



Supplementary Material

Quantum Artificial Neural Network Approach to Derive a Highly Predictive 3D-QSAR Model for Blood–Brain Barrier Passage

Taeho Kim,¹ Byoung Hoon You,² Songhee Han,² Ho Chul Shin,² Kee-Choo Chung,^{1,*} Hwangseo Park^{1,*}

¹ Department of Bioscience and Biotechnology, Sejong University, 209 Neungdong-ro, Kwangjin-gu, Seoul 05006, Korea

² Whan In Pharmaceutical Co., Ltd., 11, Beobwon-ro 6-gil, Songpa-gu, Seoul 05855, Korea


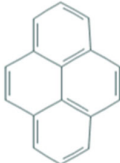
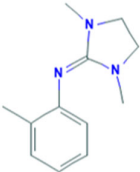
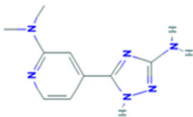
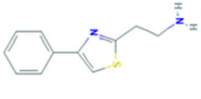
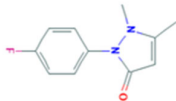
* Correspondence: Tel: +82-2-10-2963-1635 (KCC); +82-2-3408-3766 (HP); Fax: +82-2-3408-4334 (KCC); +82-2-3408-4334 (HP); E-mail: kitto28@paran.com (KCC); hspark@sejong.ac.kr (HP)

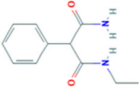
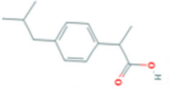
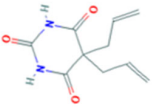
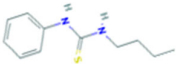
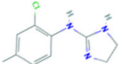
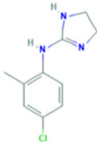
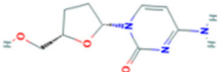
Supplementary Material

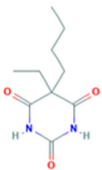
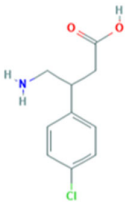
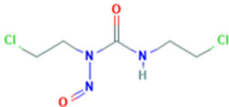
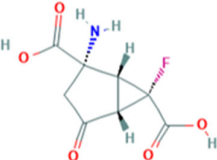
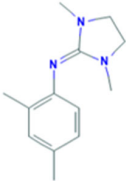
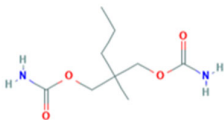
Chemical structures, molecular weights, S2-S60, S61-S84
LogBB values, and PubChem CID of all the
molecules in the dataset.

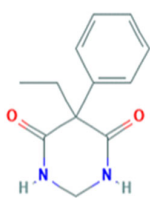
Linear diagrams showing correlation between the experimental and calculated LogBB values of Subset 1-8 molecules in the 3-fold external cross-validation.

Table S1. Chemical structures, molecular weights, experimental LogBB values, and PubChem CID of all the molecules in the dataset.

| Structure | Molecular weight | LogBB | PubChem CID |
|---|------------------|-------|-------------|
|  | 200.053 | 0.3 | 5206 |
|  | 202.255 | 0.23 | 31423 |
|  | 203.2864 | -1.39 | 12032949 |
|  | 204.234 | -1.17 | 12889418 |
|  | 204.2892 | -1.3 | 1497794 |
|  | 206.2187 | -0.05 | 94957 |

| | | | |
|---|----------|-------|-----------|
|  | 206.2438 | -0.19 | 118753220 |
|  | 206.284 | -0.18 | 3672 |
|  | 208.2164 | -0.22 | 5842 |
|  | 208.3208 | 0.03 | 3034183 |
|  | 209.6749 | -0.65 | 72138 |
|  | 209.6749 | -0.87 | 77870 |
|  | 211.22 | -1.18 | 24066 |

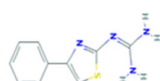
| | | | |
|---|----------|-------|----------|
|  | 212.248 | 0.19 | 6473 |
|  | 213.6603 | -1.52 | 2284 |
|  | 214.045 | -0.52 | 2578 |
|  | 217.1529 | -0.41 | 9837317 |
|  | 217.3132 | -1.3 | 21675832 |
|  | 218.2522 | -0.15 | 4064 |



218.2548

-0.07

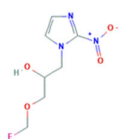
4909



218.2758

-0.18

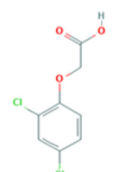
3763607



219.1717

-0.01

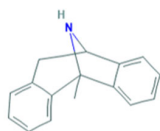
23274095



221.0336

0.15

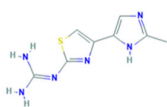
1486



221.3012

1.11

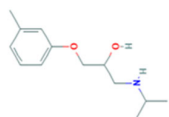
1207



222.2672

-0.04

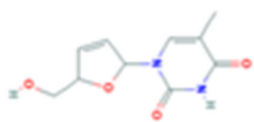
56051



223.3144

0.34

18047



224.2158

-0.48

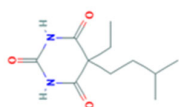
5155



225.2066

-0.84

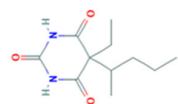
2022



226.2748

0.11

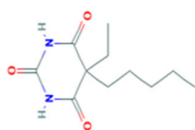
2164



226.2748

0.08

4737



226.2748

0.09

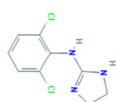
66994



228.2902

-0.12

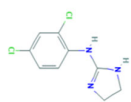
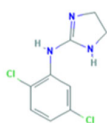
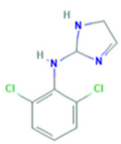
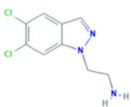
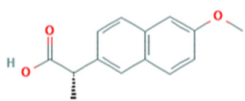
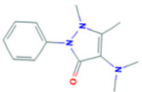
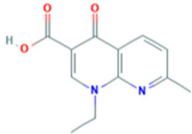
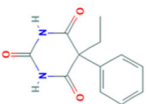
6623

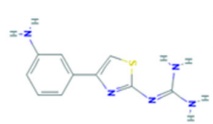


230.0902

0.12

2803

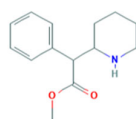
| | | | |
|---|----------|-------|----------|
|  | 230.0902 | 0.16 | 90274 |
|  | 230.0902 | 0.38 | 11777724 |
|  | 230.0902 | 0.11 | 13071367 |
|  | 230.0902 | 0.11 | 44214615 |
|  | 230.2628 | 0.1 | 156391 |
|  | 231.2968 | 0 | 6009 |
|  | 232.2384 | -0.66 | 4421 |
|  | 232.2384 | 0.12 | 4763 |



233.2904

-1.15

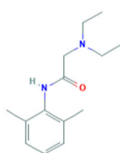
14022509



233.3096

0.88

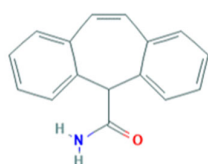
4158



234.3406

0.34

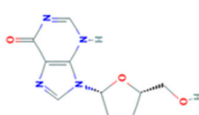
3676



235.2848

0

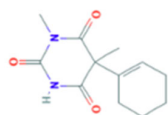
25255



236.2298

-1.301

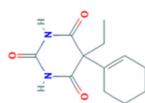
50599



236.27

0.03

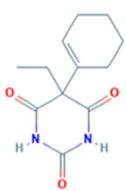
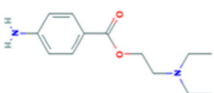
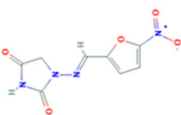
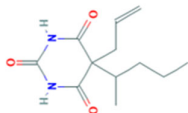
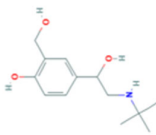
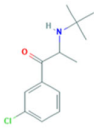
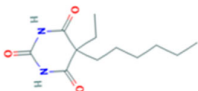
3608

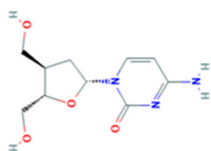


236.27

-0.301

5838

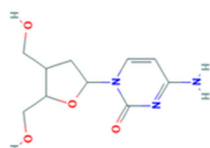
| | | | |
|---|----------|-------|---------|
|  | 236.2726 | -0.04 | 2554 |
|  | 236.3132 | 0.05 | 4914 |
|  | 238.1592 | -2.09 | 6604200 |
|  | 238.2858 | 0.2 | 5193 |
|  | 239.3138 | -1.14 | 2083 |
|  | 239.7413 | 1.4 | 444 |
|  | 240.3016 | 0.36 | 8942 |



241.2462

-0.79

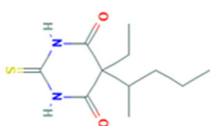
451819



241.2462

-0.79

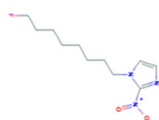
14840722



242.3354

-0.19

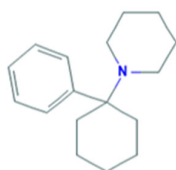
3000715



243.2801

-0.17

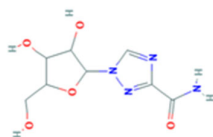
10377120



243.3912

0.58

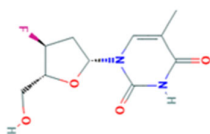
6468



244.2066

-0.67

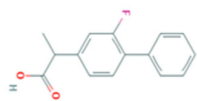
5064



244.2217

-0.59

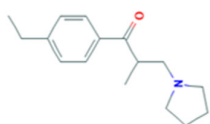
33039



244.2645

-1.68

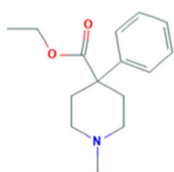
3394



245.3638

1.08

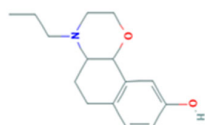
65860



247.3364

0.85

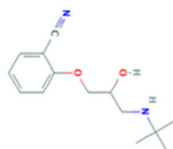
4058



247.3364

0.26

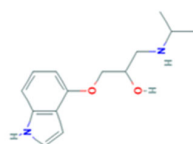
10060538



248.3242

0.38

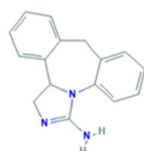
2473



248.3242

-0.14

4828



249.3146

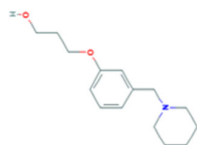
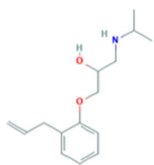
-0.16

3241

249.3522

-0.23

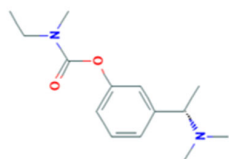
2119



249.3522

-0.02

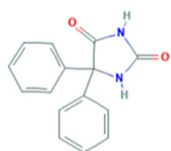
10444765



250.34

0.88

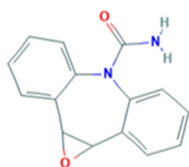
77991



252.272

-0.05

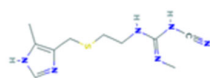
1775



252.272

-0.34

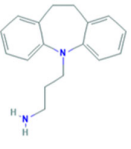
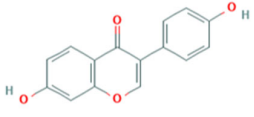
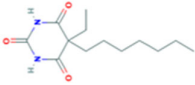
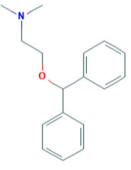
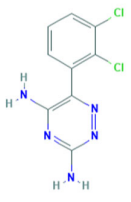
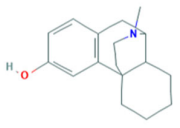
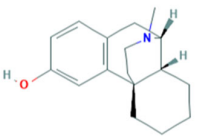
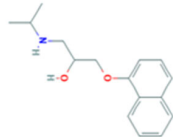
2555

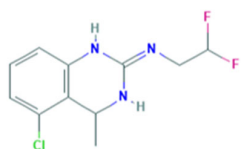


252.3366

-1.06

2756

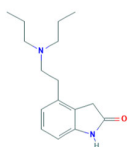
| | | | |
|---|----------|-------|---------|
|  | 252.3584 | 1.05 | 159642 |
|  | 254.2416 | -0.15 | 5281708 |
|  | 254.3284 | 0.02 | 43473 |
|  | 255.359 | 1.26 | 3100 |
|  | 256.0878 | 0.29 | 3878 |
|  | 257.3748 | 0 | 3918 |
|  | 257.3748 | 0 | 5359272 |
|  | 259.3474 | 0.84 | 4946 |



259.6819

0.6

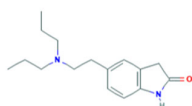
135458393



260.3784

0.08

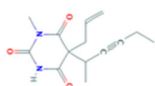
5095



260.3784

0.25

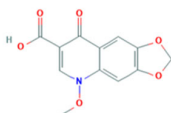
44383796



262.3078

-0.07

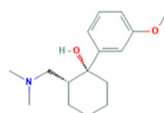
9034



263.2062

-0.92

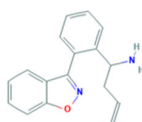
37614



263.379

0.72

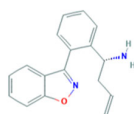
33741



264.3262

0

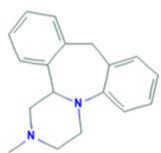
9861160



264.3262

0

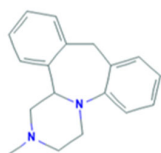
15524033



264.3694

0.99

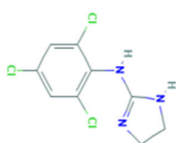
4184



264.3694

0.99

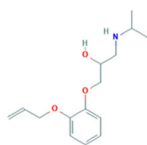
4184



264.5323

0.47

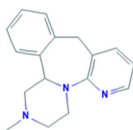
10470115



265.3516

0.02

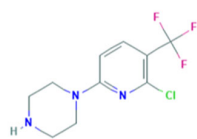
4631



265.3572

0.53

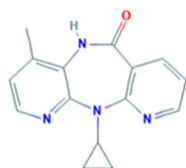
4205



265.661

1.64

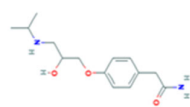
9796408



266.3018

0

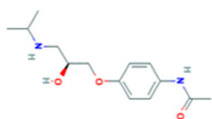
4463



266.3394

-1.14

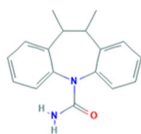
2249



266.3394

-0.55

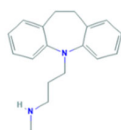
443371



266.342

-0.34

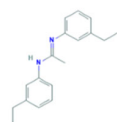
70517986



266.3852

1.08

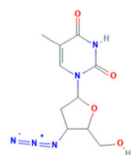
2995



266.3852

1.2

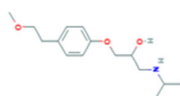
19427054



267.2438

-0.74

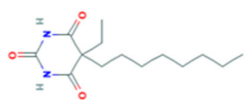
5726



267.3674

1.15

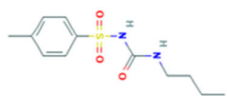
4171



268.3552

0.24

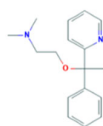
13755681



270.3458

-1.01

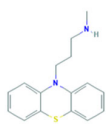
5505



270.3736

0.64

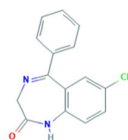
3162



270.3916

0.59

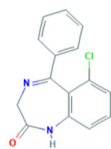
28315



270.7147

0.52

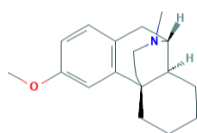
2997



270.7147

0.5

14590445



271.4016

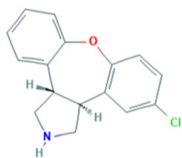
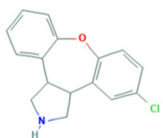
0.22

6916184

271.7427

0.39

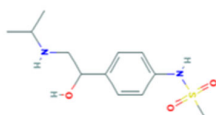
14577084



271.7427

0.39

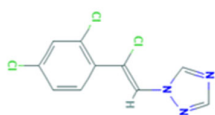
44568616



272.3616

-0.28

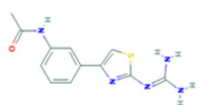
5253



274.5275

0.28

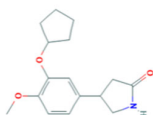
3034012



275.3276

-1.57

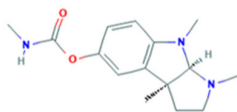
14022511



275.3468

0.61

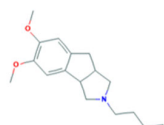
5092



275.3498

0.08

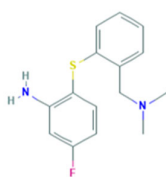
5983



275.39

0.31

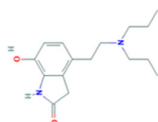
6086



276.3707

0.2

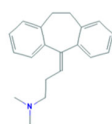
10265481



276.3778

-0.43

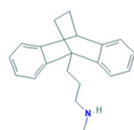
133741



277.4084

0.9

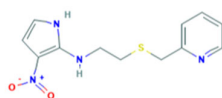
2160



277.4084

1.3

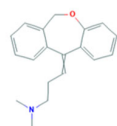
4011



278.3282

-0.66

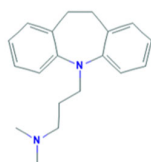
14022481



279.381

1

3158



280.412

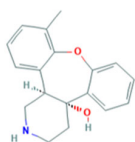
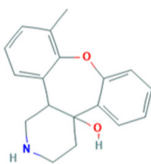
0.98

3696

281.3536

0.52

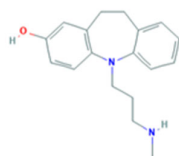
22154175



281.3536

0.52

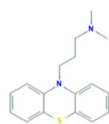
44568615



282.3846

0.53

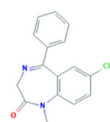
121249



284.4184

1.08

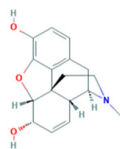
4926



284.7415

0.47

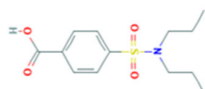
3016



285.342

-0.26

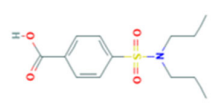
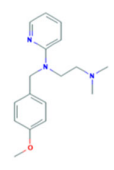
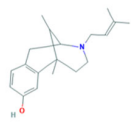
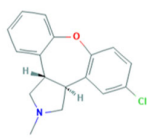
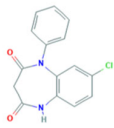
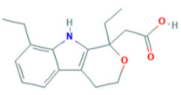
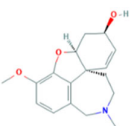
5288826

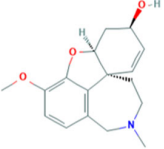
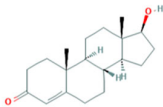
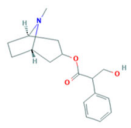
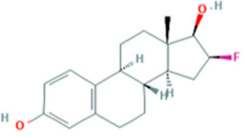
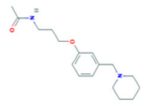
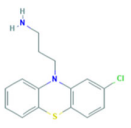
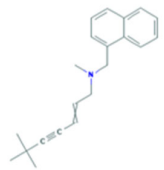


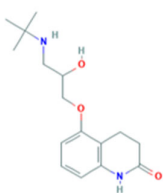
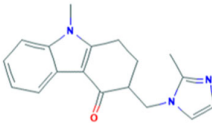
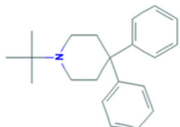
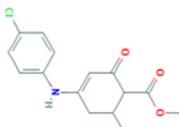
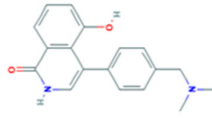
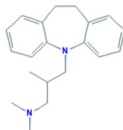
285.3574

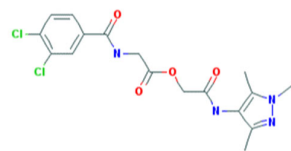
-0.4

4911

| | | | |
|---|----------|-------|--------|
|  | 285.3574 | -0.4 | 4911 |
|  | 285.3882 | 0.49 | 4992 |
|  | 285.4284 | 0.51 | 4736 |
|  | 285.7695 | 1.03 | 163091 |
|  | 286.7141 | 0.35 | 89657 |
|  | 287.3578 | -1.42 | 3308 |
|  | 287.3578 | 0.32 | 9651 |

| | | | |
|---|----------|-------|---------|
|  | 287.3578 | 0.32 | 9651 |
|  | 288.429 | 0 | 6013 |
|  | 289.3736 | -0.06 | 174174 |
|  | 290.3765 | -0.3 | 67101 |
|  | 290.4046 | -0.46 | 9971484 |
|  | 290.8069 | 0.97 | 74981 |
|  | 291.4352 | 0.08 | 5402 |

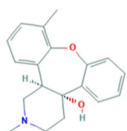
| | | | |
|---|----------|-------|---------|
|  | 292.3772 | 0.01 | 2583 |
|  | 292.4414 | -0.17 | 3035905 |
|  | 293.3676 | 0.28 | 4595 |
|  | 293.451 | 0.66 | 68778 |
|  | 293.7463 | -0.95 | 197322 |
|  | 294.3524 | -0.09 | 9839073 |
|  | 294.4388 | 0.99 | 5584 |



295.3372

-0.34

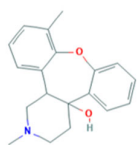
29939457



295.3804

0.82

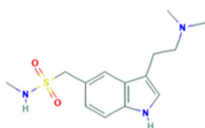
166560



295.3804

0.82

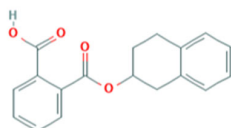
9860946



295.3988

-0.4

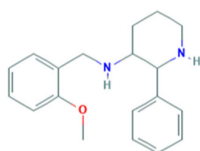
5358



296.322

0.09

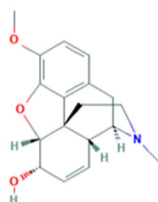
346516



296.4114

0.87

18435769



299.3688

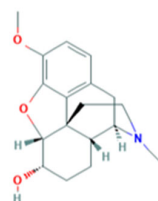
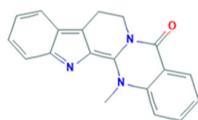
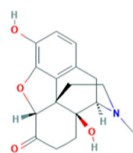
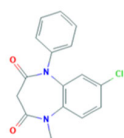
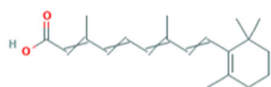
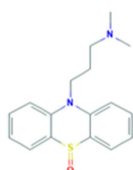
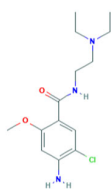
0.45

5284371

299.7967

0.9

4168



300.4178

-0.48

547559

300.44

-0.49

5538

300.7409

0.36

2789

301.3414

0.35

5284604

301.347

0.11

9817839

301.3846

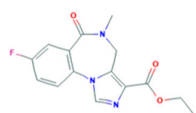
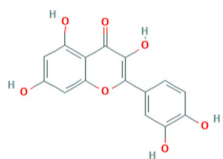
0.55

5284543

302.2398

-1.7

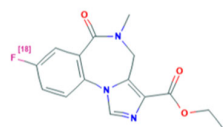
5280343



303.2919

-0.29

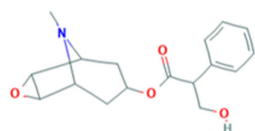
3373



303.2919

-0.095

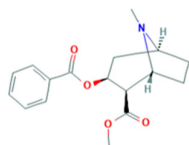
11652375



303.3572

0.23

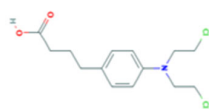
5184



303.3572

0.6

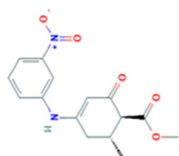
446220



304.2096

-1.7

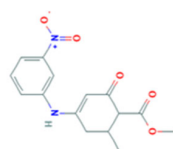
2708



304.3018

-1

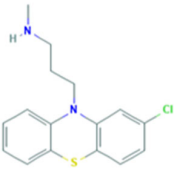
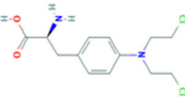
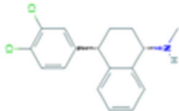
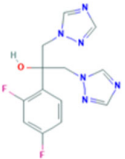
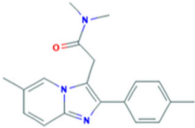
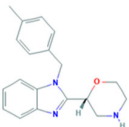
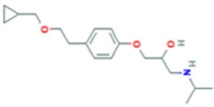
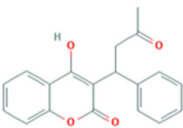
10063598

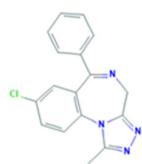


304.3018

-1

15186924

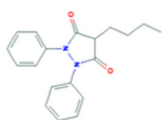
| | | | |
|---|----------|-------|----------|
|  | 304.8337 | 1.38 | 62875 |
|  | 305.1974 | -0.5 | 460612 |
|  | 306.228 | 1.6 | 68617 |
|  | 306.2734 | -0.22 | 3365 |
|  | 307.3944 | -0.48 | 5732 |
|  | 307.3944 | 0.36 | 57395287 |
|  | 307.432 | 0.39 | 2369 |
|  | 308.333 | 0 | 54678486 |



308.3792

-0.52

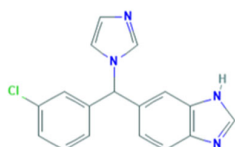
4781



308.7665

0.02

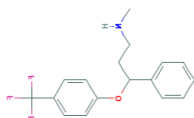
2118



308.7665

-1

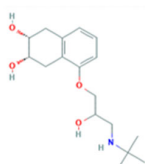
60652



309.3293

0.72

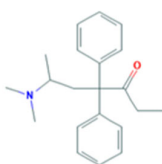
3386



309.4046

-0.95

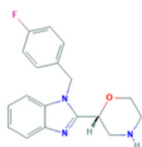
39147



309.4504

0.9

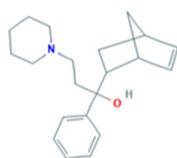
4095



311.3577

0.77

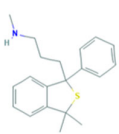
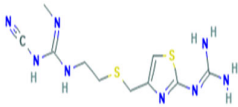
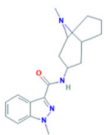
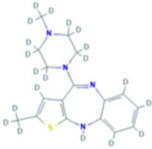
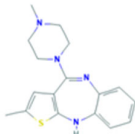
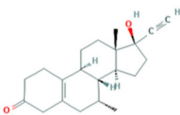
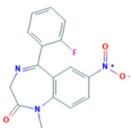
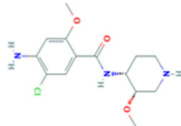
57402315

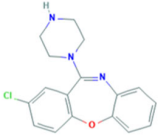
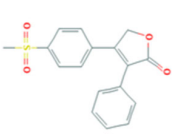
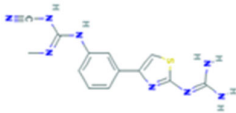

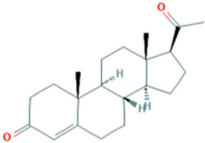
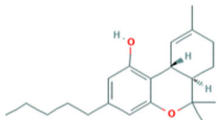
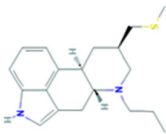
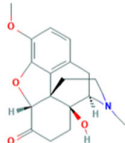


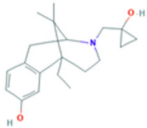
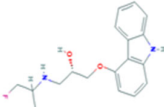
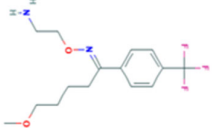
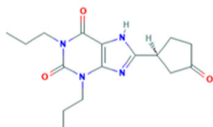
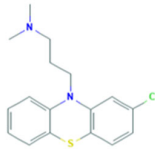
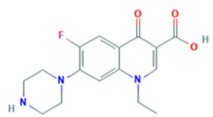
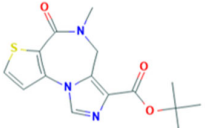
311.4662

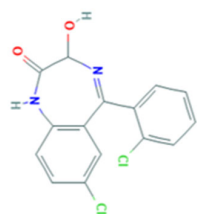
0.85

2381

| | | | |
|---|----------|-------|-----------|
|  | 311.4842 | 0.22 | 33014 |
|  | 312.41 | -0.82 | 50287 |
|  | 312.4138 | -0.69 | 3510 |
|  | 312.4318 | 0.78 | 25144104 |
|  | 312.4318 | 0.78 | 135398745 |
|  | 312.451 | 0.4 | 444008 |
|  | 313.2871 | 0.07 | 3380 |
|  | 313.7803 | -0.22 | 216236 |

| | | | |
|---|----------|-------|----------|
|  | 313.7829 | 0.6 | 2170 |
|  | 314.3552 | -0.1 | 5090 |
|  | 314.3672 | -1.54 | 14022519 |
|  | 314.4018 | -1.23 | 54429646 |
|  | 314.4668 | -0.1 | 5994 |
|  | 314.4668 | 0 | 16078 |
|  | 314.4878 | 0.3 | 47811 |
|  | 315.3682 | 0.57 | 5284603 |

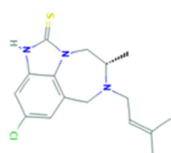
| | | | |
|---|----------|-------|----------|
|  | 315.4546 | 0.6 | 1223 |
|  | 316.3741 | 0.58 | 10358392 |
|  | 318.3371 | 0.79 | 5324346 |
|  | 318.3748 | -1.4 | 60949 |
|  | 318.8605 | 1.02 | 2726 |
|  | 319.3345 | -1.15 | 4539 |
|  | 319.3776 | -0.25 | 127382 |



321.1562

0.44

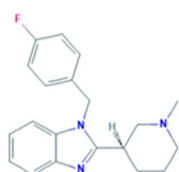
3958



321.8641

0.28

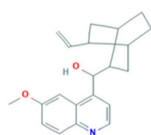
3000237



323.4119

0.43

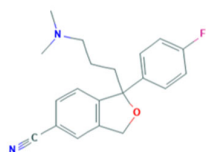
46888857



323.434

0.1

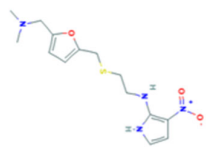
5009



324.3967

0.99

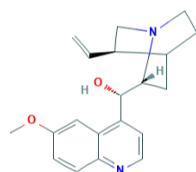
2771



324.397

-1.12

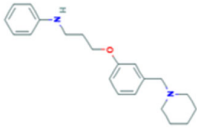
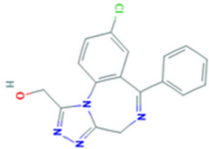
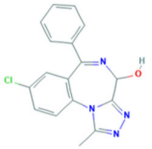
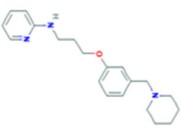

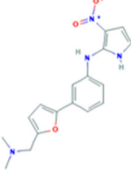
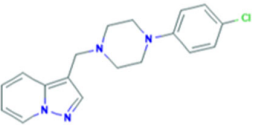
13646638

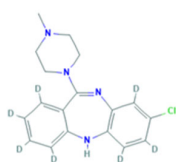


324.4218

-0.21

5953

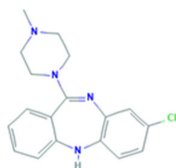
| | | | |
|---|----------|-------|----------|
|  | 324.465 | 0.69 | 10245719 |
|  | 324.7659 | -1.28 | 162244 |
|  | 324.7659 | -1.48 | 182017 |
|  | 325.4528 | 0.69 | 10019237 |
|  | 325.7688 | 0.37 | 4192 |
|  | 326.3542 | -0.27 | 14022491 |
|  | 326.8249 | 0.64 | 10404144 |



326.8249

1.3

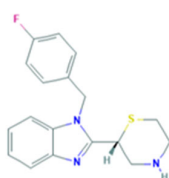
46842852



326.8249

0.7

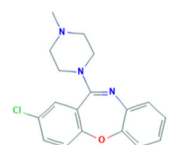
135398737



327.4183

0.89

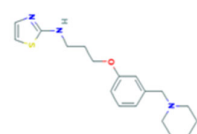
57397056



327.8097

0.8

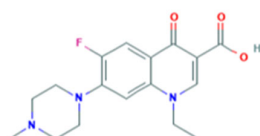
3964



331.475

0.44

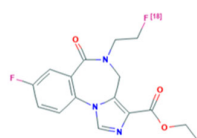
14022497



333.3613

-0.16

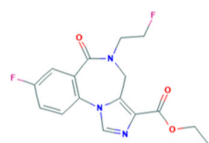
51081



335.3088

-0.14

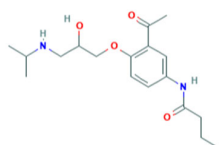
126761



335.3088

-0.14

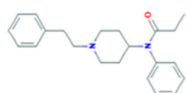
6426759



336.4302

-0.15

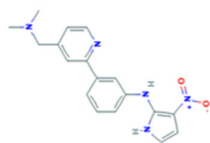
1978



336.476

0.59

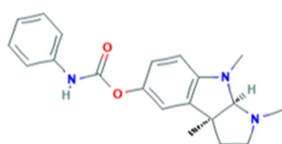
3345



337.3804

-0.28

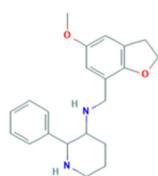
14022486



337.4206

1

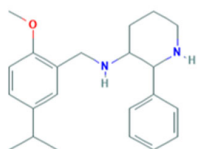
192706



338.4486

0.39

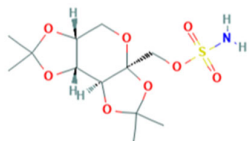
44213642



338.4918

0.92

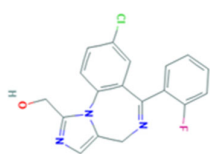
9902443



339.3598

-0.07

5284627



341.7682

-0.08

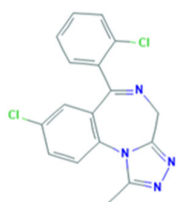
107917



341.7682

-0.22

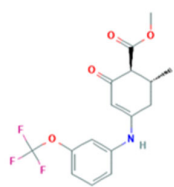
124449



343.2086

0.67

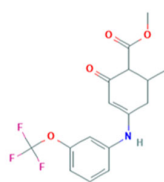
5556



343.3007

-0.17

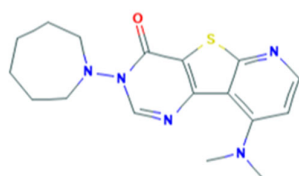
10088796



343.3007

-0.17

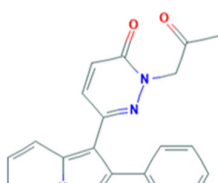
15186911

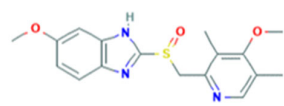
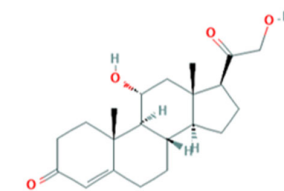
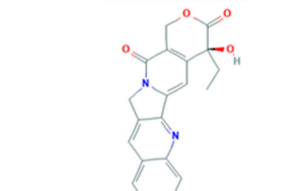
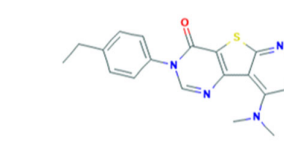
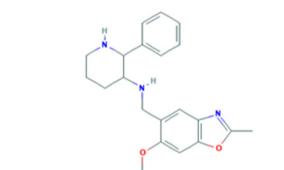
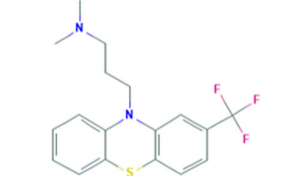


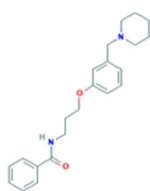
343.4458

0.43

11559235



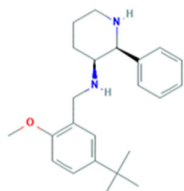
| | | | |
|---|----------|-------|----------|
| | 344.372 | -0.31 | 11110698 |
|  | 345.4154 | -0.82 | 4594 |
|  | 346.4656 | -0.5 | 256277 |
|  | 348.3574 | -0.29 | 24360 |
|  | 350.4374 | -0.47 | 11530404 |
|  | 351.4474 | 0.49 | 22620080 |
|  | 352.4155 | 1.44 | 5568 |



352.4754

-0.24

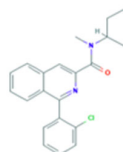
10498206



352.5186

0.98

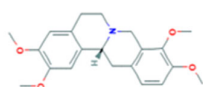
44433393



352.8597

0.48

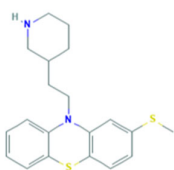
1345



355.4328

-0.07

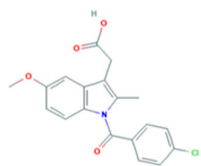
969488



356.543

0.76

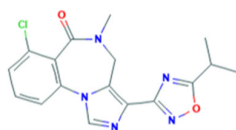
114376



357.7897

-1.26

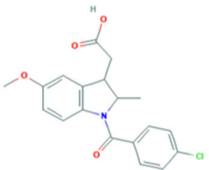
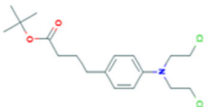
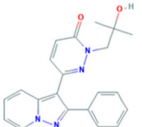
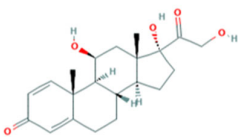
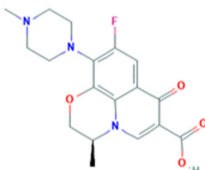
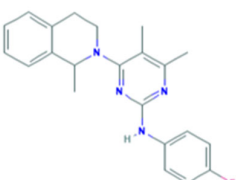
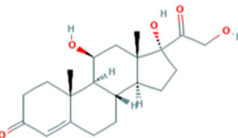
3715

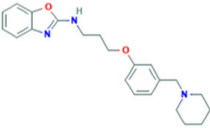
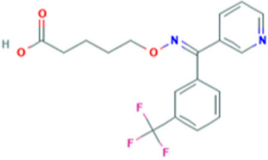
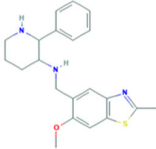
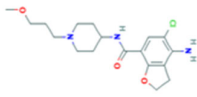
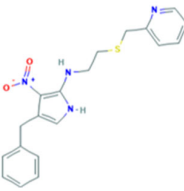
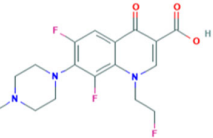
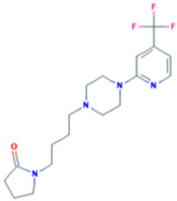


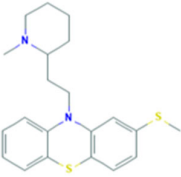
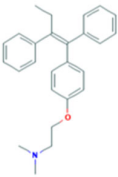
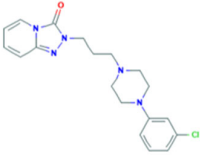
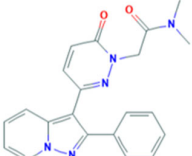
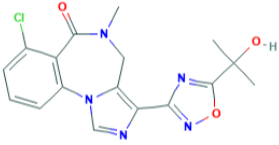
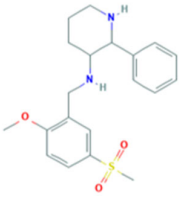
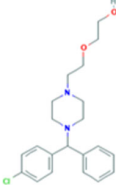
357.7957

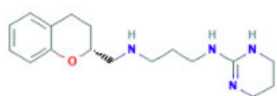
-0.3

129710

| | | | |
|---|----------|-------|----------|
|  | 359.8055 | -1.26 | 53394319 |
|  | 360.3168 | 1 | 83909 |
|  | 360.4146 | -0.23 | 10937291 |
|  | 360.4492 | -0.18 | 5755 |
|  | 361.3717 | -0.76 | 149096 |
|  | 362.4485 | 0.68 | 204104 |
|  | 362.465 | -0.22 | 5754 |

| | | | |
|---|----------|-------|----------|
|  | 365.4742 | 0.22 | 14022499 |
|  | 366.3379 | -1 | 5362391 |
|  | 367.508 | 0.48 | 22620050 |
|  | 367.8717 | -0.1 | 3052762 |
|  | 368.4526 | -0.12 | 14022483 |
|  | 369.3415 | -0.43 | 3357 |
|  | 370.4157 | 0.16 | 9907401 |

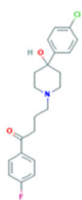
| | | | |
|---|----------|-------|----------|
|  | 370.5698 | 0.26 | 5452 |
|  | 371.5212 | 0.92 | 2733526 |
|  | 371.8657 | 0.3 | 5533 |
|  | 373.4134 | -1 | 11003252 |
|  | 373.7951 | -1.34 | 10384745 |
|  | 374.497 | -0.15 | 19696721 |
|  | 374.9065 | 0.36 | 3658 |



375.3344

-0.01

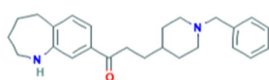
9907628



375.8662

1.33

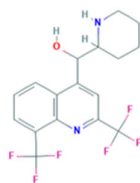
3559



376.5406

1.14

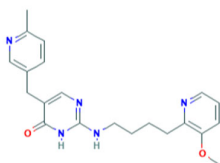
198752



378.3142

0.63

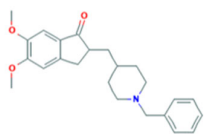
4046



379.4608

-2

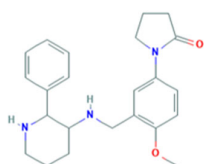
72108



379.498

0.89

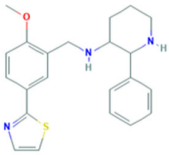
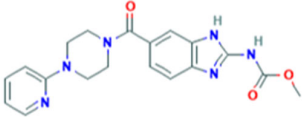
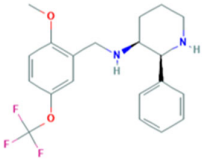
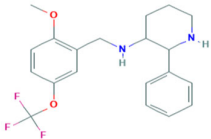
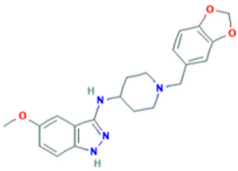
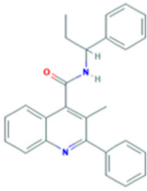
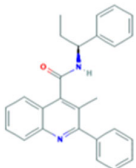
3152

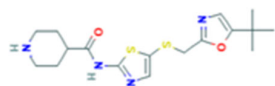


379.501

-0.22

22620062

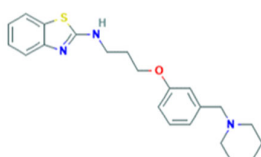
| | | | |
|---|----------|------|----------|
|  | 379.519 | 0.36 | 9907851 |
|  | 380.4054 | -1.4 | 9864646 |
|  | 380.4079 | 1.11 | 9821217 |
|  | 380.4079 | 0.63 | 9864647 |
|  | 380.4456 | 0.57 | 11531010 |
|  | 380.4884 | 0.3 | 3946663 |
|  | 380.4884 | 0.3 | 6604009 |



380.5222

-0.01

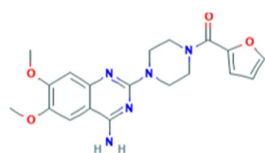
3025986



381.5348

0.14

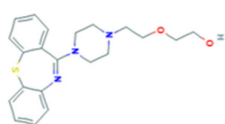
91769



383.406

-0.9

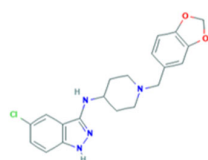
4893



383.5074

0.7

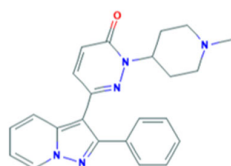
5002



384.8615

0.83

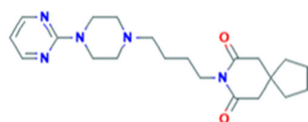
11653882



385.4676

0.06

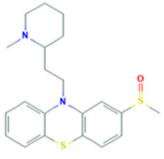
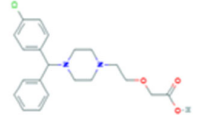
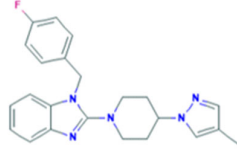
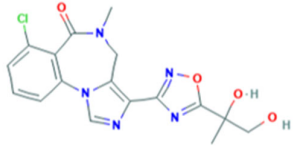
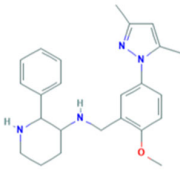
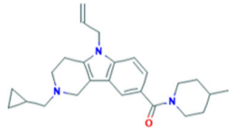
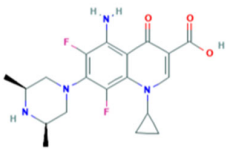
9821511

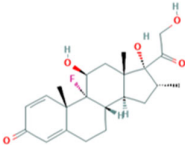
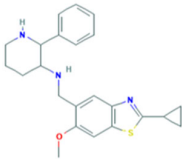
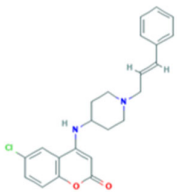
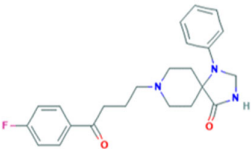
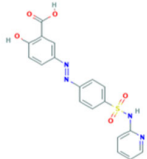
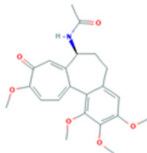
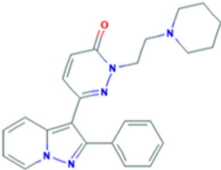


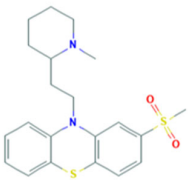
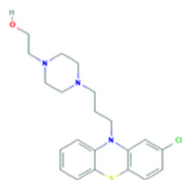
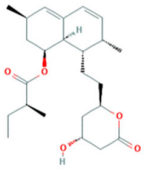
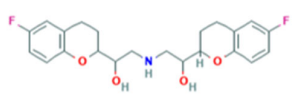
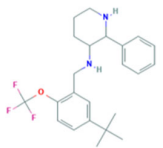
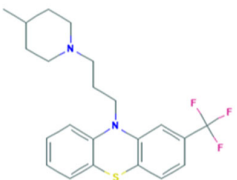
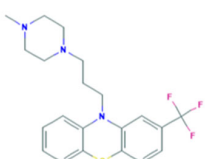
385.5082

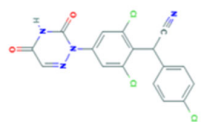
0.49

2477

| | | | |
|---|----------|-------|----------|
|  | 386.5692 | -0.28 | 4078 |
|  | 388.8901 | -2.15 | 2678 |
|  | 389.4741 | 0.32 | 45272895 |
|  | 389.7945 | -1.82 | 10091748 |
|  | 390.5272 | 0.11 | 22620075 |
|  | 391.5552 | -0.13 | 11502034 |
|  | 392.4038 | 0.41 | 60464 |

| | | | |
|---|----------|-------|----------|
|  | 392.4661 | -0.15 | 5743 |
|  | 393.5458 | 0.62 | 22620085 |
|  | 394.8969 | 0.13 | 11545677 |
|  | 395.4753 | 0.26 | 5265 |
|  | 398.3924 | -2.69 | 5339 |
|  | 399.4426 | -0.8 | 6167 |
|  | 399.4944 | 0.38 | 10884606 |

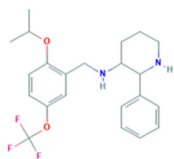
| | | | |
|---|----------|------|----------|
|  | 402.5686 | 0.18 | 31765 |
|  | 403.9659 | 0.7 | 4748 |
|  | 404.5454 | 0.85 | 53232 |
|  | 405.4398 | 0.57 | 71301 |
|  | 406.4889 | 0.96 | 9909299 |
|  | 406.5069 | 1.44 | 21440942 |
|  | 407.4947 | 1.43 | 5566 |



407.6337

-1.3

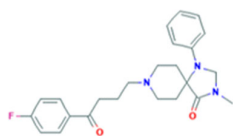
456389



408.4615

0.41

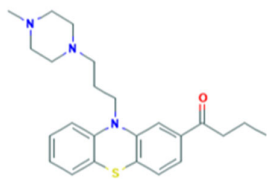
9866153



409.5021

0.46

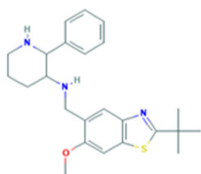
119146



409.5884

0.83

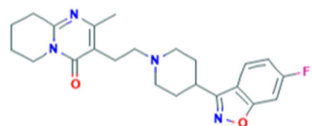
12598



409.5884

0.85

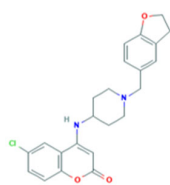
22620091



410.4899

-0.02

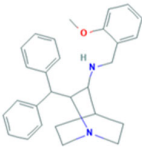
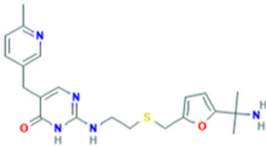
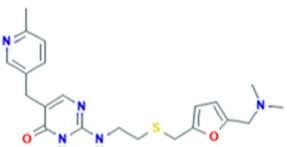
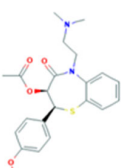
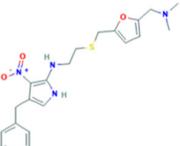
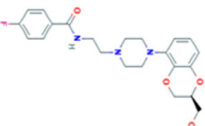
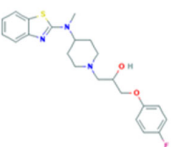
5073

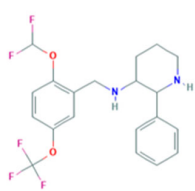
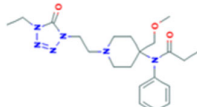
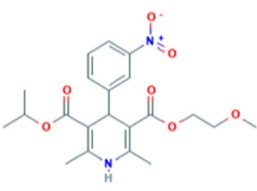
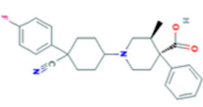
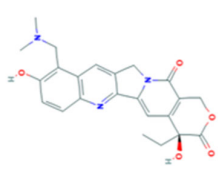
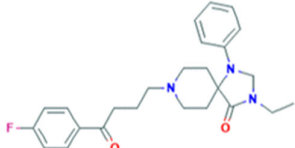
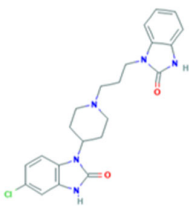


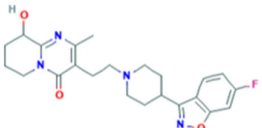
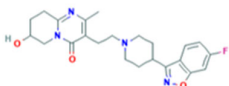
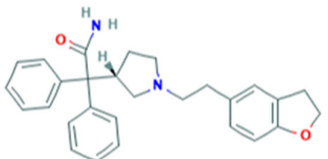
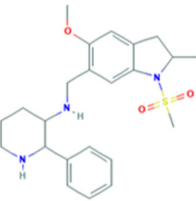
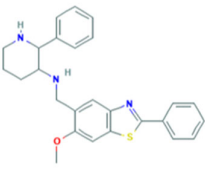
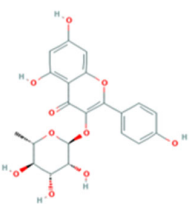
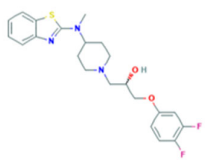
410.8963

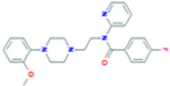
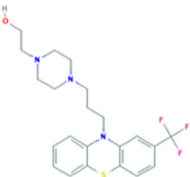
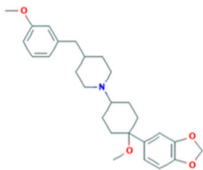
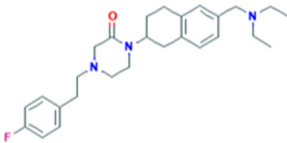
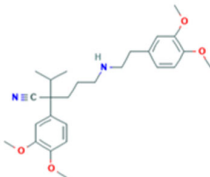
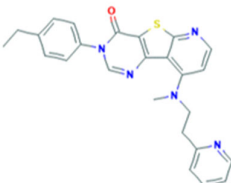
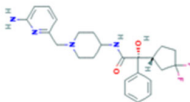
-0.14

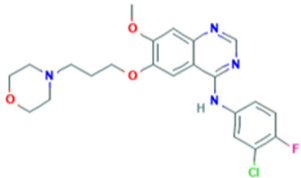
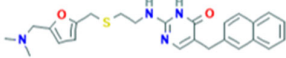
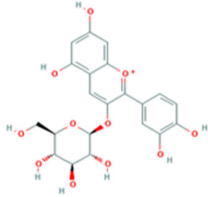
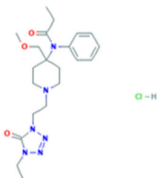
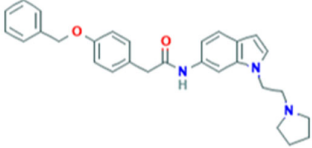
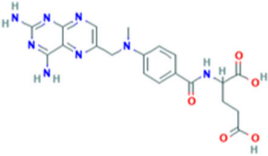
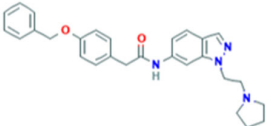
11531660

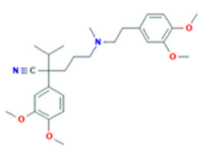
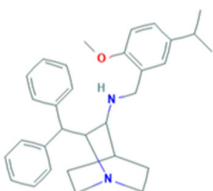
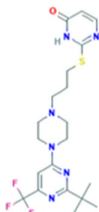
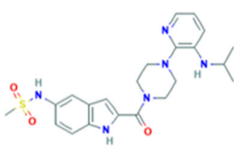
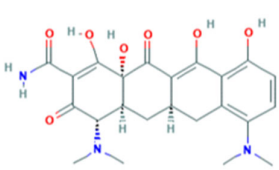
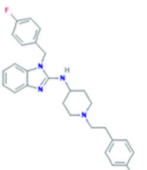
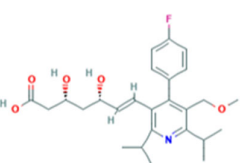
| | | | |
|---|----------|-------|----------|
|  | 412.5736 | 0.37 | 9931510 |
|  | 413.5366 | -1.06 | 51671 |
|  | 413.5366 | -1.06 | 4375468 |
|  | 414.5184 | 0.3 | 39186 |
|  | 414.5214 | -0.73 | 14022484 |
|  | 415.4631 | -0.45 | 57347 |
|  | 415.5243 | 0.78 | 59823 |

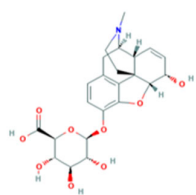
| | | | |
|---|----------|-------|----------|
|  | 416.3881 | 0.88 | 10201984 |
|  | 416.5222 | -0.74 | 51263 |
|  | 418.4456 | 0.08 | 4497 |
|  | 420.5253 | -0.7 | 54385 |
|  | 421.4518 | -0.42 | 60700 |
|  | 423.5289 | -0.01 | 13497176 |
|  | 425.9139 | -0.85 | 3151 |

| | | | |
|---|----------|-------|----------|
|  | 426.4893 | -0.67 | 115237 |
|  | 426.4893 | -0.67 | 475100 |
|  | 426.5572 | -0.62 | 444031 |
|  | 429.5762 | -0.42 | 19696654 |
|  | 429.5788 | 1.26 | 22620066 |
|  | 432.383 | 0.548 | 5316673 |
|  | 433.5144 | 0.59 | 65998 |

| | | | |
|---|----------|-------|----------|
|  | 434.5119 | 0.09 | 6603915 |
|  | 437.5209 | 1.51 | 3372 |
|  | 437.5778 | 0.74 | 10388384 |
|  | 437.5989 | 0.48 | 44592215 |
|  | 440.5814 | -0.64 | 104972 |
|  | 441.5496 | -0.8 | 44416780 |
|  | 444.5226 | -0.89 | 9846311 |

| | | | |
|---|----------|-------|----------|
|  | 446.9046 | -0.5 | 123631 |
|  | 448.5818 | -1.3 | 14022522 |
|  | 449.3903 | 0.15 | 441667 |
|  | 452.9801 | -0.82 | 64761 |
|  | 453.5828 | -0.59 | 70691333 |
|  | 454.4444 | -1.51 | 4112 |
|  | 454.5706 | -0.2 | 11775399 |

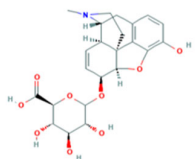
| | | | |
|---|----------|-------|----------|
|  | 454.6082 | -0.64 | 2520 |
|  | 454.654 | 0.48 | 6426143 |
|  | 456.5269 | 0.3 | 9916104 |
|  | 456.5616 | -1.52 | 5625 |
|  | 457.4822 | -0.52 | 54675783 |
|  | 458.5771 | 1.1 | 2247 |
|  | 459.5563 | -1.3 | 446156 |



461.4676

-2.15

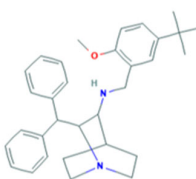
5484731



461.4676

-2.09

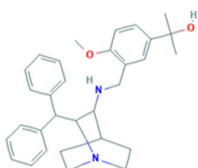
9847115



468.6808

0.46

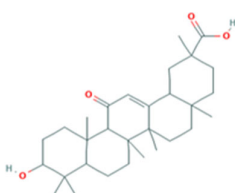
17905241



470.6534

-0.89

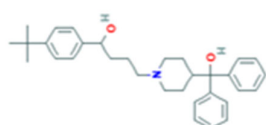
6426129



470.691

-1.4

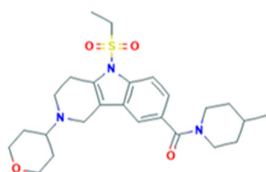
3230



471.6814

0.64

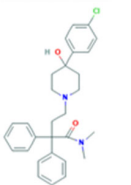
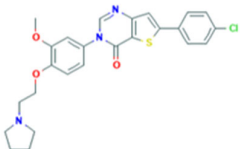
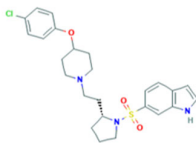
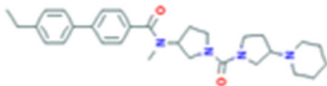
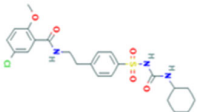
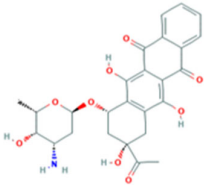
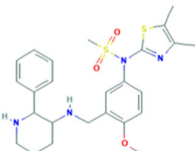
5405

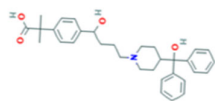


473.6292

-1.15

24894028

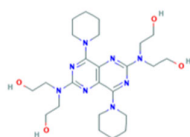
| | | | |
|---|----------|-------|----------|
|  | 477.0419 | 0.77 | 3955 |
|  | 481.9929 | 0.78 | 9826520 |
|  | 488.0403 | -0.04 | 10028436 |
|  | 488.6716 | 0.81 | 73226213 |
|  | 494.0013 | -0.9 | 3488 |
|  | 497.5006 | 0 | 42890 |
|  | 500.6728 | -0.37 | 19696689 |



501.6644

-0.98

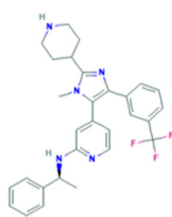
3348



504.6312

0

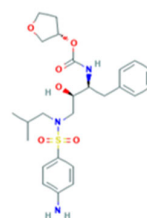
3108



505.5835

0.01

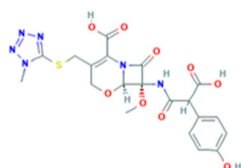
9806182



505.628

-0.56

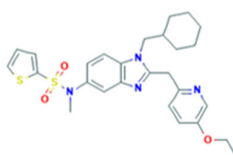
65016



520.4728

-2.52

47499



524.6948

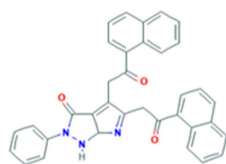
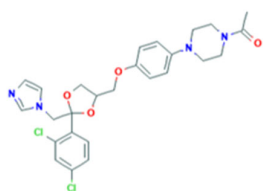
-1.15

57390958

531.4316

-0.63

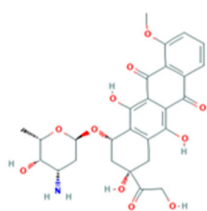
3823



535.6008

0.02

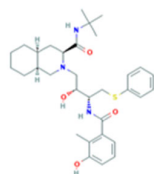
343473



543.5262

-0.83

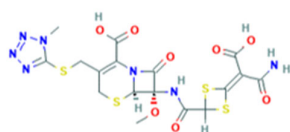
31703



567.7852

-0.93

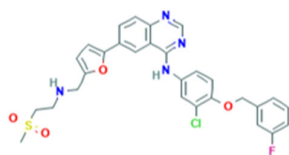
64143



575.6034

-1.89

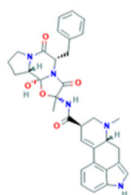
53025



581.0568

-0.03

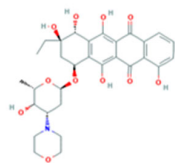
208908



581.67

-1.1

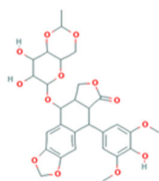
8223



585.6066

0.56

6917994

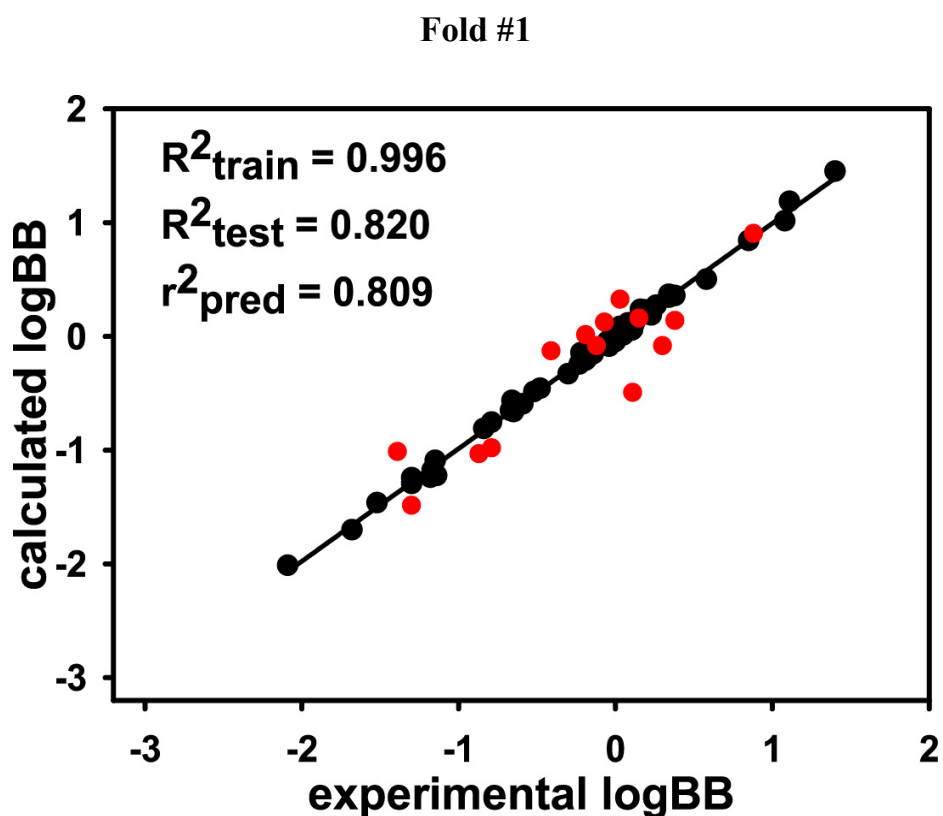


588.564

-2

3310

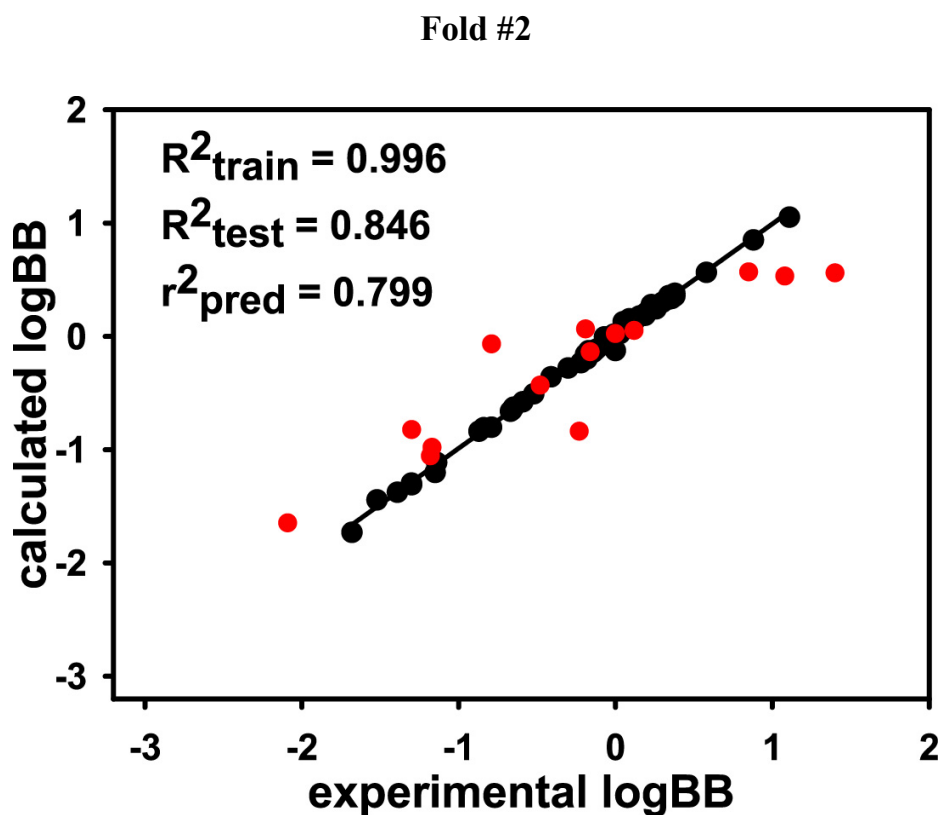
Figure S1. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 1 molecules in the training (black) and the test set (red).



Compounds in the training set: 444, 1207, 2022, 2083, 2119, 2164, 2284, 2554, 2578, 2803, 3241, 3394, 3672, 3676, 4058, 4064, 4421, 4737, 4763, 4828, 4914, 5064, 5155, 5193, 5838, 5842, 6009, 6468, 6473, 8942, 18047, 24066, 25255, 31423, 33039, 56051, 65860, 66994, 72138, 90274, 94957, 156391, 451819, 1497794, 3034183, 3763607, 6604200, 10060538, 10377120, 10444765, 11777724, 12889418, 13071367, 14022509, 21675832, 23274095, 118753220.

Compounds in the test set: 1486, 2473, 3608, 4158, 4909, 5206, 6623, 50599, 77870, 3000715, 9837317, 12032949, 14840722, 44214615.

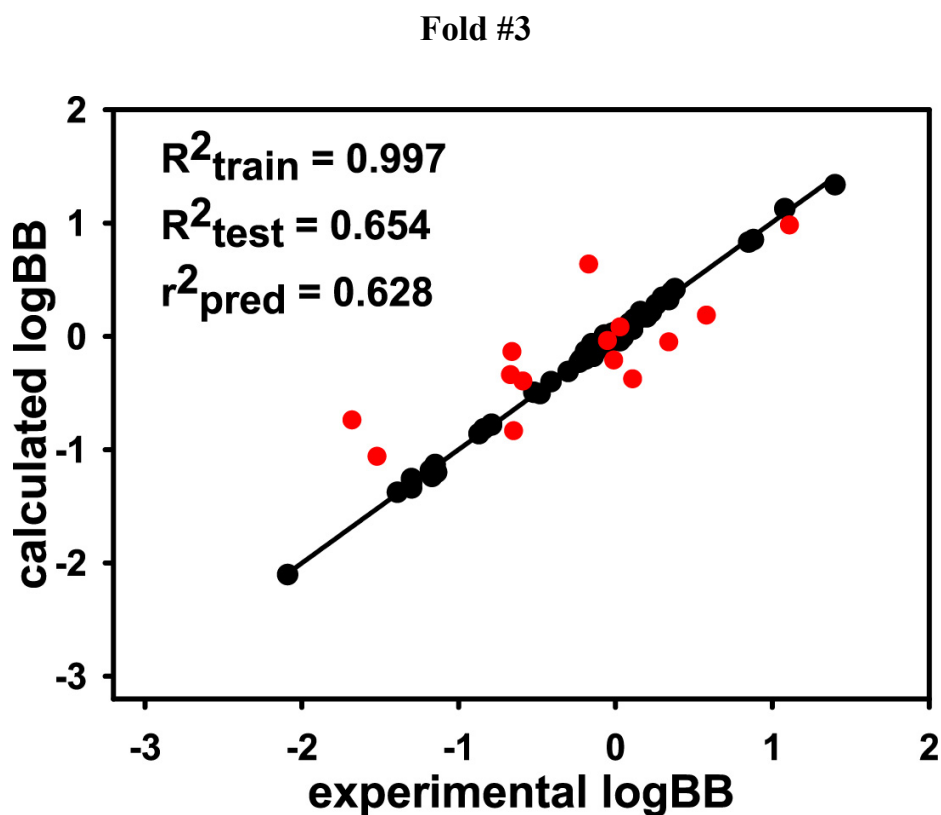
Figure S2. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 1 molecules in the training (black) and the test set (red).



Compounds in the training set: 1207, 1486, 2022, 2083, 2164, 2284, 2473, 2554, 2578, 2803, 3394, 3608, 3672, 3676, 4064, 4158, 4421, 4737, 4828, 4909, 4914, 5064, 5193, 5206, 5838, 5842, 6468, 6473, 6623, 8942, 18047, 25255, 31423, 33039, 50599, 56051, 66994, 72138, 77870, 90274, 94957, 156391, 1497794, 3000715, 3034183, 3763607, 9837317, 10060538, 10377120, 10444765, 11777724, 12032949, 13071367, 14022509, 14840722, 23274095.

Compounds in the test set: 444, 2119, 3241, 4058, 4763, 5155, 6009, 24066, 65860, 451819, 6604200, 12889418, 21675832, 118753220.

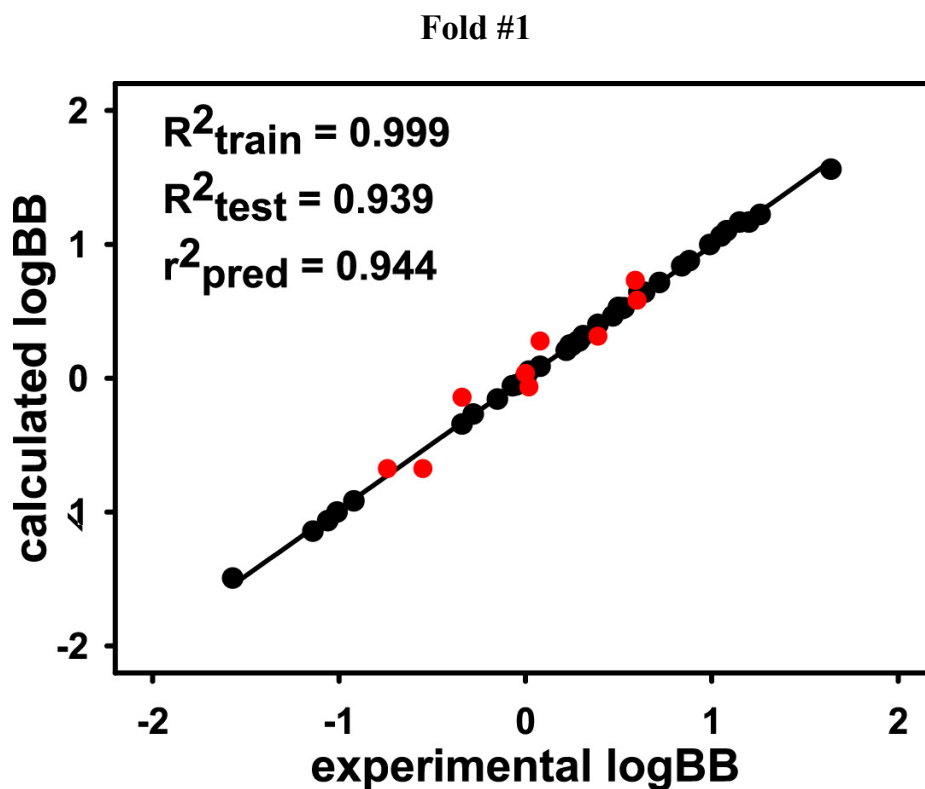
Figure S3. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 1 molecules in the training (black) and the test set (red).



Compounds in the training set: 444, 1486, 2022, 2083, 2119, 2164, 2473, 2554, 2578, 2803, 3241, 3608, 3672, 3676, 4058, 4064, 4158, 4737, 4763, 4828, 4909, 4914, 5155, 5193, 5206, 5838, 5842, 6009, 6473, 6623, 8942, 24066, 25255, 31423, 50599, 56051, 65860, 66994, 77870, 90274, 156391, 451819, 1497794, 3000715, 3763607, 6604200, 9837317, 10060538, 10444765, 11777724, 12032949, 12889418, 14022509, 14840722, 21675832, 44214615, 118753220.

Compounds in the test set: 1207, 2284, 3394, 4421, 5064, 6468, 18047, 33039, 72138, 94957, 3034183, 10377120, 13071367, 23274095.

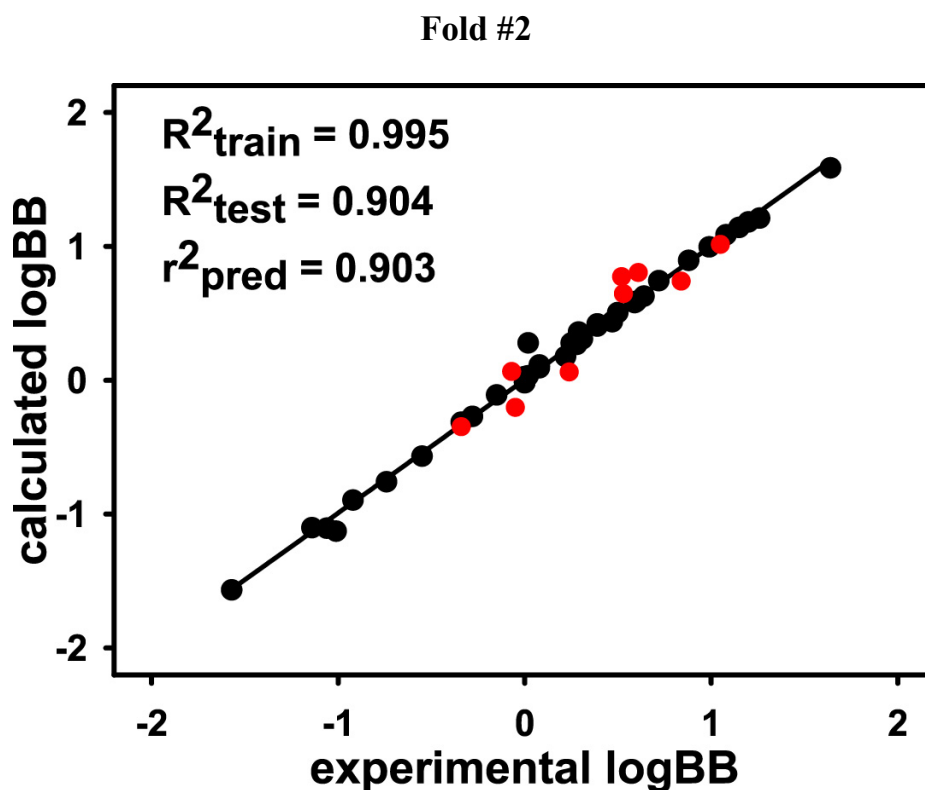
Figure S4. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 2 molecules in the training (black) and the test set (red).



Compounds in the training set: 1775, 2249, 2756, 2995, 2997, 3100, 3162, 3878, 3918, 4171, 4184, 4205, 4463, 4946, 5092, 5095, 5253, 5505, 6086, 9034, 33741, 37614, 43473, 77991, 159642, 3034012, 5281708, 5359272, 6916184, 9796408, 10470115, 13755681, 14022511, 14577084, 14590445, 15524033, 19427054, 44383796, 70517986.

Compounds in the test set: 2555, 4631, 5726, 5983, 28315, 443371, 9861160, 44568616, 135458393.

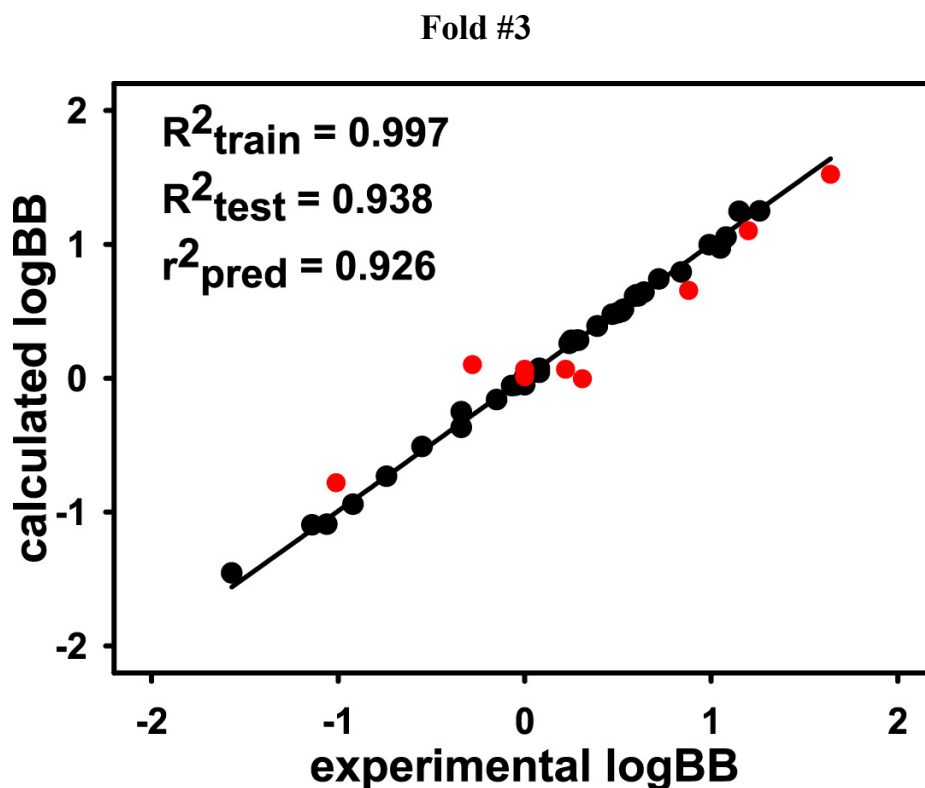
Figure S5. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 2 molecules in the training (black) and the test set (red).



Compounds in the training set: 2249, 2555, 2756, 2995, 3100, 3162, 3878, 3918, 4171, 4184, 4463, 4631, 5095, 5253, 5505, 5726, 5983, 6086, 28315, 33741, 37614, 43473, 77991, 443371, 3034012, 5281708, 5359272, 6916184, 9796408, 9861160, 10470115, 14022511, 14577084, 14590445, 15524033, 19427054, 44383796, 44568616, 135458393.

Compounds in the test set: 1775, 2997, 4205, 4946, 5092, 9034, 159642, 13755681, 70517986.

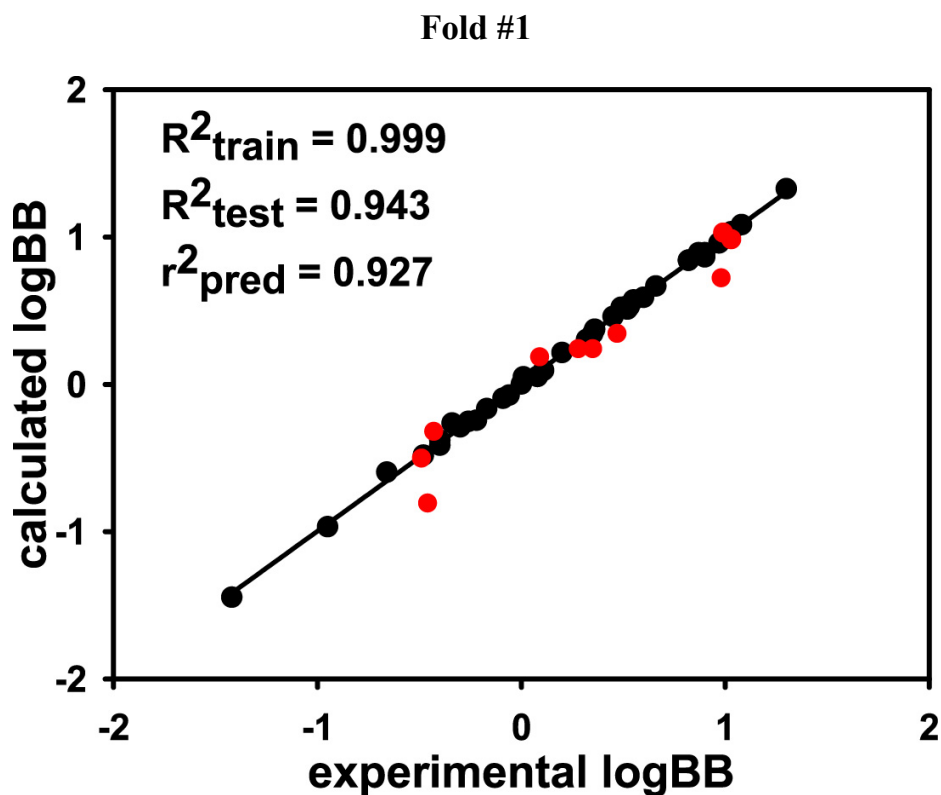
Figure S6. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 2 molecules in the training (black) and the test set (red).



Compounds in the training set: 1775, 2249, 2555, 2756, 2995, 2997, 3100, 3162, 3878, 3918, 4171, 4184, 4205, 4463, 4631, 4946, 5092, 5095, 5726, 5983, 9034, 28315, 33741, 37614, 43473, 159642, 443371, 3034012, 5281708, 9861160, 10470115, 13755681, 14022511, 14577084, 14590445, 44383796, 44568616, 70517986, 135458393.

Compounds in the test set: 5253, 5505, 6086, 77991, 5359272, 6916184, 9796408, 15524033, 19427054.

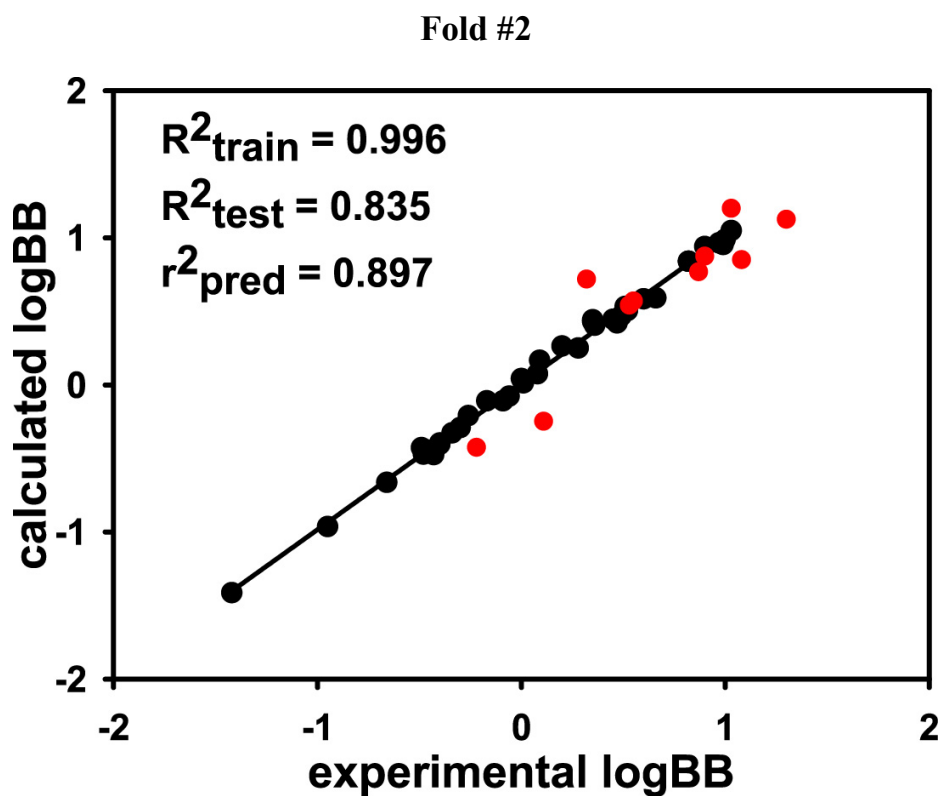
Figure S7. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 3 molecules in the training (black) and the test set (red).



Compounds in the training set: 2160, 2583, 2789, 3158, 3308, 4011, 4168, 4616, 4736, 4911, 4926, 4992, 5358, 5402, 6013, 9651, 67101, 68778, 74981, 121249, 166560, 174174, 197322, 441300, 547559, 3035905, 5284371, 5284543, 5284604, 5288826, 9817839, 9839073, 9860946, 9903970, 10265481, 14022481, 18435769, 22154175, 29939457, 44568615.

Compounds in the test set: 3016, 3696, 4595, 5538, 5584, 89657, 133741, 163091, 346516, 9971484.

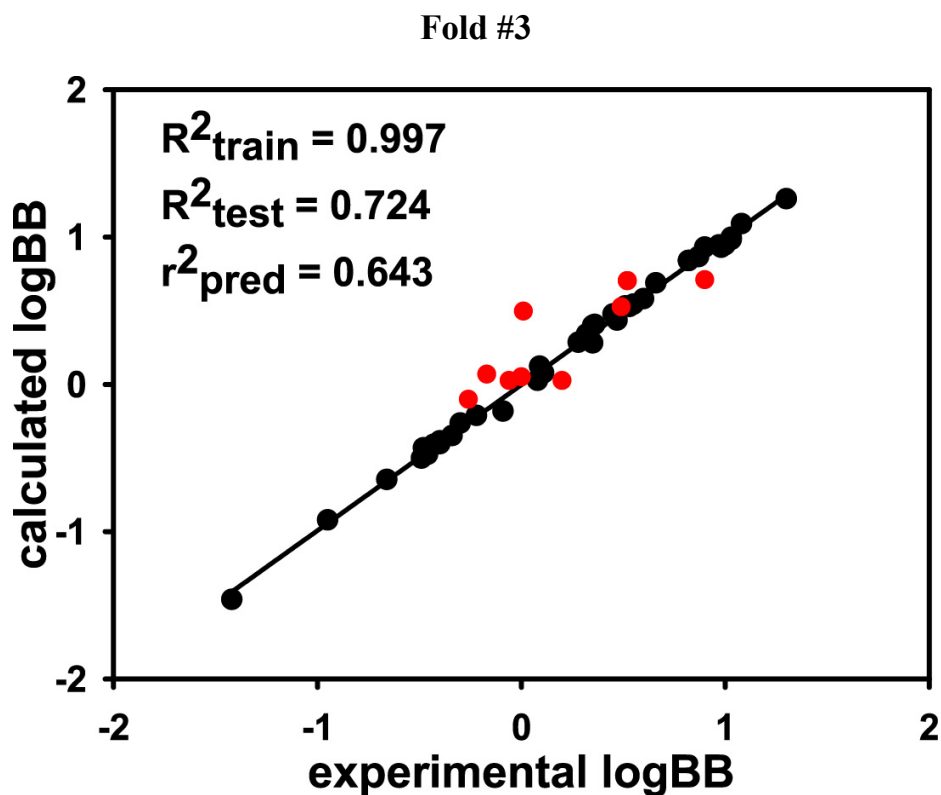
Figure S8. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 3 molecules in the training (black) and the test set (red).



Compounds in the training set: 2583, 2789, 3016, 3158, 3308, 3696, 4168, 4595, 4616, 4736, 4911, 4992, 5358, 5402, 5538, 5584, 6013, 67101, 68778, 74981, 89657, 133741, 163091, 166560, 174174, 197322, 346516, 547559, 3035905, 5284371, 5284604, 5288826, 9839073, 9860946, 9971484, 10265481, 14022481, 22154175, 29939457, 44568615.

Compounds in the test set: 2160, 4011, 4926, 9651, 121249, 441300, 5284543, 9817839, 9903970, 18435769.

Figure S9. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 3 molecules in the training (black) and the test set (red).

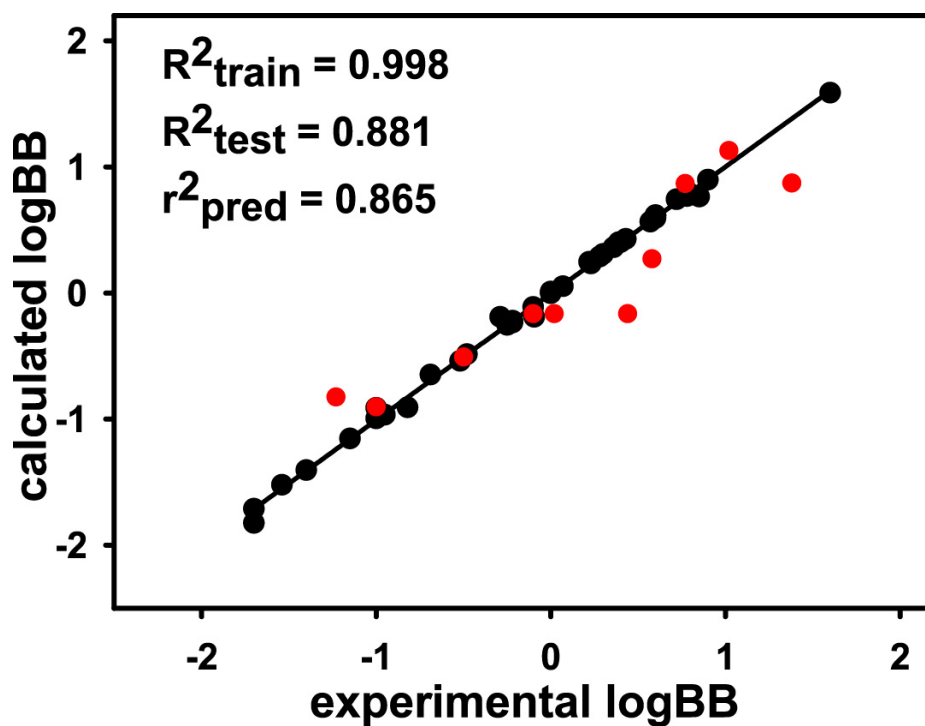


Compounds in the training set: 2160, 2789, 3016, 3158, 3308, 3696, 4011, 4595, 4616, 4736, 4911, 4926, 5358, 5402, 5538, 5584, 9651, 67101, 68778, 74981, 89657, 121249, 133741, 163091, 166560, 197322, 346516, 441300, 547559, 5284371, 5284543, 5284604, 9817839, 9839073, 9860946, 9903970, 9971484, 14022481, 18435769, 29939457.

Compounds in the test set: 2583, 4168, 4992, 6013, 174174, 3035905, 5288826, 10265481, 22154175, 44568615.

Figure S10. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 4 molecules in the training (black) and the test set (red).

Fold #1

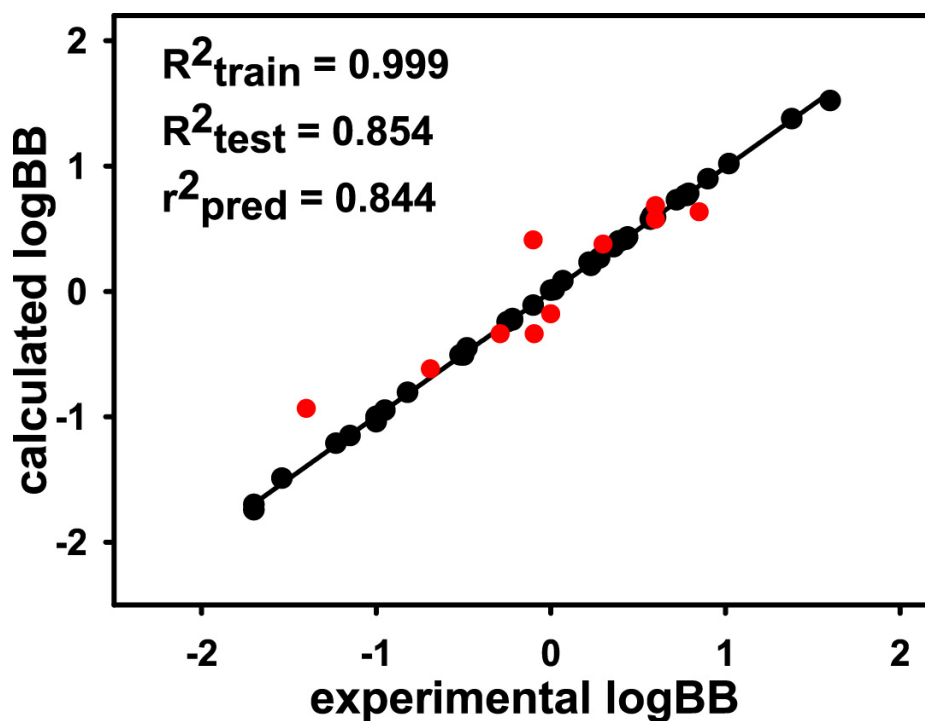


Compounds in the training set: 1223, 2170, 2369, 2381, 2708, 3365, 3373, 3380, 3386, 3510, 4095, 4539, 4781, 5090, 5184, 5732, 16078, 33014, 39147, 47811, 50287, 60652, 60949, 68617, 127382, 216236, 444008, 446220, 3000237, 5280343, 5284603, 5324346, 10063598, 11652375, 14022519, 25144104, 46888857, 54678486, 57395287, 135398745.

Compounds in the test set: 2118, 2726, 3958, 5994, 62875, 460612, 10358392, 15186924, 54429646, 57402315.

Figure S11. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 4 molecules in the training (black) and the test set (red).

Fold #2

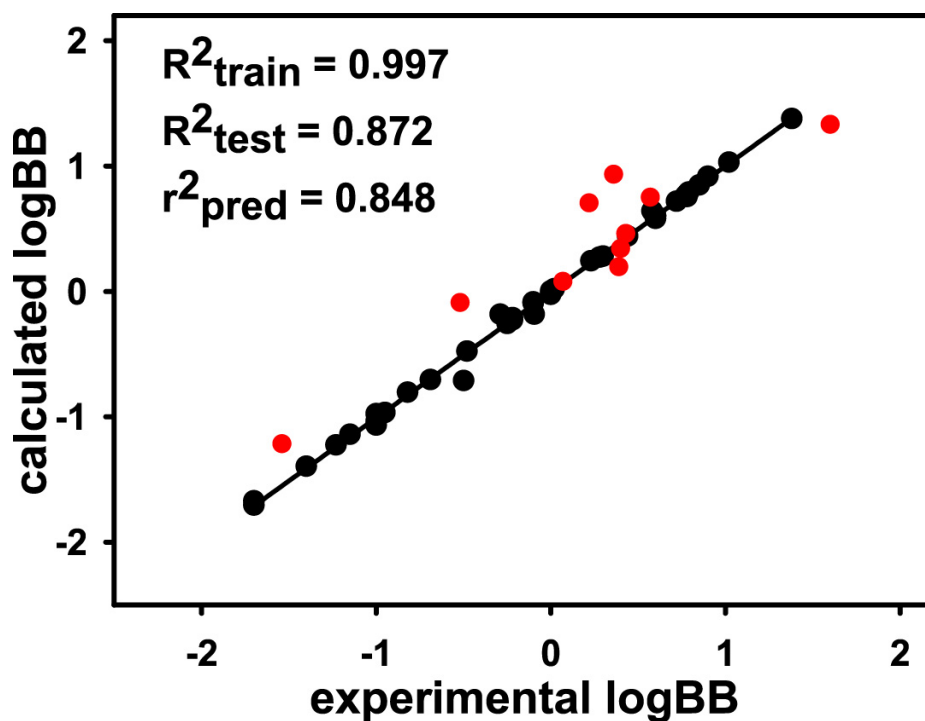


Compounds in the training set: 2170, 2369, 2708, 3365, 3380, 3386, 4095, 4539, 4781, 5184, 5732, 33014, 39147, 50287, 60652, 68617, 127382, 216236, 444008, 3000237, 5280343, 5284603, 5324346, 10063598, 14022519, 25144104, 46888857, 54678486, 57395287, 135398745, 2118, 2726, 3958, 5994, 62875, 460612, 10358392, 15186924, 54429646, 57402315.

Compounds in the test set: 1223, 2381, 3373, 3510, 5090, 16078, 47811, 60949, 446220, 11652375.

Figure S12. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 4 molecules in the training (black) and the test set (red).

Fold #3

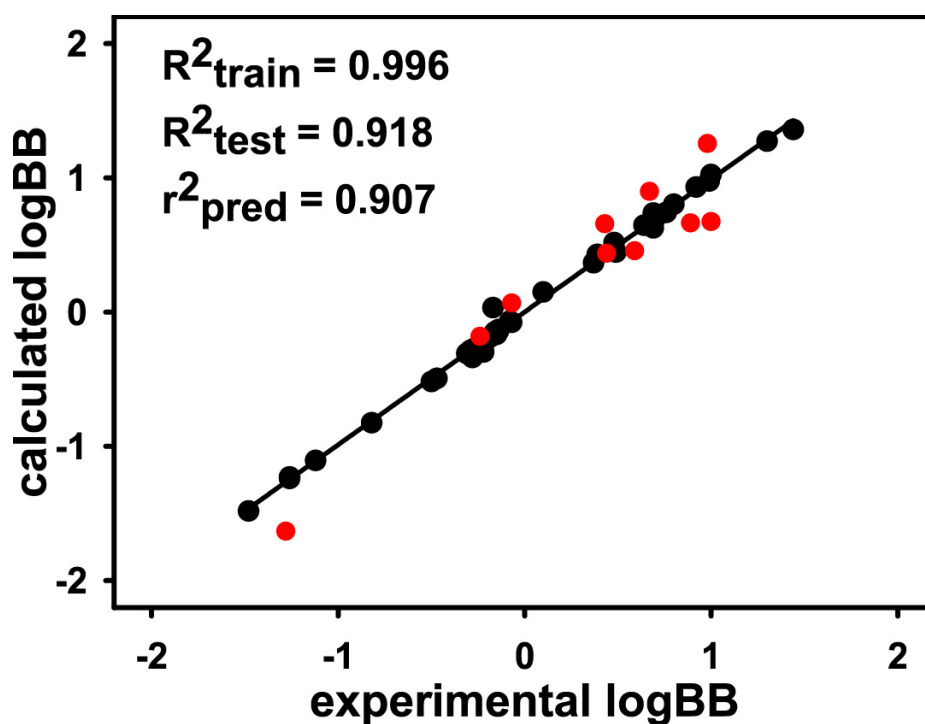


Compounds in the training set: 1223, 2118, 2170, 2381, 2708, 2726, 3365, 3373, 3386, 3510, 3958, 4095, 4539, 5090, 5184, 5732, 5994, 16078, 39147, 47811, 50287, 60652, 60949, 62875, 127382, 216236, 446220, 460612, 3000237, 5280343, 5324346, 10063598, 10358392, 11652375, 15186924, 25144104, 54429646, 54678486, 57402315, 135398745.

Compounds in the test set: 2369, 3380, 4781, 33014, 68617, 444008, 5284603, 14022519, 46888857, 57395287.

Figure S13. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 5 molecules in the training (black) and the test set (red).

Fold #1

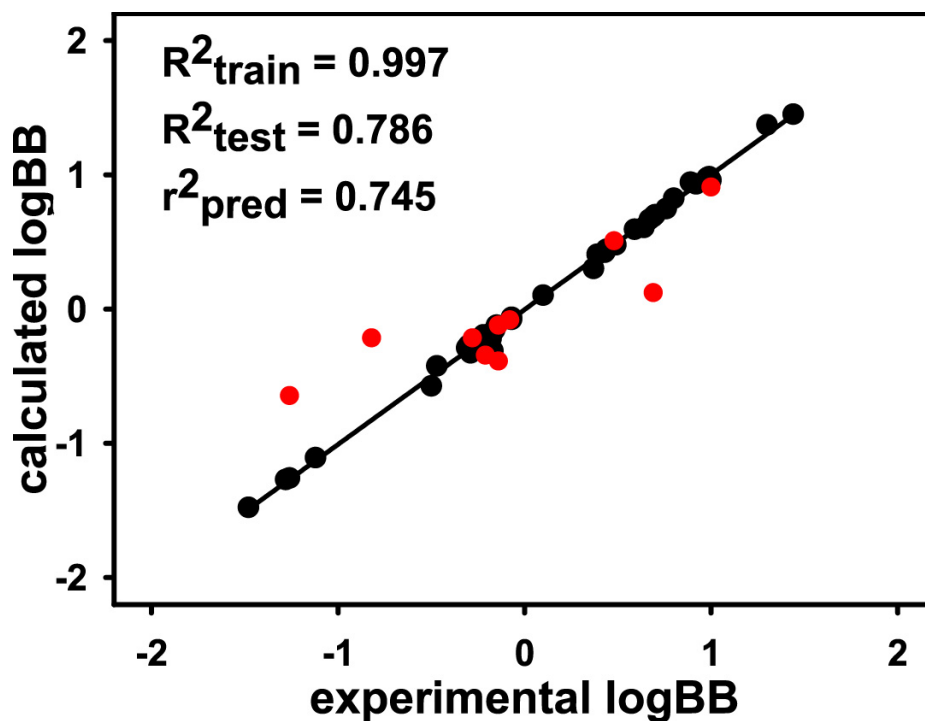


Compounds in the training set: 1345, 1978, 2771, 3715, 3964, 4192, 4594, 5009, 5568, 5755, 5953, 24360, 51081, 107917, 114376, 124449, 126761, 129710, 182017, 192706, 256277, 969488, 6426759, 9902443, 10019237, 10088796, 10245719, 10404144, 10937291, 11110698, 11530404, 13646638, 14022486, 14022491, 15186911, 22620080, 44213642, 46842852, 53394319, 135398737.

Compounds in the test set: 3345, 5556, 83909, 162244, 5284627, 10498206, 11559235, 14022497, 44433393, 57397056.

Figure S14. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 5 molecules in the training (black) and the test set (red).

Fold #2

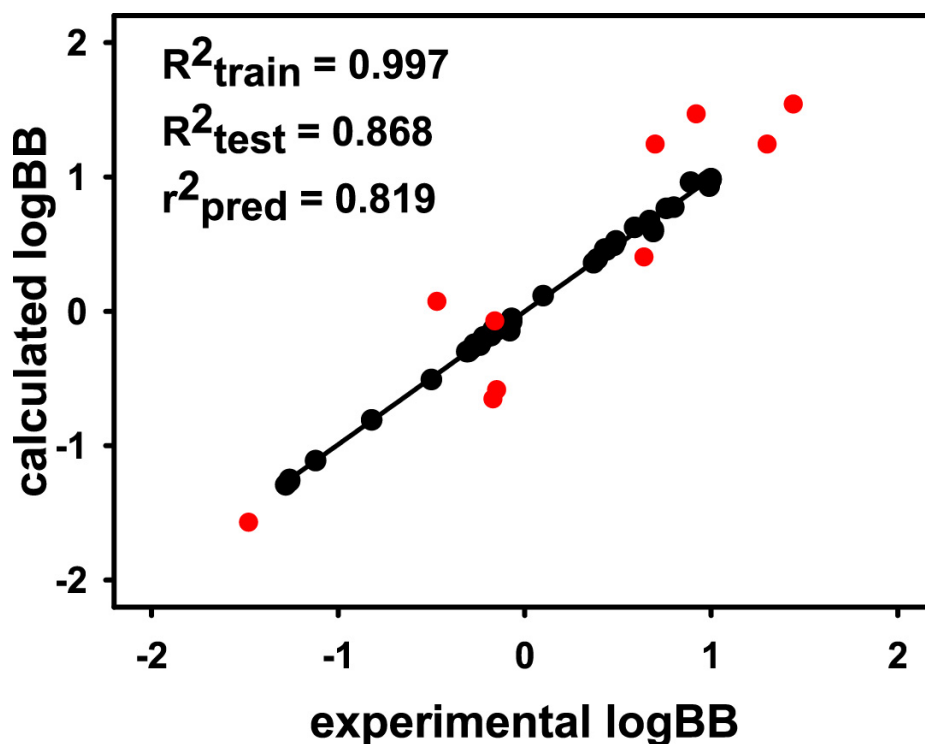


Compounds in the training set: 1978, 2771, 3345, 3964, 4192, 5009, 5556, 5568, 5755, 24360, 51081, 83909, 114376, 124449, 129710, 162244, 182017, 256277, 969488, 5284627, 9902443, 10019237, 10088796, 10404144, 10498206, 10937291, 11110698, 11530404, 11559235, 13646638, 14022491, 14022497, 15186911, 22620080, 44213642, 44433393, 46842852, 53394319, 57397056, 135398737.

Compounds in the test set: 1345, 3715, 4594, 5953, 107917, 126761, 192706, 6426759, 10245719, 14022486.

Figure S15. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 5 molecules in the training (black) and the test set (red).

Fold #3

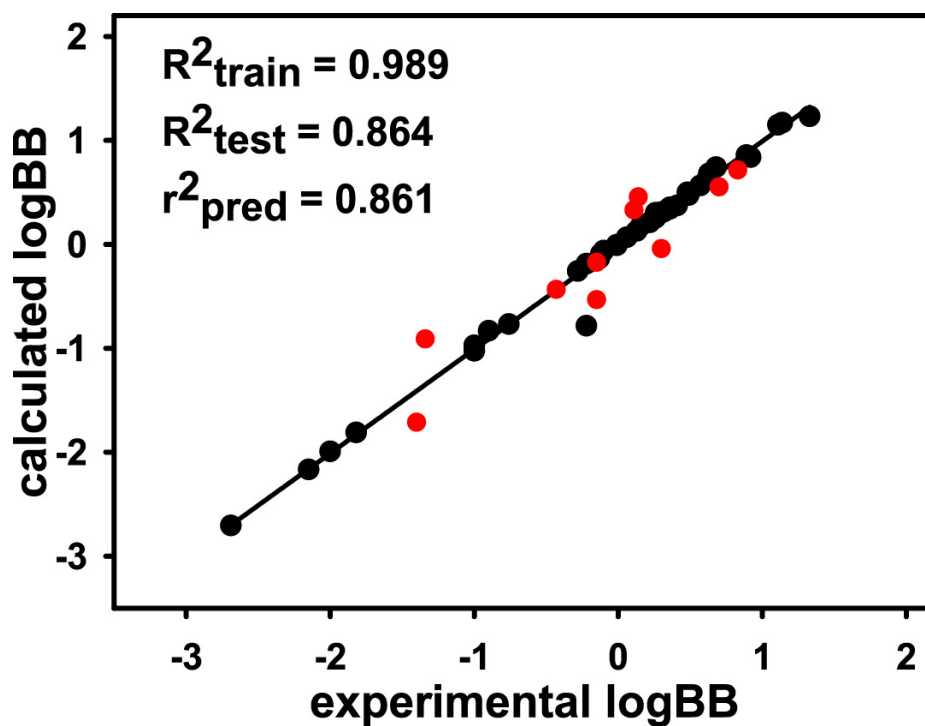


Compounds in the training set: 1345, 2771, 3345, 3715, 3964, 4192, 4594, 5009, 5556, 5755, 5953, 24360, 83909, 107917, 114376, 124449, 126761, 129710, 162244, 192706, 256277, 969488, 5284627, 6426759, 10019237, 10088796, 10245719, 10498206, 10937291, 11110698, 11559235, 13646638, 14022486, 14022491, 14022497, 22620080, 44213642, 44433393, 53394319, 57397056.

Compounds in the test set: 1978, 5568, 51081, 182017, 9902443, 10404144, 11530404, 15186911, 46842852, 135398737.

Figure S16. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 6 molecules in the training (black) and the test set (red).

Fold #1

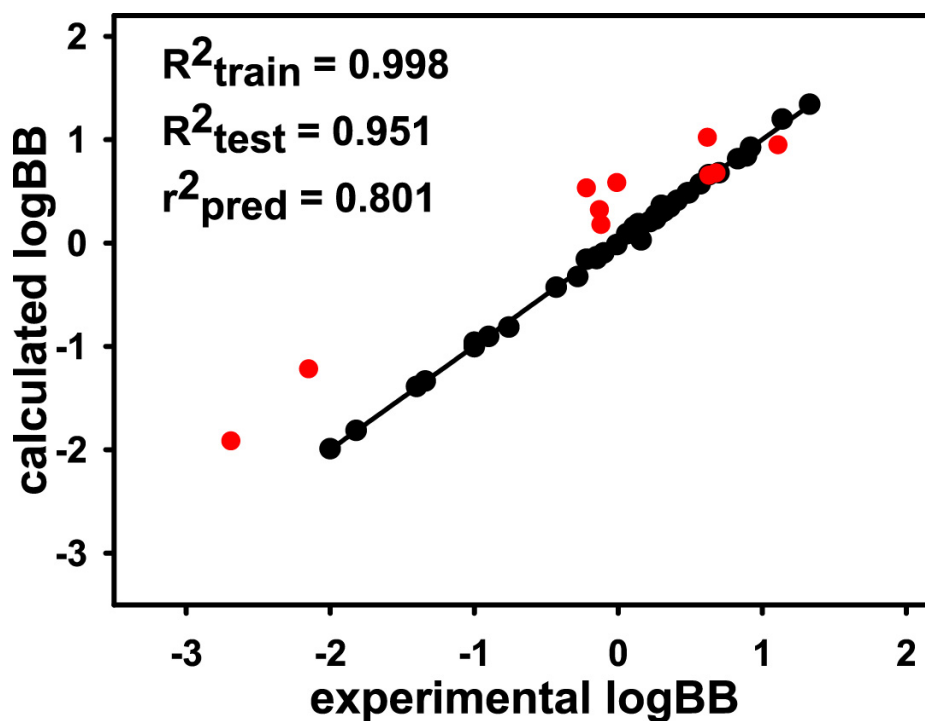


Compounds in the training set: 2477, 2678, 3152, 3559, 3658, 4046, 4078, 4893, 5265, 5339, 5452, 5533, 5754, 60464, 72108, 149096, 198752, 204104, 2733526, 3025986, 3052762, 5362391, 6604009, 9821217, 9821511, 9864647, 9907401, 9907628, 9907851, 10091748, 11003252, 11502034, 11531010, 11545677, 14022483, 14022499, 22620050, 22620062, 22620085, 45272895.

Compounds in the test set: 3357, 5002, 5743, 91769, 3946663, 9864646, 10384745, 11653882, 19696721, 22620075.

Figure S17. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 6 molecules in the training (black) and the test set (red).

Fold #2

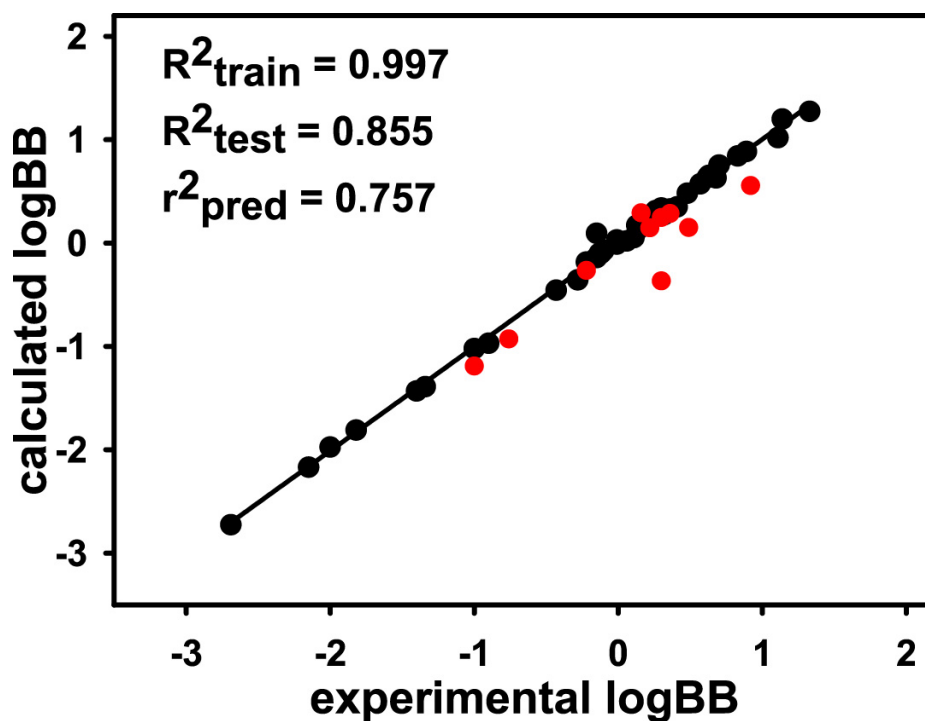


Compounds in the training set: 2477, 3152, 3357, 3559, 3658, 4078, 4893, 5002, 5265, 5452, 5533, 5743, 60464, 72108, 91769, 149096, 198752, 2733526, 3025986, 3052762, 3946663, 5362391, 6604009, 9821511, 9864646, 9864647, 9907401, 9907851, 10091748, 10384745, 11003252, 11531010, 11545677, 11653882, 14022499, 19696721, 22620050, 22620062, 22620075, 45272895.

Compounds in the test set: 2678, 4046, 5339, 5754, 204104, 9821217, 9907628, 11502034, 14022483, 22620085.

Figure S18. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 6 molecules in the training (black) and the test set (red).

Fold #3

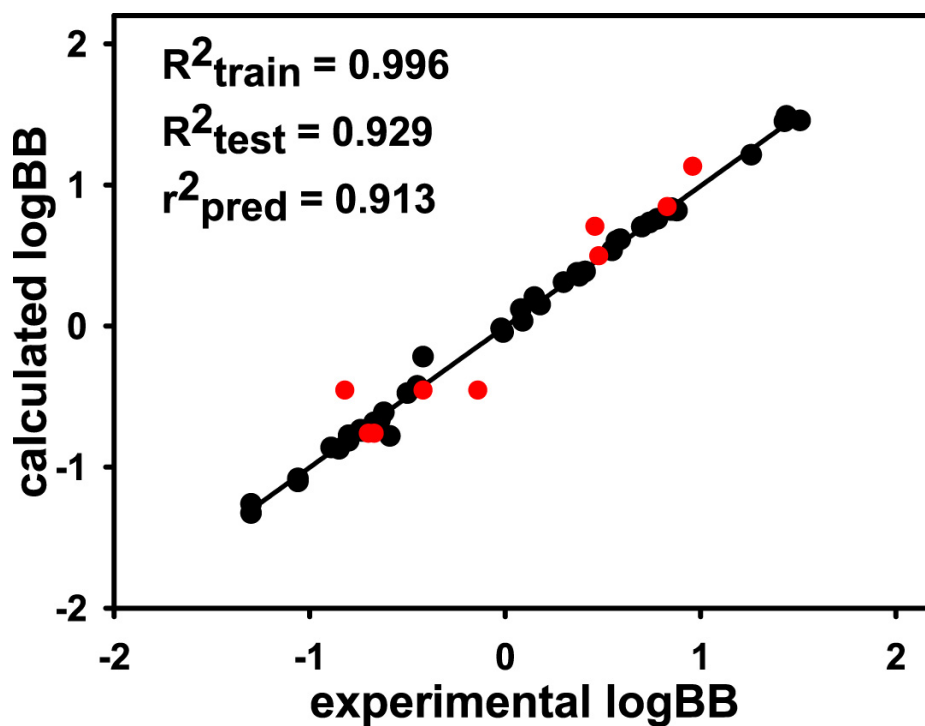


Compounds in the training set: 2678, 3152, 3357, 3559, 4046, 4078, 4893, 5002, 5265, 5339, 5452, 5743, 5754, 60464, 72108, 91769, 198752, 204104, 3025986, 3052762, 3946663, 5362391, 9821217, 9821511, 9864646, 9864647, 9907628, 9907851, 10091748, 10384745, 11502034, 11531010, 11545677, 11653882, 14022483, 19696721, 22620050, 22620075, 22620085, 45272895.

Compounds in the test set: 2477, 3658, 5533, 149096, 2733526, 6604009, 9907401, 11003252, 14022499, 22620062.

Figure S19. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 7 molecules in the training (black) and the test set (red).

Fold #1

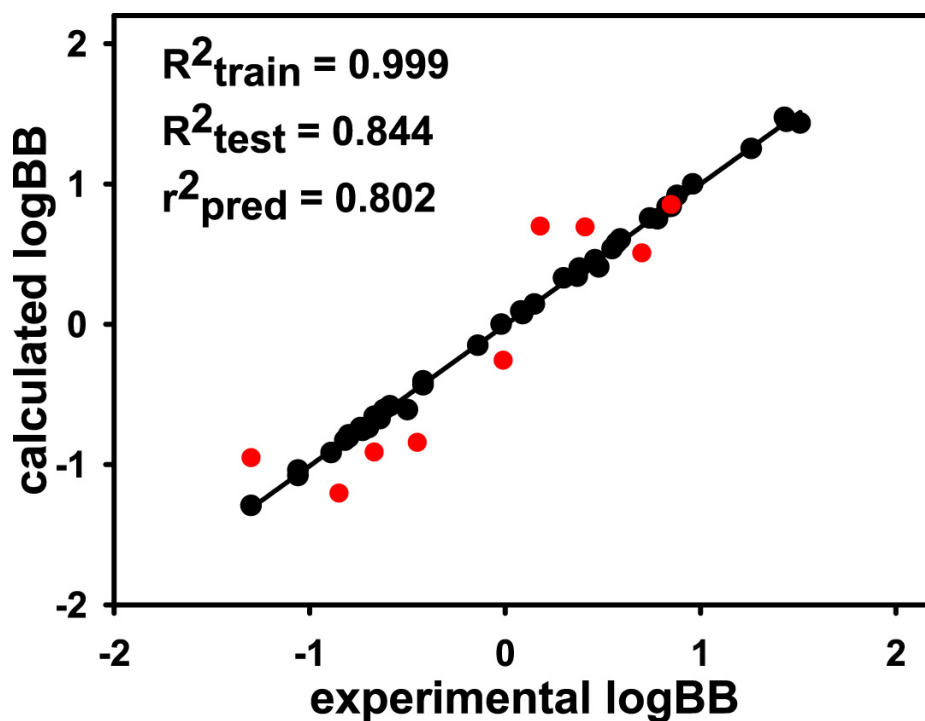


Compounds in the training set: 3151, 3372, 4497, 4748, 5073, 5566, 6167, 31765, 39186, 51263, 51671, 53232, 57347, 59823, 60700, 65998, 71301, 104972, 115237, 123631, 441667, 444031, 456389, 4375468, 5316673, 6603915, 9846311, 9866153, 9931510, 10201984, 10388384, 10884606, 13497176, 14022484, 14022522, 21440942, 22620066, 22620091, 44416780, 70691333.

Compounds in the test set: 12598, 54385, 64761, 119146, 475100, 9909299, 11531660, 19696654, 44592215.

Figure S20. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 7 molecules in the training (black) and the test set (red).

Fold #2

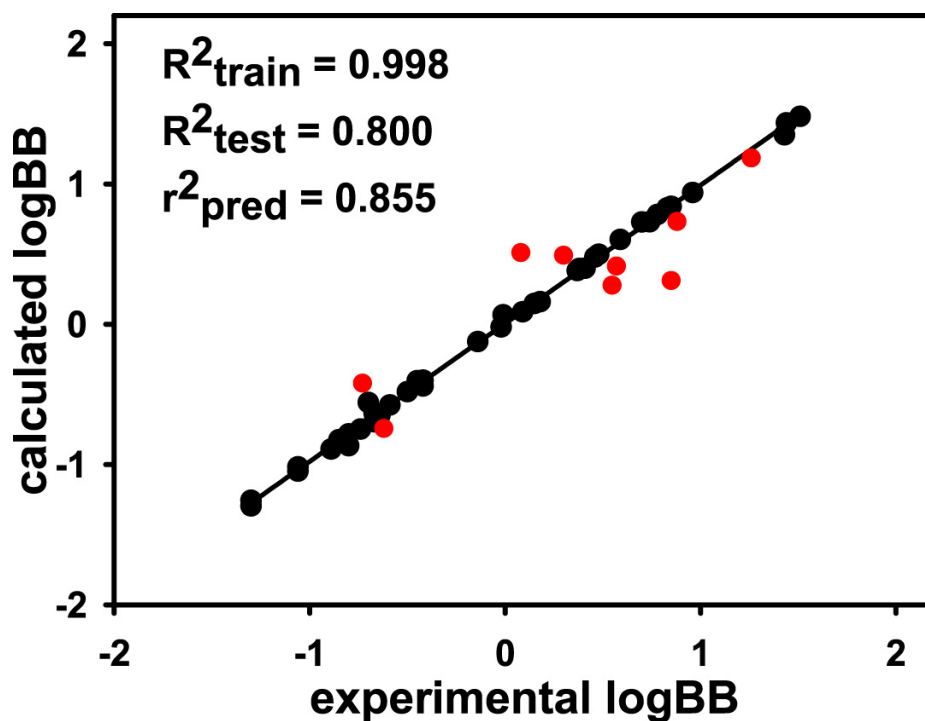


Compounds in the training set: 3372, 4497, 5073, 5566, 6167, 12598, 39186, 51263, 51671, 53232, 54385, 59823, 60700, 64761, 65998, 71301, 104972, 119146, 123631, 441667, 444031, 475100, 4375468, 5316673, 6603915, 9846311, 9909299, 9931510, 10201984, 10388384, 10884606, 11531660, 14022484, 14022522, 19696654, 21440942, 22620066, 44416780, 44592215, 70691333.

Compounds in the test set: 3151, 4748, 31765, 57347, 115237, 456389, 9866153, 13497176, 22620091.

Figure S21. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 7 molecules in the training (black) and the test set (red).

Fold #3

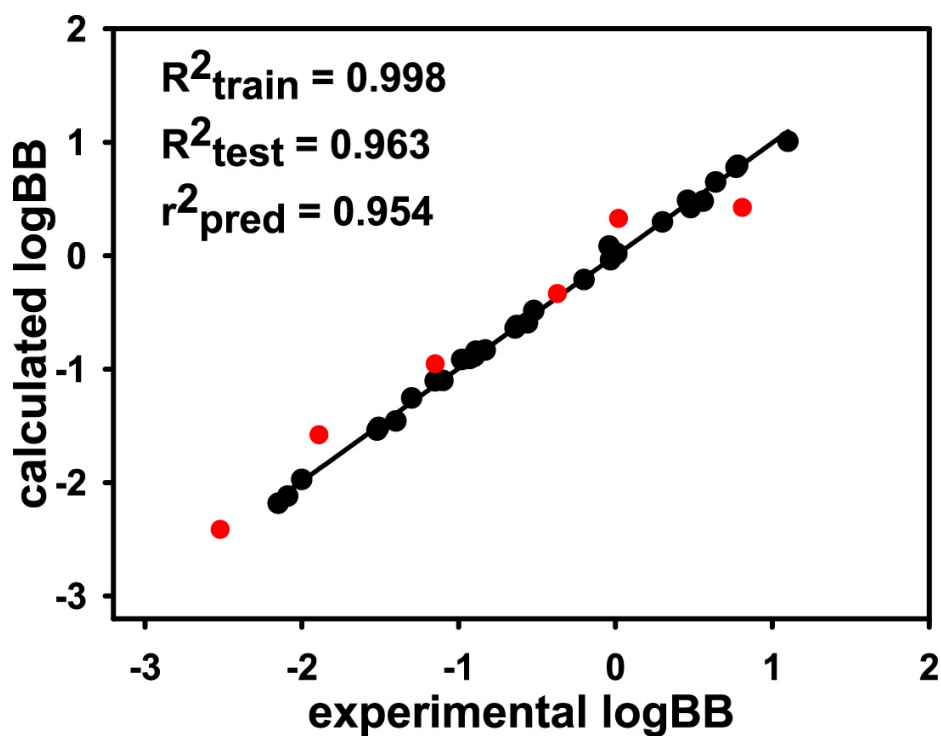


Compounds in the training set: 3151, 3372, 4748, 5073, 5566, 6167, 12598, 31765, 51263, 51671, 54385, 57347, 59823, 60700, 64761, 65998, 104972, 115237, 119146, 123631, 441667, 456389, 475100, 4375468, 6603915, 9846311, 9866153, 9909299, 9931510, 10388384, 10884606, 11531660, 13497176, 14022522, 19696654, 21440942, 22620091, 44416780, 44592215, 70691333.

Compounds in the test set: 4497, 39186, 53232, 71301, 444031, 5316673, 10201984, 14022484, 22620066.

Figure S22. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 8 molecules in the training (black) and the test set (red).

Fold #1

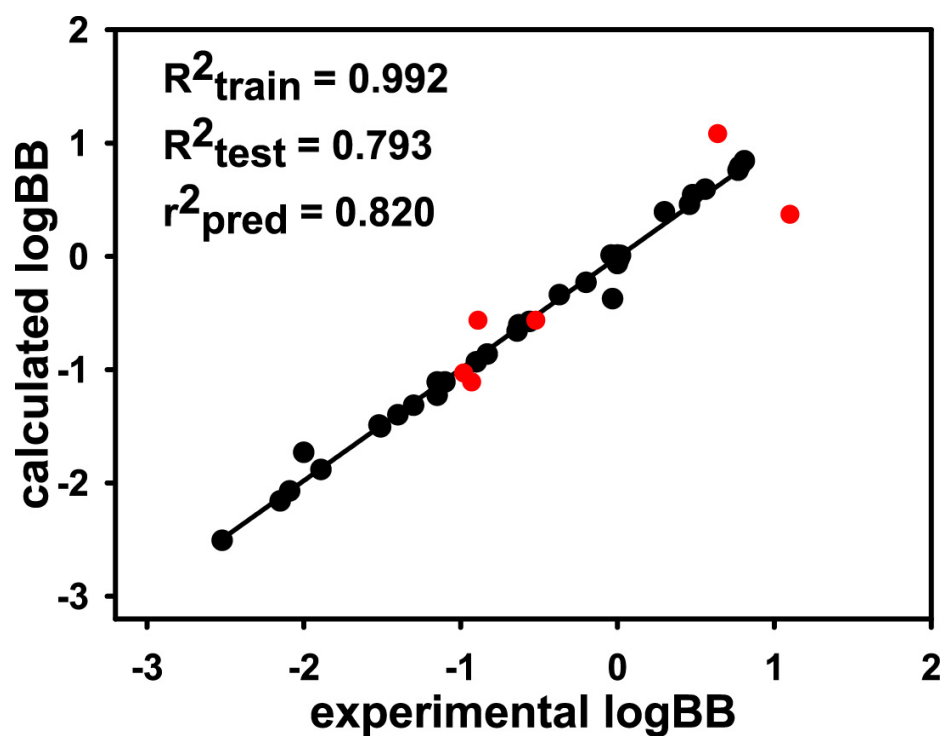


Compounds in the training set: 2247, 2520, 3108, 3230, 3310, 3348, 3488, 3823, 3955, 4112, 5405, 5625, 8223, 31703, 42890, 64143, 65016, 208908, 446156, 5484731, 6426129, 6426143, 6917994, 9806182, 9826520, 9847115, 9916104, 10028436, 11775399, 17905241, 54675783, 57390958.

Compounds in the test set: 47499, 53025, 343473, 19696689, 24894028, 73226213.

Figure S23. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 8 molecules in the training (black) and the test set (red).

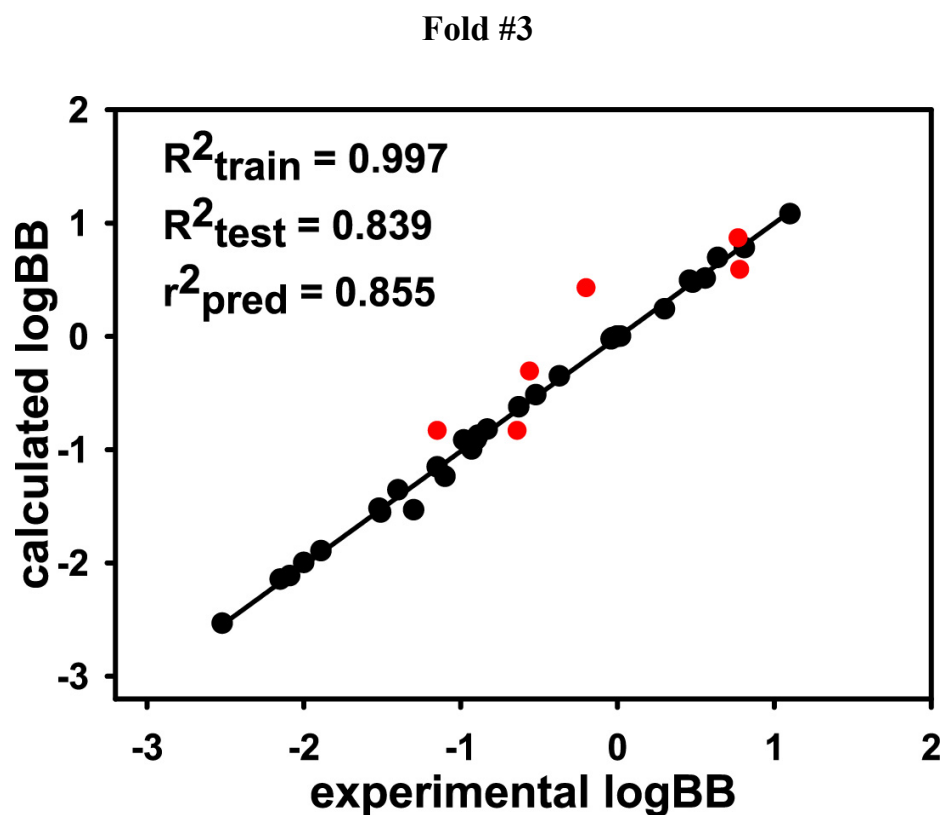
Fold #2



Compounds in the training set: 2520, 3108, 3230, 3310, 3488, 3823, 3955, 4112, 5625, 8223, 31703, 42890, 47499, 53025, 65016, 208908, 343473, 446156, 5484731, 6426143, 6917994, 9806182, 9826520, 9847115, 9916104, 10028436, 11775399, 17905241, 19696689, 24894028, 57390958, 73226213.

Compounds in the test set: 2247, 3348, 5405, 64143, 6426129, 54675783.

Figure S24. Linear diagram showing correlation between the experimental and calculated LogBB values of the Subset 8 molecules in the training (black) and the test set (red).



Compounds in the training set: 2247, 3108, 3230, 3310, 3348, 3488, 3823, 4112, 5405, 5625, 8223, 31703, 42890, 47499, 53025, 64143, 208908, 343473, 446156, 5484731, 6426129, 6426143, 6917994, 9806182, 9847115, 9916104, 10028436, 17905241, 19696689, 24894028, 54675783, 73226213.

Compounds in the test set: 2520, 3955, 65016, 9826520, 11775399, 57390958.