A Full Computational Evaluation of Two Novel Chalcone Derivatives as Inhibitors for Colon Cancer Related Proteins.

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**S1 Table:** Residue-Specific binding probability of the studied proteins.

**S2 Table:** Bond lenghts of the Xanthohumol and 8-Prenylnaringenin derivatives.

**S3 Table:** Bond angles of the Xanthohumol and 8-Prenylnaringenin derivatives.

**S4 Table:** Atomic charges of the Xanthohumol and 8-Prenylnaringenin derivatives.

**S1 Table:** Residue-Specific binding probability of the studied proteins.

**3F6U**

r=LEU;n=1 :prob\_ions=0.000;prob\_organic=0.028

r=ILE;n=2 :prob\_ions=0.044;prob\_organic=0.029

r=ASP;n=3 :prob\_ions=0.002;prob\_organic=0.027

r=GLY;n=4 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=5 :prob\_ions=0.000;prob\_organic=0.027

r=MET;n=6 :prob\_ions=0.000;prob\_organic=0.027

r=THR;n=7 :prob\_ions=0.000;prob\_organic=0.029

r=ARG;n=8 :prob\_ions=0.000;prob\_organic=0.032

r=ARG;n=9 :prob\_ions=0.001;prob\_organic=0.032

r=GLY;n=10 :prob\_ions=0.000;prob\_organic=0.035

r=ASP;n=11 :prob\_ions=0.000;prob\_organic=0.034

r=SER;n=12 :prob\_ions=0.000;prob\_organic=0.037

r=PRO;n=13 :prob\_ions=0.000;prob\_organic=0.037

r=TRP;n=14 :prob\_ions=0.000;prob\_organic=0.036

r=GLN;n=15 :prob\_ions=0.001;prob\_organic=0.034

r=VAL;n=16 :prob\_ions=0.000;prob\_organic=0.030

r=VAL;n=17 :prob\_ions=0.013;prob\_organic=0.029

r=LEU;n=18 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=19 :prob\_ions=0.076;prob\_organic=0.030

r=ASP;n=20 :prob\_ions=0.000;prob\_organic=0.033

r=SER;n=21 :prob\_ions=0.000;prob\_organic=0.027

r=LYS;n=22 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=23 :prob\_ions=0.004;prob\_organic=0.028

r=LYS;n=24 :prob\_ions=0.000;prob\_organic=0.032

r=LEU;n=25 :prob\_ions=0.000;prob\_organic=0.060

r=ALA;n=26 :prob\_ions=0.000;prob\_organic=0.191

r=CYS;n=27 :prob\_ions=0.000;prob\_organic=0.124

r=GLY;n=28 :prob\_ions=0.000;prob\_organic=0.028

r=ALA;n=29 :prob\_ions=0.000;prob\_organic=0.028

r=VAL;n=30 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=31 :prob\_ions=0.000;prob\_organic=0.028

r=ILE;n=32 :prob\_ions=0.000;prob\_organic=0.027

r=HIS;n=33 :prob\_ions=0.000;prob\_organic=0.027

r=PRO;n=34 :prob\_ions=0.000;prob\_organic=0.027

r=SER;n=35 :prob\_ions=0.000;prob\_organic=0.026

r=TRP;n=36 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=37 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=38 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=39 :prob\_ions=0.000;prob\_organic=0.027

r=ALA;n=40 :prob\_ions=0.000;prob\_organic=0.029

r=ALA;n=41 :prob\_ions=0.000;prob\_organic=0.027

r=HIS;n=42 :prob\_ions=0.000;prob\_organic=1.000

r=CYS;n=43 :prob\_ions=0.000;prob\_organic=0.059

r=MET;n=44 :prob\_ions=0.000;prob\_organic=0.028

r=ASP;n=45 :prob\_ions=0.000;prob\_organic=0.056

r=GLU;n=46 :prob\_ions=0.000;prob\_organic=0.033

r=SER;n=47 :prob\_ions=0.000;prob\_organic=0.028

r=LYS;n=48 :prob\_ions=0.000;prob\_organic=0.027

r=LYS;n=49 :prob\_ions=0.000;prob\_organic=0.028

r=LEU;n=50 :prob\_ions=0.000;prob\_organic=0.032

r=LEU;n=51 :prob\_ions=0.000;prob\_organic=0.029

r=VAL;n=52 :prob\_ions=0.002;prob\_organic=0.027

r=ARG;n=53 :prob\_ions=0.909;prob\_organic=0.032

r=LEU;n=54 :prob\_ions=0.087;prob\_organic=0.031

r=GLY;n=55 :prob\_ions=0.146;prob\_organic=0.033

r=GLU;n=56 :prob\_ions=0.983;prob\_organic=0.038

r=TYR;n=57 :prob\_ions=0.195;prob\_organic=0.031

r=ASP;n=58 :prob\_ions=0.499;prob\_organic=0.030

r=LEU;n=59 :prob\_ions=0.213;prob\_organic=0.031

r=ARG;n=60 :prob\_ions=0.050;prob\_organic=0.030

r=ARG;n=61 :prob\_ions=0.789;prob\_organic=0.032

r=TRP;n=62 :prob\_ions=0.966;prob\_organic=0.030

r=GLU;n=63 :prob\_ions=0.725;prob\_organic=0.029

r=LYS;n=64 :prob\_ions=0.060;prob\_organic=0.027

r=TRP;n=65 :prob\_ions=0.048;prob\_organic=0.028

r=GLU;n=66 :prob\_ions=0.995;prob\_organic=0.031

r=LEU;n=67 :prob\_ions=0.069;prob\_organic=0.028

r=ASP;n=68 :prob\_ions=0.012;prob\_organic=0.029

r=LEU;n=69 :prob\_ions=0.000;prob\_organic=0.027

r=ASP;n=70 :prob\_ions=0.000;prob\_organic=0.028

r=ILE;n=71 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=72 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=73 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=74 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=75 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=76 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=77 :prob\_ions=0.000;prob\_organic=0.027

r=PRO;n=78 :prob\_ions=0.000;prob\_organic=0.027

r=ASN;n=79 :prob\_ions=0.000;prob\_organic=0.027

r=TYR;n=80 :prob\_ions=0.000;prob\_organic=0.038

r=SER;n=81 :prob\_ions=0.000;prob\_organic=0.028

r=LYS;n=82 :prob\_ions=0.000;prob\_organic=0.045

r=SER;n=83 :prob\_ions=0.000;prob\_organic=0.508

r=THR;n=84 :prob\_ions=0.000;prob\_organic=0.781

r=THR;n=85 :prob\_ions=0.000;prob\_organic=0.997

r=ASP;n=86 :prob\_ions=0.000;prob\_organic=0.027

r=ASN;n=87 :prob\_ions=0.000;prob\_organic=0.027

r=ASP;n=88 :prob\_ions=0.000;prob\_organic=0.056

r=ILE;n=89 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=90 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=91 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=92 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=93 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=94 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=95 :prob\_ions=0.000;prob\_organic=0.027

r=GLN;n=96 :prob\_ions=0.000;prob\_organic=0.027

r=PRO;n=97 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=98 :prob\_ions=0.000;prob\_organic=0.027

r=THR;n=99 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=100 :prob\_ions=0.000;prob\_organic=0.027

r=SER;n=101 :prob\_ions=0.000;prob\_organic=0.029

r=GLN;n=102 :prob\_ions=0.000;prob\_organic=0.032

r=THR;n=103 :prob\_ions=0.000;prob\_organic=0.035

r=ILE;n=104 :prob\_ions=0.000;prob\_organic=0.031

r=VAL;n=105 :prob\_ions=0.000;prob\_organic=0.032

r=PRO;n=106 :prob\_ions=0.000;prob\_organic=0.031

r=ILE;n=107 :prob\_ions=0.000;prob\_organic=0.029

r=CYS;n=108 :prob\_ions=0.000;prob\_organic=0.030

r=LEU;n=109 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=110 :prob\_ions=0.000;prob\_organic=0.027

r=ASP;n=111 :prob\_ions=0.000;prob\_organic=0.027

r=SER;n=112 :prob\_ions=0.000;prob\_organic=0.027

r=GLY;n=113 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=114 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=115 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=116 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=117 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=118 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=119 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=120 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=121 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=122 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=123 :prob\_ions=0.000;prob\_organic=0.027

r=GLN;n=124 :prob\_ions=0.000;prob\_organic=0.028

r=GLU;n=125 :prob\_ions=0.000;prob\_organic=0.028

r=THR;n=126 :prob\_ions=0.000;prob\_organic=0.028

r=LEU;n=127 :prob\_ions=0.000;prob\_organic=0.029

r=VAL;n=128 :prob\_ions=0.000;prob\_organic=0.028

r=THR;n=129 :prob\_ions=0.000;prob\_organic=0.028

r=GLY;n=130 :prob\_ions=0.000;prob\_organic=0.027

r=TRP;n=131 :prob\_ions=0.067;prob\_organic=0.030

r=GLY;n=132 :prob\_ions=0.000;prob\_organic=0.028

r=TYR;n=133 :prob\_ions=0.000;prob\_organic=0.042

r=HIS;n=134 :prob\_ions=0.000;prob\_organic=0.027

r=SER;n=135 :prob\_ions=0.000;prob\_organic=0.027

r=SER;n=136 :prob\_ions=0.000;prob\_organic=0.024

r=ARG;n=137 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=138 :prob\_ions=0.000;prob\_organic=0.027

r=LYS;n=139 :prob\_ions=0.000;prob\_organic=0.027

r=GLU;n=140 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=141 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=142 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=143 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=144 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=145 :prob\_ions=0.000;prob\_organic=0.027

r=THR;n=146 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=147 :prob\_ions=0.002;prob\_organic=0.027

r=VAL;n=148 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=149 :prob\_ions=0.000;prob\_organic=0.031

r=ASN;n=150 :prob\_ions=0.000;prob\_organic=0.027

r=PHE;n=151 :prob\_ions=0.000;prob\_organic=0.027

r=ILE;n=152 :prob\_ions=0.023;prob\_organic=0.029

r=LYS;n=153 :prob\_ions=0.004;prob\_organic=0.029

r=ILE;n=154 :prob\_ions=0.178;prob\_organic=0.030

r=PRO;n=155 :prob\_ions=0.014;prob\_organic=0.027

r=VAL;n=156 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=157 :prob\_ions=0.030;prob\_organic=0.027

r=PRO;n=158 :prob\_ions=0.000;prob\_organic=0.027

r=HIS;n=159 :prob\_ions=0.000;prob\_organic=0.027

r=ASN;n=160 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=161 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=162 :prob\_ions=0.001;prob\_organic=0.027

r=SER;n=163 :prob\_ions=0.000;prob\_organic=0.027

r=GLU;n=164 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=165 :prob\_ions=0.003;prob\_organic=0.027

r=MET;n=166 :prob\_ions=0.004;prob\_organic=0.037

r=SER;n=167 :prob\_ions=0.000;prob\_organic=0.040

r=ASN;n=168 :prob\_ions=0.000;prob\_organic=0.902

r=MET;n=169 :prob\_ions=0.000;prob\_organic=0.055

r=VAL;n=170 :prob\_ions=0.000;prob\_organic=0.027

r=SER;n=171 :prob\_ions=0.000;prob\_organic=0.027

r=GLU;n=172 :prob\_ions=0.000;prob\_organic=0.027

r=ASN;n=173 :prob\_ions=0.000;prob\_organic=0.027

r=MET;n=174 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=175 :prob\_ions=0.000;prob\_organic=0.027

r=CYS;n=176 :prob\_ions=0.006;prob\_organic=0.028

r=ALA;n=177 :prob\_ions=0.640;prob\_organic=0.032

r=GLY;n=178 :prob\_ions=0.871;prob\_organic=0.031

r=ILE;n=179 :prob\_ions=0.900;prob\_organic=0.031

r=LEU;n=180 :prob\_ions=0.432;prob\_organic=0.029

r=GLY;n=181 :prob\_ions=0.049;prob\_organic=0.027

r=ASP;n=182 :prob\_ions=0.879;prob\_organic=0.030

r=ARG;n=183 :prob\_ions=0.421;prob\_organic=0.030

r=GLN;n=184 :prob\_ions=0.890;prob\_organic=0.033

r=ASP;n=185 :prob\_ions=0.522;prob\_organic=1.000

r=ALA;n=186 :prob\_ions=0.025;prob\_organic=1.000

r=CYS;n=187 :prob\_ions=0.000;prob\_organic=1.000

r=GLU;n=188 :prob\_ions=0.000;prob\_organic=1.000

r=GLY;n=189 :prob\_ions=0.000;prob\_organic=0.943

r=ASP;n=190 :prob\_ions=0.000;prob\_organic=0.293

r=SER;n=191 :prob\_ions=0.000;prob\_organic=1.000

r=GLY;n=192 :prob\_ions=0.000;prob\_organic=0.029

r=GLY;n=193 :prob\_ions=0.000;prob\_organic=0.028

r=PRO;n=194 :prob\_ions=0.000;prob\_organic=0.027

r=MET;n=195 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=196 :prob\_ions=0.000;prob\_organic=0.027

r=ALA;n=197 :prob\_ions=0.000;prob\_organic=0.028

r=SER;n=198 :prob\_ions=0.000;prob\_organic=0.028

r=PHE;n=199 :prob\_ions=0.000;prob\_organic=0.027

r=HIS;n=200 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=201 :prob\_ions=0.000;prob\_organic=0.028

r=THR;n=202 :prob\_ions=0.000;prob\_organic=0.028

r=TRP;n=203 :prob\_ions=0.000;prob\_organic=0.030

r=PHE;n=204 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=205 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=206 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=207 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=208 :prob\_ions=0.000;prob\_organic=0.028

r=VAL;n=209 :prob\_ions=0.000;prob\_organic=0.994

r=SER;n=210 :prob\_ions=0.000;prob\_organic=1.000

r=TRP;n=211 :prob\_ions=0.001;prob\_organic=1.000

r=GLY;n=212 :prob\_ions=0.001;prob\_organic=1.000

r=GLU;n=213 :prob\_ions=0.003;prob\_organic=0.870

r=GLY;n=214 :prob\_ions=0.001;prob\_organic=1.000

r=CYS;n=215 :prob\_ions=0.018;prob\_organic=0.968

r=GLY;n=216 :prob\_ions=0.199;prob\_organic=0.052

r=LEU;n=217 :prob\_ions=0.662;prob\_organic=0.039

r=LEU;n=218 :prob\_ions=0.134;prob\_organic=0.029

r=HIS;n=219 :prob\_ions=0.063;prob\_organic=0.029

r=ASN;n=220 :prob\_ions=0.898;prob\_organic=0.041

r=TYR;n=221 :prob\_ions=0.739;prob\_organic=0.041

r=GLY;n=222 :prob\_ions=0.541;prob\_organic=1.000

r=VAL;n=223 :prob\_ions=0.007;prob\_organic=0.171

r=TYR;n=224 :prob\_ions=0.020;prob\_organic=0.071

r=THR;n=225 :prob\_ions=0.000;prob\_organic=0.027

r=LYS;n=226 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=227 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=228 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=229 :prob\_ions=0.000;prob\_organic=0.027

r=TYR;n=230 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=231 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=232 :prob\_ions=0.000;prob\_organic=0.027

r=TRP;n=233 :prob\_ions=0.000;prob\_organic=0.027

r=ILE;n=234 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=235 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=236 :prob\_ions=0.000;prob\_organic=0.027

r=HIS;n=237 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=238 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=239 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=240 :prob\_ions=0.000;prob\_organic=0.026

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r=MET;n=1 :prob=0.026

r=HIS;n=2 :prob=0.026

r=HIS;n=3 :prob=0.026

r=HIS;n=4 :prob=0.026

r=HIS;n=5 :prob=0.026

r=HIS;n=6 :prob=0.026

r=HIS;n=7 :prob=0.026

r=SER;n=8 :prob=0.026

r=SER;n=9 :prob=0.026

r=GLY;n=10 :prob=0.026

r=VAL;n=11 :prob=0.026

r=ASP;n=12 :prob=0.026

r=LEU;n=13 :prob=0.026

r=GLY;n=14 :prob=0.026

r=THR;n=15 :prob=0.026

r=GLU;n=16 :prob=0.026

r=ASN;n=17 :prob=0.028

r=LEU;n=18 :prob=0.026

r=TYR;n=19 :prob=0.026

r=PHE;n=20 :prob=0.026

r=GLN;n=21 :prob=0.026

r=SER;n=22 :prob=0.026

r=MET;n=23 :prob=0.026

r=LYS;n=24 :prob=0.026

r=ILE;n=25 :prob=0.026

r=ALA;n=26 :prob=0.026

r=ILE;n=27 :prob=0.026

r=MET;n=28 :prob=0.027

r=GLY;n=29 :prob=0.031

r=ALA;n=30 :prob=0.363

r=MET;n=31 :prob=0.167

r=PRO;n=32 :prob=0.027

r=GLU;n=33 :prob=0.031

r=GLU;n=34 :prob=0.091

r=ILE;n=35 :prob=0.026

r=SER;n=36 :prob=0.026

r=PRO;n=37 :prob=0.026

r=ILE;n=38 :prob=0.026

r=LEU;n=39 :prob=0.026

r=GLU;n=40 :prob=0.026

r=LYS;n=41 :prob=0.026

r=ILE;n=42 :prob=0.026

r=GLY;n=43 :prob=0.026

r=SER;n=44 :prob=0.026

r=TYR;n=45 :prob=0.026

r=LYS;n=46 :prob=0.026

r=SER;n=47 :prob=0.026

r=THR;n=48 :prob=0.026

r=SER;n=49 :prob=0.026

r=TYR;n=50 :prob=0.026

r=ALA;n=51 :prob=0.028

r=GLY;n=52 :prob=0.027

r=ASN;n=53 :prob=0.026

r=LYS;n=54 :prob=0.026

r=TYR;n=55 :prob=0.026

r=TYR;n=56 :prob=0.026

r=GLU;n=57 :prob=0.026

r=ALA;n=58 :prob=0.026

r=THR;n=59 :prob=0.026

r=TYR;n=60 :prob=0.026

r=GLN;n=61 :prob=0.026

r=GLY;n=62 :prob=0.026

r=VAL;n=63 :prob=0.026

r=GLU;n=64 :prob=0.026

r=LEU;n=65 :prob=0.026

r=VAL;n=66 :prob=0.026

r=ILE;n=67 :prob=0.026

r=ALA;n=68 :prob=0.026

r=TYR;n=69 :prob=0.027

r=SER;n=70 :prob=0.031

r=LYS;n=71 :prob=0.033

r=ILE;n=72 :prob=0.919

r=GLY;n=73 :prob=0.037

r=LYS;n=74 :prob=0.029

r=VAL;n=75 :prob=0.027

r=PHE;n=76 :prob=0.027

r=SER;n=77 :prob=0.028

r=ALA;n=78 :prob=0.028

r=LEU;n=79 :prob=0.027

r=SER;n=80 :prob=0.026

r=ALA;n=81 :prob=0.027

r=ALA;n=82 :prob=0.026

r=THR;n=83 :prob=0.026

r=MET;n=84 :prob=0.026

r=ILE;n=85 :prob=0.027

r=GLU;n=86 :prob=0.026

r=HIS;n=87 :prob=0.026

r=PHE;n=88 :prob=0.026

r=GLY;n=89 :prob=0.026

r=ALA;n=90 :prob=0.026

r=THR;n=91 :prob=0.027

r=LYS;n=92 :prob=0.027

r=LEU;n=93 :prob=0.027

r=LEU;n=94 :prob=0.026

r=PHE;n=95 :prob=0.175

r=SER;n=96 :prob=0.030

r=GLY;n=97 :prob=0.059

r=VAL;n=98 :prob=1.000

r=ALA;n=99 :prob=1.000

r=GLY;n=100 :prob=1.000

r=ALA;n=101 :prob=0.029

r=ILE;n=102 :prob=0.027

r=SER;n=103 :prob=0.026

r=THR;n=104 :prob=0.026

r=ASN;n=105 :prob=0.026

r=LEU;n=106 :prob=0.026

r=LYS;n=107 :prob=0.026

r=VAL;n=108 :prob=0.026

r=GLY;n=109 :prob=0.026

r=ASP;n=110 :prob=0.026

r=LEU;n=111 :prob=0.026

r=ILE;n=112 :prob=0.027

r=VAL;n=113 :prob=0.026

r=ALA;n=114 :prob=0.027

r=THR;n=115 :prob=0.027

r=LYS;n=116 :prob=0.027

r=LEU;n=117 :prob=0.029

r=SER;n=118 :prob=0.029

r=GLN;n=119 :prob=0.032

r=HIS;n=120 :prob=0.031

r=ASP;n=121 :prob=0.028

r=LEU;n=122 :prob=0.029

r=ASP;n=123 :prob=0.026

r=ILE;n=124 :prob=0.027

r=THR;n=125 :prob=0.026

r=ALA;n=126 :prob=0.026

r=PHE;n=127 :prob=0.027

r=GLY;n=128 :prob=0.026

r=HIS;n=129 :prob=0.027

r=PRO;n=130 :prob=0.026

r=TYR;n=131 :prob=0.027

r=GLY;n=132 :prob=0.029

r=TYR;n=133 :prob=0.028

r=VAL;n=134 :prob=0.029

r=PRO;n=135 :prob=0.027

r=GLU;n=136 :prob=0.028

r=GLY;n=137 :prob=0.028

r=SER;n=138 :prob=0.030

r=VAL;n=139 :prob=0.029

r=PHE;n=140 :prob=0.029

r=VAL;n=141 :prob=0.031

r=GLU;n=142 :prob=0.031

r=ALA;n=143 :prob=0.030

r=ASP;n=144 :prob=0.030

r=LYS;n=145 :prob=0.028

r=ASP;n=146 :prob=0.028

r=MET;n=147 :prob=0.027

r=ILE;n=148 :prob=0.027

r=GLU;n=149 :prob=0.026

r=LEU;n=150 :prob=0.026

r=SER;n=151 :prob=0.026

r=LYS;n=152 :prob=0.026

r=LYS;n=153 :prob=0.026

r=VAL;n=154 :prob=0.026

r=ALA;n=155 :prob=0.026

r=LEU;n=156 :prob=0.026

r=GLU;n=157 :prob=0.026

r=MET;n=158 :prob=0.026

r=GLY;n=159 :prob=0.026

r=LYS;n=160 :prob=0.026

r=SER;n=161 :prob=0.026

r=VAL;n=162 :prob=0.026

r=GLN;n=163 :prob=0.026

r=GLU;n=164 :prob=0.026

r=GLY;n=165 :prob=0.026

r=ILE;n=166 :prob=0.026

r=ILE;n=167 :prob=0.029

r=ALA;n=168 :prob=0.031

r=THR;n=169 :prob=0.036

r=GLY;n=170 :prob=0.091

r=ASP;n=171 :prob=0.030

r=GLN;n=172 :prob=0.384

r=PHE;n=173 :prob=1.000

r=VAL;n=174 :prob=0.995

r=ALA;n=175 :prob=0.581

r=ASN;n=176 :prob=0.041

r=GLU;n=177 :prob=0.033

r=GLU;n=178 :prob=0.026

r=ARG;n=179 :prob=0.034

r=LYS;n=180 :prob=0.036

r=ASN;n=181 :prob=0.029

r=TRP;n=182 :prob=0.026

r=ILE;n=183 :prob=0.027

r=GLY;n=184 :prob=0.026

r=THR;n=185 :prob=0.026

r=THR;n=186 :prob=0.026

r=PHE;n=187 :prob=0.027

r=GLY;n=188 :prob=0.026

r=ALA;n=189 :prob=0.027

r=ASP;n=190 :prob=0.027

r=ALA;n=191 :prob=0.029

r=LEU;n=192 :prob=1.000

r=GLU;n=193 :prob=1.000

r=MET;n=194 :prob=1.000

r=GLU;n=195 :prob=0.979

r=GLY;n=196 :prob=0.029

r=GLY;n=197 :prob=0.031

r=SER;n=198 :prob=0.030

r=VAL;n=199 :prob=0.029

r=GLY;n=200 :prob=0.031

r=VAL;n=201 :prob=0.032

r=VAL;n=202 :prob=0.029

r=CYS;n=203 :prob=0.030

r=ASN;n=204 :prob=0.031

r=ALA;n=205 :prob=0.028

r=LEU;n=206 :prob=0.027

r=ASN;n=207 :prob=0.029

r=ILE;n=208 :prob=0.031

r=PRO;n=209 :prob=0.030

r=PHE;n=210 :prob=0.030

r=PHE;n=211 :prob=0.028

r=ILE;n=212 :prob=0.028

r=LEU;n=213 :prob=0.027

r=ARG;n=214 :prob=0.153

r=SER;n=215 :prob=0.029

r=ILE;n=216 :prob=0.028

r=SER;n=217 :prob=1.000

r=ASP;n=218 :prob=1.000

r=ALA;n=219 :prob=0.034

r=ALA;n=220 :prob=0.811

r=ASP;n=221 :prob=0.030

r=MET;n=222 :prob=0.026

r=ASP;n=223 :prob=0.033

r=ALA;n=224 :prob=0.064

r=SER;n=225 :prob=0.035

r=PHE;n=226 :prob=0.029

r=SER;n=227 :prob=0.048

r=PHE;n=228 :prob=0.871

r=ASP;n=229 :prob=0.041

r=GLU;n=230 :prob=0.026

r=PHE;n=231 :prob=0.043

r=LEU;n=232 :prob=0.038

r=GLU;n=233 :prob=0.027

r=SER;n=234 :prob=0.026

r=SER;n=235 :prob=0.027

r=ALA;n=236 :prob=0.027

r=LYS;n=237 :prob=0.026

r=GLU;n=238 :prob=0.026

r=SER;n=239 :prob=0.026

r=ALA;n=240 :prob=0.026

r=GLU;n=241 :prob=0.026

r=PHE;n=242 :prob=0.026

r=ILE;n=243 :prob=0.026

r=MET;n=244 :prob=0.026

r=LYS;n=245 :prob=0.026

r=MET;n=246 :prob=0.026

r=VAL;n=247 :prob=0.026

r=ASP;n=248 :prob=0.026

r=GLU;n=249 :prob=0.026

r=LEU;n=250 :prob=0.026

r=VAL;n=251 :prob=0.026

r=ALA;n=252 :prob=0.026

r=LEU;n=253 :prob=0.027

r=PRO;n=254 :prob=0.026

r=LEU;n=255 :prob=0.027

r=GLN;n=256 :prob=0.027

r=ASP;n=257 :prob=0.026

r=ILE;n=258 :prob=0.026

r=LYS;n=259 :prob=0.026

**4UYA**

r=SER;n=1 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=2 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=3 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=4 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=5 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=6 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=7 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=8 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=9 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=10 :prob\_ions=0.000;prob\_organic=0.027

r=GLU;n=11 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=12 :prob\_ions=0.000;prob\_organic=0.057

r=LYS;n=13 :prob\_ions=0.000;prob\_organic=0.038

r=GLU;n=14 :prob\_ions=0.000;prob\_organic=0.051

r=LEU;n=15 :prob\_ions=0.000;prob\_organic=0.043

r=ILE;n=16 :prob\_ions=0.003;prob\_organic=1.000

r=GLY;n=17 :prob\_ions=0.004;prob\_organic=0.907

r=ALA;n=18 :prob\_ions=0.000;prob\_organic=0.415

r=GLY;n=19 :prob\_ions=0.000;prob\_organic=0.096

r=GLN;n=20 :prob\_ions=0.000;prob\_organic=0.043

r=VAL;n=21 :prob\_ions=0.018;prob\_organic=1.000

r=TYR;n=22 :prob\_ions=0.000;prob\_organic=0.032

r=ARG;n=23 :prob\_ions=0.000;prob\_organic=0.038

r=ALA;n=24 :prob\_ions=0.000;prob\_organic=0.028

r=THR;n=25 :prob\_ions=0.000;prob\_organic=0.028

r=TRP;n=26 :prob\_ions=0.000;prob\_organic=0.028

r=GLN;n=27 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=28 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=29 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=30 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=31 :prob\_ions=0.000;prob\_organic=0.029

r=ALA;n=32 :prob\_ions=0.002;prob\_organic=1.000

r=VAL;n=33 :prob\_ions=0.000;prob\_organic=0.050

r=LYS;n=34 :prob\_ions=0.024;prob\_organic=1.000

r=ALA;n=35 :prob\_ions=0.000;prob\_organic=0.031

r=ALA;n=36 :prob\_ions=0.000;prob\_organic=0.035

r=ALA;n=37 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=38 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=39 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=40 :prob\_ions=0.000;prob\_organic=0.028

r=VAL;n=41 :prob\_ions=0.000;prob\_organic=0.031

r=ARG;n=42 :prob\_ions=0.000;prob\_organic=0.027

r=ARG;n=43 :prob\_ions=0.000;prob\_organic=0.028

r=GLU;n=44 :prob\_ions=0.000;prob\_organic=0.157

r=ALA;n=45 :prob\_ions=0.000;prob\_organic=0.033

r=ARG;n=46 :prob\_ions=0.000;prob\_organic=0.028

r=LEU;n=47 :prob\_ions=0.000;prob\_organic=0.035

r=PHE;n=48 :prob\_ions=0.000;prob\_organic=0.268

r=ALA;n=49 :prob\_ions=0.000;prob\_organic=0.029

r=MET;n=50 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=51 :prob\_ions=0.000;prob\_organic=0.040

r=ARG;n=52 :prob\_ions=0.000;prob\_organic=0.027

r=HIS;n=53 :prob\_ions=0.000;prob\_organic=0.027

r=PRO;n=54 :prob\_ions=0.001;prob\_organic=0.026

r=ASN;n=55 :prob\_ions=0.167;prob\_organic=0.027

r=ILE;n=56 :prob\_ions=0.017;prob\_organic=0.039

r=ILE;n=57 :prob\_ions=0.066;prob\_organic=0.982

r=GLU;n=58 :prob\_ions=0.000;prob\_organic=0.033

r=LEU;n=59 :prob\_ions=0.000;prob\_organic=0.055

r=ARG;n=60 :prob\_ions=0.000;prob\_organic=0.028

r=GLY;n=61 :prob\_ions=0.000;prob\_organic=0.028

r=VAL;n=62 :prob\_ions=0.000;prob\_organic=0.027

r=CYS;n=63 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=64 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=65 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=66 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=67 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=68 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=69 :prob\_ions=0.000;prob\_organic=0.027

r=CYS;n=70 :prob\_ions=0.000;prob\_organic=0.028

r=LEU;n=71 :prob\_ions=0.000;prob\_organic=0.234

r=VAL;n=72 :prob\_ions=0.000;prob\_organic=0.031

r=LEU;n=73 :prob\_ions=0.005;prob\_organic=1.000

r=GLU;n=74 :prob\_ions=0.001;prob\_organic=1.000

r=PHE;n=75 :prob\_ions=0.000;prob\_organic=1.000

r=ALA;n=76 :prob\_ions=0.023;prob\_organic=1.000

r=ARG;n=77 :prob\_ions=0.000;prob\_organic=0.654

r=GLY;n=78 :prob\_ions=0.001;prob\_organic=0.086

r=GLY;n=79 :prob\_ions=0.033;prob\_organic=0.893

r=ALA;n=80 :prob\_ions=0.141;prob\_organic=0.917

r=LEU;n=81 :prob\_ions=0.227;prob\_organic=0.027

r=ASN;n=82 :prob\_ions=0.006;prob\_organic=0.031

r=ARG;n=83 :prob\_ions=0.001;prob\_organic=0.119

r=ALA;n=84 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=85 :prob\_ions=0.001;prob\_organic=0.026

r=ALA;n=86 :prob\_ions=0.000;prob\_organic=0.027

r=GLY;n=87 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=88 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=89 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=90 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=91 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=92 :prob\_ions=0.000;prob\_organic=0.027

r=HIS;n=93 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=94 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=95 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=96 :prob\_ions=0.000;prob\_organic=0.027

r=ASN;n=97 :prob\_ions=0.000;prob\_organic=0.026

r=TRP;n=98 :prob\_ions=0.037;prob\_organic=0.026

r=ALA;n=99 :prob\_ions=0.002;prob\_organic=0.026

r=VAL;n=100 :prob\_ions=0.001;prob\_organic=0.026

r=GLN;n=101 :prob\_ions=0.030;prob\_organic=0.026

r=ILE;n=102 :prob\_ions=0.730;prob\_organic=0.026

r=ALA;n=103 :prob\_ions=0.010;prob\_organic=0.026

r=ARG;n=104 :prob\_ions=0.001;prob\_organic=0.026

r=GLY;n=105 :prob\_ions=0.009;prob\_organic=0.026

r=MET;n=106 :prob\_ions=0.043;prob\_organic=0.027

r=LEU;n=107 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=108 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=109 :prob\_ions=0.003;prob\_organic=0.033

r=HIS;n=110 :prob\_ions=0.000;prob\_organic=0.027

r=GLU;n=111 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=112 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=113 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=114 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=115 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=116 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=117 :prob\_ions=0.000;prob\_organic=0.032

r=LEU;n=118 :prob\_ions=0.000;prob\_organic=0.030

r=HIS;n=119 :prob\_ions=0.060;prob\_organic=0.052

r=ARG;n=120 :prob\_ions=0.000;prob\_organic=0.034

r=ASP;n=121 :prob\_ions=0.010;prob\_organic=0.080

r=LEU;n=122 :prob\_ions=0.390;prob\_organic=0.032

r=LYS;n=123 :prob\_ions=0.486;prob\_organic=0.045

r=SER;n=124 :prob\_ions=0.339;prob\_organic=0.028

r=SER;n=125 :prob\_ions=0.508;prob\_organic=0.960

r=ASN;n=126 :prob\_ions=0.786;prob\_organic=0.932

r=ILE;n=127 :prob\_ions=0.996;prob\_organic=0.030

r=LEU;n=128 :prob\_ions=0.712;prob\_organic=1.000

r=LEU;n=129 :prob\_ions=0.031;prob\_organic=0.030

r=LEU;n=130 :prob\_ions=0.001;prob\_organic=0.027

r=GLU;n=131 :prob\_ions=0.000;prob\_organic=0.027

r=LYS;n=132 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=133 :prob\_ions=0.000;prob\_organic=0.027

r=GLU;n=134 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=135 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=136 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=137 :prob\_ions=0.000;prob\_organic=0.028

r=CYS;n=138 :prob\_ions=0.000;prob\_organic=0.053

r=ASN;n=139 :prob\_ions=0.000;prob\_organic=0.069

r=LYS;n=140 :prob\_ions=0.000;prob\_organic=0.034

r=THR;n=141 :prob\_ions=0.009;prob\_organic=0.028

r=LEU;n=142 :prob\_ions=0.386;prob\_organic=0.029

r=LYS;n=143 :prob\_ions=0.882;prob\_organic=0.029

r=ILE;n=144 :prob\_ions=0.858;prob\_organic=0.041

r=THR;n=145 :prob\_ions=0.569;prob\_organic=0.990

r=ASP;n=146 :prob\_ions=0.148;prob\_organic=1.000

r=PHE;n=147 :prob\_ions=0.002;prob\_organic=0.115

r=GLY;n=148 :prob\_ions=0.000;prob\_organic=0.033

r=ALA;n=149 :prob\_ions=0.000;prob\_organic=0.033

r=TYR;n=150 :prob\_ions=0.000;prob\_organic=0.030

r=ALA;n=151 :prob\_ions=0.000;prob\_organic=0.029

r=TRP;n=152 :prob\_ions=0.000;prob\_organic=0.033

r=MET;n=153 :prob\_ions=0.000;prob\_organic=0.034

r=ALA;n=154 :prob\_ions=0.000;prob\_organic=0.031

r=PRO;n=155 :prob\_ions=0.000;prob\_organic=0.027

r=GLU;n=156 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=157 :prob\_ions=0.000;prob\_organic=0.031

r=ILE;n=158 :prob\_ions=0.000;prob\_organic=0.028

r=LYS;n=159 :prob\_ions=0.000;prob\_organic=0.027

r=SER;n=160 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=161 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=162 :prob\_ions=0.000;prob\_organic=0.028

r=PHE;n=163 :prob\_ions=0.000;prob\_organic=0.031

r=SER;n=164 :prob\_ions=0.000;prob\_organic=0.028

r=LYS;n=165 :prob\_ions=0.000;prob\_organic=0.027

r=GLY;n=166 :prob\_ions=0.000;prob\_organic=0.027

r=SER;n=167 :prob\_ions=0.000;prob\_organic=0.031

r=ASP;n=168 :prob\_ions=0.000;prob\_organic=0.030

r=ILE;n=169 :prob\_ions=0.000;prob\_organic=0.028

r=TRP;n=170 :prob\_ions=0.000;prob\_organic=0.029

r=SER;n=171 :prob\_ions=0.001;prob\_organic=0.033

r=TYR;n=172 :prob\_ions=0.007;prob\_organic=0.028

r=GLY;n=173 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=174 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=175 :prob\_ions=0.163;prob\_organic=0.027

r=LEU;n=176 :prob\_ions=0.000;prob\_organic=0.027

r=TRP;n=177 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=178 :prob\_ions=0.001;prob\_organic=0.027

r=LEU;n=179 :prob\_ions=0.004;prob\_organic=0.026

r=LEU;n=180 :prob\_ions=0.000;prob\_organic=0.027

r=THR;n=181 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=182 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=183 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=184 :prob\_ions=0.000;prob\_organic=0.027

r=PRO;n=185 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=186 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=187 :prob\_ions=0.000;prob\_organic=0.027

r=GLY;n=188 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=189 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=190 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=191 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=192 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=193 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=194 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=195 :prob\_ions=0.000;prob\_organic=0.027

r=TYR;n=196 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=197 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=198 :prob\_ions=0.000;prob\_organic=0.027

r=ALA;n=199 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=200 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=201 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=202 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=203 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=204 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=205 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=206 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=207 :prob\_ions=0.000;prob\_organic=0.027

r=PRO;n=208 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=209 :prob\_ions=0.000;prob\_organic=0.027

r=THR;n=210 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=211 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=212 :prob\_ions=0.000;prob\_organic=0.027

r=GLU;n=213 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=214 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=215 :prob\_ions=0.000;prob\_organic=0.027

r=ALA;n=216 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=217 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=218 :prob\_ions=0.000;prob\_organic=0.026

r=MET;n=219 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=220 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=221 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=222 :prob\_ions=0.000;prob\_organic=0.026

r=TRP;n=223 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=224 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=225 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=226 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=227 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=228 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=229 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=230 :prob\_ions=0.000;prob\_organic=0.027

r=PRO;n=231 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=232 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=233 :prob\_ions=0.000;prob\_organic=0.027

r=ALA;n=234 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=235 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=236 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=237 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=238 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=239 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=240 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=241 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=242 :prob\_ions=0.000;prob\_organic=0.026

r=MET;n=243 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=244 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=245 :prob\_ions=0.000;prob\_organic=0.026

r=MET;n=246 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=247 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=248 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=249 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=250 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=251 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=252 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=253 :prob\_ions=0.000;prob\_organic=0.026

r=MET;n=254 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=255 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=256 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=257 :prob\_ions=0.000;prob\_organic=0.026

r=TRP;n=258 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=259 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=260 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=261 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=262 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=263 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=264 :prob\_ions=0.000;prob\_organic=0.026

r=MET;n=265 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=266 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=267 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=268 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=269 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=270 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=271 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=272 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=273 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=274 :prob\_ions=0.000;prob\_organic=0.026

**6MFQ**

r=LEU;n=1 :prob\_ions=0.000;prob\_organic=0.030

r=SER;n=2 :prob\_ions=0.000;prob\_organic=0.030

r=LEU;n=3 :prob\_ions=0.000;prob\_organic=0.028

r=SER;n=4 :prob\_ions=0.000;prob\_organic=0.028

r=THR;n=5 :prob\_ions=0.006;prob\_organic=0.031

r=ALA;n=6 :prob\_ions=0.021;prob\_organic=0.033

r=VAL;n=7 :prob\_ions=0.004;prob\_organic=0.030

r=LYS;n=8 :prob\_ions=0.037;prob\_organic=0.031

r=GLU;n=9 :prob\_ions=0.829;prob\_organic=0.370

r=LEU;n=10 :prob\_ions=0.320;prob\_organic=0.462

r=VAL;n=11 :prob\_ions=0.033;prob\_organic=0.034

r=GLU;n=12 :prob\_ions=0.214;prob\_organic=0.033

r=ASN;n=13 :prob\_ions=0.874;prob\_organic=1.000

r=SER;n=14 :prob\_ions=0.061;prob\_organic=0.617

r=LEU;n=15 :prob\_ions=0.003;prob\_organic=0.033

r=ASP;n=16 :prob\_ions=0.093;prob\_organic=0.117

r=ALA;n=17 :prob\_ions=0.002;prob\_organic=1.000

r=GLY;n=18 :prob\_ions=0.000;prob\_organic=0.030

r=ALA;n=19 :prob\_ions=0.000;prob\_organic=0.029

r=THR;n=20 :prob\_ions=0.000;prob\_organic=0.027

r=ASN;n=21 :prob\_ions=0.000;prob\_organic=0.027

r=ILE;n=22 :prob\_ions=0.000;prob\_organic=0.027

r=ASP;n=23 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=24 :prob\_ions=0.000;prob\_organic=0.027

r=LYS;n=25 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=26 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=27 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=28 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=29 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=30 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=31 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=32 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=33 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=34 :prob\_ions=0.000;prob\_organic=0.027

r=GLU;n=35 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=36 :prob\_ions=0.000;prob\_organic=0.107

r=SER;n=37 :prob\_ions=0.000;prob\_organic=0.029

r=ASP;n=38 :prob\_ions=0.000;prob\_organic=1.000

r=ASN;n=39 :prob\_ions=0.000;prob\_organic=0.028

r=GLY;n=40 :prob\_ions=0.000;prob\_organic=0.034

r=CYS;n=41 :prob\_ions=0.000;prob\_organic=0.531

r=GLY;n=42 :prob\_ions=0.000;prob\_organic=0.996

r=VAL;n=43 :prob\_ions=0.000;prob\_organic=1.000

r=GLU;n=44 :prob\_ions=0.000;prob\_organic=0.162

r=GLU;n=45 :prob\_ions=0.000;prob\_organic=0.028

r=GLU;n=46 :prob\_ions=0.000;prob\_organic=0.027

r=ASN;n=47 :prob\_ions=0.000;prob\_organic=0.050

r=PHE;n=48 :prob\_ions=0.000;prob\_organic=0.036

r=GLU;n=49 :prob\_ions=0.000;prob\_organic=0.031

r=GLY;n=50 :prob\_ions=0.001;prob\_organic=0.115

r=LEU;n=51 :prob\_ions=0.023;prob\_organic=0.996

r=THR;n=52 :prob\_ions=0.001;prob\_organic=0.096

r=LEU;n=53 :prob\_ions=0.001;prob\_organic=0.079

r=GLU;n=54 :prob\_ions=0.804;prob\_organic=0.795

r=ALA;n=55 :prob\_ions=0.894;prob\_organic=0.981

r=LEU;n=56 :prob\_ions=0.408;prob\_organic=1.000

r=SER;n=57 :prob\_ions=0.013;prob\_organic=0.125

r=SER;n=58 :prob\_ions=0.002;prob\_organic=0.031

r=LEU;n=59 :prob\_ions=0.038;prob\_organic=0.040

r=CYS;n=60 :prob\_ions=0.000;prob\_organic=0.030

r=ALA;n=61 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=62 :prob\_ions=0.000;prob\_organic=0.030

r=SER;n=63 :prob\_ions=0.000;prob\_organic=0.028

r=ASP;n=64 :prob\_ions=0.000;prob\_organic=0.027

r=VAL;n=65 :prob\_ions=0.000;prob\_organic=0.032

r=THR;n=66 :prob\_ions=0.000;prob\_organic=0.030

r=ILE;n=67 :prob\_ions=0.001;prob\_organic=0.061

r=SER;n=68 :prob\_ions=0.000;prob\_organic=0.032

r=THR;n=69 :prob\_ions=0.000;prob\_organic=0.036

r=CYS;n=70 :prob\_ions=0.000;prob\_organic=0.029

r=HIS;n=71 :prob\_ions=0.000;prob\_organic=0.045

r=ALA;n=72 :prob\_ions=0.000;prob\_organic=0.027

r=SER;n=73 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=74 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=75 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=76 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=77 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=78 :prob\_ions=0.000;prob\_organic=0.028

r=ARG;n=79 :prob\_ions=0.000;prob\_organic=0.027

r=LEU;n=80 :prob\_ions=0.000;prob\_organic=0.046

r=MET;n=81 :prob\_ions=0.000;prob\_organic=0.027

r=PHE;n=82 :prob\_ions=0.000;prob\_organic=0.034

r=ASP;n=83 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=84 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=85 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=86 :prob\_ions=0.000;prob\_organic=0.028

r=LYS;n=87 :prob\_ions=0.000;prob\_organic=0.027

r=ILE;n=88 :prob\_ions=0.000;prob\_organic=0.028

r=ILE;n=89 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=90 :prob\_ions=0.000;prob\_organic=0.027

r=LYS;n=91 :prob\_ions=0.000;prob\_organic=0.027

r=THR;n=92 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=93 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=94 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=95 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=96 :prob\_ions=0.000;prob\_organic=0.028

r=PRO;n=97 :prob\_ions=0.000;prob\_organic=0.027

r=ARG;n=98 :prob\_ions=0.000;prob\_organic=0.027

r=GLY;n=99 :prob\_ions=0.000;prob\_organic=0.031

r=THR;n=100 :prob\_ions=0.000;prob\_organic=1.000

r=THR;n=101 :prob\_ions=0.000;prob\_organic=0.034

r=VAL;n=102 :prob\_ions=0.004;prob\_organic=0.689

r=SER;n=103 :prob\_ions=0.000;prob\_organic=0.030

r=VAL;n=104 :prob\_ions=0.000;prob\_organic=0.030

r=GLN;n=105 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=106 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=107 :prob\_ions=0.000;prob\_organic=0.029

r=PHE;n=108 :prob\_ions=0.000;prob\_organic=0.029

r=SER;n=109 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=110 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=111 :prob\_ions=0.000;prob\_organic=0.027

r=PRO;n=112 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=113 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=114 :prob\_ions=0.000;prob\_organic=0.027

r=HIS;n=115 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=116 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=117 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=118 :prob\_ions=0.000;prob\_organic=0.027

r=GLN;n=119 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=120 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=121 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=122 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=123 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=124 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=125 :prob\_ions=0.000;prob\_organic=0.027

r=TYR;n=126 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=127 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=128 :prob\_ions=0.000;prob\_organic=0.026

r=MET;n=129 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=130 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=131 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=132 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=133 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=134 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=135 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=136 :prob\_ions=0.000;prob\_organic=0.027

r=CYS;n=137 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=138 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=139 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=140 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=141 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=142 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=143 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=144 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=145 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=146 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=147 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=148 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=149 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=150 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=151 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=152 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=153 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=154 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=155 :prob\_ions=0.000;prob\_organic=0.029

r=ARG;n=156 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=157 :prob\_ions=0.000;prob\_organic=0.029

r=PRO;n=158 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=159 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=160 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=161 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=162 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=163 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=164 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=165 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=166 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=167 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=168 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=169 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=170 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=171 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=172 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=173 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=174 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=175 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=176 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=177 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=178 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=179 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=180 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=181 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=182 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=183 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=184 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=185 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=186 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=187 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=188 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=189 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=190 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=191 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=192 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=193 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=194 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=195 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=196 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=197 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=198 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=199 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=200 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=201 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=202 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=203 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=204 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=205 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=206 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=207 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=208 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=209 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=210 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=211 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=212 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=213 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=214 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=215 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=216 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=217 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=218 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=219 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=220 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=221 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=222 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=223 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=224 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=225 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=226 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=227 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=228 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=229 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=230 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=231 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=232 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=233 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=234 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=235 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=236 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=237 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=238 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=239 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=240 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=241 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=242 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=243 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=244 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=245 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=246 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=247 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=248 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=249 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=250 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=251 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=252 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=253 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=254 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=255 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=256 :prob\_ions=0.000;prob\_organic=0.026

r=MET;n=257 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=258 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=259 :prob\_ions=0.000;prob\_organic=0.026

r=ARG;n=260 :prob\_ions=0.000;prob\_organic=0.026

r=HIS;n=261 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=262 :prob\_ions=0.000;prob\_organic=0.026

r=TYR;n=263 :prob\_ions=0.000;prob\_organic=0.026

r=PRO;n=264 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=265 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=266 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=267 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=268 :prob\_ions=0.000;prob\_organic=0.026

r=ASN;n=269 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=270 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=271 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=272 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=273 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=274 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=275 :prob\_ions=0.000;prob\_organic=0.026

r=CYS;n=276 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=277 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=278 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=279 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=280 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=281 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=282 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=283 :prob\_ions=0.000;prob\_organic=0.026

r=GLN;n=284 :prob\_ions=0.000;prob\_organic=0.026

r=GLU;n=285 :prob\_ions=0.000;prob\_organic=0.035

r=GLU;n=286 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=287 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=288 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=289 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=290 :prob\_ions=0.000;prob\_organic=0.026

r=ALA;n=291 :prob\_ions=0.000;prob\_organic=0.026

r=VAL;n=292 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=293 :prob\_ions=0.000;prob\_organic=0.026

r=LYS;n=294 :prob\_ions=0.000;prob\_organic=0.026

r=THR;n=295 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=296 :prob\_ions=0.000;prob\_organic=0.026

r=LEU;n=297 :prob\_ions=0.000;prob\_organic=0.026

r=ILE;n=298 :prob\_ions=0.000;prob\_organic=0.026

r=GLY;n=299 :prob\_ions=0.000;prob\_organic=0.026

r=MET;n=300 :prob\_ions=0.000;prob\_organic=0.026

r=PHE;n=301 :prob\_ions=0.000;prob\_organic=0.026

r=ASP;n=302 :prob\_ions=0.000;prob\_organic=0.026

r=SER;n=303 :prob\_ions=0.000;prob\_organic=0.026

**S2 Table:** Bond lenghts of the Xanthohumol and 8-Prenylnaringenin derivatives.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Atom**  **Xanthohumol Derivative** | **Bond Length Actual (Å)** | **Bond Length Optimal (Å)** | **Bond Angle Actual** | **Bond Angle Optimal** |
| O(34)-H(67) | 0.9602 | 0.9610 | H(67)-O(34)-C(33) | 109.2515 |
| C(33)-H(66) | 1.1133 | 1.1110 | H(66)-C(33)-H(65) | 109.4346 |
| C(33)-H(65) | 1.1121 | 1.1110 | H(66)-C(33)-O(34) | 107.1432 |
| C(33)-O(34) | 1.4146 | 1.4080 | H(66)-C(33)-C(32) | 111.2957 |
| C(32)-H(64) | 1.1149 | 1.1130 | H(65)-C(33)-O(34) | 106.4787 |
| C(32)-H(63) | 1.1161 | 1.1130 | H(65)-C(33)-C(32) | 112.8275 |
| C(32)-C(33) | 1.5297 | 1.5140 | O(34)-C(33)-C(32) | 109.3932 |
| O(31)-H(62) | 0.9603 | 0.9610 | H(64)-C(32)-H(63) | 107.1842 |
| C(30)-H(61) | 1.1134 | 1.1110 | H(64)-C(32)-C(33) | 108.6036 |
| C(30)-H(60) | 1.1124 | 1.1110 | C(33)-C(32)-N(28) | 113.8698 |
| C(30)-O(31) | 1.4147 | 1.4080 | H(62)-O(31)-C(30) | 109.3392 |
| C(29)-H(59) | 1.1162 | 1.1130 | H(61)-C(30)-H(60) | 109.5652 |
| C(29)-H(58) | 1.1155 | 1.1130 | H(61)-C(30)-O(31) | 107.1315 |
| C(29)-C(30) | 1.5299 | 1.5140 | H(61)-C(30)-C(29) | 111.3585 |
| N(28)-C(32) | 1.4621 | 1.4380 | H(60)-C(30)-O(31) | 106.3492 |
| N(28)-C(29) | 1.4619 | 1.4380 | H(60)-C(30)-C(29) | 112.7064 |
| C(27)-H(57) | 1.1044 | 1.1130 | O(31)-C(30)-C(29) | 109.4585 |
| C(27)-H(56) | 1.1154 | 1.1130 | H(59)-C(29)-H(58) | 107.0890 |
| C(27)-N(28) | 1.4638 | 1.4380 | H(59)-C(29)-C(30) | 109.1427 |
| O(26)-H(55) | 0.9709 | 0.9720 | C(33)-C(32)-N(28) | 113.8698 |
| C(25)-C(27) | 1.5260 | 1.4970 | H(62)-O(31)-C(30) | 109.3392 |

**S3 Table:** Bond angles of the Xanthohumol and 8-Prenylnaringenin derivatives.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Atom**  **8-Prenylnaringenin Derivative** | **Bond Length Actual (Å)** | **Bond Length Optimal (Å)** | **Bond Angle Actual** | **Bond Angle Optimal** |
| O(33)-H(64) | 0.9601 | 0.9610 | H(64)-O(33)-C(32) | 109.3757 |
| C(32)-H(63) | 1.1131 | 1.1110 | H(63)-C(32)-H(62) | 109.4744 |
| C(32)-H(62) | 1.1121 | 1.1110 | H(63)-C(32)-O(33) | 107.2782 |
| C(31)-H(61) | 1.1144 | 1.1130 | H(63)-C(32)-C(31) | 111.3428 |
| C(31)-H(60) | 1.1157 | 1.1130 | H(62)-C(32)-O(33) | 106.5672 |
| O(30)-H(59) | 0.9602 | 0.9610 | H(62)-C(32)-C(31) | 112.6167 |
| C(29)-H(58) | 1.1118 | 1.1110 | O(33)-C(32)-C(31) | 109.3117 |
| C(29)-H(57) | 1.1117 | 1.1110 | H(61)-C(31)-H(60) | 106.4268 |
| C(28)-H(56) | 1.1151 | 1.1130 | H(61)-C(31)-C(32) | 109.4620 |
| C(28)-H(55) | 1.1168 | 1.1130 | H(59)-O(30)-C(29) | 109.4713 |
| C(26)-H(54) | 1.1070 | 1.1130 | H(58)-C(29)-H(57) | 109.0734 |
| C(26)-H(53) | 1.1166 | 1.1130 | H(58)-C(29)-O(30) | 106.6903 |
| C(25)-H(52) | 1.1132 | 1.1130 | H(58)-C(29)-C(28) | 112.5453 |
| C(25)-H(51) | 1.1081 | 1.1130 | H(57)-C(29)-O(30) | 106.5982 |
| C(25)-H(50) | 1.1133 | 1.1130 | H(57)-C(29)-C(28) | 112.5316 |
| O(24)-H(49) | 0.9708 | 0.9720 | O(30)-C(29)-C(28) | 109.0664 |
| O(23)-H(48) | 0.9642 | 0.9720 | H(56)-C(28)-H(55) | 103.8769 |
| O(22)-H(47) | 0.9709 | 0.9720 | H(56)-C(28)-C(29) | 108.9133 |
| C(20)-H(46) | 1.1029 | 1.1000 | H(59)-O(30)-C(29) | 109.4713 |
| C(18)-H(45) | 1.1028 | 1.1000 | C(31)-N(27)-C(28) | 113.6412 |
| C(17)-H(44) | 1.1030 | 1.1000 | C(31)-N(27)-C(26) | 110.6734 |

**S4 Table:** Atomic charges of the Xanthohumol and 8-Prenylnaringenin derivatives.

|  |  |  |  |
| --- | --- | --- | --- |
| **Atom (Xanthohumol Derivative)** | **Huckel Charges** | **Atom (8-Prenylnaringenin Derivative)** | **Huckel Charges** |
| C(1) | 0.253132 | C(1) | -0.135827 |
| C(2) | -0.210702 | C(2) | 0.0544411 |
| C(3) | 0.283483 | C(3) | -0.106989 |
| C(4) | -0.135689 | C(4) | -0.075156 |
| C(5) | 0.256933 | C(5) | -0.0915145 |
| C(6) | -0.096558 | C(6) | 0.263514 |
| O(7) | -0.28014 | C(7) | -0.218512 |
| O(8) | -0.284228 | C(8) | 0.274666 |
| O(9) | -0.264119 | C(9) | -0.161194 |
| C(10) | 0.0907518 | C(10) | 0.264306 |
| C(11) | -0.0700673 | O(11) | -0.230673 |
| C(12) | -0.10036 | C(12) | 0.207376 |
| C(13) | 0.0558938 | C(13) | -0.130401 |
| C(14) | -0.135778 | C(14) | 0.436209 |
| C(15) | -0.139015 | O(15) | -0.625994 |
| C(16) | 0.392511 | C(16) | -0.0392965 |
| C(17) | -0.164622 | C(17) | -0.0397658 |
| O(18) | -0.702263 | C(18) | -0.118305 |
| C(19) | 0.0847444 | C(19) | 0.243305 |
| C(20) | -0.0304084 | C(20) | -0.133341 |
| C(21) | 0.0114225 | C(21) | 0.0534758 |
| C(22) | -0.112686 | O(22) | -0.267755 |
| C(23) | 0.27799 | O(23) | -0.250495 |
| C(24) | -0.128902 | O(24) | -0.243384 |
| C(25) | 0.0994122 | C(25) | -0.14531 |
| O(26) | -0.231647 | C(26) | 0.00754896 |
| C(27) | -0.000756697 | N(27) | -0.115866 |
| N(28) | -0.107473 | C(28) | 0.0163106 |
| C(29) | 0.0153326 | C(29) | 0.119224 |
| C(30) | 0.146912 | O(30) | -0.372973 |

**S5 Table:** Docking detailed results

#PMS2 CLEAR H-M-SER-34 H-S-ASP-55 H-S-SER-69 H-M-ASP-70 H-S-ASN-71 H-S-ARG-134 H-S-TYR-149 H-S-ARG-151 H-M-ARG-153 H-S-THR-156 H-S-SER-158 H-S-ARG-169 H-M-PHE-173 H-S-ASN-176 H-M-GLY-228 H-M-TYR-255 H-S-TYR-255 H-S-ASP-261 H-M-LEU-266 H-S-SER-270 H-M-GLY-271 H-S-THR-285 H-S-ARG-294 H-S-ASP-298 H-M-VAL-309 H-M-TYR-310 H-M-HIS-311 H-M-ASP-328 H-S-ASP-328 H-M-LYS-349 H-M-LYS-356 H-S-LYS-356 H-M-THR-357 H-S-THR-357 H-S-THR-52 H-S-LYS-59 H-S-ASN-71 H-S-THR-121 H-S-ARG-153 H-S-LYS-183 H-S-ARG-199 H-S-THR-285 H-M-PHE-290 H-S-CYS-303 V-M-LEU-33 V-S-LEU-33 V-M-SER-34 V-S-SER-34 V-M-LEU-35 V-M-SER-36 V-S-SER-36 V-M-THR-37 V-S-THR-37 V-M-ALA-38 V-M-LYS-40 V-S-LYS-40 V-M-GLU-41 V-S-GLU-41 V-M-THR-52 V-S-THR-52 V-M-ASN-53 V-S-ASN-53 V-M-ILE-54 V-M-ASP-55 V-S-ASP-55 V-S-LYS-57 V-S-GLU-67 V-M-SER-69 V-S-SER-69 V-M-ASP-70 V-S-ASP-70 V-M-ASN-71 V-S-ASN-71 V-M-GLY-72 V-M-THR-121 V-S-THR-121 V-M-ILE-122 V-M-SER-123 V-S-SER-123 V-M-ARG-134 V-S-ARG-134 V-S-TYR-149 V-M-PRO-150 V-M-ARG-151 V-S-ARG-151 V-M-PRO-152 V-S-PRO-152 V-M-ARG-153 V-S-ARG-153 V-M-GLY-154 V-M-THR-155 V-M-THR-156 V-S-THR-156 V-M-VAL-157 V-M-SER-158 V-S-SER-158 V-S-PHE-163 V-S-LEU-166 V-M-VAL-168 V-S-VAL-168 V-M-ARG-169 V-S-ARG-169 V-M-HIS-170 V-M-LYS-171 V-M-GLU-172 V-S-GLU-172 V-M-PHE-173 V-S-PHE-173 V-M-GLN-174 V-M-ARG-175 V-S-ARG-175 V-M-ASN-176 V-S-ASN-176 V-M-ILE-177 V-M-LYS-179 V-S-LYS-179 V-M-GLU-180 V-S-GLU-180 V-M-ALA-182 V-M-LYS-183 V-S-LYS-183 V-M-MET-184 V-M-GLN-186 V-S-GLN-186 V-M-VAL-187 V-S-VAL-187 V-M-LEU-188 V-M-ALA-190 V-S-ALA-190 V-M-TYR-191 V-S-TYR-191 V-S-ALA-196 V-M-GLY-218 V-S-SER-220 V-M-PRO-221 V-M-SER-222 V-S-SER-222 V-M-ILE-223 V-S-ILE-223 V-M-LYS-224 V-S-LYS-224 V-M-GLU-225 V-S-GLU-225 V-M-ASN-226 V-M-ILE-227 V-S-ILE-227 V-M-GLY-228 V-M-SER-229 V-S-SER-229 V-M-GLY-232 V-M-GLN-233 V-S-GLN-233 V-S-LEU-236 V-S-GLN-237 V-M-PRO-241 V-S-PRO-241 V-M-PHE-242 V-S-PHE-242 V-M-VAL-243 V-S-VAL-243 V-M-GLN-244 V-S-GLN-244 V-M-PRO-247 V-S-PRO-247 V-M-SER-248 V-S-SER-248 V-M-SER-250 V-M-VAL-251 V-S-VAL-251 V-M-CYS-252 V-S-CYS-252 V-M-GLU-253 V-S-GLU-253 V-M-GLU-254 V-S-GLU-254 V-M-TYR-255 V-S-TYR-255 V-M-GLY-256 V-M-LEU-257 V-S-LEU-257 V-M-SER-260 V-S-SER-260 V-M-ASP-261 V-S-ASP-261 V-M-LEU-263 V-M-HIS-264 V-S-HIS-264 V-M-ASN-265 V-S-ASN-265 V-M-LEU-266 V-S-LEU-266 V-M-PHE-267 V-S-PHE-267 V-M-TYR-268 V-S-TYR-268 V-M-ILE-269 V-S-ILE-269 V-M-SER-270 V-S-SER-270 V-M-GLY-271 V-M-PHE-272 V-S-PHE-272 V-S-ILE-273 V-M-THR-285 V-S-THR-285 V-M-ASP-286 V-M-GLN-288 V-S-GLN-288 V-M-PHE-289 V-S-PHE-289 V-M-PHE-290 V-S-PHE-290 V-M-PHE-291 V-S-PHE-291 V-S-ARG-294 V-M-ARG-295 V-M-PRO-296 V-S-PRO-296 V-M-CYS-297 V-S-CYS-297 V-M-ASP-298 V-S-ASP-298 V-M-PRO-299 V-S-PRO-299 V-M-ALA-300 V-S-ALA-300 V-M-LYS-301 V-S-LYS-301 V-M-VAL-302 V-S-VAL-302 V-S-CYS-303 V-M-ARG-304 V-S-ARG-304 V-M-LEU-305 V-S-LEU-305 V-M-VAL-306 V-S-VAL-306 V-M-ASN-307 V-S-ASN-307 V-M-GLU-308 V-S-GLU-308 V-M-VAL-309 V-S-VAL-309 V-M-TYR-310 V-S-TYR-310 V-M-HIS-311 V-S-HIS-311 V-M-MET-312 V-S-MET-312 V-M-TYR-313 V-S-TYR-313 V-M-ASN-314 V-S-PRO-319 V-M-VAL-322 V-S-VAL-322 V-M-ASN-324 V-S-ASN-324 V-M-SER-326 V-S-SER-326 V-M-VAL-327 V-S-VAL-327 V-M-ASP-328 V-S-ASP-328 V-M-SER-329 V-M-CYS-331 V-S-CYS-331 V-S-ILE-334 V-M-GLN-342 V-S-GLN-342 V-M-ILE-343 V-S-ILE-343 V-M-LEU-344 V-S-LEU-344 V-M-LEU-345 V-S-LEU-345 V-M-GLN-346 V-S-GLN-346 V-M-GLU-347 V-S-GLU-347 V-M-GLU-348 V-S-GLU-348 V-M-LYS-349 V-S-LYS-349 V-M-LEU-350 V-S-LEU-350 V-M-LEU-351 V-S-LEU-351 V-M-LEU-352 V-S-LEU-352 V-M-ALA-353 V-S-ALA-353 V-M-VAL-354 V-S-VAL-354 V-M-LEU-355 V-S-LEU-355 V-M-LYS-356 V-S-LYS-356 V-M-THR-357 V-S-THR-357 V-M-SER-358 V-M-LEU-359 V-S-LEU-359 V-M-ILE-360 V-S-ILE-360 V-S-PHE-363 V-M-SER-36 V-S-LYS-40 V-M-GLY-50 V-M-ALA-51 V-M-THR-52 V-S-THR-52 V-M-ASN-53 V-S-ASN-53 V-S-LYS-57 V-S-LYS-59 V-M-ASP-64 V-S-ASP-64 V-M-LEU-65 V-S-LEU-65 V-S-GLU-67 V-M-ASN-71 V-S-ASN-71 V-M-ASP-119 V-S-ASP-119 V-M-VAL-120 V-M-THR-121 V-S-THR-121 V-S-ARG-134 V-S-GLN-145 V-S-PRO-148 V-S-TYR-149 V-S-PRO-152 V-M-ARG-153 V-S-ARG-153 V-M-SER-158 V-S-SER-158 V-M-VAL-159 V-M-GLN-160 V-S-GLN-160 V-S-LYS-183 V-M-GLN-186 V-S-GLN-186 V-M-VAL-187 V-S-VAL-187 V-M-ALA-190 V-S-ALA-190 V-S-TYR-191 V-M-ALA-196 V-M-GLY-197 V-M-ILE-198 V-S-ILE-198 V-S-ARG-199 V-M-GLY-218 V-M-GLY-219 V-M-SER-220 V-S-SER-220 V-M-PRO-221 V-S-PRO-221 V-M-THR-285 V-S-THR-285 V-M-ASP-286 V-M-ARG-287 V-M-GLN-288 V-S-GLN-288 V-M-PHE-289 V-S-PHE-289 V-M-PHE-290 V-S-PHE-290 V-S-PHE-291 V-M-PRO-296 V-S-PRO-296 V-M-CYS-297 V-S-CYS-297 V-M-ASP-298 V-S-ASP-298 V-M-CYS-303 V-S-CYS-303 V-S-ASN-307

APC Clear-6-PRENYLNARINGENIN-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-6Prenylnaringenin2CoCl-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2.19221 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.0564275 0 -0.2856 0 0 0 0 0 -2.87993 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.18504 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-6PRENYLNARINGENIN2ZnCl-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-8-PRENYLNARIGENIN-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-8PRENYLNARINGENIN2CoCl-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.115916 0 2.18606 -0.0603694 0.310595 -0.175537 16.9982 -0.578848 -6.55947 -0.27136 -0.817429 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.378297 -1.12538 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-8PRENYLNARINGENIN2ZnCl-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-AVASTIN-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-ISOXANTHOHUMOL-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-OXALILPLATIN-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.80193 0 0 0 0 0 0 0 0 -0.75359 -3.09827 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.164953 -2.73039 -4.8206 8.54684 -0.446968 25.5639 218.158 -2.05478 0 0 -3.61256 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.414124 0 -4.05203 -1.14133 -3.02306 4.33181 -0.0908593 0 -0.00209141 0 0 0 0 0 0 0 0 0 0 0 0 -0.00416053 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-XANTHOHUMOL-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1.13587 -0.25644 -3.52106 -3.13569 0 -0.696853 -1.92983 0 0 0 0 0 -0.174503 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.358341 -0.706552 0 0 0 0 0 0 0 0 0 -3.77907 23.8861 -3.48647 104.156 0 0 0 0 0 -0.358161 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC Clear-XELODA-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC-6-PRENYLNARINGENIN-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC-6Prenylnaringenin2CoCl-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC-6PRENYLNARINGENIN2ZnCl-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.03807 -3.86136 0 0 0 0 0 0 0 -1.04173 19.168 -2.54352 0 0 0 -2.91114 -3.5 -1.02824 -0.66467 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1.45948 -1.58929 -0.907169 -0.385675 -0.0442811 -7.21697 21.6083 -1.4969 -0.350912 -0.233467 0 -4.51611 173.602 -0.86785 462.855 -0.259492 0 -0.432424 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.0964841 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.107601 -0.045465 0 0 0 -0.435791 0 -5.02214 63.1654 -2.63815 -0.104893 -4.53451 0 16.0395 84.6231 190.324 187.596 74.4516 8.02742 -2.67496 -0.774025 -2.04127 -4.74771 -0.250802 -1.19648 -0.0406962 -0.225412 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.296591 0 -5.01173 -1.41113 -1.0457 -0.12096 -1.53847 0 10.2741 0.448435 107.879 20.6765 11.2364 -1.04236 -9.49812 -1.10949 98.0118 196.454 12.1986 -3.8606 -0.728709 -2.11926 -6.7402 -2.0727 3.98329 -2.68739 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC-8-PRENYLNARIGENIN-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.304167 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.00378574 0 -0.510224 -0.922383 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC-8PRENYLNARINGENIN2CoCl-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.104486 0 -2.93942 -2.60164 -0.125766 0 -0.239628 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.187025 -0.0333595 -0.553536 -0.551927 -1.71503 2.24874 -0.435023 -0.484728 0 0 -0.0211744 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.251849 -0.637227 -1.53354 0 -0.589177 -0.161707 -1.84465 -0.597585 0 0 -1.05642 0 -7.77166 135.2 -4.23771 4.63374 -0.0276945 0 0 -0.303533 -0.000509425 -4.0908 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC-8PRENYLNARINGENIN2ZnCl-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC-AVASTIN-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

APC-ISOXANTHOHUMOL-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

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cavMLK4 Kinase\_AGS-ISOXANTHOHUMOL-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavMLK4 Kinase\_AGS-OXALILPLATIN-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavMLK4 Kinase\_AGS-XANTHOHUMOL-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavMLK4 Kinase\_AGS-XELODA-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-6-PRENYLNARINGENIN-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-6Prenylnaringenin2CoCl-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-6PRENYLNARINGENIN2ZnCl-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-8-PRENYLNARIGENIN-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-8PRENYLNARINGENIN2CoCl-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-8PRENYLNARINGENIN2ZnCl-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-AVASTIN-0.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-ISOXANTHOHUMOL-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-OXALILPLATIN-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-XANTHOHUMOL-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

cavPMS2\_AGS-XELODA-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-6-PRENYLNARINGENIN-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2.38544 0 -1.14828 -3.5 -2.48997 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.0308583 -4.1063 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.06055 -0.246379 -1.63376 -1.39949 -4.00316 -0.438036 -1.32087 -0.38168 0 0 0 0 0 0 0 0 0 0 0 -2.387 -2.89068 -0.266393 -0.0748985 -1.70574 -5.71469 -1.64356 -3.23846 -4.03233 -6.82532 -0.936864 -5.60166 -2.24157 -11.4322 -0.189136 -3.09748 -8.18212 -0.10344 -1.99856 -0.477164

PMS2 CLEAR-6Prenylnaringenin2CoCl-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2.5 0 -2.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.0145237 0 -2.7449 -2.84834 -4.38129 -3.45908 -0.178032 -0.638644 -7.36438 -0.236146 -3.15476 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.0626702 -4.18293 0.137095 -0.162804 -3.49141 -6.91199 -5.08486 -4.03064 -0.128801 -0.659951 -1.18006 -0.109456 -0.558464 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.08085 -1.83846 -0.114805 -3.09929 -3.70762 -0.482291 -0.38354 -1.29087 -0.894042 -0.02831 -0.53569 0 -0.0294953 -7.41591 -1.43791 -12.9755 -2.154 -9.29533 -5.2564 -0.0267226 0 0 0 0 0 0 0 -1.38184 0 0 0 0 0 0 0 -0.414612 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.00830289 -0.678766 0 -0.288039 -0.182291 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-6PRENYLNARINGENIN2ZnCl-1.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.34527 0 -2.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.0554285 -0.474937 0 0 -0.890888 0 0 -4.01324 -10.8946 -8.449 -16.1344 -0.512068 -0.696773 -0.0484814 0.543163 -2.30963 -2.5217 -0.146836 -0.154805 -12.4628 -0.311416 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.949512 -5.53347 -0.0553275 -0.0101499 -0.0878994 -4.59383 -6.62913 0 0 -0.86285 -0.0713796 -0.455148 -0.92 -2.26477 -1.90101 0 0 -0.0768529 0 0 0 -3.15254 -3.33447 -0.898228 -1.19788 -1.2906 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-8-PRENYLNARIGENIN-2.pdb 0 -2.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.171818 -1.65803 -3.00095 -4.05838 -0.415331 -0.104083 -1.50394 0 0 -1.91009 -1.4456 -5.33047 -0.120823 -8.80377 -9.0609 -0.31118 0 0 0 0 0 0 0 0 0 0 -0.922353 -5.43865 -4.14621 -8.55538 -8.9151 -0.0809662 0 0 -0.0333377 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.424824 0 -0.403173 -5.75669 -0.00306705 -3.10517 0 0 0 0 0 0 0 0 -2.66181 0 0 0 0 0 0 0 0 0 -0.000469208 -0.430363 -8.57076 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1.22175 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-8PRENYLNARINGENIN2CoCl-0.pdb -1.01013 0 0 0 0 0 0 0 0 0 0 0.23206 -1.53975 -3.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -6.6423 -2.32621 -2.59351 -1.07941 -0.0700876 0 -0.101085 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1.56024 -0.208498 -6.61649 -1.16069 4.0993 175.342 -1.35924 -1.52864 34.3346 24.6923 8.70832 -2.14432 -0.502609 -0.354565 -0.0583069 -3.37422 -3.88127 -0.0118477 -2.40799 -0.418556 -2.20852 -6.26392 0 -0.331209 -0.626929 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-8PRENYLNARINGENIN2ZnCl-2.pdb 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -2.5 -3.5 0 -6.73823 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.170118 0 0 -1.8913 -5.64538 -1.78056 -6.70003 -9.02023 -4.10145 -4.48386 -0.641846 -0.477787 0 0 0 0 0 0 0 0 0 0 0 -2.29416 -1.75698 -1.55669 -0.399387 -0.18653 -0.044279 -0.288648 -1.37379 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.211487 0 -4.11938 -9.15574 -3.78221 -0.150836 -5.28038 -6.69858 -6.62403 -0.581959 -9.30862 0 0 0 0 0 0 0 0 0 0 0 0 -6.25501 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.132549 -0.139166 -0.0648593 -0.271296 0 -0.148801 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-AVASTIN-2.pdb 0 0 -0.770322 0 0 -7 0 0 0 -2.43683 -3.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -8.34824 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0.13142 -7.4632 -0.108437 -2.71286 0 0 0 0 0 -1.97533 -3.08259 -2.35687 -3.18567 -1.47996 -0.0145018 -5.18207 -7.87912 -0.512634 -1.42658 -8.10275 -0.961955 -1.59919 0 0 0 0 -3.4012 -6.5245 -0.787662 -0.799057 -1.47771 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.0193792 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.389087 0 0 -5.68912 2.7218 -3.0328 -0.84823 -0.384137 -0.0264266 -0.106643 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-ISOXANTHOHUMOL-2.pdb 0 -2.5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.154565 -1.60277 -2.9959 -4.04946 -0.441926 -0.112525 -1.49514 0 0 -2.09058 -1.57726 -5.7911 -0.211194 -8.96055 -8.6 -0.310388 0 0 0 0 0 0 0 0 0 0 -1.16655 -5.78567 -3.62274 -8.81173 -8.82776 -0.114319 0 0 -0.0714578 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.692612 0 -0.461922 -5.26574 0 -3.35966 0 0 0 0 0 0 0 0 -2.46312 0 0 0 0 0 0 0 0 0 0 -0.395074 -9.26577 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1.27125 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-OXALILPLATIN-0.pdb 0 0 -3.89908 0 0 0 0 -10.4586 -3.5 -1.67452 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.5 0 0 0 0 0 -7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.230099 -1.89366 0 0 -0.246987 0 0 -1.47131 -1.40415 -4.96317 -0.0305197 -2.7408 -2.5571 -0.156248 0 0 0 0 0 0 0 0 0 0 -2.22365 -4.04606 -7.46548 -4.52581 -0.55654 -0.911246 -0.374286 -0.0941443 -0.935488 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.157422 -0.0277934 -1.35007 -1.49392 -0.105798 -2.03579 0 0 0 0 0 0 0 -0.6587 -2.73974 0 0 0 0 0 0 0 0 0 0 0 -2.34826 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.144519 0 0 -2.55564 0 -0.0452358 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-XANTHOHUMOL-2.pdb 0 0 -0.864737 0 -7 0 0 -4.45302 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.0774 0 -4.65808 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.581388 -0.00427072 -3.56311 0 0 -0.939449 0 0 -1.0679 -1.13071 -4.15254 0 -5.44763 -9.1532 0 0 0 0 0 0 0 0 0 0 -0.229005 -2.73139 -6.21711 -4.62039 -5.99864 -2.8919 -0.037011 -0.0859386 0 -0.587804 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1.24141 0 -1.07086 -8.12778 -0.111451 -3.38352 0 0 0 0 0 0 0 -1.31198 -3.53829 0 0 0 0 0 0 0 0 0 0 -0.090988 -7.15858 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -3.95362 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

PMS2 CLEAR-XELODA-0.pdb 0 0 -6.70721 -3.5 0 0 -2.5 -4.8143 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -8.06408 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.997406 -0.991412 -0.0942861 -0.123347 0.193697 0 0 -3.89815 -1.19949 2.66818 -0.5466 -2.46774 -1.67217 0 0 0 0 0 0 0 0 -5.68693 -2.12786 -1.66389 -7.19458 -2.82913 -8.88545 -1.26187 0 -0.695464 -0.908297 -0.108184 -1.24482 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.832196 -4.92849 0 -1.73886 0 0 0 0 0 0 0 0 -0.221699 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -0.02424 -1.54562 -0.434677 -0.039004 -7.72709 0 -0.941184 0 0 -2.23164 -3.6437 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0