

## Mary Fedarko Roberts

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### Education:

Bryn Mawr College, Bryn Mawr PA	A.B.	1969	Chemistry
Stanford University, Stanford CA	Ph.D.	1974	Chemistry
University of Illinois, Urbana IL	Post-doc	1974-1975	Biochemistry
University of California, La Jolla CA	Post-doc	1975-1978	Biochemistry

### Academic Positions:

1978-1983	Assistant Professor, Chem. Dept., Massachusetts Institute of Technology
1983-1986	Associate Professor, Chem. Dept., M.I.T.
1986-1987	Staff Scientist, Francis Bitter National Magnet Laboratory, M.I.T.
1987-1990	Visiting Scientist, Francis Bitter National Magnet Laboratory, M.I.T.
1987-1991	Associate Professor, Department of Chemistry, Boston College
1991-2017	Professor, Department of Chemistry, Boston College
1993-1999	Chair, Chemistry Graduate Admissions, Boston College
2002-2006	Vice-Chair, Department of Chemistry, Boston College
2002-2015	Visiting Scientist, Department of Biochemistry, Brandeis University
2017-	Professor Emerita, Boston College

### Awards/Honors:

- ASBMB Fellow, elected 2022
- Boston College Distinguished Senior Research Award, 2008
- AAAS Fellow, elected 2007
- N.S.F. Faculty Award for Women, 1991-1997
- Alfred P. Sloan Fellow, 1982-1984
- Dreyfus Teacher / Scholar, 1980

### Professional Activities:

- Member of Biophysical Chemistry (BBCB) Study Section, N.I.H., 1984-1987
- Member of Biophysics Panel, N.S.F., 1989-1992
- Member of CRUI Panel, N.S.F., 1994-1996
- Scientific Advisory Committee, Damon Runyon-Walter Winchell Foundation Cancer Fund, 1993-1997
- Biophysical Society Council Member, 1994-1997
- Advisory Board, FASEB Summer Research Conference on Phospholipases
- Member of Physiological Chemistry (PC) Study Section, N.I.H., 2000-2004, (Chair 2002-2004)

DOE Biosciences Review Panel, 2000; 2012; BES Early Career Review 2009  
Editorial Board, *Journal of Biological Chemistry*, 2003-2007  
Ad hoc member, N.I.H. Protein Structure Initiative special emphasis panel, 2005  
Member of Biomembranes (BBM) Study Section, 2005-2009 (Chair 2007-2009)  
Editorial Board, *Biochemical Journal*, 2009-2017  
Co-Chair of the 2010 ASBMB Annual Meeting in Anaheim  
Co-Chair of the 2015 ASBMB Annual Meeting in Boston  
AAAS Chair of General Medical Sciences, 2020; Interim Chair 3/1/2022=12/31/2022  
AAAS Kavli journalism award reviewer, 2020, 2021  
Member of working group for AIMBE diversity summit “Equity and Anti-Racism: A Roadmap to Policy Transformation in BME” 01/28-29/2021 (<https://aimbe.org/diversity-summit/>)

## PUBLICATIONS:

256. Roberts, M.F., and Hedstrom, L. (2022) High resolution  $^{31}\text{P}$  field cycling NMR reveals unsuspected features of enzyme-substrate-cofactor dynamics. *Front. Mol. Biosci.*, under review.
255. Moutoussamy, E.E., Khan, H.M., Roberts, M.F., Gershenson, A., Chipot, C., and Reuter, N. (2022) Standard binding free energy and membrane desorption mechanism for a phospholipase C. *J. Chem. Theory Comput.*, under review.
254. Roberts, M.F., Cai, J., Natarajan, S.V., Khan, M.K., Reuter, N., Gershenson, A., and Redfield, A.G. (2021) Phospholipids in motion: High resolution  $^{31}\text{P}$  NMR field cycling studies. *J. Phys. Chem. B* **125**, 8827-8838.
253. Rosenberg, M.M., Yao, T., Patton, Redfield, A.G., Roberts, M.F., and Hedstrom, L. (2020) Enzyme-substrate-cofactor dynamical networks revealed by high-resolution field cycling relaxometry. *Biochemistry* **59**, 2359-2379.
252. Waheed, Q., Khan, H.M., He, T., Roberts, M.F., Gershenson, A., and Reuter, N. (2019) Interfacial aromatics mediating cation- $\pi$  interactions with choline-containing lipids can contribute as much to peripheral protein affinity for membranes as aromatics inserted below the phosphates. *J. Phys. Chem. Lett.*, **10**, 3972-3977.
251. Roberts, M.F., Khan, H.M., Goldstein, R., Reuter, N., and Gershenson, A. (2018) Search and subvert: minimalist bacterial phosphatidylinositol-specific phospholipase C (PI-PLC) enzymes. *Chem. Rev.*, **118**, 8435-8473 (2018).
250. Rosenberg, M.M., Redfield, A.G., Roberts, M.F., and Hedstrom, L. (2018) Dynamic characteristics of guanosine-5'-monophosphate reductase complexes revealed by high resolution  $^{31}\text{P}$  field-cycling NMR relaxometry. *Biochemistry* **57**, 3146-3154.
249. Roberts, M.F. (2018) High-resolution applications of shuttle field-cycling NMR. Chapter 15 in *Field Cycling NMR Relaxometry: Instrumentation, Model Theories and Applications* (R. Kimich, editor), in series: New Developments in NMR No. 18, Royal Society Press.
248. Roberts, M.F. (2017) Defining a viral membrane-binding complex on an atomic level. *Structure* **25**, 3-4.
247. Gradziel, C.S., Jordan, P.A., Jewel, D., Dufort, F.J., Miller, S.J., Chiles, T.C., and Roberts M.F. (2016) D-3-Deoxy-dioctanoylphosphatidylinositol induces cytotoxicity in human MCF-7 breast cancer cells via a mechanism that involves downregulation of the D-type cyclin-retinoblastoma pathway. *Biochim. Biophys. Acta* **1861**, 1808-1815.

246. Rosenberg, M.M., Redfield, A.G., Roberts, M.F., and Hedstrom, L. (2016) Substrate and cofactor dynamics on guanosine monophosphate reductase probed by high resolution field cycling  $^{31}\text{P}$  NMR relaxometry. *J. Biol. Chem.* **291**, 22988-22998.
245. Huang, Q., Gershenson, A., and Roberts, M.F. (2016) Recombinant broad-range phospholipase C from *Listeria monocytogenes* exhibits optimal activity at acidic pH. *Biochim. Biophys. Acta* **1864**, 697-705.
244. Khan, H.M., He, T., Fuglebakk, E., Grauffel, C., Yang, B., Roberts, M.F., Gershenson, A., and Reuter, N. (2016) A role for weak electrostatic interactions in peripheral membrane protein binding. *Biophys. J.* **110**, 1367-1378.
243. He, T., Gershenson, A., Eyles, S.J., Lee, Y.-J., Liu, W. R., Wang, J., Gao, J., and Roberts, M. F. (2015) Fluorinated aromatic amino acids distinguish cation- $\pi$  interactions from membrane insertion. *J. Biol. Chem.* **290**, 19334-19342.
242. Mitchell, G., Ge, L., Huang, Q., Chen, C., Kianian, S., Roberts, M.F., Schekman, R., and Portnoy, D.A. (2015) Avoidance of autophagy mediated by PlcA or ActA is required for *Listeria monocytogenes* growth in macrophages. *Infect. Immun.* **83**, 2175-2184.
241. Wei, Y., Stec, B., Redfield, A.G., Weerapana, E., and Roberts, M.F. (2015) Phospholipid binding sites of PTEN: Exploring the mechanism of PIP<sub>2</sub> activation. *J. Biol. Chem.* **290**, 1592-1606.
240. Yang, B., Pu, M., Khan, H., Friedman, L., Reuter, N., Roberts, M.F., and Gershenson, A. (2015) Quantifying transient interactions between *Bacillus* phosphatidylinositol-specific phospholipase C and phosphatidylcholine-rich vesicles. *J. Am. Chem. Soc.* **137**, 14-17.
239. Meidenbauer, J.J., and Roberts, M.F. (2014) Reduced glucose utilization underlies seizure protection with dietary therapy in epileptic EL mice. *Epilepsy & Behavior* **39**, 48-54.
238. Gradziel, C.S., Wang, Y., Stec, B., Redfield, A.G., and Roberts, M.F. (2014) Cytotoxic amphiphiles and phosphoinositides bind to two discrete sites on the Akt1 PH domain. *Biochemistry* **53**, 462-472.
237. Cai, J., Guo, S., Lomasney, J.W., and Roberts, M.F. (2013) Ca<sup>2+</sup>-independent binding of anionic phospholipids by phospholipase C 81 EF-hand domain. *J. Biol. Chem.* **288**, 37277-37288.
236. Kurnasov, O.V., Luk, H.-J.D., Roberts, M. F., and Stec, B. (2013) Structure of the inositol-1-phosphate cytidylyltransferase from *Thermotoga maritima*. *Acta Cryst. D* **69**, 1808-1817.
235. Cheng, J., Goldstein, R., Gershenson, A., Stec, B., and Roberts, M.F. (2013) The cation- $\pi$  box is a specific phosphatidylcholine membrane targeting motif. *J. Biol. Chem.* **288**, 14863-14873.
234. Grauffel, C., Yang, B., He, B., Roberts, M.F., Gershenson, A., and Reuter, N. (2013) Cation- $\pi$  interactions as lipid-specific anchors for phosphatidylinositol-specific phospholipase C. *J. Am. Chem. Soc.* **135**, 5740-5750.
233. Cheng, J., Karri, S., Grauffel, C., Reuter, N., Roberts, M.F., Wintrode, P.L., and Gershenson, A. (2013) Does changing the predicted dynamics of a phospholipase C alter activity and membrane binding? *Biophys. J.* **104**, 185-195.
232. Cheng, J., Goldstein, R., Stec, B., Gershenson, A., and Roberts, M.F. (2012) Competition between anion binding and dimerization modulates *S. aureus* phosphatidylinositol-specific phospholipase C enzymatic activity. *J. Biol. Chem.* **287**, 40317-40327.

231. Goldstein, R., Cheng, J., Stec, B., and Roberts, M.F. (2012) An intramolecular  $\pi$ -cation latch controls substrate access in the phosphatidylinositol-specific phospholipase C from *Staphylococcus aureus*. *Biochemistry* **51**, 2579-2587.
230. Haynie, S.L., Hinkle, A.S., Jones, N.L., Martin, C.A., Olsiewski, P.J., and Roberts, M.F. (2011) Reflections on the journey: Six short stories. *Chemistry Central Journal* 5:69 doi: 10.1186/1752-153X-5-69.
229. Neelon, K., Roberts, M.F., and Stec, B. (2011) Crystal structure of a trapped catalytic intermediate suggests that forced atomic proximity drives the catalysis of mIPS. *Biophys. J.* **101**, 2816-2824.
228. Strelko, C.L., Lu, W., Dufort, F.J., Seyfried, T.N., Chiles, T.C., Rabinowitz, J.D., and Roberts, M.F. (2011) Itaconic acid is a mammalian metabolite during macrophage activation. *J. Amer. Chem. Soc.* **133**, 16386-16389.
227. Pu, M., Orr, A., Redfield, A.G., and Roberts, M.F. (2010) Defining specific lipid binding sites for a membrane protein in situ using subtesla field-cycling. *J. Biol. Chem.* **285**, 26916-26922.
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225. Wang, Q., Wei, Y., Roberts, M.F., and Krilov, G. (2010) Understanding the stereospecific interactions of 3-deoxyphosphatidylinositol derivatives with the PTEN phosphatase domain. *J. Molec. Graphics Model.* **29**, 102-114.
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223. Pu, M., Feng, J., Redfield, A.G., and Roberts, M.F. (2009) Enzymology with a spin-labeled phospholipase C: Soluble substrate binding by  $^{31}\text{P}$  NMR from 0.005 to 11.7 Tesla. *Biochemistry* **48**, 8282-8284.
222. Pu, M., Roberts, M.F., and Gershenson, A. (2009) Fluorescence correlation spectroscopy of phosphatidylinositol-specific phospholipase C monitors the interplay of substrate and activator lipid binding. *Biochemistry* **48**, 6835-6845.
221. Pu, M., Fang, X., Gershenson, A., Redfield, A.G., and Roberts, M.F. (2009) Correlation of vesicle binding and phospholipid dynamics with phospholipase C activity: Insights into phosphatidylcholine activation and surface dilution inhibition. *J. Biol. Chem.* **284**, 16099-16107.
220. Shi, X., Shao, C., Zhang, X., Zambonelli, C., Redfield, A.G., Head, J.F., Seaton, B.A., and Roberts, M.F. (2009) Modulation of *Bacillus thuringiensis* phosphatidylinositol-specific phospholipase C activity by mutations in the putative dimerization interface. *J. Biol. Chem.* **284**, 15607-15618.
219. Longo, C.M., Wei, Y., Roberts, M.F., and Miller, S.J. (2009) Asymmetric syntheses of L,L- and L,D-di-myo-inositol-1,1'-phosphate and their behavior as stabilizers of enzyme activity at extreme temperatures. *Angew. Chem. Int. Ed.* **48**, 4158-4161.
218. Roberts, M.F., Mohanty, U., and Redfield, A.G. (2009) Phospholipid reorientation at the lipid/water interface measured by high resolution field cycling  $^{31}\text{P}$  NMR spectroscopy. *Biophys. J.* **97**, 132-141.

217. Chen, W., Goldfine, H., Ananthanarayanan, B., Cho, W., and Roberts, M.F. (2009) *Listeria monocytogenes* phosphatidylinositol-specific phospholipase C: Kinetic activation and homing in on different interfaces. *Biochemistry* **48**, 3578-3592.
216. Sivanandam, V.N., Cai, J., Redfield, A.G., and Roberts, M.F. (2009) Phosphatidylcholine “wobble” in vesicles assessed by high-resolution  $^{13}\text{C}$  field cycling NMR spectroscopy. *J. Am. Chem. Soc.* **131**, 3420-3421.
215. Wang, Y.K., Chen, W., Blair, D., Pu, M., Xu, Y., Miller, S.J., Redfield, A.G., Chiles, T.C. and Roberts, M. F. (2008) Insights into the structural specificity of the cytotoxicity of 3-deoxy-phosphatidylinositols. *J. Am. Chem. Soc.* **130**, 7746-7755.
214. Guo, S., Zhang, X., Seaton, B.A., and Roberts, M.F. (2008) Role of helix B residues in interfacial activation of a bacterial PI-PLC. *Biochemistry* **47**, 4201-4210.
213. Klauda, J.B., Roberts, M.F., Redfield, A.G., Brooks, B.R., and Pastor, R.W. (2008) Rotation of lipids in membranes: MD simulation,  $^{31}\text{P}$  spin-lattice relaxation, and rigid-body dynamics. *Biophys. J.* **94**, 3074-3083.
212. Bleiman, B.F., Dufort, F.J., Gumina, M.R., Blair, D., Wagner, D.J., Roberts, M.F., and Chiles, T.C. (2007) Interleukin-4-mediated protection of primary B lymphocytes from apoptosis via Stat6-dependent regulation of glycolytic metabolism. *J. Immunol.* **179**, 4953-4957.
211. Wang, Y.K., Stieglitz, K.A., Bubunenko, M., Court, D.L., Stec, B., and Roberts, M.F. (2007) The structure of the R184A mutant of the inositol monophosphatase encoded by *suhB* and implications for its functional interactions in *E. coli*. *J. Biol. Chem.* **282**, 26989-26996.
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209. Crouch, E., McDonald, B., Smith, K., Roberts, M., Cafarella, T., Seaton, B., and Head, J. (2007) Critical role of Arg/Lys343 in the species-dependent recognition of phosphatidylinositol by pulmonary surfactant protein D. *Biochemistry* **46**, 5160-5169.
208. Rodionov, D.A., Kurnasov, O.V., Stec, B., Wang, Y., Roberts, M.F., and Osterman, A (2007) Genomic identification and in vitro reconstitution of a complete biosynthetic pathway for the osmolyte di-myo-inositol phosphate. *Proc. Natl. Acad. Sci. U.S.A.* **104**, 4279-4284.
207. Shao, C., Shi, X., Wehbi, H., Zambonelli, C., Head, J.F., Seaton, B.A., and Roberts, M.F. (2007) Dimer structure of an interfacially impaired phosphatidylinositol-specific phospholipase C. *J. Biol. Chem.* **282**, 9228-9235.
206. Faber, A.C., Dufort, F.J., Blair, D., Wagner, D., Roberts, M.F., and Chiles, T.C. (2006) Inhibition of phosphatidylinositol 3-kinase-mediated glucose metabolism coincides with resveratrol-induced cell cycle arrest in human diffuse large B-cell lymphomas. *Biochem. Biopharm.* **29**, 1561-1566.
205. Doughty, C.A., Bleiman, B.F., Wagner, D.J., Dufort, F.J., Mataraza, J.M., Roberts, M.F., and Chiles, T.C. (2006) Receptor-mediated changes in glucose metabolism in B lymphocytes: Role of phosphatidylinositol-3-kinase signaling in the glycolytic control of growth. *Blood* **107**, 4458-4465.
204. Wang, Y.K., Morgan, A.J., Stieglitz, K.A., Stec, B., Thompson, B., Miller, S.J., and Roberts, M.F. (2006) Temperature dependence of the inositol monophosphatase  $K_m$  correlates with di-myo-inositol-1,1'-phosphate accumulation in *Archaeoglobus fulgidus*. *Biochemistry* **45**, 3307-3314.
203. Roberts, M.F. (2006) Inositol in bacteria and archaea. *Subcell. Biochem.* **39**, 103-133.

202. Roberts, M.F. (2006) Characterization of organic compatible solutes of halotolerant and halophilic organisms. *Meth. Microbiol.* **35**, 615-647.
201. Neelon, K., Schreier, H.J., Meekins, H., Robinson, P.M., and Roberts, M.F. (2005) Compatible solute effects on thermostability of glutamine synthetase and aspartate transcarbamylase from *Methanococcus jannaschii*. *Biochim. Biophys. Acta* **1753**, 164-73.
200. Roberts, M.F. (2005) Organic compatible solutes of halotolerant and halophilic microorganisms. *Saline Systems* **1**: 5.
199. Kobayashi, M., Gryczynski, Z., Malick, J., Feng, J., Roberts, M.F., Lakowicz, J.R., and Lomasney, J.W. (2005) Spectroscopic characterization of the EF-hand domain of phospholipase C- $\delta$ 1: Identification of a lipid interacting domain. *Arch. Biochem. Biophys.* **440**, 191-203.
198. Neelon, K., Wang, Y., Stec, B., and Roberts, M.F. (2005) Probing the mechanism of *Archaeoglobus fulgidus* inositol-1-phosphate synthase. *J. Biol. Chem.* **280**, 11475-11482.
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196. Stieglitz, K., Yang, H., Roberts, M.F., and Stec, B. (2005) Reaching for mechanistic consensus across kingdoms: Structure and insights into catalysis of the inositol-1-phosphate synthase (mIPS) from *Archaeoglobus fulgidus*. *Biochemistry* **44**, 213-224.
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185. Feng, J., Stieglitz, K., and Roberts, M.F. (2004) Mutation of two active site residues converts a phosphatidylinositol-specific phospholipase C to a glucose phosphatase. *J. Amer. Chem. Soc.* **126**, 1008-1009.
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