Joan-Emma Shea

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	A Venue for Advances in Experimental and Theoretical Methods in Physical Chemistry. Journal of Physical Chemistry A, 2022, 126, 177-179.	1.1	0
2	The Journal of Physical Chemistry: Looking Back on Our 125th Anniversary and Looking Ahead to 2022. Journal of Physical Chemistry A, 2022, 126, 1-2.	1.1	0
3	The Journal of Physical Chemistry: Looking Back on Our 125th Anniversary and Looking Ahead to 2022. Journal of Physical Chemistry B, 2022, 126, 1-2.	1.2	0
4	50 and 100 Years Ago in <i>The Journal of Physical Chemistry</i> . Journal of Physical Chemistry B, 2022, 126, 2609-2611.	1.2	0
5	50 and 100 Years Ago in <i>The Journal of Physical Chemistry</i> . Journal of Physical Chemistry A, 2022, 126, 2149-2151.	1.1	0
6	Confronting Racism in Chemistry Journals. ACS ES&T Engineering, 2021, 1, 3-5.	3.7	0
7	Celebrating the 125th Anniversary of The Journal of Physical Chemistry. Journal of Physical Chemistry A, 2021, 125, 1-2.	1.1	0
8	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimer's Disease, Parkinson's Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. Chemical Reviews, 2021, 121, 2545-2647.	23.0	406
9	Catalytic Cross Talk between Key Peptide Fragments That Couple Alzheimer's Disease with Amyotrophic Lateral Sclerosis. Journal of the American Chemical Society, 2021, 143, 3494-3502.	6.6	10
10	Evolving Sections of The Journal of Physical Chemistry to Reflect an Ever-Changing Field. Journal of Physical Chemistry A, 2021, 125, 2019-2020.	1.1	0
11	Evolving Sections of The Journal of Physical Chemistry to Reflect an Ever-Changing Field. Journal of Physical Chemistry B, 2021, 125, 2465-2466.	1.2	3
12	Evolving Sections of The Journal of Physical Chemistry to Reflect an Ever-Changing Field. Journal of Physical Chemistry C, 2021, 125, 5425-5426.	1.5	0
13	Protein Cold Denaturation in Implicit Solvent Simulations: A Transfer Free Energy Approach. Journal of Physical Chemistry B, 2021, 125, 5222-5232.	1.2	10
14	Force Field Parameterization for the Description of the Interactions between Hydroxypropyl-β-Cyclodextrin and Proteins. Journal of Physical Chemistry B, 2021, 125, 7397-7405.	1.2	9
15	Pressure Unfolding of Proteins: New Insights into the Role of Bound Water. Journal of Physical Chemistry B, 2021, 125, 8431-8442.	1.2	11
16	Molecular Context of Dopa Influences Adhesion of Mussel-Inspired Peptides. Journal of Physical Chemistry B, 2021, 125, 9999-10008.	1.2	5
17	CORE-MD II: A fast, adaptive, and accurate enhanced sampling method. Journal of Chemical Physics, 2021, 155, 104114.	1.2	2
18	Celebrating the 125th Anniversary of The Journal of Physical Chemistry. Journal of Physical Chemistry B, 2021, 125, 1-2.	1.2	0

#	Article	IF	CITATIONS
19	Celebrating the 125th Anniversary of The Journal of Physical Chemistry. Journal of Physical Chemistry C, 2021, 125, 1-2.	1.5	1
20	Confronting Racism in Chemistry Journals. Biochemistry, 2020, 59, 2313-2315.	1.2	0
21	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Biomaterials Science and Engineering, 2020, 6, 2707-2708.	2.6	0
22	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Central Science, 2020, 6, 589-590.	5.3	0
23	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Chemical Biology, 2020, 15, 1282-1283.	1.6	Ο
24	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Chemical Neuroscience, 2020, 11, 1196-1197.	1.7	0
25	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Earth and Space Chemistry, 2020, 4, 672-673.	1.2	Ο
26	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Energy Letters, 2020, 5, 1610-1611.	8.8	1
27	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Macro Letters, 2020, 9, 666-667.	2.3	Ο
28	Update to Our Reader, Reviewer, and Author Communities—April 2020. , 2020, 2, 563-564.		0
29	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Nano, 2020, 14, 5151-5152.	7.3	2
30	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Photonics, 2020, 7, 1080-1081.	3.2	0
31	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Pharmacology and Translational Science, 2020, 3, 455-456.	2.5	Ο
32	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Sustainable Chemistry and Engineering, 2020, 8, 6574-6575.	3.2	0
33	Update to Our Reader, Reviewer, and Author Communities—April 2020. Analytical Chemistry, 2020, 92, 6187-6188.	3.2	Ο
34	Update to Our Reader, Reviewer, and Author Communities—April 2020. Chemistry of Materials, 2020, 32, 3678-3679.	3.2	0
35	Update to Our Reader, Reviewer, and Author Communities—April 2020. Environmental Science and Technology Letters, 2020, 7, 280-281.	3.9	1
36	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Chemical Education, 2020, 97, 1217-1218.	1.1	1

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37	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Proteome Research, 2020, 19, 1883-1884.	1.8	0
38	Confronting Racism in Chemistry Journals. Langmuir, 2020, 36, 7155-7157.	1.6	0
39	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Applied Polymer Materials, 2020, 2, 1739-1740.	2.0	Ο
40	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Combinatorial Science, 2020, 22, 223-224.	3.8	0
41	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Medicinal Chemistry Letters, 2020, 11, 1060-1061.	1.3	Ο
42	Editorial Confronting Racism in Chemistry Journals. , 2020, 2, 829-831.		0
43	Confronting Racism in Chemistry Journals. Journal of Physical Chemistry Letters, 2020, 11, 5279-5281.	2.1	1
44	Confronting Racism in Chemistry Journals. ACS Applied Energy Materials, 2020, 3, 6016-6018.	2.5	0
45	Confronting Racism in Chemistry Journals. ACS Central Science, 2020, 6, 1012-1014.	5.3	1
46	Confronting Racism in Chemistry Journals. Industrial & Engineering Chemistry Research, 2020, 59, 11915-11917.	1.8	0
47	Dueling Backbones: Comparing Peptoid and Peptide Analogues of a Mussel Adhesive Protein. Macromolecules, 2020, 53, 6767-6779.	2.2	16
48	Latent Models of Molecular Dynamics Data: Automatic Order Parameter Generation for Peptide Fibrillization. Journal of Physical Chemistry B, 2020, 124, 8012-8022.	1.2	6
49	CORE-MD, a path correlated molecular dynamics simulation method. Journal of Chemical Physics, 2020, 153, 084114.	1.2	6
50	Confronting Racism in Chemistry Journals. Journal of Natural Products, 2020, 83, 2057-2059.	1.5	0
51	Confronting Racism in Chemistry Journals. Journal of the American Society for Mass Spectrometry, 2020, 31, 1321-1323.	1.2	1
52	Confronting Racism in Chemistry Journals. Energy & Fuels, 2020, 34, 7771-7773.	2.5	0
53	Confronting Racism in Chemistry Journals. ACS Sensors, 2020, 5, 1858-1860.	4.0	0
54	Confronting Racism in Chemistry Journals. ACS Nano, 2020, 14, 7675-7677.	7.3	2

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55	ADD Force Field for Sugars and Polyols: Predicting the Additivity of Protein–Osmolyte Interaction. Journal of Physical Chemistry B, 2020, 124, 7779-7790.	1.2	11
56	Terminal Capping of an Amyloidogenic Tau Fragment Modulates Its Fibrillation Propensity. Journal of Physical Chemistry B, 2020, 124, 8772-8783.	1.2	17
57	Update to Our Reader, Reviewer, and Author Communities—April 2020. Biochemistry, 2020, 59, 1641-1642.	1.2	0
58	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Chemical & Engineering Data, 2020, 65, 2253-2254.	1.0	0
59	Update to Our Reader, Reviewer, and Author Communities—April 2020. Organic Process Research and Development, 2020, 24, 872-873.	1.3	0
60	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Omega, 2020, 5, 9624-9625.	1.6	0
61	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Applied Electronic Materials, 2020, 2, 1184-1185.	2.0	0
62	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Applied Materials & Interfaces, 2020, 12, 20147-20148.	4.0	5
63	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Physical Chemistry C, 2020, 124, 9629-9630.	1.5	0
64	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Physical Chemistry Letters, 2020, 11, 3571-3572.	2.1	0
65	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Synthetic Biology, 2020, 9, 979-980.	1.9	0
66	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Applied Energy Materials, 2020, 3, 4091-4092.	2.5	0
67	Confronting Racism in Chemistry Journals. Journal of Chemical Theory and Computation, 2020, 16, 4003-4005.	2.3	0
68	Confronting Racism in Chemistry Journals. Journal of Organic Chemistry, 2020, 85, 8297-8299.	1.7	0
69	Confronting Racism in Chemistry Journals. Analytical Chemistry, 2020, 92, 8625-8627.	3.2	0
70	Confronting Racism in Chemistry Journals. Journal of Chemical Education, 2020, 97, 1695-1697.	1.1	0
71	Confronting Racism in Chemistry Journals. Organic Process Research and Development, 2020, 24, 1215-1217.	1.3	0
72	Confronting Racism in Chemistry Journals. ACS Sustainable Chemistry and Engineering, 2020, 8, .	3.2	0

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73	Confronting Racism in Chemistry Journals. Chemistry of Materials, 2020, 32, 5369-5371.	3.2	Ο
74	Confronting Racism in Chemistry Journals. Chemical Research in Toxicology, 2020, 33, 1511-1513.	1.7	0
75	Confronting Racism in Chemistry Journals. Inorganic Chemistry, 2020, 59, 8639-8641.	1.9	0
76	Confronting Racism in Chemistry Journals. ACS Chemical Biology, 2020, 15, 1719-1721.	1.6	0
77	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Chemical Theory and Computation, 2020, 16, 2881-2882.	2.3	Ο
78	Protein Stability in TMAO and Mixed Urea–TMAO Solutions. Journal of Physical Chemistry B, 2020, 124, 6181-6197.	1.2	50
79	Confronting Racism in Chemistry Journals. Organic Letters, 2020, 22, 4919-4921.	2.4	4
80	Confronting Racism in Chemistry Journals. ACS Applied Materials & Interfaces, 2020, 12, 28925-28927.	4.0	13
81	Confronting Racism in Chemistry Journals. Crystal Growth and Design, 2020, 20, 4201-4203.	1.4	1
82	Confronting Racism in Chemistry Journals. Chemical Reviews, 2020, 120, 5795-5797.	23.0	2
83	Confronting Racism in Chemistry Journals. ACS Catalysis, 2020, 10, 7307-7309.	5.5	1
84	Confronting Racism in Chemistry Journals. Biomacromolecules, 2020, 21, 2543-2545.	2.6	0
85	Confronting Racism in Chemistry Journals. Journal of Medicinal Chemistry, 2020, 63, 6575-6577.	2.9	0
86	Confronting Racism in Chemistry Journals. Macromolecules, 2020, 53, 5015-5017.	2.2	0
87	Confronting Racism in Chemistry Journals. Nano Letters, 2020, 20, 4715-4717.	4.5	5
88	Confronting Racism in Chemistry Journals. Organometallics, 2020, 39, 2331-2333.	1.1	0
89	Confronting Racism in Chemistry Journals. Journal of the American Chemical Society, 2020, 142, 11319-11321.	6.6	1
90	Heightened Cold-Denaturation of Proteins at the Ice–Water Interface. Journal of the American Chemical Society, 2020, 142, 5722-5730.	6.6	59

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91	Confronting Racism in Chemistry Journals. Accounts of Chemical Research, 2020, 53, 1257-1259.	7.6	Ο
92	Confronting Racism in Chemistry Journals. Journal of Physical Chemistry A, 2020, 124, 5271-5273.	1.1	0
93	Confronting Racism in Chemistry Journals. Journal of Chemical Information and Modeling, 2020, 60, 3325-3327.	2.5	0
94	Confronting Racism in Chemistry Journals. Journal of Proteome Research, 2020, 19, 2911-2913.	1.8	0
95	Confronting Racism in Chemistry Journals. Journal of Physical Chemistry B, 2020, 124, 5335-5337.	1.2	1
96	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Agricultural and Food Chemistry, 2020, 68, 5019-5020.	2.4	0
97	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Physical Chemistry B, 2020, 124, 3603-3604.	1.2	0
98	Confronting Racism in Chemistry Journals. Bioconjugate Chemistry, 2020, 31, 1693-1695.	1.8	0
99	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Applied Nano Materials, 2020, 3, 3960-3961.	2.4	Ο
100	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Natural Products, 2020, 83, 1357-1358.	1.5	0
101	Characteristics of Impactful Computational Contributions to <i>The Journal of Physical Chemistry B, 2020, 124, 5093-5094.</i>	1.2	3
102	Confronting Racism in Chemistry Journals. ACS Synthetic Biology, 2020, 9, 1487-1489.	1.9	0
103	Update to Our Reader, Reviewer, and Author Communities—April 2020. Bioconjugate Chemistry, 2020, 31, 1211-1212.	1.8	Ο
104	Update to Our Reader, Reviewer, and Author Communities—April 2020. Chemical Research in Toxicology, 2020, 33, 1509-1510.	1.7	0
105	A New Editor-in-Chief for The Journal of Physical Chemistry. Journal of Physical Chemistry A, 2020, 124, 1-1.	1.1	1
106	A New Editor-in-Chief for The Journal of Physical Chemistry. Journal of Physical Chemistry B, 2020, 124, 313-313.	1.2	0
107	A New Editor-in-Chief for The Journal of Physical Chemistry. Journal of Physical Chemistry C, 2020, 124, 1-1.	1.5	2
108	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Applied Bio Materials, 2020, 3, 2873-2874.	2.3	0

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109	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Organic Chemistry, 2020, 85, 5751-5752.	1.7	0
110	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of the American Society for Mass Spectrometry, 2020, 31, 1006-1007.	1.2	0
111	Update to Our Reader, Reviewer, and Author Communities—April 2020. Accounts of Chemical Research, 2020, 53, 1001-1002.	7.6	0
112	Update to Our Reader, Reviewer, and Author Communities—April 2020. Biomacromolecules, 2020, 21, 1966-1967.	2.6	0
113	Update to Our Reader, Reviewer, and Author Communities—April 2020. Chemical Reviews, 2020, 120, 3939-3940.	23.0	Ο
114	Update to Our Reader, Reviewer, and Author Communities—April 2020. Environmental Science & Technology, 2020, 54, 5307-5308.	4.6	0
115	Update to Our Reader, Reviewer, and Author Communities—April 2020. Langmuir, 2020, 36, 4565-4566.	1.6	0
116	Update to Our Reader, Reviewer, and Author Communities—April 2020. Molecular Pharmaceutics, 2020, 17, 1445-1446.	2.3	0
117	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Infectious Diseases, 2020, 6, 891-892.	1.8	0
118	Update to Our Reader, Reviewer, and Author Communities—April 2020. Crystal Growth and Design, 2020, 20, 2817-2818.	1.4	1
119	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Medicinal Chemistry, 2020, 63, 4409-4410.	2.9	0
120	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Physical Chemistry A, 2020, 124, 3501-3502.	1.1	0
121	Update to Our Reader, Reviewer, and Author Communities—April 2020. Nano Letters, 2020, 20, 2935-2936.	4.5	0
122	Update to Our Reader, Reviewer, and Author Communities—April 2020. ACS Sensors, 2020, 5, 1251-1252.	4.0	0
123	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of Chemical Information and Modeling, 2020, 60, 2651-2652.	2.5	0
124	Update to Our Reader, Reviewer, and Author Communities—April 2020. Industrial & Engineering Chemistry Research, 2020, 59, 8509-8510.	1.8	0
125	Update to Our Reader, Reviewer, and Author Communities—April 2020. Journal of the American Chemical Society, 2020, 142, 8059-8060.	6.6	3
126	Update to Our Reader, Reviewer, and Author Communities—April 2020. Inorganic Chemistry, 2020, 59, 5796-5797.	1.9	0

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127	Update to Our Reader, Reviewer, and Author Communities—April 2020. Organometallics, 2020, 39, 1665-1666.	1.1	0
128	Update to Our Reader, Reviewer, and Author Communities—April 2020. Organic Letters, 2020, 22, 3307-3308.	2.4	0
129	Confronting Racism in Chemistry Journals. ACS Biomaterials Science and Engineering, 2020, 6, 3690-3692.	2.6	1
130	Confronting Racism in Chemistry Journals. ACS Omega, 2020, 5, 14857-14859.	1.6	1
131	Confronting Racism in Chemistry Journals. Journal of Agricultural and Food Chemistry, 2020, 68, 6941-6943.	2.4	Ο
132	Confronting Racism in Chemistry Journals. ACS Earth and Space Chemistry, 2020, 4, 961-963.	1.2	0
133	Confronting Racism in Chemistry Journals. Environmental Science and Technology Letters, 2020, 7, 447-449.	3.9	Ο
134	Confronting Racism in Chemistry Journals. ACS Combinatorial Science, 2020, 22, 327-329.	3.8	0
135	Confronting Racism in Chemistry Journals. ACS Infectious Diseases, 2020, 6, 1529-1531.	1.8	0
136	Confronting Racism in Chemistry Journals. ACS Applied Bio Materials, 2020, 3, 3925-3927.	2.3	0
137	Confronting Racism in Chemistry Journals. ACS Macro Letters, 2020, 9, 1004-1006.	2.3	0
138	Confronting Racism in Chemistry Journals. Molecular Pharmaceutics, 2020, 17, 2229-2231.	2.3	1
139	Confronting Racism in Chemistry Journals. ACS Chemical Neuroscience, 2020, 11, 1852-1854.	1.7	1
140	Confronting Racism in Chemistry Journals. ACS Photonics, 2020, 7, 1586-1588.	3.2	0
141	Confronting Racism in Chemistry Journals. Environmental Science & Technology, 2020, 54, 7735-7737.	4.6	Ο
142	The <i>JPC</i> Periodic Table. Journal of Physical Chemistry A, 2019, 123, 5837-5848.	1.1	2
143	The <i>JPC</i> Periodic Table. Journal of Physical Chemistry B, 2019, 123, 5973-5984.	1.2	1
144	The <i>JPC</i> Periodic Table. Journal of Physical Chemistry Letters, 2019, 10, 4051-4062.	2.1	2

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#	Article	IF	CITATIONS
145	Small ion effects on self-coacervation phenomena in block polyampholytes. Journal of Chemical Physics, 2019, 151, 034904.	1.2	46
146	Distinct and Nonadditive Effects of Urea and Guanidinium Chloride on Peptide Solvation. Journal of Physical Chemistry Letters, 2019, 10, 7406-7413.	2.1	23
147	Young Scientists Virtual Special Issue. Journal of Physical Chemistry C, 2019, 123, 20689-20690.	1.5	Ο
148	The Mitochondrial Peptide Humanin Targets but Does Not Denature Amyloid Oligomers in Type II Diabetes. Journal of the American Chemical Society, 2019, 141, 14168-14179.	6.6	17
149	Young Scientists Virtual Special Issue. Journal of Physical Chemistry A, 2019, 123, 7335-7336.	1.1	1
150	Young Scientists Virtual Special Issue. Journal of Physical Chemistry B, 2019, 123, 7241-7242.	1.2	0
151	Editorial for January 2019 for JPC A/B/C. Journal of Physical Chemistry B, 2019, 123, 1-9.	1.2	2
152	The Classifying Autoencoder: Gaining Insight into Amyloid Assembly of Peptides and Proteins. Journal of Physical Chemistry B, 2019, 123, 5256-5264.	1.2	5
153	Complete Phase Diagram for Liquid–Liquid Phase Separation of Intrinsically Disordered Proteins. Journal of Physical Chemistry Letters, 2019, 10, 1644-1652.	2.1	204
154	Editorial for January 2019 for JPC A/B/C. Journal of Physical Chemistry A, 2019, 123, 1-9.	1.1	2
155	Editorial for January 2018 for JPC A/B/C. Journal of Physical Chemistry A, 2018, 122, 1-7.	1.1	1
156	Editorial for January 2018 for JPC A/B/C. Journal of Physical Chemistry B, 2018, 122, 1-7.	1.2	2
157	New Sections for <i>JPC A</i> / <i>B</i> / <i>C</i> . Journal of Physical Chemistry A, 2018, 122, 2611-2611.	1.1	0
158	New Sections for JPC A/B/C. Journal of Physical Chemistry B, 2018, 122, 2703-2703.	1.2	0
159	Trimethylamine <i>N</i> -oxide Counteracts Urea Denaturation by Inhibiting Protein–Urea Preferential Interaction. Journal of the American Chemical Society, 2018, 140, 483-492.	6.6	94
160	Effect of Surfactants on Surface-Induced Denaturation of Proteins: Evidence of an Orientation-Dependent Mechanism. Journal of Physical Chemistry B, 2018, 122, 11390-11399.	1.2	33
161	Systematic derivation of implicit solvent models for the study of polymer collapse. Journal of Computational Chemistry, 2017, 38, 1353-1361.	1.5	7
162	An adaptive bias – hybrid MD/kMC algorithm for protein folding and aggregation. Physical Chemistry Chemical Physics, 2017, 19, 17373-17382.	1.3	8

#	Article	IF	CITATIONS
163	Virtual Issue in Honor of the 150th Birthday of Marie Curie: Highlighting Female Physical Chemists. Journal of Physical Chemistry A, 2017, 121, 8185-8187.	1.1	Ο
164	Virtual Issue in Honor of the 150th Birthday of Marie Curie: Highlighting Female Physical Chemists. Journal of Physical Chemistry Letters, 2017, 8, 5306-5308.	2.1	0
165	Not Physical Chemistry (in the Eyes of the Journal of Physical Chemistry). Journal of Physical Chemistry A, 2017, 121, 8188-8188.	1.1	0
166	Not Physical Chemistry (in the Eyes of the <i>Journal of Physical Chemistry</i>). Journal of Physical Chemistry B, 2017, 121, 10199-10199.	1.2	1
167	Virtual Issue in Honor of the 150th Birthday of Marie Curie: Highlighting Female Physical Chemists. Journal of Physical Chemistry B, 2017, 121, 9983-9985.	1.2	0