

Information Subset	Mean chemical shift/ppm	Validity value	Concentration/ (mmol/l)
A	1.174	0.90	1.1
B	1.310	0.95	4.2
C	2.132	0.97	3.5
D	2.198	0.91	2.1
E	2.330	0.85	1.6
F	2.513	0.76	0.4
G	2.767	0.78	8.5
H	3.096	0.93	4.2
I	3.105	0.95	1.5
J	3.222	0.97	3.6
K	3.378	0.91	5.1

FIG 1