

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, vpug, 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, xsof0vo, xsof0ug, xsof0az, xsof0ki, xsof0ft, xsof0fo, xsof0se, xsof0h, xsof0b, xsof0yo, xsnef0vo, xsnef0ug, xsnef0az, xsnef0ki, xsnef0ft, xsnef0fo, xsnef0se, xsnef0h, xsnef0b, xsnef0yo, xsnof0vo, xsnof0ug, xsnof0az, xsnof0ki, xsnof0ft, xsnof0fo, xsnof0se, xsnof0h, xsnof0b, xsnof0yo

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, xvug, xvfaz, xvfki, xvfft, xvffo, xvffe, xvfh, xvfb, xvfo, xvpvo, xvpug, xvpaz, xvpki, xvpft, xvpfo, xvpse, xvph, xvpb, xvpyo, xvfrvo, xvfrug, xvfraz, xvfrki, xvfrft, xvfrfo, xvfrse, xvfrh, xvfrb, xvfrfo, xefvo, xefug, xefaz, xefki, xefft, xeffo, xeffse, 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, xseffe, xsefh, xsefb, xsefyo, xsofvo, xsofug, xsofaz, xsofki, xsofft, xsoffo, xsoffe, xsofh, xsofb, xsofyo, xsnefvo, xsnefug, xsnefaz, xsnefki, xsnefft, xsneffo, xsneffe, xsnefh, xsnefb, xsnefyo, 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, xneffe, xnefh, xnefb, xnefyo, xnofvo, xnofug, xnofaz, xnofki, xnofft, xnoffo, 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.

lvf0vo, lvf0ug, lvf0az, lvf0ki, lvf0ft, lvf0fo, lvf0se, lvf0h, lvf0b, lvf0yo, lvp0vo, lvp0ug, lvp0az, lvp0ki, lvp0ft, lvp0fo, lvp0se, lvp0h, lvp0b, lvp0yo, lvf0rvo, lvf0rug, lvf0raz, lvf0rki, lvf0rft, lvf0rfo, lvf0rse, lvf0rh, lvf0rb, lvf0ryo, lef0vo, lef0ug, lef0az, lef0ki, lef0ft, lef0fo, lef0se, lef0h, lef0b, lef0yo, lof0vo, lof0ug, lof0az, lof0ki, lof0ft, lof0fo, lof0se, lof0h, lof0b, lof0yo, lnef0vo, lnef0ug

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, lsnef0vo, lsnef0ug, lsnef0az, lsnef0ki, lsnef0ft, lsnef0fo, lsnef0se, lsnef0h, lsnef0b, lsnef0yo, 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, lvug, lvfaz, lvfki, lvfft, lvffo, lvffe, lvfh, lvfb, lvfo, lvpvo, lvpug, lvpaz, lvpki, lvpft, lvpfo, lvpse, lvph, lvpb, lvpyo, lvfrvo, lvfrug, lvfraz, lvfrki, lvfrft, lvfrfo, lvfrse, lvfrh, lvfrb, lvfrfo, lefvo, lefug, lefaz, lefki, lefft, leffo, leffe, lefh, lefb, lefyo, lofvo, lofug, lofaz, lofki, lofft, loffo, loffe, lofh, lofb, lofyo, lnefvo, lnefug

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

lsefvo, lsefug, lsefaz, lsefki, lsefft, lseffo, lseffe, lsefh, lsefb, lsefyo, lsofvo, lsofug, lsofaz, lsofki, lsofft, lsoffo, lsoffe

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

4. MERA. Molecular descriptors for enzyme.

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