LIST OF APPENDICES

APPENDIX - A

List of Publications

[1] B. Bagchi, S. Sharma, A. Chatterjee, P. Ghosh, A.K. Bothra, QSAR Study and Molecular Docking of 23-hydroxybetulinic Acid Derivatives as RMGPa and HeLa Cells Inhibitors, Commun. Comput. Chem., 3 (2015) 75-102.

[2] B. Bagchi, T. Goswami, P. Ghosh, A.K. Bothra, Computational study on the redox reaction of puupehenone in aqueous solution by density functional theory, Asian J. Chem., 28 (2016) 2199-2203.

[3] B. Bagchi, A. Chatterjee , P. Ghosh, A.K. Bothra, A theoretical investigation of cytotoxic activity of halogenated monoterpenoids from plocamium cartilagineum, JOCPR, 4 (2012) 5076-5080.

[4] B. Bagchi, A.K. Bothra , Quantum chemical study of halomon by the DFT and MP2 Methods, IUP Journal of Chemistry, 4 (2011) 41-47.

[5] A QSAR study of sesquiterpene lactones from Inula falconeri as potent anti-inflammatory agents, B. Bagchi, P. Ghosh, A.K. Bothra, JOCPR, 7 (2015) 907-912.

[6] P. Ghosh, B. Bagchi, S. Sharma, A. Chatterjee, A.K. Bothra , Molecular docking and DFT based QSAR study on oleanolic acid derivatives as Protein–tyrosine phosphatase 1B inhibitors. (Manuscript under communication)

[7] S. Sharma, B. Bagchi, S. Mukhopadhyay, A.K. Bothra, Theoretical study of lysophosphatidic acid acyltransferase 2 inhibitors, JOCPR, 5 (2013) 348-355.

APPENDIX - B

Software used in the present study

Name	Executable	Description
GAMESS	Windows/Linux	AB initio quantum chemistry package.
Firefly	Linux	AB initio and DFT computational chemistry program
MOPAC	Windows/Linux	Semiempirical quantum chemistry program
AutoDock 4.0	Windows/Linux	Suite of automated docking tools
UCSF Chimera	Windows	Molecular visualization program
Molegro Molecular Viewer	Windows	Molecular visualization program
MATLAB	Windows	Numerical computing environment
Gabedit	Windows	Graphical user interface

APPENDIX - C

Web address used in present study

Name	Web address	Description
NCBI	http://www.ncbi.nlm.nih.gov/	For molecular chemistry information
PDB	www.rcsb.org/	Repository of 3D protein structures
Binding DB	www.bindingdb.org/	Focusing chiefly on the interactions of protein considered to be drug-targets with small, drug-like molecules
DendroUPGMA	http://genomes.urv.cat/	A dendrogram construction utility
Cambridge Crystallographic Data Centre	www.ccdc.cam.ac.uk	A database of small molecule crystal structures

APPENDIX - D

List of Abbreviations

IPP: Isopentenyl diphosphate

GP: Glycogen phosphorylase

PTP1B: Protein tyrosine phosphatase 1B

QSAR: Quantitative structure-activity relationship

CoMFA: Comparative molecular field analysis

IC: Mean information content

SIC: Structural information content

CIC: Complementary information content

RMGPa: Rabbit muscle glycogen phosphorylase a