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@attribute 2DACorr_Ident_7 numeric
@attribute 2DACorr_Ident_8 numeric
@attribute 2DACorr_Ident_9 numeric
@attribute 2DACorr_LpEN_1 numeric
@attribute 2DACorr_LpEN_10 numeric
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@attribute 2DACorr_LpEN_7 numeric
@attribute 2DACorr_LpEN_8 numeric
@attribute 2DACorr_LpEN_9 numeric
@attribute 2DACorr_PiChg_1 numeric
@attribute 2DACorr_PiChg_10 numeric
@attribute 2DACorr_PiChg_11 numeric
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@attribute 2DACorr_Polariz_2 numeric
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@attribute 3DACorr_Ident_99 numeric
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@attribute ASPH numeric
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@attribute Aliphatic_bond_count numeric
@attribute Aliphatic_ring_count numeric
@attribute Aromatic_atom_count numeric
@attribute Aromatic_bond_count numeric
@attribute Aromatic_ring_count numeric
@attribute Asymmetric_atom_count numeric
@attribute Atom_count numeric
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@attribute Bond_count numeric
@attribute Carbo_ring_count numeric
@attribute Carboaromatic_ring_count numeric
@attribute Chain_atom_count numeric
@attribute Chain_bond_count numeric
@attribute Chi0 numeric
@attribute Chi1 numeric
@attribute Cyclomatic_number numeric
@attribute Diameter numeric
@attribute Dipole numeric
@attribute ECC numeric
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@attribute E_ALIPHATIC_AMINE_COUNT numeric
@attribute E_AROMATIC_AMINE_COUNT numeric
@attribute E_BASIC_NITROGEN_COUNT numeric
@attribute E_GUANIDINE_COUNT numeric
@attribute E_PRIMARY_ALIPHATIC_AMINE_COUNT numeric
@attribute E_PRIMARY_SECONDARY_ALIPHATIC_AMINE_COUNT numeric
@attribute E_SECONDARY_ALIPHATIC_AMINE_COUNT numeric
@attribute E_SULFONAMIDE_CO_COUNT numeric
@attribute E_TERTIARY_ALIPHATIC_AMINE_COUNT numeric
@attribute E_TPSA numeric
@attribute Fused_aliphatic_ring_count numeric
@attribute HAcc numeric
@attribute HDon numeric
@attribute Harary_index numeric
@attribute Hetero_ring_count numeric
@attribute Heteroaromatic_ring_count numeric
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@attribute IYY numeric
@attribute IZZ numeric
@attribute Kappa1 numeric
@attribute Kappa2 numeric
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@attribute Maxdist2 numeric
@attribute Maxdist3 numeric
@attribute PSA numeric
@attribute Polariz numeric
@attribute RGYR numeric
@attribute Radius numeric
@attribute Randic numeric
@attribute Randic_index numeric
@attribute Refractivity numeric
@attribute Ring_atom_count numeric
@attribute Ring_bond_count numeric
@attribute Rotatable_bond_count numeric
@attribute SPAN numeric
@attribute Shape numeric
@attribute Smallest_ring_size numeric
@attribute Szeged_index numeric
@attribute TPSA numeric
@attribute Weight numeric
@attribute Wiener numeric
@attribute Wiener_index numeric
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@attribute acceptorcount numeric
@attribute accsitecount numeric
@attribute apKa1 numeric
@attribute bpKa1 numeric
@attribute count numeric
@attribute donorcount numeric
@attribute donsitecount numeric
@attribute logP numeric
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@attribute pH=3.00 numeric
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@attribute pH=6.00 numeric
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0525,-0.000764,-0.000179,-0.003496,-
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1982,1982,38,5,8,3.18,5.49,21,2,2,-0.67,39.42,-0.67,-1.58,-0.67,-0.67,-0.68,-
0.77,-1.15,-1.5,-1.57,-1.58,CYP3A
49,53,30,52,102,161,199,213,169,112,75,27.5495,0,13.646,0,0,0,0,0,0,0,0,0.01967,
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0.000813,0.000138,-
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148.36,4601.37,2875.48,0.387821,-0.136426,0.157122,-0.207833,0.007282,0.114336,-
0.116582,-
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08,-10,6,1,1,3.69,35.61,3.69,3.69,3.69,3.69,3.69,3.69,3.69,3.69,3.69,3.69,CYP3A
61,113,105,63,112,153,156,141,124,119,114,331.703,40.6739,59.7803,161.856,95.980
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27,2.8,2.39,2.3,2.29,2.29,CYP3A
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47.5,14416.7,13458.2,11790.7,10615.9,1.26448,0.176512,-0.388789,-
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1.01,CYP3A
51,58,31,54,108,172,212,236,190,121,83,27.3153,0,13.5111,0,0,0,0,0,0,0,0,0.01949
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41,205.017,279.594,264.902,3040.37,3810.52,3317.92,4029.55,6921.54,8673.79,9010.
39,8220.34,6860.3,5919.46,4580.54,0.605983,0.316135,-0.137692,-
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3930.74,4424.44,18.3673,7.55265,5.7363,6,5.44009,3.56672,51.37,40.918,3.80248,6.
72684,12.1177,22.38,101.81,16,19,3,6.45642,0.779135,5,2587,51.37,338.447,1442,14
42,45,2,3,11.62,7.07,4,2,2,2.47,39.82,-1.51,2.46,-1.35,-1.17,-
0.54,0.4,1.36,2.13,2.42,2.46,CYP3A
67,166,133,71,135,193,245,275,261,246,212,40.4376,12.6953,13.2064,0,0,0,0,0,0,0,
0,0.031855,0.007996,0.002437,-0.00951,0.004404,-0.007144,-0.005163,-0.001793,-
0.002981,0.007885,-
0.002416,515.446,299.175,208.54,418.829,420.37,366.949,262.15,343.116,425.297,47
0.796,410.959,4044.07,6749.26,4908.05,5502.37,9995.13,13835.9,15730.1,15924.2,14
310.7,12274.2,9619.54,0.480168,0.041618,-0.093843,-0.193249,-0.009993,0.057976,-
0.174868,0.034687,0.063862,-0.022272,-
0.006338,4290.33,10826.5,8668.73,4676.45,8722.9,12442.1,15369.8,16943.3,16139.2,
15412.9,13580.5,0.546297,0.047696,-0.038894,-0.256115,0.055548,0.032444,-
0.165286,0.031148,0.025947,0.012263,-

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1,50,29,25,24,32,1,22,18,18,18,29,41,18,20,34,28,1,29,20,28,40,19,29,43,30,41,50
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2,12,9,12,9,8,11,4,5,1,3,607.403,0.030238,26,30,4,6,6,1,5,67,1.46,71,5,1,9,10,22
.673,15.2708,5,13.1032,4.21382,0.471525,0,0,1,0,0,0,0,0,0,0,40.54,4,3,1,141.92,0
,0,9882,3679.44,4172.4,6360.07,23.7284,8.89668,6.17751,6,8.6521,4.67651,40.54,50
.255,4.06708,7.46083,15.2708,29.21,132.58,23,26,3,7.21499,0.756261,5,4848,40.54,
429.594,2590,2590,65,3,4,12.79,4.89,10,1,1,5.2,50.04,1.45,5.2,2.32,3.3,4.26,4.95
,5.17,5.19,5.2,5.2,CYP3A
30,2,0,31,54,74,77,79,67,39,12,53.552,0,0,0,42.9151,0,35.0512,0,0,0,0,0.127979,0
,0,-0.02169,-0.022214,-0.019786,-0.000084,0.000164,-
0.00038,0,0,429.193,0,0,344.009,385.188,528.963,540.045,341.158,134.233,0,0,1422
.6,38.4784,0,1824.05,2974.86,3711.74,3542.2,3005.49,2073.76,991.497,270.076,0.50
1413,0.00705,0,-0.297836,0.117445,-0.282251,0.395301,-0.161272,-0.029606,-
0.031503,0.031966,2253.9,113.659,0,2344.7,4020.99,5675.48,6088.13,5766.4,4389.45
,2401.61,703.475,0.83193,0.00705,0,-0.406098,0.170182,-0.501388,0.575692,-
0.219378,-0.03116,-
0.043047,0.032181,12,2,0,0,0,0,0,0,0,0,0,0,8,0,0,0,0,0,0,0,0,0,0,19,0,0,0,0,0,0,
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30,1.94,31,1,1,4,5,11.596,7.71438,2,8.65098,4.39865,0.903054,0,0,0,0,0,0,0,0,0,0
,58.2,0,4,2,49.68,1,0,938,515.775,1200.8,1203.71,12.4567,5.10417,3.02973,6,3.574
53,2.28915,58.2,23.796,2.58654,4.98532,7.71438,13.31,59.04,12,12,2,4.91342,0.735
29,6,637,58.2,218.252,385,385,29,2,4,11.13,-
3.81,3,2,2,1.49,23.07,1.49,1.46,1.49,1.49,1.49,1.49,1.49,1.49,1.49,1.48,CYP3A
32,32,18,34,51,69,73,64,55,48,40,125.937,35.0994,35.2859,0,0,52.798,91.2111,40.2
486,52.6648,47.8589,12.4455,0.084012,0.004163,0.000612,-0.023487,0.023281,-
0.036997,0.01191,-0.006021,0.004747,-0.010996,-
0.00922,797.406,299.443,118.616,813.425,1223.3,1463.03,1294.69,994.606,862.342,7
13.55,462.823,1982.58,1030.87,472.794,2494.26,3821.14,4542.71,4198.34,3521.38,28
59.32,2260.14,1642.15,1.40908,0.300521,0.074569,-0.732754,-
0.104005,0.025798,0.328614,-0.338951,0.036972,0.306978,-
0.459998,2811.67,2550.87,1451.12,3059.12,4570.6,6109.78,6391.58,5598.22,4765.25,
4081.04,3325.37,1.43638,0.172007,0.087608,-0.834525,0.15183,-0.244153,0.486895,-
0.386572,0.028635,0.303386,-
0.364801,5,5,3,0,2,2,1,0,2,0,0,0,0,1,1,0,0,0,0,0,0,0,0,0,10,0,0,0,0,0,0,0,0,0,0,17
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,34,2,2,6,7,16.0161,10.3799,3,12.0614,2.57664,0.976053,0,0,0,0,0,0,0,0,0,0,127.4
5,0,7,5,79.35,1,0,3199,777.514,3574.2,4184.07,16.8438,6.48148,4.75,6,3.62598,2.1
648,127.45,30.354,3.7578,6.39255,10.3799,15.19,76.86,16,17,1,6.47803,0.886784,6,
1846,127.45,302.236,986,986,40,7,8,4.55,-
10,4,5,5,0.58,28.48,0.58,0.01,0.58,0.58,0.58,0.58,0.58,0.58,0.57,0.48,CYP3A
52,88,62,55,97,130,133,142,137,141,126,74.8733,13.5601,19.0362,0,4.90897,30.5748
,23.1393,2.00233,19.7441,9.43837,4.03849,0.081587,0,0,-0.021112,0.000075,-
0.014062,0.003341,-0.005704,-
0.003389,0.000057,0,547.301,82.0602,117.805,592.757,821.587,965.364,704.199,509.
007,289.448,164.192,70.7394,2986.93,3427.84,2549,3830.56,6220.56,7994.24,7819.85
,7867.26,7330.91,6494.36,4924.95,0.684933,0.048542,-0.048303,-0.249739,-
0.255705,0.245223,-0.043384,-0.095836,0.081762,-
0.082794,0.025234,3513.45,5710.01,4197.79,3925.43,6786.11,9014.98,9103.59,9561.5
2,9124.61,9057.81,7944.48,0.833852,0.003483,-0.088771,-0.365803,-
0.151508,0.214749,-0.094489,-0.054633,0.057924,-
0.131082,0.12051,24,0,9,8,9,2,1,6,4,4,7,7,9,4,3,4,3,2,5,6,2,3,2,43,1,4,3,0,1,3,2

,1,1,3,15,39,11,19,23,9,0,4,11,5,8,33,4,12,4,16,22,1,12,22,18,20,9,13,23,20,19,2
2,13,18,13,13,12,14,9,12,16,19,21,10,12,16,16,25,16,17,10,20,13,13,4,9,20,14,12,
8,18,17,8,9,12,1,15,14,18,15,7,6,5,8,9,14,10,5,6,15,6,8,7,8,3,6,8,0,9,6,7,7,5,7,
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,15.0054,1.10942,0.96832,0,1,0,1,0,0,0,0,0,1,48.3,0,5,1,102.48,2,0,8420,1590.13,
6367.88,7219.96,20.28,10.1563,7.39556,7,7.17413,4.32019,73.6,43.341,4.44841,7.79
188,13.3477,23.13,114.09,21,23,5,8.56493,0.925778,6,3233,48.3,383.508,1956,1956,
45,6,6,15.31,8.16,1,1,1,2.42,42.83,-3,2.41,-3,-2.97,-2.73,-1.69,-
0.09,1.18,2.02,2.36,CYP3A
57,110,78,61,111,153,162,165,153,157,150,105.395,13.9132,26.1274,0,35.2869,6.976
9,0,44.6963,5.58558,0,8.96928,0.236969,0.041996,0.03723,-0.010592,-0.106393,-
0.016129,-0.000635,0.016074,0.003634,-0.012966,-
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,326.544,277.363,3567.96,5210.77,4056.57,4672.76,7878.23,9709.43,10020.2,9822.98
,9017.12,8255.96,7037.44,0.634724,0.019295,-0.143901,-0.380408,0.176092,-
0.01524,-0.29562,0.23581,-0.018836,-
0.0392,0.035361,4054.76,7449.71,5694.85,4437.51,7843.95,10567.3,10976.8,10898.1,
10323.9,10682.2,9996.07,0.831087,0.042246,-0.058755,-0.483168,0.237647,-
0.041896,-0.258937,0.221816,-0.089571,-
0.022777,0.007571,25,0,8,8,4,8,5,4,7,7,5,9,3,5,4,5,8,6,6,4,6,9,7,50,8,6,6,0,2,4,
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22,2897.6,10632.1,13095.5,22.7755,10.092,9.79592,6,8.51545,2.66954,40.51,48.937,
5.49467,8.74578,15.0805,25.28,131.77,26,27,5,9.69218,0.928838,5,4591,39.99,440.9
41,2921,2921,49,4,5,12.17,8.95,2,1,1,3.57,48.12,-0.25,3.53,-0.25,-0.25,-0.22,-
0.01,0.66,1.61,2.56,3.29,CYP3A
28,20,12,29,46,58,57,47,36,35,29,249.995,0,0,155.902,48.9357,21.9462,10.9853,50.
2184,40.8856,0,5.75545,0.366835,0.005487,-0.002521,-0.211782,0.067121,-
0.161767,0.176954,-0.04008,0.002081,-0.0088,-
0.01011,739.951,74.8818,19.3793,789.256,957.555,958.252,821.895,689.48,484.154,2
83.985,173.346,1574.14,664.24,326.612,1929.41,2920.93,3303.06,2984.48,2408.45,18
73.16,1568.9,1122.85,0.467238,-0.063247,-0.012379,-0.335474,0.225588,-
0.160259,0.014126,-0.056861,0.280742,-
0.307876,0.160989,2350.93,1324.64,781.149,2467.79,3945.75,4789.74,4805.49,4018.8
7,3051.06,2710.27,1933.47,1.25917,-0.136904,0.026576,-0.926098,0.621065,-
0.703549,0.571167,-0.32738,0.494943,-
0.481416,0.214053,8,0,0,0,0,0,0,0,0,0,0,0,4,0,0,0,0,0,0,0,0,0,0,0,15,0,0,0,0,0,0,0
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4,29,1,1,5,6,12.3031,8.07732,2,9.4831,5.64993,0.860386,0,0,1,0,0,0,0,0,0,0,85.08
,0,5,3,51.29,1,1,1649,779.777,1530.05,1979.21,13.4321,5.76,5.92817,6,5.05921,3.2
0232,93.46,26.613,2.933,6.12364,8.07732,12.74,65.75,12,12,2,5.44683,0.548604,6,8
18,85.08,249.29,536,536,23,5,7,8.54,3.96,6,2,3,1.21,25.45,-1.73,0.22,-
0.75,0.2,0.91,1.15,1.19,1.18,1.09,0.69,CYP3A
57,93,72,59,100,126,140,152,173,178,143,44.8554,20.9767,0,0,0,7.13306,0,0,0,0,0,
0.003725,0.000114,0.000001,-0.000605,-0.000064,-0.000244,-0.000228,-0.000346,-
0.000324,-
0.000216,0.00005,693.625,225.779,64.6323,723.741,943.748,951.169,876.017,1065.19
,1128.17,879.745,496.946,3564.21,4178.08,3394.87,4518.96,7119.76,8849.07,9483.75
,10196.5,10390.7,8980,6359.36,0.394058,0.048288,0.004153,-0.074768,-
0.158928,0.057294,-0.015569,-0.027827,0.028333,-0.006998,-
0.031836,3699.12,6033.89,4654.15,4002.47,6698.25,8344.94,9131.42,9992.14,11315.1
,11533.6,9214.76,0.37636,0.045775,0.010456,-0.082696,-0.133578,0.048138,-

0.021684,-0.005707,0.024002,-0.019887,-
0.034209,28,1,12,9,8,4,11,9,7,4,7,4,4,9,3,6,5,5,5,3,8,7,4,46,3,6,3,4,6,4,1,0,3,0
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4.1859,3,16.4134,2.94749,0.954587,0,1,0,1,0,0,0,0,0,1,12.47,0,2,0,111.48,0,0,992
8,2069,6944.55,8321.14,23.6587,12.7575,10.7302,6,5.23928,2.35582,12.47,50.334,4.
62064,8.37265,14.1859,25.33,133.41,18,18,9,9.03132,0.960357,6,3338,12.47,405.959
,2330,2330,42,3,3,20,8.51,1,0,0,6.35,48.24,2.53,6.34,2.53,2.54,2.61,3,3.84,4.81,
5.71,6.23,CYP3A
34,28,30,34,60,73,92,82,70,63,29,15.9982,0,0,0,0,0,0,0,0,5.49631,0,0.012415,0,0,
-0.001409,-0.001643,-0.000573,-
0.002582,0,0,0,0,197.305,0,0,202.393,220.055,140.232,36.514,15.4444,8.6801,5.496
31,0,1310.81,600.309,415.778,1653.26,2638.52,3150.36,3281.99,2820.33,2092,1461.8
9,780.909,0.264863,-0.076163,0.070701,-0.094686,-0.016608,-0.050763,0.04636,-
0.006497,-0.114752,0.184978,-
0.075002,2059.24,1632.83,1677.7,2158.36,3760.25,4574.13,5576.9,4944.08,4171.21,3
637.42,1714.11,0.240193,-0.076163,0.070701,-0.107068,0.0289,-
0.04641,0.012348,0.034332,-0.154261,0.168688,-
0.051164,20,1,0,0,0,0,0,0,0,0,0,0,8,0,0,0,0,0,0,0,0,0,0,21,0,0,0,0,0,0,0,0,0,0,9
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39,34,1,1,8,8,10.7152,6.50291,1,10.3019,1.32047,0.977467,0,1,1,1,0,1,1,0,0,0,29.
26,0,2,2,37.55,0,0,870,308.453,1461.26,1649.13,12.0714,5.1856,4.88889,6,4.02419,
2.25775,29.26,24.272,2.98149,5.54011,6.50291,14.66,63.18,6,6,3,5.29475,0.859505,
6,461,29.26,192.301,316,316,18,2,2,20,10.2,1,1,2,2.56,23.93,-4.88,2.15,-4.14,-
3.17,-2.2,-1.35,-0.89,-0.46,0.38,1.33,CYP2D6
42,52,57,43,77,100,119,96,86,80,70,33.0469,0,0,0,0,20.0837,7.07538,0,0,0,0,0.017
341,0,0,0.002693,-0.010351,0.000032,-
0.001044,0,0,0,0,258.353,0,0,260.479,351.693,269.516,150.228,54.6032,54.7561,17.
8228,0,1832.29,1849.98,1709.27,2344.88,3822.79,4473.99,4524.15,3842.4,3322.26,29
26.55,2504.52,0.594789,0.01426,-0.024143,-0.289225,-0.091796,0.205548,-
0.133191,-0.005102,0.079927,-
0.108632,0.024483,2712.99,3139.74,3293.49,2925.56,5166.17,6649,7706.67,6315.96,5
703.46,5218.57,4393.55,0.521154,0.01211,-0.027954,-0.276625,-0.065548,0.180654,-
0.123755,0.013045,0.074598,-
0.097347,0.019771,22,0,2,4,2,0,2,2,0,1,3,0,4,1,0,1,0,0,0,0,0,0,0,29,0,0,0,0,0,0,
0,0,0,6,5,33,8,22,23,6,0,4,17,4,8,16,11,2,14,22,6,0,9,11,11,22,10,6,11,12,13,8,8
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,1,0,1,0,0,1,1,0,0,45.4,0,3,2,60.27,1,1,2489,652.986,3185.47,3407.58,15.39,6.185
49,6.81657,6,5.78115,2.78815,45.4,31.168,3.7232,7.04018,8.904,18.34,77.43,9,10,5
,6.65347,0.721143,5,964,45.4,261.359,741,741,26,2,2,13.23,9.09,1,2,2,2.94,31.54,
-0.67,2.89,-0.67,-0.67,-0.65,-0.54,-0.03,0.86,1.82,2.59,CYP2D6
38,46,13,39,67,86,100,94,95,87,76,34.4275,0,0,0,0,0,0,2.79826,0,9.25277,8.71614,
0.018479,-0.000002,0,-0.010104,0.004294,-0.002797,-0.001588,0.001767,0.000054,-
0.001975,0.00111,455.502,33.5909,0,446.527,511.467,415.685,335.422,386.922,342.3
48,226.95,112.014,1853.97,1088.97,261.079,2332.68,3707.45,4522.78,4640.24,4426.1
9,4071.59,3213.23,2225.59,0.242272,0.065598,-0.02105,-0.040087,-0.09587,-
0.022648,0.010761,0.11372,-0.056228,-
0.118284,0.042952,2491.42,2878.44,907.237,2654.07,4464.84,5649.52,6334.79,6014.1
4,6182.36,5700.38,4816.13,0.318666,0.065796,-0.016858,-0.079606,-0.084546,-
0.031073,0.004076,0.141474,-0.082604,-
0.120844,0.044853,19,0,0,1,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,34,0,0,0,0,0,0,

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17,7,8,0,12,12,2,1,38,1.72,39,1,1,7,8,13.6649,9.1647,2,11.0251,2.95835,0.922488,
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9527,7.3728,6,6.89411,2.97366,16.13,31.839,3.61919,6.00811,9.1647,16.79,80.85,12
,12,5,6.29696,0.83504,6,1042,16.13,274.788,718,718,25,3,3,20,9.42,1,0,0,3.5,31.6
2,-2.01,3.39,-1.96,-1.66,-0.96,-0.36,0.19,1.07,2.04,2.92,CYP2D6
56,102,76,59,102,140,156,158,166,164,130,6.001,0,0,0,0,2.99918,0,0,0,0,0,0.00003
6,0.000014,0.000001,-0.000002,0.000003,-0.000018,-0.000005,-0.000004,0.000004,-
0.000009,0.000012,633.205,333.121,448.109,627.033,718.572,584.584,393.764,412.98
7,318.624,245.958,258.448,3032.89,4492.55,3632.15,3882.29,6301.65,7930.16,8372.5
2,8219.32,8000.4,7186.53,5599.18,0.311699,0.00114,0.004917,-0.04205,-
0.170688,0.061689,0.00315,-0.013412,-0.00271,-
0.023582,0.012986,3509.89,6239.05,4713.66,3883.91,6625.8,8884.3,9743.72,9863.37,
10318.5,10067.5,7954.56,0.311111,0.001345,0.006358,-0.041777,-
0.168965,0.061559,0.001536,-0.013544,-0.003378,-
0.023301,0.012899,28,1,6,5,11,2,6,8,9,9,1,5,3,10,4,4,2,10,3,2,11,4,7,53,7,4,3,1,
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9.0205,13.899,4,16.3655,0.027387,0.979918,0,2,0,2,0,0,0,0,0,2,6.48,0,2,0,104.12,
1,0,10862,1516.27,7604.2,8585.11,21.2404,11.4075,10.5625,6,7.27723,2.86695,6.48,
46.714,4.90132,8.29733,13.899,25.08,119.86,24,24,6,9.15862,0.972378,6,3571,6.48,
368.514,2320,2320,40,2,2,20,8.32,1,0,0,6.14,46.58,0.75,6.13,1.65,2.2,2.42,2.94,3
.84,4.8,5.65,6.06,CYP2D6
26,3,0,27,46,61,66,60,33,18,11,31.7238,0,0,0,18.3717,0,0,0,0,0,0,0.175224,0,0,-
0.029249,-0.058691,-0.000358,0.001369,-0.000668,0.000303,-
0.000319,0,304.536,0,0,286.442,272.744,179.472,179.666,211.582,148.619,54.3832,0
,1167.21,49.154,0,1488.33,2413.74,2891.85,2654.58,1968.01,1012.97,495.004,233.91
8,0.372819,0.026743,0,-0.277295,0.284332,-0.26307,-0.004361,0.072626,0.026184,-
0.044505,-
0.007064,1736.1,182.986,0,1891.74,3147.03,4092.39,4310.37,3811,2156.7,1211.44,70
7.457,0.688881,0.026743,0,-0.513118,0.427253,-0.295694,-
0.048341,0.073603,0.058802,-0.051376,-
0.022312,10,1,0,0,0,0,0,0,0,0,0,0,0,4,0,0,0,0,0,0,0,0,0,0,0,18,0,0,0,0,0,0,0,0,0,0,1
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,3,9.25915,6.27086,2,8.84468,3.4806,0.959863,0,0,0,1,1,0,0,0,0,0,53.11,0,3,3,35.
22,1,0,580,272.279,970.793,1164.52,9.55102,4.02216,3.7037,6,3.25867,2.79726,53.1
1,20.888,2.62103,5.35674,6.27086,11.65,63.85,10,11,0,4.58426,0.651132,6,462,53.1
1,175.23,238,238,18,3,3,20,11.37,1,2,3,1.39,19.88,-1.84,0.01,-1.83,-1.83,-1.83,-
1.83,-1.83,-1.8,-1.6,-0.92,CYP2D6
31,13,4,31,53,67,83,78,56,50,29,3.03322,0,0,0,0,0,0,0,0,0,0,0.000024,-
0.000001,0,-0.000013,0.000002,-0.000001,0,-0.000005,0.000011,-
0.000008,0.000003,253.916,31.4957,0,219.52,197.868,113.655,19.4777,50.8022,103.6
67,125.377,94.2446,1184.63,270.882,71.496,1475.19,2326.55,2770.83,2850.28,2431.7
8,1767.86,1357.16,715.683,0.174974,0.001104,0.00026,-0.026703,-0.06559,-
0.005383,0.014207,-0.001578,-
0.026271,0.013543,0.001922,1933.22,819.924,254.595,2017.41,3365.03,4184.2,5036.6
1,4742.54,3487.31,3062.93,1807.03,0.174869,0.001201,0.000415,-0.0266,-0.064927,-
0.006625,0.014764,-0.001797,-
0.025915,0.013629,0.001419,17,0,1,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,27,0,0
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,6,1,1,31,2.2,31,1,1,8,8,10.3889,6.73638,1,11.8539,0.873225,0.991448,0,1,0,1,0,0
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,6,2.43184,2.33699,3.24,23.526,3.20159,6.03648,6.73638,13.6,61.35,6,6,5,6.43335,
0.963714,6,436,3.24,187.281,337,337,16,1,1,20,7.47,1,0,0,2.87,23.64,-0.95,2.87,-
0.94,-0.86,-0.44,0.42,1.39,2.27,2.76,2.86,CYP2D6
56,102,76,59,102,140,156,158,166,164,130,53.6937,16.6647,23.8464,0,0,2.99916,0,0
,17.1666,0,0,0.002575,0.000458,0.000539,-0.000757,0.000211,-0.000374,0.000314,-
0.00084,0.000825,-0.000495,-
0.001145,706.176,421.936,483.857,693.746,849.248,721.916,458.07,408.648,405.685,
383.097,395.431,3021.12,4473.31,3618.45,3867.88,6279.26,7903.2,8346.42,8190.11,7
963.44,7148.08,5568.2,0.39439,-0.027752,0.036507,-0.110908,-0.13044,0.095365,-
0.046272,-0.150616,0.130212,0.10473,-
0.100168,3770.32,6890.48,4975.61,4089.35,6930.18,9285.28,10028.3,10072.4,10751.6
,10710.3,8894.72,0.389272,-0.028309,0.034087,-0.120213,-0.112448,0.082129,-
0.028672,-0.14874,0.106969,0.096467,-
0.075691,26,0,6,8,3,6,5,11,3,5,5,11,3,9,8,2,1,3,8,3,3,5,7,49,3,2,4,4,1,3,0,3,4,3
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8.47281,14.6867,25.08,120.3,24,24,6,9.49376,0.956603,6,4305,6.48,404.495,2790,27
90,44,4,4,20,8.05,1,0,0,6.42,45.69,1.01,6.41,1.92,2.47,2.7,3.2,4.09,5.06,5.92,6.
33,CYP2D6
56,123,106,59,107,144,161,165,150,135,122,145.774,25.4346,24.7172,0,76.3729,34.5
262,7.88576,71.0362,89.8725,17.3176,0,0.028117,0,0,0.003686,-0.012082,-
0.006187,-
0.003699,0.001166,0.002568,0.000489,0,513.881,142.974,63.2337,481.035,821.999,79
8.651,599.313,470.444,400.07,276.086,205.923,3224.56,5588.14,4516.89,4189.86,695
3.76,8648.5,8874.88,8491.32,7587.84,6652.59,5919.46,0.793437,0.036757,0.148423,-
0.355158,-0.195725,0.225608,-0.115922,-0.043771,0.086479,0.033904,-
0.089672,4002.27,8616.86,7260.3,4339.01,7672.73,9826.85,10933.9,10972.9,10115.4,
9342.71,8652.41,0.746979,0.084591,0.101851,-0.350115,-0.189483,0.246807,-
0.086911,-0.08398,0.091789,0.034988,-
0.113902,25,0,6,7,4,9,5,5,3,10,2,0,6,5,7,6,5,0,4,2,2,4,1,47,1,4,2,0,1,1,2,1,0,4,
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13,7,8,11,7,7,8,9,6,513.896,0.081438,18,21,2,12,12,2,0,56,1.22,59,2,2,10,11,21.1
396,14.4528,4,14.0449,1.61088,0.896709,0,2,1,2,0,0,0,0,0,2,29.95,0,4,1,118.6,2,0
,11825,3037.01,6861.43,9320.99,23.168,10.2924,8.81633,6,5.66506,3.47159,55.25,45
.227,4.68657,7.65375,14.4528,24.64,117.27,20,22,7,8.50572,0.835033,6,4387,29.95,
437.523,2618,2618,49,8,8,15.69,9.05,1,1,1,4.28,43.84,-1.97,4.23,-
0.8,0.04,0.42,0.65,1.29,2.23,3.19,3.95,CYP2D6
51,89,67,54,96,133,140,131,110,113,112,37.1294,12.1869,0,0,12.0439,0,6.6697,5.08
075,5.02115,0,0,0.133703,0.041946,0.017191,-0.007615,-0.049237,-0.005179,-
0.002726,-0.002096,0,-0.010034,-
0.012559,549.862,197.349,330.452,562.371,695.039,543.177,296.473,101.134,39.8448
,47.1107,92.5083,2697.51,3885.86,3055.72,3470.38,5697.19,6874.3,6689.16,5991.81,
5359.58,5363.04,4927.16,0.546828,0.076856,-0.131418,-0.262625,-0.007269,-
0.020921,0.037373,-0.007305,-0.016653,-0.000589,-
0.03317,3417.06,5693.4,4392.57,3737.95,6494.02,8798.54,9255.11,8615.01,7176.02,7
185.61,7130.85,0.627675,0.04147,-0.023558,-0.279781,0.047957,-
0.073124,0.070122,-0.119234,0.014902,0.041113,-
0.066496,23,0,5,5,6,4,8,5,3,1,2,3,4,6,5,6,2,5,5,2,3,6,3,47,3,6,6,3,2,3,4,1,2,6,8

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207977,11,13,1,15,16,3,0,51,0.98,54,2,2,5,7,17.7694,12.7928,4,18.2195,1.30583,0.
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.3222,9.46746,9.67714,6,4.66343,2.83277,48.13,42.183,5.41398,9.67937,12.7928,22.
7,105.94,21,22,5,9.51711,0.882306,5,3030,48.13,347.454,2016,2016,37,2,3,14.4,9.6
4,2,2,2,3.05,41.63,-0.78,2.89,-0.77,-0.77,-0.77,-0.71,-0.37,0.44,1.4,2.32,CYP2D6
52,110,72,54,97,139,155,162,142,130,131,30.631,0,0,0,0,0,12.5185,0,0,0,13.5811,0
.012284,-0.000173,-0.000025,-0.006241,0.003333,-0.002618,0.000658,-0.001275,0,-
0.000232,0.000487,512.571,333.199,425.286,468.235,517.544,409.253,213.2,108.661,
37.8763,73.3468,197.65,2458.87,4011.24,2657.66,3170.85,5283.45,6792.53,6987.62,6
747.79,6087.84,5588.61,5129.62,0.478046,0.032738,0.039469,-0.164367,-0.083081,-
0.109057,0.166086,0.063983,-0.061859,-
0.158352,0.064269,3374.09,6826.18,4655.68,3601.64,6332.49,8963.74,9913.93,10289.
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0.13363,0.206669,0.056591,-0.071862,-
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7,3,4,14.4,9.11,2,1,1,3.72,39.83,-0.1,3.67,-0.1,-0.1,-
0.08,0.08,0.69,1.62,2.58,3.37,CYP2D6
30,12,0,30,52,62,70,70,60,47,32,20.9077,0,0,0,0,0,0,6.71191,0,0,0,0.0034,0,0,-
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1.62,-1.62,-1.61,-1.5,-0.98,-0.08,0.88,CYP2D6
40,18,3,43,78,109,131,135,117,91,55,17.1477,0,0,0,0,6.31173,0,0,0,0,0,0.011677,0
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55,114,44,57,117,183,190,184,195,210,183,2.5027,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
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45,80,82,46,83,103,111,124,108,83,85,84.8544,0,0,0,11.4147,26.2731,78.4346,55.0308,0,14.714,7.59179,0.085234,0,0,-0.025388,-0.003033,-0.012076,0.001784,-0.003904,0,0,0,413.318,0,0,394.427,544.213,626.382,495.671,176.264,20.1561,40.2865,18.0304,1971.8,2903.91,2209.22,2490.69,4036.3,4823.9,4771.39,4582.86,3921.16,3353.54,3250.44,0.704347,-0.20353,-0.03295,-0.26399,-0.117967,-0.237974,0.438925,0.004443,-0.379592,0.28443,0.064763,3164.36,5341.09,5118.61,3344.63,5853.06,7339.52,7955.65,8703.74,7728.25,5942.17,5759.68,0.841459,-0.197116,-0.027822,-0.387248,0.103392,-0.490808,0.487874,0.134044,-0.435254,0.250273,0.048463,22,0,0,0,0,0,0,0,2,0,0,0,12,0,0,0,0,0,0,0,0,0,0,29,0,0,0,0,0,0,0,0,0,2,17,28,6,20,13,13,0,9,14,3,10,22,10,9,11,13,12,1,10,17,17,14,12,22,16,19,19,17,7,21,15,14,22,12,11,18,11,10,13,9,16,17,10,14,17,8,15,11,12,19,6,11,16,9,16,11,5,14,7,5,9,0,7,15,7,7,9,4,7,9,3,4,14,9,4,2,4,1,2,3,2,1,4,1,5,1,3,0,3,0,2,2,1,1,454.832,0.106971,16,17,1,6,6,1,1,45,1.77,46,1,1,11,12,16.1125,10.6169,2,11.5727,6.49447,0.959564,0,1,0,1,0,0,0,0,0,1,50.8,0,5,1,74.77,1,0,3788,1303.4,4630.34,5186.4,18.3403,8.74089,6.57439,6,4.47234,2.90815,50.8,34.824,3.86986,5.87322,10.6169,19.48,90.56,11,11,6,7.25955,0.970424,5,1372,50.8,371.27,1080,1080,34,4,5,12.36,9.13,2,1,1,1.95,34.73,-1.87,1.89,-1.87,-1.87,-1.85,-1.7,-1.1,-0.17,0.79,1.58,CYP2D6
43,32,8,46,96,150,168,152,121,76,54,5.70966,0,0,0,0,0,2.85483,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,5.70966,0,0,0,0,0,2.85483,0,0,0,0,2005.27,759.677,156.18,2763.59,5225.03,7266.43,7408.48,6102.39,4375.2,2570.69,1581.49,0.213909,0.010308,0.005426,-0.023838,-0.081459,-0.043354,0.00949,0.028728,-0.009935,-0.009986,0.007664,2475.67,1740.08,430.079,2756.28,5699.99,8787.4,9703.17,8663.87,6851.91,4274.68,2984.9,0.213909,0.010308,0.005426,-0.023838,-0.081459,-0.043354,0.00949,0.028728,-0.009935,-0.009986,0.007664,26,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,56,0,0,0,0,0,0,0,0,0,1,5,69,14,15,27,11,0,9,10,4,20,14,25,9,12,22,20,0,9,25,23,24,19,20,20,13,21,17,0,14,10,19,11,10,14,17,10,11,13,6,13,9,16,9,12,8,8,8,8,6,14,7,4,7,4,9,5,4,6,6,2,0,1,4,5,3,2,6,0,0,1,3,11,0,3,1,0,0,1,1,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,338.462,0.084132,17,20,4,0,0,0,4,43,1.56,46,0,0,0,0,11.2423,8.41582,4,9.50154,0.913566,0.942575,0,2,0,2,0,0,0,0,0,2,6.48,4,2,0,56.22,4,0,1207,528.018,1580.92,1654.7,10.88,4.28062,3.48444,6,4.10628,3.00726,6.48,27.905,2.83353,5.52847,8.41582,18.23,71.82,17,20,0,4.9669,0.718658,6,1180,6.48,234.38,458,458,30,2,2,20,9.46,1,0,0,1.75,28.52,-5.89,1.64,-5.88,-5.81,-5.41,-4.49,-3.09,-1.33,0.16,1.15,CYP2D6
41,67,53,44,82,114,119,99,59,64,70,44.841,0,0,0,14.6102,0,32.7221,0,5.18763,0,5.32566,0.144975,0,0,-0.012672,-0.028584,0.012114,-

0.053342,0.00748,0.002516,0,0,396.936,18.2141,9.2505,390.861,538.38,499.198,397.277,202.365,100.113,19.417,23.9557,2138.57,2866.84,1903.33,2803.8,4787.33,5758.13,5228.84,3961.6,3181.28,3430.05,3429.36,0.577747,-0.046393,-0.026658,-0.282304,0.006384,-0.184919,0.314268,-0.172457,0.051817,-0.057531,0.085875,2837.17,4173.04,3218,3138.7,5672.65,7713.57,8123.44,6887.36,4475.29,4529.49,4600.45,0.678902,-0.00856,-0.001807,-0.392496,0.216683,-0.218942,0.164106,-0.198398,0.174836,-0.069369,-0.020394,19,0,3,2,0,2,1,2,2,1,1,0,3,0,2,0,0,0,0,1,0,0,1,35,0,0,0,0,0,0,0,0,0,9,14,30,13,17,13,10,0,12,5,13,7,23,19,6,13,10,18,1,17,13,13,14,10,9,16,12,12,10,9,19,8,8,10,7,13,0,13,4,7,7,7,11,5,7,6,5,8,9,7,12,7,7,7,3,6,9,6,10,11,3,2,0,4,8,7,8,5,5,1,3,8,6,7,12,5,4,0,4,8,3,3,5,2,2,2,4,4,3,2,1,2,1,0,3,359.558,0.152734,12,14,2,9,10,2,2,41,1.12,44,1,1,4,5,14.397,10.2203,4,12.8124,5.54712,0.986274,0,1,1,1,0,0,0,0,0,1,45.33,2,4,1,72.65,3,1,3288,538.668,3262.37,3519.54,14.5833,5.89388,5.95041,6,3.33879,2.94972,45.33,32.744,3.5878,6.71917,10.2203,18.09,81.5,17,19,3,6.72514,0.906847,5,1429,45.33,284.353,944,944,33,2,3,12.18,9.34,2,1,1,2.74,32.94,-1.08,2.65,-1.08,-1.08,-1.07,-0.97,-0.48,0.41,1.38,2.24,CYP2D6
52,102,94,55,98,133,142,147,129,113,103,76.4485,0,9.48456,0,0,8.36028,0,30.0522,5.47389,9.41925,9.02542,0.001739,0,0,0.000333,-0.000742,-0.000783,-0.000033,0.00026,0.000267,-0.000214,0.000044,526.099,56.3079,66.1106,569.249,826.745,880.146,677.311,495.264,306.345,185.705,81.3645,3279.59,5196.62,4325.83,4225.78,6901.3,8479.95,8395.58,7956.2,7006.11,6139.45,5534.54,0.484628,-0.022593,-0.008355,-0.151366,-0.186385,0.121892,-0.040666,-0.044,0.064939,0.001252,0.001024,3433.55,6654.62,6118.06,3781.86,6595.31,8765.56,9164.7,9363.55,8317.53,7347.56,6743.65,0.47835,-0.024144,-0.006252,-0.151121,-0.185838,0.12137,-0.032711,-0.041075,0.05621,-0.000023,0.002099,24,0,3,5,4,5,2,5,1,1,5,1,5,4,4,1,4,4,3,1,4,1,3,45,2,2,2,1,2,4,1,0,0,1,9,49,12,25,24,12,0,7,10,6,6,33,3,4,9,16,20,0,13,37,17,15,11,12,20,14,15,33,13,26,16,14,9,12,16,2,11,12,9,9,18,15,21,15,16,21,15,9,14,13,5,23,19,13,14,13,9,10,11,7,9,0,10,17,15,9,11,17,15,9,16,10,13,12,10,10,13,7,9,7,3,8,7,3,5,3,10,10,6,6,5,6,7,6,497.238,0.112125,15,18,2,12,12,2,0,52,1.3,55,2,2,7,8,18.6396,13.2415,4,14.9501,2.51274,0.959679,0,2,0,2,0,0,0,0,0,2,26.71,0,3,1,101.28,2,0,8675,2008.72,7145.96,8439.28,20.28,9.66686,8.09951,6,5.86807,3.17779,52.01,45.759,4.68396,7.62304,13.2415,23.09,127,20,22,5,8.42846,0.961177,6,3418,26.71,400.965,2000,2000,43,5,5,15.69,9.07,1,1,1,4.45,45.35,-1.55,4.41,-0.58,0.23,0.59,0.82,1.45,2.39,3.35,4.12,CYP2D6
36,42,29,37,59,75,74,73,69,70,62,151.687,0,0,0,35.1874,90.2293,28.8995,70.8396,0,0,130.79,0.10614,-0.008181,0.010459,-0.021022,-0.029851,0.011736,-0.023012,0.00217,0.001491,0.015217,-0.010326,774.499,324.038,310.79,676.054,822.043,893.148,892.36,893.429,771.093,771.19,724.771,2142.48,1456,951.076,2641.25,3996.49,4692.44,4433.09,4102.62,3755.62,3308.35,2414.27,0.831084,-0.198672,-0.241567,-0.494287,0.024908,0.24645,-0.460759,0.497508,-0.18952,-0.334831,0.543206,3034.88,3477.55,2507.03,3119.83,4841.72,6089.56,5928.25,5841,5622.22,5528.46,4949.99,1.05984,-0.225059,-0.239294,-0.63262,0.143023,0.222216,-0.671967,0.692258,-0.238334,-0.347413,0.569951,11,1,0,0,0,0,0,0,1,0,0,0,4,0,0,0,0,0,0,0,0,0,0,20,0,0,0,0,0,0,0,0,0,2,16,16,4,13,15,8,0,2,8,3,2,22,7,5,13,7,12,2,5,7,10,10,13,7,14,14,10,12,16,11,9,5,12,8,13,10,4,9,11,1,6,6,10,5,10,10,5,11,5,8,3,12,7,5,6,8,10,1,4,3,6,0,6,8,9,2,7,4,2,2,3,3,4,4,5,1,0,2,2,0,4,1,1,0,3,2,0,1,0,1,2,2,1,0,414.552,0.056981,11,12,0,12,12,2,0,36,1.87,37,2,2,11,12,16.8196,10.9692,2,11.5181,1.04017,0.842455,1,0,1,0,0,0,0,0,0,0,75.63,0,5,2,78.1,0,0,4853,1684.21,3126.05,4138.21,19.3264,9.47461,8.59375,6,7.37042,2.64034,75.63,35.301,3.55422,6.76935,10.9692,16.34,86.32,12,12,7,6.98835,0.701513,6,1742,75.63,354.184,1278,1278,32,6,8,3.44,-2.18,7,2,2,1.36,33.67,0.5,-0.14,-0.02,-0.13,-0.14,-0.14,-0.14,-0.14,-0.14,-0.14,CYP2C9

56,143,110,58,99,136,148,152,169,173,165,89.0291,24.7163,16.1566,0,16.9276,0,37.
9562,9.88762,27.374,24.3805,0,0.09747,-0.019889,-0.001822,-0.004845,-
0.036317,0.00183,-0.007436,-
0.006676,0.000838,0.006379,0.01273,707.752,352.105,484.751,672.691,858.302,825.1
83,814.196,742.441,723.577,493.744,396.663,3552.21,5477.72,3903.61,4613.66,7553.
31,9332.08,10022.5,10026.1,9581.09,8551.02,7096.26,0.964515,0.302465,-0.162885,-
0.54197,0.196644,-0.335374,0.469168,-0.424866,0.121904,0.114152,-
0.281397,4009.68,9700.18,7887.54,4258.43,7083.75,9570.67,10323.7,10559,11385.6,1
1540.8,10999.2,1.02151,0.218518,-0.157083,-0.605799,0.277713,-
0.402734,0.529993,-0.526582,0.283498,0.006733,-
0.233172,23,3,8,0,4,6,5,3,2,5,6,1,7,4,3,5,2,1,2,2,4,1,2,37,4,1,2,4,1,0,1,1,2,8,1
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23,21,19,18,21,22,20,20,18,19,7,31,17,20,20,22,27,28,14,24,15,7,16,14,15,19,19,1
2,12,17,15,11,0,9,18,6,19,7,17,9,21,12,14,8,10,8,9,11,17,3,11,11,10,6,0,5,7,7,5,
7,2,2,7,7,9,534.581,0.105223,15,16,0,15,16,3,2,56,1.7,58,2,2,15,16,21.8361,14.27
38,3,15.9347,2.76957,0.946484,1,0,1,0,0,0,0,0,0,0,0,82.69,0,5,3,119.31,1,1,10358,2
120.54,6570.17,8273.91,24.6387,11.2277,9.58262,6,4.90278,3.6982,82.69,47.059,4.5
4036,8.2177,14.2738,25.11,114.86,15,16,8,8.57826,0.939074,5,3167,82.69,411.466,2
476,2476,47,5,6,4.56,-
10,2,3,3,4.46,46.03,2.44,0.78,1.52,0.94,0.8,0.78,0.78,0.78,0.78,0.78,CYP2C9
33,38,20,35,57,69,76,69,61,47,46,355.506,8.88281,0,152.179,95.4607,164.966,351.6
25,216.584,28.9852,64.2684,0,0.47418,0.008189,0.002699,-0.224371,-
0.03302,0.054415,-0.00916,-0.010352,-0.105634,0.129635,-
0.048843,926.628,322.09,131.664,964.375,1254.15,1322.21,1351.44,1102.19,833.884,
780.808,568.767,2464.45,1788.13,885.561,3101.6,4889.04,5448.19,5329.33,4310.2,35
57.8,2911.11,2502.7,0.789174,0.009545,0.005827,-0.496717,0.185731,-0.006784,-
0.318529,0.371947,-0.132856,0.039823,-
0.051941,3111.53,2993.38,1505.41,3290.18,5362,6580.76,7471.43,6587.63,5326.37,41
62.52,3767.55,1.77939,0.011477,-0.032248,-1.10388,0.52009,-0.032862,-
0.918198,1.04019,-0.614995,0.319801,-
0.08086,8,4,2,0,1,2,2,1,0,0,2,0,6,0,0,1,0,2,0,0,2,0,0,9,0,1,0,0,0,1,0,0,0,2,14,1
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,0,0,8,9,16.7757,10.8194,3,14.1032,1.93271,0.98554,1,0,0,0,0,0,0,0,0,0,0,99.6,0,7,
2,84.69,3,2,3723,876.751,5174.33,5876.36,17.8112,6.71884,5.23498,6,3.66167,2.960
67,136.22,35.404,4.0049,7.37809,10.8194,15.07,87.9,15,16,2,7.94355,0.911493,5,16
97,99.6,371.821,1115,1115,41,8,11,0.89,4.45,8,2,2,-0.72,33.47,-2.07,-3.62,-
1.87,-1.26,-0.72,-0.96,-1.79,-2.72,-3.39,-3.59,CYP2C9
33,32,8,34,55,68,78,81,61,57,54,54.7953,0,0,0,15.4558,0,37.7645,0,0,0,0,0.084095
,0,0,-0.01698,-0.007958,-0.003595,-0.010734,-0.019415,0.016958,-
0.005752,0.005429,540.694,0,0,549.75,707.722,688.272,597.229,541.517,470.935,322
.617,107.308,1793.55,752.609,137.551,2245.45,3448.19,4084.09,4043.44,3614.67,287
1.19,2404.59,1708.85,0.500651,-0.063444,0.041228,-0.323416,0.120058,-
0.110188,0.208064,-0.245047,0.082204,0.051302,-
0.011086,2376.71,2135.02,477.124,2510.12,3960.99,4891.59,5498.77,5566.65,4262.92
,4013.05,3733.47,0.623191,-0.097064,0.041228,-0.42859,0.289107,-
0.285636,0.276811,-
0.298063,0.148515,0.017296,0.024799,13,2,0,0,0,0,0,0,0,0,0,0,2,0,0,0,0,0,0,0,0,0
,0,20,0,0,0,0,0,0,0,0,0,0,1,8,25,8,8,12,6,0,1,6,3,8,21,7,5,7,11,12,1,7,2,8,18,1,11
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,2,0,1,2,5,1,6,0,1,0,2,3,6,2,5,1,0,0,2,0,2,0,1,1,0,1,1,0,0,1,0,0,0,0,327.082,0.0
81282,6,7,0,12,12,2,0,33,1.83,34,2,2,6,7,13.121,8.59222,2,10.4572,2.26816,0.9362
85,1,0,1,0,0,0,0,0,0,0,49.33,0,3,2,56.36,0,0,1799,633.439,1803.43,1953.17,14.41,
6.43787,5.26749,6,4.47907,3.07155,49.33,28.887,3.01616,5.72195,8.59222,14.89,71.
88,12,12,3,5.48048,0.827551,6,930,49.33,241.285,602,602,27,3,4,3.89,-
1.68,3,2,2,3.85,26.92,3.58,0.72,2.82,1.88,1.09,0.77,0.72,0.72,0.72,0.72,CYP2C9

43,77,54,45,78,105,102,102,107,108,94,117.311,0,0,50.6702,40.2307,40.2307,7.9855
1,0,0,0,0,0.276535,0.001217,0,0.081227,-0.116536,-
0.216482,0.062043,0.020528,0.007904,0.022184,-
0.00035,647.611,28.1543,0,668.785,890.879,1004.65,922.47,844.142,610.071,317.393
,119.311,2393.31,2393.7,1328.66,3068.38,4968.25,5997.87,5934.35,5880.88,5568.79,
4777.5,3562.83,0.400215,-0.00662,0.006031,-0.160113,-0.025873,-
0.060565,0.012481,0.060888,0.067063,-0.081418,-
0.029983,3101.74,4525.82,3102.92,3317.85,5689.04,7711.8,7812.16,7977.02,8055.6,7
370.1,5750.95,0.842909,-0.020021,0.003449,-0.169576,-0.039684,-
0.597546,0.214047,0.239281,0.087954,-0.087705,-
0.064989,20,0,0,2,3,0,3,3,2,0,1,1,0,0,0,3,0,0,1,0,0,0,1,38,0,0,0,0,0,0,0,0,0,0,7,1
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9,11,10,8,13,12,10,0,11,12,12,5,13,12,8,11,10,12,6,11,10,8,15,12,5,7,5,4,12,0,13
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11,13,1,12,12,2,0,43,1.71,45,2,2,6,8,16.2338,11.2364,3,12.8408,1.30141,0.883225,
0,0,0,0,0,0,0,0,0,0,40.62,0,4,0,83.37,1,0,3588,1303.79,2780.23,3763.73,17.8112,8
.39273,6.42805,6,6.46054,2.89239,40.62,36.379,3.56713,7.39259,11.2364,19.17,88.7
6,17,17,5,7.45782,0.736981,5,1571,40.62,308.374,1109,1109,37,2,4,5.13,-
6.55,2,0,0,4.22,34.47,4.22,0.99,4.22,4.22,4.19,3.98,3.3,2.37,1.51,1.07,CYP2C9
27,21,14,28,45,51,53,41,32,33,22,296.848,8.19188,0,164.52,105.422,119.028,85.576
,65.868,42.1768,0,28.4415,0.471233,-0.003402,0,-0.171043,0.013432,-
0.220276,0.134669,0.029752,-0.007226,0.007703,-
0.019226,715.795,51.219,0,745.617,903.873,818.442,745.293,617.272,356.529,221.60
1,112.783,1614.11,688.648,385.889,1974.39,2974.39,3122.4,2937.79,2285.78,1747.3,
1527.55,948.08,0.465806,-0.044334,0.010872,-0.354646,0.270479,-0.172262,-
0.007405,-0.091606,0.340045,-
0.323452,0.148037,2423.38,1420.88,938.042,2545.53,4080.02,4504.05,4786.16,3712.6
1,2793.41,2957.11,1621.54,1.4512,-0.099491,0.0023,-0.900205,0.624839,-
0.80155,0.384954,-0.251384,0.613421,-
0.514758,0.217895,7,0,0,0,0,0,0,0,0,0,0,0,3,0,0,0,0,0,0,0,0,0,0,0,11,0,0,0,0,0,0,0
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5,0,1,1,0,2,1,0,0,1,0,0,0,1,0,0,0,0,0,297.647,0.070475,6,7,0,11,11,2,0,27,1.85,2
8,1,1,6,7,12.4663,7.97116,2,10.3931,6.12341,0.890331,0,0,1,0,0,0,0,0,0,0,0,97.97,0
,6,3,51.45,1,1,1646,881.596,1936.24,2477.56,13.4321,5.32544,6.47934,6,5.48366,2.
09547,134.59,26.961,3.12957,6.64609,7.97116,12.21,66.84,11,11,2,5.78396,0.563791
,5,731,97.97,270.333,535,535,22,7,9,5.51,1.95,6,2,3,0.03,25.13,-1.05,-1.11,-
0.25,-0.01,0.01,-0.08,-0.5,-0.97,-1.09,-1.11,CYP2C9
30,23,23,31,50,63,64,61,46,33,26,81.3281,47.5804,0,0,16.9558,21.2478,0,0,0,0,30.
6084,0.064313,-0.005815,-0.001681,-0.020684,0.003616,-0.014145,0.001915,-
0.00493,0.006728,-
0.021768,0.024607,588.16,183.453,171.86,517.274,631.152,651.219,677.863,499.112,
290.954,246.682,258.813,1654.49,923.839,692.041,2052,3119.56,3472.63,3213.53,279
9.47,2133.32,1531.42,1141.89,0.523151,0.058116,-0.007925,-
0.303206,0.00928,0.035827,0.079931,-0.014137,-0.059568,-
0.142075,0.121947,2368.46,1809.18,1687.92,2446.06,3840.03,4835.19,4950.74,4494.7
1,3319.64,2520.82,2187.38,0.762522,0.00066,0.011756,-
0.439345,0.076206,0.012723,0.090261,-0.055697,-0.024627,-
0.271019,0.267989,11,2,1,0,0,1,0,1,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,18,0,0,0,0,0,0,
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1.69,31,1,1,7,8,13.121,8.59222,2,11.7269,3.22598,0.97882,1,0,0,0,0,0,0,0,0,0,54.
37,0,3,1,55.2,1,1,2194,570.628,2787.32,3151.07,14.41,6.43787,6.144,6,4.50805,3.4
8189,82.61,28.009,3.53588,6.10024,8.59222,13.62,69.41,11,11,4,6.14198,0.922365,5
,924,54.37,260.309,653,653,25,4,6,3.46,-10,3,1,1,2.88,26.69,-0.15,-0.8,-0.67,-
0.79,-0.8,-0.8,-0.8,-0.8,-0.8,-0.8,CYP2C9

33,38,20,35,57,69,76,69,61,47,46,322.434,0,0,152.379,62.6219,161.152,272.56,130.
948,28.9918,19.2221,0,0.472412,0.013404,0.000518,-0.224425,-0.023812,0.048566,-
0.019997,-0.000867,-0.109092,0.132267,-
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703.897,532.554,2301.57,1655.41,781.929,2903.9,4583.1,5131.65,5008.41,4041.18,33
48.04,2741.55,2362.58,0.771814,-0.045159,-0.003586,-0.473067,0.12013,-0.005284,-
0.128433,0.14992,0.009313,-
0.06216,0.03427,3013.97,2885.11,1381.55,3212.15,5245.38,6437.52,7298.9,6330.04,5
157.38,3972.68,3670.59,1.76155,-0.076643,-0.024568,-1.08003,0.46402,-0.111644,-
0.613988,0.775227,-
0.474723,0.217843,0.03045,9,4,2,0,1,2,2,0,1,0,2,0,6,1,1,0,0,3,0,0,0,0,1,9,0,0,0,
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671,6,3.6432,2.93254,136.22,33.476,3.64285,7.37916,10.4256,15.07,83.93,15,16,2,7
.32106,0.823003,5,1513,99.6,337.376,988,988,39,7,10,1.32,4.45,8,2,2,-
1.11,31.41,-2.52,-4.06,-2.32,-1.69,-1.11,-1.25,-2.03,-2.97,-3.73,-4.02,CYP2C9
39,54,42,40,65,69,87,97,89,92,61,88.5554,32.5226,16.298,0,19.4131,37.2704,38.234
6,0,0,58.2549,29.1932,0.1253,0.007366,0.002807,-0.071301,0.037647,-0.007995,-
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0.005029,590.073,113.034,24.8353,586.521,768.047,736.331,500.692,463.854,563.897
,534.462,283.272,1659.25,1429.68,901.072,2059.82,3166.32,3673.32,3905.76,3714.76
,3151.94,2662.94,1845.86,0.937963,-0.061081,-0.008882,-0.535054,0.052749,-
0.003736,0.356001,-0.398072,-0.384189,0.668302,-
0.144641,2917.88,3997.54,3006.37,3186.98,5079.24,5513.63,6540.83,7080.46,6367.32
,6315.14,4487.88,1.10824,-0.206981,-0.031401,-0.780833,0.512933,-
0.365893,0.372098,-0.212218,-0.616101,0.789408,-
0.073994,14,1,0,0,0,0,0,0,0,0,0,0,0,18,0,0,0,0,0,0,0,0,0,0,0,9,0,0,0,0,0,0,0,0,0,0,2
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22,5.95041,6,5.39374,5.03643,105.51,30.881,3.47273,6.77798,10.0832,17.37,81.51,1
2,12,5,6.04904,0.553641,6,1466,105.51,290.318,946,946,33,7,7,20,7.16,6,2,4,1.05,
29.8,-0.27,1.05,-0.26,-0.26,-0.26,-0.21,0.09,0.69,0.99,1.04,CYP2C9
74,182,158,78,137,176,191,185,179,167,180,331.556,23.2817,74.8133,160.365,111.11
1,42.645,21.66,48.4769,72.461,53.3744,21.9813,0.567455,0.019457,0.078786,-
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345.5,9959.67,9951.98,1.09431,-0.191026,0.135978,-0.717911,0.411043,-0.28742,-
0.082558,0.271266,-0.253704,0.216287,-
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58,26,27,8,9.61104,0.750406,5,9240,115.73,575.676,6548,6548,66,7,11,4.29,-1.08,6,2,2,6.19,61.71,6.19,5.05,6.19,6.17,6.03,5.54,5.14,5.06,5.05,5.05,CYP2C9