

Supporting information

Phosphate Prodrugs Derived From N-Acetylglucosamine Have Enhanced Chondroprotective Activity in Explant Cultures and Represent a New Lead in Anti-Osteoarthritis Drug Discovery.

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Microanalytical data on target compounds

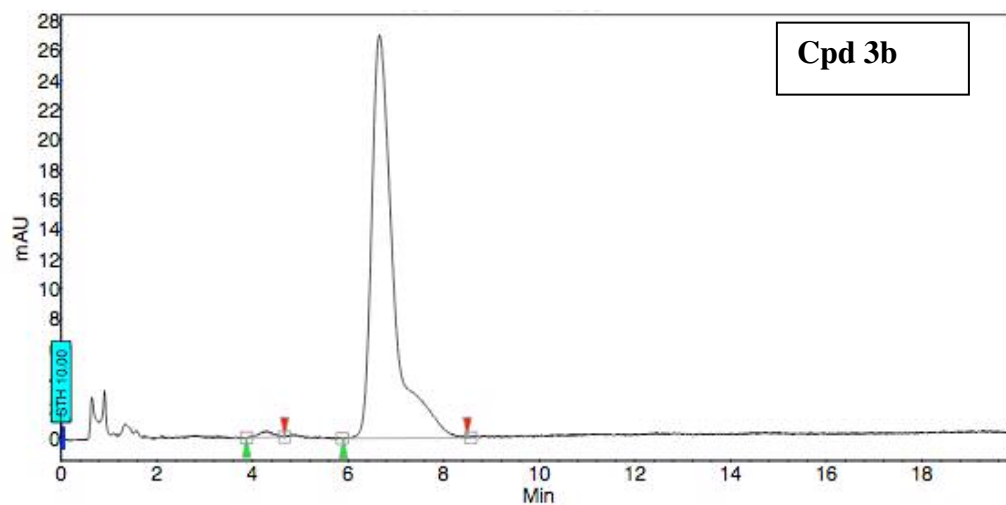
Cpd	Formula	Calculated %	Found %
3a	C ₂₅ H ₃₃ N ₂ O ₁₁ P. 1.5 H ₂ O	C 50.42%, H 6.09%, N 4.70%.	C 50.73 %, H 6.42 %, N 4.79%.
3q	C ₂₆ H ₄₁ N ₂ O ₁₁ P	C 53.06%, H 7.02%, N 4.76%.	C 52.90%, H 7.09 %, N 4.54%.

Analytical reverse phase HPLC data on selected target compounds

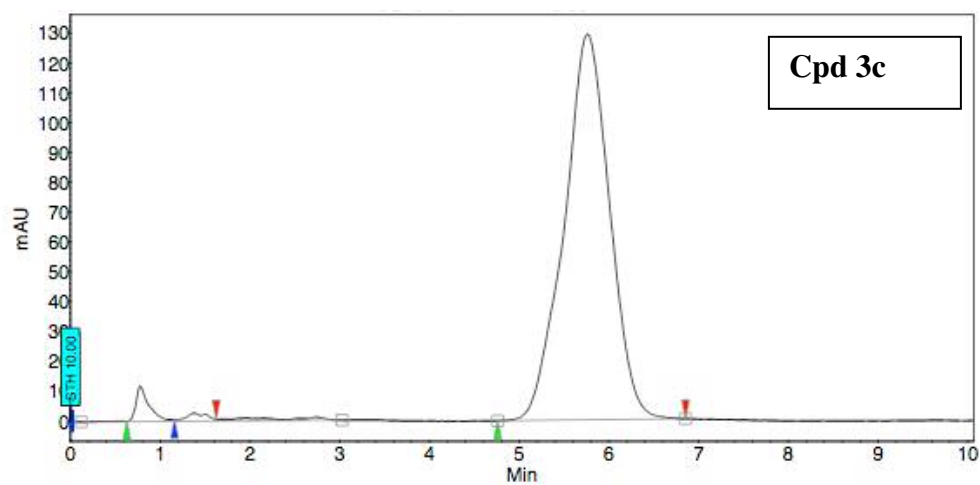
Cpd	Elution conditions	tR (mins)	λ_{max}	Purity
3b	a	6.65	288	99%
3c	b	5.76	278	97%
3g	c	6.31, 6.63, 7.55	274	100 %
3i	c	6.55, 7.05, 7.81	274	96 %
3k	c	6.66, 7.40	273	96 %
3m	c	6.85	273	96 %
3n	c	7.35, 7.79	274	97 %
3r	c	6.32, 7.64	275	95 %

a) 85% H₂O : 15% CH₃CN; b) 68% H₂O: 32% CH₃CN;

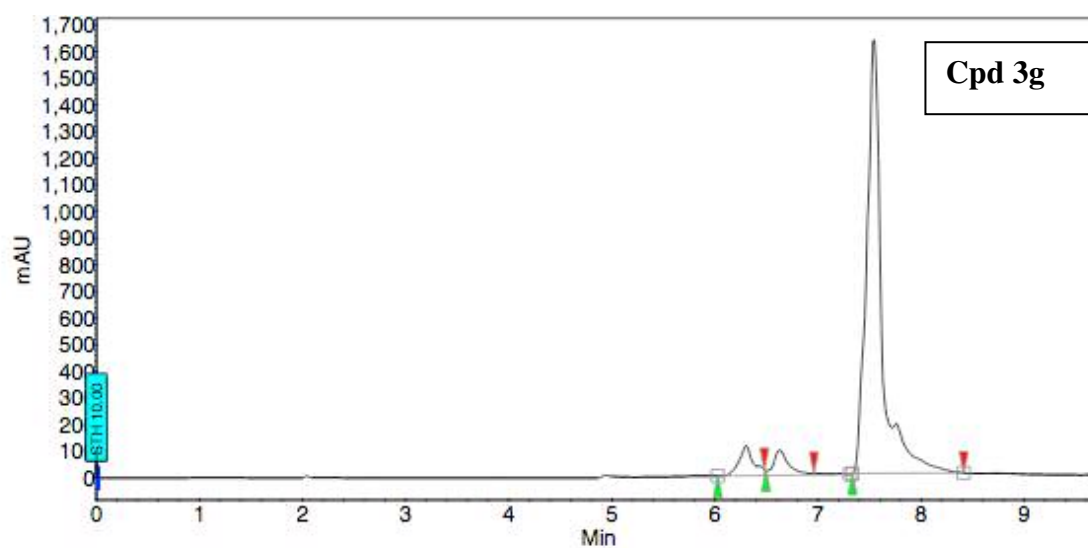
c) 100% H₂O : 0% CH₃CN to 0% H₂O : 100% CH₃CN in 10 mins



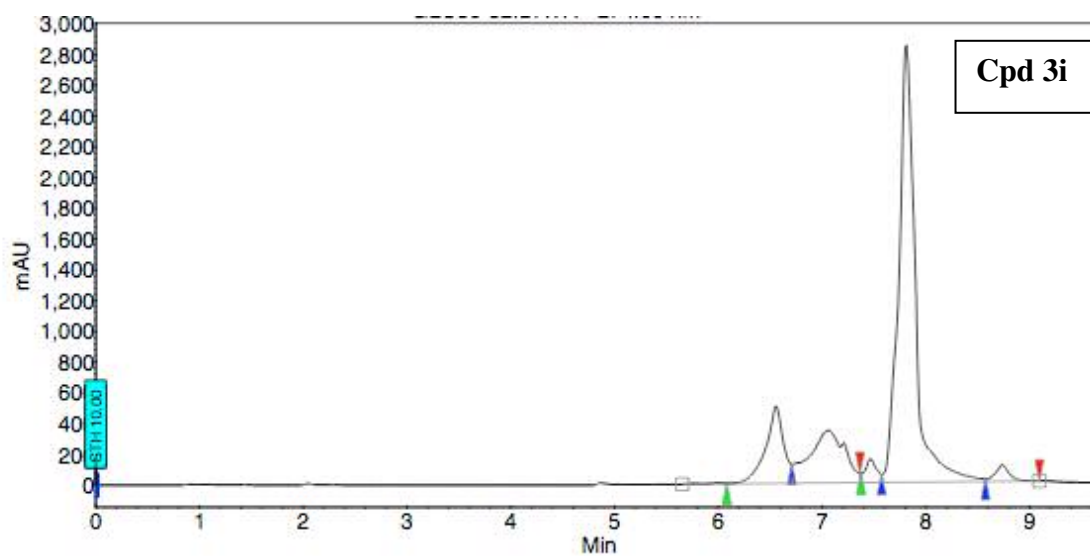
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	4.29	1.01	0.4	0.1	1.007
2	UNKNOWN	6.65	98.99	27.0	14.2	98.993
Total			100.00	27.4	14.3	100.000



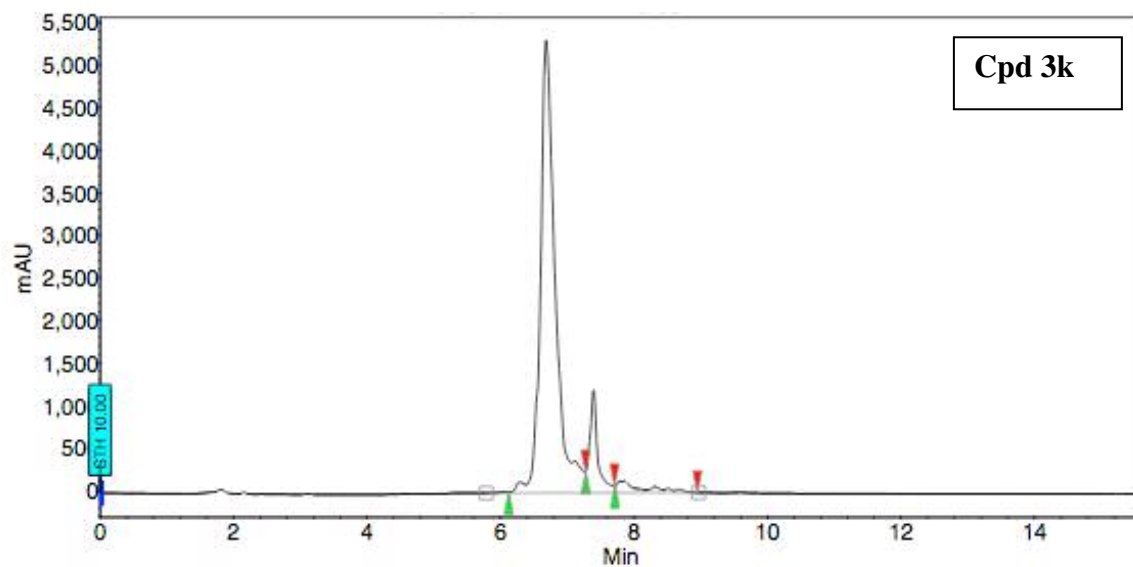
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	0.77	2.53	11.9	2.0	2.533
2	UNKNOWN	1.37	0.91	2.6	0.7	0.915
3	UNKNOWN	5.76	96.55	129.3	75.8	96.552
Total			100.00	143.8	78.5	100.000



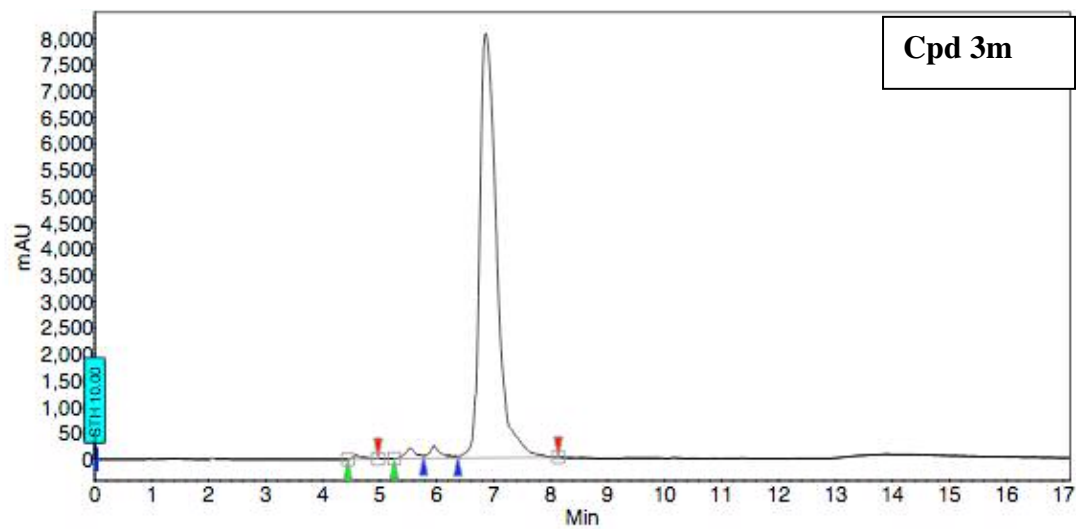
Index	Name	Time (Min)	Quantity (% Area)	Height (mAU)	Area (mAU.Min)	Area % (%)
1	UNKNOWN	6.31	5.74	112.6	18.0	5.739
2	UNKNOWN	6.63	5.00	96.6	15.7	5.001
3	UNKNOWN	7.55	89.26	1625.9	280.0	89.259
Total			100.00	1835.0	313.7	100.000



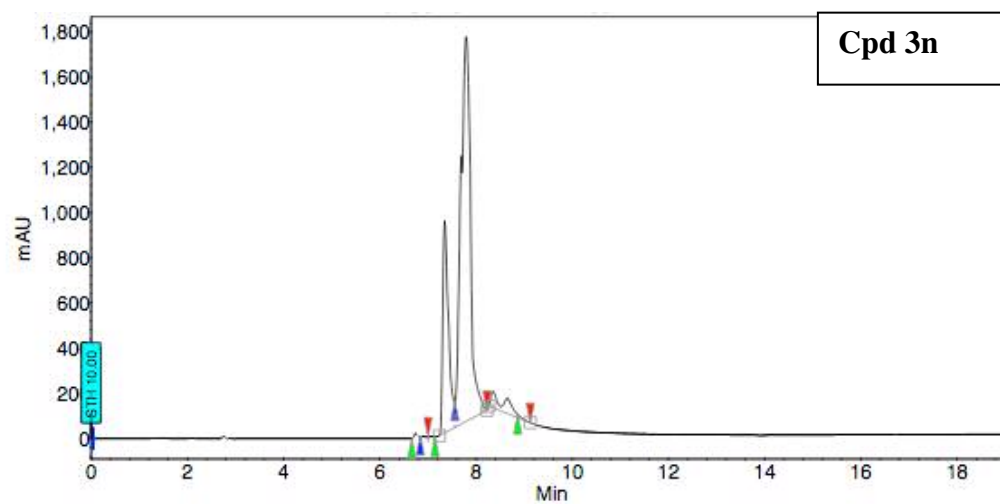
Index	Name	Time (Min)	Quantity (% Area)	Height (mAU)	Area (mAU.Min)	Area % (%)
1	UNKNOWN	6.56	12.55	503.1	100.4	12.545
2	UNKNOWN	7.05	16.81	341.4	134.6	16.807
3	UNKNOWN	7.47	2.42	154.9	19.4	2.420
4	UNKNOWN	7.81	66.18	2840.5	529.8	66.184
5	UNKNOWN	8.73	2.04	109.5	16.4	2.043
Total			100.00	3949.2	800.5	100.000



Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	6.68	85.68	5322.3	1381.2	85.681
2	UNKNOWN	7.40	10.47	1204.0	168.7	10.468
3	UNKNOWN	7.85	3.85	141.8	62.1	3.852
Total			100.00	6668.1	1612.1	100.000



Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	4.59	0.50	71.3	14.4	0.497
2	UNKNOWN	5.53	1.47	200.4	42.5	1.469
3	UNKNOWN	5.95	1.90	235.3	55.0	1.901
4	UNKNOWN	6.85	96.13	8070.8	2781.7	96.134
Total			100.00	8577.8	2893.6	100.000



Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	6.73	1.72	66.1	9.4	1.724
2	UNKNOWN	6.84	0.92	41.1	5.0	0.918
3	UNKNOWN	7.35	23.73	940.1	129.4	23.730
4	UNKNOWN	7.79	73.43	1703.5	400.5	73.426
5	UNKNOWN	8.87	0.20	13.1	1.1	0.202
Total			100.00	2763.9	545.5	100.000