The o2h Discovery Green Chemistry Model – A Project Lifecycle Approach

o2h Discovery understands the responsibility it has to develop green and sustainable technologies for its company and the collaborators during a formative stage of the discovery process. The purpose of this document is to detail the green chemistry/sustainable processes that o2h Discovery has in place across the life cycle of a chemical product starting from design to procurement of raw materials, synthesis, analysis, dispatch and disposal to provide the necessary level of confidence for the collaborators to enter into or extend an existing collaboration with o2h Discovery.

The o2h Discovery green chemistry model is a design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances and possess little or no toxicity to human health and environment. This module will also benefit our collaborators as we adopt bio-degradable, eco-friendly green packaging material. Hence, the o2h discovery green chemistry model is developed with an aim to improve the efficiency of our chemical product by changing how chemicals are designed, manufactured and used by preventing or reducing the generation of harmful substances.

No.	Stage/Step	Process/Policy	Risk Level (1-High)	Resp.
A. Design				
A1	In-house chemistry check	o2h team evaluate the chemistry targets in effective manner to ensure the route of synthesis supported very well by reported literature procedures. o2h team has prepared in-house chemistry check via Chemfinder method to ensure to check the same/similar chemistry carried out within team or projects @ o2h.	2	TLs, HS
A2	Effective literature search	o2h team have an access of Sci-finder literature search tool which helps to find out the effective literature around the requested chemistry targets from the collaborators. o2h team believe in provide plan-A, B & C however they would go with best synthesis route which is proposed via strong literature route. o2h team only propose chemical ordering for preferred route first to reduce the chemicals inventory.	2	TLs, HS
A3	Scientific peer review	o2h team have strong scientific leadership team in UK and India. For the novel and exploratory chemistry, o2h team believe in discussing the novel and exploratory chemistry targets with scientific leadership team and get their feedback and make the most effective synthetic routes. o2h team also has scientific peer review meeting every Friday where o2h team discuss their chemistry challenges/learnings with larger team and exchange the knowledge and ideas. This process found very effective and help for quick troubleshooting the chemistry challenges.	2	TLs, HS
B. Chemical Procurement				
B1	In-house check	o2h SCM team always prefer to check the chemicals availability in o2h projects/store inventory before ordering. Majority of the o2h projects are offering the FTEs cost including the chemical cost with the threshold limit so there is no harm to use some chemical internally to save the cost and chemical waste.	3	SCM team
B2	Vendor Selection	o2h SCM team prefer to order chemical from the local/domestic vendor first which can save the unnecessary packaging waste and hazardous. If the chemical is not available in local/domestic vendor, o2h team then go with the selected international vendors who are well trusted and provide high quality material and packaging. o2h SCM team ensure to order the chemical in single pack where possible to prevent to generate unnecessary glass/plastic waste.	2	SCM team

B3	Common Chemicals	o2h SCM team make the strong inventory of common chemicals and solvent so they can utilize on the requirement basis and prevent their unnecessary ordering.	2	SCM team
B4	Hazardous chemicals	o2h team has developed & implemented the separate process for use of Hazardous chemicals in the laboratory. o2h team has identify the list of hazardous chemicals (HRC) and consider their minimum procurement of general use across the team. o2h has provided the separate fire proof cabinets for the storage of those hazardous chemicals and have assigned one dedicated in charge person who takes care of the HRC chemicals inventory monitoring and issuing process. For example, if chemist have planned the synthesis of any target which includes the use of HRC then firstly chemist have to fill the HRC checklist appendix-2 design by the R & D project/group leaders and get issue the hazardous chemical from the store. As o2h stores all the HRC chemicals separately at dedicated place and not inside the lab. After that a scientist will have to process the reaction in presence of either senior team member, safety officer or a person nominated in list of HRC handler (Appendix-3). o2h has implemented this process to prevent the risk of incidents cause by use of HRC inside the lab and to ensure that all the measured safety standards are followed well to handle HRC as per our "CORA Policy (chemical Operations Risk Assessment)" appendix-4. **Note:** *o2h team consider or use the large quantity of hazardous chemicals only if the chemistry goes well on small scale.*	1	TLs, safety team
B5	Solvents	o2h SCM team process the solvent procurement from nearby vendors on daily requirement basis to avoid un-necessary storage.	2	SCM team
C. Chemical Synthesis				
C1	Prevent Waste	Prevent Waste is a best practice that encourages chemists to minimize the amount of waste that is generated to avoid having to manage its downstream impacts. It is better to avoid a problem than try to fix it later. o2h team design chemical synthesis to prevent waste. Leave no waste to treat or clean up. o2h team ensure the chemical labelling with the proper code with expiry date so the chemical is use on time before it starts degrading and converted into waste. o2h team check the internal inventory for any chemical before making new purchases. o2h team practice to share the excess materials (which are not client approved materials) with a colleague or other lab. o2h has also recently donate some old chemicals to a local university for their research work. o2h team follow the proper segregation process of waste generated during the laboratory operations (e.g., halogenated solvent from non-halogenated, non-biohazardous from bio-hazardous).	1	TLs, scientists, YS, KS
C2	Maximize atom efficiency	o2h team design the synthetic routes which are shorter and cost effective. o2h team prefer the close reaction monitoring to ensure that the starting materials are consumed and reaction turned into maximum yield conversion to product and produce less waste. For the scale up projects, o2h team validate the chemistry in the fashion that produce the high conversion rate to the product and	1	TLs & scientists

		produce minimum waste and then apply the same process for the scale up.		
C3	Design less hazardous chemical synthesis	o2h team prefer to use less hazardous chemicals as much as possible during the route designing and synthesis rather o2h prefer to use the less hazardous and greener route for the synthesis. Since o2h team dealing with the majority of the MedChem project at small scale using the hazardous chemicals which are not suitable for scale up handling thus o2h team consider their alternative plans for the scale up synthesis to ensure safe operations and prevent the waste. o2h team more focus on the catalysis approach which are safe in handling and generate very minimum waste which can be re-cycle at certain points.	1	TLs
C4	Design safer chemicals and products	o2h team dealing with the majority MedChem and scale up projects which are novel so o2h team don't have major idea about the toxicology of the intermediate and final products. Thus, o2h team arrange a kick off meeting with the collaborator to understand the MedChem progress and toxicology the molecules designed by the collaborator and take necessary preventive measurement before execution of the project. If possible, o2h team come up with the alternative synthesis options where possible i.e., TMS-diazomethane is good and safer alternative of diazomethane. o2h team not consider use of NaCN, KCN rather they use other safer cynation reagent like TMS-CN etc where possible. During the chemistry execution, o2h team take all safety majors in the laboratory and if any they observed any toxic property of any intermediate/final product, o2h team immediately inform to the collaborator and discuss the issue on real time basis.	1	TLs
C5	Use safer solvents and reaction conditions	The use of auxiliary substances (e.g. solvents, separation agents, etc.) should be made unnecessary wherever possible and innocuous when used. Solvents are most commonly use in the laboratory for different purposes i.e. reaction media, extraction, purification, trituration, washing etc. Thus, use of right, minimum and safer solvent (green solvent – Ref- Byrne et al. Sustain Chem Process (2016) 4:7, Appendix-5, Ref-1) is very necessary to prevent the toxic environment and waste. o2h team consider the best and greener solvent for the chemical reactions, extractions and purifications. o2h team avoid carcinogenic solvents for their routing work where possible or handle with proper care. o2h team consider minimum volume of solvent for the reaction and purification. o2h team mostly consider the purification via trituration and flash purification to ensure minimum solvent waste. For large scale projects, o2h team consider the recycling of the solvents and reuse them.	1	TLs, scientists

C6	Increase energy efficiency	o2h team prefer to run chemical reactions at room temperature and pressure whenever possible. o2h team prefer more use of Microwave reaction for quick screening and then use the successful condition for scale up at convention method. o2h use the photochemistry where possible in the chemistry to reduce the energy consumptions. o2h laboratory facility and infrastructure has fully running LEDs lights with sensor which consume minimum power.	2	TLs, scientists
C7	Use renewable feedstocks	o2h team believe in renewable feedstocks. o2h team do the recycling of the solvents where possible and reuse them. o2h team prefer to use the protic solvents i.e., MeOH, EtOH, IPA which can be produces from the natural resources via fermentation. o2h team use the MeOH for the labware washing and re-distilled the used MeOH and reuse it again for the glassware washing.	2	TLs, safety team
C8	Avoid chemical derivatives	o2h team are strong in route designing and propose most efficient and shorter synthetic routes for novel MedChem molecules. o2h team prefer and ensure not to proposal unnecessary protection-deprotection which increase the number of steps which reduce the associated hazardous waste. o2h team prefer and store the intermediates/final compound at certain stage where they are stable at room temperature.	1	TLs & QA
C9	Use catalysts and not stoichiometric reagents	o2h team mostly prefer to use catalyst during the route designing and execution which minimize the waste generated by using catalytic reactions. Catalysts are effective in small amounts and can carry out a single reaction many times. Catalysts are preferable to stoichiometric reagents, which are used in excess and carry out a reaction only once. Some catalyst waste i.e., Pd-C are collected by the vendor and re-cycle it.	1	TLs, safety team
C10	Design chemicals and products to degrade after use	o2h team prefer to check the stability of each intermediate and final compounds synthesized during the chemistry execution at small scale first prior to scale up. o2h team prefer to store the intermediate/final compound at certain stage where they show good stability at room temperature. In some cases where intermediates/final compounds are not stable at room temperature, o2h team stored them at -80˚C refrigerator to avoid degradation which is again a source of hazardous waste.	1	TLs
C11	Analyse in real time to prevent pollution:	o2h team always prefer to do real time reaction monitoring by TLC, LCMS and HPLC analysis and conclude the reaction completion to ensure real-time monitoring and control during synthesis to minimize or eliminate the formation of by-products. o2h team prefer to identify the by-products formed during the synthesis by structural confirmation and discuss with the collaborator and supply them if they are key of their interest. o2h also consider the possible route to convert the by-product back to desired product where possible.	1	TLs
C12	Minimize the potential for accidents	o2h team always prefer to design the synthetic routes which includes less hazardous. Where possible, o2h team design experiments to use and generate substances that have the lowest health, safety and environmental impacts so risk of accidental	1	TLs, safety team

		expose or harm. o2h team prefer to use all preventive controls in the laboratory operations. These controls include personal protective equipment like gloves or lab coats; engineering controls like a fume hood, active cooling, or maximum reaction volumes. o2h team has established the process for hazardous reactions and scale up handling where senior support team help the chemist for the safe chemistry operation – for more detail please read section **B4**. o2h team has also identify the emergency response team for prevention of large incident. A strong EHS team of o2h always keep close eyes and regular audit of all the laboratories and entire facility of o2h discovery to ensure the smooth site operation. An automatic fire suppression and alarm system @ o2h keep site secure and prevent the major incident. o2h discovery site also have fire hydrant system which is the most effective and common firefighting solution.		
D. Chemical Analysis				
D1	Reducing amount and number of samples	o2h analytical team is effectively use the very less quantity of the sample for the analysis and also run the sample in generic method to fulfil the requirement of the chemistry and confirm the end results. The team always ensure to avoid the repeat analysis and confirm the result in sure shot method to indirectly helps to minimize the energy as well as solvent.	2	ADL team
D2	Combining analytical Process	o2h analytical team is always use hyphenated technique to confirm the product formation which will help to reduce the time consumption as well as cost of analysis. This also helps to reduce the solvent uses.	2	ADL team
D3	Reducing or avoiding pre-treatment steps and using direct method	o2h analytical team always prefer to use suitable technique which can easily identify/quantify the trace level impurities as well as product by adopting suitable detector and generally avoiding derivatization method to avoid reagent uses as well as solvent to minimize the waste generation.	1	ADL team
D4	Reducing reagent and waste	o2h analytical team trying to prefer SFC for the purification where CO_2 is used as mobile phase and other organic solvent with very less amount can be used to minimize the waste. Also help us to reduce the solvent evaporation in environment due to less uses of organic solvent.	2	ADL team
D5	Promoting simultaneously detection of multiple analytes	o2h analytical team prefer to use combined techniques to detect the multiple analytes in single analysis which help us to reduce the analysis time as well as solvent consumption. Also reduce the operation cost to save the energy.	2	ADL team
D6	Increase miniaturization and automation	o2h analytical team is using fully automated system to avoid error in the analysis and also help to avoid repeat analysis. Team is capable enough to develop the purification method in shorter column in automated system to improve the productivity as well as reduce the solvent consumption which help us to reduce waste solvent generation.	2	ADL team
E. Chemical Packaging/Dispatch				
It is better to prevent waste or non-biodegradable waste material than to treat or clean up waste material after it is formed and o2h understand it's responsibility to protect the environment by using the sustainable or green packing material. We encourage use of bio-degradable packaging and ensuring procurement through vendors empanelling this policy in their packaging to ensure compliance.				

E1	Use of environment friendly green packaging or sustainable packing material	Green packaging or sustainable packaging material refers to the sourcing, development and use of packaging solutions that have minimal environmental impact and footprint. We at o2h, encourage our chemist & project team to use such kind of packing materials to minimize the level of harmful or non-biodegradable packing material as much as possible and to follow this we use variety of biodegradable or recyclable materials which are available in different forms like, Use of starch based packaging derives, plant base bio-materials, bio-plastic, use of corrugated bubble wrap instead of using traditional plastic bubble wrap which is fun to pop but because it is non-biodegradable plastic, its less fun for the environment when it ends up in landfills, than use of 100 % recycled bulk bags. All these are lightweight and inexpensive, and they won't harm marine life if they end up in rivers, lakes or oceans. Thus, use of above all material does not include any material in their manufacturing that are harmful to the earth and all these gives excellent choices for their bio-degradability and they are incredibly eco-friendly.	1	TLs, SCM team
E2	Use of green packing solutions	Use of green packing solutions also one of the good option that offers a wide range of benefits to protect the environment. Below are few sustainable packaging examples: ● **Packaging that includes renewable resources:** Cellulose, for example, which derives from wood pulp, is an attractive alternative to petroleum-derived polymers such as PET, PE and PP. Starch-based biomaterial is also an appealing alternative. ● **Packaging with additives:** Packaging additives, primarily biodegradable, Oxo-degradable and photodegradable materials, help the packaging biodegrade faster and reduce the accumulation of packaging waste. ● **Recyclable materials:** These include familiar materials such as cardboard, plastic and metals. ● **Compostable materials:** These include the materials like the compostable molded-fiber bowls that some fast-casual restaurants now offer their patrons. ● **Packaging reduction:** Have you ever opened a bag of cookies or chips, only to realize that the amount of food takes up only half the space inside the package? Green packaging strives to reduce the amount of packaging per product it contains. Even if manufacturers cannot switch the type of material used in their packaging, they can take steps to optimize the packaging by reducing the amount of material used to make it.	2	SCM team
E3	Benefits of using green packaging	Use of green packaging at o2h can offer a wide array of benefits for both client and the environment like… 1) **Increased use of recycled product:** the more we can re-cycle material, the less energy and fewer resources we waste on creating all new packaging. Moreover, recycled	1	SCM team, TLs

		product use less water and less energy than brand new material. Green packaging often strives to meet goals such as using 100% post-consumer recycled paper products and plastics 2) **Diminished reliance on fossil fuels:** Green packaging strives to use as little fossil fuel energy as possible to reduce the carbon footprint of packaging manufacturing. 3) **Reduced use of natural resources:** By designing minimal packaging, green packaging manufacturers help reduce the consumption of natural resources. This reduction helps ensure resources will remain on our planet for future generations. 4) **More energy-efficient manufacturing methods:** Instead of relying on fossil fuels, green packaging strives to use alternative power, such as wind or solar energy. 5) **Increased use of renewable resources:** Instead of using paper derived from cutting down trees, for example, some green packaging manufacturers use paper that comes from agricultural fibres instead.		
F. Chemical Disposal				
F1	Collection of chemical waste	The collection of waste chemicals/materials at o2h includes not only the gathering of different categories of waste and recyclable materials but also the transport of these materials after collection to the location vehicle is emptied. This location may be GPCB approved chemical processing facility, a transfer station or a landfill disposal site.	1	Safety team
F2	Handling, separation, storage & processing of chemical/waste disposal	At o2h, our chemistry team is well trained and aware on the handling, separation & storage of chemical waste. We follow our internal SOP of "Waste Management" to handle and dispose waste appropriately. From waste origin to waste disposal it is o2h responsibility to ensure generation, collection, transfer, storage and disposal of waste appropriately. Our chemistry team at o2h separates the waste according to state & nature of waste produced before, during & after the synthesis process. Segregating waste from, the origin of generation to follow waste segregation protocol & informing EHS & team leader for any specific disposal of chemical. We have categorized the generated waste in two main categories: 1) Hazardous waste 2) Solid non-hazardous waste **1) Hazardous waste:** ● all the generated hazardous waste like process residue silica, organic solvent waste, empty glass containers or chemical bottles, PPEs, syringes, needles, capillaries etc. are collected in dedicated labelled waste containers and stored at dedicated place only with label "Hazardous waste only". ● once the hazardous waste collected, it is transport to the GPCB (Gujarat Pollution Control Board) authorized waste disposal facility as per the statutory requirement given in the guideline of "Transport Storage Disposal Facility" to control the accumulation at each site of o2h. in the	1	Safety team, TLs

		conclusion o2h makes sure that all the generated hazardous waste are further treated, recycled and reused to save the environment & gain the ecological benefits. ● Moreover, waste collected in ETS/STP collection tank are further treated through various process step to recover the treated water and that recovered treated water are further used in gardening, toilet flush & utility. The remaining waste i.e. ETP sludge collected & packed separately and transported to the TSDF (landfill facility) for disposal or landfilling. **2) Solid non-hazardous waste:** All the generated solid non-hazardous waste like stationary waste, food/canteen waste, packing cartoons etc. are stored separately in dedicated waste bin & transferred to the authorized recycler on daily or weekly basis to control the waste accumulation at o2h.		
G. Engineering and Infra				
G1	Glass façade	o2h has chosen glass with a U value 2.8W/m2K for the façade for its Shirish Research Park. The glass with this U value (i) provides higher natural light transmission thereby reducing the need for artificial lights in specific areas of the building and (ii) comes with a low solar factor whereby the heat load in the pertinent areas of the building (adjacent to the façade) is reduced which in turn leads to lower cooling requirement in that area.	3	Eng. team
G2	Cavity brickwork	In exterior walls we used cavity type brickwork for insulation. The air in the cavity wall acts as a non-conductor of heat and hence minimizes the transmission of heat from the outer leaf to the internal face of the interior leaf. Thus, cavity walls help in maintaining the thermal insulation of a premise.	3	Eng. team
G3	Skylight	We have large skylights on top floor labs. Which provides higher natural light transmission. Whereas using 2.8W/m2K u value glass maintain the solar factor.	3	Eng. team
G4	Slant walls	Slant walls/partition on top floor maximise the natural sunlight which helps in energy efficiency.	3	Eng. team
G5	Furniture material	Using reclaimed wood for furniture, which can help reduce air pollution and the potential for leaching into local waterways.	2	Eng. team
G6	Building material	For RCC structure used fly ash content in concrete to reduce cement usage, results in decreasing concrete's carbon footprint, while increasing its strength and workability. Also, reduce water demand and superplasticizer needs. Also, using fly ash brick to reduction in energy use and greenhouse gas and other adverse air emissions.	2	Eng. team
G7	Tree plantation	Implementing use of high vegetation for reducing heat absorption. Plantation of >5 trees/200sqm area.	2	Eng. team
G8	Rainwater harvesting	Average rainfall of Ahmadabad is 753mm. In 6,323 sqm area of o2h premises possible water collection per year is 2, 857 m3 and form roof top 1256 m3/year. Overflow water is connected to 2 borewells to increase the water level in surrounding area. After filtration water is collected in storage tank which is used for domestic, irrigation & HVAC make-up. It also reduces the chances	2	Eng. team

		of flooding around building. It not only reduces the water bills but also reduces the carbon footprint.		
G9	ETP/STP plant	We have zero discharge ETP/STP plant. The plant discharges no liquid effluent into surface waters, in effect completely eliminating the environmental pollution associated with treatment. Process also makes effective use of wastewater treatment, recycling, and reuse, thereby contributing to water conservation through reduced intake of fresh water.	2	Eng. team
G10	HVAC	Using AHUs with Plate Heat Exchanger along with EC fans for energy efficiency. In exhaust blower I3 efficient motors are used. Also has auto temperature control to minimise chiller electric load. Used ultra-high-performance fume hoods with VAV (variable air-volume) configuration to reduce HVAC capacity and operations.	2	Eng. team
G11	Scrubber system	Used scrubber system to remove harmful materials from labs exhaust gases before they are released into the environment.	1	Eng. team
G12	VOC sensors	In order to keep the working environment healthy, safe, and risk-free we have VOC sensors configured in labs.	1	Eng. team
G13	Daylight & motion sensors	Installed daylight sensors in office area & motion sensors in labs to reduce electricity consumption by eliminating the possibility that the lights will accidentally be left on. As mentioned before, energy consumption uses fossil fuels and produces CO2 emissions that are harmful to the environment.	2	Eng. team
G14	Solar panels	We are working on implementing solar panels on rooftop with 72kW installation capacity. A renewable source of power, solar energy has an important role in reducing greenhouse gas emissions and mitigating climate change, which is critical to protecting humans, wildlife, and ecosystems. Solar energy can also improve air quality and reduce water use from energy production.	2	Eng. team
G15	EV charging station	Working on EV charger's implementation on site to encourage use electric vehicles.	3	Eng. team
G16	Smart Toilet	Installed eco-efficient sanitary ware with sensors for toilet flushing system & wash basin tap. With the use of sensors water wastage is minimal as the flush strictly regulates the amount of water used to flush, and it automatically stops every time after it is used.	3	Eng. team

Appendix:

Appendix-1: Legends

Abbreviation	Full Name	Designation
TLs	Team leaders	Including group leaders & Project leaders
HS	Hemal Soni	Head of Chemistry
YS	Yasir Shehravi	Assistant Manager- EHS

KS	Kiran Soni	Assistant Manager- EHS
SCM Team	Supply Chain Management team	-
o2h	o2h Discovery Pvt. Ltd.	-
ETP	Effluent Treatment Plant	-
STP	Sewage Treatment Plant	-
EV station	Electric Vehicle charging station	-
Kw	Kilowatt	-
FTE	Full Time Employee	-
HRC	High Risk Chemicals	-
CORA	Chemical Operations Risk Assessment	-
MeoH	Methanol	-
EtoH	Ethanol	-
IPA	Isopropyl Alcohol	-
TLC	Think Layer Chromatography	-
LCMS	Liquid Chromatography-Mass Spectrometry	-
HPLC	High Performance Liquid Chromatography	-
ADL	Analytical Development Laboratory	-
GPCB	Gujarat Pollution Control Board	-
PPEs	Personal Protection Equipment	-
TSDF	Transport Storage Disposal Facility	-
HVAC	Heating Ventilation Air-conditioning system	-
AHU	Air Handling Unit	-
VAV	Variable Air Volume	-
VOC sensors	Volatile Organic Compound sensors	-

Appendix-2: HRC checklist

o2h - Chemical Operations Safety C

Appendix-3: HRC handler list

HRC handler list.pdf

Appendix-4: CORA Policy

O2h Guidelines - Chemical Operation

Appendix-5: Sustainable chemical process

Byrne et al. Sustain Chem Process (2016)