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Supplementary Material

A series of imidazolyl-containing bisphosphonates with abundant hydrogen-bonding interactions: syntheses, structures and bone-binding affinity

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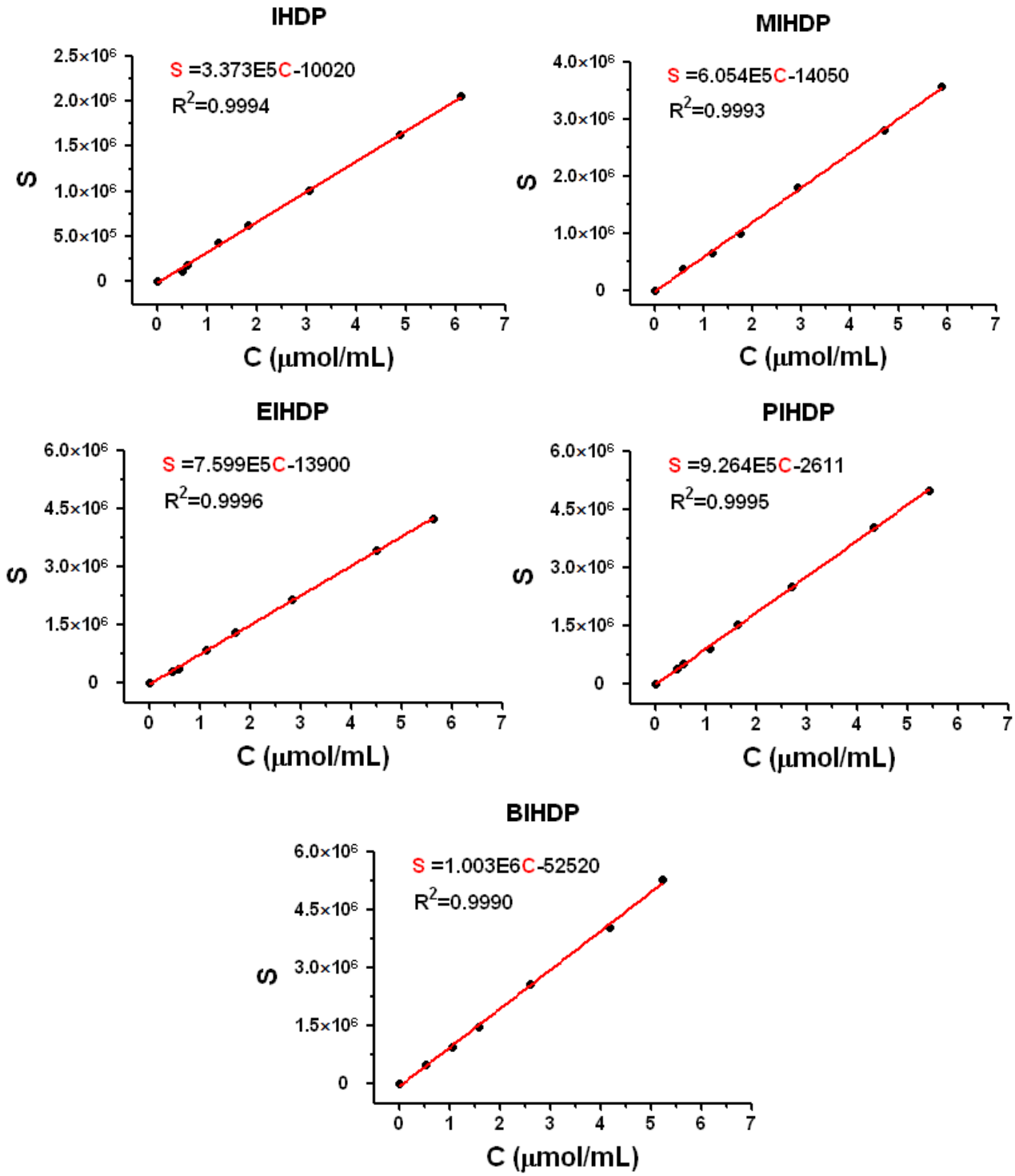

Fig. 1S. Standard concentration-area curves of BPs 3a-3e determined by HPLC.

Table S1. Selected Bond Lengths (Å) and Bond Angles (deg) for 3a-3e

	3a	3b	3c	3d	3e
P1—C9	1.8465(17)	1.842(2)	1.8494(14)	1.8451(16)	1.842(3)
P2—C9	1.8358(18)	1.832(2)	1.8513(13)	1.8491(17)	1.856(3)
P1—O1	1.5277(13)	1.5517(17)	1.5655(11)	1.5785(13)	1.5514(19)
P1—O2	1.5622(13)	1.5341(17)	1.5433(11)	1.5529(13)	1.562(2)
P1—O3	1.4934(14)	1.4985(17)	1.4916(11)	1.4764(13)	1.486(2)
P2—O4	1.5148(12)	1.5212(16)	1.5055(10)	1.5309(12)	1.511(2)
P2—O5	1.5118(13)	1.5100(16)	1.5103(11)	1.4948(13)	1.514(2)
P2—O6	1.5703(13)	1.5622(17)	1.5663(11)	1.5728(12)	1.5605(19)
C1—C2	1.336(3)	1.347(4)	1.353(2)	1.346(2)	1.346(4)
N1—C1	1.374(2)	1.389(3)	1.383(2)	1.382(2)	1.386(3)
N1—C3	1.334(3)	1.332(3)	1.3366(19)	1.338(2)	1.338(4)
N2—C2	1.363(3)	1.379(3)	1.378(2)	1.377(2)	1.381(4)
N2—C3	1.313(3)	1.325(3)	1.334(2)	1.335(2)	1.332(4)
P1—C9—P2	113.89(9)	114.69(11)	111.82(7)	110.20(8)	109.58(13)
C8—C9—O7	107.31(13)	109.55(16)	104.16(10)	112.73(12)	111.3(2)
O1—P1—O2	110.78(7)	110.05(9)	107.01(7)	104.22(7)	105.43(11)
O1—P1—O3	113.32(8)	112.18(10)	112.45(6)	111.61(7)	113.73(12)
O2—P1—O3	108.60(7)	111.17(10)	110.75(6)	115.38(8)	112.03(11)
C9—P1—O1	110.69(7)	107.39(9)	104.67(6)	104.78(7)	109.20(11)
C9—P1—O2	106.87(8)	108.69(10)	108.05(6)	107.89(7)	105.26(12)
C9—P1—O3	106.28(8)	107.18(10)	113.51(6)	112.15(7)	110.72(11)
O4—P2—O5	114.52(7)	113.60(9)	114.33(6)	113.78(7)	115.31(11)
O4—P2—O6	110.42(7)	110.87(10)	108.25(6)	109.11(7)	110.77(11)
O5—P2—O6	108.02(8)	107.42(9)	111.12(5)	108.77(7)	108.10(11)
C9—P2—O4	111.25(8)	108.04(9)	107.58(6)	107.20(7)	107.11(11)
C9—P2—O5	107.22(7)	111.85(9)	110.12(6)	111.80(7)	109.00(11)
C9—P2—O6	104.89(8)	104.72(9)	104.96(6)	105.86(7)	106.16(11)