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Scientometric Portrait of Nobel Laureate Arieh Warshel

Sonia Bansal*
Assistant Librarian, Guru Angad Dev Veterinary and Animal Sciences University, Ludhiana, Punjab, India

Abstract

This study presents an analysis of publication productivity of Arieh Warshel, recipient of 2013 Nobel Prize in Chemistry. During 1968-2016, he had contributed 393 publications including 25 book chapters. His publications are analyzed by year, authorship pattern and channels of communication used etc.

Keywords: *Scientometric, bibliometric, Arieh Warshel.*

****Author for Correspondence*** Email: soniapta@gmail.com

INTRODUCTION

Arieh Warshel was awarded the 2013 Nobel Prize in chemistry for the development of multiscale models for complex chemical systems. He shared the prize with American British Israeli chemist Michael Levitt and American Austrian chemist Martin Karplus. He was born on November 20, 1940 in the Sde Nahum kibbutz in what was then British Palestine (now Israel). He received his doctorate in chemical physics from the Weizmann Institute of Science in Rehovot, Israel, in 1969. In the 1970s, Martin Karplus, Michael Levitt, and Arieh Warshel successfully developed methods that combined quantum and classical mechanics to calculate the courses of chemical reactions using computers [1, 2].

Warshel, distinguished professor of chemistry and biochemistry at the University of Southern California, is famous for his work on computational biochemistry and biophysics. He pioneered computer simulations of the functions of biological systems, and for developing what is known today as computational enzymology [3]. Quantum mechanics/molecular mechanics is now a state-of-the-art approach used by scientists and engineers for simulating chemical processes. Scientists and engineers use this approach not only for drug discovery and tracking reaction mechanisms but also to improve fundamental understanding of chemical structure and bonding [4].

OBJECTIVES OF THE STUDY

- To ascertain year-wise productivity and authorship pattern.
- To identify channels of communication used by Arieh Warshel for publishing his research work.
- To identify most prolific authors associated with Arieh Warshel.

METHODOLOGY

The research publications of Arieh Warshel published during 1968-2016 were downloaded from the website (http://laetro.usc.edu/research.html). Arieh Warshel had published 393 publications during 1968-2016. Out of 393 publications, he published 368 journal articles and 25 book chapters.

Table 1 depicts that Arieh Warshel had published 89.57% papers in collaboration and remaining 10.43% as sole author. The first publication of Warshel was published under joint authorship at the age of 28 years in the year 1968. He had published maximum number of papers in joint authorship (151) followed by three authored (104), four authored (63), five authored (15), six authored (12), and seven authored (2) articles. Arieh Warshel had published a paper in 2006 with 68 collaborators.

Table 2 depicts various channels of communication used by Arieh Warshel for publishing his research publications. It is clear from Table 2 that Arieh Warshel had published maximum number of papers in *The Journal of Physical Chemistry B* (57), followed by *Proceedings of the National Academy of Sciences of the United States of America* (43), *Journal of the American Chemical Society* (37),

Biochemistry (30), *Journal of Chemical Physics* (23), *Proteins: Structure, Function, and Bioinformatics* (16), *Chemical Physics Letters* (14), *Journal of Physical Chemistry* (12), *Journal of Molecular Biology* (8), and *Chemical Physics* (7).

Table 1: *Year-Wise Productivity of Arieh Warshel*

Age, in years	Year	Authorship pattern												Total multi-authored publications	TP	Collaboration rate	Publishing age
		1	2	3	4	5	6	7	9	11	13	36	68				
28	1968		1											1	1	1.00	1
29	1969		2	1										3	3	1.00	2
30	1970		2	3										5	5	1.00	3
31	1971	2												0	2	0	4
32	1972		2											2	2	1.00	5
33	1973	1												0	1	0	6
34	1974		4	1	2									7	7	1.00	7
35	1975	1	4	1	1									6	7	0.86	8
36	1976	3	2	1										3	6	0.50	9
37	1977	4	1	1										2	6	0.33	10
38	1978	4	2	1					1					4	8	0.40	11
39	1979	3	2											2	5	0.40	12
40	1980	1	1											1	2	0.50	13
41	1981	3	4											4	7	0.57	14
42	1982	1	1											1	2	0.50	15
43	1983		1	1	1									3	3	1.00	16
44	1984	1	1	1										2	3	0.67	17
45	1985		6											6	6	1.00	18
46	1986	1	4	2										6	7	0.86	19
47	1987	3	4											4	7	0.57	20
48	1988		2	3	1	2								8	8	1.00	21
49	1989	2	4	4	2			1						11	13	0.85	22
50	1990	2	4	1	1		1							7	9	0.78	23
51	1991		4	2	3									9	9	1.00	24
52	1992		5	4	1	1	1							12	12	1.00	25
53	1993		4	2	1									7	7	1.00	26
54	1994		2	4	1	1	2							10	10	1.00	27
55	1995		2	1	2		1							6	6	1.00	28
56	1996		3	2	2	2								9	9	1.00	29
57	1997	1	6	7		1								14	15	0.93	30
58	1998	1	7	5	2									14	15	0.93	31
59	1999		3	4	1	1								9	9	1.00	32
60	2000	1	2	4	4	1	2					1		14	15	0.93	33
61	2001		4	1	1									6	6	1.00	34
62	2002	1		3	2									5	6	0.83	35
63	2003	1	3	5	2									10	11	0.91	36
64	2004		7	3	1									11	11	1.00	37
65	2005	1	2	3	3									8	9	0.89	38
66	2006	1	3	6	1	1	1						1	13	14	0.93	39
67	2007		2	2	4	2					1			11	11	1.00	40
68	2008		3	5	3	3				1				15	15	1.00	41
69	2009		5	5	4									14	14	1.00	42
70	2010		7	5	2		2							16	16	1.00	43
71	2011		6	2	3		1							12	12	1.00	44
72	2012		4	2	3			1						10	10	1.00	45
73	2013	1	6	2	4									12	13	0.92	46
74	2014	1	2	1	2		1							6	7	0.86	47
75	2015		4	2	3									9	9	1.00	48
76	2016		1	1										2	2	1.00	49
	Total	**41**	**151**	**104**	**63**	**15**	**12**	**2**	**1**	**1**	**1**	**1**	**1**	**393**			

Note. TP = Total publications

Table 2: *Channels of Communication Used by Arieh Warshel*

Channels of communication	Number of papers published	Percentage
The Journal of Physical Chemistry B	57	14.50
Proceedings of the National Academy of Sciences of the United States of America	43	10.94
Journal of the American Chemical Society	37	9.41
Biochemistry	30	7.63
Journal of Chemical Physics	23	5.85
Proteins: Structure, Function, and Bioinformatics	16	4.07
Chemical Physics Letters	14	3.56
Journal of Physical Chemistry	12	3.05
Journal of Molecular Biology	8	2.04
Chemical Physics	7	1.78
FEBS Letters	5	1.27
Protein Engineering	5	1.27
Journal of Computational Chemistry	5	1.27
Photochemistry and Photobiology	5	1.27
Israel Journal of Chemistry	5	1.27
Biochimica et Biophysica Acta-Bioenergetics	5	1.27
Chemical Reviews	4	1.03
Proteins	4	1.03
Quarterly Reviews of Biophysics	4	1.03
Nature	4	1.03
Physical Chemistry Chemical Physics	3	0.76
Photosynthesis Research	3	0.76
Theoretical Chemistry Accounts	3	0.76
Accounts of Chemical Research	3	0.76
Chembiochem	3	0.76
Faraday Discussions	3	0.76
Journal of Biological Chemistry	2	0.52
Chemphyschem	2	0.52
Journal of Organic Chemistry	2	0.52
The FASEB Journal	2	0.52
Journal of Biological Inorganic Chemistry	2	0.52
Journal of Chemical Theory and Computation	2	0.52
Journal of Cellular Biochemistry	2	0.52
Bulletin of the American Physical Society	2	0.52
Biophysical Journal	2	0.52
Science	2	0.52
Nature Structural Biology	2	0.52
Angewandte Chemie International Edition	2	0.52
Annual Review of Physical Chemistry	2	0.52
Biochimica et Biophysica Acta	1	0.25
Biochim Biophys Acta	1	0.25
Current Opinion Chemical Biology	1	0.25

Journal of Biomolecular Structure and Dynamics	1	0.25
Biochimica et Biophysica Acta: Biomembranes	1	0.25
Journal of Physical Organic Chemistry	1	0.25
Biotechnology Journal	1	0.25
Biochimica et Biophysica Acta: Proteins and Proteomics	1	0.25
Philosophical Transactions of the Royal Society B: Biological Sciences	1	0.25
Journal of Computational and Theoretical Nanoscience	1	0.25
Annual Review of Biophysics and Biomolecular Structure	1	0.25
Advances in Protein Chemistry	1	0.25
Biopolymers	1	0.25
Journal of Molecular Graphics & Modelling	1	0.25
International Journal of Quantum Chemistry	1	0.25
Inorganic Chemistry	1	0.25
Structural Chemistry	1	0.25
Journal of Photochemistry and Photobiology A: Chemistry	1	0.25
Biological Chemistry Hoppe-Seyler	1	0.25
Annual Review of Biophysics and Biophysical Chemistry	1	0.25
Computational Molecular Science	1	0.25
Chemistry & Biology	1	0.25
Current Opinion in Structural Biology	1	0.25
Annual Review of Physical Chemistry	1	0.25
Computers & Chemistry	1	0.25
Trends in Biochemical Sciences	1	0.25
Journal of Molecular Structure	1	0.25
Journal of Molecular Spectroscopy	1	0.25
Phosphorus, Sulfur, and Silicon and the Related Elements	1	0.25
Structure	1	0.25
Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials	1	0.25
Book Chapters	25	6.36

Table 3: *Most Prolific Authors Associated with Arieh Warshel*

Name of the collaborator	Period of association	Total years	Total publications
Z. T. Chu	1989–2015	27	39
J. Florian	1997–2012	16	32
S. C. L. Kamerlin	2008–2013	6	24
W. W. Parson	1987–2009	23	24
J. K. Hwang	1985–1999	15	22
J. Aqvist	1989–2007	19	15
M. H. M. Olsson	2003–2008	6	14
M. F. Goodman	1995–2012	18	13
T. Schweins	1992–1998	7	10
P. K. Sharma	2005–2013	9	10
M. Kato	2003–2008	6	10
E. Rosta	2005–2012	8	9
S. Creighton	1988–1990	3	9
J. Villa	2000–2001	2	9
S. Mukherjee	2012–2015	4	8

It is clear from Table 3 that Arieh Warshel collaborated with Z. T. Chu for 27 years and published 39 articles. J. Florian follows next with 32 publications, followed by S. C. L. Kamerlin and W. W. Parson (24 articles each), J. K. Hwang (22 publications), J. Aqvist (15 publications), and M. H. M. Olsson (14 publications), M. F. Goodman (13 publications), T. Schweins, P. K. Sharma, and M. Kato (10 publications each), E. Rosta, S. Creighton, and J. Villa (9 publications each). Arieh Warshel and S. Mukherjee had 8 publication in collaboration during 2012-2015.

CONCLUSION

Arieh Warshel had contributed 393 papers during 1968-2016 and his first paper was published under joint authorship in the year 1968. The percentage of solo research articles was only 10.43%, which makes it clear that he preferred to work in collaboration. He published 368 publications in 70 journals and remaining 25 as book chapters. Arieh Warshel and Z.T. Chu collaborated for 27 years and published 39 research papers.

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