Comprehensive additive release and bioaccessibility model for risk assessment of micro- and nano-plastics in the environment

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Primary Objective: *Create a robust and generalizable model to predict polymer additive release, transformation (where relevant), and bioaccessibility in context of realistic aquatic environments*

This objective will be addressed through the following work packages (WP):

WP #1: Compile a comprehensive literature review of polymer additive chemical space, application by polymer type, transformation, and leachability in context of ambient waters and ecological receptor ingestion.

WP #2: Build and test a quantitative model to predict additive distribution among environmental compartments including polymer particles, water, and digestive environments representing deposit feeders, filter feeders, aquatic predators, and humans.

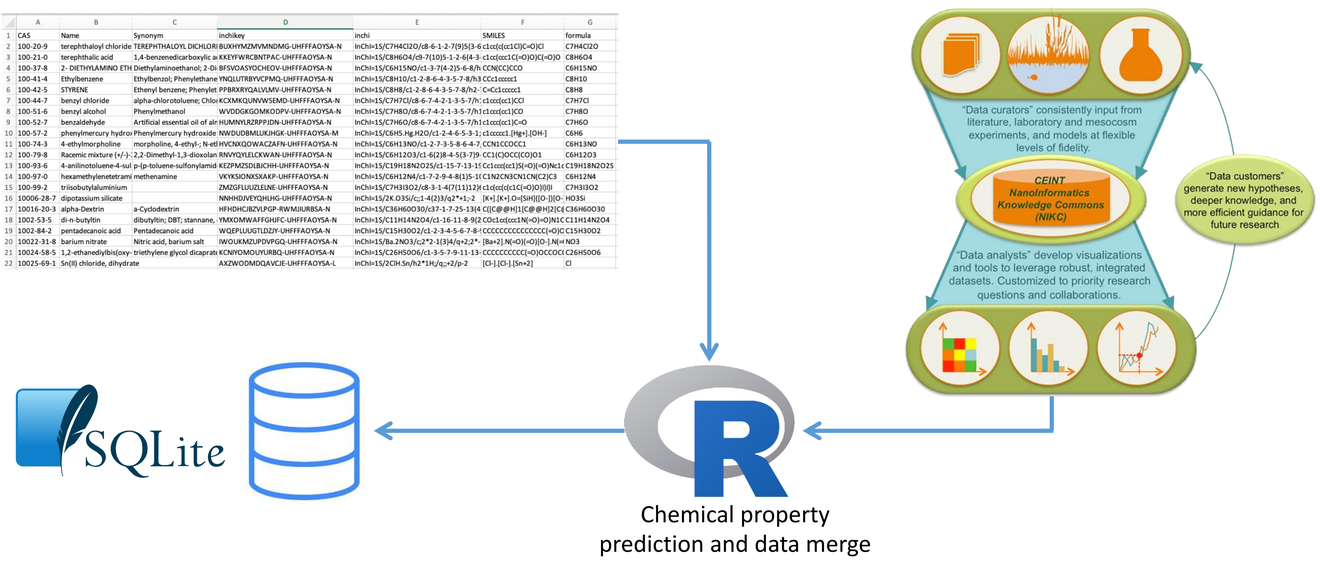
WP #3: Perform laboratory-based polymer additive leaching/bioaccessibility experiments designed to parameterize, validate, and test the model built in WP# 2.

Literature review and additive database

The primary output will be a three-element database designed to capture current knowledge associated with three data types:

- Data Type 1: Additive properties, based on measured or predicted molecular/material parameters
- Data Type 2: Polymer properties, based on bulk performance/manufacturing parameters of common-use and performance plastics
- Data Type 3: Environmental/receptor properties, describing relevant parameters of natural waters and receptor organism gut physiology

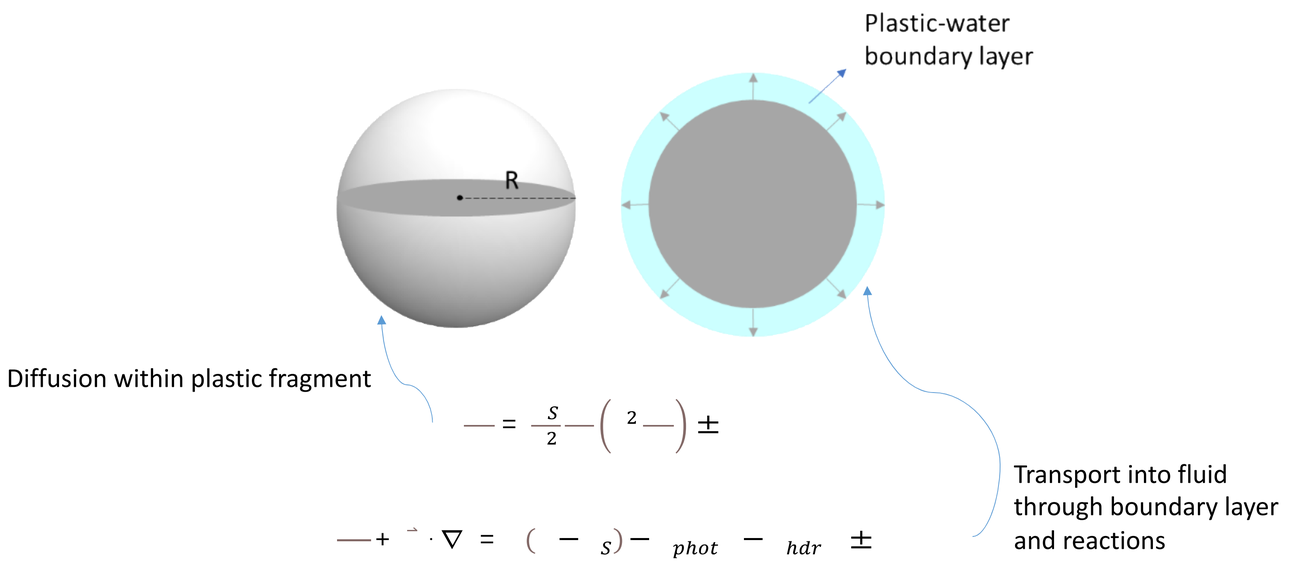
	A	B	C	D	E	F	G
1	CAS	Name	Synonym	inchikey	inchi	SMILES	formula
2	100-20-9	terephthaloyl chloride	TEREPHTHALOYL DICHLOR	BUXHYMZMVMNDMG-UHFFFAOYSA-N	InChI=1S/C7H4Cl2O/c8-6-1-2-7(9)5(3-6	c1cc(c(cc1Cl)C=O)Cl	C7H4Cl2O
3	100-21-0	terephthalic acid	1,4-benzenedicarboxylic a	KKEYFWRCBNTPAC-UHFFFAOYSA-N	InChI=1S/C8H6O4/c9-7(10)5-1-2-6(4-3-	c1cc(ccc1C(=O)O)C(=O)O	C8H6O4
4	100-37-8	2- DIETHYLAMINO ETH	Diethylaminoethanol; 2-Di	BFSVOASYOCHEOV-UHFFFAOYSA-N	InChI=1S/C6H15NO/c1-3-7(4-2)5-6-8/h	CCN(CC)CCO	C6H15NO
5	100-41-4	Ethylbenzene	Ethylbenzol; Phenylethane	YNQLUTRBYVCPMQ-UHFFFAOYSA-N	InChI=1S/C8H10/c1-2-8-6-4-3-5-7-8/h3	CCc1ccccc1	C8H10
6	100-42-5	STYRENE	Ethenyl benzene; Phenylet	PPBRXRYQALVLMV-UHFFFAOYSA-N	InChI=1S/C8H8/c1-2-8-6-4-3-5-7-8/h2-	C=Cc1ccccc1	C8H8
7	100-44-7	benzyl chloride	alpha-chlorotoluene; Chlo	KCXMKQUNVWSEMD-UHFFFAOYSA-N	InChI=1S/C7H7Cl/c8-6-7-4-2-1-3-5-7/h	c1ccc(cc1)CCl	C7H7Cl
8	100-51-6	benzyl alcohol	Phenylmethanol	WVDDGKGOMKODPV-UHFFFAOYSA-N	InChI=1S/C7H8O/c8-6-7-4-2-1-3-5-7/h	c1ccc(cc1)CO	C7H8O
9	100-52-7	benzaldehyde	Artificial essential oil of alr	HUMNYLRZRPPJDN-UHFFFAOYSA-N	InChI=1S/C7H6O/c8-6-7-4-2-1-3-5-7/h	c1ccc(cc1)C=O	C7H6O
10	100-57-2	phenylmercury hydrox	Phenylmercury hydroxide	NWDUDBMLUKJHGK-UHFFFAOYSA-M	InChI=1S/C6H5.Hg.H2O/c1-2-4-6-5-3-1;	c1ccccc1.[Hg+].[OH-]	C6H6
11	100-74-3	4-ethylmorpholine	morpholine, 4-ethyl-; N-et	HVCNXQOWACZAFN-UHFFFAOYSA-N	InChI=1S/C6H13NO/c1-2-7-3-5-8-6-4-7/	CCN1CCOCC1	C6H13NO
12	100-79-8	Racemic mixture (+/-)-;	2,2-Dimethyl-1,3-dioxolan	RNVYQYLELCKWAN-UHFFFAOYSA-N	InChI=1S/C6H12O3/c1-6(2)8-4-5(3-7)9-	CC1(C)OCC(CO)O1	C6H12O3
13	100-93-6	4-anilinotoluene-4-sul	p-(p-toluene-sulfonylamid	KEZPMZSDLBJCHH-UHFFFAOYSA-N	InChI=1S/C19H18N2O2S/c1-15-7-13-1	Cc1ccc(cc1)S(=O)(=O)Nc1c	C19H18N2O2S
14	100-97-0	hexamethylenetetrami	methenamine	VKYKSIONXSXAKP-UHFFFAOYSA-N	InChI=1S/C6H12N4/c1-7-2-9-4-8(1)5-1(	C1N2CN3CN1CN(C2)C3	C6H12N4
15	100-99-2	triisobutylaluminium		ZMZGFLUUZLELNE-UHFFFAOYSA-N	InChI=1S/C7H13O2/c8-3-1-4(7(11)12)9	c1c(cc(c1C(=O)O)[O])	C7H13O2
16	10006-28-7	dipotassium silicate		NNHHDJVEYQHLHG-UHFFFAOYSA-N	InChI=1S/2K.O3Si/c;;1-4(2)3/q2*+1;-2	[K+].[K+].O=[SiH]([O-])[O-	HO3Si
17	10016-20-3	alpha-Dextrin	a-Cyclodextrin	HFHDHCJBZVLPGP-RWMJIURBSA-N	InChI=1S/C36H60O30/c37-1-7-25-13(4	C([C@@H]1[C@@H]2[C(	C36H60O30
18	1002-53-5	di-n-butyltin	dibutyltin; DBT; stannane,	YMXOMWAFFGHJFC-UHFFFAOYSA-N	InChI=1S/C12H26O4Sn/c1-5-9-13-17(1	CCCCO[Sn](=O)(=O)OCCCC	C12H26O4Sn
19	1002-84-2	pentadecanoic acid	Pentadecanoic acid	WQEPLUUGTLDZJY-UHFFFAOYSA-N	InChI=1S/C15H30O2/c1-2-3-4-5-6-7-8-	CCCCCCCCCCCCCC(=O)O	C15H30O2
20	10022-31-8	barium nitrate	Nitric acid, barium salt	IWOUKMZUPDVPGQ-UHFFFAOYSA-N	InChI=1S/Ba.2NO3/c;2*2-1(3)4/q+2;2*	[Ba+2].[N+](=O)([O-])[N+](=O)[O-	BaN2O6
21	10024-58-5	1,2-ethanediylbis(oxy-	triethylene glycol dicaprat	KCNYOMOUYURBQ-UHFFFAOYSA-N	InChI=1S/C26H50O6/c1-3-5-7-9-11-13-	CCCCCCCCCC(=O)OCCOCCOC	C26H50O6
22	10025-69-1	Sn(II) chloride, dihydrate		AXZWODMDQAVCJE-UHFFFAOYSA-L	InChI=1S/2ClH.Sn/h2*1H;/q;;+2/p-2	[Cl-].[Cl-].[Sn+2]	Cl



Additive release model development and testing

The primary output will be numerical code that can be integrated as a subroutine in a larger particle- population model for particulate plastics.

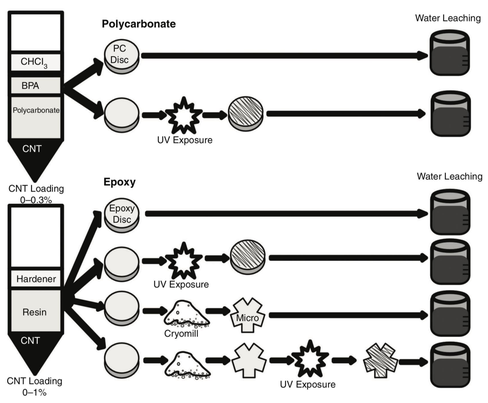
- Mathematical formulation for several cases:
  - Non-reactive additives
  - Reactive additives and pertinent degradation reactions
  - Non-homogeneous distribution within fragments
- Calculation of additive release in a variety of media including:
  - Ocean water
  - Fresh water
  - Representative vertebrate gut environments



Additive leaching and bioaccessibility experiments

Experiments will be designed to explore:

- Influence of additive chemical structure on leachability (QSAR approach)
- Polymer type/geometry/chemistry as a driving factor for leachability
- Impact of type and extent of weathering (e.g. physical vs. chemical vs. photolytic) on additive leaching
- Additive localization on/in polymer and its influence on leaching
- Gut digestive fluid parameters and their importance to additive leaching from polymers
- Reactivity and transformation of leachable additives



Adapted from: Walker, I. et al., *Environ. Chem.* 2021, 18, 131–141

Additive Type	• Surface-coating (e.g. PFAS components for stain resistance/water-repellency) • Intrinsic additive (e.g. disperse azobenzene dyes in polyester microfibers) • Performance additive (e.g. antioxidants such as Irgafos 168 or UV inhibitors such as Tinuvin 770)
Polymer Type	• Polyolefin (relatively inert to direct UV degradation, e.g. polypropylene) • Aromatic thermoplastic (glassy and UV-active, e.g. polystyrene) • Elastomer (rubbery and subject to oxidation, e.g. polyurethane)
Weathering Treatment	• UV exposure (pre-treatment of polymer with SUNTEST XLS+ in laboratory) • Physical abrasion/fragmentation (laboratory abrader or cryomill) • Oxidant exposure (pre-treatment with ozone or peroxide)
Leaching Treatment	• Water (fresh-to-brackish, pH 5-8, dissolved organic matter, temperature 4º - 40º C) • Simulated or actual digestive fluid (bile salt surfactants, lipase, pepsin, other enzymes, pH 2-7)

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