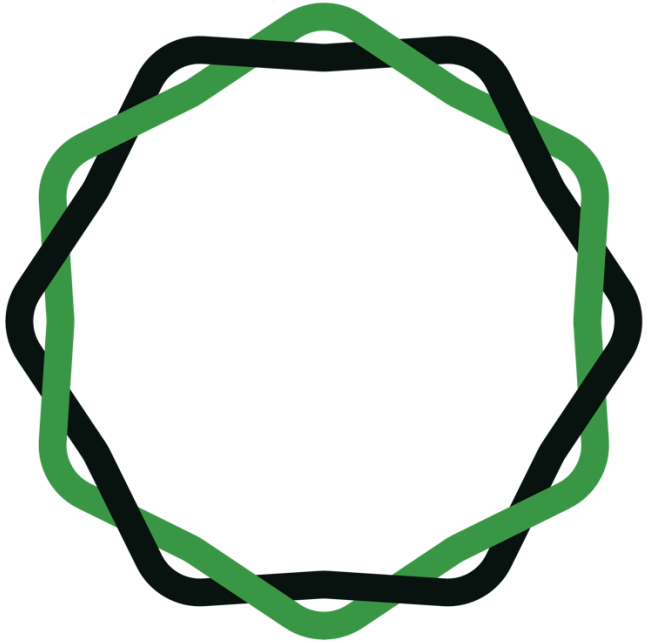


Approaching Substitution

Green Chemistry Change Management

Tabitha Petchey
Green Rose Chemistry
18 Sep 2024

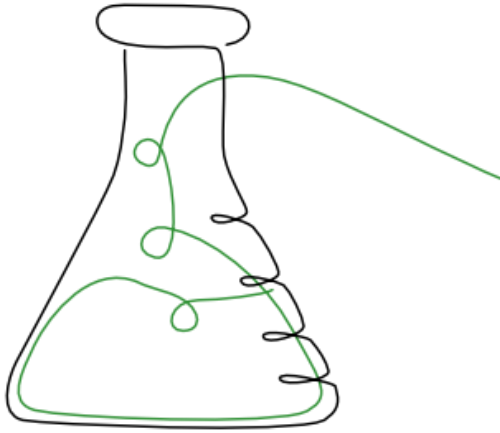
Agenda

- Introduction
- Types of Substitution
- Getting Started
- Challenges in Practice
- Conclusions and Further Reading

GREEN ROSE CHEMISTRY

GREEN ROSE CHEMISTRY

What is Alternatives Assessment?



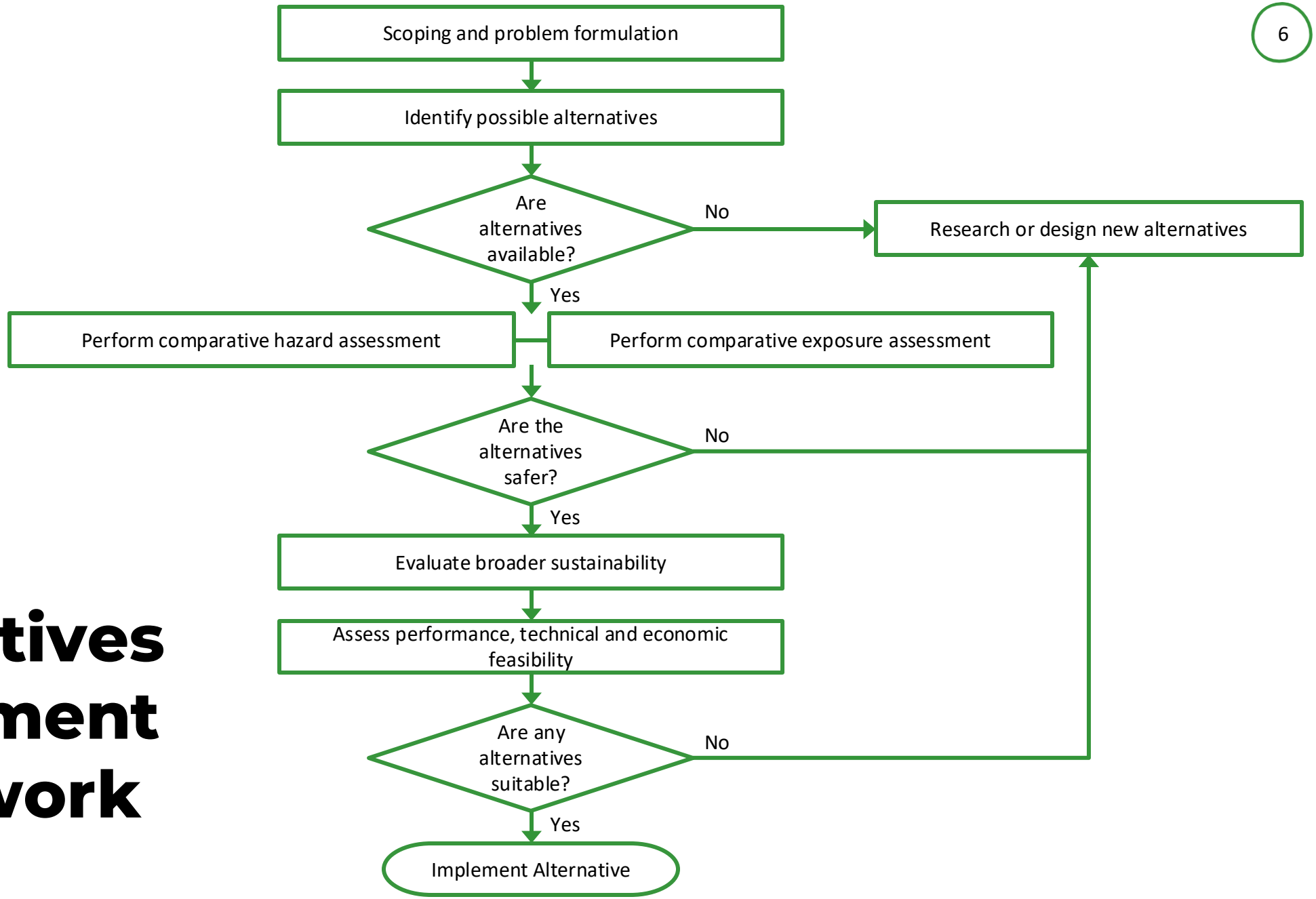
Alternatives Assessment (AA)

- Process for identifying, comparing, and selecting safer alternatives to chemicals of concern
- Based on hazards, performance, and economic viability
- Historically focused on safety rather than other sustainability characteristics
- Sustainability aspects can be added as needed
- Sometimes called “functional substitution”

AA Principles

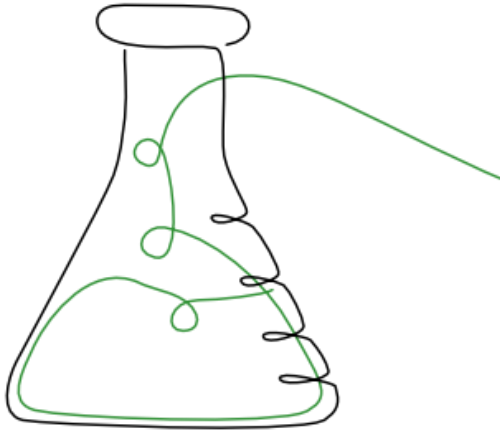
- Reduce hazard
- Minimise exposure
- Use best available information
- Require disclosure and transparency
- Resolve trade-offs
- Take action

Alternatives Assessment Framework



GREEN ROSE CHEMISTRY

Types of Substitution



Beyond Chemical Function

	Product Example BPA in thermal paper receipts	**Process Example** DCM in degreasing metal parts
Chemical Function Change the chemical	Could we use a different chemical developer? Result: drop-in chemical replacement, e.g. BPS	Could we use a different degreasing solvent? Result: drop-in chemical replacement, e.g. acetone
End Use Function Change the product or process	Could we create a printed image without a chemical developer? Result: Printing system that doesn't use thermal paper	Could we degrease metal parts without a solvent? Result: Solvent-free system, e.g. ultrasonic or aqueous surfactants
Function as Service Change the system	Are receipts necessary? Could we provide a record of sale to the customer in a different way? Result: Electronic receipts	Is degreasing necessary? Could we find another way to provide clean metal parts for end use? Result: Lubricant-free cutting methods

Source: Tickner et al. 2014

Chemical Function

- What is the primary function being provided?
  - Are there any secondary functions?
- Which functions are necessary, and which are desirable?
- Which chemical properties produce the function?
- Is the chemical structure linked to the function?
  - Is it possible to create the function with a different structure?
- Is the chemical structure linked to the hazard?
  - Will related structures be similarly hazardous?

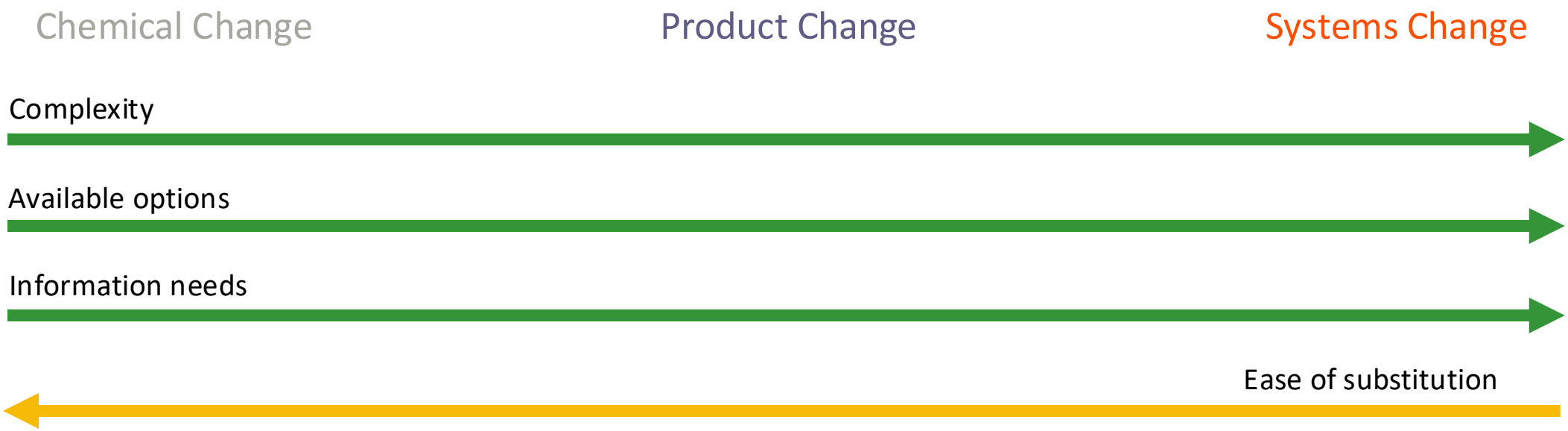
End Use Function

- What is the primary purpose the chemical is serving?
  - Are there any secondary purposes?
- Which purposes are necessary, and which are desirable?
- Are there other ways the same purpose could be served?
  - Material choices
  - Process redesign
- Broader range of choices makes it easier to step away from hazardous chemistry

Function as Service

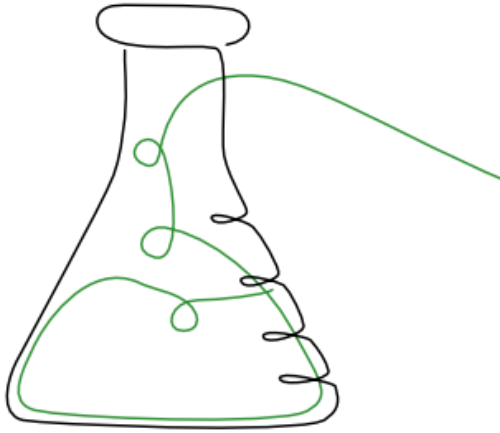
- What primary service is the chemical product providing?
  - Are there any secondary services?
- Is it a necessary service, or just desirable?
- Could the system be redesigned to provide the service in a different way?
- Requires cooperation between many different stakeholders
- Can lead to disruptive tech and competitive advantage

Functional Substitution



GREEN ROSE CHEMISTRY

Getting Started



Scoping

- Talk with stakeholders!
- Identify and write down the goal of your assessment
- Evaluate your resources (time, money, expertise)
  - Can you enlist help from internal teams? External experts?
- Choose a type of substitution based on resource limitations
- Define the properties, hazards, and characteristics of your current chemical, the ideal replacement, and a minimally acceptable replacement

Finding Alternatives

- There is no one database for replacement chemicals
- Often information about alternatives on Google is unreliable (content marketing)
  - Has gotten worse with rise of AI copywriting
- Finding options can involve deep literature searches, attending conferences, critically searching multiple databases, networking, talking with other industry sectors, reading case studies

Assessing Chemical Hazard

- Screen out highly problematic alternatives using authoritative lists
  - Ozone-depleting substances, persistent organic pollutants, REACH SVHC, etc.
- Use GHS criteria for chemical hazards
- Create and use decision rules – what is “safer”?
  - E.g. Avoid CMRs, PBTs, vPvB
- Take note of data gaps and address uncertainty

Assessing Chemical Exposure

- May not be necessary if physicochemical properties of alternatives are similar
- Identify exposure pathways and reasonably foreseeable exposure scenarios
  - e.g. volatile solvent can escape into air, non-volatile solid won't
- Talk to stakeholders about storage, processing, use
- Compare exposure potential of alternatives

Broader Sustainability Metrics

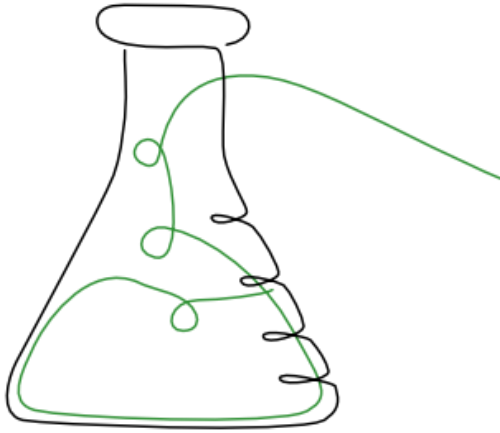
- Identify sustainable characteristics that are important for your application and industry
- Talk to stakeholders
  - Marketing labels? Regulatory requirements? Corporate goals?
- Identify relevant metrics and search for data
- Certifications and labels can be helpful

Feasibility

- Performance
  - Usually involves some sort of testing
  - If no internal labs, look at open access labs and services
- Technical feasibility
  - Does the alternative work with existing equipment?
  - Does it meet all technical requirements?
- Economic feasibility
  - Is the alternative within budget?
  - Can you justify a cost increase using savings from improved safety?
  - Scale and reliability of supply

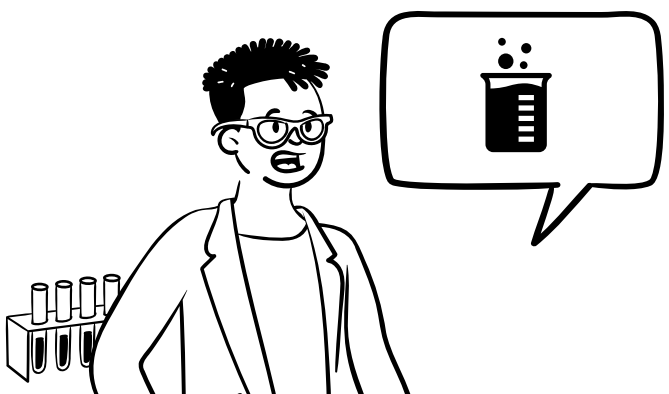
GREEN ROSE CHEMISTRY

Challenges in Practice



Isolated Expertise

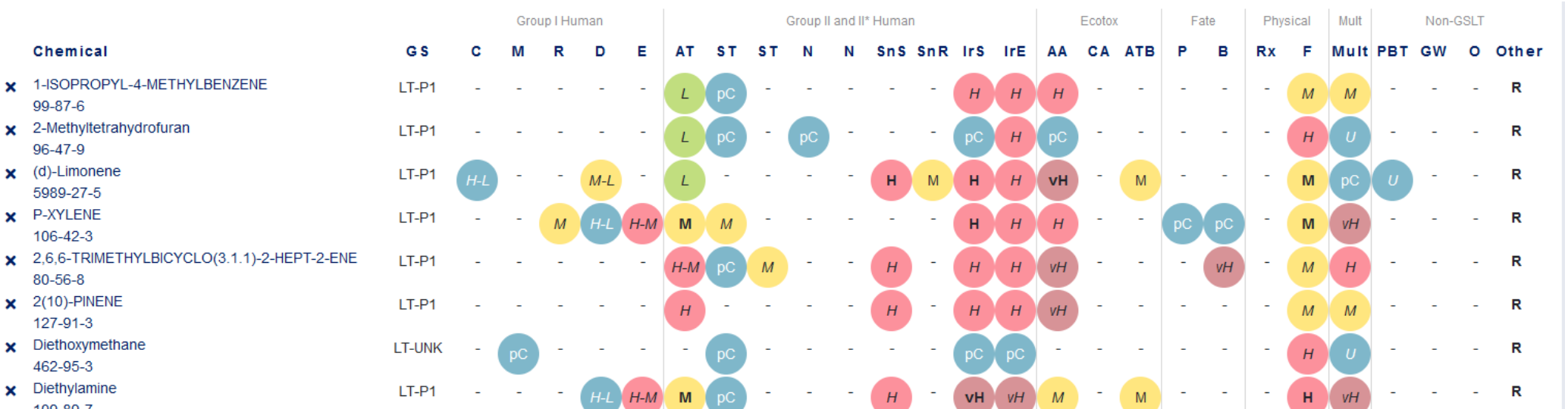
- Demand for substitution comes from end user
- Substitution requires deep chemical expertise
- Formulators and product designers are not equipped to ask or answer questions like “are there other potential proton donors with configurations similar to BPA that are unlikely to bind to estrogen?”



Data Gaps

- Not enough data on chemical hazards
- Other types of data are even harder to get
  - Performance characteristics
  - Sustainability data
  - Chemical use volumes

			Group I Human					Group II and II* Human									Ecotox			Fate		Physical		Mult	Non-GSLT			
	Chemical	GS	C	M	R	D	E	AT	ST	ST	N	N	SnS	SnR	IrS	IrE	AA	CA	ATB	P	B	Rx	F	Mult	PBT	GW	O	Other
×	1-ISOPROPYL-4-METHYLBENZENE 99-87-6	LT-P1	-	-	-	-	-	L	pC	-	-	-	-	-	H	H	H	-	-	-	-	-	M	M	-	-	-	R
×	2-Methyltetrahydrofuran 96-47-9	LT-P1	-	-	-	-	-	L	pC	-	pC	-	-	-	pC	H	pC	-	-	-	-	-	H	U	-	-	-	R
×	(d)-Limonene 5989-27-5	LT-P1	H-L	-	-	M-L	-	L	-	-	-	-	H	M	H	H	vH	-	M	-	-	-	M	pC	U	-	-	R
×	P-XYLENE 106-42-3	LT-P1	-	-	M	H-L	H-M	M	M	-	-	-	-	-	H	H	H	-	-	pC	pC	-	M	vH	-	-	-	R
×	2,6,6-TRIMETHYLBICYCLO(3.1.1)-2-HEPT-2-ENE 80-56-8	LT-P1	-	-	-	-	-	H-M	pC	M	-	-	H	-	H	H	vH	-	-	-	vH	-	M	H	-	-	-	R
×	2(10)-PINENE 127-91-3	LT-P1	-	-	-	-	-	H	-	-	-	-	H	-	H	H	vH	-	-	-	-	-	M	M	-	-	-	R
×	Diethoxymethane 462-95-3	LT-UNK	-	pC	-	-	-	-	pC	-	-	-	-	-	pC	pC	-	-	-	-	-	-	H	U	-	-	-	R
×	Diethylamine	LT-P1	-	-	-	H-L	H-M	M	pC	-	-	-	H	-	vH	vH	M	-	M	-	-	-	H	vH	-	-	-	R



Essential vs. Desirable

- Must identify essential vs. desirable functions, properties, characteristics
- Challenging to get stakeholder agreement

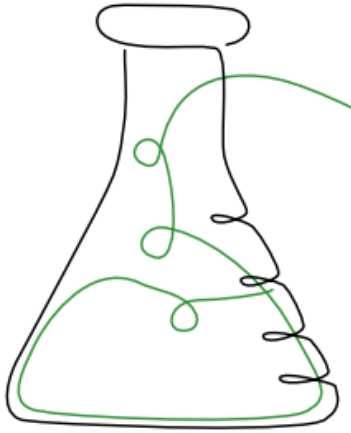
		Current Solvent	Ideal Replacement	Acceptable Replacement
ID	Name	[redacted]	n/a	n/a
	CAS		n/a	n/a
	EC		n/a	n/a
cal Charact	Freezing Point (°C at 101 kPa)		< - 30	< -15
	Boiling Point (°C at 101 kPa)		>250	120-249
	Vapour Pressure (Pa at 25°C)		Low vapour pressure	Low vapour pressure
	Dynamic Viscosity (mPa·s at 20°C		0.5-1.0	1.0-1.5
	Density (g/cm³ at 25°C)		<1	not critical
	Surface Tension (mN/m at 25°C)		20-30	>30 is also fine
	Water Solubility (g/L at 20°C)		<1	<100
	Must Dissolve...	polyurethane, polyols, isocyanates	olyurethane, polyols, isocyanat	olyurethane, polyols, isocyanates
	Other	no reaction with isocyanates	no reaction with isocyanates or	no reaction with isocyanates or pol
Commerc ial	Colour	clear, colourless	colourless or white	pale yellow
	Odour	ethereal, fruity	no odour	quickly dispersing, pleasant

Trade-Offs

- Often there is no ideal substitute
- Must use essential vs. desirable criteria to compromise
- If all options are hazardous, use exposure assessment to identify relatively safer options
- For newer alternatives, cost and scale of supply can be a challenge
  - Can be overcome with partnerships

GREEN ROSE CHEMISTRY

Conclusions



To sum up…

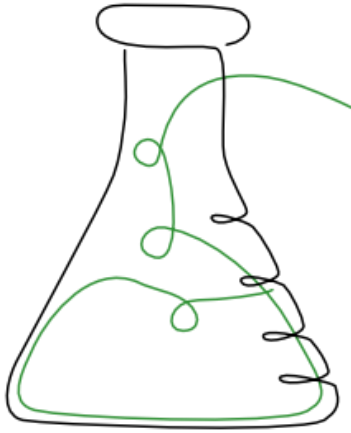
- Substitution of chemicals is a multi-disciplinary exercise
- Communication between stakeholders and different experts is essential
- Identifying potential alternatives and finding sufficient data can be challenging
- Many tools and resources freely available to help

Further Reading

- Advancing Safer Alternatives through Functional Substitution
  http://dx.doi.org/10.1021/es503328m
- OECD Guidance on Safer Chemical Alternatives
  https://www.oecd.org/chemicalsafety/risk-management/guidance-on-key-considerations-for-the-identification-and-selection-of-safer-chemical-alternatives.pdf
- ECHA Online Training on Alternatives Analysis
  https://echa.europa.eu/online-training-on-analysis-of-alternatives
- OECD Toolbox
  https://www.oecd.org/chemicalsafety/risk-management/substitution-of-hazardous-chemicals/

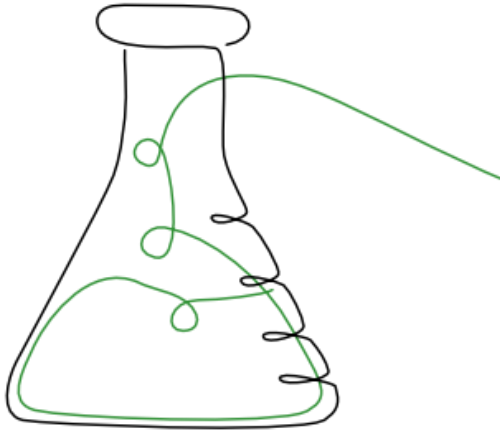
GREEN ROSE CHEMISTRY

Break



GREEN ROSE CHEMISTRY

Exercise: Scoping



Scoping a Substitution (45 min)

- Open the Identification of Chemical Requirements spreadsheet
- Identify a chemical you'd like to substitute (hexane is filled in as an example)
- If no ideas come to mind, open Safer Alternative Nail Polish Removers and use this example
- Start by identifying ideal and minimally acceptable characteristics for an alternative – aim for 30% completion
- Qualitative metrics are okay, if quantitative are unknown
- Try to identify potential alternatives and their characteristics

GREEN ROSE CHEMISTRY

Questions?

Contact Tabitha Petchey at tabitha.petchey@greenrosechemistry.com.