



Journal of Applicable Chemistry

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(International Peer Reviewed Journal)



Knowledge Inn (in nature)

Research Profile of Frances Arnold, NL2018Chem

Process knowledge discovery

Knowledge-Based Conformer Generation



Nobel Laureate

Frances Arnold

Chemistry

2018

Research Profile Frances of Hamilton Arnold

Frances Hamilton Arnold



Born on July 25, 1956
Edgewood, Pennsylvania, U.S.

Linus Pauling Professor of Chemical Engineering,
Bioengineering and Biochemistry
California Institute of Technology, CA, USA;
email: cheme.caltech.edu

	All	Since 2014
Citations	46,361	15,188
h-index	118	63
# Publications	> 600	
Accessed on 13-01-2019		

Directed enzyme evolution technique

- ▶ Evolved enzymes were used to make compounds with bonds that do not occur in biology, Ex. Bonds between carbon and silicon; argon and boron
- ▶ Various types of plants, animals, and other living things on Earth have their origin in other pre-existing types. Evolution, fundamental keystone of modern system biology explains

distinguishable differences in species arising due to modifications in successive generations.

- + Unprecedented impact in biocatalysis by redesign of the catalysts of life to match process requirements in terms of specificity, activity and robustness

Academic profile of Frances Hamilton Arnold

Graduation

Mechanical and aerospace engineering	Princeton University	1979
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Doctoral research

Chemical engineering	University of California at Berkeley Ph D Director: Harvey Warren Blanch Thesis: Design and Scale-Up of Affinity Separations	1985
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Post-Doctoral research

One year	Postdoctoral fellow at Berkeley	
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Progeny

Academic	Christopher Voigt, Huimin Zhao, Ulrich Schwaneberg
Biological	William A. Lange Joseph I. Lange James Bailey

Companies started based on her research outcome

Gevo	<ul style="list-style-type: none"> ▪ Uses yeast to make isobutanol + can be used instead of ethanol in making fuel 	2005
Provivi	Alters insect pheromones so that pests harmful to crops will be unable to mate with each other	2013

Employment

Assistant professor	1987
Associate professor	1992
Full professor	1996

Year Awards (to Frances Hamilton Arnold)

2018 Nobel Prize in Chemistry

2017	Raymond and Beverly Sackler Prize in Convergence Research
2016	Millennium Technology Prize
2013	National Medal of Technology and Innovation
2011	Draper Prize
2007	FASEB Excellence in Science Award
2005	Garvan–Olin Medal

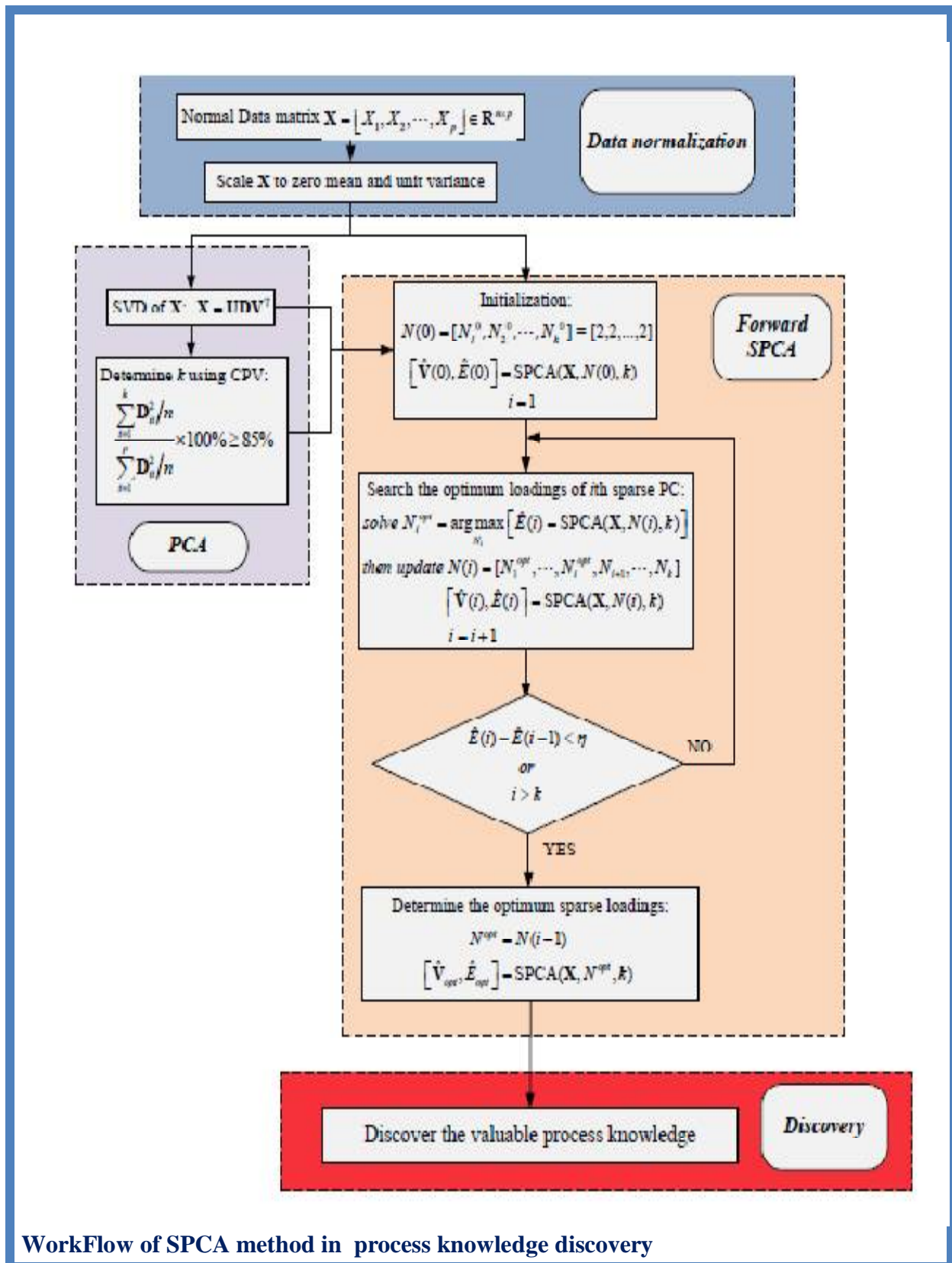
Typical Publications	# Citations	Year of pub
<p>Dynamic pattern formation in a vesicle-generating microfluidic device T Thorsen, RW Roberts, FH Arnold, SR Quake Physical review letters 86 (18), 4163</p>	1950	2001
<p>Molecular evolution by staggered extension process (StEP) in vitro recombination H Zhao, L Giver, Z Shao, JA Affholter, FH Arnold Nature biotechnology 16 (3), 258</p>	1007	1998
<p>Protein stability promotes evolvability JD Bloom, ST Labthavikul, CR Otey, FH Arnold Proceedings of the National Academy of Sciences 103 (15), 5869-5874</p>	799	2006
<p>Why highly expressed proteins evolve slowly DA Drummond, JD Bloom, C Adami, CO Wilke, FH Arnold Proceedings of the National Academy of Sciences 102 (40), 14338-14343</p>	634	2005
<p>Why highly expressed proteins evolve slowly DA Drummond, JD Bloom, C Adami, CO Wilke, FH Arnold Proceedings of the National Academy of Sciences 102 (40), 14338-14343</p>	634	2005
<p>Design by directed evolution FH Arnold Accounts of chemical research 31 (3), 125-131</p>	622	1998
<p>Directed evolution of a thermostable esterase L Giver, A Gershenson, PO Freskgard, FH Arnold Proceedings of the National Academy of Sciences 95 (22), 12809-12813</p>	582	1998
<p>Exploring protein fitness landscapes by directed evolution PA Romero, FH Arnold Nature reviews Molecular cell biology 10 (12), 866</p>	580	2009
<p>Directed evolution of a para-nitrobenzyl esterase for aqueous-organic solvents JC Moore, FH Arnold Nature biotechnology 14 (4), 458</p>	555	1996
<p>Laboratory evolution of peroxide-mediated cytochrome P450 hydroxylation H Joo, Z Lin, FH Arnold Nature 399 (6737), 670</p>	480	1999
<p>Directed evolution of a genetic circuit Y Yokobayashi, R Weiss, FH Arnold Proceedings of the National Academy of Sciences 99 (26), 16587-16591</p>	454	2002
<p>Directed evolution of enzyme catalysts O Kuchner, FH Arnold Trends in biotechnology 15 (12), 523-530</p>	434	1997
<p>How enzymes adapt: lessons from directed evolution FH Arnold, PL Wintrode, K Miyazaki, A Gershenson Trends in biochemical sciences 26 (2), 100-106</p>	416	2001

Typical Publications	# Citations	Year of pub
Directed evolution of biocatalysts FH Arnold, AA Volkov Current opinion in chemical biology 3 (1), 54-59	400	1999
Laboratory evolution of a soluble, self-sufficient, highly active alkane hydroxylase A Glieder, ET Farinas, FH Arnold Nature biotechnology 20 (11), 1135	391	2002
Directed evolution converts subtilisin E into a functional equivalent of thermitase H Zhao, FH Arnold Protein Engineering 12 (1), 47-53	374	1999
Directed evolution of subtilisin E in Bacillus subtilis to enhance total activity in aqueous dimethylformamide L You, FH Arnold Protein Engineering, Design and Selection 9 (1), 77-83	361	1996
Evolving strategies for enzyme engineering JD Bloom, MM Meyer, P Meinhold, CR Otey, D MacMillan, FH Arnold Current opinion in structural biology 15 (4), 447-452	349	2005
In the light of directed evolution: pathways of adaptive protein evolution JD Bloom, FH Arnold Proceedings of the National Academy of Sciences 106 (Supplement 1), 9995-10000	345	2009
Directed enzyme evolution ET Farinas, T Bulter, FH Arnold Current opinion in biotechnology 12 (6), 545-551	306	2001
Directed evolution study of temperature adaptation in a psychrophilic enzyme1 K Miyazaki, PL Wintrode, RA Grayling, DN Rubingh, FH Arnold Journal of molecular biology 297 (4), 1015-1026	302	2000
Directed enzyme evolution: climbing fitness peaks one amino acid at a time CA Tracewell, FH Arnold Current opinion in chemical biology 13 (1), 3-9	286	2009
Functional expression of a fungal laccase in Saccharomyces cerevisiae by directed evolution T Bulter, M Alcalde, V Sieber, P Meinhold, C Schlachtbauer, FH Arnold Applied and environmental microbiology 69 (2), 987-995	282	2003
Directed enzyme evolution: screening and selection methods FH Arnold, G Georgiou Springer Science & Business Media	250	2003
Exploring nonnatural evolutionary pathways by saturation mutagenesis: rapid improvement of protein function K Miyazaki, FH Arnold Journal of molecular evolution 49 (6), 716-720	245	1999

Typical Publications	# Citations	Year of pub
<p>Strategies for the in vitro evolution of protein function: enzyme evolution by random recombination of improved sequences¹</p> <p>JC Moore, HM Jin, O Kuchner, FH Arnold Journal of molecular biology 272 (3), 336-347</p>	240	1997
<p>Computational method to reduce the search space for directed protein evolution</p> <p>CA Voigt, SL Mayo, FH Arnold, ZG Wang Proceedings of the National Academy of Sciences 98 (7), 3778-3783</p>	215	2001
<p>Directed evolution: creating biocatalysts for the future</p> <p>FH Arnold Chemical engineering science 51 (23), 5091-5102</p>	167	1996
<p>A high-throughput digital imaging screen for the discovery and directed evolution of oxygenases</p> <p>H Joo, A Arisawa, Z Lin, FH Arnold Chemistry & biology 6 (10), 699-706</p>	133	1999
<p>A general mechanism for network-dosage compensation in gene circuits</p> <p>M Acar, BF Pando, FH Arnold, MB Elowitz, A Van Oudenaarden Science 329 (5999), 1656-1660</p>	92	2010

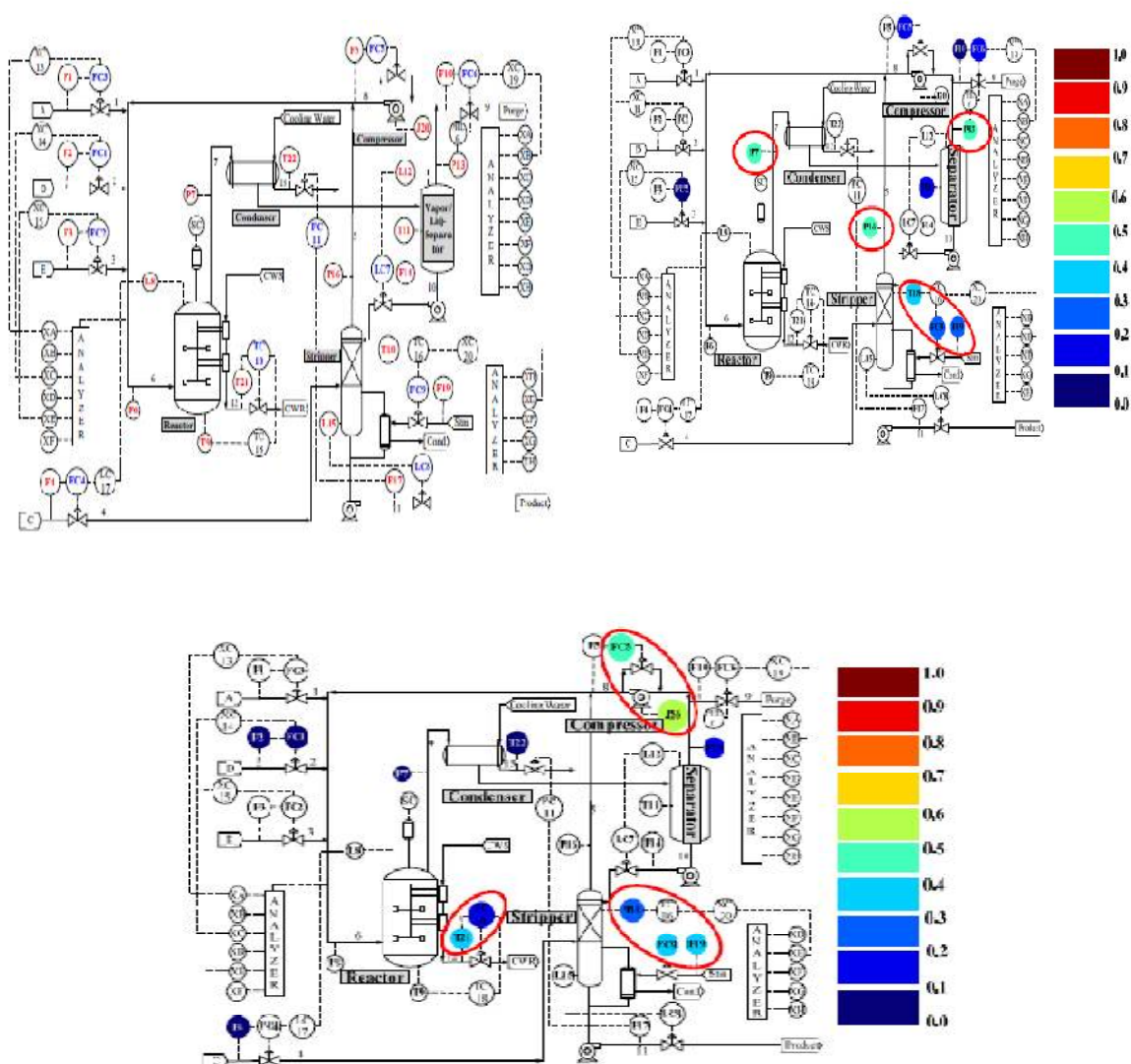
Tennessee Eastman process

<p style="text-align: center;"> Historical process data ↓ Forward Sparse Principal Component Analysis (Forward SPCA) ↓ Process knowledge discovery ↓ </p>	<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 30%; padding: 5px;">Major components for unit operation</td> <td style="width: 10%; text-align: center; vertical-align: middle;">:</td> <td style="padding: 5px;">[exothermic reactor; product condenser; vapor-liquid separator; recycle compressor; reboiled product stripper]</td> </tr> <tr> <td style="padding: 5px;"> <ul style="list-style-type: none"> ▶ 22 continuous process measurements, ▶ 12 manipulated variables ▶ 19 composition measurements </td> <td style="padding: 5px;"></td> <td style="padding: 5px;"> <ul style="list-style-type: none"> ▶ Total # variables (=33) selected in this study: [22 continuous process measurements + 11 manipulated variables ▶ # samples: 960 normal samples with sampling rate of 3 min ▶ SPCA mode </td> </tr> <tr> <td style="padding: 5px;">Input to reactor: Four gaseous reactants (A, C, D, E) + inert B</td> <td style="width: 10%; text-align: center; vertical-align: middle;">→</td> <td style="padding: 5px;">Two liquid products (G, H) + one byproduct F</td> </tr> </table>	Major components for unit operation	:	[exothermic reactor; product condenser; vapor-liquid separator; recycle compressor; reboiled product stripper]	<ul style="list-style-type: none"> ▶ 22 continuous process measurements, ▶ 12 manipulated variables ▶ 19 composition measurements 		<ul style="list-style-type: none"> ▶ Total # variables (=33) selected in this study: [22 continuous process measurements + 11 manipulated variables ▶ # samples: 960 normal samples with sampling rate of 3 min ▶ SPCA mode 	Input to reactor: Four gaseous reactants (A, C, D, E) + inert B	→	Two liquid products (G, H) + one byproduct F
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Workflow of SPCA method in process knowledge discovery

Process flow diagram of Tennessee Eastman process



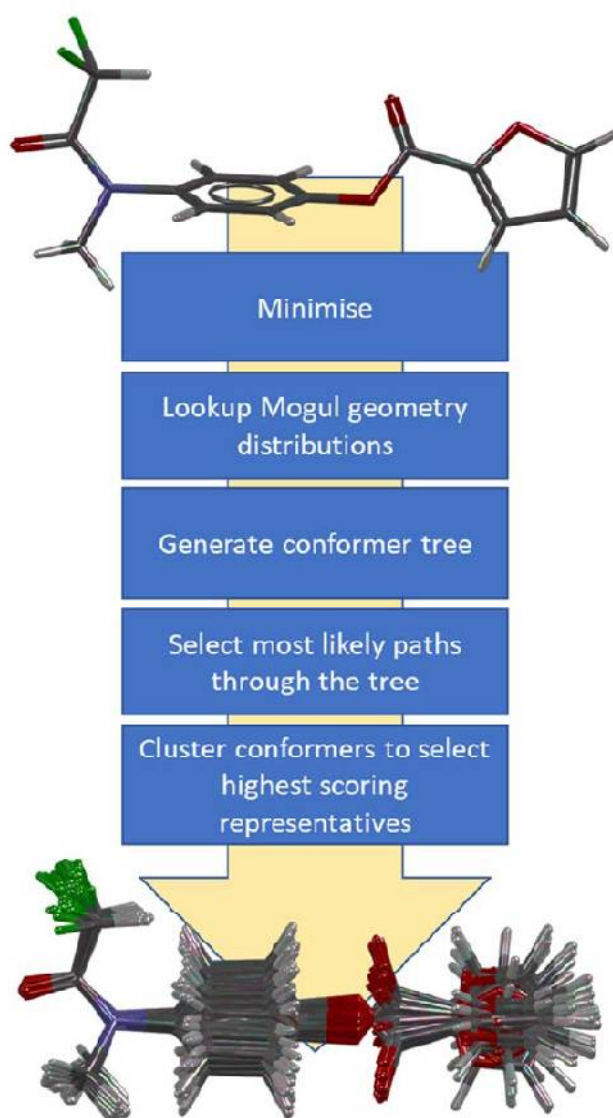
Information Source (is) [ACS.org](https://doi.org/10.1021/acs.chemlett.8b00001) ;

Ti: Process Knowledge Discovery Using Sparse Principal Component Analysis

Au: Huihui Ga, Shiram Gajjar, Murat Kulahci, Qunxiong Zhu, Ahmet Palazoglu

JO: Industrial & Engineering Chemistry Research, 2018

Knowledge-Based Conformer Generation



Information Source (is) ACS.org ;

Ti: Knowledge-Based Conformer Generation
Using the
Cambridge Structural Database

Au: Jason C. Cole, Oliver Korb, Patrick McCabe,
Murray Read, and Robin Taylor

JO: J. Chem. Inf. Model., 2018, 58 (3), pp 615–
629

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R. Sambasiva Rao, School of Chemistry
Andhra University, Visakhapatnam
rsr.chem@gmail.com