

Supporting Information

for

Anion– π interactions influence pK_a values

Christopher J. Cadman and Anna K. Croft*

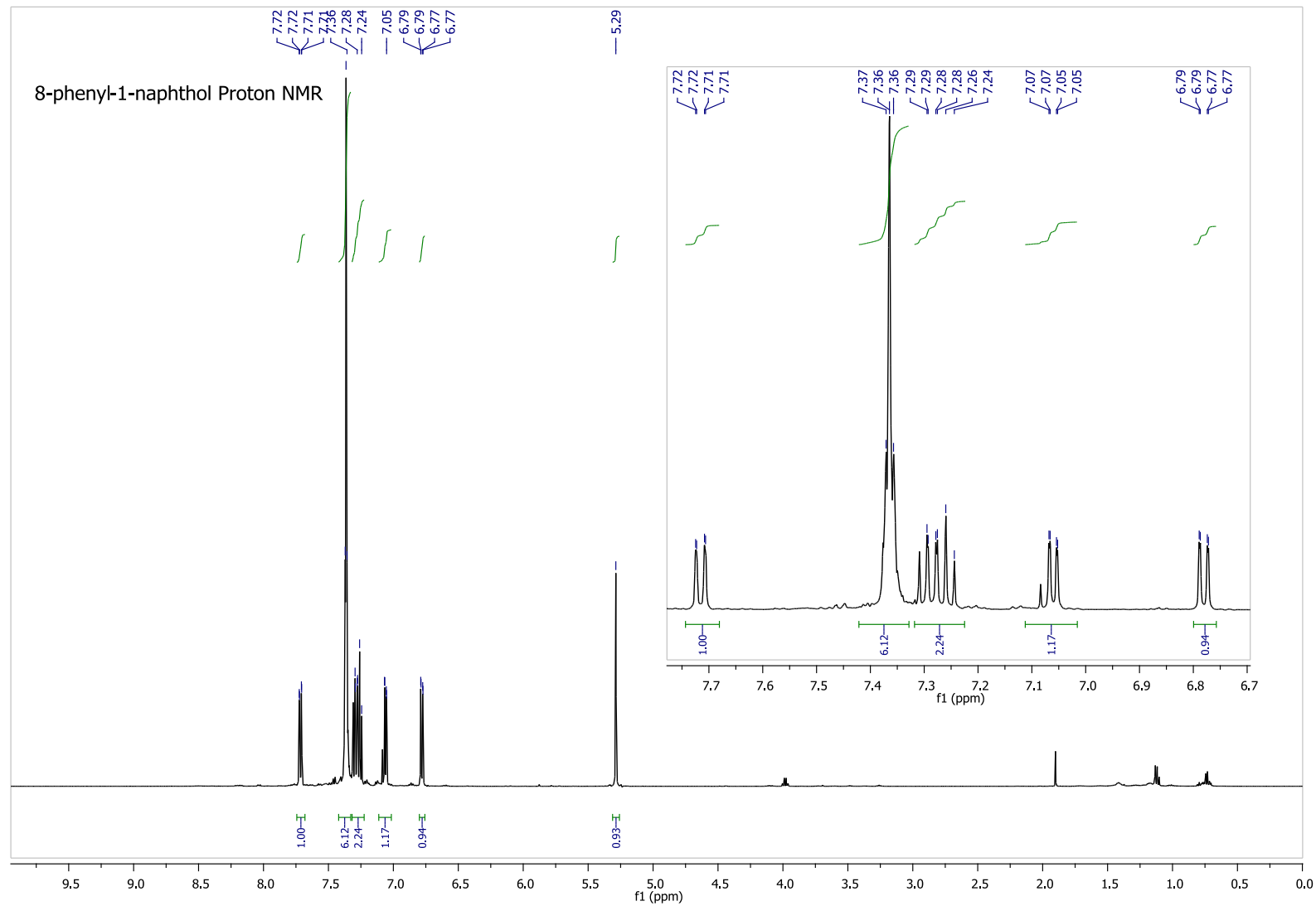
Address: School of Chemistry, University of Wales Bangor, Bangor, Gwynedd, LL57 2UW, United Kingdom. Fax: +44 1248 370 528. Tel: +44 1248 382 375.

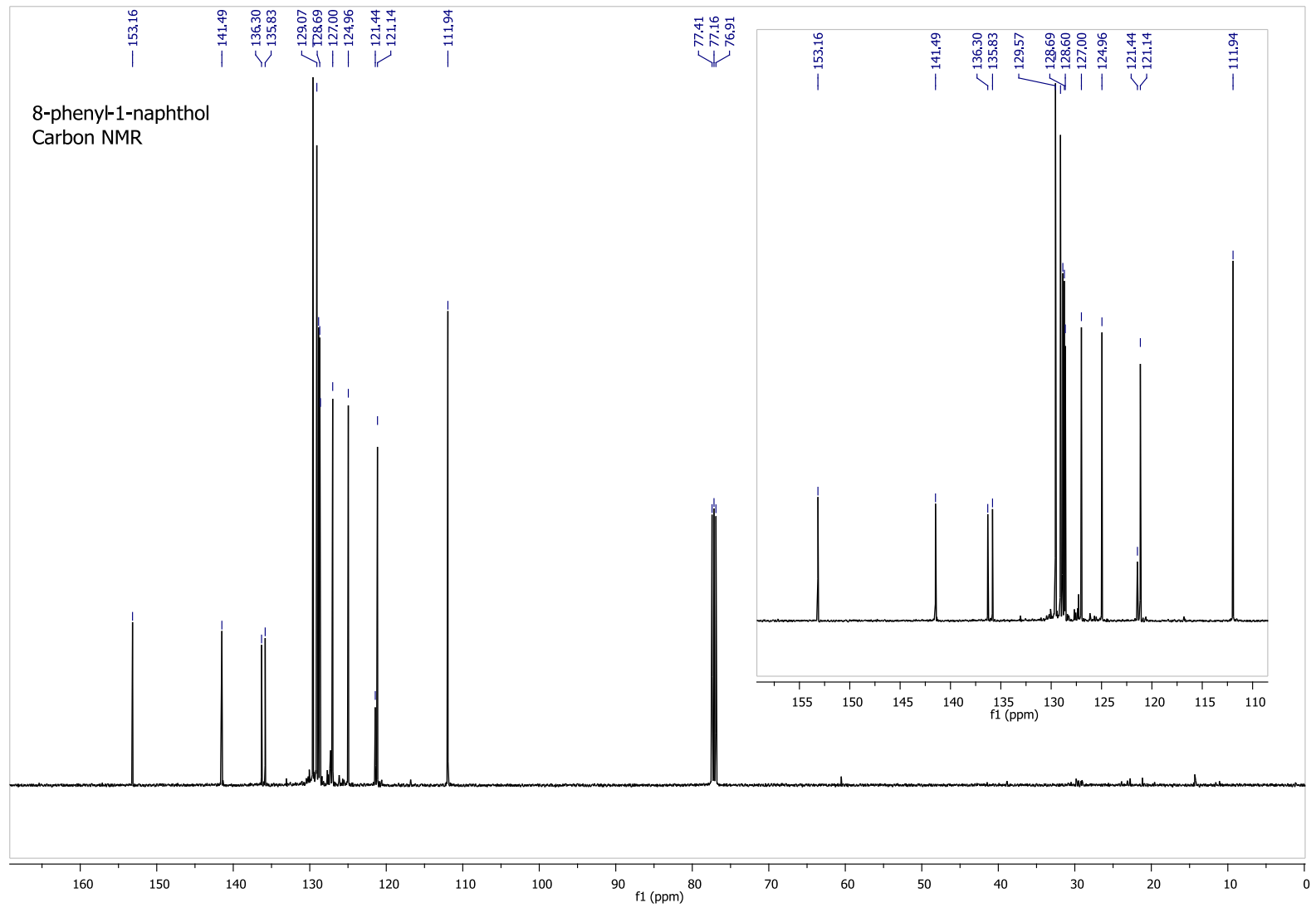
Email: Anna K. Croft - a.k.croft@bangor.ac.uk

*Corresponding author

Original spectral data for compounds 1–5

Compound 1: 8-phenyl-1-naphthol





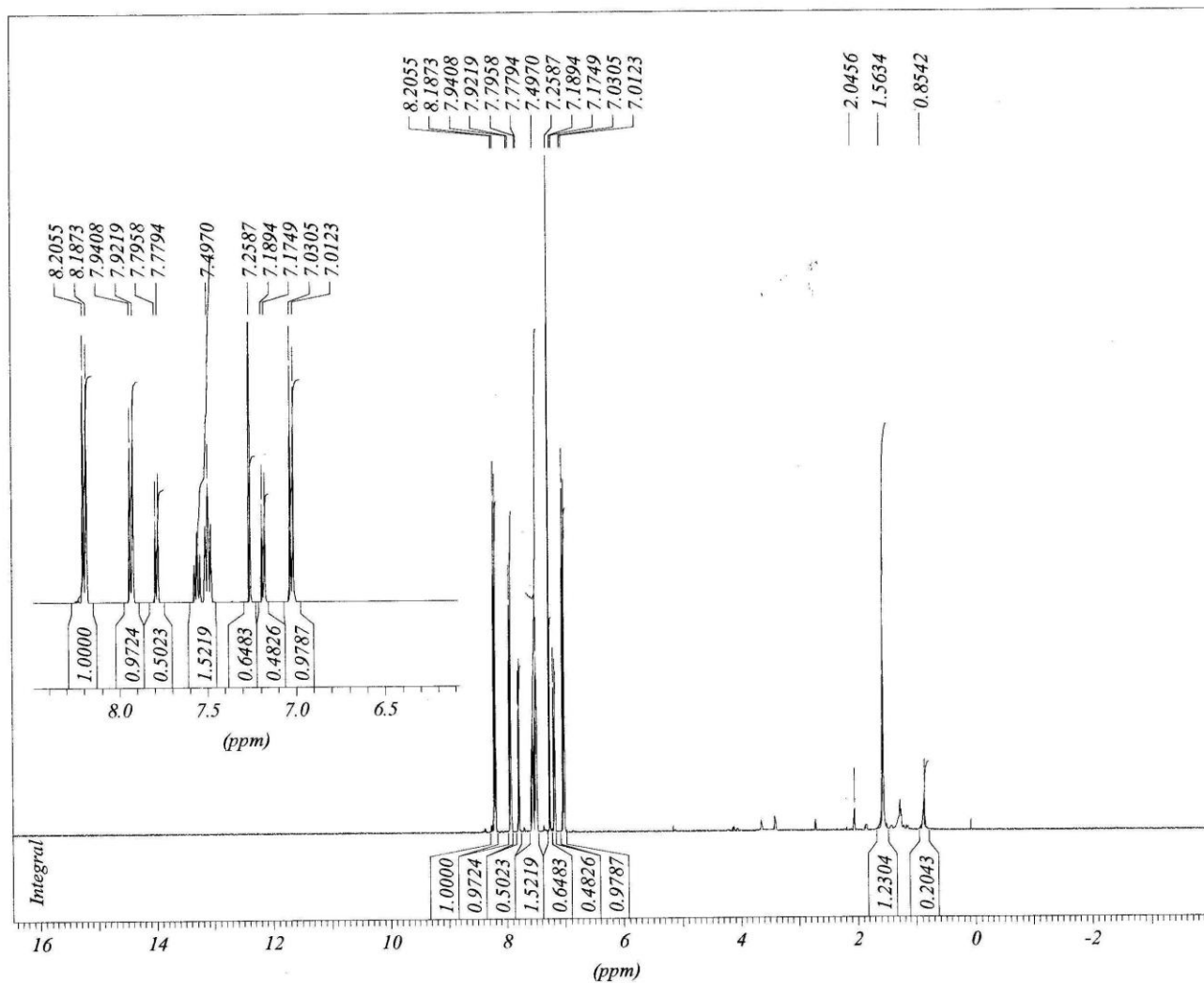
Compound 2: 8-(4-nitrophenyl)-1-naphthol

Research group AKC
Project name 500110519
CA0011



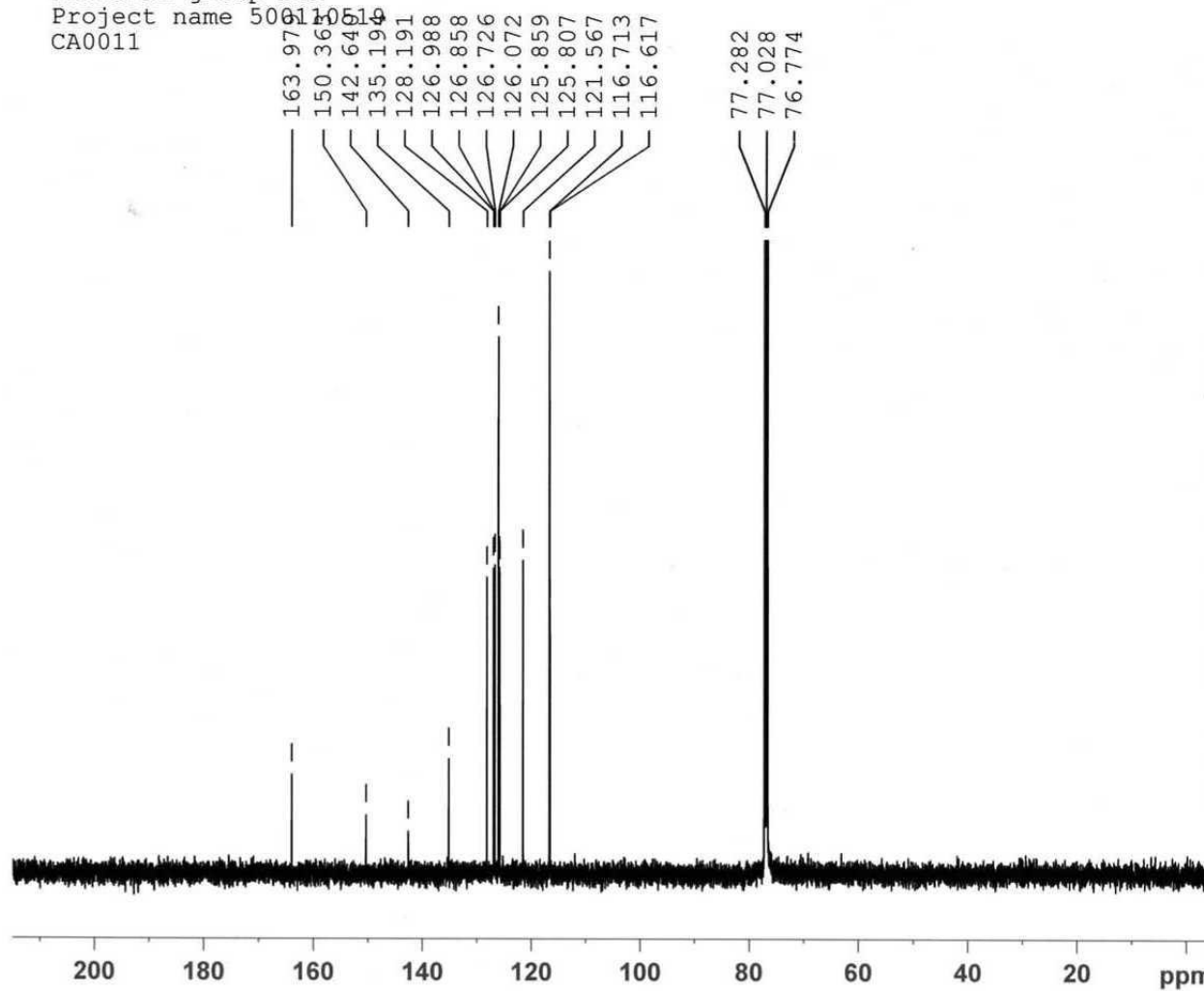
*** Current Data Parameters ***

NAME : oc2808
EXPNO : 80
PROCNO : 1



8-(4-nitrophenyl)-1-naphthol Proton NMR

Research group AKC
Project name 500110
CA0011



Current Data Parameters
NAME oc2808
EXPNO 81
PROCNO 1

F2 - Acquisition Parameters
Date_ 20081029
Time_ 7.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 912.3
DW 16.650 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

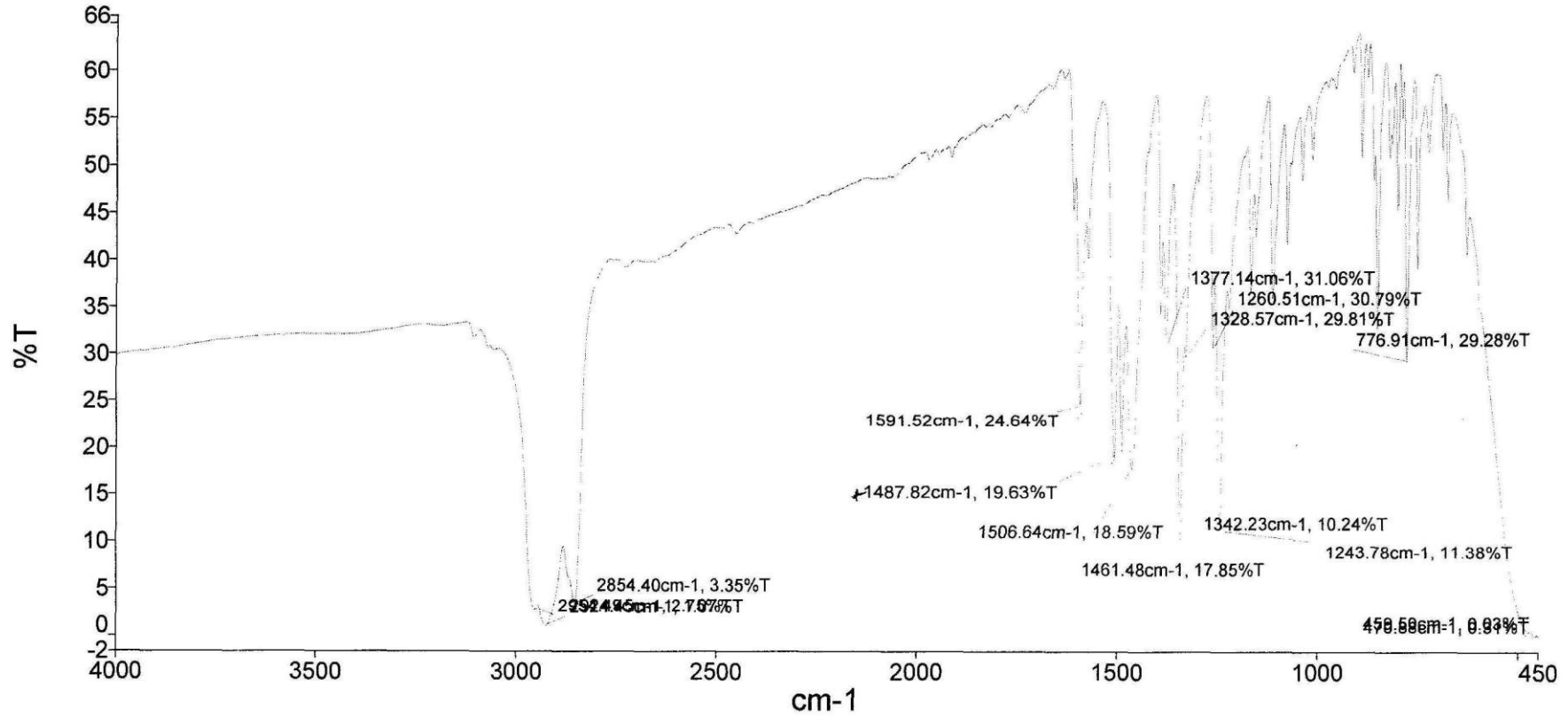
===== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 1.00 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 16.00 dB
PL13 17.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

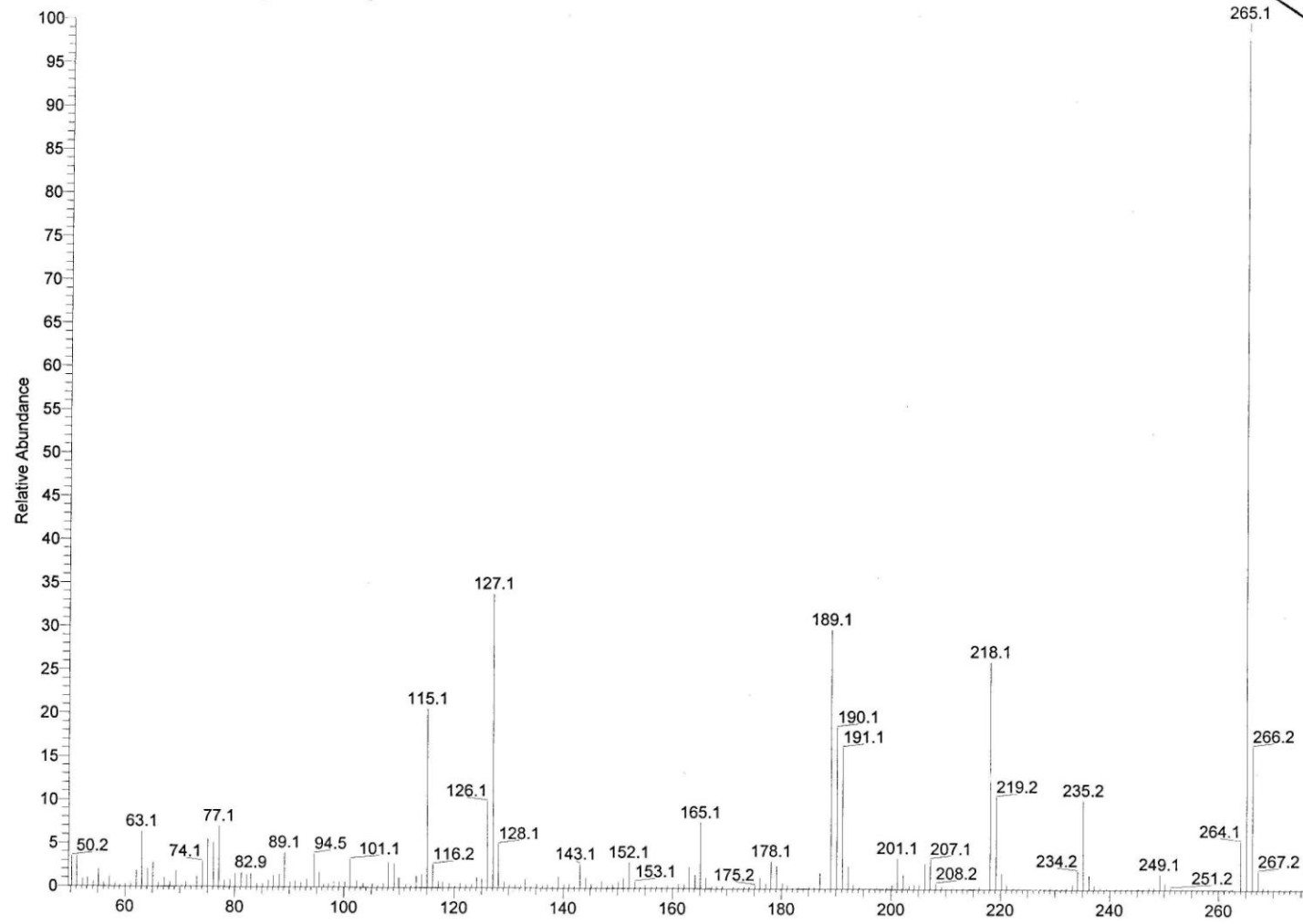
8-(4-nitrophenyl)-1-naphthol Carbon NMR

Analyst Administrator
Date 03 November 2008 12:43

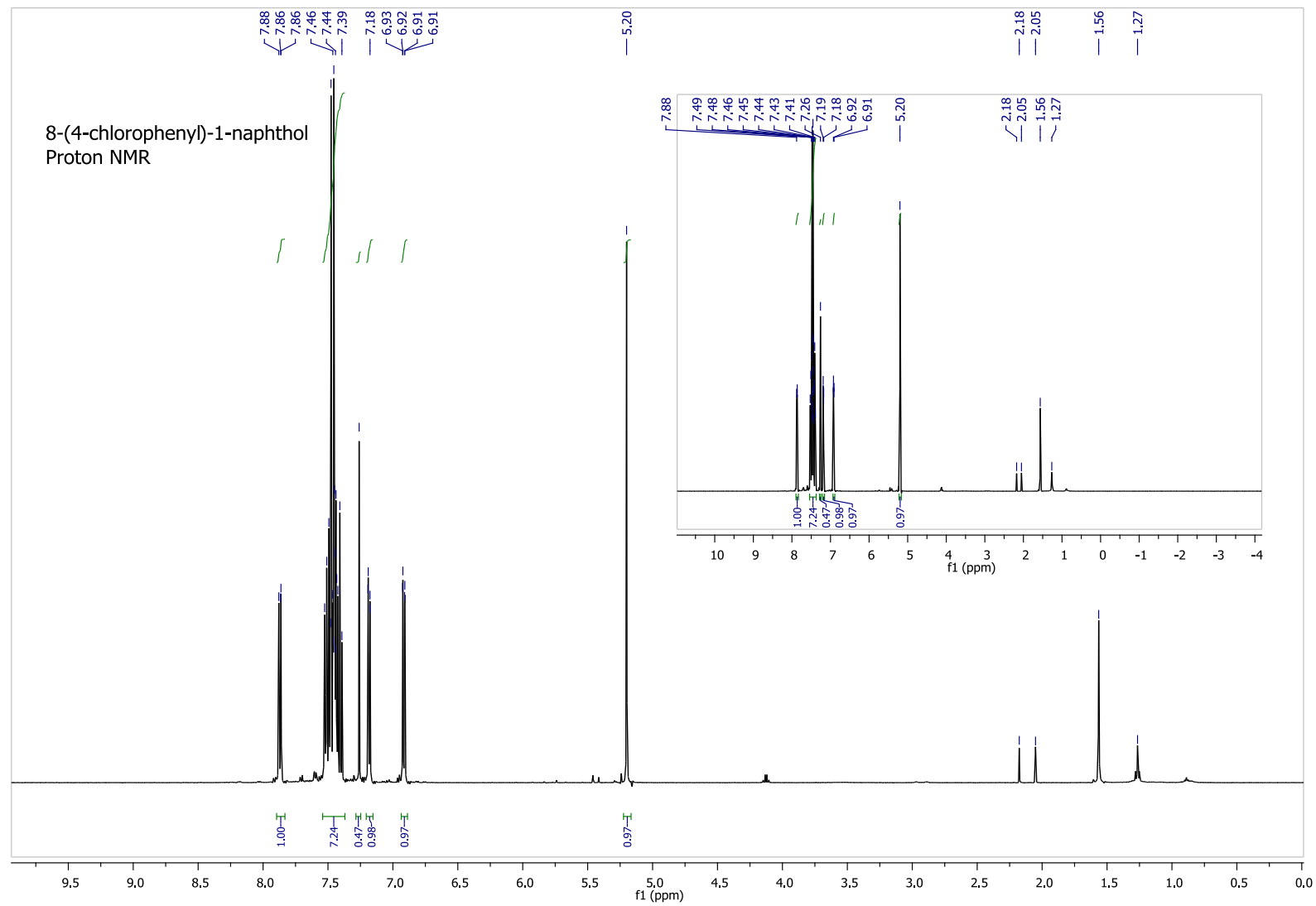


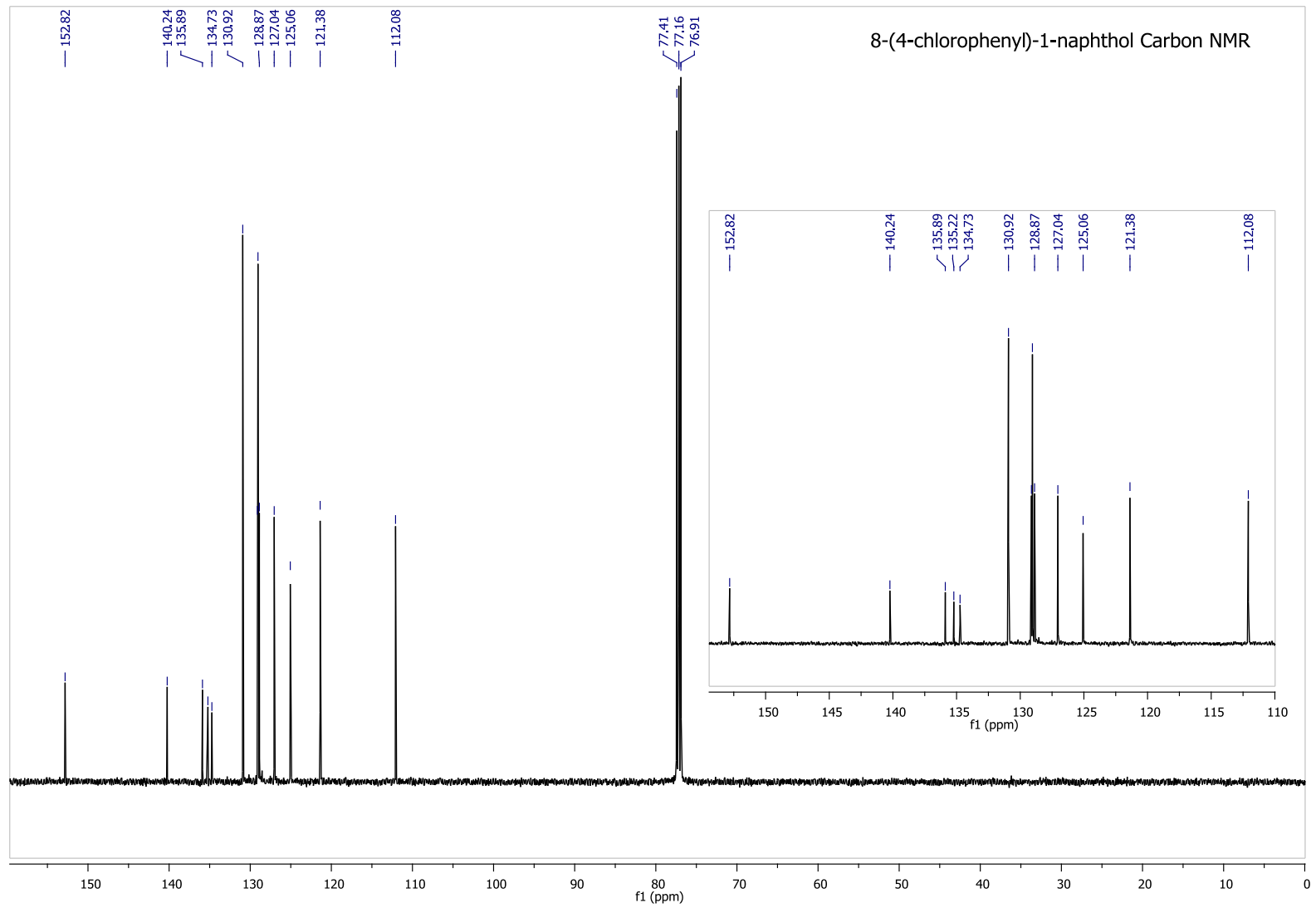
Administrator 62 Sample 062 By Administrator date Monday, November 03 2008

cad02 #1299 RT: 24.65 AV: 1 NL: 2.58E5
T: {0,0} + c EI det=350.00 Full ms [50.00-650.00]

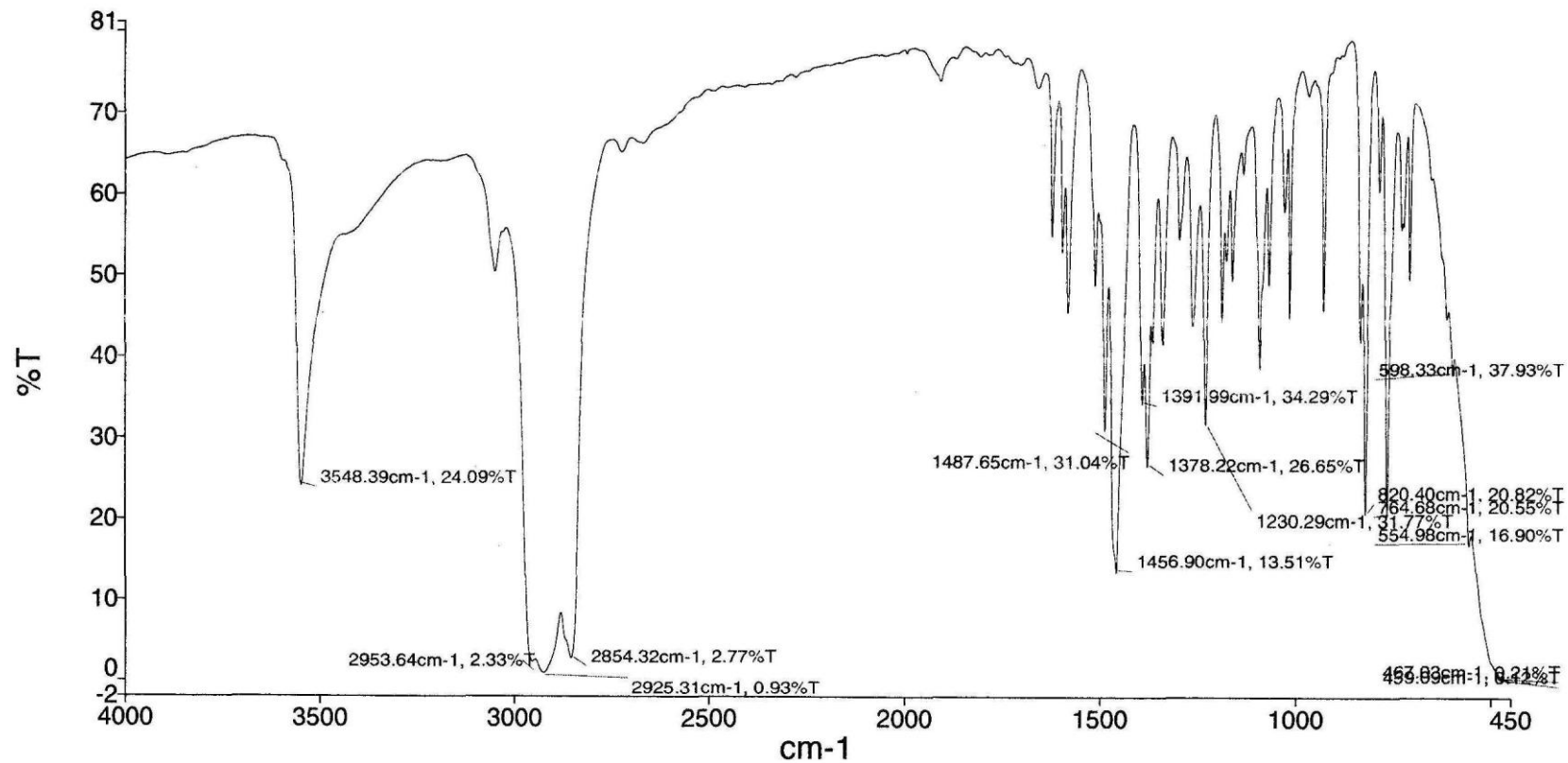


Compound 3: 8-(4-chlorophenyl)-1-naphthol



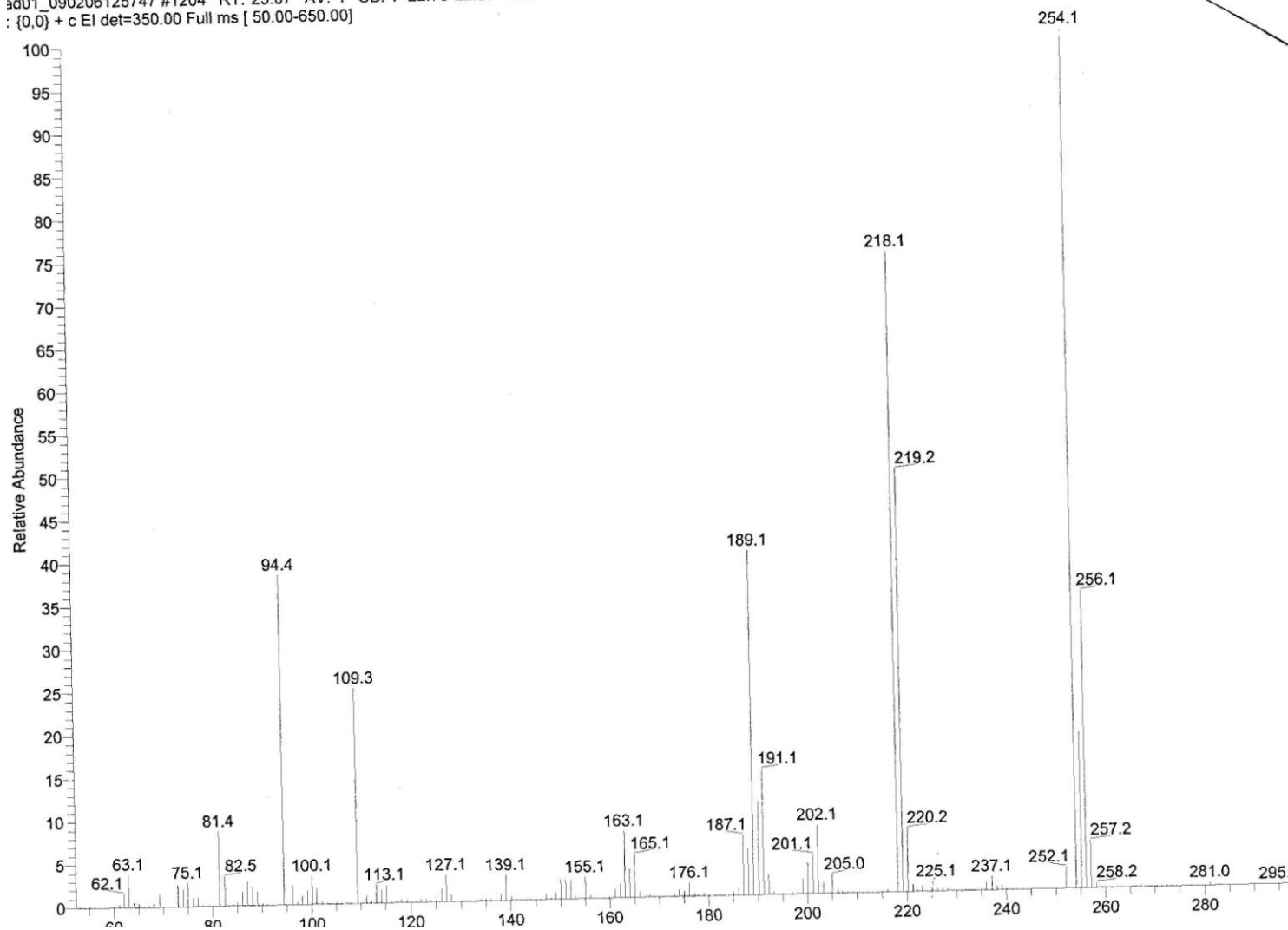


Analyst Administrator
Date 26 January 2009 14:42

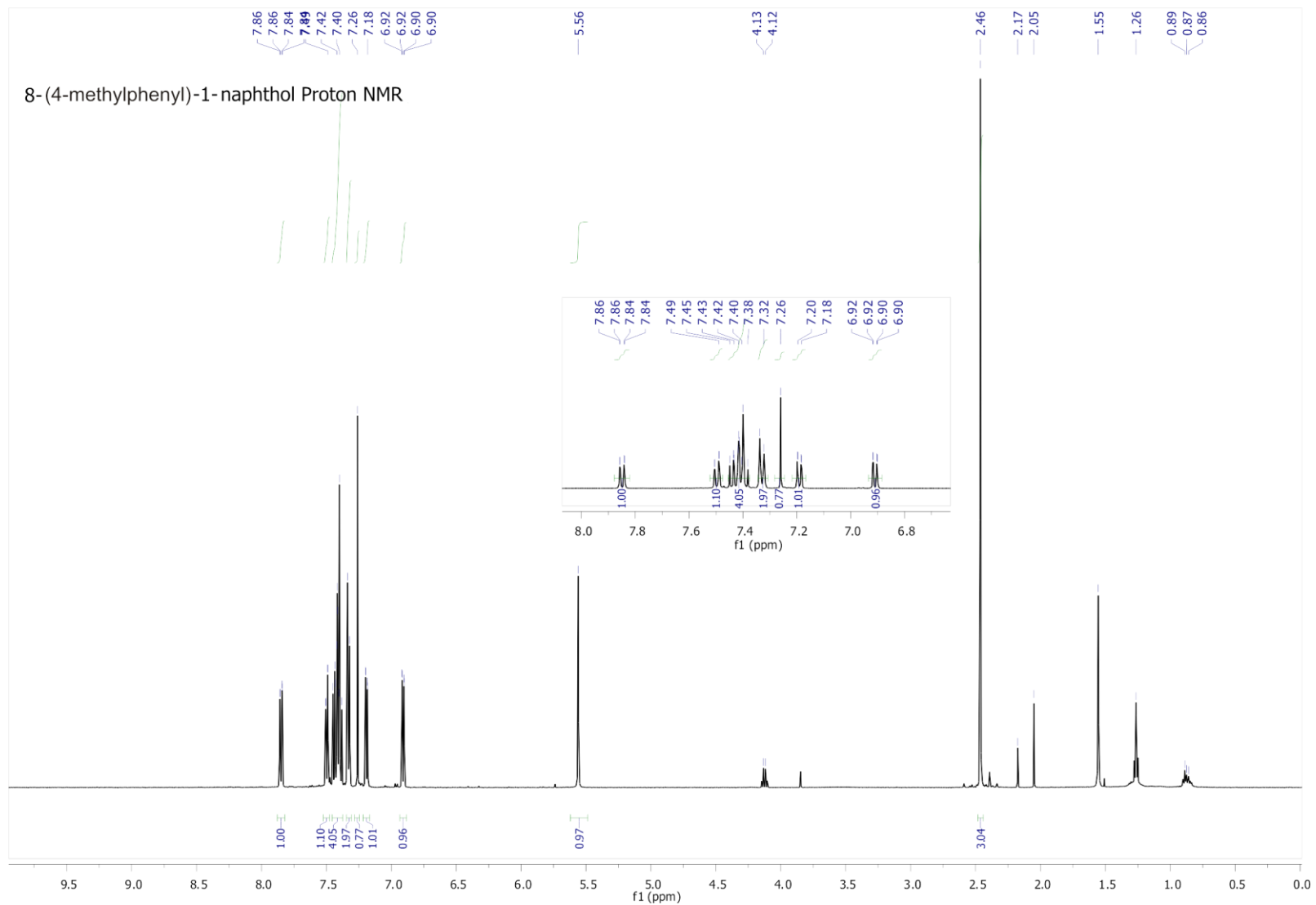


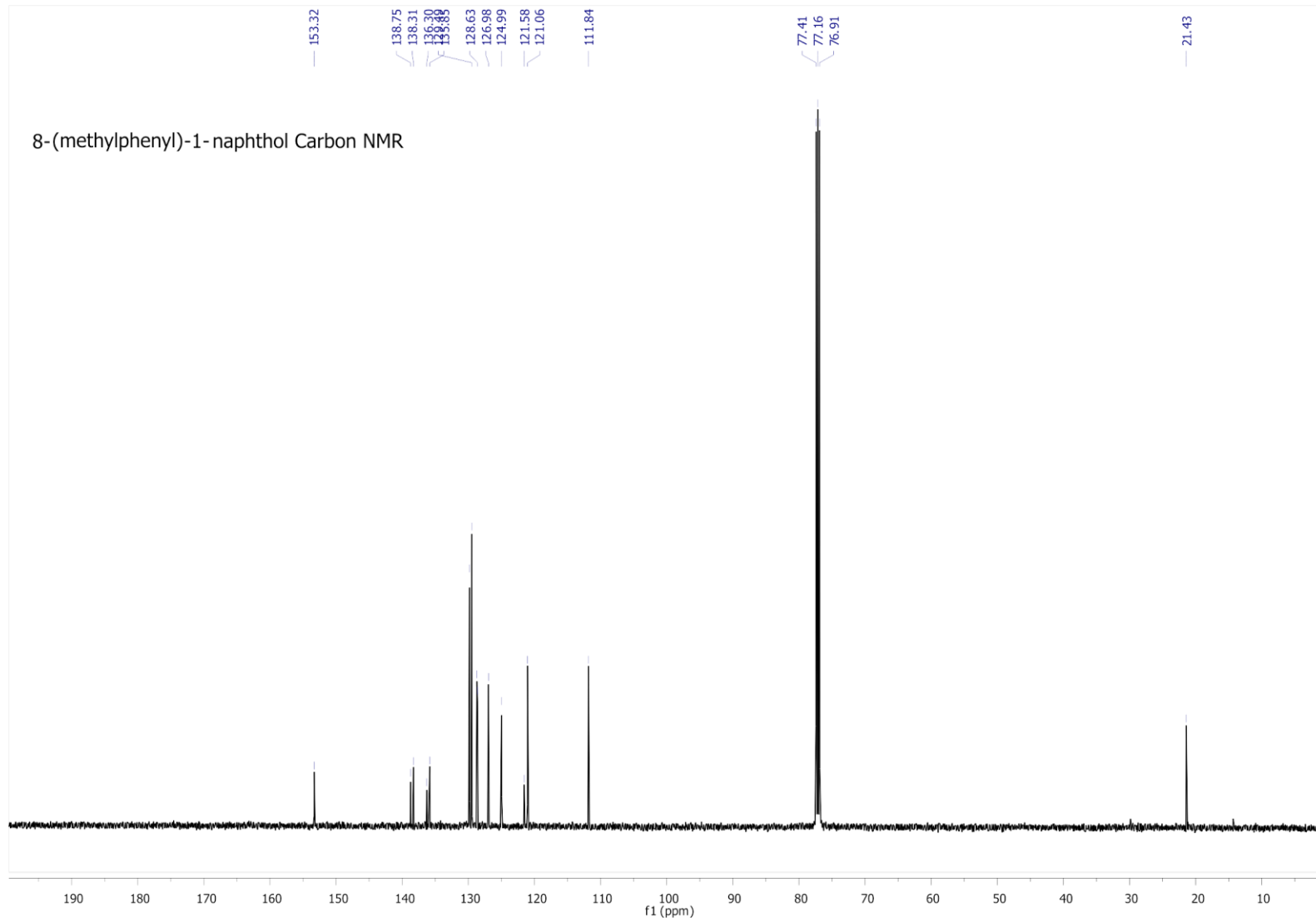
Administrator 10 Sample 010 By Administrator date Monday, January 26 2009

ad01_090206125747 #1204 RT: 23.07 AV: 1 SB: 7 22.79-22.89 NL: 3.01E6
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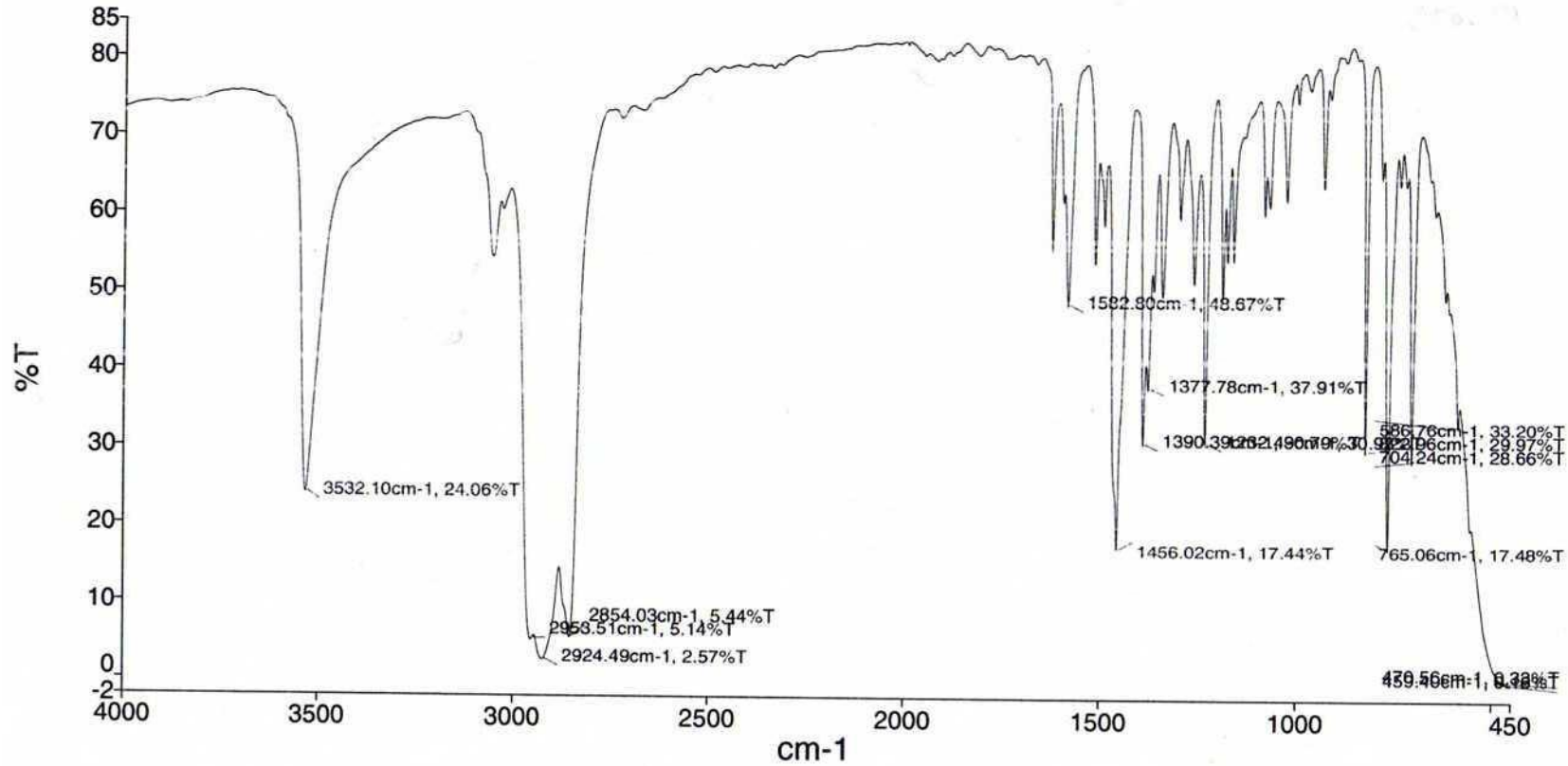
Compound 4: 8-(4-methylphenyl)-1-naphthol





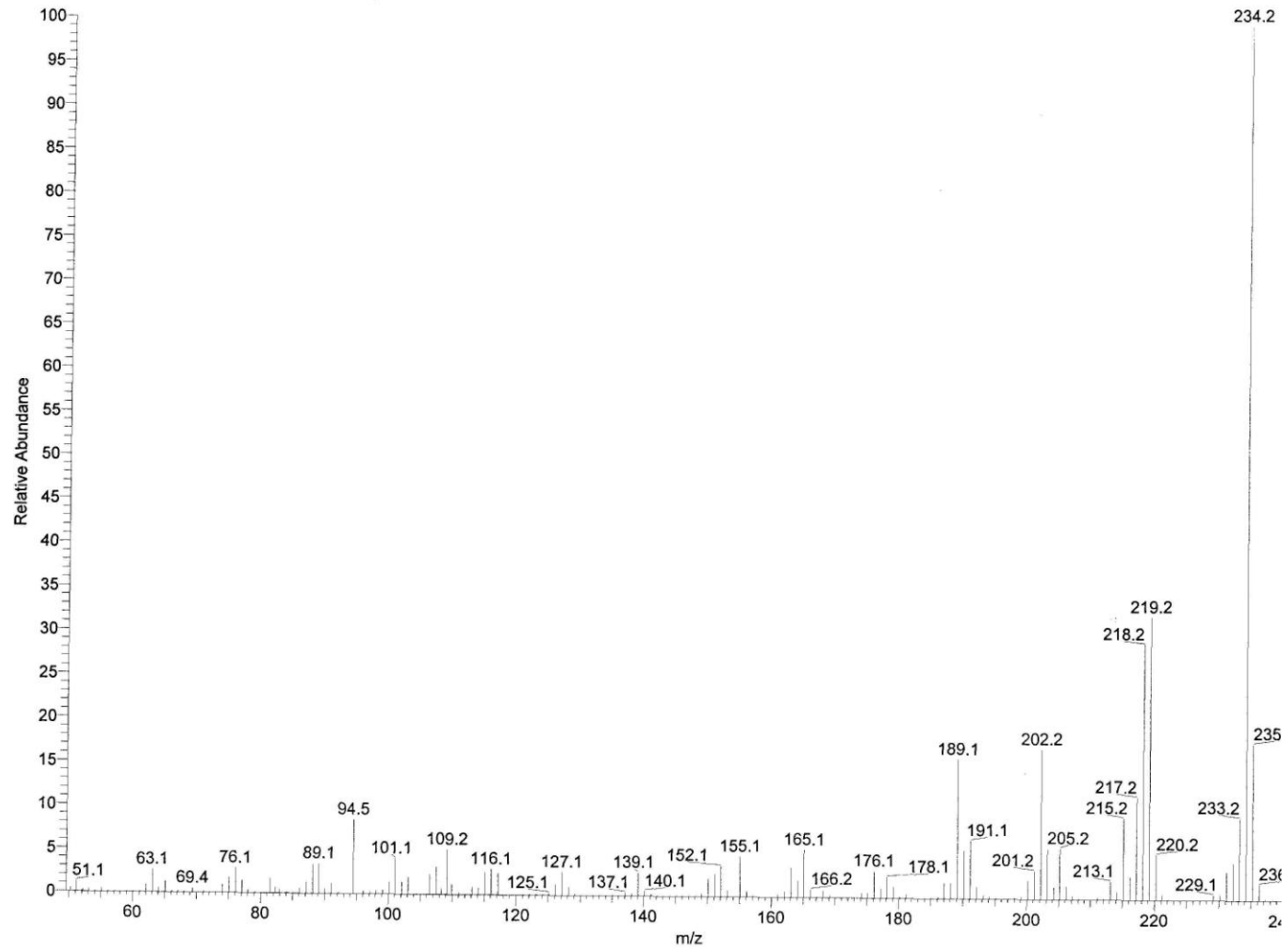
Analyst
Date

Administrator
26 January 2009 14:54

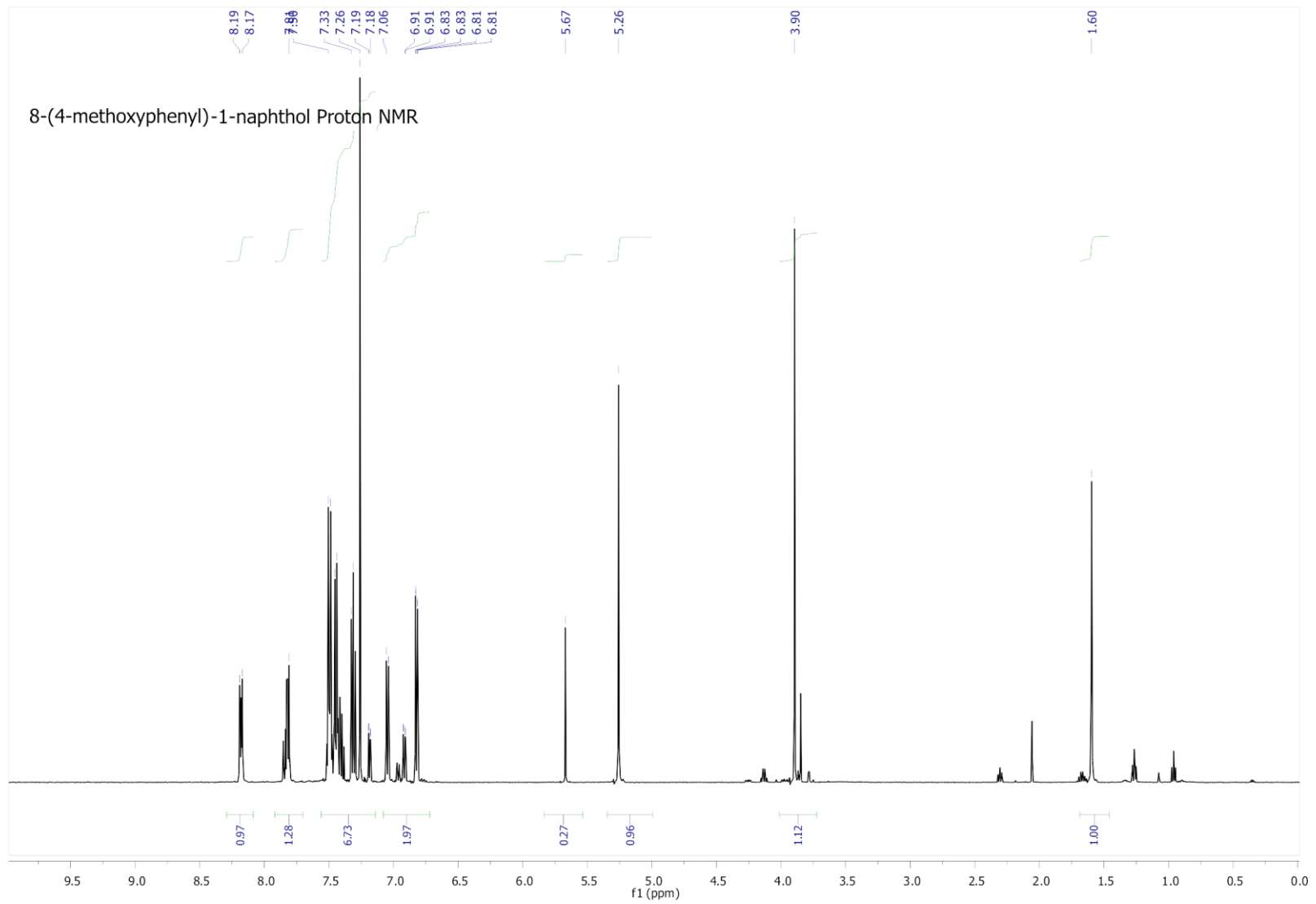


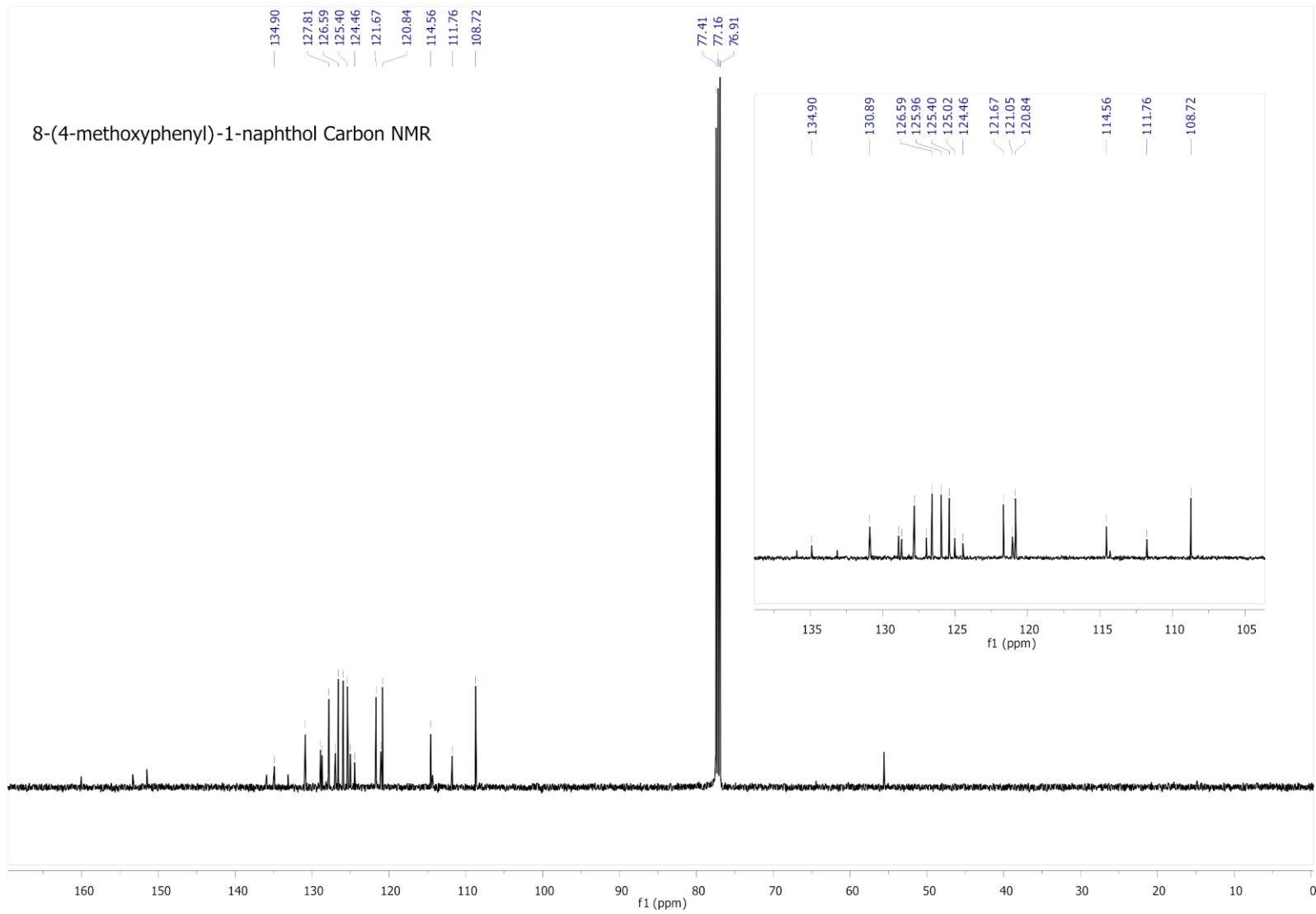
Administrator 12 Sample 012 By Administrator date Monday, January 26 2009

cad04 #1140 RT: 22.00 AV: 1 NL: 1.69E6
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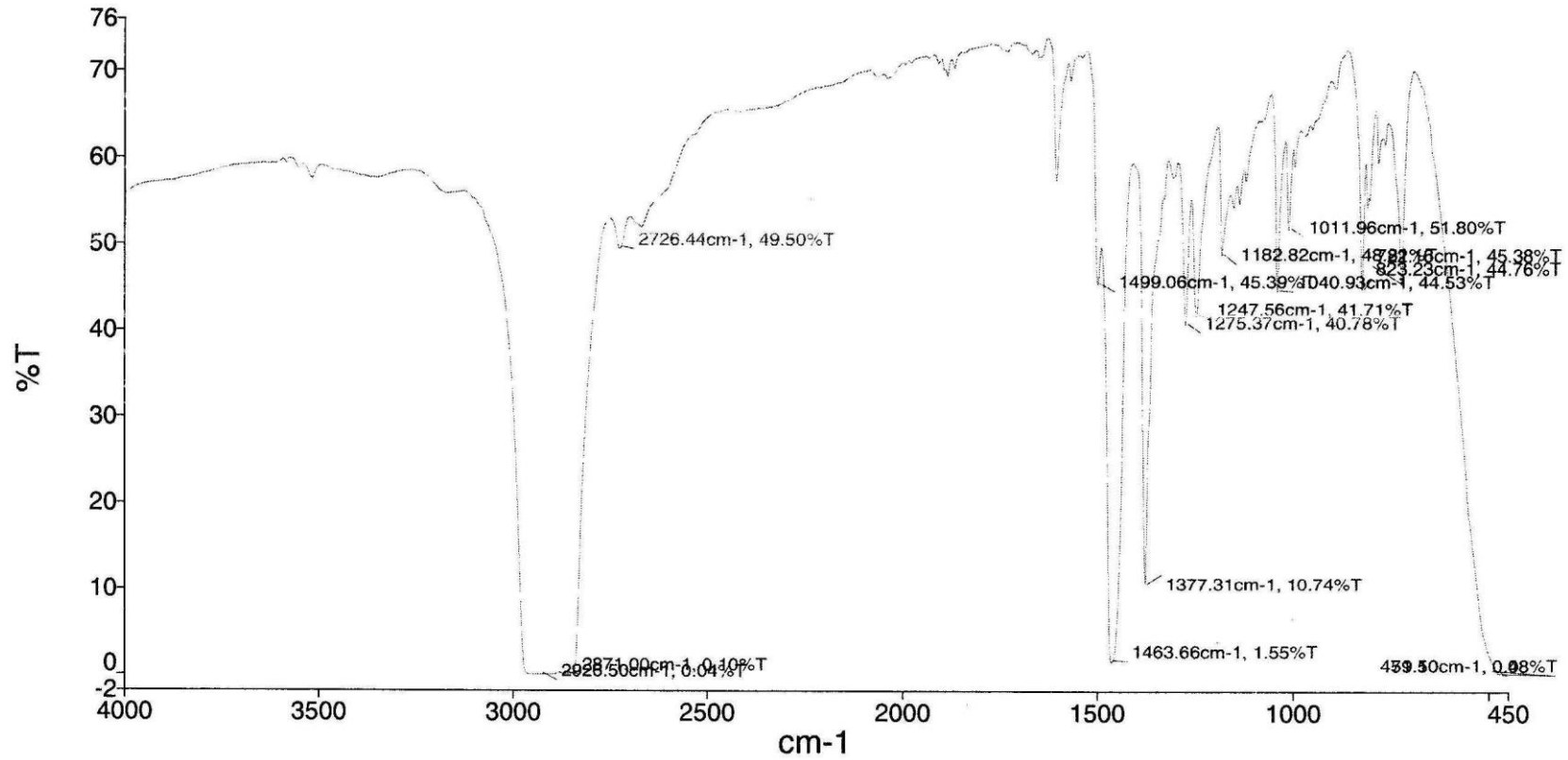
Compound 5: 8-(4-methoxyphenyl)-1-naphthol





Analyst
Date

Administrator
26 January 2009 14:48



Administrator 11 Sample 011 By Administrator date Monday, January 26 2009

cad03 #1228-1230 RT: 23.47-23.50 AV: 3 SB: 11 23.25-23.42 NL: 1.47E4

T: {0,0} + c EI det=350.00 Full ms [50.00-650.00]

