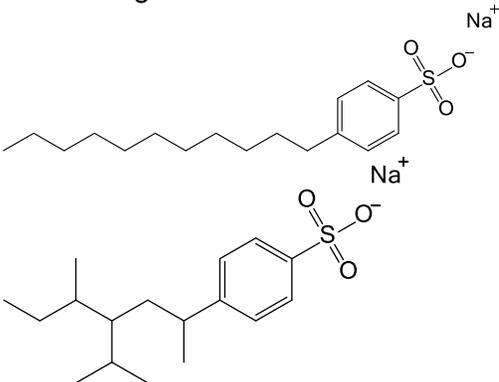
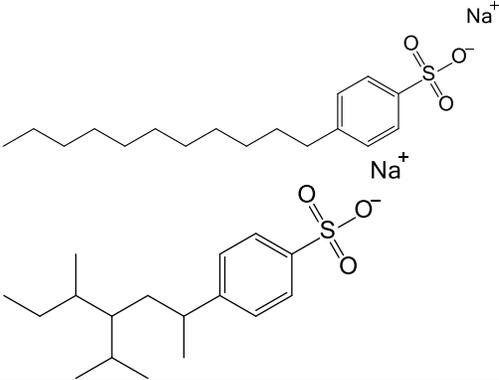
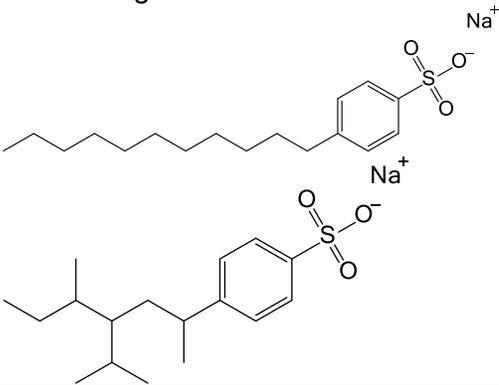
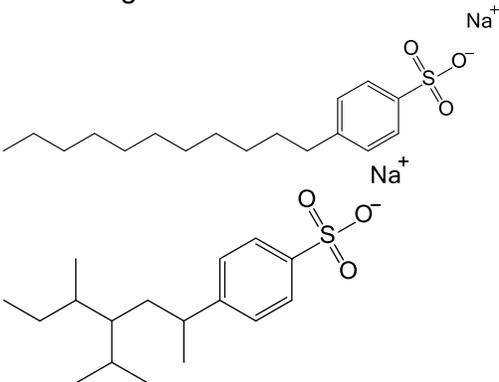


Activity 3 Print Files

Activity 3 – Keywords: A waste and hazard reduction puzzle

Question	Response	Team/Group	Letter	Colour Dots								
What is the expression that defines E-factor?	Kg waste/Kg product	1	G	Green								
What is the expression that defines E-factor?	Kg waste/Kg product	2	G	Blue								
What is the expression that defines E-factor?	Kg waste/Kg product	3	C	Yellow								
What is the expression that defines E-factor?	Kg waste/Kg product	4	H	Red								
LD50 is a metric on chemical SDS pages, which is a measure that determines the dosage of that chemical that is lethal to 50% of a population. Using the following LD50 data; determine which of these compounds is the most toxic? <table border="1"> <tr> <td>Potassium Hydroxide</td> <td>ORAL 333 mg/kg (rat, male)</td> </tr> <tr> <td>Ammonium</td> <td>ORAL 350 mg/kg (rat)</td> </tr> <tr> <td>Potassium Carbonate (anhydrous)</td> <td>ORAL 2000 mg/kg (rat, male and female)</td> </tr> <tr> <td>Triethylamine</td> <td>ORAL 460 mg/kg (rat)</td> </tr> </table>	Potassium Hydroxide	ORAL 333 mg/kg (rat, male)	Ammonium	ORAL 350 mg/kg (rat)	Potassium Carbonate (anhydrous)	ORAL 2000 mg/kg (rat, male and female)	Triethylamine	ORAL 460 mg/kg (rat)	Potassium Hydroxide	1	O	Green
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What is one advantage of using water as a solvent in a reaction at a temperature below 100°C?	Minimal VOC emissions generated from reaction	1	F	Green								
What is one disadvantage of using water as a solvent in a reaction at a temperature below 100°C?	Limits reaction to only utilizing reactants that are air- and water-stable	2	E	Blue								
What is one advantage of using water as a solvent in a reaction at a temperature below 100°C?	Lowers the cost of the reaction	3	O	Yellow								
What is one disadvantage of using water as a solvent in a reaction at a temperature below 100°C?	Product could be difficult to isolate due to costs of separation, distillation or boiling off solvent	4	N	Red								
Which of the reactions on page 36 of the handbook has the highest turnover number?	Product 6	1	O	Green								
Which of the reactions on page 37 of the handbook has the highest turnover number?	Product 7	2	E	Blue								
Which of the reactions on page 36 of the handbook has the lowest turnover number?	Product 3	3	L	Yellow								
Which of the reactions on page 37 of the handbook has the lowest turnover number?	Product 4	4	D	Red								
<p>Which of these two compounds has a slower degradation rate?</p> 	Linear product	1	R	Green								

<p>Which of these two compounds has a faster degradation rate?</p> 	Branched product	2	N	Blue
<p>Which of these two compounds has a slower degradation rate?</p> 	Linear product	3	C	Yellow
<p>Which of these two compounds has a faster degradation rate?</p> 	Branched product	4	E	Red

Which of these processes will have a lower E-factor? a. Cumene route to phenol (scheme 1.1) b. Sulfonation route to phenol (scheme 1.2)	Cumene route to phenol	1	G	Green
Which of these processes will have a higher E-factor? a. Cumene route to phenol (scheme 1.1) b. Sulfonation route to phenol (scheme 1.2)	Sulfonation route to phenol	2	E	Blue
Which of these processes will have a lower E-factor? a. Current pathway to Ibuprofen (scheme 2.1) b. Boots pathway to Ibuprofen (scheme 2.2)	Current pathway to Ibuprofen	3	A	Yellow
Which of these processes will have a higher E-factor? a. Current pathway to Ibuprofen (scheme 2.1) b. Boots pathway to Ibuprofen (scheme 2.2)	Boots pathway to Ibuprofen	4	R	Red
Identify one of the by-products from the reaction scheme 1.1 (handbook page 39)	CO ₂	1	R	Green
Identify one of the by-products from the reaction scheme 1.1 (handbook page 39)	Na ₂ SO ₃	2	R	Blue
Identify one of the by-products from the reaction scheme 2.1 (handbook page 40)	Al(OH) ₃	3	T	Yellow
Identify one of the by-products from the reaction scheme 2.1 (handbook page 40)	C ₂ H ₅ OH	4	H	Red
Using the information in the handbook - which of these metals is the most abundant on earth? Chromium (Cr), Titanium (Ti), Gold (Au), Gallium (Ga)	Ti	1	E	Green
Using the information in the handbook - which of these metals is the most abundant on earth? Ruthenium (Ru), Nickel (Ni), Iron (Fe), Zinc (Zn)	Fe	2	C	Blue
Using the information in the handbook - which of these metals is the most abundant on earth? Chromium (Cr), Titanium (Ti), Gold (Au), Gallium (Ga)	Ga	3	A	Yellow
Using the information in the handbook - which of these metals is the most abundant on earth? Ruthenium (Ru), Nickel (Ni), Iron (Fe), Zinc (Zn)	Zn	4	A	Red

What does a reaction run "neat" mean?	A reaction is performed in which a reactant is in a liquid state at the temperature of the reaction, and behaves as a solvent for other reactants.	1	E	Green												
What does a reaction run "neat" mean?	A reaction is performed in which a reactant is in a liquid state at the temperature of the reaction, and behaves as a solvent for other reactants.	2	H	Blue												
How can a reaction be run without the use of a solvent?	Mechanochemistry - using the kinetic energy of either ball-milling or mortar and pestle to break and form bonds	3	L	Yellow												
How can a reaction be run without the use of a solvent?	Running a reaction "neat" - a reactant is a liquid at the temperature of the reaction and acts as a solvent for other reactants	4	Z	Red												
Using the handout provided, on page 41 and 42, find a reaction that has generates no by-product and has an atom economy of 100%	Claisen rearrangement	1	N	Green												
Using the handout provided, on page 41 and 42, find a reaction that has generates no by-product and has an atom economy of 100%	Beckmann rearrangement	2	E	Blue												
Using the handout provided, on page 41 and 42, find a reaction that has generates no by-product and has an atom economy of 100%	Claisen rearrangement	3	Y	Yellow												
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Listed are the flash points of 4 solvents. Which solvent poses the largest fire risk if it were to be used?	Acetone	1	E	Green												
<table border="1"> <thead> <tr> <th>Solvents</th> <th>Flash point (°C)</th> </tr> </thead> <tbody> <tr> <td>Methanol</td> <td>9.7</td> </tr> <tr> <td>Ethanol</td> <td>13</td> </tr> <tr> <td>Isopropanol</td> <td>12</td> </tr> <tr> <td>Ethyl acetate</td> <td>-4</td> </tr> <tr> <td>Acetone</td> <td>-17</td> </tr> </tbody> </table>					Solvents	Flash point (°C)	Methanol	9.7	Ethanol	13	Isopropanol	12	Ethyl acetate	-4	Acetone	-17
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$A + B \rightarrow C$ $C + X \rightarrow Y$	$A + B \rightarrow C + D$ $C + X \rightarrow Y$															
Blank Question	Blank answer	4	D	No colour given, but will be with team with Red answers												

Activity 4 Questions

What is the expression that defines E-factor?

LD50 is a metric on a chemical's SDS, which is a measure that determines the dosage of that chemical that is lethal to 50% of a population. Using the LD50 data below (also on page 35 of the handbook, and the handout for this activity), determine which compound is the **MOST** dangerous if ingested?

Potassium Hydroxide	ORAL 333 mg/kg (rat, male)
Ammonium	ORAL 350 mg/kg (rat)
Potassium Carbonate (anhydrous)	ORAL 2000 mg/kg (rat, male and female)
Triethylamine	ORAL 460 mg/kg (rat)

What is one advantage of using water as a solvent in a reaction at a temperature below 100°C?

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LD50 is a metric on a chemical's SDS, which is a measure that determines the dosage of that chemical that is lethal to 50% of a population. Using the LD50 data below (also on page 35 of the handbook, and the handout for this activity), determine which compound is the **MOST** dangerous if ingested?

Hydrochloric acid	ORAL 238 mg/kg (rat)
Formic acid	ORAL 738 mg/kg (rat)
Glacial acetic acid	ORAL 3310 mg/kg (rat)
Citric acid	ORAL 6730 mg/kg (rat)

LD50 is a metric on a chemical's SDS, which is a measure that determines the dosage of that chemical that is lethal to 50% of a population. Using the LD50 data below (also on page 35 of the handbook, and the handout for this activity), determine which compound is the **MOST** dangerous if ingested?

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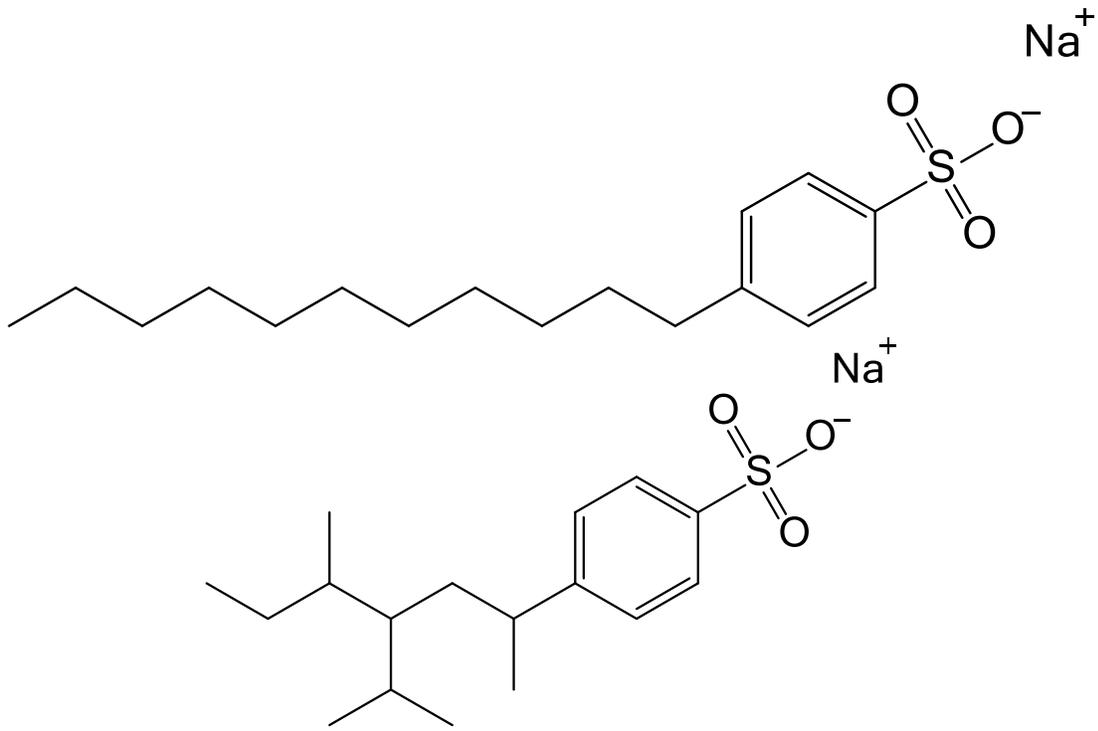
Which of the reactions on page 36 of the handbook has the **highest** turnover number?

Which of the reactions on page 37 of the handbook has the **highest** turnover number?

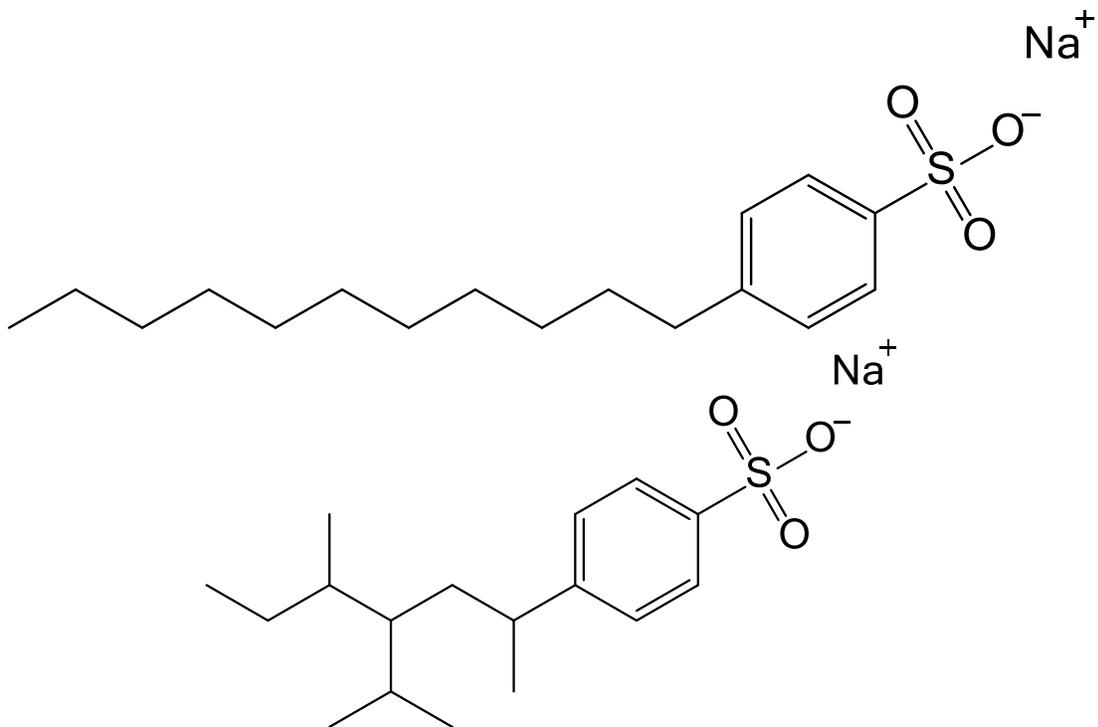
Which of the reactions on page 36 of the handbook has the **lowest** turnover number?

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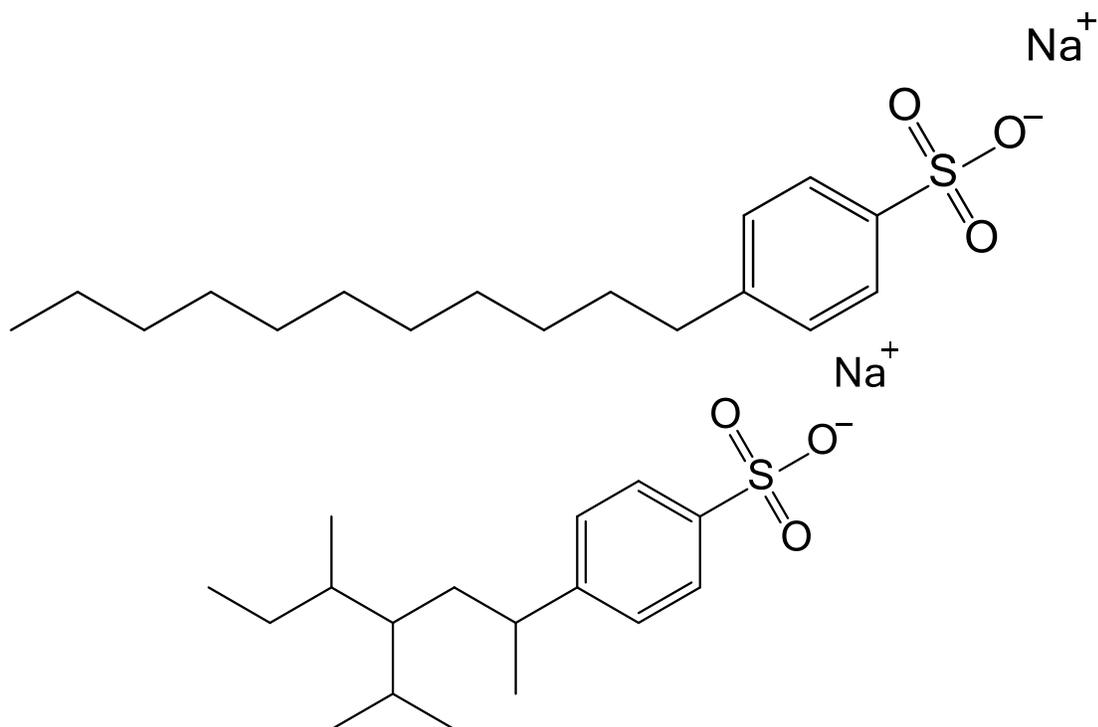
Which of these two compounds has a faster degradation rate?



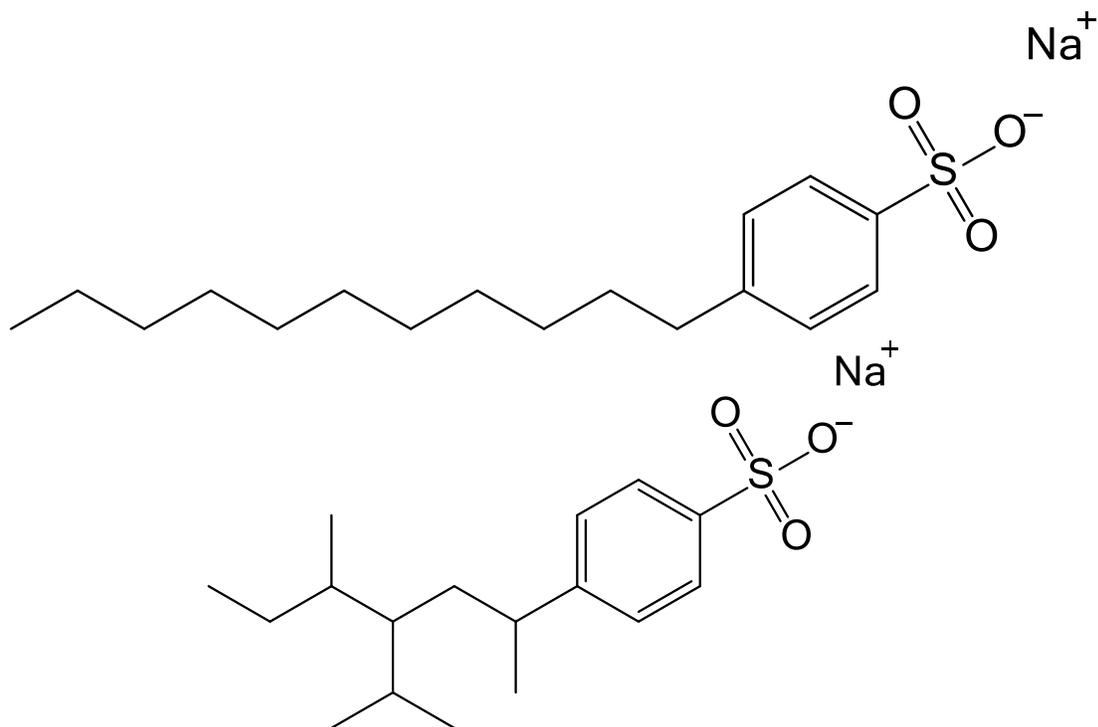
Which of these two compounds has a faster degradation rate?



Which of these two compounds has a faster degradation rate?



Which of these two compounds has a faster degradation rate?



See page 39 in the handbook or activity handout.

Which of these processes (scheme 1.1 or 1.2) will have a lower E-factor?

- a. Cumene route to phenol (scheme 1.1)
- b. Sulfonation route to phenol (scheme 1.2)

See page 39 in the handbook or activity handout.

Which of these processes (scheme 1.1 or 1.2) will have a lower E-factor?

- a. Cumene route to phenol (scheme 1.1)
- b. Sulfonation route to phenol (scheme 1.2)

See page 40 in the handbook or activity handout.

Which of these processes (scheme 2.1 or 2.2) will have a higher E-factor?

- a. Current pathway to Ibuprofen (scheme 2.1)
- b. Boots pathway to Ibuprofen (scheme 2.2)

See page 40 in the handbook or activity handout.

Which of these processes (scheme 2.1 or 2.2) will have a lower E-factor?

- a. Current pathway to Ibuprofen (scheme 2.1)
- b. Boots pathway to Ibuprofen (scheme 2.2)

Identify one of the by-products from the reaction scheme 1.1 (handbook page 39)

Identify one of the by-products from the reaction scheme 1.1 (handbook page 39)

Identify one of the by-products from the reaction
scheme 2.1
(handbook page 40)

Identify one of the by-products from the reaction
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Using the information in the handbook - which of these
metals is the most abundant on earth?

Chromium (Cr), Titanium (Ti),
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What does a reaction run "neat" mean?

What does a reaction run "neat" mean?

How can a reaction be run without the use of a solvent?

How can a reaction be run without the use of a solvent?

Using the handout provided, on page 41 and 42, find a reaction that has generates no by-product and has an atom economy of 100%

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Using the handout provided, on page 41 and 42, find a reaction that has generates no by-product and has an atom economy of 100%

Listed are the flash points of 5 common solvents. Which solvent poses the **largest** fire risk if it were to be used?

Solvents	Flash point (°C)
Methanol	9.7
Ethanol	13
Isopropanol	12
Ethyl acetate	-4
Acetone	-17

Listed are the flash points of 5 common solvents. Which solvent poses the **largest** fire risk if it were to be used?

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Methanol	9.7
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Which of these reactions will have the greater percent atom economy?



Which of these reactions will have the greater percent atom economy?



Activity 4 Answers

Kg waste/Kg product

Kg waste/Kg product

Kg waste/Kg product

Kg waste/Kg product

Hydrochloric acid

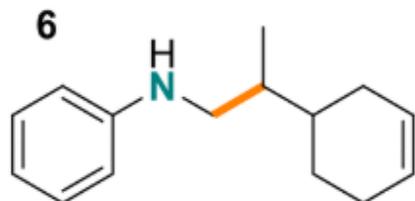
Potassium
Hydroxide

Potassium
Carbonate
(anhydrous)

Citric Acid

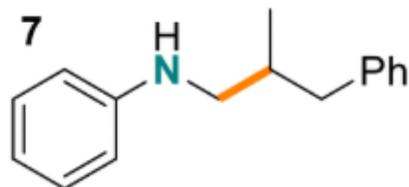
<p>Minimal VOC emissions generated from reaction</p>	<p>Limits the reaction to utilizing reactants that are water-stable (and, usually air-stable)</p>
<p>Lowers cost of reaction</p>	<p>Product could be difficult to isolate based on solubility</p>

Product 6



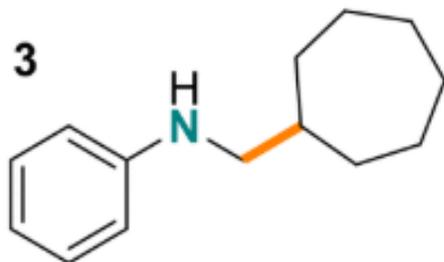
5%
8 h
97%
>99:1

Product 7



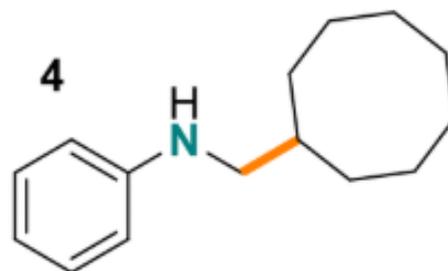
10%
48 h
82%
>99:1

Product 3



10%
48 h
91%

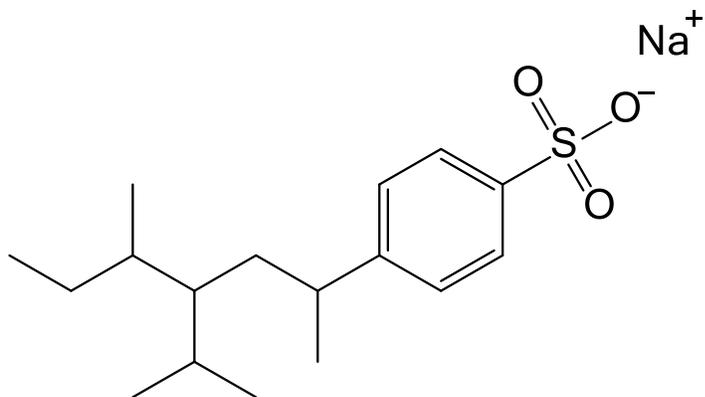
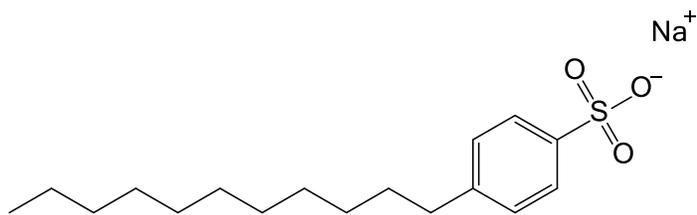
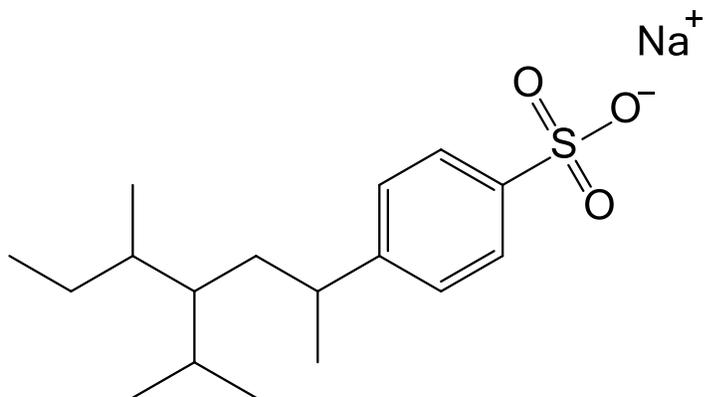
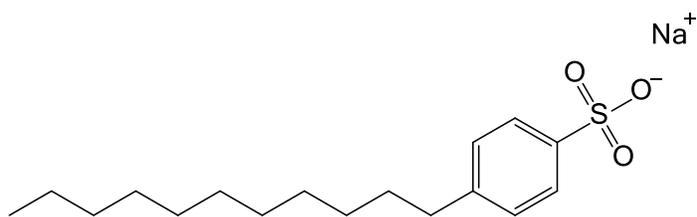
Product 4



10%
48 h
78%

Activity 4 – Questions and Answers Print-off document

Refer to question and answer document for allocation of Q → A → Letter → Team



Sulfonation route to phenol synthesis

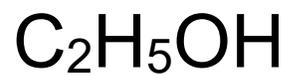
Cumene route to phenol synthesis

Current process for Ibuprofen synthesis

Boots process for Ibuprofen synthesis

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Ti

Fe

Zn

Ga

<p>A reaction is performed in which a reactant is in a liquid state at the temperature of the reaction, and is used as a solvent for other reactants</p>	<p>A reaction is performed in which a reactant is in a liquid state at the temperature of the reaction, and behaves as a solvent for other reactants</p>
<p>Mechanochemistry - using the kinetic energy of either ball-milling or mortar and pestle to break and form bonds</p>	<p>Running a reaction "neat" - a reactant is a liquid at the temperature of the reaction and acts as a solvent for other reactants</p>

Claisen rearrangement

Beckmann
rearrangement

Claisen rearrangement

Beckmann
rearrangement

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Acetone

Acetone

Ethanol

Ethanol

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