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1P005: Predictive Automated Combustion Chemistry: from Molecule to Rate Coefficients using KinBot

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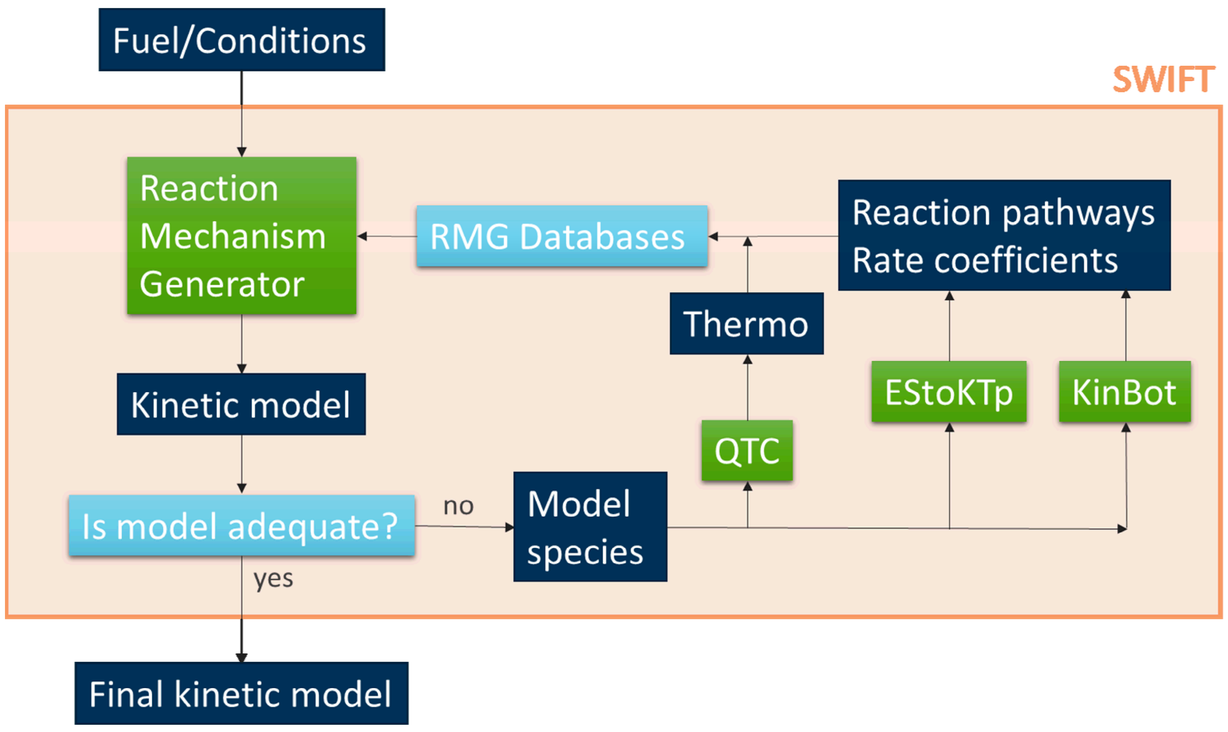
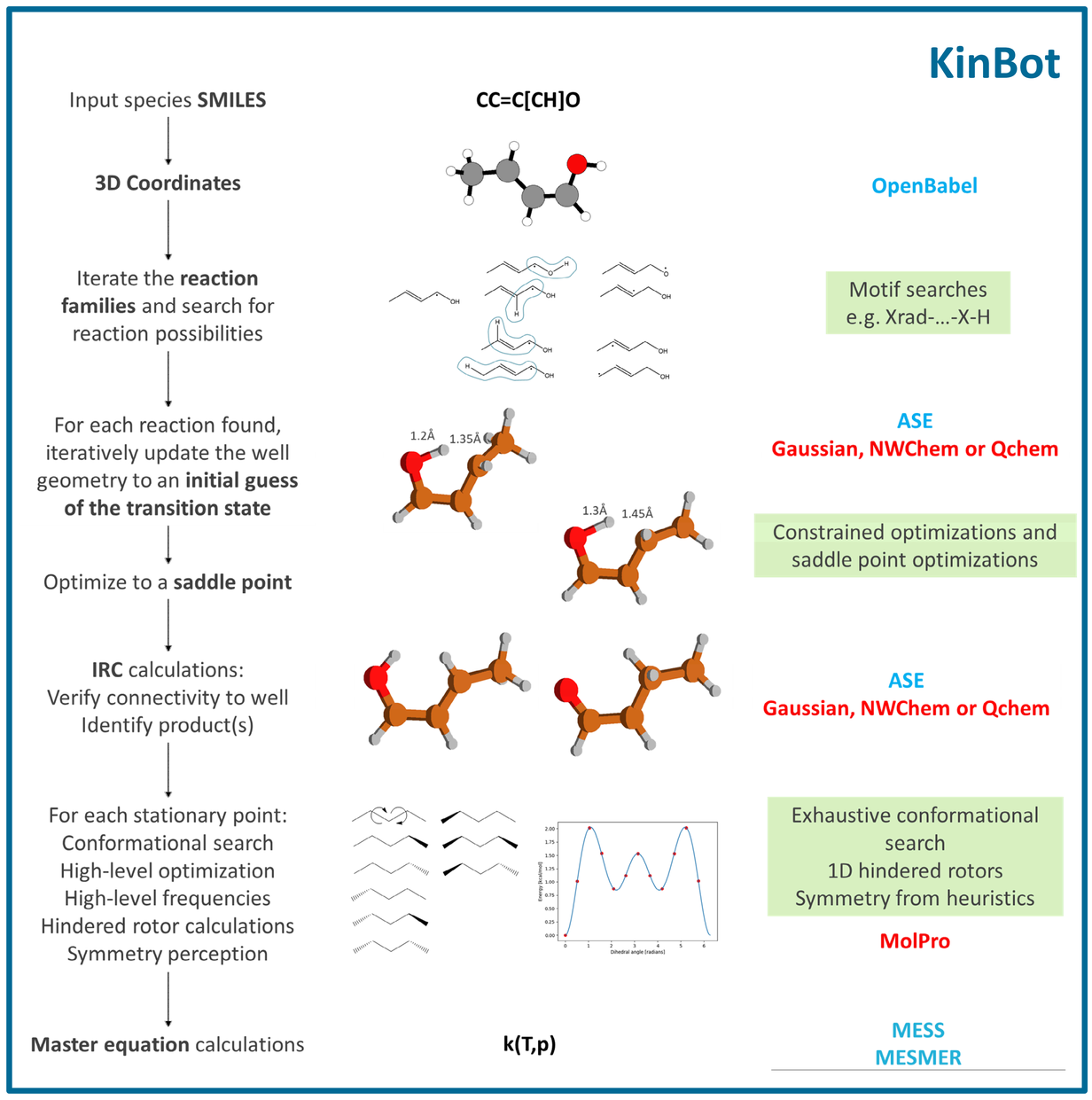
Introduction

- **Aim: automatically build predictive kinetic models from combustion**
- **Challenges: Discover unexpected reaction pathways and build accurate databases for key parameters**
- **Solution: Development of the KinBot code which automatically crawls on Potential Energy Surfaces to identify pathways and calculate rate coefficients**

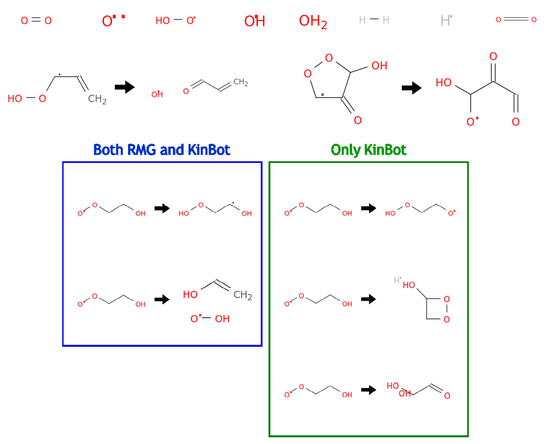


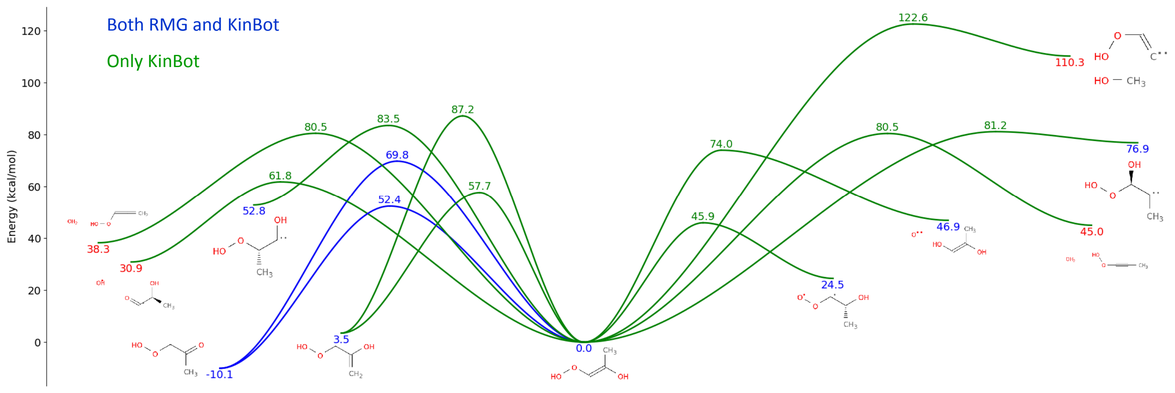


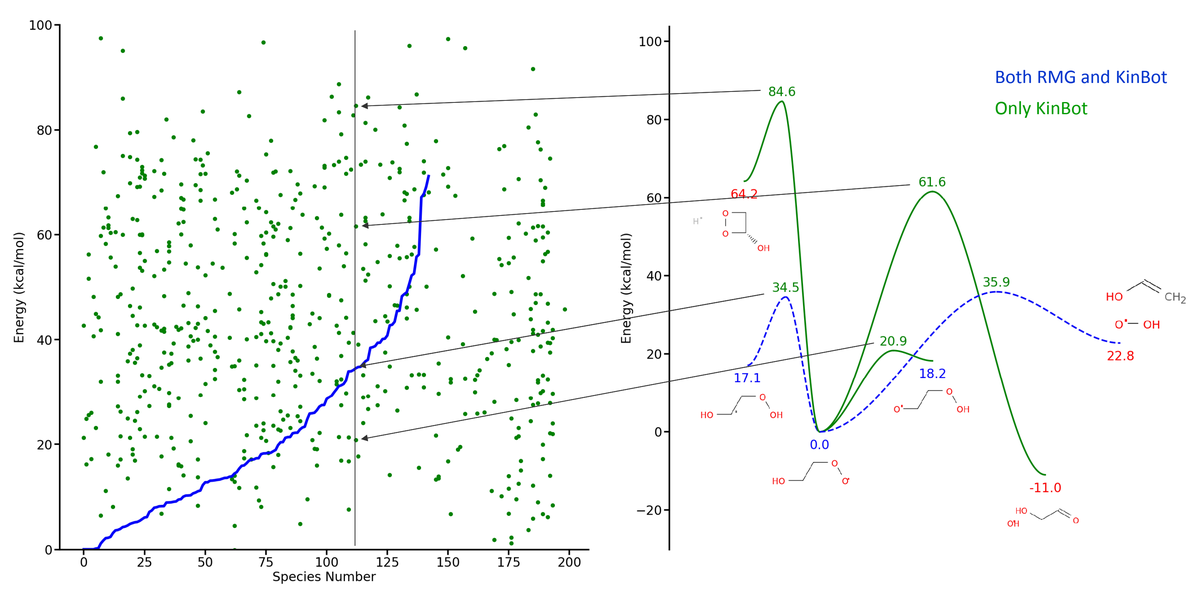
Results

Propane combustion model from RMG: 11589 reactions between 320 species
b3lyp/6-31G reaction searches in Gaussian
Note: no bimolecular reactions nor barrierless reactions considered

20	Species without any reaction
36	Species that do not exist
567	Reactions reported by RMG
1332	Reactions found by KinBot
330	Reactions in KinBot and RMG
1002	"New" reactions
237	Reactions missed by KinBot







Conclusions

KinBot explores full PES's for all species in a kinetic model in order to identify unexpected pathways and to calculate temperature and pressure dependent rate coefficients.

Note: KinBot will soon be open source

Acknowledgments

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