

Water mediated synthesis of *N'*-arylmethylene ,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide library

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Spectral Data

***N'*-phenylmethylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4a**

White solid; IR (KBr): 3626, 3593, 2889, 297, 2852, 1666, 155, 192, 18, 1261, 709, 630 cm⁻¹; ¹H NMR (DMSO); 12.36 (S, 1H, NH), 10.78 (S, 1H, NH), 8.3 (s, 1H, =CH), 7.76-7.67 (m, 2H, Ar), 7.0-7.37 (m, 3H, Ar), 3.15-2.78 (m, H, CH₂), 1.81-1.75 (m, H, CH₂); MS (*m/z*): 268 (M⁺); Anal. Calcd for C₁₅H₁₆NO: C, 67.15; H, 6.01; N, 20.88. Found: C, 67.10; H, 6.12; N, 20.8.

***N'*-(-methoxyphenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4b**

White solid; IR (KBr): 3628, 2989, 2966, 293, 2033, 1905, 1680, 1627, 1605, 1508, 160, 1251, 835 cm⁻¹; ¹H NMR (DMSO); 12.6 (S, 1H, NH), 10.81 (S, 1H, NH), 8.57 (s, 1H, =CH), 7.76-7.62 (m, 2H, Ar), 7.29-7.26 (m, 2H, Ar), 3.81 (s, 3H, OCH₃), 3.01-2.68 (m, H, CH₂), 1.80-1.75 (m, H, CH₂); MS (*m/z*): 298 (M⁺); Anal. Calcd for C₁₆H₁₈NO₂: C, 6.1; H, 6.08; N, 18.78. Found: C, 6.58; H, 5.93; N, 18.56.

***N'*-(-methylphenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4c**

White solid; IR (KBr): 3628, 291, 286, 1681, 1529, 198, 152, 126, 85 cm⁻¹; ¹H NMR (DMSO); 12.57 (S, 1H, NH), 10.85 (S, 1H, NH), 8.31 (s, 1H, =CH), 7.75-7.62 (m, 2H, Ar), 7.20-7.18 (m, 2H, Ar), 2.97-2.77 (m, 2H, CH₂), 2.66-2.58 (m, 2H, CH₂), 2.37 (s, 3H, CH₃), 1.80-1.7 (m, H, CH₂); MS (*m/z*): 282 (M⁺); Anal. Calcd for C₁₆H₁₈NO: C, 68.06; H, 6.3; N, 19.8. Found: C, 68.18; H, 6.50; N, 19.77.

***N'*-(3,-dimethoxyphenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4d**

Yellow solid; IR (KBr): 3628, 2905, 287, 1681, 155, 128, 1221, 836 cm⁻¹; ¹H NMR (DMSO); 12.5 (S, 1H, NH), 10.69 (S, 1H, NH), 8.55 (s, 1H, =CH), 7.59-7.13 (m, 3H, Ar), 3.83 (s, 3H, OCH₃), 3.81 (s, 3H, OCH₃), 2.97-2.78 (m, H, CH₂), 1.81-1.75 (m, H, CH₂); MS (*m/z*): 328 (M⁺); Anal. Calcd for C₁₇H₂₀NO₃: C, 62.18; H, 6.1; N, 17.06. Found: C, 62.38; H, 6.29; N, 17.01.

***N'*-(2,5-dimethoxyphenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4e**

Pale-yellow solid; IR (KBr): 3650, 3128, 2991, 2883, 166, 155, 1508, 192, 127, 1255, 889 cm⁻¹; ¹H NMR (DMSO); 12.50 (S, 1H, NH), 10.60 (S, 1H, NH), 8.61 (s, 1H, =CH), 7.57 (t, 1H, Ar), 6.90 (t, 2H, Ar), 3.83 (s, 3H, OCH₃), 3.79 (s, 3H, OCH₃), 2.80 (d, 2H, CH₂), 2.65 (t, 2H, CH₂), 1.81-1.7 (m, H, CH₂); MS (*m/z*): 328 (M⁺); Anal. Calcd for C₁₇H₂₀NO₃: C, 62.18; H, 6.1; N, 17.06. Found: C, 62.31; H, 6.25; N, 17.02.

***N'*-(3-bromophenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4f**

White solid; IR (KBr): 368, 2998, 2915, 1678, 161, 1595, 1539, 15 cm⁻¹; ¹H NMR (DMSO); 12.51 (S, 1H, NH), 10.75 (S, 1H, NH), 8.6 (s, 1H, =CH), 7.76-7.2 (m, H, Ar), 2.86-2.62 (m, H, CH₂), 1.80-1.7 (m, H, CH₂); MS (*m/z*): 36 (M⁺); Anal. Calcd for C₁₅H₁₅BrNO: C, 51.89; H, .35; N, 16.1. Found: C, 51.92; H, .17; N, 16.53.

***N'*-(hydroxyphenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4g**

White solid; IR (KBr): 3621, 297, 1691, 1619, 155, 1507, 128 cm⁻¹; ¹H NMR (DMSO); 12.57 (S, 1H, NH), 10.87 (S, 1H, NH), 10.08 (s, 1H, OH), 8.31 (s, 1H, =CH), 7.67-7.61 (m, 2H, Ar), 7.31-7.27 (m, 2H, Ar), 2.82-2.59 (m, H, CH₂), 1.81-1.75 (m, H, CH₂); MS (*m/z*): 28 (M⁺); Anal. Calcd for C₁₅H₁₆NO₂: C, 63.37; H, 5.67; N, 19.71. Found: C, 63.6; H, 5.5; N, 19.69.

***N'*-(2-hydroxyphenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4h** White solid; IR (KBr): 361, 2978, 299, 2853, 1678, 1660, 159, 128 cm⁻¹; ¹H NMR (DMSO); 12.61 (S, 1H, NH), 10.8 (S, 1H, NH), 10.01 (s, 1H, OH), 8.32 (s, 1H, =CH), 7.77-7.28 (m, H, Ar), 2.91-2.7 (m, H, CH₂), 1.80-1.75 (m, H, CH₂); MS (*m/z*): 28 (M⁺); Anal. Calcd for C₁₅H₁₆NO₂: C, 63.37; H, 5.67; N, 19.71. Found: C, 63.58; H, 5.51; N, 19.80.

***N'*-[-(dimethylamino)phenyl]methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4i** Yellowish-orange solid; IR (KBr): 361, 2998, 2989, 2850, 2828, 1680, 11 cm⁻¹; ¹H NMR (DMSO); 12.9 (S, 1H, NH), 10.88 (S, 1H, NH), 8.5 (s, 1H, =CH), 7.56-7.51 (m, 2H, Ar), 7.23-7.12 (m, 2H, Ar), .03 (s, 6H, CH₃), 2.98-2.70 (m, H, CH₂), 1.80-1.7 (m, H, CH₂); MS (*m/z*): 311 (M⁺); Anal. Calcd for C₁₇H₂₁N₅O: C, 65.57; H, 6.80; N, 22.9. Found: C, 65.68; H, 6.69; N, 22.67.

***N'*-(3-chlorophenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4j**

Pale-yellow solid; IR (KBr): 3672, 2938, 2886, 1671, 160, 156, 1539, 139 cm⁻¹; ¹H NMR (DMSO); 12.53 (S, 1H, NH), 10.78 (S, 1H, NH), 8.1 (s, 1H, =CH), 7.5-7.29 (m, H, Ar), 2.85-2.57 (m, H, CH₂), 1.81-1.7 (m, H, CH₂); MS (*m/z*): 302 (M⁺); Anal. Calcd for C₁₅H₁₅ClNO: C, 59.51; H, .99; N, 18.51. Found: C, 59.35; H, 5.17; N, 18.19.

***N'*-(chlorophenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4k**

White solid; IR (KBr): 359, 2928, 2865, 1678, 160, 1528, 160 cm⁻¹; ¹H NMR (DMSO); 12.53 (S, 1H, NH), 10.91 (S, 1H, NH), 8.39 (s, 1H, =CH), 7.79-7.71 (m, 2H, Ar), 7.0-7.37 (m, 2H, Ar), 2.87-2.61 (m, H, CH₂), 1.81-1.7 (m, H, CH₂); MS (*m/z*): 302 (M⁺); Anal. Calcd for C₁₅H₁₅ClNO: C, 59.51; H, .99; N, 18.51. Found: C, 59.39; H, 5.06; N, 18.27.

***N'*-(2-chlorophenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4l**

Pale-yellow solid; IR (KBr): 3656, 355, 301, 2978, 291, 2856, 1678, 1505, 128 cm⁻¹; ¹H NMR (DMSO); 12.3 (S, 1H, NH), 10.75 (S, 1H, NH), 8.39 (s, 1H, =CH), 7.51-7.37 (m, H, Ar), 2.83-2.68 (m, H, CH₂), 1.81-1.7 (m, H, CH₂); MS (*m/z*): 302 (M⁺); Anal. Calcd for C₁₅H₁₅ClNO: C, 59.51; H, .99; N, 18.51. Found: C, 59.2; H, .91; N, 18.0.

N'-(*-*fluorophenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4m

White solid; IR (KBr): 3626, 297, 1629, 1506, 113, 1228, 829 cm⁻¹; ¹H NMR (DMSO); 12.9 (S, 1H, NH), 10.67 (S, 1H, NH), 8.7 (s, 1H, =CH), 7.70-7.8 (m, H, Ar), 2.87-2.71 (m, H, CH₂), 1.81-1.7 (m, H, CH₂); MS (*m/z*): 286 (M⁺); Anal. Calcd for C₁₅H₁₅FNO: C, 62.93; H, 5.28; N, 19.57. Found: C, 62.78; H, 5.39; N, 19.55.

N'-(*-*nitrophenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4n

Yellow solid; IR (KBr): 3671, 2950, 2888, 166, 161, 128 cm⁻¹; ¹H NMR (DMSO); 12.56 (S, 1H, NH), 10.68 (S, 1H, NH), 8.33 (s, 1H, =CH), 7.6-7.30 (m, H, Ar), 3.02-2.78 (m, H, CH₂), 1.80-1.7 (m, H, CH₂); MS (*m/z*): 313 (M⁺); Anal. Calcd for C₁₅H₁₅N₅O₃: C, 57.50; H, .83; N, 22.35. Found: C, 57.29; H, .7; N, 22.6.

N'-(3-nitrophenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4o

Yellow solid; IR (KBr): 3619, 291, 2855, 165, 1515, 196, 17, 1221 cm⁻¹; ¹H NMR (DMSO); 12.51 (S, 1H, NH), 10.78 (S, 1H, NH), 8.9 (s, 1H, =CH), 7.69-7.19 (m, H, Ar), 2.97-2.79 (m, H, CH₂), 1.81-1.75 (m, H, CH₂); MS (*m/z*): 313 (M⁺); Anal. Calcd for C₁₅H₁₅N₅O₃: C, 57.50; H, .83; N, 22.35. Found: C, 57.0; H, .99; N, 22.21.

N'-pyridin-3-ylmethylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4p

White solid; IR (KBr): 361, 2927, 289, 1675, 1589, 1528, 156, 1205 cm⁻¹; ¹H NMR (DMSO); 12.61 (S, 1H, NH), 11.2 (S, 1H, NH), 8.5 (s, 1H, =CH), 8.8 (d, 1H, Ar), 8.57-8.55 (m, 1H, Ar), 8.17 (d, 1H, Ar), 8.38-8.35 (m, 1H, Ar), 2.97-2.77 (m, 2H, CH₂), 2.67-2.57 (m, 2H, CH₂), 1.82-1.75 (m, H, CH₂); MS (*m/z*): 269 (M⁺); Anal. Calcd for C₁₁H₁₅N₅O: C, 62.; H, 5.61; N, 26.01. Found: C, 62.5; H, 5.38; N, 25.88.

N'-2-furylmethylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4q

White solid; IR (KBr): 3629, 297, 2889, 1692, 1606, 1519, 168, 127, 1221 cm⁻¹; ¹H NMR (DMSO); 12.61 (S, 1H, NH), 10.98 (S, 1H, NH), 8.5 (s, 1H, =CH), 8.59-8.5 (m, 2H, Ar), 8.21-8.17 (m, 1H, Ar), 2.97-2.62 (m, H, CH₂), 1.81-1.75 (m, H, CH₂); MS (*m/z*): 258 (M⁺); Anal. Calcd for C₁₃H₁₁NO₂: C, 60.5; H, 5.6; N, 21.69. Found: C, 60.36; H, 5.36; N, 21.61.

N'-1-naphthylmethylen-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4r

White solid; IR (KBr): 3626, 3593, 3028, 2978, 2912, 2852, 1668, 155, 192, 18, 1282 cm⁻¹; ¹H NMR (DMSO); 12.60 (S, 1H, NH), 10.68 (S, 1H, NH), 8.35 (s, 1H, =CH), 7.96-7.62 (m, 7H, Ar), 2.89-2.58 (m, H, CH₂), 1.80-1.75 (m, H, CH₂); MS (*m/z*): 318 (M⁺); Anal. Calcd for C₁₉H₁₈NO: C, 71.68; H, 5.70; N, 17.60. Found: C, 71.78; H, 5.6; N, 17.51.

N'-(3-hydroxyphenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4s

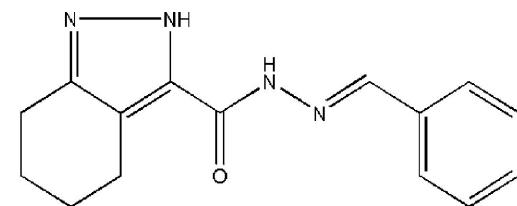
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N'-(2-methoxyphenyl)methylene-,5,6,7-tetrahydro-2*H*-indazole-3-carbohydrazide 4t

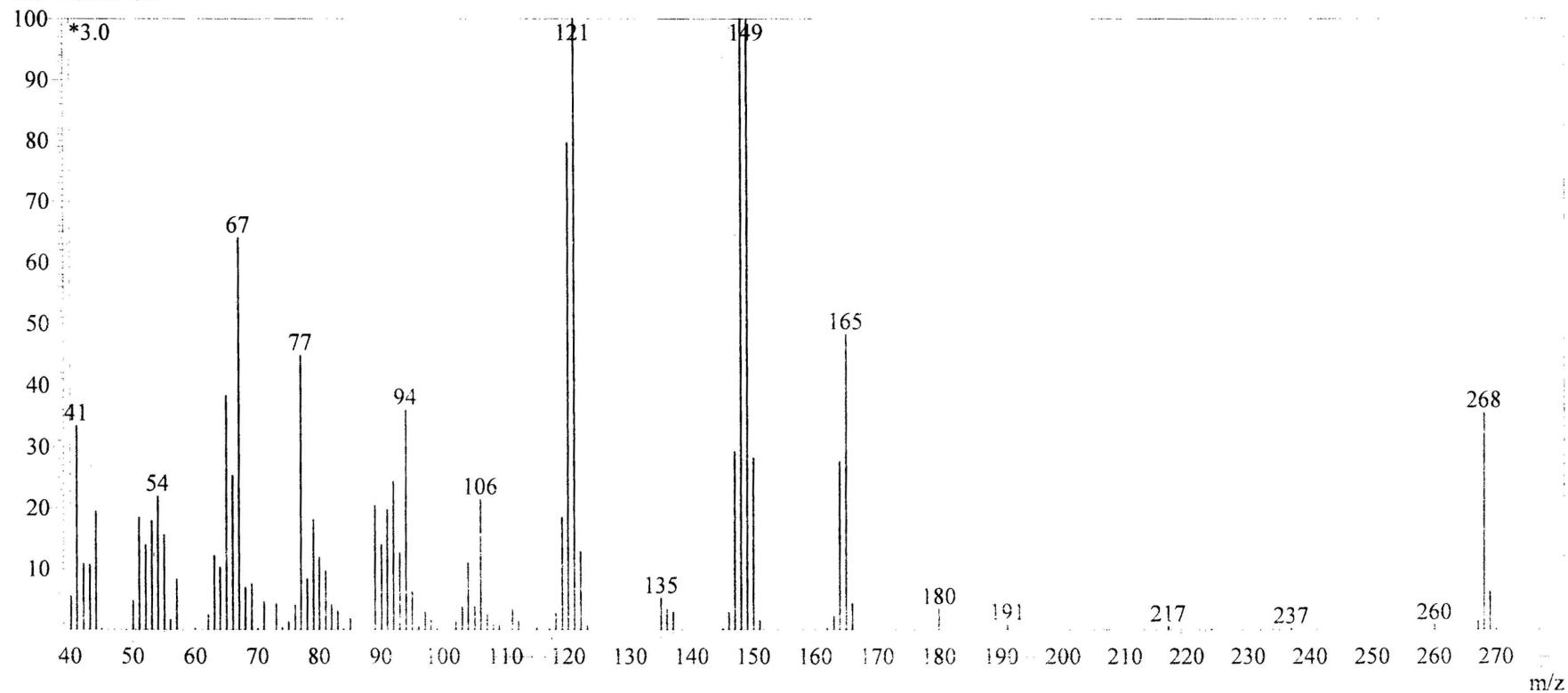
White solid; IR (KBr): 3609, 2970, 296, 1668, 165, 1568, 13 cm⁻¹; ¹H NMR (DMSO); 12.57 (S, 1H, NH), 10.70 (S, 1H, NH), 8.5 (s, 1H, =CH), 7.60-7.28 (m, H, Ar), 3.79 (s, 3H, OCH₃), 2.87-2.55 (m, H, CH₂), 1.81-1.75 (m, H, CH₂); MS (*m/z*): 298 (M⁺); Anal. Calcd for C₁₆H₁₈NO₂: C, 6.1; H, 6.08; N, 18.78. Found: C, 6.32; H, 5.91; N, 18.66.

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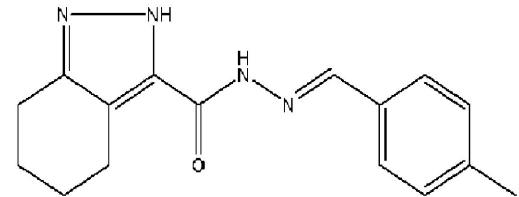
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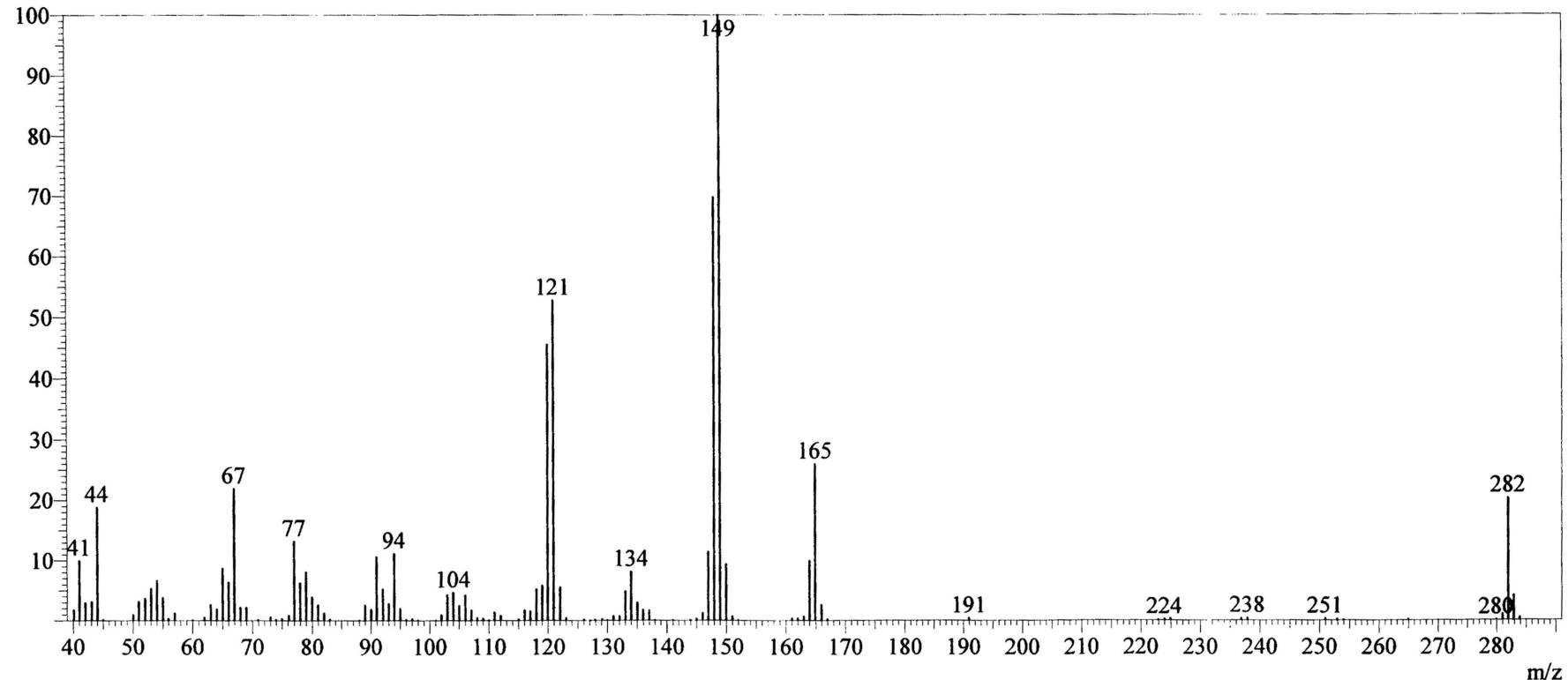
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Sample Information

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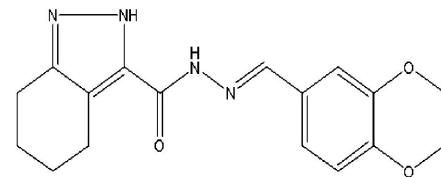
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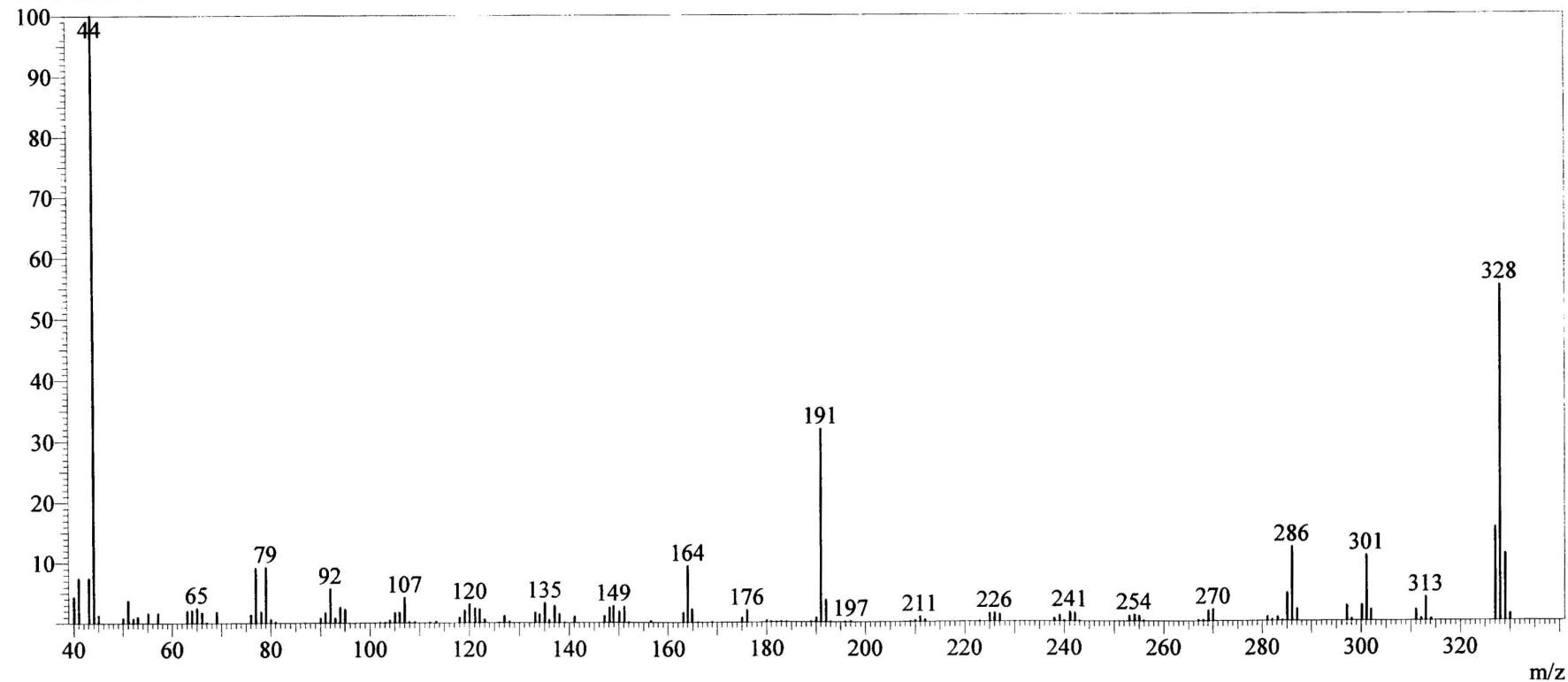
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RAJKOT-360005**

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Sample Information



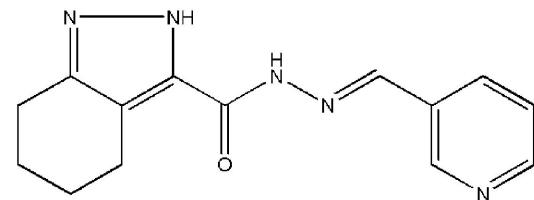
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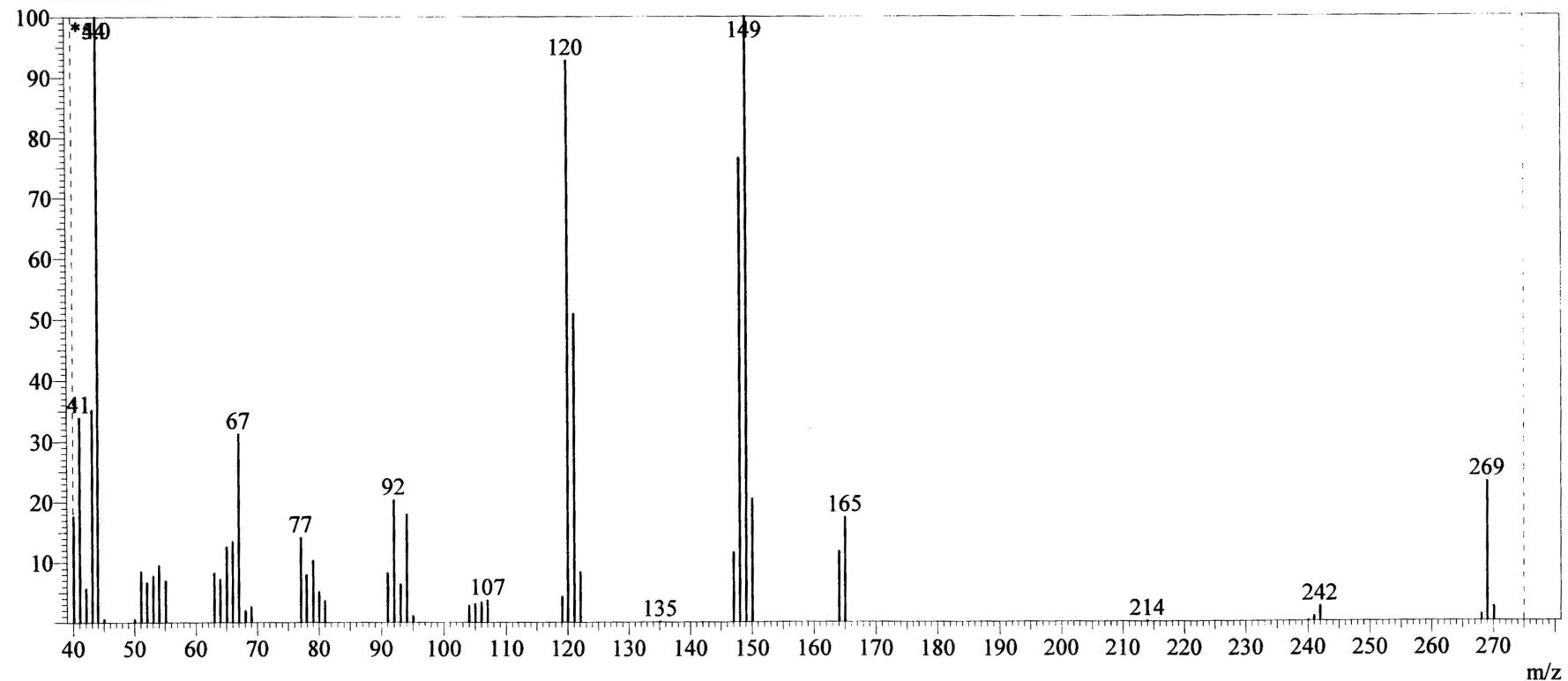
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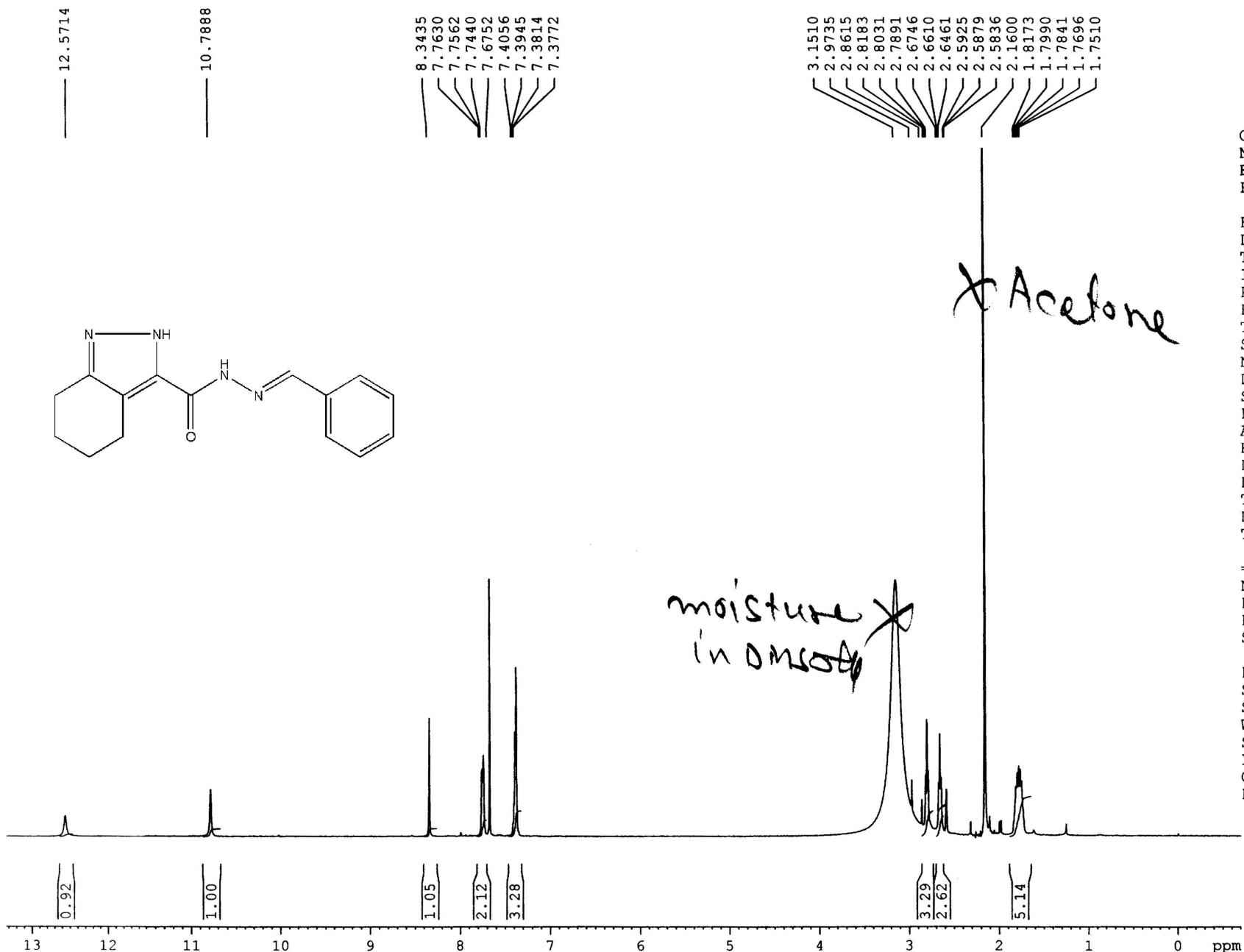
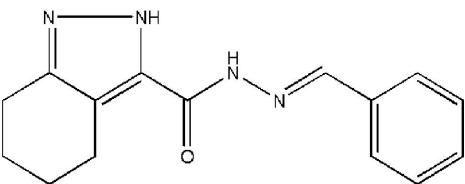
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SAIF
Panjab University
Chandigarh

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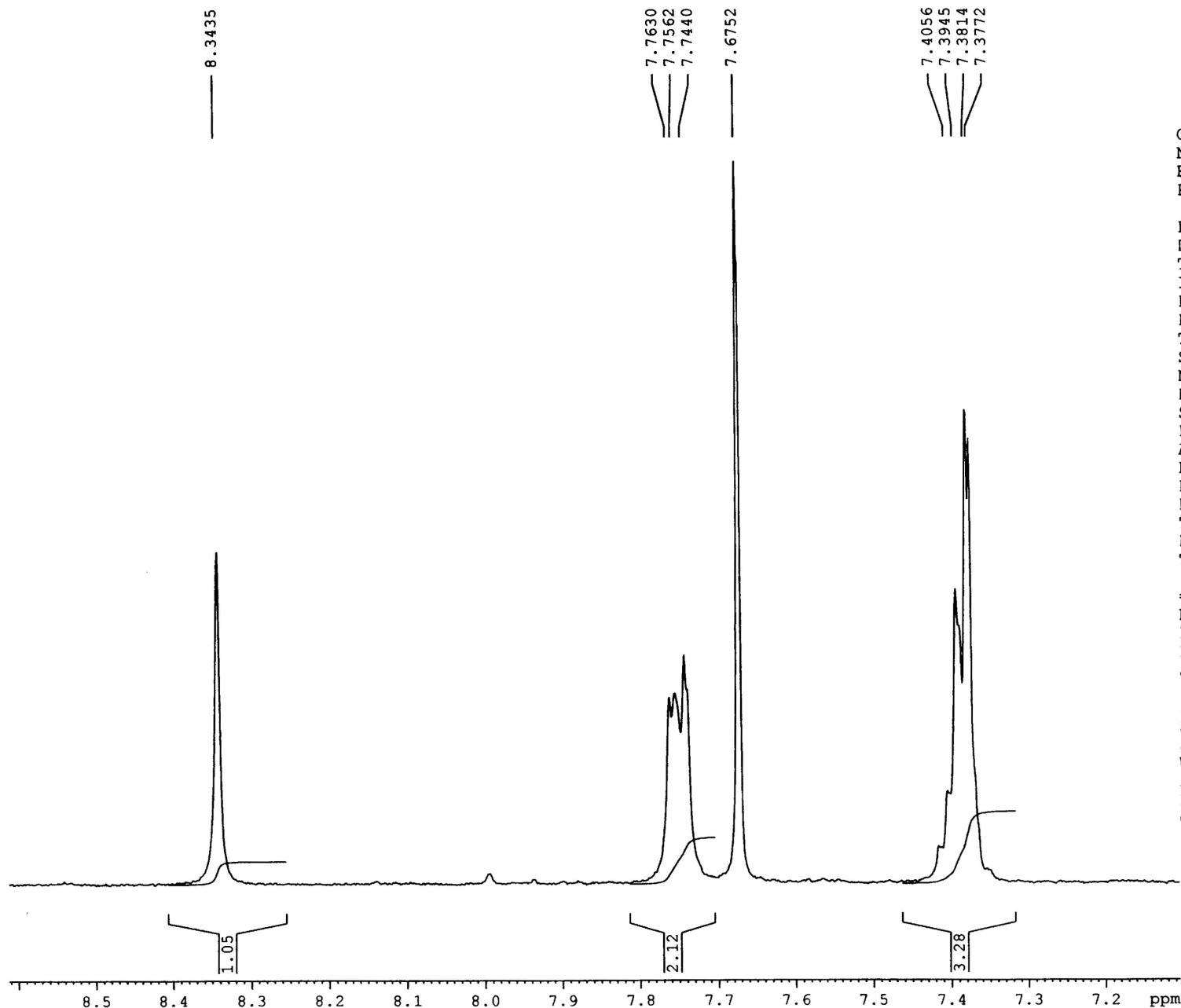
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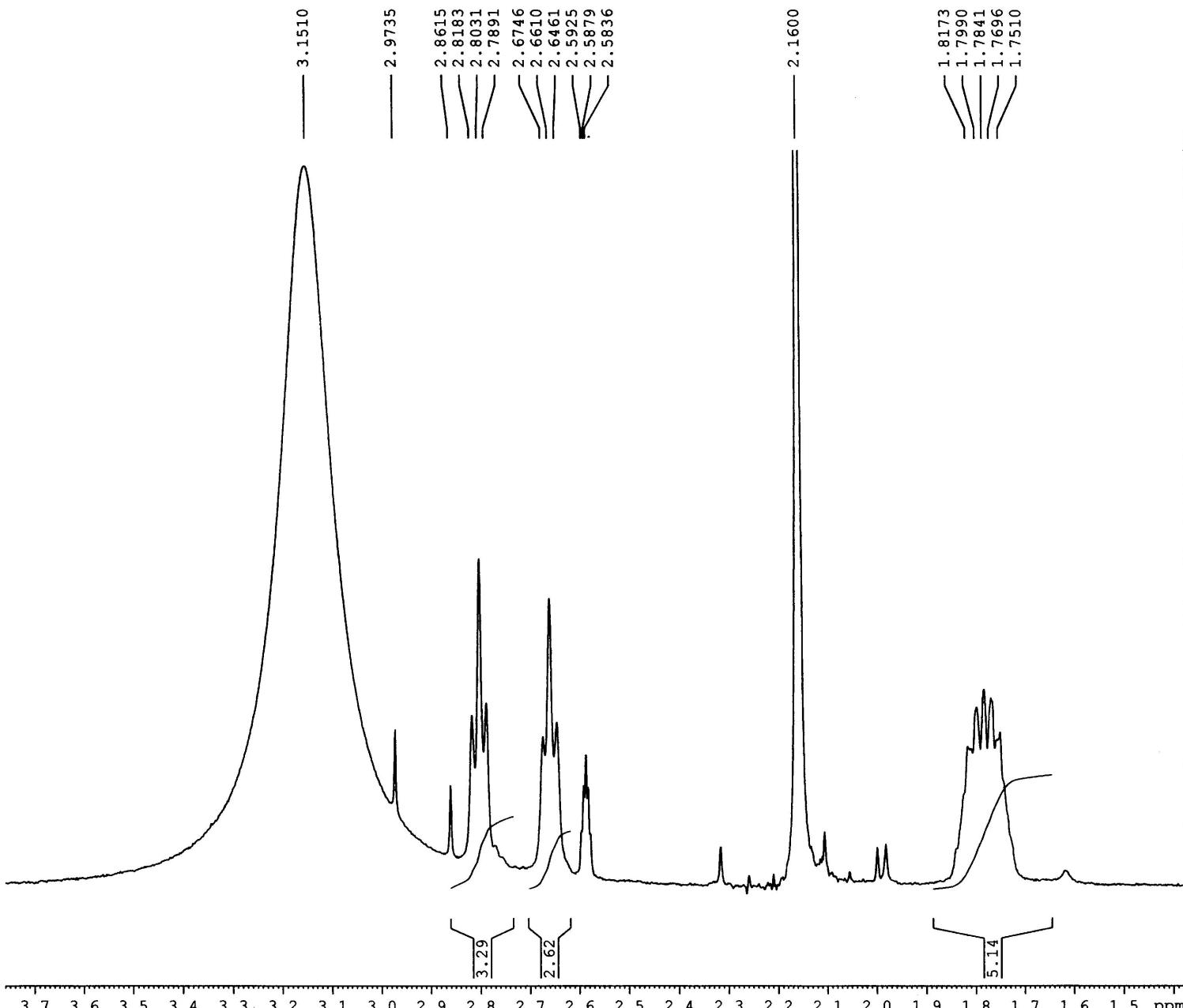
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Spectrometer
SAIF
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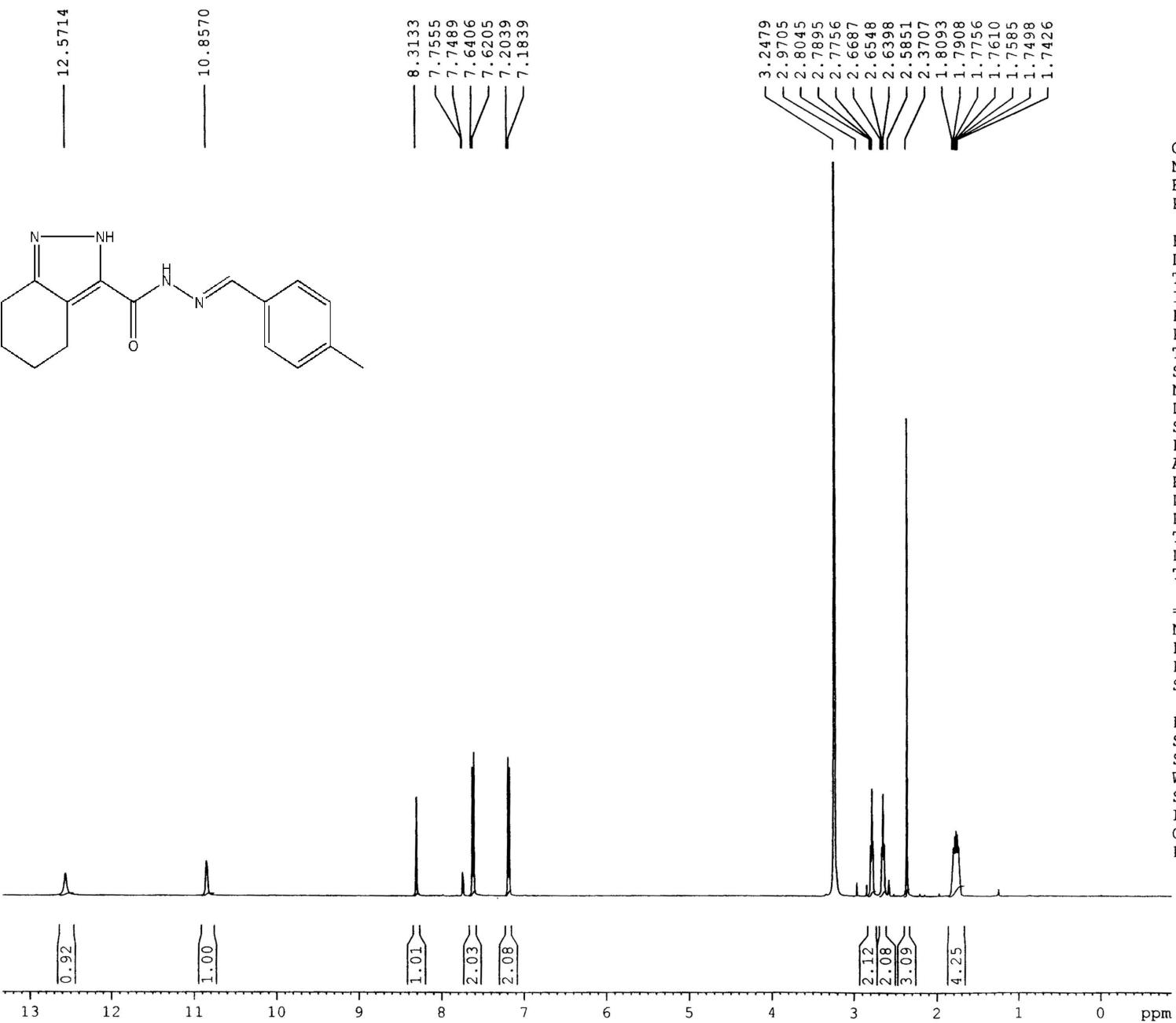
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GB 0
PC 1.00



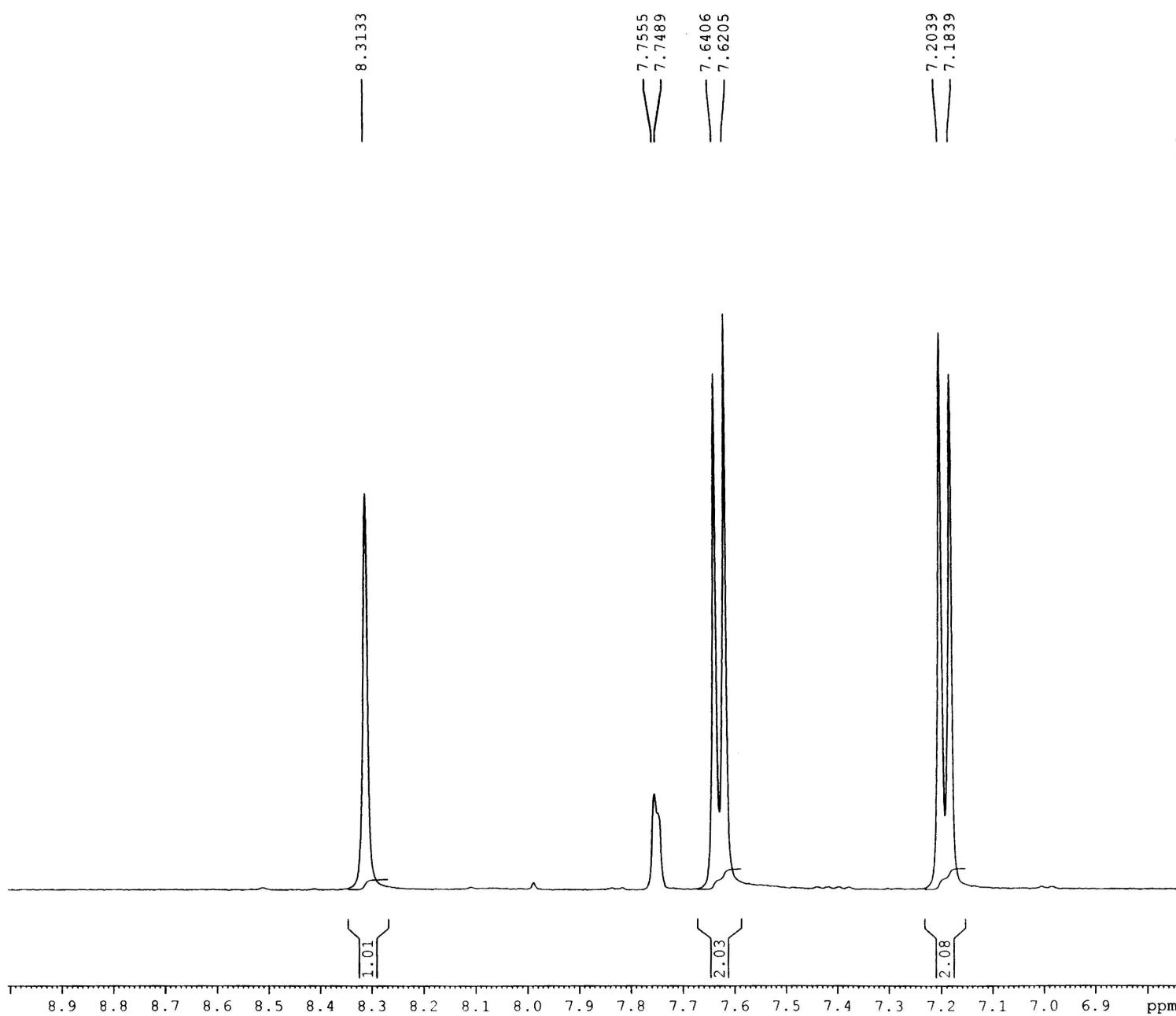
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME Sep25-2008
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080925
Time 21.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 228
DW 41.600 usec
DE 6.00 usec
TE 294.8 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1299701 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



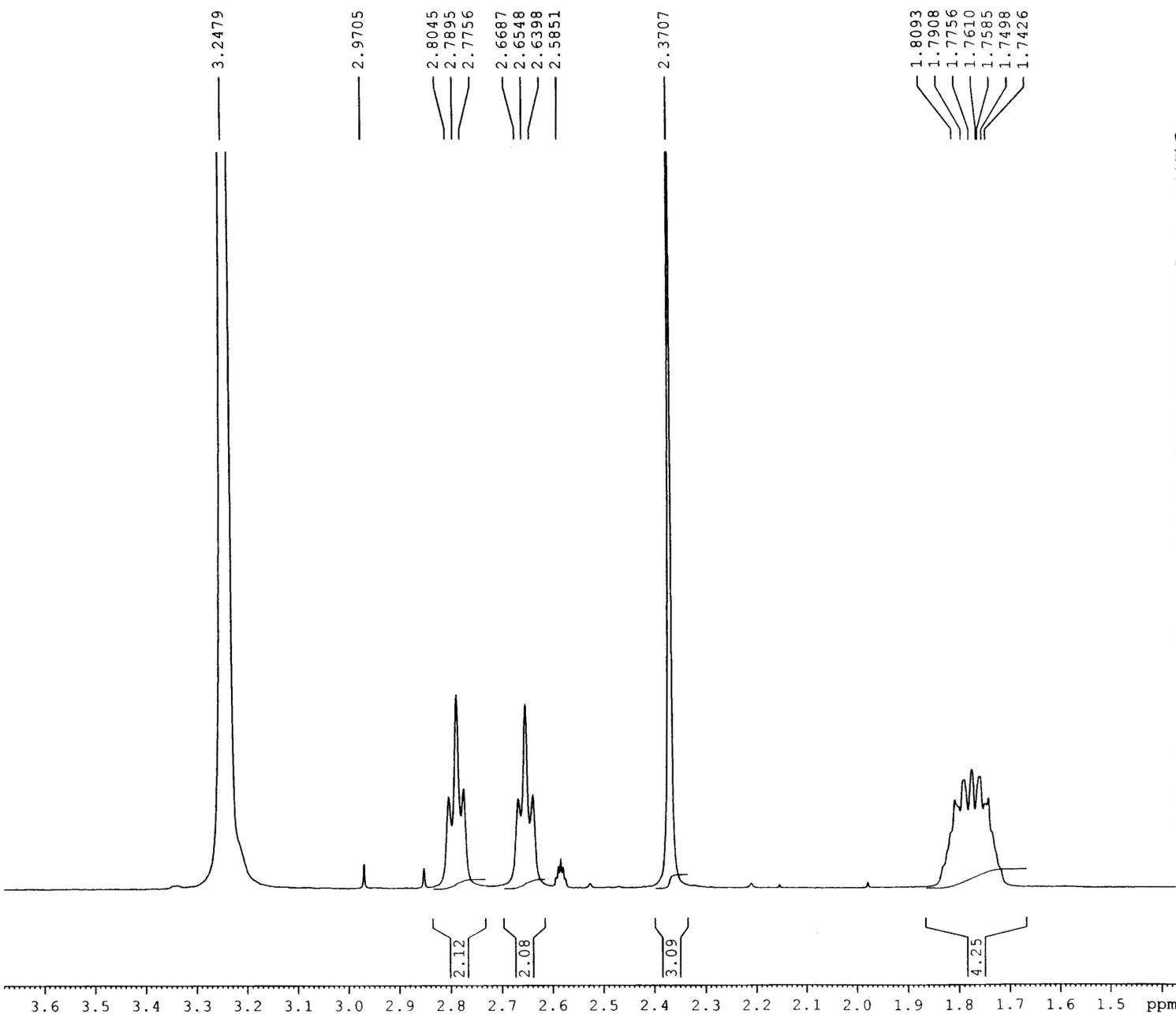
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME Sep25-2008
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080925
Time_ 21.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
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TD 65536
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NS 16
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AQ 2.7263477 sec
RG 228
DW 41.600 usec
DE 6.00 usec
TE 294.8 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1299701 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME Sep25-2008
EXPNO 31
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080925
Time_ 21.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 228
DW 41.600 usec
DE 6.00 usec
TE 294.8 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SF01 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1299701 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME Sep25-2008
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080925
Time 21.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 287
DW 41.600 usec
DE 6.00 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1299677 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

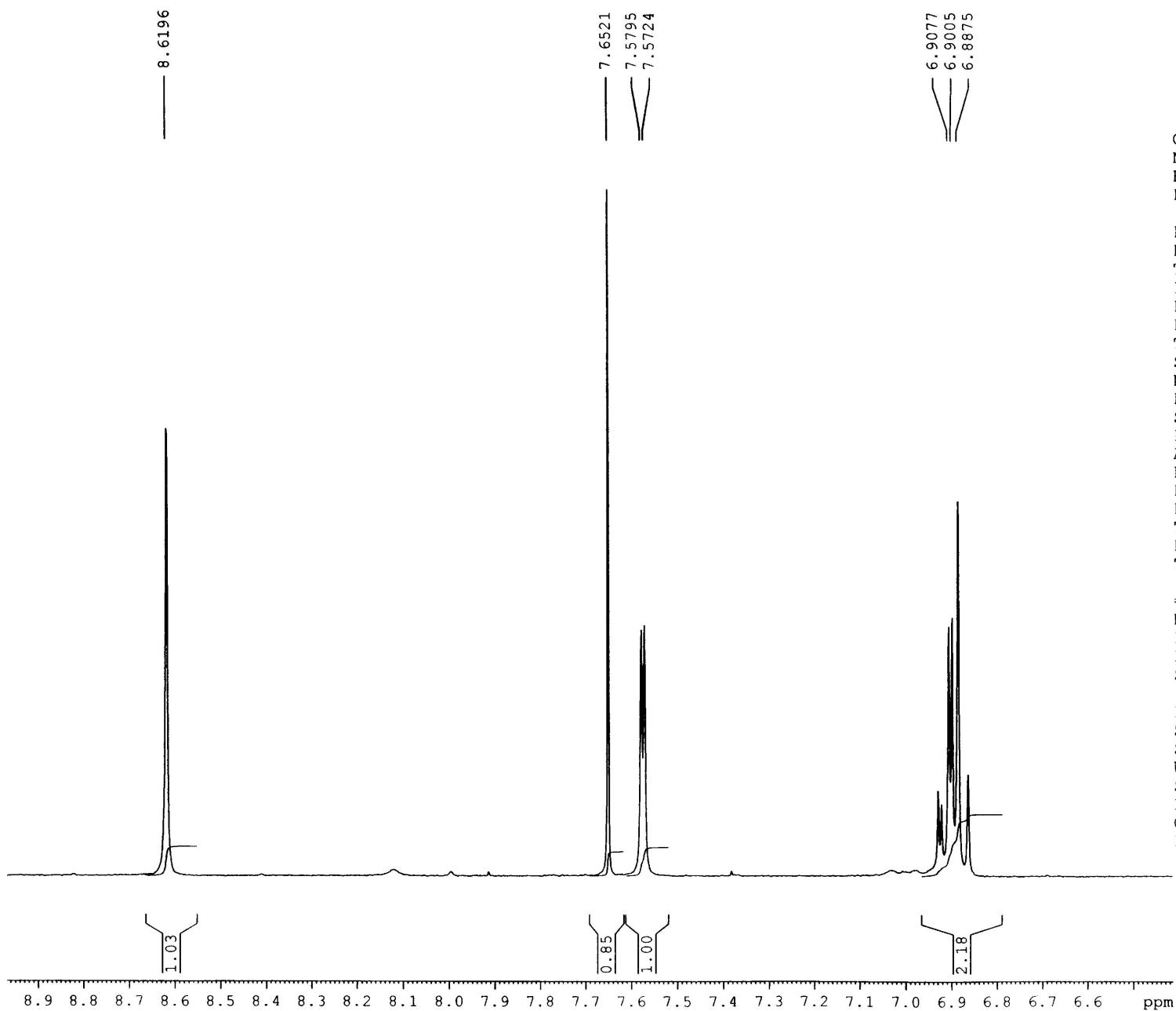
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

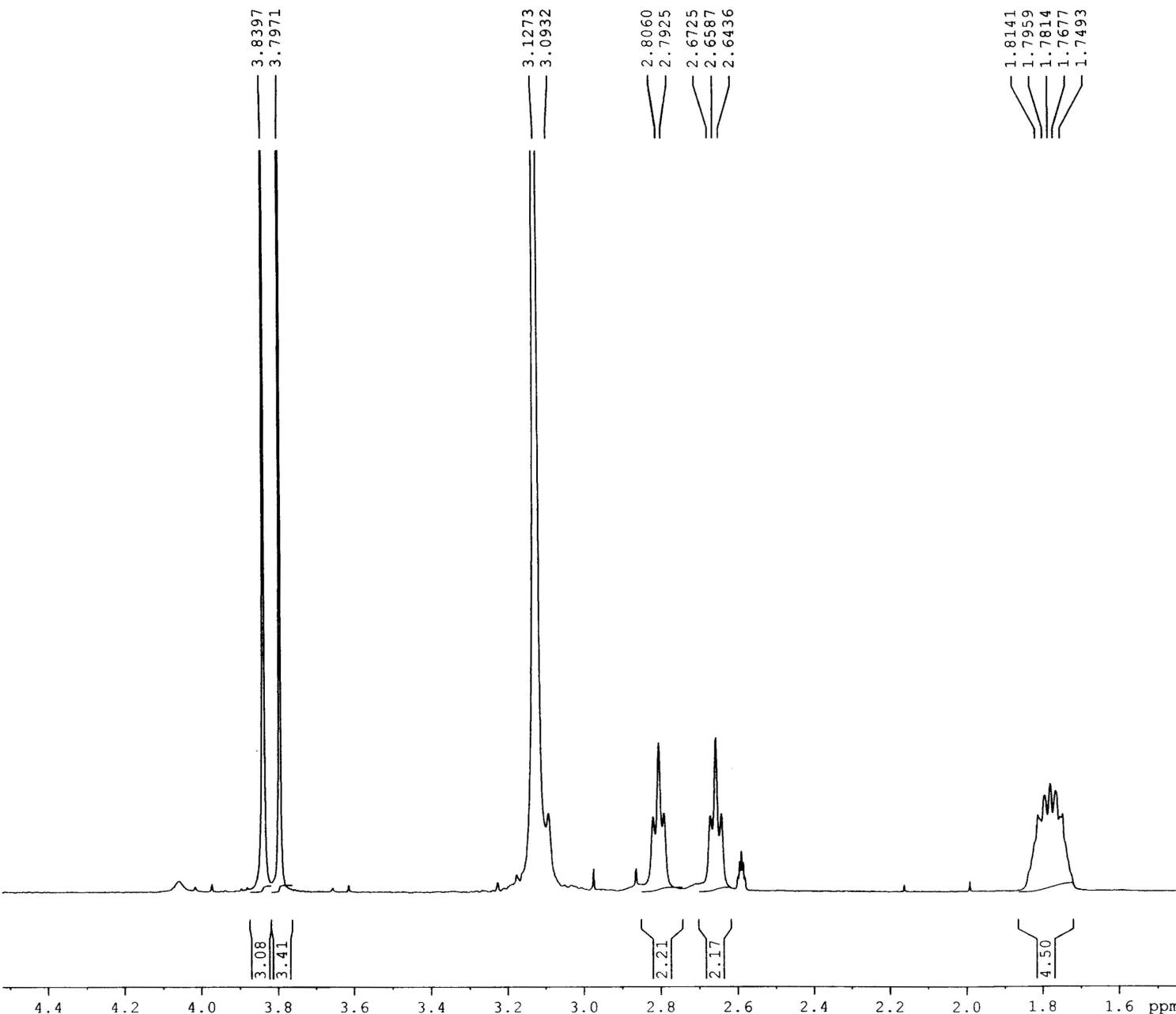
Current Data Parameters
NAME Sep25-2008
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080925
Time 21.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 287
DW 41.600 usec
DE 6.00 usec
TE 294.8 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PLL -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1299677 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





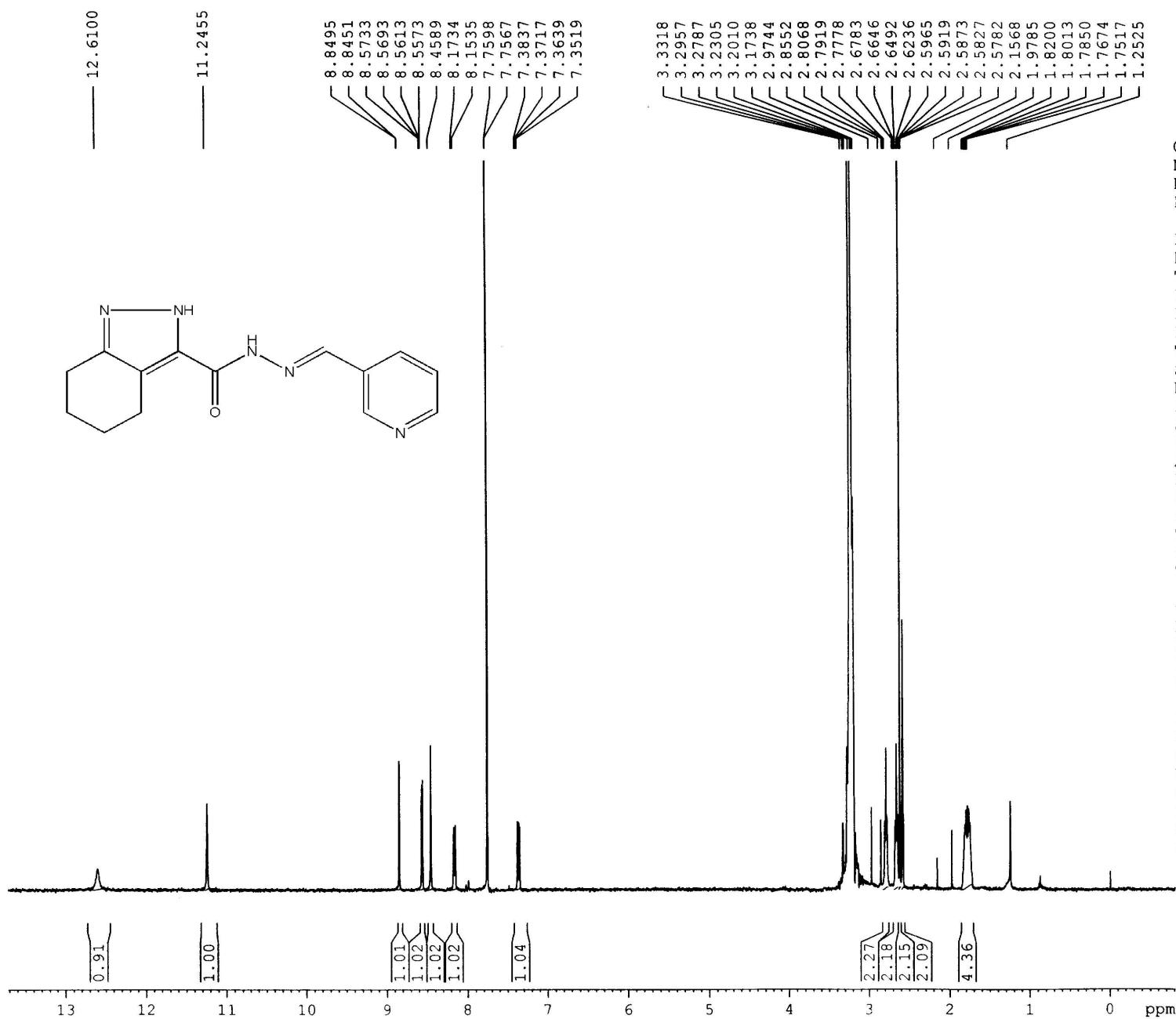
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current Data Parameters
NAME Sep25-2008
EXPNO 41
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080925
Time 21.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 287
DW 41.600 usec
DE 6.00 usec
TE 294.8 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1299677 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER
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Spectrometer
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Current Data Parameters

NAME Sep25-2008
EXPNO 51
PROCNO 1

F2 - Acquisition Parameters

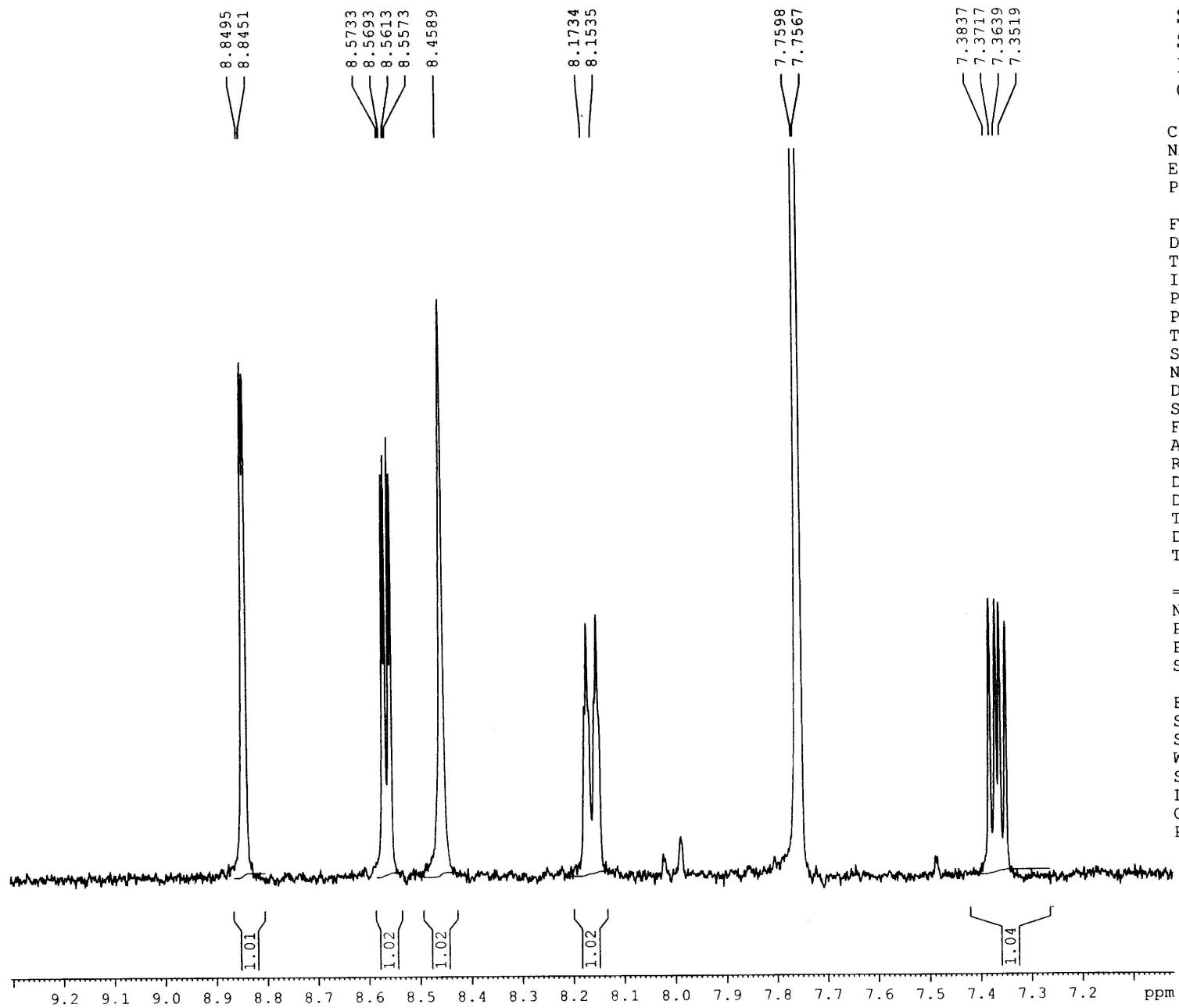
Date_ 20080925
Time_ 21.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 322
DW 41.600 usec
DE 6.00 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1

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

NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SF01 400.1324008 MHz

F2 - Processing parameters

SI 32768
SF 400.1299692 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh

Current	Data	Parameters
NAME	Sep25-2008	
EXPNO		51
PROCNO		1

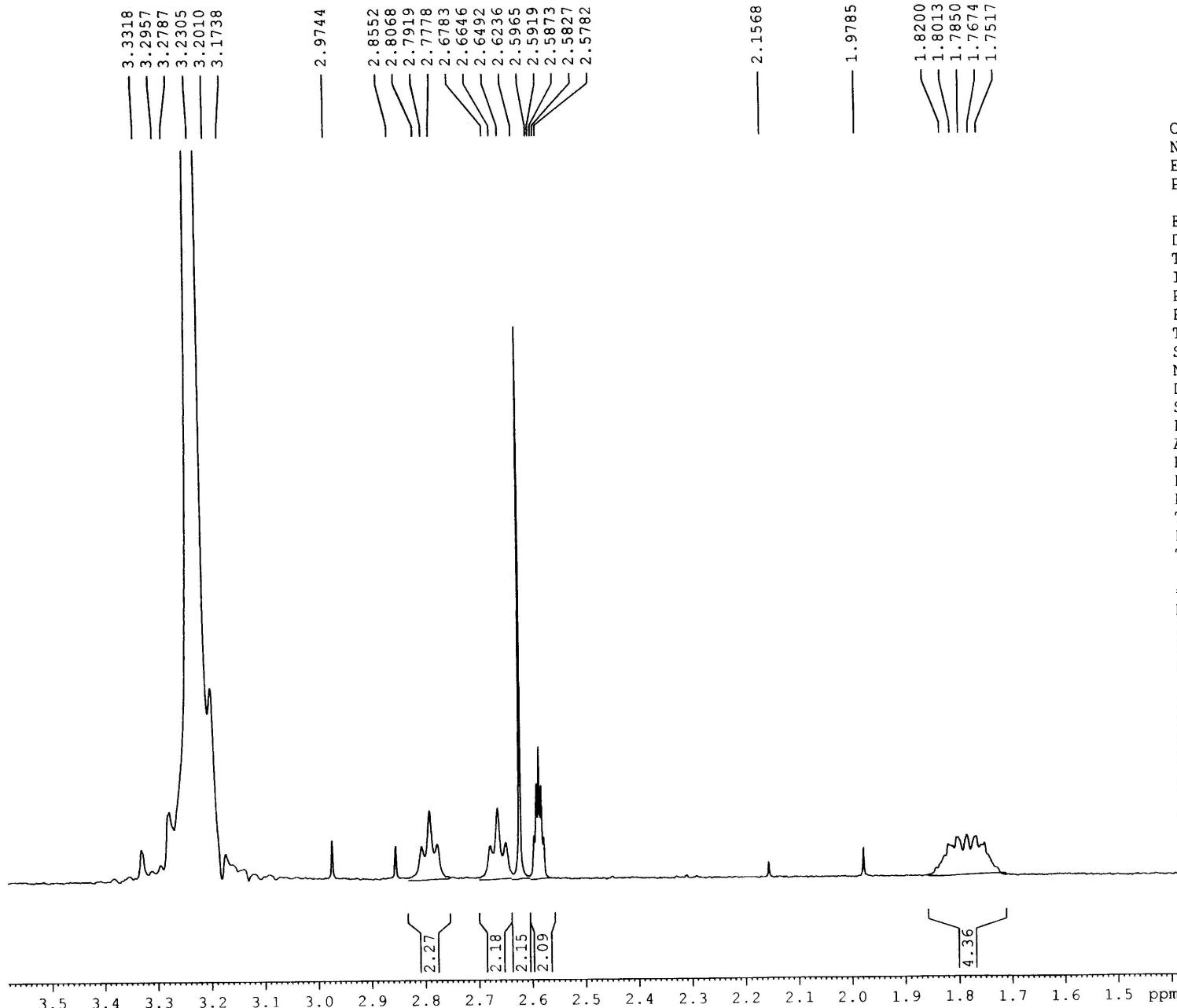
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F2 - Acquisition Parameters
Date_           20080925
Time_           21.29
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zg30
TD             65536
SOLVENT        DMSO
NS              16
DS              2
SWH             12019.230 Hz
FIDRES         0.183399 Hz
AQ             2.7263477 sec
RG              322
DW              41.600 usec
DE              6.00 usec
TE              294.8 K
D1             1.00000000 sec
TD0                 1

```

===== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SEQ1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1299692 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER
AVANCE II 400 NMR
Spectrometer
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Panjab University
Chandigarh

Current Data Parameters
NAME Sep25-2008
EXPNO 51
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080925
Time 21.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 322
DW 41.600 usec
DE 6.00 usec
TE 294.8 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SF01 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1299692 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

