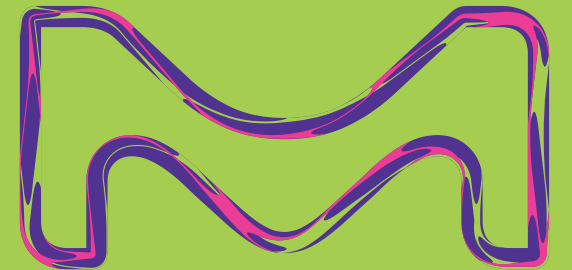


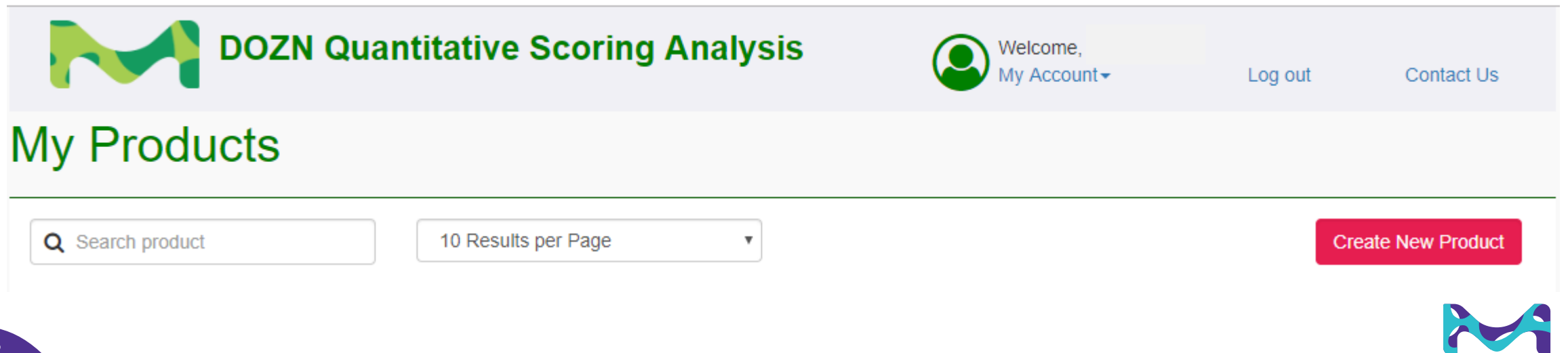
HOW TO OPERATE DOZN™ 2.0?



Beginning DOZN™ 2.0 Entry

<https://green.milliporesigmabioinfo.com/dozn/>

- Register on the DOZN™ 2.0 website and provide the requested information
 - You will receive further email instructions to complete the registration
- After account is created and approved click the red “Create New Product” button to begin
- Each product entered will be found under My Products section in the Home tab



The screenshot shows the top navigation bar of the DOZN website. On the left is the logo, a stylized 'M' shape in green and yellow, followed by the text 'DOZN Quantitative Scoring Analysis'. On the right, there is a user profile icon with the text 'Welcome, My Account' and a dropdown arrow. Further right are links for 'Log out' and 'Contact Us'. Below the navigation bar is a section titled 'My Products'. Under this title, there is a search bar with a magnifying glass icon and the text 'Search product', a dropdown menu showing '10 Results per Page', and a prominent red button labeled 'Create New Product'. In the bottom right corner of the page, there is a smaller version of the 'M' logo.

Product and Coproduct Information

- The product name will become the name shown in the My Products section of the Home screen. The product name can be anything; the name does not effect scoring.
- If no product brand/number available search for product:
<https://www.sigmaaldrich.com>
- Mass should be the mass of the final product/coproduct obtained not the theoretical yield
- Only add coproducts if the side product is kept for sale or further production

Product Information ⓘ

*Product Name	*Mass	*Unit
<input type="text"/>	<input type="text"/>	<input type="text" value="g"/>
*Product Number	*Brand	
<input type="text"/>	<input type="text" value="Select"/>	

Coproducts ⓘ

Coproduct #1			Remove
*Coproduct Name	*Mass	*Unit	
<input type="text"/>	<input type="text"/>	<input type="text" value="g"/>	



Reaction Conditions

- Reaction conditions are considered if temperature and/or pressure deviate from ambient conditions. Only consider conditions if work is used to change the conditions, exclude conditions caused by a chemical reaction (ex: exclude heating from exothermic reactions)
- Reaction conditions will be assigned to raw materials, so name each to differentiate from similar steps (example: Reflux 1, Reflux 2, Filter ether mixture, Filter DCM layer, etc.)
- If the same reaction conditions are used twice in the same procedure, the condition must be entered twice to properly assign reaction conditions to raw materials
- If time is not explicitly stated in procedure, one hour should be assumed unless this time is deemed unreasonable (ex: "filter off solid" would likely be counted as one hour unless the amount of solid is small in which one hour could be deemed unreasonable)

Reaction Condition #1 Remove

Name of Synthesis Step	Time	Time Unit
<input type="text"/>	<input type="text"/>	min <input type="text"/>

Pressure Input Method


<input type="radio"/>	<input type="radio"/>
Exact Value	General Conditions

Temperature Input Method

<input type="radio"/>	<input type="radio"/>
Exact Value	General Conditions



Reaction Conditions (cont.)

- Pressure and temperature of each reaction condition can be entered as exact or general conditions
- Hovering over the  icon will show the corresponding pressure or temperature ranges corresponding to each general condition

Reaction Condition #1

Name of Synthesis Step


Time

Time Unit

Pressure Input Method

Exact Value

General Conditions

Pressure Score 


No mention of vacuum or pressure change

Pressure Ranges (Torr)	Pressure Ranges (mBar)	Pressure Ranges (atm)	General Condition
760	1013	1	No mention of vacuum or pressure change
560 - 760	747 - 1013	0.737 - 1	Reduced pressure
260 - 560	347 - 747	0.342 - 0.737	Under vacuum, rotovap, or unspecified
40 - 260	53 - 347	0.052 - 0.342	Vacuum oven
0 - 40	0 - 53	0 - 0.052	High vacuum, vacuum oven

Temperature Input Method

Exact Value

General Conditions

Temperature Score 




Room temperature

Temperature Ranges (°C)	Temperature Ranges (°F)	Temperature Ranges (K)	General Condition
< -20	< -4	< 253	Below -20°C
-20 - 0	-4 - 32	253 - 273	Technical Cooling
0 - 10	32 - 50	273 - 283	Ice Cooling
10 - 20	50 - 68	283 - 293	Water Cooling
20 - 30	68 - 86	293 - 303	Room Temperature
30 - 90	86 - 194	303 - 363	Hot Water Heating
90 - 160	194 - 320	363 - 433	Steam Heating
160 - 280	320 - 536	433 - 553	Hot Oil or Electrical Heating
> 280	> 536	> 553	Above 280°C

ADD A REACTION CONDITION



Raw Materials

- Enter product name and number as they appear on SDS sheet, then select what each is Used As by referencing the  icon
- A raw material is only considered to be waste if it is discarded entirely in the process
 - If waste, select waste severity based on information in section 13.1 of SDS
 - Waste is a derivative if it is the product of a non-synthetic step (ex: blocking/unblocking reactions)
- A material is renewable if it fits the USDA definition of a biobased product
- Water is never considered a solvent in this tool, only organic solvents are considered
- To determine B score see section 10.6 and 12 of SDS and reference the  icon
- Add reaction condition to each material by checking the box next to the condition;  each raw material is not required to have a reaction condition to contribute to scoring


Raw Material #2 Remove

*Product Name *Product Number *Brand

*Mass Is Waste? Yes No Is Renewable? Yes No Is Solvent? Yes No B Score

Used As

Reactant	An integral reagent that is incorporated into the product, or an acid or base used to change the pH of the product.
Recovered Reactant	A reagent that is recovered and reused.
Auxiliary	Anything besides a reagent, e.g. water, washing solutions, and non-reacting solvents.
Recovered Auxiliary	An auxiliary material that is recovered and reused.

Reaction Conditions 

Element	GHS Category 1	GHS Category 2	GHS Category 3	GHS Category 4
Acute aquatic toxicity	≤ 1.00 mg/l	> 1.00 but ≤ 10.0 mg/l	> 10.0 but ≤ 100.0 mg/l	> 100 mg/l
Chronic aquatic toxicity, NOEC (fish, daphnia)	≤ 1.00 mg/l	> 1.00 but ≤ 10.0 mg/l	> 10.0 but ≤ 100.0 mg/l	> 100 mg/l
B score	4	3	2	1

Locate the SDS and check section 10.6 for hazardous decomposition products. If there is no data, use the B score for the material. If there are hazardous decomposition products, check section 12 of the SDS and use the table for the B score. If you would arrive at different B scores for different degradation products, use the highest number for the B score in DOZN.

Reaction Conditions

- Reflux 1
- Reflux 2
- Filter ether mixture
- Filter DCM layer

ADD A RAW M



Process Information

- If product is non-degradable enter the final mass of the product for Mass used for B score of Product
 - If the product is readily degradable, determine the mass of desired product used to determine B score; this mass can be estimated based on the ratio of separation
- The reaction is considered monitored if analytical methods were in place to alert chemist if the formation of hazardous chemicals or spills were to occur
- Anytime the Save bottom can be used to save the entry; the entry will not be scored
- To score the reaction: click the Save & Calculate bottom. The page will reload after score is processed
- Score and score breakdown will be found after the entry

Process Information

*B score of Product ⓘ <input type="text" value="Select"/>	*Mass used for B score of Product <input type="text"/>	*Unit <input type="text" value="g"/>
*Number of Catalytic Steps <input type="text"/>	*Number of Synthesis Steps <input type="text"/>	
Is Monitored? ⓘ <input type="radio"/> Yes <input type="radio"/> No		



DOZN™ 2.0 Results

- Aggregate score gives overall “greenness” of procedure
- Scores are broken down by each of the 12 principles of green chemistry
- Scores are also broken down to The Three Groups for easy comparison of procedures
- To save entry as Excel file, click the white “Download” box to the right of the results

DOZN SCORE RESULT

 Download

Aggregate Score



Scoring Matrix



Principle	Score
#1 Prevention	10.00
#2 Atom Economy	39.09
#3 Less Hazardous Chemical Synthesis	75.57
#4 Designing Safer Chemicals	2.89
#5 Safer Solvents and Auxiliaries	0.00
#6 Design for Energy Efficiency	202.61
#7 Use of Renewable Feedstocks	39.09
#8 Reduce Derivatives	0.00
#9 Catalysis	1.00
#10 Design for Degradation	2.20
#11 Real-time analysis for Pollution Prevention	1.00
#12 Inherently Safer Chemistry for Accident Prevention	57.47

Groups	Principles	Score
#1 Improved Resource Use	1, 2, 7, 8, 9, 11	15.03
#2 Increased Energy Efficiency	6	202.61
#3 Reduced Human and Environmental Hazards	3, 4, 5, 10, 12	27.63

Note: The intent of the DOZN tool is to compare relative “greenness” for similar products or processes, as indicated by a lower DOZN score.

