Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

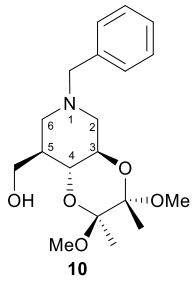
Coumarin-azasugar-benzyl conjugates as non-neurotoxic dual inhibitors of butyrylcholinesterase and cancer cell growth

I. Caroline Vaaland Holmgard,[a] Aday González-Bakker,[b] Eleonora Poeta,[c] Adrián Puerta,[b] Miguel X. Fernandes,[d] Barbara Monti,[c] José G. Fernández-Bolaños,[e] José M. Padrón,*[b] Óscar López,*[e] and Emil Lindbäck*[a]

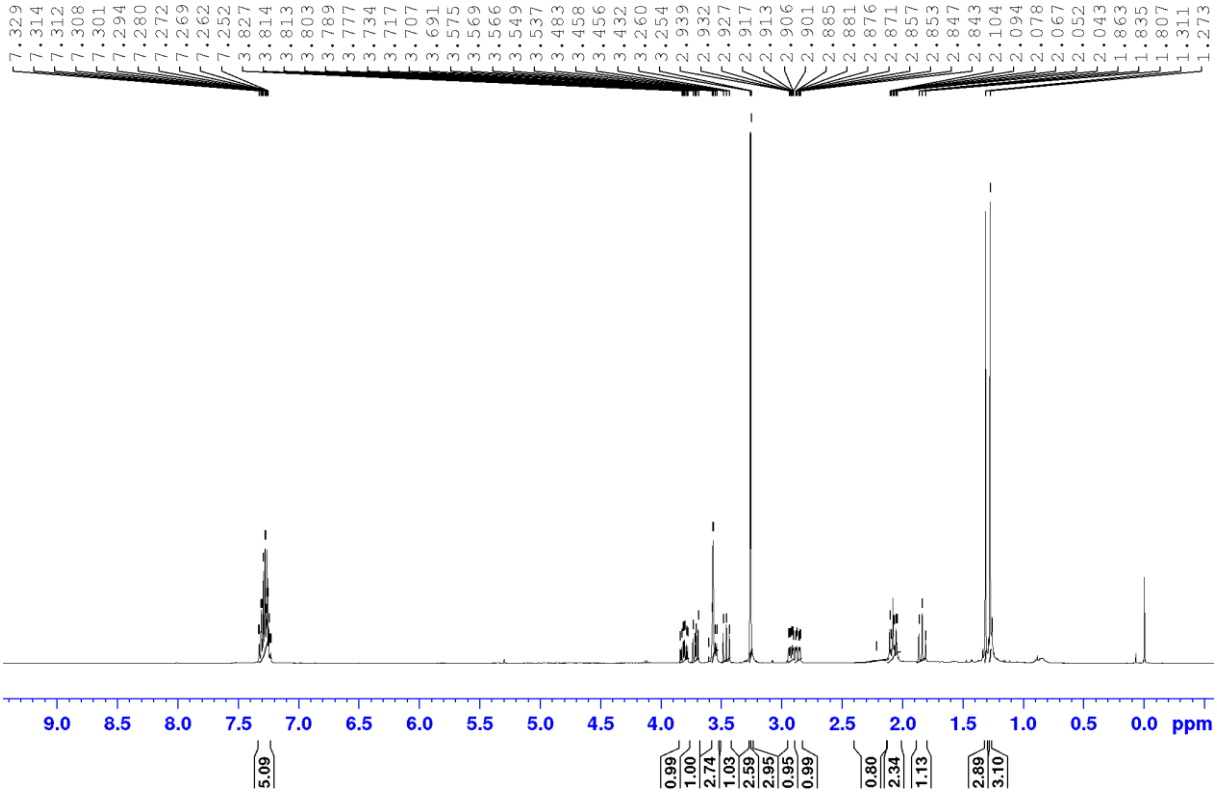
[a]Department of Chemistry, Bioscience and Environmental Engineering, Faculty of Science and Technology, University of Stavanger, Stavanger, Norway
[b]BioLab, Instituto Universitario de Bio-Orgánica "Antonio González" (IUBO-AG), Universidad de La Laguna, c/Astrofísico Francisco Sánchez 2, La Laguna, E-38206, Spain
[c]Department of Pharmacy and Biotechnology, University of Bologna, Bologna, Italy
[d]Department of Engineering and Chemical Sciences, Karlstad University, Karlstad, Sweden
[e]Departamento de Química Orgánica, Facultad de Química, Universidad de Sevilla, Seville, Spain.

Table of content

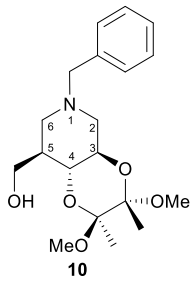
^{1}H-NMR spectra of compound **10** ($CDCl_3$, 400.13 MHz)



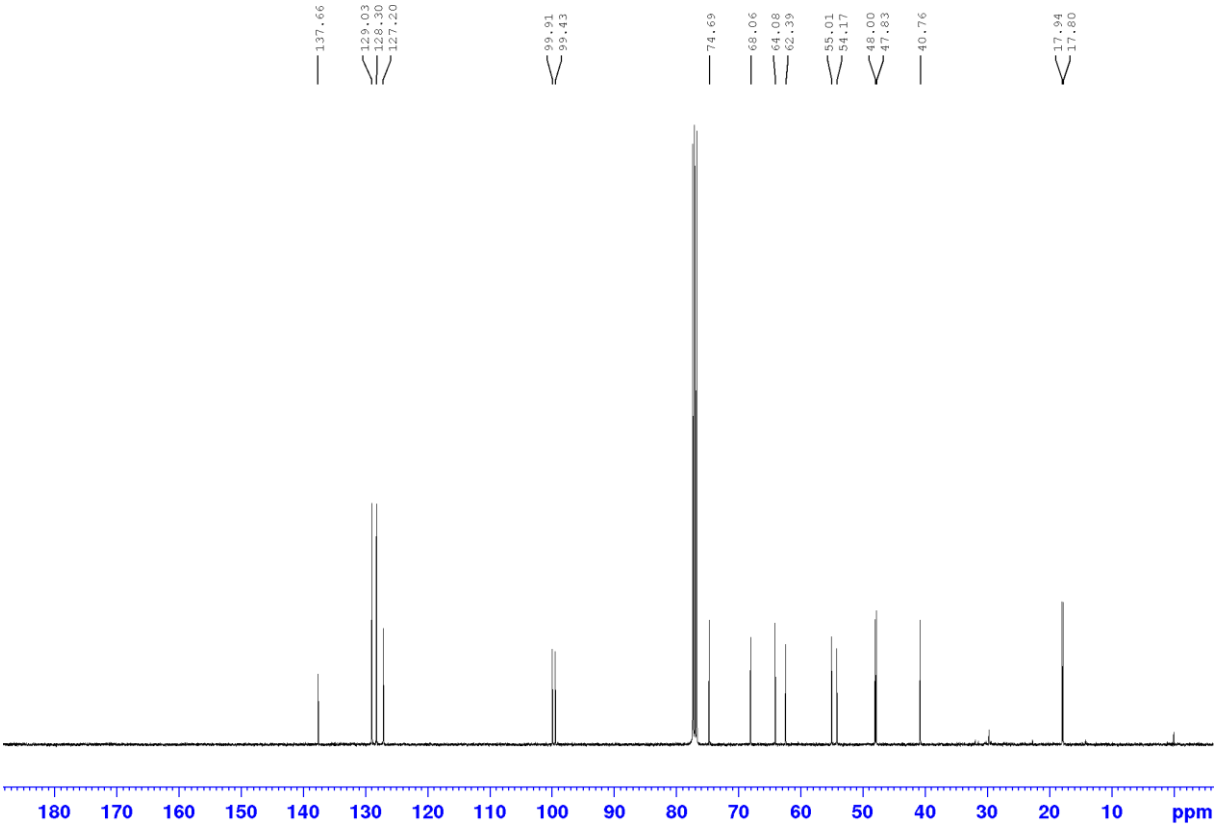
10



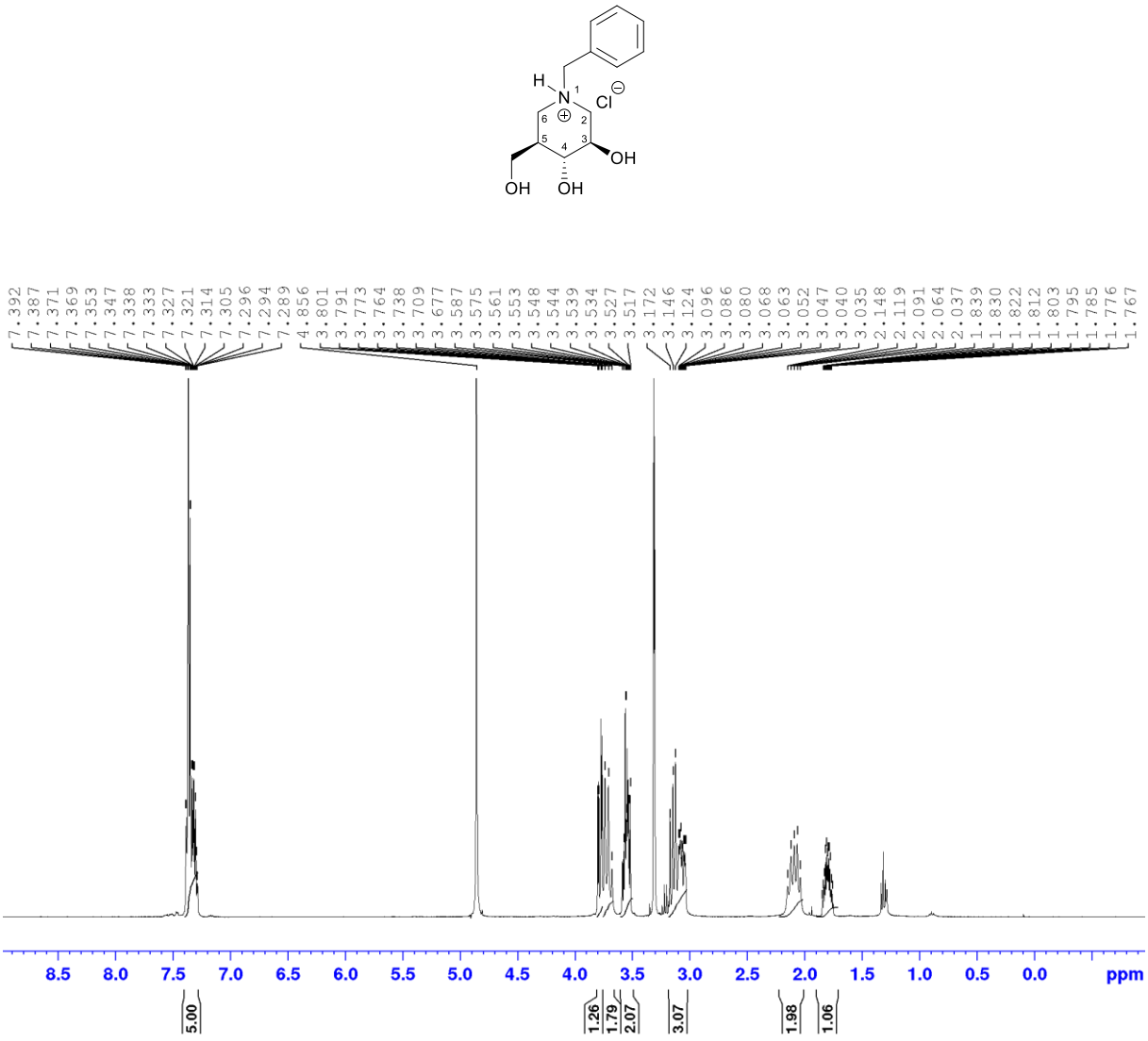
^{13}C-NMR spectra of compound **10** ($CDCl_3$, 100.61 MHz)



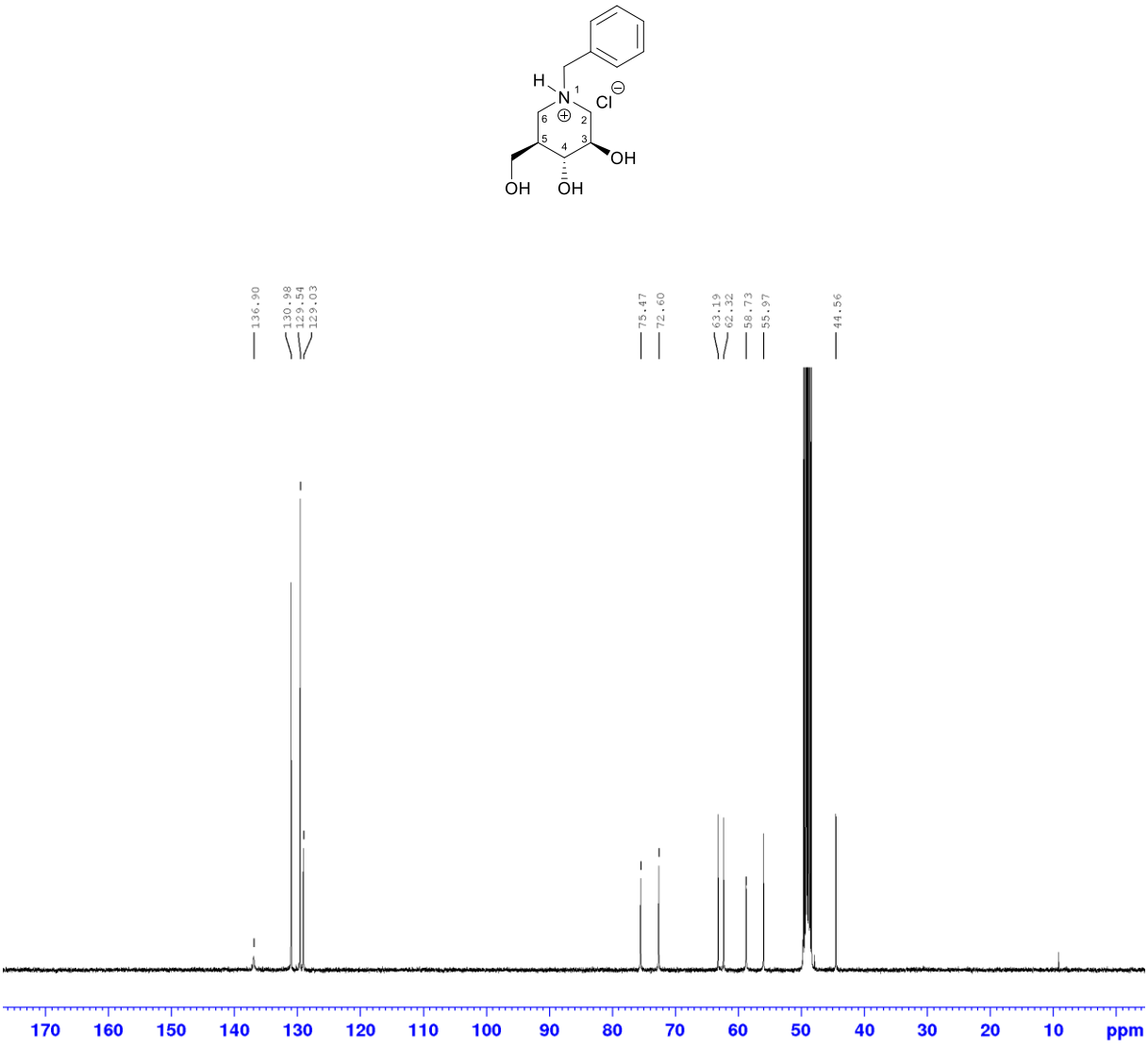
10



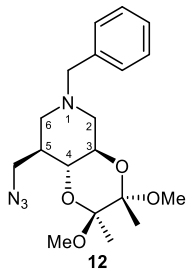
^{1}H-NMR spectra of compound **11** (CD_3OD, 400.13 MHz)



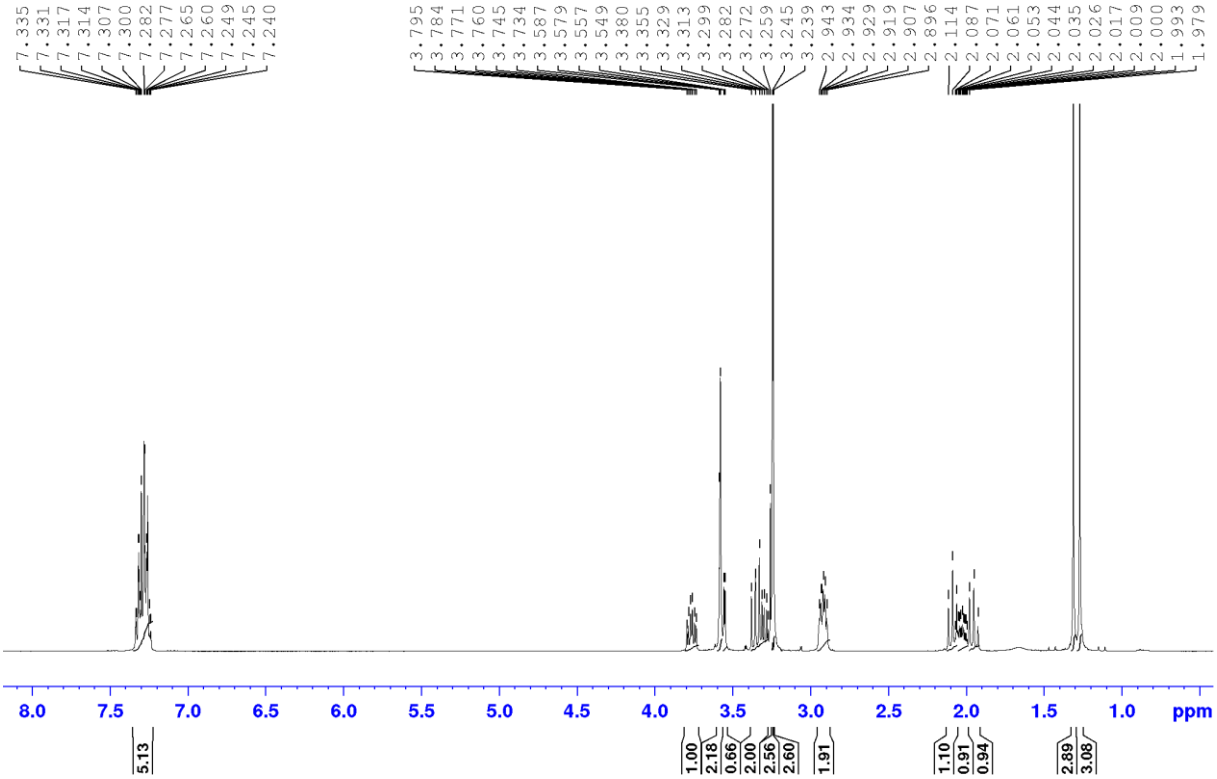
^{13}C-NMR spectra of compound **11** (CD_3OD, 100.61 MHz)



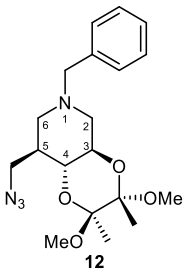
^{1}H-NMR spectra of compound **12** ($CDCl_3$, 400.13 MHz)



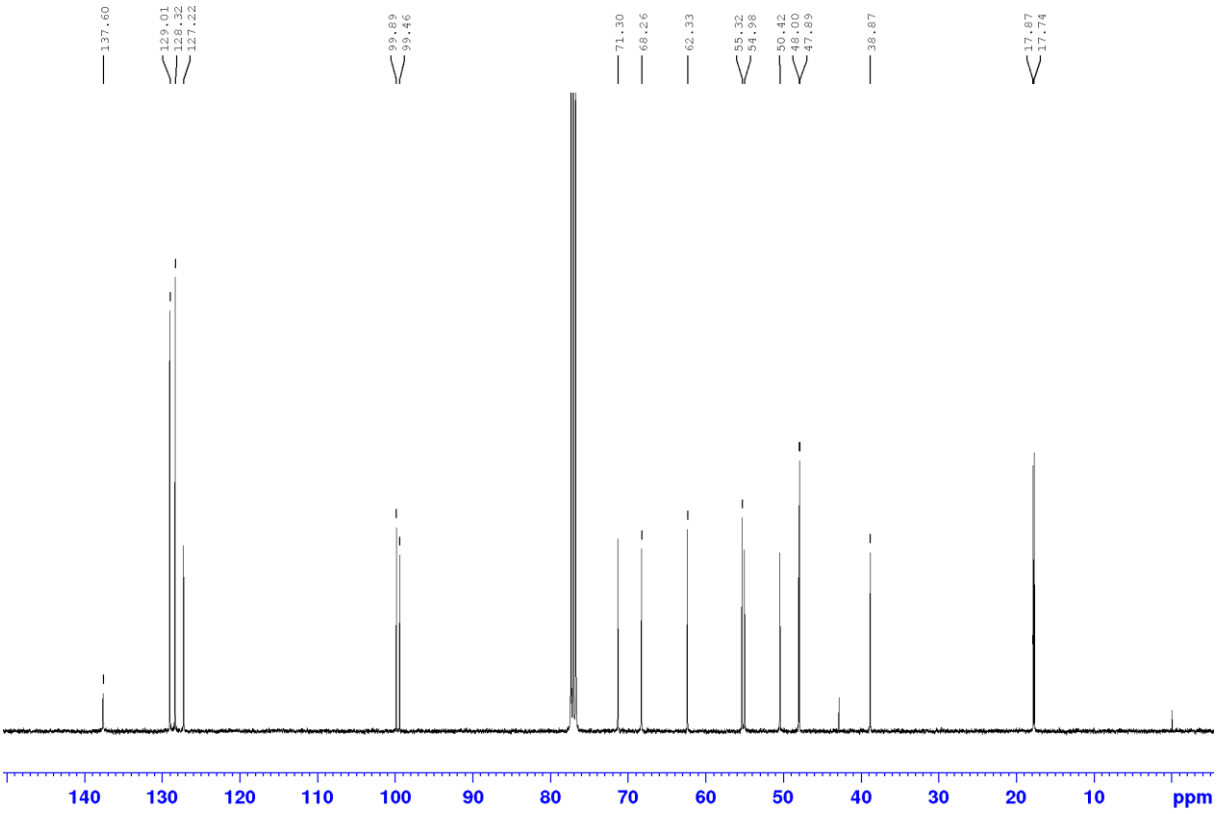
12



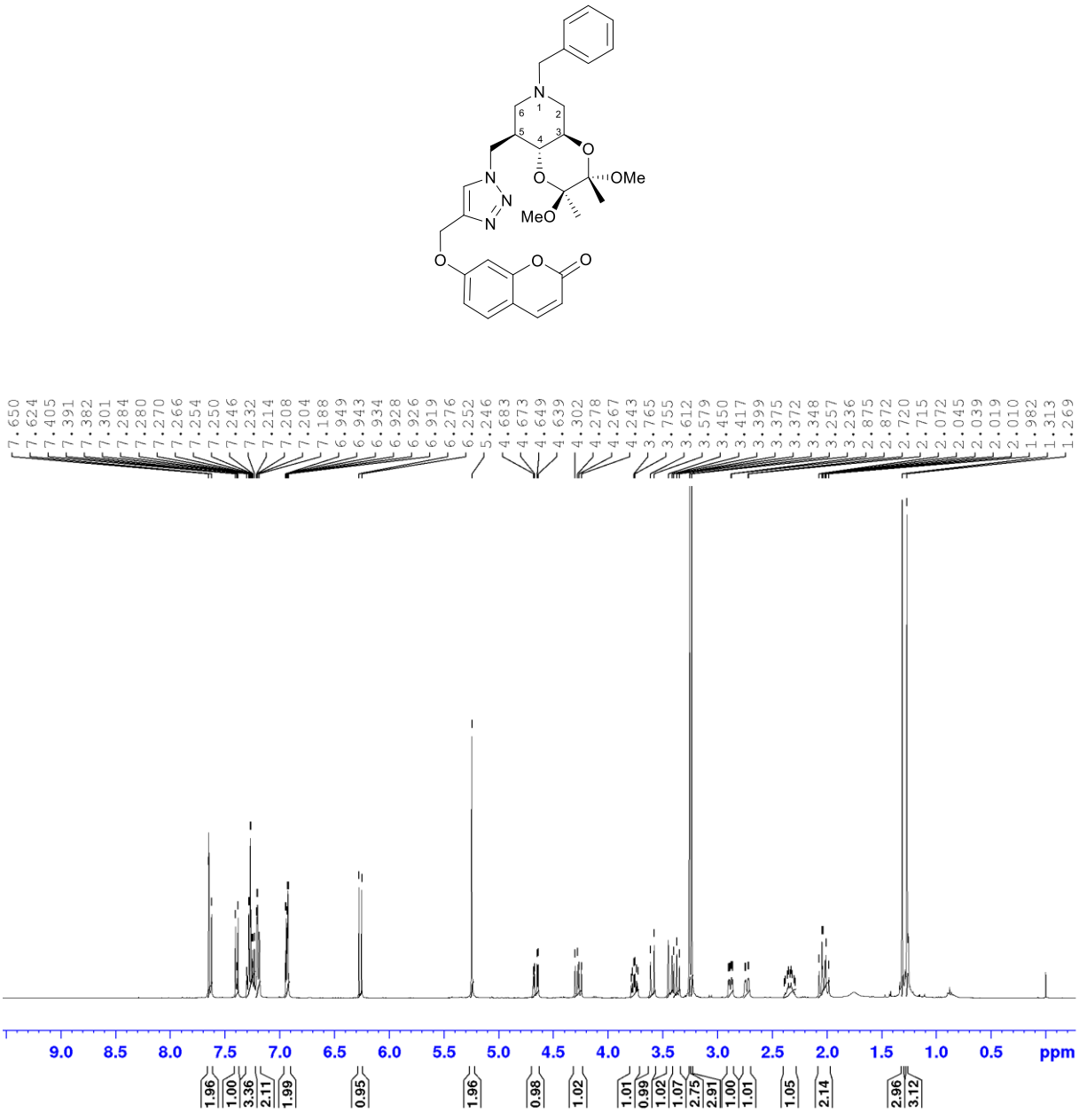
^{13}C-NMR spectra of compound **12** ($CDCl_3$, 100.61 MHz)



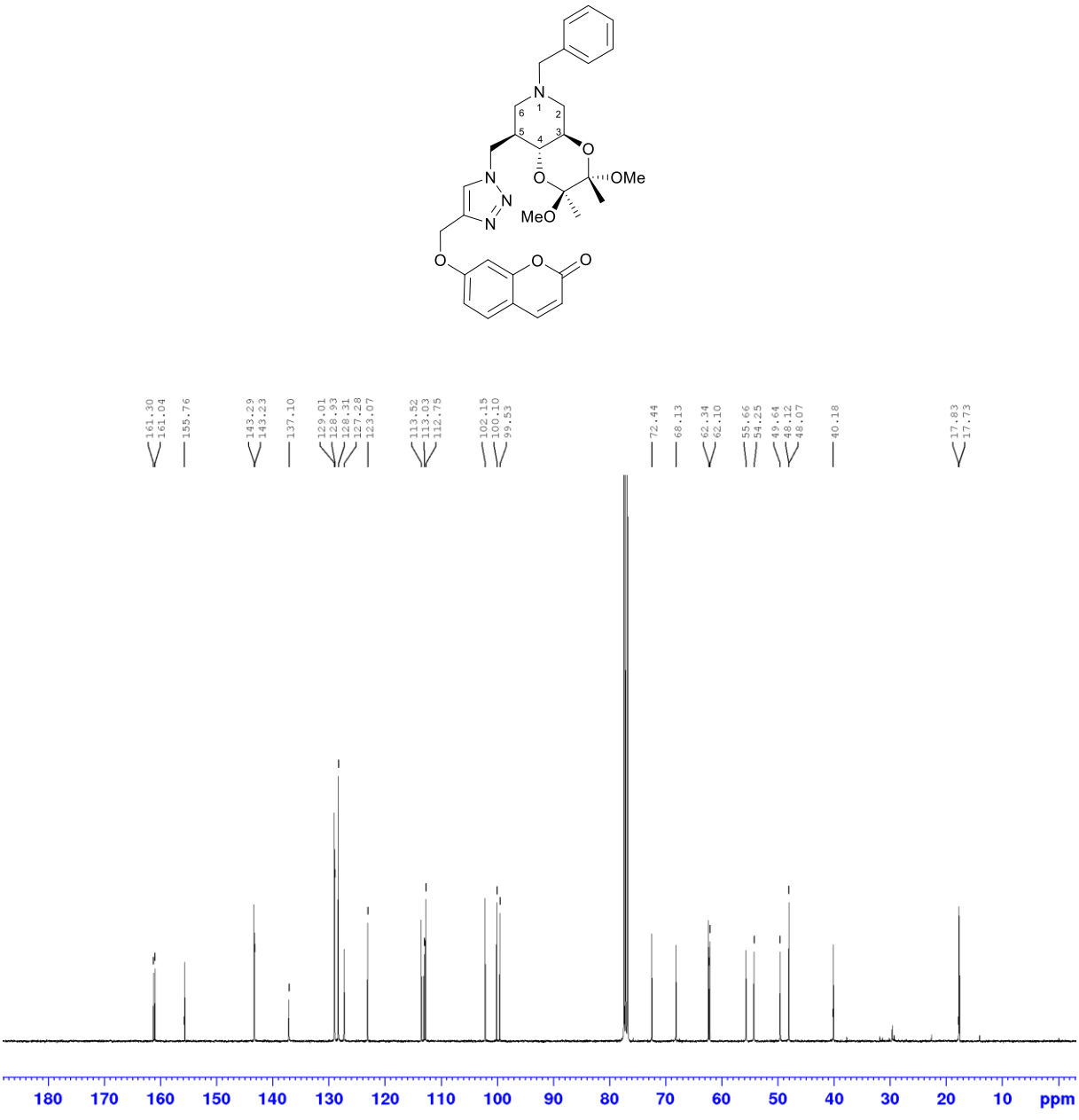
12



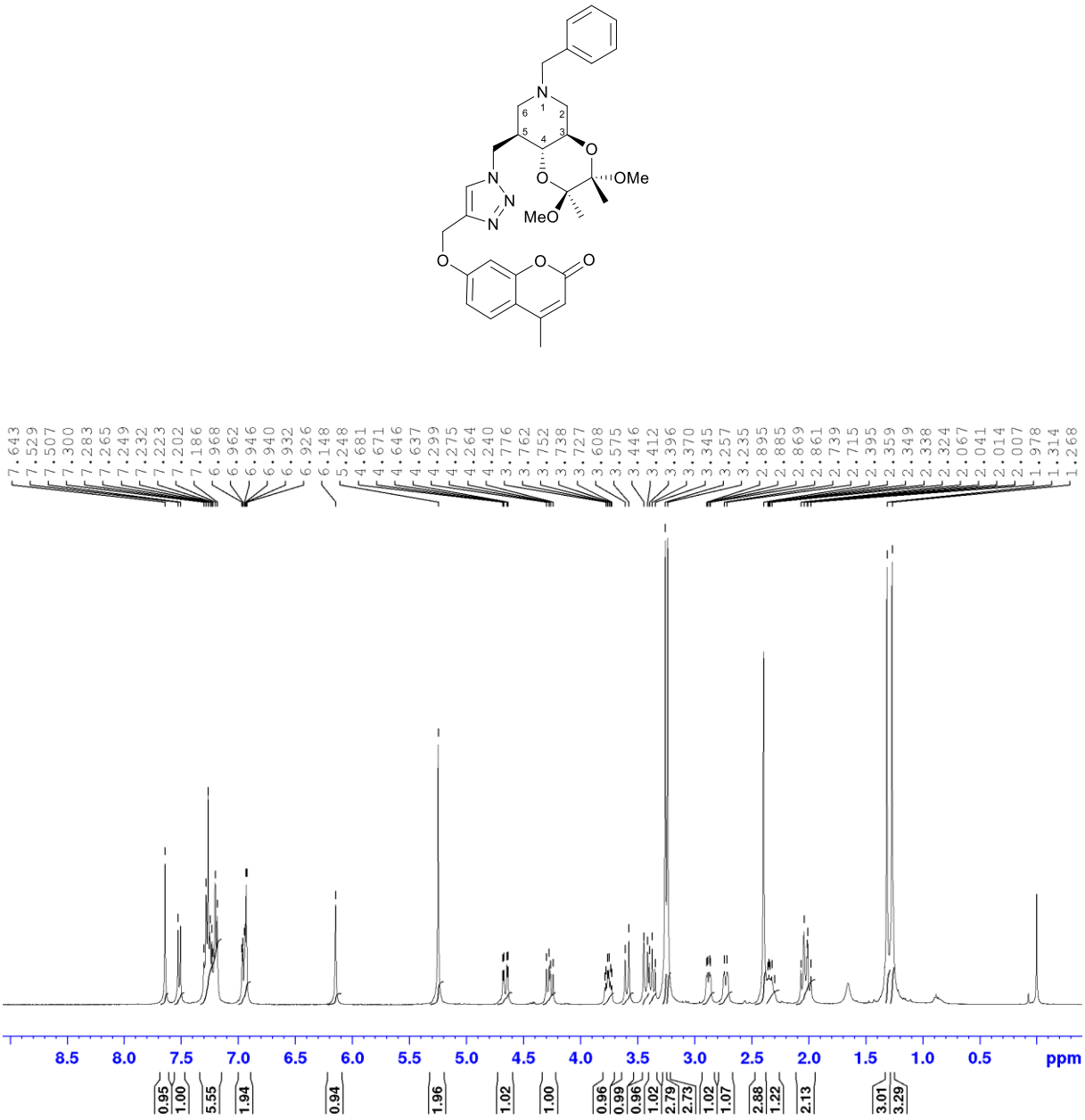
^{1}H-NMR spectra of compound **17a** ($CDCl_3$, 400.13 MHz)



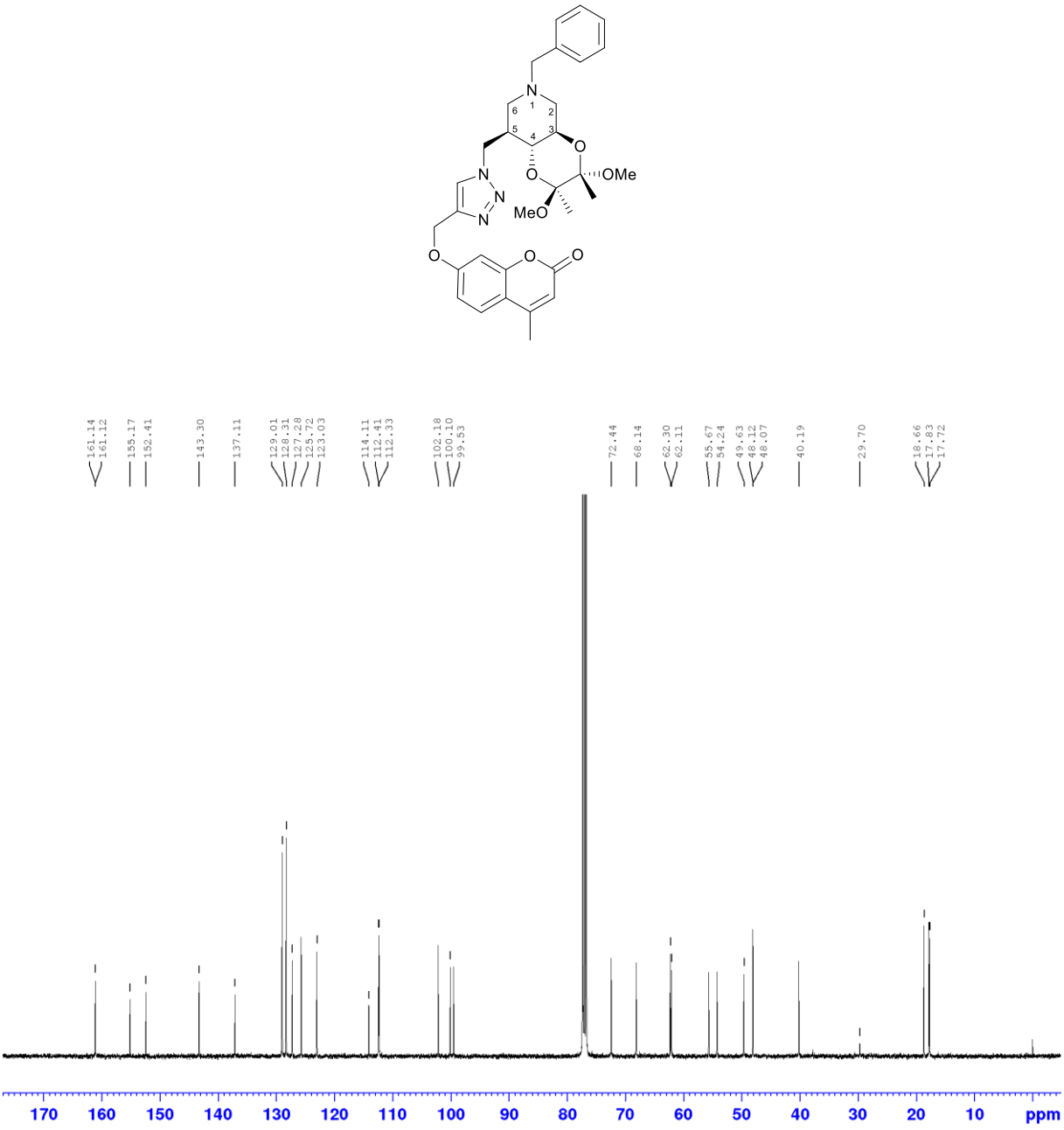
^{13}C-NMR spectra of compound **17a** ($CDCl_3$, 100.61 MHz)



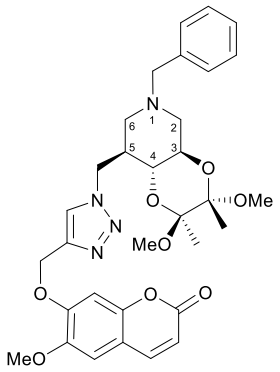
^{1}H-NMR spectra of compound **17b** ($CDCl_3$, 400.13 MHz)

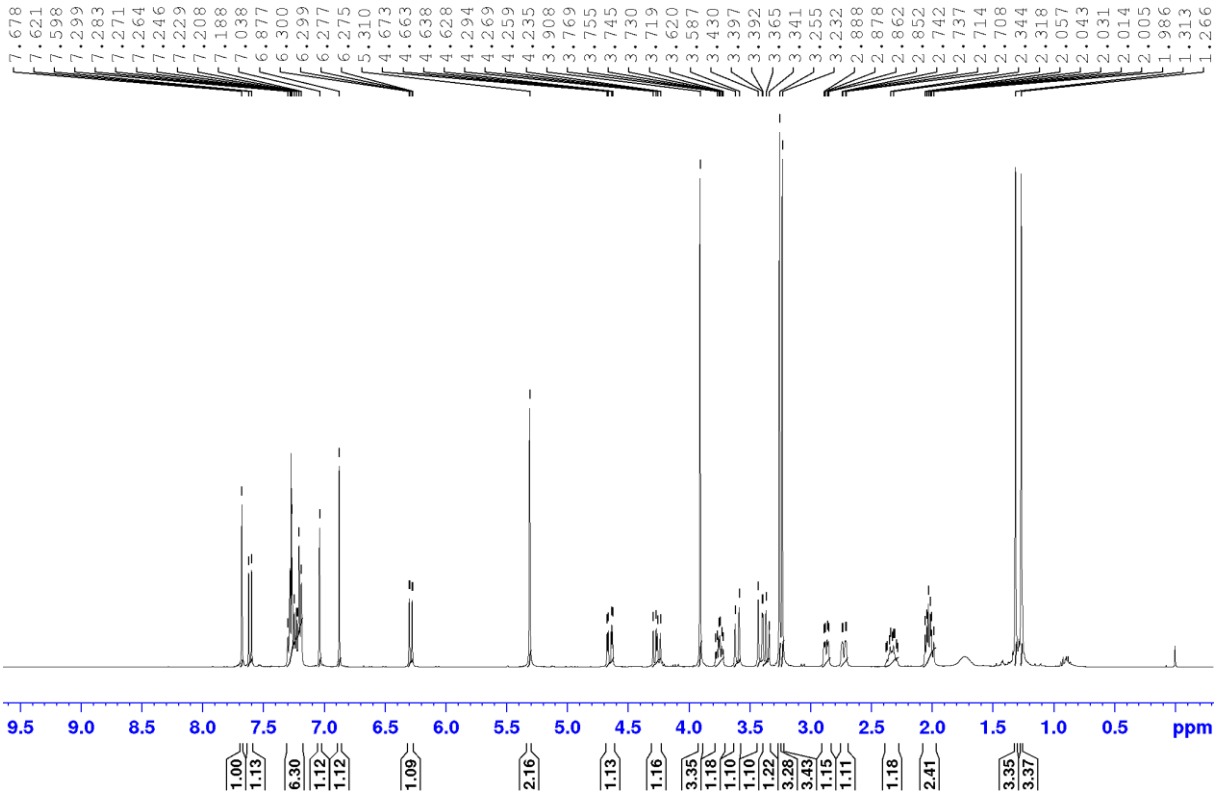


^{13}C-NMR spectra of compound **17b** ($CDCl_3$, 100.61 MHz)

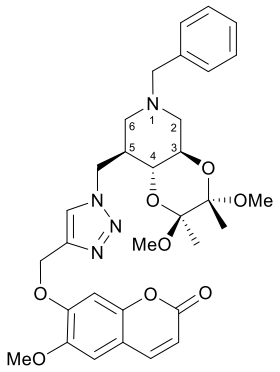


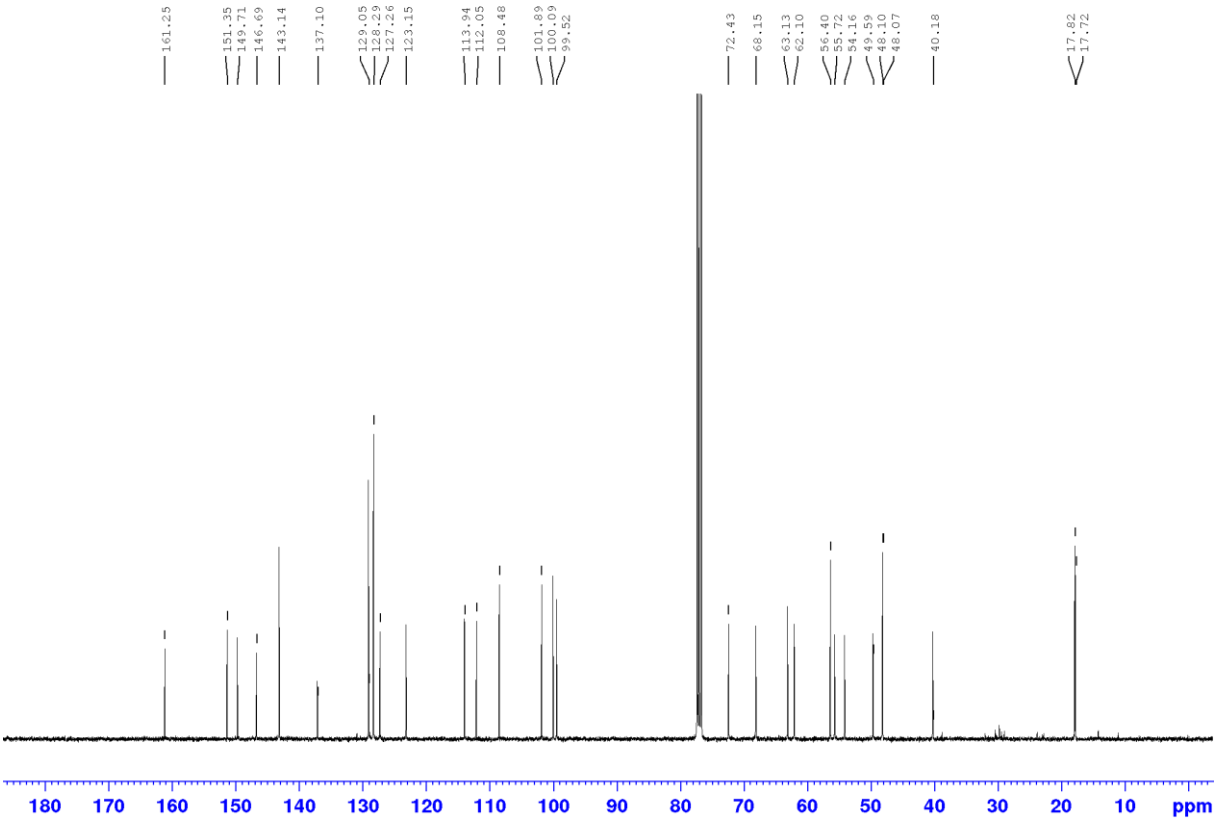
^{1}H-NMR spectra of compound **17c** ($CDCl_3$, 400.13 MHz)



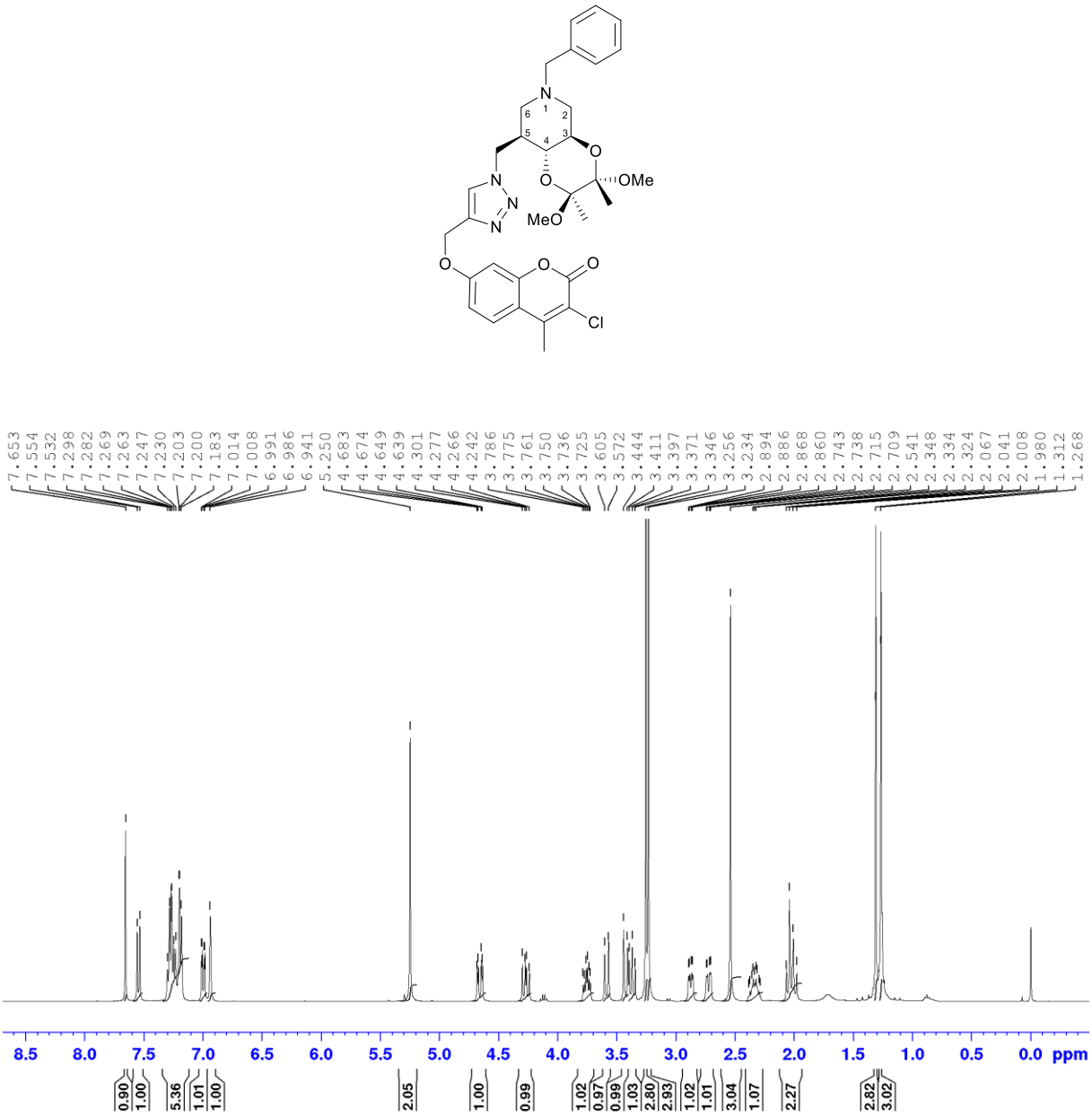


^{13}C-NMR spectra of compound **17c** ($CDCl_3$, 100.61 MHz)

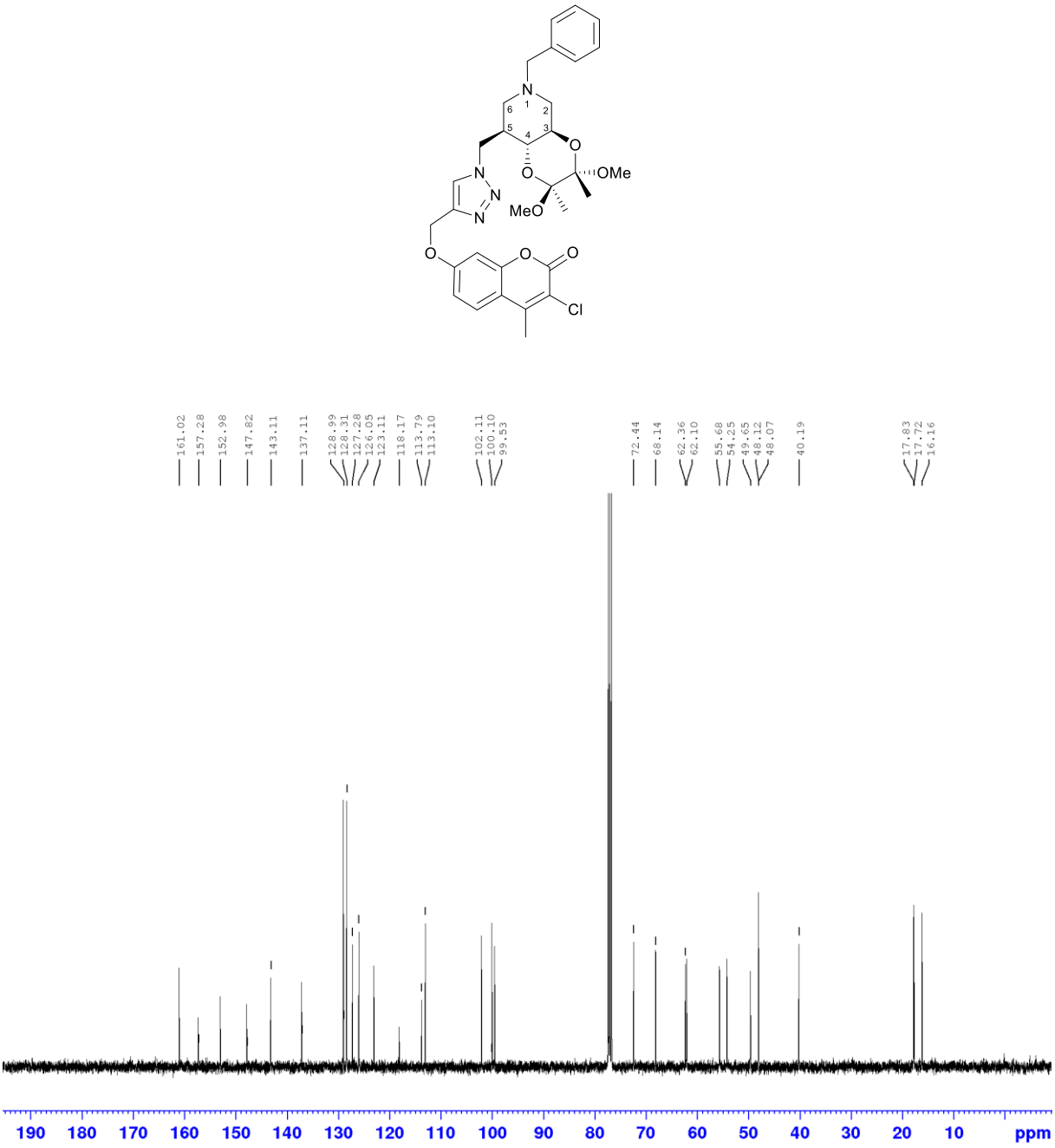




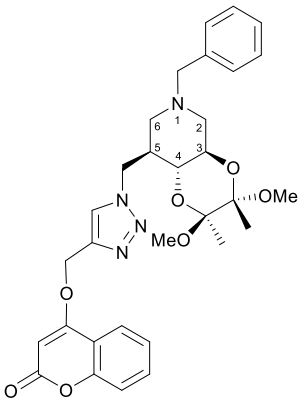
^{1}H-NMR spectra of compound **17d** ($CDCl_3$, 400.13 MHz)

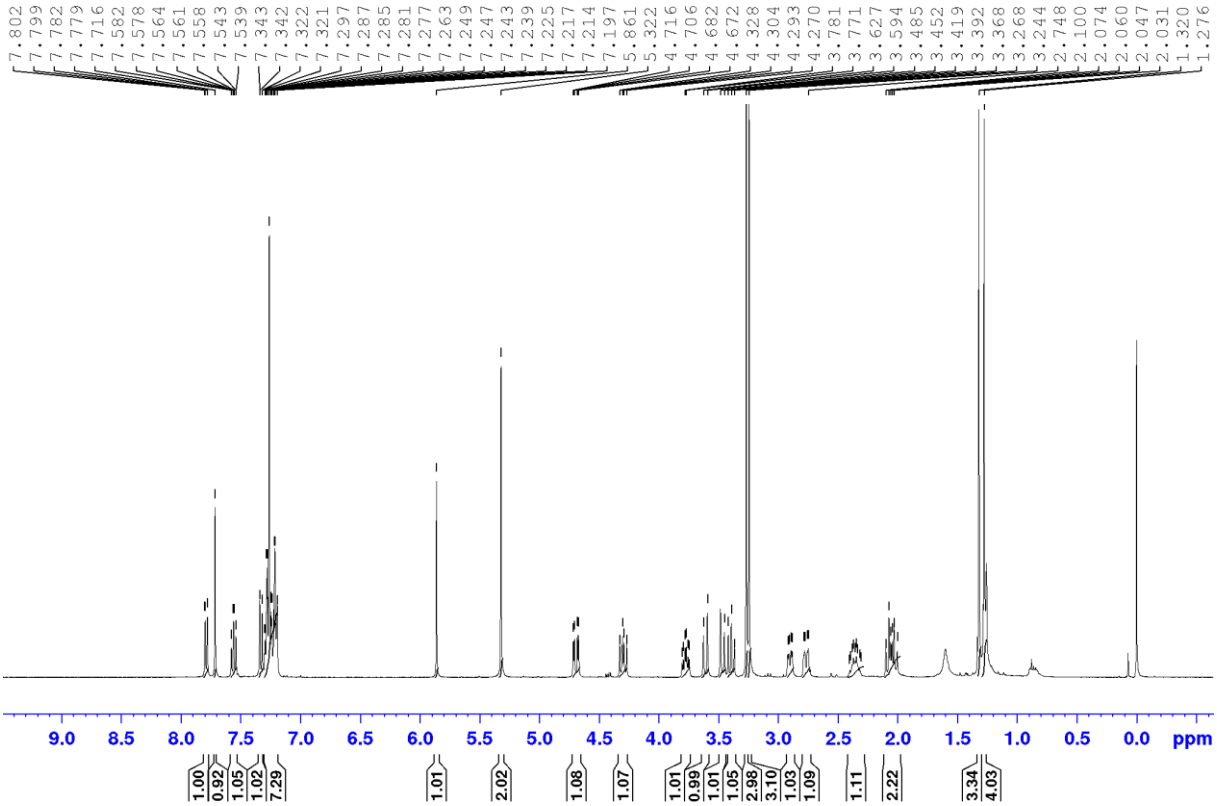


^{13}C-NMR spectra of compound **17d** ($CDCl_3$, 100.61 MHz)

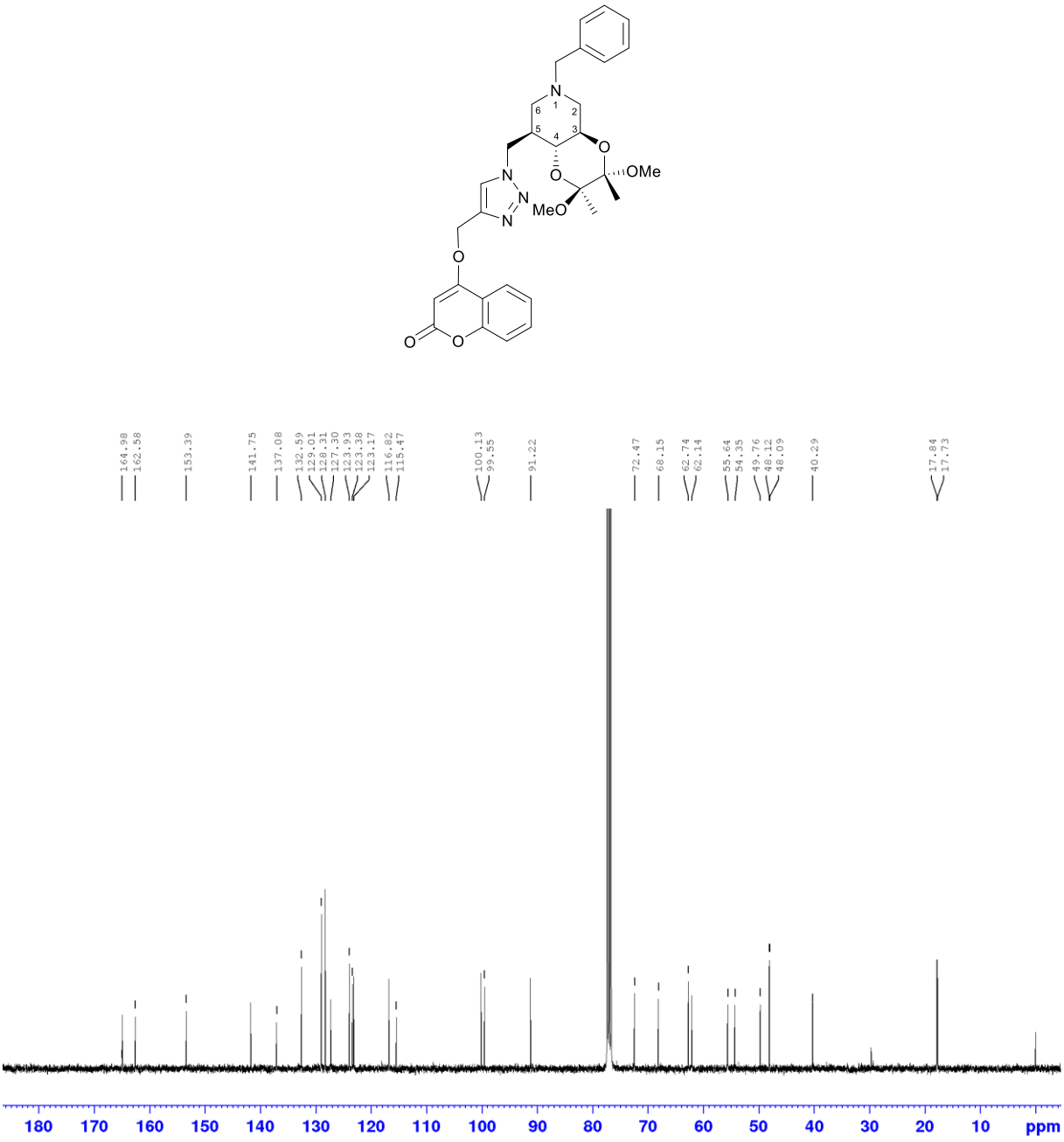


^{1}H-NMR spectra of compound **17e** ($CDCl_3$, 400.13 MHz)

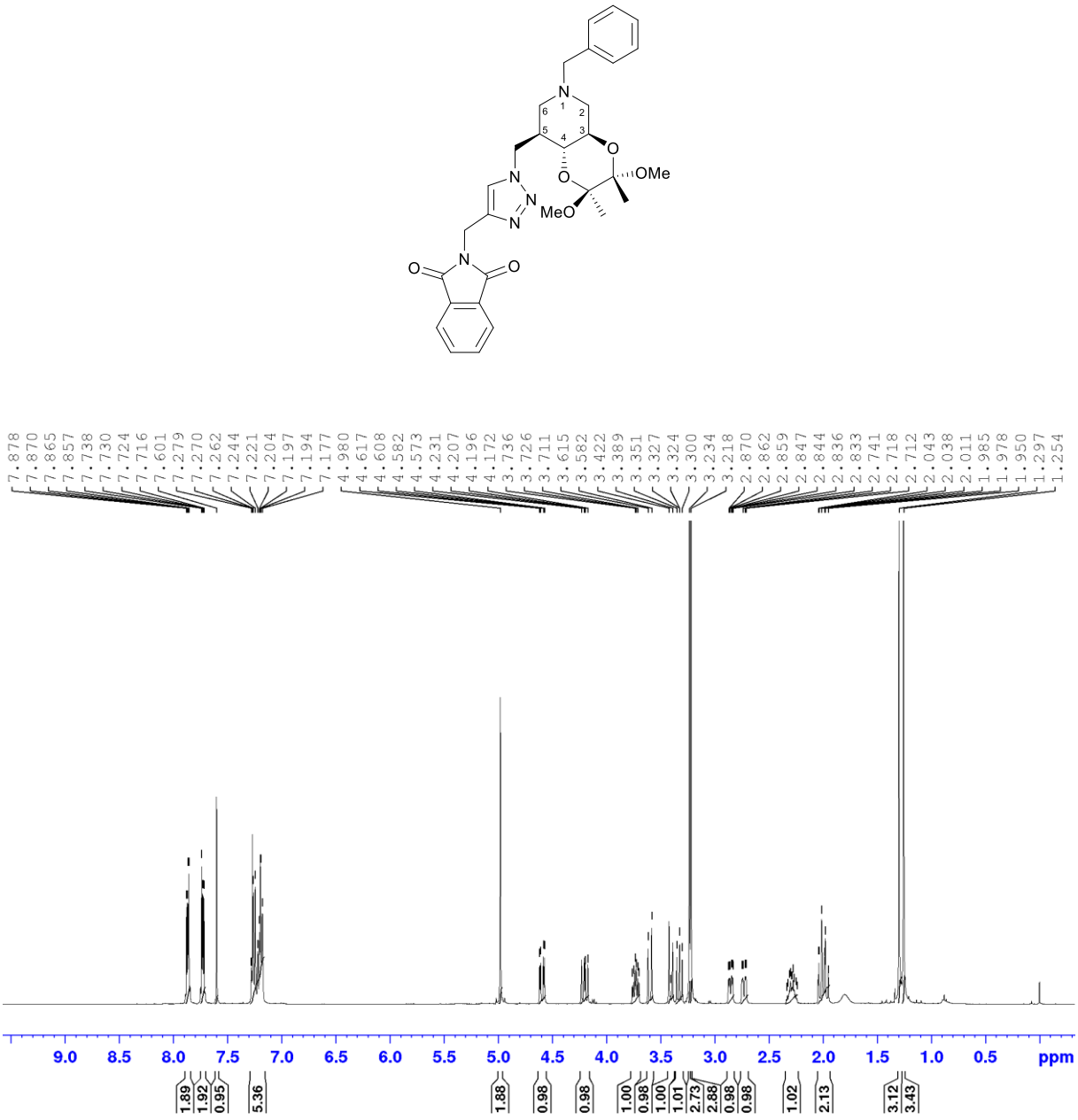




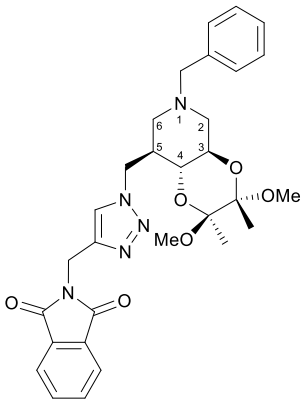
^{13}C-NMR spectra of compound **17e** ($CDCl_3$, 100.61 MHz)

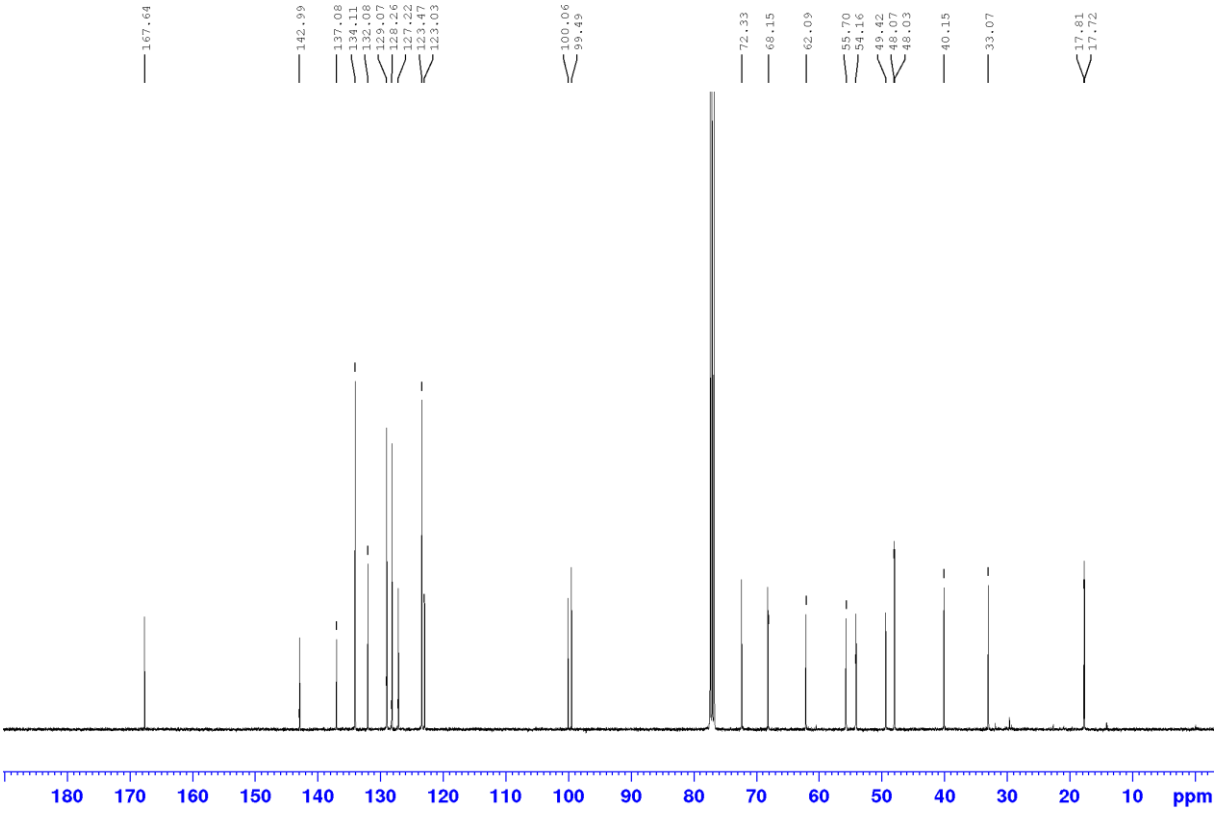


^{1}H-NMR spectra of compound **20** ($CDCl_3$, 400.13 MHz)

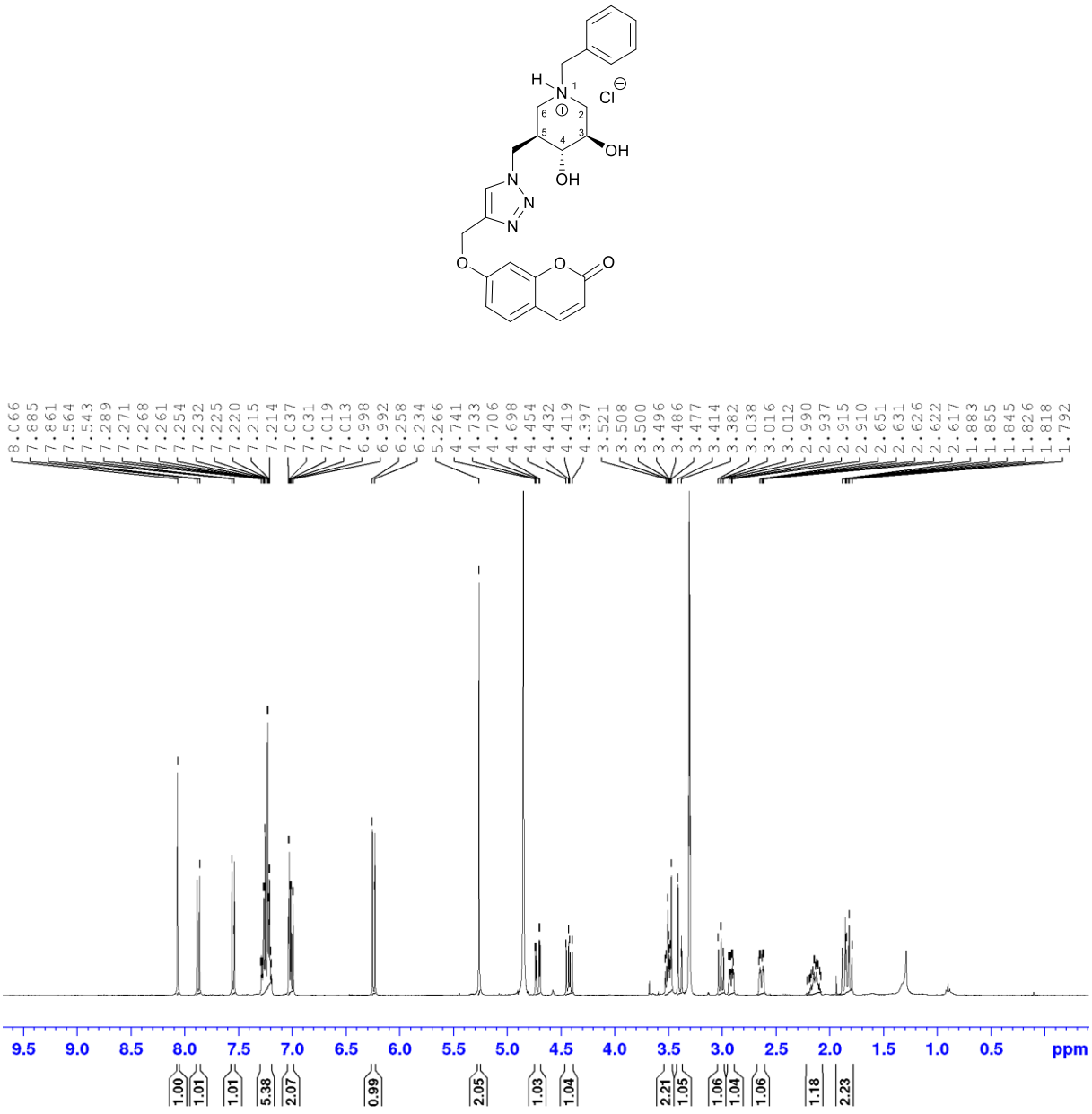


^{13}C-NMR spectra of compound **20** ($CDCl_3$, 100.61 MHz)

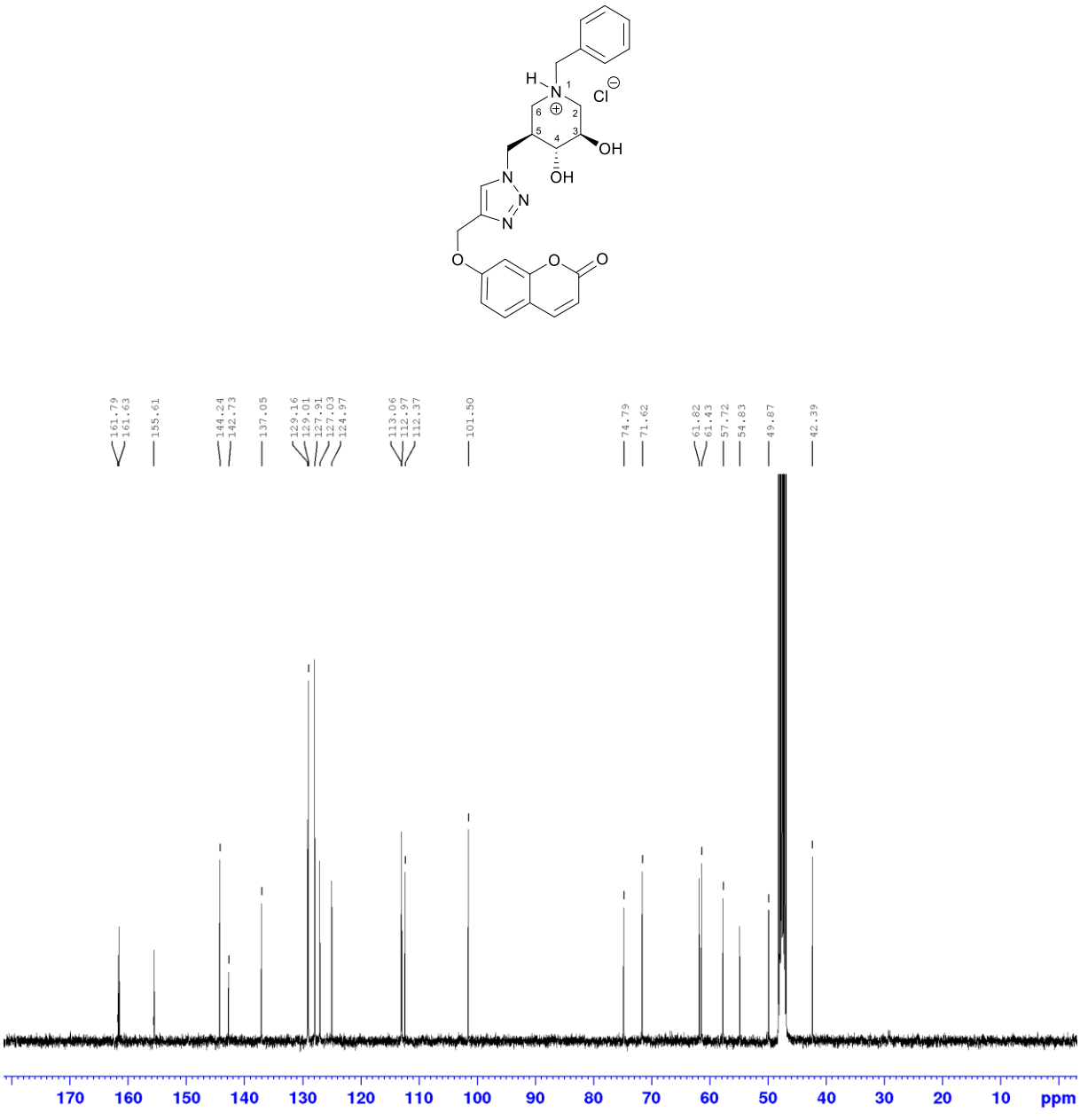




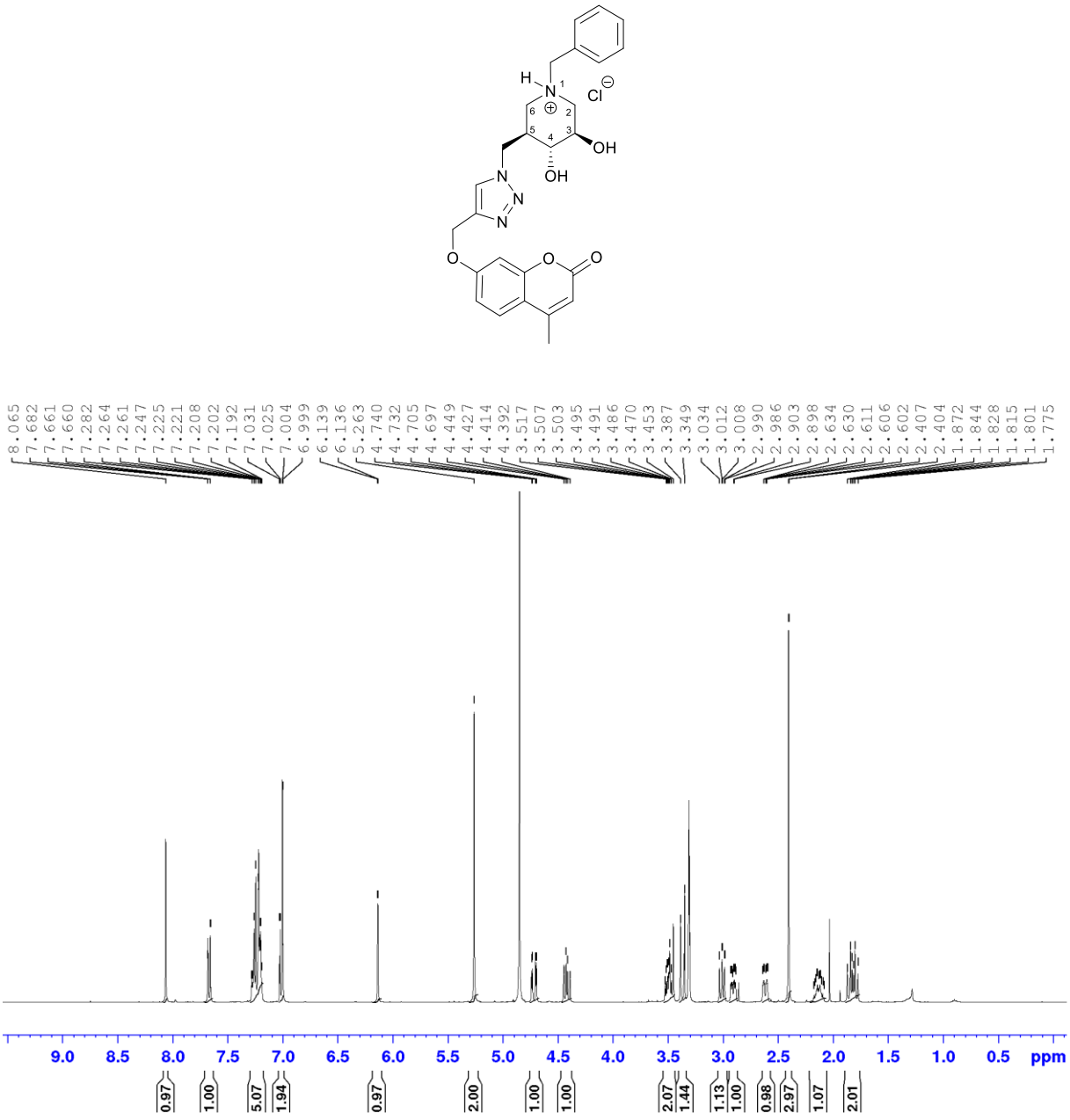
^{1}H-NMR spectra of compound **8a** (CD_3OD, 400.13 MHz)



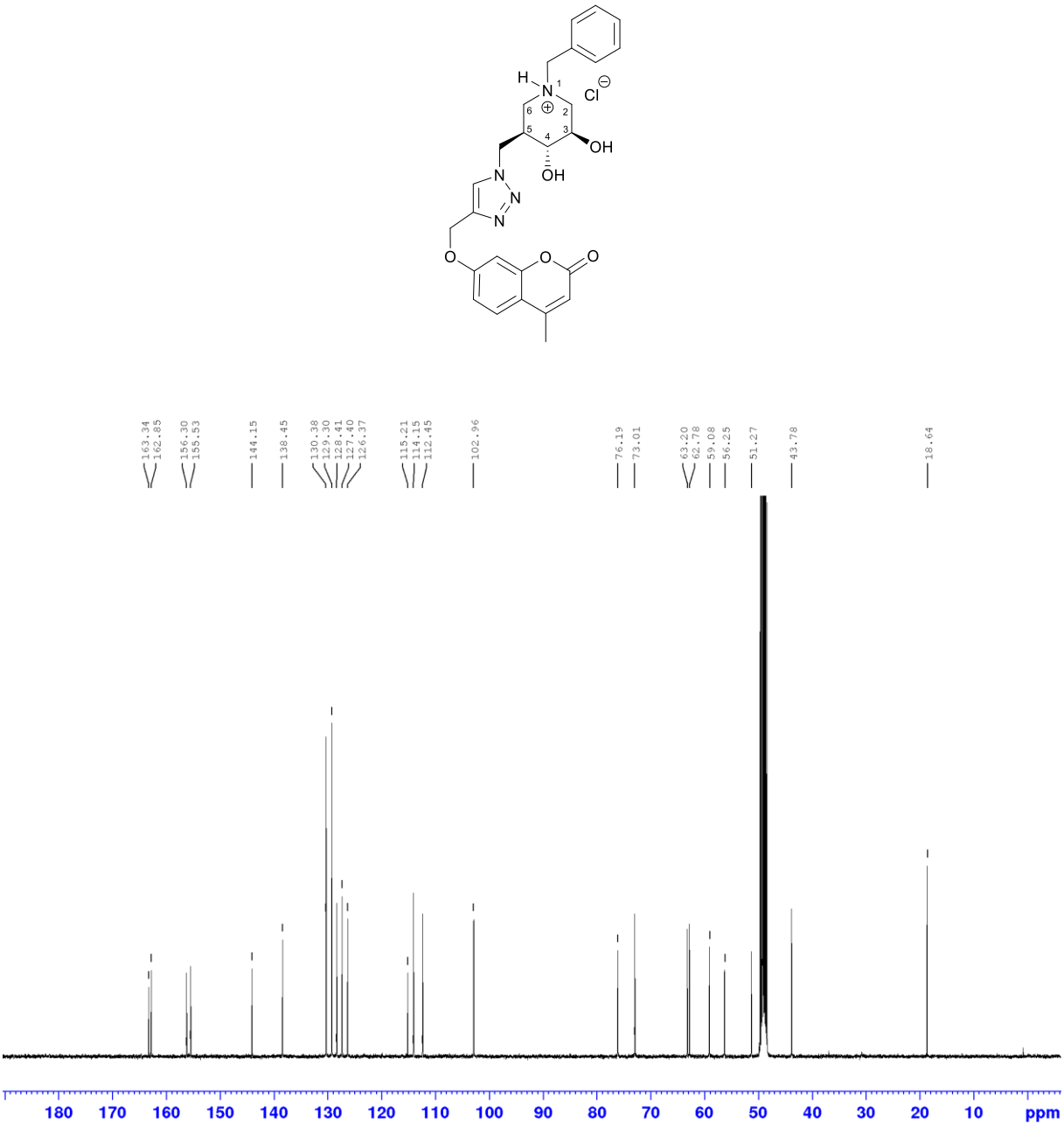
^{13}C-NMR spectra of compound **8a** (CD_3OD, 100.61 MHz)



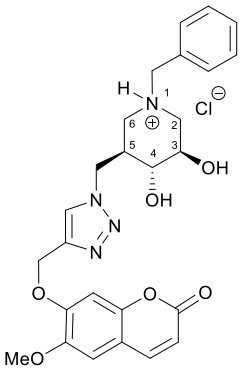
^{1}H-NMR spectra of compound **8b** (CD_3OD, 400.13 MHz)

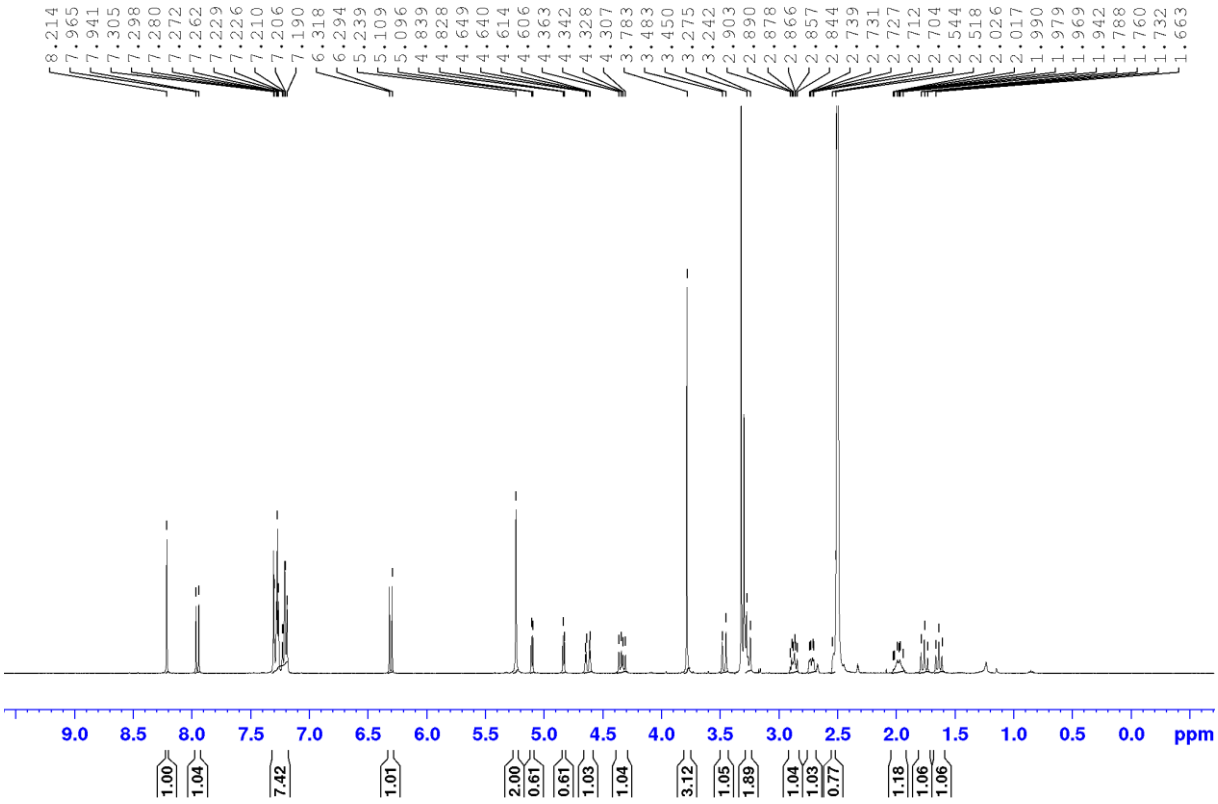


^{13}C-NMR spectra of compound **8b** (CD_3OD, 100.61 MHz)

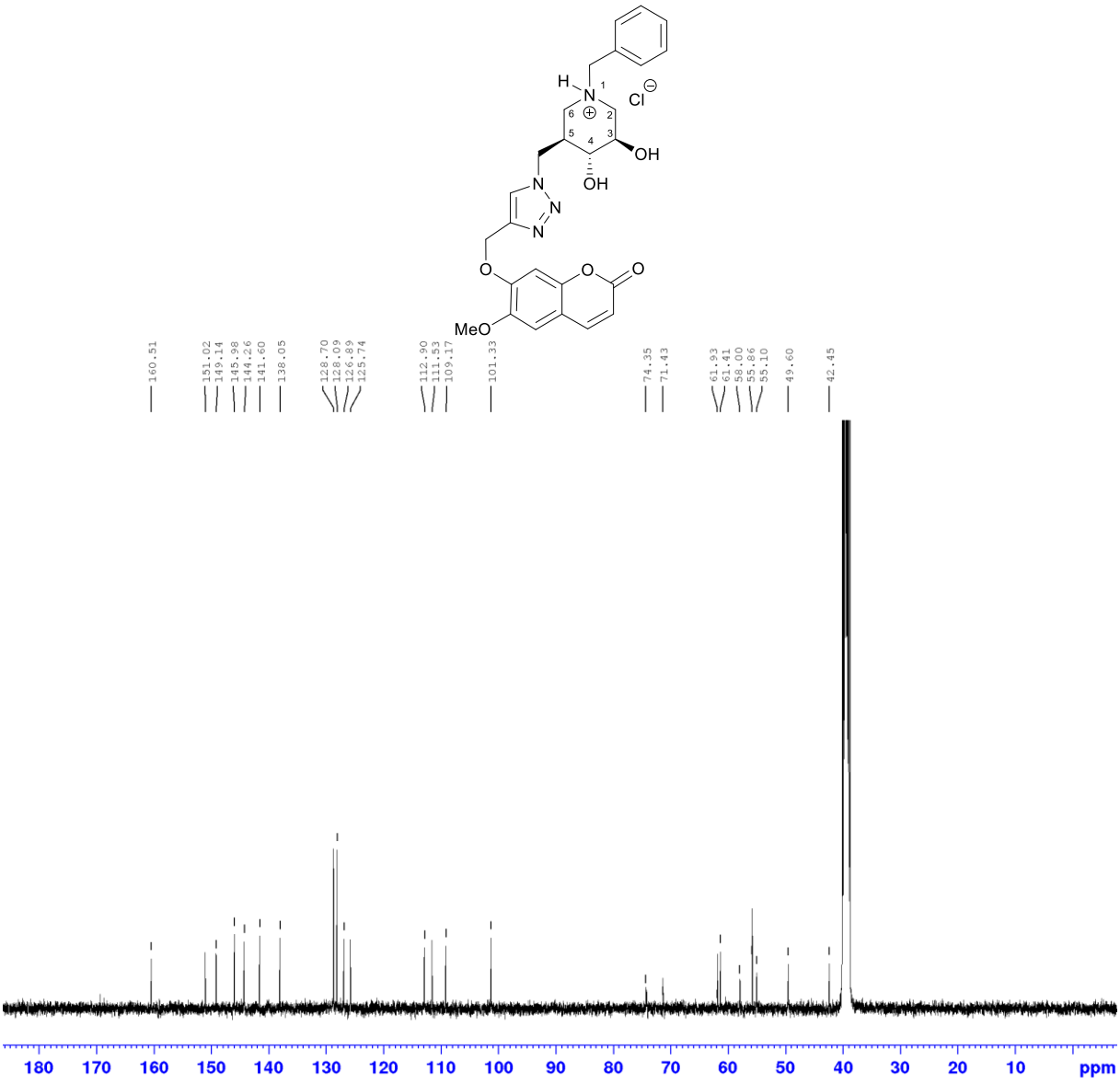


[1]H-NMR spectra of compound **8c** (DMSO, 400.13 MHz)

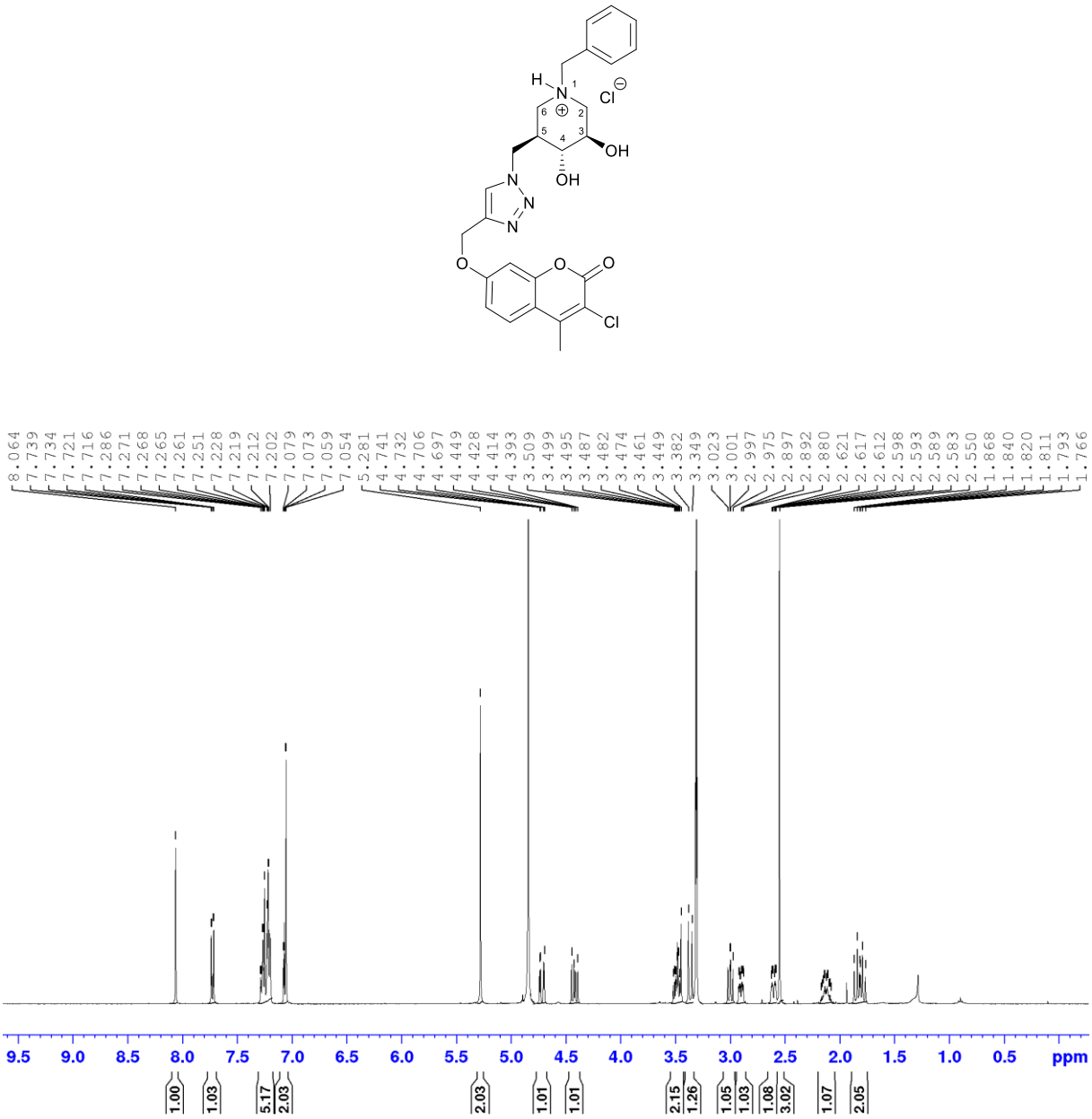




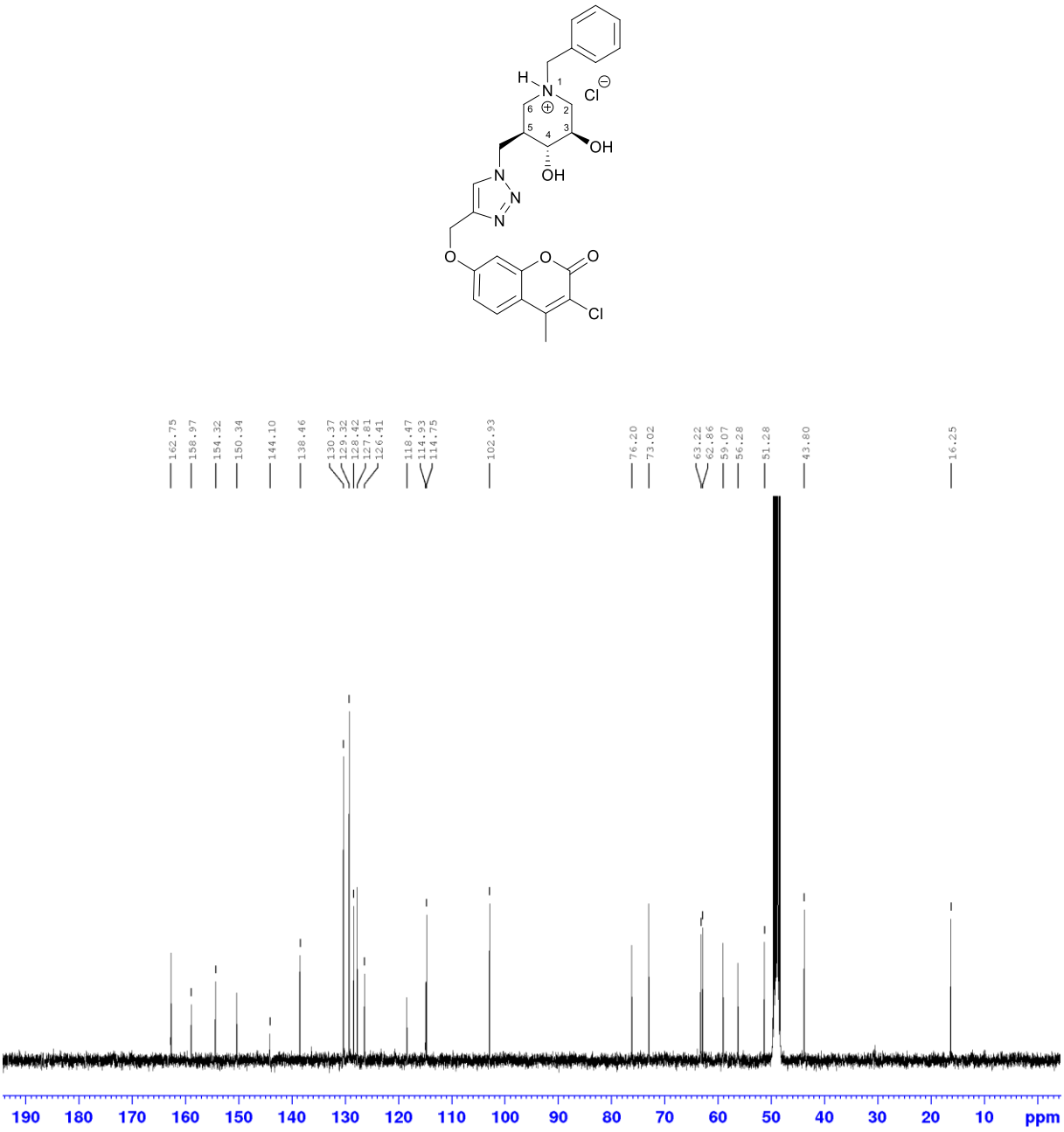
^{1}H-NMR spectra of compound **8c** (DMSO, 400.13 MHz)



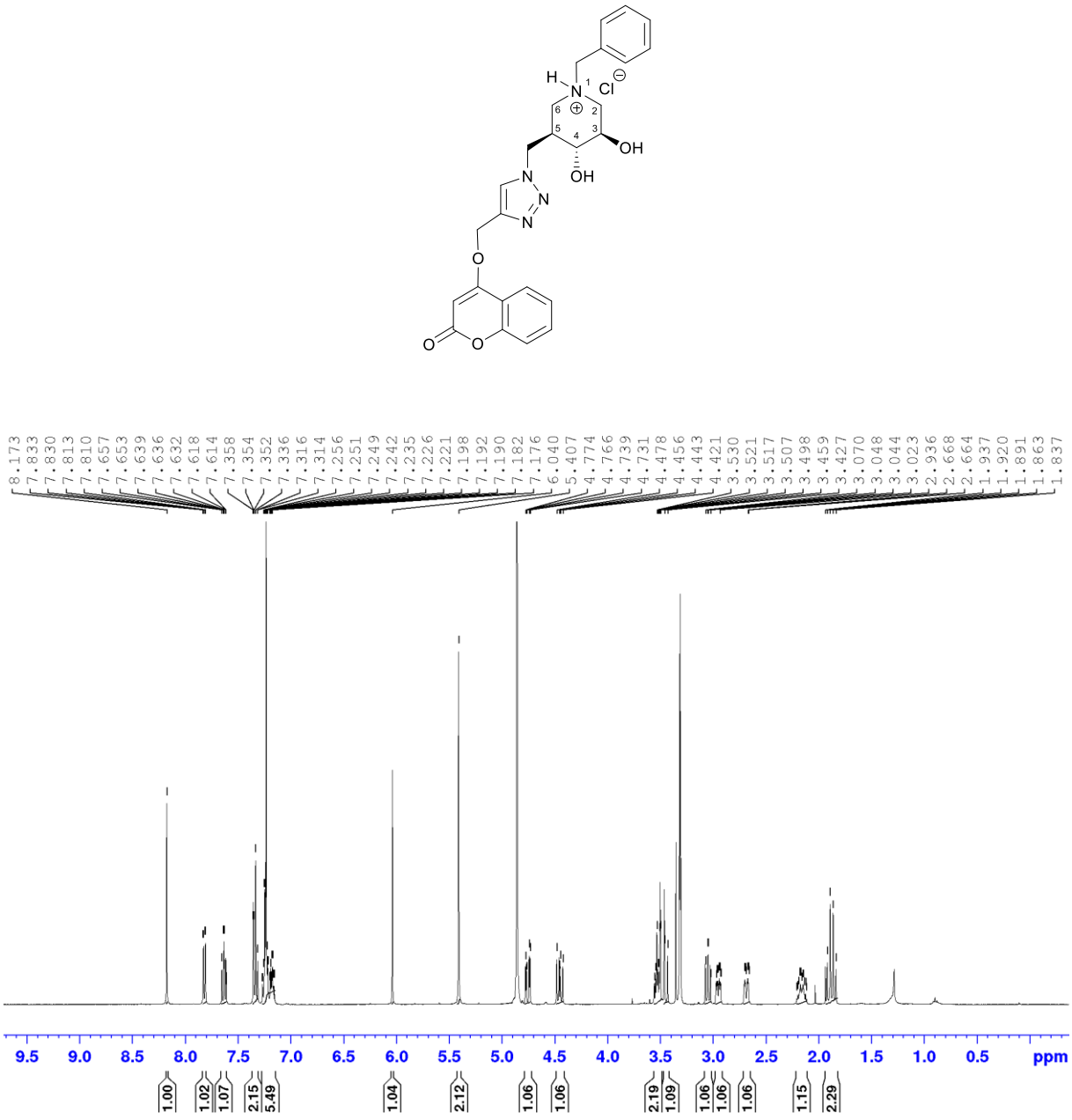
^{1}H-NMR spectra of compound **8d** (CD_3OD, 400.13 MHz)



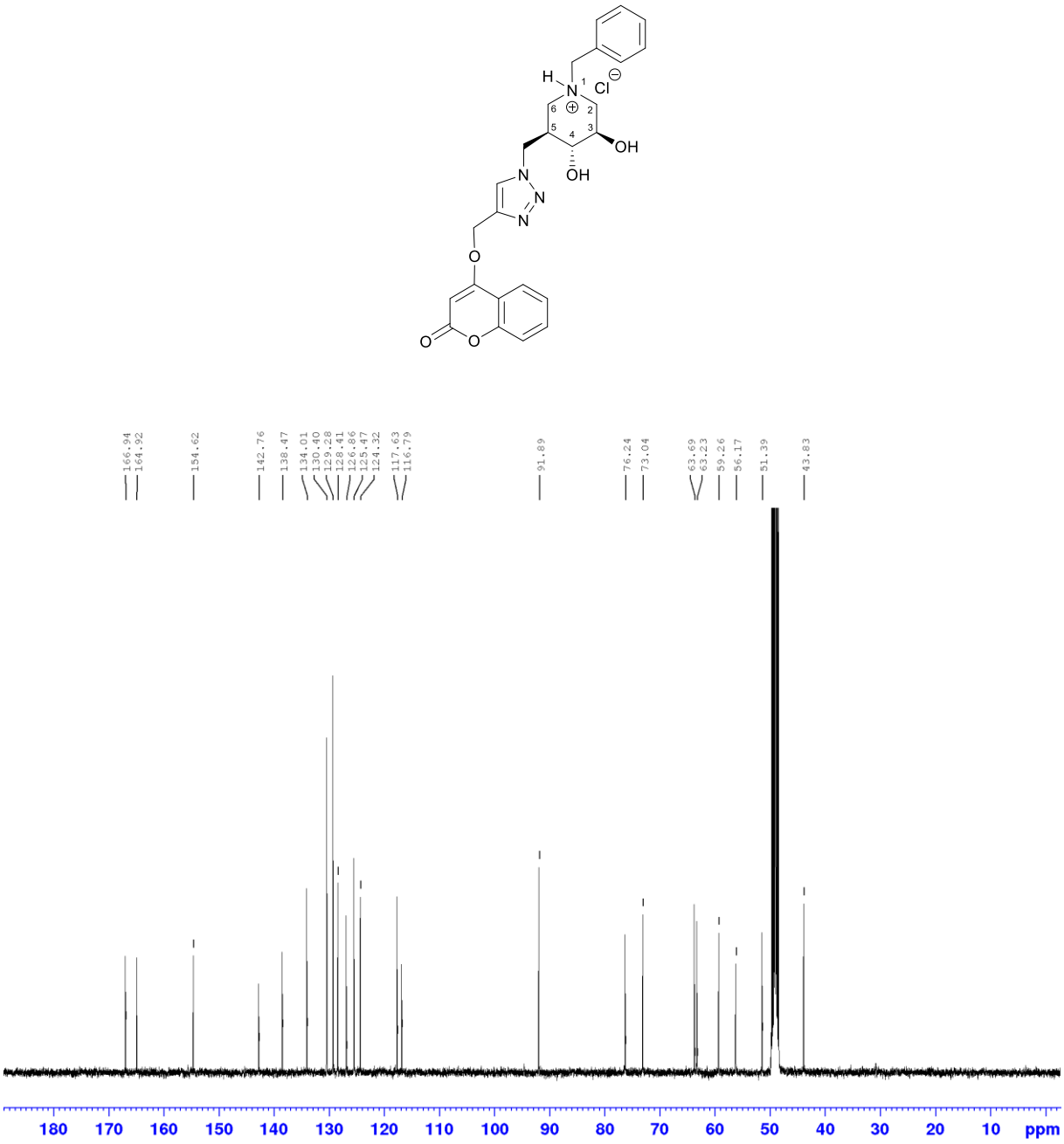
^{1}H-NMR spectra of compound **8d** (CD_3OD, 400.13 MHz)



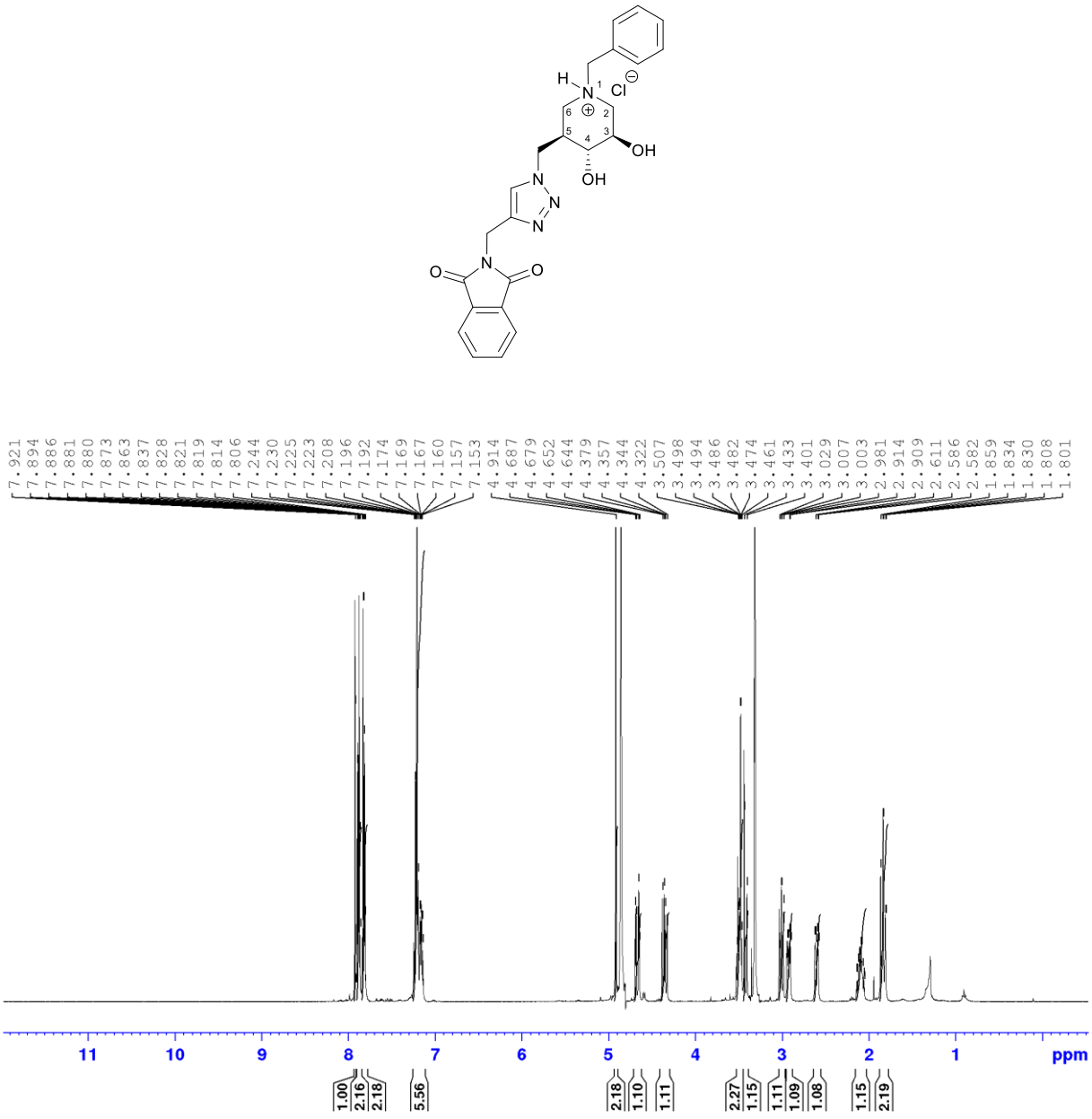
^{1}H-NMR spectra of compound **8e** (CD_3OD, 400.13 MHz)



^{13}C-NMR spectra of compound **8e** (CD_3OD, 100.61 MHz)



^{1}H-NMR spectra of compound **21** (CD_3OD, 400.13 MHz)



^{1}H-NMR spectra of compound **21** (CD_3OD, 400.13 MHz)

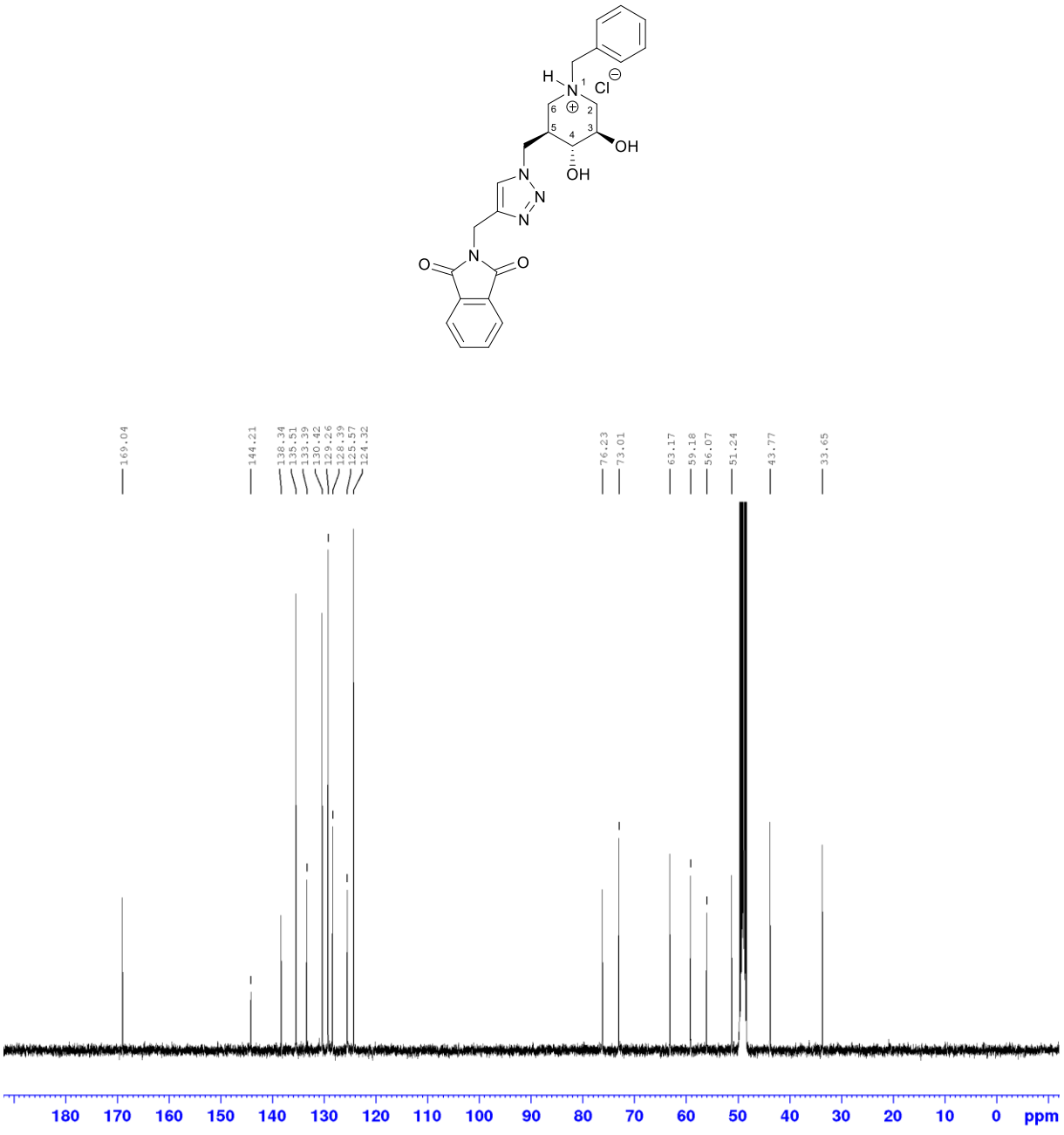


Table S1. Antiproliferative activity (GI_{50}, μM)[a] against human solid tumor cell lines**.**

Comp.	Cell line (origin)					
	A549 (lung)	**HBL-100 (breast)**	**HeLa (cervix)**	**SW1573 (lung)**	**T-47D (breast)**	**WiDr (colon)**
11	>100	>100	>100	>100	>100	>100
10	>100	>100	>100	>100	>100	>100
8a	>100	>100	44±2.9	89±17	>100	67±12
17a	93±9.8	47±4.8	25±6.5	46±13	>100	40±11
8b	>100	97±6.6	83±20	94±12	>100	>100
17b	97±4.0	52±7.3	48±22	96±8.4	>100	95±2.1
8c	95±12	89±28	88±30	85±36	>100	88±30
17c	89±27	66±32	45±22	77±36	>100	39±9.7
8d	70±2.2	56±18	53±22	98±3.0	78±16	47±7.4
17d	90±20	82±35	>100	95±9.9	n.t.[b]	5.6±1.1
8e	>100	>100	98±3.9	97±5.5	>100	>100
17e	88±8.0	40±3.2	34±11	60±11	66±4.9	44±15
21	>100	84±39	85±37	85±37	>100	84±39
20	73±21	89±28	58±21	84±28	>100	54±19
Cisplatin	4.9±0.2	1.9±0.2	1.8±0.5	2.7±0.4	17±3.3	23±4.3

[a]Values ± standard deviation from two to six representative experiments. [b]n.t. = not tested.