

Supporting information

Finding lead compounds for dengue antivirals from a collection of old drugs through *in silico* target prediction and subsequent *in vitro* validation

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Supporting Information S1

Supplementary tables

Variance percentage of the first 10 Principal Components (PCs)

Table S1. Explained variance percentage of the first 10 Principal Components (PCs).

PCs	Value
Explained variance percentage of PC1	19.217
Explained variance percentage of PC2	5.348
Explained variance percentage of PC3	5.092
Explained variance percentage of PC4	3.226
Explained variance percentage of PC5	2.625
Explained variance percentage of PC6	2.227
Explained variance percentage of PC7	2.04
Explained variance percentage of PC8	1.872
Explained variance percentage of PC9	1.697
Explained variance percentage of PC10	1.549

The eigenvalues of the training set according to the chemical structures from PCA

Table S2. The eigenvalues of the training set according to the chemical structures. The eigenvalues describe the total variance explained by each principal component. There were 512-bit binary string with respective PCAs value.

Variable Name	pc1	pc2	pc3
Structure of smiles [FragFp] bit 0	0.019613	-0.06599	0.039135
Structure of smiles [FragFp] bit 1	0.075367	0.009896	0.005492
Structure of smiles [FragFp] bit 10	0.051698	-0.07758	0.018239
Structure of smiles [FragFp] bit 100	0.072073	-0.01529	0.021822
Structure of smiles [FragFp] bit 101	0.046917	0.002419	-0.02372
Structure of smiles [FragFp] bit 102	0.063902	-0.02106	0.029623
Structure of smiles [FragFp] bit 103	-0.02278	-0.00604	0.122796
Structure of smiles [FragFp] bit 104	0.034826	0.060547	0.018474
Structure of smiles [FragFp] bit 105	0.063278	-0.04539	0.034258
Structure of smiles [FragFp] bit 106	0.073721	0.01903	0.001499
Structure of smiles [FragFp] bit 107	0.071974	0.027832	0.014552
Structure of smiles [FragFp] bit 108	0.009034	0.020733	-0.00982
Structure of smiles [FragFp] bit 109	0.072336	0.003478	0.005936
Structure of smiles [FragFp] bit 11	0.078983	-0.02374	-8.67E-04
Structure of smiles [FragFp] bit 110	0.061818	-0.00293	0.008195
Structure of smiles [FragFp] bit 111	0.079669	-0.0145	-0.0095
Structure of smiles [FragFp] bit 112	0.036881	-0.05491	0.022848

Structure of smiles [FragFp] bit 113	0.069186	0.045472	0.009443
Structure of smiles [FragFp] bit 114	0.064249	-0.06462	0.003885
Structure of smiles [FragFp] bit 115	0.069148	-0.05192	-0.01664
Structure of smiles [FragFp] bit 116	0.010476	0.013516	0.028497
Structure of smiles [FragFp] bit 117	0.080444	-0.01705	-5.15E-04
Structure of smiles [FragFp] bit 118	0.072605	-0.03934	-0.00937
Structure of smiles [FragFp] bit 119	0.068194	0.042348	0.02217
Structure of smiles [FragFp] bit 12	0.078954	-0.02935	0.010759
Structure of smiles [FragFp] bit 120	0.072155	-0.04395	-0.01023
Structure of smiles [FragFp] bit 121	0.05751	0.042772	-0.02567
Structure of smiles [FragFp] bit 122	0.046113	-0.10379	-0.0153
Structure of smiles [FragFp] bit 123	0.043329	-0.10273	-0.00913
Structure of smiles [FragFp] bit 124	0.007868	-0.04271	0.034956
Structure of smiles [FragFp] bit 125	0.058365	-0.04128	0.033946
Structure of smiles [FragFp] bit 126	0.050277	-0.05379	0.046309
Structure of smiles [FragFp] bit 127	0.074562	0.006511	0.005103
Structure of smiles [FragFp] bit 128	0.06562	-0.03831	-0.01886
Structure of smiles [FragFp] bit 129	-0.01014	0.033772	0.090405
Structure of smiles [FragFp] bit 13	-0.00213	0.023151	0.068301
Structure of smiles [FragFp] bit 130	0.073059	0.014696	-0.0098
Structure of smiles [FragFp] bit 131	0.057864	-0.0226	0.035209
Structure of smiles [FragFp] bit 132	0.061353	0.057819	0.012535
Structure of smiles [FragFp] bit 133	0.012332	0.009707	0.005238
Structure of smiles [FragFp] bit 134	-0.00889	0.024692	0.064695
Structure of smiles [FragFp] bit 135	-0.00471	-0.00378	0.017042
Structure of smiles [FragFp] bit 136	0.034755	-0.10213	-0.01941
Structure of smiles [FragFp] bit 137	-0.0054	0.019425	0.104899
Structure of smiles [FragFp] bit 138	0.076576	0.020559	-1.86E-04
Structure of smiles [FragFp] bit 139	0.030256	0.01667	0.036157
Structure of smiles [FragFp] bit 14	0.066122	-0.06332	0.002424
Structure of smiles [FragFp] bit 140	-0.01004	-0.00415	0.132058
Structure of smiles [FragFp] bit 141	-0.00727	0.011029	0.101681
Structure of smiles [FragFp] bit 142	0.06466	0.060542	0.00158
Structure of smiles [FragFp] bit 143	0.03632	0.064576	-0.00816
Structure of smiles [FragFp] bit 144	0.06883	0.071363	0.010253
Structure of smiles [FragFp] bit 145	0.068454	-0.0334	0.024787
Structure of smiles [FragFp] bit 146	-0.01428	-0.01572	0.119135
Structure of smiles [FragFp] bit 147	0.056954	0.083205	0.014125
Structure of smiles [FragFp] bit 148	0.059091	-0.02984	0.039114
Structure of smiles [FragFp] bit 149	0.010844	-0.09532	0.05123
Structure of smiles [FragFp] bit 15	0.059073	-0.07767	9.60E-04
Structure of smiles [FragFp] bit 150	0.032696	0.053519	-0.01741
Structure of smiles [FragFp] bit 151	0.065504	0.024519	0.005364
Structure of smiles [FragFp] bit 152	0.059393	-0.00262	-0.01503
Structure of smiles [FragFp] bit 153	0.072332	0.015326	0.010148
Structure of smiles [FragFp] bit 154	0.059959	-0.03097	-0.01842

Structure of smiles [FragFp] bit 155	0.073918	0.044684	0.015035
Structure of smiles [FragFp] bit 156	0.044785	-0.00528	-3.05E-05
Structure of smiles [FragFp] bit 157	0.049053	0.063571	0.003024
Structure of smiles [FragFp] bit 158	0.071026	0.054091	0.012251
Structure of smiles [FragFp] bit 159	0.069649	-0.03437	0.019209
Structure of smiles [FragFp] bit 16	-0.02312	-0.00233	0.117006
Structure of smiles [FragFp] bit 160	0.072955	0.039602	0.002204
Structure of smiles [FragFp] bit 161	0.048555	-2.74E-04	-0.03047
Structure of smiles [FragFp] bit 162	-0.00496	-0.11012	-0.0081
Structure of smiles [FragFp] bit 163	0.076743	0.031581	-0.00538
Structure of smiles [FragFp] bit 164	0.05587	-0.08333	-0.0468
Structure of smiles [FragFp] bit 165	0.067609	-0.03849	-0.02847
Structure of smiles [FragFp] bit 166	0.010096	-0.02594	0.058558
Structure of smiles [FragFp] bit 167	0.066306	-0.06407	-0.00612
Structure of smiles [FragFp] bit 168	0.046758	0.049865	-0.00285
Structure of smiles [FragFp] bit 169	0.027004	0.053539	0.026677
Structure of smiles [FragFp] bit 17	0.071214	0.002764	0.005214
Structure of smiles [FragFp] bit 170	0.052739	0.01778	-0.03227
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Structure of smiles [FragFp] bit 177	-0.012	0.029688	0.117351
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Structure of smiles [FragFp] bit 181	-0.00604	-0.05901	0.014899
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Structure of smiles [FragFp] bit 183	0.019001	-0.05516	0.038105
Structure of smiles [FragFp] bit 184	0.041747	0.041049	-0.03029
Structure of smiles [FragFp] bit 185	0.059238	-0.04851	0.038348
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Structure of smiles [FragFp] bit 187	0.069143	0.036992	0.012245
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Structure of smiles [FragFp] bit 189	0.075045	0.035047	-0.00267
Structure of smiles [FragFp] bit 19	0.065737	-0.061	0.002616
Structure of smiles [FragFp] bit 190	0.035317	0.067713	0.037542
Structure of smiles [FragFp] bit 191	-0.01022	-0.02505	0.052538
Structure of smiles [FragFp] bit 192	0.042016	-0.08942	-0.03538
Structure of smiles [FragFp] bit 193	0.060154	0.045447	2.95E-04
Structure of smiles [FragFp] bit 194	0.016209	-0.00578	9.00E-04
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Structure of smiles [FragFp] bit 197	0.057254	-0.04223	0.033802
Structure of smiles [FragFp] bit 198	0.063569	0.06653	0.01349
Structure of smiles [FragFp] bit 199	0.011911	-0.08069	0.030842
Structure of smiles [FragFp] bit 2	0.073896	-0.03366	-0.01977
Structure of smiles [FragFp] bit 20	8.32E-04	-0.00555	0.095339
Structure of smiles [FragFp] bit 200	0.002732	0.01883	0.06655
Structure of smiles [FragFp] bit 201	0.027639	0.045034	-0.00167
Structure of smiles [FragFp] bit 202	-0.00719	0.032311	0.102397
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Structure of smiles [FragFp] bit 204	0.03611	0.054836	-0.01976
Structure of smiles [FragFp] bit 205	0.076176	-0.01088	-5.34E-04
Structure of smiles [FragFp] bit 206	0.060502	-0.03362	-0.01405
Structure of smiles [FragFp] bit 207	0.034481	0.033963	-0.03134
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Structure of smiles [FragFp] bit 21	0.065085	0.026137	0.022803
Structure of smiles [FragFp] bit 210	0.058693	-0.06243	-0.00927
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Structure of smiles [FragFp] bit 213	0.062932	0.033529	0.023548
Structure of smiles [FragFp] bit 214	0.058954	0.056785	0.012444
Structure of smiles [FragFp] bit 215	0.017474	-0.02862	0.069538
Structure of smiles [FragFp] bit 216	0.015626	0.022433	-0.01648
Structure of smiles [FragFp] bit 217	0.005775	0.002976	-0.00873
Structure of smiles [FragFp] bit 218	0.073742	0.035618	3.53E-04
Structure of smiles [FragFp] bit 219	-0.01372	-0.02951	0.104677
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Structure of smiles [FragFp] bit 223	-0.00524	-0.05692	2.14E-04
Structure of smiles [FragFp] bit 224	0.030902	0.03515	-0.03613
Structure of smiles [FragFp] bit 225	0.067879	0.059344	0.002184
Structure of smiles [FragFp] bit 226	-0.01823	-0.07378	0.073772
Structure of smiles [FragFp] bit 227	0.065442	-0.02465	0.027087
Structure of smiles [FragFp] bit 228	-0.0146	-0.02864	0.093439
Structure of smiles [FragFp] bit 229	0.063933	-0.06207	-0.02413
Structure of smiles [FragFp] bit 23	0.071359	-0.04852	-0.01005
Structure of smiles [FragFp] bit 230	0.031476	0.053854	-0.01825
Structure of smiles [FragFp] bit 231	0.035379	0.072847	0.042145
Structure of smiles [FragFp] bit 232	0.027122	0.043809	-0.02179
Structure of smiles [FragFp] bit 233	0.061063	-0.02057	0.011373
Structure of smiles [FragFp] bit 234	0.025966	0.029127	-0.00255
Structure of smiles [FragFp] bit 235	0.06513	0.046612	-0.02599
Structure of smiles [FragFp] bit 236	0.025541	0.037624	-0.02262
Structure of smiles [FragFp] bit 237	-0.01753	0.001295	0.138356

Structure of smiles [FragFp] bit 238	0.042724	-0.06481	0.017643
Structure of smiles [FragFp] bit 239	-0.00942	0.029423	0.1263
Structure of smiles [FragFp] bit 24	0.071265	-0.04908	-0.01268
Structure of smiles [FragFp] bit 240	0.062804	0.003845	0.031129
Structure of smiles [FragFp] bit 241	0.05356	-0.03712	0.034959
Structure of smiles [FragFp] bit 242	-0.01406	-0.04869	0.044937
Structure of smiles [FragFp] bit 243	0.037639	-0.05354	0.022083
Structure of smiles [FragFp] bit 244	0.065844	0.017896	0.00733
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Structure of smiles [FragFp] bit 246	0.014574	-0.00406	0.038152
Structure of smiles [FragFp] bit 247	0.035501	0.006244	-0.01043
Structure of smiles [FragFp] bit 248	-0.00763	-0.04423	0.060263
Structure of smiles [FragFp] bit 249	0.069625	0.028373	9.96E-04
Structure of smiles [FragFp] bit 25	0.009157	-0.05014	0.037698
Structure of smiles [FragFp] bit 250	0.073478	0.043811	-4.42E-04
Structure of smiles [FragFp] bit 251	0.064084	-0.05447	-0.03776
Structure of smiles [FragFp] bit 252	0.036221	-0.06294	0.004027
Structure of smiles [FragFp] bit 253	0.067371	0.009239	0.010244
Structure of smiles [FragFp] bit 254	0.066809	0.046202	-0.02366
Structure of smiles [FragFp] bit 255	0.068476	0.045784	0.012031
Structure of smiles [FragFp] bit 256	0.035517	0.049937	-0.01776
Structure of smiles [FragFp] bit 257	0.025493	-0.054	9.05E-04
Structure of smiles [FragFp] bit 258	-0.00822	-0.02468	0.052121
Structure of smiles [FragFp] bit 259	0.062693	-0.01751	-0.00358
Structure of smiles [FragFp] bit 26	0.038904	-0.07247	0.020285
Structure of smiles [FragFp] bit 260	-0.00765	0.020286	0.07309
Structure of smiles [FragFp] bit 261	-0.00168	-0.11276	-0.01111
Structure of smiles [FragFp] bit 262	0.064505	-0.0516	-0.02431
Structure of smiles [FragFp] bit 263	0.039406	-0.09514	-0.01458
Structure of smiles [FragFp] bit 264	0.064806	0.027111	0.016707
Structure of smiles [FragFp] bit 265	0.024108	0.032562	-0.00918
Structure of smiles [FragFp] bit 266	0.04419	0.021081	-0.0209
Structure of smiles [FragFp] bit 267	0.056843	-0.00745	-0.01901
Structure of smiles [FragFp] bit 268	0.006451	0.028412	0.00737
Structure of smiles [FragFp] bit 269	-0.01622	0.023979	0.110472
Structure of smiles [FragFp] bit 27	0.059597	0.03163	-0.00823
Structure of smiles [FragFp] bit 270	-0.00806	0.004178	0.119447
Structure of smiles [FragFp] bit 271	0.058762	0.028934	0.023582
Structure of smiles [FragFp] bit 272	0.020849	-0.00837	0.03503
Structure of smiles [FragFp] bit 273	-0.00147	-0.07325	-0.01769
Structure of smiles [FragFp] bit 274	0.048209	-0.05975	0.048029
Structure of smiles [FragFp] bit 275	0.036754	-0.07027	-0.0288
Structure of smiles [FragFp] bit 276	0.03497	-0.00226	0.061439
Structure of smiles [FragFp] bit 277	-0.01185	-0.06379	0.072416
Structure of smiles [FragFp] bit 278	0.066996	-0.01982	-0.02244
Structure of smiles [FragFp] bit 279	0.025373	0.025031	0.011109

Structure of smiles [FragFp] bit 28	0.033371	-0.05569	0.027876
Structure of smiles [FragFp] bit 280	0.057399	0.040317	0.025778
Structure of smiles [FragFp] bit 281	0.007551	-0.12029	-0.01181
Structure of smiles [FragFp] bit 282	0.034167	0.062612	0.042472
Structure of smiles [FragFp] bit 283	0.061023	-0.03066	-0.01857
Structure of smiles [FragFp] bit 284	0.060232	0.023788	0.025577
Structure of smiles [FragFp] bit 285	0.025968	0.035573	-0.01409
Structure of smiles [FragFp] bit 286	0.059143	-0.04335	-0.05096
Structure of smiles [FragFp] bit 287	0.068775	0.044519	4.01E-04
Structure of smiles [FragFp] bit 288	0.060717	0.019331	-0.02502
Structure of smiles [FragFp] bit 289	0.063751	-0.01408	0.03087
Structure of smiles [FragFp] bit 29	0.057152	0.028501	-0.00162
Structure of smiles [FragFp] bit 290	0.049007	0.077229	0.01064
Structure of smiles [FragFp] bit 291	0.066876	0.050969	0.017264
Structure of smiles [FragFp] bit 292	0.053231	0.075176	0.020438
Structure of smiles [FragFp] bit 293	-0.00994	-0.07863	0.043019
Structure of smiles [FragFp] bit 294	-0.00991	0.026257	0.114869
Structure of smiles [FragFp] bit 295	0.072654	0.001403	0.007261
Structure of smiles [FragFp] bit 296	0.064889	0.031499	-0.01606
Structure of smiles [FragFp] bit 297	0.061064	0.06738	0.015802
Structure of smiles [FragFp] bit 298	0.04213	0.010055	-0.00565
Structure of smiles [FragFp] bit 299	-0.01496	0.028615	0.073678
Structure of smiles [FragFp] bit 3	0.081358	-0.01382	0.001266
Structure of smiles [FragFp] bit 30	0.018224	0.032445	0.017406
Structure of smiles [FragFp] bit 300	0.002691	-0.04093	0.006703
Structure of smiles [FragFp] bit 301	0.032744	0.023348	0.032239
Structure of smiles [FragFp] bit 302	0.04762	0.033702	-0.04407
Structure of smiles [FragFp] bit 303	0.001569	0.011382	0.036667
Structure of smiles [FragFp] bit 304	0.031208	0.023589	0.06984
Structure of smiles [FragFp] bit 305	0.041404	-0.03731	-0.00727
Structure of smiles [FragFp] bit 306	0.055904	0.083877	0.016563
Structure of smiles [FragFp] bit 307	-0.01585	0.006328	0.10313
Structure of smiles [FragFp] bit 308	-0.01297	-0.08574	0.039564
Structure of smiles [FragFp] bit 309	0.067855	0.067724	0.012523
Structure of smiles [FragFp] bit 31	0.074327	-0.03913	0.016433
Structure of smiles [FragFp] bit 310	0.02432	0.056573	-0.00207
Structure of smiles [FragFp] bit 311	0.061774	-0.06564	-0.03699
Structure of smiles [FragFp] bit 312	-0.00781	0.014743	0.118217
Structure of smiles [FragFp] bit 313	0.060495	-0.0067	0.015594
Structure of smiles [FragFp] bit 314	0.060755	0.003265	-0.02143
Structure of smiles [FragFp] bit 315	-0.00552	-0.06608	0.048672
Structure of smiles [FragFp] bit 316	0.048915	0.035725	0.026165
Structure of smiles [FragFp] bit 317	0.073451	0.016081	0.003509
Structure of smiles [FragFp] bit 318	0.065039	0.031444	0.009404
Structure of smiles [FragFp] bit 319	0.059151	-0.0598	-0.02978
Structure of smiles [FragFp] bit 32	0.060499	0.025861	0.023262

Structure of smiles [FragFp] bit 320	0.027193	-0.01969	0.045769
Structure of smiles [FragFp] bit 321	0.062454	-0.02953	0.020486
Structure of smiles [FragFp] bit 322	0.063605	0.024255	0.006598
Structure of smiles [FragFp] bit 323	0.060985	-0.01173	-0.02794
Structure of smiles [FragFp] bit 324	-0.00752	0.022813	0.094452
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Structure of smiles [FragFp] bit 326	-0.01364	-0.02901	0.088997
Structure of smiles [FragFp] bit 327	0.026048	0.016554	-0.01209
Structure of smiles [FragFp] bit 328	0.057941	0.064173	0.014896
Structure of smiles [FragFp] bit 329	0.062053	-0.0015	-0.03485
Structure of smiles [FragFp] bit 33	0.044265	-0.08495	0.011937
Structure of smiles [FragFp] bit 330	-0.00113	-0.04458	0.040036
Structure of smiles [FragFp] bit 331	-0.01749	-0.02766	0.104299
Structure of smiles [FragFp] bit 332	0.019516	-0.1197	0.01821
Structure of smiles [FragFp] bit 333	-0.00902	0.018965	0.090081
Structure of smiles [FragFp] bit 334	-0.00984	-0.03744	0.097286
Structure of smiles [FragFp] bit 335	-0.01101	0.028785	0.119455
Structure of smiles [FragFp] bit 336	0.010302	-0.04052	0.03458
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Structure of smiles [FragFp] bit 338	-0.01994	-0.08868	0.03996
Structure of smiles [FragFp] bit 339	0.057908	0.028973	0.022253
Structure of smiles [FragFp] bit 34	0.054936	-0.07769	0.017379
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Structure of smiles [FragFp] bit 396	-0.01091	0.008215	7.69E-04
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Structure of smiles [FragFp] bit 406	0.026402	0.025175	-0.00239
Structure of smiles [FragFp] bit 407	0.018122	-0.01475	0.021809
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Structure of smiles [FragFp] bit 41	0.052778	0.022857	-7.31E-04
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Structure of smiles [FragFp] bit 427	7.04E-04	-0.02728	0.071382
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Structure of smiles [FragFp] bit 463	0.014178	0.068851	0.029946
Structure of smiles [FragFp] bit 464	0.009471	0.032077	-0.00387
Structure of smiles [FragFp] bit 465	0.00628	0.006637	-0.01655
Structure of smiles [FragFp] bit 466	0.005922	0.017613	0.003679
Structure of smiles [FragFp] bit 467	0.007769	-0.02005	0.007276
Structure of smiles [FragFp] bit 468	0.009165	0.022962	-0.01115
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Structure of smiles [FragFp] bit 473	0.020214	-0.01816	-0.00626
Structure of smiles [FragFp] bit 474	-0.01497	-0.01399	0.082444
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Structure of smiles [FragFp] bit 50	0.004542	-0.02831	0.022595
Structure of smiles [FragFp] bit 500	-0.00689	0.029519	0.1002
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Structure of smiles [FragFp] bit 62	0.01096	-0.01489	0.008928
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Structure of smiles [FragFp] bit 66	0.070601	0.016543	0.002905
Structure of smiles [FragFp] bit 67	0.053315	-0.08033	0.024577

Structure of smiles [FragFp] bit 68	0.071216	0.05137	0.003775
Structure of smiles [FragFp] bit 69	0.078314	0.014096	-0.01256
Structure of smiles [FragFp] bit 7	0.064309	0.041418	-0.00803
Structure of smiles [FragFp] bit 70	0.074053	0.011525	-0.00561
Structure of smiles [FragFp] bit 71	0.015454	0.020771	0.023996
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Structure of smiles [FragFp] bit 73	0.074912	0.024141	0.00226
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Structure of smiles [FragFp] bit 8	0.037065	-0.05974	0.03826
Structure of smiles [FragFp] bit 80	0.078227	0.019773	-0.0036
Structure of smiles [FragFp] bit 81	0.061679	-0.08758	-0.02717
Structure of smiles [FragFp] bit 82	0.051546	0.062695	-0.00461
Structure of smiles [FragFp] bit 83	0.036994	0.062891	-0.00798
Structure of smiles [FragFp] bit 84	0.071374	-0.04927	-0.00689
Structure of smiles [FragFp] bit 85	0.077728	-0.00577	0.003742
Structure of smiles [FragFp] bit 86	0.057399	-0.0876	-0.02805
Structure of smiles [FragFp] bit 87	-0.01683	-0.06502	0.070407
Structure of smiles [FragFp] bit 88	-0.00592	0.020237	0.073192
Structure of smiles [FragFp] bit 89	0.07164	0.043027	0.022176
Structure of smiles [FragFp] bit 9	0.002598	0.015081	0.050432
Structure of smiles [FragFp] bit 90	0.062137	-0.03696	0.029905
Structure of smiles [FragFp] bit 91	0.049644	-0.07313	0.021795
Structure of smiles [FragFp] bit 92	0.045274	-0.09562	-0.00747
Structure of smiles [FragFp] bit 93	0.043885	-0.10483	-0.00516
Structure of smiles [FragFp] bit 94	-0.00904	0.026708	0.101655
Structure of smiles [FragFp] bit 95	0.037642	0.069642	0.023564
Structure of smiles [FragFp] bit 96	0.050472	-0.05451	0.046834
Structure of smiles [FragFp] bit 97	0.035709	-0.04265	0.075028
Structure of smiles [FragFp] bit 98	-0.0158	0.006608	0.128745
Structure of smiles [FragFp] bit 99	0.042709	-0.08189	0.028348

Supplementary figures

Chemical space visualization using PCA

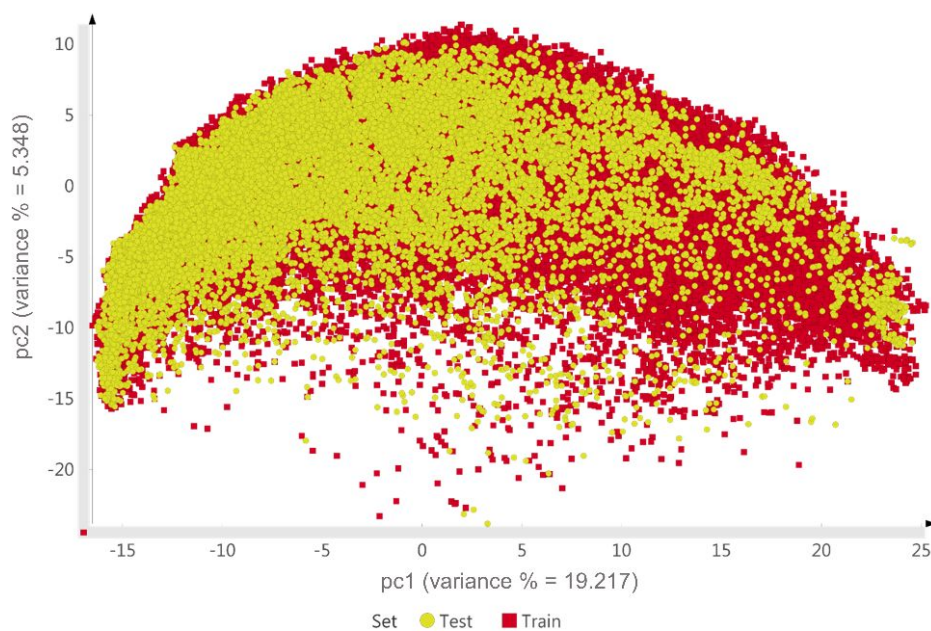


Figure S1. The chemical space visualization using PCA. Test set compounds were mostly mapped within the training set chemical space boundaries which confirms the prediction quality of the PCM and L-B model.

Scatter plot of PCA of screened drugs and active compounds of P14337 (dengue NS3 protein) from the training set

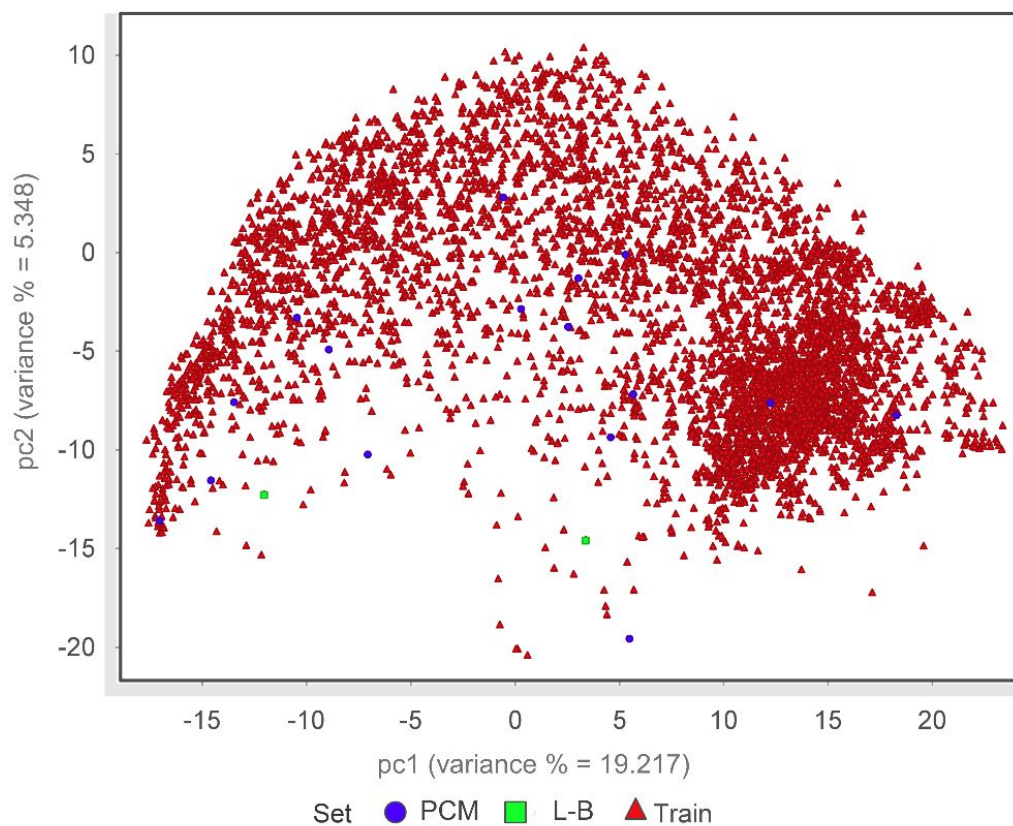


Figure S2. Scatter plot of PCA of screened drugs and active compounds of P14337 (dengue NS3 protein) from the training set. Drugs/substances which scored 0.99 from PCM model and ≥ 0.5 for L-B model were subjected to PCA to determine their position in the chemical space covered by the training set. Most of drugs predicted using PCM model (blue) lies within the training set boundaries, while the drugs predicted using the L-B model lies close to the compounds but not in the heavily populated area.