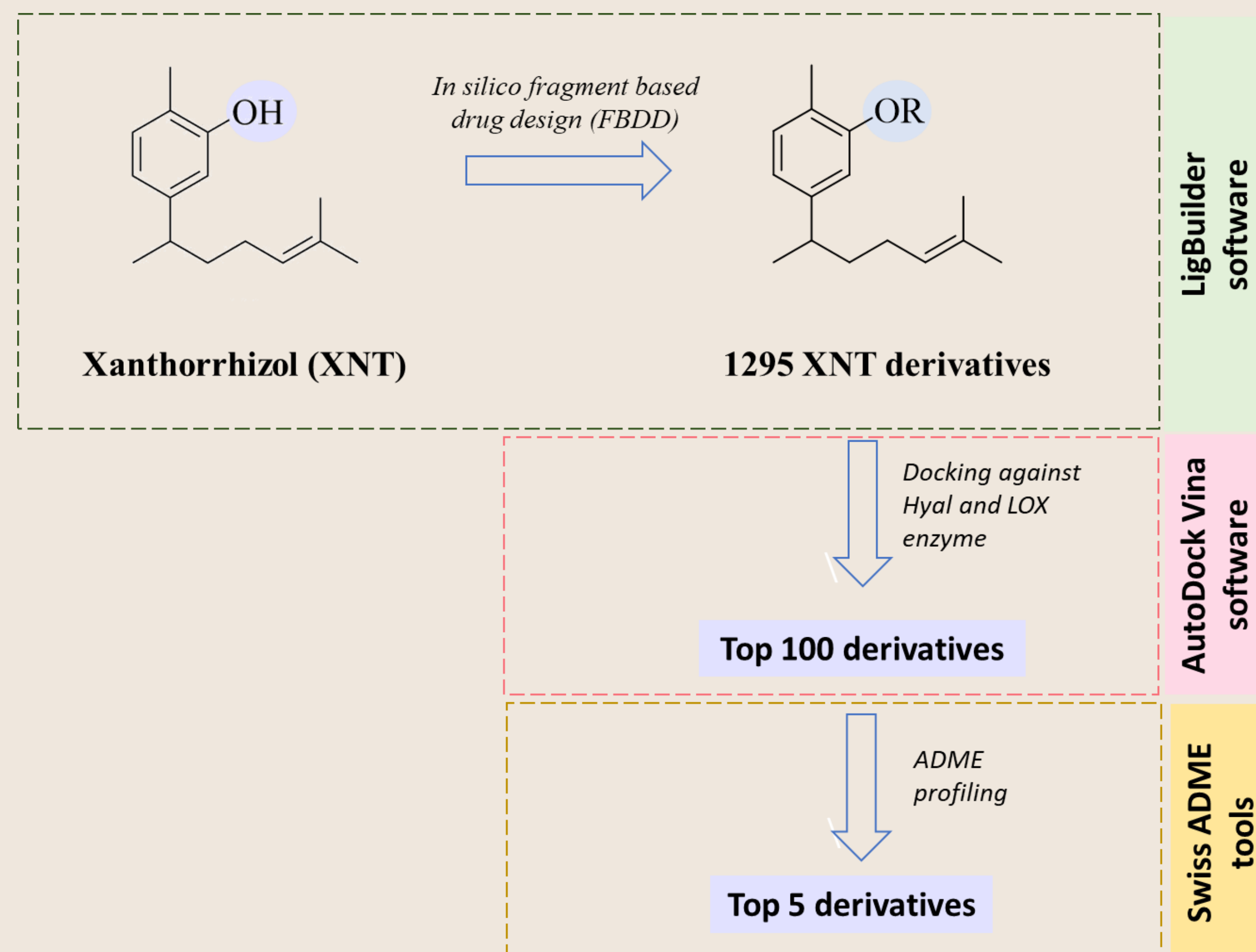


DESIGN OF XANTHORRHIZOL DERIVATIVES USING *IN SILICO* FRAGMENT BASED DRUG DESIGN (FBDD) APPROACH AS HYALURONIDASE INHIBITORS

AN INTERNATIONAL AWARD-WINNING INSTITUTION FOR SUSTAINABILITY

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 Department of Chemistry, Kulliyah of Science, International Islamic University Malaysia (IIUM), 25200, Kuantan, Pahang, Malaysia
 *Corresponding author (e-mail: nuruliman@iium.edu.my)

GRAPHICAL ABSTRACT



INTRODUCTION

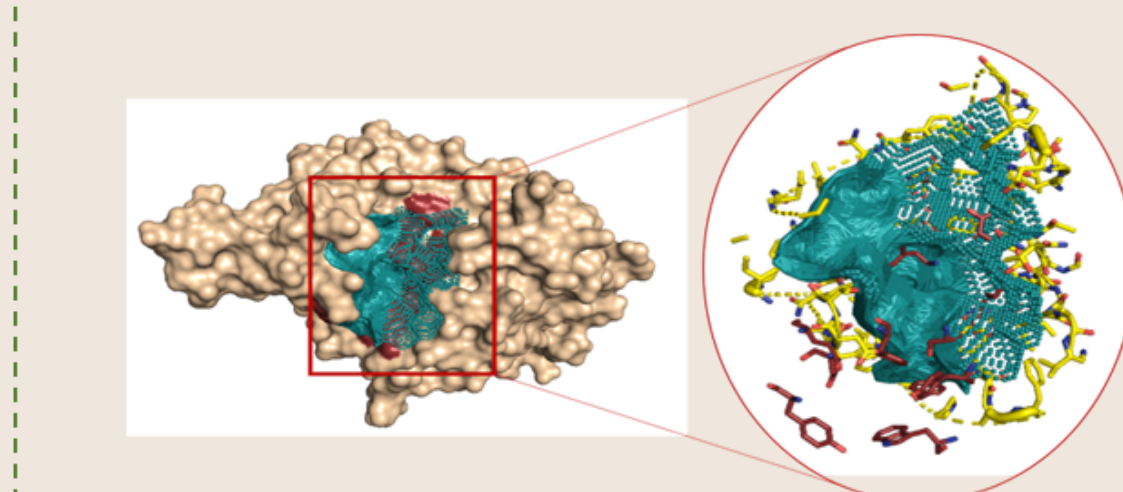
Xanthorrhizol (XNT) is a type of bisabolene sesquiterpenoids and can be isolated from rhizome part of *Curcuma xanthorrhiza* essential oil¹. Various biological activities of XNT were reported in literature, including anti-inflammatory properties through inhibition of pro-inflammatory enzymes, such as cyclooxygenase (COX) and inducible nitric oxide synthase (iNOS)². Due to its small molecular weight (MW = 281.33 g/mol) and biological benefits, XNT is a suitable candidate to be further optimized as a more potent drug compound. Preliminary *in vitro* and *in silico* inhibitory studies showed that XNT exhibited low activity (8.79 % inhibition at concentration 100 µg/mL, binding energy = -6.5 kcal/mol) towards hyaluronidase (Hyal), an enzyme responsible for the degradation of hyaluronic acid (HA), resulting in the formation of small, low-molecular weight hyaluronic acid fragments that can induce inflammatory response towards human body³. In this study, *in silico* fragment-based drug design (FBDD) approach was utilized to optimize XNT by modifying the hydroxyl (-OH) group, generating new derivatives with stronger affinity towards Hyal enzyme, as well as better ADME and druglikeness properties, which are crucial for the drug absorption in human body.

METHODOLOGY

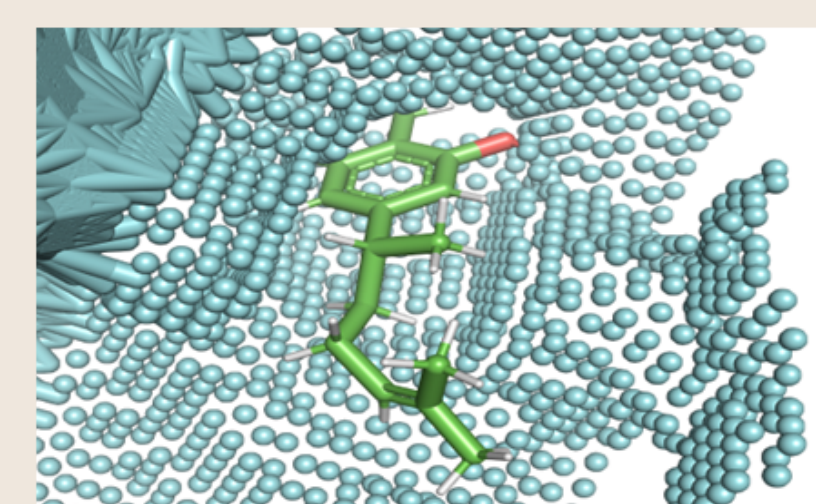
1. *In silico* FBDD using XNT as "seed" structure via LigBuilder software



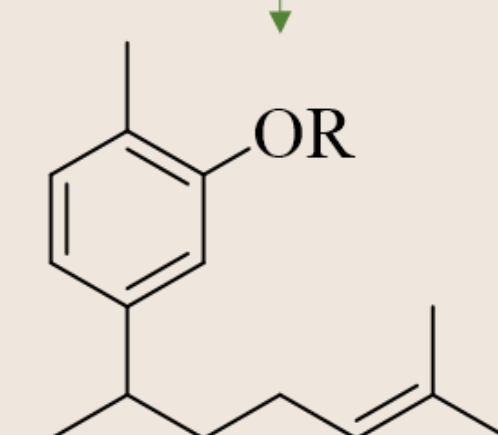
Crystal structure of human hyaluronidase-1 from Protein Data Bank (PDB ID: 2PE4)



Active pocket detection of Hyal enzyme

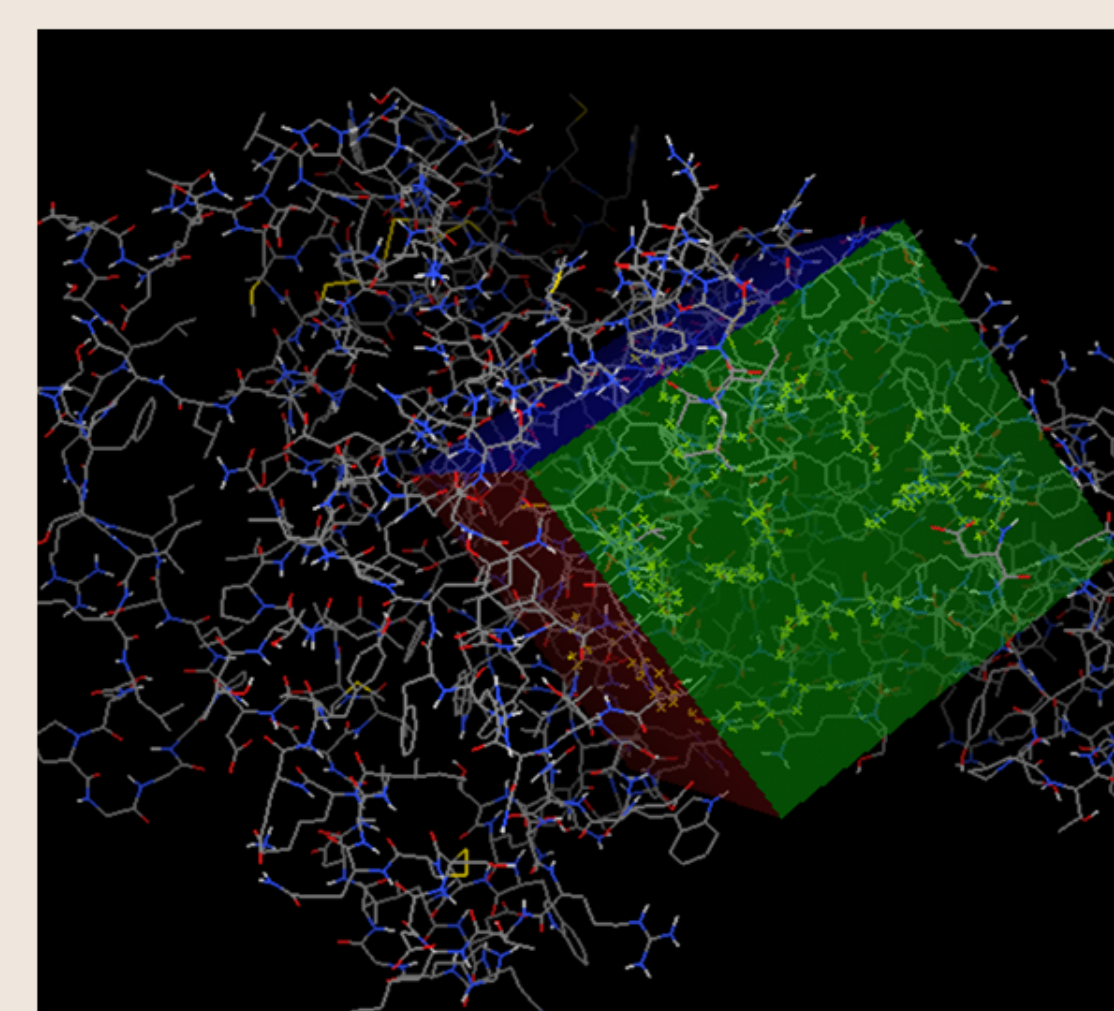


Seed growing using pre-docked XNT



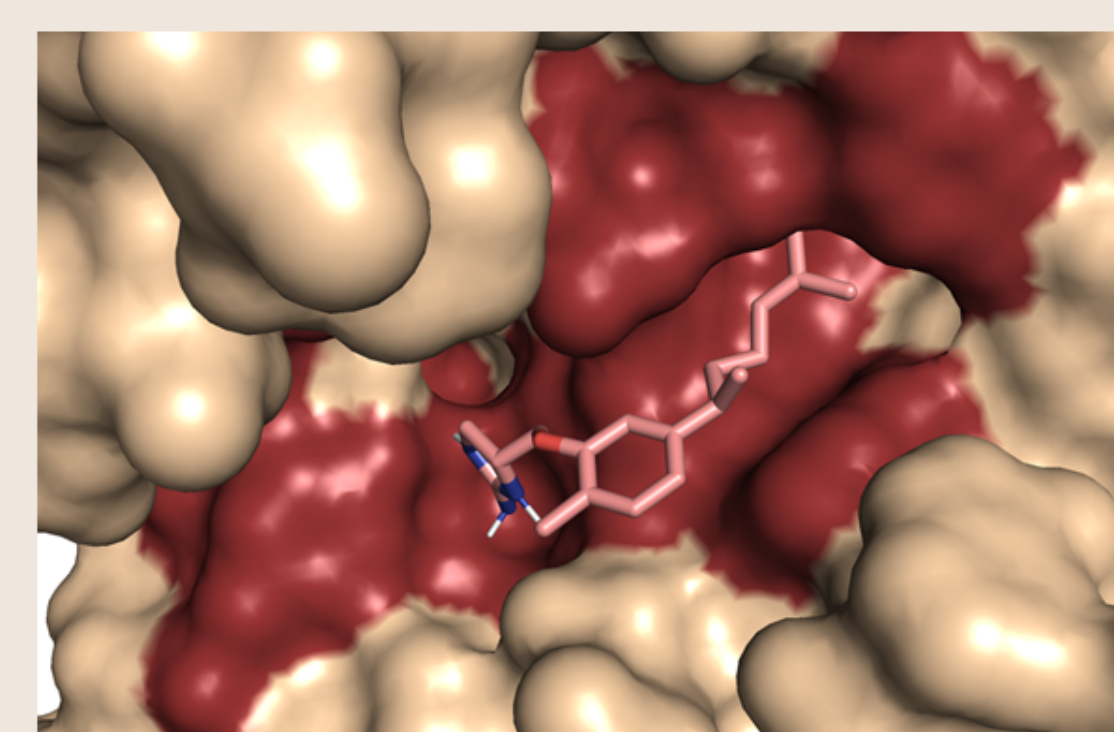
R = fragments from LigBuilder database

2. Molecular docking of XNT derivatives against Hyal enzyme using AutoDock Vina



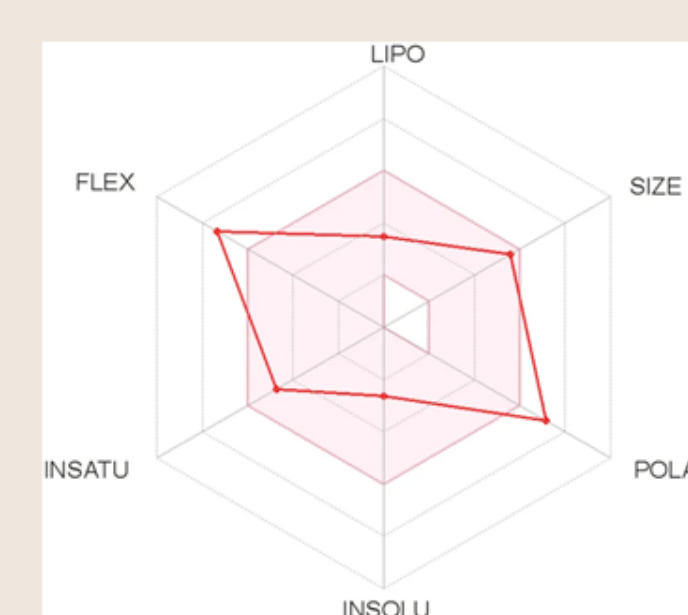
Grid box specification

Center; No. of points;
 x= 37.045 x= 62
 y= -17.292 y= 58
 z= -10.421 z= 58



Site-targeted docking

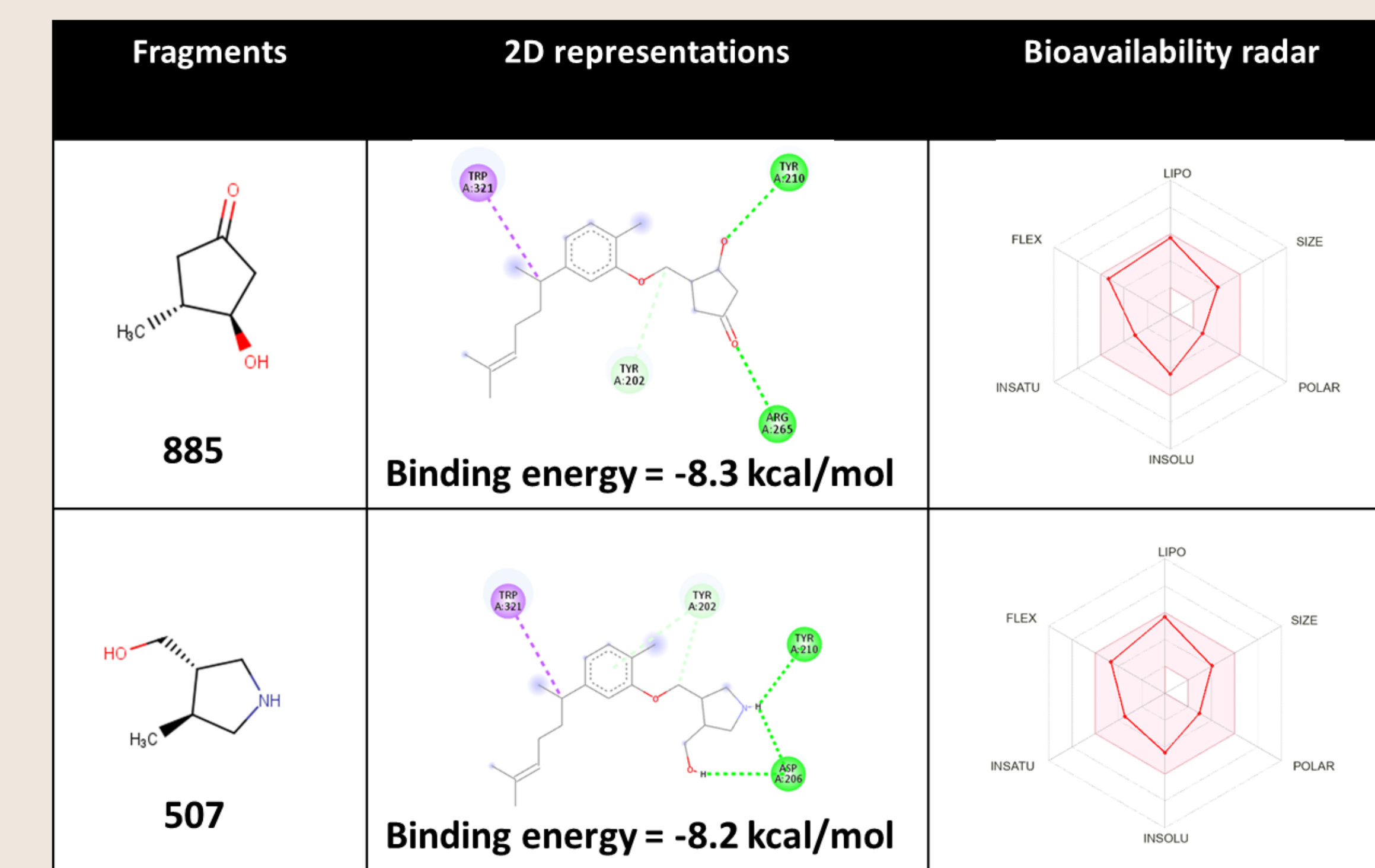
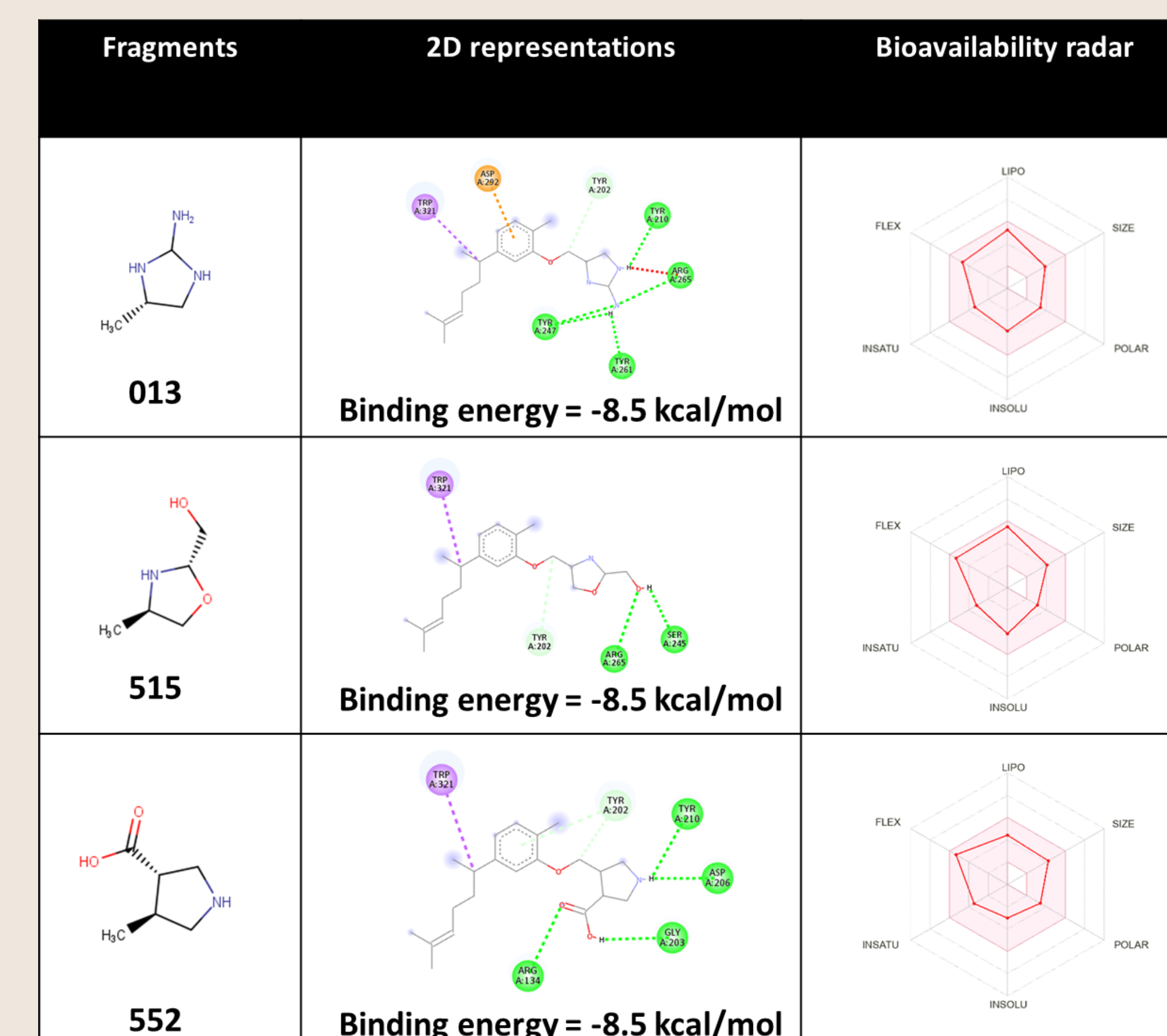
3. *In silico* ADME prediction using SwissADME tools



Bioavailability radar diagram

RESULTS AND ANALYSIS

1295 XNT derivatives were generated through *in silico* FBDD approach in LigBuilder, and molecular docking studies revealed that the derivatives were bound to Hyal enzyme with binding energies ranging from -8.5 kcal/mol to -6.2 kcal/mol. Then, top 100 derivatives with best binding energies were further screened to remove duplicates and predict their druglikeness properties using SwissADME tools. Five fragments, **013**, **515**, **552**, **885**, and **507** substituted to the -OH group of XNT showed improved binding affinity and drug likeness properties compared to XNT. From the 2D representation of the docking result, it can be observed that derivatives composed of pentacyclic ring fragment exhibited higher energy and favourable binding through hydrogen bonding and pi-interactions. Moreover, the presence of heteroatoms such as nitrogen and oxygen not only contributed to the protein-ligand interactions, but also towards optimized ADME properties.



CONCLUSION

- 1295 derivatives were successfully generated by modifying the -OH group of XNT using *in silico* FBDD approach
- Substitution to pentacyclic ring fragment improved the binding affinity towards Hyal and were also predicted to satisfy all the important parameters for drug absorption in human body.
- Through the incorporation of computational tools, this work greatly helped in the exploration of chemical space for site-targeted drug design as well as providing a more efficient approach in term of time and cost consumption for drug modification towards more potent drug candidates.

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P49	Silver Nanodumbbell Electrochemical Surface Kinetics And Mechanisms Of Interactions With Targeted Molecules Of Environmental And Biological Significance Olayemi Jola Fakayode <i>UNISA, South Africa</i>	Water and Environmental Chemistry
P50	Synthesis And Anticancer Activities Of Tricyclic And Angular Tetracyclic [1,2,4]-Benzothiadiazine Dioxides Via Metal-Free Sp³-C-H Activation. Oluwole Familoni <i>University of Lagos, Nigeria</i>	Health and Wellbeing
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P53	Electrochemical Impedance Spectroscopy Study Of Ni Coating Electroplated From Deep Eutectic Solvent At Different Current Densities Of Pulse Electrodeposition Mehry Fattah <i>York University, Canada</i>	Energy and Materials
P54	A Fluorescent Covalent Organic Cage For Selective Sensing Of Co²⁺ Ion And Picric Acid. Dr. RAMESH KUMAR Gajula <i>KG REDDY COLLEGE OF ENGINEERING AND TECHNOLOGY HYDERABAD, India</i>	Energy and Materials
P55	Dehydrogenative Methanol Activation And Its Application As Transfer Hydrogenating Reagent Under Homogeneous Catalysis Nidhi Garg <i>IIT KANPUR INDIA, India</i>	Green Chemistry and Catalysis
P56	In-Vitro Cell Migration Activity Of Some Lupeol Esters G. M. Kamal B Gunaherath <i>The Open University of Sri Lanka, Sri Lanka</i>	Health and Wellbeing
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P63	<p>Microwave Irradiation Suppresses The Jahn-Teller Distortion In Spinel LiMn_2O_4 Cathode Material For Lithium-Ion Batteries Aderemi Haruna <i>University of the Witwatersrand, South Africa</i></p>	Energy and Materials
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P70	Highly Sensitive Electrochemical Sensor For The Detection Of Tetracycline In Urine Opeyemi Iresemowo <i>University of Kwazulu-Natal, South Africa</i>	Energy and Materials
P71	Impact Of Natural Hydrocolloids Addition On The Physicochemical, Antioxidant And Digestive Enzymes Inhibitory Properties Of Sorghum Bicolor Flour Emmanuel Anyachukwu Ironi <i>Kwara State University, Nigeria</i>	Food and Agriculture
P72	Endogenous Proteins And Lipids Influence The Phenolics Profile, Anti-Nephrolithiatic And Antioxidant Activities Of Monodora Myristica Seed Extract Emmanuel Anyachukwu Ironi <i>Kwara State University, Nigeria</i>	Food and Agriculture
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P76	Physico-Chemical Analysis Of Moringa Oleifera Seeds: Harnessing Its Industrial Application Potentials Oghomwen Christie Ize-Iyamu <i>Rubber Research Institute of Nigeria, Nigeria</i>	Biodiversity and Natural Products
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P79	Promising Activity Of Tetrahydroisoquinolines Against Multidrug-Resistant Clinical Salmonella Isolates And Cytotoxicity Against Monkey Kidney Cells Ngo Hanna Joelle <i>University of Douala, Cameroon</i>	Health and Wellbeing
P80	Amine And Imine-Functionalized Mn-Based Mof As Unusual Turn-On And Turn-Off Sensor For D¹⁰ Heavy Metal Ions And Efficient Adsorbent To Capture Iodine. Samrah Kamal <i>ALIGARH MUSLIM UNIVERSITY, India</i>	Water and Environmental Chemistry



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P83	Investigation Of Thermal Degradation Mechanism In Thermoplastic Polystyrene Tetramer Model By Dft Method Baggya Karunaratna <i>Eastern University Sri Lanka, Sri Lanka</i>	Water and Environmental Chemistry
P84	Lactobionic Acid Engineered Iron Oxide Nanoparticles For Enhancing Oral Bioavailability Of Ceftriaxone. Muhammad Kawish <i>H.E.J Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi, Pakistan, Pakistan</i>	Health and Wellbeing
P85	Heterogenization Of Niau Nanoparticles Into Nanoporous Carbon Derived From Covalent Triazine Frameworks: An Efficient Catalyst For Hydrogenation Reactions Nithya Kesavan <i>Madurai Kamaraj University, India</i>	Green Chemistry and Catalysis
P86	Antimicrobial Peptides Of Temporin Sha For Targeting Mdr S. Aureus (Nctc 13277) And H.Pylori (Atcc 43504) Arif Khan <i>H.E.J. University of Karachi, Pakistan</i>	Biodiversity and Natural Products
P87	Investigation Of The "Memory Effect" Of Thf-Hydrate Formation On Different Surfaces Meem Noshin Nawal Khan <i>Gettysburg College, USA</i>	Energy and Materials
P88	New Bioactive Monoterpene Indole Alkaloids From Rinorea Yaundensis Engl. Bushra Khatoun	Biodiversity and Natural Products



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P92	Production Of Nano-Composites From Agriculture And Industrial Waste. A Green Approach. Sunil Kumar <i>Chaudhary Devi Lal University sirsa haryana, India</i>	Green Chemistry and Catalysis
P93	Evaluation And Purification Of Betalain Pigments From Red-Purple Variety Of Atriplex Hortensis "Rubra" That Exhibit Antioxidant And Cardioprotective Activity Agnieszka Kumorkiewicz-Jamro <i>South Australian Health and Medical Research Institute / Cracow University of Technology, Australia</i>	Food and Agriculture
P94	Transfer Hydrogenation Of Pyridinium And Quinolinium Species Using Ethanol As A Hydrogen Source Malleswara Rao Kuram <i>CSIR-Central Drug Research Institute, India</i>	Green Chemistry and Catalysis
P95	Chlorpyrifos And Lambda-Cyhalothrin Residue Analysis Of Newly Cultivated Genotype Of Cowpea Using Gc-Ecd Martin Kwesi Beyamfui <i>University Of Cape Coast, Ghana</i>	Food and Agriculture



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