

Name: Dr Subhash Agarwal

Designation: Scientist E and Head

Division/Department: Bioinformatics

Educational Qualification: M.Sc, ADPGD, PhD

Work Experience: 15 Years



Research Interests: Cancer informatics, Machine learning, Database Development, Structure based Drug Design and Chemoinformatics,

Membership of Professional Societies:

- Life Member, Indian Association for Cancer Research (IACR)
- Member, The National Academy of Sciences (NASI, Allahabad)

Member of any national/international research/academic committee:

- Member, Area Advisory Board - Bioinformatics, Amity University, Noida
- Reviewer for DBT BIRAC (2012-2018)
- DBT-NER (North East Region) Screening committee member
- M.Sc / M.Tech Paper Setter for various Universities

Fellowships/Awards/Patents (academic/national/international):

- 2019. Selected as Member, The National Academy of Sciences (NASI, Allahabad)
- 2017. Shakuntala Amir Chand Award (ICMR) for the year 2015
- 2017. BiosolveIT Scientific Spring Challenge Winner (International Award)
- 2013. Awarded Department of Health Research (DHR) Fellowship
- 2012. Recipient of DBT Innovative Young Biotechnologist Award
- 2008. Awarded DST Young Scientist Project
- 2006. Recipient of IUBMB- Young Scientist Award, Japan (International Award)
- 2002. Awarded scholarship by DBT during ADPGD in Bioinformatics, JNU
- 2001. Recipient of CSIR-UGC NET scholarship for pursuing PhD
- 2001. GATE Qualified

Projects:

- **Ongoing**

S. No	Title of Project	Funding Agency	Role	Duration
1	Identifying anti-cancerous phytomolecule combinations against cancers for leveraging traditional drug discovery	Indian Council of Medical Research (ICMR)	Principal Investigator	Oct 2021 - Oct 2023
2	Predicting the anti-cancer potential of phyto-molecules against different cancers using knowledge of natural products.	Indian Council of Medical Research (ICMR)	Principal Investigator	Jan 2020- Jan 2023

- **Completed**

S. No	Title of Project	Funding Agency	Role	Duration
1	Next generation EGFR inhibitor identification using ligand based QSAR technique	Department of Health Research (DHR)	Principal Investigator	Sep 2016- Sep 2019
2	Identification of novel inhibitors targeting EGFR using an integrated ligand and structure based approach	Department of Biotechnology (DBT)	Principal Investigator	Aug 2012- Aug 2015
3	Prediction of drug targets of chemical constituents present within non-codified medicinal plants	National Innovation Foundation (NIF)	Principal Investigator	Apr 2011- Sep 2014
4	Development of an automated system for differentiating slowly and rapidly evolving human genes to facilitate medical research	Department of Science and Technology (DST)	Principal Investigator	Jan 2010 - Jan 2013
5	Virtual screening of chemical libraries with the key cysteine biosynthetic pathway enzymes in Entamoeba histolytica for novel inhibitor identification	Department of Science and Technology (DST)	Principal Investigator	Apr 2008 - Mar 2011

Publications: (latest first and in Vancouver style with latest impact factor):

SNo	Paper Details	DOI	IF
1	Agarwal SM, Nandekar P, Saini R. Computational identification of natural product inhibitors against EGFR double mutant (T790M/L858R) by integrating ADMET, machine learning, molecular docking and a dynamics approach. RSC Adv. 2022 Jun 7;12(26):16779-16789. doi: 10.1039/d2ra00373b. PMID: 35754875	10.1039/d2ra00373b	4.036

2	Das AP, Saini S, Agarwal SM . A comprehensive meta-analysis of non-coding polymorphisms associated with precancerous lesions and cervical cancer. <i>Genomics</i> . 2022 Feb 25;114(3):110323. doi: 10.1016/j.ygeno.2022.110323.	10.1016/j.ygeno.2022.110323	4.31
3	Das AP, Chopra M, Agarwal SM . Prioritization and Meta-analysis of regulatory SNPs identified IL6, TGFB1, TLR9 and MMP7 as significantly associated with cervical cancer. <i>Cytokine</i> . 2022 Sep; 157: 155954. doi: 10.1016/j.cyto.2022.155954	10.1016/j.cyto.2022.155954	3.93
4	Das AP, Saini S, Tyagi S, Chaudhary N, Agarwal SM . Elucidation of Increased Cervical Cancer Risk Due to Polymorphisms in XRCC1 (R399Q and R194W), ERCC5 (D1104H), and NQO1 (P187S). <i>Reprod Sci</i> . 2022 Oct 4. doi: 10.1007/s43032-022-01096-6.	10.1007/s43032-022-01096-6	2.92
5	Saini R, Agarwal SM . EGFRisopred: a machine learning-based classification model for identifying isoform-specific inhibitors against EGFR and HER2. <i>Mol Divers</i> . 2022 Jun;26(3):1531-1543. doi: 10.1007/s11030-021-10284-6.	10.1007/s11030-021-10284-6	3.36
6	Ansari MF, Inam A, Ahmad K, Fatima S, Agarwal SM , Azam A. Synthesis of metronidazole based thiazolidinone analogs as promising antiamebic agents. <i>Bioorganic Med Chem Lett</i> . 2020;30(23):127549. Available from: http://doi.org/10.1016/j.bmcl.2020.127549	doi.org/10.1016/j.bmcl.2020.127549	2.94
7	Saini R, Fatima S, Agarwal SM . TMLRpred: A machine learning classification model to distinguish reversible EGFR double mutant inhibitors. <i>Chem Biol Drug Des</i> . 2020;96(3):921–30. Available from: http://doi.org/10.1111/cbdd.13697	10.1111/cbdd.13697	2.873
8	Fatima S, Gupta P, Sharma S, Sharma A, Agarwal SM . ADMET profiling of geographically diverse phytochemical using chemoinformatic tools. <i>Future Med Chem</i> . 2019 Dec;12(1):69–87. Available from: https://doi.org/10.4155%2Ffmc-2019-0206	10.4155%2Ffmc-2019-0206	4.767
9	Fatima S, Agarwal SM . Structure-activity Relationship Study on Therapeutically Relevant EGFR Double Mutant Inhibitors. <i>Med Chem (Los Angeles)</i> . 2019;16(1):52–62. Available from: http://doi.org/10.2174/1573406415666190206204853	10.2174/1573406415666190206204853	2.75
10	Fatima S, Pal D, Agarwal SM . QSAR of clinically important EGFR mutant L858R/T790M pyridinylimidazole inhibitors. <i>Chem Biol Drug Des</i> . 2019;94(1):1306–15.	10.1111/cbdd.13505	2.873
11	Fatima S, Agarwal SM . Exploring structural features of EGFR–HER2 dual inhibitors as anti-cancer agents using G-QSAR approach. <i>J Recept Signal Transduct</i> . 2019;39(3):243–52.	10.1080/10799893.2019.1660896	2.579

12	Fatima S, Gupta P, Agarwal SM . Insight into structural requirements of antiameobic flavonoids: 3D-QSAR and G-QSAR studies. <i>Chem Biol Drug Des</i> . 2018;92(4):1743–9.	10.1111/cbdd.13343	2.873
13	Fatima S, Agarwal SM . Unraveling structural requirements of amino-pyrimidine t790m/1858r double mutant egfr inhibitors: 2d and 3d qsar study. <i>J Recept Signal Transduct</i> . 2018;38(4):299–306.	10.1080/10799893.2018.1494740	2.579
14	Sharma A, Sharma S, Gupta M, Fatima S, Saini R, Agarwal SM . Pharmacokinetic profiling of anticancer phytochemicals using computational approach. <i>Phytochem Anal</i> . 2018;29(6):559–68.	10.1002/pca.2767	3.37
15	Sharma S, Gupta M, Sharma A, Agarwal SM . Oral Bioavailability of Naturally Occurring Anticancer Phytomolecules. <i>Lett Drug Des Discov</i> . 2018;15(11):1180–8.	www.eurkaselect.com/article/87789	1.15
16	Agarwal SM , Pal D, Gupta M, Saini R. Insight into Discovery of Next Generation Reversible TMLR Inhibitors Targeting EGFR Activating and Drug Resistant T790M Mutants. <i>Curr Cancer Drug Targets</i> . 2017;17(7):617–36.	10.2174/1568009617666170330112842	3.43
17	Malik MZ, Alam MJ, Ishrat R, Agarwal SM , Singh RKB. Control of apoptosis by SMAR1. <i>Mol Biosyst</i> . 2017;13(2):350–62.	10.1039/c6mb00525j	4.212
18	Sheriff SA, Shaik Ibrahim S, Devaki T, Chakraborty S, Agarwal S , Pérez-Sánchez H. Lycopene Prevents Mitochondrial Dysfunction during d -Galactosamine/Lipopolysaccharide-Induced Fulminant Hepatic Failure in Albino Rats. <i>J Proteome Res</i> . 2017;16(9):3190–9.	10.1021/acs.jproteome.7b00176	5.37
19	Dhiman K, Agarwal SM . NPred: QSAR classification model for identifying plant based naturally occurring anti-cancerous inhibitors. <i>RSC Adv</i> . 2016;6(55):49395–400.	10.1039/C6RA02772E	3.36
20	Agarwal SM , Sharma M, Fatima S. VOCC: a database of volatile organic compounds in cancer. <i>RSC Adv</i> . 2016;6(115):114783–9.	10.1039/C6RA24414A	4.036
21	Leeza Zaidi S, Agarwal SM , Chavalitshewinkoon-Petmitr P, Suksangpleng T, Ahmad K, AVECILLA F, et al. Thienopyrimidine sulphonamide hybrids: Design, synthesis, antiprotozoal activity and molecular docking studies. <i>RSC Adv</i> . 2016;6(93):90371–83.	10.1039/C6RA15181G	4.036
22	Sharma VK, Nandekar PP, Sangamwar A, Pérez-Sánchez H, Agarwal SM . Structure guided design and binding analysis of EGFR inhibiting analogues of erlotinib and AEE788 using ensemble docking, molecular dynamics and MM-GBSA. <i>RSC Adv</i> . 2016;6(70):65725–35.	10.1039/C6RA08517B	4.036

23	Singh H, Singh S, Singla D, Agarwal SM , Raghava GPS. QSAR based model for discriminating EGFR inhibitors and non-inhibitors using Random forest. Biol Direct. 2015;10(1).	10.1186/s13062-015-0046-9	4.54
24	Ansari MF, Siddiqui SM, Agarwal SM , Vikramdeo KS, Mondal N, Azam A. Metronidazole hydrazone conjugates: Design, synthesis, antiamebic and molecular docking studies. Bioorganic Med Chem Lett. 2015;25(17):3545–9.	10.1016/j.bmcl.2015.06.091	2.94
25	Inam A, Van Zyl RL, Van Vuuren NJ, Chen CT, Avecilla F, Agarwal SM , et al. Chloroquinoline-acetamide hybrids: A promising series of potential antiprotozoal agents. RSC Adv. 2015;5(60):48368–81.	10.1039/C5RA05472A	4.036
26	Azam A, Agarwal SM . Heterocyclic lead compounds against amebiasis. Amebiasis Biol Pathog Entamoeba. 2015;565–81.	link.springer.com/chapter/10.1007/978-4-431-55200-0_33	-
27	Mangal M, Imran Khan M, Mohan Agarwal S . Acetogenins as Potential Anticancer Agents. Anticancer Agents Med Chem. 2015;16(2):138–59.	10.2174/1871520615666150629101827	2.527
28	Yadav IS, Nandekar PP, Srivastava S, Sangamwar A, Chaudhury A, Agarwal SM . Ensemble docking and molecular dynamics identify knoevenagel curcumin derivatives with potent anti-EGFR activity. Gene 539, (2014) 82-90.	10.1016/j.gene.2014.01.056	3.913
29	Yadav I, Singh H, Khan M, Chaudhury A, Raghava GPS, Agarwal S . EGFRIndb: Epidermal Growth Factor Receptor Inhibitor Database. Anticancer Agents Med Chem. 2014;14(7):928–35.	10.2174/1871520614666140323203140	2.527
30	Chauhan JS, Dhanda SK, Singla D, Agarwal SM , Raghava GPS. QSAR-based models for designing quinazoline/imidazothiazoles/pyrazolopyrimidines based inhibitors against wild and mutant EGFR. PLoS One. 2014;9(7).	10.1371/journal.pone.0101079	3.752
31	Sharma G, Dua P, Agarwal S . A Comprehensive Review of Dysregulated miRNAs Involved in Cervical Cancer. Curr Genomics. 2014;15(4):310–23.	10.2174/1389202915666140528003249	2.689

32	Srivastava P, Mangal M, Agarwal SM . Understanding the transcriptional regulation of cervix cancer using microarray gene expression data and promoter sequence analysis of a curated gene set. <i>Gene</i> . 2014;535(2):233–8.	10.1016/j.gene.2013.11.028	3.913
33	Sharma G, Agarwal S . Identification of Critical MicroRNA Gene Targets in Cervical Cancer Using Network Properties. <i>MicroRNA</i> . 2014;3(1):37–44.	10.2174/2211536603666140417214659	-
34	Arora A, Gera S, Maheshwari T, Raghav D, Alam MJ, Singh RKB, et al. The Dynamics of Stress p53-Mdm2 Network Regulated by p300 and HDAC1. <i>PLoS One</i> . 2013;8(2).	10.1371/journal.pone.0052736	3.752
35	Salahuddin A, Inam A, Van Zyl RL, Heslop DC, Chen CT, Avecilla F, et al. Synthesis and evaluation of 7-chloro-4-(piperazin-1-yl)quinoline- sulfonamide as hybrid antiprotozoal agents. <i>Bioorganic Med Chem</i> . 2013;21(11):3080–9.	10.1016/j.bmc.2013.03.052	3.64
36	Alam MJ, Devi GR, Ravins, Ishrat R, Agarwal SM , Singh RKB. Switching p53 states by calcium: Dynamics and interaction of stress systems. <i>Mol Biosyst</i> . 2013;9(3):508–21.	10.1039/c3mb25277a	4.212
37	Raghav D, Sharma V, Agarwal SM . Structural investigation of deleterious non-synonymous SNPs of EGFR gene. <i>Interdiscip Sci Comput Life Sci</i> . 2013;5(1):60–8.	10.1007/s12539-013-0149-x	3.492
38	Mangal M, Sagar P, Singh H, Raghava GPS, Agarwal SM . NPACT: Naturally occurring plant-based anti-cancer compound-activity-target database. <i>Nucleic Acids Res</i> . 2013;41(D1):D1124-9.	10.1093/nar/gks1047	19.16
39	Salahuddin A, Agarwal SM , Avecilla F, Azam A. Metronidazole thiosalicylate conjugates: Synthesis, crystal structure, docking studies and antiamebic activity. <i>Bioorganic Med Chem Lett</i> . 2012;22(17):5694–9.	10.1016/j.bmcl.2012.06.083	2.94
40	Younus Wani M, Athar F, Salauddin A, Agarwal SM , Azam A, Choi I, et al. Novel terpene based 1,4,2-dioxazoles: Synthesis, characterization, molecular properties and screening against <i>Entamoeba histolytica</i> . <i>Eur J Med Chem</i> . 2011;46(9):4742–52.	10.1016/j.ejmech.2011.06.005	7.088
41	Agarwal SM , Raghav D, Singh H, Raghava GPS. CCDB: A curated database of genes involved in cervix cancer. <i>Nucleic Acids Res</i> . 2011;39(SUPPL. 1). 975-9.	10.1093/nar/gkq1024	19.16
42	Baniulis D, Liobikas J, Agarwal SM , Frercks B, Vaitiekaitis G, Stanys V. Phylogeny of structural domains of plant serine β -lactamase family proteins. <i>Biologija</i> . 2010;56(1):41–8.	www.lm aleidykla .lt/ojs/ind ex.php/bi ologija/a rticle/vie	-

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43	Agarwal SM, Srivastava PK. Human intronless disease associated genes are slowly evolving. <i>BMB Rep.</i> 2009;42(6):356–60.	2-s2.0-68349146848	5.041
44	Abid M, Agarwal SM , Azam A. Synthesis and antiamebic activity of metronidazole thiosemicarbazone analogues. <i>Eur J Med Chem.</i> 2008;43(9):2035–9.	10.1016/j.ejmech.2007.12.007	7.088
45	Agarwal SM. Rapidly Evolving Regions of the Human Genome. In: <i>eLS.</i> 2008.	10.1002/9780470015902.a0020802	-
46	Agarwal SM, Grover A. Nucleotide Composition and Amino Acid Usage in AT-Rich Hyperthermophilic Species. <i>Open Bioinforma J.</i> 2008;2(1):11–9.	10.2174/1875036200802010011	-
47	Agarwal SM, Jain R, Bhattacharya A, Azam A. Inhibitors of <i>Escherichia coli</i> serine acetyltransferase block proliferation of <i>Entamoeba histolytica</i> trophozoites. <i>Int J Parasitol.</i> 2008;38(2):137–41.	10.1016/j.ijpara.2007.09.009	4.33
48	Azam A, Agarwal SM. Targeting amoebiasis: Status and developments. <i>Curr Bioact Compd.</i> 2007;3(2):121–33.	10.2174/157340707780809590	-
49	Athar F, Husain K, Abid M, Agarwal SM , Coles SJ, Hursthouse MB, et al. Synthesis and anti-amoebic activity of gold(I), ruthenium(II), and copper(II) complexes of metronidazole. <i>Chem Biodivers.</i> 2005;2(10):1320–30.	10.1002/cbdv.200590104	2.745
50	Agarwal SM, Jain M, Grover A. Genomic distribution of genes encoding 68 cytoplasmic ribosomal protein families in rice. <i>Acta Physiol Plant.</i> 2005;27(4):439–46.	2-s2.0-28244443304	2.736
51	Agarwal SM. Evolutionary rate variation in eukaryotic lineage specific human intronless proteins. <i>Biochem Biophys Res Commun.</i> 2005;337(4):1192–7.	10.1016/j.bbrc.2005.09.172	3.58
52	Agarwal SM, Gupta J. Comparative analysis of human intronless proteins. <i>Biochem Biophys Res Commun.</i> 2005;331(2):512–9.	10.1016/j.bbrc.2005.03.209	3.58

Popular articles/op-ed/media-coverage: (latest first and provide title and link):

- Shashi Sharma and **Subhash Mohan Agarwal.** Environmental risk factors associated with emergence of breast cancer. *University News*, 48(24), 69-72, **2010**

- **Subhash Mohan Agarwal***. Polymerase Chain Reaction- A biological Xerox machine. *Invention Intelligence* 44(1), 8-14, **2009**
- **Subhash Mohan Agarwal***. Patenting human genes- the post genome sequencing issues. *Invention Intelligence* 43(1), 3-9, **2008**

Presentations/Talks/Lectures: (latest first, title of the presentation, organized by and date)

- **2022**. Talk on Drug Discovery. UGC-HRDC, Jamia Millia Islamia, New Delhi. 16th August.
- **2021**. Applications of Bioinformatics in Drug Discovery. Amity Institute of Biotechnology, Noida. 29th October
- **2021**. Role of QSAR and Machine Learning in Drug Discovery ATAL Faculty Development Program on “Computer Science and Biology: Impact of Bioinformatics and Molecular Biology on Drug Discovery” - 04th - 08th, October, 2021 (Online Mode) organized by Department of Biotechnology, IILM.
- **2019**. Advancing drug discovery from plant based natural products using computational approach. Interdisciplinary Science Conference on Big Data and Computational Biology, Jamia Millia Islamia, New Delhi. 21-22nd October.
- **2018**. Bioinformatics and its role in drug designing. Jaipur National University, Jaipur. 17th September.
- **2017**. Exploring anticancer therapeutics from natural products using in-silico methods. 36th Annual Conference of Indian Association of Cancer Research, Kerala. February 9 – 11.
- **2015** Biological databases and its application in Cancer. (Technical session: Big Data Biology and Cyberinfrastructure). Conference on Computational Biology: Back to the Future. Jawaharlal Nehru University, New Delhi, December 26 - 27.
- **2015** Prediction of protein structure: Homology modeling and fold recognition methods (Theory cum Practical). National workshop on “In silico approaches to drug designing”. Banaras Hindu University, Varanasi, March 23-28.
- **2014** Homology modeling and its applications (Theory cum Practical). Two day National workshop on “Pharmacoinformatics – Insilico tools for next generation biological and drug research”. JSS College of Pharmacy, Ooty. October 17-18.
- **2014** Transcriptional regulation of cervix cancer using microarray gene expression data and promoter sequence analysis of a curated gene set. 33rd Annual Convention of Indian Association of Cancer Research, Thiruvananthapuram, February 13-15.

- **2013** Identification of Inhibitors against EGFR secondary mutant from Natural product library, National Conference on Recent Trends in Protein Structural Biology, New Delhi, December 16-18.
- **2013** Bioinformatics and its Applications. Invited Lecture at *Department of Bioinformatics, DAV College, Sector 10, Chandigarh.*
- **2011** Sequence and Structural analysis enables prediction of functionally important residues responsible for regulating Epidermal Growth Factor Receptor Tyrosine Kinase activity. *International Interdisciplinary Science Conference, November 15-17, Jamia Millia Islamia, New Delhi.*
- **2011** Introduction to Bioinformatics. Workshop on *Application of Statistical Software's in Medical Research*, January 19-21, Institute of Cytology and Preventive Oncology, Noida.
- **2010** Evolutionary aspects of Human Genome deciphered using Sequence Conservation. Invited Lecture at Banasthali University, Rajasthan.

Brief Biosketch (not more than 100 words):

Dr. Agarwal has acted as an enabler for cancer drug discovery by introducing new computational resources and tools. He has been working towards creation of new knowledge like Databases, Webservers and Standalone software applications. The creation of these knowledge driven web-resources has enabled solving scientific questions in Cancer drug discovery. Dr Agarwal has received grants from various scientific agencies and several national as well as international awards for his work. Overall, Dr. Agarwal has implemented highly innovative and powerful computational tools in order to accelerate cancer drug discovery process.

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