

FIGURE 1

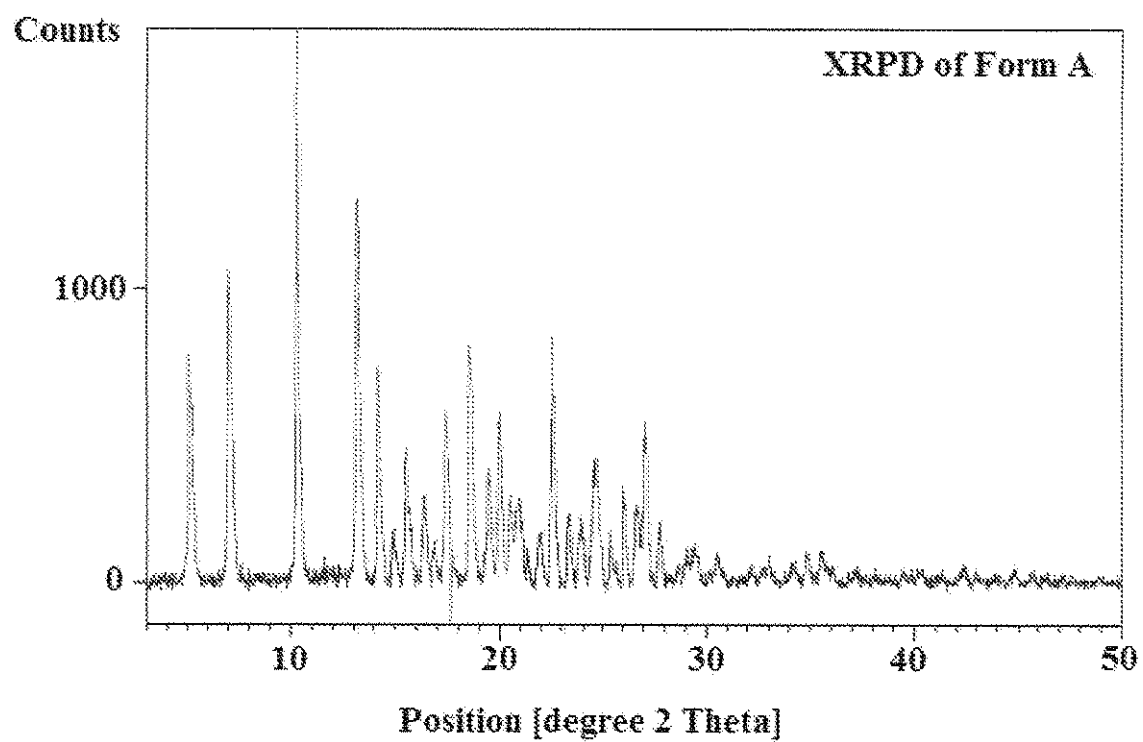
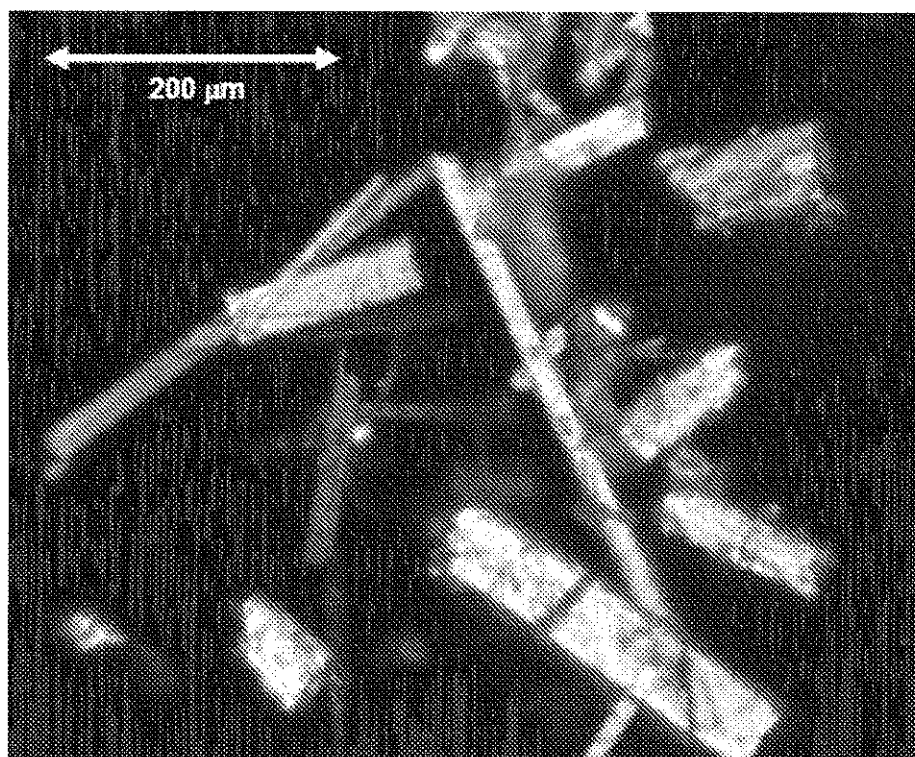
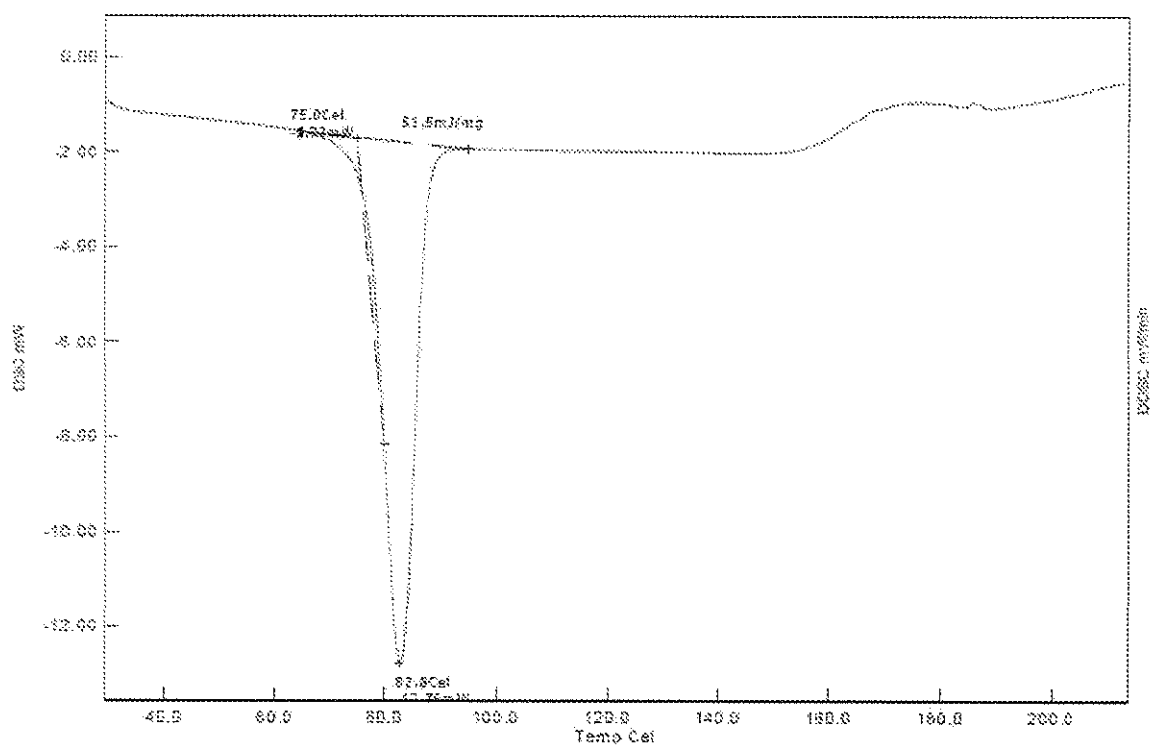


FIGURE 2



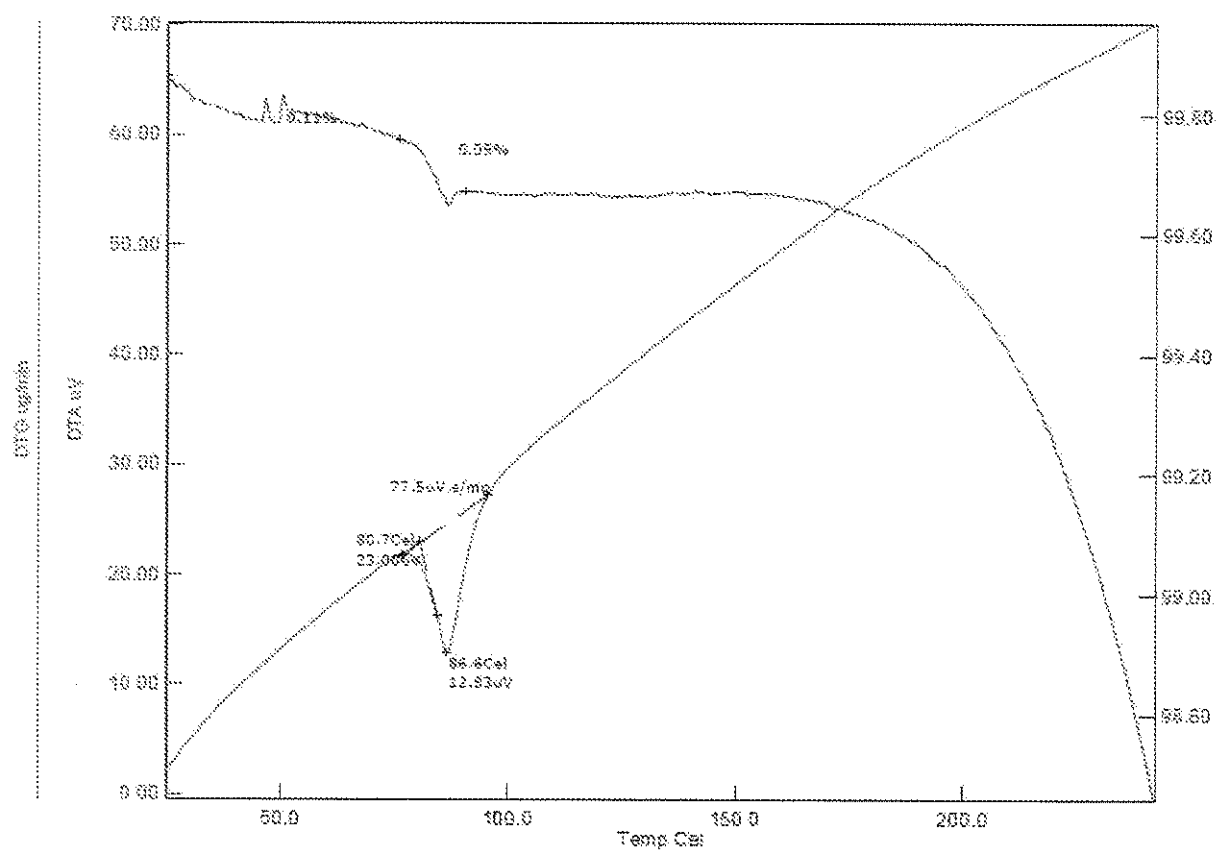
Form A

FIGURE 3



DSC of Form A

FIGURE 4



TG/DTA of Form A

FIGURE 5

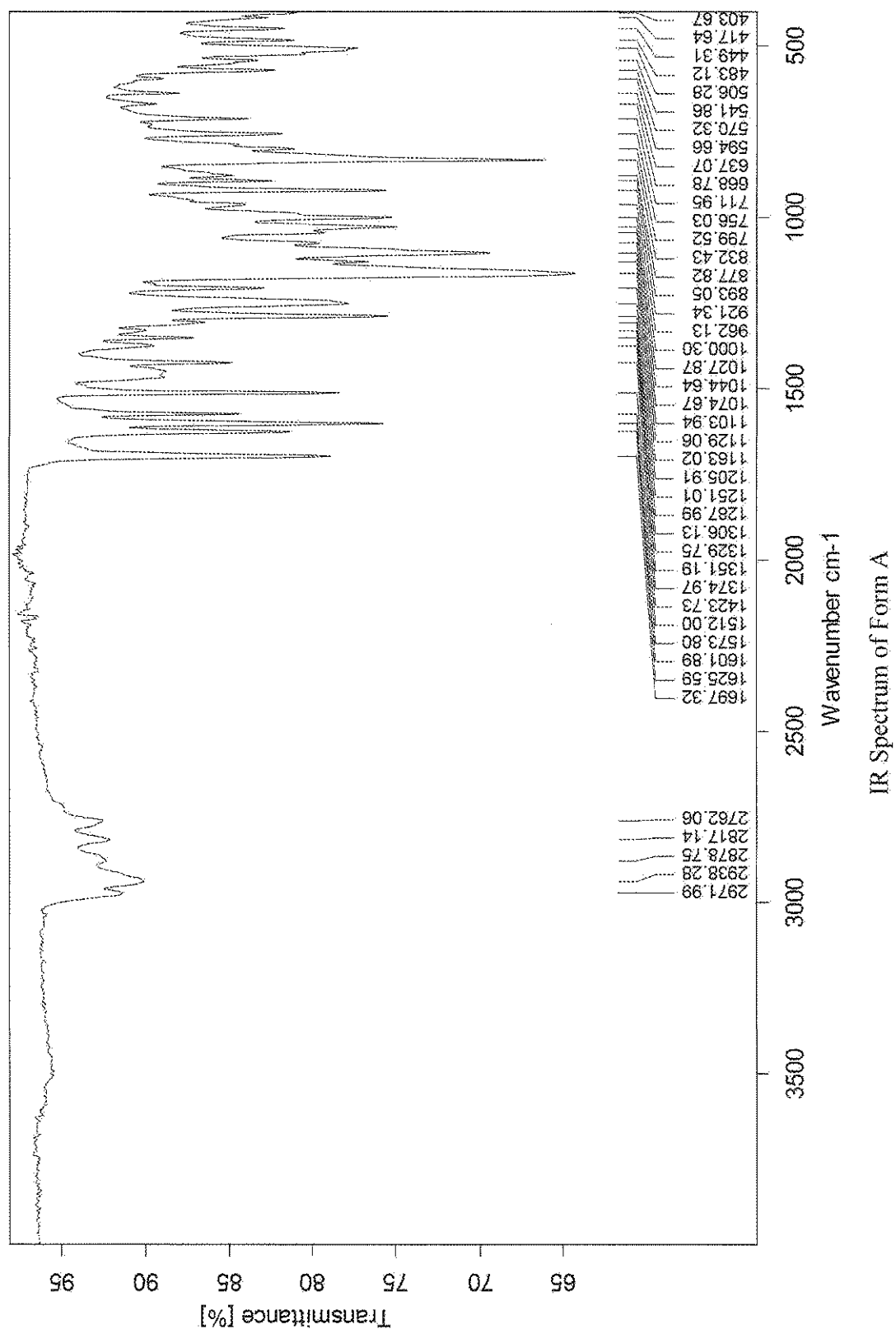


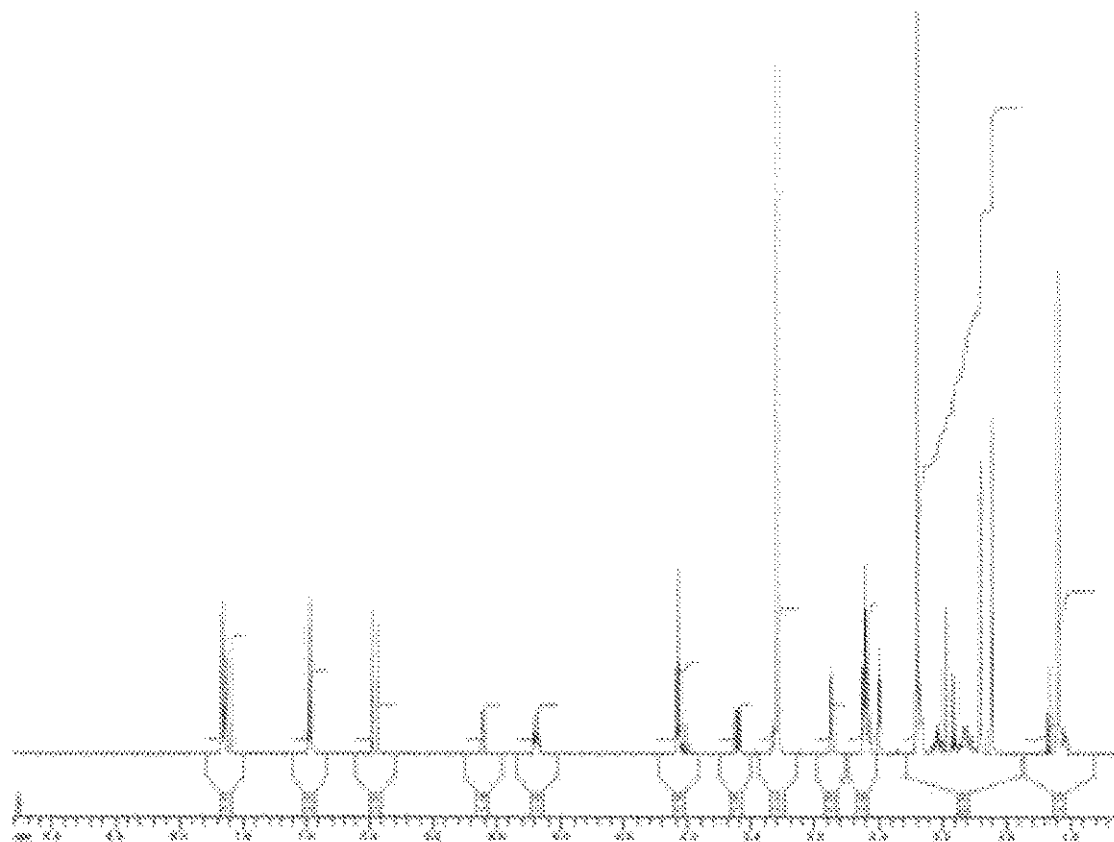
FIGURE 6 ^1H NMR Spectrum of Form A

FIGURE 7

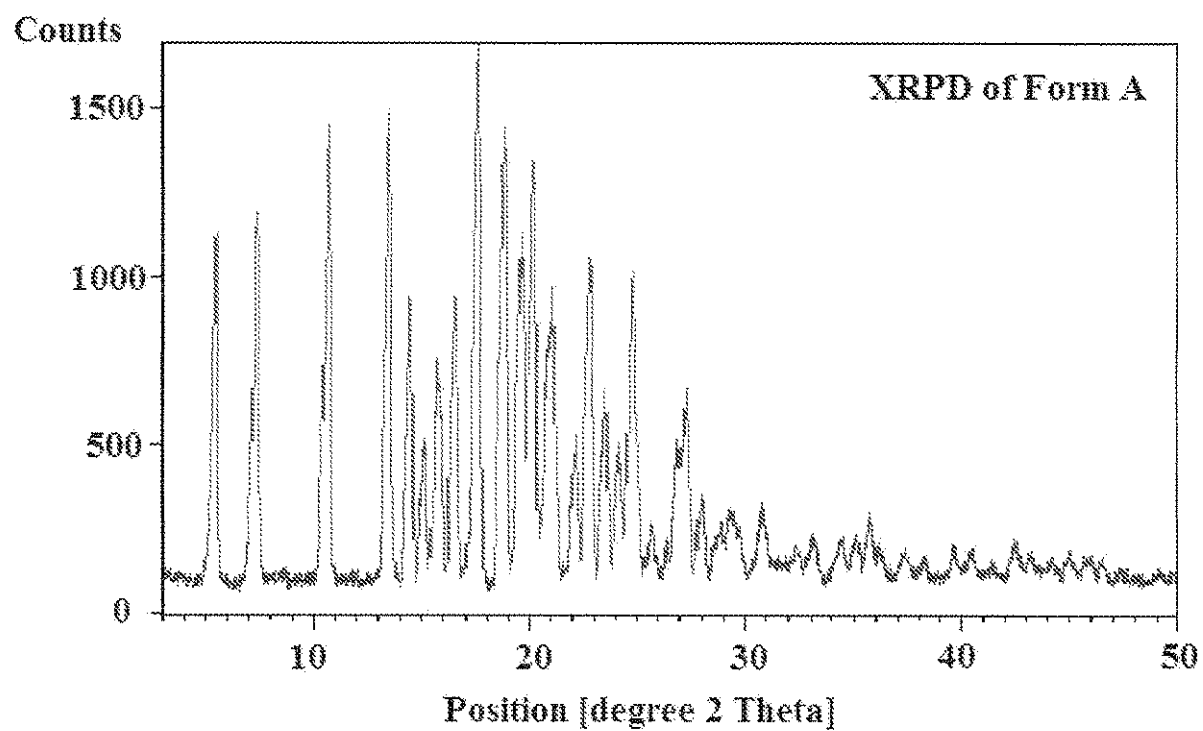


FIGURE 8

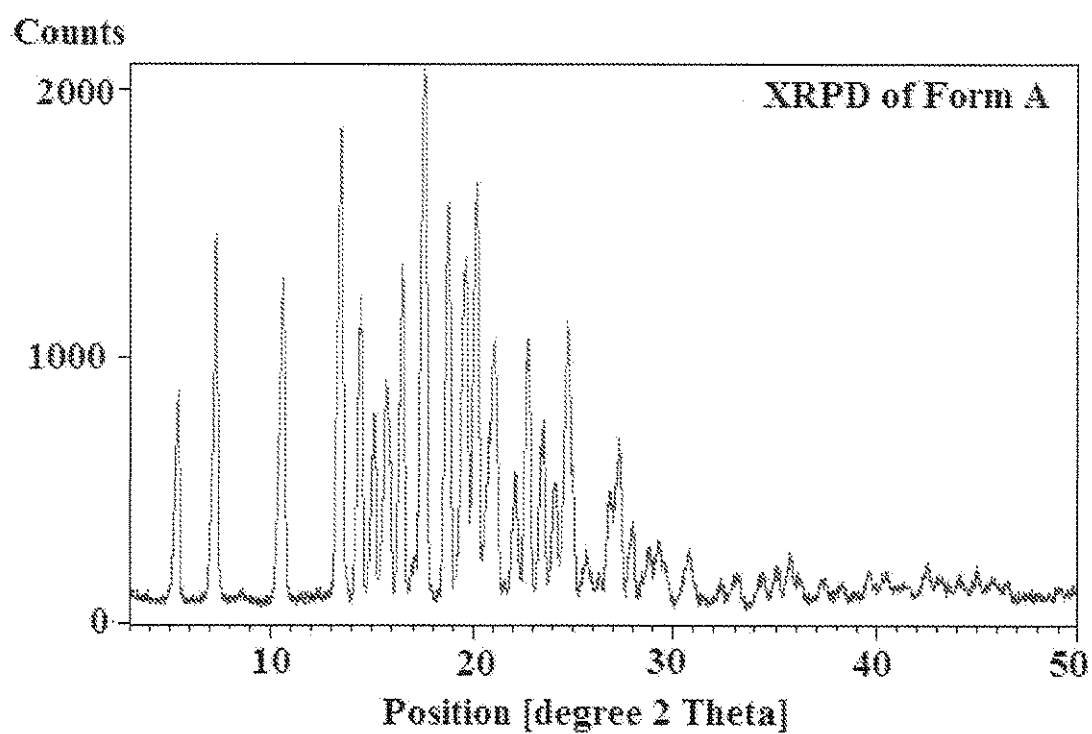


FIGURE 9

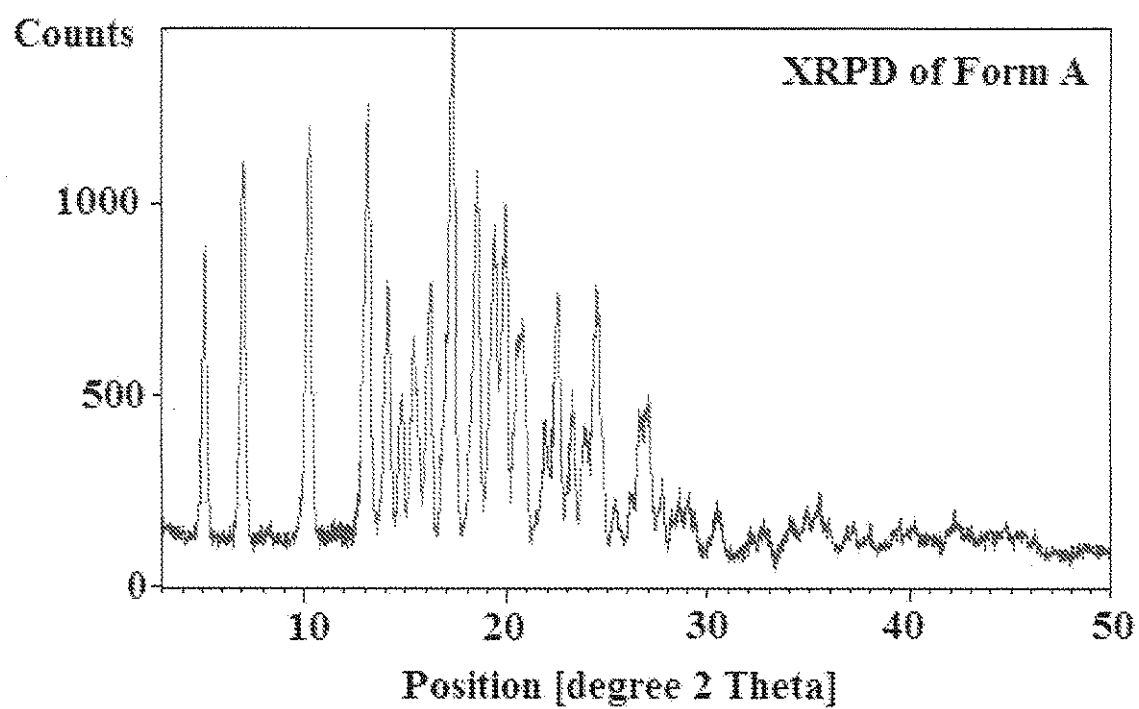
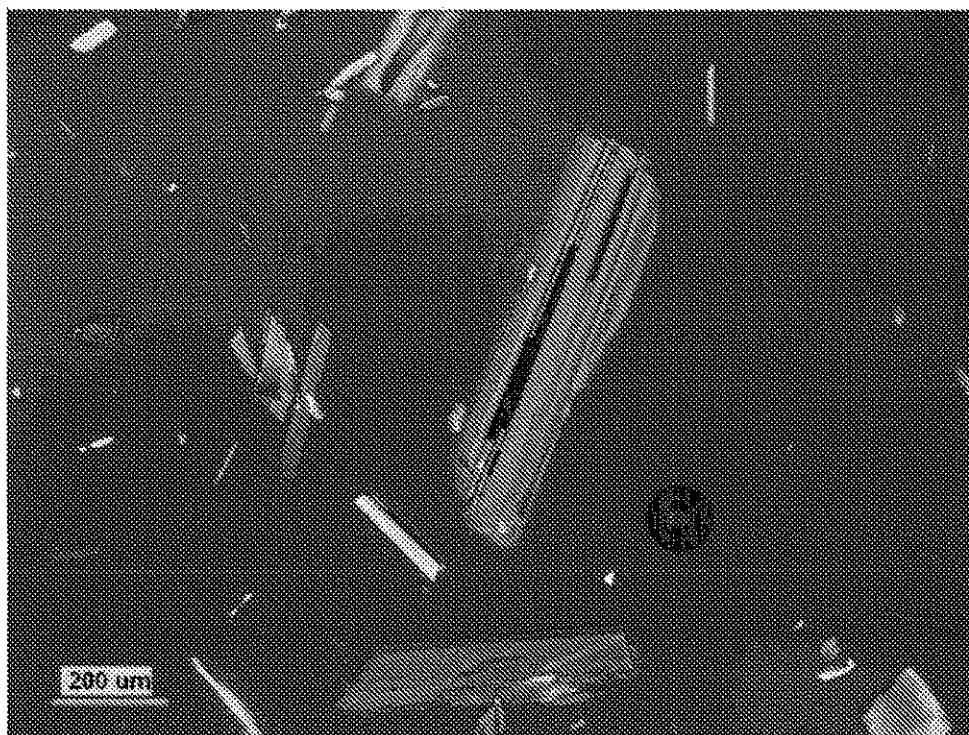


FIGURE 10



Form A

FIGURE 11

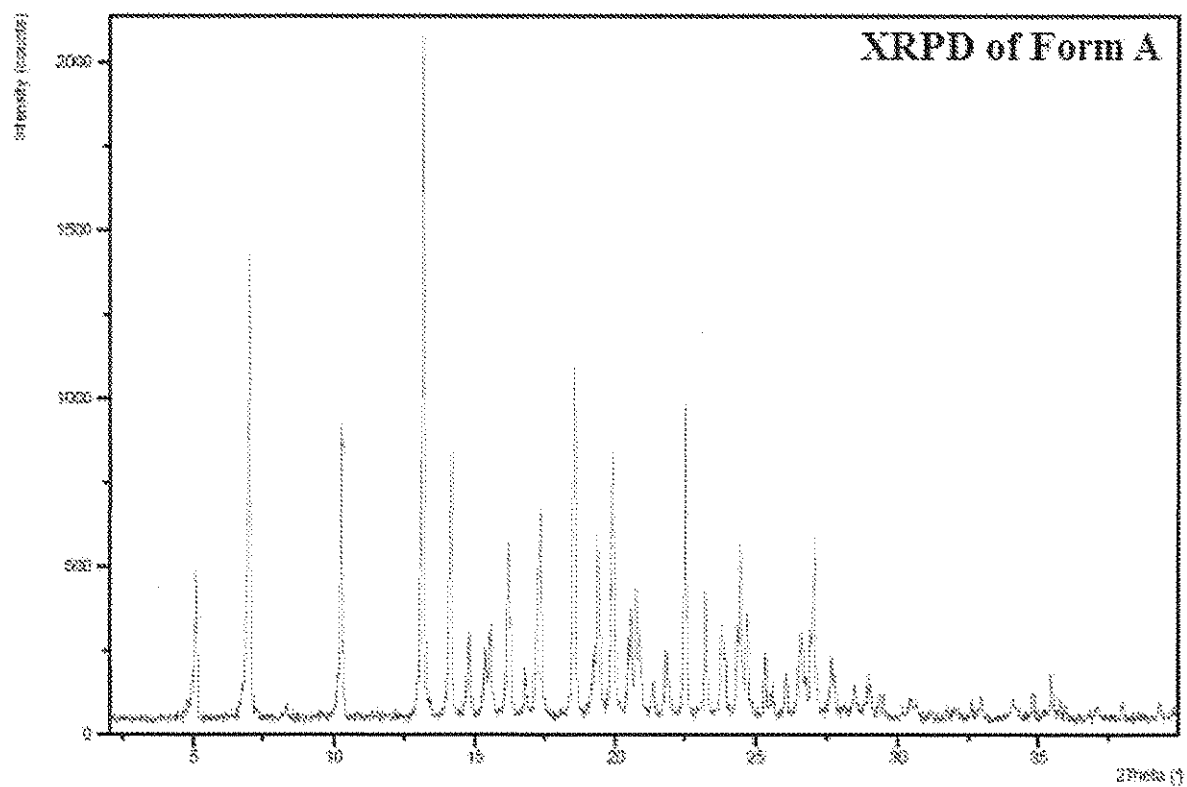




FIGURE 12C

Atomic coordinates:

Atom	x	y	z	U _{iso} /equiv
C1	-0.1127(18)	1.1185(7)	1.1007(2)	0.094(3)
C2	-0.3725(17)	1.2183(9)	1.0646(4)	0.136(5)
N1	-0.1933(13)	1.1504(5)	1.06128(19)	0.092(2)
C3	-0.2113(16)	1.0738(7)	1.0352(2)	0.060(2)
C4	0.0287(14)	1.0412(6)	1.02090(16)	0.089(3)
N1'	-0.1933(13)	1.1504(5)	1.06128(19)	0.092(2)
C3'	-0.086(4)	1.1506(17)	1.0236(5)	0.060(2)
C4'	0.0287(14)	1.0412(6)	1.02090(16)	0.089(3)
O1	-0.0318(7)	0.9727(4)	0.99048(9)	0.0640(12)
C5	0.1200(8)	0.9063(4)	0.97610(12)	0.0402(10)
C6	0.0536(8)	0.8492(4)	0.94357(12)	0.0376(9)
C7	0.1931(7)	0.7804(3)	0.92688(11)	0.0328(8)
C8	0.4015(7)	0.7685(3)	0.94139(10)	0.0295(8)
C9	0.4625(7)	0.8252(3)	0.97435(10)	0.0316(8)
C10	0.3234(8)	0.8950(3)	0.99168(11)	0.0347(9)
C11	0.5571(7)	0.7016(3)	0.92295(12)	0.0343(9)
C12	0.5384(8)	0.6466(3)	0.88989(12)	0.0357(9)
O2	0.8898(7)	0.5771(3)	0.89201(10)	0.0578(11)
C13	0.7224(8)	0.5875(4)	0.87535(12)	0.0395(10)
O3	0.6792(5)	0.5470(2)	0.83956(7)	0.0330(6)
C14	0.8585(7)	0.4973(3)	0.81960(11)	0.0322(8)
C15	0.7599(6)	0.4229(3)	0.78977(10)	0.0265(7)
O4	0.6306(5)	0.3479(2)	0.80816(8)	0.0315(6)
C16	0.6204(6)	0.4779(3)	0.75913(10)	0.0244(7)
C17	0.7485(6)	0.5638(3)	0.73992(11)	0.0277(7)
O5	0.8823(5)	0.5355(2)	0.70669(8)	0.0328(6)
C18	0.8583(7)	0.6342(3)	0.76912(12)	0.0343(8)
C19	0.9929(7)	0.5762(3)	0.79856(12)	0.0360(9)
C20	0.7511(9)	0.2702(3)	0.82708(15)	0.0450(11)
C21	0.7026(7)	0.6041(3)	0.70070(12)	0.0352(9)
C22	0.5198(6)	0.4023(3)	0.73014(10)	0.0244(7)
O6	0.3053(4)	0.3699(2)	0.74204(8)	0.0286(6)
C23	0.6613(7)	0.3168(3)	0.71524(11)	0.0304(8)
C24	0.3266(6)	0.4348(3)	0.70809(10)	0.0263(7)
C25	0.2617(7)	0.3923(3)	0.66842(11)	0.0319(8)
C26	0.3771(7)	0.4465(3)	0.63557(11)	0.0338(8)
C27	0.3002(7)	0.5187(3)	0.61231(11)	0.0353(9)
C28	0.0725(8)	0.5565(4)	0.61362(13)	0.0421(11)
C29	0.4372(9)	0.5661(4)	0.58149(12)	0.0467(12)
H1A	-0.1046	1.178	1.1181	0.14
H1B	0.0304	1.0883	1.0979	0.14
H1C	-0.2107	1.068	1.1121	0.14
H2A	-0.3422	1.2698	1.0849	0.204
H2B	-0.5006	1.1796	1.0721	0.204
H2C	-0.3972	1.252	1.0392	0.204
H3A	-0.2975	1.096	1.0122	0.072

H3B	-0.2842	1.0149	1.0476	0.072
H4A	0.1114	1.0999	1.0107	0.107
H4B	0.1106	1.0069	1.0421	0.107
H3'1	0.0207	1.2062	1.0222	0.072
H3'2	-0.1909	1.1593	1.0019	0.072
H4'1	0.1849	1.0532	1.0184	0.107
H4'2	0.0055	1.0061	1.0464	0.107
H6	-0.0866	0.8577	0.9331	0.045
H7	0.1471	0.7403	0.9051	0.039
H9	0.6018	0.816	0.9852	0.038
H10	0.3675	0.9341	1.0138	0.042
H11	0.691	0.6961	0.9362	0.041
H12	0.4065	0.6457	0.8758	0.043
H14	0.9482	0.4593	0.8392	0.039
H15	0.8793	0.3876	0.7755	0.032
H16	0.4996	0.5106	0.7739	0.029
H18A	0.9508	0.6827	0.7546	0.041
H18B	0.7482	0.6742	0.7834	0.041
H19A	1.0541	0.6243	0.8181	0.043
H19B	1.1132	0.5423	0.7847	0.043
H20A	0.653	0.2208	0.8391	0.067
H20B	0.8419	0.3005	0.8476	0.067
H20C	0.8416	0.2355	0.8076	0.067
H21A	0.5752	0.5772	0.6867	0.042
H21B	0.7346	0.6768	0.6957	0.042
H23A	0.7807	0.3064	0.7336	0.046
H23B	0.718	0.3346	0.6891	0.046
H23C	0.5769	0.2539	0.7133	0.046
H24	0.2834	0.5073	0.7126	0.032
H25A	0.2958	0.3186	0.6674	0.038
H25B	0.1049	0.4002	0.6649	0.038
H26	0.5215	0.4265	0.631	0.041
H28A	0.0527	0.6098	0.5937	0.063
H28B	0.042	0.5845	0.6399	0.063
H28C	-0.0256	0.4998	0.6082	0.063
H29A	0.3541	0.6175	0.5671	0.07
H29B	0.4864	0.5134	0.563	0.07
H29C	0.5616	0.5985	0.594	0.07

Anisotropic displacement parameters:

Atom	u^{11}	u^{22}	u^{33}	u^{12}	u^{13}	u^{23}
C1	0.122(7)	0.090(5)	0.069(4)	0.010(6)	0.001(5)	-0.012(4)
C2	0.085(7)	0.138(8)	0.184(11)	0.054(7)	-0.004(7)	-0.070(8)
N1	0.112(6)	0.077(4)	0.086(4)	0.053(4)	0.038(4)	0.010(3)
C3	0.066(5)	0.071(5)	0.043(3)	0.027(4)	-0.015(3)	-0.023(3)
C4	0.125(6)	0.106(5)	0.037(2)	0.085(5)	-0.022(3)	-0.032(3)
N1'	0.112(6)	0.077(4)	0.086(4)	0.053(4)	0.038(4)	0.010(3)
C3'	0.066(5)	0.071(5)	0.043(3)	0.027(4)	-0.015(3)	-0.023(3)
C4'	0.125(6)	0.106(5)	0.037(2)	0.085(5)	-0.022(3)	-0.032(3)

O1	0.061(2)	0.099(3)	0.0319(15)	0.046(2)	-0.0023(16)	-0.0104(18)
C5	0.047(3)	0.049(2)	0.0251(16)	0.013(2)	0.0076(18)	0.0025(16)
C6	0.033(2)	0.052(2)	0.0282(17)	0.003(2)	0.0048(16)	0.0066(17)
C7	0.037(2)	0.0367(19)	0.0251(16)	-0.0071(18)	-0.0005(15)	0.0001(15)
C8	0.034(2)	0.0314(18)	0.0230(15)	-0.0049(16)	0.0025(15)	-0.0031(14)
C9	0.034(2)	0.0379(19)	0.0234(15)	-0.0032(17)	0.0010(15)	-0.0043(15)
C10	0.041(2)	0.040(2)	0.0231(15)	0.0066(19)	0.0024(16)	-0.0031(15)
C11	0.036(2)	0.036(2)	0.0307(18)	-0.0010(18)	0.0003(16)	-0.0057(15)
C12	0.036(2)	0.040(2)	0.0312(18)	-0.0021(19)	-0.0014(17)	-0.0096(16)
O2	0.049(2)	0.076(2)	0.0479(18)	0.017(2)	-0.0205(17)	-0.0357(18)
C13	0.042(2)	0.043(2)	0.035(2)	-0.002(2)	-0.0025(18)	-0.0178(17)
O3	0.0317(14)	0.0404(14)	0.0270(12)	0.0019(13)	-0.0009(12)	-0.0114(11)
C14	0.030(2)	0.0346(18)	0.0321(17)	0.0033(17)	-0.0020(16)	-0.0124(15)
C15	0.0225(17)	0.0301(17)	0.0270(16)	0.0051(15)	-0.0022(14)	-0.0062(13)
O4	0.0359(15)	0.0277(12)	0.0309(12)	0.0040(12)	-0.0059(12)	0.0007(10)
C16	0.0220(16)	0.0238(15)	0.0274(15)	0.0017(14)	-0.0017(13)	-0.0055(13)
C17	0.0235(17)	0.0260(16)	0.0335(17)	0.0034(15)	0.0028(15)	-0.0065(14)
O5	0.0279(13)	0.0406(15)	0.0299(12)	0.0069(13)	0.0035(11)	-0.0020(11)
C18	0.031(2)	0.0310(18)	0.041(2)	-0.0042(17)	0.0030(17)	-0.0109(16)
C19	0.029(2)	0.042(2)	0.0371(19)	-0.0030(18)	-0.0038(17)	-0.0141(17)
C20	0.054(3)	0.032(2)	0.049(2)	0.009(2)	-0.015(2)	0.0018(19)
C21	0.029(2)	0.0306(18)	0.046(2)	0.0002(17)	-0.0042(17)	0.0026(16)
C22	0.0218(17)	0.0267(16)	0.0247(15)	0.0029(14)	0.0012(13)	-0.0038(13)
O6	0.0240(13)	0.0326(13)	0.0293(12)	-0.0030(11)	0.0013(10)	-0.0025(10)
C23	0.031(2)	0.0294(17)	0.0311(17)	0.0065(16)	-0.0016(15)	-0.0122(14)
C24	0.0231(17)	0.0296(17)	0.0263(15)	-0.0011(15)	-0.0001(14)	-0.0036(13)
C25	0.028(2)	0.0386(19)	0.0289(17)	0.0009(17)	-0.0056(15)	-0.0053(15)
C26	0.0281(19)	0.045(2)	0.0281(17)	-0.0012(18)	-0.0024(15)	-0.0081(16)
C27	0.038(2)	0.042(2)	0.0259(16)	-0.0026(19)	-0.0048(16)	-0.0090(16)
C28	0.047(3)	0.044(2)	0.035(2)	0.009(2)	-0.0111(19)	-0.0067(18)
C29	0.060(3)	0.052(3)	0.0278(18)	-0.009(2)	-0.002(2)	-0.0013(18)

Bond lengths:

C1-N1	1.487(10)	C15-H15	1
C1-H1A	0.98	O4-C20	1.420(5)
C1-H1B	0.98	C16-C17	1.527(5)
C1-H1C	0.98	C16-C22	1.529(5)
C2-N1	1.433(10)	C16-H16	1
C2-H2A	0.98	C17-O5	1.449(4)
C2-H2B	0.98	C17-C21	1.457(5)
C2-H2C	0.98	C17-C18	1.516(5)
N1-C3	1.344(10)	O5-C21	1.451(5)
C3-C4	1.629(12)	C18-C19	1.509(6)
C3-H3A	0.99	C18-H18A	0.99
C3-H3B	0.99	C18-H18B	0.99
C4-O1	1.418(7)	C19-H19A	0.99
C4-H4A	0.99	C19-H19B	0.99
C4-H4B	0.99	C20-H20A	0.98
C3'-H3'1	0.99	C20-H20B	0.98

C3'-H3'2	0.99	C20-H20C	0.98
O1-C5	1.375(6)	C21-H21A	0.99
C5-C10	1.382(7)	C21-H21B	0.99
C5-C6	1.395(6)	C22-O6	1.460(5)
C6-C7	1.375(6)	C22-C24	1.479(5)
C6-H6	0.95	C22-C23	1.514(5)
C7-C8	1.397(6)	O6-C24	1.436(4)
C7-H7	0.95	C23-H23A	0.98
C8-C9	1.394(5)	C23-H23B	0.98
C8-C11	1.450(6)	C23-H23C	0.98
C9-C10	1.390(6)	C24-C25	1.509(5)
C9-H9	0.95	C24-H24	1
C10-H10	0.95	C25-C26	1.503(6)
C11-C12	1.337(5)	C25-H25A	0.99
C11-H11	0.95	C25-H25B	0.99
C12-C13	1.470(6)	C26-C27	1.322(6)
C12-H12	0.95	C26-H26	0.95
O2-C13	1.194(6)	C27-C29	1.484(6)
C13-O3	1.350(5)	C27-C28	1.504(7)
O3-C14	1.459(5)	C28-H28A	0.98
C14-C19	1.511(6)	C28-H28B	0.98
C14-C15	1.533(5)	C28-H28C	0.98
C14-H14	1	C29-H29A	0.98
C15-O4	1.415(5)	C29-H29B	0.98
C15-C16	1.534(5)	C29-H29C	0.98

Bond angles:

N1-C1-H1A	109.5	C15-C16-H16	106.9
N1-C1-H1B	109.5	O5-C17-C21	59.9(2)
H1A-C1-H1B	109.5	O5-C17-C18	113.7(3)
N1-C1-H1C	109.5	C21-C17-C18	117.5(3)
H1A-C1-H1C	109.5	O5-C17-C16	116.3(3)
H1B-C1-H1C	109.5	C21-C17-C16	123.6(3)
N1-C2-H2A	109.5	C18-C17-C16	114.1(3)
N1-C2-H2B	109.5	C17-O5-C21	60.3(2)
H2A-C2-H2B	109.5	C19-C18-C17	112.0(3)
N1-C2-H2C	109.5	C19-C18-H18A	109.2
H2A-C2-H2C	109.5	C17-C18-H18A	109.2
H2B-C2-H2C	109.5	C19-C18-H18B	109.2
C3-N1-C2	116.9(8)	C17-C18-H18B	109.2
C3-N1-C1	114.1(6)	H18A-C18-H18B	107.9
C2-N1-C1	111.6(7)	C18-C19-C14	110.4(4)
N1-C3-C4	108.3(7)	C18-C19-H19A	109.6
N1-C3-H3A	110	C14-C19-H19A	109.6
C4-C3-H3A	110	C18-C19-H19B	109.6
N1-C3-H3B	110	C14-C19-H19B	109.6
C4-C3-H3B	110	H19A-C19-H19B	108.1
H3A-C3-H3B	108.4	O4-C20-H20A	109.5
O1-C4-C3	97.9(6)	O4-C20-H20B	109.5

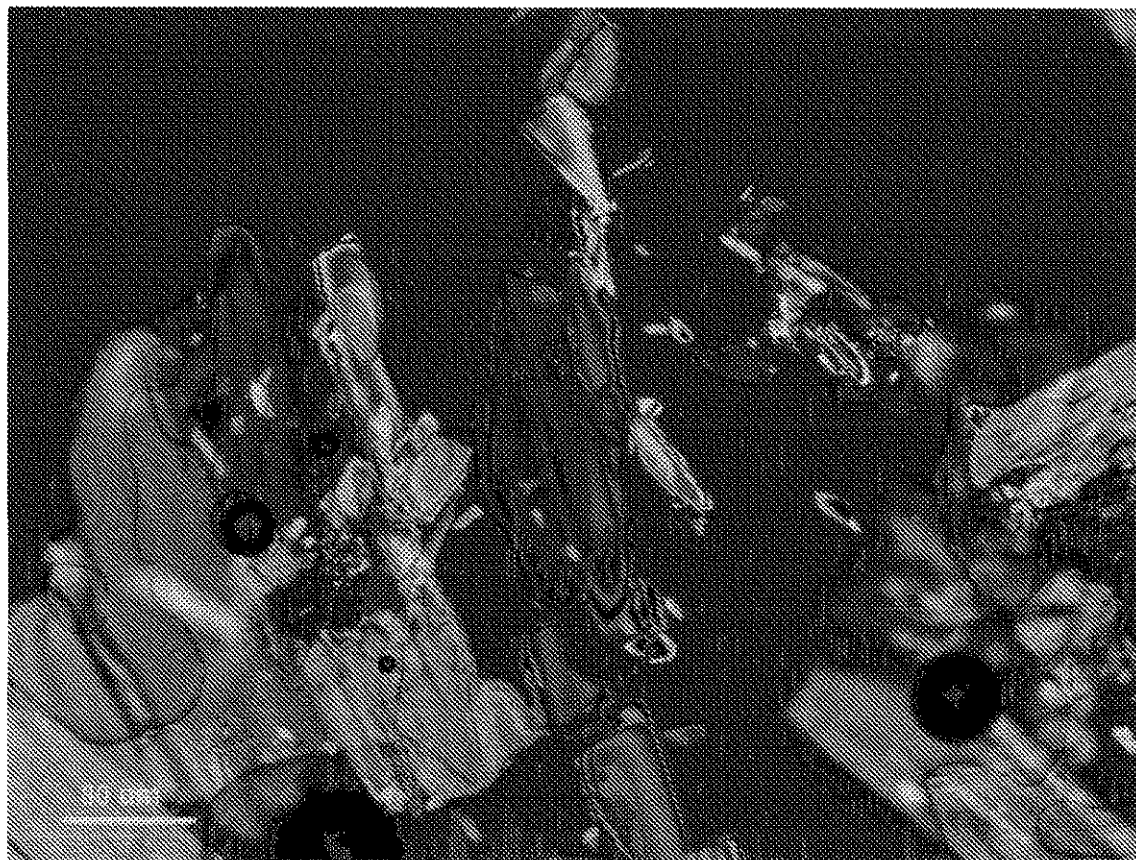
O1-C4-H4A	112.2	H20A-C20-H20B	109.5
C3-C4-H4A	112.2	O4-C20-H20C	109.5
O1-C4-H4B	112.2	H20A-C20-H20C	109.5
C3-C4-H4B	112.2	H20B-C20-H20C	109.5
H4A-C4-H4B	109.8	O5-C21-C17	59.8(2)
H3'1-C3'-H3'2	108.9	O5-C21-H21A	117.8
C5-O1-C4	118.4(5)	C17-C21-H21A	117.8
O1-C5-C10	124.4(4)	O5-C21-H21B	117.8
O1-C5-C6	114.6(4)	C17-C21-H21B	117.8
C10-C5-C6	121.0(4)	H21A-C21-H21B	114.9
C7-C6-C5	119.3(4)	O6-C22-C24	58.5(2)
C7-C6-H6	120.3	O6-C22-C23	114.2(3)
C5-C6-H6	120.3	C24-C22-C23	121.3(3)
C6-C7-C8	121.1(4)	O6-C22-C16	112.8(3)
C6-C7-H7	119.4	C24-C22-C16	118.1(3)
C8-C7-H7	119.4	C23-C22-C16	117.1(3)
C9-C8-C7	118.4(4)	C24-O6-C22	61.4(2)
C9-C8-C11	119.0(4)	C22-C23-H23A	109.5
C7-C8-C11	122.6(4)	C22-C23-H23B	109.5
C10-C9-C8	121.3(4)	H23A-C23-H23B	109.5
C10-C9-H9	119.4	C22-C23-H23C	109.5
C8-C9-H9	119.4	H23A-C23-H23C	109.5
C5-C10-C9	118.8(4)	H23B-C23-H23C	109.5
C5-C10-H10	120.6	O6-C24-C22	60.1(2)
C9-C10-H10	120.6	O6-C24-C25	117.9(3)
C12-C11-C8	129.0(4)	C22-C24-C25	124.1(3)
C12-C11-H11	115.5	O6-C24-H24	114.5
C8-C11-H11	115.5	C22-C24-H24	114.5
C11-C12-C13	119.8(4)	C25-C24-H24	114.5
C11-C12-H12	120.1	C26-C25-C24	110.8(3)
C13-C12-H12	120.1	C26-C25-H25A	109.5
O2-C13-O3	123.6(4)	C24-C25-H25A	109.5
O2-C13-C12	125.8(4)	C26-C25-H25B	109.5
O3-C13-C12	110.6(4)	C24-C25-H25B	109.5
C13-O3-C14	116.0(3)	H25A-C25-H25B	108.1
O3-C14-C19	109.7(3)	C27-C26-C25	127.3(4)
O3-C14-C15	106.4(3)	C27-C26-H26	116.3
C19-C14-C15	110.4(3)	C25-C26-H26	116.3
O3-C14-H14	110.1	C26-C27-C29	120.7(4)
C19-C14-H14	110.1	C26-C27-C28	124.1(4)
C15-C14-H14	110.1	C29-C27-C28	115.2(4)
O4-C15-C14	112.4(3)	C27-C28-H28A	109.5
O4-C15-C16	107.5(3)	C27-C28-H28B	109.5
C14-C15-C16	111.9(3)	H28A-C28-H28B	109.5
O4-C15-H15	108.3	C27-C28-H28C	109.5
C14-C15-H15	108.3	H28A-C28-H28C	109.5
C16-C15-H15	108.3	H28B-C28-H28C	109.5
C15-O4-C20	113.4(3)	C27-C29-H29A	109.5
C17-C16-C22	114.8(3)	C27-C29-H29B	109.5
C17-C16-C15	109.8(3)	H29A-C29-H29B	109.5

C22-C16-C15	111.2(3)	C27-C29-H29C	109.5
C17-C16-H16	106.9	H29A-C29-H29C	109.5
C22-C16-H16	106.9	H29B-C29-H29C	109.5

Torsion angles:

C2-N1-C3-C4	153.9(8)	C22-C16-C17-O5	-41.0(4)
C1-N1-C3-C4	-73.5(10)	C15-C16-C17-O5	85.1(4)
N1-C3-C4-O1	-172.1(6)	C22-C16-C17-C21	28.9(5)
C3-C4-O1-C5	-164.0(5)	C15-C16-C17-C21	155.0(3)
C4-O1-C5-C10	6.2(8)	C22-C16-C17-C18	-176.4(3)
C4-O1-C5-C6	-173.7(5)	C15-C16-C17-C18	-50.3(4)
O1-C5-C6-C7	-180.0(4)	C18-C17-O5-C21	-109.2(4)
C10-C5-C6-C7	0.1(7)	C16-C17-O5-C21	115.2(4)
C5-C6-C7-C8	-1.4(6)	O5-C17-C18-C19	-84.1(4)
C6-C7-C8-C9	2.5(6)	C21-C17-C18-C19	-151.2(4)
C6-C7-C8-C11	-175.9(4)	C16-C17-C18-C19	52.5(5)
C7-C8-C9-C10	-2.4(6)	C17-C18-C19-C14	-55.6(4)
C11-C8-C9-C10	176.1(4)	O3-C14-C19-C18	-58.4(4)
O1-C5-C10-C9	-179.9(4)	C15-C14-C19-C18	58.6(4)
C6-C5-C10-C9	0.0(7)	C18-C17-C21-O5	102.9(4)
C8-C9-C10-C5	1.1(6)	C16-C17-C21-O5	-103.2(4)
C9-C8-C11-C12	-174.7(4)	C17-C16-C22-O6	-140.9(3)
C7-C8-C11-C12	3.7(7)	C15-C16-C22-O6	93.7(4)
C8-C11-C12-C13	176.8(4)	C17-C16-C22-C24	-75.6(4)
C11-C12-C13-O2	5.8(8)	C15-C16-C22-C24	159.0(3)
C11-C12-C13-O3	-173.0(4)	C17-C16-C22-C23	83.6(4)
O2-C13-O3-C14	-6.3(7)	C15-C16-C22-C23	-41.8(4)
C12-C13-O3-C14	172.5(4)	C23-C22-O6-C24	-113.1(3)
C13-O3-C14-C19	-82.9(4)	C16-C22-O6-C24	110.0(3)
C13-O3-C14-C15	157.7(4)	C22-O6-C24-C25	115.3(4)
O3-C14-C15-O4	-60.5(4)	C23-C22-C24-O6	100.9(4)
C19-C14-C15-O4	-179.4(3)	C16-C22-C24-O6	-100.8(3)
O3-C14-C15-C16	60.6(4)	O6-C22-C24-C25	-105.2(4)
C19-C14-C15-C16	-58.3(4)	C23-C22-C24-C25	-4.3(6)
C14-C15-O4-C20	-76.2(4)	C16-C22-C24-C25	153.9(4)
C16-C15-O4-C20	160.2(3)	O6-C24-C25-C26	-155.3(3)
O4-C15-C16-C17	176.9(3)	C22-C24-C25-C26	-84.1(5)
C14-C15-C16-C17	53.0(4)	C24-C25-C26-C27	-101.4(5)
O4-C15-C16-C22	-55.0(4)	C25-C26-C27-C29	178.9(4)
C14-C15-C16-C22	-178.8(3)	C25-C26-C27-C28	-3.3(6)

FIGURE 13



Form C

FIGURE 14

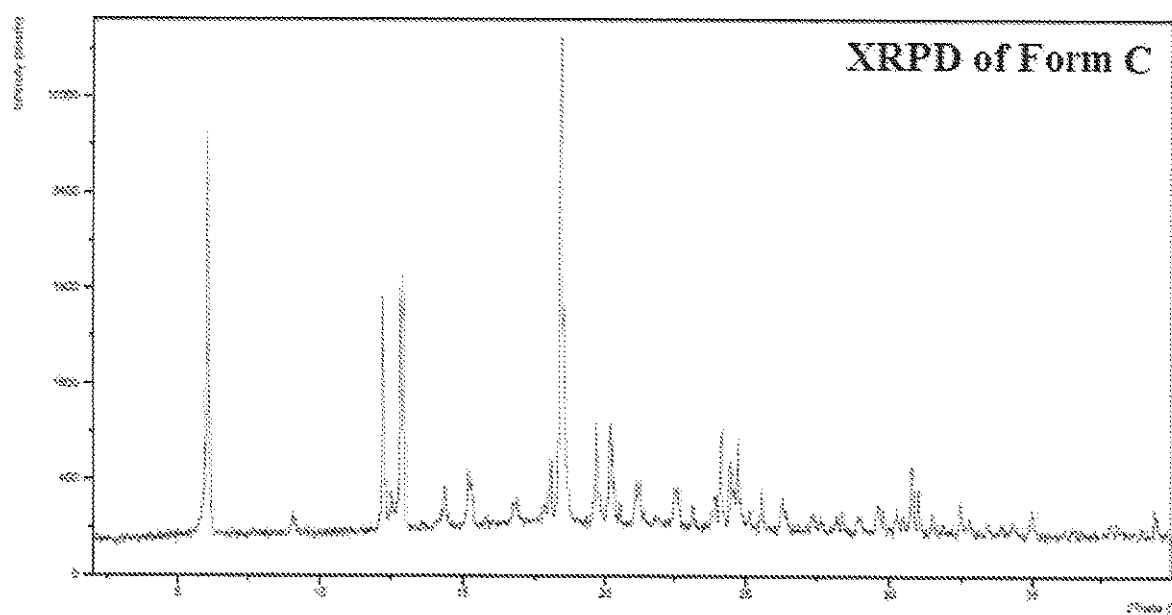


FIGURE 15

