The data set is saved in SOM_PAK format (used in SOM_Toolbox: http://www.cis.hut.fi/projects/somtoolbox/) in a text file readable in Notepad (MS Windows).

The first line in the file has only one number. It represents number of variables (in this case: descriptors and the modeled property). The second line starts with '#n' after this the names (or abbreviations) of the variables are given separated by spaces. Third line (which does not have to be present) starts with '#l'. This means that after this sign the names of the labels are given.

The structure of the abbreviation for the atom-based descriptors is for example:

'a_av_El_Affinity'

The first letter 'a' shows that the descriptor this is an atom-based descriptor. The second two letters 'av' or 'su' shows that the descriptor is based on the arithmetic mean of the values in the columns of the Laplacian-transformed property matrix (M). In the case of 'su' the final descriptors are obtained as a sum of the columns of M. The remaining part of the abbreviation represents the atomic property on which the descriptor is based. In this case, it is electron affinity.

In the case of bond-based descriptors (calculated from the line graphs) the structure of the abbreviations is:

'b_su_dif_VdW_radius'

Here the first letter 'b' shows that this is bond-based descriptor. 'su' represents that the descriptor was calculated as a sum of the columns of M. The next three letters ('sum' or 'dif') shows whether the bond property was calculated as a sum or absolute value of the differences of the atomic properties. The remaining part (in this case 'VdW_radius') represents the atomic property on which the descriptor is based.

This data set has 54 descriptors. The column number 55 corresponds to the modeled property (-log(LD50) in this case). The last column starts with '1' and ends with '69' this column has the labels for the structures as presented on Table 2.

55

#n a_av_Z a_av_Ar a_av_Elneg a_av_1st_ion_pot a_av_El_Affinity a_av_Ion_radius a_av_Atom_radius a_av_VdV_radius a_av_Polariz a_av_Atom_vol a_av_Vert_degree a_su_Z a_su_Ar a_su_Elneg a_su_1st_ion_pot a_su_El_Affinity a_su_Ion_radius a_su_Atom_radius a_su_VdV_radius a_su_Polariz a_su_Atom_vol a_su_Vert_degree b_av_dif_Ar b_av_dif_Elneg b_av_dif_El_Affinity b_av_dif_Ion_radius b_av_dif_Atom_radius b_av_dif_VdV_radius b_av_dif_Polariz b_av_dif_Atom_vol b_su_dif_Ar b_su_dif_Elneg b_su_dif_El_Affinity b_su_dif_Ion_radius b_su_dif_Atom_radius b_su_dif_VdV_radius b_su_dif_Polariz b_su_dif_Atom_vol b_av_sum_Ar b_av_sum_Elneg b_av_sum_El_Affinity b_av_sum_Ion_radius b_av_sum_Atom_radius b_av_sum_VdV_radius b_av_sum_Polariz b_av_sum_Atom_vol b_su_sum_Ar b_su_sum_Elneg b_su_sum_El_Affinity b_su_sum_Ion_radius b_su_sum_Atom_radius b_su_sum_VdV_radius b_su_sum_Polariz b_su_sum_Atom_vol property

labels

48 96.088 20.4 90.08 10.08 1.28 7.28 1360 14.4 36.64 80 288 576.528 122.4 540.48 60.48 7.68 43.68 8160 86.4 219.84 480 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 192.176 40.8 20.16 2.56 14.56 2720 28.8 73.28 1153.06 244.8 120.96 15.36 87.36 16320 172.8 439.68 3.4 1

70.9948 150.223 20.3567 89.8043 11.6218 2.739 7.31703 1346.96 15.202 53.2727 74.5776 496.963 1051.56 142.497 628.63 81.3525 19.173 51.2192 9428.69 106.414 372.909 522.043 34.6411 0.209207 1.07155 0.918469 0.107155 7.65391 0.663339 10.7257 242.488 1.46445 7.50083 6.42929 0.750083 53.5774 4.64337 75.0798 260.241 40.9396 22.1681 4.38203 14.6749 2716.7 29.9313 94.2601 1821.69 286.577 155.177 30.6742 102.724 19016.9 209.519 659.821 3.89 2

57.8133 113.603 20.5215 89.8046 11.8277 2.61542 7.19345 1338.72 14.4606 46.1053 74.5776 404.693 795.222 143.651 628.632 82.7942 18.308 50.3542 9371.02 101.224 322.737 522.043 11.96 0.311259 1.19911 0.84193 0.0306156 2.5513 0.204104 6.28641 83.72 2.17881 8.39379 5.89351 0.21431 17.8591 1.42873 44.0049 214.814 41.144 22.4236 4.22873 14.5216 2706.48 29.0116 85.3689 1503.7 288.008 156.965 29.6011 101.651 18945.4 203.081 597.582 3.77 3

48.7511 97.5787 20.7522 90.3401 10.0565 2.27765 6.92983 1319.77 13.3014 43.7162 78.8749 341.258 683.051 145.265 632.381 70.3954 15.9436 48.5088 9238.38 93.11 306.013 552.124 2.03492 0.454132 0.102052 0.632723 0.132668 9.18469 0.513833 4.80666 14.2444 3.17892 0.714365 4.42906 0.928675 64.2929 3.59683 33.6466 194.936 41.4302 20.2263 3.80972 14.1946 2682.98 27.5736 82.4052 1364.55 290.011 141.584 26.668 99.362 18780.8 193.015 576.836 3.51 4

47.1035 94.2933 20.019 88.3975 9.89173 1.25609 7.14402 1334.6 14.131 35.9556 78.8749 329.724 660.053 140.133 618.782 69.2421 8.79264 50.0082 9342.18 98.9173 251.689 552.124 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 190.86 40.5206 20.0219 2.54247 14.4603 2701.37 28.6028 72.7782 1336.02 283.644 140.154 17.7973 101.222 18909.6 200.219 509.447 3.32 5

64.8787 126.208 20.598 89.5555 13.0852 3.57981 7.12686 1322.58 14.4963 52.9254 78.0689 519.029 1009.66 164.784 716.444 104.682 28.6385 57.0149 10580.6 115.971 423.403 624.551 20.0926 0.522909 2.01449 1.41443 0.0514337 4.28614 0.342891 10.561 160.741 4.18327 16.1159 11.3154 0.411469 34.2891 2.74313 84.4884 229.499 41.2498 23.889 5.34713 14.4506 2688.93 29.0651 93.3015 1835.99 329.998 191.112 42.777 115.605 21511.5 232.521 746.412 4.4 6

65.122 126.651 20.6174 89.6242 13.1298 3.60858 7.13108 1323.26 14.5095 53.1521 78.0005 520.976 1013.21 164.939 716.994 105.039 28.8686 57.0487 10586.1 116.076 425.217 624.004 20.7508 0.540039 2.08048 1.46076 0.0531186 4.42655 0.354124 10.907 166.006 4.32031 16.6438 11.6861 0.424949 35.4124 2.83299 87.2562 231.747 41.5091 24.1194 5.44387 14.5353 2704.44 29.2467 94.3276 1853.97 332.073 192.955 43.551 116.282 21635.5 233.973 754.621 4.3 7

65.186 126.765 20.618 89.6217 13.1412 3.61733 7.13046 1323.11 14.5098 53.214 78.0053 521.488 1014.12 164.944 716.974 105.13 28.9386 57.0437 10584.9 116.078 425.712 624.042 20.93 0.544703 2.09845 1.47338 0.0535774 4.46478 0.357183 11.0012 167.44 4.35763 16.7876 11.787 0.428619 35.7183 2.85746 88.0098 231.984 41.476 24.1422 5.4726 14.5204 2701.55 29.2227 94.4828 1855.87 331.808 193.138 43.7808 116.164 21612.4 233.782 755.862 4.62 8

57.073 112.405 20.7967 90.0168 11.5596 3.28887 6.89979 1306.26 13.4979 50.8676 78.0689 456.584 899.242 166.373 720.134 92.4765 26.311 55.1983 10450.1 107.983 406.941 624.551 11.7556 0.642921 1.09297 1.23869 0.137156 9.85812 0.60306 9.31807 94.0448 5.14337 8.74373 9.90956 1.09725 78.865 4.82448 74.5445 212.851 41.4894 22.0488 4.99622 14.1767 2669.25 27.8609 90.8194 1702.81 331.915 176.39 39.9697 113.414 21354 222.887 726.555 4.02 9

55.7859 109.818 20.1793 88.3976 11.4421 2.42362 7.08799 1319.67 14.2222 44.3044 78.0005 446.288 878.543 161.434 707.181 91.5372 19.389 56.704 10557.4 113.778 354.436 624.004 10.3754 0.27002 1.04024 0.730381 0.0265593 2.21328 0.177062 5.45351 83.0032 2.16016 8.32192 5.84305 0.212474 17.7062 1.4165 43.6281 211.101 40.9718 22.0494 3.99047 14.4824 2700.04 28.8943 83.4755 1688.8 327.774 176.395 31.9237 115.859 21600.3 231.155 667.804 3.84 10

55.8148 109.869 20.1783 88.3905 11.4472 2.42791 7.08721 1319.51 14.2214 44.333 78.0053 446.519 878.949 161.426 707.124 91.5775 19.4233 56.6977 10556.1 113.772 354.664 624.042 10.465 0.272352 1.04922 0.736689 0.0267887 2.23239 0.178591 5.50061 83.72 2.17881 8.39379 5.89351 0.21431 17.8591 1.42873 44.0049 211.114 40.9329 22.0497 4.00343 14.467 2697.1 28.8666 83.513 1688.91 327.463 176.398 32.0274 115.736 21576.8 230.933 668.104 4.33 11

49.3225 98.713 21.0195 90.5578 10.0417 3.01969 6.67146 1290.23 12.4886 48.9868 78.0005 394.58 789.704 168.156 724.463 80.334 24.1575 53.3717 10321.8 99.9089 391.895 624.004 3.53062 0.787926 0.177062 1.09778 0.230181 15.9356 0.891508 8.33962 28.2449 6.30341 1.4165 8.78228 1.84145 127.485 7.13206 66.717 197.48 42.0024 20.3317 4.72157 13.9715 2663.92 26.7679 89.2187 1579.84 336.019 162.654 37.7726 111.772 21311.4 214.144 713.75 3.04 12

49.8904 99.8478 21.2662 91.4383 10.1318 3.19247 6.68276 1296.4 12.4455 50.4688 72.2985 449.014 898.63 191.396 822.944 91.186 28.7322 60.1449 11667.6 112.01 454.22 650.687 4.84196 1.08058 0.242826 1.50552 0.315674 21.8544 1.22263 11.4371 43.5776 9.72519 2.18544 13.5497 2.84107 196.689 11.0037 102.934 197.743 42.0853 20.2227 5.46773 13.6397 2621.06 25.8033 94.2617 1779.69 378.768 182.004 49.2096 122.757 23589.5 232.23 848.355 3.21 13

47.8481 95.7728 20.3638 88.8047 9.89198 2.11802 6.85721 1302.71 13.2141 42.1252 78.0689 382.785 766.182 162.911 710.438 79.1359 16.9441 54.8577 10421.7 105.713 337.002 624.551 1.70931 0.381466 0.0857228 0.531481 0.11144 7.71505 0.431614 4.03754 13.6745 3.05173 0.685782 4.25185 0.891517 61.7204 3.45291 32.3004 192.79 40.9673 20.0375 3.584 14.1254 2664.97 27.5186 80.2749 1542.32 327.739 160.3 28.672 113.003 21319.7 220.148 642.199 3.77 14

47.8862 95.849 20.3804 88.8644 9.89811 2.12918 6.85818 1303.15 13.2118 42.2218 78.0005 383.09 766.792 163.043 710.915 79.1849 17.0334 54.8655 10425.2 105.694 337.774 624.004 1.76531 0.393963 0.088531 0.548892 0.11509 7.96779 0.445754 4.16981 14.1225 3.1517 0.708248 4.39114 0.920723 63.7423 3.56603 33.3585 193.967 41.2184 20.1556 3.62932 14.2005 2679.78 27.655 80.9211 1551.74 329.747 161.244 29.0346 113.604 21438.2 221.24 647.369 3.29 15

47.8854 95.8473 20.3801 88.8591 9.89734 2.13236 6.85653 1302.93 13.2072 42.2425 78.0053 383.083 766.778 163.041 710.873 79.1787 17.0589 54.8523 10423.4 105.658 337.94 624.042 1.78055 0.397366 0.0892956 0.553633 0.116084 8.03661 0.449604 4.20582 14.2444 3.17892 0.714365 4.42906 0.928675 64.2929 3.59683 33.6466 193.795 41.1822 20.1354 3.63836 14.1821 2676.62 27.6138 80.9308 1550.36 329.458 161.083 29.1069 113.457 21413 220.91 647.446 3.58 16

50.7234 101.506 21.6929 94.1353 8.86216 4.96707 6.38944 1262.35 11.3872 64.5883 73.395 507.234 1015.06 216.929 941.353
88.6216 49.6707 63.8944 12623.5 113.872 645.883 733.95 3.80546 0.83853 1.63621 1.40429 0.240904 15.733 0.913697 11.7967
38.0546 8.3853 16.3621 14.0429 2.40904 157.33 9.13697 117.967 202.672 43.2782 17.4648 8.85033 13.4191 2607.32 24.5827 122.55
2026.72 432.782 174.648 88.5033 134.191 26073.2 245.827 1225.5 3.36 17

50.3307 100.727 21.4577 92.1119 10.2002 3.33394 6.68794 1300.71 12.4019 51.6679 65.0865 503.307 1007.27 214.577 921.119
102.002 33.3394 66.8794 13007.1 124.019 516.679 650.865 5.91094 1.31914 0.296436 1.83791 0.385367 26.6793 1.49256 13.9622
59.1094 13.1914 2.96436 18.3791 3.85367 266.793 14.9256 139.622 197.778 42.1152 20.1132 6.08298 13.3512 2582.99 24.9773
98.3668 1977.78 421.152 201.132 60.8298 133.512 25829.9 249.773 983.668 3.07 18

46.4289 92.9428 19.7323 87.1315 9.75006 1.2381 7.04171 1315.48 13.9287 35.4407 78.0689 371.431 743.543 157.858 697.052
78.0005 9.90482 56.3337 10523.9 111.429 283.526 624.551 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 189.376 40.2056 19.8663 2.5227
14.3479 2680.37 28.3804 72.2124 1515.01 321.645 158.93 20.1816 114.783 21443 227.043 577.699 3.48 19

46.4437 92.9725 19.7386 87.1593 9.75317 1.2385 7.04396 1315.9 13.9331 35.452 78.0053 371.549 743.78 157.908 697.274 78.0254
9.90798 56.3517 10527.2 111.465 283.616 624.042 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 190.244 40.3897 19.9573 2.53426 14.4136
2692.65 28.5104 72.5431 1521.95 323.118 159.658 20.2741 115.309 21541.2 228.083 580.345 4.21 20

49.5782 99.223 21.1827 92.7876 8.75646 4.24086 6.54387 1273.4 11.9802 59.0773 69.026 495.782 992.23 211.827 927.876 87.5646
42.4086 65.4387 12734 119.802 590.773 690.26 2.35712 0.515015 1.54997 0.946212 0.146284 9.15689 0.546704 8.30548 23.5712
5.15015 15.4997 9.46212 1.46284 91.5689 5.46704 83.0548 199.3 42.5291 17.3076 7.90518 13.5787 2614.61 25.2651 115.223 1993
425.291 173.076 79.0518 135.787 26146.1 252.651 1152.23 3.57 21

49.5847 99.236 21.1859 92.8013 8.75166 4.25047 6.54201 1273.2 11.9735 59.1522 68.9771 495.847 992.36 211.859 928.013 87.5166
42.5047 65.4201 12732 119.735 591.522 689.771 2.3767 0.519578 1.5622 0.958034 0.147691 9.2713 0.5525 8.40457 23.767 5.19578
15.622 9.58034 1.47691 92.713 5.525 84.0457 200.074 42.6952 17.3578 7.9579 13.6257 2623.99 25.3458 115.838 2000.74 426.952
173.578 79.579 136.257 26239.9 253.458 1158.38 3.63 22

49.57 99.2065 21.1797 92.7754 8.74682 4.25198 6.53938 1272.73 11.9679 59.1559 73.395 495.7 992.065 211.797 927.754 87.4682
42.5198 65.3938 12727.3 119.679 591.559 733.95 2.38101 0.520638 1.56477 0.961386 0.148037 9.30373 0.554014 8.43207 23.8101
5.20638 15.6477 9.61386 1.48037 93.0373 5.54014 84.3207 199.831 42.6442 17.3223 7.96705 13.6043 2620.14 25.3 115.84 1998.31
426.442 173.223 79.6705 136.043 26201.4 253 1158.4 3.76 23

51.6931 103.44 22.1559 96.5808 8.1036 6.23623 6.21571 1245.98 10.6903 74.7927 64.9791 620.317 1241.29 265.871 1158.97
97.2432 74.8347 74.5886 14951.8 128.284 897.513 779.749 3.91992 0.856244 2.57815 1.57033 0.243117 15.1968 0.908154 13.7876
47.039 10.2749 30.9379 18.844 2.9174 182.361 10.8978 165.451 205.992 44.0931 15.6345 11.4648 13.0787 2572.81 23.2217 143.697
2471.9 529.117 187.614 137.578 156.944 30873.7 278.66 1724.36 5.45 24

51.6746 103.403 22.149 96.5548 8.08312 6.25834 6.20674 1244.62 10.6659 74.9492 64.97 620.095 1240.84 265.788 1158.66 96.9974
75.1001 74.4809 14935.4 127.991 899.391 779.64 3.96116 0.865963 2.60367 1.59672 0.246151 15.4522 0.920833 14.0076 47.5339
10.3916 31.244 19.1607 2.95381 185.426 11.05 168.091 206.502 44.2055 15.6144 11.5691 13.0916 2576.52 23.2192 144.63 2478.03
530.466 187.373 138.829 157.1 30918.3 278.63 1735.56 4.38 25

51.6542 103.362 22.1404 96.5195 8.07593 6.26097 6.203 1243.95 10.6577 74.9586 68.7829 619.85 1240.35 265.685 1158.23 96.9111
75.1316 74.436 14927.4 127.893 899.503 825.394 3.96835 0.867729 2.60796 1.60231 0.246728 15.5062 0.923356 14.0535 47.6203
10.4128 31.2955 19.2277 2.96073 186.075 11.0803 168.641 206.223 44.1472 15.5657 11.5889 13.0648 2571.8 23.1598 144.705
2474.68 529.767 186.788 139.067 156.778 30861.6 277.917 1736.46 5.22 26

49.3904 98.8462 21.1261 93.1765 8.14785 4.75352 6.44387 1257.75 11.6728 63.1496 69.3159 543.294 1087.31 232.387 1024.94
89.6264 52.2887 70.8825 13835.2 128.401 694.645 762.474 2.76079 0.619898 1.77749 1.34007 0.182521 12.9684 0.713722 11.4885
30.3687 6.81888 19.5524 14.7408 2.00774 142.652 7.85094 126.374 198.94 42.4736 16.7402 8.35538 13.4994 2601.82 25.0187
118.839 2188.34 467.21 184.142 91.9092 148.494 28620 275.206 1307.23 3.48 27

49.3923 98.8499 21.1274 93.1842 8.13975 4.7653 6.44091 1257.36 11.6635 63.2393 66.6608 543.315 1087.35 232.401 1025.03
89.5373 52.4183 70.85 13830.9 128.299 695.633 733.269 2.78282 0.625086 1.79113 1.3541 0.184139 13.1042 0.720476 11.6056
30.6111 6.87595 19.7024 14.8952 2.02553 144.147 7.92524 127.661 199.602 42.6161 16.7721 8.41345 13.5366 2609.42 25.0782
119.465 2195.62 468.777 184.493 92.548 148.903 28703.6 275.86 1314.12 3.24 28

49.3903 98.846 21.1264 93.1778 8.14209 4.76225 6.44123 1257.39 11.6649 63.2143 63.0381 543.293 1087.31 232.391 1024.96
89.563 52.3848 70.8535 13831.3 128.314 695.357 693.419 2.77727 0.623724 1.78782 1.3498 0.183695 13.0625 0.71853 11.5702
30.55 6.86096 19.666 14.8477 2.02064 143.688 7.90383 127.272 199.584 42.6117 16.7827 8.39967 13.5381 2609.55 25.0844 119.352
2195.42 468.729 184.61 92.3963 148.919 28705.1 275.928 1312.87 3.35 29

49.3792 98.824 21.1207 93.14 8.16111 4.73625 6.44565 1257.91 11.6806 63.0079 69.3159 543.172 1087.06 232.327 1024.54 89.7722
52.0988 70.9021 13837 128.487 693.086 762.474 2.73235 0.612916 1.76053 1.31798 0.180242 12.7547 0.703748 11.3073 30.0558
6.74208 19.3658 14.4978 1.98266 140.301 7.74123 124.38 198.882 42.4593 16.775 8.31 13.5041 2602.26 25.0392 118.466 2187.7
467.052 184.526 91.41 148.545 28624.8 275.431 1303.13 3.8 30

49.3954 98.8563 21.128 93.1801 8.15475 4.74731 6.44593 1258.07 11.6785 63.1036 73.2712 543.35 1087.42 232.408 1024.98
89.7022 52.2204 70.9052 13838.8 128.464 694.139 805.983 2.75283 0.617945 1.77274 1.33389 0.181884 12.9086 0.710931 11.4378
30.2812 6.79739 19.5002 14.6728 2.00072 141.995 7.82025 125.816 199.647 42.623 16.8308 8.34753 13.5563 2612.29 25.1355
118.972 2196.12 468.853 185.139 91.8228 149.12 28735.2 276.49 1308.69 3.8 31

49.4062 98.878 21.1327 93.2015 8.15585 4.74886 6.44731 1258.34 11.6809 63.1218 69.2568 543.469 1087.66 232.459 1025.22
89.7144 52.2375 70.9204 13841.7 128.49 694.339 761.825 2.75446 0.618344 1.77371 1.33515 0.182014 12.9208 0.711501 11.4482
30.299 6.80178 19.5108 14.6867 2.00215 142.129 7.82652 125.93 199.732 42.6409 16.8389 8.3482 13.5633 2613.56 25.1496 119.003
2197.05 469.05 185.227 91.8302 149.196 28749.1 276.645 1309.03 3.79 32

50.4403 100.94 21.5933 94.4427 8.24574 5.39976 6.31256 1248.97 11.1582 68.0764 69.2568 554.844 1110.34 237.526 1038.87
90.7031 59.3973 69.4382 13738.7 122.74 748.84 761.825 4.01135 0.899446 1.8515 1.73854 0.264362 18.675 1.03153 14.5254
44.1248 9.89391 20.3665 19.124 2.90798 205.425 11.3468 159.78 202.218 43.1969 16.9278 9.1469 13.4004 2602.17 24.5164 125.096
2224.4 475.166 186.206 100.616 147.404 28623.9 269.681 1376.06 3.65 33

49.4167 98.8989 21.1378 93.2359 8.14337 4.76511 6.44563 1258.18 11.6736 63.2551 69.2568 543.584 1087.89 232.516 1025.59
89.5771 52.4162 70.902 13840 128.41 695.806 761.825 2.78148 0.624978 1.78983 1.35614 0.18418 13.1239 0.720979 11.6204
30.5963 6.87476 19.6881 14.9175 2.02598 144.363 7.93077 127.824 199.787 42.6544 16.8059 8.39108 13.5588 2613.14 25.1302
119.355 2197.66 469.199 184.865 92.3019 149.147 28744.6 276.432 1312.9 3.77 34

70.341 135.954 20.6592 89.3726 14.0575 4.32483 7.0762 1310.26 14.5255 58.1971 77.429 633.069 1223.58 185.933 804.354 126.518
38.9235 63.6858 11792.3 130.729 523.774 696.861 26.3704 0.68629 2.6439 1.85636 0.0675039 5.62533 0.450026 13.8608 237.334

6.17661 23.7951 16.7072 0.607535 50.628 4.05024 124.747 240.977 41.3798 25.0356 6.20683 14.4137 2678.76 29.1408 99.4653
2168.79 372.418 225.32 55.8615 129.723 24108.8 262.267 895.188 4.89 35

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126.944 39.2014 63.7222 11798.1 130.848 525.947 696.259 27.003 0.702753 2.70733 1.90089 0.0691232 5.76027 0.460821 14.1933
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3024.32 501.28 312.335 91.1826 170.06 31766.5 342.289 1313.56 6.06 69