Pyridinium-1-yl Bisphosphonates are Potent Inhibitors of Farnesyl Diphosphate Synthase and Bone Resorption

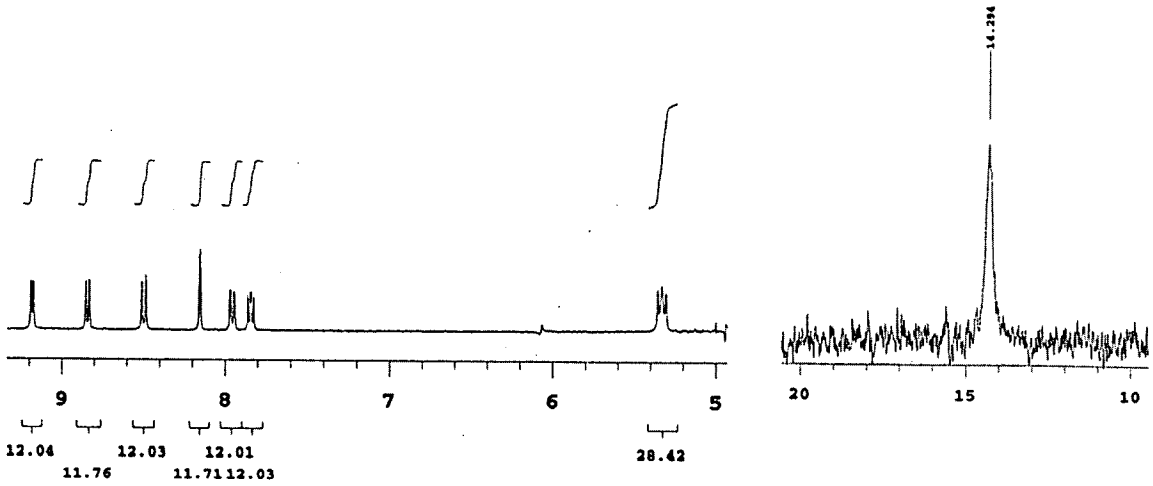
John M. Sanders, Yongcheng Song, Julian M. W. Chan, Yonghui Zhang, Samuel Jennings, Thomas Kosztowski, Sarah Odeh, Ryan Flessner, Christine Schwerdtfeger, Evangelia Kotsikorou, Gary A. Meints, Aurora Ortiz Gómez, Dolores González-Pacanowska, Amy M. Raker, Hong Wang, Ermond R. van Beek, Socrates E. Papapoulos, Craig T. Morita and Eric Oldfield

Supporting Information

C/H/N Microanalytical data.....S2

NMR spectra for **14**.....S3

Appendix: Analytical Data for Pyridinium-1-yl Bisphosphonates.

Compound Number	Molecular Formula	Calculated			Found		
		Carbon (%)	Hydrogen (%)	Nitrogen (%)	Carbon (%)	Hydrogen (%)	Nitrogen (%)
5	$C_7H_{11}NP_2O_7$	29.70	3.92	4.95	29.36	3.80	4.84
7	$C_8H_{13}NP_2O_7$	32.34	4.41	4.71	32.48	4.34	4.63
8	$C_{13}H_{13}NP_2O_7Na_2$ • 2 H_2O	35.55	3.90	3.19	35.88	4.12	3.27
9	$C_{13}H_{11}NP_2O_8Na_4$ • 3 H_2O	30.19	3.31	2.71	30.44	3.34	2.61
10	$C_{14}H_{14}NP_2O_7Na_3$ • 1.5 H_2O	36.07	3.68	3.00	36.00	3.91	2.95
11	$C_{15}H_{16}NP_2O_7Na_3$ • 2.5 H_2O	36.16	4.25	2.81	36.01	4.00	2.79
12	$C_{19}H_{19}NP_2O_7$ • 0.5 H_2O	51.36	4.54	3.15	50.94	4.37	3.15
13	$C_{11}H_{13}NP_2O_7$ • 0.25 H_2O	39.13	4.03	4.15	39.17	3.81	4.16
14	$C_{11}H_{12}NP_2O_7Cl$ • H_2O	32.41	3.21	3.44	32.05	3.41	3.34
15	$C_9H_{15}NP_2O_7$	34.74	4.86	4.50	34.67	4.84	4.42
16	$C_{11}H_{19}NP_2O_7$ • 0.25 H_2O	38.44	5.72	4.08	38.29	5.49	4.11
17	$C_8H_{13}NP_2O_7$ • H_2O	29.02	4.57	4.23	28.99	4.25	4.17
18	$C_{14}H_{16}NP_2O_7Na$ • 0.5 H_2O	41.60	4.24	3.47	41.41	4.16	3.34
20	$C_7H_{10}FNP_2O_7$	27.92	3.35	4.65	28.41	3.34	4.62

Appendix: ^{1}H and ^{31}P NMR spectra for **14**.