| DATE        | FORMULA | MOLECULAR WEIGHT | SLIDE | MOLECULAR SHAPE | NAME                                                                 | CHARGED(validate) | DB | DATA | META | GROUP | STACK | NAME | CONTACTS |
|------------|---------|------------------|-------|-----------------|----------------------------------------------------------------------|------------------|----|------|------|-------|-------|------|-----------|
| 2019-01-01 | C21H22F5N3O3S | 547.659           |       | 1 9 10 11       | (3Z)-6-(4-HYDROXY-3-METHOXYPHENYL)-3-(1H-PYRROL-2-YLMETHYLENE)-1,3-DIHYDRO-2H-INDOL-2-ONE | -11.85           | 36 | -6.603 | 66   | 1     |       |       |           |
| 2019-01-02 | C18H12Cl2N2O3  | 344.360           |       | 1 8 9 10 11     | C18H12Cl2O4                                                         | -11.9          | 33 | -5.683 | 55   | 1     |       |       |           |
| 2019-01-03 | C26H20ClFN2O2  | 418.358           |       | 1 8 9 10 11     | C26H20ClFN2O2                                                       | -12.02         | 35 | -7.487 | 71   | 1     |       |       |           |
| 2019-01-04 | C18H14N4O3S2   | 390.421           |       | 1 8 9 10 11     | C18H14N4O3S2                                                       | -12.09         | 37 | -7.412 | 75   | 1     |       |       |           |
| 2019-01-05 | C27H28F3N7O3   | 628.563           |       | 1 8 9 10 11     | C27H28F3N7O3                                                       | -12.17         | 40 | -8.782 | 87   | 1     |       |       |           |
| 2019-01-06 | C22H27FN4O2    | 420.476           |       | 1 8 9 10 11     | C22H27FN4O2                                                       | -12.18         | 41 | -8.312 | 83   | 1     |       |       |           |
| ChemID   | Common Name                      | CAS Number | MW (g/mol) | Tp (°C) | Kp (atm) | pKa | pKb | Ref. |
|----------|----------------------------------|------------|------------|----------|----------|-----|-----|------|
| DB15247  | Vorolanib                        | 439.491    |            | -11.83   | -7.156   | 2   | 63  |      |
| DB02466  | BMS-181156                       | 362.4614   |            | -11.81   | -8.19    | 2   | 58  |      |
| DB05197  | Sofalcone                        | 450.5235   |            | -11.80   | -9.211   | 4   | 89  |      |
| DB05943  | Resatorvid                       | 361.81     |            | -11.79   | -5.836   | 0   | 48  |      |
| DB06412  | Oxymetholone                     | 332.484    |            | -11.78   | -6.649   | 1   | 35  |      |
| DB08407  | Platensimycin                    | 441.4737   |            | -11.74   | -8.199   | 5   | 75  |      |
| DB07156  | (4Z)-6-bromo-4-({[4-(pyrrolidin-1-ylmethyl)phenyl]amino}methylidene)isoquinoline-1,3(2H,4H)-dione | 426.306   |            | -11.74   | -8.518   | 1   | 63  |      |
| DB07615  | Tranilast                        | 327.3313   |            | -11.68   | -7.194   | 2   | 49  |      |
| Compound                                                                 | Experimental | Approved |
|-------------------------------------------------------------------------|--------------|----------|
| (3Z)-N,N-DIMETHYL-2-OXO-3-(4,5,6,7-TETRAHYDRO-1H-INDOL-2-YLMETHYLIDENE)-2,3-DIHYDRO-1H-INDOLE-5-SULFONAMIDE | experimental | approved |
| (4Z)-2-[(1R,2R)-1-Amino-2-hydroxypropyl]-4-[(4-amino-1H-indol-3-yl)methylene]-5-oxo-4,5-dihydro-1H-imidazol-1-yl}acetic acid | experimental | approved |
| 5-(4'-AMINO-1'-ETHYL-5',8'-DIFLUORO-1'H-SPIRO[PIPERIDINE-4,2'-QUINAZOLINE]-1-YLCARBONYL)PICOLINONITRILE | experimental | approved |
| 1-METHYL ETHYL 1-CHLORO-5-[(5,6DIHYDRO-2-METHYL-1,4-OXATHIIN-3-YL)CARBONYL]AMINO]BENZOATE | experimental | approved |
| (2Z)-2-(Benzoylamino)-3-[4-(2-bromophenoxy)phenyl]acrylic acid | experimental | approved |
| (3E)-2,6-DIOXO-6-PHENYLHEX-3-ENOATE | experimental | approved |
| VTP-194204 | experimental | approved |
| Enzacamene | experimental | approved |
| Alitretinoin | experimental | approved |
| Orantinib | experimental | approved |
| Amiloxate | experimental | approved |
| Ozagrel | experimental | approved |
| DB     | Compound                          | molecular formula | formula weight | Experimental | Approval | 1 | 2 |
|-------|-----------------------------------|-------------------|----------------|--------------|----------|---|---|
| DB08186 | C13H13NO                            |                 | 199.2484       | -9.46        | -7.328   | 26 |
| DB04769 | C12H7N3O2S                          |                 | 257.268        | -9.45        | -6.747   | 26 |
| DB13504 | C14H15N5O5S2                       |                 | 397.42         | -9.38        | -5.846   | 24 |
| DB02816 | C10H10N4O3S                        |                 | 266.276        | -9.33        | -6.031   | 28 |
| DB15201 | C24H28O4                           |                 | 380.484        | -9.33        | -7.46    | 26 |
| DB01332 | C13H13N5O5S2                       |                 | 383.403        | -9.32        | -6.412   | 26 |
| DB03428 | C13H11N3O2                         |                 | 241.2453       | -9.31        | -5.536   | 26 |
| DB07516 | C12H9ClO4                          |                 | 252.65         | -9.29        | -5.798   | 46 |
| DB04657 | C12H13NO2S                         |                 | 235.302        | -9.28        | -6.181   | 59 |
| DB04347 | C7H8O5                            |                 | 172.1354       | -9.25        | -6.179   | 24 |
| DB03991 | C11H17NO8                          |                 | 291.2546       | -9.25        | -6.321   | 26 |
| DB07960 | C12H19NO6                          |                 | 273.2824       | -9.23        | -6.25    | 24 |
| DB07503 | C11H5F2NO4S                        |                 | 285.224        | -9.19        | -4.93    | 23 |
| DB03321 | C11H18N2O7                         |                 | 290.2698       | -9.09        | -6.255   | 18 |
| DB08587 | C11H12O5                          |                 | 224.21         | -9.09        | -5.871   | 21 |
| DB03981 | C6H8O9S                           |                 | 256.187        | -9.06        | -6.357   | 17 |
| DB14184 | C9H8O                             |                 | 132.1592       | -9.05        | -6.323   | 32 |
| DB07788 | C19H22O7                           |                 | 362.3738       | -9.02        | -5.879   | 35 |