

Supporting information : Small chemical causes, drastic structural effects : the case of calcium glutarate

Table 1: Fractional atomic coordinates for BioMIL-2

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
Ca	-0.1171 (3)	0.20243 (8)	0.4140 (4)	0.0060 (4)
O1	-0.1536 (8)	0.1648 (3)	0.8015 (7)	0.0120 (4)
O2	0.2783 (6)	-0.1811 (3)	0.9551 (9)	0.0120 (4)
O3	-0.0395 (5)	-0.1847 (3)	0.8915 (14)	0.0120 (4)
O4	-0.0329 (6)	0.2753 (3)	0.0998 (10)	0.0120 (4)
O5	-0.1182 (8)	0.1077 (3)	0.1273 (8)	0.0120 (4)
C1	0.1195 (14)	-0.1480 (4)	0.8966 (17)	0.0167 (4)
C2	0.1250 (15)	-0.0699 (4)	0.7807 (14)	0.0167 (4)
C3	-0.0005 (12)	-0.0249 (4)	0.9239 (13)	0.0167 (4)
C4	0.0042 (14)	0.0443 (4)	0.7932 (12)	0.0167 (4)
C5	-0.0940 (13)	0.1098 (4)	0.9170 (15)	0.0167 (4)

Table 2: Fractional atomic coordinates for bioMIL-2ht

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
Ca	0.6063(2)	0.01536(3)	1.00168(5)	0.0157(4)
O1	0.61447(5)	-0.03613(5)	0.75749(2)	0.0217(3)
O2	0.53125(2)	0.06483(6)	0.91358(5)	0.0308(5)
O3	0.69664(7)	0.11466(1)	0.86398(3)	0.0261(5)
O4	0.63936(2)	0.08696(4)	1.22311(1)	0.0352(3)
C1	0.51444(3)	0.09672(4)	0.80966(2)	0.0204(6)
C3	0.57472(4)	-0.09979(2)	0.69476(5)	0.0181(3)
C4	0.52104(1)	-0.16407(6)	0.79481(5)	0.0303(7)
C5	0.5702(1)	0.14771(3)	0.6919(2)	0.0224(5)
C6	0.56857(4)	-0.18454(6)	0.9052(4)	0.0288(8)

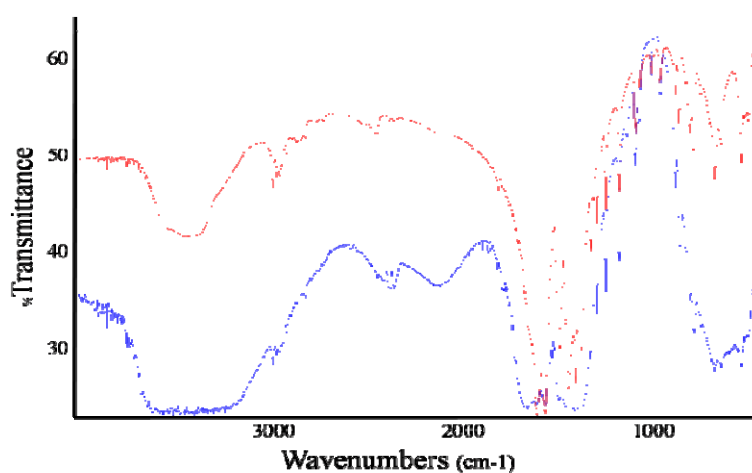


Figure 1: IR spectra for BioMIL-2 (blue) and BioMIL-2ht (red)