Basak modification of discussion based on Mircea input:

Regarding the influential indices from the Diudea lab of descriptors, the topological indices (Sum.of.topological.distances.between.O..O; E.state.topological.parameter; Sum.of.topological.distances.between.N..O) are descriptors developed at Topo Group Cluj, Romania, and others. These are based on topological distance and detour, then on molecular graph fragmentation and collection of this information as fragmental property indices. Such indices express the presence of heteroatoms, by atomic radii and Sanderson electronegativities, then converted in topological partial charges on the heavy atoms in the molecule. ALOGP3 is a quantifier of hydrophobicity and so may aid in passage of chemicals through biological membranes (Li et al, the source of our data). Both polar surface area (PSA) and hydrophobicity calculated by the ClogP program have been found to be influential in the prediction of blood-brain barrier entry of chemicals [ refs: Li et al; and

1) Medicinal Chemical Properties of Successful Central Nervous System Drugs, Hassan Pajouhesh\* and George R. Lenz; Vol. 2, 541–553, October 2005 © The American Society for Experimental NeuroTherapeutics, Inc. 541; The Journal of the American Society for Experimental NeuroTherapeutics

2) Accurate Prediction of the Blood–Brain Partitioning of a Large Set of Solutes Using Ab Initio Calculations and

Genetic Neural Network Modeling

BAHRAM HEMMATEENEJAD,1,2\* RAMIN MIRI,2 MOHAMMAD A. SAFARPOUR,3 AHMAD R. MEHDIPOUR2;

Hemmateenejad et al. l Vol. 27, No. 11 l Journal of Computational Chemistry, 27: 1125–1135, 2006

Dear Friend Subhash,

I answered to this query:

“This is a scientific paper. Provide proper references for the variable importance measure. Please provide a credible reference to the scientific literature rather than a company web page. ”

1. MV Diudea, G Katona, I Lukovits, N Trinajstić, Detour and Cluj-detour indices. *Croatica Chemica Acta*, **1998**, 71 (3), 459-471
2. L Jäntschi, G Katona, MV Diudea, Modeling molecular properties by Cluj Indices. *MATCH, Commun. Math. Comput. Chem*. **2000**, 41, 151-188
3. OM Minailiuc, G Katona, MV Diudea, M Strunje, A Graovac, I Gutman, Szeged fragmental indices. *Croatica Chemica Acta*, 1998, 71 (3), 473-488.
4. MV Diudea, OM Minailiuc, G Katona, I Gutman, Szeged matrices and related numbers. *MATCH, Commun. Math. Comput. Chem.* 1997, 35, 129-143.
5. O Ivanciuc, T Ivanciuc, MV Diudea, Molecular graph matrices and derived structural descriptors. *SAR and QSAR in Environmental Research*, **1997**, 7 (1-4), 63-87.
6. MV Diudea, S Klavžar, Omega polynomial revisited. *Acta Chim. Slov*. **2010**, 57, 565-570.
7. PV Khadikar, S Karmarkar, VK Agrawal, J Singh, A Shrivastava, I Lukovits, Szeged index-applications for drug modeling. *Letters in Drug Design & Discovery*, **2005**, 2 (8), 606-624

Mircea

citations 11 and 12  should  be replace with

11.CN Lungu C-C CHEMOKINE RECEPTOR TYPE 3 INHIBITORS: BIOACTIVITY PREDICTION USING LOCAL VERTEX INVARIANTS BASED ON THERMAL CONDUCTIVITY LAYER MATRIX, , STUDIA UBB CHEMIA, LXIII, 1,  ,177-188, 2018

12..CN. Lungu, S. Ersali, B. Szefler, A. Pirvan-Moldovan, S. C. Basak and M. V. Diudea, "Dimensionality of big data set explored by cluj descriptors," Studia UBB Chemia, 62(3), 197-204, 2017.

 and an extra one for Schrodinger descriptors added

13.Lungu CN, Bratanovici IB, Mirabela GM, Antoci V, Mangalagiu II., Hybrid imidazole-pyridine derivatives: an approach to novel anticancer DNA intercalators. Curr Med Chem. 2018.