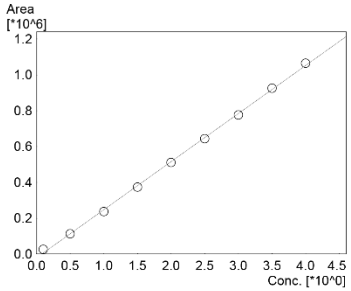
Supplementary material

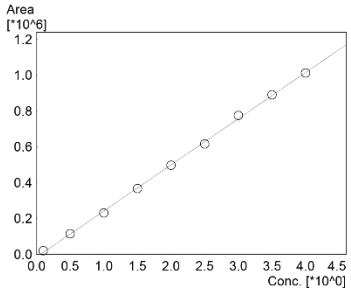
==== Shimadzu LabSolutions Calibration Curve ====

ID# : 1
Name : Cellobiose
Quantitative Method : External Standard
Function : f(x)=268565*x-21427.1
Rr1=0.9995679 Rr2=0.9991360 RSS=9.111441e+008
MeanRF: 2.519031e+005 RFSD: 1.320872e+004 RFRSD: 5.243573
FitType : Linear
ZeroThrough : Not Through
Weighted Regression : None
Detector Name : Detector A



#	Conc.(Ratio)	MeanArea	Area
1	0.1	25489	24967
			25823
			25675
2	0.5	112329	112265
			111229
			113491
3	1	236764	232132
			238099
			240062
4	1.5	373406	383581
			367051
			369587
5	2	510326	514103
			502929
			513947
6	2.5	643751	643159
			652680
			635416
7	3	775679	773794
			771235
			782007

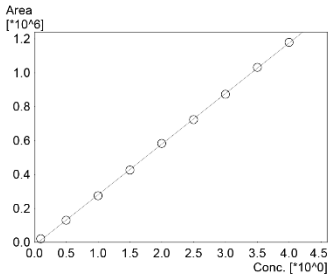
ID# : 2
Name : Glucose
Quantitative Method : External Standard
Function : f(x)=257802*x-15920.0
Rr1=0.9995992 Rr2=0.9991986 RSS=7.787030e+008
MeanRF: 2.409830e+005 RFSD: 1.679015e+004 RFRSD: 6.967357
FitType : Linear
ZeroThrough : Not Through
Weighted Regression : None
Detector Name : Detector A



#	Conc.(Ratio)	MeanArea	Area
1	0.1	20298	20165
			20584
			20143
2	0.5	115031	115194
			114777
			115122
3	1	230378	230763
			229399
			230973
4	1.5	367622	367206
			369811
			365850
5	2	496745	498390
			498027
			493817
6	2.5	615692	609752
			612242
			625082
7	3	775478	784035
			781496
			760901

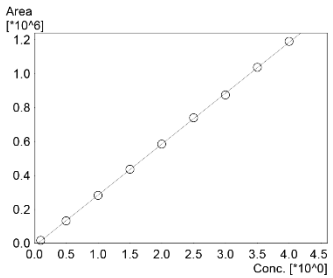
Figure S1 Carbohydrate calibration-1

ID# : 3
Name : Xylose
Quantitative Method : External Standard
Function : f(x)=298393*x-17868.2
Rr1=0.9999107 Rr2=0.9998214 RSS=2.323244e+008
MeanRF: 2.764211e+005 RFSD: 2.683019e+004 RFRSD: 9.706274
FitType : Linear
ZeroThrough : Not Through
Weighted Regression : None
Detector Name : Detector A



#	Conc.(Ratio)	MeanArea	Area
1	0.1	20853	20418
			21296
			20844
2	0.5	129894	128947
			129652
			131084
3	1	274586	272839
			275269
			275650
4	1.5	426150	429225
			424521
			424702
5	2	582703	582481
			579573
			586056
6	2.5	722941	721579
			727010
			720234
7	3	872250	865934
			870240
			880576

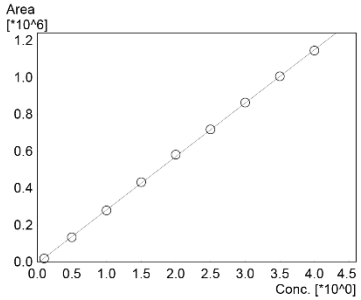
ID# : 4
Name : Galactose
Quantitative Method : External Standard
Function : f(x)=300719*x-16257.2
Rr1=0.9999283 Rr2=0.9998566 RSS=1.894707e+008
MeanRF: 2.758890e+005 RFSD: 3.913491e+004 RFRSD: 14.185020
FitType : Linear
ZeroThrough : Not Through
Weighted Regression : None
Detector Name : Detector A



#	Conc.(Ratio)	MeanArea	Area
1	0.1	17138	16680
			17832
			16900
2	0.5	131777	130898
			131112
			133322
3	1	282468	278245
			285902
			283258
4	1.5	437070	438080
			433120
			440011
5	2	584789	579981
			580876
			593509
6	2.5	740033	741123
			748266
			730711
7	3	874836	863397
			871450
			889660

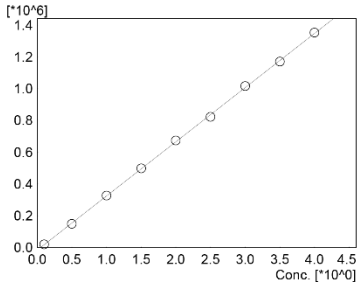
Figure S2 carbohydrate calibration-2

ID# : 5
Name : Arabinose
Quantitative Method : External Standard
Function : f(x)=289664*x-7828.21
Rr1=0.9999285 Rr2=0.9998570 RSS=1.753046e+008
MeanRF: 2.727462e+005 RFSD: 3.304902e+004 RFRSD: 12.117135
FitType : Linear
ZeroThrough : Not Through
Weighted Regression : None
Detector Name : Detector A



#	Conc.(Ratio)	MeanArea	Area
1	0.1	18317	17876
			18486
			18589
2	0.5	133586	130954
			134358
			135446
3	1	278592	277375
			280694
			277708
4	1.5	431334	428056
			431655
			434292
5	2	580611	579225
			579444
			583165
6	2.5	717575	709562
			722542
			720623
7	3	862620	867046
			862925
			857890

ID# : 6
Name : Mannose
Quantitative Method : External Standard
Function : f(x)=340995*x-16184.6
Rr1=0.9998631 Rr2=0.9997262 RSS=4.651460e+008
MeanRF: 3.143239e+005 RFSD: 4.504760e+004 RFRSD: 14.331585
FitType : Linear
ZeroThrough : Not Through
Weighted Regression : None
Detector Name : Detector A

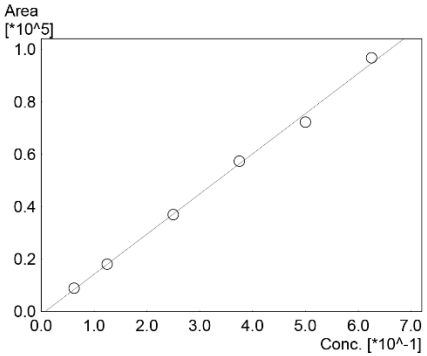


#	Conc.(Ratio)	MeanArea	Area
1	0.1	19527	18847
			19898
			19837
2	0.5	149340	143944
			152033
			152044
3	1	326758	334922
			333539
			311814
4	1.5	497879	472794
			509837
			511006
5	2	673674	657800
			678003
			685219
6	2.5	821462	798781
			820213
			845393
7	3	1015701	1029015
			1006319
			1011770

Figure S3 carbohydrate calibration – 3

==== Shimadzu LabSolutions Calibration Curve ====

ID# : 1
Name : Acetic acid
Quantitative Method : External Standard
Function : f(x)=153298*x-1156.90
Rr1=0.9985355 Rr2=0.9970732 RSS=1.639262e+007
MeanRF: 1.476569e+005 RFSD: 4.805890e+003 RFRSD: 3.254769
FitType : Linear
ZeroThrough : Not Through
Weighted Regression : None
Detector Name : Detector A



#	Conc.(Ratio)	MeanArea	Area
1	0.0625	8886	8886
			8886
			8886
2	0.125	18006	18006
			18006
			18006
3	0.25	36924	36924
			36924
			36924
4	0.375	57296	57296
			57296
			57296
5	0.5	72209	72209
			72209
			72209
6	0.625	96753	96753
			96753
			96753

Figure S4 Acetate calibration

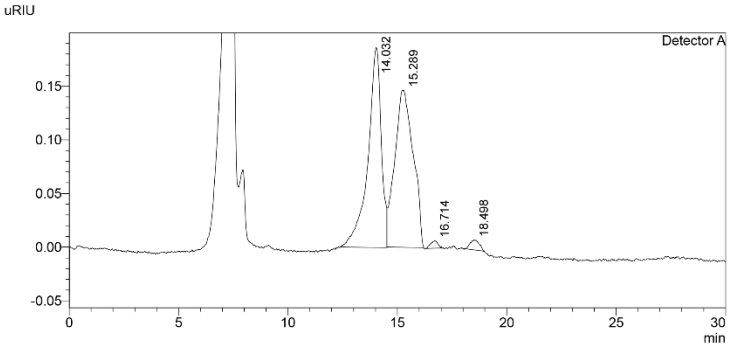
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: CO2-structural-25ulin1ml-apr21		
Sample ID	: CO2-structural-25ulin1ml-apr21		
Data Filename	: CO2-structural-25ulin1ml-apr21.lcd		
Method Filename	: Cb-Glc-Xyl-Gal-Ara-Man-RezexPb+2-80C-50C-calibration.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 5 uL	Level	: 1
Date Acquired	: 4/15/2021 9:20:26 PM	Acquired by	: NIT
Date Processed	: 5/27/2021 10:26:04 AM	Processed by	: Pradeep

<Chromatogram>



<Peak Table>

Detector A

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	14.032	7924	187	0.092	mg/ml	M	Glucose
2	15.289	8617	147	0.089	mg/ml	M	Xylose
3	16.714	161	7	0.055	mg/ml	M	Galactose
4	18.498	276	9	0.028	mg/ml	M	Arabinose
Total		16978	349				

Figure S5 Structural carbohydrates-CO

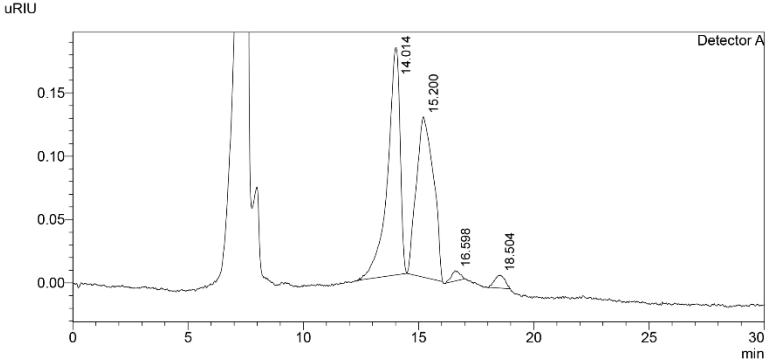
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: CP2-structural-25ulin1ml-apr21		
Sample ID	: CP2-structural-25ulin1ml-apr21		
Data Filename	: CP2-structural-25ulin1ml-apr21.lcd		
Method Filename	: Cb-Glc-Xyl-Gal-Ara-Man-RezexPb+2-80C-50C-calibration.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 5 uL	Level	: 1
Date Acquired	: 4/15/2021 10:33:09 PM	Acquired by	: NIT
Date Processed	: 5/27/2021 10:33:41 AM	Processed by	: Pradeep

<Chromatogram>



<Peak Table>

Detector A

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	14.014	6746	180	0.088	mg/ml	M	Glucose
2	15.200	6530	127	0.082	mg/ml	M	Xylose
3	16.598	208	8	0.055	mg/ml	M	Galactose
4	18.504	321	10	0.028	mg/ml	M	Arabinose
Total		13805	325				

Figure S6 Structural carbohydrates – CP

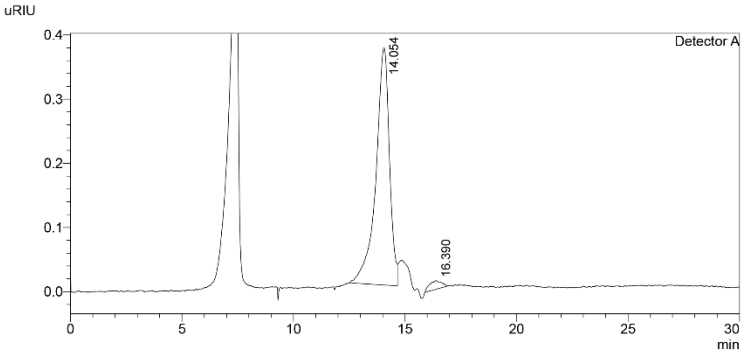
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: Avicel1-structural-25ulin1ml-apr21		
Sample ID	: Avicel1-structural-25ulin1ml-ap		
Data Filename	: Avicel1-structural-25ulin1ml-apr21.lcd		
Method Filename	: Cb-Glc-Xyl-Gal-Ara-Man-RezexPb+2-80C-50C-calibration.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 5 uL	Level	: 1
Date Acquired	: 4/16/2021 12:12:00 AM	Acquired by	: NIT
Date Processed	: 5/27/2021 10:45:32 AM	Processed by	: Pradeep

<Chromatogram>



<Peak Table>

Detector A

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	14.054	15679	370	0.123	mg/ml	M	Glucose
2	16.390	516	14	0.056	mg/ml	M	Galactose
Total		16195	383				

Figure S7 Structural carbohydrates -AC

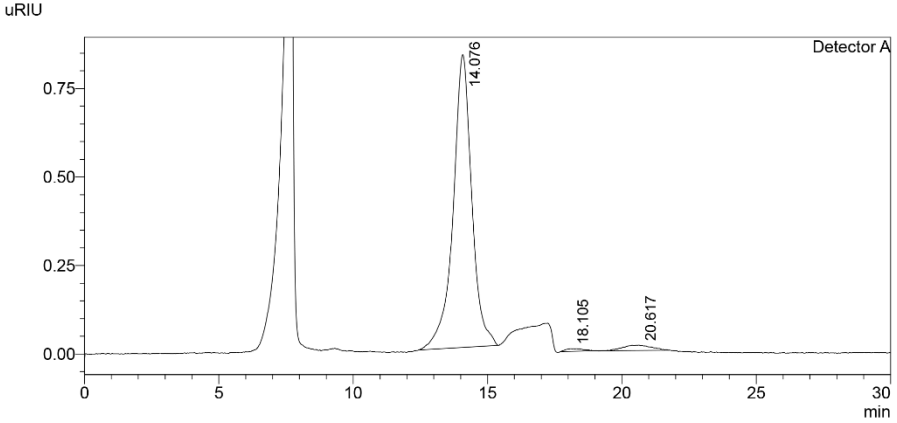
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: Cellulose1-structural-25ulin1ml-apr21		
Sample ID	: Cellulose1-structural-25ulin1ml		
Data Filename	: Cellulose1-structural-25ulin1ml-apr21.lcd		
Method Filename	: Cb-Glc-Xyl-Gal-Ara-Man-RezexPb+2-80C-50C-calibration.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 5 uL	Level	: 1
Date Acquired	: 4/15/2021 11:06:30 PM	Acquired by	: NIT
Date Processed	: 5/27/2021 10:47:50 AM	Processed by	: Pradeep

<Chromatogram>



<Peak Table>

Detector A

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	14.076	40126	828	0.217	mg/ml	M	Glucose
2	18.105	330	8	0.028	mg/ml	M	Arabinose
3	20.617	1089	15	0.051	mg/ml	M	Mannose
Total		41545	850				

Figure S8 Structural carbohydrates – CL

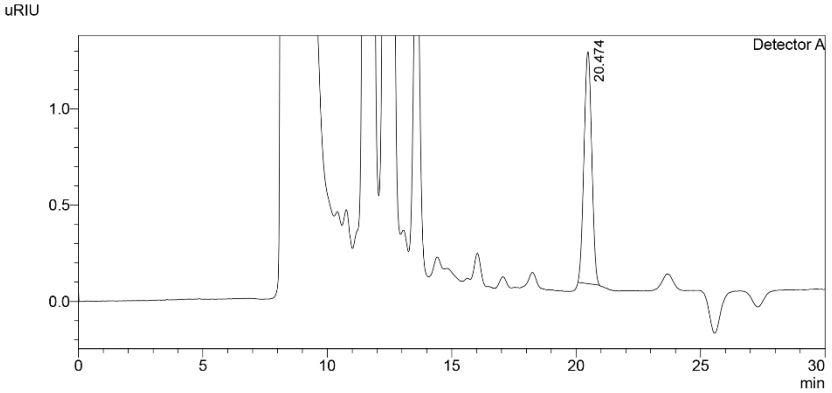
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: CO-no dilution		
Sample ID	: CO-no dilution		
Data Filename	: CO-no dilution.lcd		
Method Filename	: Acetate calibration curve.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 5 uL	Level	: 1
Date Acquired	: 5/27/2021 7:29:05 PM	Acquired by	: NIT
Date Processed	: 7/28/2021 1:00:13 PM	Processed by	: Pradeep

<Chromatogram>



<Peak Table>

Detector A

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.474	25600	1205	0.184	mg/ml		Acetic acid
Total		25600	1205				

Figure S9 Acetate -CO

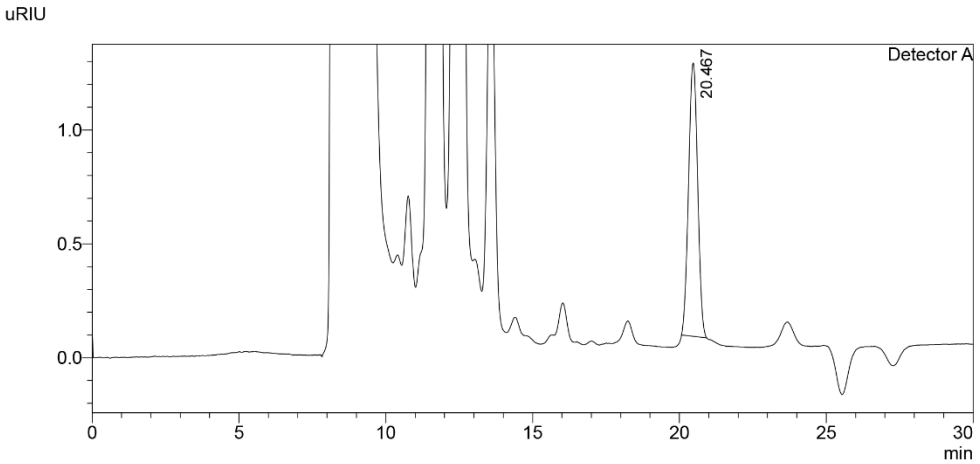
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: CP-no dilution		
Sample ID	: CP-no dilution		
Data Filename	: CP-no dilution.lcd		
Method Filename	: Acetate calibration curve.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 5 uL	Level	: 1
Date Acquired	: 5/27/2021 6:52:38 PM	Acquired by	: NIT
Date Processed	: 7/28/2021 12:58:36 PM	Processed by	: Pradeep

<Chromatogram>



<Peak Table>

Detector A

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	20.467	25366	1200	0.182	mg/ml		Acetic acid
Total		25366	1200				

Figure S10 Acetate – CP

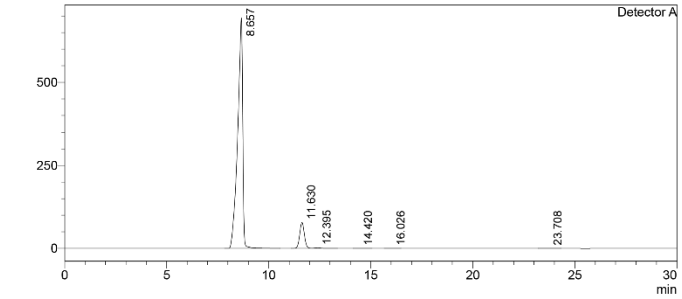
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: Avicel-no dilution		
Sample ID	: Avicel-no dilution		
Data Filename	: Avicel-no dilution001.lcd		
Method Filename	: organic acids -Repromer H - pradeep.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 5 uL	Level	: 1
Date Acquired	: 5/27/2021 5:32:27 PM	Acquired by	: NIT
Date Processed	: 5/27/2021 6:02:31 PM	Processed by	: NIT

<Chromatogram>



<Peak Table>

Detector A

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	8.657	11959112	694055	0.000			
2	11.630	1253413	78142	0.000			
3	12.395	43572	2005	-0.000	mg/ml	V	RT:12.150
4	14.420	2442	125	0.000			
5	16.026	5747	303	0.000			
6	23.708	7737	263	0.000			
Total		13272024	774894				

Figure S11 Acetate – AC

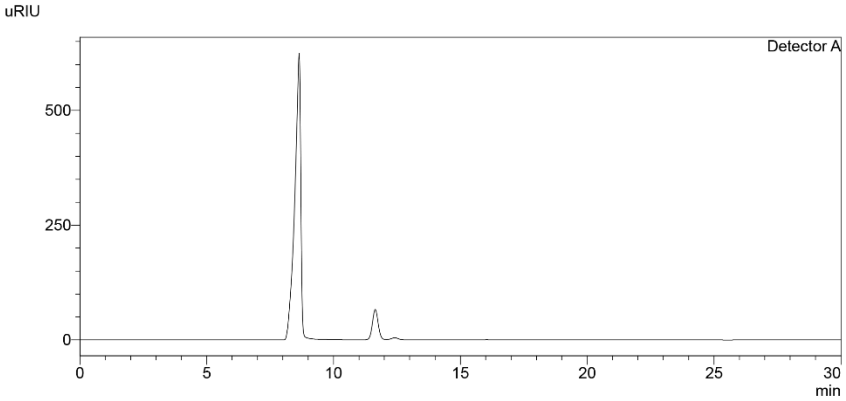
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

Sample Name	: Cellulose-no dilution		
Sample ID	: Cellulose-no dilution		
Data Filename	: Cellulose-no dilution.lcd		
Method Filename	: Acetate calibration curve.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 5 uL	Level	: 1
Date Acquired	: 5/27/2021 6:13:52 PM	Acquired by	: NIT
Date Processed	: 7/28/2021 1:01:03 PM	Processed by	: Pradeep

<Chromatogram>



<Peak Table>

Detector A

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
Total							

Figure S12 Acetate - CL

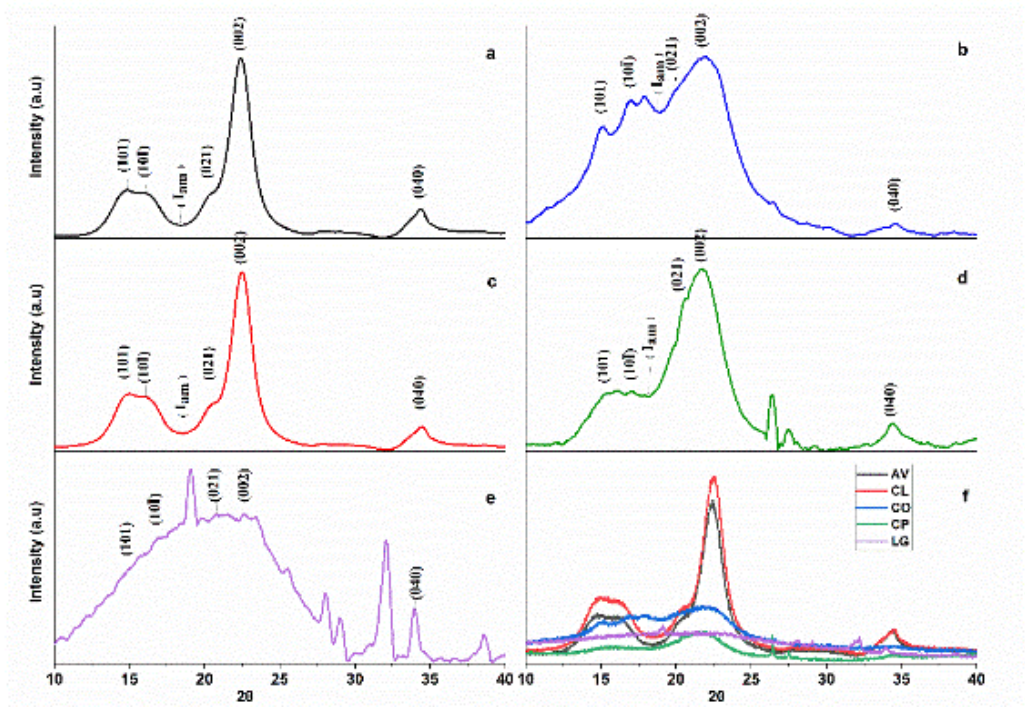


Figure S13 XRD profiles of the samples

Note: a) AC; b) CO; c) CL; d) CP; e) LG; f) all