Table 2: List of all descriptors used for feature selection. “Neutral” refer to the neutral form of the molecule, whereas “prot” refers to the protonated form.

ACD_pKaMA
ACD_pKa1
ACD_pKa2
prot_li
prot_n_ion
prot_n_pdN
prot_n_pH
prot_n_PI
prot_n_plN
prot_n_pN
prot_n_pol
prot_n_tautomers
prot_PDist
prot_Qamines
prot_QMAXN
prot_QMAXneg
prot_QMAXpos
prot_QMEANN
prot_QMINN
prot_QSUM
prot_QSUMH
prot_QSUMN
prot_QSUMneg
prot_QSUMO
prot_QSUMpos
prot_mpc
neutral_I3
neutral_li
neutral_n_amines
neutral_n_COOH
neutral_n_hal
neutral_n_ion
neutral_n_OpN
neutral_n_pdN
neutral_n_pH
neutral_n_PI
neutral_n_plN
neutral_n_pN
neutral_n_pol
neutral_n_qN
neutral_n_tautomers
neutral_n_XpC
neutral_PDist
neutral_Qamines
neutral_QMAXN
neutral_QMAXneg
neutral_QMAXpos
neutral_QMEANN
neutral_QMINN
neutral_QSUM
neutral_QSUMH
neutral_QSUMN
neutral_QSUMneg
neutral_QSUMO
neutral_QSUMpos
neutral_mpc
prot_apol
prot_a_acc
prot_a_acid
prot_a_aro
prot_a_base
prot_a_count
prot_a_don
prot_a_heavy
prot_a_hyd
prot_a_IC
prot_a_ICM
prot_a_nB
prot_a_nBr

prot_a_nC
prot_a_nCl
prot_a_nF
prot_a_nH
prot_a_nI
prot_a_nN
prot_a_nO
prot_a_nP
prot_a_nS
prot_balabanJ
prot_BCUT_PEOE_0
prot_BCUT_PEOE_1
prot_BCUT_PEOE_2
prot_BCUT_PEOE_3
prot_BCUT_SLOGP_0
prot_BCUT_SLOGP_1
prot_BCUT_SLOGP_2
prot_BCUT_SLOGP_3
prot_BCUT_SMR_0
prot_BCUT_SMR_1
prot_BCUT_SMR_2
prot_BCUT_SMR_3
prot_bpol
prot_b_1rotN
prot_b_1rotR
prot_b_ar
prot_b_count
prot_b_double
prot_b_heavy
prot_b_rotN
prot_b_rotR
prot_b_single
prot_b_triple
prot_chi0
prot_chi0v
prot_chi0v_C
prot_chi0_C
prot_chi1
prot_chi1v
prot_chi1v_C
prot_chi1_C
prot_chiral
prot_chiral_u
prot_density
prot_diameter
prot_FCharge
prot_GCUT_PEOE_0
prot_GCUT_PEOE_1
prot_GCUT_PEOE_2
prot_GCUT_PEOE_3
prot_GCUT_SLOGP_0
prot_GCUT_SLOGP_1
prot_GCUT_SLOGP_2
prot_GCUT_SLOGP_3
prot_GCUT_SMR_0
prot_GCUT_SMR_1
prot_GCUT_SMR_2
prot_GCUT_SMR_3
prot_Kier1
prot_Kier2
prot_Kier3
prot_KierA1
prot_KierA2
prot_KierA3
prot_KierFlex
prot_lip_acc
prot_lip_don
prot_lip_druglike
prot_lip_violation

prot_logPow
prot_logS
prot_mr
prot_mutagenic
prot_nmol
prot_opr_brigid
prot_opr_leadlike
prot_opr_nring
prot_opr_nrot
prot_opr_violation
prot_PCplus
prot_PCminus
prot_PEOE_PCplus
prot_PEOE_PCminus
prot_PEOE_RPCplus
prot_PEOE_RPCminus
prot_PEOE_VSAplus0
prot_PEOE_VSAplus1
prot_PEOE_VSAplus2
prot_PEOE_VSAplus3
prot_PEOE_VSAplus4
prot_PEOE_VSAplus5
prot_PEOE_VSAplus6
prot_PEOE_VSAminus0
prot_PEOE_VSAminus1
prot_PEOE_VSAminus2
prot_PEOE_VSAminus3
prot_PEOE_VSAminus4
prot_PEOE_VSAminus5
prot_PEOE_VSAminus6
prot_PEOE_VSA_FHYD
prot_PEOE_VSA_FNEG
prot_PEOE_VSA_FPNEG
prot_PEOE_VSA_FPOL
prot_PEOE_VSA_FPOS
prot_PEOE_VSA_FPPOS
prot_PEOE_VSA_HYD
prot_PEOE_VSA_NEG
prot_PEOE_VSA_PNEG
prot_PEOE_VSA_POL
prot_PEOE_VSA_POS
prot_PEOE_VSA_PPOS
prot_petitjean
prot_petitjeanSC
prot_pKa
prot_Q_PCplus
prot_Q_PCminus
prot_Q_RPCplus
prot_Q_RPCminus
prot_Q_VSA_FHYD
prot_Q_VSA_FNEG
prot_Q_VSA_FPNEG
prot_Q_VSA_FPOL
prot_Q_VSA_FPOS
prot_Q_VSA_FPPOS
prot_Q_VSA_HYD
prot_Q_VSA_NEG
prot_Q_VSA_PNEG
prot_Q_VSA_POL
prot_Q_VSA_POS
prot_Q_VSA_PPOS
prot_radius
prot_reactive
prot_rings
prot_RPCplus
prot_RPCminus
prot_rsynth
prot_SlogP
prot_SlogP_VSA0

prot_SlogP_VSA1
prot_SlogP_VSA2
prot_SlogP_VSA3
prot_SlogP_VSA4
prot_SlogP_VSA5
prot_SlogP_VSA6
prot_SlogP_VSA7
prot_SlogP_VSA8
prot_SlogP_VSA9
prot_SMR
prot_SMR_VSA0
prot_SMR_VSA1
prot_SMR_VSA2
prot_SMR_VSA3
prot_SMR_VSA4
prot_SMR_VSA5
prot_SMR_VSA6
prot_SMR_VSA7
prot_TPSA
prot_VAdjEq
prot_VAdjMa
prot_VDistEq
prot_VDistMa
prot_vdw_area
prot_vdw_vol
prot_vsa_acc
prot_vsa_acid
prot_vsa_base
prot_vsa_don
prot_vsa_hyd
prot_vsa_other
prot_vsa_pol
prot_Weight
prot_weinerPath
prot_weinerPol
prot_zagreb
neutral_apol
neutral_a_acc
neutral_a_acid
neutral_a_aro
neutral_a_base
neutral_a_count
neutral_a_don
neutral_a_heavy
neutral_a_hyd
neutral_a_IC
neutral_a_ICM
neutral_a_nB
neutral_a_nBr
neutral_a_nC
neutral_a_nCl
neutral_a_nF
neutral_a_nH
neutral_a_nI
neutral_a_nN
neutral_a_nO
neutral_a_nP
neutral_a_nS
neutral_balabanJ
neutral_BCUT_PEOE_0
neutral_BCUT_PEOE_1
neutral_BCUT_PEOE_2
neutral_BCUT_PEOE_3
neutral_BCUT_SLOGP_0
neutral_BCUT_SLOGP_1
neutral_BCUT_SLOGP_2
neutral_BCUT_SLOGP_3
neutral_BCUT_SMR_0
neutral_BCUT_SMR_1
neutral_BCUT_SMR_2
neutral_BCUT_SMR_3
neutral_bpol
neutral_b_1rotN

neutral_b_1rotR
neutral_b_ar
neutral_b_count
neutral_b_double
neutral_b_heavy
neutral_b_rotN
neutral_b_rotR
neutral_b_single
neutral_b_triple
neutral_chi0
neutral_chi0v
neutral_chi0v_C
neutral_chi0_C
neutral_chi1
neutral_chi1v
neutral_chi1v_C
neutral_chi1_C
neutral_chiral
neutral_chiral_u
neutral_density
neutral_diameter
neutral_FCharge
neutral_GCUT_PEOE_0
neutral_GCUT_PEOE_1
neutral_GCUT_PEOE_2
neutral_GCUT_PEOE_3
neutral_GCUT_SLOGP_0
neutral_GCUT_SLOGP_1
neutral_GCUT_SLOGP_2
neutral_GCUT_SLOGP_3
neutral_GCUT_SMR_0
neutral_GCUT_SMR_1
neutral_GCUT_SMR_2
neutral_GCUT_SMR_3
neutral_Kier1
neutral_Kier2
neutral_Kier3
neutral_KierA1
neutral_KierA2
neutral_KierA3
neutral_KierFlex
neutral_lip_acc
neutral_lip_don
neutral_lip_druglike
neutral_lip_violation
neutral_logPow
neutral_logS
neutral_mr
neutral_mutagenic
neutral_nmol
neutral_opr_brigid
neutral_opr_leadlike
neutral_opr_nring
neutral_opr_nrot
neutral_opr_violation
neutral_PCplus
neutral_PCminus
neutral_PEOE_PCplus
neutral_PEOE_PCminus
neutral_PEOE_RPCplus
neutral_PEOE_RPCminus
neutral_PEOE_VSAplus0
neutral_PEOE_VSAplus1
neutral_PEOE_VSAplus2
neutral_PEOE_VSAplus3
neutral_PEOE_VSAplus4
neutral_PEOE_VSAplus5
neutral_PEOE_VSAplus6
neutral_PEOE_VSAminus0
neutral_PEOE_VSAminus1
neutral_PEOE_VSAminus2
neutral_PEOE_VSAminus3
neutral_PEOE_VSAminus4

neutral_PEOE_VSAminus5
neutral_PEOE_VSAminus6
neutral_PEOE_VSA_FHYD
neutral_PEOE_VSA_FNEG
neutral_PEOE_VSA_FPNEG
neutral_PEOE_VSA_FPOL
neutral_PEOE_VSA_FPOS
neutral_PEOE_VSA_FPPOS
neutral_PEOE_VSA_HYD
neutral_PEOE_VSA_NEG
neutral_PEOE_VSA_PNEG
neutral_PEOE_VSA_POL
neutral_PEOE_VSA_POS
neutral_PEOE_VSA_PPOS
neutral_petitjean
neutral_petitjeanSC
neutral_pKa
neutral_Q_PCplus
neutral_Q_PCminus
neutral_Q_RPCplus
neutral_Q_RPCminus
neutral_Q_VSA_FHYD
neutral_Q_VSA_FNEG
neutral_Q_VSA_FPNEG
neutral_Q_VSA_FPOL
neutral_Q_VSA_FPOS
neutral_Q_VSA_FPPOS
neutral_Q_VSA_HYD
neutral_Q_VSA_NEG
neutral_Q_VSA_PNEG
neutral_Q_VSA_POL
neutral_Q_VSA_POS
neutral_Q_VSA_PPOS
neutral_radius
neutral_reactive
neutral_rings
neutral_RPCplus
neutral_RPCminus
neutral_rsynth
neutral_SlogP
neutral_SlogP_VSA0
neutral_SlogP_VSA1
neutral_SlogP_VSA2
neutral_SlogP_VSA3
neutral_SlogP_VSA4
neutral_SlogP_VSA5
neutral_SlogP_VSA6
neutral_SlogP_VSA7
neutral_SlogP_VSA8
neutral_SlogP_VSA9
neutral_SMR
neutral_SMR_VSA0
neutral_SMR_VSA1
neutral_SMR_VSA2
neutral_SMR_VSA3
neutral_SMR_VSA4
neutral_SMR_VSA5
neutral_SMR_VSA6
neutral_SMR_VSA7
neutral_TPSA
neutral_VAdjEq
neutral_VAdjMa
neutral_VDistEq
neutral_VDistMa
neutral_vdw_area
neutral_vdw_vol
neutral_vsa_acc
neutral_vsa_acid
neutral_vsa_base
neutral_vsa_don
neutral_vsa_hyd
neutral_vsa_other
neutral_vsa_pol

neutral_Weight
neutral_weinerPath
neutral_weinerPol
neutral_zagreb
RotatableBondCount
MolecularWeight
TotalFormalCharge
HydrogenBondDonorCount
HydrogenBondAcceptorCount
Complexity
HeavyAtomCount
AtomChiralCount
TPSA
ACD_pKa1_plus_pKa2
ACD_pKa1_plus_pKa2mod
prot_logPow_logWeight
neutral_logPow_logWeight
si_Weight_ACD_pKaMA
si_Weight_ACD_pKa1
si_Weight_ACD_pKa2
si_Weight_prot_li
si_Weight_prot_n_ion
si_Weight_prot_n_pdN
si_Weight_prot_n_pH
si_Weight_prot_n_PI
si_Weight_prot_n_plN
si_Weight_prot_n_pN
si_Weight_prot_n_pol
si_Weight_prot_n_tautomers
si_Weight_prot_PDist
si_Weight_prot_Qamines
si_Weight_prot_QMAXN
si_Weight_prot_QMAXneg
si_Weight_prot_QMAXpos
si_Weight_prot_QMEANN
si_Weight_prot_QMINN
si_Weight_prot_QSUM
si_Weight_prot_QSUMH
si_Weight_prot_QSUMN
si_Weight_prot_QSUMneg
si_Weight_prot_QSUMO
si_Weight_prot_QSUMpos
si_Weight_prot_mpc
si_Weight_neutral_I3
si_Weight_neutral_li
si_Weight_neutral_n_amines
si_Weight_neutral_n_COOH
si_Weight_neutral_n_hal
si_Weight_neutral_n_ion
si_Weight_neutral_n_OpN
si_Weight_neutral_n_pdN
si_Weight_neutral_n_pH
si_Weight_neutral_n_PI
si_Weight_neutral_n_plN
si_Weight_neutral_n_pN
si_Weight_neutral_n_pol
si_Weight_neutral_n_qN
si_Weight_neutral_n_tautomers
si_Weight_neutral_n_XpC
si_Weight_neutral_PDist
si_Weight_neutral_Qamines
si_Weight_neutral_QMAXN
si_Weight_neutral_QMAXneg
si_Weight_neutral_QMAXpos
si_Weight_neutral_QMEANN
si_Weight_neutral_QMINN
si_Weight_neutral_QSUM
si_Weight_neutral_QSUMH
si_Weight_neutral_QSUMN
si_Weight_neutral_QSUMneg
si_Weight_neutral_QSUMO
si_Weight_neutral_QSUMpos
si_Weight_neutral_mpc

si_Weight_prot_apol
si_Weight_prot_a_acc
si_Weight_prot_a_acid
si_Weight_prot_a_aro
si_Weight_prot_a_base
si_Weight_prot_a_count
si_Weight_prot_a_don
si_Weight_prot_a_heavy
si_Weight_prot_a_hyd
si_Weight_prot_a_IC
si_Weight_prot_a_ICM
si_Weight_prot_a_nB
si_Weight_prot_a_nBr
si_Weight_prot_a_nC
si_Weight_prot_a_nCl
si_Weight_prot_a_nF
si_Weight_prot_a_nH
si_Weight_prot_a_nI
si_Weight_prot_a_nN
si_Weight_prot_a_nO
si_Weight_prot_a_nP
si_Weight_prot_a_nS
si_Weight_prot_balabanJ
si_Weight_prot_BCUT_PEOE_0
si_Weight_prot_BCUT_PEOE_1
si_Weight_prot_BCUT_PEOE_2
si_Weight_prot_BCUT_PEOE_3
si_Weight_prot_BCUT_SLOGP_0
si_Weight_prot_BCUT_SLOGP_1
si_Weight_prot_BCUT_SLOGP_2
si_Weight_prot_BCUT_SLOGP_3
si_Weight_prot_BCUT_SMR_0
si_Weight_prot_BCUT_SMR_1
si_Weight_prot_BCUT_SMR_2
si_Weight_prot_BCUT_SMR_3
si_Weight_prot_bpol
si_Weight_prot_b_1rotN
si_Weight_prot_b_1rotR
si_Weight_prot_b_ar
si_Weight_prot_b_count
si_Weight_prot_b_double
si_Weight_prot_b_heavy
si_Weight_prot_b_rotN
si_Weight_prot_b_rotR
si_Weight_prot_b_single
si_Weight_prot_b_triple
si_Weight_prot_chi0
si_Weight_prot_chi0v
si_Weight_prot_chi0v_C
si_Weight_prot_chi0_C
si_Weight_prot_chi1
si_Weight_prot_chi1v
si_Weight_prot_chi1v_C
si_Weight_prot_chi1_C
si_Weight_prot_chiral
si_Weight_prot_chiral_u
si_Weight_prot_density
si_Weight_prot_diameter
si_Weight_prot_FCharge
si_Weight_prot_GCUT_PEOE_0
si_Weight_prot_GCUT_PEOE_1
si_Weight_prot_GCUT_PEOE_2
si_Weight_prot_GCUT_PEOE_3
si_Weight_prot_GCUT_SLOGP_0
si_Weight_prot_GCUT_SLOGP_1
si_Weight_prot_GCUT_SLOGP_2
si_Weight_prot_GCUT_SLOGP_3
si_Weight_prot_GCUT_SMR_0
si_Weight_prot_GCUT_SMR_1
si_Weight_prot_GCUT_SMR_2
si_Weight_prot_GCUT_SMR_3
si_Weight_prot_Kier1
si_Weight_prot_Kier2

si_Weight_prot_Kier3
si_Weight_prot_KierA1
si_Weight_prot_KierA2
si_Weight_prot_KierA3
si_Weight_prot_KierFlex
si_Weight_prot_lip_acc
si_Weight_prot_lip_don
si_Weight_prot_lip_druglike
si_Weight_prot_lip_violation
si_Weight_prot_logPow
si_Weight_prot_logS
si_Weight_prot_mr
si_Weight_prot_mutagenic
si_Weight_prot_nmol
si_Weight_prot_opr_brigid
si_Weight_prot_opr_leadlike
si_Weight_prot_opr_nring
si_Weight_prot_opr_nrot
si_Weight_prot_opr_violation
si_Weight_prot_PCplus
si_Weight_prot_PCminus
si_Weight_prot_PEOE_PCplus
si_Weight_prot_PEOE_PCminus
si_Weight_prot_PEOE_RPCplus
si_Weight_prot_PEOE_RPCminus
si_Weight_prot_PEOE_VSAplus0
si_Weight_prot_PEOE_VSAplus1
si_Weight_prot_PEOE_VSAplus2
si_Weight_prot_PEOE_VSAplus3
si_Weight_prot_PEOE_VSAplus4
si_Weight_prot_PEOE_VSAplus5
si_Weight_prot_PEOE_VSAplus6
si_Weight_prot_PEOE_VSAminus0
si_Weight_prot_PEOE_VSAminus1
si_Weight_prot_PEOE_VSAminus2
si_Weight_prot_PEOE_VSAminus3
si_Weight_prot_PEOE_VSAminus4
si_Weight_prot_PEOE_VSAminus5
si_Weight_prot_PEOE_VSAminus6
si_Weight_prot_PEOE_VSA_FHYD
si_Weight_prot_PEOE_VSA_FNEG
si_Weight_prot_PEOE_VSA_FPNEG
si_Weight_prot_PEOE_VSA_FPOL
si_Weight_prot_PEOE_VSA_FPOS
si_Weight_prot_PEOE_VSA_FPPOS
si_Weight_prot_PEOE_VSA_HYD
si_Weight_prot_PEOE_VSA_NEG
si_Weight_prot_PEOE_VSA_PNEG
si_Weight_prot_PEOE_VSA_POL
si_Weight_prot_PEOE_VSA_POS
si_Weight_prot_PEOE_VSA_PPOS
si_Weight_prot_petitjean
si_Weight_prot_petitjeanSC
si_Weight_prot_pKa
si_Weight_prot_Q_PCplus
si_Weight_prot_Q_PCminus
si_Weight_prot_Q_RPCplus
si_Weight_prot_Q_RPCminus
si_Weight_prot_Q_VSA_FHYD
si_Weight_prot_Q_VSA_FNEG
si_Weight_prot_Q_VSA_FPNEG
si_Weight_prot_Q_VSA_FPOL
si_Weight_prot_Q_VSA_FPOS
si_Weight_prot_Q_VSA_FPPOS
si_Weight_prot_Q_VSA_HYD
si_Weight_prot_Q_VSA_NEG
si_Weight_prot_Q_VSA_PNEG
si_Weight_prot_Q_VSA_POL
si_Weight_prot_Q_VSA_POS
si_Weight_prot_Q_VSA_PPOS
si_Weight_prot_radius
si_Weight_prot_reactive
si_Weight_prot_rings

si_Weight_prot_RPCplus
si_Weight_prot_RPCminus
si_Weight_prot_rsynth
si_Weight_prot_SlogP
si_Weight_prot_SlogP_VSA0
si_Weight_prot_SlogP_VSA1
si_Weight_prot_SlogP_VSA2
si_Weight_prot_SlogP_VSA3
si_Weight_prot_SlogP_VSA4
si_Weight_prot_SlogP_VSA5
si_Weight_prot_SlogP_VSA6
si_Weight_prot_SlogP_VSA7
si_Weight_prot_SlogP_VSA8
si_Weight_prot_SlogP_VSA9
si_Weight_prot_SMR
si_Weight_prot_SMR_VSA0
si_Weight_prot_SMR_VSA1
si_Weight_prot_SMR_VSA2
si_Weight_prot_SMR_VSA3
si_Weight_prot_SMR_VSA4
si_Weight_prot_SMR_VSA5
si_Weight_prot_SMR_VSA6
si_Weight_prot_SMR_VSA7
si_Weight_prot_TPSA
si_Weight_prot_VAdjEq
si_Weight_prot_VAdjMa
si_Weight_prot_VDistEq
si_Weight_prot_VDistMa
si_Weight_prot_vdw_area
si_Weight_prot_vdw_vol
si_Weight_prot_vsa_acc
si_Weight_prot_vsa_acid
si_Weight_prot_vsa_base
si_Weight_prot_vsa_don
si_Weight_prot_vsa_hyd
si_Weight_prot_vsa_other
si_Weight_prot_vsa_pol
si_Weight_prot_Weight
si_Weight_prot_weinerPath
si_Weight_prot_weinerPol
si_Weight_prot_zagreb
si_Weight_neutral_apol
si_Weight_neutral_a_acc
si_Weight_neutral_a_acid
si_Weight_neutral_a_aro
si_Weight_neutral_a_base
si_Weight_neutral_a_count
si_Weight_neutral_a_don
si_Weight_neutral_a_heavy
si_Weight_neutral_a_hyd
si_Weight_neutral_a_IC
si_Weight_neutral_a_ICM
si_Weight_neutral_a_nB
si_Weight_neutral_a_nBr
si_Weight_neutral_a_nC
si_Weight_neutral_a_nCl
si_Weight_neutral_a_nF
si_Weight_neutral_a_nH
si_Weight_neutral_a_nI
si_Weight_neutral_a_nN
si_Weight_neutral_a_nO
si_Weight_neutral_a_nP
si_Weight_neutral_a_nS
si_Weight_neutral_balabanJ
si_Weight_neutral_BCUT_PEOE_0
si_Weight_neutral_BCUT_PEOE_1
si_Weight_neutral_BCUT_PEOE_2
si_Weight_neutral_BCUT_PEOE_3
si_Weight_neutral_BCUT_SLOGP_0
si_Weight_neutral_BCUT_SLOGP_1
si_Weight_neutral_BCUT_SLOGP_2
si_Weight_neutral_BCUT_SLOGP_3
si_Weight_neutral_BCUT_SMR_0

si_Weight_neutral_BCUT_SMR_1
si_Weight_neutral_BCUT_SMR_2
si_Weight_neutral_BCUT_SMR_3
si_Weight_neutral_bpol
si_Weight_neutral_b_1rotN
si_Weight_neutral_b_1rotR
si_Weight_neutral_b_ar
si_Weight_neutral_b_count
si_Weight_neutral_b_double
si_Weight_neutral_b_heavy
si_Weight_neutral_b_rotN
si_Weight_neutral_b_rotR
si_Weight_neutral_b_single
si_Weight_neutral_b_triple
si_Weight_neutral_chi0
si_Weight_neutral_chi0v
si_Weight_neutral_chi0v_C
si_Weight_neutral_chi0_C
si_Weight_neutral_chi1
si_Weight_neutral_chi1v
si_Weight_neutral_chi1v_C
si_Weight_neutral_chi1_C
si_Weight_neutral_chiral
si_Weight_neutral_chiral_u
si_Weight_neutral_density
si_Weight_neutral_diameter
si_Weight_neutral_FCharge
si_Weight_neutral_GCUT_PEOE_0
si_Weight_neutral_GCUT_PEOE_1
si_Weight_neutral_GCUT_PEOE_2
si_Weight_neutral_GCUT_PEOE_3
si_Weight_neutral_GCUT_SLOGP_0
si_Weight_neutral_GCUT_SLOGP_1
si_Weight_neutral_GCUT_SLOGP_2
si_Weight_neutral_GCUT_SLOGP_3
si_Weight_neutral_GCUT_SMR_0
si_Weight_neutral_GCUT_SMR_1
si_Weight_neutral_GCUT_SMR_2
si_Weight_neutral_GCUT_SMR_3
si_Weight_neutral_Kier1
si_Weight_neutral_Kier2
si_Weight_neutral_Kier3
si_Weight_neutral_KierA1
si_Weight_neutral_KierA2
si_Weight_neutral_KierA3
si_Weight_neutral_KierFlex
si_Weight_neutral_lip_acc
si_Weight_neutral_lip_don
si_Weight_neutral_lip_druglike
si_Weight_neutral_lip_violation
si_Weight_neutral_logPow
si_Weight_neutral_logS
si_Weight_neutral_mr
si_Weight_neutral_mutagenic
si_Weight_neutral_nmol
si_Weight_neutral_opr_brigid
si_Weight_neutral_opr_leadlike
si_Weight_neutral_opr_nring
si_Weight_neutral_opr_nrot
si_Weight_neutral_opr_violation
si_Weight_neutral_PCplus
si_Weight_neutral_PCminus
si_Weight_neutral_PEOE_PCplus
si_Weight_neutral_PEOE_PCminus
si_Weight_neutral_PEOE_RPCplus
si_Weight_neutral_PEOE_RPCminus
si_Weight_neutral_PEOE_VSAplus0
si_Weight_neutral_PEOE_VSAplus1
si_Weight_neutral_PEOE_VSAplus2
si_Weight_neutral_PEOE_VSAplus3
si_Weight_neutral_PEOE_VSAplus4
si_Weight_neutral_PEOE_VSAplus5
si_Weight_neutral_PEOE_VSAplus6

si_Weight_neutral_PEOE_VSAminus0
si_Weight_neutral_PEOE_VSAminus1
si_Weight_neutral_PEOE_VSAminus2
si_Weight_neutral_PEOE_VSAminus3
si_Weight_neutral_PEOE_VSAminus4
si_Weight_neutral_PEOE_VSAminus5
si_Weight_neutral_PEOE_VSAminus6
si_Weight_neutral_PEOE_VSA_FHYD
si_Weight_neutral_PEOE_VSA_FNEG
si_Weight_neutral_PEOE_VSA_FPNEG
si_Weight_neutral_PEOE_VSA_FPOL
si_Weight_neutral_PEOE_VSA_FPOS
si_Weight_neutral_PEOE_VSA_FPPOS
si_Weight_neutral_PEOE_VSA_HYD
si_Weight_neutral_PEOE_VSA_NEG
si_Weight_neutral_PEOE_VSA_PNEG
si_Weight_neutral_PEOE_VSA_POL
si_Weight_neutral_PEOE_VSA_POS
si_Weight_neutral_PEOE_VSA_PPOS
si_Weight_neutral_petitjean
si_Weight_neutral_petitjeanSC
si_Weight_neutral_pKa
si_Weight_neutral_Q_PCplus
si_Weight_neutral_Q_PCminus
si_Weight_neutral_Q_RPCplus
si_Weight_neutral_Q_RPCminus
si_Weight_neutral_Q_VSA_FHYD
si_Weight_neutral_Q_VSA_FNEG
si_Weight_neutral_Q_VSA_FPNEG
si_Weight_neutral_Q_VSA_FPOL
si_Weight_neutral_Q_VSA_FPOS
si_Weight_neutral_Q_VSA_FPPOS
si_Weight_neutral_Q_VSA_HYD
si_Weight_neutral_Q_VSA_NEG
si_Weight_neutral_Q_VSA_PNEG
si_Weight_neutral_Q_VSA_POL
si_Weight_neutral_Q_VSA_POS
si_Weight_neutral_Q_VSA_PPOS
si_Weight_neutral_radius
si_Weight_neutral_reactive
si_Weight_neutral_rings
si_Weight_neutral_RPCplus
si_Weight_neutral_RPCminus
si_Weight_neutral_rsynth
si_Weight_neutral_SlogP
si_Weight_neutral_SlogP_VSA0
si_Weight_neutral_SlogP_VSA1
si_Weight_neutral_SlogP_VSA2
si_Weight_neutral_SlogP_VSA3
si_Weight_neutral_SlogP_VSA4
si_Weight_neutral_SlogP_VSA5
si_Weight_neutral_SlogP_VSA6
si_Weight_neutral_SlogP_VSA7
si_Weight_neutral_SlogP_VSA8
si_Weight_neutral_SlogP_VSA9
si_Weight_neutral_SMR
si_Weight_neutral_SMR_VSA0
si_Weight_neutral_SMR_VSA1
si_Weight_neutral_SMR_VSA2
si_Weight_neutral_SMR_VSA3
si_Weight_neutral_SMR_VSA4
si_Weight_neutral_SMR_VSA5
si_Weight_neutral_SMR_VSA6
si_Weight_neutral_SMR_VSA7
si_Weight_neutral_TPSA
si_Weight_neutral_VAdjEq
si_Weight_neutral_VAdjMa
si_Weight_neutral_VDistEq

si_Weight_neutral_VDistMa
si_Weight_neutral_vdw_area
si_Weight_neutral_vdw_vol
si_Weight_neutral_vsa_acc
si_Weight_neutral_vsa_acid
si_Weight_neutral_vsa_base
si_Weight_neutral_vsa_don
si_Weight_neutral_vsa_hyd
si_Weight_neutral_vsa_other
si_Weight_neutral_vsa_pol

si_Weight_neutral_Weight
si_Weight_neutral_weinerPath
si_Weight_neutral_weinerPol
si_Weight_neutral_zagreb
si_Weight_RotatableBondCount
si_Weight_MolecularWeight
si_Weight_TotalFormalCharge
si_Weight_HydrogenBondDonorCount
si_Weight_HydrogenBondAcceptorCount

si_Weight_Complexity
si_Weight_HeavyAtomCount
si_Weight_AtomChiralCount
si_Weight_TPSA
si_Weight_ACD_pKa1_plus_pKa2
si_Weight_ACD_pKa1_plus_pKa2mod
si_Weight_prot_logPow_logWeight
si_Weight_neutral_logPow_logWeight