=C(N)C2=CC=C(OC)C=C2)C	0.299499	0.265177
PTTFBJMAXQDBBB	CC1=CC=C(O1)C=N\N2CCN(CC2)C3C4=C(C=CC=C4	0.250765	0.226551
CESGXMOSNLYWMO	O=C(CN1CCCCC1)NC2=CC=C(OC3=CC=CC=C3)C=C	0.24623	0.270643
YPVMVWFHOJLRSK	CN1C(CC(=O)NC2=CC=C(Br)C=C2)C3=C(CC1(C)C)C=	0.268624	0.250508
XWBHWYITYBXWOS	CN1CCN(CC1)C2=NC=NC3=C2C=C(S3)C4=CC=CC=C	0.294347	0.289633
ZLHWFOFDJUOUMH	COC1=CC=C(NC2=NC(CN3CCN(CC3)C4=CC=C(F)C=C	0.302261	0.262487
CKEIFXSNZGOKPW	CCC1C(NC(C(C)C1=NO)C2=CC=CC=C2)C3=CC=CC=	0.267964	0.242368
WXCGHDFZRVFFLV	CCCN1C(=NC2=C1C=CC=C2)N3CCN(CC4=CC=C(CI)(0.241457	0.237568
TYBAKKFHVSVDKH	COC1=CC(CN2CCN(CC3=CC=C(SC)C=C3)CC2)=C(OC	0.269203	0.273619
ZZFRROOYRMMSET	CC1=NC(N=C(N)N)=NC2=C(C)C=CC=C12	0.26533	0.241739
ASDMBUDPVLVAHA	COC1=CC=C(C=C1)N2CCC3=C(C)N=C4C(OC)=CC=CC	0.292048	0.28571
NFZVJHWAJYJGOY	CN1CCN(CC1)C2=CC=C(C=C2)C3=NC4=C(C=CC=C4	0.278393	0.259369
XYFRLVLKALKQQZ	COC(=O)C1CCN(CC2=CC=C(OCCCN3CCN(CC3)C4=C	0.260239	0.230887
HUNJLBDDZDWCKK	COCCCNCCC(CCC(C)C)C1=CC2=C(OCO2)C=C1	0.282553	0.252634
JBGHJXWBNDFTSA	CN(C)CCCNC1=C2CCCC2=NC3=C(C(C)=NN13)C4=	0.288982	0.266451
OWGLMKKLVSBNQO	CCN1CCN(CC1)C2=CC(=NC3=C(C(C)=NN23)C4=CC=	0.254957	0.232975
XMQCHSRAEXBLI	CC1=NN2C(N=C3CCCC3=C2NCCN4CCOCC4)=C1C	0.261232	0.231113
JMOFBGHQYQUSHG	CN(C)CCCNC1=CC(=NC2=C(C=NN12)C3=CC=CC=C3	0.239629	0.233864
GISIYNAFXBOWDC	CC1=CC=C(C=C1)C2=C[N+](CC3=CC(CI)=CC=C3)=C4	0.2569	0.26113
OBYWVKBVUSCYQS	CN(C)CCCNC1=NC(=NC2=C1C3=C(CCCC3)S2)N4N=	0.270503	0.246747
QELWKQFMKISWQR	CN(C)CCNC1=NC(=NC2=C1C3=C(COC(C)(C)C3)S2)N	0.265749	0.23
JEXXVBQPAVICRW	CCN(CC(=O)NC1=C(C=CC=C1)C2=CC=CC=C2)CC3=N	0.252206	0.235624
UNMDHILIMVHBQR	CCN(CC)CCNC(=O)C1=CC=C(NC(=O)C2=CC=C(CI)C=	0.249184	0.235051

ZEUJCYADFATLCX	NC(N)=NC(S)=NC1=CC=C(Cl)C=C1	0.27714	0.263459
XHNDJXVUEBFYGM	CC1=C(C)C2=C(N1)C=CC3=C2C=CC=N3	0.249907	0.228631
AJTPQUQBGRYBEE	C1NCC2=C3C=CC=CC3=CC=C2C1C4=CC=CC=C4	0.337474	0.290287
XLFUVMNKHCIQDM	CN1C=NC(=C1)SC2=CC=C(Br)C=C2)[N+](O)=O	0.252251	0.223628
SYLIEQPXLCNFKC	[O-][N+](=O)C1=CC2=C(OC3=C(C=CC=C3)N=C2)C=C	0.253406	0.232689
GUYLKDVAVXYBGJ	CS\C(S)=N\C1=CN=CC=C1	0.253795	0.246864
LISDNWVJPBZAES	COC1=CC=C(C=C1)C2=NNC(=C2)C3CCN(CC4=CC=C(0.263799	0.2401
XZRWTNCPHHCOSV	FC(F)(F)C1=CC(CN2CCC(CC2)C3=CC(=NN3)C4=CC=C	0.247942	0.236525
DKFBCULBTJRMBM	COC1=CC=C(C=C1)C2=NC(=NC=C2)C3=CC=C(O)C=C	0.252528	0.27386
FFBROMLEGXOUHZ	COC1=CC=C(C=C1)S(=O)(=O)N2C(C)COC3=C2C=CC=	0.248219	0.22579
NOPGOGLCTNBNT	CN1N=CC2=C1N=C(NC3=C(Cl)C=CC=C3)N=C2NC4=	0.253357	0.231839
BVTCELZGBMCJOG	COC1=C(C)C(C)=C(C=C1)C2=NC(CN3CCCC3C4=NC	0.261985	0.246452
NKVJFSGYMQEBRF	CN1C=CN=C1CN2CCN(CC3=CN(N=C3C4=CC=C(F)C:	0.27814	0.253552
BKWIAAHRGPGSJH	CN1C=CN=C1CN2CCN(CC3=CN(N=C3C4=CC(F)=CC:	0.261297	0.263301
HVQSTRGEJFIASM	COCCN(C)CC1=CN(N=C1C2=C(C)C=CC=C2)C3=C(F)C	0.240854	0.247228
JEJASUKMKLSUAG	COC1=CC2=C(NC(CN3CCC(CO)(CCOC4=CC=CC=C4)	0.254969	0.244162
LQILTFJSNUBKIM	CC1=C(CN2CCN(CC2)C3=C4C=CC=CC4=NC=N3)N=C	0.240454	0.233574
VUPZYWWTUXURLT	COC1=CC=CC(OC)=C1CN2CCCC(C2)C(=O)C3=C(SC)(0.279529	0.275708
ZVTIQPCPFQIKLD	CN(CC1=NC(CC2=C(Cl)C=CC=C2)=NO1)CC3=C(C)C=	0.272423	0.254967
RHHUEMKHXMZVIG	OC(COC1=CC=C(CNCCC2=CC=C(C=C2)C(F)(F)F)C=C1	0.2749	0.243953
ATLFDMCREQQYDN	CC(C)N(CC1=CN=C1C2=CC=C(C=C2)C3=CC=CC=C:	0.298228	0.278083
NGHHORJGYXYTFP	CN(CC1=NC=CN1)CC2=CN(N=C2C3=CC(C)=CC=C3)(0.292327	0.298266
SHPMMJCTFKAWSG	COC1=CC(OC)=C(C=C1)C(=O)C2CCCN(CC3=CC=CN3	0.280121	0.255535
SCKXXJKTIMSHFN	CC1=CC(C)=NN1CCNCC2=CN(N=C2C3=CC=C(F)C=C	0.284936	0.318493
LWWQELLQYMRXGU	COC1=CC=C(C=C1)N2C=C(CNCCC3=NC(C)=CC(C)=N	0.298839	0.268858
AZCGPYGJRIQRDE	CC(C)CCC1=NOC(CN(CC2=C(C)N(C)N=C2)C(C)C)=N	0.333518	0.327707
BJKHXRFRWQAEJY	OCC2(CC1=CC=CC=C1)CCN(CC3=CN=C(N=C3)C4=C	0.269714	0.242582
CRQIKGNLEOGTIN	CCOC1=CC=C(CN2CCN(CC3=C(C)C4=C(N3)C=CC(OC	0.272365	0.239301
ZFVPIXKVMQGBF	CN(CC1=CN(N=C1C2=CC3=C(OC3)C=C2)C4=CC=C	0.247279	0.247783
NXEZLRVOZPTHCO	FC1=C(C=CC=C1)C2N(CC3=CC=CN3C4=NC=CC=N4)	0.25786	0.237856
DPXMBHSCQSNZNF	CCN1C=C(CN2CCC3=C(NC4=C3C=CC=C4)C2C5=CC	0.255505	0.244387
FZZITNVNCBBRBU	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC(OC)=	0.298234	0.260206
SXOOYBILAWOAI	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC(=CC:	0.2896	0.25803
UFLOKYHSVZBTGE	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=C4OC(O	0.264064	0.24745
KTCKKCPJMYCGME	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC=C(C)	0.292606	0.286626
VTCZAKBGYDAQQS	CCOC(=O)C2(CC1=CC(OC)=CC=C1)CCN(C\C=C\C3=C	0.259105	0.240581
RPSOYZFVEBMXDL	CC1=CC=C(C=C1)C2(CCCC2)C3=NOC(CN4CCC(CC4	0.258556	0.247739
TXJZLJKSHRENRC	CCOC1=CC=C(C=C1)C2=NC(CN(C[C@@H]3CCC(=O	0.240256	0.246538
ZKQMCVOQCUTTRA	CCOC(=O)C2(CCCC1=CC=CC=C1)CCN(CC3=CN(CC)N	0.275591	0.265289
AAKWMGDOOVHENN	CCOC1=CC=C(C=C1)C2N(CCCN3C=CC=N3)CCC4=C:	0.287418	0.272472
WDDPZZJXKJWGGZ	CCOC(=O)C2(CCCC1=CC=CC=C1)CCN(CC3=CN=C(C)	0.270092	0.260165
FWCRHJYCKFZIAA	COC1=CC=C(C=C1)N2C=C(CN(C)C(C)C3=NC=NC=C3	0.313366	0.337073
UUIFWRRRIYLZGPG	CN1N=C(C)C(CN(CC2=C(C)OC(=N2)C3=C(C)C=CC=C:	0.242598	0.235796
URHPYQXCXXUSFX	COC1=C(C=C(F)C=C1)C(=O)C2CCCN(CC3=CN(C)C4=	0.261262	0.249949
HOMIBDDRDRDEFOM	CN1C=C(CN2CCN(CC2)C3=CC=CC(C)=N3)C(=N1)C4	0.295833	0.294717
NJDIJLHVGRJXHQ	CCN1N=C(C)C(CN2CCC3=C(NC4=C3C=CC=C4)C2C5	0.241632	0.241331
WTEOAHRLJGTWRZ	CC1=CC=C(C=C1)N2C=C(CNCCC3C=CC=N3)C(=N2	0.326539	0.286632
ZMNCFUGXZWTEJY	CCOC1=CC=C(CN2CCN(CC3=CN=C(S3)C4=CC=CC=C	0.258687	0.246593

FYLLKYZNUBYPTL	CCOC1=CC=C(CN2CCN(CC3=C(C)C4=C(N3)C=CC=C4	0.263892	0.241241
WLSLGSJWJNXZXCC	FC1=C(C=CC=C1)C2N(CC3=COC=C3)CCC4=C2NC5=	0.25177	0.235691
UWUPTKFUSXZFGD	CCOC(=O)C2(CC1CC1)CCN(CC3=C(F)C=C(OC)C=C3)C	0.260745	0.250654
SXMJDSFQLMRDNK	CC(C)(O)C#CC1=CC=C(CN2CCCC(CO)(CC3=CC(CI)=C	0.270848	0.280665
QUKGSOVSHLCELK	CN(CC1=CN(N=C1C2=CC(F)=CC=C2)C3=CC(C)=CC=C	0.251654	0.236351
YDAHVNIORWJIV	CCN1C=CN=C1CN(C)CC2=CN(N=C2C3=CC=CC=C3)C	0.259199	0.260277
BCGMXKJUZYVGMJ	CCOC(=O)C2(CCCC1=CC=CC=C1)CCN(CC3=NC=CN3	0.258787	0.237047
MDPMYGUAEAFIOS	CC(C)N1CCC(CC1)N2CCN(CC3=CC=C(O3)C4=CC=C(C	0.301944	0.283331
ZFWTTCOXZVMVOQ	COC1=CC(OC)=C(C=C1)C2=NC(CN3CCN(CC3)C4=C5	0.287302	0.271653
WJBXZNPTDXCVCV	CN(CC(O)COC1=CC=C(CNCC2=CC=C(CI)S2)C=C1)CC	0.27998	0.26714
VVEYWVLTXOWUHL	FC1=CC=C(C=C1)N2C=C(CNCCC3=NC=CC=C3)C(=N:	0.240448	0.230318
DQWOYLXISLTHQD	ClC1=CC=C(C=C1)C(=O)C2CCCN(CC3=CN(N=C3)C4=	0.264797	0.242637
YZSCVGMHSCGXIL	ClC1=CC=C(C=C1)C(=O)C2CCCN(CC3=CC=CN3C4=N	0.268223	0.26
JBYLARROVLVBI	COC1=C(CN2C=CC=N2)C=C(CN3CCCC(C3)C(=O)C4=	0.272578	0.244856
QCAJALZNRVYHKS	COC1=CC=C(C=C1)N2C=C(CNC3CCOCC3)C(=N2)C4	0.269882	0.255683
IJFWMGUGQKMKQO	COC1=CC=C(CC2(CO)CCN(CC3=CC4=C(OC3)C=CC(C	0.241667	0.232226
QWVDJMDVHANWSM	CCN1C=CN=C1CN(C)CC2=CN(N=C2C3=C(F)C=C(OC	0.28318	0.294583
GMQBGSKUGGMPAM	CC(=C)[C@H]1CCC(CN2CCC(CC2)N3CCC(CC3)C(=O	0.256356	0.225917
AFVLYIBFUZRBPV	CN(C)CCCNCC1=CN(N=C1C2=C(C)C=CC=C2)C3=C(F	0.309858	0.29561
ZKGRBJTINVQJAX	CSC1=CC=C(C=C1)C2=NC(CN3CCCCC3C4=CN=CC=C	0.264526	0.281828
RTUWXPJUIDPBCJ	COC1=CC(=CC=C1)C2CCCN2CC3=C(C)OC(=N3)C4=C	0.283431	0.281323
NRBUOGJEVXEQAN	CC1=CC(N2C=C(CNCCC3C=CC=N3)C(=N2)C4=CC=	0.308348	0.30825
SZSCDZKFQNVGHY	CC1=NC=CN1CCCNCC2=CN(N=C2C3=CC=C(F)C=C3	0.257305	0.244487
DESKVDNHFKWY	CC1=NC(CN2CCCC(C2)C(=O)C3=C4C=CC=C5CCC(C	0.251009	0.225967
LOHJNFDYGMTSN	O=C(C1CCCN(CC2=NC=CC=C2)C1)C3=C4C=CC=C5C	0.245029	0.244134
CQUHQOPIXROFE	FC1=CC=C(C=C1)N2C=C(CNCCC3=CN=CC=C3)C(=N:	0.245442	0.231721
OHKFNYSXZJVFSQ	COC1=C(OC)C=C(CC2=NOC(CN3CCN(CC3)C4=NC=C	0.274912	0.255529
NPRLULMTXBRZO	C(N1CCN(CC1)C2CCC3=C(C2)C=CC=C3)C4=NC(CC5	0.258106	0.249856
BAASLYURXOHEG	ClC1=CC=C(C=C1)C(=O)C2CCCN(CC3=CC4=C(C=C3)	0.275734	0.246109
MBPRRILZKATBFW	CC1=C(C)C=C(C=C1)C2=NNC=C2CNCCC3=CN(N=C3	0.328881	0.297658
CYWIWKYWLQBNBA	CN1CCN(CC1C2=CC=CC=C2)C(=O)C3=NOC(COC4=C	0.266356	0.239293
NQYQOXQABBZQSE	OCCC1CN(CC2=NC3=C(C=C2)C=C(CI)C=C3)CCN1CC	0.244151	0.224524
HBJGKNBCHGRSOA	ClC1=CC=C(C=C1)C(=O)C2CCCN(CC3=C4N=CC=CC4	0.291363	0.284108
NKGPKGBJGOADMH	FC(F)(F)C1=CC(CC2=NOC(CN3CCC(CC3)C4=CC=NC=	0.280798	0.263281
FHCZAQUUNSLAQY	OCC2(CC1=CC(=CC=C1)C(F)(F)F)CCN(CC3=CC(F)=CC	0.248576	0.225438
NZEIDBTTWSYLCM	COC1=CC=C(C=C1)N2C=C(CNC3CCN(C)CC3)C(=N2)	0.321016	0.323617
HMXGHYPMLPTBOS	CSC1=CC=C(CN2CCC(CO)(CC3=CC=C(CI)C=C3)CC2)C	0.310945	0.289902
WOZVHZFFMRRFAK	COC1=C(C=CC=C1)C2CCCN2CC3=C(C)OC(=N3)C4=C	0.285006	0.256603
XASOOGGPNWVOCZ	CSC1=CC(CN2CCC(CO)(CC3=CC(=CC=C3)C(F)(F)F)C	0.243689	0.227497
BPMSQKCYNZZCDL	COCC1=CC=C(CN2CCC3=C(NC4=C3C=CC=C4)C2CC	0.246559	0.231843
ZUYMJOIZOUJQTC	CCN1C=C(CNCC2=CN(C)N=C2C3=CC=C(C=C3)C4CC	0.278854	0.288496
VCCRFAZUYUPLNS	COC1=C(C=C)CN2CCCC(CO)(CC3=CC(CI)=CC=C3)C	0.26524	0.242025
GBGWEVIXWLGSZR	COC1=CC=C(C=C1)N2C=C(CN(C)C3CCOCC3)C(=N2)	0.294175	0.289015
JIUQYIJYFWHPQM	CCN1C=CN=C1CN2CCCC(C2)C(=O)C3=CC4=C(C=C3)	0.24044	0.23146
NWYWRJMNFOBIMX	CC(CC1=NC=CN=C1)NCC2=CN(N=C2C3=CC(C)=CC=	0.250031	0.240456
JBNWRZAPHBAVBQ	COC1=C2N=CC=CC2=C(CN(C)CC3=NC(CC4=CC(F)=C	0.295917	0.275856
DVVMTXGLVWUGGB	COCC1CCN(CC2=CN(CC3=CC=CC=C3)N=C2C4=CC5	0.273896	0.250579
LCRFBQZLFWFDCF	COCCN1CCCC(CNCC2=CN(C)N=C2C3=CC=C(OC4=C	0.256728	0.239629

LRMNRVWEHOCALO	COCC1CCCN(CC2=CN(CC3=CC=CC=C3)N=C2C4=CC	0.253022	0.262312
GKNIJVSASFJETKG	CC(C)CC1=CC(CN2CCCC(CO)(CC3=CC(Cl)=CC=C3)C	0.272795	0.24517
LXRHZPIGVAAUCI	CCC(O)C1CCN(CC2=CN(N=C2C3=CC(F)=CC=C3)C4=	0.262783	0.246725
VDQDSCLUERDOST	COC1=CC(OC)=C(C=C1)C(=O)C2CCCN(C\C=C\C3=C(0.256299	0.23388
KQFDPMQZRUTXPA	COC1=CC2=C(C=C1)C=C(C=C2)C(=O)C3CCCN(CC4=	0.242492	0.228318
KXEYVFAGHLNOEV	CC1=CC(=C(C)S1)C2=NN(C=C2CN3CCN(CC3)C4=NC	0.315825	0.30232
NBFTWNLATVAUAM	CN1C=C(CN2CCN(CC2)C3=CC(C)=NC(C)=C3)C(=N1)	0.351717	0.317014
JNTZDXUUXYAWMU	C1CCN(CC1)C2=C(NC3=NC4=C(C=CC=C4)N5C=NN=	0.278726	0.256042
FEGIRYMCKCJPBY	COC1=CC=C(CNC(=O)C2CCCN(CC3=C(C)OC(=N3)C4	0.262053	0.250767
XHQUMJLPQUTNMD	N#CC1=CC(NC2=C3C=CC=CC3=NC4=C2CCCC4)=CC	0.273336	0.241627
LBXANFQOQNCQEL	COC1=CC=C(C=C1)N2N=C(C(NC3CCN(CC4=CC=CC=	0.255715	0.266417
YJJJRJVBTWWBNG	CC1CCN(CCCNC(S)=NC2=CC3=C(C=C2)N=C(C=C3C)	0.262216	0.235064
OJMCRNNZWOYFQJ	[O-][N+](=O)C1=CC=C(NC(=O)NCCCN2CCN(CC2)C3=	0.258754	0.242245
MBKCLKGGOYNYQAP	CCCN(CC)CCCN(C(S)=NC1=CC2=C(C=C1)N=C(C=C2)	0.258662	0.255857
NZORQKRPSGFQLE	CN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)NCCCN4	0.284264	0.286762
XKGYMEZDXUIVFP	CN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)N4CCN(0.252002	0.245936
LMOVQMOCYLFXKH	CC1CN(CCN1C2=CC(C)=CC=C2)C(\S)=N\C3=CC4=C(0.247228	0.227676
WYYHHQCZFNMOCC	COC1=CC=C(CNC(S)=NC2=CC3=C(C=C2)N=C(C=C3C)	0.271419	0.255258
OOAYGBZBQZEBNW	CN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)NCC4=C	0.254174	0.222461
CPMGALIDDQAPP	CN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)N4CCN(0.257033	0.252008
HLWSDOKFCOSYBI	CCN(CC)C(\S)=N\C1=CC2=C(C=C1)N=C(C=C2C)N3C(0.271394	0.237871
RZCWMDFCFUXRLU	CCCN1CCN(CC1)C(\S)=N\C2=CC3=C(C=C2)N=C(C=C	0.296176	0.262633
XXUIMDJNJTYWQD	CCN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)N4CCC	0.244559	0.248819
UNNVTXBVMHXGU	CCN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)N4CCN	0.290335	0.280486
BNVIHRYZPJVFAS	CCC(C)NC(S)=NC1=CC2=C(C=C1)N=C(C=C2C)N3CC(0.259532	0.246874
UQNIQQMLYLZLQM	CSC1=CC(=CC=C1)N=C(S)N(CCCN2CCN(C)CC2)CC3=	0.291621	0.296929
RWYJVSJPESENBE	COC1=C(Cl)C=C(C=C1)N=C(S)N(CCCN2CCC(C)CC2)C	0.276651	0.247328
YZEQNCRVOVLQHO	CC1=C(Cl)C=C(C=C1)N=C(S)N(CCN2CCCC2)CC3=C	0.25734	0.242072
JHHUBMUZFNWBWF	CCOC(=O)C1=CC=C(C=C1)N=C(S)N(CCCN2CCC(C)CC	0.262501	0.251372
LRDUMMRCSWWHSH	CC1=C(C=CC=C1)\N=C(/S)N(CC2=NC=CC=C2)CC3=C	0.256488	0.229267
SEALYCBSEQDAOV	CN1CCN(CCCNC(=O)C2=C3C=CC=CC3=C(NC4=CC(C	0.26436	0.24613
SXFVOOSWOKCVKQ	FC1=NC(F)=C(F)C(NCCCNC2=C(F)C(F)=NC(F)=C2F)=(0.254022	0.247994
FXWJYMLMEYQWMJ	C[N+]=C2SCC(=NN2C3=C1C=CC=C3)C4=CC=CC=C	0.239411	0.234227
JRMYQNXXMWDWDFW	CC1=CC(OCCCCCN2C=CN=C2)=CC(C)=C1Cl	0.240322	0.223772
AFYSBOFSBZXDRD	FC(F)S(=O)(=O)C1=CC(=CC=C1)N=C(S)N2CCN(CC2)C	0.239131	0.265842
ANWUINNDMYCNDD	CC(N=C(S)NCCC1=CC=CC=C1)C(N2CCN(CC3=CC=CC	0.257279	0.244379
OQEFVFGCTVHSMGW	COC1=CC(CN(CCC2=C(C)NC3=C2C=C(Cl)C=C3)C(S)=	0.241638	0.24943
HCGFCVYNUZHUCW	CN1CCN(CC1)C(=S)C2=CN(CC3=CC=C(Br)C=C3)C4=	0.249888	0.239238
WKXMREPQLQSTHK	[O-][N+](=O)C1=C(CN2CCN(CC3=CNC4=C3C=CC=C4	0.252779	0.241325
PADZYLUAUOMXDT	COC1=C(CNCC2=C(OC)C=CC(Br)=C2)C=CC=C1	0.278444	0.287123
BFUYCBZDDJDIOZ	[O-][N+](=O)C1=CC=C(CN2CCN(CC3=CNC4=C3C=CC	0.246226	0.248185
KHXYGMHITFMSSB	[O-][N+](=O)C1=CC(=CC=C1)C2=CC=C(O2)\C=N\NC3	0.268501	0.252761
QDCSZEPGRRVZLO	CCOC1=CC2=C(C=C1)N=CC(=C2N3CCC4(CC3)OCCC	0.238532	0.225095
PNFMIJKJNPCKGZ	CCOC1=CC2=C(C=C1)N=CC(=C2N3CCN(CC3)C4=CC	0.245611	0.235363
YGQOFHZHVHYTLN	CCOC(=O)C1=C(\N=C(/S)N2CCN(CC2)C3=C(OC)C=C1	0.244656	0.226149
MRNQMYQVAKMUSY	CN(C)CC1=C(N=C2C=CC=CN12)C3=CC=C(Cl)C=C3	0.253422	0.247562
MYNKYKFAAVZKFR	CC1=CC=C(CNCC(O)C2=CC=CC=C2)C3=CC=C(Cl)C=	0.242086	0.239388
ZZJOTYVKOBLDMI	CN(C)CCCN(C(=O)\C=C\C1=CC=C(OCC2=C(Cl)C=CC=	0.258783	0.222475

RTVDPQBHFPOHDW	[O-][N+](=O)C1=C(SC2=CC=C(Cl)C=C2)C=CC(CN3CC	0.307609	0.264825
HRGXNVAXDCCHTJ	CN1CCN(CC2=CC(=C(SC3=CC=C(Cl)C=C3)C=C2)[N+	0.298616	0.284681
JOXFOVKOHKFZNG	COC1=C2N=C(C)C3=C(N(CC3)C4=CC=CC=C4)C2=CC	0.29155	0.276597
XWBNXNPYMCYTKF	CCS(=O)(=O)C1=NC(=C(S1)N2CCC3=C(C2)C=CC=C3)	0.245572	0.241612
MZVDBDZUJDCBSC	CN(C)C1=NC(=NC(N\N=C\C2=CC=C(Cl)C=C2)=C1)N(0.272075	0.263776
KGYVKILQXKVVWJ	COC1=C(\C=N\NC2=NC(=NC(=C2)N(C)C)N(C)C)C=CC	0.245308	0.225241
XQRNYCRKOMTZFY	BrC1=CC=C(\C=N\NC2=NC=CC=C2)C=C1	0.248384	0.255253
IHAPMOBRYZOQFE	CN(C1CCS(=O)(=O)C1)C2=NC(=CS2)C3=CC=C(Br)C=I	0.256848	0.256779
KRDOFMHJLWKXIU	C1CN(CCN1)C2=NSC3=C2C=CC=C3	0.346153	0.312153
HIFUXKJUQAFAJU	CC1=CC=C(CN2CCN(CC3=C(F)C=CC=C3)CC2)C=C1	0.257033	0.272488
WPKKEQCPXUTCDZ	CCOC(=O)C1=C(C)C(C(=O)OCC)=C(N1)C=O	0.243017	0.22557
RYSOBSPYPVTLDS	CC(=O)C1=CC=C(NC2=C3C=C(C)C=CC3=NC(C)=C2)C	0.259518	0.224786
FTFFGSFIZWGJIM	[O-][N+](=O)C1=CC=C(C=C1)C2=CC=C(C=C2)S(=O)(=	0.315625	0.285612
AYRFKQUXGIWEFY	FC1=CC=C(CN2C(=O)NC3=C2C=CC(=C3)C(=O)NC4C	0.278456	0.234759
WAWROLBZXUSKFC	CCN1C(=NC2=C1C=CC=C2)N3CCN(CC3)S(=O)(=O)C.	0.267299	0.233339
JPLCIFZYVVSLL	COC1=CC2=C(C=C1)N(C(C)C)C=C2)S(=O)(=O)C3=C	0.270344	0.236725
IRCARNCHRGIKND	ClC1=CC=C(C=C1)S(=O)(=O)NC2C(N3CCNCC3)C4=C	0.2799	0.25851
SLQXSPDKMZEODT	CC1=CC=C(C=C1)C2=C(O)C(CN3CCCC3)=CC(CN4C	0.262782	0.256331
YFVRUSSYKPOITK	CC1=CC(CN2CCN(CC2)C3=CC=C(Cl)C=C3)=CC=C1	0.239212	0.223985
ZKUBYEOCFYGKNL	CCCCCCCCNC(S)=NCCN1CCCCC1	0.24313	0.231461
FEXQYNVUMVIVGE	O=C(CN1CCN(CC2=CC=CC=C2)CC1)NC3=C(C=CC=C	0.286331	0.272813
LLAWTBLIBJUONA	OC(C1CN2CCC1CC2)(C3=CC(Cl)=CC=C3)C4=CC(Cl)-	0.27959	0.282767
NJFAWKDEUTVGF	COC1=CC(OC)=C(C=C1)\N=C(/S)N2CCN(CC2)C(C3=(0.299635	0.299326
KQFAYSOEMKUZBH	COC1=C(C=CC=C1)N2CCN(CC2)C(=O)C3=C(OC)C=C1	0.258672	0.229533
NTQGEZJOMVFLMK	CC1C(N(C)C(CC1(O)C2=CC=C(F)C=C2)C3=CC=CC=C:	0.258431	0.265185
ISXPELHAGSCOTH	CCOC1=C(NC2=C3C=CC(Cl)=CC3=NC=C2)C=CC=C1	0.29311	0.27042
XSGLKSWEYRBHSW	[O-][N+](=O)C1=CC(CN2CCN(CC3=CC=C(Cl)C=C3)CC	0.240172	0.24337
SMIOHXYOEZYTOZ	CN(C)C1=CC=[N+](CC(=O)NC2=CC=C(OC3=CC=CC=C	0.251263	0.237694
GHWBMURKXUDZMP	COC1=C(C=CC=C1)C(CC(=O)C2=CC=CC=C2)CC(=O)C	0.239785	0.226754
NJNAIDUQVFTTBZ	CCN(CC)CC#CC(OC)(C1=CC=CC=C1)C2=CC=CC=C2	0.279764	0.270153
FVFRHLHSSWBPELS	COC1=CC(CN2CCN(CC3=C4C=CC=CC4=CC=C3)CC2	0.266086	0.272563
LRXTUBHKBZJFDW	CC1=CC(C)=NC(=N1)\N=C(/N)NCCC2=CNC3=C2C=C	0.250318	0.234308
QCXXSOISNANRNA	CC1=C(OCC2=NN=C(SCCN3CCCC3)N2)C4=CC=CC=C	0.263748	0.266668
TWCMTPLQZRXYOY	CCOC1=CC2=C(C=C1)N=C(NCC\N=C(/S)NCCCN(C)C'	0.250379	0.23992
IHZFFUAIKZYKBM	CCC1=CC=C(C=C1)N=C(S)NC2CC3CCCC(C2)N3CC4-	0.292323	0.291478
IEZSNPNKNGWEET	CC(C)CCN1N=NN=C1CN2CCN(CC2)C(C3=CC=CC=C:	0.244306	0.24019
NGRYFJUARYBAHQ	COC1=CC=C(C=C1)C2=C(N=CO2)C(=O)N3CCN(CC3)	0.246788	0.247485
SXZLFLGASKUCKZ	CC1=CC(C)=NC(\N=C(/N)NC2=CC=C(C=C2)C3=CC=C	0.285035	0.240165
APGLINRJTWKNDT	CN(C)C1=NC(=NC(N\N=C\C2=CC=CC=C2)=C1)N(C)C	0.250581	0.226467
POGJCPKDTDNXJG	SC(=NCCCC1CCOCC1)N2CCN(CC2)C3=NC(=CS3)C4	0.312367	0.291551
VLTIUAUCHIASBMZ	CCNC1=NC(=NC(NC(C)C)C)=N1)N2CCCCC2	0.284845	0.282266
BTGJNQZJPRUNAF	COC1=CC(OC)=C(NC2=NC(=NC(NC(C)C)C)=N2)N3C	0.25456	0.223657
WOSAORHVEAJOFC	CC1=NC2=C(C=CC=C2)N1C3CCN(CC(=O)NC4=C(Br)	0.284494	0.266751
GTCJGLXECMCTOG	CN(C)CCNC1=C(C)C(C)=NC2=CC(=NN12)C3=CC=C(C	0.243241	0.225897
BUMLQGZXHOSJCC	COC1=CC(=CC=C1)C2=C(C#N)C(=NC(=N2)C3=CC=C(0.296987	0.269863
QFHIFJRXZPZTA	CN1CCN(CC1)C2=C(C#N)C(=NC(=N2)C3=CC=CC=C3	0.270185	0.255549
JAIcceXMYCENQ	COC1=C(C=CC=C1)C2=C(C#N)C(=NC(=N2)C3=CC=C(0.260517	0.235179
QRAVHOBHERRTSC	ClC1=CC=C(SCC2=NC(=NC(=C2)N3CCOCC3)C4=NC-	0.25652	0.243087

QWKVLFZMMXCIJ	CC1=CC=C(CN2CCC(CC2)C3=CC(=NN3)C4=CC=CS4	0.253645	0.232882
FKEBRCPVZPTAMC	ClC1=CC(Cl)=C(C=C1)C2=NNC(=C2)C3CCNCC3	0.319792	0.328759
LNOMSJXJZOIPW	NC(N)=NC1=NC2=C(C=C(F)C=C2)C(=N1)C3=CC=CC=	0.244809	0.250059
ACSLIDFTZZIDFE	SC(=NCC1CCCO1)N2CCN(CC2)C3=NC(=CS3)C4=CC:	0.240433	0.224647
XAAQJGCFNFXKST	CCN(CC)CCCN(C(=O)C1=CC=CO1)C2=NC(=CS2)C3=(0.269896	0.25182
KTJNUFKBFSSJSB	CN(C)CCCN(C(=O)C1=CC=CO1)C2=NC(=CS2)C3=CC:	0.263753	0.240424
GGQOVVCIKFWMM	CCN1CCN(CC1)C2=C(Cl)C=C(NC(=O)C3=CC=C(O3))	0.240272	0.235826
UNAWHUIPJQHFOG	CN(C)CC1=C(SC2=C(Cl)C=CC(Cl)=C2)C=C(F)C=C1	0.249136	0.272714
FGNAPWDGOUVUBN	CN(C)CCN(C)CC1=C(SC2=C3C=CC=CC3=CC=C2)C=C	0.273895	0.278928
QZJSTFQILYOCCT	CC1C2=C(SC(CCCN(C)C)C3=C1C=CC=C3)C=CC=C2	0.335755	0.341638
HVBFDMQTIYPSNN	O=C1CC2=C(SC3=C1C=CC(OCCCN4CCCC4)=C3)C=	0.251251	0.227296
CBYVLYPUADKSDZ	CN1CCC(CC1)OC2=C(SC3=CC=CC=C3)C=CC=C2	0.315954	0.287168
HTQNTTWSGOYWOJ	CN1CCN(CCOC2C3=C(CSC4=C2C=C(Cl)C=C4)C=CC=	0.323286	0.304419
VGDJMCOVGPXEGS	COC1=C(OCC2=CC=C(Cl)C=C2)C(Br)=CC(CNC(C)C)C	0.251032	0.235164
FCHFYDCSAICDEA	COC1=C(C=CC=C1)N2CCN(CC(O)COCCOC3=CC=C(B	0.280406	0.252001
BMQGWQJMFCYXPU	ClC1=CC2=C(SCC3=C(C=CC=C3)C2OC4CN5CCC4CC	0.322556	0.303729
CCBMGCPPZDFKPKQ	CC1=CC(C)=NC(NN=C(C2=CC=CC=C2)C3=CC=CC=C3	0.27305	0.284865
BVSAILCTPWDKAT	CCN(CC)CCN(CC1=CC2=CC=C(C)C=C2NC1=O)C(\S)=	0.25092	0.22305
REHMQQADKYVDHV	CNC(S)=N\N=C\C1=CC(Br)=C(OCC2=CC=CC=C2)C=C	0.242463	0.279242
KWSJNROGXMPADP	CCOCCCNCC1=CC=C(OCC2=C(Cl)C=CC=C2)C=C1	0.255571	0.245106
LAADJKRGIQNHQR	[O-][N+](=O)C1=CC(=C(C=C1)N2N=NN=C2C3=CC=C1	0.258616	0.226826
HUMOBQPLLCZOHC	CCC1=CC=C(OCCOCC(O)CN2CCN(CC3=CC=C(Cl)C=C	0.250814	0.238179
VFJLWYJYPAVLE	COC1=C(OCC(O)CN2CCN(CC3=CC=C(Cl)C=C3)CC2)	0.259195	0.263504
PEDWTSPDIWXPOU	COC1=CC=C(NC2=NCC(CC3=CC=C(Br)C=C3)S2)C=C:	0.268625	0.26494
DGZUNQTZDDPLAE	CN(C)CC1=C(SC2=C3C=CC=CC3=CC=C2)C=CC=C1	0.299987	0.30102
PIRXOVWZBWSEMM	FC1=C(CN2C(=N)N(CCC3=CC=CC=C3)C4=C2C=CC=C	0.252453	0.269021
YAPHWQFSXRJHAD	OCCCN1=C(N=NC(=N1)C2=CC=C(Cl)C=C2)C3=CC=	0.240447	0.237094
YEJLKGBVTVLUJU	BrC1=CC=C(CN2C3=C(CCC3)C(=N)C4=C2CCCC4)C=	0.274666	0.270142
NBDSXQFFUYCQTN	CCCC1=NC(=C(N1CC(C)C)S(=O)(=O)C2=CC=CC=C2)	0.251224	0.229472
QRLIGEHLZYBXOP	CC1=CC=C(SCCOCCN2CCC3=C(C2)C=CC=C3)C=C1	0.244674	0.24244
JFUFOHQSLUKCSH	CN1CCC2=C(\N=C3/CCCN3CC4=CC=CC=C4)C5=C(C	0.246444	0.222821
FXMCSZOBLACMJZ	ClC1=C(Cl)C(NC(=O)NC2=CC=CC=C2)=CC=C1	0.248275	0.248025
SEUJBLRENKKWQS	CN(C)C1=CC=C(\C=N\N=C(/S)NCC2=CC=CO2)C=C1	0.239495	0.22328
FNFERHAIGOPDW	CCN(CC)S(=O)(=O)C1=C(C=CN=C1)N2CCN(CC2)C3=	0.242626	0.243129
VIEAOLWFSGPFPM	N=C1N(CC2=CC=CC=C2)C3=C(C=CC=C3)N1CC4=CC	0.305787	0.287584
MNSXBNKPPDYZMT	CCOC(=O)C1=C(C)N(C)C(C)=C(C1C2=CC=C(Cl)C=C2)	0.273268	0.287081
XXHHSTVXSOGSM	ClC1=CC(Br)=C(OCCCCCN2CCCC2)C=C1	0.32767	0.301302
IJGCPZWDASZGQN	CN(C)CCOC(C1CCCC1)C2=C(C)C=CC=C2C	0.277709	0.262598
RUWJWJOWWHKQPF	CC(C)NCCOC(C1=CC=CC=C1)C2=C(C)C=C(C)C=C2C	0.276389	0.264634
NPMCVFRTRDHRA	CO\N=C\C1=CC(OC)=C(OC2=C(C=C(C=C2))[N+][O-])	0.266407	0.280669
APJRCYYMTABKQQ	CC1=CC=C(C=C1)C2=NC(=C(O2)N3COCC3)P(=O)(C	0.240825	0.250364
HPWRLPQMPREEMM	OCl(=O)(=O)=O.CC1=CC=C(C=C1)C2=CC(C3=CC=C(C	0.244044	0.245103
UPGPCOREBWFJLY	COC1=CC=C(C=C1)N2CCN(CC2)C3=NC(NC4=CC=C(I	0.259064	0.252913
GPLGXZOMVXBMDO	COC1=C(OC)C=C2C(=C1)N=C(N=C2N3CCN(CC3)C4:	0.249084	0.25767
GLWJYTMHGSPNN	C1COCCOCCOC2=C(OCCOCCOCCOC3=C(OCCOCCC	0.294678	0.297417
MABYJMBBOLWQDW	CC1=CC(C)=C(C[N+]=CC(=CC=C2)C3=CC=CC=C3)C:	0.276327	0.265793
QTGLIGIORIFWRD	OC(COCCOC1=CC=C(Br)C=C1)CN2CCN(CC3=CC=CC	0.272882	0.231642
UOAKYFGDTSZLLF	CCOC1=CC=C(NC2=NC(=NC(Cl)=N2)N3CCN(CC3)C4	0.252391	0.251175

APABSGRYLLJSEU	CCOC1=C(OCC)C(CI)=CC(CNCCC2=CNC3=C2C=CC=C	0.257183	0.226437
NATUZEAPAOKDTI	CC(NCC1=CC=C(C=C1)C2=CC=CC=C2)C(O)C3=CC=C	0.254034	0.258486
FYXJNIGRTLZK GK	CSC1=CC=C(OC2CCN(CC3=CC=CC=C3)CC2)C=C1	0.290161	0.274481
DCZIXOHFCAHNKD	ClC1=C2SC3=C(CC(N4CCNCC4)C2=CC=C1)C=CC=C:	0.266916	0.284026
WLBMFXSDDL BRAZ	CN1CCC(CC1)OC2=CC=C(SC3=CC=CC=C3)C=C2	0.274859	0.264406
JEXBWN OUCUFHHS	BrC1=CC2=C(SCC3=C(C=CC=C3)C2C4=NCCN4)C=C:	0.281691	0.260188
BJZHTQLHPCJNND	CN1CCN(CCOC2CC3=C(SC4=C2C=C(CI)C=C4)C=CC=	0.277337	0.265931
FYGXUYJSSXOBBL	COC1=CC=C(C=C1)N=C(N)SCC2=NC=CC=C2	0.240432	0.225797
DPBGOHFPUVYOPM	CN1CCC(CC1)OC2=C(SC3=C(C=CC=C3)C(F)(F)F)C=C	0.263932	0.253246
LVUDIWHCHFHYEK	BrC1=CC2=C(SCC3=C(C=CC=C3)C2OC4CN5CCC4C	0.287	0.2743
RHUQQLBVJSNVLJ	CC1CC(C)CN(CCOCSC2=CC=CC=C2)C1	0.288523	0.305026
GYRJRIXBTMXCKY	CCCCOC1=CC=C(C=C1)C(=O)N\N=C\C2=CC(OC)=C(C	0.24434	0.225932
YGECTRZNNKKYOAY	N=C1C=CN(CC(=O)C2=CC=C(C=C2)C3=CC=CC=C3)C	0.249493	0.22735
VCRYKKJSLYCBHY	CC1=NN(C(C)=C1SC2=CC=C(C=C2)[N+][[O-]]=O)S(=C	0.249569	0.23347
FNNSJXWEFTXZSZ	COC1=CC(=CC=C1)N=C(S)N(CCC2=C(C)NC3=C2C=C	0.25207	0.254383
FVZIWOKPRSIM EC	COC1=CC(=CC=C1)N=C(S)N(CCC2=C(C)NC3=C2C=C	0.241235	0.22633
ASNILPDOVJQAO	FC1=CC=C(C=C1)N2CCN(CC2)C(CNC(=O)OCC3=CC=	0.263687	0.223543
GIYGBHMNMCHJIT	CN(C)CCCN(C(=O)CCC1=CC=CC=C1)C2=NC3=C(S2)C	0.243178	0.223254
GRIXINIGTYIHSN	ClCC(=O)N(C1=CC=CC=C1)C2=CC=CC=C2	0.239837	0.229801
OBMKABNHORJNQU	CSC1=NC2=C(C=CC=C2)C(=N1)N3CCN(CC3)C4=C(C	0.238956	0.224641
GGDHOWPTGBRPMC	ClC1=CC=C(C=C1)C2=CSC(=N2)N3CCOCC3	0.252233	0.255445
XPPTXMKRVXHUMG	COC1=CC=C(C=C1)C2=NOC(COC3=CC=CC=C3)=C2	0.24965	0.241469
JCTOPHRZYRAFTP	ClC1=CC=C(CNC(NC2CCCC2)=NC3=CC=CC=C3)C=	0.310109	0.274694
AJZXPBSDWPVYBE	COC1=CC=C(C=C1)N2CCN(CC2)C3=NC4=C(C=CC=C	0.251219	0.248394
MIYOOJWODFLYKL	BrC1=CC=C(C=C1)S(=O)(=O)C2=NC3=C(C=CC=C3)N:	0.244515	0.25154
SKEPZBWZVMRFSJ	CCN(CC)C1=C(C#N)C(=NC(=N1)C2=NC=CC=C2)C3=(0.273678	0.261758
QJRPMZWTWYPYKW	ClC1=CC2=C(C=C1)C(=CC=N2)N3CCN(CC3)S(=O)(=	0.262286	0.247335
ILZJYRDFLDSWFU	CCOC(=O)C2(CCC1=CC=CC=C1)CCN(CC3=C(OC)C=C	0.267072	0.225252
FTOZHDVIBQNOEF	CC1=CC(NC2=NC(C)(C)N=C(N)N2)=CC=C1	0.313043	0.313036
ZNQQBOBENQFAGZ	CC1=NC(SCC2=NN=C(O2)C3=C(C=CC=C3)[N+][[O-]]:	0.23879	0.234222
MDMGFFNYPHLZDG	FC1=CC=C(C=C1)N2CCN(CC2)C(S)=NC(=O)C3=CC=C	0.252733	0.232192
GPJBSEDRPMPHS	BrC1=CC=C(C=C1)C2=CN3CCSC3=N2	0.270047	0.269575
HHWOVFWQFLUAI	COC1=C(N=C(N=C1)C2=NC=CC=C2)N(C)C	0.243733	0.251547
XWXIIFYKAGUANZ	CCN(CC)CCNCC(O)(C1=CC=C(CI)C=C1)C2=CC=C(CI)	0.308828	0.307814
AYBYPRNGUZVMQV	CN1CCN(CC(O)(C2=CC=C(CI)C=C2)C3=CC=C(CI)C=C	0.273876	0.277202
GAAVXFWCTHXPOI	NC(=S)N1OC[C@H]2COC3=C([C@H]12)C4=C(C=C	0.242142	0.240979
UECKKYNEEBRMIL	OC(CNCC1=CC=C(C=C1)C2=CC=CC=C2)C3=CC(O)=C	0.264068	0.23066
QUIXMYIKMXDKJF	CCCCN(CC)CC1=CC=C(CNC(S)=NC2=C(CI)C=C(C)C=C	0.255719	0.240974
CAMZJWMMMLZD LSE	CCCCN(CC)CC1=CC=C(CNC(=O)NC2=CC=C(CI)C=C2)	0.315242	0.274555
KUSMJVHRBZPAHQ	CSC1=CC(=CC=C1)N=C(S)N(CCN(C)C)C(C)C2=NC=CC	0.297771	0.28478
GKNZLDCSKLKLX	CN(C)CCNC(=O)C1=CC(=C(SC2=CC=C(Br)C=C2)C=C1	0.264189	0.227712
IKHJSFHAHLFWOV	N1N=C(C2=CC=NC=C2)C3=CC=C4C=CC=CC4=C3N=	0.251114	0.256468
RQZVZXMZBKLHPE	OCl(=O)(=O)=O.C1=CC=C(C=C1)C2=CC(C3=CC=CC=C	0.263497	0.285008
XJLAUUGAEXMSTE	CC1=CC(C)=NC(\N=C(/N)NC2=C(C=CC=C2)C3=CC=C	0.2489	0.241787
KGIUVVMKTGEIGN	CN(C)C1=CC=[N+](CC(=O)C2=CC=C(C=C2)C3=CC=CC	0.260262	0.246816
YWF DALCOUZEVS L	COC1=CC=C(C=C1)C2=[N+](CC3=CC=CC=C3)C4=C(C	0.256195	0.255945
KTKSHXRVVYJPI	CC1=CC=C(NC2=NCC(CC3=CC=C(Br)C=C3)S2)C=C1	0.307179	0.302039
UXKVVUPOXFJTFJ	COC1=C(C=CC=C1)N2CCN(CC2)C(\S)=N\C3=CC(C)=	0.291936	0.26786

BPKDNYUQUUDNJX	CC1=CC=C(C=C1)S(=O)(=O)CC(CN2CCCC2)N3CCC(0.274295	0.244978
MMPSNKSYGQWBD	CSC1=CC=C(CN2CCN(CC3=CC=C(C=C3))[N+](O)=O	0.286772	0.27437
KAIBCOJELXAENF	CCN(CC)CCNC(=O)C1=C(C)C2=C(N1)C=CC(OCC3=CC	0.244651	0.22916
BRBRPRUPAFZBRK	COC1=C(OC)C=C2C(CC3(CCCC3)N=C2SC)=C1	0.279439	0.245644
AOUWTGIEFIEWFQ	CCC1C(N(C)C(CC1(O)C2=CC=CC=C2)C3=CC=CC=C3)	0.28987	0.263592
AYUJSXPEEOWVIP	COC1=C(CN2CCN(CC3=CC=C(Cl)C=C3)CC2)C=CC=C	0.262443	0.259336
OAWBNSFACJTGRK	CC1CN(CCN1)C2=CC(NCCOC3=CC=CC=C3)=C(C=C2	0.29042	0.25824
NJCPKBULCCSCOS	CC1=CC(C=C)N2CCN(CC2)C3=CC=CC=C3)=CC=C1	0.250023	0.242383
HZJFUUXNALQFED	CN(C)CCCN(C(=O)COC1=CC=C(Cl)C=C1)C2=NC3=C(0.242125	0.242744
FYFMMYDSPMPQTP	CC1=CC=CC(C)=C1\N=C(/S)NCCSC2=CC=C(Cl)C=C2	0.270257	0.263177
NKWQFTAEPAINSK	CC(C)CCN(C1CCN(CC1)C(C)C(\S)=N\C2=CC(F)=CC	0.26838	0.236183
BJOSXOWNVQPBLO	CN(C)CCOCCOC1=C(C=C(Cl)C=C1)C(C)(C)C	0.260209	0.234881
UZVYOKPDOYMPGP	NC(N)=N\N=C\C1=CC=C(OS(=O)(=O)C2=CC=CC=C2)	0.248389	0.227361
KYQYSANJUCXXCA	COC1=C(OCC2=CC=C(Cl)C=C2)C=CC(C=C)N(N)N	0.279473	0.268695
OZISUZNBRLJW	COC1=CC=C(C=C1)C(=O)C2=C(C=CC(=C2)[N+](O)=	0.243982	0.251975
UXHDQIRZKBKYO	FC1=C(Cl)C=C(C=C1)N=C(S)NC2=CC(=NN2)C3=CC=C	0.245369	0.231409
UPXSQTKCJWIRJW	CC1=C(Cl)C=C(C=C1)N=C(S)N(CCCN2CCCC2)CC3=C	0.277865	0.263356
MXLFJBAJDFTZCN	SC(=NC1=CC(Cl)=CC=C1)N(CCCN2CCCC2)CC3=CC=C	0.256214	0.24587
YWLOVUQANAXWLU	CC1=CC(=CC=C1)N=C(S)N(CCCN2CCCC2)CC3=CC=C	0.265289	0.271058
JKUNUPFGZSGECC	COC1=CC(=CC=C1)N=C(S)N(CCCN2CCCC2)CC3=CC=C	0.274749	0.262708
BMCGWOGJNBHUIB	CSC1=CC(=CC=C1)N=C(S)N(CCCN2CCCC2)CC3=CC=C	0.259339	0.251738
SCAPUKMLNDPVEH	CC1=CC=C(C=C1)N=C(S)N(CCCN2CCCC2)CC3=CC=C	0.297633	0.280122
FTODNNJQFPXFFV	CSC1=CC(=CC=C1)N=C(S)N2CCCN(CC3=CC(Cl)=CC=C	0.301718	0.287258
YSIBDEVVZTYCIB	COC1=CC=C(C=C1)N=C(S)N2CCCN(CC3=CC(Cl)=CC=C	0.269014	0.243639
PFLGULRHQNYPMN	CSC1=CC(=CC=C1)N=C(S)N2CCCN(CC3=CC=C(F)C=C	0.283816	0.251518
CVPTVBGYWXRAP	COC1=CC(=CC=C1)N=C(S)N2CCCN(CC3=CC=C(F)C=C	0.262712	0.265507
BNCOSJBYOFDSSY	CC1=CC(C)=C(C=C1)\N=C(/S)N2CCCN(CC3=CC=C(F)	0.247881	0.228058
RZRDGLIUVFCRMT	CC1=CC(=CC=C1)N=C(S)NCCN(C2CCCC2)C3CCCCC:	0.270818	0.239922
LQKHIQAPCZVYRQ	CC1=C(C)C=C(C=C1)N=C(S)NCCN(C2CCCC2)C3CCC(0.303435	0.281904
KUIDKYKLCWSCLF	C(C1CCC=CC1)N2CCN(CC2)C3CCCCC3	0.261824	0.229514
HFDQYVFKIRDR	CC1CN(CC(C)O1)C2=NC=NC3=C2C(=CN3)C4=CC=C(0.240337	0.22334
WMKPTGOSRIGQDX	CCOC(=O)C1=C(C)N(CCC(=O)NC2CCN(CC3=CC=CC=C	0.277979	0.262764
UEAXCDRBRBTKKU	CC(N1CCC(CNC(S)=NC2=CC(Cl)=CC=C2)C1)C3=CC=C	0.310152	0.318703
POGXRPWJRVAECM	CC1=C(C)C=C2C(CC(=O)NC2=C1)C3=C(F)C=CC(Br)=	0.25696	0.224692
PDNZQQNYZWNULD	CN1CCN(CC1)\N=C\C2=CC=C(O2)C3=C(Cl)C=C(C=C	0.243344	0.238795
BZKFKMJKMGZZKC	COC1=C(OCC2=CC=CC=C2)C=C(CNCCC3=CC=C(Cl)C	0.246708	0.259606
MDFLWFCCFITZCN	CCC1=CC=C(CN2CCN(CC3=CC=C(SC)C=C3)CC2)C=C	0.239952	0.233899
GFICLCROZVLVCW	CCC1=CC=C(C=C1)C2=NN(C=C2)CSC(N)=N)C3=CC=C	0.241776	0.237277
WYSDYHBYVSQBCE	CCCCN1C(=N)N(CCOCC2=CC=C(C)C=C2)C3=C1C=CC:	0.252407	0.226997
GEVANJBQYBIITO	ClC1=CC=C(CN2CCC(CC2)C(=O)N3CCN(CC3)C(C4=C	0.240773	0.228704
VTMSWKGMQBMIIO	CCC(C)NCCOCCOC1=C(C)C=C(Br)C=C1	0.279214	0.247871
VDTIHKPXBJSNY	CC(C)C1=C(OCCCN(C)CC2=CC=CC=C2)C=C(C)C=C1	0.257489	0.24113
YMHIDQHPRVTLET	CC1CC(C)CN(CCOCC2=C(Cl)C(Cl)=CC=C2)C1	0.289051	0.265768
ZTLJFBUPZUQPQC	CC(C)(C)C1=CC=C(OCCCNCC2=CC=CC=C2)C=C1	0.267942	0.237643
VGOLDQYBUBVZFOS	CCC(C)NCCOCC1=C(Br)C=C(C)C=C1C	0.306087	0.276455
ZSSRJISHTMTSOJ	CC1CCCN(CCOCCOC2=C(Cl)C=C(Br)C=C2)C1	0.284211	0.25793
XXNKKQHOPHTSDT	CC1CCCN(CCOCC2=C(Br)C=C(Cl)C=C2)C1	0.279689	0.254649
PSCYBUVYHUPSDO	CC1CCCN(CCOCCOC2=C(C=CC=C2)C3=CC=CC=C3)C	0.294623	0.270111

RDCDECHOIHHUNU	CCC(C)NCCCOC1=C(CC=C)C=C(Cl)C=C1	0.266973	0.227033
SSWTVYLFQUWTFI	CCC(C)NCCOCCOC1=C(C)C(C)=C(Cl)C=C1	0.268861	0.24365
BCBIOKIGGQEXNQ	CCC(C)NCCCCOC1=C(C)C=C(Cl)C=C1	0.295595	0.280705
OCLXWBHRPPKPNW	CCC(C)NCCCCOC1=CC(=CC(C)=C1)C(C)C	0.267416	0.228165
AEWAFEBQAPEWDL	CN(CCCOC1=C(Br)C=C(C)C=C1)CC2=CC=CC=C2	0.269297	0.236967
FFFYLIDSAKFNSD	CC(C)C1=CC=C(C=C1)\C=N\NC2=NC(=NC(=C2)N3CC	0.250712	0.226584
LCCTUHKKBTVVSS	CC1CCN(CCCOC2=C(Br)C=C(C)C=C2)CC1	0.290084	0.29107
JIZJRSNIKWMADT	CCOC1=C(OCC2=CC=C(Cl)C=C2)C=CC(\C=N\N=C(N)	0.258974	0.252464
MQTHJNMKFYHZQJ	COC1=C(OCCCCN2CCC(C)CC2)C=CC(CC=C)=C1	0.258372	0.257134
JBOZAMBUQYKIHA	COC1=C(OCC2=CC=CC=C2)C(CNC34CC5CC(CC(C5)	0.249752	0.227372
YAJVHXYYTXCAO	CCN(CC)C1=CC=C(CNCCC2=CC=C(F)C=C2)C=C1	0.312575	0.299334
XIDROJXYFJREQL	CCCCNCC1=CC(OC)=C(OC2CCCC2)C(Br)=C1	0.281569	0.240341
FMTHLQDBSCILBQ	CC(C)C1CCC(C)CC1OCC(O)CN2CCCC(C)C2	0.30052	0.2713
NNICULATGKYIKY	OCCN1CCN(CC(O)COC2=CC=C(C=C2)C34CC5CC(CC	0.24477	0.234799
YVUSAXKSOPPPJJ	CCOC(=O)C1=CC(NC(=O)C2=CC=C(C=C2)N(C)C)=CC=	0.255709	0.250367
FTUASJMDPFCADW	CC1=CC(C)=C(NC(N)=NC2=NC(=CC(C)=N2)N3CCCC	0.243061	0.228128
QYJSXKKODPSROV	CN1CCN(CC1)C2=C(C=C(C=C2)C(=O)C3=CC=C(Br)C=	0.264935	0.232691
RZHPANYKRJPBKP	CC1=C(CSCCNC(S)=NC2=CC=CC=C2)C=CC=C1	0.245776	0.234923
FKKFVJQSKCKZDV	SC(NC1CC2CCC(C1)N2CC3=CC=CC=C3)=NC4=CC=C	0.288318	0.277753
SDGYUCWQEJQFMK	COC1=CC(OC)=C(NC2=NC(=NC(NC3=C(OC)C=C(OC)	0.258781	0.248614
SENPBBUJCAQOCZ	COCCCNCCCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.288337	0.266713
GCRAXYJYGWUDKD	CC(C)NCCCCOC1=CC(=CC(C)=C1)C(C)C	0.253494	0.228483
NIRXFWNBVKSCOD	ClC1=C(Cl)C=C(OCCCN2CCCC2)C=C1	0.293234	0.263165
KEDCFLQUPOQSMN	[O-][N+](=O)C1=C(NC2CC2)C=C(C=C1)N3CCCC3	0.269224	0.234187
UZZSBHPQFNQHIB	SC(NCC1=C(Cl)C=C(Cl)C=C1)=NC2=CC=CC=C2	0.246935	0.234499
OXHLKKWMHZCRJW	CN1CCN(CC1)C2=C(C=C(F)C(=C2)N3CCCCC3)[N+]	0.314115	0.297859
NQJZRCYVUAQNMJ	CSC1=C(C=CC=C1)C(=O)N2CCN(CC2)C3=CC(Cl)=CC=	0.262496	0.254547
UXHDUFIOVXVIJL	CC1CCCN(CCCOC2=C(Cl)C=C(Br)C=C2)C1	0.289427	0.266875
AIMUFYVOHLVFCJ	CC1CCCN(CCOC2=C(Br)C3=C(C=CC=C3)C=C2)C1	0.246445	0.233804
ZRNCPTILWBFYFU	COC1=C(OCCCN2CC(C)CC(C)C2)C=CC(CC=C)=C1	0.241081	0.235488
FERNBCFSUGMRRK	CC1CCCN(CCOCCOC2=C(Br)C=C(C)C=C2Cl)C1	0.274565	0.263583
DXLYNCCYRVAILX	CCC(C)NCCOCCOC1=CC(C)=C(Cl)C(C)=C1	0.25958	0.243842
SFDHNSVBQLVGV	CN(C)CCCCOC1=C(Cl)C=C(Br)C=C1	0.299419	0.291009
FSQNAVGZOIOEFD	CN(C)CCOCCOC1=C2C=CC=CC2=C(Cl)C=C1	0.2702	0.27816
NDESNAGGEMBXFS	CC1CCCN(CCCOC2=C(C=C(C)C=C2)[N+](O)C1	0.259129	0.243587
SFMLQAVQSGBTMM	CC1CC(C)CN(CCOCCSC2=CC=C(Cl)C=C2)C1	0.310249	0.30551
DJZUMTSRGAGZJZ	CC1CCCN(CCCOC2=C(C=CC=C2)C3=CC=CC=C3)C1	0.287789	0.283609
RMJFYGBCYRSVGX	CCC(C)NCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.262095	0.242653
XCHSDYOLWFHBLV	CN(C)CCOCCOC1=C(CC=C)C=C(Cl)C=C1	0.254642	0.257398
XJPDYOUONEOAM	COC1=C(OCCCN2CC(C)CC(C)C2)C=CC(\C=C\C)=C1	0.263305	0.252305
YFJPAZGBYRDQGG	CN(C)CCOCCOC1=C(Br)C=C(Cl)C=C1	0.269487	0.267639
FHEMKPMORHQQQS	CCC(C)NCCOCCOC1=C(Br)C=C(Cl)C=C1	0.239061	0.230399
ZQEXXTHWIUDAAP	CN(CCCOC1=C(Cl)C=CC(C)=C1)CC2=CC=CC=C2	0.264787	0.276318
HMTNZOGZNYHIEQ	CC1CC(C)CN(CCCNC(=O)C2=CC3=C(N2C)C4=C(NC3	0.242299	0.232016
VEULKRYMXABOMR	FC1=CC(=CC=C1)C(=O)NC2=NN(CC3=CC=CC=C3)C=	0.261788	0.250131
OLFLPZGIJLSZFG	NC1=NC(NC2=CC=C(Cl)C=C2)=NC(CN3CCN(CC3)C4	0.248582	0.223963
ISWRJPQPLRUCHM	CCOC1=CC=C(NC2=NC(CN3CCN(CC3)C4=C(F)C=CC=	0.259823	0.222612
IJMNDTSCUAZHRX	CC1=CC(Br)=C(NC(=O)NC2=CC=C(Cl)C=C2)C=C1	0.239674	0.254674

GVZFKHPHBTYJJ	CC(C)C1=CC=C(C=C1)C(=O)NCCCN2CCN(CCCNC(=O	0.279832	0.249779
QCHPJBPMPZWYTRW	BrC1=C(OCCCCN2C=NC3=C2C=CC=C3)C=CC=C1	0.24023	0.224594
XPBPUSHVNFQNMN	COC1=C(OC)C(OC)=C(CN2CCN(CC2)C(=O)C3=C4C=C	0.281435	0.263733
KVGWUIURYEHAX	FC1=CC=C(COC2=C(CNCC3CCCO3)C=C(Br)C=C2)C=	0.252469	0.231549
JUUPROSNCWGZHL	CCN(CC)C1=CC=C(CNCCC2=C(F)C=CC=C2)C=C1	0.280332	0.261686
DKOLTNOMOCFJKI	C(COC1=C(C=CC=C1)C2=CC=CC=C2)OCCN3CCC4=C	0.283539	0.288377
JFVXGMCWCRFNIA	CC1CCCC(NCCCCOC2=C(C)C=C(C)C=C2)C1C	0.268055	0.247814
RNXXMVAWNIQIAY	ClC1=CC=C(SCCOCCN2CCC3=C(C2)C=CC=C3)C=C1	0.252131	0.260133
YQLVICLGJVP GCZ	CNCCCO1=CC(OC2=CC=CC=C2)=CC=C1	0.239548	0.26342
VFEHOEAMKLDHI	CNCCCO1=C(C)C(C)=CC(C)=C1	0.286983	0.277352
MYMDEOZVGRYQND	C(CNC1CCCC1)COC2=CC=C(C=C2)C3=CC=CC=C3	0.257826	0.23473
YXPAJJOQUGLWAW	CC(C)C1=CC=C(OCCCN2CCCC2)C=C1	0.289971	0.289828
GJUQNXFCNZTWKL	O=S(=O)(CC(CN1CCCC1)N2CCCC2)C3=CC4=C(C=C	0.260979	0.252264
AJOSLCKWHYXIGZ	COC1=C(OC)C=C(NC(=O)N2CCN(CC2)C3=CC=C(C=C	0.267161	0.256293
LGFBWSZKHBLEG	FC1=CC(F)=C(C=C1)\N=C(S)N2CCN(C\C=C\C3=CC=	0.244442	0.228391
UWHKGMMAZFDNPR	[O-][N+](=O)C1=CC=C(C=C1)S(=O)(=O)CC(CN2CCCC	0.243772	0.238481
GRSGNBWLJCPRMF	C(COC1=C(C=CC=C1)C2=CC=CC=C2)CN3CCCC3	0.292605	0.301258
LIVWJOWBAOASLL	COC1=C(OCCCN2CCN(CC2)C(C3=CC=CC=C3)C4=C	0.278028	0.268791
WBHITXUPZPJNFQ	C(COC1=C(C=CC=C1)C2=CC=CC=C2)CN3CCCC3	0.319771	0.281161
AZGMNIZEDJYOTG	COCCCNCCCCSC1=CC=C(Cl)C=C1	0.281148	0.267614
ZPRZGEJEFRDCKP	CN1CCN(CCCCO2=C(C=CC=C2)C3=CC=CC=C3)CC1	0.25213	0.275875
VKEYFEWCJZVRR	CC1CCN(CCCCO2=C(C)C=C(Br)C=C2)CC1	0.303653	0.279976
SUNKWBDBFBWFSC	ClC1=CC(Br)=C(OCCCN2CCCC2)C=C1	0.27154	0.26377
PXOSRXIRTZFHEM	C(CCN1CCCC1)COC2=CC=C(OCC3=CC=CC=C3)C=C2	0.251254	0.259188
FKJMV DLMELUKBZ	CC1CCN(CCO2=CC=C(OCC3=CC=CC=C3)C=C2)CC1	0.283294	0.255162
JTYGCCQWYOUAE	CC1=C(OCCCN2CCCC2)C=CC(Br)=C1	0.28034	0.2539
MRZZAIYUACOFLA	CC1CCN(CCCCO2=C(C=CC=C2)C3=CC=CC=C3)CC1	0.289411	0.275886
CVVWFILCNQEOER	CC1CCN(CCOCCOC2=C(C=CC=C2)C3=CC=CC=C3)C	0.29845	0.290438
DKDIUWSBBSRHRQ	COCCCNCCCCOC1=C(C)C=C(Br)C=C1	0.30462	0.273488
XSWNRULUPLYDX	COCCCNCCOC1=CC=C(C=C1)C(C)C2=CC=CC=C2	0.282331	0.255119
YCEKXMFYKWKGW	C(COC1=CC=C(OCC2=CC=CC=C2)C=C1)CN3CCCC3	0.265854	0.268415
GQFUPFFSXYFHP	CC1=C(C=C(Cl)C=C1)N2CCN(CC2)C(\S)=N\CC3=CC=	0.243689	0.228385
UWHNHEHALYKFPX	COCCCNCCOCCOC1=C(C=C(Cl)C=C1)C(C)C	0.249457	0.234186
HPECOWXNRPSDOW	COCCCNCCCCOC1=C(C=C(Cl)C=C1)C(C)C	0.264703	0.273275
IQVIKDPDRJNOIH	CCCCNCCOCCOC1=C(Br)C=C(Cl)C=C1	0.272648	0.240176
VQTJEOYKUQLCLX	COCCCNCCCCOC1=C(Cl)C=C(Br)C=C1	0.292792	0.262647
YHGWRZQMLHASHX	CC1CCN(CCOCCSC2=CC=C(Cl)C=C2)CC1	0.299409	0.287499
RNV DZTFWEXPPCU	CC(C)NCCCO1=C(CC=C)C=C(Cl)C=C1	0.248372	0.232933
BBUWRFSVSNYDB	C(CN1CCCC1)OC2=CC=C(OCC3=CC=CC=C3)C=C2	0.26432	0.249781
SHFSYRGBXUYCKE	C(CCN1CCCC1)COC2=C(C=CC=C2)C3=CC=CC=C3	0.287195	0.266463
GQYQARJPAMYJJ	COCCNCCCCOC1=C(C)C=C(Br)C=C1	0.265047	0.238236
FQFVOMNQSZAVLR	COCCCNCCOCCSC1=CC=C(Cl)C=C1	0.268521	0.27148
LXYASAOAWTZRBQ	COCCCNCCCCOC1=CC=C(C=C1)C(C)C2=CC=CC=C2	0.250181	0.240685
PGDQVXNYFYSOFA	CC1=CC(OCCCN2CCCC2)=C(C=C1)C(C)C	0.247002	0.233335
WFTUOFGLKWFNW	C(CN1CCCC1)OC2=CC=C(OCC3=CC=CC=C3)C=C2	0.255922	0.241962
KRTDFHGFQAZYDV	COC1=C(OCC2=C(Cl)C=CC=C2)C=CC(\C=N\O)=C1	0.24406	0.231238
FPUGRWXWXIKFML	COC(=O)C1=C(NC(S)=NN2CCN(C)CC2)SC3=C1CCC(C	0.250021	0.22973
PQLCXUPBVIKFFG	FC1=CC(Cl)=C(CN2CCN(CC2)C(\S)=N\CCC3=CC=CC=	0.260144	0.254048

JWEFANVNEHLLDH	CC1=C(C=CC=C1Cl)\N=C(/S)NCC2=C(Cl)C=CC=C2	0.27421	0.25685
HAGMIUXRVWGUFA	CC(C)CN(CC(C)C)CC(O)COC1=C(Br)C=CC=C1	0.280409	0.234662
SXABAObUANMHV	[O-][N+](=O)C1=C(C=C(C=C1)N2CCNCC2)N3CCCCC1	0.276368	0.252458
ZOFUEPAECUOZJV	COC1=C(OCCN2CCC(CC3=CC=CC=C3)CC2)C=CC(=C	0.249796	0.249778
VIGCGDJDZNXXPV	COC1=CC=CC(OC)=C1OCCCN2CCC(CC3=CC=CC=C	0.306588	0.293636
LPVWEORWKBYMBI	CC1(C)COC(\C=C\C2=CC=C(C=C2)[N+](O)=O)=N1	0.253011	0.238994
OQVAJQUCTXKXMW	COC1=C(OC2CCCC2)C=C(Br)C(CNC3CCCC3)=C1	0.299756	0.264901
WXTWEJNFZDBKHN	CCN1CCN(CCCOC2=C(Br)C=C(Cl)C=C2)CC1	0.312912	0.308787
QXCLZDQCQVDKAR	CCN1CCN(CCOC2=C(Cl)C(Cl)=CC=C2)CC1	0.28001	0.281582
BEJVCYTZJSCWPG	CSC1=CC(=CC=C1)N2CCN(CCCNC(S)=NC3=CC=C(F)C	0.304939	0.272583
GOKKDJRZUCAPLS	CCOC(=O)C1=CC=C(NC(=O)COC2=C(OC)C=C(CNC3C	0.261515	0.225615
VBTJJBPDUUBLAN	ClC1=CC(=CC=C1)C2=NC3=C(C=CC=C3)C(NCCCN4C	0.245956	0.223726
KGWDIYMLQDNMQP	[O-][N+](=O)C1=NN(C2=CC=CC=C2)[N+](O)=C1NC	0.253968	0.25453
ZXKOMYIPTDBCFK	COC1=C(OC)C=C(C=C1)C2=CSC(=N2)N3CCN(CC3)C	0.258838	0.263783
FXBLCNQDCJPYSD	CC1=CC(OCCN2CCC(CC3=CC=CC=C3)CC2)=C(C=C1	0.248075	0.248504
PSLFLFQJOCYNET	CCOC(=O)C1=CC=C(NC(=O)COC2=C(CNC3CCCC3)C	0.258681	0.229007
FBTMLLNWEFZLSO	CC1=C(NC(=O)C2=CC=C(CN3CCOCC3)C=C2)C=CC(C	0.24567	0.225868
ORZXAVVYGYBRFH	CCOC1=C(OCC2=CC=C(C)C=C2)C=CC(\C=N\O)=C1	0.243047	0.230162
CGEQTVNVVCKVDH	CCOC(=O)C1=C(NC(=O)CCN2CCOCC2)SC(C)=C1C3=	0.240918	0.229164
GWGXKLPOBVUBID	COC1=CC=C(C=C1)N2N=CC3=C2N=CN=C3N4CCN(C	0.251578	0.242526
REDCWBMFJVHFM	COC1=C(C=CC=C1)N2CCN(CC2)C(\S)=N\C3=CC=C(C	0.250757	0.230206
QYBAPVCAKUOYGY	CCN(CC1=CC=CC=C1)C2CCN(CC3=CC=C(SC)C=C3)C	0.248344	0.233515
YHLDLUMVWQSJHW	CN(C)C1=CC=C(C=C1)C(\S)=N\C2=CC=CC=C2	0.269719	0.285022
XFKBVJQHHPASKP	C(NC12CC3CC(CC(C3)C1)C2)C4=C(OCC5=CC=CC=C	0.273062	0.260994
ASYZTKCDBLULEQ	CCOC1=CC=C(OCC2=CC(=CC=C2)C(=O)N(CC)CC)C=C	0.251408	0.24072
GRRZJWOHVXGXDO	COC1=C(OC)C(OC)=C(CN2CCN(CCCOC3=CC=C(Cl)C	0.280721	0.274779
HEOAYOJFWWSGBM	C(COC1=C(C=CC=C1)C2=CC=CC=C2)CN3CCCCC3	0.24312	0.264845
GOCMETWPMPECCN	C(CCN1CCCCC1)COC2=C(C=CC=C2)C3=CC=CC=C3	0.257208	0.274502
IVLBYNZHIIIHOH	BrC1=C(OCCCN2CCCCC2)C=CC=C1	0.287149	0.277064
QESYMHDXPQJEHR	CC1=CC(C)=C(OCCCN2CCCCC2)C=C1	0.274998	0.277677
YHUXMSLWZYFUGT	BrC1=CC(OCCCN2CCCCC2)=CC=C1	0.278371	0.288886
WIWWIBIRURAGMD	CC(C)(C1=CC=CC=C1)C2=CC=C(OCCCN3CCNCC3)C	0.255968	0.241522
FDGXABIAEZTJCM	CN1CCN(CCCOC2=C(C(=O)C=CC=C2)CC1	0.254354	0.236972
PXUMPNLLASGJTF	CN1CCN(CC1)C2=CC=C(NC(=O)C3=CC=C(O3)C4=CC	0.256301	0.237967
BDHYQZLCEYRYHZ	SC(NCC1=CC=C(Cl)C=C1)=NC2CCN(CC3=CC=CC=C3	0.309635	0.302226
LAMJXNKMRSGCNB	SC(NC1CCN(CC2=CC=CC=C2)CC1)=NC3=C(Cl)C=C(B	0.266653	0.277495
UWONKTWTNIYPQE	CC1=NN(C2=C1C(C)=C(CCC(=O)NC3=CC=C(CN4CCC	0.247465	0.22406
JXONPPKRYJENMO	[O-][N+](=O)C1=CC=C(NC(=O)NC2=C(F)C=C(Cl)C=C2	0.243554	0.267384
FGBRKEJLQWBLOX	CC1=C(OCC(O)CN2C(=N)N(CC3=CC=CC=C3)C4=C2C	0.255959	0.232625
UMGOIUGWGIDDRY	CCCN1CCN(CC1)C2=NC=NC3=C2C(=CS3)C4COC5=	0.247438	0.228813
RZMBLYFTQCGNPA	FC1=C(COC2=C(CNCC3=CN=CC=C3)C=C(Br)C=C2)C	0.243795	0.232864
YFMJHHNGMFMMOI	CCOC1=C(OCC2=CC=CC=C2)C(Br)=CC(CNCCO)=C1	0.305343	0.278431
SNQXWEDASGPDRO	COC1=C(OC2CCCC2)C=C(Br)C(CNCC3=CC=CC=C3)=	0.24946	0.227139
SESBBJCQFFBCAQ	CCN1CCN(CCCOC2=C(C=CC=C2)C3=CC=CC=C3)CC1	0.293022	0.345001
IDNLDKVZUUKPKO	[O-][N+](=O)C1=C2N=CC=C(N3CCCC3)C2=CC=C1	0.304587	0.271771
WUXPIHKVMXGSCO	CNCC1=C2C=CC=CC2=CC=C1OCC3=C(F)C=CC=C3	0.307403	0.314703
CNXCLIWQKBUJL	CC1CCN(CC1)C(C2=C(NC(=O)C3=CC=CO3)SC(C)=C2	0.243639	0.247278
SGMXFQFNCTRIYGN	OC(CON=C1C2=C(C=CC=C2)C3=C1C=CC=C3)CN4CC	0.246131	0.237344

DARZMOVEAYAQSU	CN1N=CC2=C1N=CN=C2N3CCN(CC3)C4=CC(Cl)=C	0.25375	0.246013
MDANCUAEFSMZMJ	S=C1SCN(CC2=CN=CC=C2)CN1CC3=CC=CC=C3	0.280685	0.266313
BULMODKVYZUWGQ	CN1CCN(CC1)C2=NC=NC3=C2C(=CN3C4=CC=C(F)C	0.278904	0.270623
KIQMPLDUQLNUGR	CC1CCN(CCCN2C(=O)C3=C(C=CC=C3)N=C2SCC(=O)	0.283203	0.272499
ZXRLMFHUUUIQRE	[O-][N+](=O)C1=CC=C(C=C1)S(=O)(=O)CC(CN2CCOC	0.255581	0.273682
JLIOYJUFXPJOPJ	CCOC1=CC=C(C=C1)C(C)\N=C(/S)NCC2=CC=C(Cl)C=	0.239325	0.241323
IHTNUABIDOQQHY	CC1=NN(C(NC2=C(Cl)N=C3C=CC=CC3=N2)=C1)C4=	0.278906	0.279603
CRXCHEDZFDDCMS	COC1=C(OC)C=C(NP(=O)(OC2=CC=C(Cl)C=C2)OC3=	0.254441	0.231137
GXADDOMJEKODJM	COC1=CC(NP(=O)(OC2=CC=C(Cl)C=C2)OC3=CC=C(C	0.269779	0.251623
PUMKUBDFETUMHR	COC1=NC(=NC(NC2CCCCC2)=N1)N3CCCCC3	0.261627	0.233131
KYXFQLGXQKEFTL	CN(C)C1=CC=C(CNC2C3CC4CC(C3)CC2C4)C=C1	0.286285	0.227154
UBKHTBJCEMMIX	COC1=C(OCCCCN2CC(C)OC(C)C2)C=CC(CC=C)=C1	0.252836	0.229731
VSUZUIHQHXKTNZ	CN(C)CCOC1=CC=C(C=C1)C(C)(C)C2=CC=CC=C2	0.26092	0.269817
NKFFSZDJFBWGNX	CCC(C)NCCCOC1=C(Cl)C=CC(Cl)=C1	0.269631	0.239411
OJXUTEQKYARIAE	CC1CC(C)CN(CCOC2=C(Cl)C=C(Cl)C=C2)C1	0.296377	0.272046
WXIZYRMWFYFBOF	COC1=CC=C(CN2CCN(CC(O)CN3C4=C(C=CC=C4)C5	0.267142	0.233093
HTESIOSNBHFBPG	ClC1=CC(OCCN2CCN(CCOC3=CC(Cl)=CC=C3)CC2)=	0.312233	0.306687
CCBNQKADENDQLT	COC1=CC(=CC(OC)=C1)C(=O)NC2=NC(=C(O2)C3=CC	0.243914	0.246207
JDWQBGIYOHYBSR	CC1=CC=C(C=C1)C2=NNC=C2\C=N\N3C(=O)C4=C(C	0.244381	0.237106
AQRXEBHCTMZRIO	CCCCCCCC[N+](C)(C)CC#C	0.287953	0.244199
QFOMORMHDMJFDX	CSC1=NC(N(C)C)=C(CC2=CC=C(OC(C)C)C=C2)C(Cl)=	0.250421	0.248477
KIYSHYZINRZPMH	CN1CCN(CC1)\N=C\C2=CC(Cl)=C(Cl)C=C2	0.276025	0.269605
QSHVRKJQAHHUCK	CN1C=NC(=C1OC2=CC3=C(C=CC=C3)C=C2)[N+](O-	0.242453	0.236611
TWMNSQGYKDIDRO	CC1=NC(NCC2=CC=CC=C2)=NC(N\N=C\C3=CC=CC=	0.241967	0.234717
UOIUXZCCHBUOLE	CCN1CCC(CC1)C2=NC(=CS2)C3=CC(Br)=CC=C3	0.300804	0.305275
WDPCUABBFTUIEB	CCCCOP(=O)(C(NC1=CC=CC=C1)C2=CC=CC=C2)C3=	0.256409	0.267365
KSJMFXRFOAAIJ	ClC1=CC=C(C=C1)C2=CC=C(O2)C(=O)NC3=C(C=CC=	0.241076	0.233036
FFIIZXTWAHLAAR	CN1CCN(CC1)C(=S)SCC(=O)NC2=C(C=C(Cl)C=C2)C(=	0.246141	0.231761
RMGDBFVOOAVQD	COC1=CC=C(C=C1)C2CC(=NN2C(=O)C3=CN=CC=C3	0.246916	0.235763
LUMFRFYQKACABY	COC1=CC=C(C=C1)[N+]2=C3SCCN3C(=C2)C4=CC=C	0.274562	0.246439
APZKSDJWVXIYBG	CC1=CC=CC2=NC(CSC(N)=N)=C(Br)N12	0.241004	0.223738
JTPOILAPENLVRK	COC1=CC=C(C=C1)C2=C[N+](=C3SCCN23)C4=CC=C	0.255911	0.229592
HAYUDLNFDROBAK	COC1=C(C=CC=C1)C(=O)N2C3=C(SC4=C2C=CC=C4)	0.241875	0.227876
RQWPMCHDZCMYDY	COC1=CC=C(C=C1)C2=CN3CCCCC3=[N+]2C4=CC=	0.256581	0.241486
VJBSUZOYIXRIG	CCOC1=CC=C(C=C1)[N+]2=C3CCCCCN3C=C2C4=CC	0.265072	0.251878
RYGOLMQJSCPBKD	CCOC1=CC=C(C=C1)C2=CN3CCCCC3=[N+]2C4=CC	0.311433	0.309765
NLKQOQPQCOLHSP	COC1=CC=C(CN2C(=C[N+]3=C2C=CC=C3)C4=CC=C(0.283579	0.248736
IVCMVLQWGVGYGX	COC1=CC=C(CN2C(=C[N+]3=C2C=CC=C3)C4=CC=C(0.240943	0.224559
FJGJMPKHRVYXRC	CCOC1=CC=C(CC2=C(N=C(SC)N=C2Cl)N(C)C)C=C1	0.243981	0.241016
RNTOYPHAKLFIHA	CCOC1=C(CSC(N)=N)C=C(Br)C=C1	0.250913	0.281559
AOFTWMZIZMOCQH	CCCCOC1=C(CSC(N)=N)C=C(Br)C=C1	0.259564	0.244658
BBKCBPMHPQHHEM	CCOC(=O)C1(CCN(CC(=O)NC2=C3C=CC=CC3=CC=C	0.249615	0.243584
MGLURDBJAAAYHC	CCN1CCN(CC1)C2=C(C=C(F)C(=C2)N3CCCC3)[N+](F	0.309815	0.285525
HIRFJJHUBGHUDC	CN1CCN(CC1)C2=C(C=C(F)C(=C2)N3CCC4=C(C3)C=	0.320135	0.292647
VMOSPCSOWBEFCJ	COC1=CC=C(C=C1)C(=O)O[C@H](C2CC3CCN2CC3C	0.259909	0.247125
AZIQVQCACXYRFM	COC1=CC=C(C=C1)C(=O)ON2C(=O)C3=C(C=CC=C3)N	0.248724	0.254929
PMAPSVKQSNRJJJO	CN(C)C1=CC=C(\C=N\NC(=O)C2=C(Cl)C=CC=C2)C=C	0.241303	0.242734
IOXREBLQQCZGU	COC1=CC(=CC=C1)N=C(S)N(CCCN2CCOCC2)CC3=C	0.246702	0.246285

PBXSCDGXPXQLPX	COC1=CC=C(C=C1)N=C(S)N(CCCN2CCOCC2)CC3=Cl	0.242174	0.237429
JZWQVKCQOJKTEF	CN1C=C(CN(CCCN2CCOCC2)C(\S)=N\C3=CC(Cl)=CC	0.273638	0.241543
LRSFFDRYGFKPIL	COC1=C(OCC2=CC=C(Cl)C=C2)C=CC(CNCC3=NC=CC	0.250802	0.239049
FGXORRWATASCLIV	CCN1CCN(CC1)C(\S)=N\C2=CC3=C(C=C2)N=C(C=C3	0.275326	0.249005
ULVCFGLOBJJNMH	FC1=CC=C(COC2=C(CNCC3=CC=NC=C3)C=C(Br)C=C	0.260672	0.223059
AKKNPBZYGQDLY	COC1=C(OC)C=C(CNCCC(C(C)C)C2=CC=C(OC(C)C)C=	0.329125	0.302934
GYJOCYVSODNABJ	COC(=O)C1=C(C=C(OC)C(OC)=C1)\N=C(/S)N2CCN(C	0.268947	0.240424
JDHQMNQTFMMAOM	CCN1CCN(CC1)C(=O)C2=CC=C(CSC3=CC=C(C)C=C3	0.291987	0.26379
JHUZXKHQDVCOQQ	COC1=CC=C(NS(=O)(=O)C2=CC(N(C)S(=O)(=O)C3=CC	0.24814	0.236764
VUBFUAHKEBCMTF	OC(C1CCN(CC(=O)NC2=CC=CC=C2)CC1)(C3=CC=CC	0.289131	0.239741
UUVNYPCBBXOBP	CCC(=O)NC(S)=NC1=C(N2CCCC2)C(Cl)=CC=C1	0.246681	0.230184
VILROXNCRXPOMD	CCOC(=O)N1CCN(CC1)C2=C(C=C(F)C(=C2)N3CCN(0.293572	0.269898
PKSMIXVRARBJHK	COC1=C(OCC2=C(Cl)C=CC=C2)C(Cl)=CC(CNC3CCCC	0.311122	0.262724
QWZQCJLVBHCNJU	SC(=NC1CCCC1)N2CCN(CC(=O)NC3=CC=C(OC4=CC	0.241204	0.23057
APLGOPMDXTVZMI	COCCC\N=C(/S)N1CCN(CC1)C2=CC=C(C=C2)[N+](C	0.24403	0.228351
IHLQVRGYCNKFET	CCC(C)C1=CC=C(C=C1)N=C(S)NC2CCN(CC3=CC=CC	0.263159	0.249581
LFRDEVWAMJRBPU	FC(F)(F)C1=CC(=CC=C1)N=C(S)N2CCN(CC2)C3=CC(=	0.273375	0.256044
FTJTUQRVWVOUOA	COC1=C(OCC2=C(Cl)C=CC=C2)C(Br)=CC(CNCCO)=C	0.267821	0.234578
PNTVSUDFVUTGCM	CC1=C(NC(=O)CN2CCC(CC2)C(O)(C3=CC=CC=C3)C4	0.262191	0.231028
IRZCIGMOYMHWKF	COC1=CC=C(C=C1)C2=NN(C(C2)C3=CC=C(C=C3)N(C	0.265347	0.305934
FXVGRPNJSDXZBY	COC1=CC=C(NC(S)=NC2=CC=C(OC3=CC=CC=C3)C=C	0.259271	0.269469
LPGWRSRDJVSZKN	CCCCNCC1=CC(OC)=C(OCC2=CC=CS2)C(Br)=C1	0.309526	0.243135
YHZWZMLROKXOTC	CN1CCN(CC1)C(=O)C2=CC=C(CSC3=CC=C(Cl)C=C3)	0.262886	0.25615
OXBGNWDZXDFSIY	CCOC1=C(OCC2=CC=CC=C2)C(Cl)=CC(CNC3CCCC3)	0.290736	0.288666
GFLZAPCJCWPPDY	COC1=C(OCC2=CC=C(F)C=C2)C(Cl)=CC(CNC3CCCC3	0.307247	0.306424
RRSLQLMRWNJBR	ClC1=CC(NC(=O)C2C3CCC4C(CCC23)C4(Cl)Cl)=CC=	0.248728	0.23168
ZNYSNAVINDASLY	BrC1=C(NC(=O)C2=C(C=CC=C2)C3=CC=CC=C3)C=CC	0.245358	0.235187
NMILQIXJUCLYPM	ClC1=CC=C(SCC(=O)NC2=C(C=CC=C2)N3CCN(CC3)C	0.240815	0.250899
OPFYPRZIJSHSD	ClC1=CC(Cl)=C(OCCOCCN2CCC3=C(C2)C=CC=C3)C=	0.240304	0.245768
HHIZRUCKMDETPC	COC1=C(C=C(C=C1)S(=O)(=O)N2CCCCC2)N(C)S(=O	0.254042	0.236371
MZQGFOWHHQGHQE	CCN1CCN(CC1)C2=C(C=C(F)C(=C2)N3CCC4=C(C3)C	0.270726	0.249015
MFJHMTFOCRVPES	CC(C)C1CC(CCNCC2=CC=C(C=C2)N(C)C)(CCO1)C3=	0.26237	0.243453
JIWPBHDLXKHUIY	O=C(N1N=C(CC1C2=CC=CC=C2)C3=CC=CC=C3)C4=	0.238729	0.26335
CBZLKDOSMRWOF	CC(N(C)C)C1=C(C=CC=C1)C(O)(C2=CC=CC=C2)C3=C	0.301328	0.285554
FGJSCJRVOKNQRT	COC1=C(OC)C=C(C=C1)C(=O)ON=C(N)CC2=CC=C(Cl)	0.24087	0.24142
HTWRVXQXRQFGJO	ClC1=CC=C(SCCCCN2CCNCC2)C=C1	0.276743	0.277375
SAJUMWGDQUCTNA	[O-][N+](=O)C1=CC(C(=O)NC2=C(F)C=CC=C2)=C(NC	0.243909	0.224004
XQNKEFPXJRALFI	CC1=C(NC(=O)C2=CC=C(CN3C=C(Cl)C=N3)C=C2)C=	0.242182	0.2297
QJPYARHRMNJIKM	CNC1=C(NC)N=C2C=C(C=CC2=N1)[N+](C([O-])=O)[N+	0.272746	0.240023
ZOUZBYNFKZTCNL	CC1N(C(C)=O)C2(CCCCC2)CC(C)(C)C3=C1C=CC=C3	0.251064	0.241683
RJRWCDQVJJBARX	COC1=C(OC)C=C(C=C1)C2=NOC(=N2)C3=C(C=C(Cl))	0.273981	0.256925
DAOGNIPTKRWQJW	COC1=CC=C(C=C1)C2=C(CN(C)C)C(C3=CC=CC=C3)C	0.278685	0.258549
KQINOEXPQWEJAM	BrC1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(CC3=CC=NC	0.240033	0.226413
MWXKPEOYDRTWIC	CCN(CC)CCN(C)C1CCC(CC1)C2=CC=CC=C2	0.310398	0.311834
SQFIEPRJZMJXRF	COC1=CC=C(\C=C2\C(=O)OCC3=C2C=C(OC)C(OC)=	0.253443	0.245448
MHRGHFADWRHYKY	CCC(C)NCCOCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.301892	0.232626
ODXWTIQZKBOZDX	CN(C)CCOC1=C(Br)C=C(Cl)C=C1	0.272005	0.238658
NCXKSMOKOSHEEE	ClC1=C(OCCCNCC2=CC=CC=C2)C=CC(Br)=C1	0.264843	0.242828

WTJDIXPHKATLQB	CN(C)CCCCOC1=C(C)C=C(Br)C=C1C	0.305926	0.276265
KNTZMAYDEMUNCX	CN(C)CCCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.339629	0.302217
ZBBUAIZGIYNBOY	CC1=CC(CI)=C(OCCCCNCC2=CC=CC=C2)C(C)=C1	0.307363	0.252166
XETJGRBNXWFOH	CC1=CC(Br)=C(OCCCCNCC2=CC=CC=C2)C(CI)=C1	0.27672	0.252872
WHIGUJZLRRODIW	COC1=C(CCN2CCC(CC2)C(C)(C)C)C=CC=C1	0.297601	0.270705
WJQZLOXABWPCAW	COC1=C(OC)C=C(CCN(C)CC2=CC(OCC3=CC=CC=C3)	0.339181	0.271889
YYDFKGIJNPKQQQ	COC1=C(OCC2=CC=CC=C2)C=CC(CN(C)CCC3=CC=C	0.401605	0.360606
ITNUOBZVVCQYIR	CCN(CC)C1=CC=C(CN(C)CCC2=CC(OC)=C(OC)C=C2)	0.334503	0.299884
XEYKJRJBLPXUCX	COC1=C(OC)C=C(CCN(C)CC2=CC(OC)=C(OCC3=CC=C	0.325147	0.282293
MLIFNSQYMKISJW	CC1CC(C)CN(C\C=C\C2=C(C=CC=C2)[N+][O-])=O)C1	0.281585	0.227441
QMPBAKPCKCRGHI	CC1=C(C)C(=CC=C1)N2CCN(CCC3=CC=CC=C3)CC2	0.25568	0.226921
IUBPKAQOGIZZMD	CC1=CC=C(C=C1)N2CCN(CCC3=CC=CC=C3)CC2	0.288821	0.250854
WRRZWDSPRAYBPJ	COCCCNCCCOC1=C(Br)C=C(CI)C=C1	0.299634	0.233344
PCXONJJXYHRMLO	CCCCNCCOCCOC1=C(Br)C=C(C)C=C1	0.282992	0.266048
QFJSLSKIXKEPTJ	COCCNCCCOC1=C(Br)C=C(C)C=C1CI	0.267079	0.223332
SZDOLPMWCLBLPB	CC1=C(OCCCCNCC=C)C=CC(Br)=C1	0.248674	0.229995
INVREHUUDVSVED	CC(C)(C)NCCOCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.238834	0.227292
UWUNEDSBUNJFED	CC(C)NCCCOC1=C(Br)C=C(CI)C=C1	0.239915	0.241699
WVFCDXUZPLZEQW	CC1=CC(C)=C(C=C1)\N=C(/S)NCCC(C2=CC=CC=C2)C	0.24037	0.229318
ZDJIVOYTTMIHIB	SC(NCCC1=CC=CC=C1)=NC2CCCCC2	0.255591	0.234471
PTNNZVXQWGI VTC	COC1=CC(OC)=C(C=C1)\N=C(/S)NCCC(C2=CC=CC=C	0.246382	0.227297
JYJAYGWGJVISOU	COC1=C(OCC2=CC=C(CI)C=C2)C(Br)=CC(\C=N\O)=C	0.27093	0.272407
WTJCHZPEHFPZBV	O\N=C\C1=C(OCC2=C(CI)C=CC=C2)C=CC(CI)=C1	0.250658	0.250519
KDTYLDXGROQMAF	CCOC1=CC(C=NO)=CC(Br)=C1OCC2=CC=C(CI)C=C2	0.246765	0.233795
UDJLUJZUDPOEGL	SC(NCCSCC1=C(CI)C=C(CI)C=C1)=NC2=CC=CC=C2	0.248655	0.227818
DUUYHYIRJTUWIV	CN(C1CCCC1NS(=O)(=O)C2=CC=C(CI)C=C2)C3=CC	0.291317	0.289375
GRHHTAWTWPMOCU	COC1=C(C=CC=C1)C2=C(N=C3C=CC=CC3=N2)C4=C	0.272994	0.275834
WXTQEVVFWKQQN	CC1=CC=C(C=C1)C(=O)C2=C(C=CC(=C2)[N+][O-])=O	0.248788	0.234146
XLFGZKSNBLRCLB	CC1=C(C)C=C(C=C1)C(=O)C2=C(C=CC(=C2)[N+][O-])	0.249252	0.240692
ZTQVXCWBAVXCSE	COC1=CC(=CC=C1)N=C(S)NCCC(C2=CC=CC=C2)C3=	0.254426	0.237341
UUKRSZSKURUMHQ	CCS(=O)(=O)N1CCN(CC1)C2=CC(NC(C)C3=CC=CC=C	0.254859	0.250009
AMNSTBWPBHSZPR	CN1CCN(CC1)C2=C(C=C(C=C2)[N+][O-])=O)C(=O)C3	0.283707	0.267488
MJYRMLLWMCTTIQ	CN1CCN(CC1)C2=C(C=C(C=C2)[N+][O-])=O)C(=O)C3	0.293635	0.287741
PQYVCNAZBXRPCW	COC1=C(OC)C=C(C=C1)C(=O)ON=C(N)CC2=C(CI)C=C	0.276635	0.253194
PFUGFBVKYUACM	ClC1=CC=C(CN2CCC(CC3=CC=CC=C3)CC2)C=C1	0.277424	0.272434
CMKIHTVZYQPCON	CC1=CC=C(C=C1)C2=NN(C=C2CSC(N)=N)C3=CC=CC	0.270936	0.278969
WTPMCLVFWZNZLZ	CCN1CCN(CC1)C2=C(C=C(C=C2)[N+][O-])=O)C(=O)C	0.301531	0.273319
JKMSYEBQUVJADV	COC1=CC=C(OCC(O)CN2CCC(CN3C(=O)C4=CC=CC5	0.262012	0.240932
AQXXEMGKTDAVAP	CCCCN(CCCC)CC(O)CN(C1=C(OC)C=CC(=C1)[N+][O-	0.288332	0.237776
ABHCKRUQSBLDMN	NC(N)=N\N=C\C1=CC=C(OCC2=C(CI)C=CC=C2)C=C1	0.257896	0.245632
JVWWXYXUTLHZCP	CC1=C(NC(=O)C2=CC=C(CN3CCC(CC4=CC=CC=C4)C	0.319018	0.292276
TUWASWOKSINXMU	NC(N)=N\N=C\C1=CC=C(OCC2=CC=CC=C2)C=C1	0.325212	0.307717
VOHLOXVZTUDANM	N\C(CC1=CC=C(C=C1)[N+][O-])=O)=N/OC(=O)C(C2=	0.252031	0.269748
YGTWHYDKFQWMCH	NC(N)=N\N=C\C1=CC=C(OCC2=CC=C(CI)C=C2)C=C1	0.241435	0.242204
BBIHYZVVPNDFEM	CC1CCN(CCOCCOC2=C(Br)C=C(CI)C=C2)CC1	0.298705	0.259711
UDGMUTVGJWZWCW	CC1CCN(CCOCCOC2=C(CI)C=C(Br)C=C2)CC1	0.244909	0.257697
UMJQMNYMVGJEGV	COC1=C(CCNCC2=CC(OCC3=CC=CC=C3)=C(OC)C=C	0.263698	0.254971
FYHJDLFXHYHVCBK	CC(C)C1=C(OCCNC(S)=NC2=C3C=CC=CC3=CC=C2)C	0.239342	0.227725

GXOGKKIFMLZWLU	CC(=O)OC1=C(C(NC(=O)CC2=CC=CC=C2)C3=CC=CC	0.293168	0.256774
FQYQIFZGAFMKAJ	CC1CN(CC(=O)NC2=CC=CC(=C2)C(=O)NC3=CC=CC(=	0.238652	0.226907
BJWLIQNCLGRWV	CC(C)C1CCC(C)CC1OCC(O)CN2CCN(CC3=CC=CC=C	0.257906	0.225113
LRIADFAHJSIJAO	CCOC1=CC=C(C=C1)C2N(C(=O)CC3=C2C=C(OC)C(O	0.249514	0.239915
IMSXHNJZMPDAEB	[O-][N+](=O)C1=CC(=CC=C1)C2=NC(=NO2)C3=CC=N	0.239749	0.258163
OUFLODBNKFDTL	[O-][N+](=O)C1=CC=C(OC\C=C2/OC3=C(C=C(C=C3))	0.253403	0.227211
DLFJEYJDKJLRAF	CC1=C(NC(=O)C2=CC=C(CN3CCC4=C(C3)C=CC=C4)	0.24334	0.23137
FXPMPLOCTNNVFP	COC1=C(C=CC=C1)N2CCN(CC2)C(=O)C(SC3=CC=CC	0.282973	0.251696
JYHAMVSBYCEZJP	CC(=O)NC1=C(CN2CCN(CC2)C3=CC=C(F)C=C3)C4=C	0.247098	0.23522
NVPULQRBTOUZRC	CCN(CC)C1=CC=C(NC(=O)C2=CN=C(Cl)C=C2)C=C1	0.256886	0.237046
GKMONRSASOZVEV	ClC1=CC(NC(=O)CN2C=CSC2=N)=C(OC3=CC=CC=C3	0.256225	0.224262
LMEPYNNZHODNKD	ClC1=CC=C(C=C1)C(=O)ON=C2CCCCCN2	0.261029	0.244546
UADSTFVNKMVGDE	N(\N=C\C1=NC=CC=C1)C(=NC2=CC=CC=C2)C3=NC=	0.286497	0.292809
KQYMEUWGNWTQNR	CCOC1=C(CSC(N)=N)C=C(Br)C=C1	0.281344	0.279148
WDUWPOZKU AURIE	CC1=CC=C(C=C1)C(C)(CC=C)NCC2=CC=CC=C2	0.262989	0.278159
JTKBDFHJBRBLSV	COC(=O)C1=CC=C(C=C1)N=C(S)N2CCN(CC3=CC=C(C	0.269151	0.244285
LDEYTFPHRHGQRH	COC1=CC(OCCNC2=C(C=CC(=C2)N3CCCCC3)[N+](0.249056	0.233926
LSUAQIXSFSVXIF	CN(C)CCCN\C=C1\C(=O)N(CC2=CC=CC=C2)C(=O)C3	0.247202	0.239207
YPLQRLFGAHJJMA	C(N1CCC(CC1)NC2=C3C=CC=CC3=NC(=N2)C4=CC=	0.289017	0.263103
GQKRTCAGSAQWNB	CCN(CC)CCCN\C=C1\C(=O)N(CC2=CC=CC=C2)C(=O)	0.258025	0.244755
KQXYFFACRYKBSU	CC1=C(C)C2=C(S1)N=CN=C2NCC(C)(C)N3CCOCC3	0.244776	0.234025
KDHMYSSPRFRNGI	COC1=CC=C(\C=N\NC2=NC(=NC(=C2)N(C)N(C)C	0.266296	0.24128
NSQKAUNDMZCXQV	CC1=C(C=CC=C1)N2N=NN=C2SC3=NN=NN3C4=CC	0.291403	0.27816
FCZRGYLWLUFHGZ	COC1=C(OC)C=C(C=C1)C2=NN3C(SC2)=NN=C3C4=C	0.245332	0.247939
RRQBCJDYYQAJST	CCN1CCN(CC1)C2=NC3=C(S2)C=CC=C3	0.24037	0.229621
RBHZGVFTWLUADV	OCl(=O)(=O)=O.CCN(CC)C1=NC(C2=C1C=CC=C2)=[N	0.245852	0.22294
ZWNRUJRFBJWEW	BrC1=CC=C(\C=N\NC(=O)C2=C(C=CC=C2)N3C=CC=C	0.260385	0.238299
OWDUKYZZXKSFOO	C1CCC(CC1)NC2=N\C(=N/C3CCCCC3)C4=C2C=CC=	0.360836	0.294729
ROCHHJNADQTSRD	CCNC(S)=NC1=CC=C(C=C1)N(C(C)C)C2=CC=CC=C2	0.270387	0.262171
MORMFMXGUXFXPZ	COCCNC(S)=N\N=C(/C)C1=CC=C(C=C1)N2C=CN=C2	0.292075	0.228418
MJKRXXRUOWINKG	CSC1=NC(=NC(=N1)C(Cl)Cl)C2=CC=CC=C2	0.250071	0.25862
LWYDHIFSDUAOND	CC1=CC=C(C=C1)C(N2CCC3=C2C=CC=C3)C4=NN=N	0.244246	0.232952
BVSQAVPIRWSWLO	COC1=CC=CC(=C1)C(=O)OC2=C(CN3CCOCC3)C=C(C	0.244879	0.227579
WQWNBRGPFIQDJL	COC1=CC=C(OCCNC2=C(C=CC(=C2)N3CCCCC3)[N+	0.251808	0.244449
JLLCHARGIPYMIT	CN(C#N)C1=NC(NC2=CC=C(C)C=C2)=NC(Cl)=N1	0.262774	0.260843
SMEHUBTZJNZVHX	CCN(CC)CC#CCC(C)(C1=CC=CC=C1)C2=CC=CC=C2	0.38835	0.336544
YZEUWNDTGFSRCI	CC1=NC(N\N=C\C2=CC=C(C=C2)[N+](O)=O)=NC(=	0.247765	0.260534
PURCLPLAJBDPSN	[O-][N+](=O)C1=C(\C=N\N2CCN(CC2)C3=NC=CC=C3	0.259568	0.253784
MBMXWDHGHXRCPM	NC1=NN=NN1\N=C\C2=CC(=C(C=C2)N3CCCCC3)[N	0.238929	0.234311
QJZSHERJMUXCMW	CC1=CC(C)=NC(SC2=C(C=C(C=C2)[N+](O)=O)[N+](0.257076	0.234556
HFBVLGXCYLGKMD	CN(CC#CCC(C1=CC=CC=C1)C2=CC=CC=C2)C(C)(C)C	0.372097	0.314107
GFBQXPRGIHEBLZ	CCN(CC)CCSC1=NC2=C(N=N1)C3=C(C=CC(C)=C3)N	0.259049	0.247738
BOPZIFGDYDKFKQ	CN1CCN(CC1)C2=CC(=NC3=C(C(C)=NN23)C4=CC=C	0.264005	0.244663
MGRKMZUXHDFOOZ	COC1=CC=C(C=C1)N2C(=O)C3=C(SC4=C3CCCC4)N	0.281702	0.230283
WJVYVQYNRUSJKO	CN(C(=S)OC1=CC=C(C=C1)C(=O)NC2=CC=CC=C2)C3	0.246119	0.223807
IBAJVZQIEQKVFA	CCN1CCN(CC1)C2=CC(=NC3=C(C(C)=NN23)C4=CC=	0.240913	0.22458
NIVKYFMSODCHBA	CN1CCN(CC1)C2=C3C=CC=CC3=NC(=N2)C4=NC=C	0.329415	0.282151
RSVSVTFVNBBOUK	[O-][N+](=O)C1=CC(=CC(=C1)C2=NNC(=N2)C3=CC=C	0.263427	0.264576

XFUOWSIVPDOZPZ	CC(C(=O)C1=CC=C(C=C1)C2=CC=CC=C2)[N+] ³ =CC=C	0.268108	0.23712
XTOYWMZBOPJBBF	N=C1N(CC2=CC=CO2)C=NC3=C1C(=C(O3)C4=CC=C	0.248664	0.248202
JVYMSPPKDODTNF	ClC1=CC=C(C=C1)C2=NN3C(SC2)=NN=C3C4=CC(=N	0.2496	0.244768
PRCHRZJMNMUBL	CN(C)CCSC1=NC(=NC2=C1C3=C(CCCC3)S2)N4N=C	0.253736	0.222428
RWEAXGZDJDTGQE	CN(C)CCSC1=NC(=NC2=C1C3=C(COC(C)(C)C3)S2)N	0.280864	0.236126
IYUNTXJINBRJRQ	CCCCN1C(=O)NC(=O)\C(=C(\CC)NC2=C(OC)C=C(OC)	0.245617	0.225867
JHWCAUPFKZRTML	CN(C)CCCN(C(=O)C1=CC(C)=CC=C1)C2=NC(CC(=O)N	0.338251	0.282082
HQHQLMLBBPGIHNK	CN1C2CCC1C=C(C2)N(CCC3=CNC4=C3C=CC=C4)C	0.285992	0.24881
GROOKPHVLDTGUFU	CC1=CC(CC(CC2=NC3=C(N2)C=CC=C3)C4=NC5=C(N	0.246313	0.227245
PYRRMLCJNCDFH	SC(NC1CC2CCCC(C1)N2C3CC3)=NC4=CC=C(Cl)C=C	0.302018	0.269984
OUERQWUICBAUMO	COC1=CC2=C(C=C1)N3CCN(CC4=CC=CC=C4)\C(=N,	0.265921	0.259951
GRNUHFOJCOJSEC	ClC1=CC(=CC=C1)N2C(=O)N=C3SC4=C(C=CC=C4)N:	0.240184	0.236639
YWNDEYAFFWAJB	CCOC(=O)C1=CC=C(C=C1)N=C(S)NC2CC(C)(C)NC(C)	0.295499	0.229362
YTCMZQLKSYRJL	CCOC1=CC=C(C=C1)C2=NC3=C(C=CC=C3)C(=NN2)C	0.24939	0.254651
GEWWLRYGMYJUOD	NC(CC1=CC=C(Cl)C=C1)=NOC(=O)C2=CC3=C(C=CC=	0.248826	0.273662
IYHJBMSFLDJGMU	CC1=C(C(=O)CN2CCN(C\C=C\C3=CC=CC=C3)CC2)C	0.263794	0.237549
LVIRGEJLFCULO	CCN1C2=C(C=C(Cl)C=C2)[N+](CC)=C1\C=C\N(C)C3=	0.254182	0.273631
BJFQOTJNLNGRAJ	COC1=CC=C(C=C1)C2=NC(=NC(=C2)C#N)N3CCN(C)	0.255563	0.262139
GDKCAAWSNQLXNX	CC1=NC(NCC2=CC=CC=C2)=NC(NC3CCCCC3)=C1	0.264837	0.256431
HUJNAXQVFZTBDR	SC(NC1=CC=CC=C1)=NC2=CC=C(OCC3=C(Cl)C=C(Cl)	0.255	0.266112
BKIOGOWYGSGBSJ	CC1=CC2=C(C=C1)N=C(N2)C3CCN(CC4=NN=NN4)	0.280227	0.238798
OBKYREAEPMNVOJ	ClC1=CC=C(CN2CCC(CC2)C3=NC4=C(N3)C=CC(Cl)=	0.303523	0.273599
OCXSAVQTZUMWDB	CC1=CC=C(CN2CCC(CC2)C3=NC4=C(N3)C=CC(Cl)=C	0.331812	0.278622
DOLRSKODGZOLBF	CC1=CC=C(CN2N=NN=C2CN3CCC(CC3)C4=NC5=C	0.247172	0.236633
ONORYECFZPCHNK	CCOC(=O)NC1=CC2=C(SC3=C(C=CC=C3)N2C(=O)CC	0.245448	0.233303
CKIKNERKNNTMPA	CCN(CC)C1=C2N=CN=C2N(CC3=C(Cl)C=CC=C3Cl)C:	0.267831	0.242575
YGUJRTGZNGUEFD	CCN1C2=C(C=CC=C2)C3=C1C=CC(CN4CCN(CC4)S(C	0.267513	0.24145
MBZRJXDWSXXRPA	C1CN(CCN1C(C2=CC=CC=C2)C3=CC=CC=C3)C4=NC	0.248705	0.233439
YCGSVDGHSBHCMU	COC1=C(C=CC=C1)N2CCN(CCCCOC3=C4C=CC=CC4	0.313558	0.279757
VOHCIXMVPQJCBT	CC(CNCC1CCCO1)COC2=C3C=CC=CC3=CC=C2	0.251533	0.241533
GTWFZIQZWKDHQG	COC1=C(C=CC=C1)N2CCN(CCCCCOC3=CC=C(F)C=	0.298113	0.263616
MDXWCEKNISCBOB	CCN(CC)C1=C(C2=CC=CC=C2)C(N)=C3C=CC=CC3=N	0.240425	0.230594
QLHAVMTYLGFGPT	ClC1=CC(Cl)=C(CN2C=CC(=N)C=C2)C=C1	0.271441	0.243274
WVTBKMSZTWLEJF	ClC1=C(CN2C=CC(=N)C=C2)C=CC=C1	0.271074	0.262528
HUYPSQORIFAKE	CCCCCCN1C=CC(=N)C=C1	0.262247	0.244402
IYHZRMBBRCHWHH	COC1=CC=C(C=C1)C(=O)C(CCCCC(CN(C)C)C(=O)C2=	0.281717	0.242561
XPUBUHIUUWTNML	O=C(NC1=CC=C(C=C1)C2=CSC(=N2)C3=CC=CC=C3)	0.246698	0.246927
OEXXRKSNZNGLHY	COC1=C(OCCN2CSC(=S)N(C)C2)C=CC=C1	0.253816	0.264487
BNHBFAPJZHNXTE	CCOC1=CC=C(C=C1)C2=CN=C3CCCN23	0.272677	0.235484
ZJCAADTWXGBVBW	CCCCCOC1=C(C=C(CSC(N)=N)C=C1)[N+](O)=O	0.249218	0.22495
BJBBLXXEJYVLNN	CCOC1=C(C=C(Br)C=C1)C(\C)=N\NC2=NCCN2	0.26512	0.254706
AYTQUIGQFYMRK	CCOC1=NC(=NC(SCCOC2=C(Cl)C=C(Cl)C=C2)=N1)N	0.267378	0.243543
CYTLIRHZWTZIJZ	C(C1=CC=CC=C1)[N+] ² =C3C=CC4=C(C=CC=C4)C3=C	0.2487	0.231302
JXOJPBJBHDCLFP	CCOC(=O)C1=C(OC2=C1C(CN3CCN(C)CC3)=C(O)C=C	0.246573	0.225478
SKOYRHCAKHQCLN	COC1=CC=C(C=C1)N2CCN(CC2)C(=O)CN3CCN(CC3	0.259455	0.223898
QQFAOBCJMZDGFZ	CN(CC1=C(C)N(C)N=C1)S(=O)(=O)C2=CC3=C(C=CC	0.239592	0.259298
GBXSKDSBFPTQMT	CCN1C(=NC2=C1C=CC=C2)N3CCN(CC3)C(\S)=N\CC	0.267151	0.240905
YULJENCEDMKCBO	CCC1=CC=C(C=C1)N=C(S)NC2CC3CCCC(C2)N3CC4:	0.284357	0.250846

HQFPUAJGLRNHNO	CC1=CC=C(C=C1)N=C(S)NC2CC3CCCC(C2)N3CC4=C	0.295065	0.257934
WBVWGGCUSNNYOF	CC1=CC(=CC=C1)N=C(S)NC2CC3CCCC(C2)N3CC4=C	0.308497	0.270967
SNFOZKYWNCUNHB	CC1=C(C)C=C(C=C1)N=C(S)NC2CC3CCC(C2)N3CC4=C	0.283641	0.227691
HKTRXPBQEMJXKL	C(CC1OC2=C(SC3=C1C=CC=C3)C=CC=C2)CN4CCCC	0.316914	0.30781
VCPJENOVITMSR	C(C1=NC2=C(O1)C=CC=C2)C3=CC=C(CC4=NC5=C(C	0.299757	0.275173
PGECPCGYLPPUBG	CC1=C(C=CC(=C1)S(=O)(=O)N(CC2=CC=CS2)CC3=C(I	0.252013	0.228872
NERDWIVQEVZSNB	CCN1C(CN2CCN(CC2)C3=CC=C(CI)C=C3)=NC4=C1C	0.252168	0.234743
MSELVEFUVDXEPF	COC1=CC(OC)=C(C=C1)N2CCC3=C(C)N=C4C(OC)=C	0.276135	0.245015
ZVCLXPNROWCWPR	COC1=CC=CC2=C3N(CCC3=C(C)N=C12)C4=C(OC)C:	0.268771	0.230743
BQVHJQPCNMOJBF	ClC1=CC=C(C=C1)N2N=NN=C2C3=C(N=C(N=C3)C4:	0.243665	0.229535
MXYNGMIPFOZVCR	CC1=NC2=NC(=CN2C(=C1)N3CCN(CC3)C4=C(CI)C=	0.244122	0.243705
BTDUZNAUJSTJOU	CO\N=C\C1=CC(=C(C=C1)N2CCN(CC2)C(=O)C3=CC:	0.240237	0.227143
RITAQUDKGCTMA	C1CCCCC1.OCCN2CCN(CC2)C3CC4=C(SC5=C3C=C	0.28294	0.266781
IAMLCAUGORULLB	CN1CCN(CC1)C2=CC3=C(SC4=C2C=C(F)C=C4)C=C(C	0.293028	0.284276
WWRPLVWWTUOKJ	CN(CC\C=C1/C2=C(CSC3=C1C=CC=C3)C=CC=C2)CC	0.324258	0.310959
YKTFPDPMGVDHHH	COC1=CC=C(C=C1)N2N=CC(=C2C3=CC=C(CI)C=C3):	0.269567	0.255814
HMRMLANCYBERPV	ClC1=CC=C(C=C1)C2=C(C=NN2C3=CC=CC=C3)S(=O,	0.254434	0.239178
IGIHZEVHFLGLQF	COC1=CC=C(C=C1)C2=CC=NC3=NC(=NN23)N4CCN	0.246951	0.228403
UHVLSVIMQYIHDO	CC1=C(C(=O)N\N=C(/N)COC2=CC=C(CI)C=C2)C(=NC	0.272981	0.243256
OUETVWDFEBXIIG	CC(C)(C)N(NC(=O)NC1=CC(CI)=C(CI)C=C1)C(=O)C2=	0.251624	0.230376
PXIVFERFHLBIGX	ClC1=CC2=C(NC=C2C3=NN=NN3C4=CC=CC=C4)C=	0.240473	0.233035
MVHXEQFYJFVGQN	FC1=CC=C(C=C1)N2N=NN=C2C3=C(N=C(N=C3)C4=	0.260204	0.231116
NOGWKIKUGIOGRI	CC1=CC2=C(C=C1)N=C(C)C=C2NC3=CC4=C(OCCO4	0.268129	0.225097
ZJALJNUPIKLBOV	CCOC1=C(OCC2=CC=C(F)C=C2)C(CI)=CC(CNC3CCCC	0.269672	0.258111
GXEKCEZPKBONE	OCCCCNCC1=CC=C(OCC2=CC=C(CI)C=C2)C=C1	0.270147	0.246912
QOOVZEKTHKXNJ	OCCCCNCC1=CC=C(OCC2=C(CI)C=C(CI)C=C2)C=C1	0.26296	0.243654
CANIKTZQFIBYRL	COC1=C(OCC2=C(F)C=CC=C2)C(CI)=CC(CNC3CCCC	0.287985	0.268563
MRYDXMIUFMHLSD	BrC1=CC=C(C=C1)C2=NC(N3CCSCC3)=C(N=N2)C4=	0.262059	0.264087
IZGSUERWAGXCGI	CCN1CCN(CC1)C2=NC(=NC(SC(C)C)=C2)C3=CC=C(C	0.240543	0.229686
PMNWGMNJCRIDQV	CCN1CCN(CC1)C(C2=C(NC(=O)C3=CC=CC=C3)SC(C)	0.276969	0.238416
CJKCFLYRDSJZME	COC1=CC(\C=N\NC2=NC(=NC(NC3=CC=C(C)C=C3)=	0.255239	0.235452
WVBGVKOFVTPUES	CN(C)C1=C(N=C(O1)C2=C(CI)C=CC=C2)P(=O)(C3=CC	0.253342	0.227641
DGSLNAYNGJCLCL	CC1CN(CC(C)N1)C2=C(N=NC(=N2)C3=CC=C(Br)C=C	0.303237	0.293099
WRPDQUCFOSSPJS	CN1CCN(CC1)C2=C(N=NC(=N2)C3=CC=C(Br)C=C3)(0.251378	0.240815
GYLHKEZFHVNIOV	ClC1=CC(OP(=O)(NC2=CC=CC=C2)NC3=CC=CC=C3):	0.298656	0.249435
AUILCEXTYULELM	COC1=CC(C2=NNC(=C2)C3CCN(CC3)C4=C(C=CC=N	0.252365	0.243057
PLHQKCFXFAHOHFS	BrC1=CC=C(OC2=NC=C(CN3CCN(CC3)C4=CC=CC=C	0.254929	0.229893
OEFIQMOFTOGRZ	Cl.CCOC1=CC(CNCCC2=CC=C(C=C2)S(N)(=O)=O)=CC	0.241554	0.222518
GFQBXMRQGFENBF	O=S(CC1=NC(=NC(SC2=CC=CC=C2)=C1)C3=CC=CC=	0.240356	0.226956
CENHMPXIORHGRL	ClC1=CC=C(C=C1)S(=O)(=O)C2=C(N=NS2)C3=CC=CC	0.242191	0.235364
XWPUVAJJDJDDX	COC1=CC(=CC=C1)N2CCN(CC2)C3=C(C#N)C(=NN3(0.247449	0.222598
OGPAHBYNEJBWTE	CNS(=O)(=O)C1=C(C=CN=C1)N2CCN(CC2)C3=CC(=C	0.256322	0.232834
LFTVZXRUGJNGFT	COC1=CC=C(C=C1)N2CCN(CC2)C3=C4NC5=CC=CC:	0.254583	0.223995
XMFRZFUHINORMI	OC(N\C=N\OCC1=C(CI)C=C(CI)C=C1)=NOCC2=C(CI)	0.283842	0.281888
YSKUMRJOXCGCBL	CC1=C(CS(=O)(=O)C2=NC3=C(C=CC=C3)N=C2)C=CC	0.277092	0.257727
YHXAHRDOPRQCT	CN1CCN(CC1)C2=C(NC(=O)C3=CC=C(O3)C4=C(CI)C	0.272445	0.236843
ODCWNXRKYVORLL	CN(C)C1=NC(=CS1)C2=CC=C(C=C2)[N+](=[O-])=O	0.284667	0.274167
QZPDHIOGDDQVGR	CC1=CC(C)=C(NC(=O)C2=CC=C(CN3CCC4=C(C3)C=C	0.293524	0.255487

HQYYPEABZCQIEL	C1C1=CC=C(COC2=C(CNCC3=CN=CC=C3)C=CC=C2)(0.30036	0.254454
KTTXGCPAHAFTBD	CCC(=O)N1CCN(CC1)C2=CC=C(NC(=O)COC3=C(Cl)C	0.255071	0.226537
ZCHSTDVIRRYJIR	CC1=CC=C(C=C1)N2C(SCC3=NC(=NO3)C4=CC=C(C)I	0.255798	0.248343
RSFJKZMNGBNBFH	CCOC1=C(OCC2=CC=C(Cl)C=C2)C(Br)=CC(CNCCO)=	0.258411	0.245762
BTIJWSSNPZJRY	CCN(CC)CCN1C(=N)N(CCO2=CC=CC=C2)C3=C1C=	0.341264	0.311611
HMVDPSBMURUMKW	CC1=CC=C(C=C1)C2=NOC(CSC3=NN=C(CC4=CC=CC	0.259091	0.269486
DWJBIVQOEBBMFX	C1C1=CC=C(C=C1)C2=NOC(CSC3=NN=C(N3C4=CC=	0.242136	0.243139
QPNWPFVICLCAAX	CCCN(CCC)C1=NC(=NC(N)=N1)C2=C(OC)C=CC(Cl)=	0.266316	0.25953
QRDQOMFEFIBBJS	CN(C)CC1=C(C=CC=C1)C2(O)C3=C(CSC4=C2C=CC=C	0.271217	0.23783
QOVIQRJRTXKFJU	C1C1=CC=C(NC(=O)NCCCN2CCC3=C(C2)C=CC=C3)C	0.296091	0.246647
MDDRWSNZRGJWKC	COC1=C(CC(=O)NC2CC(C)(C)NC(C)(C)C2)C3=C(C=C1	0.258583	0.224234
FEOPHKIAPXXDQZ	CSC1=CC=C(C=C1)C(=S)N2CCN(CC3=CC=CC=C3)CC:	0.245074	0.225781
OLYZPQGCRYWJMC	COC1=C(OCC2=CC=C(Cl)C=C2)C=CC(CNCCN3CCOC	0.302001	0.246019
VUEWAEOLVLURHX	CCCSC1=NC(=NC(=C1)N2CCN(C)CC2)C3=CC=C(OC)I	0.277369	0.264384
NWCOFZGRQWJPBX	C(COC1=CC2=C(CCC2)C=C1)CN3C=NC4=C3C=CC=C	0.274285	0.263966
YLBHFMBUTMFLKO	CN(C)CCNC(=O)C1=CC=C(COC2=C(Cl)C=C(Cl)C=C2)(0.277685	0.255412
JNXNYTVXYJGSGV	COC1=C(OCC2=CC=C(F)C=C2)C(CNCCC3=CNC4=C3	0.268576	0.252809
MCMRMQBQACIYAS	COC1=C(OCC2=CC(Cl)=CC=C2)C=CC(CNCC3=NC=CC	0.277395	0.239589
PAPIOPHQCDRZNX	C1C1=CC=C(CN2CCN(CC2)C3=NC=NC4=C3C(=CS4)C	0.250623	0.229843
HZOUVFXIEDZQBR	CC1=CC2=C(N=C(N=C2NCCCN3CCOCC3)C(F)(F)F)C	0.258292	0.22447
WARDEZUQTYBQRX	CCN(CC(=O)NC1=CC(C)=NN1C2=NC(C)=CC(C)=N2)C	0.24035	0.226414
VYOSGODVAZSQCF	NC1=NC(NC2=CC=CC=C2)=NC(CN3CCC(CC4=CC=C	0.288962	0.237617
YAYHYWWKCFAPKI	COC1=CC=C(C=C1)C(CNC(=O)C2=C(OC)C=C3C=CC=	0.264231	0.253994
QUHMQOAHHLRDNE	COC1=C(OCCCN2CCCC2)C=CC(\C=C\C)=C1	0.255939	0.238356
NUODQPXIBAZSKZ	C(CCN1CCCC1)COC2=CC=C(OCC3=CC=CC=C3)C=C	0.257634	0.240084
MPADXQRDLMSCFA	CCCN(CS)=NC1=CC=C(NC2=CC=CC=C2)C=C1	0.288323	0.251095
CFPFBAMQBRZFTB	CCCN(CCC)CC#CCOC1=CC=C(OC)C=C1	0.271162	0.247791
ZHTQDAFKFNIAEJ	C(COC1=CC=C(OCC2=CC=CC=C2)C=C1)CN3CCCCC:	0.257222	0.2592
YBDBDLJYQGTTEL	CC1=C(OCCCCN2CCCC2)C(=CC=C1)C(C)(C)C	0.243866	0.224456
KVXDMAVJTSWXQE	COC1=CC(OCCSC2=NC(N)=CC(N)=N2)=CC=C1	0.239818	0.223623
RECJWNWZVDPHTR	CC1=C(C=O)C(C=O)=C(C)N1CC2=CC=CC=C2	0.244862	0.232724
MLCOUDSAHVZGSZ	CCOC1=NC(=NC(NC2=CC(Cl)=C(OC)C=C2)=N1)N3C	0.269773	0.255403
IZPMIQXCORNEBS	CCN(CCC(=O)NC1=CC(C)=C(Br)C=C1)CC2=CC=CC=C	0.256573	0.23563
PAEBNEQLSFRKPA	O=C(NC1=CC=C(C=C1)C(=O)OC2CCCC2)C3CCCCC:	0.25204	0.237197
NZQDIZLTOXEKBJ	CCNC1=NC(SCCOC2=CC=C(C)C=C2)=NC(NC(C)C)=N:	0.265105	0.242753
VCAFBCJZFWGQQ	CC1CCN(CC1)C(=O)N2C3=C(SC4=C2C=CC=C4)C=CC	0.250991	0.227216
KZMNEUDJPXGUHK	C1C1=CC(Cl)=C(CN2C=C(\C=N\N3C=NN=C3)C4=C2C	0.244947	0.235614
NCCDUMYZJREKV	CCN(CC)C1=CC=C(C=C1)N2C(C)=CC(C=O)=C2C	0.256139	0.243559
ZZAZHFYLWKJNNT	CC(C)(C)CC(C)(C)NCC(O)COC1=C(F)C=C(Br)C=C1F	0.245399	0.225201
XCWZVWQOWUAVHN	CCOC(=O)C1=C(C)SC2=C1N(C(=O)CN(CC)CC)C3=C(S	0.294352	0.252865
CXEOXHFRVSMJHA	CC1=CC(CN2CCN(CC3=CC=C(Cl)C=C3)CC2)=CC=C1	0.259853	0.250702
BIEBYLJZXQGHFD	CC1=CC(=CC=C1)C(=O)O\N=C(/N)CC2=CC=C(C=C2)[0.273664	0.266462
IIRYXZKXMAAGME	C(N1CCN(CC1)C2=NC3=CC=CC=C3C4=C2C=CC=C4	0.241336	0.232658
OMLVVIWJFYCDRC	CC(C)NCCOCCOC1=CC(C)=C(Cl)C(C)=C1	0.254571	0.247578
XBVINISZBXHUEW	COC1=CC=C(C=C1)C(N)=NOC(=O)C2=CC(=CC=C2)[N	0.251064	0.236771
FYDXTSDJPHQUMZ	CC1(C)CC2=C(C=CC=C2)C(NNC(=O)C3=NC=CC=C3)=	0.258864	0.259171
BIEKBOAPWJBVSP	CCCN(\N=N\C1=CC(=CC=C1)[N+][[O-])=O)C2=CC=C	0.261652	0.282121
CKMYOVXRWBUCBE	COC1=CC2=C(C=C1)C(C)=CC(=N2)N3CCN(CC3)C4=C	0.255031	0.25855

PAWJOLDYSVNDLF	CCCCCOC1=CC=C(CN2CCN(CC)CC2)C=C1	0.286693	0.245299
DEIZXTGKXXFXFL	COC1=C(C=CC=C1)N2CCN(CC3=C(Cl)C=C(Cl)C=C3)C	0.238949	0.231574
JFDUNNTVXUDHSF	CCN(CC)C1=CC=C(CN2CCC(=CC2)C3=CC=C(F)C=C3)	0.283119	0.243135
YLHNXEFEKGQGGX	ClC1=C(C=CC=C1)C2=CC=C(CN3CCN(CC3)C4=CC=C	0.270965	0.243345
HXAALNHUNDFNAG	ClC1=CC(NC(=O)NC2=CC=CC=C2)=CC(Cl)=C1	0.245722	0.249688
VWJAYGIZVFLNFB	CN1CCCN(CC2=C(Cl)C=C(Cl)C=C2)CC1	0.251786	0.259278
TWFBQVYJVVPGEV	CCN1CCN(CC2=CC(OC3=CC=C(Cl)C=C3)=CC=C2)CC	0.306901	0.293709
RHTVLVDZUFGCM	CN1CCN(CC2=CC(OC3=CC=C(Cl)C=C3)=CC=C2)CC1	0.307474	0.271274
YQZHTUZDSCIWGT	CC1=C(C=CC=C1)N2CCN(CC3=CNC4=C3C=CC=C4)C	0.285961	0.245243
CCNHJWKQNZUWBC	CN(C)C1=C(C#N)C(=NC=C1)N(CC2=CC=CC=C2)CC3=	0.27707	0.261018
HLWGQPDMRUMUBC	CC1CCN(CC(O)COCCC2CC4CC(CC(C4)C2)C3)CC1	0.348043	0.277936
UXFUFUAMAGXED	CCN(CC)CCN1C(NC(=O)C2=CC=C(Cl)C=C2)=NC3=C1	0.248297	0.253075
XHNLICSHYXRRRU	CCCCN1CCC2=C(N)C3=C(C=CC(Br)=C3)N=C12	0.260035	0.228709
MIQFBVNMSNEFFS	O=S(=O)(OC1=CC=CC=C1)\C=C\C2=CC=CC=C2	0.295943	0.250122
GUFZUGXNBXBWFF	CC1=NC2=C(C=CC=C2)C(=C1)N3CCN(CC3)S(=O)(=O	0.253497	0.22249
LRGXJHPESRPBJJ	CCOC(=O)C1=C(NS(=O)(=O)C2=CC=C(OCC)C=C2)C(=	0.272353	0.241055
SADMOYKKNMBFNC	COC1=C(OC)C=C(C=C1)C2=C(C)NN=C2C3=C(O)C=C(0.244513	0.229336
JPWJXSIDSZJDAS	COC1=C(C=CC=C1)N2CCN(CC2)C3CCN(CC3)S(=O)(=	0.287977	0.247834
MXPFZKGBTAPXGI	COC1=C(Br)C=C(CN2CCN(CC2)S(=O)(=O)C3=CC=C(C	0.243764	0.263949
QJJDJGGXMIKHG	CCN(CC)S(=O)(=O)C1=CC=C(C=C1)C2=CC=C(C=C2)S(0.241129	0.245988
SGYJJYITWMLWJY	CC(C)(C)N1N=NN=C1C(N(CC2=CC=CS2)CC3=CC=CC	0.307727	0.271183
ZYWQCSWVZKNUOJ	N#CC1=CC(=CC=C1)C(N2CCCCC2)C3=NN=NN3C4	0.258296	0.249588
XJGLRLPMNQYBO	COC1=C(C=CC=C1)C(N2CCCCC2)C3=NN=NN3CCC	0.302162	0.264554
KYDHPCWYILKKLP	FC1=CC=C(CN(CC2=CC=CC=C2)C(C3=CC=CS3)C4=N	0.247757	0.231548
PHLXQWKNUVUFUHP	FC1=CC=C(C=C1)C(N2CCCC3=C2C=CC=C3)C4=NN=	0.247492	0.234254
NUUCIGIMSHFSTN	CC(C)(C)N1N=NN=C1C(N(CC2=CC=CC=C2)CC3=CC=	0.319273	0.309759
FSBUWEPMPXKRBG	COC1=CC(=CC(OC)=C1OC)C2=NN=C(O2)C3=CC=CC:	0.257155	0.336998
HUQUQRMXRCGVHV	CCOC1=NC(OCC)=NC(NC2=CC(Cl)=C(OC)C=C2)=N1	0.260138	0.265169
KQFQDPQDZXEMJO	CN1CCN(CC1)C2=CC(=NC3=CC(=NN23)C4=CC=C(F)	0.246146	0.242567
KNLBJJWWKPSMLJ	CCN1CCN(CC1)C2=CC(=NC3=CC(=NN23)C4=CC(F)=	0.244057	0.242604
DTAVDUKDVHWDGI	N(C1=NC(=CS1)C2=CC=NC=C2)C3=CC=CC=C3	0.254201	0.241849
LLZBBUSYDDCIHI	CCN(CC1=CC=CC=C1)C(C2=NN=NN2C(C)(C)C)C3=C(0.24289	0.23784
PUUZKSNYSNKYBU	CCN(CC1=CC=CC=C1)C(C2=NN=NN2C(C)(C)CC)C3=	0.298531	0.295844
DSIJIWPKYALVPW	CCOC1=CC2=C(C=C1)N=C(NN=C2C3=CC=C(C)C=C3)	0.244884	0.276015
QBMPNWRHTXHPPC	CCCCOC(=O)CC(N1CCCC1)C(=O)OCCCC	0.239931	0.226294
JQMVBGTGLWRZBN	COC1=C2C=CC=CC2=C(C=C1)C(=O)C3=CC=C(C=C3)	0.252312	0.257148
BKDOYQAYQBPWCW	CCN1C(CNC2=CC=C(Cl)C=C2)=NN=C1SCC3=CC=C(C	0.245259	0.225344
ZPHWBMFZZUNXAS	CC1=CC(NC2=NC(=NC(=N2)N3CCCC3)N4CCCC4	0.241051	0.237882
VLOLDCVHFBJWEG	CC1=CC=C(CN2CCN(CC3=C(C=CC=C3)C(F)(F)CC2)	0.264588	0.243797
YZUYACPEASIANE	CCOC1=CC2=C(C=C1)N=C(NN=C2C3=CC=C(C)C=C3)	0.24471	0.25416
JWOKQHIWSOTUTQ	CC1=C(NC2=NC(SC3=NCCS3)=NC(NC4=C(C)C=CC=C	0.241394	0.237423
KQEROGTWFRRPRET	FC(F)(F)C1=C(CN2CCN(CC3=CC=CC=C3)CC2)C=CC=	0.257027	0.251673
RPSUUNBXYWODIB	COC1=C(OC)C=C2C(CC(C)(C)N=C2SC)=C1	0.280025	0.267
ICSZZKJAACPKQV	CCN(CC)CCCNC1=C2C=CC=CC2=NC(=N1)C3=CC=CC	0.32861	0.267006
NXFVZVNBQJQOMR	CC=1C=C(N(N1)C=2N=C(N=C(N2)N(C3=CC=CC=C3))	0.256645	0.227422
XXNRZZXPXAFYRJ	CC1C(N(C)C(CC1(O)C2=CC=CC=C2)C3=CC=CC=C3)C	0.281737	0.241458
XANBEVHQLOSTKB	CC(C)C1C(N(C)C(CC1(O)C2=CC=CC=C2)C3=CC=CC=	0.309184	0.265047
GMKOTCDQUJTHJW	ClC1=CC=C(CN(CC2CCCO2)C(C3=CC=CS3)C4=NN=	0.317542	0.271964

ZSXLRXQCIPPUBL	CN1CCN(CC1)C2=NC(C)=NC3=C2C(C)=C(S3)C(=O)N	0.253299	0.236367
CPIGJVVUIMHDJX	FC1=CC=C(CN2CCCN(C2)C(=O)NC3=CC=C(CI)C=C3)	0.323143	0.301427
KSQQBSHUOFGFPY	FC1=C(C=CC=C1)N2CCN(CCCNC(=O)CCS(=O))(=O)CC	0.30267	0.254028
MOUCFYOVUVZKGO	CCN1C=C(C2=NC(C)CO2)C3=C1C=CC=C3	0.272297	0.278909
IUQFASBFPJNXNL	C(NC1CCCCC1)C2=CNC3=C2C=CC=C3	0.2695	0.228095
WAORDGOWMGVLES	ClC1=C(NC(=O)C2CCN(CC3=C(N4C=CC=C4)N(N=C3	0.256367	0.257249
XXJNZRSVXFNCF	CC1=CC2=C(N=C(S2)N3CCC(CC3)C(=O)NCCCN4CC	0.258055	0.242893
XDJPIAZHJWEVFX	CCN(CC)C(C(=O)NC1=CC=C(C=C1)C(C)C)C2=CC3=C(0.255766	0.233078
ZOXGTPAJSZQQQL	CN(C1CCN(C)CC1)C2=C3C=CC=CC3=NC(=N2)C4=C(0.320793	0.261622
GUUNSUFKFQVCAM	CC1=C(C)C=C(C=C1)N=C(S)NC2CCN(CC3=CC=CC=C:	0.282272	0.258388
FBPUSSTVPEHJZ	CN1CCN(CC1)\N=C\C2=CC=C(C=C2)C3=CC=CC=C3	0.265678	0.262224
CAKMYIPQMBADR	CC\C(=N/NC(S)=NC(C)C)C1=CC(OC)=C(OC)C=C1	0.246971	0.249029
JTFAPYUEBOLXAA	CC(C)C1CCC(C)CC1OCC(O)CNC(C)C2=CC=CC=C2	0.270461	0.24232
PZBQWXVZZSOME	CC1=CC=C(C=C1)[N+]2=C3CCCN3C=C2C4=CC=CC=	0.257894	0.235865
DSNJWBWIHZBKBY	CC1=CC=C(C=C1)C23CC4CC(CC(CN))(C4)C2)C3	0.295495	0.248977
JSJDJVKIJBHDEV	CC1=C(CCN(CC2=CN=CC=C2)C(\S)=N\C3=CC(F)=CC:	0.248433	0.2402
IOQOTMJQIOAEGE	ClC1=C(CC2=CN=C(NC(=O)C3=NCCN3)S2)C=CC=C1	0.241567	0.234102
RGXQSTAXYTZFAH	CNC1=C(C=CC=C1)C(C)(C)C2=CC(=NO2)C3=CC=C(F)	0.254339	0.222917
FFZPOJBEZPEIS	CCOC1=CC=C(OCC(O)CNC2CCN(CC3=CC=CC=C3)C(0.303127	0.270691
RGERENBIMAVPHU	CN(C)CCCN(CC1=CC=CC=C1)C(\S)=N\C2=CC(=CC=C	0.260451	0.272783
MITHIUBSAMMSKI	CCCN1CCC(CC1)=NNC2=C(C=C(C=C2)S(=O))(=O)N3C	0.261202	0.237231
APGNGCGMAUPNGB	COC1=C(C=CC=C1)N2CCN(CC2)C3=C(CI)C=C(C=C3)	0.243243	0.22657
WGDSAFOTCQLQRE	CC1=C(C=CC=C1Cl)\N=C(/S)NC2CCN(CC3=CC=CC=C(0.30783	0.278931
DSYPCNCZRPTQR	SC(NC1CCN(CC2=CC=CC=C2)CC1)=NC3=C(CI)C=C(C	0.28007	0.269249
UMMYMWVAVAFBMI	COC1=CC=C(C=C1)C(\C)=N\N=C(/S)NCC(C)=C	0.276752	0.254756
MUDFBKCKCRBPPG	CC1CN(CC(O)COC(C2=CC=C(CI)C=C2)C3=CC=C(CI)C	0.252275	0.249417
HNUKTONMTDKSNL	CC(C)(C)CC(C)(C)\N=C(/S)NC1CCN(CC2=CC=CC=C2)	0.287308	0.270425
ZTSTZMCJXAIHKT	COC1=CC=C(C=C1)C(CNC2=C(C=C(C=C2)S(=O))(=O)N	0.26057	0.233946
GYEAWEXUZSBOFM	CCN(CC)C1=CC(CC(C)(C)C1)=[N+]2CCCC2	0.282649	0.251619
KOLGEUCXCXNGKF	CC(CCC1=CC=CC=C1)NC(S)=NC2=C(C)C=CC=C2C	0.249077	0.231689
IRLFCKFNNDZJQF	CCCCNC(S)=N\N=C\C1=C(F)C=CC=C1	0.25943	0.253975
WGAIKQUMPSQOC	COC1=CC(NP(=O)(OC2=C(CI)C=CC=C2)OC3=C(CI)C=	0.241621	0.244178
JHLURTREAGIFPK	CC1(C)CC(=CC(C1)=[N+]2CCCC2)N3CCCC3	0.253277	0.231637
WJMIMXYRGJRXJX	CC(NC(=O)NC1=CC(CI)=C(CI)C=C1)C(N2CCOCC2)C3	0.257532	0.248355
XMHYKWUTXHOZPS	CC(NC(S)=NC1=C(CI)C=C(CI)C=C1)C(N2CCCC2)C3=C(0.252378	0.233179
XIRMZKNKBAGVWMK	OC(COC(C1=CC=C(CI)C=C1)C2=CC=C(CI)C=C2)CN3C	0.271347	0.261525
RFDWBDBJZPGSDV	OC(COC(C1=CC=C(CI)C=C1)C2=CC=C(CI)C=C2)CN3C	0.260448	0.244901
SVSVLBHIFZWSRG	CC1=C(NC2=NN=C(CS2)C3=C(F)C=CC=C3)C=CC=C1	0.254433	0.244371
UJRLZGIGEHBNG	NC(=O)C1=C(NC(=O)CN2CCCC2)SC(=C1)C3=CC=C(0.245546	0.245693
WHJMAVKRZMGXCB	COC1=CC(OC)=C(\C=N\OCC(=O)NC(C2=CC=CC=C2)(0.244935	0.23488
CZHISYXHAMLNPP	COC1=C(OC)C=C2CN(CCC2=C1)C3=NC(CN4CCCC4	0.244448	0.248398
RATWPNWVUUMXKZ	CC1CCN(CC1)C2=NC(CN3CCCC3)=NC4=C2C(=CS4	0.269432	0.251373
GTMGOATVZUJYOY	COC1=C(OC)C=C(C=C1)C2=NN(C=C2\C=N\NC3=NC:	0.241144	0.249326
WIHHAAMSUSMUNX	COC1=C(OC)C=C(CN(C)C(C)C(=O)NC2=C(CI)C=C(C=C	0.247926	0.226956
FFRXGZVWUXIOFC	CCC1=CC=C(C=C1)N=C(S)NC2CCN(CC3=CC=CC=C3)	0.265847	0.252621
UHKRNZBRPHNBOS	COC1=CC(=CC(OC)=C1OC)C2=NN=C(CSC3=NN=C(N	0.248032	0.235106
UPICNCXVCNWBJJ	FC1=CC(\C=N\NC(S)=NC2=C(CI)C=CC=C2)=CC=C1	0.243045	0.231542
SBDIXHSCQKEGEH	CCN(CC1=CC=CC=C1)C2=CC=C(\C=N\N=C(N)N)C=C:	0.25771	0.262021

SLVVATXCONJWRI	FC1=C(NC(=O)NC2=CC(Cl)=CC=C2)C=CC(Br)=C1	0.244086	0.248123
GDTXUEISIGTSKV	CC(C)C(C)NC(=O)COC1=CC=C(SC2=CC=C(OCC(=O)N	0.247817	0.240641
UQSMUJOGDKXYLDZ	CC(C)C1=CC=C(C=C1)N=C(S)NC2CCN(CC3=CC=CC=C	0.262555	0.250498
YISSDERVCSJHT	C1CC2=C(CN1C3=NC=NC4=C3C(=CS4)C5=CC=CC=C	0.253868	0.234918
RQLJXERUJHJDFLW	CN(CC1=NC(NC2=C(C)C=CC=C2)=NC(N)=N1)CC3=C	0.280409	0.255483
STTBDSZTRDAOTP	[O-][N+](=O)C1=CC(C(=O)N2CCC3=C2C=CC=C3)=C(C	0.258773	0.238622
BRYADXWQXOCNNO	CCNC1=NC(CN2CCCC2)=NC3=C1C(=CS3)C4=CC=C	0.288609	0.266619
GQJNFXFTZTBLZ	OC(CNC1CCCC2=C1C=CC=C2)COC3=C(Cl)C=CC=C3	0.242803	0.256259
JSDVJMOIUAOCKP	COC1=C(OC)C=C(CNCCC(C2=CC=C(F)C=C2)C3=CC=C	0.268216	0.26088
UILQWCDDYAJXJZ	COC1=CC=C(C=C1)N2N=NN=C2C3N(C)C(C)(C)CC4=	0.325976	0.300529
QLJKULLHBGHQDQ	CCN(CC)CC1=CC=C(NC(=O)C2=C(Cl)C3=C(S2)C=C(Cl	0.25698	0.236475
QOAGYTJZVXSXHX	CC(C)OP(=O)(C(NC1=CC=CC=C1)C2=CC=CC=C2)C3=	0.264216	0.227045
WSPSTYUUVYFNI	COC1=CC=C(C=C1)C(CCNCC2=CC=C(F)C=C2)C3=CC	0.25584	0.251794
LTARLXNMDBFWOI	COC1=CC=C(C=C1)C(CCNCC(C)C2=CC=CC=C2)C3=CC	0.242686	0.238863
JKQHGOLFKHLBOU	COC1=CC=C(C=C1)C(CCNCC2=CC=CC=C2)C3=CC=C	0.258667	0.238005
VKNDOFXTCCPRML	COC1=CC=C(CNCCC(C2=CC=C(F)C=C2)C3=CC=C(OC	0.268539	0.246418
KQVIYHJSXGPHKZ	COC1=CC=C(C=C1)C(CCNCC2=C(F)C=CC=C2)C3=CC	0.242441	0.263106
RCNXXRUYIDGGD	COC1=CC=C(C=C1)S(=O)(=O)N2C(COC3=C2C=CC=C	0.281529	0.223582
DVXFIGSTXDVTMY	CN(C)CCCNS(=O)(=O)C1=CC=C(OC2=C(Cl)C=C(C=N2	0.267121	0.258557
WDPAIMDQTHEXQA	CN1C2=C(C=CC=C2)C(\C=N\OC(=O)C3=CC=C(F)C=C	0.247936	0.23362
LKVPXJLABQUOEI	COC1=CC=C(CNCC(O)(C2=CC=CC=C2)C3=CC=C(Cl)C	0.267791	0.254083
ZMIRPKQRKYFMDH	COC(=O)C1=CC=C(C=C1)N2CCC(CC2)C3=CC(=NN3	0.243653	0.23307
SLDHMWQQBRXOPJ	CCOC(=O)C1(CCN(CC2=CC=C(Cl)C=C2)CC1)S(=O)(=	0.263577	0.255117
BPJVHYKTKRZBIP	ClC1=C(Cl)C=C(CN2C=C(CCN3CCS(=O)(=O)CC3)C4=	0.240144	0.226402
DEAUJTDWFWZDHU	CC1=CC=C(C=C1)S(=O)(=O)C2=C(OC3=C(C)C(C)=CC=	0.253902	0.239316
XWRNYKBJTXUZEB	CC1=CC2=NC(=C(CN3CCOCC3)N2C=C1)C4=CC=CC=	0.263791	0.24596
FXMKRHIUUZIFV	COC1=CC(=CC=C1)C(=C\C2=C(N=C3N2C=CC=C3)C	0.253718	0.227124
ZECTTYWBFIVMLX	CN(C)C1=C(C#N)C(OC2=CC=C(C=C2)C(C)(C)C)=NC=C	0.285124	0.260584
DIKNWBKZSAJDIQ	CN(C)C1=C(C#N)C(OC2=CC=C(Cl)C=C2)=NC=C1	0.254382	0.246646
SCNLPUFJULYTHF	COC1=C(SC2=CC(Cl)=CC=C2)N=C(N=C1)C3=NC=CC=	0.275853	0.241239
UUDMVIMMEVTSAD	COC1=C(SC2=C(Cl)C=CC=C2Cl)N=C(N=C1)C3=NC=C	0.26492	0.263236
QKSGRSQVRBFEB	COC1=C(OC)C=C(CNCC(O)(C2=CC=C(Cl)C=C2)C3=C	0.248013	0.238731
NMEOYLUNPQMPFS	COC1=C(CNCC(O)(C2=CC=C(Cl)C=C2)C3=CC=C(Cl)C	0.271317	0.234187
BGVKRGSSHQCQDF	COC1=CC=C(CNCC(O)(C2=CC=C(Cl)C=C2)C3=CC=C	0.262525	0.242372
LZZXJXVVDIPROL	COC1=C(SC2=CC=C(Cl)C=C2)N=C(N=C1)C3=NC=CC=	0.270523	0.238542
ALSLDYJTFGXFLD	CN(C)C1=NC(C2=C(Cl)C=C(Cl)C=C2)=C(C=N1)S(=O)(0.252113	0.245953
JBGNGFJSYNQYML	OC(CSC1=C(Cl)C=CC=C1)CN2CCN(CC2)C3=CC=C(F)	0.340483	0.279504
JLCZXQCYGWUHC	CCOC1=C(OCC)C(Br)=CC(CNCC2=CC=CS2)=C1	0.291985	0.238563
JJKQQRKSKAEBE	COC1=C(OCC2=C(Cl)C=C(Cl)C=C2)C=CC(CNCC3=NC	0.250162	0.224856
NOEWXKXWASRWJB	COC1=C(OCC2=C(Cl)C=C(Cl)C=C2)C=CC(CNCCN3CC	0.318243	0.282092
YBVSECASAQHRMH	FC1=C(COC2=C(CNCC3=CC=NC=C3)C=CC=C2)C=CC	0.29238	0.240816
QFESFPVBIJPECI	O=C1CC(=C(C2=CC=CC=C2)C3=CC=CC=C3)C(=O)N1	0.238684	0.222769
AIXGNQFHVKZCMK	ClC1=CC(Cl)=C(OCC(=O)N2CCCN(CC2)C(=O)COC3=C	0.25451	0.235772
JGIYPOIEJZBYNH	OC1=C2N=CC=CC2=C(CN3CCN(CC3)C4=CC=CC=C4	0.268944	0.230745
CCHLMSUZHFPSC	CC1=C(CSC2=NC3=C(N2)C=CC=C3)N=CC=C1OCC(F)	0.248925	0.227032
OMVOIQOJAQKYML	ClC1=CC=C(C=C1)C(N2CCSCC2)C3=NN=NN3CCC4=	0.266275	0.252164
SKJFQDYGDDOQEC	CC(C)(C)N1N=NN=C1C(N(CC2=CC=CO2)CC3=CC=C	0.281621	0.269151
ZSCFGJKUZUBHLP	FC1=CC=C(NC(=O)CN2CCC(CC2)C(=O)C3=CC=C(F)C	0.275539	0.268205

BXIXXXYDDJVHDL	<chem>Nc1cc(Cl)ccc1N</chem>	4-Chloro-1,2-diaminobenzene	0.228573
VVBLNCFGVYUYGU	<chem>CN(C)C1=CC=C(C=C1)C(=O)C2</chem>	Michler's ketone	0.240754
USSIQXCVUWKGNF	<chem>Cl.CCC(=O)C(CC(C)N(C)C)(c1c</chem>	Methadone hydrochloride	0.285051
VYZAHLCBVHPDDF	<chem>O=[N+](O-)]c1cc(ccc1Cl)[N+](</chem>	1-Chloro-2,4-dinitro	0.24828
OUPZKGBUJRBP GC	<chem>O=C1N(CC2CO2)C(=O)N(CC3C</chem>	1,3,5-Triglycidyl isocyanurate	0.225639
STJLVHWMYQXCPB	<chem>CCCC1COC(CN2C=NC=N2)(O1</chem>	Conazole Mix II (116	0.241877
TXUZVZSFRXZGTL	<chem>Oc1ccc(cc1)C(\c2ccc(OCCN(C</chem>	(Z)-4-Hydroxytamoxifen	0.227634
OPNUROKCU BTKLF	<chem>Cc2ccccc2NC(=N)Nc1ccccc1</chem>	1,3-Bis(2-methylphe	0.244254
VYWPPRLJNVHPEU	<chem>O=C(CCl)c1ccc(Cl)cc1Cl</chem>	2,2',4'-Trichloroacetophenone	0.222392
JAWNWEKHDFBPSG	<chem>N=C1NC(=N)C2=C1C=C3C=CC</chem>	1,3-Diiminobenz(f)-isoindoline	0.265547
NAZZKEZTSOOC SZ	<chem>CC1=CC=NC2=C1C=CC3=CC=CN=C23</chem>		0.25202
BRPQDJPIBCQFSR	<chem>CC1=C(C)C2=C(N=CC=C2)C3=NC=CC=C13</chem>		0.241215
GHYKV VHGPCZVOG	<chem>C1COCCOC2=CC=CC=C2OCCOCCOCCOC3=CC=CC=C3OCCOCCO</chem>		0.337227
IYZPSKNKXWSFJB	<chem>CC(CC1=C(SC2=C(O)C=CC=C2)</chem>	Specs, AE-641/30177025, NSC-2	0.236716
BTMBDRIKPNQIGA	<chem>CN1CC2CC3=CC=CC=C3SC4=CC=CC(=C24)C1</chem>		0.27999
ODRWNMOVHUSDRV	<chem>NCC/C=C1/C2=CC=CC=C2CSC3=CC=CC=C13</chem>		0.309386
HCENOERZKIRXPE	<chem>FC1=CC=C(C=C1)C(OCCN2CCCC2)C3=CC=C(Br)C=C3</chem>		0.327283
GHZNNDWKJRHDC K	<chem>CC(OCCN1CCCC1)(C2=CC=C(F)C=C2)C3=CC=C(F)C=</chem>		0.267714
HLSOHEMSDNNTJI	<chem>ClC1=CC=C2SCC3=CC=CC=C3(\C4=N\CCN4)C2=C1</chem>		0.351451
DQOHSEZYXSACCG	<chem>CN(C)CC1=CC=C(SC2=CC=CC(=C2)Cl)C=C1</chem>		0.233094
LRJYCOXCGLJCLI	<chem>CN(C)CC1=CC=CC(=C1)SC2=CC=CC=C2Cl</chem>		0.298488
DGDOAYXAWGZZMH	<chem>CN(C)CC1=C(C)[N](CC2=CC=CC=C2)C3=C1C4=CC(=CC=C4C3=O)</chem>		0.234983
UNTIDFUZYGXBI	<chem>OC(C1CN2CCC1CC2)(C3=CC=CC=C3)C4=CC=C(Cl)C=C4</chem>		0.304612
VWJJD NBPVIMITE	<chem>CCCOC1=CC=C(C=C1Cl)\C2=C\ S\C3=N\CCN23</chem>		0.256073
LNWZCAHWXGGAY	<chem>CCN(CC)C1=CC=C(C=C1)\C=N\N=C(S)\NCC2=CC=C(OC)C=C2</chem>		0.243089
WHVNGICQKYBDDP	<chem>FC(F)(F)C1=CC2=C(SC3=C(C=CC=C3)N2CCCN4CCN(CCCl)CC4)C=</chem>		0.226867
VBWVJZYUPVDPN	<chem>FC1=CC=C(C=C1)C(=O)CCCN2CCC3=C(C2)C4=CC(F)</chem>		0.248005
AIEOARPRTKSOKM	<chem>CC1=CC=C(C=C1)C(O)(C2CN: Chem Div, D090-015</chem>		0.249766
DJCAGMWMFPMXHO	<chem>CCN1CSC(=S)N(C1)CC2=CC=CC=C2</chem>		0.280821
RUAJRKRPPGDWBK	<chem>NCCC1=C([N](C2=CC=CC=C2)C3=CC=CC=C13)C4=CC=CC=C4</chem>		0.225931
LURMIKVZJSMXQE	<chem>CCN(CC)CCN1C2=C(SC3=C1C=CC=C3)C=CC=C2</chem>		0.271419
QUXNTLCQMWWQBGC	<chem>CCOC(=O)C1=C(C)[N](C2=CC=C(C)C=C2)C3=CC=C(O)C(=C13)CN(</chem>		0.226335
SNBUOLJXURTGNE	<chem>NC1=NC=NC(=C1\N=N\C2=CC=CC=C2)N</chem>		0.249263
CSJUPLAKKSKSQQ	<chem>CC[N]1C2=CC(=C(Cl)C=C2[N+](=C1\C=C\NC3=CC=C</chem>		0.239913
NWDOJCD SZHOIRR	<chem>COC1=CC(=CC(=C1OC)OC)C2=NOC(=C2C#CC3=CC=</chem>		0.23847
RABUWGWSP OYGN O	<chem>BrC1=CC=C(CN2CC[C@H]3\C=C/CC4=CC=CC(=C34)C2)C=C1</chem>		0.24224
OVPXVDTVZJWVGC	<chem>O=C1CCN(CCC2=CC=CC=C2)CCN1[C@H](CSC3=CC=CC=C3)C4=</chem>		0.228265
CDWTXYBGOGVCD S	<chem>CNC(C)C#CC1=C(C)ON=C1C2=CC(=C(OC)C(=C2)OC)</chem>		0.242049
YNCQFVAVWUBVJA	<chem>COC1=CC(=CC(=C1OC)OC)C2=NOC(=C2C#CC3=NC=C[N]3C)C</chem>		0.223615
ZBHN VUQCYBDIJW	<chem>COC1=CC(=CC(=C1OC)OC)C2=NOC(=C2\C=C\C3=CC</chem>		0.250499
DOZLGCD BIUCXPZ	<chem>COC1=CC(=CC=C1F)C2=C(C)ON=C2C3=CC(=C(OC)C(=C3)OC)OC</chem>		0.253951
LNFIOWKUVKUCNC	<chem>O=C1CCN(CCN1[C@H](COC2=CC=CC=C2)CC3=CC=</chem>		0.25847
OCAXFDULERPAJM	<chem>CN1C2CCC1CC(C2)OC(C=3C= 3-alpha-[(4-CHLOROPHENYL)PHI</chem>		0.224289
XDOMZLKSZGWQDP	<chem>CCN(CC)CCCNC1=N[C@@H](C2=CC(F)=CC=C2)C(C(=O)OC)=C(C</chem>		0.244843
BNHZZSKSDXENCK	<chem>COC1=CC(CNCCC2=CNC3=C2C=CC=C3)=CC=C1</chem>		0.229179
ILTDMXMXER GEPX	<chem>CCOC(=O)C1=C(N2CCN(CC2)C3=CC=CC=C3)C4=C(C=CC(OCC)=C</chem>		0.233785
SWZOJT TWWCZKTG	<chem>COC1=C(C=CC=C1)C2CCN(CC3=C4C=CC=CC4=CC=C3)CC2</chem>		0.284454
RLJCULGZUPDOJI	<chem>N1C(=NC(=C1C2=CC=CC=C2)C3=CC=CC=C3)C4=CC=CS4</chem>		0.224551

SSWHDVCIDUKFPK	C1CCN(CC1)C2=C3C=CC=CC3=NC(=C2)C4=CC=CS4	0.231976
KZKWTMMRPCTLNF	COC1=CC=C(SC[C@H])(CC2=CC=CC=C2)N3CCN(CCC	0.246608
ACIVIROIWGWZTE	CCC(CC)COC(=O)C(C#N)C1=N(Vitas-M Laboratory,STK920545	0.237099
ICPHJSKVAZMKIV	[H][C@@]1(CN(C)CCC2=CC(O R(-)-SCH-12679 mal€	0.263916
LCYDVASONUXCGX	OC[C@@H]1[C@H](C=NN1C2=CC=CC=C2)C3=CC(Cl)=CC=C3)C	0.222724
QVEISLUVGUTKAZ	C(N1C[C@@H]2C(C3=CC=CC=C3)C4(CC2(C4))[C@F	0.244223
YZVGXJBXRGLPRH	OC(COC1=CC=CC=C1)CN2C(=N)N(CCN3CCCCC3)C4=C2C=CC=C	0.22865
XCQBEENDHMMMRU	CSC1(S\C2=N\CCN2)SC3(NCCN3)S1	0.276481
HDIJLRXRAJUXQB	CCC1=C(CC2NCCC3=C2C=CC=C3)CC4N(CCC5=C4C=C(OC)C(OC	0.236854
ZIJYGZOMZWSARO	CN(C)CC1=C(C=CC(=C1)C(F)(F)F)C(O)(C2=CC=CC=C2)C3=CC=CC=	0.24649
FVXMKGRYMOKOFX	OC1CC2CCC(C1)N2CCCN3C4=C(SC5=C3C=C(Cl)C=C5)C=CC=C4	0.229326
GGRMGYJBCRHKM	[O-][S+]1(=O)CCN(CC1)C2=C(CC(C3=C[NH]C4=C3C=CC=C4)C5=C	0.263386
YQQOWRFAYJNTDF	CN(C)CCCN1C2=CC=C3C=CC=CC3=C2SC4=CC=CC(=C14)Cl	0.247082
VKJJBAAUCOSHBQ	CCN(CC)CCN1C2=C(SC3=CC=C4C=CC=CC4=C13)C=CC=C2	0.234646
IUBMTYVIPGXROV	ClC1=CC2=C(C=C1)C(NCCN3CCCCC3)=CC=N2	0.249189
LCHYXWHFOJGIHN	CN(C)C1=CC=C(C=C1)C(C2=CC=C(C=C2)N(C)C)C3=CC=C(C=C3))F	0.22254
AAOYLOCWJSLIJU	OC1=C(C=C(Br)C=C1)C(=O)C(=O)C2=C(O)C=CC(Br)=C	0.256861
ABWVZIKPCCNRGU	CN1CCN(CC(=O)N2C3=C(C=CC=C3)C(C)(CC2(C)C)C4	0.268061
ACAYSFZBEWEESJ	CCN(CC(=O)NC1=C(OC)C=C(C=C1)[N+][O-])=O)C2=C(0.240661
ACEBDVMGZIEHJD	CN1C=C(CN2CCCC(C2)C(=O)NC3=CC(=CC=C3)C4=C	0.246922
ACOCVPBXFYMYNV	COC1=CC(=CC=C1)N2CCN(CC2)C(=O)C3=C(C)NC(=C	0.240103
AGCCYFQBWLFIQI	ClC1=CC(=CC=C1)N2CCN(CC2)C(=S)C3=CC4=C(OCC	0.248475
AICDQXIWWSLIDU	CC1=CC=C(SCCN2CCN(CC3=CC=CC=C3)CC2)C=C1	0.239281
AJIKMVRVZGINJ	CCOC1=CC=C(OCCOCCN2CCC3=C(C2)C=CC=C3)C=C	0.246674
AKWKXFMCOJEAHL	CC1=CN=C(SC2=C(C=C(C=C2)[N+][O-])=O)[N+][O-]	0.248802
AKYVRGYXXUMSTM	COC1=CC=C(OC)C2=C1SC(=N2)N(CCN(C)C)C(=O)C3	0.239841
ALOCSDLPLYPB	CC1=CC=C(NS(=O)(=O)C2=C(C)C=CC(=C2)C(=O)NCC	0.242532
ALUAIUOWXSRNSF	COC1=CC2=C(SC=C2C3=CC=C(O)C=C3)C4=CC=C(S	0.241882
AMCHGSHJMDQEAO	CN(C1=CC=C(C=C1)C(=O)N2CCN(CC3=CC=CC=C3)C	0.241391
AMWRRGYURMZDDM	CC1(C)CCCC(C)(C)N1CC(O)COCCOC2=CC=C(Br)C=C	0.284319
ANCNMIYALYWRQU	CCNC(S)=N\N=C\C1=CN(CC2=CC=C(F)C=C2)C3=C1C	0.248215
ANQGVGTXLLOAND	CCCC1=CC=C(C=C1)C(C)NC(S)=NC2CCCCC2	0.239583
AODUIAGAJDMVAK	CN(C)C1=CC=C(\C=N\NC2=NC=CC=C2)C=C1	0.240398
AOGSEIZPHCFJRK	COC1=C(OC(F)F)C=CC(CN(C)C2=NC=C(C=C2)S(=O))(=	0.24829
ASHAMCREPXTDMT	CC1=CC(OCCSCC2=NC3=C(N2)C=CC=C3)=CC=C1	0.246707
ASPBUIUVBTWTAK	CC1=CC=C(C=C1)S(=O)(=O)NCC2=CC=C(C=C2)C(=O)	0.253775
ASYHJCPZWQIFAK	NC(=O)C1=C(NC(=O)C2=CC=C(O2)[N+][O-])=O)C3=C(0.238706
ATKYHVZXLZCIR	OCCN1CCN(CC2=CC(OC3=CC=C(Cl)C=C3)=CC=C2)C	0.26551
AUQGAUMQKXUNEM	CC(C)CCNC(S)=NC1=CC2=C(C=C1)N=C(C=C2)N3CC	0.244129
AUZXBFTVQZNSY	COC1=C2N=C3C=CC=C(C(=O)NCCN(C)C)C3=NC2=C1	0.254113
AWHPVVQJIDGCTK	COC1=CC(CN2CCCC(C2)C(=O)C3=CC=C(C=C3)C(C)(0.244715
AWILWAIEQYZUEQ	CCC(C)C1=C(OCCCN2CCCC2)C=CC=C1	0.244828
AWPWKYKUKZMFHZ	CN1CCN(CC2=C3C=CC(Br)=CC3=CC=C2O)CC1	0.242968
AYWMOOPWNCZFLH	CCCCCCN1[C@@H](CC2=CC=CC=C2)CN=C1NC3=	0.251073
AZWWKRAUFGDLEV	CC1=CC(C)=NC2=CC(=NN12)C3=CC=CC=C3	0.241632
AZYYTGPPGUBKMK	C(CN1CCN(CC1)C2=CC=CC=C2)SC3=CC=CC=C3	0.256086
BCLKQHNNVNSIB	CCOC1=CC2=C(C=C1)N=C(S2)N3CCCC(C3)C(=O)NC	0.239822
BCQUHCBKPBGUBW	CC1CCN(CC1)C2=CC=C(NC(=O)C3=CC=C(O3)[N+][C	0.23985

BDIWRLFHQNJQPS	NC1=NC(NC2=CC=C(F)C=C2)=NC(CSC(=S)N3CCN(CC	0.245061
BEDWAXDWZAFXKE	CC1=C(CN2CCC(CC2)C(=O)NCCCN3CCOCC3)N=C(O	0.254238
BENHUXHIBFRHAF	COC1=CC(CCC(C)NCCC(C2=CC=CC=C2)C3=CC=CC=C	0.244852
BGXBASVKZMVIMZ	COC1=CC=C(C=C1)C2=CSC3=C2C(=NC=N3)N4CCN(0.243959
BGYAWMGHQKHEHV	COC1=C(CC(N)=NOC(=O)C2=C(C)C(=CC=C2))[N+][[O-	0.264888
BIHVOVYTUAZKHG	CC(C)CCOC1=CC=C(\C=N\NC(S)=NC2=C(C)C=CC=C2	0.242393
BKLVNZQTBJAKRV	CCN(CC)C(=O)OC1=C(Br)C2=C(C=CC=C2)C=C1	0.243203
BLKXRHHHEWFOMN	COC1=CC=C(\C=N\NC(=O)CSC2CN(C2)C(C3=CC=CC	0.239228
BMKCEUMCZXRNL	ClC1=CC=C(CON2C3=C(C=CC=C3)N=C2C4=CC=C(Cl	0.256292
BOGBUFCJECXELS	CC1=CC=C(C=C1)C(=O)N=C(S)N2CCN(CC2)C3=C(C)C	0.240413
BPOGDFBKCFMJIQ	COCCN1CCC(CNCC2=CN(N=C2C3=CC=CC=C3)C4=C	0.250322
BQDQCUMFHPQCKL	COC1=CC(OC)=C(CNCC2=CC(OC)=CC(OC)=C2)C=C1	0.24597
BRKYBGNMHLZFKM	CC1=C(C)C2=C(C=CC=C2)C(=O)NCCCN3CCOCC3)N	0.248916
BROKBQPCAUXVOP	CSC1=NC(N2CCOCC2)=C(CC3=CC=C(OC(C)C)C=C3)C	0.239626
BSIIBCCVRXMNQU	C1CC[N+](C1)(CC#CC2=CC=CC=C2)CC#CC3=CC=CC:	0.256301
BTNXMDVVSFARFLG	OCCN(CCO)C1=CC2=C(C=CC3=CC=CC=C23)C4=C1C	0.251465
BUFSPPRZEBZAIM	CN(C)CCNC1=NC2=C(C3=C(CCCCC3)S2)C(=O)N1CC	0.249634
BWJGIXLFNCIUSJ	CN(C)C1=CC=C(C=C1)P(=O)(COC2=CC=C(C=C2))[N+]	0.249217
BWPADOCCBNXFAX	[O-][N+](=O)C1=CC=C(C=C1)C(=O)C[N+](=O)C	0.242521
BWRDWZMTGISINW	CCCCC1=CC=C(NC(=N)NC2=N Chem Div,4477-280	0.245996
BWUREMXPYRLHH	CC1=CC=C(CNC2=NC3=C(CS2)C=CC=C3)C=C1	0.243892
BYFVAWVWHDPHGP	CC1=CCCC2C(CN3CCCC3)C(=O)OC2C=C(C)CC1	0.276248
BYIUAKQEWUPRQD	FC(F)(F)C1=CC2=C(SC3=C(C=CC=C3)N2C(=O)CN4CC	0.239393
CASXYKFSVICGKG	COC1=CC=C(C=C1)C2=CC=C(C=C2)C(=O)C3CC3	0.250906
CBBCXYFTKWGBGY	COCCC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC(O	0.242312
CCVGPSSIPPYTFZ	COC1=CC=C(C=C1)C2=NN(C=C2C(=O)N3C4CCN(C)C	0.239189
CDTKKVKZZGALS	CC1=CC=C(CN2N=CC3=C2N=CN=C3NN)C=C1	0.240821
CDUPTXNAHOCCGC	COC1=C(OC)C(CNCC2=CC=C(SC)C=C2)=CC=C1	0.258411
CEYHTCEQRVERQ	CC1=C(CO\N=C(/C#N)C2=C(Cl)C=CC=C2Cl)C(=NO1)	0.23992
CHGRYVDOMCDAOT	CC1=CC=C(C=C1)\N=C2/SC3=C(CN2CCN4CCOCC4)	0.250226
CINVZWPFSYWSJX	CN(C)CCCN(C(=O)C1=CC=C(C=C1)S(=O)(=O)N(C)C2C	0.240131
CIUKMZPIIFWZBP	SC(=N\N=C(\C1=CC=CC=C1)C2=NC=CC=C2)N(CC3=	0.248271
CIXVTQBZSGIERE	COC1=C(OCC2=C(Cl)C=CC=C2)C=CC(CNCCN3CCOC	0.319475
CJKPBSUQNAAOAI	O=S(=O)(NCC1=CC=CC=C1)C2=CC=C(C=C2)S(=O)(=C	0.258834
CKBPBVOQBKBRML	CN(C)CCC(=O)C(CC1=CC=CC=C1)C2=CC=CC=C2	0.240612
CKFKBFSZCBLKGT	CN(C)CCCN(C(=O)C1=CC2=C(CCCC2)C=C1)C3=NC4:	0.255609
CLOUJGMPFHDOX	COC1=C(C=CC=C1)C2=NC3=C(C=CC=C3)C(=C2)C(=C	0.24031
CLTJAEIXEDUHGG	CC1CN(CCN1C2=CC=C(C)C=C2)C(=O)NC3=CC(=CC=	0.251023
CNAPXSVYNCJBGH	OC1=C(CN2CCN(CC3=CC=CC=C3)CC2)C=C(Br)C=C1	0.258066
CNRGCQAEKZRVAQ	COC1=C(C=CC=C1)N2CCN(CC2)C(=O)C3=C(C)C4=C	0.241572
CQVBTZIRVOVNHJ	O=C(CN1CCN(CC1)S(=O)(=O)C2=CC=CC=C2)NC3=C	0.246688
CRPZJMIZBLMWCK	C1CCN(CC1)C2=NC3=CC=CC=C3C4=C2C=CC=C4	0.247016
CTHMZUGHOXRSPZ	CCCC1=C(CC)C(N)=C2C=C(C)C=C(C)C2=N1	0.247874
CUNGLMWGFPBDBG	COC1=CC(O)=C(C=C1)C2=C(C(C)=NO2)C3=CC4=C(O	0.242813
CUPVITJALNDBTF	CCCN(CCC)C1=C2C=CC=CC2=NC(=N1)C3=NC=CC=C	0.24429
CVRJHVAQAVRFMR	CN(C)CCCN(C(=O)C1=CC=C(C=C1)S(=O)(=O)N2CCCC	0.238698
CWLOYLAJKOSCN	COC1=CC=C(C=C1)N2CCN(CC2)C(=O)CC3=CSC(NC:	0.245959
CYHNHIXLALJCGX	COC1=CC(=CC=C1)C(=O)NCC(N2CCC3=C2C=CC=C3	0.258374

CZTLMENWYKDRIV	CC1=C(C=CC(CI)=C1)\N=C(/S)NCCC2=CC=C(CI)C=C2	0.242948
DALXANAQFPUVST	CN(CC1=CC=C(C=C1)C(F)(F)F)C2=C(C=C(C=C2)S(=O)	0.252192
DBYCDKBEVKWZNL	NNC1=NC(=CC(=N1)C2=CC=CC=C2)C3=CC=CC=C3	0.240298
DDCMMHFKQIPWRB	CCOC(=O)CN1C=C(N=C1[N+](=[O-])=O)[N+](=[O-])=O	0.24977
DDEPXLQZTPGPRT	FC1=CC=C(CN2C=C(CCN3CCS(=O)(=O)CC3)C4=C2C:	0.246374
DEXCOBKOWPYHFL	O=S(=O)(\C=C\C=C\S(=O)(=O)C1=CC=CC=C1)C2=CC:	0.240965
DGJHXQSBRSJUQL	CC1=C(C)C2=C(S1)N=CN=C2N3CCN(CC3)S(=O)(=O)(0.241923
DGLAWAKKMLEAPT	OC(CSC1=C(CI)C=CC=C1CI)CN2CCN(CC2)C3=C(F)C=	0.281209
DLWFEKNOTMFPDS	CC1=CC=C(C=C1)C2=CSC3=C2C(NCCN4CCOCC4)=N	0.244188
DMCGEDUQPQSKBS	CC1=CC=C(SC2=C(C=C(CN3CCCC3)C=C2)[N+](=[O-]	0.261137
DMFRUFZGJWUTPH	ClC1=CC(NS(=O)(=O)C2=C(Br)C=CC(Br)=C2)=C(C=C1	0.256414
DPMVOLXFUXSYFM	O=C(CC1=CC=CC=C1)NCC2=CC=C(C=C2)N3C=CC=C	0.247482
DQCQUKZQVRZXPQ	COC1=CC=C(C=C1)N2CCN(CC3=C(O)C=C4CCCC4=C	0.249493
DQFZMCBEFYMOEH	ClC(\C=N\N1C=NN=C1)=C\C2=CC=CC=C2	0.243187
DSRGSSHFKNBGB	OCCNC1=C(C=C(C(=C1)N2CCCCC2)[N+](=[O-])=O)[N	0.239699
DSTKAXBTHYRORR	CCNS(=O)(=O)C1=CC=C(CCC(=O)N2CCN(CC2)C3=C(I	0.245618
DTLUOQNGNUEEPA	CC1=NN(C(NC2=NC3=C(C=CC=C3)N=C2)=C1)C4=CC	0.245045
DUIITUKMHKGDFO	CCN1CCN(CC1)C2=C3C=CC=CC3=NC(=N2)C4=NC=C	0.260907
DVAUHDRQKGLXCV	CC1=CC2=C(C=C1)N=C3CCCC3=C2NC4=CC5=C(OC	0.251805
DWCJGYVSROLRDX	CC1CCN(CC(O)CN2C3=C(CCCC3)C4=C2C=CC(C)=C4	0.247155
DXFQOZH IWCKOFB	ClC1=CC=C(CSC2=NC=CN2CC3=CC=CC=C3)C=C1	0.244906
FALDMNVTRFXNIT	N=C1N(CCCN2CCOCC2)C=NC3=C1C(=C(N3CC4=CC	0.238794
FBELSXQLSAVMRE	CNC(S)=N\N=C\C1=CC=C(C=C1)C(C)C	0.238467
FBGRTVMOJNNXSR	CC1=NC2=C(OC3=C2C=CC=C3)C(=N1)N4CCN(CC5=	0.24069
FBKVMQMNKXKDOJ	NC(N\N=C\C1=CNC2=C1C=CC=C2)=NC3=CC=CC=C:	0.247782
FESEYQAWPFCPT	CN1CCN(CCCNC(=O)C2=CC=C(CSCC3=CC(CI)=CC=C	0.240524
FEQSHWFAEKVGMW	CCOC1=CC2=C(C=C1)N=C(S2)N(CCCN(C)C)C(=O)C3:	0.251793
FIAOAIAXJRLEKI	FC(F)(F)C1=CC(=CC=C1)N2CCN(CC3CC4CC3C=C4)C	0.260866
FKIMWLJCPAASGO	CC1=CC=C(C=C1)C2=NOC(CCC(=O)NCCCN3CCN(CC	0.244652
FKPPLKWOEVXWOX	COC1=CC(=CC=C1)N2CCN(CC2)C(=O)CN3C(=O)NC(I	0.248671
FLDNBQIVOBCKJJ	COC1=CC(OCC(O)CN2CCC(CC3=CC=CC=C3)CC2)=C	0.259112
FLOVYJLTXSWHOB	COC1=C(F)C(F)=C(C(=O)NC2=CC=C(C=C2)N3CCN(CC	0.251271
FLZMETVYJNPQMX	CCOC1=CC=C(C=NN=C(S)NC2=C(C)C=CC=C2)C=C1	0.249328
FMKZPYAVQWBLSF	COC(=O)C1CC2=C(NC3=C2C=CC=C3)C4(CCN(CC5=C	0.242341
FQMNXKJTBWHTO	CC1CC(C)CN(C1)C2=CC(CC(C)(C)C2)=[N+]3CCCC3	0.24274
FRBOSQJLOCHVIY	COC1=CC(OC)=C(NC2CCN(CCC3=CC=CC=C3)CC2)C:	0.249057
FRIIXSFULMALB	O=S(=O)(CC(CN1CCCCC1)N2CCCCC2)C3=CC=CC=C:	0.252818
FSSMNMJYMDGYBK	CCCCN=C1N=C(S)N(C2=CC=CC=C2)C(C)=C1C(C)=O	0.244951
FUGFLZGGLPTLSE	CC1CCN(CCCOC2=C(C=CC=C2)[N+](=[O-])=O)CC1	0.255591
FUXHOSSLOMXVJP	CC[C@H](C)[C@H]1CNCCN1CCC2=CC(=CC(=C2)(0.24793
FVCSHCORWAOAEB	CC1C(C)N(C(=O)CCl)C2=C(C=CC=C2)N1C(=O)CCl	0.251725
FYBPVKZVCGENMO	COC1=CC2=C(SC(=N2)N(CCCN(C)C)C(=O)C3=CC=C(I	0.254923
FYQPQRIFFTINR	CC1=CC2=C(NC(=N2)C3CCCN(C3)C(\S)=N\C4=C(C)C	0.238614
GAIRREYVAQANTA	CCCCCCCN1C(=N)N(CC(=O)C2=CC=CO2)C3=C1C=C	0.244677
GANLGRNROBRFHX	CCCCCCCN1C(=N)N(CC(O)C2=CC=CO2)C3=C1C=CC	0.240287
GAPPGYVPJUGIHP	C\C(=N/N=C(S)SCC1=CC=CC=C1)C2=NC=CC=C2	0.2526
GASXTRAPCWRQAH	CC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC(OC)=C	0.259376
GBPRGJDUEMKMOK	CC1=C(OCCNC(S)=NC2=CC=CC=C2)C=CC=C1	0.25386

GBQCHUUUTXAHAS	FC1=C(CN2CCC(CC3=CC=CC=C3)CC2)C=CC=C1	0.239105
GCEIBLLNWJRDPK	FC(F)(F)C1=CC(=CC=C1)N2CCN(CC2)C(\S)=N\CC3CC	0.243729
GCNZGZROTNFCTM	CN1C(=N)N(CC(=O)C2=CC=CC=C2)C3=C1C=CC=C3	0.249861
GDIRMWOXEPARKY	CN(C)C1=C(C=C(C=C1)\C=N\N=C(N)N)[N+](([O-])=O	0.264454
GDPSFDWQTOIHIX	CC1=CC(C)=NC(=N1)N(CCOC2=CC=C(Cl)C=C2)C#N	0.248629
GDRWQEOJSGTFNQ	CC(N)CC1=CN(CC2=CC=CC=C2)C3=C1C=CC=C3	0.248511
GEMARUXNGYWZLQ	COC1=C(OC)C=C(C=C1)C2CC(=NN2C3=CC=CC=C3)C	0.238929
GGHXKKZQNZKZCW	NC(N\N=C\C1=CC=C(Br)C=C1)=N\N=C\C2=CC=C(Br	0.252097
GHJPBLCHQJHST	CN(C(C1=CC=CC=C1)C2=CC=CC=C2)C(\S)=N\C3=CC	0.240522
GHODQHWTFMVZTK	OC(=NOC(=O)C1=CC=CC=C1)C2C3CC(C=C3)C2C(O):	0.24691
GHONBSJAWLVFJJ	COC1=CC(=CC=C1)C2=NN3C(=C2)N=C4CCCC4=C3	0.243534
GKJOALAKKFHGH	COCCN(CCOC)C1=C2C=CC=CC2=NC(=N1)C3=CC=C(C	0.23867
GLUWQMOOSFQALM	CC1=NN(CC2=C(Cl)C=CC=C2)C3=C1C=C(S3)C(=O)N	0.25364
GMQRKHSIRSGZOM	CCNC1=NC(N\N=C(/C)C2=CC=C(OC)C=C2)=NC(NCC	0.24387
GMSMBWMTBLESFN	CC1=CC(NP(=O)(OC2=CC=CC=C2)OC3=CC=CC=C3)=	0.243246
GOZIJUKIJBIAGS	CCOC(=O)C1(CCN(CC2=CC=C(C)C=C2)CC1)S(=O)(=O	0.290491
GPIDCJLWCBZGQE	CN(CCCNC(=O)CS(=O)(=O)CC1=C(C)OC(=N1)C2=C(F	0.24684
GPMDFBYMHJZBTF	FC(F)(F)COC1=NC(=NC(=N1)N(C2=CC=CC=C2)C3=C(C	0.247497
GQPPEZBDSBAORQ	CN1CCN(CCOC2=C(C=C(C)C=C2)[N+](([O-])=O)CC1	0.242559
GQTPRLWQZDUWKJ	CC1CC(O)C=C(C)CCC=C(C)CC(O)C2CC1OC(=O)C2=C	0.245148
GRBXMROQYUPWNC	CC1=CC=C(NS(=O)(=O)C2=CC(=CC=C2)C(=O)NC3CC1	0.242855
GRLRRRSNDWCBML	CCN1C(C)=C(C)C2=C1C=CC(=C2)C(=O)NCCCN3CCCC	0.257058
GRTZXYPGLGOPL	C1OC2=C(O1)C=C(C=C2)C3=NC4=C(N3)C=CC=C4	0.243044
GSDPWYVVVAWAJZ	CCOC1=CC=C(C=C1)N=C(S)N(CC2=CC=CO2)CC3=CC	0.243829
GTHQDOILWCWUMQ	CCOC(=O)C1=C(C)C2=C(O1)C=CC(CNC3CCCC3)=C:	0.254931
GUAYXBOHGZCCLV	CCOC(=O)C1=CC(=NC2=C1SC(=N2)N(CC)CC)C3=CC:	0.240767
GVIRQIICSFDKFT	CSC1=C(OCC2=CC(=NO2)C(=O)N3CCN(CC3C)C4=CC	0.251824
GVTRMONEEFLKOO	CCOC1=C(OCC2=C(F)C=CC=C2)C(Br)=CC(CNCCSC3=	0.272622
GVUMMKJZZLDOJB	CN(C)CCCNC(=O)COC1=CC(C)=C(Br)C(C)=C1	0.24314
GWAVODRMPDBYNC	OC1(=O)(=O)=O.CC1=CC=C(C=C1)C2=CC(C3=CC=C(C	0.242569
GWBUAFKAMVXNPW	CCOC(=O)C1=CC2=C(C=C1)N(CC)C(COC3=CC4=C(C:	0.26049
GWHJFGPDVVLVBPL	COC1=C(OCC2=C(F)C=CC=C2)C(CNCCC3=CNC4=C3	0.240128
GXDYIGGSLLQOSL	CNC(S)=NC1=CC=C(C=C1)C2(CCCCC2)C3=CC=C(C=C	0.24061
GXTKJIKDRWVCSN	COC1=C(OC)C=C(C=C1)C2=NC(=C(N2)C3=CC=CC=C:	0.2428
GZHJDXCKHQLJST	COC1=C(C=CC=C1)C2=NC(N=C2C)C3=CC=C(F)C=C3	0.24945
GZHYISGBALYJAE	C\C(CC(C)(C)C1CCCC1)=N/N ChemBridge,56490:	0.245806
GZRSQMRGRMVOML	CC1=[N+](CC2=CC=CC=C2)C3=C(C=CC=C3)N1CC4=	0.248847
GZUJTINYQUYPAL	CO\N=C(/CS(=O)(=O)CC1=C(Cl)C=CC=C1)C2=C(Cl)C:	0.241248
HAMZZMBVWRGPBJ	CCN1CCCC1CN(CC2=CC3=CC=C(C)C=C3NC2=O)C(\	0.255605
HARBGVJRGOLCBC	CN(C)CCNC1=C2CCCC2=NC3=C(C(C)=NN13)C4=C	0.261083
HAWMIBLMDHZFKN	CN(C1CCCC1)C(\S)=N\C2=CC=C(OC3=CC=CC=C3)C	0.24415
HBDAYDNADGUJSK	CCC1=CC2=C(C=C1)N=C(S2)N(CCCN(C)C)C(=O)C3=C	0.240651
HBIXGQWYCSADMV	CC(\C=N\N1CCN(CC2=CC=CC=C2)CC1)=C/C3=CC=C	0.239198
HCHIBSZBHRTYPN	CC1=C(C)C=C(C=C1)N2CCN(CC2)C(=O)N3CCOCC3	0.241626
HCNCHPUSRLRNJS	C\C(=N/N=C(S)N1CC2CCC(CC2)C1)C3=NC=CN=C3	0.248035
HDBULXQOJUCQLD	CC(C)OC(=O)C1=CN=C(C=C1)N2CCN(CC2)C3=C(F)C:	0.245399
HESDAJYAHONPSE	OC1=N/C/C=C/C2=C/C=C\C(OCC=C)=C/2)=N\C3=C	0.24716
HFXFDAATZIEGHQ	CN1N=NN=C1SCCNCC2=C(OCC3=CC=CC=C3)C=CC(0.256254

HGSRDXHNGMLSSA	CN(C)CCCN(C(=O)C1=CC=C(C=C1)S(=O)(=O)N(C)CC2	0.25369
HITBEPQTTWWGIFI	COC1=CC=C(C=C1)C2=C(C#N)C(=NC(=N2)C3=CC(C):	0.241214
HIZIGRVGOMXQPT	C(N1CCN(CC2=CC3=C(C=CC=C3)C=C2)CC1)C4=CC=	0.244768
HJVIUZHNRJYUTG	COC1=CN=C(C=C)C2=C1C3=CC=CC=C3[NH]2	0.247243
HKHVMNDUQXYNBE	OC(CNC1=C2C=CC=CC2=NC(=N1)C3=CN=CC=C3)C4	0.245378
HLNNKQLCUWHCKE	NC1=C(C=C(C#N)C(=N1)N2CCN(CC2)C3=NC=CC=C3	0.244638
HLQFMKXVPCAVOZ	CCN(CC)CCNCC1=C(OCC2=C(F)C=CC=C2)C=CC(Cl)=	0.297131
HMVBHXZQCYGYHH	CC(=O)C1=CC=C(C=C1)S(=O)(=O)N2CCN(CCOC3=CC	0.239774
HNGIURSRGBTUKQ	CCCCNCCOCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.246513
HONMOBIEAAPGC	BrC1=CC=C(CNC2=NC3=C(C=CC=C3)N2CCN4CCCC	0.249366
HOVJAXXECPOCKW	CN1CCN(CC1)C(=O)CCCN2C(=S)S\C(=C/C3=CC=CC=	0.248739
HOZQYTNOQZBRCS	CN1CC[C@H]2[C@@H](C1)C3=C(C=CC(C)=C3)N2S	0.24631
HQFMIOZYIHXA	O=C1N(CCN2CCCC2)C3=C(C4=C(CCCCC4)S3)C(=C	0.255787
HRLXLJKVPAVREE	CC1=NC2=C(S1)N(CCN3CCCC3)C4=C2C=C(Cl)C=C	0.2554
HVMUWHZAZGTMJK	CN1C=NC2=C1C(Cl)=NC(Cl)=N2	0.255414
HVSPWFLNYUPLJA	COC1=CC=CC2=C1N=C(S2)N(CCCN(C)C)C(=O)C3=C(0.241245
HWFVHZCQEAUGJY	CCOC(=O)C1=CC=C(N\C(=N/S(=O)(=O)C2=C(C)C=CC:	0.280309
HWKCJOOJJUUWFA	CC(C)(C)C1=CC=C(OCCNCC2=CC=CC=C2)C=C1	0.246489
HWPVZTDNLUJHLN	C1CN(CCN1\N=C\C2=NC=CC=C2)C3C4=C(C=CC=C4	0.28263
HXNWDPAZQILIRT	O=C(N\N=C\C1=CC=CC=C1)C2=NC=CC=C2)C3=CC=	0.240343
HXWRRNFFOQYTF	CC1=NC(=CC=C1)\N=C(/S)NC2=CC=C(OC3=CC=CC=	0.241556
HXWVJOJFQXWXFE	CCCC[C@H](CN[C@@H](CNC)[C@H](C)CC)NCCC1:	0.238683
HXYZFUQPQOAXCW	CCCCN(CC)C(\S)=N\C1=CC=C(C=C1)N=C(C=C2)N:	0.240003
HYAAMKCMNGCQSE	CC1=CC(=CC(C)=C1)C(=O)NC2=CC=C(NC(=O)C3=CC:	0.247619
HYEHHPSWLBIMKF	BrC1=CC(=CC=C1)C(=O)NCC2(CCCC2)C3=CC=CC=C:	0.240276
IBSYIUYMCKJKTNI	BrC1=CC=C(NS(=O)(=O)C2=CC(=CC=C2)C(=O)NC3CC	0.24767
ICZZTNOOMSQNCH	CC1=C(C)C(OC2=NC=C(C=N2)C3=CC=C(Cl)C=C3)=C(0.239346
IDIBHZDYXUVINB	CCC1(ON(C1=O)C2=C(Br)C=CC=C2Br)C3=CC=CC=C:	0.242542
IDPUFKCIPCGYIL	OC(CC1CC12C3=C(C=CC=C3)C4=C2C=CC=N4)(C5=(0.239604
IFHMUNAIFQSUDX	CC1=CC=C(C=C1)C(=O)CN2C=C(C3=CC=C(C)C=C3)[N	0.246793
IGVFFEWTONRZIO	CCCN1C(C)=NC2=C1C=C(N3CCN(CC3)C4=NC(=CS4)	0.240387
IIIQJAKHUZXUHB	CC1=CC=C(SCCN(C)S)=NC2=C(C)C=CC(C)=C2)C=C1	0.252163
IINYNPFZSWDMKO	CCN(CC)CCSC1=NC2=C(C=CC=C2)C(=S)N1C3=CC=C	0.25934
IJAMBXTZXRKPN	CC1=NN(C(NC2=C(Cl)N=C3C=CC=CC3=N2)=C1)C4=	0.243722
IJEBYZKDEQWNC	CCN1CCN(CC1)C2=C(NC(=O)COC3=C(Cl)C=CC(C)=C	0.243455
IJLFPQDXCYIPKB	COC1=C(C=CC=C1)\N=C(/S)N2CCN(CC2)C(C3=CC=C	0.243529
ILOMPUSPHRMHIA	FC1=CC=C(C=C1)N2C(CC3=CC=CC=C3)=NN=C2SCC.	0.247291
IMCTTYPKPVYSTH	FC1=CC=C(NC(=O)C#CC2=CC=CC=C2)C=C1	0.24821
IMQWZNFAGK POT	CCCS(=O)(=O)NC1=CC(=C(C=C1)N2CCCC2)S(=O)(=	0.253413
INFUTCKSYWEKNB	COCC(C)NC(=O)CSC1=NC=C(C(Enamine, T5231205	0.249535
IOLHLRYDZRF SJM	COC1=CC=C(C=C1)N2CCN(CCCNC(=O)C3=CC4=C(C:	0.241928
IPBRVYOVATUEHJ	CC1=CC=CC=C1C2=NC(=C(NCCN3CCOCC3)O2)S(=C	0.258273
IPIFRBxBBIBXHI	CC1=C(OCCCCN(C)(C)C)C=CC(Br)=C1	0.271454
IPURTGGCIASEME	CC(C)NC(NCC1=C(Cl)C=C(Cl)C=C1)=NC2=CC=CC=C2	0.240724
IQNAWOZPXCRDHI	CCN1CCN(CC1)C2=NC3=C(C=C(NC(=O)C4=CC=CS4)	0.244411
IRBACGKLN DLBLX	CC1=C(C(=O)OCCOC2=C(C)C=CC=C2)C(=NO1)C3=C(0.247156
IRCTUCGANJLJNZ	CC(C)NCC(O)COC1CCC(CC1)C(C)(C)C	0.25426
ITGNZSJYGD PB MN	CCN1CCN(CC1)C2=CC=C(NC(- Vitas-M Laboratory,'	0.240915

ITGWHCJBHDFZBN	CCCN1CCN(CCCNC(S)=NC2=CC3=C(C=C2)N=C(C=C:	0.248948
IUENWZALYXA EGL	CN(C)C1=CC=C(NC(=S)N(CCC2=CC=CC=C2)C3CC=C	0.238609
IUZQRMQBYP SNOP	CCCCN1C(NCC2=CC3=C(OCO3)C=C2)=NC4=C1C=C	0.242351
IVTVJPLZMWA ZDG	CCN1CCN(CC1)C2=C(Cl)C=C(NC(=O)C3=CC(F)=CC=C	0.244352
IWAQYICUTFQLPL	CCOC(=O)C1=C(SC2=C1CCCC2)N3C(C)=CC(C=O)=C	0.258475
IWBVPWPPANA UJF	CC1=CC(C)=NN1CCCN2CCC(CC2)C(=O)NC3=CC(=CC	0.24587
IXDMDZYRFMQNAZ	COC1=C(OC)C(OC)=C(CN2CCN(CC2)S(=O)(=O)C3=C	0.241046
IXEJOJCKIOCKJP	COC(=O)C1=C(C[C@H]2CC[C@H]1N2C(=O)NC3C	0.24375
IZCJMEWSRTWZMW	CCN(CC)C1=NC2=C(C=C(NC(=O)C3=CC=C(Br)O3)C=C	0.251794
JAIFWJBLUVGTN	CC1=CC=CC(C)=C1NC(=O)C2=CC=C(CN3CCC4=C(C3	0.287829
JAVKUZLFYJVUCI	CC(C)(C)C1=CC=C(OCCC(=O)NC2=C(C=C(C=C2)N3C	0.239309
JBSPVQWXYLGO FN	CC1CCCN(CCOC2=CC(OC3=CC=CC=C3)=CC=C2)C1	0.265656
JCJSOROVNUFQFY	NC1=C(C=CC=C1)C#CC2=CC=C(C=C2)[N+][O-]=O	0.283265
JEMZTFFTDNRKRS	CC1=CC(N2CCN(CC2)C3=NN=NN3C4=CC=CC=C4)=	0.238868
JGQSQTHHVYQNZ	C1CN(CCN1)N=C\C2=CN=CC=C2)C3C4=C(C=CC=C4	0.242869
JHIDMNKFGHQ TND	COC1=CC=C(C=C1)C2=NOC(=N2)C3=C(C=CC=C3)C4	0.242429
JIFCJGRLNKKNO	CC1=CC(=CC=C1)N2C=C(CNCCC3=NC(C)=CC(C)=N3	0.24467
JKDLOGLNPDVUCX	CC1=C(N2CC2)C(=O)C(CO)=C(N3CC3)C1=O	0.250889
JKMMTFLYXNGCTP	CC(C)(C)NC1=NC(=NC(=N1)N2CCCC2)N3CCCC3	0.295199
JLOWBNWESRIHFY	CN(C)CC1=C(SC2=C(Cl)C=C(Cl)C=C2)C=C(F)C=C1	0.253444
JMBDCADTM YGNQO	COC1=CC2=C(C=C1)N=C(N\N=C(/C)C3=NC=CC=C3)	0.246816
JMUQRGSDGTX YBZ	OC1=CC=C(C[C@H]2CN=C(S)N2C[C@H]3CCCN3C(C	0.239684
JMWYNZLUZZSLNI	CCN(CC)CCNC(S)=NC(=O)C1=CN(N=C1C2=CC=C(OC	0.240686
JMYQPHVQYYQNOG	CC1CCCC(C)N1CC(O)COC2=C(F)C=C(Br)C=C2F	0.256946
JNRDKMLQIYZVBV	FC1=C(CN2CCN(CC2)C3=NC4=C(S3)C=CC=C4)C(Cl):	0.242399
JRIKLERLKODIGN	CC(C)C1=CC=C(OCCC2=C(C)NN=C2C)C=C1	0.244843
JSTHCNBJOWNOBT	O=C(NC1=CC(=CC=C1)N2C=CC=N2)C3CCCN(CC4=C	0.242008
JTGNGCIGAYRRAG	CC1=C(C=CC=C1Cl)\N=C(/S)N2CCCN(CC3=C(F)C=CC	0.24166
JVFUNOJJRFQCJP	CC(C)(C1=CC=CC=C1)C2=CC=C(OCCCNCC=C)C=C2	0.257874
JWDKDEOZWRNCJP	COC1=CC(=CC(OC)=C1OC)C2=CC(C(=O)NC3=C(OC)C	0.298189
JWQJZUUTXPAMDH	COC1=CC(CN2CCN(CC3=CC=C(C=C3)C(F)(F)F)CC2)=	0.239327
JXSYVEMDOJHZNA	CC1=CC(C)=C(C=C1)C(=O)NC(S)=NC2=CC=C(CN3CC	0.248124
JYDNZIKPNQPVLU	CC1=CC(C)=C(CN2C=NC(=C2)C3=CC=C(C=C3)[N+][O-	0.241776
JYWQNPPIDJENSS	CNC(=O)OCC1=C(COC(=O)NC)N(C)C(SSC(C)(C)C)=N1	0.245017
JZCVNTHDAGQJFQ	CC1CCN(CC(=O)C2=C(C)N(C(C)=C2)C3=CC=C(F)C=C:	0.2416
KAZKIRQPJHCOPZ	CCOC1=C(OCC2=CC=CS2)C(Br)=CC(CNCCO)=C1	0.294901
KBUIURUSSHIMGT	ClC1=CC(\C=N\N2CCN(CC3=CC=CC=C3)CC2)=CC=C	0.243531
KBXMQGWYLAULEO	CCN(CC)C1=NC(=NC(=C1)C(F)(F)F)C2=NC=CC=C2	0.265827
KBXOFUBAOLRVGO	CCN(CC)CCCNC(=O)C1=CC2=C(S1)C3=C(C=CC=C3)N	0.243599
KCZCJQZQLKECEE	CCOC1=CC=CC2=C1N=C(S2)N(CCCN(C)C)C(=O)C3=C	0.245055
KDUQFKQFOXKDG D	COC1=CC=C(C=C1)C2=C(C)NN=C2C3=C(O)C(C)=C(O	0.241444
KDWDAFPKFGQPMO	CCN1C(COC2=CC=C(Cl)C=C2)=NN=C1SCC3=NC4=C	0.250622
KECRXLZQHIYBOU	CC1CCCN1C2=C(N=C(S2)S(C)(=O)=O)S(=O)(=O)C3=	0.239469
KEDNXCYSCLGKU	COCC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC=C(C	0.24491
KELRDBMULRYLAZ	COC1=C(OC)C=C(C=C1)C2CCCN2\C(S)=N\C3=C(C)C	0.2389
KFEUHMSTVKWZAL	COC1=CC(OC)=C(OC)C=C1C(=O)C(=C)CN(C)C	0.255135
KFNHMGQTOQVWQC	CC1=C(NC(=O)CN2CCC(CC2)C(O)(C3=CC=CC=C3)C4	0.251142
KGCUCBMHEBZAAR	CCOC1=C(C=C(CN(CCC)CC)C)C=C1)C(=O)OC	0.258968

KGEZINBWNGJLSR	CCOC1=C(OCC2=C(F)C=CC=C2)C(Br)=CC(CNCC3=CC	0.245798
KITYONMJHHLPCF	COC1=CC2=C(C=C1)C=C(N=C2)C3=C(F)C=CC=C3	0.241012
KKSZVUGVKVEOAK	COC1=C(C=CC=C1)C(C[N+](O)=O)C2=CNC3=C2C=	0.244857
KTPBMRRITWYSQL	[O-][N+](=O)C1=C(C=CC(=C1)C(=O)N2CCN(CC3=CC=	0.238782
KTRMCWILXYBTEP	COC(=O)C1=C(OCCC(C)C)C=CC(CSC(N)=N)=C1	0.246335
KUTCXVUIOVBICM	CN1CCN(CC2=C(O)C=CC3=C2C(=CO3)C(=O)C4=CC=	0.239865
KYIAUZRDCLQACY	CCC1=CC(CNCCNCC2=C(O)C=CC(CC)=C2)=C(O)C=C:	0.249759
LAANVYLBPQYPTP	CC(O)CNCNCC1=C2C=CC=CC2=CC=C1OCC3=CC=(0.256271
LBNKQGYGRTRRD	CC(=O)C1=CC=C(NC2=C3C=C(C)C=C(C)C3=NC(C)=C:	0.239888
LCFWFLDEKVUPBD	CN(C)CCCNC1=NC=NC2=C1C(=CN2C3=CC=CC=C3)(0.246811
LDOKEGXRBPYRMH	COC1=CC=C(C=C1)C2=NN3C=NN(CC(=O)NCCCN4C	0.238992
LDUYFILRMTVKOD	COC1=CC=C(C=C1)C(N2CCN(CC2)C3=CC=CC=C3)C4	0.241215
LGFPCLMEHARZNY	CCCCN(CC(O)COC1=CC(C)=CC=C1)CC(O)COC2=CC(0.245166
LGUOGKPIPWKSHA	CCOC1=C(OCC2=CC=CC=C2)C=CC(CNC3=CC=C(CNC	0.238487
LGZSGCSPVHESJN	CCOC(=O)CN1C(=NC(=C1C2=CC=CC=C2)C3=CC=CC:	0.244604
LHILIMCFIJCSHA	C(NC1=NCCN1)C2=C(SC3=C4C=CC=CC4=CC=C3)C=	0.24399
LHMWCEVVOVBYIR	OC(COCCC12CC3CC(CC(C3)C1)C2)CN4CCCCC4	0.269473
LIAIKEXLWCJQDH	CC(C)NCCOCCSC1=CC=C(CI)C=C1	0.252018
LJJRLLVBPWZLT	COC1=C(Br)C=C(C=C1)C(=O)NC2=C(C=CC=C2)N3CC	0.244091
LKPOXZKRWJOAIR	CNC(S)=NC1=CC(=CC=C1)C2=NC3=C(C=CC=C3)N=C	0.240411
LLABXOYGKIUMRT	FC(F)(F)C1=CC(CI)=C(N=C1)N2CCCN(CC2)C(\S)=N\C	0.244024
LMDLYWVZOYMTET	CCOC1=CC=C(CSCCNC(S)=NC2=CC=C(OC)C=C2)C=C	0.24042
LMMAFKCGZFAZEO	COC1=C(OC)C=C(\C=N\OCC(=O)NC(C2=CC=CC=C2)(0.256539
LOGCDTPZMHGKMP	COC1=CC=C(C=C1)N2C(COC3=C4C=CC=CC4=CC=C:	0.272134
LONMBINMTRDROA	FC1=C(OCCCCCN2CCCC2)C=CC=C1	0.278776
LPHZYWPMOGWFEC	SC(=NC1=CC=CC(Br)=C1)N2CCN3C=CC=C3C2C4=C	0.241593
LRCLIANPNGHBFMA	CN(CC(=O)NC1=CC(F)=CC=C1)CC(=O)NC2=CC(=CC=	0.24794
LTJWZEHNLIIVCEG	CC1=CC(=CC(C)=C1)N=C(S)NC2CC3CCCC(C2)N3CC	0.263803
LUMYCUHRVRSNFU	C\C(=N/NC1=NC(=CC(C)=N1)C2=CC=CC=C2)C3=CC:	0.247445
LUURBQJWILSPPZ	CCN(CC)C1=NC=NC2=C1C(=CS2)C3COC4=C(O3)C(0.245265
LWHZXTWETGZAPA	C(N1CCOCC1)C2=C3C=CC4=CC=CC5=C4C3=C(C=C:	0.245078
LXSKJZACELIGDN	CC(=O)N1CCN(CC1)C2=CC=C(OC3=CC(=C(C=C3))[N+	0.239359
LYANQLBZUJALFT	COC1=C2N=C(C)C=C(NC3=C(C)C=CC=C3)C2=CC=C1	0.239763
LYESBOJVXBJVBZ	NCCNC[C@@H]1COC2(CCCCCCCCCC2)O1	0.24317
LYIUREYWAKPINL	C\C(=N/N=C(S)N1CCCCC1)C2=NC=CC=C2	0.25581
MBUIARAVKHOPSP	ClC1=CC(CI)=C(CN2C3=C(CCCC2=O)C=CC=C3)C=C1	0.242927
MEDNNPLNMHHDHL	CCN1CCN(CCCNC(=O)C2=CSC3=C2CCCC3)CC1	0.249148
MFELZSOBTNRDDQ	FC1=CC=C(CN2CCC(CC2)C(=O)N(CCC3=CC=CC=C3))	0.24431
MFGGANWOTSXZQA	COC1=CC(C)=C(C=C1)C(=O)C2CCCN(CC3=CC=CN3C	0.24396
MIZYLCBOZXMRKC	COC1=CC=C(C=C1)C2=NC3=C(C=CC=C3)C(NCCCN(C	0.242413
MJUBMNNENZFDBB	NC1=NC(NC2=CC=CC=C2)=NC(CSC(=S)N3CCN(CC3)	0.255684
MKZLUAVLJPHTCA	COC1=C(C=C(CI)C=C1)C(=O)C2CCCN(CC3=CN=C(C):	0.244612
MNEUHRLPCBNVQP	NNC1=NC(=NC(NC2=CC=CC=C2)=N1)N3CCCCC3	0.241306
MNVFUIZSSLMYRD	CCOC1=C(CNCCNCCO)C=C(CI)C=C1Cl	0.240959
MOWXKVLGLKIYPZ	CC1=CC(OCCCCN2C=CN=C2)=C(C)C=C1	0.282184
MROUMGHYRREOGE	COC1=CC(\C=C2\SC3=C(NC2=O)C=C(C=C3)C(=O)NC	0.249325
MRYPRGFFMVYDJW	COC(=O)C1=CN(CC2=CC(OC)=C(OC)C=C2)C=C(C1C3	0.239912
MTKWLELVFSBWIP	CCC1=CC=C(C=C1)C(CNC2=C3C=CC=CC3=NC(=N2)(0.242766

MVNJVZVXVJTEKU	CN(C)CCCN(C(=O)C1=CC=C(C=C1)S(=O)(=O)N2CCCC	0.240783
MVXZVUIEUSJAIH	CN(C1=CC=C(C=C1)C(=O)N2CCN(CC3=CC=C4OCOC	0.243333
MXEAGZWZLNDZPO	CC(C)C1=CC=C(OCC(O)CNC(C)C2=CC=CC=C2)C=C1	0.258284
MXJYBHVYFCOGNA	CCN(CC)S(=O)(=O)C1=CC(NC(=O)C2=CC=C(C=C2)N3	0.240819
MYCMIKJKPAZFJD	COC1=CC=C(C=C1)N2CCN(CC2)C(CNS(=O)(=O)C3=C	0.247104
MYJSZVZCIZXXGZ	CC(C)C1=C(NC(S)=NN(CC2=CC=CC=C2)C3=CC=CC=C	0.24939
MZFVOAWLTVMEPG	CCN(CC)S(=O)(=O)C1=CC(=C(C=C1)N2CCN(CC2)C3=	0.243228
NAACUODJWGVTLU	CN1CCN(CC1)C(=O)\C=C\C2= Enamine,T0508-118	0.262658
NAHGSCRAUMNHIA	CC1CC(C)CN(CCCSC2=CC=CC=C2)C1	0.244583
NAUVDUAFMRTQQN	CC1=CC=C(NC2=C3CCCC3=N(Chem Div,3130-153	0.242692
NBJSYTGLGDBHFD	C(NCC1=CC=C(OCC2=CC=CC=C2)C=C1)C3=CC=CS3	0.239236
NBLBHHZNRGQSQN	COC1=C(NC(=O)NC2=NC(CC(=O)N3CCN(CC3)C4=CC	0.238996
NCGHKOPCIZUFJ	CCOC1=C(NC(=O)C2=CC(NC(=O)C3CCCC3)=CC=C2)C	0.253609
NCRALVTUDQJLGN	CC1=C(CN2CCC(CC2)C(=O)NC Chem Div,C522-089	0.25194
NDCGYKFGYLNZCW	COC1=C(OCC(=O)NC(C)(C)C)C=CC(CNC(C)C23CC4C	0.240674
NESFIPBVVKVOMY	CCN(CC1CCCN(CCC2=CC(F)=CC=C2)C1)C(=O)C3=CC	0.242793
NFSMEYMZCSXINM	COC1=CC=C(C=C1)C2=NC(=NC(=C2)C#N)N3CCNCC:	0.247035
NGGRXCCACIAMPB	CCN(CC)C1=CC=C(NC(=O)NC2=CC=CC=C2)C=C1	0.249869
NJMAOFNJCLSNQY	COC1=CC=C(OC)C=C1)C2=C(C#N)C(N)=NC(=C2)C3=	0.241555
NKZYWBMSMZJJKO	CCCOC1=C(C)C=C(CCCN=C(N)N)C=C1	0.246797
NLJHFNAOINRWEU	CCCCOC1=C(C=C(CSC(N)=N)C=C1)[N+][[O-]]=O	0.250474
NNFCFDYRIJDRTR	[O-][N+](=O)C1=CC(=C(NC2=CN=CC=C2)C(=C1)[N+](0.250621
NNWLPSHIRKXURN	CCN(CC1=CC=CC=C1)S(=O)(=O)C2=CC=C(C=C2)C(=C	0.238789
NORPBVDKCPDMPW	COC1=C(C=CC=C1)N2CCN(CC2)C(=O)C3=CC=C(COC	0.260129
NPGHSFFDDMHHIK	COC1=CC=C(C=C1)N2CCN(CC2)C3=NC=NC4=C3C(=	0.259817
NPGUYIWHZCFXDH	CC1=C(C)C2=C(S1)N=C(CN3CCCC3)N=C2C1	0.250321
NPQZNMPPUASIAY	COC1=CC(OC)=C2N=C(C)C3=C(N(CC3)C4=CC=C(O)C	0.260844
NRSZLJFVHLGBKL	CN(C)CCCN(C(=O)CCC1=CC=CC=C1)C2=NC3=C(S2)C	0.248565
NRVTZAOZLYXAKX	COC1=CC(=CC(OC)=C1)C2=C(C3=CC=CS3)C4=C(C=C	0.255996
NUFQQJRGQQZCOS	CCOC(=O)C1=C(NCCCN2CCOCC2)C3=C(N=C1)C(C)=	0.248123
NVZZXTOSSAESJJ	ClC1=CC=C(NC(=O)OCCN2N=NN=C2C(N3CCOCC3)C	0.247821
NWHRCFHGNQXGJD	FC1=CC=C(C=C1)N2CCN(CC2)S(=O)(=O)C3=CC(=CC=	0.25275
NXGGPCHKCYCOAX	CN(C)CC(=C)C(=O)C1=CC2=C(OCO2)C=C1	0.241777
NYLAUQJTBURUOI	C(N1CCN(CC1)\N=C\C2=CN=CC=C2)C3=C4C=CC=C	0.239698
NYZGTUCQLQLOTI	ClCC(=O)NC1=C(C=CC=C1)C(=O)NC2=CC3=C(OCO3)	0.243288
NZFUBWWCWIPTRM	CCN(CC)S(=O)(=O)C1=CN=C(C=C1)N2CCN(CC2)C3=	0.243826
NZQWATWAVUWKFN	COC1=CC(=CC=C1)C(N(C(=O)CC2=CC=CS2)C3=CC(C	0.245071
OAQPLTKFCVNYGE	CCOC1=C(C=CC=N1)C(=O)N2CCN(CC2)C(C3=CC=CC	0.242267
OCENEPXQFHBLMK	CCN(CC)CC(=O)NC1=CC2=C(CCC3=C(C=CC=C3)N2C	0.320618
OCESNVPJCFERML	CC1=CC(Cl)=C(C)C=C1S(=O)(=O)NC2=CC3=NNC=C3	0.249928
ODFHSTUCJXXLQJ	CCC1=CN=C(CNCC2=CC=C(OCC(O)CN(C)CC3=CC=C	0.251904
OEHRXJDSSPBTM	CN(C)S(=O)(=O)C1=CC=C(NC(=O)N2CCN(CC2)C3=CC	0.23896
OEKPRBMHQAEAGG	CCOC1=CC=C(C=C1)S(=O)(=O)NCC2=CC=NC=C2	0.269822
OEWOYXMHZWAPJ	CN(C)C(=S)N=C1SSC(=S)N1CC2=CC=CC=C2	0.244509
OGEQWAXKLZAXPG	CN(C)CCCN(C(=O)C1=CC=C(C=C1)C(=O)C2=CC=CC=	0.249638
OHDARSJSUPJOBG	COC1=C(CN(CC2=NC3=C(C=CC=C3)C(=O)N2)S(=O)(=	0.239646
OHTLJXYBSOWPHN	COC1=CC=C(OC)C=C1)C2=C(OC(C)(C)N=C(OC(C)(0.247273
OHUPQINJOLRADC	C\C(=N/N=C(S)N(CC1=NC=CC=C1)CC2=NC=CC=C2)C	0.241534

OIMLWOWVDNEGEN	COC1=CC(=O)C(OC)=C(OC)C1=O	0.252368
OJEVGRBYSIFLVB	CC1=C(Cl)C=C(NC(=O)CSC2=NC3=C(C=CC=C3)C(=O)	0.239759
OJGPOHOXFKPODP	CSC1=CC=C(C=C1)C(=O)C2CCCN(CC3=CC=CN3C4=C	0.239209
OJONFUYEVNZGMS	COC1=CC(OC)=C(C=C1)C2=[N+](C)CCN3C=CC=C23	0.240238
OJZCDVLJMCJDQG	CCCCSC1=NC2=C(S1)C=C(NC3=NC(=NC(=N3)N4CC(0.244021
OKUZMGPFGBTMFL	COC1=C(OCC2=CC=C(F)C=C2)C=CC(CNCCC3=CNC4	0.253418
OMMABXQBKXLFFT	CC(NCC(O)COC1=CC2=C(C=CC=C2)C=C1)C3=CC=CC	0.258012
OMNBIEFISJHBDJ	CC1=C(CCNCC2=CC=C(Cl)C=C2)C3=C(N1)C=CC(OC(0.243504
ONZSYNDJBXYAM	FC1=C(CNCCC(CC2=CC=CC=C2)C3=CC4=C(OCO4)C:	0.238638
OOAPZUSKZNTZKO	CC(C)C1=CC(OCCCCN(C)C)=CC=C1	0.261196
OOEKANWELYHCMY	CC1=C(CSC2=NN=C(N2CC3=CC=CO3)C4=CC=CS4)C	0.24976
OOJYVOXEFZVRNL	CCOC1=CC=C(C=C1)N=C(S)N2CCCN(CC3=C(C)C=CC	0.239148
OQWWABIXMUFBUI	CC(CNC1=CC=C(C=C1)[N+](O)=O)OC2=NON=C2C	0.266686
ORHQABFVUQKVIS	CN(C)CCCN(C=O)C1=CC=C(C=C1)S(=O)(=O)N2CCCC	0.24437
OSEMTBZFAUSVMB	COC1=CC(OC)=C(C=C1)N=C2/SC3=C(CN2CCN4CC(0.263174
OWHDVIBZBONORH	CC(C)C1=C(OCC(=O)NC2=CC3=C(C=C2)N(C)C(CCN4	0.246116
OWKZMPVHIVLZEX	CC(=C)C1CCC(CN2CCN(CC3=CC=CC=C3)CC2)=CC1	0.240397
OXVQORLPGKNNFZ	CCCCN(C1CC2CCC(C1)N2C)C(=O)C3=CC=C(Cl)C=C3	0.241046
PBFQBTABIKSPJC	COC1=CC(OC)=C(NC2=C3C=CC=CC3=NC4=C2CCC4	0.249054
PBNSAAZNKRYIIS	C\C(=N/OCC1=CC=C(Br)C=C1)C2=NC=CC=C2	0.240468
PBZPZRBFYOUOBJ	CCCCN(CC)CCNC(=O)C1=CC2=C(S1)C3=C(C=CC=C3)	0.249422
PDICYFOXVGFINZ	COC1=C(C=CC=C1)N2CCN(CC2)\N=C\C3=CC(=C(Cl)	0.241765
PDUPXVBNXBQTOH	C(N1CCCCC1)C2=CNC3=C2C=CC=C3	0.268109
PENGFPGDYHZNAP	COC1=C(CN2C=CC=N2)C=C(CN3CCCC(C3)C(=O)C4=	0.251591
PENXDAMCASPCMY	CCOCCC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC=	0.256306
PFUFOXKNRLGMSL	[O-][N+](=O)C1=NC=CN1CCNC2=C3C(C=CC=C3[N+	0.245174
PHKAITMLWITDDV	CCN(CC)CCSC1=NC2=C(N=N1)C3=C(C=CC=C3)N2C(0.261486
PHZMYJRNQGSBG	COC1=CC=C(C=C1N(C)S(=O)(=O)C2=CC=C(Cl)C=C2):	0.248895
PIGWDDIGMRNVDO	CC1=CC(OCC(O)CN2CCN(CC2)S(=O)(=O)C3=C(C)C=C(0.245047
PIJBYDDOCXHZFH	N=C1N(CCN2CCOCC2)C=NC3=C1C(C4=CC=CC=C4)I	0.251164
PJTXCMBEHDWJMJ	OC(CNC1CCCC1)COC2=CC=C(C=C2)C3=CC=CC=C3	0.250108
PKERGGKJACRDCQ	CC1=NN2C(N=CC(C3=CC=CC=C3)=C2N)=C1C4=CC=	0.240477
PKNFTRYZNWKASG	CCC1=CC=C(OCCCCN(C)CC2=CC=CC=C2)C=C1	0.252179
PKTDIPACDGKPY	COC1=C(NC2=C3C=CC=CC3=NC4=CC=CC=C24)C=C	0.243829
PLHTVUFOHHOCSF	CN1CCN(CC1)C2=CC=C(C(=C2)N3N=C(C4=CC=CC=C	0.245059
PMYNSLQJVYZORD	CC(C)C)C1=CC=C(C=C1)N=C(S)NCC2=CC=CS2	0.250576
POQKFFNMUPZZRK	OCl(=O)(=O)=O.Oc(CN1C2=C(C=CC=C2)C3=C1C=CC	0.256586
PTWKKKSNTGCGKY	CCCN1C(=N)N(CCOCC2=CC=C(OC)C=C2)C3=CC=CC(=	0.281532
PTYQBUIBRXMOH	CC(C)C\N=C(/S)N(CCC1=NC2=C(N1)C=C(C)C(C)=C2)	0.250122
PWPWXLHAYGEBIS	CSC1=C(OCC2=CC(=NO2)C(=O)NCCN3CCCC4=C3C=	0.243432
PWQZJFBQCSIYJG	CC1=NC2=C(C=CC=C2)C(=C1)C(=O)N3CCC(=CC3)C4	0.254396
PXBLKWLLBSFBBD	CCCOP(=O)(C(NC1=CC=CC=C1)C2=CC=C(C)C=C2)C3	0.263519
PXCQCBOGRVCHKF	C\C(=N/N1CCN(CC1)C2C3=C(C=CC=C3)C4=C2C=CC	0.266761
PYEWRVJBQXWXNV	ClCC(=O)N=C1SC=CN1CC2=C(Cl)C=CC=C2	0.239395
PZBATUNEVLSDIG	[O-][N+](=O)C1=CC(Cl)=C(NS(=O)(=O)C2=CC=CC=C2)	0.246557
QAFQNDKFLYMCFC	CCOC1=C(OCC)C=C2N3C=CC=C3C(NCC2=C1)C4=C(0.252047
QBEGUTHCSOWVOB	CCN(CC)CC(O)CN1C2=C(C=CC=C2)C3=C1C=CC=C3	0.265842
QBYRWBBTOQMSDN	CN(C)CCCN1=C2C=CC=CC2=NC3=C1CCC3	0.265487

QCMZFCTUSGZVHX	OC(CNC12CC3CC(CC(C3)C1)C2)COC4=C(Cl)C=C(C=	0.244493
QCWAHIREZGSIQK	CCC1=C(C=C(C=C1)C2=CC(C)=NO2)S(=O)(=O)N3CC1	0.259274
QECYXZZAYWHQKA	COC1=CC=C(C=C1OC)CCNC=2C3=CC(=C(C=C3N=CN	0.249205
QEKXMFPGXAXIOU	CCOC1=C(OCC2=CC=CC=C2)C(Cl)=CC(CNCCC3=CC=	0.268575
QEQSXWLGYYHTFF	COCCN(CCOCC)C1=C2C=CC=CC2=NC(=N1)C3=CC=C(0.249852
QESGNZQXHOVHR	ClC1=C(C=CC=C1)C(\N2CCOCC2)=N\C3=CC(Br)=CC	0.241862
QFBBKUKXNCERIF	C\N=C(/S)N1N=C(CC1C2=CC=C(Br)C=C2)C3=CC=C(0.292508
QFMLSARVKDKZLE	CC1=CC(=CC(C)=C1)N=C(S)NCCN(C2CCCC2)C3CCC(0.257241
QFOHGRXAODPOFZ	CC1=CC=C(C)N1C2=CC=C(C=C2)C(=O)NC3CCN(CC4	0.247484
QFTFZZJYAPSZFF	OC1CCCN(CC2=C3C=CC4=CC=CC5=C4C3=C(C=C2)C	0.241245
QHOMAMNYIIILEC	CN(C)C1=CC=C(CNC2CC(C)(C)NC(C)(C)C2)C=C1	0.268293
QIOCRCNQUZAYHU	CC1=NC(OCC(C)(C)C)=C(C(C)=C1)S(=O)(=O)C2=C(C)	0.24688
QIXGHKYUZRPJNK	COC1=CC=C(C=C1)C2=CSC3=C2C(=NC=N3)N4CCN(0.257364
QJEQNMXYYQUOAY	C\C(=N/NC(S)=NC1=CC(Cl)=CC=C1)C2=NC=CC=C2	0.250133
QJRMVLSNYMICMY	CCOC1=C(OCC2=CC=C(F)C=C2)C=CC(\C=N\O)=C1	0.239551
QKDMCYVRFPKIW	COC1=CC=C(NS(=O)(=O)C2=CC(N)=C(C=C2)N3CCCC	0.240714
QLEYAENRHBCCLS	CCCN(CCC)C1=CC(CC(C)(C)C1)=[N+]2CCCC2	0.250439
QNFAGAPWMNDJKM	ClC1=CC=C(C=C1)C2=NC(N3CCSCC3)=C(N=N2)C4=	0.238757
QNXYHIJIMBFHB	CN1CCN(CC1)C2=CC=C(NC(=O)C3=CC=C(O3)C4=C(0.251219
QOABVBAPHTTZBQ	COC1=CC=C(C=C1)C(=O)C(CN2CCOCC2)C3=CC=CC:	0.25275
QOXRKGCSSOOUCE	CCCOC1=CC=C(C=C1)C2=NC3=C(C=CC=C3)C(=N2)N	0.243833
QPAUSEFRWOAHNY	CC1=CC=C(C=C1)C2=CN3CCCC3=[N+]2C4=CC=CC=	0.257601
QPWQDQPRXBGKND	NNC1=NC2=C(N=N1)C3=C(C=CC(F)=C3)N2CC4=CC:	0.256968
QPXLVBYIKHAFPH	COC1=C(C=CC=C1)\N=C(/S)N(CCCN2CCOCC2)CC3=	0.240922
QQXBIXLVIFJHLJ	O=C(NC1=NC2=C(C=CC=C2)N1CCN3CCCC3)C4CC	0.247788
QTDHFMBDIJSUNI	ClC1=CC=C(NC(=O)C2CCCN(C2)C3=NC=NC4=C3N=	0.239898
QTHQMLMUIVEMBE	CCCCCCCCC[N+](C)(C)CC#C Vitas-M Laboratory,'	0.239958
QTLRAYBBJLKXOP	COC1=CC=C(C[N]2N=NN=C2C(N3CCN(CC3)C4CCCC	0.239186
QWKNZOOQCBSJMP	CN(C)CCCN(CC1=CC2=CC(C)=CC=C2NC1=O)C(\S)=N	0.252942
QXCVDJEJBVQMAX	OC(CNCC1=CC=C(F)C=C1)(C2=CC=C(F)C=C2)C3=CC:	0.250409
QXOKXZIVWIYPSI	COC1=CC(=CC(OC)=C1OC)C2=CC3=C(SC4=CSC=C	0.255185
QYVJNOLAQFWVNH	CC(C)N1N=C(C)C(CN2CCC(CC2)C(=O)NC3=CC(=CC=	0.245241
QZABAUGUFDUGHY	CC(=O)C(\SC1=C2N=CC=CC2=CC=C1)=N/NC3=C(Cl)	0.245095
RAJNSLIDHIYJAD	ClC(Cl)(Cl)C1=NC2=C(C=CC=C2)N3N=NC=C13	0.242011
RARVXOGFGVCHLE	CCCCOC1=C(CN(CCCl)CCCl)C=C(C)C=C1	0.243221
RBGJBTCSPSNVCP	COC1=CC=C(CN2CCN(CC2)CC3=CC=CC=C3)C(=C1)C	0.251818
RBPFQHWXRDLGK	[O-][N+](=O)C1=CC(=CC=C1)C(=O)N2CCN(CC2)C3=C	0.239194
RBRLGTLGTUBHPM	OC1=C(C=CC=C1)N2CCN(CC2)C(=O)C3=C4C=CC=CC	0.247917
REKAMGPSQSKSHW	BrC1=CC=CC=C1N2C(=N)N(CCN3CCOCC3)C4=CC:	0.245886
RFNVOGZLEKVTMA	OC(C1CCCN1)C2=C3C=CC=CC3=NC(=C2)C4=CC(C	0.260088
RHKBXWCHOOPPSM	CCN(CC)CC(C)(C)C(=O)\C=C\C1=CC=C(C=C1)\C=C\C	0.239611
RHVHUEROIBGXJT	CC(C)OC1=CC(=CC=C1)C(=O)C2CCCN(CC3=CC=CN3	0.245642
RHZUUBXOXYENX	COC1=CC=C(C=C1)C(CNC(=O)C2=CC(=CC=C2)S(=O)	0.241625
RJCIRPVSLBLECQ	CCN1N=C(C(=O)NC2=C(C=CC=C2)N3CCCC3)C4=C(C	0.247368
RJHKTRXMAXYCBF	COC1=CC=C(CCNCC2=C(N(C)C3=C2C=CC=C3)C4=C(0.246113
RJZNQJVLIVSQNQ	CC1=CC2=C(OCCN2C(=O)CCC(=O)NCCCN3CCC(CC4	0.248635
RLDJXJNLXMWGOA	CC1=CC(NC2=C3C=CC=CC3=C(N=N2)C4=CC(=C(C=C	0.23926
RNTSNHMJGYWEKC	CN(C)CCCN(C(=O)C1=CC=C(C=C1)S(=O)(=O)N(C)C2C	0.251835

RPEUIPUAHNPTTQ	CCOC(=O)C1=C(NC(=O)CSC2=NN=NN2C3=C(OCC)C:	0.241155
RQDZLDRIYAKHKPP	CCC(=O)C1=CC=C(OCC(O)CN(CCC2=CC=CC=C2)CC3	0.258557
RQVGCCGAQUDRPT	C[N+](C)(C)CC1CCCC(C[N+](C)(C)C)C1=O	0.250118
RUPBLWIJNNVTP	CN(C)C1=NC(=NC(=N1)N(C)C)N(CCOC2=CC=CC=C2)	0.243341
RVAARCEFQOBAS	CC1=C(C2C(CCN)C2(C)C)C3=C(N1)C4=C(C=CC=C4)(0.240238
RVPBSHYEMHOHLI	COC1=CC=C(C=C1)C2=NN=NN2C3=C(OC)C=CC=C3	0.301495
RWKJZYJOUFZCBE	CC1=NC2=C(C(=CS2)C3=CC=CS3)C(=N1)N4CCN(CC	0.243887
RZTBKYKQRGWYHE	O=C(CCC1=CC=CC=C1)NCC(N2CCC3=C2C=CC=C3)C	0.238874
SAELUZHUVGEPDC	CCN(C1=CC=CC=C1)S(=O)(=O)C2=CC=C(C=C2)C(=O)	0.24194
SAMHYHOPAYQFKM	CC1=C(C(=O)OCCOC2=CC(C)=CC=C2)C(=NO1)C3=C(0.253901
SBLKUDGIULXZDL	COC1=C(OC)C=C(CC(C)N2CCN(CC2)C3=CC(=CC=C3)	0.239064
SCACDDZDERNNJQ	CC(C)NCCOCCOC1=C(Br)C=C(C)C=C1	0.254607
SCDCXJKXJWWTFC	OCCC1CN(CC2=NC(=CS2)C3=CC=CC=C3)CCN1CC4=	0.247788
SCLCQHFTAHMGLY	COC1=CC=C(C=C1)C2=NC(CN3CCN(CC3)C4=C(OC)(0.247001
SCPOUXBOXZRUEC	OC1=CC=C(C=C1)N2CCN(CC2)C3=NN=NN3C4=CC=	0.24602
SCZAVKYSJQFZQE	CN1CCN(CC1)C2=C(C=C(C=C2)[N+](O-)=O)C(=O)C	0.300636
SEFPOGFLQJCNQ	COC(=O)C1=C(NC(=O)N2C3=C(SC4=C2C=CC=C4)C=	0.24457
SERARLPHLRPDEK	COC1=CC=C2C=CC=CC2=C1C3=[N+](N=C(NC4=C(O	0.251573
SESCWBOJVLPNPJ	CCOC(=O)C2(CC1=CC(OC)=CC=C1)CCN(CC3=C(O)C(0.244126
SFAMFMRSBAURBQ	CN1C=NC(=C1S(=O)(=O)OC2=C3C=CC=CC3=CC=C2)	0.240173
SFLJKYWGKSRUHI	CCC(C)(C)N1N=NN=C1C(N2CCN(CC2)C3=CC(=CC=C	0.252182
SGTHCPWGCBBTQS	CC1CN(CCCCOC2=CC(OC3=CC=CC=C3)=CC=C2)CC(0.239105
SHFSMMIREYPMIZ	COC1=CC(=CC=C1)C2=C(C3=C(S2)C=CC=C3)C4=CC:	0.253749
SHGHJFRHODQTAY	NC(=N)SCC1=C2C=CC=CC2=CC=C1	0.31074
SIXYGYZZIPIIQY	C\C(=N\NC1=C2C=CC(Cl)=CC2=NC=C1)C3=CC=C(N)	0.239027
SJULWNAGWWLFPW	CCN(CC)CC(=O)NC1=C(C(=O)C2=CC=CC=C2OC)C3=(0.241348
SLYAPTUIQBLMIT	CC1=C(OCC(=O)NC2CCCC2)C=C(C(Cl)=C1)S(=O)(=C	0.241263
SORBIQRUJDIFIF	CCOC1=CC=C(C=C1)C2=NC3=C(C=CC=C3)C(=C2)C(=	0.251804
SPSPOWPZVGSPTH	OC1=C(NC(=O)C2=C(N=NS2)C3=CC=CC=C3)C=C(Cl)	0.239784
SQBJBIZLVOLNJO	CC1=NC(=NC(NC2=CC(Cl)=C(C)C=C2)=C1)N3CCOCC	0.243064
SQJOFDOREZPAQN	COC1=C(OC)C=C(CCNC2=C(C=CC=N2)C#N)C=C1	0.240019
SRRXZDLALXNSBQ	CCN1CCN(CC1)C(=S)C2=CC=C(Br)C=C2	0.249755
SSXVQELOGLQHU	SC(=NC1CCCC1)N2CCOCCOCCN(CCOCCOCC2)C(S	0.241263
STESNBKMEHDD	ClC1=CC=C(C=C1)C2=C(CN3CCSCC3)N4C=CC=CC4:	0.241345
SVCIDLBDONIET	CN1C2=C(N=C1[N+])3=C(C=C(C=C3C4=CC=CC=C4)C	0.246654
SVXRHEZOFABMBH	C1CCC2=C(NC3=CC4=C(OCCO4)C=C3)C5=C(C=CC=	0.239439
SWGJNUIYBDWJNN	CC1=C(C)C=C(C=C1)C(=O)NCC(N2CCC3=C2C=CC=C:	0.245087
SXZBYUVSZLNKJM	COC1=C(OC)C=C(C=C1)C=C2\CSC\C=C\C3=CC(OC	0.248292
SYERUUDLJVMPLJ	CCCCN(CC)CCNC(=O)C1=CC2=C(S1)C3=C(NC2=O)C:	0.252913
SYHIJYYMOZHSNX	CC1=CC=C(OCCSCC2=NC3=C(N2)C=CC=C3)C=C1	0.250367
SYXLOOHCNOJAFE	CCC(N1CCN(CC1)C2CCCC2)C3=NN=NN3CC4=CC=	0.247569
SYYGCUJYTYVGN	[O-][N+](=O)C1=C(C=CC(=C1)C(=O)NC2=CC(Cl)=C(C=	0.251394
TVFVSMYKTZQONF	CN(CC1=CN(N=C1C2=CC=C(F)C=C2)C3=CC=C(C)C(=	0.250147
TVKRDOZXUUNQKC	CO\N=C(N1CCN(CC1)C2=C(Cl)C=C(C=C2)[N+](O-)	0.243489
TVPLXFFKIHRXIQ	CC(C)OC1=CC=C(C=C1)C(CCN' Vitas-M Laboratory,'	0.247541
TVSQUWXEZAGGAK	CC1=C(C(=O)NC2=NC3=C(CCCC3)S2)C(=NO1)C4=C(0.243021
TVTAROZZZQUKMA	[O-][N+](=O)C1=CC=C(O1)C(=C Asinex Ltd.,BAS 070I	0.241053
TYCOHDNYAYQQMC	CCOC(=O)NC1=CC2=C(C=C1)!: Chem Div,6204-000	0.240287

TYVVZRKDKNAKQL	COC1=CC2=NC(=NC(N3CCN(CC3)C4=C(OC)C=CC=C	0.244287
UAAALTLFXDOSFC	CCN1CCN(CC(=O)C2=C(C)N(CC3=CC=CC=C3)C4=C2	0.24656
UALDBRJEZANGIH	CC1=C(CN2CCC(CO)(CC3CCCCO3)CC2)NC4=C1C=C	0.244347
UBNQMQAKEHACQS	CCOC(=O)N1CCC2=C3C1=CC4=C(C=C(OC)C(OC)=C4	0.239416
UBNXZEQQZVZKGI	CCN(CC)CCN(C(=O)C1=CC2=C(CCCC2)C=C1)C3=NC	0.248484
UBQWKZBWKZJBQL	C\C(=N/NC(=O)C(C1=CC=CC=C1)C2=CC=CC=C2)C3=	0.242639
UCSWKWWBALRWHA	CN(C)S(=O)(=O)C1=CC(NC(=O)CN2CCC(CC3=CC=CC:	0.246389
UCWFKMCLVUTDNK	CN(C)CCCN(C(=O)C1=C2C=CC=CC2=NC(=C1)C3=CC	0.240713
UIJMDUXHELIQBM	CC1=CC=C(NC2=NC(=NC(N\N=C\C3=CC4=C(OCO4)N	0.241678
UINMGICZUPYDIS	CCN1CCN(CC1)S(=O)(=O)C2=CC(C(=O)N(C)CCOC3=C	0.238807
UJXNTMKNABVJLC	CC(NC1=C(C=CC(=C1)N2CCN(CC2)S(C)(=O)=O)[N+](0.239375
UJYXJHAUJAVUPS	CCOC(=O)C1=C(C)N(C2=C1C(CN(C)C)=C(O)C=C2)C3	0.247449
ULIKHOKUJARYGT	CN(C)CCNC(=O)COC1=CC=C(C=C1)C23CC4CC(CC(C	0.243786
UONONLWVMSQVOV	CC1=CC=C(C=C1)N2CCN(C2C3=CN=CC=C3)C4=CC=	0.248933
UPDYFODQZAARMC	NC1=NC2=C(C=CC=C2)N1CCOC3=C(CI)C=CC=C3	0.25916
UPYPKFGTIGBERH	COC1=CC(NC(=O)CN(CC2=CC=C(F)C=C2)C3CCCCC3	0.250012
UQGWTAWOZSDBV	CC(\N=C(/S)NCC1=CC=C(F)C=C1)C23CC4CC(CC(C4)	0.246358
UROAGBRHXNLTPV	CIC1=CC=C(C=C1)C2=CN=C3CCCN23	0.245719
USVOEAYFZSWIIR	CCOC1=CC=C(C=C1)C(=O)C(CN2CCOCC2)C3=CC=C(0.240591
USXULQFZBJCRHV	COCCC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC=C	0.24516
UTVTYBVMPOXYDT	CC1CCN(CCC2=NC3=C(C=CC(NC(=O)COC4=CC=C(CI	0.260735
UUIJAAPVQKLCRV	CCN(CC)CCCNC(=O)C1=NOC(=C1)C2=CC=C(CI)C=C2	0.244432
UUOFRWFOCBNQL	CC1=CC(C)=C(C=C1)\N=C(/S)NCCC2=CC=C(CI)C=C2	0.243255
UVPZPPRSQKHJX	CN(C)C1=CC=C(N\C(S)=N\C23CC4CC(CC(C4)C2)C3)	0.2404
UWPPLJAPAUPEGL	COC1=CC=C(C=C1)[N+] ₂ =C3SC(C)CN3C=C2C4=CC=	0.245784
UXEFRWPQRRAVAY	COC1=CC(OCC(O)CN2CCC(CN3C(=O)C4=CC=CC5=C	0.240683
UXLZBDSLOPHET	COC1=C(C=CC=C1)N2CCN(CC3=CC=C(O3)C4=C(C=C	0.250002
UYCPODUGTIKMQJ	CCOC1=CC=C(CN2CCN(CC2)C(=O)C3=C4C=CC=CC4	0.244236
UYLUHZDEWSZGQW	CC1=CC=C(OCCN2C=C(C#N)C3=C2C=CC=C3)C=C1	0.253488
UYTWVEVNIDBOOP	CN1C2CCC1\C(=C/C3=CC=CC=C3)C(=O)\C2=C/C4=	0.241929
VAJHKGKQGPAOTB	CN(C)C1=C(CI)C(=O)OC(=C1)C2=CC=C(Br)C=C2	0.244281
VBRPHTQWMPRTIL	CC1CCCC(C)N1CC(O)COC2=CC=C(CI)C=C2	0.240498
VBSXPTVMOBQJBU	FC1=CC=C(C=C1)C(=O)N=C(S)N2CCN(C\C=C\C3=CC	0.245464
VBSXUUVLWVVBGPW	C1CC2=NC3=CC=CC=C3C(NC' Chem Div,C660-081	0.252663
VBWIYMDGYOGPQH	CC1=CC=C(C=C1)C2=C3C=CC=CC3=C(N=N2)N4CCC	0.240973
VCBIEXLZPYLOK	CN1C=NC(=C1S(=O)(=O)OC2=CC=C(CI)C=C2)[N+](O	0.25181
VCSUQZLXYTZUSA	CC1=NN(C(NC2=CC=C(CI)C=C2)=C1)C3=CC(CI)=CC=	0.243027
VFTDVICZBGDMMB	COC1=CC=C(C=C1)C(=O)C2=C(OC)C=C(OC)C=C2	0.241962
VITOPYUWSHTJCP	CIC1=CC(CI)=C(OCCN2CCCC2)C=C1	0.247906
VIUARWLVOKKPBA	COC1=CC(NC(=O)CC2=CSC(NC(=O)NC3=C(OC)C=CC	0.238761
VIZQXDUFMCPNNR	CC1SC2=C(NC1=O)C=C(C=C2)S(=O)(=O)CCC(=O)N3C	0.24433
VJEYGFUKNKNUPI	C\C(=N/N=C(S)N1CC2CCC(CC2)C1)C3=NC(C)=CC=C	0.247209
VKJMTDRGVCGQAB	FC1=CC=C(NC(=O)N2CCN(CC2)C\C=C\C3=CC=CC=C	0.239329
VLRIXSOPPQTQRW	OC(COC1=CC=C(C=C1)C(=O)C2=CC=CC=C2)CN3CC	0.256471
VMFCPKMXXMFGCB	CIC1=CC(NC(=O)CSC2=C(C=C3N4CCC(CC4)C3=N2)(0.24346
VNATTZOVBANMGI	O=C(NCCCN1CCOCC1)\C=C\C2=CN(N=C2C3=CC4=	0.242623
VNHQMMKCMKFKVIK	CN(C)C1=NC(SS1)=NCC2=CC=CS2	0.248751
VPLLEOWKJGEBQ	CC1CCN(CCCNC(=O)C2=CC3=C(S2)C4=C(OC3)C=CC	0.251657

VPPSMUBPAGINDQ	COC1=CC=C(CS(=O))(=O)C2=NC(=C(N2CC#C)C3=CC=	0.249151
VPXGOSNPXCNGAI	CSC1=CC=C(COC(=O)C2=C(C=CC(=C2)[N+](O)=O)N	0.253927
VQNDYQDYUOUASP	ClC1=C(\C=C\C=N\NC2=NC(=NC(=N2)N3CCOCC3)N	0.241725
VRBRKGZQLMGDOZ	CN(C)CCCN(CCCC1=CC=C(C=C1)C(C)(C)C(C)=O	0.240452
VRJIARCVQYLUSK	OC(COC(C1=CC=CC=C1)C2=CC=CC=C2)CN3CCN(CC	0.261817
VROFFYZWONRMLJ	CN(CCNC(=O)C1=CNC2=C1C=CC3=C2C=CC=C3)CC	0.251322
VWMOAWMNLJJWES	CC1=CC=C(C=C1)S(=O)(=O)NCC2CCN(CC2)C3=CC=C	0.253024
VYYGUDPHNMYNOZ	COC1=C2C=C3C=CC=CC3=NC2=C(C=C1)C(=O)NCC	0.25093
VZJMIYLTPATHJF	NC(=NC1=C2C=CC=CC2=CC(=N1)C3=NC=CC=C3)C4	0.26062
WAOXRKSTEPNQHX	FC(F)S(=O)(=O)C1=CC(=CC=C1)N=C(S)N2CCN(CC2)C	0.240745
WAWQQSFPVMZFGI	CC1=C(C)C(=CC=C1)N2CCN(CCNC(=O)CN3C=CC=C3	0.241251
WCIBEZJZJGVGON	CCN(CC)CCN1C2=C(N=C(C)S2)C3=C1C=CC(Cl)=C3	0.263197
WCJPLNHOHLMXLW	CN1C=C(CNCC2=CN(C)N=C2C3=CC=C(C=C3)C4CCC	0.249043
WCVFHKQIKJXTB	CN(C)\N=N\C1=C(C)NN=C1C2=CN=CC=C2	0.243383
WDDZRPACTJCDQY	ClC1=CC(Br)=C(OCCCNCC2=CC=CC=C2)C=C1	0.263614
WDJCNXSMIWWVYFP	NC(N)=N\N=C\C1=CC=C(OCC2=C(Cl)C=C(Cl)C=C2)C	0.244928
WETHLXVRTCYMEM	COC1=C/C=C(CNC(=O)C(=C\C2=C\C=C/C(OC)=C\2O	0.247777
WFMOFGWKZAWYQG	COC1=C(OC)C=C2C(N)=NC(NC3=CC(Cl)=C(C)C=C3)=	0.240902
WGQPJPGVHXXIAT	O=C(NC1=CC=C(C=C1)S(=O)(=O)N2CCOCC2)C3=CC=	0.243777
WJWDTOQCLKWEQZ	COC1=CC=C(C=C1)C2=NC(NCC3=CN=CC=C3)=NC(=	0.240604
WLHYVTHSELEICV	COC1=CC2=C(SC(=N2)N(CCCN(C)C)C(=O)C3=CC=C(C	0.255516
WLVBWARTACPUQP	CCN(CC)C1=CC=C(\C=N\N2C(S)=NN=C2C3=C(Br)C=	0.243041
WMVVRGRBAZJRT	O=C(CSC1=NC2=C(S1)C=CC=C2)N3C4=C(SC5=C3C=	0.242171
WODOFYSHORIFHD	CN(C)CCCN(S(=O))(=O)C1=CC(=C(SC2=NN=C(C3CCCC	0.259931
WQIYNLPMGLCLCN	CC1=CC=C(C=C1)C2=CC(C(= Chem Div, K786-061	0.241555
WQSKZUZWWWMTWP	COC1=C(OC)C(OC)=C(CN(C)C(=O)C2=C3C=C(C)C=CC	0.245727
WRAFTAVDGKMKAB	CC1C(NC(C)C1=NO)C2=CC=C(C)C=C2)C3=CC=C(C	0.272942
WRJNPNNNXDKGIT	CN(CC1=CC=CC=C1)C2=NC(NCC3=CC=CC=C3)=C(C	0.239802
WSAFOSLUYQLSH	CC(O)=O.C\C(C1=CC(Cl)=C(Cl)C=C1)=N/N=C(N)N	0.241347
WSKQJKVCLZTFGA	SC(NCCC(C1=CC=CC=C1)C2=CC=CC=C2)=NC3=CC=C	0.243848
WSNZTMMXOCBRKK	CCN(CC1=CC=CC=C1)S(=O)(=O)C2=CC=C(C=C2)C=C	0.239883
WVIRSODSHUDUOW	COC1=CC=C(C=C1)N2CCN(CC(O)COC(C3=CC=C(F)C	0.252213
WXPPGDOWCHYFSR	CCOC(=O)C1=CCN=C1NC(S)=NC2=CC=C(Cl)C=C2	0.238522
WXQWZSULCDJOPQ	CN(C)C1=CC=C(CNC2=NC=CC=C2)C=C1	0.243964
WXVSEVMFXFCFKU	COC(=O)C1C(C(=O)OC)C(C(=O)OC)(C(=O)OC)C(C(=O)	0.251772
WYBNNZDNQBJYZ	COC1=C(C=CC=C1)C(CCNCC2=CC=C(C=C2)N(C)C)C3	0.245168
WYQBCCYUNHYXTC	COC1=CC=C(C=C1)C(=O)CC(NC2=CC=C(C=C2)[N+](O	0.239692
XBDYWBADVCXSTK	OCCN1CCN(CC1)C2=NC3=C(C=CC=C3)C(=C2)C4=C	0.250742
XCUBHVGZTRPNPL	OC(C(CN1CCOCC1)C2=CC=CC=C2)(C3CCCC3)C4=C	0.244066
XEJVOVDZHOXUAT	CN(C)C1=C(C#N)C(OC2=C(C)C=C(Cl)C=C2)=NC=C1	0.259822
XHJDLZKBWRACRS	FC1=CC=C(C=C1)N2CCN(CCCNC(=O)C3CCCN(C3)C4	0.246751
XHNKZHYGYVZHJ	CCCCOC1=CC=C(C=C1)C(\C)=N\NC2=NCCN2	0.243925
XHSAIGFLHNJOKP	CCN(CC)C1=NC2=C(C=C(NC(=O)C3=CC=CS3)C=C2)C	0.240243
XIGRAOLFCSXTG	ClC1=C(Cl)C=C(C=C1)\N=C(/N2CCOCC2)C3=CC=CC	0.260059
XIKYZTGDAQDTNU	CN(CC(O)COC1=C2C=CC=CC2=CC=C1)CC3=CC=C(O	0.249032
XIVYSLHGKXUJTD	CC1=C(SC=C1)C(=O)C2CCCN(CC3=C(C=CC(C)=C3)N	0.23915
XJHNORLJONUTKI	O=C(OCC1=CC=CC=C1)N(CCCCN(CCCNCC2=CC=CC	0.246751
XJYRYUOGCGZHDF	CC1=C(C=C(Cl)C=C1)N2CCN(CC2)C(C3=NN=NN3C4	0.245844

XKOVUBDUNUHXS0	OC(CN1C2=C(C=CC=C2)C3=C1C=CC=C3)CN4CCN(C	0.242184
XLKKCURUKPNNEA	COC1=CC2=C(C=C1)[N+](CC3=C4N=CC=CC4=CC=C3	0.244628
XLYSDMZAMKIWBN	OCCN1CCN(CC1)C2=C(C3=CC=CC=C3)C4=C(NC2=C	0.251952
XNHGVTDLRFSAPN	CC1=NOC(\C=C\C2=NC(C)=CC=C2)=C1[N+](O)=O	0.252868
XOIIRTQBVGWQOQ	CCOC(=O)C1=C(C2=C(C=CC(OC)=C2)N1CCCN(C)C)C	0.262832
XQPZUGBRDVZFDJ	COC1=CC=C(C=C1)N2C=C(CNCCCN3C=CN=C3)C(=N	0.249752
XSJWTEZTQHSADD	CCCCCCCCCCCC[N+](C)(C)CC# Vitas-M Laboratory,!	0.245582
XUHGFSQXOLWNFW	CCOC(=O)C1=CC(=NN1C2=C(F)C=C(F)C=C2)C3=CC=	0.250613
XUTNMIQLYHXVJH	CCOC1=C(OCC2=C(CI)C=CC=C2)C(Br)=CC(CNCCO)=	0.24593
XVHFFYLQYILPQM	CC1=C(N2C=CC=CC2=N1)C3=CSC(NC4=CC(C)=CC=C	0.245144
XVINKGCPRSZLX	CCC(\N=C(/S)NCC1=CC=C(F)C=C1)C2=CC=CC=C2	0.243957
XVYSWTLMGNJWKT	ClC1=CN=CC(CI)=C1N\N=C\C2=CC=NC=C2	0.262123
XXVLKDRPHSFIIB	CN(C)CCN1C(=O)C2=CC(=CC3=CC=CC(C1=O)=C23)[0.242122
XYKMESYITRVGTA	OC1=CC=C(C=C1)[N+]2=C(C=C(C=C2C3=CC=CC=C3)	0.251264
XZORRJRGPUBUJO	CCC(C)NCCOCCOC1=C(Br)C=C(C)C=C1	0.25967
YBXHHZVHHDHTOD	[O-][N+](=O)C1=CC=C(\C=N\NC(=O)CN2C3=C(SC4=C	0.240759
YDIIDGKQDPEWGP	ClC1=CC(=CC=C1)C(=O)C2CCCN(CC3=C4C=CN=CC4	0.256101
YDXNVEKPWOPIOB	CC1=NC=C(N=C1)C(=O)NNC(=O)C2=CC=C(Br)C=C2	0.251588
YECRMDXCCWJQRQ	CN(C)CCCN(C(=O)C1=CC=C(C=C1)C(=O)C2=CC=CC=	0.24065
YEZYPWUWHPIJFLE	C\C(=N/N=C(S)N1CCN(CC1)C2=NC=CC=C2)C3=NC=	0.256075
YFODDWIUJODQNJ	CC(C)OC1=CC=C(CNCCC2(CCOC(C)(C)C2)C(C)C)C=C	0.257049
YFOISQFQTXOBA	CN1\C=C/C(=O)C2=C(C)C=CC=C2)C3=C(CC1(C)C)C:	0.242321
YHTDLQUZNMNIOR	CC1=NOC(=C1)C2=CC(=C(C)C=C2)S(=O)(=O)NCCCN:	0.248604
YIJBKFVBAAGOKC	COC1=CC=C(C=C1)N=C(S)NC(N)=NC2=NC3=C(C=CC	0.239933
YINNFAZGMMIJFN	OCCCCNCC1=CC=C(OCC2=C(CI)C=CC=C2)C=C1	0.261008
YIWWVKPIIIXLBSB	COC1=C(OCCCN2CCCC(C)C2)C=CC(CC=C)=C1	0.240066
YKBOWZAAKMELLI	CN(C)CCOC(=O)C1=C[N](CC2=CC=CC=C2)C3=CC=CC	0.240295
YKKMJJGWUMHXHZ	COC1=CC=C(C=C1)C2=C(C3=C(O2)N=CN(CC4=CC=C	0.239152
YLWMAKXLSDXMED	COC1=CC(CC(=O)NC2=NC(=CS2)C3=CC(OC)=C(OC)C	0.240167
YNHWSBATNPTUPW	CC(C)(C)N1N=NN=C1C(N(CC2=CC=CO2)CC3=CC=C(0.240962
YOMCMCXNHFXHSG	CN1CCC2C(C1)C3=C(C=CC(C)=C3)N2C(=O)NC4=CC	0.299222
YPRFHJIPLZZVDN	COC1=C(C=CC=C1)C2=NC(CN2C3=CC=CC=C3)C4=C	0.247582
YRWBDZODXRMJDJ	COC1=CC(OC)=C(\C=C\C2=CC(C)(C)N=C(S)N2)C=C1	0.239335
YSVZMAWDLNAATP	CCN1CCN(CC1)S(=O)(=O)C2=CC(C(=O)NC3=C(C=CC	0.262162
YUFKRFB0VWVWJRJ	N#CC1=C(N=C(C=N1)C2=CC3=C(OCCOCCOCCOCCOCC	0.239444
YUPPELVWCBEYPQ	CN(O)C(=S)C1=CC=CC=C1	0.25317
YUQBQMYRWOFRLV	CC1(C)CC(=CC(C1)=[N+]2CCCCC2)N3CCN(CC4=CC=	0.239731
YWVAFGKAVNYSSZ	CC(C)(C)NC1=NC(NC(C)(C)C)=NC(NN)=N1	0.242922
YXSUMTZEYLAKDC	CC1=CC=C(CNC(N)=NC2=NC(C)=CC(C)=N2)C=C1	0.24048
YYILJCASTDQTHM	OC(CSC1=C(CI)C=CC=C1CI)CN2CCN(CC2)C3=CC=C(0.260717
ZANNRTNEIWXXEG	COC1=CC=C(C=C1)N(C)S(=O)(=O)C2=CC(=CC=C2)C(:	0.242384
ZBCONQPPSGNGCK	O=C(N1CCN(C\C=C\C2=CC=CC=C2)CC1)C3=NN(CC4	0.243198
ZCKCUBVQBIPCEZ	COC1=CC(OC)=C(CN2CCN(CC3=C(C=CC=C3)C(F)(F)F	0.247869
ZCMKKFLZOGVHPV	CC1=C(\N=N\N2CCOCC2)C(=NN1)C(F)(F)F	0.2494
ZCXJDVQGWDEQDD	COC1=CC2=C(C=C1)N(C)C(C)=C2C(O)CN3CCC(CC4=	0.246047
ZEDIOOZDWFAQFR	CCCCCCC(O)(C(CN1CCOCC1)C2=CC=CC=C2)C3=CC:	0.241569
ZEGIJHAYNYJTLA	CN1CCN(CC1)C(=O)CCN2C(=S)S\C(=C/C3=C(CI)C=C	0.23988
ZEGXDKXOBNMNHM	CN(C)C1=CC=C(C=C1)C2C3CCCC4=C(C=CC=C4)C3=	0.263421

ZETGWOAMKIFVCD	C1C1=CC=CC(Cl)=C1CN2C(=NC3=C2C=CC=C3)C4=C	0.247156
ZFKSUSAQDQXBQU	CCCCNCCCOC1=C(Br)C=C(C)C=C1	0.23914
ZGAVNXQAROBPJG	C\C(=N/N=C(S)N1CCN(CC1)C2CCCCC2)C3=NC=CC	0.260434
ZGSMAKABUUKIGZ	COC1=CC=C(C=C1)N2CCC3=C(C)N=C4C(OC)=CC(OC	0.250934
ZGTAJRXCMOHMGE	CC1=CC=C(C=C1)S(=O)(=O)C2=C(N=C(N=C2)C3=CC=	0.254793
ZGZKWXYPXZOLP	CCOC(=O)C1=C(C)N(C)C(C)=C(C1C2=CC=C(C=C2)C(=	0.242628
ZHSVAVLUGYWZLY	FC1=CC=C(C=C1)N2CCN(CC2)C(CNS(=O)(=O)C3=CC	0.239119
ZIADASSVEQFTPJ	C1C1=CC(CSC2=NCCN2S(=O)(=O)C3=CC=CC=C3)=CC	0.239725
ZKSCCNZKLCYNG	C\C(=N/NC(S)=NC1=CC=C(C)C=C1)C2=NC=CC=C2	0.253654
ZMEIUSLAHMLILY	C\C(=N/NC1=NC2=C(S1)C=CC=C2)C3=NC=NC=C3	0.265783
ZNKZJFNZLZIBKB	C1C1=CC(Cl)=C(CN2C=CC(C=C2)=NC=C(C#N)C#N)C=	0.250451
ZOQUZJUOXNLBG	SC(NC1CCCC1)=NC2=CC(Cl)=C(Cl)C=C2	0.24986
ZPKMAEIACURLLY	NCC(C1=CNC2=C1C=CC=C2)C3=C(Cl)C=C(Cl)C=C3	0.246432
ZQWQPIZBIBXILO	FC(F)(F)C1=CC(=C(Cl)C=C1)S(=O)(=O)N2CCN(CC2)C:	0.244144
ZRDDDLMFVDMLDV	CC1=CC(OCNC2=C(C=CC(=C)N3CCOCC3)[N+](O-	0.242109
ZRPCBSVZDYOXLU	OC(CN1C2=C(C=CC=C2)C3=C1C=CC=C3)CN4CCN(C	0.251721
ZTSHUIKUXBMWIU	COC1=C(CNCCC2=CC(Cl)=CC=C2)C=C(Br)C=C1	0.243062
ZVKRQQLIVGVTJW	CC1=C(C(C)=C(C#N)C(SC2=CC=C(Br)C=C2)=N1)[N+](0.272193
ZVLDOCMMDSEFS	CC1=NOC2=C1C(=NC=N2)N3CCN(CC3)C4=CC(Cl)=C	0.238589
ZVRFHIOZZIRX	CCN(CC)C1=CC=C(NC(=O)C2=CC3=C(N2)C=CC=C3O	0.250594
ZWLLBMKHBAHHR	CCN(CC)S(=O)(=O)C1=CC=C(CC2=C(Cl)C=C(C=N2)C(I	0.245013
ZXLYQIGBMNBIGR	CN1CCN(CC1)C2=C(NC(=O)C=C\C3=CC=C(F)C=C3)I	0.244455
ZXPRMDFCJHQDNF	C(CNC1=NC(=NC2=C1OC3=C2C=CC=C3)C4=CC=CC:	0.242826
ZYGZEBPRTVGGB	CC(C)(C)NC1=NN=C(CS1)C2=CC=C(Cl)C=C2	0.244895
ZYPWORFMWGRPSP	CCCCC1(C)CC2=C(C=CC=C2)C(S)=N1	0.246835
ZYVNVSXHLQNSKF	SC(NCCSCC1=C(Cl)C=CC=C1)=NC2=CC=CC=C2	0.243746
ZZBGZNIPTZCMW	COC1=C(C=CC=C1)C2=C(C3=C(S2)C=C4OCOC4=C3)	0.25041
ZZCOBZHGHUPJB	COC1=CC=C(C=C1)N2C(COC3=CC=C(C)C=C3)=NN=C	0.259249
AASRCBKEVNIKNS	FC1=CC=C(C=C1)C(C#N)C2=CC=C(C=C2)C(=O)C3=CC=CC=C3	0.237494
ACFMQNZEFBOBOS	COC1=CC=C(C=C1)C2CCCN2CC(O)COC3=C(C=CC=C3)C(C)C	0.289474
ACIVKCBUJZMHEJ	COC1=CC(=CC(OC)=C1)C(=O)NC2=CC=C(C=C2)N3CCN(CC3)C(=C	0.241977
ACLPGRMEXAUBOL	CSC1=CC=C(C=C1)N2CCN(CCCNC(=O)NC3=C(F)C=CC=C3)CC2	0.224886
ACYIFJVISTZKDH	CCOC(=O)C2(CC1=CC(OC)=CC=C1)CCN(CC3=C4OCOC4=CC=C3)	0.247797
ADAPKYLLFMLIQP	CCN1CCN(CC1)S(=O)(=O)C2=CC(C(=O)N(C)CC3=C(Cl)C=C(Cl)C=C	0.222704
ADPFAIWAXXBVD	CCN1CCN(CC1)S(=O)(=O)C2=CC(C(=O)N(C)CC3=C(Cl)C(Cl)=CC=C	0.231533
ADSUTYNVUAOYJE	CC1=CC=C(NC(=O)NC2=CC(Cl)=C(F)C=C2)C=C1	0.225507
ADYMNXMINSVTR	CN(C)C1=C(C2=CC=CC=C2)C(N)=C3C=CC=CC3=N1	0.232919
AEKSGFBUSUPIU	OCC2(CC1=CC=C(Cl)C=C1)CCN(CCCC3=CC=CC=C3)CC2	0.2842
AFQJSVUEYGIVJR	CCOC1=CC=C(C=C1)C2=CS\C(N2CC)=C(/C#N)C3=NN=C4CCCCC	0.226314
AFVPSEWUXQUXPL	CC1=CC2=C(C=C1)N=C([NH]2)C3CCN(CC3)CC4COC5=CC=CC=	0.224743
AFWZWCFLKWMERJ	CC1=CC=C(O1)C2=NOC(=N2)C3CCCN(C3)C(=O)C4=CC=C(Cl)C=C	0.22555
AGCVPOVKAQCEKZ	CN(C)CCOC1=CC=C(C=C1)C2=C(C(C)=C3C=CC=CN23)C4=CC=CC	0.255421
AGJXMOUNRZOAQL	CC1=CC(Br)=C(OCN2CCCC2)C(Cl)=C1	0.277172
AGMZYQRFQBWYMA	CCOC1=CC=C(C=C1)C(O)(CCC(C)C)C(CN2CCOCC2)C3=CC=CC=C:	0.241531
AGZPBADSPZYFK	COC1=CC=C(OC(=O)NC2CCN(CC3=CC=C(Cl)C=C3)C2)C=C1	0.225463
AHRRJYCTHQFNFIJ	CC1=CC=CC(C)=C1N2CCN(CC2)C(=O)NC3=CC4=C(OCCO4)C=C3	0.232099
AHSMUGYEUDLUEJ	CCOC1=C(OC)C=C(CN(C)CC2=CC(=O)OC3=C2C=CC(C)=C3)C=C:	0.230633
AIARMSZYEHLPA	CC1=CC=C(C=C1)N2CN(CCC3=CCCC3)CN=C2S	0.234144

AIAUBLZIUFOPKQ	COC1=C(OC)C=C(CC(=O)C2=C(C)C(OC)=C(OC)C=C2)C=C1	0.260861
AIHIQFKQKQRNDO	CN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)N4CCCC4)C(C)=C2	0.224537
AIPOQWXLFRZLBZ	FC1=CC=C(CN2CCC(CC2)C(=O)NC3=CC=C(OC4=CN=CC=C4)C=C	0.245715
AISCERDTBIBFLE	CCC1=NOC(CN2N=C(C=C2C(=O)NCC3=CC=CS3)C4=CC=CC=C4)=	0.228875
AIVPWARKSDFLRL	CCOP(=O)(C1=C(OC(=N1)C2=C(CI)C=CC=C2)N3CCCC3)C4=CC=	0.223151
AJYMPTJHOJJOAX	OC(CSC1=C(CI)C=CC=C1)CN2CCN(CC2)C3=C(F)C=CC=C3	0.228084
ALCDRILYESVMBT	CCOC1=CC=C(\C=N\NC(=O)COC2=C(C=CC=C2)C3=CC=CC=C3)C:	0.248478
ALIGJLBZICSLG	NC(=NOC(=O)C1=CC=CC=C1)C(CC2=CC=CC=C2)C(O)=NOC(=O)C:	0.288549
ALLWYNNQMHUNLY	COC1=CC2=C(C=C1)C(C=C(S2)C3=C(OC)C=CC=C3)C4=CC=C(OCC	0.261341
ALOLQKUQFQNHEP	COC1=C(NS(=O)(=O)C2=CC(NC(=O)NC3=CC=C(CI)C=C3)=CC=C2)	0.234222
ALSZPRQIWXWJGV	COC1=C(C)C(OC)=C(\C=N\NC(=O)C2=CC=C(COC3=C(CI)C=CC=C3	0.235823
AMJQCSLHSRWVTB	FC(F)(F)C1=CC(=CC=C1)N=C(S)N(CCCN2CCCC2)CC3=CC=CN3CC	0.230474
AMYLJMRRCMPYGD	NC(=N)SCP(=O)(C1=CC=CC=C1)C2=CC=CC=C2	0.251038
ANHCGXPONAGNRS	CC1=CC(OCC(O)CN2CC3(C)CC2CC(C)(C)C3)=CC=C1	0.234722
ANIBUTITUZXEIN	COC1=C(NC2=C3C=CC=CC3=NC4=C2CCC4)C=CC=C1	0.268164
ANOXEUSGZWSCQL	COC1=C(OC)C2=C3[C@H](CC4=CC=C(OC5=C6[C@H](CC7=CC=C	0.304396
AOMRGESQCJWXMU	CSC1=CC(NS(=O)(=O)C2=CC=C(C=C2)C3=COC(C)=N3)=CC=C1	0.255355
APBGERKKEPNJPX	NNC(S)=NCC1=CN=CC=C1	0.232993
APZNOVIGOGKSL	BrC1=CC=CC(=C1)C2=NC(=NO2)C3=CC=NC=C3	0.231923
AQBXGPHZDHQKJU	COC1=CC=C(CCC2=CC(OC)=C(OC)C(OC)=C2)C=C1	0.282749
AQDSFMDNNDYZQZ	CC1=CC=C(NC2=NC(CN3CCC4=C(C3)C=CC=C4)=NC(N)=N2)C=C:	0.269416
AQIRCFUGHKTBRW	COC1=CC(=CC(OC)=C1)C(=O)NC2=CC=C(C=C2)C(=O)NC3=C(OC)	0.230892
AQKSZPZBPSWIIF	COC1=CC=C(C=C1)C(=O)NNC(S)=NC(=O)C2=CC=CC=C2	0.22849
AQLIQOWLNIWJQK	COC1=CC=C(OCC(=O)NC2=C(C=CC=C2)C3=CC=CC=C3)C=C1	0.284975
ARFHVPIUSIFBRQ	O=C(NC1=CC2=C(CCC2)C=C1)C3=CC=CC=C3	0.234587
ASCMALAQEXFXOO	CC1=CC(NC(=O)C2=CC=C(COC3=C(CI)C=CC=C3)C=C2)=NC(C)=C:	0.22523
ASGPCSXEGIHST	CSC1=CC(CN2CCC(CC2)OC3=CC=C(C=C3)C(=O)N4CCCC4)=CC:	0.228897
ASGYLGLHJVMQSD	CC1CN(CC(=O)NC2=NC(=CS2)C3=CC=C(CI)C=C3)CC(C)O1	0.235269
ASINSSNRTKKCSK	CC1CC(C)CN(CCOC2=CC=C(Br)C=C2)C1	0.246441
ASMJXIDKPABPIX	COC1=C(C=CC=C1)C(=O)NC2=CC=NN2C3CCN(C\C=C\C4=CC=C(0.235373
ASODCVVTIYBPJW	C/N=C\1/C2=C(C3=CC(=CC=C3N2CCN1C)OC)C4=CC=CC=C4	0.229924
ASVUGFSTHMYMMZ	COC1=CC(OC)=C(CN2CCN(CC2)C(=O)COC3=CC4=C(C=CC=C4)C=	0.225911
ATEGWQFKEHLPHS	C(NC1=C2C=CC=CC2=NC(=N1)N3CCN(CC3)C4=CC=CC=C4)C5=(0.225361
ATKFQPJQNPDUHP	FC1=CC=C(C=C1)C2N(CCCN3C=CC=N3)CCC4=C2NC5=C4C=CC=	0.23311
ATSPISXBGSVNJB	CC1=CC(NC2=CC=CC(=C2)[N+ Chem Div,4248-0392	0.229545
ATTEYLKIDJNPW	CCOC1=C(OC)C=C(CNC2CCCCC2)C=C1Br	0.253714
ATWQYIPIROSCR	COC1=CC2=C(C=C1OC)C(C)N(CC3=C(OC)C=CC(\C=N\NC(=O)C4=	0.229011
ATYQDOWOVFHSBG	COC1=CC=C(C=C1)S(=O)(=O)NC2=C(OC)C=CC(CI)=C2	0.239799
AUBPAHGOPMKHON	CN1CCCN(CC2=C(Br)C=CC=C2)CC1	0.225802
AUHSCPWSQSCWHJ	CC1=NC(C)=C(S1)C2=CSC(NC3 Vitas-M Laboratory,STK135234	0.223193
AUIABNOHKCXLLO	CC1=CC(OCCN2CCC3=C(C2)C=CC=C3)=C(C=C1)[N+][O-]=O	0.232733
AUTKUCVVRPJBCM	C1=CC=C(C=C1)C2=NN=C(N=C2)C3=NC=CC=C3	0.233558
AVEBTIMALLPEHM	CCC(C)(N(N=O)C1=C(CI)C=CC=C1)C2=NN=NN2C3=C(C)C=CC=C3	0.232511
AVMIDJMCARKKQD	CCCCOC1=CC=C(CN2CCSC2)C=C1	0.223115
AVQXSVWNHJNMRC	CN(CCC(=O)NC1=CC=C(CI)C=C1)CC2=CC=CC=C2	0.246379
AVZUMYQYDQLHFF	ClC1=C(C=CC=C1)C2=CC=C(O2)\C=N\NC(=O)C3=CC=CC=C3	0.229733
AWNGFBUYGOWSNY	ClC1=CN2C=C(N=C2C=C1)C3=CC4=C(OCO4)C=C3	0.231263
AXCWVBQRHXIMP	CN1C=CN=C1SCC2=CN3C=C(Br)C=CC3=N2	0.226502

AXGPAKQCBGOPEJ	CN(C)CCCN(CC1=CC2=C(C)C=C(C)C=C2NC1=O)C(\S)=N\CC3=CC	0.229256
AXGRPWAPOGHIQD	COC1=CC(OC)=C(C=C1)C(=O)C2CCCN(C2)C3CC4=C(C3)C=CC=C4	0.269658
AXRFHVSJXDUWGD	COC1=C(C=CC=C1)N2CCN(CC3=CC(Br)=CC=C3)CC2	0.254482
AYDOMIXGYJLDMY	COC1=C(OC)C(CNCC2=C(Br)C=CC=C2)=CC=C1	0.263906
AYELFEVAWGRWJK	CN(C)CC\C=C1\C2=C(SC3=C1C=C(CI)C=C3)C=C(F)C=C2	0.377801
AYVUMJJNEANS DG	COC1=CC(=CC(OC)=C1OC)C(=O)N\N=C\C2=C(C)SC=C2	0.240669
AZJRNGLZWXWQT	COC1=CC=C(C=C1)C2=C(SC(=N2)N3CCCCC3)C(=O)C4=CC=CC=C4	0.231472
AZUPXLMDEBQPMR	CC(C)NCC(O)C1=CC=C(C=C1)C2CCCC2	0.222923
BAMHRHHJUIHVEL	CN(C)C(CNC(=O)C1=C(CI)C=CC(=C1)S(=O)(=O)N(C)C2=CC=CC=C2	0.247382
BAWIKNJTMONHPS	CC1=NOC(=C1C(=O)O\N=C(/N)C2=CC=C(C=C2)C(C)(C)C3=CC=C3	0.23184
BBNMGAAYWJNSLK	COC1=CC=C(C=C1)C(\C)=N\N=C(/S)NCC=C	0.223649
BBVAPEPYNHBXNN	CN1C=C(CN2CCN(CC2)C3=CC(C)=NC(C)=C3)C(=N1)C4=C(F)C=C4	0.24281
BCHVIOYJXOCQFG	CC1=CC=C(OC2=CC=C(C=C2)S(=O)(=O)NCC(C)(C)N3CCOCC3)C(=O)C4=CC=CC=C4	0.236161
BCVQJQQTPWRCME	CCC(N1CCN(CC1)C2=CC(=CC=C2)C)C3=NN=N[N]3C(C)(C)C	0.235798
BDDFHKQCQVEDIO	CC(C)C1=C(OCC(O)CN(C)CC2=CC=CC=C2)C=C(C)C=C1	0.254635
BDSKZGMMUZJQQT	COC1=C(OC)C=C(C=C1)C2=C(OC(C)(C)C)N=C(OC(C)(C)C)N=C2	0.319565
BDSQWOPRSMBXAT	CCOC(=O)CN1C(=N)N(CCOC2=CC3=C(C=CC=C3)C=C2)C4=C1C=C4	0.2527
BEIOTRIMEFDJST	COC1=CC=C(C=C1)C(=O)O\N=C\C2=C(SCC3=C(CI)C=CC=C3)N(C)C	0.224142
BEKLGEVQKKS NLM	CCOC1=C(C=CC=C1)N2CCN(CC3=C(OC)C(OC)=C(OC)C=C3)CC2	0.231657
BFFQFOBHPRLZCN	FC1=CC=C(C=C1)C2=NN=C(O2)C3=CC4=C(C=CC=C4)C=C3	0.29579
BFGKMEZYPPJWNA	ClC1=CC=C(COC2=CC(CNCC3=CC=NC=C3)=CC=C2)C=C1	0.226457
BFJIMBWUFKWQDO	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC(F)=CC=C3)CC2	0.248952
BFKGAYAKPZQXFE	CCSC1=NSC(NC(=O)NC2=CC(F)=CC=C2)=N1	0.22327
BGGICLDHEUSDFV	CSC1=CC=C(C=C1)S(=O)(=O)NC2=CC=C(F)C=C2	0.232207
BGOSATMJICJGCY	COC1=CC=C(C=C1)C(N2CCN(CC2)C3=CC=C(OC)C=C3)C4=NN=N4	0.232081
BHDNWYQMDQWZGK	COC1=C(CI)C=C(C=C1)C2=CC=C(CNCCCN3CCOCC3)O2	0.247144
BHGWOZJFVFCQ	CC1=CC=C(C=C1)S(=O)(=O)OC2=C(C=CC=C2)C3=CC=CC=C3	0.270688
BHPUCSXYFCWZKO	C(COC1=C2C=CC=CC2=CC=C1)CN3CCCCC3	0.265849
BIFMXJBRWDNSAA	COC1=CC=C(C=C1)C2=C(C3=C(S2)C=CC=C3)C4=CC=C(O)C=C4	0.234788
BIPYEWPIKKNUMI	CC(=O)NC1=NN(C(C)=O)C(C)(S1)C2=CC=CS2	0.223997
BISWIAQUGOELCK	CCSC1=NC2=C(C=C(OC)C(OC)=C2)C(=N)N1CCCN3CCOCC3	0.265593
BJFHJAVFRVWDQJ	COC1=CC=C(OCC2N(CCC3=C2C=C(OC)C(OC)=C3)C(S)=NC)C=C1	0.254213
BJMUGVJXKMIWFB	CC(NCC1=CC=C(OCC2=CC=C(CI)C=C2)C=C1)C(O)C3=CC=CC=C3	0.223347
BJQKWSSXUZLJHP	COC1=CC(CN2CCN(CC2)C(=O)C3=C(C)C=CC(=C3)S(=O)(=O)NC4=CC=CC=C4	0.232878
BJRMIBIDQJDYPM	CC(=O)N1CCN(CC1)C2=C(CI)C=C(NC(=O)C3=CC(=C(C=C3)N4CC=CC=CC4	0.225059
BJUZJRDGGZMYBB	CN(CC(O)COC(C1=CC=CC=C1)C2=CC=CC=C2)C3CCCCC3	0.268393
BKMXHRJXCXNEQV	CC1=NC=C(CN2CCCC(C2)C(=O)NC3=CC=C(C=C3)C4=CC(F)=CC=C4	0.226393
BLBOGNWRCZWBRL	CCC(C)C1=CC=C(N\C(S)=N\C2=C(C)C=C(OC)C=C2)C=C1	0.239345
BLCDALNXTYIDY	COC1=C(COC(=O)C2=CC(=CC=C2)N(C)C)C=C(C=C1)C(C)=O	0.22492
BLMLURKILFRZRZ	COC1=C(OCC2=C(CI)C=CC=C2F)C=CC(CNCCN(C)C)=C1	0.293234
BLSVDFZAFIAGRO	CC(=O)C1=CC(CN2CCC(CC2)C(=O)NC3=CC(=CC=C3)C4=CSC=N4	0.222908
BLZMTXKDCRAJFA	CC(C)(C)CC(C)(C)NCC(O)COCCOC1=CC=C(Br)C=C1	0.231371
BMBWRFABZOCADR	CN(CC(=O)NC1=C(C=CC=C1)C2=CC=CC=C2)CC3=C(C)C=CC=C3	0.229068
BMGYCRITAPCASD	CNCCCOC1=CC2=C(CCC2)C=C1	0.257926
BMHG UWQJWGVXMD	C(SC1=NN=C(C=C1)C2=NC=CC=C2)C3=NC=CC=C3	0.230966
BMOIQSIAAWNCHF	[O-][N+](=O)C1=CC(=CC=C1)C2=CC=C(CN3CCN(CC3)C4=CC=CC=C4	0.225686
BNDNQOBIHDSIDO	CC1=C(C)C=C(NC(=O)N2CCCN(CC3=CC=C(F)C=C3)C2)C=C1	0.258858
BOEIMGXBJBIBFB	CC1CCCCN1C2=C3C=CC=CC3=NC=N2	0.229768

BOHJXWIKYKVKNM	FC1=CC=CC(N\C(SCC2=CC=CC Vitas-M Laboratory,STK548494	0.229265
BOSGQZOGZYRDLT	SC(NCC(N1CCCCC1)C2=CC=CO2)=NCC3=CC=CO3	0.223752
BPJCPHVVMMHXPT	O=C(NCCCCCCC1CCCCC1)C(C2CCCC2)C3CCCC3	0.265998
BPSUZGWXWZLOPC	COC1=CC(NC(=O)C2=CC(=CC=C2)S(=O)(=O)N3CCN(CC4=CC=CC=	0.236329
BQODYDMJEHLGFO	CC1CC2=C(C=CC=C2)N1CC3=CC(=CC=C3)S(=O)(=O)N(C)C	0.247887
BQPQYRCBUNHGPV	CC1=C(C)C(=CC=C1)N2CCN(CC2)C(C3=CC=CS3)C4=NN=NN4C(C	0.229102
BQVXYHYXISZSEZ	ClC1=CC(NC(=O)NC2=CC=CC=C2)=CC=C1	0.257285
BQZXBDMZJFAFRA	COC1=C(OC)C=C(CNC(=O)CC2=CC=C(C=C2)C3=CC=CC=C3)C=C1	0.233526
BRTJTYYVQVSSDC	COC(=O)C1=C(C=CS1)\N=C(/S)N2CCN(CC2)C3=C(C)C=CC(C)=C3	0.24367
BRYSGTDRSIOCPS	CCOC1=CC=C(NC(=O)C2=CC=C(CN3CCC4=C(C3)C=CC=C4)C=C2	0.224761
BSMBZDDPUMOQPJ	N(C1=N\C(=N/C2=NC=CC=C2)C3=C1C=CC=C3)C4=NC=CC=C4	0.242641
BTHJSJWKKXLIKW	COC1=CC2=C(NC(=C2)C(=O)N3CCN(CC4=CC=C(F)C=C4)CC3)C=	0.225883
BTIQRDLMOKTWQC	COC1=C(CNCC2=CC=C(C)C=C2)C3=C(C=CC=C3)C=C1	0.332308
BTOPPOSOJXWFAJ	CN1C=NC=C1C#CC2=C(SC3=C2C=CC=C3)C4=CSC=C4	0.22669
BTPKXYVSPCTESF	COC1=C(OCC2=CC=CC=C2)C(Cl)=CC(CNCCC3=CC=CC=C3)=C1	0.234719
BTTVNTIBAFEWEV	OC(COC1=CC=C(Cl)C=C1)CN2CCC(CC3=CC=CC=C3)CC2	0.269172
BTVNLBYXURCKH	CCC[C@@H](CN[C@@H](CNC)C(C)C)NCCCCC1=CC=CC=C1	0.224191
BTXVDTFVASAZJF	FC(F)(F)C1=CC(=CC(CCN2CCNC[C@@H]2CC3=CC=CC=C3)=C1)(0.224064
BUAHNKMYLRTGSL	COC1=CC=C(C=C1)N2C=C(C3=C2N=CN=C3N4CCN(CCO)CC4)C5	0.241471
BUNQSOFZXWJGTL	CN(C)C1=NC(NC2=CC=C(F)C=C2)=NC(NN)=N1	0.226677
BUOCOYLLPODLCO	CN(C)C1=CC=C(C=C1)C2N(CCN2C(=O)C3=CC=C(C)C=C3)C(=O)C	0.240204
BUTMLLMFIQVESW	CC1=CC(OCCN2CCCCC2)=C(C=C1)[N+][O-]=O	0.268177
BVRMUICYAKQBCW	ClC1=CC=CC(=C1)[N]2C(=NN=C2SCC#N)COC3=CC=CC4=CC=CC=	0.224227
BVZMDKSFUGHPNM	O=C1N(CC2=CN=CC=C2)C[C@@H]3C[C@H](N4CCC[C@@]134	0.224449
BWDSMWZBQJYVLD	CN(C)CCOC1C2=C(CCC3=C1C4=C(C=CC=C4)C=C3)C=CC=C2	0.278688
BWFJFDFSCPJWFL	COC1=C(C=CC=C1)N2CCN(CC3=C(O)C=C(C)C(C)=C3)CC2	0.238928
BXDSNVDDCYESMA	CCOC1=C(OCC=C)C(Br)=CC(\C=N\O)=C1	0.242257
BXHHWAOVEHCDHF	ClC1=C(C=CC(NC(=O)C2=CN=CC=C2)=C1)N3CCN(CC3)C(=O)C4=	0.226613
BXJKOPVBUDWDQZ	FC1=CC=C(CNC(=O)COC2=CC=C(Cl)C=C2)C=C1	0.224681
BXJXHNSQWRVHT	CCC1=CC=C(C=C1)C2=NC3=C(C=CC=C3)C(=C2)C(=O)NN4CCN(C	0.228526
BXSFUKRCGLOBQQ	CN(C1=CC=CC=C1)C2=NC(=NC(=N2)[N]3C=CN=C3)N4CCCC4	0.224291
BXYINYBUTMVQPS	CC1=NC(=NC(=C1)N2CCOCC2)C3=C(O)C=CC=C3	0.252139
BXZQWBSRVZLWCC	COC1=C(OCC2=CC(Cl)=CC=C2)C=CC(CNCCN3CCOCC3)=C1	0.307172
BYTYAJKQMBGNK	CC1=CC(CN2CCC(CNC(=O)NC3=C(C)C(Cl)=CC=C3)CC2)=C(C)C=C	0.275757
BZACYZYRPQYTH	[O-][N+](=O)C1=NC=C(C=C1)N2CCN(CC2)C3=CC(Cl)=CC=C3	0.243935
BZIAEZXSQSIYSO	COC1=CC=CC=C1N2CCN(CC2)C(C3=NN=N[N]3C(C)(C)C)C4=CC=	0.248249
CACLSACREDIJKKA	CC1=CC=CC(=C1)N2CCN(CC2)C(=O)C3=CC=NC=C3	0.227805
CAHYBXRVISPHFZ	C\C=C(/C)CN1CCN(CC1)C2=CC(=CC=C2)C	0.263234
CBLQZPJUGCLDBK	CC(C)COC1=CC(=CC=C1)C(=O)NC2=CC=C(CN3CCOCC3)C=C2	0.233119
CBYUCPYFKGYOHO	COC1=CC=C(OC)C(NC(=S)N(CCC2=C(C)NC3=CC=CC=C23)CC4=C	0.226976
CCOPWNUUIGRDLJ	CCN1C(=O)C=C(OCC(=O)NCCCN2CCN(CC2)C3=CC(Cl)=CC=C3)C	0.22587
CDFYRTDHIKBKFK	CN(C)S(=O)(=O)C1=CC(=CC=C1)C2=CN3C=C(Cl)C=CC3=N2	0.227464
CDHZIABROIXFSK	CC1=CC(NC(=N)NC2=NC(C)=C Chem Div,4477-2810	0.230941
CDJKCCVJOSEVCN	COC1=CC(=CC(OC)=C1OC)C(C[N+][O-])=O)C2=C(C)NC3=C2C=C(0.227365
CDOFQIKMXHKBAM	CN(C)CCNC(=O)C1=CC(NS(=O)(=O)C2=CC=C(C)C=C2)=C(C=C1)N:	0.224304
CDQDBARFPXIBDL	CCOC1=C(C=CC=C1)N2CCN(CC3=CC=CO3)CC2	0.223888
CEBGMERQJUUHQ	COC1=CC(\C=N\NC(S)=NC2=CN=CC=C2)=CC=C1	0.223044
CEGNVVBQHXHNIS	CCN(CC)CCCN(CC1=CC=C(C)O1)CC2=CC=C(C)O2	0.246589

CELVNGSELGNMX	CN(C)CCCNC(=O)C(\NC(=O)C1=CC=CC=C1)=C/C2=CC=C(O2)C3=	0.232595
CEONVQJNAZKJEP	COC1=C(NC(=O)CN(C)C2CCCC2)C=C(Cl)C=C1	0.225634
CEZSIEYRNYQISC	OC1=CC(\C=N\N2CCN(CC2)C3C4=C(C=CC=C4)C5=C3C=CC=C5):	0.227509
CFDQVGFNCRRBHF	CC1=NN2C=C(C=NC2=C1Br)C3=CC(Cl)=CC=C3	0.231501
CFGFKGXGORLUDT	CC1=N[N](C2=CC=CC=C2)C(=C1)C(=O)NCCN3CCN(CC3)C4=CC=	0.257222
CFLROMZYSCLTKV	COC1=CC=C(NS(=O)(=O)C2=CC=C(C=C2)C(=O)N3CCCCC3)C=C1	0.231824
CFQDHJAYMGIKSH	CC(C)C(N(CC1=CC=CS1)CC2=CC=CC=C2)C3=NN=NN3C(C)(C)C	0.235233
CFRXYOYUERVVQOJ	FC1=CC=C(\C=N\NC2=C3C=CC=CC3=NC(=N2)C4=CN=CC=C4)C=	0.226378
CFVDXHSQQLTGMR	CC1=CC(OCCN2CCC3=C(C2)C=CC=C3)=C(Cl)C=C1	0.237775
CFWGNVBFHLHVDZ	CN(C)CCOC2(CC1=CC=C(C)C=C1)CCC(CC2)C(C)(C)C	0.282242
CFWRFUOXDOJOMS	CCN(CC)C1=CC=C(C=C1)C(=O)N\N=C\C2=C(OC(F)F)C=CC=C2	0.224016
CGFOMWCQKNHSDI	NC1=C(Cl)C=C(C=C1Cl)\N=N\C2=CC=CC=C2	0.255718
CGNKPCLUWSNJCD	[O-][N+](=O)C1=C(CN2CCN(CC3=CC4=C(C=CC=C4)C=C3)CC2)C=	0.23251
CHGKOYRZOJKRGJ	COC1=CC(CN(CCC2=C(C)NC3=C2C=C(C)C=C3)C(S)=NC(C)(C)C)=C	0.23517
CHJVUQSZTPIBOH	COC1=C(Br)C=C(\C=N\N2CCN(CC3=CC=C(C)C=C3)CC2)C=C1	0.265746
CHLGGFOIALNAM	O\C(CN1CCN(CC1)C2=C(F)C=CC=C2)=C(\C#N)C3=NC(=CS3)C4=	0.227847
CHWNQKIZEDLWAC	CC1=C2COC(C)(C)CC2=C(C#N)C(=N1)N3CCN(CC4=CC=CC=C4)C	0.228759
CIUJRBUERMUQIZ	COC1=CC=C(C=C1)C2=NN(C(C2)C3=CC=CC=C3)C(=O)C4=CC(=C	0.259136
CIXYZNFDMNWESE	BrC1=CC=C(C=C1)S(=O)(=O)NC2=CC(=CC=C2)C(=O)NC3CCN(CC	0.235736
CKMNSLDZNGQQFK	CC(C)CC(=O)NC(C1=C(Cl)C=CC=C1)C2=C3C=CC=CC3=CC=C2O	0.223144
CKOYRYPZEZRCO	COC1=C(C=CC=C1)C2=C(C3=C(O2)C=CC=C3)C4=CC5=C(OCO5)C	0.226234
CLBBSJHIPCURMH	CC(C)NC1CCC(CC1)NC2=C3C=CC(Cl)=CC3=NC=C2	0.267144
CLCZLSWNLPIOR	COC1=C(C=C(Cl)C=C1)C(=O)NC2=C(C=CC=C2)N3CCN(C)CC3	0.25968
CLESYUIRTDJQBD	COC1=CC=C(CN2N=NN=C2CN(CC3=CC4=CC=C(C)C=C4NC3=O)(0.223564
CLNLJBXCSNSBRR	OC1=C(CN2CCN(CC3=CC=CC=C3)CC2)C=C(Cl)C=C1	0.231376
CMEZREFGTWJCD	CCOC(=O)N1CCC(CC1)NC(S)=NC2=CC3=C(C=C2)N=C(C=C3)N4	0.226818
CMRJNXIGRAVTPW	ClC1=C(Cl)C=C(C=C1)C2=CN3CC4=C(C=CC=C4)C3=N2	0.223871
CMZLSJOICXCPRS	ClC1=C(C=CC=C1)N2CCN(CC3=CNC4=C3C=CC=C4)CC2	0.236301
CNCQKPLZYJPG	OC(=O)C(F)(F)F.C(CCNCCCNC1=CC=CC=C1)CNCCCNC2=CC=C	0.229559
CNGTZCYFEYRLDM	COC1=CC=C(OC)C(=C1)C(N2CCN(CC2)C3=CC=C(F)C=C3)C4=NN:	0.248287
CNPYOSIWMMDNAMU	CCN(CC)CCCC(C)NC1=C2C(Cl)=CC=CC2=CC=N1	0.274589
CNSRUOBRAULBTH	C(N1N=CC2=C1N=CN=C2N3CCN(CC3)C(C4=CC=CC=C4)C5=CC=	0.248017
CNYRNWBKXAGLAB	COC1=CC2=C(S(C3=C(C=C(OC)C=C3)C(C2)N4CCN(C)CC4)C=C1	0.354229
COAXYFCHSALIKC	COC1=C(OC)C=C(CCN(C=O)C2CCN(CC3=C(C)OC(=N3)C4=C(C)C=	0.227143
COCFXAMJVUWCAE	CC1=CC(C)=C(CN(\N=N\C2=NON=C2N)C3=NON=C3N)C=C1	0.233472
COEGXHSYEOXWIM	COC1=CC=C(OC2=NC3=C(C=CC=C3)C(C)=C2)C=C1	0.249312
COGWQKWMKKWWTG	CC1=CC=C(CON2C(=NC3=C2C=CC=N3)C4=C(Cl)C=C(Cl)C=C4)C=	0.222896
CPGAZACKLLWLCI	CN(CC1=CC=CC=C1)C(NC(=O)C2=CC=CC=C2)C(Cl)(Cl)Cl	0.224604
CPYUHASOANZKJ	CC1=CC(OCCOCCN2CCCC2)=C(C=C1)C(C)(C)C	0.268285
CREWBZNTQFJRTK	ClC1=CC=C(C=C1)C2(CC2)C(=O)N3CCC(CC3)N4N=C(OC4=O)C5:	0.239514
CRKWINMSRQMAMG	OCC2(CCOC1=CC=CC=C1)CCN(CC3=C(OC(F)F)C=CC=C3)CC2	0.227057
CROXNVPOHIITIU	C(NC(NCC1=CC=CC=C1)=NCC2=CC=CC=C2)C3=CC=CC=C3	0.354574
CRVUUBYQNLMAN	CSC1=CC(=CC=C1)N=C(S)(CCN2CCCC(C)C2)CC3=CC=CS3	0.320991
CSBCZTFCHKVEHH	CC1=CC(Cl)=C(OCCCCN2CCOCC2)C=C1	0.230217
CSDXZWBEXVREQ	COC1=CC=C(C=C1)C2=NC(=NO2)C3=CC=CS3	0.237659
CSVSFHSGBPJKL	CCN(CCC(=O)NC1=CC(OC)=CC(OC)=C1)CC2=CC=CC=C2	0.223142
CTABHCUZJBWUKN	CCC1=C(C(N)=NC(N)=N1)C2=CC(N=[N+]=[N-])=C(Cl)C=C2	0.233401
CTFGZCLXDDSDZSP	COC1=CC=C(C=C1)C2=CSC(=N2)N(CCCN(C)C)C(=O)C3=C(Cl)C=C	0.281027

CTHFPUVDOBFICV	CCN1CCN(CCCN(CC2=CC=CO2)C(\S)=N\N\C3=CC(CI)=C(C)C=C3)C(0.293047
CTRALNDVXGSNGG	CCOC(=O)NC1=CC2=C(SC3=C(C=CC=C3)N2C(=O)CN4CCN(C)CC2	0.244615
CTSMNTKHEBETQQ	CC(CCN1CCN(CC1)C2=CC=CC=C2)C3=CC=CC=C3	0.259407
CUCBNBGILSWLMM	COC1=CC(OC)=C(C=C1)N2CC(CC2=O)C(=O)NC3=C(C=CC=C3)N4	0.225912
CUDAUFWNWXEKQT	CCCCNC1=NC(=C2CN(C)CCC2=C1C#N)N3CCCC3	0.227067
CVDCNSWAKGHLPW	CCOC1=C(C=CC=C1)N2CCN(CC2)C(=O)C(SC3=CC=CC=C3)C4=CC	0.244386
CVLRQJYHVVASQZ	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CN=C(SC)N=C3)CC2	0.242496
CVOWBCFITZKFG	COC1=CC=C(C=C1)N(CC=C)C(=O)C2=CC=CC=C2	0.240527
CVRHZDVULXGZKK	ClC1=CC(=CC=C1)N2N=NN=C2SCC#C	0.247722
CWAOFVPMZVLPDA	CC1CCN(CCC2=NC3=C(C=CC(NC(=O)COC4=CC=C(C)C=C4)=C3)N	0.251721
CWHPCVUWPBDYDN	COC1=CC(NC(=O)CN2CCCC2)=C(OC)C=C1NC(=O)C3=CC(C)=CC	0.227559
CWJUGFJMCXYHKKH	CC1=CC(C)=C(OCC(=O)NC2=CC=C(CN3CCCC3)C=C2)C=C1	0.252238
CWLJSHKCKQBYCI	COC1=C(OCC#N)C(Br)=CC(CNC2CCCCC2)=C1	0.260064
CXGKBIKEBNIOL	CC1=NN=C(O1)C2=CC(=C(OC3=CC(C)=C(C)C=C3)C=C2)[N+](O)C	0.234553
CXWDUNHYRYDJT	COC1=C(OC)C=C(CCN(C=O)CSC2=CN(CC3=CC(C)=CC=C3)C4=C2	0.231406
CYBCSVDRVUWPDN	CC(CC1=CC=CS1)NC(S)=NC2=CC=CC=C2	0.267553
CYCYXQWOYFRCKV	COC1=C(NC(=O)C2=CC=C(C=C2)[N+](O)C=C(C=C1)C(=O)NC	0.260794
CYYQCICIVGWIRA	CC1CC(C)CN(CC(O)COCCOC2=CC=C(Br)C=C2)C1	0.253026
CZMIHGKZSLTWDH	ClC1=CC(CC2SC(N\N=C\C3=CC=CS3)=NC2=O)=CC=C1	0.227206
DAAIJRXTWDBNW	COC1=CC=C(C=C1)C2=NC(=C(O2)N3CCCCC3)C#N	0.225958
DABAZMUSWLQFIC	C(OC(CN1CCCCC1)CN2CCCCC2)C3=CC=CC=C3	0.266121
DACRAQACYIOEFP	CC(C)NC(=NS(=O)(=O)C1=CC=CC=C1)C(Cl)(Cl)Cl	0.243597
DADKYQVHBKPSMQ	CC1=CC=C(C=C1)C(N2CCN(CC2)C3=CC=CC(=C3)C)C4=NN=N[N	0.251053
DAHVKHKOXKQRNL	CC1CCCCN1CCNC(=O)C2=CC3=C(C=C2)S(=O)C4=C(C=CC=C4)C(0.223606
DAKQYIUMJPHKKX	CN(C)CC(=O)NC1=CC=C(OC2=CC=C(Cl)C=C2)C=C1	0.273482
DAKSQZZDXNAHO	COC1=C(OCC2=CC=CC=C2)C(CNCCC3=CNC4=C3C=CC=C4)=CC=	0.230967
DAOJEQLQWZKXBS	CCN(CC)C1=NC(=CC(=N1)C(N)=O)C2=CC=CC=C2	0.234698
DBCUBSHSBILWMT	CC1=C(F)C=C(C=C1)S(=O)(=O)NC2=CC(=CC=C2)C(=O)NC3CCN(C	0.232173
DBWZSMKWALMPGA	SC(NCC1CCCCC1)=NC2=CC=C(OC3=CC=CC=C3)C=C2	0.247151
DBXXUXQUEUCCQQ	COC1=CC(NC(=O)CN(C)CC(=O)NC2=C(C=CC=C2)C3=CC=CC=C3)	0.249485
DBYBMKZBIDYVCC	COC(=O)CC1=CC=C(C=C1)N=C(S)N2CCN(CC2)C3=C(C)C=CC(Cl)=	0.224785
DBYCLOFOYRQWNH	CCOC1=C(NC(=O)CN2CCC3=C(C2)C=CC=C3)C=CC=C1	0.223729
DCHIGJKFAJLWRP	CN(C)CCCNC(=O)C1=C2C=CC=CC2=NC(SC3=CC=C(C)C=C3)=C1	0.245018
DCMLHASVCBLPNN	CCC(C)NCCOCCOC1=C2C=CC=CC2=C(Cl)C=C1	0.244916
DCPQZEDTFBGXDX	CCOC(=O)N1CCN(CC1)C2=C3C=CC=CC3=NC(=N2)C4=CC=CS4	0.223667
DDNMSWYZEIZUAD	ClC1=CC=CC=C1NC(=O)CSC2=NC(=NC(=N2)N3CCOCC3)NC4=CC	0.224072
DDUMHFXTQIMXFR	CN(C)CCNC(=O)C1=C2N=C3C(F)=CC=CC3=NC2=CC=C1	0.260806
DEAURHCATALVPR	COC1=CC=C(C=C1)C(N)=NOC(=O)CC2=CC(OC)=C(OC)C=C2	0.264921
DEMDFVSPNYKHJF	CCN(CC)CCN1C(NCC2=CC=C(OC)C=C2)=NC3=C1C=CC=C3	0.223287
DEOIIOVUIGWUNZ	COC(=O)C1=CC=C(OCCOC2=CC=CC=C2)C=C1	0.226519
DEURQQYOCUQBZH	COC1=CC=CC=C1NC(=O)CN2CCN(CC2)CC(=O)NC3=CC=C(Cl)C(=	0.226257
DFAZKXXYTBVFSM	CC1=CC(N2CCN(CCCC3=CC=CC=C3)CC2)=C(C)C=C1	0.254936
DFIBKKCZVMHTRL	N\C(=N/O)C1=NC(=NC(=N1)N2CCCC2)N(C3=CC=CC=C3)C4=CC=	0.243062
DFUSOVKMCNZCRI	COC1=C(OC2=C3C=CC=CC3=C(Cl)C=C2)N=C(N=C1)C4=NC=CC(=	0.222681
DGMBGNDGWVUWFU	COC1=CC=C(C=C1)C2=C(N(C)C3=C2C=C(C=C3)C4=NNC=C4)C5=	0.222869
DGOYFIDOIXRNR	CCOC(=O)C1(SC2=C(NC1=O)C=CC(C)=C2)N(CC)CC	0.250163
DHAMFUBSTHXWDX	CCCCN(CCCC)CC(O)COC1=CC=C(Br)C=C1	0.291383
DHIINGHRFJVSJJ	CCN1CCN(CC1)C2=NC3=C(C=C(NC(=O)CCC(=O)N4CCN(CC4)C5=	0.229648

DHKNVMARWYPUJF	CCC1=CC2=C(S1)N=CN=C2N3CCN(CC3)C4=NN=C(CC)S4	0.226946
DHMMQFBVMCMNCO	FC1=CC(CN2CCN3CCCC3C2C4CCCC4)=CC=C1	0.269176
DHNWBWEYLRLFHM	CCN(CC)C1=CC=C(C=C1)\C=N\O	0.234262
DHXSBDLDCWKDPQ	CCN(CCNC(=O)NC1=CC=C(Cl)C=C1)C2=CC=CC=C2	0.234881
DIEHCOWDEVPAM	CNC(S)=N\N=C(/C)C1=CC(C)=C(C)C=C1	0.272506
DIRHJRWJLBCERZ	FC1=CC=C(C=C1)N2CCN(CC3=CN=C3C4=CC=C(F)C=C4)CC2	0.276391
DIWDJLXPQLNOOB	COC1=C(CN2CCN(CC3=CC=CC=C3)CC2)C4=C(C=CC=C4)C=C1	0.29878
DJQKPIFCGBTKDP	COC1=CC(=CC(OC)=C1OC)C(=O)NCC(N2CCC3=C2C=CC=C3)C4=	0.242341
DJXXAAZCZQAFBJ	CC(C)C1=C(C)C=C(OCCOCCN2CCCC2)C=C1	0.246021
DKEZYKPYNGDETM	CC1=CC=C(SC2=C(C=C(CN3CCCC3)C=C2)[N+][[O-]]=O)C=C1	0.232049
DKJLSDBYIWDWRK	ClC1=CC=C(C=C1)C2=NC3=C(O2)C=CC(CN4CCCC4)=C3	0.278155
DKKIFPJZIAESRV	COC1=CC=C(C[N]2N=NN=C2C(N3CCN(CC3)C4=CC(=CC=C4)Cl)	0.224872
DKNMWSHHJHRNMX	ClC1=CC=C(NC(=O)NCC2CCN(CC3=CC(Cl)=CC=C3)CC2)C=C1	0.234966
DMGILJRCIFDWJJ	CC1=NC(NCC2=CC=CC=C2)=NC(N\N=C\3=CC=C(Cl)C=C3)=C1	0.235455
DMRMUHYCIYWJAU	C(N1CCN(CC1)C(C2=CC=CC=C2)C3=CC=CC=C3)C4=NN=NN4C5	0.286486
DMTDVNHYYWDIHE	CCN1CCN(CC1)C2=NC(C3=CC Enamine, T5595253	0.275922
DMWDZPMAUFSSIX	COC1=CC=CC(=C1OC)CN2CCN(CC2)C3=CC=CC=C3OC	0.234405
DNFBNGGPAMFYIV	CCCOP(=O)(OCCC)C1=C(NCC2=CC=CC=C2)OC(=N1)C3=CC=CC=C	0.222797
DNTYWICAROEIIR	CC1=CC(OCC2=NC3=C(N2)C=CC=C3)=C(C)C=C1	0.231769
DOKQGIRVWSSXKL	COCCC\N=C(/S)NCCCNC1=C(C=C2C(C)=CC(C)=CC2=N1)C#N	0.223333
DOOBXNPTUKTSNY	ClC1=NC(CN2CCCC2)=NC3=C1C4=C(CCC4)S3	0.243598
DOUCZHOFEMSYAG	CN1CCN(CCCN(CC2=CC=CS2)C(\S)=N\3=C(C)C=CC(Cl)=C3)CC1	0.255972
DOXLERIYHMSOMJ	CCN(CC)CCC(=O)NC1=CC2=C(CCC3=C(C=CC=C3)N2C(=O)CN(CC	0.225268
DPHOJHQHHHIQCL	CN1C=C(CNCC2=CN=C3C=CC=CN23)C(=N1)C4=CC=C(OC5=CC=C	0.264586
DPYHNEPEJIWDCT	CCC(C)C1=CC=C(OCCCCN2CCOCC2)C=C1	0.239158
DQKQMQQAJZCKTQ	COC1=C(OCC2=CC=CC=C2)C=CC(=C1)C(=O)NCC3(CCCCC3)N(C)	0.232661
DREJKENLGOKNAZ	CCN1CCN(CC1)C2=C3C=CC=CC3=NC(=N2)C4=CC=CC=C4	0.279088
DRFOYVAYXQSPB	CN(C)C1=CC(Cl)=C(\C=N\NC(=O)C2=C3C=CC=CC3=CC=C2)C=C1	0.25259
DRIGLOHKSIRHTN	CCN1CCN(CC1)C2=NC=C(C(=O)NC3=CC(=CC=C3OC)Cl)C4=CC=C	0.237371
DRLOMTNFDAXLP	BrC1=CC=C(S1)C(=O)CN2C(=N)N(CC=C)C3=C2C=CC=C3	0.268558
DRNLODMFWUMQSP	NC(S)=NN=C1CCCCCCCC1	0.226479
DRPQDKIQVZBZQF	C(NC1=N/C(=N\C2=C\C=C/C=C\1\2)/C3=C/C=C\N=C/3)C4CCCC	0.236878
DRUMPVMKOJHDRC	C1CN2C=C(C3=CC=CC=C3)[N+](=C2S1)C4=CC=CC=C4	0.222801
DSMKQBURCDVYOU	C\C(CC(C)(C)N1CC1)=N/NC(=O)NC2=C3C=CC=CC3=CC=C2	0.234896
DSWJVWIYKYRPS	CN(C)CCN1=C(N=C(COC2=CC=C(C=C2)C3=CC=CC=C3)O1)C#N	0.23342
DTWXHGYNVUCCSA	CN(C)C1=C(C=NC(=N1)C2=CC=CC=C2)S(=O)(=O)C3=CC=CC=C3	0.234577
DTYPZBRQTBSMGX	COC1=C(OCC2=CN=C(Cl)C=C2)C=CC(CNCCC3=C(F)C=CC=C3)=C	0.290349
DUJGQCJQVKGBBA	[O-][N+](=O)C1=CC=C(N\N=C\C2=CC(=CC=C2)[N+][[O-]]=O)C=C1	0.26265
DUKVGVACMPFMCR	COC1=CC(=CC(OC)=C1OC)C(=O)N2CCN(CC2)C3=CC=C(C)C=C3C	0.24683
DUXONKOEFSZBRM	CCN(CC)C1CC2=C(C=CC=C2)N(C(=O)N(CC)CC)C3=C1C=CC=C3	0.265463
DVLUMXSRCLLMQ	CN(C)CC1=C(SC2=CC3=C(CCCC3)C=C2)C=CC=C1	0.271961
DVNGUIAUHYPPNY	[O-][N+](=O)C1=CC=C(C=C1)C2=CSC(NN=C3CCCC3)=N2	0.257147
DVZLRSRQJCWUDR	CCOC1=CC=C(NS(=O)(=O)C2=CC=C(C=C2)C(=O)N3CCCC(C)C3)C	0.233035
DWEHQOULYWLDKU	COC1=C(OCC2=C(F)C=CC=C2)C(Br)=CC(\C=N\N=C(/N)S)=C1	0.225147
DWKHSHKYUERWFEQ	ClC1=CC=C(C=C1)C2=NN(CC(=O)NCCC3CCN(CC4=CC=CC=C4))	0.229114
DWMKFHNGYSTTPN	CN1C=NC(=C1OC2=C3C=CC=CC3=CC=C2)[N+][[O-]]=O	0.22369
DWOMXKJFILUXON	C(N1CCN(CC1)C2CCCSC3=C2C=CC=C3)C4=CC=CC=C4	0.283428
DWZFYKRGLXCPJR	COCC\N=C(/S)N(CCC1=C(C)NC2=C1C=C(Cl)C=C2)CC3=CC=CS3	0.224178

DXCJPVMSHPSMOJ	COC1=C(NC(=O)NC2=C(C)C(=CC=C2)[N+](O-)=O)C=C(Cl)C=C1	0.231603
DXRCBRDEXSOCGK	CNC(S)=N\N=C(/C)C1=CC(Cl)=C(Cl)C=C1	0.222451
DYHFAXLRWJHHNW	CC1=CC=C(C(=C1)[N+](=O)[O-])OCC2=CC(=CC=C2OC)C=NNS(=O)	0.236306
DYVNGQCNSFPQKG	CN(C)CCOCCOC1=C(Cl)C=C(Cl)C=C1C	0.228782
DZGRLYLKYCPFRS	CCOC1=C(CN2CCN(CC3=CC4=C(N3)C=CC=C4)CC2CCO)C=CC=C	0.232523
DZMNESXMQJGKKI	COC1=C(OC)C(CN2CCC(CC2)N(CCC3=CC=CC=C3)CC4=CC=CC=C	0.228644
DZXOAZAYQQTNL	CN1N=C(C)C(CCNS(=O)(=O)C2=CC=C(F)C=C2)=C1OC3=CC=CC=C	0.228669
FAHCSUHPPAUHAJ	CC1C2=CC(=C(C=C2CCN1CC3=CC(=CC=C3OC)C4C5=C(C6=CC=C	0.226467
FAIMXTPBTXEZOU	COC1=CC=C(C=C1)N=C(S)N(CCC2=C(C)NC3=C2C=C(C)C=C3)CC4	0.22317
FAONSHXBPKBFFM	ClC1=CC2=C(C=C1)N=NN=C2C3=CC=CC=C3	0.225222
FAVNEIQETLCCMJ	COC1=C(OC)C=C(C=C1)C2CCCN2\C(S)=N\C3=CC(Cl)=C(C)C=C3	0.222572
FBDXJTMJDJGBLQ	CC1=C(C=CC=C1)\N=C(/S)N2CCN(CC2)C3=C(Cl)C=CC=C3	0.247313
FBFXKSNSAZWILX	COC1=CC(NC(=O)CN2CCCC2)=C(OC)C=C1NC(=O)C3=C(F)C=CC	0.225634
FBNFOLOPSHLEV	CN1CCN(CC1)C2=C(NC(=O)C3=CC=C(OCC4=CC=CC=C4)C=C3)C=	0.237402
FBGUSGCVXYLMEC	NC(N)=N\N=C\C1=CC=C(F)C=C1)C2=CC=C(C=C2)C(F)(F)F	0.270413
FBXCANGVJBRBNR	COCCN1CCN(CC1)C2=CC(=NC=3N2N=C(C3)C4=CC=CC(=C4)F)C	0.23319
FBZAJSFJQICZTP	COC1=CC(=CC(=C1OC)OC)C2=NOC(=N2)C3=CC=CS3	0.24484
FCMGAQVDVZZVMS	CN1CCN(CC1)/C=N/C2=C(C3=C(S2)CCCC3)C#N	0.228326
FCVKDGDZUJYPSH	COC1=CC=C(C=C1OC)C2=NC(=C(O2)N3CCOCC3)C#N	0.225593
FDOSEIDYURVHEG	N1N=C(N=C1C2=CC=CC=C2)C3=NC=CC=C3	0.2382
FDQPXONIZUKKOP	CCCC(N1CCN(CC1)C2=C(OC)C=CC=C2)C3=NN=NN3CC4=CC=C(0.256658
FEIPKKUNQNPRSR	ClC1=CC2=C(C=C1)C(N\N=C\C3=C(Br)C=CC=C3)=CC=N2	0.228784
FEJOLHSHKJVETA	CC1CCCN(CCC(=O)NC2=CC=C(Br)C=C2)C1	0.244105
FEMGCABIWSZTCY	COC1=C(OC)C=C(C=C1)C2=NC(CN3CCC(CC3)C4=CC=CC=C4)=C(0.260213
FEMIEKUWTKIHRN	CCN(CC)C1OC2=C(C=C3OCOC3=C2)C(C1C)C4=CC(OC)=C(OC)C(0.279664
FENXQLVGXFEBTI	CC(=O)OC1=C(C(NC(=O)CC2=CC=CC=C2)C3=C(Cl)C=CC=C3)C4=(0.225635
FEPLCODWFOEWGR	C=CCNC1=NC(=C(C#N)C2=C1CN(CC2)CC3=CC=CC=C3)N4CCCC(0.227234
FEQNWINUVOBUMS	CCOC1=CC=C(NC2=C(N=C(O2)Vitas-M Laboratory,STK896245	0.239817
FEYIQDUSEQEAQQ	CCN1N=NC(=N1)C2=C(NC(=O)C3=CC(OC)=C(OC)C(OC)=C3)C=CC	0.222422
FGANKVPJYTWBHR	ClC1=CC=CC(=C1C[N]2C=NC3=C(N=CN=C23)N4CCCCC4)Cl	0.224797
FHRGNLSZHKOTAT	COC1=CC=C(C=C1)N=C(S)N(CCCN2CCCC2)CC3=CC=CS3	0.226754
FIMZBUXFQJCLW	FC1=C(C=CC=C1)N2CCN(CC3CC4CC3C=C4)CC2	0.229791
FIRQIZRGCGBDIR	COC1=CC(C(N2CCN(CC2)C3=C(F)C=CC=C3)C4=NN=NN4C5CCC(0.27021
FIRVQBUFVTUCCI	CC1=NC2=C(C=CC=C2OCCOC3=C(F)C=CC=C3)C=C1	0.225962
FJAKLMISLRNGKE	COC1=CC=C(C=C1)N2CCN(CC2)C(C3=NN=NN3C4CCCC4)C5=C(0.225388
FJBYQCDEDRMELR	COC1=CC=C(OC)C(=C1)C(N2CCC3=CC=CC=C3C2)C4=NN=N[N]4	0.248204
FJDNIGBGUJFUDB	SC(=NCCCC1=CC=CC=C1)N2CCN(CC2)C34CC5CC(CC(C5)C3)C4	0.2331
FJNLHZWCZQSEM	CN1N=C(C)C(CN(CC2=C(C)OC(=N2)C3=C(F)C=CC(F)=C3)C4CC4)=	0.280836
FJSBOKGZRDNR	CCN1CCN(CC1)C(=O)C2=C3C=CC=C4C(=O)N(C(=O)C(C=C2)=C34	0.225566
FKFYQEWXJSWQAT	COC1=CC(=CC(OC)=C1OC)C(=O)N\N=C\C2=C(C)C=CS2	0.250004
FKIJJURFHQMUIJL	CCC(N(CC1=CC=CS1)CC2=CC3=CC(C)=CC=C3NC2=O)C4=NN=NN	0.23883
FKMZPBSNNGNDGN	CN1CCN(CC1)C2=CC=C(NC(=O)COC3=CC4=C(C=CC=C4)C=C3)C=	0.270037
FLJGGKMZWAHJCQ	CC1=NC(=CC(N\N=C\C2=CC=C(Br)C=C2)=N1)N3CCOCC3	0.25911
FMADPVXRTFIHAS	FC1=C(C=CC=C1)N2CCN(CC2)C(=O)C(SC3=CC=CC=C3)C4=CC=C(0.228977
FMEALALYOZMLJI	CN1CCN(CC1)C2=NC(=NC=C2F)N3CCN(CC3)C4=CC=CC=C4	0.245931
FMJZREWCDZABCY	N=C1C2=C(CCC2)N(C3=CC=CC=C3)C4=C1CCC4	0.246082
FNICKYKABLLSJL	CCN(C1=CC=CC=C1)S(=O)(=O)C2=CC(OC)=C(N)C=C2	0.248817
FNKHNBXJOKKZGR	COC1=C(C)C(C)=C(CN2CCC(CC3=CC=CC=C3)CC2)C=C1	0.315832

FNPLGUOFZNEW CZ	CCCN(CCC)C(S)=NC(=O)C1=CC=C(C=C1)C2=CC=CC=C2	0.223817
FOAQRHEMCKCECH	CC1=C(C(=O)ON=C(N)C2=CC=CC=C2)C(=NO1)C3=C(Cl)C=CC=C3	0.242067
FOBWHVBAUPMWAP	CC1=CC(C)=C(C=C1)N2N=CC3=C2N=CN=C3SCC4=CN=CC=C4	0.222844
FOCRVTZMMYEUOF	COCCNCCOC1=CC=C(C=C1)C(C)(C)C2=CC=CC=C2	0.259777
FOGDQAOHTOYVSF	CNCCCOC1=CC(OC(C)C)=CC=C1	0.241793
FORFCNAFUW TYPN	CN1CCN(CC1)\N=C\C2=C3C=CC=CC3=C(Cl)C4=CC=CC=C24	0.22839
FOWCHVLUWQUTGX	CCOC(=O)C2(CCC1=CC=CC=C1)CCN(CC3=CC4=C(OCCO4)C=C3)	0.244436
FPINGFDOQFIVJE	CCN(CCNC(=O)C1CCN(CC2=C(C)OC(=N2)C3=CC=C(Cl)C=C3)CC1	0.22433
FPJCKMLPYYNAN	FC1=C(\C=N\N2CCN(CC3=C(Cl)C=CC=C3)CC2)C=CC=C1	0.249317
FPRXCNSGMDHDM	NC(=NOC(=O)C1=CC2=C(C=CC=C2)C=C1)C3=CN=CC=C3	0.224914
FQIBZBRPAORTIW	CN(C)CCNC1=C2C=CC=CC2=NC(=N1)C3=CC=C(Cl)C=C3	0.227925
FQXIH YRHMIGVLB	COC1=CC=C(C=C1)N2CCN(CC2)C3=C4C=C(OC)C=CC4=NC=C3S(0.225272
FRHSRBZOZ FJKHM	CC(=O)N1CCN(CC1)C2=NC(=N Enamine, T5282149	0.252855
FRVKAMAPGDOAOR	FC(F)(F)C1=CC(OCCN2CCN(CC3=CC=CC=C3)CC2)=CC=C1	0.236173
FSCHTKXZGZZBEI	CC1=C(C)C2=C(S1)N=CN=C2N3CCN(CCO4=CC=C(C)C=C4)CC3	0.22336
FSKOZAKNLVZSJY	CN1CCN(CC1)\N=C\C2=C(C)N(C(C)=C2)C3=CC=C(Cl)C=C3	0.29976
FSLNQLUXMDYMQS	CC(C)(C)NC1=NC(NC2=CC=CC=C2)=NC(Cl)=N1	0.223047
FSMSIQBJGBFHOD	CC(C)[C@H](NC(=O)C1=C(Cl)C=C(C=C1)[N+](=[O-])=O)C(=O)N2CC	0.227679
FSTUGIAOYRQVER	COC1=CC(C)=C(C(=O)CC(=O)C2=C(C)C=C(OC)C=C2)C(C)=C1	0.226373
FTCZSQZSQPLFK	CN(CC(=O)NC1=C(C(N)=O)C2=C(CCC2)S1)CC(=O)NC3=CC=C(C)C	0.226939
FTNZGDP EMBMSRL	CN(C1=CC=C(OCC2=NN=C(O2)C3=CC=CC=C3)C=C1)S(=O)(=O)C4	0.227752
FTVOQPHLIRK GNE	[O-][N+](=O)C1=C(\C=N\NC2=CC=CC=C2)C=CC=C1	0.25689
FUDFOMIUCNYRPS	O=C(\C(=N\NC1=CC=CC=C1)C2=CC=CC=C2)C3=CC=CC=C3	0.247611
FULWIWRWOXIENS	CCN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)N4CCN(CC4)C5=C(0.228854
FVBRWQIUJUHLKQ	CC1=CC(C)=NC(=N1)\N=C(/N)NCCC2=CC=CC=C2	0.269376
FVMDKJMUUVLQFT	C(N1CCN(CC1)C2=NC3=C(C=CC=C3)C(=N2)N4CCOCC4)C5=CC=	0.238503
FVMHRIIKBTULDQ	CC(CN1CCNCC1)(NS(=O)(=O)C2=CC=CC=C2)C3=CC=CC=C3	0.27069
FVXJBIBSUXZZOB	CSC1=CC=C(CN2CCC(CC2)N3N=CC=C3NC(=O)CCCC4=CC=CC=C	0.240291
FWMDRV RWLSQQKS	CCOC(=O)C1=C(N2CCN(CC2)C3=NC=CC=C3)C4=C(N=C1)C(OC)=	0.245263
FWMGJOMHHMSLRH	CCOC(=O)C1=C(C)C(C(=O)OCC)=C(NC(=O)CCN2CCCCC2)S1	0.234276
FWOQORGCRAJKQQ	CCN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)NCCN(C)C)C(C)=C2	0.257098
FWTUXKISATUREG	CCN(CC)CCCN(C(C)=O)C1=NC(=CS1)C2=CC(=CC=C2OC)OC	0.243156
FXBWUMYZDFNSIT	CCOC1=C(O)C(CN2CCCC(C2)N3CCC4=C(C3)C=CC=C4)=CC=C1	0.255796
FXEQPMSYJAWBQO	COC1=CC=C(Cl)C(=C1)N2CCN(CCCNC(=O)NC3=CC=C(C)C=C3)C(0.244616
FXGLYTICQZTCBR	NN1C(CC2=C3C=CC=CC3=CC=C2)=NN=C1SCCO4=CC=C(Br)C=	0.226572
FXHJIMQXQWJNSM	[O-][N+](=O)C1=NN(C2=CC3=C(OCCO3)C=C2)[N+](=[O-])=C1NC4=	0.22461
FXIXZADJVWSXHM	COC1=C(NC(=O)C2=C(Cl)C=CC=C2)C=CC(NC(=O)C3=CC=CO3)=C	0.229207
FXJAEQYVUIYOGT	COCCNCCCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.251226
FXJLTMMMLBWKDB	FC1=C(CN2CCCN(C2)C(\S)=N\C3=CC(Cl)=CC=C3)C=CC=C1	0.292759
FXODFKSCTMISKJ	CCOC(=O)C2(CCO1=CC=CC=C1)CCN(CC3=C(Cl)C=C(O)C(OC)=C	0.223814
FYIPNJMDLPBTAZ	[O-][N+](=O)C1=CC(=CC=C1)C(=O)ON=C2CCCCN2	0.266227
FYLQXNREZWACS	CCN1C(=S)N(CC(=O)NCCC2=CC=CC=C2)N=C1C3=CC=C(C)C=C3	0.224815
FZKZQIQMQNHFF	CC(C)CCN(C(C)C1=CC=NC=C1)C(\S)=N\C2=C(Cl)C=C(C)C=C2	0.253926
FZOIGUDNUCIBHK	COC1=CC(NC(=O)CN(C)CC(=O)NC2=C(Br)C=CC=C2)=C(OC)C=C1	0.237241
GBEICOCUEFDHJG	COC1=CC=C(C=C1)C(N2CCN(CC2)C3CCCC3)C4=NN=N[N]4CCC	0.251662
GBSMJQFLFZCWRI	COC1=CC=C(C=C1)N2CCN(CCCNC(=O)CCC(=O)N3CCOC4=C3C=	0.22662
GBTWBJLHCODVDI	COC1=C(OC)C(CNC2=NC3=C(C=CC=C3)N2CCN4CCCC4)=CC=C	0.229211
GBZVAFHGNJO CMQ	CCN(CC)C(=O)OC1=C2C=CC=CC2=C(Br)C=C1	0.234698

GCVLEBDECBRVJQ	CC(COC1=CC=CC=C1)N2CCC(CO)(CCC3=CC=CC=C3)CC2	0.225569
GCWVFAKIMDGKKD	CCOC(=O)C=C1C2=CC(=CC=C2OC1CN3CCCCC3)OC	0.230634
GCZMZXAUIJZPUNB	CN1C(CSCC2=CC=C(F)C=C2)=NN=C1SCC(=O)N3CCN(CC3)C4=C(C	0.222432
GDPMPIOBOVLEFC	COC1=C(OC)C=C(C=C1)C2=NC3=C(C=CC=C3)C(=C2)C(=O)NCC(N	0.237672
GEACFDKUFUTDHQ	CCOC1=CC2=C(C=C1)N=C(CN3CCN(CC4=C(OCC)C=CC=C4)C(CC	0.237733
GECZCJFICUIMSI	COC(=O)C1=C(CN2CCN(CC2)C3=C(C)C=CC=C3C)C(=CC=C1)[N+](0.223136
GEMVZPHXNBWWMU	CCN(CC)C1=CC=C(\C=N\N=C(/S)NCC2=CC=CC=C2)C=C1	0.224972
GEQNCGFQSPMLJV	CN(C)C1=CC=C(C=C1)C(=O)OCC2=CC=C(Br)C=C2	0.243033
GERMESKNXWUMHU	COC1=CC=C(CN2CSC(=S)N(CC3=CC=CC=C3)C2)C=C1	0.247558
GERPWQVNLHBOO	COC1=CC(OC)=C(C=C1)\N=C(/S)NCC2=C(Cl)C=CC=C2	0.222553
GFBPVKIACSQGE	CC1=NC(SCC2=NN=C(O2)C3=CC=CC=C3)=C(C#N)C(C)=C1	0.236527
GDFDIMKBMBRKCK	[O-][N+](=O)C1=CC=C(C=C1)C(C2=CC=C(C=C2)[N+](O)C3=C	0.346202
GFJNNGKTSOPVAY	ClC1=CC=C(C=C1)C2=C[N]3CCCC3=N2	0.230855
GFUVCRKEKDTQLI	C\C(=N/N1CCN(CC1)C2=CC=C(Cl)C=C2)C3=CC(=CC=C3)[N+](O-	0.248697
GFUXOVBMILUFAl	CCOC(=O)C1=C(CN2CCC(C)CC2)OC3=C1C=C(OC)C=C3	0.238342
GFWQVGZOCSTMLG	CN(C)C1=CC=C(\C=N\OC(=O)NC2=CC=CC=C2)C=C1	0.225873
GGBKVCLOHXJYCD	ClC1=CC=C(C=C1)C(=O)NC2=NC3=C(C=CC=C3)N2CCN4CCCC4	0.227795
GGIWODNVLZJOOT	CN(CC1=CC=C(OC(F)F)C=C1)C(=O)C2=CC(=CC=C2)S(=O)(=O)N3C	0.242122
GGNVUUYFBLWSNA	FC1=CC=C(C=C1)C2=CSC(=N2)N3CCC(C3)C4=CC=CC=C4	0.222429
GGOPXJDIHLBUFA	COC1=C(CN2CCCC(C2)C(=O)C3=C(OC)C=CC=C3)C=CC=C1	0.281938
GGUSVJNBCCGLN	COC1=CC=C(C=C1OC)C2\N=C(\C3=CC=CC=C3)C(C)(C)N2O	0.244282
GIIGIGNNZPCHTH	COC1=CC=C(C=C1)C(OCC(O)CNC(C)C2=CC=CC=C2)C3=CC=C(OC	0.246547
GIJMFAXZRUVIID	CS(=O)C1=C(C#N)C(=CC(=N1)C2=CC=C(Br)C=C2)C3=CC=CC=C3	0.223011
GIWODWVYEOAGQV	COC1=C(C=CC=C1)N2CCN(CCC3=CNC4=C3C=C5OCOC5=C4)CC	0.233657
GJBMKWRVTJKJMB	CC1=NC2=C(C(=N[N]2)C(=C1)NCCCN3CCOCC3)C4=CC=C(F)C=C	0.242367
GJDUWIZZYNPMPM	COC1=CC(CN(C)CC2=CC=CC=C2)=CC(OC)=C1O	0.224323
GJTJFBHITMENPA	CCC1=NC(C)=CN1S(=O)(=O)C2=C(Cl)C=CC(=C2)[N+](O)C3=C	0.223281
GLHFLADPKLAAEW	CN1CCN(CC1)C2CC3=C(SC4=C2C=CC(F)=C4)C=CC(Cl)=C3	0.324472
GMGOWYUFAKEZNV	CC1=CC(CN2CCCC(C2)C(=O)C3=CC4=C(OCO4)C=C3)=C(C=C1)N	0.245182
GMHDMQBFGWPQNB	CN1CCN(CC1)C2=CC=CC=C2NC(=O)C3=CC=CC(=C3)OCC4=CC=C	0.23196
GMKWAECOPLCWIU	CCN1C=C(CNC(=O)C2=NOC(COC3=C(Cl)C=C(F)C=C3)=C2)C=N1	0.228509
GMZKPSNHHJCDHS	NC1=C2CCCCC2=NC3=C1C4=C(CCCCC4)S3	0.22569
GNERZWOWHNEPQY	COC1=CC=C(C)C2=C1N=C(S2)N(CCCN(C)C)C(=O)C3=CC4=C(OCC	0.259342
GNEYUFAQVQXLDT	CN(CC1CCCN(CCC2=CC(=CC=C2)C(F)(F)F)C1)CC3=CC=C(NC(C)=	0.244021
GNQPUMLOPMZMFD	CCN(CC)S(=O)(=O)C1=CC(NC(=O)CCSC2=CC=C(Cl)C=C2)=CC=C1	0.224485
GNUBRPMYIYQREU	O=C(COC1=C2C=CC=CC2=CC=C1)N3C4=C(CCC5=C3C=CC=C5)C	0.234402
GNYVZJXAVMJYCL	ClC1=C(CN2CCC(CC3=CC=CC=C3)CC2)C=CC=C1	0.245649
GNZNPBWUFBQNO	COC1=CC(OC)=C(C=C1)C(=O)ON=C(N)C2=NC=CC=C2	0.244099
GOTFOTVSQWHRPI	C1CN(CC2=NN=C(O2)C3=CC=CC=C3)C4=CC=CC=C4C1	0.236154
GOUYUKOYEGKQEP	CC(C)(C)CN1CCN(CC2=NC(=CS2)C3=CC=C(F)C=C3)CC1CCO	0.2497
GOYZZBUIRKBKF	ClC1=CC(SC2=NC3=C(C=CC=C3)C(=C2)C(=O)NCC4=CN=CC=C4)=	0.223758
GPHKEFTVUJXMFE	CC1=C(C=C(Cl)C=C1)\N=C(/S)\N=C\2=C3C=CC=CC3=CC=C2	0.230966
GPZVOIQOWJGZNX	CC1=C(NS(=O)(=O)C2=CC=CC=C2)C=CC(=C1Cl)[N+](O)C3=C	0.239033
GQTJICULGXVQYFK	CN1CCN(COC2=CC=C(CC3=CC=CC=C3)C=C2)CC1	0.311654
GQYYPZGNULJLX	OCCN1CCN(CC#CCN2C3=C(C=CC=C3)C4=C2C=CC=C4)CC1	0.231664
GRECSEGRAXDXTR	CN1CCN(CC2=CC=C(OCC3=CC=CC=C3)C=C2)CC1	0.266045
GRPWIUUZNMITRR	CN1CCN(CC1)C2=C(C=CC(=C2)N3CCNCC3)[N+](O)C3=C	0.319182
GRWSQAQXMPBGJF	CCOC(=O)C1=C(C)OC2=C1C=C(OCC3=C(C)OC(=C3)C(=O)OC)C=C	0.223047

GRXZPUPSNRQSLN	CC1=CC(CN2C=C(C=O)C3=C2C=CC=C3)=CC=C1	0.233392
GSAAGSUVRWCSLI	CCOC(=O)C2(CCC1=CC=CC=C1)CCN(CC3=CN=C(S3)N(C)C)CC2	0.239368
GSDKCMWRUKEVLN	CC(C)C1=NC(=CS1)C(=O)N2CCCC(C2)N3CCN(CC3)C4=CC(CI)=CC	0.222675
GSMKCRRJOLCONI	COC1=CC(OC)=C(CN2CCN(CC3=CC=C(C)C=C3)CC2)C=C1	0.282398
GSSRESKKVSYJBV	CCOC(=O)C1=C(C)N(N=C1C)C2=CC=C(NC(=O)C3=CC=CS3)C=C2	0.252283
GSTUWJWXDCPWJC	COC1=CC(NC(=O)C2=CC=CC(C Asinex Ltd.,ASN 05211794	0.235008
GTDGCZAGEYQBAY	CC1CCCN(CCOCCSC2=CC=CC=C2)C1	0.275778
GTERTOOLLXWSZ	COC1=CC=C(NS(=O)(=O)C2=C(CI)C=CC(N\C(=N\S(=O)(=O)C3=CC:	0.223055
GTLWHVUWUKACHV	CC(C)(C)C1=CC=C(C=C1)\C=N\N=C(/S)NCC=C	0.236091
GUAXLFYUHSZDEJ	CC1=C(C=CC=C1)\N=C(/S)NCC2=CC=CC=C2	0.244539
GUDCJDDWCVHWCJ	CSC1=NC=C(CN2CCC(CC2)C(=O)NC3=CC(=CC=C3)C4=CSC=N4)C	0.229672
GUFALNAJWRRFDJ	ClC1=CC=C(CCN(C(=O)NC2=CC(CI)=CC=C2)C=C1	0.229109
GUHVLTSSVAHUPR	CN(C)C1=CC=C(\C=N\C2=CC(=NN2C3=CC=CC=C3)C4=CC=CC=C	0.244955
GUJLSPBIMKSORO	COC1=C(OC)C=C(CCNCC2=CC=C(C=C2)C3=CC=CC=C3)C=C1	0.308041
GUVDQOJQJFBGOG	[O-][N+](=O)C1=CC=C(C=C1)N2CCN(CC2)C(\S)=N\C3=C(F)C=C(F)	0.226033
GVCAJCMWYITQHP	COC1=CC=C(C=C1)C2=C(C#N)C(CI)=NC(=N2)C3=CC=CC=C3	0.228478
GVHZDMRBDLOKDN	CC(C)(CN1CCN(CC1)C2=CC=CC=C2)NS(=O)(=O)C3=CC=CC=C3	0.234912
GVMJKGBKSBKKG	COC1=CC(=CC(OC)=C1OC)C2=C3C=C(Br)C=CC3=NO2	0.239147
GVUGEKWJLJBSME	CC1=C(CS(=O)CC(=O)NCCN2CCCCC2)N=C(O1)C3=CC=C(CI)C=C	0.228558
GVZJSCMVVSKDGI	CCOC(=O)C1=C(C)C(C(=O)OCC)=C(CN2CCN(CC2)C3=CC=C(OC)C:	0.239275
GWCMQHSUMBHFOV	COC1=CC=C(C=C1)C(CNC(=O)C2=CC(NS(=O)(=O)C3=CC(F)=C(C)C	0.253214
GWPBCLLSUFIEQ	CC1=CC(\C=N\NC(=O)C2=CC=CS2)=C(C)N1C3=CC(C)=CC=C3	0.231212
GWPVLAMALAXBBS	CN(C)C1=CC=C(C=C(C2=NN=NN2C3=CC=CC=C3)C4=NN=NN4C5	0.230877
GXIYXTKEJHCQKQ	CCOC1=CC2=NC(=NC(=C2C=C1OC)N3CCOCC3)C4=CC=C(OC)C(:	0.226947
GXOIDTTXZUMBPM	C1CN(CCN1)C2=NC3=C(C=CC=C3)C(=N2)C4=CC=CC=C4	0.24425
GXTQAAKFDCCZOW	ClC1=C(C=CC=C1)C(N2CCN(CC3=CC=CO3)CC2)C4=NN=NN4CC!	0.229136
GYZIRVEMCRRLN	COC1=C(OC)C=C(CC2=NOC(CN(C)CC3=CC(=CC=C3)N4C=CC=N4	0.292673
GZFKDIVFUIWLBN	CN(C)C1=C2C=CC=CC2=C(NC(=O)CC3=CC=CC=C3)C=C1	0.247074
GZSUOVWERIQSOD	COC1=CC=C(N\C(C)=C\C2=[N+](C(=CS2)C3=CC=CC=C3)C4=CC=(0.22546
HADBTEMVDIMDLW	COC1=CC=C(C=C1)C(CNC(=O)C2=CC(NS(=O)(=O)C3=CC(F)=C(C)C	0.224353
HAIISKYDVPHGQW	COC1=CC=C(C=C1)C2=NC(CN3CCN(CC4=CC(F)=CC=C4)CC3)=C(0.229503
HAJLSVZWWIZPKO	CCC1=CC=C(C=C1)S(=O)(=O)N2C3CCN(C)CC3C4=C2C=CC(C)=C4	0.237509
HBCOFKWCWJCOHJQ	COC1=CC=C(\C=N\N)2C(=NN=C2C3=CC=CC=C3)SC)C=C1C	0.228174
HBDRUYIKYFKALI	COC1=CC(CC2(CO)CCCN(CC3=CC4=C(N3)C=CC=C4)C2)=CC=C1	0.227727
HBQNDKWJHWTOSZ	C1CN=C(N1)C2C3=C(CSC4=C2C=CC=C4)C=CC=C3	0.309989
HBVIRPOPLIFNHY	CCN(CC)C1=CC=C(C=C1)C(=O)OCC(=O)NC2=C(C=CC=C2)C3=CC=	0.230662
HCAYDEBXAFFBPA	CCOC1=CC=C(OCC2=CC=C(O2)C(=O)NC(C)(C)C)C=C1	0.230292
HESAYFLMAHLMGI	COC1=CC(OC)=C(C=C1)C(N2CCC(C)CC2)C3=NN=NN3C4CCCC4	0.24583
HFKZYMPEMMAFOG	ClC1=CC(=CC=C1)C2=NN=C(O2)C3=CC=CC=C3	0.251292
HFRAYEALNRDZAA	CN(C)C1=C(N=C(O1)C2=CC=CC=C2Cl)C#N	0.252926
HFTBUYNKBJOJMS	OC(COC1=CC=C(C=C1)[S+](O-)(=O)N2CCOCC2)CN3CCN(CC3)C	0.223463
HFTYZLAWHVLZCM	CCOC(=O)C2(CCCC1=CC=CC=C1)CCN(CC2)C3CCCC3	0.273099
HGIDBTSZCANBC	OC(COC1=CC=C2C=C(Br)C=CC2=C1)CN3CCCC3	0.232547
HGQYANJAVUDYOU	O=S1(=O)CCS(=O)(=O)C1C2=CC=CC=C2	0.257122
HHLJKQAHDJERX	CN1CCC2=C(C1)SC(NC(=O)COC3=CC4=C(C=CC=C4)C=C3)=N2	0.233893
HHUNIUFQOPFKBB	CCN1CCN(CCOC2=C(OCC3=CC=CC=C3)C=CC=C2)CC1	0.288044
HHVHRBNNVYQGO	COC1=CC=C(C=C1)C2CC(=NN2C(=O)CN3CCCC3)C4=CC=C(Br)C=	0.319311
HXXBUEDUJDFQEA	CCOC(=O)C1=NC2=C(C=CC=C2)C1=[N+]=[N-]	0.225799

HIELOUZGQULWCY	CC1=C2CC(OC2=C3C=CC=CC3=N1)C(C)(Cl)Br	0.224097
HIGQBYWQSGFTR	CCOC1=CC=C(C=C1)N2N=NN=C2C3=NC4=C(S3)C=CC=C4	0.22474
HIHIGEUVECSANJ	C1CCN(CC1)C2=NC(=NC(N\C=C\3=CNC4=C3C=CC=C4)=N2)N5	0.222611
HIHZFTNEEQAKJI	CCCN(CCC)C1=NC=NC2=C1C=NN2C3=CC=C(OC)C=C3	0.235778
HIJNKVCALQPZDU	CN1N=C(C2=CC=C(C=C2)C(=O)N3CCN(CC4=CC=CC=C4)CC3)C5=	0.224705
HIWLGEQTJTUJIU	CCN1C2=C(C=C(C)C=C2)C3=C1N=C(SCCN4CCCC4)N=N3	0.234117
HIZVPOSTRMNMOK	OC1=C(C=CC=C1)C2=NC(=NN2)C3=C(O)C=CC=C3	0.222622
HIZXBECURMQHTA	COC1=CC(CN2CCN(CC2)C(=O)C3=CC=C(C=C3)C4=CC=CC=C4)=C	0.223186
HJAPVMMMLKRVJSJW	CN(C)S(=O)(=O)C1=CC(Cl)=C(C=C1)N2CCN(CC2)S(=O)(=O)C3=CC	0.247187
HJUXGLLHBMPOHN	O=C(NC1=CC=C(C=C1)N2CCOCC2)C3=C4C=CC=CC4=CC=C3	0.233315
HKLVXLJTGPBFMX	SC(NCC1=CC=C(Cl)C=C1)=NC2=CC=NC=C2	0.228346
HLARMCFCXXGSBI	OC(C(N1CCOCC1)C2=CC=CC=C2)(C3=CC=CC=C3)C4=CC=C(F)C=	0.264265
HLIKMPYBPSBSSF	COC1=C(OC)C=C(CN2CCC(CC3=CC=CC=C3)CC2)C=C1	0.26018
HLMDXVXISRHHOA	CCN(CC)CCNC(=O)C1=CC=C(NC(=O)C2=CC=C(C=C2)S(=O)(=O)N3	0.240205
HLTBWYWHWCSST	COC1=CC=C(C=C1)N=C(S)N2CCN(C\C=C\C3=CC=CC=C3)CC2	0.237644
HMLVFUWQWMPWKQ	CC1C(N(C)C(C)C1(O)C#CC2=CC=CC=C2)C3=CC=CC=C3)C4=CC	0.223413
HMWQYKGAJZEVGV	CC1=CC(N)=CC(C)=C1C2=C(Br)C=C(N)C=C2Br	0.23413
HNDBTGRZKRHNHB	CCOC1=CC2=C(NC(=N2)C3=CC=CC=C3)C=C1	0.22592
HNJQORNOYZWCSS	BrC1=CC(CNCC2=CC=NC=C2)=C(OCC3=CC=CC=C3)C=C1	0.234992
HNXVXXIPESJDSF	CCN(CC)C1=CC=C(C=C1)C2NC(=O)C3=C(N2)C=CC=C3	0.225641
HOABSRFVIVDIIQ	ClC1=C(C=CC(NC(=O)C2=CC3=C(OCCO3)C=C2)=C1)N4CCCC4	0.226264
HOSZHAPBMXUGHN	BrC1=CC=C2OCCOCCOCCOC3=CC=C(Br)C=C3OCCOCCOC2=C1	0.238855
HPBYXKYAIRHMX	FC1=CC(=CC=C1)C2=CC(NC(=O)C3CCN(CC4CCOC4)CC3)=CC=C2	0.224
HPEPXRUMTGVIPA	CN(CC(=O)NC1=C(Cl)C=CC=C1)C(=O)C2=CC(=CC=C2)S(=O)(=O)N	0.224264
HPGIERMBOVEBRN	CC1=CC=C(C=C1)S(=O)(=O)NC2=C(C=CC=C2)N3CCOCC3	0.238855
HQJNJFVKALQGS	OCC1=C/C=C(\C=N\1)C(=O)NN=CC2=C(O)/C=C\C3=C\C=C/C=C\	0.223179
HQSGVANNJFLMFK	CC1=CC=C(OCCCN2CCC3=C(C2)C=CC=C3)C=C1	0.251182
HQVSYDCPHPKQMR	CC1=CC=C(C=C1)C2=NN(C(C2)C3=C(F)C=CC=C3)C(=O)C4=C(F)C	0.228521
HRAFYRYVAHBEW	COC1=CC=C(C=C1)C2=NN(C=C2CO)C3=CC=CC=C3	0.229553
HRCITNWLOQMDGX	C(N1CCN(CC1)C2=CC=CC=C2)C3=C4C=CC=CC4=NC=C3	0.237112
HRTMRFLKYRRWRK	CC1=CC(Br)=C(OCCCCCN2CCNCC2)C=C1	0.248256
HRWZLSGNASCXOO	CN(C)CCCN(C=O)C1=CC=CO1)C2=NC3=C(S2)C=C(Cl)C=C3	0.277911
HRZJKYJOXWGSPG	COC1=CC=C(C=C1)C(N2CCN(CC2)C3=C(F)C=CC=C3)C4=NN=NN	0.269108
HSOFMPNGAGDYGZ	CCOC(=O)C1=CC(=NN1C2=CC=CC=C2)C3=CC=C(C=C3)N4CCOC	0.263362
HTHMHMCMMLGKYFL	CN1CCN(CC1)C(=O)NC23CC4CC(C2)CC(C4)(C3)C5=CC=C(C)C=C	0.246238
HUSBTGWYEQTSSS	CCOC(=O)C1=CC=C(C=C1)N=C(S)N(CCN(C)C)CC2=CC=CS2	0.232715
HVHPQMBRWAKQKF	CCOC(=O)C1=C(CN(C)C)N(C2=C1C=C(O)C(Br)=C2)C3=CC=C(C)C=	0.238977
HVMDLOCSGFODDK	CN(C)CCCN(C=O)C1=CC(C)=C(C)C=C1)C2=NC3=C(S2)C=C(Cl)C=	0.240672
HWAVRYVDKATCPW	C(CC12CC3CC(CC(C3)C1)C2)N4CCNC[C@@H]4CC5=CC=CC=C5	0.235792
HWJWHNLIKCTRLU	FC1=CC=C(C=C1)N2CCN(CC2)C(=O)C3=C(C=CC=C3)C(=O)N4CC	0.230007
HWLGXOFSMYQGBA	CC1=C(C=CC=C1)C(=O)N2CCN(CC2)C3=CC=C(NC(=O)CSC4=CC=	0.223535
HWMASQCYVGFIE	C1=CC=C(C=C1)N2C=C(C(=N2)C3=CC=C(C=C3)Br)CSC(=[NH2+])I	0.231062
HWMGCIBPEVSOIV	COC1=CC=C(C=C1)C2SCCN2\C(S)=N\C3=CC(Cl)=CC=C3	0.226449
HWTBJWYIGDBEA	CCCC[C@@H]1CNCCN1CCC2=CC(=CC=C2)C(F)(F)C(F)(F)F	0.229086
HXPLNKYQPETFS	COC1=CC(=CC=C1)C2=NN(C=C2CN(C)CC3=C(C)N=C4C=CC=CN3	0.225639
HYBVVHAETRLEFE	CN(CC(C(=O)C1=CC=CC=C1)C2=CC=CC=C2)CC3=CC(Cl)=CC(Cl)=	0.271842
HYCVPCISSUCAZ	C1CCN(CC1)C2=C3C=CC=CC3=NC(=C2)C4=CC=CC=C4	0.265106
HYOYFRGAFYROPQ	CC1=C(OCCNCC2=CC=CC=C2)C=CC(Br)=C1	0.250215

HYQLDXYGOJREDF	O=C(CCN1CCC2=C(C1)C=CC=C2)NC3=CC=CC=C3	0.236996
HZIQSBATGNZGL	CC1=CC(C)=C(C)C=C1CN2CCC(CC2)N3N=CC=C3NC(=O)C4=C(Cl)	0.224568
IAGSPPNEMBPKMI	CN(C)CCCNC1=C(N=C(O1)C2=CC=C(Cl)C=C2)C#N	0.228206
IANCZQXGGKBOTP	CCOC1=CN=C(O1)C2=CC=C(Cl)C=C2	0.244124
IBBJVLJKTNANGK	CNC(S)=N\N=C(/C)CCC\C(C)=N\N=C(S)NC	0.27159
IBGPJBXGKDMHHH	CC1=C(C)C(OCC(O)CN2CCC3=C(C2)C=CC=C3)=C(C)C=C1	0.243004
IBLVRWXMJGVKAV	COC1=CC=C(NC2=NC=NC3=C2C(=CS3)C4=CC=C(OC)C=C4)C=C1	0.23318
IBVDUESHTFZMLI	C1CN(CCO1)C2=NC(=NC3=CC=CC=C23)C4=CC=CC=N4	0.223002
ICBICEUBDGNXDW	COC1=CC=C(C=C1)N2CCN(CCNC(=O)NC3=C(OC)C=C(C=C3)[N+](0.239276
ICSBTSRZHYVGZ	CCC1C(OC2=C(C=C3OCOC3=C2)C1C4=CC(OC)=C(OC)C(OC)=C4)	0.244918
ICJCBXYUQYODIT	CC1=C(C=C(Cl)C=C1)N2CCN(CC(=O)NC3=CC=C(CN4CCCC4)C=	0.264265
IDDQIYZGJMLTCJ	CCOC(=O)C1=C(SC\C=N\NC2=CC=CC=C2)=C1C3=C(Cl)C=CC=C3	0.22699
IDFLLYMCUVPBPR	CC1CCN(CC(O)COC2=CC=C(C=C2)C3=CC=CC=C3)CC1	0.242979
IDGKROPBCDYPCE	COC1=C(OC)C=C(C=C1)C2=NC(=NO2)C3=C(OC)C=CC=C3	0.239311
IDPCEAGLYFHFT	COC1=CC=CC(=C1OC)C(N2CCN(CC2)C3CCCC3)C4=NN=N[N]4C(0.233552
IDQGIKHEHYTHX	O=C(NC1=CC=C(C=C1)S(=O)(=O)N2CCCC2)C3=CC=C(CN4CCCC5=	0.226288
IDTSOTQCVWNYBM	CC1CC(C)CN(CCCNC(=O)C2=CC=C3SC(N4CCCC4)C(=O)NC3=C(0.252097
IEAQEGSZTNJBFC	COC(=O)C1=CC=C(NC(=O)NC2=CC(Cl)=C(F)C=C2)C=C1	0.225954
IEFLQJYSYFXCQH	CN1CCN(CC1)S(=O)(=O)C2=CC=C(NC(=O)NC3=CC(Cl)=CC=C3)C=	0.246298
IEHAFFWCRXYSF	[O-][N+](=O)C1=C(F)C=CC(=C1)S(=O)(=O)CCCN2CCOCC2	0.229185
IEIJYXPXGFJHX	CN1CCN(CC1)C2=C3C=CC=CC3=NC(=N2)C4=CC(=CC=C4)[N+](C	0.285615
IENYSTZWERREFN	CCOC1=CC=C(OCCN(C)CC2=CC=CC=C2)C=C1	0.297063
IETSDSVFULQJY	CN1CCN(CC1)C2=NC(=NC3=CC=CC=C23)C4=CC=NC=C4	0.272094
IEZDTNCUMWPRTD	[O-][N+](=O)C1=C(C=C(C=C1)N2CCNCC2)N3CCCC3	0.246455
IFCJHZPIQXTBIM	COC1=CC(C2=CSC(NC(=O)CC3=CC=C(F)C=C3)=N2)=C(OC)C=C1	0.230575
IFGOXKISHLDSOC	CCC1=CC=CC=C1OCCCN2CCCC2	0.239071
IFHDQENIOFOWNT	COC1=CC=C(C=C1)N2CCN(CC2)C(C(C)NS(=O)(=O)C3=CC=CC=C3	0.22349
IGFDWKFTWISJQF	COC1=CC=C(C=C1)C2=NN(C(C2)C3=C(Cl)C=CC=C3)C(S)=NC	0.242451
IGHSNESWYQWJKG	OCCN1CCN(CC1)C2=NC=NC3=C2C(=CN3C4=CC=C(Br)C=C4)C5=	0.228464
IGPUFUHRMWSPGW	COC1=CC(=CC(OC)=C1OC)C2=NC3=C(C=CC=C3)C(=C2)C4=NN=C(0.25795
IGVDXOCVFAZDBF	CCC1=C(CC)N=C2C=C(C=CC2=N1)C(=O)NCCCN3CCN(CC3)C4=C	0.268431
IHPAPQFVGNWMBN	CCOC(=O)C1=CC=C(C=C1)N=C(S)N(CCCN2CCCCC2)CC3=CC=C(0.27345
IIEOHBPTLRILF	CCCCN1C(=NC(=O)C2=CC=CO2)C(=CC3=C1N=C4C=CC=CN4C3=	0.283521
IINVJSTLHFZNN	CCC1CCCCN1CCCNC(=O)C2=CC3=C(C=C2)N(C)C(C)=C3C	0.244205
IISUIBFUGHJUBG	CSC1=C(C=CC=C1)C2=NN=C(O2)C3=CC=C(Cl)C=C3	0.229771
IYJBJQVZSYERE	O1N=C(N=C1C2=CC=CC=C2C3=CC=CC=C3)C4=CC=CN=C4	0.241204
IJBZONJMXCXSXW	CCN(CC)CC(O)C1=CC2=C(C=C1)C=CC3=C2C=C(O)C=C3	0.247328
IJGSXXQMYBXCHB	CCN(CC)CCN1C(=N)N(CC(O)COC2=CC(C)=CC=C2)C3=C1C=CC=C	0.230852
IJYHPISIGXOPFY	CC1=C(C)C2=C(N1)C=CC(=C2)C(=O)N3CCN(CC3)C4=C(C)C(C)=C(0.225112
ILHXEMLHKPZGJK	CCN(CC)C1=C2C=C(Br)C=CC2=NC=N1	0.231026
ILNJPDOMRDGGOM	CCOC1=CC=C(C=C1)S(=O)(=O)NC2=C(OC)C=CC(OC)=C2	0.262369
IMNKEUHUAVZSTA	C1C1=CC=C(CN/2\C=C/C(=N)/C=C2)C=C1	0.277878
IMYIETUJQGZVGC	COC1=NC(OC2=CC(=C(C=C2)[N+](O-)=O)[N+](O-)=O)=NC(OC)=	0.229258
INATXWGGHFJGIQ	SC(=NC1CCCC1)N2CCN(CC2)C3=CC=C(Cl)C=C3	0.222872
INDGKFWVKZOQMH	CN1C(=O)N(C)C2=C1C=C(N3CCN(CC3)C(=O)C4=C(Br)C=CC=C4)(0.236768
INPNMBZFXUQZPZ	CCOC1=CC=C(C=C1)C2=NN=C(NC3=NCCCC3)O2	0.224476
INVMJJKFELVUKU	CC1CCN(CCOC2=CC(Br)=CC=C2)CC1	0.289189
IOCCMLDPNDBVDE	C\C(=N/N=C(\S)NCC1=CC=CC=C1)C2=CC3=C(C=CC=C3)C=C2	0.241372

IOENYQZRXBUTBA	C(OC1=CC2=C(C=CC=C2)C=C1)C3=NC4=C(N3)C=CC=C4	0.245987
IOWSODAHYNSLUK	CCCOC1=CC=C(CNC(S)=NCC2=CC=C(OC(C)C)C=C2)C=C1	0.289754
IPBGOGJVRVDOMV	FC(F)OC1=CC=C(CN2CCC(CC2)N3N=CC=C3NC(=O)C4CCCC4)C=	0.232826
IPCDJMHCUSAOOJ	CCCN(CCC)CC(C)(C)NS(=O)(=O)C1=CC=C(Cl)C=C1	0.222592
IPNYWESNDBXTQP	SC(=NCC=C)N(CC1=CC=CC=C1)CC2=CC=CC=C2	0.230858
IPWIMNYYYYMAPFC	COC1=CC=C(C=C1)C2=NC(=C(C#N)C(=C2)C3=CC=CC=C3)S(C)=O	0.228943
IQJMUBVOUOHXRP	OP(O)(=O)CN1CCNCCN(CP(O)(O)=O)CCNCC1	0.276209
IQRNBJJJJYIMT	CN(C)C1=NC(N\N=C\C2=CC(Br)=CC=C2)=NC(NCC3=CC=CC=C3):	0.223559
IRMLBVBGBZYXZNV	C([C@H]1CNCCN1CC2(CC2)C3=CC=CC=C3)C4=C5C=CC=CC5	0.272189
IRMNUGAFPPNLKP	CCN(CC)C(=S)SCC(=O)NC1=NC(=C(O1)C2=CC=CC=C2)C3=CC=CC	0.239021
IRRUJGMCBGBHEH	CCOC(=O)C1=C(C)NC(C(=O)OCC2=C(C)ON=C2C)=C1C	0.244914
IRVJESCRIBTULW	CC1=CC2=C(NC(=O)C(CN(CC3=CC=CC=C3)CC4=NN=NN4CC5=CC=C	0.250181
IRXYWNURKDCDAW	NC(=O)C(C1=CC=C(Br)C=C1)C2=CC=C(C=C2)C(=O)C3=CC=CC=C3	0.244057
ISDZPMGIXQBLRG	CC1=C(OC2=C1C=C(C)C=C2Cl)C(=O)N3CCN(CC3)C4=CC=NC=C4	0.230948
ISTFTATZQQNYEU	COC1=C(C=CC=C1)\N=N\C2=NC(=C(N2)C3=CC=CC=C3)C4=CC=C	0.225884
ISWBJEGHXZRLFP	CC1=CC(=NN1CC2=CC=C(C)C=C2)C(=O)NC3=CC=C(Br)C=C3	0.223222
ITAHKLCZQWHDIN	COC1=C(NC(=O)C2=CC=C(CN3CCN(CC3)C4=CC=CC=C4)C=C2)C=	0.223709
ITEMLMXMYOMKQF	CC1=NN(C(C)=C1\C=N\N2CCN(CC2)C3=CC=CC=C3)C4=CC=CC=C	0.243253
ITEQRTWMTYJAE	FC(F)(F)C1=C(C=NC(=N1)N2CCCC2)C3=NN=NN3C4=CC=C(Cl)C=	0.225736
ITMSURDFRPXGBI	COC1=CC=C(C=C1)N2CCN(CC(=O)NC3=C(SC)C=CC=C3)CC2	0.231605
ITOIFNLKDKMKOA	CCOC(=O)C1=C(OC2=C1C(CN(C)C)=C(O)C(CN(C)C)=C2)C3=CC=C	0.228546
ITWKHNKRPIXIABE	CC1=CC=C(C=C1)N2C=C(CNCCC3=CSC=N3)C(=N2)C4=CC=C(F)C	0.287142
IUFSXUHCYBGFAM	CCOC1=CC=C(C=C1)S(=O)(=O)N2CCN(CC(O)COC3=CC(=CC=C3))	0.248236
IUQGXMQYGXRRDW	COC(=O)C1=CN(C=C(C1C2=CC(=CC=C2)[N+][O-])=O)C(=O)OC)C3	0.229494
IVAWCVDHOTUAQF	CSCCC(NC(=O)C1=CC=CC=C1)C(=O)N2CCN(CC3=CC=C(Cl)C=C3)	0.231273
IVPPXEYDMTEQN	COC1=C(OC)C=C(C=C1)C2=CN=C2C3=C(O)C=C(OCC(C)=C)C=C3	0.233355
IVYFMXZYAAQEV	CCOC1=CC=C(NC(=O)CN2CCN(CC(=O)NC3=CC(=C(Cl)C=C3)C(F)(0.22742
IWDGWQZJFLVDSG	COC(=O)C1=CN(CC2=CC=C(C)C=C2)C=C(C1C3=CC(F)=C(F)C=C3)	0.2247
IWNVURXZAIYEGZ	Cl.CCCC(N1CCN(CC1)C2=CC(Cl)=CC=C2)C3=NN=NN3CC4=CC=C	0.234048
IXHRPSIJGXCI OH	COC1=C(C=CC=C1)C2=C3N=C(C)C=C(N3N=C2)N4CCCCC4	0.249195
IXRFXROGXPJAGZ	[O-][N+](=O)C1=C(Br)C=C(N2CCCC2)C(F)=C1	0.278176
IYINIJNBCAQUCX	CCCN(CC1=CC=CC=C1)C2CCN(CCC3=CC=CC=C3)CC2	0.328276
IYLYIQZUZPGQNN	CC1=CC=C(CN2CCN(CC2)\N=C\C3=CC=CC=C3)C=C1	0.230406
IYRBMNSXGNPBSQ	ClC1=CC(=CC=C1)C2CC(=O)NC3=C2C=C4CCCC4=C3	0.229454
IYWGNQQLTCZOTC	CC1=NN(C(C)=C1\C=N\NC(=O)CSC2=NN=C(N2C3=CC=C(Cl)C=C3	0.242196
IZFAYTPVDGJXAT	C(CC(CC1=CC=CC=C1)C2=CC=CO2)NCC3=CC=CC=C3	0.23848
JAOSEIAJTQKXPZ	CC1=CC=C(C=C1)S(=O)(=O)NCCC(C2=CC=CO2)C3=CC=CC=C3	0.232106
JATLPCOUVWPKNJ	FC1=C(CNC(C2=CC=CC=C2)C3=CC=CC=C3)C(Cl)=CC=C1	0.262315
JAXHRWLWPCLFRN	CN1CCN(CC1)C2=C(NS(=O)(=O)C3=C(Cl)C=CC=C3)C=C(Cl)C=C2	0.261911
JBBSWMJFTCEOLT	CN(C)CCCN1C(=O)C2=C(C=CC=C2)N=C1SCC(=O)NC3=NC(=CS3)	0.225498
JBCQAORKQPODRW	CC(=O)C1=C(C)NC(C(=O)OCC2=C(F)C=CC=C2)=C1C	0.232526
JBLNZNDTQWAJDN	COCCCNCCOCCOC1=C(Br)C=C(Cl)C=C1	0.243436
JBPDVHTSPXTOM	O=C(C1CCCN(CC2CC2)C1)C3=C4C=CC=C5CCC(C=C3)=C45	0.229581
JBSAJONOVKCGOQ	C1CCCN(CC1)C2=NC(=CS2)C3=CC=CC=C3	0.254869
JBXVXHBWBMJGIP	N#CC1=C(N=C(C=N1)C2=CC3=C(OCCOCCOCCOCCOCCO3)C=C2	0.226725
JCDSUXLNHJBRFG	CCOC1=CC=C(C=C1)C2=NN=C(SCC3=NN=C(O3)C4=CC=CC=C4)N	0.228542
JCLWLOGOGKBEGR	CC1=CC=C(C=C1)C2=NOC(CCC(=O)NCCCN3CCN(CC3)C4=CC(Cl)	0.255822
JCMQQNRPYKUQNS	CCOC(=O)C1=CC=C(NC(=O)CCC2=NC(=NO2)C3=CC=CC=C3Cl)C=	0.222626

JCSBDYJALPKIB	CCN(CC)S(=O)(=O)C1=CC=C(C=C1)C2=NOC3(C2)N(C)C4=C(C=CC	0.23393
JCTUXAQXOAUKHI	CC1=C(C)C2=C(C=C1)C(=CC(=N2)C3=CN=CC=C3)C(=O)N4CCN(C	0.223557
JDQNUEOWXXAZHW	COC1=CC(OC)=C(C=C1)C(=O)NC2=CC3=C(C=C2)N=C(C=C3C)N4C	0.224456
JDWJAJQDBOFSCS	CC1=C(C=CC=C1)\N=C(/S)NCCSC2=CC=C(Cl)C=C2	0.229814
JEDYDGPKXXCAMR	COC1=CC=C(CN2N=NN=C2C(N3CCN(CC3)C4CCCC4)C5=CC=CC	0.267008
JEEPBTWHGGAFCL	COC1=C(OC)C(OC)=C(CNCCC2=CC=C(Cl)C=C2)C=C1	0.28257
JEFKGGPWVUONSR	COC1=CC=C(C=C1)C2=CSC(CCN3N=C(C)C=C3C)=N2	0.23095
JEJWQCTZDAJWOX	CC1=CC=C(C=C1)S(=O)(=O)NCCC2=CC=C(C=C2)C(=O)NCCN(CC3=	0.225909
JEOAQTNLXBCMAF	OC1=C(C=CC=C1)N2CCN(CC2)C3=C(Cl)C=C(C=C3)[N+][[O-]]=O	0.223471
JEWNHEWDQGXKSB	C(CCN1CCCC1)COC2=CC(OC3=CC=CC=C3)=CC=C2	0.264553
JEWOVFPNPJKWHN	OC(CNC1CCCC1)CNC2=C3C=CC(Cl)=CC3=NC=C2	0.23801
JEXHFRROVBBQCA	CN(C)CCCN(C(=O)C1=CC2=C(C=CC=C2)C=C1)C3=NC4=C(S3)C=C	0.230169
JEXNGXDZDIALR	CCOC1=C(OCC2=C(Cl)C=C(Cl)C=C2)C(CNCCO)=CC=C1	0.226174
JFECUBGECCGCS	CN1C=C(CN2CCCC(C2)C(=O)C3=C(F)C=CC(F)=C3)C4=C1C=CC=C	0.263816
JFIGKXRBNOWCTJ	NC(N)=NN=C(N=NC1=CC=CC=C1)C2=CC=C(Cl)C=C2	0.302471
JFOVJQCUIHRYOI	CN(CC1COC2=C(O1)C=CC=C2)C3=C4C=CC=CC4=NC(=N3)C5=C	0.237136
JFXJZFHPBYCODG	CC1CCN(CC1)C(=S)C2=CC=C(C=C2)N(C)C	0.229105
JGXMWNIVIDLSHR	COC1=C(C2=C(N=C(C)C=C2)C(=C1)[N+][[O-]]=O)[N+][[O-]]=O	0.242647
JGYJCRUVWAQTJL	CCCCOC1=CC=C(C=C1)C(=O)C(CN2CCOCC2)C3=CC=CC=C3	0.226408
JGZOWIZUUCOWBI	COC1=C(OCCCC2=C(Br)C=C(C)C=C2C)C=CC=C1	0.237929
JHGXRJAFYGXXHM	CC(C)OC(=O)NC1=CC2=C(CCC3=C(C=CC=C3)N2C(=O)N4CCN(C)	0.236299
JINAMQIRPMDXCD	CN1CCN(CC1)C(=S)C2=CN(CC3=CC(F)=CC=C3)C4=C2C=CC=C4	0.239978
JIWLATPWTJVSEH	OC(COC1=CC=CC=C1)CN(C2=CC=CC=C2)S(=O)(=O)C3=CC=CC=C	0.224047
JJRKCJKZOGFYPI	CC1=C(CC=C)C(N\N=C\C2=CC=NC=C2)=NC(=N1)C3=CC=CC=C3	0.226694
JJTYWBMDBLXULI	ClC1=CC2=C(C=C1)C(N\N=C\C3=CC(Br)=CC=C3)=CC=N2	0.239082
JKBNVHANVPUPKE	CCN1C=CN=C1CN(C)CC2=CN(N=C2C3=CC(C)=CC=C3)C4=CC=C(0.223254
JKHAICNBAJGKSQ	CN(C)CCCN(C(=O)C1=CC2=C(S1)C3=C(S2)C=CC=C3	0.242284
JLOBHBFPMZARDU	CC1=NN=C(C2=CN(N=C12)C3=CC=CC=C3)C4=CC(Br)=CC=C4	0.235778
JLSLZBCBNKGSPP	COC1=C(OC)C=C(C=C1)N=C(S)N2CCN(C\C=C\C3=CC=CC=C3)CC	0.226982
JLTONPRENNPEAR	COC1=CC=C(NC2=NC(=NC(=N Asinex Ltd.,BAS 07354379	0.246747
JLTXVLMENAZLNM	CCN1CCN(CC2=CC=C(OCC3=CC=CC=C3)C=C2)CC1	0.261234
JNIDCDDMCZGKCX	COC1=CC=C(C=C1)C2(O)CCN(CCCCOC3=CC=CC=C3)CC2	0.228036
JOGWHDSFGXCBJM	CN1CCN(CC1)C2=NC3=C(C=C(C=C3)N=C(S)N4CCCCC4)C(C)=C	0.238026
JOIDIVUDKPRITIS	[O-][N+](=O)C1=CN=C(C=C1)N2CCN(CC3=CC=CC=C3)CC2	0.226207
JOJSQJRJKUTDEU	CCN1CCN(CC1)C(=O)C2=C(C=CC=C2)N(CC3=CC=CC=C3)S(=O)(=	0.272356
JOWHAUBDIRDYTL	CCCN(CCC)CCCN(C(S)=NC1=CC2=C(C=C1)N=C(C=C2C)N3CCN(C	0.233333
JPBNGWPHLUZKBL	CCOC1=C(OCCN2CCC(CC3=CC=CC=C3)CC2)C=CC=C1	0.301886
JPHOMPNOKNRQQR	FC(F)(F)C1=NN=C(NC2=CC=C(Cl)C=C2)S1	0.2367
JPJOVOODFZGOBN	OC(COC1=CC=CC=C1)CN2CCN(CC2)C3=CC=C(C=C3)[N+][[O-]]=C	0.234928
JPPIQETUUBNFCC	CCOC1=CC=C(C=C1OCC)C2=NC(=NO2)C3=CC=CC=C3	0.230526
JPURAYRMIBQZRY	CC(C)N(CCOC(C1=CC=CC=C1)C2=C(C)C=CC=C2)C(C)C	0.269919
JQAJLVIVGYEBAG	OCCN1CCN(CC1)C2C(NS(=O)(=O)C3=CC=CC=C3)C4=C5C2=CC=C	0.240437
JQCRYKFJQAXIGC	CC1CCCC(C1)N2CCN(CC2)C3=C(C)C=CC(C)=C3	0.247982
JQPRWNFWMSGCNX	C(NC1CCCC1)C2=C(OCC3=CC=CC=C3)C=CC=C2	0.269498
JQUOFAHAMJITJLC	CC(C)N(CC1=NC(=NO1)C2=CC=C(C)C=C2)C(=O)C(C3=CC=CC=C3	0.229363
JQWSTJBTMKYCEO	COC1=CC(NC2=C3C=C(C)C=CC3=NC(C)=C2)=C(OC)C=C1	0.303287
JRALGXVGNCFV	CCOC1=CC=C(CNC(=O)NC2=CC=CC=C2)C=C1	0.232954
JRYZLOINKNIRJT	CCOC(=O)C1=C(C)[N](CCN2CCN(C)CC2)C3=CC=C(OC)C=C13	0.227162

JSGLPQUQCAJGX	CC1=C(CN2CCCC2C3=NC=CS3)N=C(O1)C4=C(F)C=C(F)C=C4	0.228689
JSJBMZPEAGTQLQ	COC1=C(NC(=O)NCC2CCN(CC3=C(C)C=CC(C)=C3)CC2)C=C(C)C=	0.231271
JSNNVLCYCHVEHC	CCCCOC1=CC=CC(=C1)C(=O)NC2=CC=C(C=C2)N3CCN(CC)CC3	0.225637
JTFWJZSDIREVFS	CSC1=C(OC2CCN(CC3=CC=CC=C3)CC2)C=CC=C1	0.340908
JTMQGPLGCCHGPD	ClC1=CC=C(NC(=O)NC2=CC(=C(C=C2)N3CCCC3)S(=O)(=O)NC4=	0.236982
JTMZNFHJPKPQDT	CC1=CC(CN2C(=CC3=C2N=CC=C3)C(C)(C)C)=CC=C1	0.271131
JUEAKQUMMBNRJE	CC1=C2C=CC=CC2=NC(NCC3=CC=CC=C3)=C1	0.231729
JUNITZPKTVZOBL	CN(CCCOC(C)=O)CC\C=C1\C2=C(CSC3=C1C=CC=C3)C=CC=C2	0.288524
JUUBFXIMFOJFOF	CCC1=C(C(N)=NC(N)=N1)C2=CC(=C(CI)C=C2)[N+](O)=O	0.250458
JVLGQDDHLXXDIU	CC(C)(C)C1=CC=C(CN(CC2=CC=CO2)CC3=NN=NN3C4CCCC4)C=	0.22253
JVMNOSIVRDMOOI	CCOC1=CC(NC(=O)CN2CCC(CC2)NC(=O)C3=CC(F)=CC=C3)=C(O	0.251416
JWIQRHJOQFUKQG	[O-][N+](=O)C1=CC=C(C=C1)N=C(S)NCC2=CC=NC=C2	0.247205
JWLVUMDTLQKCBN	CCC(C)NC(=O)NC1=C(CI)C=C(Br)C=C1	0.240564
JWUZFQWYBYNHLW	CCCCOC1=C(C=NN2C(C)=NN=C2N3N=C(C)C=C3C)C4=C(C=CC=C4	0.22541
JXKGRWTUSHVHIN	CC1=C(C)C=C(C=C1)N=C2N=C(N)C3=C2C=CC=C3	0.239148
JXLWBGZKWDKAY	O=S(=O)(N1CCC(CC1)OC2=CC=C(C=C2)N3C=NN=N3)C4=CC=CC	0.242508
JXNJCTVONYQNOB	CC1=CC(=CC(C)=C1)N=C(S)NC2CC3CCC(C2)N3CC4=CC=CO4	0.237643
JXPRESUBWIPPEI	CN(C)CCN[C@H]1CCC2C3CC=C4C[C@H](O)CC[C@]4(C)C3C	0.223278
JYGQRLQMJKRAQM	C(SC1=NN=C(O1)C2=CC=NC=C2)C3=CC=CC=C3	0.236171
JYPNBRZXZWBVCJ	COC1=C(OC)C=C(\C=N\NC(=O)CCN2C=NC(=C2C3=CC=CC=C3)C	0.225151
JZJDBAQXXFLGET	CCC1=C(OCCCCN2CCCC2)C=CC=C1	0.262105
JZXKGDVUHZCZAG	CCOC(=O)C1=C(N=C(N2CCN(CC2)C3=NC=CC=C3)C(=C1)C#N)C4	0.233248
JZMQVIHLDJAZFB	ClC1=CC(CI)=C(CSCCNC(=O)C2=CC=C(CN3CCOCC3)C=C2)C=C1	0.223441
KAPNTNCOCCNYHW	C\C(=N/N=C(\S)NCC1=CC=CC=C1)C2=CC=C(CI)C=C2	0.228087
KATBYCBPLVGOSL	O=C(CN1CCN(CC1)C2CCCC2)NC3=C(C=CC=C3)N4CCCC4	0.233509
KBGPTRHFZMERIT	CN(C)CC(O)C1=CC=C(\C=C\C2=CC=C(CI)C=C2)C=C1	0.27744
KBJNMSFZNNKLAR	CN1CCN(CC1)C2=NC(=NC(=N2)N3CCOCC3)NC4=CC=CC(=C4)C(0.227634
KBSCTGNEANFMTI	CC1=C(C[N]2C=CC=C2\C3=N\C(CO3)C4=CC=CC=C4)N=C(O1)C5	0.229886
KCANVEYUHCAMAP	CN(C)P(=O)(N(C)C)C(CI)=C(N1CCCCC1)N2CCCCC2	0.222743
KCGKYNZVRUJZQT	COC1=CC(OC)=C(C=C1)C(=O)C2CCN(CC3=CC=C(C)S3)C2	0.281642
KCQPDQZKZHYEG	CNC(S)=N\N=C\C1=CC(OCC2=C(F)C=CC=C2)=CC=C1	0.240951
KCXHNZGGTPMYAO	O\N=C\C1=CN(N=N1)C2=CC=C(CI)C=C2	0.26659
KDBMTBGGSOYBFT	FC1=CC=C(OCC2=NC(=C(O2)N3CCN(CC3)CC4=CC=CC=C4)C#N)(0.224811
KDFDQZTQJHHPU	CC1=CC(C(=O)ON=C(N)C2=CC=C(Br)C=C2)=C(C)C=C1	0.260282
KDMMSLIGTXPHPC	C(CC1=NC=CC=C1)NC2=CC3=C(C=C2)C4=C(C3)C=CC=C4	0.233774
KDOOEZRRXACFFT	CC1=NN(CC(O)COC2=CC3=C(CCC3)C=C2)C(C)=C1Br	0.23467
KDXXZHBZHFASCN	CCN1C=C(CN2CCC(CC2)C(=O)NC3=CC=C(OC4=C(F)C=CC=C4)C=	0.22428
KDZAFEAXRMURGE	CC1=CC(C)=NC(=N1)N(CCOC2=CC=CC=C2)C#N	0.265341
KEDKUNDQJRZHCY	COC1=CC(OC)=C(Br)C=C1CN2CCN(C)CC2	0.261326
KEMGTVYZPCBGOZ	BrC1=CC=C(NC(=O)C2=CC(OC(=S)N3CCOCC3)=CC=C2)C=C1	0.244464
KEPUOYACJXZYTQ	CCN1CCN(CC1)C2=CC=C(N)C=C2	0.253997
KETQGNPDHAUPMQ	COC1=CC=C(\C=C\CN2CCCC(CO)(CC3=CC(CI)=CC=C3)C2)C=C1	0.224285
KFAYLGCSTUTEDG	ClC1=CC=CC=C1OCCCCN2CCCC2	0.223001
KFLNUTIUYWTQNV	OC1=C(C=CC=C1)C(=O)NC2=CC3=C(C=CC=C3)C=C2	0.222884
KFMJDJOTJHGYPD	COC1=CC=C(C=C1)S(=O)(=O)NC2=C(OC)C=CC(=C2)[N+](O)=O	0.232696
KFQVNFHNLPHYDBU	CC1=C[N+](CC(=O)C2=CC=C(C=C2)C3=CC=CC=C3)=CC(C)=C1	0.234019
KGCBYKIMDOLQAS	N=C1N(CCCN2CCOCC2)C=NC3=C1C(=C(O3)C4=CC=CC=C4)C5=	0.274316
KGHCKYAADOQTDL	COC1=CC=CC2=C1N=C(S2)N(CCCN(C)C)C(=O)C(C3=CC=CC=C3)(0.22428

KGXPAEXNOWUTLY	[O-][N+](=O)C1=CC(C(=O)C2=CC=C(Br)C=C2)=C(C=C1)N3CCCCC:	0.223041
KHBXLWYPAHPKPS	CCOC1=C(OCCOCCN2CCN(CC3=CC=CC=C3)CC2)C=CC=C1	0.232553
KHKINSFQHMMKAG	COC1=CC(NS(=O)(=O)C2=CC=C(SC)C=C2)=C(OC)C=C1	0.259358
KHQBLGXKDHEXLY	FC1=CC=C(CN2CCC(CC2)C(=O)N3CCN(C\C=C\C4=CC=CC=C4)CC	0.224606
KHWOFOKQCKHWOQ	CCC1=CC=C(C=C1)C2=NN=C(NC3=CC(=CC=C3)S(=O)(=O)N(C)C)S	0.223699
KHZZMTAJRIDFIB	CCN(CC)C1=CC=C2C3=C(OC)C(OC)=C(OC)C=C3CC[C@H](NC)C2	0.223766
KIGGDAAHNWHMSMB	C(N1CCN(CC1)C(C2=CC=CC=C2)C3=CC=CC=C3)C4=NN=NN4C5	0.294418
KIUBOTVFTXCRLM	CC1=C(CSCC2=NC3=C(N2)C=CC=C3)C=CC=C1	0.229887
KIUJEASPRLEBRK	COC1=CC=C(CC2(CO)CCN(CC2)C(C)COC3=CC=CC=C3)C=C1	0.238843
KIYVHIIADWNBLP	COC1=C(OC2=CC(Cl)=CC=C2)N=C(N=C1)C3=NC=CC=C3	0.225048
KJCOJSQXSSWBOW	C1CC(CCN1)C2=CC(=NN2)C3=C4C=CC=CC4=CC=C3	0.295404
KJJNTQIFGZQDBH	CC1=C(CS(=O)CC(=O)NCCC2CCN(CC3=CC=CC=C3)CC2)N=C(O1	0.25136
KJXSVDPEQQZMBQ	COC1=CC=C(OC2=C3C=CC=CC3=NC(SC)=N2)C=C1	0.226344
KKEGVNCPHQPGEI	CN1C2=C(OC3=C1C=C(N=N3)N4CCN(CC5=CC=CC=C5)CC4)C=C1	0.226999
KKJZHOSFNMOHED	O=C(N1CCN(CC1)C2=CC=CC=C2)C3=CC(=CC=C3)S(=O)(=O)N4C(C	0.242551
KKUPAQXIWRJBGX	CC\C(=N/NC1=C2C=CC=CC2=CN=N1)C3=CC=C(F)C=C3	0.245846
KLCDQSGLLRINH	NC1=C(\N=N\C2=CC=CC=C2)C3=C(C=CC=C3)C=C1	0.225048
KLDJVUCROBXZPY	COC1=C(C)C=C(CN2CCC(CC3=CC=CC=C3)CC2)C(C)=C1	0.264482
KLNDWVFAKPPOLR	CC(NC(=O)C1=CC(=CC=C1)S(=O)(=O)N2CCN(C)CC2)C3=C(Cl)C=C	0.226613
KLTOIPJAYFPKPX	ClC1=CC=C(OCCSCC2=NN=C(NC(=O)NC3=CC(Cl)=CC=C3)S2)C=C	0.223317
KLYSZBKELNHMBM	COC1=CC(=CC(OC)=C1OC)C(=O)N\N=C\C2=CC=C(C=C2)N(CCCl)	0.249804
KMEORUDTMIYUQO	CN1CCN(CC1)C(=S)C2=CC=C(OCC(=O)NC3=CC(=CC=C3)C(F)(F)F)	0.222909
KMJAIOIQANQPJDX	COC1=CC=C(CC2(CO)CCN(CC3=CC=C(OC(F)(F)F)C=C3)CC2)C=C1	0.263187
KNHQDHACCVXHFJ	COC1=CC=C(C=C1OC)C2=NN=C(O2)C3=CC=CN=C3	0.228933
KOEKRBDZZOVZ	COC1=CC=C(OCC(O)CN2C(=N)N(CC3=CC=CC=C3)C4=CC=CC=C2	0.225321
KOFWLPMUYUZFP	CN(CCOC1=CC=C(Cl)C=C1)CC(O)C2=CC=CC=C2	0.274452
KOGKLWVBRDGOX	C1CN(CCN1C2=CC=CC=C2)C3=NC(=NC(=N3)C4=CC=CC=C4)N5C	0.244484
KORDZYYEBBVDAZ	COC1=CC=C(NC2=NC=NC3=C2C=N[N]3CC4=CC=CC=C4)C=C1O	0.248243
KOUOYJYRICGOSC	N1C=CC2=C1C=CC(=C2)C3=CN=CC=C3	0.225907
KOVIKBQUWRXSED	COC1=CC(=CC=C1)C2=C(C3=C(S2)C=CC=C3)C4=CC=C(OCCN5C	0.230043
KPFNCQBDQIVSJG	CCOC1=C(OC)C(Br)=CC(=C1)C(=O)NC2=CC=C(F)C=C2	0.25203
KPMYNDOTFPMRGX	CSC1=CC=C(CN(C)C(=O)C2=CC(=CC=C2)S(=O)(=O)N3CCN(CC4=C	0.225111
KPXBSOCMUBSBS	COC1=CC=C(CN2CCN(CC2)S(=O)(=O)C3=CC=C(Br)C=C3)C=C1	0.294165
KQERGFNGNIWLDR	CC[N]1C2=CC=CC=C2N=C1C3=CC=C(C=C3)N(C)C	0.271357
KQIHSDIGUBVIJR	COC1=CC=C(SC2=C(OC)C=NC(=N2)C3=NC=CC=C3)C=C1	0.232626
KQIYRTRYFJCLHP	COC1=CC2=C(OC(C)=C2C(=O)N3CCN(CC3)C4=CC=CC=C4)C=C1I	0.23112
KRFARVYVEIJXSQ	CC1=CC(=CC(C)=C1)N=C(S)NCC2=CC=C(F)C=C2	0.239387
KTBYFABLDEWPS	[O-][N+](=O)C1=C(N=CC=C1)N2CCC(CC2)C3=CC(=NN3)C4=CC=C	0.230744
KTHPCIRABJFDML	C1CN(CCN1)C2=NC(NC3=CC=CC=C3)=NC(NC4=CC=CC=C4)=N2	0.283197
KTWSKIQUAVAPQO	OC1=C(CNCCCNC2=C(O)C=CC=C2)C=CC=C1	0.23918
KUGLEHGRXKMLME	CCCCNC1=NC(=NC(=N1)N(C)C2=CC=CC=C2)N3C=CN=C3	0.228386
KUKMFSKXMCRUCL	COC1=C(OC)C=C(C=C1)C2=NN=C(COC3=CC4=C(C=CC=C4)C=C3	0.277756
KUSKQSLFNPHSJH	CC1=CC(Br)=C(OCCCCN2CCCCC2)C=C1	0.287186
KVFRNVSKTWFZLZ	FC(F)OC1=CC=C(C=C1)N=C(S)N2CCN(CC3=CC=CC=C3)CC2	0.226878
KVHRLKBZRBQJDR	FC1=C(\C=N\NC(S)=NC2=C(Cl)C=C(Cl)C=C2)C=CC=C1	0.232812
KWWTUELROYQXKO	CC1=C(C)C(NC(=O)C2=NN(C(=N2)C3=CC=CC=C3)C4=CC=CC=C4	0.23416
KWYQGFAGMNSBQW	ClC1=CC(=CC=C1)N2CCN(CCCN3CCN(CC3)C4=CC=CC=C4)CC2	0.360586
KXEZBQTZEBDTNH	CC1=C(C#N)C(Cl)=NC(N)=C1C#N	0.223116

KXFYGCOGCADHLM	COC1=C(C=CC=C1)C2CCN(CC3=CC(Cl)=C(Cl)C=C3)CC2	0.277491
KXPJBGWZIZEBLM	CCC1=CC=C(C=C1)C2=NC(CN3CCC(CC3)C(=O)NCCC4=CC(OC)=C	0.222641
KXTYPELBHVVWFC	ClC1=C(CN2CCN(CC2)\N=C\3=CC=NC=C3)C=CC=C1	0.256583
KYAKSESTNXAPNO	CC(CCCN(C)C)C(CC1=CC=CC=C1)C2=CC=CC=C2	0.32244
KYXSKURMRIMYFM	CC1=C(CSCC(=O)NC2=C(C=CC(Cl)=C2)N3CCCC3)C(C)=NO1	0.253731
KYZWFXSCKYQHNC	CN1CCN(CC1)C2=C3C=CC=CC3=NC(=N2)C4=CC=CS4	0.235735
KZNNKGUYBGZWFY	COC1=CC=C(C=C1)N2CCN(CC2)C3=C4C=CC(Cl)=CC4=NC=C3	0.224033
KZWNTXVNZWECJU	O=C(OCCN1CCCC1)C2(CCCC2 Vitas-M Laboratory,STK555169	0.230883
KZXCSEFVNVIGEKX	CCN(CC1=CC=CC=C1)C(C2=CC=CC(=C2)C#N)C3=NN=N[N]3C(C)(0.240999
LAENUZQHPWDHFN	COC1=CC=C(C=C1OC)C(=O)N2CCN(CC2)C3CCC(CC3)C4=CC=CC	0.22541
LAGZXGNBDUFGPI	COC1=C(OC)C=C(NC(=O)C(=O)NCC(N2CCC3=C(C2)C=CC=C3)C4=	0.226278
LAJIJUOIBRLOMO	OCCC1CN(CC2=CN=C(S2)C3=CC=CC=C3)CCN1CC4=CC=CC=C4	0.251236
LAPZPUGWSBIQQC	CN(CCC1=NC=CC=C1)C2CCCN(C2)S(=O)(=O)C3=C(C)C=C(Cl)C(C)	0.224566
LBAFURBQIAJSLW	COC1=C(SC2=CC(Cl)=CC=C2)N=C(N=C1)N(C)C	0.227098
LBEQPUMCFYHPIM	CC1=CC=C(C=C1)S(=O)(=O)N2CCC3=C(CC2)C=CC=C3	0.28032
LBSIRYRCMMQUAB	COC1=CC=C(C=C1)C(O)C(CN2CCCC2)C3=CC=CC=C3)C4CCCC	0.240791
LBVFWJILNBYIOO	COC1=CC2=C(C=C1)C=C(C=C2)C3=NNC=C3CN4CCCC4C5=NON	0.233937
LCKMLQCVCBPQQI	CCCCNCCCOC1=C(Cl)C(Cl)=CC=C1	0.268276
LCKUBQBEDRQTRC	ClC1=CC2=C(NC3=C2CNCC3)C=C1	0.242494
LCLHNZWVBURZBA	[O-][S+](=O)(CC(CN1CCCC1)N2CCCC2)C3=CC=C4C=CC=CC4=C3	0.227339
LCRABWZMGNEZJV	CC1=C2C=CC=CC2=NC(=C1)N3CCNCC3	0.249301
LCVIGDYZEMTQLA	COC1=CC=CC=C1N2CCN(CC2)C(=O)C3=C(C)ON=C3C4=CC=CC(=	0.244093
LCWXCNKXPUOIIU	CC1=CC=CC2=C1N3N=NN=C3C(CN(CC4=NN=NN4C5CCCC5)C	0.240954
LCYPBPWKIODAKD	CCN(CC)C1=CC=C(C=C1)\C=N\NC2=NC=C(C=C2)[N+][[O-]]=O	0.228141
LDBGXYHYHGCKLH	CCCC(N1CCN(CC1)C2=CC=CC(=C2)C)C3=NN=N[N]3CC4CCCC	0.230956
LDNFVOBONUXXME	CN1C(=N)N(CC(O)C2=CC=CC3=CC=CC=C23)C4=CC=CC=C14	0.231279
LDSNGCZYDAXOBG	CCOC1=CC=C(C=C1)\C2=C\3C(N2CC=C)C(=O)C#N)C3=NN=C4CC	0.224932
LDZQSFJRJWGBZEP	CCOC1=C(C(=O)N2CCN(CC2)C3=CC=CC=C3)C4=C(C=CC=C4)C=C	0.231223
LEGVQFQAMCUMQW	COC1=CC(=CC(OC)=C1OC)C(=O)C2=CC(OC)=C(OC)C=C2	0.252156
LEJHIUNKJREDRV	CC1=C(C=CC(Cl)=C1)C(=O)C2CCCN(C2)C3CCSCC3	0.254048
LEQWXTTZROBKHE	CC1=CC(=NC(OC2=CC=CC(C)=C2C)=C1S(C)(=O)=O)C3=CC=CC=C:	0.229139
LERFXNHGOBLKHJ	CCOC(=O)C1=C(N=C(N2CCCC2)C(=C1)C#N)C3=CC=CC=C3	0.229874
LFCRESUTNYKKS	CC1=CC=C(C)C(=C1)N2N=NN= Enamine,T5334664	0.228731
LFGYSWPEUKSZOQ	COC1=CC=C(OC)C(CN2CCCC Vitas-M Laboratory,STK138773	0.248713
LFXFFBJIBSLMNJ	CC(C(=O)C1=CC=C(C=C1)C2=CC=CC=C2)[N+]=3=CC=C(C)C=C3	0.233274
LGBBDZXRVTQNU	CN(C)CCCOC1=CC(Cl)=CC=C1	0.271559
LGDWSMMLDYQYJBZ	CC(=O)OC1=CC(SCCCCCN2CCOCC2)=C(OC(C)=O)C=C1	0.223794
LGEINYZXOUVJFZ	CC(C)C)C1=CC=C(OCCCCCN2CCNCC2)C=C1	0.262373
LGGGUQCRIDQESW	CCOC1=CC=C(C=C1)N(CCC#N)[S+][[O-]](=O)C2=CC=C(OC)C=C2	0.23064
LGLCVGFUDURYVOD	OCC1=C(OCCCN2CCC(CC3=CC=CC=C3)CC2)C=CC=C1	0.239661
LHFHPCWQLUDMAB	CCN(CC)CCNC(=O)C1=CC(NS(=O)(=O)C2=CC=C(C)C=C2)=C(C=C1	0.235214
LHPDDBGADQDQLZ	O=C(NC1=CC=CC(=C1)NC(=O)N2CCN(CC2)C3=CC=CC=C3)N4CC	0.234123
LHTCYYGJZPGMG	CCC1=CC(OCCCCNCCCOC)=CC=C1	0.241458
LJPALRNNMOQAQU	CC1=C(Cl)C=CC(OCC(O)CN2CCC3=C(C2)C=CC=C3)=C1	0.234759
LKJBCQWMMWWEHB	COC1=CC2=C(SC(=C2)C3=CC=C(O)C=C3)C4=CC(OC)=CC(OC)=C4)	0.23419
LKTVCBAYEHDGNF	ClC1=CC(=CC=C1)N2CCN(CC2)C(=O)CCC(=O)N3CCN(CC3)C4=C(0.23013
LLYNLQDHLONHOO	CN1CCN(CC1)C(=O)CCN2C(=S)\C(=C\3=CC=C(C)C=C3)C2=O	0.230163
LMBGOBJQESYQAC	CC1=CC=C(NC2=C3C=CC=C(C)C3=NC(C)=C2)C=C1	0.262498

LMGOXKZSDSQEGF	CSC1=C(NC(=O)CN(C)CC(=O)NC2=CC(Br)=CC=C2)C=CC=C1	0.276047
LMNMFISQCMTDB	CN(C)CCCCOC1=C(Cl)C=C(Cl)C=C1C	0.28833
LMYPKWMJCDIHHF	O=C(CSC1=NC(=NC(=N1)N2CCCC2)N3CCCC3)N4CCN(CC4)C!	0.222507
LNFXLMNTXMDCOI	COC1=C(OC)C(Cl)=CC(CNC2CCCCCCC2)=C1	0.284939
LOLQYDGGGAQMCGH	CCC(C)C1=C(OCCCCN2CCCC2)C=CC=C1	0.280798
LOQNMLHIQHBJV	FC1=CC(CN2C=C(C=O)C3=C2C=CC=C3)=CC=C1	0.228063
LOZNUSRYBQAASV	CC(N(CCN(C)C)\S)=N\C1=C(C)C(Cl)=CC=C1)C2=CC=CO2	0.243494
LPAJESSQHVIDM	CCN(CC)CCNC(=O)C(Cl)=C1C(Cl)=C(Cl)C(Cl)=C1Cl	0.248022
LQWYEXCCDMWGMB	O=C(NC1=CC=C(C=C1)N2CCN(CC2)C(=O)C3=CC=CC=C3)C4=CC!	0.239672
LQZDYPHFVGRHKD	CC1=NC2=C(C=C1)C=CC3=C2N=CC=C3	0.306735
LRRFOPNECJYNMY	FC1=CC(Br)=C(OCC(=O)NC2=C(C=CC=C2)N3CCOCC3)C=C1	0.242739
LRXLNMZQHJZBB	CN(C)CC(C)(C)CNC(=O)C1CCN(CC2=C(O)C=CC=C2)CC1	0.227419
LRYLEYCCZSAPD	CC1=C(CCCNC2CCCC2)C3=C(N1)C=CC=C3	0.272759
LSJRRRNUMMUDPM	ClC1=C(\C=N\N2CCN(CC3=CC=CC=C3)CC2)C=CC=C1	0.239589
LSKZDQMPCSMAOG	ClC1=C(Cl)C=C(NC(=O)NC2=NOC=C2)C=C1	0.230615
LSQQORZIBMVTDA	CCN(CC)CCNC(=O)C1=CC=C(NC(=O)CC2=C3C=CC=CC3=CC=C2)(0.255062
LSYYZRIAKZKIKI	COC1=C(C)C=CC(NC(=O)NCCN2CCN(CC2)C3=CC=C(Cl)C=C3)=C1	0.234338
LTBKHBIPKHIHLF	NC1=NC(=NC2=CC=CC=C2)C3=C1C=CC=C3	0.225725
LTLPHMSJMFUGED	COC1=CC(OC)=C(NC2=C3C=C(Br)C=CC3=NC=N2)C=C1	0.229156
LTRBEDXMFQKQZ	COC1=C(\C=C\C2=N\C=C(N(C)C)C(=O)O2)C=CC=C1	0.236253
LTZOIUVFTDNHAC	CN(CCOCCOC1=C(Br)C=C(Cl)C=C1)CC2=CC=CC=C2	0.280401
LUWUGYXTIVKHKC	ClC1=C(NC2=NC(=CS2)C3=CN=CC=C3)C=CC=C1	0.232263
LVGSNEOJUMDTFM	CCOC(=O)C1=C(NC(=O)CCN2CCC(C)CC2)C3=C(N1)C=CC(Br)=C3	0.227107
LVPMCHZTOXKOHN	CCN1CCN(CC1)C2=C(N=C(O2)C3=CC=CC=C3)S(=O)(=O)C4=CC=(0.272528
LVUNXLQSNWTIHG	CC1=CC=C(C=C1)C2CC3CCC(C2)N3CC4=C(F)C=CC=C4	0.280467
LVZJHCULSIRZLW	CC(C)OC1=C(OCCOC2=C3N=CC=CC3=CC=C2)C=CC=C1	0.228203
LWBFQYZDAH HQOY	C(CN1CCNCC1)NC2CCCCCCCCC2	0.354122
LWHUJWSFJIYWGH	ClC1=CC(NC(=O)OCCOC(=O)NC2=CC(Cl)=CC=C2)=CC=C1	0.240284
LWLWWFQDABJJFE	O=C(CN1CCN(CC1)C2=CC=CC=C2)NC3=C(SC4=CC=CC=C4)C=CC	0.243553
LWWPJRYUNFTHPP	CC(C)(CN1CCC2=C(C1)C=CC=C2)NS(=O)(=O)C3=CC=C(Cl)C=C3	0.224593
LWWPQTIAHAKPKT	CC1CCN(CC(=O)N2C3=C(CCCC3)C4=C2C=CC=C4)CC1	0.226767
LXLLBCDJEITFLG	COC1=C(NC(=O)CN2CCN(CC2)C3=C(F)C=CC=C3)C=C(C)C=C1	0.235255
LXLKXSWZSSPDT	CC(C)CN1C(\C=N\NC2=NC3=C(N2)C=CC=C3)=NC4=C1C=CC=C4	0.234595
LYHNXOLTRNCOGM	FC1=CC=C(C=C1)C2=NN=C(CN3CCC(CC3)C4=NC5=C(S4)C=CC=(0.223361
LYSTXBLNUSUUQY	CN1CCN(CC1)C2CC3=C(SC4=C2C=CC(=C4)C(F)(F)F)C=CC=C3	0.329511
LYVCFZODSMSCFI	CCN1C(=NC2=C1C=CC=C2)N3CCN(CC3)S(=O)(=O)C4=CC=C(OC)	0.263297
LZCNZJRG NPKXNZ	CC1=CC=C(C=C1)N2C=C(CN3CCN(CC3)C4=NC=CC=C4)C(=N2)C!	0.33371
LZHKJGDGNDVNAT	CC1CCN(CC1)CC(O)COC2=C(C)C=CC(=C2C)C	0.23389
LZTFBZHIRAVIKX	ClC1=CC(Cl)=C(OCC2=CC(=NO2)C3=CC=CC=C3)C=C1	0.225416
MAAFYYHIGLBPFM	CC(C)NC(=O)O\N=C(/C)C1=C(C)N=C(S1)C2=CC=C(Cl)C=C2	0.226658
MASXUXOPBHEMES	CCC(C)NCCCCOC1=CC=C(Br)C=C1	0.26531
MATVQBKTCQLKHX	CCOC1=C(C=CC=C1)N2CCN(CC2)C(=O)C3=C(OC)C=C4C=CC=CC	0.229418
MAZMDDQJPLHOGX	COC1=CC(=CC(OC)=C1OC)C(=O)OCCC2=CC3=C(C=CC=C3)C(=O)(0.232859
MBFJXJXTFLDDHM	COC1=CC=C(NS(=O)(=O)C2=CC(N\C(=N)\S(=O)(=O)C3=CC=CC=C3	0.239287
MBJXWDYDOGMUJI	COC1=C(OC)C=C(CCN(C)S)=NCCC2=CC(OC)=C(OC)C=C2)C=C1	0.244022
MBYRHGK OUBURHB	[O-][N+](=O)C1=CC=C(C=C1)C2=CSC(=N2)N3CCCCC3	0.223195
MCELMSQHTKQYLN	CCN(CC)CC(=O)NC1=NC(=CS1)C2=CC=C(Cl)C=C2	0.227735
MCOOYONNVNRHBQ	COC1=CC=C(C=C1)C(CNC(=O)C2=CC(NS(=O)(=O)C3=CC=C(Br)C=	0.225793

MCRQBNZKVVYOII	CN(C)CC\C=C1/C2=C(SC3=C1C=C(CI)C(F)=C3)C=CC=C2	0.289403
MCTCFRQYPIHWTI	CCN(CC)CCCNC1=C(N=C(O1)C2=CC=CC(=C2)CI)C#N	0.227528
MCYLLDYDHQBNTN	CCN(CC)C1=CC=C(NC(=O)C2=CC(=CC(=C2)OC)OC)C(=C1)C	0.222697
MCYRPWJNPNZAT	CCCCOC1=CC=C(NC2=NC3(CCCC3)N=C(N)N2)C=C1	0.230198
MDNVEDZFPGSWSN	CCN(CC)CCOCCOC1=CC(C)=C(CI)C(C)=C1	0.258201
MDSZVKQTJAQFFG	COC1=C(OC2CCCC2)C(Br)=CC(CNCC(C)C)=C1	0.234232
MEEFFYUZIUCGGQ	COC(=O)\C1=C(/C)N(C)\C=C(/C1C2=CC=C(F)C(=C2)Br)C(=O)OC	0.224829
MENNRQXMFWMWAH	CCNC1=NC(=CS1)C2=CC=C(CI)C=C2	0.258612
MFDISVMGGKXHMR	CC1=C(C)C(C(N2CCN(CCO)CC2)C3=CC=C(CI)C=C3)=C(NC(=O)C4	0.230014
MFKATAJWLKTKPM	CCN(CC)CCNC1=NC(=C(S1)C2=CC=C(OC)C=C2)C3=CC=C(OC)C=C	0.260814
MFPKDUIMNIPMSH	CCCCNCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.266096
MFROXXGQCVDJFE	CIC1=C(CN(CC2=CC=CC=C2)C(C3=CC=CS3)C4=NN=NN4C5CCCC	0.272057
MFSFAIBGVJXGNV	CC(C)C1=CC(OCC(O)CN2CCC3=C(C2)C=CC=C3)=CC(C)=C1	0.225313
MFTIGMUEIADPNR	CIC1=C(C=CC(NC(=O)C2=CC=CS2)=C1)N3CCCC3	0.231409
MFUANMKFOSVLLJ	COC1=CC2=C(C=C1OC)C(=C(S2)C3=C(OC)C=CC=C3)C4=CC=C(O	0.226152
MFUCBYRUQFMVJU	COC1=C(SC2=CC=C(F)C=C2)N=C(N=C1)C3=NC=CC=C3	0.223398
MGAPEMLRADUNBX	COC1=C(OC)C=C(CN2CCCC(O)(CC3=CC(CI)=CC=C3)C2)C(CI)=C	0.237476
MGXNYBVKEOWFQD	FC1=CC=C(C=C1)N2CCN(CC2)C(=O)C3=CC(=CC=C3)C(=O)N4CC	0.241059
MHXGKAPEFLBBDT	CC1=NC2=C(C=CC=C2)C(NC3=CC(Br)=CC=C3)=C1	0.24724
MISTWAYDZLXUKR	FC1=CC=C(C=C1)C(N2CCN(CC2)C3=CC=CC=C3)C4=NN=NN4CC	0.262698
MJHDJQNJJVZMOI	N=C1N(CCN2CCCC2)C3=C(C=CC=C3)N1CC(=O)C4=CC=CS4	0.284813
MJWWSXOBWDMJJP	SC(NC1CCCC1)=NC2=CC=C(OC3=CC=CC=C3)C=C2	0.222387
MKBPIXLWYBWKRN	CIC1=NC(=NC(CS(=O)(=O)C2=CC=CC=C2)=C1)C3=CC=CC=C3	0.2423
MKCPUDVEFDAXLS	O=S(=O)(OC1=C(C=CC=C1)C2=CC=CC=C2)C3=CC=CC=C3	0.299698
MLADKRXBDKHQRM	N#CC(C#N)=C1SC(=N/C2=CC=CC=C2)\C(N1C3=CC=CC=C3)=N\C	0.269445
MLLXHGHZOGOBQS	CCCC(=O)N1CCN(CC1)C2=NC3=C(S2)C=C(Br)C=C3	0.225281
MLSJRXCETXEQCG	CIC1=C(C=CC=C1)C(=O)NC2=CC=C(C=C2)N3CCN(CC3)C(=O)C4=	0.235173
MLUXVLCNFWSIJG	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=C(OC)C=CC(OC)=C3)	0.225335
MMOBBISAVIKZPP	C(CN1CCCC1)N2C(NCC3=NC4=C(C=CC=C4)N3CC5=CC=CC=C5	0.232415
MMPRERRXDROFNS	CC1=CC(NC(=O)N2CCN(CC3=CC=C(CI)C=C3)CC2)=CC=C1	0.238198
MMROUTXCZBZOQOB	FC1=CC=C(CN(CC2=CC=CC=C2)C(\S)=N\CC=C)C=C1	0.225568
MNMXYGUYRMIBKV	CC1=C(C=C(CI)C=C1)N2CCN(CC2)C(\S)=N\CCC3=CC=CC=C3	0.223377
MNTVKKVDXXLKKV	CCOC(=O)N\N=C\C1=CC(OCC)=C(OCCSC2=CC=C(CI)C=C2)C=C1	0.244565
MOQCKKLCFQKGQK	CN1C=C(CN2CCN(CC2)C3=CC=CC=C3)C4=CC=CC=C14	0.274214
MOUFAXAHQFOEA	FC1=CC=C(NC(=O)NC2=NN=C(COC3=C(F)C=CC=C3)S2)C=C1	0.225951
MPGPLWGAOFVVRH	CN(CC\C=C1/C2=C(CSC3=C1C=CC=C3)C=CC=C2)CC=C	0.329983
MPXWIWCJZHUHQR	CN1CCC(CC1)OC2=C(SC3=CC=C(C=C3)C(F)(F)F)C=CC=C2	0.234346
MQRVZQONLUTKMA	CCC(COC)NCC1=CN(N=C1C2=CC(F)=CC=C2)C3=CC=C(OC)C=C3	0.245043
MQTJTRXFDSDSOO	O=C(OC1CN2CCC1CC2)C34CC5CC(CC(C5)C3)C4	0.24313
MQVPADVOISVUVJ	CC[N+]=C(OC2=C1C=CC=C2)\C=C\N(C)C3=CC=CC=C3	0.243358
MSEWEKWTCTRFOSN	[O-][N+](=O)C1=C(\C=N\NC(S)=N\N=C\C2=C(C=CC=C2)[N+][[O-]	0.264813
MSWDFRIWVJZPPP	Cl.CCN(CC)CCN(C(=O)C1=C/C=C(\C=C\1)S(=O)(=O)N2CCCC2)C3	0.377831
MSXJLGPMPFKMAX	CC1=CC=C(C=C1)S(=O)(=O)OC2=C(\C=N\N=C(/N)S)C=CC=C2	0.234305
MSZIWZSPLVWFC	CC1CCN(CCNC(S)=NC2=CC=C(CI)C=C2)CC1	0.293474
MTTFIFPOMXQPCT	NC(=O)N\N=C/C(CCCCC\C(C1=CC=CC=C1)=N/NC(N)=O)C2=CC=C	0.239284
MTUAPGDJRRQAHE	CCOC(=O)C1=C(CN2CCCC2)[N](C)C3=CC=C(OC)C=C13)Br	0.252439
MUBRJekkjanjnx	CN(C)CCCC1SC2=C(SC3=C1C=CC=C3)C=CC=C2	0.361686
MUJWOXGLZLOSIV	CN(CCOC1=CC=CC=C1)CC(O)COCC2=C(F)C=CC=C2	0.242121

MUWHRGFVOPWZOJ	COC1=C(O)C=C(\C=N\N2CCN(CC2)C3C4=C(C=CC=C4)C5=C3C=C	0.25729
MVFCUKAAQGQILZ	CN1CCN(CC1)C(\S)=N\C2=CC(CI)=C(CI)C=C2	0.24753
MVFPBEURBHRCAM	CCOC(=O)C1=C(C)N(C)C(C)=C(C1C2=CSC=C2)C(=O)OCC	0.236852
MVZKFDJVVINAQD	CCOC(=O)C2(CC1=CC(OC)=CC=C1)CCN(CC3=C(OC)C=CC=C3)CC	0.269732
MWIAMPGAACPVE	COC1=CC(OC)=C(Br)C=C1CN2CCN(CC2)C3=CC=C(F)C=C3	0.238368
MWNXWDMQBOTMKX	CC(C)COC1=C(CI)C=C(C\N=C(/N)N=C(N)N)C=C1	0.23559
MWXFTOXDRVAKHI	[O-][N+](=O)C1=C(CI)C=CC(NC(=O)CN(C2CCCC2)C(=O)C3=C(CI)	0.222791
MXBMUNASOBPHAY	COC1=CC=C(C=C1)N=C(S)N\C(=N\S(=O)(=O)C2=CC=C(CI)C=C2)C	0.223534
MXHWGHJBQPQAJ	CC1CCCN(C1)C2=C(N)C=C(F)C=C2	0.249301
MXJXDBQPBACLHB	C(N1CCN(CC1)C2=NC3=C4C2=CC=CC4=CC=C3)C5=CC=CC=C5	0.238792
MXXNAZFNHJOMJ	CC1=C(C=CC(F)=C1)S(=O)(=O)NC2=C(C=CC=C2)C(=O)NC3CCN(C	0.222566
MXXPOBMGINPDNZ	CN(C)CCCNC(=O)C(\NC(=O)C1=CC=C(C)C=C1)=C\C2=CC=C(O2)C	0.241409
MYUVOPXZMCGDAD	CC1=CC=CC2=C3N(CCC3=C(C)N=C12)C4=C(F)C=CC=C4	0.270714
MZGDYPYPJYRXIN	CN(C)CCCNC1=CC(C)=C(C#N)C2=NC3=C(C=CC=C3)N12	0.223842
MZJADLNSIFQRAD	OC(COCC1=CC=CS1)CN2CCN(CC2)C3=CC(=CC=C3)C(F)(F)F	0.240154
MZLZAPCURITIDY	NC1=CC(=NN1CC2=CC=CC=C2)C3=CC(Br)=CC=C3	0.227613
MZPFILZBJZGYHV	CN1\C(SC2=C1C=C(C)C=C2)=C\C3=[N+](C)C=CC=C3	0.231265
MZYURQUUEUMCEN	CCN(CC)CCN1CCN(CC1)C2=NC(=CN=C2)C3=CC4=C(C=CC=C4)C	0.236176
NAVBYVMNDQAODN	CSC1=C(C=CC=C1)C(=O)C2CCCN(CC3=CN(N=C3)C4=CC=CC=C4)	0.266511
NAVODTIWKOIFKW	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC=C(OC)C=C3)CC2	0.251465
NBASXBUUNPZFKJ	O=C(N1CCN(CC1)C(C2=CC=CC=C2)C3=CC=CC=C3)C4=CC=C(C=C	0.224915
NBGRRSVGTIFHDF	CN1CCN(CC1)C(=O)C2=CC=C(\C=C3/SC4=C(C=CC=C4)N(CC5=C	0.243335
NBKOLADYUCUELK	COC1=CC(=CC(OC)=C1OC)C2NC(S)=NC(=C2)C34CC5CC(CC(C5)C	0.229427
NBRRQUKYSKMP CJ	CCCCCCN1C2=NCCCN2C3=C1C=CC=C3	0.26022
NBSBWIMTXRSXFJ	CCN(CCCCN(C)C)CC1=CC2=C(O1)C=CC=C2	0.290093
NCFXAMQSYIPRDN	COC1=C(C=CC=C1)C(=O)NC(CCSC)C(=O)NCCCSC2=CC=CC=C2	0.231126
NCIAFIKSYBXAIL	COC1=CC=C(C=C1)C2=NOC(=N2)N3CCC(CC3)C(=O)NC4=CC(OC	0.224304
NCSSTRALCUMWTF	[O-][N+](=O)C1=CC=C(NC(=O)NCCN2CCC3=C(C2)C=CC=C3)C=C1	0.225946
NCVYEHIMKMRBGA	CIC1=CC=C(\C=N\NC(=O)CN2C3=C(SC4=C2C=CC=C4)C=CC=C3)	0.224977
NDPZKSDUMMEMSO	COC1=CC=C(C=C1)C2=C3C=C(CI)C=CC3=NO2	0.227716
NEAXSQKYNELCG	COC1=CC=C(C=C1)C2=NOC(=N2)C3=CC=C(CI)C=C3	0.263806
NEFUEHMALDWNGS	COC1=CC(=CC(OC)=C1)C2=C(C3=C(C=CC(=C3)C4=CC=CC5=C4C	0.230977
NEKJZJSWJMAZRZ	COC1=C(C=CC=C1)N2CCN(CC3=C(OC)C(OC)=C(OC)C=C3)CC2	0.242823
NEXKTFZNLLSLEA	CC1N(CCC2=C1C=C3OCCOC3=C2)C(=O)C4=CC=C(CI)C=C4	0.227404
NEYNGVZPW CJUMP	CCN1CCN(CCCOC2=C(OC)C=C(C=C2)\C=C\C)CC1	0.252141
NFFRAGZFPYNZGL	CC1=CC(N2CCN(CC2)C3=C(C=CC=N3)[N+](O)=C(C)C=C1	0.291482
NFWFNKQJHIUIBD	N#CC1=C2CCN(CC3=CC=CC=C3)CC2=C(N=C1N4CCCC4)N5CC	0.228373
NGDDKXSLDUONKY	O=C(CN(CC1=CC=CC=C1)CC2=CC=CC=C2)NC3=C(C=CC=C3)C#N	0.231371
NGLCJCLFLUWKGH	COC1=NC(=NC(=N1)N2CCOCC2)N3C=CC=C3	0.249403
NGSKLXHESMVWCC	CC(=O)C1=C(C)NC(C(=O)OCC2=CC=C(Br)C=C2)=C1C	0.232204
NGXUEHOVTWDIHS	COC1=C(OCC2=C(CI)C=C(CI)C=C2)C=CC(=C1)C(=O)NCCC(C)C	0.226166
NHGOPUUUGHBRSD	CC(=C)CNC(S)=N\N=C\C1=CC=C(C=C1)N2CCOCC2	0.234985
NHGRAHAVFNGAOG	C[C@H](CO)N1C[C@H](C)[C@H](CN(C)CC2=CC=CC=C2)OC3=C	0.228438
NHXXAIOLFGICFD	CN1CCN(CC1)C2=C(NC(=O)CCC3=NC(=NO3)C4=CC=C(C)C=C4)C	0.23216
NHYVUVPOXQKFDX	CC1=C(CN2CCC(CC2)C(=O)N3CCN(CC3)CC4=CC=CC=C4)N=C(O	0.233755
NHZBQJDEXLJZPQ	COC1=C(OCC2=CC=CC=C2)C=CC(CN3CCC(C)CC3)=C1	0.250758
NIJTUDCAEFZYJX	CC(C)NS(=O)(=O)C1=CC=C(OC2=C(CI)C=C(C=N2)C(F)(F)F)C=C1	0.247566
NIKUGIVXOLBYIT	C(N1N=NN=C1C(N2CCN(CC3=CC=CC=C3)CC2)C4=CC=CC=C4)C	0.334247

NIUUWDFMVWJKAN	CC1=C(C)C(CN2CCCCC2)=C(NC(=O)C3=CC=C(F)C=C3)S1	0.258062
NIWPGRIRBQXFLJ	COC1=CC=C(C=C1OC)C2=CC(Chem Div,C130-0360	0.233245
NJPYPBRTHCCIND	CN(CC1COCCO1)CC2=NC(=NO2)C(C3=CC=CC=C3)C4=CC=CC=C	0.223789
NJSCBCNYQNEEFZ	COC1=C(OCC2=CC=CC=C2)C=C(CN3CCN(CC3)C4=NC=CC=C4)C:	0.230855
NJSNJYYYFPTSXR	CN1N=NN=C1SCCNCC2=C(OCC3=CC=C(Cl)C=C3)C=CC=C2	0.269951
NJSSNAKBDXXDTB	COC1=CC(OC)=C(C=C1)C2C(C)C(OC3=C2C=C4OCOC4=C3)N5CC	0.249421
NJVIJAZYKLEPBH	OCl(=O)(=O)=O.CC1=[N+](CCC2=CC=CC=C2)C(=CC(=C1)C3=CC=C	0.235902
NJYXCXKGCXKMB	COC1=C(OS(=O)(=O)C2=CC=CC=C2)C=CC(\C=N\NC(=O)C3=CC=C	0.240582
NKEAWKMGMDMDQI	OC(COCC1=CC=C(Cl)C=C1)CN2CCN(CC2)CC(O)COCC3=CC=C(Cl)	0.2552
NKHPIUHDBXIEIT	COC1=CC=C(N\C(S)=N\N(C)C(\S)=N\C2=CC=C(OC)C=C2)C=C1	0.225608
NKLGHVMBNHNNG	OC1=CC=C(C[C@H]2CNCCN2CCCC3CCCC3)C=C1	0.257142
NKYSCFSNEBARFK	CCN(CC)S(=O)(=O)C1=CC=C(OC2=CC=C(C=C2)S(=O)(=O)N(CC)CC	0.249693
NLBCTXFSWJUTED	COCCCN1=NN=C(CS1)C2=C(C)N(C(C)=C2)C3=CC=CC=C3F	0.243912
NLCXYBYOMZRHXHQ	COC1=C(O)C=CC(CN(C)CC2CCN(CCC3=CC(=CC=C3)C(F)(F)F)C2	0.236994
NLEDPRHIQSRERF	C\C(=N\NC1=CC(Cl)=C(Cl)C=C1)C2=CC=C(C=C2)N3C=CN=C3	0.235946
NLPGJEYPMXWQX	COC1=C(OC)C(CN(C)CC2CCN(CCC3=CC=C(Cl)C=C3)C2)=CC=C1	0.322405
NMCKETLUGKTIKJ	CN(C)S(=O)(=O)C1=CC=CC(CSCC2=CC=CC(=C2)S(=O)(=O)N(C)C)=	0.26485
NMGVVVOTFVENON	CCOC1=CC=C(C=C1)S(=O)(=O)N(C)C2=CC=C(OC(=O)NCC3CCCC	0.24759
NNAYUDQWATWDIH	CN(CCOC1=CC(Cl)=C(Cl)C=C1)CC2=CC=CC=C2	0.239553
NNBOWLVAZHNNP	CCOC(=O)C1(CCOC)CCN(CC2=CC(OC3=CC=CC=C3)=CC=C2)CC:	0.233504
NNMIYIGWDKMLNX	ClC1=CC=C(NC(=O)NC2=NN=C(CSC3=CC=C(Cl)C=C3)S2)C=C1	0.230715
NNPNQLZPNNQNSI	COC1=CC=C(CN2CCN(CC3=C(F)C=CC=C3)CC2)C=C1	0.262034
NNQVKTYGEHCQRH	CCCN1CCN(CC1)C2=NC=NC3=C2N=N[N]3CC4=CC=CC=C4	0.238649
NODDDZXVWVZZRD	CCSC1=NC2=C(C=CC=C2)N1CC3=CC(=CC=C3)[N+](O)=O	0.222439
NOOFIJSXSDSEBF	COC1=CC(O)=C(C=C1)C2=NOC(C)=C2C3=NC4=C(C=CC=C4)C=C3	0.227127
NOWWAJANJXDNIM	CN(CCCNC(=O)CSC1=CC(=O)N(C)C2=C1C=C(Cl)C=C2)CC3=CC=C	0.227526
NOYMGARZIVMHHD	CCN1C(=S)N=C(N2CCN(CC2)C(C3=CC=CC=C3)C4=CC=CC=C4)C(0.226482
NPAULTDWEBGYBH	CCCCOC1=CC=C(CN2CCN(CC)CC2)C=C1	0.259732
NPFJSHWFQCKVOT	FC1=C(C=CC=C1)C(N2CCN(CC3=CC=CC=C3)CC2)C4=NN=NN4C	0.240869
NPKXHGFROMICTD	[I-].CC[N+]=C(\C=C\C2=C\C(=C/C=C\2O)[N+](O)=O)/C=C\C3=	0.290346
NPLRQONUDJNTDV	COC1=C(OCC2=C(Cl)C=CC=C2Cl)C(Br)=CC(CNN3N=NN=C3N)=C	0.240794
NQAPTYPIVMULPE	CC1=C(\C=N\NC2=C3C=CC(Cl)=CC3=NC=C2)C=CC=C1	0.231179
NQLJNUIURVHLKPA	CCN(CC1CCN(CCC2=CC(F)=CC=C2)C1)CC3=CC=C(O)C=C3	0.245332
NQTKVLVVQBKXOK	CCOC(=O)C1=CC=C(C=C1)N=C(S)N(CCCN2CCCC(C)C2)CC3=CC=C	0.260099
NQUWDWKVYGPVAA	COC1=CC=C(C=C1)C(N2CCC(C)CC2)C3=NN=NN3C4CCCC4	0.241849
NQVKNMMSJMBTSN	CCN1C2=C(C=C(Cl)C=C2)C3=C1N=C4C=CC=CC4=N3	0.231015
NRAHRUHGPGBWSI	N1C=CC(=N1)C2=CN=C(S2)C3=CC=CC=C3	0.226261
NRIBYXIOCGUVEW	CCC1=NC(SCC2=CC=C(OC(C)C)C=C2)=NN1	0.227726
NRTOUGPMXLJETQ	COC1=CC(=CC(OC)=C1O)C2=CC(OC)=C(O)C(OC)=C2	0.251874
NRXCJQXKEIOFHO	COC(=O)C1=CC=C(CSC(N)=N)O1	0.264993
NTDIRJAXHHBYGY	CC1=CC(NC(=O)COC2=COC(CN3CCC4=C(C3)C=CC=C4)=CC2=O):	0.225776
NTRYPVBJLOOHU	CCN1CCN(CC1)C(C(C)NS(=O)(=O)C2=CC=C(Br)C=C2)C3=CC=CC=C3	0.235383
NUDBAUWWKREJBT	ClC1=CC=C(CN2C3=NCCCN3C4=C2C=CC=C4)C=C1	0.248707
NUFCKOACLZMZR	CC1=CC=C(CSCC2=NC3=C(N2)C=CC=C3)C=C1	0.229795
NUFNKYNBZYIQDG	CCC1=C(C(N)=NC(N)=N1)C2=CC(=C(C=C2)N(C)CC3=CC=CC=C3)[0.244423
NUYMLBCETWIHJM	C[N]1C=C(CN2CCC3=CC=CC=C3C2)C4=CC=CC=C14	0.22958
NVJHCEJHMDWDFNV	CN(C)C(CNC1=NC=C(C=C1)C(F)(F)F)C2=CC=CC=C2	0.22731
NWDMYZDYCGOYAZ	CCOC1=C(\C=N\N2CCCCC2)C=CC=C1	0.256487

NWFHWIJRCYRLGB	CC1=CC(C)=NC(N\N=C\C2=C(OCC3=CC=CC=C3)C=CC=C2)=N1	0.240984
NWSJIQYNDOWTDK	COC1=C(C=CC=C1)N2CCN(CC3=C(Br)C=C4OCCOC4=C3)CC2	0.248846
NWVBMKUDSFGYDY	C1CCN(C1)C2=NC=NC3=C2C(=CS3)C4COC5=C(O4)C=CC=C5	0.246918
NWVGHEMPUOSLMU	CC1=CC(N=C(S)N\N=C2/CCCCC3=C2C=CC=C3)=C(C)C=C1	0.232984
NXHUITDSVPREHK	CCOC1=CC2=C(NC(=O)C(CN(CC3=CC=CS3)CC4=NN=NN4C(C)(C)	0.230964
NYAWOVVANLFBCL	CC1=C(C=CO1)C(=O)NC2CCCN(CC3=CC=C(Cl)C=C3)C2	0.228514
NYFOZLVGZIFOIG	COC1=C(OC)C=C(CC2=NC3=C(O2)C=C(C=C3)C(=O)N4CCN(C)C(C	0.233072
NYKHZQZVEDDAKR	COC1=C(OC)C=C(CCN2=NC(=NC(=N2)N3CCCCC3)N4CCCCC4)(0.253609
NYRBOWGJJQEQOK	COC1=C(C=CC=C1)N2CCN(CC(O)COC3=CC4=C(OCO4)C=C3)CC2	0.223953
NYWREHRGJLDICR	COC1=C(COC2=CC=C(F)C=C2)C=C(C=C1)C3NCCC4=C3NC5=C4C	0.226179
NYXUKPHUZOEPNR	CN1CCN(CC1)C(=O)COC2=CC=C(C=C2)C3=NC4=CC=CC=C4S3	0.226416
NZBRDGAGPLPQPH	CCN(CC1=CC=CC=C1)C2=CC=C(C=N\NC(S)=NC(C)C)C=C2	0.265238
NZH0HWSINPTXPQ	COC1=CC=C(CN2N=NN=C2C(C(C)C)N3CCN(CC3)C4=C(OC)C=CC	0.244259
NZIGRAASRJILNH	COC1=C(OC)C=C2CN(CC(=O)NC3=C(Cl)C=C(Cl)C=C3)CCC2=C1	0.227193
NZJWCUHISVYEOK	CC1=CC=CC(NC(=O)C2=NC=C(C=C2)C(=O)NC3=CC=CC(C)=C3)=C	0.241218
NZZYIRXZGXNWJR	CCOC(=O)C2(CC1=CC(OC)=CC=C1)CCN(CC3=C(OC)C(OC)=CC=C3	0.290667
OAHORWXWNJJTCJ	OC(COC1=CC=CC=C1)CN=C2SC3=C(C=CC=C3)N2CC(O)COC4=C(C	0.22637
OAKVQEUFBQIFTE	CC(C)NC1=NC(=NC(NC(C)C)=N1)N(CCOC2=C(Cl)C=C(Cl)C=C2)C#	0.229525
OAPPEBNXKAKQGS	C1=CC2=C(C=C1)N=C3C(C=CC4=C3C=CC=C4)=C2	0.235269
OASVHPVKKHWSHO	FC1=CC=C(C=C1)C(=O)N=C(S)NC2CCN(CC3=CC=CC=C3)CC2	0.23711
OBAOVVRDVKOEAF	C\C(CCN1CC1)=N/NC(=O)NC2=C3C=CC=CC3=CC=C2	0.236051
OBHKLQMTGZZBU	COC1=C(OCC(=O)NC2=CC(=CC=C2)C(F)(F)F)C=CC(=C1)C(=O)NCC	0.292299
OBOZOKPRZDQAO	OC(CN1CCCC1)CN(C2=CC=CC=C2)C3=CC=CC=C3	0.238781
OBUAGBRWSIDKKW	CC1=CC=C(SCCCCN2CCNCC2)C=C1	0.224527
OCAUAABUWCCDBI	COC1=CC=C(NS(=O)(=O)C2=C(C=CC(NC(=O)C3CC3)=C2)N4CCCC	0.232637
OCCMEOCLGLVGC	COC1=C(NC2=NC=NC3=C2C(C)=C(C)N3CCCN(C)C)C=CC=C1	0.250954
OCMRFULKMXDHL	CS(=O)(=O)NC1=C(C=CC=C1)C(=O)NC2=CC(Cl)=CC(Cl)=C2	0.225392
OCPNFFSUIXBUEH	COC1=CC=C(NC(=O)C2=CC=C(C=C2)C3=CSC(C)=N3)C=C1	0.227245
OCRQTOAPOJRQHU	CN1C=C([C@H]2C[C@H]3CN(CC4=CC(Cl)=CC=C4)C(=O)[C@H]	0.240621
ODDAUEGZSNPDPQ	CCOC1=C(CN2CCN(CC3=CC4=C(OC3)C=CC(OC)=C4)CC2CCO)C=	0.226218
ODNPRNWBYSQJGS	CCCCCCCC1CC(CSC(N)=N)OC1=O	0.229392
ODXKOGOMZIMVSZ	COC1=CC=C(C=C1)C2=C(C3=C(S2)C=C(OC)C=C3)C4=CC=C(OCC1	0.240236
OEKJPBBWZWSQCJ	CC1=CC(NC2=NC(=CS2)C3=CN=CC=C3)=C(C)C=C1	0.223616
OESIOUJUQWGFHC	CC1=NC(NC2=NC(=CS2)C3=CC=C(F)C=C3)=CC=C1	0.239959
OEVWPQYNFDZFUL	CC1=CC=CC(C)=C1OCC(O)CN(CC2=C(O)C=CC=C2)C3CCCCC3	0.239052
OFRYUDPPDRCHBQ	FC1=C(F)C=C(C=C1)C2=CSC(NC(=O)CN3CCCCC3)=N2	0.237626
OFYMUOTCCXAHG	CC(C)N1CCC(CC1)N2CCN(CCCC3=CC=CC=C3)CC2CCO	0.274477
OGEGHNXZKVBMSM	CC1=CC(=NC(=N1)C2=CC=CC=C2)N3CCN(CC3)C4=CC=CC=C4	0.241954
OGMPHYQPNSUBSE	CC1=CC(C)=C(NC(=O)NCC2CCN(CC3=C(Cl)C=CC(C)=C3)CC2)C=C	0.241376
OGSIYSLYFZJQBT	CCOC(=O)C1=C(CN2CCN(CC2)C3=CC=C(F)C=C3)NC(=O)NC1C4=	0.232166
OHDXDNUPVVYWOV	CNCC1=C(SC2=C3C=CC=CC3=CC=C2)C=CC=C1	0.313421
OHRHJQXHIWOGAW	CN(C)CCCN1C(C)=C(C)C2=C1N=CN=C2NC3CCCCC3	0.223176
OHUNCUXJHFATEQ	CC1=CC(C)=C(NC(=NOCC2=C(Cl)C=C(Cl)C=C2)C3=NON=C3N)C=	0.223306
OILQRYVUKMDUKO	CN1CCN(CC1)C2=CC=C(NC(=O)COC3=C(Cl)C=C(Cl)C=C3)C=C2	0.240558
OIPUPAUENHDVRT	CCN(CC)C1=CC=C(CNC2=NC3=C(C=CC=C3)N2C(C)C)C=C1	0.228222
OIRSXCBBXUDET	CN1C=C(CCNCC2=CN=C2C3=CC=C(C=C3)C4=CC=CC=C4)C=N1	0.284319
OJMFUZETINIEJ	COC1=CC=C(CN2N=NN=C2CN(CC3=CC4=CC=CC(C)=C4NC3=O)(0.227338
OJNBWCGDUWDYIZ	COC1=CC(CN2CCN(CC3=CC=CC(OC)=C3OC)CC2)=CC(OC)=C1OC	0.232664

OJXKQCJWSXNCLH	CCOC(=O)C2(CC1=CC(OC)=CC=C1)CCN(CC3=C(OC)C=CC(OC)=C3	0.279937
OKDGOSIKJZJDTQ	BrC1=CC(=CC=C1)C(=O)NC2=CC=C(CN3CCCC3)C=C2	0.281595
OKDKHOBVYMXHNMN	CC1=CC=C(NC(C(=O)C2=CC=CC=C2)C3=CC=CC=C3)C=C1	0.228374
OKVQPIRTVQSAKV	COC1=CC=C(C=C1)C(N2CCN(CC2)C3=CC=CC=C3)C4=NN=N[N]4	0.261568
OKXJVJAKOAJGBF	CC1CN(CCOC2=C(Br)C=C(C)C=C2)CC(C)O1	0.239593
OLDOPIUASGGWJD	CC1=C(OC2=CC=CC=C2)C(=NN1)C3=C(O)C(C)=C(OCC4=CN(N=C	0.227115
OLIMZMGPCNLWIN	CC1=CC(C)=C(C=C1)\N=C(/S)\N=C\C2=C(Cl)C=CC=C2Cl	0.233239
OLRQEYHHPDXGTO	C1CCN(CC1)C2=NC3=C(C=CC=C3)C(=N2)C4=CC=CC=C4	0.234198
OMCKFLDQQYNNMS	ClC1=CC=C(CN\2C3=CC=CC=C3N4CC/N=C24)C=C1Cl	0.247929
OMFXLHYTWYKQQR	CCN(C(C)C)C1=CC=C(NC(=O)C2=CC=C(C=C2)N3CCCC3=O)C=C1	0.230672
OMSSNTRYIIEBGA	COC1=C(Br)C=C(C=C1)C2=CSC(C)=N2	0.232855
ONDBOJRMDBRDNH	CC1=CC=C(C=C1)C(N2CCSCC2)C3=NN=NN3CCC4=CC=CC=C4	0.257184
ONMJCLPUHLOIPE	NC(=NOC(=O)C1=C(Cl)C=C(Cl)C=C1)C2=CC=C(Cl)C=C2	0.234693
ONNMQUCZUHOJPE	CC\C(=C/C1=CC=C(C=C1)N(C)C)C2=CC=NC=C2	0.239138
ONQRAYLUTWMTGL	COC1=NC(=NC(=N1)N(C2=CC=CC=C2)C3=CC=CC=C3)N4C=CN(0.247572
ONTKMNGLPHNQMU	ClC1=CC=C(C=C1)C(=O)N2CCC(CC2)C(=O)NC3=C(C=CC=C3)N4C	0.246384
OODCZOSKGSOHOM	COC1=C(C=CC=C1)N2C(=O)C3=CC=C(Cl)C4=CC=CC(C2=O)=C34	0.227704
OOKVIAGCVJKVCS	CN(CCCCCN(C)CC1=C(O)C=CC=C1)CC2=C(O)C=CC=C2	0.249758
OOORMPLAZXXCBH	OC(COC1=CC=C(C=C1)C\2CC\C=C2)CN3CCCC3	0.23344
OOPQTTTHZIVMBFO	CCCN1C(CC)=NC(=C1S(=O)(=O)C2=CC=CC=C2)[N+](O)=O	0.228262
OOYDGWVHUBKVBPQ	CN1CCN(CC1)C(=O)C2=CC=C3C=CC=CC3=C2	0.239192
OPAGGJQWNIEXLG	CC1=CC=C(C=C1)C2=NN=C3SCC(=NN23)C4=C(Br)C=CC=C4	0.2245
OQAWLIMCQATBNU	ClC1=CC=C(OCC2=NN=C(SCCN3CCCC3)N2CC4=CC=CO4)C=C1	0.241346
OQILUCZKMMCJSH	CCOC(=O)C1CCCN(CC(=O)NC2=NC(=CS2)C3=CC=CC=C3)C1	0.227469
OQPYPSPSGERKU	ClC1=CC=C(C=C1)C2=NOC(=N2)CN3CCCC3	0.264712
OQRDOWLIUBNBSG	CN(C)CCN1=NC(CSC2=CC=CC=C2)=NC3=C1C(C)=C(C)S3	0.234478
ORAARQDOHVSIAU	FC1=CC(=CC=C1)C(=O)NC2=C(C=CC=C2)N3CCN(CC3)C4=CC=CC	0.237226
ORPXTNFWZCYREN	CCN(CC)C1=CC=C(C=C1)C(=O)[N]2C=NC3=CC=CC=C23	0.228426
ORRBRQWJGYRRF	[O-][N+](=O)C1=CC(NC2=NC(OCC#C)=NC(OCC#C)=N2)=CC=C1	0.22958
OSSDAJIOWFKNQ	COC1=CC=C(C=C1)C2=NN3C(S2)=NN=C3C4=CC=C(F)C=C4	0.266293
OSFHFLPITLKMLA	CC1=CC=C(CN2N=C(N=C2C3=CC=CC=C3)C4=CC=CC=C4)C=C1	0.233843
OSTARNDTDVKCCZ	ClC1=CC(=CC=C1)N2CCN(CC2)C(=O)C3=CC=C(CS(=O)CC4=C(Cl)	0.22971
OSUVDSBKOMZSNS	CCN(CC)CCOC1=CC(Cl)=C(Cl)C=C1	0.278416
OSUYXBHXTKKQEJ	OC1=C2N=CC=CC2=C(CN3CCC(CC4=CC=CC=C4)CC3)C=C1	0.225033
OTBQDOKDJFEZPM	C1CN=C(NC2=CC3=C(CCCC3)C=C2)O1	0.293452
OTFKDWIYZMRZMS	CCOC1=CC=C(C=C1)O)C2=C(C=N[NH]2)C3=CC=C(OC)C(=C3)OC	0.224468
OUNDFXNOOKXWCF	CNC1=C(N=C(O)C2=CC=C(C)C=C2)P(=O)(C3=CC=CC=C3)C4=CC	0.224935
OUTSTXGLOZDZJL	COC1=C(OC)C=C(C=C1)N=C(S)N2CCN(CC2)C(C3=CC=CC=C3)C4=	0.235942
OUMEFUOUGFYFY	CC1=C(C)C(NP(=O)(OC2=C(F)C=CC=C2)OC3=C(F)C=CC=C3)=CC=	0.248213
OZVVRXOLAXSU	CCCOP(=O)(C(O)C1=C(Cl)C=C(Cl)C=C1)C2=CC=C(C=C2)N(C)C	0.229196
OVAKAUBQMKPERV	CC1=CC(OCCCCN2C=CN=C2)=CC(C)=C1Cl	0.237724
OVCZPKQZQWRAGV	COC1=CC=C(CN2N=NN=C2C(N3CCN(CC3)C4=CC=CC=C4)C5=C(0.240429
OVHRPJNENURSDV	CCOC(=O)C2(CC1=CC=CC=C1C(F)(F)F)CCN(CC2)C3CCN(CC3)C(C	0.254699
OVOUZRZKLVFYQV	FC1=C(OCCNC(=O)C2=CC(=CC=C2)S(=O)(=O)N3CCN(CC3)C4=CC	0.226255
OVQYKMPGGSKZPK	CCCCOC1=CC(=CC=C1)C(=O)NC2=CC=C(NC(=O)C3=CC=CS3)C=C	0.229504
OVUNTSIMUSJINY	C1CCCN(CC1)\N=C\C2=NC3=C(C=CC=C3)C=C2	0.240621
OVZUSWLKWNSJOD	COC1=CC(=CC(OC)=C1OC)C2=CC(C(=O)NC3=CC(OC)=C(OC)C=C3	0.236501
OWDTUONCXUNSSA	CC(NCCCCOC1=C2C=CC=CC2=CC=C1)C3=CC=CC=C3	0.226735

OXDABQBVHMGPKN	COC1=CC(NC(=O)CCOC2=CC(C)=CC=C2)=C(OC)C=C1	0.229476
OXIUUAPQNJSCOB	COC1=C(OC)C=C(C=C1)C2=NOC(CSC3=NN=C(CC4=CC=CC=C4)N	0.237593
OXQLTPGYKFBPHQ	CN(C)C1=C(N=C(O1)C2=C(Br)C=CC=C2)S(=O)(=O)C3=CC=C(C)C=	0.233101
OYBNZMLVTNWHAG	FC1=CC=C2[N](N=NC2=C1)C3CCN(CC3)CC(=O)NC4=CC=C5CCC	0.23317
OYBUCLJKIOAAADI	CCNC(S)=N\N=C(/C)C1=CC(=CC=C1)[N+][[O-]]=O	0.228858
OZEPKGBSALEXRT	CC1=NC(=CN2C1=NC3=C2C=CC=C3)C4=CC=CC=C4	0.237274
OZQHJTWIGIWIJC	COC1=C(C=CC=C1)\N=C(/S)N(CCN2CCCCC2)CC3=CC=CS3	0.257128
OZUGAJOHMPMGBEQ	ClC1=CC2=C(NC(=N2)C3CCN(CC4=CC=CC=C4)CC3)C=C1	0.294061
OZZZNNWJPKCYDI	COC1=CC(=CC(=C1OC)OC)CN2CCN(CC2)C3=CC=CC(=C3)Cl	0.257203
PATQZWQCQOLOBF	CC(C)(C)C1=C(OCCOCCN2CCCCC2)C=CC=C1	0.236394
PAVUUPCGSDKDRN	FC1=C(F)C=C(CN2CCN3CCCC3C2C4CCCC4)C=C1	0.264503
PBEQKEQBBDWRC	CCOC1=CC=C(NC2=C3C=C(C)C=CC3=NC(C)=C2)C=C1	0.233993
PBIHNXAJBLOCMX	CC1=C(C=C(Cl)C=C1)\N=C(/S)NCCCSC2CCCC2	0.22333
PCJPGFSVSHLPA	CCOC1=CC=C(C=C1)S(=O)(=O)NC2=CC=CC(=C2)C(=O)NCC3(CCC	0.223952
PCKQHEDPQDBDDQ	ClC1=CC(=CC=C1)C2=NC3=C(C=CC=C3)C(=C2)C(=O)NC4=NC=C(0.231884
PCPKYJIEWIMBSR	COC1=CC2=C(SC=C2C3=CC=C(OCCN4CCCC4)C=C3)C5=CC=CC(0.264106
PCTVRHUKEDNDHW	CCOC1=NC=CC=C1C(=O)OCC2=CC=C(C=C2)C(=O)OC	0.225854
PCUNCOIBDCFEGQ	COC1=C(C=CC=C1)N2CCN(CC2)C(=O)C3=CC(=C(Cl)C=C3)S(=O)(=	0.223463
PDCTWJVTWDDQFM	CCN1C=CN=C1CN2CCC3=C(NC4=C3C=CC=C4)C2C(C)(C)C	0.229822
PDIBOQMOKOEPCF	COC1=CC=C(C=C1)C2=NOC(=N2)C3=CC=C(C)C=C3	0.224321
PDIPALLOXOFUBU	NC(CC1=CC=C(Cl)C=C1)=NOC(=O)C2=C3C=CC=CC3=CC=C2	0.224989
PDIQWISRAALROZ	COC1=CC=CC(CNCC2=CC(Br)=C(OC)C=C2)=C1OC	0.250639
PDMCEANFOLKQBG	CCOC1=CC=C(NS(=O)(=O)C2=CC(=CC=C2)C(=O)N3CCN(C\C=C\C	0.222877
PDMZJRHSPLGFQQ	FC1=CC=C(COC2=CC(CNCC3=CC=NC=C3)=CC=C2)C=C1	0.278316
PDSHNUNLUUHOES	CC1=CC(=C(C)S1)C2=NN(C=C2CN3CCCC(CO)C3)C4=C(F)C=CC=C	0.233648
PEDXFVUGTVCQDZ	COC1=C(CN2CCN(CC2)C3=NC=CC=N3)C=C(Br)C=C1	0.245896
PEJZJCVAZAFKKV	COC1=C(CN(C)C(=O)C2=C3C=CC=CC3=NC(=C2)C4=CC=CS4)C=C	0.234301
PENRCLWAKGETBX	CN(C)CCCN(C(=O)C1=CC=CO1)C2=NC3=C(S2)C=C(Br)C=C3	0.229385
PEUNWKYKBOFBPY	COC1=C(Cl)C=C(C=C1)N=C(S)N(CCCN2CCCC2)CC3=CC=CN3CC4	0.225206
PFCHQLSWOQFFKU	ClC1=CC=C(C=C1)S(=O)(=O)CC2=C(Cl)C=C(Cl)C=C2	0.258638
PGAOLCBUVAGNHE	CN1N=C(C=C1NC(=O)NC2=CC(Cl)=CC(Cl)=C2)C(C)(C)C	0.229301
PGMDWBTVIQYXDF	CCOC1=CC=C(C=C1)S(=O)(=O)NC2=CC(=CC=C2)C(=O)NCC(N(C)C	0.249186
PGPBUCYUXBJKLD	CN(C1CCN(C)CC1)C2=C(N=C(O2)C3=C(Cl)C=CC=C3)S(=O)(=O)C4	0.258725
PHBUHYXWJRLCBG	COC1=CC(CNCC2=C3C=CC=CC3=C(OC)C=C2)=CC(OC)=C1OC	0.233489
PHTZFBVQTCNNBO	C1CCN(CC1)C2=C3NC4=CC=CC=C4C3=NC=N2	0.239697
PIEMAKWMQOKSEB	CN1CCN(CC1)C2=C/C=C\C=C\2NC(=O)C3=C/C=C(O\3)/C4=C/C=	0.340409
PIUWHSYGOKWZOL	CC(C)C1=CC(OCCOCCN2CCCC2)=C(C)C=C1	0.223059
PJELQLUIVZHAI	CC1=NOC(=C1)C2=CC(=C(C)C=C2)S(=O)(=O)NCCCNC3CCN(CC3)C	0.226087
PJSGJCDZKKZHRB	COC1=C(C)C=C(CN2CCC(CC2)N3N=CC=C3NC(=O)CCOC4=CC=C(0.231103
PKAIJGXARQUEAV	BrC1=CC=C(CC(=O)NC2CCN(CC3=CC=CC=C3)CC2)C=C1	0.245856
PKAQMEXZOQVWHP	CC1=CC=C(C=C1)C2=NN(C=C2\C=N\O)C3=CC=CC=C3	0.272725
PKCMIINJWNKUKY	ClC1=C(C=CC=C1)C2=NC(=C(NCCCNC3CCOCC3)O2)S(=O)(=O)C4=	0.260183
PKPWGSRONAQDSI	C\C=C1\SC(=NC1=O)N2CCCC2)C3=CC=C(Br)C=C3	0.228618
PKTJMZWZUHORSIX	CC1=C(C=CC=C1)N2CCN(CC3=CC4=C(OCO4)C=C3)CC2	0.230326
PKTVGZCDARFICO	COC1=CC=CC=C1NC(=O)CN2CCN(CC2)C3C4=CC=CC=C4C5=CC=	0.229744
PKUUIPIUCXLTDX	CC(NC1=N/C=N\C2=C1\C=C/S2)C3=C/C=C\C=C\3	0.395613
PLKWIFSIXRUXPJ	COC1=C(C=C(CSC(N)=N)C=C1)[N+][[O-]]=O	0.240144
PLNWQIRHGIFOMO	CC1=CC(C)=C(OCCNCC2=CC=CC=C2)C(C)=C1	0.224857

PLQJFNMUCXTPKU	CSC1=CC(=NC(=C1)C2=CC=NC=C2)C3=CC=C(Cl)C=C3	0.237375
PLXIPEBXLVKFAJ	ClC1=CC2=C(C=C1)C(=CC=N2)N3CCN(CC3)S(=O)(=O)C4=CC(Br)=	0.222526
PMAPOQYCXJXXVRO	COC1=C(OC)C=C(C=C1)\C=N\NC(=O)N\N=C\C2=CC(OC)=C(OC)C	0.255079
PMJFTDJHOQAWCY	CNCC1=C2C=CC=CC2=CC=C1OCC3=CC=CC=C3	0.328232
PMKGRFSNNPPKJU	ClC1=CC=C(C=C1)C(=O)C2CCN(CC2)CC(=O)NC3=CC=C4OCCOC4	0.22271
PMSTUHXQPKTZSE	CN(C1CCCC1)C(=O)C2=CC=C(C=C2)C3=CC=CC=C3	0.231331
PMYJRLDFFZDOBQ	COC1=C(OC(C)C)C(Cl)=CC(=C1)C(=O)NCC(N(C)C)C2=CC=CS2	0.222704
PNDZMKGAZPUNES	COC1=CC=C(CC2=NOC(=N2)C3=CC=C(OC)C(=C3)OC)C=C1OC	0.223703
PNEFFBLLDPIINJ	CN(C)CCN(C(=O)C1=COCCO1)C2=NC3=C(S2)C=C(Cl)C=C3	0.244315
PNKRIBLRABUUOP	CSC1=CC=C(CNC2=C3C=CC=CC3=CC=C2)C=C1	0.229768
PNSVMQCTQNBWKW	SC(NCC1=CC2=C(OCO2)C=C1)=NC3CCN(CC4=CC=CC=C4)CC3	0.252833
PNTYXZGREWTUFY	OC2(CSC1=CC=C(F)C=C1)CCN(CC2)S(=O)(=O)C3=CC=CC=C3	0.226009
PNUKEUIHMNPWLA	CC1=[N+]2C=C(C3=CC=CC=C3)C(=CC2=CC=C1)C4=CC=CC=C4	0.230616
PNWANAPQVIFWRQ	OC1=CC=C(C[C@H]2CNCCN2CC3(CC3)C4=CC=CC=C4)C=C1	0.227271
POCINPNNLOIUJL	CC1=CC=C(C[N]2N=NN=C2CN3CCC(CC3)[N]4N=NC5=CC(=CC=C	0.226796
PODKYEDAHNPAGP	CC1=CC(OCCNCC2=CC=CC=C2)=C(C)C(C)=C1	0.28459
POIOHLGVMZIVHW	CN1CC2=C(N=CC=C2)N(C)CC3=C1C=CC(Cl)=C3	0.277562
PPHZEVLBHZMQJA	CN1C(=O)\C(SC2=C/C=C\C=C1\2)C(=O)NCC3CCCO3)=C\C4=C\	0.291042
PPLAOTVRDZHLS	C\C(C1=CC=CC=C1)=N/OCO\N=C(/C)C2=CC=CC=C2	0.225625
PPSGNRXSOMBVDX	CC(C)NCCCCOC1=CC(Br)=CC=C1	0.254965
PPSVWVPMRLUHQD	CC1=CC=C(CN2CCN(CC2)\N=C\C3=CC(=C(Cl)C=C3)[N+][([O-])=O)	0.29611
PPVBXIWNUGYMPA	CC1=CC2=C(C=C1)N=C(C=C2C3=CC=CC=C3)C4=CC=NC=C4	0.232688
PPXSQWLNQKTBHD	ClC1=CC=C(C=C1)C2=NOC(CCCC(=O)NC3CCCC3)=N2	0.227032
PPYHEDHGZOLTTA	CN(C)S(=O)(=O)C1=C(C)C=CC(=C1)N=C(S)NC2CCCC2	0.229823
PQCZYLWTHDSHDF	COC1=CC=CC2=C1N=C(S2)N(C)C3=CC=CC=C3	0.252448
PQJZMXBWFCAZTB	CC1=NC2=C(C=CC=C2)N1CCOC3=CC=C(C)C=C3	0.249398
PQWNLDPZLWCBA	CSC1=CC(=CC=C1)N=C(S)N(CCCN2CCCC2)CC3=CC=CS3	0.315062
PRHAGQIVBZRUBO	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC=CS3)CC2	0.23111
PRJOGZWQBKIJAU	CC(=O)NC1=CC=C(NC(=O)C(=O)NCC(N2CCC3=C(C2)C=CC=C3)C4	0.224054
PRLFTRPRRKDIAZ	COC1=CC=C(C=C1)C(\C)=N\NC2=NC(=CC(C)=N2)C3=CC=CC=C3	0.252854
PRSDSEXRDGXJPO	CCOC(=O)C1=CN=C(N=C1NC2=CC=C(C=C2)N(C)C)[N]3N=C(C)C=	0.22863
PRSZSMVFSUELRT	CNC1=C(\C=N\N=C(N)S)N=CC=C1	0.285562
PSGHMUSVWHDVRN	BrC1=CC=C(C=C1)N2N=CC3=C(C=CC=C3)C2=O	0.228571
PSUWUZOXZUGHPC	CC1CC(C)CN(CCCNC(=O)C2=CSC3=C2CCCC3)C1	0.245284
PSVJMIZHURBTDI	BrC1=CC2=C(OC3=C(N=C2)C(=NC=N3)N4CCCC4)C=C1	0.243105
PTHSETRJGDLJGD	CC1=CC(=CC=C1)C2=NC(=C(C)O2)CN3CCCC(C3)C(=O)NC4CCCC	0.233857
PTJJHGMNKVNER	CCNC1=NC(=NC(SCC2=CC=CC=C2)=N1)N3CCOCC3	0.240423
PTLMVVWYWFMSMLQ	CC1CC(C)CN(CCCOC2=C(C=CC=C2)[N+][([O-])=O)C1	0.260801
PTOHLKZGNYWIPW	COC1=CC=C(\C=C\CN2CCC(CO)(CC3=C(Cl)C=CC=C3)CC2)C=C1	0.231944
PUVXHJNHJICBBO	CN1C(=N)N(CC(=O)C2=CC=C(Br)C=C2)C3=C1C=CC=C3	0.266849
PUVZZTMYSZJISL	COC1=CC2=C(C=C1)N(CCN(C)C)C3=C(S2)C=CC=C3	0.275927
PVTUMZHWOKQGQX	ClC1=C(C=CC=C1)C(=O)N\N=C\C2=CN(N=C2C3=CC=CC=C3)C4=	0.226089
PWCMZCSGGQBFY	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC=CN3C4=CN=CC=	0.264133
PWCZINXPDHUFKO	CN1CCC(CC1)NC(=O)CCCOC2=CC=C(Cl)C=C2C	0.227755
PWSLNADMFIPISL	COC1=C(Cl)C=C(NC(=O)COC2=C(C=CC=C2)C(=O)NCC(N(C)C)C3=	0.280091
PXDJSUVMLSUBMG	[O-][N+](=O)C1=C(C=C(C=C1)N2CCCC2)N3CCCC3	0.227272
PXIYBXVBWJIZLO	CC(C)CN(CC(C)C)CC(O)CN(C1=CC=CC=C1)S(=O)(=O)C2=C(C=CC=	0.256406
PXJLCUCNAHNABV	CC1=C(C)C(NC(=O)C2=CC=C(CN3CCC4=C(C3)C=CC=C4)C=C2)=C	0.264344

PXOMUSMGYFLSLS	CCCCC1=CC=C(NC2=NCCCS2)C=C1	0.268447
PXTKIYADTRPNT	O=C(CCN1C(=O)OC2=CC=CC=C12)N3CCN(CC3)C(C4=CC=CC=C4	0.237748
PYLSWXYTNI MYDR	CN1C2CCC1CC(C2)N(CCC3=CC=CC=C3)C(=O)C4=CC(C)=CC(C)=C	0.224263
PYTRMEMFWBKJEC	CN(CC1=C(O)C=CC(C)=C1)CC2=C(O)C=CC(C)=C2	0.272894
PZDKFVOFPGYELB	COC1=CC2=C(C=C1)C=C(C=C2)C(=O)NCC3=C(CN4CCCC4)C=CC=	0.261033
PZMVHWBTAAZMTQ	COC1=C(C=CC=C1)N2CCN(CCNC(=O)NC3=C(C)C(C)=CC=C3)CC2	0.255786
PZXFYCXNAXKKKR	CN1C(NN=O)=NC2=C1C=CC=C2	0.229482
QAGYGLBDCVOGB	CC1=NN(C(CI)=C1\C=N\NC2=NC3=C(S2)C=CC=C3)C4=C(CI)C=C	0.239183
QANPJOOBDBRKDL	COC1=C(O)C(Br)=CC(CN2CCN(CC2)C3=C(C)C(C)=CC=C3)=C1	0.226082
QAPZAHBJVOOYBD	CN1CCN(CCOCCOC2=C(CI)C=C(Br)C=C2)CC1	0.256438
QAZDTBLCRVKABV	COC1=C(CI)C=C(C=C1)N=C(S)N(CCN(C)C)C(C)C2=CC=CO2	0.244801
QBORKFJAKFLCW	CC1=NC2=C(C=CC=C2)N1CC3=C(Br)C=CC=C3	0.263688
QBWFMAFOUIMMOD	CN1CCN(CC1)C(=O)C2=CC=C(O2)C3=CC=C(Br)C=C3	0.234924
QBXWXWIHOCXUHG	BrC1=CC(\C=C\C(=O)NC2CCN(CC3=CC=CC=C3)CC2)=CC=C1	0.222572
QCCDASOPVJFNAY	CC1=CC(C)=C(C(C)=C1)S(=O)(=O)OC2=C(C=CC=C2)[N+][O-]=O	0.254152
QCKHVNJOGWFAMO	[O-][N+](=O)C1=CC(OCCCN2CCC(CC3=CC=CC=C3)CC2)=CC=C1	0.265287
QCLYSNBFAOOKB	ClCCN(CCCl)C1=CC=C(\C=N\C2=CN=C(S2)C#N)C=C1	0.242627
QCPYMEACPSNFNB	ClC1=CC2=C(C=C1)N=CC(C3=NN=NN3C4=CC=CC=C4)=C2C5=C	0.257747
QDUKGM PARKWDLS	CN(C)C1=CC=C(C=C1)C(=O)N2CCN(CC2)C3=C4C=CC=CC4=NC(=	0.24316
QDUMNIXEJNBCJ	CCC1=C2CSC(C)(C)CC2=C(C#N)C(=N1)N3CCNCC3	0.236271
QDWRYKRMAKJIGF	BrC1=CC=C(C=C1)S(=O)(=O)N2CCCC(C2)C(=O)N3CCN(CC4=CC=	0.241997
QDZYWFQEOAHJRB	CC1=CC(=CC(C)=C1)N=C(S)NCCSC2=CC=C(CI)C=C2	0.238286
QEPDEESHPAOVON	CCOC(=O)C2(CC1CC1)CCN(CC3=CN(C)C4=C3C=CC=C4)CC2	0.265582
QETWCIZJGMNCR	FC1=CC=C(NC2=NC(=NC(=N2)N3CCOCC3)N4CCOCC4)C=C1	0.269651
QEUVQEMDXMIDPV	CNCCCOC1=C(OC)C=C(C=C1)\C=C\C	0.233073
QEYKVSJFGFOGHF	COC1=C(OC)C=C2CN(CCC(C)C3=CC=C(CI)C=C3)CCC2=C1	0.30947
QFBNXUJMKJRPCR	COC1=C/C=C(\C=C\1)N2\N=C3/C(=C2/C)/C(C)=N\N=C\3N4CCC	0.310009
QFVKPTZTSNICRC	COC1=CC=C(CI)C2=C1N=C(S2)N(CCN(C)C)C(=O)C3=CC4=C(OCC	0.248867
QGDPUOFWKLLFOFY	ClC1=CC(NC(=O)NC2CCN(C2)C3CCCCC3)=CC=C1	0.247944
QGNJGCSZPBNCIE	BrC1=C(CN2CCC(CC3=CC=CC=C3)CC2)C=CC=C1	0.249672
QGSFDXOMOOGDSK	C1CN(CCN1C2=CC=CC=C2)C3=NC4=C(C=CC=C4)N=C3	0.228385
QGZRBSNMXGCSFE	CC1=NC=C(CCN2=CC3=C(C=CC=C3)C=C2)C=C1	0.248293
QHBDYLBWYSEIIL	CCC1=CC=C(C=C1)N=C(S)NC2CC3CCC(C2)N3CC4=CC=CO4	0.283643
QHIVLRLOQJFRMW	ClC1=CC=C(OCC2=CC=C(C=C2)C(=O)NCC(N3CCCCC3)C4=CC=C	0.239362
QHSODUVKFCSEIW	NC(CCS(=O)(=O)C1=CC=C(CI)C=C1)=NOC(=O)C2=C(C=CC=C2)C(F	0.226734
QHZVNNJHHNXPY	S=C1SCN(CC2=CC=CO2)CN1CC3=CC=CO3	0.233732
QITKCQWRUKVTKJ	NC(N)=N\N=C\C1=CC(CI)=C(CI)C=C1	0.267985
QITXFIQUENDJAS	COC1=C(C=CC=C1)C(N2CCN(CC2)C3=CC=CC=C3)C4=NN=NN4C	0.256416
QJECGTSVNHFPFB	CN(CC(=O)NC1=C(C)C=CC=C1C)C(=O)C2=CC(=CC=C2)S(=O)(=O)N	0.222649
QJXHHRVPXGGQDG	C(CN1CCN(CC1)C(C2=CC=CC=C2)C3=CC=CC=C3)OC4=CC=CC=C	0.282191
QJZHQABIAZLOIL	CCN1CCC2=C(C#N)C(=NC(=C2C1)N3CCOCC3)N4CCCCC4	0.228215
QKBMJXWTFKVSCO	CCOC1=CC=C(C=C1)C2=CC(CCCC(=O)NC3=C(OC)C=CC(OC)=C3)-	0.229848
QKCWWARXJOJFKM	COC1=CC=C(NS(=O)(=O)C2=C3C=CC=CC3=CC=C2)C=C1	0.229362
QKGONMGEFYJKEZ	CN1CCN(CC1)C2=NC(=CC(=N2)C3=CC=CS3)C(F)(F)F	0.239952
QKYKQQMTTWZNNG	CN1C=C(CN2CCCC(C2)C(=O)C3=CC=C(C=C3)C4=CC=CC=C4)C(C	0.256473
QLIPLXZIEDFREV	CC(=O)N1CCN(CC(=O)NC2=C(SC3=CC=CC=C3)C=CC=C2)CC1	0.237003
QLPICJMQRAXDA	CCN(CC1=CC=CC=C1)C(C2=CC=CS2)C3=NN=NN3C4CCCCC4	0.234776
QLYRCNUDUMNWH	FC1=CC=C(CN2N=NN=C2C(N3CCCCC3)C4=CC=CS4)C=C1	0.244468

QMOMYIRVYSPAKB	CCOC(=O)C2(CC1CCCCO1)CCN(CC3=C(F)C=C(OC)C=C3)CC2	0.232468
QMSBNHQGBWJGQW	CC1=NN(C=C1)C(=O)NCCCN2CCN(CC2)C3=C(C)C=CC(Cl)=C3)C	0.225584
QNEQAAAVYIGQLU	CC1CCN(CC1)C2=CC(=NC(=N2)[N]3N=C(C)C=C3C)C	0.223019
QNLXJYQUWCNYBH	OC1(CCNCC1)C2=CC=C(Br)C=C2	0.254874
QNWITCFETJUORD	COC1=CC(NC2=C(C=NC=C2[N+][[O-]]=O)[N+][[O-]]=O)=CC=C1	0.245412
QNYXZWCJSLPQKO	COC1=CC(OC)=C(NC(=O)C2=C3C=CC=CC3=NC(=C2)C4=CC(OC)=	0.25241
QNZUKQBTSDHTBA	ClC1=CC=C(CN/2\C=C/C(=N)/C=C2)C=C1Cl	0.243338
QOKAIPLCDPHDIW	CC(C)C1=CC=C(C)C=C1OCC(=O)NC2=CC=CC=C2N3CCN(C)CC3	0.253497
QOTBRBTZSQDUQQ	COC1=CC=C(C=C1OC)C2=NOC(=N2)CN(C)[S+][[O-]](=O)C3=CC=C	0.232522
QPDWOBVCJVJMBU	CNC1=NC(C)=CC(C)=C1S(=O)(=O)C2=CC=C(C)C=C2	0.231738
QPFMMJLXNBJTPA	COC1=CC(OC)=C(C=C1)C(=O)O\N=C(/N)C2=CC=CC=C2	0.260934
QPKQHAOORMNUQW	CSC1=C(OCC2=CC(=NO2)C(=O)N3CCN(C)C(C3)C4=CC=CC=C4)C	0.230589
QQIUJXHQZFWLHK	CC(C)CC1=CC=C(C=C1)C(C)C(N)=NC2=CC=C(O)C=C2	0.278475
QQWPAAYLSWYFAO	CC(C)C1=C(C=CC=C1)\N=C(/S)NC2CCN(CC3=CC=CC=C3)CC2	0.275865
QRCNADYEMNSBRW	CN(CC(=O)NC1=CC=C(Cl)C=C1)CC(=O)NC2=CC(=CC=C2C#N)Cl	0.230312
QRHJAHSNXTXASJS	ClCCN(CCCl)C1=CC=C(\C=N\NC2=NC=CC=N2)C=C1	0.258981
QRKFYUKUGTZALL	[O-][N+](=O)C1=C(Cl)C=CC(=C1)S(=O)(=O)NCCCN2CCOCC2	0.222454
QRKLUICYAXZGJB	FC1=C(C=CC=C1)N2CCN(CC2)C3=NC=NC4=NNC=C34	0.239918
QRPGGRCHUPLCMK	ClCCN(CCCl)C1=CC=C(C=C1)N2C=NC3=C2N=CN=C3Cl	0.23471
QRVMQIUAEISBOS	COC1=CC=C(C=C1)N2CCN(CC3=NC(NC4=CC(Cl)=C(C)C=C4)=NC	0.222594
QRWBTPGKKOIKO	COC1=C(OC)C(CN(C)CC(=O)NC2=C(C=CC=C2)C(=O)NC3=CC=CC=	0.266088
QSARQDDLCZSVDS	COC1=C(OCC(O)CN2C(=N)N(CC3=CC=CC=C3)C4=C2C=CC=C4)C	0.23538
QTCAKMPBKAQAHZ	COC1=CC(NS(=O)(=O)C2=C(C)C(C)=C(OC)C=C2)=C(OC)C=C1Cl	0.228304
QTDWKLWXZCNFZ	CC1=CC(=C(O)C(CN2CCN(CCC#N)CC2)=C1)C3(C)CCCC3	0.225332
QTHXJXNQUMVBAG	CCCN(CC(=O)NC(=O)NC1CCCC1)CC(=O)NC2=C(Cl)C=CC(Cl)=C2	0.232627
QTKRXJOKZCYAGZ	N\C(S)=N/N=C/C1=C(OCC2=CC=CC=C2)C=CC=C1	0.225929
QTRQJBWCSNJCAU	CC1CCC\C(C1)=N\NC2=NC3=C(C=CC=C3)C=C2	0.223792
QTUKEQREUWREAO	FC1=C(NC2=NN=C(CS2)C3=CC=CC=C3)C=CC=C1	0.228594
QUDDHHSLEAGDEC	CC1=C(NC(NCCCN2CC2)=NC3=C(C)C=CC=C3)C=CC=C1	0.344403
QUMWLIWTPWCOOQ	SC(NCCN1CCOCC1)=NC2=CC=CC(=C2)S(=O)(=O)NC3=CC=C(Br)C	0.235447
QURJSJMDOQGACP	CCOC1=CC=C2N=C(O)C(=CC2=C1)CN(CC3=CC=CS3)CC4=NN=N	0.24063
QUZTWGZXAYXRIU	N\C(CC1=CC=C(C=C1)[N+][[O-]]=O)=N/OC(=O)C2=C(Br)C=CC=C2	0.225117
QVMYGMWIMBAYRRL	CN(C)CCOC(C1CCCC1)C2=C(C)C=CC=C2	0.297695
QVVQWIYNZZPAJX	C[N+][[O-]]=CC1=CC(OCCN2CCN(CC2)C3=C(Cl)C=C(C=N3)C(F)(F	0.233362
QWBIZNDBLRAIKV	CC1(C)CC2CC(C)(CN2C3=NC=NC4=CC=CC=C34)C1	0.228189
QWLZUXANZYJJ	CC1CC(C)CN(CC(=O)NC(C2=CC=CC=C2)C3=CC=CC=C3)C1	0.228138
QXFGNIAWGPBCAC	CN(CC(O)COC1=CC2=C(C=CC=C2)C=C1)CC3=CC=C(C)C=C3	0.252483
QXJSNVAFIUZCMX	ClC1=CC=CC=C1N2CCN(CC2)C(=O)CCN3C(=O)OC4=CC=CC=C34	0.226868
QXOSABCPDHNIAL	CC1=CC=C(C=C1)C2=NC(=NO2)C3=CC=CC=C3	0.23376
QXUGQXHZIXSGKU	CS(=O)(=O)C1=C(C#N)C(=CC(=N1)C2=CC=C(Br)C=C2)C3=CC=CC=	0.239663
QYAFVXAGTSETMW	COC1=CC(CC=C)=C(OCCN(C)CC2=CC=CC=C2)C=C1	0.243584
QYPSFPTUCHKUAX	CCN(CC1=CC=CC=C1)C2=CC=C(\C=N\N=C(/S)NCC=C)C=C2	0.222488
QYRFUAMRNAKEET	N(\N=C\C1=CN=CC=C1)C2=NC(=CC(=N2)C3=CC=CC=C3)C4=CC=	0.225894
QYRGRUQZJHZIFZ	CC1=C(\C=N\N=C(/N)C2=NC=CN=C2)C=CC(=C1)N(CCCl)CCl	0.253997
QYSUKZQLGIRKGW	CC(C)C1=C(OCCN2CCC3=C(C2)C=CC=C3)C=C(C)C=C1	0.229653
QZFRAGYQZYNTFT	ClC1=CN=C(NC(=O)NCC2CCCC(CNC(=O)NC3=NC=C(Cl)C=C3)C2	0.260945
RAAMDBRJYZVAQD	CN1C(CCN2CCN(C)CC2)=NC3 InterBioScreen,STOCK5S-49612	0.241497
RAERZXDPSRTSKL	COC(=O)C1=CN(CC2=CC=C(OC Chem Div, K813-0031, NSC-261	0.229548

RAESDTULQDNSBP	FC1=C(C=CC=C1)N2CCN(CC2)C(CNC(=O)COC3=CC=CC=C3)C4=C	0.25055
RAOGOTKLNJUKFF	CCN(CC)CCCNC(=O)C1=NOC(=C1)C2=CC=CC(=C2)Cl	0.286737
RBIMEIXDDYSEGP	CSC1=CC=C(CN2CCN(CC2)C(=O)C3=CC=C(C=C3)[N+](=[O-])=O)C=	0.227878
RCBSDKHPNVVQHC	NN1C(CC2=C3C=CC=CC3=CC=C2)=NN=C1SCCOC4=CC=C(F)C=C	0.243612
RCCWZWLILTAEV	FC(F)(F)C1=CC(CN2CCSCC2)=CC=C1	0.230851
RCPSBCNJFQYDLM	CC(C)C1=C(OCCCN2CCC3=C(C2)C=CC=C3)C=C(C)C=C1	0.222405
RCXPUJWOBYOJJW	NC(N)=N\N=C\C1=CN(N=C1C2=CC=CS2)C3=CC=CC=C3	0.232438
RDBGRPXIQRPBJ	CC(C)(C)NCC(O)(C1=CC=C(Cl)C=C1)C2=CC=C(Cl)C=C2	0.261453
RDHDTXRBAUHQAD	CN(CC1=CN(C)N=C1C2=CC(Cl)=CC=C2)CC3=C(C)C=NC=C3	0.26704
RDMDBLYGUNAKBH	ClCCN(CCCl)C1=CC=C(C=C1)C2=NCCC3=C2C=CC=C3	0.230053
REHRLWIZZMGLP	CN(C)C1=CC=C(C=C1)\N=N\C2=C(C=CC=C2)C(=O)OCC(=O)N(C)C	0.235514
REIKLHYZOGQSRQ	CN(C)CCNC(=O)C1=CC=CC2=C1N=C(N2)C3=CC=NC=C3	0.240144
RENAWGQIHCWXQF	FC1=CC=C(NC(=O)NC2=C(F)C=CC=C2)C=C1	0.231077
REVHAZQWZXMKQE	FC1=CC2=C(C=C1)C(CC3=C(S2)C=CC(Cl)=C3)N4CCN(CCC5OCCC	0.29474
RGBGXPAVLXGXON	ClC1=CC(Cl)=C(C=C1)C2=NC3=C(C=CC=C3)C(=C2)C(=O)NNC(=O)	0.227441
RGDNNHVBAWSEKK	COC1=CC=C(C=C1)C(CNC(=O)C2=CC(Br)=CC=C2)N3CCCC3	0.257483
RGFADXLNILIEQ	CC1=CC=C(\C=N\NC(=O)COC2=C(C=CC=C2)C3=CC=CC=C3)C=C1	0.223196
RGIJVFWDHXTTD	CCOC1=C(O)C(CN(C)CC2CCN(CCC3=CC=C(Cl)C=C3)C2)=CC=C1	0.278185
RGMAPPXLXVKJJH	COC1=CC=C(C=C1OC)C(N2CCN(CC2)C3=CC=C(F)C=C3)C4=NN=I	0.228113
RGUGPYBGFLDYN	CCOC(=O)C1=C(C)C=C(NC(=O)NC2=CC=C(Cl)C=C2)S1	0.230562
RHGRSYWNRCWBAO	ClC1=C(OC2=CC=C(C=C2)S(=O)(=O)NCCN3CCOCC3)C=CC=C1	0.244175
RHMCMTSHSSXER	FC1=CC=C(C=C1)N2CCN(CC2)C(=O)C3=CC=C(CN4CCC5=C(C4)C	0.240688
RHPYTLPXMYNISV	FC1=C(C=CC=C1)C(N2CCN(CC3=CC=CO3)CC2)C4=NN=NN4CC5	0.230674
RHTUQQMQAVBSGS	[O-][N+](=O)C1=C(NC(=O)CN2CCCCC2)C=CC(Br)=C1	0.225963
RICBSTFZGAJTFJ	FC1=C(\C=N\NC2=C(Cl)C=NC=C2Cl)C(Cl)=CC=C1	0.244707
RJHCGCBEVHOGBY	C1=CC=C(C=C1)C=2N=C(ON2)CSC3=NN=C(N3C4=CC=CC=C4)CC	0.248889
RJJINACFKMZQI	ClC1=CC2=C(SC(=N2)C3CCNCC3)C=C1	0.225809
RJQJUPDWOUTAH	C(CC1=C2C=CC=CC2=CC=C1)N3CCNC[C@@H]3CC4=CC=CC=C4	0.282706
RLECCWRYKOQKCK	CCOC1=CC(O)=C(C=C1)C2=NNC(C)=C2OC3=CC=C(OC)C=C3	0.227691
RLGJSJOPBCLECE	COC1=C(C=C2C=CC=CC2=C1)C(=O)NC3=NC=CC(C)=C3	0.236245
RLHCOHXXAVGTHB	CC(C)N(C1=CC=CC=C1)C2=CC=C(C=C2)N=C(S)NCCN(C)C	0.357731
RLHRDPKMXSPON	CN(C)CCOC1=CC=C(C=C1)C2=C(SC3=C2C=CC=C3)C4=CSC=C4	0.291268
RLJPEHJIOJINEG	CN(C)CCOC(C1=CC=C(C)C=C1)C2=CC(=CC=C2)C(F)(F)F	0.309864
RMFQIIXCTLNZRC	N(C1=NC(=NS1)C2=CC=CC=C2)C3=CC=CC=C3	0.243947
RMQVNBGPACWTMA	COC1=CC=C(C=C1)C(=O)NNC(S)=NC(=O)C2=CC=C(Cl)C=C2	0.239861
ROQMHVNDXNSVSQ	CC(C)C1=C(C=CC=C1)\N=C(/S)NC(C)C2=CC=CC=C2	0.228417
ROVVVYHPFBDPLO	CC1=CC=C(C=C1)C2=NOC(CCC(=O)NCCN3CCN(CC4=CC=CC=C4)	0.223711
RPACPATUCIVNSK	FC1=CC(=C(F)C=C1)C2=NN=C(NC3=C(F)C=CC=C3)SC2	0.251101
RPGZZXUOBIAJNE	CC1=NC2=CC=CC=C2C(=N1)SCCOC3=CC=C(C=C3)OC	0.236467
RPKPBLGOGRELES	CN1CCN(CCCN(CC2=CC=CS2)C(\S)=N\C3=CC(C)=C(C)C=C3)CC1	0.283744
RPOONTYLVSDHLY	COC1=C(OC)C(OC)=C(\C=N\N2C(SC)=NN=C2C3=CC=CC=C3)C=C	0.250711
RQAPLMHASVVSSW	CC1=NC(=CC(N\N=C\C2=CC(F)=CC=C2)=N1)N3CCOCC3	0.224611
RQDLEWXZDCLCRS	CCN(CC)CCNC(=O)C1=NN(C2=C1CCC3=C2C=CC(OC)=C3)C4=CC	0.256127
RQRCEVNKLAYFPF	CC1CCC\C(C1)=N\NC(=S)NC2: Vitas-M Laboratory,STK083070	0.223774
RRMSMKQFFNOZRL	NC(=O)CCN1CCN(CCOC2CC3=C(SC4=C2C=CC=C4)C=CC(Cl)=C3)	0.279925
RRUHRQCUOJRTHJ	COC1=CC(=C(OC)C=C1)S(=O)(=O)N2CCN(CC2)C34CC5CC(CC(C5	0.222792
RRWNGHNOEYOFFB	C(CN1C(CNC2=CC=CC=C2)=NC3=C1C=CC=C3)OC4=CC=CC=C4	0.229584
RRXRGDXVXFYRD	CC1CCCC(C)N1CC(O)COC2=CC(=CC=C2)C	0.245971

RRZJGAZTGINHFZ	FC1=CC=C(C=C1)C2=NN(C=C2CNCC3=CC=CC=C3)C4=CC=CC=C4	0.228281
RSUNVBITOJEYPG	CCC1=NC2=C(C3=C(CCCC3)S2)C(=N1)N4CCN(CC4)C(=O)C5=CC=C5	0.228761
RSWRBALYBXCPPU	ClC1=CC=C(SCCOCCN2CCCC2)C=C1	0.282325
RSXFMHFYIPOTDZ	OC(COC1=CC=C(Br)C=C1)CN2CCC(CC3=CC=CC=C3)CC2	0.252966
RTHWJTSKQJWTDG	COC1=CC=C(CN2CCC(CC2)C(=O)NC3=CC=C(OC4=CN=CC=C4)C=C4	0.226617
RTPXMZUKAWAOMU	O=C(NC1=CC=C(C=C1)N2C=CC=N2)C3CCCCN3CC4=C5N=CC=C5	0.226878
RUIVQZQTJIUASI	CC[N+](CC)(CC#CC1=CC=CC=C1)CC#CC2=CC=CC=C2	0.233061
RULBLZKSANQWSB	COC1=C(SC2=C(OC)C=NC(=N2)C3=NC=CC=C3)C=CC=C1	0.244033
RUXJQRMOHFTVDC	CC1=CC(C)=C(C=C1)N2CCN(CC2)C3=C(C=CC=N3)[N+][O-]=O	0.236116
RVBSLUQLFIASQC	N=C1N2CCCCCCCCCCCC2=NC3=C1C=CC=C3	0.237292
RVCVRTKVCVPKSD	CCOC1=C(OCC(=O)NC2=C3C=CC=CC3=CC=C2)C=CC(CNCCCN4C	0.242143
RVDGYJRNXYZSRV	CC1=CC=C(S1)C(=O)NC2=C(C=CC(Cl)=C2)N3CCCCC3	0.24688
RVGYUVJAABJREK	CCN1CCN(CC1)C(S)=N\C2=CC3=C(C=C2)N=C(C=C3C)N4CCN(C	0.295405
RVLXBSYISIMSQS	FC1=CC=C(\C=N\NC(S)=NC2=C(Cl)C=C(Cl)C=C2)C=C1	0.26197
RVOJEUDQOHLIER	CN(C)C1=CC=C(C=C1)\C=N\N2CCCCC2	0.277543
RWAJJRZLHXZLNG	CC(C)C(N1CCC2=C1C=CC=C2)C3=NN=NN3C4CCCCC4	0.239932
RWPDRRSKJTUEDJ	CCN1CCN(CC1)C(C2=NN=NN2C(C)(C)C)C3=CC(OC)=C(OC)C=C3	0.227429
RXAQMQYOIAFNIL	CCN(CC)C1=C(C=NC(=N1)C2=CC=CC=C2)S(=O)(=O)C3=CC=C(C)C	0.234048
RXMDCSNWVQQFHW	CCCCOC1=C(C=C(Br)C=C1)C(\C)=N\NC2=NCCN2	0.230369
RXVVMJTWVLQTIH	COC1=C(COC2=C(F)C=CC=C2)C=C(C=O)C=C1	0.228502
RXVXNNJBPMJSKS	CN(C1=C(C)C(=CC=C1C)S(=O)(=O)N2CCN(C)CC2)S(=O)(=O)C3=C(C	0.236139
RYCATPIUCIAASG	CCOC1=C(C=CC=C1)\N=C(/S)N(CCCN2CCOCC2)CC3=CN(C)C4=C	0.274082
RYDQMWWJIIQZSLQ	COC1=CC=C(CCNC(=NS(=O)(=O)C2=CC=C(Cl)C=C2)C3=CC=CC=C	0.228555
RYHDJWCZARFFAF	CC1=CC2=C(C=C1C)N3CCC\N Vitas-M Laboratory,STK498416	0.2618
RYKULGMWGVPEJS	CCN(CC)CCNC(=O)C1=CC=C(NC(=O)C2=CC=C(COC3=CC=CC=C3)	0.222951
RYQIVWHYPCDZML	ClC1=CC(CN2C[C@@H]3C[C@H](N4CCC[C@@]34C2=O)C5=C	0.231101
RZPVJAQOZBEKNJ	FC1=CC(F)=C(C=C1)N2CN(C3=C2N=C4C=CC=CC4=N3)S(=O)(=O)	0.224184
RZUSMBUUTPOWAW	SC(NCC1=CC=CC=C1)=NC2=C3C=CN=CC3=CC=C2	0.226722
RZWVBSYMPVCZNJ	CCOC=1N=C(N=C(N1)SCCOC=2C=CC=CC2)N(C)C	0.2247
SAWMOFBFQZCITM	CC1=NOC(=C1)C2=CC(=C(C)C=C2)S(=O)(=O)NCC3CCN(CC4=CC(F	0.239971
SBSKJQAIRJNTGA	CN1CCN(CC1)C2=C(Cl)C=C(NC(=O)COC3=CC=CC=C3)C=C2	0.243868
SBUSMVQQRPYJAD	CN(C)CCNC(=O)NC12CC3CC(C1)CC(C3)(C2)C4=CC=C(C)C=C4	0.280131
SBUXGQJJMZYVEL	CC1=CC(=CC(C)=C1)C(=O)N(NC(=O)NC2=CC=C(Cl)C=C2)C(C)(C)C	0.234594
SBUXWFCQUBSXSX	COC1=CC=C(OC)C(=C1)C(N2CCN(CC2)C3=CC=CC=C3)C4=NN=N	0.228497
SCAPGNQQZIVBLA	ClC1=C(SC2=C1C=CC=C2)C3=NN=C(O3)SCC#N	0.230897
SCDAIUAKJXSYDU	CC(C)(CN1CCNCC1)NS(=O)(=O)C2=CC=C(Cl)C=C2	0.312271
SCDIWFUXVDYCEM	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC4=C(OCCO4)C=C3	0.259966
SCPRJXKNFHBUKU	CN1CN(C)C2=C3C1=CC=CC3=C(C=C2)[N+][O-]=O	0.241958
SDGFSCPELJHBP	COC1=CC(OC)=C(C=C1)C(=O)C2=CC=C(C=C2)N(C)C	0.276096
SDWMHFRLYBCUOT	CN(C)CCNC(C(=O)NC1=CC(Cl)=CC(Cl)=C1)C2=CC=CC=C2	0.265831
SECHNLXDFGYFOW	CN1CCC2C(C1)C3=C(C=CC(C)=C3)N2\C(S)=N\C4=C(Cl)C=C(Cl)C	0.253962
SFSRKURQYUVABX	ClC1=CC(Cl)=C(CO\N=C\C2=C(N=C3SCCN23)C4=CC=CC=C4)C=C	0.24359
SGSVTCJUBQIDLH	CC1=CC=C(NC(=O)CCN2CCC(CC3=CC=CC=C3)CC2)C=C1	0.256123
SGXZHDKUJYHHBK	CCC(C)(C)[N]1N=NN=C1C(N2CCN(CC2)C3=NC4=CC=CC=C4S3)C	0.22694
SHHGHUVUBNVWJE	CN(C)CC1=C(C)C=C2C=CC3=C(C=CC=C3)C2=C1	0.292332
SHOJTIXYLTWTNM	CCC1=C(NC(=O)C2=CC=C(CN3CCC4=C(C3)C=CC=C4)C=C2)C(C)=	0.225847
SIBQPTPZFXIELI	CN(CCOC1=C(Br)C=C(C)C=C1C)CC2=CC=CC=C2	0.324147
SIJGYHUCFYARBW	COC1=C(Br)C=C(CN2CCC3=C(C2)C=CC=C3)C=C1	0.228239

SIXSFDVHDGTUML	COC1=CC=C(C=C1)N(CC2=CC=CC=C2)S(=O)(=O)C3=CC=C(C)C=C:	0.230172
SJIJWGNUPUGTPQ	CCOC1=C(NC(S)=NC2=C(C)C=CC=N2)C=CC=C1	0.226866
SJKTXCSMIYIWAD	[O-][N+](=O)C1=C(OCC(=O)NC2=CC=C(C=C2)N3CCN(CC3)C(=O)C	0.222439
SJMBNLLHJPEHNV	CC12CNCC(C)(CN(C1)C(C3=CC=CC=C3)C4=CC=CC=C4)C2	0.318074
SKFXGBGSVNETSS	[O-][N+](=O)C1=C(\C=N\NC2=C(CI)N=CC=N2)C=CC=C1	0.234284
SKIIMHFNSMYMPI	COC1=CC=CC(=C1OCCN2CCN(CC2)C3=CC=CC=C3OC)OC	0.226412
SKSQMTDHWXDWFS	COC1=CC(=CC=C1)C2=NN=C(O2)C3=CC4=C(C=CC=C4)C=C3	0.257457
SKZOLTHIWBTQAL	N#CC1=CC=C(C=C1)C(N2CCCCC2)C3=NN=NN3CCC4=CC=CC=(0.237535
SLFDFJFMZDAKGZ	FC1=CC=C(CN2N=NN=C2CN3CCC4=C(C3)C=CC=C4)C=C1	0.279396
SLFYZNIJPKHGX	COC1=CC=CC(=C1)CN2CCCN(CC2)[S+](O)C3=CC=C(Br)C=(0.239848
SLGDRZFZLVKLF	CC1=NC=C(CN2CCCC(C2)C(=O)NC3=CC=C(C=C3)C4=CC(F)=CC=(0.269775
SLIGTSUZRAYWEB	COC1=C(OCC2=C(C)NN=C2C3=C(O)C=C(OCC(C)=C)C=C3)C=CC=C:	0.265367
SMDGYUXIZWCCHF	COC1=CC(=CC(OC)=C1OC)C2C(C)C(C)(OC3=C2C=C4OCOC4=C3)	0.233743
SMFDUNBACDAAQN	CC(C)CCN1CCN(CC1CCO)C2CCN(CC2)C3=C(C)C=C(F)C=C3	0.289713
SMLCPCWGRWUNBJ	C\C(=N/NC1=NC(=CC(C)=N1)C2=CC=CC=C2)C3=CC=C(F)C=C3	0.241021
SMMTWFIETYPVPP	CCCSC1=NN=C(NC(=O)NC2=CC=C(F)C=C2)S1	0.227694
SMNKTCOQJWBYKJ	COC(=O)C1=CN(CC2=CC=C(OC)C=C2)C=C(C1C3=CSC=C3)C(=O)C	0.228406
SNAHHWCKTZHBIF	COC1=CC(CN2C3=CC=CC=C3N=C2C4=NON=C4N)=CC=C1C	0.229971
SNXVQBVEXISXBT	CC1=C(C)C=C(C=C1)N=C(S)N(CCN2CCCCC2)CC3=CC=CO3	0.260038
SOBCWJYTJRLCNZ	CC1CCC2=C(C1)C=C(S2)C(=O)NC3CCN(CC4=CC=CC=C4)CC3	0.229835
SODCEZKWFNCHA	FC1=C(N=C(N=C1)N2CCN(CC2)C3=CC=CC=C3)N4CCN(CC4)C5=	0.233829
SODRUIDWSWLJID	CC1=CC=C(NC2=NC(CN3CCN(CC3)C4=C(F)C=CC=C4)=NC(N)=N2	0.224837
SOHYSAFTNSGPSU	CC1=C(OCCCCNCCO)C=CC(Br)=C1	0.239562
SOLYWHCJVJWXIT	CCCCN\1C2=CC(=C(C)C=C2N3CCC/N=C13)C	0.227488
SOPMCVVZQSETBN	ClC1=CC(NC2=NC(=CS2)C3=CC=NC=C3)=CC=C1	0.264193
SOWKVQZIOZWAFE	CCC1CCC2=C(C1)C=C(S2)C(=O)NCC(N3CCCC3)C4=CC=C(OC)C=(0.229872
SPDVYPXXDOLSOS	SC(NC1=CC=CC(CI)=C1)=NC2=C(OC3=CC=CC=C3)C=CC=C2	0.222748
SPEODCKLJMQURM	CC(C)(CO)NCC1=CC(OCC2=CC=C(CI)C=C2)=CC=C1	0.270805
SPNMGEIUCZRX	CN1C2=C(C=CC=C2)[N+](C)=C1C3=CC=CS3	0.228592
SPQJBAUZMNPEHF	COC(=O)C1=NN(C=C1)C2=CC=C(F)C=C2)C3=CC=CC=C3	0.237425
SQJMTMUXLOOMQG	CCN1CCN(CC1)C2=C(F)C=C(C(=C2)N3CCCC3)[N+](O)=O	0.251381
SQNLWISAIKBTCW	CN(C)CCNC(=O)C1=CC2=C(S1)C3=C(S2)C=CC=C3	0.230815
SQOBYFYNVVYZFE	CCN(CC)CCCNC(=O)CSC1=NC(=C2CCC3=C(C=CC=C3)C2=N1)C(F	0.249817
SRABAOQNRRWRGL	CC1CCN(CCCN(CC2=CC=CO2)C(\S)=N\C3=CC(C)=C(C)C=C3)CC1	0.229185
SRBUJRGGRVRZGS	COC1=C(C=C(C=C1)C(=O)NC(S)=NC2=C(C=CC=C2)N3CCCCC3)[N	0.229767
SRGGYFLVHOMED	COC1=C(C=CC=C1)C(N2CCN(CC3=CC=CC=C3)CC2)C4=NN=NN4	0.254717
SROKXKMTKYUSNU	CCCOC1=CC=C(C=C1)C(O)(CCC)CCN2CCCCC2	0.250776
SRSJAHDVWZQQKC	CC1CCN(CCCCOC2=CC(Br)=CC=C2)CC1	0.300761
SRUOOXMQYNVKRL	COC1=C(OCC2=C(C)C=CC=C2)C(Br)=CC(\C=N\N=C(/N)C3=NON=	0.223747
SSMQZBSIFHOKN	COC1=C(OC)C=C(C=C1)C2=CCN=C2C3=C(O)C=C(OCC4=CC=C(F)	0.22766
SSOBWXXBISJORZ	CCOC1=CC=C(CN2CCN(CC3=NC4=C(C=C3)C=C(F)C=C4)CC2CCO	0.263558
SSYNOGPIXQTMAK	CCN(CC)C1=C(N=C2C=CC=CC2=N1)N3N=C(C)C=C3C	0.22775
STAITCCRXGTZFI	CCC=1C(=NC2=CC(=NN2C1N3CCN(CC3)CCOCC)C4=CC(=CC=C4	0.240156
STAYAOSZGBKRN	CN(CCOC1=CC=C(CI)C=C1)C(=O)C2=CC(=CC=C2)S(=O)(=O)N3CC	0.233672
STMONZKXTMQUDL	CN1CCN(CC1)C2=NN=C(C=C2)C3=CC(NC(=O)COC4=CC=CC=C4)	0.240116
STSCGJBSYJCJODA	ClC1=CC=C(C=C1)S(=O)(=O)N2CCC(CC2)C(=O)NC3CCN(CC4=CC:	0.227713
STWOTKSCFBVDML	COCCCNCCCOC1=C(Br)C=C(C)C=C1	0.232711
SUBZWAAAYBCLAA	CCOC1=C(C=C(CSC(N)=N)C=C1)[N+](O)=O	0.225058

SUEDPLSNXHDQJF	CC1=NC2=C(C=NN2C(=C1)N3CCOCC3)C4=CC=CC=C4	0.234217
SUFVJHJHUVFGTCI	CCCN1C2=C(C=CC=C2)C3=C1N=C(SCCN4CCOCC4)N=N3	0.230144
SUIUMUSHEQVQDC	CSC1=CC=C(C=C1)CN2CCN(CC2)CC3=CC=CC=C3Cl	0.230586
SUSCYIMTNZLQLZ	OC(COC1=CC=C(OCC(O)CN2CCN(CC3=CC=CC=C3)CC2)C=C1)CN	0.291084
SVLPCMOIRWXVAU	[O-][N+](=O)C1=CC(=C(NCC2CCS(=O)(=O)C2)C(=C1)[N+](=[O-])=O)	0.250459
SVSODTYOBUHQ	C1CCC(C1)NC2=NN=C(NC3CCCC3)C4=CC=CC=C24	0.246278
SVUZFUZSRNJFGG	CC1=NC(SC2=C(Cl)C=C(Cl)C=C2)=CC(CS(=O)(=O)C3=CC=CC=C3):	0.224671
SVXFWFLYWFSIIF	COC1=CC(=CC(OC)=C1OC)C2=NN=C3SCC(=NN23)C4=CC=CC=C4	0.254294
SWFVWROOFHMFAB	CN(C)CCOC1=NC(=NC2=C1OC3=CC=CC=C23)C4=CC=CC=C4	0.248053
SWMNAVUFFAWFPO	CC1=C2SC3=C(C=C(C=C3)C(=O)NCCCN4CCOCC4)N=C(C)C2=C(C	0.24096
SWXRBPVQQRSUMH	CC1=NN(C(N2CCCC2)=C1\C=N\NC(S)=NC3=CC=C(F)C=C3)C4=C	0.229524
SXAAYAUYDIBLCP	CC(C)C1=CC=C(OCCCCN2CCCC2)C=C1	0.27658
SXARXBQACQASGW	COC1=C(OC)C=C(CCN2N=NN=C2C(N3CCN(C)CC3)C4=CC=C(Cl)C	0.224473
SXJVGQSBOLALOD	CC1=CC(N2CCN(CC3CCC=CC3)CC2)=C(C)C=C1	0.26558
SXMCYZLUBNHAQI	COC1=CC2=C(SC(=C2C3=CC=C(O)C=C3)C4=CC=CC(OC)=C4)C=C	0.227515
SXZXL SUWQJLZSZ	CC1=CC=C(CSC(NC2=CC=C(F)C=C2)=C(C#N)C#N)C=C1	0.224435
SYHIEICQBFXOKW	CN(C)C1=CC(=CC=C1)C(=O)N\N=C\C2=C(F)C=CC=C2	0.227903
SYMSQEWZPYSKKR	CC(C)CC1N(CCCN2C=CC=N2)CCC3=C1NC4=C3C=CC=C4	0.250745
SYQCMWPYFILWCG	CC1CCN(CC1)CC(O)COC2CCC(CC2)C(C)C(C)C	0.224093
SYSBSGFAVACICZ	COC1=C(C=C(Cl)C=C1Cl)C(=O)NC2=CC=C(NC(=O)C3=CC=CC=C3)C=	0.22248
SYXYVMYQTPAUFA	C(COC1=C(\C=N\N2C=NN=C2)C=CC=C1)OC3=CC=CC=C3	0.232239
TTXFUXPVMCFAY	O=C(NC1=CC=CC=C1)NC2=CC3=C(SN=N3)C=C2	0.242241
TUPKRMNNUUAPMH	COC1=CC=C(C=C1)C2=NOC(CCC(=O)NCCCN3CCN(CC3)C4=CC=C	0.224992
TUSPGVCIGOGKHY	OC(=NCCN(CCN=C(O)C1=C(N=CN1)C(O)=NC2=CC=CC=C2)CCN=	0.238881
TUSPHNIBXFMXQW	CCOC(=O)C1=C(N=NN1C2=NC(=NC(OCC)=N2)N3CCCCC3)C4=C	0.223789
TVHQVHWADWPAQA	COC1=CC=C(CNC(C2=CC=CC=C2)C3=CC=C(Cl)C=C3)C=C1	0.222592
TVLRFWWJOSJVOK	COC1=C(NC(=O)NC2=NC(=CS2)C(C)(C)C)C=CC=C1	0.231039
TVTUIXLOHKOCR	FC1=CC=C(C=C1)C(N2CCN(CC2)C3CCCCC3)C4=NN=NN4CC5=C	0.229027
TVXDYAKPKQXHU	CCOC1=C(OCC2=C3C=CC=CC3=CC=C2)C(Br)=CC(C=NN=C(N)C4:	0.253391
TWMMEMILQOBTQO	COC1=C(C=C(F)C=C1)C(=O)C2CCCN(CC3=CC=CN3C4=NC=CC=C	0.26871
TWPSAPBHHKSMAC	CN1N=C(C(CO)=C1OC2=CC=C(C)C=C2)C3=CC=CC=C3	0.249467
TWUPBEURXSAWHI	C1CN(CCN1\N=C\C2=CC=NC=C2)C3=CC=CC=C3	0.250533
TWZCZLLZJDKWFN	C(N1CCC2=C(C1)C3=C(N2)C=CC=C3)C4=CC=CC=C4	0.276059
TXASOBSTKPCXCN	CCC1=CC=C(C=C1)C2=NC(CN3CCCC(C3)C(=O)NCCC4=CC(OC)=C	0.222944
TYDLBYKMMQYLSJ	ClC1=CC(=CC=C1)C2=CSC(NC3=CN=CC=C3)=N2	0.223337
TYPXMHPYLJAKBQ	COC1=CC=C(C=C1)C(CNC(=O)C2=CC(=CC=C2)S(=O)(=O)N(CC=C)	0.240687
TYBKIMJCGAKGV	COC1=CC=C(C=C1)N2CCN(CC3=CSC(C)=C3C4=CC=C(C)C=C4)CC	0.260633
TYZFXKXKXPDBDS	COC1=CC2=C(C=C1)C=C(C=C2)C3=NOC=C3	0.226146
TZAMHKUTURYHSL	CN(C)C1=CC=C(\C=N\N=C(/C)C2=CC=CC=C2)C=C1	0.22863
TZHKRJCKNDDAQ	CC(C)CC(N1CCN(CC1)C2=CC=CC(=C2)Cl)C3=NN=N[N]3C(C)C	0.258861
TZPXEOGKYBYFGZ	CCN1CCN(CCOC2=C(C)C=C(Br)C=C2)CC1	0.237829
TZQOONHGOXXLRH	CC(C)C\N=C(/S)NCCC1=CC=CC=C1)C\N=C(/S)NCCC2=CC=CC=C	0.237783
TZTGPKPSFAHZFS	SC(=NC1=CC=CC=C1)N2CCN(C\C=C\C3=CC=CC=C3)CC2	0.252838
TZYDMNYEWNWIMB	COC1=CC=C(C=C1)C2=C(OC)C(OC)=C(OC)C=C2	0.292608
UABBWJCLLKRGRS	CC(CCC1=CC=CC=C1)NCC2=C3C=CC=CC3=CC=C2	0.224529
UAJVAORBEDZLAX	COC1=C(OC)C=C(C=C1)C2=NN(C=C2\C=N\N=C(N)N)C3=CC=CC=	0.22442
UAOWSVXZZRQDCR	ClC1=CC(=CC=C1)N2CCN(CC3=CC=C(Br)O3)CC2	0.24388
UARULYQGELQFIJ	ClC1=CC=C(C=C1)C(=O)NC2=CC(Cl)=C(NC(=O)CN3CCCCC3)C=C	0.225005

UAVZHNLWRFYHRJ	COC1=C(OC)C=C(C=C1)C(=O)ON=C(N)CC2=CC(Cl)=C(Cl)C=C2	0.224525
UAZRCPGTJUHM	COC1=C(CN2CCN(CC2)S(=O)(=O)CC3=CC=CC=C3)C=C(Br)C=C1	0.235987
UBADSFILNXXBV	COC(=O)C1=C(Cl)C=CC(NC(=O)C2=C(C)C(=CC=C2)[N+][O-])=O	0.22785
UBDCCMAHHCNWAM	COCCNCCCOC1=C(Cl)C=C(Br)C=C1	0.238917
UBSIOKKUUBUUDQ	C(COC1=C2C=CC=CC2=CC=C1)OCCN3CCN(CC4=CC=CC=C4)CC3	0.231137
UBWUXHOFFJJAQR	COC1=C(OC2CCCC2)C(Br)=CC(CNCCC3=CC=CC=C3)=C1	0.231905
UCKMAYAEGOOXBZ	CC1=C(OCC2=CC=C(F)C=C2)C=C3C=CC=CC3=N1	0.22725
UCMPHCIVJPSYNB	CC1=CC=C(CN(CC2=NC=CC=C2)C(=O)NC3=CC(C)=C(C)C=C3)C=C	0.237066
UCTQIAQYQMZDRZ	CCS(=O)(=O)C1=C(Cl)C(Cl)=C(C=C1)C2=CSC(=N2)C3=CC=CC=C3	0.227233
UDANXCXZROPWNT	CC\N=C(/S)N1CCN(CC1)C2=NC(=CS2)C3=CC=C(F)C=C3	0.257535
UDFFTDNEEOMUIJ	NC(=NOC(=O)C1=CC=CC(Br)=C1)C2=CC=CC=C2	0.229103
UDFMQZYEQSHYMP	CCOC(=O)C1=CC=C(C=C1)N=C(S)N(CCCN2CCN(CC)CC2)CC3=CC	0.307398
UDHRPRPURNIQMQ	CCNCC1=CC(OCC)=C(OCC2=CC=CC=C2)C(Cl)=C1	0.340142
UDUFXXPTEYCARI	CCOC1=CC=CC=C1N2CCN(CC2)CC3=CC=CC(=C3O)OC	0.236764
UELMMVWGHYBUEJB	CN(C)C1=CC=C(CN2CCC(CC2)C(=O)NC(C3=CC=C(F)C=C3)C4=NC	0.229652
UERPRDFAJRYSTQ	CC1=CC(CN2CCC(CNC(=O)NC3=CC(Cl)=C(F)C=C3)CC2)=C(C)C=C	0.252388
UFAPJKMCCIXKKB	COCC1=C(C(C)=NC(NCC2=CC(OC)=C(OC)C(OC)=C2)=C1C#N)[N+]	0.223386
UFJPPAGASFRWDR	CSC1=CC(=CC=C1)N=C(S)N(CCC(C)C)C2CCN(CC2)C(C)C	0.320631
UFZQAGRTXJPCDT	CC1=C(C=CC=C1)C(=O)ON=C(N)CC2=CC=CS2	0.225834
UGFOMFGCDBVENN	N=C1CC2=C(C=CC=C2)C3=C(C=CC=C3)C1C#N	0.282917
UGWJKFXHNUAPCR	CCOC1=CC=C(C=C1)S(=O)(=O)N2C(C)CC3=C2C=CC=C3	0.23545
UHMGEDKDEHYEM	FC1=CC=C(CNCCC(CC2=CC=CC=C2)C3=CC=CO3)C=C1	0.234256
UHOUTQDPMVNNCK	CC1=CC=C(C=C1)C(N)=NOC(=O)C2=CC=C(F)C=C2	0.230032
UHQIKTAVLMIABA	CC1=CC=C(C=C1)C2=NN=C(O2)C3=CC=CC=C3	0.222371
UIEWVWYZJIFDVLQ	ClC1=CC=C(OCCN2CCN(CC2)S(=O)(=O)C3=CC=CS3)C=C1	0.226347
UIKPUZFLXMCXPJ	CC1=NN(CC=C)C=C1CN2CCC(CC2)C(=O)NC3=CC(=CC=C3)C4=C	0.238199
UIMNDLRADBDQMF	CC1=C(SC(NC2=CC=CC=C2)=N1)C3=CC=CC=C3	0.226862
UIOJEXKHUHMUQHC	CC(C)C1=CC(CN2CCN(CC2)C3=CC=CC=C3)=C(O)C=C1	0.225467
UJCIPDXIDCSKPT	COC1=C(C)C=C(C=C1)C2N(CC3=CC=CN3C4=NC=CC=N4)CCC5=C	0.225151
UJKFQZSNQANFHU	CC1=CC2=C(C=C1)N=C(C)C=C2NC3=CC=C(C=C3)[N+][O-]=O	0.228615
UJMNNEJCRDDBRG	ClC1=CC=C(OCC(=O)N(C2CN3CCC2CC3)C4=C(Cl)C=CC=C4)C=C	0.249973
UKEFQPMJYGFDRU	C#CCN1C2=C(SC3=C1N=CC=C3)C=CC=C2	0.237102
UKOHEKHUXHXZTA	CN(C)CCCN(C(=O)C1=CC=CS1)C2=NC(=CS2)C3=CC=CC=C3	0.234956
UKRHIDLFLAPLNSM	CC1=C(OC2=C1C=C(Br)C=C2)C(=O)NC3CCN(CC4=CC=CC=C4)C3	0.236277
ULFSEZIPIRNWAN	COC1=CC(CN2CCN(CC2)C(\S)=N\CC3=CC=C(Cl)C=C3)=CC=C1	0.244107
ULIXOOTVKPGXGZ	COC1=CC=C(C=C1)C2=CN3CCSC3=[N+][O-]C4=CC=CC=C4	0.285598
UMODPOHVGVSVALO	CC1=CN(N=C1)C2=NC(=CC(=N2)C3=CC=CC=C3)C4=CC=CC=C4	0.259397
UMPMUQBARDZLPN	ClC1=CC=C(CS(=O)CC2=CC=C(O2)C(=O)N3CCN(CC3)C4=CC(Cl)=	0.229628
UMQWNKFKRKGDF	CN1CCN(CC1)C(CNS(=O)(=O)C2=CC=C(C=C2)[N+][O-])=O)C3=C	0.248769
UMWGOJZIKKYVDB	COC1=C(CN2CCC(CC2)C(=O)NC3=CN=C(OC4=CC=CC=C4)C=C3)	0.251397
UNFZPHVBNJIVHW	[O-][N+](=O)C1=C(NCC2=CN=CC=C2)C=C(C=C1)N3CCNCC3	0.263107
UNSTZRRKYTHBG	CN1CCN(CC1)C2=C(F)C=C(C=C2)N3CCCC3[N+][O-]=O	0.230546
UOBXJBRVEDGTQK	CN1C(=O)N(CC2=CC=C(Br)C=C2)C3=C1C=CC=C3	0.226894
UOERYGBEQSEUMT	O=C(C1CCCN(CC2=CC=NC=C2)C1)C3=CC=C(C=C3)C4=CC=CC=C	0.240574
UOUCABRMBXRKU	C=CCOC1=C(CN2CCC(CC3=CC=CC=C3)CC2)C=CC=C1	0.28902
UPAABZKHOOUFQ	CC1CCC(=C(C)C)\C(C1)=N\N=C(N)S	0.250581
UPTXRAZTDIKWML	CC1=C(C)C=C(C=C1)N=C(NC2=CC=C(Br)C=C2)N3CCOCC3	0.277502
UQBBTDSGUQJIBT	CC1\C(=N/OC2=C(C=CC=C2)[N+][O-])=O)C(C)CN1C	0.263871

UQLSPHPMYIIASW	COC1=C(OS(=O)(=O)C2=CC=CC=C2)C=C(\C=N\NC(=O)C3=CC=CC	0.230974
UQLXYFJZJNEABU	CCN1CCN(CC1)C2=C3C=CC=CC3=C(C=N2)C(=O)NC4=C(Br)C=C(0.234521
URDRIRMZCBLBOX	CCN(C1=CC=CC=C1)S(=O)(=O)C2=CC(C(=O)NC3CCN(CC4=CC=C(0.262264
URIZHJIIRUNCCY	CCNC1=NC(=NC(OC)=N1)N2CCC(CC3=CC=CC=C3)CC2	0.233164
URQARMKEOXBUIM	COC1=CC(CN2CCCC(C2)C(=O)C3=C(SC)C=CC=C3)=C(OC)C=C1	0.262924
URSNYSFIPOXJAM	COC1=CC=C(OC2=C3C=CC=CC3=C(C)N=N2)C=C1	0.224013
URTZTFXEBYPGOC	CN(C)CCSC1C2=C(CSC3=C1C=CC=C3)C=CC=C2	0.319743
USVCHZHSFHTEBE	CON1C2=C(C=CC(Cl)=C2)N=C1C3=CC=CC=C3	0.223858
USZCTAGGFGBSBS	CC1=CC=CC(=C1)OCCCN2CCCCC2	0.281326
UTCCOJHKHVSQRA	COC1=CC(=CC(OC)=C1OC)C(=O)N\N=C(\CC2=NC=CN2)C3=CC=C	0.256123
UTHZDDBVRIOCTD	CC(NC(=O)C1=CC=CO1)C(N2CCN(CC2)C3=CC=CC=C3F)C4=CC=(0.224145
UTJXCXGBYVFOGTA	CC1CCCCN1CCNC(=O)C2=CC3=C(C)N=C4C=CC=CC4=C3O2	0.23141
UTLMVRAUAPUKKC	CC(NCC(O)COC(C1=CC=CC=C1)C2=CC=C(C)C=C2)C3=CC=CC=C3	0.228106
UTVLFQJTGRGDDM	COC1=CC(=CC=C1)C2=NC(=NO2)C3=NC=CC=C3	0.2254
UTVPIKGLRUSJLF	CC1CCCN(CC2=CC=C(OCC3=CC=CC=C3)C=C2)C1	0.2854
UUAKCBNXSFFFOQ	NCC1CCN(CC1)C2=C3CCCCC3=C4C=CC=CC4=N2	0.272257
UUAMTSUZPHSPON	ClC1=CC(NP(=O)(OC2=CC=CC=C2)OC3=CC=CC=C3)=CC=C1	0.222487
UUDXRZFRPOKNDK	CC1=CNC(\N=N\C2=CC=CC=C2)=N1	0.27957
UULGWBFYZWLCQ	CN(CCOC1=CC=C(Cl)C=C1)CC2=CC(=CC=C2)S(=O)(=O)N(C)C	0.299868
UUUARVJLSFKTBK	COC1=C(OCC(=O)N(CC2=NC(=NO2)C3=CC=CC=C3)C(C)C)C=CC=	0.252512
UVRAZDREJLUWDD	COC1=CC(=CC(OC)=C1OC)C(=O)OC2=C(\C=N\NC(=O)C3=CC(Cl)=	0.25152
UWGFPAZMTGWPGY	OCl(=O)(=O)=O.BrC1=CC=C(C=C1)[N+]2=C(C=C(C=C2)C3=CC=CC=	0.274806
UWWWKQWDZQPHGT	CCOC1=CC=C(C=C1)N=C(S)NCCN2CCN(CC3=CC=CC=C3)CC2	0.26217
UXAAYSJSLOREOB	COC1=C2C=CC=CC2=C(C=C1)C3=NC(CN4CCN(CC4)C5=CC(C)=N	0.3111
UXRGUAUTVYRKBY	COC1=CC=C(CN2C(=O)NC3=C2C=CC(=C3)C(=O)NC4=CC=C(C=C4	0.224244
UYCURXFNUKLQAE	CN(C)C(CNC1=NC(C)=NC2=C1C(C)=C(C)S2)C3=CC=CC=C3	0.253729
UYLFNXPBGVPRB	CCOC(CNCC1=C(C)C2=C(NC3=C2C=CC=C3)C(C)=C1)OCC	0.235899
UYLNSTPDYDTCZ	CCN(CC)CCCNC1=NC=C(C=C1)C2=NN=C(O2)C3=CC=C(OCC(C)C)	0.231389
UYRGDWPZKLPRE	CC1=C2N=C(C=C(C(=O)NCCN3CCCC3)C2=CC=C1Cl)C4=NC=CC	0.224527
UZQSVAXISNJXMA	COC1=CC(=CC=C1)C2=C(C3=C(S2)C=C(OC)C(OC)=C3)C4=CC=C(C	0.236983
VAEYKRLNDAXEIH	ClC1=CC=C(\C=N\N2CCN(CC3=C(Cl)C=CC=C3)CC2)C=C1	0.269961
VAQAQAYEBXLZSE	[O-][N+](=O)C1=CC(C(=O)OCC2=CC(Cl)=CC=C2)=C(C=C1)N3CCO	0.237614
VBJLFSJKTRLLS	COC1=CC=C(CC2(CO)CCN(CC3=CC4=C(O3)C=CC=C4)CC2)C=C1	0.224892
VBLUFGYBAPIWMI	CC1CCN(CC1)S(=O)(=O)C2=CC3=C(C=C2)C4=C(C=C(C=C4)S(=O)(0.229549
VBMSCPYQFYJUOP	CCCCN1C(=N)N(CC(O)COC2=CC=CC=C2)C3=C1C=CC=C3	0.226303
VBNDDKRLJXHRTH	FC1=CC(=CC=C1)C(=O)C2=CC=C(C=C2)N3CCN(CC3)C(=O)C4=CC	0.225671
VBQUUEMYGITEBQ	CC(OC1=CC=C(Br)C=C1)C(=O)NC2CCN(CC3=CC=CC=C3)CC2	0.27203
VCBQAQSPQLQFBHJ	COC1=CC=C(C=C1)C(N2CCN(CC2)C3=NC4=C(S3)C=CC=C4)C5=N	0.259868
VCFHSOOCBVZOEW	COC1=CC=C(C=C1)N2C=C(CN3CCCC3)C(=N2)C4=CC(F)=CC=C4	0.269208
VCIXBQMJJQHSNKL	NC(CC1=CC=CC=C1)=NOC(=O)C2=C3C=CC=CC3=CC=C2	0.224553
VCKPFJMALJNJOS	CC(=O)NC1=CC=C(CC(=O)NCCC(C2=CC=CC=C2)C3=CC=CC=C3)C	0.232554
VCPJOSLAPPPDGI	BrC1=CC(=CC=C1)C(=O)NC2=CC=C(C=C2)C(=O)OC[C@@H]3CC(0.231481
VCPRSFYZZOYOEQ	CN(C)CC\C=C1\C2=C(SC3=C1C=C(Cl)C=C3)C=CC(F)=C2	0.378891
VDENOZWXPIFATJ	COCCN(CCOC)C1=C2C=CC=CC2=NC(=N1)C3=CC=C(C)C=C3	0.242662
VDNMALJFIDGEGE	SC(NCCC1=CC=CC=C1)=NC2CC3CCC(C2)N3CC4=CC=CC=C4	0.276554
VDONTZRAAXPZEC	CC1CCCN(CCCCOC2=CC(Br)=CC=C2)C1	0.286989
VESGNTBUUJOFAR	CC1=C(C=CC=C1)C(OCC(O)CN2CCCCC2CCO)C3=CC=CC=C3	0.225969
VEZHCVAZNDLXQA	C\C(=N/N=C(\S)NCC1=CC=CC=C1)C2=CC(Br)=CC=C2	0.240851

VFCZSWPNOOGGAJ	SC(NC1=C2C=CC=CC2=CC=C1)=NC3=C4C=CC=CC4=CC=C3	0.272478
VFFOKZZMLPKPMY	C\N=C(/S)N1N=C(CC1C2=CC=C(CI)C=C2)C3=CC=C(C)C=C3	0.228373
VFQQMNPIPMXSQY	CC1=CC(=CC=C1)N=C(S)N\N=C\C2=CC(=C(CI)C=C2)[N+][[O-]]=O	0.246745
VGJHJGQIUUCBNW	NC1=C(\C=N\N=C\C2=C(N)C=CC=C2)C=CC=C1	0.239199
VGJLNUWAZCMSLC	CN1CCN(CC1)C2=C(F)C=C(NC(=O)CSC3=C(C)C=C(C)C=C3)C=C2	0.229282
VGQNNZAKPVUEGN	CN(C)C1(CCCCC1)C2=NN=N[N]2CCOC(=O)NC3=CC=C(CI)C=C3	0.25121
VGWUFXZDHVMWPU	COC1=C(OCC(O)CN2CCC3=C(C2)C=CC=C3)C=CC(CC=C)=C1	0.223321
VHCZYBSUTHBEDK	COC1=C(OC)C=C2CN(CCC2=C1)C3=C(CI)C=C(C=C3)[N+][[O-]]=O	0.228948
VHLPETZIMDPZJC	CCOC1=CC=C(C=C1)N=C(S)NCCCN2CCN(CC2)C3=CC=C(OC)C=C:	0.246732
VHMYRIWZTCFOPT	C[N+]=C(\C=C2/SC3=C(C=CC=C3)N2CCO)C=CC=C1	0.227264
VHPBVWQHJKKNCD	CC1=C(OC2=C1C=CC=C2CI)C(=O)NC3CCN(CC4=CC=CC=C4)C3	0.22587
VHQBZODDZCAPDD	COC1=CC(=CC=C1)C2=CC=C(NC(=O)C3CCCN(CC4=CN=C(C)N4C	0.222943
VIEGMAUCXWHBOZ	COC1=CC2=CC(=C(O)N=C2C=C1OC)C(N(C)C3CCCC3)C4=NN=N	0.226796
VIFYHPTYIUPYQF	CN(CC1=CN(N=C1C2=CC(C)=CC=C2)C3=CC=C(C)C=C3)CC4=NC=	0.251472
VIOBTPHIMFHDZ	CC1=CC=CC(C)=C1N2CCN(CC2)S(=O)(=O)C3=CC(C)=C(F)C=C3	0.253418
VITWUYWKAAXNIA	FC(F)(F)C1=C/C=C(\C=C\1)S(=O)(=O)NC2=C/C=C\C(=C\2)\C3=C\	0.239315
VIXLKURPAFTTTK	COC1=CC=CC=C1C(C2=NN=NN2CC3=CC=CC=C3)N4CCN(CC4)C	0.243379
VIYPCMSAFNCFIA	CC1=CC=C(S1)\C=N\NC2=C(CI)C=C(CI)C=N2	0.241553
VJUNLCDAPXNXGM	CCN(CC)C1=CC=C(\C=N\N=C(/S)NCC2=CC=CO2)C=C1	0.233016
VJXSSYDSOJBUAV	COC1=CC(CC2=C(C)C3=C(N=C2)N=C(N)N=C3N)=C(OC)C=C1	0.239802
VKCHACDTSFSPJM	C1CC(CCC1N2CCN(CC2)C3=CC=CC=C3)C4=CC=CC=C4	0.274237
VKIYIHWONRLGDU	CC1=C(OCCN2CCCC2)C(CI)=CC=C1	0.227673
VLAPRQOFMVJAIG	CN(CCCO)CC\C=C1\C2=C(CSC3=C1C=CC=C3)C=CC=C2	0.311595
VLCFEOVOOOOSGK	OCCN(CCO)C1=CC(CI)=C(C=C1)C(C2=C(CI)C=CC=C2)C3=C(CI)C=	0.241192
VLKBTYIEMXMZDV	CC1=C(NC2=NC3=C(CS2)C=CC=C3)C=CC=C1	0.22625
VLLYOPWHMGRPFM	CC(C)NC(=O)C1=CN=C(N2CCN(CC2)C3=CC=CC=N3)C4=CC=CC=(0.224177
VLVCQMWGNONVHX	COC1=C(CN2CCN(CC2)C(=O)C3=CC=CO3)C4=C(C=CC=C4)C=C1	0.237342
VLXDGXQTILRZDH	CC1=C2SC3=C(CC(N4CCNCC4)C2=CC=C1)C=C(CI)C=C3	0.255853
VLXKKLBPHRIRN	[O-][N+](=O)C1=CC(CN2CCC(=CC2)C3=CC=C(F)C=C3)=CC=C1	0.225704
VMBKXMUODGBTIE	NC1=NC(NC2=CC=CC=C2)=NC(CN3CCN(CC3)C4=C(F)C=CC=C4):	0.225367
VMPRULWEVWCPNB	COC1=CC(OC)=C(C=C1)C(=O)C2CCCN(CC3=CC=CN3C4=NC=C(CI	0.222896
VMYPXLBUMROAIU	[O-][N+](=O)C1=CC=CC=C1NN=CC2=CC=CC=C2CI	0.244684
VNFUBVNOOAIKTF	N#CC1=C(NCCCN2CCOCC2)O Vitas-M Laboratory,STK876204	0.224171
VNTNPCOBOYPBLS	CC1=CC(C)=C(C)C=C1CN2CCC(CO)(CCOC3=CC=CC=C3)CC2	0.30468
VNYLGEAYZFFEEM	CN(CC1=CN(C)N=C1C2=C(F)C=CC=C2)CC3=C(C)C4=C(N3)C=CC=	0.241921
VOAUQLPXJRAWTL	CCN(CC)C1=NC(=NC(=N1)OCC#N)NC2=CC=C(CI)C=C2	0.237123
VOJFJMFACGUGRG	FC1=CC=C(CN2CCN(CC2)C(C3=CC=CC=C3)C4=CC=CC=C4)C=C1	0.255935
VOUMVHRAVBACH	COC1=C2C3COC4C5CC(C(C(C2=CC=C1)N34)N5C)C(O)=O	0.244998
VPAPYTJZDRDDX	ClC1=CC(NC(=O)C2=CC=CS2)=CC=C1N3CCN(CC3)C(=O)C4=CC=	0.23989
VPBFGUWKZZRKKM	CCN(CC)CC#CCC(O)(C1=CC=CC=C1)C2=CC=CC=C2	0.302
VPIDANAIZIMNGX	CC1=CC=C(C=C1)S(=O)(=O)NC2=C(C=CC=C2)C3=CC=CC=C3	0.227896
VOXSNYFYCZTJJ	FC1=C(F)C=C(C=C1)S(=O)(=O)NC2=CC(=CC=C2)C(=O)N3CCN(CC:	0.225476
VRLXBGWQMKWOLJ	NC1=NC(NC2=CC=CC=C2)=NC(CN3CCN(CC3)C(C4=CC=CC=C4)C	0.255889
VRMAPIMDRVKGOM	FC1=C(C=CC=C1)C2CC(=NN2C(=O)C3=C(Br)C=CC=C3)C4=CC=C(C	0.226985
VRTKXFMWBVSAET	CCN1CC[N]2C3=CC=C(Br)C=C3C4=C2C1CCC4	0.266972
VRWQYDQWMLAJJC	CCOC1=C(NC(=O)C2=C3C=CC=CC3=NC(=C2)C4=CC(OC)=C(OC)C	0.232549
VRWXAWXVRQECLB	CCC1=C2SC3=C(CC(N4CCNCC4)C2=CC=C1)C=CC=C3	0.235068
VRZUALFDZNDYNG	COC1=CC=C(C=C1)C(=O)NCC2=CC=C(C=C2)N3CCN(CC3)C(=O)O	0.234594

VSVJBELYLNOYHK	NC(=NOC(=O)C1=C(Cl)C=CC=C1)C2=CN=CC=C2	0.235064
VTIAMSIKHJIUCA	COC1=C(OC)C=C(C=C1)S(=O)(=O)N2CCN(CCOC3=C(Cl)C=CC=C3)C=C1	0.264699
VTNHOKYMZDRTPA	COC1=CC=C(OC2=NC(SC)=NC3=C2SC=C3)C=C1	0.245579
VUDAAHGTVVULMQ	CC1=C(C)C(CN2CCN(CC3=CC=CC=C3)CC2)=C(NC(=O)C4=CC=CO	0.251893
VUXGKEMXGHIQPD	CN(C(=O)COC1=C(C=CC=C1)C(=O)NCCOC2=CC=CC=C2)C3=CC=C(0.22389
VVGLBONFTONOKG	COC1=C(OC)C(OC)=C(CN(C)CC Enamine,T5403811	0.23806
VVQZMWXNTUVBQK	C(C1CCCC1)N2CCNC[C@H]2CC3=C4C=CC=CC4=CC=C3	0.259398
VVUGUCNNBSFPHH	COC1=CC2=C(C=C1)N=CC(=C2N3CCN(CC3)C4=CC=CC=C4)S(=O)	0.222652
VVWJBEYLLMPLAH	COC1=CC=C(C=C1)C(CNC(=O)C2=CC(=CC=C2)S(=O)(=O)NC3=CC	0.235246
VWBMQAOJOWMESA	CC(C)CC1=CC=C(CN2CCCC(C2)NC(=O)C3=CC=NN3C)C=C1	0.229517
VWDKYMHHRGVWMZ	OCC2(CCOC1=CC=CC=C1)CCN(CC3=CC4=C(OC3)C=CC(Cl)=C4)C	0.230783
VWGZOWRGLFRLIU	FC(F)OC1=C(\C=N\NC(=O)CCN2CCN(CC2)C3=CC=CC=C3)C=CC=	0.238981
VWTJMQOMKFZCEP	COC1=C(NC(=O)N2CCN(CC2)C3=C4C=CC=CC4=NC(C)=C3)C(Cl)=	0.249826
VWXIJCRXGJVNDM	C1CN(CCN1)C2=NC(=NC(NC3=CC=CC=C3)=N2)N4CCOCC4	0.254108
VXEVEODGFIABW	CC(C)(C)C1CCC(CN2[C@@H](CC3=CC=CC=C3)CN=C2NC4=CC=C	0.232467
VXVGANJCDDDWQK	FC1=C(C=CC=C1)N2CCN(CC2)C3=NC4=C(C=CC=C4)N=C3	0.224621
VXXFUXPTNRIHFJ	COC1=CC=C(CS\C2=N\CCN2)C=C1Cl	0.229044
VYDWXPSVGKFSAK	COC1=CC(=CC(OC)=C1OC)C(=O)OC2=C(\C=N\NC(=O)C3=CC=C(C	0.23307
VYOKUUZWHNNMIR	CC(C)CNC1=C2C=CC=CC2=NC3=C1CCC3	0.26963
VYSLSSWHAOVRU	CN1C2=C(C=CC=C2)C(C)(C)C13CC(=NO3)C4=CC(=CC=C4)S(=O)(:	0.225272
VYWUQQFSUNSR	COC1=C(OC)C=C2CN(CCC2=C1)C(\S)=N\C3=C(Cl)C=CC=C3	0.230343
VZYMVGKXGSEFDE	CCCN(CCC)S(=O)(=O)C1=CC(=C(Cl)C=C1)[N+](O-)=O	0.230161
WAPTVQITJCEQMB	CN1C=CC=C1\C=N\N2CCN(CC3=C(Cl)C=CC=C3)CC2	0.252386
WAVQNOTWADWNLX	COC1=CC=C(CCC(C)NC2C3CC4CC(C3)CC2C4)C=C1	0.236771
WAZQANLJTOAIOI	CCOC(=O)C1=C(SC2=C(Cl)C=CC=C2)N=C(N=N1)C3=CC=CC=C3	0.22417
WBDSXISQIHMTGL	CC1=NC(=C(N1)C2=CC=CC=C2)C3=CC=CC=C3	0.236879
WBJVNHWOQYRUQG	CN(C)CC\C=C1/C2=C(SC3=C1C=C(Cl)C(F)=C3)C=C(F)C=C2	0.263942
WBMNPSAUXXIQBE	CCOC(=O)NC1=CC2=C(SC3=C(C=CC=C3)N2C(=O)N4CCN(C)CC4)	0.224097
WBNMCRJMDFWRBV	COC1=CC=C(C=C1)N2CCN(CC2)C(=O)COC(=O)C3=C(OCC4=CC=C	0.223932
WBPKXTWRJ CZAKT	C1CCC(C1)[N]2N=NN=C2C(N3CCC(CC3)CC4=CC=CC=C4)C5=CC	0.232175
WCCQTVAMVQMWWQG	CCCCOC1=C(OC)C=C(CNCCCN2CCOCC2)C=C1Br	0.265046
WCNGLYKQWKVZKW	COC1=C(C=C2C=CC=CC2=C1)C(=O)NCC(N(C)C)C3=CC=CS3	0.237268
WDFKKHNNOXFTJQ	COC1=CC(=CC=C1)C(=O)NCC(N2CCN(CC2)C3=CC=C(F)C=C3)C4=	0.226701
WDHFYKXRZMEJO	CCOC(=O)C1=C(C)C=C(NC(=O)NC2=CC(Cl)=CC=C2)S1	0.240383
WDYIDAUIWRIEAK	COC1=CC=C(NC2=NC(CN3CCC(CC4=CC=CC=C4)CC3)=NC(N)=N2	0.223259
WDZOOWQENASWEG	CCN(CC)C1=C2N=CC=CC2=C(C=C1)[N+](O-)=O	0.229091
WECQZDGNZQWMJJ	COC1=C(C=C(Br)C=C1)C(\C)=N\NC2=NCCN2	0.235469
WEXBZFNAXBELQT	CCN(CC(O)COC(C1=CC=C(OC)C=C1)C2=CC=C(OC)C=C2)CC3=CC:	0.295646
WFCLXYFMXYSPQT	CN(C)C1=CC=[N+](CC2=CC=CC=C2)C=C1	0.254305
WFJQERALKFVBNW	CCC(C)(C)N1N=NN=C1C(N2CCC(CC3=CC=CC=C3)CC2)C4=CN=C	0.25369
WFPXFGCECGKRBQ	COC1=CC2=C(CCN=C2C3=CC=C(C=C3)N(CCC1)CC1)C=C1	0.255494
WFTNLTBSNBUOPC	CC1=CC=C(C=C1)P(=O)(CSC(N)=N)C2=CC=C(C)C=C2	0.228855
WFZDQZHEMCUHBQ	COC1=CC(NC(=O)C2=CC=C(CN3CCC4=C(C3)C=CC=C4)C=C2)=CC	0.227027
WGBAOHIEBXQJGQ	FC(F)(F)C1=C(Cl)C=CC(NC(=O)NC2CC3CCCC(C2)N3CC4=CC=CC=	0.224295
WHLKLDZLPQJBJK	CC1=CC=C(C=C1)S(=O)(=O)NCCSC2=NN=NN2C3=C(C)C=CC(C)=C	0.243034
WHPFYKPRHEFSL	CCC(C)(C)CC1=CC(=CC=C1)C2(O)CCN(CC2)S(=O)(=O)C3=CC(C):	0.241887
WIFQZKFWPZEZCK	CCCN1CCCC(C1)C(=O)C2=CC(C)=C(OC)C(C)=C2	0.229926
WIGYQBIRHHDRBO	NC(=NOC(=O)C1=C(Cl)C=CC=C1)C2=CC=C(Cl)C=C2	0.224912

WIKOYZFVDYYDNM	O=C1CC(SC(=N1)N(C2=CC=CC=C2)C3=CC=CC=C3)C4=CC=CC=C4	0.228811
WIOYPCBJJRBFS	CCCN(CCC)C1=NC2=CC=CC=C2[N]3C(=NN=C13)C	0.231311
WIPBFPCDERGUGD	CC(NC1=N/C=N\C2=C\C=C/C=C\C1\2)C3=C/C=C\C=C\3	0.36322
WJQFDPLKXZMOK	NS(=O)(=O)C1=CC=C(CCNCC2=C(OCC3=CC=CC=C3)C=CC(Br)=C2	0.223011
WJSYQWGVCFCKI	CN(C)C1=NC(=NS1)C2=CC=CC=C2	0.260304
WJVMMRROWJDULS	COC1=CC=C(CN(CCC2=CNC3=C2C=CC=C3)CC4=CC=C(OC)C=C4	0.249681
WKBOJNOIWJKTEM	CCCNCC1=C(Br)C=C(OCC2=CC=CC=C2)C(OC)=C1	0.242492
WKMNILFJGKLWSI	C(=C1C2=C(C=CC=C2)C3=C1C=CC=C3)C4=NC=CC=C4	0.274173
WKZLOBWJQCENOT	COC1=CC(OC)=C(OC)C=C1C(=O)ON=C(N)C2=CC=C(C)C=C2	0.314167
WLBSGYDYSHNKOZ	O=C(CN1C(=S)S\C1=C/C2=CC=CC=C2)C1=O)N3CCN(CCC4=NC=C	0.222881
WLFDIVSMVXWZBA	CC(C)CCC(CCN1CCCC1)C2=CC3=C(OCO3)C=C2	0.253038
WLIPRXHZDQOVQS	FC1=C(Cl)C=C(C=C1)N=C(S)N2CCN(CC2)S(=O)(=O)C3=CC4=C(C=	0.232304
WLUKJQQTEJCLN	FC1=CC(CNC2=C3C=CC(Cl)=CC3=NC=N2)=C(F)C=C1	0.225206
WLZFOHOTRBTTSJ	COC1=C(OC)C=C(C=C1)C2=NC(C#N)=C(O2)N3CCC4=C(C3)C=CC	0.229211
WLZXVTQJXVOGAD	CN(CCOC1=CC(=CC=C1)C(F)(F)CC2=CC=CC=C2	0.244934
WMRUUYUPEGDWAJ	FC1=CC=C(\C=C\CN2CCC(CC2)OC3=CC=C(C=C3)C(=O)N4CCCC	0.22332
WNEILMVLUGZDDP	COC1=C(OC)C(Cl)=CC(CN(C)CC2CCCN(CCC3=C(F)C=CC=C3)C2)=	0.327497
WNMYWKYVLNNOFF	COC1=CC=CC=C1N2CCN(CC2)C(C3=NN=NN3C(C)(C)C)C4=CC=C	0.269633
WNYKCRPUNXMPY	CCOC(=O)C1=C(NS(=O)(=O)C2=CC=C(OC)C=C2)C=CC=C1	0.224172
WOFILWXIKKUJDP	CCCCN1C(=N)N(CC(O)COC2=CC=CC=C2OC)C3=CC=CC=C13	0.229144
WOHOPYMSIBACDV	CSC1=CC=C(NC(=O)NCCCN2CCN(CC2)C3=C(F)C=CC=C3)C=C1	0.225119
WOOTZOPDGUAGF	FC1=CC=C(SC2=C(CNC3=NCCN3)C=CC=C2)C=C1	0.229485
WOPJLGVIKBDAJE	CCN1CCN(CC1)C2=CC3=C(C=C2NC(=O)C4=C(F)C=CC=C4)C(=O)N	0.225603
WOWRJXYZJITKFL	CC1=CC(OCCCN2CCC(CC3=CC=CC=C3)CC2)=C(C=C1)[N+](O)=	0.235655
WPBQNAPISRQAAY	COC1=C(OC)C=C(C=C1)S(=O)(=O)N2CCN(CCOC3=CC=C(Br)C=C3	0.228231
WPHIDJCIKTYNE	FC1=CC=CC=C1N2CCN(CC2)C(C3=CC=CS3)C4=NN=N[N]4CCCC5	0.240113
WPNCEUSBTRQOHS	SC(NC1CCN(CC2=CC=CC=C2)CC1)=NC3=CC=CC(Cl)=C3Cl	0.278473
WSPHXZZWGGJJK	OC1=C(C=C(Br)C=C1)C2(OC(=O)C3=C2C=CC=C3)C4=CC=CC=C4	0.234783
WPUKMPYLKBAQPP	CCCC(=O)OC1=C(C(C)=NN1C(C)(C)C)S(=O)(=O)C2=CC=C(C)C=C	0.225919
WQDCHJQTDZAOTQ	COC1=C(OC)C=C(CCN(C)C(=O)CC2=CC=C(C=C2)C3=CC=CC=C3)C	0.225168
WQGZHPROJLLTMO	COC1=CC(=CC=C1)C(=O)NC2=CC=C(C=C2)N3CCN(CC3)C(=O)C4	0.229794
WQOSKDXGMMHOKK	CCOC1=C(CN2C3CCC2CC(C3)C4=CC=C(C)C=C4)C=CC=C1	0.23264
WQUDFRHRBHJOGE	CC1=C(C)C(NCC2=NN=C(O2)C3=CC=CC=C3)=CC=C1	0.252841
WQYNNMCZNHWKPY	CN1N=C(C(CSC2=CC(Cl)=CC=C2)=C1Cl)C3=CC=CC=C3	0.234121
WRQAZKMHSYJKQE	COC1=CC=CC(=C1OC)C(N2CCN(CC2)C3=CC=CC(=C3C)C)C4=NN	0.246926
WRQGZJRDFGPJKX	SC(=NC1CCCC1)N2CCC3=C(C2)C=CC=C3	0.223809
WRZMZVAIXOZXPO	COC1=CC=C(C=C1)C2=CSC3=C2C(=NC=N3)N4CCN(CC4)S(=O)(=	0.22951
WSAQWMOUISYVFR	CCCCN1CCC2=C(C1)C3=C(C=CC=C3)N2CC4=CC=CC=C4	0.231566
WSGYVSIBSVBFRD	CCN(CC)CCNC(=O)C1=CC=C(NC(=O)NC2=C3C=CC=CC3=CC=C2)C	0.232296
WSHGVPVUMULZJFU	CCOC1=C(OCC2=C(Cl)C=CC=C2)C=CC(CNCCN3CCOCC3)=C1	0.293271
WSKWRSVOYUZDNM	CC1=C(CN2CCN(CC3=NC(=NO3)C(C4=CC=CC=C4)C5=CC=CC=C5	0.234463
WSPUPKXQOSRPIB	CCN1C=CN=C1CN2CCCC(C2)C(=O)C3=C(OC)C=CC(Cl)=C3	0.231671
WTJBFLDUSUCDMV	ClC1=CC=C(C=C1)C2=NN=C(NC3=NCCCC3)O2	0.248857
WTVCSVAQQCCHLN	[O-][N+](=O)C1=C(C=CC=C1)S(=O)(=O)NC2CCCCCCC2	0.233406
WTWTXGRZMUQXMI	ClC1=C(NC(=O)NC2=CC3=C(CCC3)C=C2)C=CC=C1	0.226058
WUCYLECPMWLREK	CCN1CCN(CC1)C2=C3C=CC=CC3=C(C=N2)C(=O)NC4=C(C=CC=C	0.255955
WUEUITYGIMFDKP	COC1=C(C)C(OC)=C(CNCCC2=C(F)C=CC=C2)C=C1	0.233672
WUFSIDXHZXRVAW	SC(=NC1=CC=CC=C1)N2CCC(CC3=CC=CC=C3)CC2	0.257299

WUYSOFHLTPJEGK	C1CN=C(C1)NC2=NN=C(O2)C3=CC=CC=C3	0.225391
WVUKBGUNJPPZKT	COC1=C(C=CC=C1)N2CCN(CC2)C(=O)C3=C(C)ON=C3C4=C(Cl)C=	0.245562
WVXCLKIMORBOGJ	CC1=CC=C(NCSC2=CC=C(Cl)C=C2)C=C1	0.232499
WWJNOIHSOVGFHS	CCC1=NN=C2SCC(=NN12)C3=CC=C(OC)C=C3	0.226705
WWWQLEMJBXHDDN	CN1CCN(CC1)C2=C(F)C=C(NC(=O)CSC3=CC=CC=C3)C=C2	0.239555
WXIAPDQHCQQEEP	CCN(CC)C1=C2CN(CC)CCC2=C(C#N)C(NCC3=CC=CC=C3)=N1	0.245069
WXLHGVADSVDFPI	FC1=CC(COC2=C(CNC3=CC=CC=C3)C=CC=C2)=CC=C1	0.241011
WXMWPVRVZDVLPI	C(CN1CCN(CC1)C2=NC=CC=N2)OC(C3=CC=CC=C3)C4=CC=CC=C	0.248522
WXVYHMAMNABJEM	FC1=C(NC(=O)C(=O)NCC(N2CCC3=C2C=CC=C3)C4=CC=CO4)C=C	0.225348
WYDUPMJEJGLJZ	COC1=CC=C(C=C1)N2CCN(CC2)C(CNS(=O)(=O)C3=CC=C(C)C=C3	0.249279
WYLWVVBBCWZWLQ	CN1N=CC(Cl)=C1C(=O)N2CCN(CC2)C3=CC=CC(C)=C3C	0.237419
WZJWDOBVMVCUFQV	CCN1C=CN=C1CN(C)CC2=CN(N=C2C3=CC=C(F)C=C3)C4=CC=C(I	0.230251
WZQCPYUVPQREPF	CN1CCN(CC1)S(=O)(=O)C2=CC=C(C=C2)N3CCN(CC3)C4=C(O)C=	0.251302
XAYBGZWXMSUFMR	COC1=CC=C(NC(=O)CSC2=NC3=C(S2)C=C(NC4=NC(=NC(=N4)N5	0.223728
XBMYNVZJGFJCAE	C\C(=N/NC1=NC(=CC(C)=N1)C2=CC=CC=C2)C3=CC=CO3	0.223491
XBUMEOXSWOGGLL	ClC1=C(SC2=C1C=CC(Cl)=C2)C(=O)NC3CC3	0.229072
XCEVZULHCRZQMO	[O-][N+](=O)C1=CC=C(S1)C(=O)NCC(N2CCCC2)C3=CC=CO3	0.247269
XCLJMZPIMGHSRQ	COC1=C(OC)C=C(CCN2=C(C=CC(=C2)N3CCN(CC3)C(=O)C4=C(C	0.245013
XDJJNYNUDCVIHO	COC1=CC(OC)=C(CN2CCN(CC3=C(F)C=CC=C3)CC2)C=C1	0.227156
XDLHAHDPPCGSAH	CCOC1=C(NC(=O)NCCC2=CNC3=C2C=CC=C3)C=CC=C1	0.230131
XEDVBYLUISOGOO	[O-][N+](=O)C1=CC=C(OCCCCN2CCC3=C(C2)C=CC=C3)C=C1	0.252232
XEGDMEBEXWICKV	CN(C)CCCNC1=CC(=NC2=CC(=N[N]12)C3=CC=CC(=C3)C)C	0.23619
XEHCNLUYVHHNQK	CC1CN(CCN1C2=CC(C)=CC=C2)C3=C(C#N)C(C)=CC(C)=N3	0.247572
XEHZGYNIGPCKHJ	O=C(NC1CCCC1)N2CCN(CC2)C3=NC(=CS3)C4=CC=CC=C4	0.237399
XEIKLIBXIDFFRZ	ClC1=CC(Br)=C(OC(=O)NCC(N2CCCC2)C3=CC=CO3)C=C1	0.240251
XEMIIHFCHKQMEP	CC1=NC2=C(C=NN2C3=C1CCC3)C4=CC=C(F)C=C4	0.235875
XEXJCSNBUIARJF	COC1=CC=C(NC2=C3C=CC=CC3=NC=C2)C=C1	0.240198
XEFWWGGXLFVFR	COC1=CC=C(C=C1)N=C(S)N(CCCN2CCC(C)CC2)CC3=CC=CS3	0.288579
XFFKNCXOGHDQDV	CCN(CC(=O)NC1=CC(=CC=C1)S(=O)(=O)N(C)C2=CC=CC=C2)CC3=	0.227728
XFOMWTKVHWXVRS	COC1=CC=C(C=C1)C2=NOC(CSC3=NN=C(CC4=CC=CC=C4)N3C5	0.223917
XFPRVFPKQLFBJ	OC(COCC1=CC=C(Cl)C=C1)CN2CCC3=C(C2)C=CC=C3	0.230016
XFRKOROYPDUFGL	CCCCC1CN2CCC3=C(NC4=C3C=CC=C4)C2(C)C1	0.259466
XGAGHBMKLFMKNK	C=1C=C(C=CC1SCC2=CN3C=CSC3=N2)Cl	0.233886
XGCVRMWOJYNHRT	CC1=CC2=C(C=C1)[N+](CC3=CC=CC=C3)=CC=C2C	0.237677
XGYJQKQULCSLIR	C(COC1=CC=CC=C1)OCCN2CCN(CC2)C(C3=CC=CC=C3)C4=CC=C	0.234357
XHURKZDJGLSJEZ	COC1=CC=C(CCC(C)NC2CCCCC2)C=C1	0.274606
XIGKSTOGNSHTNH	COC1=CC=C(C=C1)C2=NN(C=C2\C=C\C(=O)N3CCN(CC3)C4=NC=	0.225272
XINRDZSLRJVSV	CC(=O)NC1=CC2=C(C=C1)C3=C(C=CC=C3)C2N4CC5CCC(CC5)C4	0.236251
XIOZDCDYRARUFM	CC1=C(CN2CCN(CC2)C3=CC(C)=NC(C)=C3)N=C(O1)C4=CC=C(Cl	0.320242
XKIFTEHOCFPRJE	CCN(CC)CCOC1=CC=C(Br)C=C1	0.235505
XKIPMVXDDDLWCQ	ClC1=CC(=CC=C1N2CCOCC2)NC(=O)C3CCCC3	0.231995
XKVSASJQGCZUIK	CCN(CC)CC(=O)NC1=CC=C(C=C1)C2=NC3=CC(=CC=C3O2)NC(=C	0.226503
XLIQQHXGYXNKJK	Cl.CC(C)CCC(O)(C(CN1CCOCC1)C2=C/C=C\C=C\2)C3=C/C=C\C=C	0.229004
XLKCZXTWMUKOPW	CCC(=O)N(CCCN(C)C)C1=NC(=CS1)C2=CC(=CC=C2OC)OC	0.230786
XMBVYHDHLZZLBV	COC1=CC(NC(=O)CN2CCCC2)=C(OC)C=C1NC(=O)C3=CC=C(F)C	0.233753
XMHNKNSRQRXIGV	COC1=C(OC)C=C(CNC2=NC3=C(C=CC=C3)N2CC4=CC=CC=C4)C=	0.254193
XMNODAOMCZBXC	ClC1=C(C=C(Br)C=C1)C(=O)NC2=CC=C(C=C2)N3CCN(CC3)C(=O)	0.251374
XMZLNSMXWQVWPG	COC1=CC=C(OC)C(=C1)CN2CCN(CC2)C3=CC=CC=C3OC	0.225576

XMZXFBNWTRFDHM	CSC1=NN=C(N1C)C2=CC3=C(S2)N(C)N=C3C4=CC=CC=C4	0.234533
XNBYSSAJBPEUKS	COC1=C(OCC2=C(Cl)C=CC=C2)C(Cl)=CC(CNCCO)=C1	0.23044
XNSBJXRQWVZUOP	CCC1=CC=C(OCC(=O)NCC(N2CCCC2)C3=CC=C(Cl)C=C3)C=C1	0.234307
XNZVPGGSVXSUSN	COC1=CC=C(C=C1)\C=N\[N]2N=NC3=CC=CC=C23	0.223457
XOAHCZLVGODQES	COC1=C(C)C(OC)=C(CN2CCCN(C)CC2)C=C1	0.254227
XOLWHVLUFVZICJ	FC1=CC=C(C=C1)N2CCN(CCCNC(=O)NC34CC5CC(CC(C5)C3)C4)	0.277956
XOPKXVAUECUSFM	CNC1=C(N=NC(=N1)C2=NC=CC=C2)C3=CC=CC=C3	0.257234
XOSNMLBMTVINPR	C=CCC1=C(OCCCCN2CCCC2)C=CC=C1	0.251863
XPOIPIVHRYJHLA	CN(C)C1=NC(NC2=CC=C(F)C=C2)=NC(N\N=C\C3=CC(=C(Cl)C=C3)	0.238663
XQMYCQQCDKZGI	CC1=NN(C2=CC=C(Br)C=C2)C(=O)C3=C1C=CC=C3	0.22243
XQRAEIQSGHFRC	FC1=CC=C(C=C1)C2N(CC3=CC=CN3C4=NC=CC=N4)CCC5=C2NC	0.286568
XQRGYPGMSXNSLK	CCNC1=NC(=NC(SCCOC2=C(Cl)C=C(Cl)C=C2)=N1)N(C)C	0.227039
XQSONAFMYBJTGJ	COC1=C(OCCNC2=C(C=CC(=C2)N3CCCC3)[N+](O)=O)C=CC(0.226328
XQWPPFJWBZMAGP	FC1=CC=C(\C=N\N2CCN(CC3=CC=CC=C3)CC2)C=C1	0.2462
XRCKKZPNRBOXOH	C(SC1=NC(C2=CC=CC=C2)=C(N=N1)C3=CC=CC=C3)C4CCCCO4	0.283175
XRJDYIVGHNOQNU	COC1=CC=C(CN2CCCCC2)C(=C1)C	0.232936
XROYHKODSHBIJX	CC1CCN(CCOCCOC2=C(Br)C=C(C)C=C2Cl)CC1	0.289022
XRTLIRBMJKGLAX	CCN(CC)CCCC(C)NC1=C2C=CC=C(Cl)C2=CC=N1	0.279719
XRYRDSCHVPEDDZ	COC1=CC=C(CC2(CO)CCN(CC2)C(C)CC3=CC=C(Cl)C=C3)C=C1	0.26003
XSDCKVSJIPPTLU	COC1=CC(=CC(OC)=C1OC)C2=NN=C(O2)C3=CC(OC)=C(OC)C=C3	0.271856
XTVRXXHHMRQUOD	CCOC1=C(NC(=O)C2=C(C=CC=C2)C3=NC(=NO3)C4=C(OC)C=CC=	0.236184
XTWWYLPZORXWTF	COC1=CC=C(CN(C)C2C3=C(C=CC=C3)C4=C2C=CC=C4)C=C1	0.243167
XTYXZJSDLRFGGW	CC1CCN(CCCNC(=O)C2=CC3=C(C=C2)C(Cl)=C4CCCC4=N3)CC1	0.260185
XUPRUNUGPGVWPP	CN1C(C)=C(CN2CCC(CO)(CC3=CC(=CC=C3)C(F)(F)F)CC2)C4=C1C	0.224862
XUWYSQMGAWAZQW	O=C(N1CCN(CC1)C2=NC=CC=C2)C3=CN(N=C3C4=CC=CC=C4)C!	0.227142
XVDDBSXNXPJEM	CN(C1=CC=CC=C1)C2=CC=C(\C=N\NC(=O)CC#N)C=C2	0.238236
XVMDUCPLYPUKEG	CC1=NN(C(N2CCCC2)=C1\C=N\NC(S)=NC3=C(F)C=CC=C3)C4=C1	0.251711
XVVBDUOUGLIMR	CN(C)C1=NC(=NC(=N1)N(C)C)N(CCOCC2=C(C)C=CC=C2)C#N	0.24046
XWZUSZPPQUXYNV	FC1=CC=C(C=C1)N=C(S)N2CCN(CC2)C3=CC(=CC=C3)C(F)(F)F	0.254867
XXCFJIHBZYKRJW	NC(=N)SCC1=NC=CC=C1	0.241112
XXEVSQAQCVZSPDL	CN1CCN(CC1)S(=O)(=O)C2=CN=C(SCCOC3=CC=C(Cl)C=C3)C=C2	0.234732
XXLDPDOCCFMHIA	COC1=CC2=C(C=C1)C=C(C=C2)C(=O)C3CCCN(CC4=NC(C)=CC=C	0.230503
XYEXGCQCDHETHC	CCN(CC)CC(O)COC1=CC2=C(C=C1)N(C(C)=C2C(C)=O)C3=CC=CC	0.241645
XYSDIGROKUHACN	COC1=C(OCC2=C(Cl)C=CC=C2)C=CC(\C=N\N=C(N)N)=C1	0.234591
XYXKHGAQYACMPR	COC1=CC(OC)=C(CN(C)CC(=O)NC2=C(C=CC=C2)C3=CC=CC=C3)(0.222502
XYZXEIUKQGUHB	ON=C1C2=C(C=CC(=C2)S(=O)(=O)N3CCCC3)C4=C1C=C(C=C4)S	0.224278
XZCQCHRLIZPEIN	CC1=NC(NCC2=CC=CC=C2)=NC(N\N=C\C3=CC(Cl)=CC=C3)=C1	0.224395
XZDFNIDCZGYSMU	CCOC1=CC=C(CN(CC2=CC=CO2)C(C3=CC=CS3)C4=NN=NN4C(C	0.232895
XZHFWCWADXWVLL	COC1=CC=C(Cl)C=C1NC(=O)Cl Enamine, T5324190	0.245539
XZOZBBDBFWCZCC	COC1=CC=C(C=C1)C(CNC(=O)C2=CC=C(O2)C3=C(Cl)C=CC=C3)N	0.236303
XZTPUNHHNWXMLJ	CCOC(=O)C1CN(C)CCC1=O	0.245831
XZZUXWKCGOUDZ	COC1=C(OCC2=CN=C(Cl)C=C2)C=CC(CNCCC3=CC=C(F)C=C3)=C:	0.29799
YACADTMYZRABHM	CN1N=C(C(C#N)=C1N2CCN(CC2)C3=CC=C(F)C=C3)C(F)(F)F	0.235865
YAEUAZNKYXGVKH	COC1=CC(CN2CCN(CC2CCO)C3CCN(CC3)C4=C(C)C(C)=CC=C4)=	0.227092
YAQAMRXMQVIDBU	COC1=CC=CC(OC2=NC(=NC3= Vitas-M Laboratory, STK553023	0.234725
YAVBNHNDCLVGOW	COC1=CC(OC)=C(CN(CCN(C)C)CC2=CC=CC=C2)C=C1	0.228011
YBGHYHKRKJSQHV	C(N1C=CC(=N1)C2=CN=C(S2)C3=CC=CC=C3)C4=CC=CC=C4	0.22958
YBNZHOBZGSLGG	CC1CCN(CCOCC2=CC(Cl)=C(Cl)C=C2)CC1	0.240935

YCHCRFRAIDBMRW	CCOC1=CC=C(NC2=NC(CSC(=S)N3CCN(CC3)C4=CC=CC=C4)=NC	0.224948
YCIJUAKRNMVHFQ	ClC1=CC(NC(=O)NCCN2CCN(CC2)C3=CC=CC=C3)=CC=C1	0.233079
YCNJFNRSARUTEH	[O-][N+](=O)C1=C(Cl)C=CC(=C1)C2CC(=O)NC3=C4C=CC=CC4=CC	0.224618
YCQUKKCTTOZLLL	COC1=C(CC(N)=NOC(=O)C2=CC=CS2)C=CC=C1	0.25362
YCTVRLVATDMYPU	CCCCCCCC[N+]=C2C=CC3=C(C=CC=C3)C2=CC=C1	0.225564
YDADTNARCJIMQM	OC1=CC(=CC=C1)C2=NN=C(N=N2)C3=CC(O)=CC=C3	0.294578
YDQUEQNSRJTDHO	CN(C)C1=NC(=NC(=N1)OCC#N)NC2=CC=C(Cl)C=C2	0.230697
YEFOWGFKCOZUDR	[O-][N+](=O)C1=CC=C(C=C1)\C=N\N2CCCCC2	0.239733
YEQQSYNQFNIVQJ	COC1=C(OC)C=C(C=C1)C2=NOC(CCCOC3=CC=CC=C3)=N2	0.271667
YFXVIJAMQNMHR	CN1CCN(CC1)[S+][O-](=O)C2 Vitas-M Laboratory,STK409218	0.238345
YGBFCWQOXYENNE	O=C(N1CCCCC1)C2=CC(=CC=C2)S(=O)(=O)N3CCN(CC3)C4=C	0.235688
YGEMUJHRXZSIBA	ClC1=CC=CC(=C1)N2CCN(CCCNC(=O)C3CCC(=O)N3CC4=CC=CC	0.223234
YGGOBODDGKFPLE	O=S(=O)(N1CCN(CCOC2=CC=CC=C2)CC1)C3=CC=CS3	0.223601
YGLXNWNMISTXHH	CCOC(=O)C1=C(C)N(CCC(=O)N2CCN(CC2)C3=C(OC)C=CC=C3)C(0.23313
YGWFWAPUTWVGDK	COC1=CC(NC(=O)C2CC(=NO2)C3=CC=CC(OC)=C3OC)=CC(OC)=C	0.234433
YGWSMQFKFPYRRP	CC1=CC=C(C=C1)C2=NN(C=C2CNCC3=CC=CC=C3)C4=CC=CC=C	0.223296
YHAIUXOOUWRJIE	CN1CCN(CCOCCOC2=C(Cl)C=C(Cl)C=C2Cl)CC1	0.250417
YHVDSLJVICOSOM	COC1=CC=CC2=C1C3=C(N=CN3)C4=C2C=CC=C4OC	0.230999
YHZKIEWEQQRAHY	C(N1CCN(CC2=CC=CC=C2)CC Vitas-M Laboratory,STK146865	0.272495
YIBWFLHBLUUTEL	O=C(NC(C1=CC=C(C=C1)C2=CC=CC=C2)C3=NC=CN=C3)C4CCN(0.234033
YIIQGQGVJVFUGR	CC(NC(S)=NC1=C(C)C(C)=CC=C1)C(N2CCN(C)CC2)C3=CC=CC=C3	0.285682
YIPQJDIPICHMBD	C[N]1C(=CC2=C1C=CC3=[N+][O-]ON=C23)C4=CC=CC=C4	0.230987
YJAKNSVSOFNUEU	C1CCN2C(CC1)=NC=C2C3=CC=C(C=C3)C4=CC=CC=C4	0.242055
YJBWNJQTWJVEDN	CC(C)CCNC(S)=NC1=CC(C)=CC=C1	0.231895
YJCNXTICFCJHSA	CCN1CCN(CC2=CC=C(NC(=O)NC3=C(Cl)C=CC=C3)C=C2)CC1	0.239704
YJFVNNCYAHNNJN	CSC1=CC=C(NC(=O)NCCN2CCC3=C(C2)C=CC=C3)C=C1	0.224092
YJOAHLWLYTVYGJ	ClC1=CC=CC(=C1)N2CCN(CC2)CC3=NC(=NO3)C4=CC=CC=C4	0.223707
YJSATLBWFLERNZ	NC1=C(\C=C\C2=C(N)C=CC=C2)C=CC=C1	0.234456
YJXVBAMNAUTWBU	COC1=CC=C(NC2=NC3=C(C=CC=C3)C(=N2)N4CCCC4)C=C1	0.225531
YKATUCHACQFGBL	ClC1=C(Cl)C=C(CN2CCCCC2)C=C1	0.233431
YKJWAZAPTHMAIX	CCN(CC)C1=CC=C(CNC2=NC=C(Br)C=C2)C=C1	0.241442
YKJYNHWALGMAIC	ClC1=CC(=CC=C1)N2CCN(CC2)C(=O)C3=C(NC(=O)C4=CSCCO4)C	0.227475
YKWJBTXSMBSCM	CC(C)(CN1CCN(CC1)C(C2=CC=CC=C2)C3=CC=CC=C3)NS(=O)(=O	0.266636
YLDDBXFNJPDEFG	COC1=CC=C(C=C1)C2=NNC=C2\N=N\C3=CC=CC=C3	0.232943
YLQCIDVEFQMREC	CCOC1=C(OCC2=CC=CC=C2)C=CC(\C=N\NC(=O)C3=CC=C(CN4C	0.227145
YMRIBQFQMYWELA	ON(C(=O)CF)C1=CC=C(\C=C\C2=CC=CC=C2)C=C1	0.252226
YMSXBMKZFMDQFV	COC1=C(C=CC=C1)C2=C(C3=C(S2)C=CC=C3)C4=CC=C(OCCN5C	0.248383
YMZVLZHCYJIACQ	ClC1=CC=C(CON2C(=NC3=C2C=CC=N3)C4=C(Cl)C=C(Cl)C=C4)C	0.22634
YNBSSBNRDINQBO	CC1=CC(C)=C(NS(=O)(=O)C2=CC(=CC=C2)C(=O)NC3CCN(CC4=CC	0.227804
YNUKFHCQPMDEIC	CC1=CC(N\C(S)=N\C2=NC=CC=C2)=CC(C)=C1	0.230106
YNZWVGC MZYGYOV	CN1C(NC2=CC(Cl)=CC=C2)=NC3=C1C=CC=C3	0.236738
YOQPNFAYDVSJIE	COC1=C(OCC2=NC(=NO2)C3=CC(=CC=C3)[N+][O-]C=CC=C1	0.229033
YPDFVIZRPIOETL	CN1CCN(CCOCCOC2=C(Cl)C=C(C)C=C2C)CC1	0.232407
YPDNPMKGMDEINC	COC1=C(C=C(C=C1)C(=O)NC2=CC=C(C=C2)N3CCN(CC3)C(=O)C4	0.226413
YPDVXRQZIAHANI	CN(C)CCC1(CC\C=C\C2=CC=C NCI Chemotherapeutic Agents R	0.235455
YPIFHZHPFBNDDA	CC1=CC(Cl)=C(OCC(O)CN2CCN(CC(O)COC3=C(Cl)C=C(C)C=C3)C	0.231733
YPMIXQBDVYQRG	COC1=NC(=NN=C1C2=CC=CC=C2)C3=CC=CC=C3	0.234186
YQJNGUIVACYDCQ	COC1=C(C)C(OC)=C(CN2CCN(CC2)C3=NC=CC=C3)C=C1	0.223707

YQUZBSAZFAVTFB	CNCCOC1=CC(Cl)=C(Cl)C=C1	0.258295
YRCLNXAIBPJRBO	CN1CCN(CC1)C2=C(NC(=O)C3=CC=C(C=C3)S(=O)(=O)N4CCCCC(0.23079
YROSPBQXYVDYAU	OCCN1CCN(CC(O)COC(C2=CC Enamine,T5387682	0.250185
YRUFWIJTPCWFSO	CC1=N[N](C(=C1)C)C2=NC(=CS2)C3=CC=CC(=C3)Cl	0.231552
YRWYXGXPZQBKW	COC1=C(F)C=C(C=C1)C(=O)C2CCCN(CC3=CC=CN3C4=NC=CS4)C	0.235309
YSVVNZDXGKELPV	[O-][N+](=O)C1=CC=C(NCCCN(S(=O)(=O)C2=CC=CC=C2)C=C1	0.226359
YSWDVDXLKARVHE	CC1=C(C)C(=CC=C1)N2CCN(CC2)C(C3=NN=NN3CC4CCCO4)C5=	0.256678
YTBLBUCXWXBYTR	SC(NC1=CC=CC=C1)=NC2=C(Cl)C=C(Cl)C=C2	0.23132
YTCYEKCFMOMEJ	CC1(C)COC(=N1)C2=CC=C(F)C=C2)[N+][[O-]]=O	0.234968
YTKCEXKGQFVUGH	COC1=CC(=CC(OC)=C1OC)C(=O)NC2=CC3=C(CCC4=C(C=CC=C4)	0.278147
YTLJAXHEKBPJQN	CC1=CC(=CC=C1)N=C(S)NC2CCSC3=C2C=CC=C3	0.255988
YTPFRDGVWSSNF	CN(CCOC1=CC=C(Br)C=C1)CC(O)COC2=CC=C(C=C2)C#N	0.326304
YTRGFQPXRJRJV	C1CN(C(N1C2=CC=CC=C2)C3=CN=CC=C3)C4=CC=CC=C4	0.224447
YTZREVYYYUASL	COC1=CC(OC)=CC(CN2CCN(CC3=C(OC)C(OC)=CC=C3)CC2)=C1	0.243109
YUAAKHMUHFDSQF	CC1=NC2=C(C=CC=C2)N1CC3=C(C)C=CC=C3	0.276316
YUASKPYMGRGXGC	CN1CCN(CC1)C2=CC(NCCOC3=CC(C)=CC=C3)=C(C=C2)[N+][[O-]	0.268209
YUEHBYHERLEJFD	CC(C)(C)[N]1N=NN=C1C(N(CC2CCCO2)CC3=CC=CO3)C4=CC=CC	0.226421
YURSBVUJARRCNH	COC1=CC(OC)=C(C=C1)C(=O)ON=C(N)CC2=CC=C(C=C2)[N+][[O-]	0.240587
YVFSPCXAFARSTI	CCN1CCN(CC1)C2=C(NC(=O)C(C)OC3=CC=C(F)C=C3)C=C(C=C2)!	0.224237
YVNXXZDHQCSSQMR	C(=C1C2=C(C=CC=C2)C3=C1C=CC=C3)C4=CC=NC=C4	0.225737
YVPHSJUQTKQEGB	COC1=CC=C(CN2N=NN=C2CN(CC3=CC4=CC(C)=CC=C4N=C3O)(0.223807
YVSYLHWDHCXCTK	C1OC2=CC=C(CN3CCN(CC3)C(C4=CC=CS4)C5=NN=N[N]5CCC6:	0.248013
YVXIXZJFMGMWDW	CCN(CC)CCNC(S)=NC1=CC2=C(C=C1)N=C(C=C2)N3CCN(C)CC3	0.267182
YWBVLUMOMXAOPU	CN1CCN(CC1)C2=NC(CSC3=CC=CC=C3)=NC4=C2C(C)=C(C)S4	0.238684
YWLNLLOBROCLLKK	CC1CN(CC(C)N1)C2=CC(NCCOC3=C(C)C=CC=C3)=C(C=C2)[N+][[O-	0.228437
YWNFILIWSMKDLW	CCN(CC)CCNC1=NC(SC)=NC2=C1C3=C(CN(C)CC3)S2	0.242075
YWOOXOMNPREADPY	FC(F)(F)C1=CC(=CC=C1)N=C(S)NC(C2=CC=CC=C2)C3=CC=CC=C3	0.223711
YXHPXFQFVVHCME	ClC1=C(Cl)C=C(C=C1)N2N=NN=C2C3=CC(Cl)=C(Cl)C=C3	0.242267
YYEWCRIJAUKIKEQ	CCOC(=O)C1=C(N=C(OC2=CC=C(F)C=C2)C(=C1)C#N)C3=CC=CC=	0.255482
YYFIPTVPONYMFK	FC(F)(F)C1=CN=C(C=C1)N2CCN(CC2)C3=CC(=NC4=NC=NN34)C!	0.227304
YYHQUEROCIPNHFR	COC1=CC(=CC=C1)C2=NOC(=N2)C3=CN=C(Cl)C=C3	0.245487
YYVASTQFSXAUPG	ClC1=CC=C(NC(=O)NC2=CC=C(C=C2)C#N)C=C1	0.238012
YYVCSTQMHUYFGD	CC(C)(C)NC(=O)CN(C1CCN(CC1)CC2=CC=CC=C2)C(=O)CN3N=C(I	0.22948
YZBPKQBEEHXFCA	CC1=CC=C(OCCSC2=C3N=CNC3=NC=N2)C=C1	0.225552
YZEDAXTWYXOVDJ	[O-][N+](=O)C1=C(NCC2=CN=CC=C2)C=C(C=C1)N3CCN(CC3)C(=	0.238716
YZULJWWBOANRNC	C1CCCN(CC1)\C=C\C2=NN=NN2C3=CC=C(C=C3)C4=CC=CC=C4	0.283704
YZZZCDZBYLHNLN	O=C(C1CCCN(C1)C2CCC2)C3=C4C=CC=CC4=CC=C3	0.239325
ZABIMHRWORHDFC	CCOC(=O)C1=C(NC(=O)CN2CCCC2)SC(CN(C)C)=C1C3=CC=CC=	0.252603
ZASVDCRANMSGBG	FC1=CC=C(CN2CCN(CC2)C3=NC=NC4=C3C(=CS4)C5=CC=CC=C!	0.255687
ZATCHDAVJHRYTK	COC1=CC(CC(=O)NC2=NC(=CS2)C3=CC(F)=C(F)C=C3)=CC(OC)=C	0.22806
ZBFZRHMNASCPJB	CCN(CC)CCNC(=O)C1=C2C=CC=CC2=NC(NC3=CC(OC)=C(OC)C=C	0.224364
ZBNGBSRKPXQTGI	FC1=CC=C(C=C1)N2CCN(CC2)P(=O)(OC3=CC=CC=C3)OC4=CC=C	0.280635
ZBRAZSSUZUUNKU	COC1=CC=C(C=C1)C(=O)NCC(N2CCC3=C2C=CC=C3)C4=CC=CO4	0.231729
ZBTPFTLDGWUGCW	CN1CCN(CC2=C(OC(=O)C3=CC=CS3)C4=C(C=CC=N4)C(Cl)=C2)C	0.236591
ZBUFFWHKOVJHW	COC1=C(OC)C(OC)=C(CN2CCN(CC2)C(=O)C3CCC(CNS(=O)(=O)C4	0.241472
ZBZQCRFWASEUCI	COC1=CC=C(C=C1)C(=O)NNC(S)=NC(=O)C2=CC=CS2	0.222673
ZCOHOUIKFBCXOF	COC1=CC(=CC(=C1OC)OC)CSC2=NN=N[N]2C3=CC=C(C)C=C3	0.265188
ZDVMNCRUFXKDP	COC1=C(CNC(=O)CC2=CSC(NC(=O)NC3=C(OC)C=CC=C3)=N2)C=	0.227433

ZDXDTRDQJPEQRA	CC1=CC=C(C=C1)[S+][([O-])=O]C2(CCCC2)[S+][([O-])=O]C3=CC=C	0.251796
ZDJZTQJMGWRFBP	FC1=CC=C(C=C1)C(NC(=O)C2CCN(CCOC3=CC=C(Cl)C=C3)CC2)C	0.224153
ZEMAHOYXOAHHGN	CC(C)CN1CCN(CC2=CC=C(C)S2)CC1CCO	0.231621
ZFAVZYVAYDNLNT	COC(=O)C1=CC(NC(=O)NC23CC4CC(CC(C4)C2)C3)=CC=C1	0.241076
ZFHBIKVGKIVQB	CCOC(=O)C1CCN(CC2=CC(OCC3=CC=CC=C3)=C(OC)C=C2)CC1	0.239505
ZFTWMJHRJKDXSR	CC(N(C)CC(=O)NC1=C(Br)C=CC=C1)C(=O)NC2=CC=C(C=C2)C#N	0.262513
ZGIUFOVBQWVHDX	CCOCCN1CCN(CC1)C2C3=C(CSC4=C2C=CC=C4)C=CC=C3	0.291077
ZGSQBSCXVDPEMV	CN(C)CCOC1=CC2=C(C=CC=C2)C=C1	0.224761
ZGWMOSSZJKBYAW	CN(CCCNC(=O)C1=CN=C(\C=N\O)C=C1)CCN(C)CC2=CC=CC=C2	0.224946
ZGWXCNXAALTBR	CC1=CC(N=C(S)NCCSC2=CC=C(Cl)C=C2)=C(C)C=C1	0.233804
ZHBZKSPOQFXRSY	C=CCNC1=NC(=NC2=CC=CC=C12)N3CCCC3	0.229569
ZHILCVPERMUCCT	C=CCN(CCOC1=C2C=CC=CC2=CC=C1)CC=C	0.24662
ZHRFLBVUJAQJHO	COC1=CC=C(OCCN2CCN(CC2)S(=O)(=O)C3=C(C=CC=C3)C(F)(F)F	0.241299
ZHXZWDYFYZQMN	CCCCN(C)CCNC(=O)C1=CC2=C(S1)N(C)N=C2C3=C(F)C=CC=C3	0.226072
ZIDPTDWLCMNPFO	FC1=CC=C(C=C1)C2=C(C=NN2C3=CC=CC=C3)S(=O)(=O)C4=CC=C	0.258907
ZIDVFGTVNOAXTE	COC1=C(OCCOCCN(C)CC2=CC=CC=C2)C=CC(C)=C1	0.232924
ZITAWLJLIBKOH	CC1CCN(CCOC2=CC=C(C=C2)C(=O)C3=CC=CC=C3)CC1	0.230691
ZJLXFJDCINNRNW	CN1C(Br)=C(Br)N=C1S(=O)(=O)C2=CC=C(C=C2)[N+][([O-])=O	0.237302
ZJZRYLBMXBZUGD	COC1=CC=C(C=C1)N2CCN(CC3=NC(=NO3)C4=C(Cl)C=C(Cl)C=C4	0.222332
ZKBVDJKPVBCIEC	CC(C)(C)CNC1=C(C=CC=C1)N2CCOCC2)[N+][([O-])=O	0.23567
ZKMJZXOMSGVIQP	[O-][N+]1=C2CCC3=[N+][([O-])N(N=C3C2=NO1)C4=C(Cl)C=CC=C4	0.237064
ZKRWGPGVLZYPQJ	CC1=NC2=NC=NN2C(=C1)N3CCN(CC3)C4=NC5=C(S4)C=CC=C5	0.2231
ZKWRDHCBHIAZKI	COC1=CC=CC(=C1)CN(CC2=CC=CO2)C(C3=CC=C(F)C=C3)C4=NN	0.235664
ZKZWUEUAOWRWKC	CN1CC2=C(N=C(SCC3=CC=CC=C3)C(=C2CC1(C)C)C#N)N4CCOC	0.224863
ZLAZENKFQYTDGL	CCOC1=CC=CC(=C1)[N]2N=NN=C2C3=CC=C(OC)C=C3	0.249213
ZLPGMNPGWZWWCLN	FC(F)SC1=CC=C(C=C1)N=C(S)N2CCN(CC2)C3=NC=CC=C3	0.24509
ZLTYBEKAYYHILM	ClC1=CC=C(C=C1)S(=O)(=O)NCC(NC2=CC=CC=C2)C3=CC=CC=C3	0.253751
ZMGHADYRVNWWLD	CC1=NN2C=C(C=NC2=C1Cl)C3=CC(Cl)=CC=C3	0.222776
ZMGNVVUFDUOJQI	COC1=CC(=CC=C1)N=C(S)N2CCN(CC2)C(C3=CC=CC=C3)C4=CC=	0.244555
ZMWKFSKLWQPAOQ	CCN1CCN(CCOC2=CC(OC3=CC=CC=C3)=CC=C2)CC1	0.271432
ZNFQWIJKUZYKJ	CCOC(=O)C2(CCOC1=CC=CC=C1)CCN(CC3=CC(OC)=C(F)C=C3)C	0.293047
ZNFUABFFPMZGHF	COC1=C(Br)C=C(C=C1)C2=CN3C=C(C)C=CC3=N2	0.231774
ZNPYASUNUPFMLC	[O-][N+](=O)C1=CC=C(C=C1)N2CCN(CC3CCCC3)CC2	0.247842
ZNQJZQNOZIAORO	CCN(CC)C1=CC=C(C=C1)C2=C(C#N)C(OC)=NC(N)=C2C#N	0.232027
ZNQPBWPWNXLKKI	OCCCN1C2=CC=CC=C2NC3=NN=C(C=C13)C4=CC=CC=C4	0.244288
ZNZUODPKZHQQOI	COC1=CC=C(C=C1)N2CCN(CC2)C(C3=CC=CC=C3)C4=NN=N[N]4	0.226943
ZODNOJAQEVPKOW	CCN1CCN(CCCNC(=O)C2=CC3=C(S2)C4=C(NC3=O)C=CC=C4)CC	0.234911
ZOEGUHLNLRALRO	CC1=CC(C2=NNC=C2CN3CCCC(CO)(CC4=C(C)C=CC=C4)C3)=C(C	0.264631
ZOGOKWMZPSMNOR	C\N=C(/S)N1CCN(CC1)C2=CC(Cl)=C(Cl)C=C2	0.227522
ZOJJVSZFIYSTHC	COC1=CC=CC(OC)=C1OCCCN2CCN(CC2)C3=C(OC)C=CC=C3	0.277358
ZOQSXBXNFXEJQF	S=C1SCN(CC2=CN=CC=C2)CN1CC3=CN=CC=C3	0.228235
ZORVKOINJWFODK	COC1=CC=C(C=C1)C2CC(=NN2C(=O)C3=CC(=C(Cl)C=C3)[N+][([O-	0.23357
ZOSTWKQFNTANW	O=C(NC1=CC2=C(C=CC=C2)C=C1)C(C3CCCC3)C4=CC=CC=C4	0.238594
ZOZZSEQNQKZZGQ	CC1=C(C=CC(OCCCN2CCN(CC3=CC=CC=C3)CC2)=C1)[N+][([O-])=	0.230648
ZPOIPOCHHDZVHE	CCN1CCN(CC1)C2=C(C(N)=NC(NC3=CC(C)=CC=C3)=N2)[N+][([O-	0.256342
ZPVOJBNNZLIFED	ClC1=CC=C(C=C1)N2CCN(CC3=CC=C(Br)O3)CC2	0.244694
ZQIAXDULHBLZJE	CC1=C(C=O)C=CC(=C1)N(CCCl)CCCl	0.267939
ZQJXZFKBPDFCDC	COC1=C(NS(=O)(=O)C2=C(C=CC(NC(=O)C3=CN=CC=C3)=C2)N4C	0.234906

ZQQBASAIFGTMSU	COC1=CC(=CC(OC)=C1OC)C2=NN=C(O2)C3=CC=C(C=C3)N4CCO	0.272232
ZRHSCMXFOILLCB	CC1CCCC(NCC(O)COC(C2=CC=C(F)C=C2)C3=CC=C(F)C=C3)C1C	0.223447
ZRPJIHBJJOQXBX	SC(=NC1=C(OC2=CC=CC=C2)C=CC(Cl)=C1)N3CCN(CC3)C4=NC=	0.282632
ZSCIEDIHFGRRIK	COCCCNCCOCCOC1=C(C=CC=C1)C2=CC=CC=C2	0.24549
ZSHCLQJTSSARQ	CC1=CC(=CC=C1)N2C(SCC3=CC=C(C=C3)C#N)=NN=C2C4=CNC5	0.224595
ZSNQFQRLXCCVTP	CC1=C(CN2CCCC(C2)C(=O)NCCCN3CCOCC3)N=C(O1)C4=CC=C(0.229227
ZTWXGQRMVGRICE	CN(CC1=CN(C)C2=C1C=CC=C2)C(\S)=N\C3=CC=C(C)C=C3	0.257878
ZTZHQEVUDFQCKW	CC1=C(C=CC=C1)C2=C(N=CO2)C(=O)NC3=C(NC(=O)C4=NC=CC=	0.236923
ZUFBFBOOLBCCCM	CCCCNC(S)=NC1=CC2=C(C=C1)N=C(C=C2C)N3CCN(CC)CC3	0.251118
ZUGMTXDCVONBCH	CN(C)CCNC=C(C(=O)NC1=CC=C(Cl)C=C1Cl)C(=O)NC2=CC=C(Cl)C	0.225081
ZUJRILFEGPWBCR	COC(=O)C1=CC=C(NC(=O)NC2=C(F)C=CC=C2)C=C1	0.251432
ZUVIQGVPQYCQRJ	CC1=NC(N2CCN(CCOC3=CC=C(Cl)C=C3)CC2)=C(C#N)C(C)=C1	0.248173
ZUWVDYUCNFGIJG	COC1=C(OCC2=CN=C(Cl)C=C2)C=CC(CNCCC3=CC=CC=C3)=C1	0.262597
ZVFNTPHUFQNXLT	CCCC(N1CCN(CC1)C2=CC=CC=C2F)C3=NN=N[N]3C4CCCC4	0.237118
ZVGLSKOEGXKKZ	NC1=NC(=NC2=CC=C(Br)C=C2)C3=C1C=CC=C3	0.229685
ZVHFPVLLVIJCMW	CC1=CC(OCC(O)CN2CCN(CC3=CC4=C(OCO4)C=C3)CC2)=CC(C)=	0.243523
ZWFDVHHCQGZZQC	CN1CCN(CC1)C2=C(NC(=O)CSCC(=O)NC3=CC(C)=CC=C3)C=C(Cl)	0.242685
ZWRGSLGTWZRDMP	NC(S)=N\N=C1\C2=C(C=CC=C2)C3=C1C=CC(Br)=C3	0.24359
ZWWBESRHLHFGRU	COC1=CC=C(C=C1)C2=C(C)SC(NC3=NCCCC3)=N2	0.255238
ZXVNJVRAbsCRGU	OC1=C(C=CC=C1)C2=NNC(=C2)C3=CC=C(Cl)C=C3	0.235764
ZYCASFPOFAJMAJ	COC1=CC=C(C=C1)C2=C(C)N3CC4=C(C=CC=C4)C3=N2	0.226015
ZYKOBPNQNWRTTE	COC1=CC=C(CCNCC2=C3C=CC=CC3=CC=C2OC)C=C1	0.258682
ZYLLLUVNOGFKZ	CCN(CC)CCNC(=O)C1=CC2=C(S1)C=CC(Br)=C2	0.261627

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