Regioselective one-pot synthesis, biological activity and molecular docking studies of novel conjugates *N*-(p-aryltriazolyl)-1,5-benzodiazepin-2-ones as potent antibacterial and antifungal agents

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- Thus, the formation of the triazole unit in **4b** chosen as an example was confirmed by the disappearance in the ^{1}H NMR spectra of a triplet (t, H-3", 2.35 ppm) corresponding to the acetylenic proton in front of the appearance of the characteristic singlet (s, H-5", 8,05 ppm) which is directly attributed to the proton of the triazole ring.

  Moreover the deshielding alkynes functions characteristic signals at 4.30 ppm (d, 2H, CH2-1', *J* = 15.6 Hz), to the signals corresponding to the methylene alpha to the triazole ring at 4.96 ppm (d, 1H, H-1a ", *J* = 14.7 Hz) and 5.27 ppm (d, 1H, H-1b", *J* = 15 Hz), as can be seen when compared with their displacements in the starting molecules. Note also the presence of a singlet at 3.89 ppm directly attributed to the methoxy group and signals in the aromatic region at (δH 6,98-8,16 ppm, 12H) corresponding to the aromatic protons of both diazepine and the phenyl ring of the azide used.

Additional supports for our assignments arose from the HMBC spectrum which revealed significant long range correlation between the triazolic proton (s, H-5", 8.01 ppm) and both quaternary carbons C-4" and C-1"' at 144.6 ppm and 154.2 ppm respectively. Also, the proton H-3"' (7,62 ppm) correlates with carbons OCH_3, C-2"' et C-1"' appearing at 55,6 ppm, 122,0 ppm and 154,2 ppm respectively. Thus came supporting the obtention of the proposed molecular structures.

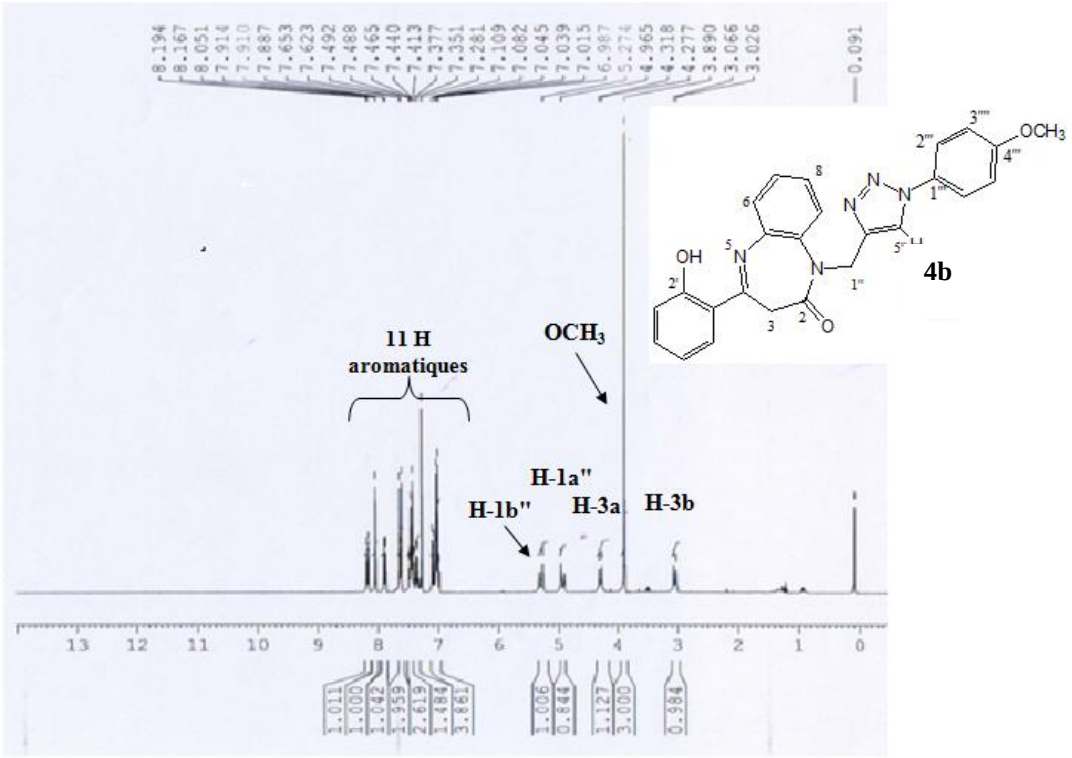


Figure S1 . NMR spectra ^1H (300 MHz, $CDCl_3$) of compound **4b**

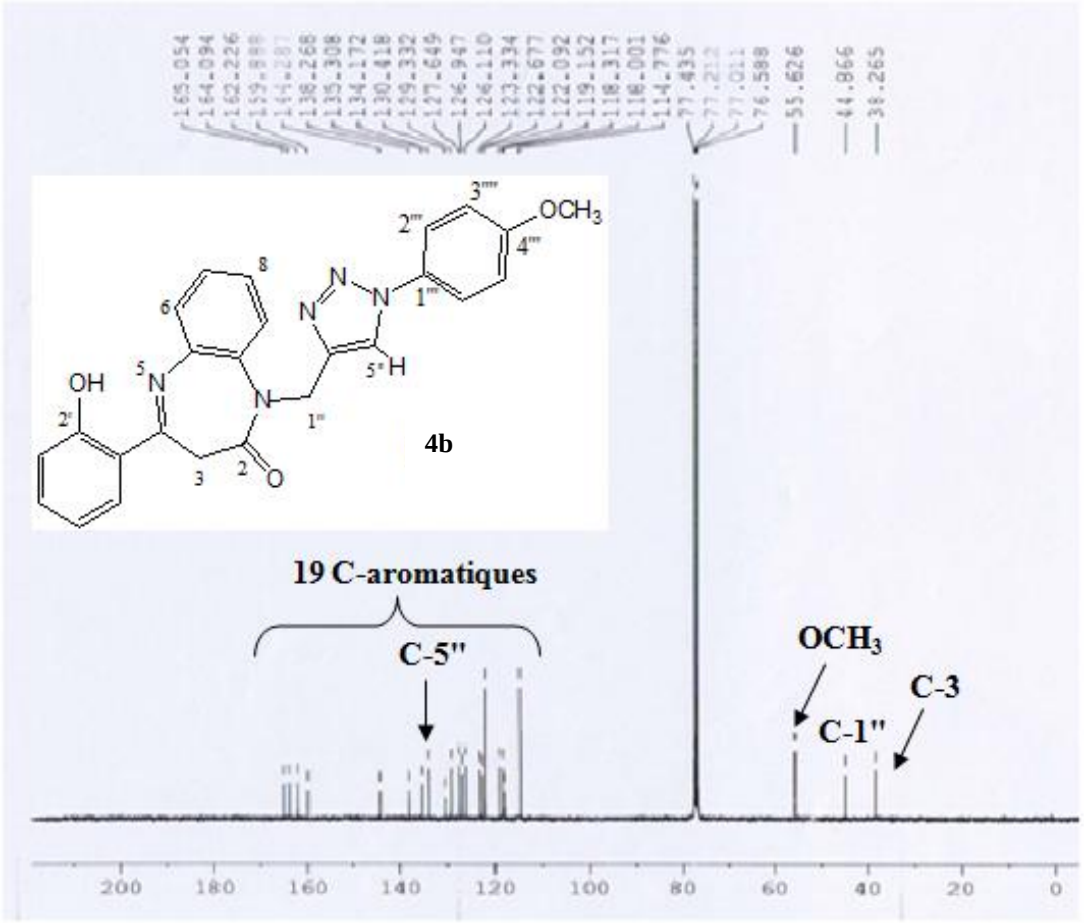


Figure S2 . NMR spectra ^{13}C (75,47 MHz, $CDCl_3$) of compound **4b**

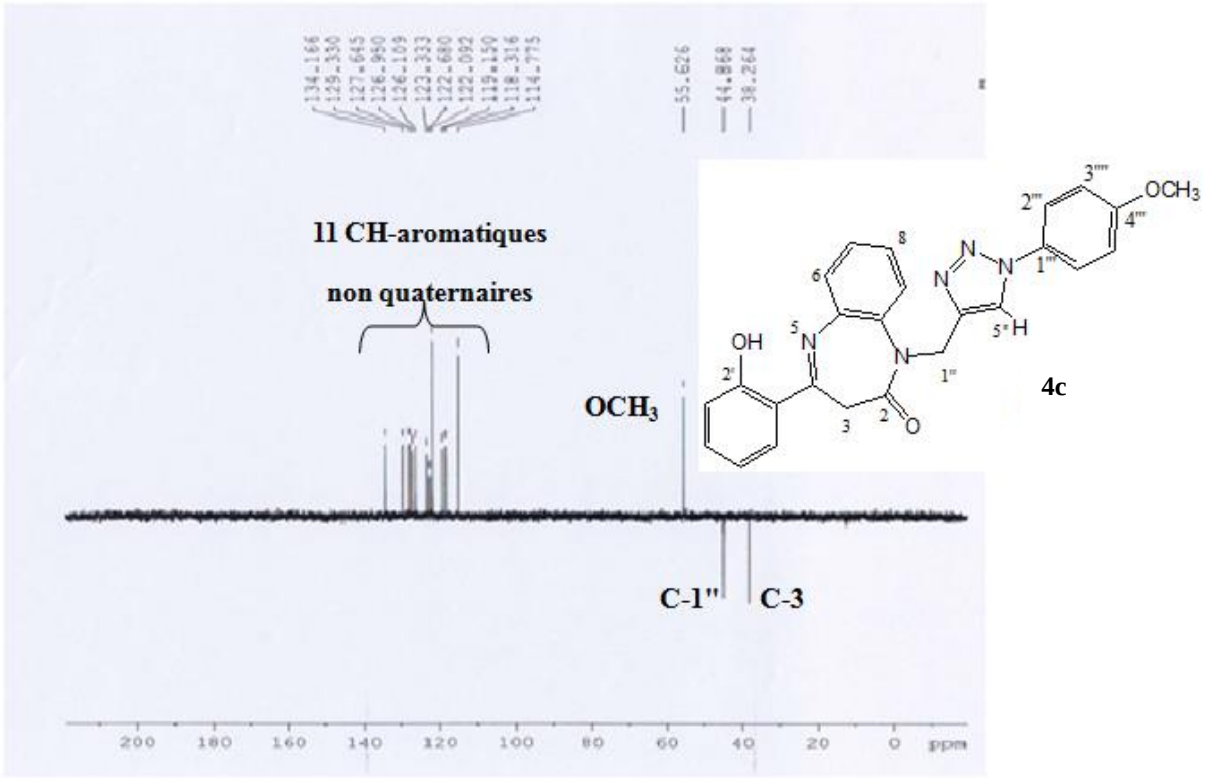


Figure S3 . DEPT 135 of compound **4b**

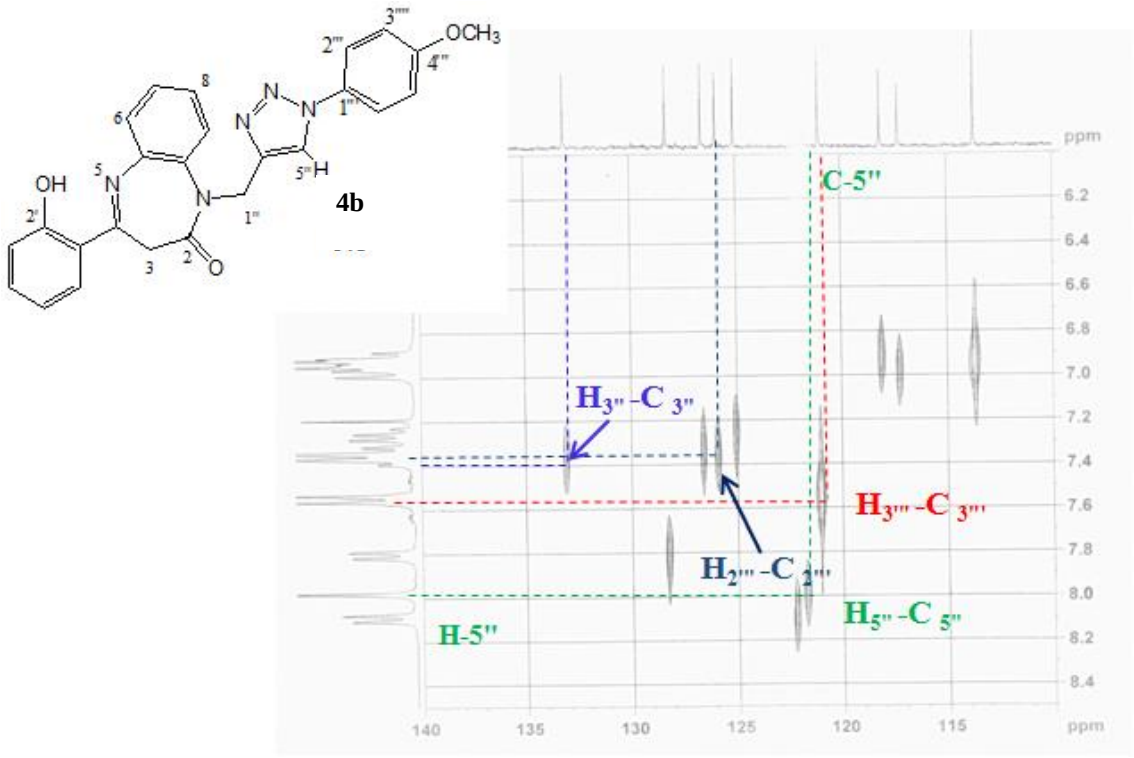


Figure S4 . CHcorr spectra of compound **4b**

- The ^{1}H NMR spectrum of the *N*-galactosyl-triazoles **6b** showed chemical shifts of H-1''' (anomeric proton) at 5.40 ppm (doublet, *J*= 4.8 Hz) downfield compared to the precursor azide at 5.56 ppm.
  Except these characteristic signals taken from the ^{1}H NMR spectrum of compound **6b**, ^{13}C NMR (75.4 MHz in $CDCl_3$) was used and more particularly the DEPT 135 experiment. In addition to the observed peaks for the starting compound, four peaks appeared between 22.6 and 25.9 ppm corresponding to the methyl of the galactopyranosyl part. Moreover, the peaks at δ= 66.8(C-2'''),67.1(C-3'''), 70.2(C-4'''), 70.7(C-5'''), 96.2(C-1'''), 109.9(C-isop), 109.9(C-isop) ppm are assigned to the introduced galactosyl moiety. The peak at 50.56 ppm is attributed to the C-6 '''carbon. A signal at 126.9 ppm is related to carbon C-5 "of the triazole ring.

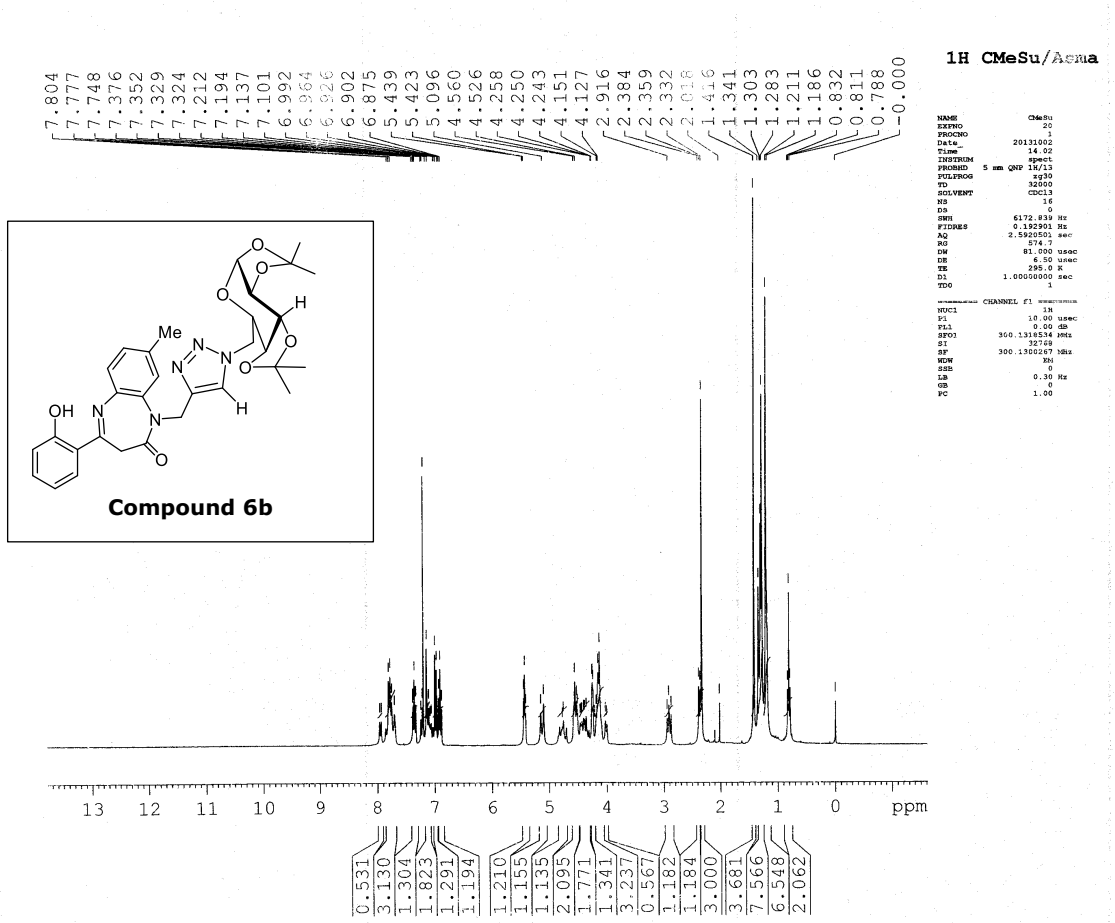


Figure S5. NMR spectra ^{1}H (300 MHz, $CDCl_3$) of compound **6b**

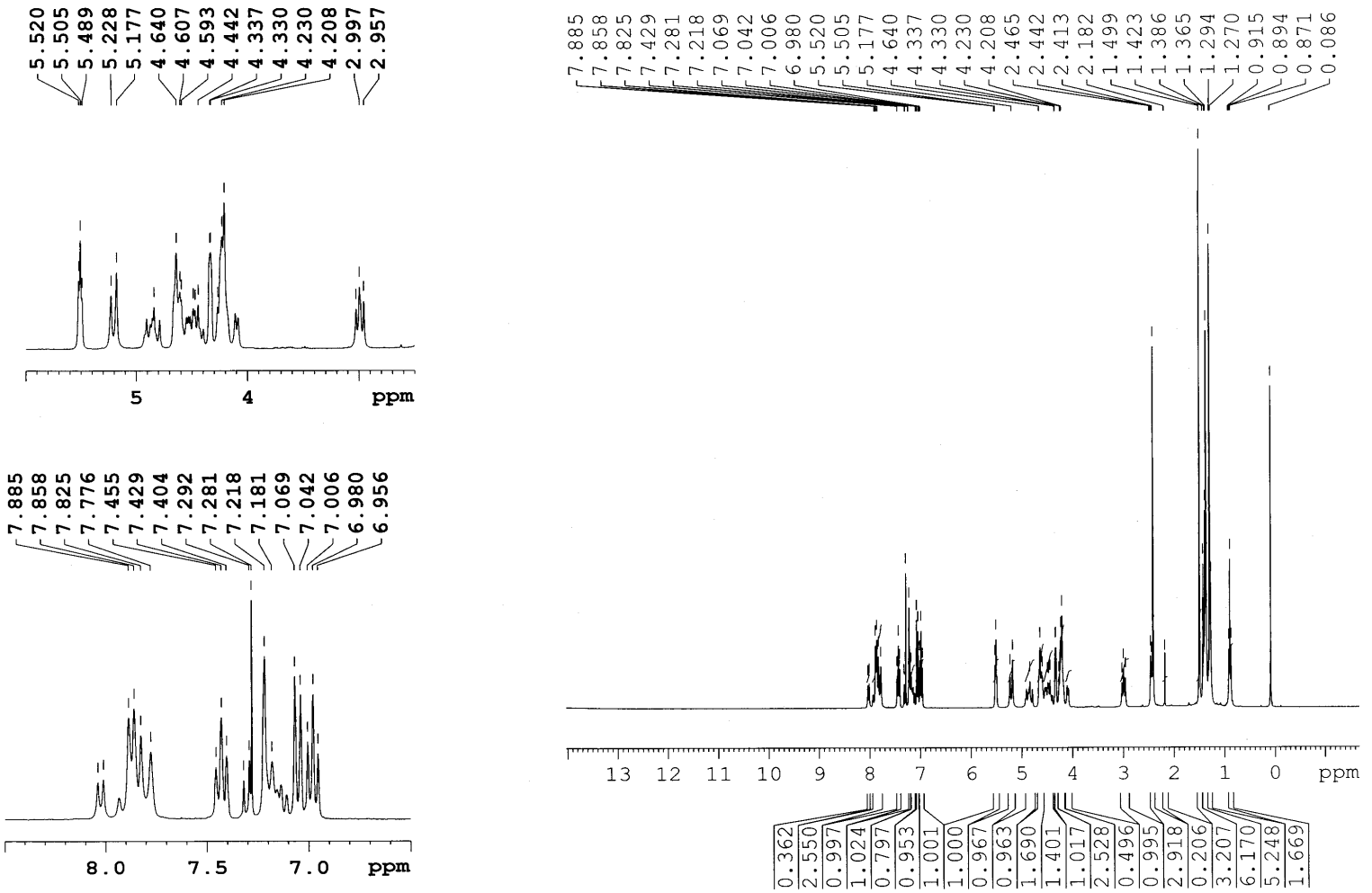


Figure S6. NMR spectra ^{1}H (300 MHz, $CDCl_3$) of compound **6b**

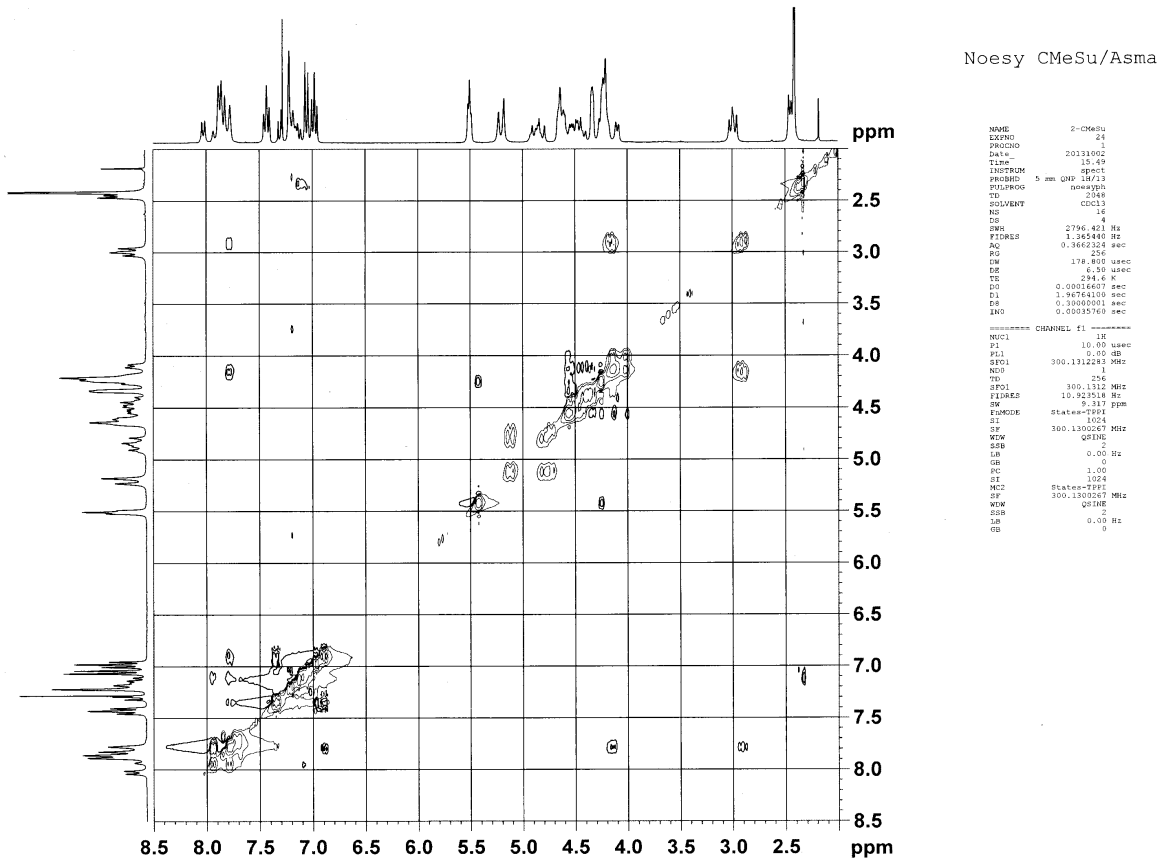


Figure S7. NOESY Spectra of compound **6b**

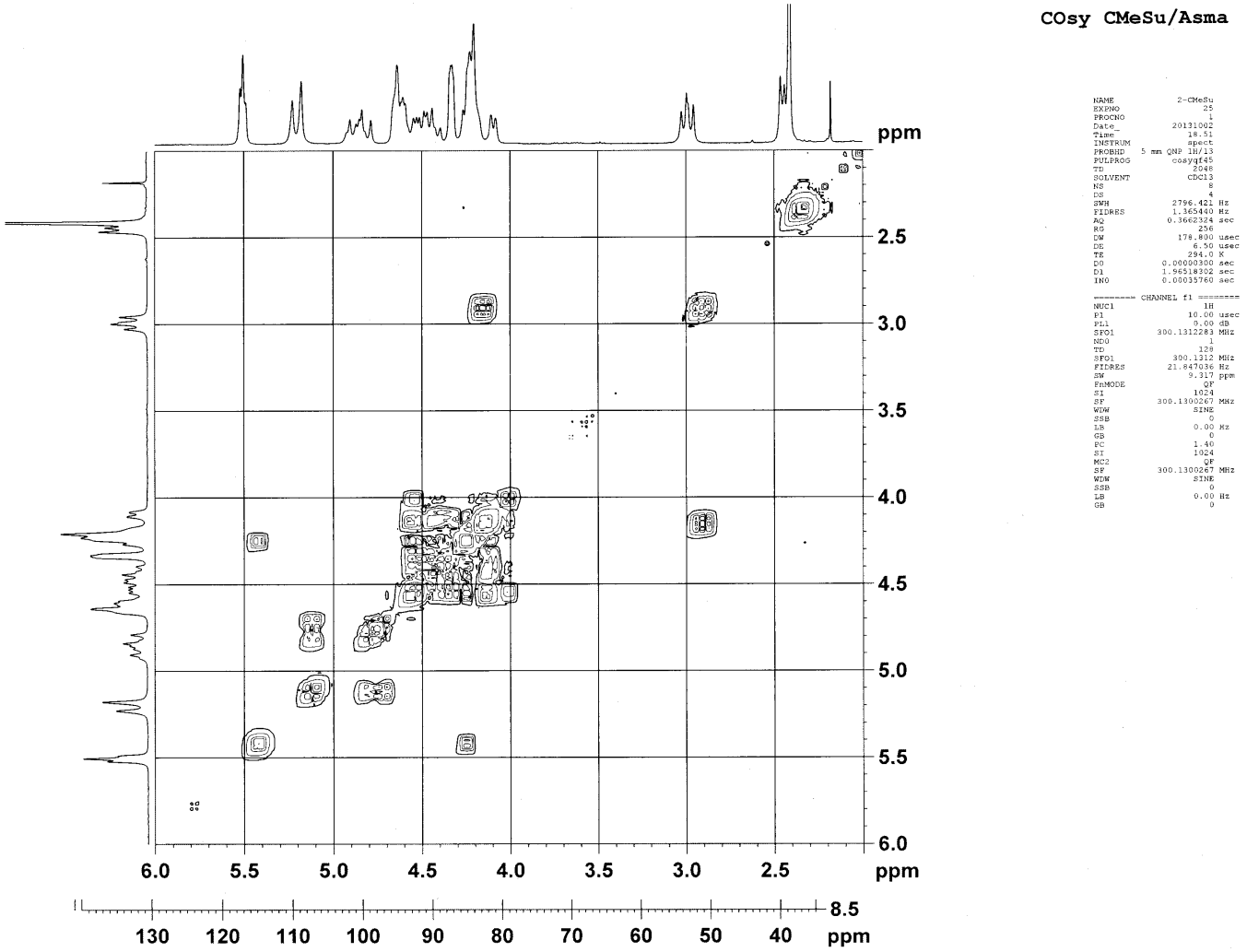
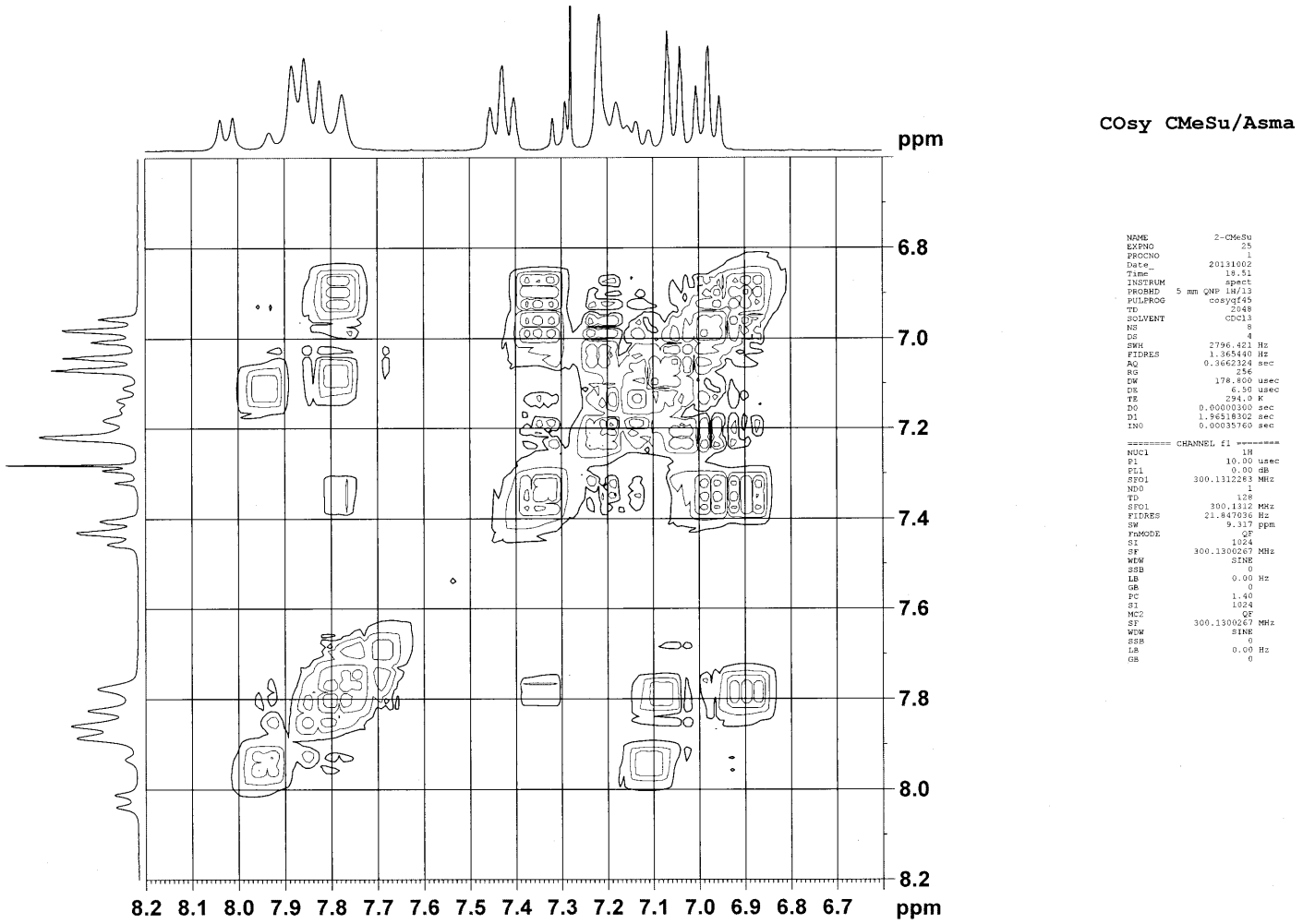


Figure S8 . COSY ^{1}H-^{1}H spectra of compound **6b**



COsy CMeSu/Asma

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FIDRES	1.365440 Hz
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DE	6.50 usec
TE	294.0 K
D0	0.00000300 sec
D1	1.96518302 sec
IN0	0.00035760 sec
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ND0	1
TD	128
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SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
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WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

Figure S9 . COSY ^{1}H-^{1}H spectra of compound **6b**

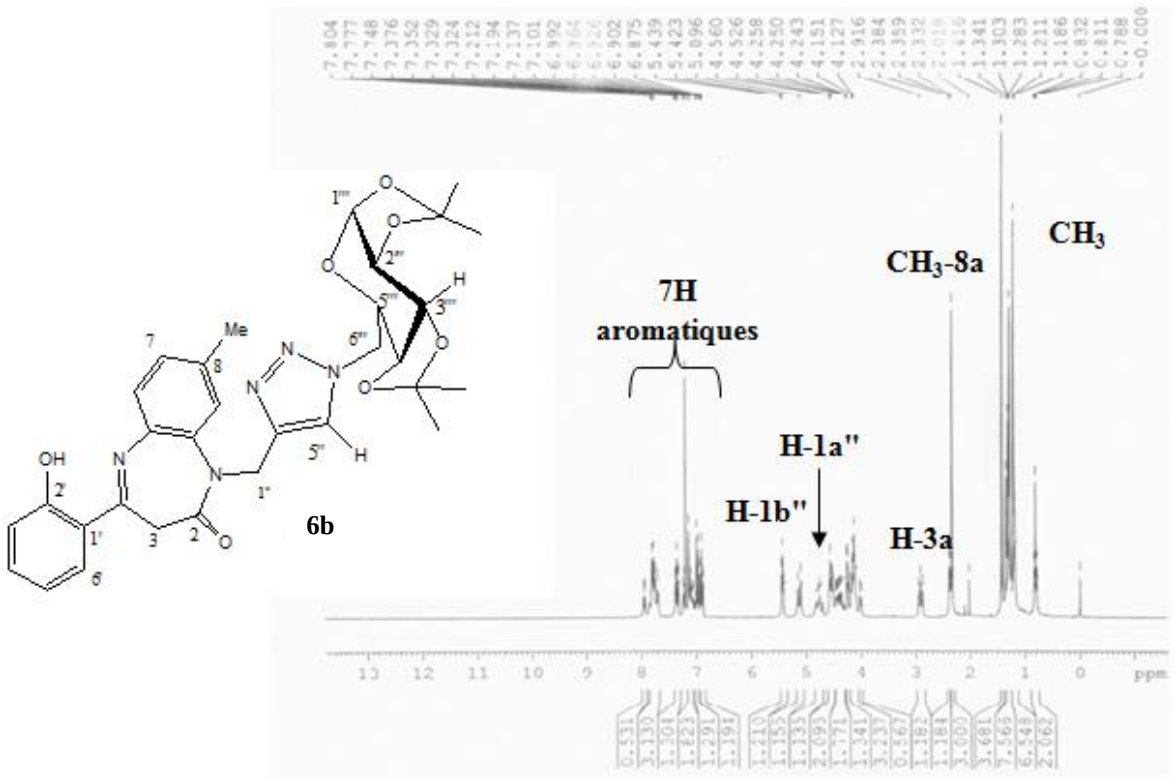


Figure S10. NMR spectra ^{1}H (300 MHz, $CDCl_3$) of compound **6b**

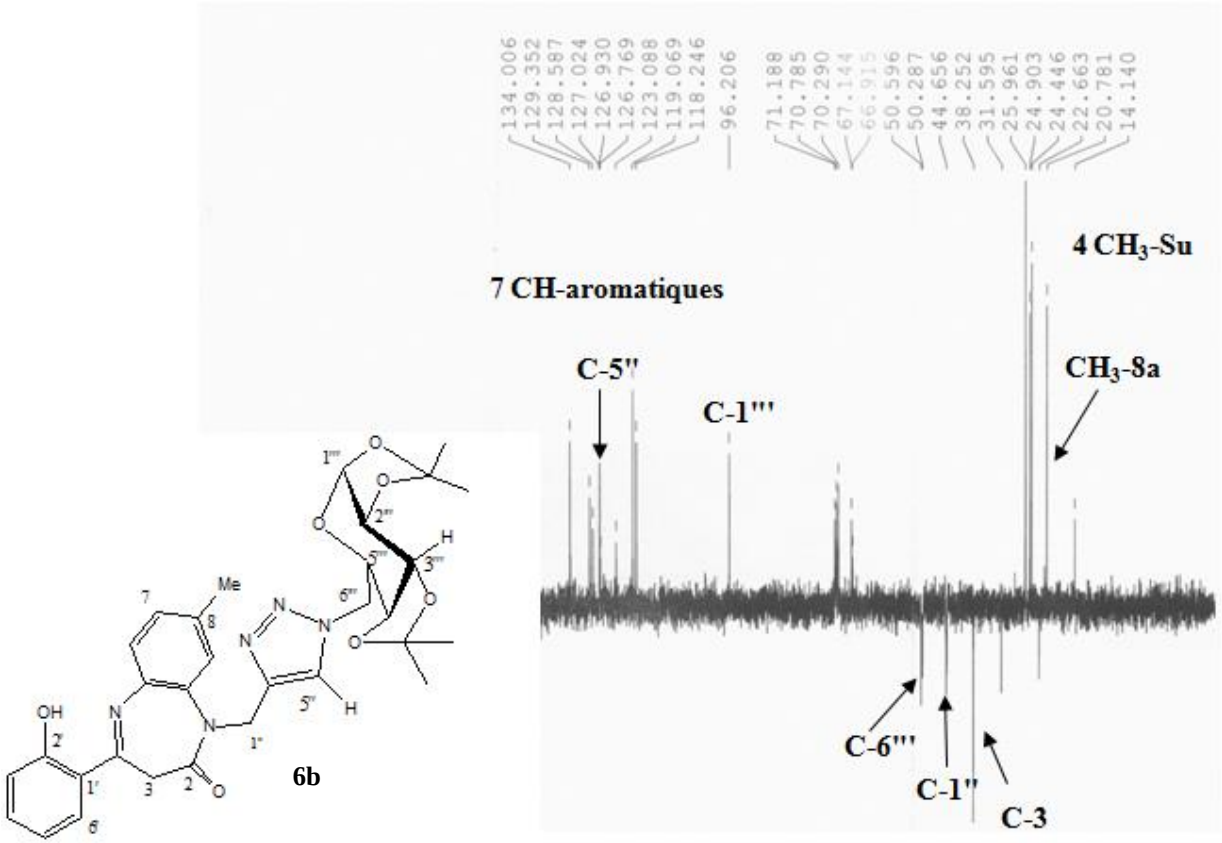


Figure S11. DEPT 135 (75,47 MHz, $CDCl_3$) of compound **6b**

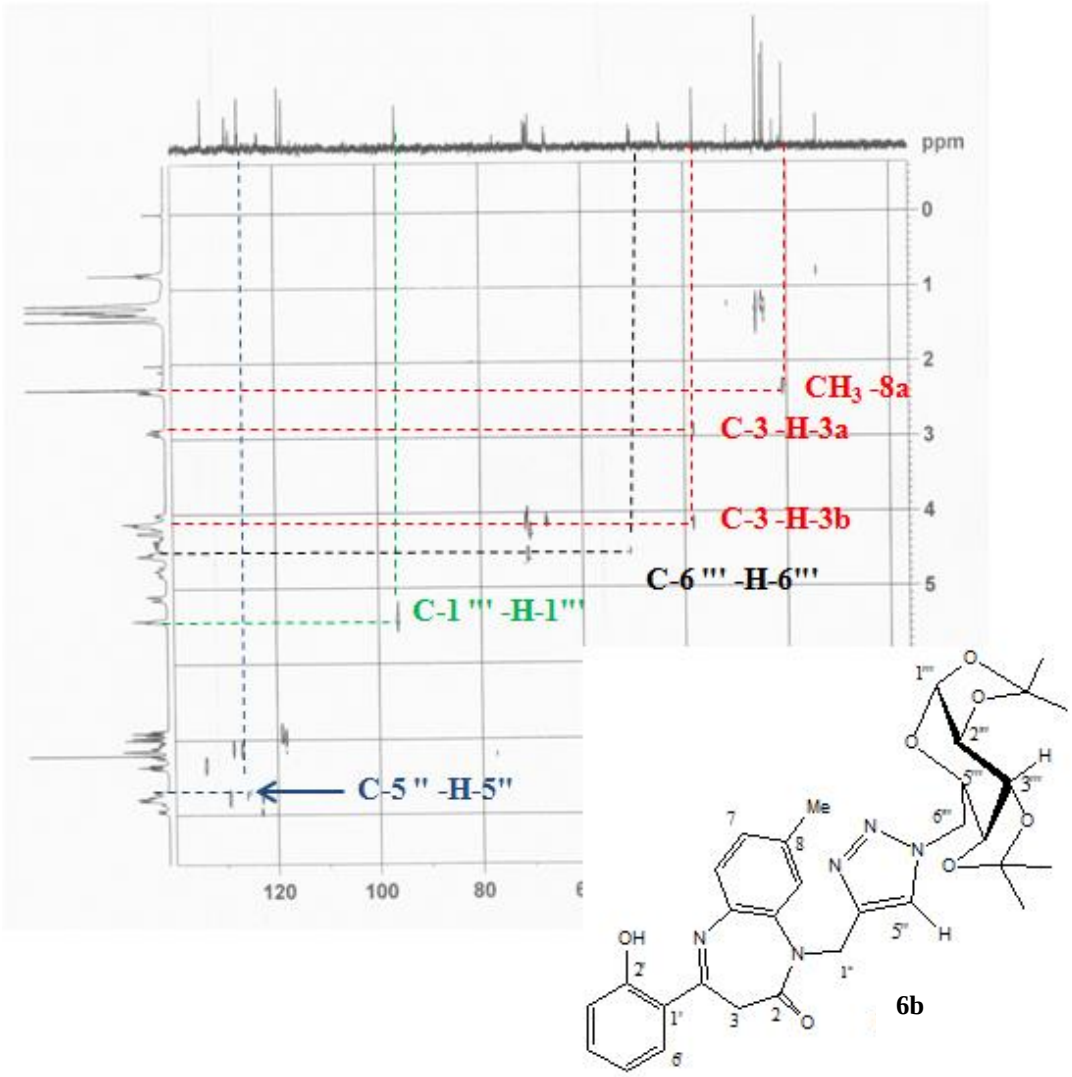


Figure S12 . CHcorr Spectra of compound **6b**

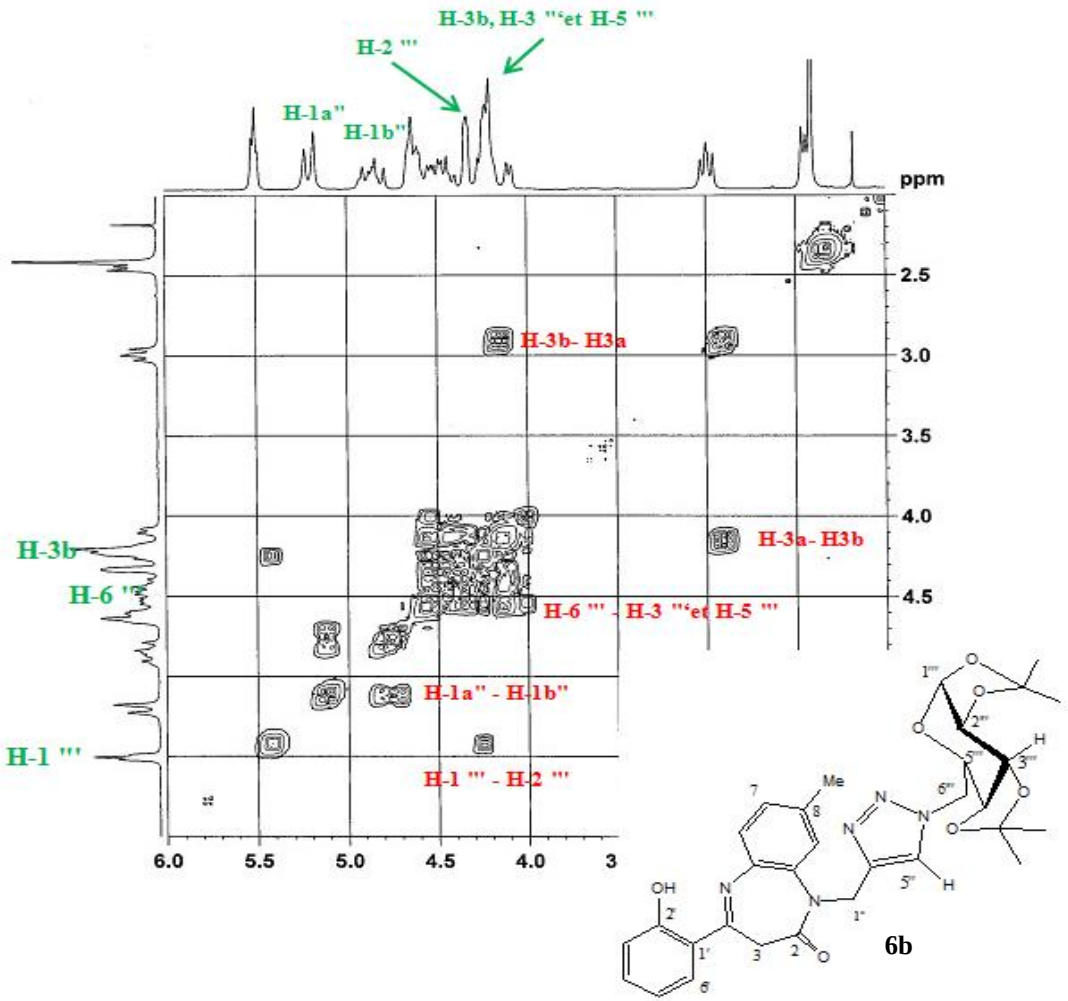


Figure S13. COSY Spectra of compound **6b**

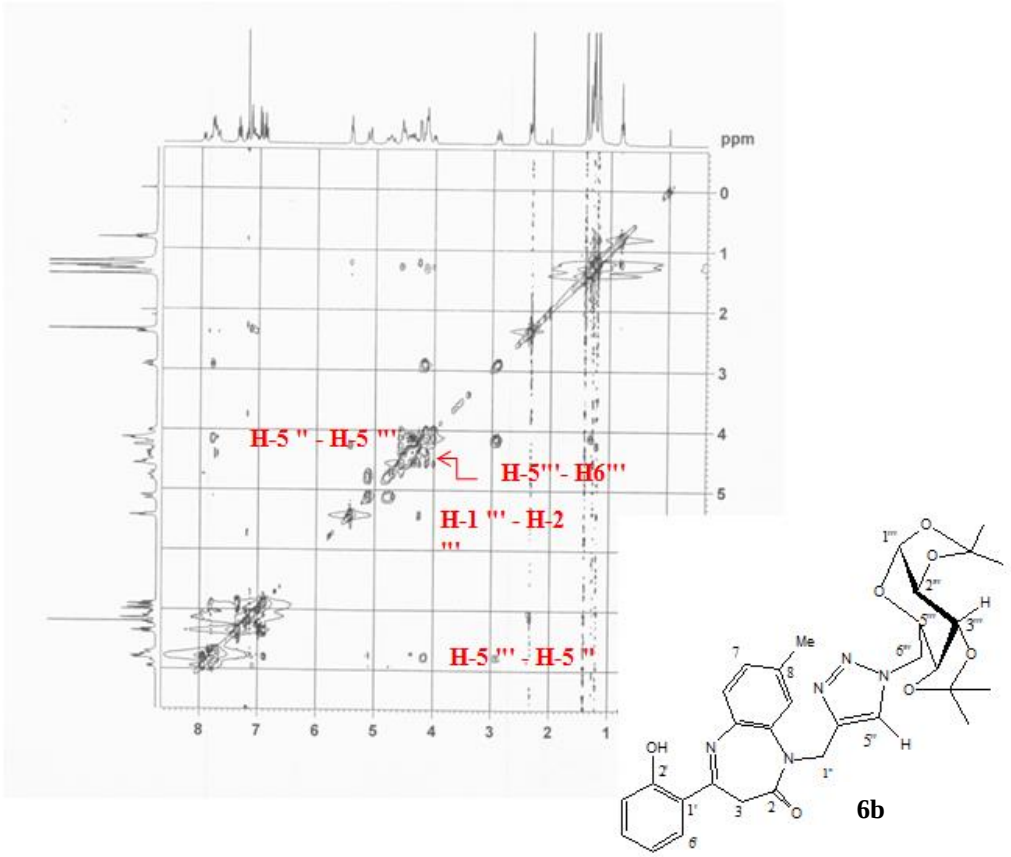


Figure S14. NOESY Spectra of compound **6b**

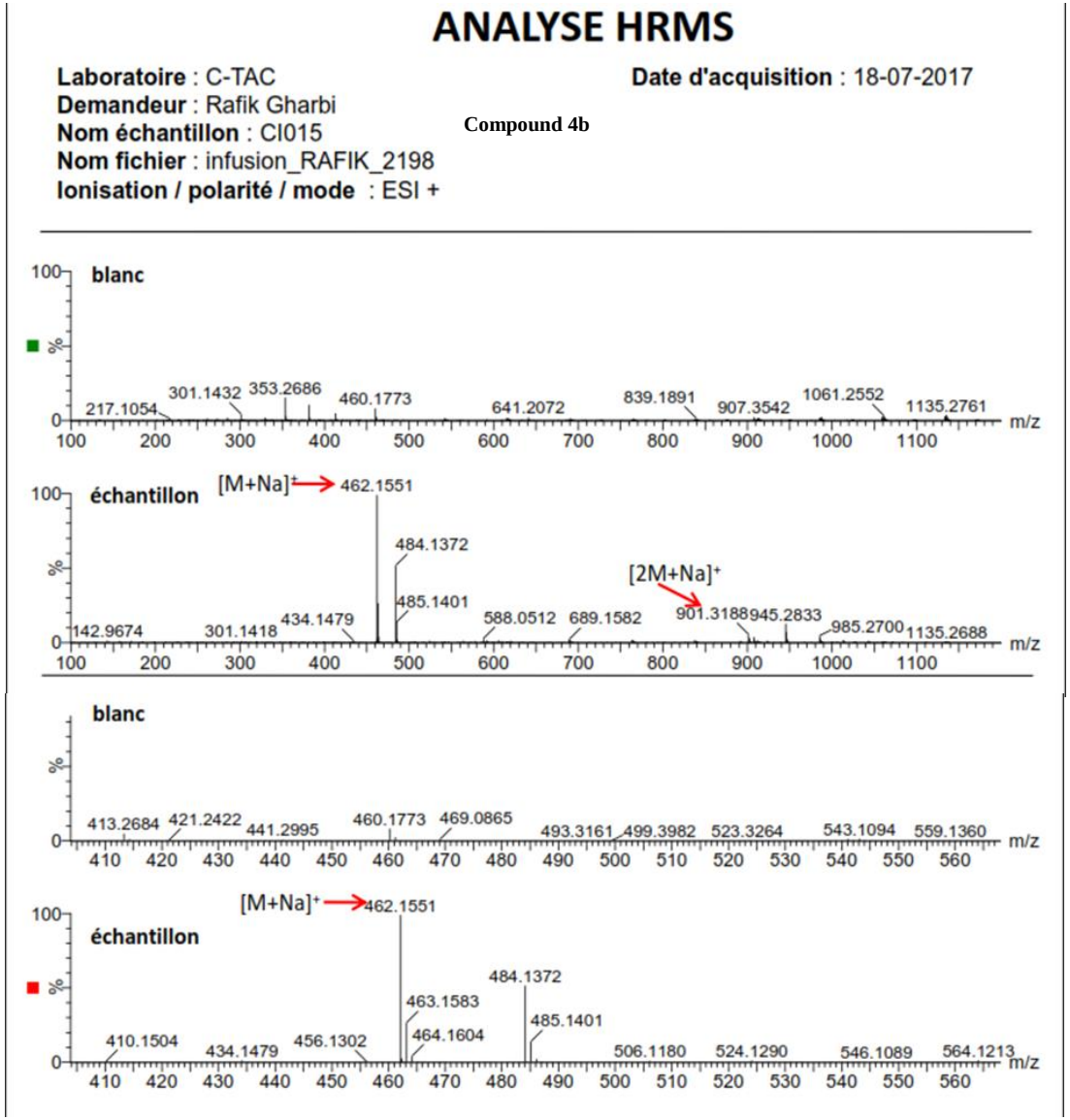


Figure S15. HRMS Spectra of compound **4b**

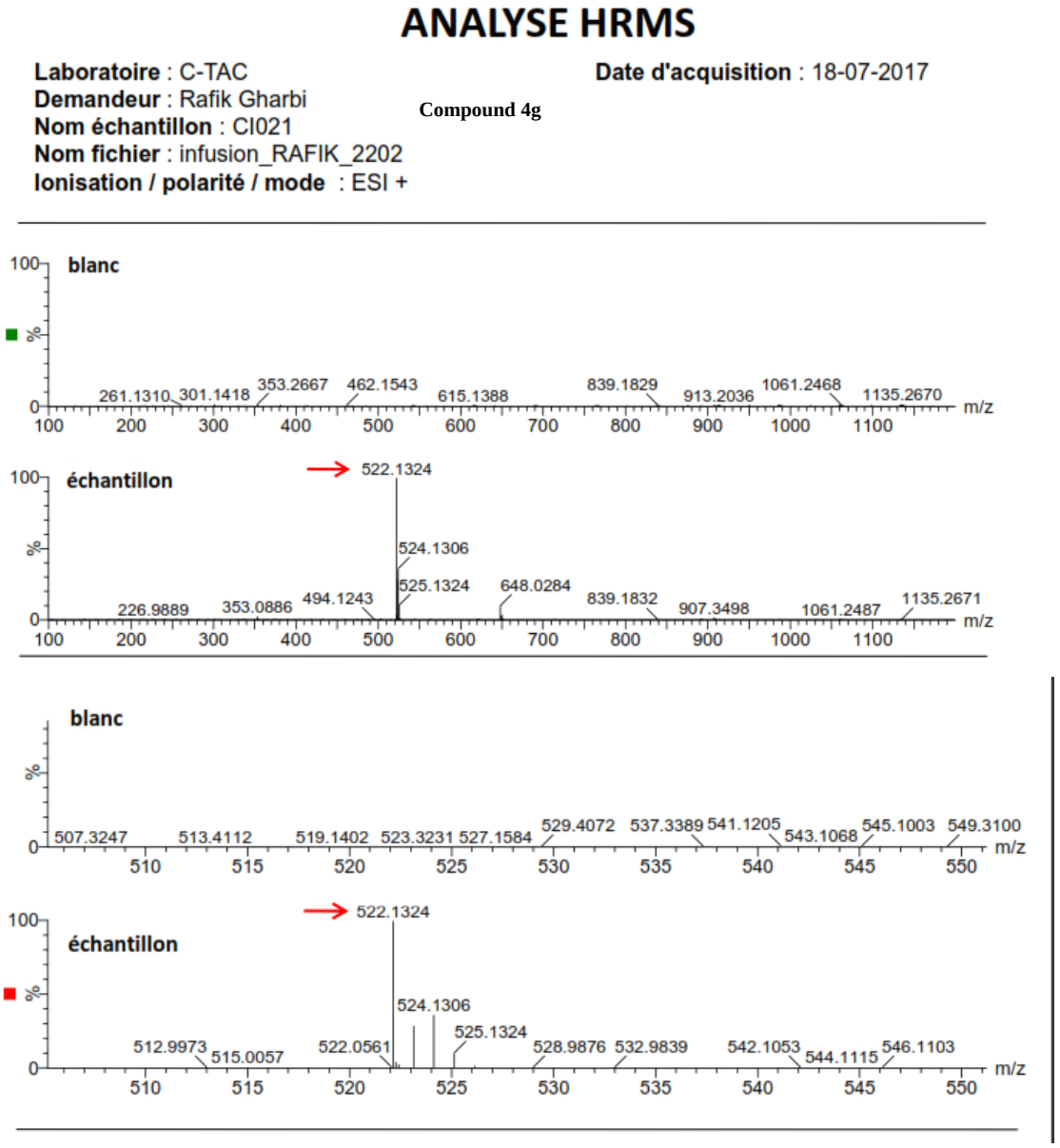
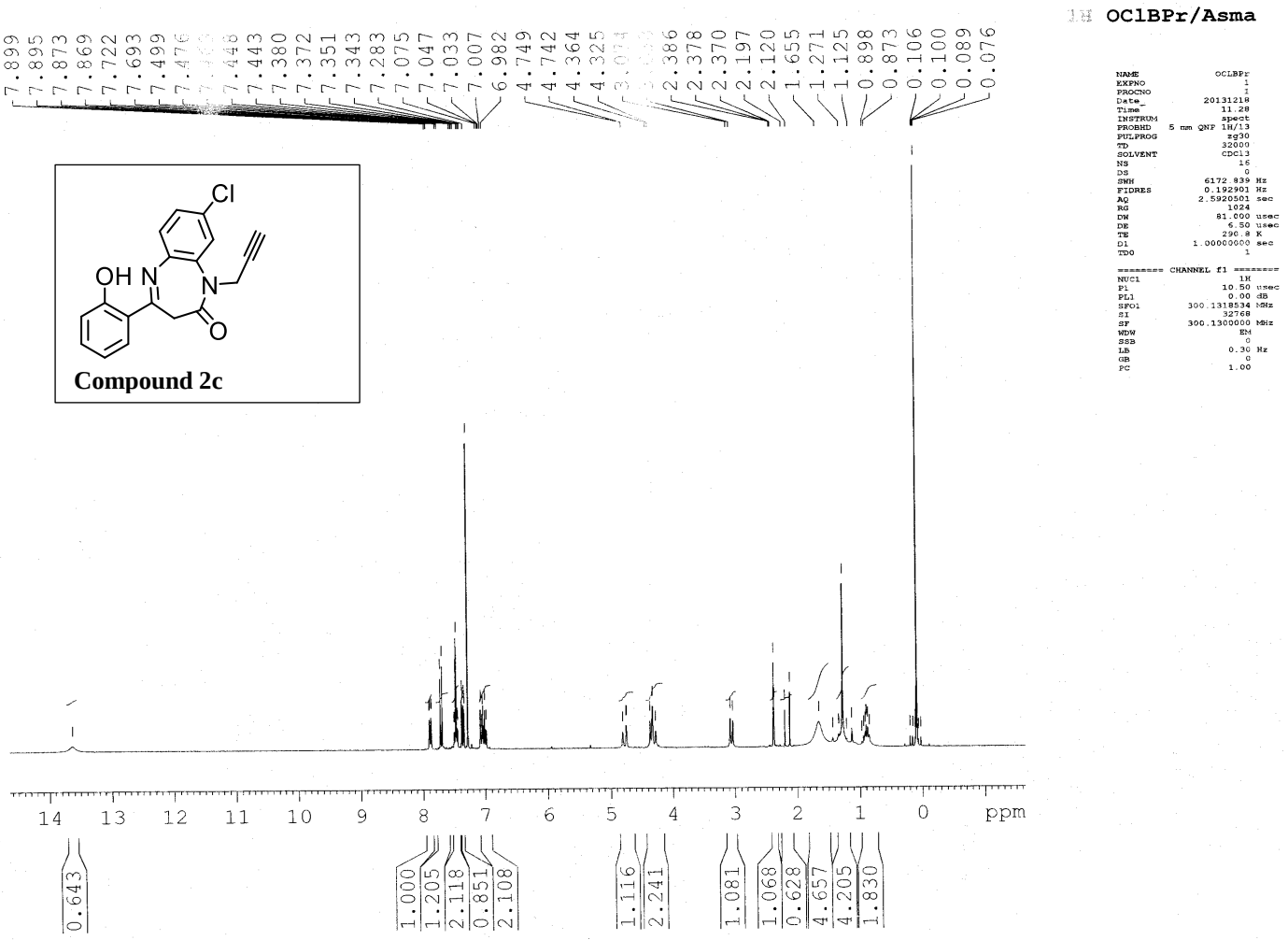


Figure S16. HRMS Spectra of compound **4g**



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PROCNO	1
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FIDRES	0.192901 Hz
AQ	2.5920501 sec
RG	1024
DW	81.000 usec
DE	6.50 usec
TE	290.8 K
D1	1.00000000 sec
TD0	1
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P1	10.50 usec
PL1	0.00 dB
SFO1	300.1318534 MHz
SI	32768
SF	300.1300000 MHz
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Figure S17. NMR spectra ^{1}H (300 MHz, $CDCl_3$) of compound **2c**

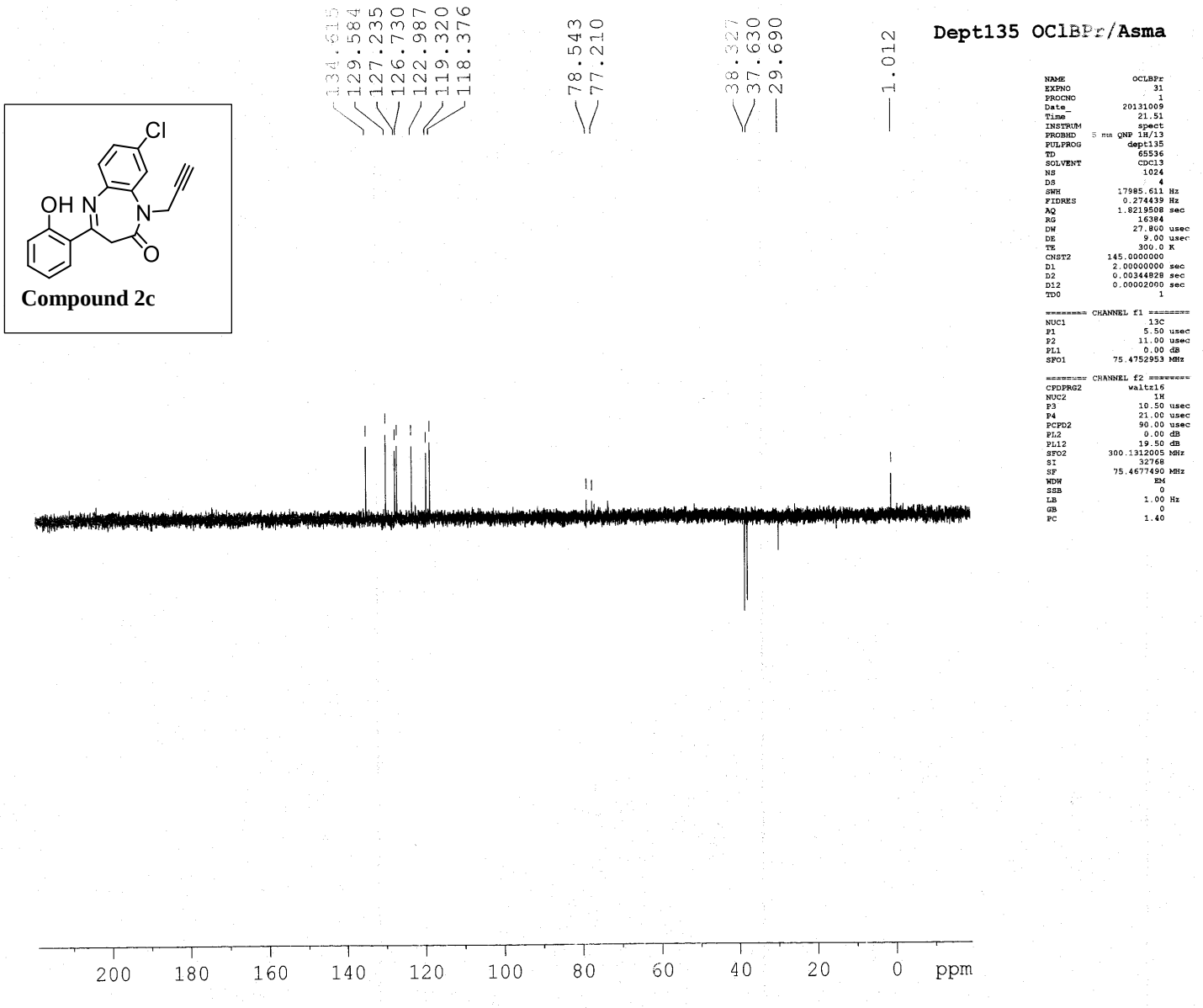


Figure S18 . DEPT 135 of compound **2c**

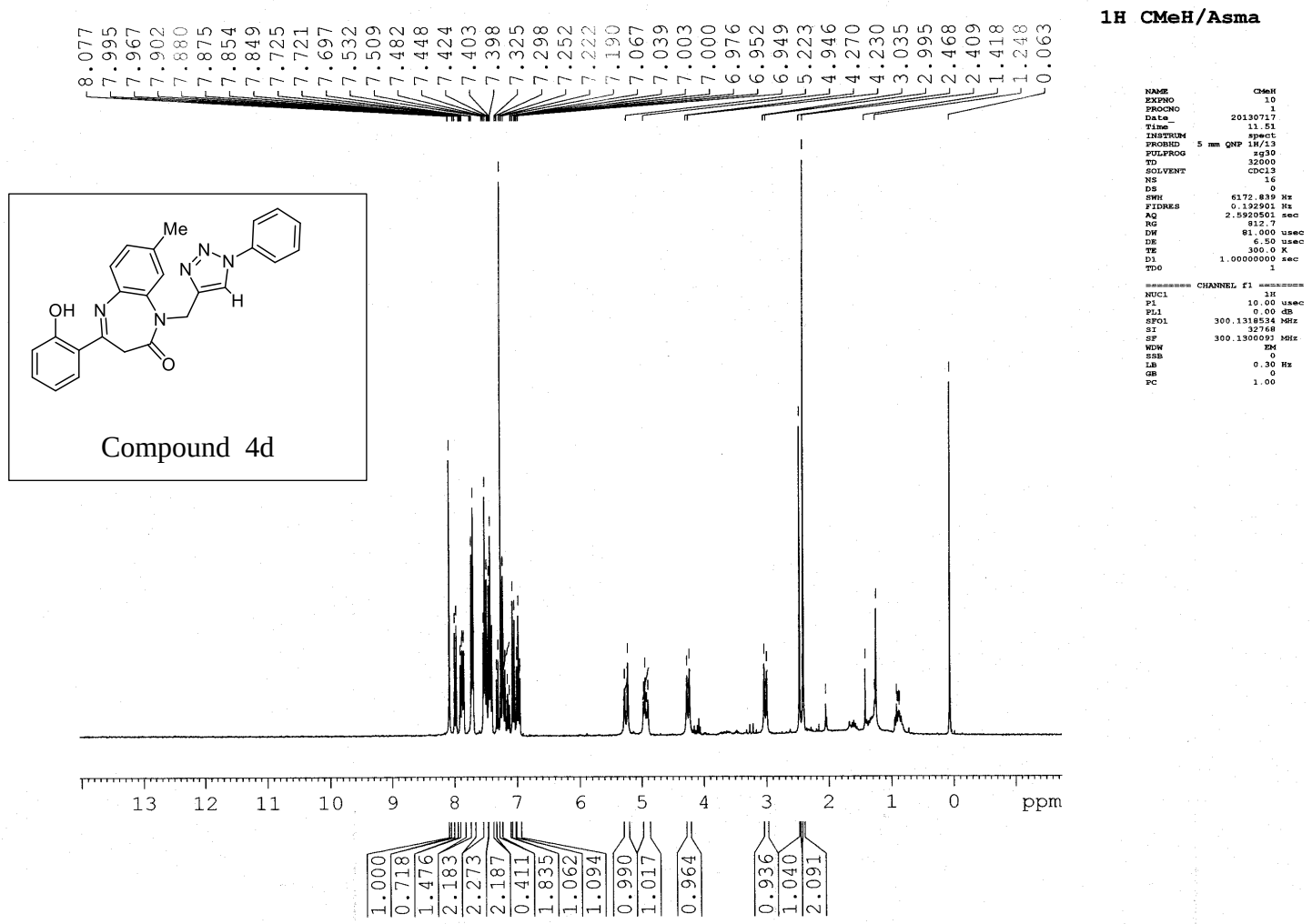


Figure S19. NMR spectra ^{1}H (300 MHz, $CDCl_3$) of compound **4d**

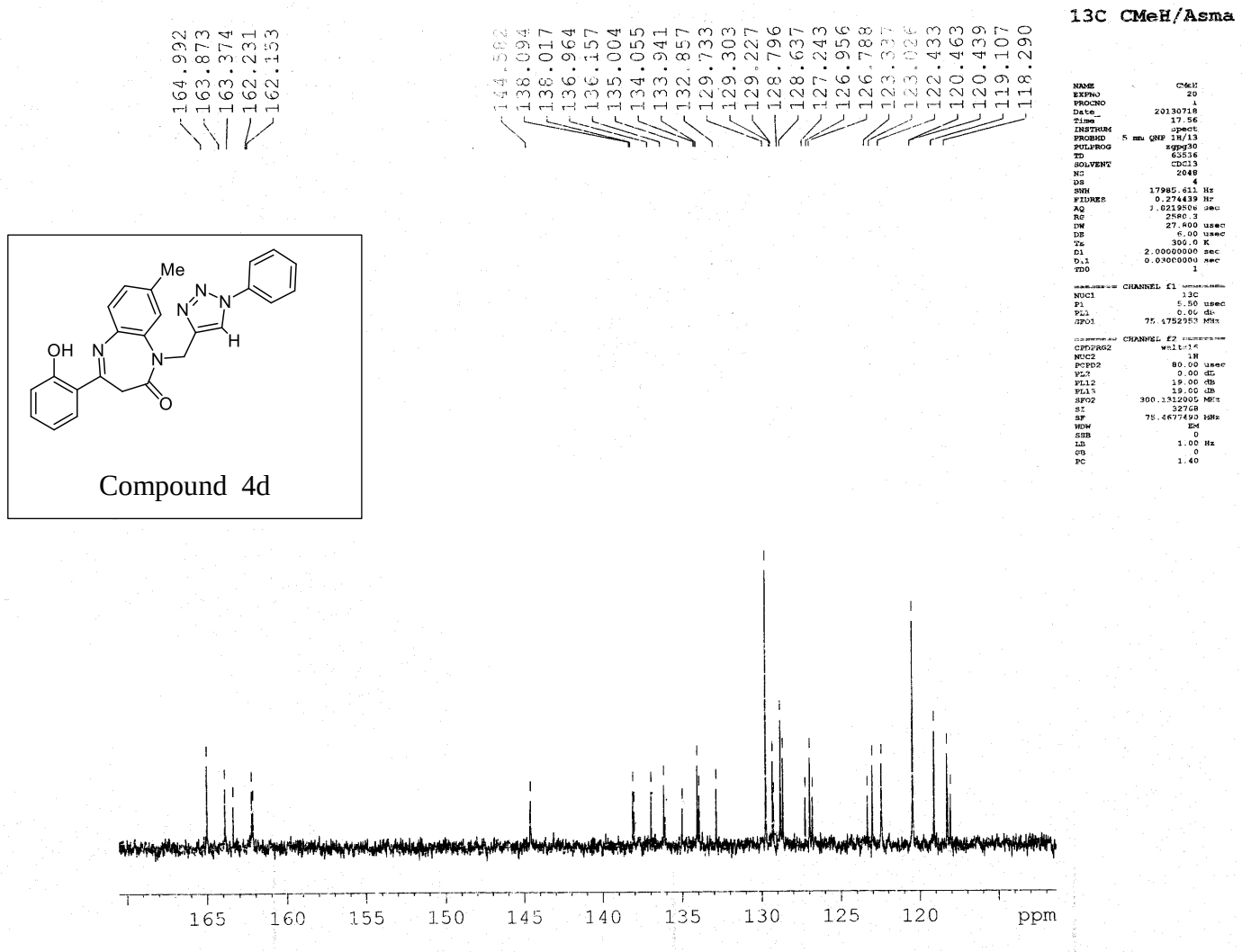


Figure S20. NMR spectra ^{13}C (75,47 MHz, $CDCl_3$) of compound **4d**

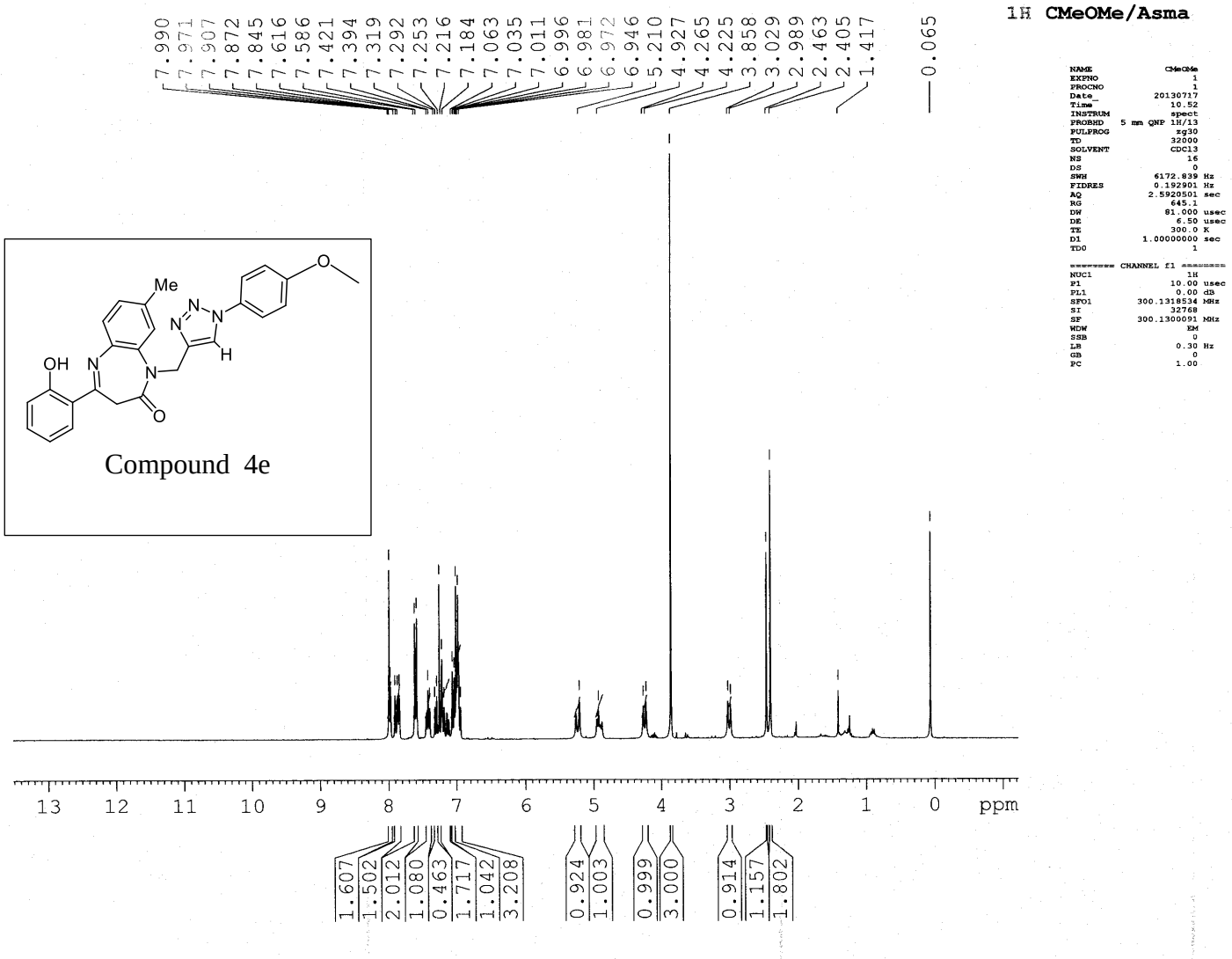


Figure S21. NMR spectra ^{1}H (300 MHz, $CDCl_3$) of compound **4e**

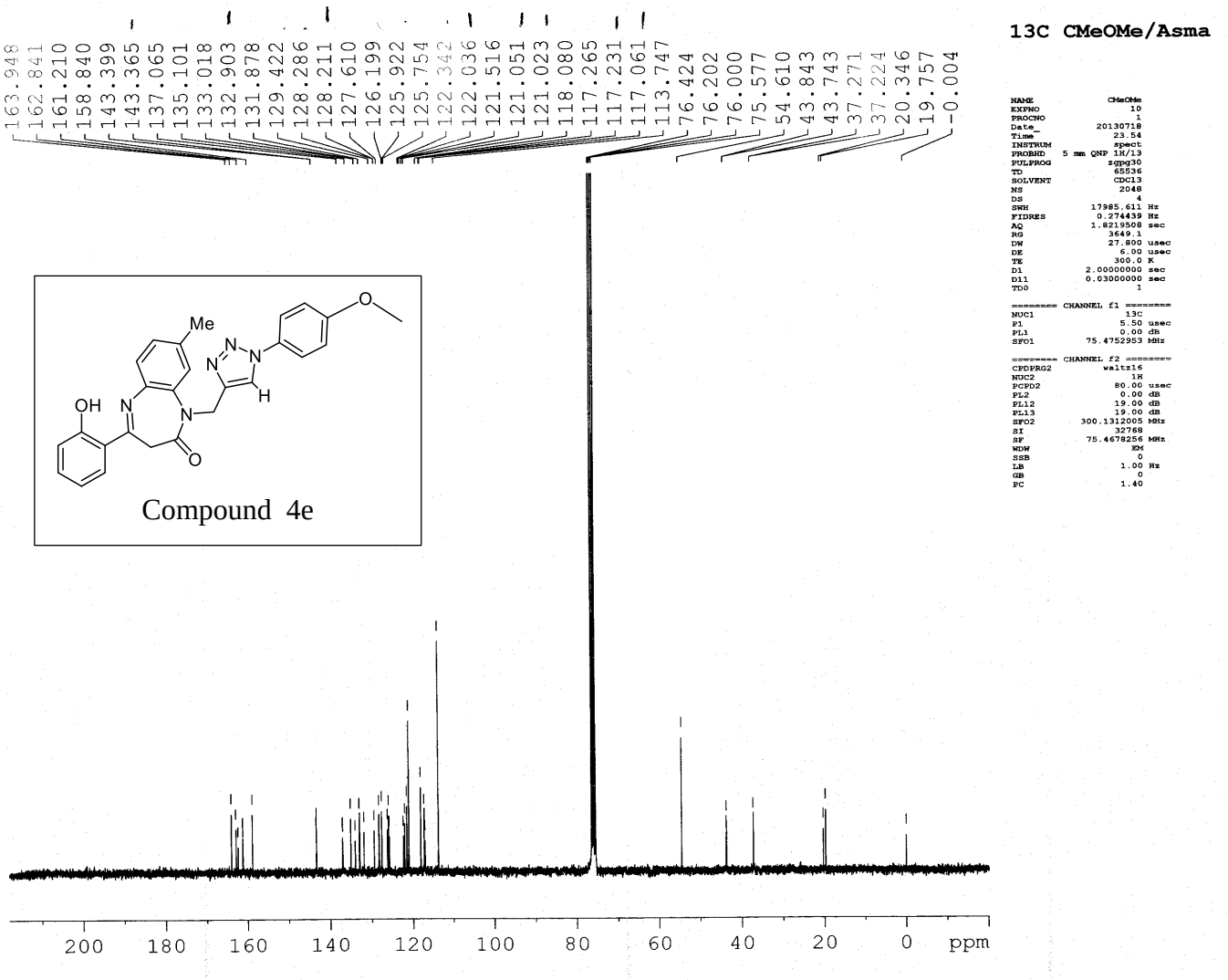


Figure S22. NMR spectra ^{13}C (75,47 MHz, $CDCl_3$) of compound **4e**

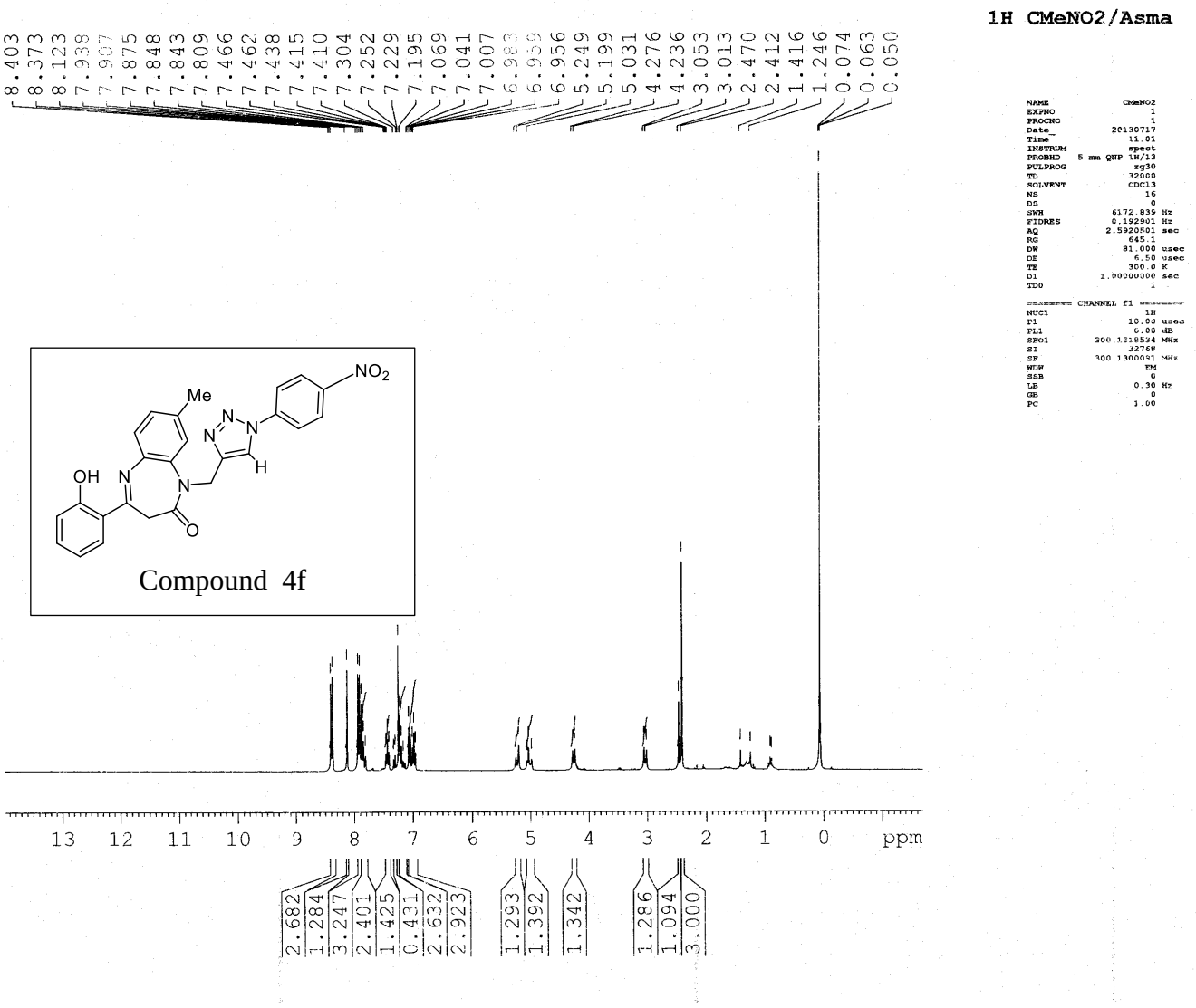


Figure S23. NMR spectra ^{1}H (300 MHz, $CDCl_3$) of compound **4f**

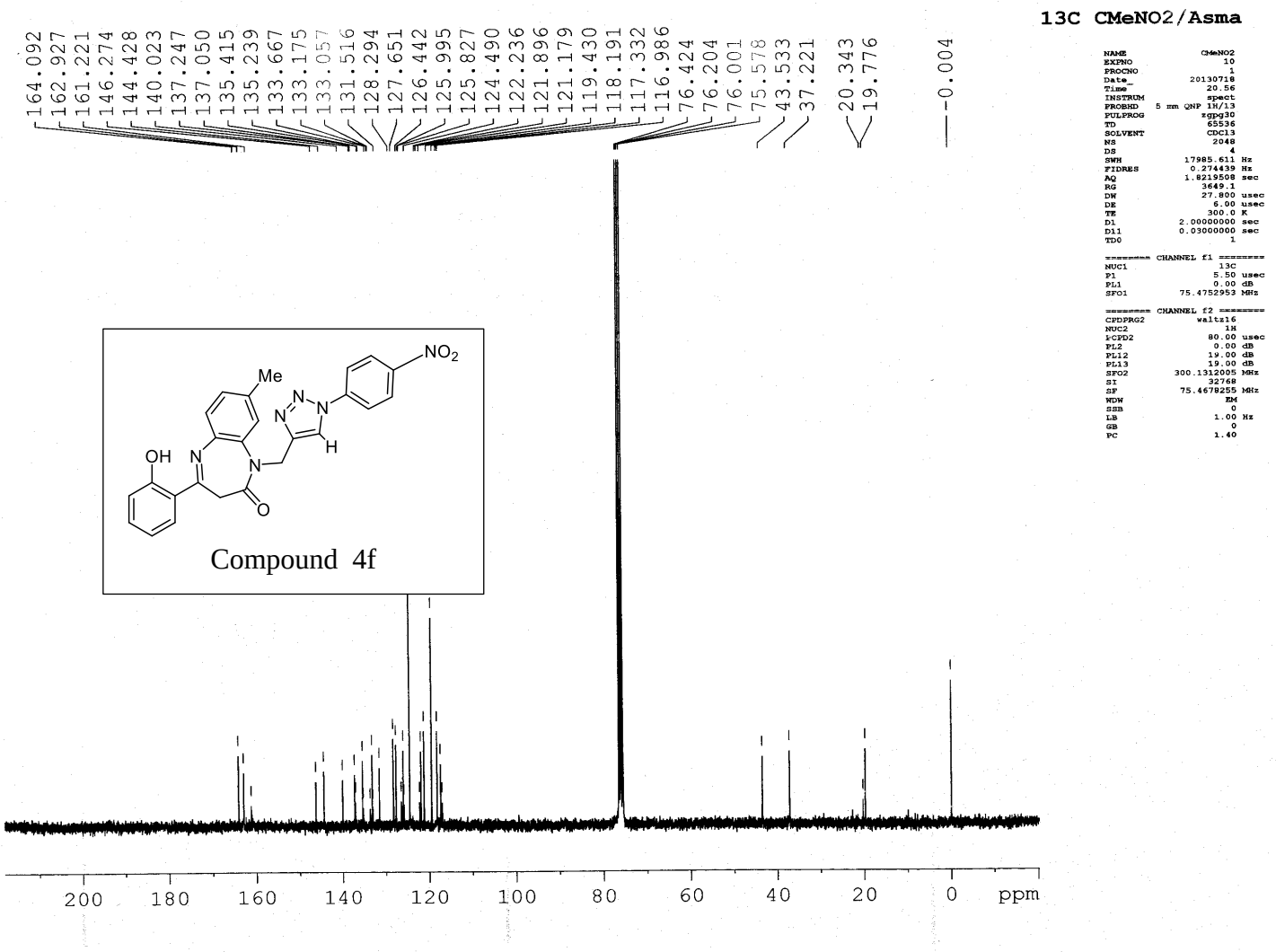


Figure S24. NMR spectra ^{13}C (75,47 MHz, $CDCl_3$) of compound **4f**

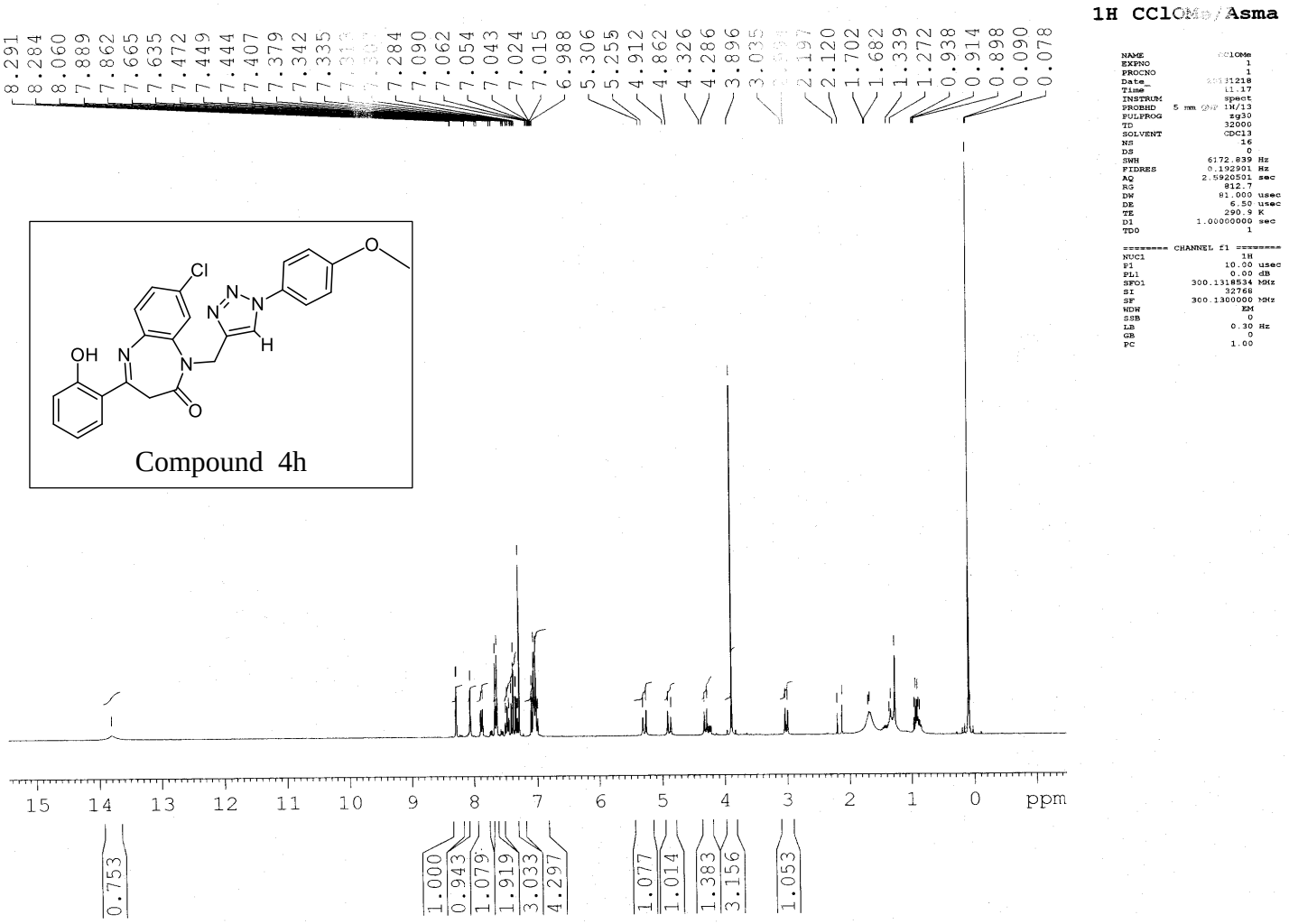
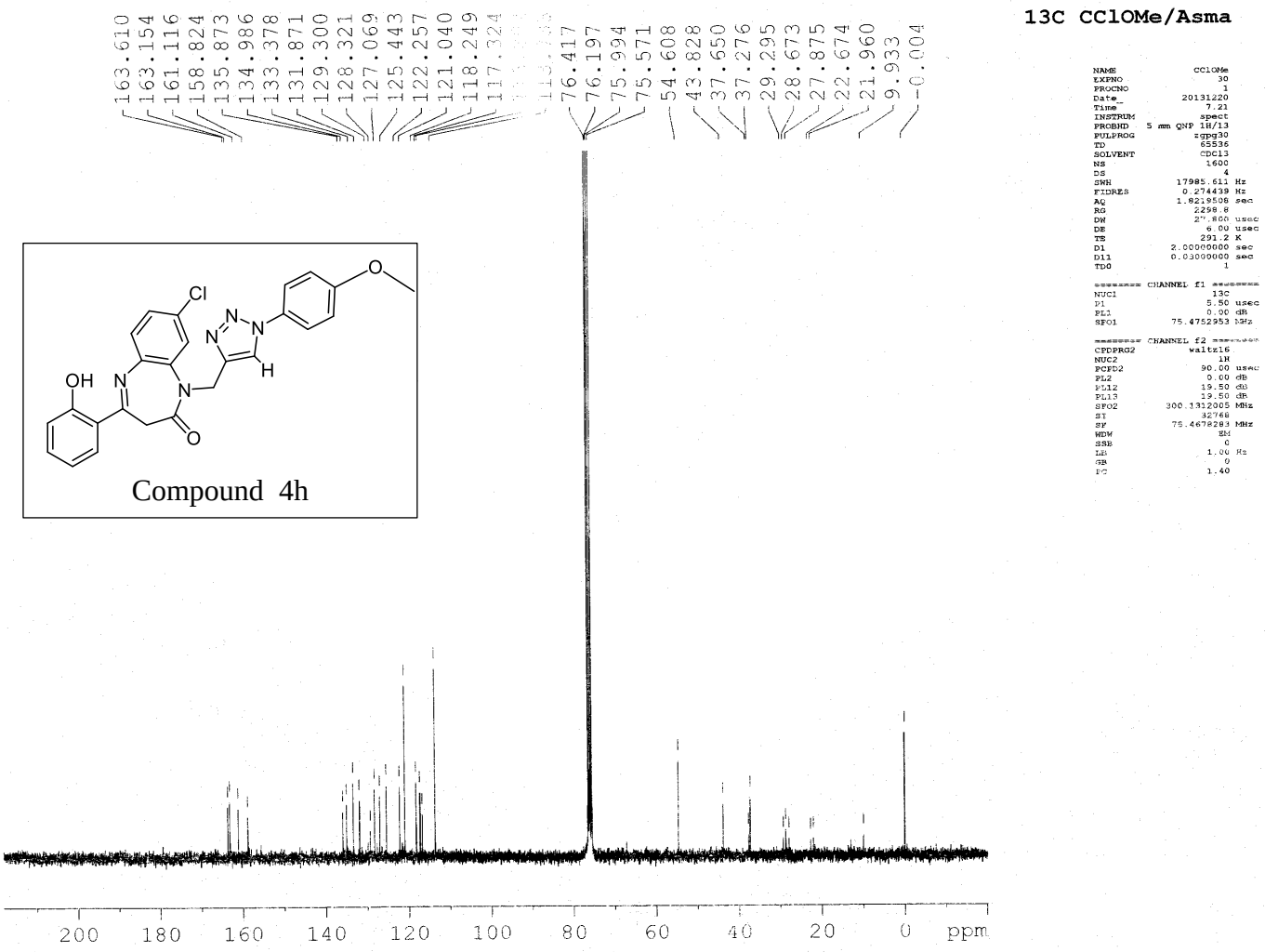


Figure S25. NMR spectra ^{1}H (300 MHz, $CDCl_3$) of compound **4h**



13C CClOMe/Asma

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PROCNO	1
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TE	291.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
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NUC1	13C
P1	5.50 usec
PL1	0.00 dB
SFO1	75.4752953 MHz
======== CHANNEL f2 ========	
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NUC2	1H
PCPD2	90.00 usec
PL2	0.00 dB
PL12	19.50 dB
PL13	19.50 dB
SFO2	300.1312005 MHz
SI	32768
SF	75.4678293 MHz
WDW	EM
SSB	0
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PC	1.40

Figure S26. NMR spectra ^{13}C (75,47 MHz, $CDCl_3$) of compound **4h**

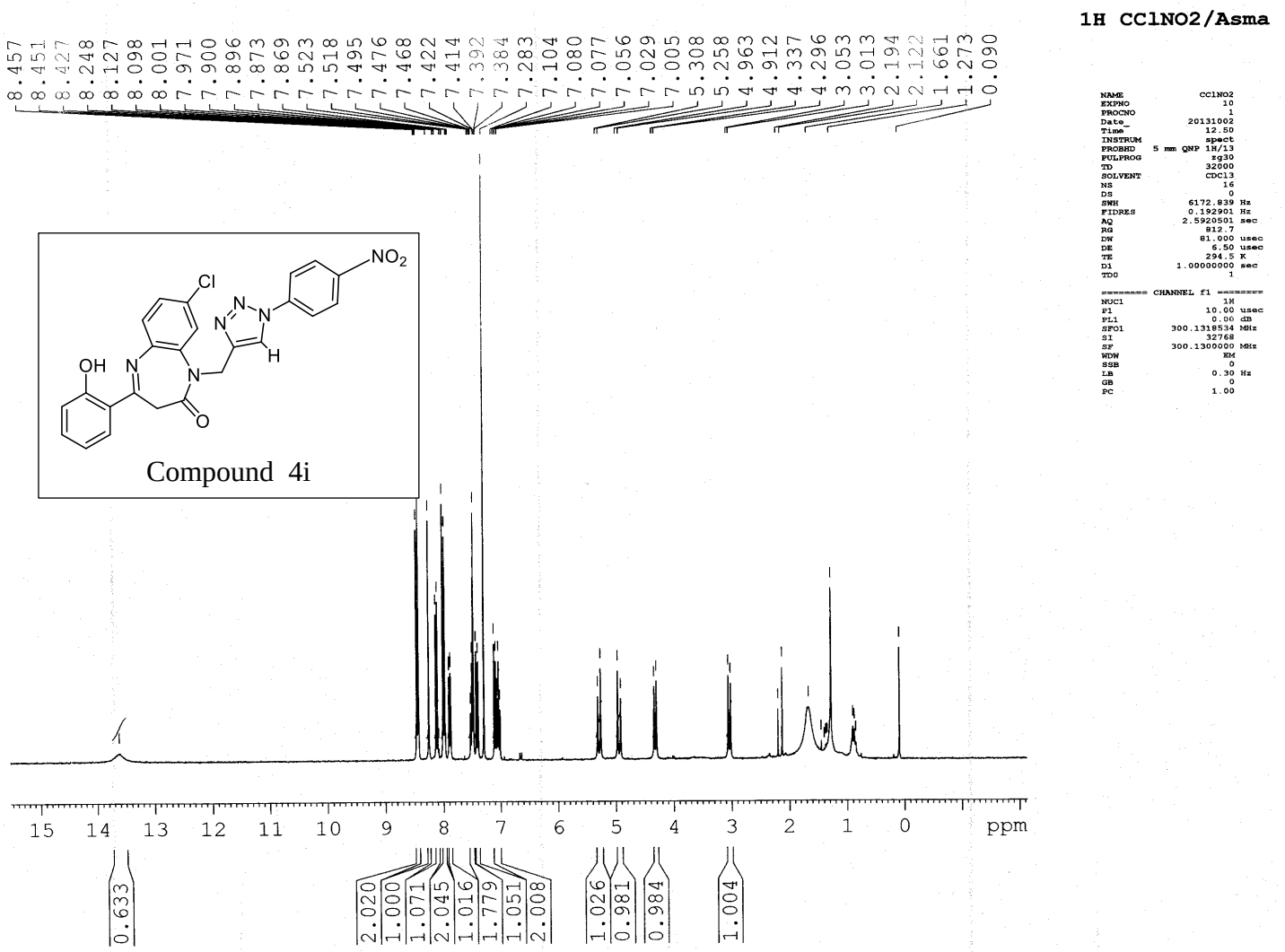

Figure S27. NMR spectra ^{1}H (300 MHz, $CDCl_3$) of compound **4i**

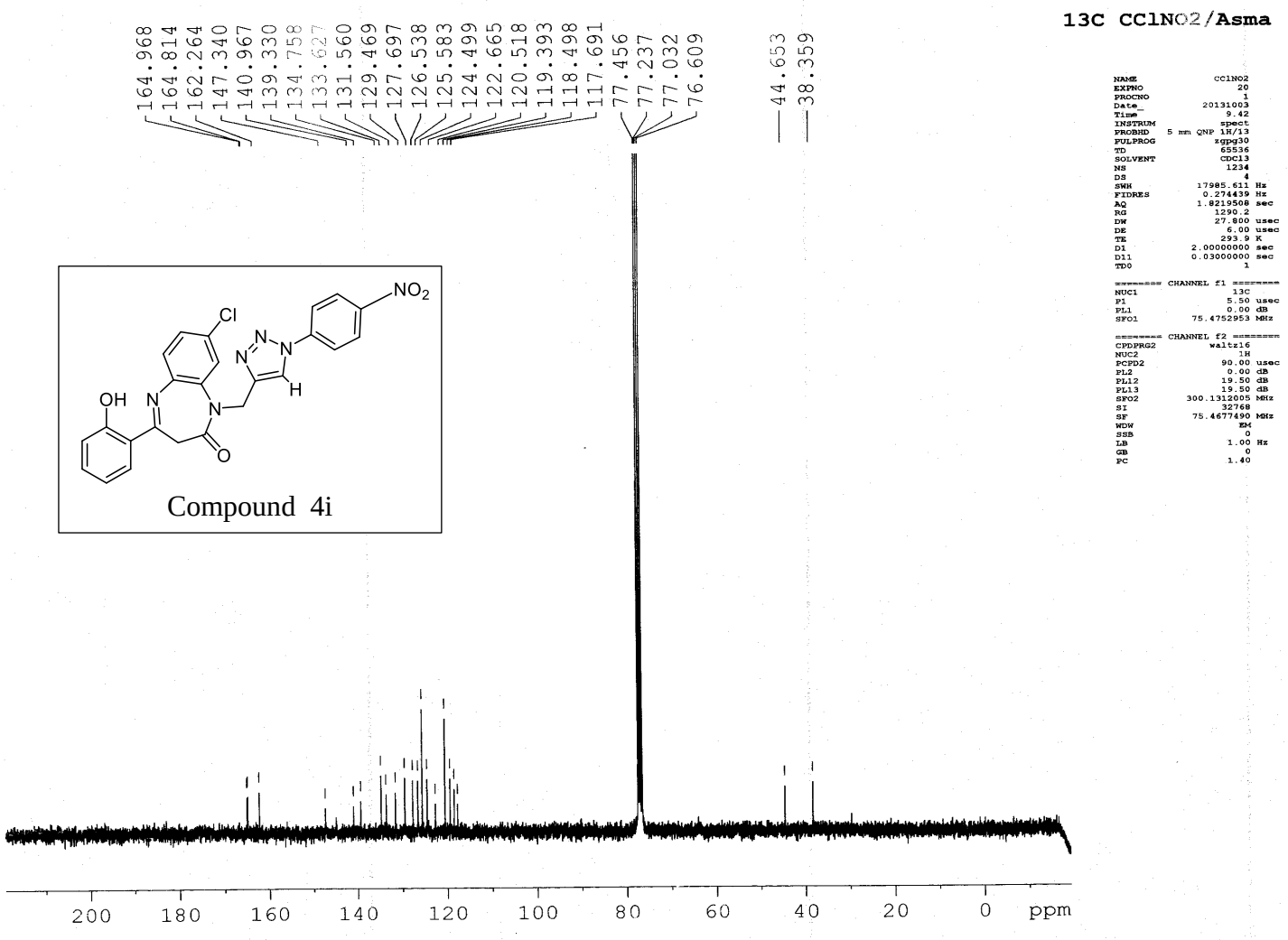

Figure S28. NMR spectra ^{13}C (75,47 MHz, $CDCl_3$) of compound **4i**