

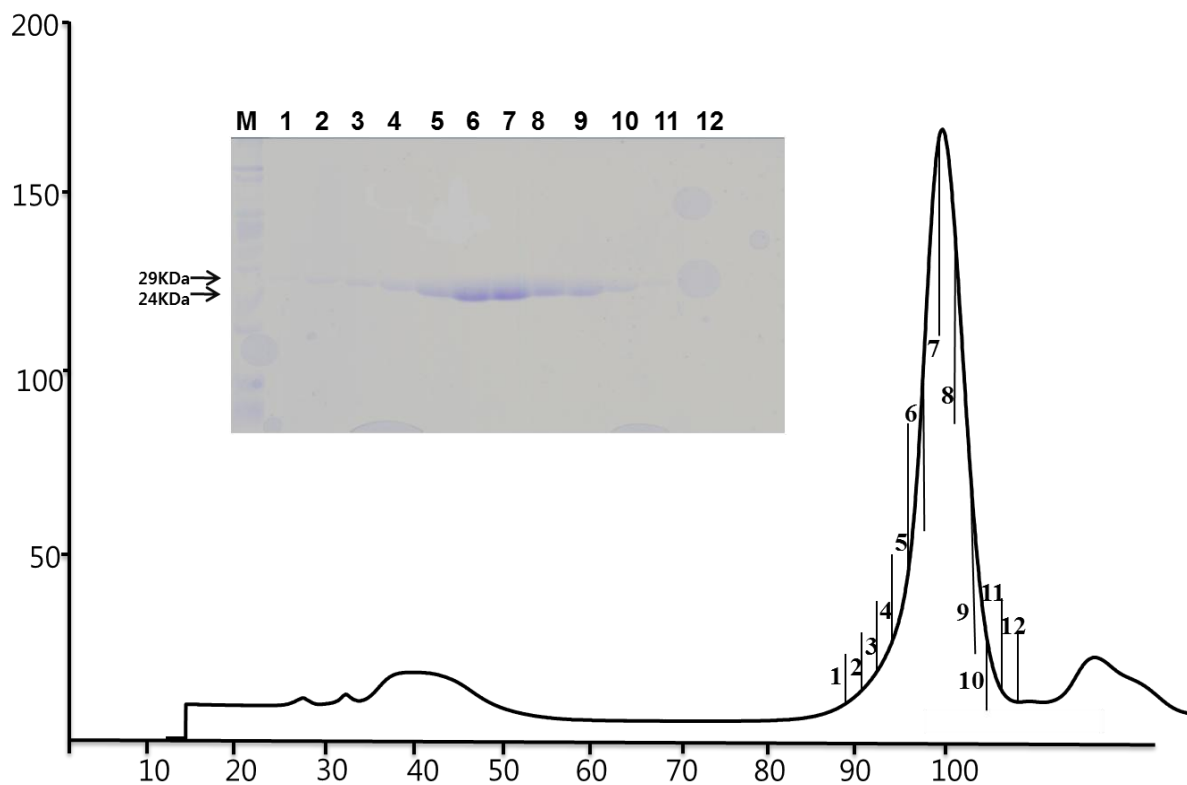
# Acta Crystallographica Section D

Volume 70 (2014)

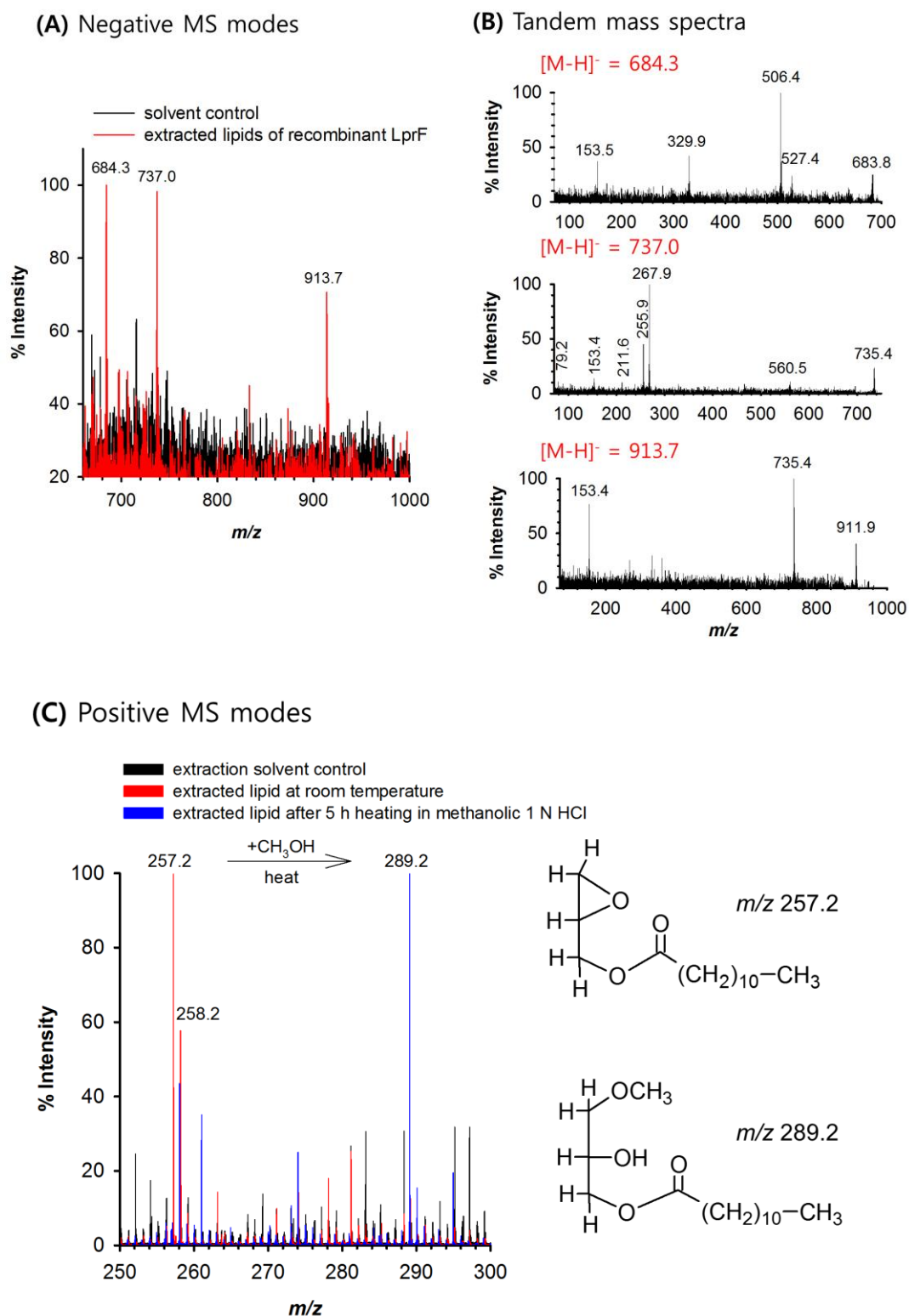
Supporting information for article:

Crystal structure and functional implications of LprF from  
*Mycobacterium tuberculosis* and *bovis*

Jin-Sik Kim, Li Jiao, Jeong-II Oh, Nam-Chul Ha and Yong-Hak Kim



**Figure S1** The elution profile of the purified LprF protein (residues 40–261) on a size exclusion chromatographic column (Hiload Superdex 16/60 200). The molecular size of the protein was calculated to be ~24 kDa based on the elution volume of the protein.



**Figure S2** Mass analysis of lipid extracted from LprF purified from *E. coli*. (A) Monoisotopic mass signals and (B) tandem mass spectra of negative ions at  $m/z$  684.3, 737.0 and 913.7 are assigned to fragment ions formed by the hydrolysis of 1,2-glycero-diacyl-3-phospho *myo*-inositol di-(L- $\beta$ -D-heptose). (C) Mass signal changes of positive ions at  $m/z$  257 and 289 derived from lipid extraction at

room temperature and 80°C, which indicate that LprF-bound phospholipid forms 1-lauryl deoxyglycerol ( $m/z$  257.2) by dephosphorylation under matrix-assisted laser desorption/ionization condition and that a methylated derivative of 1-lauryl glyceride is formed during a 5 h period of heating in chloroform-methanol-1 N HCl solution.

**Table S1** Profiles of fatty acid methyl esters of *Mycobacterium smegmatis* strains containing LprF, LprF A110Y and empty pNbv1 vector.

*Note.* Strains were grown in tryptic soy broth. Fatty acid methyl esters derived from two independent cell cultures were analyzed using a Hewlett-Packard 6890 gas chromatograph installed with Microbial Identification Software (MIDI, Newark, DE). Percentages of fatty acid components are reported as mean  $\pm$  standard deviation.

Fatty acid components	pNbv1	LprF	A110Y
14:0	2.99 $\pm$ 0.11	2.63 $\pm$ 0.49	3.15 $\pm$ 0.35
16:1 $\omega$ 9c	0.80 $\pm$ 0.56	0.78 $\pm$ 0.11	0.76 $\pm$ 0.05
16:1 $\omega$ 6c/ 16:1 $\omega$ 7c	3.71 $\pm$ 1.58	5.27 $\pm$ 0.34	3.17 $\pm$ 1.51
16:0	46.89 $\pm$ 1.63	46.93 $\pm$ 0.51	52.98 $\pm$ 5.78
16:0 10-methyl	1.03 $\pm$ 0.05	0.76 $\pm$ 0.06	0.89 $\pm$ 0.18
17:0	0.29 $\pm$ 0.14	0.35 $\pm$ 0.01	0.40 $\pm$ 0.06
18:1 $\omega$ 9c	14.44 $\pm$ 0.13	14.72 $\pm$ 2.60	7.86 $\pm$ 4.05
18:0	2.70 $\pm$ 0.30	4.10 $\pm$ 0.06	2.93 $\pm$ 0.47
18:0 10-methyl	25.76 $\pm$ 4.20	23.26 $\pm$ 0.52	26.06 $\pm$ 3.85
20:0	1.39 $\pm$ 0.19	1.20 $\pm$ 0.18	1.80 $\pm$ 0.14