

Supporting Information

Rapid assembly of heterocycles grafted macrocycles *via* tandem one-pot double 1,3-dipolar cycloaddition reaction

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Table of Contents

1. ORTEP diagram of 11a	S2
2. Scanned copy of ^1H , ^{13}C and HRMS Spectra	S3-S63

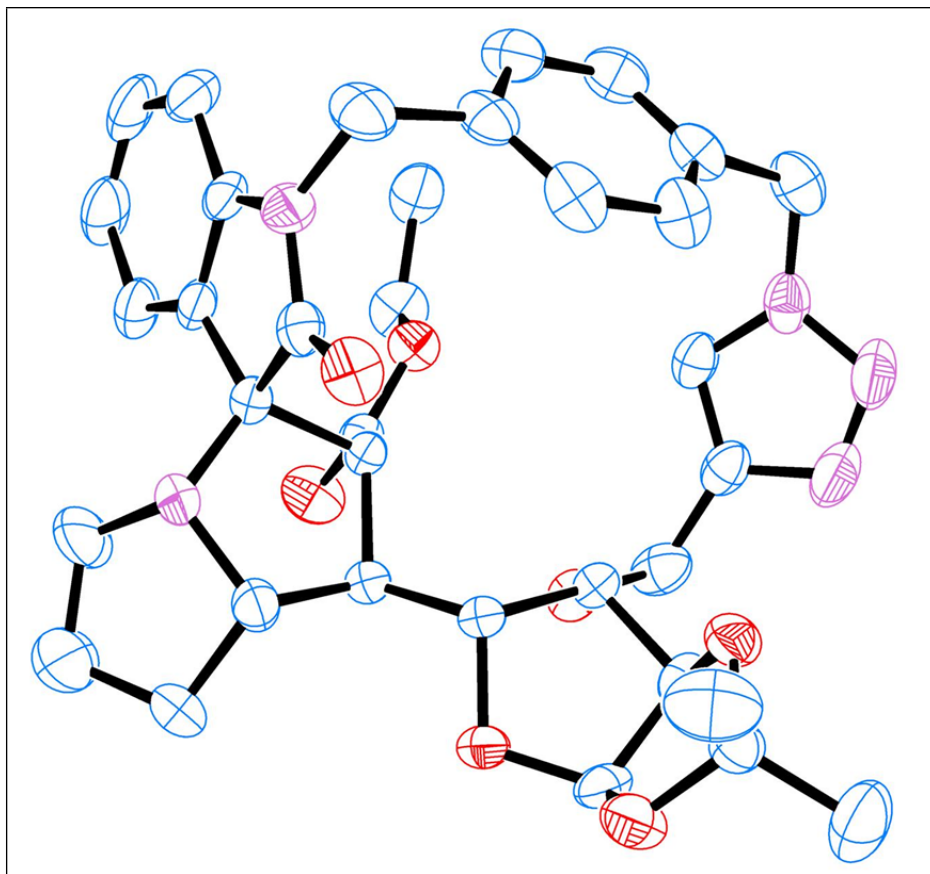


Figure 1. ORTEP diagram of **11a**. Thermal ellipsoids drawn at 30% probability. (For clarity purpose hydrogen atoms are not shown)

Scanned copy of ^1H , ^{13}C and HRMS Spectra

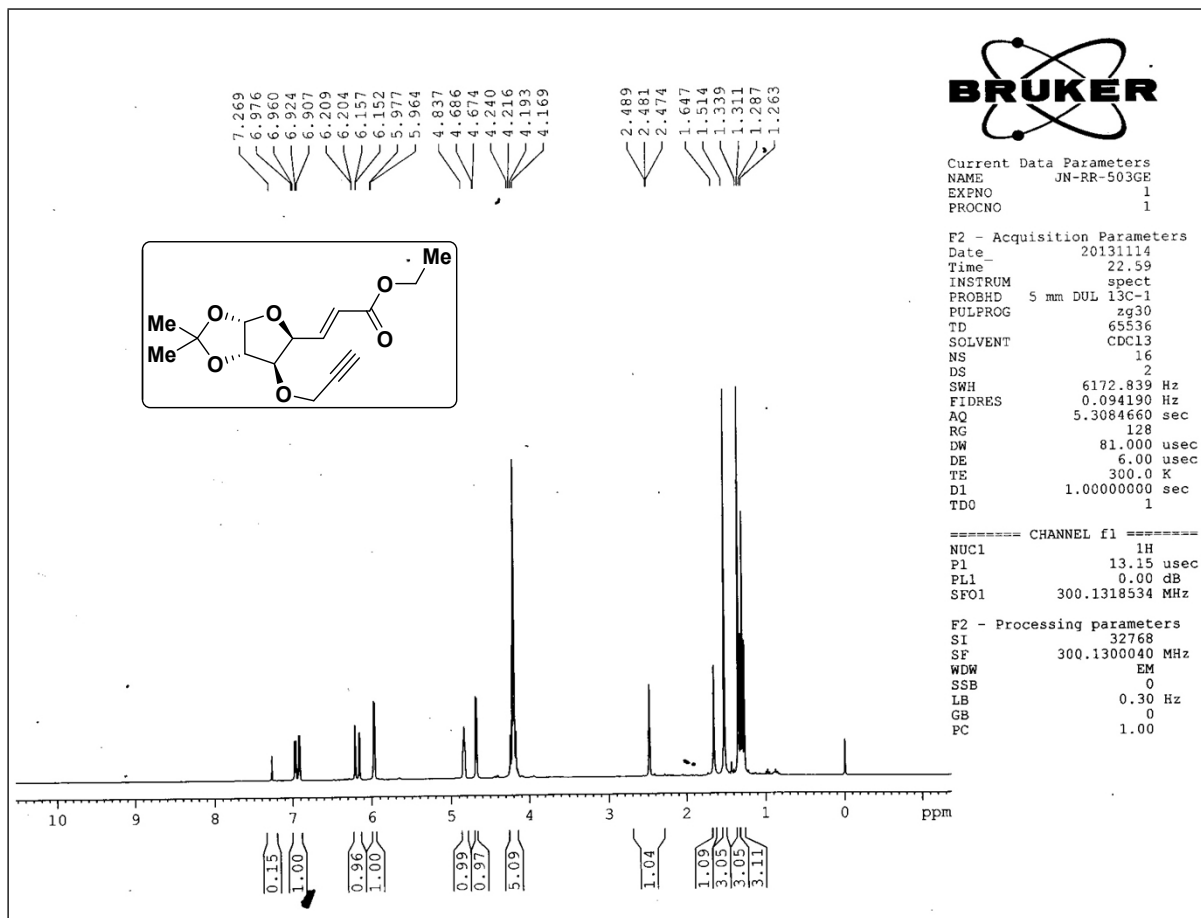


Figure 3.1a. ^1H NMR (300MHz, CDCl_3) spectrum of **3a**

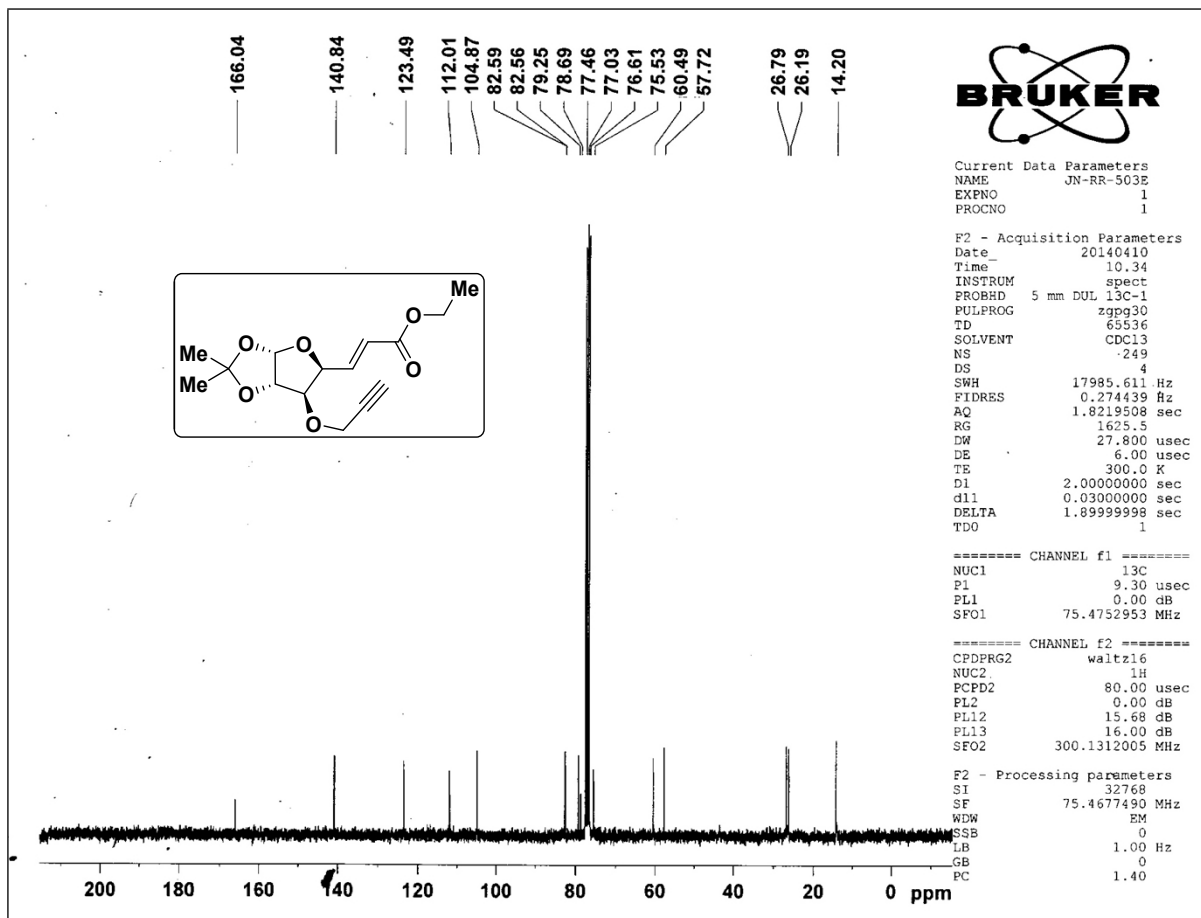


Figure 3.1b. ¹³C NMR (CDCl₃, 75MHz) of 3a

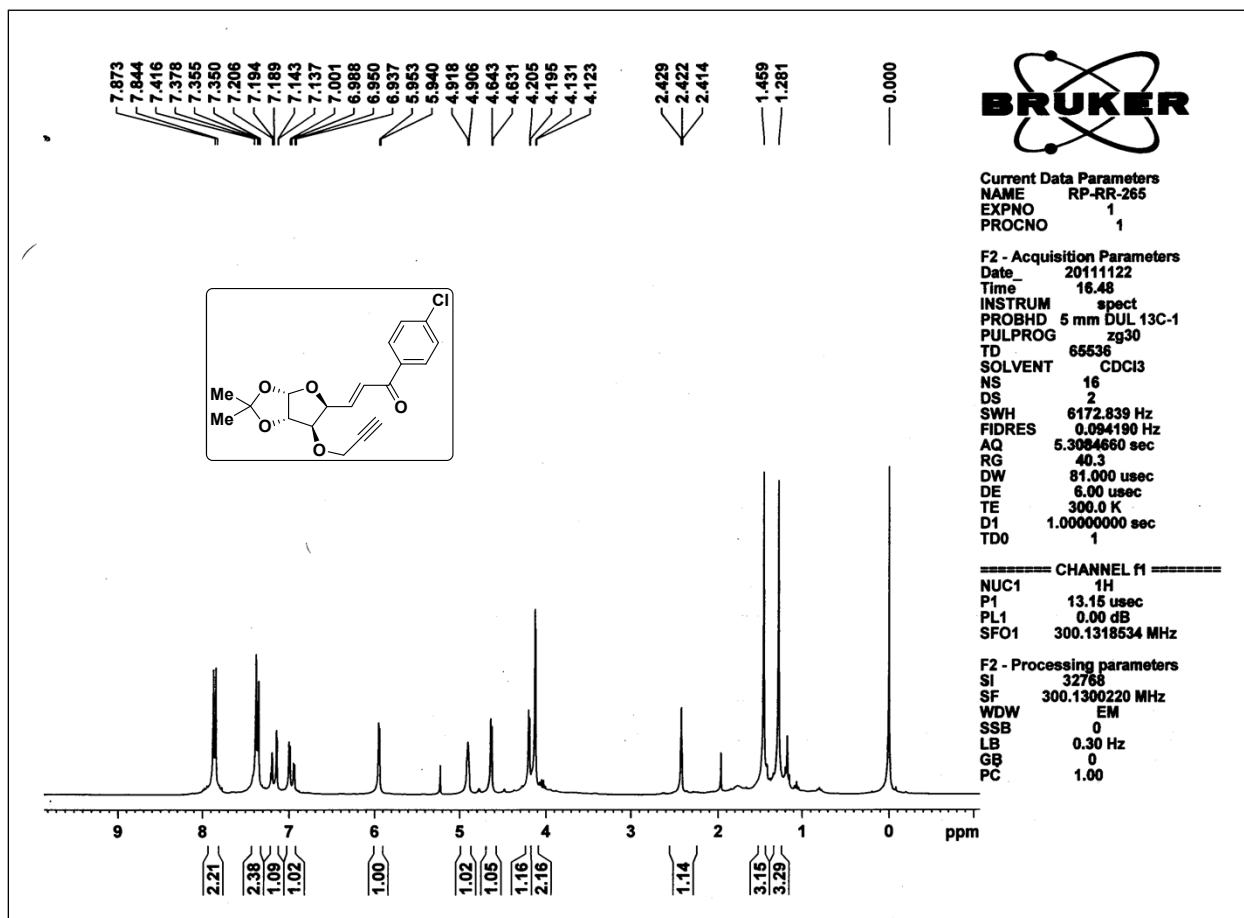


Figure 3.2a. ^1H NMR (300MHz, CDCl_3) spectrum of **3b**

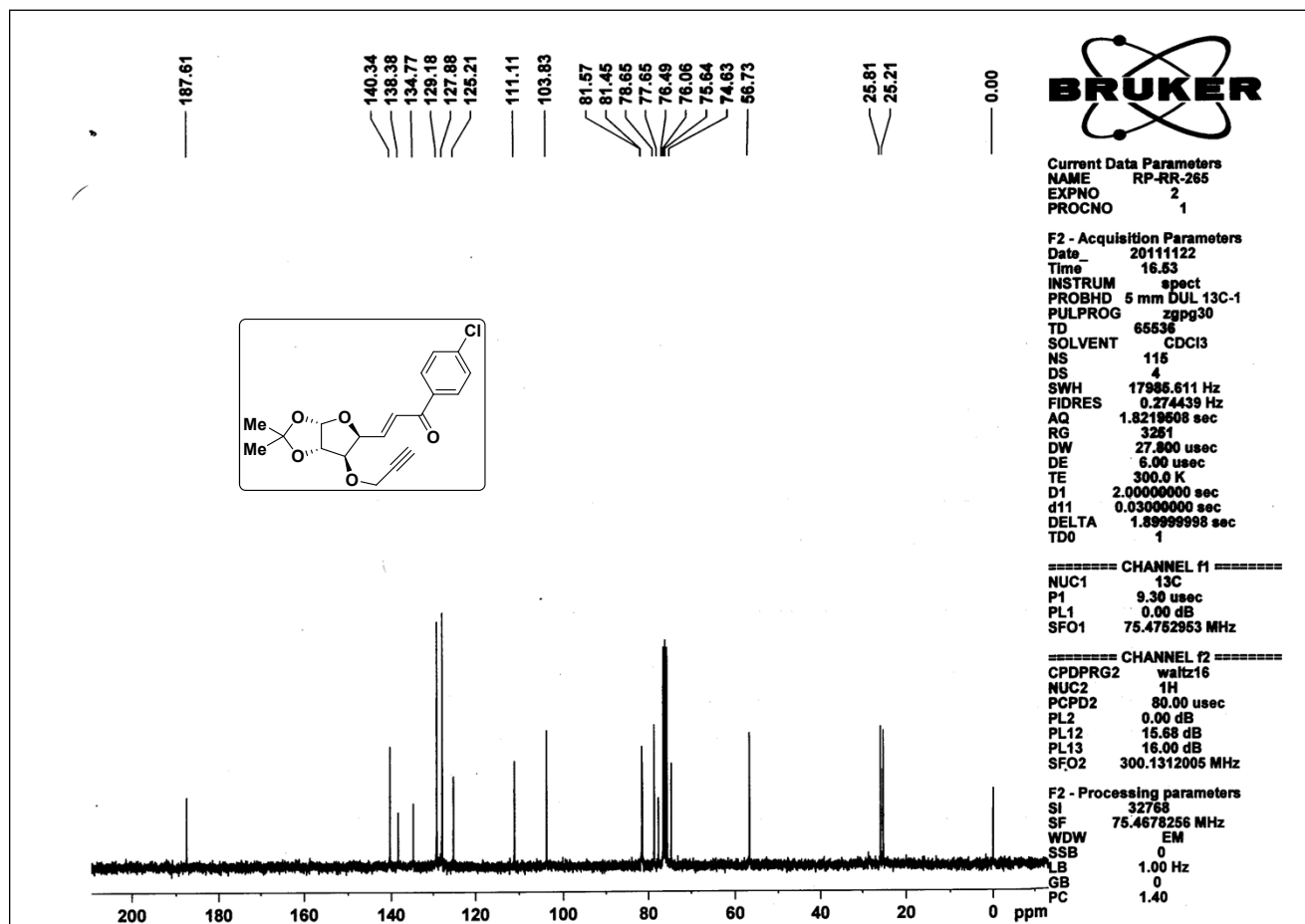


Figure 3.2b. ^{13}C NMR (CDCl_3 , 75MHz) of 3b

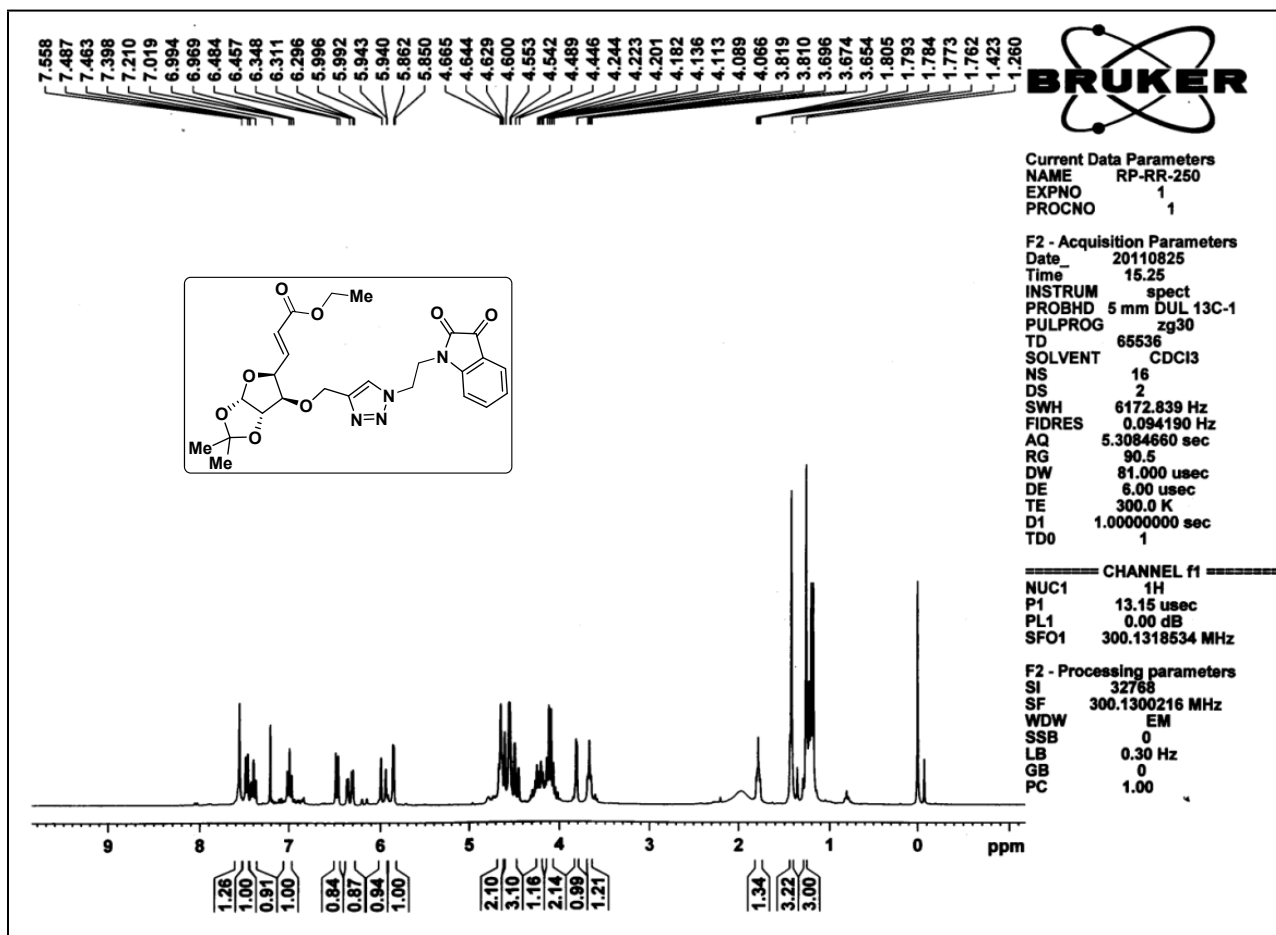


Figure 3.3a. ¹H NMR (300MHz, CDCl₃) spectrum of 8a

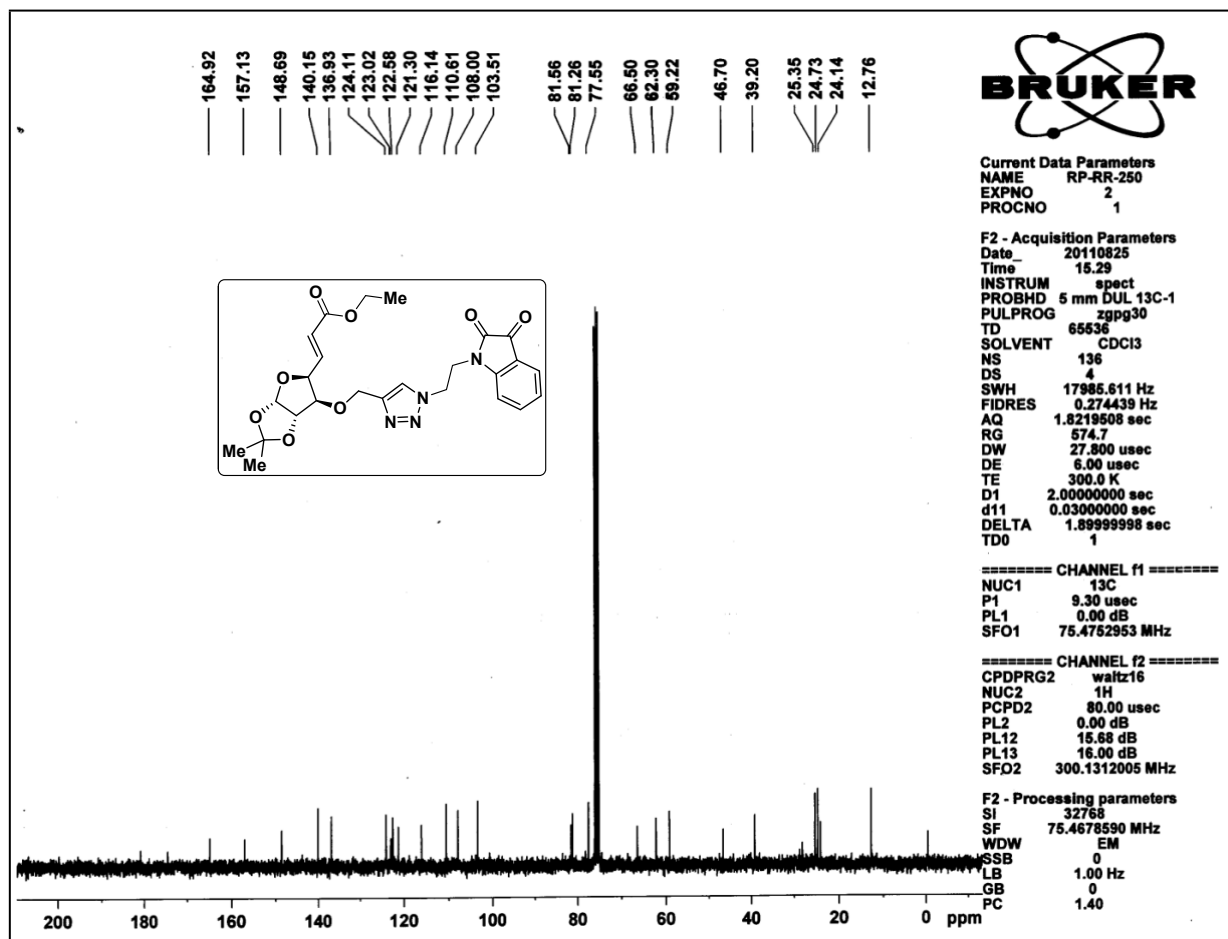


Figure 3.3b. ^{13}C NMR (CDCl_3 , 75MHz) of 8a

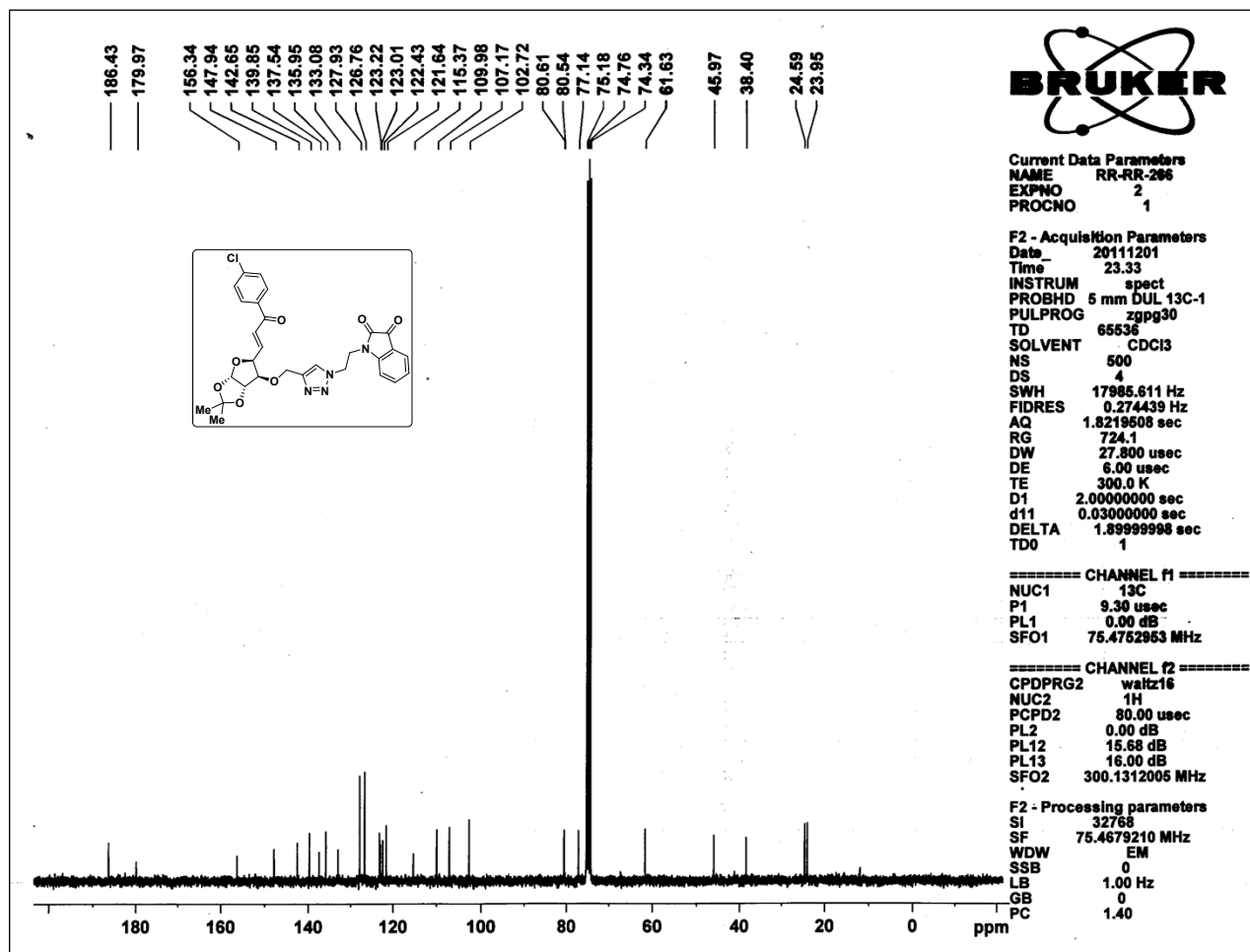


Figure 3.4b: ^{13}C NMR (CDCl_3 , 75MHz) of 8b

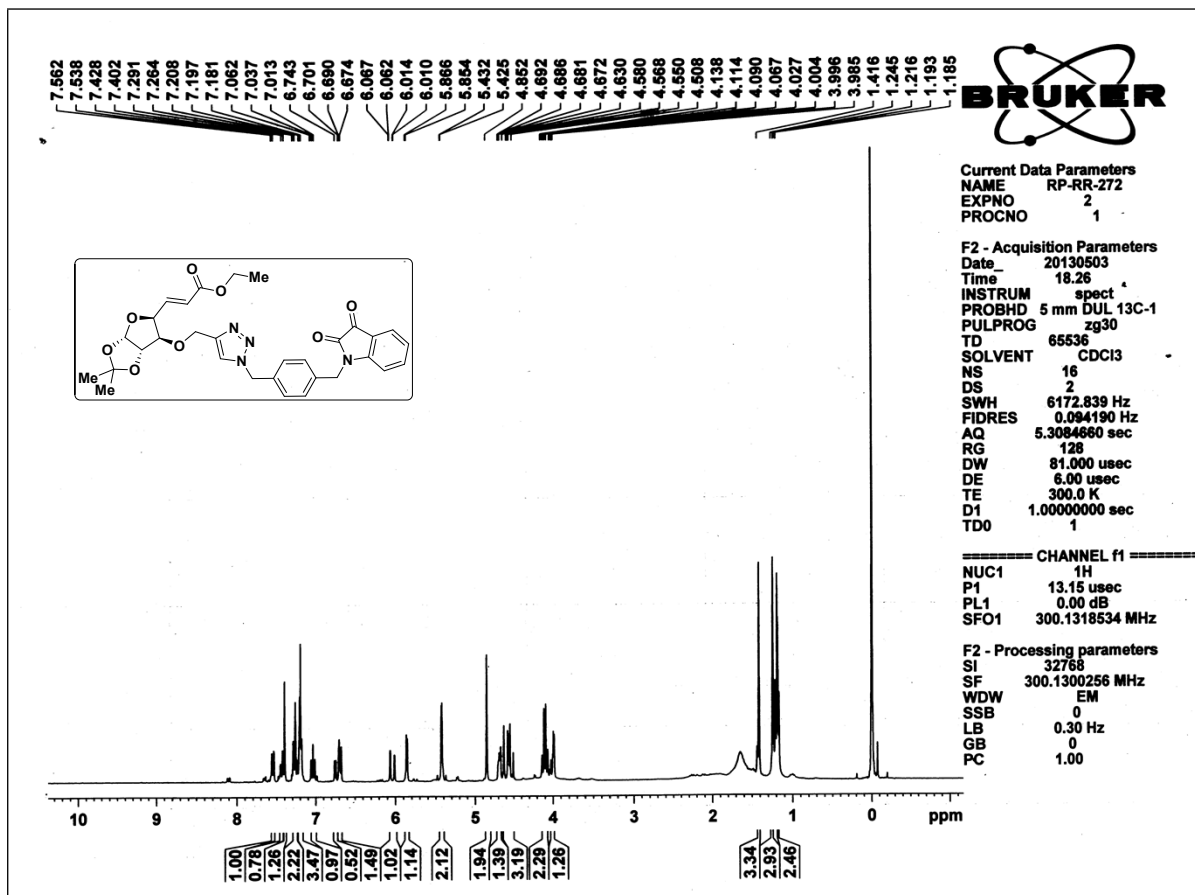
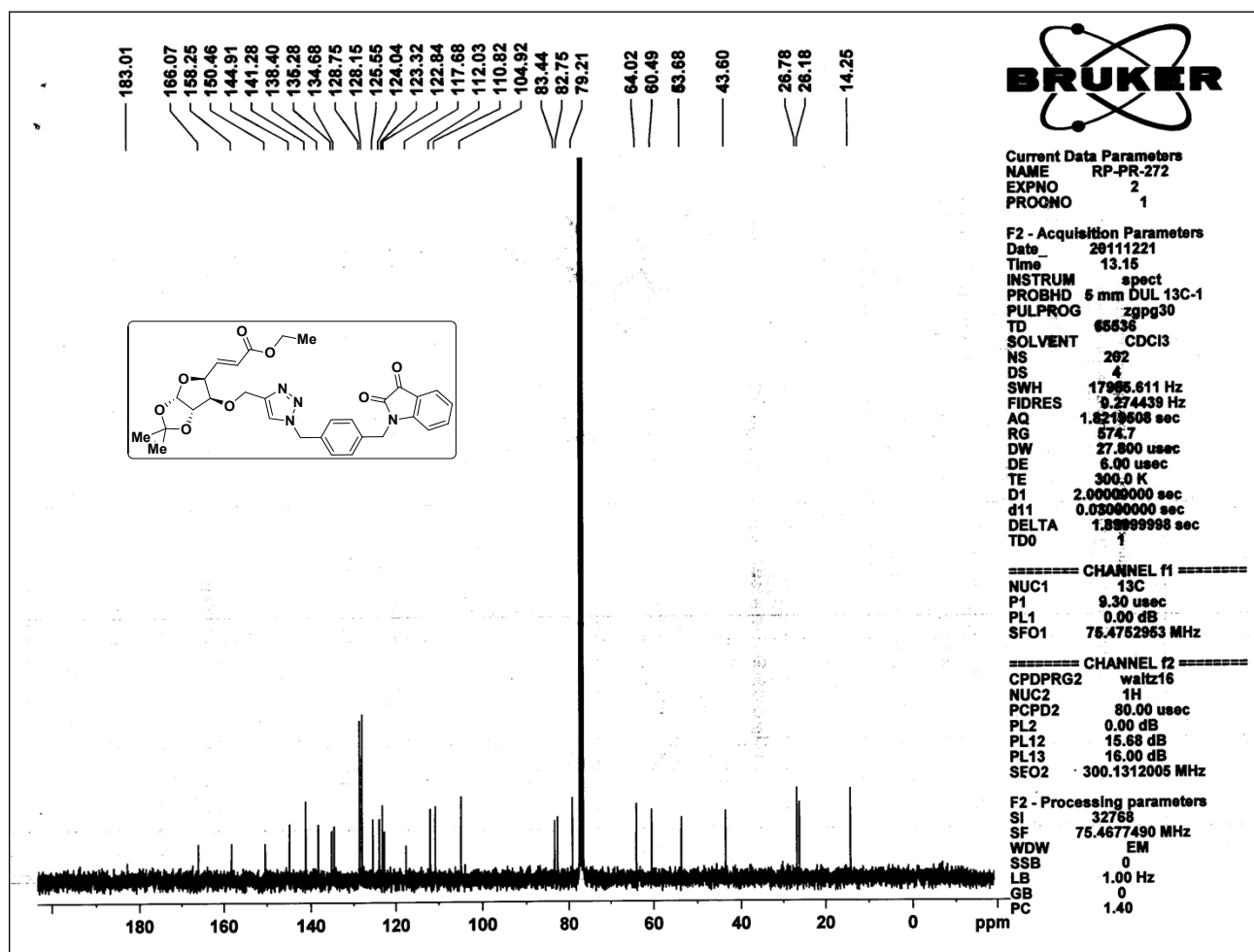


Figure 3.5a: ^1H NMR (300MHz, CDCl_3) spectrum of 8c



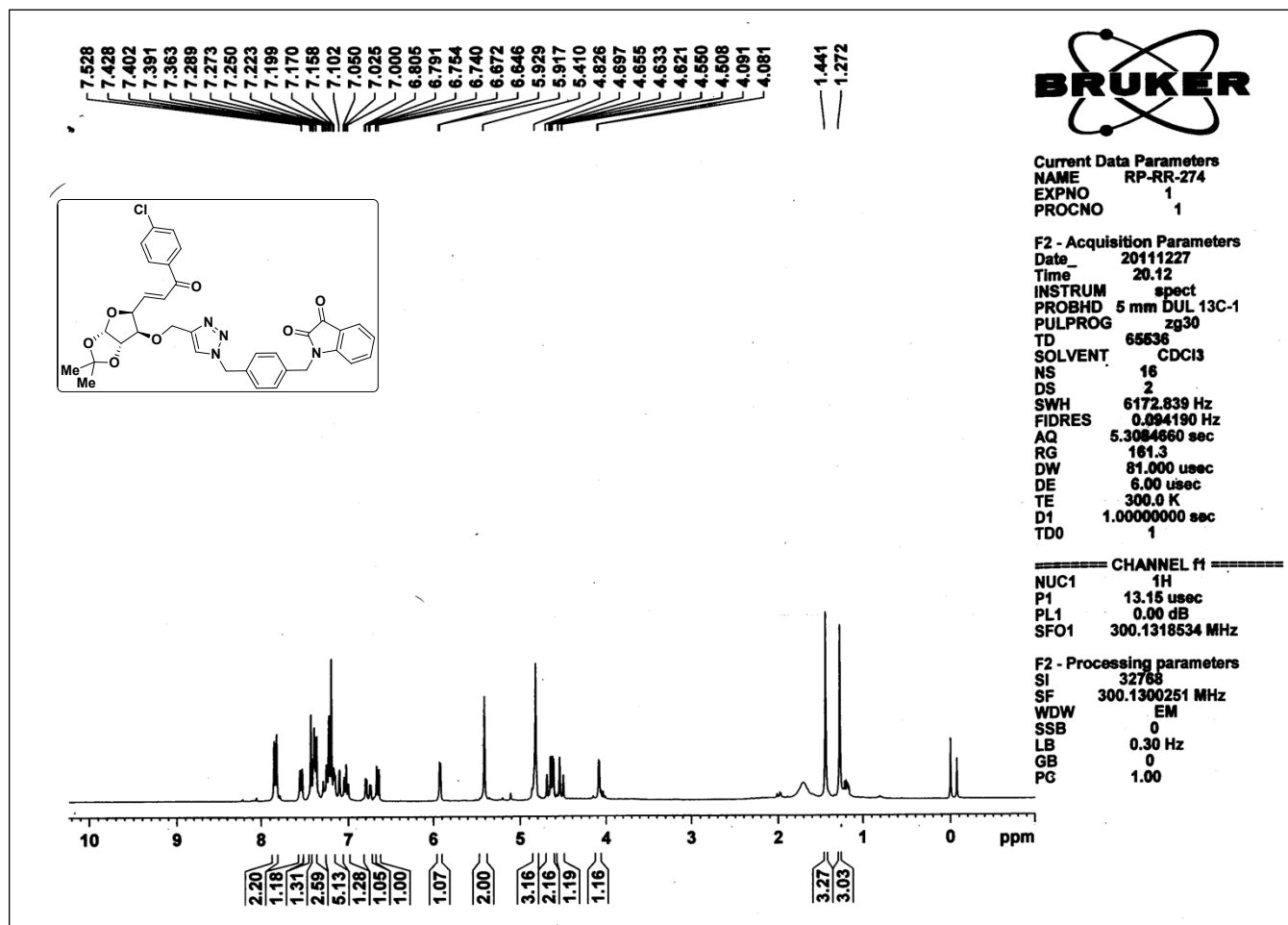


Figure 3.6a. ¹H NMR (300MHz, CDCl₃) spectrum of **8d**

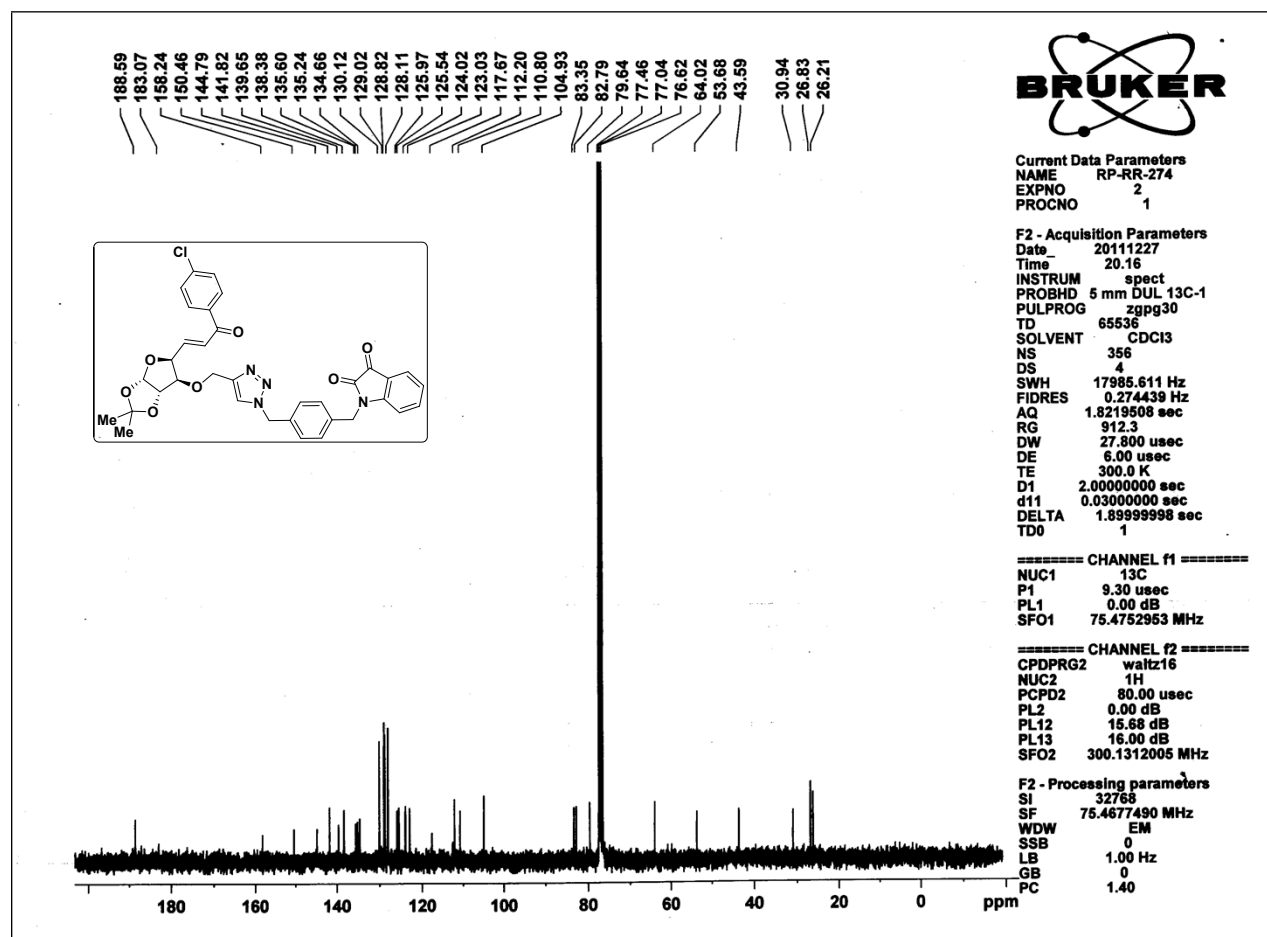
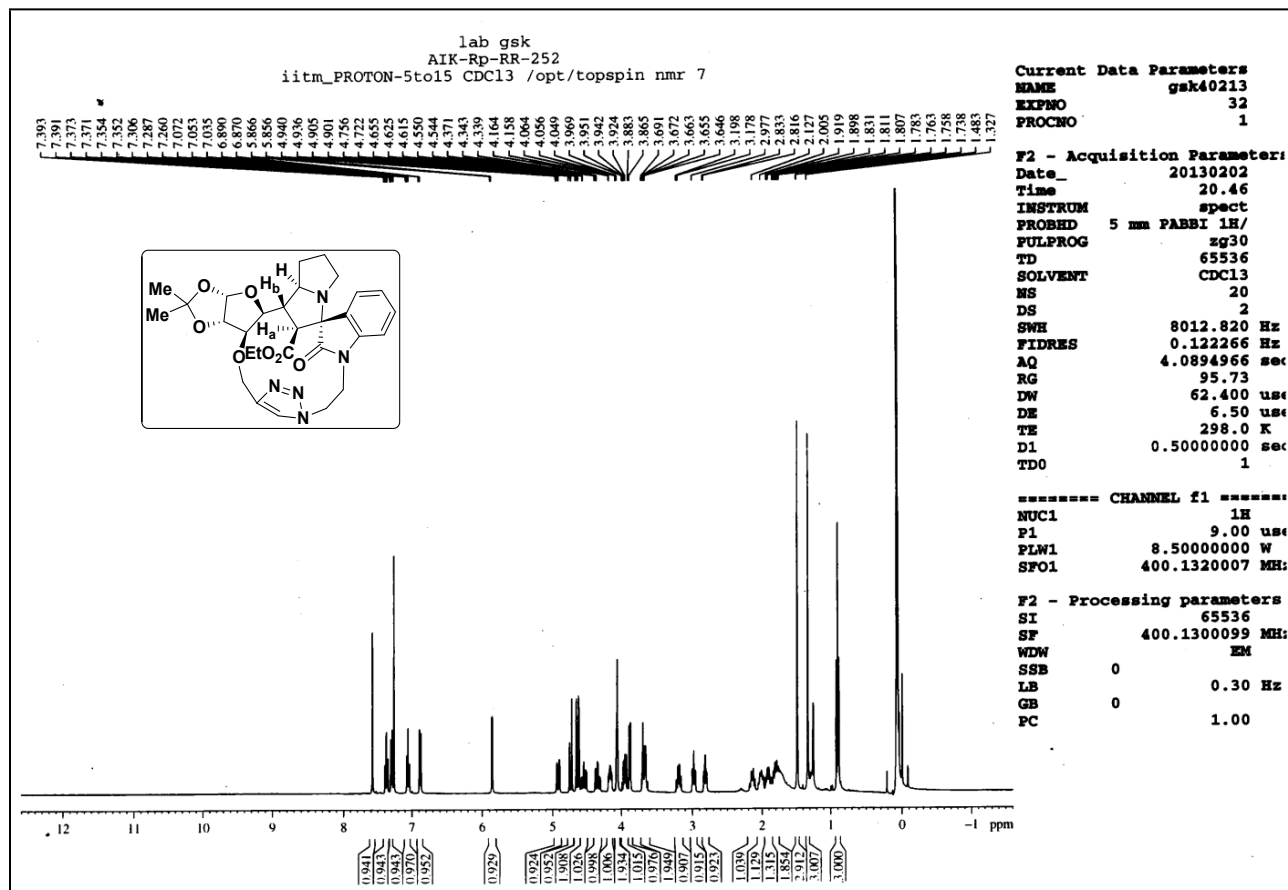


Figure 3.6b. ¹³C NMR (CDCl₃, 75MHz) of 8d



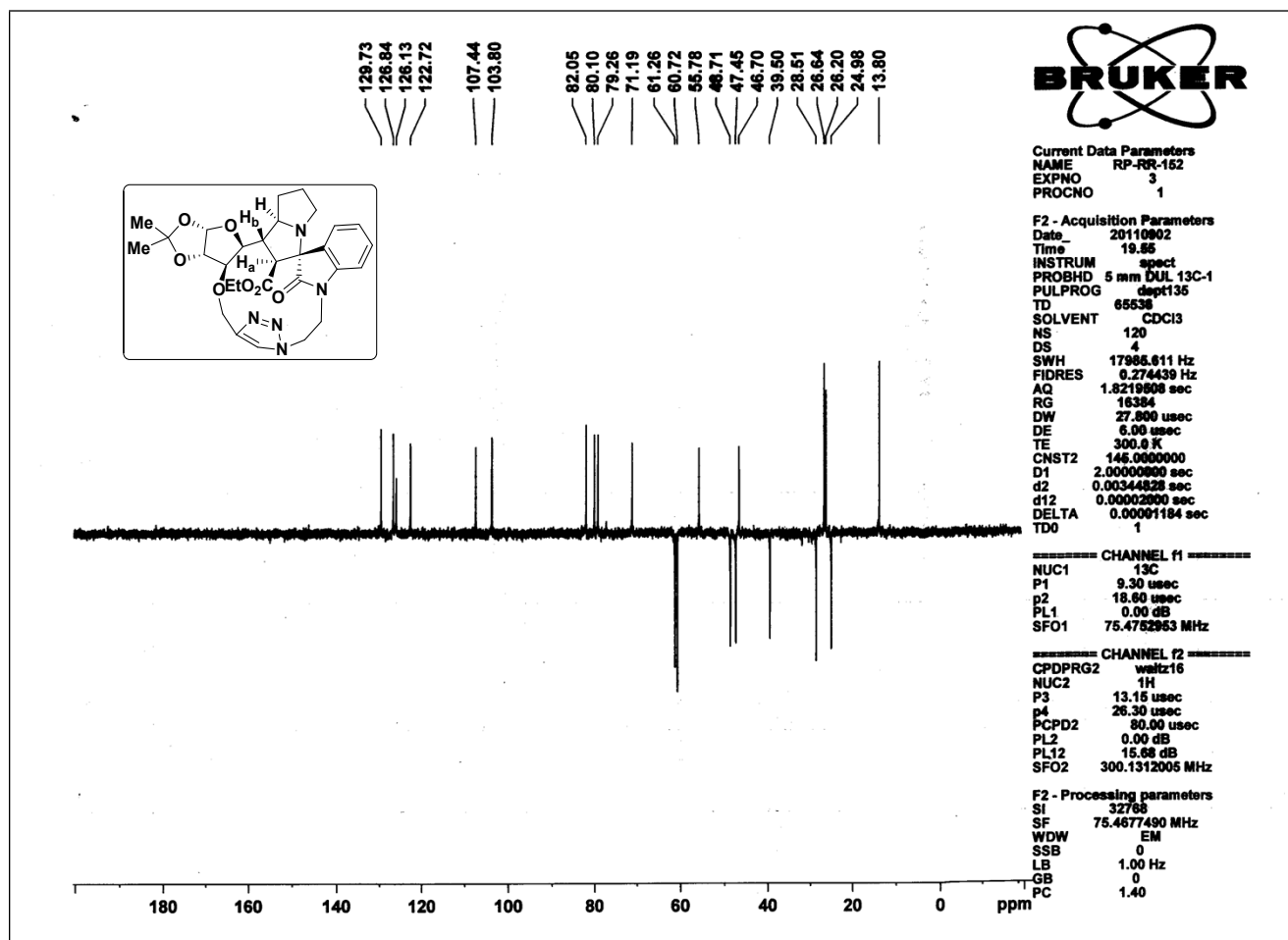


Figure 3.7c. DEPT 135 (CDCl₃, 75MHz) of 10a

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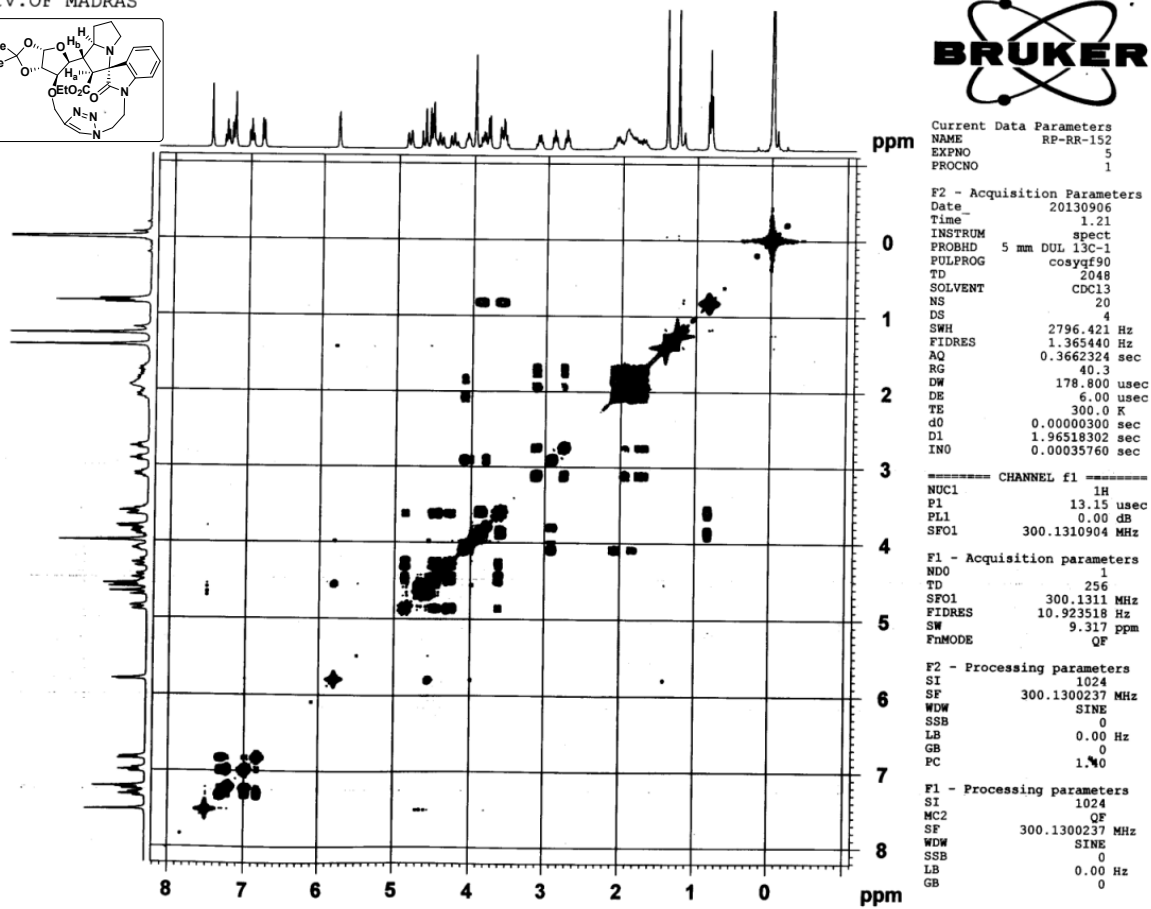
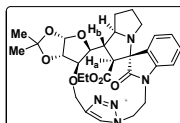
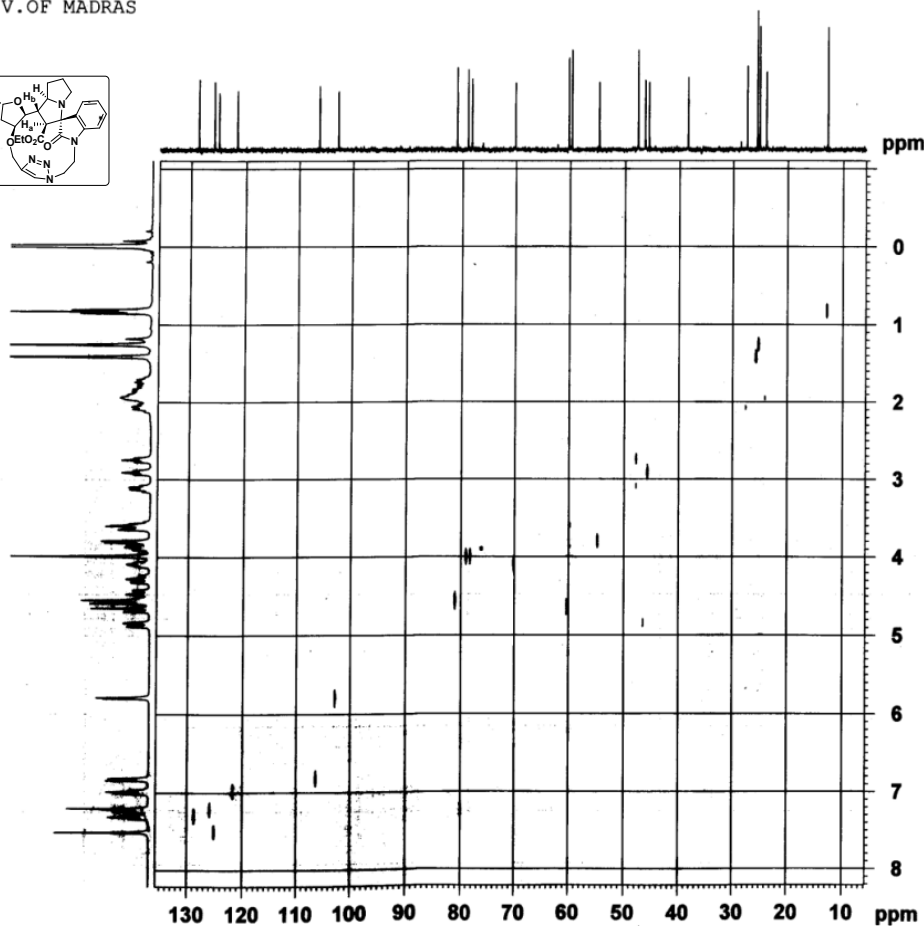
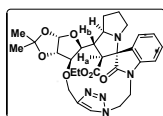


Figure 3.7d. H-H COSY spectrum of 10a

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EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
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Time 23.28
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PULPROG hxcqf
TD 4096
SOLVENT CDCl3
NS 20
DS 4
SWH 9803.922 Hz
FIDRES 2.393536 Hz
AQ 0.2089460 sec
RG 26008
DW 51.000 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.000000
CNST11 3.000000
d0 0.00000300 sec
d1 1.95821595 sec
d2 0.00344828 sec
d3 0.00229885 sec
d11 0.03000000 sec
d12 0.00002000 sec
INO 0.00017880 sec

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P1 9.30 usec
p2 18.60 usec
PL1 0.00 dB
SFO1 75.4731657 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 13.15 usec
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
SFO2 300.1310904 MHz

F1 - Acquisition parameters
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FIDRES 18.642803 Hz
SW 9.317 ppm
FnMODE QF

F2 - Processing Parameters

Figure 3.7e. C-H COSY spectrum of 10a

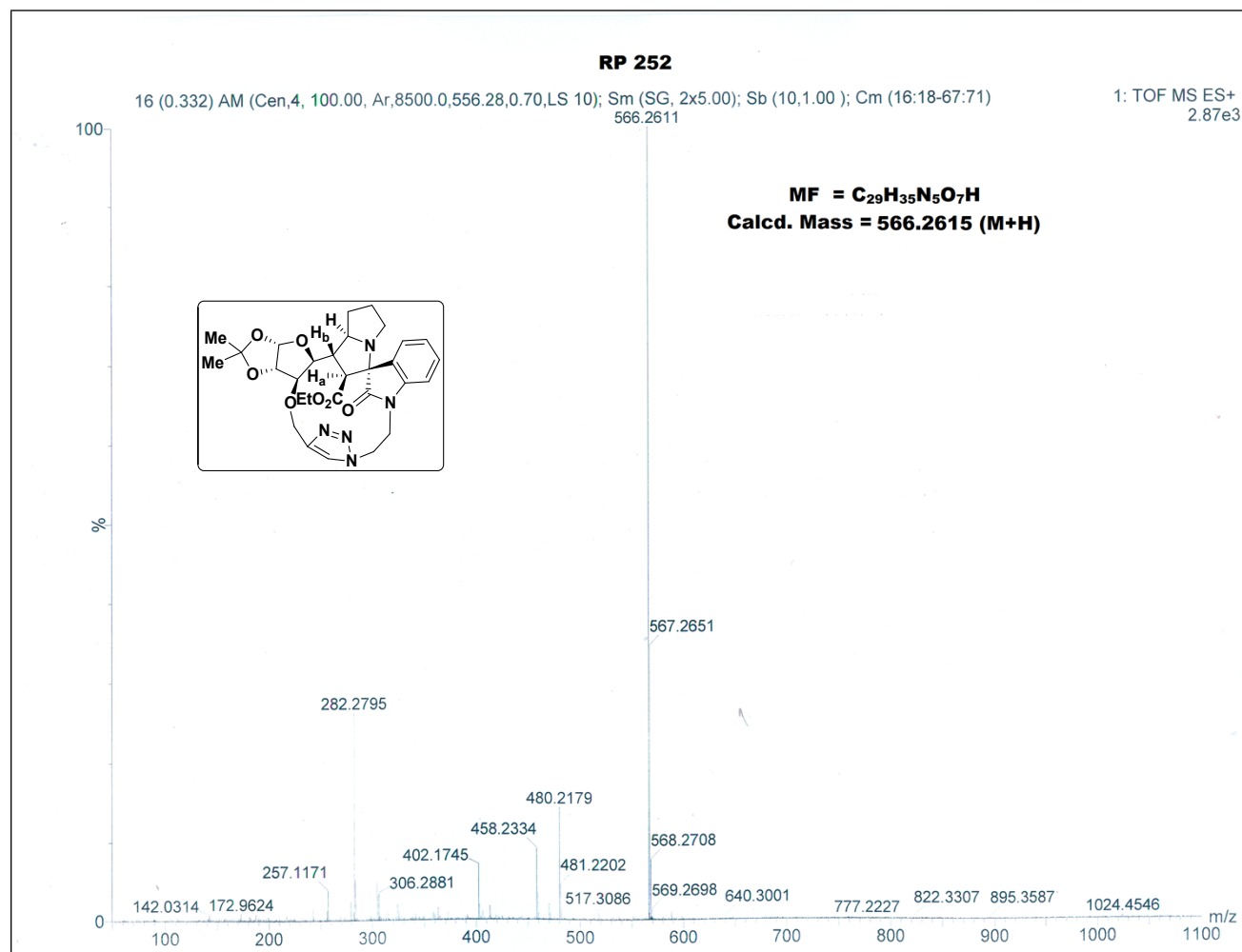


Figure 3.7f. HRMS spectrum of 10a

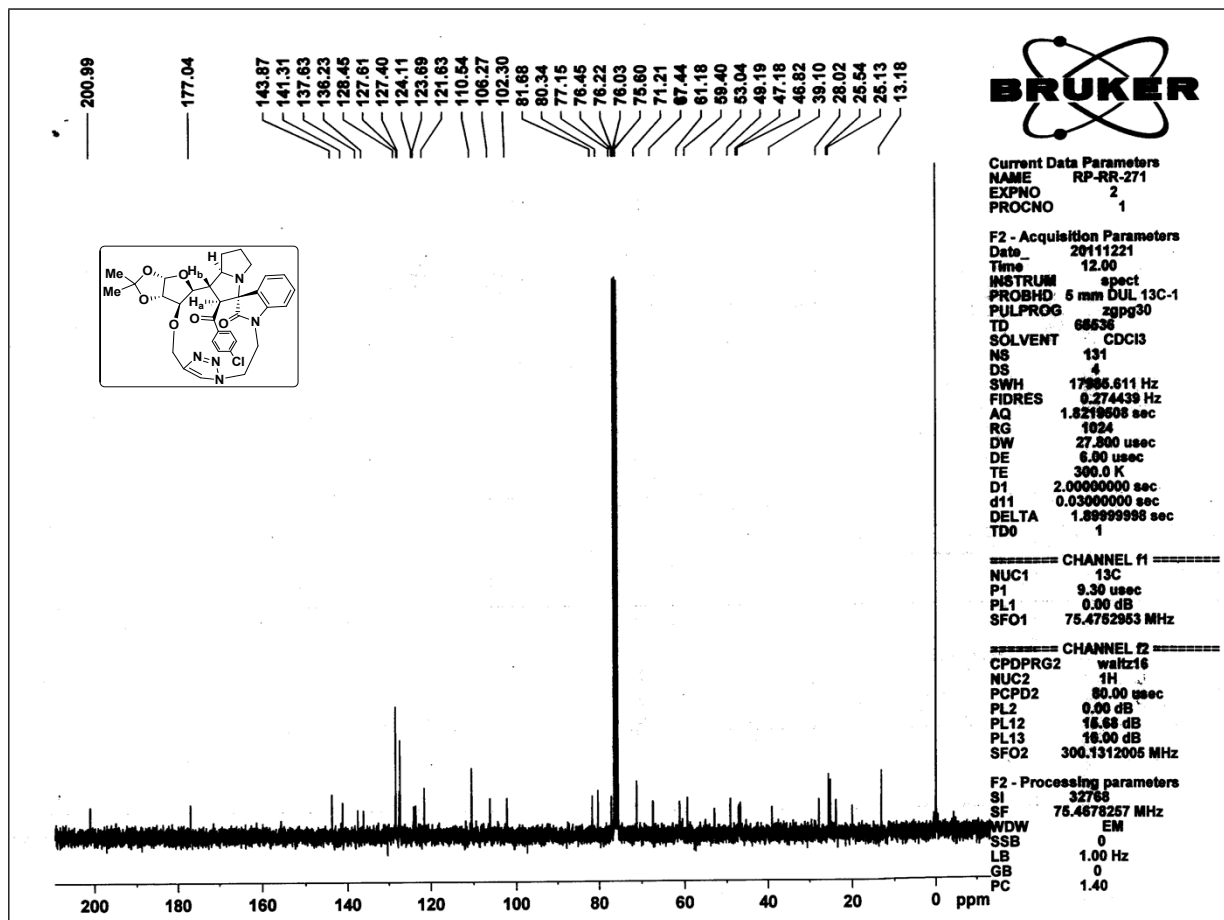


Figure 3.8b. ^{13}C NMR (CDCl_3 , 75MHz) of 10b

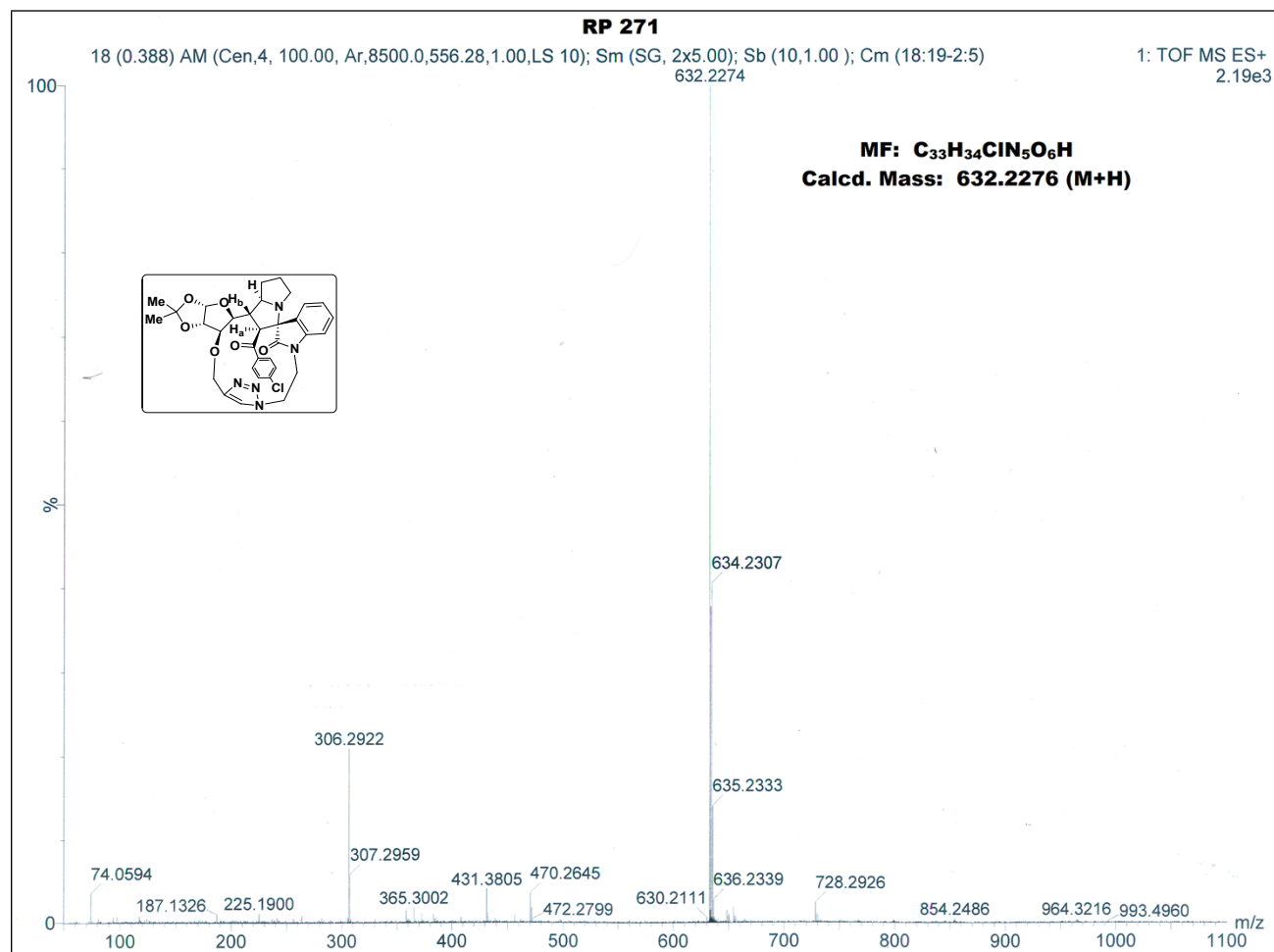
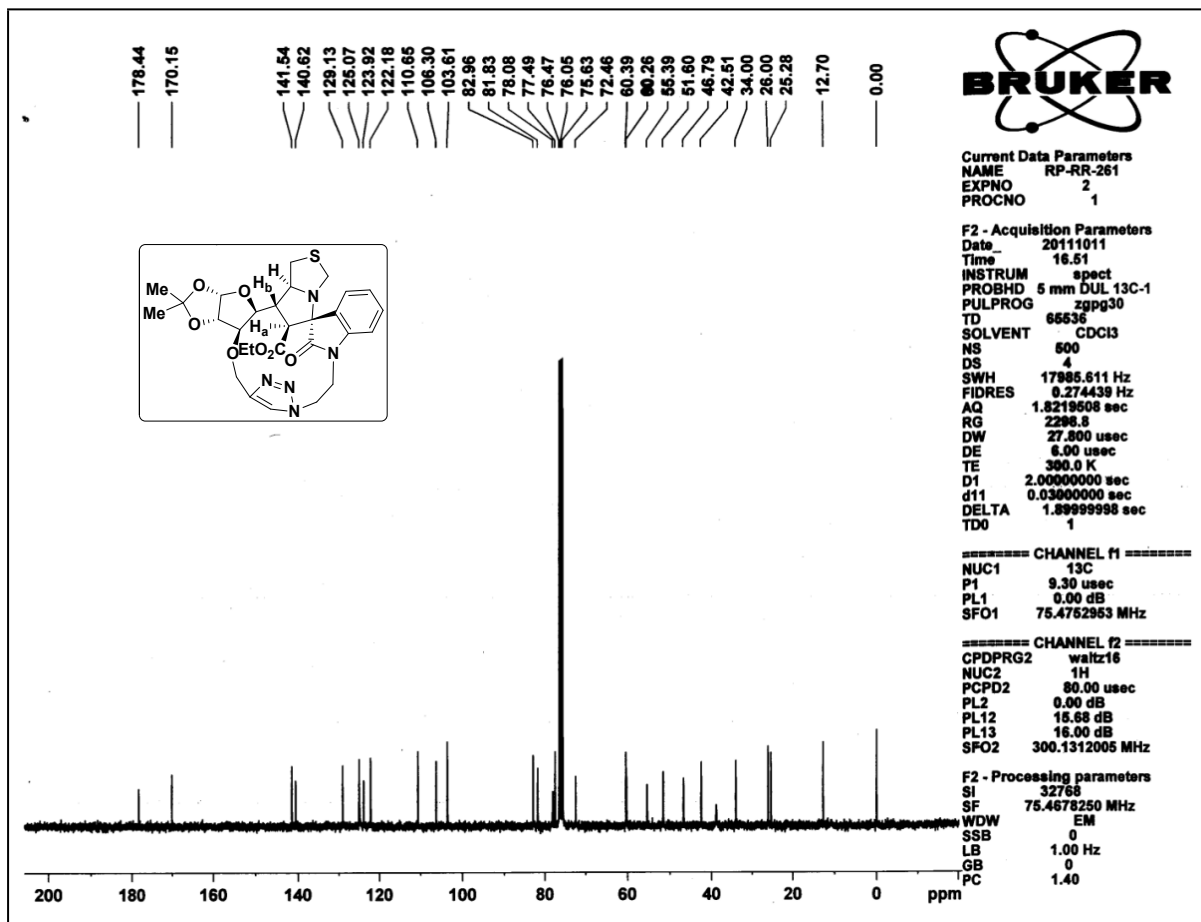


Figure 3.8d. HRMS spectrum of 10b



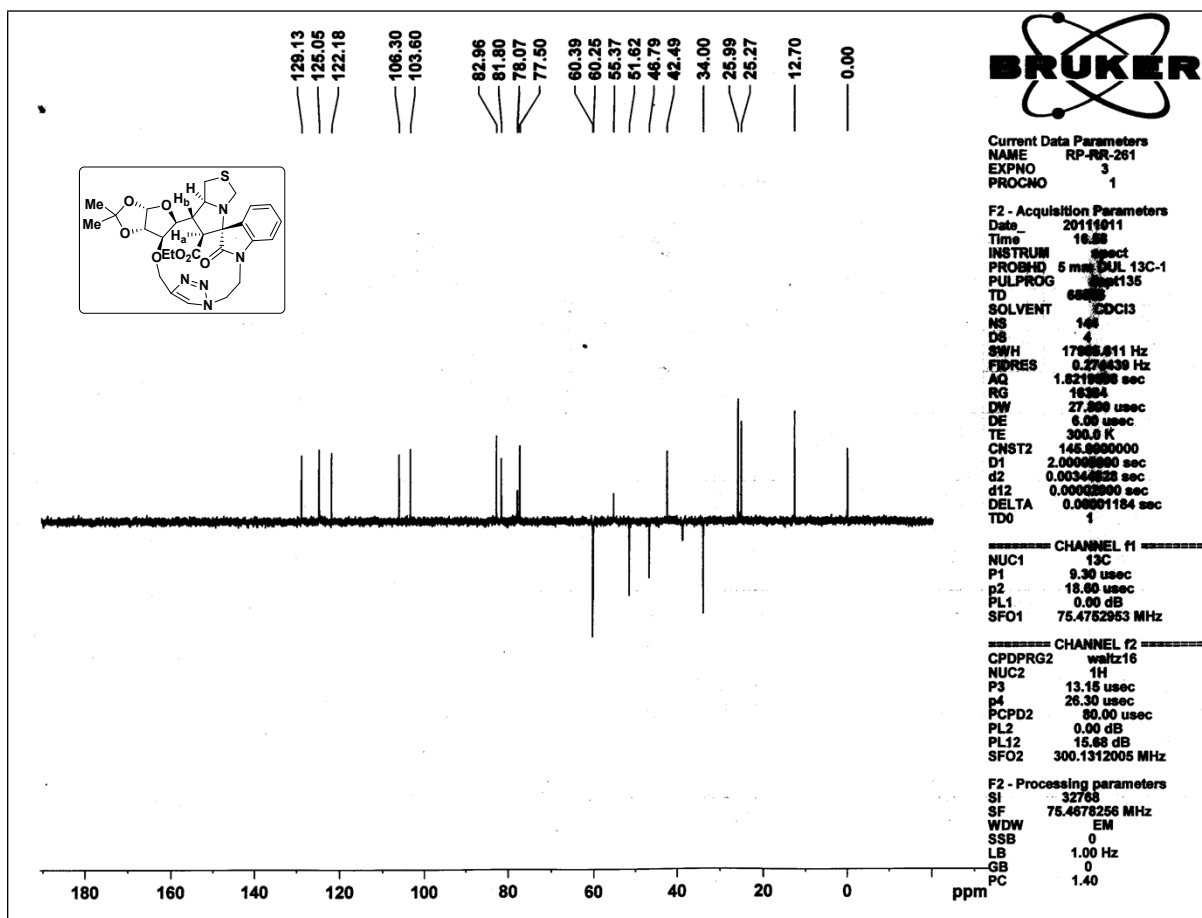


Figure 3.9c. DEPT 135 (CDCl₃, 75MHz) of 10c

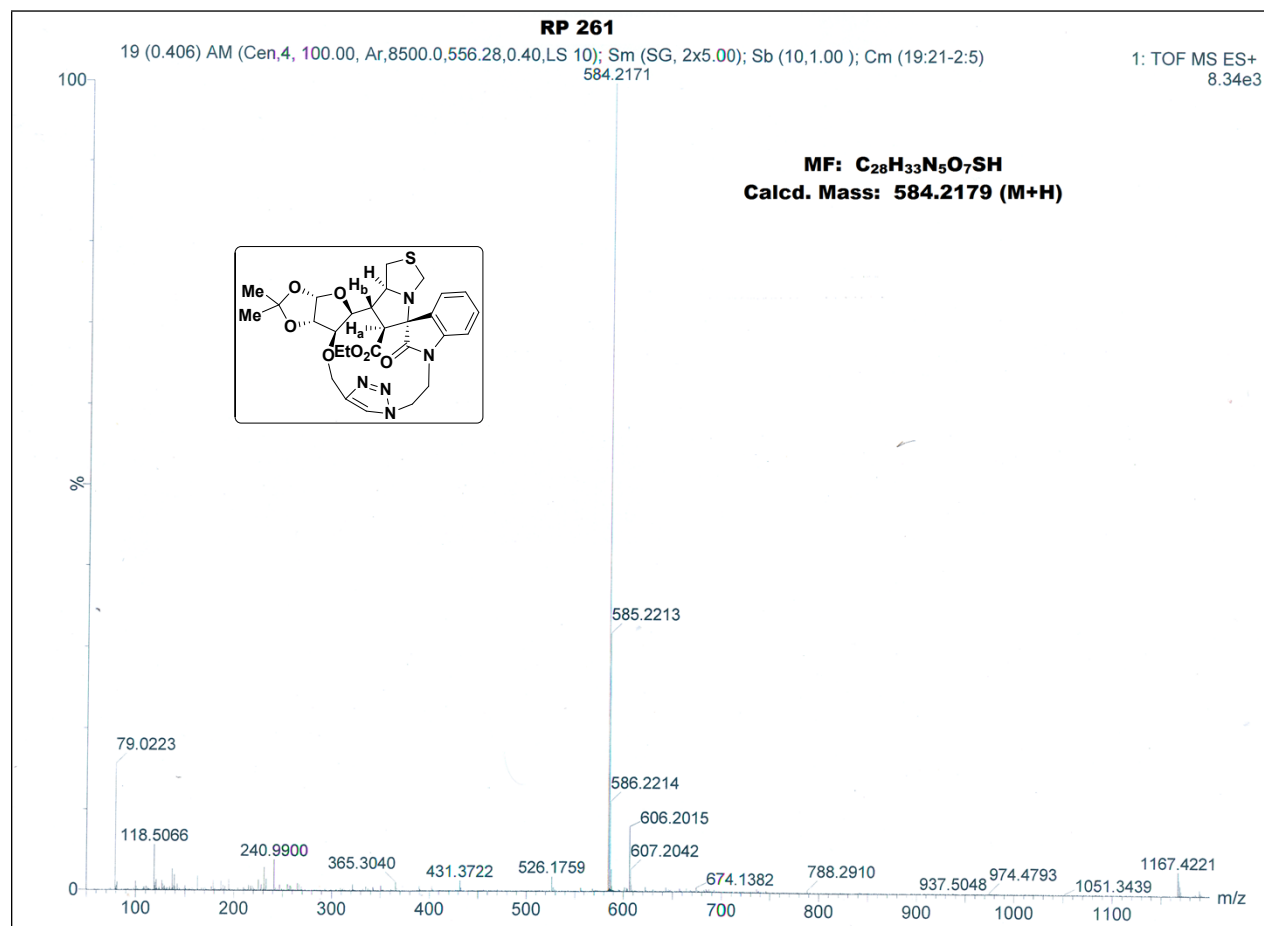


Figure 3.9d. HRMS spectrum of 10c

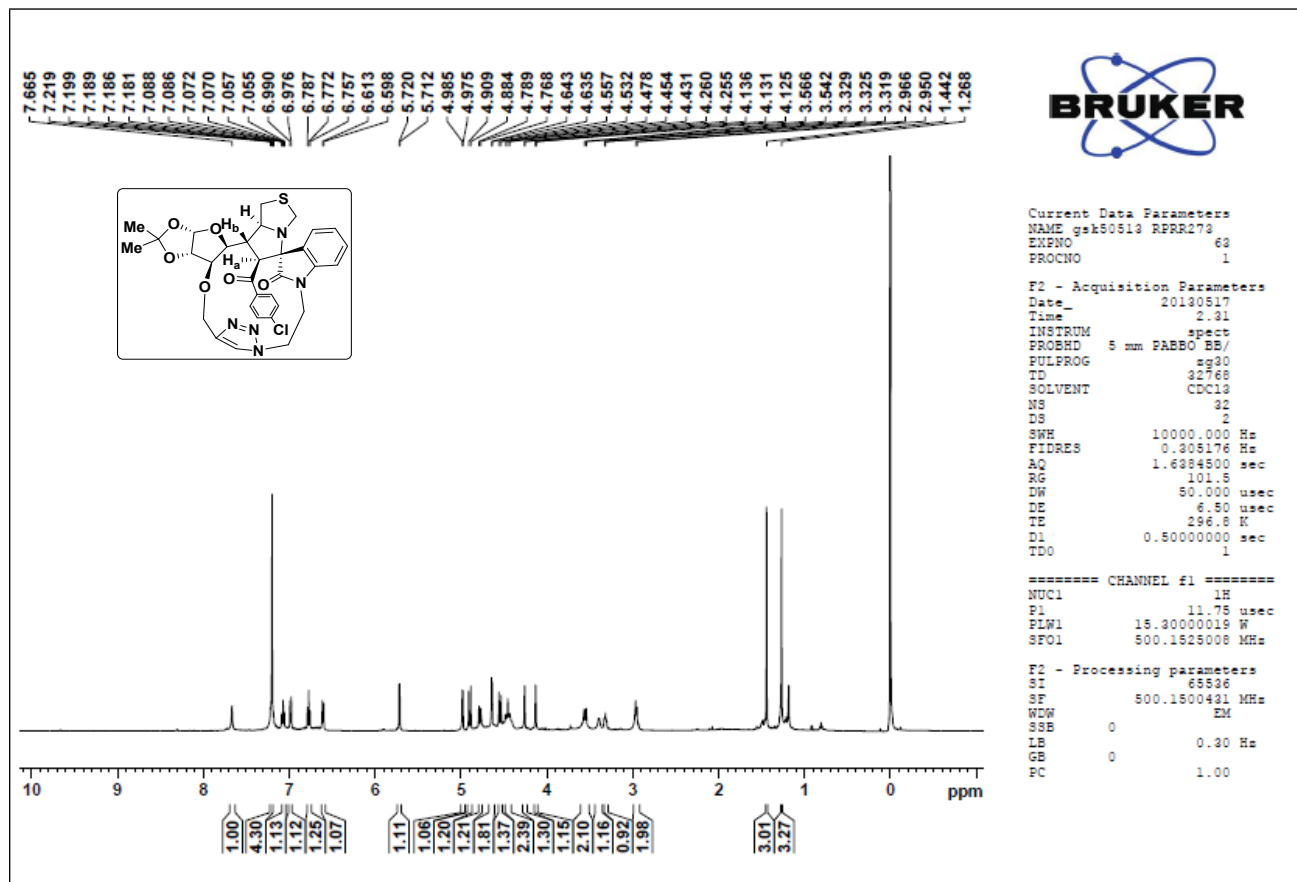


Figure 3.10a. ^1H NMR (500MHz, CDCl_3) spectrum of **10d**

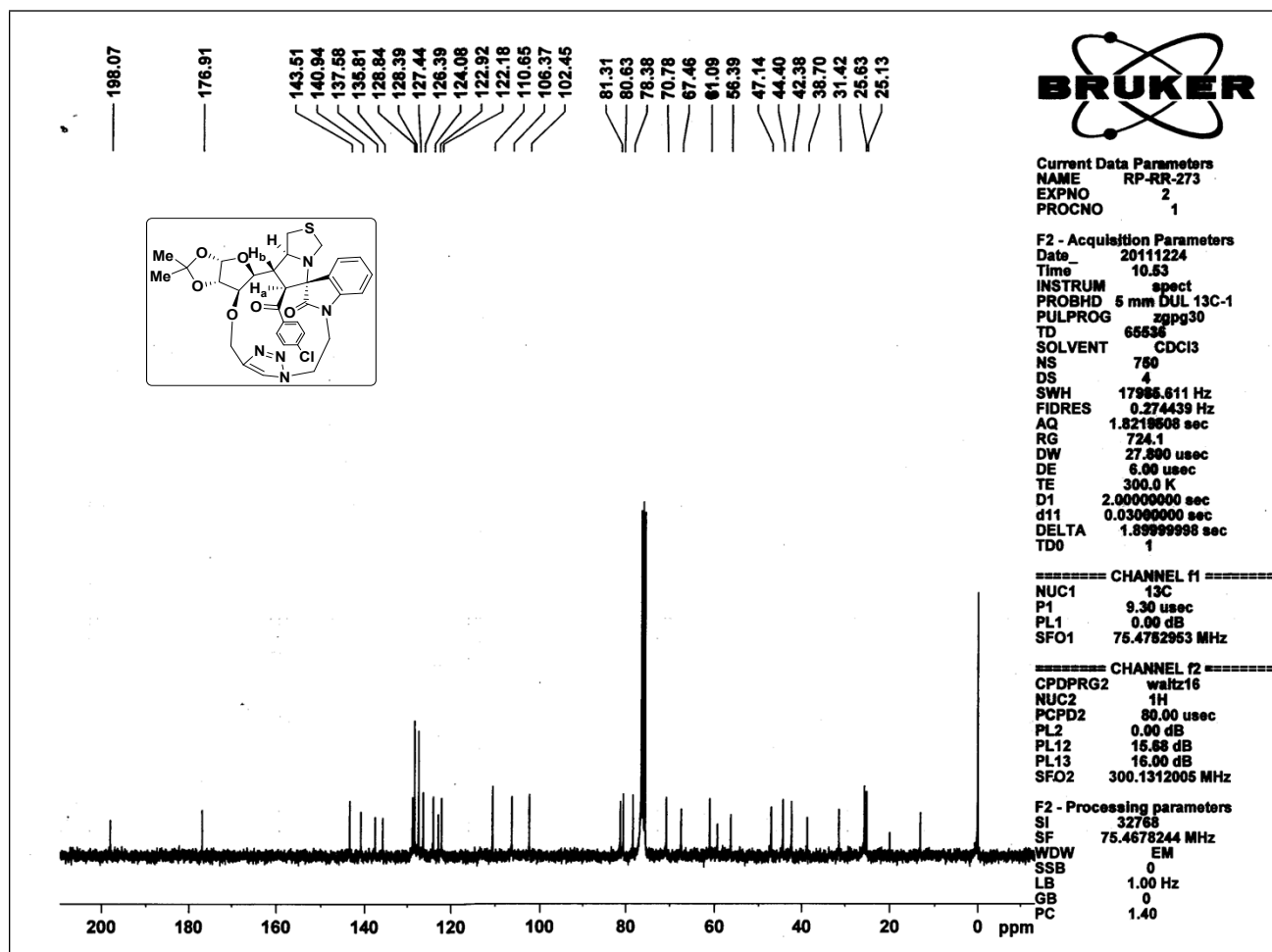


Figure 3.10b. ¹³C NMR (CDCl₃, 75MHz) of 10d

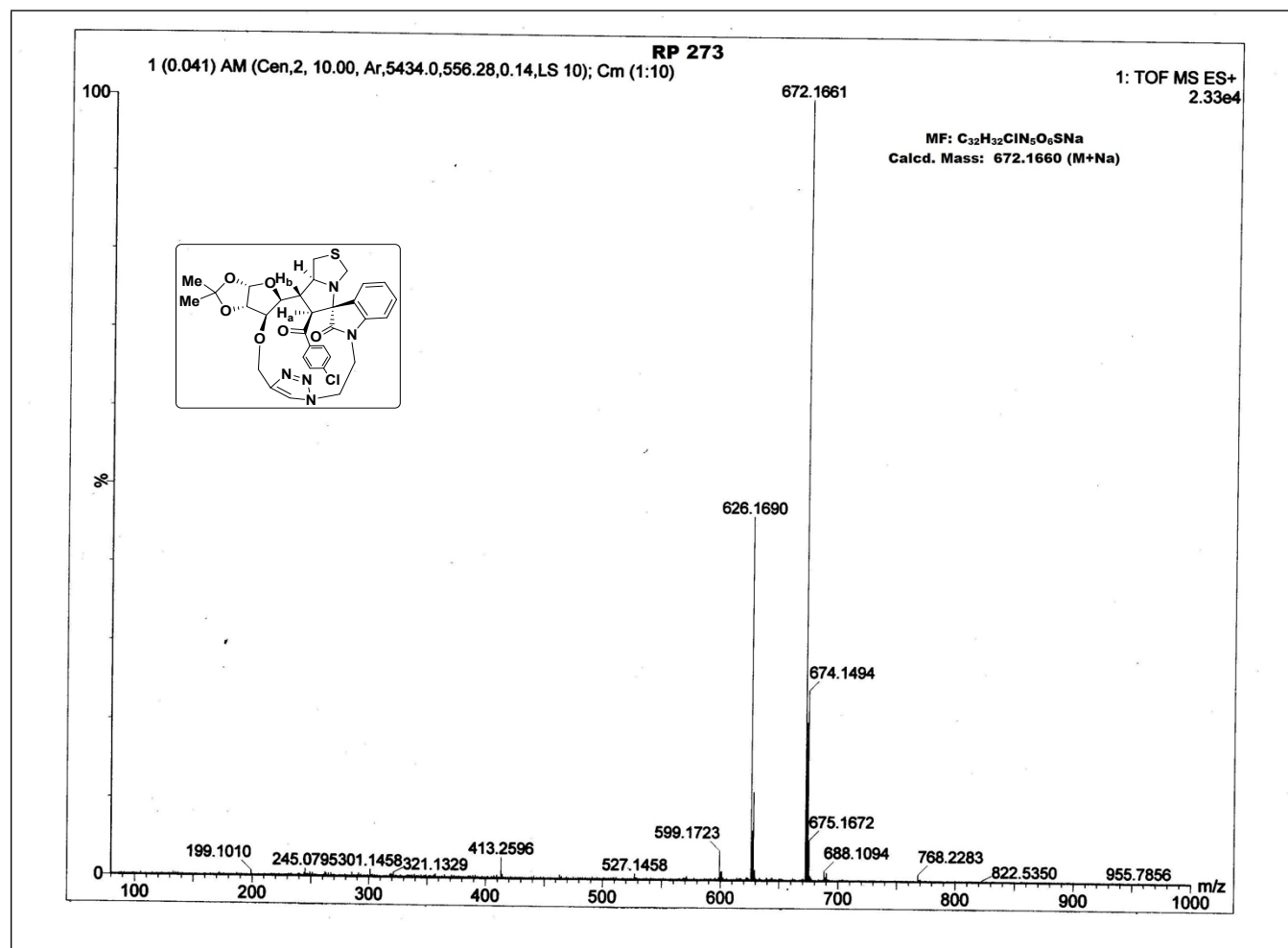
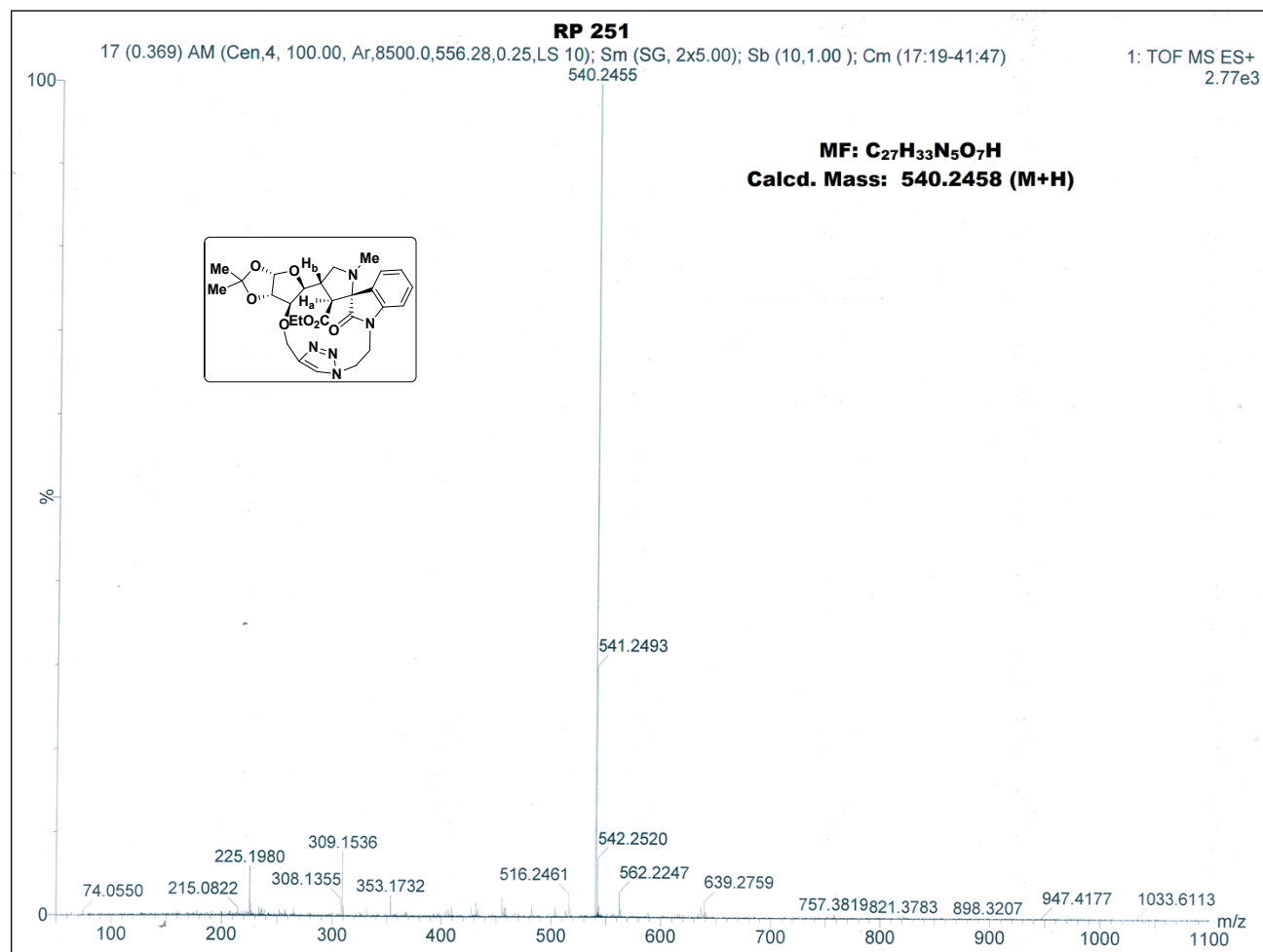


Figure 3.10d. HRMS spectrum of 10d



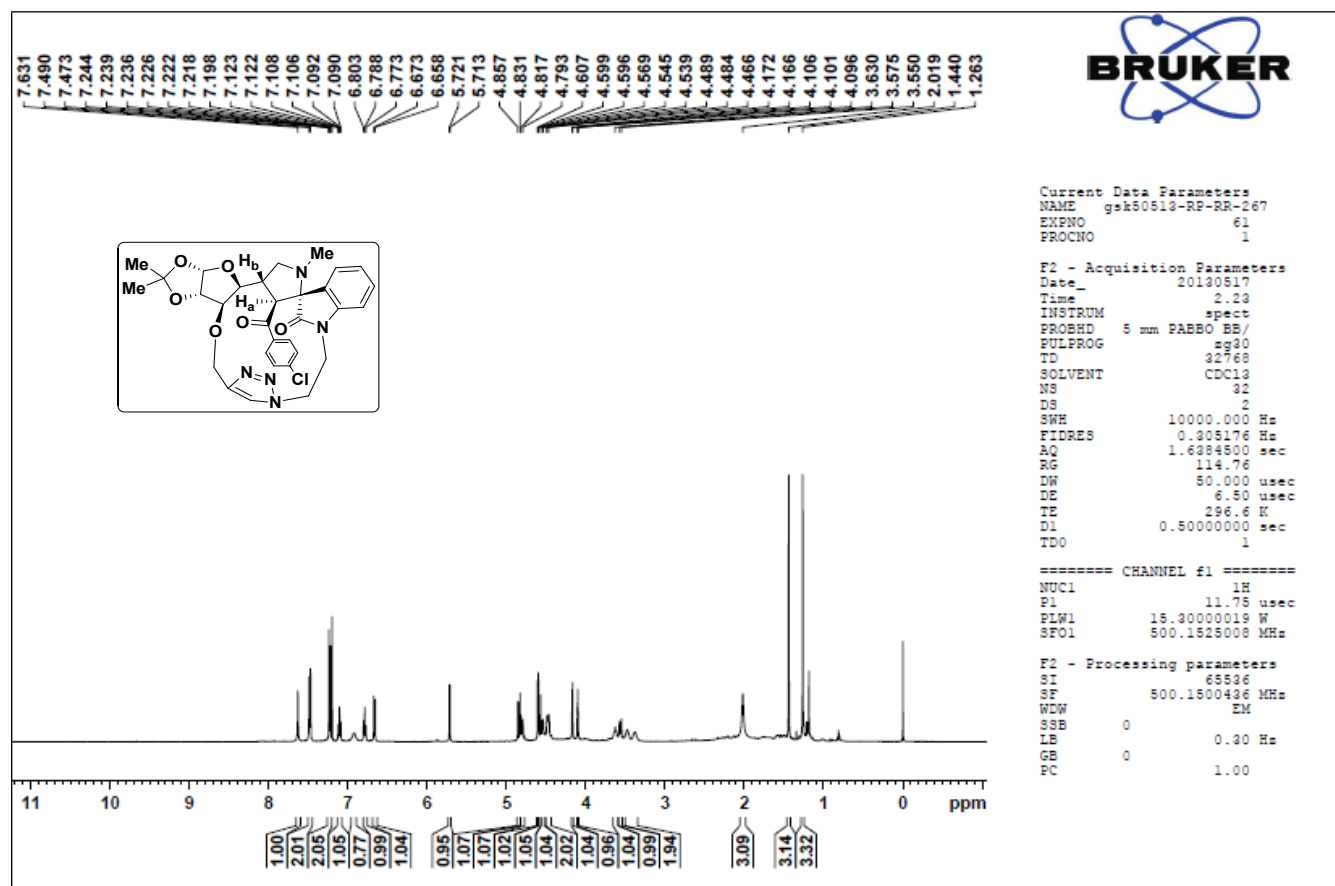
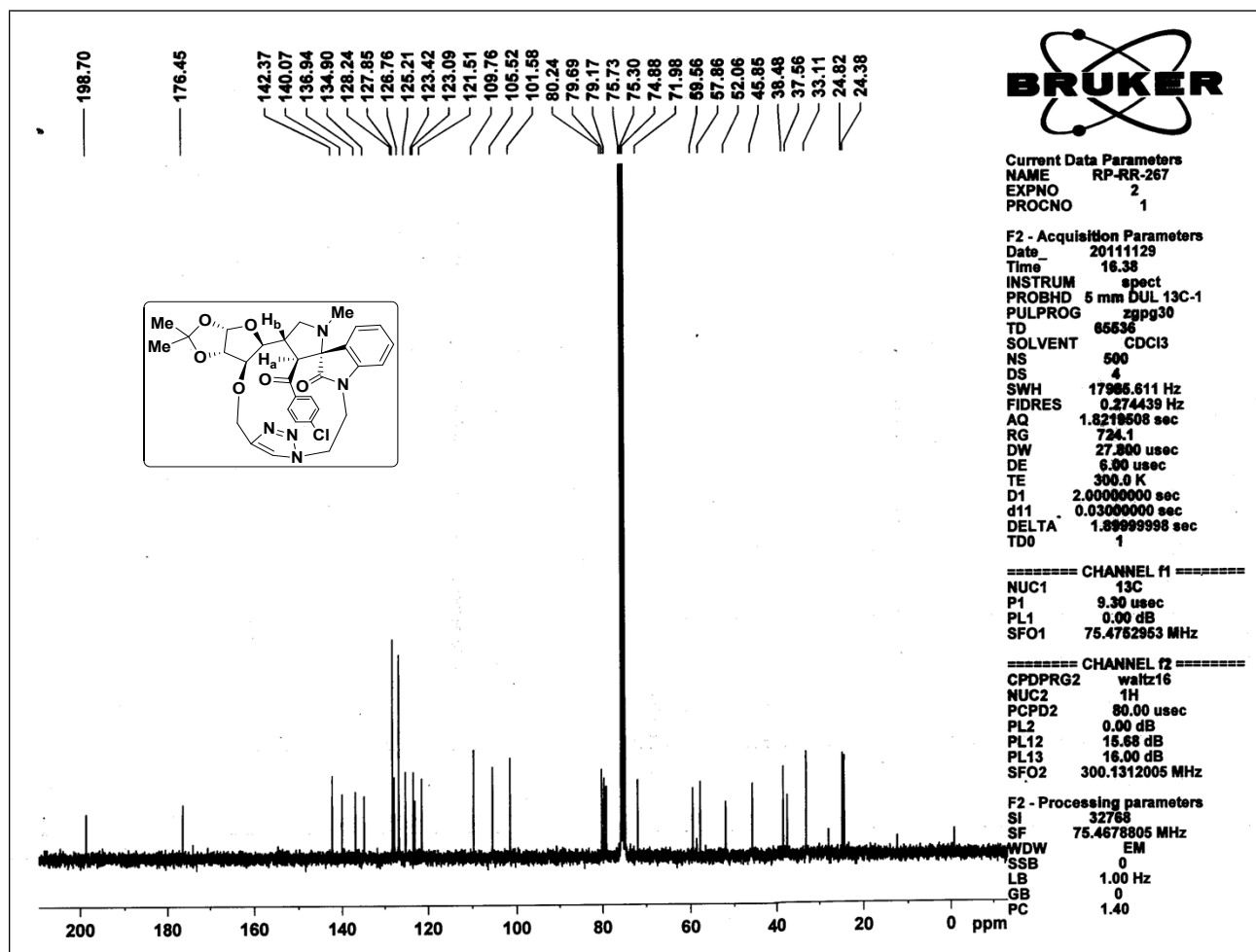


Figure 3.12a. ^1H NMR (500MHz, CDCl_3) spectrum of **10f**



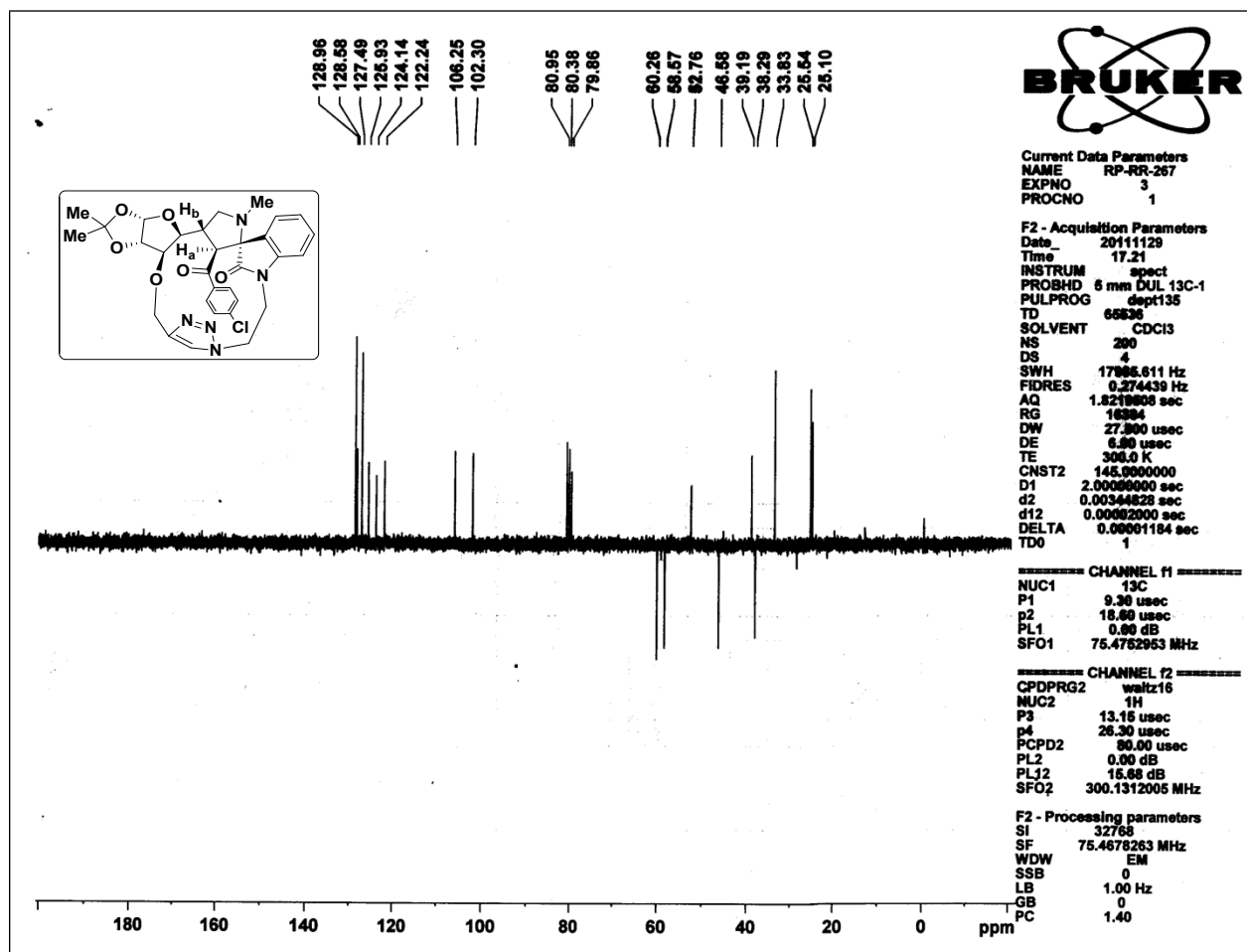


Figure 3.12c. DEPT 135 (CDCl₃, 75MHz) of 10f

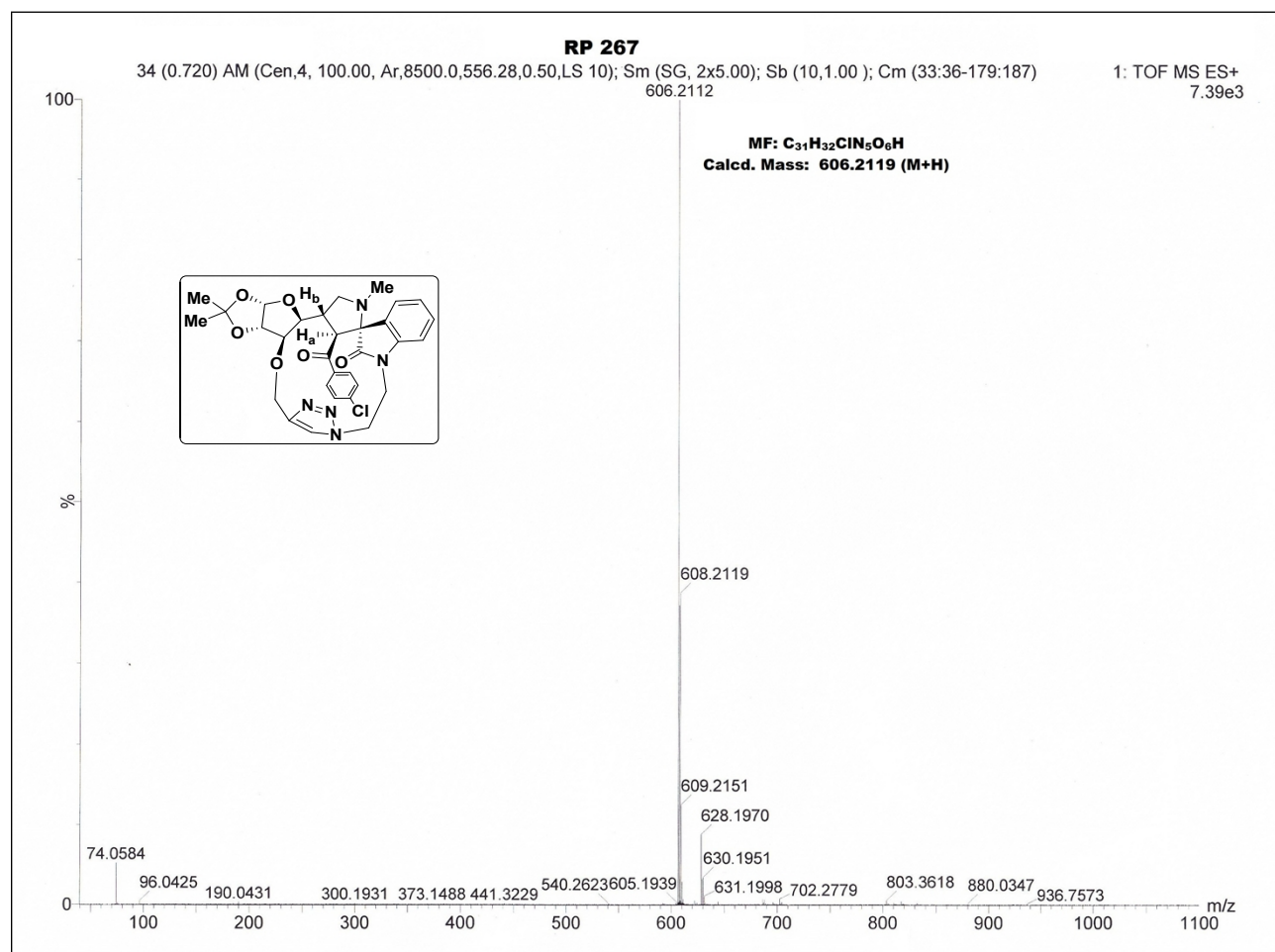


Figure 3.12d. HRMS spectrum of 10f

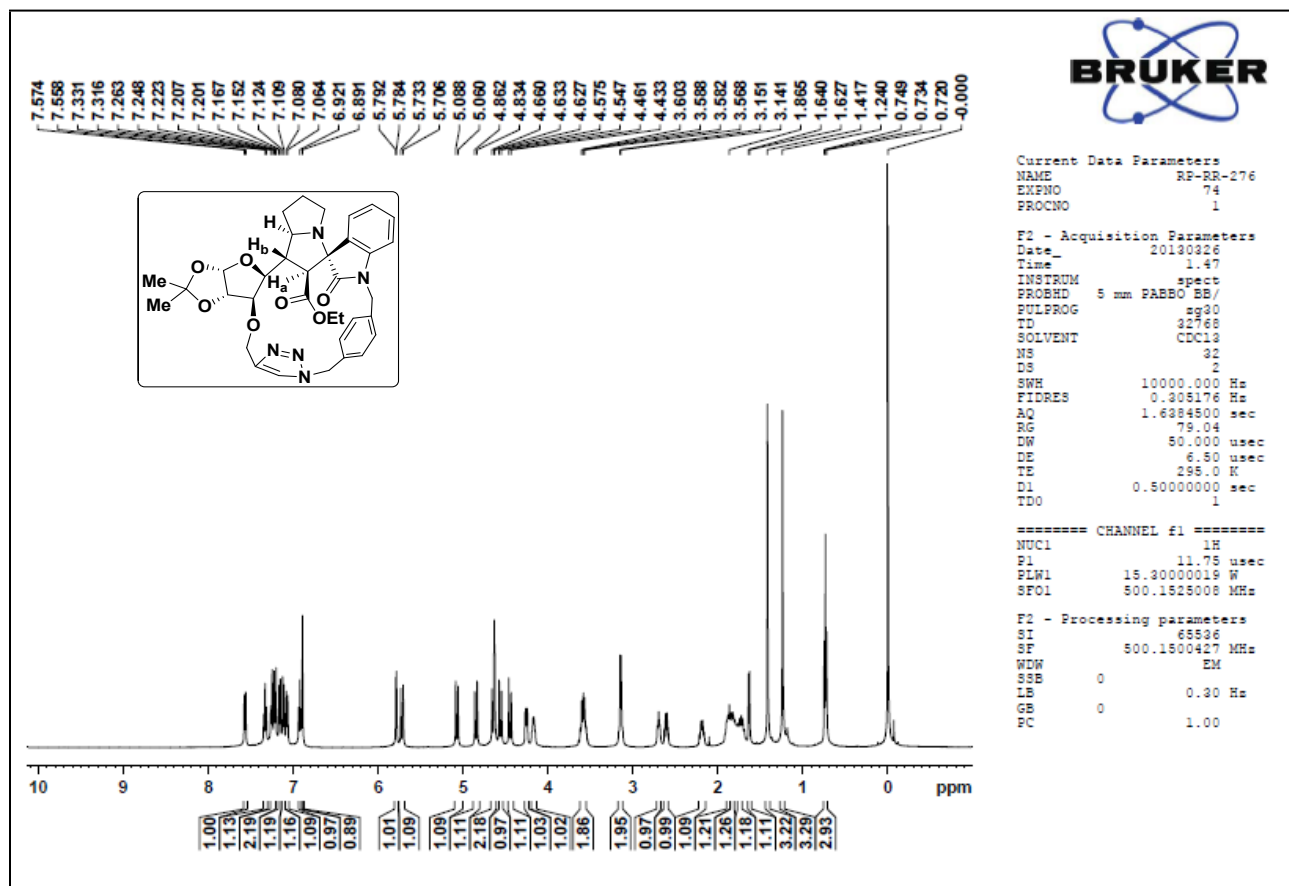


Figure 3.13a. ¹H NMR (500MHz, CDCl₃) spectrum of 11a

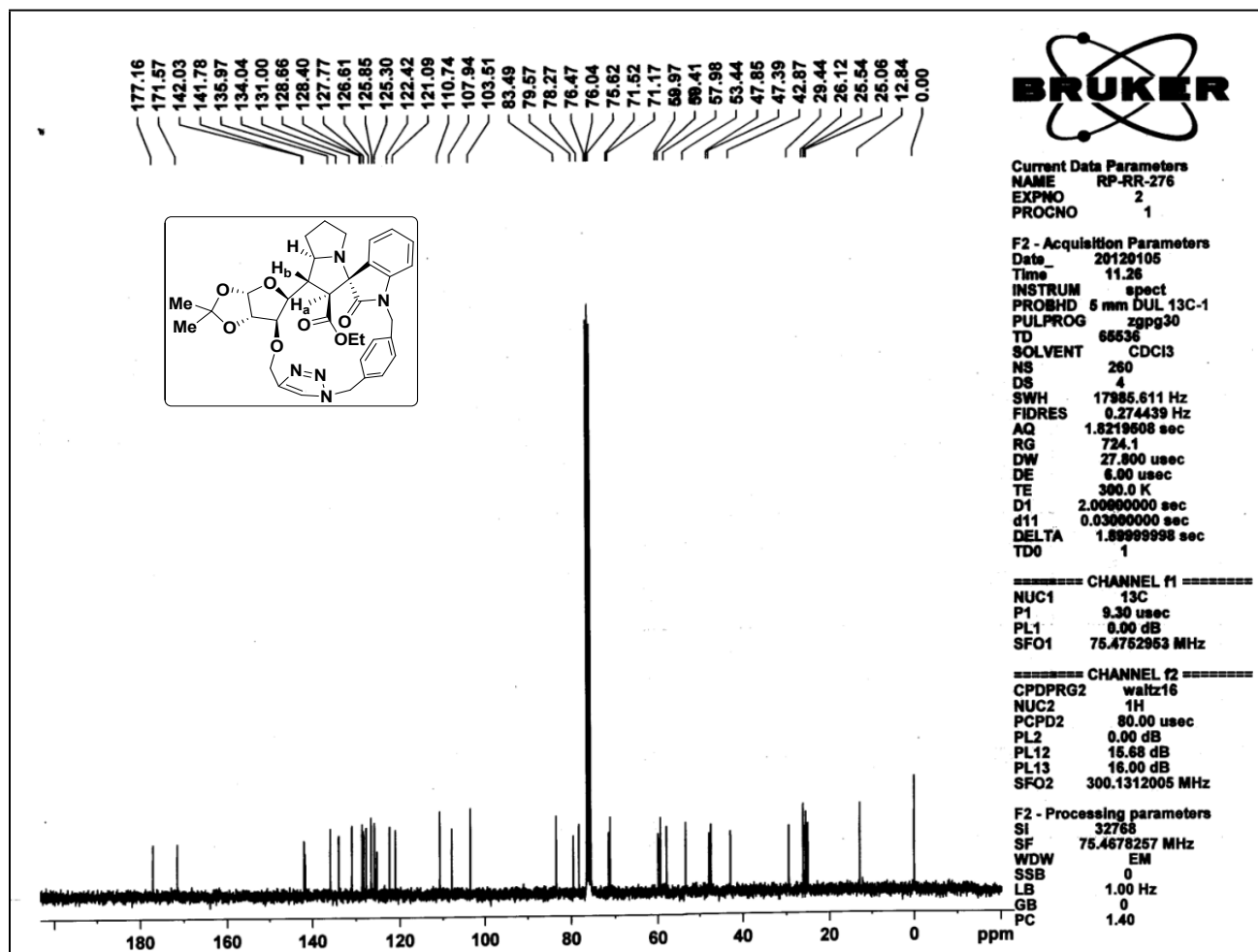
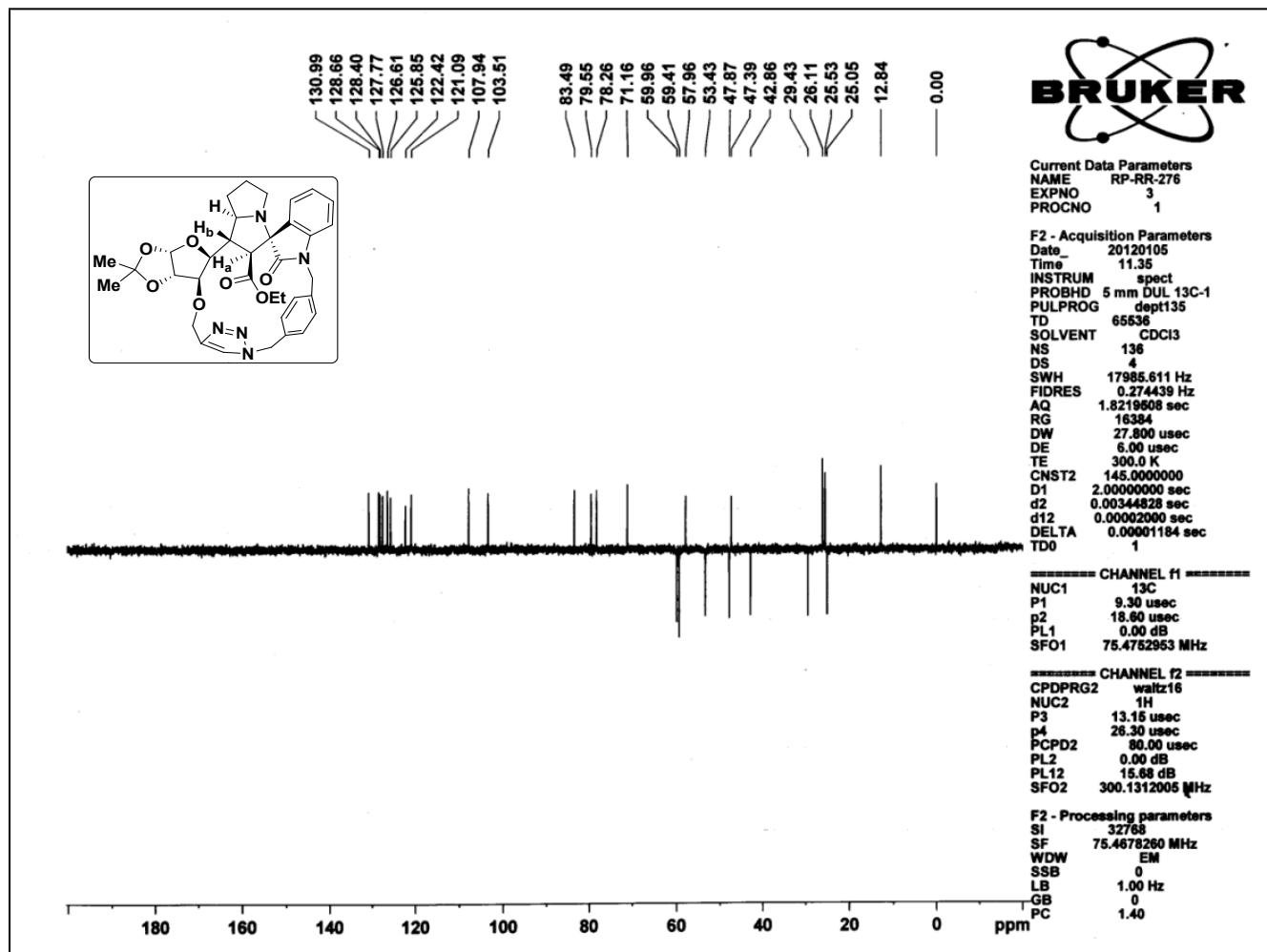


Figure 3.13b. ¹³C NMR (CDCl₃, 75MHz) of 11a



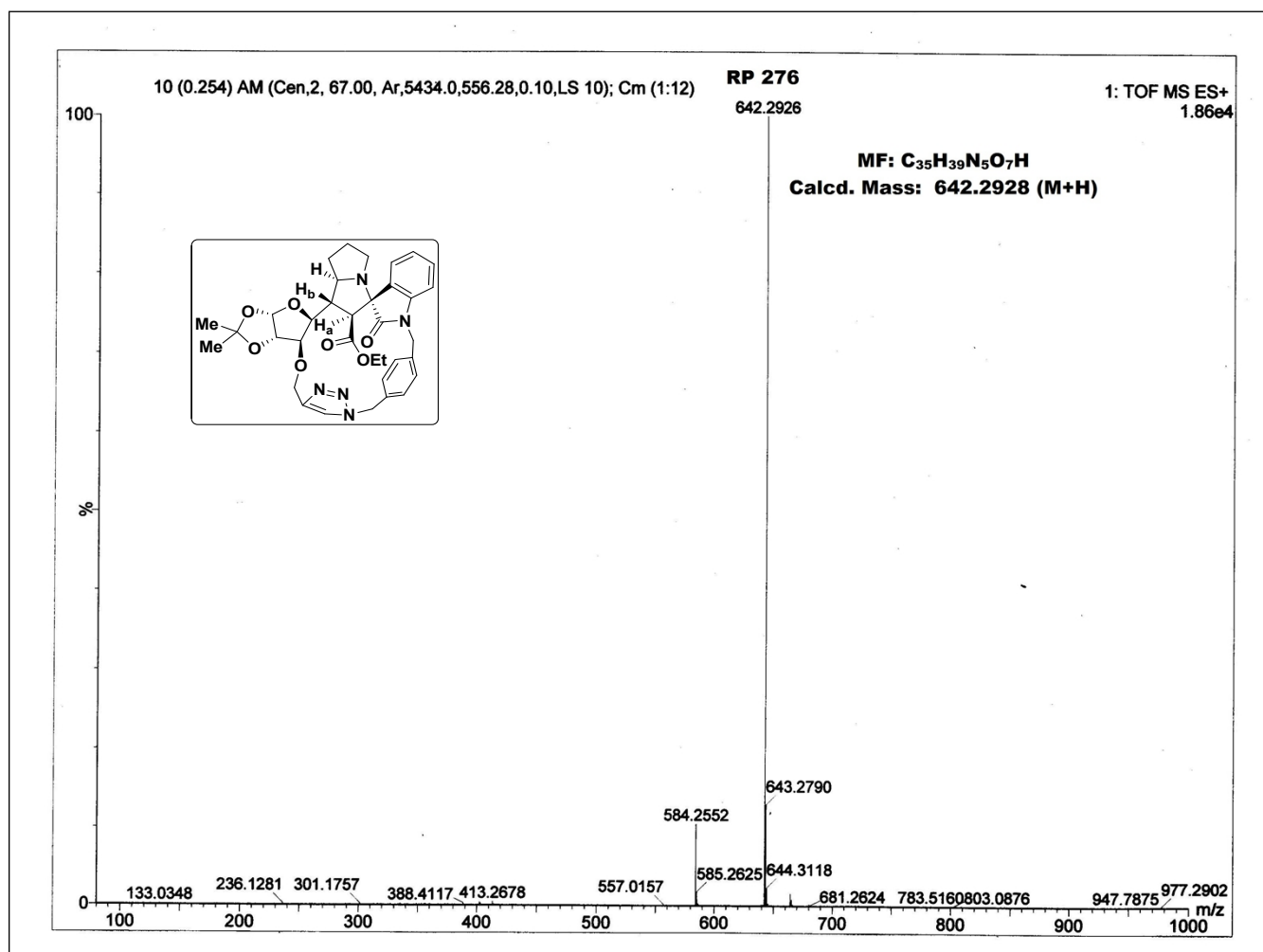
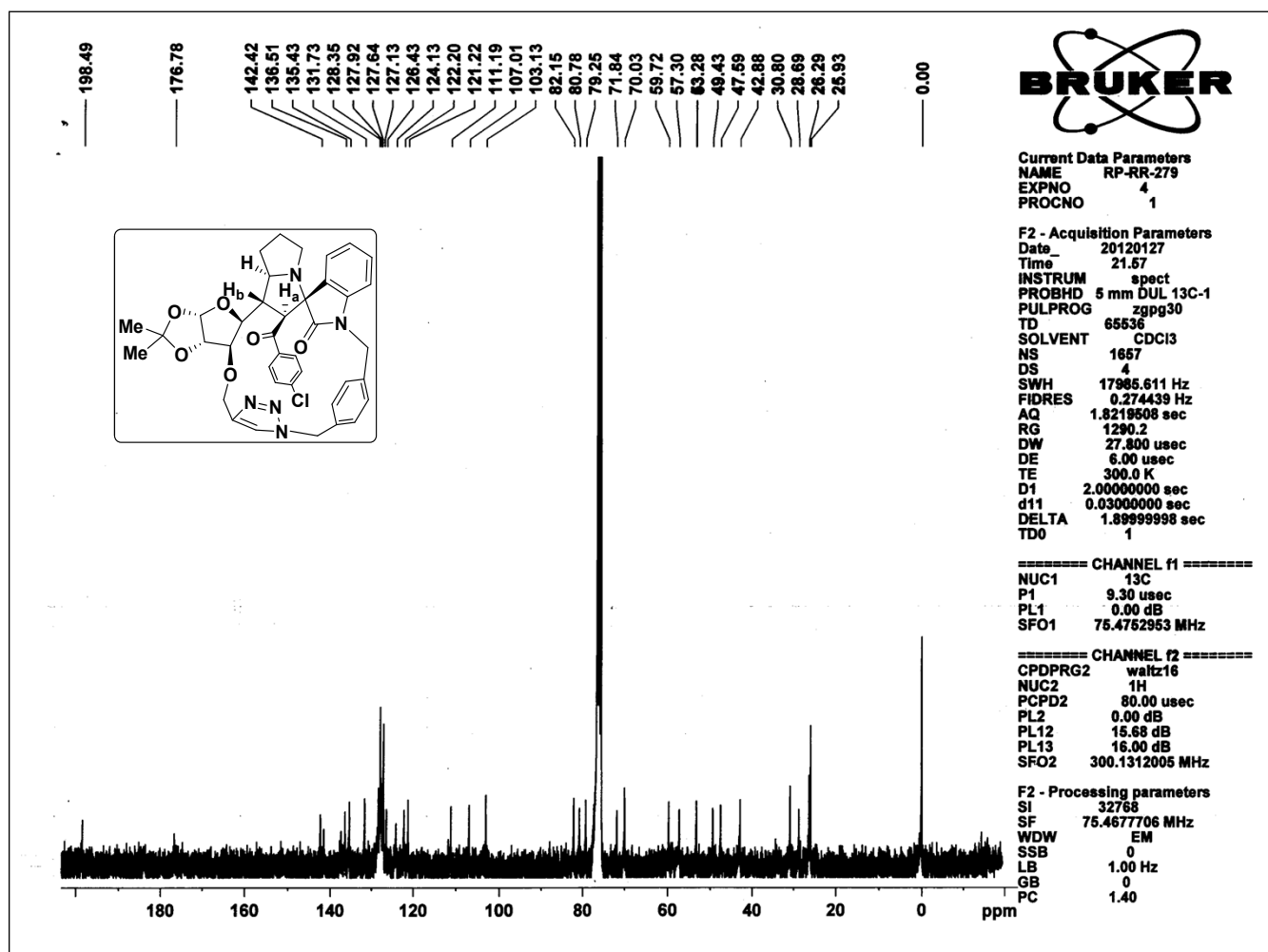
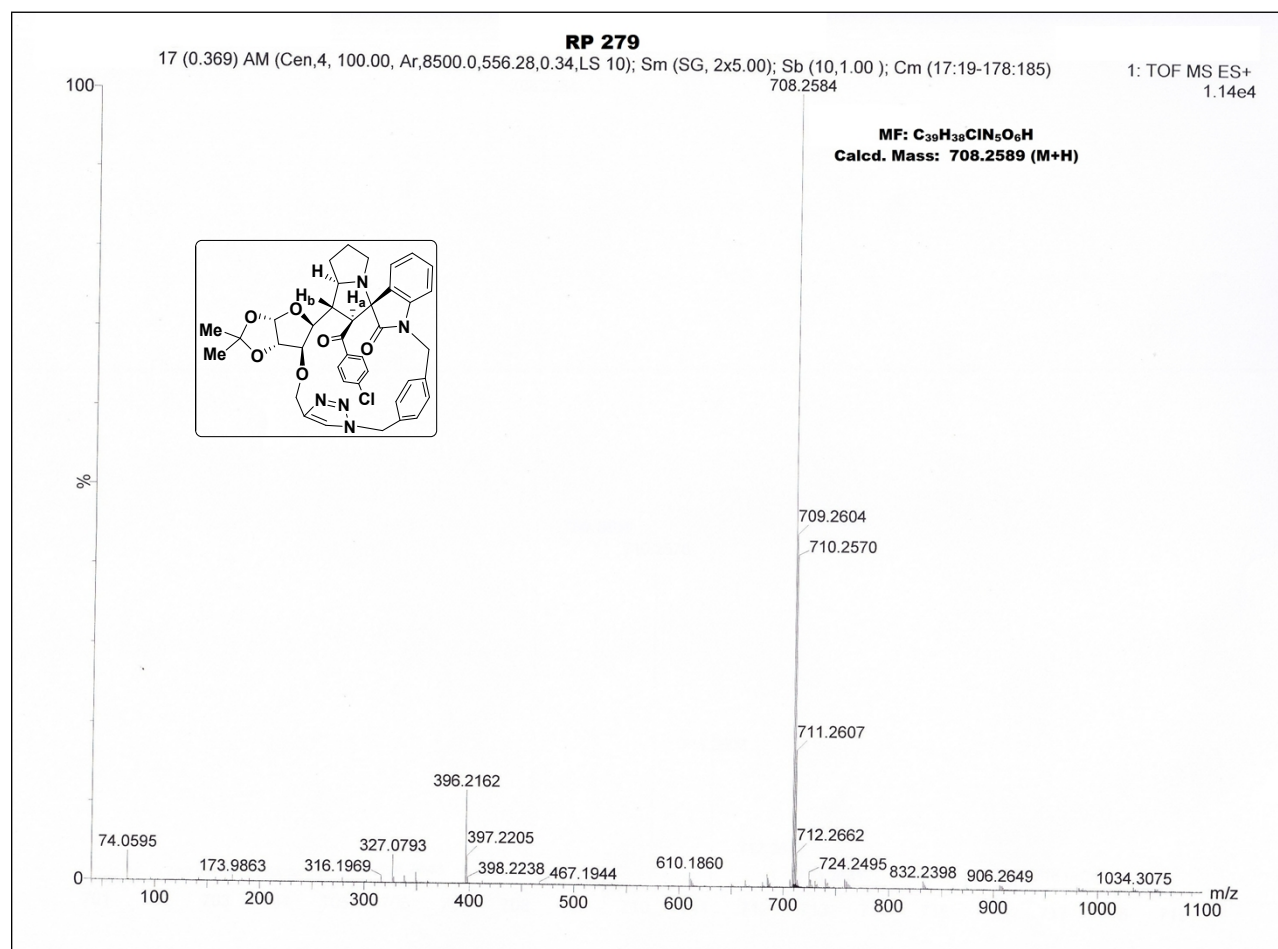


Figure 3.13d. ESI-MS spectrum of 11a





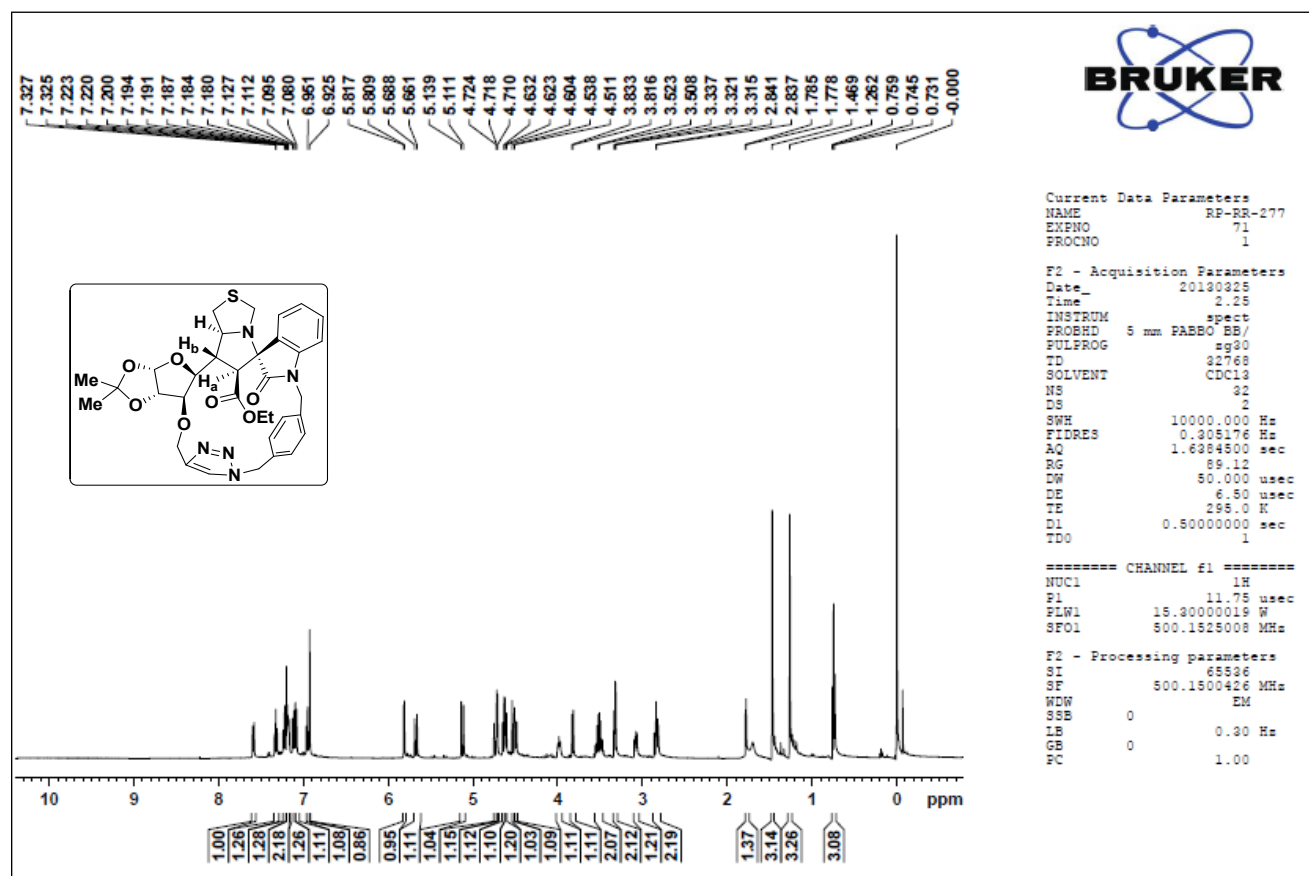


Figure 3.15a. ¹H NMR (500MHz, CDCl₃) spectrum of 11c

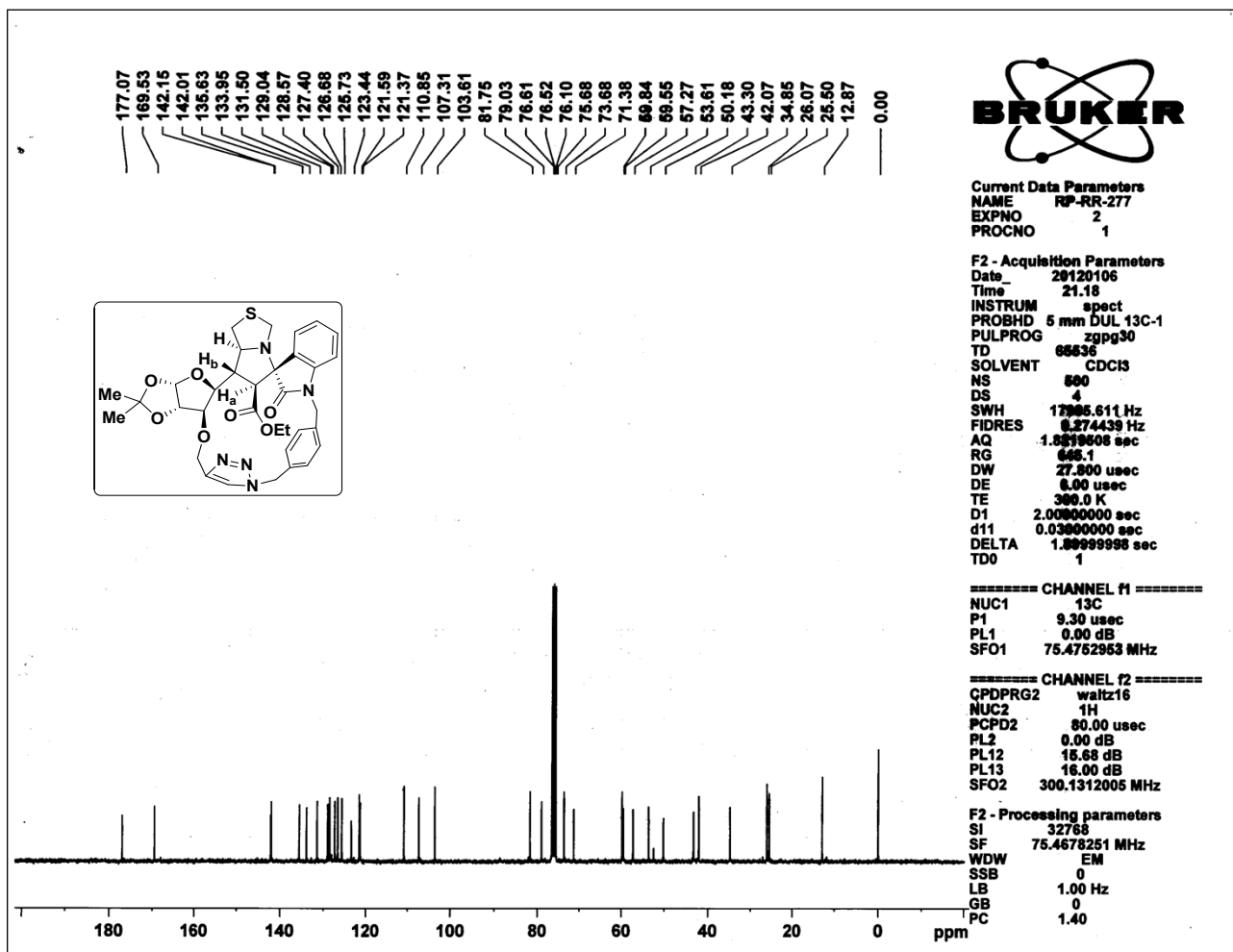


Figure 3.15b. ^{13}C NMR (CDCl_3 , 75MHz) of 11c

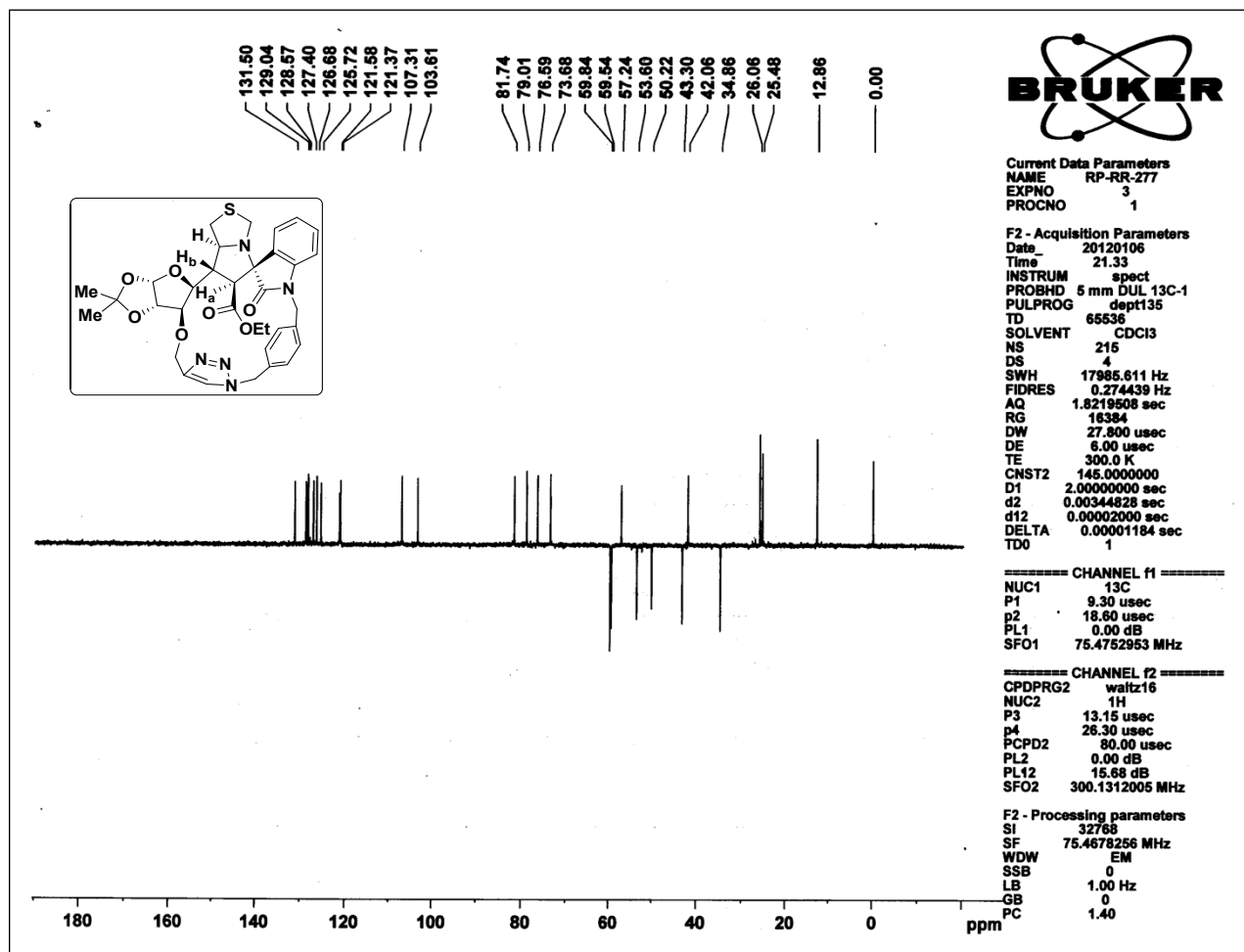


Figure 3.15c. DEPT 135 (CDCl₃, 75MHz) of 11c

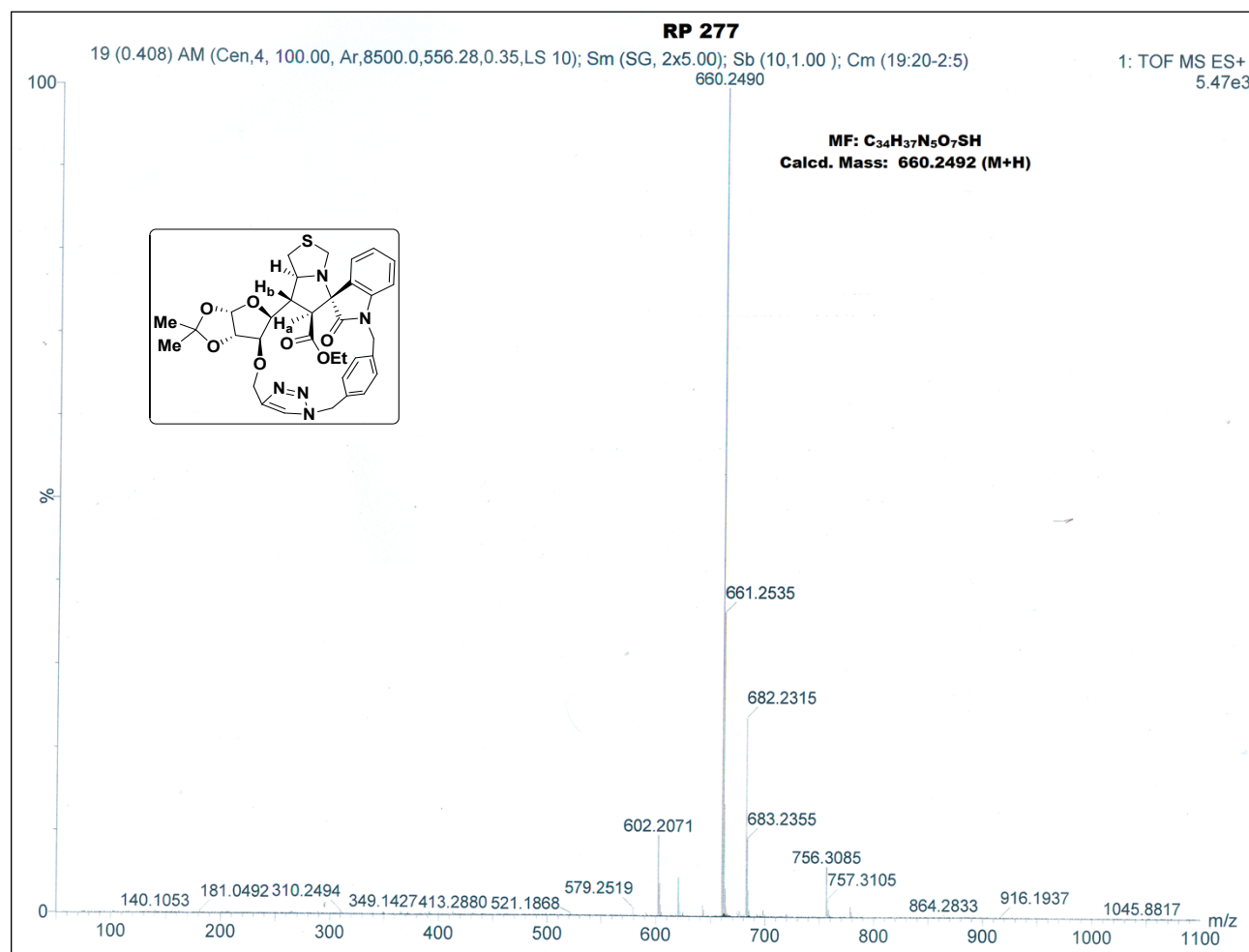


Figure 3.15d. ESI-MS spectrum of 11c

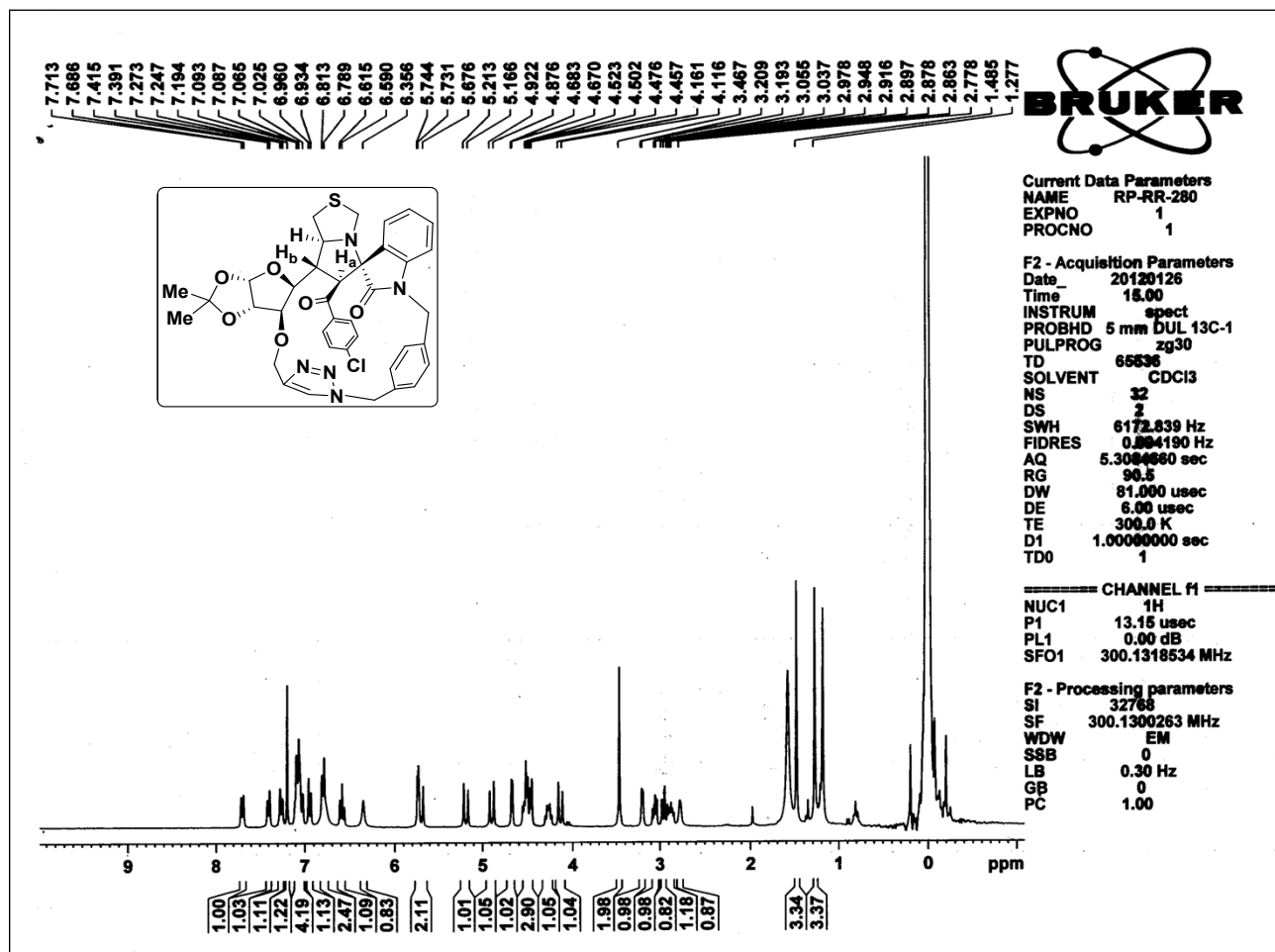


Figure 3.16a. ¹H NMR (300MHz, CDCl₃) spectrum of 11d

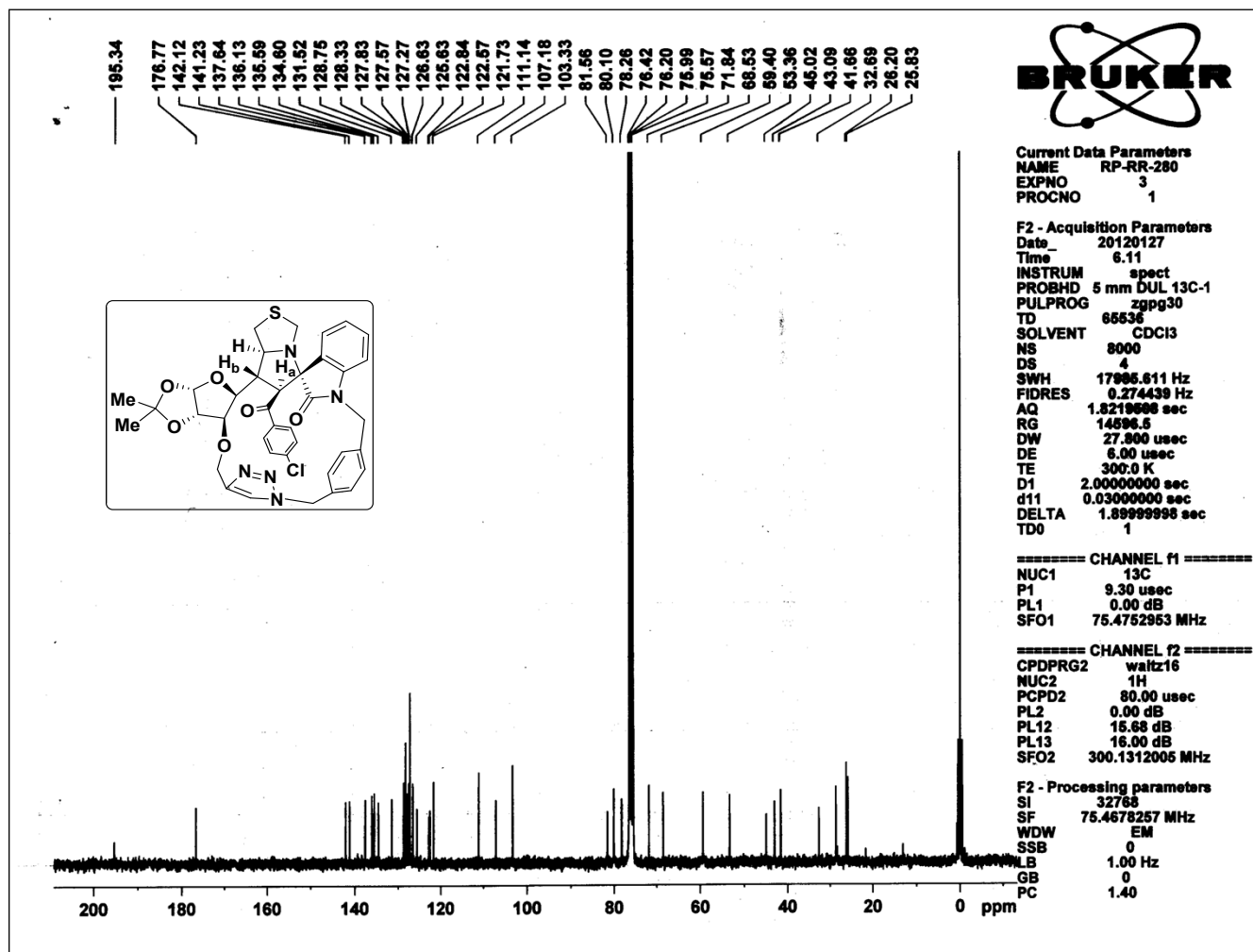


Figure 3.16b. ^{13}C NMR (CDCl_3 , 75MHz) of 11d

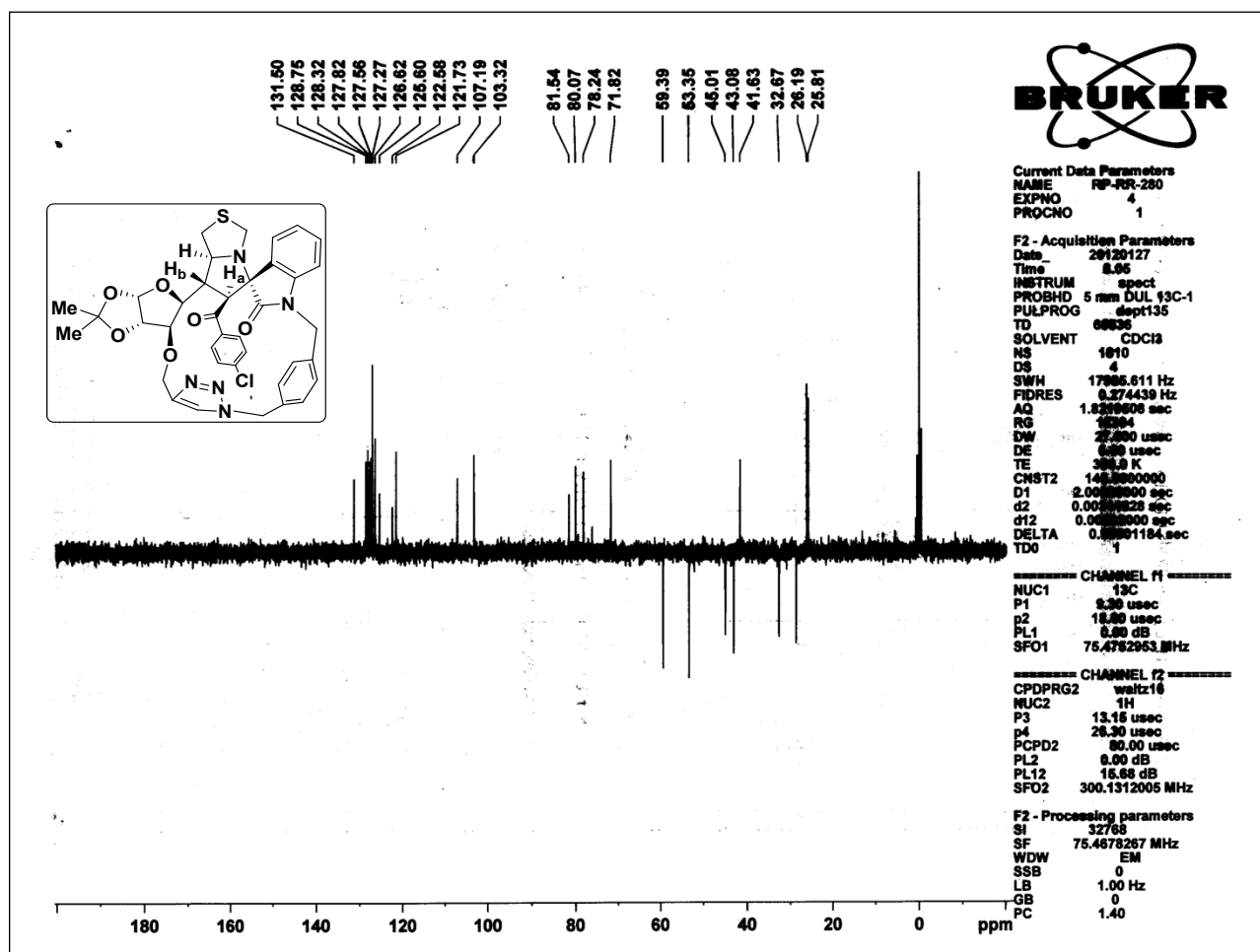
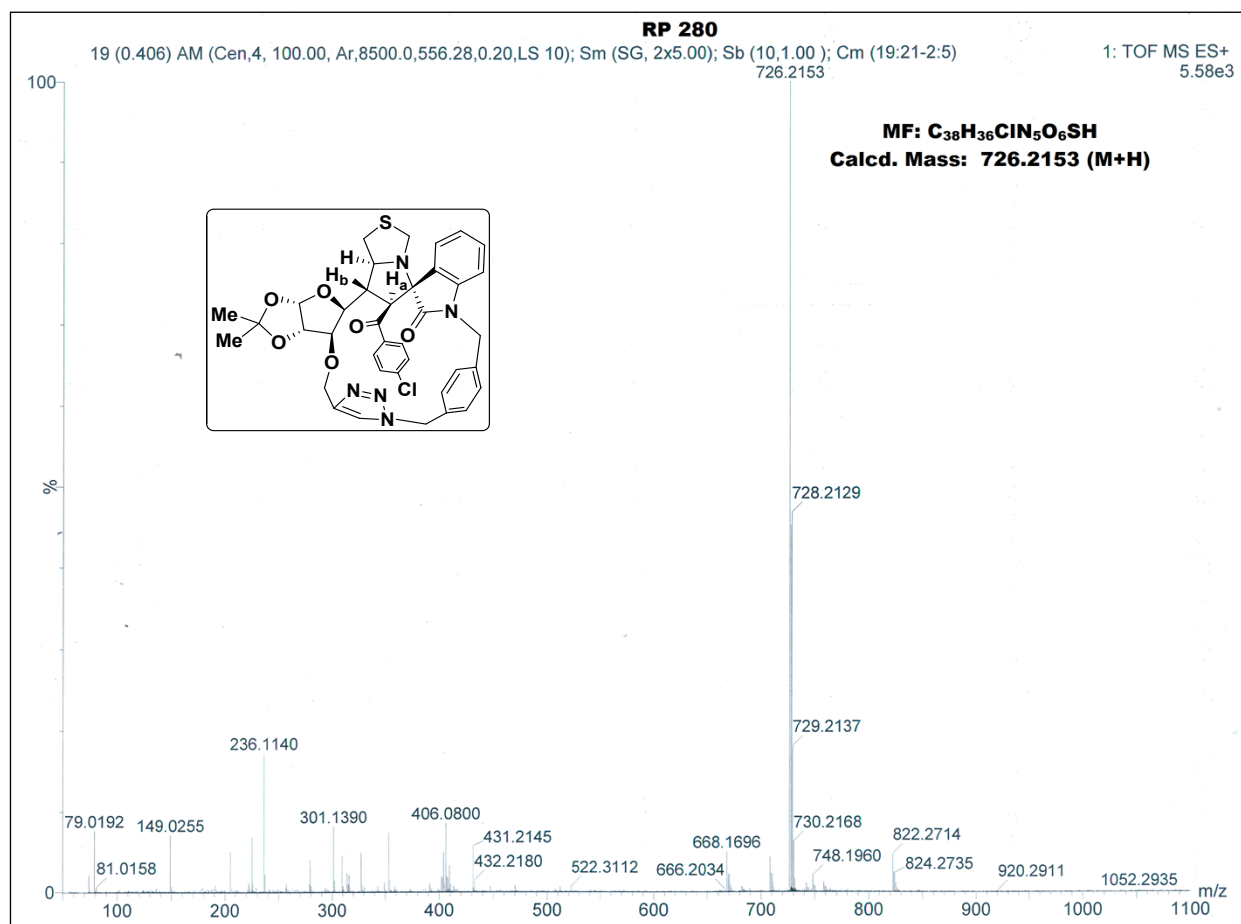


Figure 3.16c. DEPT 135 (CDCl₃, 75MHz) of 11d



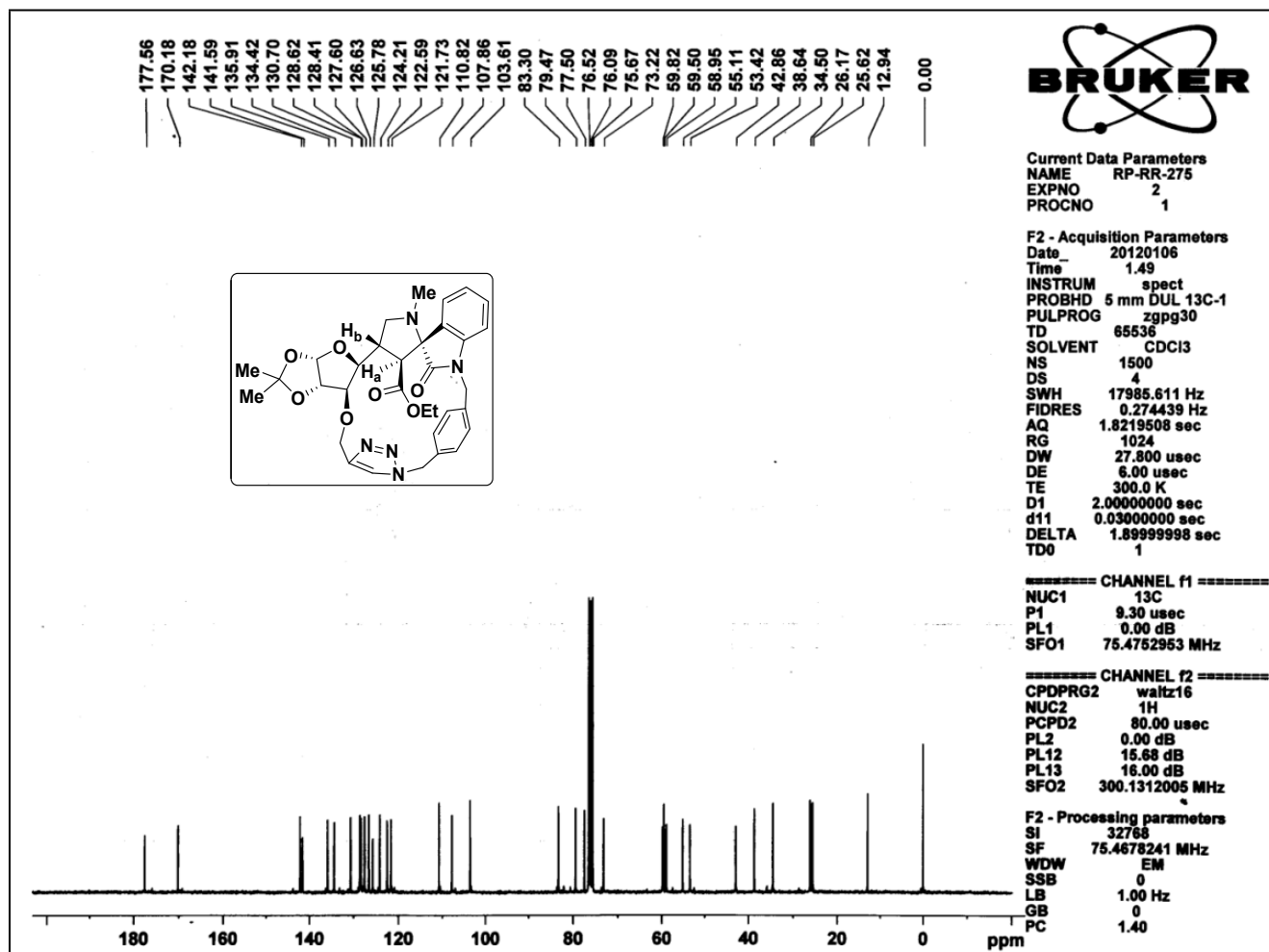


Figure 3.17b. ¹³C NMR (CDCl₃, 75MHz) of 11e

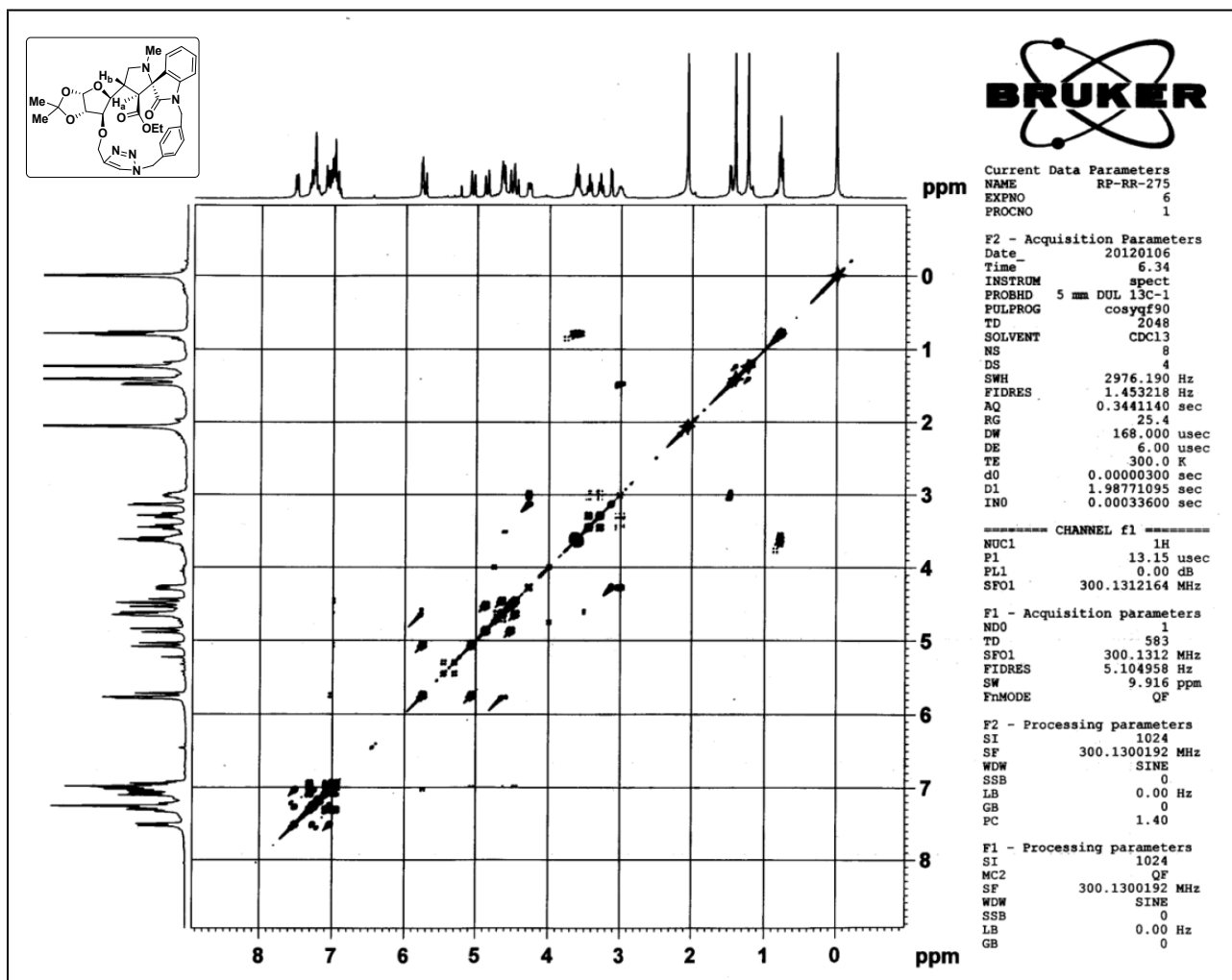


Figure 3.17c. H-H COSY spectrum of 11e

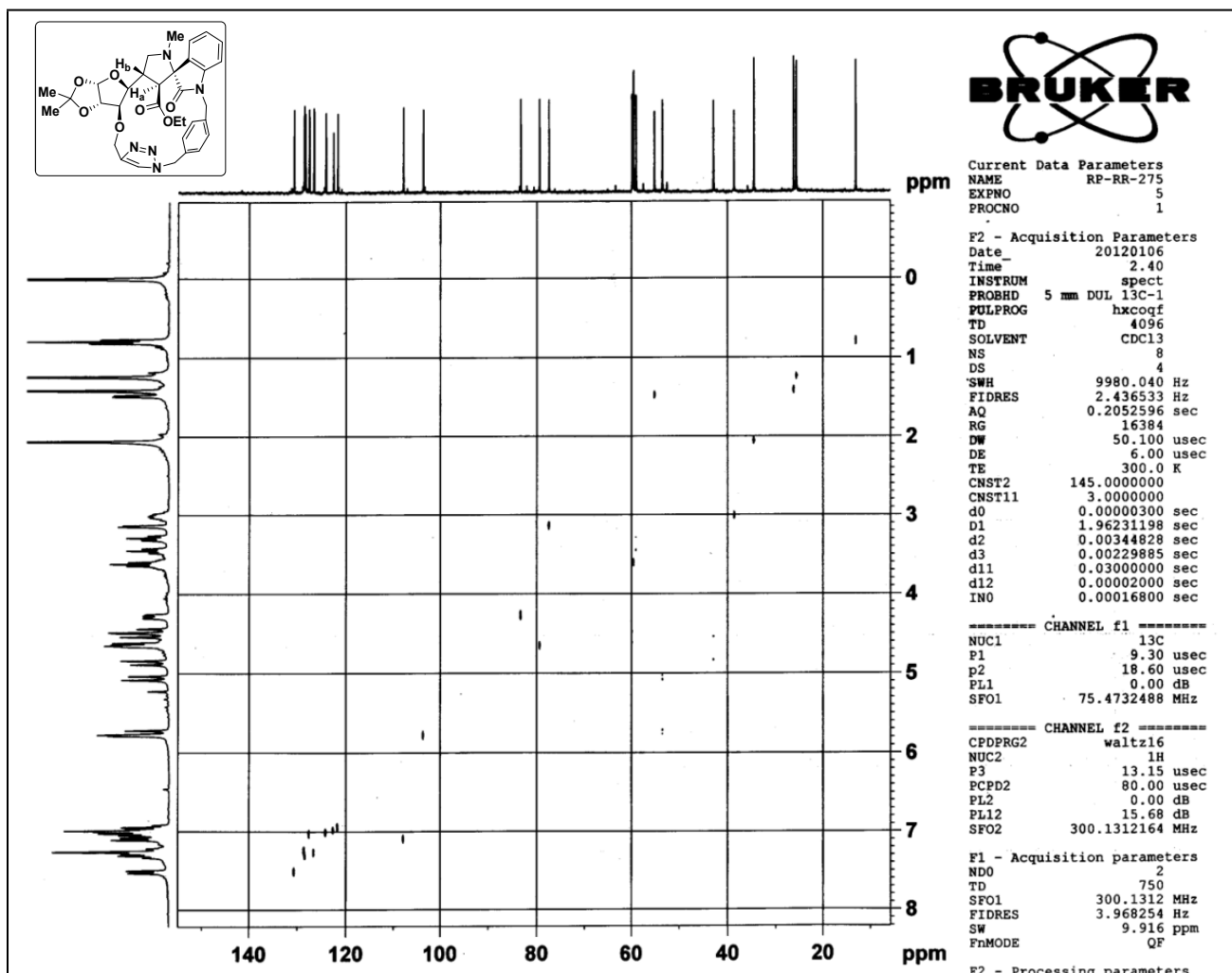
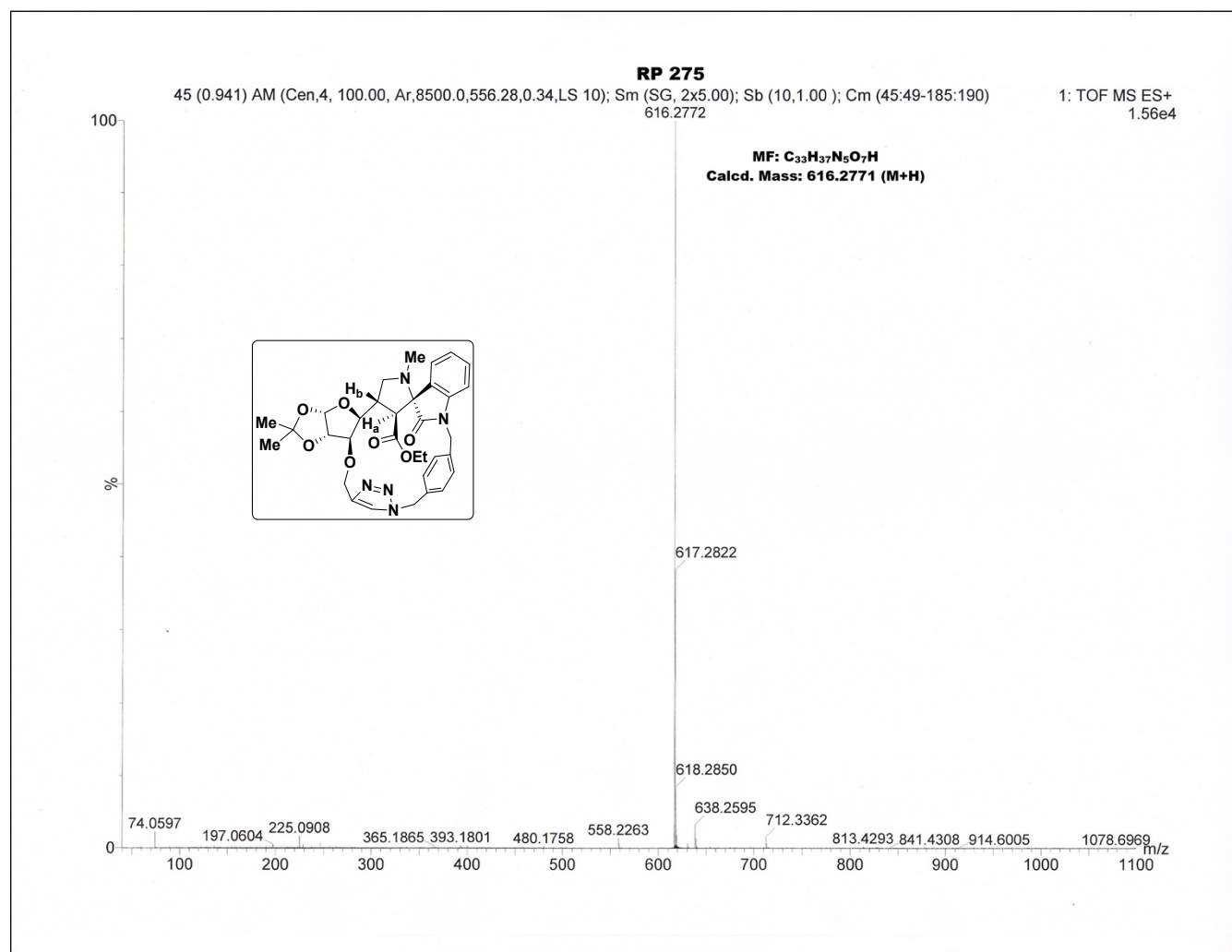
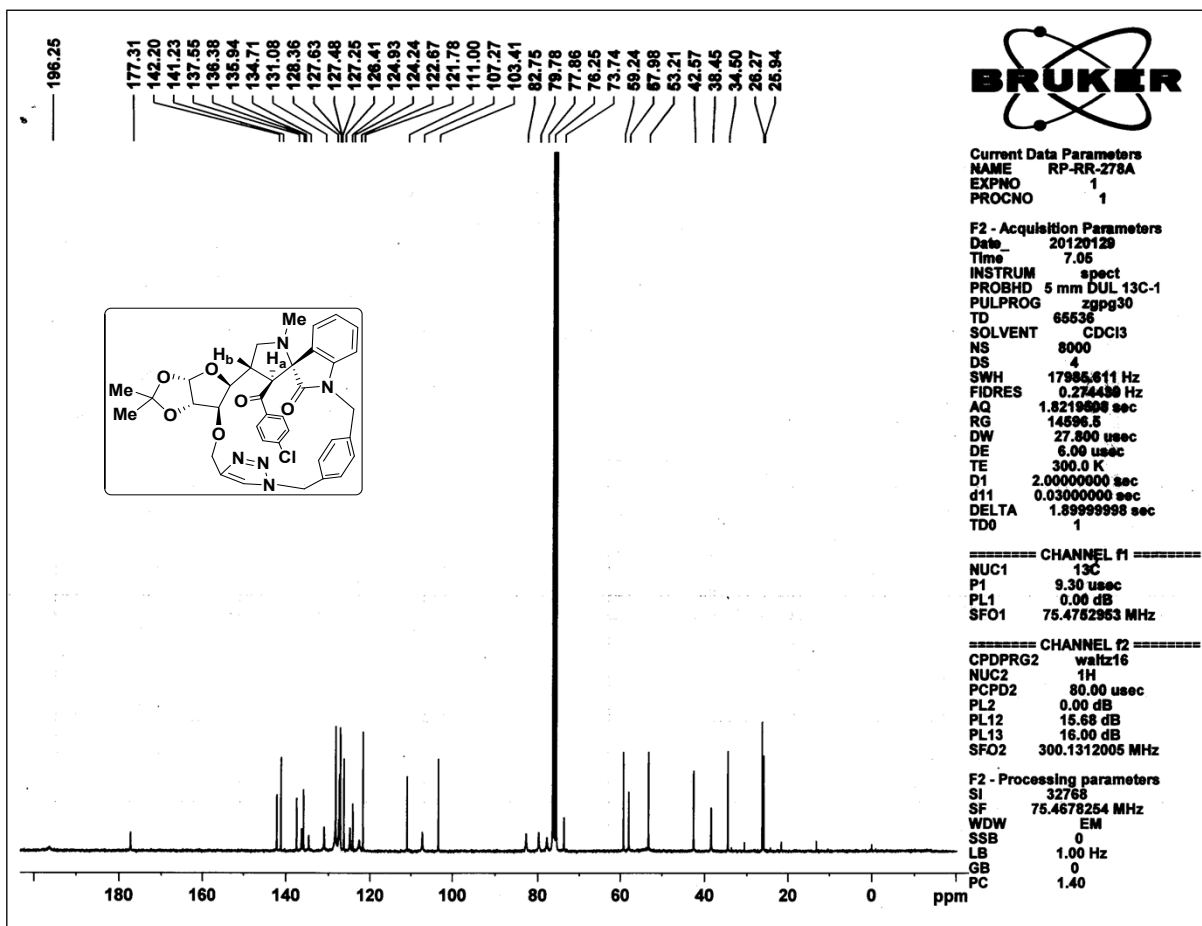


Figure 3.17d. C-H COSY spectrum of 11e





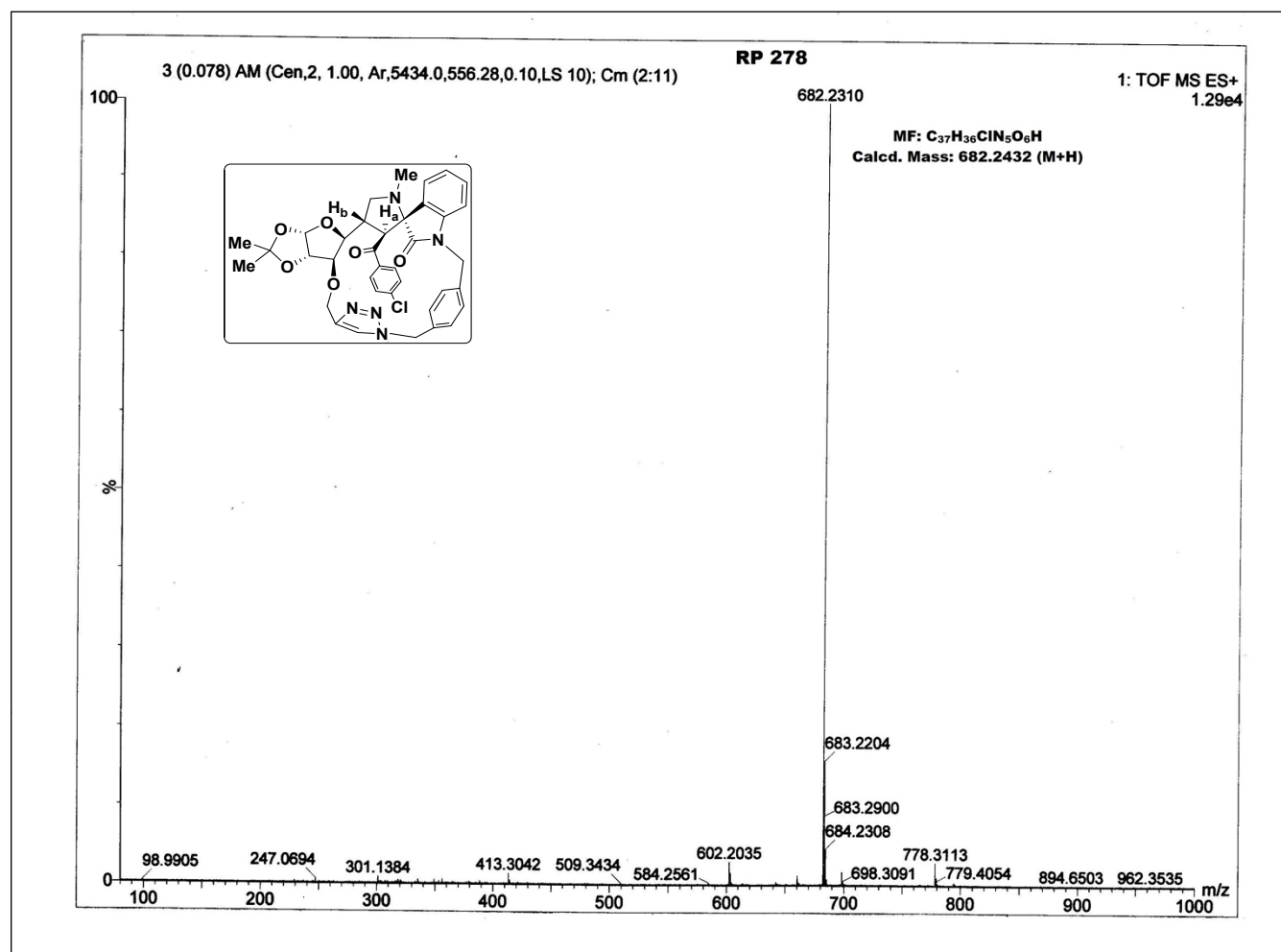


Figure 3.18c. ESI-MS spectrum of 11f