Subscription Agency
Exploring and Distributing Knowledge Globally

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

In-Silico Driven Exploration of *Coccinia grandis*: A Dual Shield against Kidney Stones and Nephrotoxicity

Prajyot Ravat*, Mahesh J Patil
ASPM College of Pharmacy Sangulwadi, Vaibhavwadi, Dist- Sindhudurg, India 416810.

****Corresponding Author***
EMail Id- *prajyotravat1999@gmail.com*

ABSTRACT

Coccinia grandis, a medicinal plant traditionally used in Indian herbal remedies, was investigated for its phytochemical profile, anti-urolithiatic, nephroprotective, and in-silico drug-likeness potential. Sequential extraction of its leaves using n-hexane, chloroform, ethyl acetate, and methanol revealed the highest yield in the methanolic extract (7.9% w/w), which was further subjected to qualitative phytochemical analysis. Methanolic extract demonstrated the presence of flavonoids, phenols, glycosides, saponins, and phytosterols. TLC analysis confirmed one major spot at Rf = 0.33 using Methanol: Ethyl Acetate: Water (6:3:1) solvent system. UV-visible and FTIR spectroscopy confirmed the presence of phenolic and alcoholic groups. In-vitro anti-urolithiatic activity was tested using the crystal aggregation assay against COM (calcium oxalate monohydrate) crystals. The extract showed moderate inhibition (up to 59.09%) in comparison to the standard Cystone (81.81%).

Nephroprotective activity using NRK-52E kidney cell lines indicated cell viability >79% across concentrations, indicating safety on normal kidney cells. In-silico docking against kidney disease-related proteins 1V97 and 1UZE showed that quercetin, cucurbitacin B, and kaempferol possessed high binding affinities (-10.1 to -9.1 kcal/mol) with strong hydrogen bonding and hydrophobic interactions. All active phytochemicals mostly followed Lipinski's rule and demonstrated promising ADME properties. This integrated in-vitro and in-silico approach highlights C. grandis as a potential nephroprotective and anti-urolithiatic agent, supported by its favorable chemical profile and bioactivity.

Keywords- *Coccinia grandis***,** *Anti-urolithiatic***,** *Nephroprotective***,** *Molecular docking Phytochemicals.*

INTRODUCTION

Coccinia grandis (L.) Voigt, commonly known as ivy gourd, is widely used in traditional medicine for the treatment of various ailments including kidney disorders. Recent advances in herbal drug development focus on natural plant-based products due to their multi-target actions and minimal side effects. Given the increasing burden of urolithiasis and nephrotoxicity caused by synthetic drugs, exploring plant-derived compounds is critical. The New Year brings worldwide interest in the research and use of traditional medicine. Therefore, governments are trying to cooperate to identify and use effective and efficient medicines in national health systems.[1] Since ancient times, people have studied nature, especially plant,to find new medicines, which has led to the use of traditional medicine, many species of plants aeeffective in treating various diseases.[2] In India, about 95% of traditional medicine is like this. Unani, Ayurveda, Homeopathy and Sadhana are herbs.[3] Plants produce primary and secondary metabolites with different functions. Coccinia is a plant from the Cucurbitaceae family. It is in Central Africa, Asia, and india. It is a perennial climbing plant that can be propagated vegetatively from seeds. Seeds can be an excellent source of oil and

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

protein that can meet the needs of the market and the consumer. The stalks are either perennially thin climbers or herbaceous climbers, and occasionally, adventitious roots sprout along ground. Branches are long, taut and flexible and can wrap around the entire length of the host. Its leaves are arranged together, its flowers are large, star shaped, white, and its fruit is dark red. The leaves and fruits that were used in foods.[4]

Coccinia grandis (ivy gourd) is rarely grown as a garden vegetable in tropical and subtropical climates worldwide. Its homeland is thought to be Central Africa, India and Asia. Its long history of human use, cultivation, and transportation obscures its origins. It is a plant species that grows in Southeast Asia.[5-6] Urolithiasis is the formation of calculi, or condition associated with urinary calculi. The term calculi are synonymous with uroliths, stones, or crystals. These calculi are formed by deposits of polycrystalline aggregates composed of varied amount of crystalloid and organic matrix. Common components of calculi include Calcium oxalate (pure), Calcium oxalate in combination with as part ate, uric acid (pure), Calcium oxalate in combination with uric acid, Calcium oxalate dihydrate in combination calcium phosphate. In this present study three plants are selected for the anti urolithiasis study[7-12]. This study aims to evaluate the phytoconstituents, anti-urolithiatic potential, nephroprotective effects, and computational drug-likeness profile of C. grandis using a combination of in-vitro and in-silico methods.

MATERIALS AND METHODS

Collection:

The whole plant of *Coccinia* Grandis was collected in the month of April 2025 from Sangulwadi, Dist Sindhudurg, India.

Extraction & Phytochemical Screening

Leaves of *C. grandis* were dried, powdered, and subjected to Soxhlet extraction using solvents in increasing polarity: n-hexane, chloroform, ethyl acetate, and methanol. The methanolic extract was chosen for further analysis. Preliminary phytochemical tests were conducted using standard chemical reagents.

TLC, UV, and FTIR

TLC profiling was performed using methanol: ethyl acetate: water (6:3:1). UV absorption and FTIR spectra identified functional groups and chromophores in the methanolic fraction.

Anti-Urolithiatic Assay

Calcium oxalate monohydrate (COM) crystal aggregation was assessed using the spectrophotometric method. Cystone was used as the standard.

Nephroprotective Assay

NRK-52E kidney cell lines were treated with extract concentrations (20–100 µg/mL), and cell viability was measured using MTT assay.

In-silico Docking

Bioactive compounds were docked against proteins 1V97 and 1UZE. Binding affinities, hydrogen bonding, and ADME profiles were evaluated using CB-Dock and Lipinski's filters.

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

RESULTS

Qualitative chemical examination of plant-based constituents in *Coccinia grandis* leaf extracts as shown in Table 1.

Table 1: Phytochemical screening of Coccinia grandis

Sr.No	TEST	n-Hexane	Chloroform	Ethyl acetate	Methanol
1	Alkaloids	-	-	+	-
2	Carbohydrate	-	-	+	-
3	Glycosides	-	+	-	+
4	Phytosterol	-	-	-	+
5	Fixed oils and Fats	-	-	-	-
6	Tannins	-	-	-	-
7	Phenols	-	-		+
8	Proteins	-	-	+	-
9	Gums and Mucilages	-	-	-	-
10	Flavonoids	-	-	-	+
11	Terpenoids	-	-	-	+
12	Steroids	-	+	-	-
13	Saponins	-	-	+	+

Note: + ve indicates positive result, whereas – ve indicates negative result

Qualitative preliminary phytochemical analysis of Coccinia grandis was performed initially with different chemical reagents to detect the nature of phytoconstituents and their presence in each extract.

Thin Layer Chromatography

Table no: 2 The TLC studies of methanol extracts of Coccinia grandis.

S.No	Name of the Extract	Solvent system	No of spots	R_f Values
1	Methanol (CGM)	Methanol : Ethyl acetate: Water (6:3:1)	01	0.33

Fig. No. 1. TLC of isolated compound

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

Column Chromatography

Fig. 2 Column chromatography of a) Chloroform b) Methanol c) n-Hexane extract

- Adsorbent: Silica for column chromatography activated at 110^{0c} for 1 hour
- Length of column: 40 cm
- Length of adsorbent: 25 cm

UV SPECTRUM:- Fraction In Pet Methanol

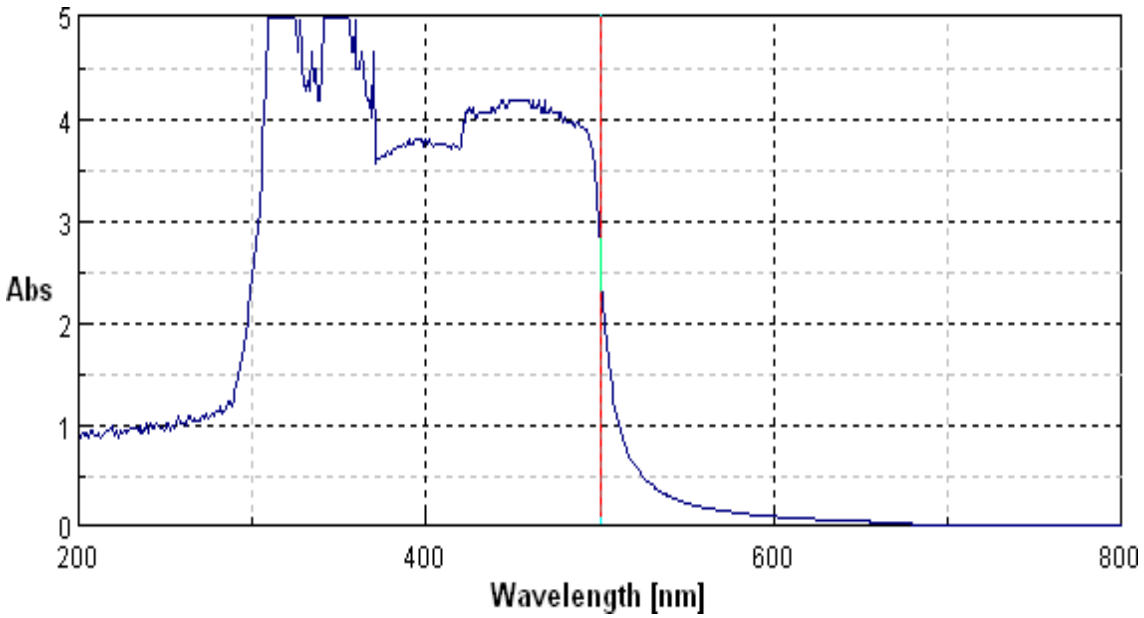


Fig. No. 3. The UV spectrum showed characteristic bands of fraction in methanol at λ= 352

The UV spectra of isolated cextract from *Coccinia grandis* was performed using methanol. The UV spectrum showed characteristic bands of fraction in methanol at λ= 321, 352, 413 The UV spectra of standard showed one characteristic peak at λ= 352.

FTIR of *Coccinia grandis* extract

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

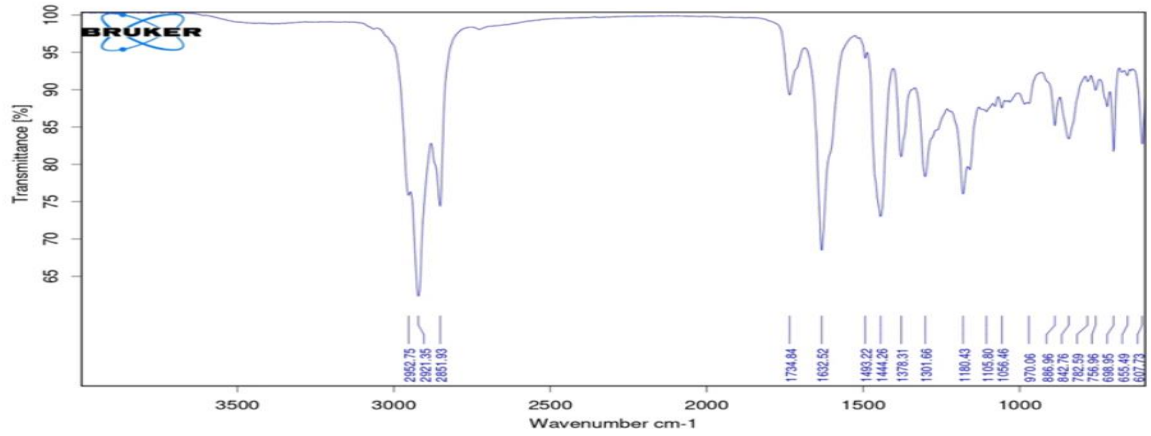


Fig. No. 4. FTIR Spectrum of Coccinia grandis extract

Table no: 5 FTIR Spectrum analysis

Sr.No.	Peak Values	Bonds	Functional groups
1	2952.75	O–H stretch, H–bonded	Alcohols, Phenols
2	2921.35	C–H stretch	Alkanes
3	1493.22	C–C stretch (in–ring)	Aromatics
4	1378.31	C–O stretch	Alcohols
5	842.46, 698.95	C–H “oop”	Aromatics

In-Vitro Anti-Urolithiatic
Crystal Aggregation assay
COM crystal

Table no: 6- Std drug Cystone tab conc.(1mg/ml)

Std drug Cystone tab conc.(1mg/ml)	Concentration	O.D	% Inhibition
Control		0.22	
5 min	10	0.10	54.54
	20	0.11	50.00
	30	0.10	54.54
	40	0.12	45.45
	50	0.12	45.45
10 min	10	0.09	59.09
	20	0.10	54.54
	30	0.09	59.09
	40	0.07	68.18
	50	0.08	63.63
	10	0.09	59.09

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

15 min	20	0.07	68.18
	30	0.07	68.18
	40	0.08	63.63
	50	0.07	68.18
20 min	10	0.06	72.72
	20	0.07	68.18
	30	0.06	72.72
	40	0.07	68.18
	50	0.06	72.72
25 min	10	0.05	77.27
	20	0.06	72.72
	30	0.04	81.81
	40	0.05	77.27
	50	0.04	81.81

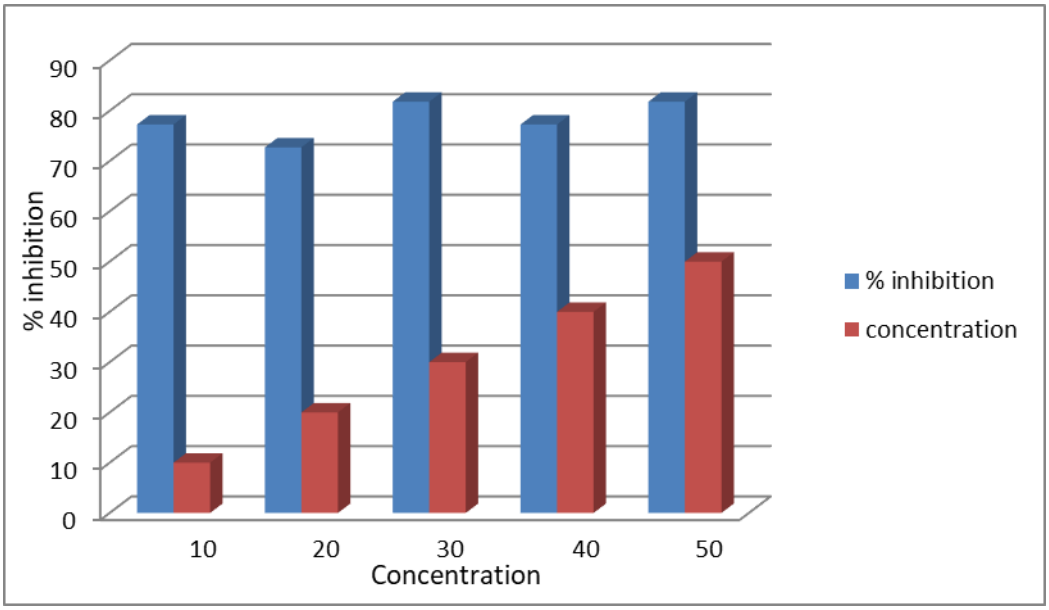


Fig. No. 5. Graphical representation of anti-urolithiatic using STD drugCystone tabconc.

Table no: 7- Sample *Coccinia grandis extract*

Sample *Coccinia grandis extract*	Concentration	O.D	% inhibition
Control	0.22		
5 min	10	0.21	4.51
	20	0.20	9.09
	30	0.21	4.51
	40	0.20	9.09
	50	0.20	9.09
10 min	10	0.19	13.63
	20	0.18	18.18
	30	0.18	18.18
	40	0.17	22.72
	50	0.17	22.72
	10	0.16	27.27

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

15 min	20	0.15	31.81
	30	0.15	31.81
	40	0.16	27.27
	50	0.16	27.27
20 min	10	0.14	36.36
	20	0.13	40.90
	30	0.13	40.90
	40	0.12	45.45
	50	0.12	45.45
25 min	10	0.10	54.54
	20	0.09	59.09
	30	0.10	54.54
	40	0.10	54.54
	50	0.09	59.09

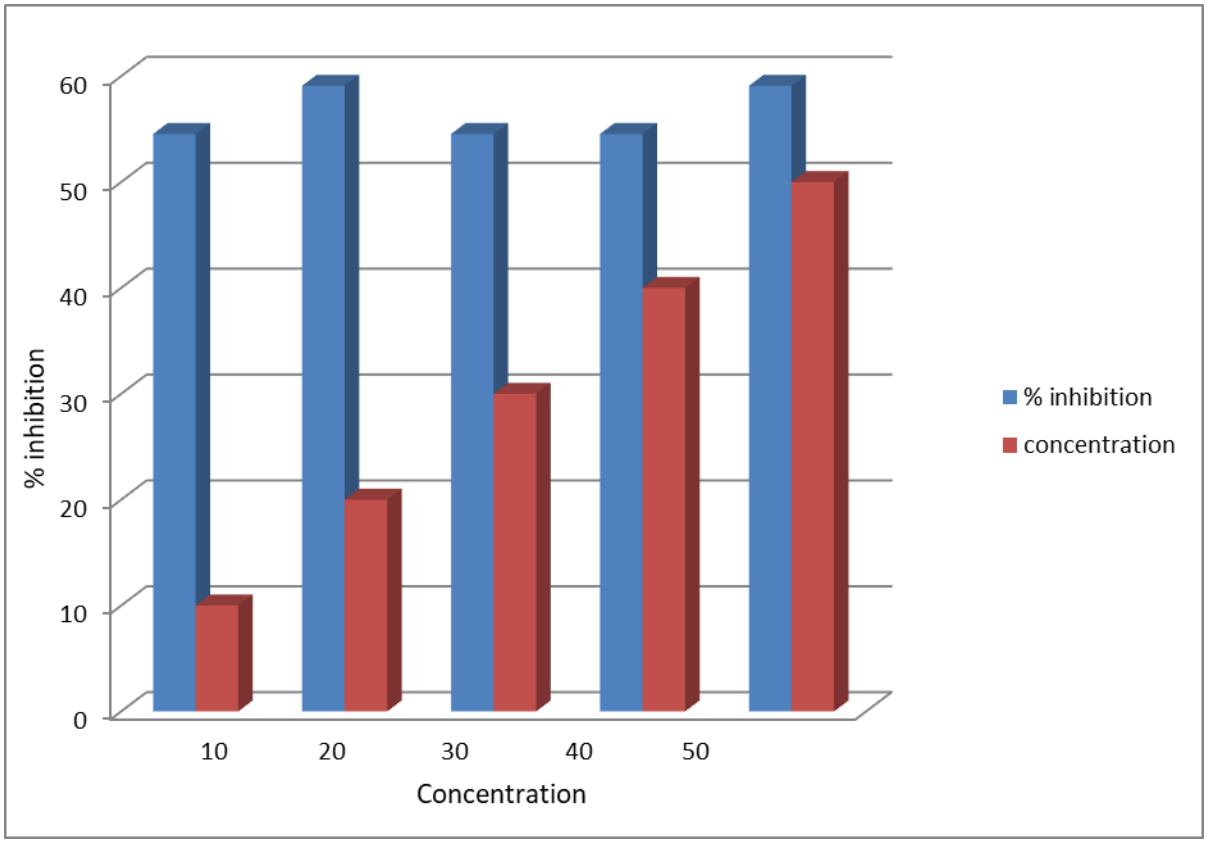


Fig. No. 6. Graphical representation of anti-urolithiatic using methanolic extract of Coccinia grandis

Investigation of protein 1UZE is done by using PDB sum software with the help of Ramchandran plot procheck analysis. According to Ramchandran plot statistics for 1UZE most favoured regions is 94.3%, additional allowed region is 5.5% generally allowed region is 0.2% and disallowed region is 0.0% which are shown in fig. no 7

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

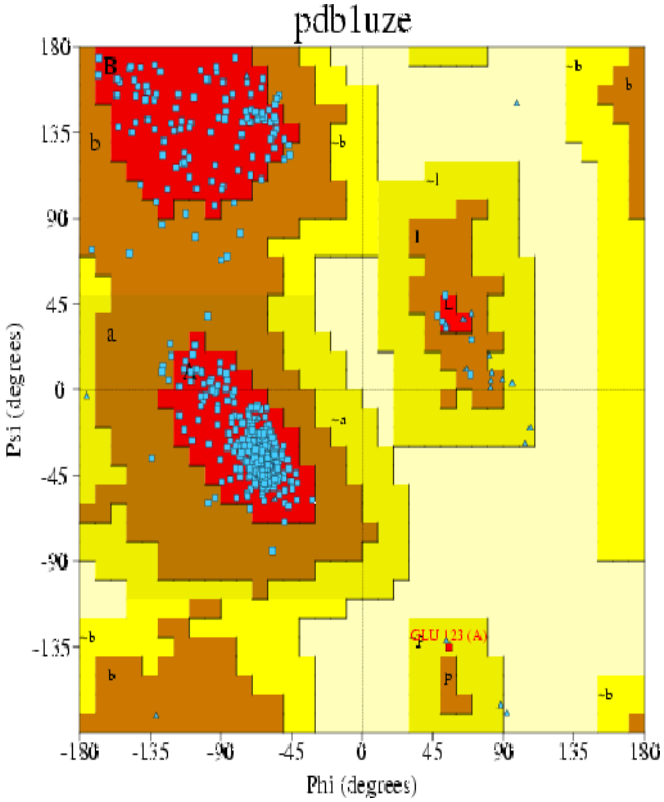
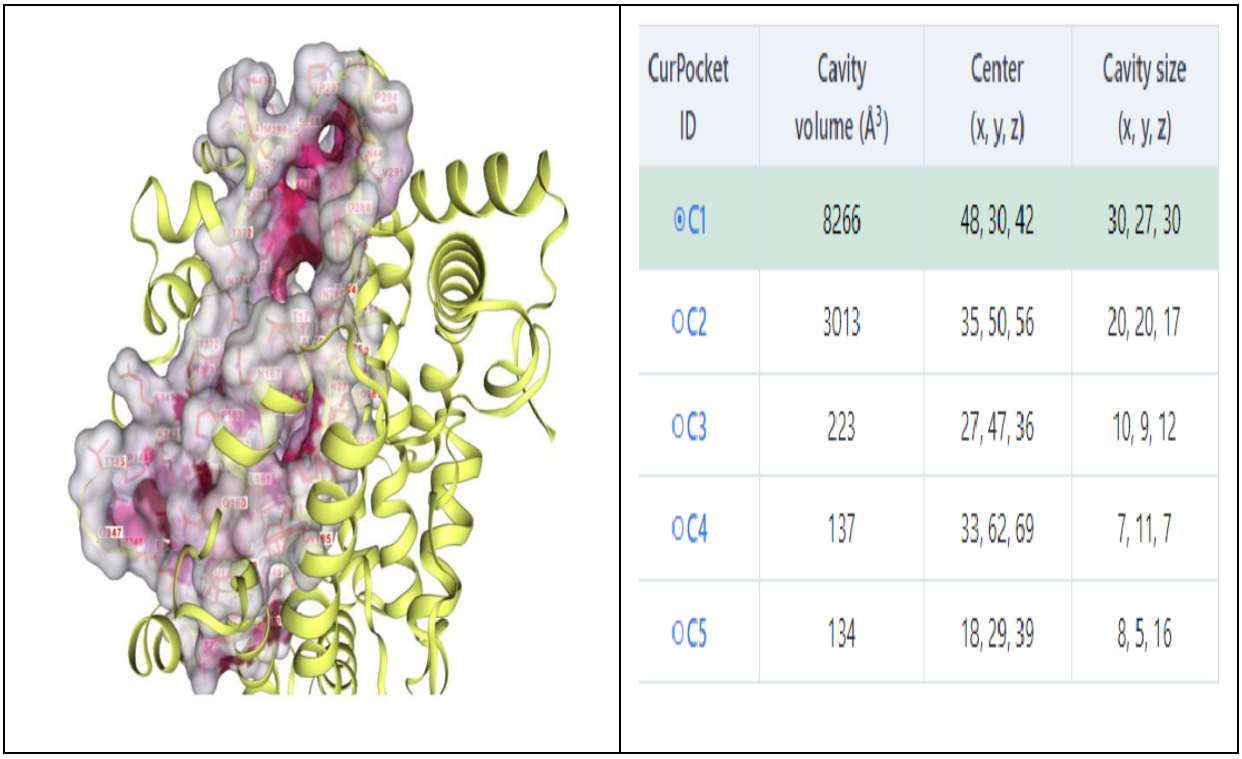


Fig. No. 7. Ramchandran plot of 1UZE



CurPocket ID	Cavity volume (Å^3)	Center (x, y, z)	Cavity size (x, y, z)
◉C1	8266	48, 30, 42	30, 27, 30
○C2	3013	35, 50, 56	20, 20, 17
○C3	223	27, 47, 36	10, 9, 12
○C4	137	33, 62, 69	7, 11, 7
○C5	134	18, 29, 39	8, 5, 16

Fig. No. 8. Cavity detection of protein 1UZE

All data obtained from molecular docking of both proteins with ligands are depicted in Table 8.

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

Table 8. Lipinski properties of bioactive compounds from C.grandisleaves

Sr. no.	Compound name	Molecular weight	Log p	H-bond donar	H-bond acceptor	Molar refractivity
1	Betasitosterol	414.71 g/mol	4.79	1	1	133.23
2	Cucurbitacin B	558.70 g/mol	1.46	3	8	150.94
3	Kaempferol	286.24 g/mol	1.47	4	6	76.01
4	Thiamine	265.35 g/mol	-1.60	2	3	73.12
5	Ferulic Acid	194.18 g/mol	1.62	2	4	51.63
6	Quercetin	302.24 g/mol	1.63	5	7	78.03
7	Ombium	330.29 g/mol	2.83	3	7	51.63
8	Ascorbic acid	176.12 g/mol	0.39	4	6	35.12
9	Trans pcoumaric acid	164.16 g/mol	0.95	2	3	45.13
10	Carbonic Acid	62.02 g/mol	-0.22	2	3	10.65

Table 9. ADME properties of various bioactive compounds

Sr no	Compound name	Formula	Distribution	Absorption				Toxicity
			BBB Pearmiability	GI Absorption	Human intestinal absorption	Skin pearmiability	CACO-2 Pearmiability	Toxicity predicted LD 50
1	Betasitosterol	C29H50O	0.781	Low	94.464	-2.783	1.201	2.552
2	Cucurbitacin B	C32H46O8	-1.003	Low	89.52	-3.496	0.588	2.381
3	kaempferol	C15H10O6	-0.939	High	74.29	-2.735	0.032	2.449
4	Thiamine	C12H17N4O5	-0.368	High	100	-2.792	0.867	2.672
5	Ferulic Acid	C10H10O4	-0.239	High	93.685	-2.72	0.176	2.282
6	Quercetin	C15H10O7	-1.098	High	77.207	-2.735	-0.229	2.471
7	Ombiun	C17H14O7	-1.089	High	87.47	-2.735	0.402	2.272
8	Ascorbic acid	C5H8O6	-0.985	High	39.154	-2.955	-0.255	1.063
9	trans p comedic acid	C9H8O3	-0.225	High	93.494	-2.715	1.21	2.155
10	Carbonic Acid	CH2O3	-0.428	High	83.064	-2.737	1.12	1.439
11	Niacin	C6H2ON4O6	-0.323	High	94.099	-2.735	1.17	2.24

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

Table no: 10 Moleculardocknig result examination of bioactive substances of *coccinia grandis* against the protein 1UZE

Compound Name	Binding affinity (kcl/mol)	Conventional H- bond Interaction	Pi Sigma Interaction	Pi Alkyl Interaction	Van- der -Waals Interaction	Other Interaction
Betasitosterol	-9.3	GLU 411	-	VAL518,LEU81, LEU140 , LEU139	GLU143,TYR69, ASN70, ASN 66, VAL351,ASN136, ASN85 ARG124, SER516, TRP357, SER355, TYR523	-
Cucurbitacin B	-10	ILE 204, ASN211, GLU124	-	-	ALA 207, TRP220, TYR135, LEU139, SER219, ALA208	-
Kaempferol	-8.2	ASP415, TYR520, LYS511, GLN281, ASP377	VAL380	ALA 354	GLN369, GLU162, HIS353, HIS513, PHE457, TYR523, PHE527, HIS383	-
Thiamine	-6.9	TYR 62, SER 355	-	- LEU 82, LEU 139,LEU 81, LEU 140	TYR 69, VAL 351, TRP 357 ,GLU 143 ,ASN 70, PHE 512, VAL 518 ,ASN 85,ASN 136	Other C- H bond- LYS 368, SER 516
Ferulic Acid	-6.5	ARG 124, SER 517	-	ILE 204, ALA 207	LEU 139, TYR 135, SER 219, TYR 213,ASP 121,ALA 208	Other Pi-anion – GlU123 Amide-pistacked – TRP 220
Quercetin	-8.3	THR 301, ASP 453	-	LYS 449, LEU 375	THR 302, ASP 300, MET 299, LEU 433, SER 298 ,GIU 376, VAL 379, MET 450,SER 284, ASN 285	-
Ombiun	-8.5	GLY 404 ,GLU 384. TYR 523, ARG 522	-	MET 223, PRO 407, PHE 512, HIS 353, VAL 518	ASN 406, PHE 391, ALA 356, SER 355	Other Pi-cation - GLU 411 Pi-Anion- GLU 403C-H bond HIS 410, HIS 387, HIS 513
Ascorbic acid	-5.7	ASP 121, TRP 220	-	-	TYR 213, ALA 208, ALA 207, ILE 204,ARG 124, TYR 135 ,GLU 123,ASN 211, SER 219	
Trans p coumaric acid	-6.2	ARG 124, SER 517	-	ALA 207	LEU 139, TYR 135,SER 219,ASP 121 ,TYR 213, ASN 211, TRP 220, ILE 204	Other Pi-anion- GLU 123
Carbonic Acid	-3.3	HIS 353, CYS 352, SER 147, VAL 350	-	-	PHE 512, VAL 351, LEU 161, TYR 146	-
Niacin	-5.4	ASN 85, ARG 124	-	- LEU 139	LEU 81, TYR 62, ASN 136 ,LEU 140, GLU 143	-
Quercetin	-8.3	THR 301, ASP 453	-	LYS 449, LEU 375	THR 302, ASP 300, MET 299, LEU 433, SER 298 ,GIU 376, VAL 379, MET 450,SER 284, ASN 285	-

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

Table no: 11 Drug likeliness properties of isolated ligand from *coccinia grandis*

Sr. no.	Compound	Lipinski	Ghose	Veber	Egan	Muegge
1	Betasitosterol	Yes	No	Yes	No	No
2	Cucurbitacin B	Yes	No	Yes	No	Yes
3	Kaempferol	Yes	Yes	Yes	Yes	Yes
4	Thiamine	Yes	Yes	Yes	Yes	Yes
5	Ferulic Acid	Yes	Yes	Yes	Yes	No
6	Quercetin	Yes	Yes	Yes	Yes	Yes
7	Ombium	Yes	Yes	Yes	Yes	Yes
8	Ascorbic acid	Yes	No	Yes	Yes	No
9	Trans p coumaric acid	Yes	Yes	Yes	Yes	No
10	Carbonic Acid	Yes	No	Yes	Yes	No
11	Niacin	Yes	No	Yes	Yes	No

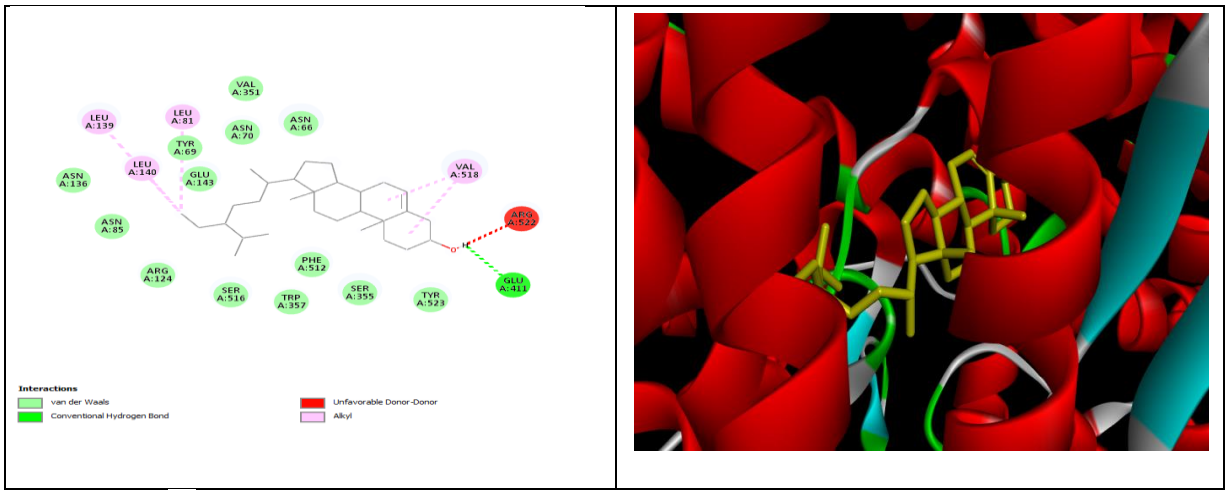


Fig. No. 9. B. Two dimensional and Three-dimensional interactions of β-Sitosterol against receptor 1UZE

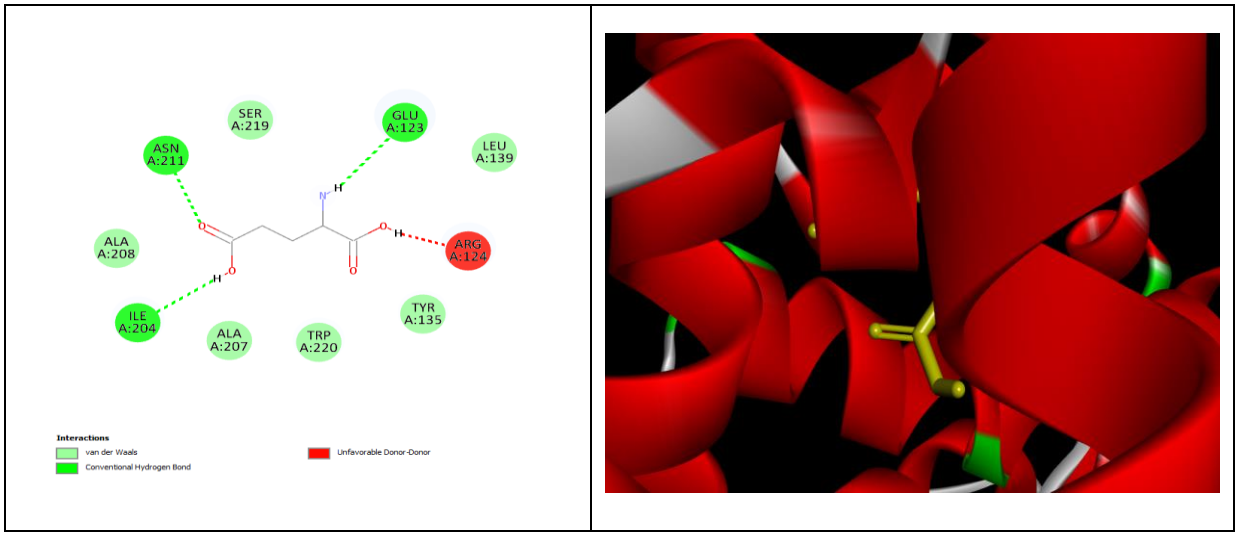


Fig. No. 10. D. Two dimensional and Three-dimensional interactions of Cucurbitacin B against receptor 1UZE

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

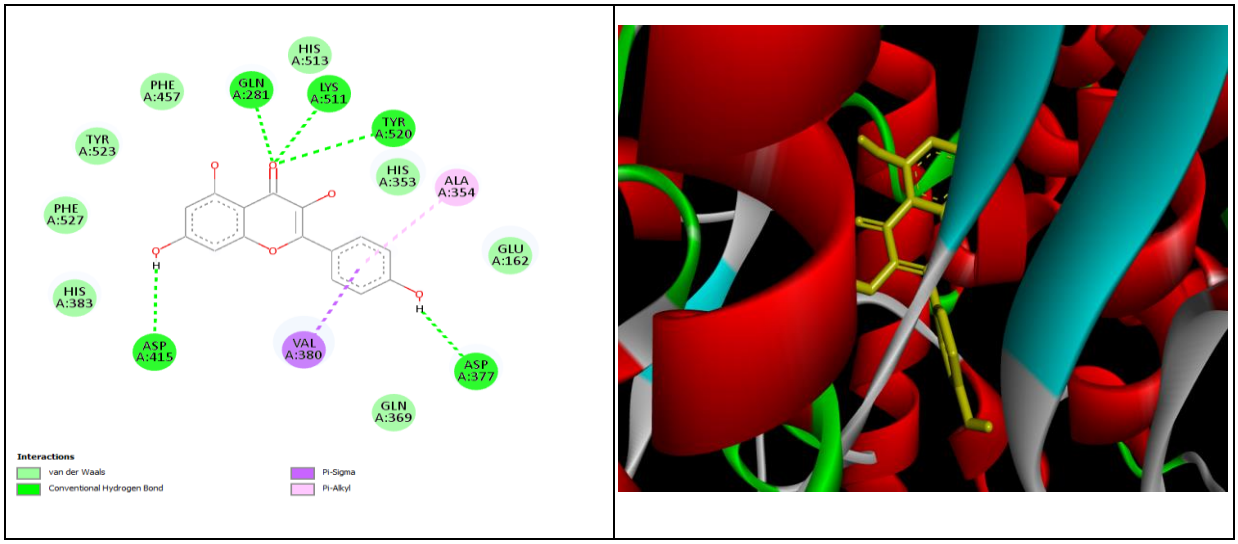


Fig. No. 11. F. Two dimensional and three-dimensional interactions of Kaempferol against receptor 1UZE

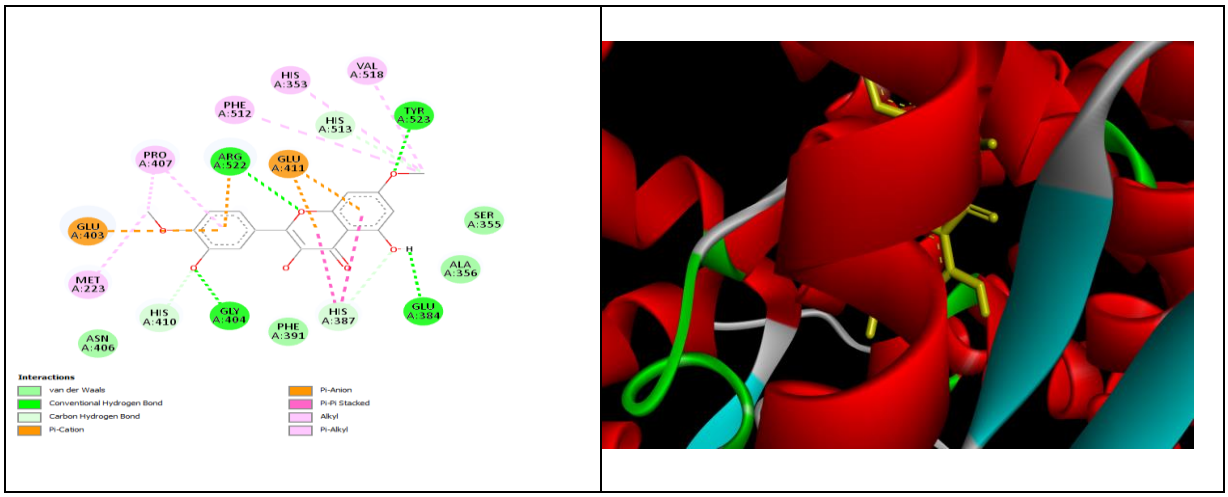


Fig. No. 12. L. Two dimensional and three-dimensional interactions of Ombiun against receptor 1UZE

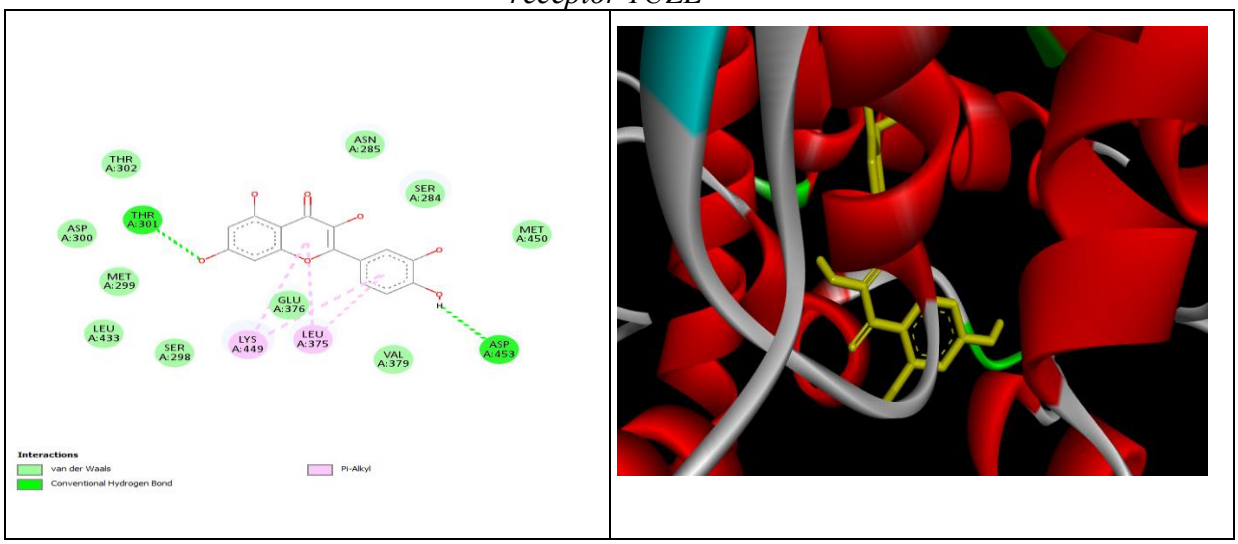


Fig. No. 13. J. Two dimensional and three-dimensional interactions of Quercetin against receptor 1UZE

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

CONCLUSION

This research confirmed that *Coccinia grandis* leaf extract, especially the methanolic fraction, contains bioactive phytochemicals with potential anti-urolithiatic and nephroprotective activities. The in-vitro crystal aggregation assay demonstrated moderate inhibition of COM crystals, while nephrotoxicity studies using NRK-52E cells indicated that the extract is non-toxic and may offer protective effects against renal damage. Spectral analyses (UV, FTIR) supported the presence of functional groups related to antioxidant and anti-inflammatory actions. In-silico molecular docking revealed strong binding affinities of compounds such as quercetin, kaempferol, and cucurbitacin B with renal disease-associated proteins (1V97 and 1UZE), validating the potential of these phytochemicals in kidney disease treatment. These compounds also complied with Lipinski's rule and showed good ADME properties, strengthening their candidacy for further drug development.

The integration of experimental and computational findings provides significant evidence that *C. grandis* may serve as a valuable natural source for developing phytopharmaceuticals aimed at treating or preventing urolithiasis and associated nephrotoxicity. Further in-vivo and clinical evaluations are needed to confirm these findings and determine dosage and formulation safety for therapeutic use.

REFERENCES

1) Kumari P., Kumari C., Shekhar Singh P.;Phytochemical Screening of Selected Medicinal Plants for Secondary Metabolites;SSR Institute of International Journal of Life Sciences Res.;2017;*3*(4);1151-1157.
2) Shahriar M., Bahar M., Hossain I., Akhter S., Haque M. A., Bhuiyan M.A.; Preliminary phytochemical screening.: *In vitro* Anti-oxidant and cytotoxic activity of five different extracts of *Withania somnifera* root. International Journal of Pharmacy; 2012; 2: 450-453.
3) Satyavati G.V., Gupta A. K., Tandon N.; Medicinal plants of India, Indian Council of Medical Research, New Delhi, India; 1987.
4) Amir Hossain S.K., Uddin N., Salim Abu M., Haque R.; Phytochemical and Pharmacological screening of *Coccinia grandis Linn*;Journal of Scientific and Innovative Research; 2014; 3 (1): 65-71.
5) Ivy gourd (Coccinia grandis) - Technigro. Available from : www.technigro.com.au/wp-content/uploads/2016/10/24- Ivy-Gourd.pdf, Assessed on : May 2011.
6) Ivy Gourd Risk Assessment - Department of Agriculture and Fisheries. Available from: https://www.daf.qld.gov.au/- data/assets/pdf.../IPA-Ivy-Gourd-Risk-Assessment.pdf. Steve Csurhes. First published 2008, Updated 2016.
7) Suresh V Chennupati, Narayana Rao Alla*, M S C Bose, Anusha G, Sravani A, Study On Anti Urolithiasis Activity Of Some Common Medicinal Plantsalcoholic Extracts, An International Journal of Advances in Pharmaceutical Sciences, 2015, 6 (2):2784-2789.
8) S umaryono W, Proksch P, Wray V, Witte L L Qualitative and Quantitative analysis of the phenolic constituents from Orthosiphon aristatus. Planta medica : 1991:57:176- 180.
9) D ouglar Skoog A., James Holler., Fer Nieman., and Timothy, A "Principles of Instrumental Analysis", London, Thomson Brook, 2005; pp. 350-432.
10) W illard, "Instrumental Methods of Analysis", New York: D. Van Nostrand company (cannada) Ltd, 4th ed,1965 pp. 180-445.

Pharmaceutical Sciences
Volume 5 Issue 2, 2025
eISSN No.: 2582-8371

11) Silverstein., "Spectrometric Identification of Organic Compounds", New York, John willey & sons, 6th ed., 1998;pp. 1-48.
12) Mezei M. A new method for mapping macromolecular topography. *J Mol Graph Model.* 2003;21(5):463–472.