Computer Vision Lab

http://vision.unipv.it/

A DATA STRUCTURE FOR PROTEIN-LIGAND MORPHOLOGICAL MATCHING

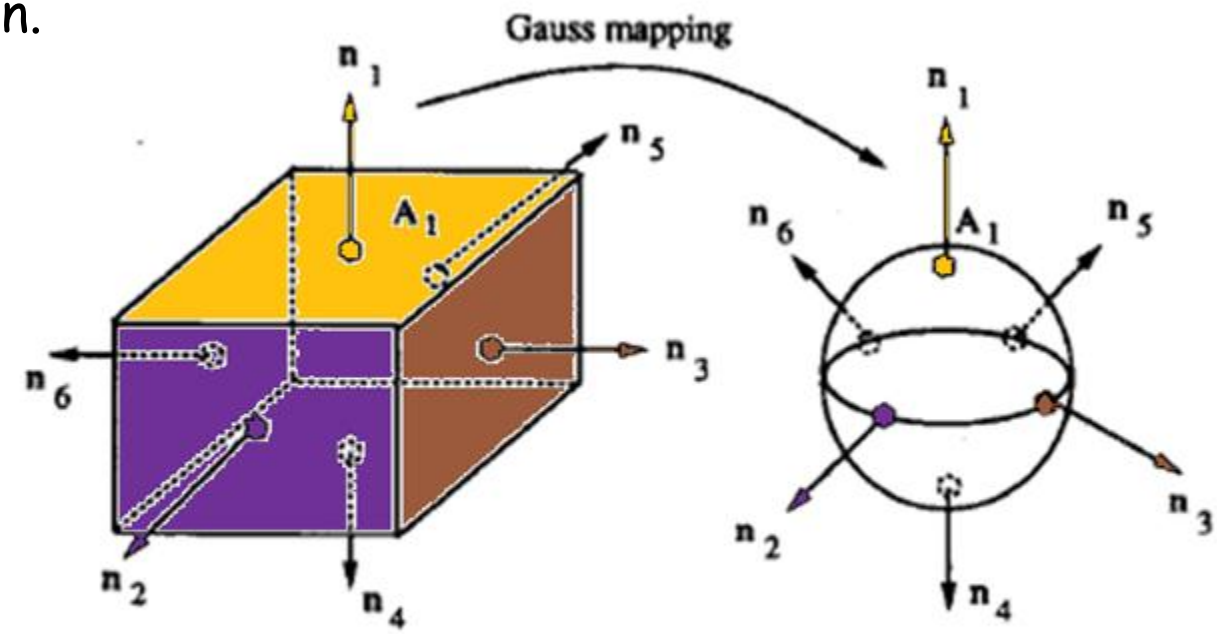
VIRGINIO CANTONI, LUCE LOMBARDI, ALESSANDRO GAGGIA
Dipartimento di Informatica e Sistemistica, Università di PAVIA,
{virginio.cantoni, luca.lombardi, alessandro.gatti}@unipv.it

Overview

- Study the interaction between structures and other molecules (Protein Docking)
  - Molecular surface representation
  - Protein surface analysis
  - Geometric shape descriptors
  - Shape matching algorithms

Extended Gaussian Image

The EGI of a 3D object or shape is an orientation histogram that records the distribution of surface area with respect to surface orientation.

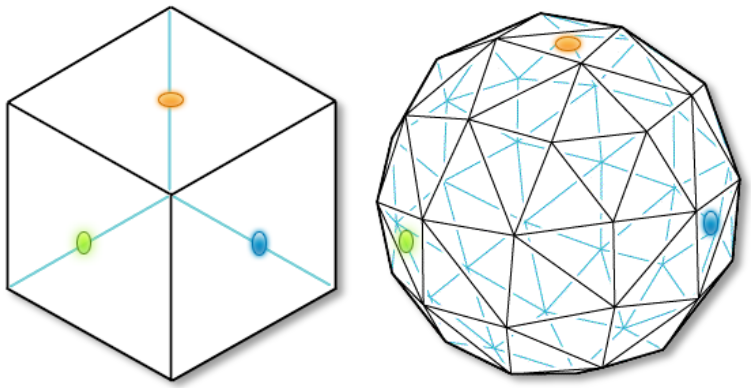


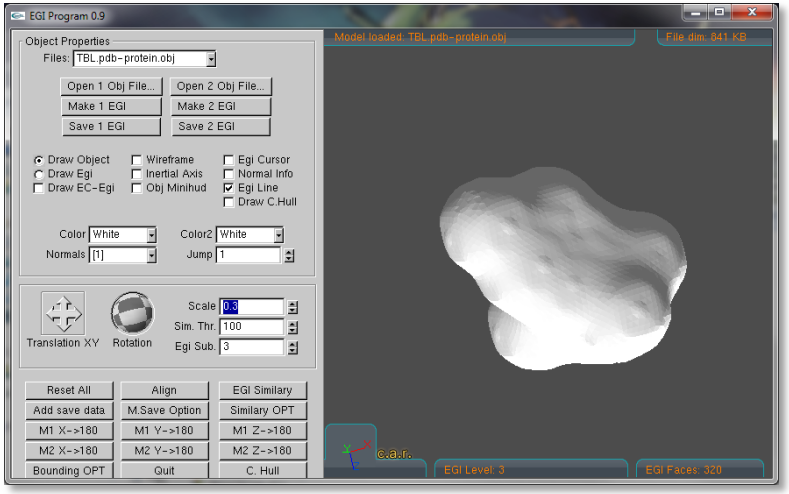
(a) Cube (b) EGI of cube

(Note: The weight is shown only for normal n_1 for clarity)

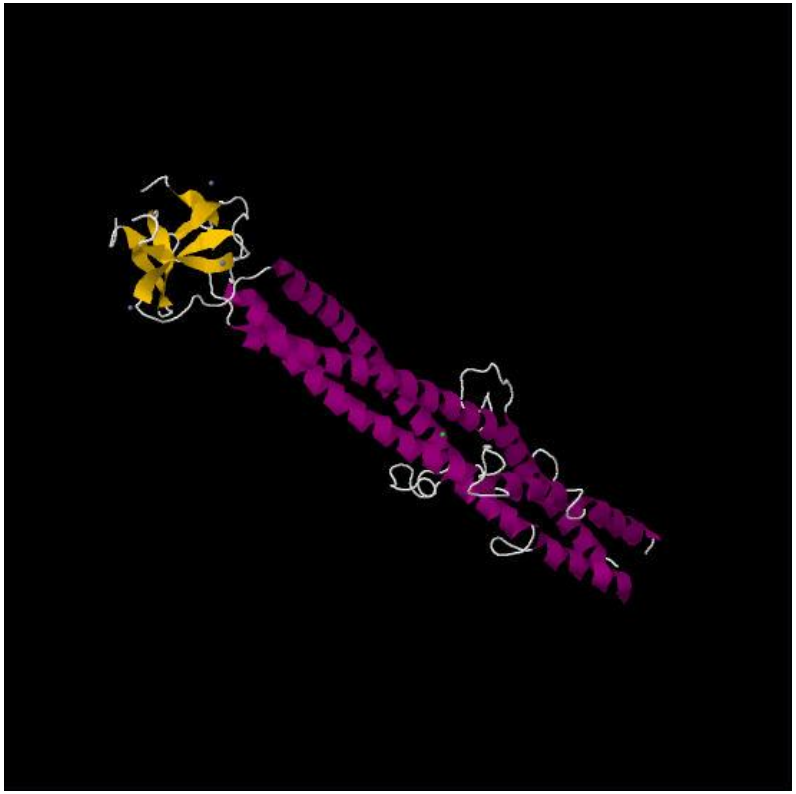
B.K.P. Horn, Extended Gaussian Images, 1984

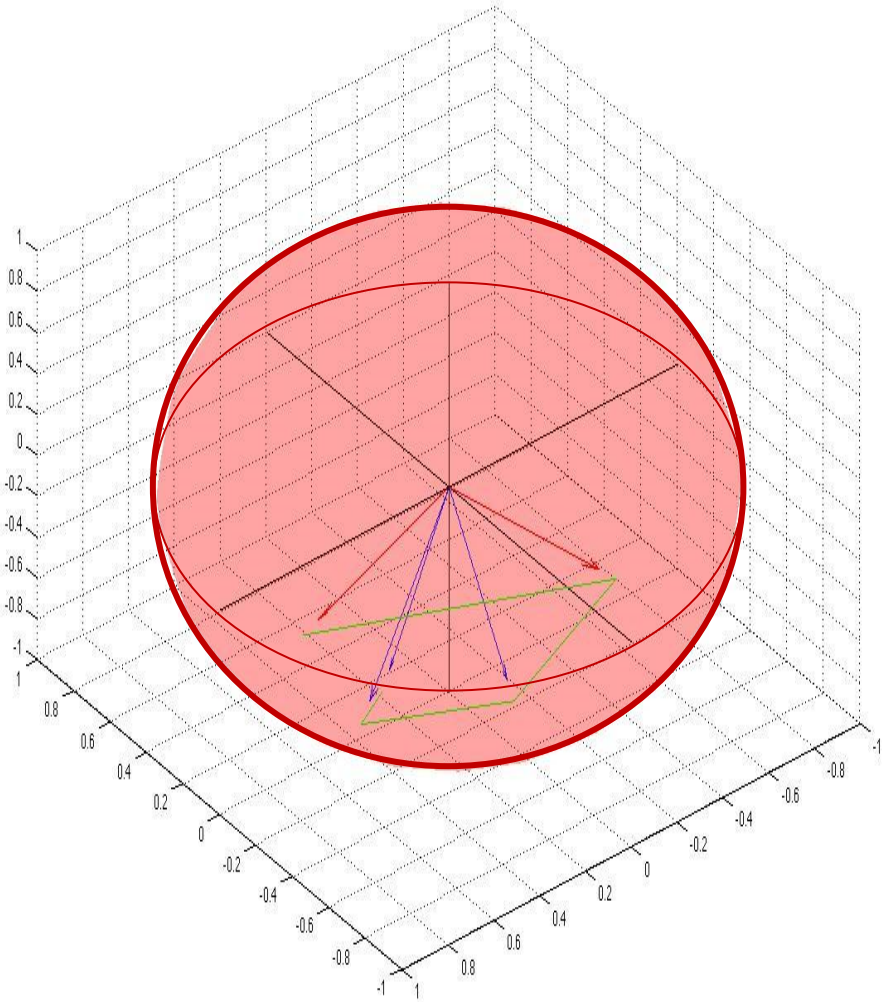
Extended Gaussian Image



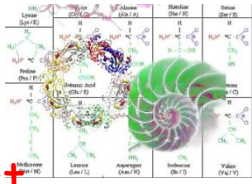


EGI - protein 1aa01





Extended Gaussian Image



- EGI The EGI of a 3D object or shape is an orientation histogram that records the distribution of surface area with respect to surface orientation.

Horn, B.K.P.: Extended Gaussian images. In: Proceedings of the IEEE 72, 1671–1686 (1984).

- CEGI The Complex EGI encodes each surface patch's signed perpendicular distance from the reference coordinate center.

Kang, S.B., Ikeuchi, K.: Determining 3-D object pose using the complex extended Gaussian image. In: IEEE Computer Society Conference on Computer Vision and Pattern Recognition, pp. 580–585 (1991).

- MEGI The More Extended Gaussian Image (MEGI) model consists of a set of position vectors for surfaces and their normal vectors.

H. Matsuo and A. Iwata, "3-D Object Recognition Using MEGI Model from Range Data." Proc. 12th Int'l Conf. Pattern Recognition, pp. 843-846, Jerusalem, Israel, Oct. 1994.

- MSEGI The multi shell EGI

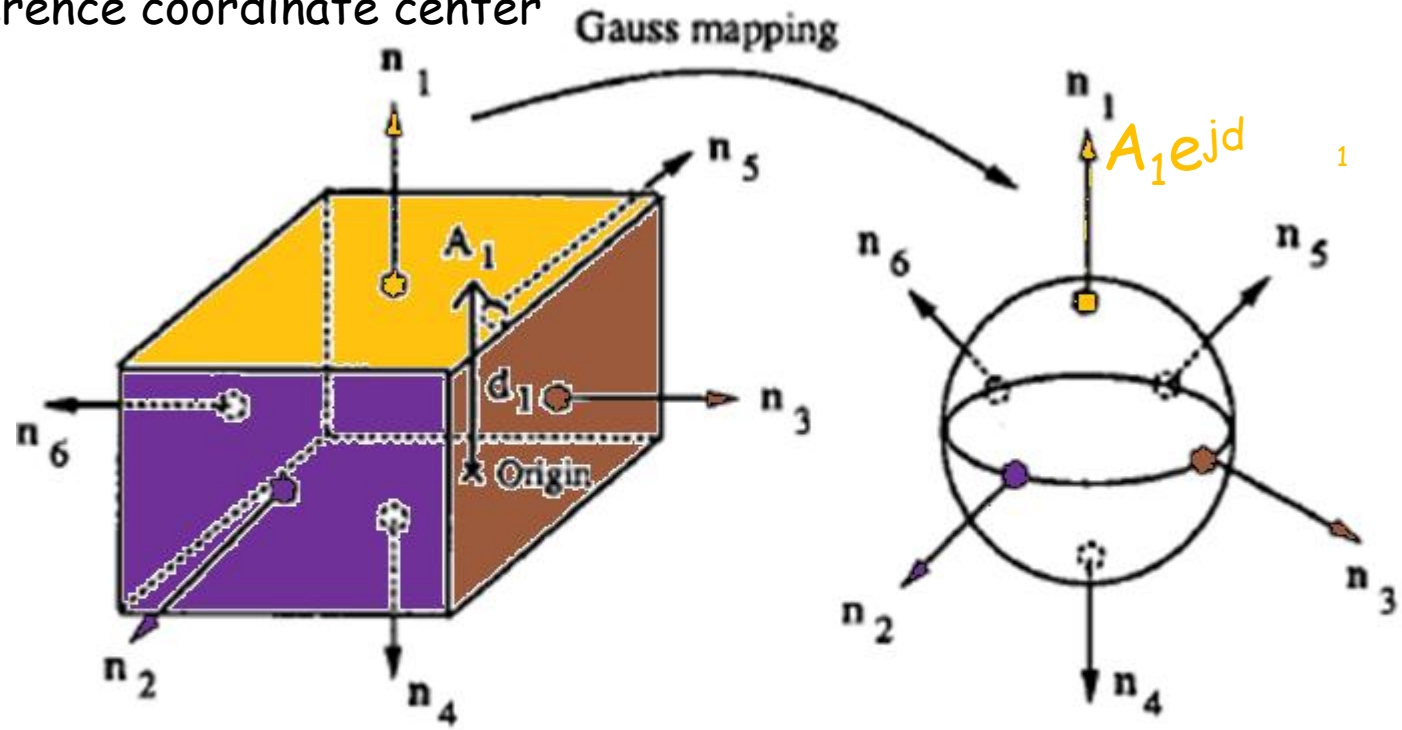
Dingwen Wang1,2, Jiqi Zhang2, Hau-San Wong2, and Yuanxiang Li, 3D Model Retrieval Based on Multi-Shell Extended Gaussian Image, G. Qiu et al. (Eds.): VISUAL 2007, LNCS 4781, pp. 426–437, 2007.

- ECEGI The Enriched CEGI encodes each surface patch's signed with its 3D position.

Zhaozheng Hu · Ronald Chung · Kenneth S. M. Fung: EC-EGI: enriched complex EGI for 3D shape registration, Machine Vision and Applications (2010) 21:177–188.

Complex EGI (C-GEI)

CEGI encodes each surface patch's signed perpendicular distance from the reference coordinate center

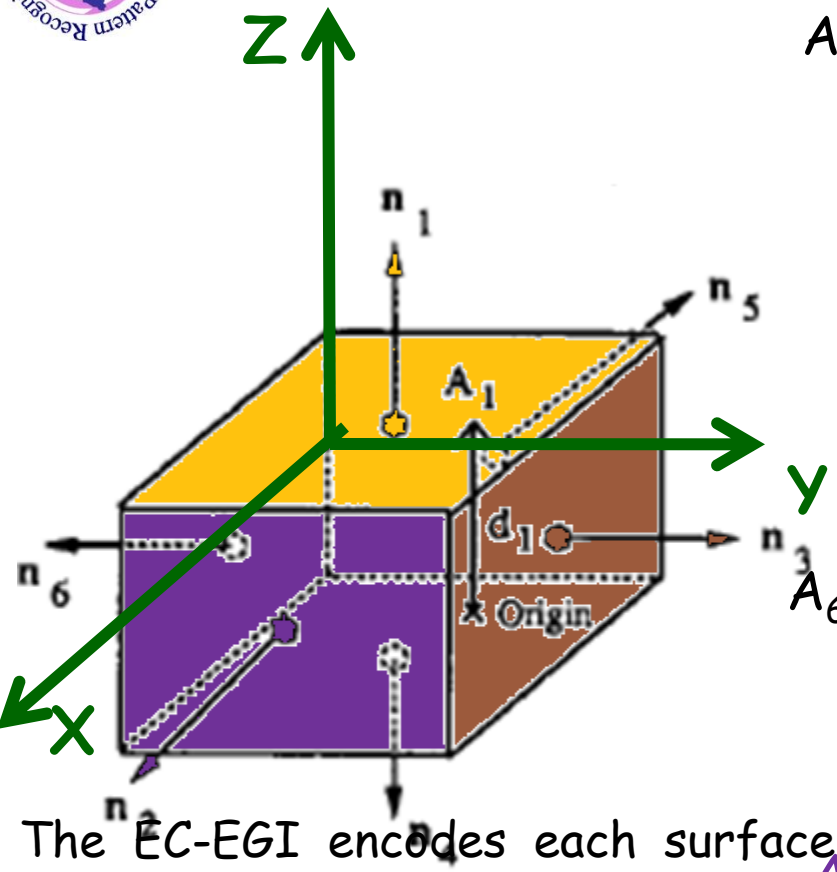


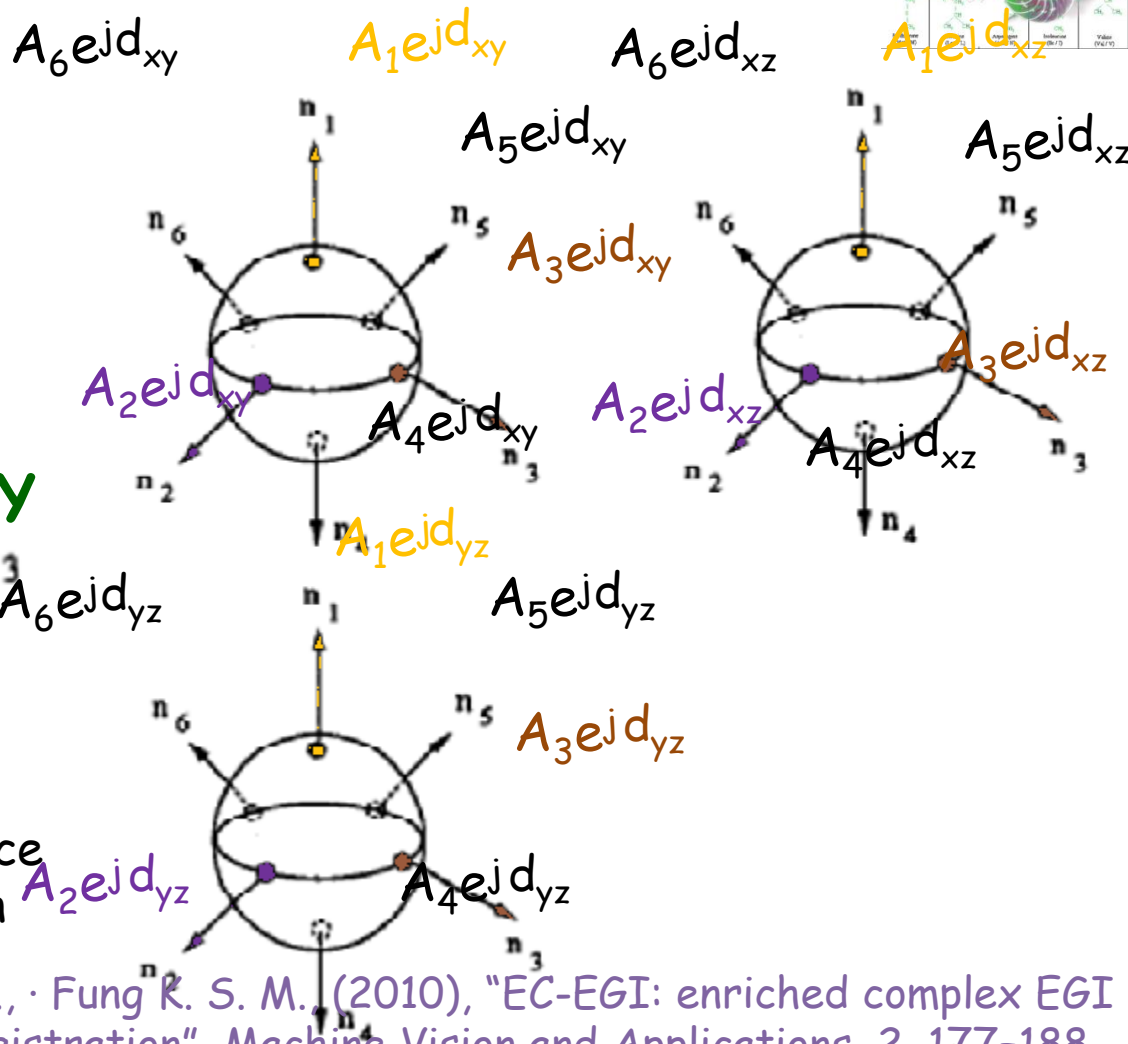
(a) Cube (b) CEGI of cube

(Note: The weight is shown only for normal n_1 for clarity)

Sing Bing Kang and Katsushi Ikeuchi, 3-D Object Pose Determination Using Complex EGI, 1993

Enriched C-EGI (EC-EGI)

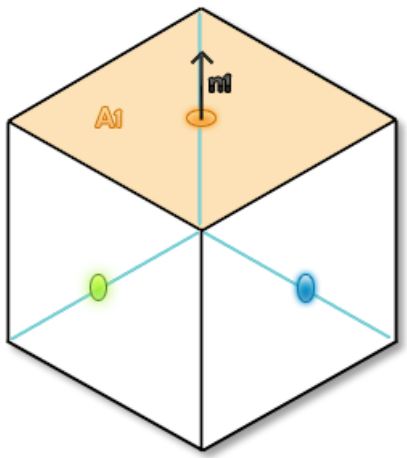


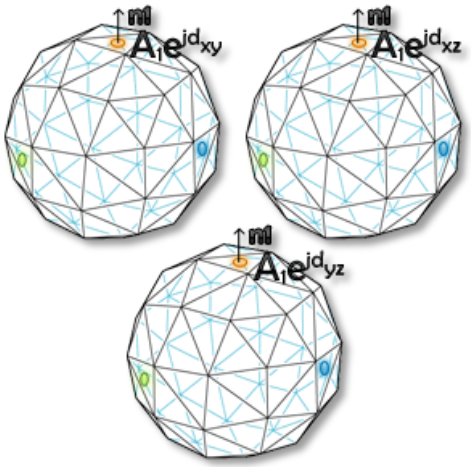


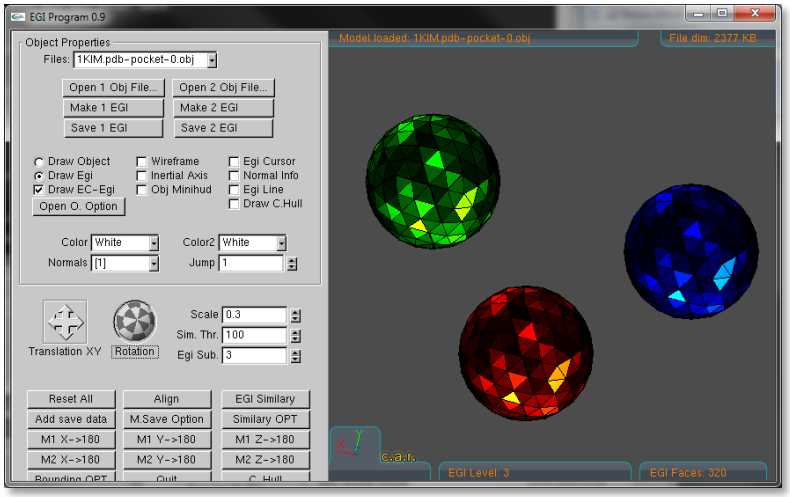
The EC-EGI encodes each surface patch's signed with its 3D position

Hu, Z., · Chung, R., · Fung K. S. M. (2010), "EC-EGI: enriched complex EGI for 3D shape registration", Machine Vision and Applications, 2, 177–188.

Enriched C-E.G.I.

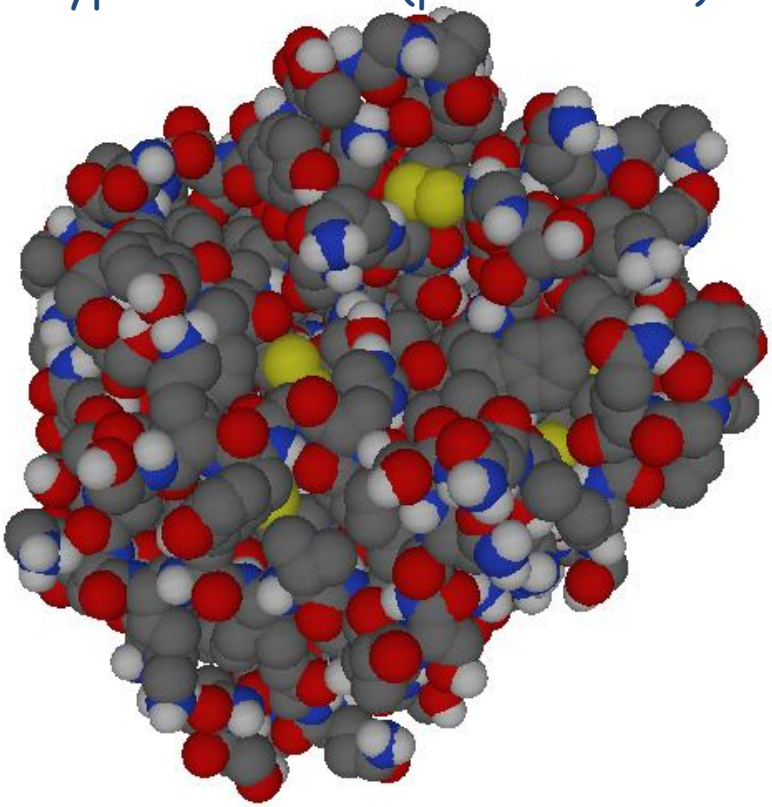


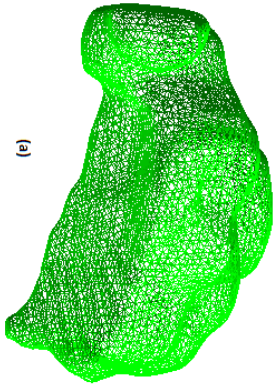


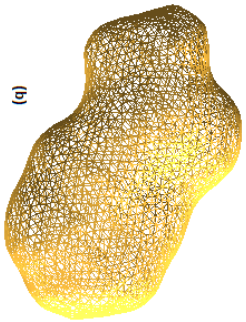


Protein-Lingand Interaction

Trypsin molecole (pdbID 1TNL).

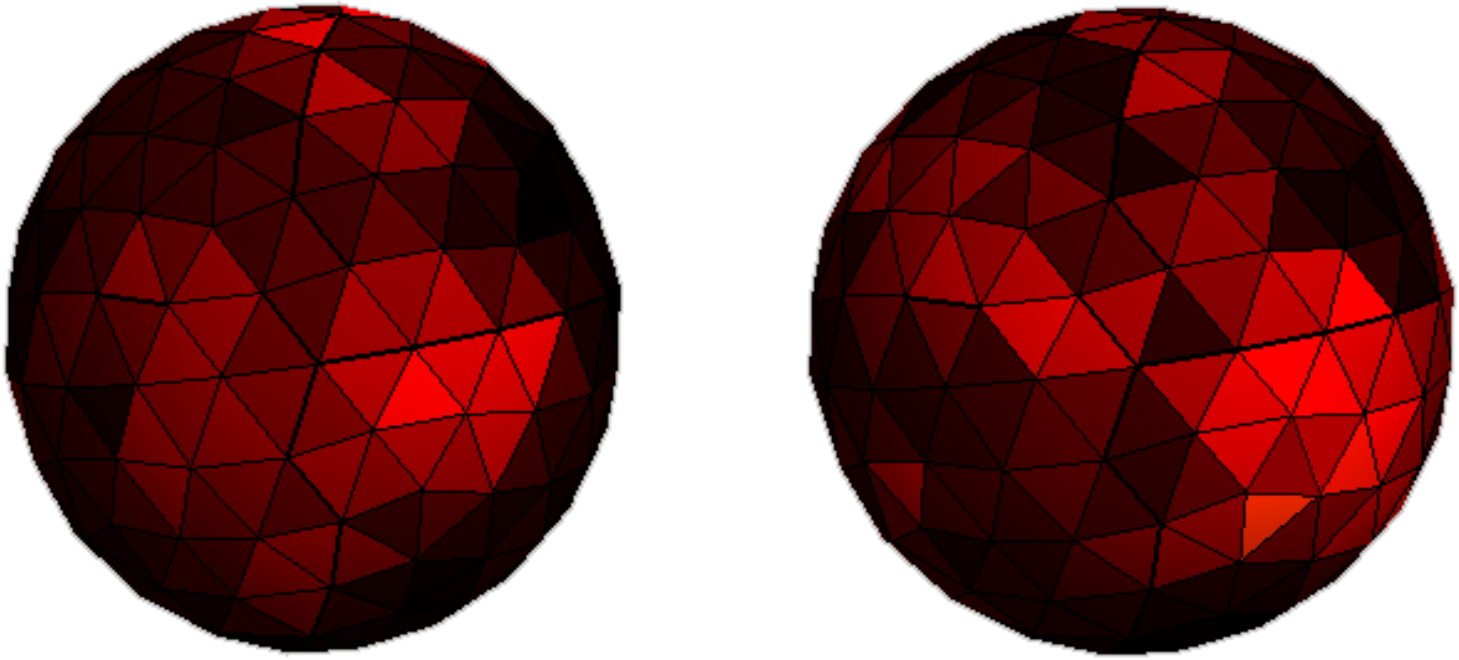






a) Pocket candidate of 1TNL protein
b) and (b) TPA ligand properly aligned

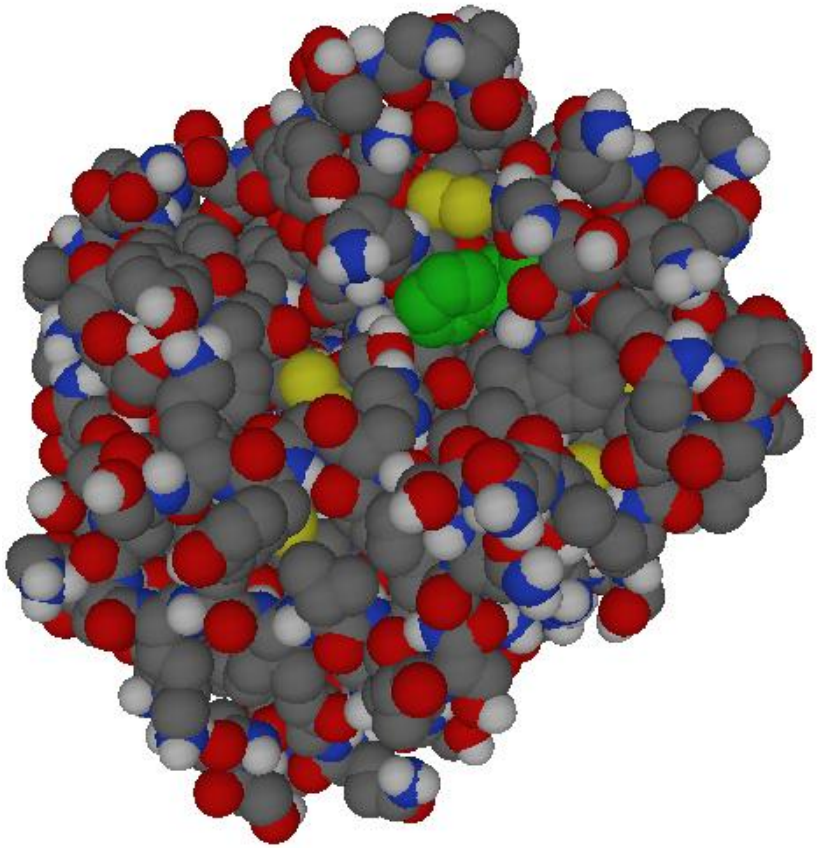
Protein-Lingand Interaction



(a) (b)

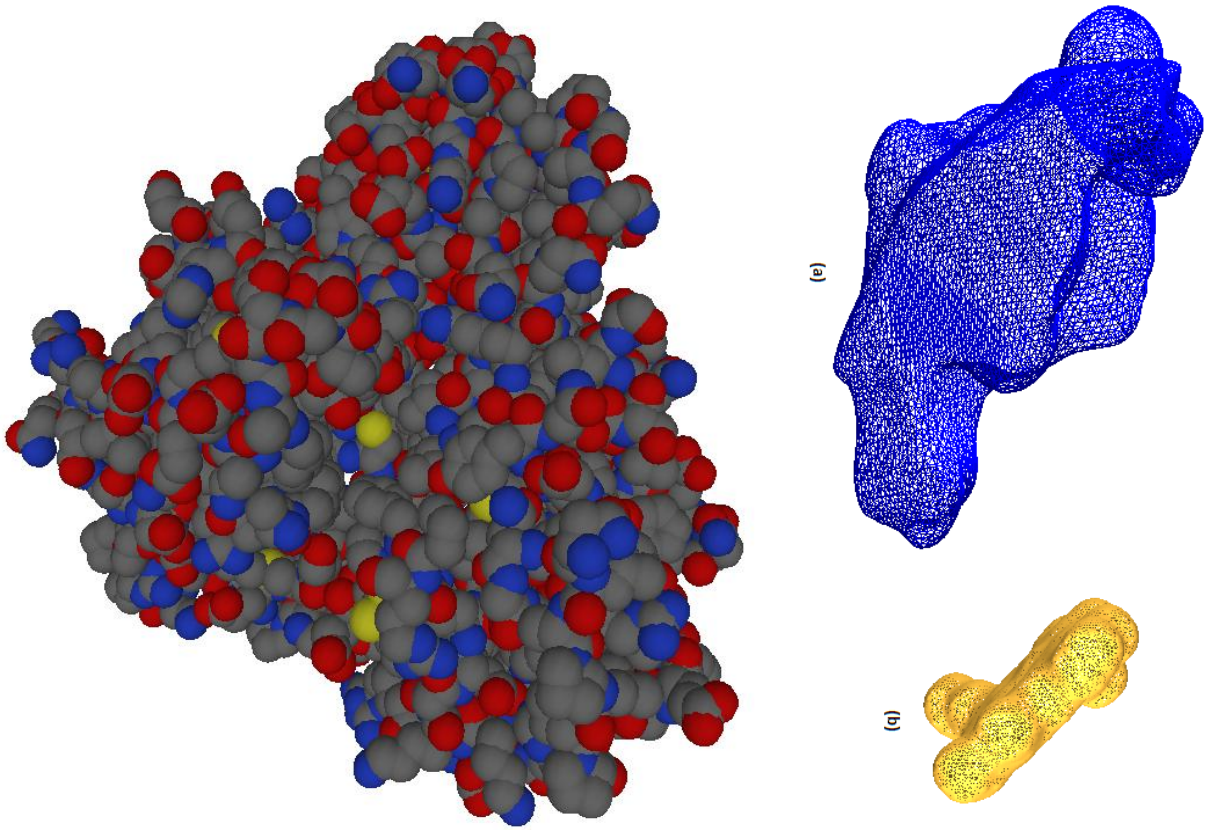
EGIs of (a) Pocket candidate of 1TNL protein and (b) TPA ligand properly aligned.

Protein-Lingand Interaction



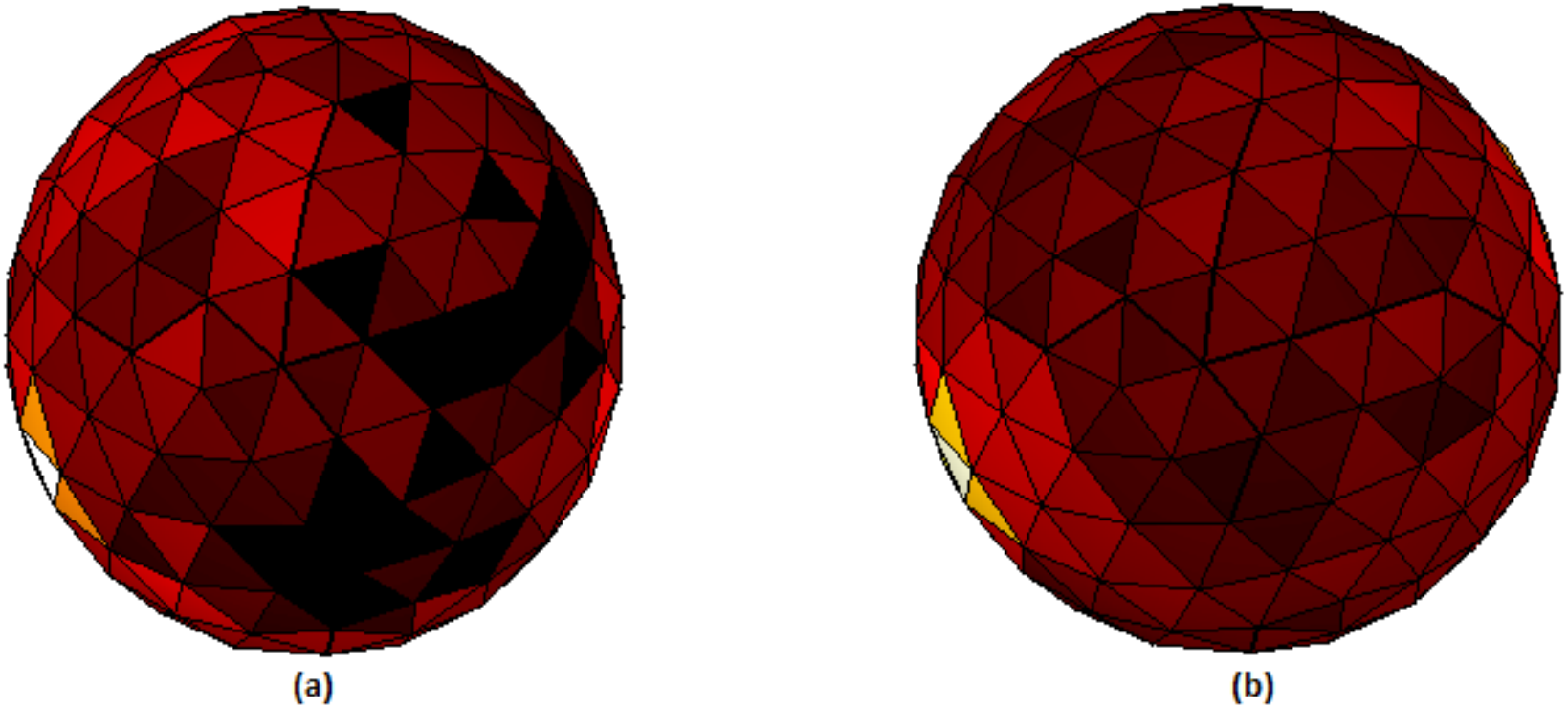
Protein-Lingand Interaction

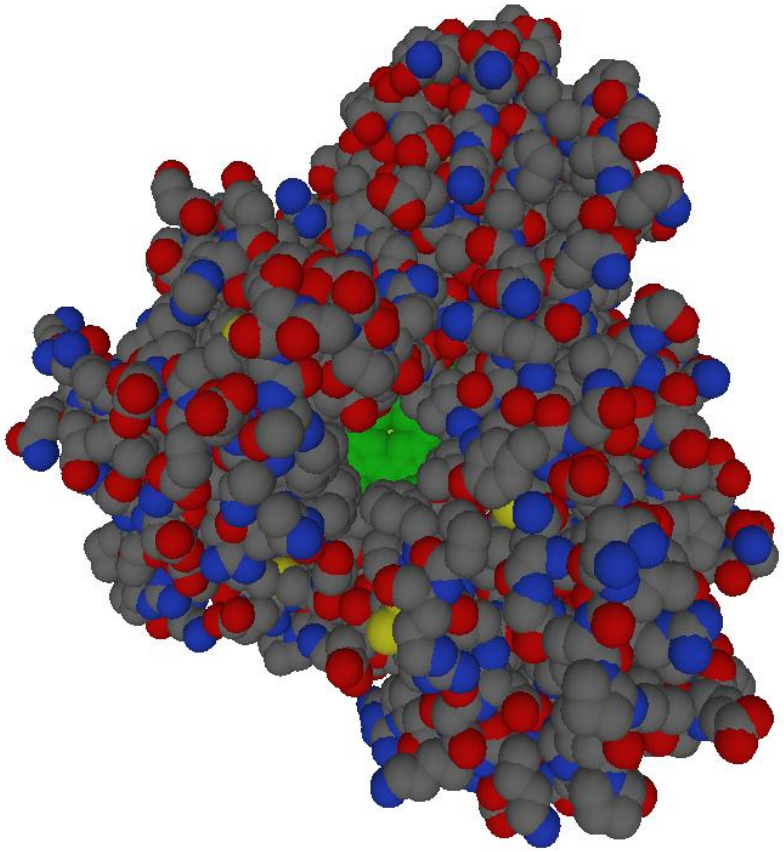
Camphor 5-monooxygenase (pdbID 3L62).



a) Pocket candidate of 3L62 protein
b) and (b) HEM ligand properly aligned

Protein-Lingand Interaction



EGIs of (a) Pocket candidate of 3L62 protein and (b) HEM ligand properly aligned.

Protein-Lingand Interaction