

## Supplementary material

Development of QSAR model based on Monte Carlo optimization for predicting GABA<sub>A</sub> receptor binding of newly emerging benzodiazepines

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Table S1. The SMILES notation of the studied molecules, calculated values for the DCW, experimental data (Ac) – Expr, the values of Ac calculated with the application of CORAL software – Calc, the difference between Expr and Calc – Diff for the built QSPR model.

| SMILES notation |                                                                   | Expr | Split 1  |        |         |     | Split 2  |        |         |     | Split 3  |        |         |     |
|-----------------|-------------------------------------------------------------------|------|----------|--------|---------|-----|----------|--------|---------|-----|----------|--------|---------|-----|
|                 |                                                                   |      | DCW      | Calc   | Diff    | Set | DCW      | Calc   | Diff    | Set | DCW      | Calc   | Diff    | Set |
| 1               | <chem>O=C1CN=C(c2c(N1)ccc(c2)F)c1ccccc1</chem>                    | 7.4  | 101.1253 | 7.186  | 0.214   | Ts  | 100.6693 | 7.2401 | 0.1599  | Tr  | 116.3149 | 6.9378 | 0.4622  | Ts  |
| 2               | <chem>Fc1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1</chem>                   | 7.77 | 106.7292 | 7.457  | 0.313   | Tr  | 117.8567 | 8.1067 | -0.3367 | Tr  | 128.8443 | 7.8145 | -0.0445 | Tr  |
| 3               | <chem>O=C1CN=C(c2c(N1)ccc(c2)F)c1ccccc1F</chem>                   | 8.13 | 119.3758 | 8.0687 | 0.0613  | Ts  | 115.9169 | 8.0088 | 0.1212  | Tr  | 131.1118 | 7.9732 | 0.1568  | Ts  |
| 4               | <chem>Fc1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1F</chem>                  | 8.29 | 117.3058 | 7.9685 | 0.3215  | Tr  | 127.5444 | 8.5951 | -0.3051 | Tr  | 133.4748 | 8.1386 | 0.1514  | Tr  |
| 6               | <chem>Clc1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1</chem>                  | 8.09 | 105.4703 | 7.3961 | 0.6939  | Tr  | 103.239  | 7.3696 | 0.7204  | Tr  | 125.6977 | 7.5944 | 0.4956  | Tr  |
| 7               | <chem>O=C1CN=C(c2c(N1)ccc(c2)Cl)c1ccccc1F</chem>                  | 8.7  | 124.9688 | 8.3392 | 0.3608  | Ts  | 125.0547 | 8.4696 | 0.2304  | Ts  | 140.5174 | 8.6313 | 0.0687  | Ts  |
| 8               | <chem>O=C1CN=C(c2c(N1)ccc(c2)Cl)c1ccccc1Cl</chem>                 | 8.74 | 127.5987 | 8.4664 | 0.2736  | Tr  | 120.4986 | 8.2399 | 0.5001  | Tr  | 139.0339 | 8.5275 | 0.2125  | Tr  |
| 9               | <chem>Ic1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1F</chem>                  | 8.54 | 129.6591 | 8.566  | -0.026  | Tr  | 131.2378 | 8.7813 | -0.2413 | Tr  | 137.2344 | 8.4016 | 0.1384  | Ts  |
| 10              | <chem>O=C1CN=C(c2c(N1)ccc(c2)C(F)(F)F)c1ccccc1</chem>             | 7.89 | 108.7634 | 7.5554 | 0.3346  | Tr  | 111.6874 | 7.7956 | 0.0944  | Tr  | 132.6692 | 8.0822 | -0.1922 | Tr  |
| 11              | <chem>[N-]=[N+]=Nc1ccc2c(c1)C(=NCC(=O)N2)c1ccccc1F</chem>         | 8.28 | 119.4535 | 8.0724 | 0.2076  | Ts  | 125.6113 | 8.4976 | -0.2176 | Tr  | 135.0366 | 8.2478 | 0.0322  | Tr  |
| 12              | <chem>O=C1CN=C(c2c(N1)ccc(c2)[N+](=O)[O-])c1ccccc1</chem>         | 8    | 116.3432 | 7.922  | 0.078   | Tr  | 109.5585 | 7.6883 | 0.3117  | Tr  | 124.8828 | 7.5373 | 0.4627  | Ts  |
| 13              | <chem>O=C1CN=C(c2c(N1)ccc(c2)[N+](=O)[O-])c1ccccc1F</chem>        | 8.82 | 134.1369 | 8.7826 | 0.0374  | Tr  | 126.2376 | 8.5292 | 0.2908  | Ts  | 142.0448 | 8.7382 | 0.0818  | Tr  |
| 14              | <chem>CN1C(=O)CN=C(c2c1ccc(c2)[N+](=O)[O-])c1ccccc1F</chem>       | 8.42 | 124.0742 | 8.2959 | 0.1241  | Tr  | 123.7266 | 8.4026 | 0.0174  | Tr  | 139.27   | 8.5441 | -0.1241 | Tr  |
| 15              | <chem>O=C1CN=C(c2c(N1)ccc(c2)[N+](=O)[O-])c1ccccc1Cl</chem>       | 8.74 | 136.1017 | 8.8776 | -0.1376 | Tr  | 127.6169 | 8.5988 | 0.1412  | Tr  | 140.1404 | 8.605  | 0.135   | Tr  |
| 16              | <chem>CN1C(=O)CN=C(c2c1ccc(c2)[N+](=O)[O-])c1ccccc1Cl</chem>      | 8.66 | 126.039  | 8.3909 | 0.2691  | Tr  | 125.106  | 8.4722 | 0.1878  | Ts  | 137.3656 | 8.4108 | 0.2492  | Tr  |
| 17              | <chem>O=C1CN=C(c2c(N1)ccc(c2)[N+](=O)[O-])c1ccccc1C(F)(F)F</chem> | 8.46 | 120.3649 | 8.1165 | 0.3435  | Ts  | 123.1451 | 8.3733 | 0.0867  | Tr  | 147.4209 | 9.1144 | -0.6544 | Ts  |
| 18              | <chem>ONc1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1F</chem>                 | 7.02 | 101.5265 | 7.2054 | -0.1854 | Tr  | 101.5447 | 7.2842 | -0.2642 | Tr  | 119.3312 | 7.1489 | -0.1289 | Ts  |
| 19              | <chem>O=C1CN=C(c2c(N1)ccc(c2)N)c1ccccc1</chem>                    | 6.41 | 86.9203  | 6.4989 | -0.0889 | Tr  | 85.52164 | 6.4763 | -0.0663 | Tr  | 104.9922 | 6.1455 | 0.2645  | Tr  |
| 20              | <chem>Nc1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1</chem>                   | 6.34 | 89.06178 | 6.6025 | -0.2625 | Ts  | 85.36918 | 6.4686 | -0.1286 | Tr  | 113.5069 | 6.7413 | -0.4013 | Tr  |
| 21              | <chem>Nc1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1F</chem>                  | 7.19 | 101.628  | 7.2103 | -0.0203 | Tr  | 98.75224 | 7.1434 | 0.0466  | Tr  | 123.8373 | 7.4642 | -0.2742 | Tr  |
| 22              | <chem>O=C1CN=C(c2c(N1)ccc(c2)N)c1ccccc1Cl</chem>                  | 7.12 | 109.1252 | 7.5729 | -0.4529 | Ts  | 105.844  | 7.501  | -0.381  | Ts  | 123.5845 | 7.4465 | -0.3265 | Tr  |
| 23              | <chem>CNC(=O)Nc1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1F</chem>           | 6.34 | 84.87083 | 6.3998 | -0.0598 | Tr  | 82.5501  | 6.3265 | 0.0135  | Tr  | 106.6328 | 6.2603 | 0.0797  | Tr  |
| 24              | <chem>N#Cc1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1</chem>                 | 6.42 | 87.83343 | 6.5431 | -0.1231 | Tr  | 87.74372 | 6.5883 | -0.1683 | Tr  | 110.8522 | 6.5556 | -0.1356 | Tr  |
| 25              | <chem>N#Cc1ccc2c(c1)C(=NCC(=O)N2C)c1ccccc1F</chem>                | 7.52 | 103.8997 | 7.3201 | 0.1999  | Tr  | 101.4748 | 7.2807 | 0.2393  | Ts  | 121.7892 | 7.3209 | 0.1991  | Tr  |
| 26              | <chem>CCc1ccc2c(c1)C(=NCC(=O)N2)c1ccccc1</chem>                   | 7.44 | 103.0088 | 7.2771 | 0.1629  | Tr  | 98.45323 | 7.1283 | 0.3117  | Tr  | 118.4718 | 7.0888 | 0.3512  | Ts  |
| 27              | <chem>C=Cc1ccc2c(c1)C(=NCC(=O)N2)c1ccccc1</chem>                  | 7.62 | 101.1965 | 7.1894 | 0.4306  | Tr  | 106.0138 | 7.5095 | 0.1105  | Tr  | 121.5353 | 7.3031 | 0.3169  | Tr  |
| 28              | <chem>O=Cc1ccc2c(c1)C(=NCC(=O)N2)c1ccccc1</chem>                  | 7.37 | 104.4454 | 7.3465 | 0.0235  | Tr  | 103.106  | 7.3629 | 0.0071  | Ts  | 121.7371 | 7.3172 | 0.0528  | Tr  |
| 29              | <chem>O=C1CN=C(c2c(N1)ccc(c2)C(=O)C)c1ccccc1F</chem>              | 7.74 | 112.5801 | 7.74   | 0       | Ts  | 109.2882 | 7.6746 | 0.0654  | Tr  | 128.2297 | 7.7715 | -0.0315 | Tr  |
| 30              | <chem>NCCc1ccc2c(c1)C(=NCC(=O)N2)c1ccccc1</chem>                  | 6.59 | 101.2863 | 7.1937 | -0.6037 | Ts  | 98.36473 | 7.1239 | -0.5339 | Ts  | 115.967  | 6.9135 | -0.3235 | Tr  |

|    |                                                        |      |          |        |         |    |          |        |         |    |          |        |         |    |
|----|--------------------------------------------------------|------|----------|--------|---------|----|----------|--------|---------|----|----------|--------|---------|----|
| 31 | NCCOCc1ccc2c(c1)C(=NCC(=O)N2Cl)c1ccccc1                | 7.2  | 98.60179 | 7.0639 | 0.1361  | Tr | 99.30224 | 7.1711 | 0.0289  | Ts | 115.659  | 6.8919 | 0.3081  | Tr |
| 32 | Clc1ccc2c(c1)C(=NCC(=O)N2CC(F)(F)F)c1ccccc1            | 7.04 | 105.6961 | 7.407  | -0.367  | Ts | 100.9574 | 7.2546 | -0.2146 | Tr | 119.2892 | 7.1459 | -0.1059 | Tr |
| 33 | C#CCN1C(=O)CN=C(c2c1ccc(c2)Cl)c1ccccc1                 | 7.03 | 101.635  | 7.2106 | -0.1806 | Tr | 96.87775 | 7.0489 | -0.0189 | Tr | 115.5979 | 6.8877 | 0.1423  | Ts |
| 34 | Clc1ccc2c(c1)C(=NCC(=O)N2CC1CC1)c1ccccc1               | 6.96 | 104.9538 | 7.3711 | -0.4111 | Tr | 98.27384 | 7.1193 | -0.1593 | Ts | 115.7426 | 6.8978 | 0.0622  | Tr |
| 35 | COCc1ccc2c(c1)C(=NCC(=O)N2[N+](=O)[O-])c1ccccc1        | 6.37 | 88.77176 | 6.5885 | -0.2185 | Ts | 86.11369 | 6.5062 | -0.1362 | Tr | 107.956  | 6.3529 | 0.0171  | Tr |
| 36 | ClN1C(=O)CN=C(c2c1ccc(c2)C(C)(C)C)c1ccccc1             | 6.21 | 79.48409 | 6.1393 | 0.0707  | Tr | 84.88412 | 6.4442 | -0.2342 | Tr | 110.387  | 6.523  | -0.313  | Ts |
| 37 | NCCc1ccc2c(c1)C(=NCC(=O)N2Cl)c1ccccc1F                 | 8.08 | 110.393  | 7.6342 | 0.4458  | Tr | 106.9536 | 7.5569 | 0.5231  | Tr | 127.1724 | 7.6976 | 0.3824  | Ts |
| 38 | CCN(CCN1C(=O)CN=C(c2c1ccc(c2)Cl)c1ccccc1F)CC           | 7.83 | 117.8589 | 7.9953 | -0.1653 | Ts | 111.165  | 7.7693 | 0.0607  | Tr | 129.8279 | 7.8834 | -0.0534 | Tr |
| 39 | OCCc1ccc2c(c1)C(=NCC(=O)N2Cl)c1ccccc1F                 | 7.61 | 111.2895 | 7.6776 | -0.0676 | Tr | 102.1798 | 7.3162 | 0.2938  | Tr | 124.4458 | 7.5068 | 0.1032  | Tr |
| 40 | NC(=O)OCCc1ccc2c(c1)C(=NCC(=O)N2Cl)c1ccccc1F           | 7.37 | 103.0204 | 7.2776 | 0.0924  | Tr | 107.656  | 7.5923 | -0.2223 | Tr | 122.5124 | 7.3715 | -0.0015 | Tr |
| 41 | OCC(Cc1ccc2c(c1)C(=NCC(=O)N2Cl)c1ccccc1F)O             | 6.85 | 101.7846 | 7.2178 | -0.3678 | Tr | 94.50891 | 6.9294 | -0.0794 | Tr | 118.165  | 7.0673 | -0.2173 | Tr |
| 42 | Clc1ccccc1C1=NCC(=O)N(c2c1cc(cc2)C(C)(C)C)[N+](=O)[O-] | 6.52 | 89.37593 | 6.6177 | -0.0977 | Tr | 80.902   | 6.2434 | 0.2766  | Tr | 103.0317 | 6.0084 | 0.5116  | Ts |
| 43 | O=C1CN=C(c2c(N1)cccc2)c1ccccc1                         | 6.45 | 91.65655 | 6.728  | -0.278  | Ts | 78.4495  | 6.1197 | 0.3303  | Tr | 104.1813 | 6.0888 | 0.3612  | Tr |
| 44 | O=C1CN=C(c2c(N1)cccc2)c1ccccc1F                        | 6.51 | 101.2352 | 7.1913 | -0.6813 | Tr | 96.66492 | 7.0382 | -0.5282 | Tr | 120.649  | 7.2411 | -0.7311 | Tr |
| 45 | CN1C(=O)CN=C(c2c1cccc2)c1ccccc1F                       | 7.47 | 111.4916 | 7.6873 | -0.2173 | Tr | 103.7609 | 7.3959 | 0.0741  | Ts | 127.147  | 7.6958 | -0.2258 | Tr |
| 46 | CN1C(=O)CN=C(c2c1cccc2)c1ccccc1Cl                      | 7.47 | 113.4564 | 7.7824 | -0.3124 | Tr | 105.1403 | 7.4655 | 0.0045  | Tr | 125.2425 | 7.5625 | -0.0925 | Ts |
| 47 | Clc1ccc2c(c1)C(=NC(C(=O)N2)C)c1ccccc1F                 | 8.46 | 128.2194 | 8.4964 | -0.0364 | Tr | 126.1309 | 8.5238 | -0.0638 | Tr | 139.9689 | 8.593  | -0.133  | Tr |
| 48 | CC1N=C(c2c(NC1=O)ccc(c2)[N+](=O)[O-])c1ccccc1Cl        | 8.92 | 127.3835 | 8.456  | 0.464   | Ts | 128.8961 | 8.6633 | 0.2567  | Ts | 144.472  | 8.908  | 0.012   | Tr |
| 49 | CC1N=C(c2cccc2)c2c(N(C1=O)C)ccc(c2)[N+](=O)[O-]        | 8.15 | 125.2411 | 8.3523 | -0.2023 | Tr | 117.4019 | 8.0837 | 0.0663  | Tr | 133.5996 | 8.1473 | 0.0027  | Tr |
| 50 | Clc1ccc2c(c1)C(=NC(C(=O)N2)C)c1ccccc1                  | 7.31 | 111.9265 | 7.7084 | -0.3984 | Tr | 107.5642 | 7.5877 | -0.2777 | Tr | 125.1609 | 7.5568 | -0.2468 | Tr |
| 51 | O=C1Nc2ccc(cc2C(=NC1O)c1ccccc1)Cl                      | 7.74 | 114.203  | 7.8185 | -0.0785 | Tr | 114.5141 | 7.9381 | -0.1981 | Tr | 131.8923 | 8.0278 | -0.2878 | Ts |
| 52 | Clc1ccc2c(c1)C(=NC(C(=O)N2)O)c1ccccc1                  | 7.8  | 104.8369 | 7.3655 | 0.4345  | Tr | 109.8591 | 7.7034 | 0.0966  | Tr | 121.8595 | 7.3258 | 0.4742  | Ts |
| 53 | Clc1ccc2c(c1)C(=NC(C(=O)N2)O)c1ccccc1Cl                | 8.46 | 120.6802 | 8.1317 | 0.3283  | Ts | 118.9995 | 8.1643 | 0.2957  | Tr | 136.9945 | 8.3848 | 0.0752  | Tr |
| 54 | Clc1ccc2c(c1)C(=NC(C(=O)N2)OC(=O)N(C)C)c1ccccc1        | 6.05 | 78.77849 | 6.1051 | -0.0551 | Tr | 78.4015  | 6.1173 | -0.0673 | Tr | 103.2123 | 6.021  | 0.029   | Tr |
| 55 | Clc1ccc2c(c1)C(=NC(C(=O)N2)Cl)c1ccccc1                 | 8.28 | 122.596  | 8.2244 | 0.0556  | Tr | 117.4596 | 8.0866 | 0.1934  | Tr | 131.3666 | 7.991  | 0.289   | Ts |
| 56 | CN=C1CN(O)C(=c2c(=N1)ccc(c2)Cl)c1ccccc1                | 6.45 | 86.6492  | 6.4858 | -0.0358 | Ts | 84.29003 | 6.4142 | 0.0358  | Tr | 106.683  | 6.2639 | 0.1861  | Tr |
| 57 | Clc1ccc2=NC(=O)CN(C(=c2c1)c1ccccc1)O                   | 6.51 | 88.37786 | 6.5694 | -0.0594 | Tr | 85.1556  | 6.4578 | 0.0522  | Tr | 107.9526 | 6.3527 | 0.1573  | Tr |
| 58 | O=C1CN=C(c2c(N1)ccc(c2)Cl)C1=CCCCC1                    | 7.47 | 107.5074 | 7.4946 | -0.0246 | Tr | 105.4026 | 7.4787 | -0.0087 | Tr | 119.5776 | 7.1661 | 0.3039  | Tr |
| 59 | Clc1ccc2c(c1)C(=NCC(=O)N2)C1=CCCCC1                    | 7.47 | 107.258  | 7.4826 | -0.0126 | Tr | 104.2785 | 7.422  | 0.048   | Tr | 125.3409 | 7.5694 | -0.0994 | Tr |
| 60 | O=C1CN=C(c2c(N1)ccc(c2)Cl)c1ccccc1                     | 7.06 | 105.5992 | 7.4023 | -0.3423 | Tr | 104.5346 | 7.4349 | -0.3749 | Tr | 119.8093 | 7.1823 | -0.1223 | Tr |
| 61 | O=C1CN=C(c2c(N1)ccc(c2)Br)c1ccccc1                     | 7.74 | 113.8425 | 7.801  | -0.061  | Tr | 109.7621 | 7.6985 | 0.0415  | Tr | 128.0785 | 7.761  | -0.021  | Tr |
| 62 | Clc1ccccc1C1=NCc2n(c3c1cccc3)c(nn2)C                   | 8.37 | 122.8921 | 8.2387 | 0.1313  | Tr | 116.1411 | 8.0202 | 0.3498  | Tr | 131.323  | 7.988  | 0.382   | Ts |
| 63 | Clc1ccc2c(c1)C(=NCc1n2cnn1)c1ccccc1                    | 8.07 | 114.2231 | 7.8194 | 0.2506  | Ts | 114.8866 | 7.9569 | 0.1131  | Ts | 132.085  | 8.0413 | 0.0287  | Ts |
| 64 | Clc1ccc2c(c1)C(=NCc1n2c(C)nn1)c1ccccc1                 | 7.7  | 115.0443 | 7.8592 | -0.1592 | Tr | 111.2989 | 7.776  | -0.076  | Ts | 128.8562 | 7.8154 | -0.1154 | Tr |
| 65 | Clc1ccc2c(c1)C(=NCc1n2c(C)nn1)c1ccccc1Cl               | 8.4  | 126.1215 | 8.3949 | 0.0051  | Tr | 127.1135 | 8.5734 | -0.1734 | Tr | 138.9785 | 8.5237 | -0.1237 | Tr |

|    |                                                                       |      |          |        |         |    |          |        |         |    |          |        |         |    |
|----|-----------------------------------------------------------------------|------|----------|--------|---------|----|----------|--------|---------|----|----------|--------|---------|----|
| 66 | <chem>OCc1nnc2n1c1ccc(cc1C(=NC2)c1ccccc1Cl)Cl</chem>                  | 8.38 | 120.7965 | 8.1374 | 0.2426  | Tr | 122.0982 | 8.3205 | 0.0595  | Tr | 137.1678 | 8.397  | -0.017  | Tr |
| 68 | <chem>CN(Cc1nnc2n1c1ccc(cc1C(=NC2)c1ccccc1Cl)C</chem>                 | 7.94 | 111.5666 | 7.691  | 0.249   | Tr | 115.1032 | 7.9678 | -0.0278 | Ts | 134.0504 | 8.1788 | -0.2388 | Tr |
| 69 | <chem>Clc1ccc2c(c1)C(=NC(c1n2c(C)nn1)C)c1ccccc1F</chem>               | 8.48 | 127.4537 | 8.4593 | 0.0207  | Tr | 116.5818 | 8.0424 | 0.4376  | Ts | 135.0692 | 8.2501 | 0.2299  | Tr |
| 70 | <chem>Fc1ccccc1C1=NC(C)c2n(c3c1cc(cc3)[N+](=O)[O-])c(nn2)C</chem>     | 8.4  | 129.1348 | 8.5407 | -0.1407 | Tr | 109.6306 | 7.6919 | 0.7081  | Ts | 123.2466 | 7.4229 | 0.9771  | Tr |
| 73 | <chem>Clc1ccccc1C1=NCc2n(c3c1ccs3)c(nn2)C</chem>                      | 8.46 | 129.8522 | 8.5754 | -0.1154 | Tr | 122.9393 | 8.3629 | 0.0971  | Tr | 138.1504 | 8.4657 | -0.0057 | Tr |
| 74 | <chem>CCc1cc2c(s1)n1c(CN=C2c2ccccc2Cl)nnc1C</chem>                    | 8.51 | 126.3515 | 8.406  | 0.104   | Tr | 124.6172 | 8.4475 | 0.0625  | Tr | 139.465  | 8.5577 | -0.0477 | Tr |
| 75 | <chem>Clc1sc2c(c1)C(=NCc1n2c(C)nn1)c1ccccc1Cl</chem>                  | 8.85 | 137.2693 | 8.9341 | -0.0841 | Ts | 123.4417 | 8.3883 | 0.4617  | Ts | 142.1631 | 8.7465 | 0.1035  | Ts |
| 76 | <chem>Brc1cc2c(s1)n1c(CN=C2c2ccccc2Cl)nnc1C</chem>                    | 8.92 | 125.1083 | 8.3459 | 0.5741  | Ts | 131.9837 | 8.819  | 0.101   | Tr | 142.8283 | 8.793  | 0.127   | Ts |
| 77 | <chem>Ic1cc2c(s1)n1c(CN=C2c2ccccc2Cl)nnc1C</chem>                     | 8.82 | 128.7619 | 8.5226 | 0.2974  | Tr | 138.4802 | 9.1465 | -0.3265 | Tr | 143.0561 | 8.809  | 0.011   | Tr |
| 78 | <chem>NCc1nnc2n1c1sc(cc1C(=NC2)c1ccccc1Cl)Cl</chem>                   | 8.54 | 135.0493 | 8.8267 | -0.2867 | Tr | 129.5855 | 8.698  | -0.158  | Tr | 139.7722 | 8.5792 | -0.0392 | Tr |
| 79 | <chem>Clc1ccc2c(c1)C(=NCc1n2c(C)nc1)c1ccccc1F</chem>                  | 8.32 | 129.9942 | 8.5822 | -0.2622 | Ts | 118.8455 | 8.1565 | 0.1635  | Ts | 136.9768 | 8.3836 | -0.0636 | Tr |
| 80 | <chem>OCc1ncc2n1c1ccc(cc1C(=NC2)c1ccccc1F)Cl</chem>                   | 8.35 | 123.275  | 8.2572 | 0.0928  | Tr | 117.2999 | 8.0786 | 0.2714  | Ts | 133.8036 | 8.1616 | 0.1884  | Tr |
| 81 | <chem>CCOC(=O)c1ncn2c1CN=C(c1c2ccc(c1)Cl)c1ccccc1</chem>              | 7.82 | 112.8481 | 7.7529 | 0.0671  | Ts | 111.8575 | 7.8042 | 0.0158  | Tr | 131.194  | 7.979  | -0.159  | Tr |
| 82 | <chem>O=C(c1ncn2c1CN=C(c1c2ccc(c1)Cl)c1ccccc1)OC(C)(C)C</chem>        | 7.85 | 115.1187 | 7.8628 | -0.0128 | Tr | 112.125  | 7.8177 | 0.0323  | Ts | 125.9912 | 7.6149 | 0.2351  | Ts |
| 83 | <chem>COC(=O)c1ncn2c1CN=C(c1c2ccc(c1)Cl)c1ccccc1F</chem>              | 8.13 | 124.6252 | 8.3225 | -0.1925 | Tr | 120.3645 | 8.2331 | -0.1031 | Tr | 135.3792 | 8.2718 | -0.1418 | Ts |
| 84 | <chem>CC(OC(=O)c1ncn2c1C[N+](=C(c1c2ccc(c1)Cl)c1ccccc1F)[O-])C</chem> | 7.92 | 115.2999 | 7.8715 | 0.0485  | Tr | 114.6547 | 7.9452 | -0.0252 | Tr | 132.6716 | 8.0823 | -0.1623 | Tr |
| 85 | <chem>Clc1ccc2c(c1)C(=NCc1n2cnc1C(=O)O)c1ccccc1Cl</chem>              | 7.89 | 122.4748 | 8.2185 | -0.3285 | Tr | 120.8465 | 8.2574 | -0.3674 | Tr | 133.127  | 8.1142 | -0.2242 | Tr |
| 86 | <chem>Clc1ccc2c(c1)C(=NCc1n2cnc1C(=O)N)c1ccccc1F</chem>               | 8.46 | 120.8606 | 8.1405 | 0.3195  | Tr | 119.5825 | 8.1937 | 0.2663  | Ts | 134.1157 | 8.1834 | 0.2766  | Tr |
| 87 | <chem>Clc1ccc2c(c1)C(=NCc1n2cnc1C(=O)N)c1ccccc1Cl</chem>              | 8.42 | 123.4905 | 8.2677 | 0.1523  | Tr | 115.0264 | 7.9639 | 0.4561  | Tr | 132.6322 | 8.0796 | 0.3404  | Tr |
| 88 | <chem>CN(Cc1nc(c2n1c1ccc(cc1C(=NC2)c1ccccc1Cl)Cl)C(=O)N)C</chem>      | 7.59 | 109.9006 | 7.6104 | -0.0204 | Tr | 102.6099 | 7.3379 | 0.2521  | Tr | 122.495  | 7.3703 | 0.2197  | Ts |

Table S2. The statistical quality of the developed QSAR models for benzodiazepines binding activity

|                                                                                                                                                                                                                                                                                                                                                                                |       | Training set |        |        |        |       |       |     | Test set |        |        |        |       |       |     |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------|--------------|--------|--------|--------|-------|-------|-----|----------|--------|--------|--------|-------|-------|-----|
|                                                                                                                                                                                                                                                                                                                                                                                |       | $r^2$        | IIC    | CCC    | $q^2$  | s     | MAE   | F   | $r^2$    | IIC    | CCC    | $q^2$  | s     | MAE   | F   |
| Split 1                                                                                                                                                                                                                                                                                                                                                                        | 1 run | 0.9221       | 0.9595 | 0.9302 | 0.9175 | 0.204 | 0.161 | 722 | 0.9254   | 0.9525 | 0.9619 | 0.9104 | 0.261 | 0.213 | 236 |
|                                                                                                                                                                                                                                                                                                                                                                                | 2 run | 0.8836       | 0.9382 | 0.8545 | 0.8772 | 0.249 | 0.188 | 463 | 0.9228   | 0.9484 | 0.9606 | 0.9049 | 0.270 | 0.224 | 227 |
|                                                                                                                                                                                                                                                                                                                                                                                | 3 run | 0.8895       | 0.9415 | 0.8044 | 0.8840 | 0.243 | 0.185 | 491 | 0.9311   | 0.9167 | 0.9647 | 0.9171 | 0.323 | 0.266 | 257 |
|                                                                                                                                                                                                                                                                                                                                                                                | Av    | 0.8984       | 0.9464 | 0.8630 | 0.8929 | 0.232 | 0.178 | 559 | 0.9264   | 0.9392 | 0.9624 | 0.9108 | 0.285 | 0.234 | 240 |
| Split 2                                                                                                                                                                                                                                                                                                                                                                        | 1 run | 0.8975       | 0.9460 | 0.8360 | 0.8917 | 0.259 | 0.186 | 543 | 0.8703   | 0.8923 | 0.9328 | 0.8429 | 0.297 | 0.231 | 127 |
|                                                                                                                                                                                                                                                                                                                                                                                | 2 run | 0.8662       | 0.9283 | 0.8743 | 0.8557 | 0.296 | 0.208 | 401 | 0.8740   | 0.8790 | 0.9348 | 0.8479 | 0.302 | 0.227 | 132 |
|                                                                                                                                                                                                                                                                                                                                                                                | 3 run | 0.8825       | 0.9376 | 0.7306 | 0.8756 | 0.278 | 0.200 | 466 | 0.8868   | 0.8744 | 0.9417 | 0.8637 | 0.305 | 0.236 | 149 |
|                                                                                                                                                                                                                                                                                                                                                                                | Av    | 0.8821       | 0.9373 | 0.8136 | 0.8743 | 0.278 | 0.198 | 470 | 0.8770   | 0.8819 | 0.9364 | 0.8515 | 0.301 | 0.231 | 136 |
| Split 3                                                                                                                                                                                                                                                                                                                                                                        | 1 run | 0.8788       | 0.9355 | 0.9082 | 0.8720 | 0.285 | 0.195 | 442 | 0.8520   | 0.9071 | 0.9230 | 0.8081 | 0.325 | 0.270 | 115 |
|                                                                                                                                                                                                                                                                                                                                                                                | 2 run | 0.8339       | 0.9094 | 0.8302 | 0.8245 | 0.334 | 0.236 | 306 | 0.8426   | 0.8660 | 0.9179 | 0.8133 | 0.339 | 0.285 | 107 |
|                                                                                                                                                                                                                                                                                                                                                                                | 3 run | 0.8540       | 0.9213 | 0.8952 | 0.8459 | 0.313 | 0.210 | 357 | 0.8416   | 0.8939 | 0.9174 | 0.7866 | 0.325 | 0.276 | 106 |
|                                                                                                                                                                                                                                                                                                                                                                                | Av    | 0.8556       | 0.9221 | 0.8779 | 0.8475 | 0.311 | 0.214 | 368 | 0.8454   | 0.8890 | 0.9194 | 0.8027 | 0.330 | 0.277 | 109 |
| $r^2$ – Correlation coefficient<br>$q^2$ – Cross-validated correlation coefficient<br>CCC - Concordance correlation coefficient<br>IIC - Index of ideality of correlation<br>s – Standard error of estimation<br>MAE – Mean absolute error<br>F – Fischer ratio<br>Av – Average value for statistical parameters obtained from three independent Monte Carlo optimization runs |       |              |        |        |        |       |       |     |          |        |        |        |       |       |     |

Table S3. Y-randomization of the best QSAR model (best optimization run) for three independent splits

|                                                          | Split 1  |        | Split 2  |        | Split 3  |        |
|----------------------------------------------------------|----------|--------|----------|--------|----------|--------|
|                                                          | Training | Test   | Training | Test   | Training | Test   |
| 0                                                        | 0.8895   | 0.9311 | 0.8825   | 0.8868 | 0.8788   | 0.852  |
| 1                                                        | 0.0038   | 0.0803 | 0.0152   | 0.1631 | 0.0001   | 0.0079 |
| 2                                                        | 0.0424   | 0.0007 | 0.0204   | 0.0666 | 0.0124   | 0.029  |
| 3                                                        | 0.0038   | 0.4131 | 0        | 0.0216 | 0.0093   | 0.3571 |
| 4                                                        | 0.0915   | 0.1749 | 0.0072   | 0.1384 | 0.0008   | 0.0012 |
| 5                                                        | 0.015    | 0.148  | 0.0258   | 0.0012 | 0.0168   | 0.1138 |
| 6                                                        | 0.0016   | 0.1234 | 0.0186   | 0.1    | 0.0033   | 0.0039 |
| 7                                                        | 0.0166   | 0.1174 | 0.0028   | 0.0176 | 0.0257   | 0.0114 |
| 8                                                        | 0.0061   | 0.0002 | 0.0323   | 0.044  | 0.0175   | 0.3167 |
| 9                                                        | 0.0075   | 0.0606 | 0.0231   | 0.0733 | 0.0151   | 0.0086 |
| 10                                                       | 0.0183   | 0.0444 | 0.0102   | 0.0093 | 0.0007   | 0.086  |
| $R_r^2$                                                  | 0.0207   | 0.1163 | 0.0156   | 0.0635 | 0.0102   | 0.0936 |
| $^cR_p^2$                                                | 0.8791   | 0.871  | 0.8747   | 0.8545 | 0.8737   | 0.8039 |
| $^cR_p^2 = R \times (R^2 - R_r^2)^{1/2}$ should be > 0.5 |          |        |          |        |          |        |

Table S4. The list of SAKs together with their correlation weights for the three runs of the Monte Carlo optimization.

| SAk              | CW(SAk)  |          |          | SAk           | CW(SAk)  |          |          | SAk          | CW(SAk)  |          |          | SAk           | CW(SAk)  |          |          |
|------------------|----------|----------|----------|---------------|----------|----------|----------|--------------|----------|----------|----------|---------------|----------|----------|----------|
|                  | Run 1    | Run 2    | Run 3    |               | Run 1    | Run 2    | Run 3    |              | Run 1    | Run 2    | Run 3    |               | Run 1    | Run 2    | Run 3    |
| #.....           | -0.9425  | 0.28501  | -0.89738 | N...C...(...  | 0.81914  | 0.40602  | 0.12287  | S2E0N...11-. | 0.29704  | 2.56259  | -0.86578 | VS2-Br..4...  | 0.24291  | 0.43306  | 0.05662  |
| \$10,010,000,100 | 0.40715  | 0.43923  | 0.71419  | N...C.....    | -2.05706 | -1.6258  | -1.84325 | S2E0N...2-.. | 0.04833  | 0.0408   | -0.28906 | VS2-L...4...  | -0.05507 | 0.82038  | 1.89532  |
| \$10,010,001,100 | 1.46209  | 2.42734  | 0.10136  | N...C...1...  | 0.0567   | 0.11121  | 0.13086  | S2E0N...3-.. | -0.19273 | 0.12433  | 0.44593  | VS2-Cl...4... | 0.04699  | -0.1339  | 0.36329  |
| \$10,011,000,000 | -0.59615 | -0.14552 | 0.07521  | N...C...2...  | -0.53809 | -0.50439 | -1.01193 | S2E0N...5-.. | 0.32106  | 0.28615  | 0.3287   | VS2-Cl...5... | -0.07849 | 0.09636  | 2.05853  |
| \$10,011,000,010 | 0.22878  | 0.35755  | 0.68644  | N...C...C...  | 2.70165  | 1.7596   | 1.99086  | S2E0N...6-.. | 0.0095   | 0.46188  | 0.20054  | VS2-Cl...6... | 0.30169  | 0.18934  | 0.47611  |
| \$10,011,000,100 | 0.49669  | -0.51653 | 0.2201   | N...Cl.....   | -0.02036 | -0.63911 | -0.86927 | S2E0N...7-.. | 0.33865  | -0.92192 | 0.29413  | VS2-N...10..  | 1.27767  | -0.22058 | 0.3332   |
| \$10,011,001,000 | 0.29873  | -1.39398 | 0.4544   | N...[...(...  | 0.45869  | 1.33392  | 1.1709   | S2E0N...8-.. | -0.26573 | 0.49621  | 0.34922  | VS2-N...11..  | -2.13509 | -2.9531  | -0.86344 |
| \$10,011,001,001 | 2.1295   | 0.59585  | 2.34823  | N...[...C...  | -1.08019 | -0.89491 | -0.88696 | S2E0N...9-.. | -0.53782 | -0.5563  | -0.61306 | VS2-N...12..  | 0.2503   | -1.18898 | -1.74091 |
| \$10,011,001,100 | 0.55113  | -0.16156 | 0.23416  | N...c...1...  | 0.42214  | 0.26782  | -0.05268 | S2E0O...1-.. | 0.31267  | 0.12383  | -0.23124 | VS2-N...13..  | 1.23494  | 0.39573  | -0.10463 |
| \$11,011,000,000 | -0.19488 | -0.90043 | -0.77938 | N...c...2...  | -1.12707 | 2.35764  | 0.32177  | S2E0O...2-.. | 0.24178  | 0.35491  | -0.80458 | VS2-N...14..  | -0.88032 | 0.38813  | -0.31673 |
| \$11,011,000,100 | 0.41393  | -0.11985 | 0.14128  | O...(.....    | 0.00433  | -0.5025  | -0.67227 | S2E0O...3-.. | 0.08546  | 0.21375  | 0.08068  | VS2-N...2...  | 0.36276  | 0.15925  | 0.14951  |
| \$11,011,001,000 | -0.57588 | 0.71072  | 1.25564  | O...(....1... | -0.03743 | 0.05086  | 0.25658  | S2E0O...4-.. | -0.86088 | 0.25135  | -0.93105 | VS2-N...3...  | -0.83194 | 0.26084  | -0.55155 |
| (...(.....       | -0.84302 | -0.38317 | -0.27029 | O...(....C... | -0.03683 | -0.7111  | -0.70792 | S2E0O...5-.. | 1.90437  | 0.45322  | 0.26994  | VS2-N...4...  | 0.15803  | 0.25115  | 0.01103  |
| (.....           | -0.68012 | -0.68069 | -0.84875 | O...(....F... | -0.7498  | -0.38077 | -0.84193 | S2E0O...7-.. | -0.32348 | -0.13344 | -0.57289 | VS2-N...6...  | 0.29352  | 0.08542  | -0.06382 |
| (...C...(...     | -0.55408 | 0.49199  | 0.31231  | O...(....N... | 0.28813  | 0.08955  | 0.20759  | S2E0s...6-.. | 0.54003  | 2.14317  | 0.07648  | VS2-N...7...  | 0.4405   | 2.10132  | -0.74176 |
| (...F...(...     | -0.2912  | 0.41635  | 0.23655  | O...(....O... | 0.30005  | 0.39911  | 0.46618  | S2E0s...7-.. | 1.26769  | -0.73784 | 0.21752  | VS2-N...8...  | 0.47076  | 2.23661  | 0.48979  |
| (...Br...(...    | 0.07604  | -0.07335 | 2.60933  | O...-.....    | 2.35027  | 1.53325  | 1.21156  | S2E0s...8-.. | 0.06279  | 2.13422  | 2.27775  | VS2-N...9...  | -0.09882 | 1.41224  | -0.87773 |
| (...Cl...(...    | -0.4944  | 0.35865  | -0.60805 | O.....        | -0.12354 | 0.1187   | 0.22597  | S3E0C...0-.. | 0.35316  | -0.68119 | -0.56735 | VS2-O...2...  | 0.12813  | 0.49378  | 2.08309  |
| (...N...(...     | -0.99635 | -0.05273 | 0.13273  | O...1.....    | 0.13194  | 0.03564  | 2.1093   | S3E0C...1-.. | -1.09052 | -1.99115 | 0.48873  | VS2-O...3...  | -0.37969 | -0.45471 | -0.71189 |
| (...O...(...     | -0.54595 | -0.62412 | 0.41241  | O...1...C...  | 0.19515  | 0.02261  | 1.49852  | S3E0C...10-  | 0.38644  | 0.08473  | -0.50813 | VS2-O...4...  | -0.68757 | -0.45726 | 0.33931  |
| (...c...(...     | 0.07111  | 2.46591  | 0.0851   | O...=...(...  | 0.1355   | -0.11296 | 0.31098  | S3E0C...11-  | -1.74697 | -0.77641 | -1.94483 | VS2-O...5...  | 0.3199   | -0.63087 | -0.05573 |
| ++++B2--B3==     | -0.0457  | 1.16076  | -0.32873 | O...=.....    | 0.28563  | 0.06381  | 0.25411  | S3E0C...12-  | 0.23292  | 1.62067  | 1.23674  | VS2-O...6...  | 0.32883  | 0.22099  | 0.31083  |
| ++++F--B2==      | -0.09671 | 0.75173  | 0.0278   | O...=...1...  | 2.03724  | 0.32938  | -0.19349 | S3E0C...13-  | 0.5995   | 0.10246  | 0.28925  | VS2-O...9...  | -1.05251 | -0.61321 | -0.05607 |
| ++++F--B3==      | 0.37371  | -0.20354 | 0.86029  | O...=...C...  | 0.43349  | -0.62828 | 0.35686  | S3E0C...14-  | 0.10586  | 0.1228   | 2.4107   | VS2-s...10..  | 0.16503  | 0.08417  | -0.06385 |
| ++++F--Cl==      | 0.03835  | 0.43852  | 0.11726  | O...C...(...  | -0.89576 | -0.46426 | -0.49578 | S3E0C...15-  | -1.09856 | -0.31686 | -1.09824 | VS2-s...8...  | 0.91499  | 2.07785  | 0.166    |
| ++++F--N===      | 0.6771   | 0.38845  | 1.47888  | O...C.....    | -0.96971 | -3.77972 | -0.99799 | S3E0C...16-  | -0.96573 | -0.92041 | -0.4164  | VS2-s...9...  | 0.35372  | 0.34427  | 0.27422  |
| ++++F--O===      | 2.42591  | 0.26056  | -0.24909 | O...C...C...  | -0.69097 | -0.77087 | 0.28473  | S3E0C...17-  | 0.09607  | 1.45689  | 0.15087  | VS3-C...10..  | 0.44127  | 1.31966  | 0.30806  |
| ++++CL--N===     | 0.05403  | 0.19967  | -0.2412  | O...N.....    | -0.50361 | 0.22627  | -0.53459 | S3E0C...2-.. | 0.1844   | 0.30491  | -0.57802 | VS3-C...11..  | 0.10714  | 0.4708   | 1.328    |
| ++++CL--O===     | 0.17301  | 0.32373  | 0.34928  | O...[...(...  | 0.72748  | 1.22129  | -1.55355 | S3E0C...18-  | -0.77035 | -0.52424 | -0.9506  | VS3-C...12..  | 0.00743  | 0.4882   | 0.17878  |
| ++++CL--S===     | 0.499    | -0.03327 | 0.61755  | P2E0C...0-..  | 0.44391  | 0.4464   | 0.19022  | S3E0C...3-.. | -0.64352 | -0.24358 | -0.06379 | VS3-C...13..  | 0.47368  | 0.03512  | 0.47931  |
| ++++Br--B2==     | 0.40398  | 2.41533  | 0.07628  | P2E0C...1-..  | -0.78745 | 0.33096  | 0.6991   | S3E0C...4-.. | 0.48822  | 0.44117  | -0.94594 | VS3-C...14..  | 1.3899   | 0.17161  | 0.07872  |
| ++++Br--N===     | 0.3491   | -0.42548 | 0.84843  | P2E0C...2-..  | 0.34354  | 0.08846  | -0.831   | S3E0C...5-.. | 1.12455  | 0.49593  | 0.4927   | VS3-C...15..  | 0.38974  | 0.17467  | 0.39061  |

|               |          |          |          |               |          |          |          |               |          |          |          |               |          |          |          |
|---------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|
| ++++Br--O===  | 2.14475  | -0.94098 | 2.30836  | P2E0C...3-..  | 0.22332  | 0.04106  | 0.30942  | S3E0C...6-..  | 0.18539  | 0.2943   | 0.1753   | VS3-C...16..  | -0.26859 | 0.49146  | 1.40125  |
| ++++I---B2==  | 0.84071  | 0.13731  | 0.10499  | P2E0F...1-..  | 0.21876  | 2.13528  | 0.08915  | S3E0C...7-..  | 0.19694  | 0.4943   | 0.43434  | VS3-C...17..  | 0.45113  | -0.03949 | 0.32687  |
| ++++I---F===  | 0.00048  | 1.29256  | 2.25946  | P2E0F...2-..  | -0.05268 | 0.34175  | 0.13516  | S3E0C...8-..  | 0.60053  | 0.10475  | 0.13996  | VS3-C...2...  | -1.23026 | 0.1025   | 0.56092  |
| ++++I---N===  | -0.71919 | 1.92276  | 2.17859  | P2E0Br...1-.. | 1.12805  | 0.24951  | 1.32348  | S3E0C...9-..  | 0.09268  | 0.07128  | 0.45392  | VS3-C...18..  | -0.7916  | -0.12267 | 0.38216  |
| ++++I---O===  | 2.28559  | 0.20447  | 2.24823  | P2E0I...1-..  | 0.13979  | -0.18864 | -0.3681  | S3E0F...3-..  | 1.3889   | 0.50391  | 0.15416  | VS3-C...19..  | 0.73728  | 2.23093  | -0.78761 |
| ++++Cl--B2==  | 0.31289  | -0.33852 | 0.0905   | P2E0Cl...1-.. | 0.031    | 0.08965  | 2.34996  | S3E0F...4-..  | 0.26273  | 0.09662  | 0.18042  | VS3-C...20..  | 0.10863  | -0.84178 | 0.2181   |
| ++++Cl--B3==  | -0.24619 | 0.3986   | -0.31395 | P2E0N...0-..  | 0.17765  | -0.97677 | 0.43672  | S3E0F...6-..  | 2.08234  | 0.485    | 0.47151  | VS3-C...21..  | 0.00997  | 0.09387  | 0.19329  |
| ++++N---B2==  | 0.65137  | 5.0548   | 6.58089  | P2E0N...1-..  | 0.47575  | 0.09461  | 0.42529  | S3E0Br...4-.. | 2.03213  | 1.12308  | -0.17327 | VS3-C...3...  | 0.18403  | 0.34009  | -0.72373 |
| ++++N---B3==  | -0.64123 | -0.79214 | 0.08895  | P2E0N...2-..  | 0.0472   | 1.27389  | 0.26919  | S3E0I...4-..  | 2.27508  | 2.21193  | 1.96269  | VS3-C...4...  | 0.14826  | -0.2549  | -0.23668 |
| ++++N---O===  | -0.23967 | 1.03721  | -1.62073 | P2E0N...3-..  | -0.65803 | -0.80678 | -0.765   | S3E0Cl...4-.. | 0.716    | 0.05816  | 0.4924   | VS3-C...5...  | -0.24373 | -0.84812 | -0.82214 |
| ++++N---S===  | 2.46787  | 2.10398  | 0.13912  | P2E0O...0-..  | 0.08185  | 0.47285  | 0.31584  | S3E0Cl...5-.. | 0.8363   | -0.04618 | -0.16375 | VS3-C...6...  | -0.54437 | -0.11888 | 0.68668  |
| ++++O---B2==  | -0.75139 | 2.01397  | 0.03827  | P2E0O...1-..  | -0.50991 | -0.7751  | -0.84914 | S3E0Cl...6-.. | 2.55864  | 0.68109  | -0.38624 | VS3-C...7...  | 0.36844  | 0.26462  | 0.38967  |
| ++++O---B3==  | 0.16786  | 0.24797  | 0.0641   | P2E0O...2-..  | 0.23214  | -0.67253 | -0.59084 | S3E0Cl...7-.. | 0.29693  | 0.45015  | 0.38961  | VS3-C...8...  | 0.44484  | 0.22646  | 0.12122  |
| ++++S---B2==  | -0.69493 | 0.31078  | 0.49604  | P2E0s...1-..  | 1.17247  | -0.92472 | 1.95606  | S3E0Cl...8-.. | -0.01608 | -1.09028 | -0.17293 | VS3-C...9...  | 0.11844  | 0.47572  | 1.3631   |
| +.....        | 2.22593  | 0.49813  | 2.05787  | P2E0s...2-..  | 0.26098  | -0.84002 | 0.60375  | S3E0N...0-..  | -0.9593  | -0.94197 | 0.29324  | VS3-F...4...  | 0.38954  | 0.48488  | 0.12     |
| +...[(...)    | 1.7616   | 1.97339  | 2.30782  | P3E0C...0-..  | 3.32683  | 1.41193  | 2.37127  | S3E0N...1-..  | -0.85206 | 0.36162  | -0.85512 | VS3-F...5...  | 0.07381  | 0.04047  | -0.80746 |
| -.....        | 0.22255  | 2.12158  | 2.31305  | P3E0C...1-..  | 0.23058  | -0.58957 | -0.82713 | S3E0N...10-   | -0.28617 | 0.20409  | -1.31194 | VS3-F...7...  | 0.08257  | 0.71984  | 0.41043  |
| -...[(...)    | 1.81901  | 0.20386  | 0.34355  | P3E0C...2-..  | 0.14138  | -0.85033 | 0.1728   | S3E0N...11-   | 0.35536  | -0.04769 | 0.26612  | VS3-Br...5... | 0.16027  | -0.5115  | 0.26279  |
| 1...(.....)   | 0.09699  | 1.74967  | -0.40593 | P3E0C...3-..  | 0.24694  | 1.09448  | 0.39222  | S3E0N...12-   | -0.30825 | -0.9588  | 0.38711  | VS3-I...5...  | 0.3605   | 2.58735  | 2.36225  |
| 1.....        | 0.45182  | 1.23708  | 0.49858  | P3E0C...4-..  | 0.14506  | -0.01097 | -0.59412 | S3E0N...13-   | 0.40738  | -0.09583 | 0.28532  | VS3-Cl...5... | 2.10464  | 2.41584  | 0.4995   |
| 1...C...(...  | 0.48256  | -0.68962 | 0.14833  | P3E0C...5-..  | 0.49875  | -0.55308 | -0.99506 | S3E0N...14-   | 0.18123  | -0.77654 | 0.06082  | VS3-Cl...6... | 0.37212  | 0.3932   | 2.01037  |
| 1...C...1...  | 0.639    | -0.38035 | -0.62487 | P3E0C...6-..  | 0.26577  | -1.54837 | -0.59778 | S3E0N...15-   | -0.19469 | -1.0013  | -0.0605  | VS3-Cl...7... | 0.58241  | 2.08619  | -0.61792 |
| 1...F...(...  | -0.64507 | 0.09895  | -0.56648 | P3E0F...1-..  | 2.38492  | 2.13095  | 0.11951  | S3E0N...17-   | -0.26994 | 0.39851  | -0.79002 | VS3-Cl...8... | -0.92249 | 0.42325  | 0.12391  |
| 1...Cl...(... | 0.32135  | 0.10337  | -2.0617  | P3E0F...2-..  | -0.15017 | 0.13488  | 0.24471  | S3E0N...2-..  | 0.41472  | 0.2873   | 0.2241   | VS3-Cl...9... | 0.18621  | -0.42424 | -0.89139 |
| 1...N...(...  | -0.04494 | 2.27425  | -0.71342 | P3E0Br...1-.. | 2.12029  | 0.38173  | 0.50676  | S3E0N...3-..  | -4.75169 | -1.85525 | -0.80837 | VS3-N...10..  | 2.04821  | 4.03444  | -1.4662  |
| 1...O...(...  | 0.25136  | 0.35691  | 0.1536   | P3E0I...1-..  | 0.04164  | 0.16114  | 0.46678  | S3E0N...4-..  | -2.52656 | -0.08064 | -0.79534 | VS3-N...11..  | 0.29058  | 0.49464  | -0.6484  |
| 1...c...(...  | 0.65931  | 0.47327  | 2.35049  | P3E0Cl...1-.. | 2.4418   | -0.07795 | 0.45618  | S3E0N...5-..  | 0.1777   | 0.04339  | -0.64999 | VS3-N...12..  | 0.93353  | 0.88179  | 2.34902  |
| 1...c...1...  | 2.11036  | 0.52844  | -0.68052 | P3E0Cl...2-.. | -0.64958 | -0.1324  | 0.09955  | S3E0N...6-..  | -0.80573 | 0.10037  | -0.2445  | VS3-N...13..  | -0.04232 | 0.1999   | 1.05988  |
| 1...n...(...  | 2.25824  | 0.07411  | 0.13583  | P3E0Cl...3-.. | 0.32682  | 0.29809  | 0.23623  | S3E0N...7-..  | 0.0475   | 0.33601  | 2.38986  | VS3-N...14..  | 0.07263  | 0.45932  | 0.4145   |
| 1...s...(...  | 0.08329  | 2.08489  | 0.17473  | P3E0N...0-..  | 0.21471  | 0.20008  | 0.46015  | S3E0N...8-..  | 0.35509  | -0.0069  | 1.09761  | VS3-N...15..  | 0.21272  | -0.36394 | 0.26042  |
| 2...(.....)   | 0.16267  | 0.46431  | 0.97841  | P3E0N...1-..  | 0.2886   | 0.45735  | 0.01183  | S3E0N...9-..  | 0.08948  | 0.37809  | 0.25053  | VS3-N...16..  | 0.03134  | 0.22001  | 0.38078  |
| 2.....        | -0.32623 | 0.44705  | 0.20212  | P3E0N...2-..  | -0.51664 | 0.23149  | 0.05053  | S3E0O...1-..  | 0.00816  | 0.42186  | 0.06449  | VS3-N...17..  | 0.08053  | 0.40108  | 0.19627  |
| 2...C...(...  | 0.10823  | 0.15628  | 0.39816  | P3E0N...3-..  | 0.30292  | 0.10676  | 0.74298  | S3E0O...2-..  | -1.90717 | -0.90715 | -0.51167 | VS3-N...2...  | 2.24801  | 0.08703  | 0.22389  |
| 2...Cl...(... | 0.77274  | 0.45795  | 0.02941  | P3E0N...4-..  | 0.0228   | 2.27192  | 0.47349  | S3E0O...3-..  | 0.04047  | 0.12422  | 2.33648  | VS3-N...18..  | 1.14172  | 0.24454  | 1.12419  |
| 2...N...(...  | 0.20974  | -0.9441  | 0.17815  | P3E0N...5-..  | -0.71787 | 0.3488   | -0.91423 | S3E0O...4-..  | 0.19869  | 0.24217  | 1.00129  | VS3-N...20..  | -0.65275 | 0.38438  | -0.01903 |



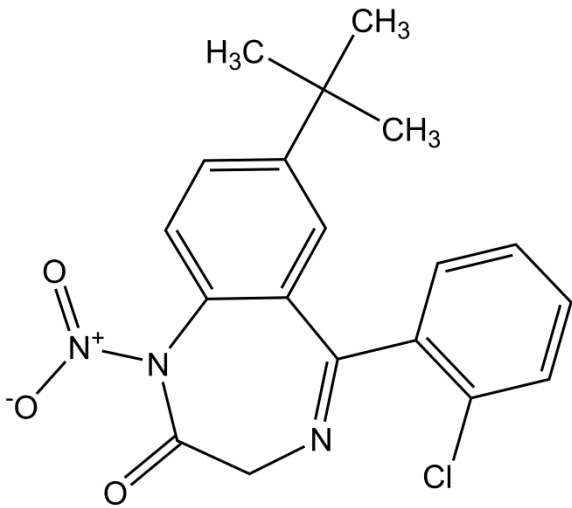
|                |          |          |          |               |          |          |          |               |          |          |          |              |          |          |          |
|----------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|--------------|----------|----------|----------|
| 2...c...(...   | 0.26522  | 0.01513  | 0.30611  | P3E0O...0-..  | -0.42217 | -0.01583 | 0.28789  | S3E0O...5-..  | -0.70119 | 0.28165  | 0.38163  | VS3-N...3... | 0.14537  | 0.00774  | -0.97681 |
| 2...c...1...   | 0.14952  | 0.22738  | -0.10852 | P3E0O...1-..  | -0.08736 | 0.32232  | 0.21236  | S3E0O...6-..  | -0.78404 | 0.19906  | 1.17101  | VS3-N...4... | -0.04969 | 1.24628  | -0.21656 |
| 2...c...2...   | 2.25878  | -0.17368 | -0.41698 | P3E0O...2-..  | 0.18374  | -0.76844 | -0.70505 | S3E0O...7-..  | -0.61722 | -1.50662 | -0.6365  | VS3-N...5... | 0.67073  | 0.42602  | 0.88174  |
| 2...n...(...   | 2.39254  | 2.44937  | 2.10799  | P3E0O...3-..  | 0.02976  | -0.6118  | -0.22475 | S3E0O...8-..  | -0.03661 | 0.7127   | -0.37762 | VS3-N...6... | 0.23947  | -0.12225 | -0.60051 |
| 2...n...1...   | -0.00211 | 0.20317  | 0.22411  | P3E0s...3-..  | 0.36864  | 2.10493  | 2.31426  | S3E0s...12-.  | 0.27403  | 0.45202  | 2.41183  | VS3-N...8... | 0.26629  | 0.27616  | 0.21284  |
| 3...(.....     | 0.49045  | 1.24487  | -0.27979 | P3E0s...4-..  | 0.13092  | 0.36056  | 0.33625  | S3E0s...13-.  | -0.49355 | -0.704   | 1.0284   | VS3-N...9... | 2.24655  | 2.164    | 1.26149  |
| 3.....         | 0.31744  | 0.46607  | 0.09754  | P4E0C...0-..  | 0.05824  | -0.76911 | -0.92764 | PT2-C...1...  | 0.25941  | 0.23315  | 0.10145  | VS3-O...2... | -0.08789 | -0.90574 | 2.08639  |
| 3...c...(...   | -0.32488 | -0.25644 | -0.83223 | P4E0C...1-..  | 0.41267  | 0.39341  | -0.91271 | PT2-C...2...  | 0.26155  | -0.07039 | -0.02017 | VS3-O...3... | -0.84926 | -0.0937  | 0.41212  |
| 3...c...1...   | 0.1497   | 2.35923  | -0.66312 | P4E0C...10-.  | 0.84725  | -0.55256 | -0.62718 | PT2-C...3...  | 0.32589  | 0.31746  | 0.49884  | VS3-O...4... | -0.47304 | 1.94582  | -0.00037 |
| =...(.....     | 1.19939  | -0.2257  | 0.02301  | P4E0C...11-.  | 0.32052  | -0.31234 | 0.3235   | PT2-C...4...  | 0.36168  | -0.70498 | 0.28567  | VS3-O...5... | -0.01138 | -0.80195 | -0.63011 |
| =.....         | 0.26353  | -0.71124 | 0.28523  | P4E0C...12-.  | 2.74662  | -1.69051 | 2.37105  | PT2-C...5...  | 0.4424   | 0.17694  | 0.28931  | VS3-O...6... | 0.26976  | 0.41566  | 0.07697  |
| =...1.....     | 0.35147  | 2.23502  | 0.22732  | P4E0C...13-.  | -0.16051 | 0.17736  | -0.67043 | PT2-C...6...  | -0.63626 | 0.30534  | 0.20012  | VS3-O...7... | 3.19332  | 0.42573  | -0.63162 |
| =...2.....     | 0.32079  | -1.0458  | -0.69201 | P4E0C...14-.  | 0.23629  | 0.13162  | 2.19403  | PT2-F...2...  | 1.71443  | 2.36398  | 2.23143  | VS3-O...8... | 0.34926  | -1.06406 | -3.29642 |
| =...C...(...   | 0.46627  | 1.42318  | 0.44227  | P4E0C...16-.  | -0.52584 | 0.2494   | -0.95324 | PT2-F...3...  | 2.31311  | 0.58209  | 0.46505  | VS3-O...9... | 0.40996  | 0.0261   | 0.05613  |
| =...C...1...   | 0.51994  | 0.4258   | 0.16395  | P4E0C...2-..  | 0.22058  | 0.42916  | 0.07932  | PT2-Br...2... | 2.1059   | 2.00911  | 0.20754  | VS3-s...14.. | 0.2398   | 0.25427  | 2.23273  |
| =...C...2...   | 2.24084  | -0.86121 | 0.43001  | P4E0C...3-..  | 0.45241  | 0.42456  | 0.45355  | PT2-I...2...  | 2.08851  | 0.59407  | 0.08455  | VS3-s...15.. | 0.20445  | 0.389    | -0.08702 |
| =...N...1...   | 0.50171  | 0.31512  | -0.67175 | P4E0C...4-..  | -0.2065  | 1.26034  | -0.32726 | PT2-Cl...2... | 2.22863  | 0.49583  | 0.34215  | Smax.0.....  | 6.18715  | 6.11152  | 9.51047  |
| =...O...(...   | 0.1699   | 0.0204   | 0.3067   | P4E0C...5-..  | -0.88451 | 0.03266  | 0.20004  | PT2-N...1...  | 0.66415  | 0.38459  | 0.26072  | [...(.....   | 0.36139  | 0.48404  | 0.14963  |
| =...c...2...   | -0.06736 | -0.8107  | 0.15517  | P4E0C...6-..  | 0.2096   | -0.78501 | 0.12788  | PT2-N...2...  | 0.01369  | 0.14472  | 0.13714  | [...(2...    | 5.76073  | 6.01444  | 8.17923  |
| C...#.....     | -0.76624 | 0.13273  | 0.25155  | P4E0C...7-..  | 0.06     | 0.49146  | 0.15339  | PT2-N...3...  | -1.07901 | -1.72915 | -0.2696  | [...(3...    | -0.27298 | -1.48943 | 1.25815  |
| C...#...C...   | 0.22139  | 0.0079   | -1.07332 | P4E0C...8-..  | 0.61851  | 2.27456  | 0.90439  | PT2-N...4...  | 0.22047  | 0.13058  | 0.30921  | [...(=...    | 0.0727   | 2.34663  | -0.50254 |
| C...(...(...   | 0.59911  | 0.56012  | 0.23966  | P4E0C...9-..  | -0.31297 | -0.75761 | 0.19502  | PT2-N...5...  | -0.75619 | -0.05213 | -0.45069 | [...(C...    | -0.56806 | 0.21179  | -0.99216 |
| C...(...(..... | -0.74243 | 0.3646   | 0.39949  | P4E0F...1-..  | 0.06604  | 2.20726  | 2.25438  | PT2-N...6...  | -0.54134 | 0.20813  | -0.71538 | [...(F...    | 0.32411  | -0.61002 | -0.9447  |
| C...(...1...   | 0.48309  | 1.3696   | 2.20659  | P4E0F...3-..  | 1.04979  | 0.33686  | 0.05996  | PT2-O...1...  | -1.07369 | -0.24513 | -0.38386 | [...(O...    | 1.10631  | 2.42078  | 0.16868  |
| C...(...2...   | 0.14906  | 0.48597  | 2.49392  | P4E0F...4-..  | 0.36657  | 0.77109  | -0.56899 | PT2-O...2...  | 0.11168  | 0.30925  | -0.98615 | [...+.....   | 0.27015  | 0.7297   | 0.22203  |
| C...(...=...   | 0.31024  | 1.02504  | 0.3811   | P4E0Br...1-.. | 0.40966  | 0.12875  | 0.81449  | PT2-O...3...  | -0.4502  | -0.61669 | -0.98935 | [...+...N... | 2.4252   | 0.47536  | 0.07726  |
| C...(...C...   | 0.78025  | -0.11754 | -0.4531  | P4E0I...1-..  | 0.48414  | 0.36843  | 0.21732  | PT2-O...4...  | -0.04983 | 0.22531  | -0.74371 | [...-.....   | -0.60974 | 0.11966  | 0.17435  |
| C.....         | 0.02042  | 0.22207  | 0.11506  | P4E0Cl...1-.. | 0.27439  | 0.40528  | 0.01256  | PT2-s...3...  | 1.67527  | 0.26743  | 0.37685  | [...-...O... | 0.37799  | 0.08618  | 0.27909  |
| C...1...(...   | -0.71481 | -0.63674 | -0.7937  | P4E0Cl...4-.. | 2.45772  | 0.21324  | 0.28324  | PT2-s...4...  | 2.25496  | 0.00843  | 0.28773  | [.....       | -0.06016 | 0.22799  | -0.19788 |
| C...1.....     | -0.51987 | 0.31226  | 0.18685  | P4E0Cl...7-.. | 0.41334  | -0.71616 | -0.75033 | PT3-C...1...  | -0.74926 | 1.94534  | 0.94886  | [...C.....   | -0.07724 | -0.06836 | 0.62915  |
| C...1...=...   | -0.84906 | -0.07781 | 0.0724   | P4E0N...0-..  | 0.47023  | -0.10624 | -0.44222 | PT3-C...2...  | 0.24602  | -0.00682 | 0.28132  | [...C...1... | 0.13241  | 0.00257  | -0.12394 |
| C...1...C...   | -0.45649 | -0.99081 | 0.34468  | P4E0N...1-..  | -1.60506 | -4.58375 | -4.37682 | PT3-C...3...  | 0.22946  | 0.32212  | 0.49375  | [...N...+... | -0.43481 | 0.12309  | 2.32499  |
| C...2...(...   | -0.23807 | 0.21446  | 0.41923  | P4E0N...10-.  | 1.03136  | 0.02095  | 0.41855  | PT3-C...4...  | 0.286    | 0.33142  | 0.28885  | [...N.....   | 0.4465   | 0.88983  | 0.48011  |
| C...2.....     | 0.316    | 1.1649   | 0.39512  | P4E0N...11-.  | -0.00982 | -0.89123 | -1.00471 | PT3-C...5...  | 0.18786  | -0.48713 | 0.2764   | [...O...-... | 0.47197  | 0.34126  | -0.86526 |
| C...=...(...   | -0.71403 | -0.64961 | -0.56111 | P4E0N...2-..  | -0.96476 | 0.29831  | 0.18404  | PT3-C...6...  | 0.34021  | 0.06905  | -0.59089 | [...O.....   | -0.15631 | 1.27245  | 0.24331  |

|              |          |          |          |              |          |          |          |              |          |          |          |              |          |          |          |
|--------------|----------|----------|----------|--------------|----------|----------|----------|--------------|----------|----------|----------|--------------|----------|----------|----------|
| C...=.....   | 0.28428  | 0.05536  | -0.2804  | P4E0N...3-.. | 0.01066  | 0.39601  | 0.59805  | PT3-C...7... | -0.04237 | 0.03623  | 2.11964  | c...(.....   | 2.21058  | 2.05023  | 0.49679  |
| C...=...1... | 1.47788  | 2.27307  | 2.46165  | P4E0N...4-.. | 0.15693  | -0.32512 | 0.58104  | PT3-C...8... | 0.00641  | 0.18463  | 0.20404  | c...(1...    | 0.26838  | 0.44697  | -0.19152 |
| C...=...C... | 0.3658   | 2.60327  | 0.7337   | P4E0N...5-.. | 0.21021  | 0.47192  | 0.32595  | PT3-C...9... | 0.31588  | 0.1173   | 0.08968  | c...(2...    | 0.33339  | 0.59975  | 2.15616  |
| C...C...#... | 0.30392  | -1.52709 | -0.27863 | P4E0N...6-.. | 0.29975  | -0.05395 | 0.13659  | PT3-F...2... | -0.85169 | 0.34789  | 0.31191  | c...(3...    | -0.58575 | 0.06242  | 2.11416  |
| C...C...(... | 0.86757  | 0.71673  | -0.1399  | P4E0N...7-.. | 0.26858  | 0.39213  | -2.60916 | PT3-F...3... | 0.48454  | 0.08898  | 0.04069  | c...(C...    | -0.69636 | 0.92037  | 0.19025  |
| C...C.....   | 0.14536  | 0.19862  | 0.40143  | P4E0N...8-.. | 0.33884  | 0.15285  | -0.63462 | PT3-Br..2... | -0.35256 | 0.52314  | 1.12811  | c...(F...    | 0.55721  | 0.21347  | 0.30918  |
| C...C...1... | -0.89833 | 0.36461  | -0.82763 | P4E0N...9-.. | 2.00814  | -0.62668 | 0.11     | PT3-I...2... | 0.3773   | 0.39752  | 0.44747  | c...(Br...   | 0.17962  | 1.15259  | -0.04887 |
| C...C...2... | -0.48287 | 1.31699  | 2.44584  | P4E0O...0-.. | 0.37752  | 0.73812  | -0.63316 | PT3-Cl..2... | 0.07447  | 2.2554   | 0.00176  | c...(Cl...   | -0.26486 | 2.40788  | 0.5002   |
| C...C...=... | -0.94273 | -1.06643 | 1.34639  | P4E0O...1-.. | -0.13763 | 0.10474  | 0.06491  | PT3-Cl..3... | 0.04526  | 2.13855  | 0.21473  | c...(N...    | 0.16512  | -0.85572 | 0.29406  |
| C...C...C... | 0.28752  | 0.4084   | 0.32034  | P4E0O...2-.. | -0.83863 | 0.43738  | -0.60164 | PT3-Cl..4... | 0.30762  | 0.18666  | 0.11752  | c...(O...    | -0.22133 | 1.13925  | 0.98132  |
| C...N...(... | 0.38969  | 0.24799  | 0.19563  | P4E0O...3-.. | -0.57645 | -0.63989 | 0.34886  | PT3-N...1... | -1.05204 | -0.47574 | -0.08701 | c...( [...   | 0.079    | 0.1431   | -0.43554 |
| C...N...1... | 2.0125   | 2.31159  | 1.09808  | P4E0O...4-.. | -0.03017 | -0.58128 | 0.35214  | PT3-N...2... | 0.28622  | 0.07251  | 0.19507  | c...(c...    | 0.18497  | 0.37788  | 0.12407  |
| C...N...=... | -0.20902 | 0.95981  | 1.01811  | P4E0O...7-.. | 0.03299  | 0.02382  | 0.22863  | PT3-N...3... | -0.67211 | -1.07623 | -0.94546 | c.....       | 0.47505  | -0.14287 | -0.01543 |
| C...N...C... | -1.27927 | -0.50309 | -0.78415 | P4E0s...7-.. | 0.47751  | -0.66532 | 2.37755  | PT3-N...4... | -0.56649 | 0.37818  | -0.66269 | c...1...(... | 0.36353  | 0.33088  | 0.22828  |
| C...O...(... | -0.19363 | -1.09569 | 0.24675  | P4E0s...8-.. | -0.00579 | 2.74364  | 2.18784  | PT3-N...5... | 0.54351  | 1.09074  | -0.35072 | c...1.....   | 0.07046  | -0.00236 | 0.11494  |
| C...O...C... | 3.65293  | 2.70976  | 4.3615   | NNC-C...101. | -0.70999 | -0.62663 | 0.03245  | PT3-N...6... | 2.26149  | 0.32028  | 0.20424  | c...1...C... | -1.41939 | -0.75787 | 1.30722  |
| C...C...1... | 0.14224  | 0.29723  | 0.19286  | NNC-C...110. | 0.99462  | -0.86714 | -0.17245 | PT3-N...7... | -0.3301  | -0.35336 | -0.81163 | c...1...F... | 0.4985   | 0.47145  | 0.40676  |
| C...c...2... | 2.0545   | 0.3872   | -0.23985 | NNC-C...202. | 0.46674  | -0.03963 | -1.18063 | PT3-N...8... | -0.61241 | -0.64824 | -0.65244 | c...1...Cl.. | 0.75511  | 1.08297  | 0.11422  |
| C3.....0...  | -0.99032 | 2.72035  | 1.33651  | NNC-C...211. | 0.08115  | 0.25217  | 0.14     | PT3-O...1... | 0.3974   | 0.0793   | 0.04916  | c...1...C... | 0.28035  | 0.02097  | -0.26369 |
| C3.....1...  | -0.83123 | -0.58132 | -0.93114 | NNC-C...220. | -0.63124 | 0.00332  | 0.20102  | PT3-O...2... | -0.84157 | 0.47222  | 0.28972  | c...2...(... | 0.22507  | -0.35859 | 0.56556  |
| C4.....0...  | 5.24155  | 5.8158   | 5.52398  | NNC-C...303. | -0.72789 | -0.57357 | 0.20384  | PT3-O...3... | 0.23651  | -0.57911 | 0.36811  | c...2.....   | 0.37702  | 0.42513  | 0.1574   |
| C5.....0...  | -0.18128 | -0.65181 | 0.6165   | NNC-C...312. | -0.05253 | 2.35893  | 0.22579  | PT3-O...4... | 0.13537  | 0.09406  | 0.21105  | c...2...=... | -0.72045 | 1.25916  | -0.87902 |
| C5...AH.1... | 1.36634  | 0.21312  | 0.20854  | NNC-C...321. | 0.0841   | 0.40393  | 0.8382   | PT3-O...5... | 0.41296  | -0.48063 | 0.16945  | c...2...C... | -0.78609 | 0.71163  | 2.42362  |
| C5...AH.2... | 0.04821  | 0.24829  | -0.99149 | NNC-C...330. | -0.92901 | -0.68504 | -0.62281 | PT3-s...5... | 0.35494  | 0.12634  | 0.05824  | c...2...Cl.. | 0.47393  | 0.13954  | 0.4661   |
| C6...A.1...  | 0.07112  | -0.02993 | 2.30999  | NNC-C...413. | 0.19268  | 0.45351  | 0.4153   | PT3-s...6... | 0.51725  | 0.46482  | 0.09419  | c...2...c... | 1.11927  | 0.2208   | 0.04856  |
| C6...A.2...  | 3.16493  | -1.73178 | -0.54518 | NNC-C...440. | -0.68832 | -1.05998 | -0.87211 | PT4-C...1... | 0.98424  | -0.31496 | -0.51027 | c...3...(... | 0.15772  | 2.74818  | -0.00135 |
| C6...AH.2... | -0.22467 | 0.46633  | -0.63088 | NNC-F...110. | 0.31392  | 0.16703  | -0.44159 | PT4-C...10.. | 0.21261  | 0.31663  | 0.35737  | c...3.....   | 0.33476  | 0.48044  | 0.40973  |
| C7...AH.1... | 4.99866  | 6.1289   | 11.53368 | NNC-Br..110. | 0.46516  | 0.41633  | -0.93074 | PT4-C...11.. | 2.38673  | 0.08377  | -0.07329 | c...3...c... | 0.20128  | 2.36642  | 2.2907   |
| BOND10000000 | -0.92608 | 0.47973  | -0.40856 | NNC-I...110. | 2.21589  | 0.49118  | 0.1568   | PT4-C...12.. | 0.49447  | -0.7494  | 0.49132  | c...=...(... | -0.0207  | 0.38297  | 0.43622  |
| BOND11000000 | 0.13973  | 0.5138   | -0.77334 | NNC-Cl..101. | -0.5967  | 2.11139  | 0.30662  | PT4-C...13.. | 2.52635  | 0.35305  | -0.02159 | c...=.....   | -0.72844 | -1.07835 | 0.33492  |
| F...( [...   | -0.8231  | 0.27548  | -0.3273  | NNC-Cl..110. | 0.3882   | 0.43162  | 0.28245  | PT4-C...14.. | -0.59505 | 0.16983  | 1.45121  | c...C...#... | 0.48051  | 0.06532  | 0.01223  |
| F...(.....   | 0.14196  | 0.03349  | 0.09006  | NNC-N...110. | 0.45372  | 0.05799  | -0.63245 | PT4-C...16.. | 0.44546  | -0.03464 | 0.11299  | c...C...(... | 0.98137  | 0.75768  | 0.89608  |
| F...(C...    | 0.3065   | 2.25163  | 0.17832  | NNC-N...211. | -0.08324 | -0.20948 | 0.3092   | PT4-C...17.. | -0.88046 | 0.07163  | 0.70414  | c...C.....   | 0.67335  | 0.45678  | -0.00096 |
| F...(F...    | -0.89602 | 0.3453   | 0.32583  | NNC-N...220. | 0.4863   | 0.67397  | 0.12037  | PT4-C...18.. | 0.49905  | -0.05299 | -0.88013 | c...C...=... | 0.04276  | 2.35824  | 0.33268  |
| F.....       | 0.23898  | 0.1689   | -0.62548 | NNC-N...303. | -0.66301 | 0.7113   | -0.93047 | PT4-C...2... | 0.43828  | -0.79704 | 0.4013   | c...C...C... | 2.32838  | 1.45428  | 2.20175  |

|                |          |          |          |               |          |          |          |               |          |          |          |               |          |          |          |
|----------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|---------------|----------|----------|----------|
| F...1.....     | 0.18059  | -0.09947 | 1.26469  | NNC-N...312.  | 0.00303  | 2.42333  | 2.01363  | PT4-C...3...  | 0.07186  | 0.36695  | 0.11755  | c...C...N...  | 0.64571  | 0.19366  | 0.28324  |
| F...c...1...   | 2.3975   | 0.3181   | 2.44006  | NNC-N...321.  | -0.55091 | 0.56123  | 0.30017  | PT4-C...4...  | -1.07338 | 0.36705  | -0.82918 | c...C...O...  | 0.1432   | 0.41401  | 0.01951  |
| EC0-C...1...   | -0.64992 | 0.23455  | 0.04459  | NNC-N...330.  | 0.2263   | 0.365    | 0.23132  | PT4-C...5...  | 0.64494  | -0.00546 | -0.18128 | c...F.....    | 0.09262  | 2.41992  | 0.48891  |
| EC0-C...2...   | 0.25453  | 2.24233  | 0.14056  | NNC-O...101.  | -0.06771 | -0.90931 | 0.26824  | PT4-C...6...  | 0.16486  | 0.06199  | -0.64571 | c...I.....    | 2.39023  | 2.38992  | 2.25328  |
| EC0-C...3...   | 0.10994  | 2.42891  | 0.33485  | NNC-O...110.  | -0.36    | -0.77724 | -0.53859 | PT4-C...7...  | 1.00108  | 3.29234  | 0.21082  | c...Cl.....   | 0.21276  | 0.74516  | 0.47065  |
| EC0-C...4...   | 0.03683  | 0.47604  | -0.04786 | NNC-O...220.  | -0.12406 | -0.80484 | 0.89074  | PT4-C...8...  | 0.35668  | -0.55889 | 0.26542  | c...N...(...  | -0.87991 | -0.90779 | -1.20753 |
| EC0-F...1...   | 0.12092  | 0.38459  | -0.06398 | NNC-s...220.  | -0.53457 | 0.03345  | 1.20298  | PT4-C...9...  | 2.08892  | 0.09678  | 1.40339  | c...N.....    | -1.51319 | 0.40076  | -1.4552  |
| EC0-Br...1...  | 1.42802  | 0.44539  | 2.11696  | NNE0C...100-  | 0.30814  | 0.50412  | -0.58323 | PT4-F...2...  | 0.01345  | 0.25397  | 1.13699  | c...N...1...  | -0.44879 | 0.09151  | 0.07878  |
| EC0-I...1...   | 2.39325  | 0.44174  | 0.57905  | NNE0C...109-  | 0.25665  | 0.1831   | -0.95115 | PT4-F...4...  | -0.42071 | 0.49197  | 0.45662  | c...N...O...  | 0.15299  | 0.09764  | -0.24708 |
| EC0-Cl...1...  | -0.22395 | 2.15566  | 1.30146  | NNE0C...200-  | -0.66979 | 0.10332  | -0.22716 | PT4-F...5...  | 0.29486  | 1.35249  | 0.4767   | c...c...(...  | 0.06308  | 0.16481  | 0.32495  |
| EC0-N...1...   | -1.40924 | -0.51262 | -0.8534  | NNE0C...209-  | 0.17516  | 0.44211  | 0.24282  | PT4-Br...2... | 0.316    | 0.45144  | 0.38029  | c...c.....    | -0.73807 | 0.00535  | 0.308    |
| EC0-N...2...   | 0.10716  | 0.21324  | -0.46325 | NNE0C...218-  | 0.08353  | 0.13001  | -0.53705 | PT4-I...2...  | 0.02033  | 1.15533  | 0.23436  | c...c...1...  | -0.70135 | 0.4353   | 0.12833  |
| EC0-N...3...   | 0.43536  | 0.21171  | 0.26626  | NNE0C...300-  | -0.92511 | -0.56625 | -0.89636 | PT4-Cl...2... | 0.61726  | 0.3909   | 0.19101  | c...c...2...  | -0.65924 | 1.564    | 1.49618  |
| EC0-O...1...   | 0.08565  | -0.96463 | -0.81615 | NNE0C...309-  | 1.63713  | 1.3667   | -0.67411 | PT4-Cl...5... | 0.32578  | 0.41683  | 2.31623  | c...c...3...  | 1.96913  | 0.37836  | 0.04142  |
| EC0-O...2...   | 0.47291  | -0.9811  | -0.18091 | NNE0C...318-  | 0.25245  | 0.39275  | 1.37414  | PT4-Cl...8... | 0.41757  | 0.09583  | 0.33538  | c...c...C...  | -0.57625 | 0.02302  | 0.23599  |
| EC0-s...2...   | 1.20321  | 2.31762  | 0.25204  | NNE0C...327-  | 1.0827   | -0.97056 | -0.73471 | PT4-N...1...  | -0.75546 | 0.20211  | 0.23466  | c...n...(...  | 0.93071  | 0.29674  | 0.72929  |
| Br...(.....    | 0.01412  | 0.24557  | 2.69694  | NNE0C...409-  | -0.45629 | -0.06778 | -0.2038  | PT4-N...10..  | -0.64376 | -0.88031 | 0.30345  | c...n...1...  | -1.10228 | -0.97684 | -0.976   |
| Br...(....2... | 0.47528  | 2.14116  | -0.88305 | NNE0C...436-  | -0.51825 | -0.19038 | -0.76562 | PT4-N...11..  | 0.09761  | 0.41666  | 0.25595  | c...n...2...  | -3.00867 | -1.98027 | -0.70973 |
| Br.....        | 0.76272  | 0.09818  | -0.48572 | NNE0F...109-  | 0.36277  | 0.14975  | 0.11822  | PT4-N...12..  | 0.28849  | -0.75546 | 0.41599  | c...n...C...  | 1.26071  | 2.42531  | 0.37279  |
| I.....         | 0.83793  | 2.38714  | 1.43187  | NNE0Br...109- | 0.56129  | 0.27823  | -0.64168 | PT4-N...13..  | 0.14618  | -1.11455 | -0.90355 | c...s...1...  | 0.43603  | 1.76015  | 2.37284  |
| I...c...1...   | 0.44162  | 2.47459  | 0.37384  | NNE0I...109-  | 0.32686  | 2.46674  | -0.83512 | PT4-N...2...  | 0.33633  | 0.37285  | -0.73514 | c...s...3...  | 2.08677  | 0.27454  | -0.6954  |
| Cl...(.....    | -0.15832 | -0.89226 | 2.48093  | NNE0Cl...100- | 0.42003  | 0.47462  | 0.63847  | PT4-N...3...  | -1.09571 | -0.99341 | -0.56259 | n...(.....    | -1.79632 | -0.52846 | 1.85439  |
| Cl...(....1... | -0.65256 | 0.45835  | 0.28015  | NNE0Cl...109- | 0.50865  | 2.48713  | 1.04315  | PT4-N...4...  | -0.05345 | -0.59466 | 0.05761  | n...(....1... | 0.05859  | -0.1985  | 0.00009  |
| Cl...(....2... | 0.49489  | -0.6384  | 0.23266  | NNE0N...109-  | -0.8033  | -0.80541 | 0.97709  | PT4-N...6...  | 3.02725  | 5.69533  | 1.0258   | n...(....C... | 0.41817  | 0.4406   | 2.08171  |
| Cl...(....C... | 1.26437  | -0.65543 | -0.02267 | NNE0N...209-  | 1.81454  | 0.36568  | -0.60771 | PT4-N...7...  | 0.43641  | 0.02905  | -0.64811 | n...(....Cl.. | 0.27847  | 2.08643  | 0.00225  |
| Cl...(....Cl.. | 0.27164  | -0.11655 | 0.32861  | NNE0N...218-  | 2.35208  | 0.3152   | 0.47244  | PT4-N...8...  | -0.46412 | 0.15206  | 0.27874  | n...(....c... | 0.37203  | 0.04434  | 0.47368  |
| Cl.....        | 0.09546  | 0.39923  | 0.55021  | NNE0N...300-  | 0.27916  | -0.37541 | 0.04238  | PT4-N...9...  | 1.04196  | 1.17096  | 1.49924  | n.....        | 0.20122  | 0.37389  | 0.29904  |
| Cl.1.....      | 1.67878  | 2.3335   | 0.37297  | NNE0N...309-  | 2.23976  | 0.57644  | 2.09794  | PT4-O...1...  | 0.25497  | 0.22438  | 1.30433  | n...1...(...  | -0.03481 | 0.39819  | 0.40288  |
| Cl.2.....      | -0.49585 | 1.6052   | -0.73154 | NNE0N...318-  | -0.69037 | 0.23094  | -0.95559 | PT4-O...2...  | -0.32249 | 0.44547  | -0.05101 | n...1.....    | 0.45606  | -0.08219 | 0.13958  |
| Cl.N...1...    | -0.70687 | -0.6722  | -0.73719 | NNE0N...327-  | 0.44779  | 0.20278  | 0.3541   | PT4-O...4...  | -0.92567 | 0.37631  | 0.07581  | n...1...c...  | 0.43602  | -0.99188 | -0.74236 |
| Cl.c...1...    | 0.12165  | 0.73953  | 1.08635  | NNE0O...100-  | -1.39582 | 0.54192  | -0.12881 | PT4-O...5...  | 0.0418   | 0.38266  | 0.41029  | n...2...(...  | 0.04454  | 2.4732   | -0.48854 |
| Cmax.2.....    | 0.14983  | 0.06211  | 1.16054  | NNE0O...109-  | -0.07268 | 0.4124   | 0.43339  | PT4-O...8...  | 0.47285  | 2.28781  | 0.48495  | n...2.....    | -0.01761 | 0.28547  | 0.32216  |
| Cmax.3.....    | 0.09222  | 2.11294  | -0.90444 | NNE0O...218-  | 2.26615  | 3.49874  | -0.74113 | PT4-O...9...  | -0.39072 | -1.53139 | -0.88127 | n...2...C...  | 0.31181  | 0.32329  | -0.08748 |
| HALO00000000   | 0.46176  | -0.22167 | 0.29119  | NNE0s...218-  | 1.17038  | 2.34931  | 0.38723  | PT4-s...10..  | 0.25939  | -0.08321 | 0.6636   | n...c...(...  | -0.18898 | 0.14391  | 1.35855  |
| HALO00100000   | -0.09801 | 0.29965  | 2.14227  | NOSP10000000  | 0.08265  | 2.26442  | 1.30107  | PT4-s...9...  | 0.28622  | 0.34739  | 0.02531  | n...c.....    | -0.33466 | 0.16211  | -0.27468 |

|              |          |          |          |               |          |          |          |              |          |          |          |              |          |          |          |
|--------------|----------|----------|----------|---------------|----------|----------|----------|--------------|----------|----------|----------|--------------|----------|----------|----------|
| HALO01000000 | -0.52411 | 0.47277  | 0.15312  | NOSP11000000  | -0.30303 | 2.00868  | 0.06713  | Nmax.1.....  | 0.48297  | -0.08085 | 0.25605  | n...c...1... | -0.424   | -0.45381 | -1.56857 |
| HALO10000000 | 0.12992  | 0.45115  | 0.64397  | S2E0C...0-..  | -0.56104 | 0.39082  | 0.18504  | Nmax.2.....  | 0.31311  | 2.47145  | 0.25796  | n...c...2... | -0.09694 | 0.30069  | 2.41095  |
| HALO10010000 | -0.09421 | 2.9342   | 2.01539  | S2E0C...1-..  | -0.17081 | -0.576   | -0.06634 | Nmax.3.....  | -0.53295 | 0.07474  | 0.0948   | n...c...C... | 0.33645  | 2.12156  | 0.74798  |
| HALO11000000 | 0.35382  | 1.26753  | -0.11673 | S2E0C...10-.  | -0.09033 | -0.64877 | 0.36635  | Nmax.4.....  | -0.90464 | -0.70357 | -0.02867 | n...c...n... | -2.2077  | -2.50781 | -1.37733 |
| N...#......  | -0.99739 | 0.20648  | 2.08389  | S2E0C...11-.  | 0.03435  | 0.20036  | 0.29038  | Omax.0.....  | 0.42096  | 2.44391  | 1.31901  | n...n...(... | 2.28307  | 2.47609  | 0.45735  |
| N...#...C... | 0.53454  | 2.49201  | -0.57888 | S2E0C...2-..  | 0.45111  | 0.39747  | 0.18809  | Omax.1.....  | 0.06414  | 2.24114  | 0.30391  | n...n.....   | 2.2705   | -0.70216 | 0.32399  |
| N...(.....   | 0.07954  | -1.31943 | -0.41829 | S2E0C...3-..  | 0.28391  | 0.6988   | -0.91616 | Omax.2.....  | -0.71391 | 0.03027  | 0.18361  | n...n...1... | 0.12037  | 2.42495  | 0.25984  |
| N...(2...    | -1.16364 | -0.06058 | 0.16118  | S2E0C...4-..  | -0.81205 | -0.67405 | -0.3228  | Omax.3.....  | 0.24872  | 2.2394   | 0.19457  | n...n...2... | 0.05592  | 2.43741  | 0.38789  |
| N...(C...    | -0.66657 | 0.43719  | 0.07967  | S2E0C...5-..  | 0.34703  | 0.02301  | 1.3756   | VS2-C...10.. | -0.12804 | 0.28136  | 0.09195  | n...n...C... | 0.05562  | 2.06322  | 0.05835  |
| N...+.....   | 1.77774  | 0.18688  | 0.26278  | S2E0C...6-..  | 0.04758  | 0.1415   | 0.42876  | VS2-C...11.. | 0.54568  | 0.08323  | 0.39957  | s...(.....   | 1.44047  | 0.23643  | 0.37259  |
| N.....       | -0.91553 | 0.4313   | -0.66125 | S2E0C...7-..  | -0.30252 | 2.00545  | 0.22129  | VS2-C...12.. | 0.18111  | 0.13446  | 0.48598  | s...(C...    | -0.84112 | 2.17644  | 0.06012  |
| N...1...(... | 0.11351  | 0.13338  | 0.1982   | S2E0C...8-..  | 0.20676  | 0.43014  | 0.02846  | VS2-C...13.. | 0.25762  | -0.49518 | -0.95557 | s.....       | 0.03576  | 0.82833  | -0.60087 |
| N...1.....   | 0.02569  | 0.0696   | 0.33531  | S2E0C...9-..  | 2.47038  | 0.09114  | 0.31897  | VS2-C...14.. | 2.31896  | -0.76238 | 0.4721   | s...1...(... | 2.43089  | 0.32161  | 0.46363  |
| N...1...C... | -0.77694 | 2.1376   | -1.1316  | S2E0F...3-..  | 0.22297  | 0.2719   | -0.87095 | VS2-C...2... | -0.64164 | -0.4946  | 0.30117  | s...1.....   | -0.85486 | 2.74597  | 2.3901   |
| N...2...(... | 2.4951   | 1.3729   | 1.23734  | S2E0F...4-..  | 0.27036  | 0.62909  | 2.21036  | VS2-C...3... | -3.5157  | -0.84638 | 0.19638  | s...1...C... | 0.12502  | -0.03432 | 1.45315  |
| N...2.....   | 2.04929  | 0.40196  | 0.4173   | S2E0Br...3-.. | 0.23976  | 0.32731  | 0.23844  | VS2-C...4... | 0.24414  | 0.22736  | 0.23913  | s...3...(... | 0.21085  | 1.119    | 0.25912  |
| N...2...C... | 0.25412  | -0.71223 | 0.70088  | S2E0I...3-..  | 1.0505   | 1.38067  | 0.07189  | VS2-C...5... | -1.20561 | -1.0335  | 0.27889  | s...3.....   | 0.16373  | -0.15173 | -0.30332 |
| N...2...Cl.. | 1.51833  | 0.06359  | 0.25235  | S2E0Cl...3-.. | 1.1806   | 0.31149  | 0.11968  | VS2-C...6... | 0.33313  | -0.02224 | 0.18883  | s...c...(... | -0.99542 | 0.25679  | 1.22492  |
| N...=...(... | 0.3576   | 0.1723   | 2.08311  | S2E0Cl...4-.. | 0.50074  | -0.04346 | -0.24136 | VS2-C...7... | 0.076    | 0.3333   | 0.25076  | s...c.....   | -0.12005 | 0.23778  | 0.21762  |
| N...=.....   | 0.4581   | 0.48439  | -0.95322 | S2E0Cl...5-.. | 0.36091  | -0.3093  | 0.14344  | VS2-C...8... | 0.15604  | 0.28555  | 2.35471  | s...c...2... | 0.18156  | 0.66354  | 2.33977  |
| N...=...1... | 0.3797   | -0.81739 | -0.66147 | S2E0N...0-..  | 0.21513  | -0.97807 | 0.24405  | VS2-C...9... | -0.99118 | 0.42312  | -0.87787 | s...c...C... | -0.46635 | 0.35848  | 2.24935  |
| N...=...2... | 0.25688  | -0.41137 | 1.46051  | S2E0N...1-..  | -0.25311 | 0.3072   | 1.19278  | VS2-F...4... | 0.2892   | 0.03547  | 2.47596  |              |          |          |          |
| N...=...C... | -0.95334 | 0.42753  | 0.33939  | S2E0N...10-.  | -0.81456 | -1.43022 | 0.15553  | VS2-F...5... | -0.20939 | 0.46458  | 0.0698   |              |          |          |          |

Table S5. Example of DCW (1,12) calculation

|  <p>SMILES notation: <chem>Clc1ccccc1C1=NCC(=O)N(c2c1cc(cc2)C(C)(C)C)[N+](=O)[O-]</chem></p> <p>DCW: 89.37593</p> <p>Ac(calc.) = 6.6177</p> |         |             |         |            |         |               |         |              |         |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|-------------|---------|------------|---------|---------------|---------|--------------|---------|
| SAk                                                                                                                                                                                                                           | CW(SAk) | SAk         | CW(SAk) | SAk        | CW(SAk) | SAk           | CW(SAk) | SAk          | CW(SAk) |
| Cl.....                                                                                                                                                                                                                       | 0.5502  | C.....      | 0.1151  | =...(...   | 0.023   | [...O.....    | 0.2433  | (...C...(    | 0.3123  |
| c.....                                                                                                                                                                                                                        | -0.0154 | (.....      | -0.8488 | O...=..... | 0.2541  | O...-.....    | 1.2116  | C...(...C... | -0.4531 |
| 1.....                                                                                                                                                                                                                        | 0.4986  | (.....      | -0.8488 | O...(..... | -0.6723 | [...-.....    | 0.1744  | (...C...(    | 0.3123  |
| c.....                                                                                                                                                                                                                        | -0.0154 | C.....      | 0.1151  | N...(..... | -0.4183 | Cl...C...1... | 1.0863  | C...(...(    | 0.2397  |
| c.....                                                                                                                                                                                                                        | -0.0154 | (.....      | -0.8488 | N...(..... | -0.4183 | c...1...c...  | -0.2637 | C...(...(    | 0.2397  |
| c.....                                                                                                                                                                                                                        | -0.0154 | C.....      | 0.1151  | c...(..... | 0.4968  | c...c...1...  | 0.1283  | (...C...(    | 0.3123  |
| c.....                                                                                                                                                                                                                        | -0.0154 | (.....      | -0.8488 | c...2..... | 0.1574  | c...c...c...  | 0.236   | C...(...C... | -0.4531 |
| c.....                                                                                                                                                                                                                        | -0.0154 | [.....      | -0.1979 | c...2..... | 0.1574  | c...c...c...  | 0.236   | (...C...(    | 0.3123  |
| 1.....                                                                                                                                                                                                                        | 0.4986  | N.....      | -0.6612 | c...1..... | 0.1149  | c...c...c...  | 0.236   | [...(...C... | -0.9922 |
| C.....                                                                                                                                                                                                                        | 0.1151  | +.....      | 2.0579  | c...1..... | 0.1149  | c...c...1...  | 0.1283  | N...[...(... | 1.1709  |
| 1.....                                                                                                                                                                                                                        | 0.4986  | [.....      | -0.1979 | c...c..... | 0.308   | c...1...C...  | 1.3072  | [...N...+... | 2.325   |
| =.....                                                                                                                                                                                                                        | 0.2852  | (.....      | -0.8488 | c...(..... | 0.4968  | 1...C...1...  | -0.6249 | [...+...N... | 0.0773  |
| N.....                                                                                                                                                                                                                        | -0.6612 | =.....      | 0.2852  | c...(..... | 0.4968  | C...1...=...  | 0.0724  | +...[...(... | 2.3078  |
| C.....                                                                                                                                                                                                                        | 0.1151  | O.....      | 0.226   | c...c..... | 0.308   | N...=...1...  | -0.6615 | [...(...=... | -0.5025 |
| C.....                                                                                                                                                                                                                        | 0.1151  | (.....      | -0.8488 | c...2..... | 0.1574  | C...N...=...  | 1.0181  | O...=...(... | 0.311   |
| (.....                                                                                                                                                                                                                        | -0.8488 | [.....      | -0.1979 | 2...(..... | 0.9784  | N...C...C...  | 1.9909  | =...O...(... | 0.3067  |
| =.....                                                                                                                                                                                                                        | 0.2852  | O.....      | 0.226   | C...(..... | 0.3995  | C...C...(...  | -0.1399 | [...(...O... | 0.1687  |
| O.....                                                                                                                                                                                                                        | 0.226   | -.....      | 2.313   | C...(...   | 0.3995  | C...(...=...  | 0.3811  | O...[...(... | -1.5535 |
| (.....                                                                                                                                                                                                                        | -0.8488 | [.....      | -0.1979 | C...(...   | 0.3995  | O...=...(...  | 0.311   | [...O...-... | -0.8653 |
| N.....                                                                                                                                                                                                                        | -0.6612 | c...Cl..... | 0.4706  | C...(...   | 0.3995  | =...O...(...  | 0.3067  | [...-...O... | 0.2791  |
| (.....                                                                                                                                                                                                                        | -0.8488 | c...1.....  | 0.1149  | (...(...   | 0.2703  | O...(...N...  | 0.2076  | Cmax.2.....  | 1.1605  |
| c.....                                                                                                                                                                                                                        | -0.0154 | c...1.....  | 0.1149  | C...(...   | 0.3995  | (...N...(...  | 0.1327  | Nmax.3.....  | 0.0948  |
| 2.....                                                                                                                                                                                                                        | 0.2021  | c...c.....  | 0.308   | C...(...   | 0.3995  | c...(...N...  | 0.2941  | Omax.3.....  | 0.1946  |
| c.....                                                                                                                                                                                                                        | -0.0154 | c...c.....  | 0.308   | C...(...   | 0.3995  | 2...c...(...  | 0.3061  | Smax.0.....  | 9.5105  |

|        |         |            |         |            |         |               |         |              |         |
|--------|---------|------------|---------|------------|---------|---------------|---------|--------------|---------|
| 1..... | 0.4986  | c...c..... | 0.308   | C...(..... | 0.3995  | c...2...c...  | 0.0486  | NOSP11000000 | 0.0671  |
| c..... | -0.0154 | c...c..... | 0.308   | [...(..... | 0.1496  | 2...c...1...  | -0.1085 | HALO01000000 | 0.1531  |
| c..... | -0.0154 | c...1..... | 0.1149  | [...N..... | 0.4801  | c...1...c...  | -0.2637 | BOND10000000 | -0.4086 |
| (..... | -0.8488 | C...1..... | 0.1868  | N...+..... | 0.2628  | c...c...1...  | 0.1283  | ++++CL--N=== | -0.2412 |
| c..... | -0.0154 | C...1..... | 0.1868  | [...+..... | 0.222   | c...c...(...  | 0.325   | ++++CL--O=== | 0.3493  |
| c..... | -0.0154 | =...1..... | 0.2273  | [...(..... | 0.1496  | c...(c...c... | 0.1241  | ++++N---O=== | -1.6207 |
| 2..... | 0.2021  | N...=..... | -0.9532 | =...(..... | 0.023   | c...c...(...  | 0.325   | ++++Cl--B2== | 0.0905  |
| (..... | -0.8488 | N...C..... | -1.8432 | O...=..... | 0.2541  | c...c...2...  | 1.4962  | ++++O---B2== | 0.0383  |
| C..... | 0.1151  | C...C..... | 0.4014  | O...(..... | -0.6723 | c...2...(...  | 0.5656  | ++++N---B2== | 6.5809  |
| (..... | -0.8488 | C...(..... | 0.3995  | [...(..... | 0.1496  | C...(c...2... | 2.4939  | 10011000100  | 0.2201  |

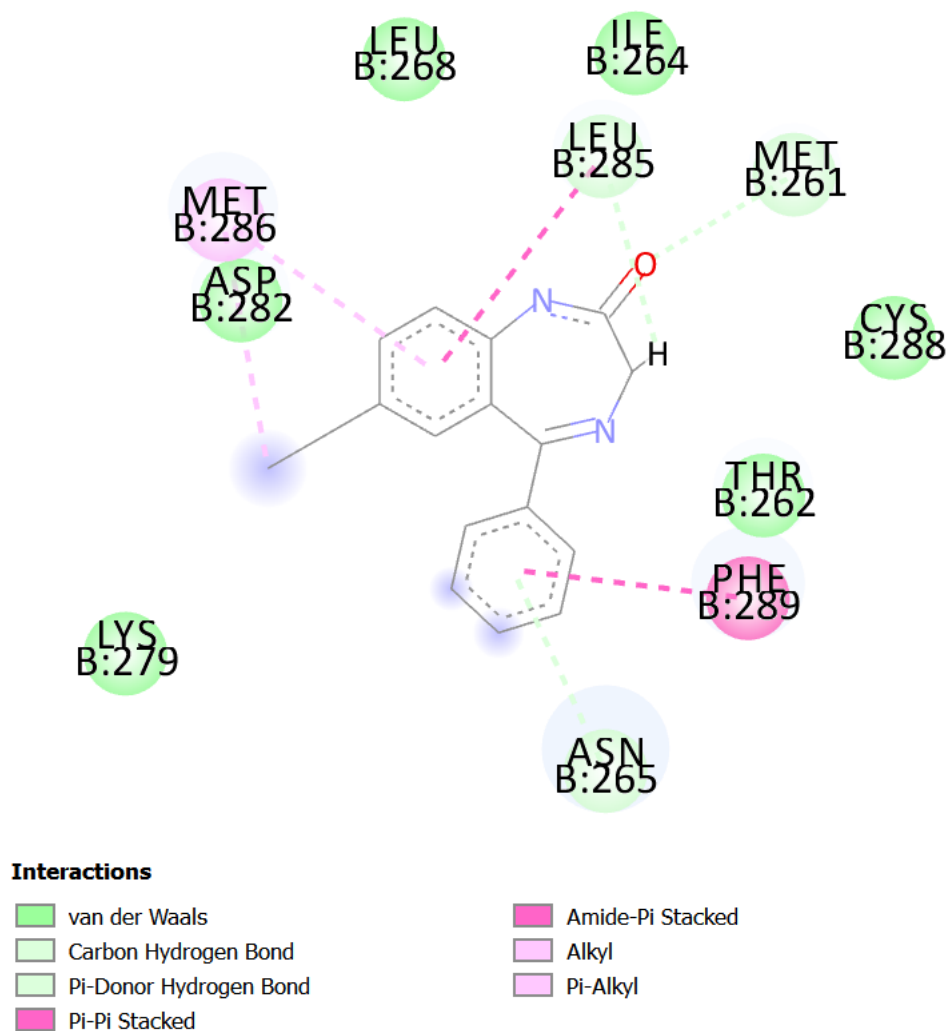
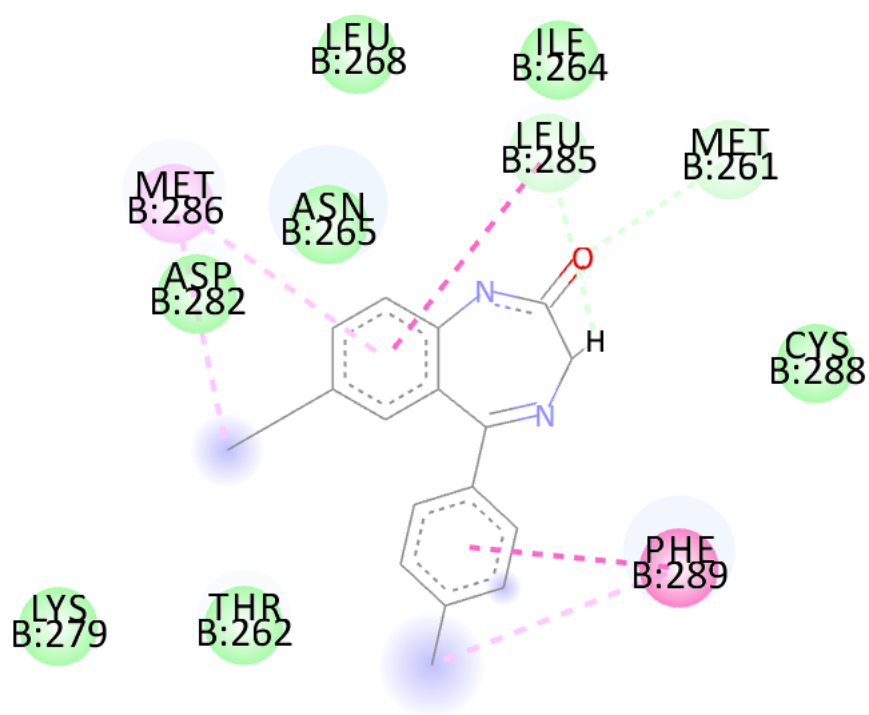


Figure S1. Two-dimensional representation of the interaction between molecule A and amino acids inside GABA<sub>A</sub>.



#### Interactions

|                      |                  |
|----------------------|------------------|
| van der Waals        | Amide-Pi Stacked |
| Carbon Hydrogen Bond | Alkyl            |
| Pi-Pi Stacked        | Pi-Alkyl         |

Figure S2. Two-dimensional representation of the interaction between molecule A1 and amino acids inside GABA<sub>A</sub>.



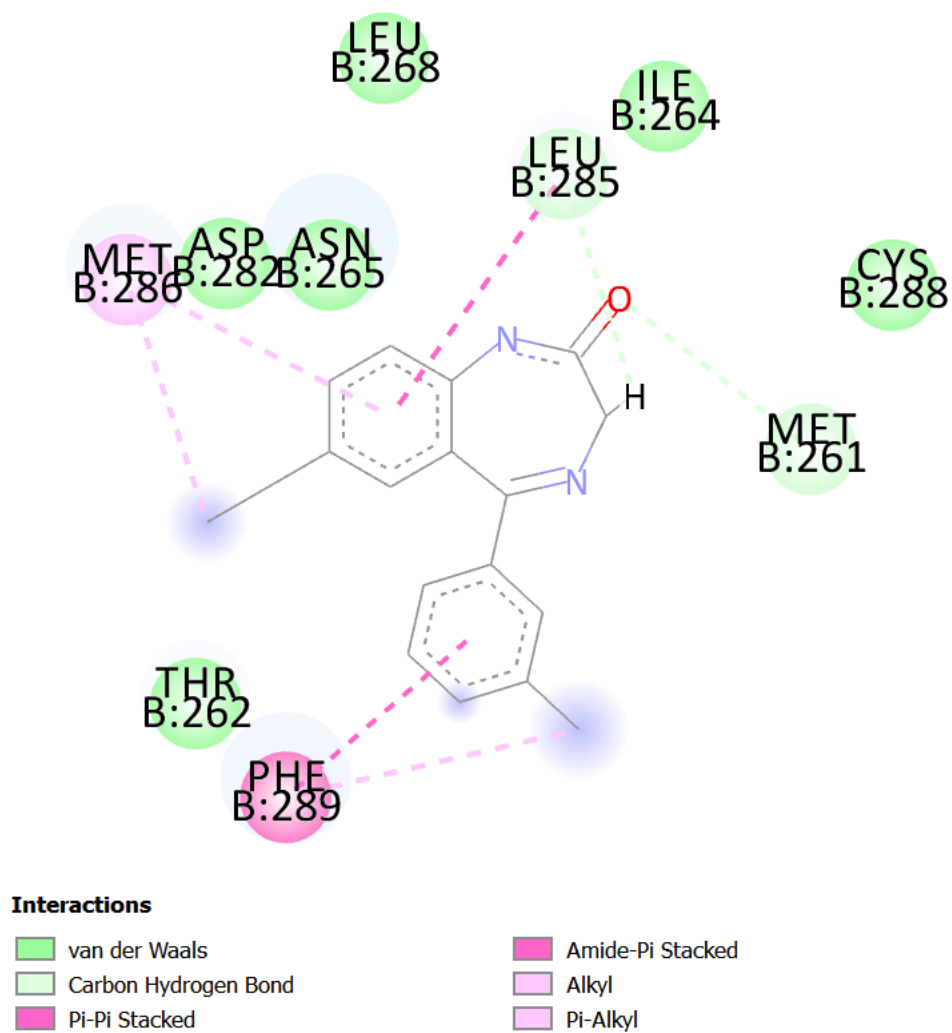


Figure S3. Two-dimensional representation of the interaction between molecule A2 and amino acids inside GABA<sub>A</sub>.

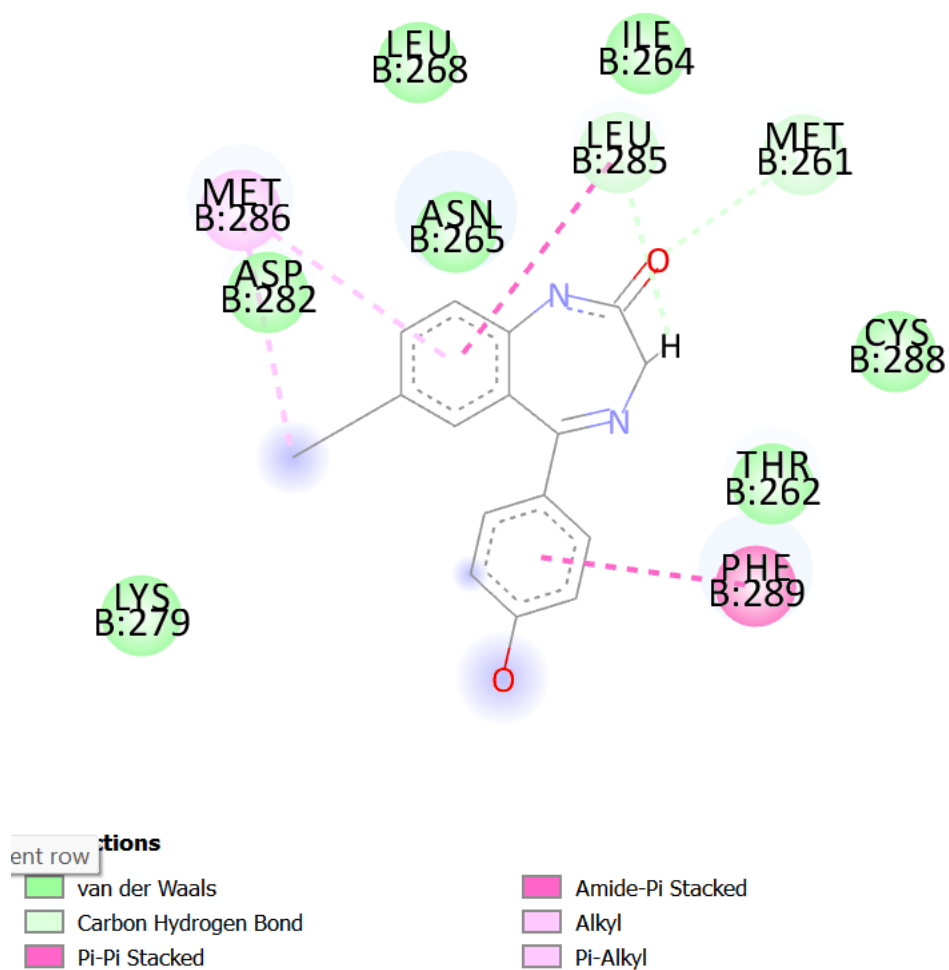


Figure S4. Two-dimensional representation of the interaction between molecule A3 and amino acids inside GABA<sub>A</sub>.

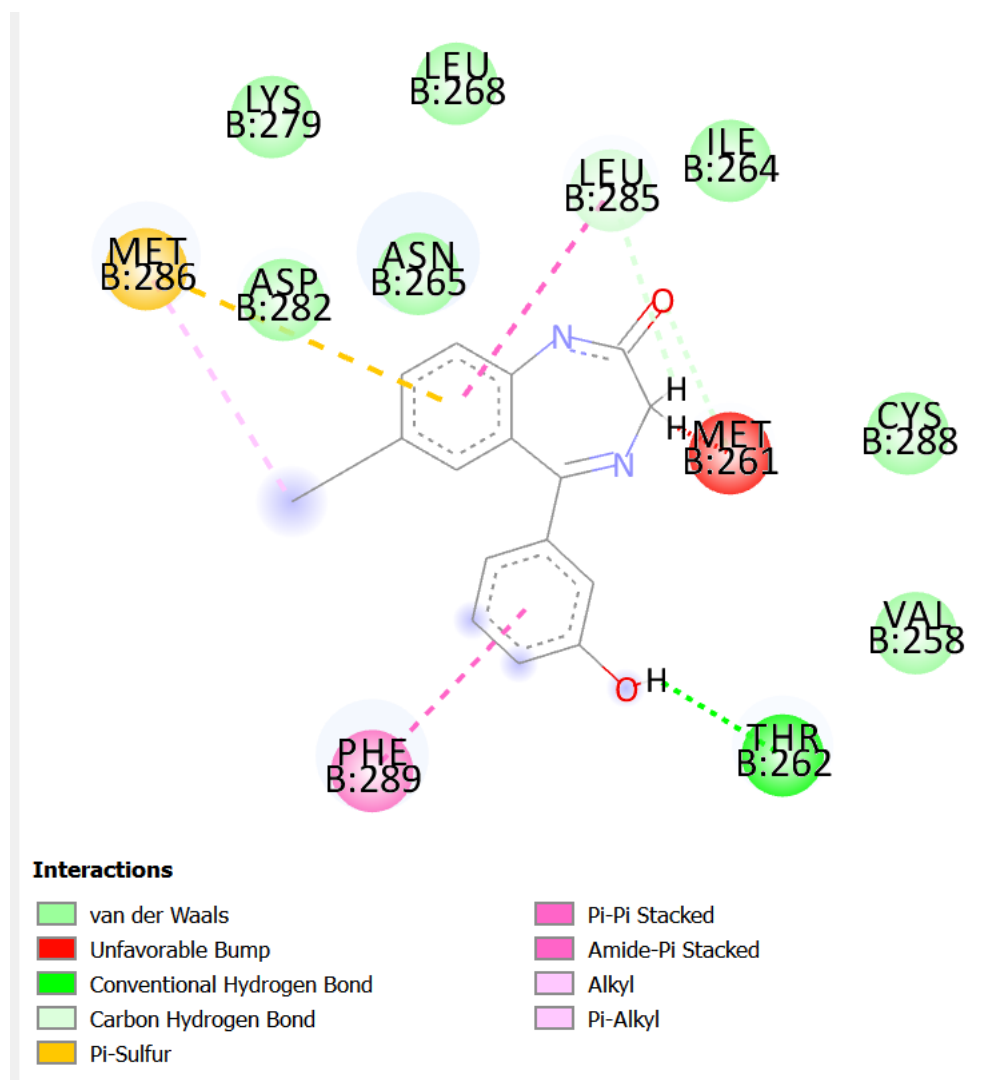
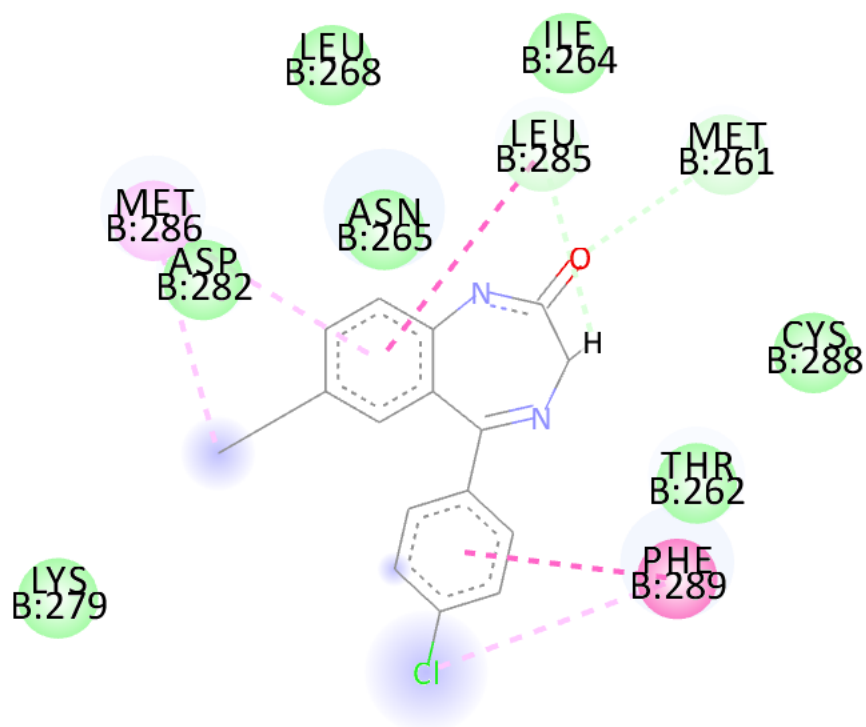


Figure S5. Two-dimensional representation of the interaction between molecule A4 and amino acids inside GABA<sub>A</sub>.



#### Interactions

|                                                                |                                                         |
|----------------------------------------------------------------|---------------------------------------------------------|
| <span style="color: green;">—</span> van der Waals             | <span style="color: magenta;">—</span> Amide-Pi Stacked |
| <span style="color: lightgreen;">—</span> Carbon Hydrogen Bond | <span style="color: pink;">—</span> Alkyl               |
| <span style="color: pink;">—</span> Pi-Pi Stacked              | <span style="color: lightpink;">—</span> Pi-Alkyl       |

Figure S6. Two-dimensional representation of the interaction between molecule A5 and amino acids inside GABA<sub>A</sub>.

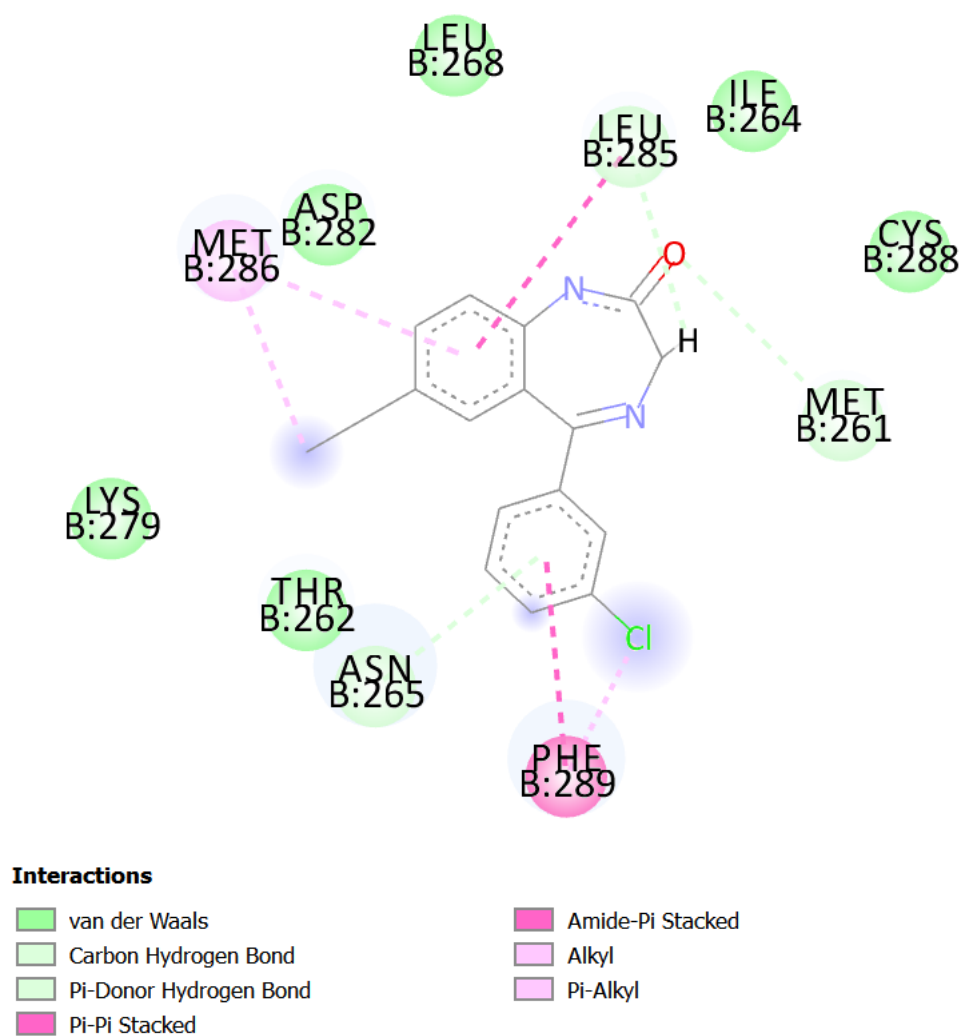


Figure S7. Two-dimensional representation of the interaction between molecule A6 and amino acids inside GABA<sub>A</sub>.