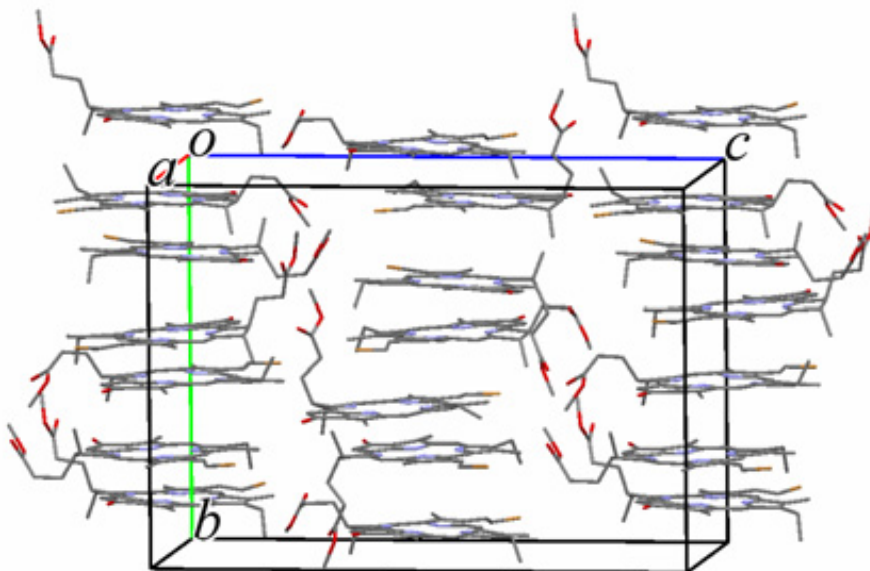


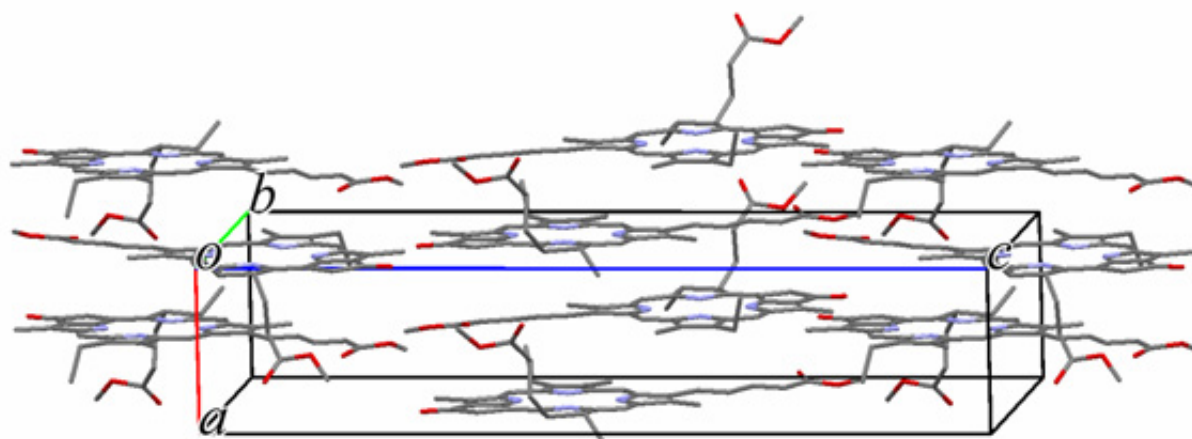
Supplementary Data

X-Ray single-crystal structures and NMR characterization of three vinyl-substituted methylpyropheophorbide *a* derivatives

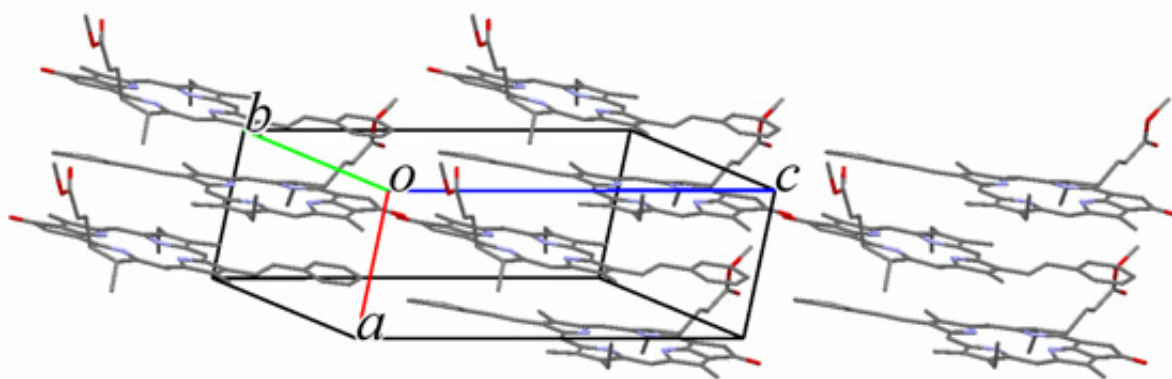
Ivan S. Lonin,^{a@} Evgeny S. Belyaev,^a Viktor A. Tafeenko,^b Vladimir V. Chernyshev,^{a, b} Elena V. Savinkina,^c Gelii V. Ponomarev^d, Oskar I. Koifman,^e and Aslan Yu. Tsivadze.^a



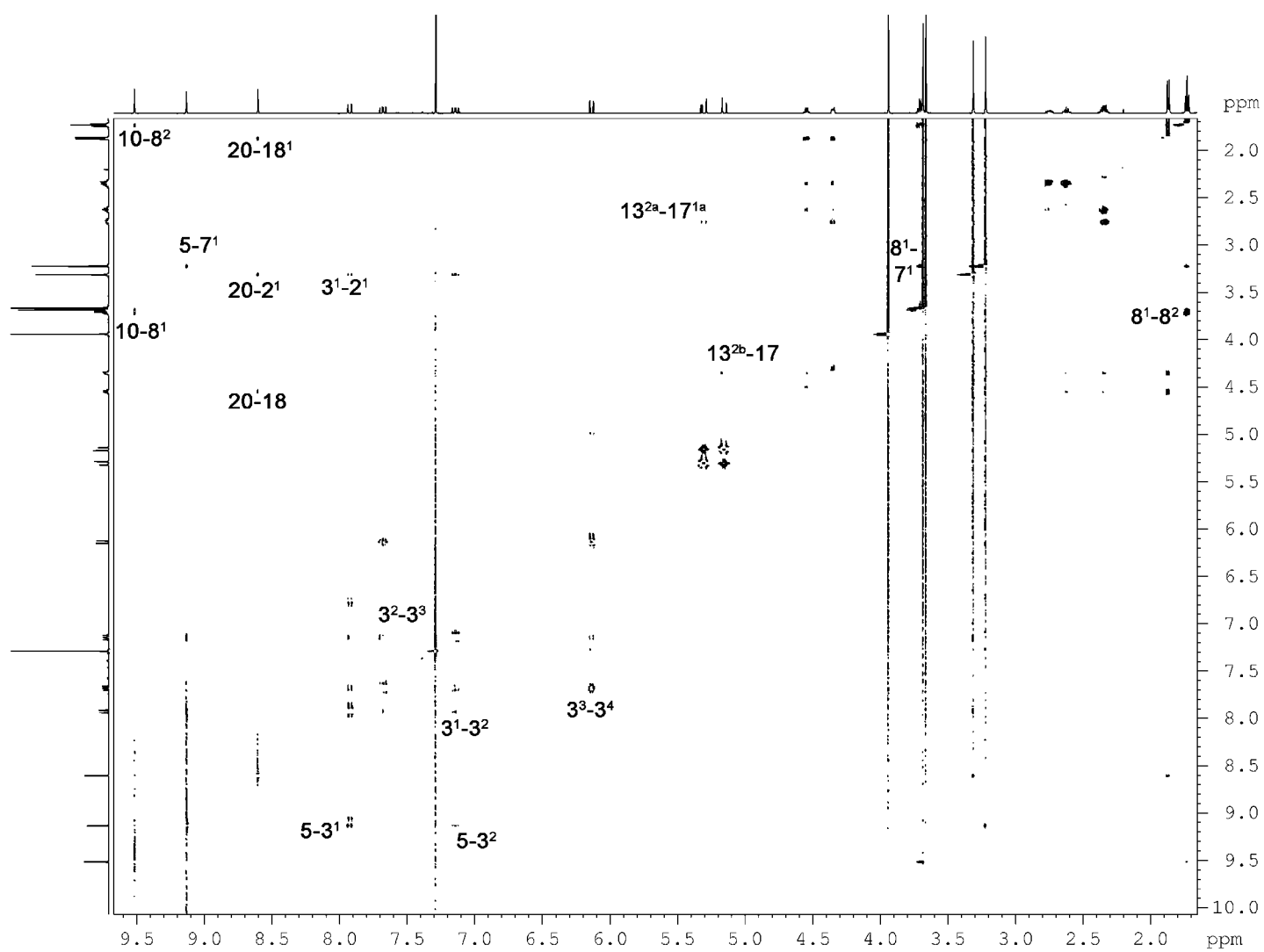
Crystal packing of **1**. H atoms omitted for clarity.



Crystal packing of **2**. H atoms omitted for clarity.



Crystal packing of **3**. H atoms omitted for clarity.



^1H - ^1H NOESY spectrum of compound **2**.

¹H and ¹³C NMR data for compounds 1–3

NMR spectral data							
¹³ C	δ, ppm			¹ H	δ, ppm, multiplicity, <i>J</i> , Hz		
	1	2	3		1	2	3
				NH(A)	0.26, bs	0.26, bs	0.08, s
				NH(B)	-1.87, bs	-1.89, bs	-1.65, bs
C-1	140.8	140.7	141.6				
C-2	130.8	132.1	131.2				
C-2 ¹ (-CH ₃)	12.3	12.6	12.4	H-2 ¹ (-CH ₃)	3.35, s	3.30, s	3.45, s
C-3	133.3	133.1	135.5				
C-4	135.1	135.5	136.4				
C-5 (-CH=)	96.9	96.5	97.1	H-5	9.19, s	9.12, s	9.40, s
C-6	154.9	154.8	155.2				
C-7	136.2	136.3	136.1				
C-7 ¹ (-CH ₃)	11.2	11.2	11.3	H-7 ¹ (-CH ₃)	3.21, s	3.20, s	3.22, s
C-8	145.0	145.0	145.0				
C-8 ¹ (-CH ₂ -)	19.5	19.5	19.5	H-8 ¹	3.67, q , 7.8	3.68, q , 7.8	3.69, q , 7.8
C-8 ² (-CH ₃)	17.4	17.4	17.4	H-8 ²	1.69, t , 7.8	1.70, t , 7.8	1.70, t , 7.8
C-9	150.9	151.1	150.8				
C-10 (-CH=)	104.1	104.0	104.1	H-10	9.48, s	9.49, s	9.50, s
C-11	138.2	138.3	137.9				
C-12	131.3	128.9	128.4				
C-12 ¹ (-CH ₃)	12.0	12.1	12.1	H-12 ¹ (-CH ₃)	3.66, s	3.66, s	3.67, s
C-13	128.8	130.9	130.5				
C-13 ¹ (>C=O)	196.8	196.1	196.2				
C-13 ² (-CH ₂ -)	48.1	48.1	48.0	H-13 ^{2a} H-13 ^{2b}	5.27, d , 19.3 5.12, d , 19.3	5.28, d , 19.1 5.13, d , 19.1	5.26, d , 19.3 5.11, d , 19.3
C-14	149.0	148.9	149.1				
C-15	106.3	106.4	106.0				
C-16	160.6	160.8	160.4				
C-17	51.8	51.8	51.7	H-17	4.31, m	4.32, m	4.29, m
C-17 ¹ (-CH ₂ -)	29.9	29.9	29.9	H-17 ^{1a} H-17 ^{1b}	2.70, m 2.30, m	2.72, m 2.32, m	2.71, m 2.31, m
C-17 ² (-CH ₂ -)	30.9	30.9	30.9	H-17 ^{2a} H-17 ^{2b}	2.57, m 2.30, m	2.59, m 2.32, m	2.58, m 2.31, m
C-17 ³ (>C=O)	173.4	173.4	173.5				
C-17 ⁴ (-OCH ₃)	51.6	51.7	51.7	H-17 ⁴ (-OCH ₃)	3.62, s	3.63, s	3.62, s
C-18	50.0	49.9	50.0	H-18	4.50, qd , 7.5, 1.4	4.51, qd , 7.5, 1.9	4.50, qd , 7.5, 1.7
C-18 ¹ (-CH ₃)	23.2	23.2	23.2	H-18 ¹	1.82, d , 7.5	1.84, d , 7.5	1.83, d , 7.5
C-19	171.1	171.0	171.4				
C-20 (-CH=)	93.3	93.4	93.0	H-20	8.57, s	8.58, s	8.57, s
C3 Substituent							
¹³ C	δ, ppm			¹ H	δ, ppm, multiplicity, <i>J</i> , Hz		
	1	2	3		1	2	3
C-3 ¹ (-CH=)	129.6	132.1	120.7	H-3 ¹	8.32, d , 14.5	7.92, d , 15.7	8.32, d , 16.5
C-3 ² (-CH=)	112.3	132.8	136.9	H-3 ²	7.25, d , 14.5	7.14, dd , 15.7, 11.1	7.59, d , 16.5
C-3 ³		145.0	137.6	H-3 ³		7.66, dd , 15.3, 11.1	
C-3 ⁴		121.7	126.8	H-3 ⁴		6.12, d , 15.3,	7.85, m
C-3 ⁵		167.4	129.0	H-3 ⁵			7.57, m
C-3 ⁶		51.8	128.4	H-3 ⁶		3.91, s	7.46, td , 7.4, 1.2