File: JM-25-2
Sample: MAHWISH / DR. M. IQBAL
Instrument: JEOL MS 600H-1

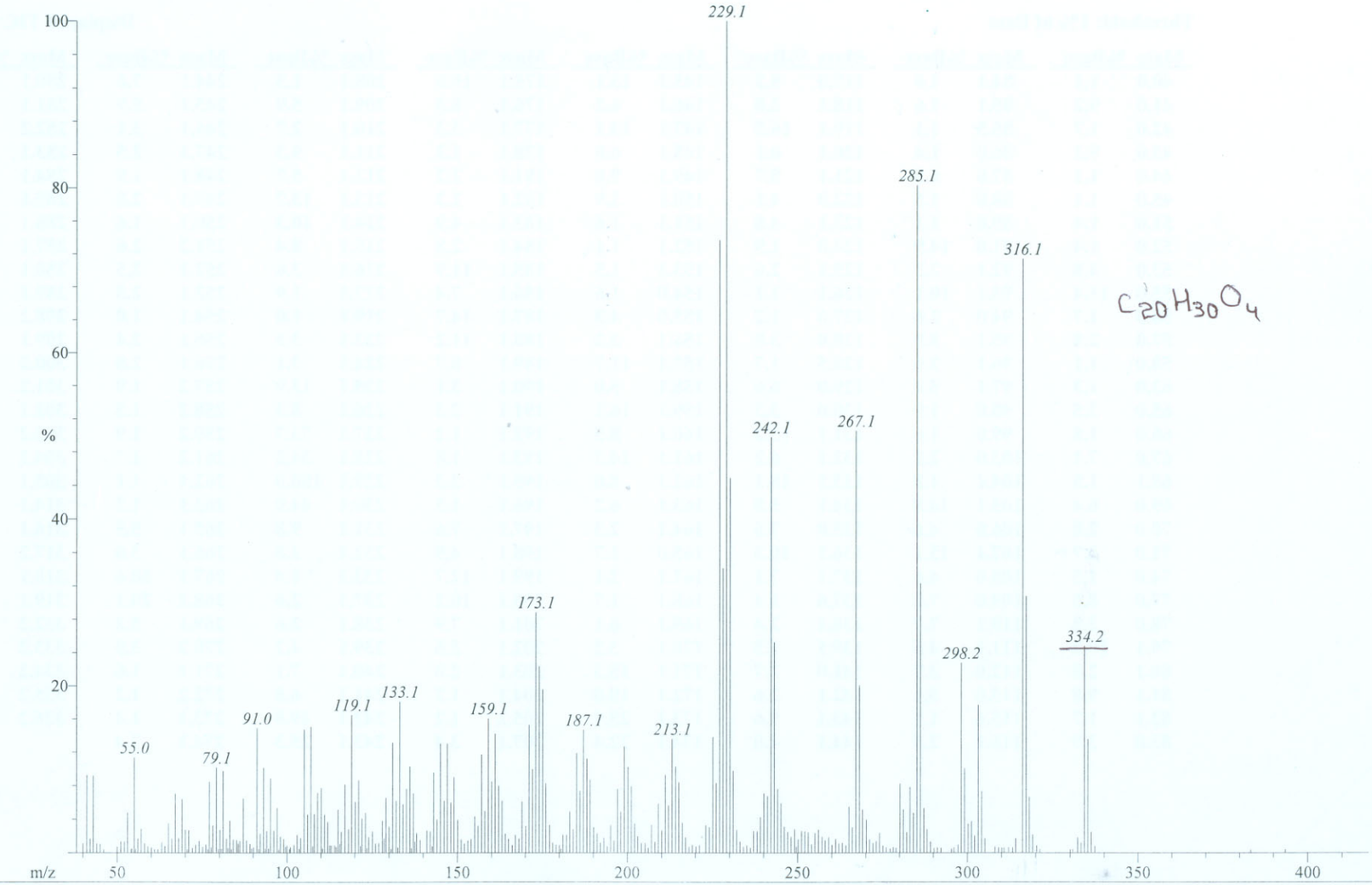
Date Run: 10-30-2015 (Time Run: 10:38:17)

Ionization mode: EI+

Scan: 13
Base: m/z 229; 29.5%FS TIC: 5723794

R.T.: 1.08

Compound 5




$C_{20}H_{30}O_4$

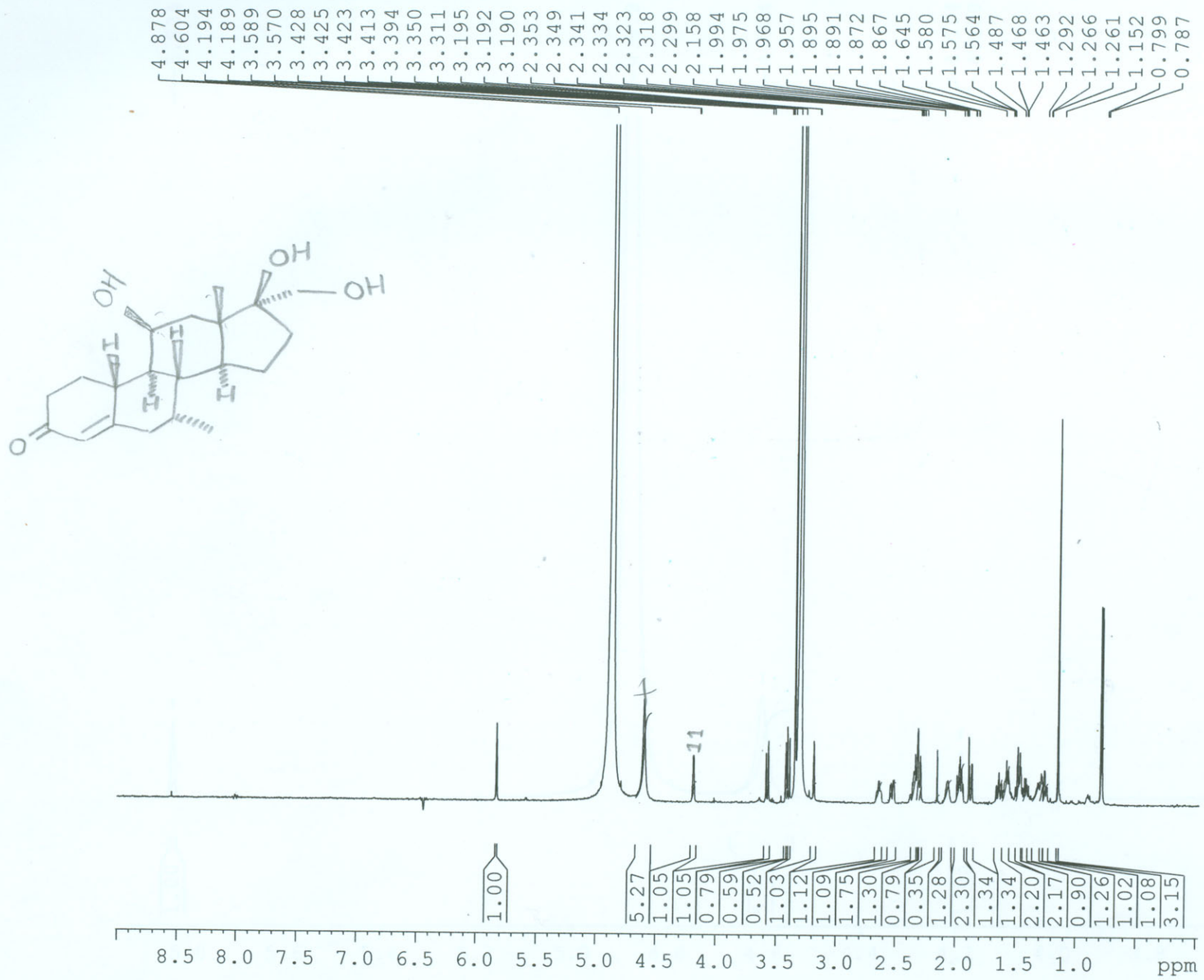
comp. 5

| Mass | Relative Intensity | Theoretical Mass | Delta [ppm] | Delta [mmu] | RDB | Composition |
|---|---|---|---|---|---|---|
| | | 265.1651 | -25.2 | -6.7 | 0.5 | $C_{12}H_{25}O_6$ |
| 266.1628 | 6.2 | 266.1671 | -16.0 | -4.3 | 9.0 | $C_{19}H_{22}O_1$ |
| 267.1735 | 39.9 | 267.1749 | -5.2 | -1.4 | 8.5 | $C_{19}H_{23}O_1$ |
| 268.1803 | 22.1 | 268.1827 | -8.9 | -2.4 | 8.0 | $C_{19}H_{24}O_1$ |
| 269.1882 | 13.6 | 269.1905 | -8.9 | -2.4 | 7.5 | $C_{19}H_{25}O_1$ |
| 270.1969 | 15.1 | 270.1984 | -5.3 | -1.4 | 7.0 | $C_{19}H_{26}O_1$ |
| 271.2025 | 5.7 | 271.2062 | -13.8 | -3.7 | 6.5 | $C_{19}H_{27}O_1$ |
| 272.1805 | 1.5 | 272.1776 | 10.6 | 2.9 | 7.0 | $C_{18}H_{24}O_2$ |
| 272.2077 | 1.6 | 272.2140 | -23.4 | -6.4 | 6.0 | $C_{19}H_{28}O_1$ |
| 279.1729 | 1.2 | 279.1749 | -7.3 | -2.0 | 9.5 | $C_{20}H_{23}O_1$ |
| | | 279.1808 | -28.3 | -7.9 | 0.5 | $C_{13}H_{27}O_6$ |
| 280.1833 | 13.5 | 280.1827 | 2.1 | 0.6 | 9.0 | $C_{20}H_{24}O_1$ |
| | | 280.1886 | -18.9 | -5.3 | 0.0 | $C_{13}H_{28}O_6$ |
| 281.1891 | 5.4 | 281.1905 | -5.1 | -1.4 | 8.5 | $C_{20}H_{25}O_1$ |
| 282.1989 | 6.6 | 282.1984 | 1.9 | 0.5 | 8.0 | $C_{20}H_{26}O_1$ |
| 283.1707 | 12.3 | 283.1698 | 3.1 | 0.9 | 8.5 | $C_{19}H_{23}O_2$ |
| 284.1778 | 8.2. | 284.1776 | 0.5 | 0.2 | 8.0 | $C_{19}H_{24}O_2$ |
| 285.1867 | 32.7 | 285.1855 | 4.5 | 1.3 | 7.5 | $C_{19}H_{25}O_2$ |
| 286.1934 | 17.7 | 286.1933 | 0.6 | 0.2 | 7.0 | $C_{19}H_{26}O_2$ |
| 287.1957 | 4.6 | 287.2011 | -18.8 | -5.4 | 6.5 | $C_{19}H_{27}O_2$ |
| 288.2089 | 1.8 | 288.2089 | -0.2 | -0.1 | 6.0 | $C_{19}H_{28}O_2$ |
| 296.1759 | 2.2 | 296.1776 | -5.9 | -1.8 | 9.0 | $C_{20}H_{24}O_2$ |
| | | 296.1835 | -25.8 | -7.6 | 0.0 | $C_{13}H_{28}O_7$ |
| 297.1836 | 1.2 | 297.1855 | -6.4 | -1.9 | 8.5 | $C_{20}H_{25}O_2$ |
| 298.1919 | 64.2 | 298.1933 | -4.6 | -1.4 | 8.0 | $C_{20}H_{26}O_2$ |
| 299.1970 | 25.2 | 299.2011 | -13.6 | -4.1 | 7.5 | $C_{20}H_{27}O_2$ |
| 300.2021 | 6.2 | 300.2089 | -22.7 | -6.8 | 7.0 | $C_{20}H_{28}O_2$ |
| | | 300.1937 | 28.1 | 8.4 | 3.0 | $C_{16}H_{28}O_5$ |
| 301.1853 | 3.4 | 301.1804 | 16.4 | 4.9 | 7.5 | $C_{19}H_{25}O_3$ |
| 302.1880 | 1.2 | 302.1882 | -0.6 | -0.2 | 7.0 | $C_{19}H_{26}O_3$ |
| 303.1958 | 7.1 | 303.1960 | -0.7 | -0.2 | 6.5 | $C_{19}H_{27}O_3$ |
| 304.1998 | 2.5 | 304.2038 | -13.1 | -4.0 | 6.0 | $C_{19}H_{28}O_3$ |
| 314.1881 | 3.1 | 314.1882 | -0.2 | -0.1 | 8.0 | $C_{20}H_{26}O_3$ |
| 315.1924 | 1.4 | 315.1960 | -11.6 | -3.7 | 7.5 | $C_{20}H_{27}O_3$ |
| 316.2037 | 23.0 | 316.2038 | -0.6 | -0.2 | 7.0 | $C_{20}H_{28}O_3$ |
| 317.2100 | 9.6 | 317.2117 | -5.1 | -1.6 | 6.5 | $C_{20}H_{29}O_3$ |
| 318.2144 | 2.0 | 318.2195 | -16.0 | -5.1 | 6.0 | $C_{20}H_{30}O_3$ |
| 334.2146 | 7.0 | 334.2144 | 0.5 | 0.2 | 6.0 | $C_{20}H_{30}O_4$ |
| 335.2197 | 2.8 | 335.2222 | -7.5 | -2.5 | 5.5 | $C_{20}H_{31}O_4$ |

Mahwish / Dr. Iqbal / JM-25-2 / MeOD
1H

Comp - 5

AVANCE AV-600-LC
CRYOPROBE
LAB NO: 108



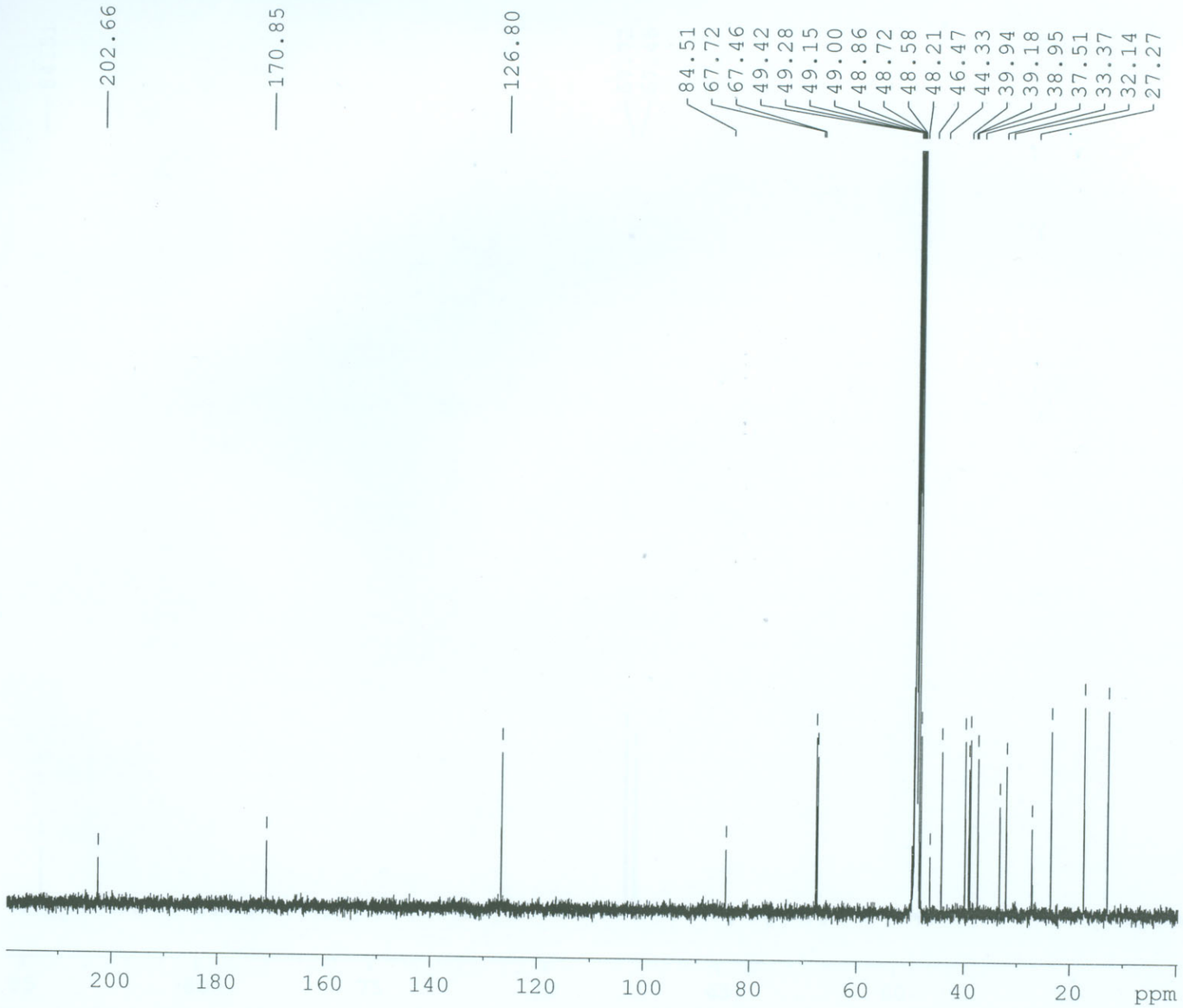

| | |
|---|---|
| NAME | oct08-15 |
| EXPNO | 3 |
| PROCNO | 1 |
| Date_ | 20151008 |
| Time | 13.13 |
| INSTRUM | spect |
| PROBHD | 5 mm CPTCI 1H- |
| PULPROG | zg30 |
| TD | 32768 |
| SOLVENT | MeOD |
| NS | 64 |
| DS | 0 |
| SWH | 12019.230 Hz |
| FIDRES | 0.366798 Hz |
| AQ | 1.3632404 sec |
| RG | 9 |
| DW | 41.600 usec |
| DE | 6.50 usec |
| TE | 298.0 K |
| D1 | 2.00000000 sec |
| TD0 | 1 |

======== CHANNEL f1 ========

| | |
|---|---|
| NUC1 | 1H |
| P1 | 8.00 usec |
| PL1 | 3.31 dB |
| PL1W | 6.79873323 W |
| SFO1 | 600.0348002 MHz |
| SI | 32768 |
| SF | 600.0300107 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 0.50 Hz |
| GB | 0 |
| PC | 1.40 |

MAHWISH / Dr. IQBAL / JM-25-2 / CD3OD
BB

comp 5

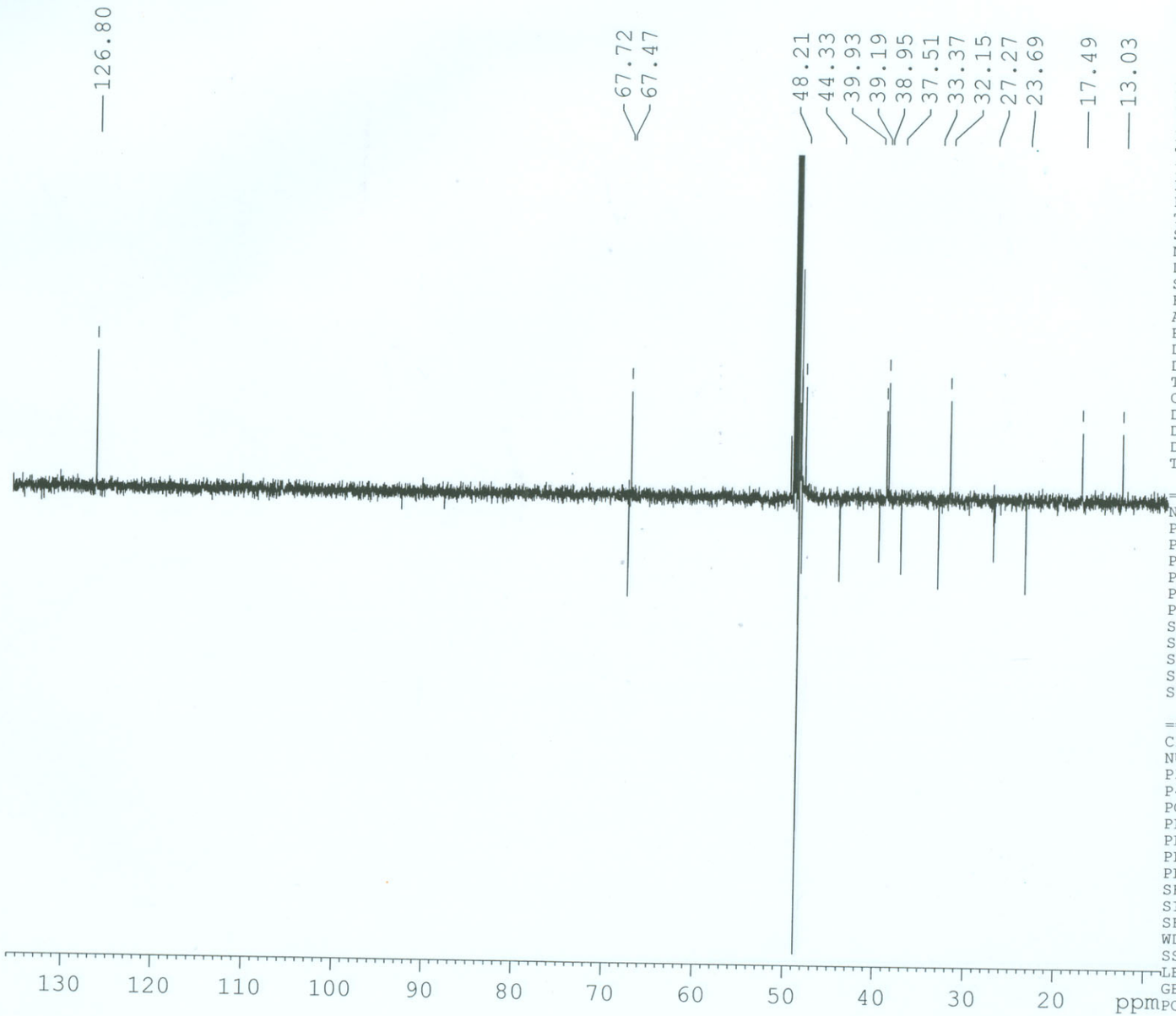



AVANCE AV-600
CRYO PROBE
LAB NO: 108

| | |
|---|---|
| NAME | oct09-15 |
| EXPNO | 6 |
| PROCNO | 1 |
| Date_ | 20151010 |
| Time | 14.26 |
| INSTRUM | spect |
| PROBHD | 5 mm CPTCI 1H- |
| PULPROG | zgpg |
| TD | 32768 |
| SOLVENT | MeOD |
| NS | 16384 |
| DS | 2 |
| SWH | 35971.223 Hz |
| FIDRES | 1.097755 Hz |
| AQ | 0.4555391 sec |
| RG | 32768 |
| DW | 13.900 usec |
| DE | 6.50 usec |
| TE | 298.0 K |
| D1 | 1.50000000 sec |
| D11 | 0.03000000 sec |
| TD0 | 16 |
| ======== CHANNEL f1 ======== | |
| NUC1 | 13C |
| P1 | 15.40 usec |
| PL1 | 1.00 dB |
| PL1W | 83.60149384 W |
| SFO1 | 150.9453107 MHz |
| ======== CHANNEL f2 ======== | |
| CPDPRG2 | waltz16 |
| NUC2 | 1H |
| PCPD2 | 65.00 usec |
| PL2 | 3.30 dB |
| PL12 | 22.06 dB |
| PL13 | 27.00 dB |
| PL2W | 9.16420078 W |
| PL12W | 0.12192553 W |
| PL13W | 0.03909260 W |
| SFO2 | 600.2336014 MHz |
| SI | 16384 |
| SF | 150.9277401 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 0.50 |

MAHWISH / Dr. IQBAL / JM-25-2 / CD3OD
DEPT135

Comp-5

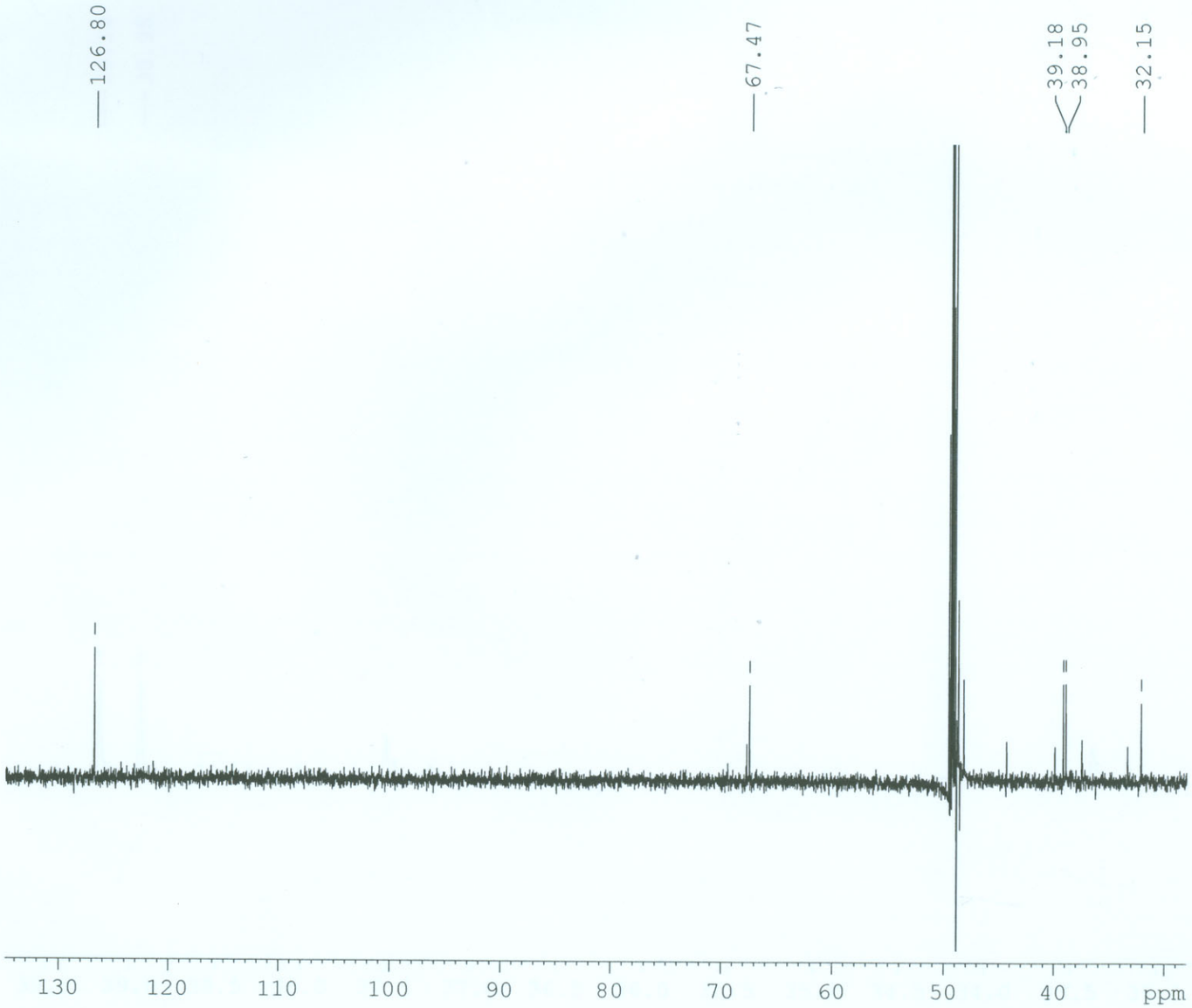



BRUKER

| | |
|---|---|
| NAME | oct09-15 |
| EXPNO | 7 |
| PROCNO | 1 |
| Date_ | 20151010 |
| Time | 23.38 |
| INSTRUM | spect |
| PROBHD | 5 mm CPTCI 1H- |
| PULPROG | deptsp135 |
| TD | 32768 |
| SOLVENT | MeOD |
| NS | 8192 |
| DS | 2 |
| SWH | 30303.031 Hz |
| FIDRES | 0.924775 Hz |
| AQ | 0.5407385 sec |
| RG | 32768 |
| DW | 16.500 usec |
| DE | 6.50 usec |
| TE | 298.0 K |
| CNST2 | 145.0000000 |
| D1 | 1.50000000 sec |
| D2 | 0.00344828 sec |
| D12 | 0.00002000 sec |
| TD0 | 8 |
| ======== CHANNEL f1 ======== | |
| NUC1 | 13C |
| P1 | 15.40 usec |
| P12 | 2000.00 usec |
| PL0 | 120.00 dB |
| PL1 | 1.00 dB |
| PL0W | 0.00000000 W |
| PL1W | 83.60149384 W |
| SFO1 | 150.9430468 MHz |
| SP2 | 5.40 dB |
| SPNAM2 | Crp60comp.4 |
| SPOAL2 | 0.500 |
| SPOFFS2 | 0.00 Hz |
| ======== CHANNEL f2 ======== | |
| CPDPRG2 | waltz16 |
| NUC2 | 1H |
| P3 | 7.50 usec |
| P4 | 15.00 usec |
| PCPD2 | 65.00 usec |
| PL2 | 3.30 dB |
| PL12 | 22.06 dB |
| PL2W | 9.16420078 W |
| PL12W | 0.12192553 W |
| SFO2 | 600.2324009 MHz |
| SI | 16384 |
| SF | 150.9277401 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.00 |

MAHWISH / Dr. IQBAL / JM-25-2 / CD3OD
DEPT90

comp - 5

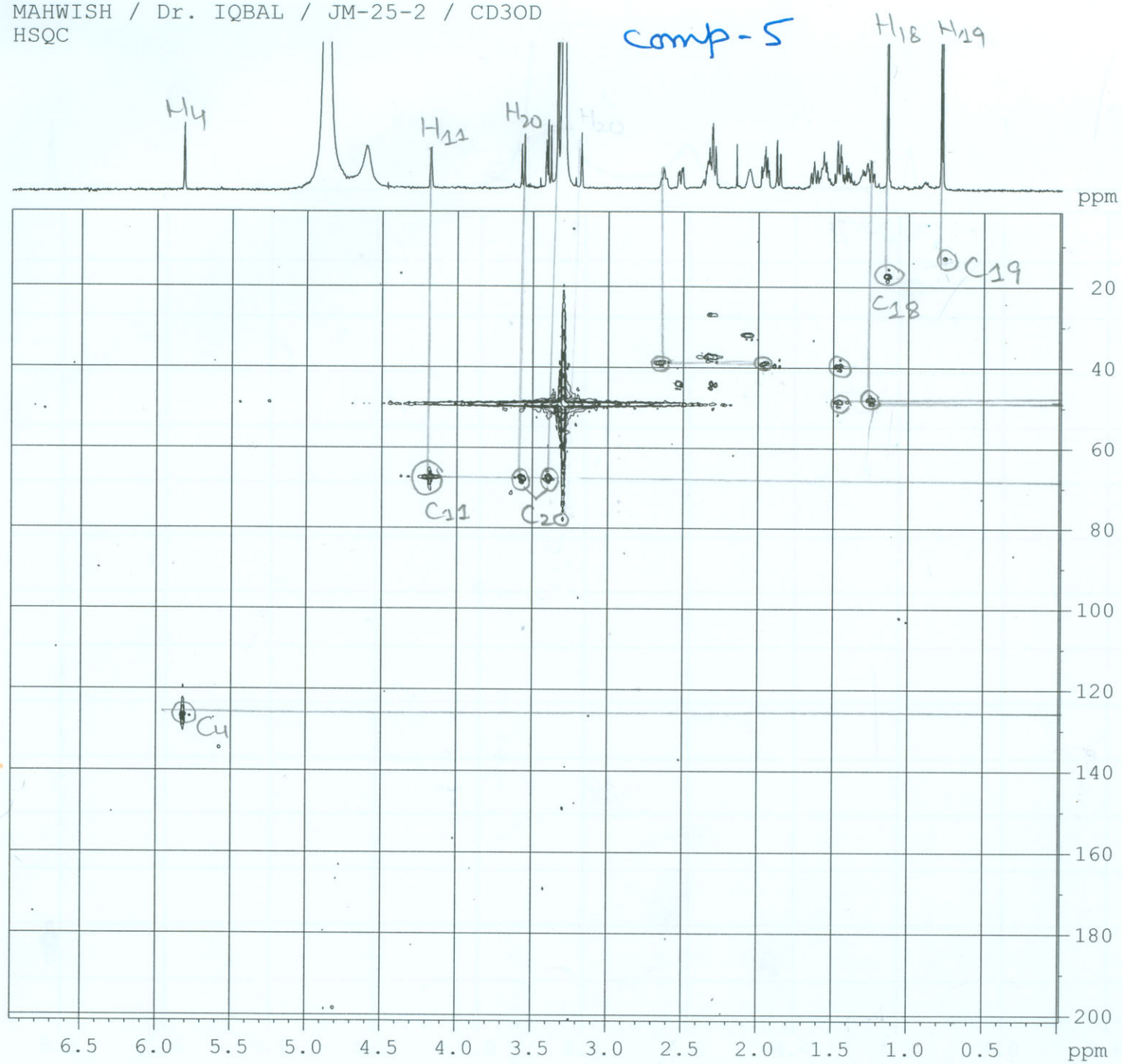



AVANCE AV-600
CRYO PROBE
LAB NO: 108

| | | |
|---|---|---|
| NAME | oct09-15 | |
| EXPNO | 8 | |
| PROCNO | 1 | |
| Date_ | 20151011 | |
| Time | 4.23 | |
| INSTRUM | spect | |
| PROBHD | 5 mm CPTCI 1H- | |
| PULPROG | deptsp90 | |
| TD | 32768 | |
| SOLVENT | MeOD | |
| NS | 4096 | |
| DS | 2 | |
| SWH | 30303.031 | Hz |
| FIDRES | 0.924775 | Hz |
| AQ | 0.5407385 | sec |
| RG | 32768 | |
| DW | 16.500 | usec |
| DE | 6.50 | usec |
| TE | 298.0 | K |
| CNST2 | 145.0000000 | |
| D1 | 1.50000000 | sec |
| D2 | 0.00344828 | sec |
| D12 | 0.00002000 | sec |
| TD0 | 4 | |
| ======== CHANNEL f1 ======== | | |
| NUC1 | 13C | |
| P1 | 15.40 | usec |
| P12 | 2000.00 | usec |
| PL0 | 120.00 | dB |
| PL1 | 1.00 | dB |
| PL0W | 0.00000000 | W |
| PL1W | 83.60149384 | W |
| SFO1 | 150.9430468 | MHz |
| SP2 | 5.40 | dB |
| SPNAM2 | Crp60comp.4 | |
| SPOAL2 | 0.500 | |
| SPOFFS2 | 0.00 | Hz |
| ======== CHANNEL f2 ======== | | |
| CPDPRG2 | waltz16 | |
| NUC2 | 1H | |
| P3 | 7.50 | usec |
| P4 | 15.00 | usec |
| PCPD2 | 65.00 | usec |
| PL2 | 3.30 | dB |
| PL12 | 22.06 | dB |
| PL2W | 9.16420078 | W |
| PL12W | 0.12192553 | W |
| SFO2 | 600.2324009 | MHz |
| SI | 16384 | |
| SF | 150.9277401 | MHz |
| WDW | EM | |
| SSB | 0 | |
| LB | 1.00 | Hz |
| GB | 0 | |
| PC | 1.00 | |

MAHWISH / Dr. IQBAL / JM-25-2 / CD3OD
HSQC

comp-5

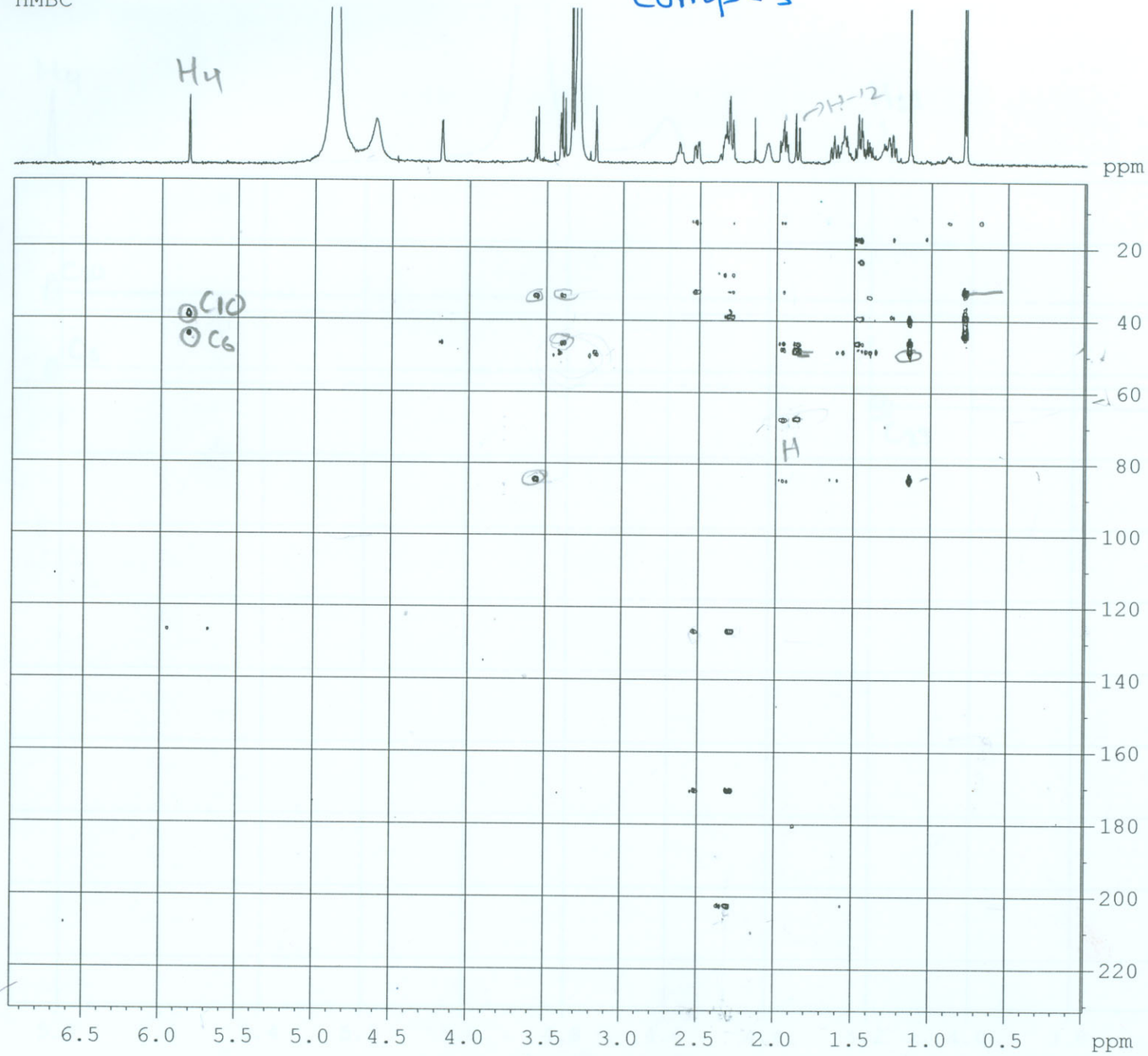



AVANCE AV-600
CRYO PROBE
LAB NO: 108

| | | |
|---|---|---|
| NAME | oct09-15 | |
| EXPNO | 4 | |
| PROCNO | 1 | |
| Date_ | 20151010 | |
| Time | 0.47 | |
| INSTRUM | spect | |
| PROBHD | 5 mm CPTCI 1H- | |
| PULPROG | hsqcetgpsi | |
| TD | 1024 | |
| SOLVENT | MeOD | |
| NS | 32 | |
| DS | 8 | |
| SWH | 4194.631 | Hz |
| FIDRES | 4.096319 | Hz |
| AQ | 0.1222300 | sec |
| RG | 29193 | |
| DW | 119.200 | usec |
| DE | 6.50 | usec |
| TE | 298.0 | K |
| CNST2 | 145.0000000 | |
| D0 | 0.00000300 | sec |
| D1 | 2.00000000 | sec |
| D4 | 0.00172414 | sec |
| D11 | 0.03000000 | sec |
| D13 | 0.00000400 | sec |
| D16 | 0.00015000 | sec |
| D24 | 0.00110000 | sec |
| IN0 | 0.00001655 | sec |
| ZGOPTNS | | |
| ======== CHANNEL f1 ======== | | |
| NUC1 | 1H | |
| P1 | 7.20 | usec |
| P2 | 14.40 | usec |
| P28 | 0.50 | usec |
| PL1 | 3.30 | dB |
| PL1W | 9.16420078 | W |
| SFO1 | 600.2321008 | MHz |
| ======== CHANNEL f2 ======== | | |
| CPDPRG2 | garp | |
| NUC2 | 13C | |
| P3 | 15.40 | usec |
| P4 | 30.80 | usec |
| PCPD2 | 61.00 | usec |
| PL2 | 1.00 | dB |
| PL12 | 13.00 | dB |
| PL2W | 83.60149384 | W |
| PL12W | 5.27489758 | W |
| SFO2 | 150.9430468 | MHz |
| ====== GRADIENT CHANNEL ===== | | |
| GPNAM1 | SINE.100 | |
| GPNAM2 | SINE.100 | |
| GPZ1 | 80.00 | % |
| GPZ2 | 20.10 | % |
| P16 | 2000.00 | usec |
| ND0 | 2 | |
| TD | 256 | |
| SFO1 | 150.943 | MHz |
| FIDRES | 117.924255 | Hz |
| SW | 200.000 | ppm |
| FnMODE | Echo-Antiecho | |
| SI | 1024 | |
| SF | 600.2300154 | MHz |
| WDW | QSINE | |
| SSB | 2 | |
| LB | 0.00 | Hz |
| GB | 0 | |
| PC | 4.00 | |
| SI | 1024 | |
| MC2 | echo-antiecho | |
| SF | 150.9277401 | MHz |
| WDW | QSINE | |
| SSB | 2 | |
| LB | 0.00 | Hz |
| GB | 0 | |

MAHWISH / Dr. IQBAL / JM-25-2 / CD3OD
HMBC

comp-5

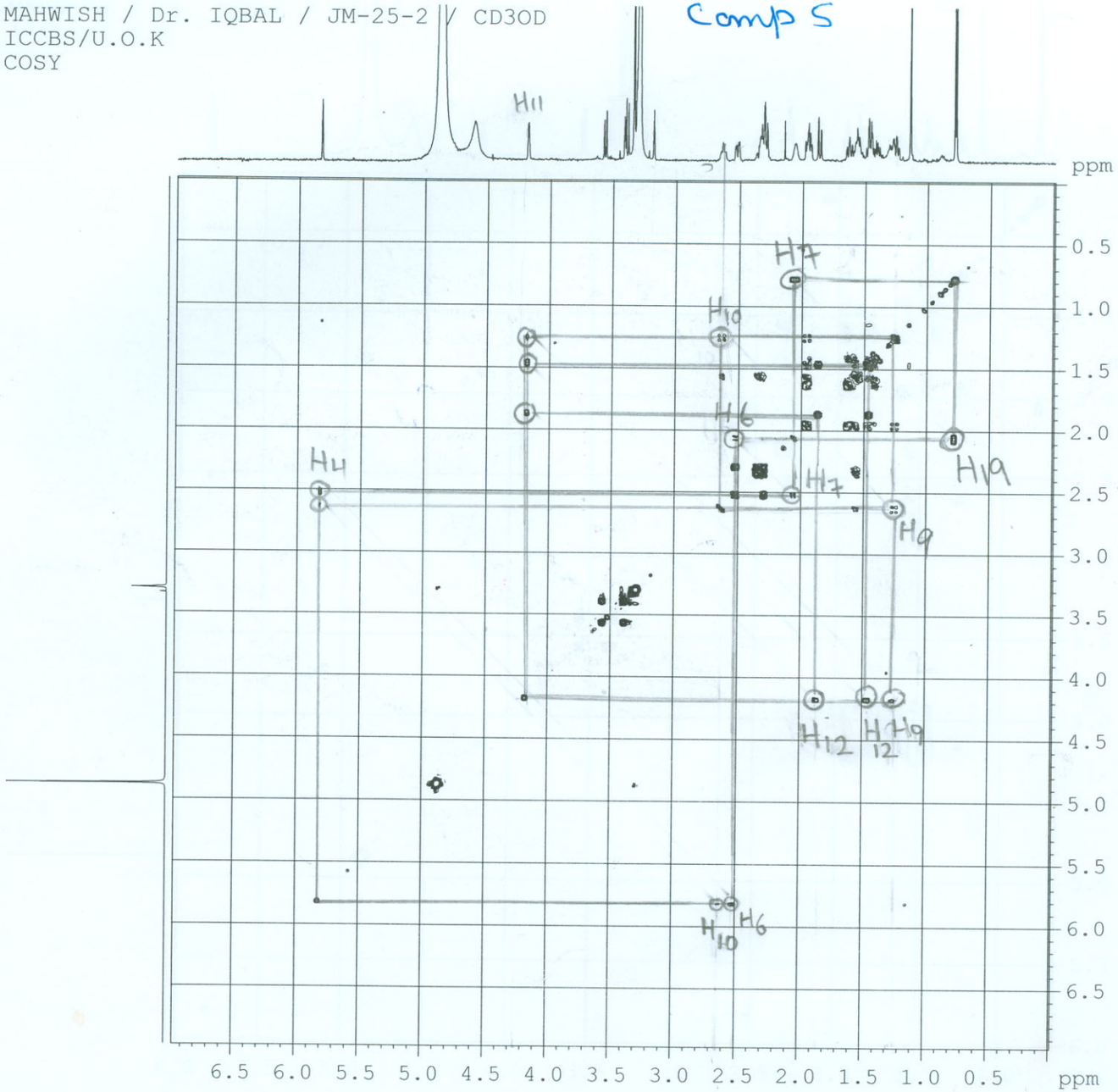



AVANCE AV-600
CRYO PROBE
LAB NO: 108

| | |
|---|---|
| NAME | oct09-15 |
| EXPNO | 5 |
| PROCNO | 1 |
| Date_ | 20151010 |
| Time | 5.41 |
| INSTRUM | spect |
| PROBHD | 5 mm CPTCI 1H- |
| PULPROG | hmbcgplpndqf |
| TD | 2048 |
| SOLVENT | MeOD |
| NS | 64 |
| DS | 16 |
| SWH | 4194.631 Hz |
| FIDRES | 2.048160 Hz |
| AQ | 0.2442908 sec |
| RG | 46341 |
| DW | 119.200 usec |
| DE | 6.50 usec |
| TE | 298.0 K |
| CNST2 | 145.0000000 |
| CNST13 | 13.0000000 |
| D0 | 0.00000300 sec |
| D1 | 1.50000000 sec |
| D2 | 0.00344828 sec |
| D6 | 0.03846154 sec |
| D16 | 0.00015000 sec |
| IN0 | 0.00001440 sec |
| ======== CHANNEL f1 ======== | |
| NUC1 | 1H |
| P1 | 7.20 usec |
| P2 | 14.40 usec |
| PL1 | 3.30 dB |
| PL1W | 9.16420078 W |
| SFO1 | 600.2321008 MHz |
| ======== CHANNEL f2 ======== | |
| NUC2 | 13C |
| P3 | 15.40 usec |
| PL2 | 1.00 dB |
| PL2W | 83.60149384 W |
| SFO2 | 150.9453107 MHz |
| ====== GRADIENT CHANNEL ===== | |
| GPNAM1 | SINE.100 |
| GPNAM2 | SINE.100 |
| GPNAM3 | SINE.100 |
| GPZ1 | 50.00 % |
| GPZ2 | 30.00 % |
| GPZ3 | 40.10 % |
| P16 | 2000.00 usec |
| ND0 | 2 |
| TD | 256 |
| SFO1 | 150.9453 MHz |
| FIDRES | 135.614929 Hz |
| SW | 230.000 ppm |
| FnMODE | QF |
| SI | 1024 |
| SF | 600.2300154 MHz |
| WDW | SINE |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.40 |
| SI | 1024 |
| MC2 | QF |
| SF | 150.9277401 MHz |
| WDW | SINE |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |

MAHWISH / Dr. IQBAL / JM-25-2 / CD3OD
ICCBS/U.O.K
COSY

Comp 5

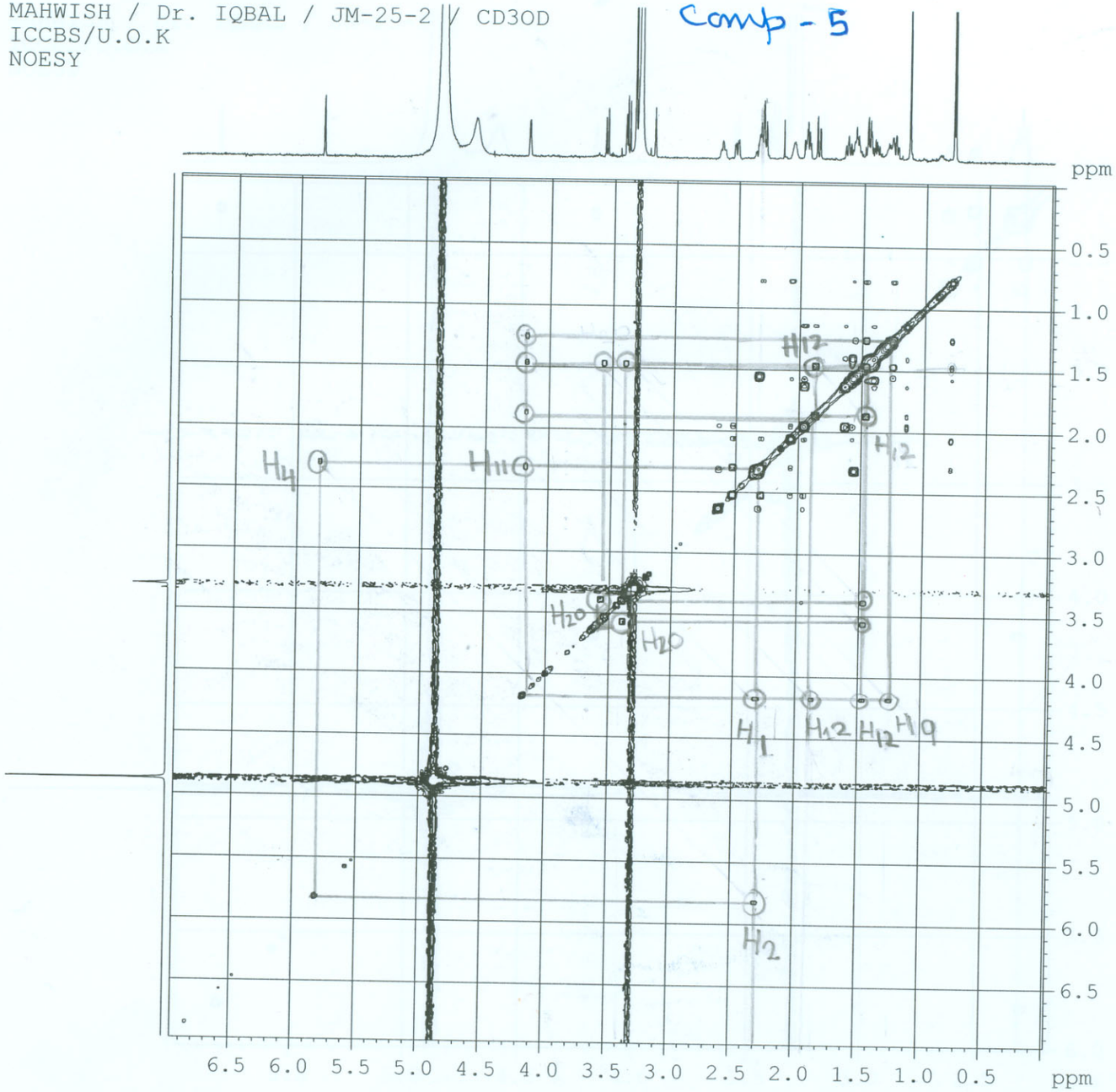



AVANCE AV-600
CRYO PROBE
LAB NO: 108

| | |
|---|---|
| NAME | oct09-15 |
| EXPNO | 2 |
| PROCNO | 1 |
| Date_ | 20151009 |
| Time | 16.02 |
| INSTRUM | spect |
| PROBHD | 5 mm CPTCI 1H- |
| PULPROG | cosydfqf |
| TD | 2048 |
| SOLVENT | MeOD |
| NS | 16 |
| DS | 4 |
| SWH | 4194.631 Hz |
| FIDRES | 2.048160 Hz |
| AQ | 0.2442908 sec |
| RG | 128 |
| DW | 119.200 usec |
| DE | 6.50 usec |
| TE | 298.0 K |
| D0 | 0.00000300 sec |
| D1 | 1.50000000 sec |
| D13 | 0.00000400 sec |
| D20 | 0.00000200 sec |
| IN0 | 0.00023840 sec |
| ======== CHANNEL f1 ======== | |
| NUC1 | 1H |
| P1 | 7.20 usec |
| PL1 | 3.30 dB |
| PL1W | 9.16420078 W |
| SFO1 | 600.2321008 MHz |
| ND0 | 1 |
| TD | 256 |
| SFO1 | 600.2321 MHz |
| FIDRES | 16.385277 Hz |
| SW | 6.988 ppm |
| FnMODE | QF |
| SI | 1024 |
| SF | 600.2300154 MHz |
| WDW | QSINE |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.40 |
| SI | 1024 |
| MC2 | QF |
| SF | 600.2300154 MHz |
| WDW | QSINE |
| SSB | 0 |
| LB | 0.00 Hz |
| GB | 0 |

MAHWISH / Dr. IQBAL / JM-25-2 / CD3OD
ICCBS/U.O.K
NOESY

Comp - 5




AVANCE AV-600
CRYO PROBE
LAB NO: 108

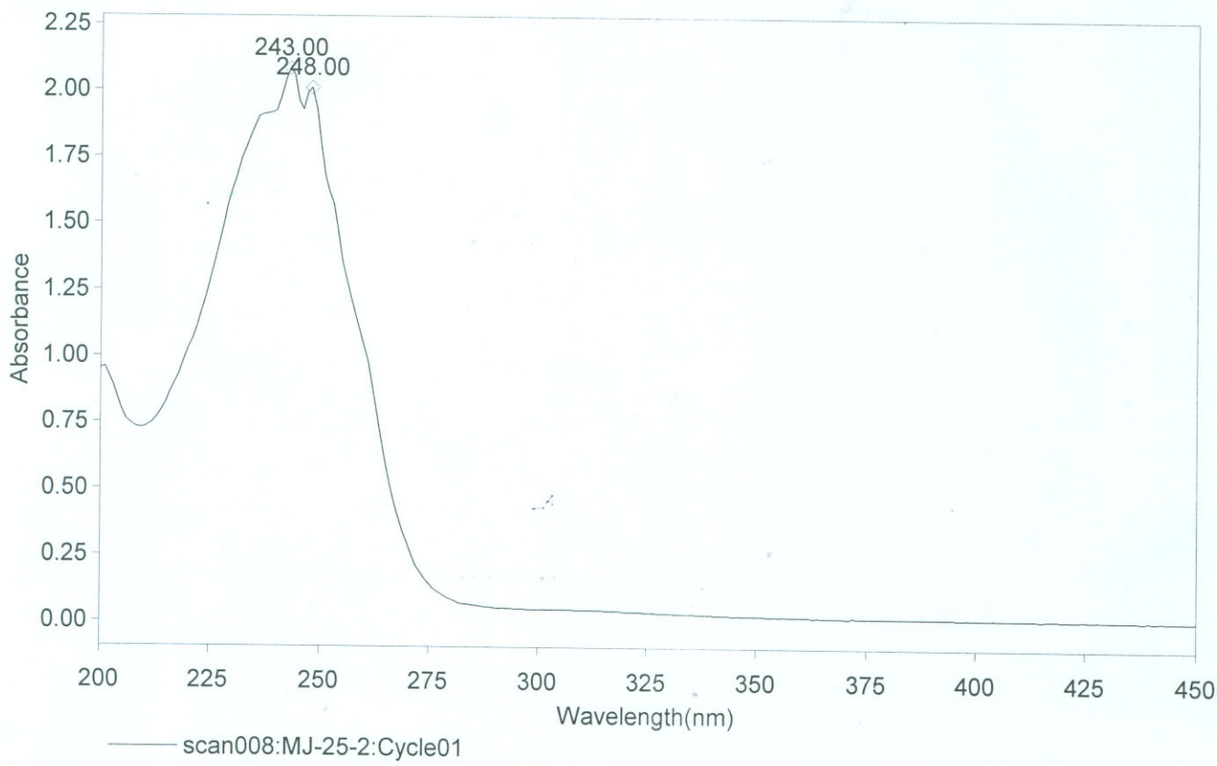
| | |
|---|---|
| NAME | oct09-15 |
| EXPNO | 3 |
| PROCNO | 1 |
| Date_ | 20151009 |
| Time | 18.05 |
| INSTRUM | spect |
| PROBHD | 5 mm CPTCI 1H- |
| PULPROG | noesygpph |
| TD | 1024 |
| SOLVENT | MeOD |
| NS | 32 |
| DS | 4 |
| SWH | 4194.631 Hz |
| FIDRES | 4.096319 Hz |
| AQ | 0.1222300 sec |
| RG | 71.8 |
| DW | 119.200 usec |
| DE | 6.50 usec |
| TE | 298.0 K |
| D0 | 0.00010978 sec |
| D1 | 2.00000000 sec |
| D8 | 0.80000001 sec |
| D16 | 0.00015000 sec |
| IN0 | 0.00023840 sec |
| ======== CHANNEL f1 ======== | |
| NUC1 | 1H |
| P1 | 7.40 usec |
| P2 | 14.80 usec |
| PL1 | 3.30 dB |
| PL1W | 9.16420078 W |
| SFO1 | 600.2321008 MHz |
| ====== GRADIENT CHANNEL ===== | |
| GPNAM1 | SINE.100 |
| GPNAM2 | SINE.100 |
| GPZ1 | 40.00 % |
| GPZ2 | -40.00 % |
| P16 | 2000.00 usec |
| ND0 | 1 |
| TD | 256 |
| SFO1 | 600.2321 MHz |
| FIDRES | 16.385277 Hz |
| SW | 6.988 ppm |
| FnMODE | States-TPPI |
| SI | 1024 |
| SF | 600.2300154 MHz |
| WDW | QSINE |
| SSB | 2 |
| LB | 0.00 Hz |
| GB | 0 |
| PC | 1.40 |
| SI | 1024 |
| MC2 | States-TPPI |
| SF | 600.2300154 MHz |
| WDW | QSINE |
| SSB | 2 |
| LB | 0.00 Hz |
| GB | 0 |

Comp - 5

## THERMO ELECTRON ~ VISIONpro SOFTWARE V4.10

| | | | |
|---|---|---|---|
| Operator Name | Arshad Alam | Date of Report | 10/8/2015 |
| Department | Analytical laboratory#004 TWC | Time of Report | 11:05:24AM |
| Organization | ICCBS.Karachi University. | | |
| Information | Porf . Dr. M. Iqbal / Mahwish. | | |

**Scan Graph**



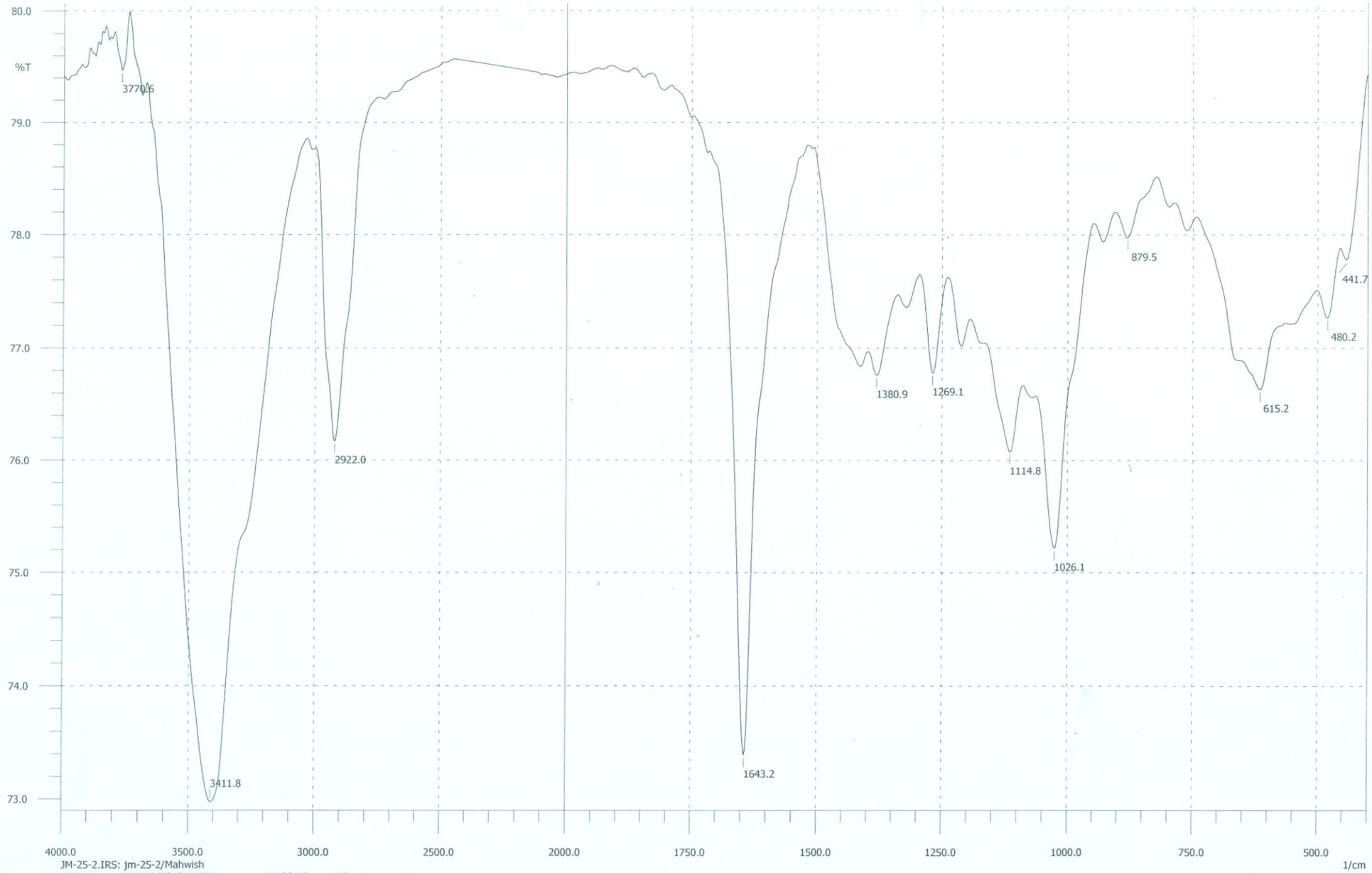

**Results Table - JM- 25-2.sre,MJ-25-2,Cycle01**

| nm | A |
|---|---|
| 243.00 | 2.083 |
| 248.00 | 2.010 |

**Peak Pick Method**
Find 8 Peaks Above -3.0000 A
Start Wavelength 200.00 nm
Stop Wavelength 450.00 nm
Sort By Wavelength

Sensitivity Medium

2 ml → 0.3 ml + 2 ml




JM-25-2.IRS: jm-25-2/Mahwish

| | | | | | |
|---|---|---|---|---|---|
| Date: | 10/12/2015 | Time: | 11:32:19 | NScans: | 5 |
| Type: | HYPER IR | User: | Zubair Ahmed | Detector: | standard |
| Abscissa: | 1/cm | Ordinate: | %T | Apodization: | Happ |
| Min: | 401.17 | Max: | 3998.16 | Range: | 1/cm |
| Ndp: | 1866 | Data Interval: | 1.92868 | Resolution: | 4.0 |
| Gain: | auto | Aperture: | auto | Mirror Speed: | 2.8(low) |

Comp - 5