

Supplementary Information

Data Fusion by Joint Non-negative Matrix

Factorization for Hypothesizing

Pseudo-chemistry Using Bayesian Networks

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S1 Process Conditions

Table S1: Process conditions for spectral data collection

Spectral sensor	Process conditions	
FTIR	Temperature($^{\circ}C$)	Residence time (<i>min</i>)
	150	66, 126, 186, 246, 306, 366, 426, 486
	200	66, 126, 186, 246, 306, 486
	250	246
	300	126, 186, 246, 306, 366, 426, 486
	340	6, 66, 126, 246, 486
	360	6, 16.02, 25.98, 36, 66, 246, 583.02
1H -NMR	400	6, 16.02, 25.98, 36, 66, 96, 126
	150	60, 120, 180, 240, 300, 360, 420, 480
	200	60, 120, 180, 240, 300, 360, 420, 480
	250	60, 120, 180, 240, 300, 360, 420, 480
1H -NMR	300	60, 120, 180, 240, 300, 360, 420, 480

S2 Highly correlated spectral channels

Table S2: Wavenumbers of FTIR spectra with correlation > 0.9

609.46	619.11	1323.07	1911.32	1448.43	2634.57	3116.74	3193.89	3242.10	3627.84	1920.96	3946.07
763.76	802.00	1810.00	1911.32	734.83	2644.21	2297.05	3203.53	1390.57	3637.48	2750.29	3946.07
783.04	841.00	1294.14	1920.96	1631.66	2644.21	2287.41	3213.17	1911.32	3637.48	3830.35	3946.07
599.82	870.00	1487.01	1930.60	2605.64	2644.21	2239.19	3222.82	2711.72	3637.48	1303.78	3955.71
648.04	937.00	1890.00	1930.60	1467.72	2653.86	1053.06	3232.46	1361.64	3647.12	1853.46	3955.71
667.32	966.00	1420.00	1940.25	1853.46	2653.86	1564.16	3232.46	3242.10	3647.12	2682.79	3955.71
898.76	1010.00	1600.00	1949.89	1949.89	2663.50	1940.25	3232.46	1409.86	3656.77	3685.70	3955.71
1014.48	1050.00	1197.71	1969.18	1062.70	2682.79	2991.37	3232.46	2557.42	3656.77	1101.27	3965.35
1014.48	1080.00	1245.92	1978.82	1650.95	2682.79	2412.77	3242.10	3637.48	3656.77	1776.31	3965.35
1081.99	1100.00	1640.00	1978.82	2615.28	2682.79	3087.81	3251.75	1487.01	3666.41	2557.42	3965.35
811.97	1140.00	1770.00	1988.46	1323.07	2692.43	1458.08	3261.39	2499.56	3666.41	3531.40	3965.35
763.76	1160.00	1700.00	2007.75	1814.88	2692.43	2769.58	3271.03	3531.40	3666.41	1004.84	3975.00
1139.85	1170.00	1020.00	2036.68	2644.21	2692.43	821.62	3280.68	3569.98	3676.05	1660.59	3975.00
1188.06	1220.00	1700.00	2036.68	1390.57	2702.07	3261.39	3280.68	1487.01	3685.70	2162.04	3975.00
898.76	1260.00	1550.00	2046.32	1882.39	2702.07	2846.72	3290.32	2499.56	3685.70	3483.19	3975.00
1101.27	1270.00	860.00	2055.97	744.47	2711.72	831.26	3309.61	3531.40	3685.70	3946.07	3975.00
1014.48	1280.00	1062.70	2075.25	1487.01	2711.72	667.32	3319.25	1294.14	3695.34	1400.22	3984.64
1101.27	1290.00	744.47	2084.90	1882.39	2711.72	2866.01	3328.89	1853.46	3695.34	1920.96	3984.64
706.00	1310.00	1487.01	2084.90	734.83	2721.36	667.32	3348.18	2624.93	3695.34	2731.00	3984.64
1024.13	1320.00	1872.74	2084.90	1525.58	2721.36	2663.50	3357.82	3656.77	3695.34	3782.13	3984.64
1101.27	1330.00	1294.14	2094.54	2499.56	2721.36	2914.23	3367.47	1400.22	3704.98	1110.92	3994.29
1207.35	1370.00	1043.41	2104.18	1110.92	2731.00	2952.80	3377.11	1901.67	3704.98	1805.24	3994.29
1280.00	1390.00	1630.00	2104.18	1795.60	2731.00	3377.11	3386.75	2721.36	3704.98	2567.07	3994.29
1332.71	1400.00	706.00	2113.83	2567.07	2731.00	3386.75	3396.40	705.90	3714.63	3550.69	3994.29
638.39	1420.00	1487.01	2113.83	1255.57	2740.65	2875.65	3406.04	2200.62	3714.63		
1313.43	1430.00	1024.13	2123.47	1824.53	2740.65	1612.37	3415.68	1380.93	3724.27		
831.26	1460.00	1795.60	2123.47	2586.35	2740.65	3299.96	3415.68	1506.30	3733.91		
1091.63	1480.00	1720.00	2142.76	1294.14	2750.29	2644.21	3425.33	1506.30	3743.56		
1101.27	1490.00	1710.00	2162.04	2094.54	2750.29	1544.87	3434.97	1352.00	3753.20		
1080.00	1500.00	1390.57	2171.69	946.98	2759.93	2084.90	3434.97	3222.82	3753.20		
1014.48	1520.00	1100.00	2181.33	1564.16	2759.93	811.97	3444.61	1323.07	3762.84		

Table S2 continued from previous page

1024.13	1530.00	908.00	2190.97	1978.82	2759.93	3261.39	3444.61	2509.21	3762.84
734.83	1540.00	2162.04	2200.62	918.05	2769.58	1390.57	3454.26	3560.33	3762.84
1525.58	1540.00	1371.29	2229.55	2316.34	2779.22	1911.32	3454.26	1294.14	3772.49
879.48	1554.51	1730.00	2248.83	821.62	2798.51	2711.72	3454.26	2036.68	3772.49
1438.79	1564.16	1371.29	2268.12	937.34	2808.15	1583.44	3463.90	2972.09	3772.49
744.47	1583.44	2258.48	2277.76	1168.78	2817.79	2538.14	3463.90	1043.41	3782.13
1290.00	1590.00	1371.29	2297.05	2769.58	2827.44	1043.41	3473.54	1920.96	3782.13
1515.94	1602.73	725.00	2316.34	2779.22	2837.08	1631.66	3473.54	2972.09	3782.13
1564.16	1612.37	975.91	2325.98	2325.98	2846.72	2596.00	3473.54	1014.48	3791.77
1602.73	1620.00	976.00	2345.27	2335.63	2856.37	1033.77	3483.19	1535.23	3791.77
1602.73	1631.66	957.00	2364.56	1959.53	2875.65	1564.16	3483.19	2084.90	3791.77
1544.87	1641.30	2350.00	2374.20	1901.67	2885.30	2104.18	3483.19	3001.02	3791.77
1303.78	1650.95	1350.00	2393.49	1949.89	2894.94	3454.26	3483.19	1361.64	3801.42
1024.13	1660.59	1747.38	2403.13	667.32	2914.23	1535.23	3492.83	3733.91	3801.42
1583.44	1660.59	2133.11	2412.77	667.32	2933.51	1930.60	3492.83	1400.22	3811.06
1294.14	1670.23	2268.12	2422.42	2904.58	2943.16	3463.90	3492.83	1901.67	3811.06
734.83	1679.88	2297.05	2432.06	1689.52	2952.80	2190.97	3502.47	2721.36	3811.06
1477.37	1679.88	1370.00	2451.35	705.90	2962.44	1091.63	3512.12	3772.49	3811.06
1053.06	1689.52	2130.00	2460.99	1438.79	2962.44	1689.52	3512.12	3222.82	3820.70
1564.16	1689.52	2210.00	2470.63	1853.46	2962.44	2547.78	3512.12	1419.50	3830.35
1400.22	1699.16	638.00	2489.92	2731.00	2962.44	744.47	3521.76	2721.36	3830.35
1361.64	1728.09	1080.00	2499.56	1400.22	2972.09	1525.58	3521.76	3811.06	3830.35
686.61	1760.00	2480.00	2499.56	2489.92	2972.09	1901.67	3521.76	3618.19	3839.99
1072.34	1776.31	1430.00	2509.21	1053.06	2981.73	3434.97	3521.76	3724.27	3849.63
1062.70	1785.95	2490.00	2509.21	1679.88	2981.73	1313.43	3531.40	1795.60	3859.28
1689.52	1785.95	1070.00	2528.49	2181.33	2981.73	1872.74	3531.40	2981.73	3859.28
1400.22	1795.60	2080.00	2528.49	1043.41	2991.37	2682.79	3531.40	1226.64	3868.92
1081.99	1805.24	1930.00	2538.14	1795.60	2991.37	1043.41	3541.05	3020.30	3868.92
1593.09	1805.24	1795.60	2547.78	2605.64	2991.37	1554.51	3541.05	1255.57	3878.56
1245.92	1814.88	1110.92	2557.42	1265.21	3001.02	1949.89	3541.05	2499.56	3878.56
1641.30	1814.88	2499.56	2557.42	2181.33	3001.02	2991.37	3541.05	3695.34	3878.56
1284.50	1824.53	1390.57	2567.07	1419.50	3010.66	1274.85	3550.69	1795.60	3888.21
1679.88	1824.53	1901.67	2567.07	3001.02	3010.66	1843.81	3550.69	3001.02	3888.21
1323.07	1834.17	1062.70	2576.71	628.75	3029.95	2605.64	3550.69	1419.50	3897.85
1814.88	1834.17	1602.73	2576.71	2788.86	3039.59	1014.48	3560.33	676.97	3907.49
1400.22	1843.81	2080.00	2576.71	783.04	3058.88	1689.52	3560.33	1699.16	3907.49
1824.53	1843.81	1290.00	2586.35	2142.76	3068.52	2528.49	3560.33	2692.43	3907.49
1490.00	1850.00	1680.00	2586.35	1197.71	3087.81	3550.69	3560.33	3762.84	3907.49
744.00	1860.00	744.00	2596.00	3058.88	3097.45	3001.02	3569.98	1776.31	3917.14
1535.23	1863.10	1480.00	2596.00	773.40	3116.74	1409.86	3579.62	2981.73	3917.14
1004.84	1870.00	1860.00	2596.00	715.54	3126.38	2123.47	3579.62	705.90	3926.78
1544.87	1870.00	1070.00	2605.64	1352.00	3136.03	3454.26	3579.62	1776.31	3926.78
1004.84	1880.00	1580.00	2605.64	773.40	3145.67	2403.13	3589.26	2702.07	3926.78
1520.00	1882.39	2080.00	2605.64	3116.74	3145.67	1265.21	3598.91	3772.49	3926.78
734.83	1890.00	1270.00	2615.28	3097.45	3155.31	1978.82	3598.91	1284.50	3936.42
1470.00	1892.03	1670.00	2615.28	2837.08	3164.96	2962.44	3598.91	1834.17	3936.42
1853.46	1892.03	706.00	2624.93	2769.58	3174.60	2248.83	3608.55	2615.28	3936.42
1467.72	1901.67	1440.00	2624.93	850.55	3184.24	2229.55	3618.19	3637.48	3936.42
1853.46	1901.67	1840.00	2624.93	773.40	3193.89	1371.29	3627.84	1110.92	3946.07

Table S3: Wavenumbers of FTIR spectra with correlation < -0.9

609.461	638.391	918.049	2094.540	2065.610	2798.507	1014.483	3107.094	2277.764	3367.465	3425.326	3753.200
705.895	783.042	773.398	2113.827	898.762	2808.150	1535.225	3107.094	2287.408	3377.109	3039.591	3762.844
821.615	898.762	1149.490	2123.470	1785.952	2808.150	1911.316	3107.094	2239.191	3386.752	1149.490	3772.487
686.608	966.266	1477.365	2142.757	2711.716	2808.150	2962.444	3107.094	1747.379	3396.396	754.112	3782.130
792.685	1024.126	1882.386	2142.757	1699.162	2817.793	1390.574	3116.738	1747.379	3406.039	2846.723	3782.130
783.042	1053.056	802.329	2162.044	2731.003	2817.793	1940.246	3116.738	1747.379	3415.682	2306.695	3791.774
754.112	1081.986	927.692	2171.687	1776.309	2827.437	2740.646	3116.738	1737.736	3425.326	1448.434	3801.417
811.972	1101.273	648.035	2190.974	2750.290	2827.437	1303.784	3126.381	1737.736	3434.969	754.112	3811.061
1043.413	1130.203	956.623	2200.617	2171.687	2837.080	1785.952	3126.381	2065.610	3444.612	3097.451	3811.061
1062.700	1149.490	889.119	2229.548	2075.254	2846.723	2644.213	3126.381	1149.490	3454.256	2046.324	3820.704
1072.343	1178.420	869.832	2268.121	2200.617	2856.367	2663.499	3136.025	3280.675	3454.256	831.259	3830.347
879.476	1226.637	1448.434	2297.051	2470.632	2866.010	1920.960	3145.668	628.748	3473.543	3280.675	3830.347
763.755	1255.567	1487.008	2306.695	2432.058	2875.653	3010.661	3145.668	715.538	3483.186	2894.940	3839.991
773.398	1274.854	1882.386	2306.695	1188.063	2894.940	1409.861	3155.311	3107.094	3483.186	2335.625	3849.634
918.049	1294.141	2181.331	2316.338	1236.280	2904.584	1853.456	3155.311	3087.808	3492.829	1178.420	3859.277
1149.490	1313.427	2065.610	2335.625	1352.001	2914.227	2702.073	3155.311	2316.338	3502.473	1959.533	3868.921

Table S3 continued from previous page

1130.203	1332.714	1988.463	2354.911	1342.357	2923.870	1284.497	3164.955	918.049	3512.116	811.972	3878.564
995.196	1371.288	1419.504	2374.198	2210.261	2933.514	2162.044	3164.955	3251.745	3512.116	3261.388	3878.564
1159.133	1390.574	1930.603	2383.842	1737.736	2943.157	898.762	3174.598	3271.032	3521.759	2798.507	3888.208
918.049	1409.861	879.476	2412.772	1728.092	2952.800	1496.651	3174.598	3078.164	3531.403	956.623	3897.851
773.398	1429.148	956.623	2441.702	821.615	2972.087	1978.820	3174.598	3029.947	3541.046	792.685	3907.494
1371.288	1448.434	648.035	2470.632	1130.203	2981.731	2972.087	3174.598	1168.777	3550.690	3145.668	3907.494
715.538	1467.721	975.909	2480.275	1178.420	2991.374	1400.218	3184.241	628.748	3560.333	1458.078	3917.138
1178.420	1496.651	1149.490	2489.919	1178.420	3001.017	2557.422	3184.241	3078.164	3560.333	811.972	3926.781
1207.350	1515.938	628.748	2509.205	1159.133	3010.661	1062.700	3193.885	937.336	3569.976	3164.955	3926.781
1216.994	1544.868	1159.133	2518.849	2933.514	3020.304	1689.519	3193.885	773.398	3579.620	2808.150	3936.424
1506.295	1573.798	1458.078	2528.492	1641.302	3029.947	2499.562	3193.885	3126.381	3579.620	840.902	3946.068
1130.203	1612.372	783.042	2547.779	2624.926	3029.947	1448.434	3203.528	3319.249	3589.263	3261.388	3946.068
1197.707	1641.302	850.545	2557.422	1255.567	3039.591	2904.584	3213.172	2808.150	3598.906	3058.878	3955.711
1207.350	1670.232	715.538	2576.709	1650.945	3039.591	763.755	3232.458	1959.533	3608.550	1458.078	3965.354
802.329	1699.162	2142.757	2586.352	2576.709	3039.591	3126.381	3232.458	2634.569	3618.193	783.042	3974.998
937.336	1708.806	715.538	2615.282	1033.769	3049.234	898.762	3251.745	2538.135	3627.836	3145.668	3974.998
1573.798	1728.092	1226.637	2634.569	1544.868	3049.234	1496.651	3251.745	811.972	3637.480	2798.507	3984.641
1438.791	1747.379	2142.757	2644.213	1920.960	3049.234	1882.386	3251.745	3164.955	3637.480	811.972	3994.285
937.336	1766.666	1969.177	2663.499	2972.087	3049.234	2759.933	3251.745	3299.962	3647.123	3164.955	3994.285
783.042	1785.952	1757.022	2673.143	1332.714	3058.878	2123.470	3261.388	2769.576	3656.767		
1458.078	1795.596	2142.757	2682.786	1805.239	3058.878	1043.413	3271.032	792.685	3666.410		
1178.420	1824.526	918.049	2702.073	2653.856	3058.878	1554.512	3271.032	3155.311	3666.410		
715.538	1853.456	773.398	2721.360	1101.273	3068.521	1978.820	3271.032	2846.723	3676.053		
715.538	1882.386	1178.420	2731.003	1612.372	3068.521	3001.017	3271.032	2837.080	3685.697		
1737.736	1901.673	831.259	2750.290	2113.827	3068.521	2094.540	3280.675	1130.203	3695.340		
1178.420	1920.960	1053.056	2769.576	946.979	3078.164	1419.504	3290.318	3251.745	3695.340		
1159.133	1940.246	1679.875	2769.576	1535.225	3078.164	1371.288	3299.962	3058.878	3704.983		
879.476	1969.177	2181.331	2769.576	1911.316	3078.164	696.251	3309.605	927.692	3714.627		
725.182	1988.463	1053.056	2779.220	2981.731	3078.164	1766.666	3319.249	619.105	3724.270		
1747.379	1998.107	1940.246	2779.220	1535.225	3087.808	1728.092	3328.892	879.476	3733.914		
599.818	2027.037	705.895	2788.863	1930.603	3087.808	1236.280	3338.535	1834.169	3733.914		
1197.707	2046.324	1487.008	2788.863	946.979	3097.451	3222.815	3338.535	3377.109	3733.914		
792.685	2065.610	2499.562	2788.863	1564.155	3097.451	2451.345	3348.179	1930.603	3743.557		
937.336	2075.254	1081.986	2798.507	1978.820	3097.451	2403.128	3357.822	879.476	3753.200		

Table S4: Chemical shifts of ^1H -NMR spectra with correlation > 0.9

-0.997	-0.956	3.031	3.642	3.316	5.595	6.042	7.548	4.415	9.460	4.415	11.943
-0.916	-0.549	1.650	3.682	4.171	5.595	1.119	7.589	5.717	9.460	7.874	11.943
-0.468	-0.427	2.584	3.682	5.554	5.595	2.218	7.629	8.158	9.460	9.745	11.943
-0.712	-0.305	3.560	3.682	4.293	5.676	4.049	7.629	5.432	9.542	8.606	11.983
-0.427	-0.224	3.070	3.723	2.136	5.717	5.595	7.629	2.340	9.583	9.054	12.024
-0.875	-0.142	2.050	3.764	3.601	5.717	2.096	7.670	3.235	9.583	5.147	12.065
-0.183	-0.102	3.230	3.764	4.659	5.717	2.991	7.670	4.049	9.583	7.019	12.065
-0.956	0.020	2.014	3.805	2.096	5.798	3.805	7.670	4.985	9.583	8.036	12.105
-0.997	0.102	2.909	3.805	2.991	5.798	4.659	7.670	7.914	9.583	11.292	12.105
-0.102	0.142	3.720	3.805	3.845	5.798	6.205	7.670	8.077	9.623	5.961	12.146
0.142	0.183	2.950	3.845	4.700	5.798	1.648	7.711	9.135	9.664	10.925	12.146
0.061	0.264	3.800	3.845	4.496	5.839	1.973	7.751	3.764	9.745	9.013	12.187
-0.956	0.346	2.750	3.886	4.008	5.880	2.869	7.751	4.740	9.745	4.822	12.227
-0.102	0.387	3.560	3.886	5.758	5.880	3.682	7.751	6.246	9.745	9.827	12.227
0.102	0.427	3.360	3.927	4.618	5.920	4.862	7.751	8.565	9.745	-0.509	12.309
0.264	0.468	2.050	3.967	4.537	5.961	1.933	7.792	8.158	9.827	10.763	12.309
0.346	0.509	2.991	3.967	3.764	6.002	3.031	7.792	4.252	9.867	8.972	12.390
0.387	0.549	3.805	3.967	5.147	6.002	3.886	7.792	8.077	9.867	2.502	12.431
0.264	0.590	3.153	4.008	3.438	6.083	4.700	7.792	9.745	9.867	6.246	12.431
0.061	0.631	1.892	4.049	5.595	6.083	6.612	7.792	3.031	9.908	7.589	12.431
-0.142	0.671	3.072	4.049	2.747	6.124	3.194	7.833	3.886	9.908	11.861	12.472
-0.956	0.712	3.927	4.049	3.601	6.124	4.049	7.833	4.700	9.908	5.107	12.594
0.671	0.712	3.030	4.089	4.618	6.124	4.862	7.833	7.792	9.908	8.525	12.594
-0.549	0.793	3.890	4.089	1.811	6.165	7.670	7.833	5.229	9.949	0.061	12.675
0.793	0.875	2.665	4.130	3.113	6.165	3.601	7.874	3.357	10.071	7.385	12.716
0.793	0.956	3.560	4.130	3.967	6.165	4.659	7.874	4.333	10.071	-0.916	12.878
-0.549	1.040	3.276	4.171	2.502	6.205	6.002	7.874	8.077	10.071	12.349	12.878
0.916	1.080	4.130	4.171	4.130	6.205	3.194	7.914	9.867	10.071		
-0.916	1.160	2.460	4.211	5.920	6.205	4.049	7.914	8.565	10.111		
0.793	1.200	3.276	4.211	2.747	6.246	4.862	7.914	2.625	10.152		
0.916	1.280	4.090	4.211	3.560	6.246	7.833	7.914	6.205	10.152		

Table S4 continued from previous page

1.038	1.360	3.190	4.252	4.700	6.246	3.805	7.955	7.548	10.152
1.404	1.530	4.049	4.252	2.258	6.287	4.740	7.955	3.560	10.274
1.445	1.690	2.502	4.293	4.415	6.287	6.246	7.955	4.496	10.274
1.648	1.770	3.360	4.293	6.246	6.287	1.933	7.996	7.467	10.274
1.811	1.851	4.211	4.293	2.258	6.327	2.828	7.996	8.931	10.274
1.770	1.973	3.438	4.333	3.194	6.327	3.642	7.996	5.920	10.356
1.690	2.050	4.293	4.333	4.903	6.327	4.496	7.996	7.548	10.396
2.055	2.096	3.110	4.374	6.002	6.368	5.920	7.996	2.828	10.518
2.014	2.177	4.089	4.374	6.246	6.409	7.833	7.996	4.374	10.518
1.811	2.260	3.600	4.415	6.287	6.449	4.130	8.036	5.961	10.518
1.973	2.299	1.970	4.456	2.177	6.490	7.833	8.036	7.670	10.518
2.055	2.340	2.950	4.456	3.113	6.490	4.293	8.077	4.985	10.559
1.648	2.502	3.760	4.456	4.659	6.490	8.036	8.077	7.019	10.559
1.485	2.543	2.299	4.496	2.462	6.531	6.490	8.118	8.077	10.600
2.462	2.543	3.642	4.496	3.276	6.531	3.967	8.158	5.391	10.640
2.177	2.584	2.096	4.537	4.415	6.531	6.083	8.158	7.711	10.681
1.933	2.625	3.357	4.537	6.124	6.531	3.479	8.199	1.038	10.763
1.648	2.665	4.250	4.537	1.973	6.571	4.415	8.199	5.920	10.763
2.543	2.665	2.140	4.578	3.113	6.571	5.880	8.199	10.559	10.763
2.136	2.706	3.030	4.578	1.933	6.612	5.758	8.240	2.909	10.925
1.770	2.747	3.850	4.578	2.828	6.612	8.077	8.280	4.252	10.925
2.665	2.747	3.190	4.618	3.642	6.612	2.991	8.321	5.798	10.925
2.218	2.790	4.330	4.618	4.618	6.612	3.845	8.321	7.792	10.925
1.811	2.828	2.180	4.659	6.124	6.612	4.659	8.321	-0.793	10.966
2.706	2.828	3.070	4.659	4.903	6.653	6.205	8.321	0.956	10.966
2.177	2.869	3.890	4.659	-0.916	6.694	4.333	8.362	8.728	11.007
1.729	2.909	1.890	4.700	0.916	6.734	3.316	8.403	9.664	11.047
2.625	2.909	3.030	4.700	5.798	6.734	4.252	8.403	3.153	11.088
2.014	2.950	3.886	4.700	4.944	6.775	5.717	8.403	4.008	11.088
2.909	2.950	1.811	4.740	1.200	6.816	8.280	8.403	5.880	11.088
2.462	2.991	2.869	4.740	2.828	6.816	2.869	8.443	8.769	11.088
1.851	3.031	3.764	4.740	6.694	6.816	3.682	8.443	9.216	11.210
2.747	3.031	4.700	4.740	6.409	6.856	4.578	8.443	9.257	11.292
2.136	3.072	4.089	4.781	1.200	6.897	8.036	8.443	9.623	11.332
3.031	3.072	2.014	4.822	2.543	6.938	2.787	8.525	0.509	11.373
2.340	3.113	3.190	4.822	5.025	6.938	5.025	8.525	2.665	11.414
1.729	3.153	4.010	4.822	6.856	6.938	6.734	8.525	3.601	11.414
2.620	3.150	2.340	4.862	2.543	6.978	4.089	8.565	4.659	11.414
1.970	3.190	3.280	4.862	1.200	7.019	5.798	8.565	9.583	11.414
2.869	3.194	4.290	4.862	2.665	7.019	8.403	8.565	5.066	11.454
2.218	3.230	1.810	4.903	5.920	7.019	7.792	8.606	6.897	11.454
3.113	3.230	2.710	4.903	1.445	7.060	4.496	8.687	5.514	11.495
2.340	3.280	3.520	4.903	2.869	7.060	8.036	8.687	8.809	11.495
3.230	3.276	4.500	4.903	6.612	7.060	5.758	8.728	6.449	11.536
2.828	3.320	2.790	4.944	1.322	7.100	1.973	8.769	11.332	11.576
2.050	3.357	4.860	4.944	2.869	7.100	3.601	8.769	1.322	11.617
2.991	3.357	3.110	4.985	-0.916	7.141	4.537	8.769	2.177	11.658
2.258	3.398	4.500	4.985	6.694	7.141	8.321	8.769	3.276	11.658
3.276	3.398	2.010	5.025	2.421	7.263	5.514	8.850	4.130	11.658
2.787	3.438	2.909	5.025	1.729	7.426	5.391	8.891	4.985	11.658
1.973	3.479	3.723	5.025	2.665	7.426	4.781	8.931	7.792	11.658
2.909	3.479	4.659	5.025	4.211	7.426	8.565	8.931	10.274	11.658
2.014	3.520	4.862	5.066	2.258	7.467	8.606	9.013	3.398	11.698
2.950	3.520	3.031	5.107	3.276	7.467	8.728	9.135	4.252	11.698
1.973	3.560	2.706	5.147	4.130	7.467	8.809	9.216	6.083	11.698
2.869	3.560	4.618	5.147	4.985	7.467	4.496	9.338	8.565	11.698
1.933	3.601	4.171	5.473	2.462	7.507	8.158	9.338	9.013	11.739
3.031	3.601	3.886	5.554	4.578	7.507	-0.509	9.420	5.636	11.820
2.014	3.642	4.985	5.554	6.531	7.507	3.520	9.460	11.292	11.820

Table S5: Chemical shifts of ^1H -NMR spectra with correlation < -0.9

1.322	2.380	2.787	7.222	0.387	9.298	0.183	11.129	9.501	12.756
1.445	2.421	5.107	7.222	-0.712	9.664	0.387	11.292	12.716	12.797
2.421	2.665	1.689	7.263	1.322	9.949	0.346	11.332		
-0.875	5.229	2.625	7.263	2.828	9.949	-0.509	11.576		
1.729	5.229	3.642	7.263	-0.671	10.030	0.509	11.576		
1.363	5.269	1.526	7.304	0.346	10.030	0.590	11.739		

Table S5 continued from previous page

1.322	5.310	2.625	7.304	9.786	10.437	0.387	11.820
0.142	5.351	6.490	7.304	0.224	10.478	0.387	11.983
0.509	5.391	7.345	7.426	0.305	10.600	0.509	12.105
5.229	6.571	7.263	7.996	0.102	10.640	10.437	12.349
5.269	7.019	0.305	8.362	5.269	10.681	10.234	12.634
1.770	7.182	0.142	8.891	0.061	10.722	11.576	12.675
2.747	7.182	0.305	9.013	7.222	10.763	3.072	12.756
5.025	7.182	0.264	9.135	1.160	10.844	3.927	12.756
1.770	7.222	0.346	9.257	0.305	11.007	5.880	12.756

Table S6: Wavenumbers of FTIR and chemical shifts of ^1H -NMR spectra with cross-correlation > 0.7

750.25	-1.00	3299.96	1.85	2960.52	3.44	3230.53	5.35	1409.86	8.24	1035.70	10.60
850.55	-0.96	1580.00	1.89	1487.01	3.48	1093.56	5.39	2096.47	8.24	1317.28	10.60
607.53	-0.92	2659.64	1.89	1679.88	3.48	2092.61	5.39	2725.22	8.24	1845.74	10.60
2864.08	-0.92	3508.26	1.89	2655.78	3.48	2752.22	5.39	3596.98	8.24	2582.49	10.60
2335.62	-0.88	1620.00	1.93	892.98	3.52	3728.13	5.39	3932.57	8.24	3454.26	10.60
935.41	-0.83	2650.00	1.93	1645.16	3.52	892.98	5.59	1610.44	8.32	3789.85	10.60
619.10	-0.79	3470.00	1.93	2879.51	3.52	1633.59	5.59	3481.26	8.32	1240.14	10.64
2933.51	-0.79	1614.30	1.97	885.26	3.56	1984.61	5.59	1247.85	8.36	2559.35	10.64
2324.05	-0.71	2678.93	1.97	1637.44	3.56	3504.40	5.59	1780.17	8.36	2910.37	10.68
854.40	-0.63	3490.00	1.97	2648.07	3.56	1247.85	5.64	2513.06	8.36	2486.06	10.72
2856.37	-0.63	1900.00	2.01	3492.83	3.56	1687.59	5.64	2983.66	8.36	3890.14	10.72
2362.63	-0.59	3300.00	2.01	1579.58	3.60	2096.47	5.64	3728.13	8.36	3338.54	10.76
2366.48	-0.55	1550.00	2.05	1880.46	3.60	2717.50	5.64	997.12	8.44	2262.34	10.84
2042.47	-0.51	2660.00	2.05	2659.64	3.60	3593.12	5.64	1629.73	8.44	931.55	10.97
777.26	-0.39	689.00	2.10	881.40	3.64	3948.00	5.64	1934.46	8.44	900.69	11.01
2042.47	-0.39	1640.00	2.10	1618.16	3.64	1444.58	5.72	2894.94	8.44	1325.00	11.01
669.25	-0.35	2879.51	2.10	1957.60	3.64	1645.16	5.72	1081.99	8.48	2177.47	11.01
2374.20	-0.35	665.39	2.14	2960.52	3.64	1911.32	5.72	2115.76	8.48	2987.52	11.01
3280.00	-0.31	1610.44	2.14	1463.86	3.68	2655.78	5.72	3531.40	8.48	3789.85	11.01
2864.08	-0.26	2632.64	2.14	3388.68	3.68	707.82	5.76	3948.00	8.48	1000.98	11.09
973.98	-0.18	3442.68	2.14	1525.58	3.72	1309.57	5.76	1070.41	8.61	1587.30	11.09
3311.53	-0.18	1568.01	2.18	1814.88	3.72	2732.93	5.76	1429.15	8.61	1849.60	11.09
2350.00	-0.14	1950.00	2.18	2574.78	3.72	3955.71	5.76	1656.73	8.61	2613.35	11.09
862.12	-0.10	3380.00	2.18	3485.11	3.72	3539.12	5.88	1903.60	8.61	3500.54	11.09
3141.81	-0.10	1483.15	2.22	1564.15	3.76	1290.28	6.08	2605.64	8.61	1112.85	11.29
923.84	-0.06	1876.60	2.22	1865.03	3.76	1687.59	6.08	2987.52	8.61	1703.02	11.29
2852.51	-0.06	2945.09	2.22	2682.79	3.76	2084.90	6.08	3681.84	8.61	2524.63	11.29
854.40	-0.02	893.00	2.26	1452.29	3.80	3454.26	6.08	946.98	8.77	3002.95	11.29
3265.25	-0.02	1960.00	2.26	2594.07	3.80	730.97	6.16	1514.01	8.77	3774.42	11.29
1140.00	0.02	3407.97	2.26	3465.83	3.80	1606.59	6.16	1687.59	8.77	703.97	11.33
3284.53	0.02	1600.00	2.30	1610.44	3.85	1903.60	6.16	1984.61	8.77	1429.15	11.33
1143.70	0.06	2880.00	2.30	2628.78	3.85	2690.50	6.16	2713.64	8.77	2524.63	11.33
3261.39	0.06	889.12	2.34	1467.72	3.89	889.12	6.33	1012.55	8.85	3569.98	11.33
1135.99	0.10	2069.47	2.34	1024.13	3.93	2945.09	6.33	1402.15	8.85	3909.42	11.33
3292.25	0.10	3420.00	2.34	1514.01	3.93	1575.73	6.49	2729.07	8.85	1490.87	11.41
1124.42	0.14	1992.32	2.38	1687.59	3.93	3396.40	6.49	3704.98	8.85	1672.16	11.41
3122.52	0.14	2435.92	2.38	1980.75	3.93	2887.23	6.57	1024.13	8.89	2536.21	11.41
916.00	0.18	1236.28	2.42	2705.93	3.93	1444.58	6.61	1305.71	8.89	3434.97	11.41
2856.37	0.18	2300.00	2.42	3936.42	3.93	607.53	6.69	1880.46	8.89	2189.05	11.58
846.69	0.22	3855.42	2.42	1614.30	3.97	2925.80	6.69	2586.35	8.89	3924.85	11.58
2833.22	0.22	2910.00	2.50	2644.21	3.97	2937.37	6.82	3512.12	8.89	2933.51	11.62
835.12	0.26	1460.00	2.54	3504.40	3.97	3342.39	6.90	3793.70	8.89	1548.73	11.66
2813.94	0.26	3430.00	2.54	1529.44	4.01	603.68	7.02	1039.56	9.01	1872.74	11.66
808.11	0.31	2910.00	2.58	1695.30	4.01	3365.54	7.02	1413.72	9.01	2690.50	11.66
2783.08	0.31	1448.43	2.62	2077.18	4.01	2941.23	7.06	2729.07	9.01	1008.70	11.70
765.68	0.35	3299.96	2.62	3434.97	4.01	2675.07	7.10	3693.41	9.01	1602.73	11.70
1170.71	0.35	1957.60	2.67	1533.30	4.05	877.55	7.14	1390.57	9.13	1861.17	11.70
3265.25	0.35	3384.82	2.67	1930.60	4.05	1359.72	7.18	2972.09	9.13	2628.78	11.70
935.41	0.39	2880.00	2.71	3481.26	4.05	2293.19	7.18	703.97	9.26	900.69	11.74
3122.52	0.39	889.00	2.75	2536.21	4.09	3816.85	7.18	1398.29	9.26	2115.76	11.74
850.55	0.43	3350.00	2.75	1579.58	4.13	1969.18	7.22	2189.05	9.26	3577.69	11.74
2829.37	0.43	2670.00	2.79	2644.21	4.13	2462.92	7.22	2995.23	9.26	615.25	11.82
831.26	0.47	689.00	2.83	1305.71	4.17	1224.71	7.26	3774.42	9.26	2169.76	11.82
2817.79	0.47	2940.00	2.83	1641.30	4.17	2297.05	7.26	1776.31	9.30	3654.84	11.82

Table S6 continued from previous page

823.54	0.51	1470.00	2.87	1915.17	4.17	3836.13	7.26	1051.13	9.50	1008.70	11.98
2802.36	0.51	3360.00	2.87	3469.69	4.17	2281.62	7.30	1514.01	9.50	1290.28	11.98
811.97	0.55	2050.00	2.91	1587.30	4.21	746.40	7.43	1865.03	9.50	1811.03	11.98
2813.94	0.55	3430.00	2.91	2648.07	4.21	3234.39	7.43	2698.22	9.50	2559.35	11.98
854.40	0.59	2680.00	2.95	3465.83	4.21	1564.15	7.47	3604.69	9.50	3006.80	11.98
3292.25	0.59	881.40	2.99	2594.07	4.25	2590.21	7.47	1552.58	9.58	3778.27	11.98
1170.71	0.63	2034.75	2.99	1575.73	4.29	865.97	7.59	1980.75	9.58	1016.41	12.11
927.69	0.67	3407.97	2.99	1980.75	4.29	2046.32	7.67	3396.40	9.58	1298.00	12.11
2351.05	0.71	2536.21	3.03	3461.97	4.29	746.40	7.75	1043.41	9.62	2000.04	12.11
2362.63	0.96	3442.68	3.03	1568.01	4.33	2046.32	7.75	1325.00	9.62	2709.79	12.11
970.12	1.00	1895.89	3.07	1853.46	4.33	3415.68	7.75	1911.32	9.62	3635.55	12.11
3346.25	1.00	3299.96	3.07	2648.07	4.33	1544.87	7.79	2624.93	9.62	3940.28	12.11
2366.48	1.04	1570.00	3.11	1444.58	4.46	1853.46	7.79	3539.12	9.62	1066.56	12.19
966.27	1.08	2880.00	3.11	1645.16	4.46	2648.07	7.79	3920.99	9.62	1402.15	12.19
3360.00	1.08	885.00	3.15	2084.90	4.46	889.12	8.00	1062.70	9.83	1849.60	12.19
2920.00	1.12	1930.00	3.15	3407.97	4.46	2894.94	8.00	1398.29	9.83	2555.49	12.19
2929.66	1.16	2960.00	3.15	1606.59	4.58	1004.84	8.04	2092.61	9.83	2983.66	12.19
2864.08	1.32	1440.00	3.19	3380.97	4.58	1301.86	8.04	2744.50	9.83	3704.98	12.19
2038.61	1.40	2880.00	3.19	1587.30	4.66	1606.59	8.04	3658.70	9.83	892.98	12.23
989.41	1.44	1470.00	3.23	2675.07	4.66	1857.31	8.04	3994.28	9.83	1267.14	12.23
3380.00	1.44	1900.00	3.23	3508.26	4.66	2601.78	8.04	1583.44	9.91	1548.73	12.23
2933.51	1.49	2950.00	3.23	1595.01	4.70	3473.54	8.04	1865.03	9.91	1814.88	12.23
1450.00	1.53	1450.00	3.28	1895.89	4.70	3971.14	8.04	2640.36	9.91	2100.33	12.23
3380.97	1.53	1980.00	3.28	2690.50	4.70	1089.70	8.08	711.68	9.95	2721.36	12.23
2914.23	1.57	3400.00	3.28	1440.72	4.82	1502.44	8.08	2266.19	9.95	3531.40	12.23
1463.86	1.61	1580.00	3.32	1641.30	4.82	1799.45	8.08	3589.26	9.95	3955.71	12.23
3388.68	1.61	2883.37	3.32	1949.89	4.82	2084.90	8.08	2181.33	10.03	2362.63	12.31
2891.08	1.65	1529.44	3.36	2952.80	4.82	2759.93	8.08	3890.14	10.03	804.26	12.67
889.12	1.69	1895.89	3.36	1463.86	4.90	3701.13	8.08	1108.99	10.07	2786.93	12.67
3377.11	1.69	2956.66	3.36	3388.68	4.90	1043.41	8.16	1533.30	10.07	1213.14	12.76
2883.37	1.73	1467.72	3.40	2879.51	5.03	1490.87	8.16	1795.60	10.07	3161.10	12.76
885.26	1.77	1656.73	3.40	1379.00	5.23	1676.02	8.16	2050.18	10.07		
2941.23	1.77	2636.50	3.40	2428.20	5.23	1953.75	8.16	2736.79	10.07		
1448.43	1.81	665.39	3.44	1236.28	5.27	2729.07	8.16	3662.55	10.07		
3361.68	1.81	1606.59	3.44	2420.49	5.27	3697.27	8.16	2007.75	10.48		
1602.73	1.85	1946.03	3.44	676.96	5.35	1074.27	8.24	3677.98	10.48		

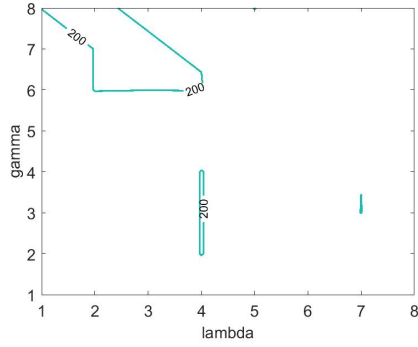
Table S7: Wavenumbers of FTIR and chemical shifts of ^1H -NMR spectra with cross-correlation < -0.7

615.247	-0.997	3569.976	0.468	1517.867	2.218	2281.622	3.682	3870.849	7.100	1182.277	11.088
3874.707	-0.997	676.965	0.509	3211.243	2.218	3851.563	3.682	2455.202	7.141	3091.665	11.088
3010.661	-0.956	2111.898	0.509	1517.867	2.258	3072.378	3.723	2069.468	7.182	808.115	11.292
2023.179	-0.916	3002.946	0.509	3249.816	2.258	1213.136	3.764	3427.254	7.182	2806.221	11.292
622.962	-0.875	3920.995	0.509	1718.449	2.299	3735.842	3.764	2910.370	7.222	781.113	11.332
2470.632	-0.875	2092.612	0.549	3245.959	2.299	2003.893	3.805	1448.434	7.263	2019.322	11.332
1988.463	-0.834	3600.835	0.549	1436.862	2.340	715.538	3.845	3380.966	7.263	3307.677	11.332
3832.276	-0.834	1699.162	0.590	3161.097	2.340	3238.244	3.845	2887.226	7.304	3072.378	11.414
2459.060	-0.793	3670.267	0.590	1452.292	2.380	1189.992	3.927	1236.280	7.426	854.403	11.576
2007.750	-0.712	1776.309	0.631	3384.824	2.380	3110.952	3.927	2412.772	7.426	657.678	11.617
3758.986	-0.712	3631.694	0.631	2925.799	2.421	1521.724	3.967	1201.564	7.467	2451.345	11.617
2189.045	-0.631	2127.328	0.671	1236.280	2.502	3735.842	3.967	3751.272	7.467	1436.862	11.658
642.249	-0.590	1386.717	0.712	2389.628	2.502	3049.234	4.008	3546.832	7.589	3743.557	11.658
3882.421	-0.590	692.394	0.956	3901.708	2.502	1197.707	4.049	1969.177	7.670	3083.950	11.698
3708.841	-0.549	3172.669	0.956	2262.335	2.543	1189.992	4.089	1213.136	7.751	819.687	11.739
2470.632	-0.509	2150.472	0.997	3627.836	2.543	1216.994	4.130	2393.485	7.751	719.396	11.820
1240.138	-0.387	3805.275	0.997	1733.878	2.584	1189.992	4.171	673.107	7.792	1151.419	11.820
2486.061	-0.387	2439.773	1.038	3026.090	2.584	3272.960	4.171	3095.522	7.792	3265.246	11.820
3720.413	-0.387	1344.286	1.078	1213.136	2.625	1749.308	4.211	1714.592	7.996	1556.440	11.983
1768.594	-0.346	2466.775	1.078	2293.194	2.625	3743.557	4.211	3566.119	7.996	3176.527	11.983
3797.560	-0.346	1942.175	1.119	3855.420	2.625	1205.422	4.293	3049.234	8.036	919.978	12.105
3797.560	-0.305	3608.550	1.119	1992.321	2.665	3731.985	4.293	1521.724	8.077	3122.524	12.105
2462.917	-0.264	2462.917	1.160	3731.985	2.665	3107.094	4.333	3272.960	8.077	1139.847	12.187
1768.594	-0.183	2219.904	1.322	1737.736	2.706	1737.736	4.456	3103.237	8.158	3103.237	12.187
3758.986	-0.183	3612.407	1.322	3195.813	2.706	3585.406	4.456	823.544	8.240	1556.440	12.227
2192.903	-0.142	2262.335	1.404	1363.573	2.747	1749.308	4.578	3049.234	8.240	3180.384	12.227
615.247	-0.102	3816.847	1.404	2405.057	2.747	3839.991	4.578	2304.766	8.321	2239.191	12.309

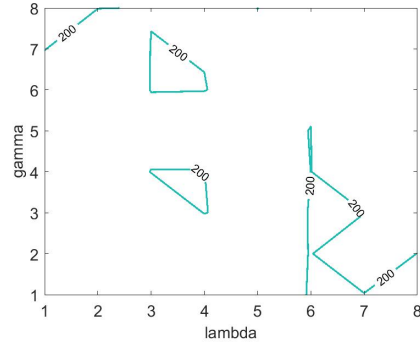
Table S7 continued from previous page

2497.633	-0.102	2277.764	1.445	3870.849	2.747	1749.308	4.659	1178.420	8.362	3905.566	12.309
3924.852	-0.102	3816.847	1.445	2254.620	2.787	3743.557	4.659	3191.956	8.362	2123.470	12.675
2162.044	-0.061	2243.048	1.485	3855.420	2.787	3026.090	4.700	3029.947	8.443	3577.691	12.675
3596.978	-0.061	3211.243	1.485	2003.893	2.828	1193.849	4.822	754.112	8.484	734.825	12.756
904.548	-0.020	1730.021	1.526	3820.704	2.828	3103.237	4.822	2802.364	8.484	1494.723	12.756
2547.779	-0.020	2416.629	1.526	1753.165	2.869	1232.423	4.903	1560.298	8.606	1676.018	12.756
676.965	0.020	680.822	1.567	3616.264	2.869	3022.233	4.903	3191.956	8.606	1980.749	12.756
2185.188	0.020	2258.478	1.567	1714.592	2.909	1359.715	5.025	3049.234	8.769	2952.800	12.756
3782.130	0.020	3245.959	1.567	3218.958	2.909	3735.842	5.025	916.120	8.850		
1706.877	0.061	1726.164	1.607	1359.715	2.950	2933.514	5.229	796.543	8.891		
2748.361	0.061	2412.772	1.607	3095.522	2.950	2667.357	5.269	2817.793	8.891		
3886.279	0.061	3901.708	1.607	1209.279	2.991	862.117	5.351	1132.132	9.013		
2165.901	0.102	2246.906	1.648	2397.342	2.991	3265.246	5.351	808.115	9.135		
3720.413	0.102	3222.815	1.648	1120.560	3.031	1132.132	5.391	2833.223	9.135		
1394.432	0.142	1375.145	1.689	2385.770	3.031	3164.955	5.391	850.545	9.257		
2505.348	0.142	2393.485	1.689	680.822	3.072	3161.097	5.595	2833.223	9.257		
3693.411	0.142	3901.708	1.689	2142.757	3.072	1178.420	5.636	2829.365	9.298		
1240.138	0.183	2235.334	1.729	3836.133	3.072	3126.381	5.636	3276.818	9.501		
2505.348	0.183	3242.102	1.729	1749.308	3.113	2304.766	5.717	2003.893	9.583		
3878.564	0.183	1359.715	1.770	3585.406	3.113	3747.414	5.717	3839.991	9.583		
1922.888	0.224	2412.772	1.770	1517.867	3.153	3107.094	5.880	2790.792	9.623		
2968.230	0.224	1201.564	1.811	3203.528	3.153	3199.671	6.083	719.396	9.827		
3874.707	0.224	2385.770	1.811	1510.152	3.194	3037.662	6.165	3041.519	9.827		
1429.148	0.264	3870.849	1.811	3731.985	3.194	1213.136	6.327	1216.994	9.908		
2543.922	0.264	2003.893	1.851	1741.593	3.235	2408.914	6.327	3188.099	9.908		
3720.413	0.264	3801.417	1.851	3801.417	3.235	1197.707	6.490	2879.511	9.949		
1078.129	0.305	1737.736	1.892	1745.450	3.276	2393.485	6.490	811.972	10.030		
2000.035	0.305	3249.816	1.892	3743.557	3.276	626.819	6.571	2856.367	10.030		
2725.217	0.305	1510.152	1.933	3195.813	3.316	2250.763	6.571	3064.664	10.071		
3685.697	0.305	3195.813	1.933	1737.736	3.357	3242.102	6.571	827.401	10.478		
3986.570	0.305	1363.573	1.973	3751.272	3.357	1733.878	6.612	2825.508	10.478		
1703.019	0.346	3095.522	1.973	3033.805	3.398	1379.002	6.694	819.687	10.600		
2532.349	0.346	1213.136	2.014	1220.851	3.438	3527.545	6.694	3056.949	10.600		
3639.409	0.346	2389.628	2.014	3735.842	3.438	2258.478	6.816	846.688	10.640		
3951.854	0.346	3870.849	2.014	3033.805	3.479	3863.135	6.816	2852.509	10.640		
1919.031	0.387	1969.177	2.055	1216.994	3.520	2451.345	6.897	757.969	10.722		
2597.924	0.387	3735.842	2.055	3195.813	3.520	2266.192	6.978	2316.338	10.722		
3782.130	0.387	1722.306	2.096	1517.867	3.560	1359.715	7.019	2216.047	10.763		
1332.714	0.427	3245.959	2.096	3211.243	3.560	2389.628	7.019	3546.832	10.763		
2185.188	0.427	1541.011	2.136	1737.736	3.601	3901.708	7.019	2061.753	10.844		
3635.551	0.427	3238.244	2.136	3751.272	3.601	2285.479	7.060	700.109	10.966		
3959.568	0.427	1521.724	2.177	2300.909	3.642	3870.849	7.060	3832.276	10.966		
2119.613	0.468	3211.243	2.177	680.822	3.682	2293.194	7.100	1170.705	11.007		

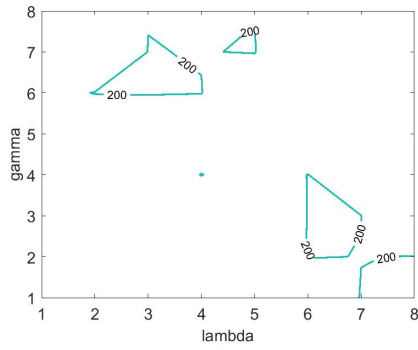
S3 For $\alpha = 10^{-3}$



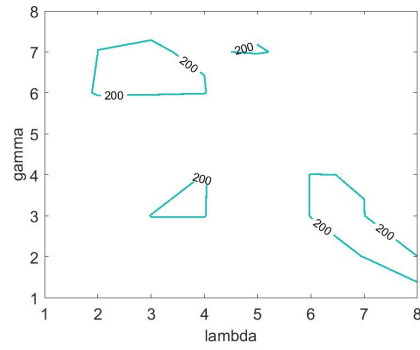
(a) $\beta = 10^{-3}$



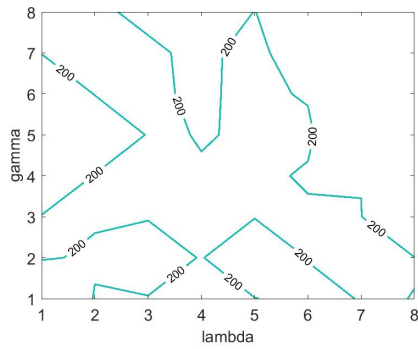
(b) $\beta = 10^{-2}$



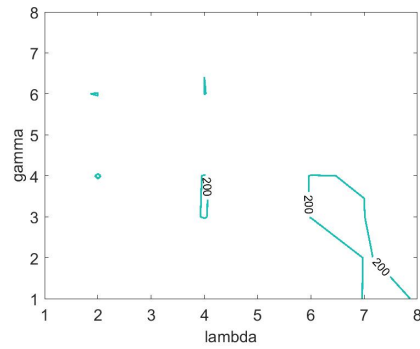
(c) $\beta = 10^{-1}$



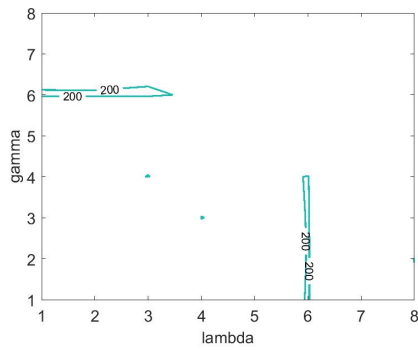
(d) $\beta = 10^0$



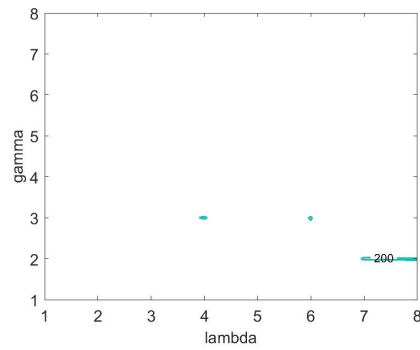
(e) $\beta = 0$



(f) $\beta = 10^1$



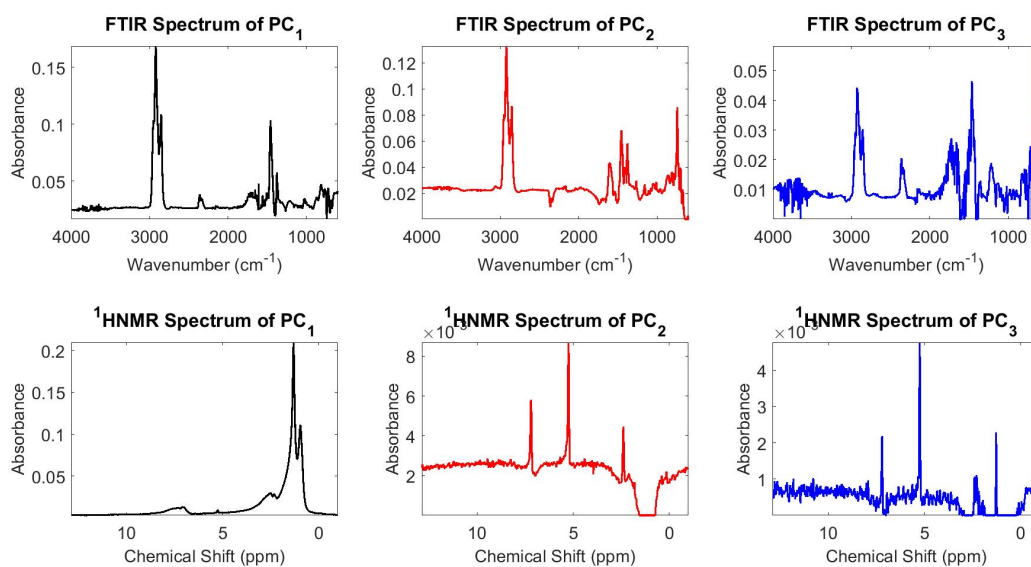
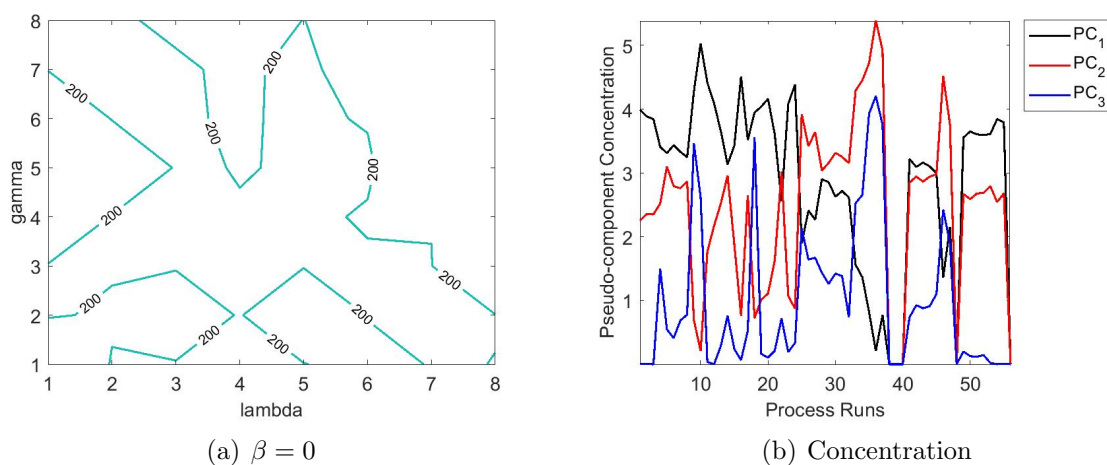
(g) $\beta = 10^2$



(h) $\beta = 10^3$

S10

Figure S1: Isocontours for reconstruction error $E \leq 200$



(c) Pseudo-component spectra

Figure S2: JNMF profiles for $\alpha = 10^{-3}, \beta = 0, \gamma = 0, \lambda = 10^{-1}$

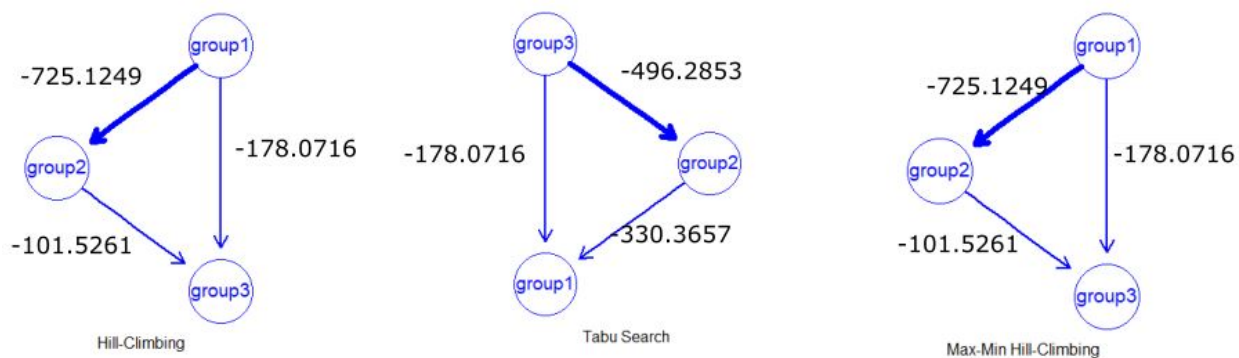
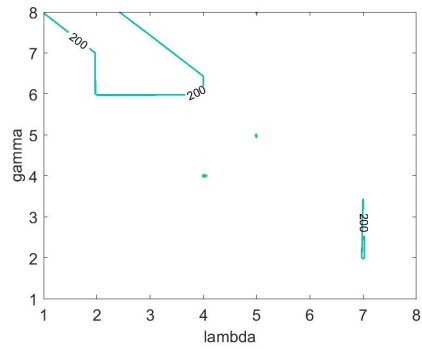
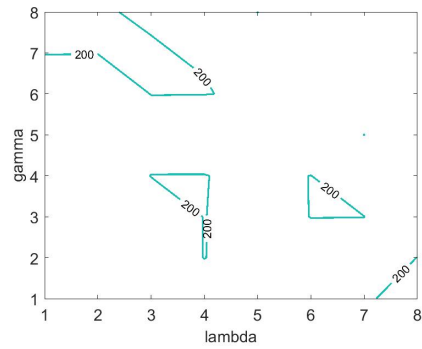


Figure S3: Bayesian networks constructed from the PC spectra

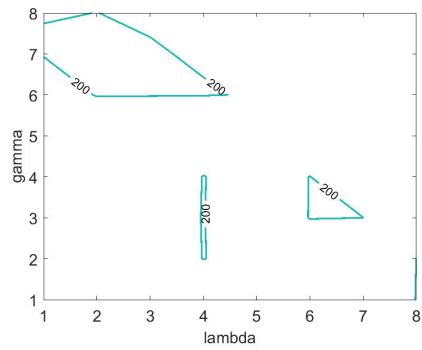
S4 For $\alpha = 10^{-2}$



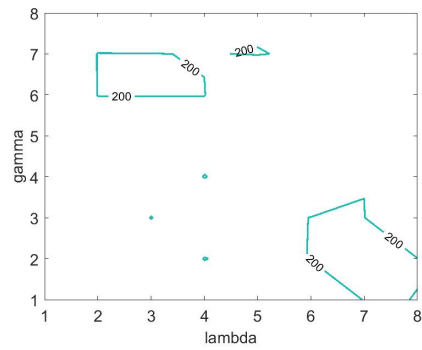
(a) $\beta = 10^{-3}$



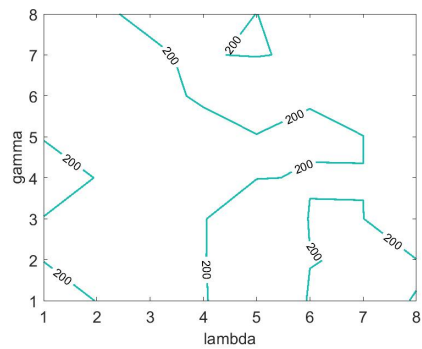
(b) $\beta = 10^{-2}$



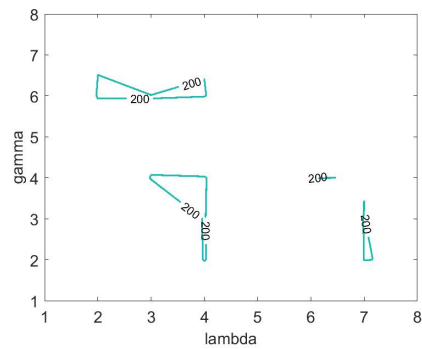
(c) $\beta = 10^{-1}$



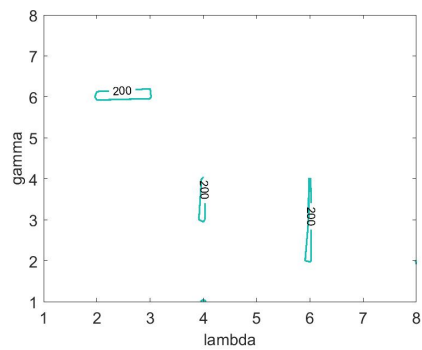
(d) $\beta = 10^0$



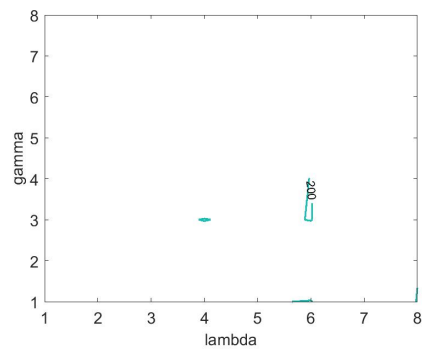
(e) $\beta = 0$



(f) $\beta = 10^1$



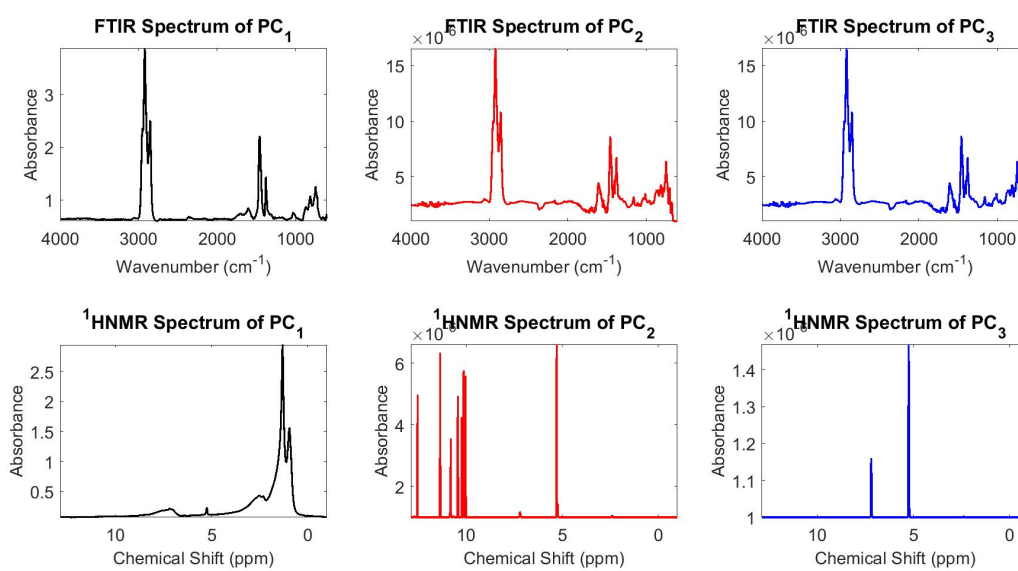
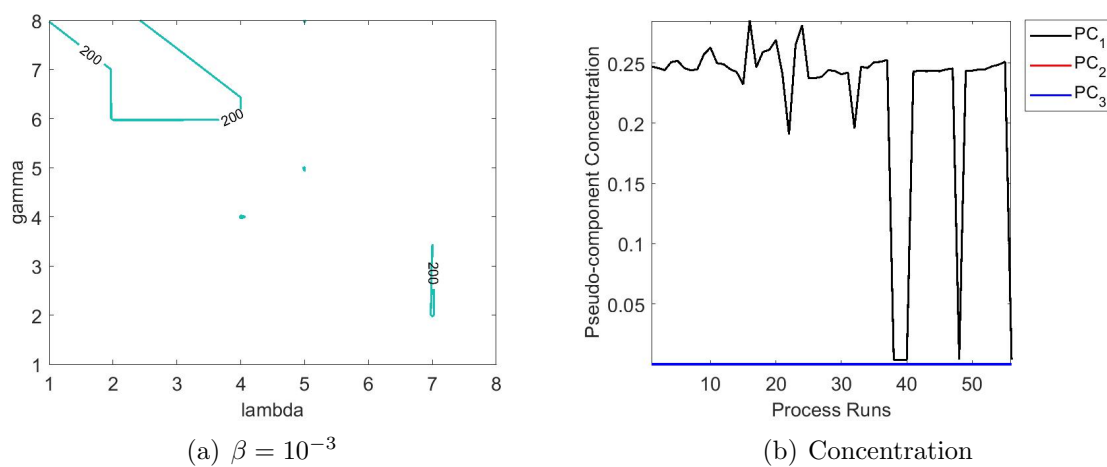
(g) $\beta = 10^2$



(h) $\beta = 10^3$

S13

Figure S4: Isocontours for reconstruction error $E \leq 200$



(c) Pseudo-component spectra

Figure S5: JNMF profiles for $\alpha = 10^{-2}$, $\beta = 10^{-3}$, $\gamma = 10^1$, $\lambda = 10^{-2}$

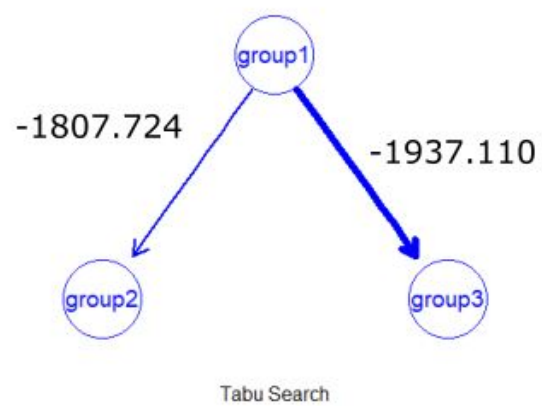
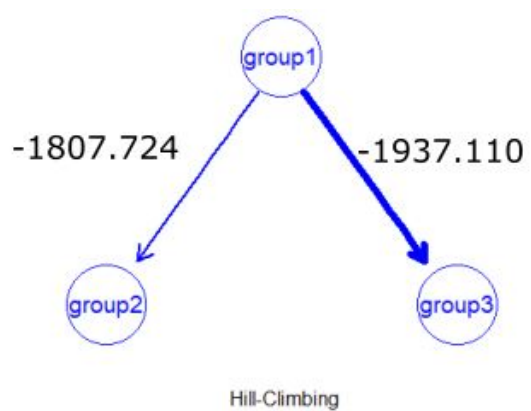
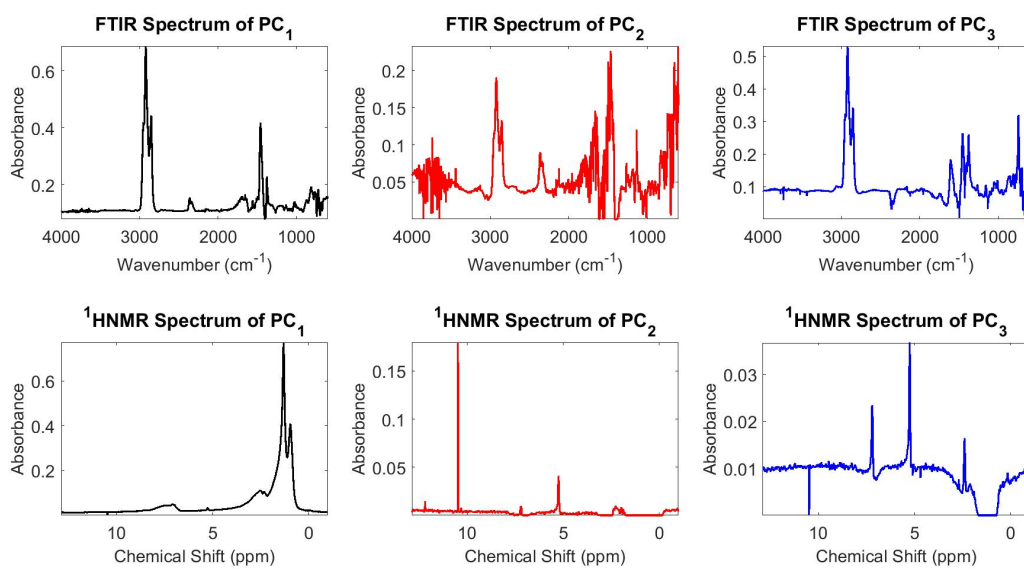
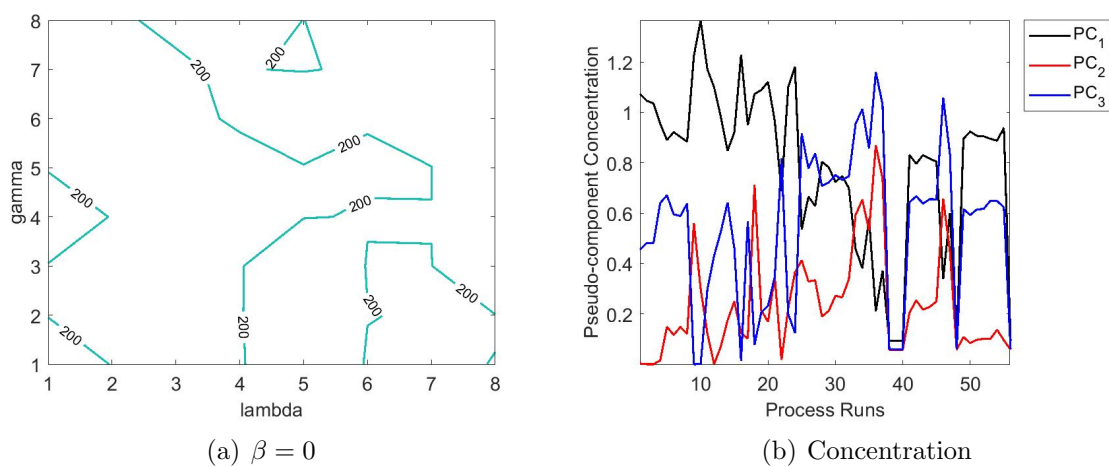


Figure S6: Bayesian networks constructed from the PC spectra



(c) Pseudo-component spectra

Figure S7: JNMF profiles for $\alpha = 10^{-2}$, $\beta = 0$, $\gamma = 10^{-1}$, $\lambda = 10^{-2}$

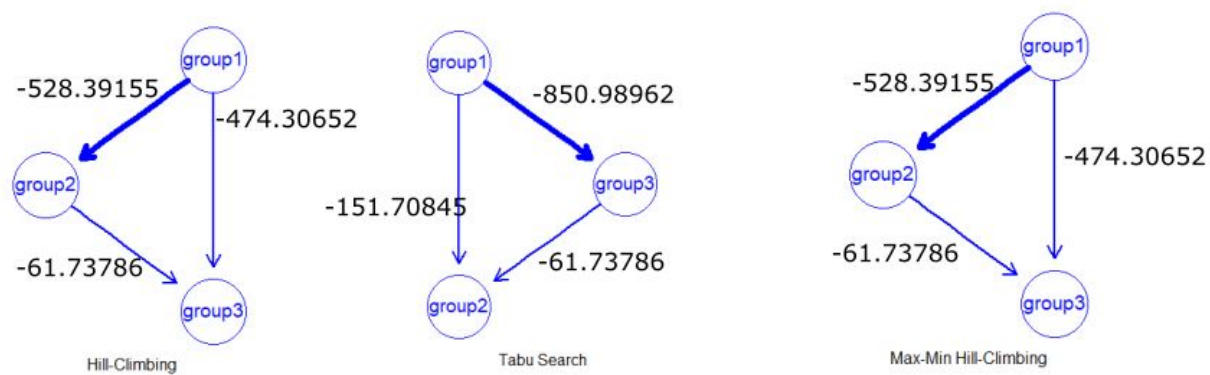
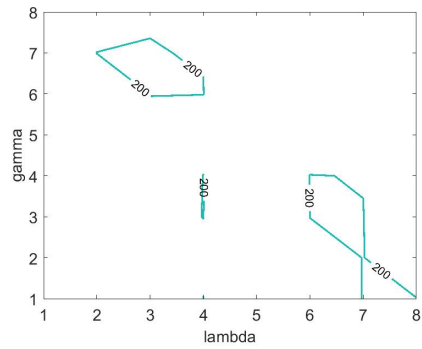
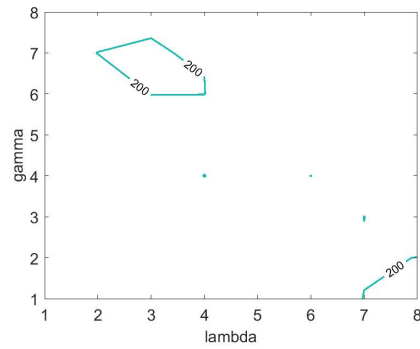


Figure S8: Bayesian networks constructed from the PC spectra

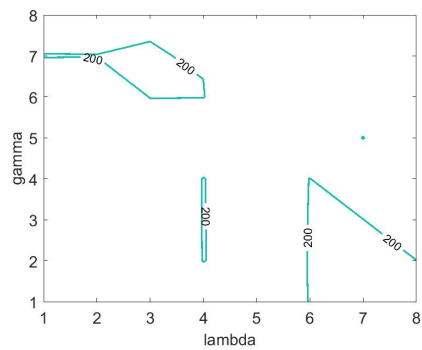
S5 For $\alpha = 10^0$



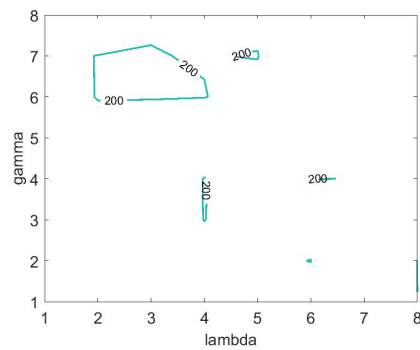
(a) $\beta = 10^{-3}$



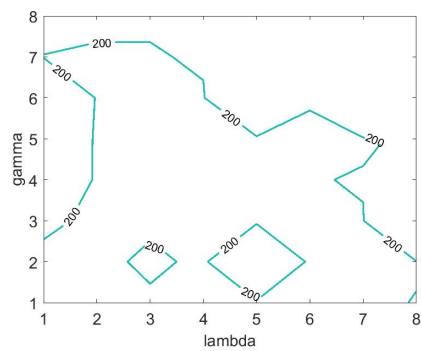
(b) $\beta = 10^{-2}$



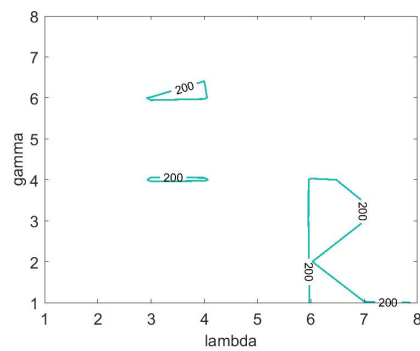
(c) $\beta = 10^{-1}$



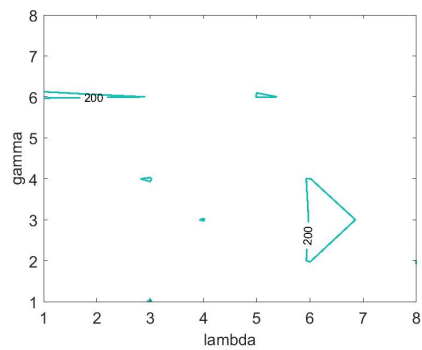
(d) $\beta = 10^0$



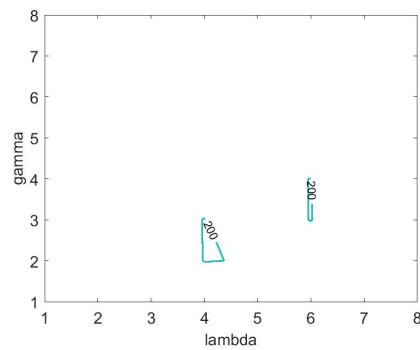
(e) $\beta = 0$



(f) $\beta = 10^1$



(g) $\beta = 10^2$



(h) $\beta = 10^3$

S19

Figure S9: Isocontours for reconstruction error $E \leq 200$

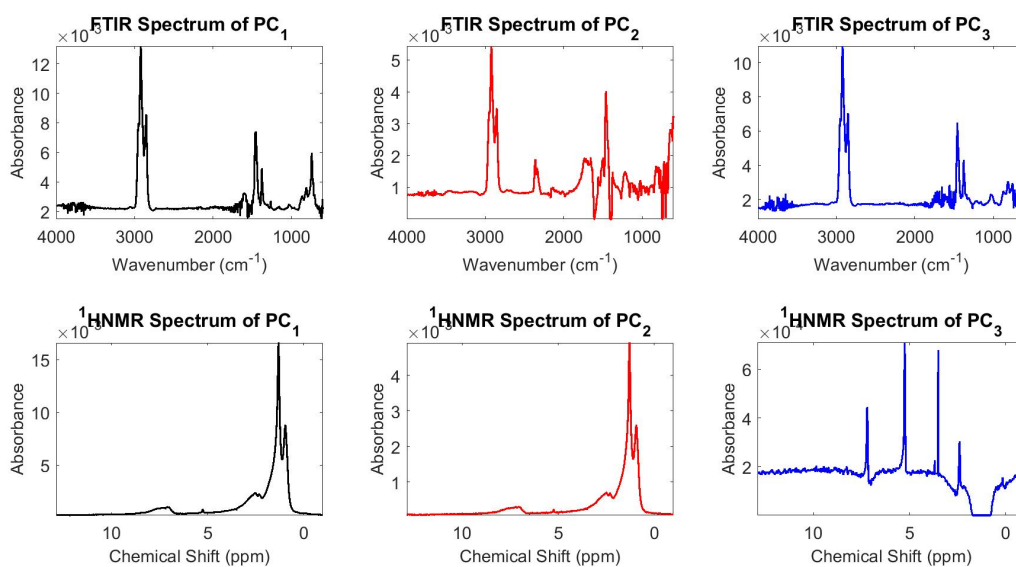
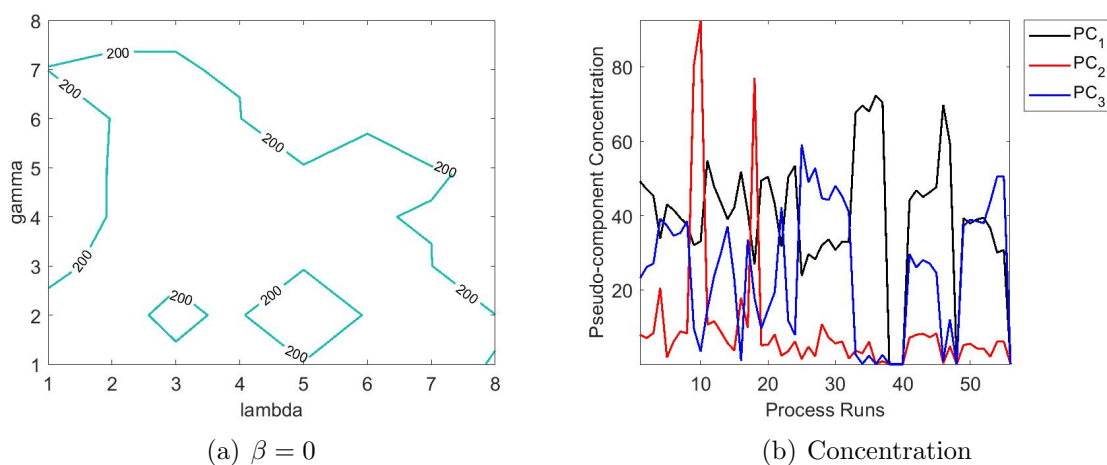


Figure S10: JNMF profiles for $\alpha = 10^0, \beta = 0, \gamma = 0, \lambda = 10^0$

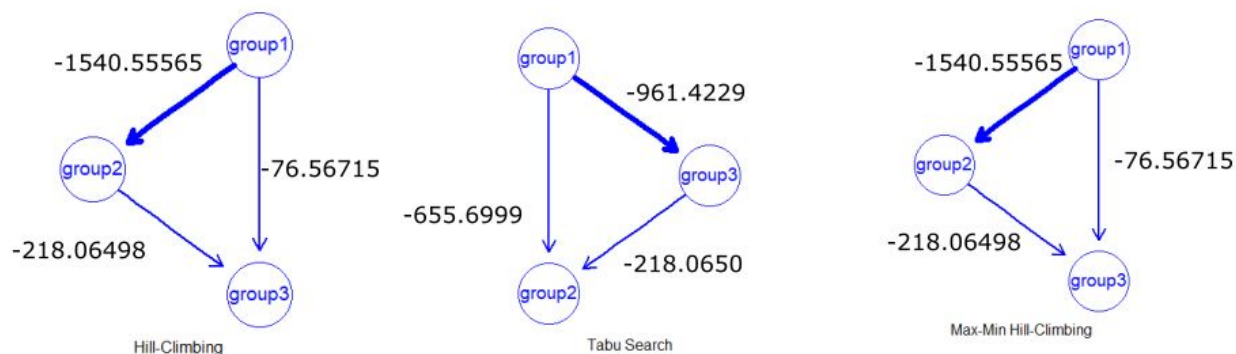
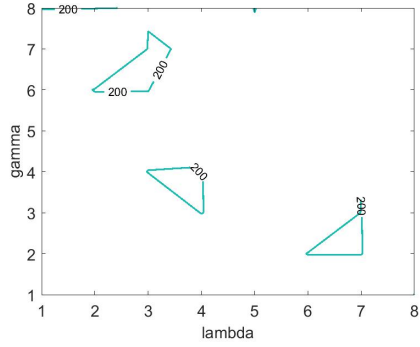
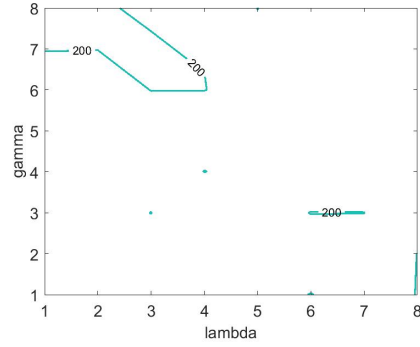


Figure S11: Bayesian networks constructed from the PC spectra

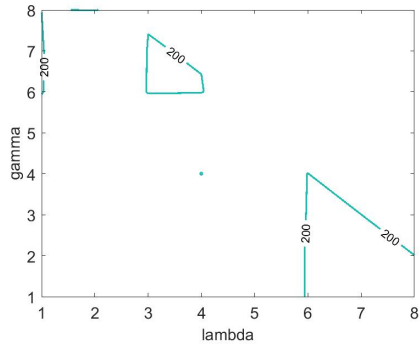
S6 For $\alpha = 0$



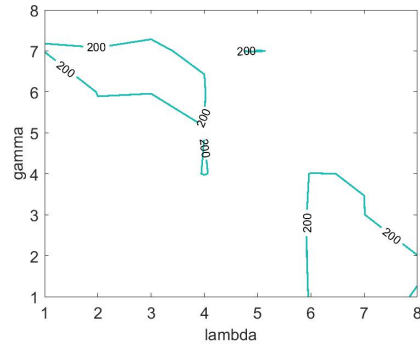
(a) $\beta = 10^{-3}$



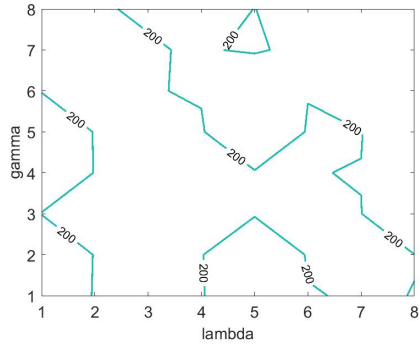
(b) $\beta = 10^{-2}$



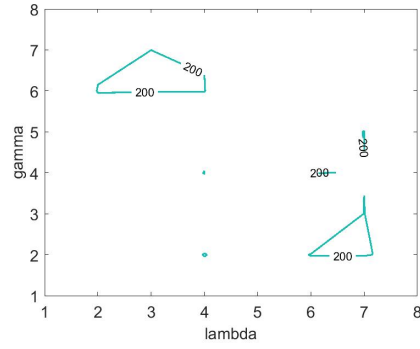
(c) $\beta = 10^{-1}$



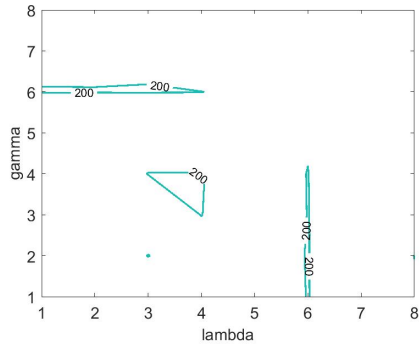
(d) $\beta = 10^0$



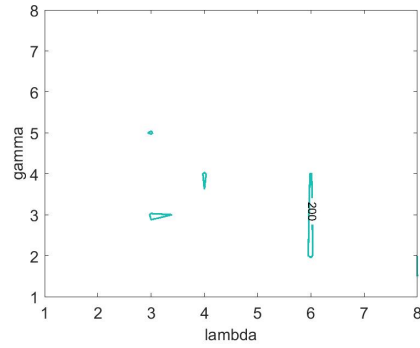
(e) $\beta = 0$



(f) $\beta = 10^1$



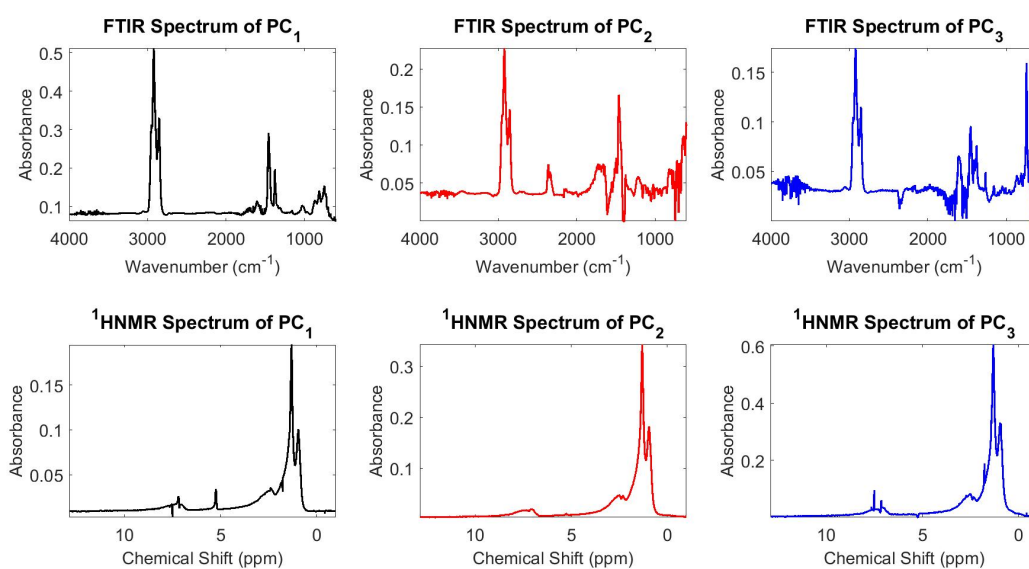
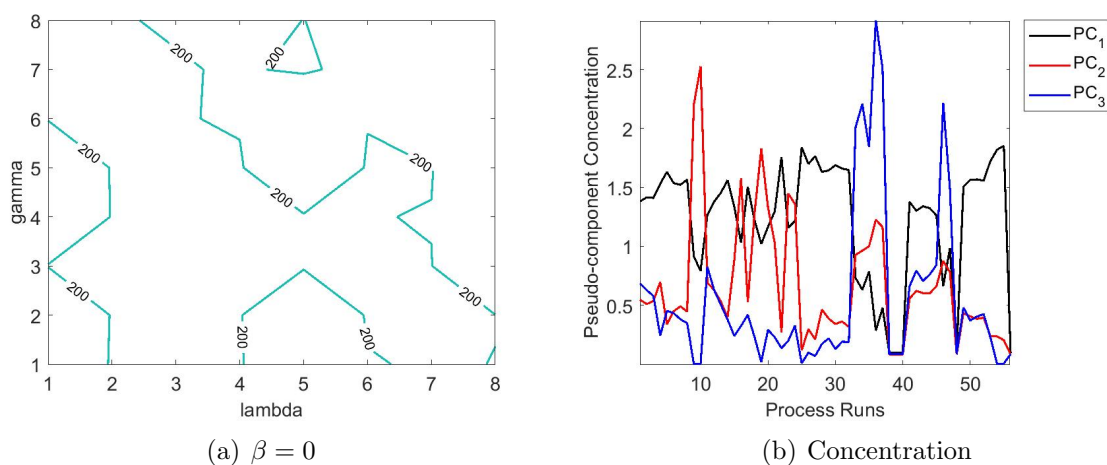
(g) $\beta = 10^2$



(h) $\beta = 10^3$

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Figure S12: Isocontours for reconstruction error $E \leq 200$



(c) Pseudo-component spectra

Figure S13: JNMF profiles for $\alpha = 0, \beta = 0, \gamma = 10^{-2}, \lambda = 10^{-2}$

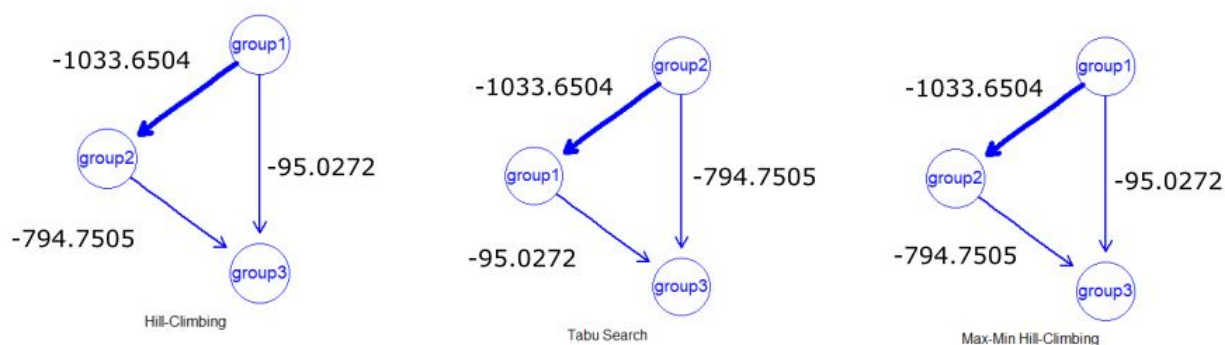
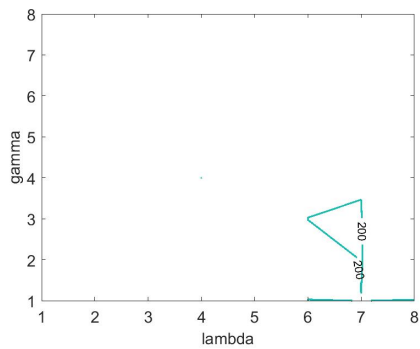
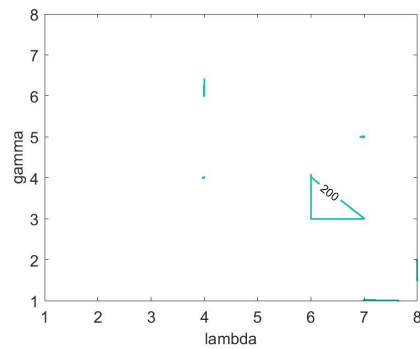


Figure S14: Bayesian networks constructed from the PC spectra

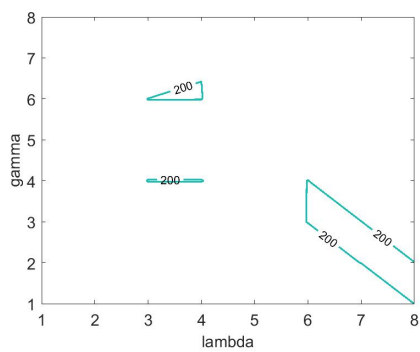
S7 For $\alpha = 10^1$



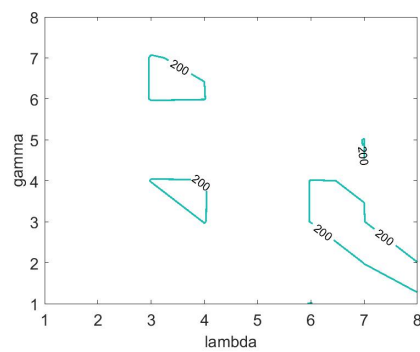
(a) $\beta = 10^{-3}$



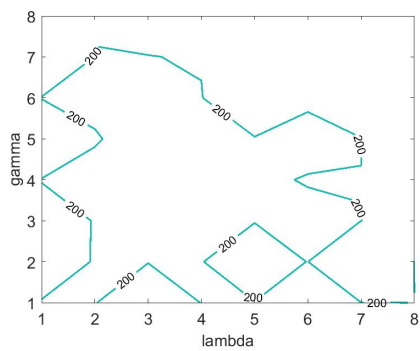
(b) $\beta = 10^{-2}$



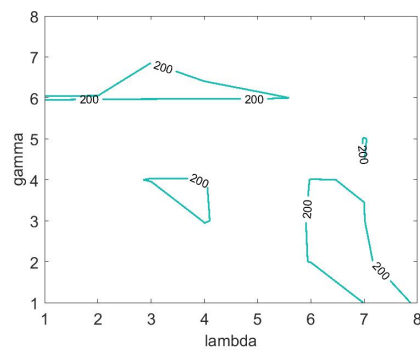
(c) $\beta = 10^{-1}$



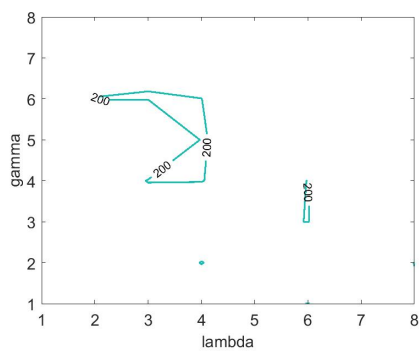
(d) $\beta = 10^0$



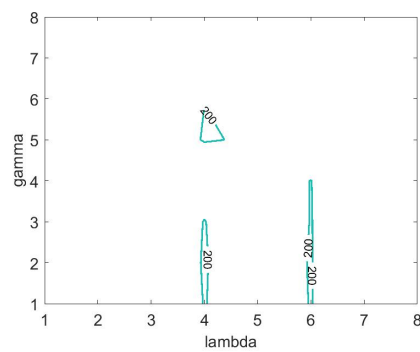
(e) $\beta = 0$



(f) $\beta = 10^1$



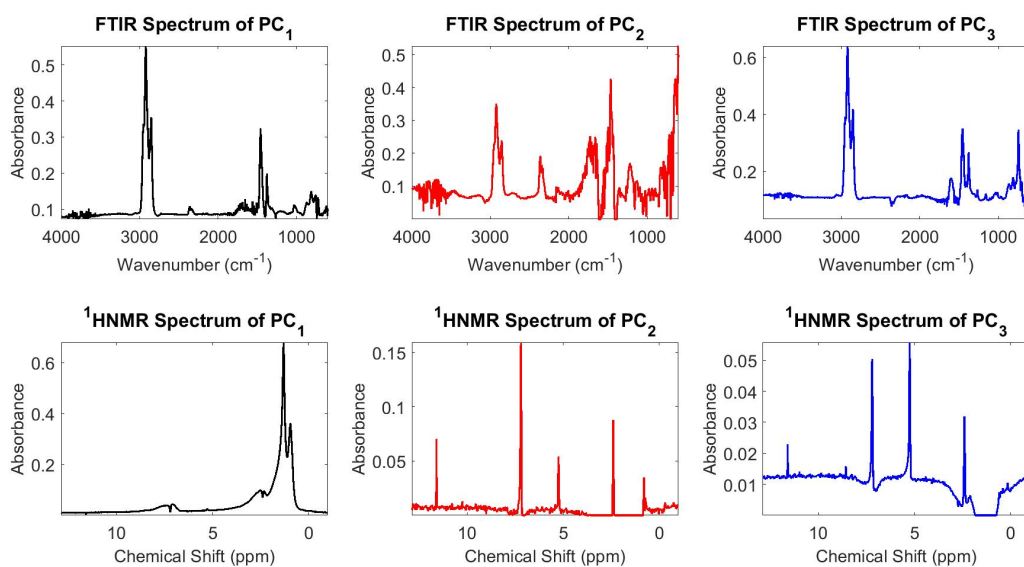
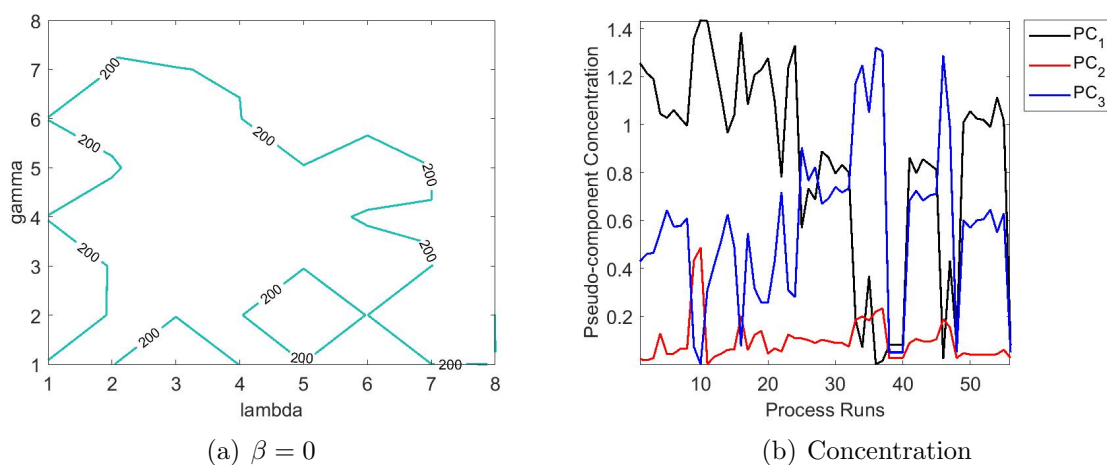
(g) $\beta = 10^2$



(h) $\beta = 10^3$

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Figure S15: Isocontours for reconstruction error $E \leq 200$



(c) Pseudo-component spectra

Figure S16: JNMF profiles for $\alpha = 10^1, \beta = 0, \gamma = 10^{-1}, \lambda = 0$

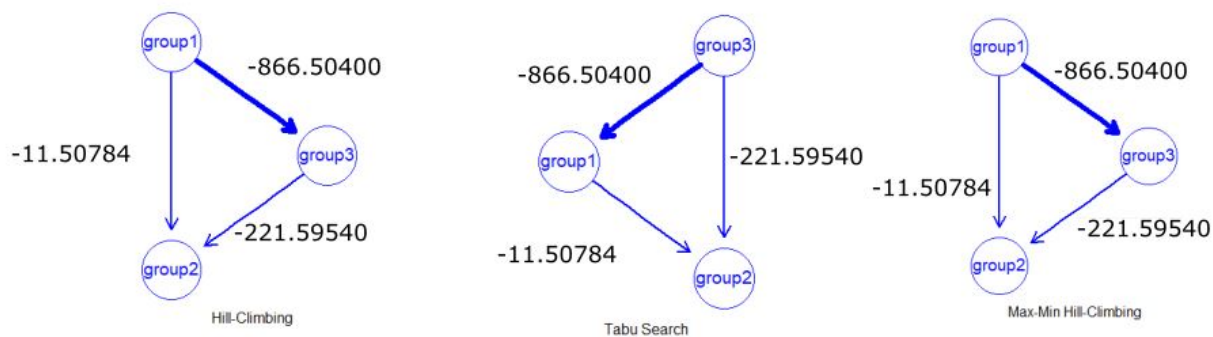
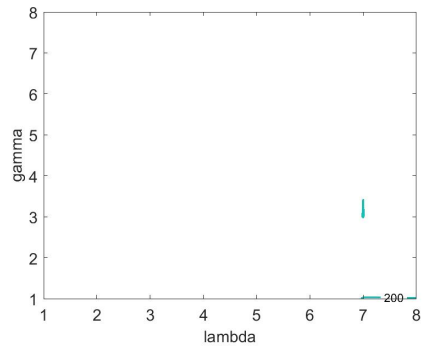
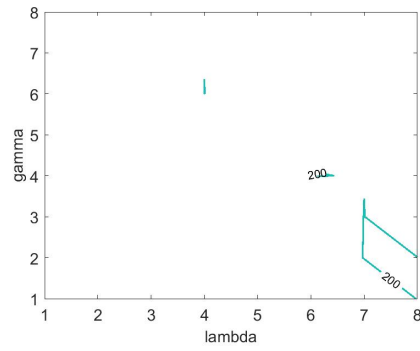


Figure S17: Bayesian networks constructed from the PC spectra

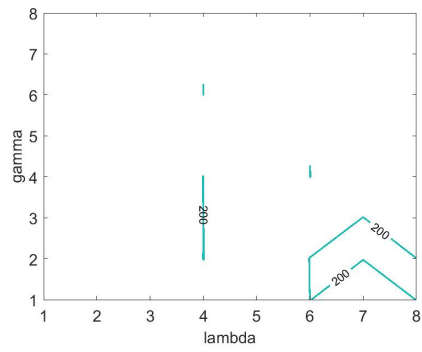
S8 For $\alpha = 10^2$



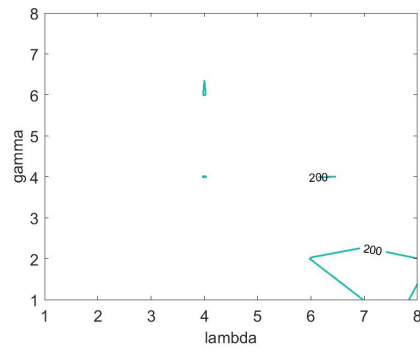
(a) $\beta = 10^{-3}$



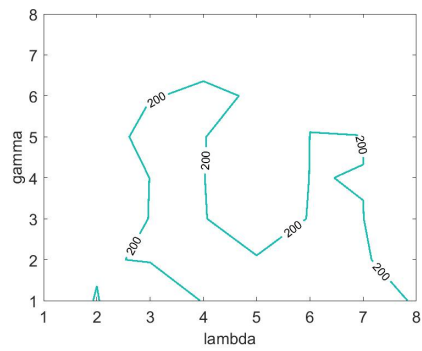
(b) $\beta = 10^{-2}$



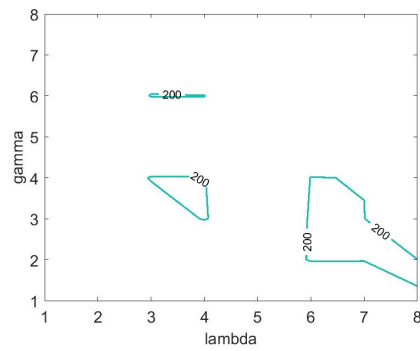
(c) $\beta = 10^{-1}$



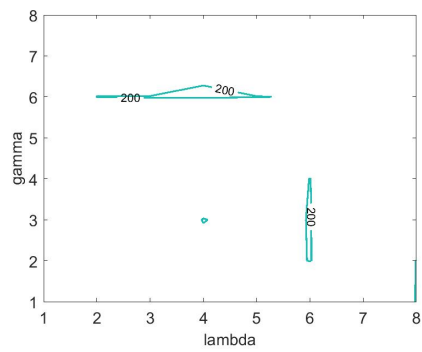
(d) $\beta = 10^0$



(e) $\beta = 0$

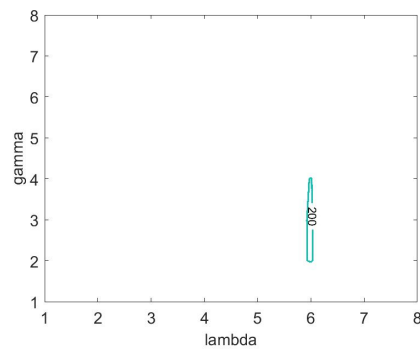


(f) $\beta = 10^1$



(g) $\beta = 10^2$

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(h) $\beta = 10^3$

Figure S18: Isocontours for reconstruction error $E \leq 200$

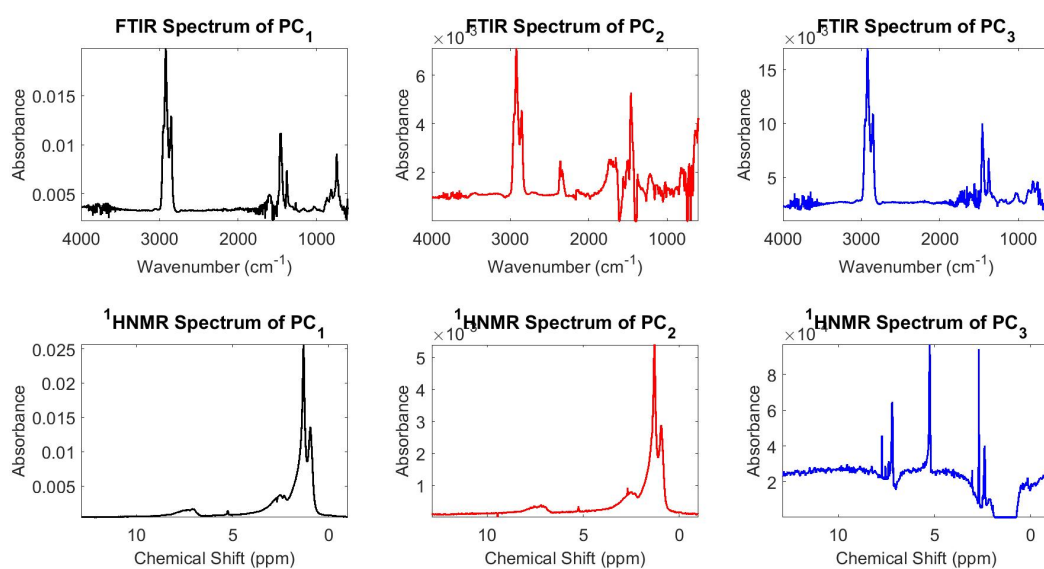
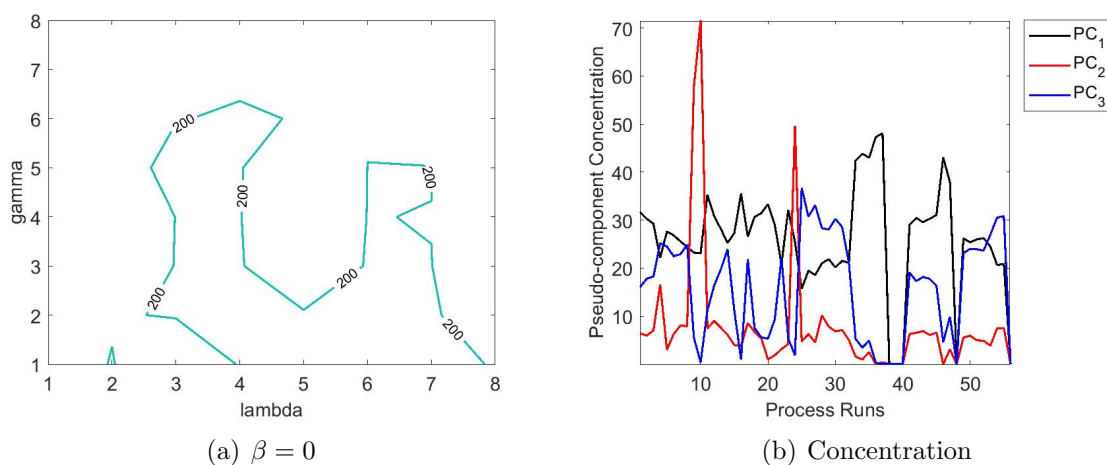


Figure S19: JNMF profiles for $\alpha = 10^2, \beta = 0, \gamma = 10^{-2}, \lambda = 10^0$

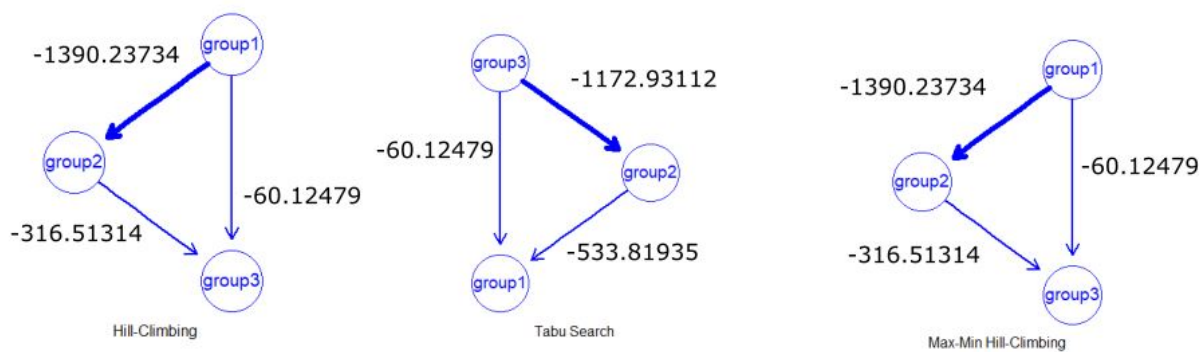
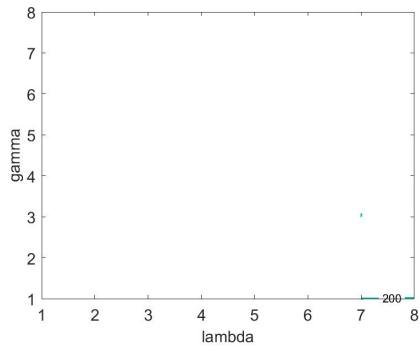
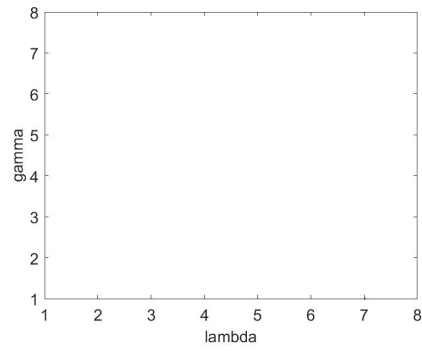


Figure S20: Bayesian networks constructed from the PC spectra

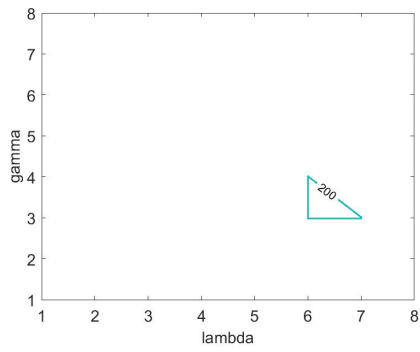
S9 For $\alpha = 10^3$



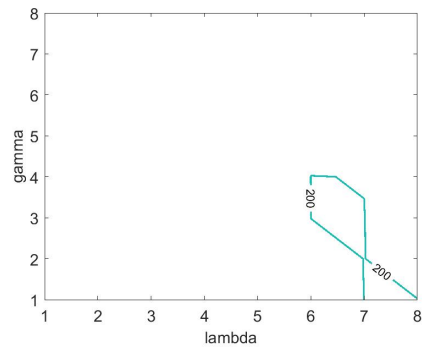
(a) $\beta = 10^{-3}$



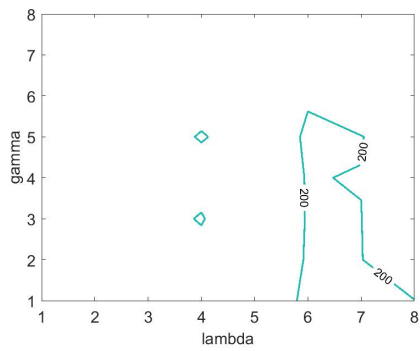
(b) $\beta = 10^{-2}$



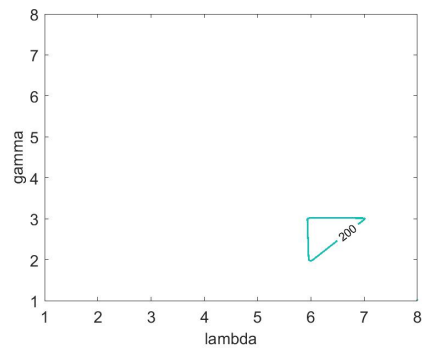
(c) $\beta = 10^{-1}$



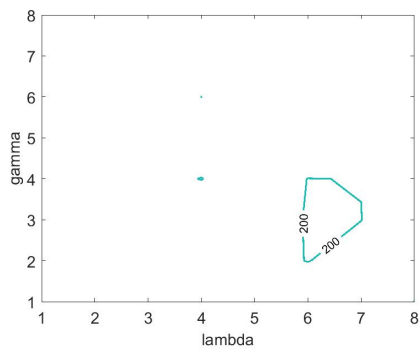
(d) $\beta = 10^0$



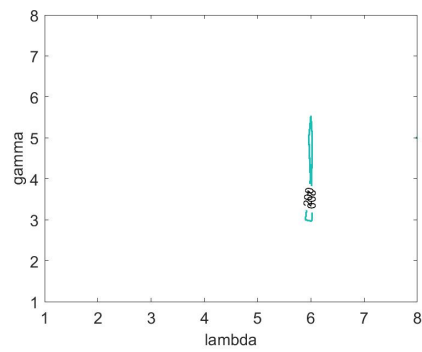
(e) $\beta = 0$



(f) $\beta = 10^1$



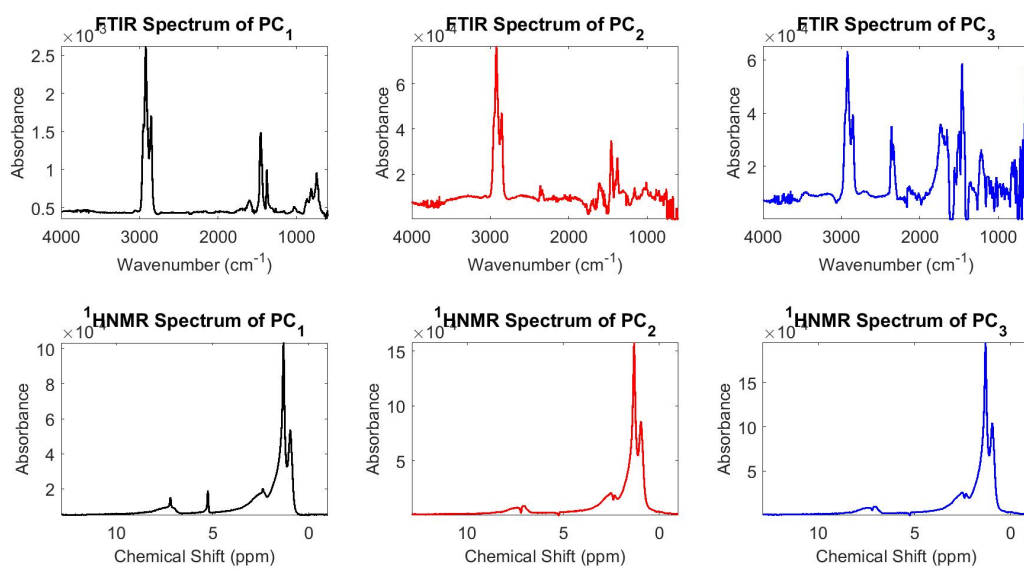
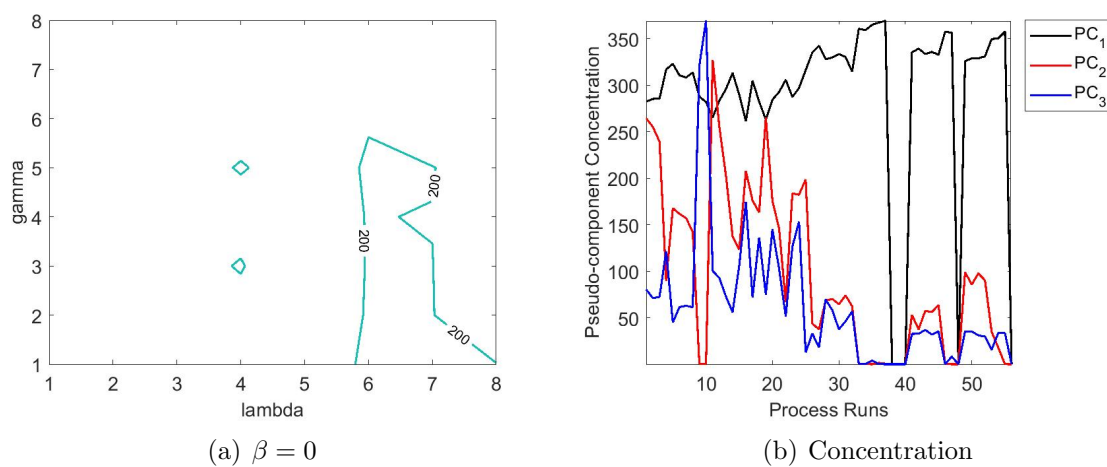
(g) $\beta = 10^2$



(h) $\beta = 10^3$

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Figure S21: Isocontours for reconstruction error $E \leq 200$



(c) Pseudo-component spectra

Figure S22: JNMF profiles for $\alpha = 10^3, \beta = 0, \gamma = 10^{-3}, \lambda = 10^1$

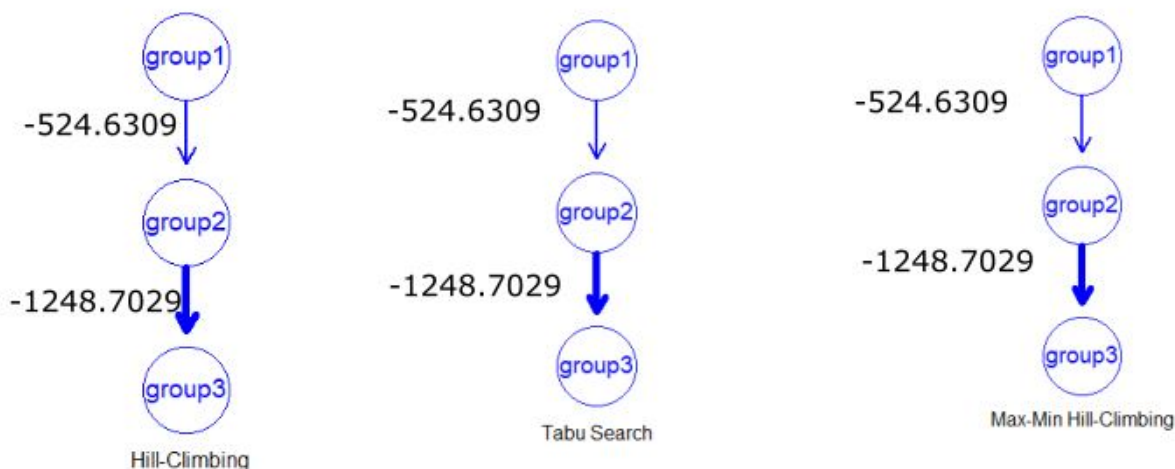


Figure S23: Bayesian networks constructed from the PC spectra

S10 ROD=4 for orthogonal case

Relaxing the rank in the factorization of the objective beyond 4 factors in noisy pseudo-components which is undesirable. The reported results of the factorization for a rank of 4 pseudocomponents given below did not satisfy the convergence criteria within 5000 iterations and had a relatively higher reconstruction error.

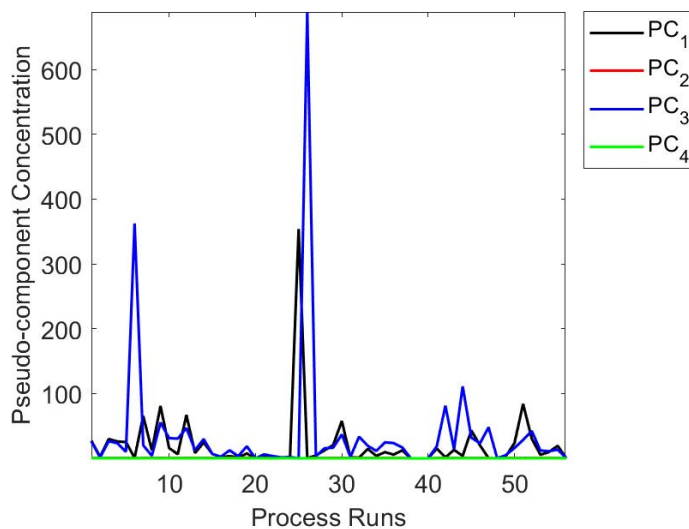


Figure S24: Concentration profiles

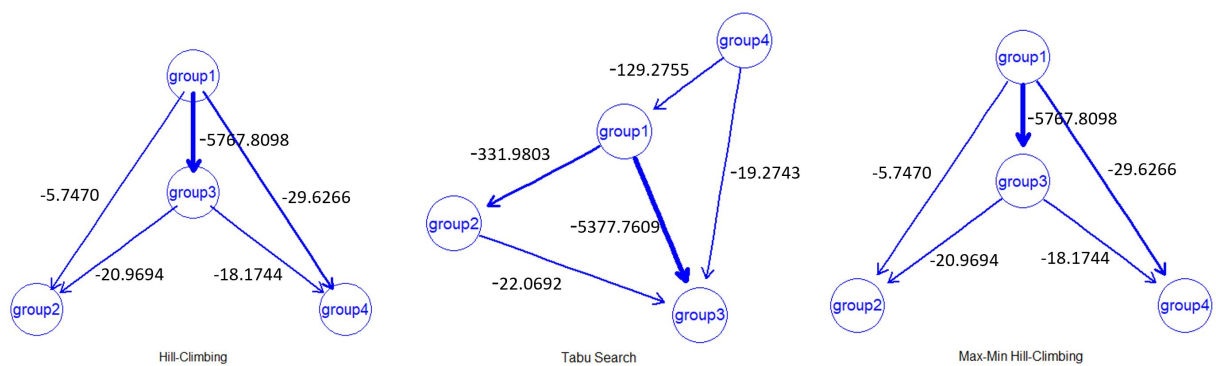
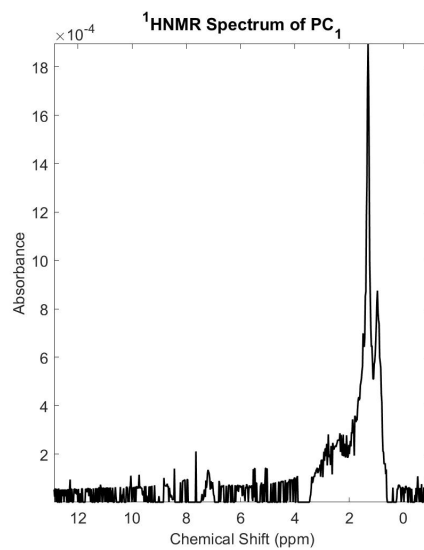
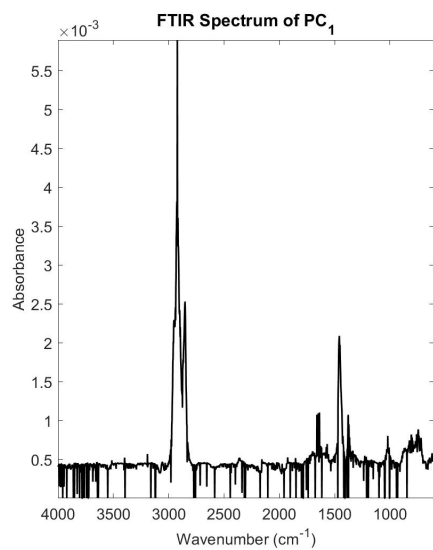
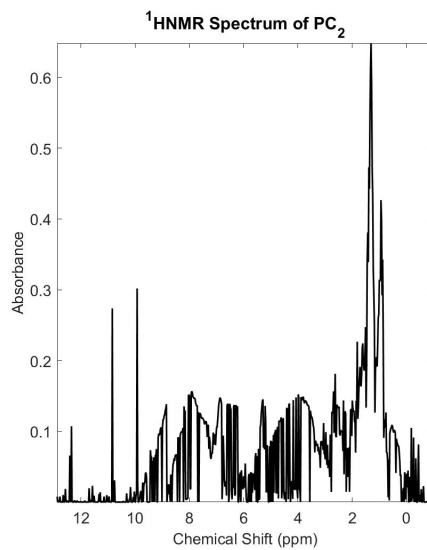
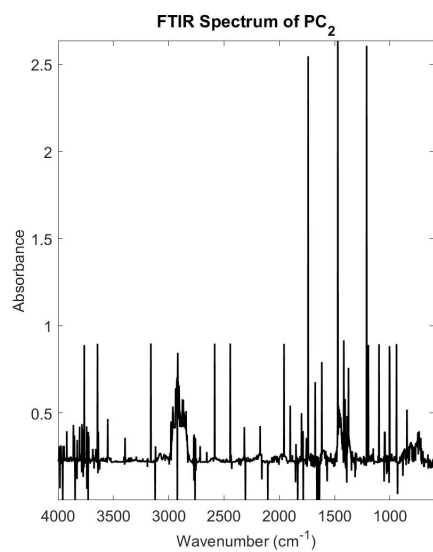


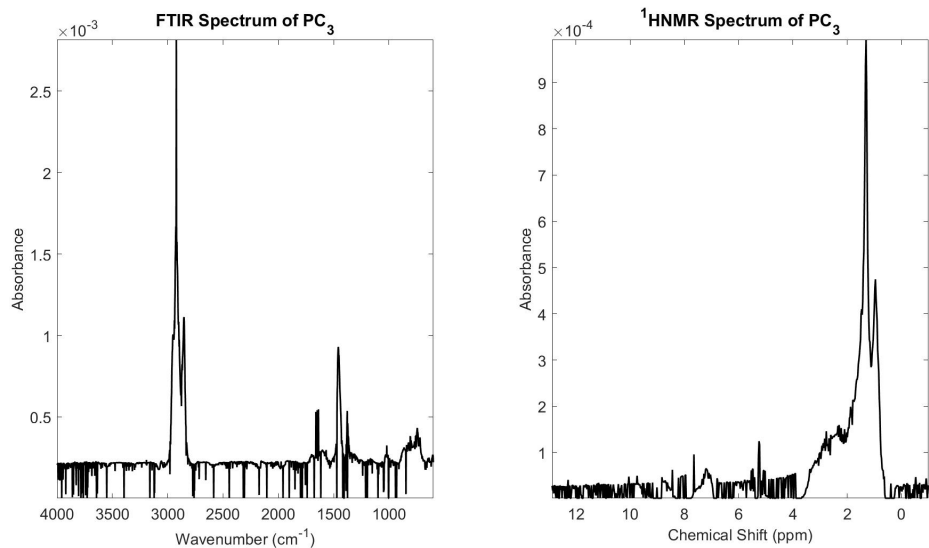
Figure S25: Bayesian networks constructed from the PC spectra



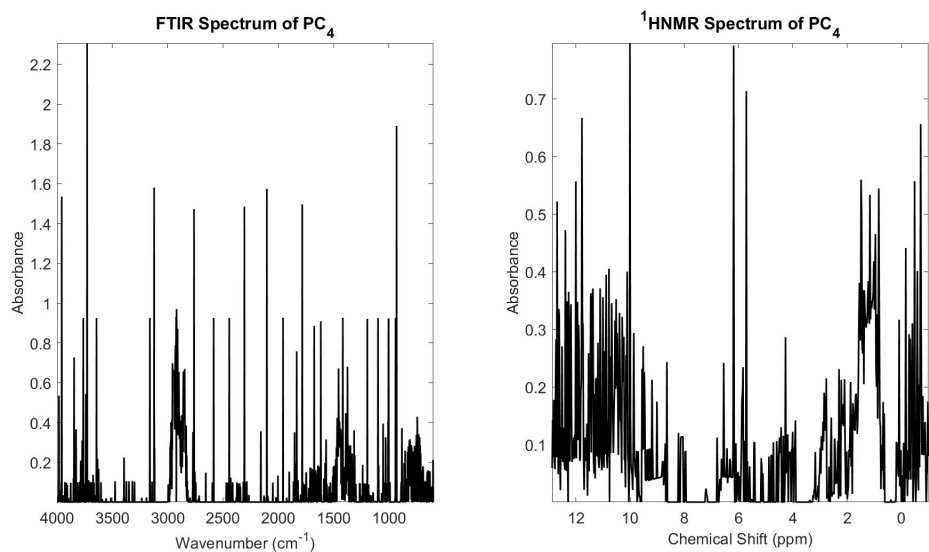
(a) PC_1



(b) PC_2



(c) PC_3



(d) PC_4

Figure S26: Pseudo-component spectra for rank= 4