

Squaramide-Tethered Sulfonamides and Coumarins: Synthesis, Inhibition of Tumor-Associated CAs IX and XII and Docking Simulations

Giulia Arrighi ¹, Adrián Puerta ², Andrea Petrini ³, Francisco J. Hicke ¹, Alessio Nocentini ³,
Miguel X. Fernandes ², José M. Padrón ², Claudiu T. Supuran ^{3,*}, José G. Fernández-Bolaños ¹
and Óscar López ^{1,*}

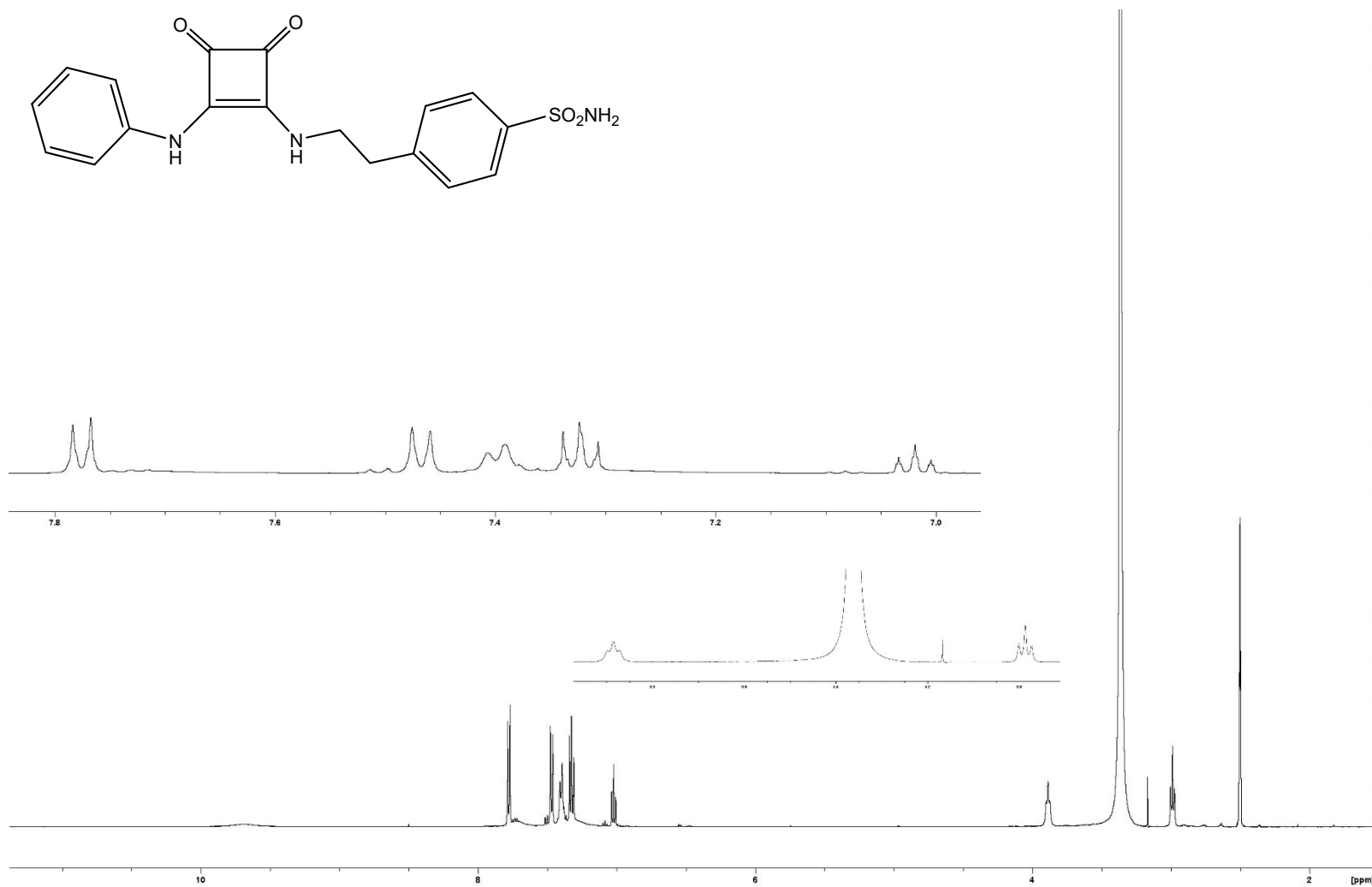
¹ Departamento de Química Orgánica, Facultad de Química, Universidad de Sevilla, Apartado 1203,
E-41071 Seville, Spain; giulia.arrighi1@stud.unifi.it (G.A.); javipoke@hotmail.es (F.J.H.);
bolanos@us.es (J.G.F.-B.)

² BioLab, Instituto Universitario de Bio-Organica Antonio González (IUBO-AG), Universidad de La Laguna,
c/Astrofísico Francisco Sánchez 2, E-38206 La Laguna, Spain; apuertaa@ull.es (A.P.);
mfernand@ull.es (M.X.F.); jmpadron@ull.es (J.M.P.)

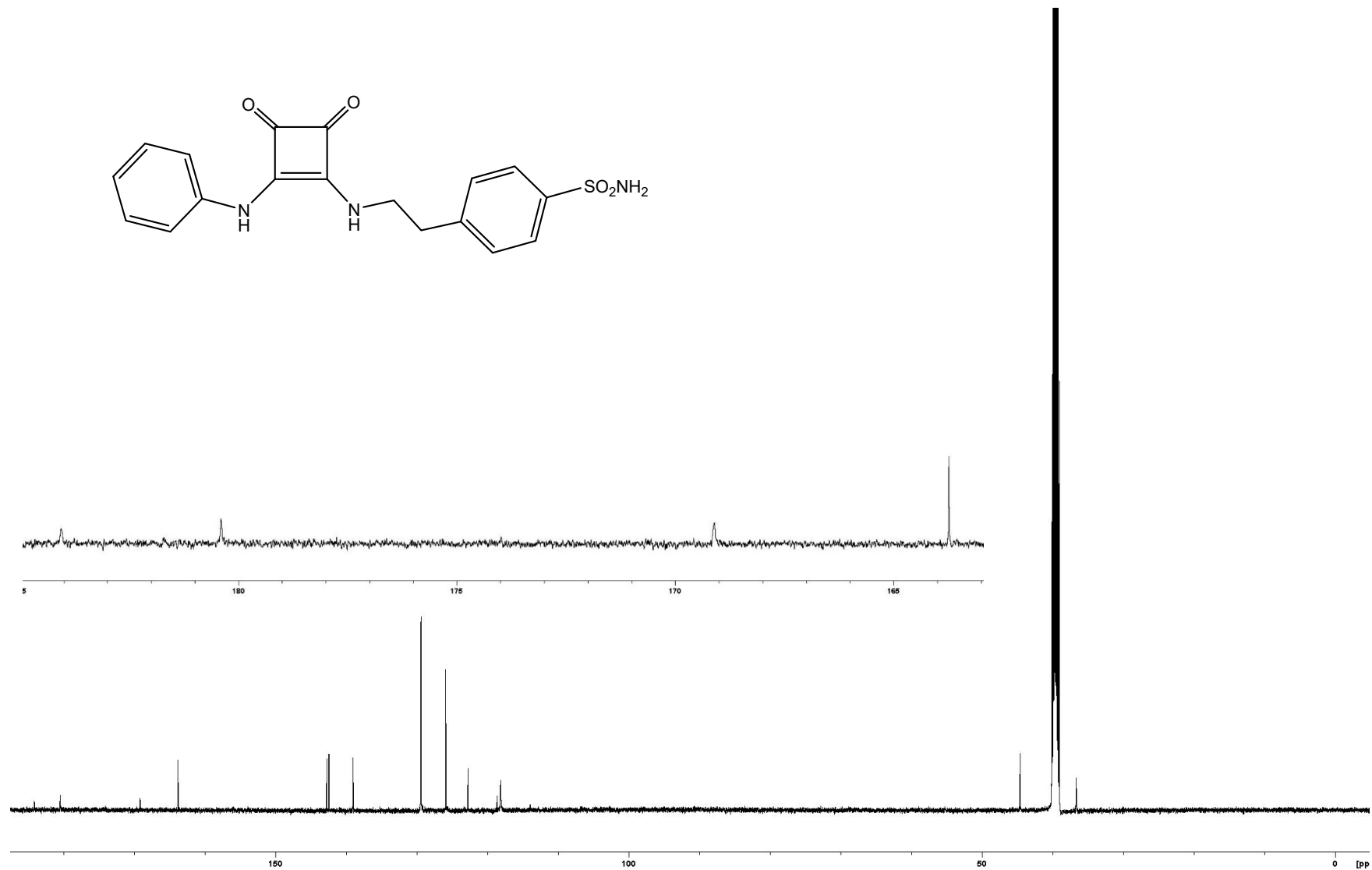
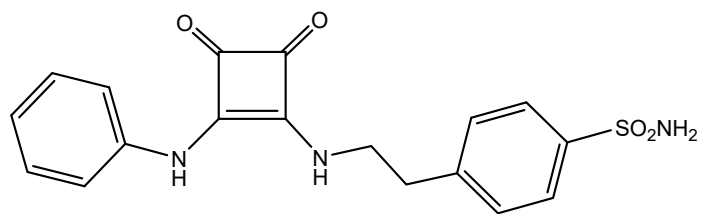
³ NEUROFARBA Department, Sezione di Scienze Farmaceutiche e Nutraceutiche, University of Florence,
50019 Florence, Italy; andrea.petreni@unifi.it (A.P.); alessio.nocentini@unifi.it (A.N.)

* Correspondence: claudiu.supuran@unifi.it (C.T.S.); osc-lopez@us.es (Ó.L.)

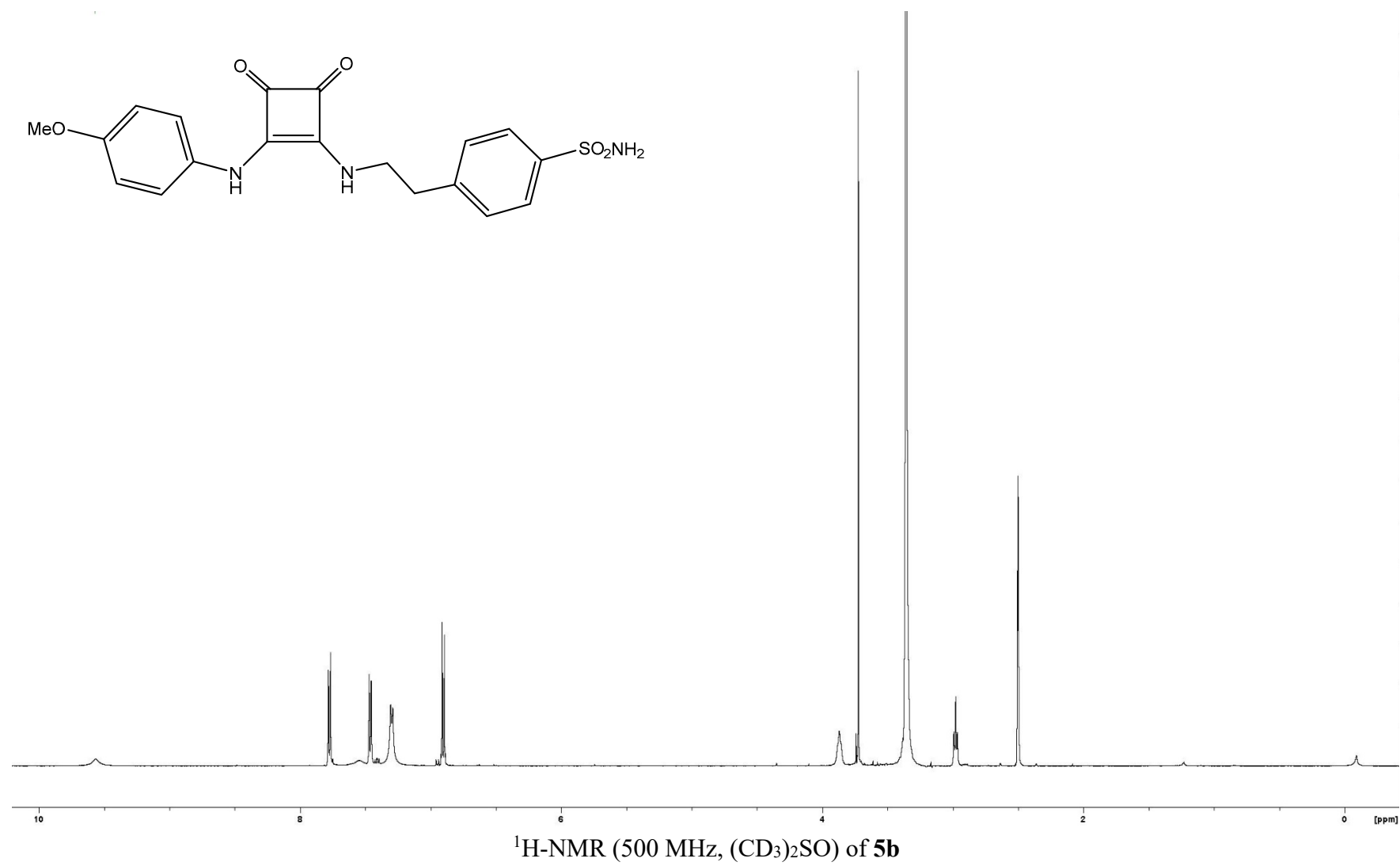
¹H- and ¹³C-NMR spectra of compounds 5, 6, 8, 10, 11, 16.....S2–S53

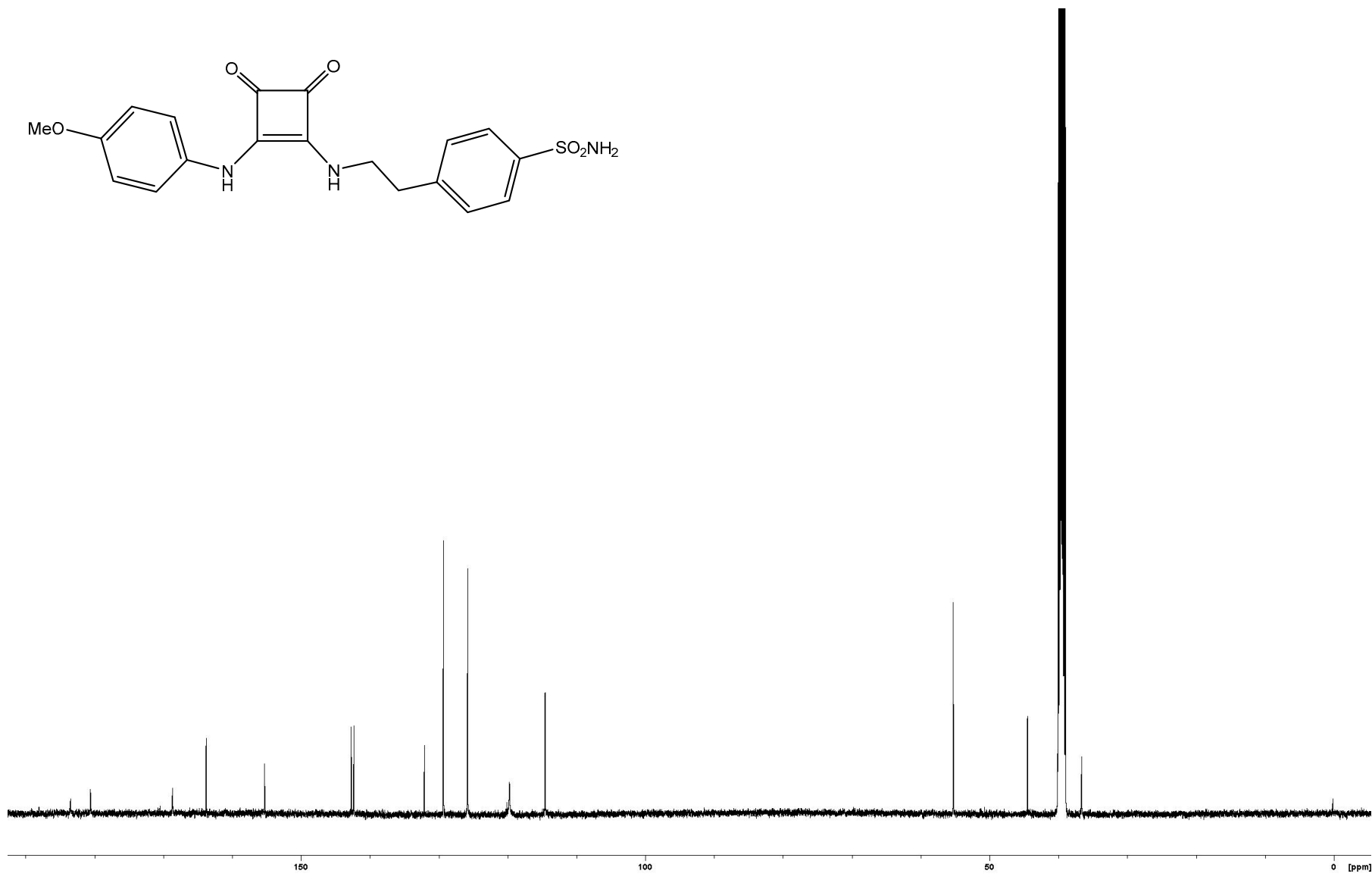


¹H-NMR (500 MHz, (CD₃)₂SO) of **5a**

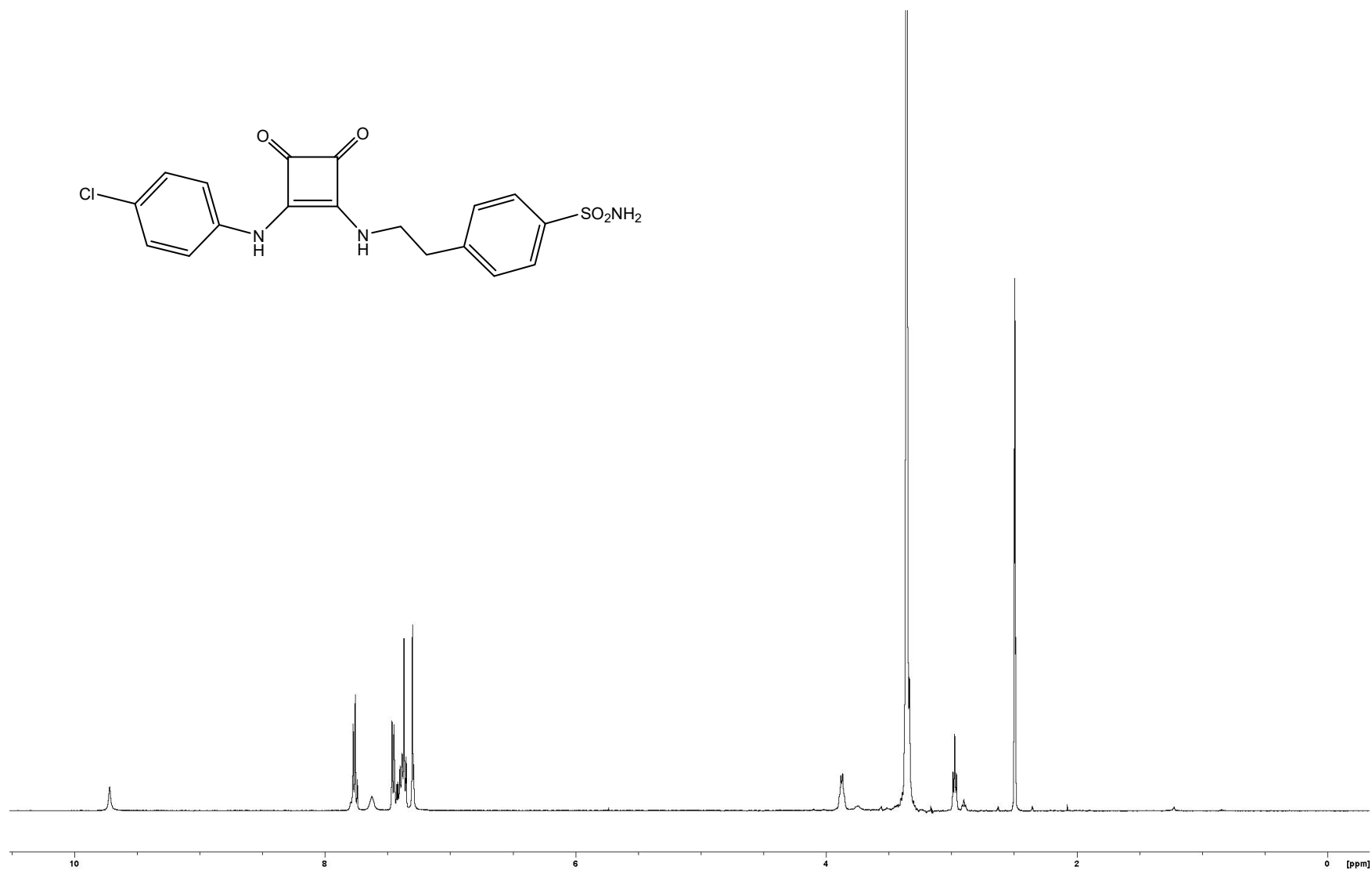
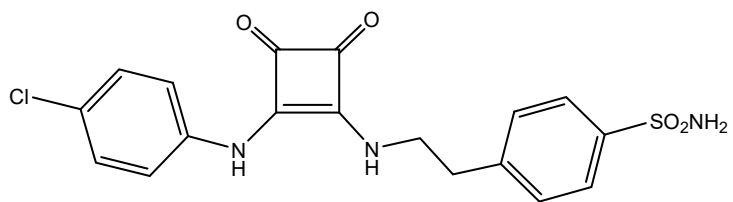


¹³C-NMR (125.7 MHz, (CD₃)₂SO) of **5a**

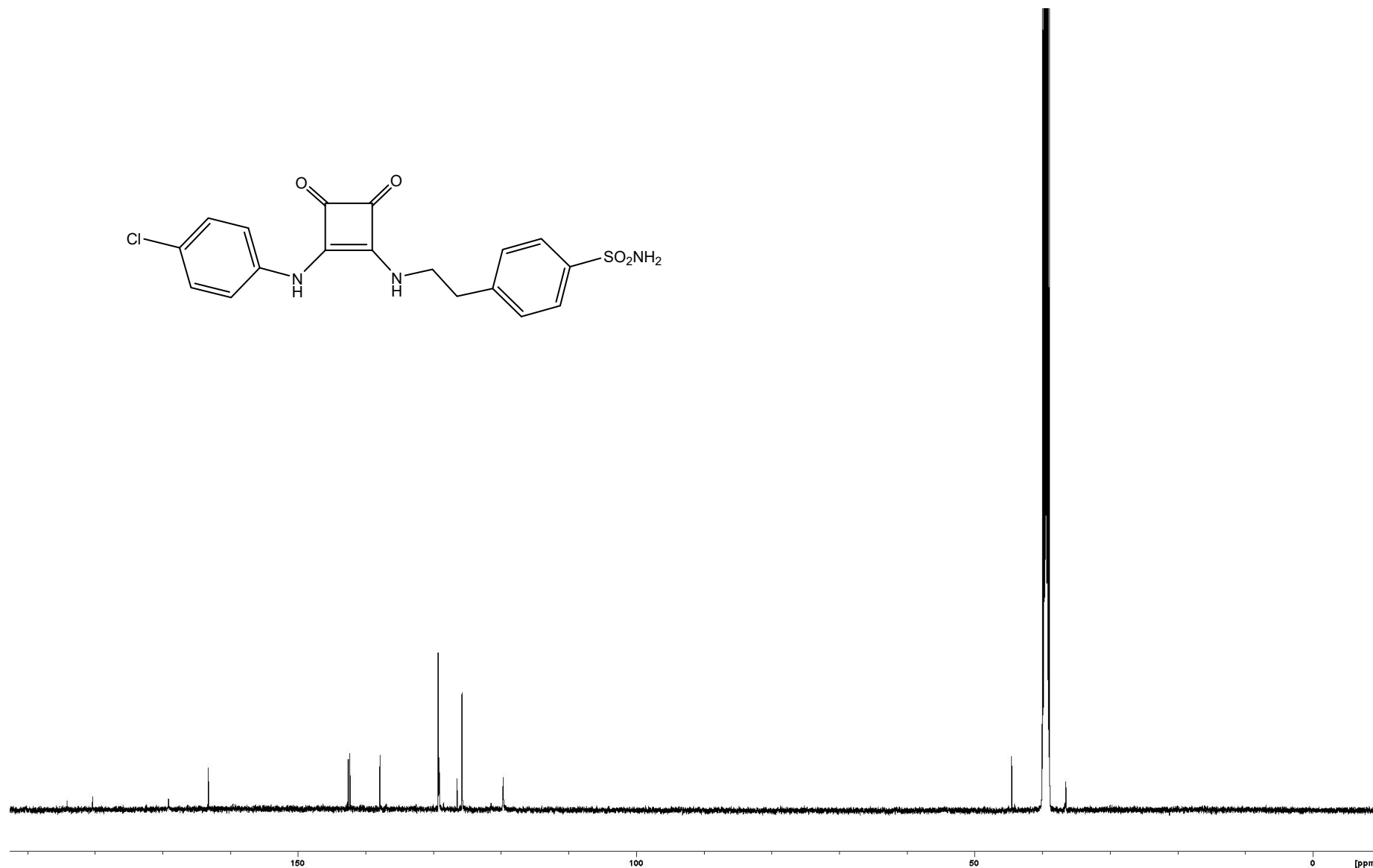
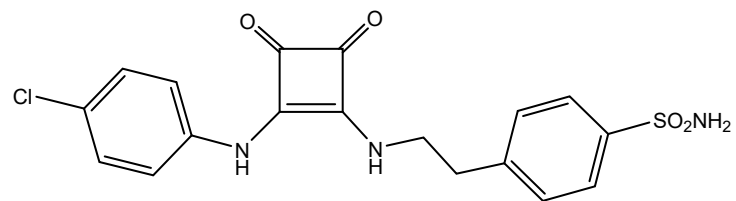




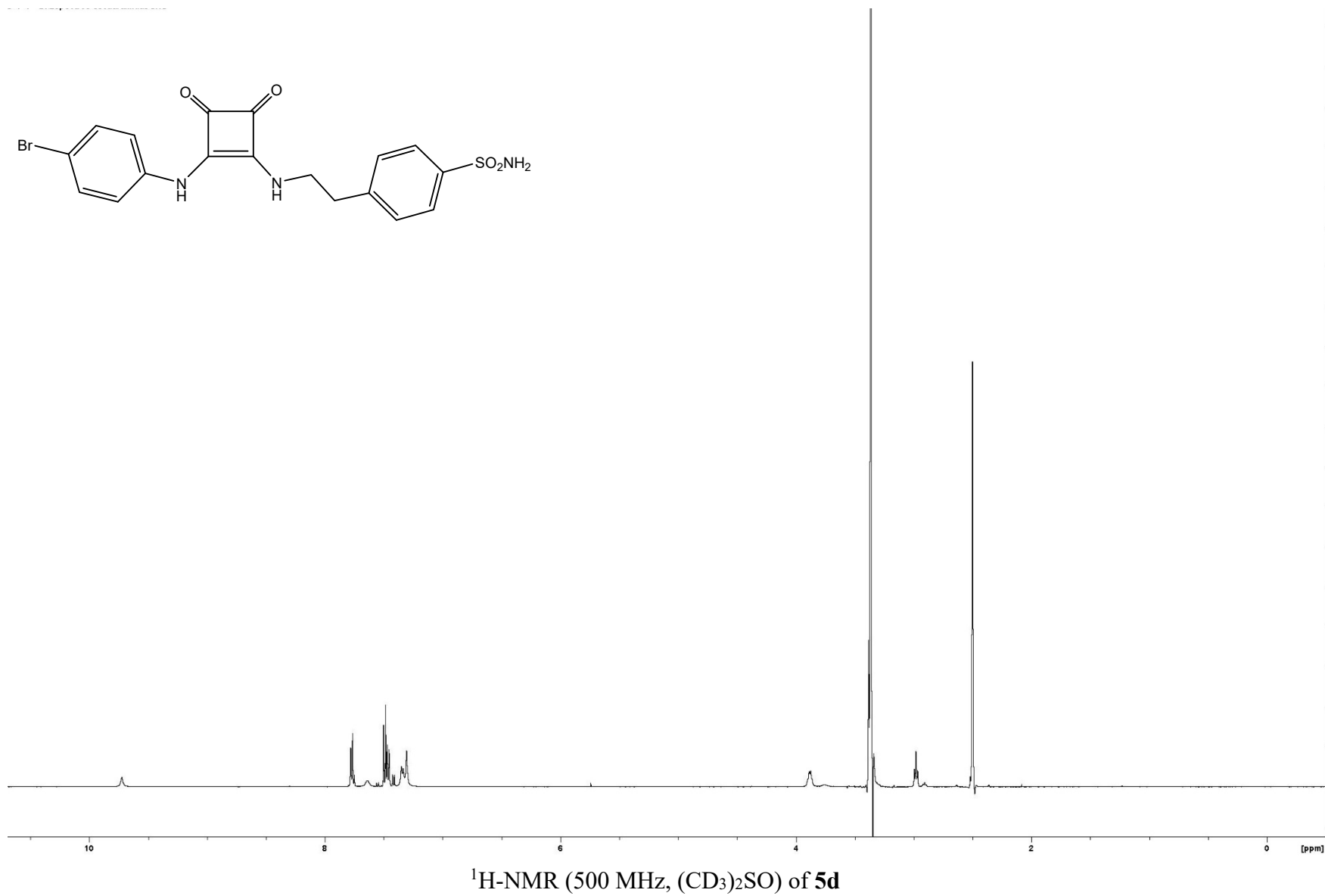
¹³C-NMR (125.7 MHz, (CD₃)₂SO) of **5b**

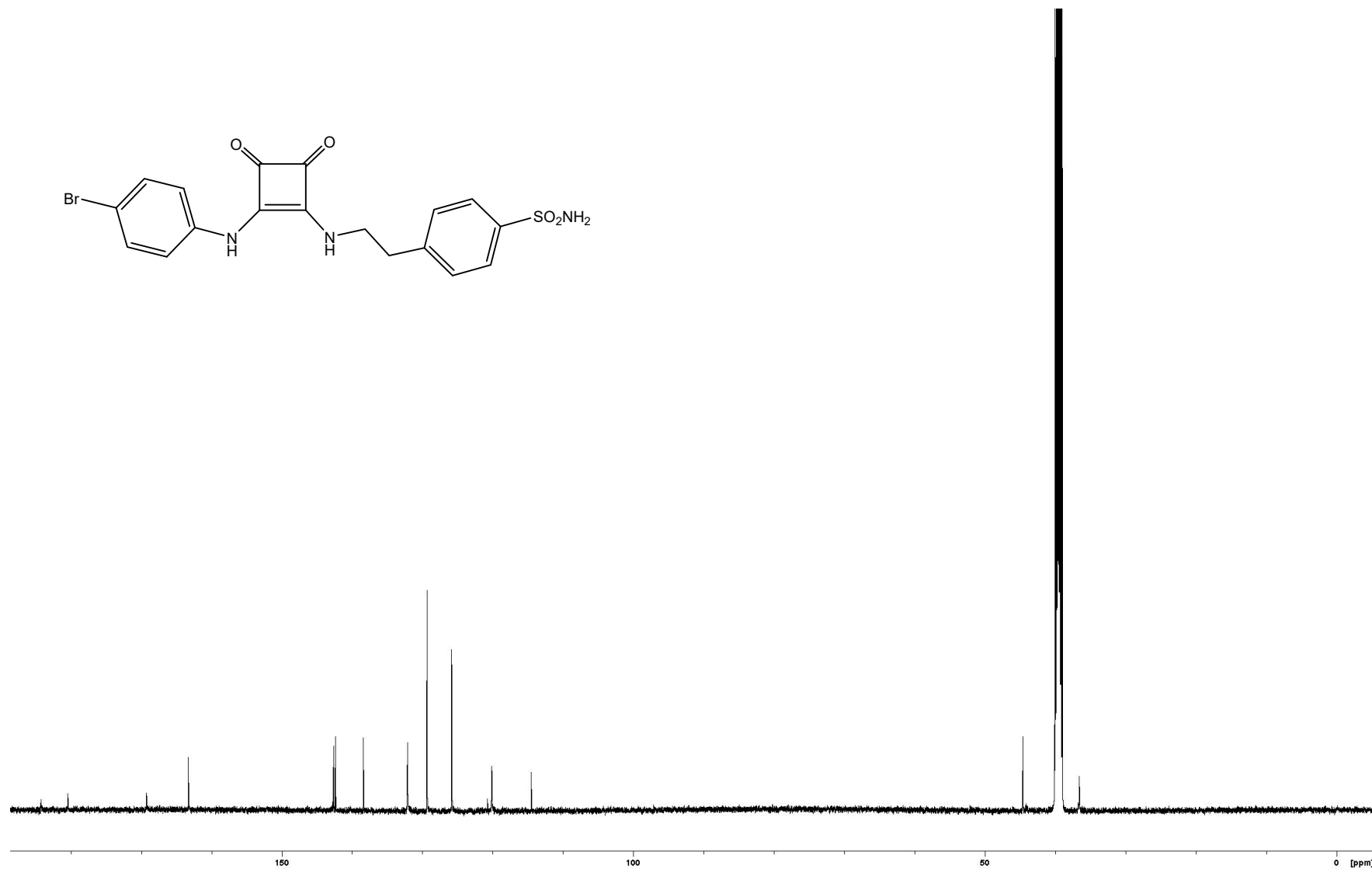
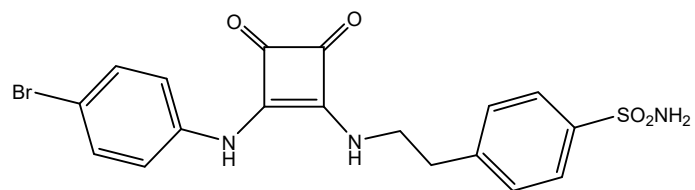


^1H -NMR (500 MHz, $(\text{CD}_3)_2\text{SO}$) of **5c**

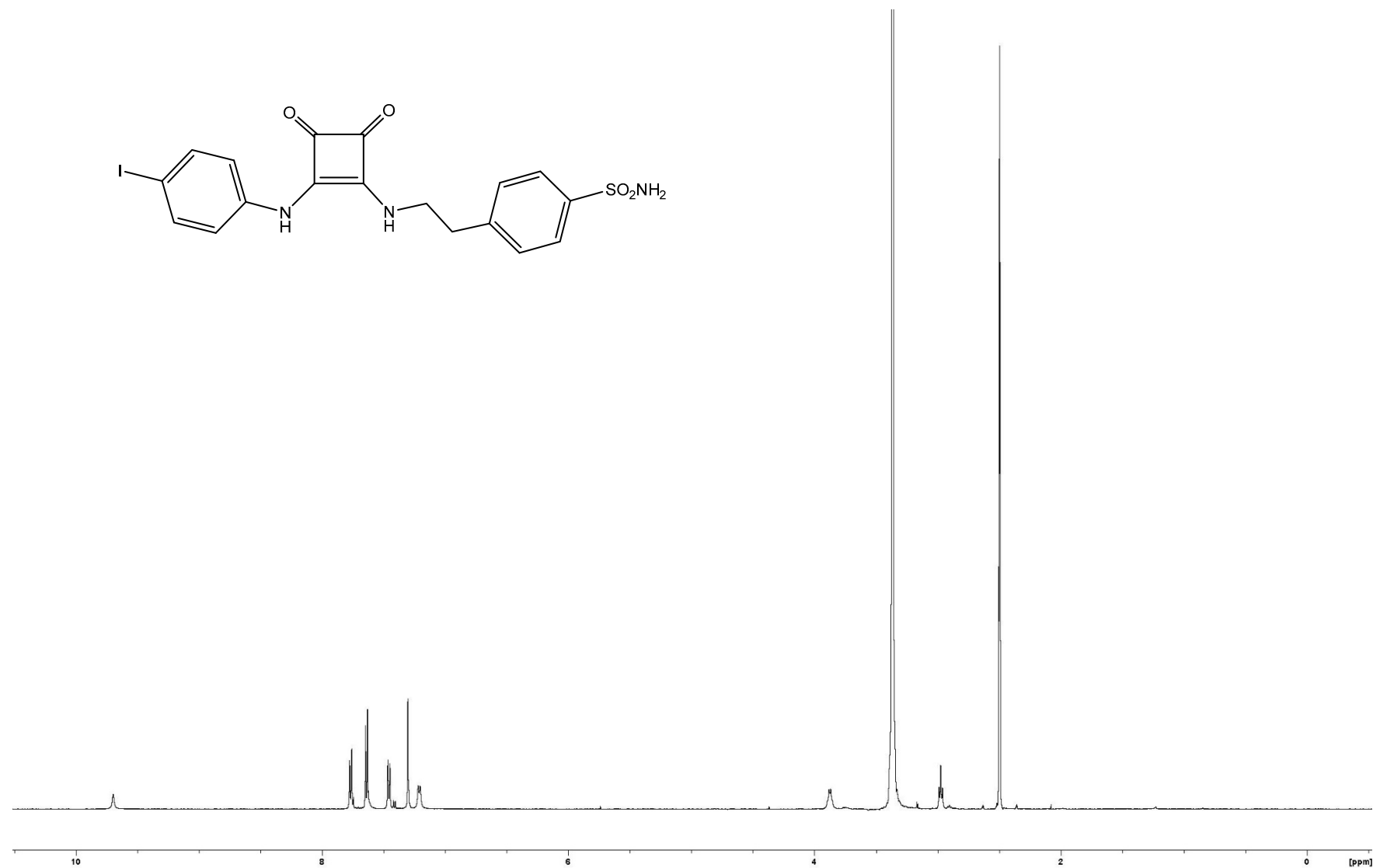


^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **5c**

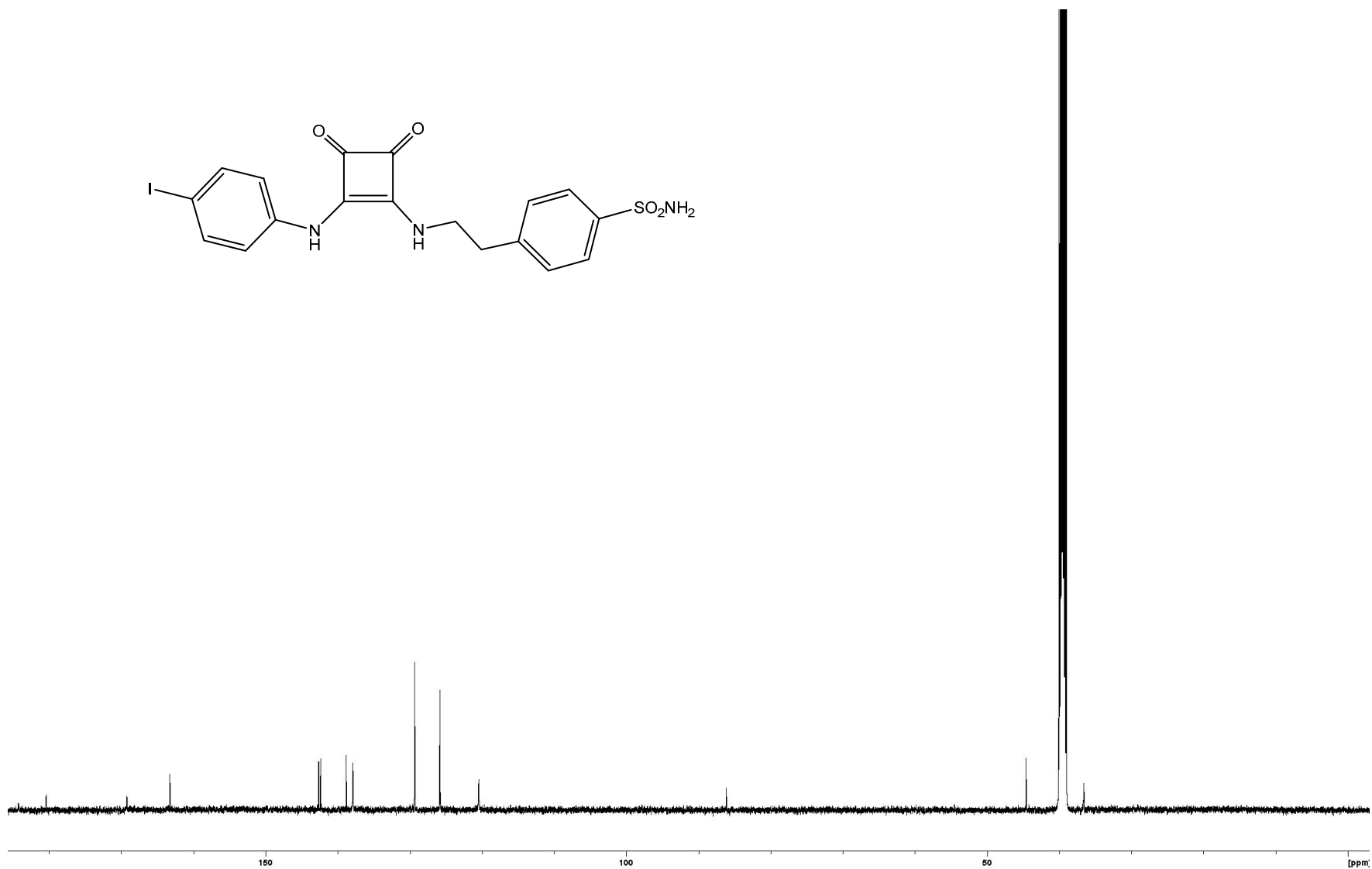
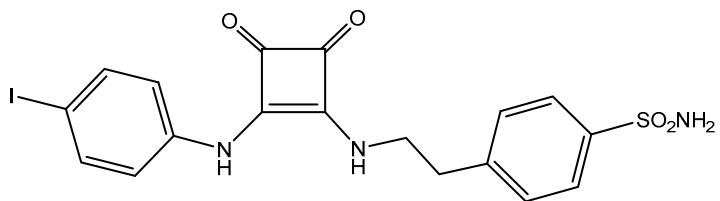




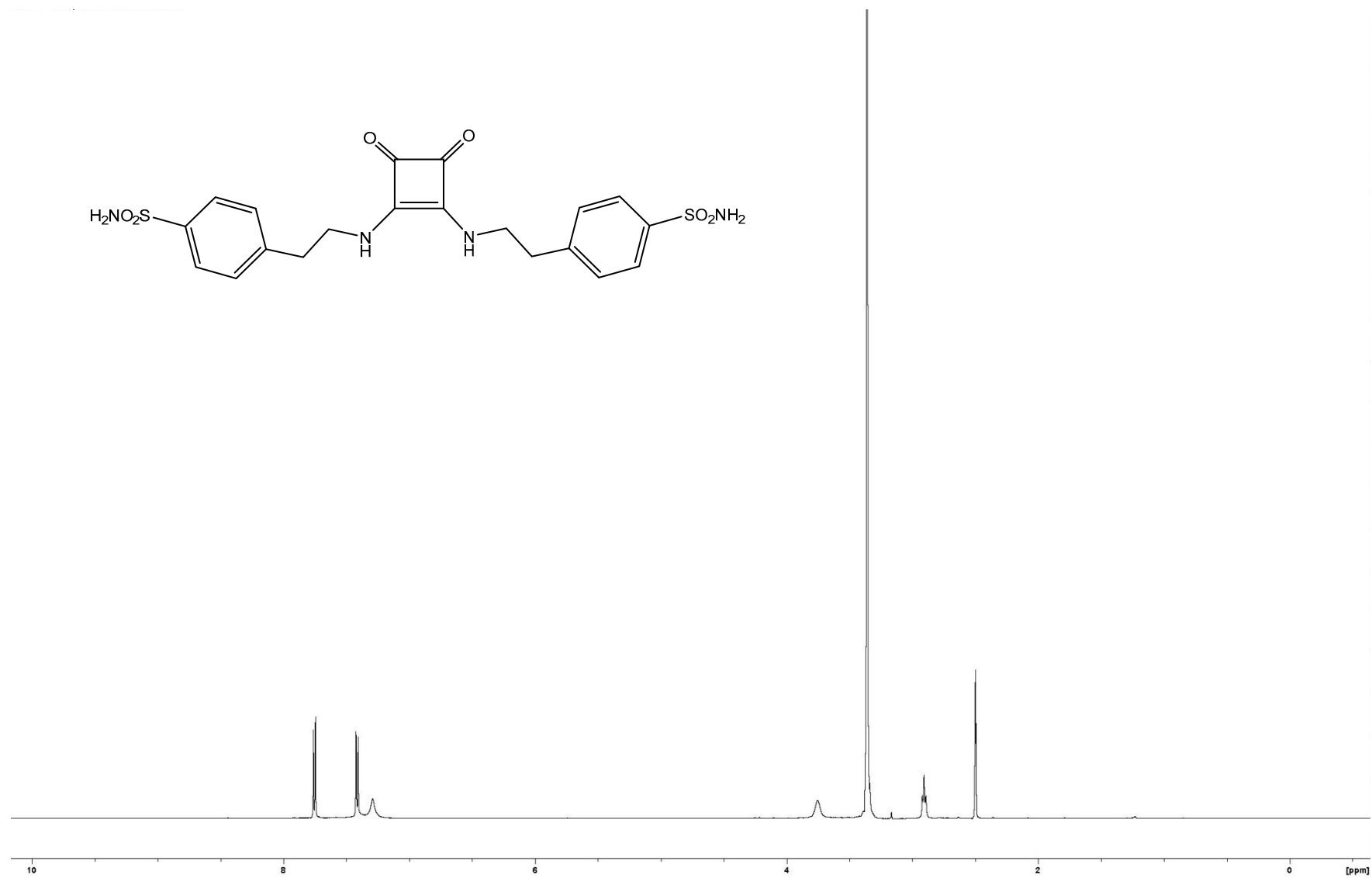
^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **5d**



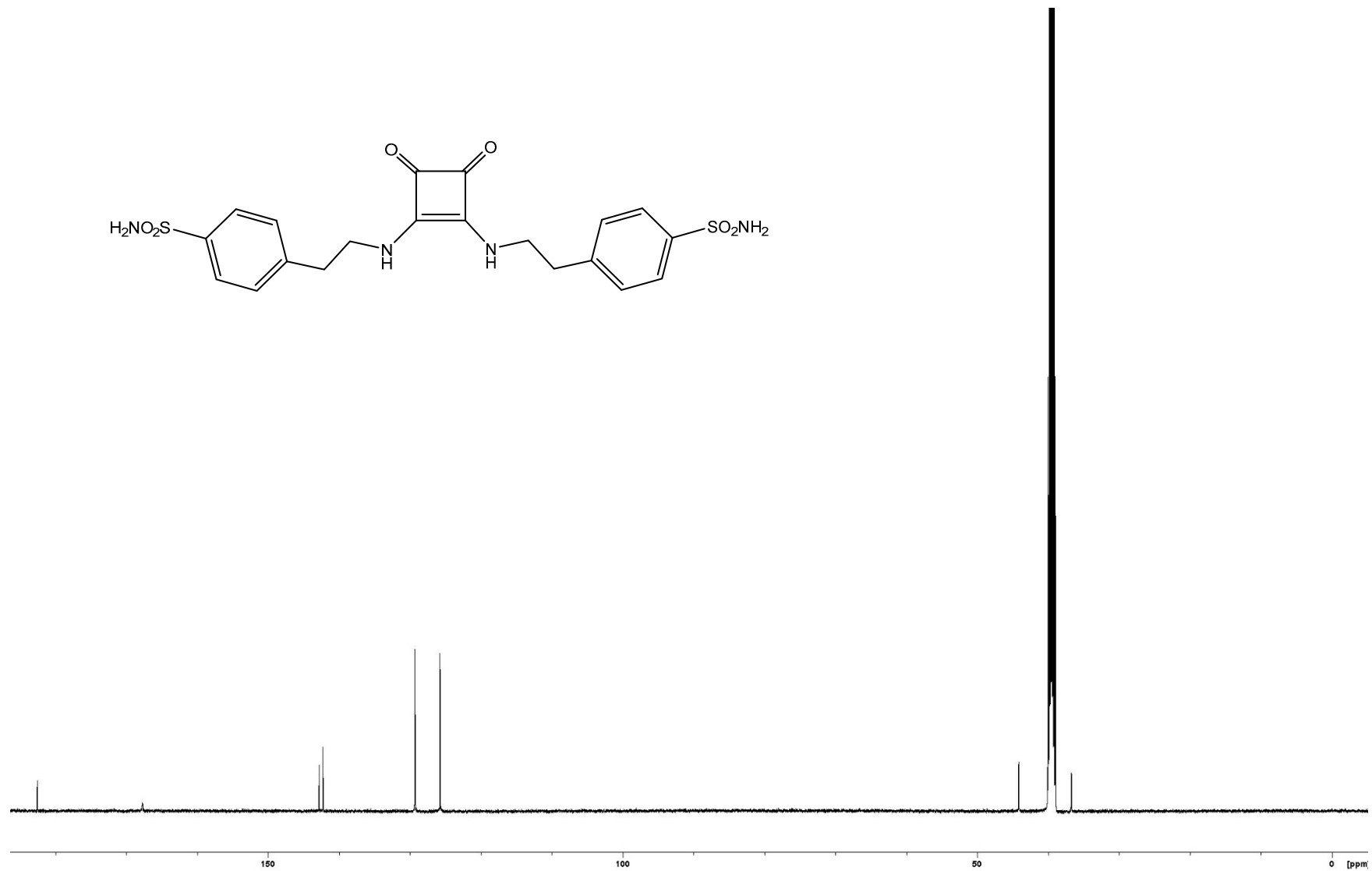
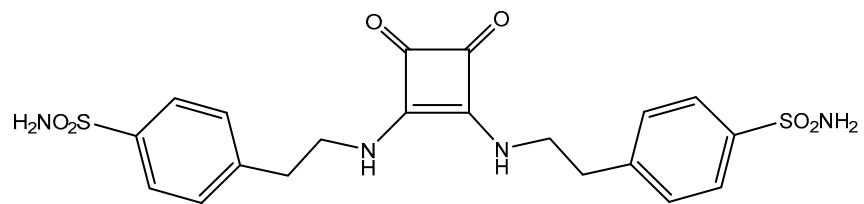
¹H-NMR (500 MHz, (CD₃)₂SO) of **5e**



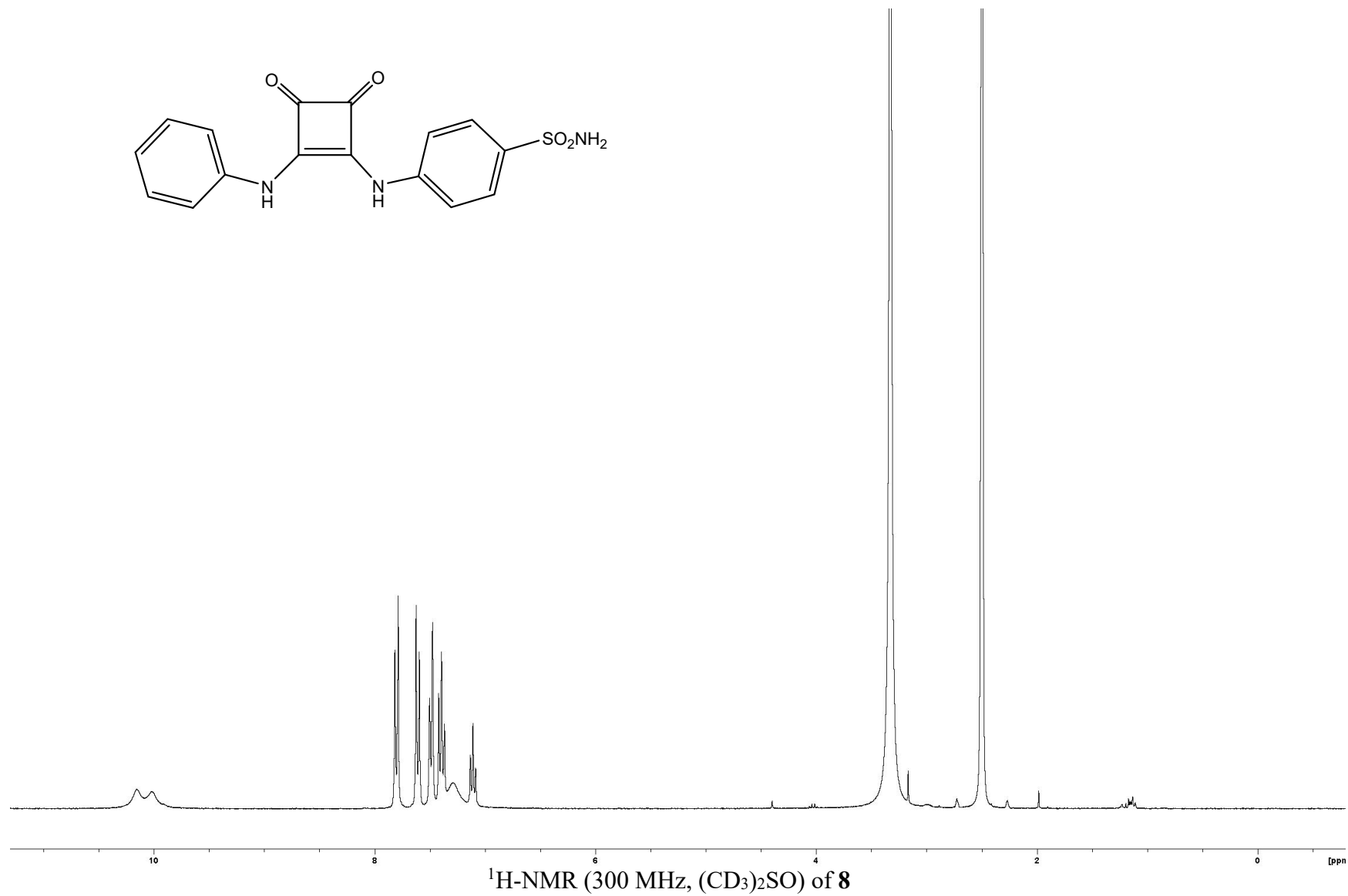
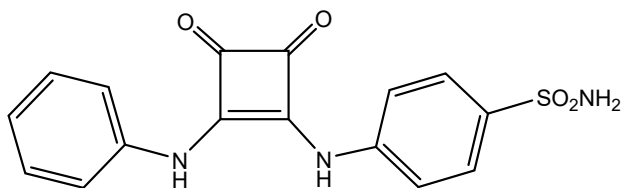
^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **5e**

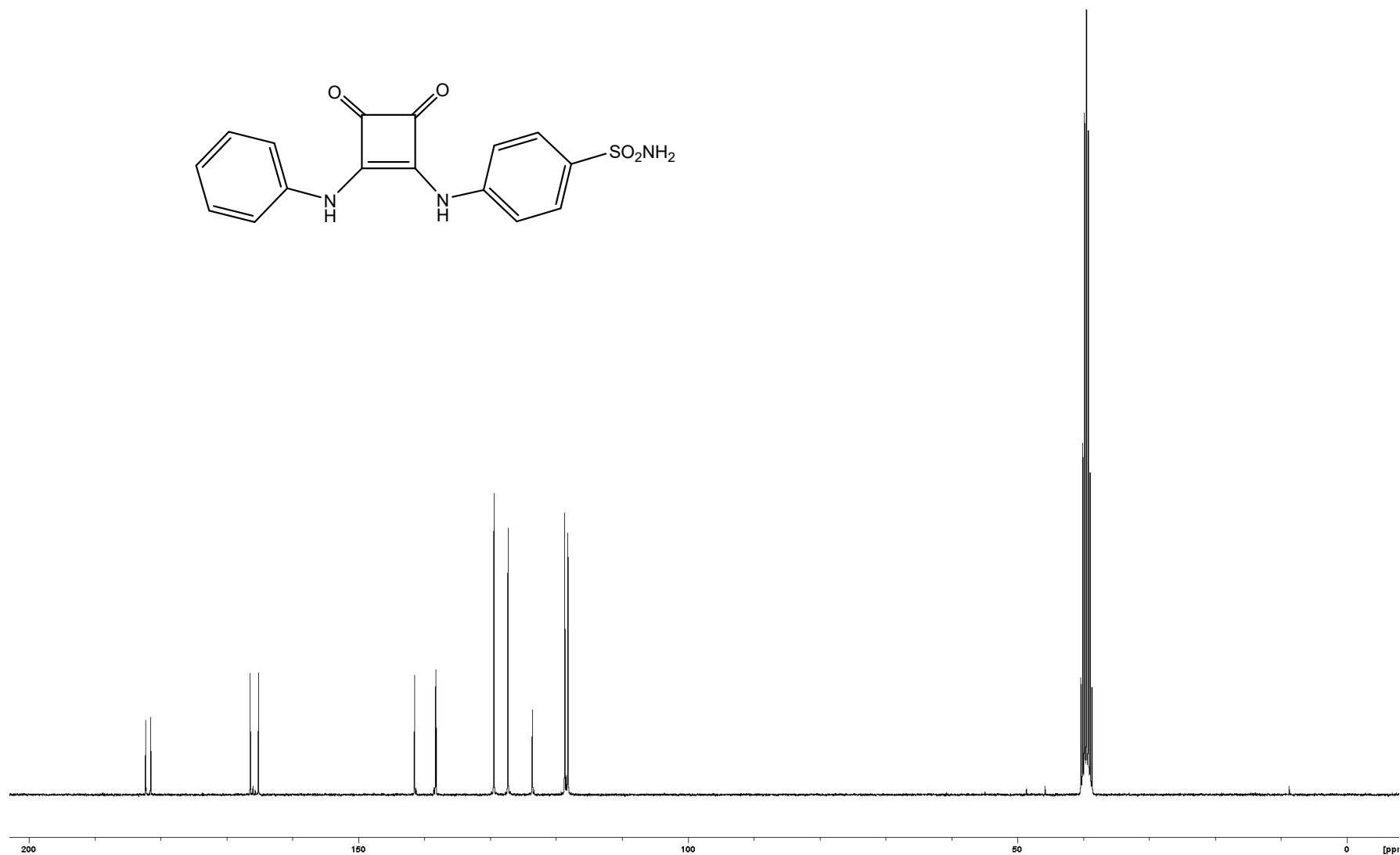
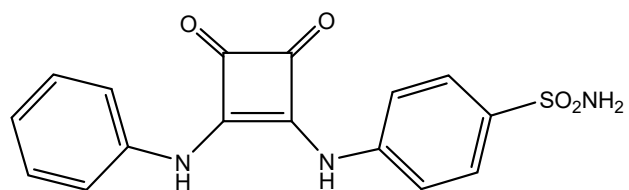


¹H-NMR (500 MHz, (CD₃)₂SO) of **6**

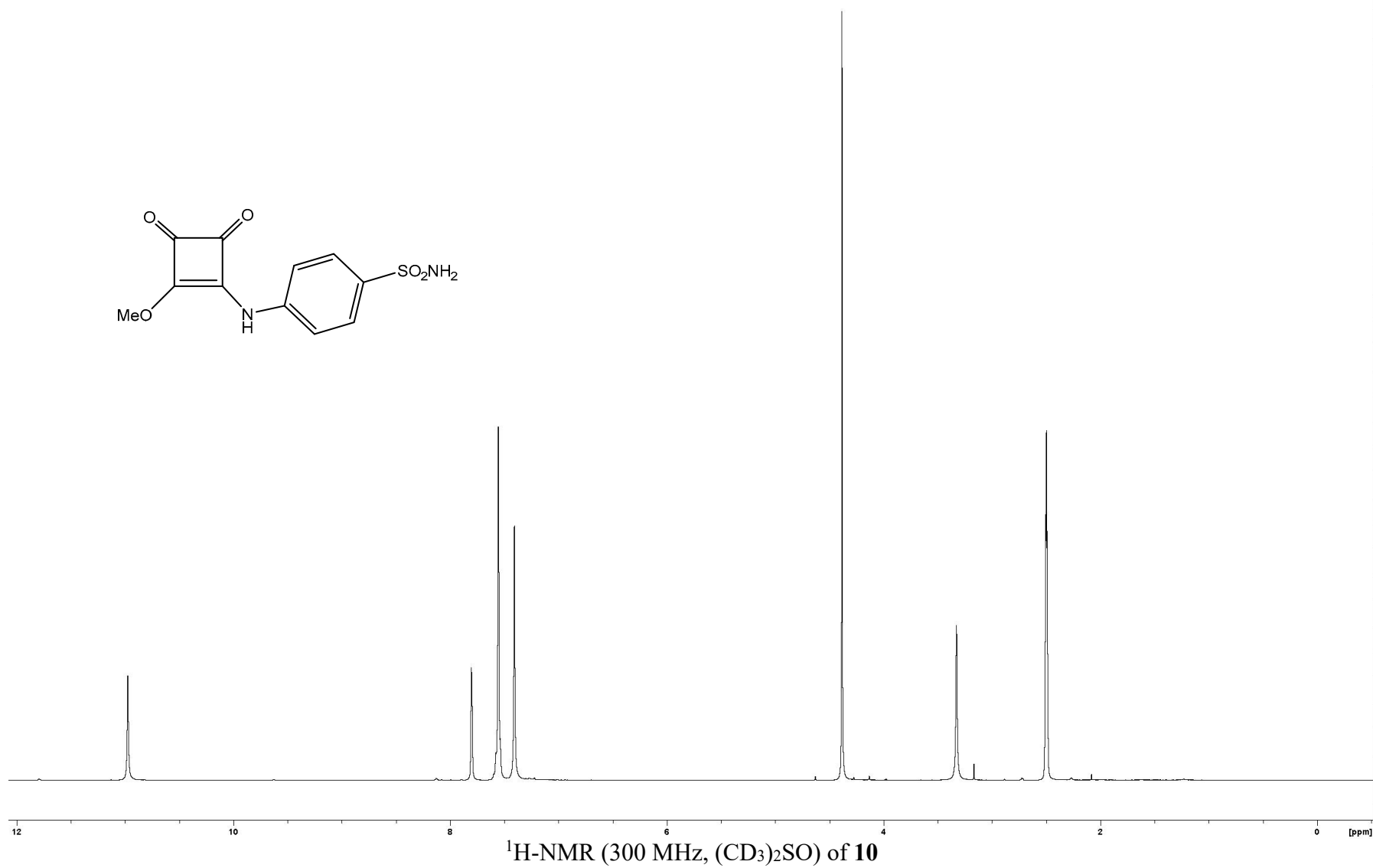
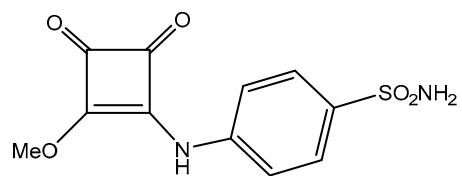


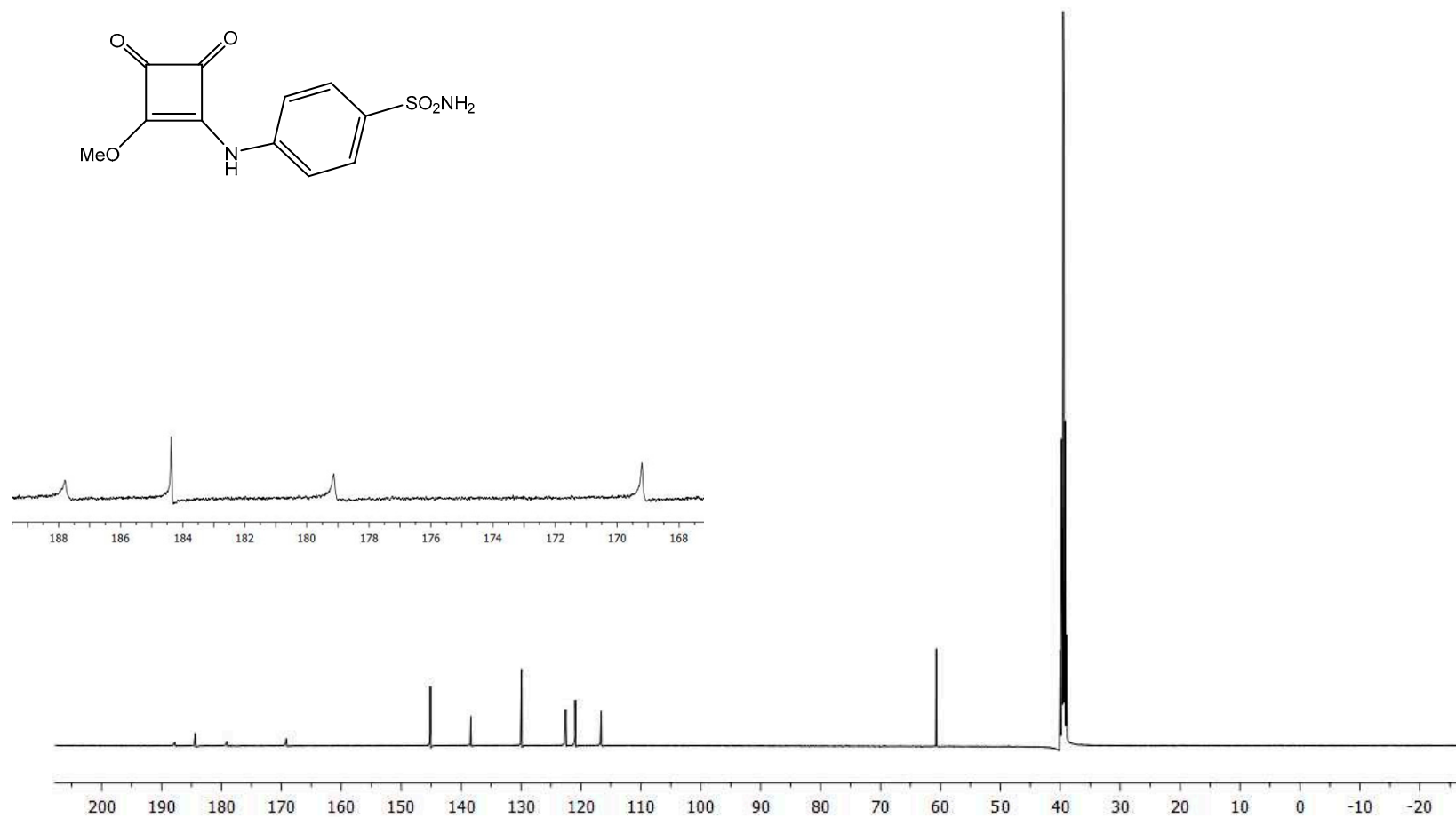
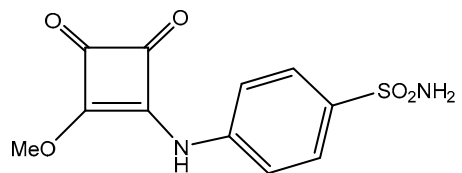
^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **6**



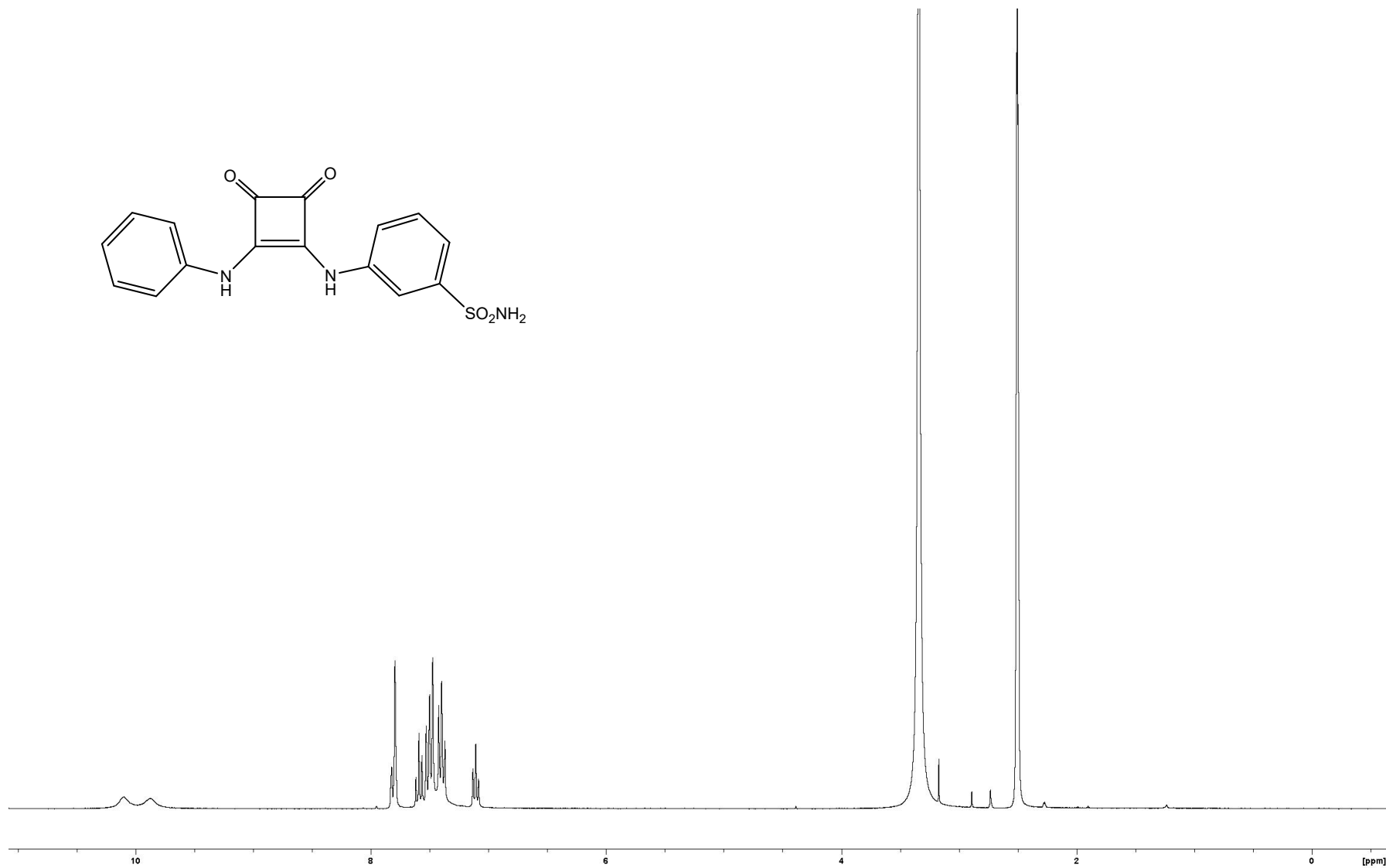
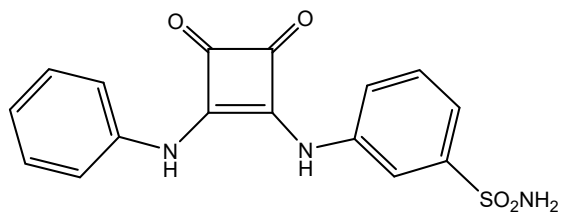


^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **8**

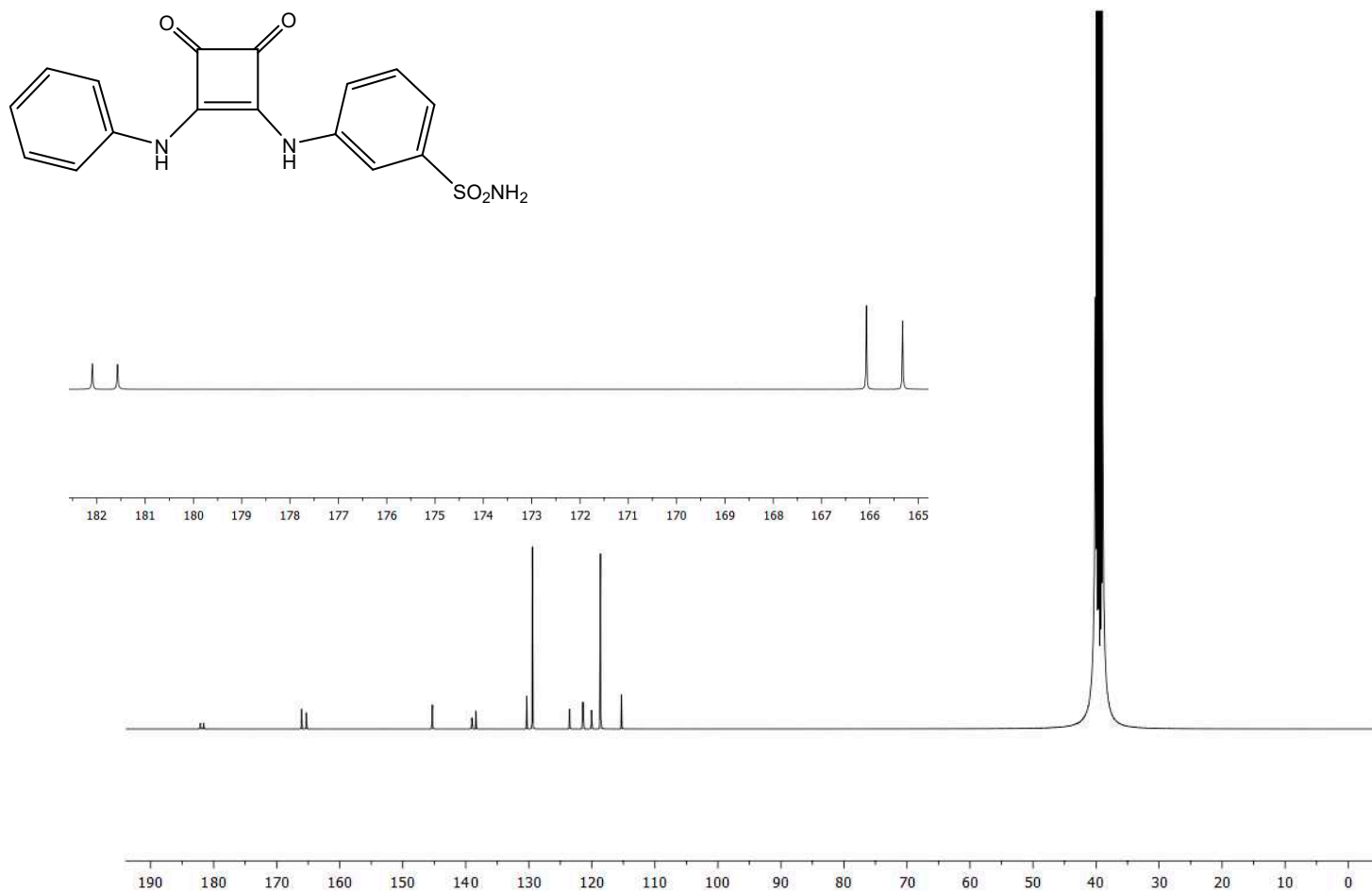


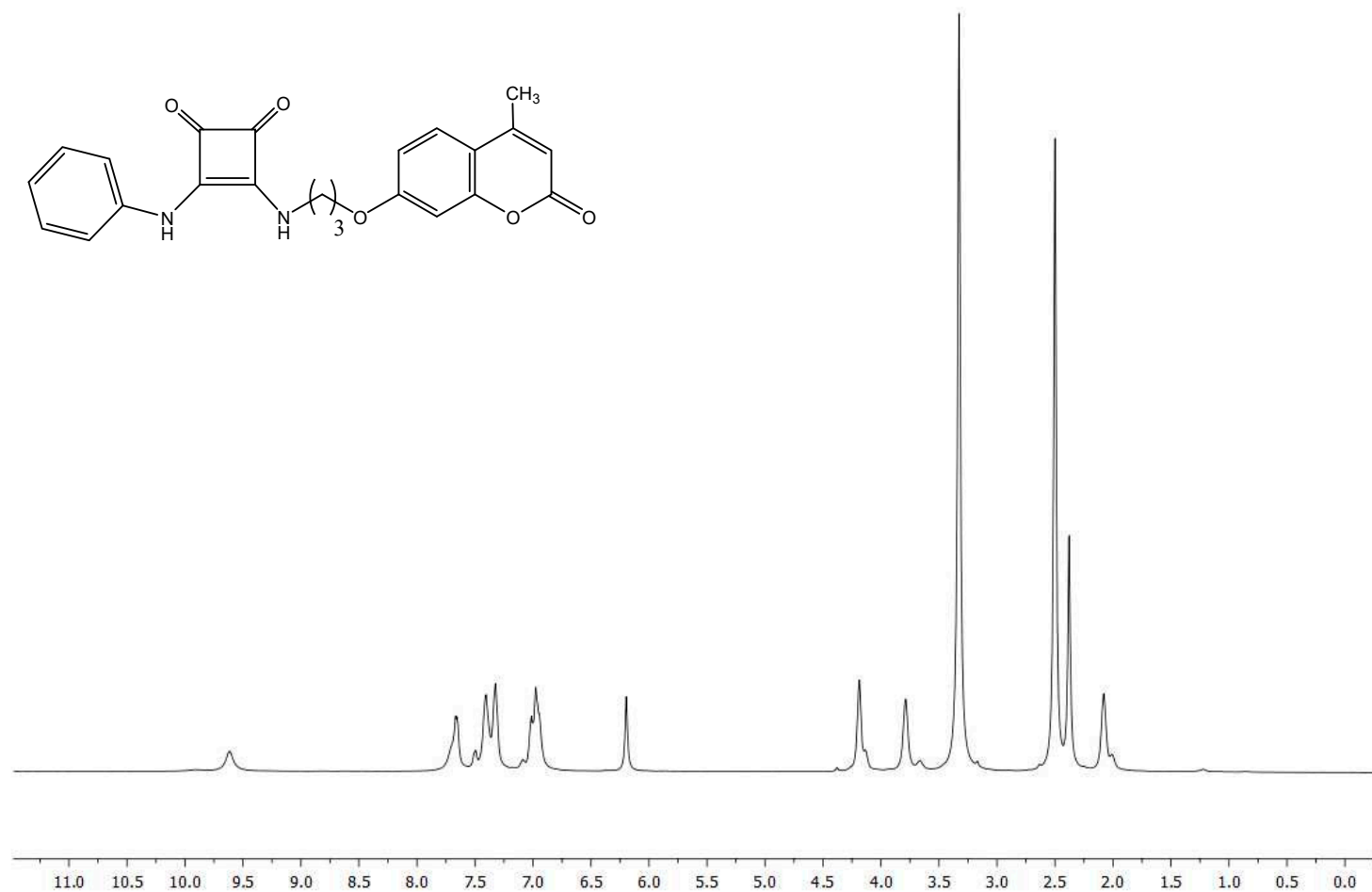


^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **10**

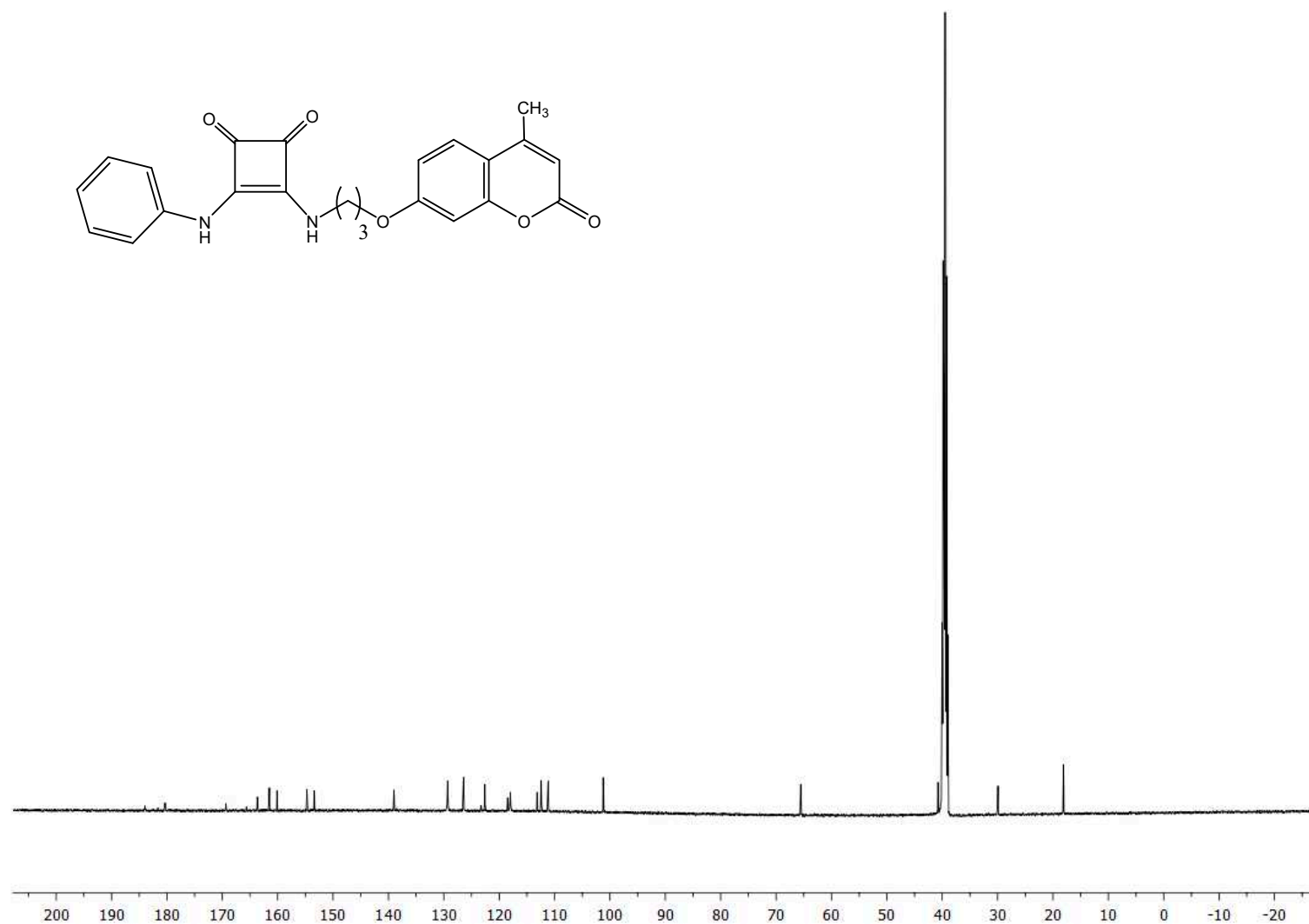


^1H -NMR (300 MHz, $(\text{CD}_3)_2\text{SO}$) of **11**

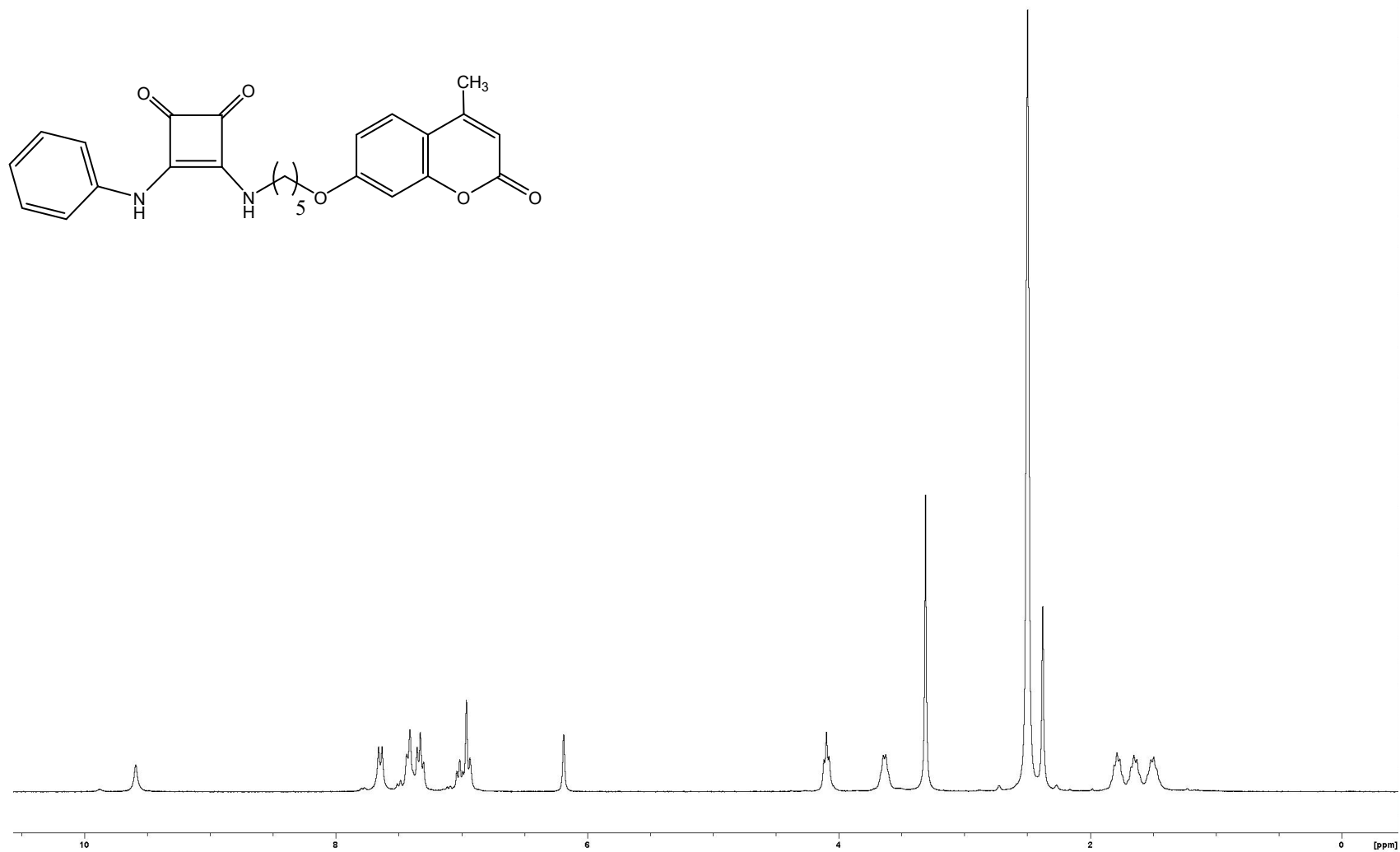




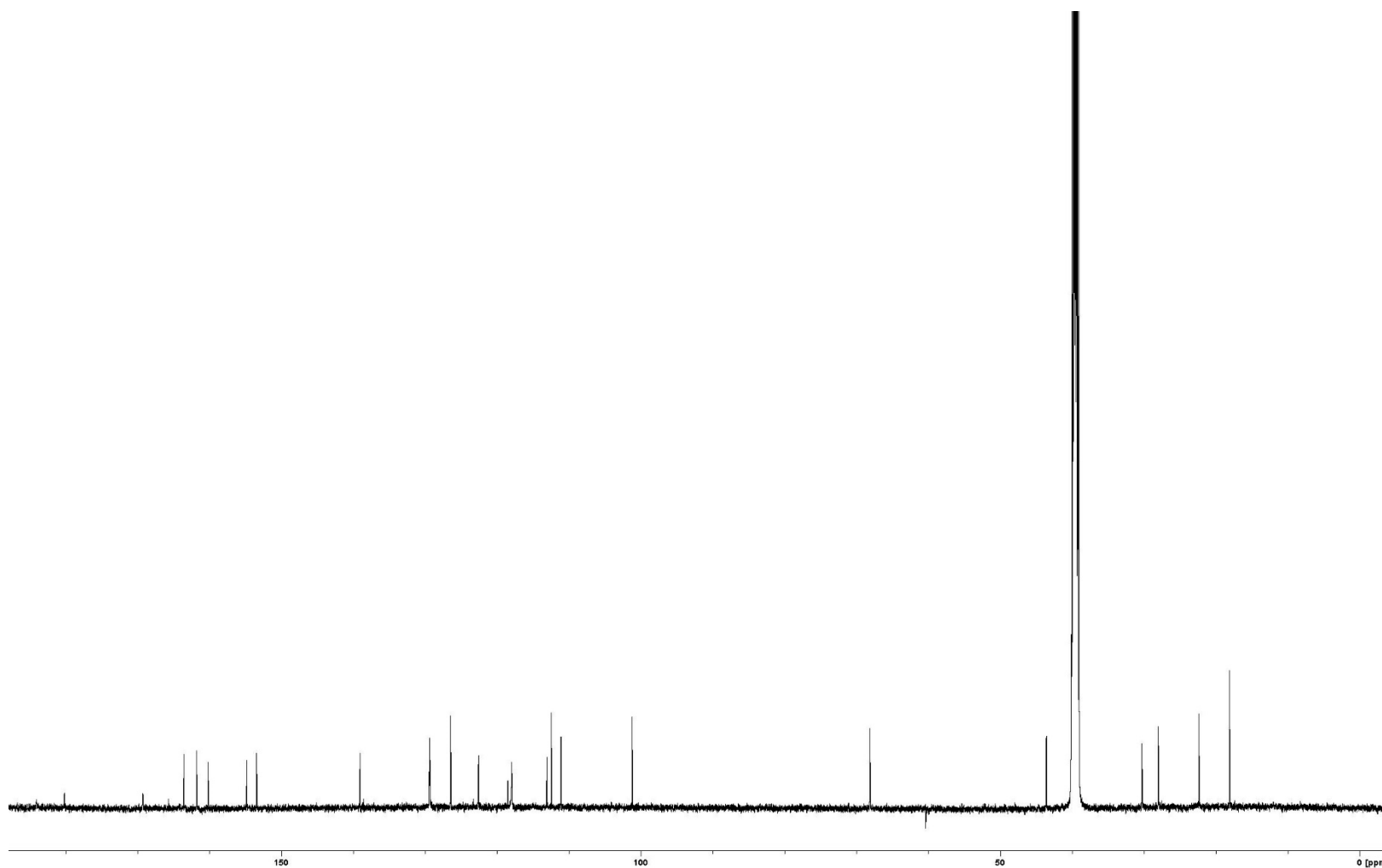
$^1\text{H-NMR}$ (500 MHz, $(\text{CD}_3)_2\text{SO}$) of **16a**



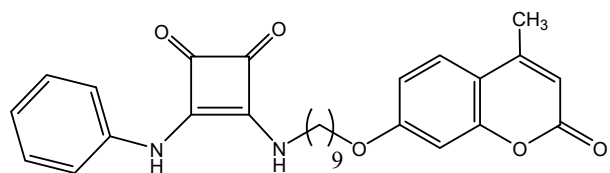
^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16a**



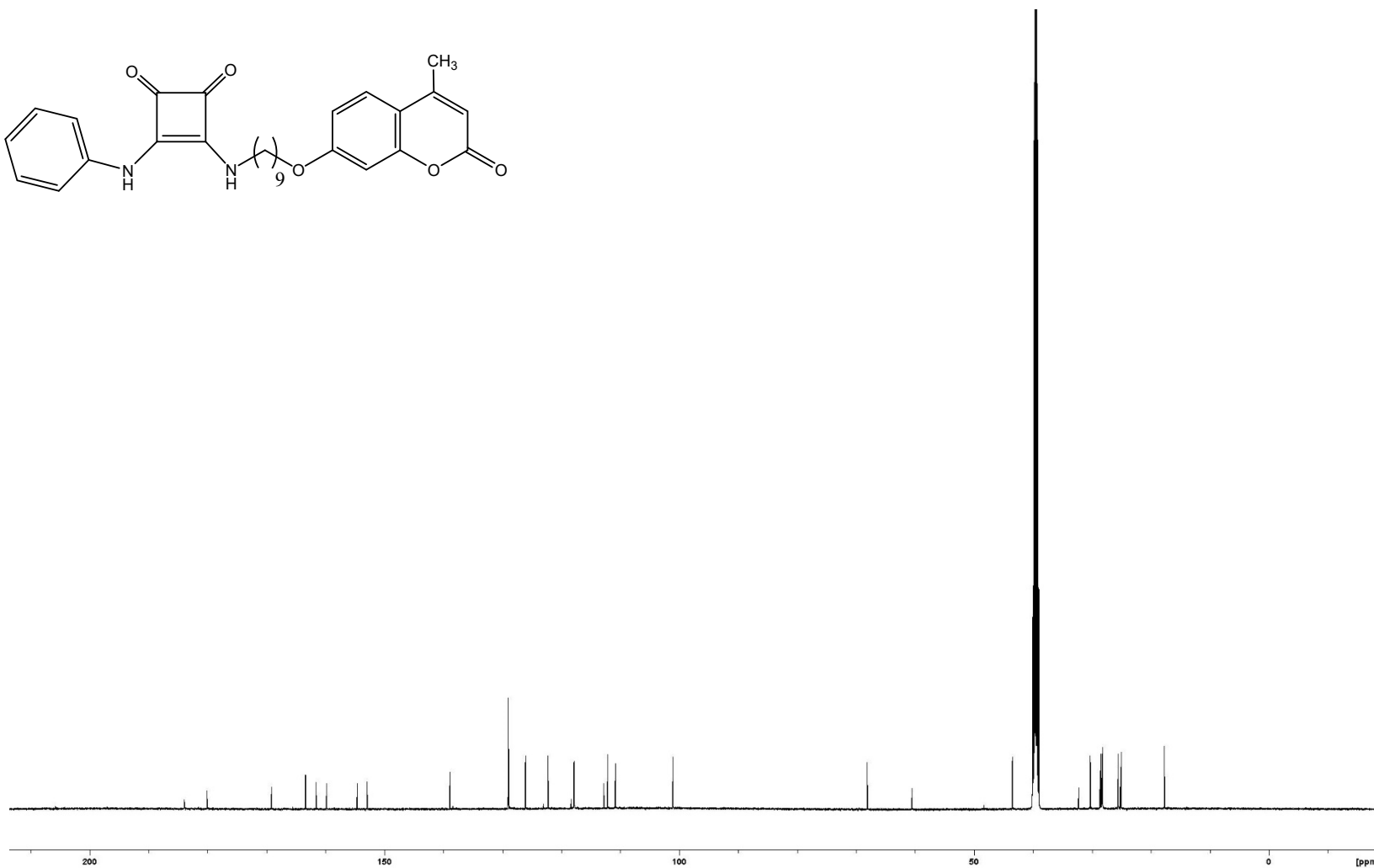
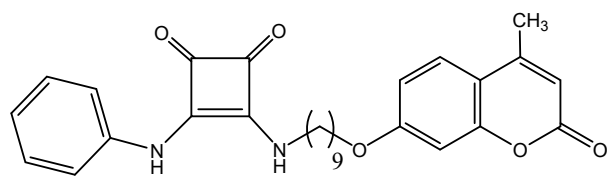
^1H -NMR (300 MHz, $(\text{CD}_3)_2\text{SO}$) of **16b**



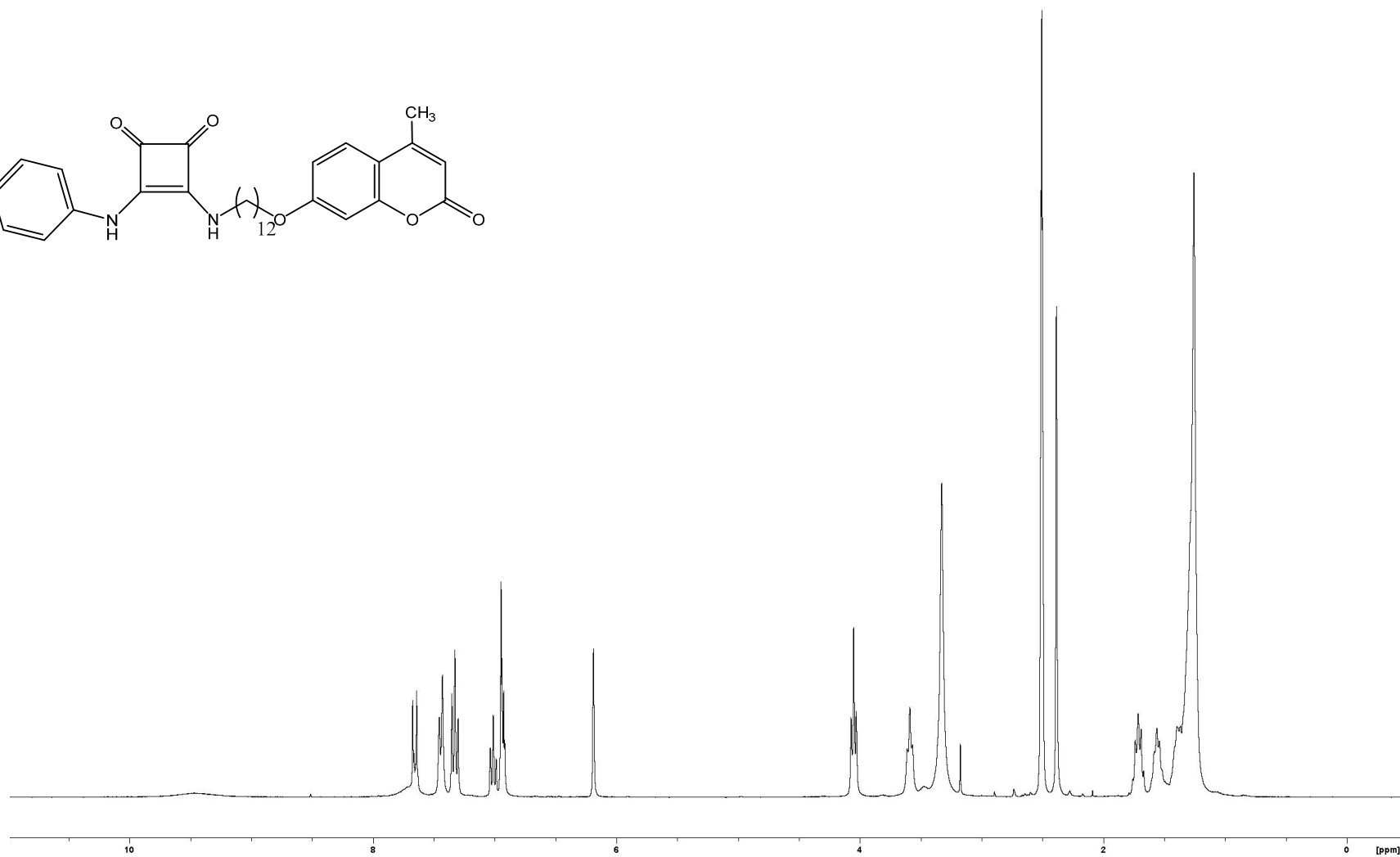
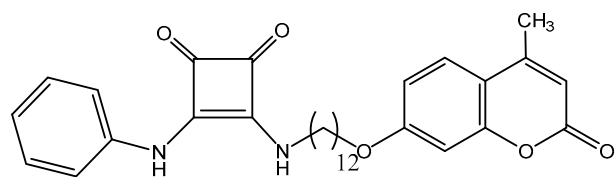
^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16b**



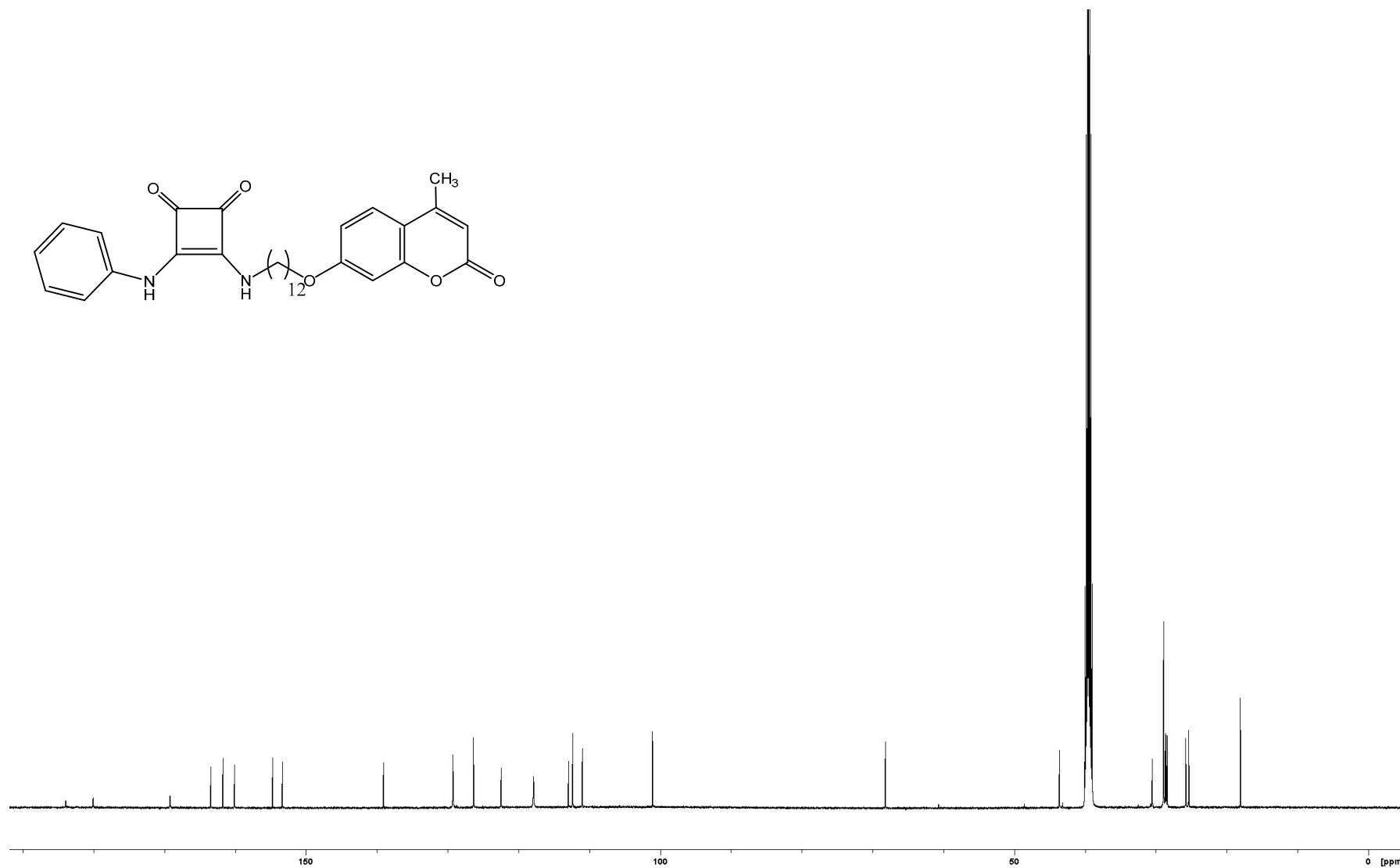
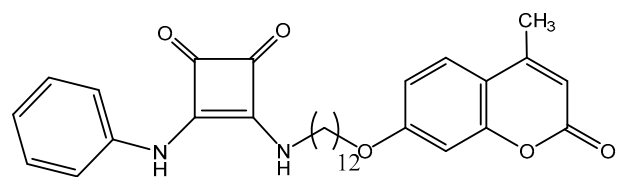
$^1\text{H-NMR}$ (300 MHz, $(\text{CD}_3)_2\text{SO}$) of **16c**



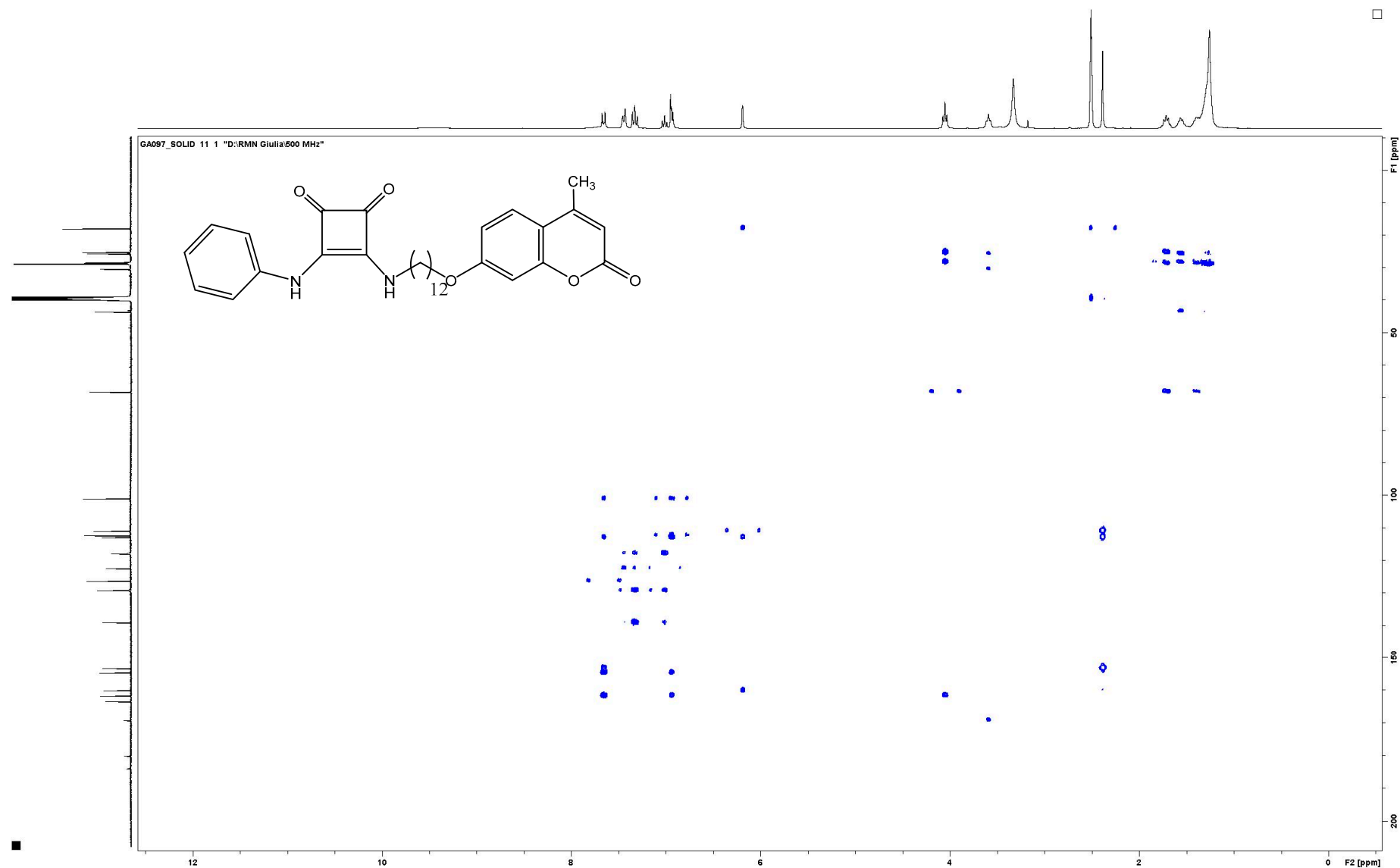
^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16c**



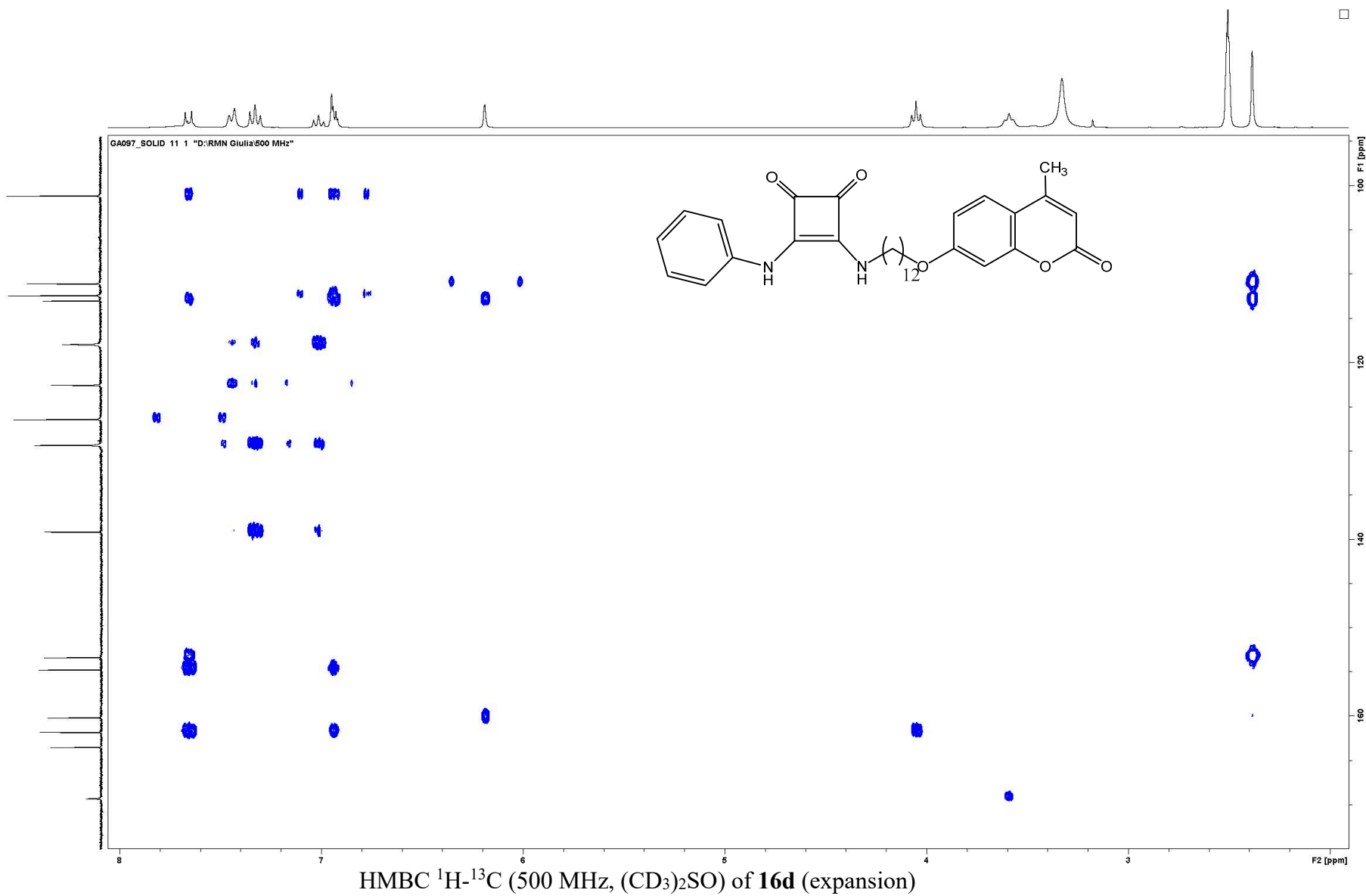
^1H -NMR (300 MHz, $(\text{CD}_3)_2\text{SO}$) of **16d**

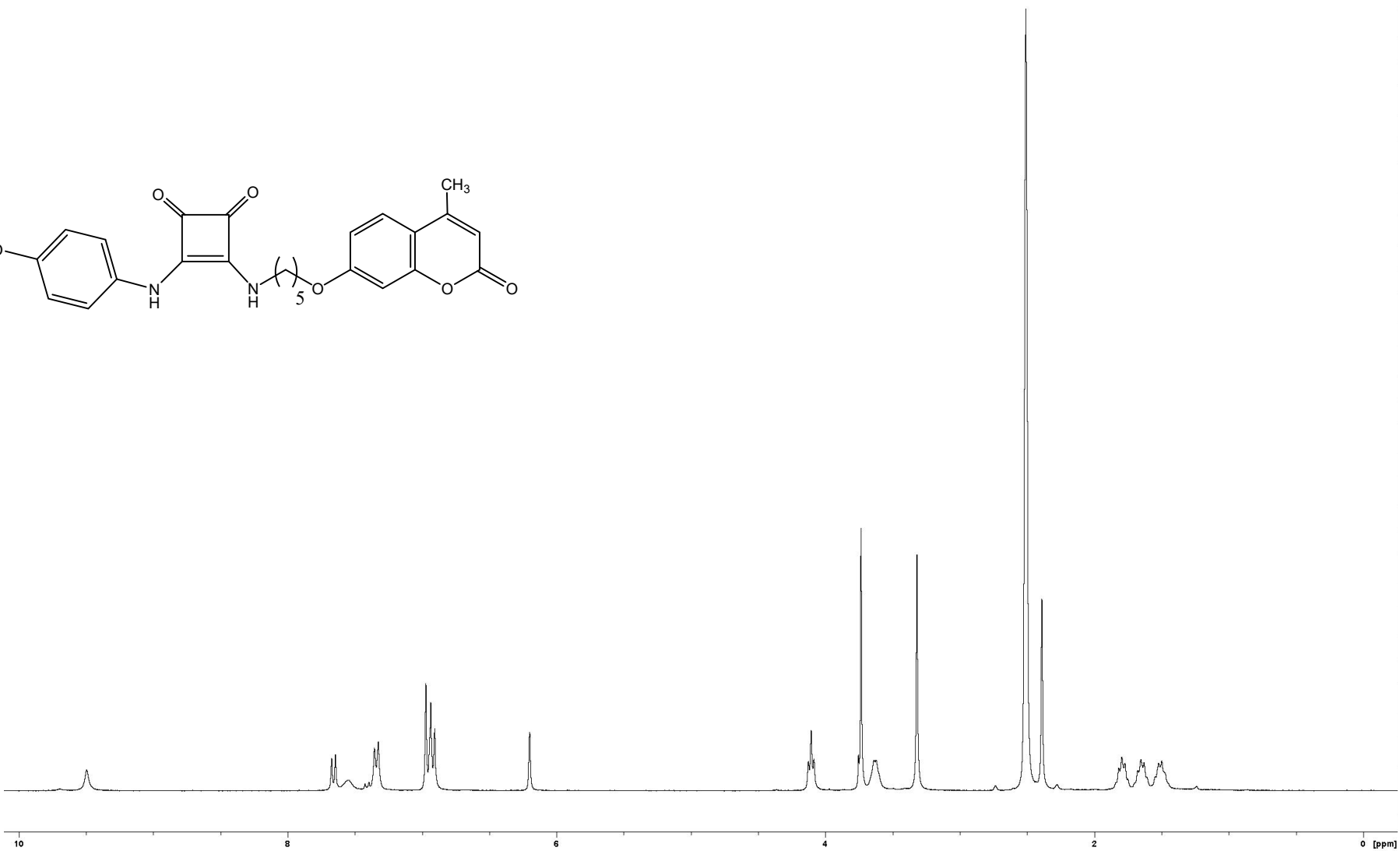


^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16d**

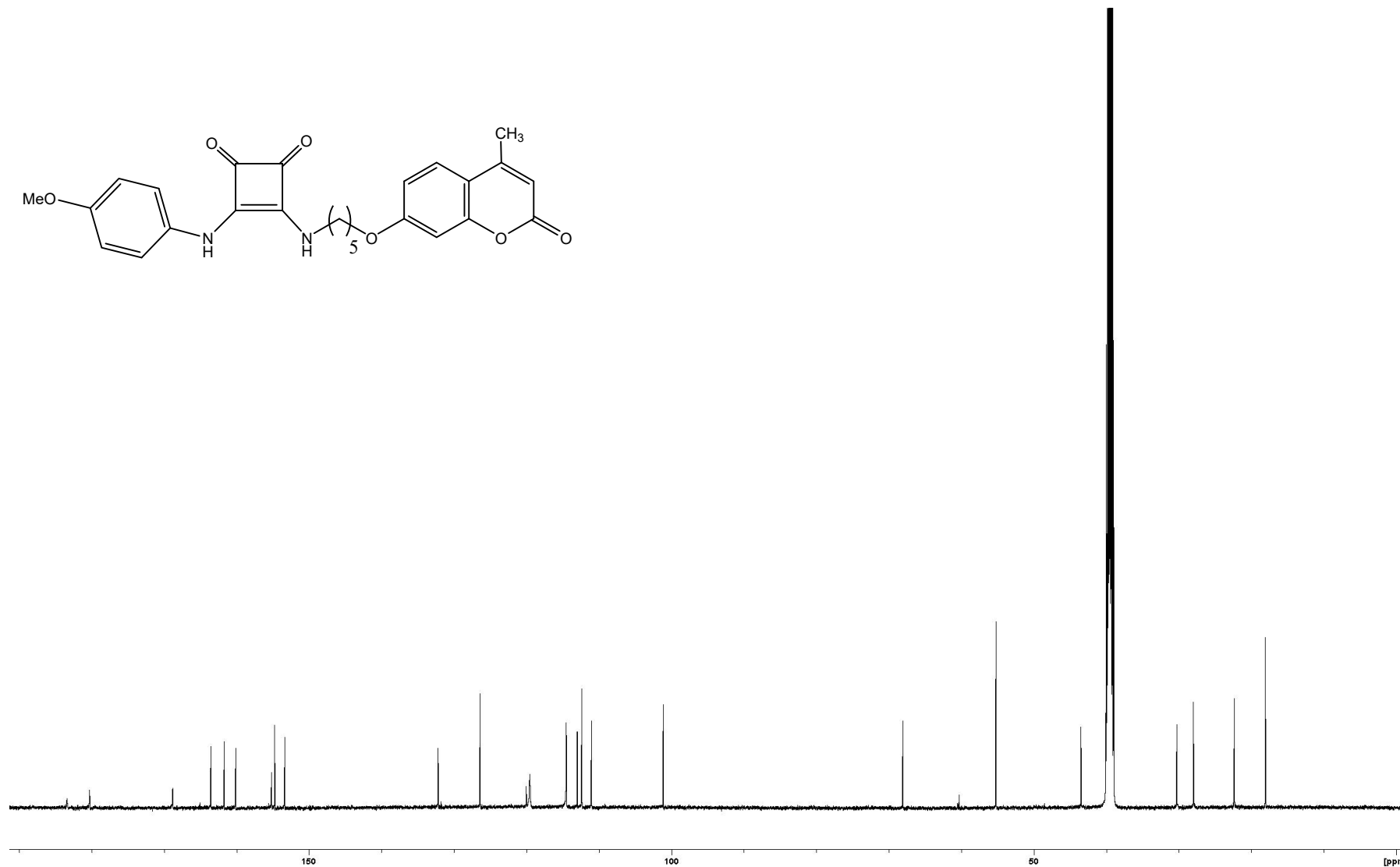
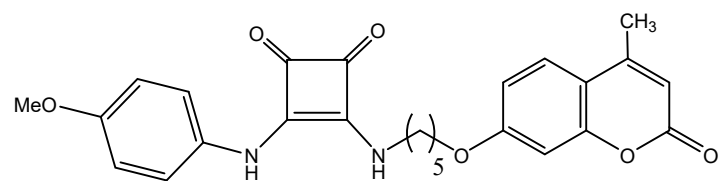


HMBC ^1H - ^{13}C (500 MHz, $(\text{CD}_3)_2\text{SO}$) of **16d**

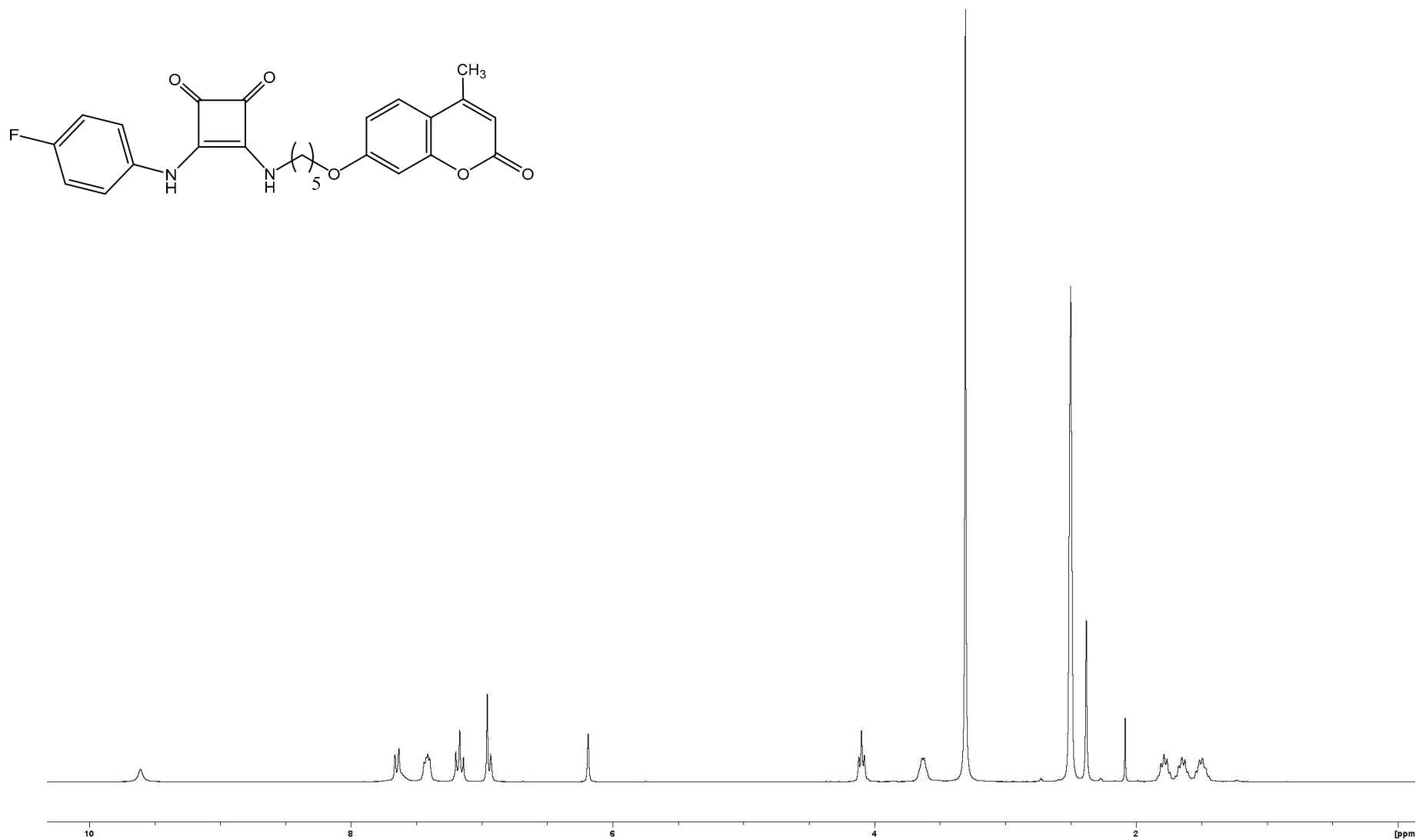




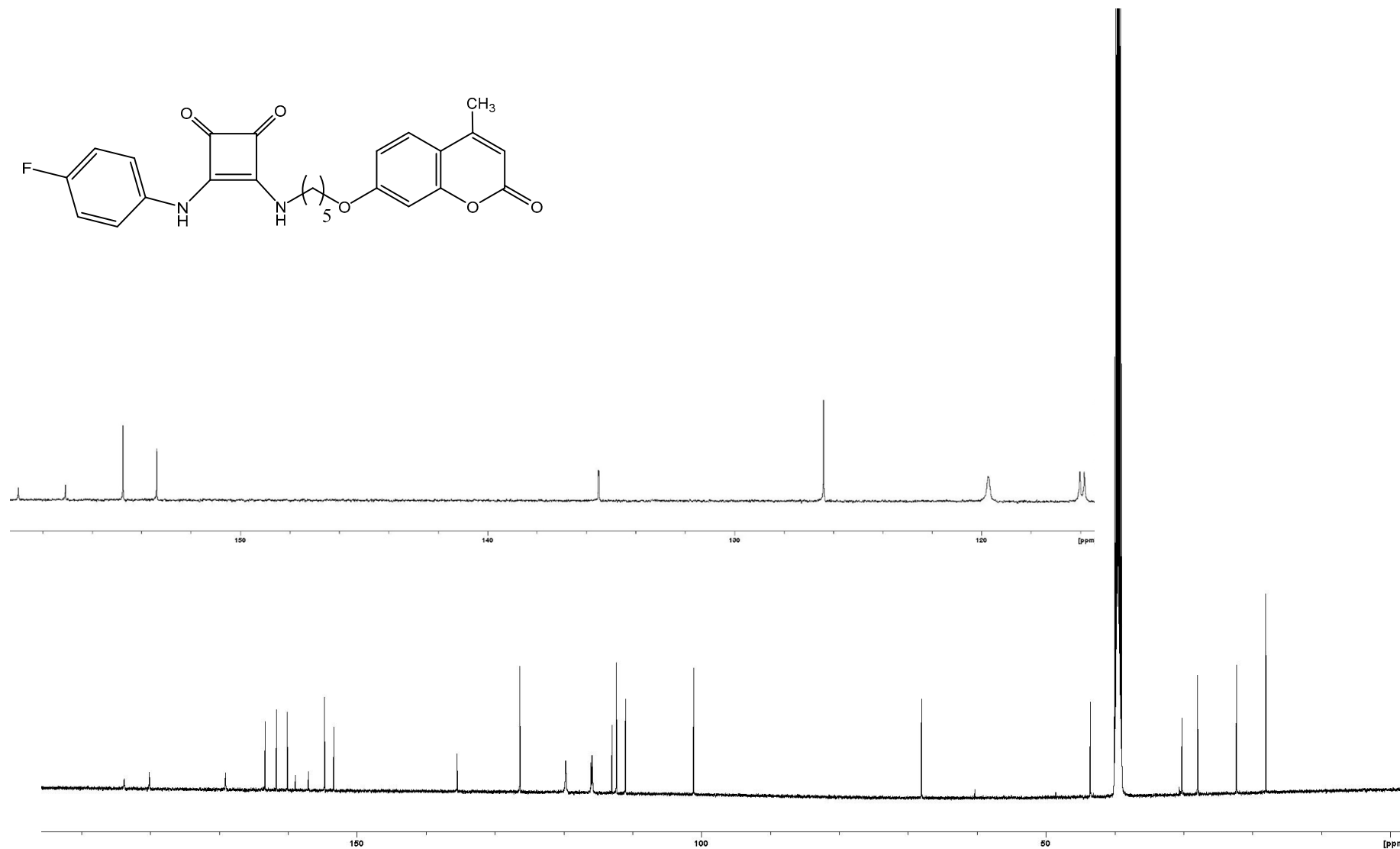
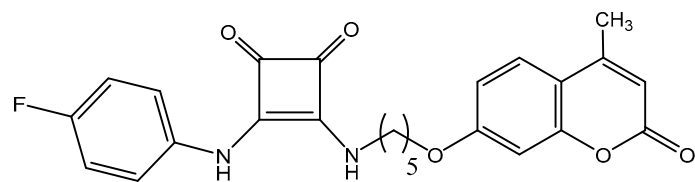
S30



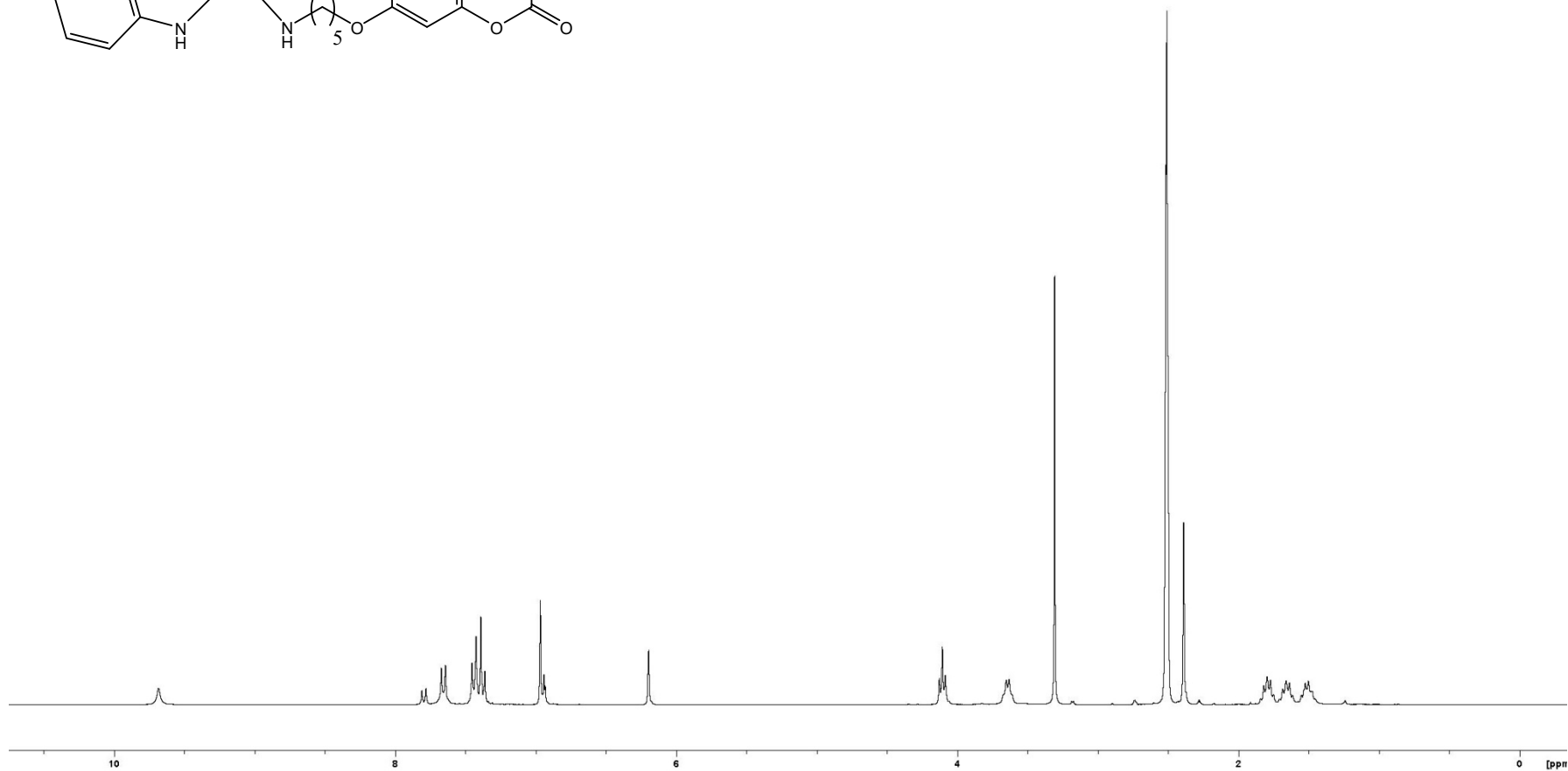
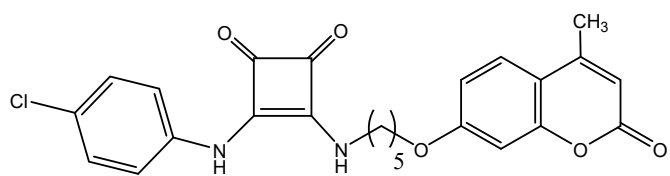
^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16e**



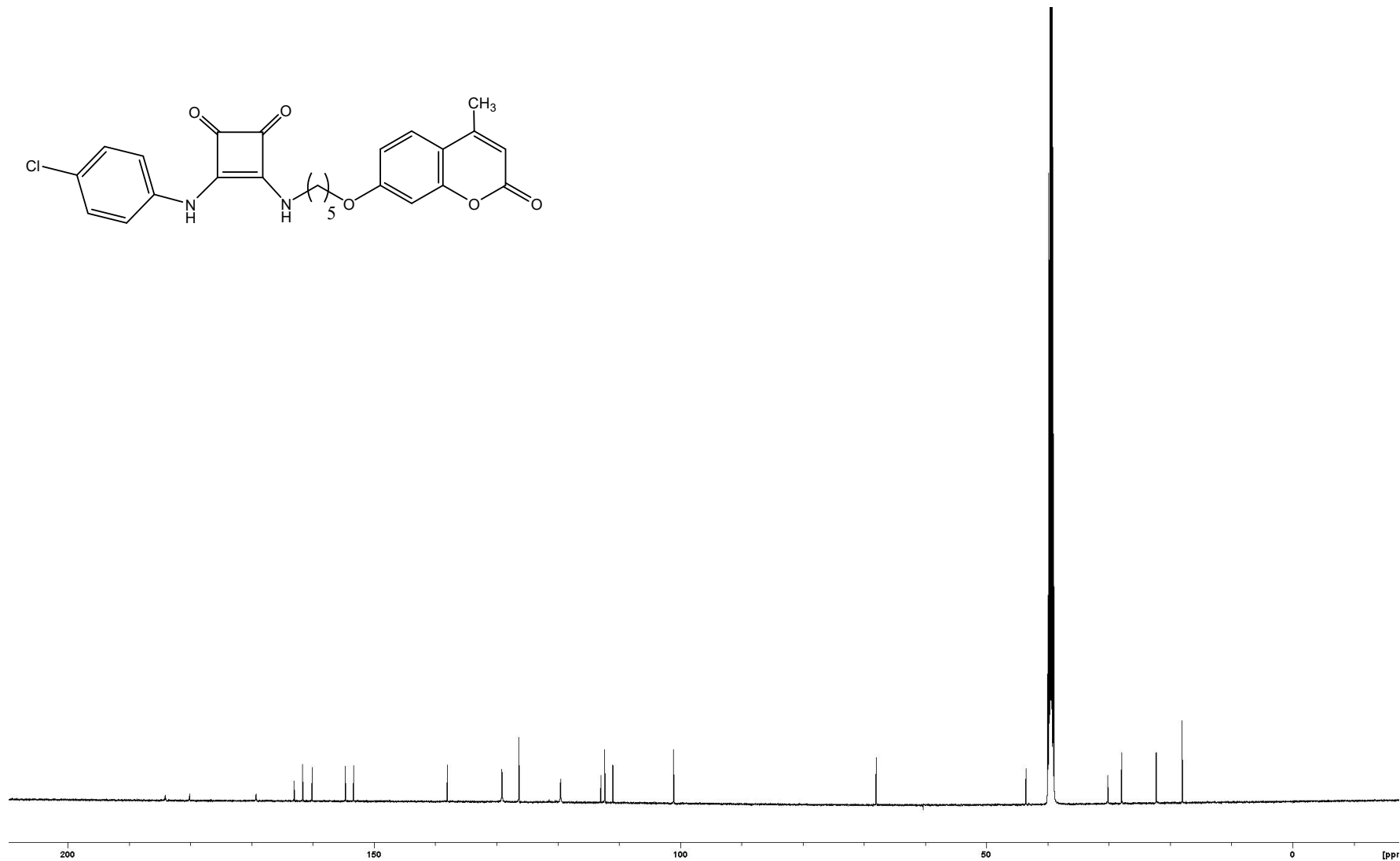
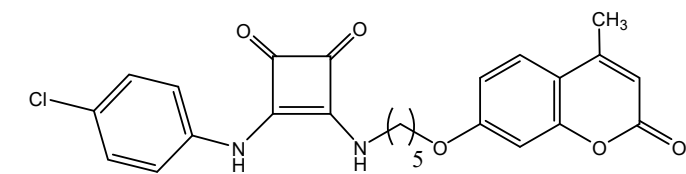
¹H-NMR (300 MHz, (CD₃)₂SO) of **16f**



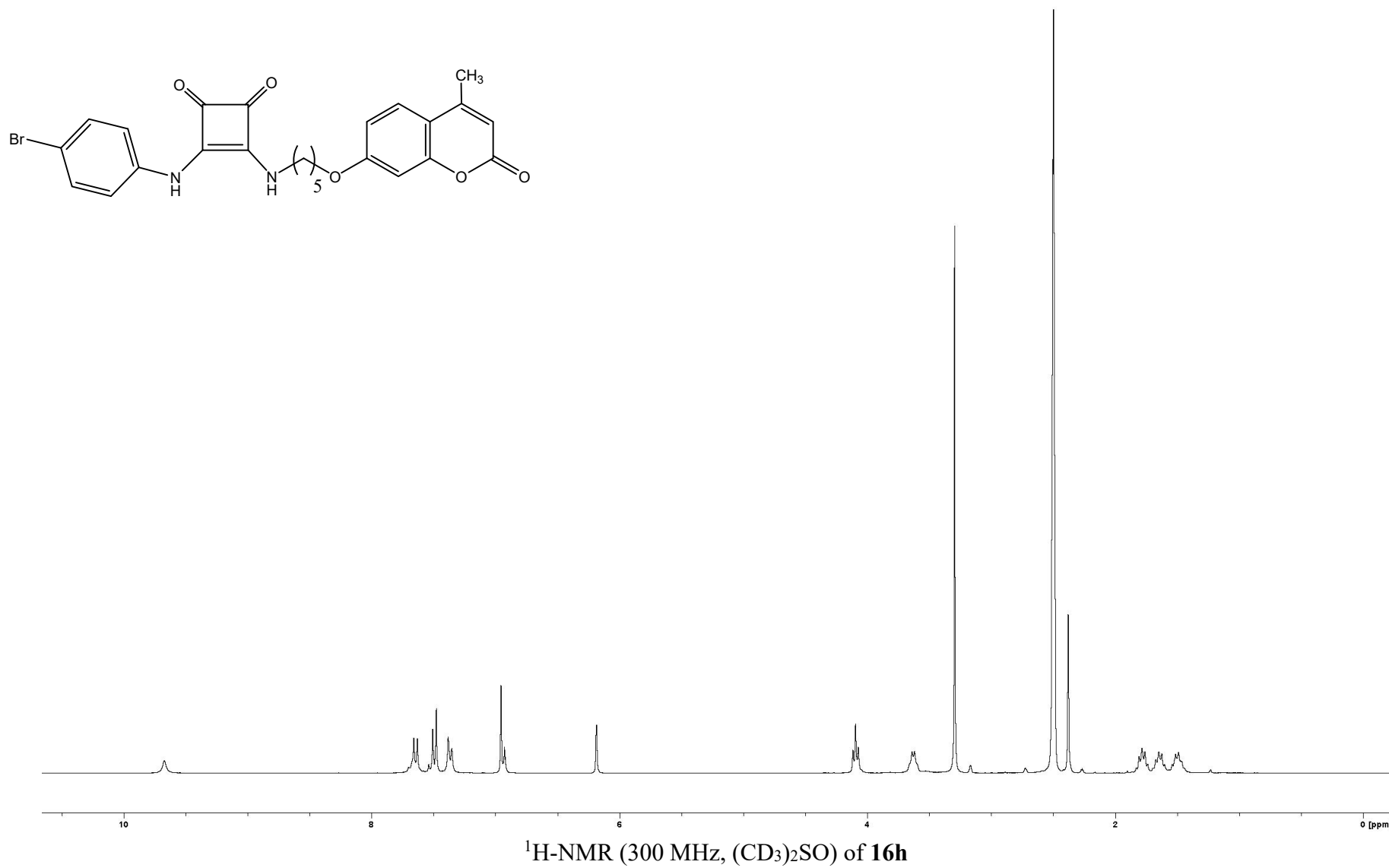
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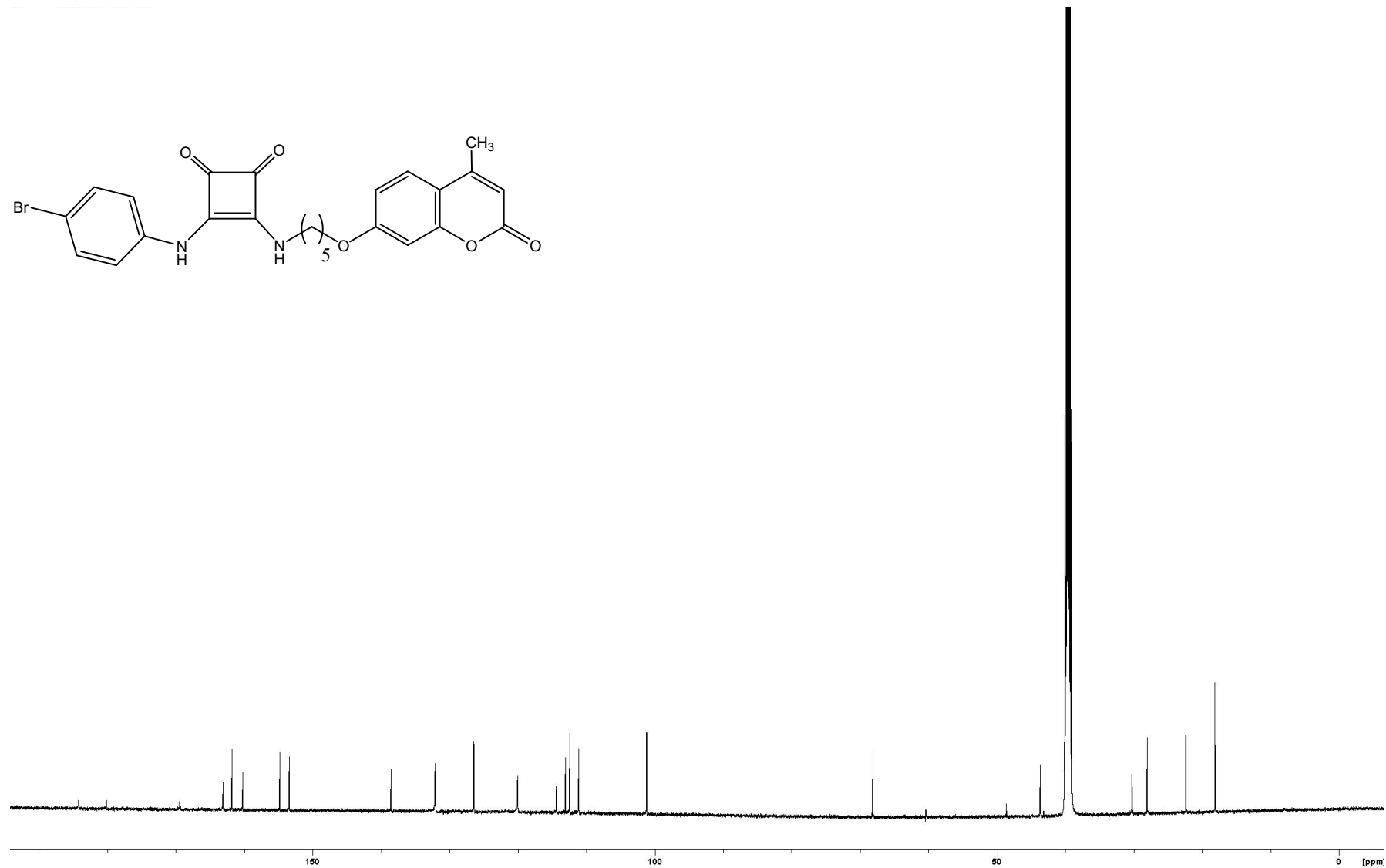
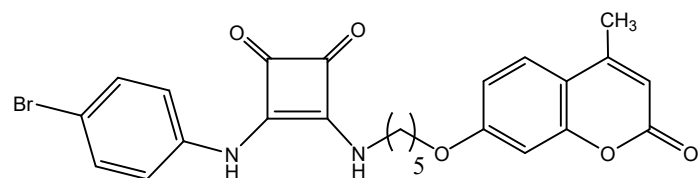


¹H-NMR (300 MHz, (CD₃)₂SO) of **16g**

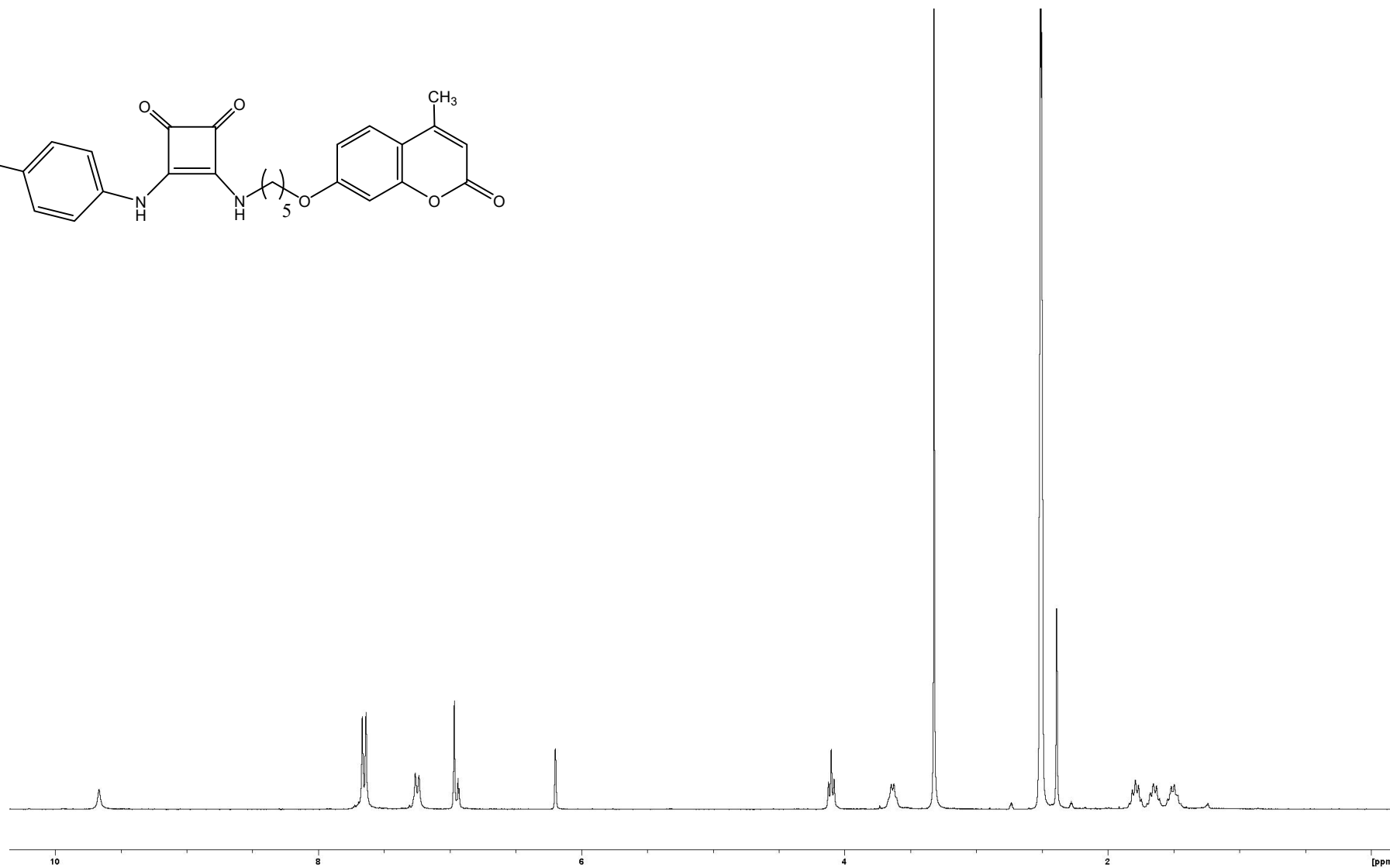
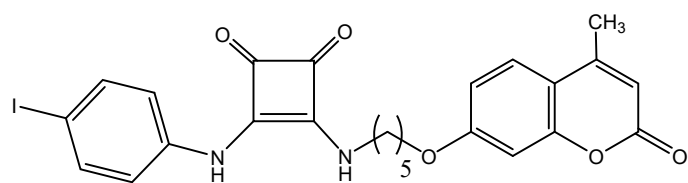


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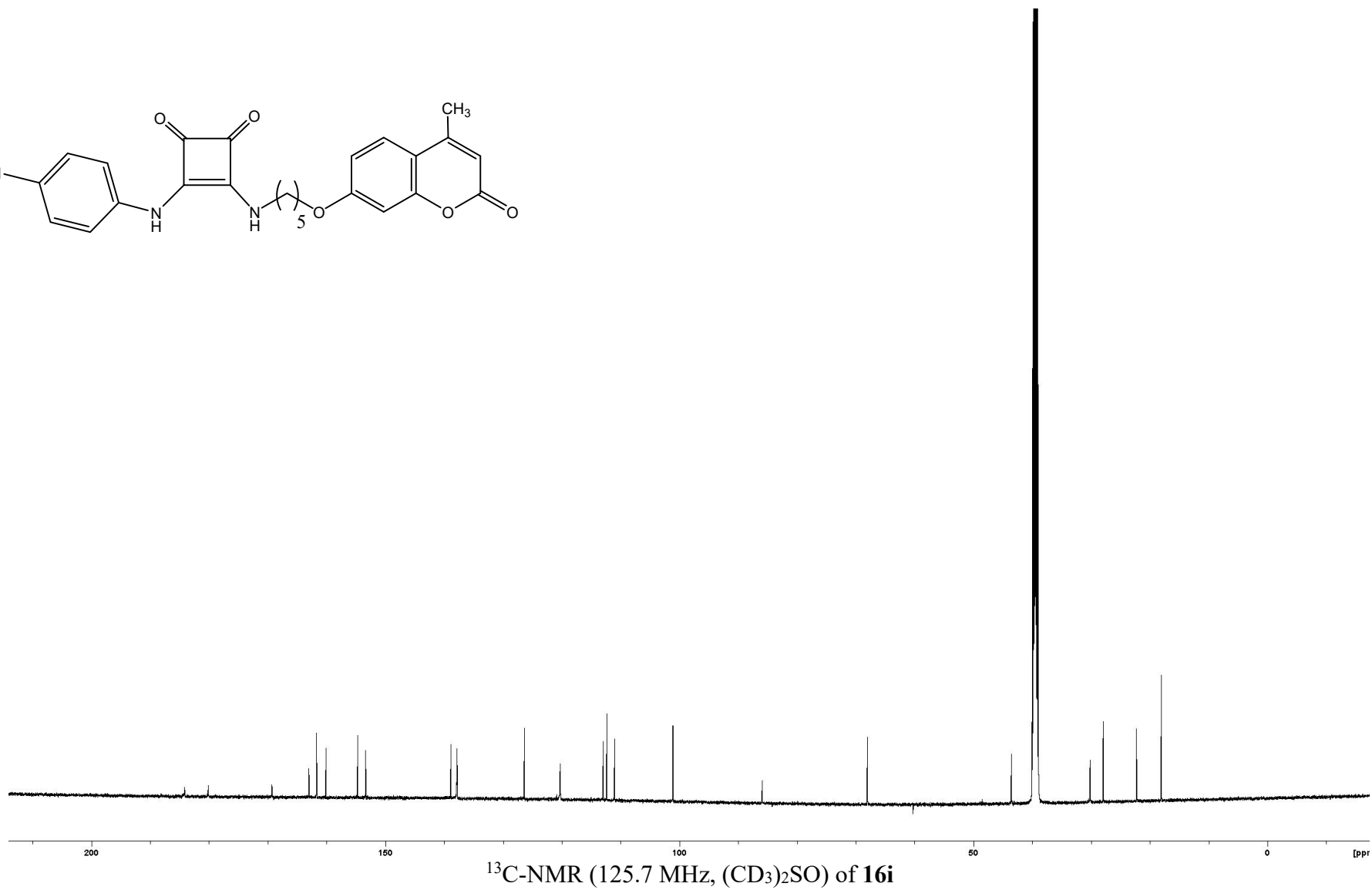
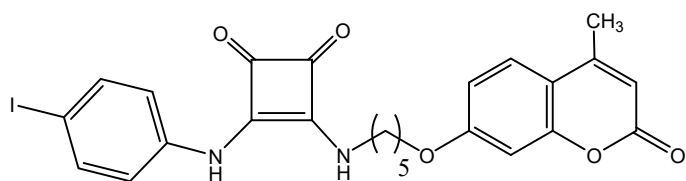


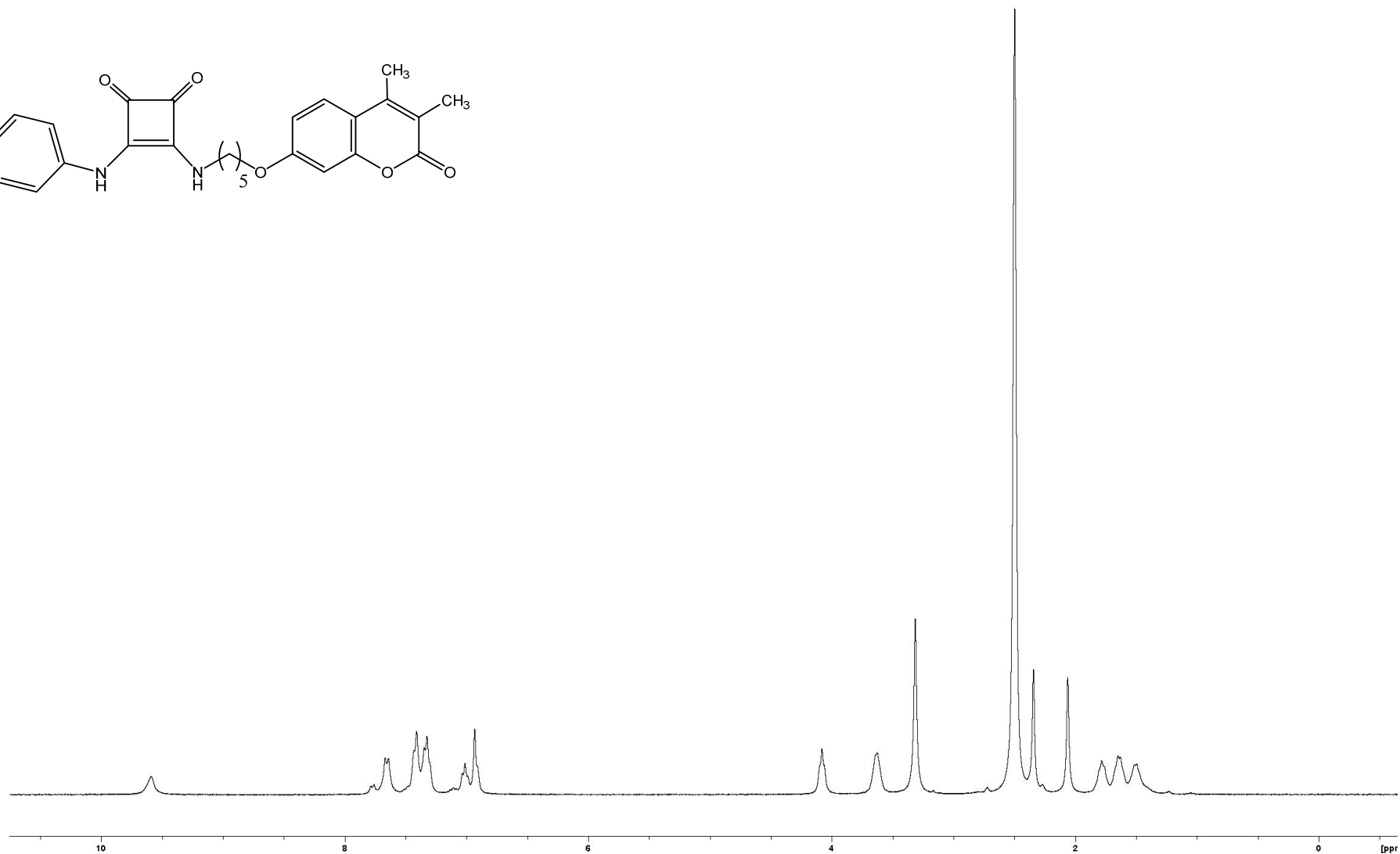
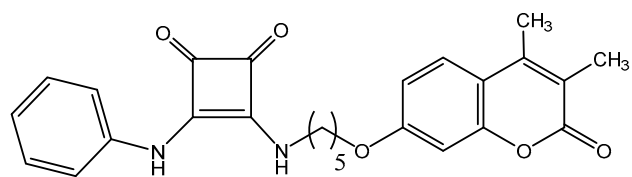


^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16h**

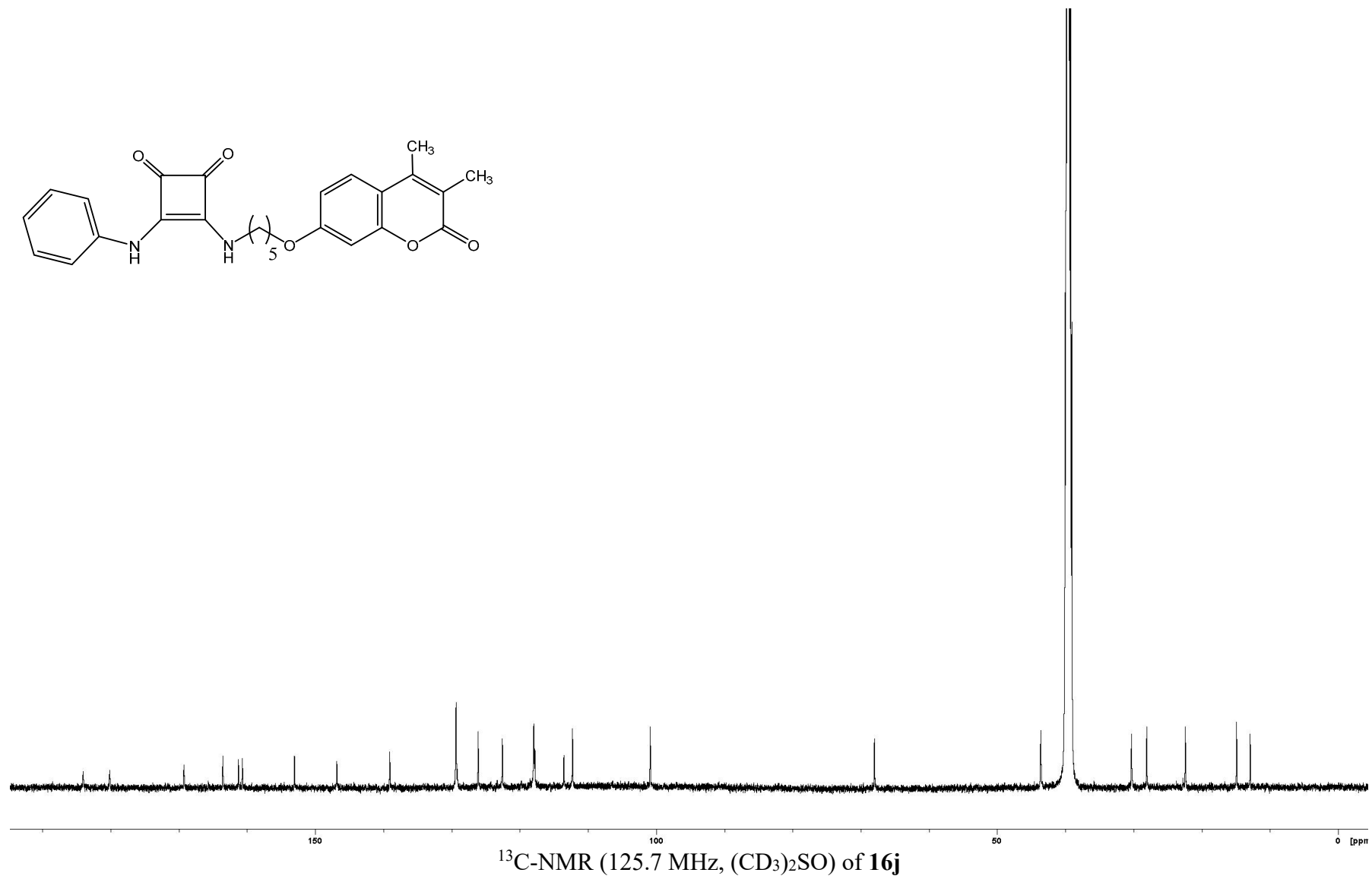


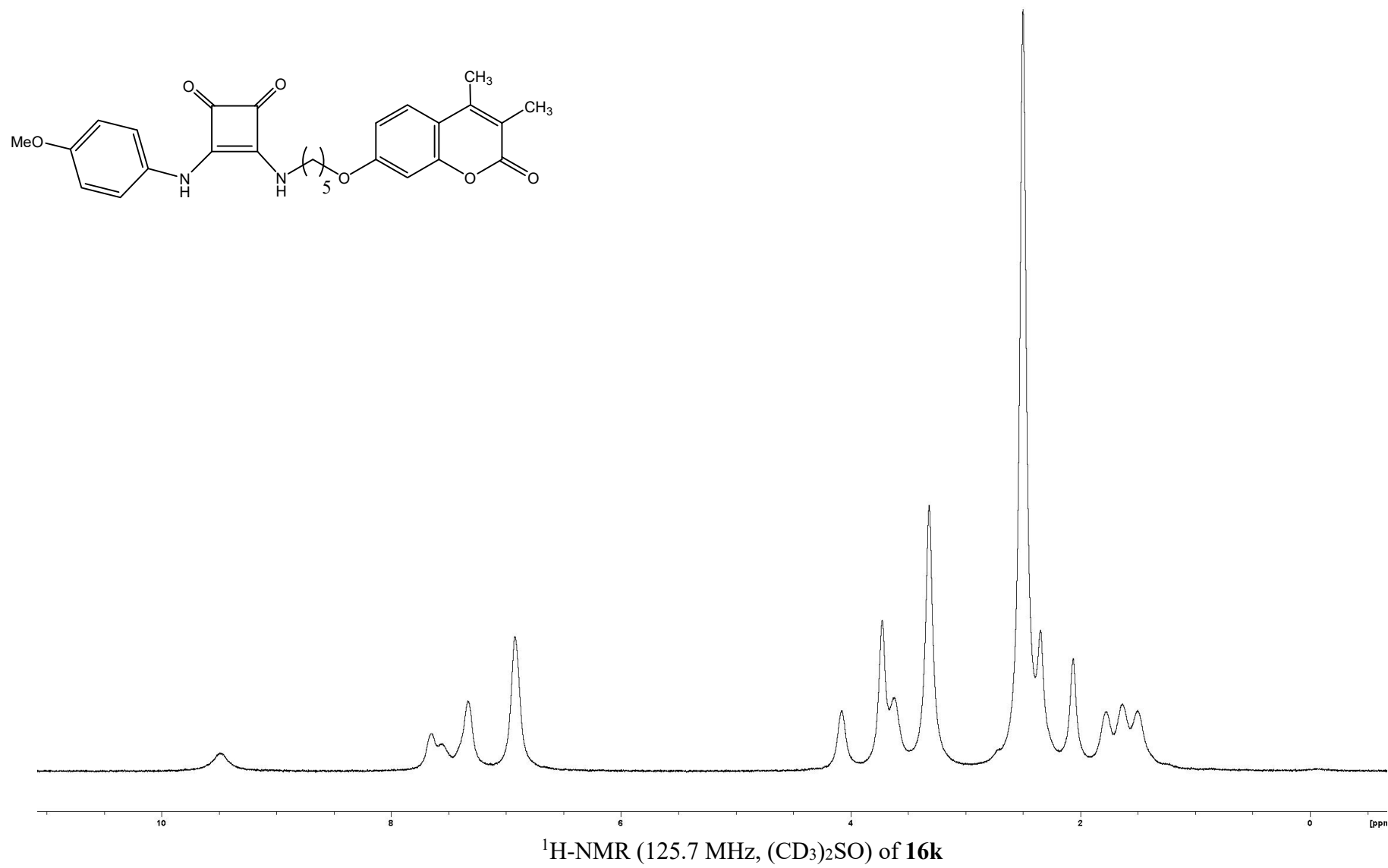
$^1\text{H-NMR}$ (300 MHz, $(\text{CD}_3)_2\text{SO}$) of **16i**

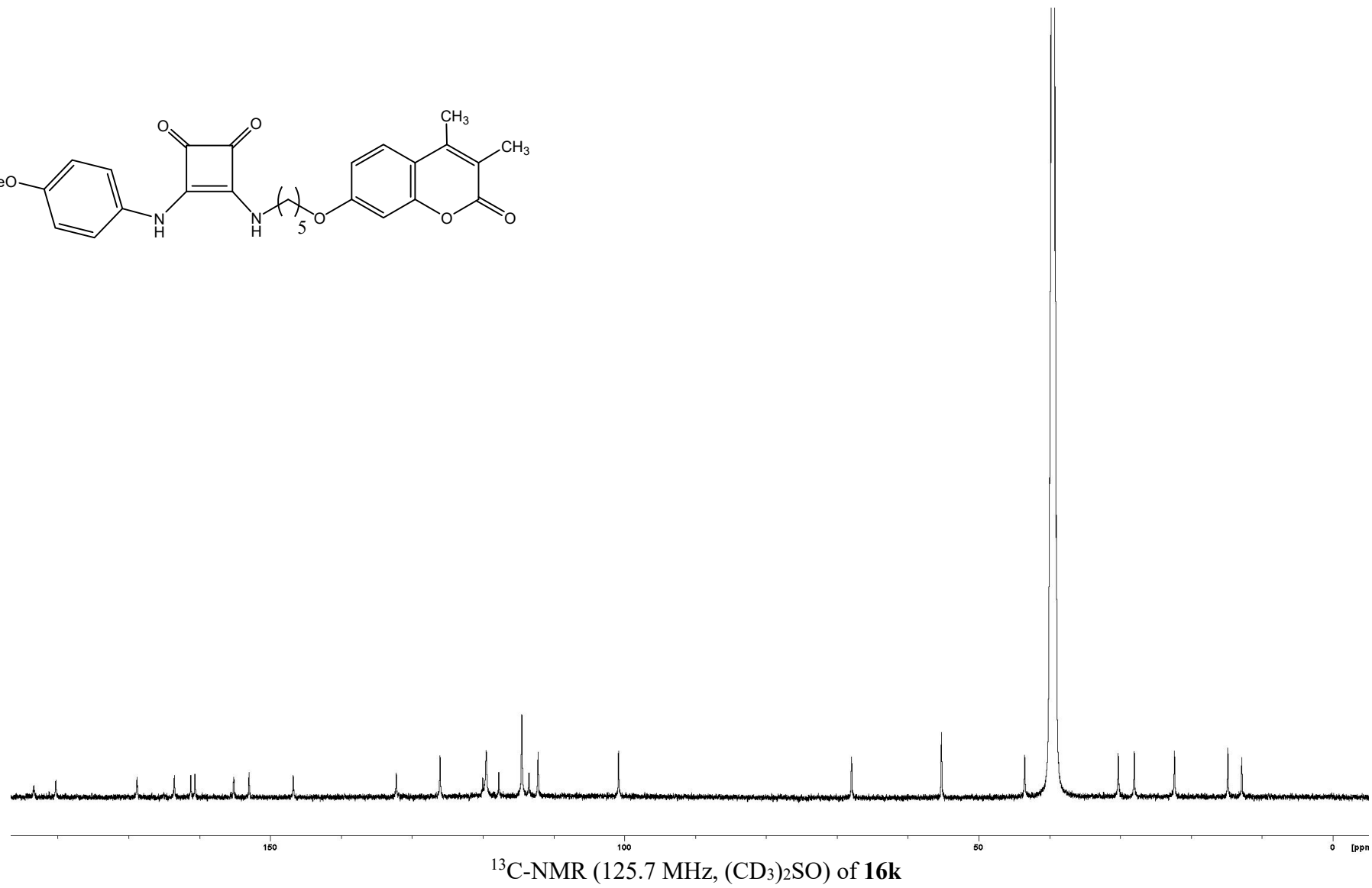
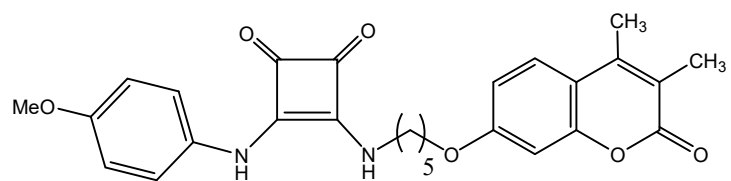


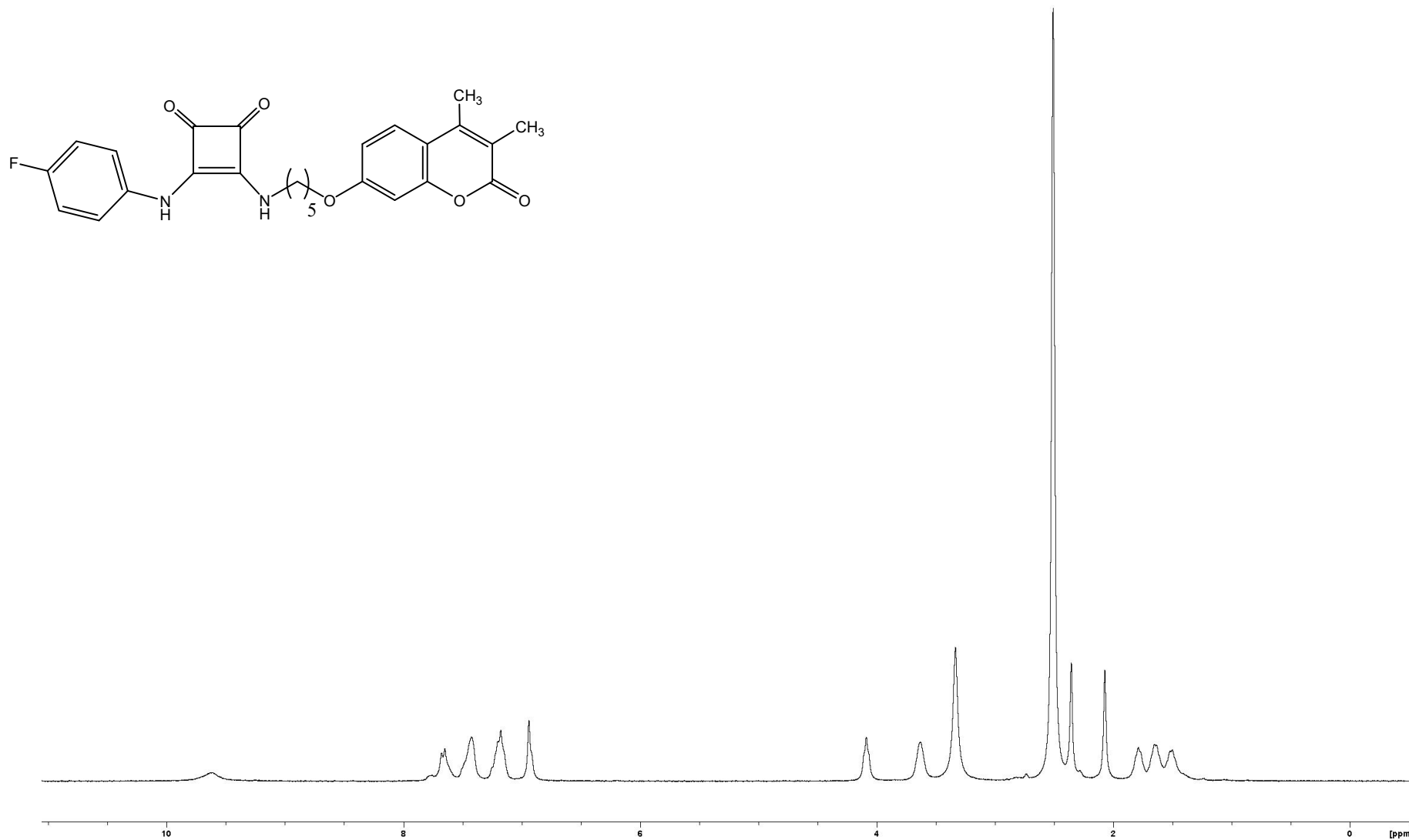


$^1\text{H-NMR}$ (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16j**

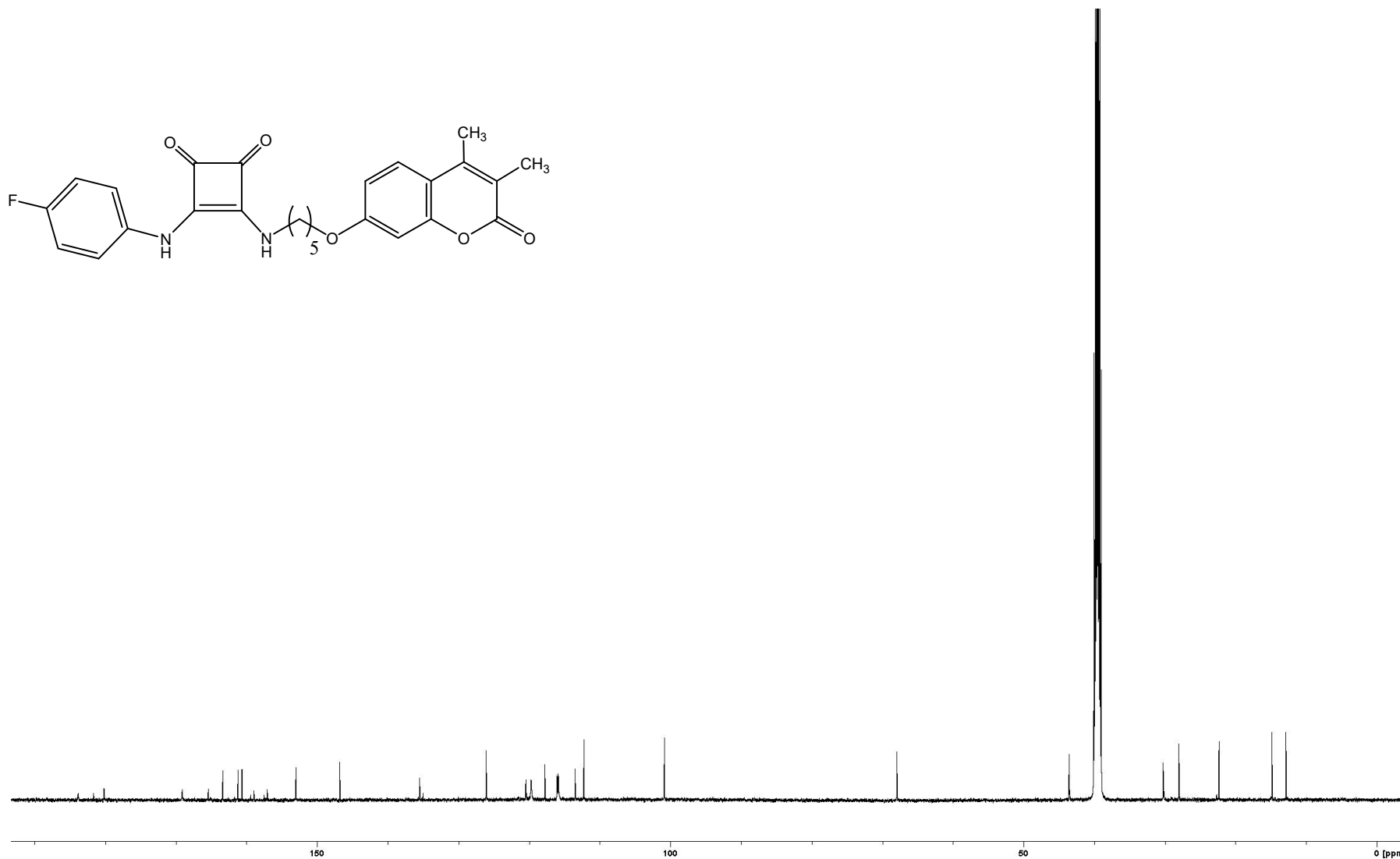
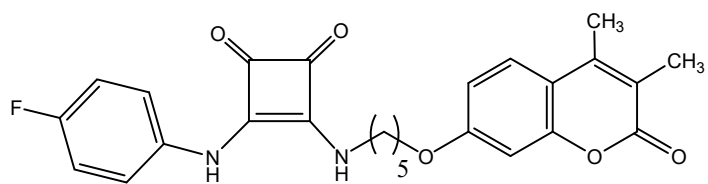




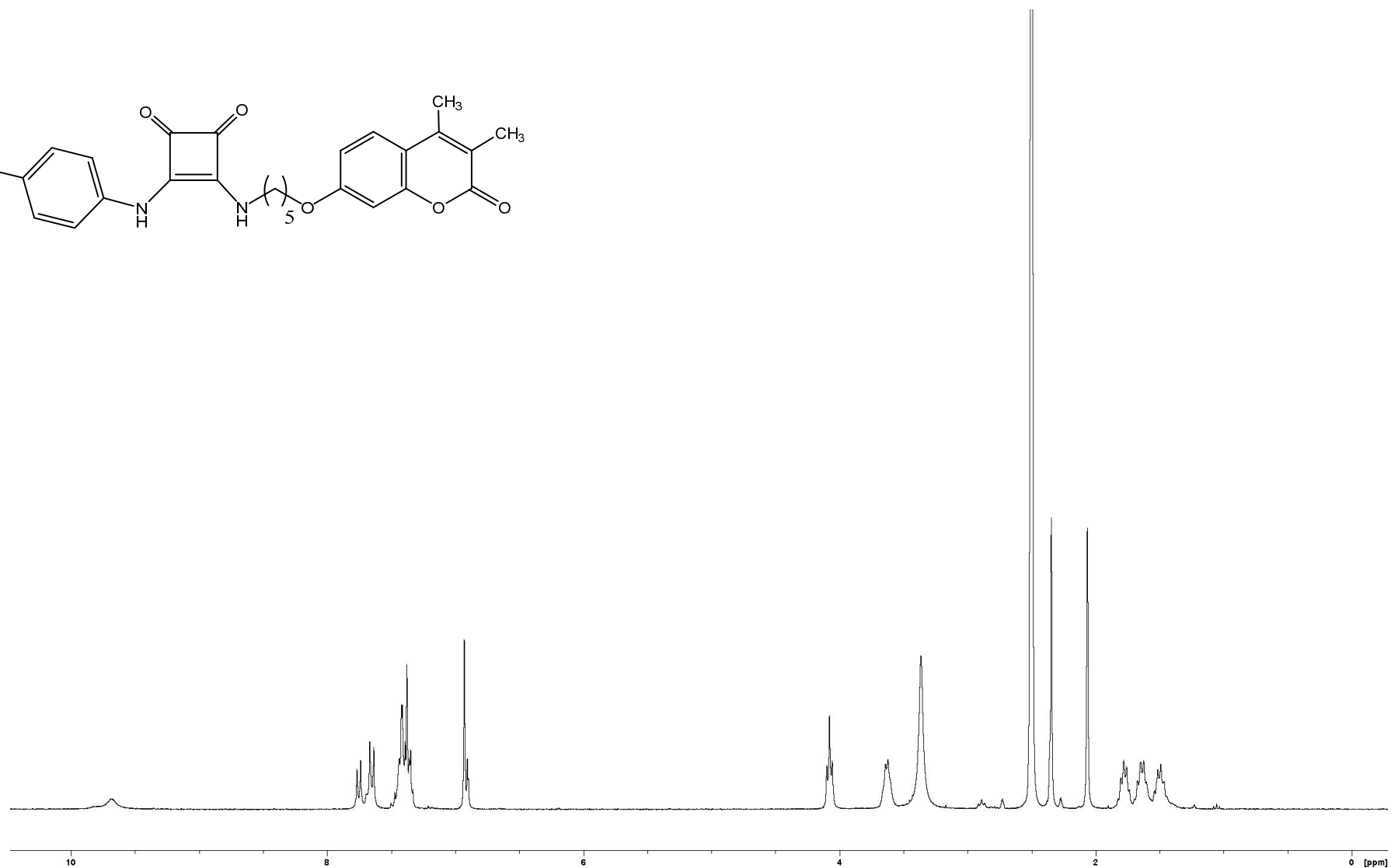
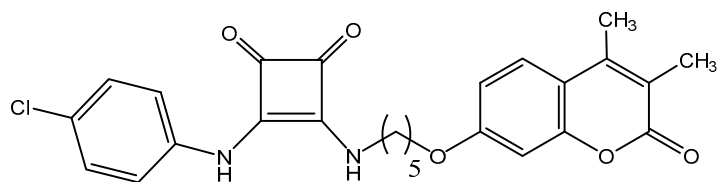




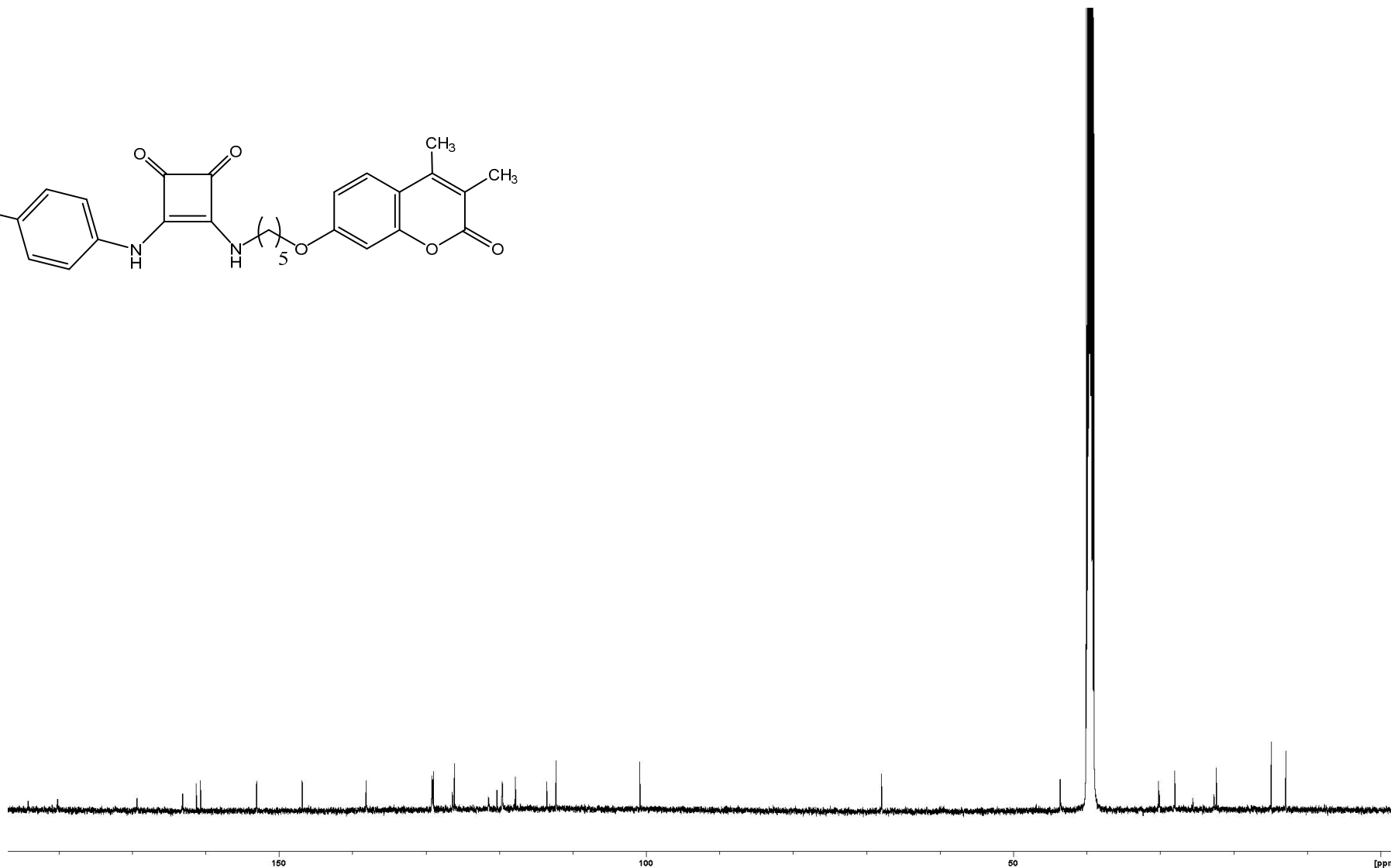
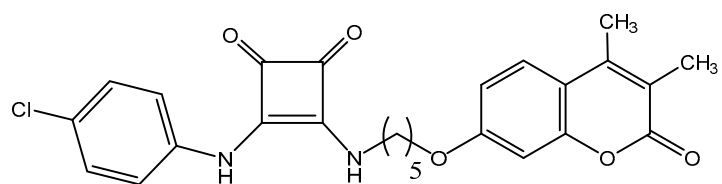
$^1\text{H-NMR}$ (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16l**



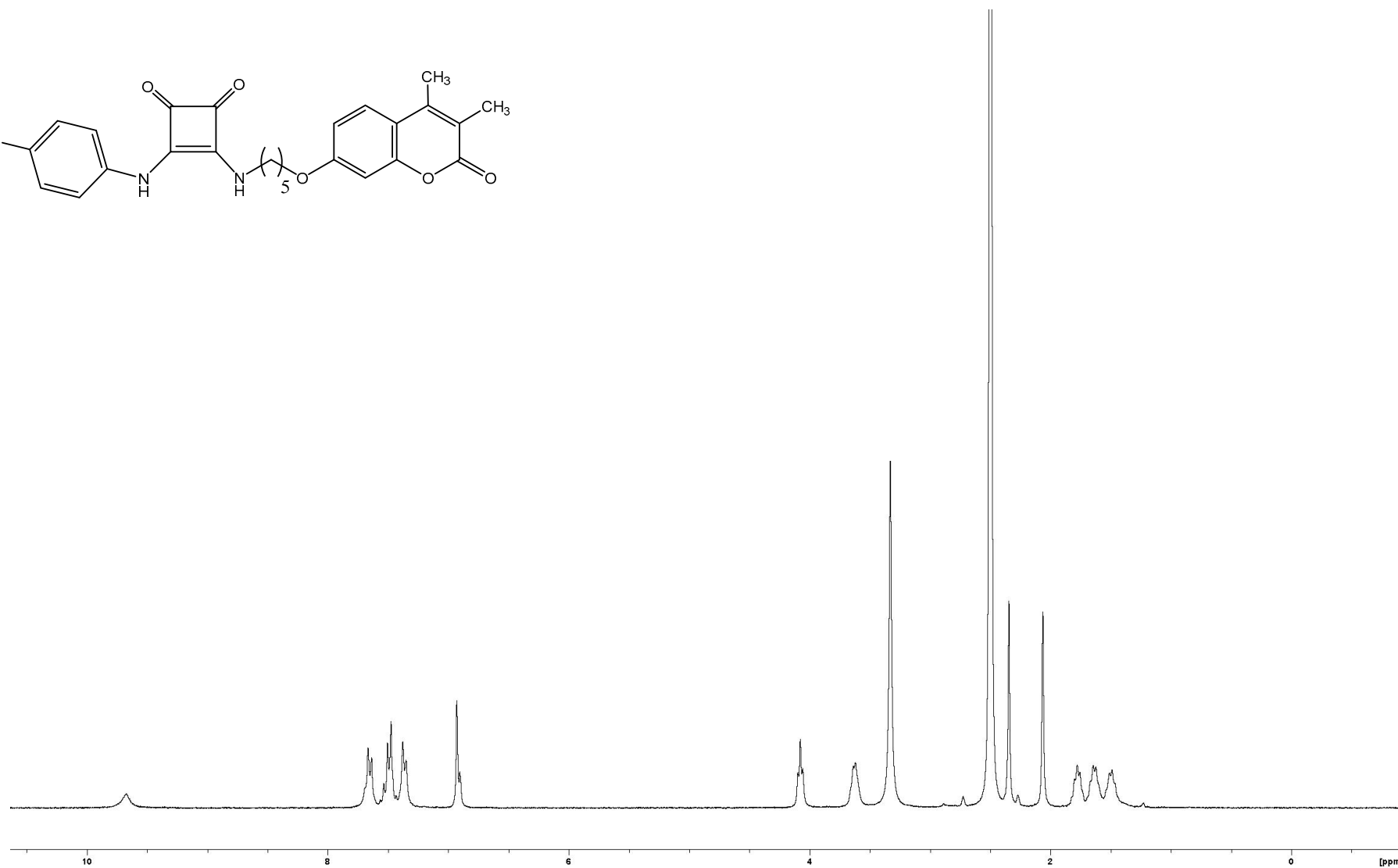
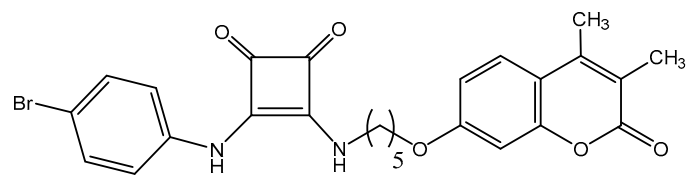
^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16l**



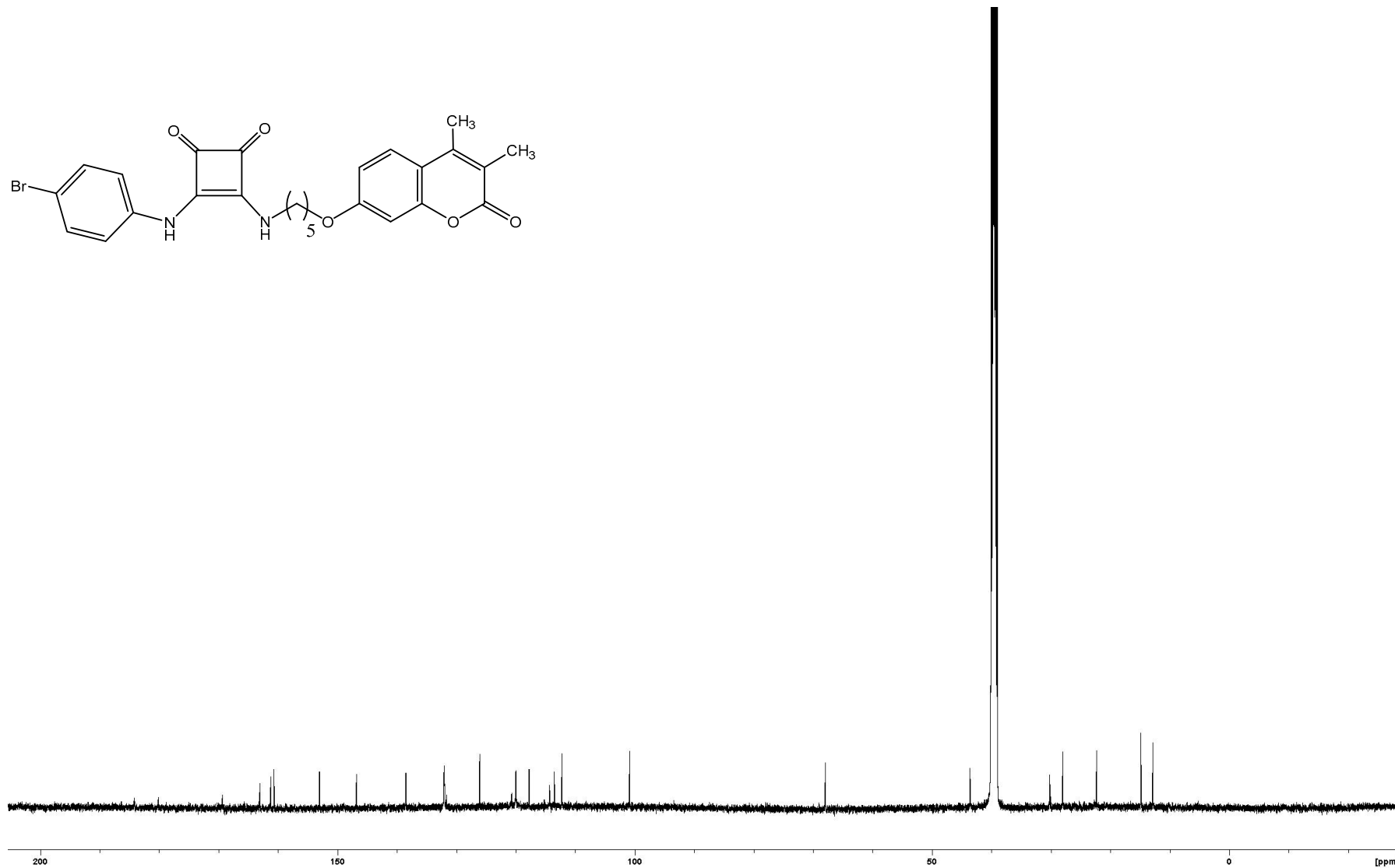
^1H -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16m**



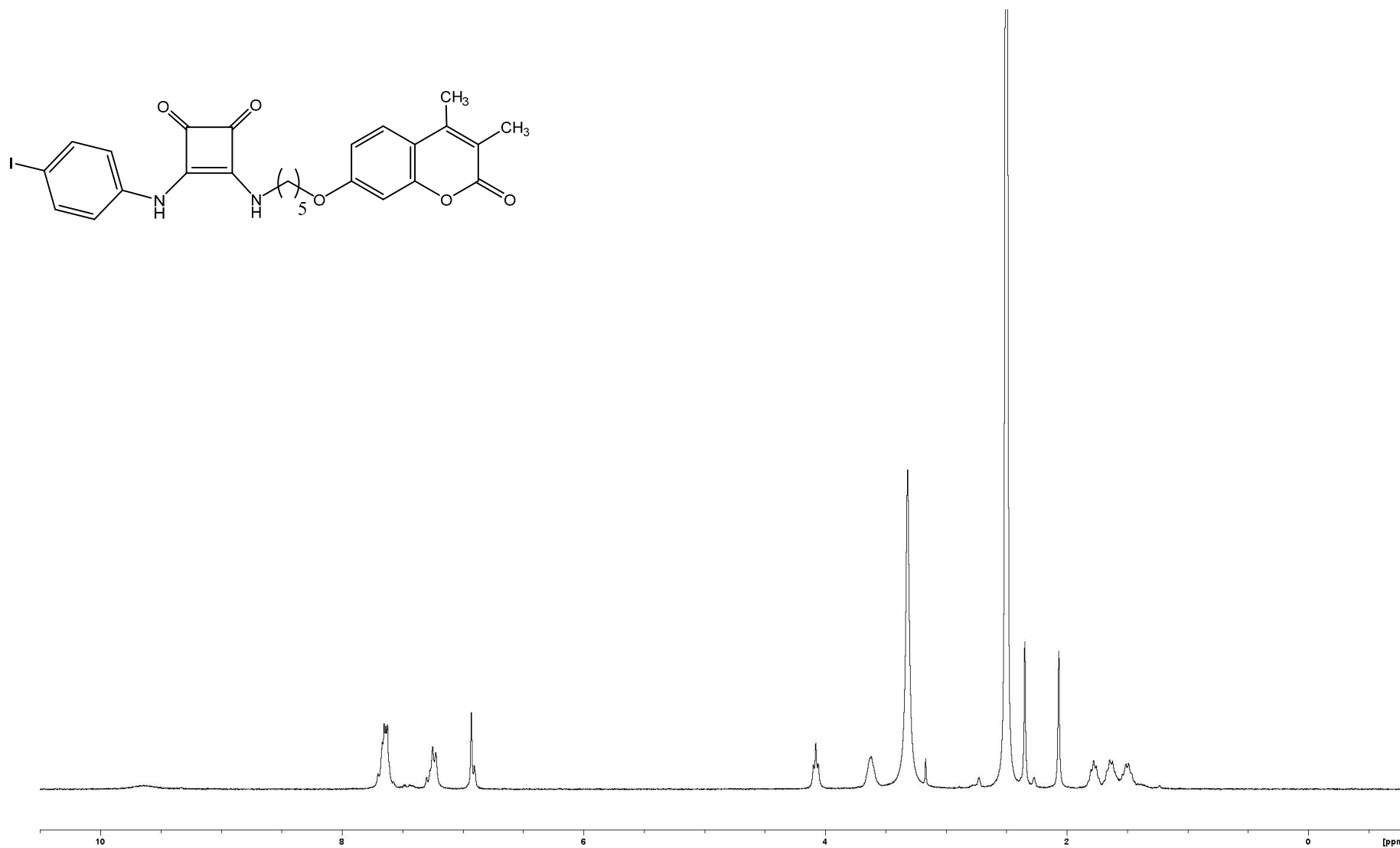
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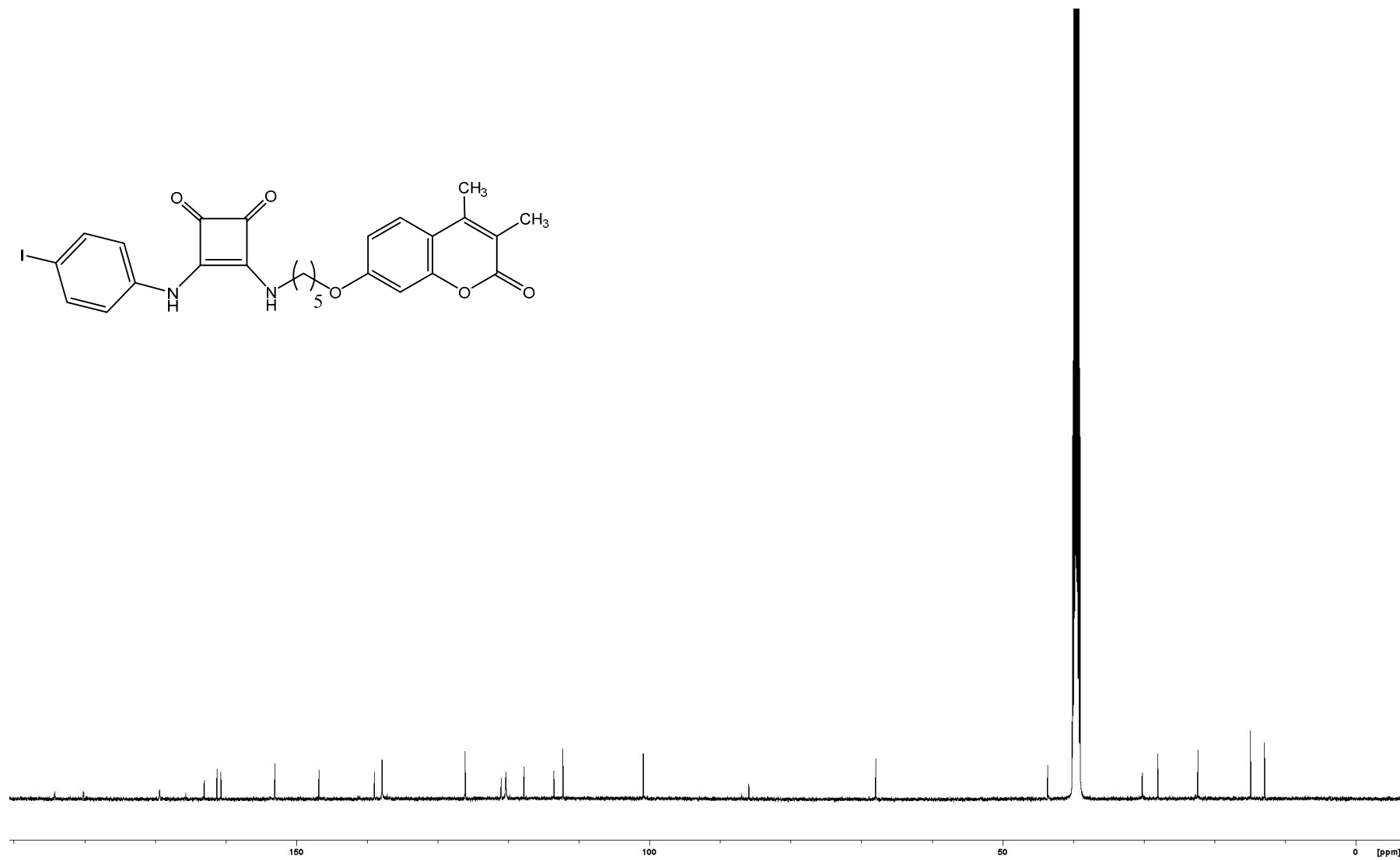
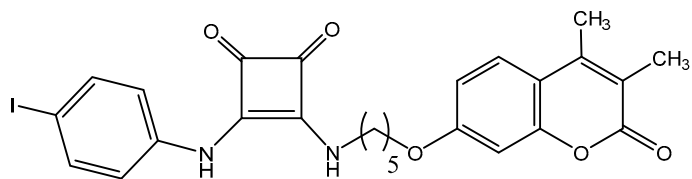
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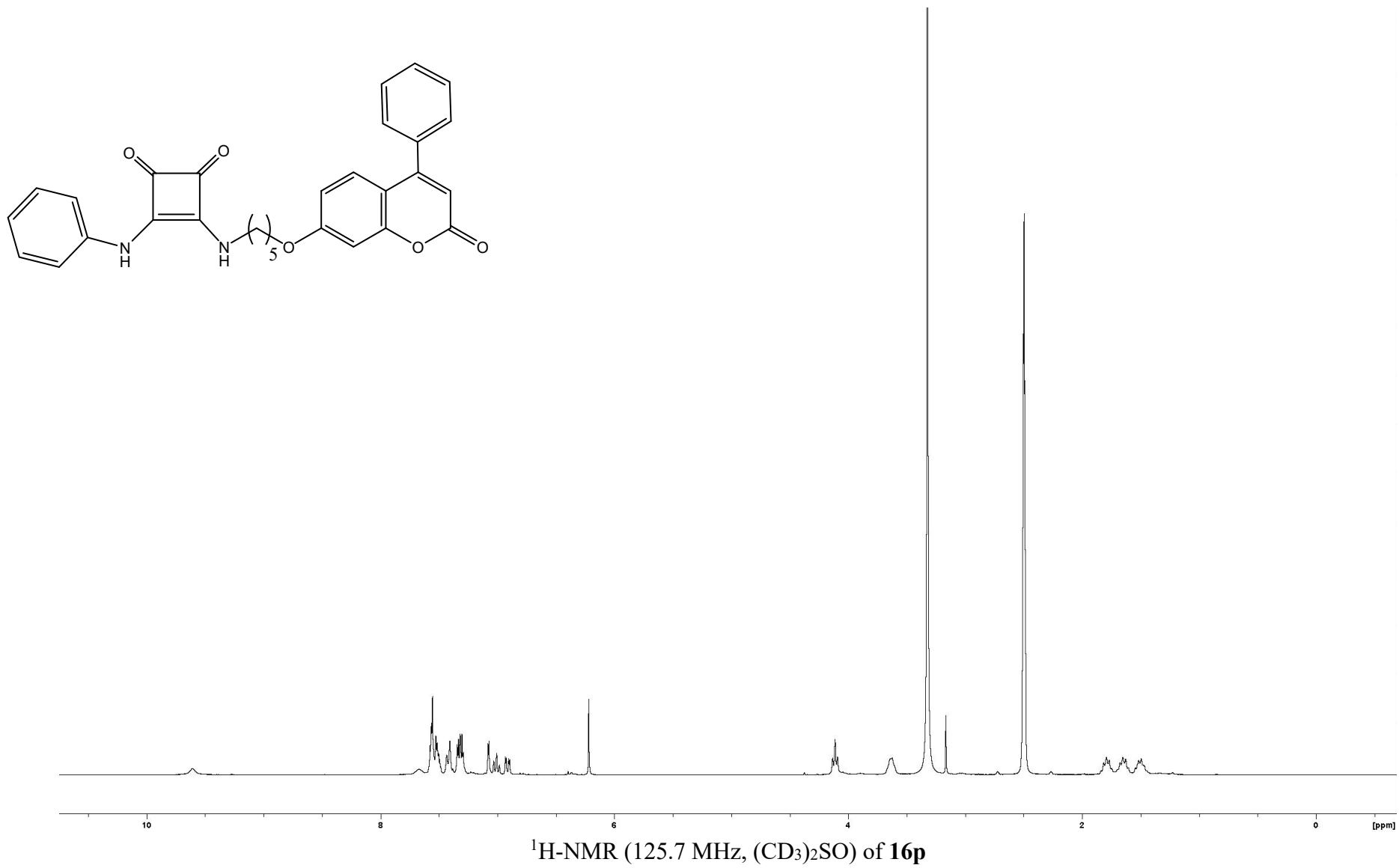
^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16n**

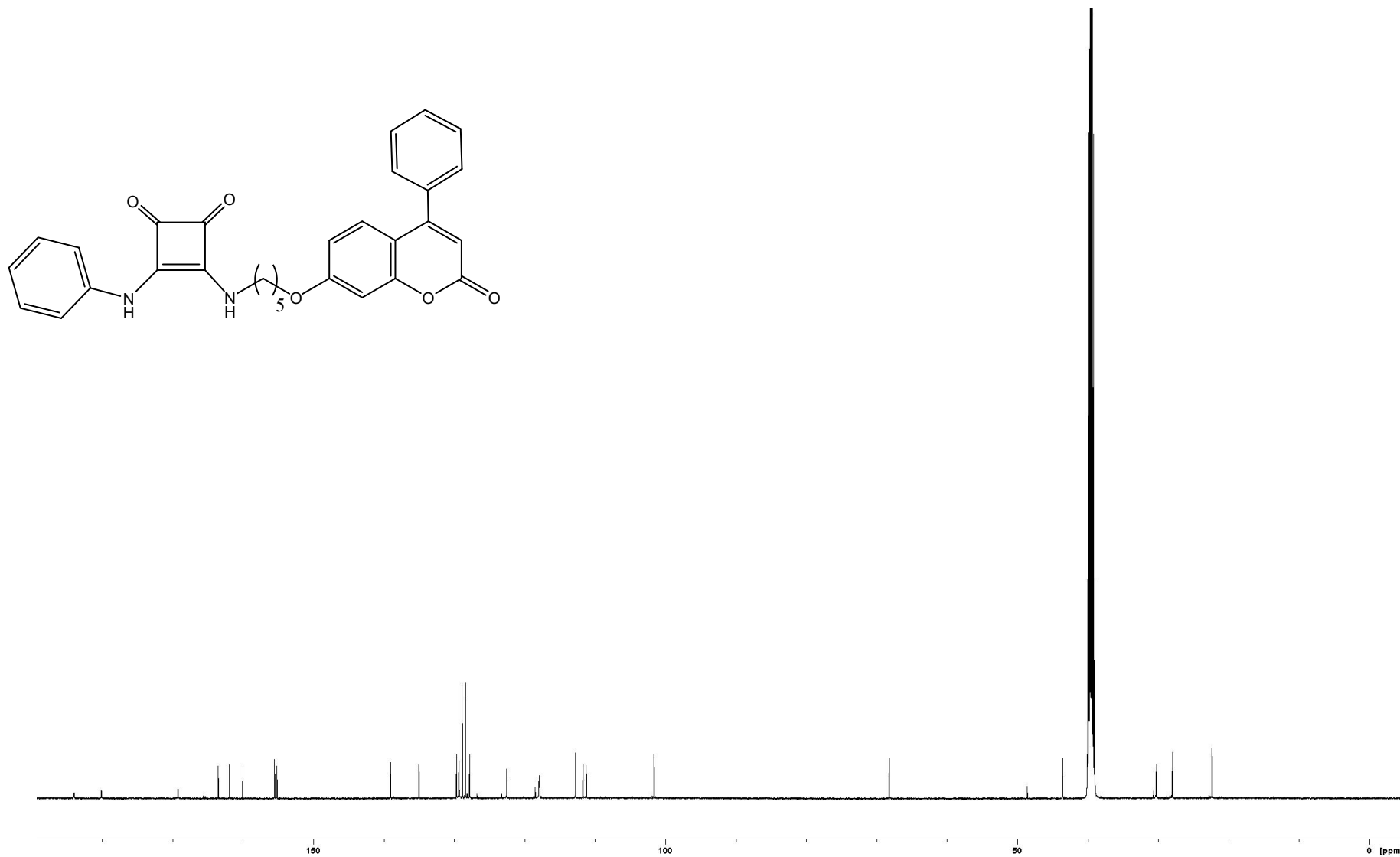


$^1\text{H-NMR}$ (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16o**



^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **160**





^{13}C -NMR (125.7 MHz, $(\text{CD}_3)_2\text{SO}$) of **16p**