

### Independent Publications:

20. A machine learning approach for prediction the reactivity power of hypervalent iodine compounds

**Saini, V.\*** Kataria, R., Rajput, S.,  
*Artif. Intell. Chem.* (2024)

[\[Link\]](#)

19. Extraction and characterization of ultrasound assisted extraction: improved functional quality of pectin from jackfruit (*Artocarpus heterophyllus* Lam.) peel waste.

Saurabh, V.; Vathsala, V.; Yadav, S. K.; Sharma, N.; Varghese, E.; **Saini, V.;**  
Singh, S. P.; Dutta, A.; Kaur, C.,  
*J. Food Meas. Charact.* (2023)

[\[Link\]](#)

18. A mechanistic investigation of metal-free allylic fluorination of styrenes for the synthesis of allyl fluoride derivatives using density functional theory.

Singh, H.; **Saini, V.\***  
*Struct. Chem.* (2023)

[\[Link\]](#)

17. Transition-Metal-Free and Selective Deconstructive Carbonyl Olefination of  $\alpha$ -Hydroxy Ketones: A Complementary Approach to Knoevenagel Reaction

Sandeep, S.; **Saini, V.**; Chayawan, C.; Chaudhary, G. R.; Venugopalan, P.;  
Kumar, A.  
*Synthesis* (2023)

[\[Link\]](#)

16. Predicting the ET(30) parameter of organic solvents via machine learning.

**Saini, V.\*** Singh, H.  
*Chem. Phys. Lett.* (2023)

[\[Link\]](#)

15. Development, Synthesis and *in silico* Investigations of Novel Acyclic Allyl Fluoride Derivatives

Chauhan, N., Singh, H., Singh, K. N., McKenna, J., **Saini, V. \***  
*Synthesis* (2022)

[\[Link\]](#)

14. A Machine Learning Approach for Predicting the Fluorination Strength of Electrophilic Fluorinating Reagents

**Saini, V. \***  
*Phys. Chem. Chem. Phys.* (2022)

[\[Link\]](#)

13. Machine Learning Prediction of Empirical Polarity Using SMILES Encoding of Organic Solvents

**Saini, V. \***  
Mol. Div. (2022)  
[\[Link\]](#)

12. A machine learning approach for predicting the empirical polarity of organic solvents

**Saini, V. \*** Kumar, R.  
New J. Chem. (2022)  
[\[Link\]](#)

11. Development, Synthesis, Computational and *in silico* investigations of Pd(II)-Catalyzed Aryl Fluorinated and Hydroxylated Sulfonamides

Singh, H.; **Saini, V. \***  
J. Mol. Struct.  
[\[Link\]](#)

10. Effective Optimization Approach for Predicting the Nucleophilicities of Organic Molecules: A Machine Learning Approach

**Saini, V. \*** Sharma, A.; Nivatia, D.  
Pb. Univ. Res. J (Sci.) (2022)  
[\[Link\]](#)

9. A machine learning approach for predicting the nucleophilicity of organic molecules.

**Saini, V. \*** Sharma, A.; Nivatia, D.  
Phys. Chem. Chem. Phys. (2022)  
[\[Link\]](#)

8. Synthesis of quinoline based molecular probes for detection of nitric oxide. Kaushik, D.; Kaur, M.; Mutreja, V.; Pathania, K.; Salunke, D. B.; Sahoo, S. C.;

**Saini, V. \*** Pawar, S. V.; Kansal, S. K.; Mehta, S. K.,  
Dyes and Pigments (2022)  
[\[Link\]](#)

7. Dehydroacetic acid derived Schiff base as selective and sensitive colorimetric chemosensor for the detection of Cu(II) ions in aqueous medium.

Vashisht D.; Sharma S.; Kumar R.; **Saini V. \***; Saini V.; Ibhadon A.; Sahoo S. C.;  
Sharma S.; Mehta S. K.; Kataria R.  
Microchem. J. (2020)  
[\[Link\]](#)

### **Ph.D. and Post-doc Publications**

6. The Development and Mechanistic Investigation of a Palladium-Catalyzed 1,3-Arylfluorination of Chromenes

**Saini, V. \***; Thornbury, R. T.; Fernandes, T. d. A.; Santiago, C. B.; Talbot, E. P. A.;  
Sigman, M. S.; McKenna, J. M.; Toste, F. D.  
Chem. Sci. (2017)

[\[Link\]](#)

5. Development and Analysis of a Pd(0)-Catalyzed Enantioselective 1,1-Diarylation of Acrylates Enabled by Chiral Anion Phase Transfer  
Yamamoto, E.; Hilton, M. J.; Orlandi, M.; **Saini, V.**; Toste, F. D.; Sigman, M. S.  
*J. Am. Chem. Soc.* (2016)

[\[Link\]](#)

4. Synthesis of Highly Functionalized Tri- and Tetrasubstituted Alkenes via Pd-Catalyzed 1,2-Hydrovinylation of Terminal 1,3-Dienes  
**Saini, V.**; O'Dair M.; Sigman, M. S.  
*J. Am. Chem. Soc.* (2015)

[\[Link\]](#)

3. Pd(0)-Catalyzed 1,1-Diarylation of Ethylene and Allylic Carbonates  
**Saini, V.**; Liao, L.; Wang, Q.; Jana, R.; Sigman, M. S.  
*Org. Lett.* (2013)

[\[Link\]](#)

2. Transition-Metal-Catalyzed Laboratory-Scale Carbon–Carbon Bond-Forming Reactions of Ethylene  
**Saini, V.**; Stokes, B. J.; Sigman, M. S.  
*Angew. Chem. Int. Ed* (2013)

[\[Link\]](#)

1. Palladium-Catalyzed 1,1-Difunctionalization of Ethylene  
**Saini, V.**; Sigman, M. S.  
*J. Am. Chem. Soc.* (2012)

[\[Link\]](#)