

Supplementary Information

¹H and ¹³C-NMR Spectra for

A remarkable temperature effect in the desymmetrization of bridged *meso*-tricyclic succinic anhydrides with chiral oxazolidin-2-ones

Narendra R. Chaubey and Sunil K. Ghosh*

Bio-Organic Division, Bhabha Atomic Research Centre, Mumbai 400085, INDIA

E-mail: ghsunil@barc.gov.in

Table of Contents

Entry	Description	Page
1	Figure-S1. ¹ H NMR Spectrum of 5a	3
2	Figure-S2. ¹³ C NMR Spectrum of 5a	4
3	Figure-S3. ¹ H NMR Spectrum of 6a	5
4	Figure-S4. ¹³ C NMR Spectrum of 6a	6
5	Figure-S5. ¹ H NMR Spectrum of 5b	7
6	Figure-S6. ¹³ C NMR Spectrum of 5b	8
7	Figure-S7. ¹ H NMR Spectrum of 6b	9
8	Figure-S8. ¹³ C NMR Spectrum of 6b	10
9	Figure-S9. ¹ H NMR Spectrum of 5c	11
10	Figure-S10. ¹³ C NMR Spectrum of 5c	12
11	Figure-S11. ¹ H NMR Spectrum of 6c	13
12	Figure-S12. ¹³ C NMR Spectrum of 6c	14
13	Figure-S13. ¹ H NMR Spectrum of 5d	15
14	Figure-S14. ¹³ C NMR Spectrum of 5d	16
15	Figure-S15. ¹ H NMR Spectrum of 6d	17
16	Figure-S16. ¹³ C NMR Spectrum of 6d	18
17	Figure-S17. ¹ H NMR Spectrum of 7a	19
18	Figure-S18. ¹³ C NMR Spectrum of 7a	20
19	Figure-S19. ¹ H NMR Spectrum of 8a	21
20	Figure-S20. ¹³ C NMR Spectrum of 8a	22
21	Figure-S21. ¹ H NMR Spectrum of 10a	23
22	Figure-S22. ¹³ C NMR Spectrum of 10a	24
23	Figure-S23. ¹ H NMR Spectrum of 11a	25
24	Figure-S24. ¹³ C NMR Spectrum of 11a	26
25	Figure-S25. ¹ H NMR Spectrum of 11b	27
26	Figure-S26. ¹³ C NMR Spectrum of 11b	28

Entry	Description	Page
27	Figure-S27. ¹ H NMR Spectrum of 12b	29
28	Figure-S28. ¹³ C NMR Spectrum of 12b	30
29	Figure-S29. ¹ H NMR Spectrum of 11c	31
30	Figure-S30. ¹³ C NMR Spectrum of 11c	32
31	Figure-S31. ¹ H NMR Spectrum of 12c	33
32	Figure-S32. ¹³ C NMR Spectrum of 12c	34
33	Figure-S33. ¹ H NMR Spectrum of 11d	35
34	Figure-S34. ¹³ C NMR Spectrum of 11d	36
35	Figure-S35. ¹ H NMR Spectrum of 12d	37
36	Figure-S36. ¹³ C NMR Spectrum of 12d	38
37	Figure-S37. ¹ H NMR Spectrum of 11e	39
38	Figure-S38. ¹³ C NMR Spectrum of 11e	40
39	Figure-S39. ¹ H NMR Spectrum of 11f	41
40	Figure-S40. ¹³ C NMR Spectrum of 11f	42
41	Figure-S41. ¹ H NMR Spectrum of 13	43
42	Figure-S42. ¹³ C NMR Spectrum of 13	44
43	Figure-S43. ¹ H NMR Spectrum of 15a	45
44	Figure-S44. ¹³ C NMR Spectrum of 15a	46
45	Figure-S45. ¹ H NMR Spectrum of 16a	47
46	Figure-S46. ¹³ C NMR Spectrum of 16a	48
47	Figure-S47. ¹ H NMR Spectrum of 15b	49
48	Figure-S48. ¹³ C NMR Spectrum of 15b	50
49	Figure-S49. ¹ H NMR Spectrum of 16b	51
50	Figure-S50. ¹³ C NMR Spectrum of 16b	52

Figure-S1. ¹H NMR spectrum of compound **5a**

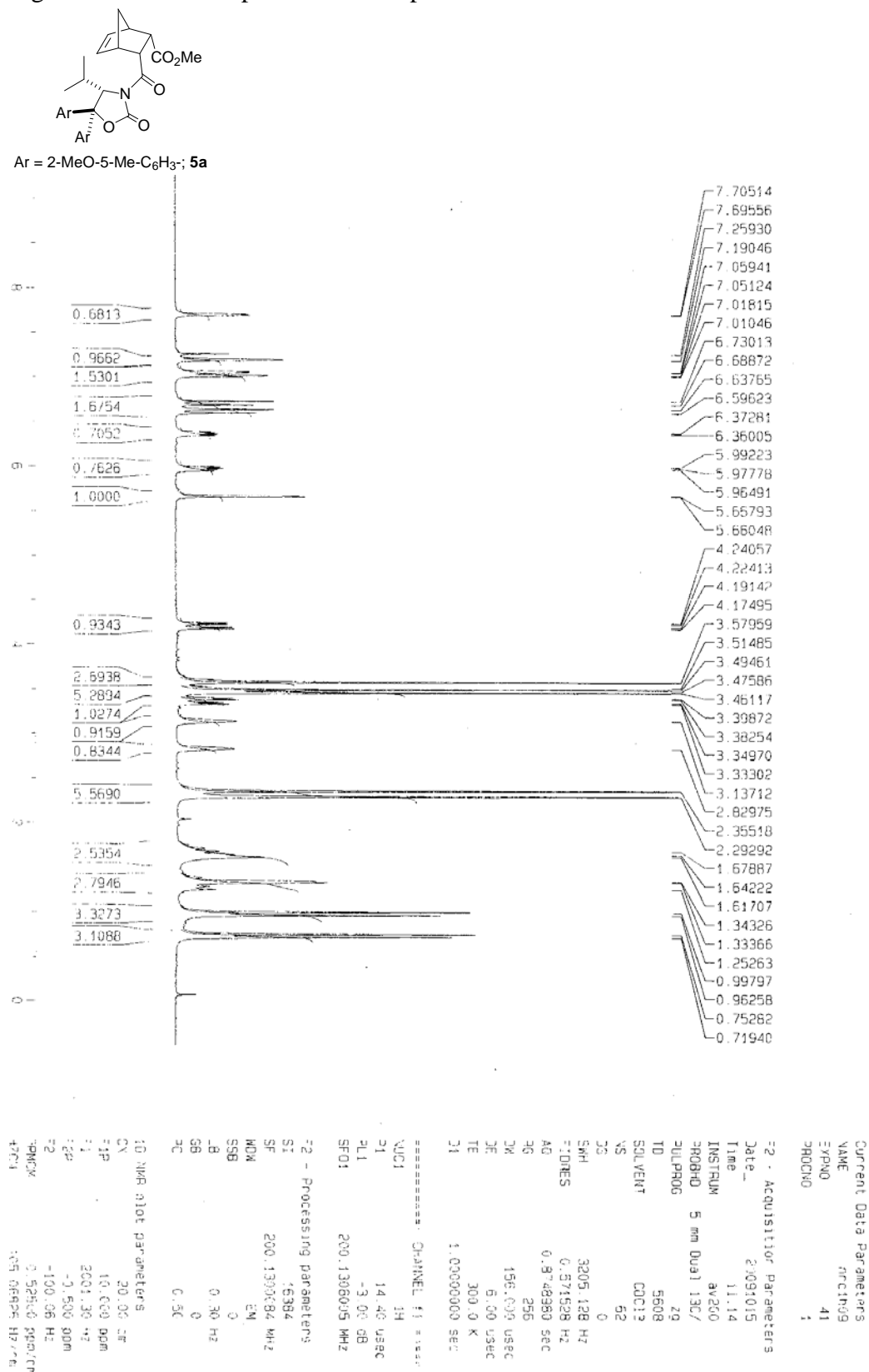
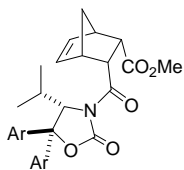


Figure-S2. ¹³C NMR spectrum of compound 5a



Ar = 2-MeO-5-Me-C₆H₃; 5a

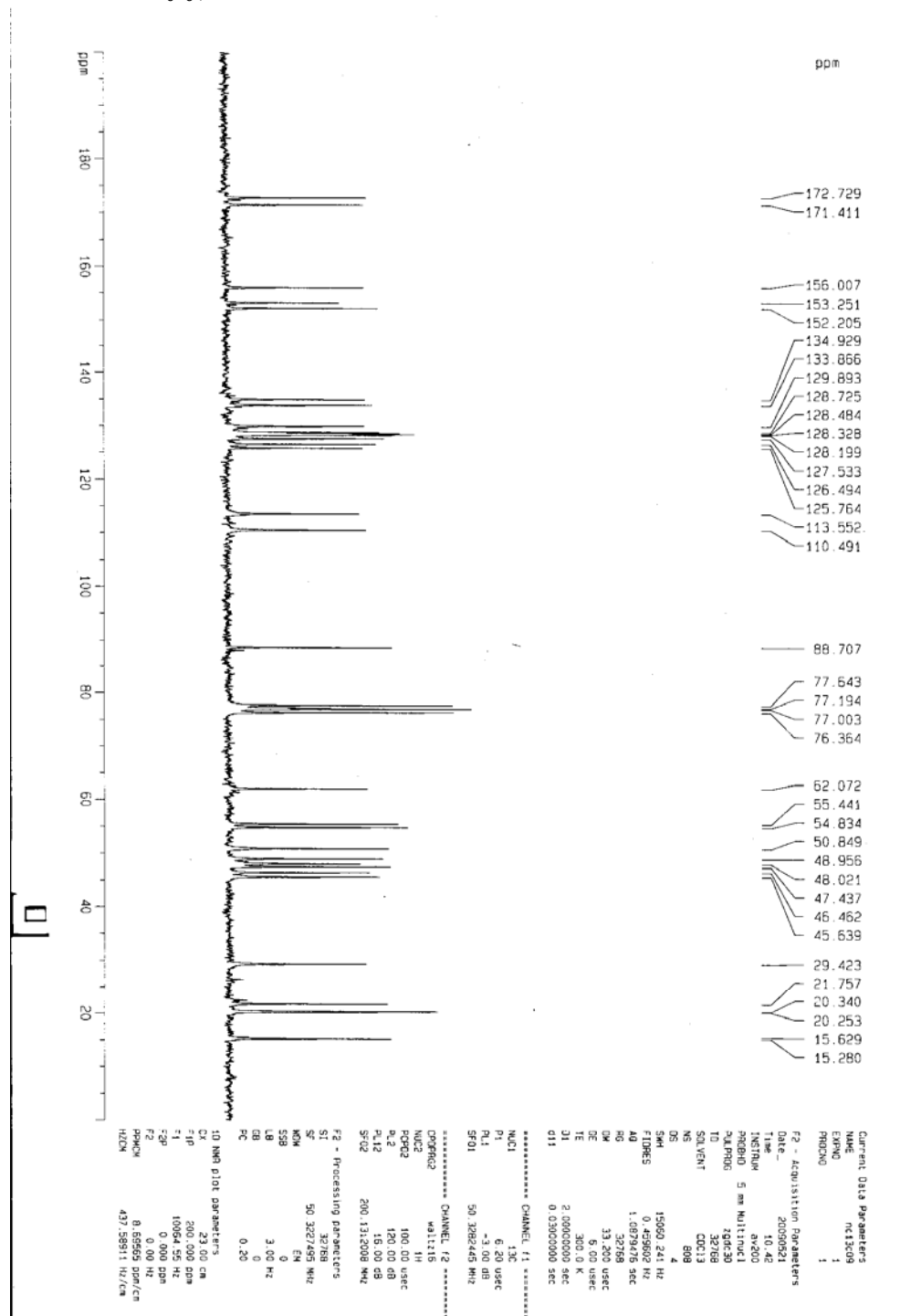


Figure-S3. ¹H NMR spectrum of compound **6a**

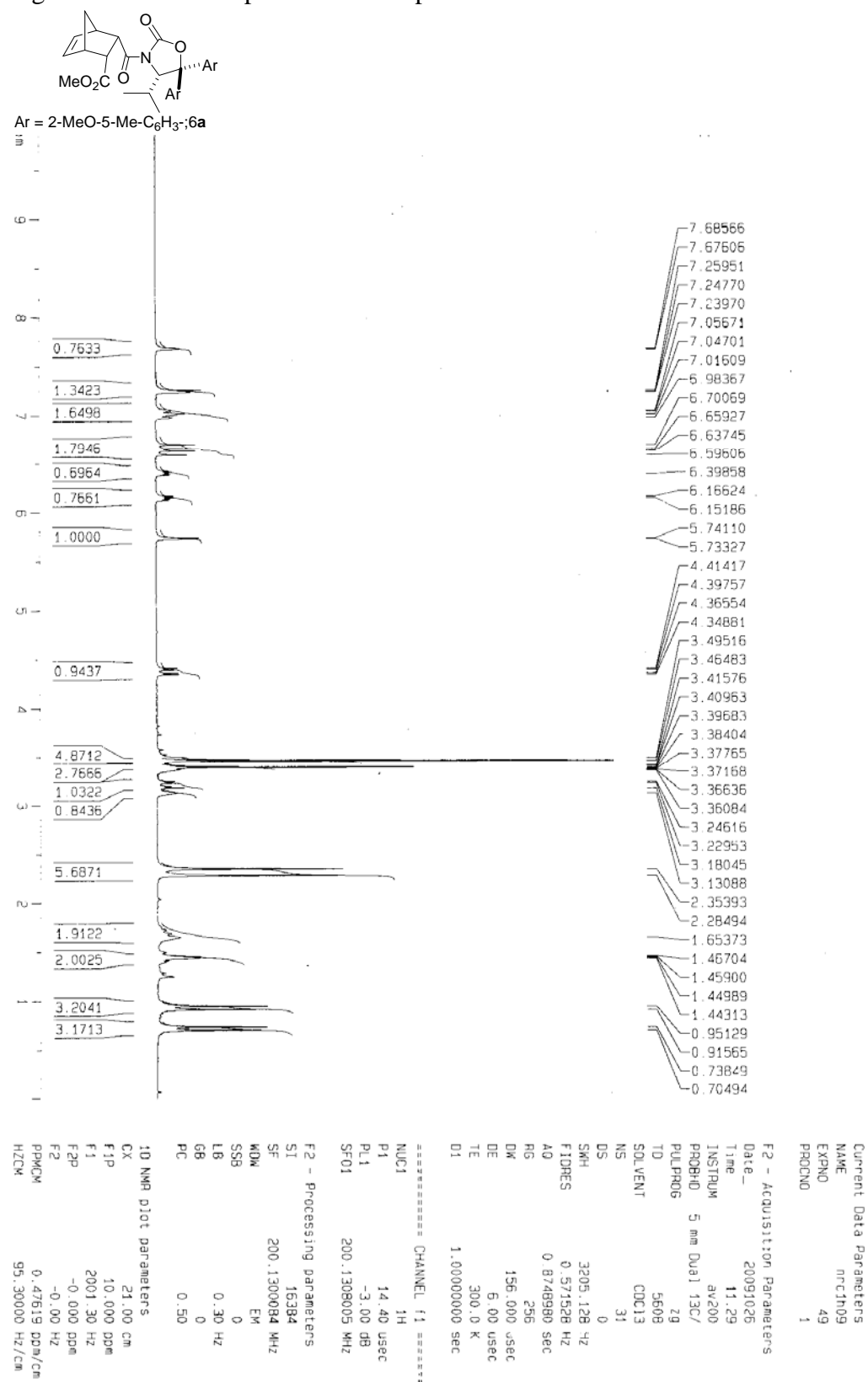


Figure-S4. ^{13}C NMR spectrum of compound **6a**

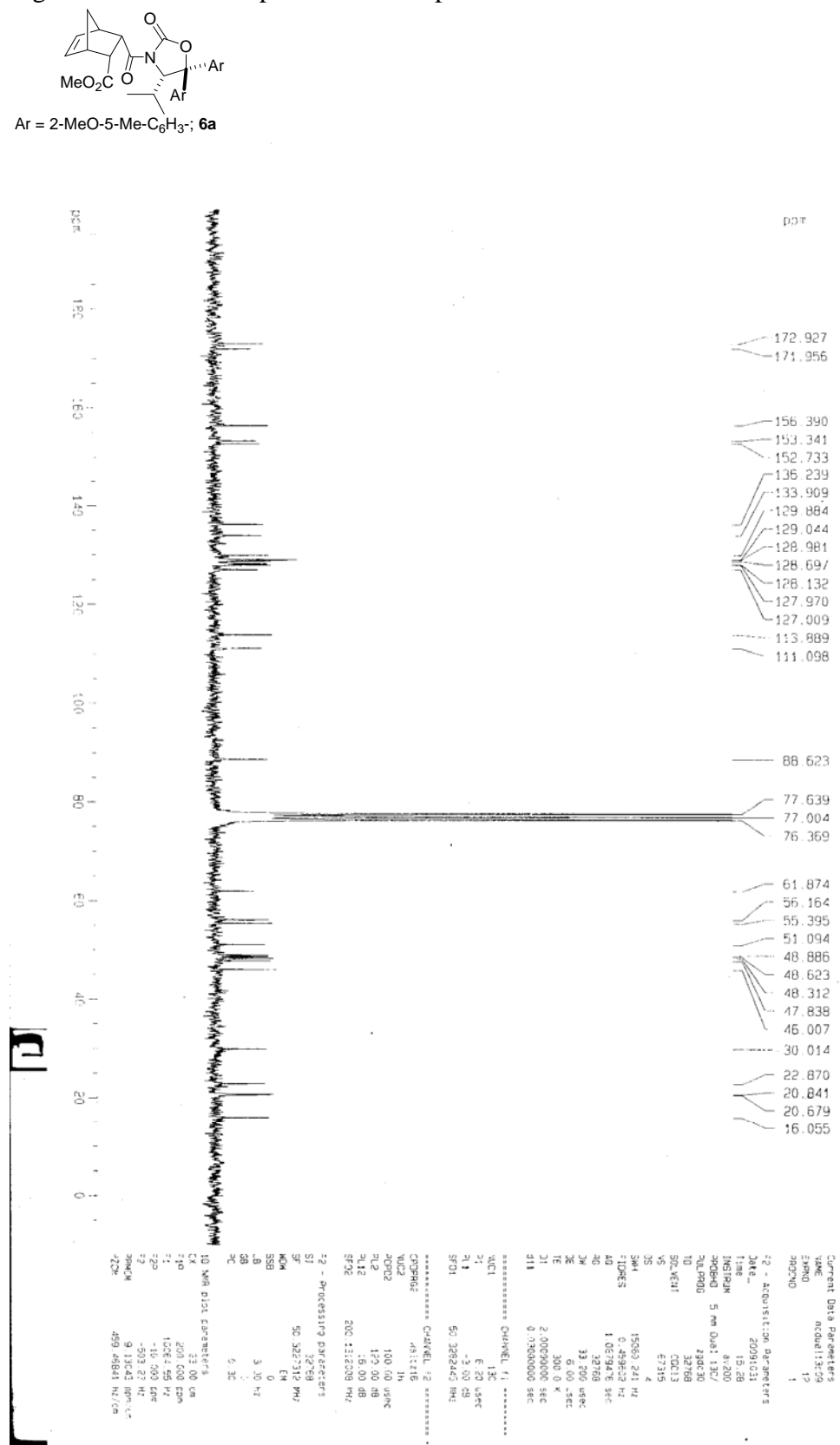
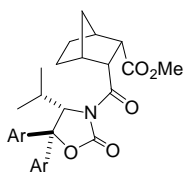
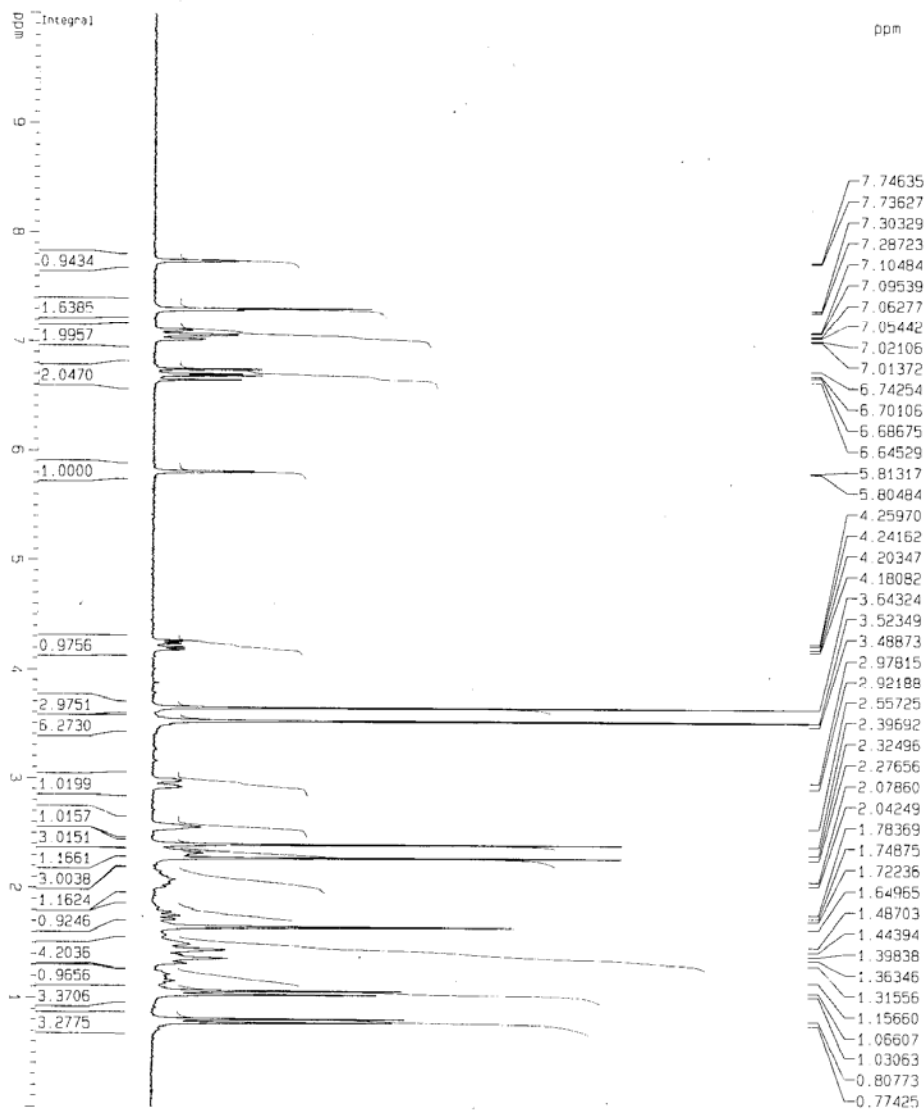


Figure-S5. ¹H NMR spectrum of compound **5b**



Ar = 2-MeO-5-Me-C₆H₃; **5b**



```

Current Data Parameters
NAME          FC-06-810
EXPNO        5
PROCNO       1

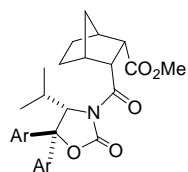
F2 - Acquisition Parameters
Date_         20100719
Time          15:22
INSTRUM      spect
PROBHD       5 mm Dual 13C/
PULPROG      zgpg30
TD           26850
SOLVENT      CDCl3
NS           24
DS           0
SWH          6176.652 Hz
FIDRES      0.250168 Hz
AQ           1.9987025 sec
RG           656
DM           80.000 usec
DE           115.00 usec
TE           0.0
AQREST      1.0000000 sec
MCREST      0.0000000 sec
MCMSK      0.01500000 sec

***** CHANNEL f1 *****
NUC1         1H
PI           14.40 usec
PL           -3.00 dB
SFO1         200.1360200 MHz

F2 - Processing parameters
SI           16384
SF           200.1360000 MHz
WDW          EM
SSB          0
LB           3.30 Hz
GB           0
PC           1.00

1D NMR plot parameters
CX           21.00 cm
CY           15.00 cm
F1P          10.000 DPM
F2P          2001.30 Hz
F3P          -0.000 Hz
PC136       0.4755 DPM/cm
PC137       95.30000 Hz/cm
    
```

Figure-S6. ^{13}C NMR spectrum of compound **5b**



Ar = 2-MeO-5-Me-C₆H₃-; **5b**

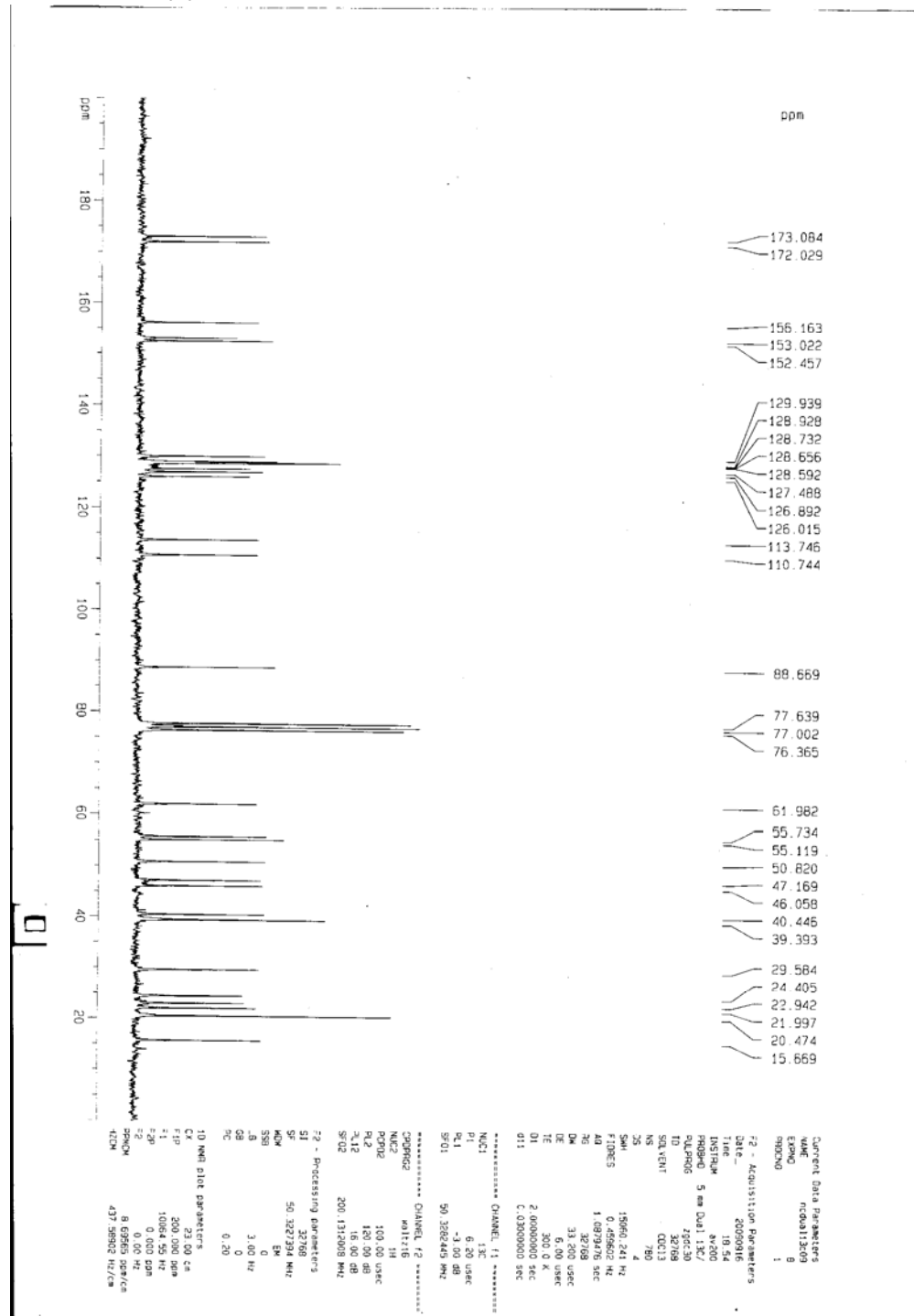
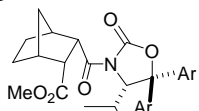


Figure-S7. ¹H NMR spectrum of compound **6b**



Ar = 2-MeO-5-Me-C₆H₃; **6b**

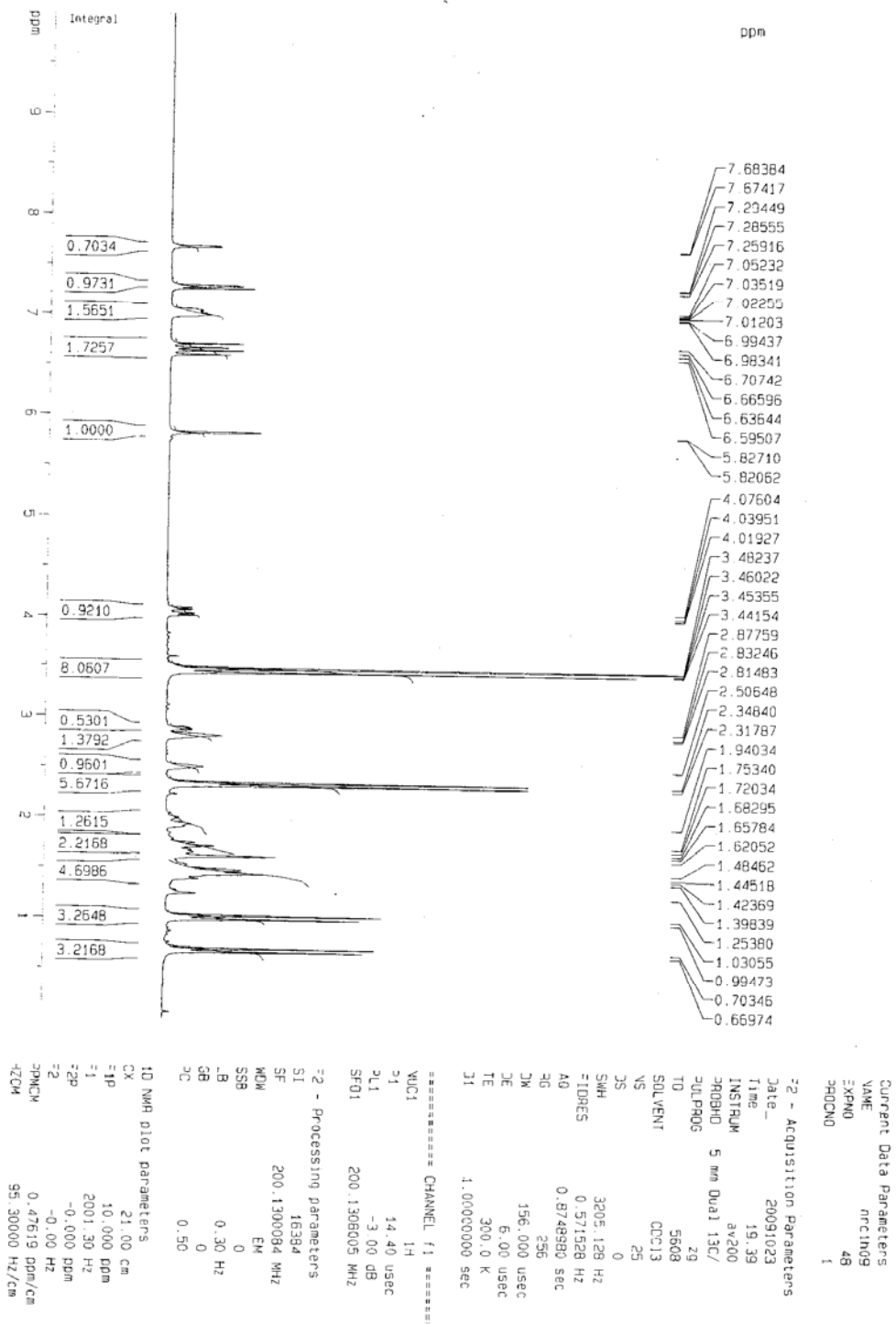
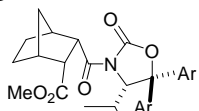


Figure-S8. ¹³C NMR spectrum of compound **6b**



Ar = 2-MeO-5-Me-C₆H₃; **6b**

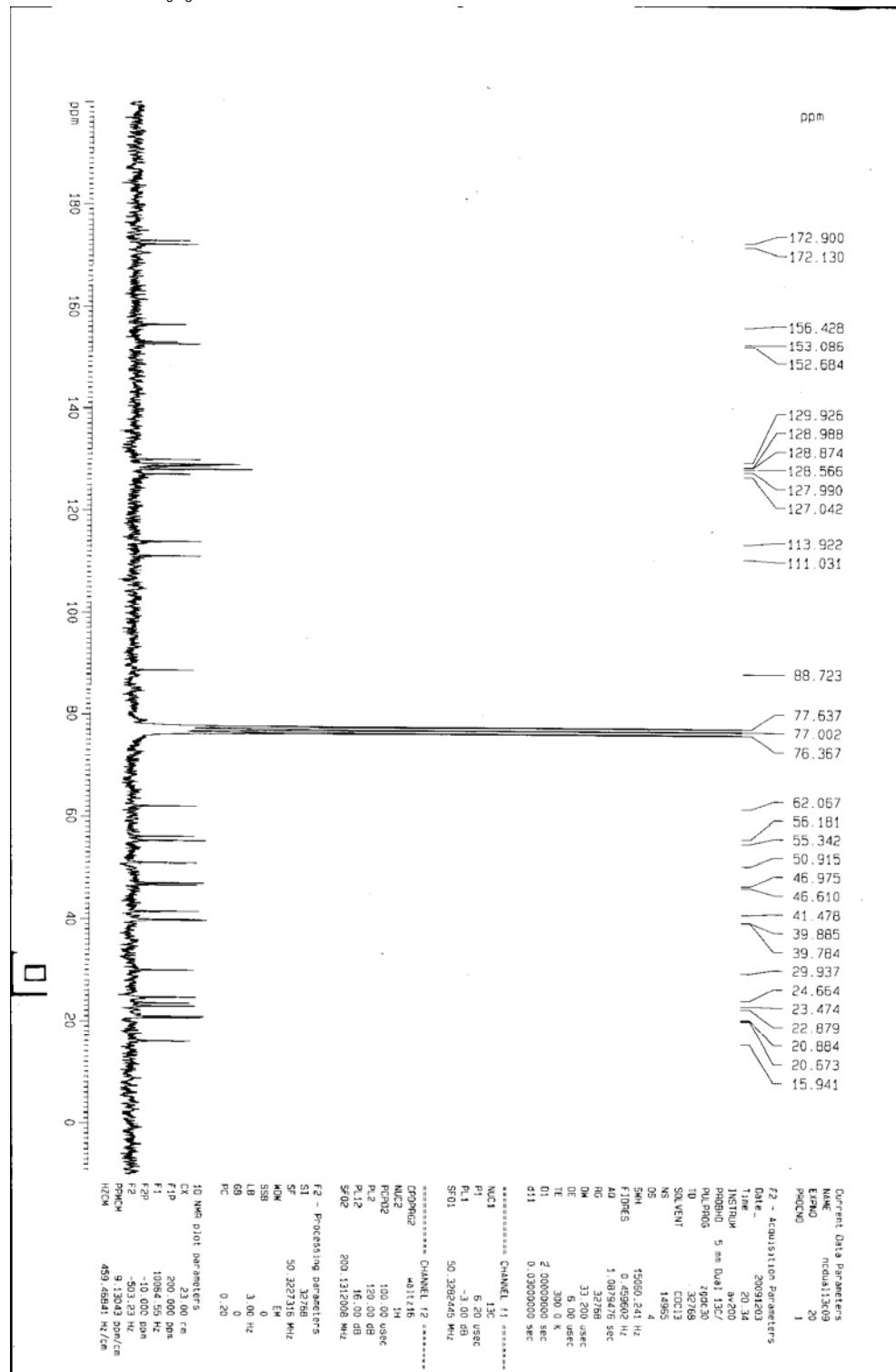
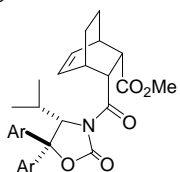
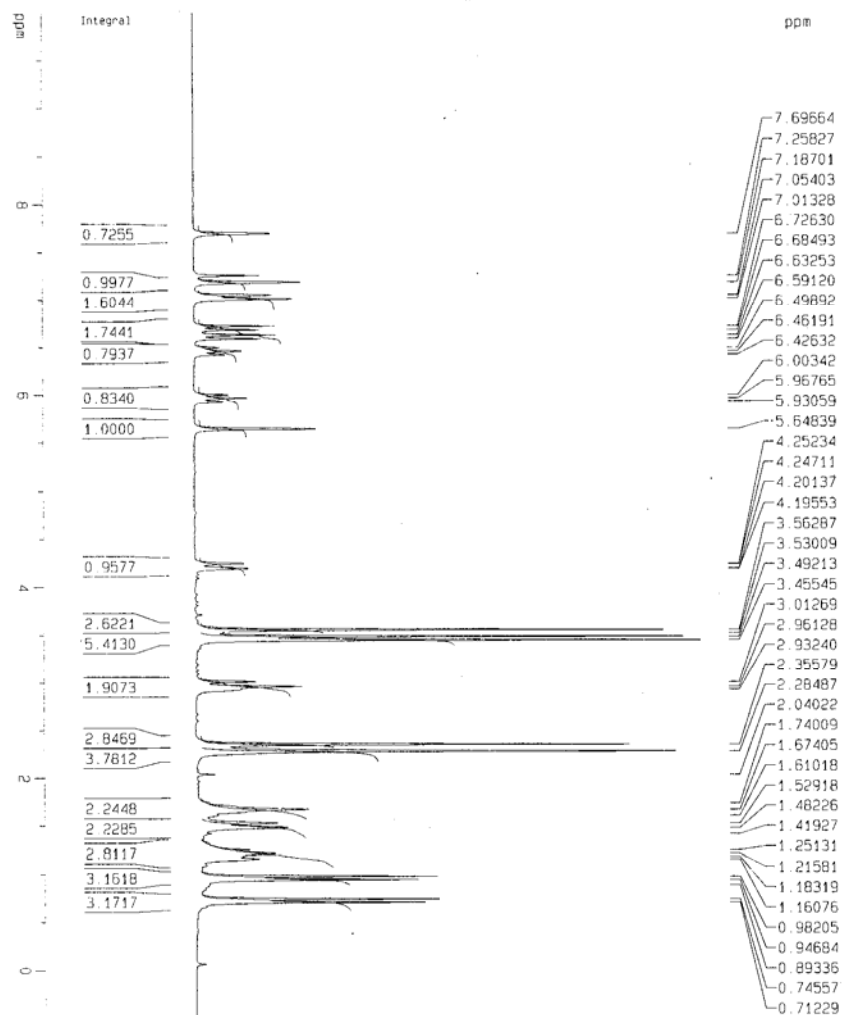


Figure-S9. ¹H NMR spectrum of compound **5c**



Ar = 2-MeO-5-Me-C₆H₃-, **5c**



```

Current Data Parameters
NAME      nrc1n09
EXPNO    39
PROCNO   1

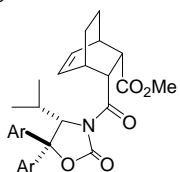
F2 - Acquisition Parameters
Date_    20091007
Time     16.40
INSTRUM  av200
PROBHD   5 mm QNP 13C/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
VS        24
SFO1     100.628150 MHz
SFO2     125.761360 MHz
SMH      3205.128 Hz
FIDRES   0.571528 Hz
AQ        0.8748980 sec
RG         256
AQ        156.000 usec
DE        6.00 usec
TE        300.2 K
JE        1.00000000 sec
J1

===== CHANNEL f1 =====
NUC1      1H
P1        14.40 usec
PL1       -3.00 dB
SFO1      200.1308005 MHz

F2 - Processing parameters
SI         16384
SF         200.1300084 MHz
WDW         EM
SSB         0
GB         0.33 Hz
GB         0
PC         0.50

10 NMR plot parameters
CX         20.00 cm
CP         10.000 ppm
F1         2001.30 Hz
F2         -0.500 ppm
PCMCN     -100.006 Hz
PCMCN     0.52506 ppm/cm
ZCM       105.06825 Hz/cm
    
```

Figure-S10. ¹³C NMR spectrum of compound 5c



Ar = 2-MeO-5-Me-C₆H₃; 5c

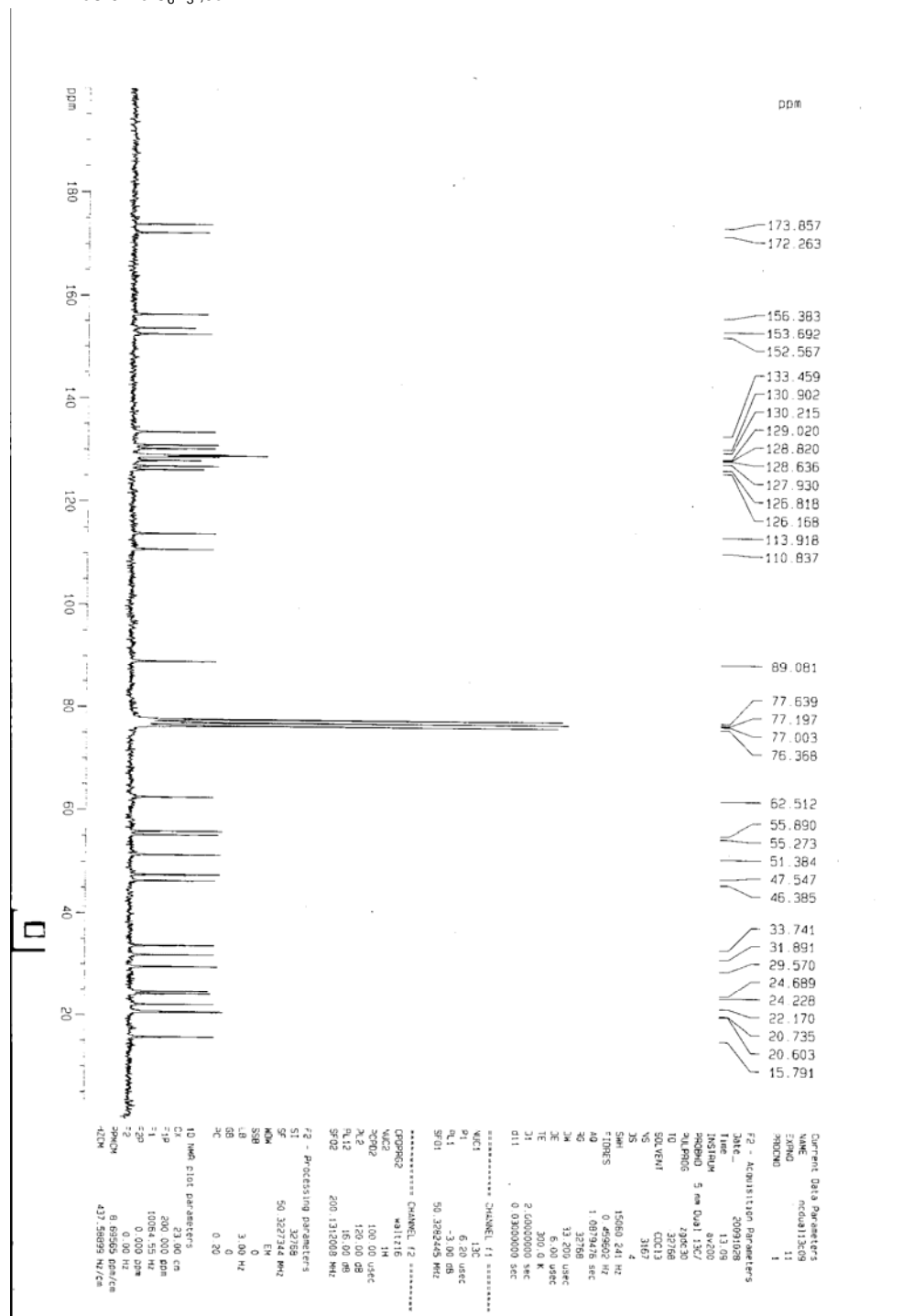
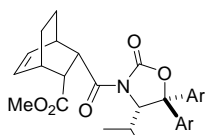


Figure-S11. ¹H NMR spectrum of compound **6c**



Ar = 2-MeO-5-Me-C₆H₃; **6c**

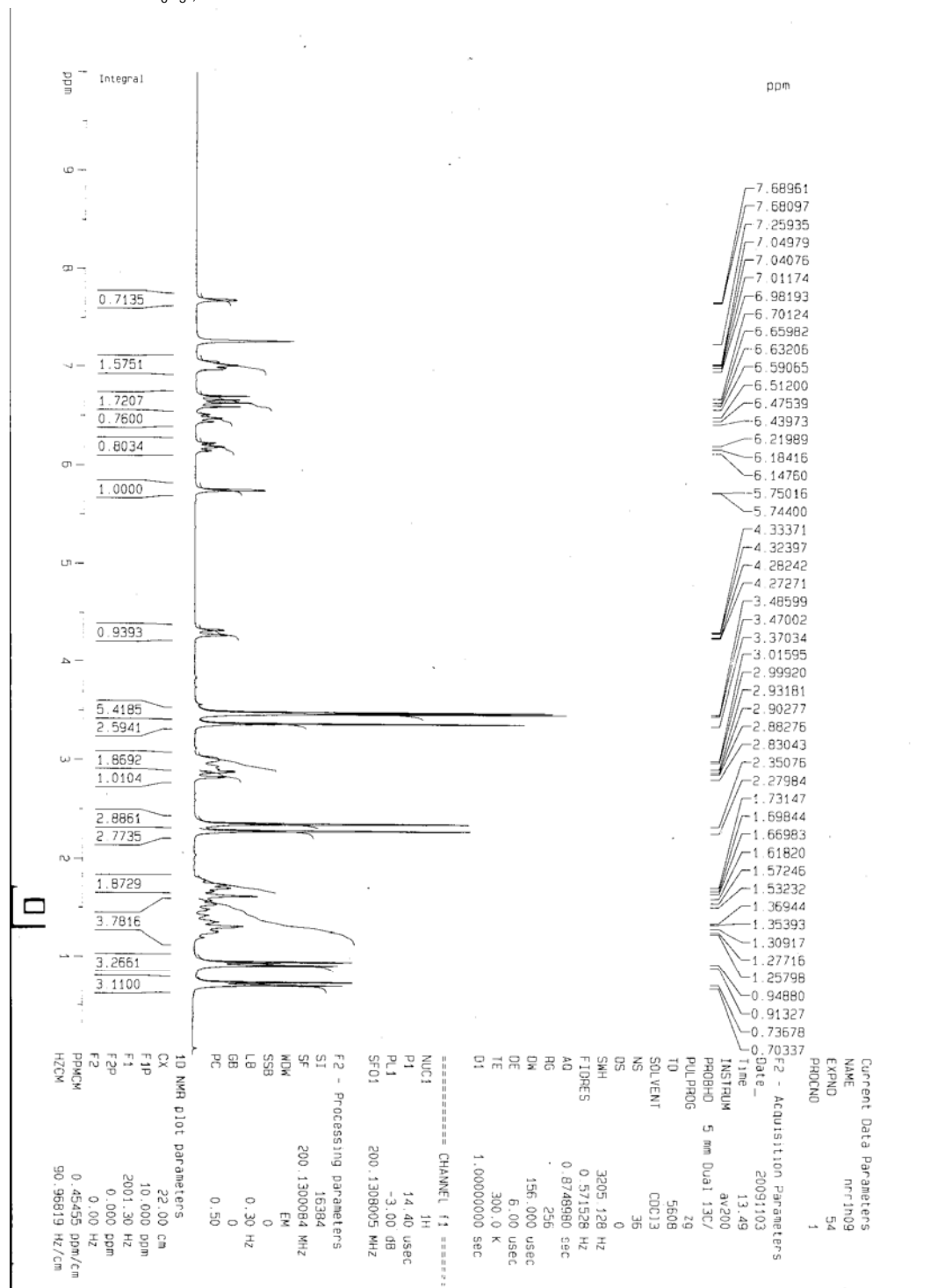
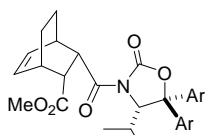


Figure-S12. ¹³C NMR spectrum of compound **6c**



Ar = 2-MeO-5-Me-C₆H₃;

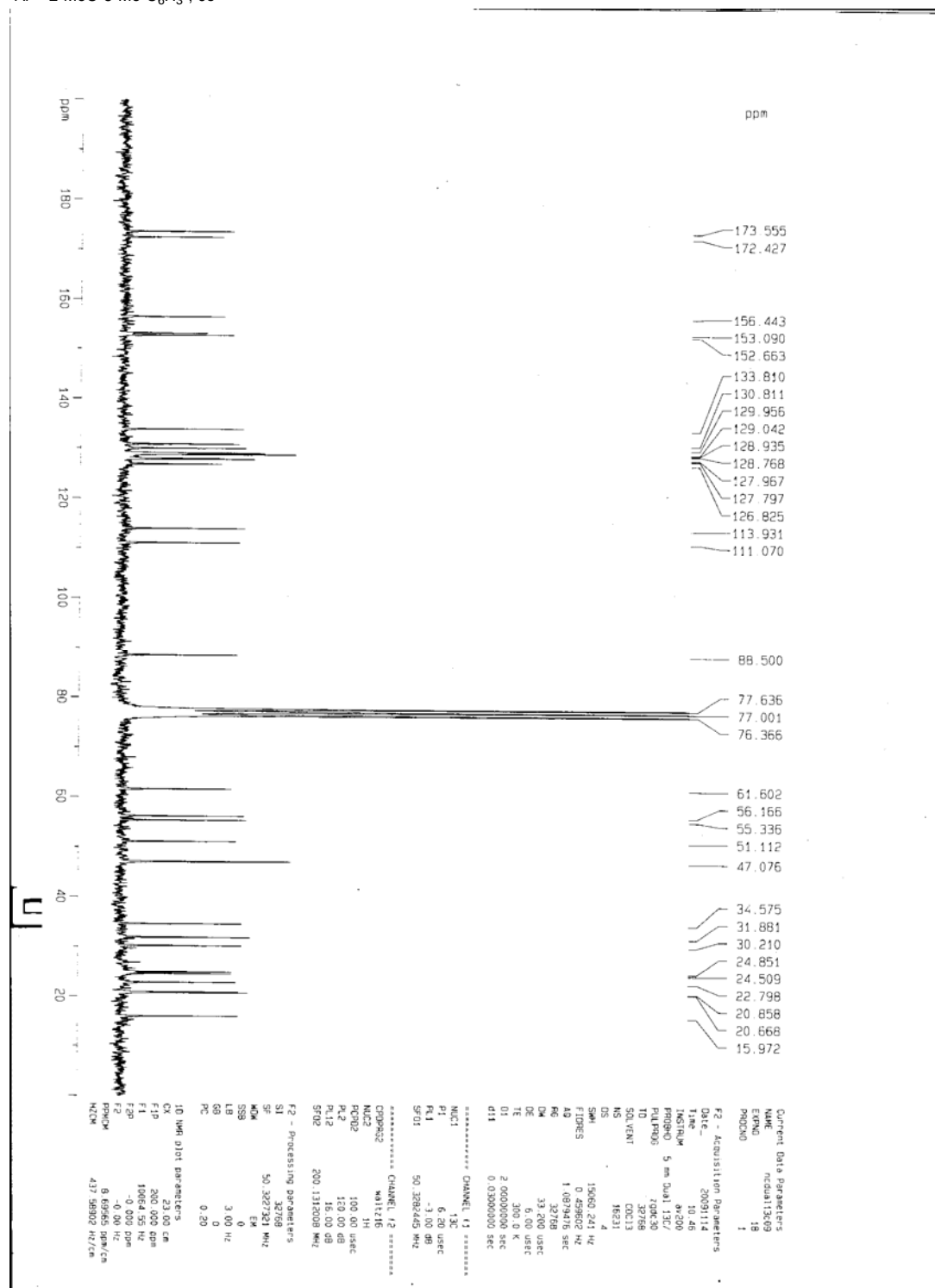
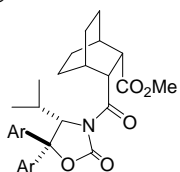


Figure-S13. ¹H NMR spectrum of compound **5d**



Ar = 2-MeO-5-Me-C₆H₃; **5d**

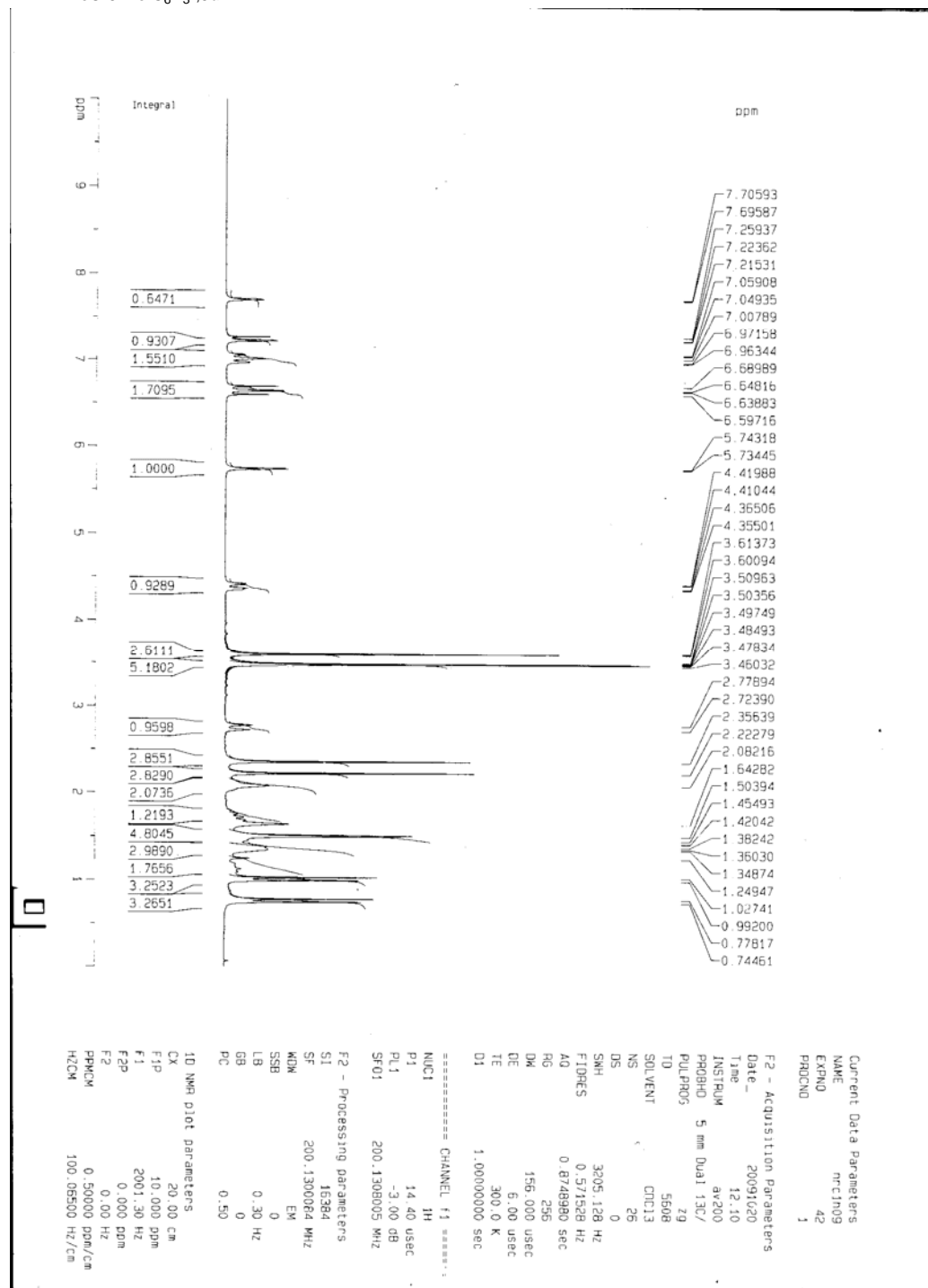
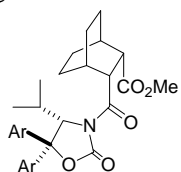


Figure-S14. ¹³C NMR spectrum of compound **5d**



Ar = 2-MeO-5-Me-C₆H₃; **5d**

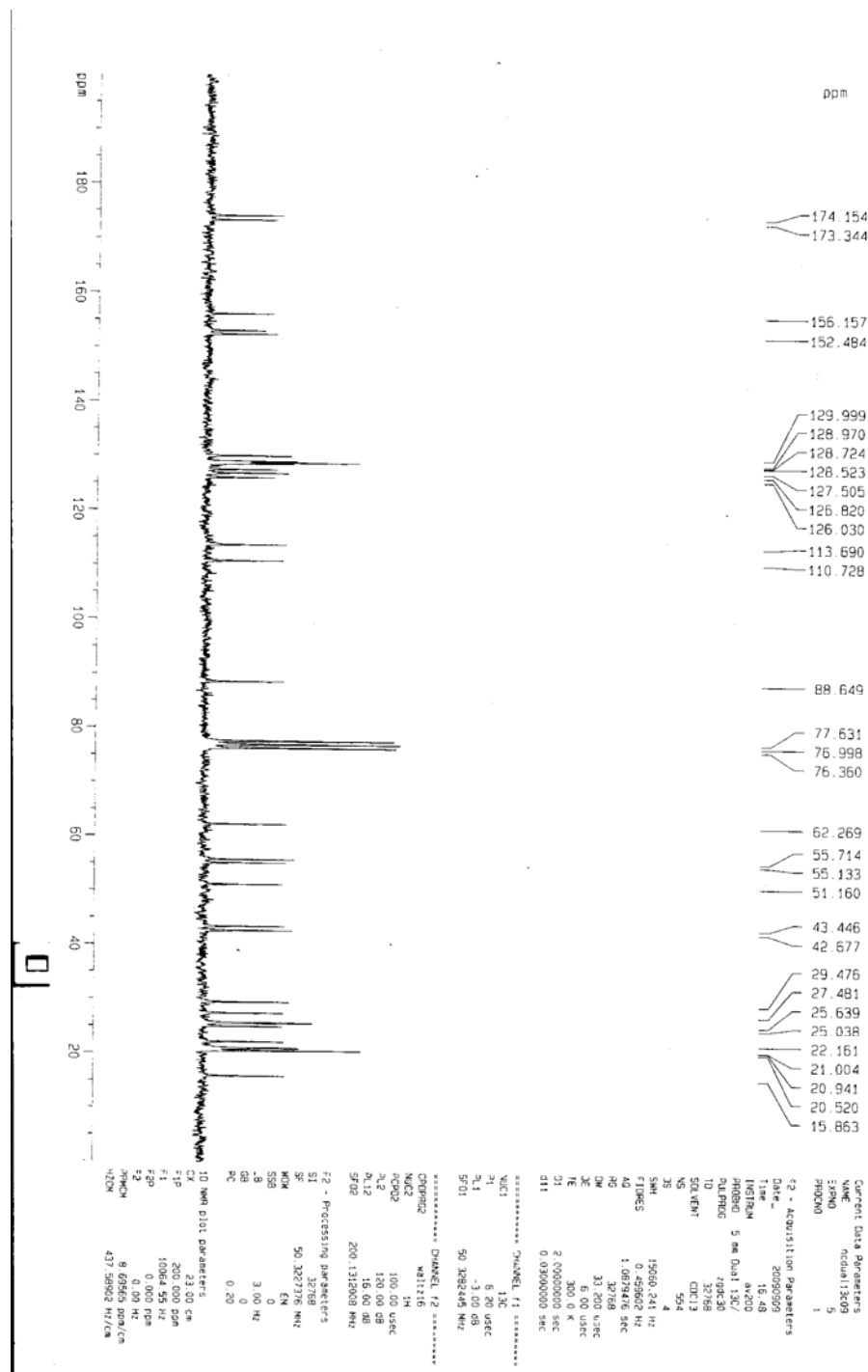
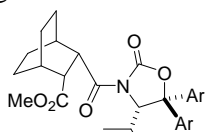
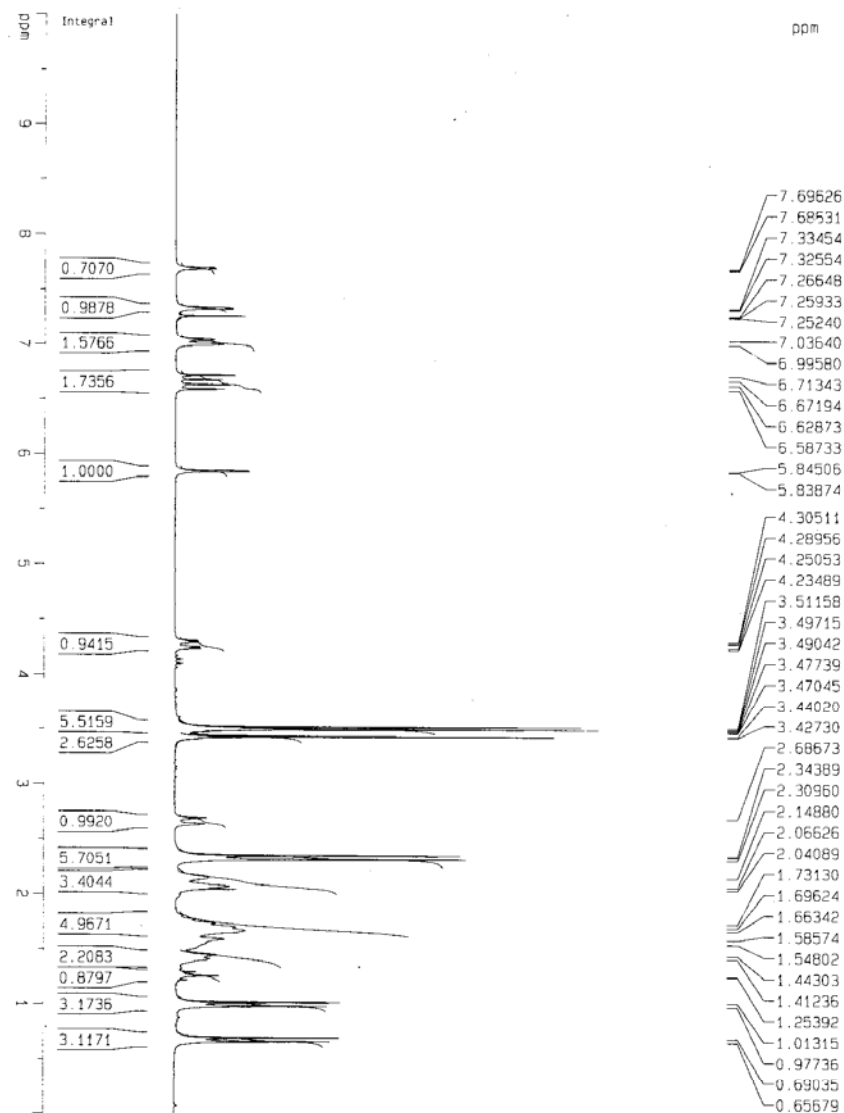


Figure-S15. ¹H NMR spectrum of compound **6d**



Ar = 2-MeO-5-Me-C₆H₃;



Current Data Parameters
 NAME nrc1h09
 EXPNO 47
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20091022
 Time 18.01
 INSTRUM av200
 PROBHD 5 mm Dual 13C/
 PULPROG zg
 TD 6608
 SOLVENT CDCl3
 NS 24
 DS 0
 SMH 3205.128 Hz
 FIDRES 0.571528 Hz
 AQ 0.8746980 sec
 RG 256
 DE 156.000 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.40 usec
 PL1 -3.00 dB
 SF01 200.1308005 MHz

F2 - Processing parameters
 SI 16384
 SF 200.1300084 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 0.50

1D NMR plot parameters
 CX 21.00 cm
 F1p 10.000 ppm
 F1 2001.30 Hz
 F2p -0.000 ppm
 F2 -0.00 Hz
 PPM/CM 0.47519 ppm/cm
 HZ/CM 95.30000 Hz/cm

Figure-S16. ¹³C NMR spectrum of compound **6d**

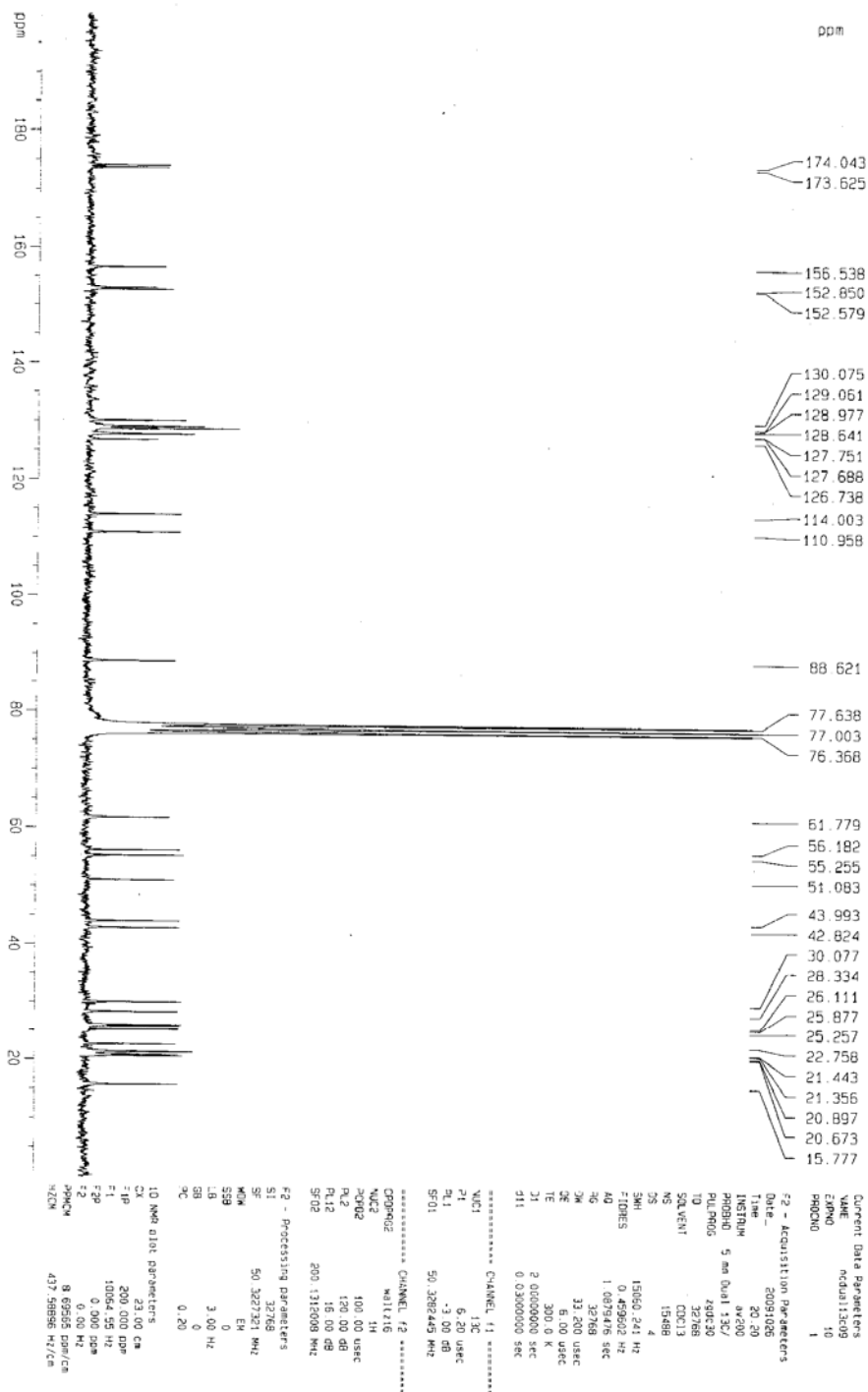
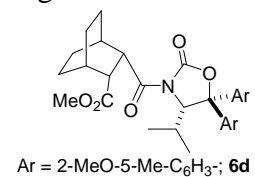


Figure-S17. ¹H NMR spectrum of compound **7a**

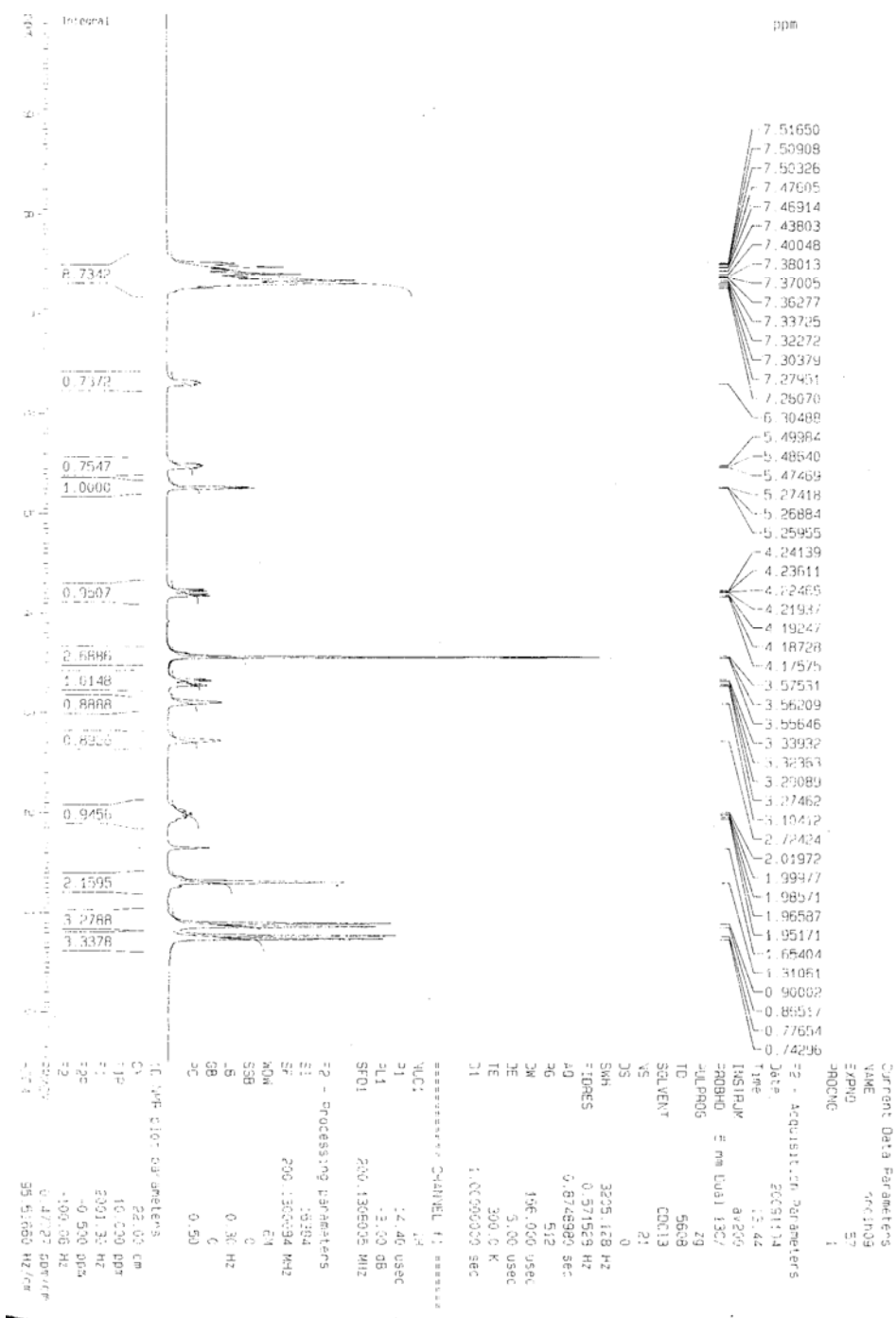
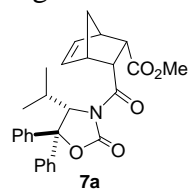


Figure-S18. ^{13}C NMR spectrum of compound **7a**

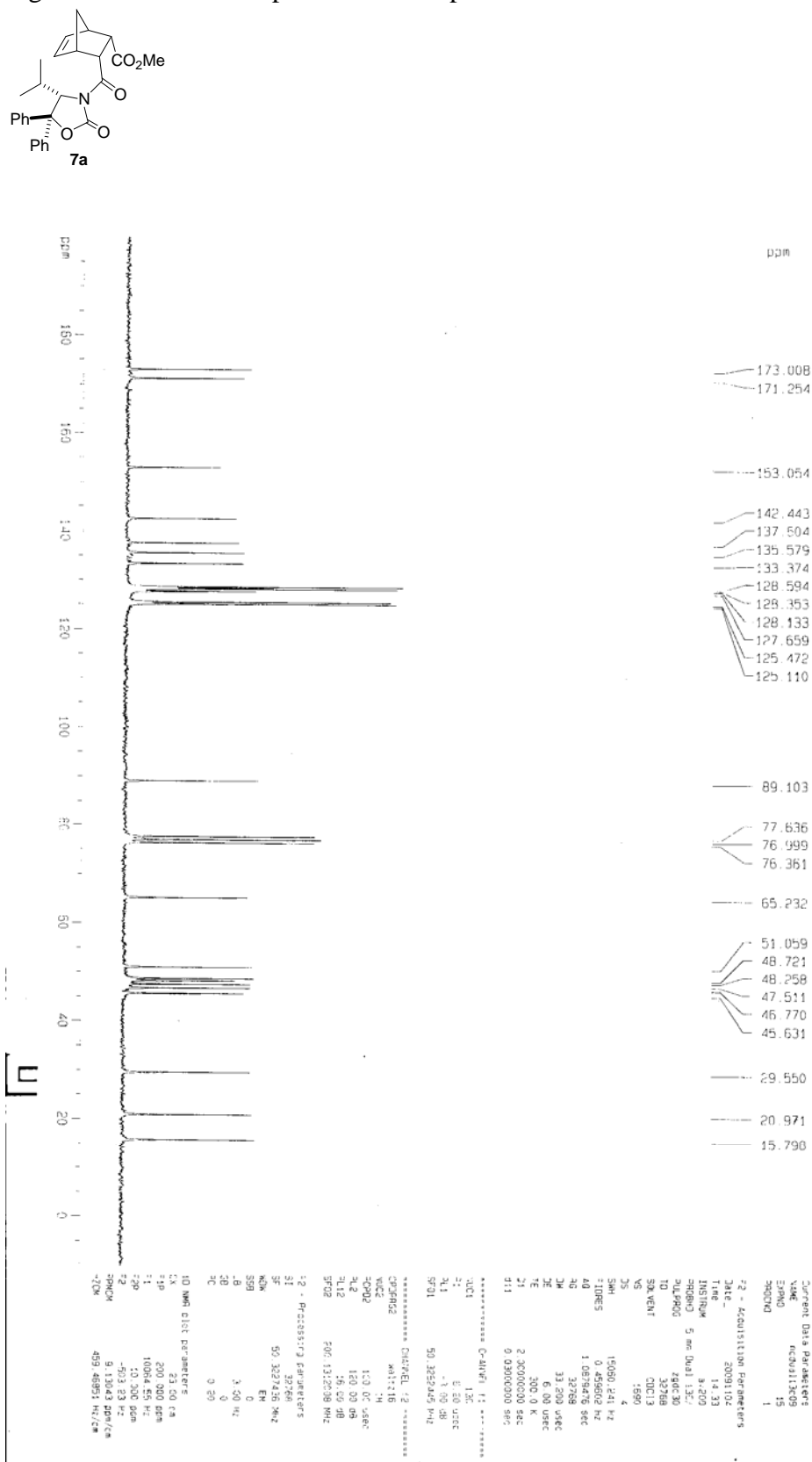


Figure-S19. ¹H NMR spectrum of compound **8a**

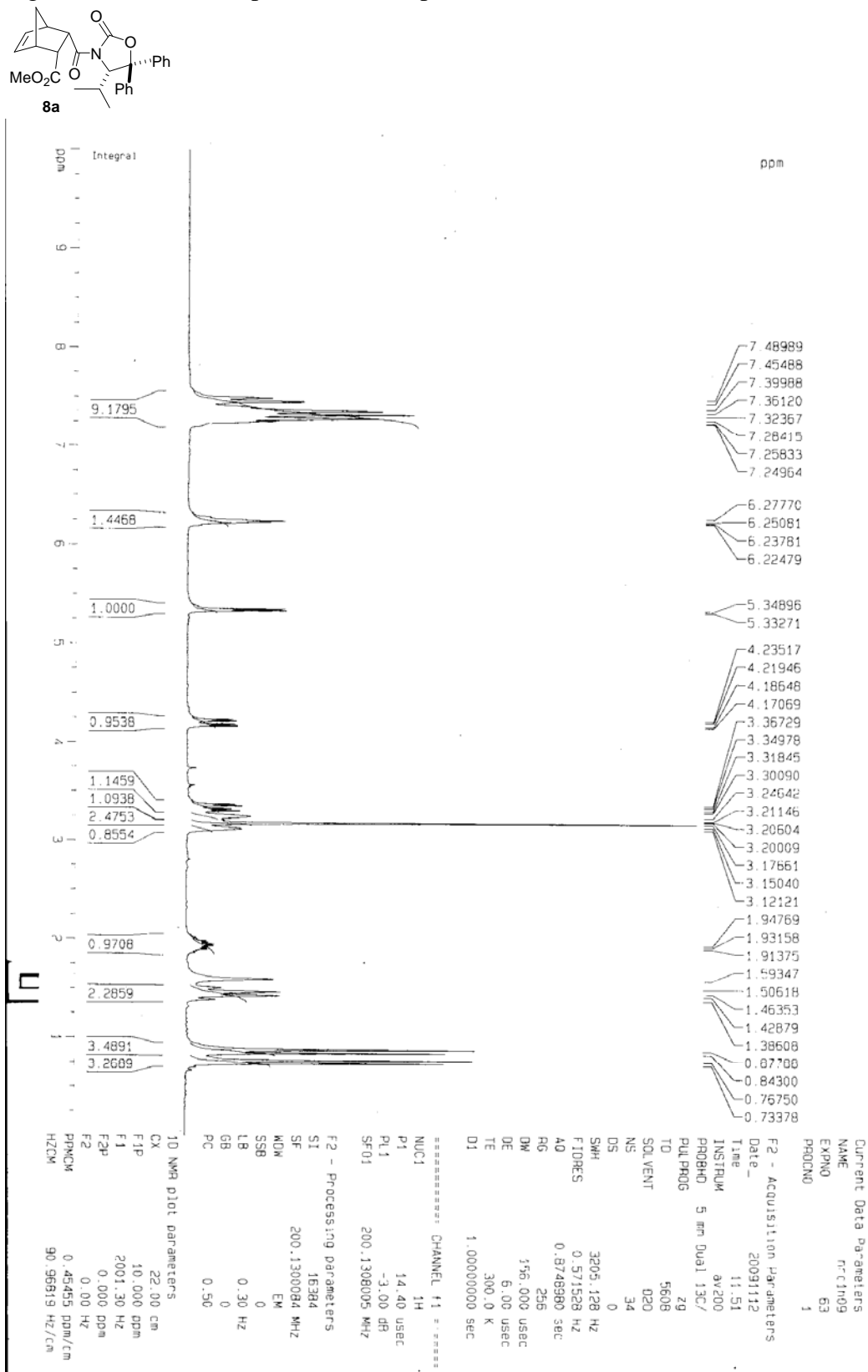


Figure-S20. ¹³C NMR spectrum of compound **8a**

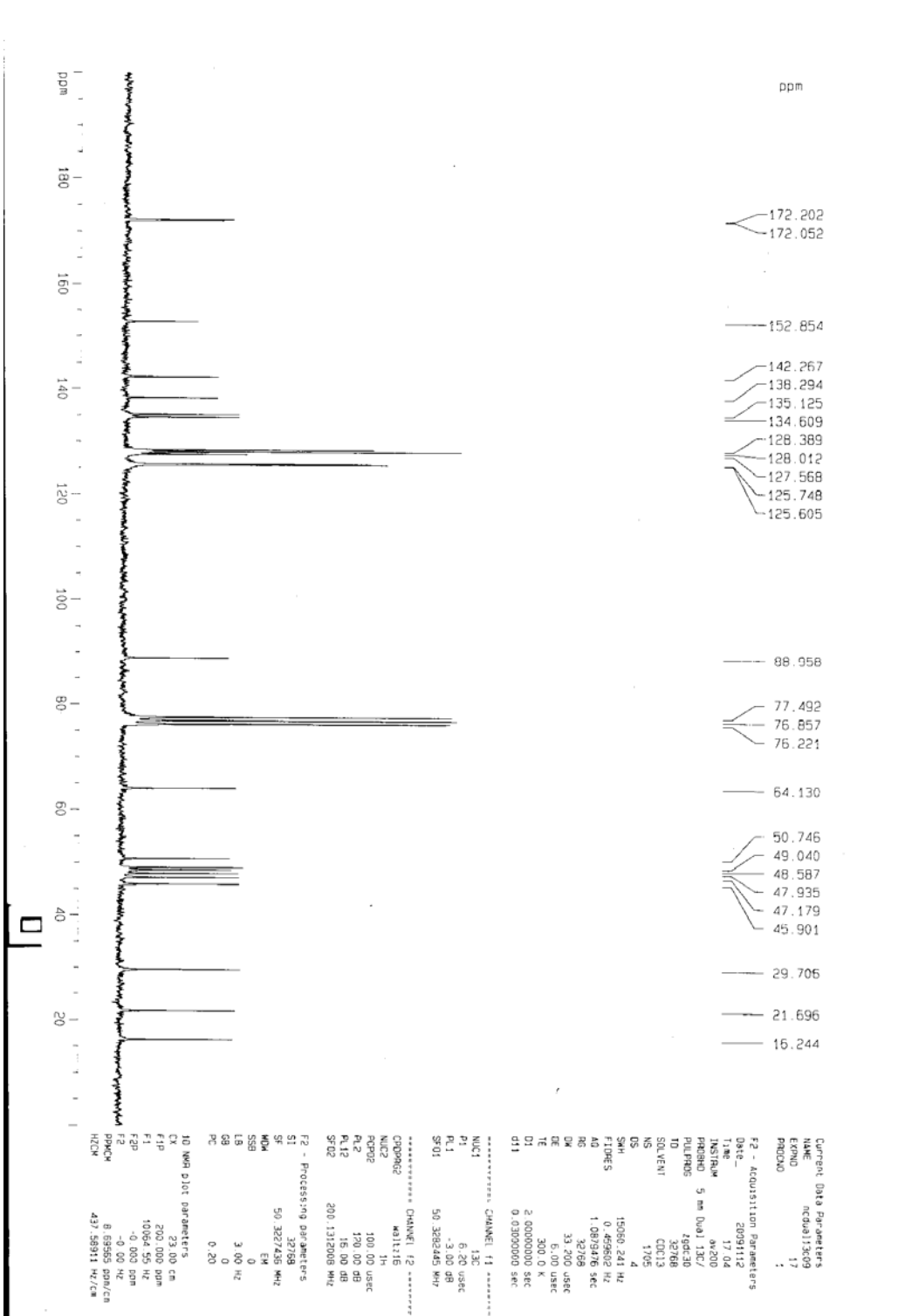
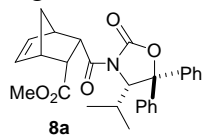


Figure-S21. ¹H NMR spectrum of compound 10a

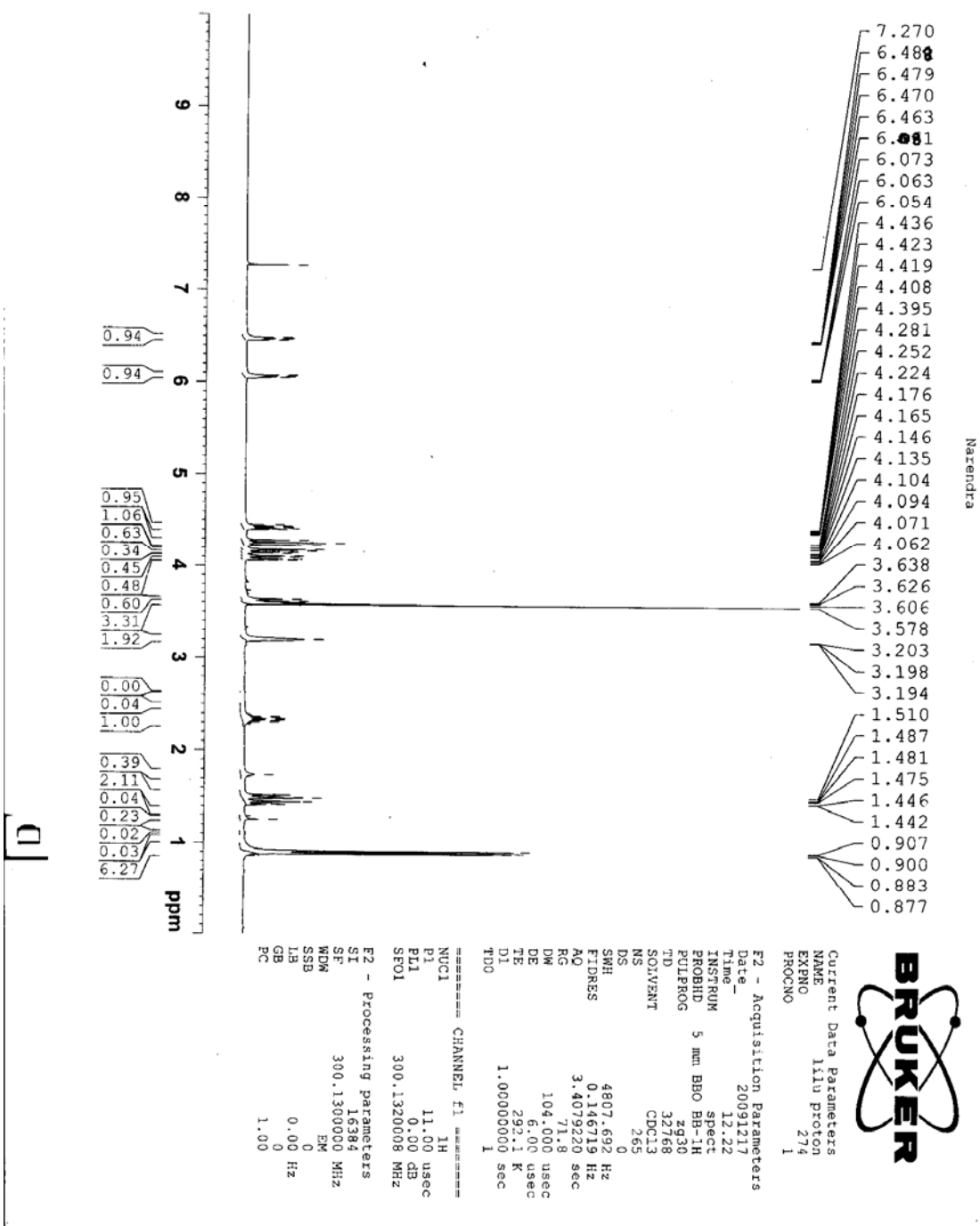
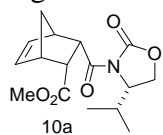


Figure-S22. ¹³C NMR spectrum of compound **10a**

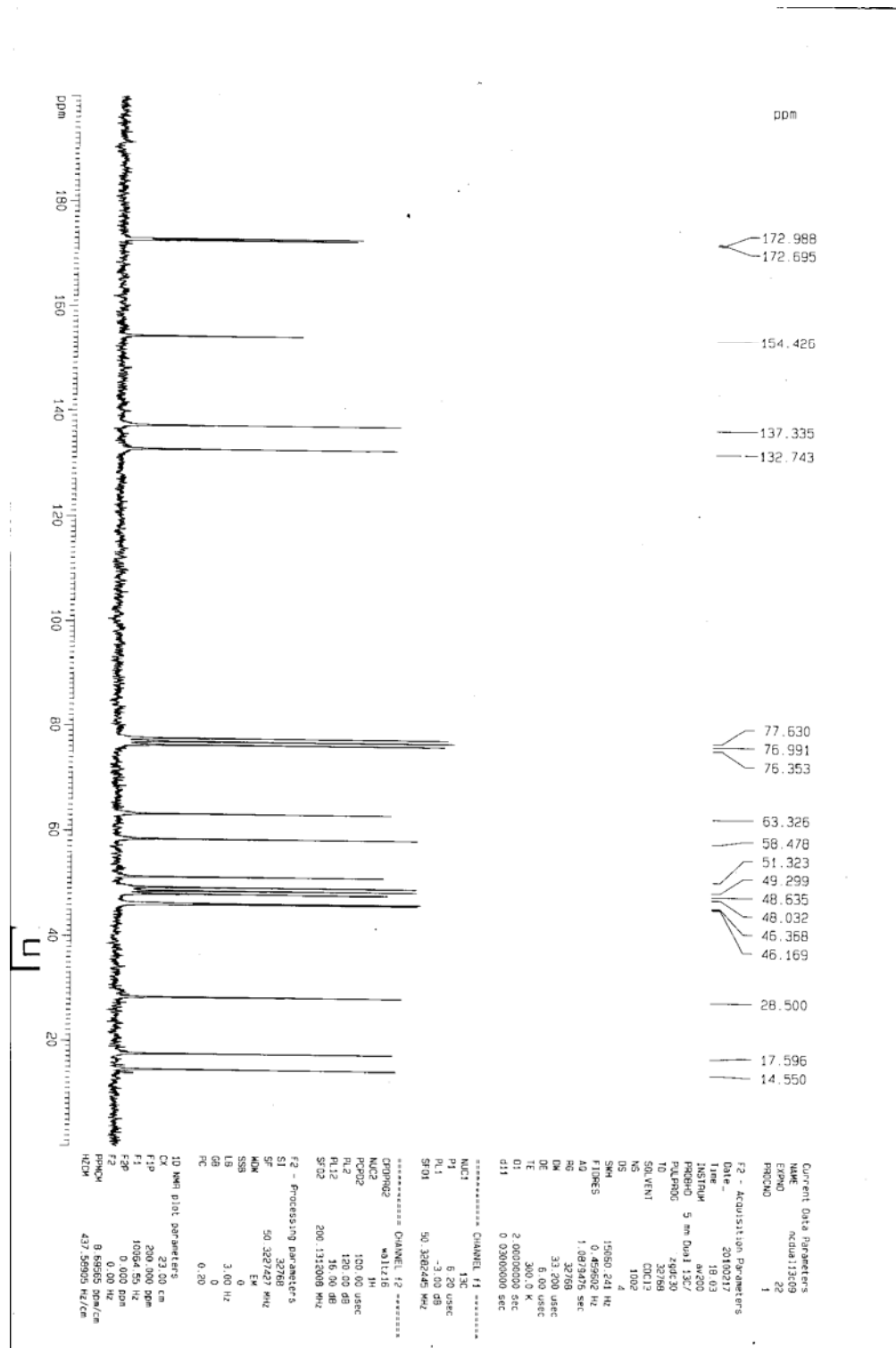
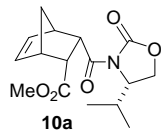


Figure-S23. ¹H NMR spectrum of compound **11a**

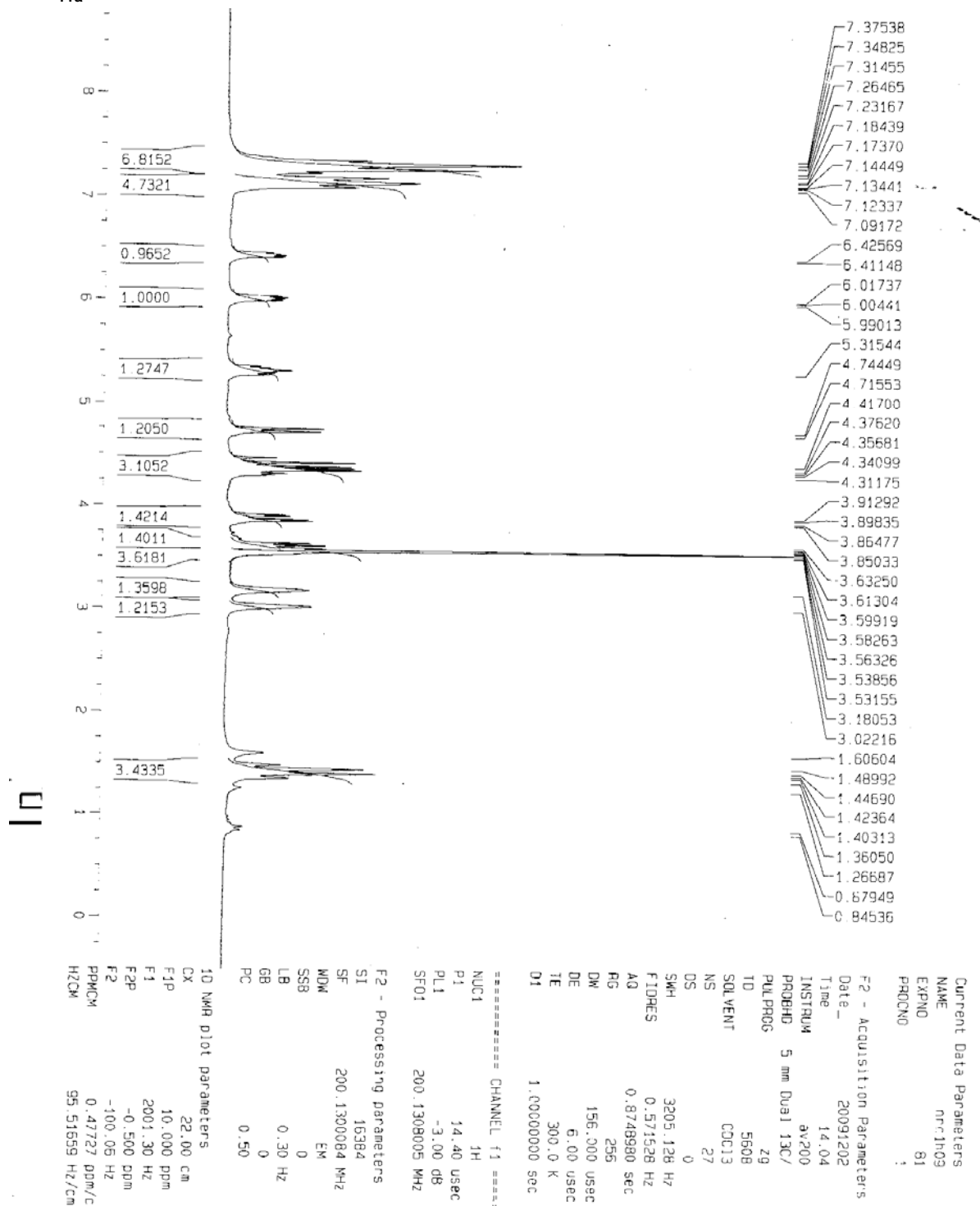
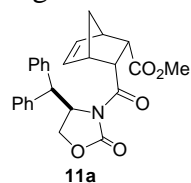


Figure-S24. ¹³C NMR spectrum of compound **11a**

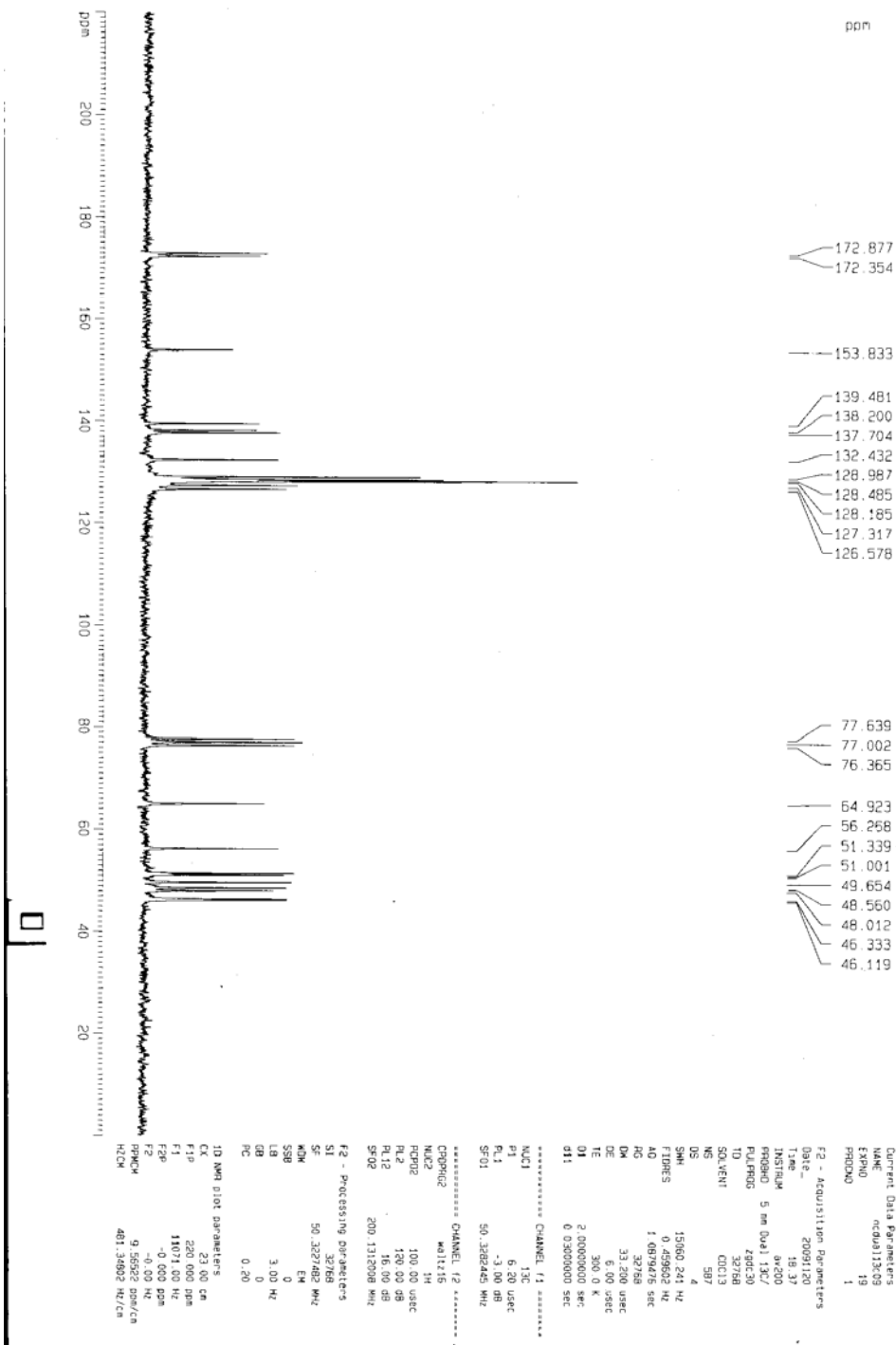
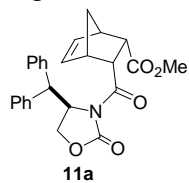


Figure-S25. ¹H NMR spectrum of compound **11b**

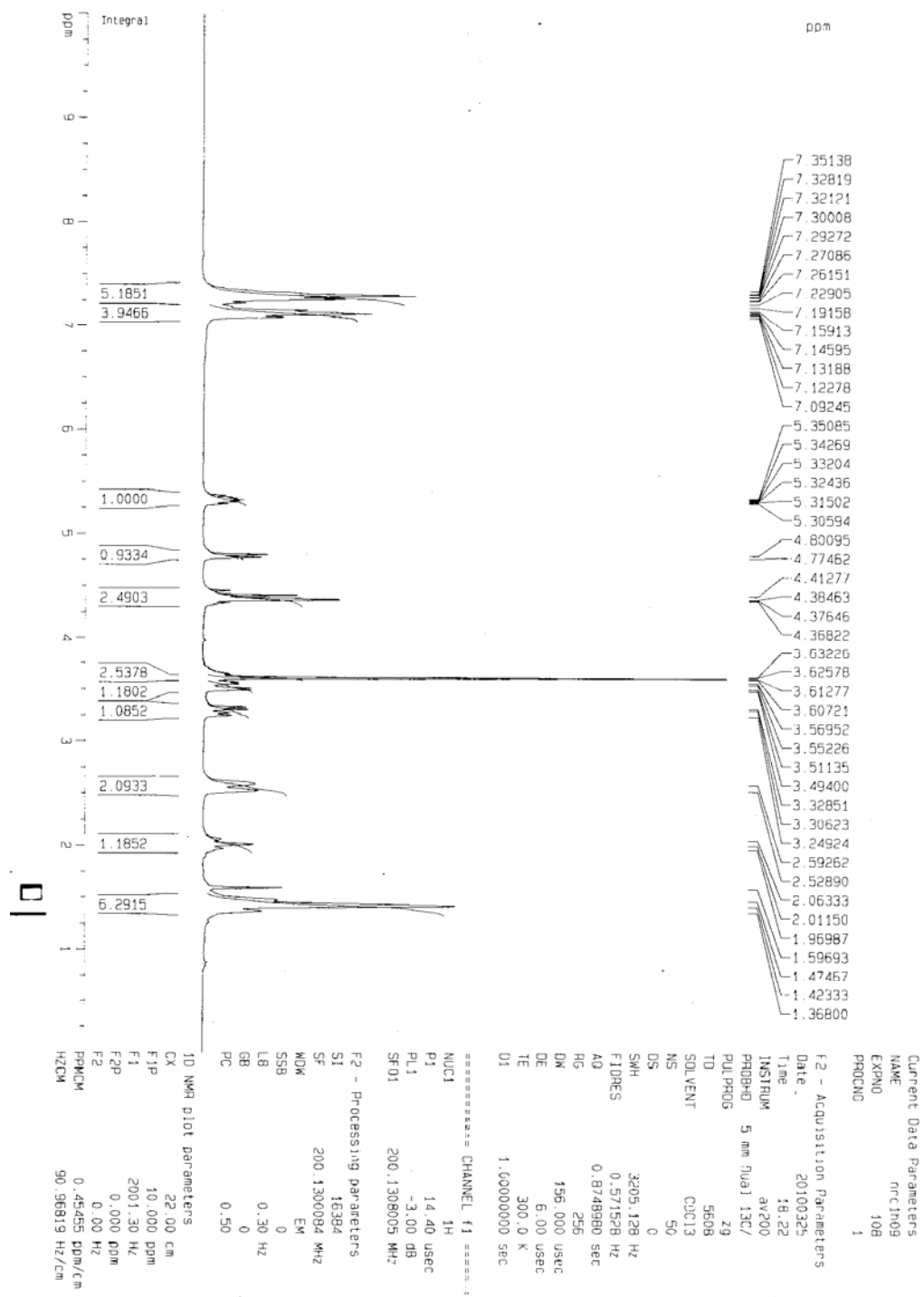
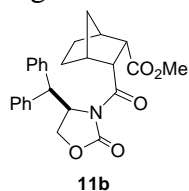


Figure-S26. ¹³C NMR spectrum of compound **11b**

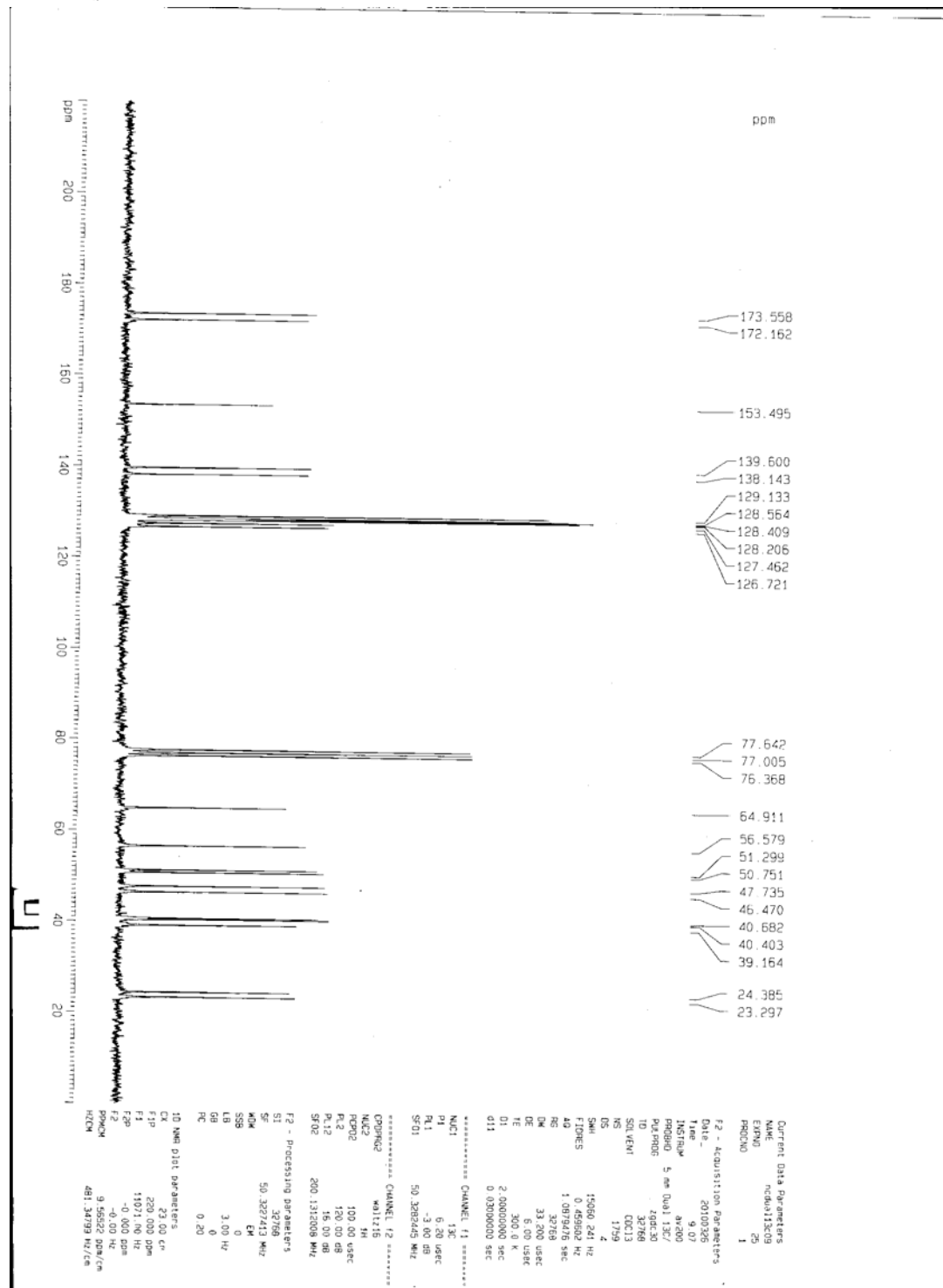
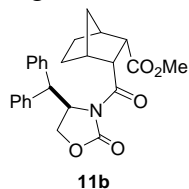


Figure-S27. ¹H NMR spectrum of compound **12b**

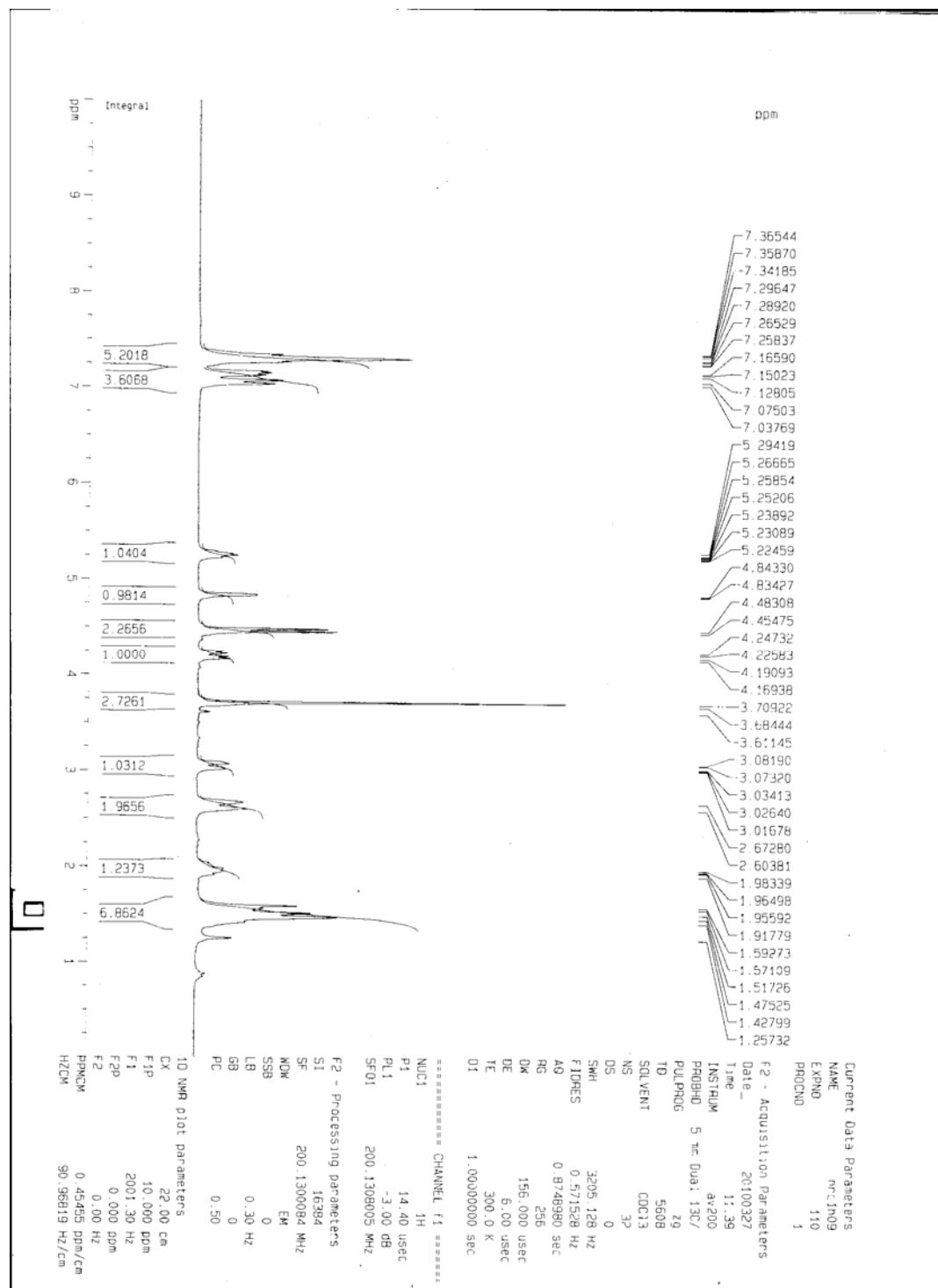
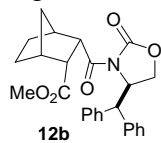


Figure-S28. ¹³C NMR spectrum of compound **12b**

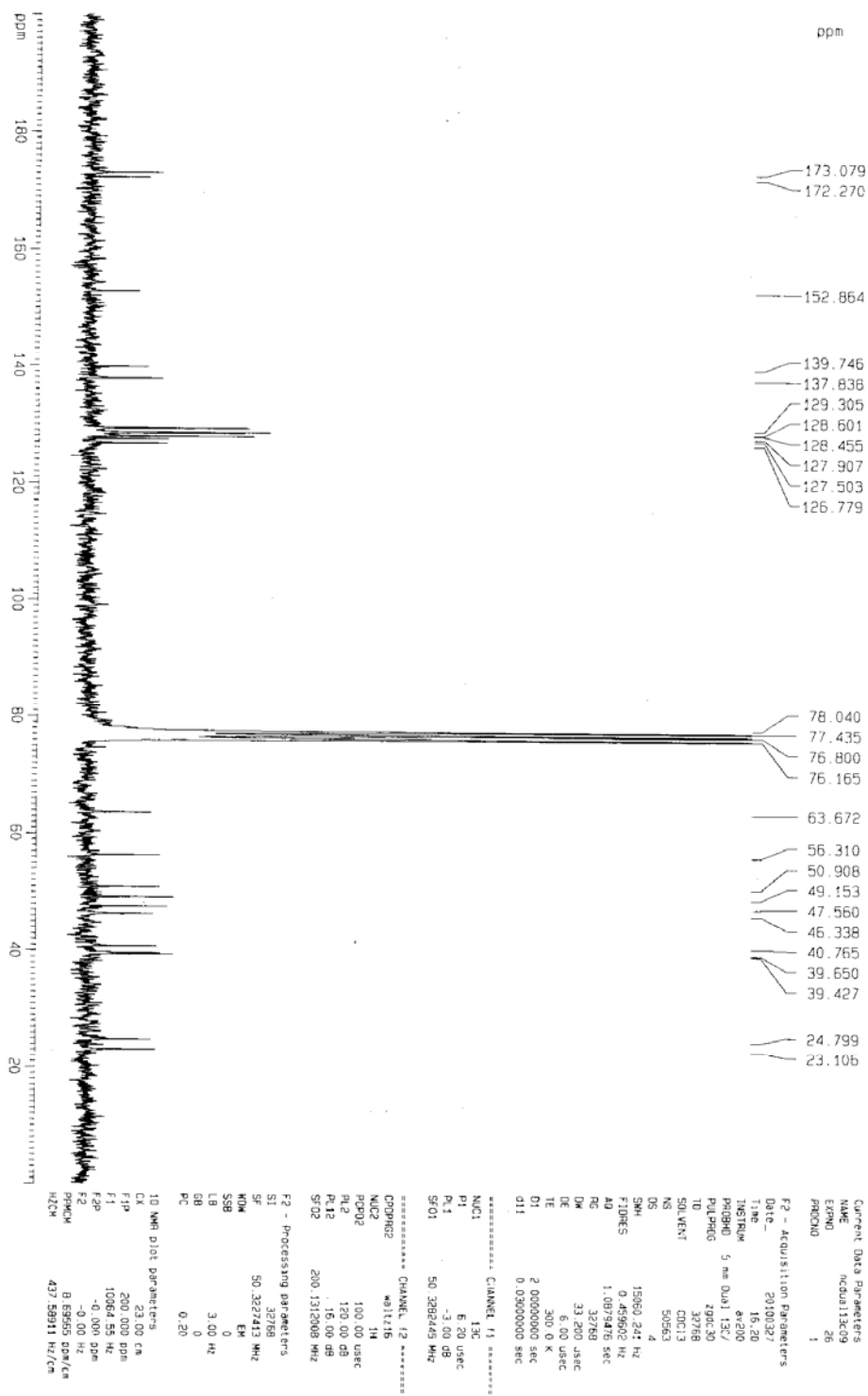
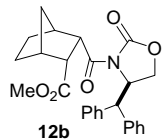


Figure-S29. ¹H NMR spectrum of compound **11c**

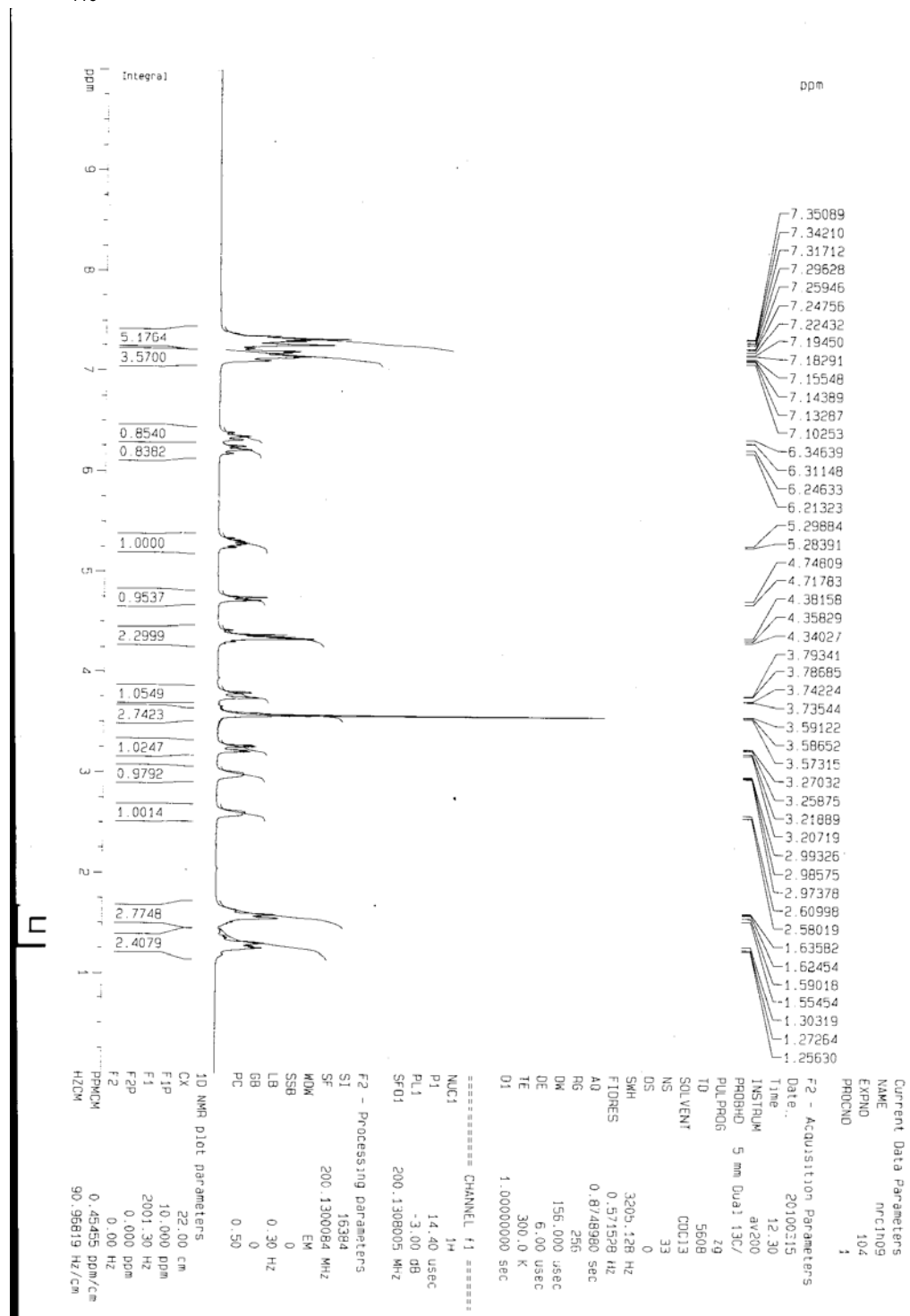
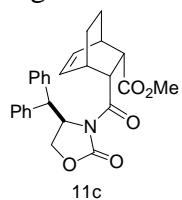


Figure-S30. ¹³C NMR spectrum of compound **11c**

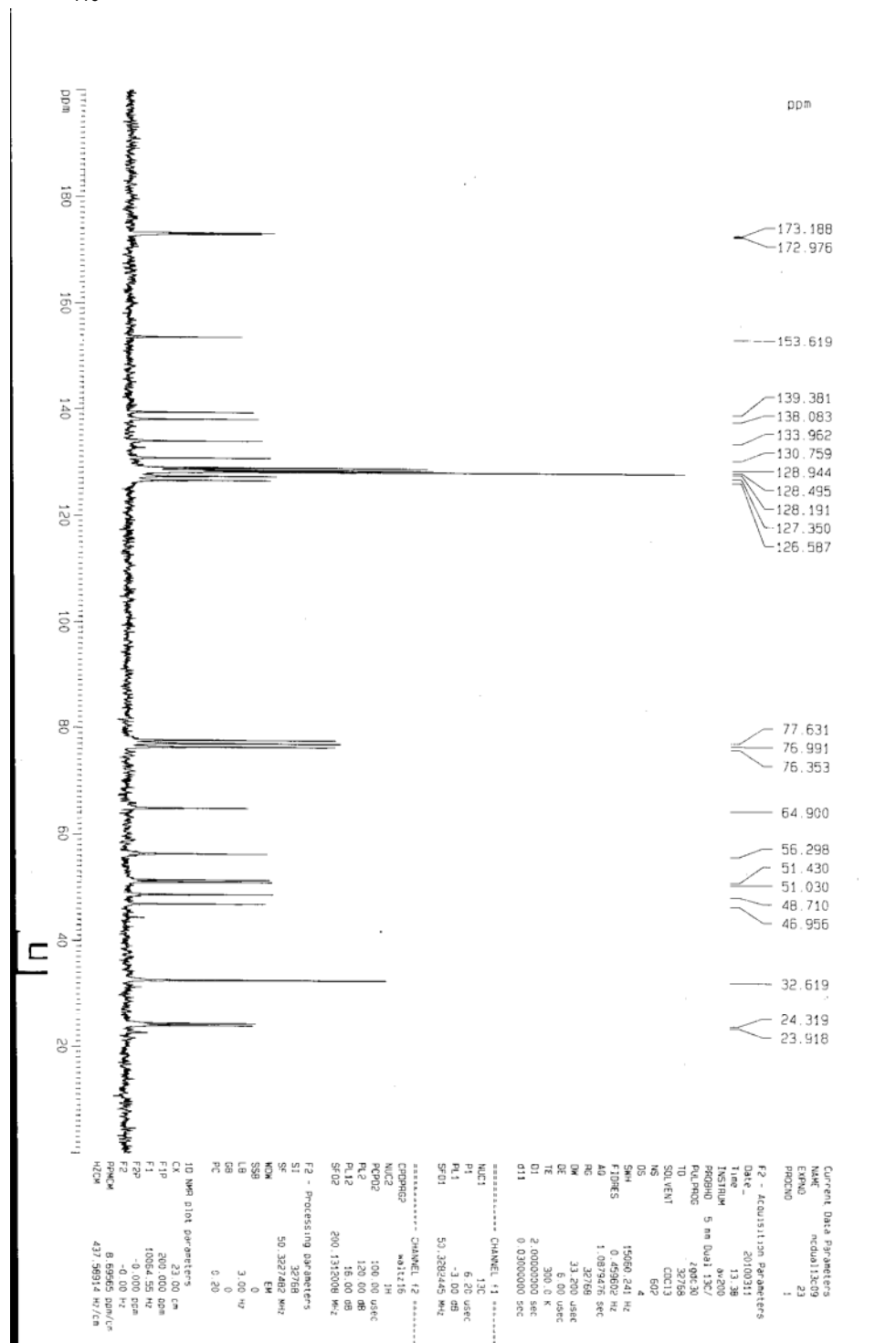
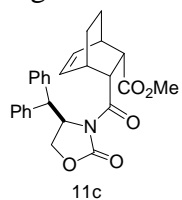


Figure-S31. ¹H NMR spectrum of compound **12c**

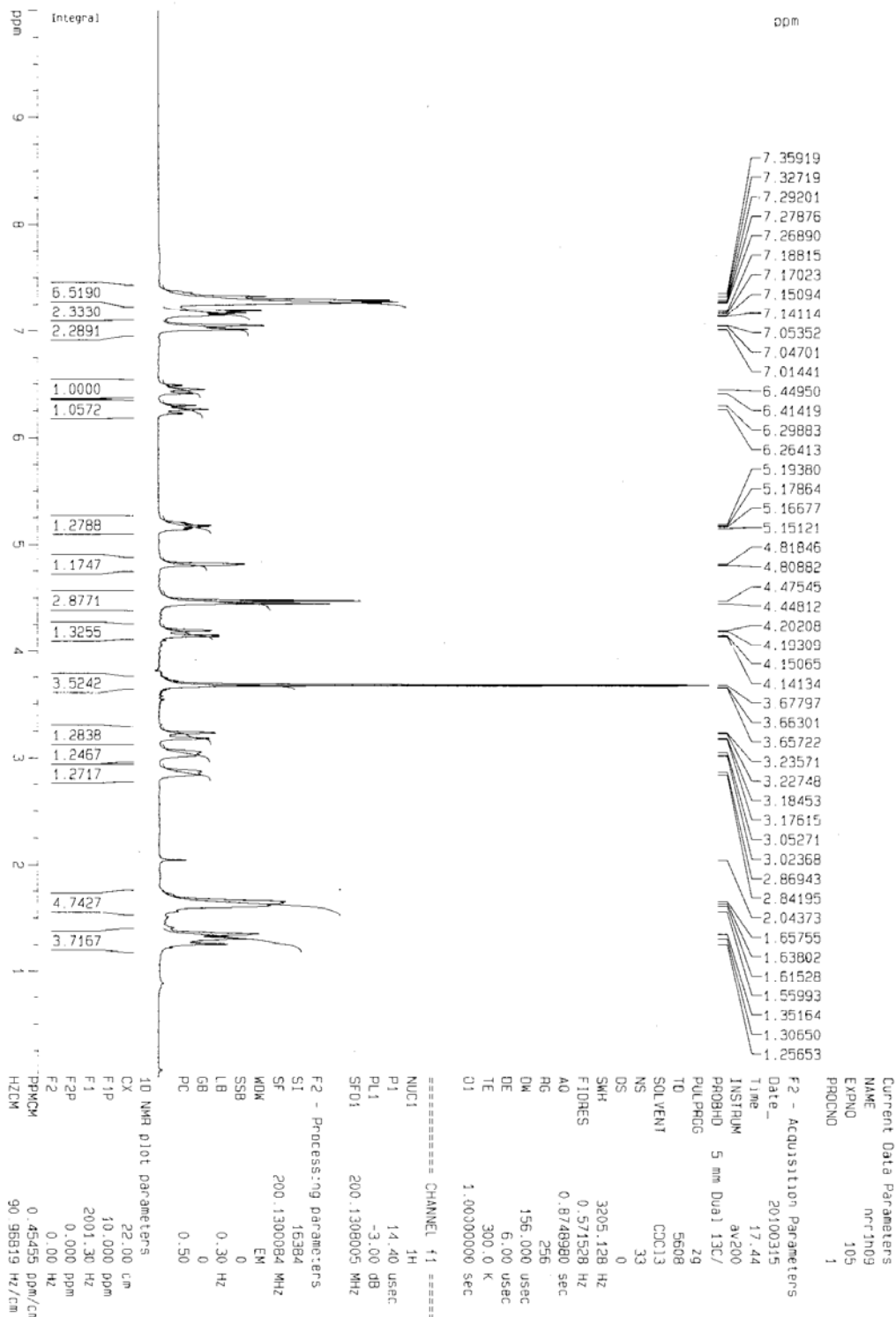
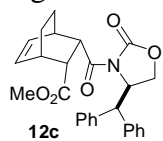


Figure-S32. ¹³C NMR spectrum of compound **12c**

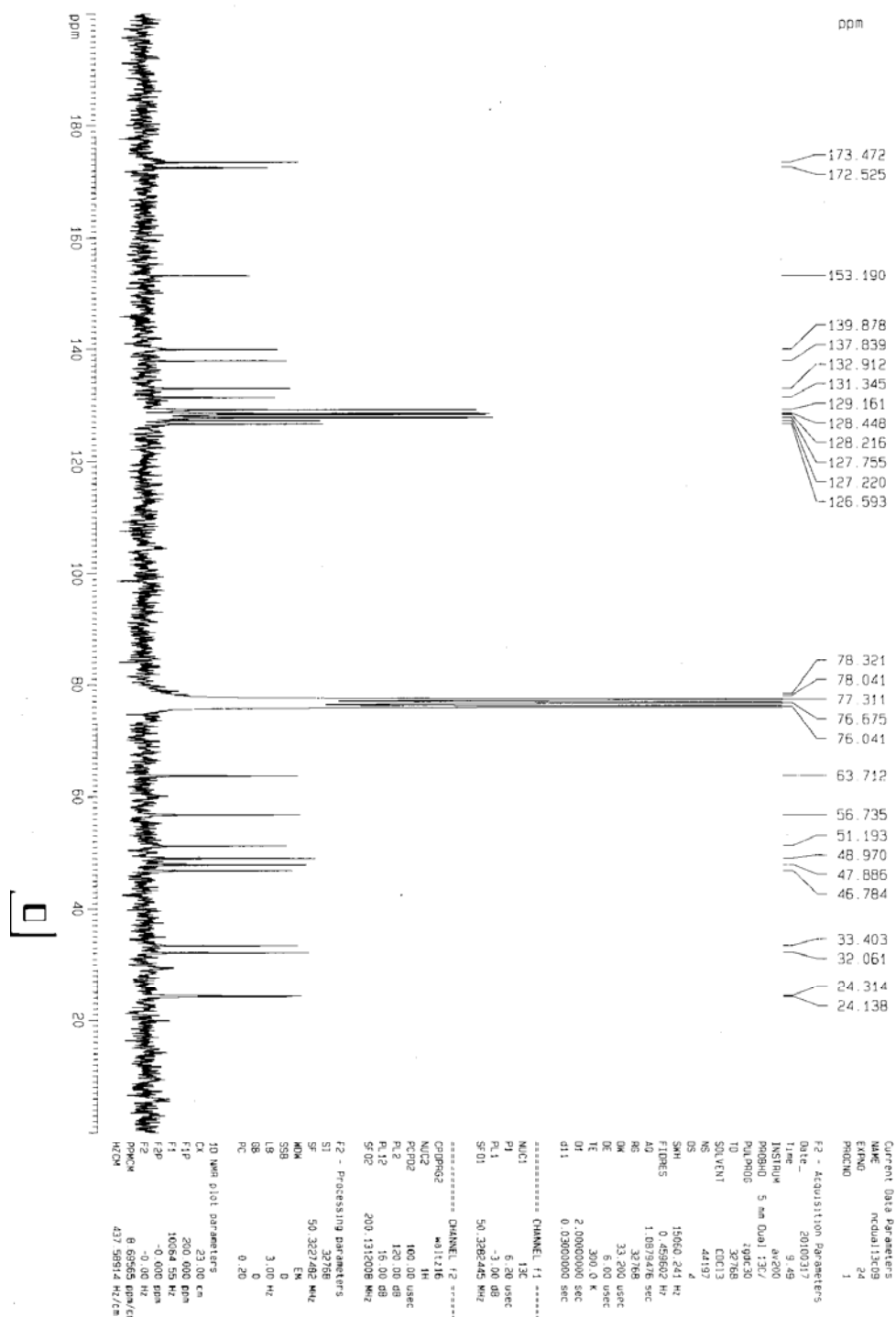
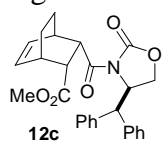


Figure-S33. ¹H NMR spectrum of compound **11d**

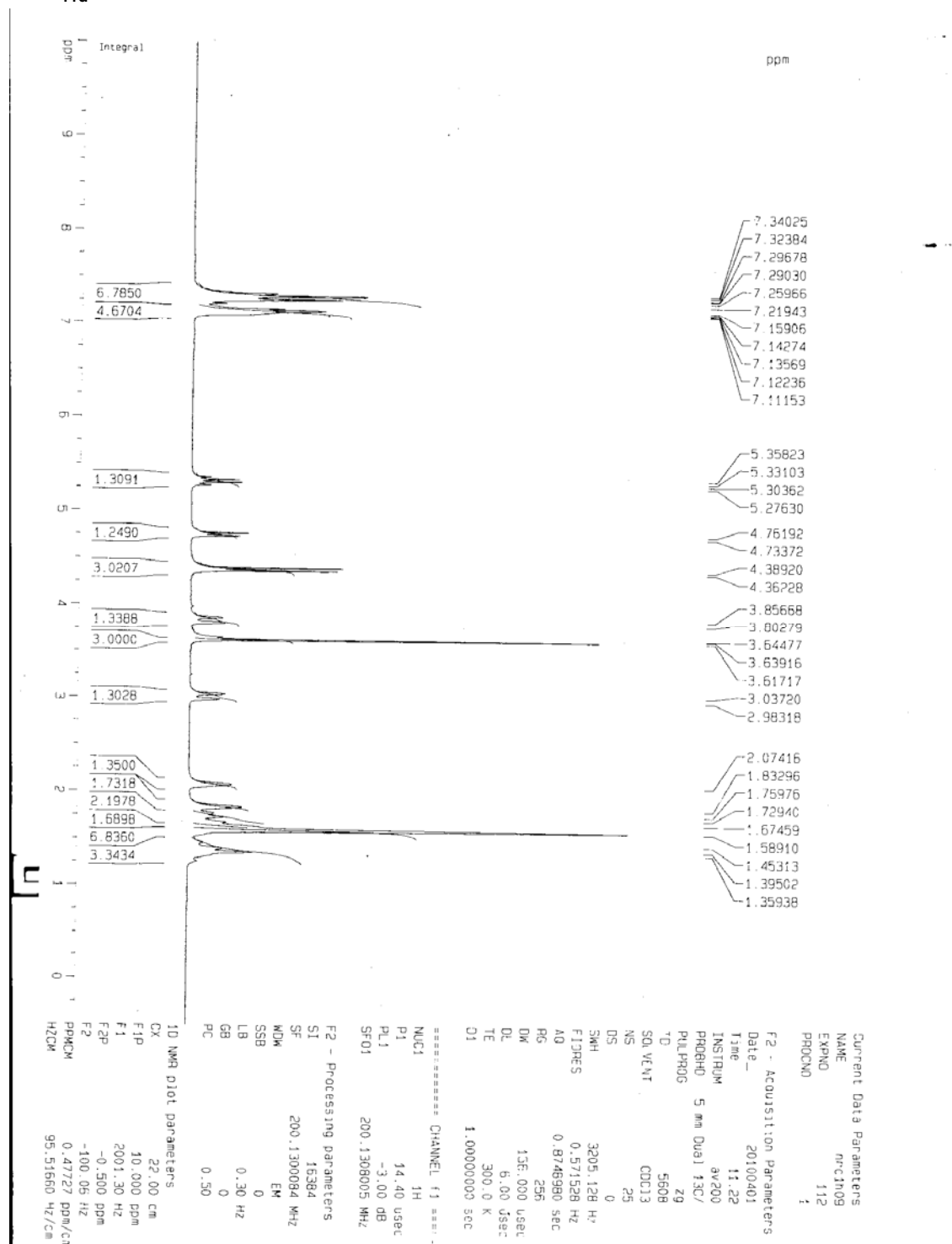
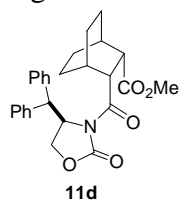


Figure-S34. ¹³C NMR spectrum of compound **11d**

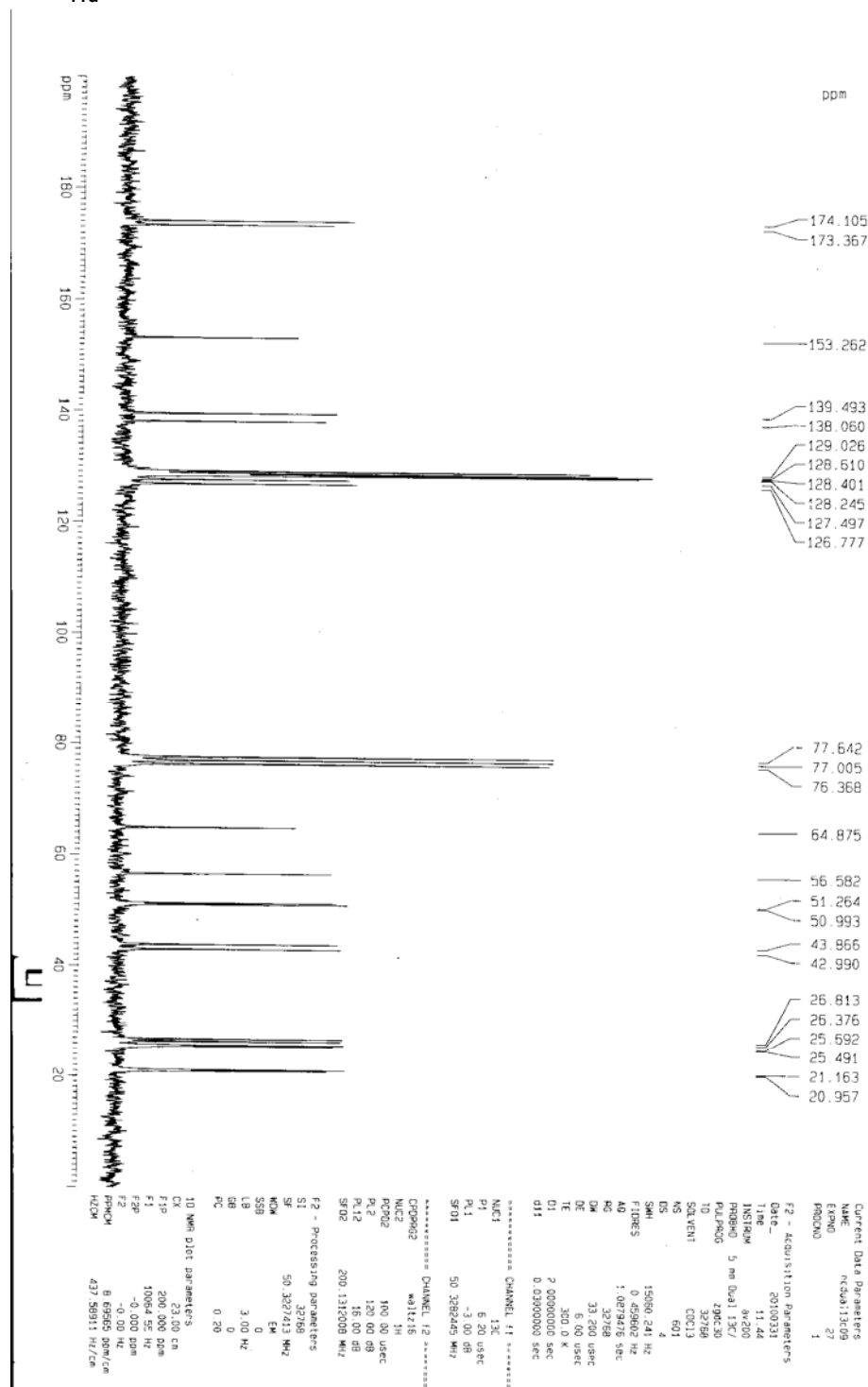
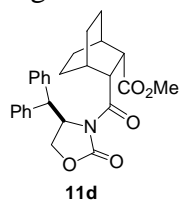


Figure-S35. ^1H NMR (500 MHz) spectrum of compound **12d**

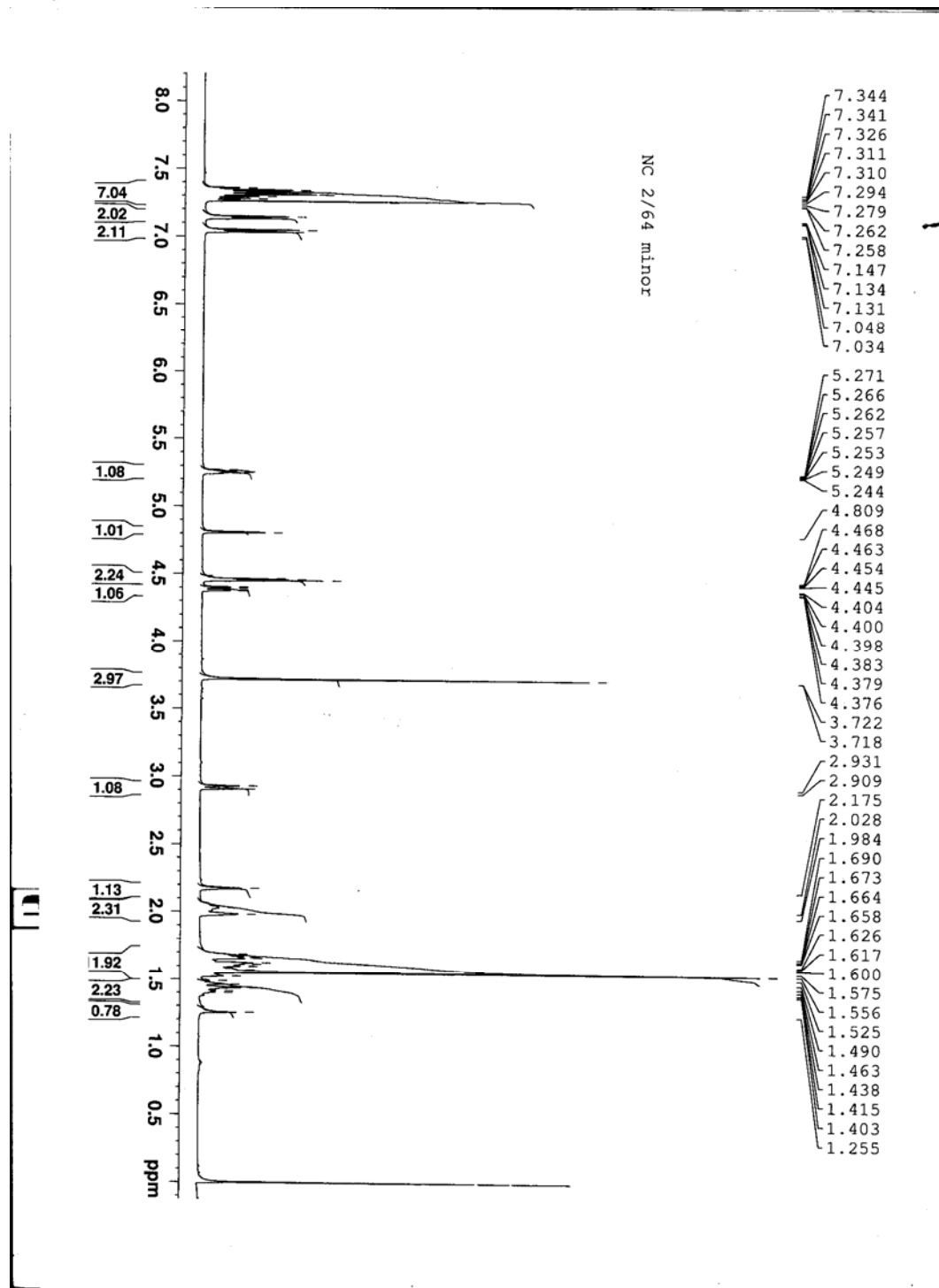
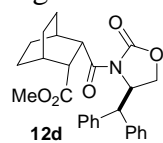


Figure-S36. ^{13}C NMR (125 MHz) spectrum of compound **12d**

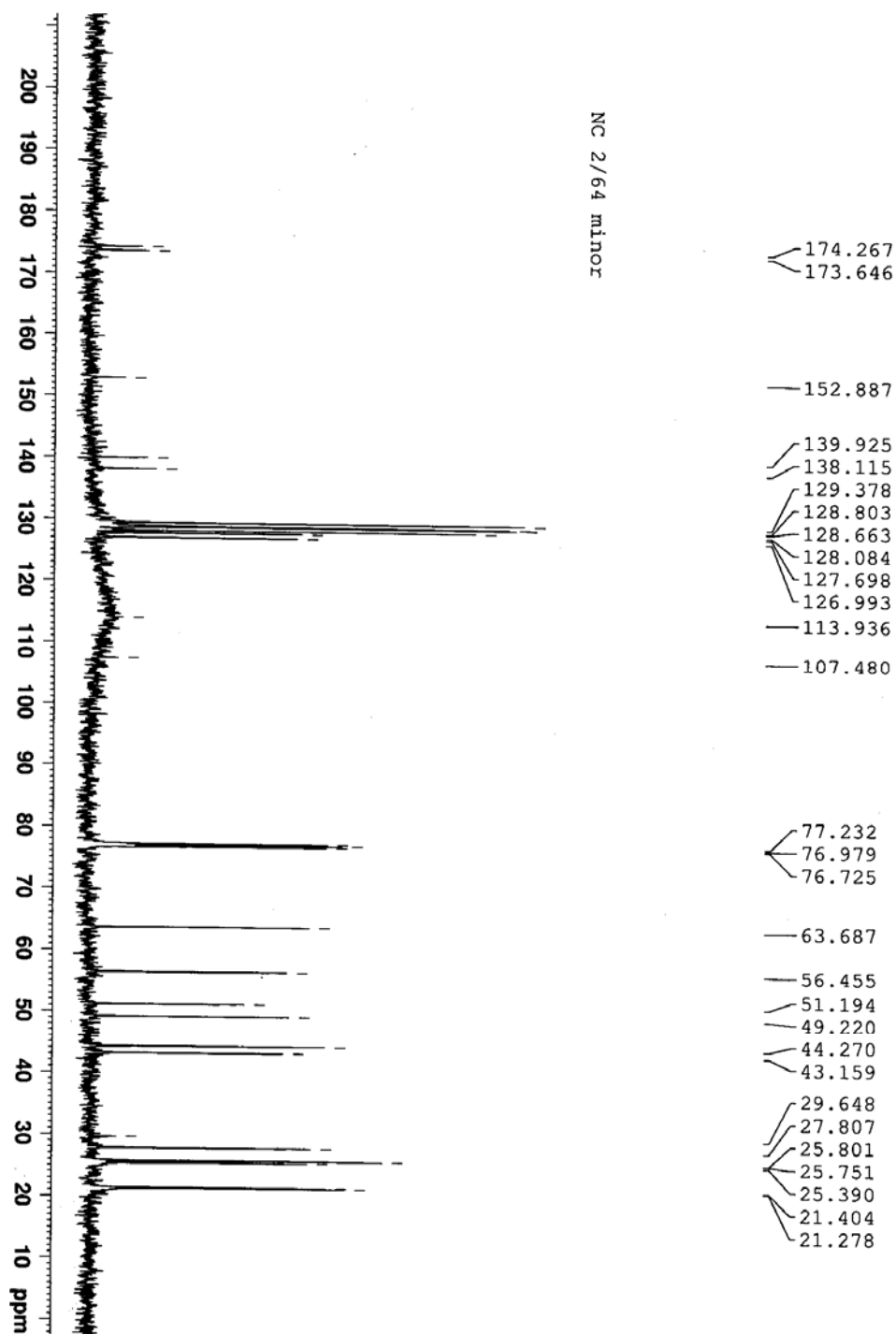
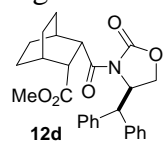


Figure-S37. ^1H NMR (500 MHz) spectrum of compound **11e**

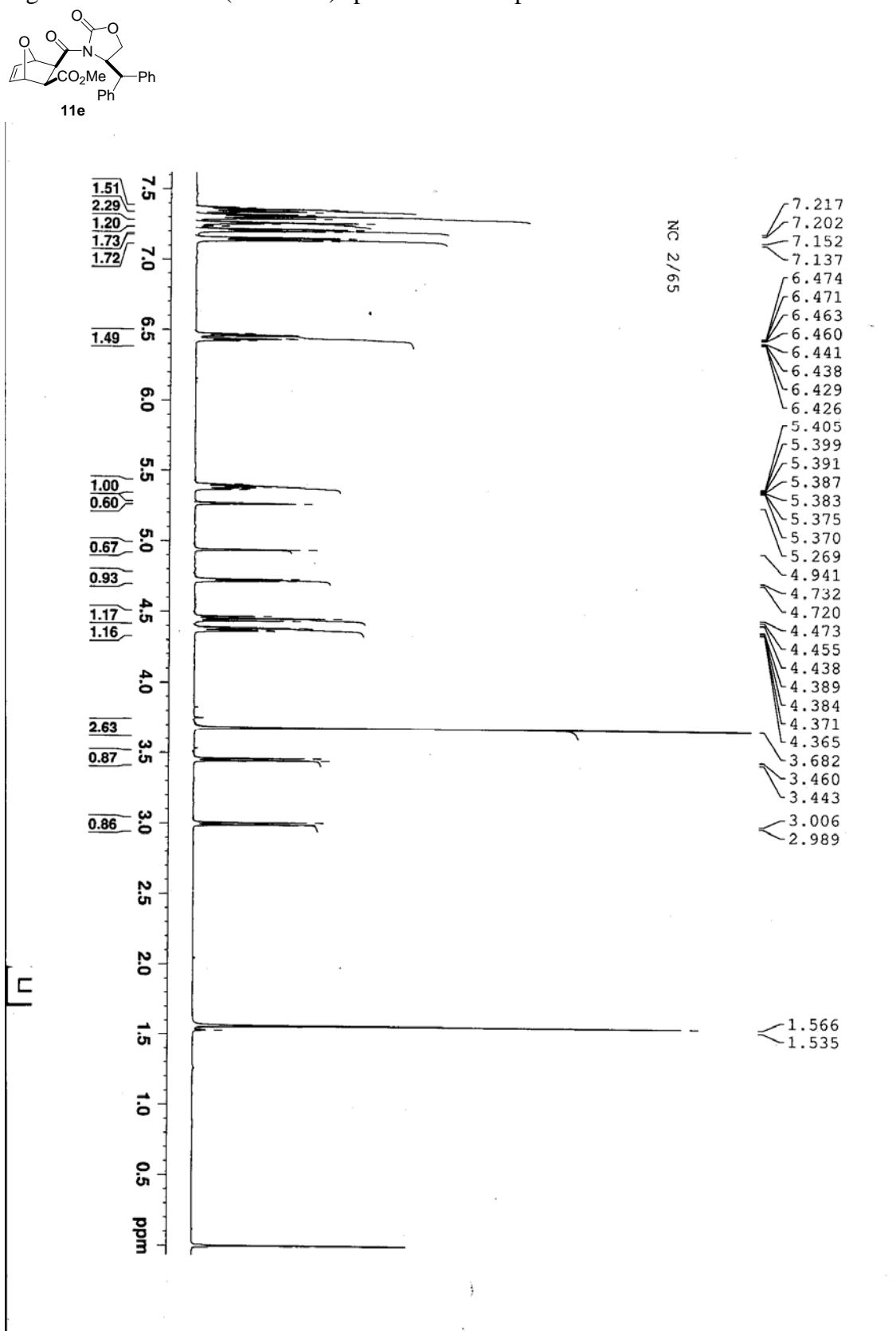


Figure-S38. ^{13}C NMR spectrum of compound **11e**

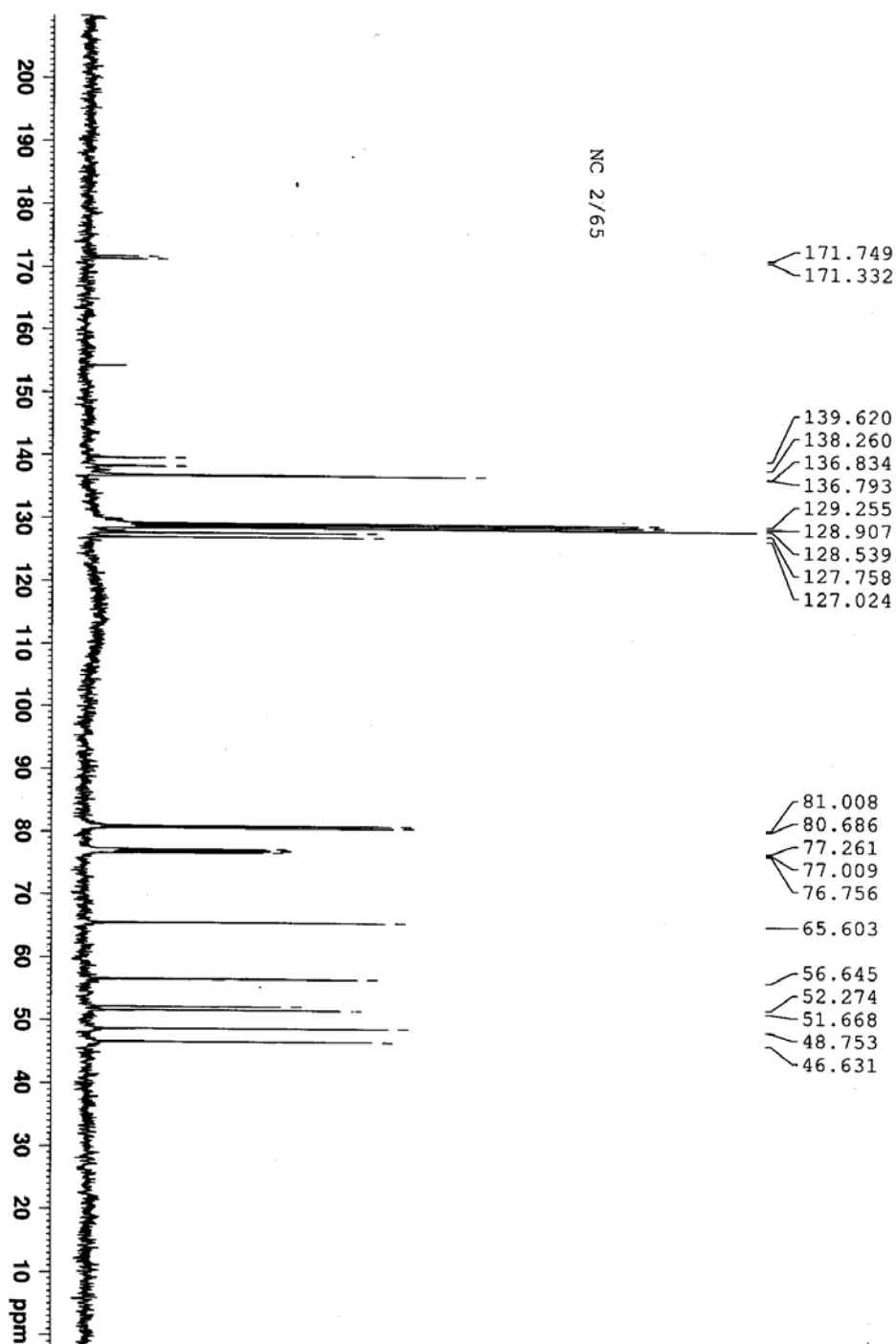
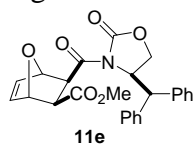


Figure-S39. ¹H NMR spectrum of compound **11f**

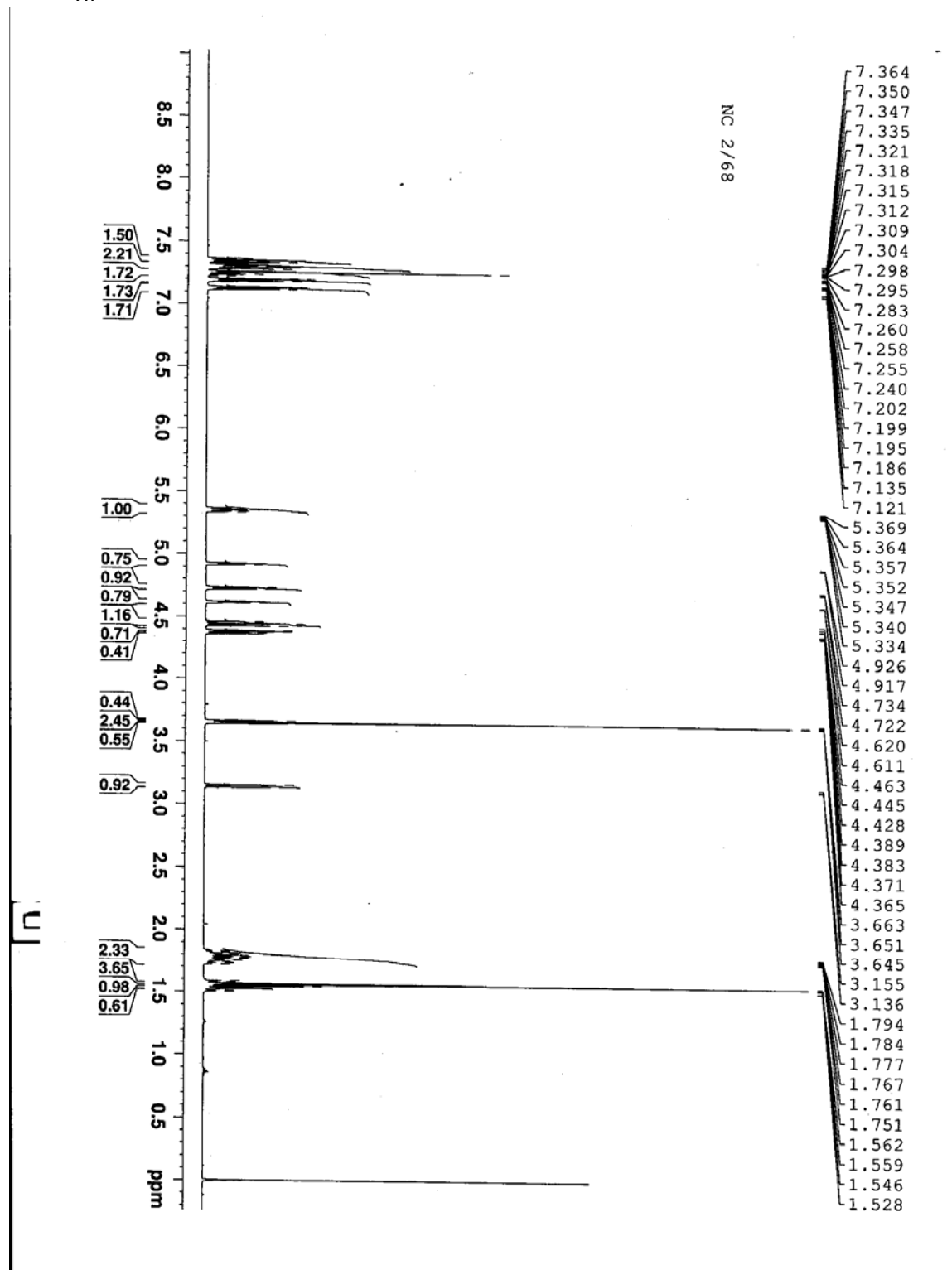
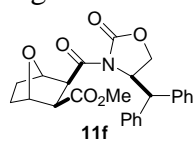


Figure-S40. ^{13}C NMR spectrum of compound **11f**

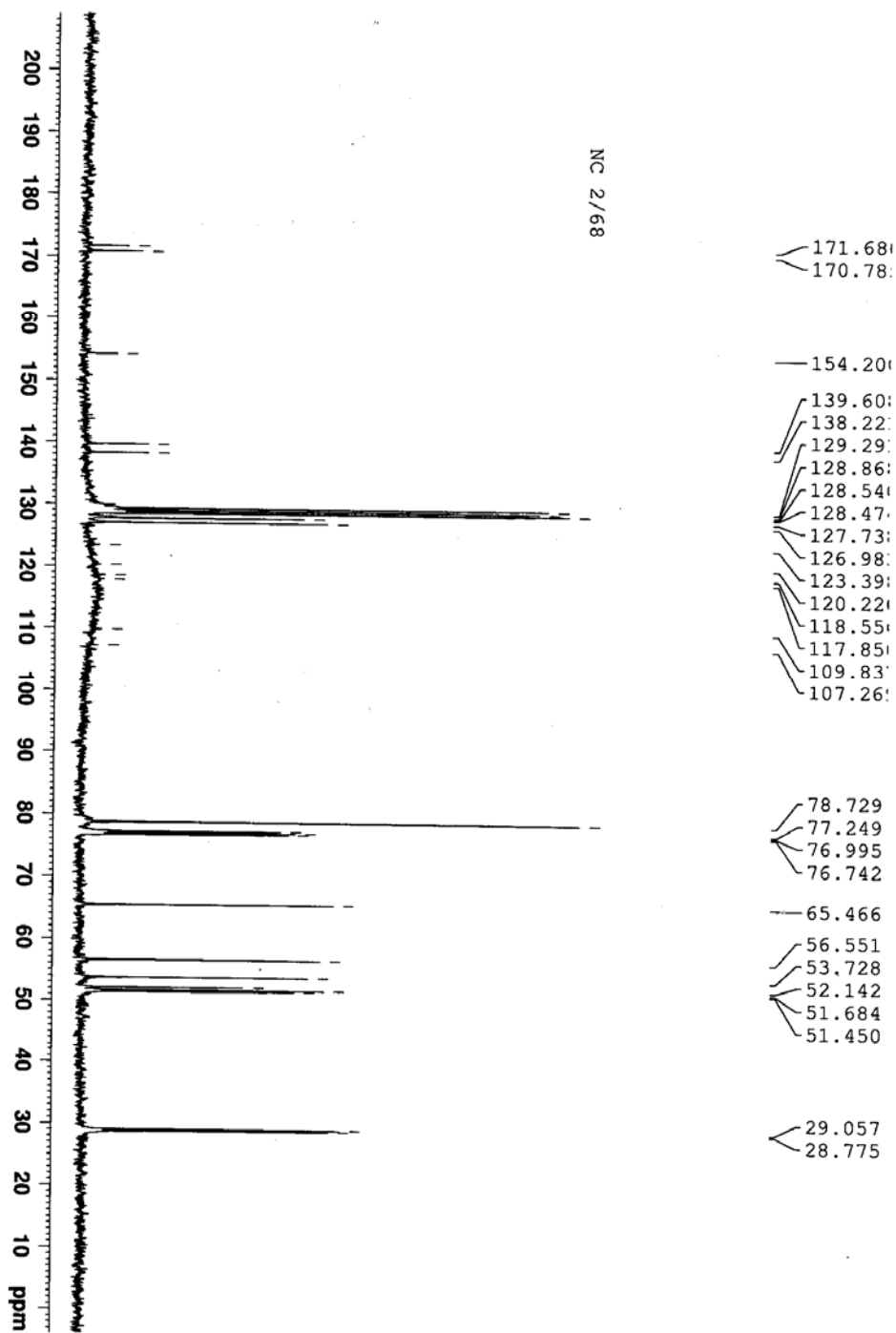
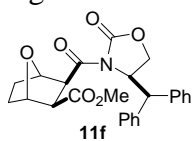


Figure-S41. ¹H NMR spectrum of compound **13**

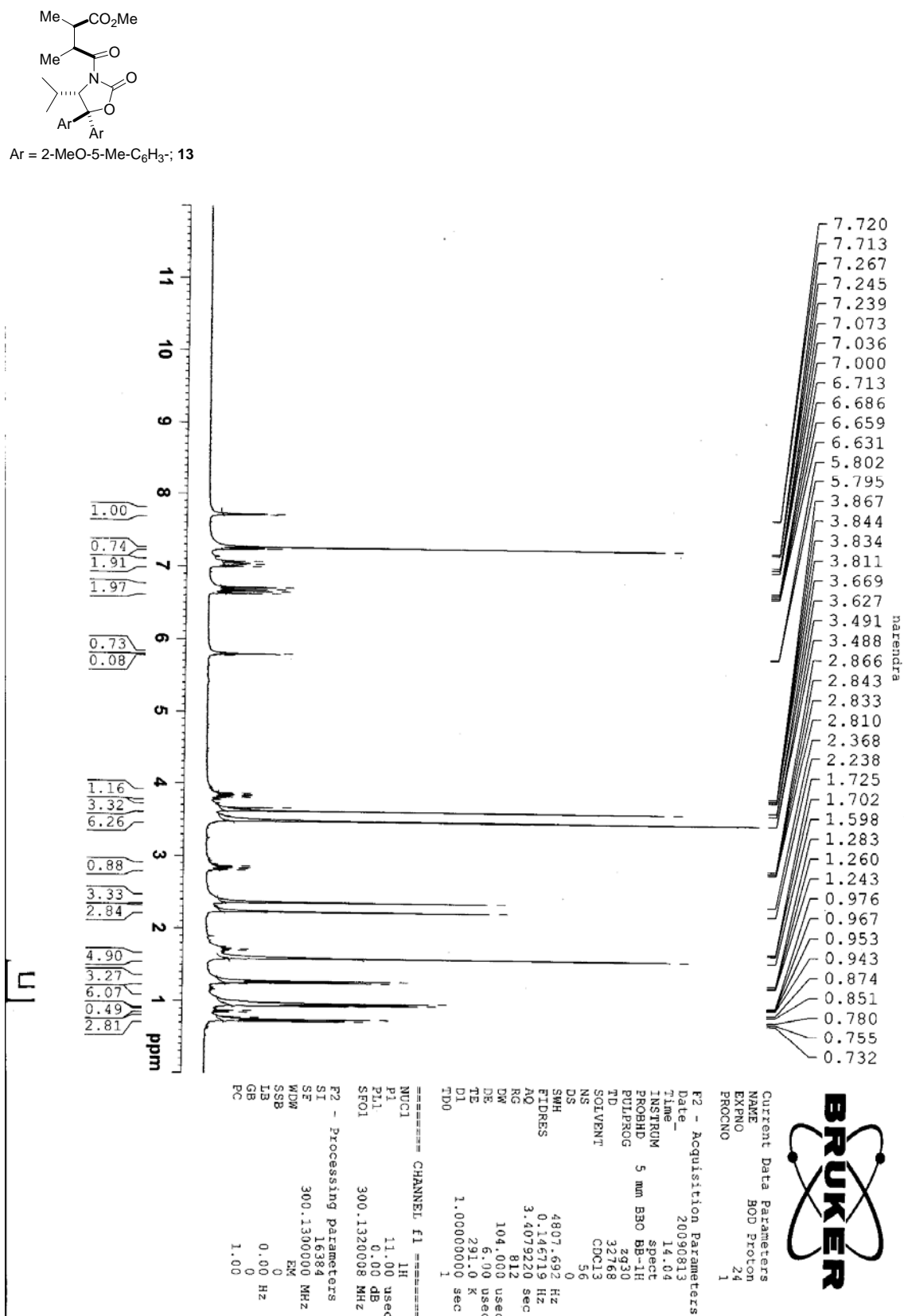


Figure-S42. ¹³C NMR spectrum of compound **13**

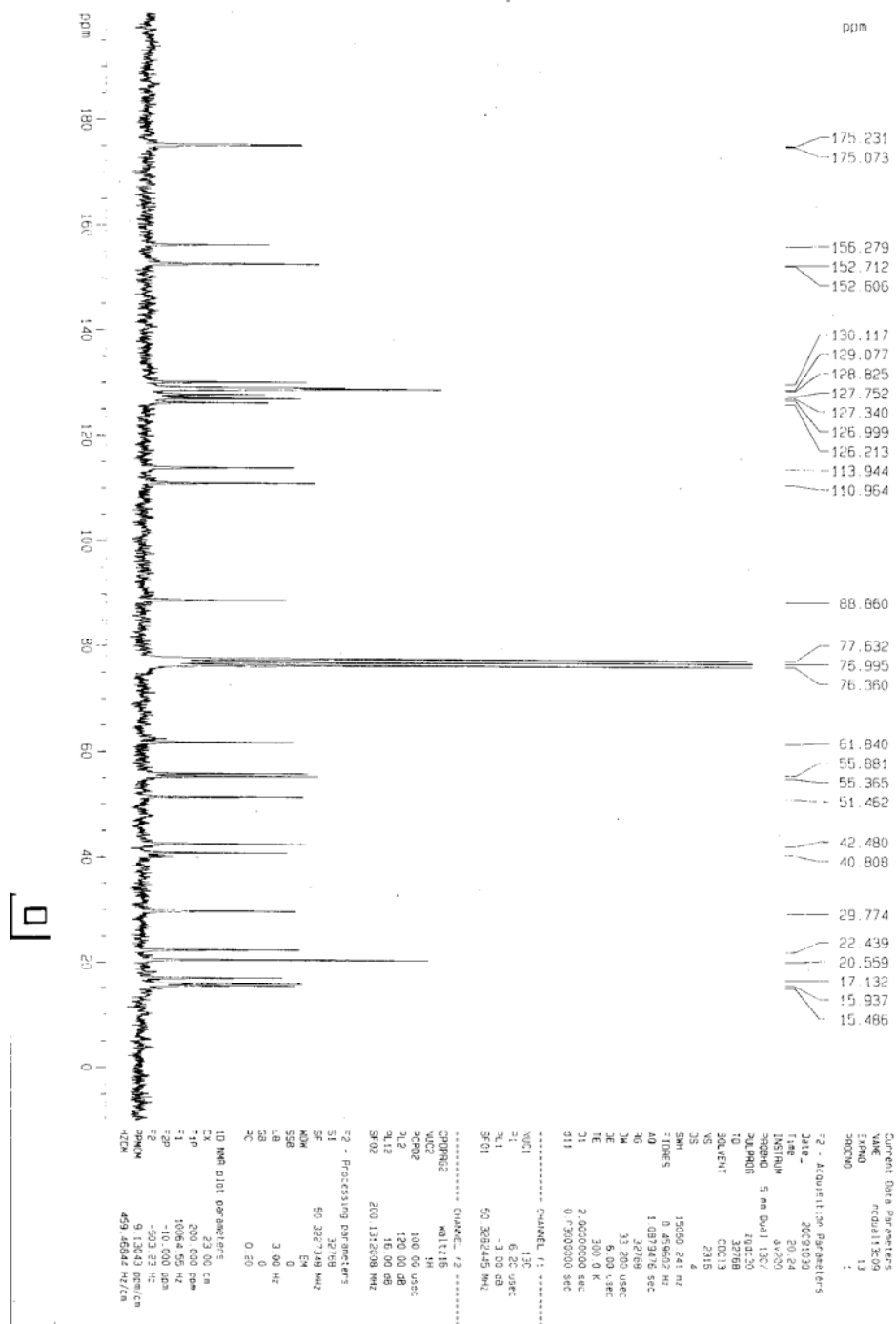
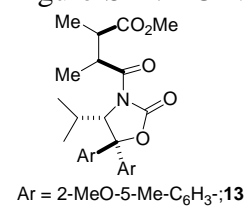
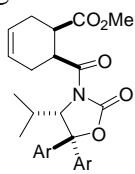


Figure-S43. ¹H NMR spectrum of compound **15a**



Ar = 2-MeO-5-Me-C₆H₃; **15a**

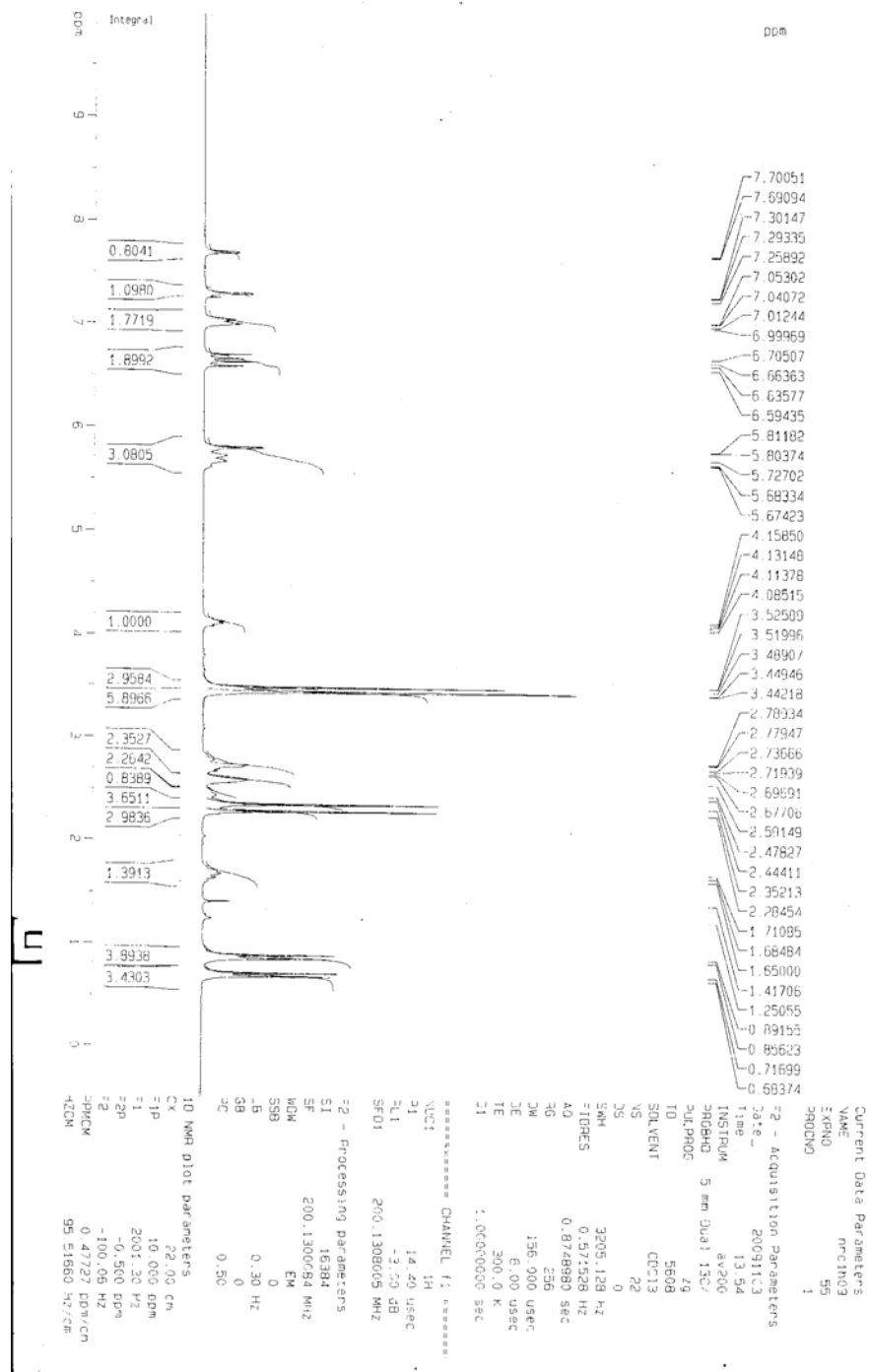
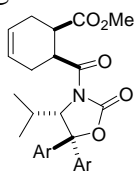


Figure-S44. ^{13}C NMR spectrum of compound **15a**



Ar = 2-MeO-5-Me-C₆H₃; **15a**

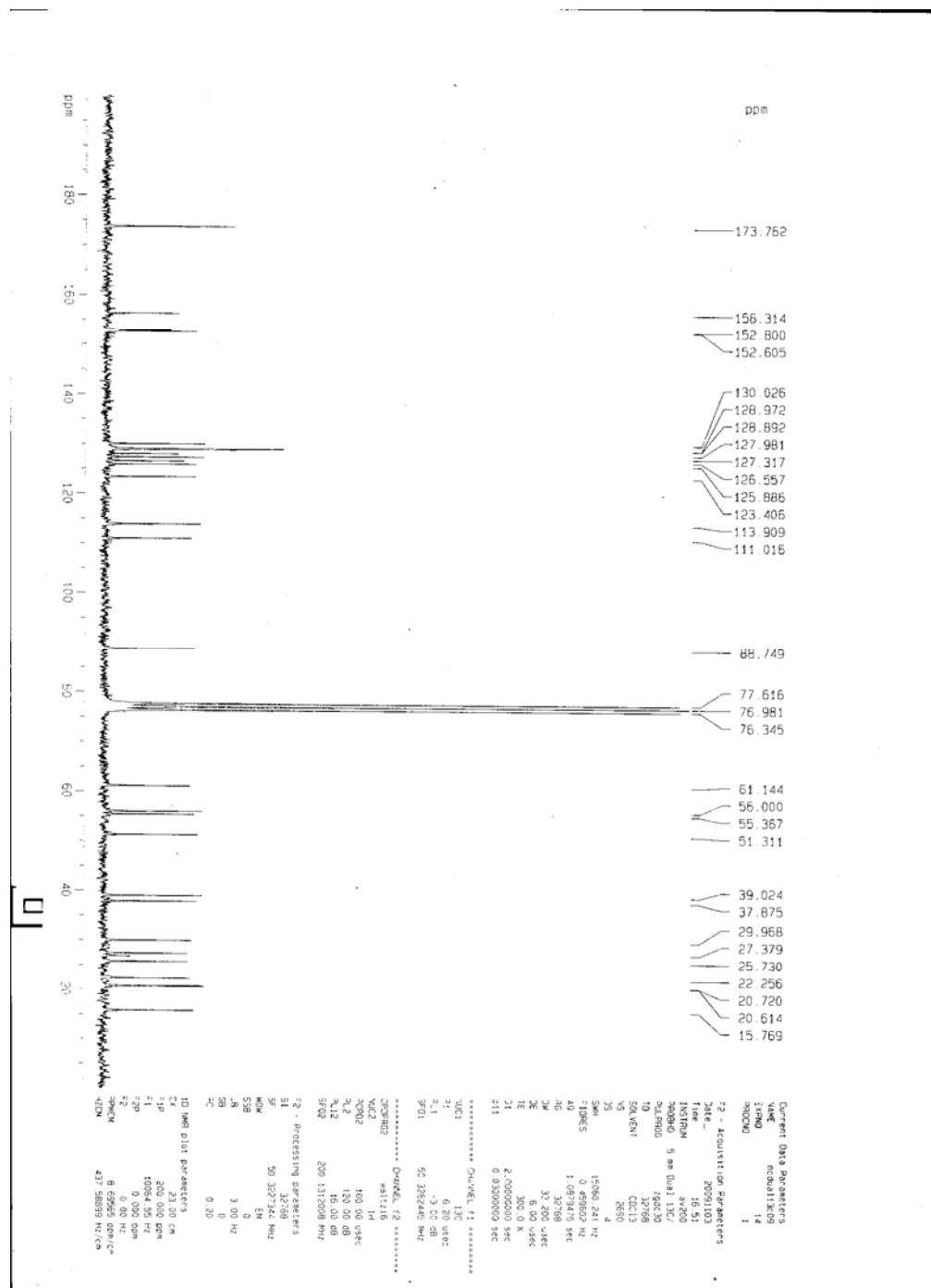
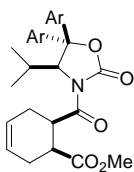


Figure-S45. ¹H NMR spectrum of compound **16a**



Ar = 2-MeO-5-Me-C₆H₃; **16a**

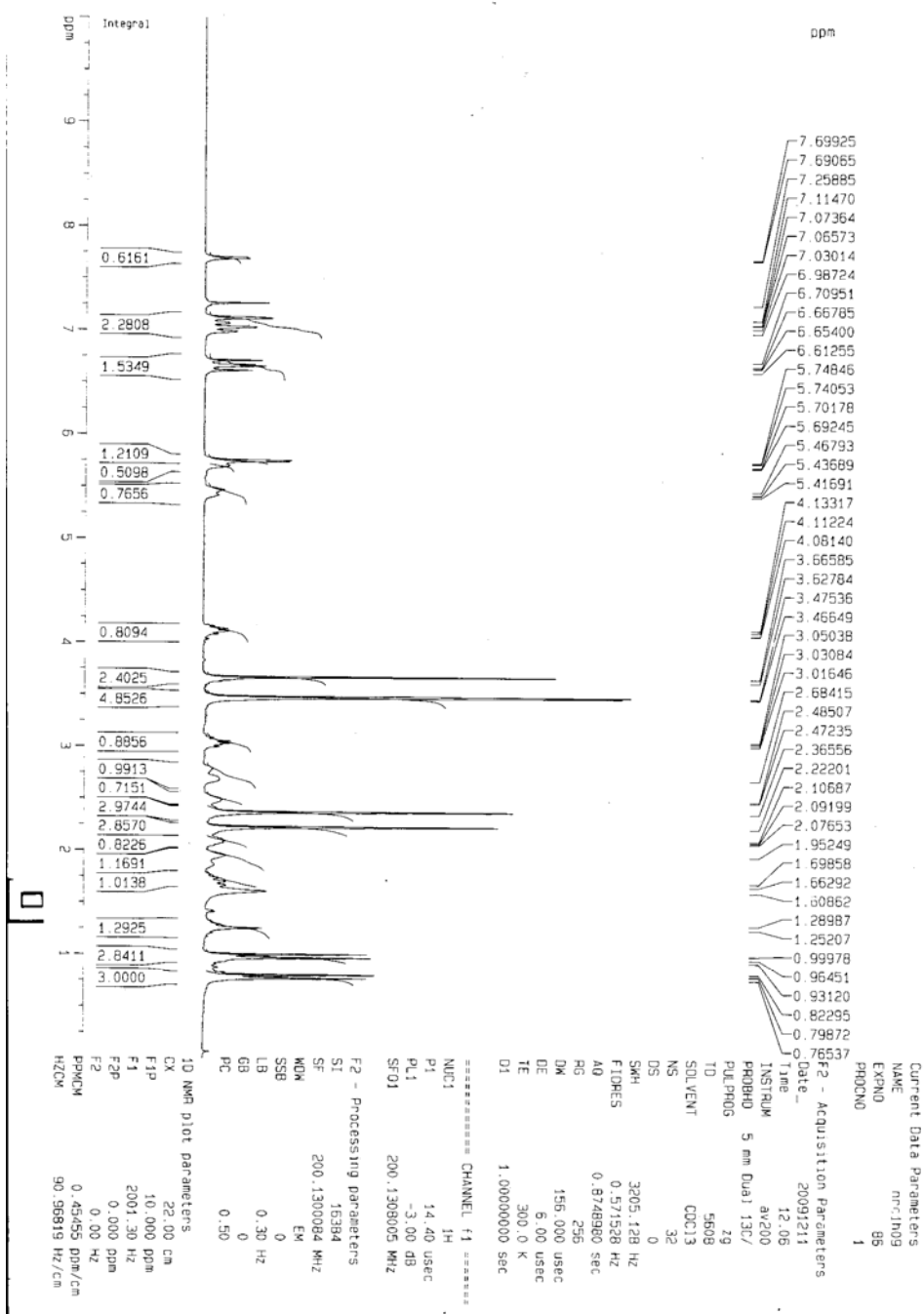
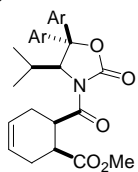
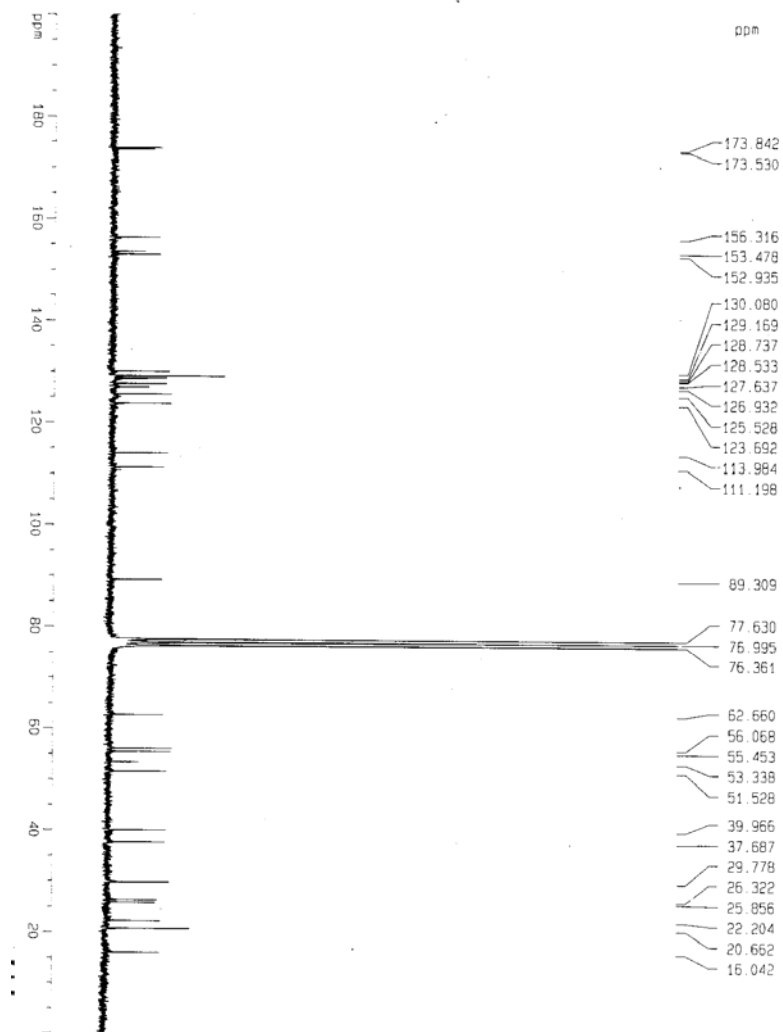


Figure-S46. ^{13}C NMR spectrum of compound **16a**

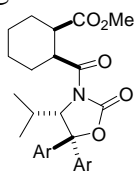


Ar = 2-MeO-5-Me-C₆H₃; **16a**



===== CHANNEL 12 =====
NAME: 16a
EXPNO: 3
PROCNO: 1
F2 - Acquisition Parameters
Date_ 20100810
Time 11:26:43
INSTRUM spect
PROBHD 5 mm QNP 1H/2
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
DS 1282
SWH 11799.427 Hz
AQ 0.260019 Hz
RG 327.500
FIDRES 0.000000 Hz
AQRES 0.000000 Hz
NUC1 13C
NUC2 13C
PC 41.700 dB
TE 300.2 K
D1 2.0000000 sec
d11 0.0500000 sec
DELTA 1.8000000 sec
DELTA2 0.0000000 sec
DELTA3 0.0000000 sec
===== CHANNEL 11 =====
NAME: 16a
EXPNO: 3
PROCNO: 1
F2 - Processing parameters
SI 32768
SF 125.760 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
NOISE 3.00 dB
===== CHANNEL 12 =====
NAME: 16a
EXPNO: 3
PROCNO: 1
F2 - Processing parameters
SI 65536
SF 125.760 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
NOISE 3.00 dB
===== CHANNEL 11 =====
NAME: 16a
EXPNO: 3
PROCNO: 1
F2 - Processing parameters
SI 32768
SF 125.760 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
NOISE 3.00 dB

Figure-S47. ¹H NMR spectrum of compound **15b**



Ar = 2-MeO-5-Me-C₆H₃; **15b**

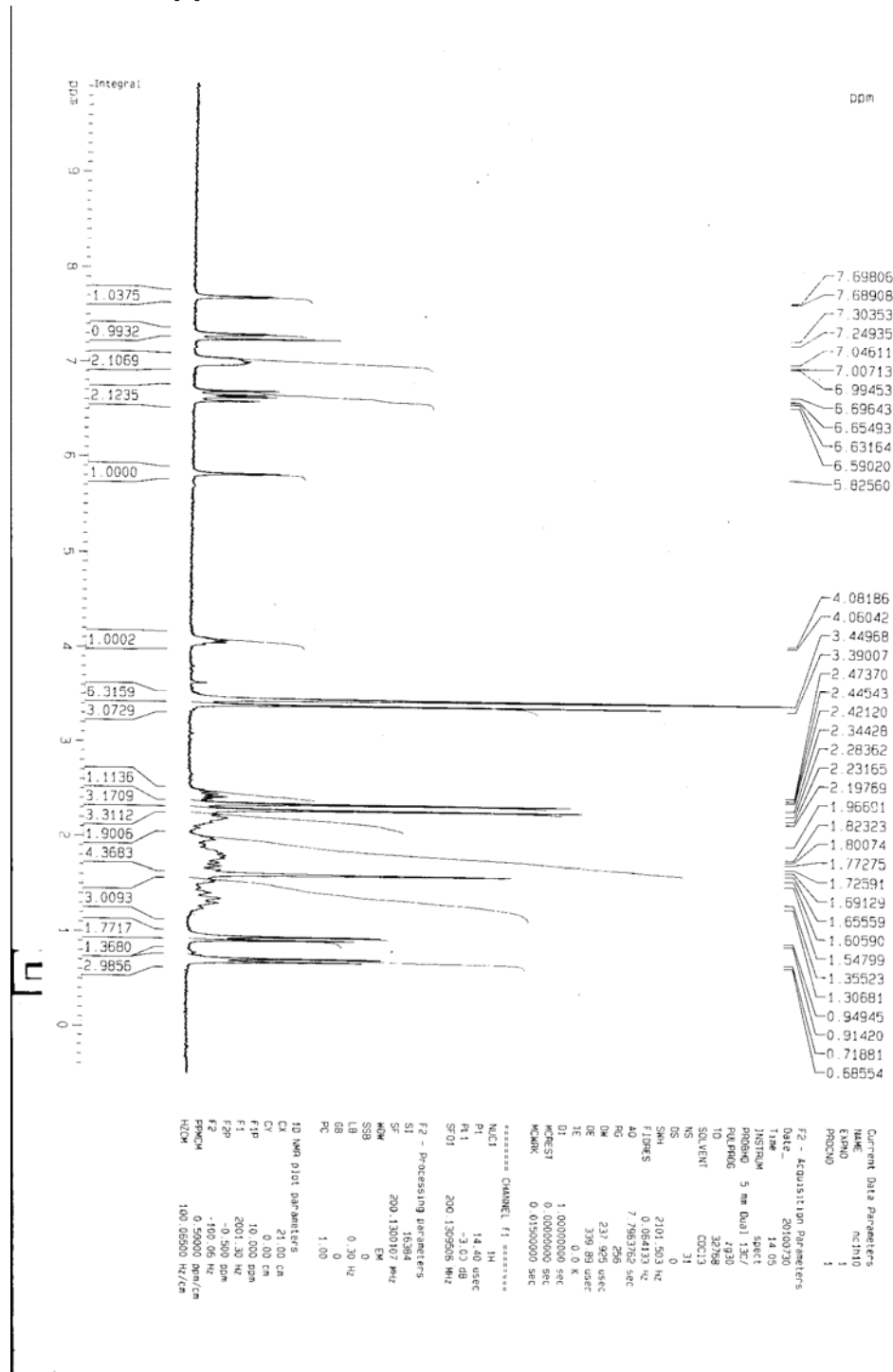
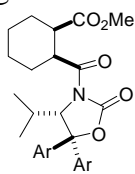


Figure-S48. ^{13}C NMR spectrum of compound **15b**



Ar = 2-MeO-5-Me-C₆H₃; **15b**

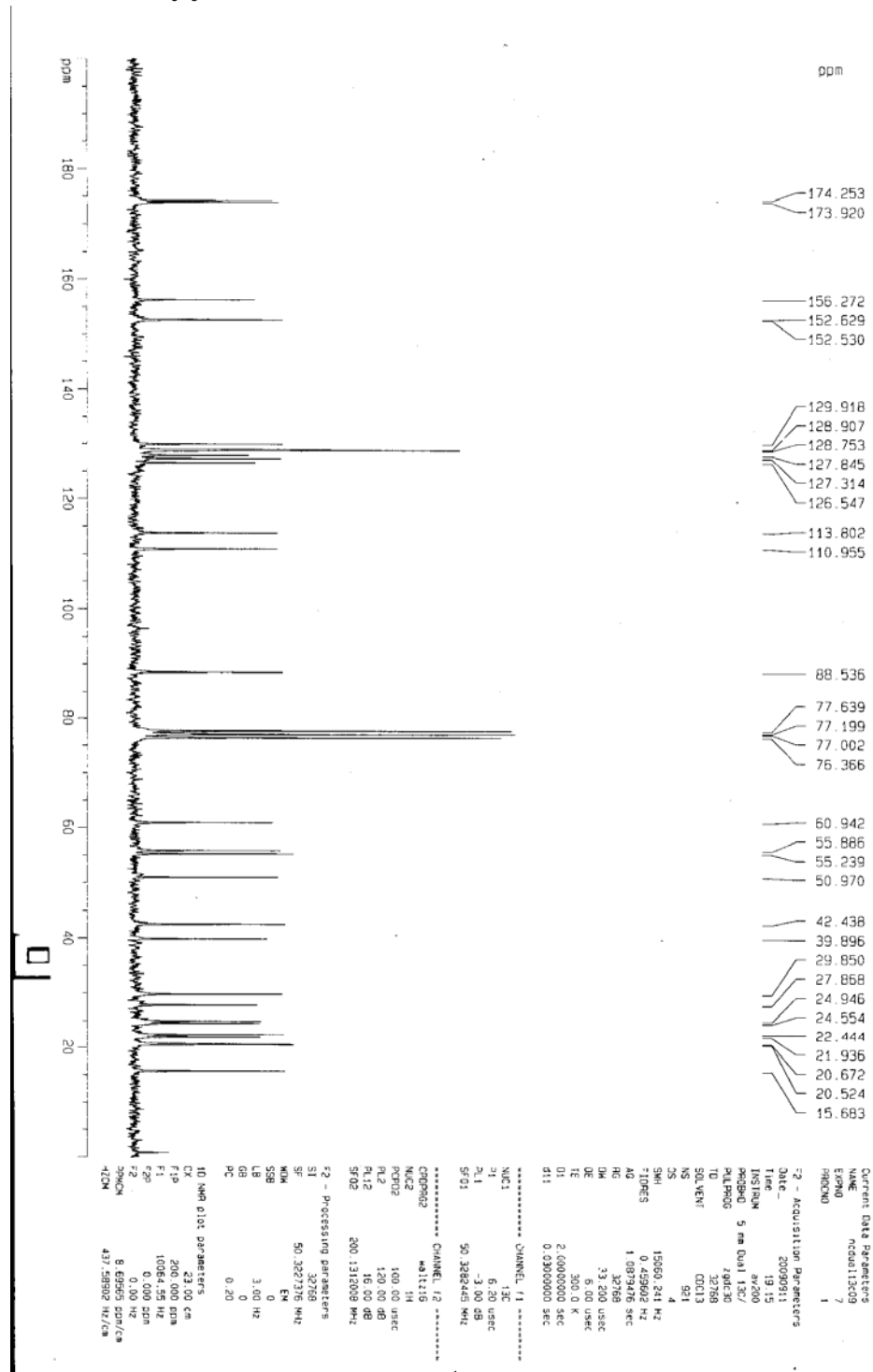
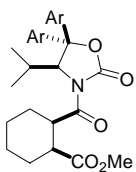


Figure-S49. ^1H NMR (500 MHz) spectrum of compound **16b**



Ar = 2-MeO-5-Me-C₆H₃; **16b**

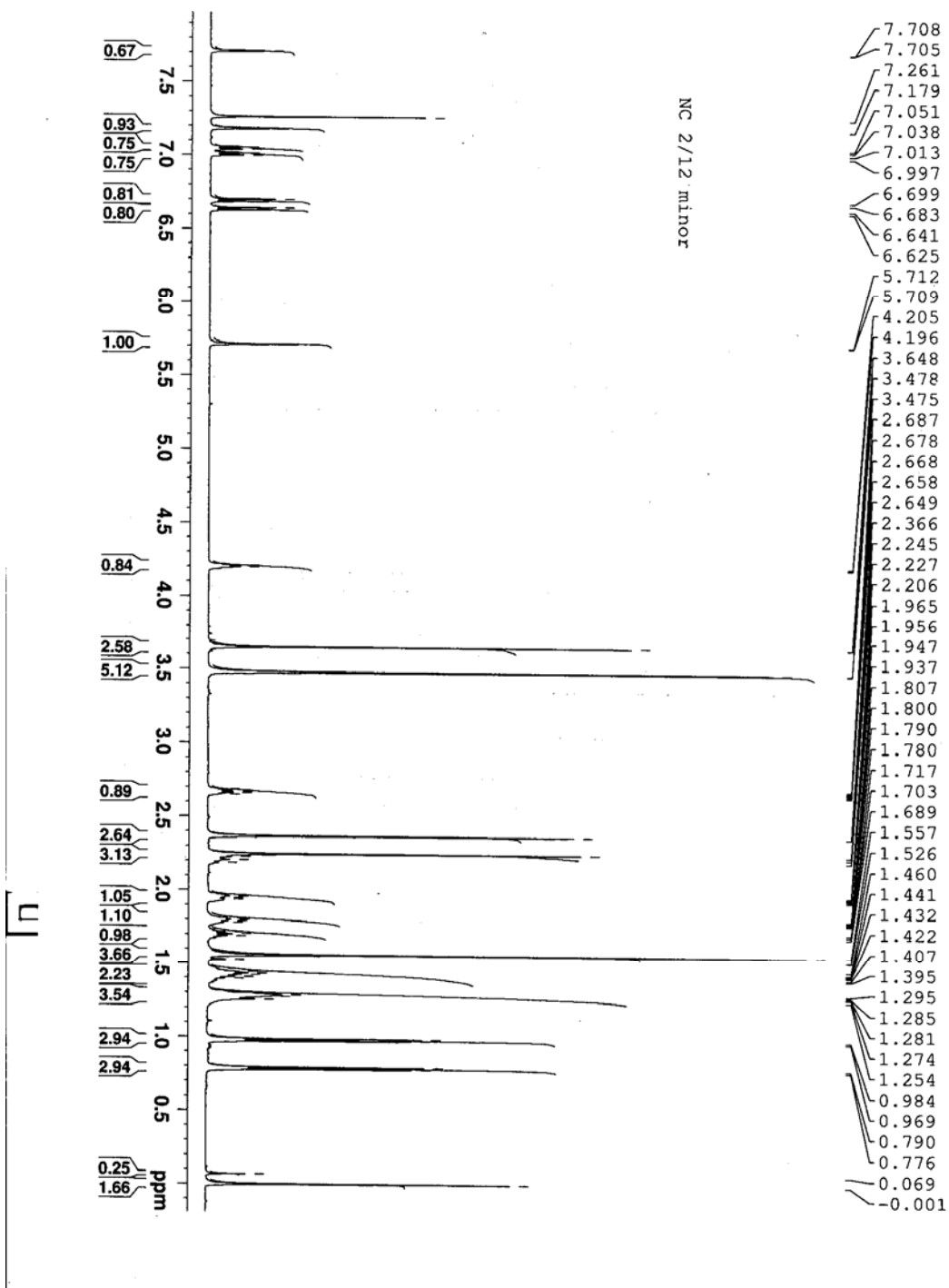


Figure-S50. ^{13}C NMR (125 MHz) spectrum of compound **16b**

