

Supporting Information

Total Synthesis of (±)-Auranthine Confirmed its Refined Structure

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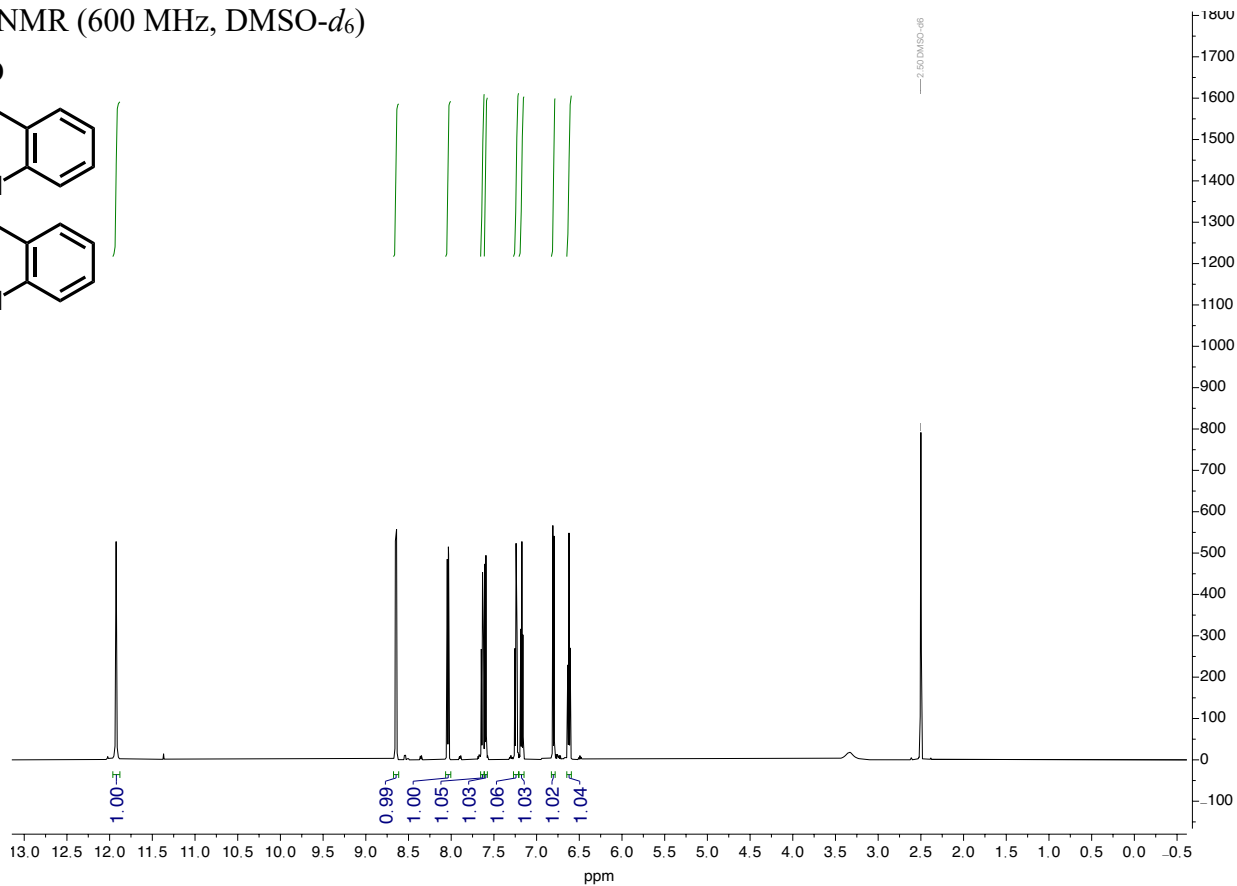
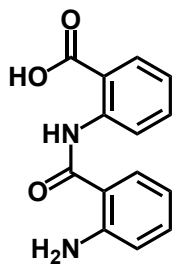
Tel.: +49-251-8333392; E-mail: s_kali03@uni-muenster.de (S.A.K.).

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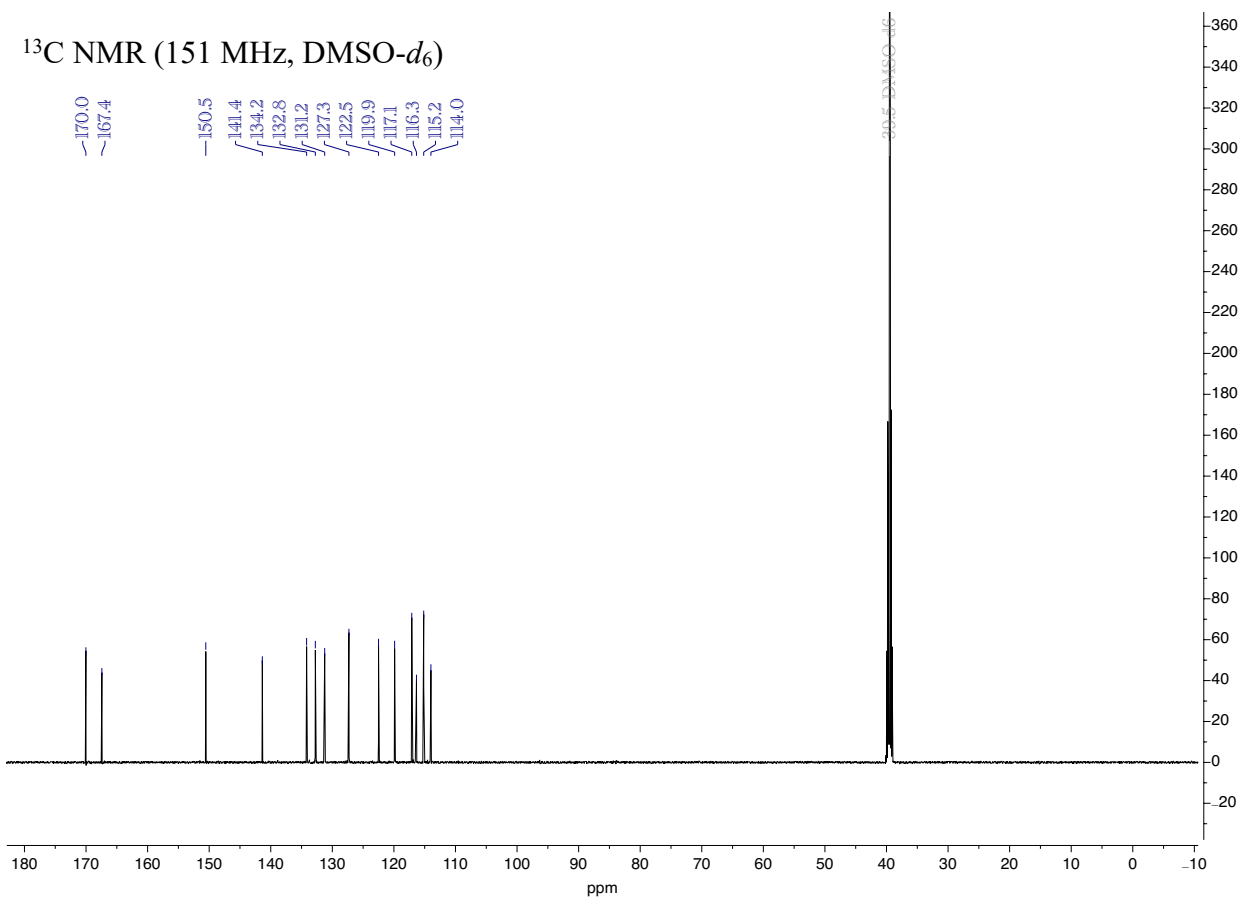
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¹³ C NMR spectrum of 10	S3
¹ H NMR spectrum of 14	S4
¹³ C NMR spectrum of 14	S4
¹ H NMR spectrum of 15	S5
¹³ C NMR spectrum of 15	S5
¹ H NMR spectrum of 11	S6
¹³ C NMR spectrum of 11	S6
¹ H NMR spectrum of 12	S7
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2-(2-Aminobenzamido)benzoic acid (10)

^1H NMR (600 MHz, DMSO- d_6)

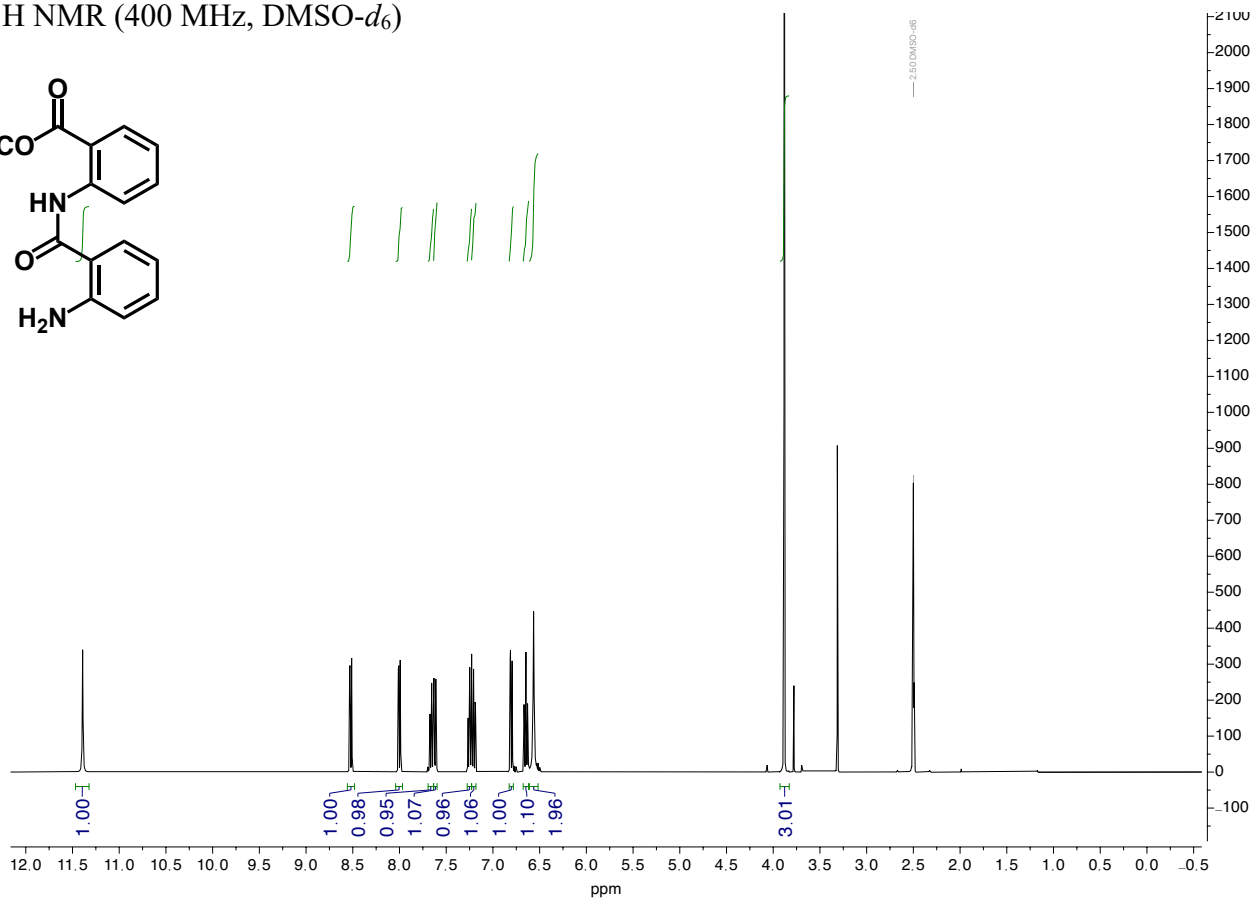
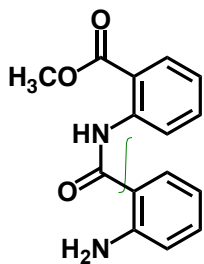


^{13}C NMR (151 MHz, DMSO- d_6)

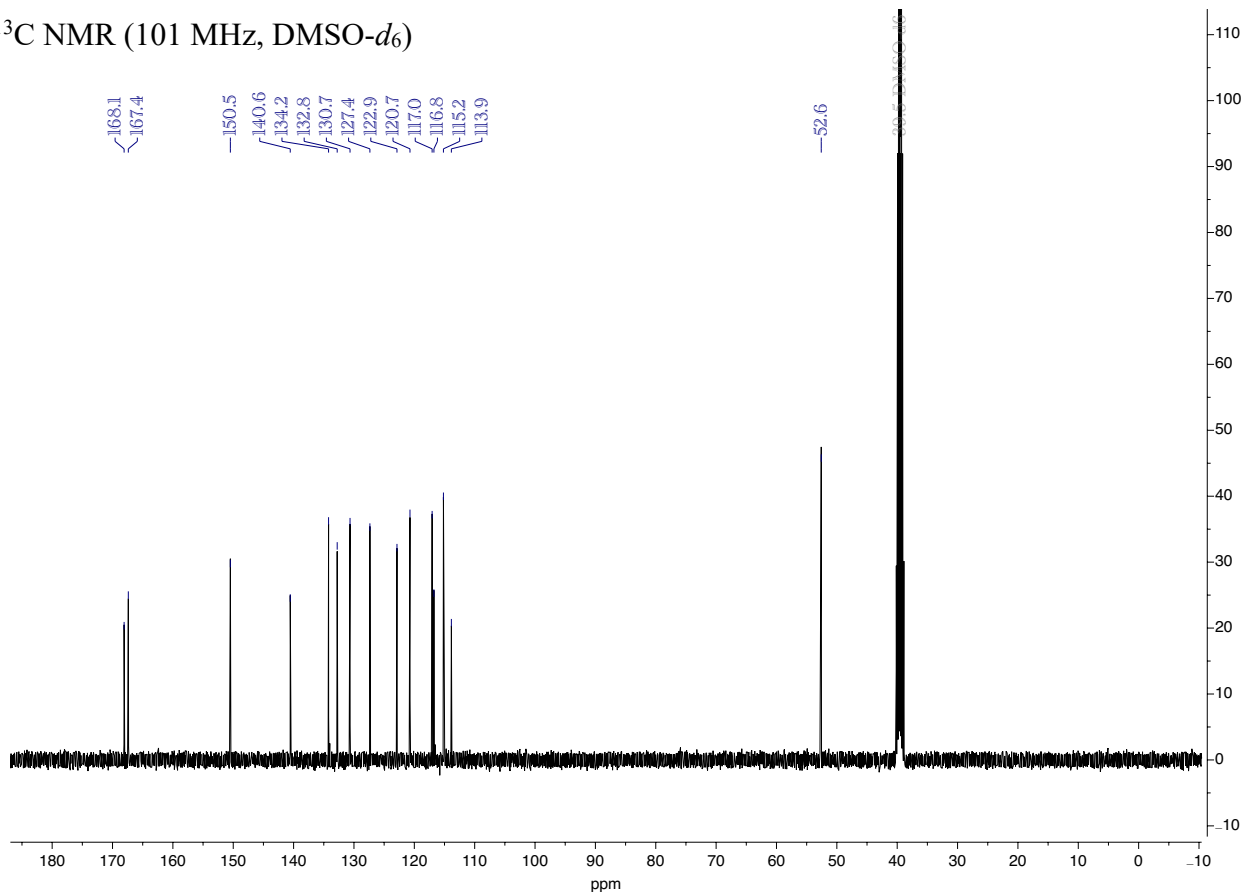


Methyl 2-(2-aminobenzoylamino)benzoate (14)

^1H NMR (400 MHz, $\text{DMSO-}d_6$)

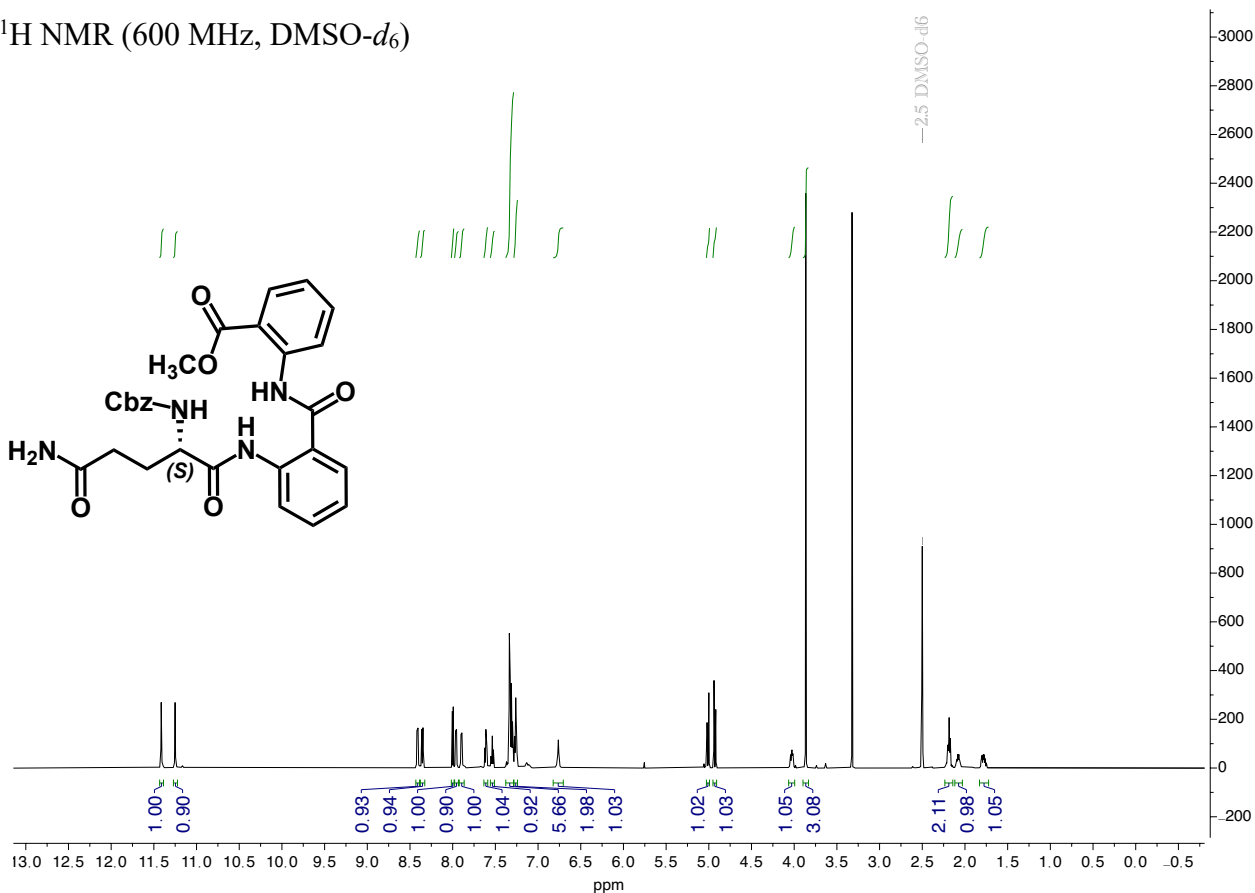


^{13}C NMR (101 MHz, $\text{DMSO-}d_6$)

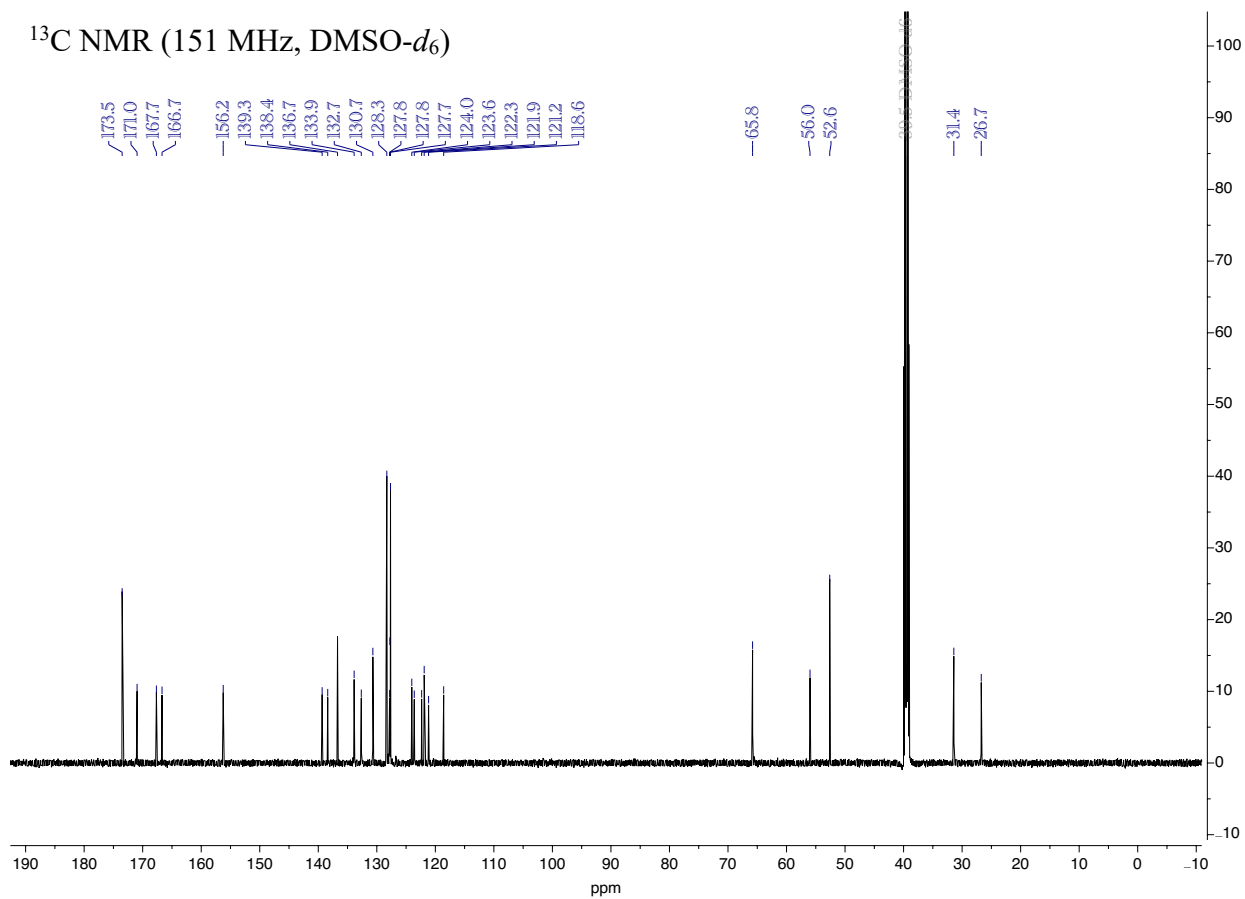


Methyl (S)-2-(2-(5-amino-2-(((benzyloxy)carbonyl)amino)-5-oxopentanamido)benzamido)benzoate (15)

¹H NMR (600 MHz, DMSO-d₆)

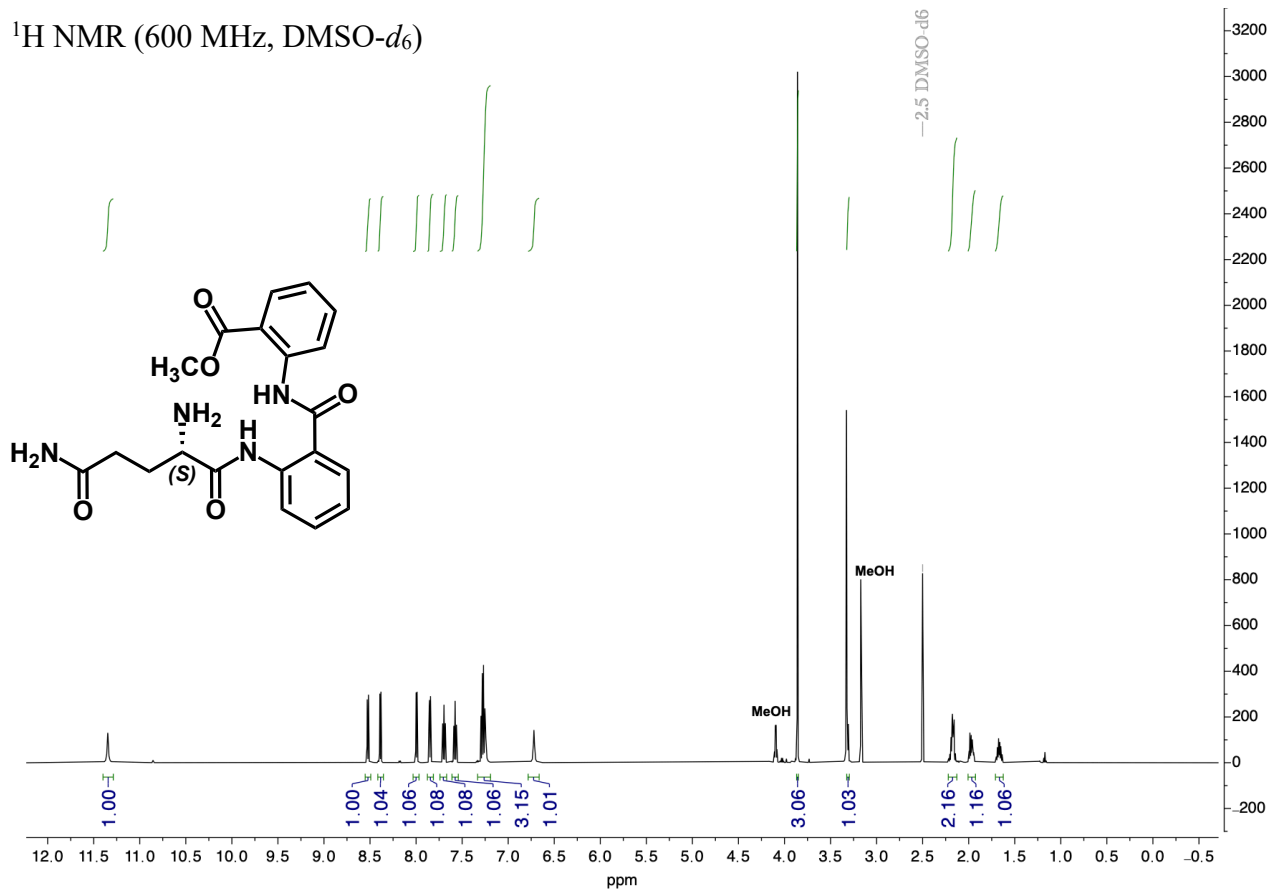


¹³C NMR (151 MHz, DMSO-d₆)

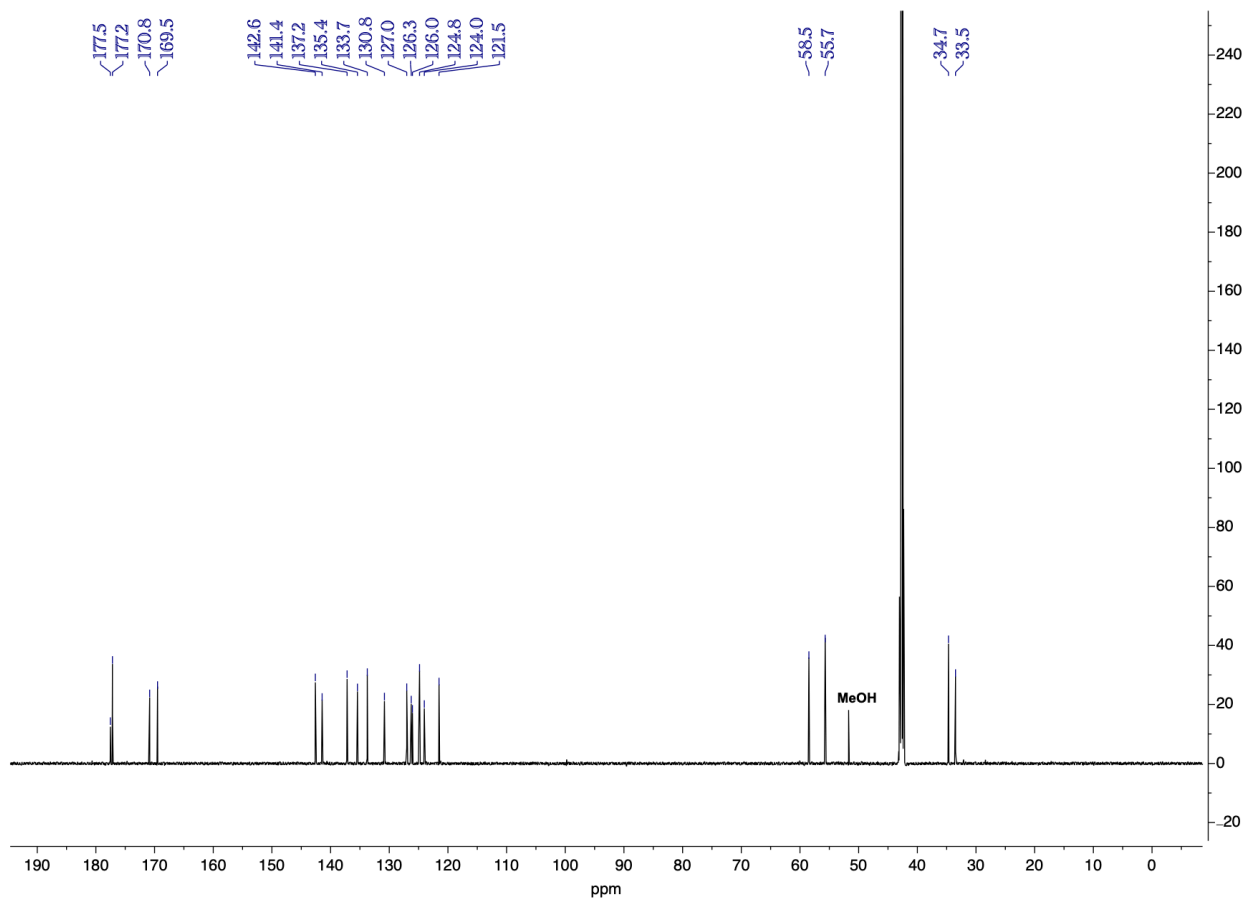


Methyl (S)-2-(2-(2,5-diamino-5-oxopentanamido)benzamido)benzoate (11)

^1H NMR (600 MHz, $\text{DMSO-}d_6$)

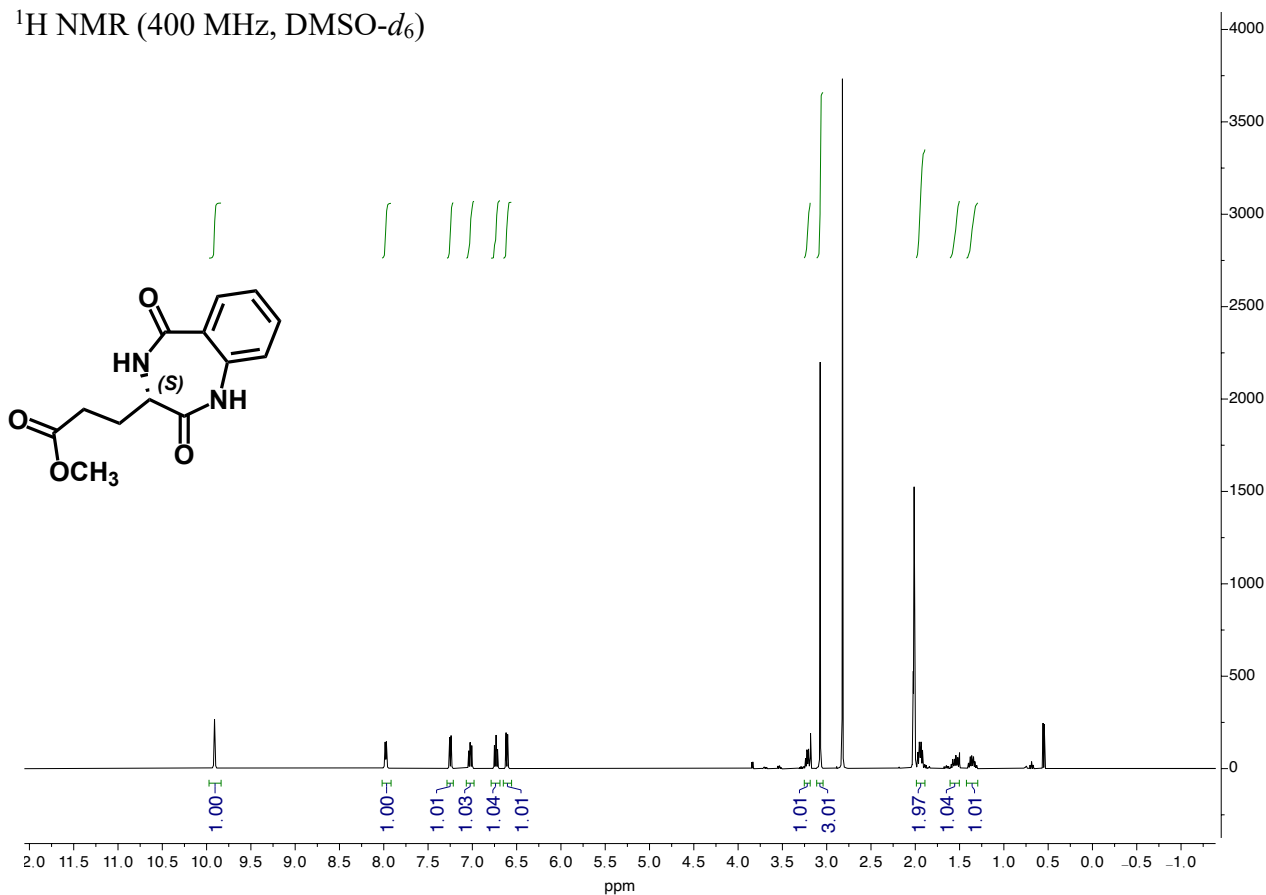


^{13}C NMR (151 MHz, $\text{DMSO-}d_6$)

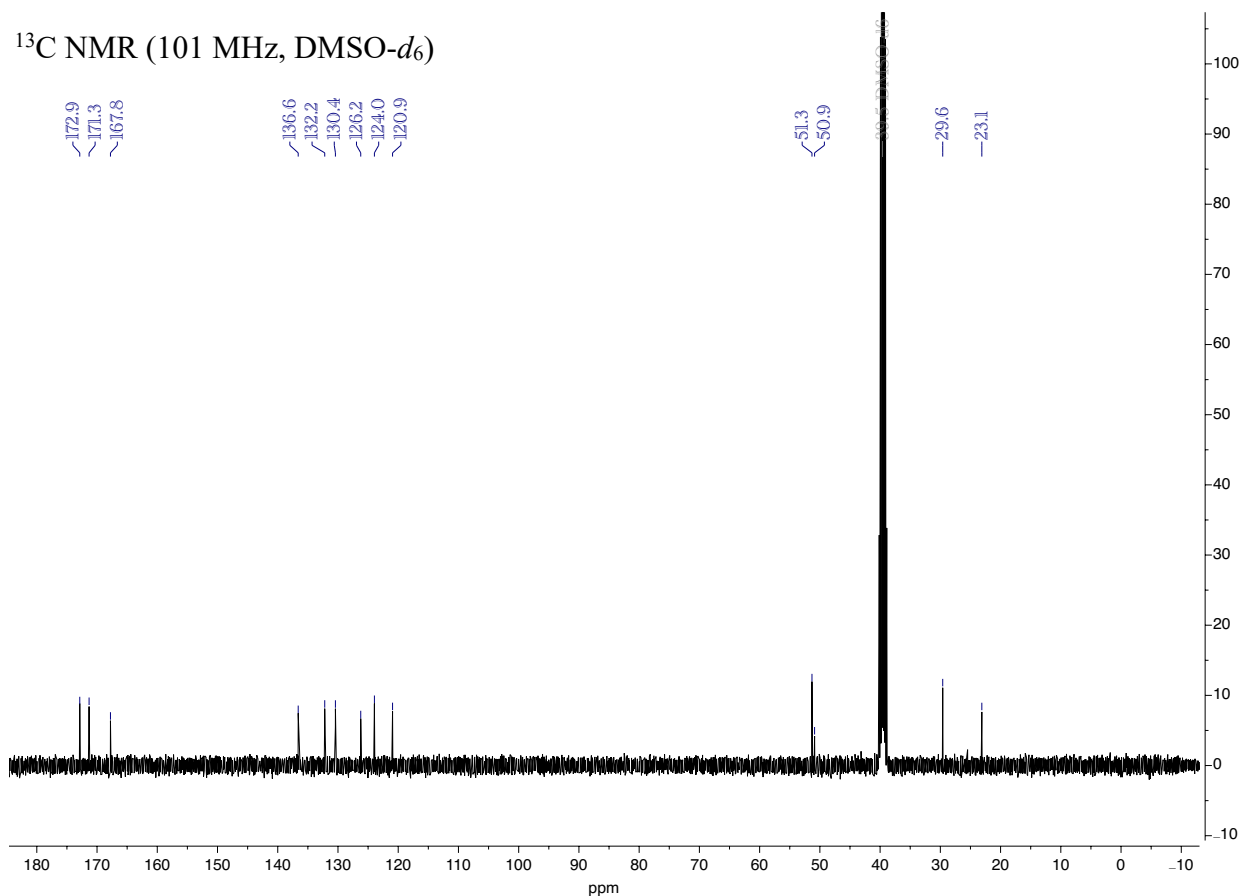


Methyl (S)-3-(2,5-Dioxo-2,3,4,5-tetrahydro-1H-1,4-benzodiazepin-3-yl) propanoate (12)

^1H NMR (400 MHz, $\text{DMSO-}d_6$)

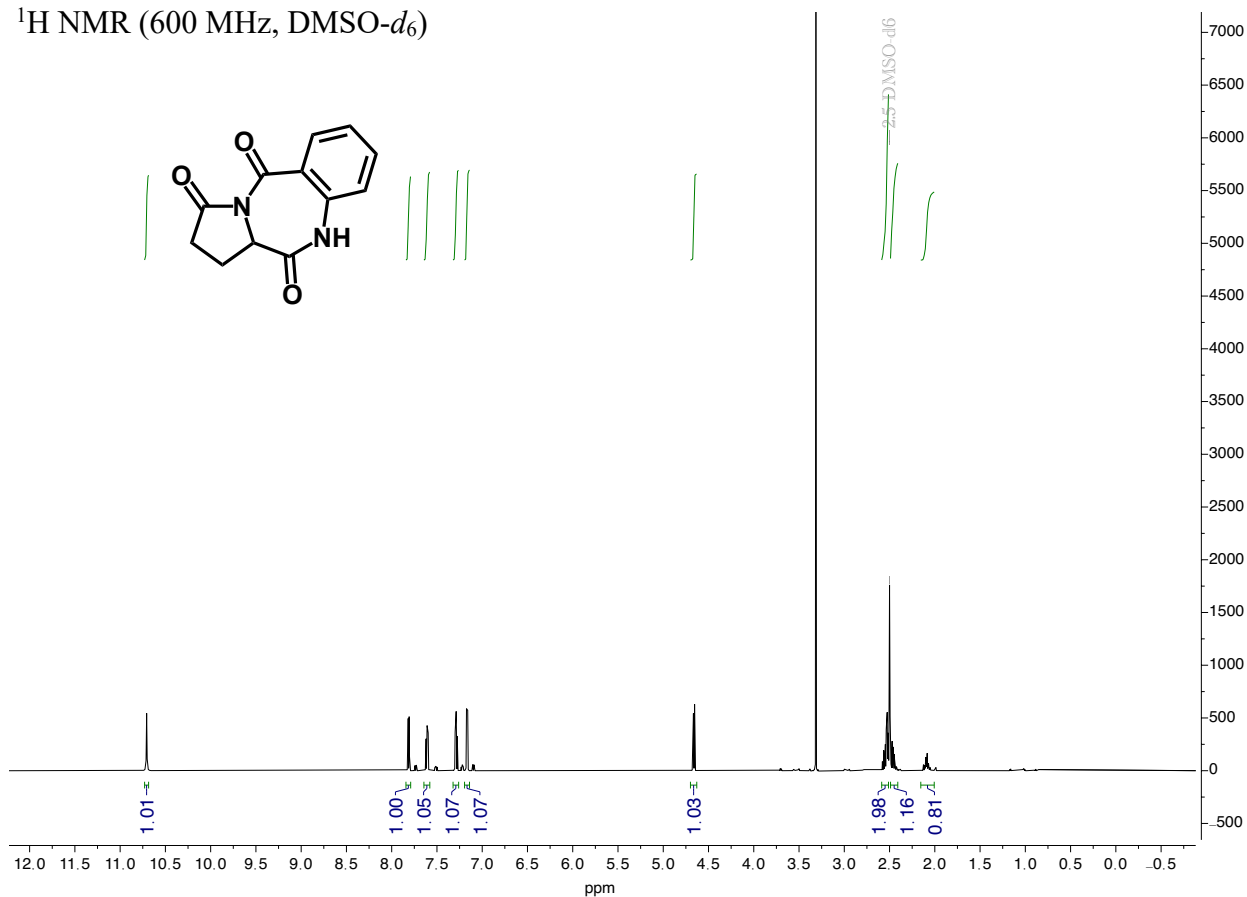


^{13}C NMR (101 MHz, $\text{DMSO-}d_6$)

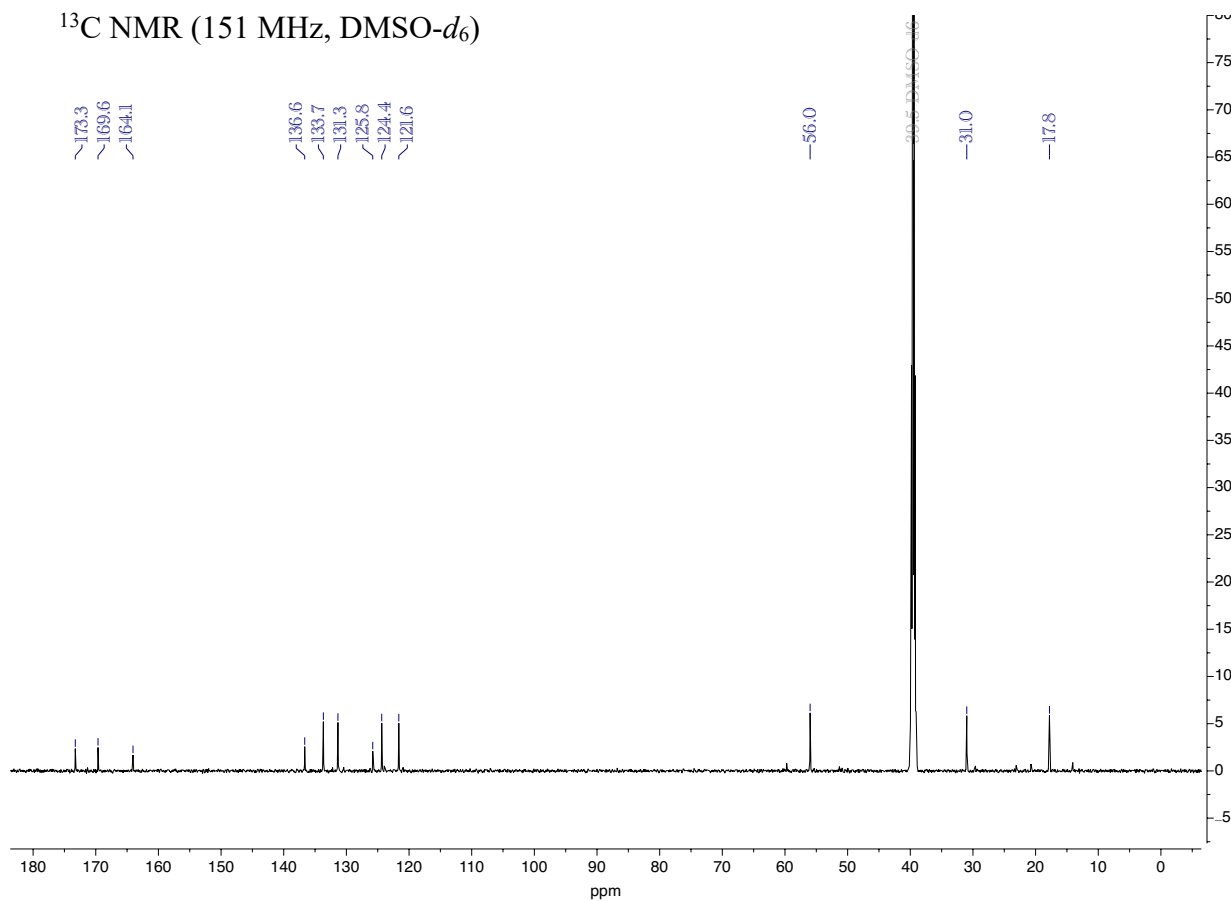


(±)-1,11a-Dihydro-3H-benzo[e]pyrrolo[1,2-a][1,4]diazepine-3,5,11(2H,10H)-trione (16)

¹H NMR (600 MHz, DMSO-*d*₆)

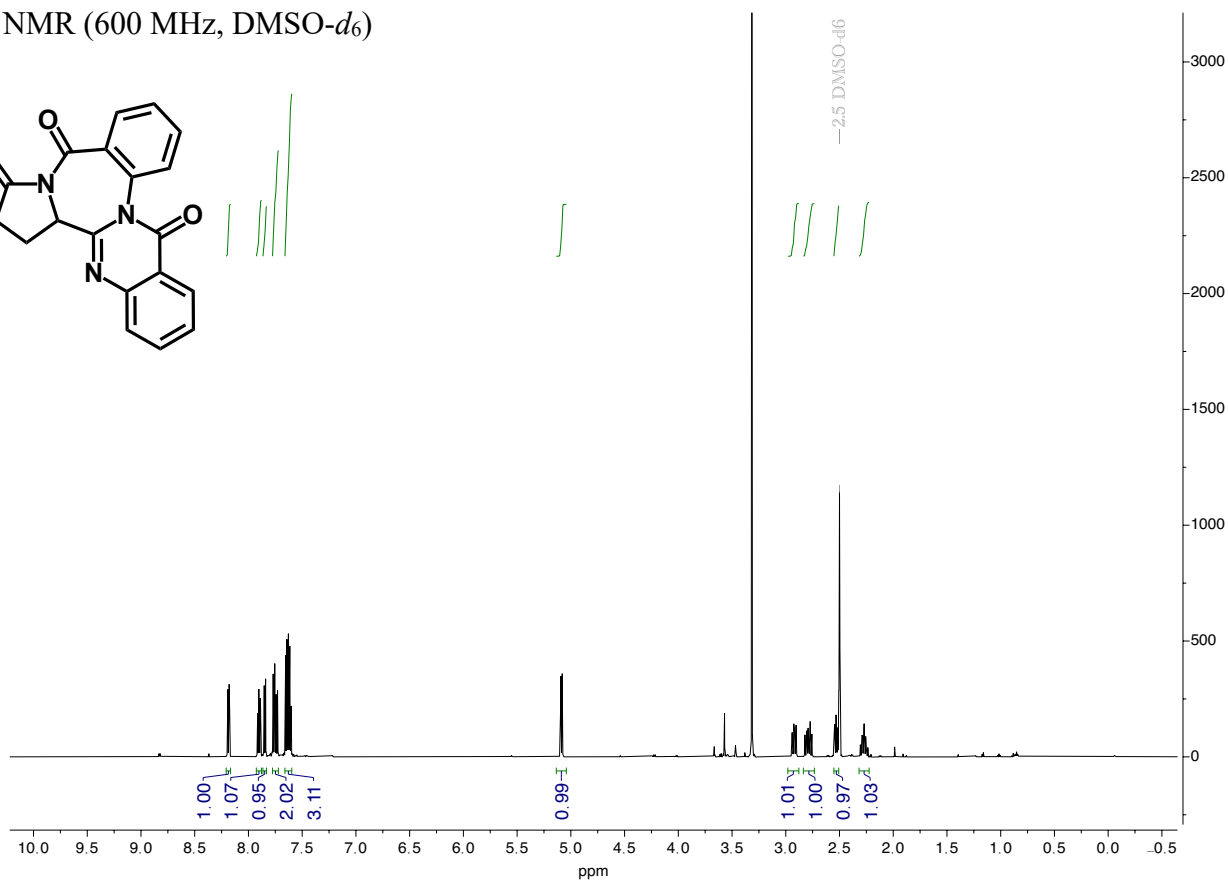
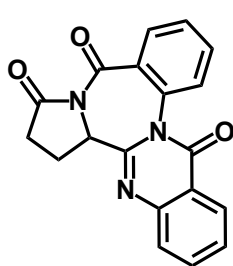


¹³C NMR (151 MHz, DMSO-*d*₆)

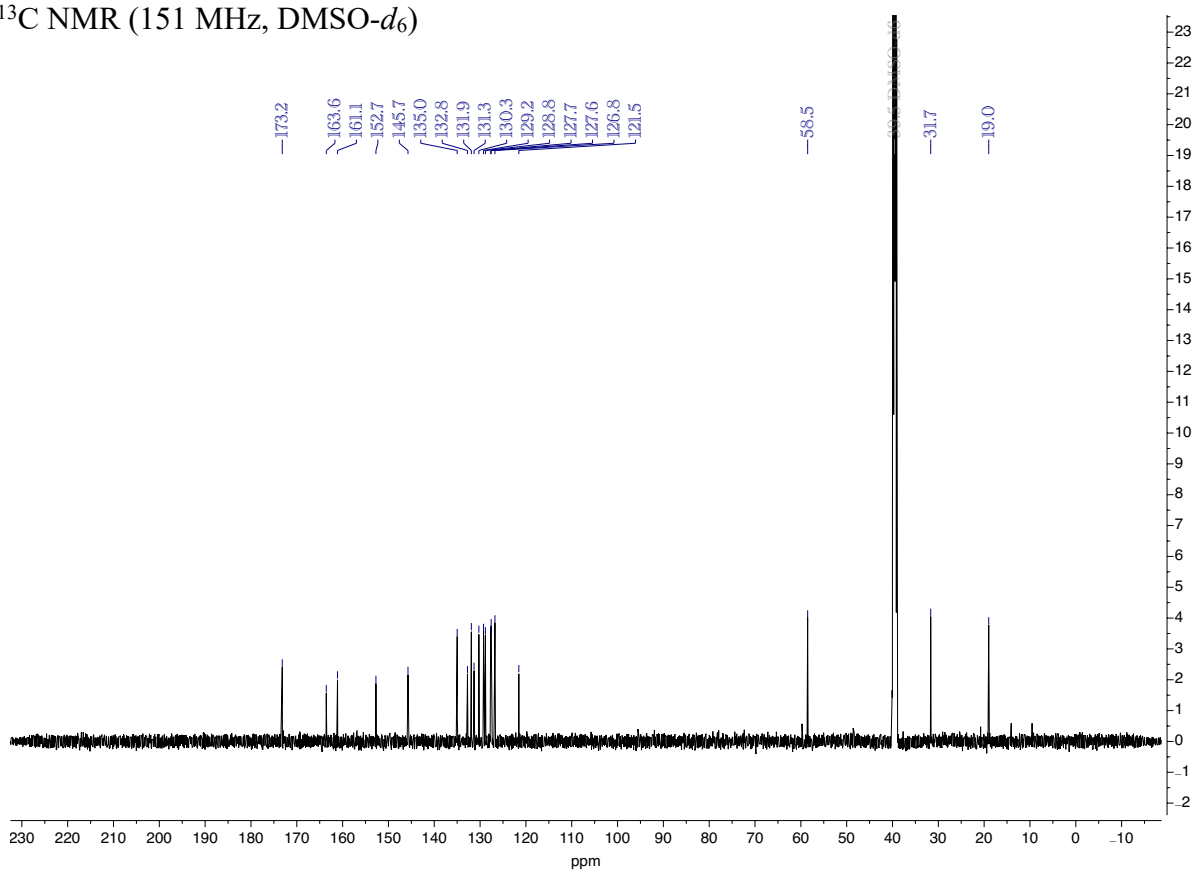


(±)-6,7-Dihydro-8*H*,10*H*-benzo[6,7]pyrrolo[2',1':3,4][1,4]diazepino[2,1-*b*]quinazoline-8,10,16(5*bH*)-trione (13')

¹H NMR (600 MHz, DMSO-*d*₆)

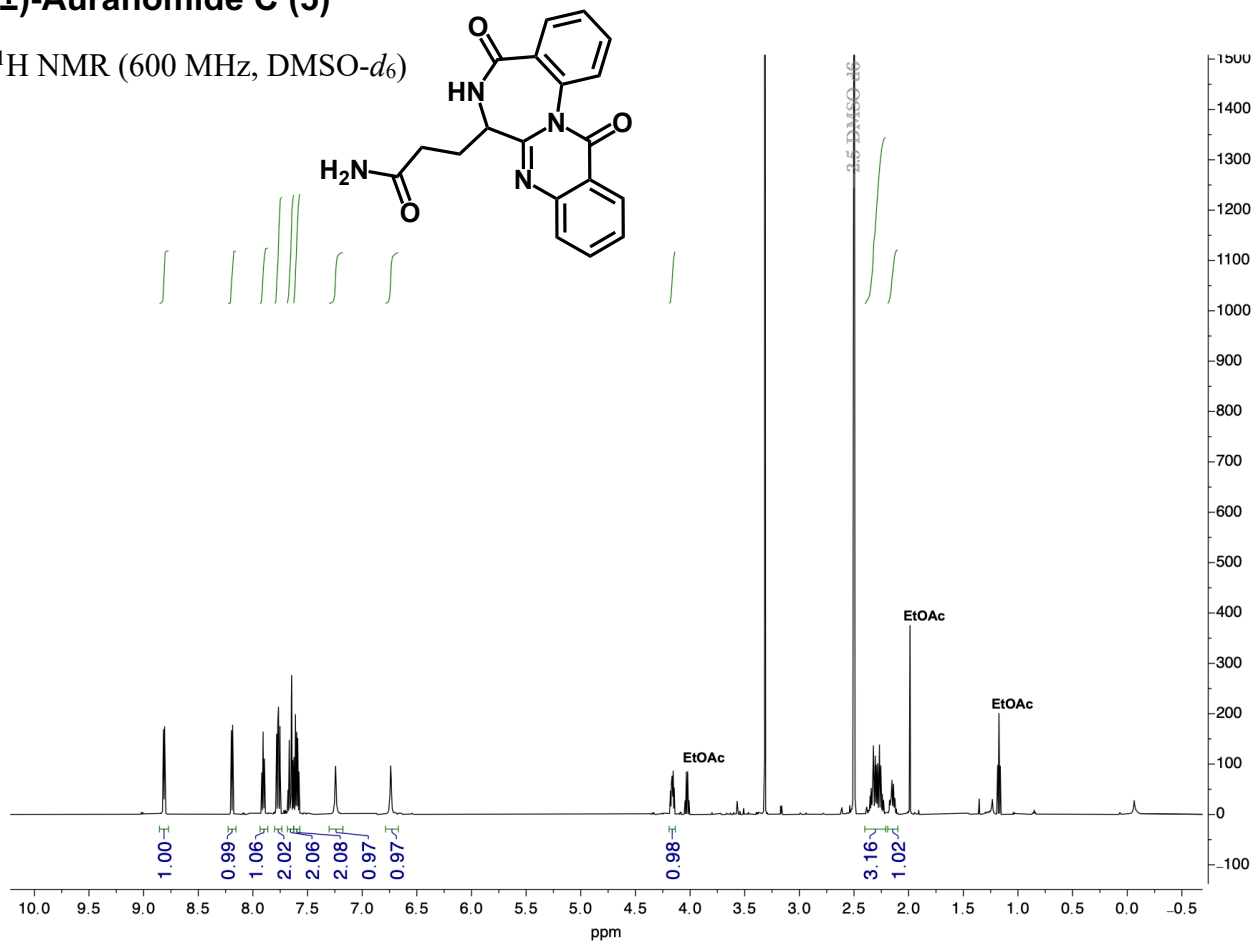


¹³C NMR (151 MHz, DMSO-*d*₆)

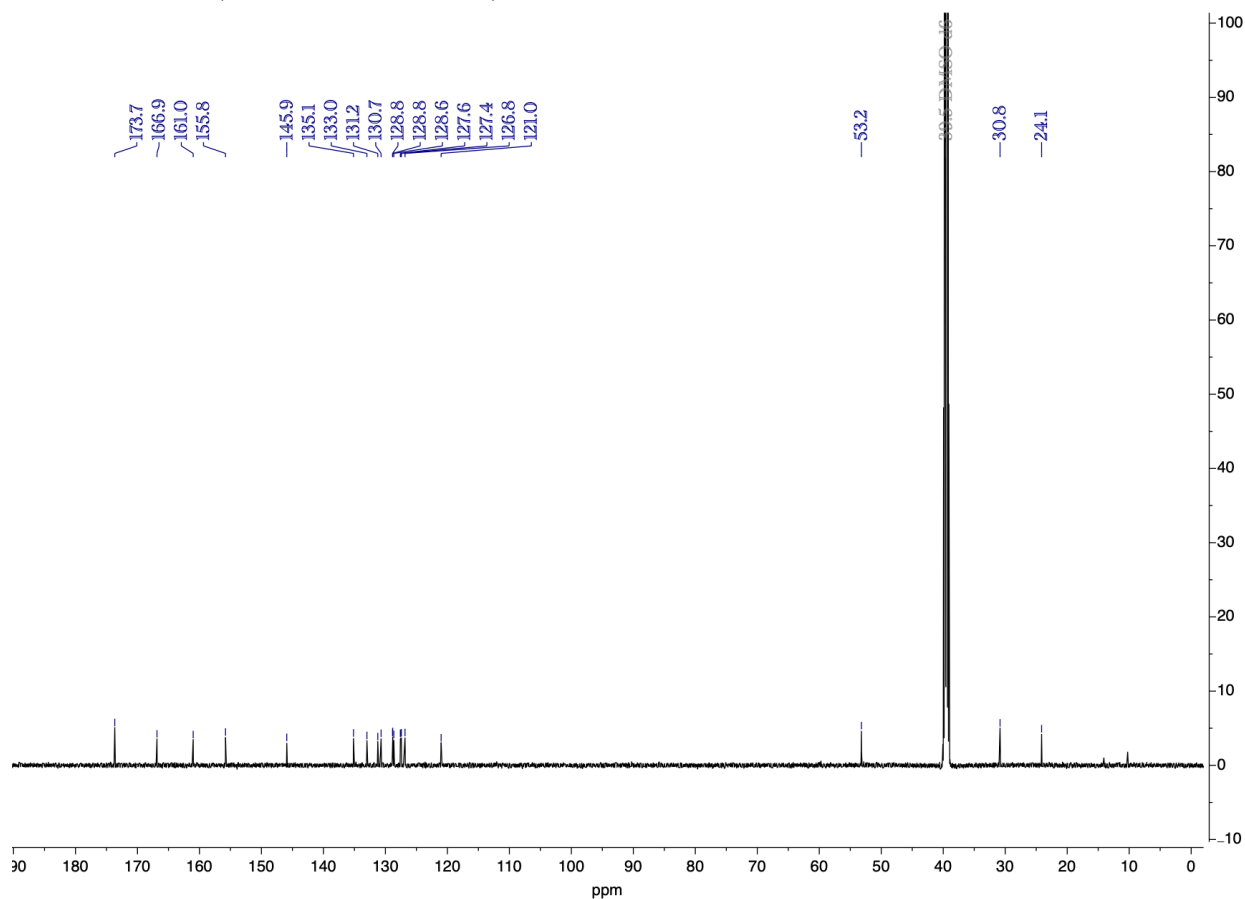


(±)-Auranomide C (5)

¹H NMR (600 MHz, DMSO-d₆)

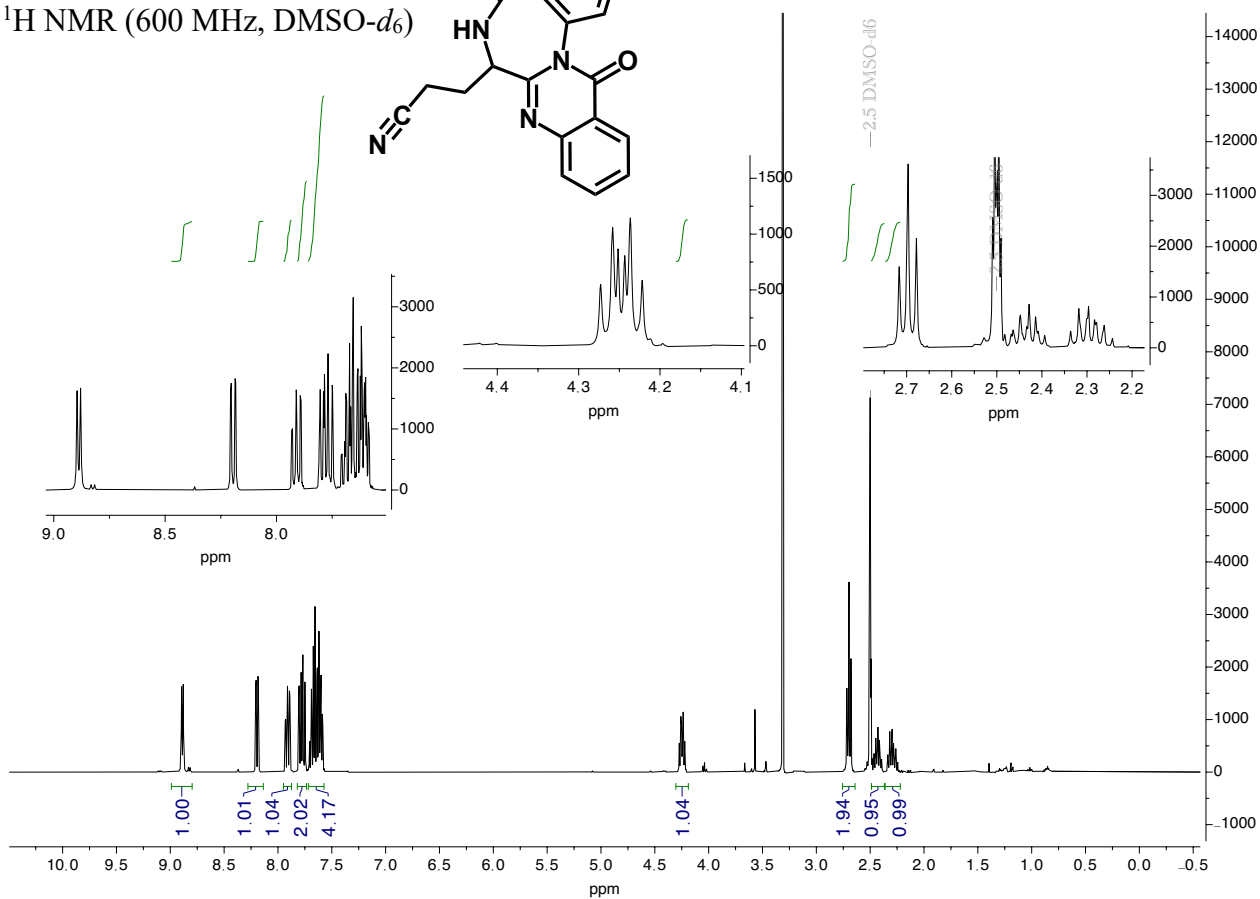
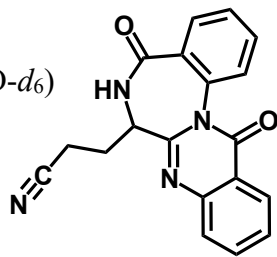


¹³C NMR (151 MHz, DMSO-d₆)

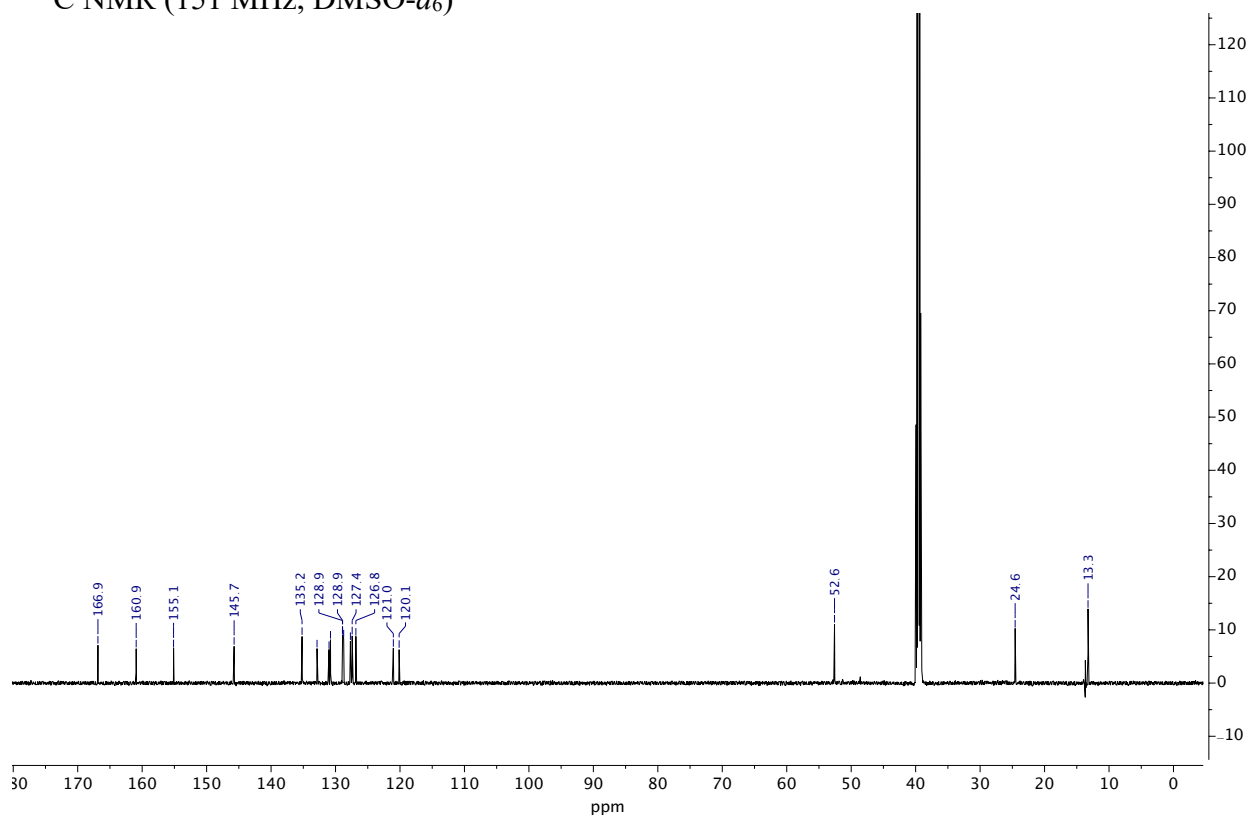


(±)-Auranthine (1)

^1H NMR (600 MHz, $\text{DMSO-}d_6$)



^{13}C NMR (151 MHz, $\text{DMSO-}d_6$)



IR spectra comparison of synthetic (\pm)-Auranthine (1) and natural (-)-Auranthine (1)

