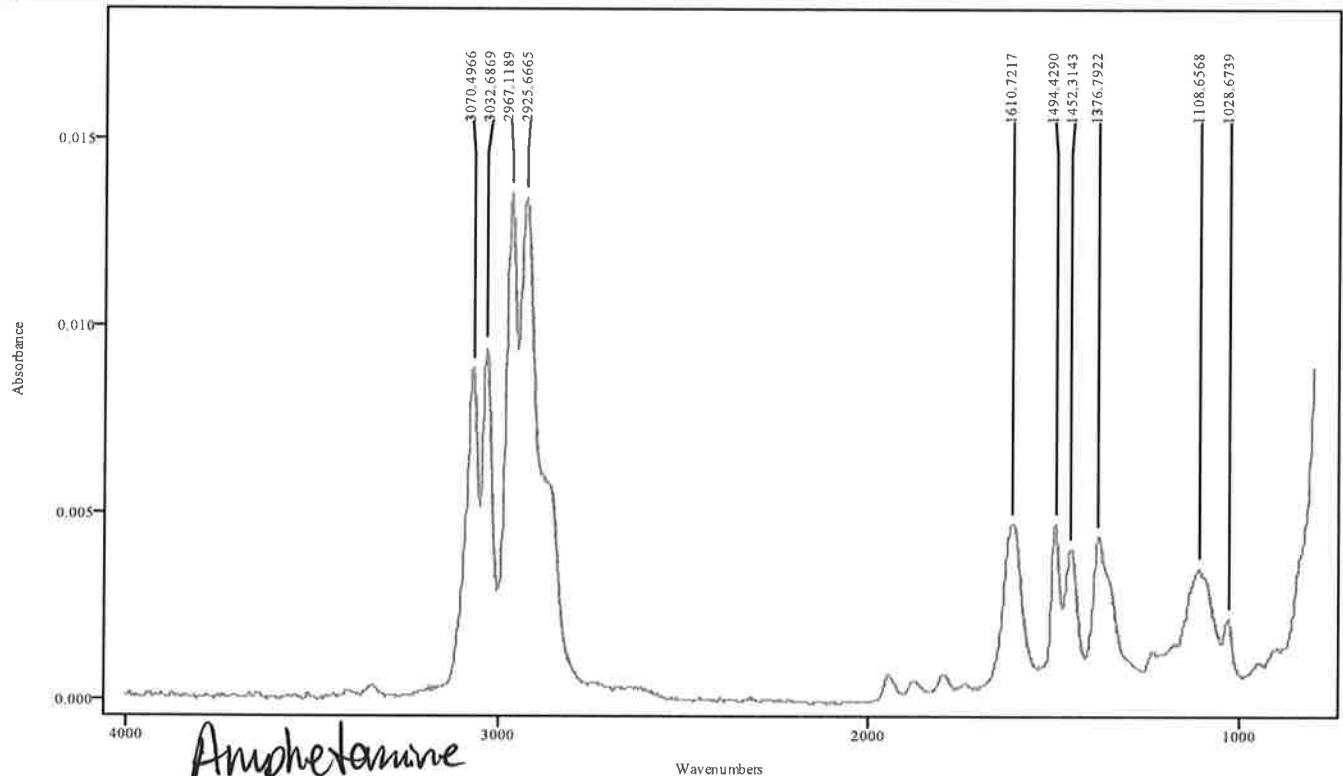


Wavenumber Accuracy

MH

Manual Peak Pick Results

Sample Filename	IRDATA.SPC
File Title	4.80 minutes: AVE (4.79: 4.81) Ref. (4.55: 4.77) of AMPHETAMINE MIX 2MGML 2020_February_21_160743.cgm
Date	Wed Mar 04 14:34:30 2020



IRDATA.SPC: 4.80 minutes: AVE (4.79: 4.81) Ref. (4.55: 4.77) of AMPHETAMINE MIX 2MGML 2020_February_21_160743.cgm

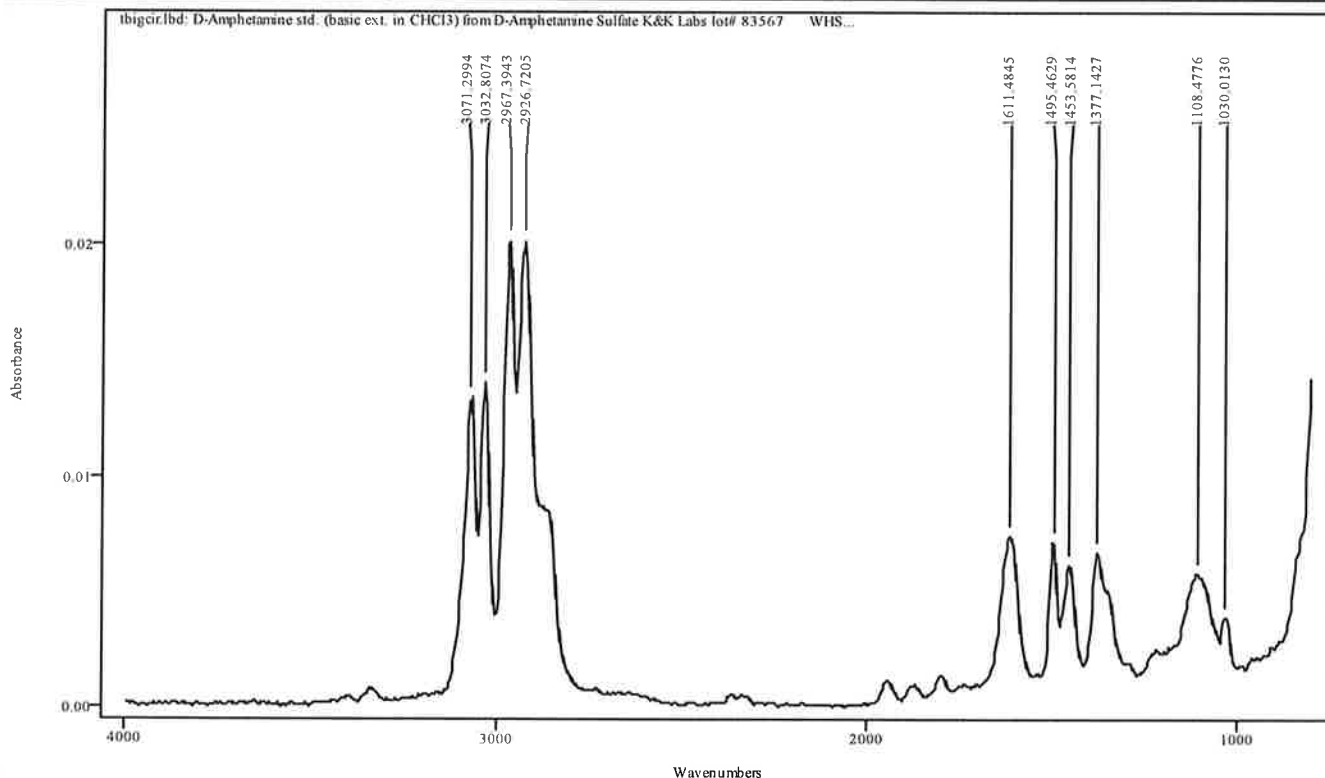
Filename	Peak At	Peak Height
IRDATA.SPC [0]	1028.6739	0.0022
IRDATA.SPC [0]	1108.6568	0.0035
IRDATA.SPC [0]	1376.7922	0.0044
IRDATA.SPC [0]	1452.3143	0.0041
IRDATA.SPC [0]	1494.4290	0.0047
IRDATA.SPC [0]	1610.7217	0.0047
IRDATA.SPC [0]	2925.6665	0.0134
IRDATA.SPC [0]	2967.1189	0.0135
IRDATA.SPC [0]	3032.6869	0.0094
IRDATA.SPC [0]	3070.4966	0.0089

Within +/- 2 cm⁻¹

MA

Manual Peak Pick Results

Sample Filename	Entry 2 from Library tbigcir.lbd
File Title	D-Amphetamine std. (basic ext. in CHCl3) from D-Amphetamine Sulfate K&K Labs lot# 83567 WHS
Date	Wed Mar 04 14:35:21 2020



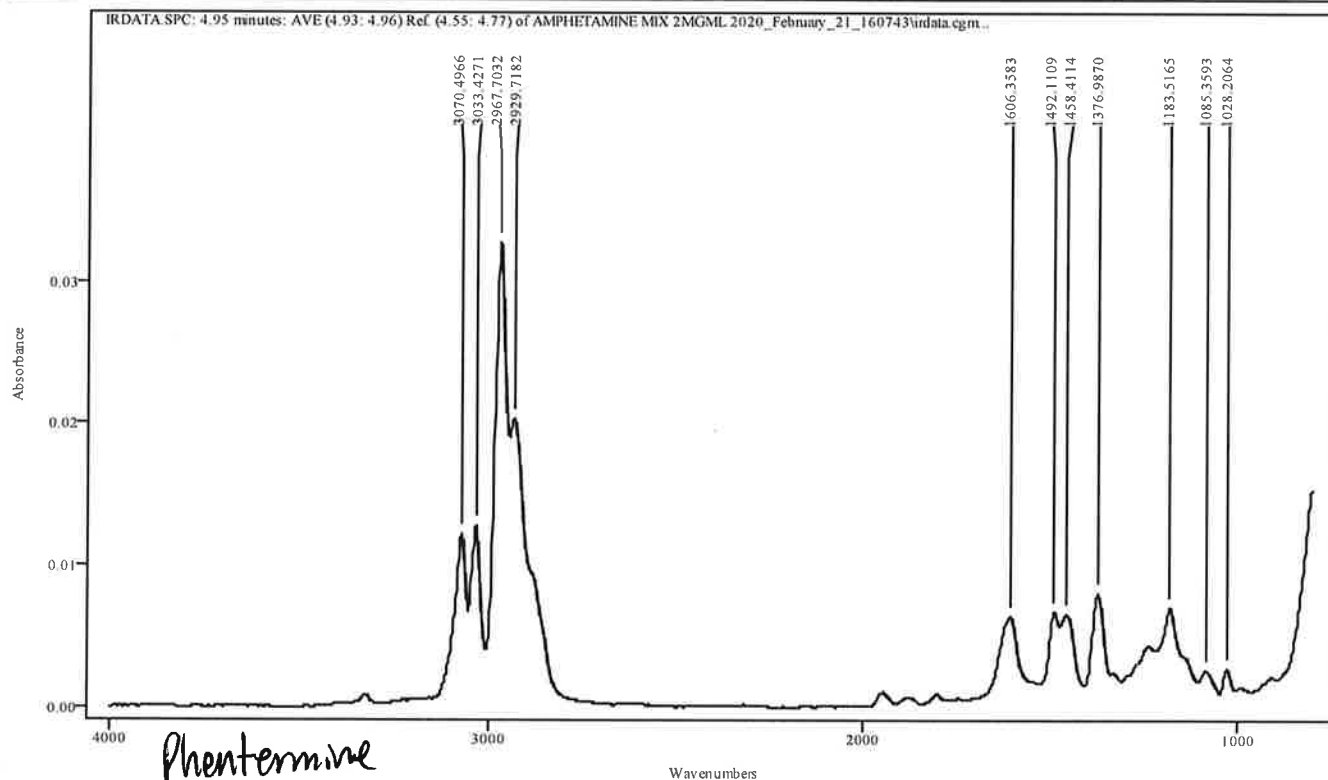
Entry 2 from Library tbigcir.lbd: D-Amphetamine std. (basic ext. in CHCl3) from D-Amphetamine Sulfate K&K Labs lot# 83567 WHS

Filename	Peak At	Peak Height
tbigcir.lbd [2]	1030.0130	0.0039
tbigcir.lbd [2]	1108.4776	0.0058
tbigcir.lbd [2]	1377.1427	0.0067
tbigcir.lbd [2]	1453.5814	0.0061
tbigcir.lbd [2]	1495.4629	0.0071
tbigcir.lbd [2]	1611.4845	0.0074
tbigcir.lbd [2]	2926.7205	0.0201
tbigcir.lbd [2]	2967.3943	0.0202
tbigcir.lbd [2]	3032.8074	0.0141
tbigcir.lbd [2]	3071.2994	0.0134

JA

Manual Peak Pick Results

Sample Filename	IRDATA.SPC
File Title	4.95 minutes: AVE (4.93: 4.96) Ref. (4.55: 4.77) of AMPHETAMINE MIX 2MGML 2020_February_21_160743.cgm
Date	Wed Mar 04 14:48:42 2020



IRDATA.SPC: 4.95 minutes: AVE (4.93: 4.96) Ref. (4.55: 4.77) of AMPHETAMINE MIX 2MGML 2020_February_21_160743.cgm

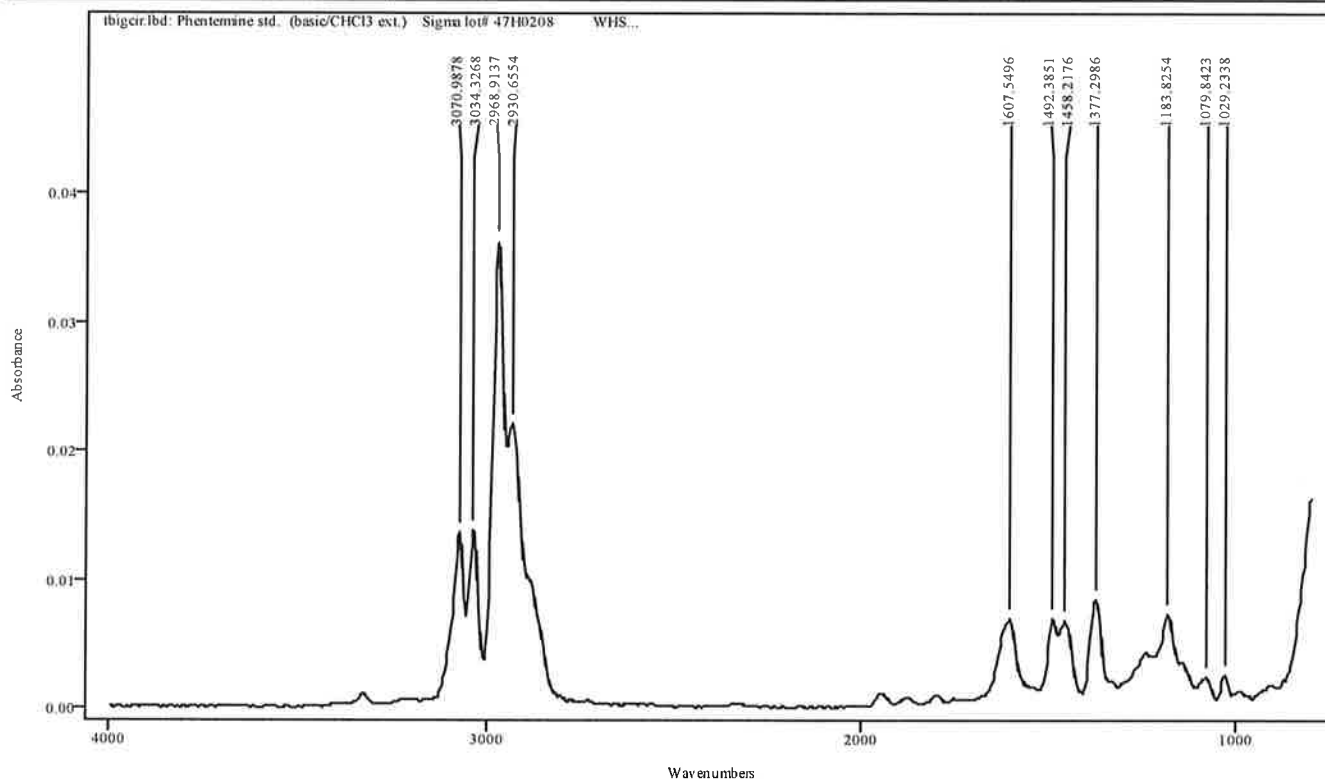
Filename	Peak At	Peak Height
IRDATA.SPC [0]	1028.2064	0.0027
IRDATA.SPC [0]	1085.3593	0.0026
IRDATA.SPC [0]	1183.5165	0.0070
IRDATA.SPC [0]	1376.9870	0.0081
IRDATA.SPC [0]	1458.4114	0.0066
IRDATA.SPC [0]	1492.1109	0.0068
IRDATA.SPC [0]	1606.3583	0.0065
IRDATA.SPC [0]	2929.7182	0.0204
IRDATA.SPC [0]	2967.7032	0.0328
IRDATA.SPC [0]	3033.4271	0.0128
IRDATA.SPC [0]	3070.4966	0.0122

within $\pm 6 \text{ cm}^{-1}$

Manual Peak Pick Results

CH

Sample Filename	Entry 5 from Library tbigcir.lbd		
File Title	Phentermine std. (basic/CHCl3 ext.)	Sigma lot# 47H0208	WHS
Date	Wed Mar 04 14:49:08 2020		



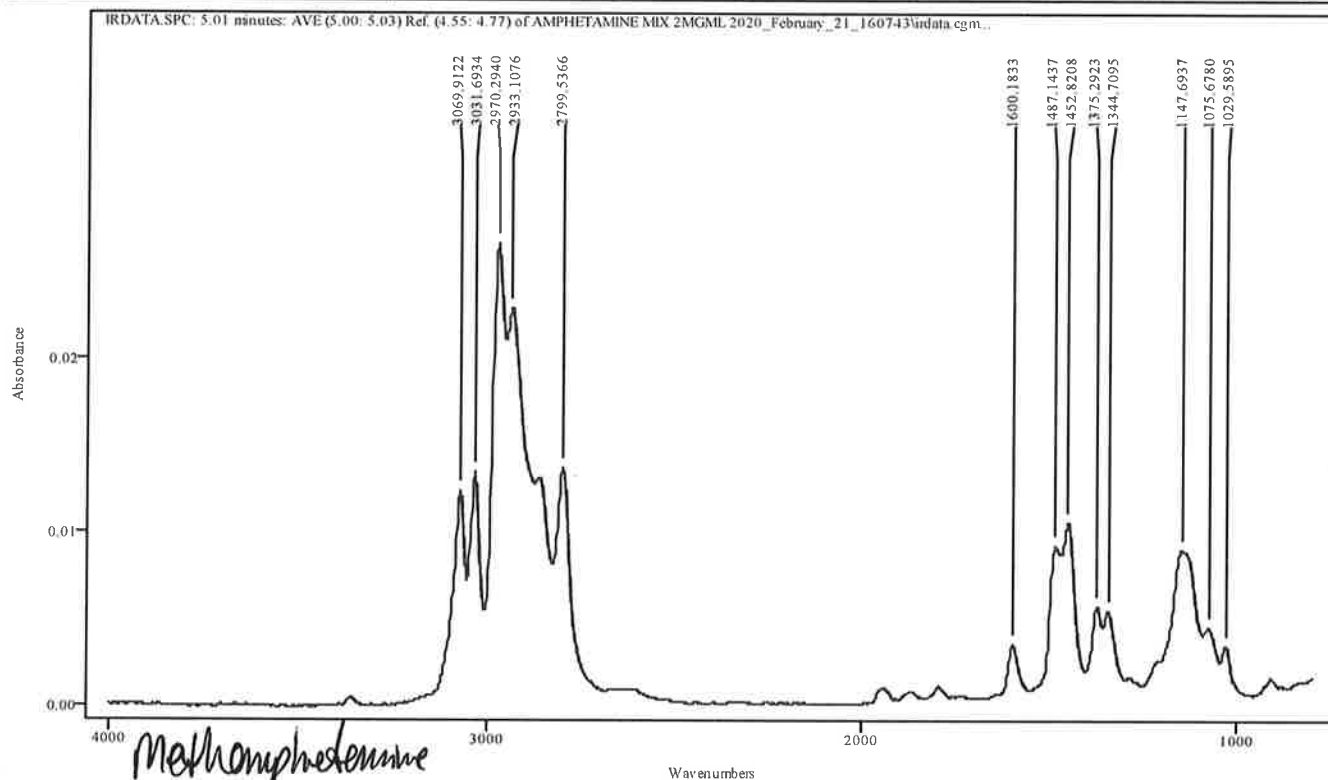
Entry 5 from Library tbigcir.lbd: Phentermine std. (basic/CHCl3 ext.) Sigma lot# 47H0208
WHS

Filename	Peak At	Peak Height
tbigcir.lbd [5]	1029.2338	0.0026
tbigcir.lbd [5]	1079.8423	0.0024
tbigcir.lbd [5]	1183.8254	0.0073
tbigcir.lbd [5]	1377.2986	0.0085
tbigcir.lbd [5]	1458.2176	0.0068
tbigcir.lbd [5]	1492.3851	0.0070
tbigcir.lbd [5]	1607.5496	0.0069
tbigcir.lbd [5]	2930.6554	0.0221
tbigcir.lbd [5]	2968.9137	0.0363
tbigcir.lbd [5]	3034.3268	0.0139
tbigcir.lbd [5]	3070.9878	0.0136

Manual Peak Pick Results

MA

Sample Filename	IRDATA.SPC
File Title	5.01 minutes: AVE (5.00: 5.03) Ref. (4.55: 4.77) of AMPHETAMINE MIX 2MGML 2020_February_21_160743.cgm
Date	Wed Mar 04 14:46:41 2020



IRDATA.SPC: 5.01 minutes: AVE (5.00: 5.03) Ref. (4.55: 4.77) of AMPHETAMINE MIX 2MGML 2020_February_21_160743.cgm

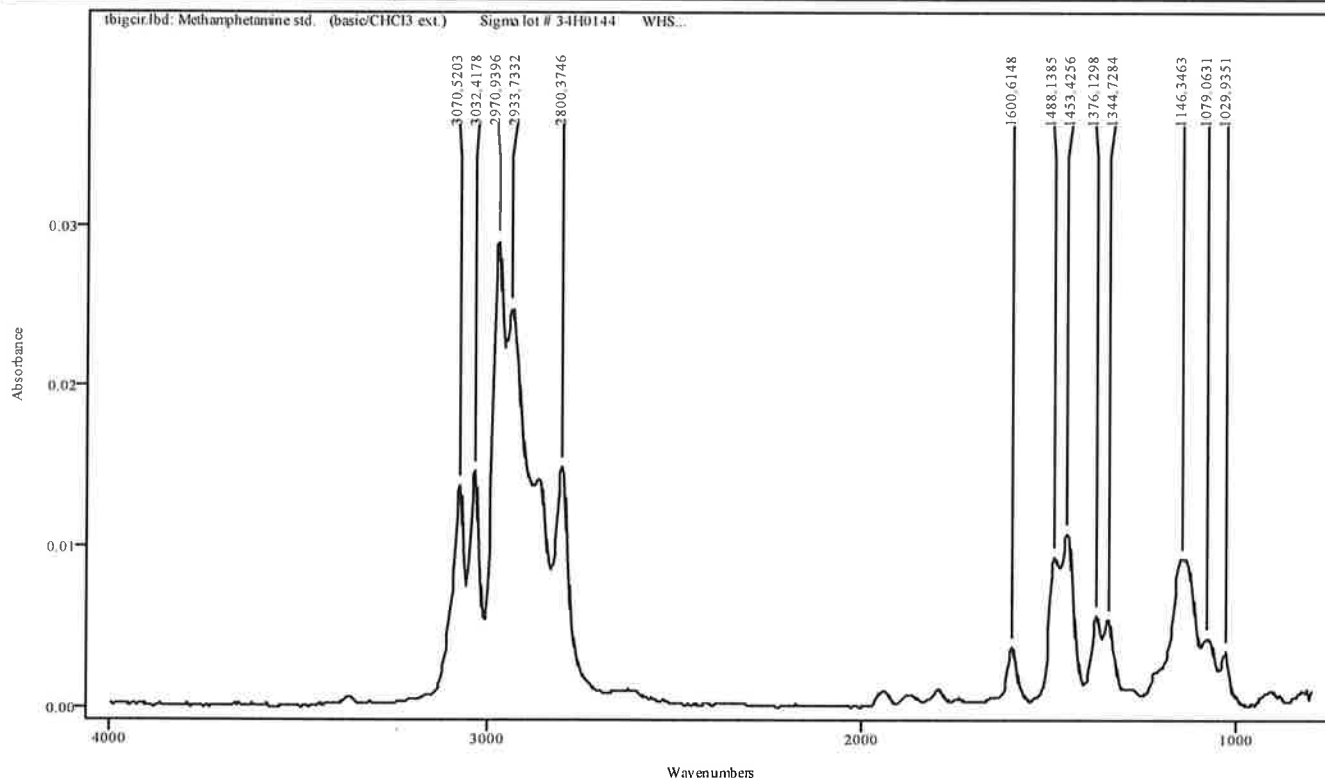
Filename	Peak At	Peak Height
IRDATA.SPC [0]	1029.5895	0.0036
IRDATA.SPC [0]	1075.6780	0.0046
IRDATA.SPC [0]	1147.6937	0.0090
IRDATA.SPC [0]	1344.7095	0.0056
IRDATA.SPC [0]	1375.2923	0.0058
IRDATA.SPC [0]	1452.8208	0.0106
IRDATA.SPC [0]	1487.1437	0.0093
IRDATA.SPC [0]	1600.1833	0.0036
IRDATA.SPC [0]	2799.5366	0.0137
IRDATA.SPC [0]	2933.1076	0.0229
IRDATA.SPC [0]	2970.2940	0.0267
IRDATA.SPC [0]	3031.6934	0.0134
IRDATA.SPC [0]	3069.9122	0.0124

within +/- 4 cm⁻¹

CH

Manual Peak Pick Results

Sample Filename	Entry 4 from Library tbigcir.lbd	
File Title	Methamphetamine std. (basic/CHCl3 ext.) WHS	Sigma lot # 34H0144
Date	Wed Mar 04 14:43:31 2020	



Entry 4 from Library tbigcir.lbd: Methamphetamine std. (basic/CHCl3 ext.)
34H0144 WHS

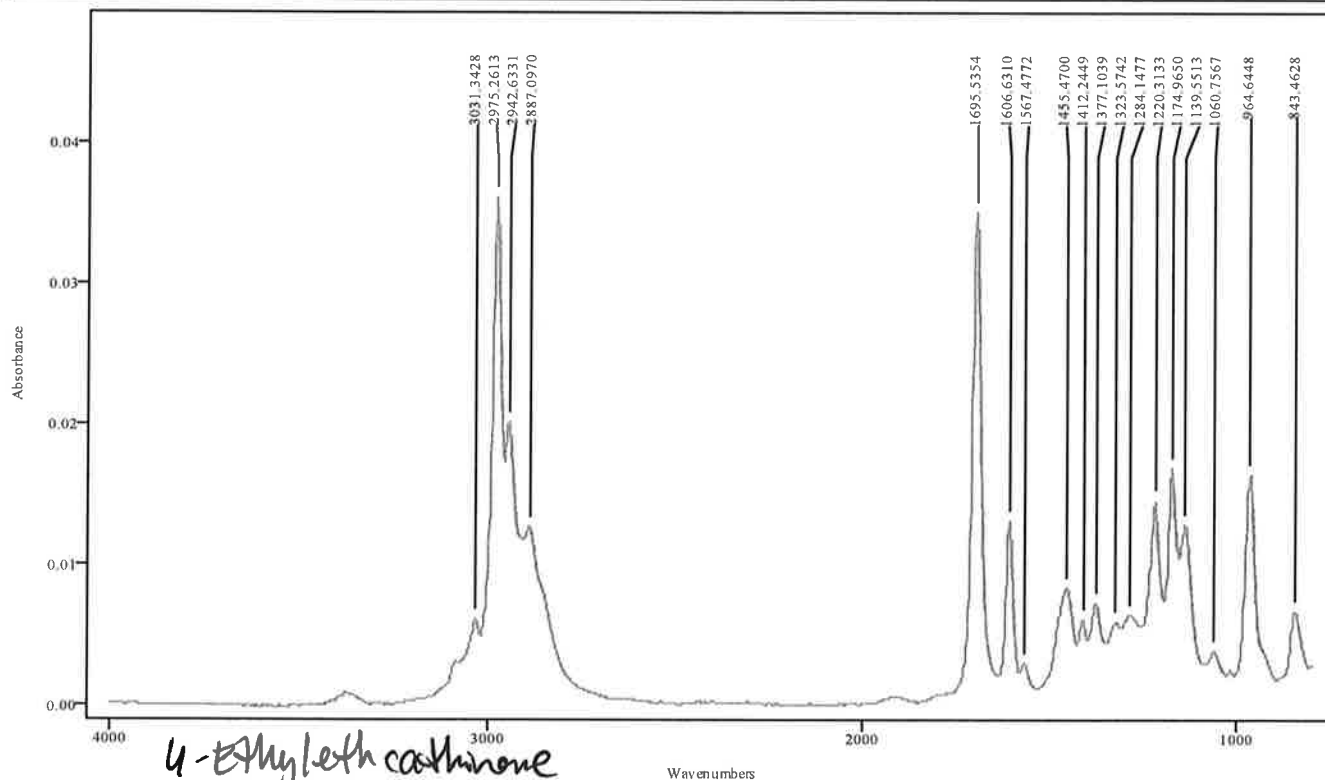
Sigma lot #

Filename	Peak At	Peak Height
tbigcir.lbd [4]	1029.9351	0.0035
tbigcir.lbd [4]	1079.0631	0.0043
tbigcir.lbd [4]	1146.3463	0.0093
tbigcir.lbd [4]	1344.7284	0.0054
tbigcir.lbd [4]	1376.1298	0.0057
tbigcir.lbd [4]	1453.4256	0.0108
tbigcir.lbd [4]	1488.1385	0.0094
tbigcir.lbd [4]	1600.6148	0.0038
tbigcir.lbd [4]	2800.3746	0.0150
tbigcir.lbd [4]	2933.7332	0.0248
tbigcir.lbd [4]	2970.9396	0.0290
tbigcir.lbd [4]	3032.4178	0.0148
tbigcir.lbd [4]	3070.5203	0.0138

Manual Peak Pick Results

MA

Sample Filename	IRDATA.SPC
File Title	4.12 minutes: AVE (4.11: 4.14) Ref. (3.82: 4.09) of 4-ETHYLETHCATH 2MGML 2020_February_21_173456.cgm
Date	Wed Mar 04 14:56:55 2020



IRDATA.SPC: 4.12 minutes: AVE (4.11: 4.14) Ref. (3.82: 4.09) of 4-ETHYLETHCATH 2MGML 2020_February_21_173456.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	843.4628	0.0068
IRDATA.SPC [0]	964.6448	0.0165
IRDATA.SPC [0]	1060.7567	0.0040
IRDATA.SPC [0]	1139.5513	0.0128
IRDATA.SPC [0]	1174.9650	0.0169
IRDATA.SPC [0]	1220.3133	0.0146
IRDATA.SPC [0]	1284.1477	0.0065
IRDATA.SPC [0]	1323.5742	0.0060
IRDATA.SPC [0]	1377.1039	0.0074
IRDATA.SPC [0]	1412.2449	0.0062
IRDATA.SPC [0]	1455.4700	0.0083
IRDATA.SPC [0]	1567.4772	0.0030
IRDATA.SPC [0]	1606.6310	0.0132

within +/- 4 cm⁻¹

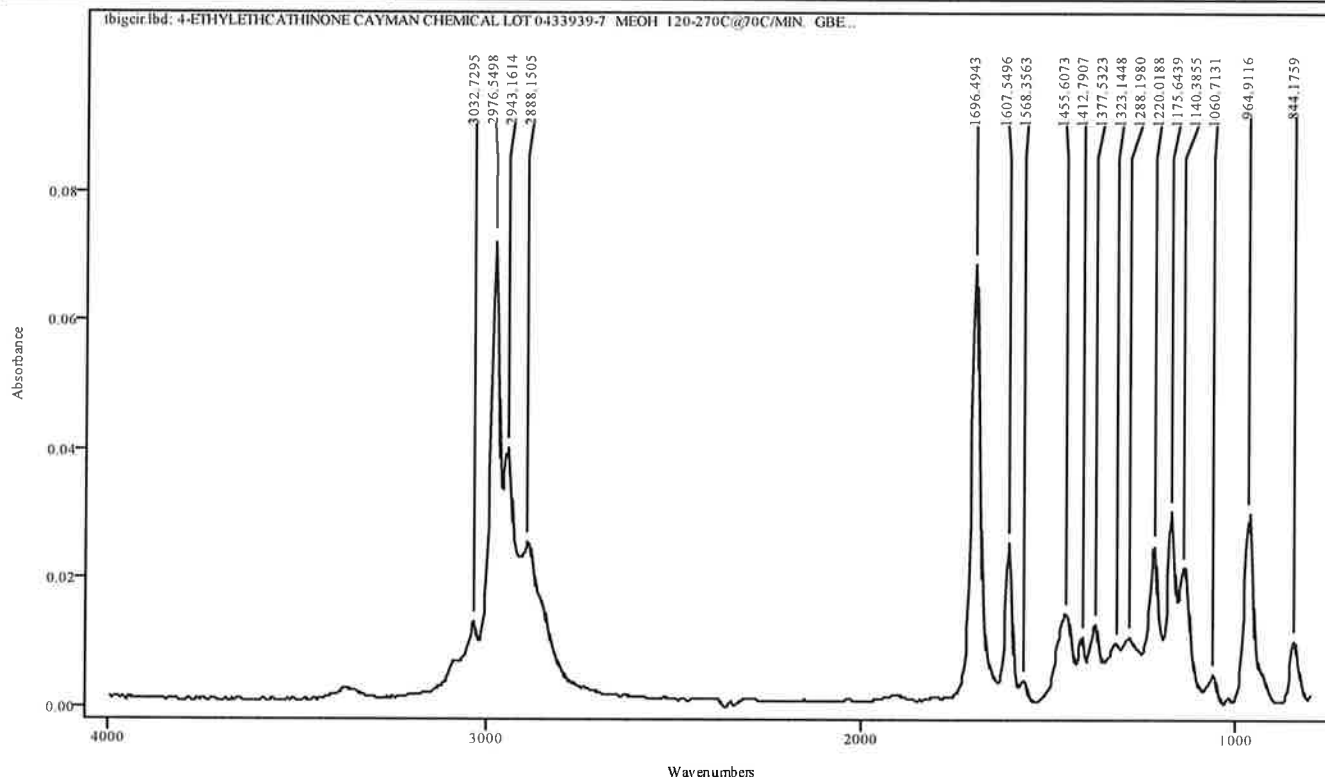
IRDATA.SPC [0]	1695.5354	0.0351
IRDATA.SPC [0]	2887.0970	0.0128
IRDATA.SPC [0]	2942.6331	0.0202
IRDATA.SPC [0]	2975.2613	0.0362
IRDATA.SPC [0]	3031.3428	0.0062

MA

MA

Manual Peak Pick Results

Sample Filename	Entry 285 from Library tbigcir.lbd
File Title	4-ETHYLETHCATHINONE CAYMAN CHEMICAL LOT 0433939-7 MEOH 120-270C@70C/MIN. GBE
Date	Wed Mar 04 14:57:33 2020



Entry 285 from Library tbigcir.lbd: 4-ETHYLETHCATHINONE CAYMAN CHEMICAL LOT 0433939-7 MEOH 120-270C@70C/MIN. GBE

Filename	Peak At	Peak Height
tbigcir.lbd [285]	844.1759	0.0105
tbigcir.lbd [285]	964.9116	0.0301
tbigcir.lbd [285]	1060.7131	0.0052
tbigcir.lbd [285]	1140.3855	0.0218
tbigcir.lbd [285]	1175.6439	0.0307
tbigcir.lbd [285]	1220.0188	0.0252
tbigcir.lbd [285]	1288.1980	0.0109
tbigcir.lbd [285]	1323.1448	0.0102
tbigcir.lbd [285]	1377.5323	0.0130
tbigcir.lbd [285]	1412.7907	0.0110
tbigcir.lbd [285]	1455.6073	0.0148
tbigcir.lbd [285]	1568.3563	0.0042
tbigcir.lbd [285]	1607.5496	0.0257

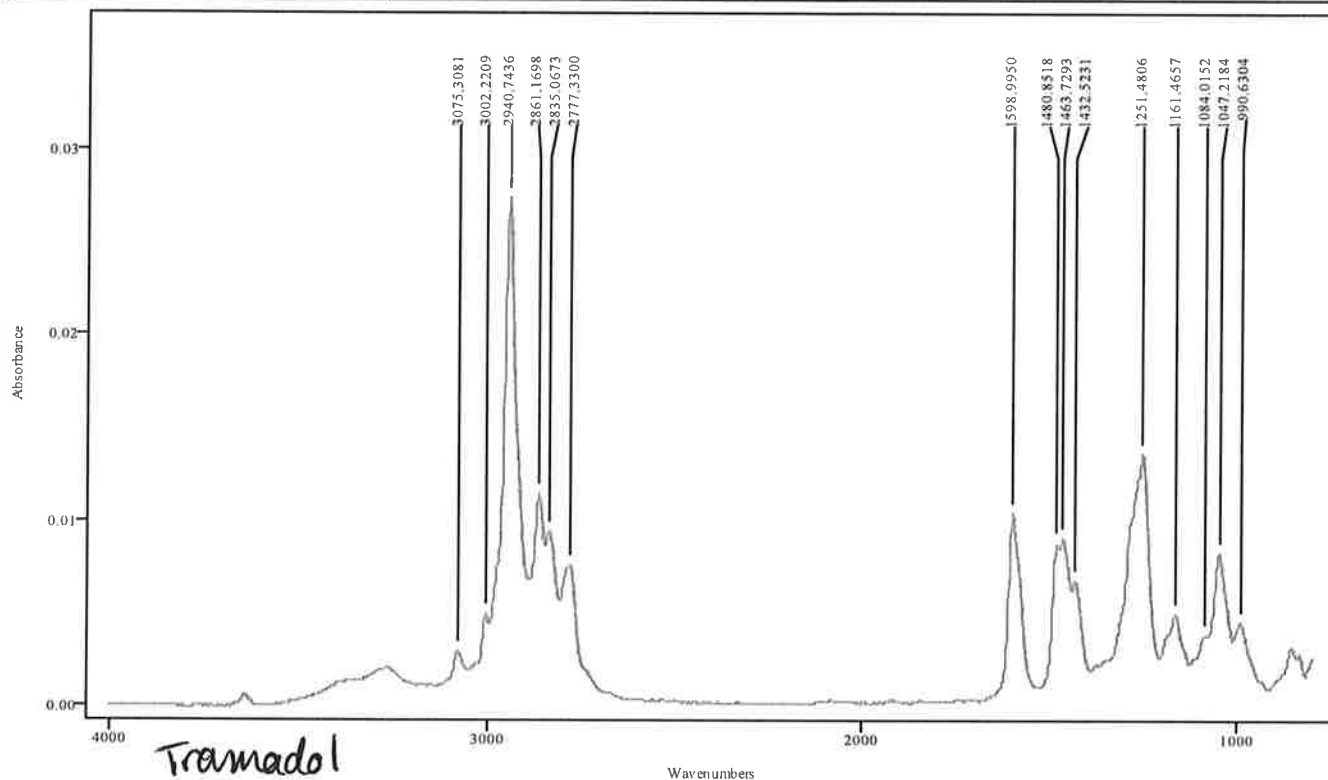
CH

tbigcir.lbd [285]	1696.4943	0.0690
tbigcir.lbd [285]	2888.1505	0.0255
tbigcir.lbd [285]	2943.1614	0.0401
tbigcir.lbd [285]	2976.5498	0.0727
tbigcir.lbd [285]	3032.7295	0.0132

Manual Peak Pick Results

Handwritten initials

Sample Filename	IRDATA.SPC
File Title	5.35 minutes: AVE (5.33: 5.37) Ref. (5.09: 5.31) of THF4A MIX 2MGML 2020_February_21_190555.cgm
Date	Wed Mar 04 15:02:06 2020



IRDATA.SPC: 5.35 minutes: AVE (5.33: 5.37) Ref. (5.09: 5.31) of THF4A MIX 2MGML 2020_February_21_190555.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	990.6304	0.0046
IRDATA.SPC [0]	1047.2184	0.0082
IRDATA.SPC [0]	1084.0152	0.0038
IRDATA.SPC [0]	1161.4657	0.0049
IRDATA.SPC [0]	1251.4806	0.0135
IRDATA.SPC [0]	1432.5231	0.0068
IRDATA.SPC [0]	1463.7293	0.0090
IRDATA.SPC [0]	1480.8518	0.0088
IRDATA.SPC [0]	1598.9950	0.0104
IRDATA.SPC [0]	2777.3300	0.0075
IRDATA.SPC [0]	2835.0673	0.0094
IRDATA.SPC [0]	2861.1698	0.0114
IRDATA.SPC [0]	2940.7436	0.0274

within +/- 1.5 cm⁻¹

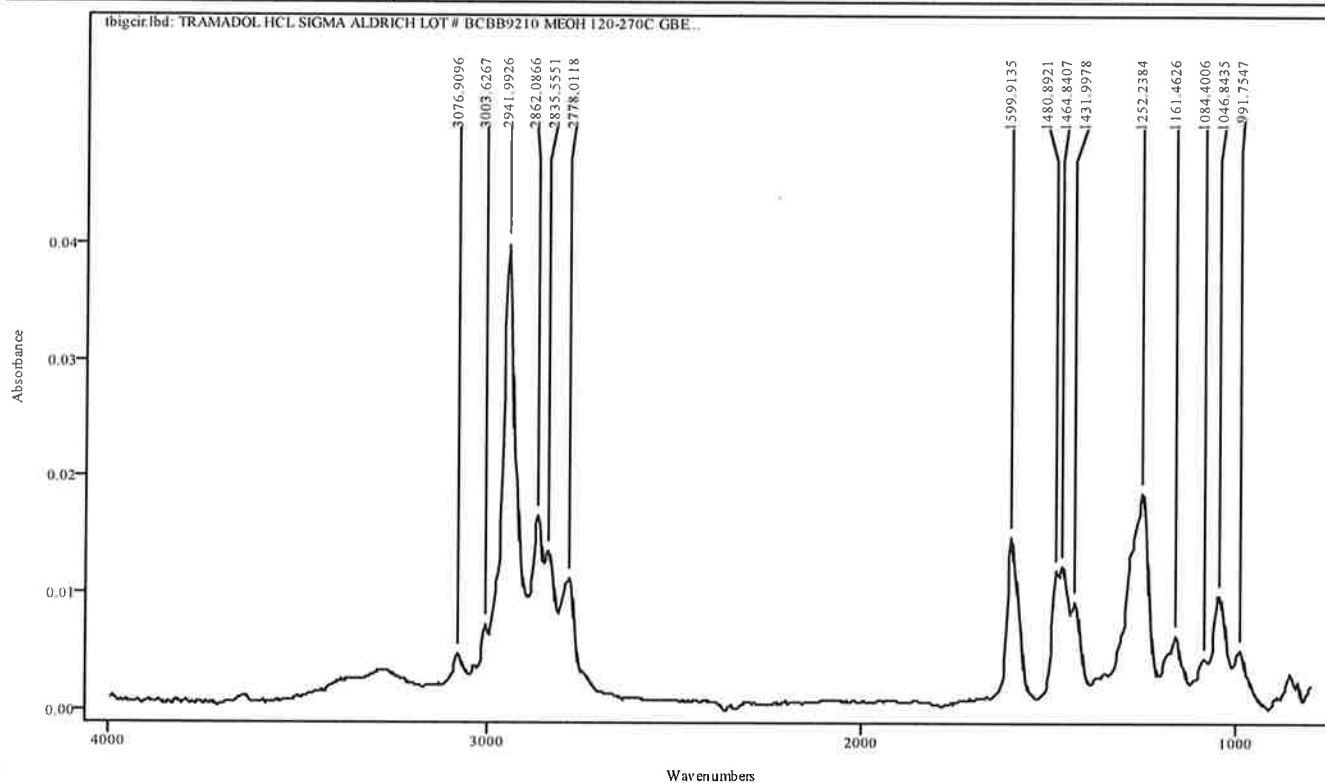
IRDATA.SPC [0]	3002.2209	0.0049
IRDATA.SPC [0]	3075.3081	0.0029

MA

Manual Peak Pick Results

MA

Sample Filename	Entry 256 from Library tbigcir.lbd
File Title	TRAMADOL HCL SIGMA ALDRICH LOT # BCBB9210 MEOH 120-270C GBE
Date	Wed Mar 04 15:02:41 2020



Entry 256 from Library tbigcir.lbd: TRAMADOL HCL SIGMA ALDRICH LOT # BCBB9210 MEOH 120-270C GBE

Filename	Peak At	Peak Height
tbigcir.lbd [256]	991.7547	0.0051
tbigcir.lbd [256]	1046.8435	0.0099
tbigcir.lbd [256]	1084.4006	0.0044
tbigcir.lbd [256]	1161.4626	0.0065
tbigcir.lbd [256]	1252.2384	0.0186
tbigcir.lbd [256]	1431.9978	0.0093
tbigcir.lbd [256]	1464.8407	0.0124
tbigcir.lbd [256]	1480.8921	0.0120
tbigcir.lbd [256]	1599.9135	0.0149
tbigcir.lbd [256]	2778.0118	0.0113
tbigcir.lbd [256]	2835.5551	0.0135
tbigcir.lbd [256]	2862.0866	0.0166
tbigcir.lbd [256]	2941.9926	0.0400
tbigcir.lbd [256]	3003.6267	0.0073

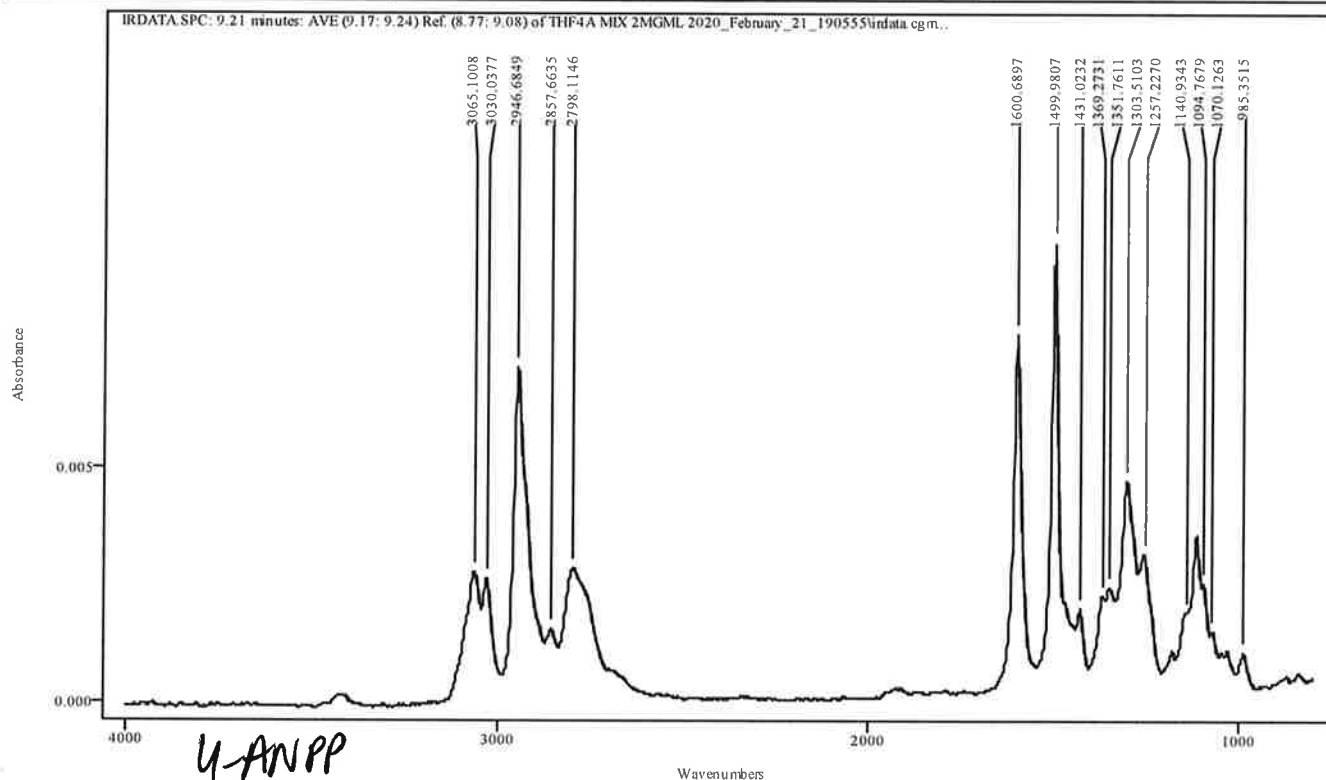
tbigcir.lbd [256]	3076.9096	0.0049
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JK

MA

Manual Peak Pick Results

Sample Filename	IRDATA.SPC
File Title	9.21 minutes: AVE (9.17: 9.24) Ref. (8.77: 9.08) of THF4A MIX 2MGML 2020_February_21_190555\irdata.cgm
Date	Wed Mar 04 15:06:24 2020



IRDATA.SPC: 9.21 minutes: AVE (9.17: 9.24) Ref. (8.77: 9.08) of THF4A MIX 2MGML 2020_February_21_190555.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	985.3515	0.0011
IRDATA.SPC [0]	1070.1263	0.0015
IRDATA.SPC [0]	1094.7679	0.0026
IRDATA.SPC [0]	1140.9343	0.0019
IRDATA.SPC [0]	1257.2270	0.0032
IRDATA.SPC [0]	1303.5103	0.0047
IRDATA.SPC [0]	1351.7611	0.0025
IRDATA.SPC [0]	1369.2731	0.0023
IRDATA.SPC [0]	1431.0232	0.0020
IRDATA.SPC [0]	1499.9807	0.0098
IRDATA.SPC [0]	1600.6897	0.0078
IRDATA.SPC [0]	2798.1146	0.0029
IRDATA.SPC [0]	2857.6635	0.0016

within 1.5 cm^{-1}

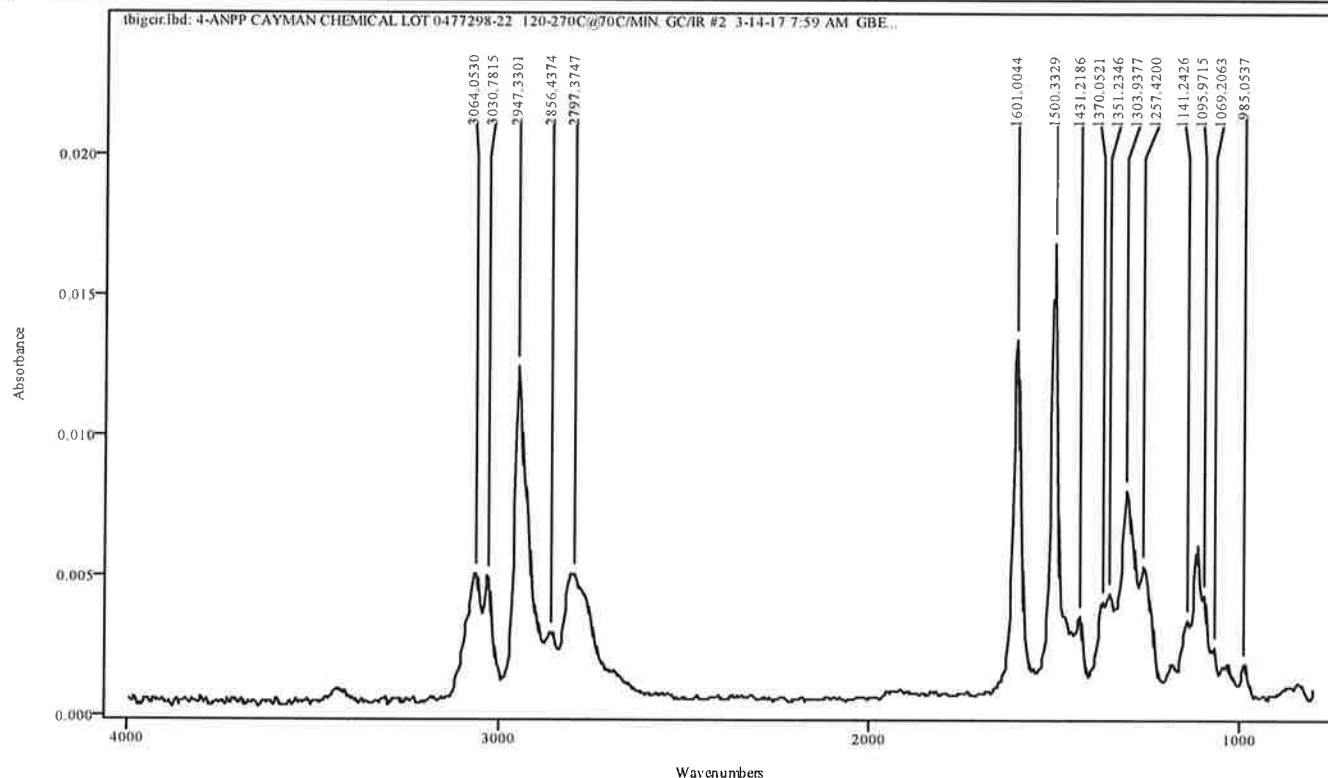
IRDATA.SPC [0]	2946.6849	0.0072
IRDATA.SPC [0]	3030.0377	0.0027
IRDATA.SPC [0]	3065.1008	0.0028

MA

MA

Manual Peak Pick Results

Sample Filename	Entry 432 from Library tbigcir.lbd
File Title	4-ANPP CAYMAN CHEMICAL LOT 0477298-22 120-270C@70C/MIN. GC/IR #2 3-14-17 7:59 AM GBE
Date	Wed Mar 04 15:07:00 2020



Entry 432 from Library tbigcir.lbd: 4-ANPP CAYMAN CHEMICAL LOT 0477298-22
120-270C@70C/MIN. GC/IR #2 3-14-17 7:59 AM GBE

Filename	Peak At	Peak Height
tbigcir.lbd [432]	985.0537	0.0019
tbigcir.lbd [432]	1069.2063	0.0025
tbigcir.lbd [432]	1095.9715	0.0043
tbigcir.lbd [432]	1141.2426	0.0034
tbigcir.lbd [432]	1257.4200	0.0054
tbigcir.lbd [432]	1303.9377	0.0080
tbigcir.lbd [432]	1351.2346	0.0044
tbigcir.lbd [432]	1370.0521	0.0041
tbigcir.lbd [432]	1431.2186	0.0036
tbigcir.lbd [432]	1500.3329	0.0169
tbigcir.lbd [432]	1601.0044	0.0135
tbigcir.lbd [432]	2797.3747	0.0051
tbigcir.lbd [432]	2856.4374	0.0030

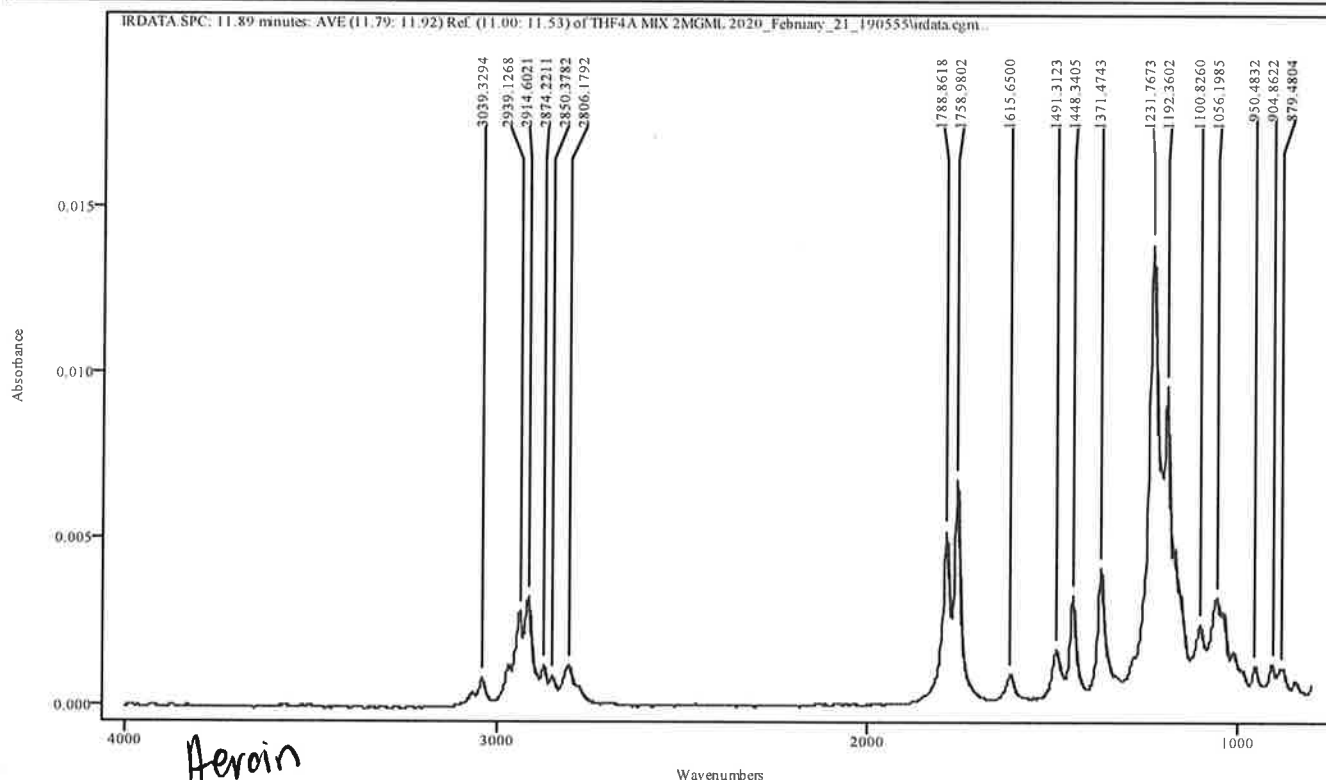
tbigcir.lbd [432]	2947.3301	0.0125
tbigcir.lbd [432]	3030.7815	0.0050
tbigcir.lbd [432]	3064.0530	0.0051

MAH

Manual Peak Pick Results

MA

Sample Filename	IRDATA.SPC
File Title	11.89 minutes: AVE (11.79: 11.92) Ref. (11.00: 11.53) of THF4A MIX 2MGML 2020_February_21_190555.cgm
Date	Wed Mar 04 15:11:16 2020



IRDATA.SPC: 11.89 minutes: AVE (11.79: 11.92) Ref. (11.00: 11.53) of THF4A MIX 2MGML 2020_February_21_190555.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	879.4804	0.0011
IRDATA.SPC [0]	904.8622	0.0012
IRDATA.SPC [0]	950.4832	0.0012
IRDATA.SPC [0]	1056.1985	0.0033
IRDATA.SPC [0]	1100.8260	0.0024
IRDATA.SPC [0]	1192.3602	0.0096
IRDATA.SPC [0]	1231.7673	0.0139
IRDATA.SPC [0]	1371.4743	0.0041
IRDATA.SPC [0]	1448.3405	0.0033
IRDATA.SPC [0]	1491.3123	0.0017
IRDATA.SPC [0]	1615.6500	0.0009
IRDATA.SPC [0]	1758.9802	0.0068
IRDATA.SPC [0]	1788.8618	0.0053

within $\pm 2 \text{ cm}^{-1}$

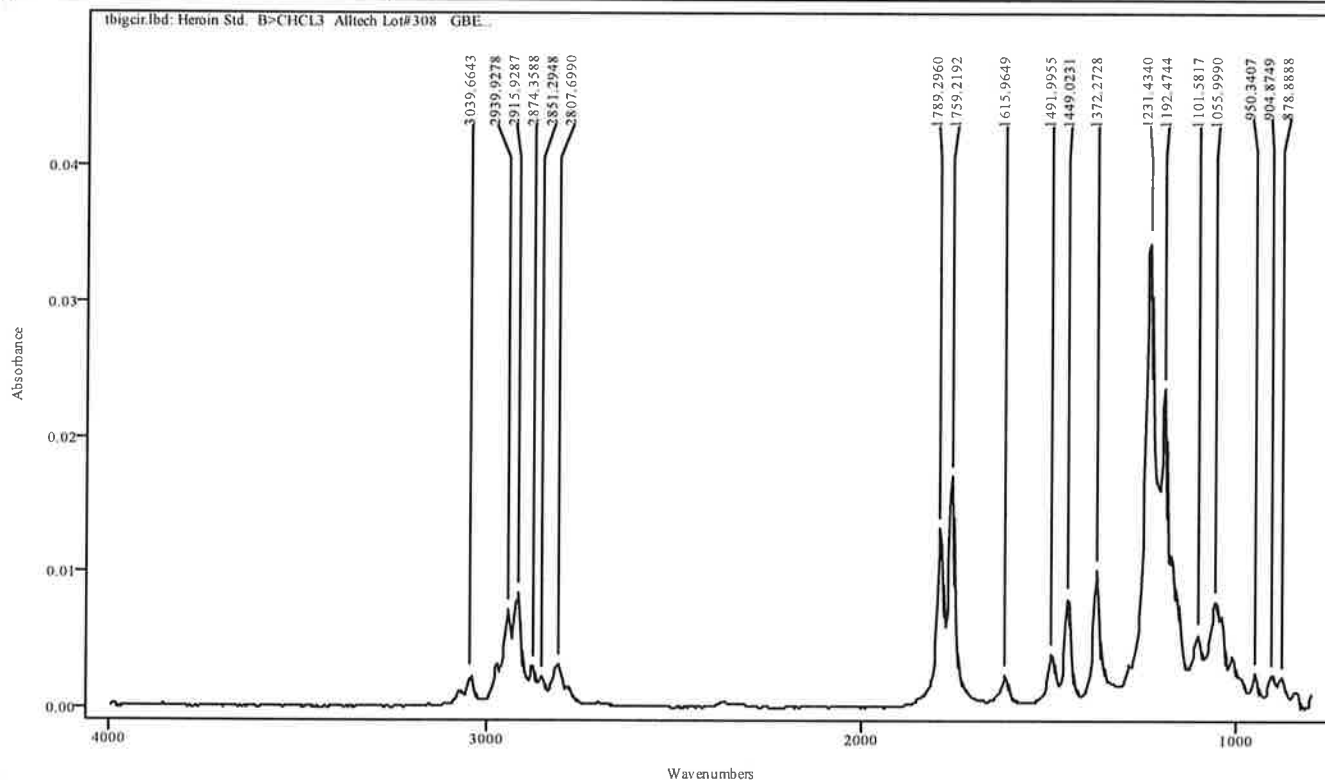
IRDATA.SPC [0]	2806.1792	0.0012
IRDATA.SPC [0]	2850.3782	0.0008
IRDATA.SPC [0]	2874.2211	0.0012
IRDATA.SPC [0]	2914.6021	0.0033
IRDATA.SPC [0]	2939.1268	0.0028
IRDATA.SPC [0]	3039.3294	0.0008

MA

Manual Peak Pick Results

Handwritten signature

Sample Filename	Entry 40 from Library tbigcir.lbd
File Title	Heroin Std. B>CHCL3 Alltech Lot#308 GBE
Date	Wed Mar 04 15:10:52 2020



Entry 40 from Library tbigcir.lbd: Heroin Std. B>CHCL3 Alltech Lot#308 GBE

Filename	Peak At	Peak Height
tbigcir.lbd [40]	878.8888	0.0024
tbigcir.lbd [40]	904.8749	0.0025
tbigcir.lbd [40]	950.3407	0.0027
tbigcir.lbd [40]	1055.9990	0.0079
tbigcir.lbd [40]	1101.5817	0.0055
tbigcir.lbd [40]	1192.4744	0.0237
tbigcir.lbd [40]	1231.4340	0.0346
tbigcir.lbd [40]	1372.2728	0.0102
tbigcir.lbd [40]	1449.0231	0.0081
tbigcir.lbd [40]	1491.9955	0.0041
tbigcir.lbd [40]	1615.9649	0.0024
tbigcir.lbd [40]	1759.2192	0.0172
tbigcir.lbd [40]	1789.2960	0.0132
tbigcir.lbd [40]	2807.6990	0.0033

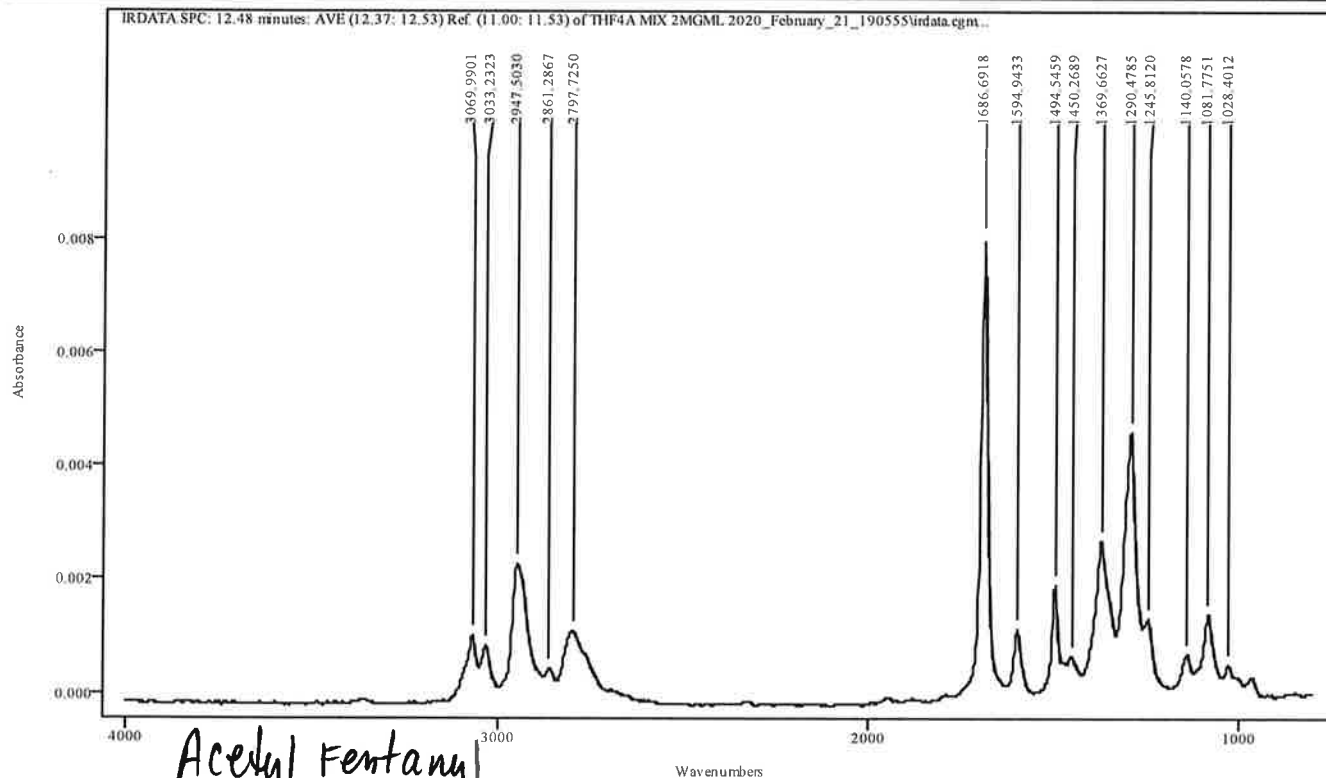
MA

tbigcir.lbd [40]	2851.2948	0.0023
tbigcir.lbd [40]	2874.3588	0.0032
tbigcir.lbd [40]	2915.9287	0.0085
tbigcir.lbd [40]	2939.9278	0.0072
tbigcir.lbd [40]	3039.6643	0.0024

Manual Peak Pick Results

NA

Sample Filename	IRDATA.SPC
File Title	12.48 minutes: AVE (12.37: 12.53) Ref. (11.00: 11.53) of THF4A MIX 2MGML 2020_February_21_190555.cgm
Date	Wed Mar 04 15:14:41 2020



IRDATA.SPC: 12.48 minutes: AVE (12.37: 12.53) Ref. (11.00: 11.53) of THF4A MIX 2MGML 2020_February_21_190555.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	1028.4012	0.0005
IRDATA.SPC [0]	1081.7751	0.0014
IRDATA.SPC [0]	1140.0578	0.0007
IRDATA.SPC [0]	1245.8120	0.0013
IRDATA.SPC [0]	1290.4785	0.0046
IRDATA.SPC [0]	1369.6627	0.0027
IRDATA.SPC [0]	1450.2689	0.0007
IRDATA.SPC [0]	1494.5459	0.0019
IRDATA.SPC [0]	1594.9433	0.0011
IRDATA.SPC [0]	1686.6918	0.0080
IRDATA.SPC [0]	2797.7250	0.0011
IRDATA.SPC [0]	2861.2867	0.0004
IRDATA.SPC [0]	2947.5030	0.0023

Within +/- 3 cm⁻¹

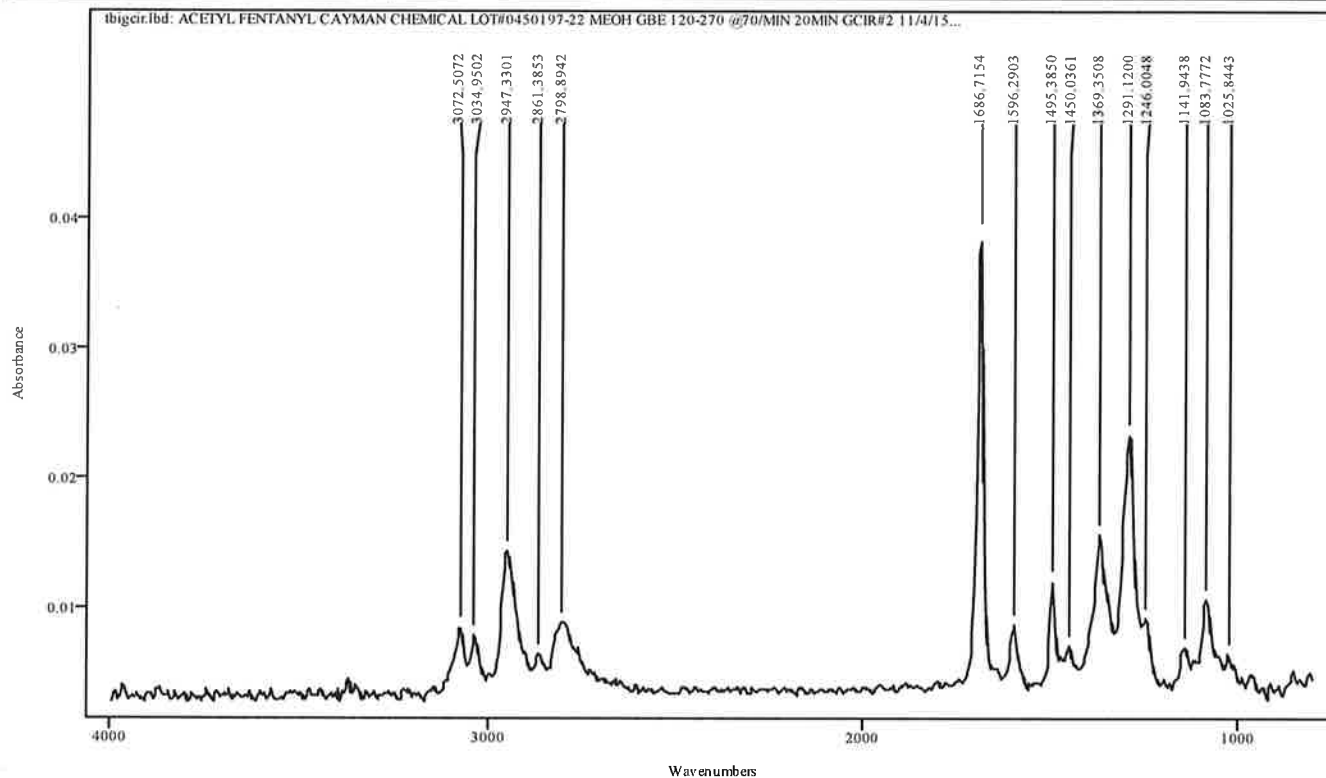
IRDATA.SPC [0]	3033.2323	0.0008
IRDATA.SPC [0]	3069.9901	0.0010

MF

11/4

Manual Peak Pick Results

Sample Filename	Entry 403 from Library tbigcir.lbd
File Title	ACETYL FENTANYL CAYMAN CHEMICAL LOT#0450197-22 MEOH GBE 120-270 @70/MIN 20MIN GCIR#2 11/4/15
Date	Wed Mar 04 15:15:40 2020



Entry 403 from Library tbigcir.lbd: ACETYL FENTANYL CAYMAN CHEMICAL LOT#0450197-22 MEOH GBE 120-270 @70/MIN 20MIN GCIR#2 11/4/15

Filename	Peak At	Peak Height
tbigcir.lbd [403]	1025.8443	0.0065
tbigcir.lbd [403]	1083.7772	0.0107
tbigcir.lbd [403]	1141.9438	0.0070
tbigcir.lbd [403]	1246.0048	0.0093
tbigcir.lbd [403]	1291.1200	0.0234
tbigcir.lbd [403]	1369.3508	0.0157
tbigcir.lbd [403]	1450.0361	0.0071
tbigcir.lbd [403]	1495.3850	0.0121
tbigcir.lbd [403]	1596.2903	0.0087
tbigcir.lbd [403]	1686.7154	0.0389
tbigcir.lbd [403]	2798.8942	0.0089
tbigcir.lbd [403]	2861.3853	0.0065
tbigcir.lbd [403]	2947.3301	0.0145

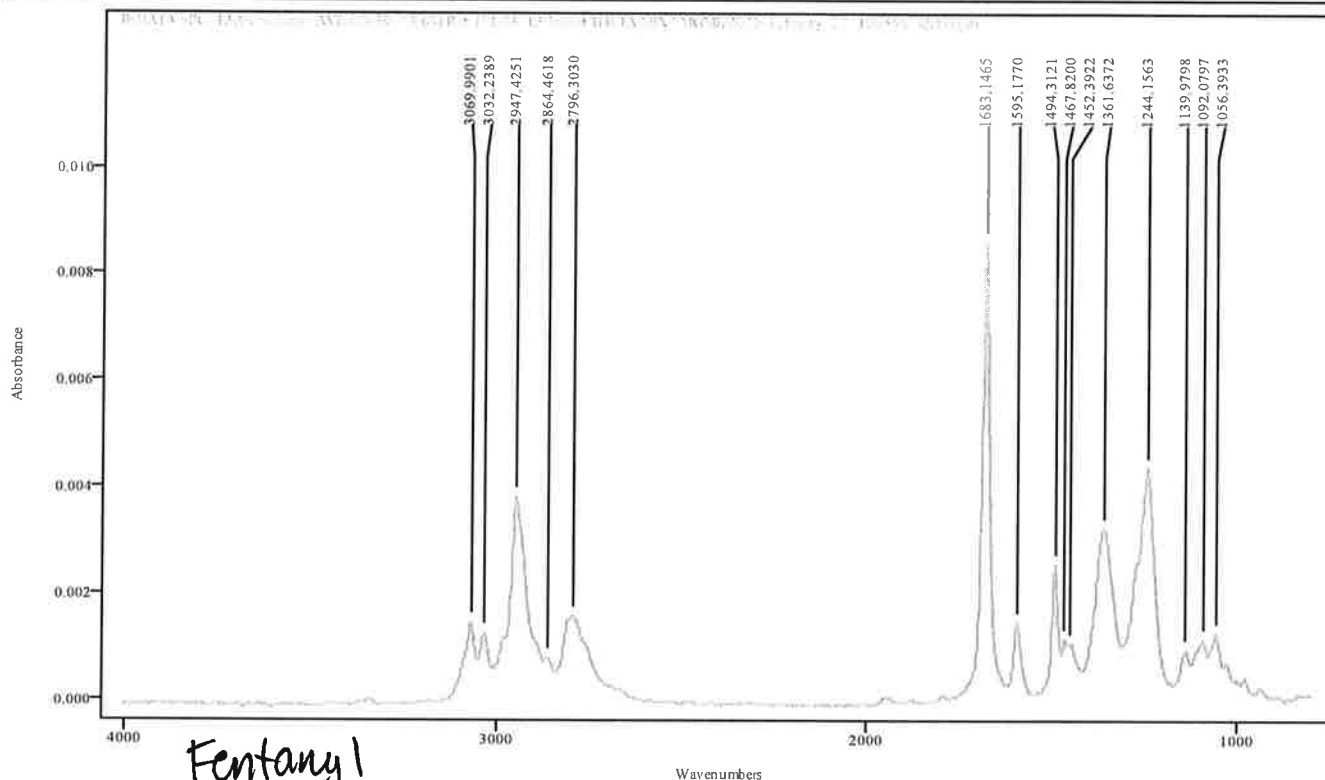
tbigcir.lbd [403]	3034.9502	0.0079
tbigcir.lbd [403]	3072.5072	0.0086

MA

MA

Manual Peak Pick Results

Sample Filename	IRDATA.SPC
File Title	13.60 minutes: AVE (13.49: 13.63) Ref. (12.73: 13.30) of THF4A MIX 2MGML 2020_February_21_190555.cgm
Date	Wed Mar 04 15:18:52 2020



IRDATA.SPC: 13.60 minutes: AVE (13.49: 13.63) Ref. (12.73: 13.30) of THF4A MIX 2MGML 2020_February_21_190555.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	1056.3933	0.0013
IRDATA.SPC [0]	1092.0797	0.0011
IRDATA.SPC [0]	1139.9798	0.0009
IRDATA.SPC [0]	1244.1563	0.0043
IRDATA.SPC [0]	1361.6372	0.0032
IRDATA.SPC [0]	1452.3922	0.0011
IRDATA.SPC [0]	1467.8200	0.0012
IRDATA.SPC [0]	1494.3121	0.0025
IRDATA.SPC [0]	1595.1770	0.0014
IRDATA.SPC [0]	1683.1465	0.0086
IRDATA.SPC [0]	2796.3030	0.0016
IRDATA.SPC [0]	2864.4618	0.0008
IRDATA.SPC [0]	2947.4251	0.0038

within +/- 1.5 cm⁻¹

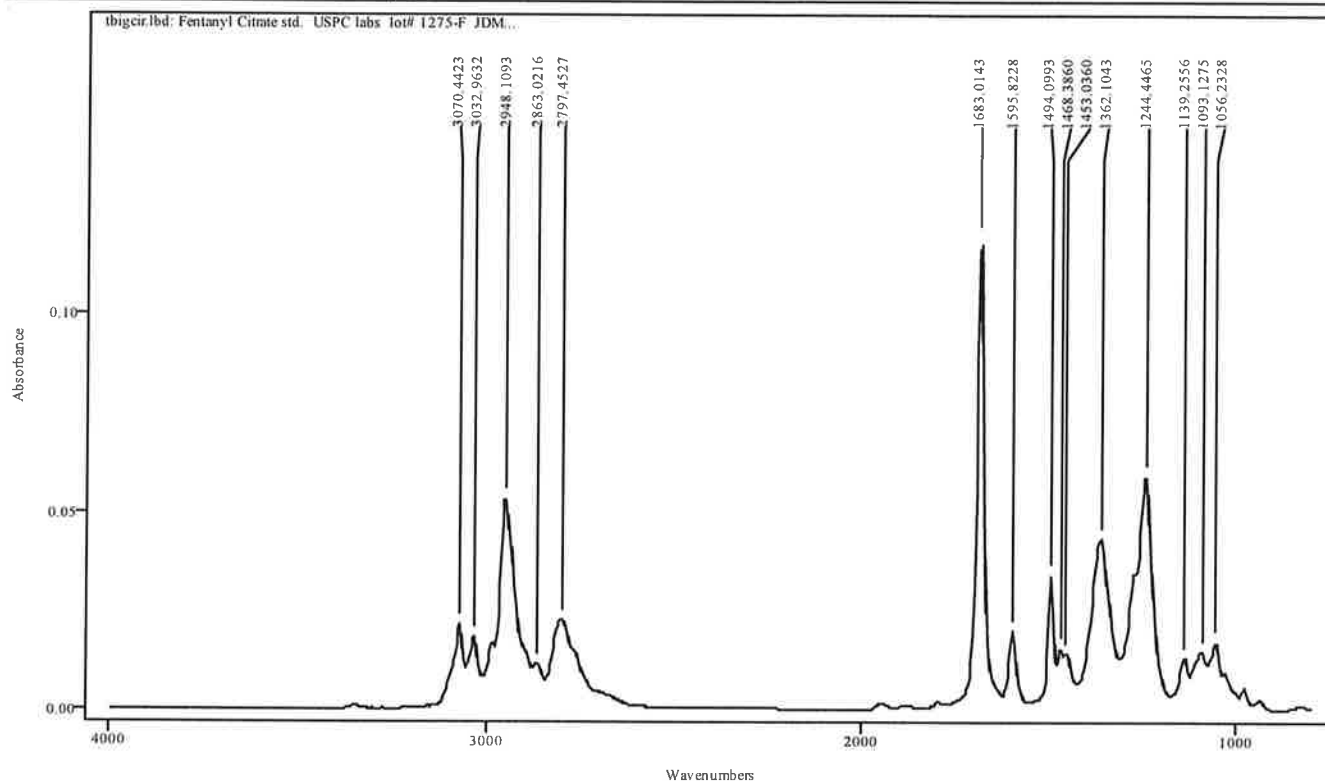
IRDATA.SPC [0]	3032.2389	0.0013
IRDATA.SPC [0]	3069.9901	0.0015

HA

Manual Peak Pick Results

JH

Sample Filename	Entry 93 from Library tbigcir.lbd
File Title	Fentanyl Citrate std. USPC labs lot# 1275-F JDM
Date	Wed Mar 04 15:19:24 2020



Entry 93 from Library tbigcir.lbd: Fentanyl Citrate std. USPC labs lot# 1275-F JDM

Filename	Peak At	Peak Height
tbigcir.lbd [93]	1056.2328	0.0172
tbigcir.lbd [93]	1093.1275	0.0149
tbigcir.lbd [93]	1139.2556	0.0133
tbigcir.lbd [93]	1244.4465	0.0592
tbigcir.lbd [93]	1362.1043	0.0436
tbigcir.lbd [93]	1453.0360	0.0145
tbigcir.lbd [93]	1468.3860	0.0157
tbigcir.lbd [93]	1494.0993	0.0344
tbigcir.lbd [93]	1595.8228	0.0202
tbigcir.lbd [93]	1683.0143	0.1196
tbigcir.lbd [93]	2797.4527	0.0227
tbigcir.lbd [93]	2863.0216	0.0118
tbigcir.lbd [93]	2948.1093	0.0535
tbigcir.lbd [93]	3032.9632	0.0185

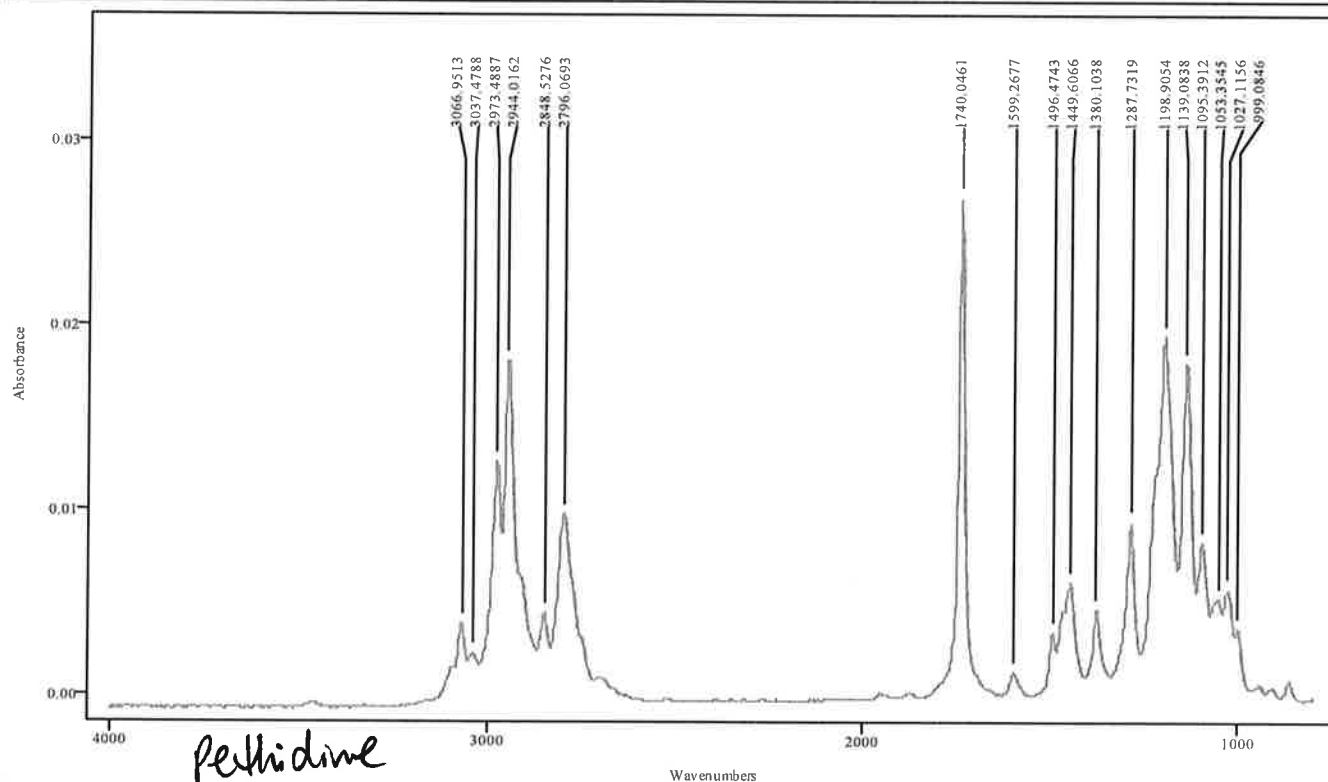
tbigcir.lbd [93]	3070.4423	0.0216
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11

Manual Peak Pick Results

CH

Sample Filename	IRDATA.SPC
File Title	2.98 minutes: AVE (2.96: 2.99) Ref. (2.75: 2.93) of GCMS MIX 2MGML 2020_February_21_211647.cgm
Date	Wed Mar 04 15:23:28 2020



IRDATA.SPC: 2.98 minutes: AVE (2.96: 2.99) Ref. (2.75: 2.93) of GCMS MIX 2MGML 2020_February_21_211647.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	999.0846	0.0036
IRDATA.SPC [0]	1027.1156	0.0057
IRDATA.SPC [0]	1053.3545	0.0052
IRDATA.SPC [0]	1095.3912	0.0083
IRDATA.SPC [0]	1139.0838	0.0180
IRDATA.SPC [0]	1198.9054	0.0194
IRDATA.SPC [0]	1287.7319	0.0094
IRDATA.SPC [0]	1380.1038	0.0046
IRDATA.SPC [0]	1449.6066	0.0061
IRDATA.SPC [0]	1496.4743	0.0033
IRDATA.SPC [0]	1599.2677	0.0012
IRDATA.SPC [0]	1740.0461	0.0269
IRDATA.SPC [0]	2796.0693	0.0098

within 1.5 cm⁻¹

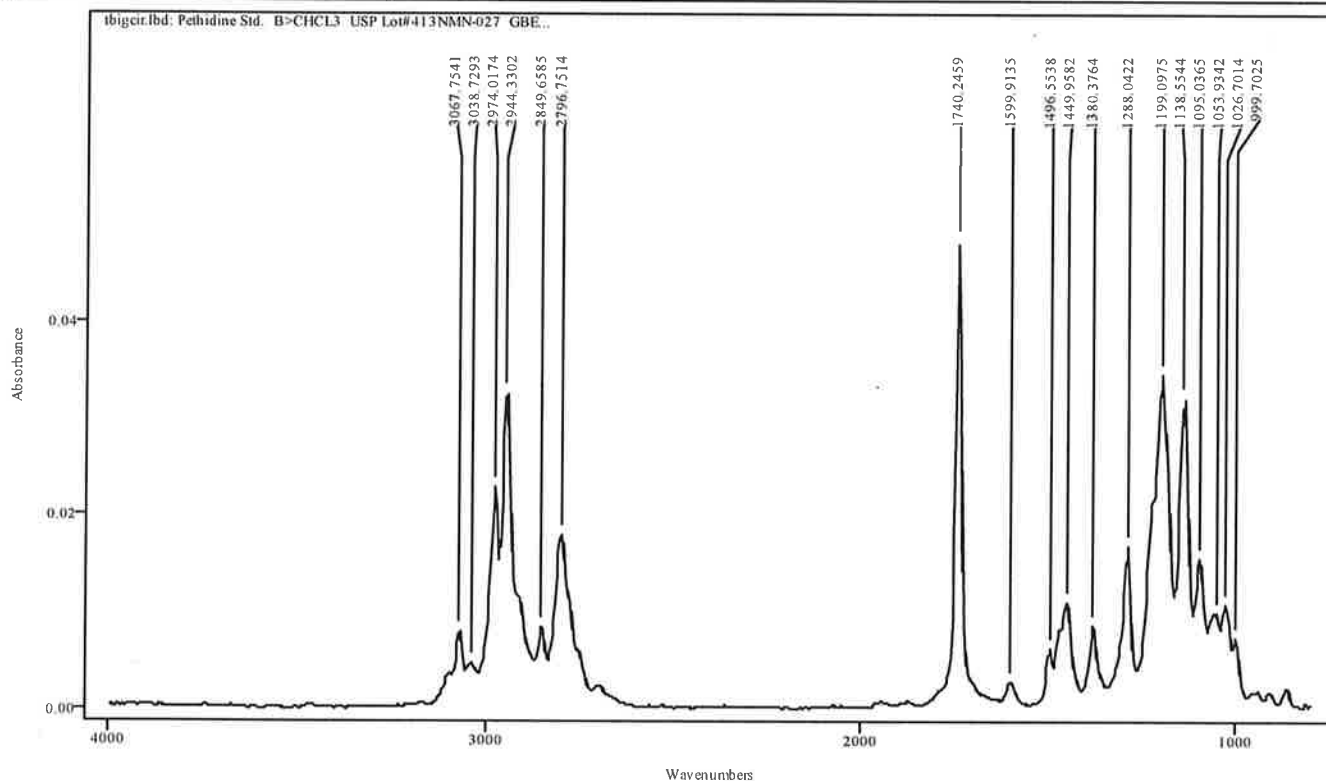
IRDATA.SPC [0]	2848.5276	0.0044
IRDATA.SPC [0]	2944.0162	0.0181
IRDATA.SPC [0]	2973.4887	0.0126
IRDATA.SPC [0]	3037.4788	0.0022
IRDATA.SPC [0]	3066.9513	0.0039

MA

MA

Manual Peak Pick Results

Sample Filename	Entry 43 from Library tbigcir.lbd
File Title	Pethidine Std. B>CHCL3 USP Lot#413NMN-027 GBE
Date	Wed Mar 04 15:24:06 2020



Entry 43 from Library tbigcir.lbd: Pethidine Std. B>CHCL3 USP Lot#413NMN-027 GBE

Filename	Peak At	Peak Height
tbigcir.lbd [43]	999.7025	0.0073
tbigcir.lbd [43]	1026.7014	0.0108
tbigcir.lbd [43]	1053.9342	0.0099
tbigcir.lbd [43]	1095.0365	0.0155
tbigcir.lbd [43]	1138.5544	0.0321
tbigcir.lbd [43]	1199.0975	0.0345
tbigcir.lbd [43]	1288.0422	0.0169
tbigcir.lbd [43]	1380.3764	0.0087
tbigcir.lbd [43]	1449.9582	0.0110
tbigcir.lbd [43]	1496.5538	0.0062
tbigcir.lbd [43]	1599.9135	0.0029
tbigcir.lbd [43]	1740.2459	0.0483
tbigcir.lbd [43]	2796.7514	0.0179
tbigcir.lbd [43]	2849.6585	0.0084

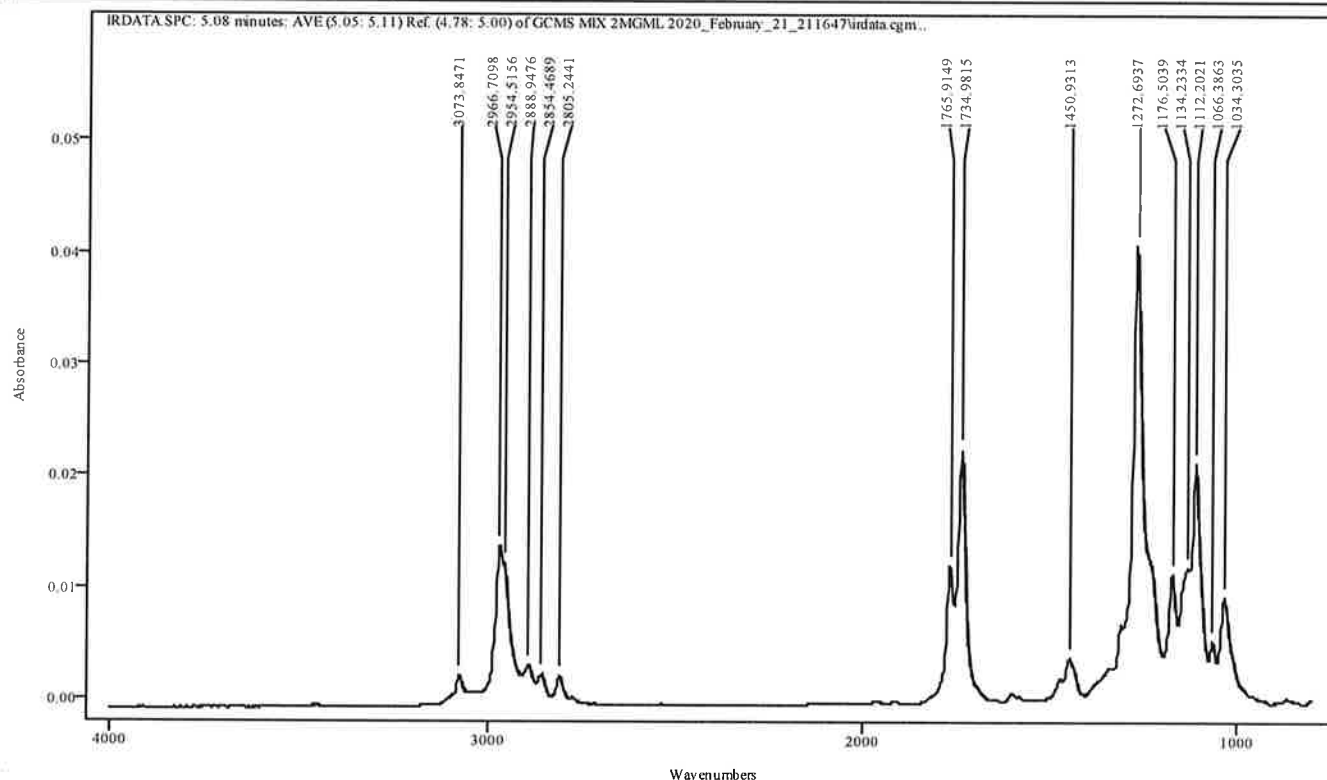
tbigcir.lbd [43]	2944.3302	0.0325
tbigcir.lbd [43]	2974.0174	0.0228
tbigcir.lbd [43]	3038.7293	0.0047
tbigcir.lbd [43]	3067.7541	0.0080

✓H

Manual Peak Pick Results

MA

Sample Filename	IRDATA.SPC
File Title	5.08 minutes: AVE (5.05: 5.11) Ref. (4.78: 5.00) of GCMS MIX 2MGML 2020_February_21_211647.cgm
Date	Wed Mar 04 15:26:47 2020



IRDATA.SPC: 5.08 minutes: AVE (5.05: 5.11) Ref. (4.78: 5.00) of GCMS MIX 2MGML 2020_February_21_211647.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	1034.3035	0.0092
IRDATA.SPC [0]	1066.3863	0.0052
IRDATA.SPC [0]	1112.2021	0.0213
IRDATA.SPC [0]	1134.2334	0.0117
IRDATA.SPC [0]	1176.5039	0.0113
IRDATA.SPC [0]	1272.6937	0.0407
IRDATA.SPC [0]	1450.9313	0.0038
IRDATA.SPC [0]	1734.9815	0.0224
IRDATA.SPC [0]	1765.9149	0.0121
IRDATA.SPC [0]	2805.2441	0.0021
IRDATA.SPC [0]	2854.4689	0.0022
IRDATA.SPC [0]	2888.9476	0.0030
IRDATA.SPC [0]	2954.5156	0.0122

within 1.5 cm⁻¹

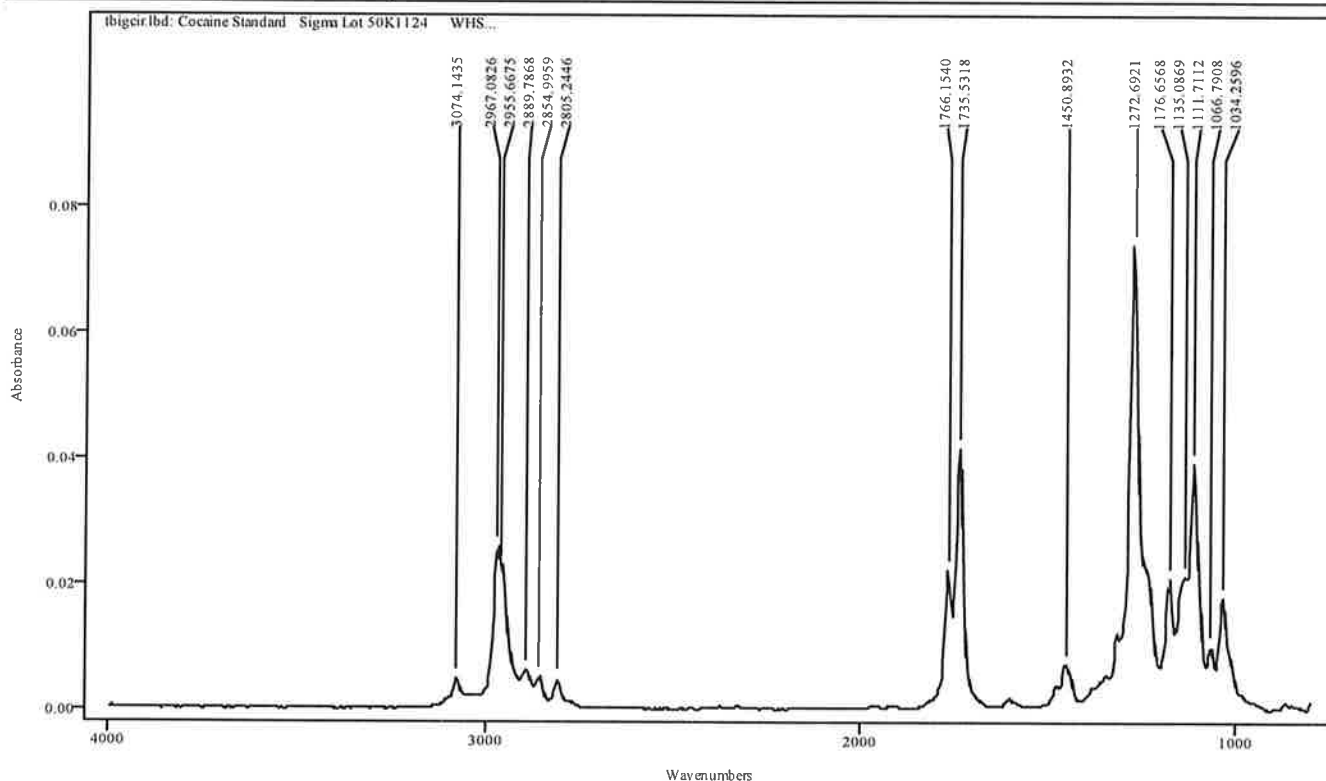
IRDATA.SPC [0]	2966.7098	0.0137
IRDATA.SPC [0]	3073.8471	0.0021

JH

MA

Manual Peak Pick Results

Sample Filename	Entry 1 from Library tbigcir.lbd
File Title	Cocaine Standard Sigma Lot 50K1124 WHS
Date	Wed Mar 04 15:27:15 2020



Entry 1 from Library tbigcir.lbd: Cocaine Standard Sigma Lot 50K1124 WHS

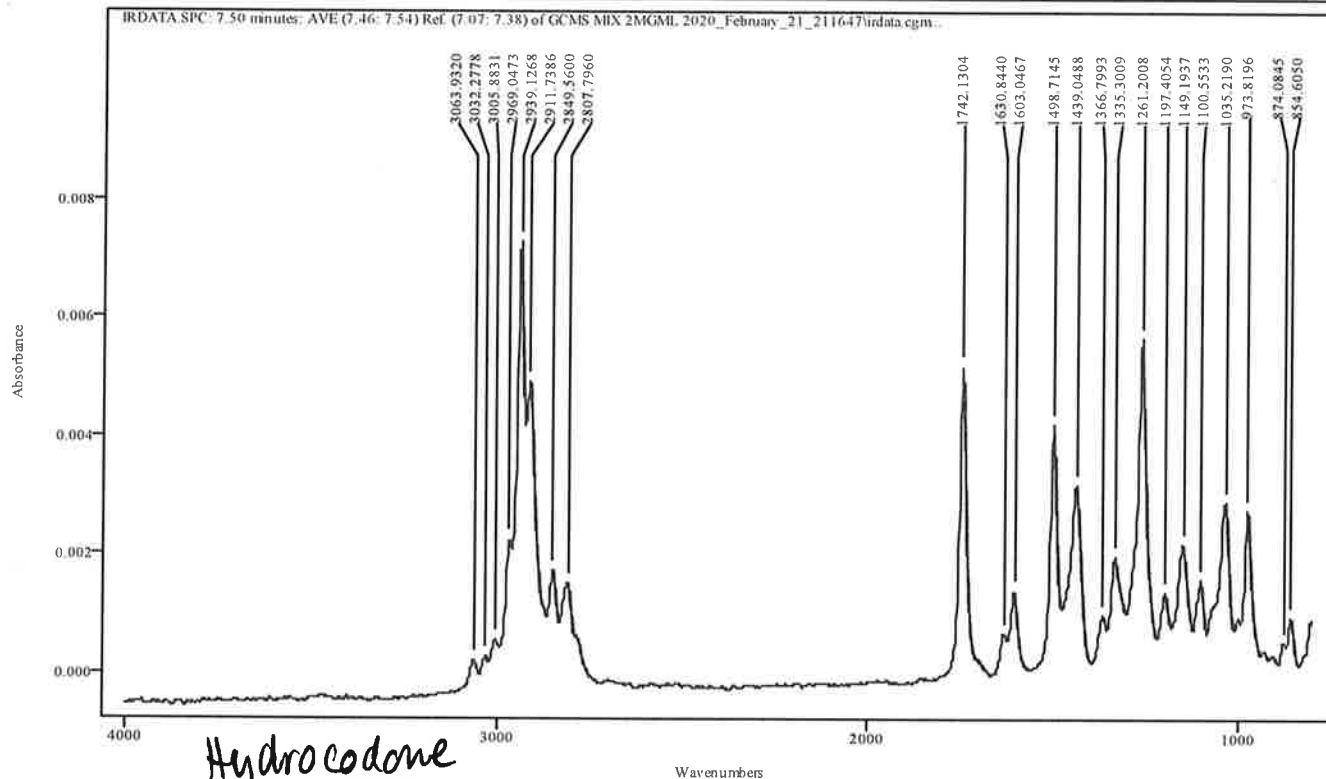
Filename	Peak At	Peak Height
tbigcir.lbd [1]	1034.2596	0.0179
tbigcir.lbd [1]	1066.7908	0.0102
tbigcir.lbd [1]	1111.7112	0.0393
tbigcir.lbd [1]	1135.0869	0.0212
tbigcir.lbd [1]	1176.6568	0.0209
tbigcir.lbd [1]	1272.6921	0.0740
tbigcir.lbd [1]	1450.8932	0.0075
tbigcir.lbd [1]	1735.5318	0.0415
tbigcir.lbd [1]	1766.1540	0.0223
tbigcir.lbd [1]	2805.2446	0.0049
tbigcir.lbd [1]	2854.9959	0.0052
tbigcir.lbd [1]	2889.7868	0.0065
tbigcir.lbd [1]	2955.6675	0.0231
tbigcir.lbd [1]	2967.0826	0.0259

tbicir.lbd [1]	3074.1435	0.0051
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MA

Manual Peak Pick Results

Sample Filename	IRDATA.SPC
File Title	7.50 minutes: AVE (7.46: 7.54) Ref. (7.07: 7.38) of GCMS MIX 2MGML 2020_February_21_211647.cgm
Date	Wed Mar 04 15:31:48 2020



IRDATA.SPC: 7.50 minutes: AVE (7.46: 7.54) Ref. (7.07: 7.38) of GCMS MIX 2MGML 2020_February_21_211647.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	854.6050	0.0009
IRDATA.SPC [0]	874.0845	0.0005
IRDATA.SPC [0]	973.8196	0.0027
IRDATA.SPC [0]	1035.2190	0.0029
IRDATA.SPC [0]	1100.5533	0.0016
IRDATA.SPC [0]	1149.1937	0.0022
IRDATA.SPC [0]	1197.4054	0.0014
IRDATA.SPC [0]	1261.2008	0.0057
IRDATA.SPC [0]	1335.3009	0.0020
IRDATA.SPC [0]	1366.7993	0.0010
IRDATA.SPC [0]	1439.0488	0.0032
IRDATA.SPC [0]	1498.7145	0.0042
IRDATA.SPC [0]	1603.0467	0.0014

within $\pm 25 \text{ cm}^{-1}$

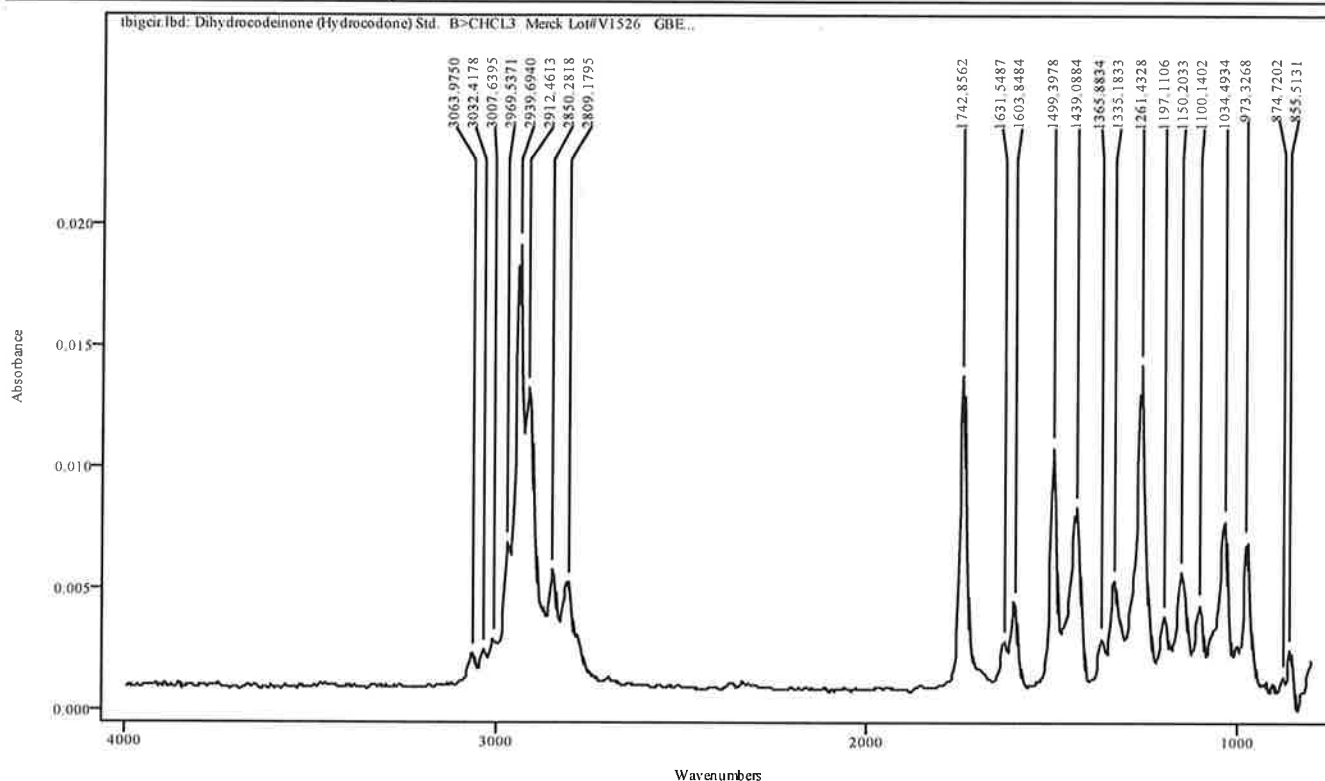
11

IRDATA.SPC [0]	1630.8440	0.0007
IRDATA.SPC [0]	1742.1304	0.0052
IRDATA.SPC [0]	2807.7960	0.0015
IRDATA.SPC [0]	2849.5600	0.0017
IRDATA.SPC [0]	2911.7386	0.0049
IRDATA.SPC [0]	2939.1268	0.0073
IRDATA.SPC [0]	2969.0473	0.0022
IRDATA.SPC [0]	3005.8831	0.0006
IRDATA.SPC [0]	3032.2778	0.0003
IRDATA.SPC [0]	3063.9320	0.0002

MA

Manual Peak Pick Results

Sample Filename	Entry 41 from Library tbigcir.lbd
File Title	Dihydrocodeinone (Hydrocodone) Std. B>CHCL3 Merck Lot#V1526 GBE
Date	Wed Mar 04 15:32:27 2020



Entry 41 from Library tbigcir.lbd: Dihydrocodeinone (Hydrocodone) Std. B>CHCL3 Merck Lot#V1526 GBE

Filename	Peak At	Peak Height
tbigcir.lbd [41]	855.5131	0.0025
tbigcir.lbd [41]	874.7202	0.0014
tbigcir.lbd [41]	973.3268	0.0070
tbigcir.lbd [41]	1034.4934	0.0078
tbigcir.lbd [41]	1100.1402	0.0044
tbigcir.lbd [41]	1150.2033	0.0057
tbigcir.lbd [41]	1197.1106	0.0039
tbigcir.lbd [41]	1261.4328	0.0143
tbigcir.lbd [41]	1335.1833	0.0054
tbigcir.lbd [41]	1365.8834	0.0030
tbigcir.lbd [41]	1439.0884	0.0083
tbigcir.lbd [41]	1499.3978	0.0109
tbigcir.lbd [41]	1603.8484	0.0045
tbigcir.lbd [41]	1631.5487	0.0029

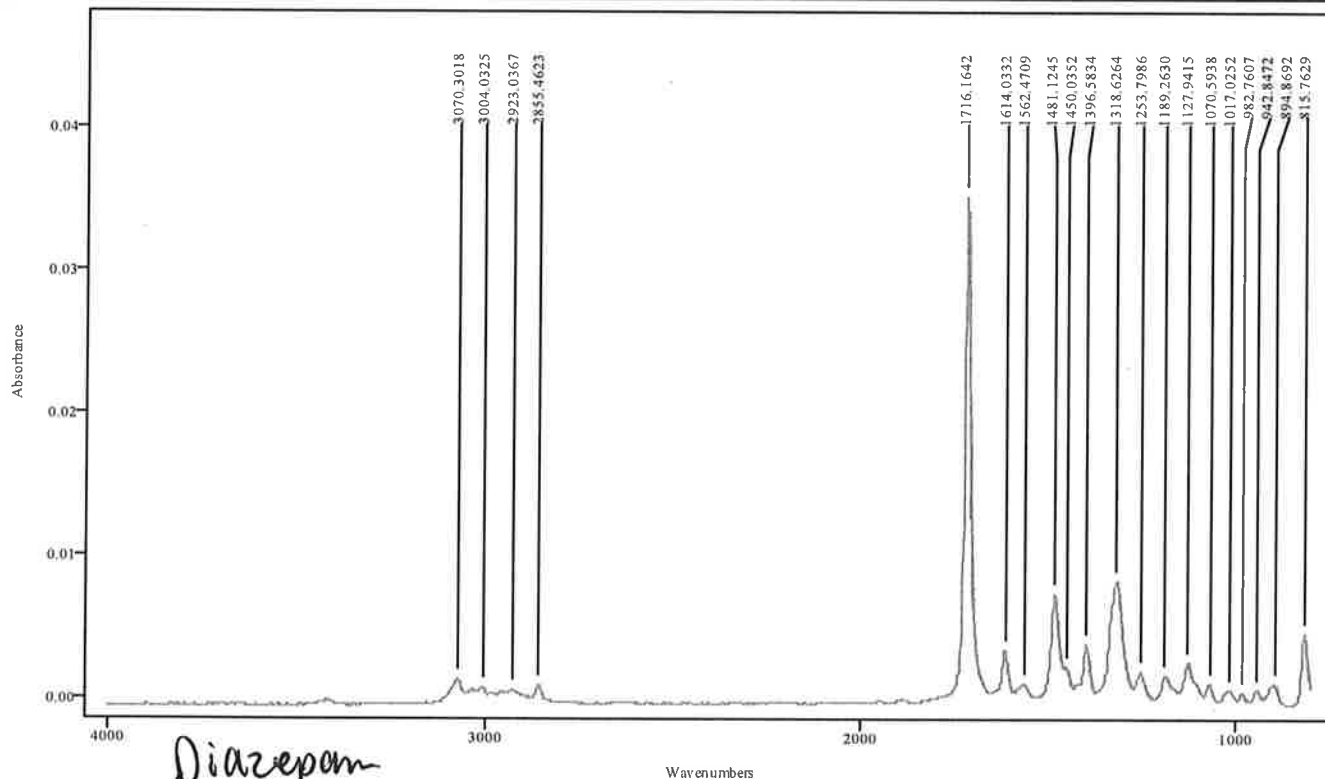
tbigcir.lbd [41]	1742.8562	0.0138
tbigcir.lbd [41]	2809.1795	0.0053
tbigcir.lbd [41]	2850.2818	0.0058
tbigcir.lbd [41]	2912.4613	0.0133
tbigcir.lbd [41]	2939.6940	0.0193
tbigcir.lbd [41]	2969.5371	0.0069
tbigcir.lbd [41]	3007.6395	0.0029
tbigcir.lbd [41]	3032.4178	0.0025
tbigcir.lbd [41]	3063.9750	0.0023

MA

MA

Manual Peak Pick Results

Sample Filename	IRDATA.SPC
File Title	7.29 minutes: AVE (7.24: 7.33) Ref. (6.74: 7.14) of DIAZEPAM 2MGML 2020_February_21_224624.cgm
Date	Wed Mar 04 15:35:52 2020



IRDATA.SPC: 7.29 minutes: AVE (7.24: 7.33) Ref. (6.74: 7.14) of DIAZEPAM 2MGML 2020_February_21_224624.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	815.7629	0.0046
IRDATA.SPC [0]	894.8692	0.0011
IRDATA.SPC [0]	942.8472	0.0007
IRDATA.SPC [0]	982.7607	0.0004
IRDATA.SPC [0]	1017.0252	0.0006
IRDATA.SPC [0]	1070.5938	0.0011
IRDATA.SPC [0]	1127.9415	0.0025
IRDATA.SPC [0]	1189.2630	0.0016
IRDATA.SPC [0]	1253.7986	0.0019
IRDATA.SPC [0]	1318.6264	0.0082
IRDATA.SPC [0]	1396.5834	0.0038
IRDATA.SPC [0]	1450.0352	0.0022
IRDATA.SPC [0]	1481.1245	0.0074

within +/- 3 cm⁻¹

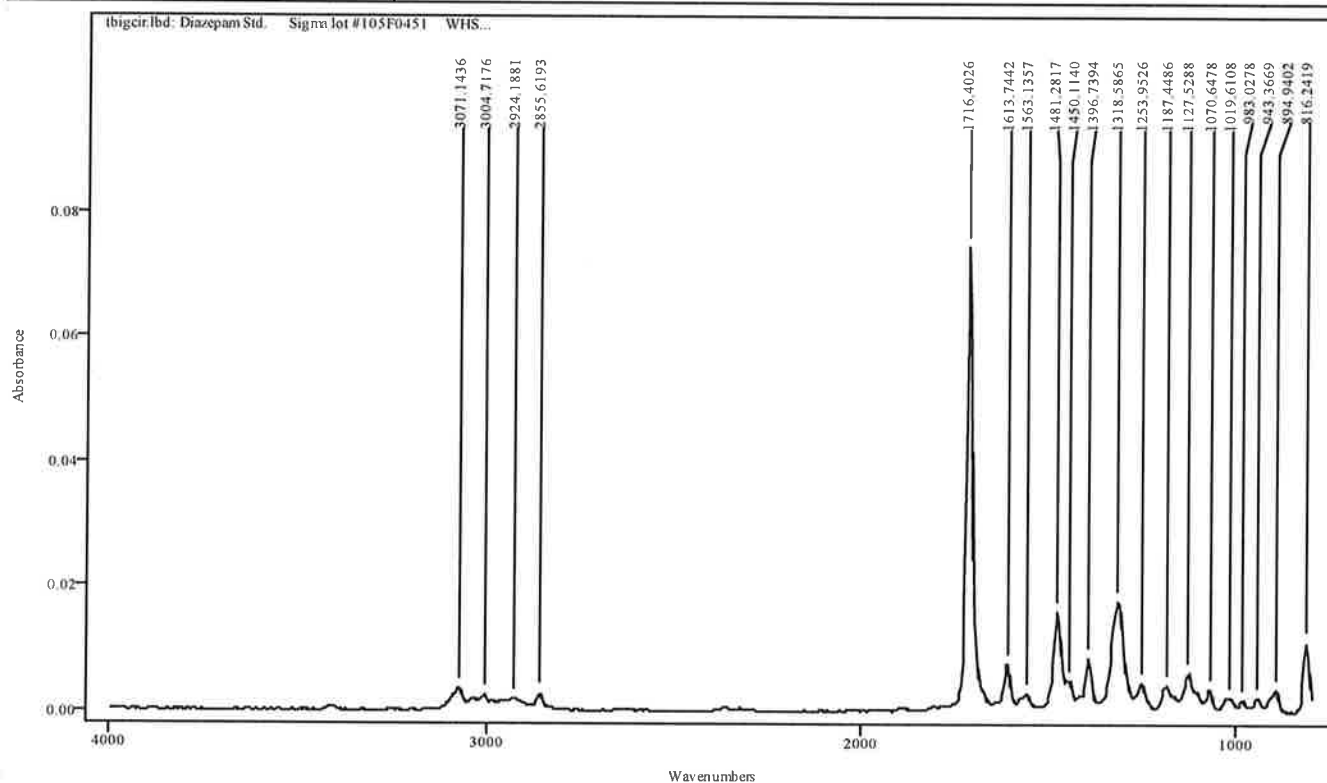
IRDATA.SPC [0]	1562.4709	0.0010
IRDATA.SPC [0]	1614.0332	0.0034
IRDATA.SPC [0]	1716.1642	0.0352
IRDATA.SPC [0]	2855.4623	0.0009
IRDATA.SPC [0]	2923.0367	0.0005
IRDATA.SPC [0]	3004.0325	0.0008
IRDATA.SPC [0]	3070.3018	0.0013

CH

Manual Peak Pick Results

CHK

Sample Filename	Entry 6 from Library tbigcir.lbd		
File Title	Diazepam Std.	Sigma lot #105F0451	WHS
Date	Wed Mar 04 15:36:20 2020		



Entry 6 from Library tbigcir.lbd: Diazepam Std. Sigma lot #105F0451 WHS

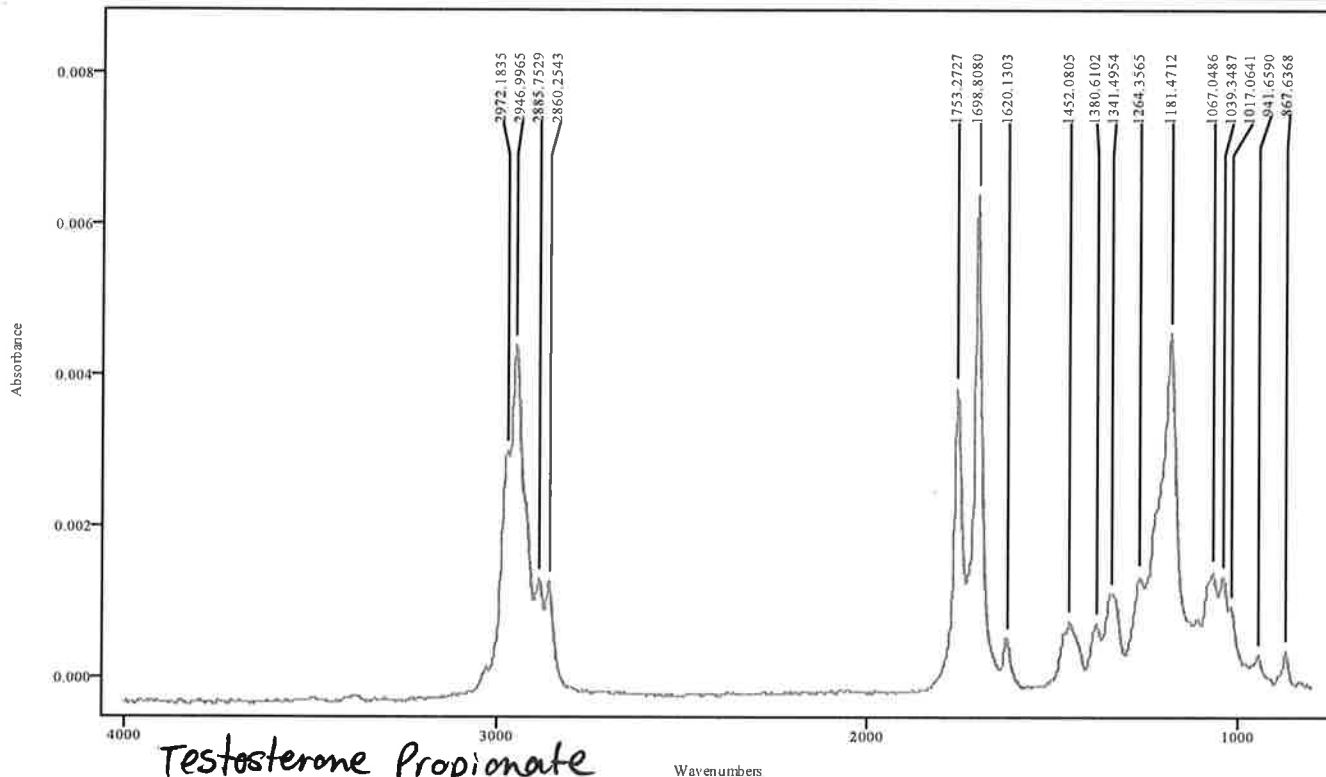
Filename	Peak At	Peak Height
tbigcir.lbd [6]	816.2419	0.0114
tbigcir.lbd [6]	894.9402	0.0036
tbigcir.lbd [6]	943.3669	0.0025
tbigcir.lbd [6]	983.0278	0.0021
tbigcir.lbd [6]	1019.6108	0.0024
tbigcir.lbd [6]	1070.6478	0.0036
tbigcir.lbd [6]	1127.5288	0.0063
tbigcir.lbd [6]	1187.4486	0.0043
tbigcir.lbd [6]	1253.9526	0.0048
tbigcir.lbd [6]	1318.5865	0.0176
tbigcir.lbd [6]	1396.7394	0.0087
tbigcir.lbd [6]	1450.1140	0.0052
tbigcir.lbd [6]	1481.2817	0.0161
tbigcir.lbd [6]	1563.1357	0.0029

tbigcir.lbd [6]	1613.7442	0.0079
tbigcir.lbd [6]	1716.4026	0.0747
tbigcir.lbd [6]	2855.6193	0.0029
tbigcir.lbd [6]	2924.1881	0.0021
tbigcir.lbd [6]	3004.7176	0.0026
tbigcir.lbd [6]	3071.1436	0.0038

MA

Manual Peak Pick Results

Sample Filename	IRDATA.SPC
File Title	13.73 minutes: AVE (13.58: 13.77) Ref. (12.50: 13.30) of TESTOST PROP 2MGML 2020_February_22_010648.cgm
Date	Wed Mar 04 15:39:00 2020



IRDATA.SPC: 13.73 minutes: AVE (13.58: 13.77) Ref. (12.50: 13.30) of TESTOST PROP 2MGML 2020_February_22_010648.cgm

Filename	Peak At	Peak Height
IRDATA.SPC [0]	867.6368	0.0004
IRDATA.SPC [0]	941.6590	0.0003
IRDATA.SPC [0]	1017.0641	0.0010
IRDATA.SPC [0]	1039.3487	0.0013
IRDATA.SPC [0]	1067.0486	0.0014
IRDATA.SPC [0]	1181.4712	0.0046
IRDATA.SPC [0]	1264.3565	0.0014
IRDATA.SPC [0]	1341.4954	0.0011
IRDATA.SPC [0]	1380.6102	0.0007
IRDATA.SPC [0]	1452.0805	0.0007
IRDATA.SPC [0]	1620.1303	0.0005
IRDATA.SPC [0]	1698.8080	0.0064
IRDATA.SPC [0]	1753.2727	0.0038

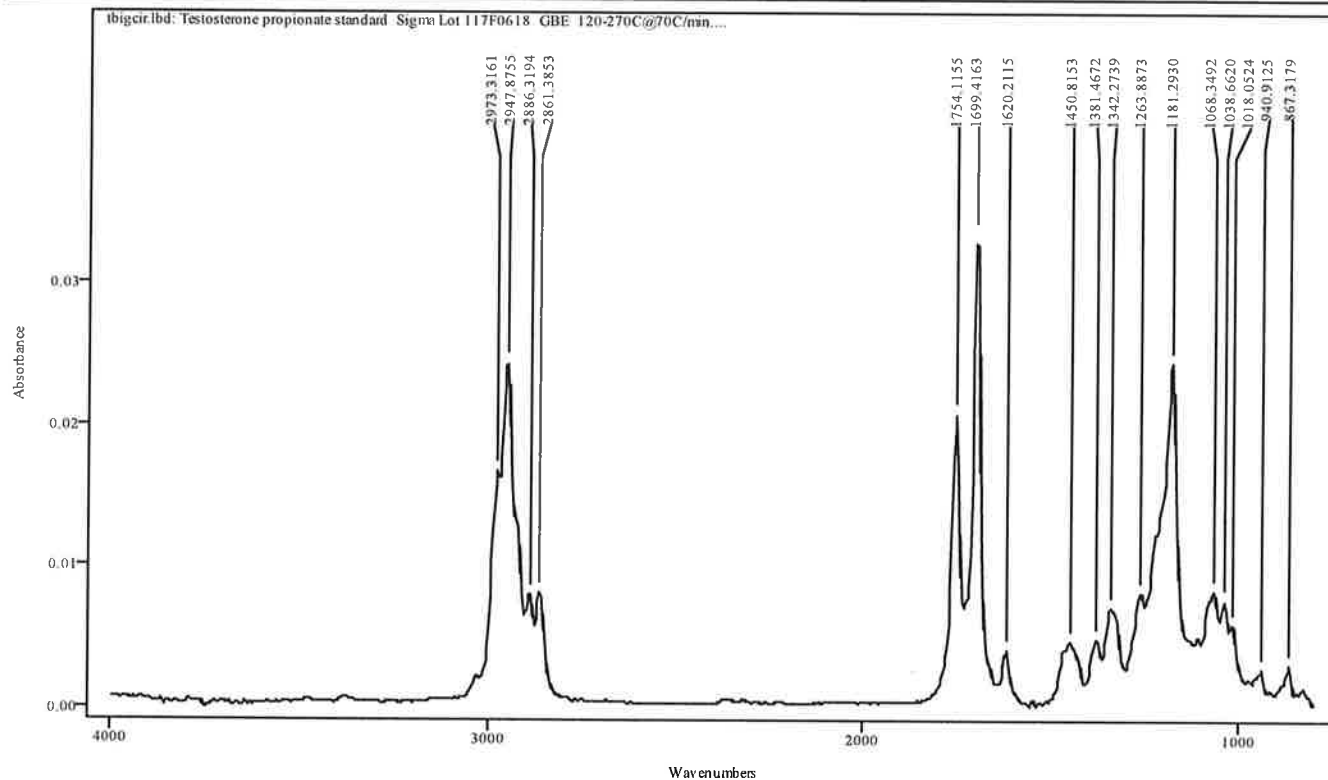
*Within ± 2 cm⁻¹
1.5*

IRDATA.SPC [0]	2860.2543	0.0013
IRDATA.SPC [0]	2885.7529	0.0013
IRDATA.SPC [0]	2946.9965	0.0044
IRDATA.SPC [0]	2972.1835	0.0030

Manual Peak Pick Results

MA

Sample Filename	Entry 63 from Library tbigcir.lbd
File Title	Testosterone propionate standard Sigma Lot 117F0618 GBE 120-270C@70C/min.
Date	Wed Mar 04 15:39:33 2020



Entry 63 from Library tbigcir.lbd: Testosterone propionate standard Sigma Lot 117F0618 GBE 120-270C@70C/min.

Filename	Peak At	Peak Height
tbigcir.lbd [63]	867.3179	0.0031
tbigcir.lbd [63]	940.9125	0.0028
tbigcir.lbd [63]	1018.0524	0.0060
tbigcir.lbd [63]	1038.6620	0.0076
tbigcir.lbd [63]	1068.3492	0.0083
tbigcir.lbd [63]	1181.2930	0.0244
tbigcir.lbd [63]	1263.8873	0.0082
tbigcir.lbd [63]	1342.2739	0.0070
tbigcir.lbd [63]	1381.4672	0.0049
tbigcir.lbd [63]	1450.8153	0.0048
tbigcir.lbd [63]	1620.2115	0.0041
tbigcir.lbd [63]	1699.4163	0.0336
tbigcir.lbd [63]	1754.1155	0.0209

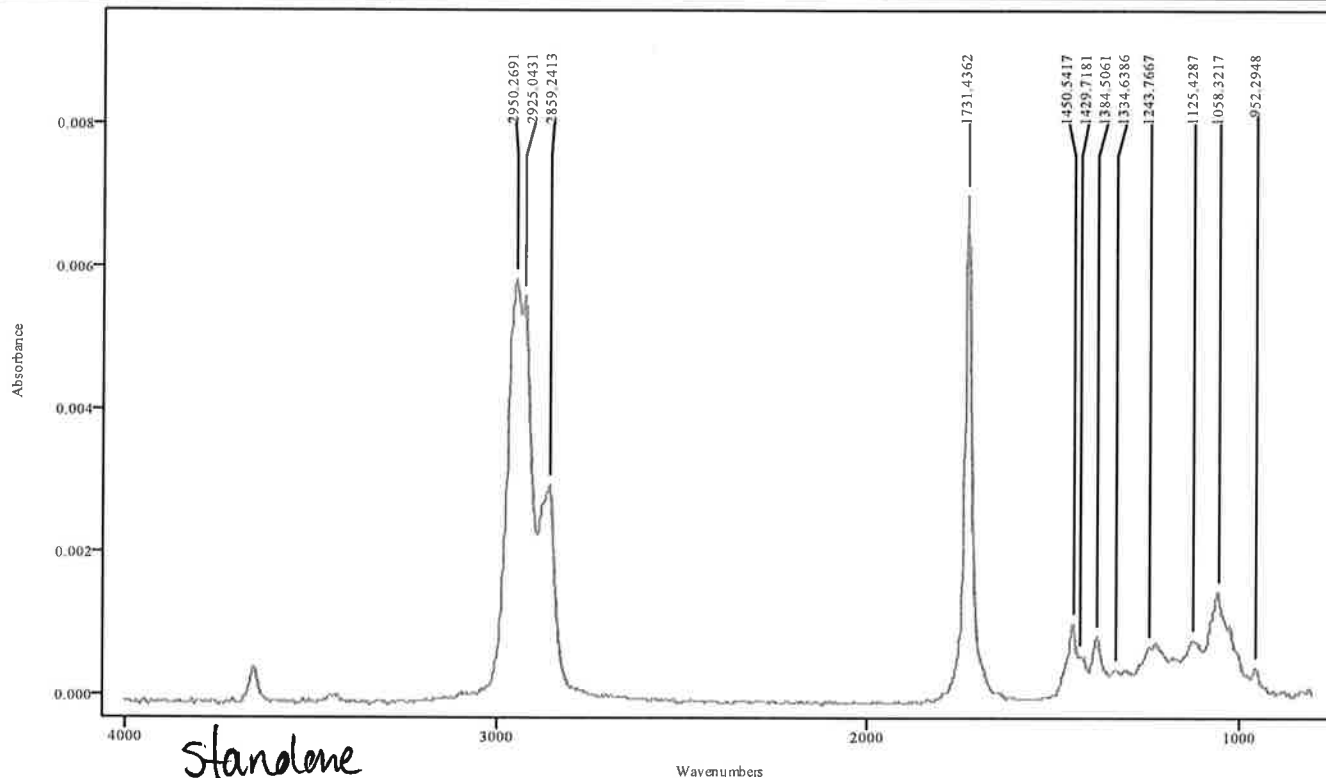
tbigcir.lbd [63]	2861.3853	0.0081
tbigcir.lbd [63]	2886.3194	0.0081
tbigcir.lbd [63]	2947.8755	0.0244
tbigcir.lbd [63]	2973.3161	0.0167

MA

MA

Manual Peak Pick Results

Sample Filename	IRDATA.SPC
File Title	7.65 minutes: AVE (7.58: 7.69) Ref. (6.98: 7.47) of STANOLONE 2MGML 2020_February_22_032910.cgm
Date	Wed Mar 04 15:44:31 2020



IRDATA.SPC: 7.65 minutes: AVE (7.58: 7.69) Ref. (6.98: 7.47) of STANOLONE 2MGML 2020_February_22_032910.cgm

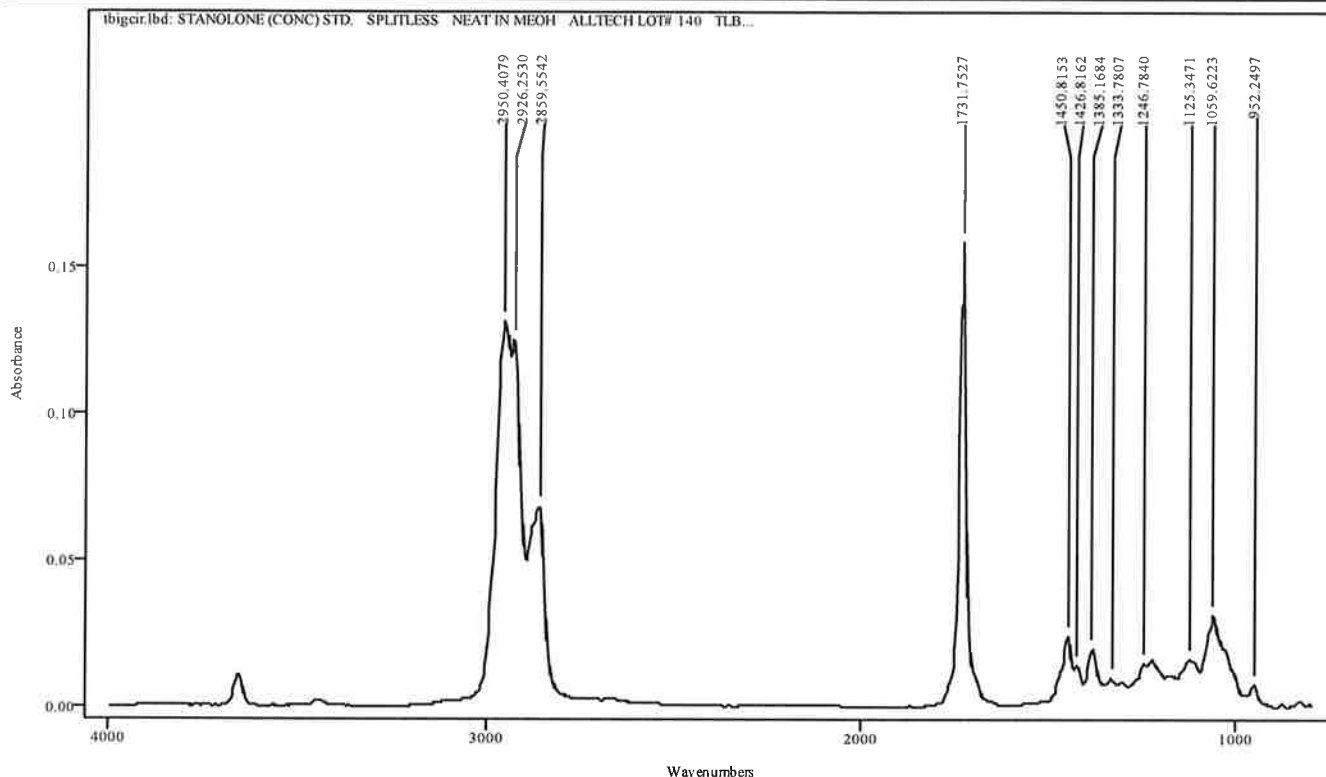
Filename	Peak At	Peak Height
IRDATA.SPC [0]	952.2948	0.0004
IRDATA.SPC [0]	1058.3217	0.0014
IRDATA.SPC [0]	1125.4287	0.0008
IRDATA.SPC [0]	1243.7667	0.0007
IRDATA.SPC [0]	1334.6386	0.0004
IRDATA.SPC [0]	1384.5061	0.0008
IRDATA.SPC [0]	1429.7181	0.0005
IRDATA.SPC [0]	1450.5417	0.0010
IRDATA.SPC [0]	1731.4362	0.0070
IRDATA.SPC [0]	2859.2413	0.0030
IRDATA.SPC [0]	2925.0431	0.0056
IRDATA.SPC [0]	2950.2691	0.0058

within +/- 3.1 cm⁻¹

AK

Manual Peak Pick Results

Sample Filename	Entry 172 from Library tbigcir.lbd
File Title	STANOLONE (CONC) STD. SPLITLESS NEAT IN MEOH ALLTECH LOT# 140 TLB
Date	Wed Mar 04 15:45:03 2020



Entry 172 from Library tbigcir.lbd: STANOLONE (CONC) STD. SPLITLESS NEAT IN MEOH ALLTECH LOT# 140 TLB

Filename	Peak At	Peak Height
tbigcir.lbd [172]	952.2497	0.0079
tbigcir.lbd [172]	1059.6223	0.0313
tbigcir.lbd [172]	1125.3471	0.0164
tbigcir.lbd [172]	1246.7840	0.0151
tbigcir.lbd [172]	1333.7807	0.0097
tbigcir.lbd [172]	1385.1684	0.0200
tbigcir.lbd [172]	1426.8162	0.0140
tbigcir.lbd [172]	1450.8153	0.0243
tbigcir.lbd [172]	1731.7527	0.1587
tbigcir.lbd [172]	2859.5542	0.0682
tbigcir.lbd [172]	2926.2530	0.1252
tbigcir.lbd [172]	2950.4079	0.1311