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Energy and Climate

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Co-optimization of Fuels and Engines:

Co-Optima Low Greenhouse Gas Fuels Team

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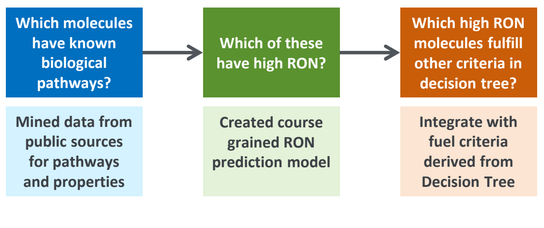
Overview

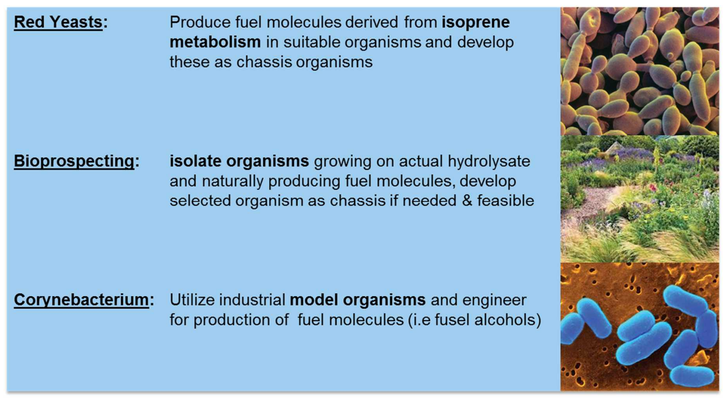
- 30 by 30: The primary objective of Co-Optima is a 30% reduction in per-vehicle petroleum consumption by 2030, beyond the "business as usual" case.
- This will be achieved through the co—optimization of both fuels and engines.
- Six teams and 10 national labs are partnering in this multi-year effort.
- Working with the engine development and other Co-Optima teams, the Sandia fuels team is using computational and biochemical methods to produce fuel molecules with optimal performance for engines optimized in this effort.

Methodologies

- Computational methods



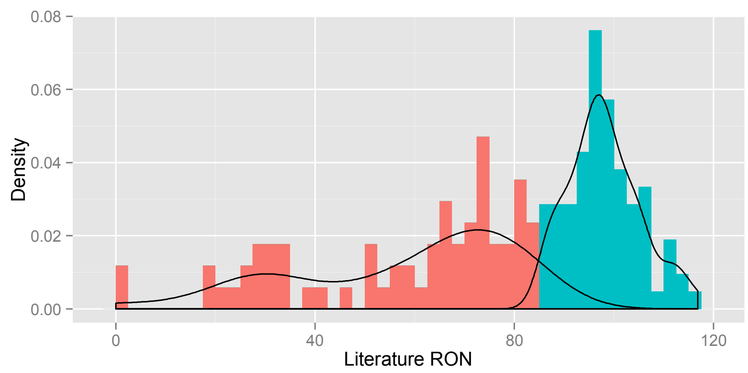
- Biochemical production



Discussion

- Thus far engine performance has been limited by the type of fuel available (i.e. petroleum). Biology allows for the production of molecules not heretofore considered as fuels. We asked the question: what fuel properties does an engine need for higher performance and efficiency?
- In Co-Optima criteria were developed for what makes a good fuel. We developed methods to screen for all known biochemical pathways to produce these fuels in chemical databases, including research octane number (RON), where available. These were used to develop a RON prediction model.
- Molecules which were predicted to have high RON were targeted for biological production, and routes to terpenes and mixed alcohols demonstrated.

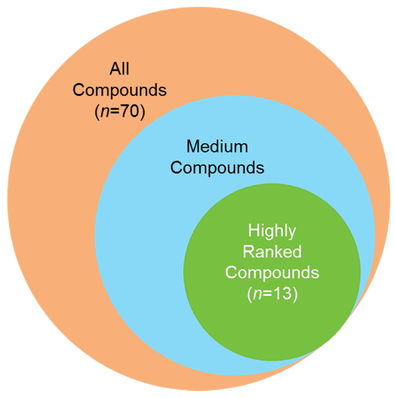
Computation Results



- Literature RON values were used with a machine learning technique to build a RON prediction model, enabling high throughput RON evaluation.
- This technique will be used to predict other largely unavailable fuel properties, such as flame speed.

Features	Weight	Type
OH Rate Constant	0.0382	Physical
Surface Tension	0.0368	Physical
SMARTS Pattern: C-C-C-C-C-C	0.0349	Structural
KOC (pH 5.5)	0.0323	Physical
Vapor Pressure (mmHg at 25°C)	0.0313	Physical
SMARTS Pattern: C-C-C-C-C	0.0313	Structural
Octanol-Water Partition Coefficient (pH 7.4)	0.0302	Physical

Metric	Mean value	Std. dev
Accuracy	0.80	0.09
Precision	0.82	0.12
Sensitivity	0.80	0.16
Receiver Operator Characteristic (AUC)	0.88	0.07

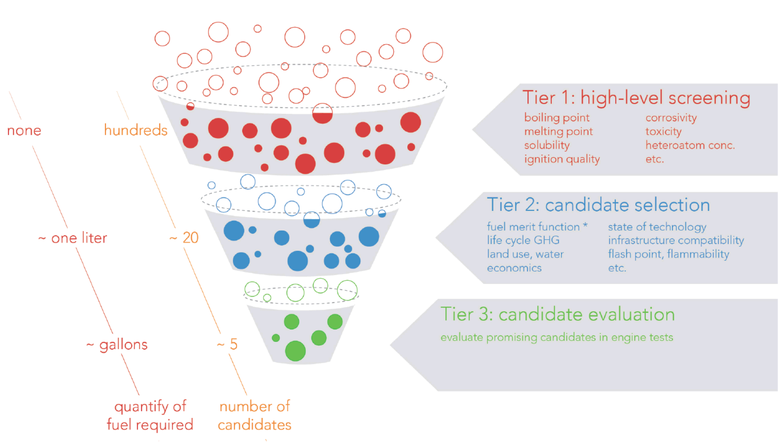


Compounds predicted to have RON > 85 in order of probability in class

1. Isooctane
2. Methylcyclopentane
3. Ethanol
4. Methyl butyrate
5. Ethyl isobutyrate
6. Methyl 2-methylbutyrate
7. 2-methyl 2 butanol
8. Isoprenol
9. Isobutanol
10. 3 methyl 1 butanol
11. Butyl acetate
12. Toluene
13. Isoamyl acetate

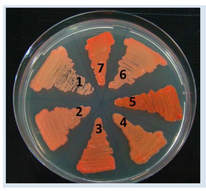
- >2000 QSAR and structural features were correlated to RON. It was possible to describe which features most heavily contributed to RON. This will enable more detailed investigation into RON chemistry and allow improved fuel selection.
- The model enables down-selection from 1000s of molecules to a number that can feasibly be investigated experimentally.

Screening and production



Red Yeasts

- Organisms producing **carotenoids** have good metabolic flow through **isoprene biosynthesis** pathways.
- A variety of fuel molecule candidates can be derived from isoprene biosynthesis pathways
- Strain engineering efforts are focused on two yeasts:

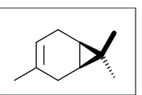
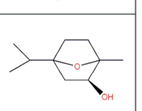
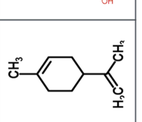
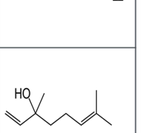


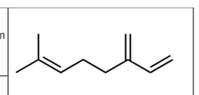
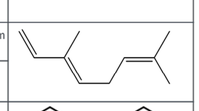
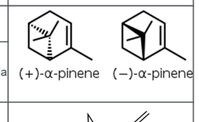
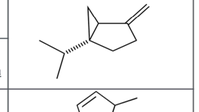
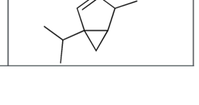
Xanthophyllomyces dendrorhous (Agaricomycotina)

- Oleaginous yeast, demonstrated to utilize xylose for growth
- Used in commercial carotenoid production
- Major Carotenoids (in this sequence): **Astaxanthin, HO-ketotorulene, Cantaxanthin**
- 20 MB genome, **published and very well annotated**
- **Lots of molecular tools for strain engineering published**, including many case studies increasing flux into carotenoid pathway

Rhodosporidium toluroides (Pucciniomycotina)

- Oleaginous yeast, demonstrated to utilize xylose for growth
- Used in commercial carotenoid production
- Major Carotenoids (in this sequence): **Torularhodin, Torulene, Beta carotene**
- 20 MB genome published
- Transformation methods established but only few methods available

Carene	PaJF67	Picea abies	
	TpsB	Salvia stenophylla	
Cineole	hyp3	Hypoxylon sp. E74060B	
	SSCG_00536	Streptomyces clavuligerus	
Limonene	ag10	Abies grandis	
Linalol	PaTPS-Lin	Picea Abies	

Myrcene	ama1e20	Antirrhinum majus	
	amaOC15		
	ag2.2	Abies grandis	
Ocimene	ama0a23	Antirrhinum majus	
	LcTPS1	Licea cubeba	
Pinene	ag3.18	Abies grandis	 (+)-α-pinene (−)-α-pinene
	pt30	Pinus taeda	
Sabinene	RlemTPS2	Citrus jambhiri	
	SabS1	Salvia pomifera	
Thujene	LcTPS2	Licea cubeba	

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