ADMET Predictor(TM) Output file  4/7/2022  5:42:22 PM

Input File Name =
S:\AGO\PD_SolidDose\FormDev_NewProducts\Projects\Steptoe\Conformer3D_CID_9444
(1).sdf

Default Hayduk-Laudie diffusivity [cm^2/s x 10^5] model
Default S+MDCK permeability [cm/s x 10^7] model
Default S+Peff permeability [cm/s x 10^4] model
Default Meylan solubility [mg/mL] model
Default S+Sw solubility [mg/mL] model
Default S+BBB permeability model
Default S+PrUnbnd percent unbound model
Default S+Vd volume of distribution [L/kg] model
ADMET Risk rules from c:\program files\simulations plus,
inc\admet_predictor\Default.ro5
pH for ionization descriptors = 7.4
pH for pH-sensitive models = 7.4

*molname PUBCHEM_COMPOUND_CID PUBCHEM_CONFORMER_RMSD
PUBCHEM_CONFORMER_DIVERSEORDER PUBCHEM_MMFF94_PARTIAL_CHARGES
PUBCHEM_EFFECTIVE_ROTOR_COUNT PUBCHEM_PHARMACOPHORE_FEATURES
PUBCHEM_HEAVY_ATOM_COUNT PUBCHEM_ATOM_DEF_STEREO_COUNT
PUBCHEM_ATOM_UDEF_STEREO_COUNT PUBCHEM_BOND_DEF_STEREO_COUNT
PUBCHEM_BOND_UDEF_STEREO_COUNT PUBCHEM_ISOTOPIC_ATOM_COUNT
PUBCHEM_COMPONENT_COUNT PUBCHEM_CACTVS_TAUTO_COUNT PUBCHEM_CONFORMER_ID
PUBCHEM_MMFF94_ENERGY PUBCHEM_FEATURE_SELFOVERLAP PUBCHEM_SHAPE_FINGERPRINT
PUBCHEM_SHAPE_MULTIPOLES PUBCHEM_SHAPE_SELFOVERLAP
PUBCHEM_SHAPE_VOLUME PUBCHEM_COORDINATE_TYPE MeltingPoint Orig.Order
Acid_Pred_pKa Base_Pred_pKa DiffCoef MlogP S+logP Outsider_of_S+logP
S+logD S+Peff Outsider_of_S+Peff S+Pavg Outsider_of_S+Pavg S+MDCK
Outsider_of_S+MDCK S+Sw Outsider_of_S+Sw S+pH S+IS S+SF
S+Sp S+BBB Outsider_of_S+BBB S+PrUnbnd Outsider_of_S+PrUnbnd
S+Vd Outsider_of_S+Vd TOX_MRTD Outsider_of_TOX_MRTD
TOX_ER_Filter Outsider_of_TOX_ER_Filter TOX_ER Outsider_of_TOX_ER
TOX_FHM Outsider_of_TOX_FHM TOX_hERG Outsider_of_TOX_hERG TOX_BRM_Rat
Outsider_of_TOX_BRM_Rat TOX_BRM_Mouse Outsider_of_TOX_BRM_Mouse S+HIVI-ST
Outsider_of_S+HIVI-ST S+HIVI-TC Outsider_of_S+HIVI-TC SimHIA_1
SimHIA_10 SimHIA_100 SimHIA_1000 ADMET_Risk ADMET_Code
Formula MWt MolVol VMcGowan N_Atoms N_Carbon N_Ntrgen
N_Oxygen N_Phsphr N_Sulfur N_Fluorn N_Chlorn
N_Bromin N_Iodine N_Halogen N_Nonorgn N_Metal N_Bonds
N_FrRotB F_SgleB F_DbleB F_TpleB F_AromB F_AFRBWF N_Rings N_AromR
N_AlipR N_Pisyms N_Kekule X0 X1 X2 Kappa1 Kappa2
Kappa3 Wiener SsCH3 SssCH2 SsssCH SssssC SdCH2 SdsCH SdssC SaaCH
SaasC SaadC SaaaC StCH SddC StsC SssssN SdsssN SsNH2 SssNH
SsssN SdNH SdsN SdssN SaaN SaaNH SaasN SddsN SaadN SaaaN StN
StsN StdN SsOH SssO SsO- SdO SaaO SdsssP SdssPH SsPH2
SssPH SsssP SssssssP SddssS SsSH SssS SssssssS SdssS SsssS SdS
SaaS SsF SsCl SsBr SsI SHsOH SHdNH SHsNH2 SHssNH SHsSH

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SHCH_321        SHdCH2  SHdsCH  SHaaCH  SHtCH   S_unknown       AlHdrxl_-OH
ArHdrxl_-OH     Carbonyl_C=O    Ether___-O-     PriAmine_-NH2   PriAmAli_-NH2
PriAmAro_-NH2   SecAmine_>NH    TerAmine_>N-    QuaAmine_>[N+]< ArNitrog_=N-
Imine___=N-     Nitrile_C#N     Isocynd_[N+]#[C-]       Thiol___-SH
ThioCrbl_C=S    Sulfide_-S-     Slfonium_>[S+]- Phsphine_>P-    HydxlAmn_>N-O-
Oxime___=N-O-   Nitroso_-N=O    Hdrzine_>N-N<   Hdrzone_=N-N<   Azo_____-N=N-
Diazo___-[N+]#N ThioAmin_>N-S-  Disulfde_-S-S-  Sulfoxde_>S=O   Thioxime_=N-S-
Nitro___-NO2    Nitrite_-O-N=O  Ntrosam_>N-N=O  Azoxy___-N(=O)=N-
Azide___-N=N#N  Sulfone_>S(=O)=O        Sulfinat_S(=O)O-        Phsporat_P(=O)O-
Triazo__-N-N-N- Oxadiazo_-N-O-N-        Thiadiaz_-N-S-N-        Triazene_-N=N-N-
Nitrate_-O-NO2  NNitro__>N-NO2  Sulfonat_-SO3-  Sulfite_-SO3<   Sulfonmd_-SO2-N<
PriSlfmd_-SO2-NH2       Phsponat_-PO3<  SPhspnat_-SPO2< Phspite_-OPO2<
Tetrazo_-NNNN-  Oxdzoxde_-N(=O)ON-      NOHydxam_-N(N=O)OH      Sulfamid_>NSO2N<
Sulfate_-OSO3   ThioSulf_-SSO3  Phspate_O=PO3<- PhspatS_O=PS(k)O(3-k)<-
SPhspat_S=PO3<- SPhspatS_S=PS(k)O(3-k)<-        PhspatN_O=PN(n)O(3-n)<<<
SPhspatN_S=PN(n)O(3-n)<<<       PhsptSN_O=PS(k)N(n)O(3-n-k)<<
SPhsptSN_S=PS(k)N(n)O(3-n-k)<<  Diphspat_O=PO2-O-PO2=O
Triphspt_O=PO2-O-PO(=O)-OPO2=O  AlCbxyl_-COOH   ArCbxyl_-COOH   Ester___C(=O)OC
Amide___C(=O)N< Thioamd_C(=S)N< Amidine_C(=N-)N<        Isocyant_-N=C=O
Thiocynt_-S-C#N Isothcnt_-N=C=S Urea____>NC(=O)N<       Carbmte_>NC(=O)O<
Guandne_>NC(=N-)N<      Imide___O=C(N-)C=O      Barbitur_C1C(=O)NC(=O)NC1=O
Unknown_        M_CX    M_NO    M_PRX   M_UB    M_HB    M_POL   M_AMP   M_ALK
M_RNG   M_QN    M_NO2   M_NCS   M_BLM   AlphaAA PrAlphAA        AlphaAE PrAlphAE
Steroid H_AlAlco        H_AlAcid        H_AlAmin        H_ArAcid        H_Phenol
H_AlPyri        H_Azo   H_Nitrle        H_HCarb H_Nitro H_SO2   H_FAlkan
H_PAH   H_MultiN        H_AmAcid        RgGrav__3D      RgGeom__3D      RadMax__3D
Propr1__3D      MIRxx___3D      MIRyy___3D      MIRzz___3D      SM2xx___3D
SM2yy___3D      SM2zz___3D      BoxX____3D      BoxY____3D      BoxZ____3D
DStokes_3D      Propr2__3D      Grav3___3D      TotASA__3D      PolASA__3D
NpoASA__3D      SolvE___3D      SolvEMt_3D      PEoED___3D      PEoEDIa_3D
PEoEDIb_3D      PEoEDIIa3D      PEoEDIIb3D      T_Rgrav T_Rgeom T_Radmax
T_Dipole        T_Grav3 FormalQ IHB     PHB     HBD     HBA     HBDo    HBAo
HBDn    HBAn    HBDch   HBAch   HBDoch  HBAoch  HBDnch  HBAnch  HBAsa___3D
HBAwsa__3D      PosASA__3D      NegASA__3D      Dipole__3D      ABSQ    ABSQon
MaxQ    MinQ    NPA_ABSQ        NPA_AQon        NPA_MaxQ        NPA_MinQ
NPA_Q1  NPA_Q2  NPA_Q3  NPA_Q4  NPA_Q5  NPA_Q6  EqualChi        N_Electr
PolarizG        PolarizM        N_IoAcAt        N_IoBaAt        AcidAtoms
BaseAtoms       FAnion  FCation FUnion  FZwitter        QAvgNeg QAvgPos F_NLP
F_HBP
9444    9444    0.6     1 12 13 7 5 14 10 2 6 11 4 9 8 3        23 1 -0.56 10 0.28
11 0.28 12 0.28 13 0.58 14 0.28 15 0.84 16 0.45 17 0.71 2 -0.68 24 0.4 25 0.4 26
0.06 27 0.4 28 0.4 29 0.4 3 -0.68 4 -0.68 5 -0.57 6 -0.42 7 -0.66 8 -0.66 9 -0.85
3       12 1 1 acceptor 1 2 acceptor 1 2 donor 1 3 acceptor 1 3 donor 1 4 acceptor
1 4 donor 1 5 acceptor 1 7 donor 1 9 donor 5 1 10 11 12 13 rings 6 6 7 8 15 16 17
rings   17      4       0       0       0       0       1       3       1.#INF
50.9521 60.962  10608611 8 18411694409049253760 11132069 177 18412541020444494778
12138202 97 18115012001220561597 12500047 106 18337105674893126407 12932764 1
17967523554309708816 12969540 114 17969481746681867365 13024252 1
16008756779798805865 14115302 16 183371210766   300.58 6.14 2.47 0.84 3.95 0.5 0.04
1.55 0.49 -1.36 0.1 -0.24 -0.17 0.57    635.496 168.2   2 5 10  0.0     1
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 3.14;-1.95;-3.60;-7.33 1.01    -1.1    -2.09   0       -2.09   0.14    0
0.51    0       59.56   0       1.44E+01        0       7.96    1.44E+01
1.21E+01        1.44E+01        Low     1       75.39   0       0.67    0
More_than_3.16  0       Nontoxic        0       0.0001  1       2429.43 1
3.51    1       22.57   0       957.72  1       3.8     0       4.11    0
                        3.0     LP_Pr_Hd_       C8H12N4O5       244.21  189.
243.5   17      8       4       5       0       0       0       0       0       0
0       0       0       18      2       0.61    0.06    0.00    0.33    0.29    2
1       1       5       1       12.58   8.04    7.35    13.43   5.33    2.56    496
0.0     -0.4729 -4.735  0.0     0.0     0.0     0.0     1.0605  -0.1963 -0.7571 0.0
0.0     0.0     0.0     0.0     0.0     5.2133  0.0     0.0     0.0     0.0     0.0
6.9566  0.0     0.9027  0.0     0.0     0.0     0.0     0.0     0.0     28.0899
5.134   0.0     11.4709 0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0
0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0
7.9055  0.0     1.7543  0.0     0.0     5.978   0.0     0.0     1.6434  0.0     0
3       0       0       1       1       0       1       0       0       0       1
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       0       0       0       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
0       0       0       0       0       8.00    9       8       4       0       2
0.00    0       1       0.00    0       0.00    0       0       0       0       0
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       2.89E+00        2.84E+00        4.75E+00
3.37E+00        4.81E-01        3.64E-01        1.54E-01        3.73E-02
2.71E-01        6.92E-01        2.11E+00        5.42E+00        7.96E+00
6.92E-01        3.60E-01        1.34E+01        3.79E+02        2.07E+02
1.72E+02        -2.20E+01       1.84E+01        16      6       2       10      4
2.89E+00        2.82E+00        4.80E+00        1.73E+00        1.50E+01        0
0       0       4       8       3       5       1       3       2.2     -4.95
1.41    -3.09   0.8     -1.87   2.07E+02        -1.36E+02       1.72E+02
2.07E+02        1.86E+00        0.47    0.47    0.24    -0.08   10.96   5.42    0.8
-0.8    -2.75   2.5     -1.67   0.85    -0.38   0.06    5.63    128     21.97
21.33   0       4       None    9(-NH2)6(-Naa)7(aNa)8(aNa)      0.0     0.0001
0.9999  0.0     0.0     0.0001  0.7647  0.2941
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