www.avmatsim.eu

/*
We are a self-funded
family business

We are people-focused
and care about Ethics
and Environment
*/

GRACE

/*
Avant-garde
Materials
Simulation
*/

/*
We have made
Crystal
Structures
Predictable
*/

/*
We push frontiers
to deliver
In Silico Material Design

We bring genuine value
to our customers
by placing facts over fictions
*/

I am polymorphic

OUR TRACK RECORD

In > 50 CSP studies, we have proven that the stable form is missing in 15-45% of the cases

Faraday Discussions
doi.org/10.1039/C8FD00069G

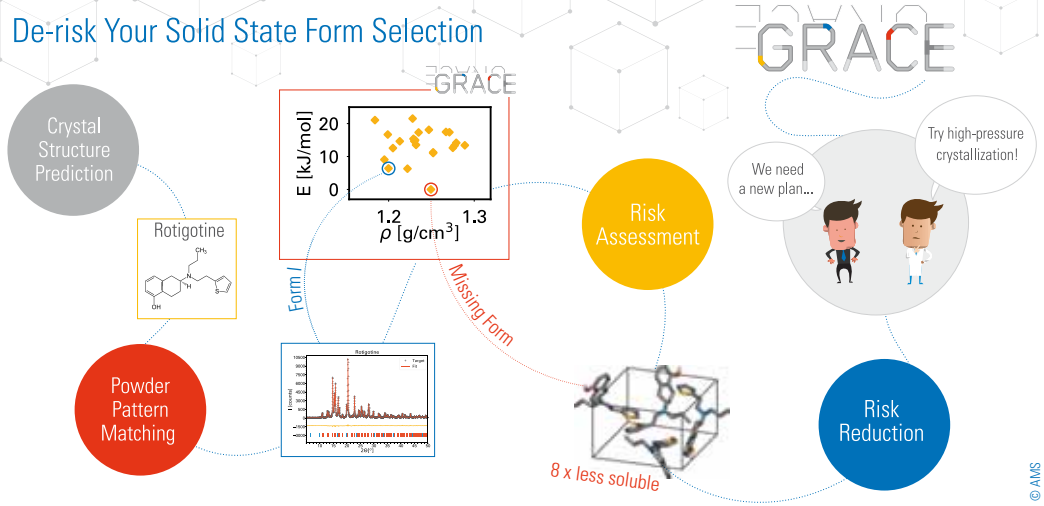
Our calculations are accurate enough to identify missing forms beyond doubt

Nature Comm. Chemistry
doi.org/10.1038/s42004-019-0171-y

We suggest crystallization experiments off the beaten track to crystallize new forms

Nature Comm.
doi.org/10.1038/ncomms8793

De-risk Your Solid State Form Selection



CONTACT US IF YOU...

Fear the appearance of a late-appearing crystal form

Want to crystallize a novel form with improved properties

Need to solve the structure of a poorly crystallizing compound

Cannot crystallize your compound at all

Have to compare the relative stability of two experimental forms

Require novel algorithms to accelerate your research

Get your quote!
GRACE
The most successful software package in the last three blind tests on organic Crystal Structures Prediction

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