

Supplementary Information

Multi-scale Computational Screening and Mechanistic insights of Cyclic Amines as Solvents for Improved Lignocellulosic Biomass Processing

Nikhil Kumar^{a,b}, Brian R. Taylor^{a,b}, Vallari Chourasia,^{a,c} Alberto Rodriguez,^{a,c} John M. Gladden,^{a,c} Blake A. Simmons^{a,d}, Hemant Choudhary^{a,c}, Kenneth L. Sale^{a,b,*}

^aJoint BioEnergy Institute, Emeryville, CA, 94608, USA

^bDepartment of Biosecurity and Bioassurance, Sandia National Laboratories, Livermore, CA, 94550, USA

^cDepartment of Biomaterials and Biomanufacturing, Sandia National Laboratories, Livermore, CA 94550, USA

^dBiological Systems and Engineering Division, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA

^eDepartment of Bioresource and Environmental Security, Sandia National Laboratories, Livermore, CA 94550, USA

*Corresponding authors:

KLS: klsale@lbl.gov; klsale@sandia.gov

Table S1. List of cyclic amines used for Screening of biopolymers using the COSMO-RS model at 140°C and 1 atm pressure.

Compound	ln(γ)_Hemicellulose	ln(γ)_Cellulose	ln(γ)_Lignin
1-methylpiperidine-1-oxide	-4.65734518	-3.67765338	-3.78372425
2,3,4,6,7,8-hexahydropyrrolo[1,2-a]pyrimidine	-1.09992543	0.14909459	-2.07635201
1-piperazineethanamine	-1.1707466	0.06397863	-1.88843785
1-acetylpyrrolidine	-1.14740511	-0.14855522	-1.86779134
4-piperidinemethanamine	-1.17393808	-0.03291426	-1.82550727
pyrrolidine-1-carbaldehyde	-1.28871533	-0.47002297	-1.81480381
n-methyl-2-pyrrolidinone	-1.17274755	-0.3421156	-1.79525607
piperazine	-1.15542004	-0.47816	-1.76929551
2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine	-0.22915426	1.22121677	-1.71452494
1,2-dimethyl-1h-imidazole	-0.8545864	-0.00145274	-1.55156023
1-piperidinecarboxaldehyde	-0.53079931	0.3868061	-1.52953727
hexahydro-1h-1,4-diazepine	-0.64141404	0.32299367	-1.52346411
1,1',1''-phosphoryltripiperidine	0.9720409	3.34703243	-1.52298858
1-acetyl piperidine	-0.31420047	0.76611631	-1.52289635
pyrrolidine-1-carbonitrile	-0.76289769	0.04005871	-1.51876566
2-methylpiperazine	-0.56877482	0.42035748	-1.49336258
1-ethyl-2-methyl-imidazole	-0.43148814	0.57355418	-1.49076521
4-methylpyridazine	-1.09820878	-0.31305958	-1.48887664
1-piperazineethanol	-0.50716262	0.54939908	-1.47766879
butyl-amine	-0.20339297	0.77180938	-1.47539286
morpholine	-0.74493565	-0.0452708	-1.45843487
4-methylpyridine-1-oxide	-1.07138162	-0.25592547	-1.45725936
1-methylimidazol	-1.06498166	-0.38357672	-1.43587296
1,4-bis(2-hydroxyethyl)piperazine	-0.10232505	1.17436115	-1.43464373
3-methylpyridazine	-0.98538479	-0.2042484	-1.42389541
3-methylpyridine 1-oxide	-0.86591087	-0.0578407	-1.40876904
1-pyrrolidineethanamine	0.06693472	1.27338459	-1.39781959
1-aminopiperidine	-0.295329	0.6541182	-1.3682526
1-piperidinecarbonitrile	-0.18922772	0.65837444	-1.35144694
1-methyl-2(1h)-pyridinone	-0.88050881	-0.09973314	-1.34442765
1-methyl-2(1h)-pyridinone	-0.88010105	-0.09939137	-1.34416186
2-pyrrolidon	-1.46659199	-0.89243394	-1.32061426
1-methylpiperazine	-0.07803549	0.91123875	-1.31967471
1-butyl-2-methyl-imidazole	0.40524961	1.72510352	-1.29914605
pentylene tetrazole	-0.51488215	0.39043419	-1.29326227

trichloromelamine	0.41403847	1.35171482	-1.23761595
2-piperidineethanol	0.23091195	1.37623703	-1.23695032
1-piperazinecarboxylicacidethylester	0.25658775	1.44993577	-1.21542571
1,3,6-trimethyl-2,4(1h,3h)-pyrimidinedione	-0.39209216	0.49855803	-1.21386752
trans-2,5-dimethylpiperazine	0.22422207	1.32948889	-1.20952513
4-methoxypyridazine	-0.90213553	-0.15123616	-1.20896044
pyridazine	-1.07760101	-0.48431262	-1.20112805
phthalazine	-0.50614725	0.44884746	-1.19405213
3-methylpyrrolidine	0.37362536	1.35524128	-1.174287
2-pyridineethanol	0.25688104	1.24711799	-1.16176362
2-methylpyrazine	0.08198536	0.88141255	-1.14787165
pyridine	0.10403722	0.82029262	-1.1437111
3-fluoropiperidine	0.10722809	0.92666375	-1.13397512
thiomorpholine	0.29587639	1.07831566	-1.13063582
Ethylmorpholine	0.49506094	1.53269984	-1.12968
4-hydroxy-2(1h)-pyridone	-0.4381341	-0.25253982	-1.11220119
pyrazine	-0.21571286	0.40312922	-1.1090704
1-(2-nitrovinyl)pyrrolidine	-0.52534694	0.25157267	-1.10887898
3-methyl-1,2,4-triazine	-0.53364658	0.13643029	-1.10604034
n-nitrosopiperidine	0.2529002	1.05609853	-1.10340828
2,6-dimethylpyrazine	0.46486634	1.44321825	-1.10301802
3-methoxypyridazine	-0.15482987	0.6262919	-1.09567818
2,5-dimethylpyrazine	0.4971016	1.48407542	-1.09417354
indol-5-ol	-0.06652964	0.40100132	-1.09033494
2-methylpyrrolidine	0.56611727	1.55374947	-1.08657766
4-hydroxy-2(1h)-pyridone	-0.4212904	-0.23408263	-1.08299487
pyrido(2,3-b)pyrazine	-0.49917029	0.39470903	-1.08021183
2,6-dimethylmorpholine	0.38636886	1.37697123	-1.07863724
1-(2-nitrovinyl)piperidine	-0.28939612	0.59114679	-1.07148238
2,3-dimethylpyrazine	0.47719178	1.42245001	-1.0644804
piperidine	0.69025197	1.48440166	-1.06389642
6-methyl-2(1h)-pyridone	-1.04569893	-0.31656308	-1.06189787
6-methyl-2(1h)-pyridone	-1.04402091	-0.3154017	-1.06146199
4-methyl-2-thiazolamine	0.04565038	0.73450492	-1.05847928
4-methyl-2-thiazolamine	0.04509075	0.73359272	-1.05834565
4,5-dihydro-2-methylthiazole	0.59842558	1.42426736	-1.0572699
4,5-dihydro-2-methylthiazole	0.59966129	1.42557277	-1.05650611
3-amino-5,6-dimethyl-as-triazine	-0.75460502	0.05593692	-1.05039966
4-hydroxy-2(1h)-pyridone	-0.42981051	-0.25460525	-1.04868919

1-methyl-3-piperidinemethanol	0.7861035	1.94348079	-1.04787615
cyromazine	-0.69254413	0.16088316	-1.04465455
isoquinolineoxide	-0.10122927	0.8428572	-1.04362534
3,3-difluoropyrrolidine	0.02040166	0.73841501	-1.03589685
indole-2-carboxylic acid	0.59278156	1.24032263	-1.02547661
1-ethyl-2,5-pyrrolidinedione	-0.07545903	0.60777199	-1.02475978
(2r)-2-fluoropyrrolidine	0.08417237	0.70515523	-1.01984966
2-methylaminopyrazine	-0.05504586	0.73628712	-1.01458556
sym-triazine	-0.39401019	0.11821421	-1.00745781
2-ethylpyrazine	0.67603617	1.63576747	-0.9886579
2-propionylthiazole	0.37707739	1.30563092	-0.98804814
5-chloro-2-pyridinamine	0.25698236	0.99130035	-0.98268351
3-(methylthio)-2-butanone	0.5822468	1.42488451	-0.98175457
6-hydroxy-4(1h)-pyrimidinone	-0.27402279	-0.07572763	-0.97847618
1,3,5-trimethyl-1,3,5-triazinane	0.86565615	2.03890784	-0.97744271
2-piperidinemethanol	0.60174076	1.5206625	-0.97644808
1-methyl-2,5-pyrrolidinedione	-0.45497295	0.05980137	-0.97561274
1-benzoylpiperidine	1.20680522	2.5589493	-0.97300502
2-thiazolamine	-0.24756381	0.27091706	-0.97087979
2-propionylthiazole	0.38616563	1.31133758	-0.97082156
2-thiazolamine	-0.24643129	0.27189687	-0.97045724
2,4,6-tripicryltriazine	4.27700376	5.92756344	-0.96747933
1-methyl-2-piperidinethione	0.56552938	1.43263795	-0.96616579
4-vinylpyridine	0.71683153	1.66699504	-0.96480654
trimethylpyrazine	0.93462286	2.0577316	-0.96255041
thiazole	0.39499817	1.01947809	-0.95276709
thiazole	0.3993209	1.02431333	-0.95189338
2-methyl-3-tetrahydrofuranthiol	0.7924588	1.62846987	-0.94182907
2-methyl-1h-imidazole	-0.88357856	-0.30177652	-0.93313846
indole	0.85877334	1.5964511	-0.93213245
3,4-dihydro-1h-isoquinoline	1.00105034	2.10502071	-0.93177052
2-aminobenzothiazole	0.55244272	1.3777595	-0.9297627
2-aminobenzothiazole	0.55414221	1.37969853	-0.92930242
2-acetylthiazole c1 43	0.06835169	0.82333376	-0.92712328
dihydromethylcyclopentapyrazine	0.99760528	2.11328342	-0.92131129
2-fluoropyrazine	0.28488016	0.94711991	-0.91838308
caffeine	0.14483656	1.15682575	-0.91595834
4-methyl-5-thiazoleethanol	0.49167182	1.42253165	-0.91391247
4-methylthiazole	0.82903772	1.6389076	-0.91250135
4-methylthiazole	0.83092404	1.64080998	-0.9119003
2,4-dimethyl-5-acetylthiazole	0.93646859	2.01178446	-0.91116553

2-methyl-thiazole	0.87131536	1.68391015	-0.90090865
2-methyl-thiazole	0.87230072	1.68405509	-0.89986231
2-ethyl-6-methylpyrazine	1.10135868	2.23934854	-0.89962358
7-azaindole	0.34371729	1.09092268	-0.89802919
2-ethyl-5-methylpyrazine	1.10986806	2.25104646	-0.89626911
1,2,4-benzotriazine	0.32094992	1.2072961	-0.89444372
2-aminopyrazine	-0.60749797	-0.07302829	-0.8939998
5-isoquinolinamine	0.29081874	1.1995046	-0.88532118
methoxypyrazine	0.76988319	1.58943724	-0.88329406
2-propylpyrazine	1.10177421	2.22438784	-0.87846567
(3s)-3-fluoro-1-methylpyrrolidine	0.90526494	1.79883964	-0.87299852
2-piperidinecarboxylicacid	0.12297184	0.81726714	-0.87286707
4-methylpiperidine	1.18201222	2.10830641	-0.87113107
2-ethoxythiazole	0.94819451	1.87705839	-0.86960756
pyrazine-ethanethiol	0.83860042	1.82840101	-0.86923818
2,4-dimethyl-5-acetylthiazole	1.16595828	2.2715123	-0.86890491
pyrazin-1-ylethan-1-one	0.54165424	1.33634235	-0.86559855
1-piperidineacetonitrile	0.90216605	1.90449753	-0.86555883
n,n'-dimethylpiperazine	1.10583039	2.24551154	-0.86250817
3-(methylthio)-2-butanone	1.06174321	1.9454027	-0.86197162
trimethylisocyanurate	0.54091249	1.33787667	-0.85675601
2-mercaptomethylpyrazine	0.59992805	1.44184676	-0.85557012
2-ethyl-3-methylpyrazine	1.13930079	2.23656874	-0.85431014
3,4-dimethyl-1,2-cyclopentadione	0.69204442	1.43444456	-0.85399384
4,5-dimethylthiazole	1.14861962	2.11582698	-0.85035013
4,5-dimethylthiazole	1.15071148	2.11827297	-0.84929352
methylimidazol	-0.78296893	-0.21736704	-0.84786149
1,2,4-triazine	-0.62804314	-0.15672423	-0.84733716
2,5-dimethylthiazole	1.23485573	2.22161888	-0.84420237
10,11-dihydro-5h-tetrazolo[1,5-b][2]benzazepine	0.39339486	1.51405024	-0.8441248
isoquinoline	1.04750608	2.08737814	-0.84410832
2,5-dimethylthiazole	1.23872812	2.2264682	-0.84287888
5-azaindole	-0.14205352	0.58658844	-0.84252018
2,4-dimethyl-5-acetylthiazole	1.30740679	2.43659763	-0.84198629
3-(methylthio)-2-butanone	1.09420618	1.97607577	-0.84040185
3,4-dimethyl-1,2-cyclopentadione	0.63324438	1.36201392	-0.83917383
chloropyrazine	0.69969515	1.45176871	-0.83686182
methylindole	1.3365621	2.25116208	-0.83519525
4-Butylmorpholine	1.36293461	2.70555449	-0.83466333
6-azaindole	-0.12135092	0.5968766	-0.83458284

3,4-dimethyl-1,2-cyclopentadione	0.61606574	1.34099201	-0.8345226
2-Morpholinoethanol	-0.25490534	0.51932925	-0.833053
1-piperidinepropanenitrile	1.13000963	2.23605819	-0.83259136
n-hydroxyphthalimide	0.34456816	0.77784986	-0.83253953
1-piperidineethanol	1.24096912	2.33164948	-0.82866401
4-azaindole	-0.08068816	0.63116826	-0.82681997
3-(methylthio)-2-butanone	1.13674755	2.01944147	-0.8219555
2-isopropylpyrazine	1.21680444	2.31588275	-0.81527927
indole-3-carboxylicacid	0.1677503	0.70027089	-0.81526487
1-morpholinopropan-2-ol	0.2475858	1.18584907	-0.80932379
methylcyclopentapyrazine	0.1826813	0.91742645	-0.80426689
2-methoxy-6-methylpyrazine	1.19540829	2.19099136	-0.80353325
2-methyl-5-vinylpyrazine	1.1871955	2.23762181	-0.80256909
2-acetyl-3-methylpyrazine	1.08839624	2.06665099	-0.8008735
1-phenylpiperazine	1.37838412	2.62587699	-0.79739331
2-methyl-5-methoxythiazole	1.27041464	2.23712162	-0.79582794
2-methoxy-5-methylpyrazine	1.21008203	2.20408269	-0.79567597
9-methyl-9h-purin-6-amine	-0.65557193	0.12956183	-0.79405626
2-methyl-5-methoxythiazole	1.27869482	2.24693375	-0.79320594
pyridine-2,5-dicarboxylicacid	0.35067187	0.7390458	-0.79265486
2-ethylpyridine	1.29560741	2.33714545	-0.79055414
tetramethylpyrazine	1.43146555	2.69380289	-0.79011155
2,4-dimethylthiazole	1.3638366	2.35325996	-0.7879851
2,4-dimethylthiazole	1.37123491	2.36003781	-0.78456745
2,4,6-trimethoxy-1,3,5-triazine	1.02481113	2.0563785	-0.78231991
1-(fluoromethyl)pyrrolidine	1.07156254	1.92346972	-0.78176757
4-pyridinecarbonitrile	0.3381409	1.09769226	-0.78058593
3,3-dimethylpiperidine	1.30587183	2.48813818	-0.78030114
1-5-dimethyluracil	-0.49721573	0.16943629	-0.77747293
4-methyl-5-thiazoleethanol	0.443816	1.31617961	-0.77745347
indol-5-ylamine	0.12535362	0.78755594	-0.77744681
4-ethyl-4-methyl-2,6-piperidinedione	0.28226265	1.09233958	-0.77694063
2-{Methyl[3-(pyrrolidin-1-yl)propyl]amino}ethan-1-ol	1.83267141	3.54836851	-0.77316132
pyrazinyl-methyl-sulfide	1.14389506	2.0797762	-0.77301904
1-Pyrrolidineethanol	0.22385857	1.16300392	-0.77042767
2(1h)-quinolinone	-0.0433952	0.82369504	-0.76991414
3-chloro-6-methoxypyridazine	0.85718528	1.74766974	-0.76727563
4-methyl-5-thiazoleethanol	0.28845856	1.1319595	-0.76649062
3,5-dimethylpiperidine	1.36919921	2.58074999	-0.76524163
2-methylindole	1.43044898	2.36509437	-0.76476744

2-methyl-5-ethylpyridine	1.52205391	2.73158286	-0.76375709
2-pipecoline	1.34467005	2.33766567	-0.76370159
2,5-difluoropyrazine	0.6906975	1.4111706	-0.76284822
isopropenylpyrazine	1.24948325	2.27307067	-0.76148051
2-aminoacridine	1.17738567	2.40017598	-0.7600105
2-aminoacridine	1.1798589	2.40253972	-0.75992246
3-cyanopyridine	0.33511781	1.08103236	-0.75706471
1h-benzimidazole	-0.22350293	0.44314109	-0.75503373
2-acetylthiazole	1.04459074	1.8571838	-0.75338367
1-Piperazineethanol	0.63119408	1.87562211	-0.75336524
2-methoxy-3-methylpyrazine	1.32424564	2.32276253	-0.75239944
4-phenylpiperidine	1.8488298	3.07830008	-0.75167938
hexahydro-1h-azepine	1.23081766	2.284433	-0.75042332
4,5-dimethyl-1,3-thiazole-2(3h)-thione	1.05387077	1.90055115	-0.75011596
2-acetylthiazole	1.06626472	1.88112132	-0.74999949
4,5-dimethyl-1,3-thiazole-2(3h)-thione	1.05514283	1.90225725	-0.7498397
2,6-difluoropyrazine	0.77857711	1.52977156	-0.7495988
4-piperidineethanol	0.21174601	1.19580098	-0.74616992
3-pyridinemethanol	-0.12121588	0.52004973	-0.7402236
4-methyl-5-thiazoleethanol	0.38534947	1.23183121	-0.74011654
1-methyl-4-piperidinol	0.49411311	1.34091229	-0.72868166
2-cyanopyridine	0.53944885	1.30066401	-0.7273434
2-vinylpyridine	1.43328603	2.22647223	-0.72596824
indoline	1.35195948	2.25501018	-0.72231776
3-(2-hydroxyethyl)-1h-indole	0.62582336	1.49749243	-0.72213179
1-Ethyl-3-hydroxypiperidine	0.52638812	1.63220878	-0.72195293
2-methyl-5-isopropylpyrazine	1.61349975	2.88867491	-0.72136997
nicotine	1.70029299	3.08252013	-0.71985679
4-methyl-5-thiazoleethanol	0.45329279	1.31095653	-0.71913976
5-ethyl-2,3-dimethylpyrazine	1.62730896	2.90690973	-0.71806372
n-methylindol-2,3-dione	0.87517892	1.74611416	-0.71396004
simazine	1.66420659	3.05091071	-0.708618
carbamazepine	0.92481751	2.33047482	-0.70847291
3-ethyl-2,6-dimethylpyrazine	1.63879365	2.90625031	-0.70809907
4-methyl-5-thiazoleethanol	0.54051753	1.40206196	-0.70382895
isoquinolone-3-methyl	1.6119865	2.81972804	-0.70145956
1-methylisoquinoline	1.56253029	2.7418748	-0.70121174
1,3-dihydro-2h-indol-2-one	0.16387114	0.88928193	-0.69780109
4-ethylpiperidine	1.64615445	2.72292928	-0.69708672
pyrazinamide	-0.40759412	0.22049511	-0.69193275

indoleaceticacid	0.41187121	1.03012579	-0.68960339
a,a-dimethyl-1-piperidineacetonitrile	1.66324932	2.93802827	-0.68817317
1-ethyl-3-piperidinol	1.50579507	2.39233306	-0.68780915
2(3h)-benzothiazolethione	1.48531177	2.39212555	-0.68135105
2(3h)-benzothiazolethione	1.48552839	2.39239881	-0.68130419
2-propionylthiazole	1.5071885	2.48454959	-0.67688808
2,4,5-trimethylthiazole	1.76320339	2.90904534	-0.67360858
2,4,5-trimethylthiazole	1.76472157	2.91157392	-0.67353104
2-methyl-1h-isoindole-1,3(2h)-dione	1.29718553	2.21695692	-0.67267874
4-pyrimidinecarbonitrile	0.29260076	0.97510619	-0.67194053
2-propionylthiazole	1.5347297	2.51422514	-0.67187946
4-thiazolecarbonitrile	0.56351699	1.23676888	-0.67075171
4-thiazolecarbonitrile	0.56315968	1.23626376	-0.6706225
pyrazinecarbonitrile	0.3556033	1.04198208	-0.66633154
4-methyl-5-vinylthiazole	1.57061347	2.6036805	-0.66509197
4-methyl-5-vinylthiazole	1.57135147	2.60475548	-0.66501518
3-Piperidino-1,2-propanediol	0.36231478	1.37925741	-0.66262146
2-pyrimidinecarbonitrile	0.43661283	1.13154354	-0.6615398
3-phenylpyridine	1.65827633	2.89507517	-0.65878466
1,2,4-trimethylpiperazine	1.60991152	2.88170007	-0.65859896
1-methyl-pyrrolidine	1.4526445	2.44506761	-0.65822192
3-Hydroxy-1-methylpiperidine	0.82246783	1.69546746	-0.65449358
2,6-pyrazinediamine	-0.96999911	-0.51527068	-0.64430049
5-hydroxyisoquinoline	0.7600022	1.50650634	-0.64390318
2,3-dimethyl-1h-indole	1.90154225	2.99337372	-0.64292039
2-acetyl-3-ethylpyrazine	1.66717435	2.80180378	-0.64226102
3,3-difluoro-1-methylpyrrolidine	1.32141123	2.24394074	-0.64148253
ethenyl-dimethylpyrazine	1.73016361	2.92238072	-0.63944472
2-methyl-3-methylthiopyrazine	1.72158661	2.82371812	-0.63842931
beta-ionone	2.1497701	3.76315993	-0.6370064
imazalil	2.29638923	4.24013128	-0.63697425
beta-ionone	2.14810459	3.76067623	-0.63692617
2,3-diethylpyrazine	1.75985706	3.01074023	-0.63652779
s-orthophenylenethiocarbamate	0.99560114	1.76108454	-0.6333915
s-orthophenylenethiocarbamate	0.99570691	1.76127052	-0.63330948
2,4-dimethylbenzaldehyde	1.73562202	2.83196401	-0.63202396
1-(1-methyl-pyrrolidin-3-yl)-ethane-1,2-diol	0.76048532	1.67788934	-0.63157573
2-methoxy-3,6-dimethylpyrazine	1.78637812	2.9571531	-0.6294699
5-(Morpholin-4-yl)pentan-1-ol	0.83284893	2.08992168	-0.62920054

1-(1h-indol-3-yl)ethanone	0.51487856	1.38144767	-0.62583207
3,3-dimethylsuccinimide	-0.04367756	0.49773401	-0.6245381
1,3,5-triazine-2,4,6-triamine	-1.5129499	-1.12375128	-0.62379968
pyrazinoicacid	0.27679974	0.79789702	-0.62316602
diethadione	0.68156894	1.48596865	-0.61806443
1,2,3-triazine	-0.78267908	-0.36185989	-0.61600049
benzothiazole	1.54355659	2.50400721	-0.61347324
benzothiazole	1.543835	2.5043045	-0.61338743
4,5-dimethyl-2-ethyl-3-thiazoline	1.93188907	3.14561504	-0.61010422
2-isobutyl-3-methylpyrazine	1.91896651	3.28430308	-0.60741383
thiabendazole	1.53773947	2.76202062	-0.60546237
thiabendazole	1.5649933	2.79102839	-0.6029155
2-ethyl-4-methylthiazole	1.93430843	3.08241877	-0.60209878
2-ethyl-4-methylthiazole	1.9368027	3.08439023	-0.6008034
cyanuricfluoride	1.06262932	1.87408977	-0.60032354
1,2-benzisothiazole	1.61028223	2.59490051	-0.5996374
1,2-benzisothiazole	1.61071215	2.59534557	-0.59950831
n,n'-trimethylenethiourea	-0.61869351	-0.12296298	-0.58818796
1h-indole-3-carboxaldehyde	0.31423785	1.0315916	-0.58184595
3-methyl-1,3-thiazole-2(3h)-thione	1.19507795	1.94080521	-0.58018138
3-methyl-1,3-thiazole-2(3h)-thione	1.19455289	1.94003292	-0.58004527
6-amino-3-methylpurine	-1.14485076	-0.41586973	-0.57997201
2,6-dimethylpiperidine	1.76278783	2.95531344	-0.57868761
theobromine	-0.28556577	0.47493324	-0.57383957
atrazine	2.17747164	3.72871106	-0.57155384
2-ethoxythiazole	1.89420915	2.88874974	-0.56701191
4,5-dimethyl-2-ethyl-3-thiazoline	2.02844428	3.2408409	-0.56648266
2-Piperidinoethanol	1.005344	1.99599158	-0.56360207
2(3h)-benzothiazolethione	2.05909649	3.14470496	-0.56121003
2-ethoxythiazole	1.96305555	2.97136689	-0.55761362
2,3-diethyl-5-methylpyrazine	2.11025378	3.53903242	-0.55654921
phenoxazine	2.2320984	3.4013193	-0.5564881
indolizine	1.80082102	2.70824856	-0.55511806
3,4,5-trimethyl-1,3-thiazole-2(3h)-thione	1.8544444	2.92949513	-0.54726543
3,4,5-trimethyl-1,3-thiazole-2(3h)-thione	1.85493904	2.93011117	-0.54723139
trifluoro-pyrazine	1.25500422	2.09723491	-0.54675993
ethyl dimethylthiazole	2.16404053	3.45143916	-0.54555366
ethyl dimethylthiazole	2.16473537	3.45187516	-0.54503334

2-isobutylthiazole	2.1112148	3.34950205	-0.54406873
3-Pyrrolidino-1,2-propanediol	0.5656083	1.46090556	-0.53756268
2-(1-methylpropyl)thiazole	2.09816167	3.32509323	-0.53619331
phthalimide	0.67216416	1.30089382	-0.53599309
3-ethyl-2-methoxypyrazine	1.9703442	3.12871249	-0.5355682
n-chlorosuccinimide	0.26353709	0.71930543	-0.52524148
2-isobutylthiazole	2.15718877	3.39541391	-0.5248907
2-phenylpyrrolidine	2.02930273	3.30537267	-0.52442464
2-bromothiazole	1.74044619	2.63306539	-0.51888363
2-bromothiazole	1.74075881	2.63341806	-0.51879159
2-Piperidineethanol	1.1317077	2.23839668	-0.51832325
2-isobutylthiazole	2.17629838	3.41694164	-0.5163586
secbumeton	2.40394732	4.13365687	-0.51631052
4,5-dimethyl-2-ethyl-3-thiazoline	2.15689692	3.367876	-0.51215955
3-Piperidino-1,2-propanediol	2.60216025	3.99681224	-0.51201605
4-chloro-n-methylpiperidine	1.81492412	2.8792015	-0.50941674
3,5-diethyl-2-methylpyrazine	2.20362344	3.63646523	-0.50910843
2,4-dimethyl-5-vinylthiazole	2.1532877	3.36158395	-0.50801179
2,4-dimethyl-5-vinylthiazole	2.15738228	3.36683495	-0.50668625
(1s)-1-methylpropyloxypyrazine	2.15837964	3.45409758	-0.50318761
cyclohexylmethyl-pyrazine	2.24972686	3.75332713	-0.50250495
2-methylbenzothiazole	2.0672198	3.21117138	-0.50047154
2-methylbenzothiazole	2.06749419	3.21145218	-0.50036521
phenanthridine	2.11933506	3.45191148	-0.5001062
2-isobutylthiazole	2.21751826	3.46024744	-0.49861556
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine	2.38749359	3.99944558	-0.49736688
2-isobutylthiazole	2.22716558	3.47230547	-0.49619553
(1r)-1-methylpropyloxypyrazine	2.19178751	3.49589855	-0.49441536
2-ethoxythiazole	2.11037892	3.113722	-0.49407606
2-ethylpiperidine	1.91699436	3.15575988	-0.49369908
prometryn	2.85250892	4.59109669	-0.49066598
1-methyl-1h-indole	1.99297094	3.00066318	-0.48957138
indomethacin	2.70081334	4.3431205	-0.48947298
prometon	2.54107751	4.30770156	-0.48742377
conhydrine	2.05522337	2.99322904	-0.48339282
terbuthylazine	2.4706649	4.11498419	-0.48256311
phenazine	2.12406165	3.45292588	-0.48229698
2,5-diethyl-3-methylpyrazine	2.26790358	3.69566127	-0.48048304
thiabendazole	0.30934979	1.45841916	-0.48027802
6-ethyl-2,3,5-trimethyl-pyrazine	2.23415502	3.6470958	-0.47849748

2-isopropyl-4-methylthiazole	2.30448895	3.57791895	-0.47279042
phenothiazine	2.4759114	3.74342071	-0.47252119
2(3h)-benzothiazolethione	2.35019965	3.48673613	-0.46832948
acridine	2.24195112	3.59046565	-0.4682654
acridine	2.24229079	3.59077789	-0.4681204
9-(n,n-dimethylamino)acridine	2.53165263	4.17316987	-0.46181491
9-(n,n-dimethylamino)acridine_	2.53310261	4.17440212	-0.46117943
2-methyl-1,2,3,4-tetrahydroisoquinoline	2.22711457	3.49570999	-0.45982163
2-(1-methylpropyl)thiazole	2.27842049	3.51226289	-0.45953998
9-(n,n-dimethylamino)acridine	2.54381526	4.18497065	-0.45595846
oxazepam	1.52096076	2.88790152	-0.45506637
4-pyridazinecarbonitrile	-0.17603259	0.42049507	-0.45383001
2,3-diethyl-5-methylpyrazine	2.31739813	3.74038763	-0.453484
beta-ionone	2.55135078	4.17514855	-0.44885031
phenazine,5-oxide	2.15681778	3.41661132	-0.4443729
2,3-diethyl-5-methylpyrazine	2.36010657	3.78354043	-0.43940544
2-phenylpyridine	2.22292597	3.449108	-0.43791454
3,5-diazaindole	-0.71140193	-0.12420784	-0.43565404
2-ethyl-3-methylthiopyrazine	2.36050428	3.61507385	-0.43287917
5-azadibenzo(a,e)cycloheptatriene	2.52978164	3.85253782	-0.43105735
N-methyl morpholineoxide	2.58497534	4.1592217	-0.43058698
beta-ionone	2.6190037	4.24362916	-0.42979281
hexahydro-1,3,5-trinitro-1,3,5-triazine	0.82023958	1.19422024	-0.42381714
1-Piperidinepropanol	1.48478395	2.62003343	-0.42315298
beta-ionone	2.63662244	4.2612252	-0.42255263
propazine	2.6968808	4.41263058	-0.41719307
1h-indole-2,3-dione	0.45518605	1.03942818	-0.41675216
1,4-Piperazinediethanol	-0.32671092	0.65294955	-0.41611136
2-(3-fluorophenyl)pyrrolidine	2.27173718	3.61281046	-0.4122555
ethenyl-ethylmethylpyrazine	2.39676534	3.74275183	-0.41028296
ametryn	3.04123561	4.75962714	-0.39817715
2-isopropyl-4-methylthiazole	2.47846588	3.7610427	-0.39762174
2-(1-methylpropyl)thiazole	2.44541486	3.68675429	-0.39473489
2-(piperidin-1-yl)propane-1,3-diol	0.60370353	1.48606975	-0.39381311
n-methylpiperidine	2.00207491	3.08577222	-0.38746543
sulfathiazole	1.03096851	1.99548114	-0.38275444
1h-isoindole-1,3(2h)-dione,4-amino-	0.40911818	1.02024806	-0.38213164
sulfathiazole	1.03744521	2.0035446	-0.38205442
sulfathiazole	1.0344926	1.99617606	-0.38101261

5-nitro-2-thiazolamine	0.07643669	0.41257516	-0.38009708
5-nitro-2-thiazolamine	0.07626506	0.41232447	-0.37999336
beta-ionone	2.70200261	4.32829555	-0.3791856
theophylline	-0.11023799	0.59005274	-0.37796014
Hygroline	1.80476741	2.99545848	-0.37706659
1,2-dimethylpyrrolidine	2.07537874	3.19203339	-0.37284584
1-ethylpyrrolidine	2.09037472	3.22443804	-0.37266672
1,2-dimethylindole	2.39885913	3.55129361	-0.37208299
1-Ethylpiperidine-3,5-diol	0.0913899	0.8608124	-0.37189008
(2r)-1,2-dimethylpyrrolidine	2.07872561	3.198203	-0.37019799
4-Isobutylmorpholine	2.24933439	3.54274031	-0.36141217
sulfathiazole	0.99811054	1.95148937	-0.35922746
1-(2-hydroxyethyl)imidazole	-0.91596681	-0.38845546	-0.3583632
2,4-thiazolidinedione	0.18006632	0.43830787	-0.35818346
2,4-thiazolidinedione	0.17923065	0.43676773	-0.35808413
3-chloromethyl-n-methylpiperidine	2.24070744	3.46181749	-0.35790905
2-methyl-3-(pyrrolidin-1-yl)propan-1-ol	1.80534877	2.92274125	-0.34972245
(1s)-1-methylbutyloxypyrazine	2.650904	4.11055689	-0.34954075
(1r)-1-methylbutyloxypyrazine	2.64817693	4.10943523	-0.34843485
2-(2-butyl)-4,5-dimethyl-3-thiazoline	2.67485102	4.11586485	-0.34192672
beta-ionone	2.79133172	4.42612159	-0.34178199
3-(hydroxymethyl)-1-piperidinepropanol	0.83035687	1.86041003	-0.33920795
molinate	2.72834102	4.17605254	-0.33805842
2-[Cyclohexyl(methyl)amino]ethanol	1.87002419	3.1265747	-0.33742523
beta-ionone	2.81072213	4.45209936	-0.3366354
1,3-dimethyl-1h-indole	2.52517423	3.70602169	-0.33450863
terbutryn	3.21009238	5.04338872	-0.33232468
1-(piperidin-1-yl)propan-2-ol	1.92470289	3.10556702	-0.33182882
2-isopropyl-4-methylthiazole	2.64498357	3.93257992	-0.33052822
isopentyl dimethylpyrazine	2.83056005	4.52960815	-0.32948678
sulfaethoxypyridazine	1.24643121	2.52274393	-0.32658547
2,3-diethyl-5-methylpyrazine	2.60252013	4.01423932	-0.32413209
4,5-dimethyl-2-isobutyl-3-thiazoline	2.80024646	4.29734707	-0.32231162
2-methoxy-3-isopropylpyrazine	2.56374079	3.86771652	-0.3205065
tropane	2.2408186	3.46009754	-0.30896765
adenine	-0.99895879	-0.51224146	-0.30858165

alpha-phenyl-1-piperidineacetonitrile	2.87135667	4.37901618	-0.3079579
1,4-dinitrosopiperazine	0.0352125	0.57107629	-0.30667144
7h-benzo[c]phenothiazine	3.18795641	4.75245127	-0.30457694
octahydroazocine	2.1691852	3.30488149	-0.30314225
2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine	3.08190724	4.83655498	-0.2975946
meperidine	3.07120279	4.84355206	-0.2942701
3-methyl-1,3-benzothiazole-2(3h)-thione_c0_99	2.53596967	3.70358218	-0.29253911
3-methyl-1,3-benzothiazole-2(3h)-thione	2.54052006	3.70961156	-0.29149713
1,3-dihydro-1-methyl-2h-imidazole-2-thione	-0.04337208	0.397984	-0.28828705
isonipetric acid	-3.40036514	-2.67806324	-0.28135841
4,5-dimethyl-2-isobutyl-3-thiazoline	2.91499768	4.41186921	-0.27029699
2-propylpiperidine	2.47846554	3.86928712	-0.26901112
1h-imidazo(4,5-b)pyridine	-0.96108847	-0.36055742	-0.26675384
sulfachlorpyridazine	0.94877172	2.01426926	-0.26204024
benz(c)acridine	3.02450922	4.66772771	-0.25784862
benz(c)acridine	3.02576227	4.66890974	-0.25733242
1h-purine-2,6-diamine	-1.19242201	-0.73445982	-0.25235137
2-isobutyl-3-methoxypyrazine	2.83136276	4.26830316	-0.24783574
1,2,3-trimethyl-1h-indole	2.89099389	4.19736867	-0.21808135
2-(2-butyl)-4,5-dimethyl-3-thiazoline	2.97592506	4.4467126	-0.21674865
4,5-dimethyl-2-isobutylthiazole	3.1201869	4.69664962	-0.21046516
4,5-dimethyl-2-isobutyl-3-thiazoline	3.0646413	4.55939497	-0.20606291
12h-benzo[c]phenothiazine	3.4042021	5.00322745	-0.20392246
2-(2-butyl)-4,5-dimethyl-3-thiazoline	3.00922932	4.47532655	-0.20234169
1-phenylpyrrolidine	2.84601835	4.09602829	-0.20106114
4,5-dimethyl-2-isobutylthiazole	3.14701776	4.72036593	-0.19765485
4,5-dimethyl-2-isobutylthiazole	3.15311123	4.7282513	-0.19366061
captan	2.91227545	4.30786287	-0.18527743
2-methoxy-3-(1-methylpropyl)pyrazine	2.95938478	4.38721471	-0.17961516
2,5-pyrrolidinedione	-0.44826611	-0.23583694	-0.16868441
7h-dibenzo[c,h]phenothiazine	3.85531551	5.7106746	-0.16423106
4,5-dimethyl-2-isobutylthiazole	3.22786965	4.80369939	-0.15645413
2-(2-butyl)-4,5-dimethyl-3-	3.14194869	4.62756209	-0.15386758

thiazoline			
2-ethoxy-3-isopropylpyrazine	3.04738023	4.51469821	-0.14778512
perphenazine	4.47083618	7.17559641	-0.14195817
2,8-dimethyl-6h,12h-5,11-methanodibenzo[b,f][1,5]diazocine	3.50781121	5.30753992	-0.14071254
sulfathiazole	0.77879074	1.67088092	-0.1329376
2-Piperidinoethanol	3.12930748	4.54506148	-0.13280983
6-azathymine	-0.19032521	0.12567405	-0.12942709
sulfathiazole	0.76290325	1.65445232	-0.12227096
1'-(Cyclohexylimino)bispropan-2-ol	2.05489895	3.54152559	-0.11861666
sulfathiazole	0.75266396	1.64480997	-0.11727875
hexahydro-1,3,5-trinitroso-1,3,5-triazine	0.51593637	1.00420649	-0.11548875
6-(Piperidin-1-yl)hexan-1-ol	2.5869878	4.18657439	-0.10277741
tryptophan	-1.23868856	-0.54980162	-0.10236447
2,2,6,6-tetramethylpiperidine	2.78711245	4.2016882	-0.1017441
n-allylpiperidine	2.87461221	4.09904552	-0.10033156
1-ethylpiperidine	2.65136133	3.87470453	-0.09992258
ethoxyquin	3.50739633	5.18068884	-0.09788905
1-ethyl-2-methylpyrrolidine	2.71918054	3.97584385	-0.08715702
pyrazine-2-one	-0.68993199	-0.37566466	-0.08703361
n-phenylpiperidine	3.19001444	4.55070339	-0.07443757
4-aminophthalimide	0.15331701	0.64438565	-0.06492099
dibenz[a,j]acridine	3.83311963	5.78078669	-0.05166745
dibenz[a,j]acridine	3.83381593	5.78111849	-0.0513402
(1s)-1-methylhexyloxy pyrazine	3.57464349	5.34010816	-0.04772935
1-4-dinitropiperazine	0.93808715	1.41762921	-0.04421916
2,3,6,7-tetrahydro-1h,5h-pyrido[3,2,1-ij]quinoline	3.23431069	4.60441873	-0.04126549
(1r)-1-methylhexyloxy pyrazine	3.59121016	5.3583409	-0.04087688
2-(3-trifluoromethylphenyl)pyrrolidine	3.14201015	4.74647952	-0.03953372
benz(a)acridine	3.64333178	5.29974627	-0.03577827
benz(a)acridine	3.64440227	5.30122649	-0.03548576
n-methyl-2-phenylpyrrolidine	3.29756811	4.72333061	-0.00698115
indolene a	4.95904788	7.61798972	0.04868619
4-hydroxy-2(1h)-pyridone	-0.34211913	-0.3074935	0.05380581
4-hydroxy-2(1h)-pyridone	-0.30943788	-0.25701576	0.05604181
pyrazine-1,4-dioxide	-0.64789953	-0.40971376	0.0576565
n-methyl-2-(3-fluorophenyl)pyrrolidine	3.50223671	4.99204983	0.08625798

14h-dibenzo[a,j]phenothiazine	4.40926116	6.34650317	0.10062181
2-thiouracil	0.09158612	0.35861901	0.11168894
(1s)-1-methylheptyloxypyrazine	4.0609831	5.9830818	0.11429265
n-propylpiperidine	3.20474872	4.58896986	0.11980692
(1r)-1-methylheptyloxypyrazine	4.08571425	6.01166618	0.12214401
dibenz(a,h)acridine	4.38776474	6.34207463	0.13691366
dibenz(a,h)acridine	4.38979127	6.34431631	0.13765032
dibenz(a,c)acridine	4.37463873	6.31103802	0.13995656
dibenz(a,c)acridine	4.37747308	6.31429458	0.14092184
thymine	-0.45431475	-0.11837676	0.14410579
n-butylpyrrolidine	3.33300957	4.76451137	0.16443491
promazine	4.62771135	6.73671453	0.18059485
(1s,2r,5s)-menthyloxypyrazine	4.21546597	6.18008812	0.19614692
(1r,2s,5r)-menthyloxypyrazine	4.2253031	6.19094278	0.19902096
3,4,5,6-dibenzacridine	4.62277064	6.60473345	0.2240091
3,4,5,6-dibenzacridine	4.62491396	6.6074156	0.22471637
1,1'-dithiobispiperidine	4.42610369	6.20386217	0.26525194
imipramine	4.79252346	6.98637793	0.27424289
1,2,4-triazine-3,5(2h,4h)-dione	-0.13332799	-0.01534352	0.29242366
1,1'-thiobispiperidine	4.1032589	5.75219891	0.29287212
chloropromazine	5.10206081	7.35174562	0.34242716
N-Decylmorpholine	4.32755357	6.35676778	0.35291406
trifluoperazine	5.48059742	8.22691539	0.40062113
n-methyl-2-(3-trifluoromethylphenyl)pyrrolidine	4.27909266	6.03292526	0.43668711
alloxane	0.31211011	0.22415775	0.48988199
1,2,2,6,6-pentamethylpiperidine	4.0072708	5.49533662	0.51056815
(s)-1-(2-methylbutyl)pyrrolidine	4.08961143	5.62419789	0.52503743
(r)-1-(2-methylbutyl)pyrrolidine	4.10507859	5.64118848	0.53267241
triflupromazine	5.54765067	7.97894559	0.56576913
2,5-piperazinedione	-1.19606529	-0.98240439	0.62150367
(r)-2-methyl-1-((r)-2-methylbutyl)pyrrolidine	4.73801091	6.38715506	0.81724588
(r)-2-methyl-1-((s)-2-methylbutyl)pyrrolidine	4.75608441	6.41636788	0.82513576
(s)-2-methyl-1-((s)-2-methylbutyl)pyrrolidine	4.76236781	6.41922953	0.82552346
(s)-2-methyl-1-((r)-2-methylbutyl)pyrrolidine	4.75526044	6.40869655	0.82742057
hypoxanthine	-0.49398567	-0.27067808	1.23931558
2,2,3,3,5,6,6-heptafluoro-3,6-dihydro-2h-1,4-oxazine	4.23903354	5.53259639	1.29665885

Table S2. Boiling points and GHS hazard classifications. Boiling points were obtained from ChemSpider (averaged from multiple measurements at standard pressure), and hazard data were retrieved from PubChem. X indicates the presence of the specified hazardous classification for each compound according to GHS criteria.

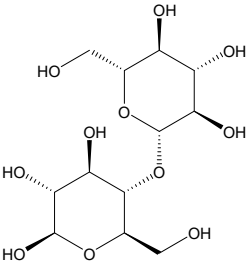
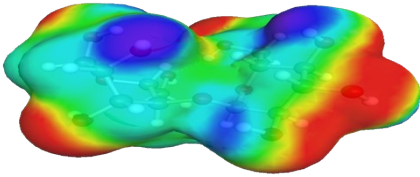
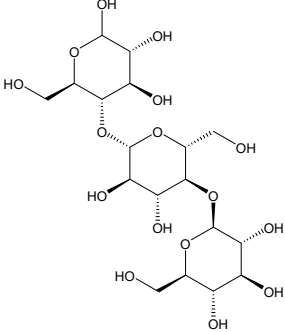
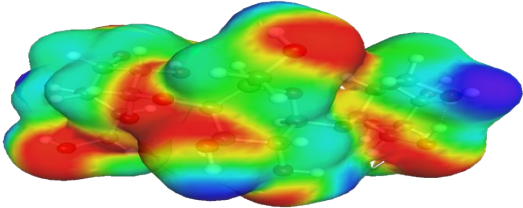
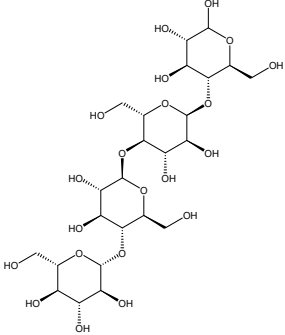
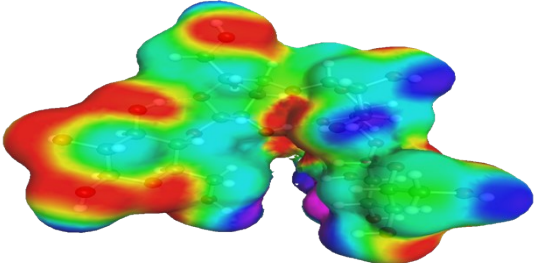
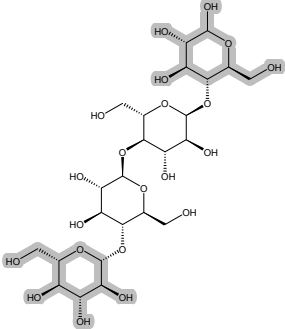
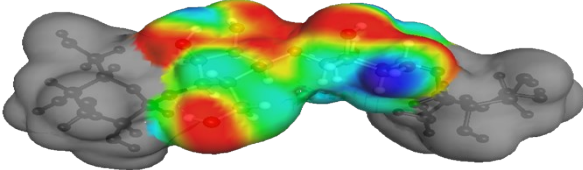
Chemical Name	Boiling Point (°C)	Acute Toxic	Corrosive	Environmental Hazard	Flammable	Health Hazard	Irritant
3-Methylpyrrolidine	101		X		X		X
3-Methylpyridine1-oxide	304						X
2-Piperidineethanol	234		X				X
3-Methylpyridazine	214						X
1-Piperidinecarboxaldehyde	222	X					X

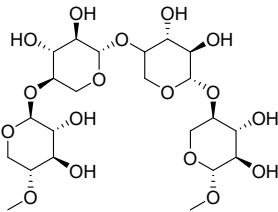
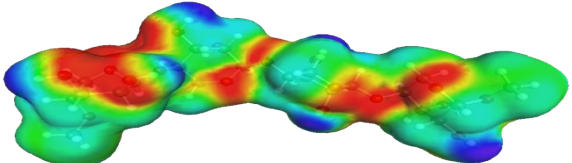
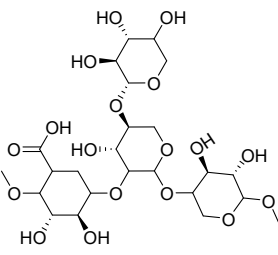
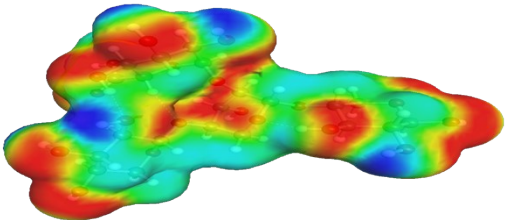
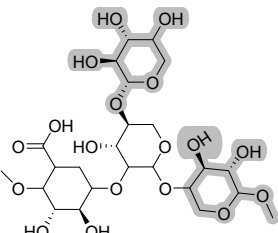
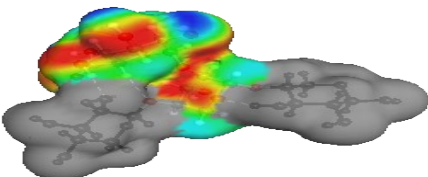
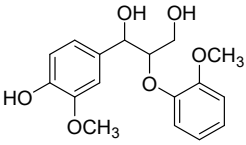
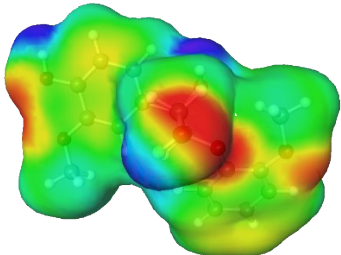
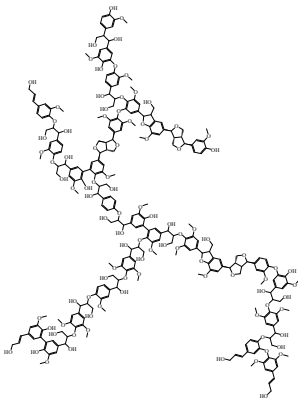
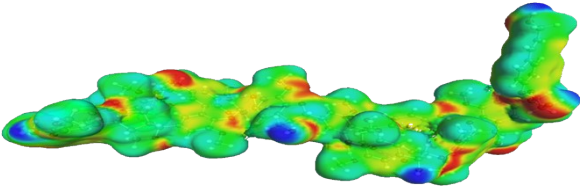
Morpholine	128	X	X	X	X	X	X
1-Methylimidazol	198	X	X			X	X
4-Methylpyridine- 1-oxide	318						X
4- Methylpyridazine	246						X
1-Butyl-2-methyl- imidazole	244						X
1-Aminopiperidine	147		X		X		X
Trans-2,5- dimethylpiperazin e	163	X	X		X		X
1- Methylpiperazine	138	X	X		X		X
1-Acetylpiperidine	226						X
1-ethyl-2-methyl-imidazole							X

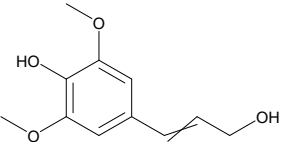
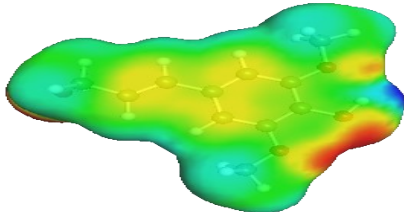
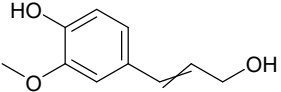
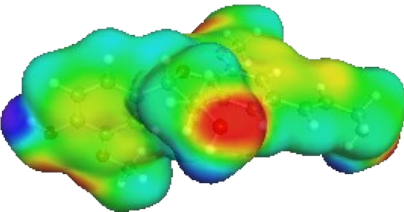
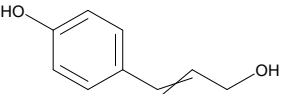
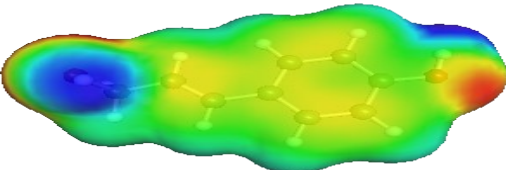
1,2-Dimethyl-1h-imidazole	204		X			X	X
1,4-Bis(2-hydroxyethyl) piperazine	340		X				
1-Piperazineethanol	242		X				X
n-Methyl-2-pyrrolidinone	234						X
1-Pyrrolidineethanamine	178		X		X		
Pyrrolidine-1-carbaldehyde	227						X
Hexahydro-1h-1,4-diazepine	169	X	X				
2-Methylpiperazine	154		X		X		X

1- Acetylpyrrolidine	212		X		X		
Piperazine	145		X		X	X	X
2,3,4,6,7,8,9,10- Octahydropyrimidin o[1,2-a]azepine	314	X	X				X
4- Piperidinemethana mine	200		X				
1- Piperazineethanam ine	218	X	X			X	X
2,3,4,6,7,8- Hexahydropyrrolo [1,2-a]pyrimidine	251	X	X				X
1,1',1''- Phosphoryltripiper idine	434	X	X		X		X

Table S3. COSMO surface images of all the biopolymers used in the present study.

Name of Biopolymers	Structure	COSMO Structure
Cellobiose		
Cellotriose		
Cellotetraose		
Cellotetraose Capped		

Xylan		
Glucuronoxylan		
Glucuronoxylan Capped		
Guaiacylglycerol-β-guaiacyl ether (GGE)		
Lignin		

Sinapyl alcohol		
Coniferyl alcohol		
Coumaryl alcohol		

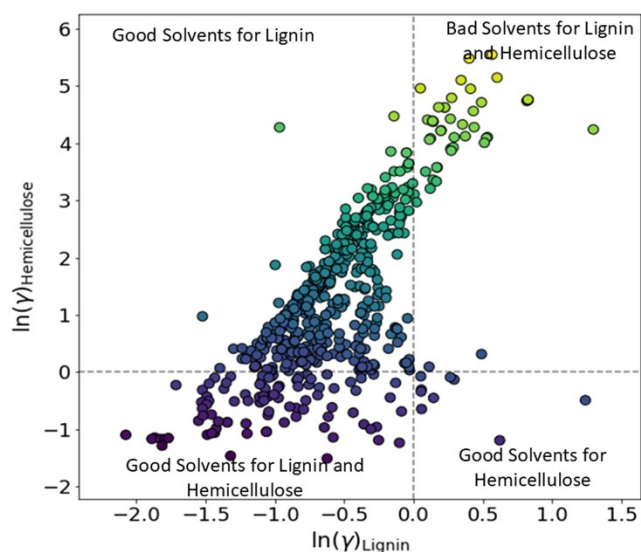


Figure S1. The combined interaction for hemicellulose and lignin for cyclic amine at 140°C and 1 atm pressure. The color represents the activity coefficients values from most negative (dark blue) to least negative (yellow).

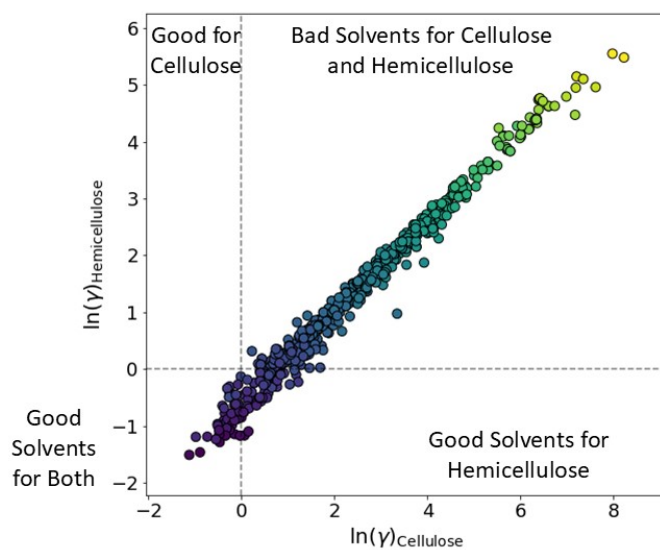


Figure S2. The combined interaction for hemicellulose and cellulose for cyclic amine at 140°C and 1 atm pressure. The color represents the activity coefficients values from most negative (dark blue) to least negative (yellow color).



Figure S3. Appearance of sorghum biomass before and after pretreatment with two studied cyclic amines.