| Var ID (Primary)                                                                 | M1.VIP [3+2+0] | M1.VIP[3]c | vSE     |
|--------------------------------------------------------------------------------|----------------|-----------|---------|
| lividomycin B                                                                   | 2.7601         | 0.796074  |         |
| synechoxanthin                                                                  | 2.7506         | 0.793319  |         |
| dihydrostreptomycin                                                             | 2.7497         | 0.79299   |         |
| 3-hydroxy-4-methyl-anthranilate pentapeptide lactone                            | 2.7486         | 0.793067  |         |
| atabrine                                                                        | 2.7477         | 0.792083  |         |
| 6''-deamino-6''-hydroxyneomycin C                                               | 2.7419         | 0.789537  |         |
| paromomycin                                                                     | 2.7419         | 0.789537  |         |
| 5-iO/i-&beta\-mycaminosyltylonolide                                            | 2.7419         | 0.789537  |         |
| sucrose-3-decanoyl-4-isoveleroyl-3''-isovalerate                                | 2.7388         | 0.789042  |         |
| simvastatin lactone                                                             | 2.737          | 0.789716  |         |
| desferrioxamine E                                                               | 2.7366         | 0.789895  |         |
| 15-oxo spinosyn macrolactone                                                    | 2.735          | 0.785635  |         |
| huvastatin lactone                                                              | 2.735          | 0.785635  |         |
| sucrose-3-(2-methyl)butyryl-4-isovaleroyl-3''-laurate                           | 2.7339         | 0.791532  |         |
| sucrose-3-lauroyl-4-isovaleroyl-3''-isovalerate                                  | 2.7339         | 0.791532  |         |
| sucrose-3-lauroyl-4-isovaleroyl-3''-(2-methyl)butyrate                          | 2.7339         | 0.791532  |         |
| iCypridina/i oxyluciferin                                                        | 2.7295         | 0.785231  |         |
| phytosphingosine 1-phosphate                                                    | 2.7295         | 0.785269  |         |
| prefusarin (open ring form)                                                     | 2.7295         | 0.784695  |         |
| carbonolide                                                                      | 2.7084         | 0.775984  |         |
| 2-palmitoyl-trehalose                                                            | 2.5357         | 0.791206  |         |
| terfenadine                                                                      | 2.521          | 0.742374  |         |
| apicidin D2                                                                      | 2.5134         | 0.755217  |         |
| (25*3R*4S)-4-hydroxy-L-isoleucine                                               | 2.4928         | 0.680832  |         |
| azaguanine                                                                       | 2.4928         | 0.680832  |         |
| &beta\-guinidooxypropionamide                                                  | 2.4928         | 0.680832  |         |
| 5-hydroxy-leucine                                                                | 2.4928         | 0.680832  |         |
| 4-hydroxy-L-leucine                                                              | 2.4928         | 0.680832  |         |
| sucrose 2-isovaleroyl-3-isodecanoyl-4-isobutanoate                              | 2.461          | 0.770946  |         |
| sucrose 3-lauroyl-4-isovaleroyl-3''-acetate                                      | 2.461          | 0.770946  |         |
| fusidate                                                                         | 2.428          | 0.75157   |         |
| 2-stearoyl-trehalose                                                             | 2.4246         | 0.722575  |         |
| &alpha\-paxitriol                                                                | 2.4244         | 0.67134   |         |
| &beta\-paxitriol                                                                 | 2.4244         | 0.67134   |         |
| digitoxigenin 3-O-&beta\-D-quinovoside                                           | 2.4145         | 0.81876   |         |
| digiproside                                                                      | 2.4145         | 0.81876   |         |
| terpendole C                                                                     | 2.4115         | 0.81786   |         |
| sucrose 3-lauroyl-3''-isovalerate                                               | 2.4013         | 0.718028  |         |
| sucrose-3-lauroyl-4-isovaleroyl                                                  | 2.4013         | 0.718028  |         |
| 2''-3''4''-iO/i-methyl-rhamnosyl tetracyclic spinosyn                            | 2.4003         | 0.716858  |         |
| 20-hydroxy-5-iO/i-mycaminosyltylactone                                          | 2.3988         | 0.716238  |         |
| &beta\-aflatrem                                                                   | 2.3785         | 0.806443  |         |
| aflatrem                                                                         | 2.3785         | 0.806443  |         |
| guadinomine B                                                                    | 2.3784         | 0.806418  |         |
| westiellamide                                                                    | 2.3706         | 0.751907  |         |
| 2''-iO/i-methyl-rhamnosyl tetracyclic spinosyn                                   | 2.3663         | 0.749702  |         |
| 1-(&alpha\-linolenoyl)-isn/i-glycero-3-phosphoethanolamine                    | 2.3543         | 0.743396  |         |
| Substance                                           | Value 1  | Value 2     |
|-----------------------------------------------------|----------|-------------|
| methymycin                                           | 2,3543   | 0,743395    |
| neomethymycin                                        | 2,3543   | 0,743395    |
| ethyl-2-methylacetoacetate                          | 2,306    | 0,621887    |
| pentachlorophenol                                    | 2,2491   | 0,761667    |
| 13-desoxypaxilline                                   | 2,1191   | 0,587208    |
| 1-acyl-sn-glycero-3-phosphoglycerol (n-C16:0)         | 2,0915   | 2,52297     |
| 2-16:0-lysophosphatidylglycerol                      | 2,0915   | 2,52297     |
| 7*8-diketopelargonate                                | 2,0495   | 0,497965    |
| 6-isobutyl-4-hydroxy-2-pyrene                        | 2,0495   | 0,497965    |
| veratral alcohol radical                             | 2,0495   | 0,497965    |
| 3-[(1S/i)-cyclohex-3-en-1-yl]-2-oxopropanoate        | 2,0495   | 0,497965    |
| ubiquinol-0                                          | 2,0481   | 0,49722     |
| veratraldehyde                                       | 2,0481   | 0,49722     |
| 3-methylcinaldehyde                                  | 2,0481   | 0,49722     |
| 3-methoxy-4-hydroxyphenylglycol                      | 2,0481   | 0,49722     |
| L-mycarose                                           | 2,0481   | 0,49722     |
| 1-(2*4-dihydroxy-3-methylphenyl)ethanone             | 2,0481   | 0,49722     |
| (IR/i)-1*3-diphenyl-pentane-1*4-dione                | 2,0155   | 1,6497      |
| (7R)-itrans/i-hinokiresinol                          | 2,0155   | 1,6497      |
| (7S)-itrans/i-hinokiresinol                          | 2,0155   | 1,6497      |
| L-alanyl-D-glutamate                                 | 1,954    | 1,49227     |
| &gamma\-L-glutamyl-D-alanine                        | 1,954    | 1,49227     |
| 20-dihydrorosaminic                                  | 1,9259   | 0,551681    |
| (3R)-3-hydroxy-16-methoxy-2*3-dihydrotabersonine    | 1,9171   | 1,57089     |
| deacetyl vindorosine                                | 1,9171   | 1,57089     |
| sphinganine 1-phosphate                              | 1,9154   | 1,57001     |
| 16-methoxytabersonine                               | 1,9148   | 1,56856     |
| 11-dehydro-15-oxo spinosyn macro lactone            | 1,9133   | 1,56605     |
| spinosyn tricyclic macro lactone                    | 1,9133   | 1,56605     |
| 12-\&alpha\-hydroxy-3 ooxochola-4*6-dienoate        | 1,9128   | 1,5624      |
| 7-\&alpha\*12-\&alpha\-dihydroxy-3-oxochol-4-enoate | 1,9128   | 1,5624      |
| 3 &beta\-hydroxy-7*12-diketocholanate               | 1,9128   | 1,5624      |
| 10&beta\*14&beta\-dihydroxytaxa-4(20)*11-dien-5&alpha\-1-oleoyl-isn/i-glycero-3-phospho-(1\-isn/i-glycerol) | 1,888   | 1,52892     |
| xylostasin                                          | 1,884    | 0,562143    |
| (behenoyl)adenylate                                 | 1,864    | 0,533323    |
| furostanol-26-alcohol                                | 1,858    | 0,707223    |
| 2*22-dideoxyecdysone                                | 1,858    | 0,707223    |
| calcitetrol                                         | 1,858    | 0,707223    |
| glycolithocholate                                    | 1,858    | 0,707223    |
| (25iR/i)-3&alpha\*7&alpha\*12&alpha\-trihydroxy-5&beta\-4*4'-diaponeurosporenoate | 1,8574   | 0,707409     |
| 7'-O-demethylcephaeline                              | 1,8573   | 0,707772    |
| solasodine                                          | 1,8572   | 0,708391    |
| piericidin A                                         | 1,8569   | 0,707224    |
| &beta\-tocotrienol                                  | 1,8569   | 0,707224    |
| &gamma\-tocotrienol                                 | 1,8569   | 0,707224    |
| 2*3-dimethyl-6-geranylgeranyl-1*4-benzoquinol        | 1,8569   | 0,707224    |
| 4*4'-diapoly copene-4-al                            | 1,8563   | 0,706824    |
| 3*7*12-trihydroxy coprostanate                      | 1,8552   | 0,708082    |
| Compound                                                   | LogP  | S  |
|------------------------------------------------------------|-------|----|
| Lyngbyatoxin C                                            | 1.855 | 0.706854 |
| Huvastatin acid                                            | 1.855 | 0.706849 |
| (i22R*23R/i)-28-homocastasterone                          | 1.854 | 0.707062 |
| Lavendomycin                                               | 1.851 | 0.538731 |
| 3-[(3Z*6Z*9Z*12Z)-pentadeca-3*6*9*12-tetraen-1-yl]-4-    | 1.851 | 0.707446 |
| [(2Z*5Z*8Z*11Z)-tetradeca-2*5*8*11-tetraen-1-yl]oxetan-2-| 1.850 | 0.707101 |
| Oleanolic aldehyde                                         | 1.850 | 0.707101 |
| (4Z*8Z*12Z*16Z*20Z)-4*8*12*16*20-pentamethyl-24-11-oxocucurbitadienol | 1.850 | 0.707101 |
| 4&alpha;\-formyl*4&beta;\-14&alpha;\-dimethyl-9&beta;\-19-cyclo-5&alpha;\-cholest-24-en-3&beta;\-ol    | 1.850 | 0.707101 |