

Supporting Information

Unveiling the potential of novel indol-3-yl-phenyl allylidene hydrazine carboximidamide derivatives as AChE/BACE 1 dual inhibitors: A combined *in-silico*, synthesis and *in-vitro* studies

Amit Sharma¹, Santosh Rudrawar^{2,3}, Ankita Sharma⁴, Sandip B. Bharate⁴, Hemant R. Jadhav^{1*}

¹Pharmaceutical Chemistry Research Laboratory, Department of Pharmacy, Birla Institute of Technology and Science Pilani, Pilani Campus, Vidya Vihar, Pilani – 333031 (RJ) India

²The Institute for Biomedicine and Glycomics, Griffith University, Gold Coast 4222, Australia

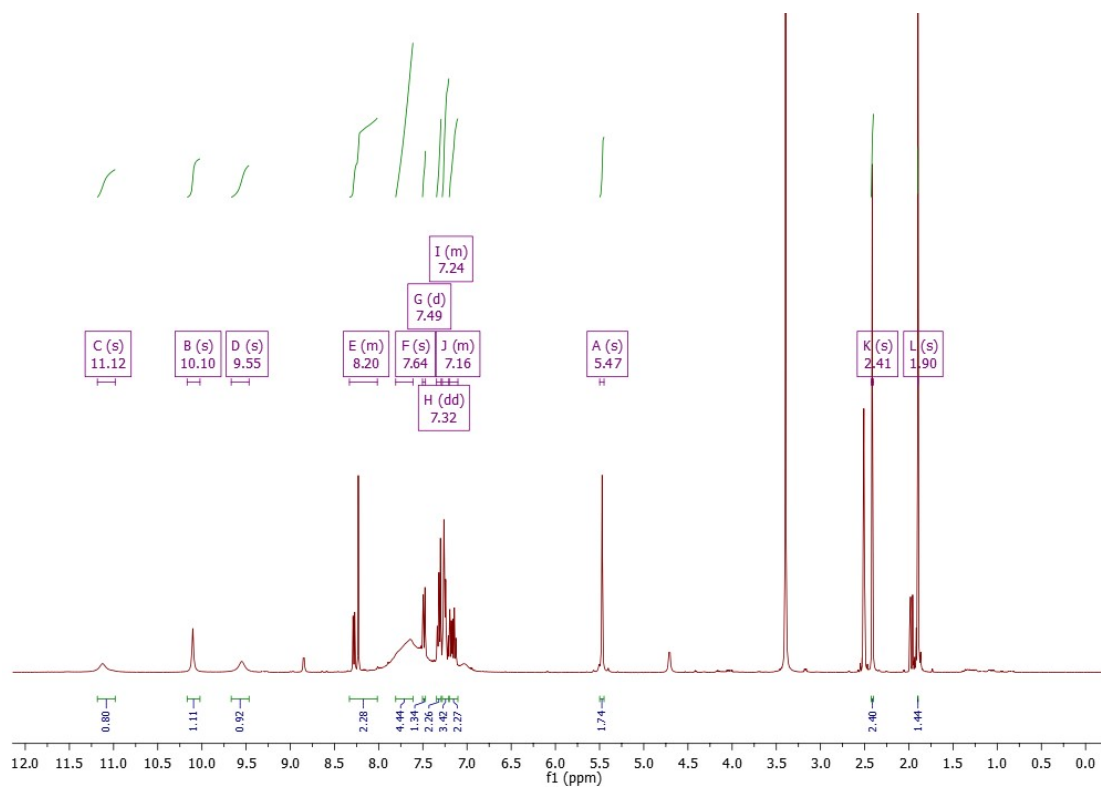
³School of Pharmacy and Medical Sciences, Griffith University, Gold Coast 4222, Australia

⁴Natural Products and Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu – 181110, India

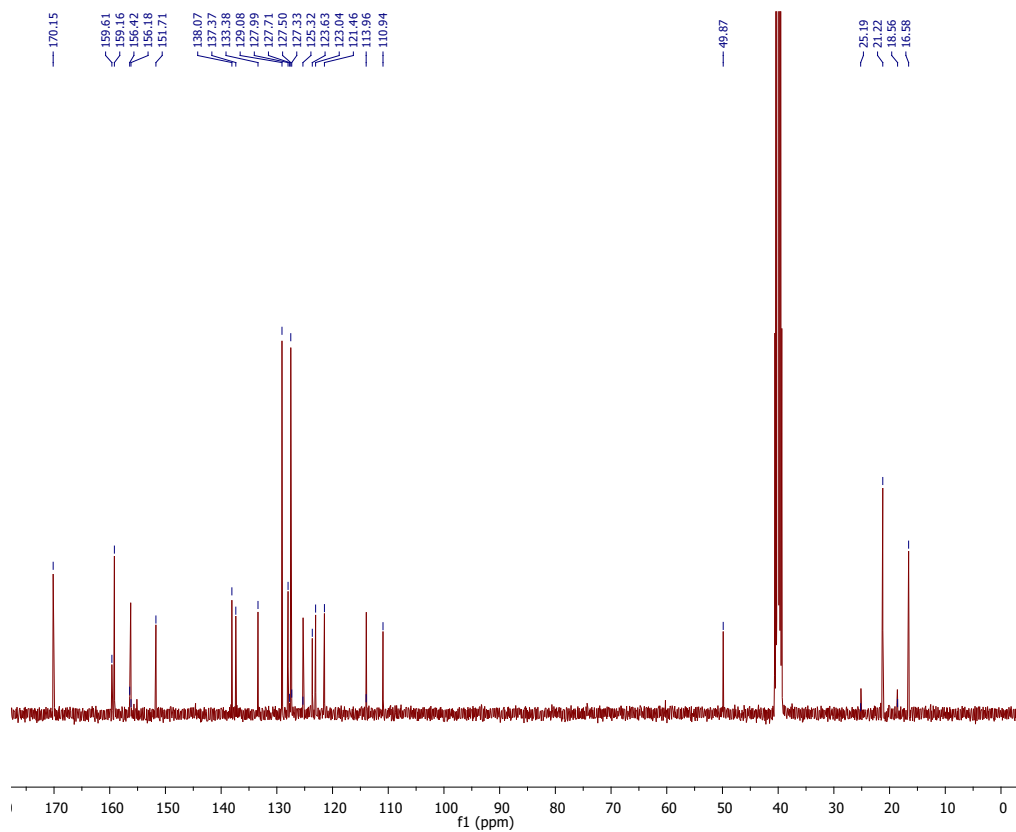
*Corresponding author: Tel: +91-1596-255 506; Fax: +91-1596-244183;

E-mail: hemantrj@pilani.bits-pilani.ac.in

^1H NMR spectrum of compound **1a** in DMSO-d_6 .

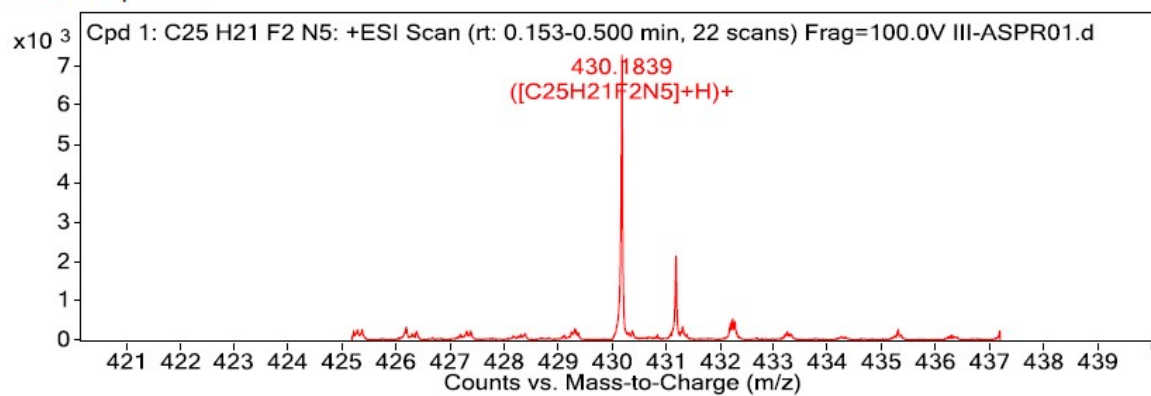


^{13}C NMR spectrum of compound **1a** in DMSO-d_6 .

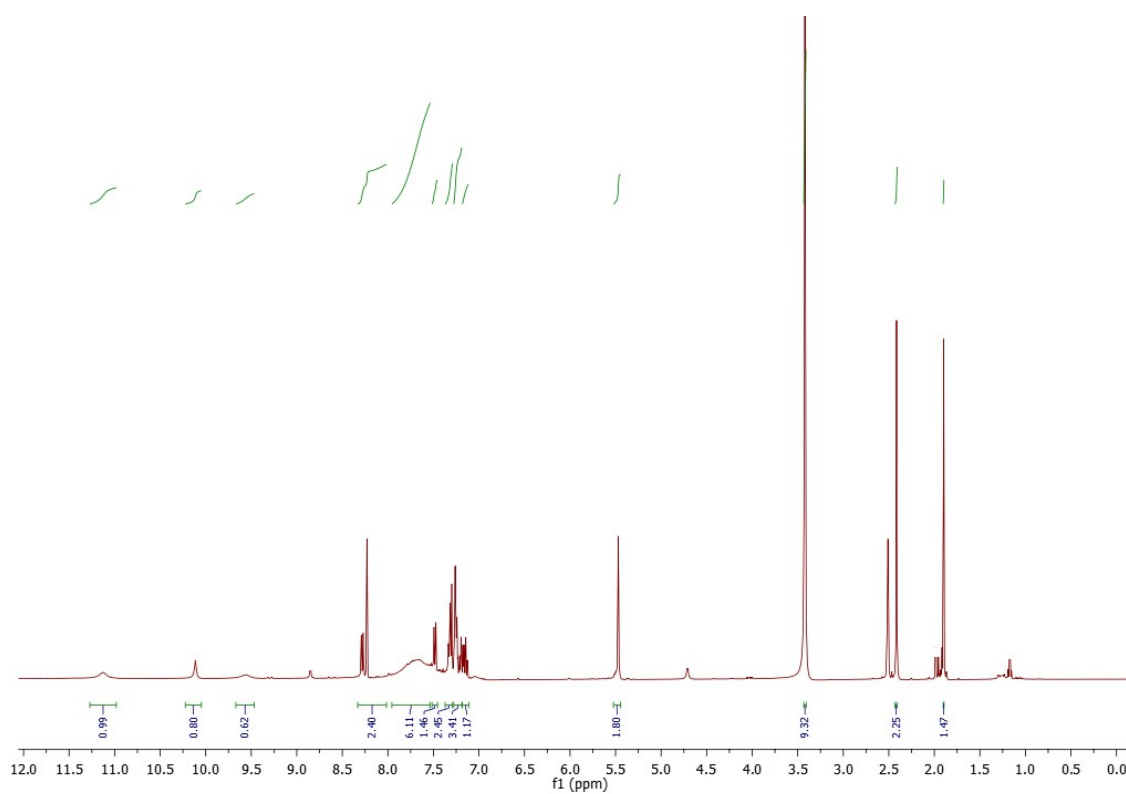


HRMS spectrum of compound **1a**.

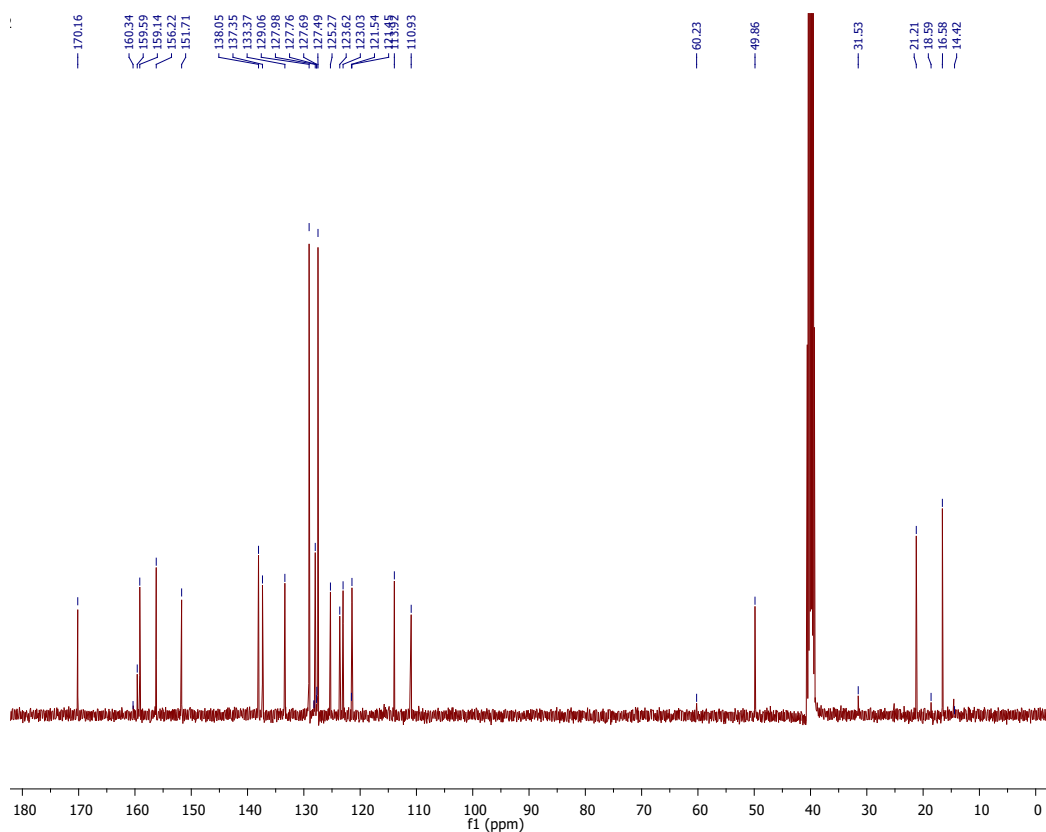
MS Zoomed Spectrum



¹H NMR spectrum of compound **1b** in DMSO-d₆.

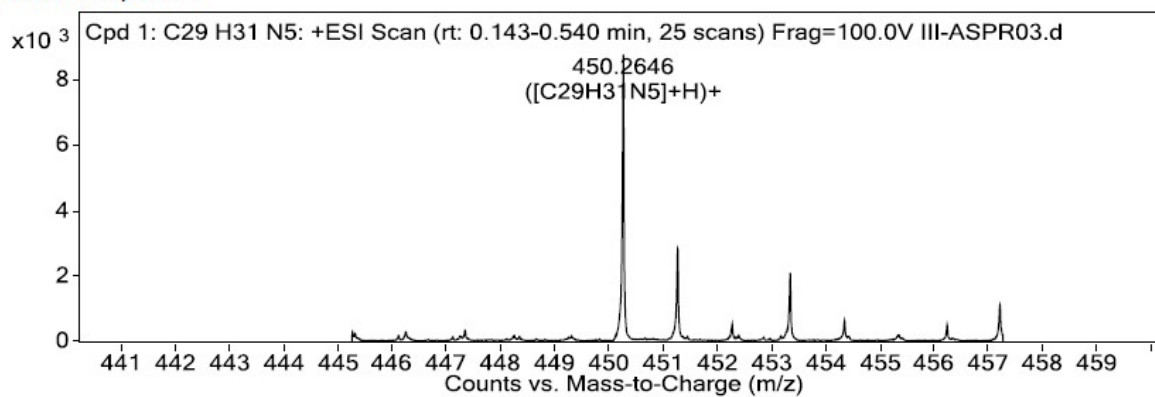


^{13}C NMR spectrum of compound **1b** in DMSO-d_6 .

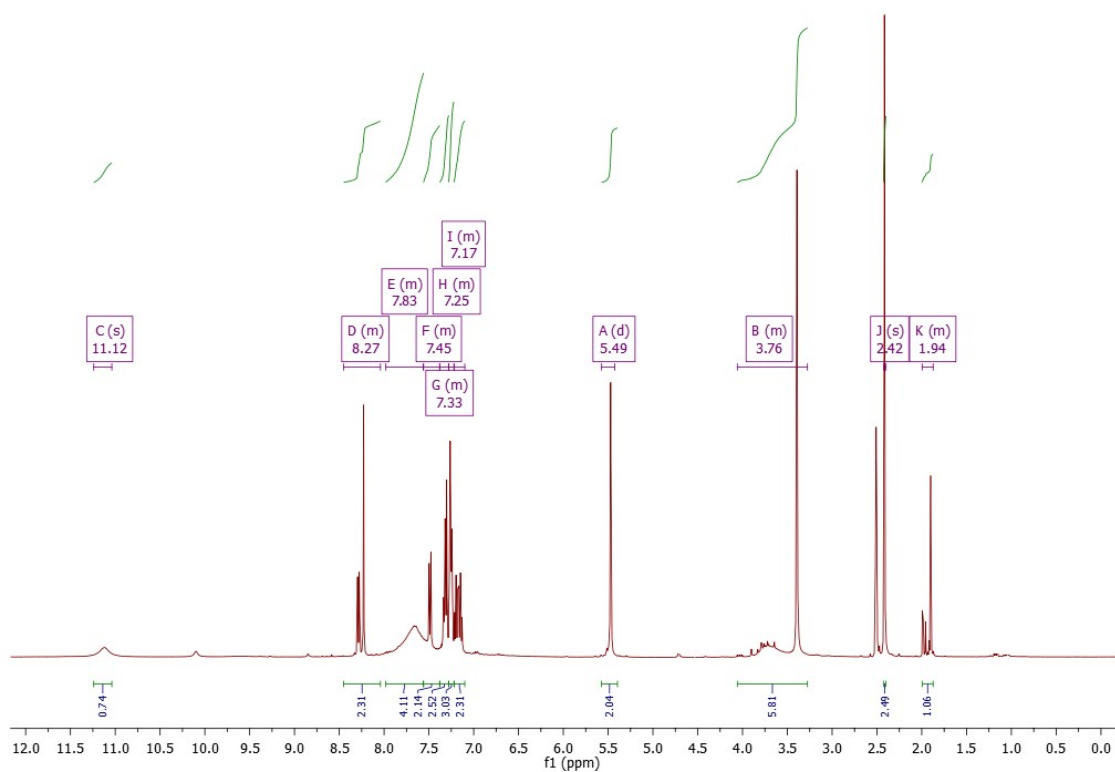


HRMS spectrum of compound **1b**.

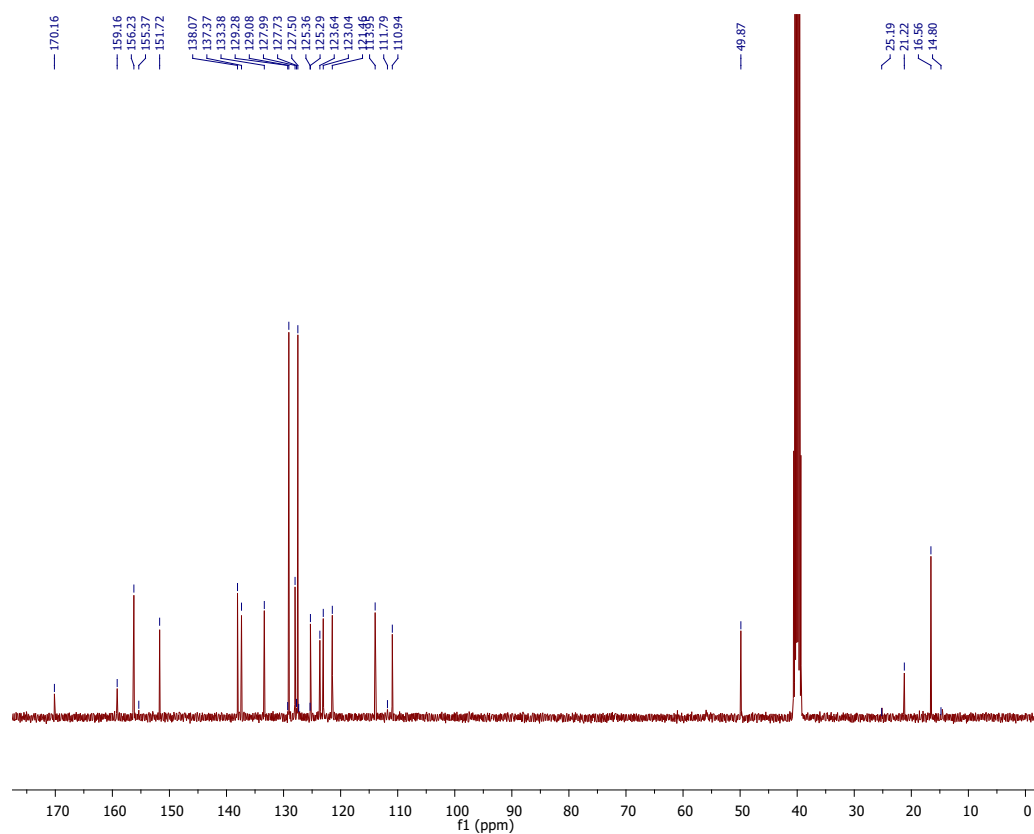
MS Zoomed Spectrum



^1H NMR spectrum of compound **1c** in DMSO-d_6 .

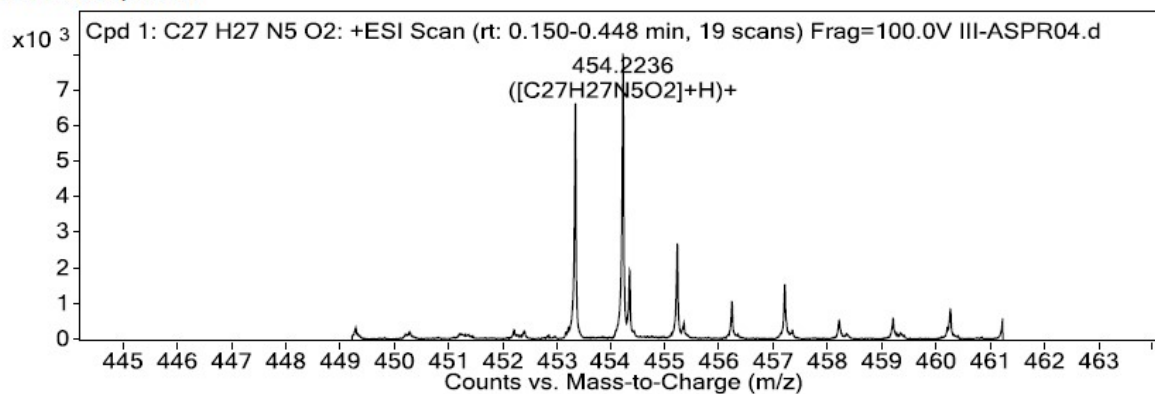


^{13}C NMR spectrum of compound **1c** in DMSO-d_6 .

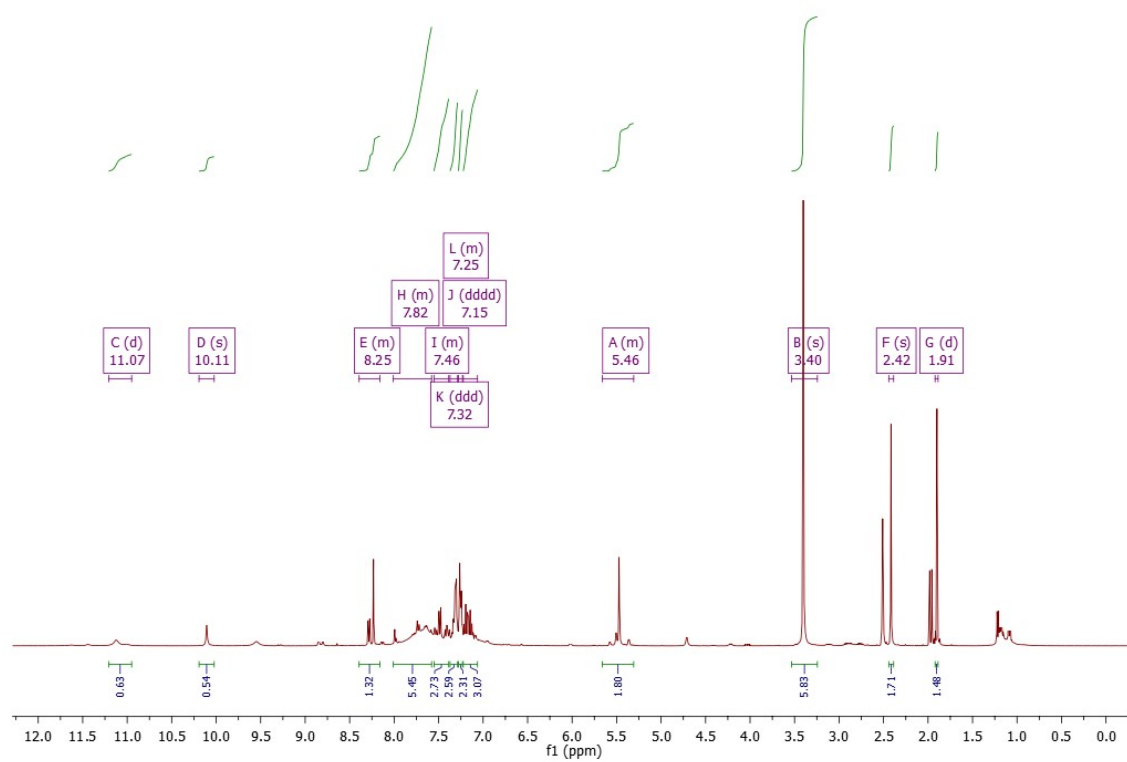


HRMS spectrum of compound **1c**.

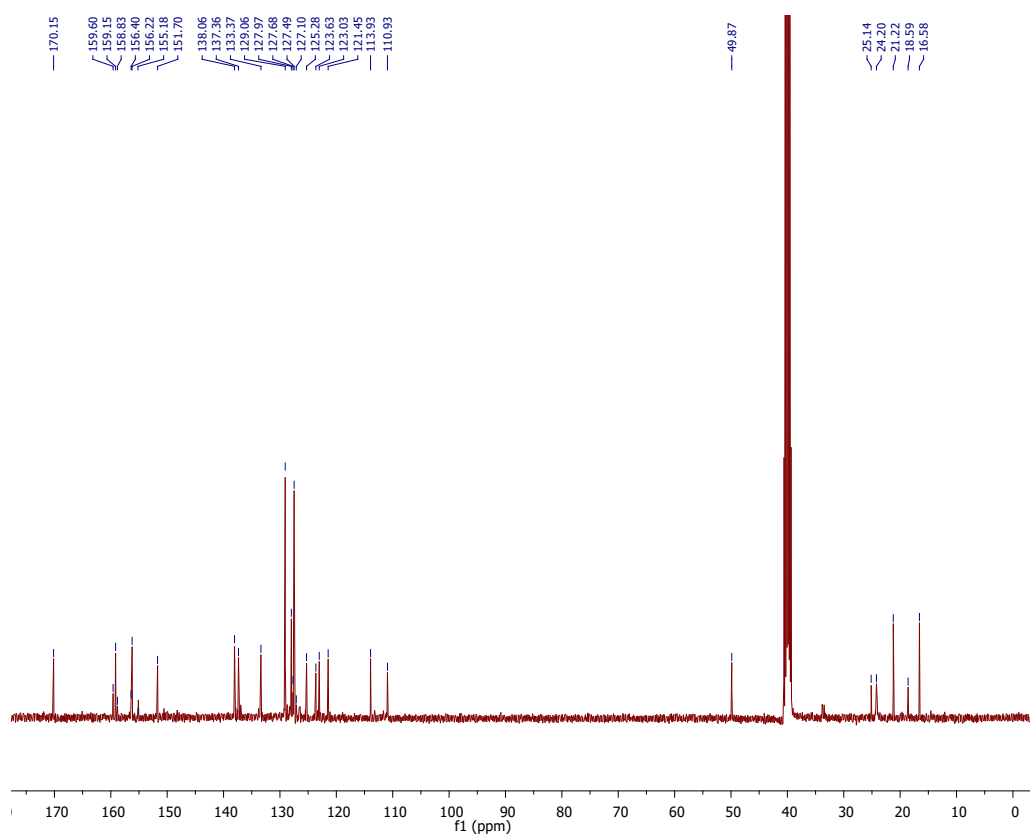
MS Zoomed Spectrum



¹H NMR spectrum of compound **1d** in DMSO-d₆.



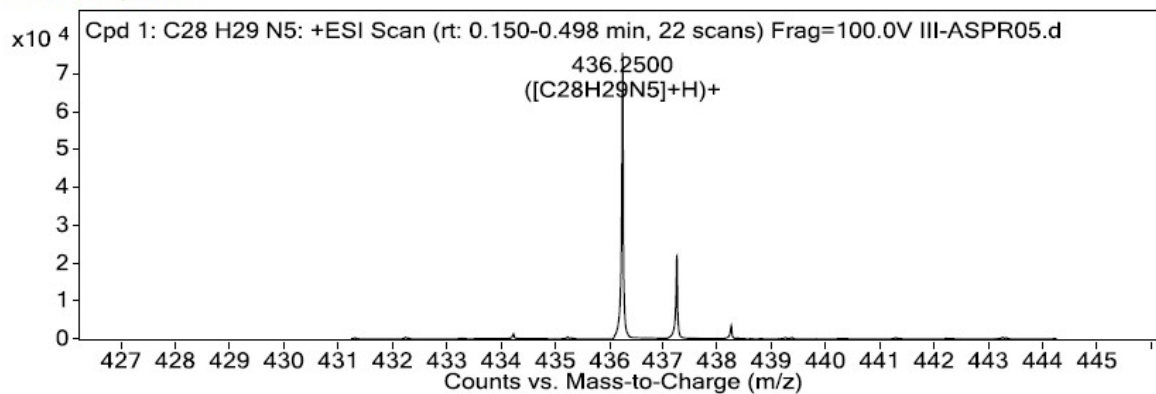
^{13}C



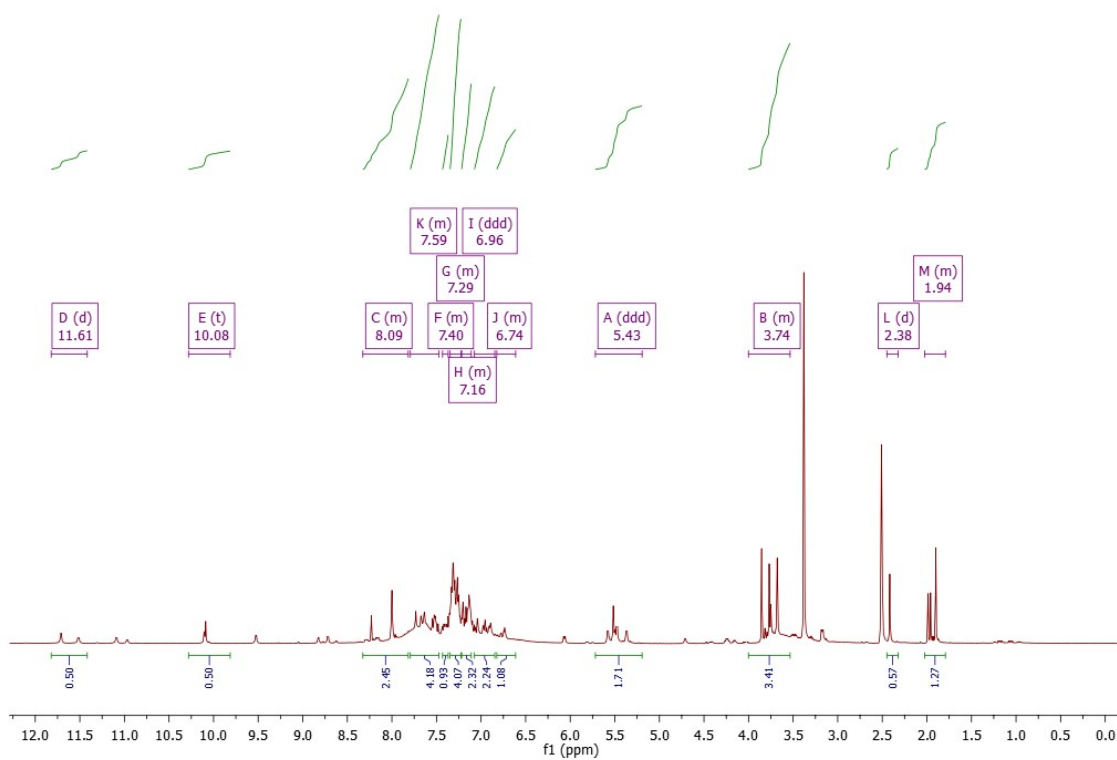
NMR spectrum of compound **1d** in DMSO-d_6 .

HRMS spectrum of compound **1d**.

MS Zoomed Spectrum



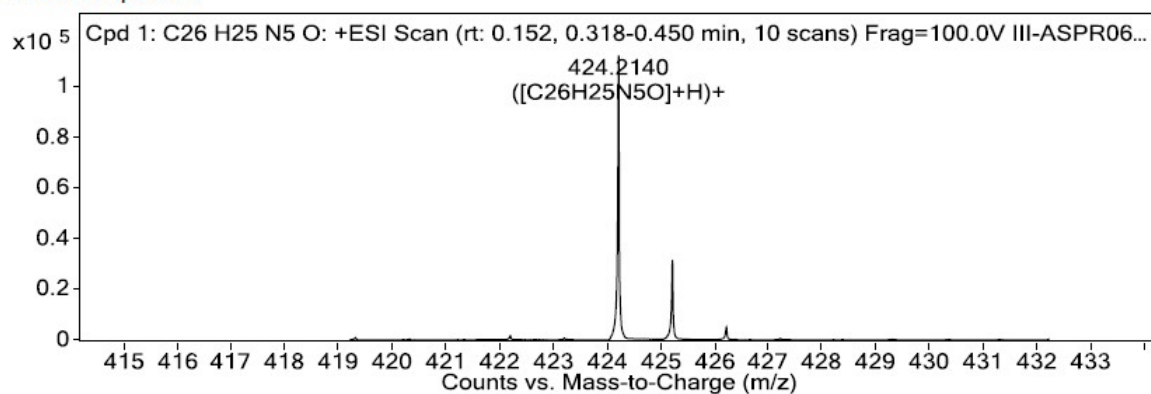
¹H NMR spectrum of compound **1e** in DMSO-d₆.



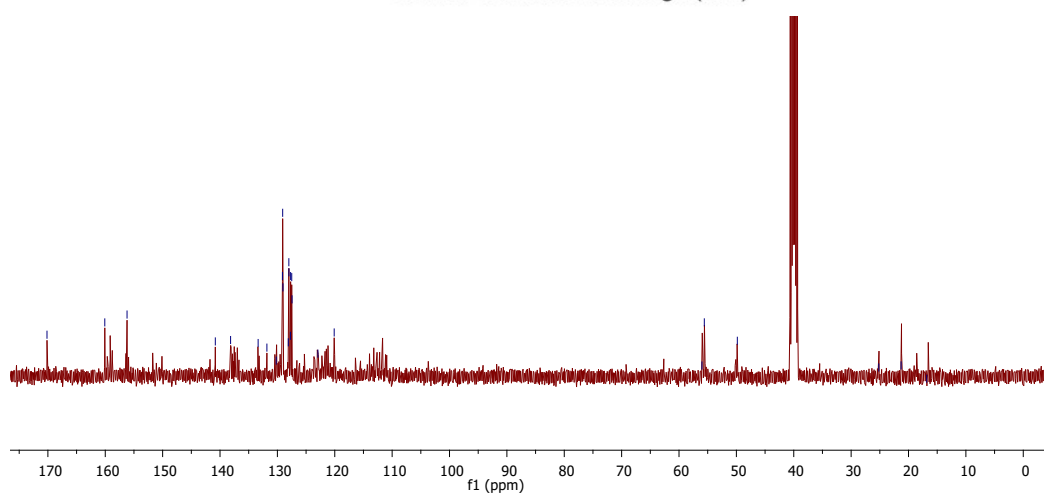
^{13}C NMR spectrum of compound **1e** in DMSO-d_6 .

HRMS spectrum of compound **1e**.

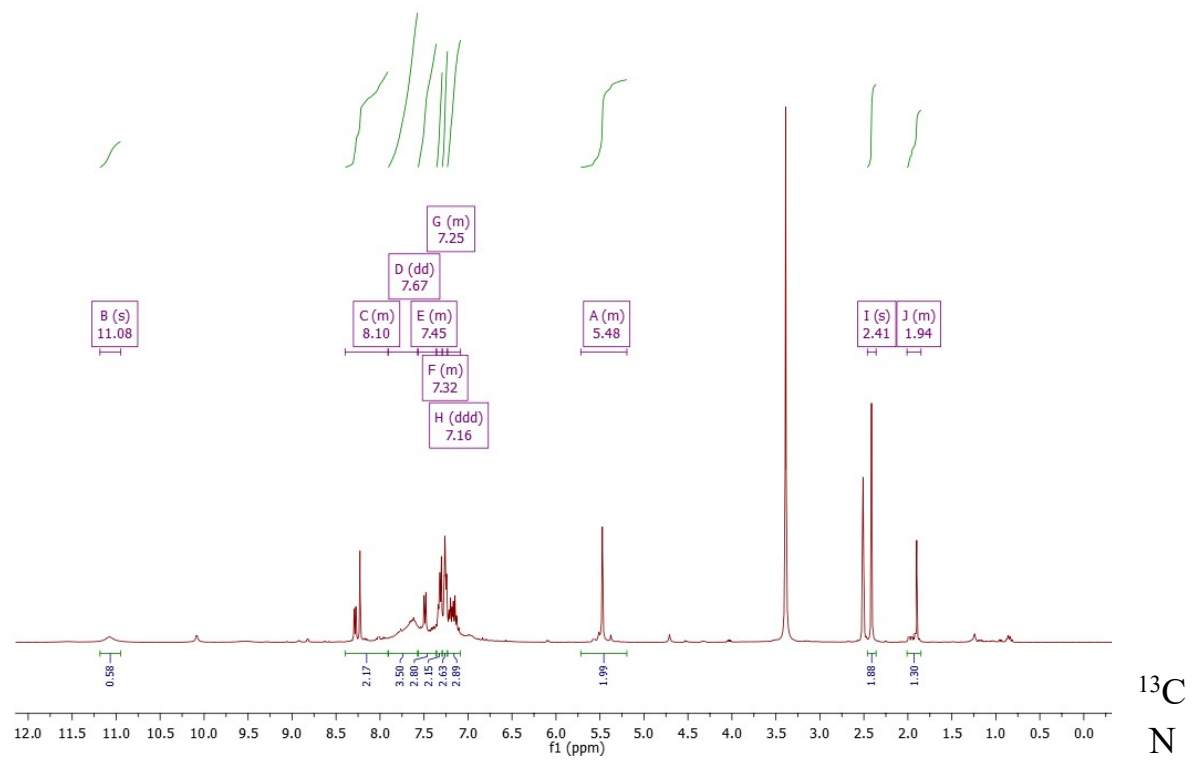
MS Zoomed Spectrum



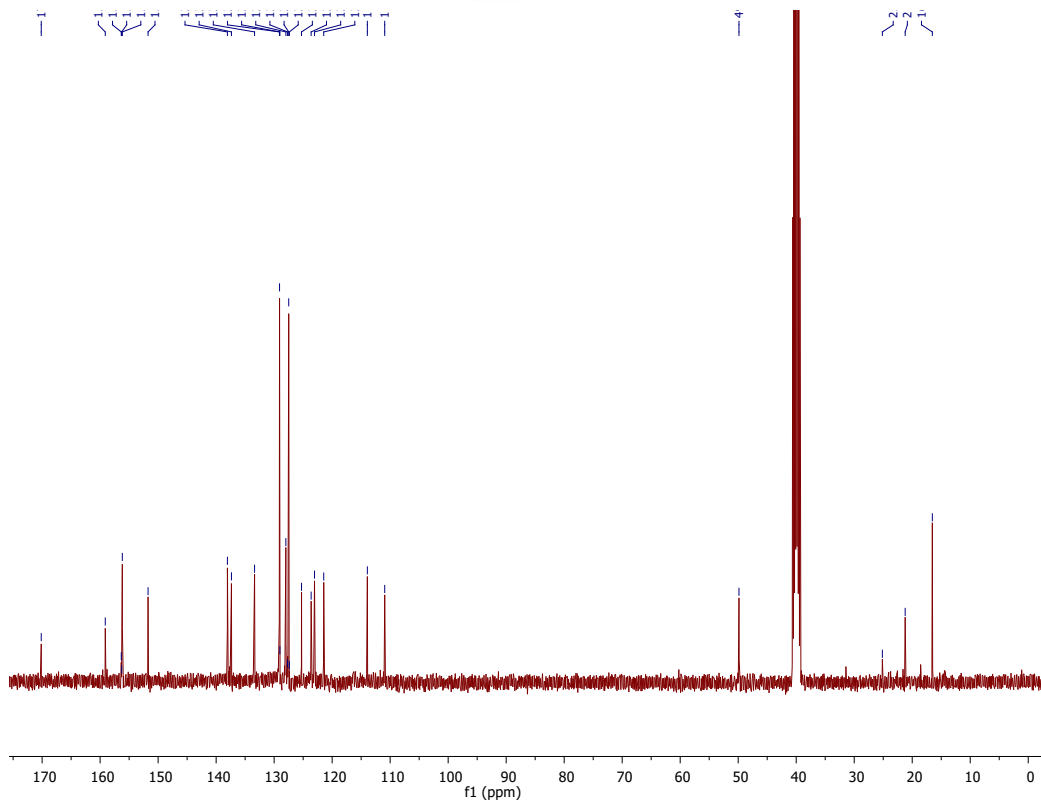
^1H



NMR spectrum of compound **1f** in DMSO-d_6 .



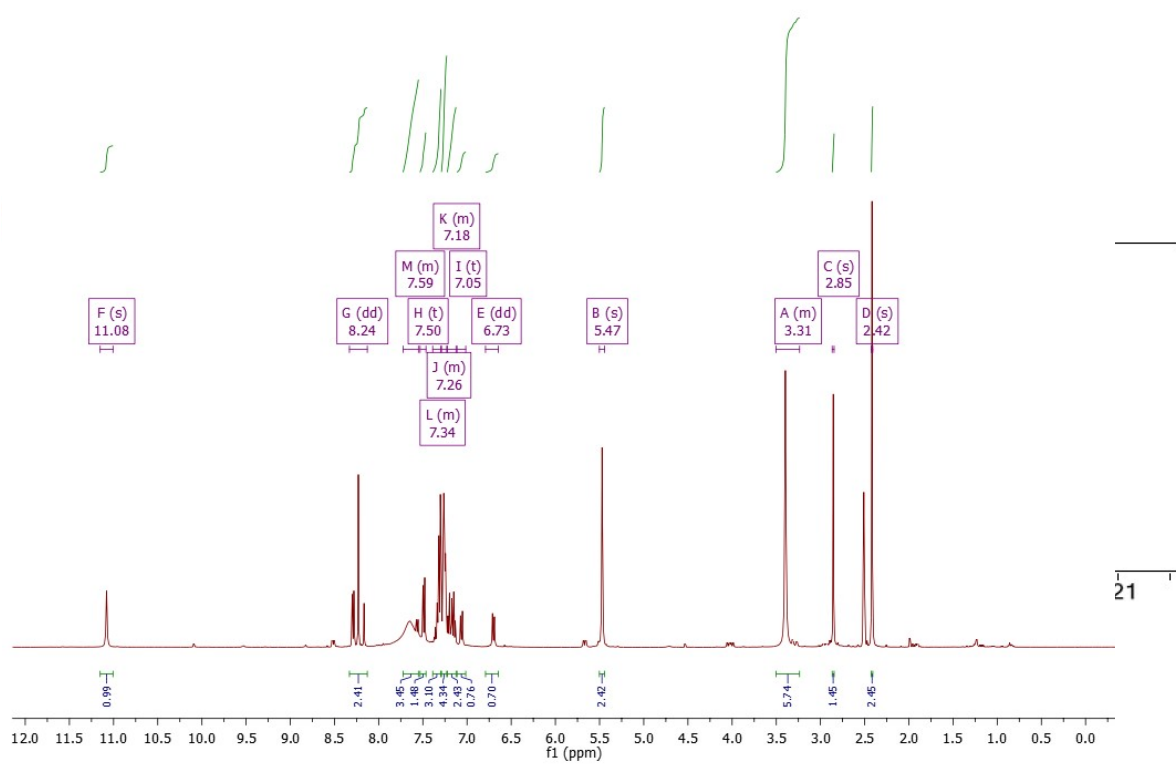
MR



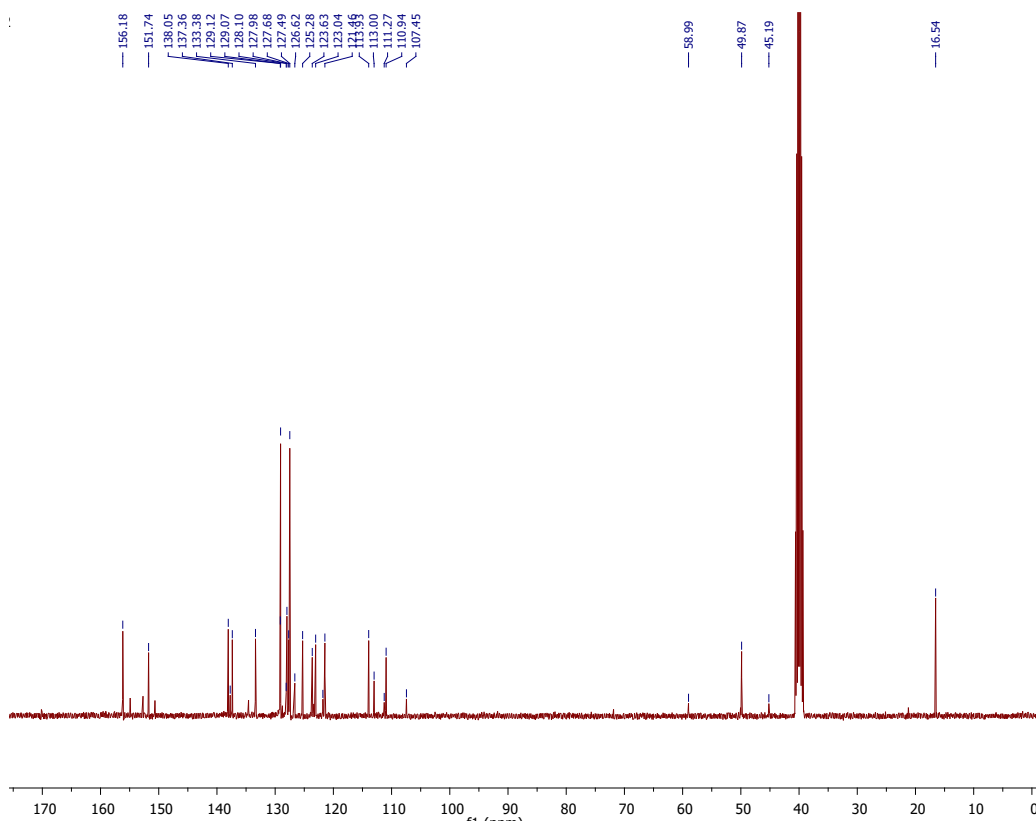
spectrum of compound **1f** in DMSO-d₆.

HRMS spectrum of compound **1f**.

^1H NMR spectrum of compound **1g** in DMSO-d_6 .

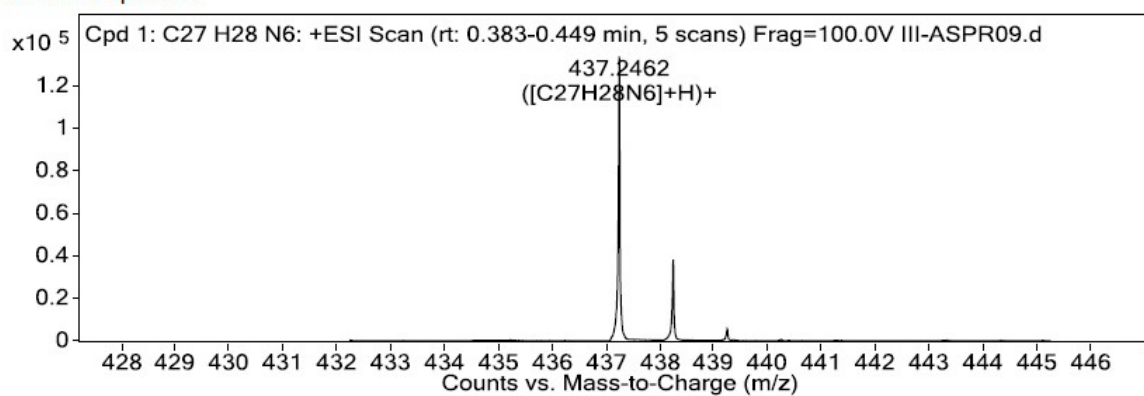


^{13}C NMR spectrum of compound **1g** in DMSO-d_6 .

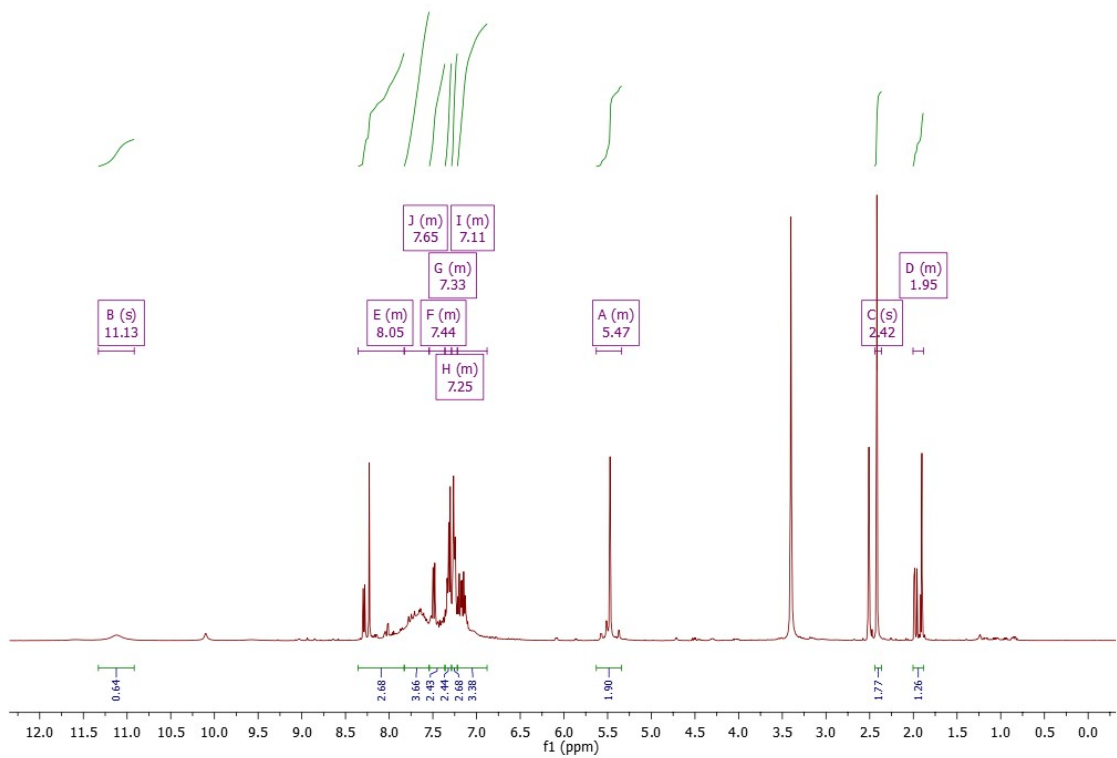


HRMS spectrum of compound **1g**.

MS Zoomed Spectrum

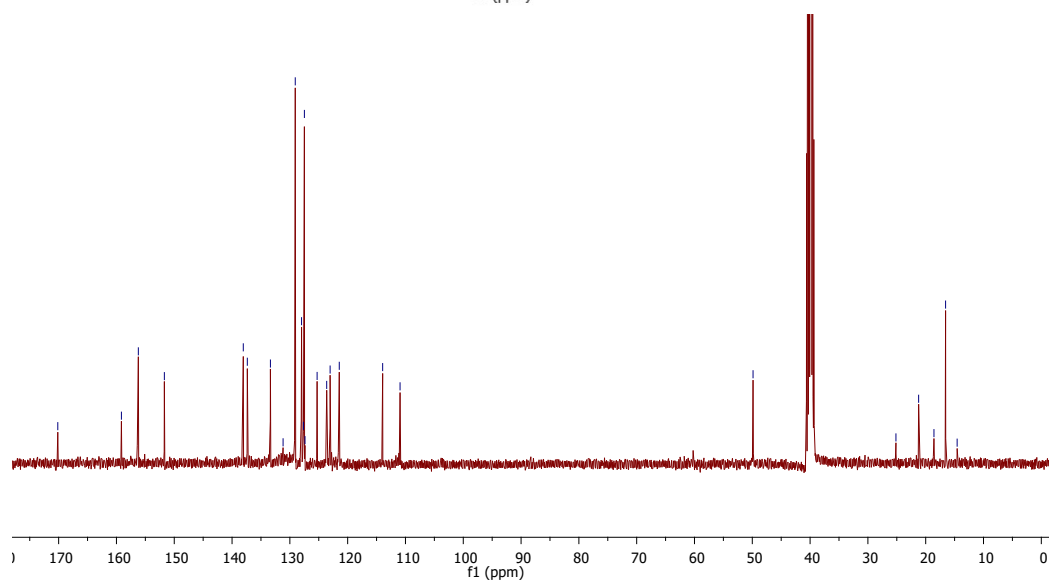


^1H NMR spectrum of compound **1h** in DMSO-d_6 .



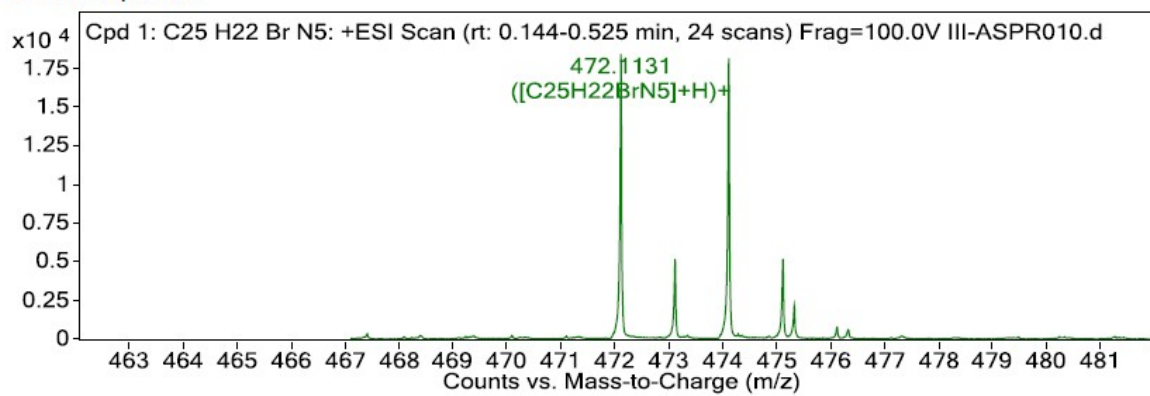
¹³C
N
M
R
spe
ctr
um

of



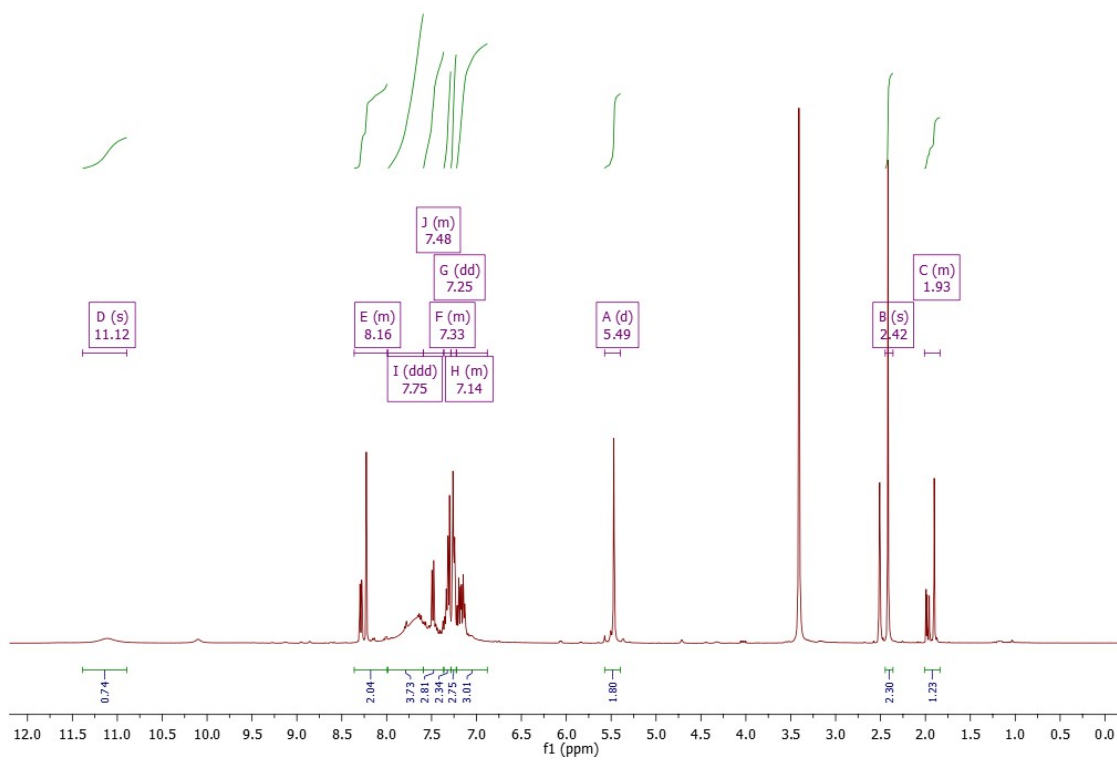
compound **1h** in DMSO-d₆.

MS Zoomed Spectrum

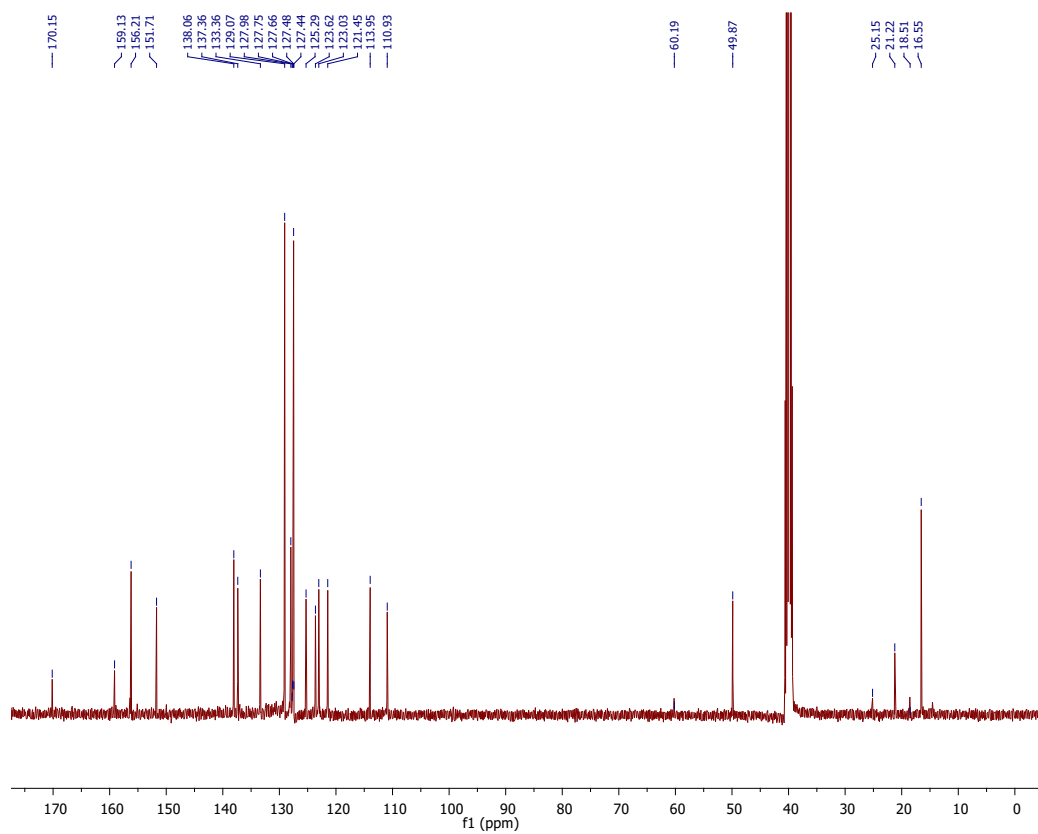


HRMS spectrum of compound **1h**.

¹H NMR spectrum of compound **1i** in DMSO-d₆.

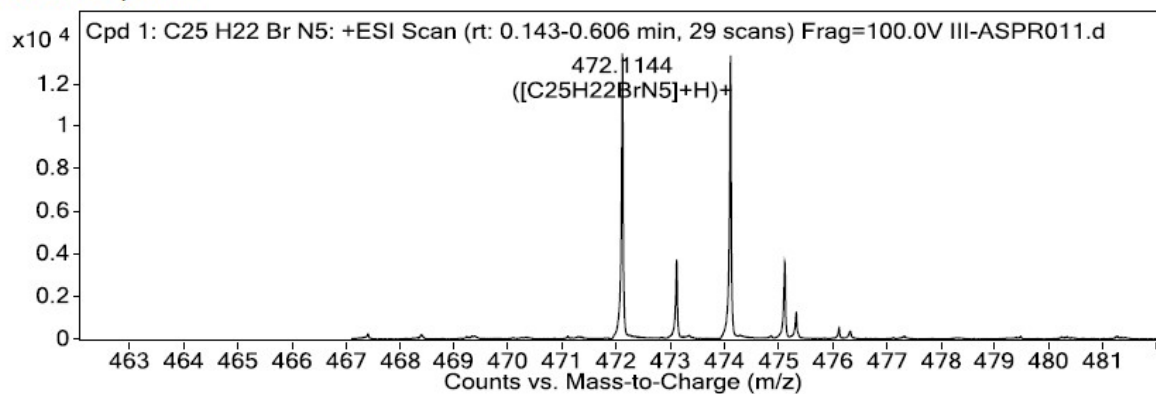


¹³C NMR spectrum of compound **1i** in DMSO-d₆.

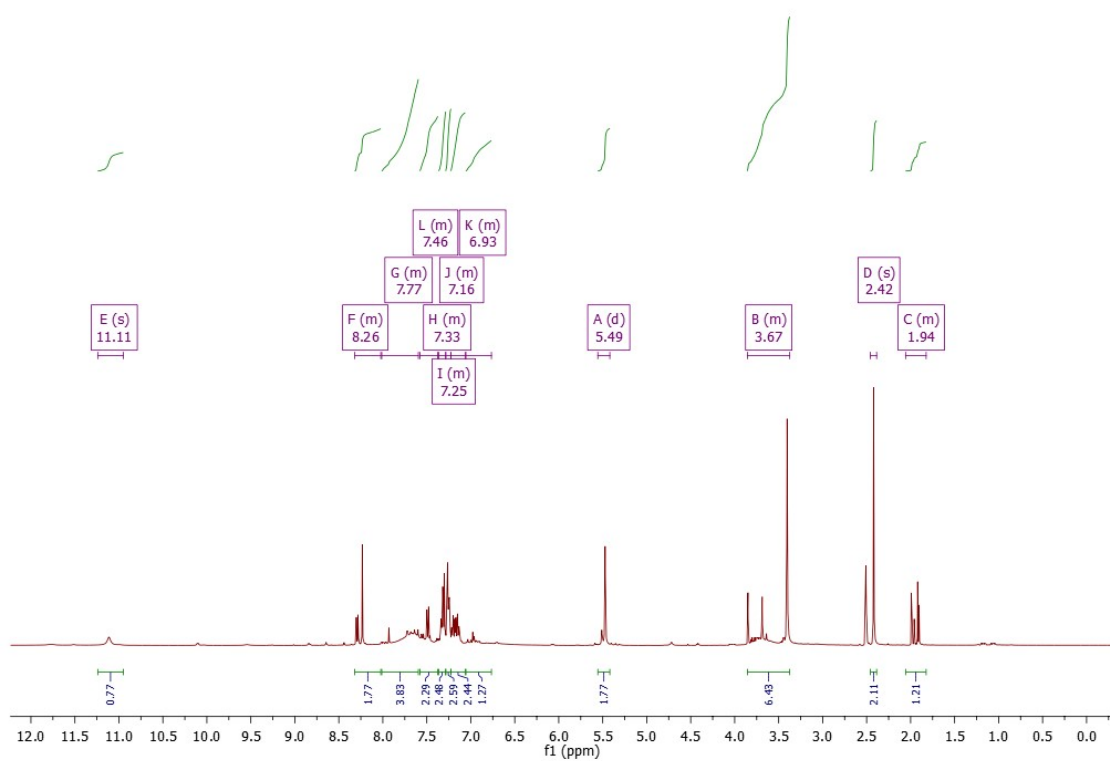


HRMS spectrum of compound **1i**.

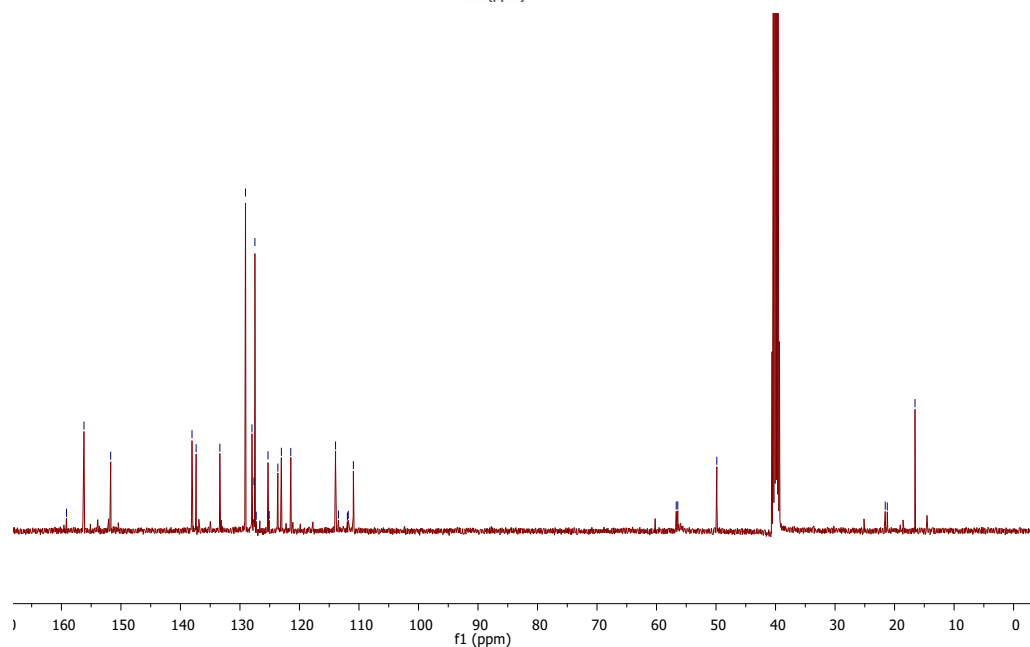
MS Zoomed Spectrum



¹H NMR spectrum of compound **1j** in DMSO-d₆.

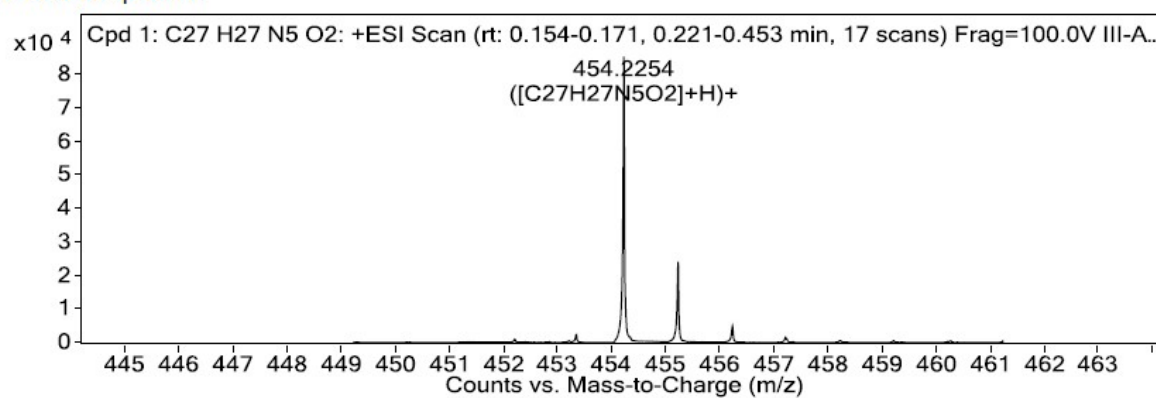


¹³C
NMR
spe
ctru
m

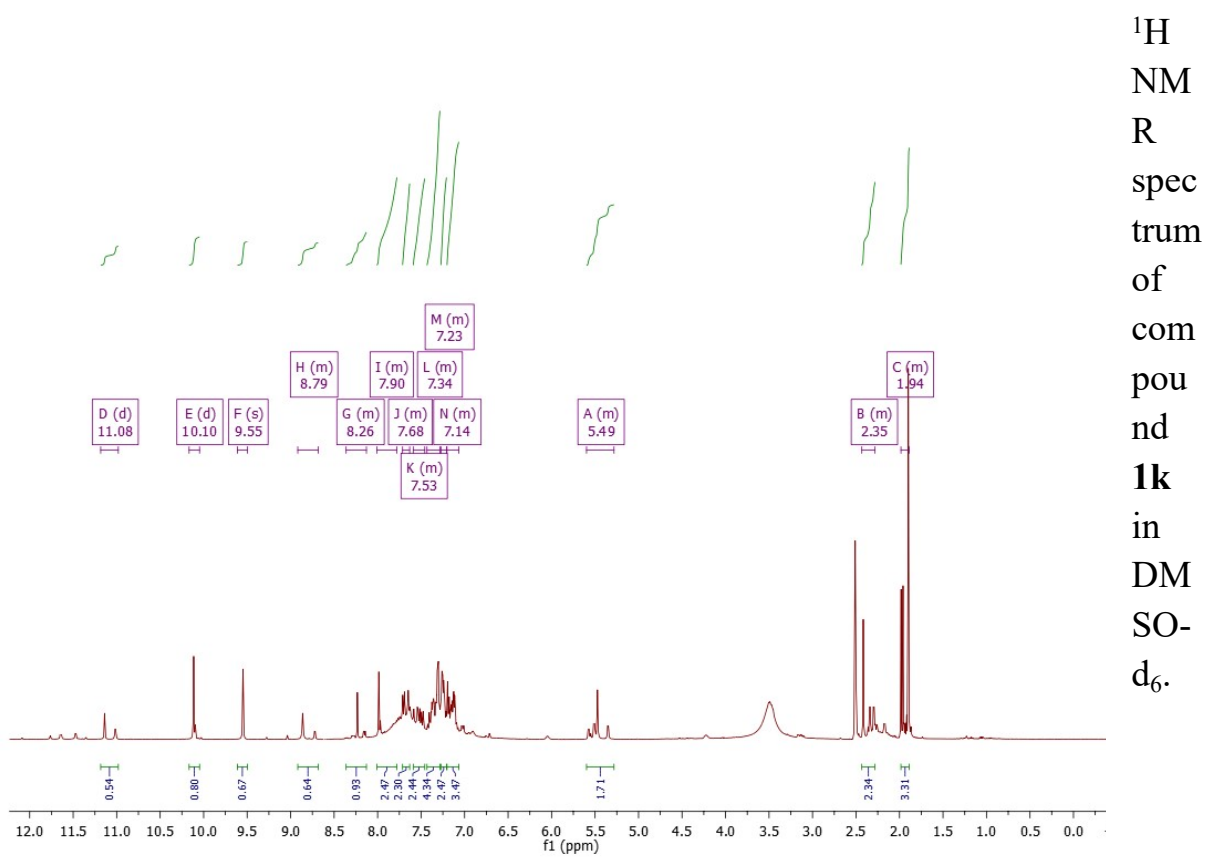


of compound **1j** in DMSO-d₆.

MS Zoomed Spectrum



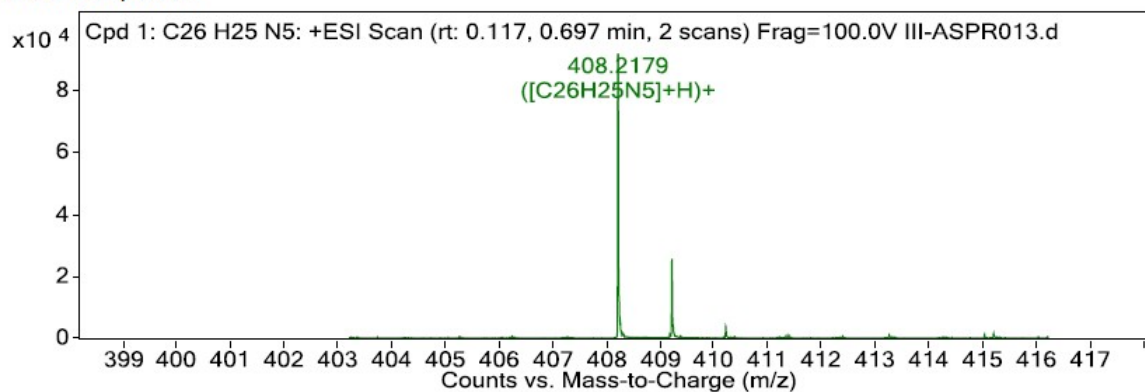
HRMS spectrum of compound **1j**.



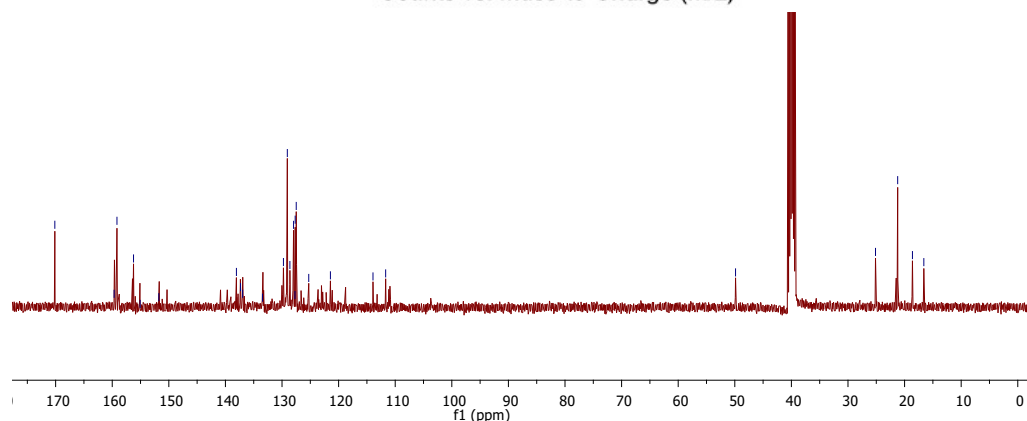
^{13}C NMR spectrum of compound **1k** in DMSO-d_6 .

HRMS spectrum of compound **1k**.

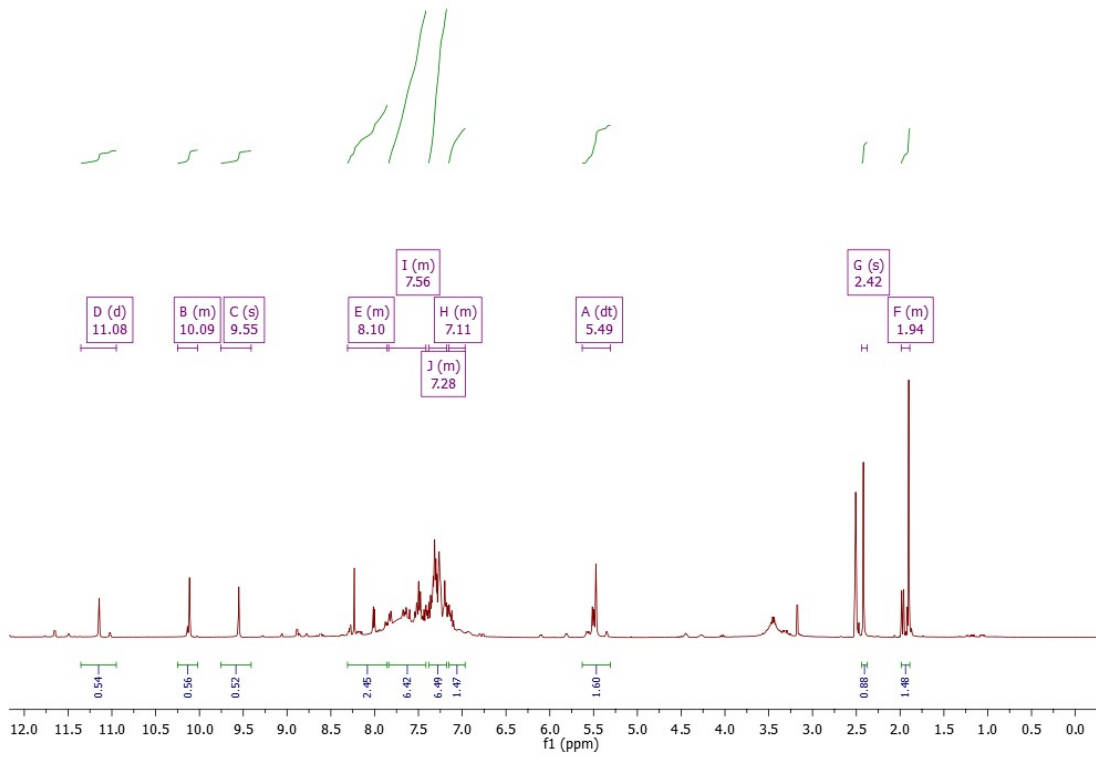
MS Zoomed Spectrum



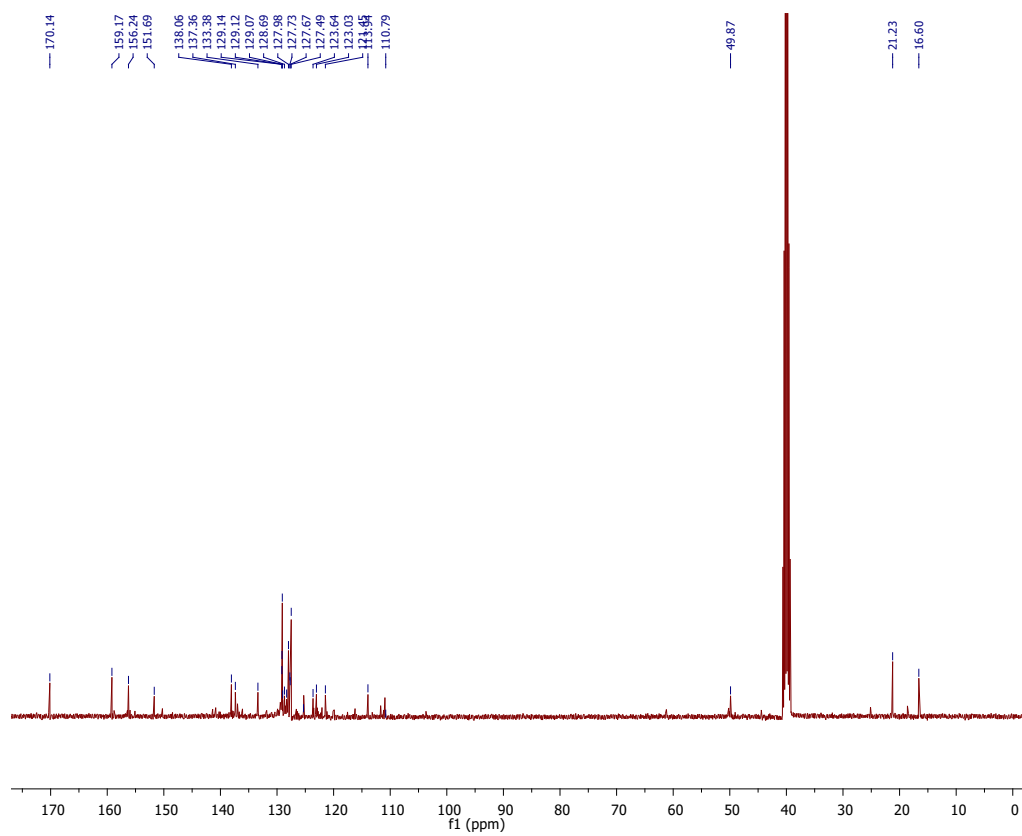
^1H



NMR spectrum of compound **1l** in DMSO-d_6 .

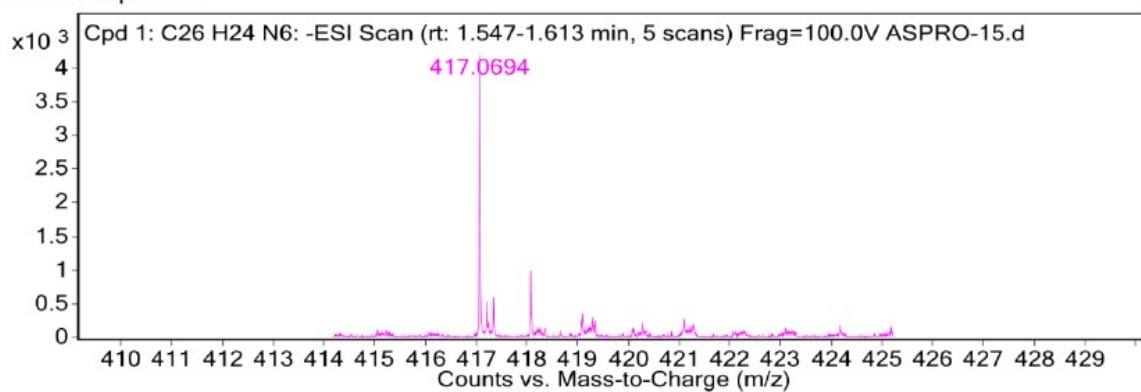


^{13}C



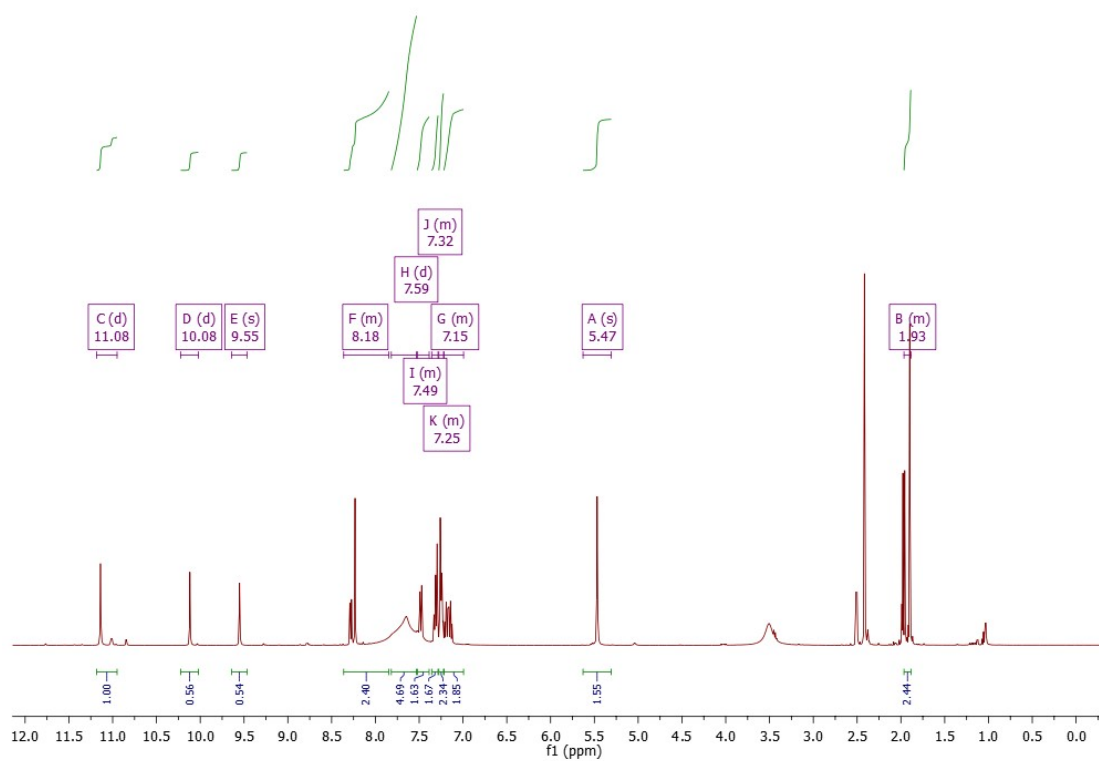
NMR spectrum of compound **11** in DMSO-d_6 .

MS Zoomed Spectrum



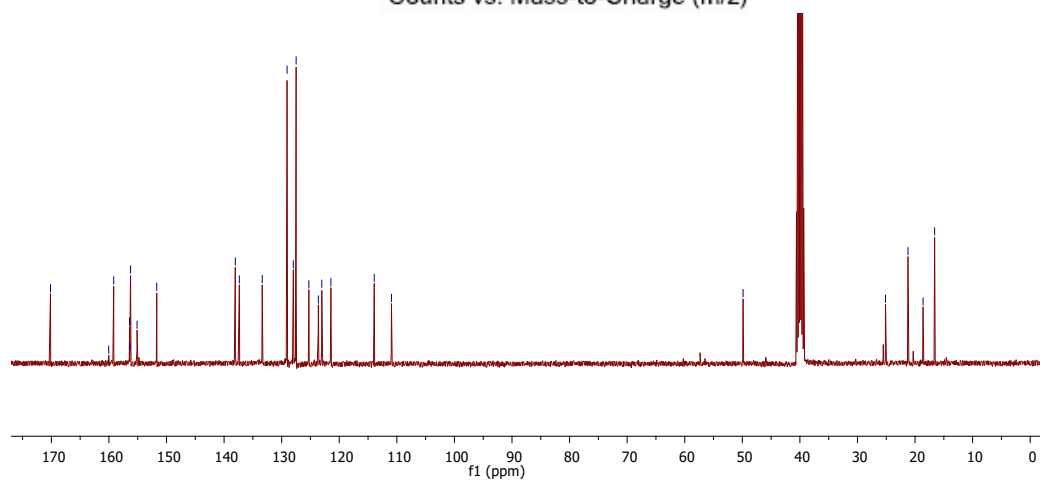
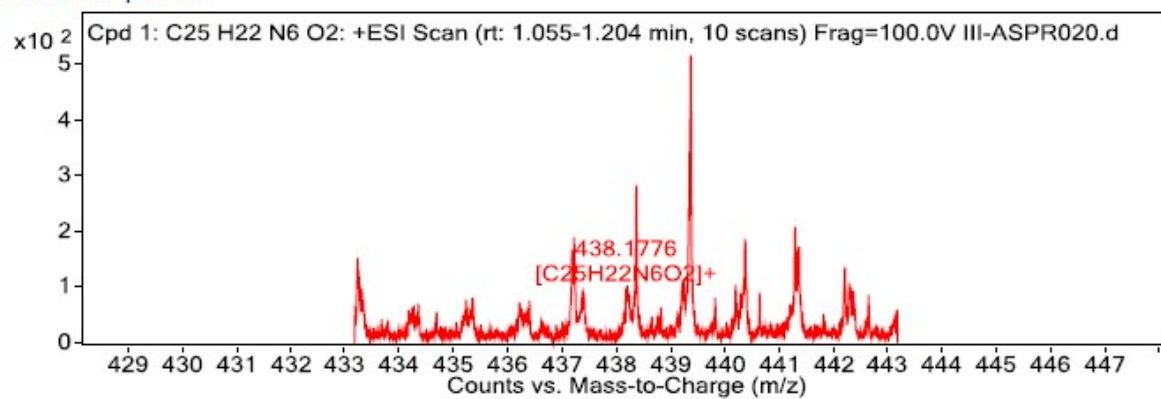
HRMS spectrum of compound **1l**.

¹H NMR spectrum of compound **1n** in DMSO-d₆.



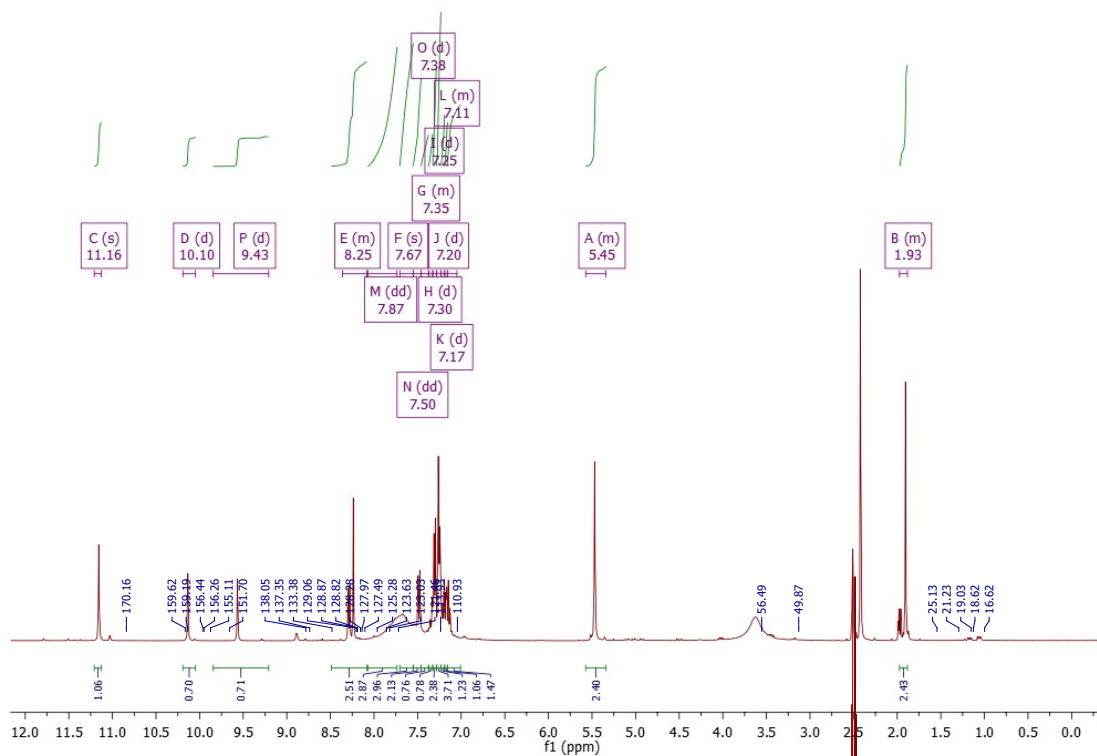
^{13}C NMR spectrum of compound **1n** in DMSO-d_6 .

MS Zoomed Spectrum



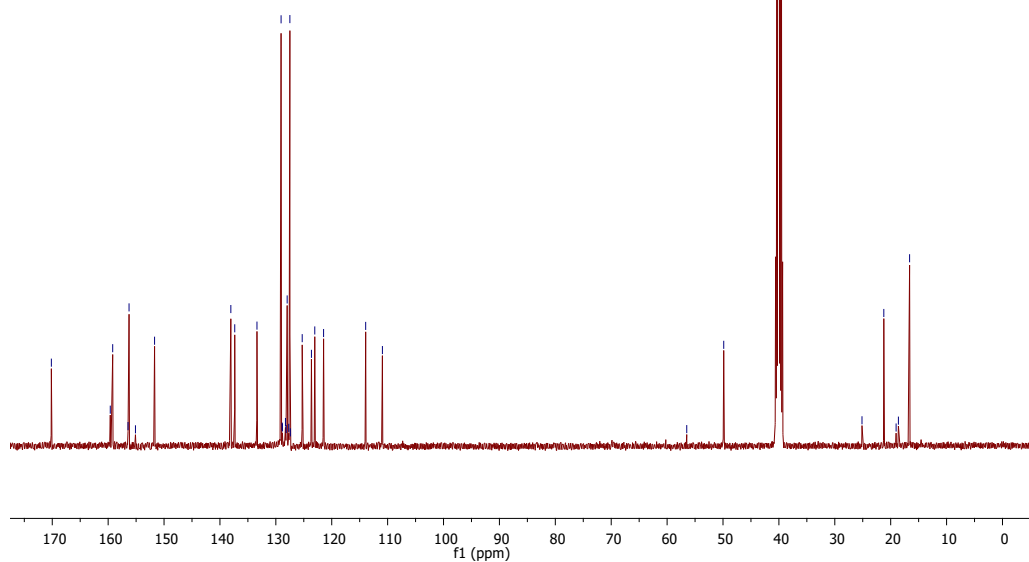
HRMS spectrum of compound **1n**.

^1H NMR spectrum of compound **1o** in DMSO-d_6 .



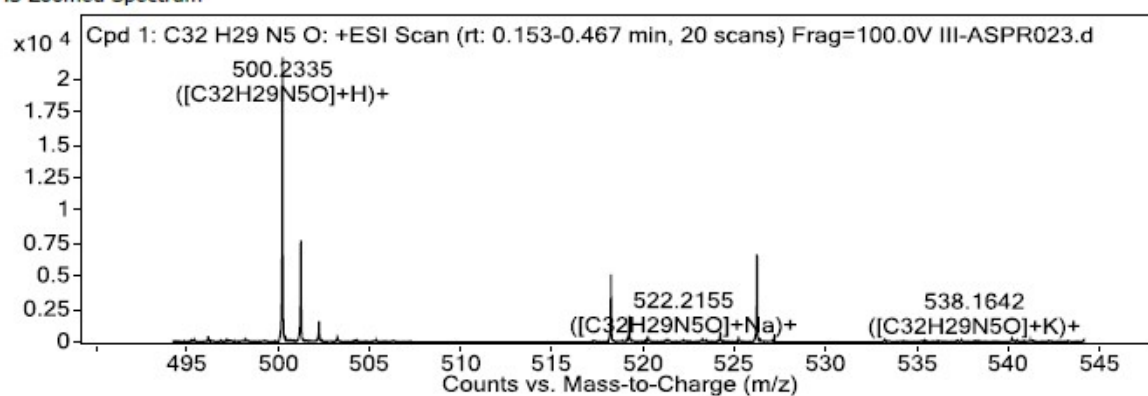
^{13}C
NMR
spe
ctru
m

of



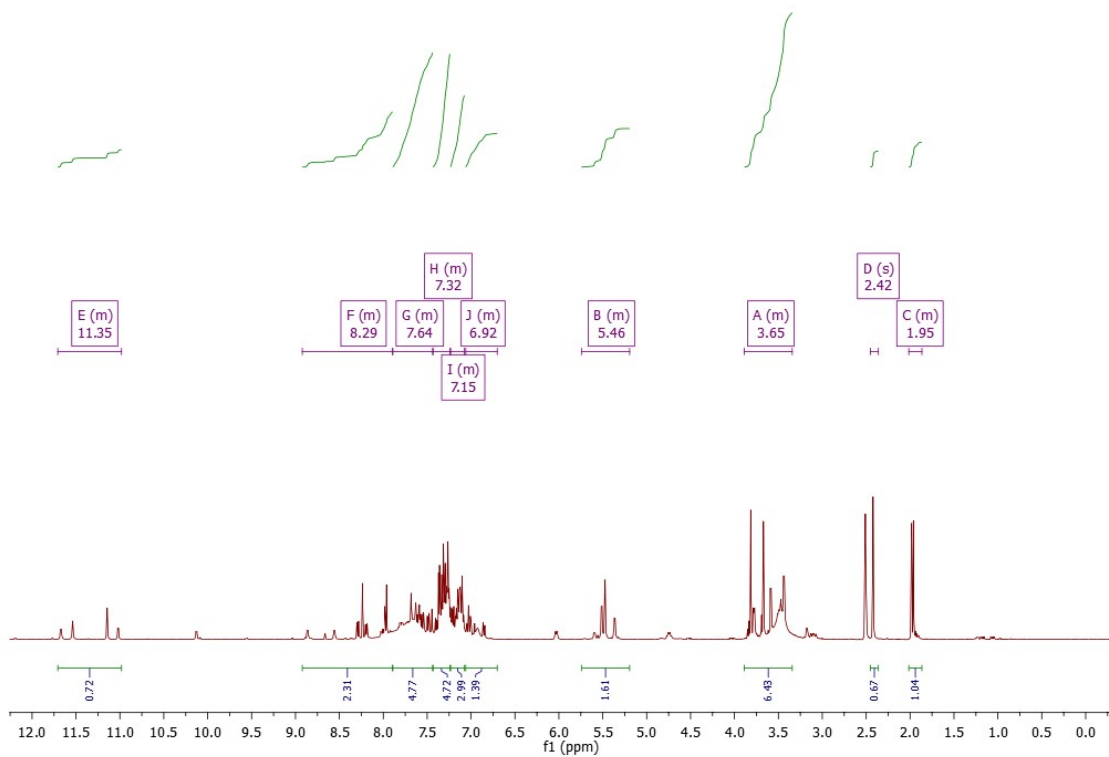
compound **1o** in DMSO-d_6 .

MS Zoomed Spectrum

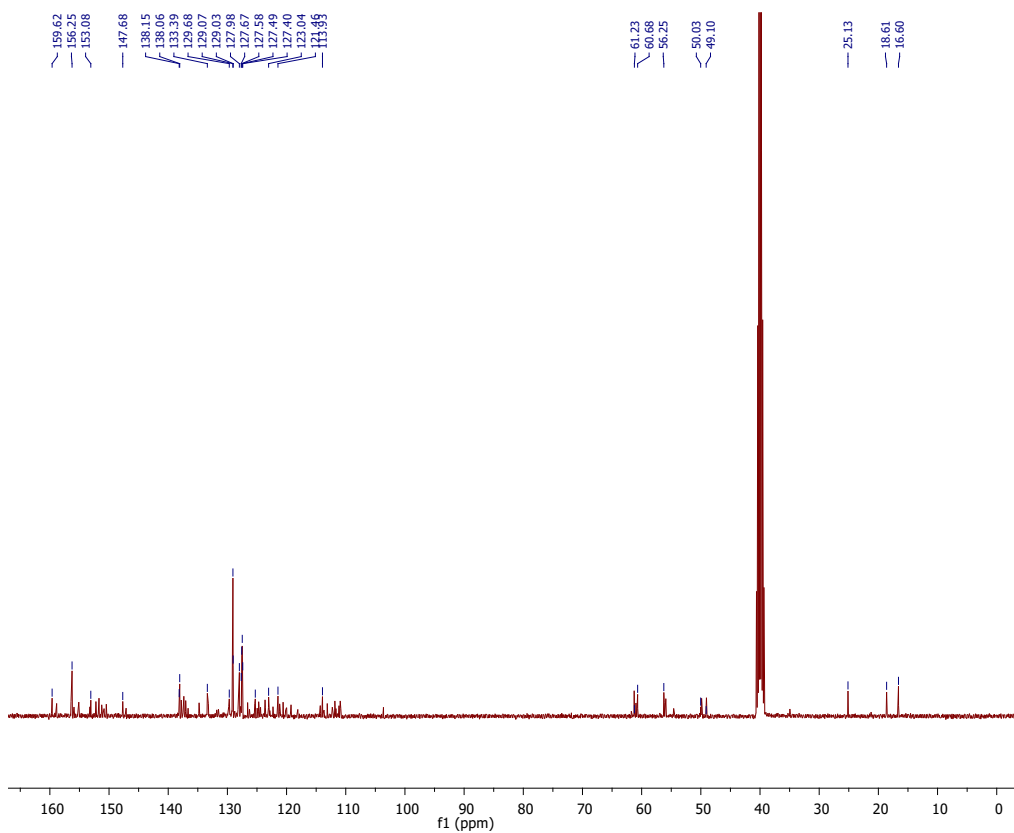


HRMS spectrum of compound **1o**.

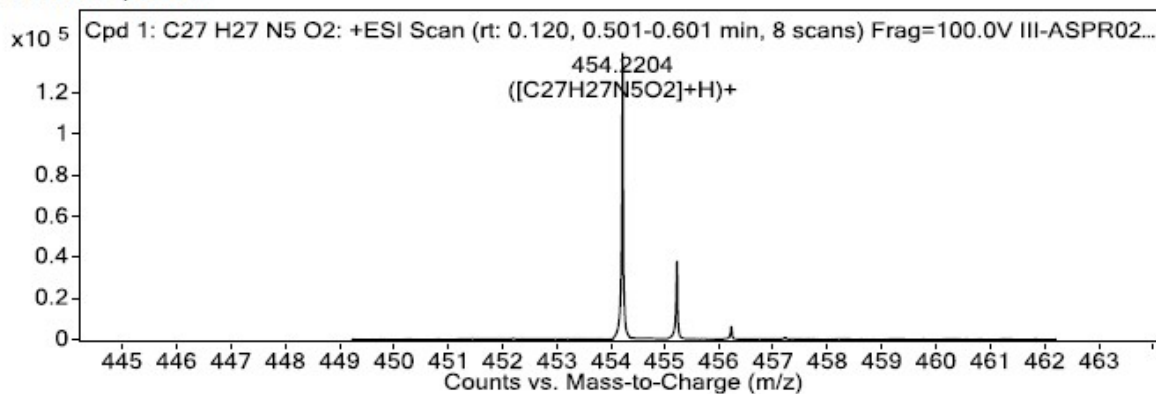
¹H NMR spectrum of compound **1p** in DMSO-d₆.



¹³C NMR spectrum of compound **1p** in DMSO-d₆.

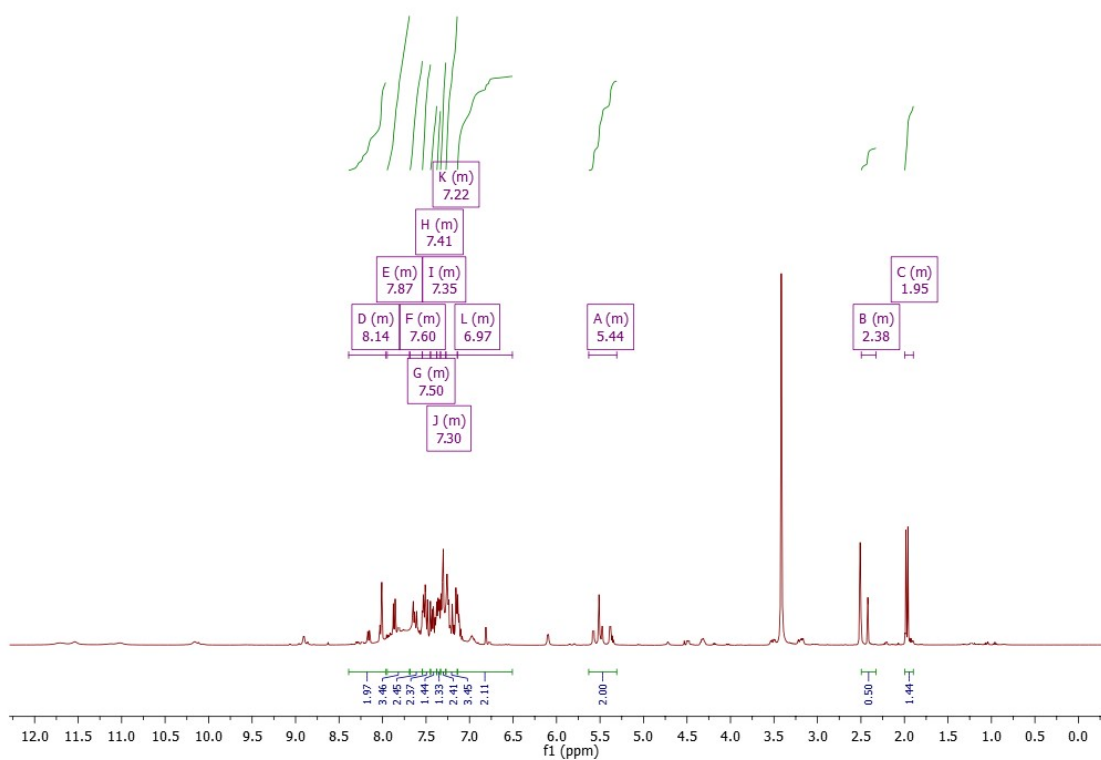


MS Zoomed Spectrum

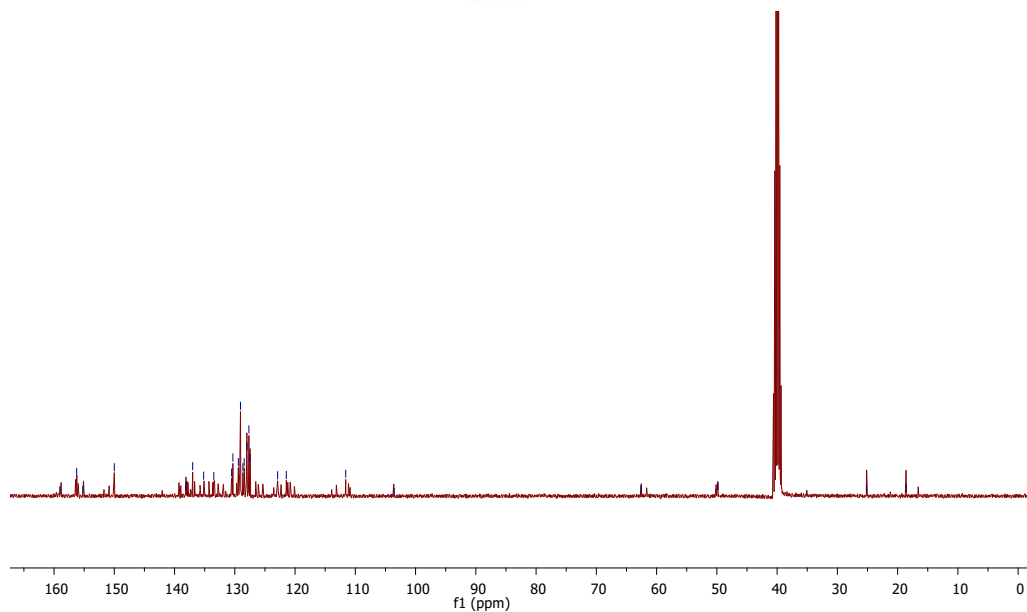


HRMS spectrum of compound **1p**.

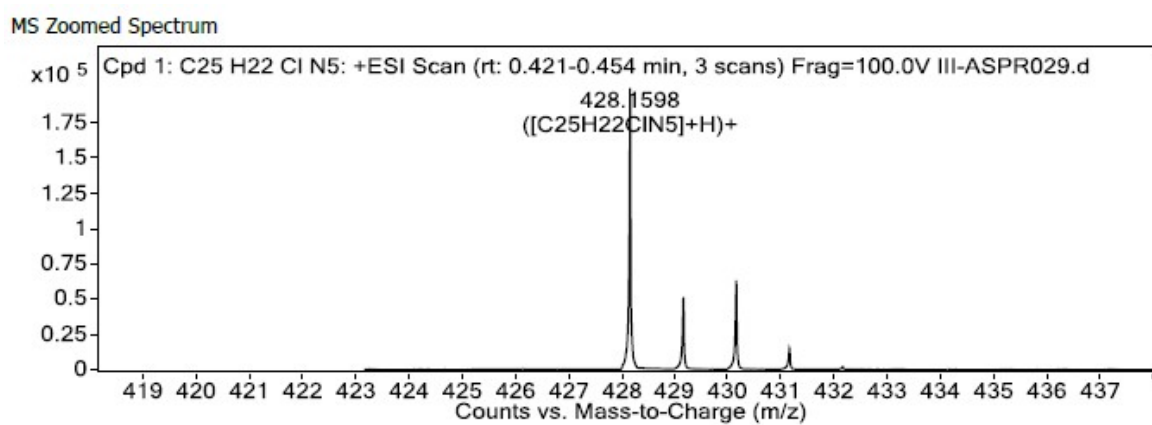
¹H NMR spectrum of compound **1q** in DMSO-d₆.



¹³C
NMR
spe
ctru
m

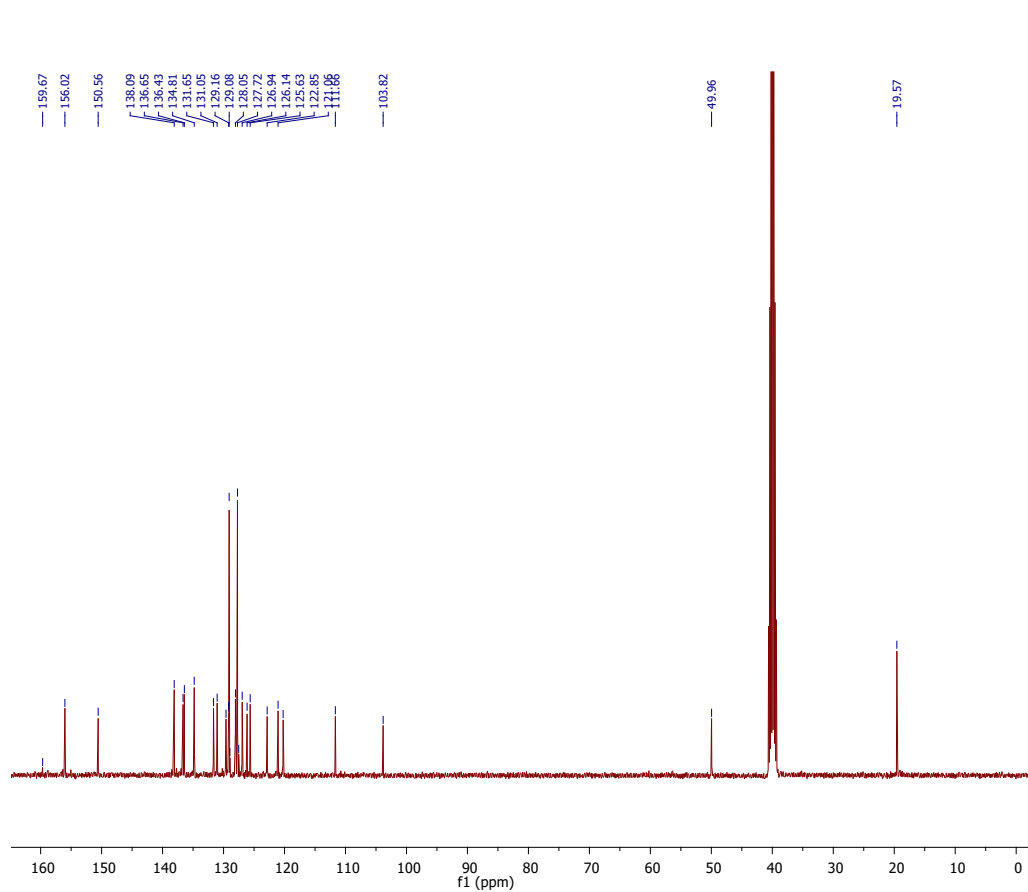
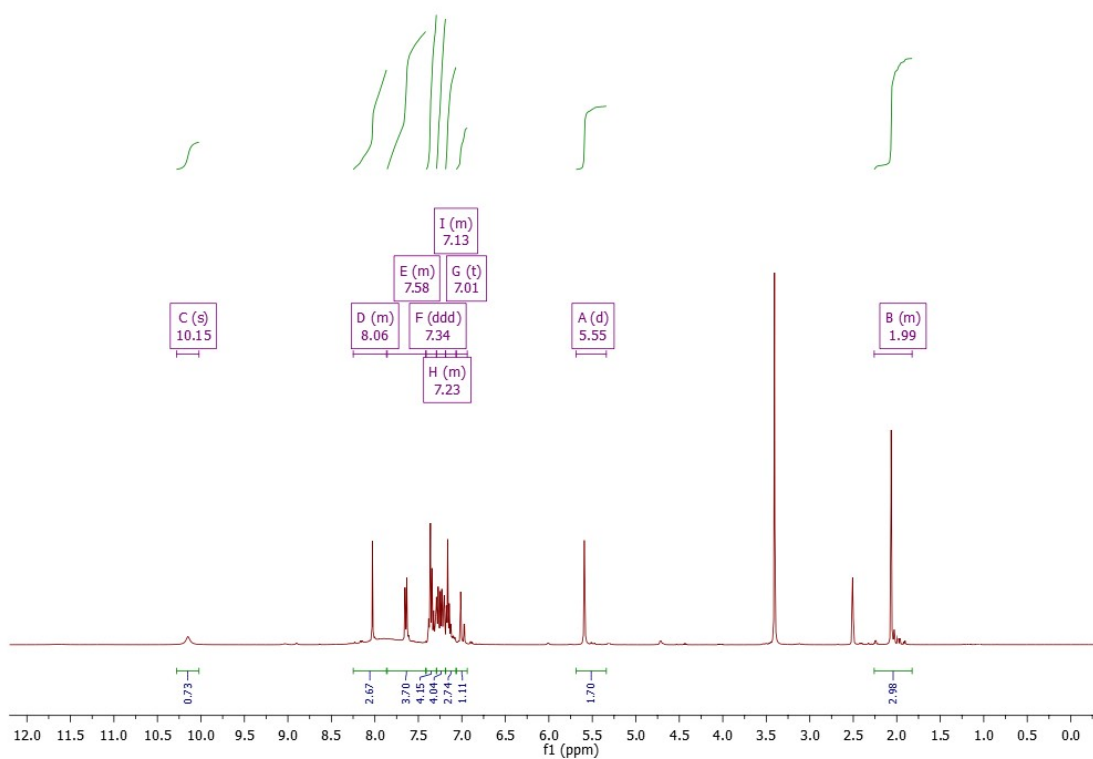


of compound **1q** in DMSO-d₆.



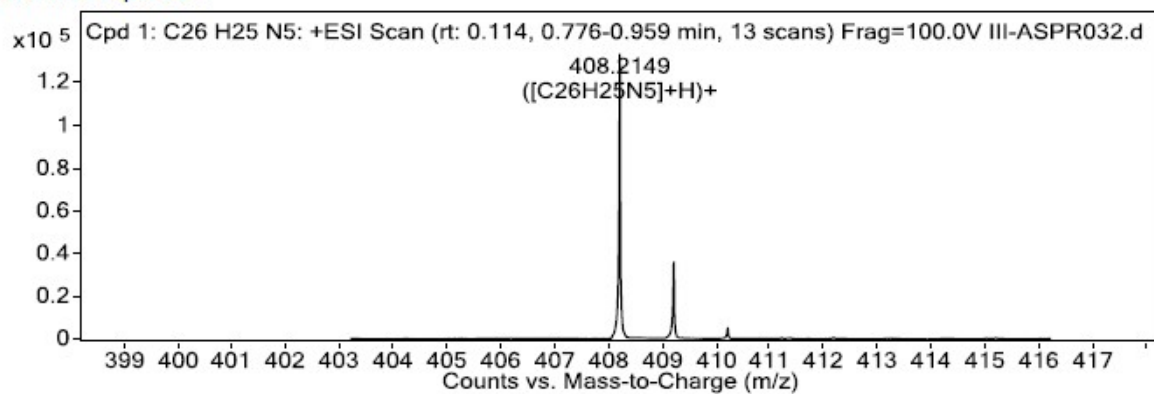
HRMS spectrum of compound **1q**.

^1H NMR spectrum of compound **1r** in DMSO-d_6 .



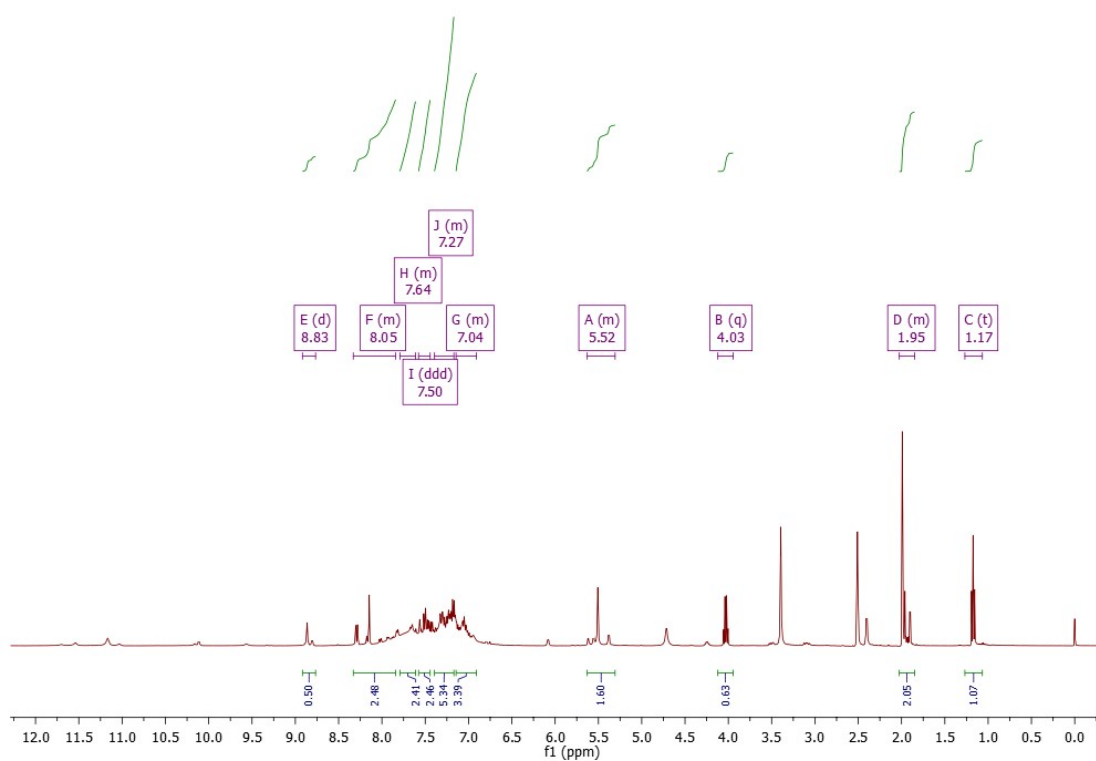
^{13}C
NMR
spectrum
of
compound
1r
in
 DMSO-d_6 .

MS Zoomed Spectrum

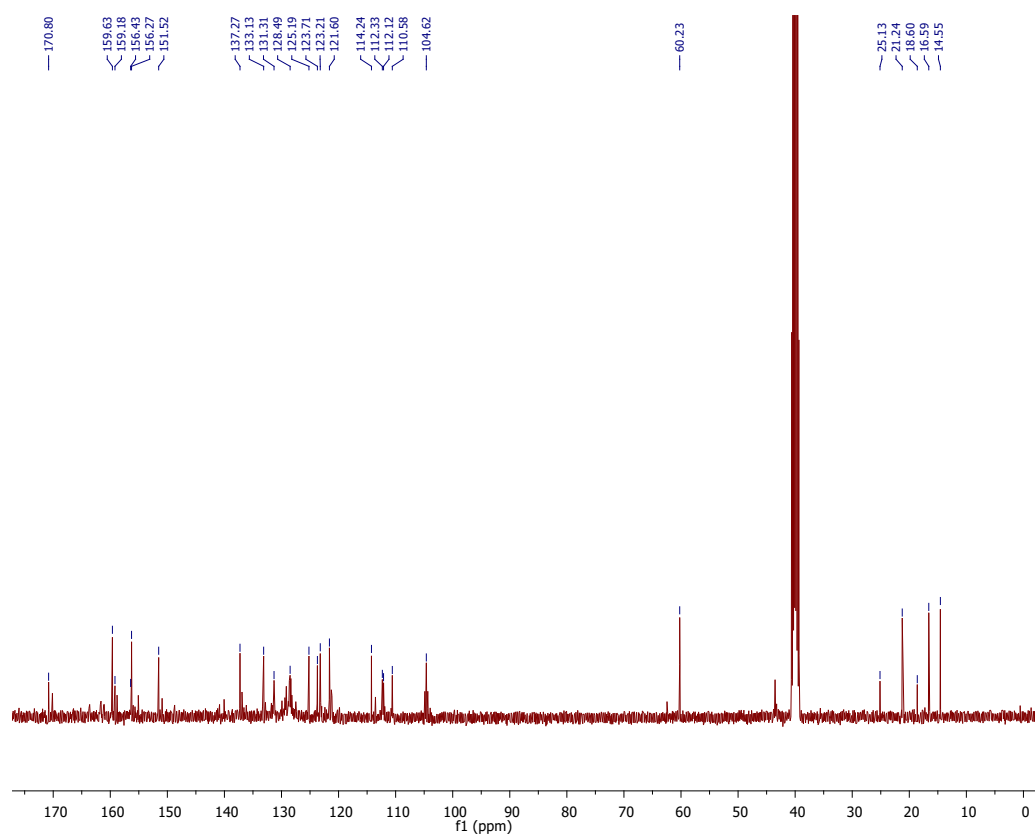


HRMS spectrum of compound **1r**.

¹H NMR spectrum of compound **2a** in DMSO-d₆.

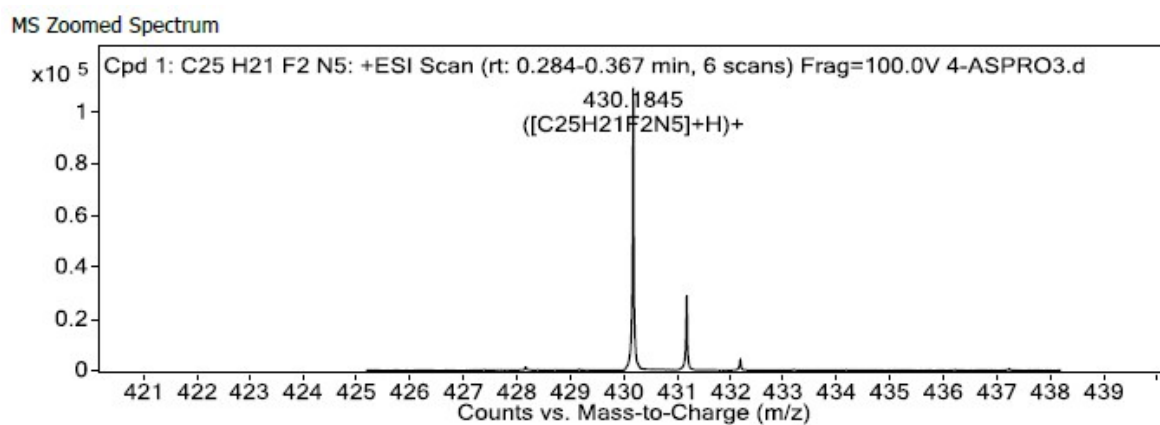


^{13}C

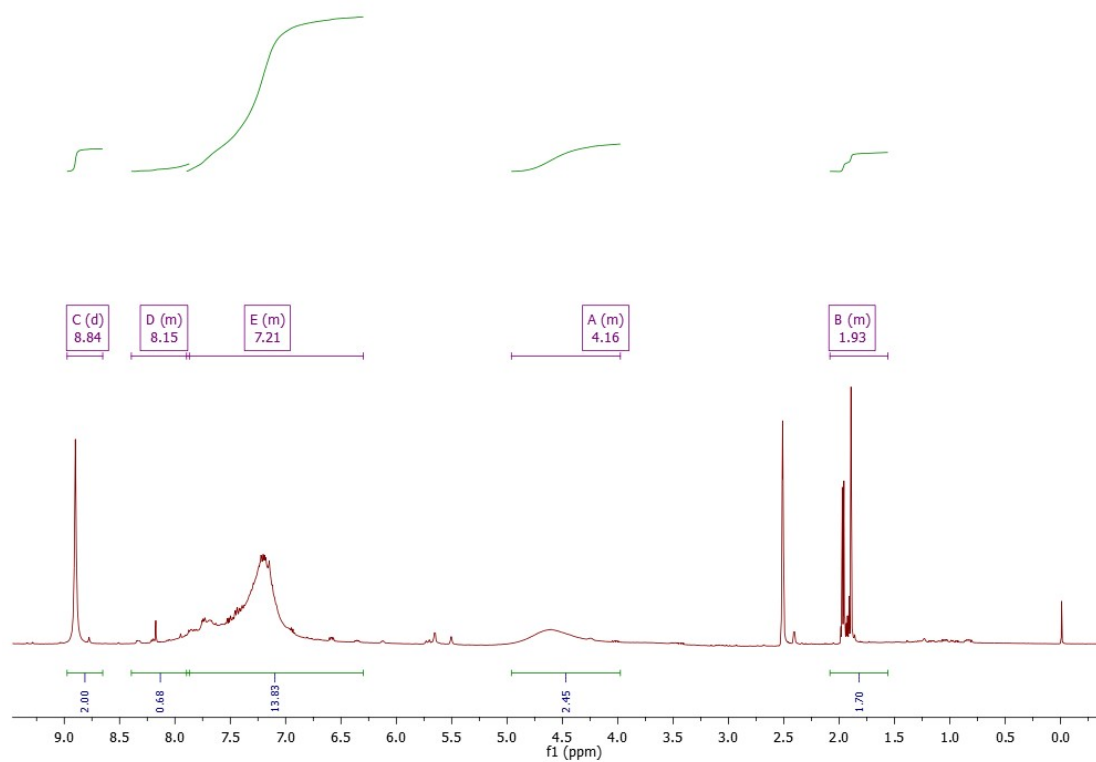


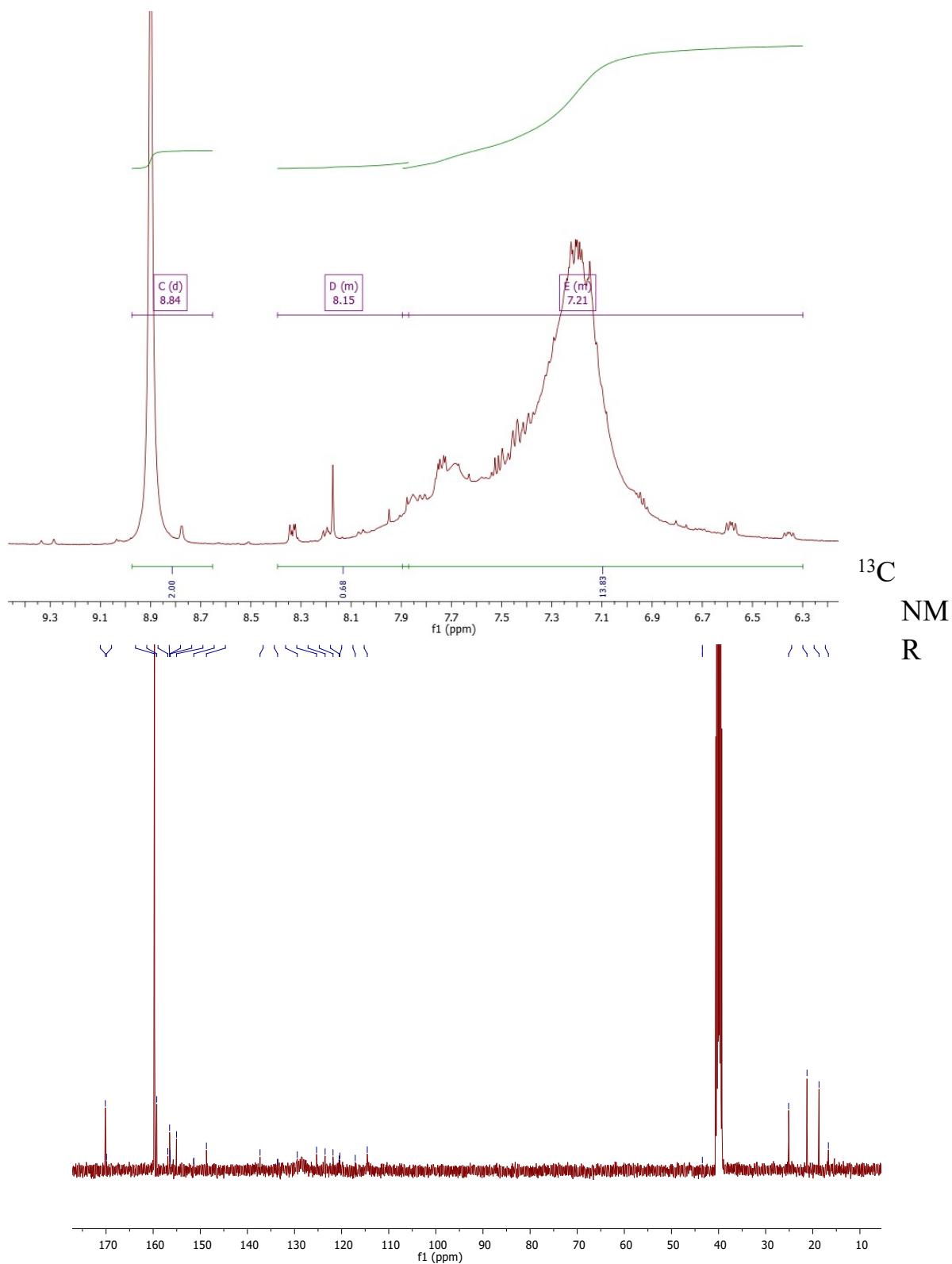
NMR spectrum of compound **2a** in DMSO- d_6 .

HRMS spectrum of compound **2a**.



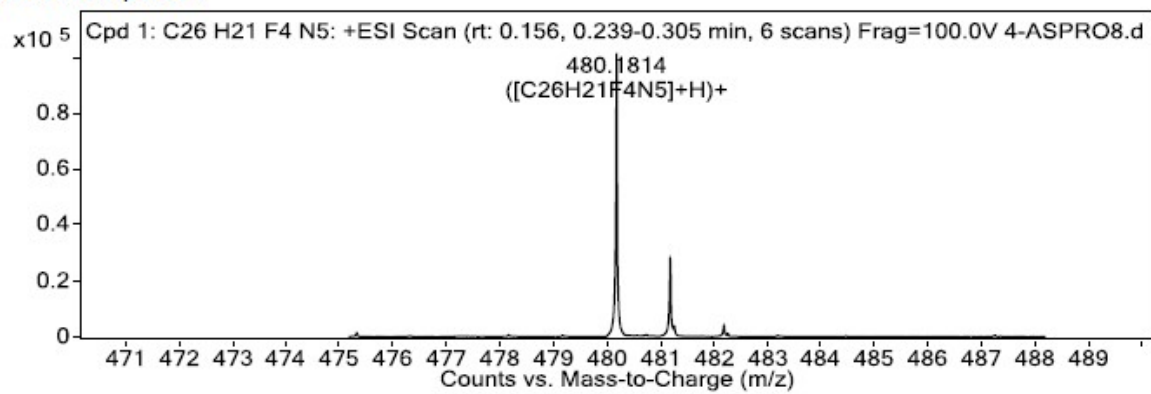
¹H NMR spectrum of compound **2d** in DMSO-d₆.





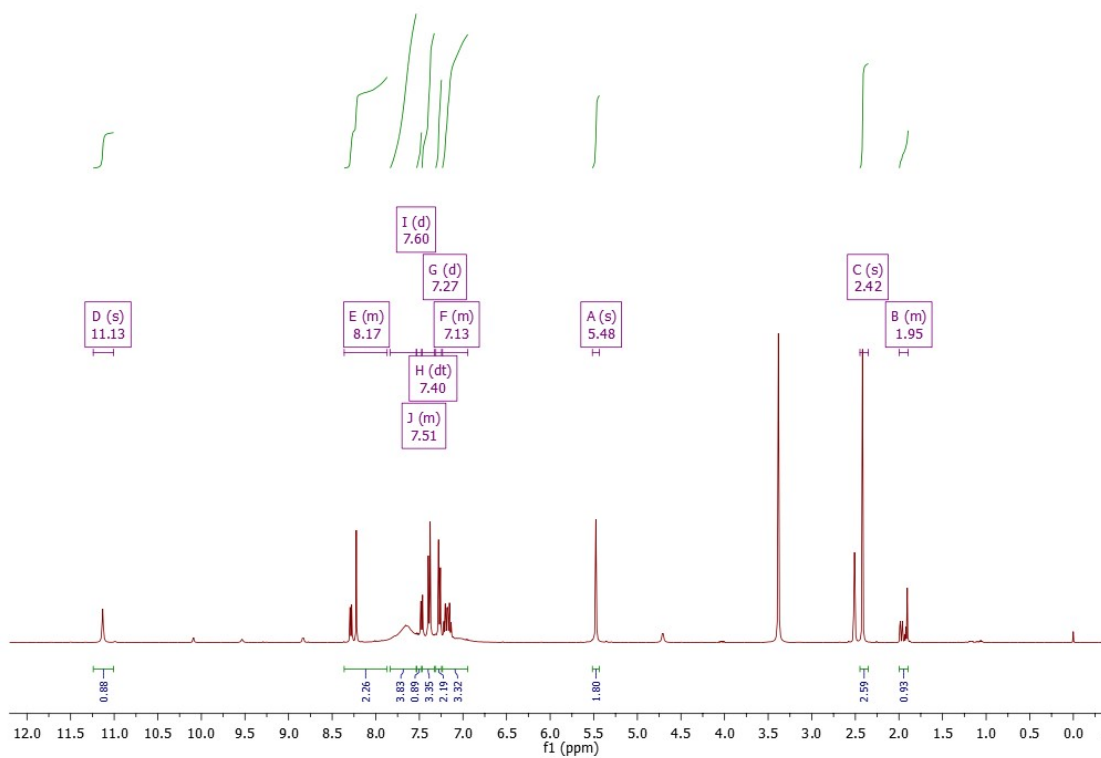
spectrum of compound **2d** in DMSO- d_6 .

MS Zoomed Spectrum

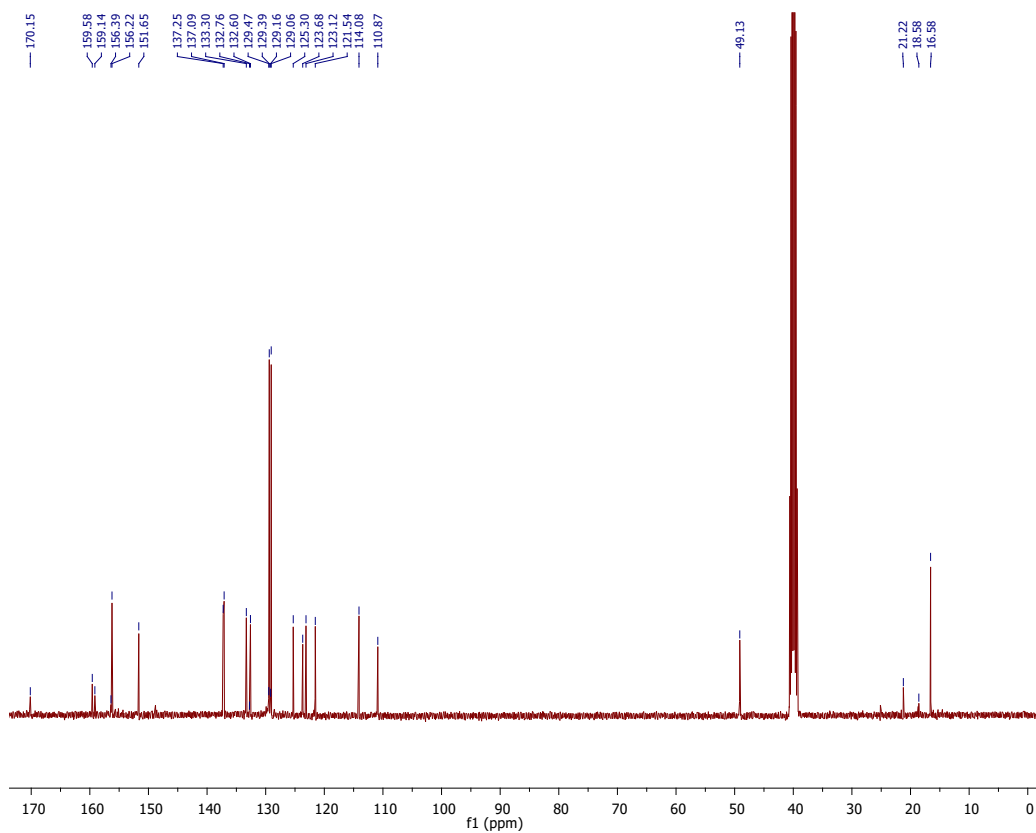


HRMS spectrum of compound **2d**.

¹H NMR spectrum of compound **2f** in DMSO-d₆.

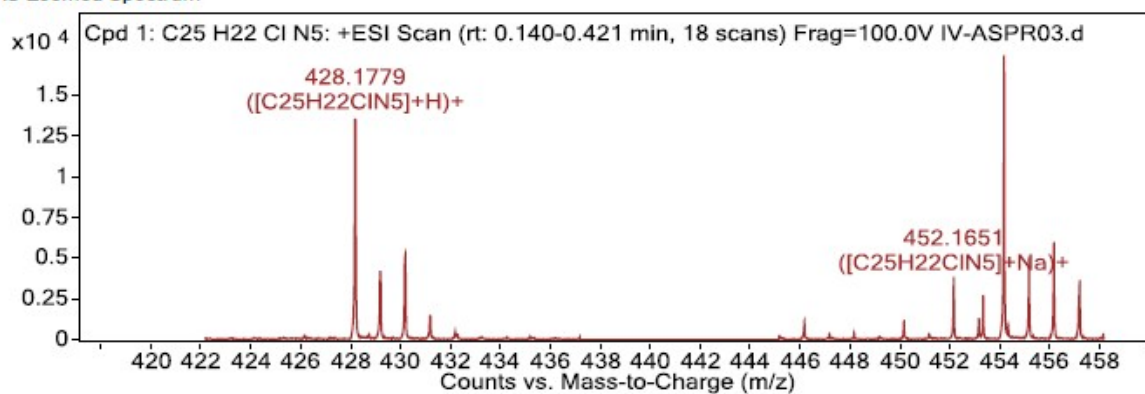


^{13}C



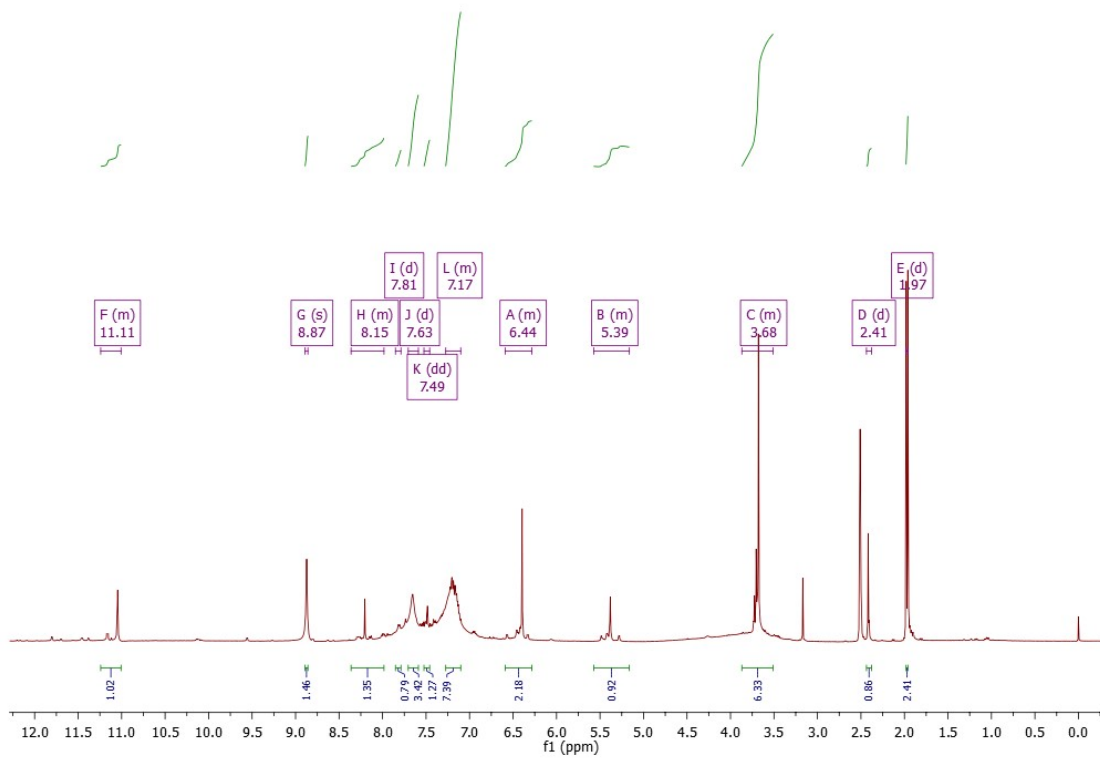
NMR spectrum of compound **2f** in DMSO-d_6 .

MS Zoomed Spectrum

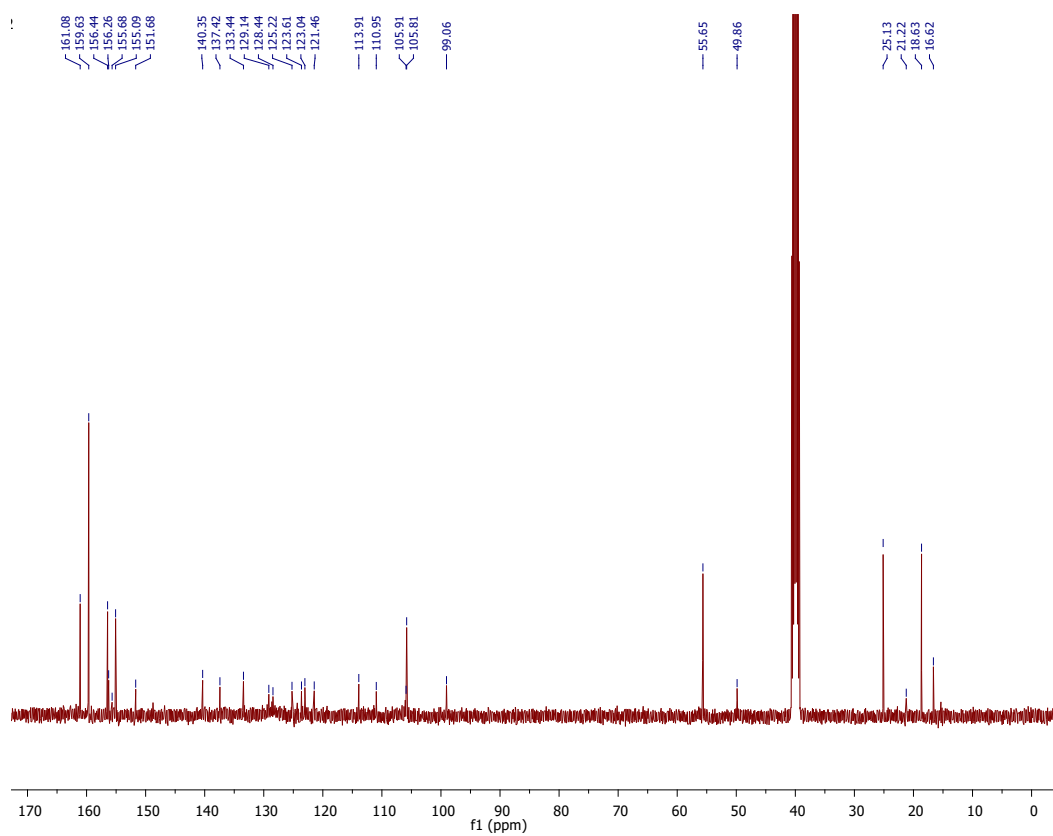


HRMS spectrum of compound **2f**.

¹H NMR spectrum of compound **2g** in DMSO-d₆.

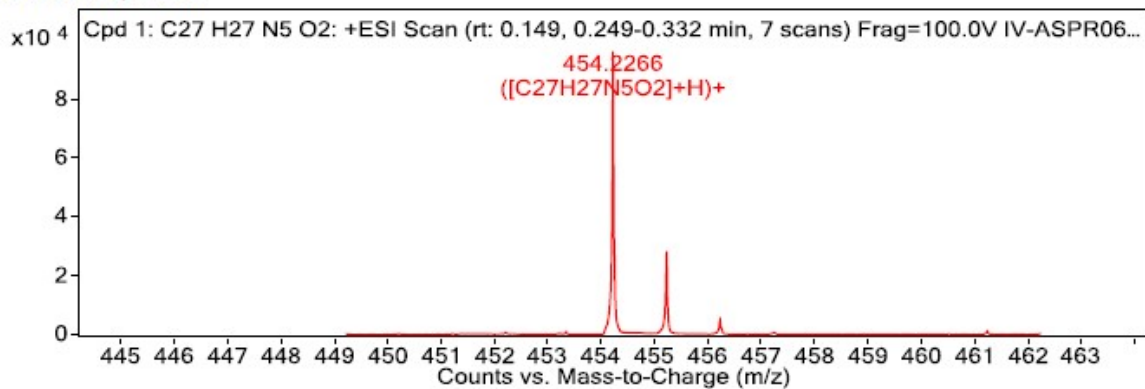


^{13}C



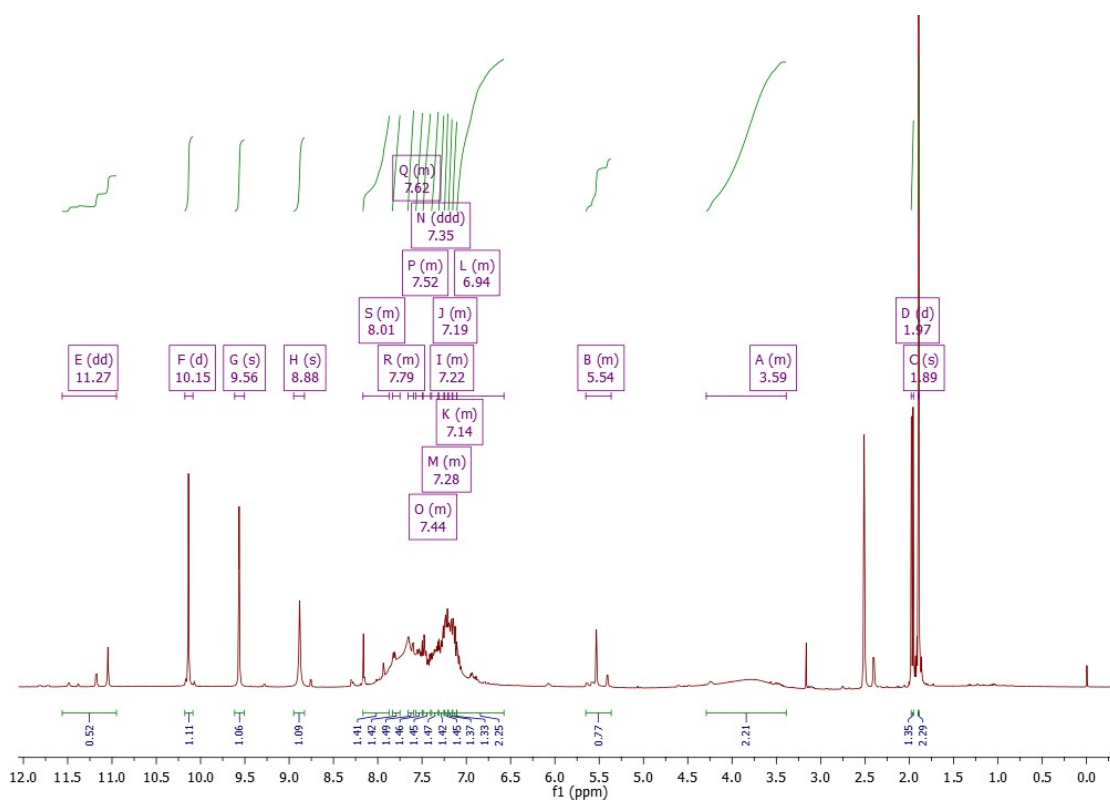
NMR spectrum of compound **2g** in DMSO-d_6 .

MS Zoomed Spectrum

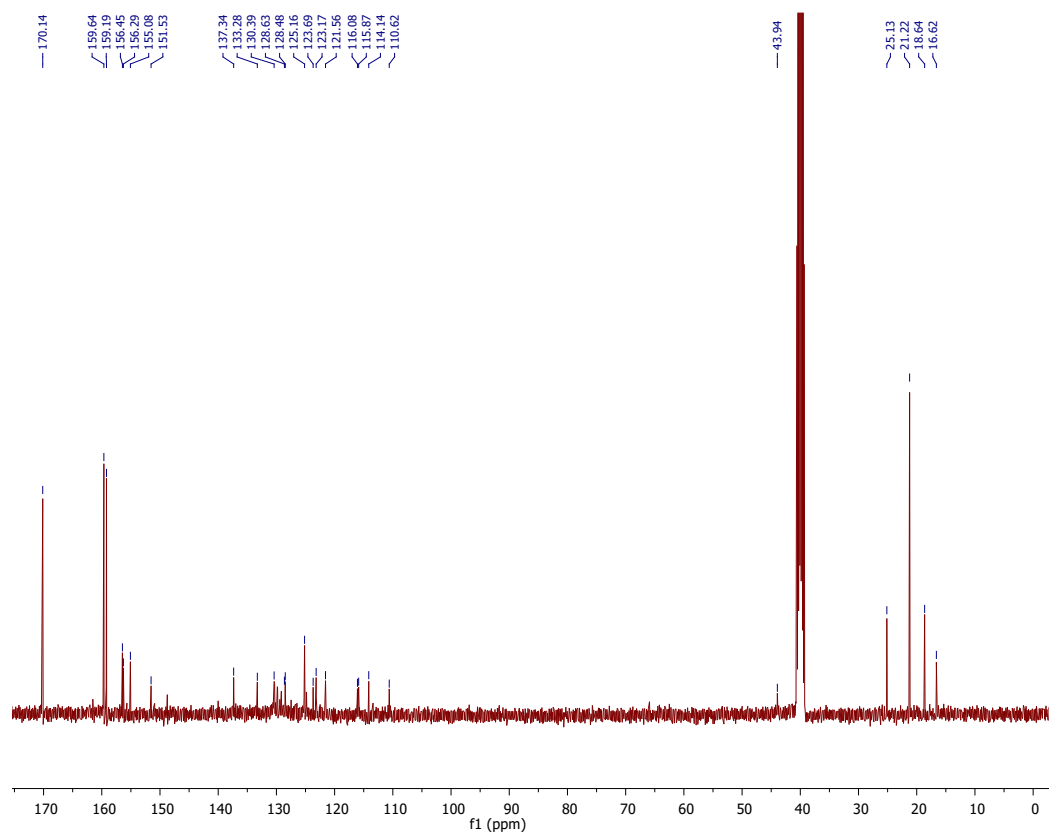


HRMS spectrum of compound **2g**.

¹H NMR spectrum of compound **2h** in DMSO-d₆.

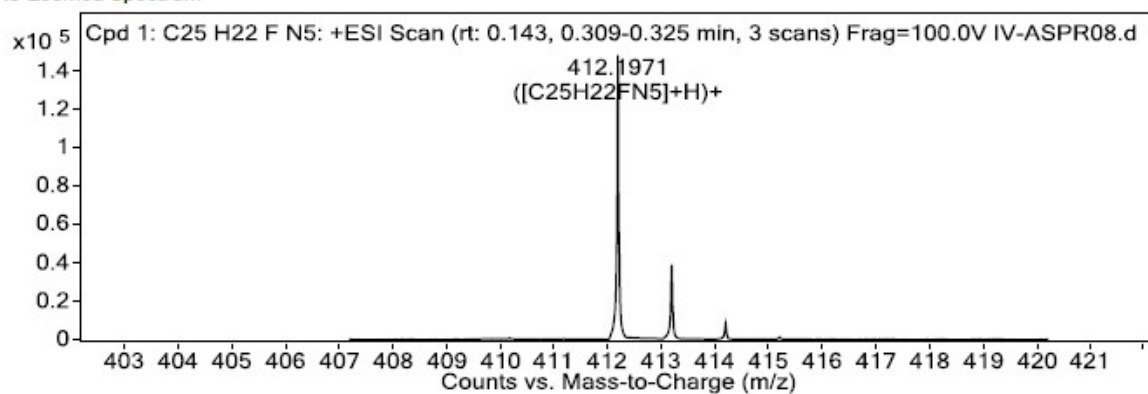


^{13}C



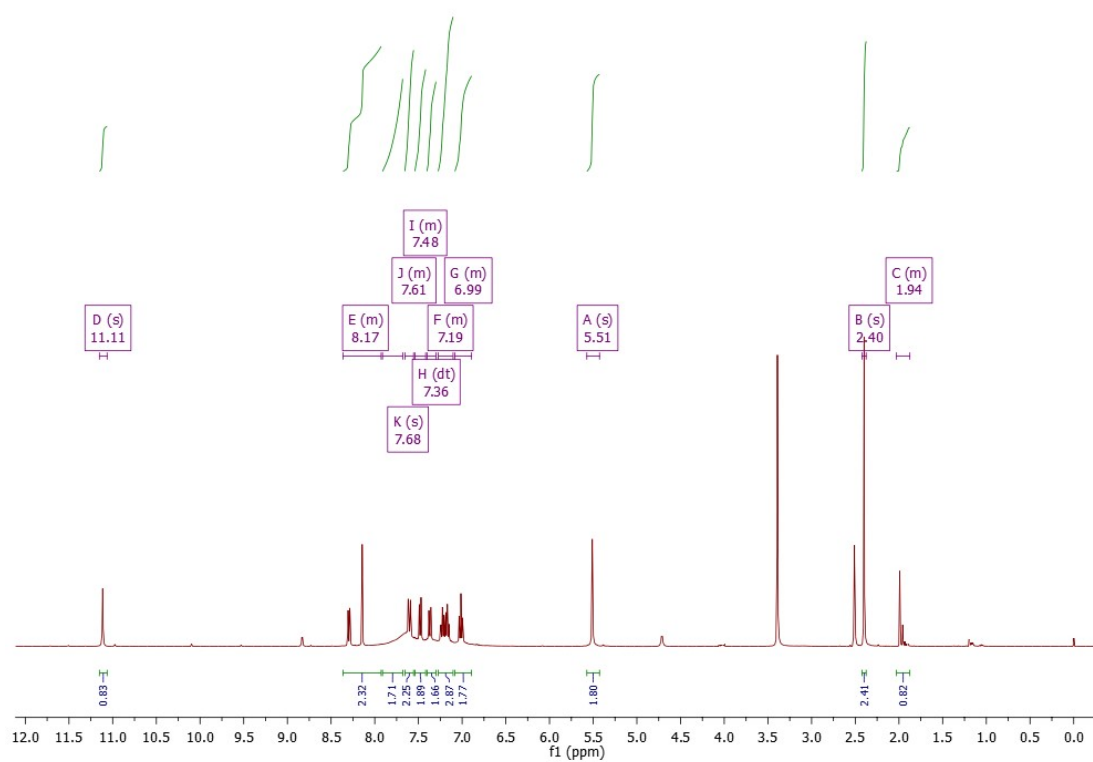
NMR spectrum of compound **2h** in DMSO-d_6 .

MS Zoomed Spectrum

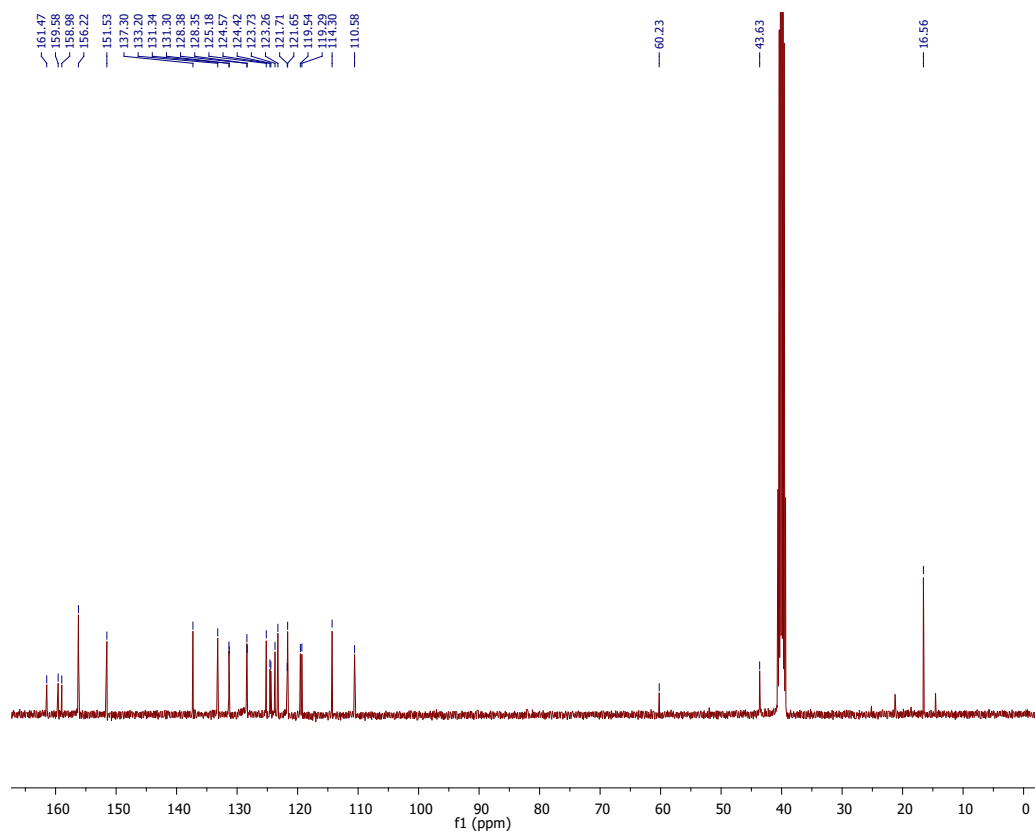


HRMS spectrum of compound **2h**.

¹H NMR spectrum of compound **2i** in DMSO-d₆.

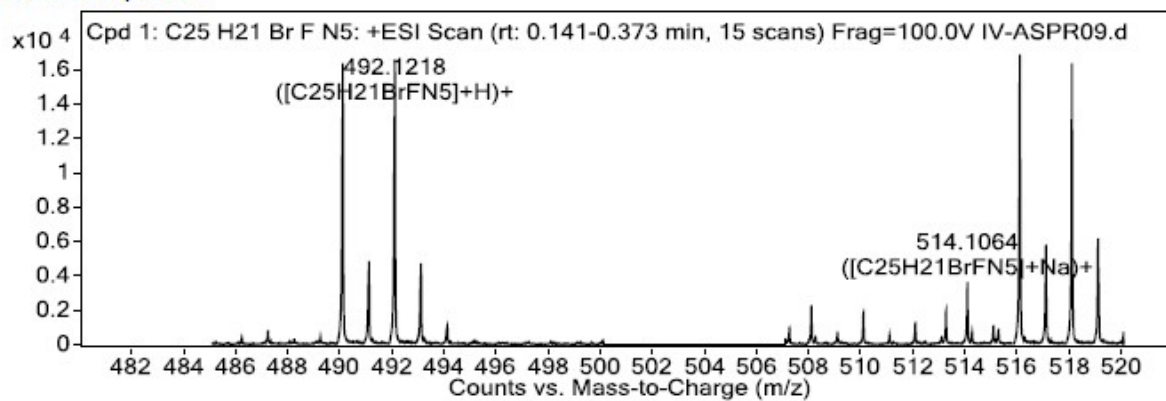


^{13}C



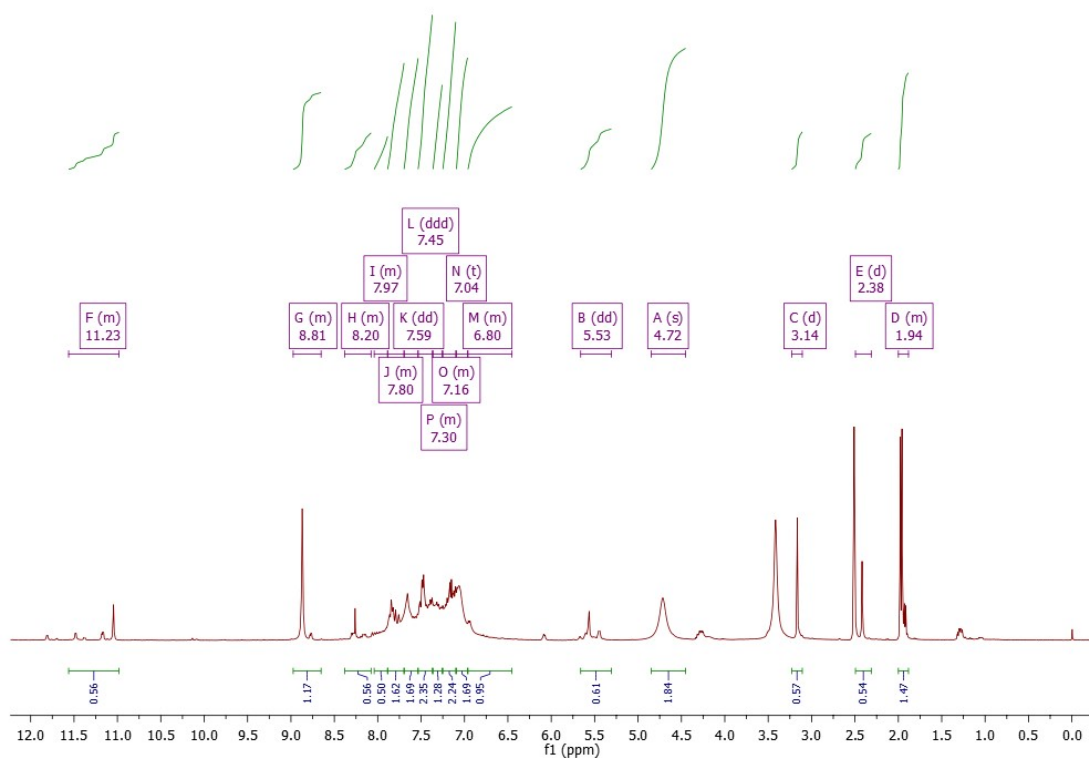
NMR spectrum of compound **2i** in DMSO- d_6 .

MS Zoomed Spectrum

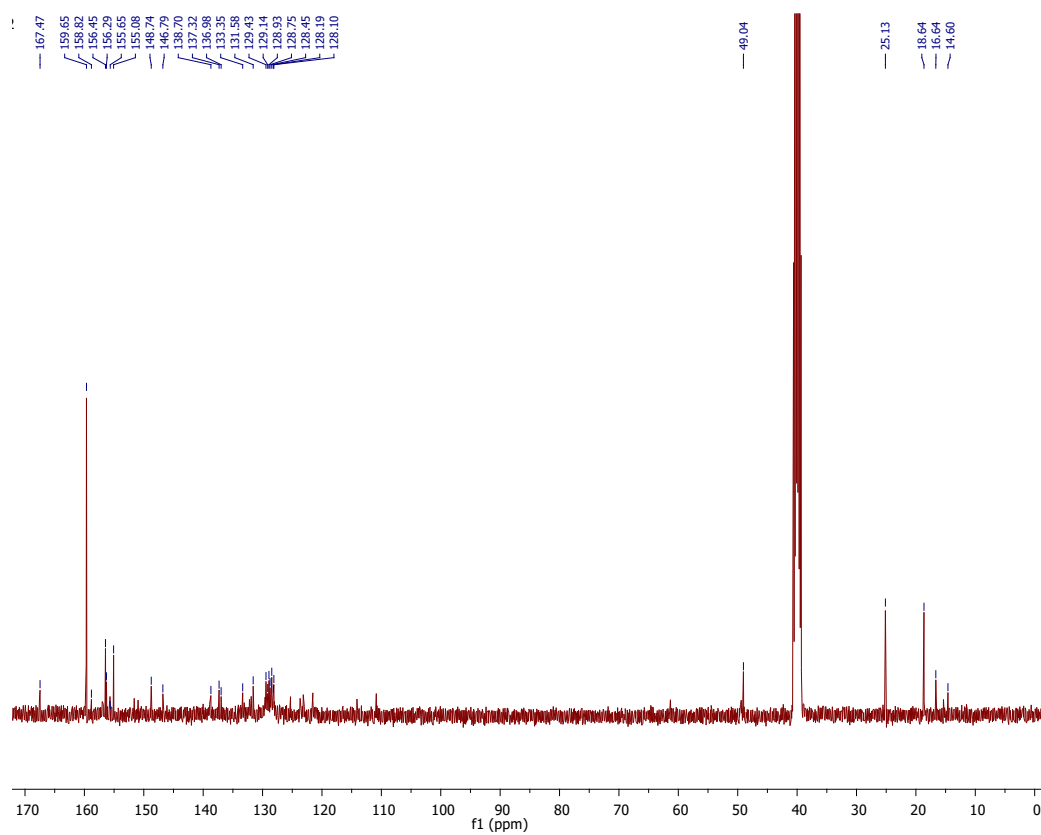


HRMS spectrum of compound **2i**.

¹H NMR spectrum of compound **2j** in DMSO-d₆.

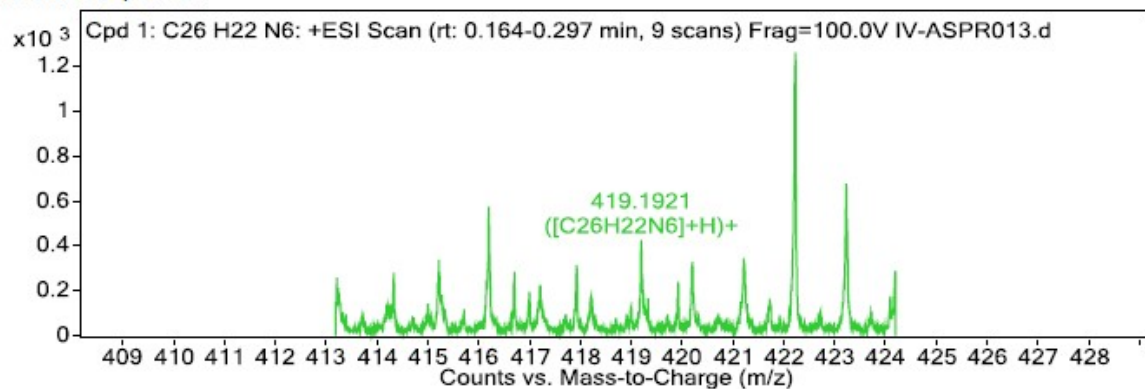


^{13}C NMR spectrum of compound **2j** in DMSO-d_6 .

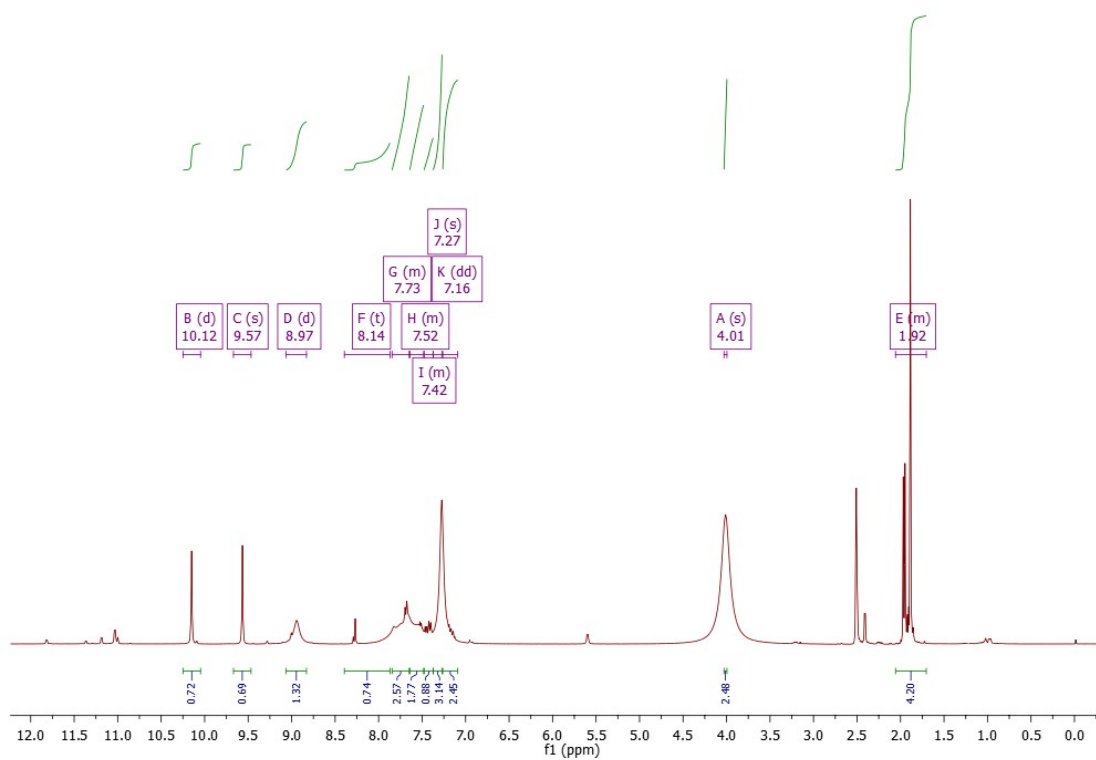


HRMS spectrum of compound **2j**.

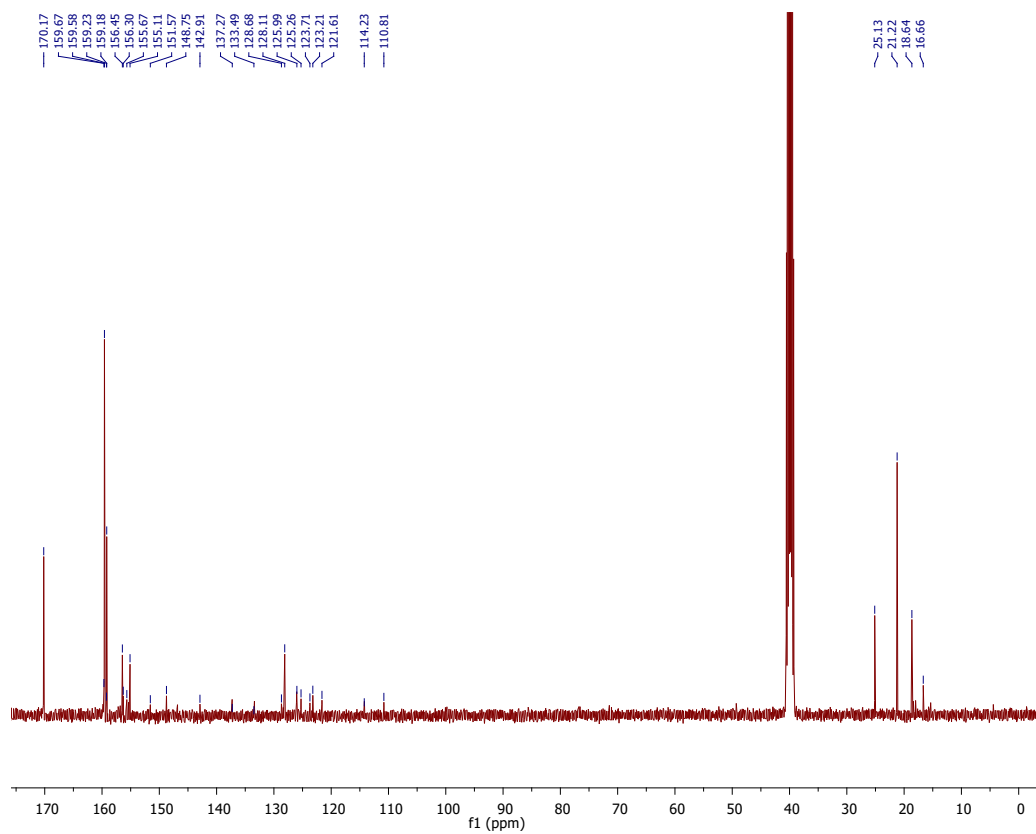
MS Zoomed Spectrum



¹H NMR spectrum of compound **3a** in DMSO-d₆.

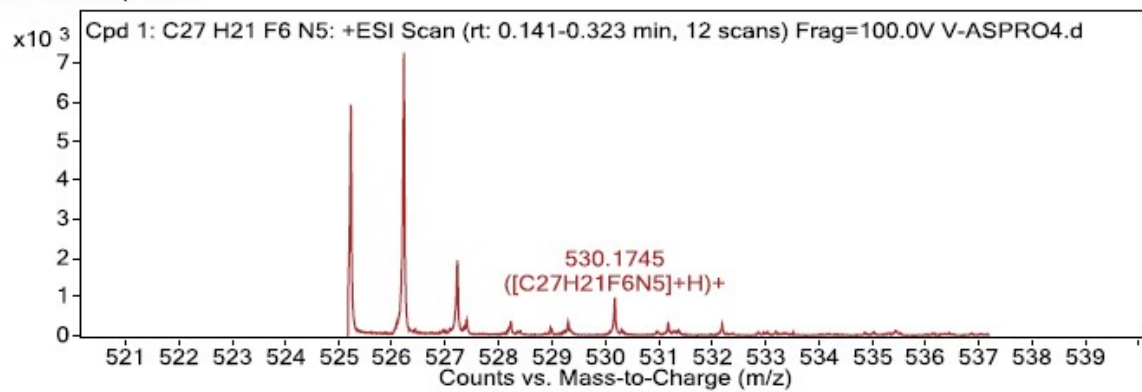


^{13}C



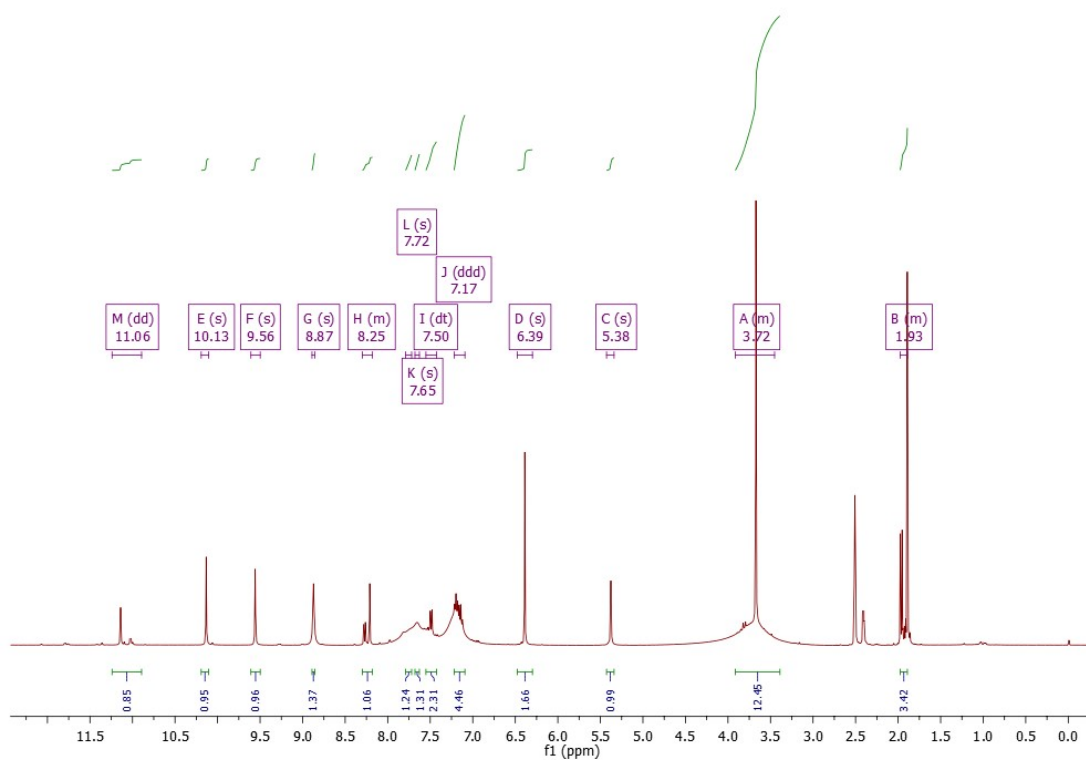
NMR spectrum of compound **3a** in DMSO- d_6 .

MS Zoomed Spectrum

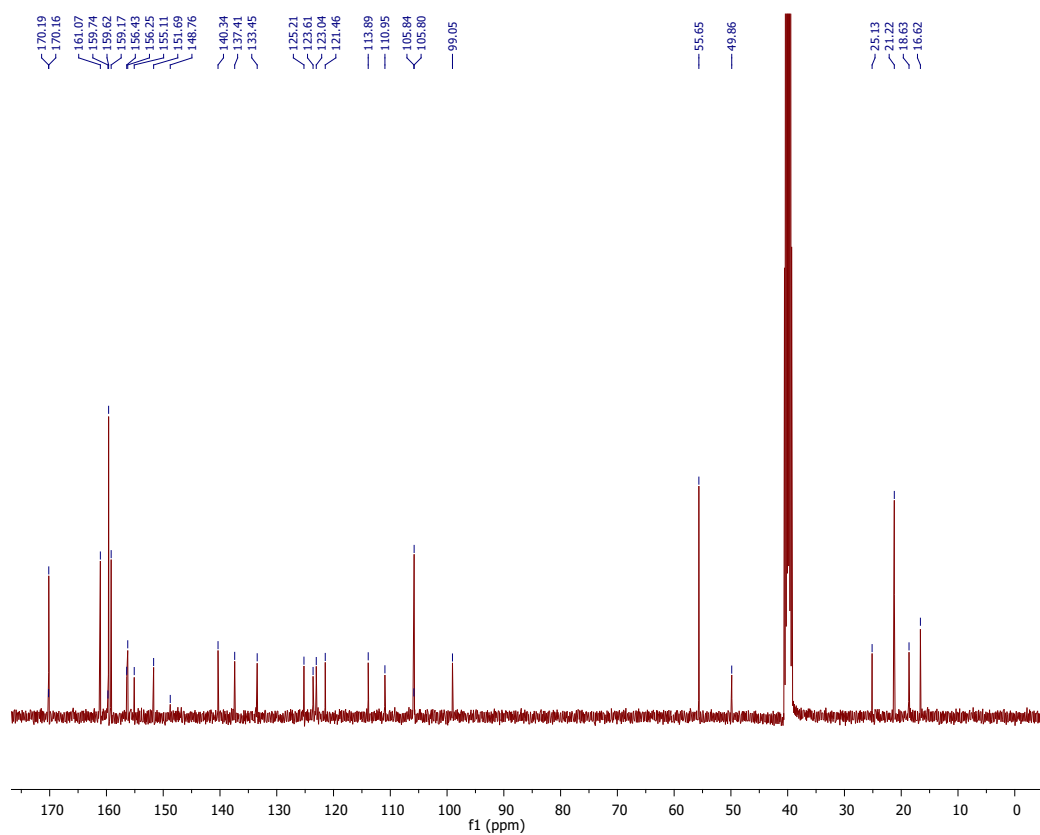


HRMS spectrum of compound **3a**.

¹H NMR spectrum of compound **3b** in DMSO-d₆.

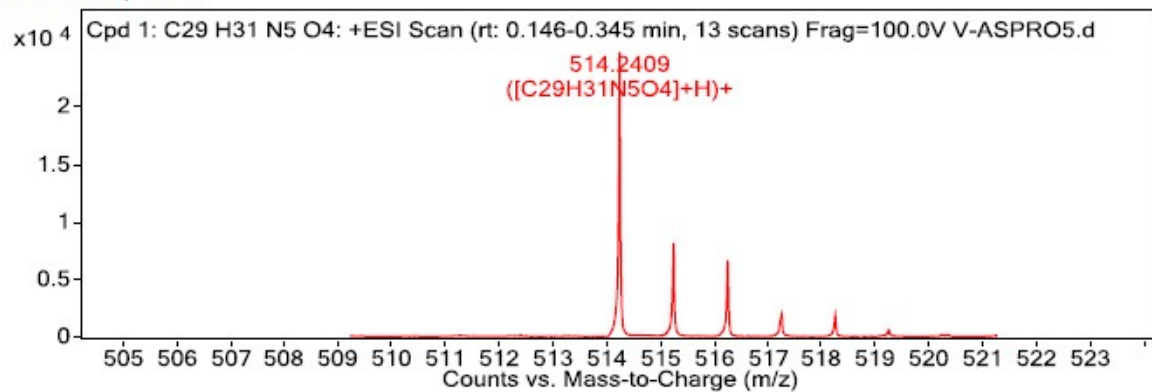


^{13}C



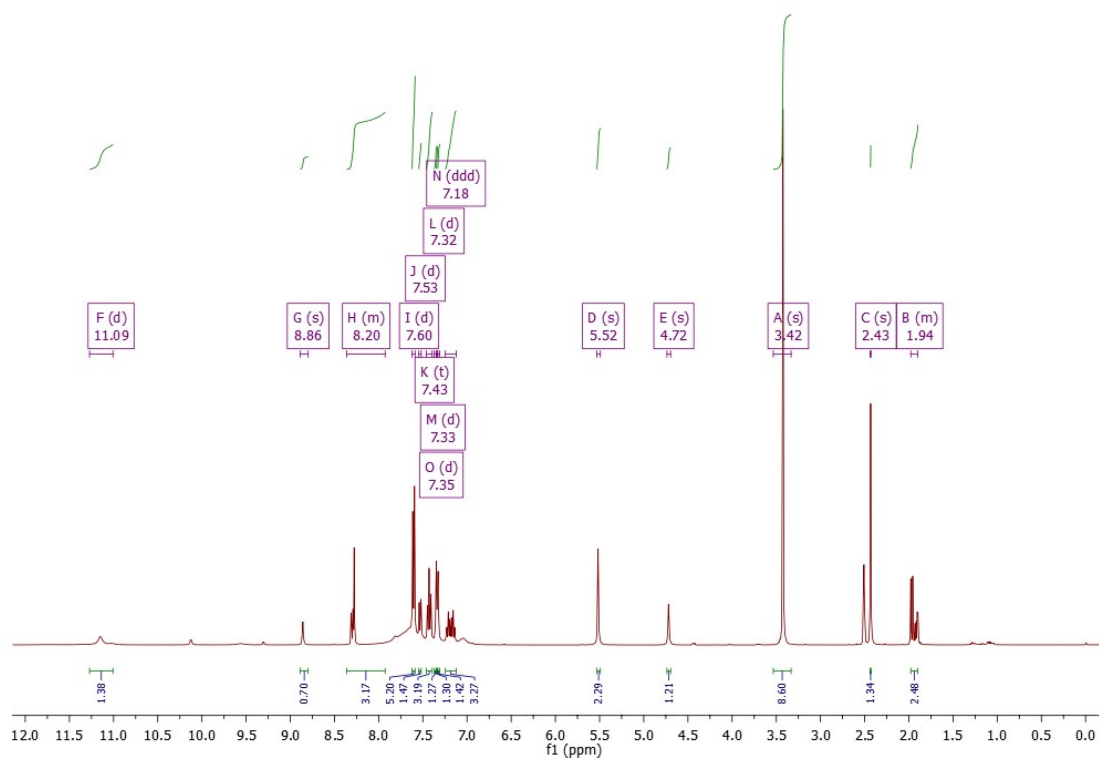
NMR spectrum of compound **3b** in DMSO-d_6 .

MS Zoomed Spectrum

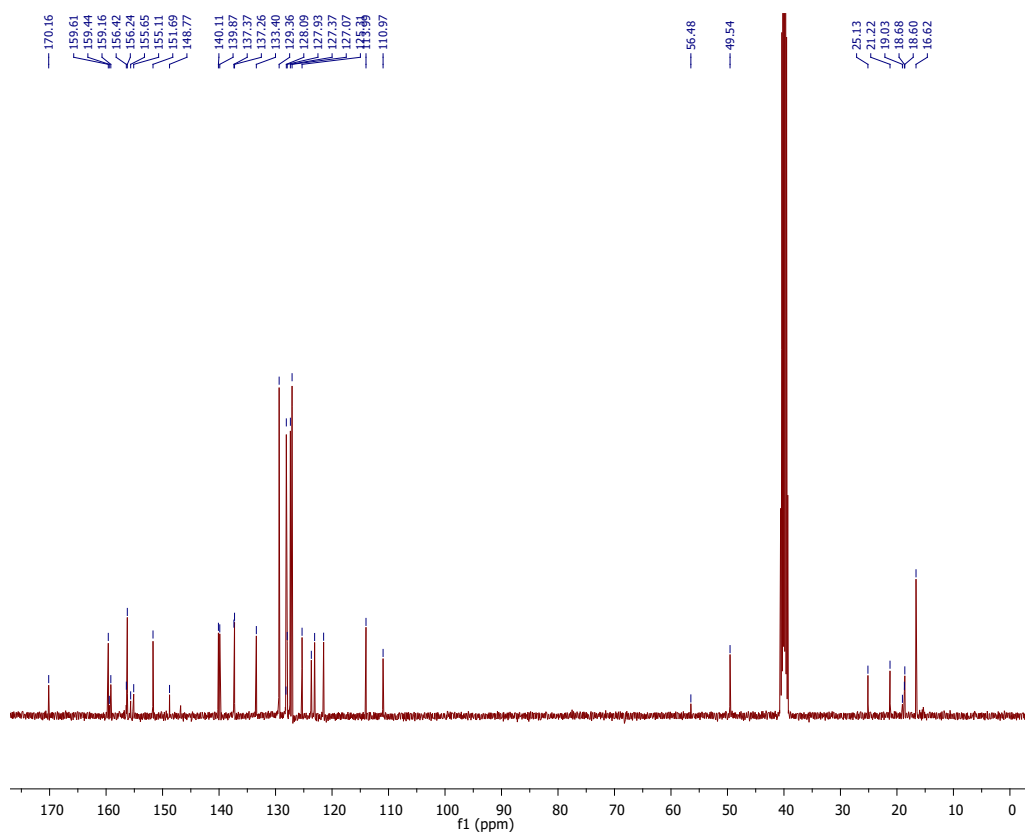


HRMS spectrum of compound **3b**.

¹H NMR spectrum of compound **3c** in DMSO-d₆.



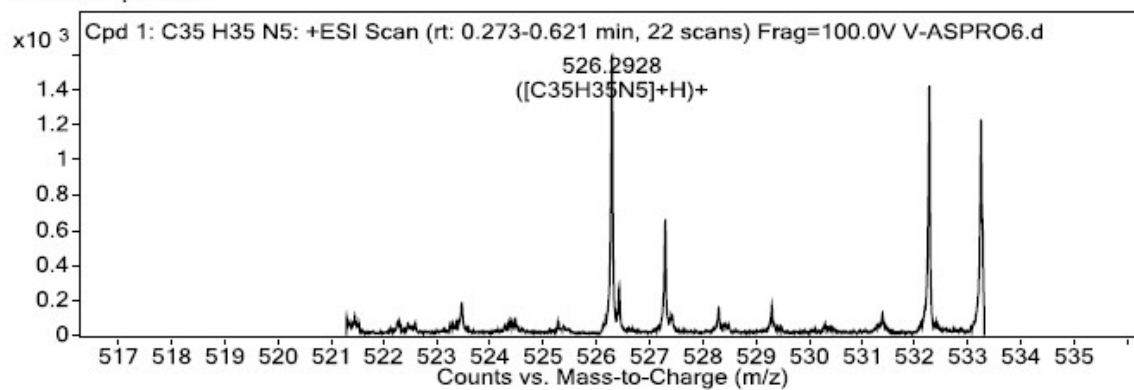
^{13}C



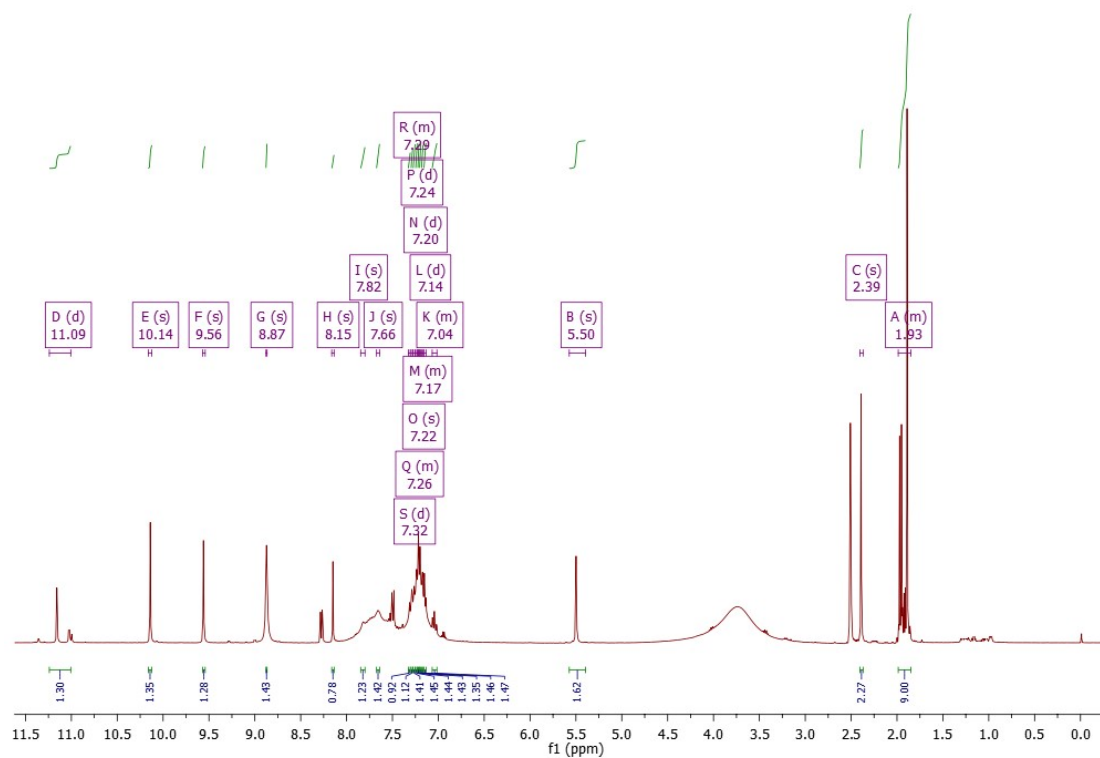
NMR spectrum of compound **3c** in DMSO-d_6 .

HRMS spectrum of compound **3c**.

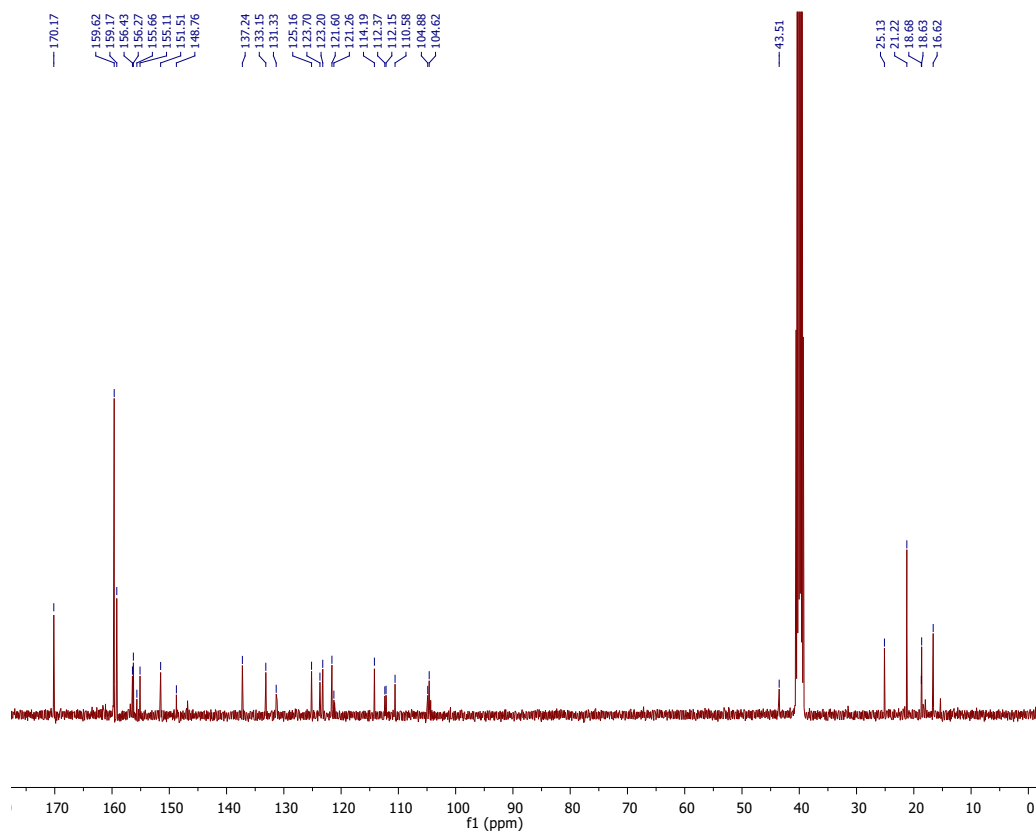
MS Zoomed Spectrum



¹H NMR spectrum of compound **3d** in DMSO-d₆.



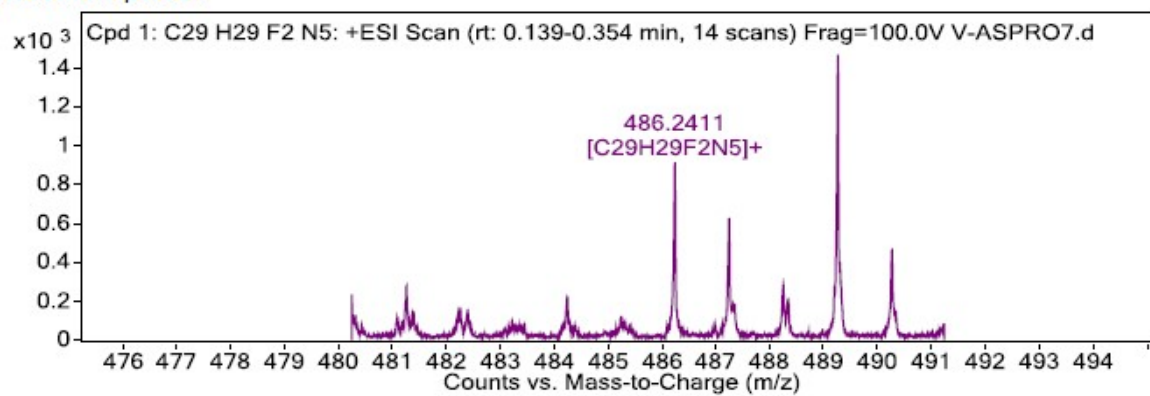
^{13}C



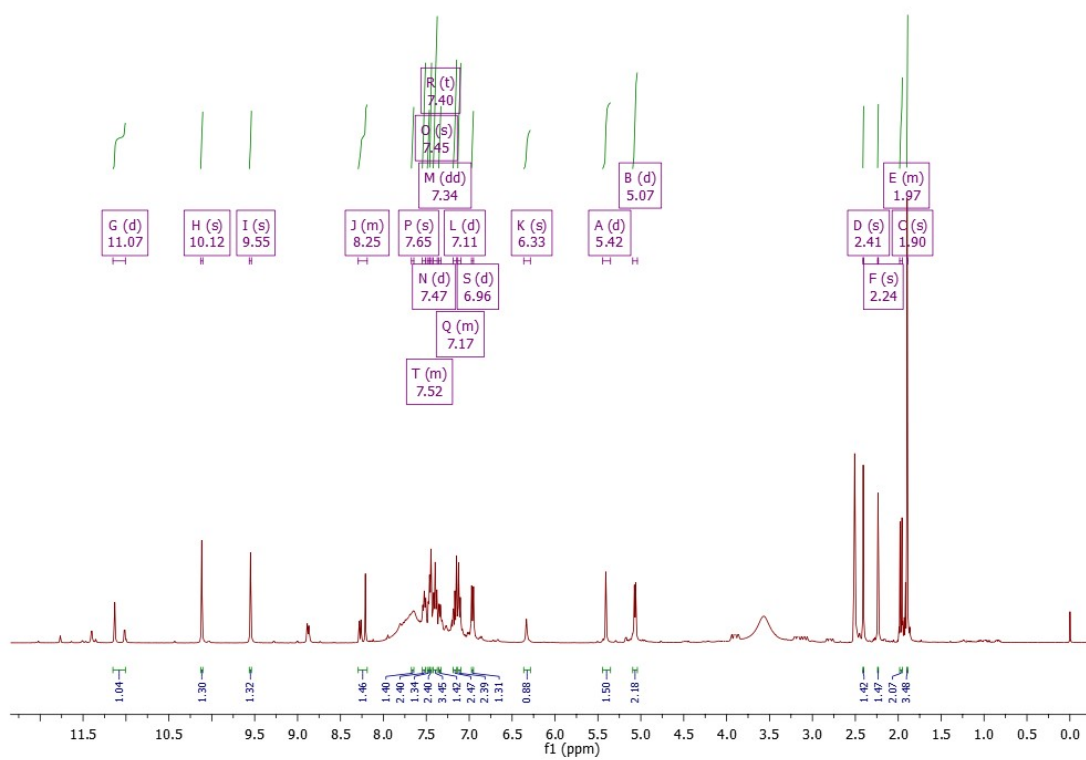
NMR spectrum of compound **3d** in DMSO-d_6 .

HRMS spectrum of compound **3d**.

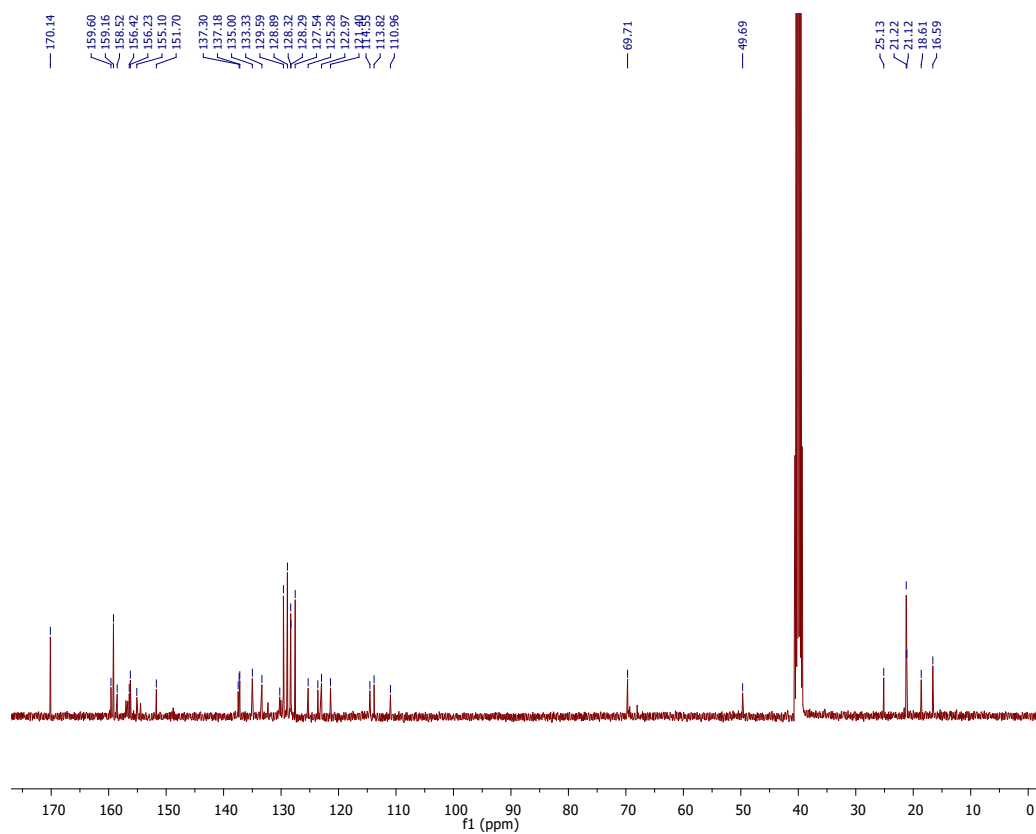
MS Zoomed Spectrum



¹H NMR spectrum of compound **3e** in DMSO-d₆.

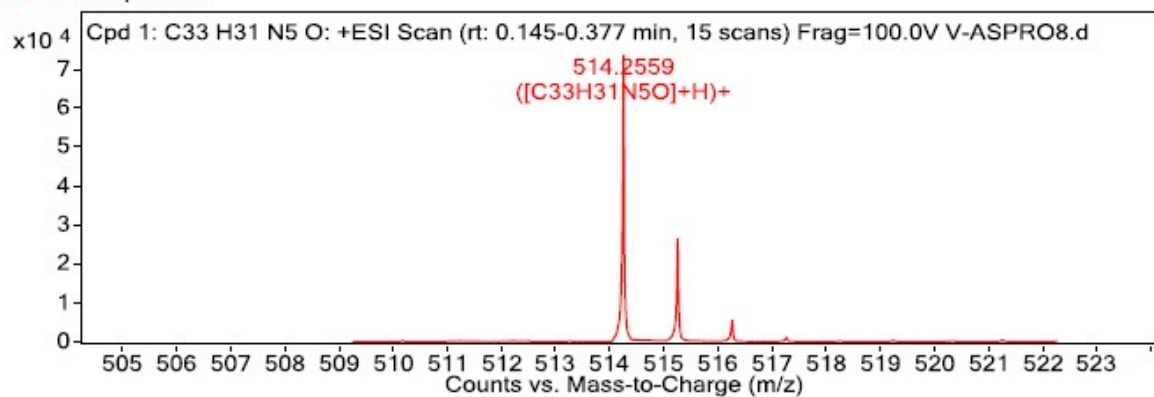


^{13}C



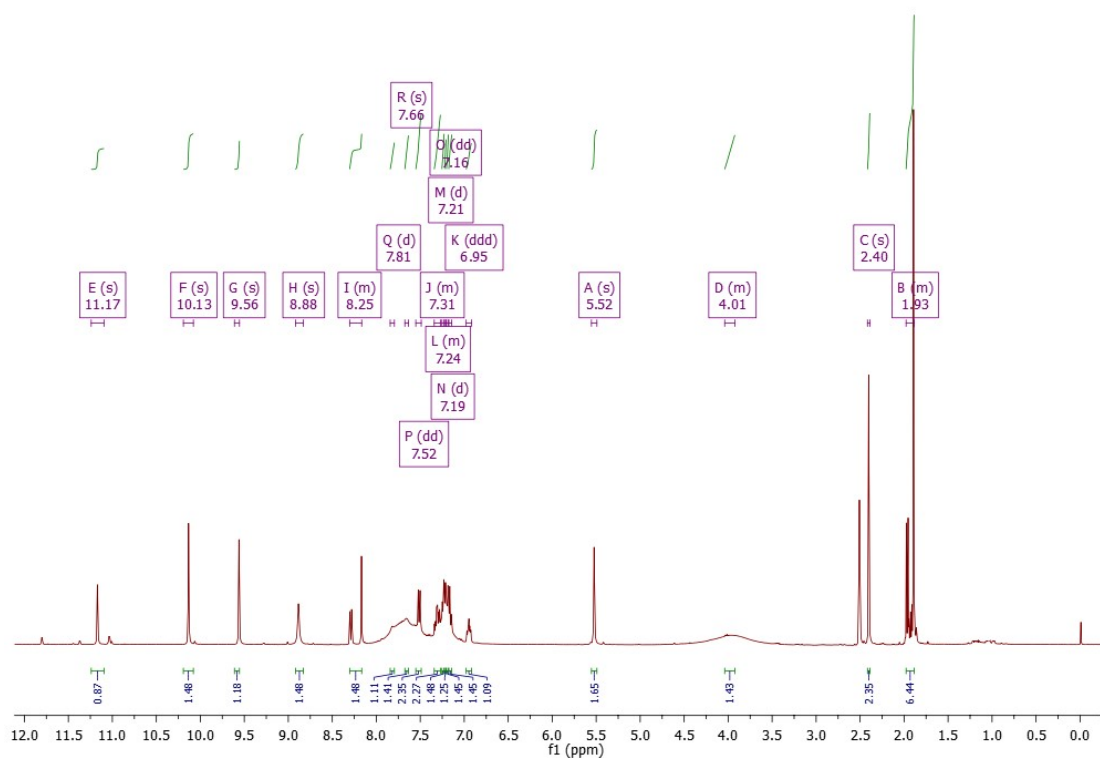
NMR spectrum of compound **3e** in DMSO- d_6 .

MS Zoomed Spectrum

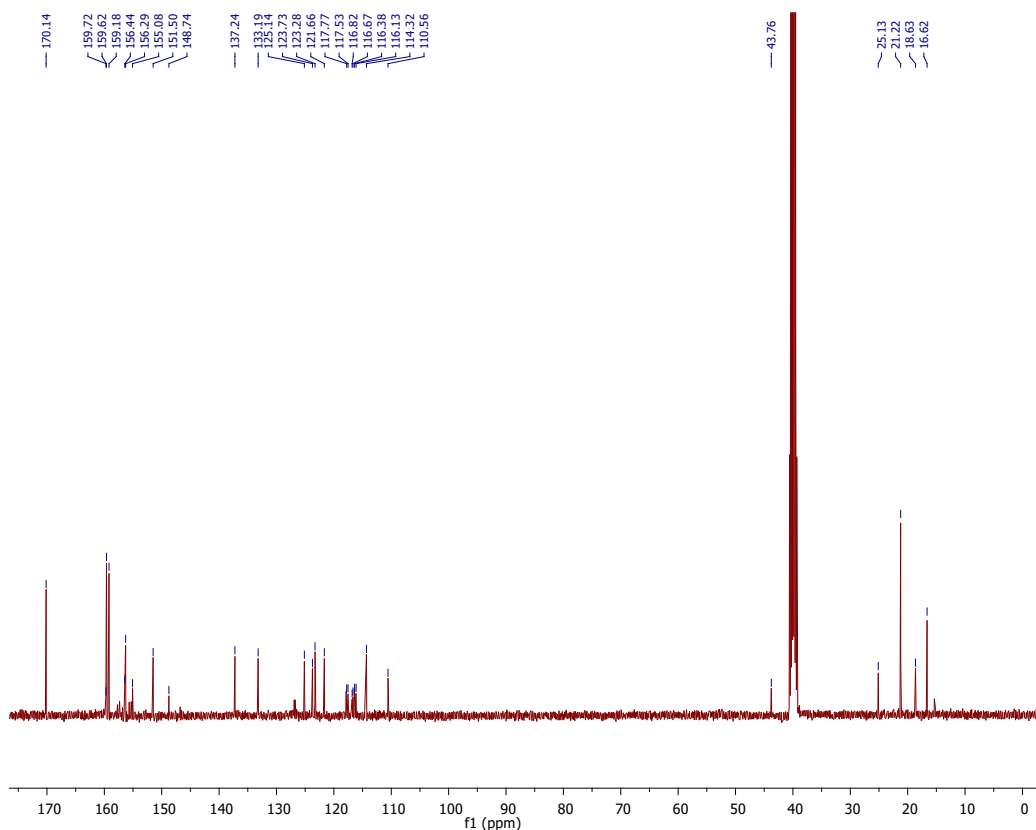


HRMS spectrum of compound **3e**.

¹H NMR spectrum of compound **3f** in DMSO-d₆.

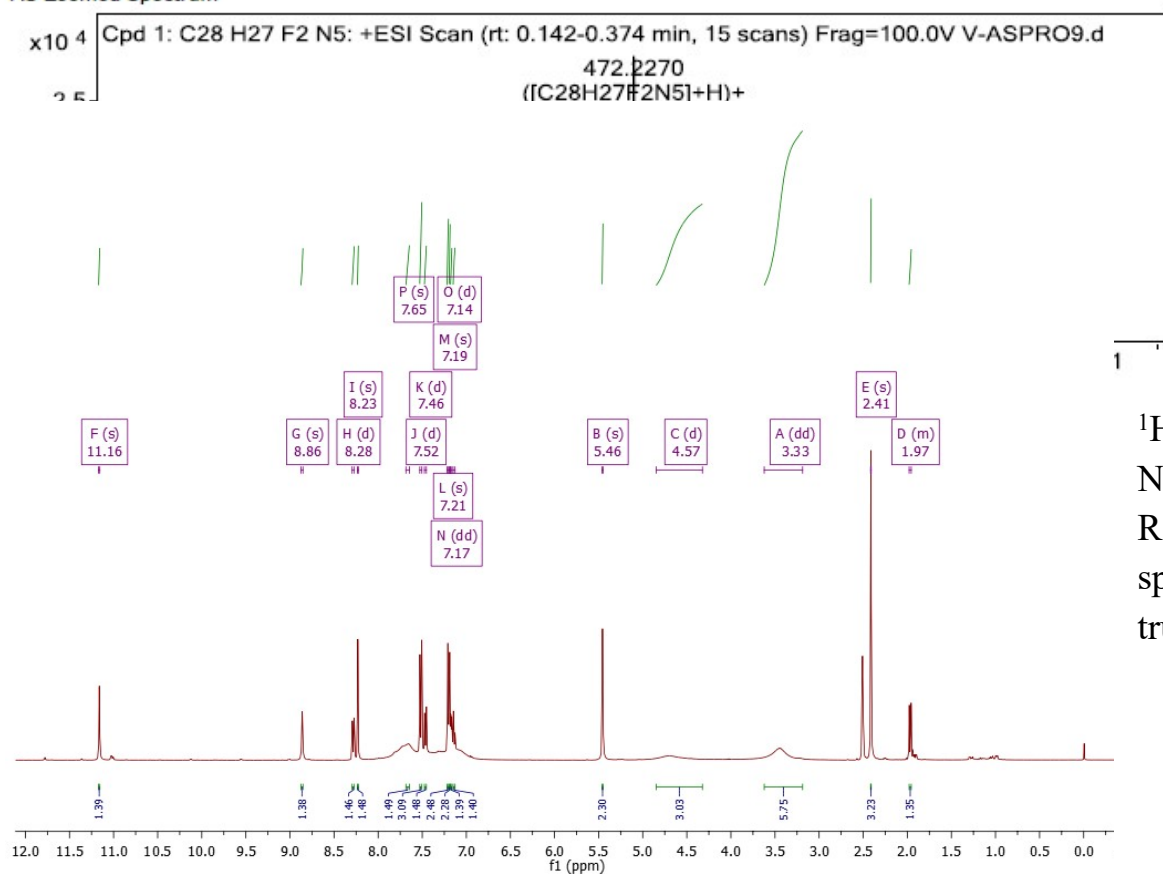


^{13}C NMR spectrum of compound **3f** in DMSO-d_6 .



HRMS spectrum of compound **3f**.

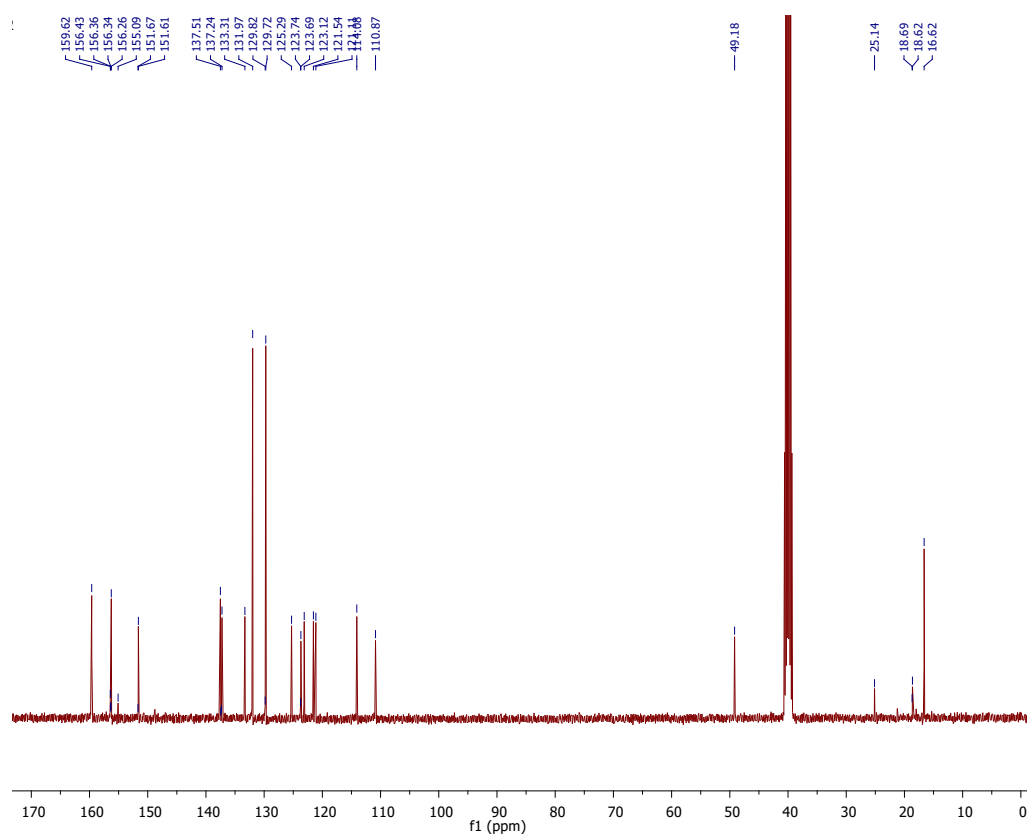
MS Zoomed Spectrum



^1H
NMR
spec
trum

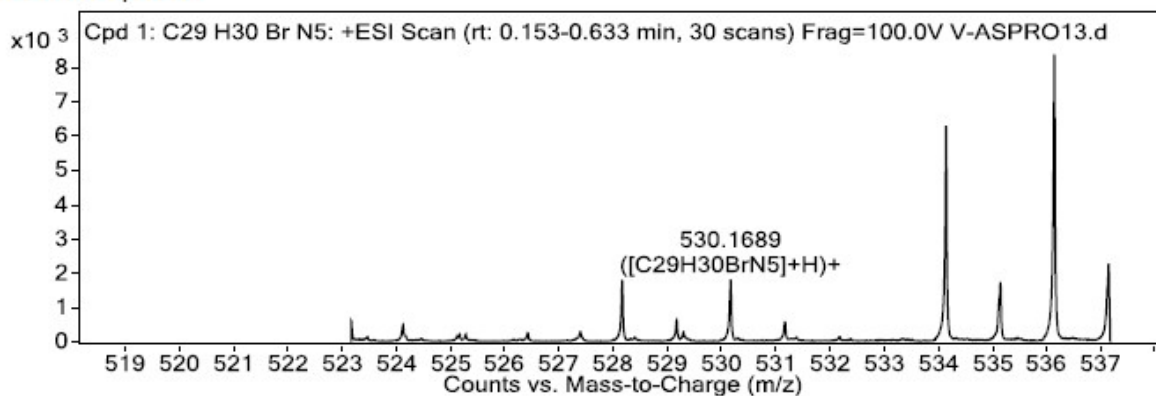
of compound **3g** in DMSO-d₆.

^{13}C



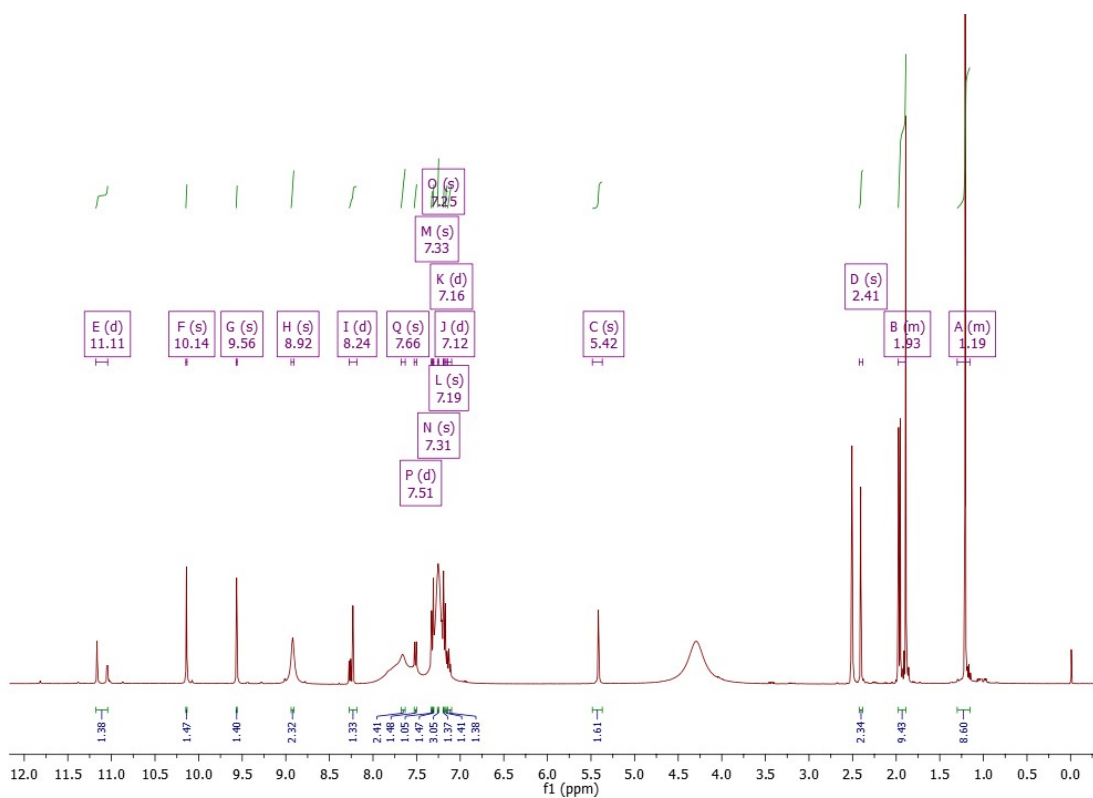
NMR spectrum of compound **3g** in DMSO-d_6 .

MS Zoomed Spectrum

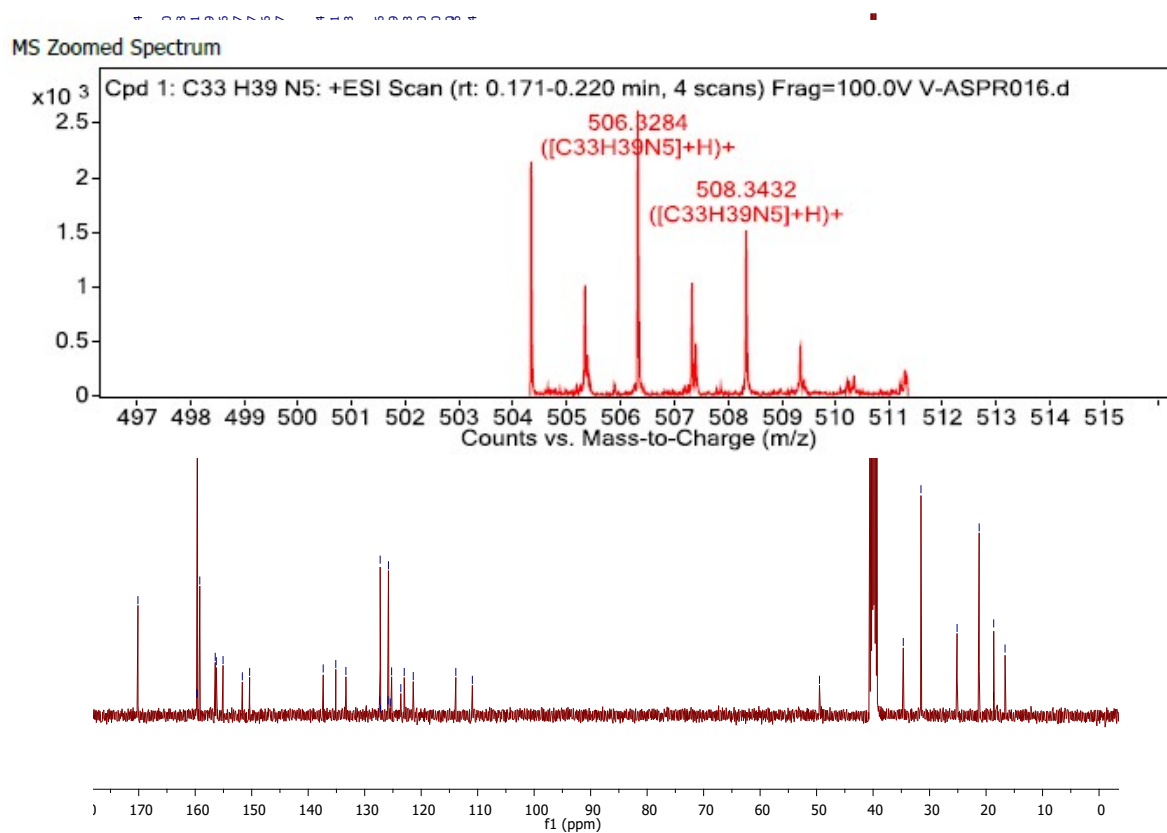


HRMS spectrum of compound **3g**.

¹H NMR spectrum of compound **3h** in DMSO-d₆.

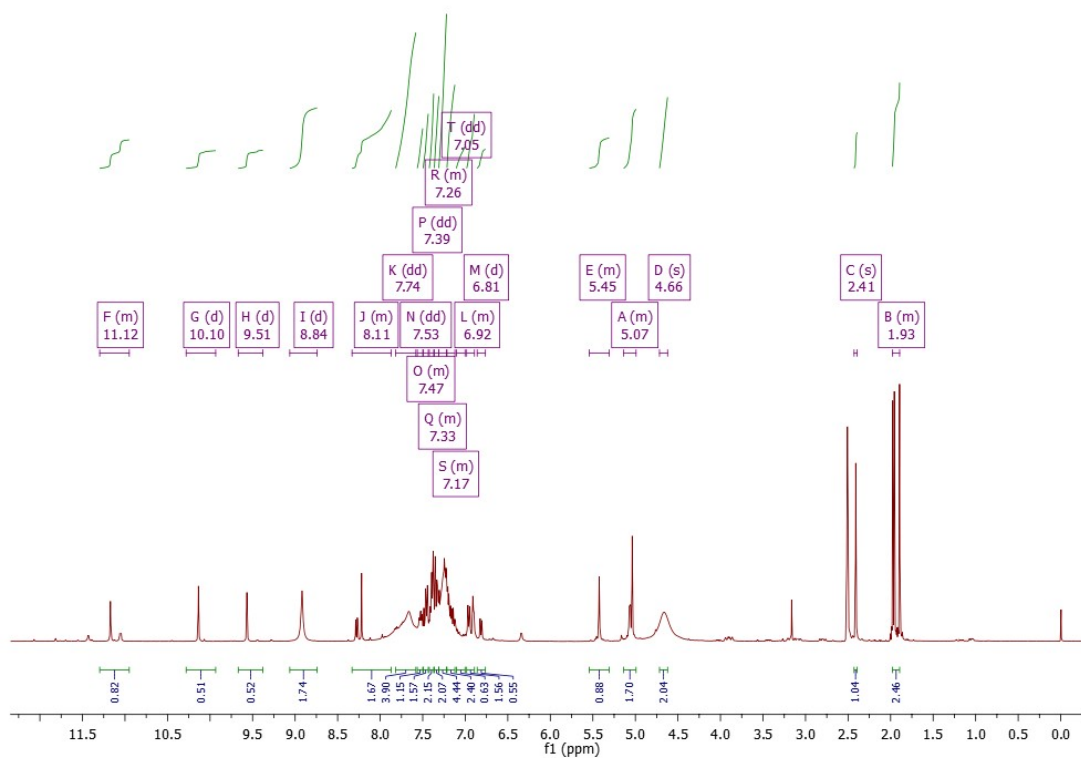


^{13}C NMR spectrum of compound **3h** in DMSO-d_6 .

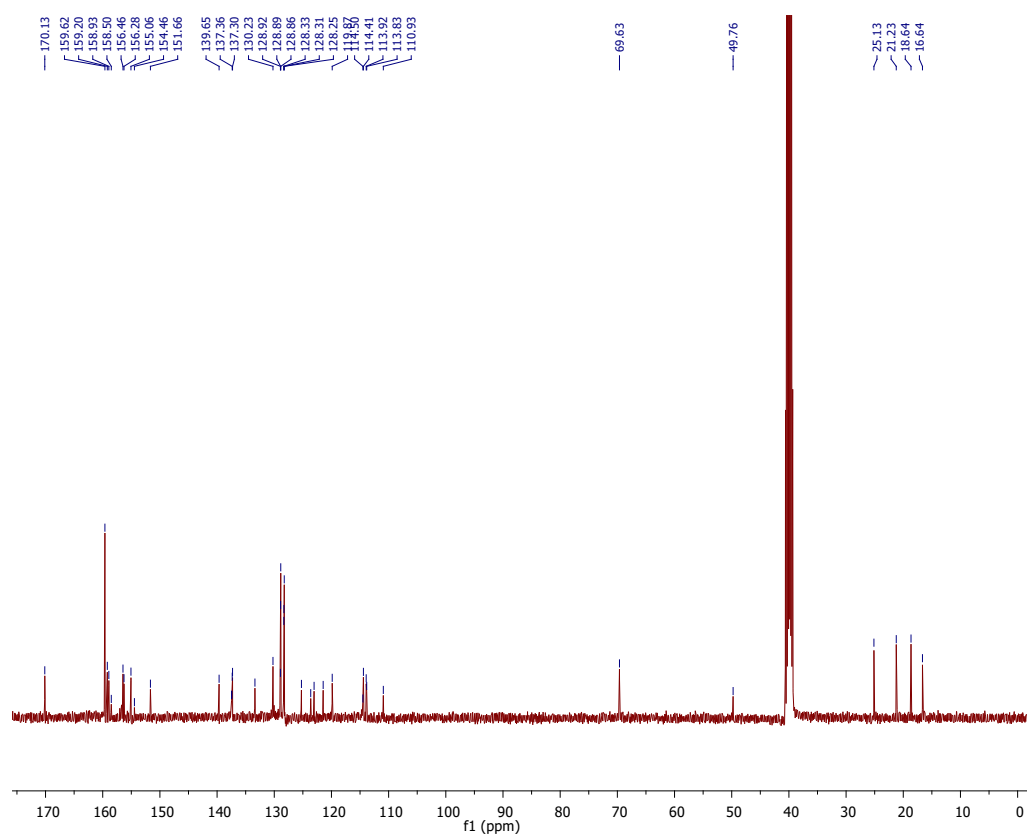


HRMS spectrum of compound **3h**.

^1H NMR spectrum of compound **3i** in DMSO-d_6 .

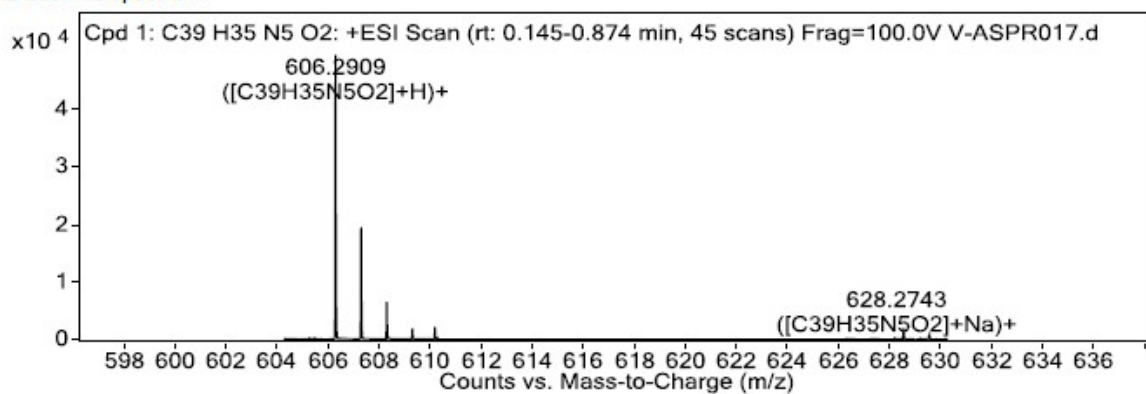


^{13}C



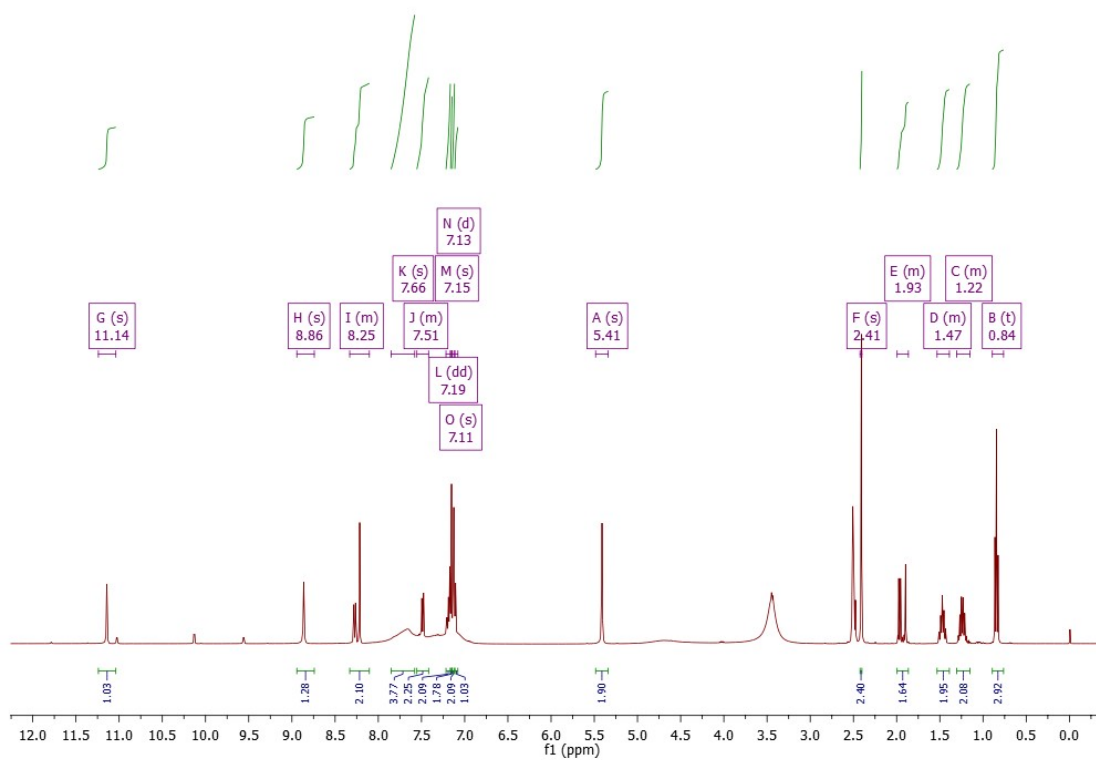
NMR spectrum of compound **3i** in DMSO- d_6 .

MS Zoomed Spectrum

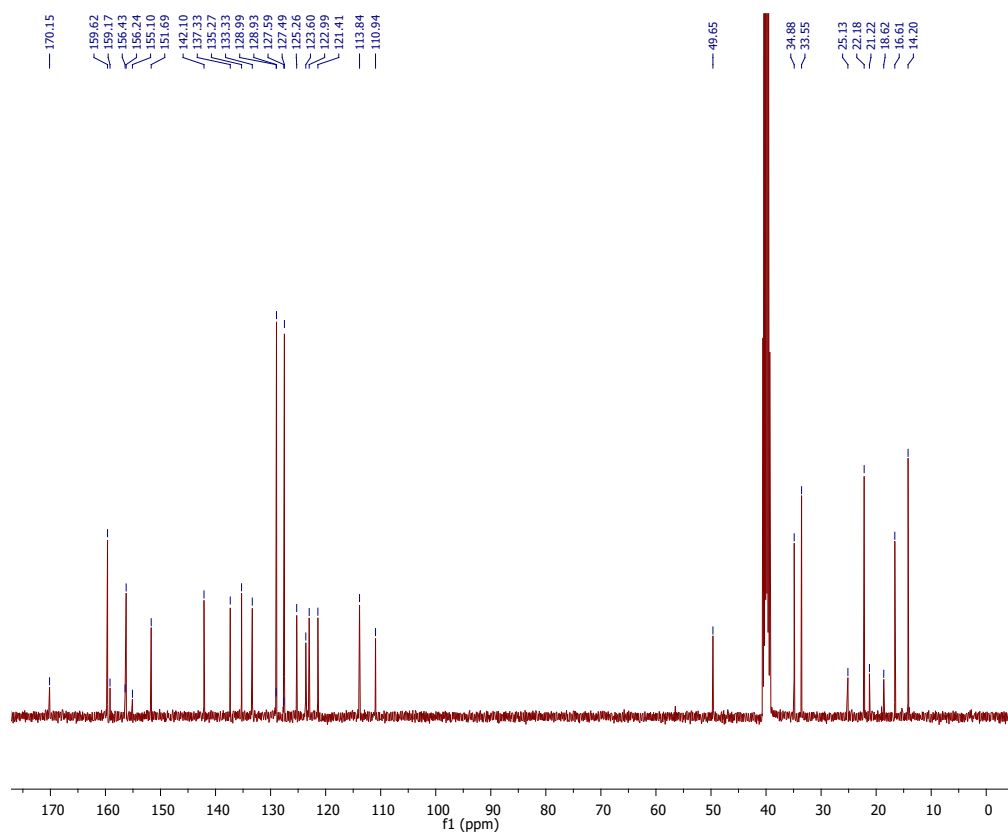


HRMS spectrum of compound **3i**.

¹H NMR spectrum of compound **3j** in DMSO-d₆.

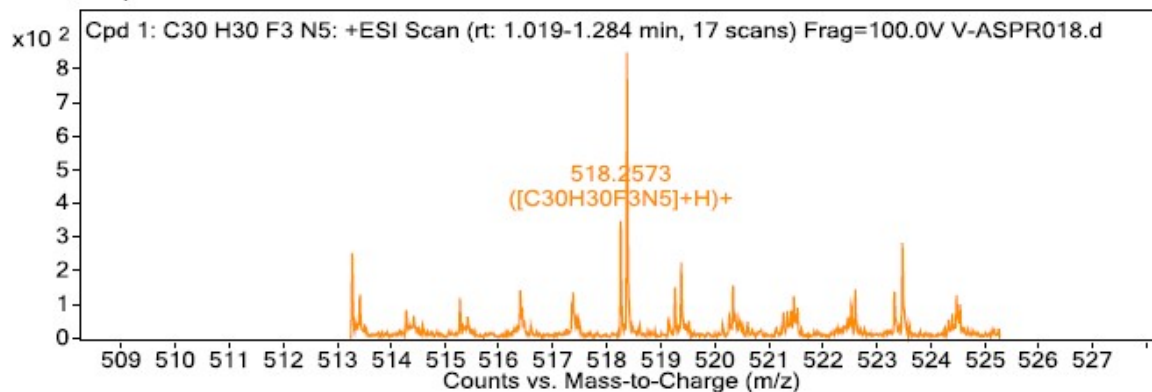


^{13}C



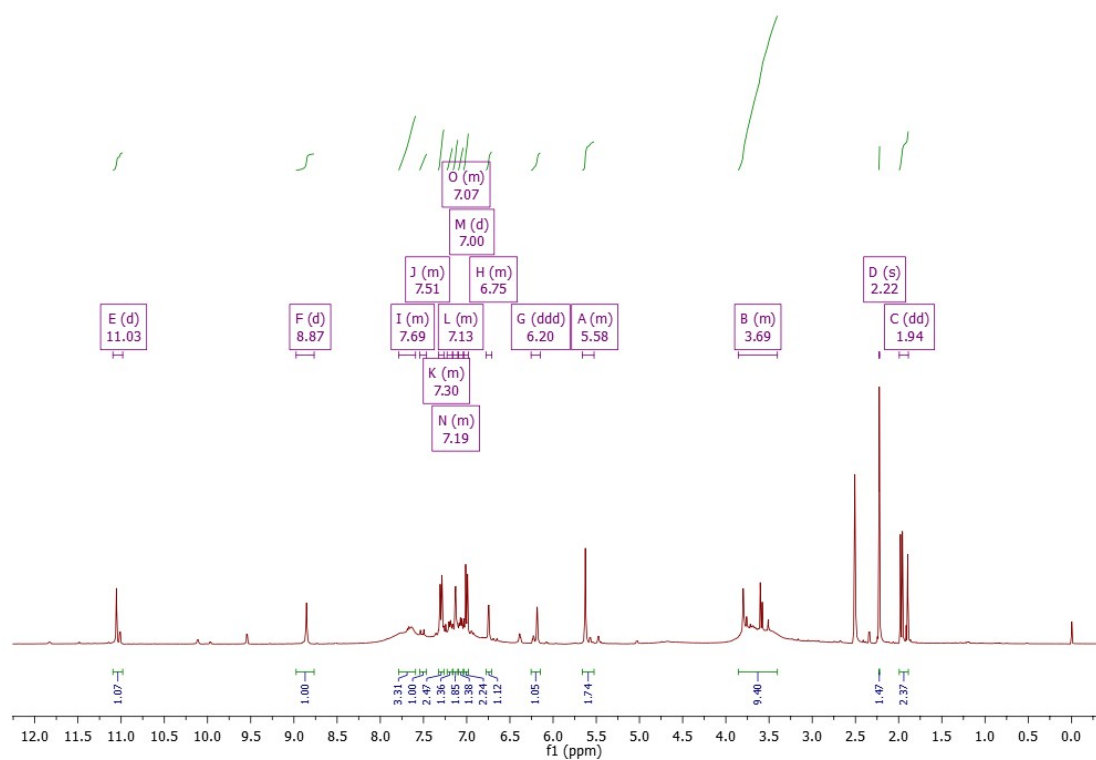
NMR spectrum of compound **3j** in DMSO- d_6 .

MS Zoomed Spectrum

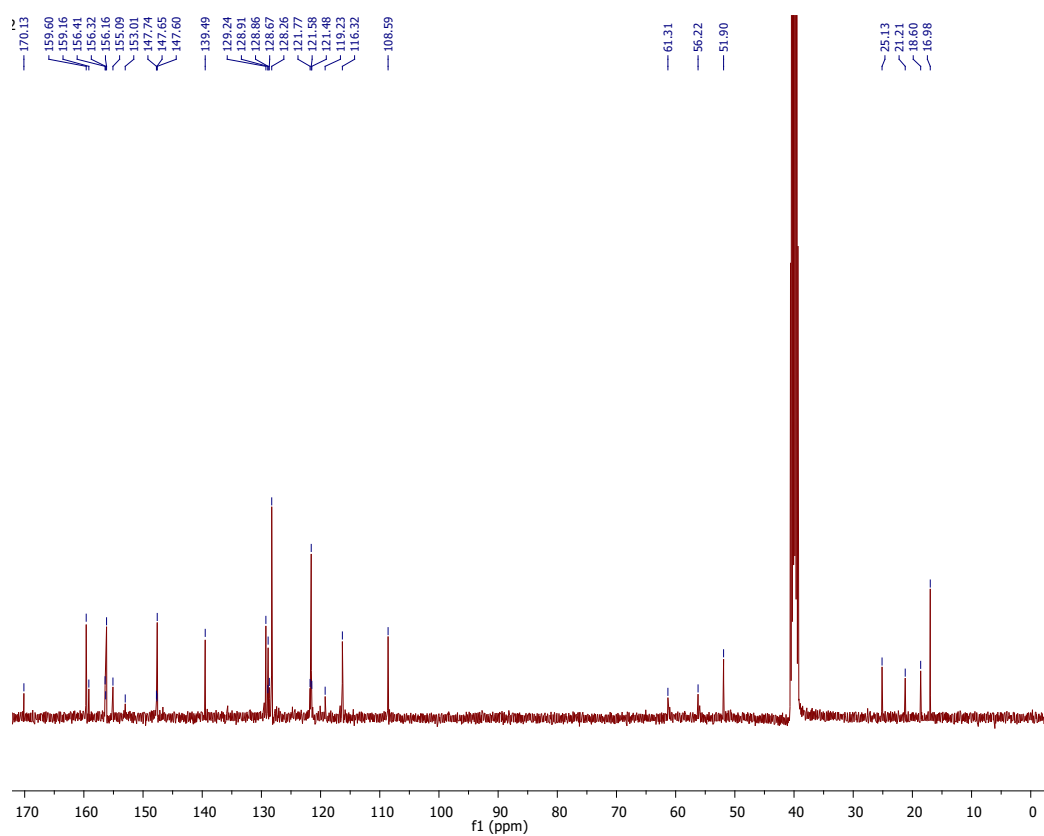


HRMS spectrum of compound **3j**.

¹H NMR spectrum of compound **3k** in DMSO-d₆.

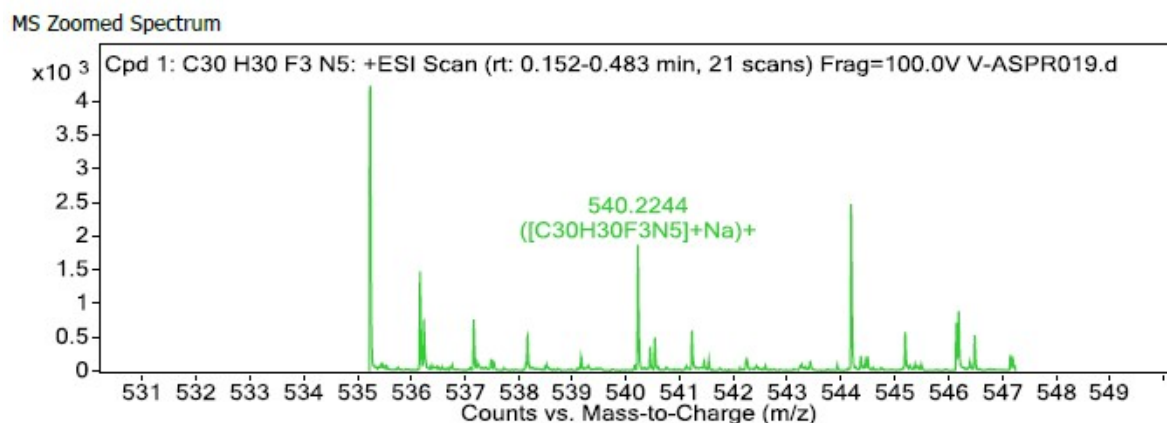


^{13}C

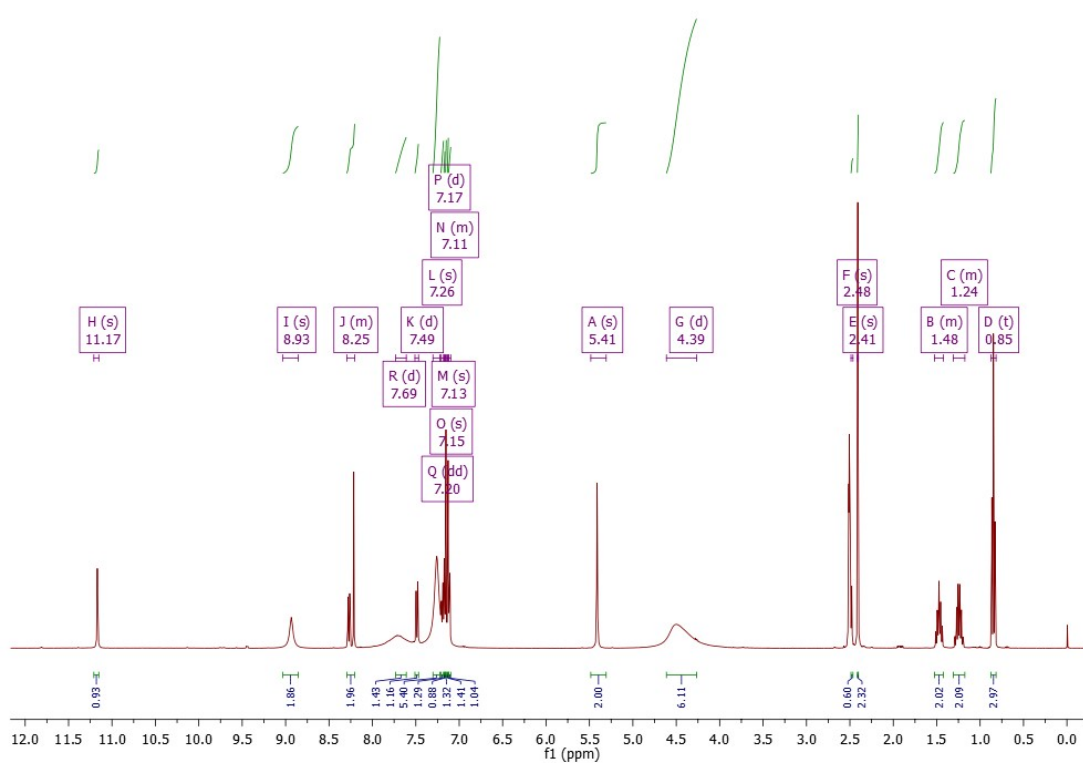


NMR spectrum of compound **3k** in DMSO-d_6 .

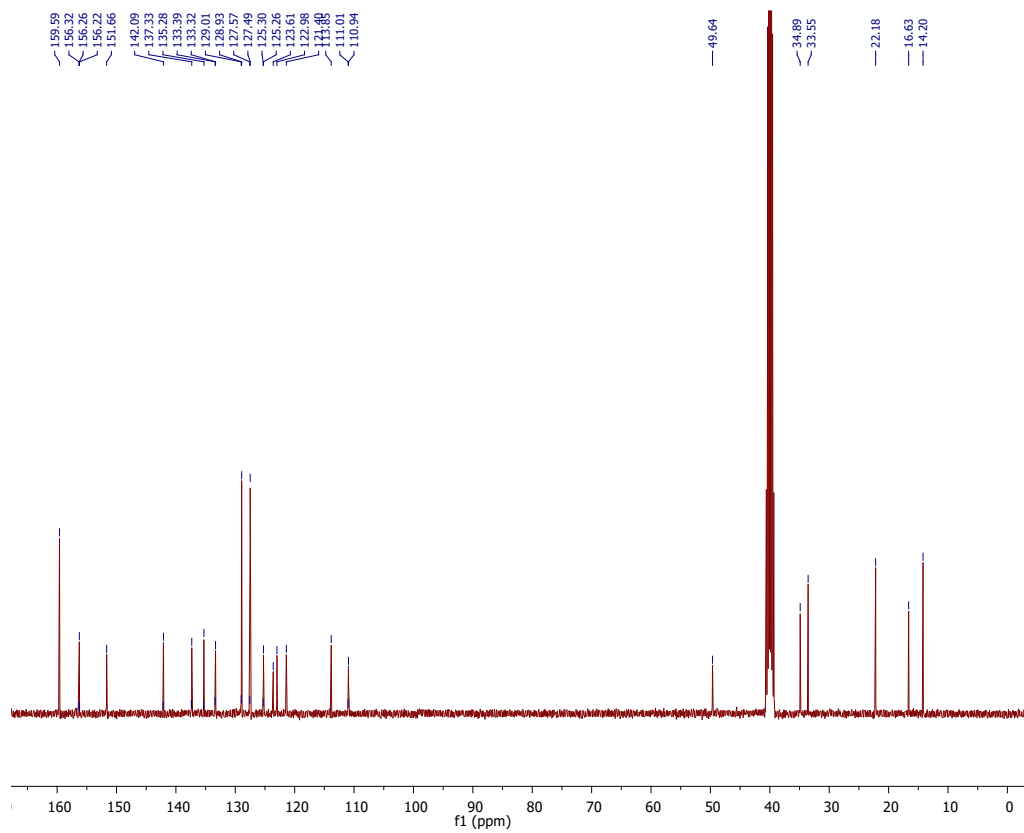
HRMS spectrum of compound **3k**.



¹H NMR spectrum of compound **3l** in DMSO-d₆.

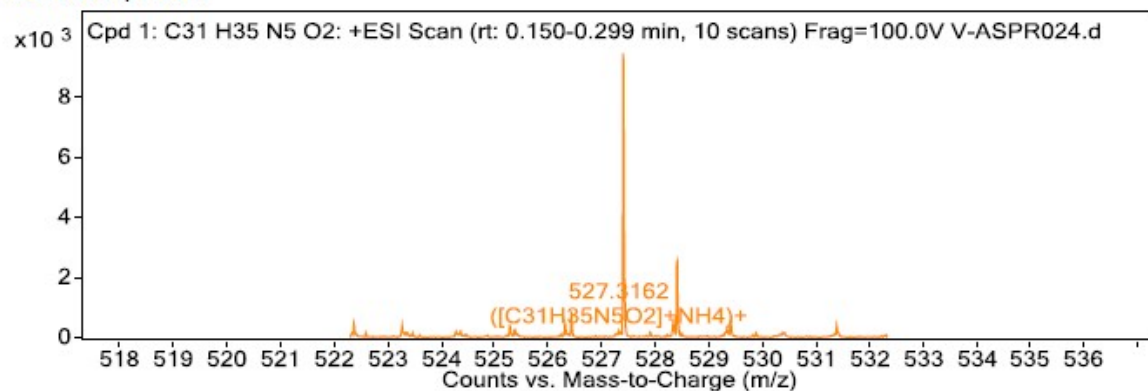


^{13}C



NMR spectrum of compound **31** in DMSO- d_6 .

MS Zoomed Spectrum



HRMS spectrum of compound **3l**.