

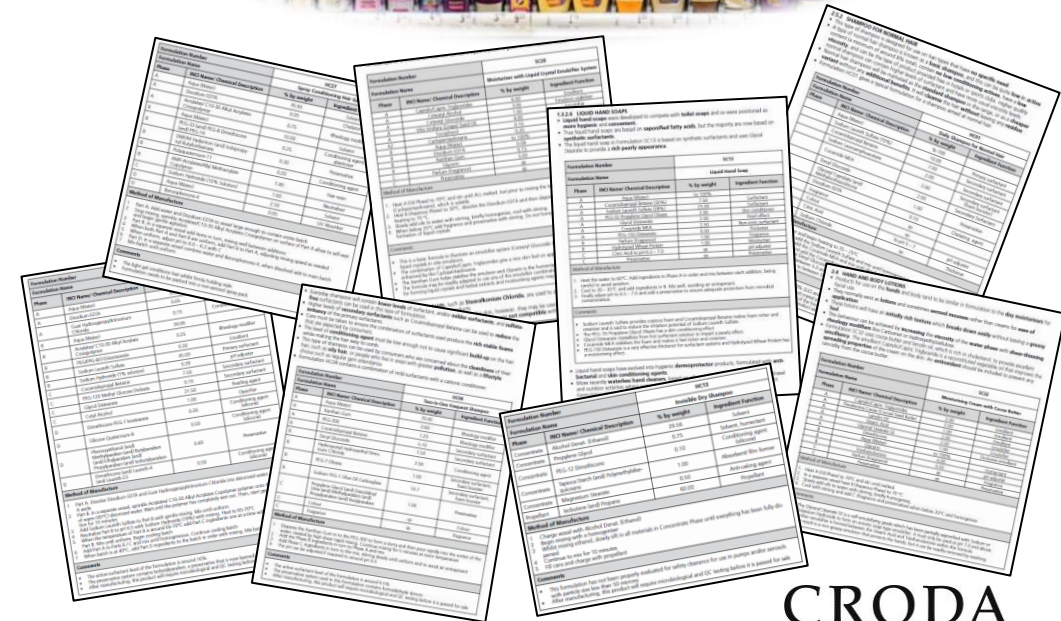
Advancing Formulation Science in Personal Care

Katy Helm



Formulating Cosmetics Is Easy...

- Over the years lots of research has been done to optimise the manufacture of cosmetic formulations
- Guidelines were developed and patented where if you use X% of ingredient A + X% of ingredient B... then you have a perfect formulation chassis
- Brands use these guidelines and the same basic formulations across a large range of products
- But what if you need to make a formulation with a new ingredient or claim!?



Formulating Cosmetics Is Very Difficult!

- The number of ingredients available to a formulator has significantly increased since these guidelines were developed
- Regulations and certifications are continuously updating
- The expectations from customers has significantly increased, from the type and amount of product claims to the sustainability of the product and ingredients
- So how do we develop new formulations to meet all of the customer demands?

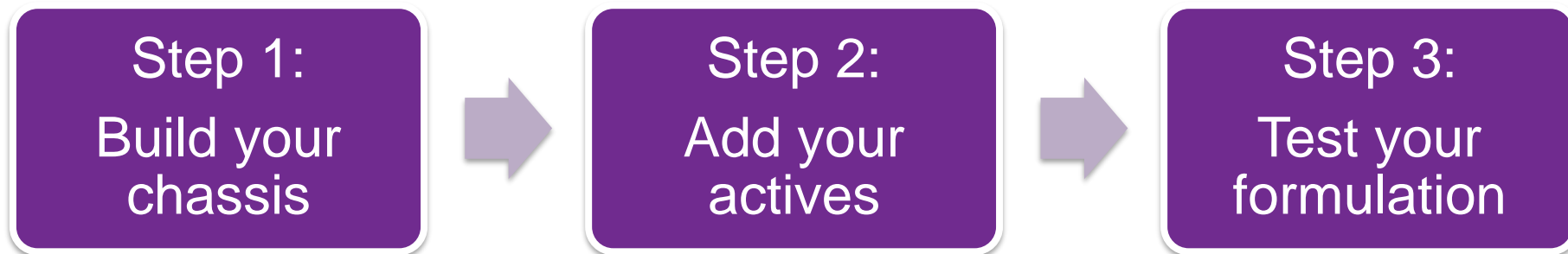


Example Formulation Brief

You've been asked to make a luxury moisturiser for Amazing Cosmetics with the following formulation requirements:

- 100% Natural
- Silicone-free
- Anti-Ageing benefits
- Luxury, silky sensory

Lets start formulating!



Step 1: Build Your Chassis

Ingredients?

Emulsifiers:

Arlacel LC
Cithrol PGTL
NatraGem EW
Super Sterol Ester
Syncrowax OSW
Cithrol PG32IS
ECO Brij S20
ECO Brij S721
Span 60
Crodafos CES
Cosmowax D
Crodex M
ECO Tween 20
Span 20
Cithrol GMS 40

Oils:

Crodamol SSA
Crodamol ISIS
Cithrol GMM
Crodamol GTIS
Crodamol SS
Crodamol GTCC
Crodamol PTC
Supermol B
Cropure Almond

Concentrations?

Emulsifier 1:

1%
2%
3%
4%
5%

Oil 1:

5%
10%
15%
20%
25%

Emulsifier 2:

1%
2%
3%
4%
5%

Oil 2:

5%
10%
15%
20%
25%

Emulsifier 3:

1%
2%
3%
4%
5%

Oil 3:

5%
10%
15%
20%
25%

Process Conditions?

Temperature:

25°C
50°C
60°C
70°C
80°C

Stirring Speed:

500rpm
600rpm
800rpm
1000rpm
1200rpm

Order of Addition:

One pot mixture
2 Part Mixture
3 Part mixture
4 Part Mixture

Stirring time:

1 minute
5 minutes
10 minutes
15 minutes
30 minutes

Homogenisation:

None
6000rpm
8000rpm
10000rpm

Stirrer Type:

Paddle
Propeller
Dissolver
Anchor
Blade

Step 1: Build Your Chassis

Ingredients?

Emulsifiers:

Arlacel-LG
Cithrol-PGTL
NatraGem EW
Super-Sterol Ester
Syncrowax-OSW
Cithrol-PG32IS
ECO-Brij-S20
ECO-Brij-S721
Span-60
Crodafos-CES
Cosmowax-D
Crodex-M
ECO-Tween-20
Span 20
Cithrol-GMS-40

Oils:

Crodamol-SSA
Crodamol-ISIS
Cithrol-GMM
Crodamol-GTIS
Crodamol-SS
Crodamol-GTCC
Crodamol-PTC
Supermol B
Cropure-Almond

Concentrations?

Emulsifier 1:

1%
2%
3%
4%
5%

Oil 1:

5%
10%
15%
20%
25%

Emulsifier 2:

1%
2%
3%
4%
5%

Oil 2:

5%
10%
15%
20%
25%

Emulsifier 3:

1%
2%
3%
4%
5%

Oil 3:

5%
10%
15%
20%
25%

Process Conditions?

Temperature:

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1-minute
5 minutes
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Homogenisation:

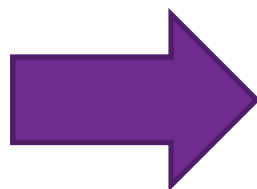
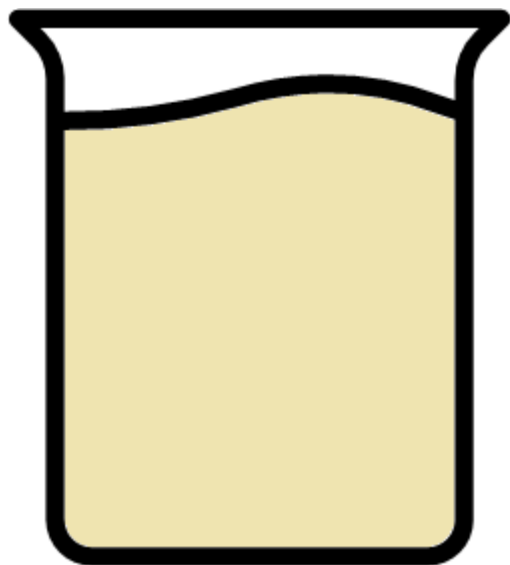
None
6000rpm
8000rpm
10000rpm

Stirrer Type:

Paddle
Propeller
Dissolver
Anchor
Blade

Decisions based on experience, marketing literature, example formulations and intuition

Step 2: Add Your Actives



Active Ingredients?

Actives:
Zanthocare
Avocadin HU25
Phytessence
Speedwell
Collasurge
Optimhyal
Essenskin
Prolevis
Sterocare PH
Siegesbeckia PH
Subliskin
Phytofleur French
Rose EC
Fruitliquid Goji EC

Concentration?

Active 1:

1%
2%
3%
4%
5%

Active 2:

1%
2%
3%
4%
5%

Process Conditions?

Temperature:

25°C
50°C
60°C
70°C
80°C

Stirring Speed:

500rpm
600rpm
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1200rpm

Stirrer Type:

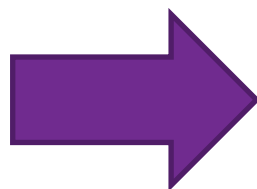
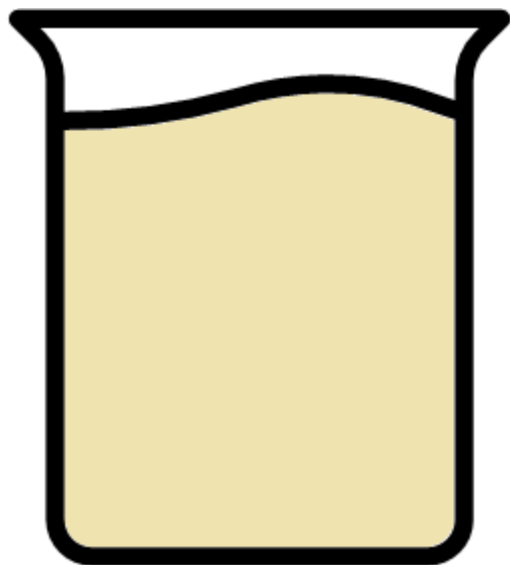
Paddle
Propeller
Dissolver
Anchor
Blade

Stirring time:

1 minute
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You make 10 formulations through trial and error until you get a stable formulation with good sensory and appearance

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Sterocare-PH
Siegesbeckia-PH
Subliskin
Phytofleur-French
Rose-EG
Fruitliquid-Goji-EC

Concentration?

Active 1:

1%
2%
3%
4%
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Active 2:

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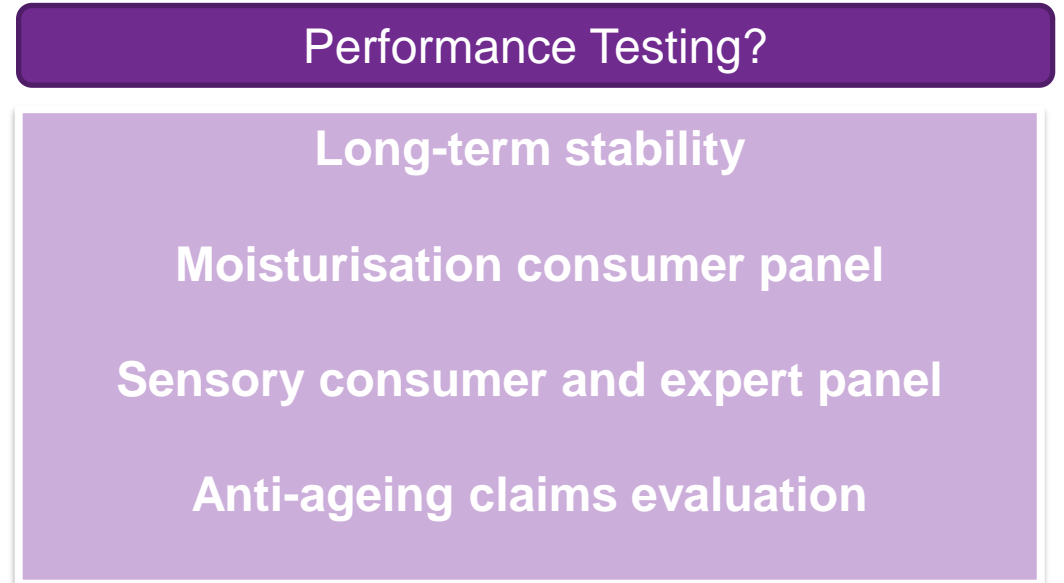
Stirring time:

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5 minutes
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You make 10 formulations through trial and error until you get a stable formulation with good sensory and appearance

Decisions based on experience, marketing literature, example formulations and intuition

Step 3: Test Your Formulation



You make 5 more formulations through trial and error until you get a formulation that hits the brief!

Step 3: Test Your Formulation



Performance Testing?

- Long-term stability ✓
- Moisturisation consumer panel ✓
- Sensory consumer and expert panel ✓
- Anti-ageing claims evaluation ✓

You make 5 more formulations through trial and error until you get a formulation that hits the brief!



Step 3: Test Your Formulation

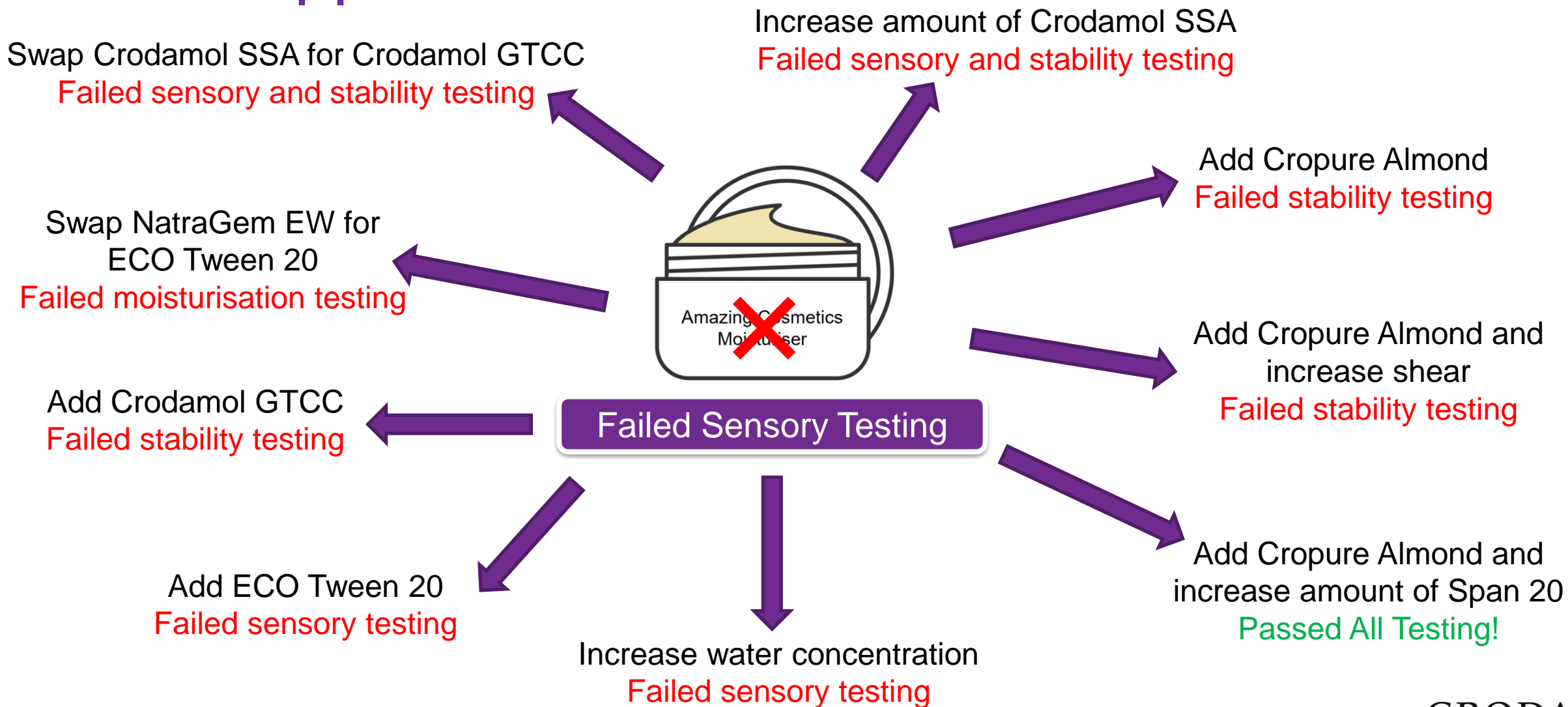


Performance Testing?

- Long-term stability ❌
- Moisturisation consumer panel ❌
- Sensory consumer and expert panel ❌
- Anti-ageing claims evaluation ❌

But what would you do if it failed?

What Happens When It Fails?



Formulation Science

Throughout the development process there was one goal: to create a formulation to meet the brief

What did the scientist learn and what did future scientists learn from this formulation development approach?

Formulating using trial and error, instinct, preferences and experience can result in opportunities being missed:

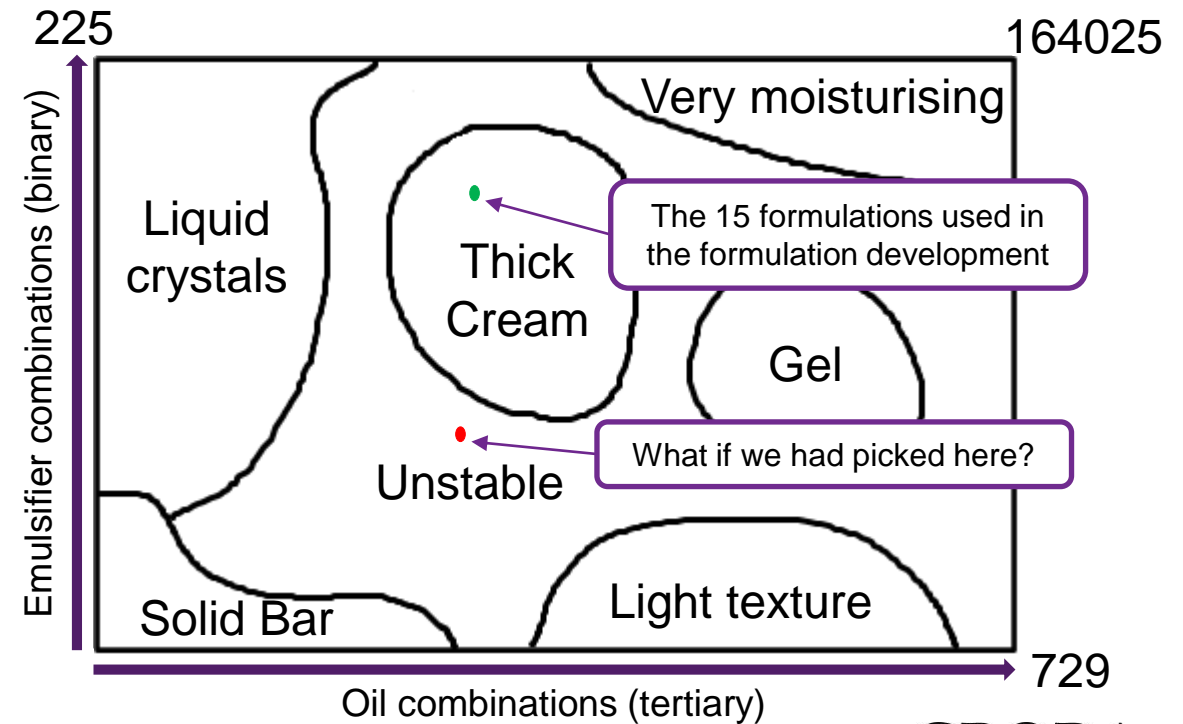
- What if other ingredients would've been better?
- What if adding more oil would've given a better sensory?
- What if stirring faster would've changed the microstructure to deliver the active better?

Because only a small number of formulations were made we cannot answer these questions

Formulation Science

- If we take all the ingredients and all the possible combinations and concentrations and all the different process conditions the formulator would've needed to make 100000's formulations
- In reality, the scientist only used a fraction of this number and missed large areas of formulation space that would give much better results

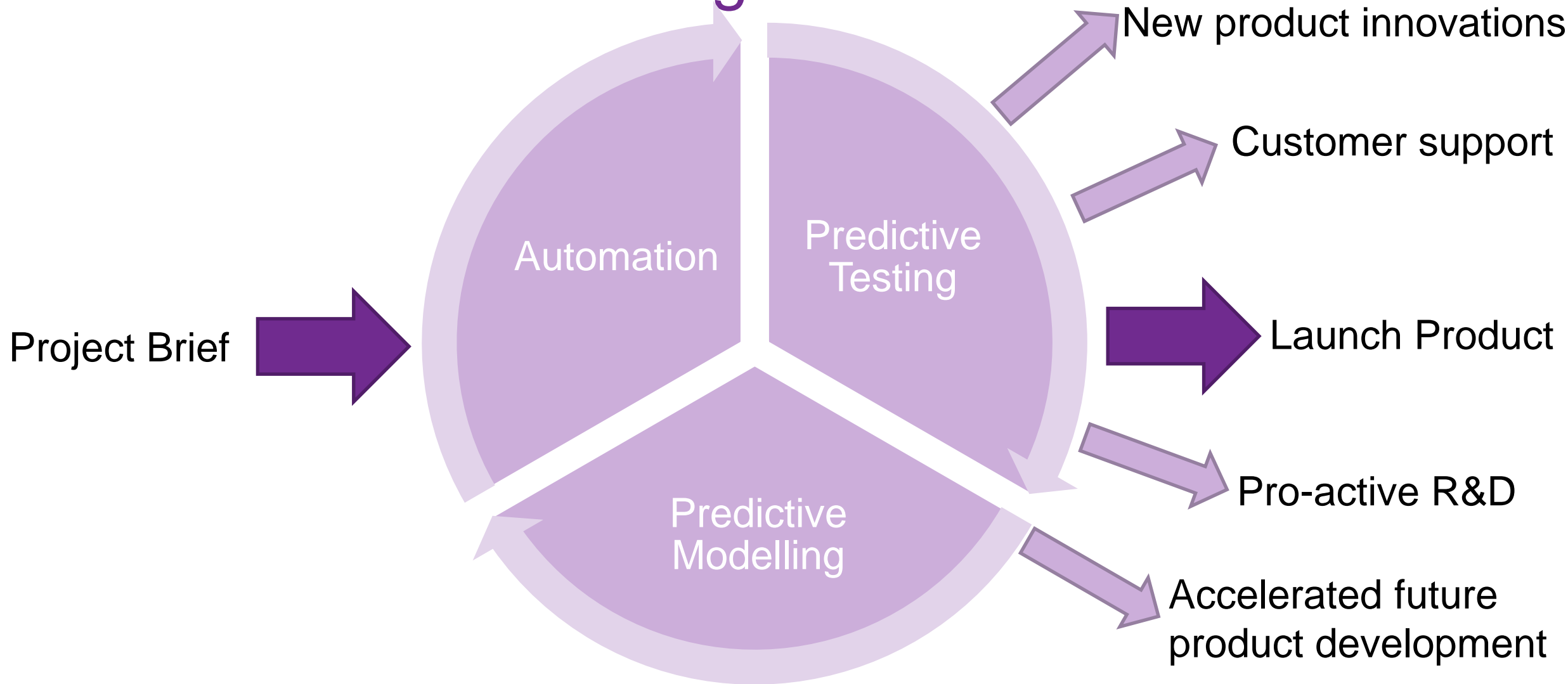
It's not realistic to expect formulators to make every possible formulation but we can approach formulation science in a better way to make better decisions and gain understanding

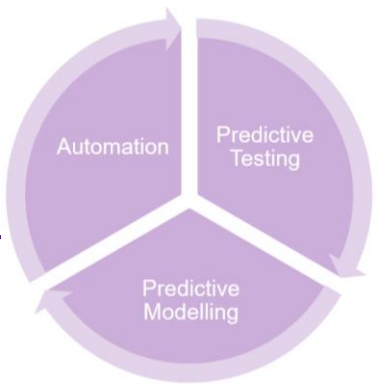


Advanced Product Design



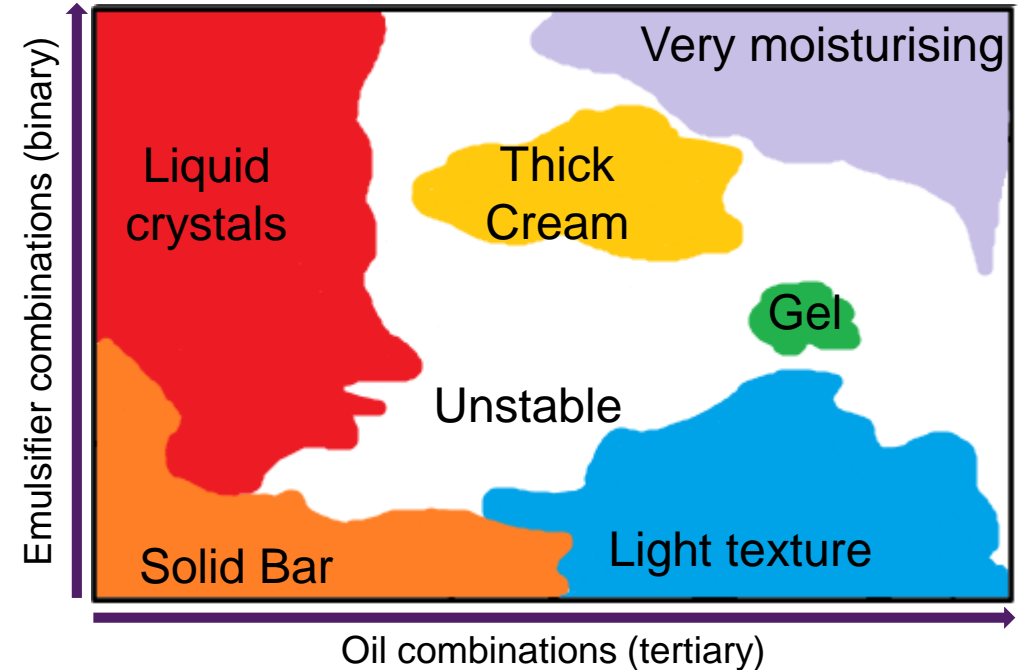
Advanced Product Design





Predictive Modelling

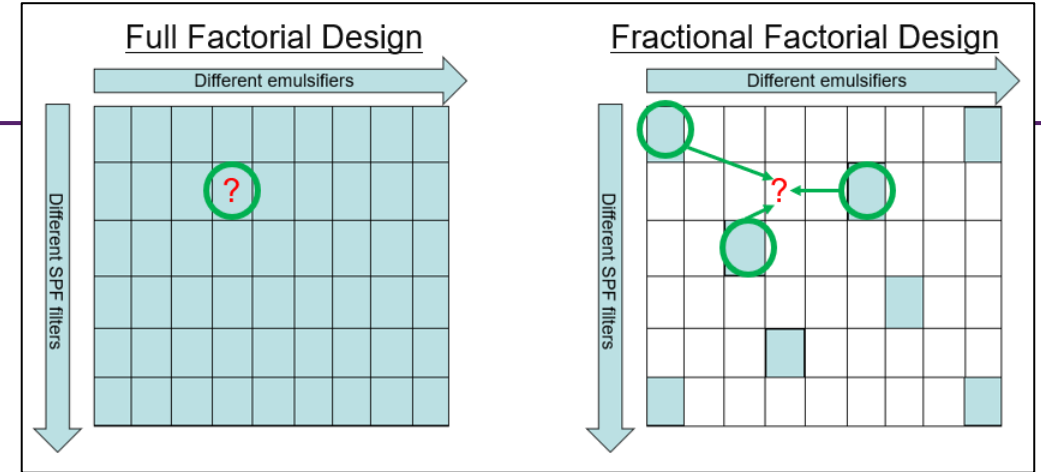
- Predictive modelling can be used to quickly gather an overview of a large area of formulation space, using trends and data analytics to predict behaviours
- This can be used as a quick screen to narrow down the formulation space so that more in-depth research is done in the right areas



We use DoE predictive modelling to understand a 'blurred' version of the formulation map quickly

Design of Experiment

- Design of Experiment (DoE) can be used to optimise experimental design
- DoE produces predictive models to understand the entire formulation space when only a few areas have been tested

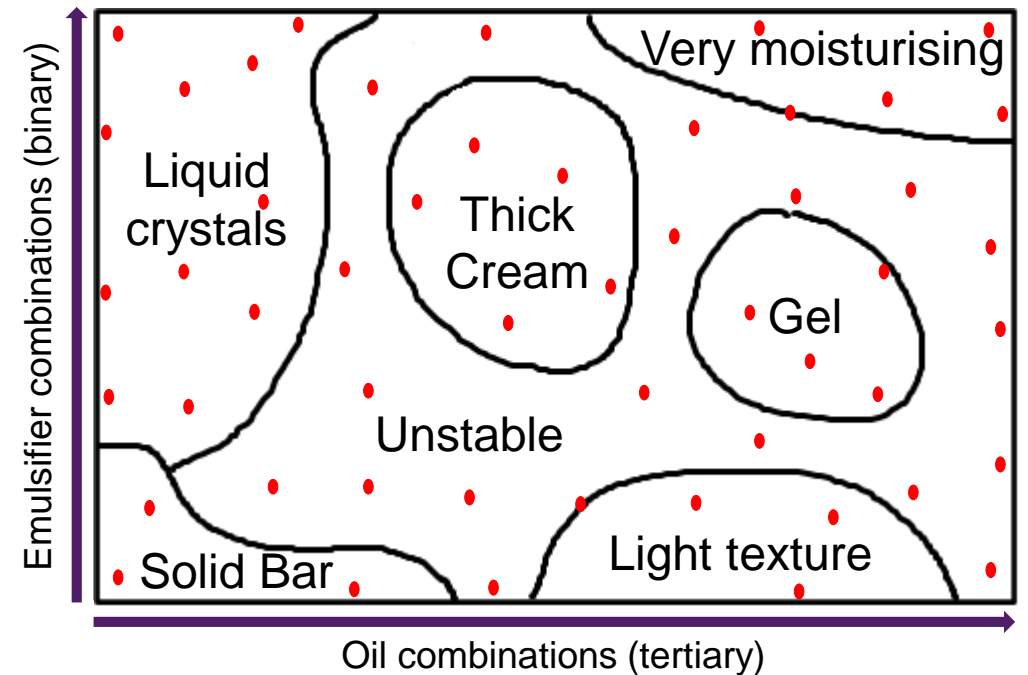


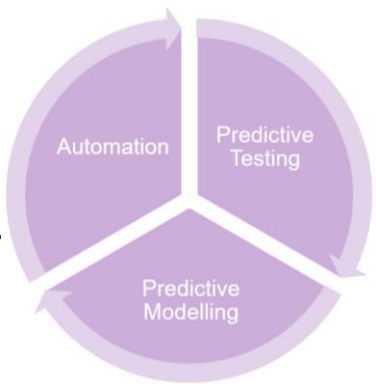
Approach 1:

15 Formulations developed through **trial and error**
= 1 final formulation which hits the brief

Approach 2:

100 formulations developed through **DoE**
= 1 final formulation which hits the brief
= Predictive map for all possible formulations





Automation

Benchtop



Vs



Automation



Using an automated formulation platform allowed formulations to be made throughout the day and into the night



Formulations were created in a controlled environment with data available on the exact amounts, stirrer speeds, temperatures and ingredient addition rates

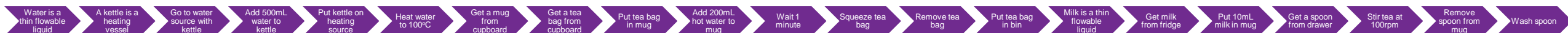
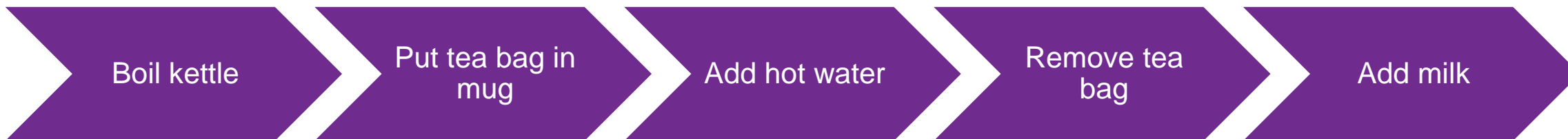


Scientist resource could be utilised on data analysis and experimental design

Automated Formulation Development

“You need to think like you don't know what you're doing”

If you were asked to provide instructions for how to make a cup of tea where would you start?

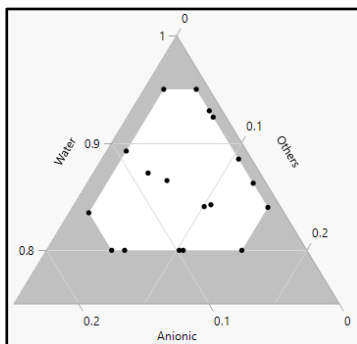


Automated Formulation Development

Its extremely important to automate the entire formulation or product development process, nobody wants to test 100+ formulations one at a time...

Predictive Modelling

Design of Experiment



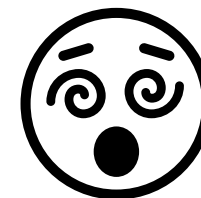
Automated
Formulation
Development

ChemSpeed Formax



Performance Testing

Manual Testing



Automated Formulation Development

Its extremely important to automate the entire formulation or product development process, nobody wants to test 100+ formulations one at a time...

Predictive Modelling



Automated Formulation Development

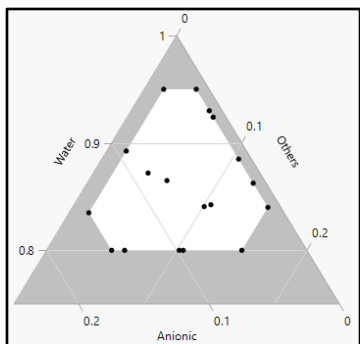


Predictive Testing



Performance Testing

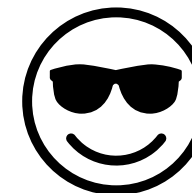
Design of Experiment

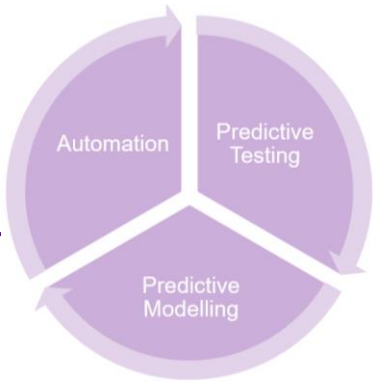


ChemSpeed Formax



Best formulations are sent for further testing





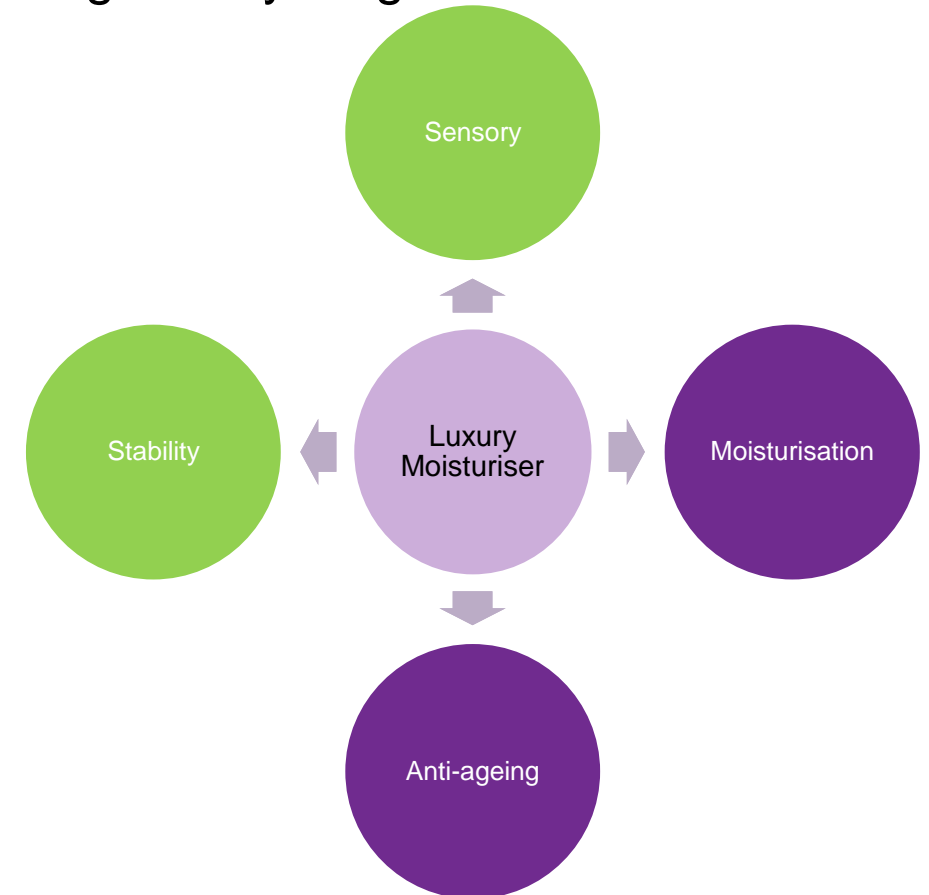
Predictive Testing - Emulsions

Formulations require a range of performance testing depending on the application and claims, therefore it would be impossible to go through everything!

Formulation Brief:

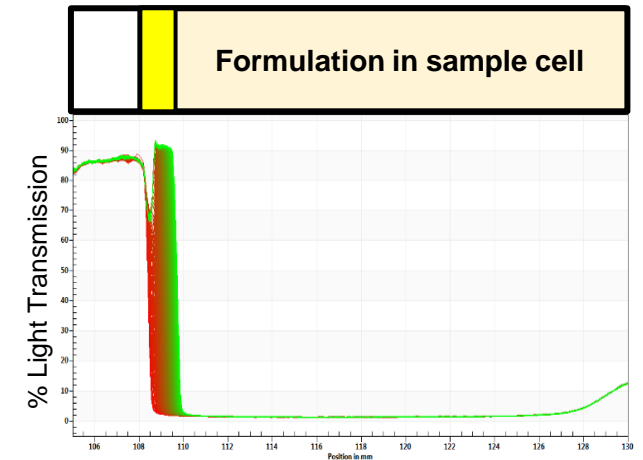
- Luxury moisturiser
- 100% Natural
- Silicone-free
- Anti-Ageing benefits
- Luxury, silky sensory

Half of our performance parameters require testing on skin whereas the other half can be easily predicted using instrumentation



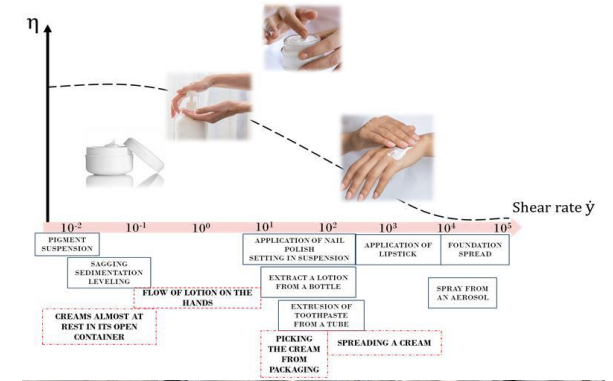
Predictive Testing – Accelerated Stability

- Traditionally, formulation stability is measured using elevated temperatures taking 3 months to determine
- The LUMiSizer can accelerate this testing giving a stability prediction after 1 hour
- The LUMiSizer is an analytical centrifuge which uses Space and Time resolved Extinction Profile (STEP) technology to generate physical stability predictions in a matter of hours
- The stability analysis is also both qualitative and quantitative and so allows for advanced stability data generation

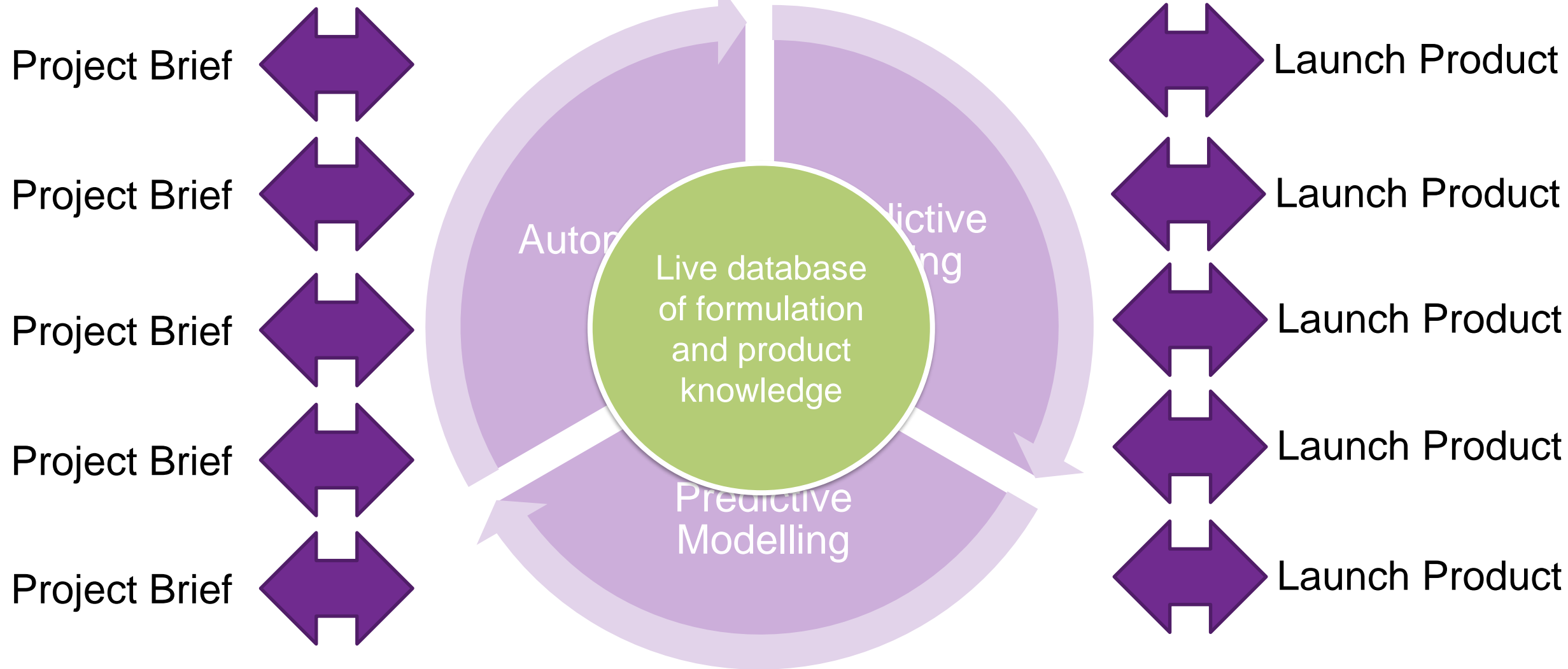


Predictive Testing – Sensory

- The rheology of a formulation can be used to evaluate the bulk viscosity and flow properties of a formulation:
 - Correlating to the sensory a consumer will experience during product application to the skin or hair
 - Identifying the most suitable packaging for the formulation
- The tribology of a formulation can be used to predict how the formulation will spread across the skin and the after-feel of the formulation after application
- Using a high-throughput rheometer accelerates the testing further



Advanced Product Design



Trial and Error Approach

Human Resource

5 days



A formulator requires a minimum of 5 days to develop a formulation to the brief using a trial and error approach.

Data Analysis

1 month



It takes a minimum of 1 month to evaluate the stability and performance of a formulation.

Lab Capacity

In use for 10 days



Lab space and equipment is in use for a minimum of 10 days and storage of formulations for 1 month preventing other tests from being conducted.

Customer engagement

Limited customer engagement



Customers can request formulations to be formulated and tested through the CWR process, or make an enquiry with the technical team.

Advanced Formulation Design

Human Resource

< 1 minute



Users of the Croda formulation databases will select the required inputs and be directed towards recommended ingredients and concentrations

Results

< 1 second



The test is simulated using Artificial Intelligence and the results are available in real-time.

Lab Capacity

~75%
reduction
(illustrative)



It will still be necessary to conduct tests in a lab, but the tool can be used to reduce lab use significantly

Customer engagement

High customer engagement



Making the Croda Formulation tool available to customers will increase awareness, engagement, lead generation and allow the customer to 'self-assess' their formulations



Thank You!

Non-warranty

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