Supplementary Information

Unveiling the knowledge of a RAFT polymerizations database obtained from an automated parallel synthesizer

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1. Example NMR spectra and SEC curves

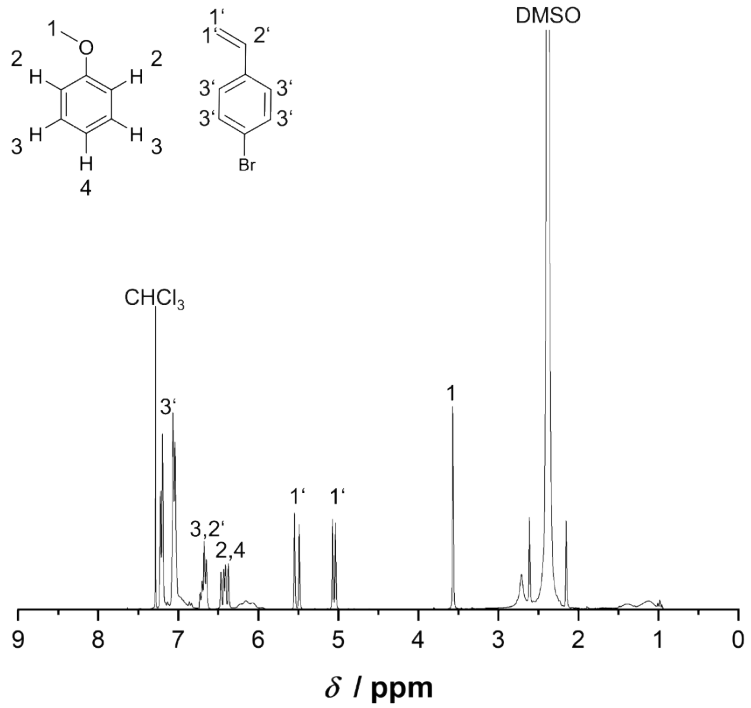

Figure S1: ^{1}H-NMR spectrum of the polymerization of 4-bromostyrene with 4-cyano-4-(phenylcarbonothioylthio)pentanoic acid in dimethyl sulfoxide utilizing anisole as standard after 15 h. The signals of the monomer and standard are assigned. The remaining signals can be attributed to polymeric species of the monomer. (300 MHz, $CDCl_3$).

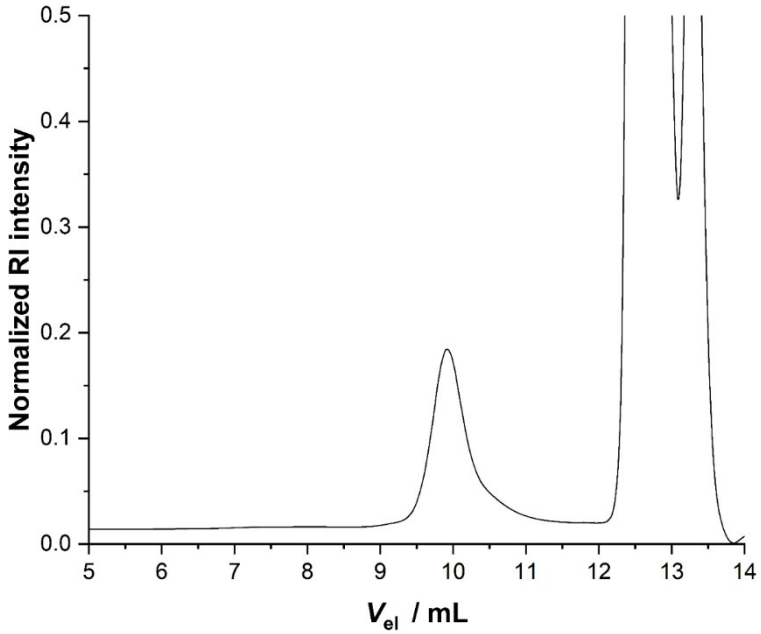

Figure S2: Zoom into normalized SEC curve of a sample retrieved after 15 h from a polymerization of 4-bromostyrene with 4-cyano-4-(phenylcarbonothioylthio)pentanoic acid in dimethyl sulfoxide utilizing anisole as standard. (Eluent = 94/4/2 vol% chloroform, triethylamine, *iso*-propanol; poly(styrene) standard).

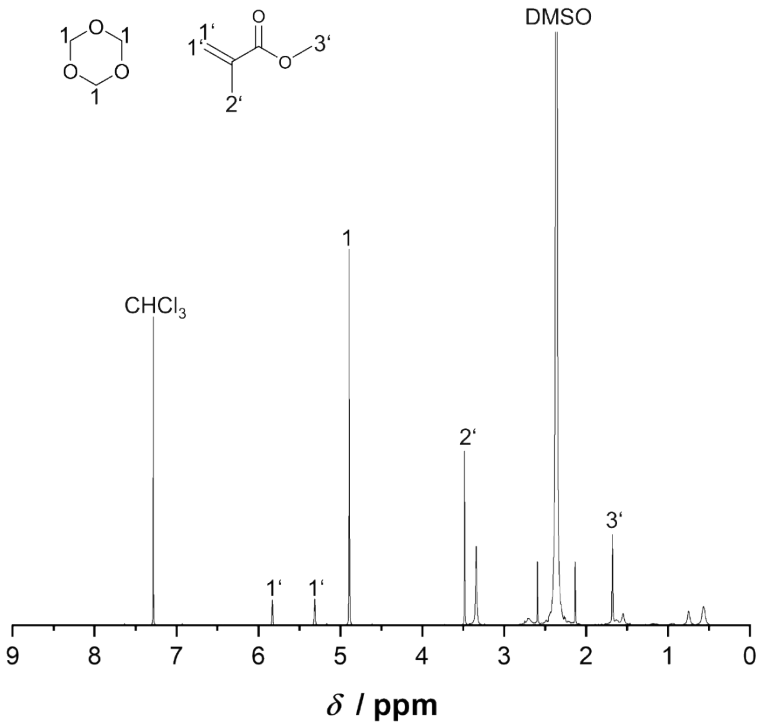

Figure S3: ^{1}H-NMR spectrum of the polymerization of methyl methacrylate with 4-cyano-4-(phenylcarbonothioylthio)pentanoic acid in dimethyl sulfoxide utilizing 1,3,5-trioxane as standard after 15 h. The signals of the monomer and standard are assigned. The remaining signals can be attributed to polymeric species of the monomer. (300 MHz, $CDCl_3$).

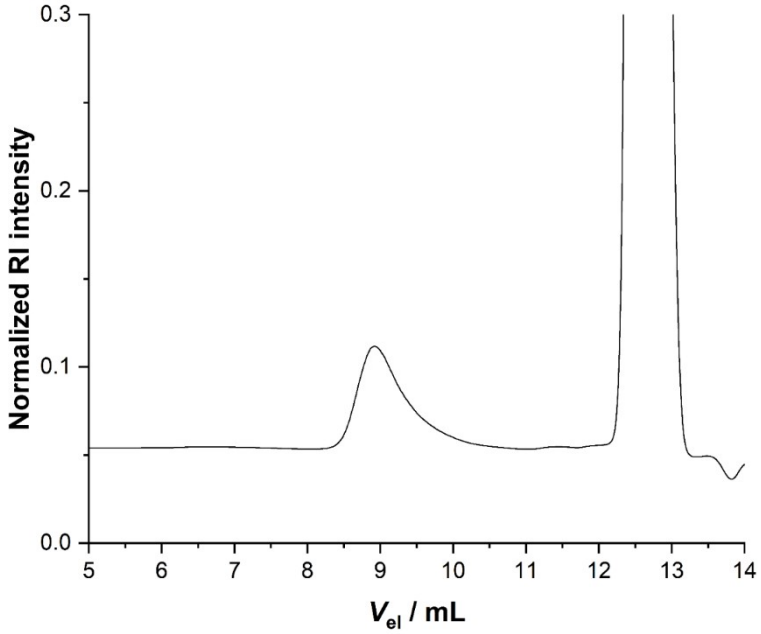

Figure S4: Zoom into normalized SEC curve of a sample retrieved after 15 h from a polymerization of methyl methacrylate with 4-cyano-4-(phenylcarbonothioylthio)pentanoic acid in dimethyl sulfoxide utilizing 1,3,5-trioxane as standard. (Eluent = 94/4/2 vol% chloroform, triethylamine, *iso*-propanol; poly(styrene) standard).

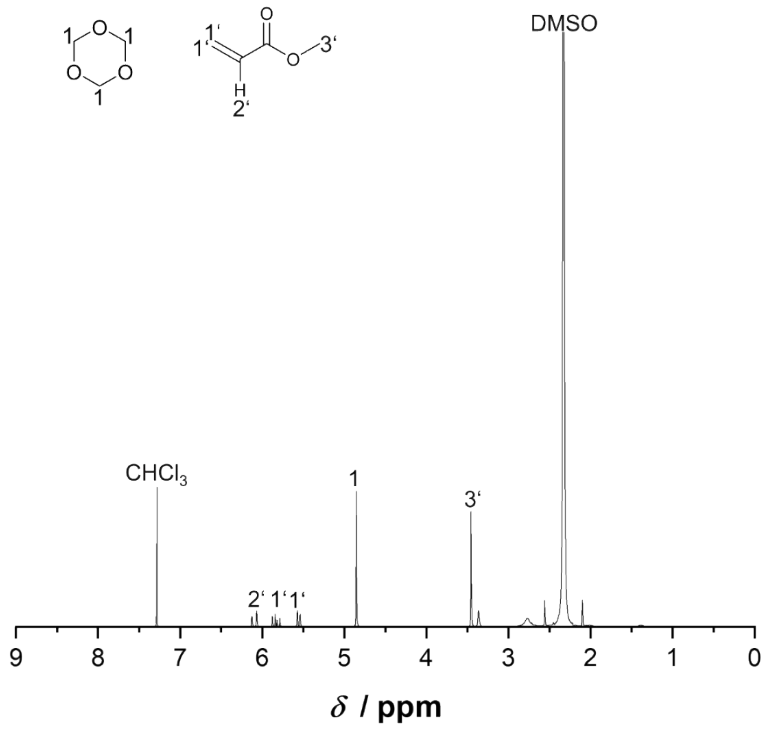

Figure S5: ^{1}H-NMR spectrum of the polymerization of methyl acrylate with 4-cyano-4-(phenylcarbonothioylthio)pentanoic acid in dimethyl sulfoxide utilizing 1,3,5-trioxane as standard after 15 h. The signals of the monomer and standard are assigned. The remaining signals can be attributed to polymeric species of the monomer. (300 MHz, $CDCl_3$).

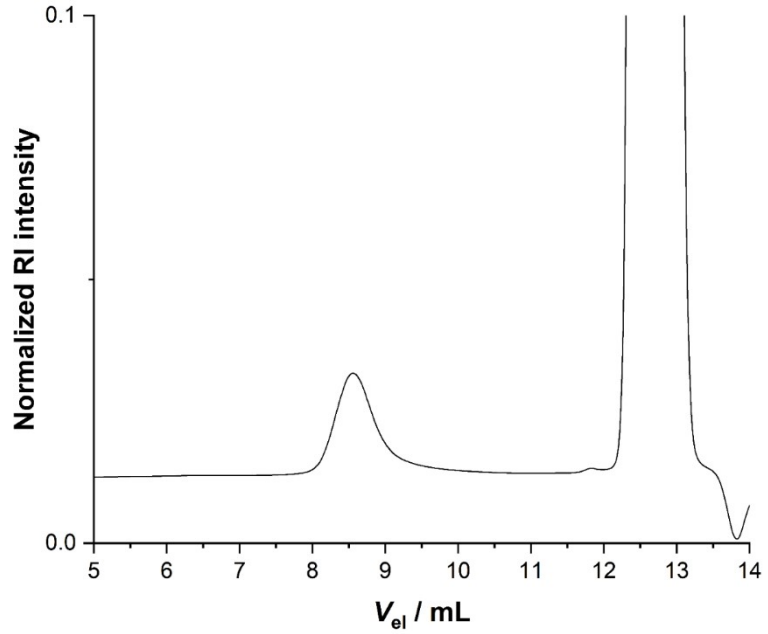

Figure S6: Zoom into normalized SEC curve of a sample retrieved after 15 h from a polymerization of methyl acrylate with 4-cyano-4-(phenylcarbonothioylthio)pentanoic acid in dimethyl sulfoxide utilizing 1,3,5-trioxane as standard. (Eluent = 94/4/2 vol% chloroform, triethylamine, *iso*-propanol; poly(styrene) standard).

2. Permutation tables and overview of performed polymerizations

In the following six tables, the information about whether or not the reactions could lead to a satisfactory result (see curation criteria) are accessible. The first tables S1, S2 and S3 provide all abbreviation-determiners. The subsequent three tables S4 to S6 are the solvent-wise monomer-RAFT-agent permutation tables. “YES” means the reaction analytics met the expected criteria of a RAFT polymerization at least once (if the reaction was carried out multiple times). “NO” means the opposite. Empty entries mean that the polymerizations have not been carried out.

Table S1: Dictionary for all monomer abbreviations in the permutation tables.

Determiner	Monomers
1	Styrene
2	4-Chlorostyrene
3	4-Bromostyrene
4	4-Methylstyrene
5	4-Methoxystyrene
6	Methyl methacrylate
7	Butyl methacrylate
8	Lauryl methacrylate
9	2-(Dimethylamino)ethyl methacrylate
10	Benzyl methacrylate
11	Methyl acrylate
12	Butyl acrylate
13	Lauryl acrylate
14	2-(Dimethylamino)ethyl acrylate
15	Benzyl acrylate
16	4-*tert*-Butylstyrene

Table S2: Dictionary for all RAFT-agent abbreviations in the permutation tables.

Determiner	RAFT-agent
A	2-Cyano-2-propyl benzodithioate

B	4-Cyano-4-(phenylcarbonothioylthio)pentanoic acid
C	2-Phenyl-2-propyl benzodithioate
D	2-Cyano-2-propyl dodecyl trithiocarbonate
E	2-(Dodecylthiocarbonothioylthio)-2-methylpropionic acid
F	Cyanomethyl dodecyl trithiocarbonate
G	Benzyl 1H-pyrrole-1-carbodithioate

Table S3: Dictionary for all solvent abbreviations in the permutation tables.

Determiner	**Solvents**
DMF	Dimethyl formamide
Tol	Toluene
DMSO	Dimethyl sulfoxide

Table S4: Permutation table for all Reactions successfully (YES, resulting in satisfiable results) and non-successfully (NO, analytic results deviated from the expected reaction) performed in dimethyl sulfoxide.

DMSO	**A**	**B**	**C**	**D**	**E**	**F**	**G**
1	YES	YES	YES	YES	YES	YES	YES
2	YES	YES	YES	YES	NO	YES	NO
3	YES	YES	YES	NO	NO	NO	NO
4	YES	YES	YES	NO	NO	NO	YES
5	NO		NO				
6	YES	YES	YES	YES	YES	NO	NO
7	NO	NO	NO	NO	NO	NO	NO
8	NO	NO	NO	NO	NO	NO	NO
9	NO	NO	NO	NO	NO	YES	NO
10	YES	YES	YES	YES	YES	NO	NO
11	YES	YES	YES	YES	NO	YES	YES
12	NO	NO	NO	NO	NO	NO	NO
13	NO	NO	NO	NO	NO	NO	NO
14	YES	NO	NO	NO	NO	NO	YES
15	YES	YES	YES	YES	NO	NO	YES
16	NO	NO	NO	NO	NO	NO	NO

Table S5: Permutation table for all reactions successfully (YES, resulting in satisfiable results) and non-successfully (NO, analytic results deviated from the expected reaction) performed in toluene.

Tol	**A**	**B**	**C**	**D**	**E**	**F**	**G**
1	YES	YES	YES	NO	YES	YES	YES
2	YES	YES	YES	YES	YES	YES	YES
3	YES	YES	NO	YES	YES	YES	YES
4	YES	YES	NO	YES	YES	YES	YES
5	NO		YES				
6	YES	YES	YES	YES	NO	NO	NO
7	YES	YES	YES	YES	YES	NO	NO
8	YES	YES	NO	NO	YES	NO	NO
9	YES	NO	NO	YES	YES	NO	NO
10	YES	YES	YES	YES	YES	NO	NO
11	YES	NO	YES	YES	NO	NO	YES
12	YES	YES	YES	YES	NO	YES	YES
13	YES	YES	YES	YES	NO	YES	YES
14	YES	NO	NO	YES	NO	YES	YES
15	YES	YES	YES	NO	NO	YES	YES
16	YES	YES	NO	YES	NO	YES	YES

Table S6: Permutation table for all reactions successfully (YES, resulting in satisfiable results) and non-successfully (NO, analytic results deviated from the expected reaction) performed in dimethylformamide.

DMF	**A**	**B**	**C**	**D**	**E**	**F**	**G**
1	YES	YES	YES	YES	YES	YES	YES
2	YES	NO	NO	YES	YES	YES	YES

3	YES	YES	NO	YES	YES	YES	YES
4	YES	YES	NO	YES	YES	YES	YES
5	NO		NO				
6	YES	YES	YES	YES	YES	NO	NO
7	YES	YES	YES	YES	YES	NO	NO
8	NO	NO	NO	NO	NO	NO	NO
9	YES	YES	NO	YES	NO	YES	NO
10	YES	YES	YES	YES	YES	NO	NO
11	YES	NO	YES	YES	NO	YES	YES
12	YES	NO	YES	YES	NO	YES	YES
13	NO	NO	NO	NO	NO	NO	NO
14	YES	NO	NO	YES	NO	NO	YES
15	YES	YES	YES	YES	NO	YES	YES
16	YES	NO	NO	YES	YES	YES	YES

3. Overview of the automated robot program

As all the polymerizations and the sampling of those was executed with minimal human intervention, it is of importance to understand, how the program was implemented inside the automated parallel synthesizer. **Table S7** presents a step-by-step overview of the tasks inside the program.

Table S7: Step-by-step protocol for addition of reaction components and sampling during the reaction inside the automated platform.

Step		Task	Description
1		**Macro Task**	**Rinsing of needles**
	1.1	Rinsing needle 1, 2, 3, 4	Rinsing of all needles with 10 mL chloroform inside and 10 mL chloroform outside
2		**Reflux**	**Manually turn reflux temperature ON (5 °C) on reactors**
3		**Macro Task**	**Addition of solvents to reactor**
	3.1	Liquid transfer	Solvent 1 to respective reactors (volumes depending on monomer molar mass)
	3.2	Liquid transfer	Solvent 2 to respective reactors (volumes depending on monomer molar mass)
	3.3	Liquid transfer	Solvent 3 to respective reactors (volumes depending on monomer molar mass)
4		**Macro Task**	**Dispense analytical solvents (NMR, SEC) to vials and tubes for 0 h sampling**
	4.1	Liquid transfer	1 mL of SEC eluent to first 15 sampling vials
	4.2	Liquid transfer	0.35 mL of deuterated chloroform to first 15 NMR tubes
5		**Macro Task**	**Dispense monomers (10 mmol) to reactors**
	5.1	Liquid transfer	10 mmol of monomer 1 to first three reactors
	5.2	Liquid transfer	10 mmol of monomer 2 to next three reactors
	5.3	Liquid transfer	10 mmol of monomer 3 to next three reactors
	5.4	Liquid transfer	10 mmol of monomer 4 to next three reactors
	5.5	Liquid transfer	10 mmol of monomer 5 to next three reactors
6		Liquid transfer	Dispense anisole (0.4 mL, 3.66 mmol) standard to reactors with fitting monomers
7		Liquid transfer	Dispense trioxane solution in toluene (2.5 mL, 3.66 mmol) to reactors with fitting monomers
8		**Macro Task**	**Dispense RAFT/AIBN solutions (1.99 mL, c(AIBN) = 8.38 mmol/L, c(RAFT) = 33.5 mmol/L) in solvents 1 to 3 to reactors**
	8.1	Liquid transfer	1.99 mL of solution in solvent 1 to reactors with solvent 1
	8.2	Liquid transfer	1.99 mL of solution in solvent 2 to reactors with solvent 2

	8.3	Liquid transfer	1.99 mL of solution in solvent 3 to reactors with solvent 3
9		**Set Drawer Valve**	**Open reactors under inert gas (N_2)**
10		**Wait**	**Wait 60 min (flushing reaction solutions for 15 to 30 min (N_2), then manual abortion)**
11		**Set Drawer Valve**	**Close reactors under inert gas (N_2)**
12		**Stir**	**Agitation ON (400 rpm)**
13		**Macro Task**	**Sampling t = 0 h for NMR and SEC**
	13.1	Sampling from reactor 1 and 2	From reactor to sampling vials and NMR tubes (0.2 mL SEC sample and 0.2 mL NMR sample)
	13.2	Sampling from reactor 3 and 4	From reactor to sampling vials and NMR tubes (0.2 mL SEC sample and 0.2 mL NMR sample)
	13.3	Sampling from reactor 5 and 6	From reactor to sampling vials and NMR tubes (0.2 mL SEC sample and 0.2 mL NMR sample)
	13.4	Sampling from reactor 7 and 8	From reactor to sampling vials and NMR tubes (0.2 mL SEC sample and 0.2 mL NMR sample)
	13.5	Sampling from reactor 9 and 10	From reactor to sampling vials and NMR tubes (0.2 mL SEC sample and 0.2 mL NMR sample)
	13.6	Sampling from reactor 11 and 12	From reactor to sampling vials and NMR tubes (0.2 mL SEC sample and 0.2 mL NMR sample)
	13.7	Sampling from reactor 13 and 14	From reactor to sampling vials and NMR tubes (0.2 mL SEC sample and 0.2 mL NMR sample)
	13.8	Sampling from reactor 15	From reactor to sampling vials and NMR tubes (0.2 mL SEC sample and 0.2 mL NMR sample)
14		**Set Timer**	**Set T = *samplingtimer***
15		**Heating/cooling**	**Thermostat ON (70 °C) on reactors**
16		**Macro Task**	**Dispense analytical solvents (NMR, SEC) to vials and tubes for 1 h and 2 h sampling**
	16.1	Liquid transfer	1 mL of SEC eluent to next 30 sampling vials
	16.2	Liquid transfer	0.35 mL of deuterated chloroform to next 30 NMR tubes
17		**Wait**	**Wait for 1 h after *samplingtimer***
18		**Macro Task**	Sampling t = 1 h for NMR and SEC
		Same subtasks as for t = 0h	
19		**Wait**	**Wait for 2 h after *samplingtimer***
20		**Macro Task**	Sampling t = 2 h for NMR and SEC

		Same subtasks as before	
21		**Macro Task**	**Dispense analytical solvents (NMR, SEC) to vials and tubes for 4 h and 6 h sampling**
	21.1	Liquid transfer	1 mL of SEC eluent to next 30 sampling vials
	21.2	Liquid transfer	0.35 mL of deuterated chloroform to next 15 NMR tubes
22		**Wait**	**Wait for 4 h after *samplingtimer***
23		**Macro Task**	**Sampling t = 4 h for NMR and SEC**
		Same subtasks as before	
24		**Wait**	**Wait for 6 h after *samplingtimer***
25		**Macro Task**	**Sampling t = 6 h only for SEC**
	25.1	Sampling from reactor 1 and 2	From reactor to sampling vials (0.2 mL SEC sample)
	25.2	Sampling from reactor 3 and 4	From reactor to sampling vials (0.2 mL SEC sample)
	25.3	Sampling from reactor 5 and 6	From reactor to sampling vials (0.2 mL SEC sample)
	25.4	Sampling from reactor 7 and 8	From reactor to sampling vials (0.2 mL SEC sample)
	25.5	Sampling from reactor 9 and 10	From reactor to sampling vials (0.2 mL SEC sample)
	25.6	Sampling from reactor 11 and 12	From reactor to sampling vials (0.2 mL SEC sample)
	25.7	Sampling from reactor 13 and 14	From reactor to sampling vials (0.2 mL SEC sample)
	25.8	Sampling from reactor 15	From reactor to sampling vials (0.2 mL SEC sample)
26		**Macro Task**	**Dispense analytical solvents (NMR, SEC) to vials and tubes for 8 h, 10 h and 15 h sampling**
	26.1	Liquid transfer	1 mL of SEC eluent to next 45 sampling vials
	26.2	Liquid transfer	0.35 mL of deuterated chloroform to next 30 NMR tubes
		Same subtasks as before	
27		**Wait**	**Wait for 8 h after *samplingtimer***
28		**Macro Task**	**Sampling t = 8 h for NMR and SEC**
		Same subtasks as before	
29		**Wait**	**Wait for 10 h after *samplingtimer***
30		**Macro Task**	**Sampling t = 10 h only for SEC**
		Same subtasks as before	
31		**Wait**	**Wait for 15 h after *samplingtimer***
32		**Macro Task**	**Sampling t = 15 h for NMR and SEC**
		Same subtasks as before	

33		**Macro Task**	**Rinsing of needles**
	33.1	Rinsing needle 1, 2, 3, 4	Rinsing of all needles with 8 mL of chloroform inside and 8 mL of chloroform outside
34		**Macro Task**	**Turn devices off**
	34.1	Stir	Agitation OFF on reactors (400 rpm)
	34.2	Heating/cooling	Thermostat OFF (70 °C) on reactors
	34.3	Reflux	Reflux temperature OFF (5 °C) on reactors
35		**Wait**	**Wait for 15 h from this point on**
36			**Manual change of NMR funnel module**
37		**Liquid transfer**	**Add 0.4 mL of deuterated chloroform to all of the NMR tubes**

4. Program diagram

The software is split into several compartments which enable the separation of the generation of the FAIR data set after a possible change of the experimenter spreadsheet from the provision of the web service (**Figure S7**). Every script file is annotated with explanatory comments and a Jupyter notebook file can be run in the same software environment showing the research data analysis progress of this whole work.

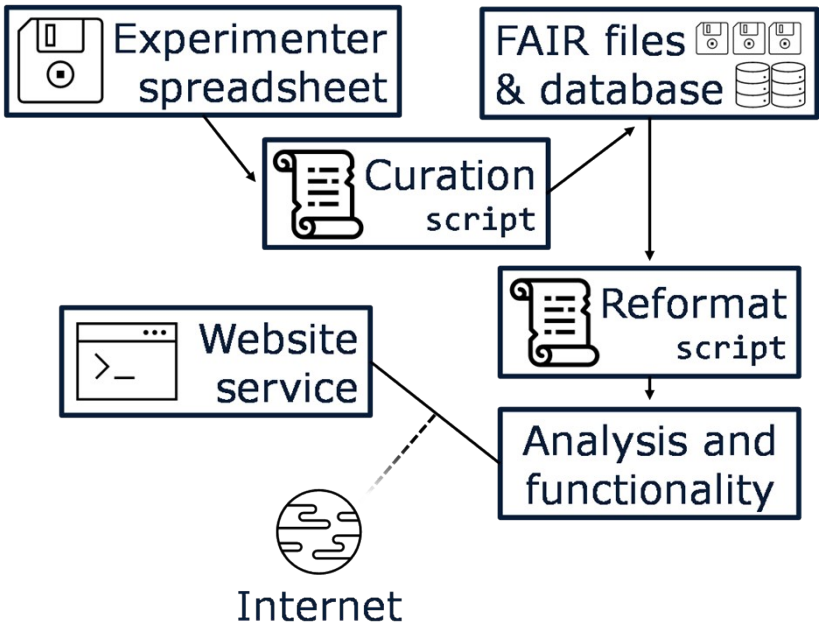

Figure S7: Flowchart of the program architecture leading from the experimental data spreadsheet to the website-service.

5. Partition of the unsuccessful kinetics into categories

As some of the kinetic profiles were marked as unsuccessful, we wanted to distinguish the reasons for this marking. Generally, the unsuccessful reactions can be divided into two categories. We named the first category "discarded" meaning that either an experimental setup error was the obvious reason for rejecting the kinetic (*e.g.*, a robot failure occurred during the experiment), or it was not possible to ensure if a successful polymerization was determined as unsuccessful because of experimental constraints (*e.g.*, sampling from gels). This category combined 257 reactions with 89 of them being repetitions of previous parameter combinations to ensure the validity of the findings. The second category is called "failed" experiments, meaning that no polymerization progress could be recorded, but could have been recognized securely according to the experimental setup. Of the 48 failed experiments, 21 were repetition experiments.

5.1. Discarded polymerizations

Within the discarded category, several subgroups could be identified (**Figure S8**):

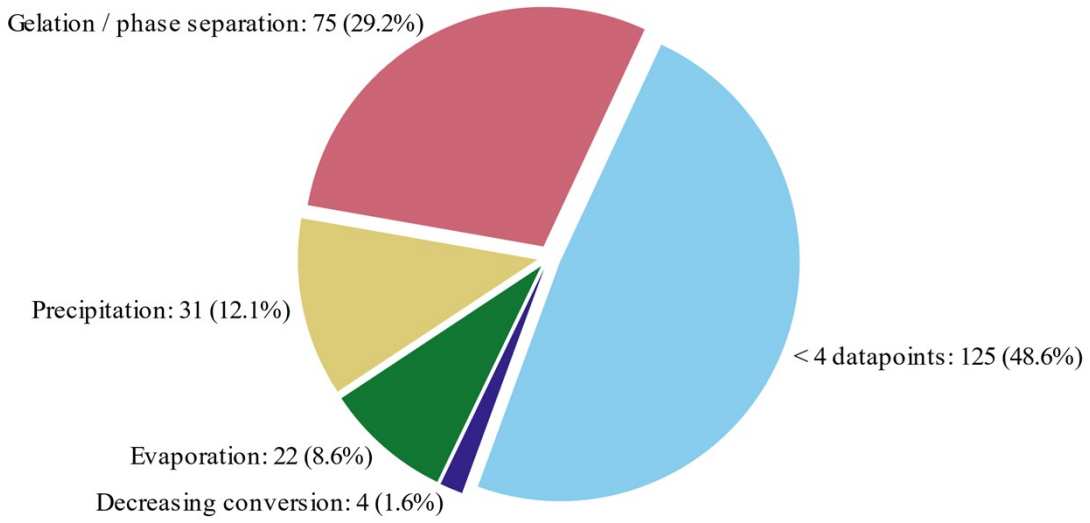

Figure S8: Classification of discarded experiments in a pie chart with their absolute amounts and relative percentages.

1. Setup errors, evaporation:

This class contains polymerizations in which reactors were not properly sealed, resulting in underfilled reactors by the end of the kinetic series. This caused altered monomer

concentrations and invalidated the corresponding data. 22 reactions (9%) fell into this subgroup.

2. Precipitation during the reaction:

In 31 reactions (ca. 12%), a solid precipitate was observed in the reactor after the 15 h sampling interval. Since the precipitate could not be sampled with the existing setup, these reactions were discarded.

3. Gelation / phase separation during the reaction:

A total of 75 reactions (ca. 29%) formed a gel (either on top of the reaction solution or gelation of the solution itself) during the kinetic run. This was particularly common in polymerizations of unpolar monomers in polar solvents such as DMSO and DMF. Although polymerization is overt, the presence of gelation made it impossible to confirm whether SEC and NMR measurements accurately reflected the reactor conditions, as they may have been perturbed by the gel phase.

4. Data loss due to measurement limitation:

The largest subgroup contained 125 reactions (ca. 49%), which were discarded based on the same criteria applied to individual data points in the main manuscript. Typical reasons included:

- Insufficient data points (<4 per kinetic run) caused by rejection of erroneous measurements as defined before.
- SEC molar mass values (M_n or M_w) exceeding the calibration range.
- Very slow polymerization rates, leading to the absence of measurable molar masses in SEC elugrams.

5. Clear measurement errors:

In a small fraction of cases (4 reactions, ca. 1%), conversions were found to decrease with reaction progress, an artifact of measurement errors.

Of the initial 168 individual discarded polymerization condition experiments 88% (or 147 experiments) were repeated to minimize the likelihood of our setup being at fault. In this effort of retrying all reactions where obvious setup related errors occurred (evaporation, measurement errors), and some of the other categories, 44 experiment replicates (ca. 30% of all 147 retried) could be categorized as successful in subsequent attempts, while 14 reactions (ca. 10% of all 147 retried) could be categorized as failed. The remaining 89 experiments remained unchanged in the discarded category after replication.

In general, only six of the original 381 reactions (without replicates) were classified as both successful and failed when comparing multiple reaction attempts. Primarily, this outcome was found because their conversion was very close to the threshold for being marked as failed due to low conversion (five out of six).

5.2. Failed polymerizations

The second category, termed “failed”, included 48 experiments (with 21 repetitions) which we considered as failed in a sense that the polymerizations did either exhibit very low conversions (on average below 1% over the course of 15 h) (8 experiments), or decreasing molar mass values by more than 10% (SEC method accuracy) over the course of the experiment (33 experiments). This behavior can be attributed to a non-compatibility of active monomer chain and RAFT-agent, effectively rendering the synthesis to an uncontrolled free radical polymerization, seemingly lowering the average molar masses as more lately initialized, short chains grow suggesting inferior control of the polymerization and a free radical polymerization character dominates within the performed reaction instead of the character of a reversible-deactivation radical polymerization.

6. Consistency of conversion for replicates

To check for the reproducibility of the successful polymerizations, the divergences of conversion for the replicates of identical experimental conditions (same monomer, solvent and RAFT-agent) were evaluated. The resulting box-plot is displayed in **Figure S9**.

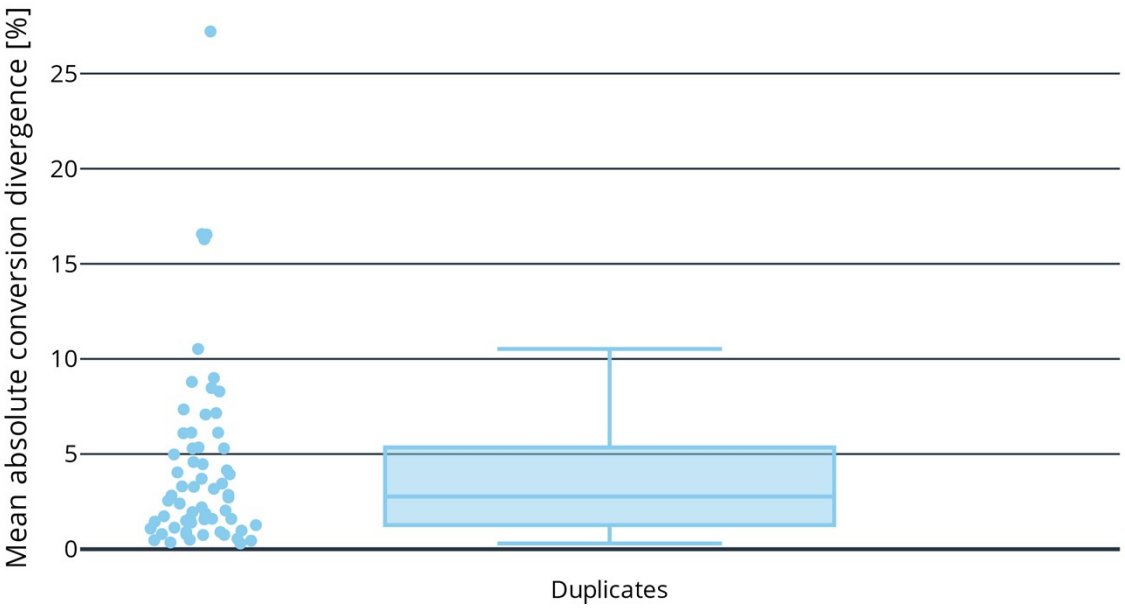

Figure S9: Divergences of the conversion of replicate experiments in comparison to the initial experiment with identical RAFT-agent, monomer and solvent. The presented data are the mean values of all absolute conversion differences over all sampling time points.

The number of replicates per identical reaction condition was typically two (in total: 29 pairs, 5 trios and 3 quartets). Each point in the plot represents the divergence between two kinetics. To be more precise, they represent the arithmetic mean of all absolute differences in conversion over all sampling time points, between two kinetics. Almost all quartiles lie within the determination accuracy of the NMR conversion measurement method (10%; upper fence 10.52%), while four points are suspected of being outliers.

7. Fit-types comparison

In **Figure S10** a rough overview on how good the different fit types can describe the kinetics is given by comparing all errors of the coefficients of determination for all 234 successful kinetic experiments. The peaks in the diagram represent experiments in which individual adjustments resulted in a poor correlation between the experimental data and the fitting function. These are most prominent for fitting with the linear growth function. On the other hand, the negative growth and sigmoidal fits generally provide a better correlation.

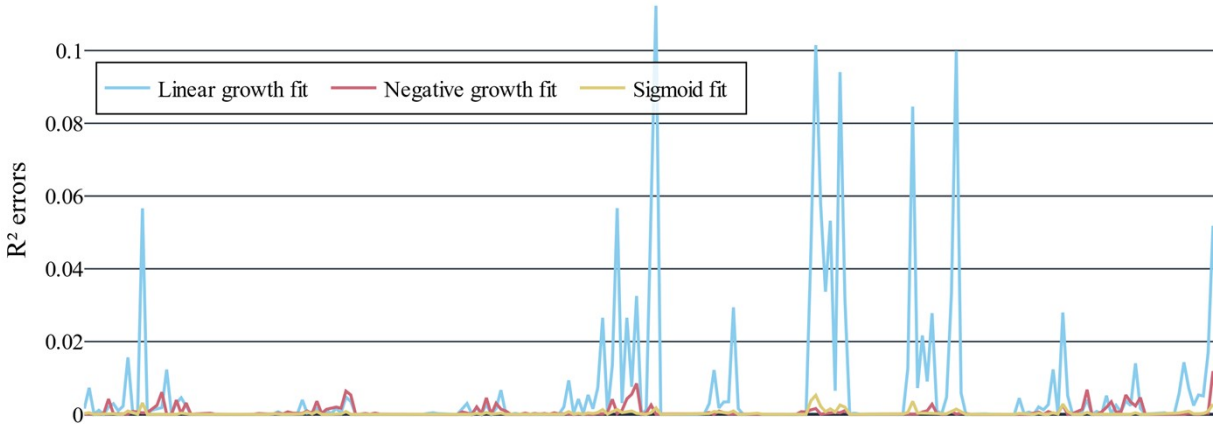

Figure S10: Comparison of all errors of coefficients of determination (R^2 errors) for three fit types for all 234 successful kinetic experiments.

There are three premises which can explain the outcome:

First: A linear course of reaction can be fitted well with all three functions considered.

Secondly: A negative growth course can be fitted with the sigmoidal and the like-called function.

Third: A sigmoidal course of reaction can only be fitted with the sigmoidal function. Since all three types of progression are evident in our set of reactions, the overall superior fitting performance with the sigmoidal function, in terms of smallest mean and total R^2 error, was expected (see **Table S8**).

Table S8: Numerical overview of the three fits in comparison by their coefficients of determination (R^2 errors).

Fit-type	Times best	Mean of R^2 error	Sum of all R^2 errors
Linear	28	0.0065	1.5127
Sigmoidal	131	0.0003	0.0668
Negative growth	75	0.0007	0.1601

However, fitting an almost or perfect linear course with a likewise linear function results in a slightly (difference in R^2 errors always less than 5×10^{-10} better fit compared to the two other functions, due to the increased number of parameters to optimize in the more sophisticated functions. Therefore, through the comparison of where which functions worked best, an estimate about the rate of termination (convergence to max conversion) / incomplete reaction

(reaction still in linear increase part at last sampling time) and speed of initiation (slow increase of conversion from timepoint zero) can be given. We summed up the errors per specific monomer, RAFT-agent or solvent and plotted their reciprocal values normalized to one to visualize the amount of the prior mentioned aspects in **Figures S11**, **S12** and **S13**.

For example, almost all reactions with 4-*tert*-butylstyrene as monomer exhibited a gradual increase in conversion with no convergence to a conclusion of the reaction within the sampling timeframe, thus, proceeding linear. In contrast, polymerizations with lauryl acrylate started with a slow initiation followed by a swift rise to high conversions and creeping in of termination at the culmination of the last few sampling points – a sigmoidal curvature.

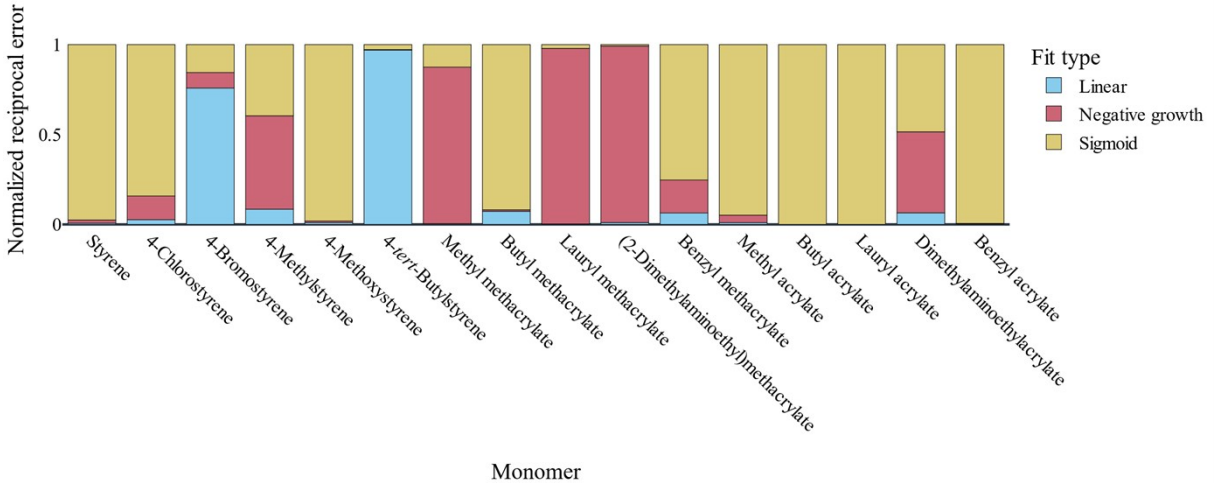

Figure S11: Visualization of linear, negative growth and sigmoidal reaction course separated by monomers.

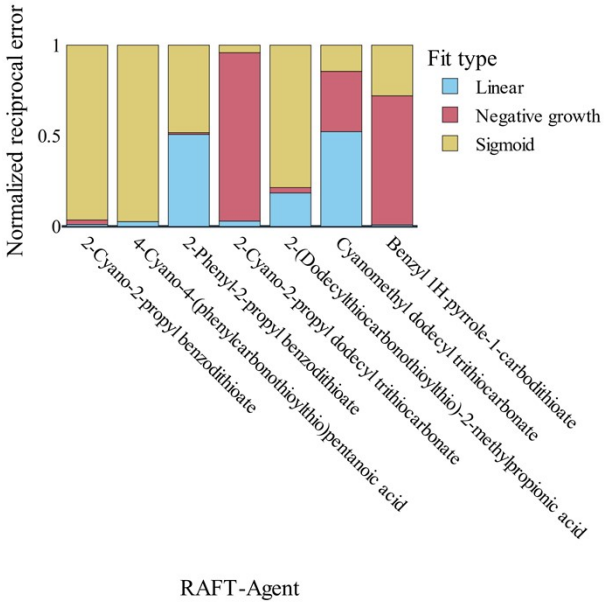

Figure S12: Visualization of linear, negative growth and sigmoidal reaction course separated by RAFT-agents.

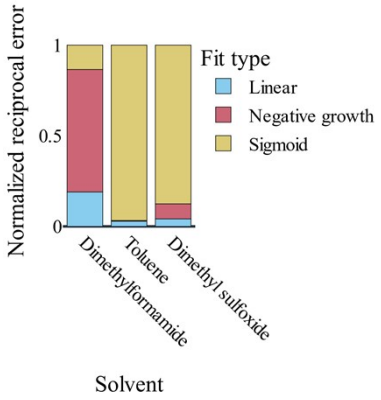

Figure S13: Visualization of linear, negative growth and sigmoidal reaction course separated by solvents.

8. Website interface

The website is responsive, i.e. it adapts to the dimensions of the user's screen, although it is optimized for use on desktop computers. An example of the website is provided in **Figure S14**. Initially, all links to data, software and research are provided, followed by a dropdown menu containing all unique reactants available to be searched for. Upon clicking the search button, a sortable table is rendered, from which the user can select and plot a number of empirical experiments in the subsequent section. These experiments include a comparison of conversion and/or M_n and M_w in interlaced or stacked fashion, as well as fitting options for the kinetic processes.

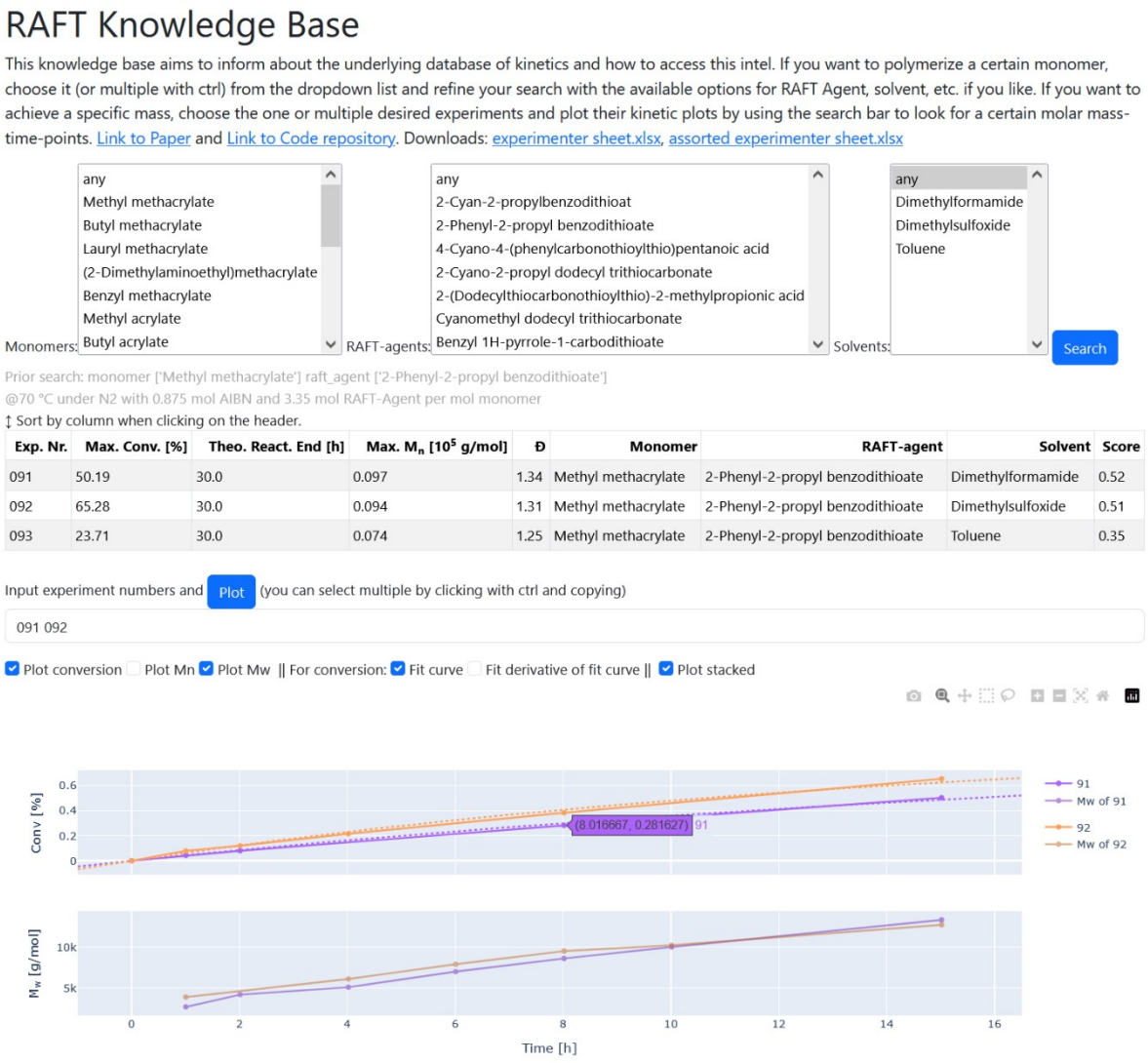

Figure S14: Example of a search query with multiple plotting options selected.