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Circular High-performance Aza-Michael Polymers as Innovative materials Originating from Nature

CHAMPION
circular bio-based polymers

WP6. High-performance Application Testing and Computational Prioritisation

CHAMPION 2021-2024

Thomas Farmer, WP6 Leader

BBI JU

Horizon 2020
European Union Funding
for Research & Innovation

Bio-based Industries Consortium

This project has received funding from the Bio Based Industries Joint Undertaking (JU) under grant agreement No 887398. The JU receives support from the European Union's Horizon 2020 research and innovation programme and the Bio Based Industries Consortium.

WP6 - High-performance Application Testing and Computational Prioritisation

Performed over 7 tasks:

- T6.1 – Computational Prioritisation (UoY) – interim and final — **finished (D6.2)**
- T6.2 – Testing Scheme (UoY) — **finished (MS4)**
- T6.3 – *Preliminary Property Screen* – all candidates (UoY, WUR) — **finished (D6.3)**
- T6.4 – Home Care High-performance Testing (UNI) — ongoing
- T6.5 – Table and Floor Coating High-performance Testing (ORI) — ongoing
- T6.6 – Structural Adhesives High-performance Testing (SBC) — ongoing
- T6.7 – Automotive Interior Surfaces High-performance Testing (STA) — ongoing

End-user led

ORINEO original renewables

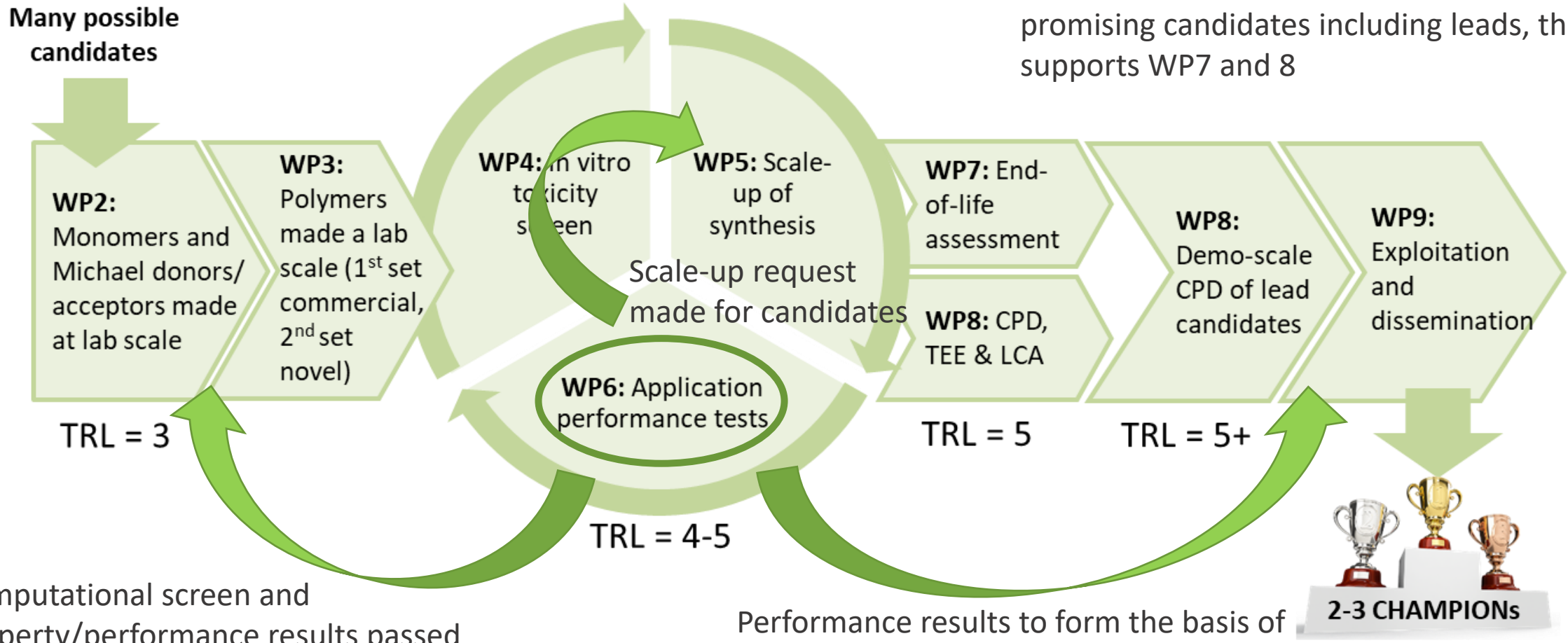
SCOTT BADER

Stahl

Unilever

Link with other WPs

Results from **WP6** aid selection of promising candidates including leads, thus supports WP7 and 8



Computational screen and property/performance results passed back to WP2/3 for iterative design

Performance results to form the basis of decisions on which candidates to patent

Project Defined Wantss of End-users Differ:

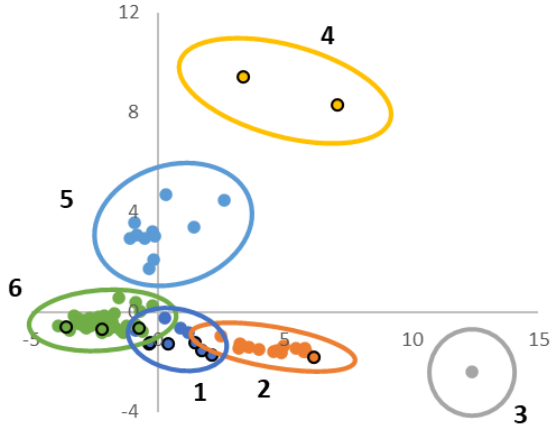
	ORI	SBC	STA	UNI
Application	Rigid coating	Structural adhesive	Flexible coating	Home care additive
Safety	Non-hazardous during cure	Non-hazardous during cure	Non-hazardous during cure	No release of hazardous chemicals in formulation & use
Processing	Needs reactive diluent	Needs reactive diluent	Needs reactive diluent	Water/formulation soluble
Stability	Stable over many years	Stable over many years	Stable over many years	Stable in formulation and use
End-of-life	Recycling	Recycling	Recycling	Biodegradation

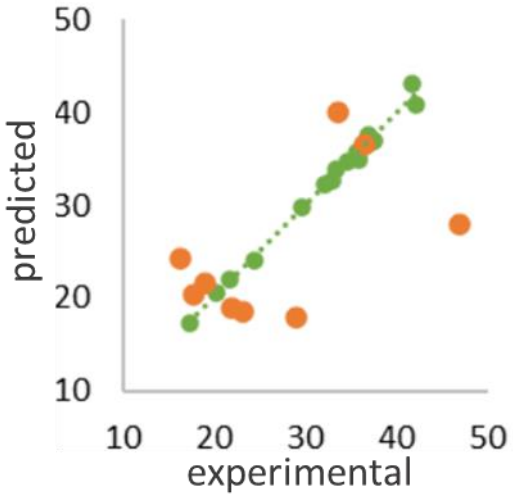
Computational Prioritisation and Preliminary Property Screen by University Partners

Task T6.1 Computational Prioritisation Prior to Synthesis + Attempt to use Principal Component Analysis with experimental data to aid future modelling

- Phase 1: CHAMPION candidates, 12 incumbent compounds, and an additional 25 amine reactants (Michael donors) modelled and electronic properties calculated
- Candidates ranked by similarity to each of the 12 targets (right)
- Phase 2: Experimental data from WP6 was combined with electronic properties in an attempt to produce a predictive model, however the accuracy was low because of the many variables in the experimental approach (see right).
- Deliverable **D6.2** submitted M27 (on time) to conclude T6.1

Phase 1: First 2 principal components of the QSAR variables, grouped into 6 clusters of similar compounds. Target (incumbent) compounds are circled in black. Other datapoints are CHAMPION compounds.

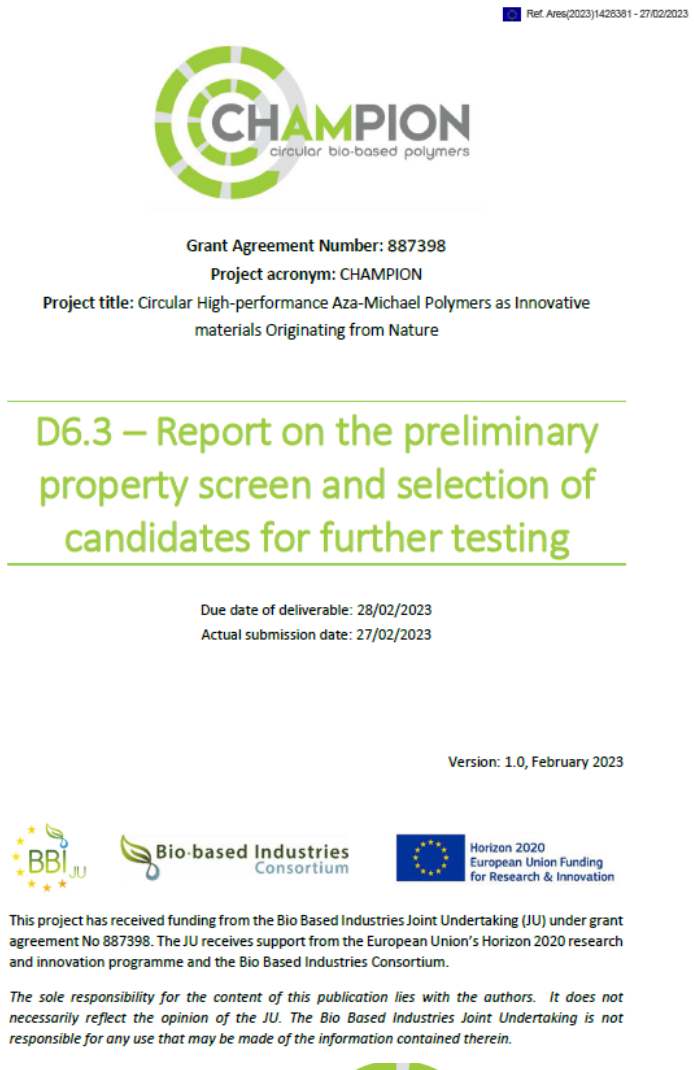




Phase 2 example: Application performance (experimental vs. prediction) of candidate materials - training set in green, validation set in orange

Task T6.3 *Preliminary property screen* of candidates. Months 4-33

- Testing scheme was established early (T6.2, MS4)
  - This was modified to increase the significance of Shore A/D and water/formulation solubility tests
- Report on the *preliminary property screen* of both Sets successfully submitted February 2023 (D6.3)
- **180 candidates screened** (99 for coatings/adhesives, 81 for water soluble polymers) + 15 pre-polymers
  - +further 19 tested as multiple batches
  - DoA set a target of 50-100
- **69 selected** for *initial performance tests*
  - 11 for coatings and adhesives as “inspiration” for end users
  - 58 for home care
  - DoA set a target of 10-40 (for testing, not selection)



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CHAMPION circular bio-based polymers

Grant Agreement Number: 887398
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D6.3 – Report on the preliminary property screen and selection of candidates for further testing

Due date of deliverable: 28/02/2023
Actual submission date: 27/02/2023

Version: 1.0, February 2023

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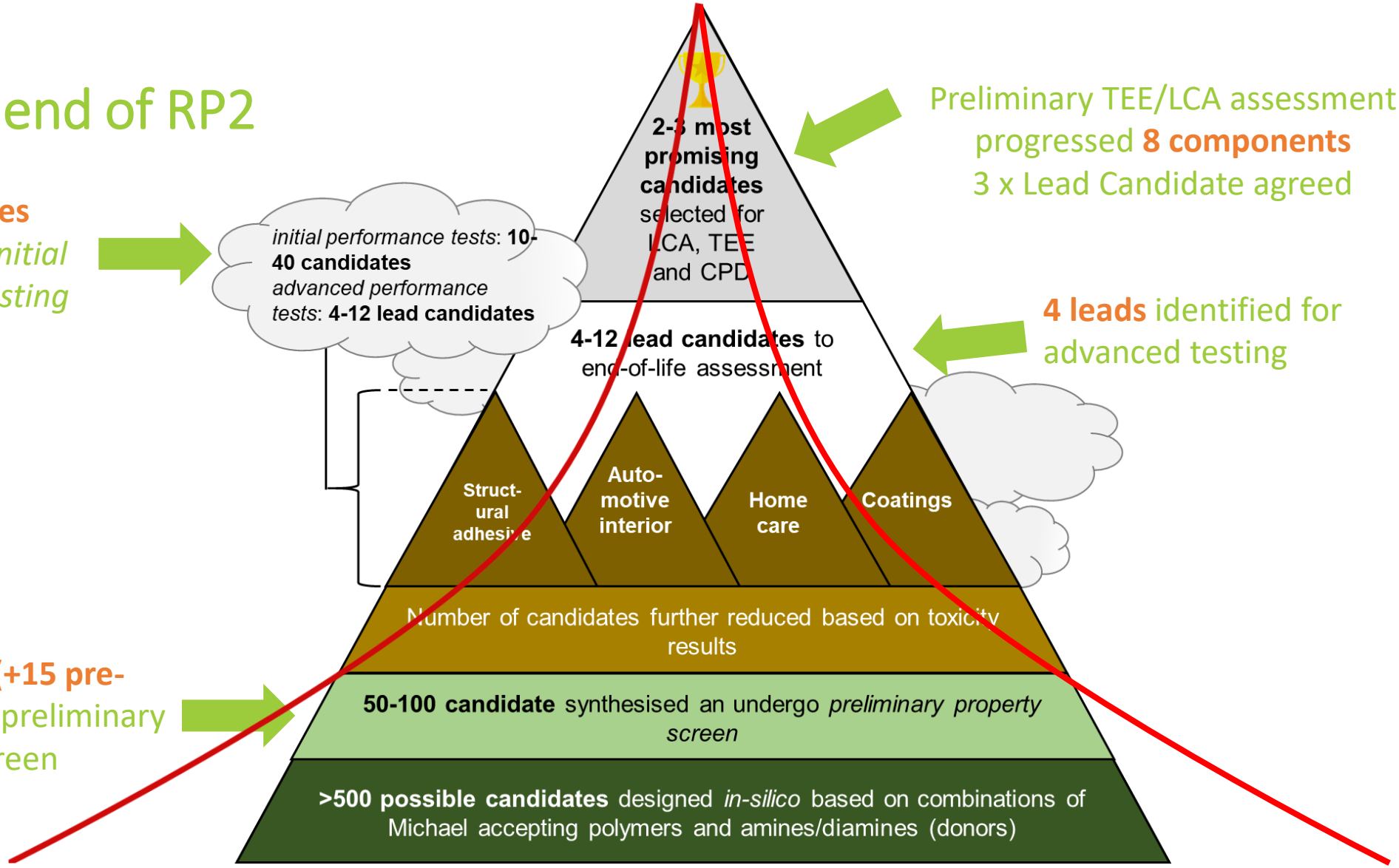
CHAMPION circular bio-based polymers

Achieved by end of RP2

69 candidates progressed to *initial performance testing*

180 candidates (+15 pre-polymers) through preliminary property screen



Preliminary TEE/LCA assessment progressed **8 components**
3 x Lead Candidate agreed

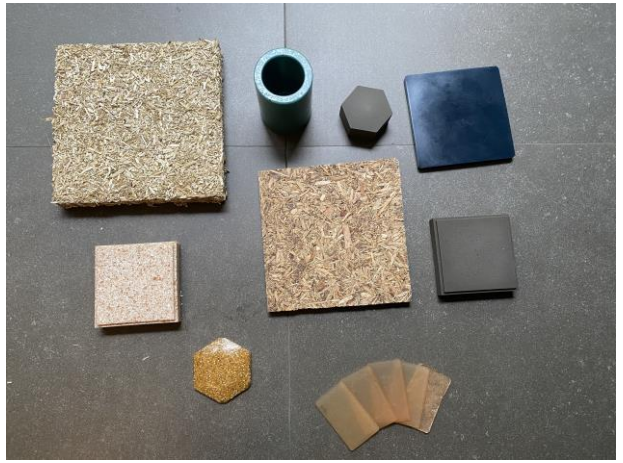
4 leads identified for advanced testing

Initial and *Advanced Performance Testing* by Industry Partners:

Hard Surfaces – Philippe Willems - Orineo

Task T6.5 Performance application testing of surface coatings.

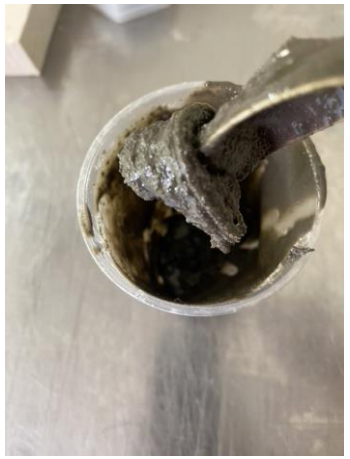
- Aza-Michael Polyester and diamine, suitable for coating and binder applications selected
- Reactive diluent used for improving processability
- Lead candidate (P46N3) evaluated in different applications (prototypes available)
  - Decorative tiles
  - Casted 3-D objects
  - Wood panels
  - Insulation panels
  - Decorative finishing sheet

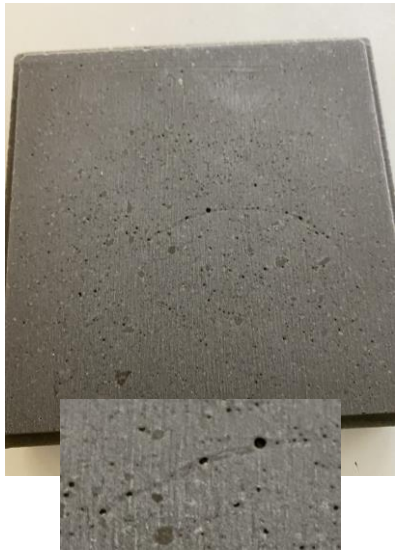


Task T6.5 Performance application testing of surface coatings

Points of improvements

- Open time: should be extended to +/-45'
- Viscosity pretty high: air bubble inclusions
- Mixing with natural fibres
- T_g is quite low





WP6 - High-performance Application Testing and Computational Prioritisation: Final Conclusions

- Computational prioritisation used to reduce targets from many hundreds down to a more achievable set of around 50 initial targets – based on similarity to incumbents
  - Challenging to align experimental performance with computational predictions
- Tiered approach to testing successful in managing project resource
  - However, our “mountain” lost candidates more rapidly than anticipated as testing became more advanced
- Feedback loop between WP6 (testing), WP7 (EOL) and WP3 (polymer design) led to enhancements in performance of several candidates
- For some end-user performance of the best CHAMPION candidates still remained below that of the incumbents – but significant achievements made in 4 years!
- Reactive diluents for some applications were necessary
  - Mid project one promising RD had to be dropped due to a shift in it’s regulatory clearance

Early testing by Industry Partners is essential for success!

Contact

- Thomas Farmer (UoY/UNI)
- James Sherwood (UoY)
- Dan Day (UoY)
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