Supporting Information for Update and Critical Reanalysis of IUPAC Benchmark Propagation Rate Coefficient Data

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1. Estimates of k_p and E_A from individual studies:

Table S1. Estimates of k_p at 25°C, A and E_A for styrene from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, T_0 = 298.15 K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A[a]	N[b]	se[c]	V(ln k_p)[c] × 10^3	V(E_A)[c]	Cov(ln k_p, E_A)[c] × 10^3
S1	25	77.0	4.34			1	0.052	2.70		
S2	25	84.0	4.43			1	0.050[d]	2.50		
S3	25	78.6	4.36			1	0.050[d]	2.50		
S4	25	92.0	4.52			1	0.050[d]	2.50		
S5	30–90	92.0	4.52	30.8	7.36	4	0.075	5.27	2.33	-95.1
S6	25–55	78.4	4.36	31.1	7.34	4	0.023	0.411	0.756	-14.2
S7	30–90	93.5	4.54	31.5	7.49	4	0.011	0.108	0.0478	-1.95
S8	-12–93	89.8	4.50	32.6	7.66	45	0.042	0.0482	0.0228	-0. 431
S9[e]	25–60	96.5	4.57	31.3	7.47	2	0.050[d]	2.50	2.78	-59.0
S10[e]	18–57	81.4	4.40	30.9	7.33	10	0.092	1.53	2.82	-43.7
S11[e]	18–57	80.7	4.39	31.8	7.48	24	0.023	0.532	0.0665	-1.23
S12[e]	30–40	88.4	4.48	32.1	7.57	4	0.0055	0.0391	0.187	-2.43
S13[e]	18–47	97.4	4.58	33.1	7.78	6	0.037	0.259	1.21	-6.49
S14[e]	25–70	79.2	4.37	30.7	7.27	4	0.022	0.355	0.313	-8.54
S15[e]	50–120	89.5	4.49	31.9	7.54	10	0.052	1.61	0.415	-23.6
S16[e]	20–60	94.4	4.55	32.4	7.65	3	0.011	0.0741	0.101	-1.84
Average		86.8[f]	4.46	31.7	7.49	16(12)[g]		6.66	0.585	32.2

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se: standard error in data points (= $\sqrt{\dfrac{SSR}{N-2}}$) where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] for studies with only one or two reported values, se was assumed to be 0.05, corresponding to a reproducibility of +/- 5% in the k_p measurement. [e] studies not included in Buback *et al.*, *Macromol. Chem. Phys.* 1995, **196**, 3267-3280 (S17). [f] Geometric mean of k$_p$ values. [g] Here N represents the number of individual studies. The number in parentheses is the number of studies reporting an E$_A$ value.
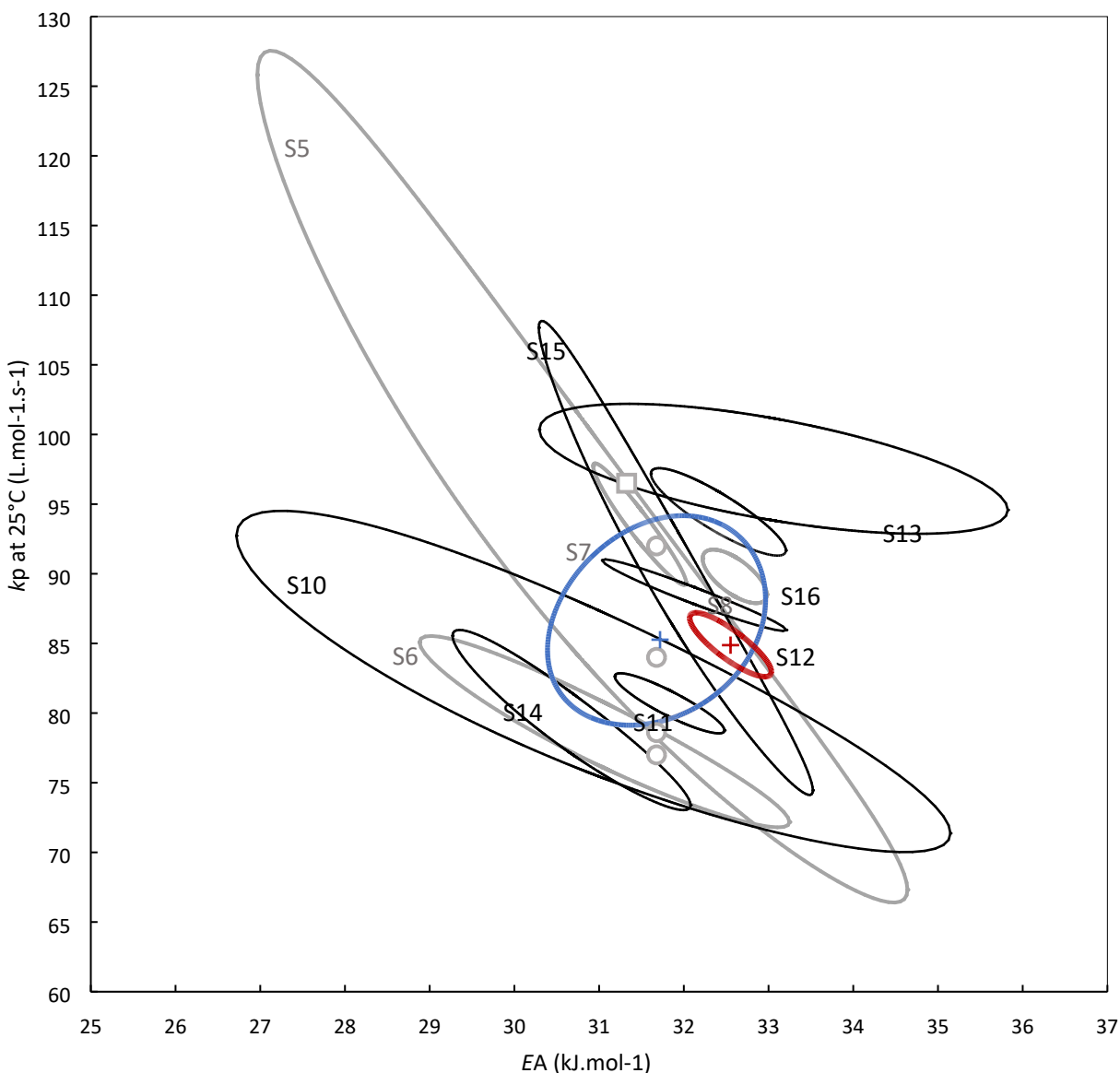
Figure S1. 95% JCRs for individual studies of k_p of styrene (grey: original data set;[S17] black: expanded data set), and for the weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S17] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red). Open circles represent the point estimates for k_p at 25°C of studies S1-S4, shown at the interlaboratory average E_A of 31.7 kJ.mol^{-1}. The open square represents the point estimate for k_p and E_A of study S9. Crosses represent the point estimates for the weighted average of studies (blue) and the original IUPAC benchmark value (red).

Table S2. Estimates of k_p at 25°C, A and E_A for methyl methacrylate from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, T_0 = 298.15 K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A^a	N^b	se^c	V(ln k_p)^c × 10^3	V(E_A)^c	Cov(ln k_p, E_A)^c × 10^3
S1	25	315	5.75				0.027	0.149		
S4	25	359	5.88				0.05^d	2.50		
S9	25–60	372	5.92	22.4	6.50	2	0.05^d	2.50	2.78	-59.0
S16	-18–25	348	5.85	24.4	6.81	3	0.013	0.151	0.0758	2.65
S18	25	294	5.69				0.012	0.0721		
S19	-1–70	317	5.76	23.9	6.69	12	0.035	0.110	0.0806	-0.727
S20	10–90	340	5.83	21.3	6.26	37	0.042	0.0871	0.0612	-1.57
S21	20–90	310	5.74	22.2	6.37	8	0.027	0.208	0.0937	-3.35
S22^d	25	316	5.75			6	0.067	4.55		
S23^d	20–25	319	5.77	24.6	6.81	11	0.030	0.185	7.17	26.9
S24^d	25–60	331	5.80	22.0	6.38	12	0.044	0.519	0.661	-15.3
S25^d	40–50	343	5.84	18.8	5.83	6	0.021	1.83	2.36	-64.4
S26^d	30–70	317	5.76	23.9	6.69	11	0.076	2.52	2.85	-75.4
S27^d	18–57	308	5.73	22.3	6.39	8	0.059	0.629	1.31	-16.2
S28^d	6–47	299	5.70	23.6	6.60	24	0.041	0.0715	0.150	-0.278
S29^d	40	338^f	5.82^f			2	0.05^d	2.53^g		
S30^d	20–60	343	5.84	22.4	6.46	8	0.063	0.748	0.811	-14.4
S31^d	11–92	344	5.84	22.9	6.54	18	0.018	0.0361	0.0202	-0.599
S32^d	10–42	328	5.79	23.1	6.55	20	0.037	0.0705	0.238	-0.535
Average		336^e	5.82	22.7	6.50	19(14)^f		15.7	2.16	-25.6

^{a} calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). ^{b} number of experimental points reported. ^{c} se:

standard error in data points (= $\sqrt{\dfrac{SSR}{N-2}}$) where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. ^{d} studies not included in Beuermann *et al.*, *Macromol. Chem. Phys.,* 1997, **198**, 1545-1560 (S33). ^{e} Geometric mean of k_p values. ^{f} Measurements at 313K adjusted to 298 K using average E_A of all studies. ^{g} Variance at 298K (V$_{298}$) calculated as V$_{298}$ = V$_{313}$ +V$_{EA}$*[1/R*(1/313-1/298)]^2 + Cov$_{kp,EA}$*[1/R*(1/313-1/298)], where V$_{313}$ is the measured variance at 313K, and V$_{EA}$ and Cov$_{kp,EA}$ are the estimated variance in E_A and covariance in E_A and ln k_p. ^{h} Here N represents the number of individual studies. The number in parentheses is the number of studies reporting an E_A value.
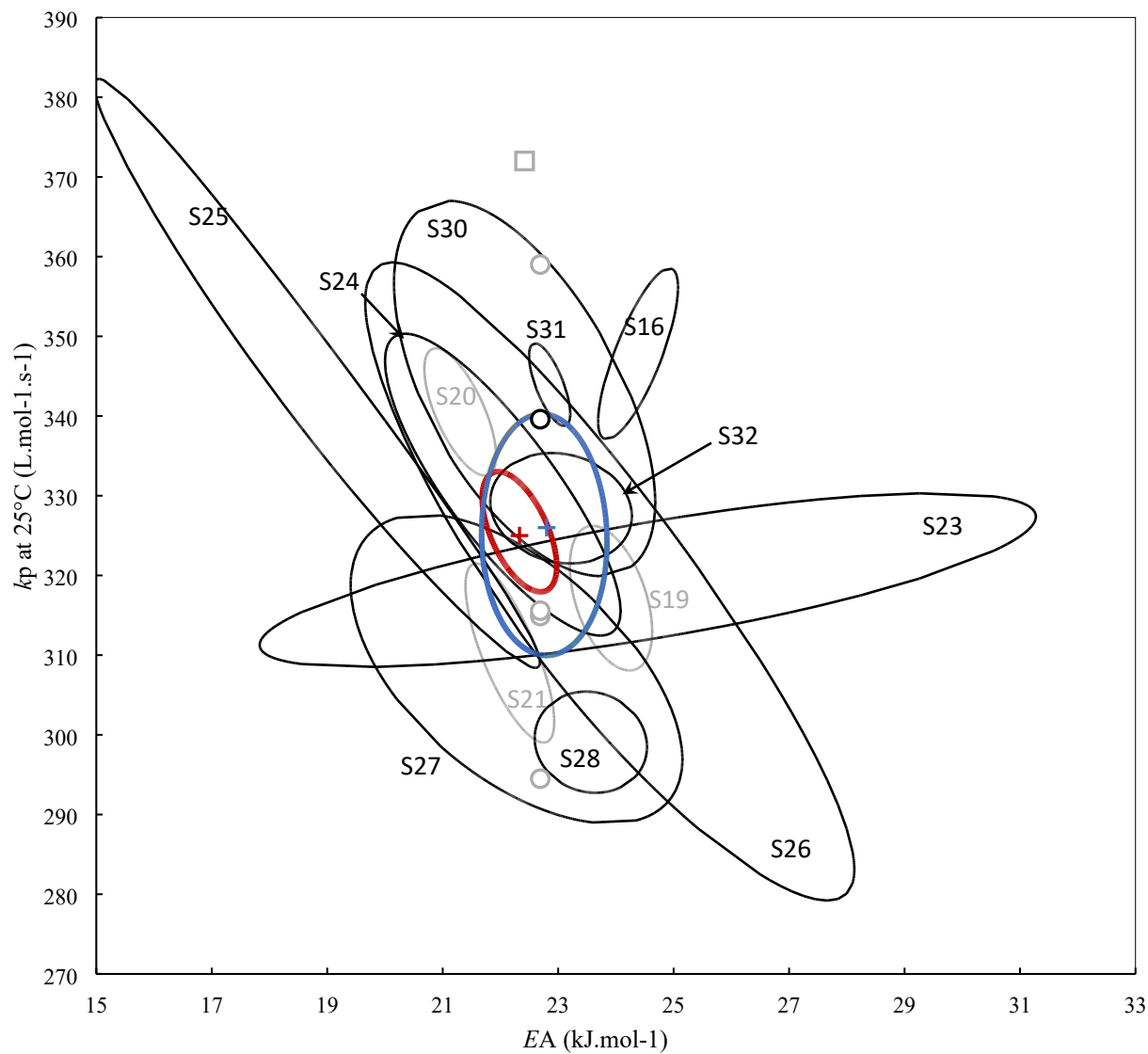
Figure S2. 95% JCRs for individual studies of k_p of methyl methacrylate (original data set:[S33] gray; expanded data set: black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S33] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red). Open circles represent the point estimates for k_p at 25°C of studies S1, S4, S18 (in gray) and S22 (in black), shown at the interlaboratory average E_A of 22.4 kJ.mol^{-1}. The open square represents the point estimate for k_p and E_A of study S9.

Table S3. Estimates of k_p at 25°C, A and E_A for ethyl methacrylate from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, $T_0 = 298.15$ K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A[a]	N[b]	se[c]	V(ln k_p)[c] × 10^3	V(E_A)[c]	Cov(ln k_p, E_A)[c] × 10^3
S28	6–47	292	5.68	23.8	6.64	30	0.041	0.0559	0.146	-0.321
S34	10–90	354	5.87	21.4	6.31	9	0.024	0.0980	0.0442	-1.21
S35	10–90	356	5.88	22.6	6.52	30	0.055	0.292	0.136	-5.11
S31[d]	1–91	352	5.86	23.5	6.66	20	0.009	0.00700	0.00406	-0.0931
Average		337[e]	5.82	22.9	6.53	4[f]		9.34	1.15	-65.7

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se: standard error in data points $(= \sqrt{\frac{SSR}{N-2}})$ where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] Study not included in Beuermann *et al.*, *Macromol. Chem. Phys.*, 2000, **201**, 1355–1364 (S36). [e] Geometric mean of k_p values. [f] Here N represents the number of individual studies.
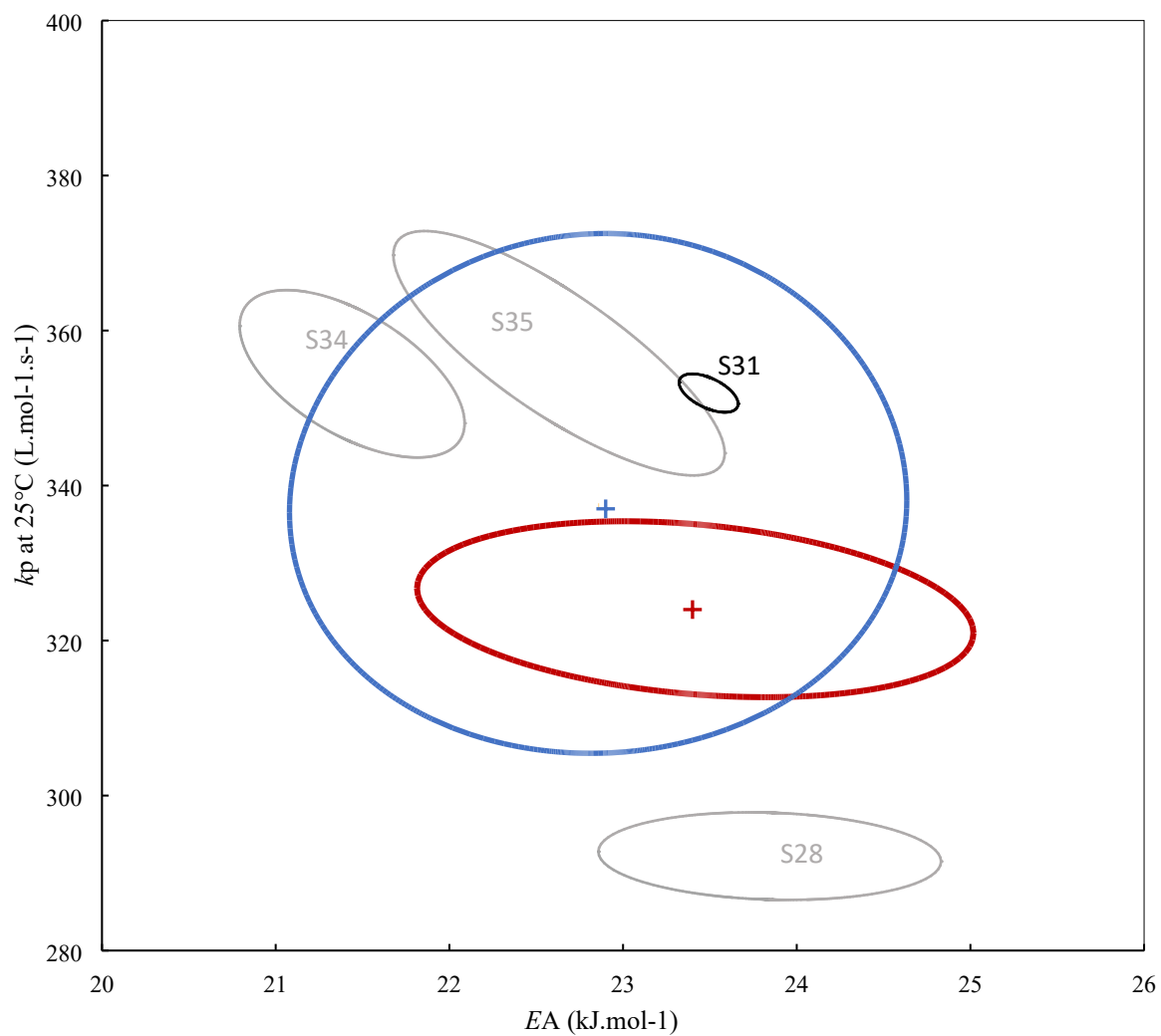
Figure S3. 95% JCRs for individual studies of k_p of ethyl methacrylate (original data set:[S36] gray; expanded data set: black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S36] obtained by pooling the data points of the original IUPAC data set (restricted to the temperature range 0-50°C and counting points of S34 and S35 twice), is shown for comparison (red).

Table S4. Estimates of k_p at 25°C, A and E_A for butyl methacrylate from individual studies obtained by linear least squares fitting of ln k_p to $(1/T − 1/T_0)$, T_0 = 298.15 K Units of E_A are kJ·mol⁻¹, while k_p and A are given in L·mol⁻¹·s⁻¹.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A[a]	N[b]	se[c]	V(ln k_p)[c] × 10³	V(E_A)[c]	Cov(ln k_p, E_A)[c] × 10³
S37	-20–50	390	5.97	22.8	6.59	17	0.050	0.178	0.165	2.35
S35	10–90	403	6.00	21.8	6.42	42	0.072	0.543	0.165	-8.31
S34	10–90	399	5.99	21.7	6.41	10	0.026	0.117	0.0464	-1.47
S28	6–47	343	5.84	23.0	6.57	30	0.037	0.0465	0.118	-0.315
S38[d]	50–80	354	5.87	24.0	6.59	6	0.045	3.26	13.2	-62.3
S39[d]	50–80	400	5.99	22.8	6.75	6	0.056	5.12	2.08	-97.8
S32[d]	0–91	402	6.00	23.3	6.69	20	0.010	0.00758	0.00438	-0.101
S40[d]	1–70	420	6.04	23.0	6.66	7	0.044	0.301	0.233	-2.26
Average		383[e]	5.95	22.2	6.58	8[f]		1.41	0.118	-7.41

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se:

standard error in data points $\left(= \sqrt{\dfrac{SSR}{N-2}}\right)$ where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] studies not included Beuermann *et al.*, *Macromol. Chem. Phys.* 2000, **201**, 1355–1364 (S36) [e] Geometric mean of k_p values. [f] Here N represents the number of individual studies.
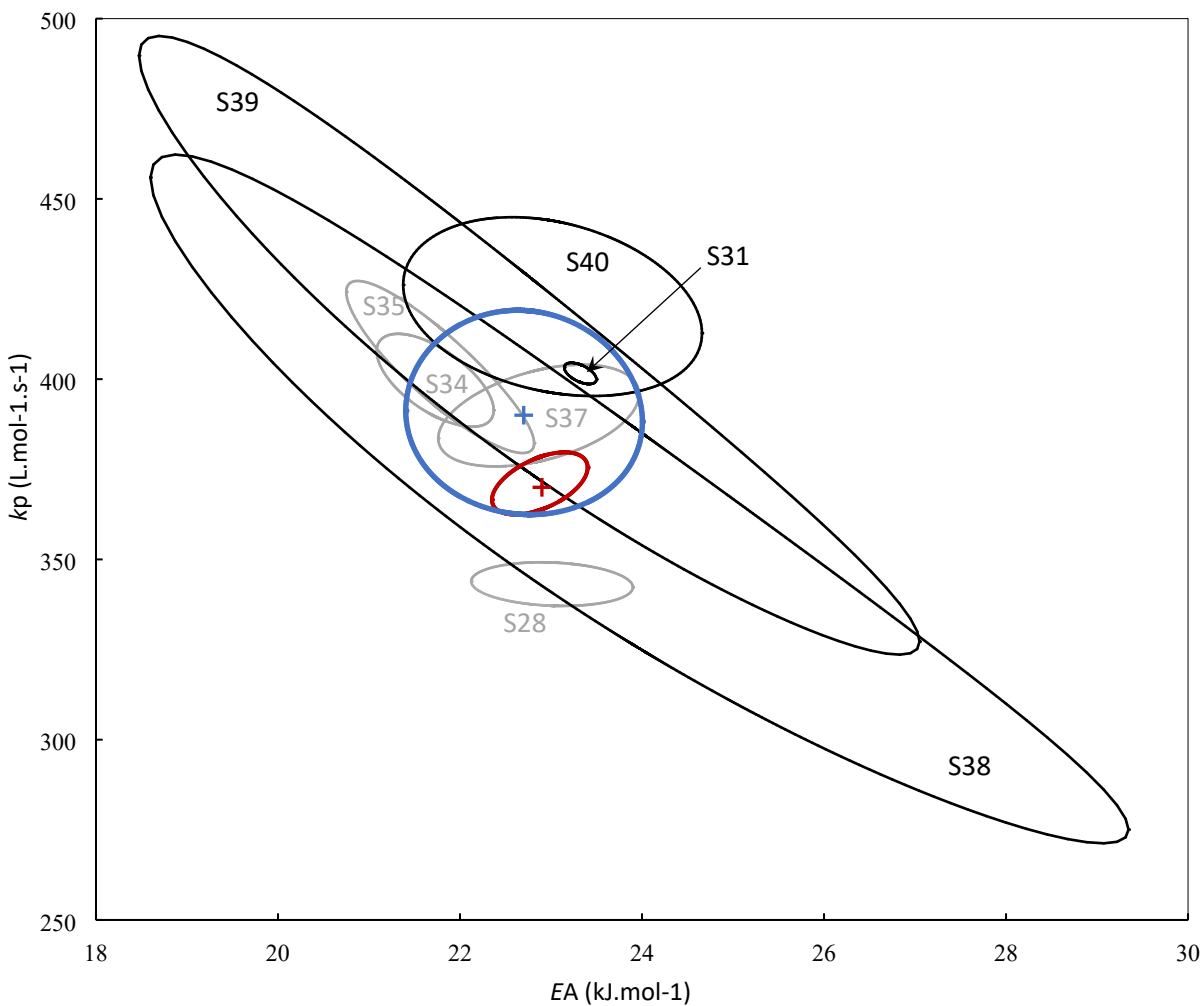
Figure S4. 95% JCRs for individual studies of k_p of butyl methacrylate (original data set:[S36] gray; expanded data set: black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S36] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red).

Table S5. Estimates of k_p at 25°C, A and E_A for dodecyl methacrylate from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, T_0 = 298.15 K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A[a]	N[b]	se[c]	V(ln k_p)[c] × 10^3	V(E_A)[c]	Cov(ln k_p, E_A)[c] × 10^3
S40	9–60	503	6.22	20.9	6.36	27	0.092	0.484	0.709	-10.9
S38	10–90	523	6.26	20.8	6.37	33	0.056	0.233	0.112	-3.95
S37	10–60	539	6.29	20.0	6.23	9	0.019	0.0436	0.0585	-0.416
Average		522[d]	6.26	20.5	6.32	3[e]		1.18	0.268	-15.5

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se: standard error in data points (= $\sqrt{\dfrac{SSR}{N-2}}$) where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] Geometric mean of k_p values. [e] Here N represents the number of individual studies.
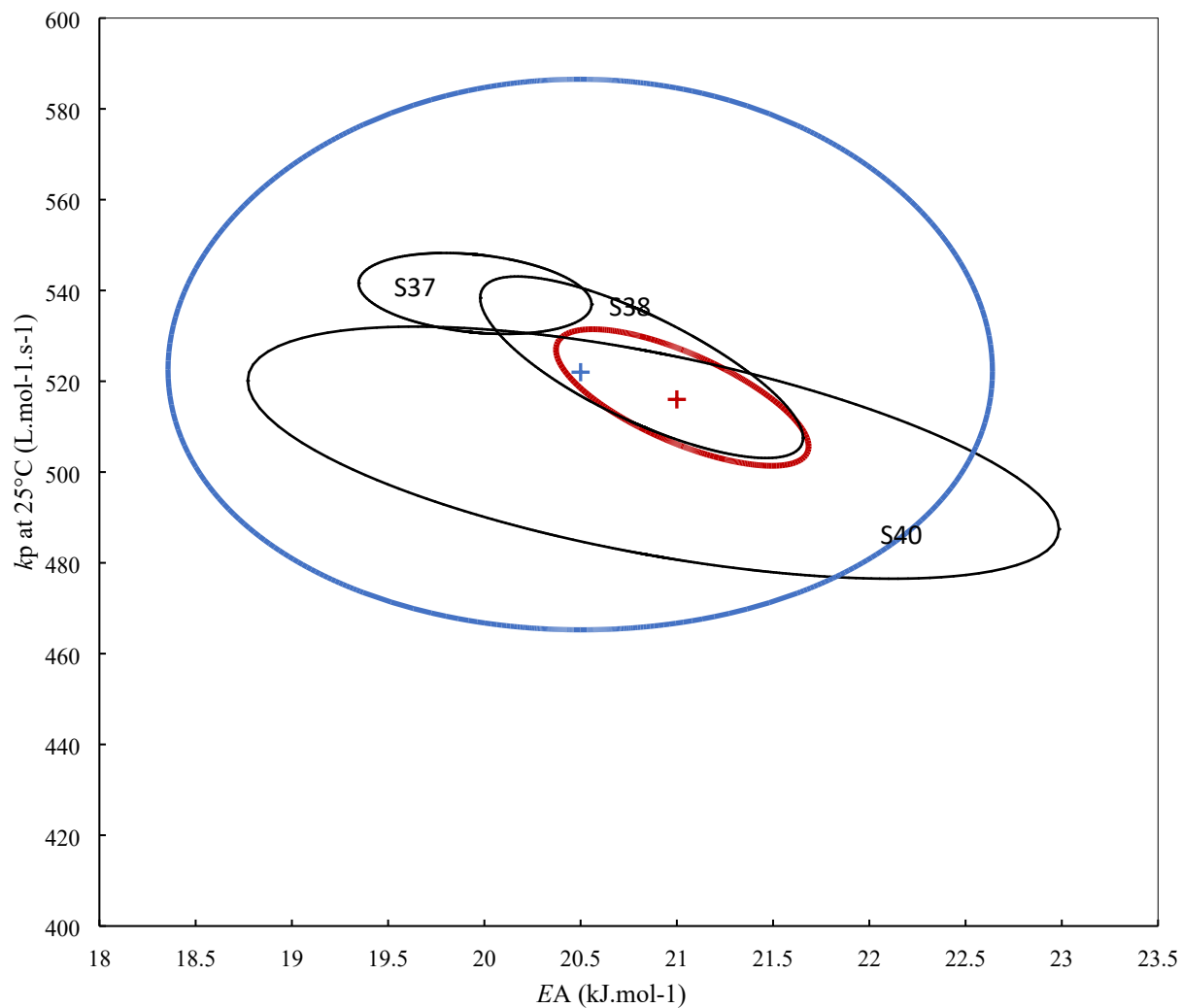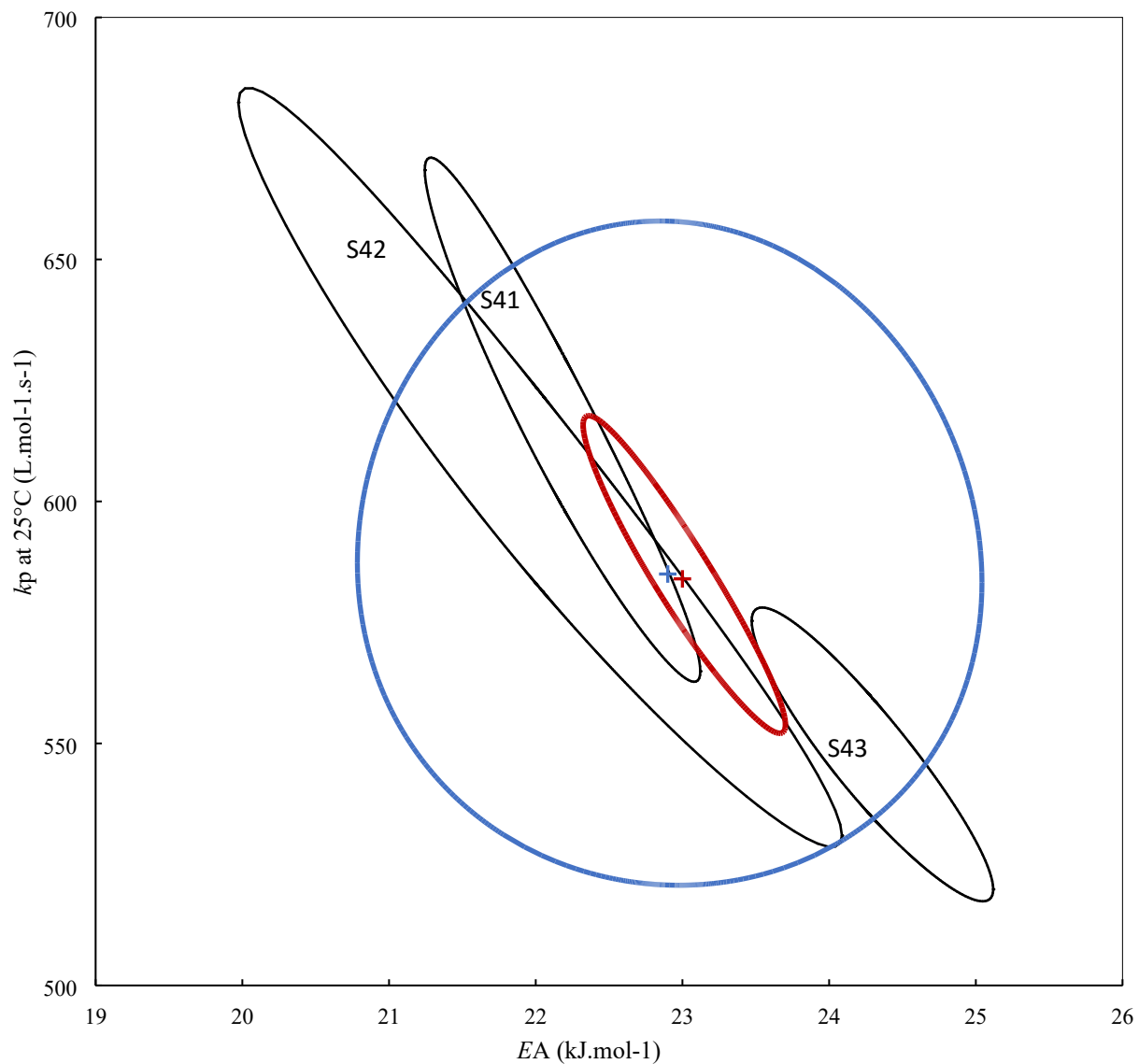
Figure S5. 95% JCRs for individual studies of k_p of dodecyl methacrylate (black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S36] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red).

Table S6. Estimates of k_p at 25°C, A and E_A for cyclohexyl methacrylate from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, $T_0 = 298.15$ K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A[a]	N[b]	se[c]	V(ln k_p)[c] × 10^3	V(E_A)[c]	Cov(ln k_p, E_A)[c] × 10^3
S41	10–90	615	6.42	22.2	6.67	34	0.059	0.372	0.135	-6.03
S42	21–91	602	6.40	22.0	6.64	10	0.037	0.618	0.516	-15.7
S43	30–70	547	6.30	24.3	6.99	18	0.036	0.162	0.0953	-2.93
Average		587[d]	6.38	22.8	6.77	3[e]		1.41	1.60	-76.7

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se: standard error in data points (= $\sqrt{\dfrac{SSR}{N-2}}$) where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] Geometric mean of k_p values. [e] Here N represents the number of individual studies.

Figure S6. 95% JCRs for individual studies of k_p of cyclohexyl methacrylate (black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S44] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red).

Table S7. Estimates of k_p at 25°C, A and E_A for glycidyl methacrylate from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, T_0 = 298.15 K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A^a	N^b	se^c	V(ln k_p)^c × 10^3	V(E_A)^c	Cov(ln k_p, E_A)^c × 10^3
S41	30–90	572	6.35	23.3	6.84	22	0.069	0.106	0.337	-16.8
S43	20–61	588	6.38	26.2	7.35	10	0.017	0.0514	0.0904	-1.46
S45^f	60–90	541	6.29	20.3	6.29	6	0.036	4.68	1.43	-80.0
Average		566^d	6.34	23.2	6.83	3^e		1.81	8.59	123

^{a} calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). ^{b} number of experimental points reported. ^{b} se:

standard error in data points (= $\sqrt{\dfrac{SSR}{N-2}}$) where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. ^{c} for studies with only one or two reported values, se was assumed to be 0.05, corresponding to a reproducibility of +/- 5% in the k_p measurement. ^{d} Geometric mean of k_p values. ^{e} Here N represents the number of individual studies. ^{f} study not included in Beuermann et al., *Macromol. Chem. Phys.* 2003, **204**, 1338–1350 (S44). Data points at temperatures >90°C were excluded to reduce interference from depropagation.
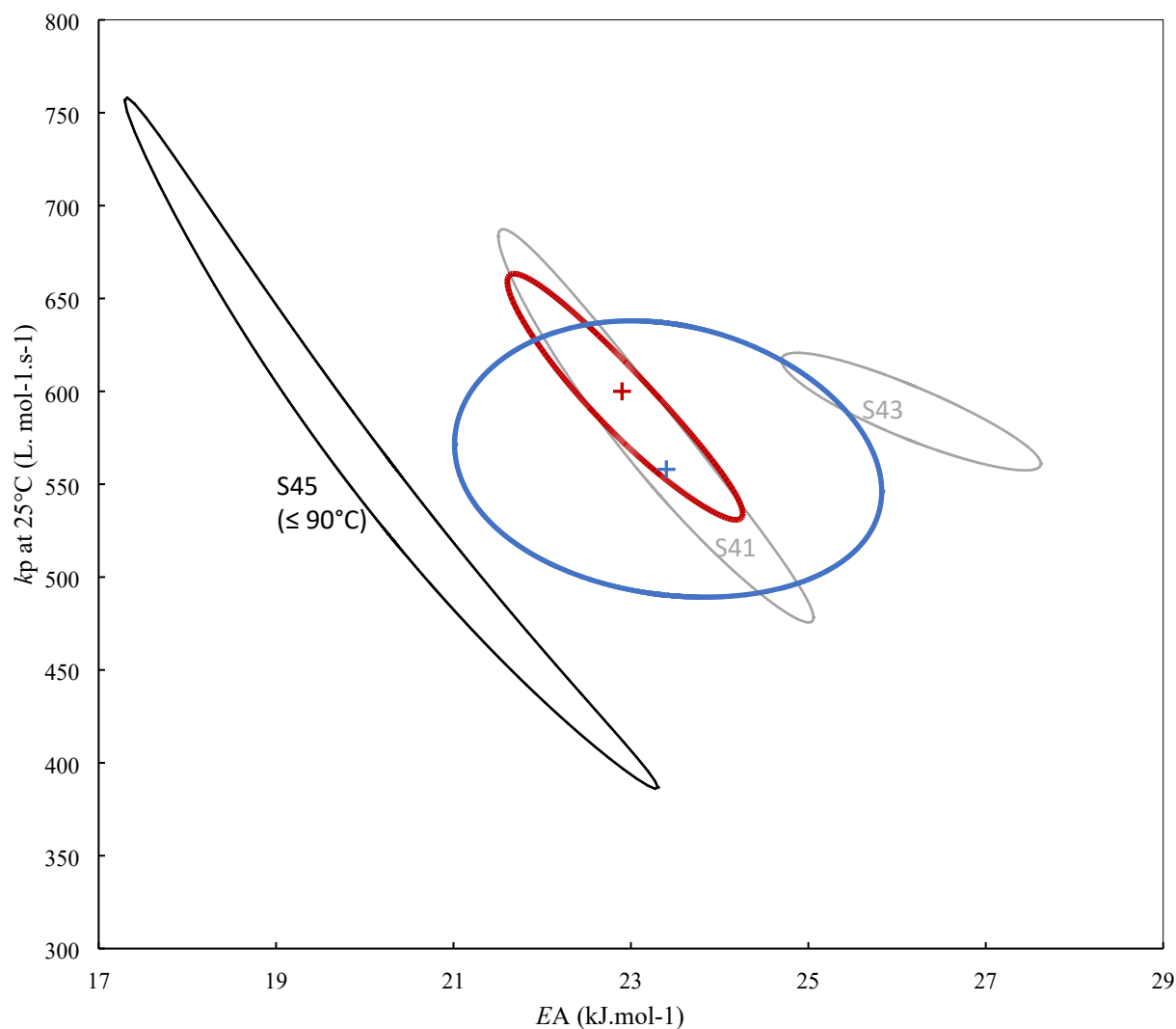
Figure S7. 95% JCRs for individual studies of k_p of glycidyl methacrylate (original data set[S44]: gray; expanded data set: black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S44] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red).

Table S8. Estimates of k_p at 25°C, A and E_A for benzyl methacrylate from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, T_0 = 298.15 K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A[a]	N[b]	se[c]	V(ln k_p)[c] × 10^3	V(E_A)[c]	Cov(ln k_p, E_A)[c] × 10^3
S41	21–90	620	6.43	22.0	6.64	10	0.043	0.523	0.230	-8.81
S42	22–70	619	6.43	23.0	6.83	10	0.018	0.0959	0.0804	-2.28
S28	6–50	723	6.58	23.2	6.92	29	0.037	0.0475	0.128	-0.412
S46[d]	13–73	648	6.47	21.1	6.51	12	0.029	0.104	0.108	-1.93
Average		651[e]	6.489	22.3	6.72	4[f]		5.28	0.928	25.9

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se:

standard error in data points (= $\sqrt{\dfrac{SSR}{N-2}}$) where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] study not included in Beuermann et al., *Macromol. Chem. Phys.* 2003, **204**, 1338–1350 (S44). [e] Geometric mean of k_p values. [f] Here N represents the number of individual studies.
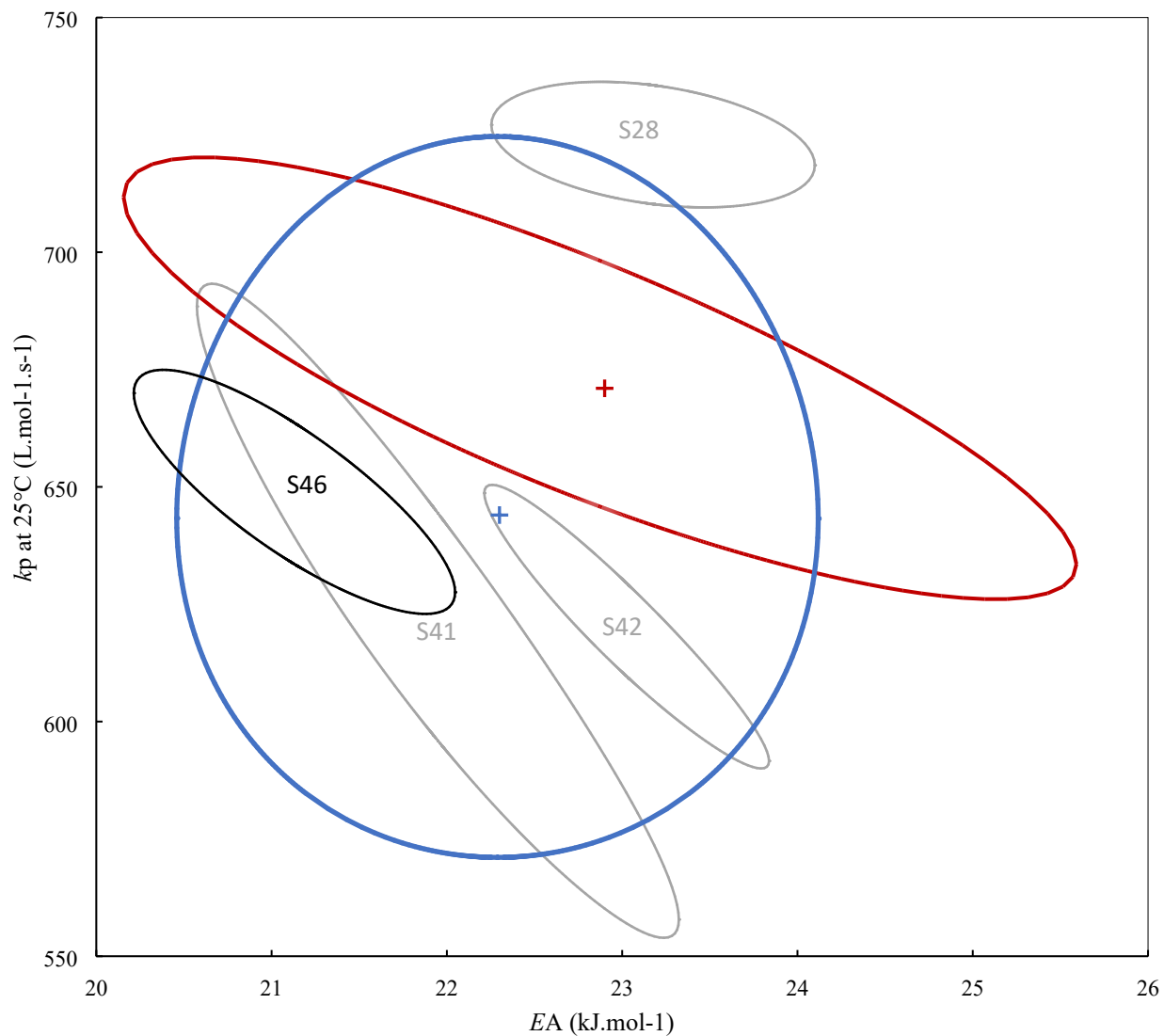
Figure S8. 95% JCRs for individual studies of k_p of benzyl methacrylate (original data set:[S44] gray; expanded data set: black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S44] obtained by pooling the data points of the original IUPAC data set in the restricted temperature range 10–55°C, and counting data from S41 and S42 twice, is shown for comparison (red).

Table S9. Estimates of k_p at 25°C, A and E_A for isobornyl methacrylate from individual studies obtained by linear least squares fitting of $\ln k_p$ to $(1/T - 1/T_0)$, $T_0 = 298.15$ K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A[a]	N[b]	se[c]	V(ln k_p)[c] × 10^3	V(E_A)[c]	Cov(ln k_p, E_A)[c] × 10^3
S41	10–90	491.3	6.20	22.9	6.71	28	0.057	0.376	0.139	-6.00
S42	0–91	588.1	6.38	23.3	6.85	15	0.021	0.0468	0.0349	-0.793
Average		538[d]	6.29	23.1	6.78	2[e]		16.1	0.0732	34.4

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se:

standard error in data points $\left(= \sqrt{\dfrac{SSR}{N-2}}\right)$ where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] Geometric mean of k_p values. [e] Here N represents the number of individual studies.
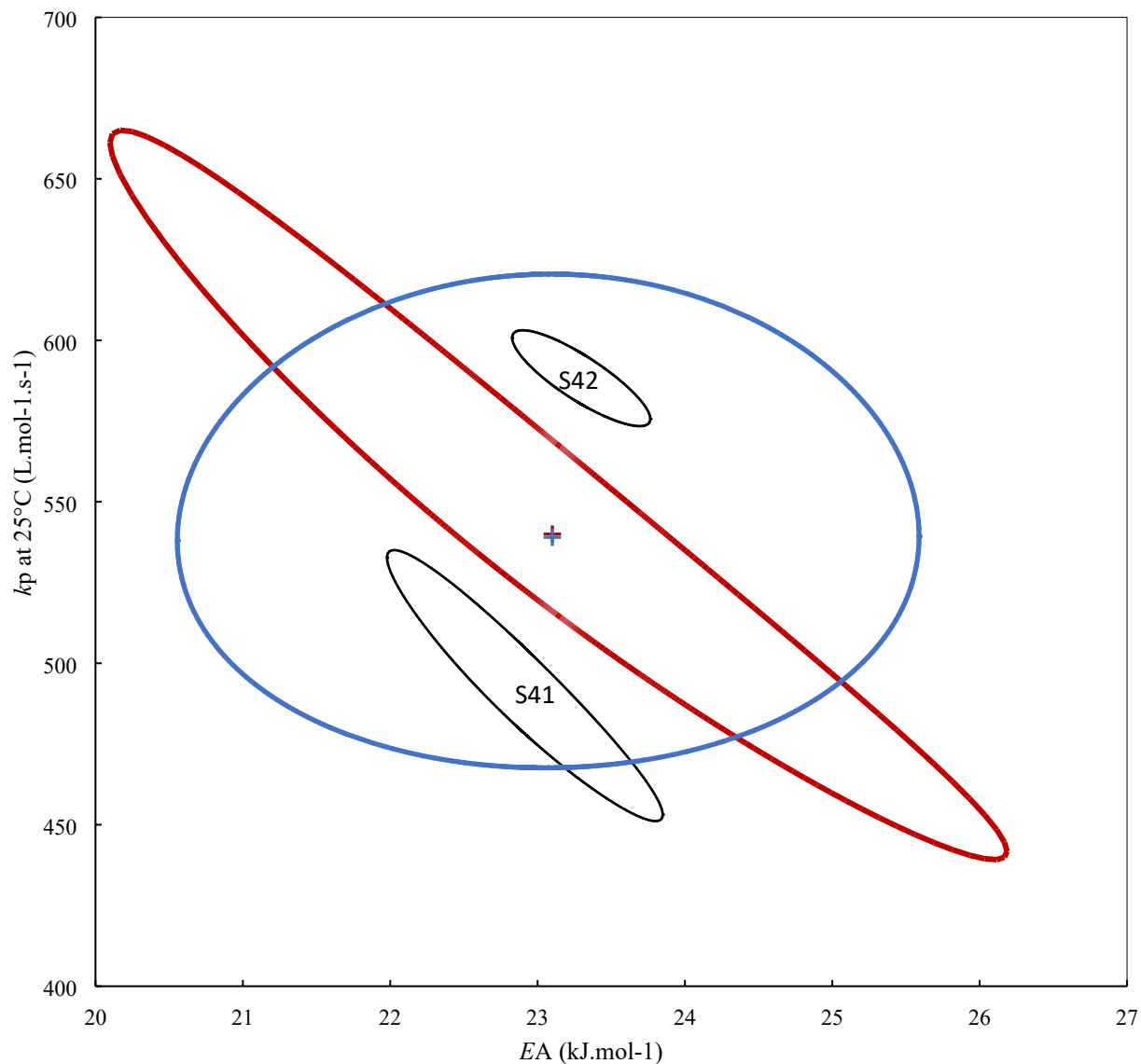
Figure S9. 95% JCRs for individual studies of k_p of isobornyl methacrylate (black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S44] obtained by pooling the data points of the original IUPAC data set in the restricted temperature range of 30–80°C and counting the data points of S42 twice, is shown for comparison (red).

Table S10. Estimates of k_p at 25°C, A and E_A for butyl acrylate from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, $T_0 = 298.15$ K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A[a]	N[b]	se[c]	V(ln k_p)[c] × 10^3	V(E_A)[c]	Cov(ln k_p, E_A)[c] × 10^3
S47	-65–-46	12.1	9.40	15.5	6.81	25	0.14	44.6	1.99	295
S48	-36–15	15.5	9.65	16.1	7.01	15	0.033	0.330	0.0865	4.73
S49	-41–15	14.8	9.60	18.0	7.33	30	0.030	0.152	0.0286	1.87
S50	-8–-7	13.5[d]	9.51[d]			4	0.15[e]	20.4[e]		
S51	11	15.7[d]	9.66[d]			2	0.083[e]	5.65[e]		
S52[f]	12–70	15.8	9.67	18.1	7.36	15	0.030	0.150	0.111	-3.16
S53[f]	30–50	17.3	9.76	14.5	6.77	4	0.050	4.10	5.53	-139
S54[f]	-25–38	15.5	9.65	18.6	7.44	17	0.013	0.0192	0.0106	0.320
S55[g]	*5–20*	*15.8*	*9.67*	*11.3*	*6.17*	*37*	*0.042*	*0.304*	*0.836*	*14.6*
Average		14.9[h]	9.61	16.9	7.12	7(5)[i]		12.1	2.73	4.92

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se:

standard error in data points $\left(= \sqrt{\dfrac{SSR}{N-2}}\right)$ where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] k_p @ 25°C adjusted from experimental temperature of -7.5°C (S50) or 10.8°C (S51) using the average activation energy of 16.9 kJ.mol^{-1}. [e] se and V(ln k_p) corrected by adding V(E_A)/[R(1/298.15-1/T)]^2+cov(E_A, ln k_p)/[R(1/298.15-1/T)] to the variance obtained at the experimental temperatures of -7.5°C and 10.8°C, where V(E_A) and cov(E_A, ln k_p) are the variance of the average activation energy and its covariance with ln k_p and T is -7.5°C or 10.8°C respectively. [f] study not included in Asua et al., *Macromol. Chem. Phys.* 2004, **205**, 2151–2160 (S56). [g] These results were excluded from the calculation of the interlaboratory mean and variance. [h] Geometric mean of k_p values. [i] Here N represents the number of individual studies. Number in parentheses is the number of studies reporting an E_A value.
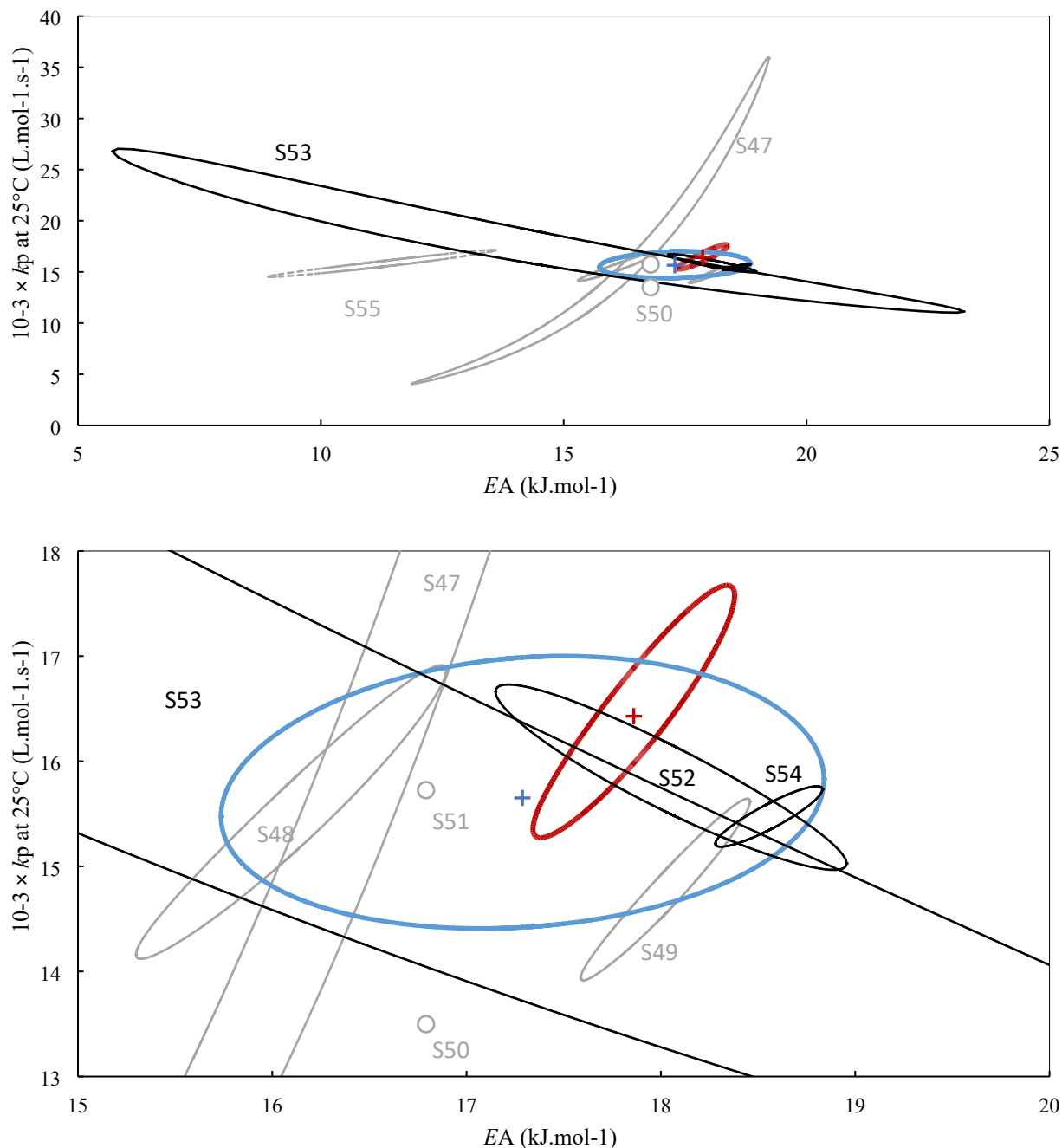
Figure S10. (a) 95% JCRs for individual studies of k_p of butyl acrylate (original data set:[S56] gray; expanded data set: black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S56] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red). The data from reference S55 (dotted line) was excluded from the calculation of the pooled interlaboratory variance. Data from references S50 and S51 were adjusted to 25°C using the average activation energy of 16.9 kJ.mol^{-1}. (b) shows an expanded view of the region containing the 95% JCRs corresponding to references S48-S49, S52 and S54 and the point estimates of references S50 and S51.

Table S11. Estimates of k_p at 25°C, A and E_A for methacrylic acid (15% aq. solution) from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, T_0 = 298.15 K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A (kJ.mol$^{-1)}$)	Log$_{10}$ A[a]	N[b]	se[c] × 10^3	V(ln k_p)[c] × 10^3	V(E_A)[c] × 10^3	Cov(ln k_p, E_A)[c] × 10^3
S57	18–89	3.60	6.24	15.3	6.71	17	43	0.212	162	-4.08
S58	20–60	3.86	6.20	14.9	6.85	12	8.7	0.0116	15.7	-0.286
Average		3.73[d]	6.22	15.1	6.22	2[e]		2.35	69	-12.8

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se: standard error in data points (= $\sqrt{\dfrac{SSR}{N-2}}$) where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] Geometric mean of k_p values. [e] Here N represents the number of individual studies.
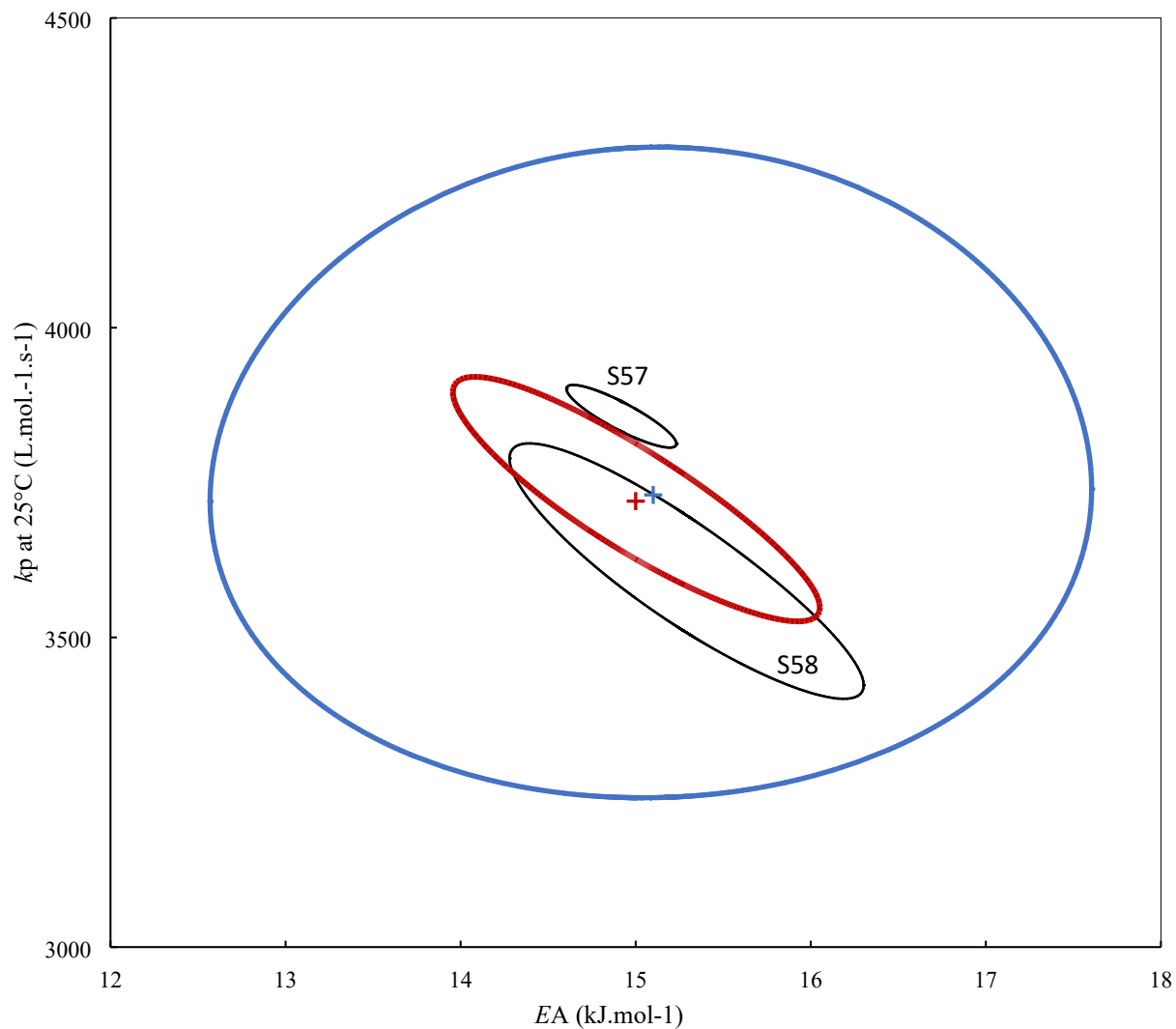
Figure S11. 95% JCRs for individual studies of k_p of methacrylic acid in 15% aqueous solution (black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S59] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red).

Table S12. Estimates of k_p at 25°C, A and E_A for methyl acrylate from individual studies obtained by linear least squares fitting of ln k_p to $(1/T - 1/T_0)$, T_0 = 298.15 K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C	Ln k_p @ 25°C	E_A	Log$_{10}$ A[a]	N[b]	se[c]	V(ln k_p)[c] × 10^3	V(E_A)[c]	Cov(ln k_p, E_A)[c] × 10^3
S60	-26–61	12.9	9.46	16.2	6.94	39	0.047	0.0666	0.0388	0.640
S50	-19–32	13.1	9.48	17.8	7.23	41	0.087	0.569	0.276	10.3
S54	-25–37	14.7	9.59	18.3	7.38	18	0.0084	0.00714	0.00413	0.115
S61[d]	*-28–-15*	*17.6*	*9.77*	*19.2*	*7.60*	*2*	*0.05[b]*	*47.2*	*8.19*	*613*
S62	11-61	14.1	9.56	19.0	7.48	12	0.059	0.391	1.48	61.6
Average		13.7[d]	9.52	17.8	7.26	4[e]		3.71	2.11	61.6

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298K)]/ln(10). [b] number of experimental points reported. [c] se:

standard error in data points ($= \sqrt{\dfrac{SSR}{N-2}}$) where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] These results, which were extrapolated from high pressure experiments, were excluded from the calculation of the interlaboratory mean and variance. [e] Geometric mean of k_p values. [f] Here N represents the number of individual studies.
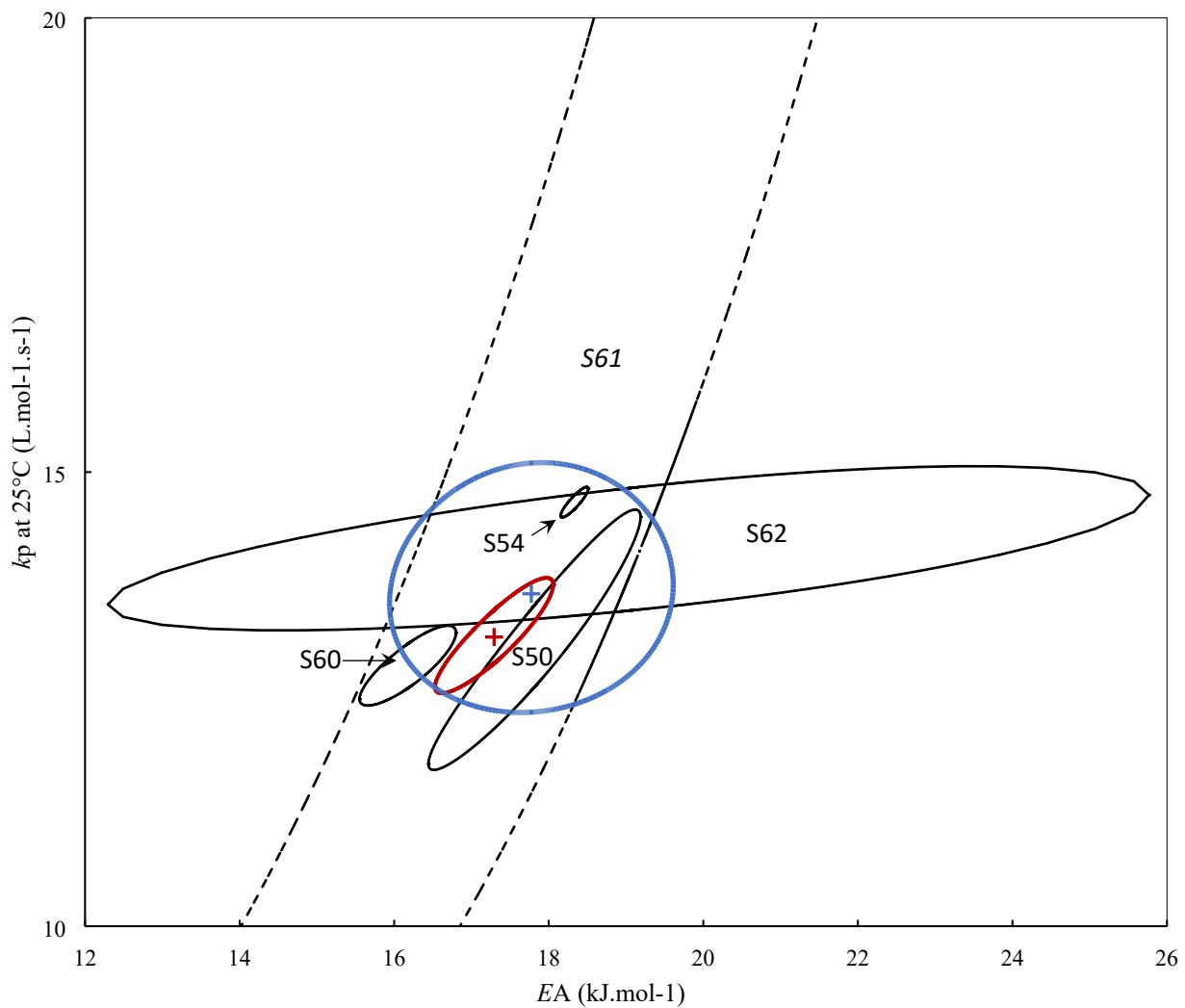
Figure S12. 95% JCRs for individual studies of k_p of methyl acrylate (black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S60] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red). The results of S61 (dashed line) were excluded from the calculations, as these results were extrapolated from high pressure experiments.

Table S13. Estimates of k_p at 25°C, A and E_A for vinyl acetate from individual studies obtained by linear least squares fitting of $\ln k_p$ to $(1/T - 1/T_0)$, $T_0 = 298.15$ K. Units of E_A are kJ·mol^{-1}, while k_p and A are given in L·mol^{-1}·s^{-1}.

Ref.	T (°C)	k_p @ 25°C × 10^3	Ln k_p @ 25°C	E_A	Log$_{10}$ A	N	se[a]	V(ln k_p) × 10^3	V(E_A)	Cov(ln k_p, E_A) × 10^3
S63	5–70	4.06	8.31	21.7	7.42	17	0.080	0.619	0.683	-12.8
S20	10–60	3.59	8.19	20.4	7.12	21	0.050	0.126	0.199	-1.21
S50	9–56	3.47	8.15	22.2	7.43	13	0.102	0.846	5.20	14.5
S64	10–60	3.89	8.26	19.1	6.93	40	0.073	0.281	0.572	-9.18
S65	25–65	3.38	8.13	21.7	7.34	53	0.093	0.585	0.717	-17.4
S66	14–61	3.38	8.13	18.6	6.78	33	0.063	0.176	0.276	-3.97
Average		3.62[d]	8.19	20.6	7.17	6[e]		5.94	2.34	6.81

[a] calculated as Log$_{10}$ A = [ln $k_{p,298K}$ + E_A/(R×298 K)]/ln(10). [b] number of experimental points reported. [c] se: standard error in data points (= $\sqrt{\dfrac{SSR}{N-2}}$) where SSR is the sum of squared residuals to the linear fit; V(X): variance of X; Cov(X, Y): covariance of X and Y. [d] Geometric mean of k_p values. [e] Here N represents the number of individual studies.
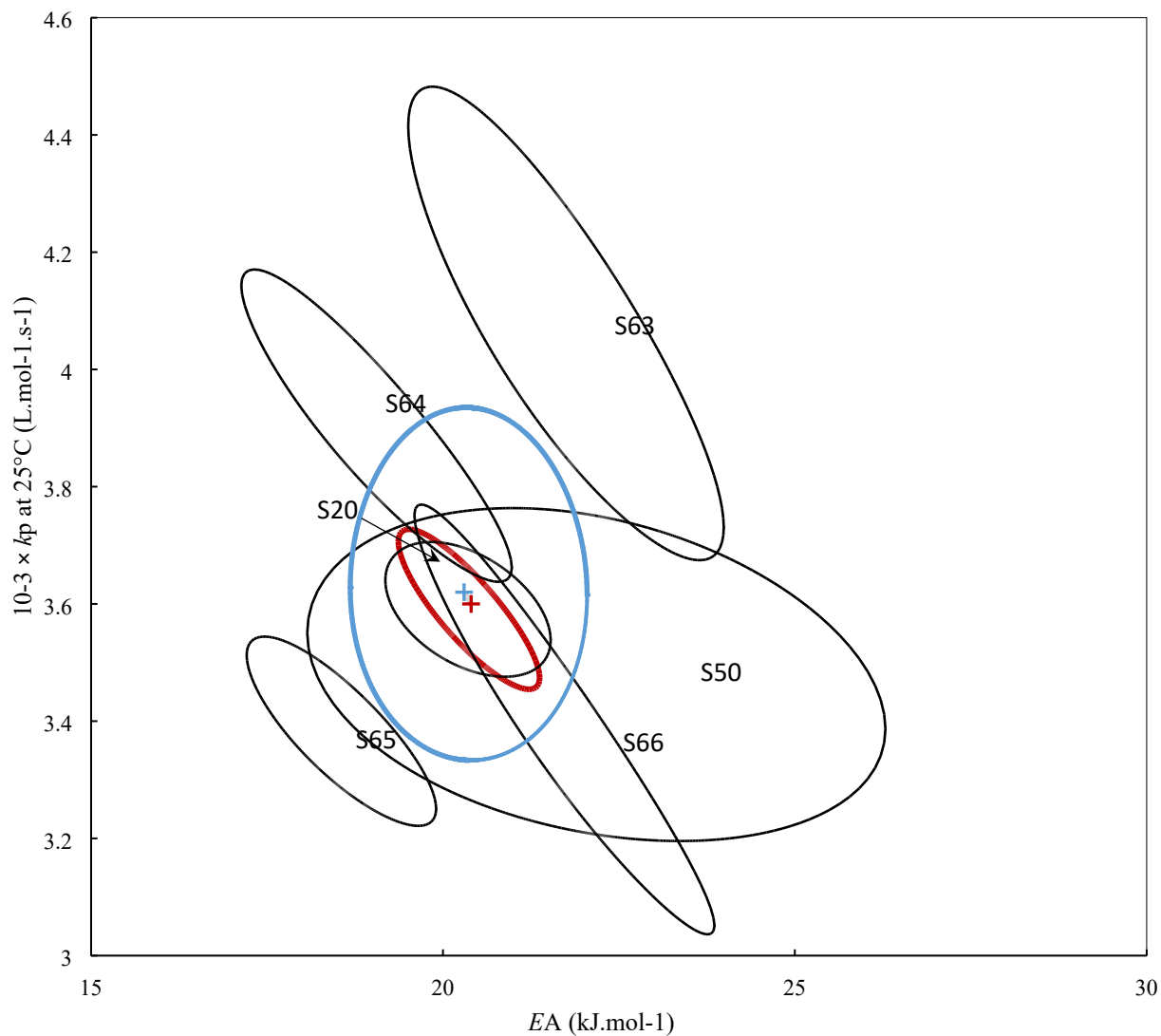
Figure S13. 95% JCRs for individual studies of k_p of vinyl acetate (black), and weighted average of studies with estimated uncertainty from the pooled interlaboratory variance (blue). The originally calculated 95% joint confidence region,[S67] obtained by pooling the data points of the original IUPAC data set, is shown for comparison (red).

2. Example calculation of 95% JCR from pooled interlaboratory variance.

The method is illustrated using the methyl acrylate data (Table S12). The pooled interlaboratory variances in ln k_p at 25°C (6.01×10^{-3}), E_A (1.88 (kJ·mol^{-1})^2) and the covariance (4.17×10^{-3} kJ·mol^{-1}) were added to the respective estimated variances and covariances from the linear fits (Table S14). The resulting covariance matrices, C_i, were inverted to form weight matrices, W_i (eq. S1)

$$W = C^{-1} = \begin{bmatrix} V(\ln k_p) & Cov(\ln k_p, E_A) \\ Cov(\ln k_p, E_A) & V(E_A) \end{bmatrix}^{-1} = \frac{1}{\det (C)} \begin{bmatrix} V(E_A) & -Cov(\ln k_p, E_A) \\ -Cov(\ln k_p, E_A) & V(\ln k_p) \end{bmatrix} \tag{S1}$$

$$\det (C) = V(E_A) \times V(\ln k_p) - [cov(\ln k_p, E_A)]^2$$

The weighted average was obtained from equation S2:

$$\begin{bmatrix} \bar{\ln k_p} \\ E_A \end{bmatrix} = \left(\sum_i W_i \right)^{-1} \sum_i W_i \begin{bmatrix} \ln k_p \\ E_A \end{bmatrix}_i \tag{S2}$$

The covariance matrix of the weighted average is given by $\left(\sum_i W_i \right)^{-1}$. This leads to a weighted average ln kp of 9.52, with estimated variance 1.56×10^{-3}, E_A of 17.8 kJ·mol^{-1} with estimated variance 0.523 (kJ·mol^{-1})^2, and estimated covariance of 2.10×10^{-3} kJ·mol^{-1}.

These variances are subsequently used to generate a 95% joint confidence region, using equation S3:[S68]

$$(\beta - \hat{\beta})^T \left(\sum_i W_i \right) (\beta - \hat{\beta}) < c \tag{S3}$$

Where β is a column vector containing ln k_p and E_A, $\hat{\beta}$ is the estimated value of β, and c is a critical value drawn from Hotelling's T^2 distribution with 2 and 58 degrees of freedom corresponding to the 95% significance level ($c = 6.44$). The 58 degrees of freedom correspond to the 71 studies for which estimates of both ln kp and E_A are available, minus the 13 monomers investigated. Use of a χ^2 distribution with 2 degrees of freedom in place of the T^2 distribution results in a slightly smaller JCR ($c = 5.99$).

A confidence band for k_p vs. temperature can be obtained from the same covariance matrix using equation S4:[S68]

$$\left| \ln \left(\frac{k_p}{\hat{k}_p} \right) \right| < \sqrt{c} \left(V(\ln k_{p0}) + \frac{V(E_A)}{R^2} \left(\frac{1}{T} - \frac{1}{T_0} \right)^2 - 2 \frac{Cov(\ln k_p, E_A)}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right) \right)^{\frac{1}{2}} \tag{S4}$$

Table S14: Calculation of weighted average and covariance matrix for ln k_p at 25°C and E_A of methyl acrylate. Units of E_A are kJ·mol^{-1}, while k_p is given in L·mol^{-1}·s^{-1}.

Ref.	ln k_p @ 25°C	E_A	C			W			weighted	
			$V(\ln k_{p,0}) \times 10^3$	$V(E_A)$	Cov. $\times 10^3$	$w_{\ln kp}$	w_{EA}	w_{Cov}	A^a	B^a
S60	9.46	16.2	6.07	1.92	4.81	165	0.521	-0.412	1553	4.53
S50	9.48	17.8	6.58	2.16	14.5	154	0.470	-1.03	1444	-1.42
S54	9.59	18.3	6.02	1.898	4.28	166	0.531	-0.378	1590	6.10
S62	9.56	19.0	6.41	2.53	12.2	158	0.400	-0.764	1491	0.31
weighted average	**9.52**	**17.8**	**1.56**	**0.523**	**2.10**	**643**	**1.92**	**-2.59**	**6078**	**9.53**

^{a} $A = w_{\ln kp} \times \ln k_p + w_{Cov} \times E_A$; $B = w_{EA} \times E_A + w_{Cov} \times \ln k_p$
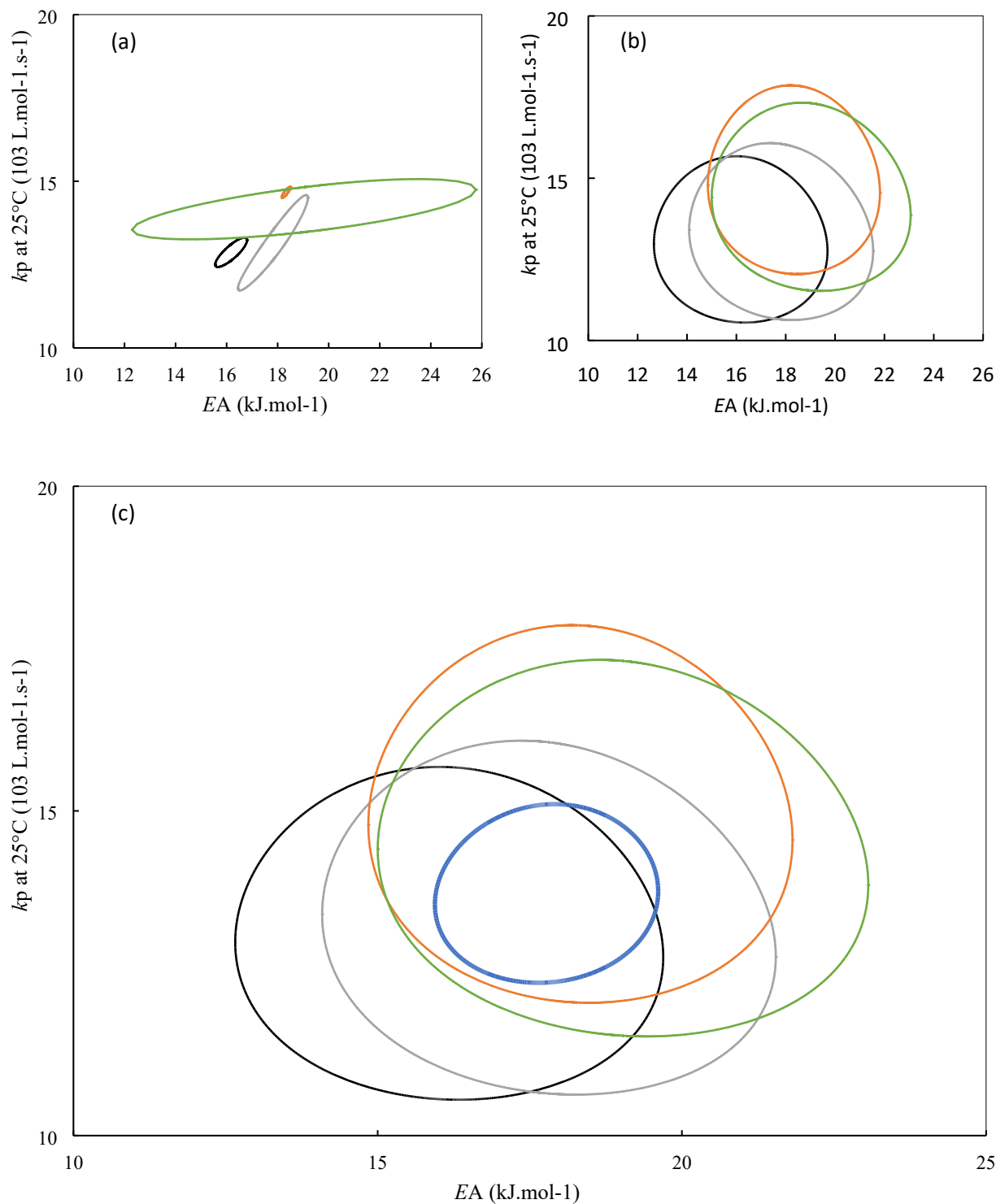
Figure S14. Process of obtaining a combined 95% joint confidence region: JCRs for the individual studies (a) are recalculated to include the interlaboratory variation (b). A combined JCR (c, shown in blue) is obtained from the weighted average of the individual estimates and the corresponding covariance matrix (Table S14)

3. Confidence bands for k_p:

The 95% confidence bands for k_p were obtained from equation S4, setting $c = 6.44$, $T_0 = 298$ K and using the values for $V(\ln k_{p,0})$, $V(E_A)$ and $Cov(\ln k_{p,0}, E_A)$ shown in Table S15

Table S15: Parameters for calculation of 95% confidence bands for k_p. Units of E_A are kJ·mol^{-1}, while $k_{p,0}$ is given in L·mol^{-1}·s^{-1}.

Monomer	$\ln k_{p,0}$	E_A	$V(\ln k_{p,0}) \times 10^3$	$V(E_A)$	$Cov(\ln k_{p,0}, E_A) \times 10^3$
STY	4.46	32.5	0.442	0.215	-0.432
MMA	5.78	22.3	0.338	0.183	-0.293
EMA	5.82	23.4	1.53	0.491	-0.643
BMA	5.97	22.9	0.834	0.274	0.819
DMA	6.26	21.0	2.08	0.713	0.0955
CHMA	6.37	23.0	2.13	0.704	-1.16
GMA	6.33	22.9	2.53	0.831	-7.81
BnMA	6.47	22.9	2.20	0.520	-0.0138
iBoMA	6.29	23.1	3.11	0.984	0.149
BA	9.66	17.9	1.05	0.374	2.74
MAA	8.22	15.0	3.06	0.985	1.05
MA	9.52	17.3	1.56	0.523	2.10
VAc	8.19	20.4	1.07	0.440	-0.460
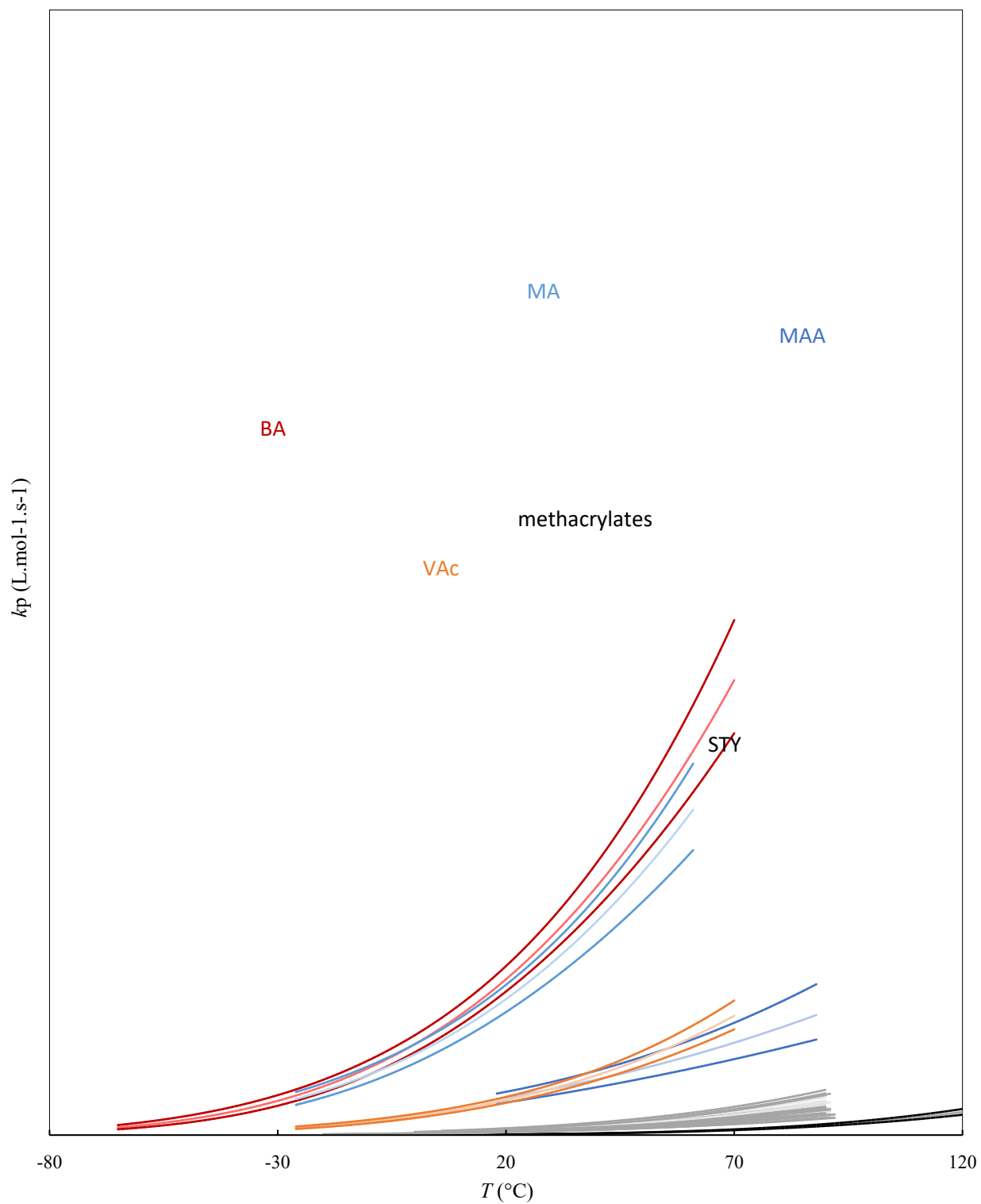
Figure S15. 95% confidence bands for k_p of styrene (STY), butyl acrylate (BA), methacrylic acid (MAA, 15% aqueous solution), methyl acrylate (MA) and vinyl acetate (VAc).
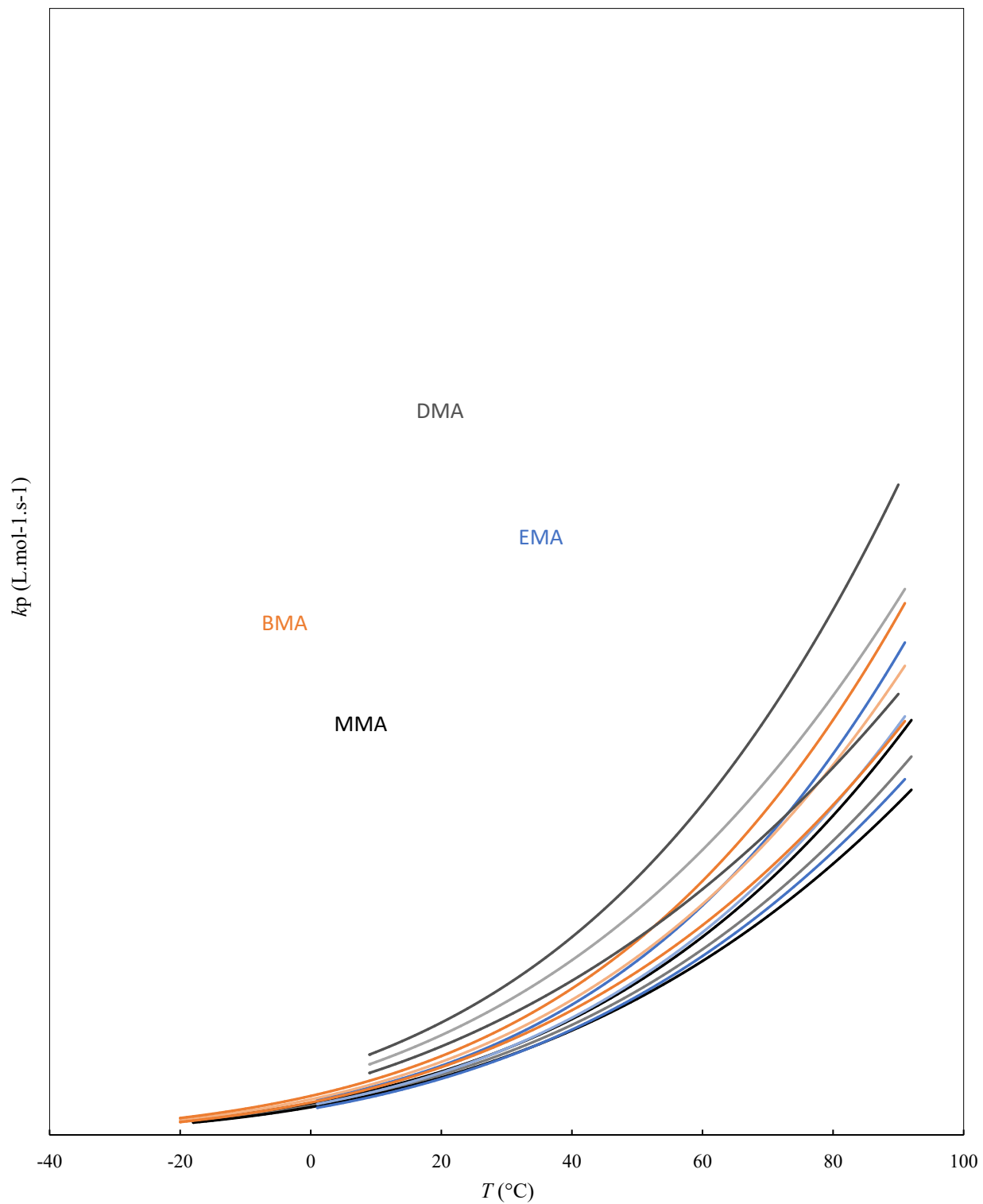
Figure S16. 95% confidence bands for k_p of linear methacrylates: methyl methacrylate (MMA), ethyl methacrylate (EMA), butyl methacrylate (BMA) and dodecyl methacrylate (DMA).
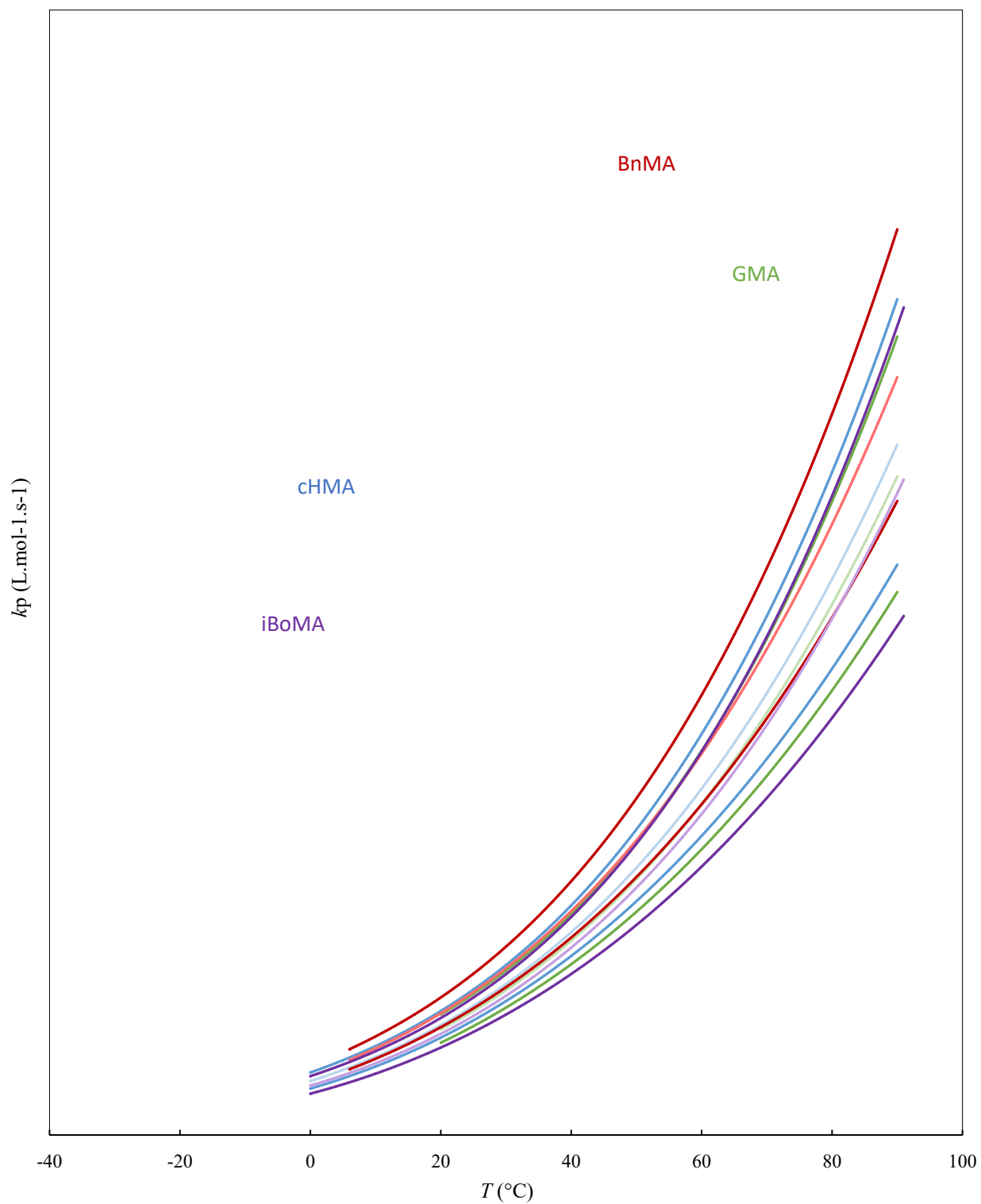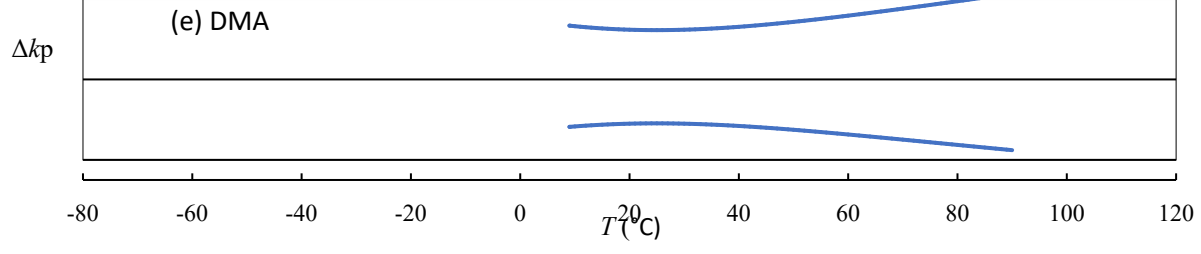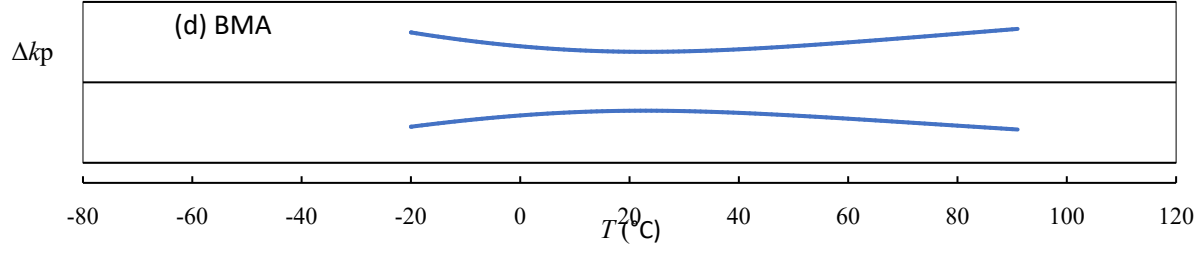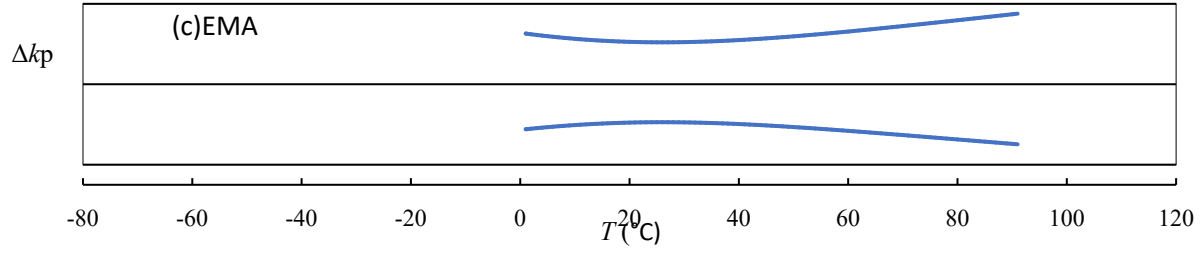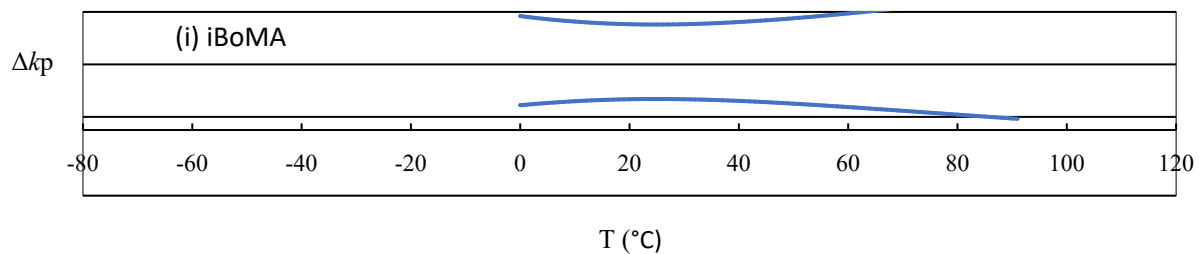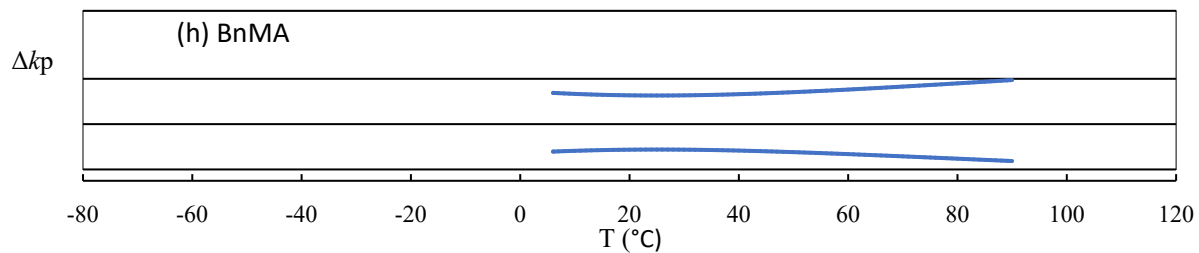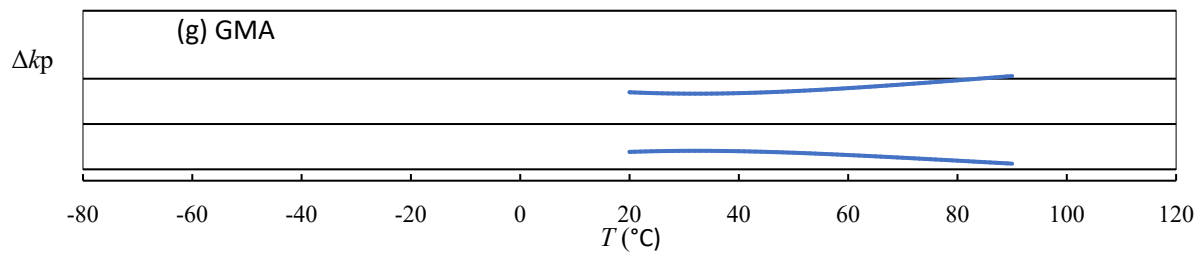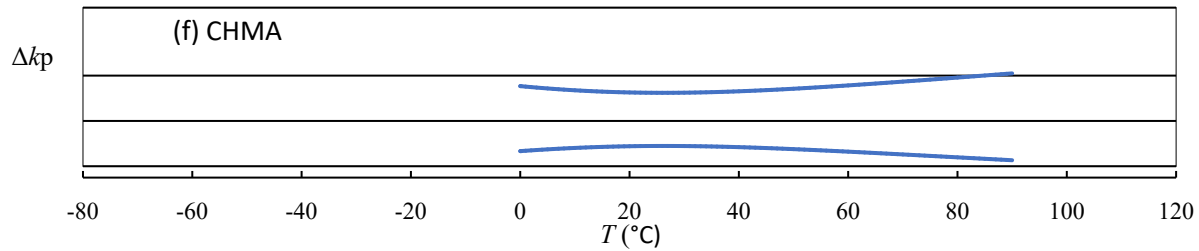
Figure S17. 95% confidence bands for k_p of cyclic methacrylates: cyclohexyl methacrylate (cHMA), glycidyl methacrylate (GMA), benzyl methacrylate (BnMA) and isobornyl methacrylate (iBoMA).

(a) STY

Δkp

-80 -60 -40 -20 0 T (°C) 20 40 60 80 100 120

(b) MMA

Δkp

-80 -60 -40 -20 0 T (°C) 20 40 60 80 100 120

(c)EMA

Δkp

-80 -60 -40 -20 0 T (°C) 20 40 60 80 100 120

(d) BMA

Δkp

-80 -60 -40 -20 0 T (°C) 20 40 60 80 100 120

(e) DMA

Δkp

-80 -60 -40 -20 0 T (°C) 20 40 60 80 100 120

35

(f) CHMA

Δkp

T (°C)

(g) GMA

Δkp

T (°C)

(h) BnMA

Δkp

T (°C)

(i) iBoMA

Δkp
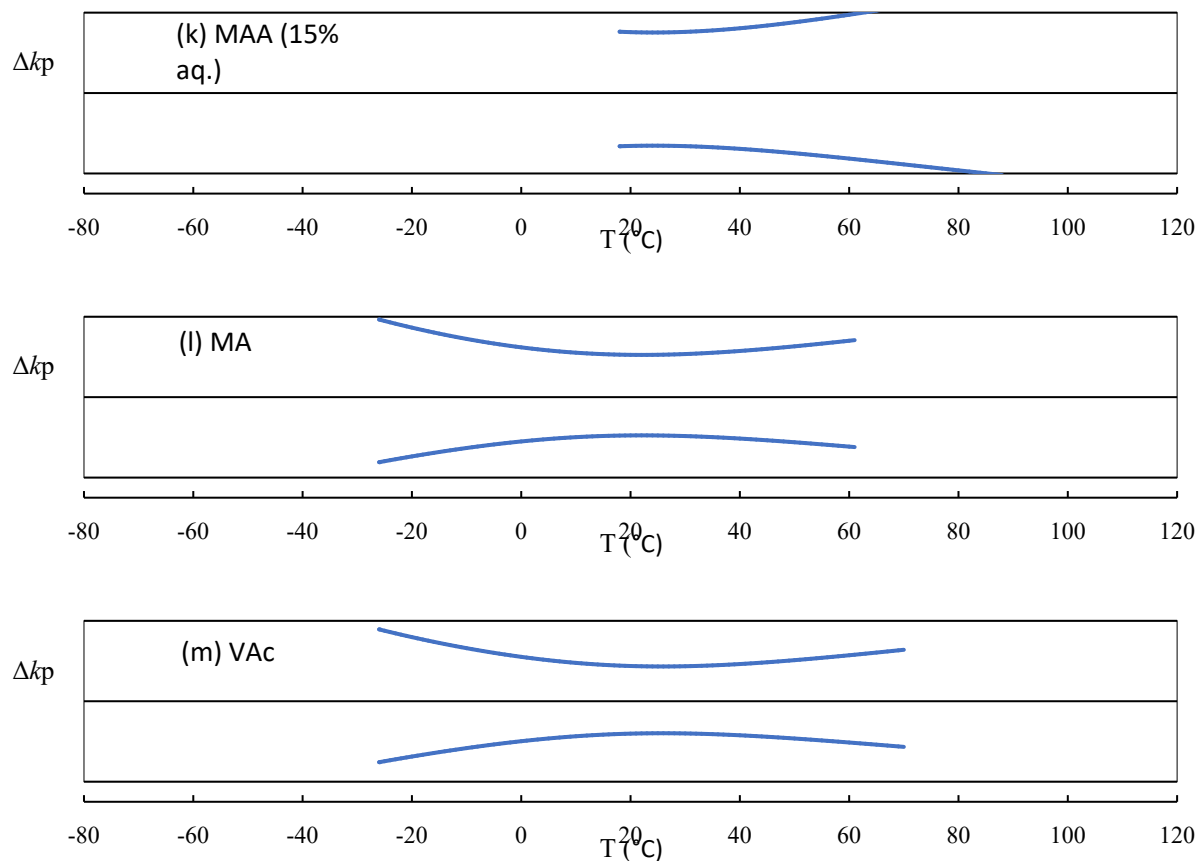
T (°C)

(j) BA

Δkp

T (°C)
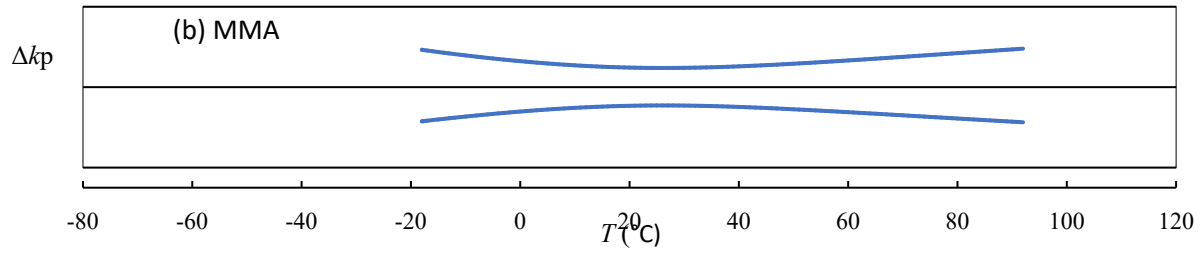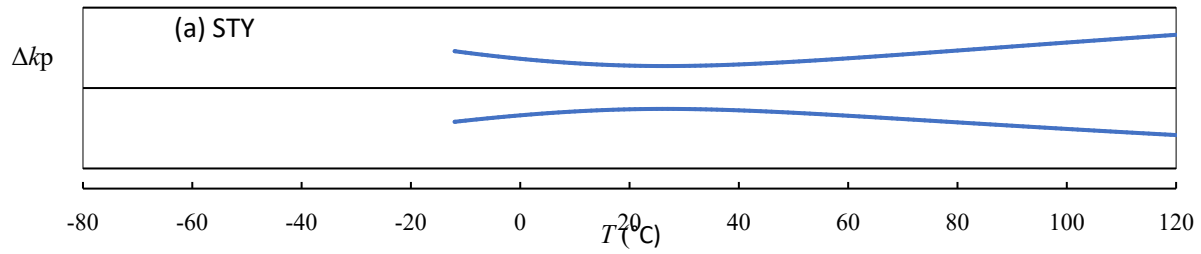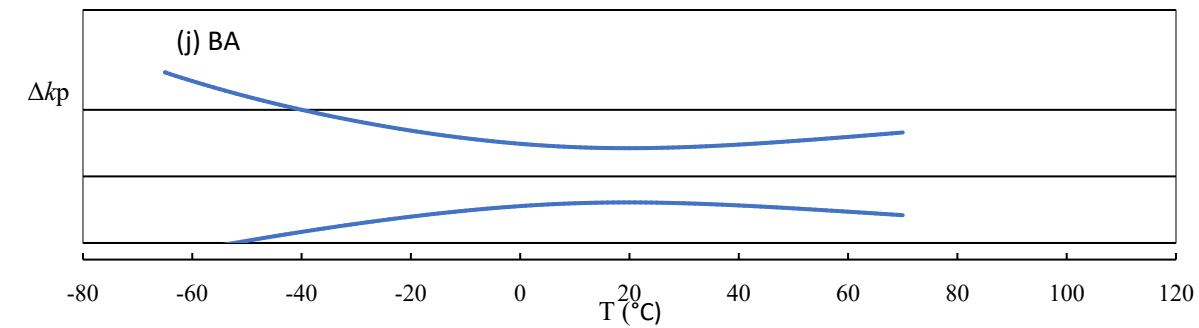
Figure S18. 95% confidence bands for k_p of vinyl monomers, expressed as relative deviation from the best fit to the experimental data ($\Delta k_p = \dfrac{k_p - \hat{k}_p}{\hat{k}_p}$). (a) styrene (STY); (b) methyl methacrylate (MMA); (c) ethyl methacrylate (EMA); (d) butyl methacrylate (BMA); (e) dodecyl methacrylate (DMA); (f) cyclohexyl methacrylate (cHMA); (g) glycidyl methacrylate (GMA); (h) benzyl methacrylate (BnMA); (i) isobornyl methacrylate (iBoMA); (j) butyl acrylate (BA); (k) methacrylic acid (MAA, 15% aqueous solution); (l) methyl acrylate (MA); (m) vinyl acetate (VAc).

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