

Electronic Supplementary Information (ESI)

Modeling ionization quenching in organic scintillators

T. A. Laplace¹, B. L. Goldblum^{1,2}, J. A. Brown¹, G. LeBlanc¹, T. Li¹, J. J. Manfredi¹,
and Erik Brubaker³

¹Department of Nuclear Engineering, University of California, Berkeley, CA 94720 USA.

²Nuclear Science Division at Lawrence Berkeley National Laboratory, Berkeley, CA, 94720 USA.

³Sandia National Laboratories, Livermore, CA, 94550 USA.

1 Proton light yield model performance

Table S1. Model goodness-of-fit for proton light yield data with no parameter constraints. The values correspond to the median χ^2 statistic from the Monte Carlo distribution divided by the number of degrees of freedom. The uncertainty is given by the median absolute deviation.

Scintillator	Birks	Chou	Hong et al.	Yoshida et al.	Voltz et al.
EJ-204	(11234 ± 1510)/31	(1878 ± 674)/30	(1851 ± 840)/29	(1270 ± 694)/28	(1411 ± 704)/28
EJ-309	(37064 ± 7857)/46	(2149 ± 1660)/45	(2369 ± 1660)/44	(1863 ± 1562)/43	(2362 ± 1453)/43
EJ-276	(1976 ± 525)/21	(129 ± 42)/20	(463 ± 145)/19	(93 ± 25)/18	(95 ± 18)/18
Organic glass	(6708 ± 1714)/52	(740 ± 205)/51	(428 ± 174)/50	(342 ± 151)/49	(376 ± 143)/49

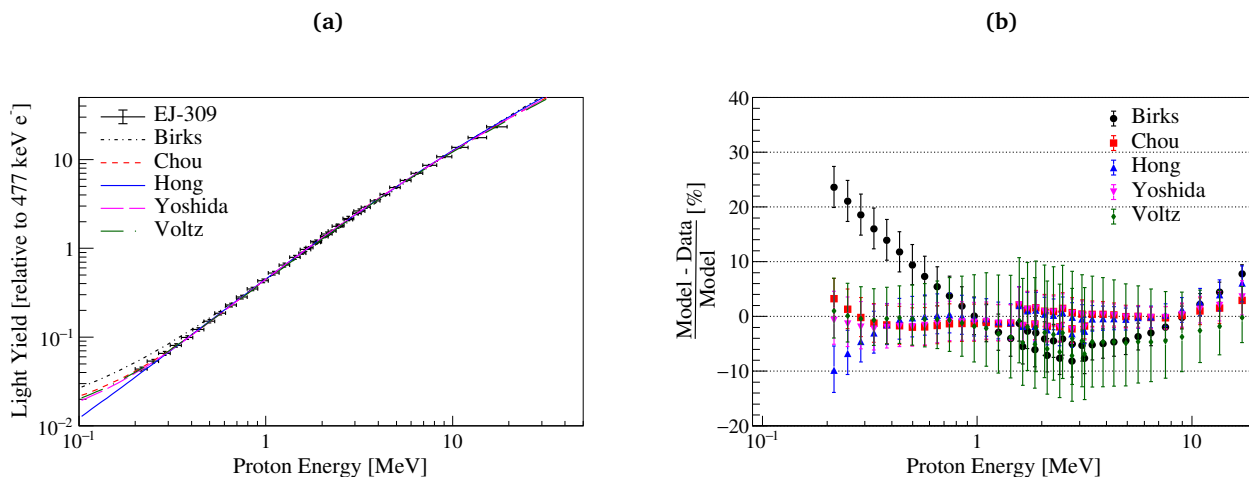


Figure S1. (a) Specific luminescence models applied to EJ-309 proton light yield data. (b) Standard deviation of model fits to the measured data.

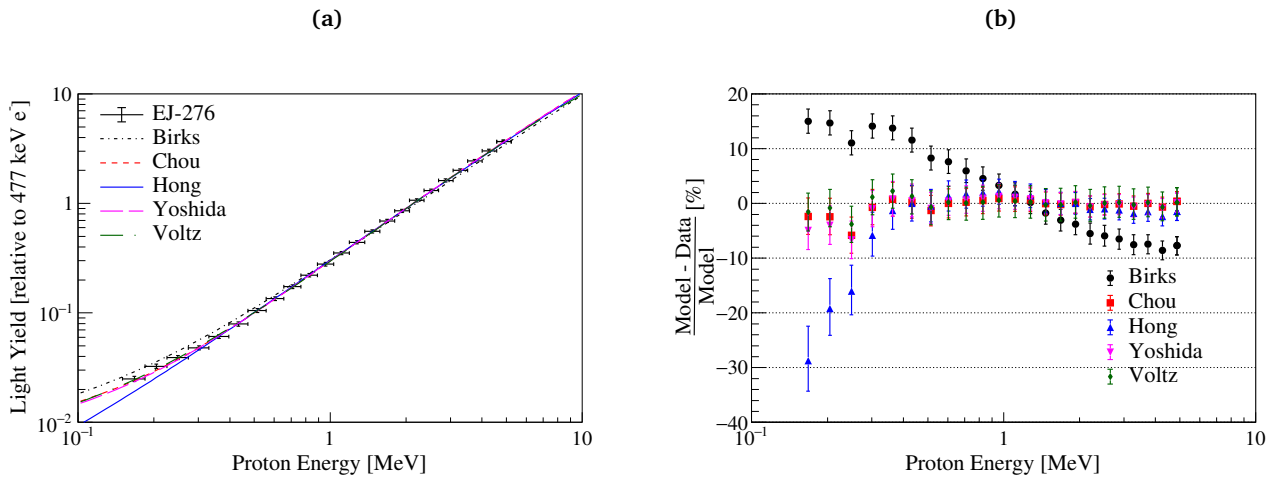


Figure S2. (a) Specific luminescence models applied to EJ-276 proton light yield data. (b) Standard deviation of model fits to the measured data.

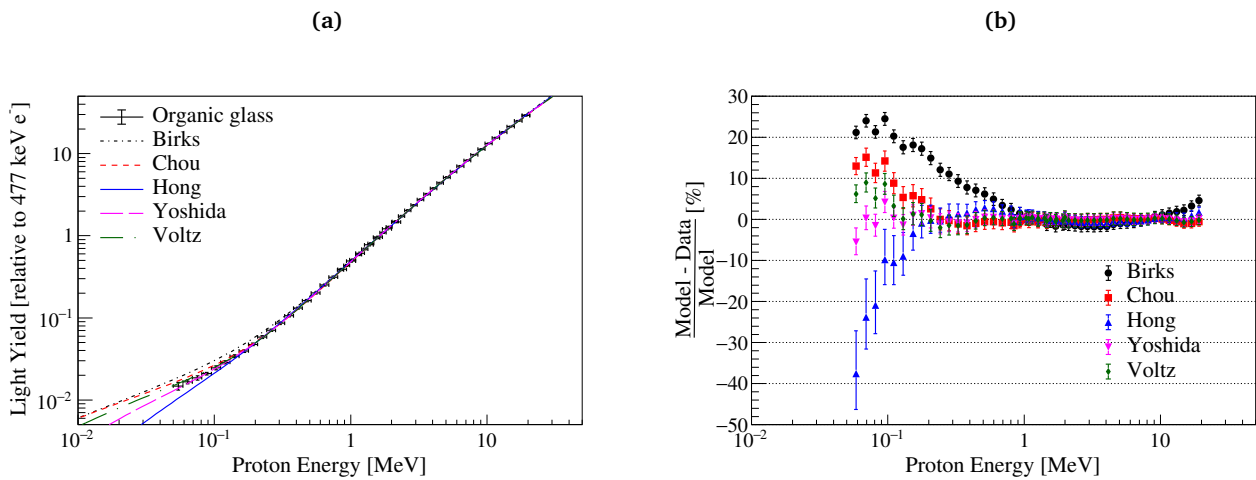


Figure S3. (a) Specific luminescence models applied to the organic glass proton light yield data. (b) Standard deviation of model fits to the measured data.

2 EJ-204 proton light yield model parameters and covariance

Table S2. EJ-204 proton light yield model parameters.

Model	S or S_e (rel. 477 keV e^-)	S_n (rel. 477 keV e^-)	kB or kB_e (mg/cm ² /MeV)	kB_n (mg/cm ² /MeV)	C (mg/cm ² /MeV) ²
Birks	2.51	—	13.1	—	—
Chou	1.86	—	5.50	—	7.93
Hong et al.	2.51	2.51	9.64	3163	—
Yoshida et al.	2.14	2.47	7.61	284	6.12

(a) Birks, Chou, Hong et al. and Yoshida et al.

S (rel. 477 keV e^-)	T_0 (keV)	B_s (mg/cm ² /MeV)	R_d	B_t (mg/cm ² /MeV)
1.79	7.40	7.93	0.409	1.74

(b) Voltz et al.

Table S3. EJ-204 proton light yield model parameter covariance matrices.

	S	kB
S	$2.09e-6$	$3.04e-5$
kB	$3.04e-5$	$9.00e-2$

(a) Birks

	S	kB	C
S	$1.62e-2$	0.104	$-1.61e-3$
kB	0.104	0.748	-0.140
C	$-1.61e-3$	-0.140	0.439

(b) Chou

	S_e	S_n	kB_e	kB_n
S_e	$4.08e-5$	$2.26e-10$	$2.76e-4$	$1.51e-2$
S_n	$2.26e-10$	$1.09e-12$	$3.68e-10$	$-2.44e-6$
kB_e	$2.76e-4$	$3.68e-10$	0.349	-319
kB_n	$1.51e-2$	$-2.44e-6$	-319	3.86e5

(c) Hong et al.

	S_e	S_n	kB_e	kB_n	C
S_e	$3.14e-2$	$2.26e-3$	0.208	13.4	$-6.98e-2$
S_n	$2.26e-3$	$3.00e-2$	$8.24e-3$	-2.96	$2.11e-2$
kB_e	0.208	$8.24e-3$	1.49	92.5	-0.646
kB_n	13.4	-2.96	92.5	$3.29e4$	-133
C	$-6.98e-2$	$-2.11e-2$	-0.646	-133	1.09

(d) Yoshida et al.

	S	T_0	B_s	R_d	B_t
S	$1.44e-2$	0.315	$9.53e-2$	$4.94e-4$	$1.17e-2$
T_0	0.315	18.8	-2.47	-0.186	-0.293
B_s	$9.53e-2$	2.47	3.83	0.143	0.474
R_d	$4.94e-4$	-0.186	0.143	$8.32e-3$	$2.52e-2$
B_t	$1.17e-2$	-0.293	0.474	$2.52e-2$	$8.68e-2$

(e) Voltz et al.

3 EJ-309 proton light yield model parameters and covariance

Table S4. EJ-309 proton light yield model parameters.

Model	S or S_e (rel. 477 keV e^-)	S_n (rel. 477 keV e^-)	kB or kB_e (mg/cm ² /MeV)	kB_n (mg/cm ² /MeV)	C (mg/cm ² /MeV) ²
Birks	2.51	—	10.4	—	—
Chou	1.94	—	4.55	—	6.91
Hong et al.	2.17	2.50	4.38	4403	—
Yoshida et al.	1.98	2.42	4.89	168	6.13

(a) Birks, Chou, Hong et al. and Yoshida et al.

S (rel. 477 keV e^-)	T_0 (keV)	B_s (mg/cm ² /MeV)	R_d	B_t (mg/cm ² /MeV)
1.86	2.54	10.9	0.54	1.90

(b) Voltz et al.

Table S5. EJ-309 proton light yield model parameter covariance matrices.

	S	kB
S	$1.00e-3$	$5.44e-3$
kB	$5.44e-3$	0.279

(a) Birks

	S	kB	C
S	$2.43e-2$	0.165	$-8.37e-4$
kB	0.165	1.25	-0.170
C	$-8.37e-4$	-0.170	0.534

(b) Chou

	S_e	S_n	kB_e	kB_n
S_e	$3.53e-2$	$4.28e-3$	0.258	-26.3
S_n	$4.28e-3$	$1.06e-2$	$3.55e-2$	-5.87
kB_e	0.258	$3.55e-2$	2.35	-629
kB_n	-26.3	-5.87	-629	$5.39e5$

(c) Hong et al.

	S_e	S_n	kB_e	kB_n	C
S_e	$2.38e-2$	$1.40e-2$	0.163	-1.74	$-2.74e-3$
S_n	$1.40e-2$	$6.86e-2$	0.101	-28.4	$8.23e-2$
kB_e	0.163	0.101	1.25	-16.2	-0.162
kB_n	-1.74	-28.4	-16.2	$5.79e4$	-165
C	$-2.74e-3$	$8.23e-2$	-0.162	-165	0.966

(d) Yoshida et al.

	S	T_0	B_s	R_d	B_t
S	$7.98e-3$	$1.93e-2$	0.265	$3.53e-4$	$5.82e-3$
T_0	$1.93e-2$	26.2	-4.90	-0.164	-0.378
B_s	0.265	-4.90	22.0	0.226	0.638
R_d	$3.53e-4$	-0.164	0.226	$8.76e-3$	$2.10e-2$
B_t	$5.82e-3$	-0.378	0.638	$2.10e-2$	$5.73e-2$

(e) Voltz et al.

4 EJ-276 proton light yield model parameters and covariance

Table S6. EJ-276 proton light yield model parameters.

Model	S or S_e (rel. 477 keV e^-)	S_n (rel. 477 keV e^-)	kB or kB_e (mg/cm ² /MeV)	kB_n (mg/cm ² /MeV)	C (mg/cm ² /MeV) ²
Birks	2.51	—	17.5	—	—
Chou	2.43	—	13.3	—	9.55
Hong et al.	2.51	2.51	12.5	5286	—
Yoshida et al.	2.46	2.51	13.6	4.18	8.95

(a) Birks, Chou, Hong et al. and Yoshida et al.

S (rel. 477 keV e^-)	T_0 (keV)	B_s (mg/cm ² /MeV)	R_d	B_t (mg/cm ² /MeV)
1.76	8.15	7.67	0.230	1.29

(b) Voltz et al.

Table S7. EJ-276 proton light yield model parameter covariance matrices.

	S	kB
S	$3.19e-5$	$3.53e-4$
kB	$3.53e-4$	0.227

(a) Birks

	S	kB	C
S	$1.90e-2$	0.165	$2.11e-2$
kB	0.165	1.72	-0.265
C	$2.11e-2$	-0.265	1.97

(b) Chou

	S_e	S_n	kB_e	kB_n
S_e	$2.81e-16$	$-2.21e-13$	$2.12e-11$	$3.65e-7$
S_n	$-2.21e-13$	$2.67e-4$	$1.31e-3$	-1.50
kB_e	$2.12e-11$	$1.31e-3$	1.13	-1283
kB_n	$3.65e-7$	-1.50	-1283	$1.78e6$

(c) Hong et al.

	S_e	S_n	kB_e	kB_n	C
S_e	$1.25e-2$	$1.45e-4$	0.110	-0.132	$9.49e-3$
S_n	$1.45e-4$	$2.44e-3$	$-7.57e-5$	-0.629	$7.18e-3$
kB_e	0.110	$-7.57e-5$	1.26	1.88	-0.392
kB_n	-0.32	-0.629	1.88	963	-14.0
C	$9.49e-3$	$7.18e-3$	-0.392	-14.0	2.10

(d) Yoshida et al.

	S	T_0	B_s	R_d	B_t
S	$1.01e-2$	0.149	$6.89e-2$	$1.08e-3$	$1.14e-2$
T_0	0.149	6.73	0.654	$1.96e-3$	0.112
B_s	$6.89e-2$	0.654	0.875	$2.80e-2$	0.180
R_d	$1.08e-3$	$1.96e-3$	$2.80e-2$	$1.63e-3$	$8.84e-3$
B_t	$1.14e-2$	0.112	0.180	$8.84e-3$	$5.32e-2$

(e) Voltz et al.

5 Organic glass proton light yield model parameters and covariance

Table S8. Organic glass proton light yield model parameters.

Model	S or S_e (rel. 477 keV e ⁻)	S_n (rel. 477 keV e ⁻)	kB or kB_e (mg/cm ² /MeV)	kB_n (mg/cm ² /MeV)	C (mg/cm ² /MeV) ²
Birks	2.44	—	9.83	—	—
Chou	2.14	—	6.69	—	4.24
Hong et al.	2.29	2.51	7.88	1058	—
Yoshida et al.	2.19	2.43	7.15	190	2.90

(a) Birks, Chou, Hong et al. and Yoshida et al.

S (rel. 477 keV e ⁻)	T_0 (keV)	B_s (mg/cm ² /MeV)	R_d	B_t (mg/cm ² /MeV)
2.05	13.2	8.91	0.453	1.73

(b) Voltz et al.

Table S9. Organic glass proton light yield model parameter covariance matrices.

	S	kB
S	$2.71e-3$	$1.28e-2$
kB	$1.28e-2$	0.101

(a) Birks

	S	kB	C
S	$2.80e-3$	$2.59e-2$	$-2.45e-2$
kB	$2.59e-2$	0.333	-0.394
C	$-2.45e-2$	-0.394	0.672

(b) Chou

	S_e	S_n	kB_e	kB_n
S_e	$2.13e-2$	$7.01e-5$	$1.47e-2$	-2.93
S_n	$7.01e-5$	$6.03e-4$	$7.50e-4$	-0.452
kB_e	$1.47e-2$	$-7.50e-4$	0.276	-159
kB_n	-2.93	0.452	-159	$1.45e5$

(c) Hong et al.

	S_e	S_n	kB_e	kB_n	C
S_e	$2.84e-3$	$2.66e-3$	$2.61e-2$	1.44	$-2.93e-2$
S_n	$2.66e-3$	$5.87e-2$	$2.41e-2$	0.434	$-2.68e-2$
kB_e	$2.61e-2$	$2.41e-2$	0.325	21.1	-0.438
kB_n	1.44	0.434	21.1	4779	-46.6
C	$-2.93e-2$	$-2.68e-2$	-0.438	-46.6	0.856

(d) Yoshida et al.

	S	T_0	B_s	R_d	B_t
S	$1.88e-3$	$9.38e-2$	$2.19e-2$	$1.10e-4$	$1.05e-3$
T_0	$9.38e-2$	15.4	0.969	$8.22e-4$	$3.13e-2$
B_s	$2.19e-2$	0.969	0.617	$1.07e-2$	$3.65e-2$
R_d	$1.10e-4$	$8.22e-4$	$1.07e-2$	$6.54e-4$	$2.17e-3$
B_t	$1.05e-3$	$3.13e-2$	$3.65e-2$	$2.17e-3$	$8.96e-3$

(e) Voltz et al.

6 Proton and Carbon Light Yield Models

Table S10. Model parameters obtained through simultaneous fit of the EJ-204 proton and carbon light yield data.

Model	S or S_e (rel. 477 keV e^-)	S_n (rel. 477 keV e^-)	kB or kB_e (mg/cm ² /MeV)	kB_n (mg/cm ² /MeV)	C (mg/cm ² /MeV) ²
Birks	2.51	—	13.2	—	—
Chou	2.51	—	12.9	—	0.416
Hong et al.	2.51	2.05	12.8	89.7	—
Yoshida et al.	2.51	2.51	12.8	86.3	$2.69e-3$

(a) Birks, Chou, Hong et al. and Yoshida et al.

S (rel. 477 keV e^-)	T_0 (keV)	B_s (mg/cm ² /MeV)	R_d	B_t (mg/cm ² /MeV)
1.68	11.0	4.32	$9.37e-2$	0.275

(b) Voltz et al.

Table S11. Covariance matrices for model parameters obtained through simultaneous fit of the EJ-204 proton and carbon light yield data.

	S	kB
S	$1.22e-20$	$-1.27e-12$
kB	$-1.27e-12$	$7.73e-2$

(a) Birks

	S	kB	C
S	$1.52e-20$	$2.68e-13$	$2.04e-13$
kB	$2.68e-13$	0.112	$-2.66e-2$
C	$2.04e-13$	$-2.66e-2$	$1.09e-2$

(b) Chou

	S_e	S_n	kB_e	kB_n
S_e	$1.17e-7$	$2.47e-6$	$1.89e-7$	$2.88e-4$
S_n	$2.47e-6$	0.154	$-4.61e-2$	5.73
kB_e	$1.89e-7$	$-4.61e-2$	0.100	-4.51
kB_n	$2.88e-4$	5.73	-4.51	433

(c) Hong et al.

	S_e	S_n	kB_e	kB_n	C
S_e	$1.01e-5$	$-3.02e-8$	$3.52e-5$	$3.09e-4$	$-5.76e-6$
S_n	$-3.02e-8$	$3.40e-4$	$-2.67e-4$	$2.31e-2$	$-3.28e-5$
kB_e	$3.52e-5$	$-2.67e-4$	0.100	-4.37	$3.88e-5$
kB_n	$3.09e-4$	$2.31e-2$	-4.37	371	$-2.03e-2$
C	$-5.76e-6$	$-3.28e-5$	$3.88e-5$	$-2.03e-2$	$1.40e-4$

(d) Yoshida et al.

	S	T_0	B_s	R_d	B_t
S	$4.37e-5$	$-9.77e-4$	$2.25e-6$	$-6.19e-7$	$-1.11e-6$
T_0	$-9.77e-4$	0.932	$7.55e-3$	$4.70e-4$	$1.69e-3$
B_s	$2.25e-6$	$7.55e-3$	$2.35e-2$	$1.23e-3$	$3.00e-3$
R_d	$-6.19e-7$	$4.70e-4$	$1.23e-3$	$9.63e-5$	$2.40e-4$
B_t	$-1.11e-6$	$1.69e-3$	$3.00e-3$	$2.40e-4$	$6.36e-4$

(e) Voltz et al.

Table S12. Model parameters obtained through simultaneous fit of the EJ-309 proton and carbon light yield data.

Model	S or S_e (rel. 477 keV e ⁻)	S_n (rel. 477 keV e ⁻)	kB or kB_e (mg/cm ² /MeV)	kB_n (mg/cm ² /MeV)	C (mg/cm ² /MeV) ²
Birks	2.51	—	10.5	—	—
Chou	2.22	—	6.81	—	5.05
Hong et al.	2.42	2.51	7.61	2258	—
Yoshida et al.	2.17	2.51	6.46	10.7	5.09

(a) Birks, Chou, Hong et al. and Yoshida et al.

S (rel. 477 keV e ⁻)	T_0 (keV)	B_s (mg/cm ² /MeV)	R_d	B_t (mg/cm ² /MeV)
1.70	1.86	5.67	0.192	0.468

(b) Voltz et al.

Table S13. Covariance matrices for model parameters obtained through simultaneous fit of the EJ-309 proton and carbon light yield data.

	S	kB
S	$2.56e-3$	$1.32e-2$
kB	$1.32e-2$	0.304

(a) Birks

	S	kB	C
S	$5.67e-2$	0.416	$-7.98e-2$
kB	0.416	3.23	-0.847
C	$-7.98e-2$	-0.847	0.951

(b) Chou

	S_e	S_n	kB_e	kB_n
S_e	$2.10e-2$	$1.99e-4$	0.165	-17.9
S_n	$1.99e-4$	$5.47e-4$	$2.70e-3$	-1.16
kB_e	0.165	$2.70e-3$	1.83	-576
kB_n	-17.9	-1.16	-576	5.20e5

(c) Hong et al.

	S_e	S_n	kB_e	kB_n	C
S_e	$6.06e-2$	$-8.92e-4$	0.443	3.15	-0.103
S_n	$-8.92e-4$	$2.46e-3$	$-7.72e-3$	-2.97	$1.50e-2$
kB_e	0.443	$-7.72e-3$	3.42	27.8	-1.01
kB_n	3.15	-2.97	27.8	$1.05e4$	-50.4
C	-0.103	$1.50e-2$	-1.01	-50.4	1.10

(d) Yoshida et al.

	S	T_0	B_s	R_d	B_t
S	$2.55e-3$	$7.69e-2$	$-1.99e-2$	$-1.29e-3$	$-1.47e-3$
T_0	$7.69e-2$	9.72	-1.12	$-5.96e-2$	$-7.38e-2$
B_s	$-1.99e-2$	-1.12	0.685	$2.76e-2$	$3.65e-2$
R_d	$-1.29e-3$	$-5.96e-2$	$2.76e-2$	$1.48e-3$	$1.92e-3$
B_t	$-1.47e-3$	$-7.38e-2$	$3.65e-2$	$1.92e-3$	$2.58e-3$

(e) Voltz et al.

Table S14. Model goodness-of-fit for proton and carbon light yield data with no parameter constraints. The values correspond to the median χ^2 statistic from the Monte Carlo distribution divided by the number of degrees of freedom. The uncertainty is given by the median absolute deviation.

Scintillator	Birks	Chou	Hong et al.	Yoshida et al.	Voltz et al.
EJ-204	$(15627 \pm 1464)/43$	$(15470 \pm 1409)/42$	$(14136 \pm 1465)/41$	$(13808 \pm 1443)/40$	$(4632 \pm 1143)/40$
EJ-309	$(56658 \pm 10261)/54$	$(18643 \pm 3376)/53$	$(13409 \pm 3364)/52$	$(10578 \pm 3164)/51$	$(4798 \pm 661)/51$