Y1 = 5.5716 - 0.0049 XMW - 0.0475 XAMW - 0.0070 XSv - 0.0771 XMv - 0.0160 XMe - 0.0793 XMp + 0.1539 XMi + 0.0812 XGD + 0.0011 XnTA - 0.0281 XnBM - 0.0181 XSCBO - 0.0302 XRBN - 0.1481 XRBF + 0.1718 XnDB + 0.0009 XnH + 0.3469 XnN - 0.0810 XnO + 0.1572 XnS + 0.1234 XnF - 0.0341 XnCL - 0.0074 XnBR - 0.0103 XnHM + 0.0552 XnHet + 0.0252 XnX + 0.0710 XH% + 0.0071 XC% + 0.0423 XN% - 0.0973 XO% + 0.0487 XnCsp3 + 0.0011 XnCIR + 0.0141 XRperim - 0.0654 XRbrid - 0.0528 XNNRS - 0.3178 XnR04 + 0.1326 XnR05 - 0.0536 XnR06 + 0.1768 XnR10 - 0.0448 XD/Dtr06 + 0.0013 XZM1 + 0.0155 XZM1V + 0.0610 XZM1Kup - 0.0270 XZM1Mad + 0.0157 XZM2V - 0.0530 XZM2Mad + 0.0016 XON0 + 0.0075 XQindex + 0.0398 XDBI - 0.0399 XHNar + 0.1302 XXt - 0.0052 XRam + 0.0573 XBLI - 0.0223 XMSD - 0.0773 XSPI + 0.1222 XPJI2 + 0.0631 XCENT + 0.0398 XGMTIV - 0.0158 XWap + 0.0012 XS1K - 0.1567 XS3K - 0.0736 XPW2 - 0.0651 XPW3 - 0.0371 XPW4 - 0.0477 XPW5 + 0.0209 XMAXDN + 0.0588 XMAXDP + 0.0354 XDELS + 0.0099 XTIE + 0.0181 XPsi\_i\_s - 0.0236 XPsi\_i\_A + 0.1305 XPsi\_i\_t - 0.1164 XPsi\_i\_0d + 0.0661 XPsi\_e\_1 + 0.2297 XPsi\_e\_t + 0.0162 XBAC - 0.0316 XLOC + 0.1940 XSRW05 - 0.0685 XSRW10 - 0.0463 XMPC03 + 0.0056 XMPC06 - 0.0467 XMPC07 + 0.0303 XMPC08 + 0.1819 XMPC09 + 0.0399 XMPC10 - 0.0111 XpiPC02 + 0.0001 XpiPC03 + 0.0572 XpiPC05 - 0.0609 XpiPC07 - 0.0074 XpiPC08 + 0.0965 XpiPC09 + 0.0156 XX4 - 0.0366 XX5 + 0.1020 XX2A - 0.2330 XX3A - 0.3098 XX4A + 0.3422 XX5A - 0.0003 XX0v - 0.0586 XX2v - 0.1314 XX3v + 0.0432 XX4v + 0.0301 XX5v + 0.0677 XX0Av + 0.0737 XX2Av - 0.0972 XX3Av - 0.1615 XX4Av + 0.0863 XX5Av - 0.0437 XX1sol - 0.0382 XX2sol - 0.1796 XX3sol - 0.0179 XXMOD + 0.0648 XIAC + 0.1470 XAAC + 0.0513 XIDDE - 0.0964 XIVDE - 0.0116 XGes - 0.0870 XrGes + 0.1414 XXindex - 0.1752 XYindex - 0.2951 XIC1 - 0.1252 XIC2 - 0.0604 XIC3 + 0.1011 XIC5 - 0.0246 XTIC2 + 0.0620 XSIC0 - 0.3235 XSIC1 - 0.2386 XSIC2 - 0.1406 XSIC3 - 0.0333 XCIC0 + 0.1656 XCIC1 + 0.1730 XCIC2 - 0.0045 XCIC3 - 0.1576 XCIC4 - 0.2781 XCIC5 - 0.0415 XSpPosA\_A - 0.0553 XVE1sign\_A - 0.0296 XVE2sign\_A + 0.0298 XJ\_D + 0.0022 XTI1\_L - 0.0728 XSpPosA\_L + 0.0594 XSpMaxA\_L - 0.0477 XSpDiam\_L - 0.0328 XSpMAD\_L - 0.0318 XAVS\_X - 0.0212 XChiA\_X + 0.0270 XSpPosA\_X - 0.1513 XSpDiam\_X + 0.0923 XSM3\_X + 0.1520 XSM5\_X - 0.0007 XWi\_Dt + 0.0430 XJ\_Dt + 0.0276 XChi\_D/Dt + 0.1177 XChiA\_D/Dt + 0.0151 XJ\_D/Dt - 0.0674 XSpPosA\_D/Dt - 0.0198 XChi\_Dz(Z) + 0.0729 XChiA\_Dz(Z) - 0.0503 XJ\_Dz(Z) - 0.0343 XH\_Dz(m) + 0.0221 XChi\_Dz(v) - 0.0516 XJ\_Dz(v) - 0.0690 XSM1\_Dz(v) + 0.0157 XChi\_Dz(e) + 0.0937 XChiA\_Dz(e) - 0.0371 XChi\_Dz(p) + 0.1083 XChiA\_Dz(p) - 0.1504 XJ\_Dz(p) + 0.0330 XSpMAD\_Dz(p) + 0.0529 XJ\_Dz(i) + 0.0425 XSM1\_Dz(i) - 0.0064 XAVS\_B(m) + 0.0450 XChiA\_B(m) + 0.0080 XHyWi\_B(m) + 0.0197 XSpPosA\_B(m) + 0.0866 XSpMax\_B(m) + 0.0957 XSpMaxA\_B(m) + 0.0815 XSpDiam\_B(m) + 0.0227 XSpAD\_B(m) + 0.0736 XSpMAD\_B(m) + 0.0287 XEE\_B(m) - 0.0494 XVE1sign\_B(m) - 0.0565 XVE2sign\_B(m) - 0.0846 XAVS\_B(v) + 0.0953 XChiA\_B(v) - 0.1201 XSpPosA\_B(v) - 0.0079 XSpDiam\_B(v) - 0.0573 XSpMAD\_B(v) - 0.1065 XVE1\_B(v) - 0.0800 XAVS\_B(e) - 0.0657 XSpPosA\_B(p) + 0.0176 XSpPosA\_B(i) + 0.0115 XWi\_B(s) - 0.0190 XWiA\_B(s) + 0.0541 XChiA\_B(s) - 0.0403 XSpMaxA\_B(s) - 0.1095 XSpDiam\_B(s) + 0.0162 XSpAD\_B(s) + 0.0009 XSpMAD\_B(s) - 0.0773 XSM2\_B(s) + 0.0230 XVE1sign\_B(s) - 0.0386 XVE2sign\_B(s) - 0.0359 XATS1m - 0.0072 XATS2m - 0.0875 XATS3m - 0.0940 XATS4m + 0.0151 XATS8m - 0.0251 XATS2v - 0.0575 XATS3v + 0.0340 XATS6v - 0.0104 XATS3e + 0.1825 XATS6e - 0.0498 XATS7e + 0.0145 XATS8e - 0.0292 XATS1s + 0.0283 XATS2s - 0.0794 XATS3s + 0.0192 XATSC1m - 0.0308 XATSC3m - 0.0933 XATSC4m + 0.0466 XATSC5m + 0.0369 XATSC6m + 0.0470 XATSC1e + 0.2318 XATSC2e - 0.0007 XATSC3e + 0.1139 XATSC4e + 0.0772 XATSC5e + 0.1017 XATSC6e - 0.0720 XATSC8e + 0.0901 XATSC1i + 0.0508 XATSC1s + 0.1252 XATSC2s + 0.0285 XATSC3s + 0.1423 XATSC4s + 0.0410 XATSC5s + 0.2714 XATSC6s - 0.0763 XATSC7s + 0.0610 XMATS1m + 0.2028 XMATS2m + 0.0268 XMATS3m - 0.0626 XMATS5m - 0.1455 XMATS6m - 0.0543 XMATS7m + 0.0640 XMATS8m - 0.0749 XMATS1v + 0.1433 XMATS2v + 0.0610 XMATS3v + 0.0709 XMATS6v + 0.0384 XMATS1e + 0.0762 XMATS2e + 0.0149 XMATS3e - 0.0460 XMATS4e - 0.0219 XMATS5e - 0.0992 XMATS1p + 0.1518 XMATS2p - 0.0629 XMATS3p + 0.0126 XMATS4p - 0.1454 XMATS5p - 0.1714 XMATS1i + 0.2187 XMATS2i - 0.0963 XMATS3i + 0.0695 XMATS1s + 0.0277 XMATS2s - 0.0858 XMATS4s + 0.0973 XMATS5s - 0.1948 XMATS6s - 0.0557 XMATS8s - 0.1156 XGATS1m - 0.1090 XGATS2m - 0.0900 XGATS3m - 0.0276 XGATS4m - 0.0251 XGATS5m + 0.3051 XGATS6m + 0.0199 XGATS1v - 0.0785 XGATS2v - 0.0809 XGATS3v + 0.1110 XGATS5v + 0.0387 XGATS6v + 0.0368 XGATS7v + 0.0828 XGATS1e - 0.0478 XGATS2e - 0.0793 XGATS3e + 0.0006 XGATS5e + 0.0048 XGATS1p + 0.0432 XGATS3p + 0.1855 XGATS1i - 0.1365 XGATS2i - 0.0016 XGATS3i + 0.0315 XGATS1s - 0.0191 XGATS2s - 0.1241 XGATS3s + 0.1308 XGATS4s - 0.1532 XGATS5s + 0.3319 XGATS6s - 0.0926 XGATS7s - 0.0989 XGATS8s + 0.0066 XGGI1 + 0.0622 XGGI2 - 0.0717 XGGI3 - 0.1554 XGGI4 - 0.0680 XGGI5 - 0.1484 XGGI6 + 0.0547 XGGI7 + 0.2694 XGGI8 - 0.0119 XGGI9 + 0.0375 XGGI10 + 0.0556 XJGI2 - 0.2114 XJGI3 - 0.1637 XJGI4 + 0.0158 XJGI5 - 0.3200 XJGI6 - 0.0709 XJGI7 + 0.3470 XJGI8 + 0.0101 XJGI9 - 0.0024 XJGI10 - 0.0274 XJGT - 0.0508 XSpMax2\_Bh(m) - 0.0257 XSpMax3\_Bh(m) - 0.1425 XSpMax4\_Bh(m) - 0.0400 XSpMax5\_Bh(m) + 0.1051 XSpMax6\_Bh(m) + 0.0271 XSpMax7\_Bh(m) - 0.0314 XSpMax1\_Bh(v) - 0.0017 XSpMax5\_Bh(v) - 0.0048 XSpMax1\_Bh(e) + 0.0057 XSpMax4\_Bh(e) - 0.0430 XSpMax7\_Bh(e) + 0.0106 XSpMax8\_Bh(e) + 0.0402 XSpMax2\_Bh(s) + 0.0008 XSpMax3\_Bh(s) - 0.0171 XSpMax4\_Bh(s) + 0.0599 XSpMin1\_Bh(m) + 0.0336 XSpMin2\_Bh(m) + 0.0329 XSpMin6\_Bh(v) - 0.1156 XSpMin7\_Bh(v) - 0.0392 XSpMin1\_Bh(e) - 0.0863 XSpMin7\_Bh(e) + 0.0075 XSpMin1\_Bh(p) + 0.0446 XSpMin8\_Bh(p) + 0.0476 XSpMin5\_Bh(i) + 0.0122 XSpMin6\_Bh(i) - 0.0622 XSpMin8\_Bh(i) + 0.0302 XSpMin1\_Bh(s) - 0.1611 XSpMin3\_Bh(s) + 0.1976 XSpMin4\_Bh(s) - 0.0054 XSpMin5\_Bh(s) - 0.0726 XSpMin6\_Bh(s) - 0.0912 XSpMin8\_Bh(s) + 0.0415 XP\_VSA\_LogP\_1 - 0.0694 XP\_VSA\_LogP\_2 - 0.1662 XP\_VSA\_LogP\_3 - 0.0456 XP\_VSA\_LogP\_4 + 0.2307 XP\_VSA\_LogP\_5 - 0.0177 XP\_VSA\_LogP\_8 + 0.1534 XP\_VSA\_MR\_2 - 0.1582 XP\_VSA\_MR\_3 + 0.1555 XP\_VSA\_MR\_5 + 0.0310 XP\_VSA\_MR\_7 - 0.0937 XP\_VSA\_MR\_8 + 0.0078 XP\_VSA\_m\_2 - 0.0307 XP\_VSA\_v\_3 + 0.2121 XP\_VSA\_i\_1 - 0.0725 XP\_VSA\_i\_2 - 0.0586 XP\_VSA\_i\_3 + 0.2798 XP\_VSA\_i\_4 - 0.2360 XP\_VSA\_s\_3 - 0.1038 XP\_VSA\_s\_4 - 0.0135 XP\_VSA\_s\_6 - 0.1789 XP\_VSA\_ppp\_D + 0.1098 XP\_VSA\_ppp\_con - 0.0111 XP\_VSA\_ppp\_cyc - 0.0390 XP\_VSA\_ppp\_ter + 0.0158 XEta\_alpha\_A + 0.0089 XEta\_betaS\_A - 0.0159 XEta\_beta + 0.0119 XEta\_C + 0.0351 XEta\_C\_A - 0.0308 XEta\_F\_A - 0.0445 XEta\_FL + 0.0023 XEta\_B\_A + 0.1140 XEta\_sh\_p - 0.1409 XEta\_sh\_y + 0.0935 XEta\_sh\_x + 0.0393 XSpMaxA\_EA + 0.0528 XSpMaxA\_EA(ed) + 0.0078 XSpAD\_EA(ed) + 0.0493 XSpMaxA\_EA(bo) - 0.0448 XSpMAD\_EA(bo) - 0.2109 XSpMaxA\_EA(dm) - 0.2388 XSpDiam\_EA(dm) + 0.0014 XSpMax\_EA(ri) - 0.0136 XSpMaxA\_EA(ri) - 0.0655 XSpDiam\_EA(ri) - 0.1397 XSpMAD\_EA(ri) + 0.0093 XSpDiam\_AEA(ed) + 0.0206 XSpMax\_AEA(bo) - 0.0723 XSpMax\_AEA(dm) - 0.1068 XSpMaxA\_AEA(dm) - 0.0175 XSpDiam\_AEA(dm) - 0.2253 XSpMAD\_AEA(dm) - 0.1686 XChi0\_EA(dm) - 0.0351 XChi1\_EA(dm) + 0.0314 XChi1\_EA(ri) + 0.0567 XSM03\_EA - 0.0342 XSM07\_EA(dm) - 0.0705 XSM02\_EA(ri) + 0.1025 XSM03\_EA(ri) - 0.0753 XSM04\_AEA(bo) - 0.1915 XSM10\_AEA(bo) + 0.1646 XSM12\_AEA(bo) + 0.0829 XSM13\_AEA(bo) - 0.2797 XSM14\_AEA(bo) - 0.0338 XSM15\_AEA(bo) - 0.3950 XSM06\_AEA(dm) + 0.0268 XSM07\_AEA(dm) + 0.1670 XSM08\_AEA(dm) + 0.1444 XSM09\_AEA(dm) - 0.1290 XSM11\_AEA(dm) + 0.0897 XSM12\_AEA(dm) - 0.0648 XSM02\_AEA(ri) - 0.0120 XSM05\_AEA(ri) - 0.1645 XSM06\_AEA(ri) - 0.2232 XSM07\_AEA(ri) + 0.1897 XEig08\_EA(bo) + 0.1605 XEig09\_EA(bo) + 0.0169 XEig10\_EA(bo) + 0.1264 XEig02\_EA(dm) + 0.1291 XEig03\_EA(dm) + 0.2115 XEig04\_EA(dm) + 0.1811 XEig05\_EA(dm) - 0.1903 XEig06\_EA(dm) - 0.1210 XEig07\_EA(dm) - 0.1121 XEig09\_EA(dm) - 0.0783 XEig10\_EA(dm) + 0.0380 XEig11\_EA(dm) - 0.0882 XEig12\_EA(dm) + 0.1011 XEig15\_EA(dm) - 0.1486 XEig02\_AEA(ed) + 0.0084 XEig03\_AEA(ed) + 0.0345 XEig04\_AEA(ed) + 0.0944 XEig07\_AEA(ed) + 0.1175 XEig08\_AEA(ed) + 0.1363 XEig09\_AEA(ed) - 0.0225 XEig10\_AEA(ed) - 0.0712 XEig11\_AEA(ed) - 0.0468 XEig12\_AEA(ed) - 0.0735 XEig15\_AEA(ed) + 0.0315 XEig03\_AEA(bo) + 0.2140 XEig04\_AEA(bo) - 0.0971 XEig07\_AEA(bo) + 0.2909 XEig08\_AEA(bo) + 0.1634 XEig09\_AEA(bo) - 0.1547 XEig10\_AEA(bo) - 0.2890 XEig11\_AEA(bo) - 0.3468 XEig02\_AEA(dm) + 0.0366 XEig03\_AEA(dm) + 0.2319 XEig04\_AEA(dm) + 0.0789 XEig05\_AEA(ri) - 0.1677 XEig06\_AEA(ri) - 0.0435 XEig07\_AEA(ri) + 0.2106 XEig08\_AEA(ri) + 0.2070 XEig09\_AEA(ri) - 0.0491 XEig10\_AEA(ri) + 0.0772 XnCp + 0.0659 XnCq + 0.0534 XnCrs + 0.0007 XnCrt + 0.0600 XnCrq + 0.2377 XnCconj + 0.0692 XnR=Cs - 0.0804 XnR=Ct + 0.0562 XnRCOOR - 0.9359 XnRCHO + 0.2902 XnRCO - 0.1819 XnOHp + 0.0641 XnOHs + 0.1642 XnHAcc + 0.0294 XC-003 + 0.3382 XC-006 - 0.0878 XC-008 - 0.1455 XC-014 + 0.6669 XC-040 - 0.0404 XH-046 + 0.1909 XH-047 - 0.3097 XH-051 + 0.1154 XH-052 + 0.0197 XO-058 - 0.0330 XO-061 + 0.3799 XN-074 + 0.0883 XF-085 - 0.1316 XSdCH2 + 0.0624 XSssCH2 - 0.1757 XSdsCH - 0.1646 XSaasC - 0.1052 XSssssC + 0.1368 XSddsN + 0.0168 XSdO + 0.0004 XSssO - 0.2658 XNdsCH + 0.0927 XNdssC + 0.0922 XNssssC - 0.0868 XCATS2D\_02\_DA - 0.0268 XCATS2D\_02\_DL + 0.0192 XCATS2D\_04\_DL - 0.4295 XCATS2D\_05\_DL - 0.0045 XCATS2D\_09\_DL + 0.0415 XCATS2D\_02\_AA - 0.0690 XCATS2D\_01\_AN - 0.0210 XCATS2D\_02\_AL + 0.1089 XCATS2D\_03\_AL + 0.1311 XCATS2D\_04\_AL - 0.0468 XCATS2D\_05\_AL - 0.2283 XCATS2D\_06\_AL - 0.0180 XCATS2D\_09\_AL - 0.2421 XCATS2D\_00\_NN - 0.0776 XCATS2D\_01\_LL - 0.0613 XCATS2D\_02\_LL - 0.0996 XCATS2D\_03\_LL - 0.0660 XCATS2D\_04\_LL - 0.0519 XCATS2D\_05\_LL + 0.0292 XCATS2D\_06\_LL - 0.0531 XCATS2D\_09\_LL + 0.1091 XT(F..Cl) - 0.0122 XT(Cl..Cl) - 0.0602 XT(Br..Br) + 0.1696 XB01[C-C] - 0.1407 XB01[C-O] + 0.1621 XB01[C-F] - 0.1542 XB01[C-Cl] - 0.1710 XB02[C-C] - 0.5957 XB02[C-O] - 0.2772 XB02[C-Cl] + 0.0321 XB02[O-O] - 0.1395 XB03[C-C] - 0.2193 XB03[Cl-Cl] + 0.3436 XB04[C-C] - 0.0031 XB05[C-C] - 0.1498 XB05[C-O] - 0.5127 XB06[C-O] - 0.0424 XB09[C-C] - 0.2651 XB09[C-O] + 0.0481 XB10[C-C] - 0.4039 XB10[C-O] + 0.4577 XF01[C-N] - 0.0242 XF01[C-O] - 0.0402 XF03[Cl-Cl] + 0.0337 XF08[C-C] - 0.0249 XF10[C-C] - 0.1739 XF10[C-O] - 0.1022 XUi + 0.0052 XHy + 0.1152 XTPSA(Tot) + 0.0175 XMLOGP - 0.0093 XMLOGP2 + 0.0144 XPDI + 0.0255 XDLS\_01 - 0.2148 XDLS\_02 + 0.0106 XDLS\_03 + 0.1026 XDLS\_04 + 0.1862 XDLS\_05 - 0.1531 XDLS\_06 + 0.0938 XDLS\_cons + 0.3246 XLLS\_01 - 0.0840 XLLS\_02