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Chemistry Space Exploration

Data and Coverage Considerations

S+ SimulationsPlus Webinar Series

IONIZATION PREDICTION SUMMIT

The 4-part webinar series will take place on consecutive Tuesdays.

- October 24th, 2023
- October 31st, 2023
- November 7th, 2023
- November 14th, 2023

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Data Contributions for:

- **Pharma substances**
- **Crop Science**

Are we saying: ?

- Pharma data contributes to model accuracy in pharma drug space
...good for our pharma/biotech clients!
- Crop Science data contributes to model accuracy in Agrochemicals space
...good for our Crop Science/AgChem clients!

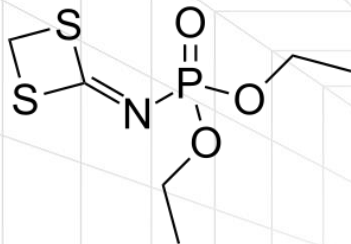


Statement

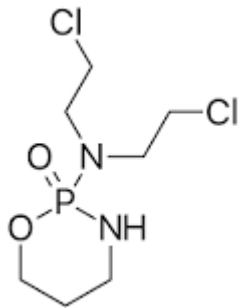
Pharma and Crop Science data altogether contribute to the more accurate modeling of pKa across chemistry space...

...The divide between Pharma and Crop Science may be more elusive than many people think.

Examples: Phosphoramids



Fosthietan: Insecticide




Cytoxan: Chemotherapeutic agent



Review

Opening up the Toolbox: Synthesis and Mechanisms of Phosphoramidates

Emeka J. Itumoh ^{1,2,3} , Shailja Data ^{1,3} and Erin M. Leitao ^{1,3,*}

- ¹ School of Chemical Sciences, The University of Auckland, 23 Symonds Street, Auckland 1010, New Zealand; eitu709@aucklanduni.ac.nz (E.J.I.); sdat751@aucklanduni.ac.nz (S.D.)
 - ² Department of Industrial Chemistry, Ebonyi State University, Abakaliki 480001, Ebonyi State, Nigeria
 - ³ The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington 6140, New Zealand
- * Correspondence: erin.leitao@auckland.ac.nz; Tel.: +64-9923-5567

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Examples

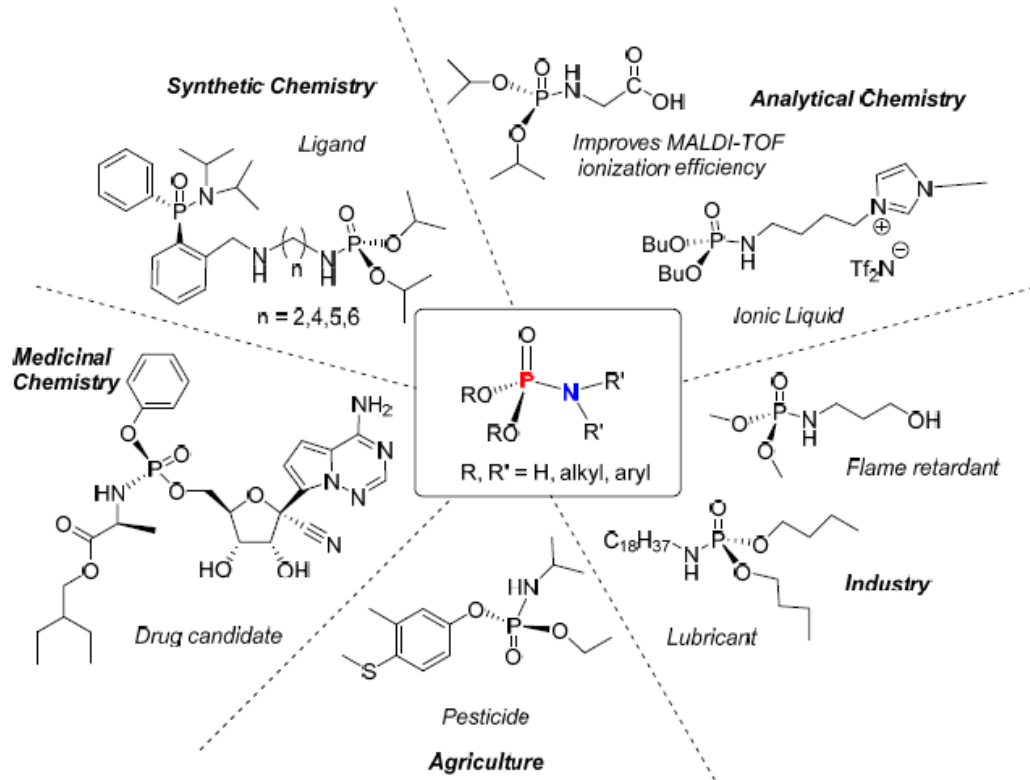
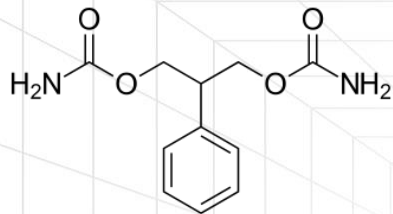
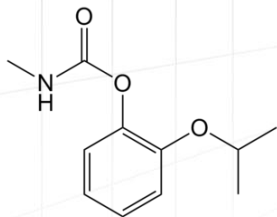


Figure 3. Applications of phosphoramidates.

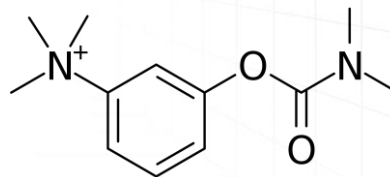
Examples: Carbamates



Felbamate: Anti-convulsant



Propoxur: Insecticide



Noestigmine: Neuro-degenerative

Journal of
**Medicinal
Chemistry**



Perspective

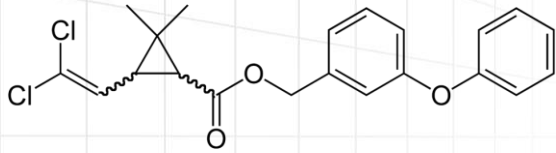
pubs.acs.org/jmc

Organic Carbamates in Drug Design and Medicinal Chemistry

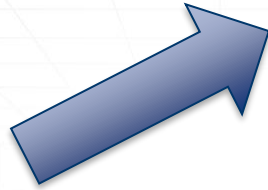
Arun K. Ghosh* and Margherita Brindisi

Department of Chemistry and Department of Medicinal Chemistry, Purdue University, West Lafayette, Indiana 47907, United States

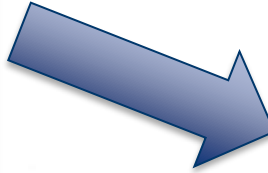
Examples: Pyrethroids



Permethrin



Medication: Applied to skin to treat scabies and lice



Insecticide: Sprayed to protect crops and livestock from parasites

Examples: PROTAC

January 19, 2023



Bayer launches new collaboration with Oerth Bio to further advance innovations in crop protection

Oerth's unique PROTAC[®] protein degradation technology is expected to be a new, game-changing generation of more sustainable crop protection products / The agreement recommits to the combination of Oerth Bio's specialized expertise designing PROTAC[®] degraders for agriculture with Bayer's global infrastructure testing, developing and commercializing leading crop protection technologies / Collaboration builds on the company launch in 2019 as a Leaps by Bayer joint-venture with Arvinas and has proven successful, meeting initial targeted milestones

Conclusion

Chemical space is a continuum.

Pharma, Crop Science and data from other industrial fields altogether can contribute to the more accurate modeling of pKa and potentially other properties.