Supporting information

Elemental analysis results for new compounds and typical dose response curves in tumor cell growth inhibition tests.

Activity of Nitrogen-Containing and Non-Nitrogen Containing Bisphosphonates on Tumor Cell Lines

Yonghui Zhang[†,¥] Annette Leon-Rossell[¶,¥] Yongcheng Song[†,¥] Danielle Studer[†], and Eric Oldfield[¶,†,*]

[†]Department of Chemistry, University of Illinois at Urbana-Champaign, 600 South Mathews Avenue, Urbana, IL 61801, USA; [¶]Department of Biophysics, University of Illinois at Urbana-Champaign, 607 South Mathews Avenue, Urbana, IL 61801, USA

[¥]These authors contributed equally to this work

*Corresponding author: Phone, 217-333-3374; Fax, 217-244-0997; email, eo@chad.scs.uiuc.edu

Table S1. Elemental analysis results of new compounds.

Compound	Formula	Calculated			Found		
		C (%)	H (%)	N (%)	C (%)	H (%)	N (%)
9	$C_{13}H_{13}FNNaO_7P_2$	39.11	3.28	3.51	39.16	3.65	3.51
10	$C_{14}H_{15}F_3NNa_2O_{8.5}P_2$	33.75	3.03	2.81	33.99	3.38	2.76
11	$C_{11}H_{19.5}NO_{7.25}P_2$	38.44	5.72	4.08	38.29	5.49	4.11
14	$C_{19}H_{19}NO_6P_2$	54.42	4.57	3.34	54.27	4.37	3.30
15	$C_{11}H_{20}NO_{6.5}P_2$	39.77	6.07	4.22	39.72	6.00	4.00
16	$C_{13}H_{15}NO_6P_2$	45.49	4.41	4.08	45.09	4.31	4.08
19	$C_7H_{11}BrNNaO_8P_2$	20.91	2.76	3.48	20.75	2.61	3.17
20	$C_8H_{14.5}NO_{6.75}P_2$	32.61	4.96	4.75	32.63	4.86	4.62
21	$C_9H_{14}NNaO_6P_2$	34.08	4.45	4.42	33.79	4.69	4.28
28	$C_7H_{11}ClNO_{6.5}P_2$	27.07	3.57	4.51	26.86	3.37	4.34
29	$C_7H_{11.5}NO_{6.25}P_2$	30.95	4.27	5.16	30.92	4.11	5.11
30	$C_7H_{11}ClNO_{6.5}P_2$	27.07	3.57	4.51	26.86	3.37	4.34
31	$C_7H_{10}INO_6P_2$	21.39	2.56	3.56	21.29	2.20	3.43
32	$C_7H_{10}BrNO_6P_2$	24.30	2.91	4.05	24.00	2.73	3.80
33	$C_{14}H_{16.25}NNa_{0.75}O_6P_2$	44.99	4.38	3.75	44.93	4.42	3.79
34	$C_8H_{10}F_3NO_6P_2$	28.76	3.01	4.18	28.41	2.92	3.97
39	$C_{19}H_{19}NO_6P_2$	54.42	4.57	3.34	54.24	4.47	3.30
40	$C_{12}H_{17}NO_8P_2$	39.46	4.69	3.84	39.33	4.50	3.82
41	$C_{19}H_{19.6}NO_{6.3}P_2$	53.73	4.65	3.30	53.38	4.47	3.37
42	$C_{12}H_{17}NO_8P_2$	39.46	4.69	3.84	39.03	4.31	4.00
44	$C_{13}H_{18}NO_{8.5}P_2$	40.43	4.70	3.63	40.34	4.49	3.25
46	$C_8H_{13}NO_8P_2$	30.68	4.18	4.47	30.32	4.05	4.38
49	$C_{12}H_{18}N_2NaO_{9.5}P_2$	33.74	4.25	6.56	33.93	4.12	6.18
50	$C_{11}H_{14}NO_{6.5}P_2$	40.50	4.33	4.29	40.64	4.11	4.30
51	$C_8H_{11}F_3NO_{6.5}P_2$	27.92	3.22	4.07	27.72	3.00	4.04
52	$C_{11}H_{19}N_2O_{8.5}P_2S$	32.28	4.68	6.84	32.13	4.38	6.62
53	$C_{19}H_{19}NO_6P_2$	54.42	4.57	3.34	54.19	4.00	3.28
54	$C_{19}H_{19}NNaO_{6.5}P_2$	50.68	4.25	3.11	50.43	4.13	3.17
56	$C_{21}H_{21}Na_3O_8P_2$	47.38	3.98		47.53	3.75	
57	$C_{20}H_{20}Na_2O_8P_2$	48.40	4.06		48.61	4.21	
58	$C_{20}H_{21}NaO_8P_2$	50.64	4.46		50.70	4.35	
59	$C_{21}H_{21}Na_2O_{7.5}P_2$	50.31	4.22		50.02	3.93	
60	$C_{21}H_{20}Na_2O_7P_2$	51.23	4.09		51.22	4.47	
61	$C_{19}H_{17.5}NaO_{7.25}P_2$	51.08	3.95		50.92	3.68	
62	$C_{20}H_{19}NaO_7P_2$	52.64	52.63		4.20	4.14	
63	$C_{20}H_{22}Na_2O_9P_2$	46.71	4.31		46.63	4.42	
64	$C_{32}H_{50}Br_2O_{14}P_2$	43.65	5.72		43.81	5.52	
65	$C_{32}H_{50}Cl_2O_{14}P_2$	48.55	6.37		48.65	4.37	

66	$C_{28}H_{42}Cl_2O_{18}P_2$	42.07	5.30		41.71	5.41	
67	$C_{28}H_{42}F_2O_{18}P_2$	43.87	5.52		43.80	5.43	
68	$C_{29}H_{43}NO_{18}P_2$	46.10	5.74		46.03	5.79	
69	$C_8H_{10}Br_2O_6P_2$	22.67	2.38		22.78	2.42	
70	$C_9H_{10}NNa_3O_7P_2$	28.82	2.69		28.83	2.76	
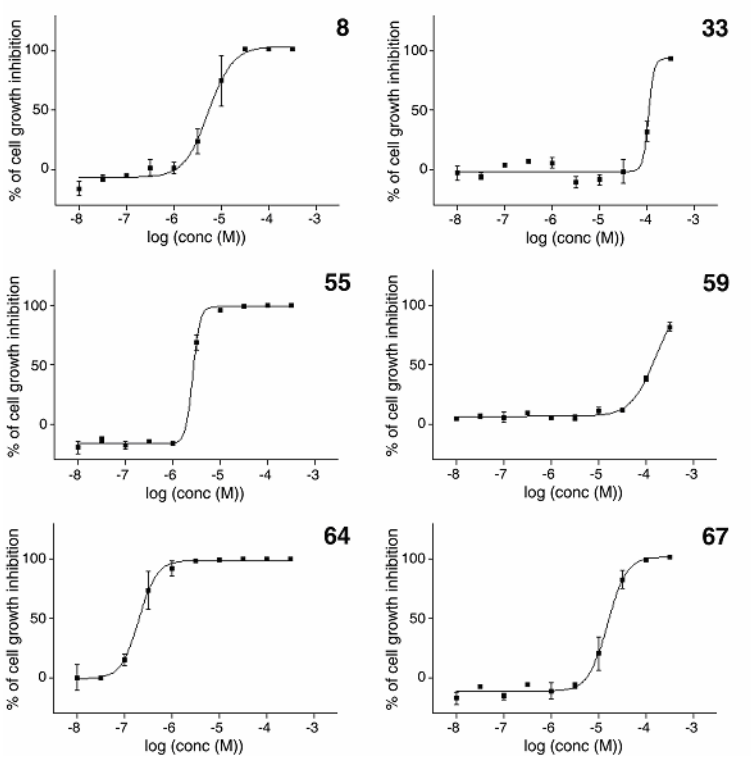
Figure S1. Representative dose response curves (for compounds **8, 33, 55, 59, 64** and **67**).