

The Relationship between Specialized Pro-resolving Lipid Mediators, Morbid Obesity and Weight Loss after Bariatric Surgery

Fabian Schulte PhD^{1,2,a}, Abdul Aziz Asbeutah MD^{3,a,b}, Peter N. Benotti MD⁴, G. Craig Wood MS⁴, Christopher Still DO⁴, Bruce R. Bistrian MD, PhD⁵, Markus Hardt PhD^{1,2} and Francine K. Welty MD, PhD^{3*}

¹ Forsyth Institute, Cambridge, MA; ² Department of Developmental Biology, Harvard School of Dental Medicine, Boston, MA; ³ Division of Cardiology, Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, MA; ⁴ Geisinger Obesity Institute; ⁵ Department of Medicine, Beth Israel Deaconess Medical Center, Harvard Medical School, Boston, MA.

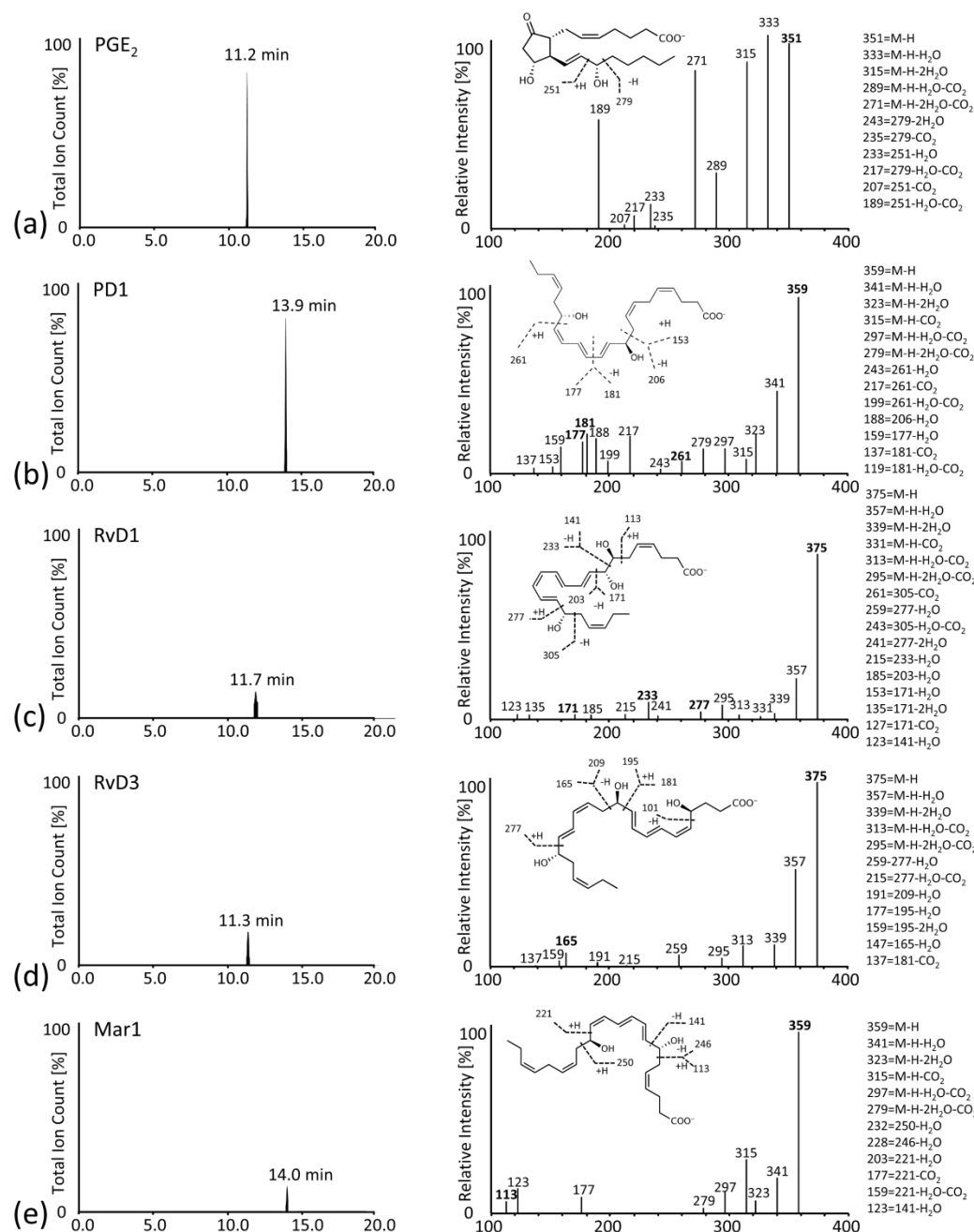
^a These authors contributed equally.

^b Current affiliation: Department of Medicine, University of Tennessee Health Science Center, Memphis, TN.

Supplementary Table S1. MRM-transitions for the detection of SPMs in human blood serum.

Compound	RT [min]	Precursor mass [m/z]	Product ions [m/z]	DP [V]	EP [V]	CXP [V]	CE [V]
d4-LTB ₄ (339.3/197.2)	14.2	339.3	197.2	-80	-10	-22	-22
d4-PGE ₂ (355.3/193.2)	11	355.3	193.2	-80	-10	-25	-25
d5-LXA ₄ (356.3/115.2)	11.7	356.3	115.2	-80	-10	-19	-19
d5-MaR ₂ (364.3/221.2)	14.6	364.3	221.2	-80	-10	-28	-28
d5-RvD ₂ (380.3/141.2)	11.1	380.3	141.2	-80	-10	-25	-25
d8-5S-HETE (327.2/116.1)	17.7	327.2	116.1	-80	-10	-17	-17
14-HDHA (343.2/205.1)	17.6	343.2	205.1	-80	-10	-17	-17
17-HDHA (343.2/245.1)	17.5	343.2	245.1	-80	-10	-17	-17
18-HEPE (317.2/259.1)	16.5	317.2	259.1	-80	-10	-16	-16
LTB ₄ (335.2/195.1)	14.2	335.2	195.1	-80	-10	-22	-22
LXA ₄ (351.2/115.1)	11.7	351.2	115.1	-80	-10	-20	-20
LXA ₄ (351.2/235.1)	11.7	351.2	235.1	-80	-10	-20	-20
LXB ₄ (351.2/221)	11.0	351.2	221.1	-80	-10	-20	-20
MaR ₁ (359.2/221.1)	14.0	359.2	221.1	-80	-10	-20	-20
MaR ₁ (359.2/250.1)	14.0	359.2	250.1	-80	-10	-20	-20
MaR ₂ (359.2/221.2)	14.6	359.2	221.2	-80	-10	-28	-28
PD ₁ (359.2/153.1)	13.9	359.2	153.1	-80	-10	-21	-21
PD ₁ (359.2/181.1)	13.9	359.2	181.1	-80	-10	-19	-19
PDX (359.1/153.1)	13.7	359.1	153.1	-80	-10	-25	-25
PDX (359.2/181.1)	13.7	359.2	181.1	-80	-10	-25	-25
PGD ₂ (351.3/233.1)	11.2	351.3	233.1	-80	-10	-16	-16
PGE ₂ (351.3/175.1)	11.0	351.3	175.1	-80	-10	-25	-25
PGE ₂ (351.3/189.1)	11.0	351.3	189.1	-80	-10	-25	-25
RvD ₁ (375.2/121.1)	11.7	375.2	121.1	-80	-10	-40	-40
RvD ₁ (375.2/215.1)	11.7	375.2	215.1	-80	-10	-26	-26
RvD ₂ (375.2/141.1)	11.1	375.2	141.1	-80	-10	-21	-21
RvD ₂ (375.2/175.1)	11.1	375.2	175.1	-80	-10	-30	-30
RvD ₃ (375.2/147.1)	11.3	375.2	147.1	-80	-10	-25	-25
RvD ₃ (375.2/181.1)	11.3	375.2	181.1	-80	-10	-22	-22
RvD ₄ (375.2/101.1)	12.7	375.2	101.1	-80	-10	-22	-22
RvD ₄ (375.2/255.1)	12.7	375.2	255.1	-80	-10	-25	-25
RvD ₅ (359.2/199.1)	13.8	359.2	199.1	-80	-10	-21	-21
RvD ₅ (359.2/261.1)	13.8	359.2	261.1	-80	-10	-20	-20
RvD ₆ (359.2/101.1)	14.3	359.2	101.1	-80	-10	-22	-22
RvE ₁ (349.2/161.1)	8.9	349.2	161.1	-80	-10	-25	-25
RvE ₁ (349.2/195.1)	8.9	349.2	195.1	-80	-10	-22	-22
RvE ₂ (333.3/199.1)	12.1	333.3	199.1	-80	-10	-24	-24
RvE ₂ (333.3/253.1)	12.1	333.3	253.1	-80	-10	-20	-20

CE Collision energy, CXP collision cell exit potential, DP declustering potential, d4-LTB₄ deuterium-labeled leukotriene B₄, d4-PGE₂ deuterium-labeled prostaglandin E₂, d5-LXA₄ deuterium-labeled lipoxin A₄, d5-MaR₂ deuterium-labeled maresin 2, d5-RvD₂ deuterium-labeled resolvin D₂, EP entrance potential, LTB₄ Leukotriene B₄, LXA₄ lipoxin A₄, LXB₄ lipoxin B₄, MaR₁ maresin 1, MaR₂ maresin 2, MRM multiple reaction monitoring, PD₁ protectin D₁, PDX protectin X, PGD₂ prostaglandin D₂, PGE₂ prostaglandin E₂, RT retention time, RvD₁ resolvin D₁, RvD₂ resolvin D₂, RvD₃ resolvin D₃, RvD₄ resolvin D₄, RvD₅ resolvin D₅, RvD₆ resolvin D₆, RvE₁ resolvin E₁, RvE₂ resolvin E₂, SPM specialized pro-resolving lipid mediators, 14-HDHA 14-hydroxy-docosahexaenoic acid, 17-HDHA 17-hydroxy-docosahexaenoic acid, 18-HEPE 18-hydroxy-eicosapentaenoic acid, [m/z] mass-over-charge.



Supplementary Figure S1. Identification of lipid mediators in human blood serum.

LC-MS/MS chromatograms (left panel) and corresponding annotated product ion spectra (right panel) of the lipid mediators PGE₂ (a), PD1 (b), RvD1 (c), RvD3 (d) and MaR1 (e) isolated from a representative human serum specimen. Identification and quantification were performed by matching retention times and MS/MS-spectra of pure synthetic standards using at least 6 diagnostic ions.

LC-MS/MS Liquid chromatography tandem mass spectrometry, *MaR1* maresin 1, *PD1* protectin D1, *PGE₂* prostaglandin E2, *RvD1* resolvin D1, *RvD3* resolvin D3.