

Full list of MERA descriptors

1. MERA. Atomic descriptors for enzyme.

nH, nC, nN, nO, nS, nHr, nCr, nNr, nOr, nSr

1.1.MERA. Atomic descriptors for enzyme. Zero order approximation. Atomic volumes. Overlapped volumes. Non-overlapped volumes.

vf0vo, vf0ug, vf0az, vf0ki, vf0se, vp0vo, vp0ug, vp0az, vp0ki, vp0se, vf0rvo, vf0rug, vf0raz, vf0rki, vf0rse, ef0vo, ef0ug, ef0az, ef0ki, ef0se, of0vo, of0ug, of0az, of0ki, of0se

1.2.MERA. Atomic descriptors for enzyme. Zero order approximation. Atomic surfaces. Overlapped surfaces. Non-overlapped surfaces.

sef0vo, sef0ug, sef0az, sef0ki, sef0se, sof0vo, sof0ug, sof0az, sof0ki, sof0se, snef0vo, snef0ug, snef0az, snef0ki, snef0se, snof0vo, snof0ug, snof0az, snof0ki, snof0se

1.3.MERA. Atomic descriptors for enzyme. Zero order approximation. Overlapped and Non-overlapped electrons.

nef0vo, nef0ug, nef0az, nef0ki, nef0se, nof0vo, nof0ug, nof0az, nof0ki, nof0se

1.4.MERA. Atomic descriptors for enzyme. First order approximation. Atomic volumes. Overlapped volumes. Non-overlapped volumes.

vfvo, vfug, vfaz, vfki, vfse, vpvo, vpub, vpaz, vpki, vpse, vfrvo, vfrug, vfraz, vfrki, vfrse, efvo, efug, efaz, efki, efse, ofvo, ofug, ofaz, ofki, ofse

1.5.MERA. Atomic descriptors for enzyme. First order approximation. Atomic surfaces. Overlapped surfaces. Non-overlapped surfaces.

sefvo, sefug, sefaz, sefki, sefse, sofvo, sofug, sofaz, sofki, sofse, snefvo, snefug, snefaz, snefki, snefse, snofvo, snofug, snofaz, snofki, snofse

1.6.MERA. Atomic descriptors for enzyme. First order approximation. Overlapped and Non-overlapped electrons.

nefvo, nefug, nefaz, nefki, nefse, nofvo, nofug, nofaz, nofki, nofse

2. MERA. Atomic descriptors for enzyme – ligand complexes.

xnH, xnC, xnN, xnO, xnF, xnP, xnS, xnCl, xnBr, xnl, xnHr, xnCr, xnNr, xnOr, xnFr, xnPr, xnSr, xnClr, xnBrr, xnlr

2.1.MERA. Atomic descriptors for enzyme – ligand complexes. Zero order approximation. Atomic volumes. Overlapped volumes. Non-overlapped volumes.

xvf0vo, xvf0ug, xvf0az, xvf0ki, xvf0ft, xvf0fo, xvf0se, xvf0h, xvf0b, xvf0yo, xvp0vo, xvp0ug, xvp0az, xvp0ki, xvp0ft, xvp0fo, xvp0se, xvp0h, xvp0b, xvp0yo, xvf0rvo, xvf0rug, xvf0raz, xvf0rki, xvf0rft, xvf0rfo, xvf0rse, xvf0rh, xvf0rb, xvf0ryo, xef0vo, xef0ug, xef0az, xef0ki, xef0ft, xef0fo, xef0se, xef0h, xef0b, xef0yo, xof0vo, xof0ug, xof0az, xof0ki, xof0ft, xof0fo, xof0se, xof0h, xof0b, xof0yo, xnef0vo, xnef0ug

2.2.MERA. Atomic descriptors for enzyme – ligand complexes. Zero order approximation. Atomic surfaces. Overlapped surfaces. Non-overlapped surfaces.

xsef0vo, xsef0ug, xsef0az, xsef0ki, xsef0ft, xsef0fo, xsef0se, xsef0h, xsef0b, xsef0yo, xsnf0vo, xsnf0ug, xsnf0az, xsnf0ki, xsnf0ft, xsnf0fo, xsnf0se, xsnf0h, xsnf0b, xsnf0yo, xsnf0vo, xsnf0ug, xsnf0az, xsnf0ki, xsnf0ft, xsnf0fo, xsnf0se, xsnf0h, xsnf0b, xsnf0yo

2.3.MERA. Atomic descriptors for enzyme – ligand complexes. Zero order approximation. Overlapped and Non-overlapped electrons.

xnef0az, xnef0ki, xnef0ft, xnef0fo, xnef0se, xnef0h, xnef0b, xnef0yo, xnof0vo, xnof0ug, xnof0az, xnof0ki, xnof0ft, xnof0fo, xnof0se, xnof0h, xnof0b, xnof0yo

2.4.MERA. Atomic descriptors for enzyme – ligand complexes. First order approximation. Atomic volumes. Overlapped volumes. Non-overlapped volumes.

xvfo, xvfg, xvfa, xvfk, xvff, xvffo, xvfa, xvfh, xvfb, xvfy, xvpo, xvpu, xvpa, xvpi, xvpt, xvpo, xvpe, xvph, xvpb, xvpy, xvfr, xvfrg, xvfrz, xvfrki, xvfrt, xvfrse, xvfrh, xvfrb, xvfryo, xefvo, xefug, xefaz, xefki, xefft, xeffo, xefse, xefh, xefb, xefyo, xofvo, xofug, xofaz, xofki, xofft, xoffo, xofse, xofh, xofb, xofyo, xnefvo, xnefug

2.5.MERA. Atomic descriptors for enzyme – ligand complexes. First order approximation. Atomic surfaces. Overlapped surfaces. Non-overlapped surfaces.

xsefvo, xsefug, xsefaz, xsefki, xsefft, xseffo, xsefse, xsefh, xsefb, xsefy, xsofvo, xsofug, xsofaz, xsofki, xsoftt, xsoffo, xsofse, xsofh, xsofb, xsofy, xsnefvo, xsnefug, xsnefaz, xsnefki, xsnefft, xsneffo, xsnefse, xsnefh, xsnefb, xsnefy, xsnofvo, xsnofug, xsnofaz, xsnofki, xsnofft, xsnoffo, xsnofse, xsnofh, xsnofb, xsnofyo

2.6.MERA. Atomic descriptors for enzyme – ligand complexes. First order approximation. Overlapped and Non-overlapped electrons.

xnefaz, xnefki, xnefft, xneffo, xnefse, xnefh, xnefb, xnefy, xnofvo, xnofug, xnofaz, xnofki, xnoftt, xnofto, xnofse, xnofh, xnofb, xnofyo

3. MERA. Atomic descriptors for ligand.

3.1.MERA. Atomic descriptors for ligand. Zero order approximation. Atomic volumes. Overlapped volumes. Non-overlapped volumes.

lvfo, lvf0ug, lvf0az, lvf0ki, lvf0ft, lvf0fo, lvf0se, lvf0h, lvf0b, lvf0yo, lvp0vo, lvp0ug, lvp0az, lvp0ki, lvp0ft, lvp0fo, lvp0se, lvp0h, lvp0b, lvp0yo, lvp0ro, lvp0rug, lvp0raz, lvp0rki, lvp0rt, lvp0rfo, lvp0rse, lvp0rh, lvp0rb, lvp0ryo, lef0vo, lef0ug, lef0az, lef0ki, lef0ft, lef0fo, lef0se, lef0h, lef0b, lef0yo, lef0vo, lef0ug, lef0az, lef0ki, lef0ft, lef0fo, lef0se, lef0h, lef0b, lef0yo, lef0vo, lef0ug

3.2.MERA. Atomic descriptors for ligand. Zero order approximation. Atomic surfaces. Overlapped surfaces. Non-overlapped surfaces.

lsef0vo, lsef0ug, lsef0az, lsef0ki, lsef0ft, lsef0fo, lsef0se, lsef0h, lsef0b, lsef0yo, lsof0vo, lsof0ug, lsof0az, lsof0ki, lsof0ft, lsof0fo, lsof0se, lsof0h, lsof0b, lsof0yo, lsnof0vo, lsnof0ug, lsnof0az, lsnof0ki, lsnof0ft, lsnof0fo, lsnof0se, lsnof0h, lsnof0b, lsnof0yo

3.3.MERA. Atomic descriptors for ligand. Zero order approximation. Overlapped and Non-overlapped electrons.

lnef0az, lnef0ki, lnef0ft, lnef0fo, lnef0se, lnef0h, lnef0b, lnef0yo, lnof0vo, lnof0ug, lnof0az, lnof0ki, lnof0ft, lnof0fo, lnof0se, lnof0h, lnof0b, lnof0yo

3.4.MERA. Atomic descriptors for ligand. First order approximation. Atomic volumes. Overlapped volumes. Non-overlapped volumes.

lvfo, lvfug, lvfa, lvfk, lvff, lvffo, lvfa, lvfh, lvfb, lvfy, lvp0, lvp0ug, lvp0az, lvp0ki, lvp0ft, lvp0fo, lvp0se, lvp0h, lvp0p, lvp0yo, lvp0ro, lvp0rug, lvp0fr, lvp0rki, lvp0rt, lvp0rfo, lvp0rse, lvp0rh, lvp0rb, lvp0ryo, lef0vo, lef0ug, lef0az, lef0ki, lef0ft, lef0fo, lef0se, lef0h, lef0b, lef0yo, lef0vo, lef0ug, lef0az, lef0ki, lef0ft, lef0fo, lef0se, lef0h, lef0b, lef0yo, lef0vo, lef0ug, lef0az, lef0ki, lef0ft, lef0fo, lef0se, lef0h, lef0b, lef0yo, lef0vo, lef0ug

3.5.MERA. Atomic descriptors for ligand. First order approximation. Atomic surfaces. Overlapped surfaces. Non-overlapped surfaces.

lsefvo, lsefug, lsefaz, lsefki, lsefft, lseffo, lsefse, lsefh, lsefy, lsofvo, lsofug, lsofaz, lsofki, lsofft, lsoffo,

Isosfse, Isosfh, Isosfb, Isosfyo, Isnefvo, Isnefug, Isnefaz, Isnefki, Isnefft, Isneffo, Isnefse, Isnefh, Isnefb, Isnefyo, Isnofvo, Isnofug, Isnofaz, Isnofki, Isnofft, Isnoffo, Isnofse, Isnofh, Isnofb, Isnofyo

3.6.MERA. Atomic descriptors for ligand. First order approximation. Overlapped and Non-overlapped electrons.

Inefaz, Inefki, Inefft, Ineffo, Inefse, Inefh, Inefb, Inefyo, Inofvo, Inofug, Inofaz, Inofki, Inofft, Inoffo, Inofse, Inofh, Inofb, Inofyo

4. MERA. Molecular descriptors for enzyme.

4.1.MERA. Molecular descriptors for enzyme. Zero order approximation. Volumes, surfaces, density, overlapped and non-overlapped volumes, overlapped and non-overlapped surfaces.

VME0, VSME0, VPME0, SME0, RO0, VOIN01, VOIN01R, VOIN02, VOIN02R, VOIN03, VOIN03R, VOIN04, VOIN04R, VOIN05, VOIN05R, MOIN02, MOIN02R, MOIN03, MOIN03R, MOIN04, MOIN04R, MOIN05, MOIN05R, EOIN02, EOIN02R, EOIN03, EOIN03R, EOIN04, EOIN04R, EOIN05, EOIN05R

4.2.MERA. Molecular descriptors for enzyme. Zero order approximation. Electronic characteristics. Number of electrons, number of bounded and unbounded electrons and their portions.

NELS0, UELS0, BELS0, UELS0r, BELS0r, UOELS0, BVEL0S, UVEL0S, BVELS0r, BOELS0r

4.3.MERA. Molecular descriptors for enzyme. First order approximation. Volumes, surfaces, density, overlapped and non-overlapped volumes, overlapped and non-overlapped surfaces, positively, negatively and neutral areas and their ratios. Sphericity.

VME, SME, SMEP, SMEN, SMED, SMEPR, SMENR, SMEDR, ESMEP, ESMEN, ESMED, d204, SPH, VOIN1, VOIN1R, VOIN2, VOIN2R, VOIN3, VOIN3R, VOIN4, VOIN4R, VOIN5, VOIN5R, VOIN6, VOIN6R, MOIN2, MOIN2R, MOIN3, MOIN3R, MOIN4, MOIN4R, MOIN5, MOIN5R, MOIN6, MOIN6R, EOIN2, EOIN2R, EOIN3, EOIN3R, EOIN4, EOIN4R, EOIN5, EOIN5R, EOIN6, EOIN6R

4.4.MERA. Molecular descriptors for enzyme. First order approximation. Electronic characteristics. Number of electrons, number of bounded and unbounded electrons and their portions. Dipole moment, weighted average positive and negative charge of surface, their sum, variations of atomic partial charges, molecular electronegativity.

NELS, UELS, BELS, UELSr, BELSr, OELS, UOELS, BOELS, UOELSr, BOELSr, DMo, QSMEP, QSMEN, QSMED, VARQ, VARSQ, HIMERA

4.5.MERA. Molecular descriptors for enzyme. First order approximation. Inertial characteristics. Inertial moments. Inertial radii. Inertial sections.

MI1, MI2, MI3, IR1, IR2, IR3, SI12, SI13, SI23, PI12, PI13, PI23

4.6.MERA. Molecular descriptors for enzyme. First order approximation. Dissymmetry, asymmetry and chirality characteristics.

DISS1, DISS2, DISS3, DISS1R, DISS2R, DISS3R, DISST, DISSTR, DISSM1, DISSM2, DISSM3, DISSM1R, DISSM2R, DISSM3R, DISSM1C, DISSM2C, DISSM3C, DISSMT, DISSMTR, DISSMTC, DISSV1, DISSV2, DISSV3, DISSV1R, DISSV2R, DISSV3R, DISSV1C, DISSV2C, DISSV3C, DISSVT, DISSVTR, DISSVTC, DISSQ1, DISSQ2, DISSQ3, DISSQ1C, DISSQ2C, DISSQ3C, DISSQT, DISSQTC, ASY1, ASY2, ASY3, ASY1R, ASY2R, ASY3R, ASYT, ASYTR, ASYM1, ASYM2, ASYM3, ASYM1R, ASYM2R, ASYM3R, ASYM1C, ASYM2C, ASYM3C, ASYMT, ASYMTR, ASYMTC, ASYV1, ASYV2, ASYV3, ASYV1R, ASYV2R, ASYV3R, ASYV1C, ASYV2C, ASYV3C, ASYVT, ASYVTR, ASYVTC, ASYQ1, ASYQ2, ASYQ3, ASYQ1C, ASYQ2C, ASYQ3C, ASYQT, ASYQTC

4.7.MERA. Molecular descriptors for enzyme. First order approximation. Geometry characteristics. Linear sizes and section in space of principal components.

DLI1, DLIB11, DLIB12, DLIB13, DLIB14, DLIB1M, DLI2, DLIB21, DLIB22, DLIB23, DLIB24, DLIB2M, DLI3, DLIB31, DLIB32, DLIB33, DLIB34, DLIB3M, DEI1, DEI2, DEI3, SG12, SG13, SG23, PG12, PG13, PG23,

NDLI1, NDLIB11, NDLIB12, NDLIB13, NDLIB14, NDLIB1M, NDLI2, NDLIB21, NDLIB22, NDLIB23, NDLIB24, NDLIB2M, NDLI3, NDLIB31, NDLIB32, NDLIB33, NDLIB34, NDLIB3M, NPOV, NPOVR, NQPOV, NQPOVR, PDLI1, PDLIB11, PDLIB12, PDLIB13, PDLIB14, PDLIB1M, PDLI2, PDLIB21, PDLIB22, PDLIB23, PDLIB24, PDLIB2M, PDLI3, PDLIB31, PDLIB32, PDLIB33, PDLIB34, PDLIB3M, PPOV, PPOVR, PQPOV, PQPOVR, FDLI1, FDLIB11, FDLIB12, FDLIB13, FDLIB14, FDLIB1M, FDLI2, FDLIB21, FDLIB22, FDLIB23, FDLIB24, FDLIB2M, FDLI3, FDLIB31, FDLIB32, FDLIB33, FDLIB34, FDLIB3M, FPOV, FPOVR, FQPOV, FQPOVR

4.8.MERA. Molecular descriptors for enzyme. First order approximation. Characteristics of interactions. Energies of Coulomb, Van der Waals, intermolecular interactions and total energy. Characteristics of association matrix, its eigen values and their combinations.

ECOUL, EVAN, EINT, EMERA, EVA1, EVA2, EVA3, NAS, SEVA, SEVAR, EVA1V0, EVA2V0, EVA3V0, SEVAV0, SEVARV0, EVA1V, EVA2V, EVA3V, SEVAV, SEVARV, HEC, SQEVA1, SQEVA2, SQEVA3, SQNAS, SQSEVA, SQSEVAR, SQEVA1V0, SQEVA2V0, SQEVA3V0, SQSEVAV0, SQSEVARV0, SQEVA1V, SQEVA2V, SQEVA3V, SQSEVAV, SQSEVARV