Supplementary Information (SI) for RSC Applied Polymers.

Supplementary Information: Convergence of high throughput experimentation and machine learning to rapidly advance application-specific polymer development

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Polymer Sample Record Checklist:

Sample Structure

- ☐ Sample ID
- ☐ Repeat unit structure
- ☐ Molecular weight
- ☐ **Polymer** Representation (SMILES, SMARTS, SELFIES, etc)

Synthesis and PurificationPurPup Conditions

- ☐ Temperature
- ☐ Pressure
- ☐ Catalyst
- ☐ pH level of reaction
- ☐ Solvent/Medium
- ☐ Concentration
- ☐ Reaction Time
- ☐ Processing conditions
- ☐ Heating medium
- ☐ Cooling Method
- ☐ Stirring Method
    - ○ Revolutions Per Minute
    - ○ Mixing time
- ☐ Batch or Flow
    - ○ Reactor type
- ☐ Purification Method

    - Type of method used (precipitation, chromatography, etc)
    - Filtration Medium (Büchner Funnel, Membrane, etc)

Sample Preparation/Conditions

- ☐ Amount used
- ☐ Annealing
    - ☐ Time
    - ☐ Temperature
    - ☐ Apparatus (oven, hot plate, etc)
- ☐ Molding conditions
    - ☐ Geometry
    - ☐ Temperature
    - ☐ Pressure
- ☐ Casting conditions
    - ☐ Solvent(s)
    - ☐ Additive(s)
    - ☐ Revolutions per minute
    - ☐ Film thickness
- ☐ Other preparation
    - ☐ Powderization (method, details, etc.)
    - ☐ Coating (material, method, amount, etc.)

Label Measurements

- ☐ Replicates
- ☐ Uncertainties
- ☐ Measurement method
- ☐ Units
- ☐ Labelling Source (Humans, AI, Automated Software)

Instrument Settings

- ☐ Calibration Metadata
- ☐ Instrument Used
- ☐ Measurement Units
- ☐ Model/serial number of instruments

Supplementary

- ☐ Labeler ID
- ☐ Raw data files

- ☐ Notes/comments
- ☐ Software/firmware version

Example Polymer Sample Record

Sample Structure	
Sample ID	PMMA-HTE-2026-03-001
Polymer Name	Poly(methyl methacrylate)
Repeat Unit Structure	–CH_2–$C(CH_3)(COOCH_3)$–
Molecular Weight	120,000 g/mol
Number Average Molecular Weight (Mn):	60,000 g/mol
Polydispersity Index (PDI):	2
Polymer Representation	Monomer SMILES: CC(=C)C(=O)OC Polymer repeating unit SMILES: [*]CC(C)(C(=O)OC)[*]

Processing and Purification Conditions	
Sample ID	PMMA-HTE-2026-03-001
Heating Medium:	Oil bath
Cooling Method:	Room temperature air cooling
Stirring Method:	Magnetic stir bar
Revolutions Per Minute (RPM):	500 RPM
Batch or Flow:	Batch reactor
Mixing Time:	10 minutes prior to polymerization
Reactor Type:	Round-bottom glass flask (250 mL) with reflux condenser
Purification Method Used:	Precipitation
Filtration Medium:	Büchner funnel with filter paper
Drying Method:	Vacuum oven (40 °C overnight)

Synthesis Conditions	
Sample ID	PMMA-HTE-2026-03-001
Polymerization Method:	Free Radical Polymerization
Temperature:	70 °C
Pressure:	1 atm
Catalyst / Initiator:	Azobisisobutyronitrile (AIBN)
pH Level of Reaction:	Neutral (~7)
Solvent / Reaction Medium:	Toluene
Monomer Concentration:	2.5 M methyl methacrylate
Reaction Time:	6 hours

Label Measurements	
Uncertainties:	Molecular weight uncertainty: ±5% Contact angle measurement uncertainty: ±2°
Measurement Method:	Gel Permeation Chromatography (GPC) for molecular weight Contact angle goniometry for surface wettability
Units:	Molecular weight → g/mol Temperature → °C Pressure → atm Contact angle → degrees (°)
Labelling Source:	Automated software + human verification

Instrument Settings	
Sample ID	PMMA-HTE-2026-03-001
Instrument Used:	Agilent 1260 Infinity II GPC
Instrument Settings	Flow rate: 1.0 mL/min Column temperature: 35 °C Detector: Light Scattering Eluent: THF
Calibration Metadata	Calibration standards: Polystyrene standards (500–500,000 g/mol) Calibration date: 2026-03-01 Calibration uncertainty: ±3%

Supplementary Information	
Sample ID	PMMA-HTE-2026-03-001
Labeler ID:	LAB-OP-23
Raw Data Files:	PMMA_HTE_2026_03_001_GPC.csv PMMA_HTE_2026_03_001_contact_angle_images/ PMMA_HTE_2026_03_001_reaction_log.txt
Storage Location:	Polymer Data Repository → HTE_Polymers → 2026 → PMMA