

Supporting Information

A Convenient Route to *N*-[2-(Fmoc)- Aminoethyl]glycine Esters and PNA Oligomerization Using a bis-Boc Nucleobase Protecting Group Strategy

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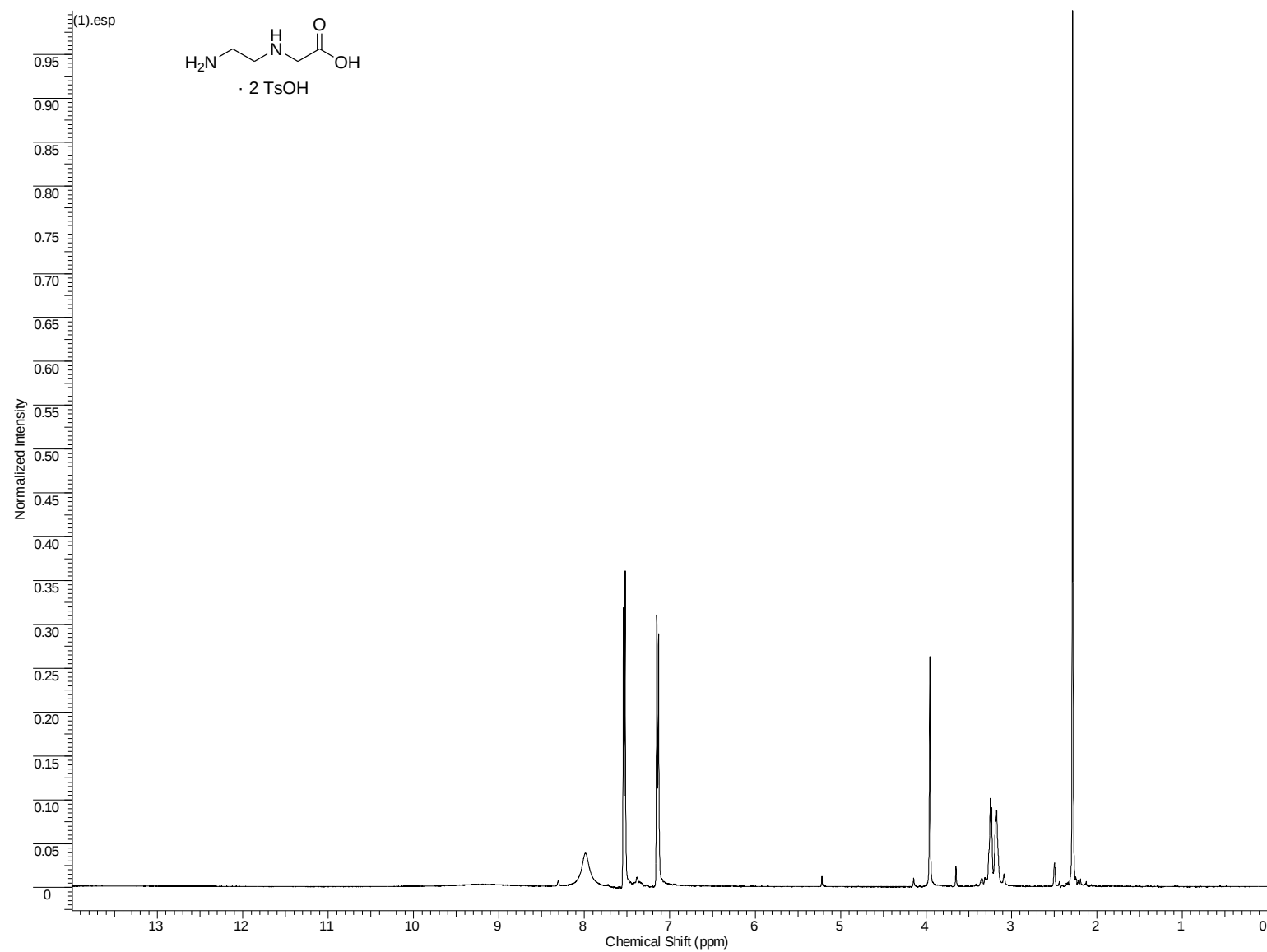
Table of Contents

General Remarks.....	S4
¹ H NMR of 1	S5
¹³ C NMR of 1	S6
¹ H NMR of 2	S7
¹³ C NMR of 2	S8
¹ H NMR of 3	S9
¹³ C NMR of 3	S10
¹ H NMR of 4	S11
¹³ C NMR of 4	S12
¹ H NMR of 5	S13
¹³ C NMR of 5	S14
¹ H NMR of 6	S15
¹³ C NMR of 6	S16
¹ H NMR of 7	S17
¹³ C NMR of 7	S18
¹ H NMR of 9	S19
¹³ C NMR of 9	S20
¹ H NMR of 10	S21
¹³ C NMR of 10	S22
¹ H NMR of 12	S23
¹³ C NMR of 12	S24
¹ H NMR of 13	S25
¹³ C NMR of 13	S26

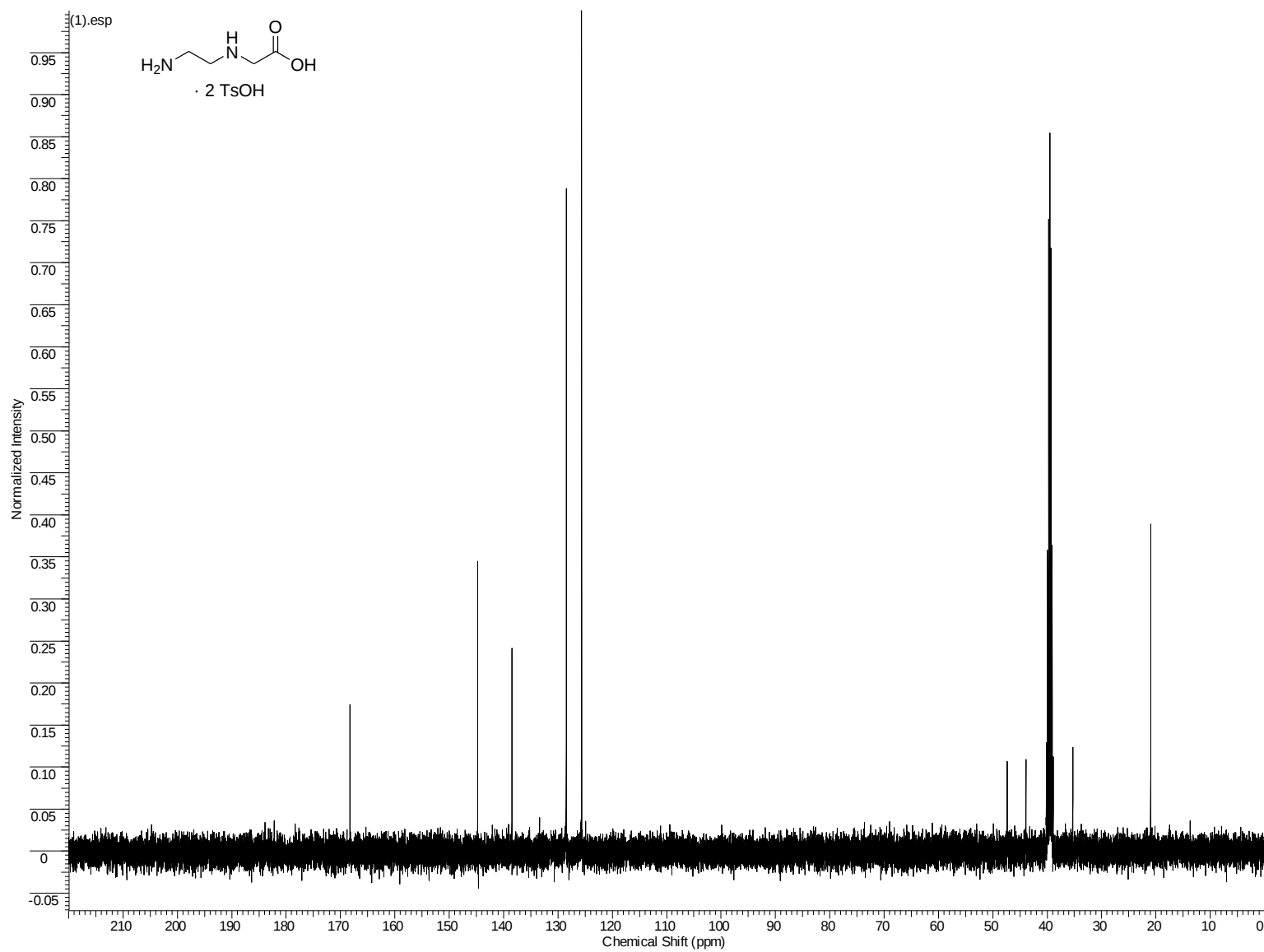
^1H NMR of 15	S27
^{13}C NMR of 15	S28
^1H NMR of 16	S29
^{13}C NMR of 16	S30
^1H NMR of 18	S31
^{13}C NMR of 18	S32
^1H NMR of 19	S33
^{13}C NMR of 19	S34
^1H NMR of 21	S35
^{13}C NMR of 21	S36
^1H NMR of 22	S37
^{13}C NMR of 22	S38
^1H NMR of 23	S39
^{13}C NMR of 23	S40
^1H NMR of 24	S41
^{13}C NMR of 24	S42
^1H NMR of 25	S43
^{13}C NMR of 25	S44
^1H NMR of 26	S45
^{13}C NMR of 26	S46
^1H NMR of 27	S47
^{13}C NMR of 27	S48
^1H NMR of 28	S49
^{13}C NMR of 28	S50
Fig. S1. HPLC chromatogram	S51

General Remarks. All chemicals were obtained from commercial sources and were of ACS reagent grade or higher and were used without further purification. Solvents for solution-phase chemistry were dried by passing through activated alumina columns. Flash column chromatography (FCC) was performed on Merck Kieselgel 60, 230-400 mesh. Thin layer chromatography (TLC) was performed on Merck Kieselgel 60 TLC plates. Chemical shifts are reported in parts per million (δ), were measured from Tetramethylsilane (0 ppm) and are referenced to the solvent CDCl_3 (7.26 ppm), $\text{DMSO}-d_6$ (2.49 ppm), D_2O (4.79 ppm) for ^1H NMR and CDCl_3 (77.0 ppm), $\text{DMSO}-d_6$ (39.5 ppm) for ^{13}C NMR. Multiplicities are described as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet) and br s (broad singlet). Coupling constants (J) are reported in Hertz (Hz). Resonances due to restricted rotation around the amide bond (rotamers) are reported as major (ma.) and minor (mi.). High resolution mass spectra (HRMS) were obtained using electron impact (EI) or electrospray (ESI).

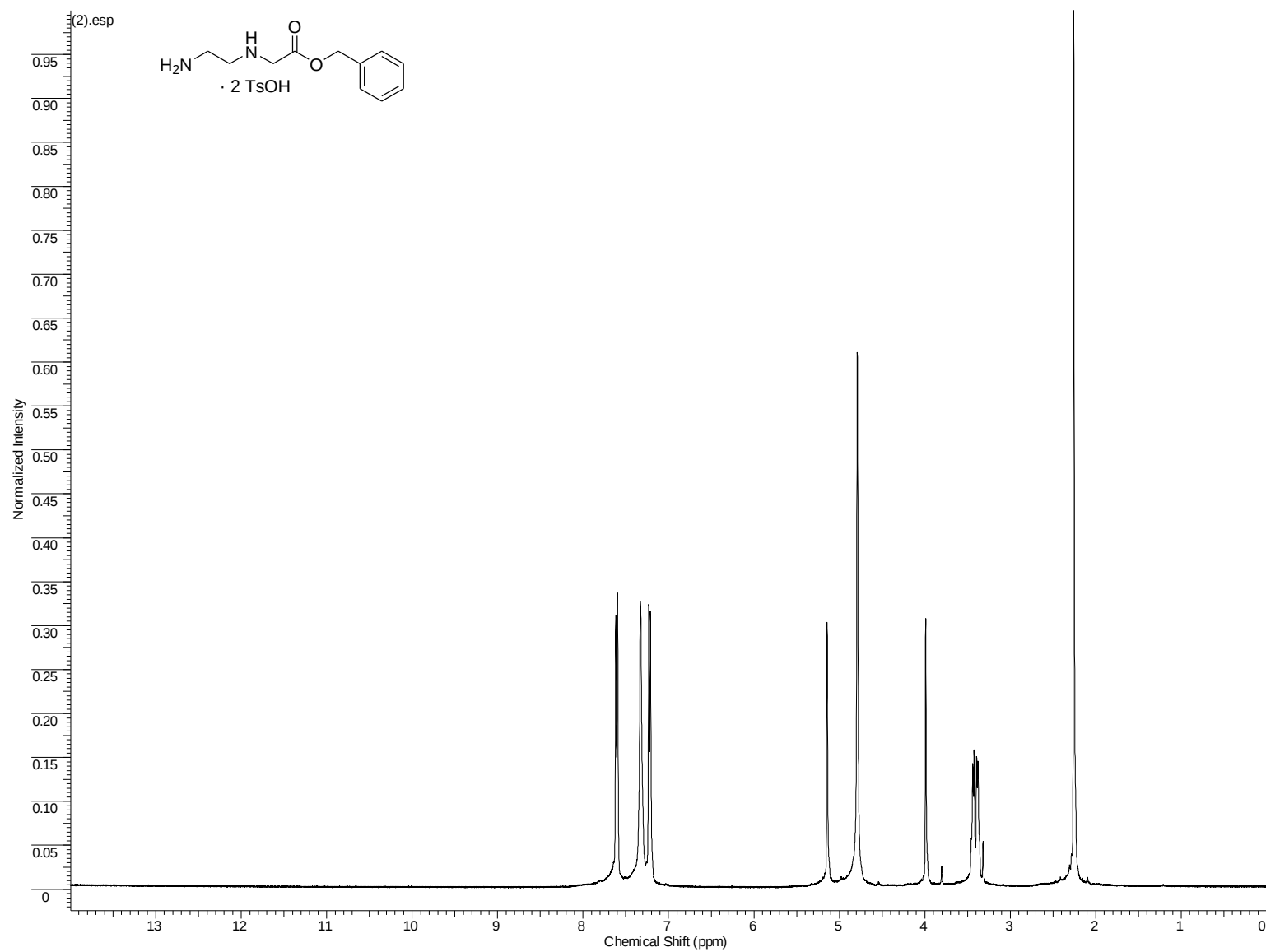
^1H NMR (400 MHz, DMSO- d_6) of **1**, *N*-(2-Aminoethyl)glycine $\cdot$ 2 TsOH



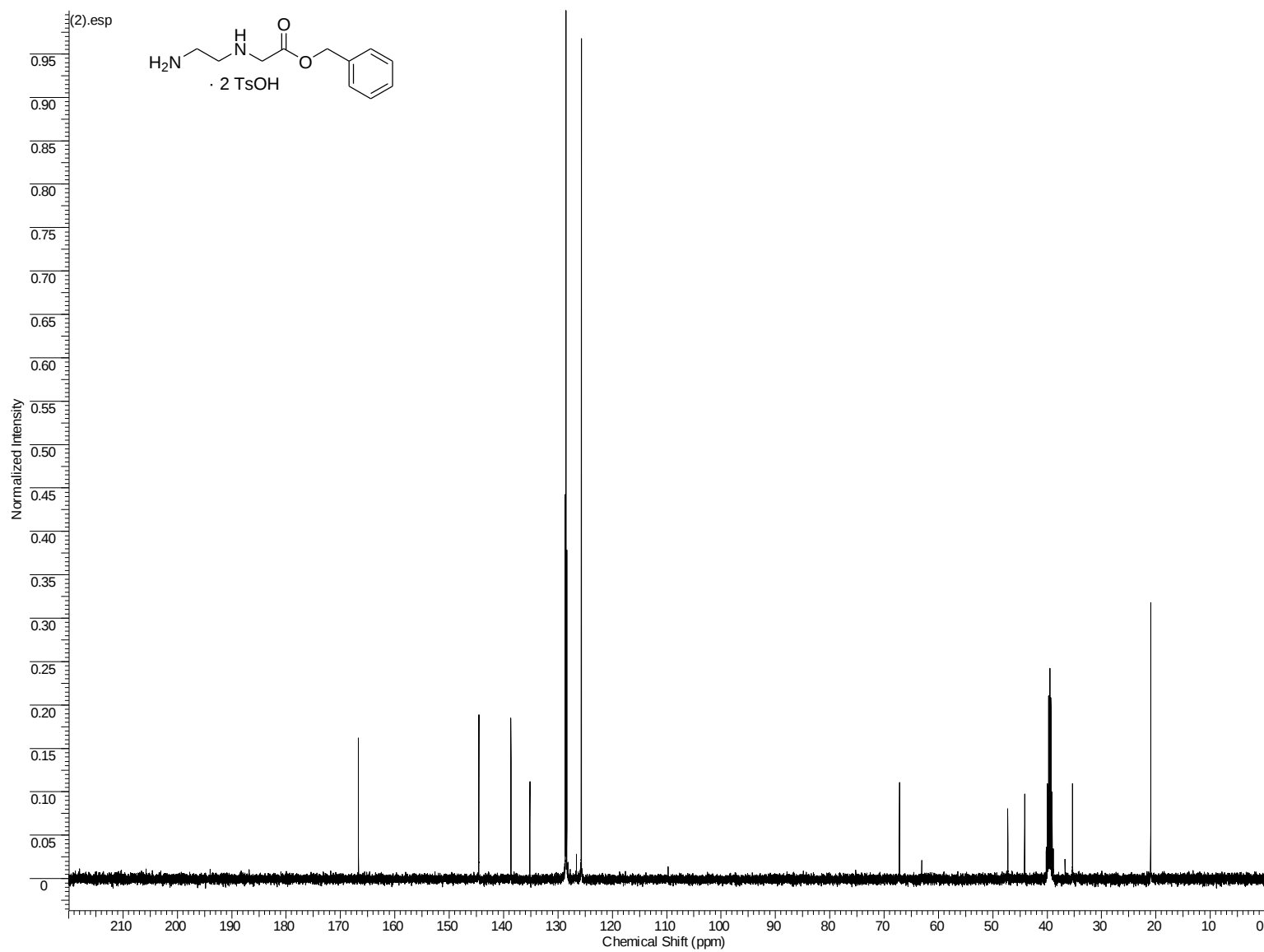
^{13}C NMR (100 MHz, DMSO- d_6) of **1**, *N*-(2-Aminoethyl)glycine · 2 TsOH



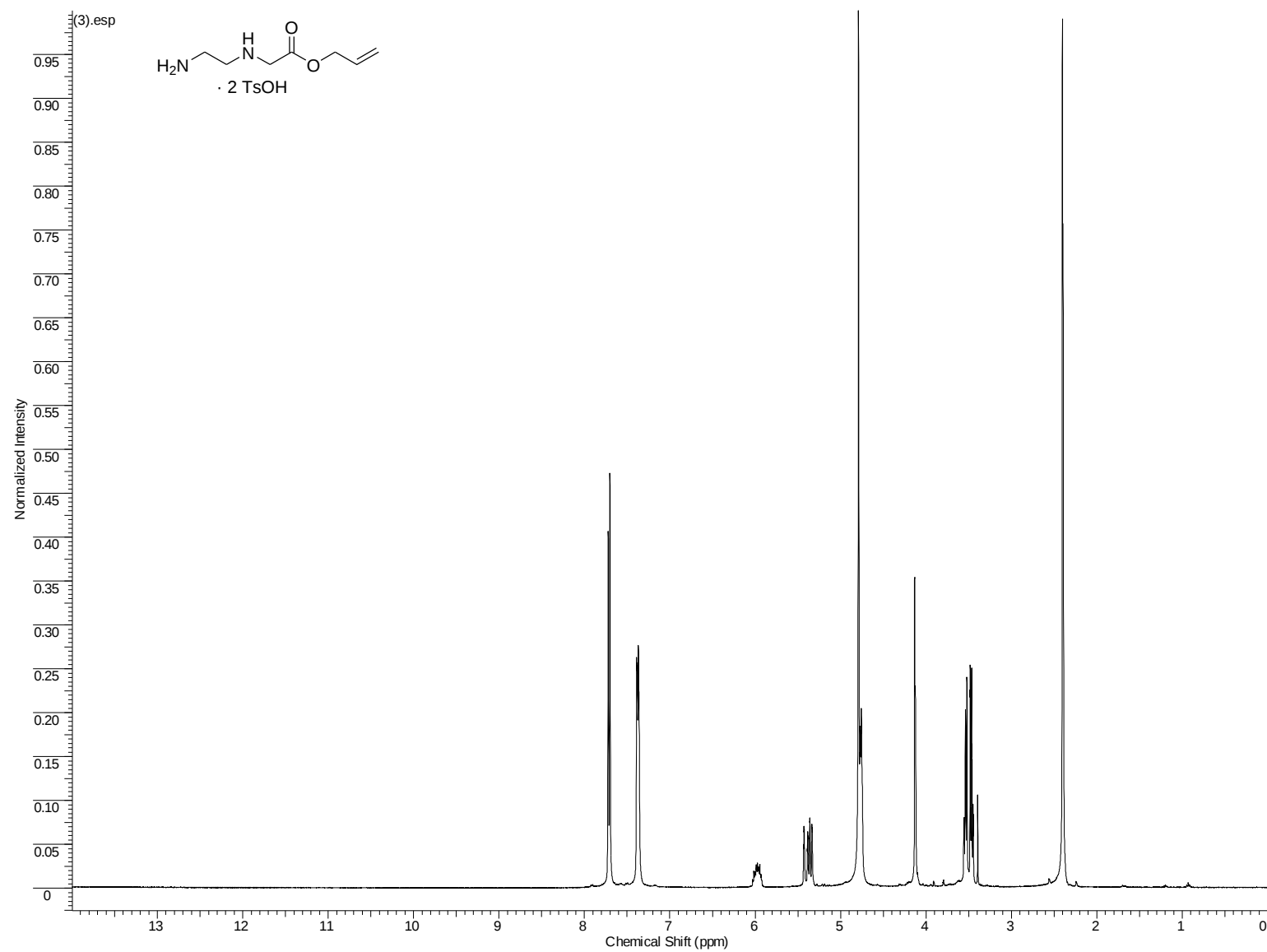
^1H NMR (400 MHz, D_2O) of 2, Benzyl *N*-(2-aminoethyl)glycinate $\cdot$ 2 TsOH



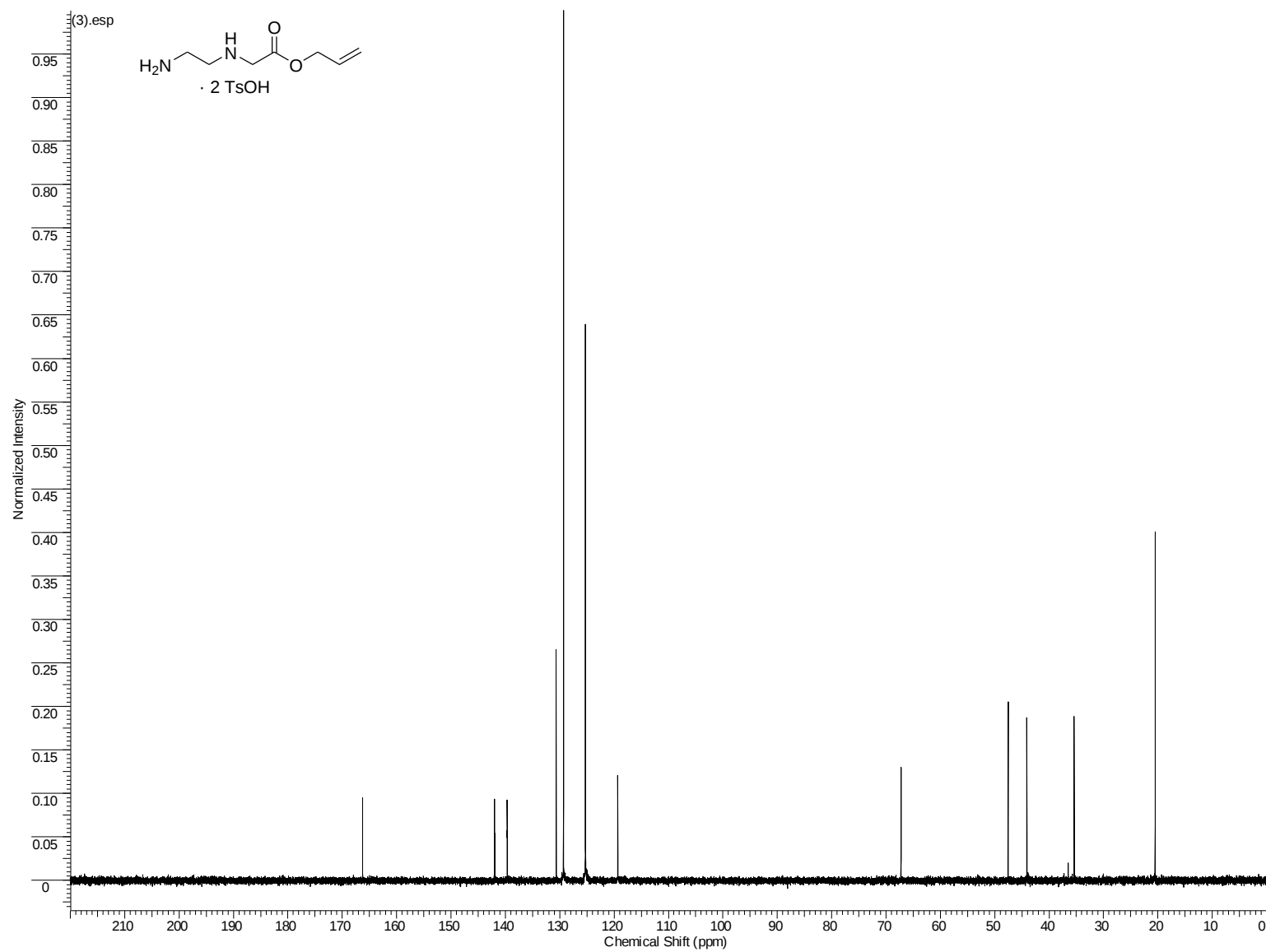
^{13}C NMR (100 MHz, DMSO- d_6) of **2**, Benzyl *N*-(2-aminoethyl)glycinate · 2 TsOH



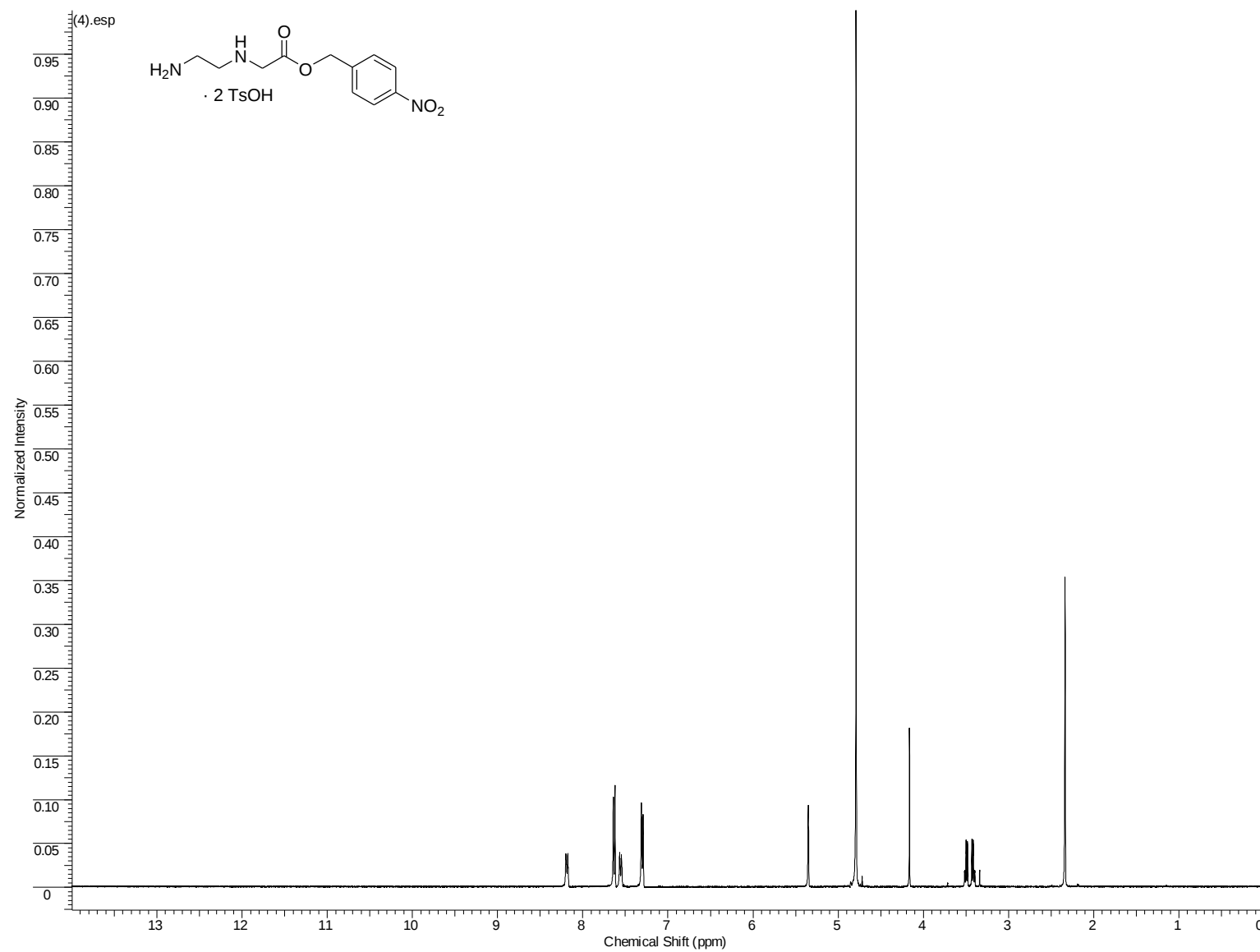
^1H NMR (400 MHz, D_2O) of **3**, Allyl *N*-(2-aminoethyl)glycinate $\cdot$ 2 TsOH



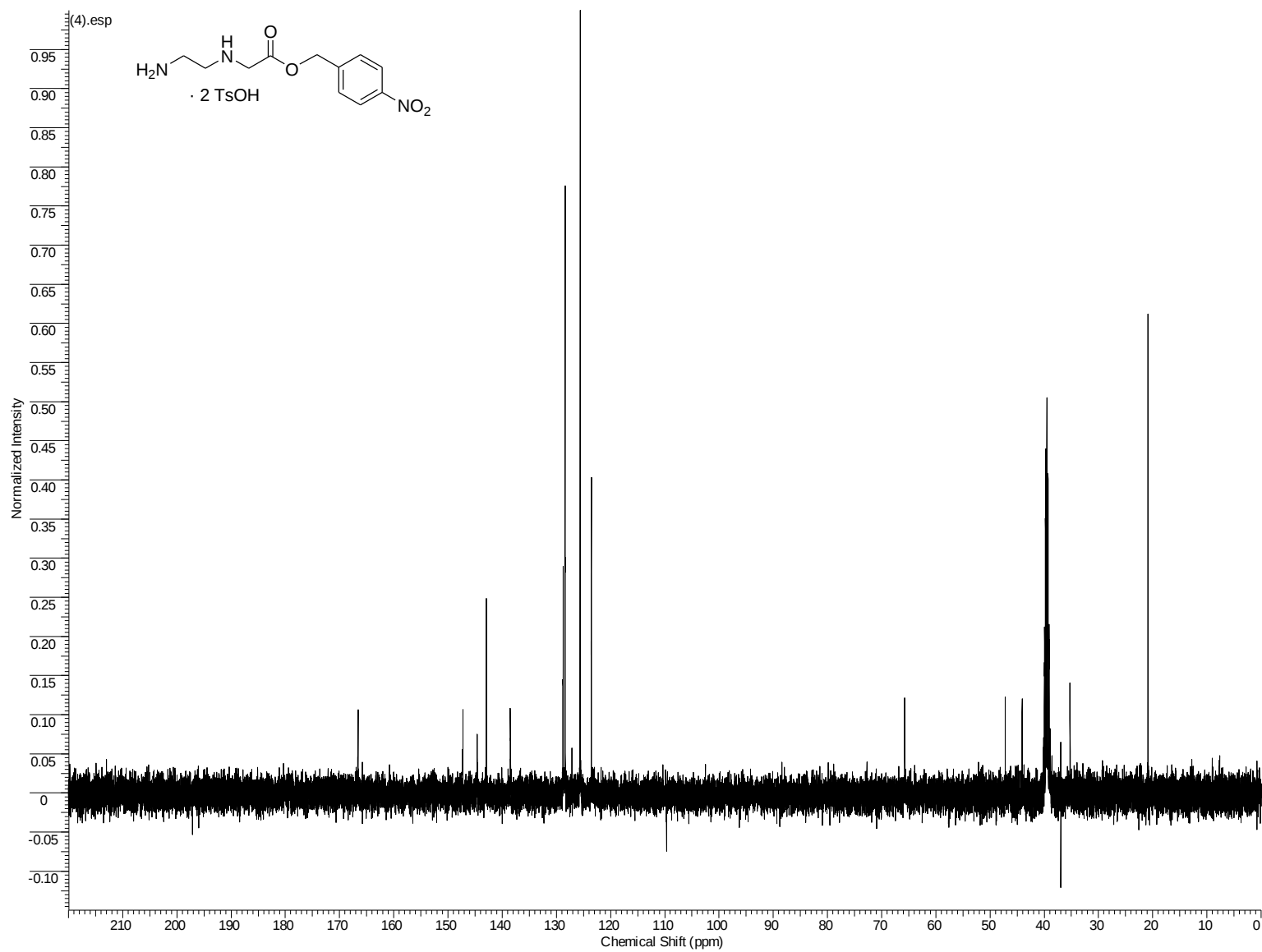
^{13}C NMR (100 MHz, D_2O) of **3**, Allyl *N*-(2-aminoethyl)glycinate · 2 TsOH



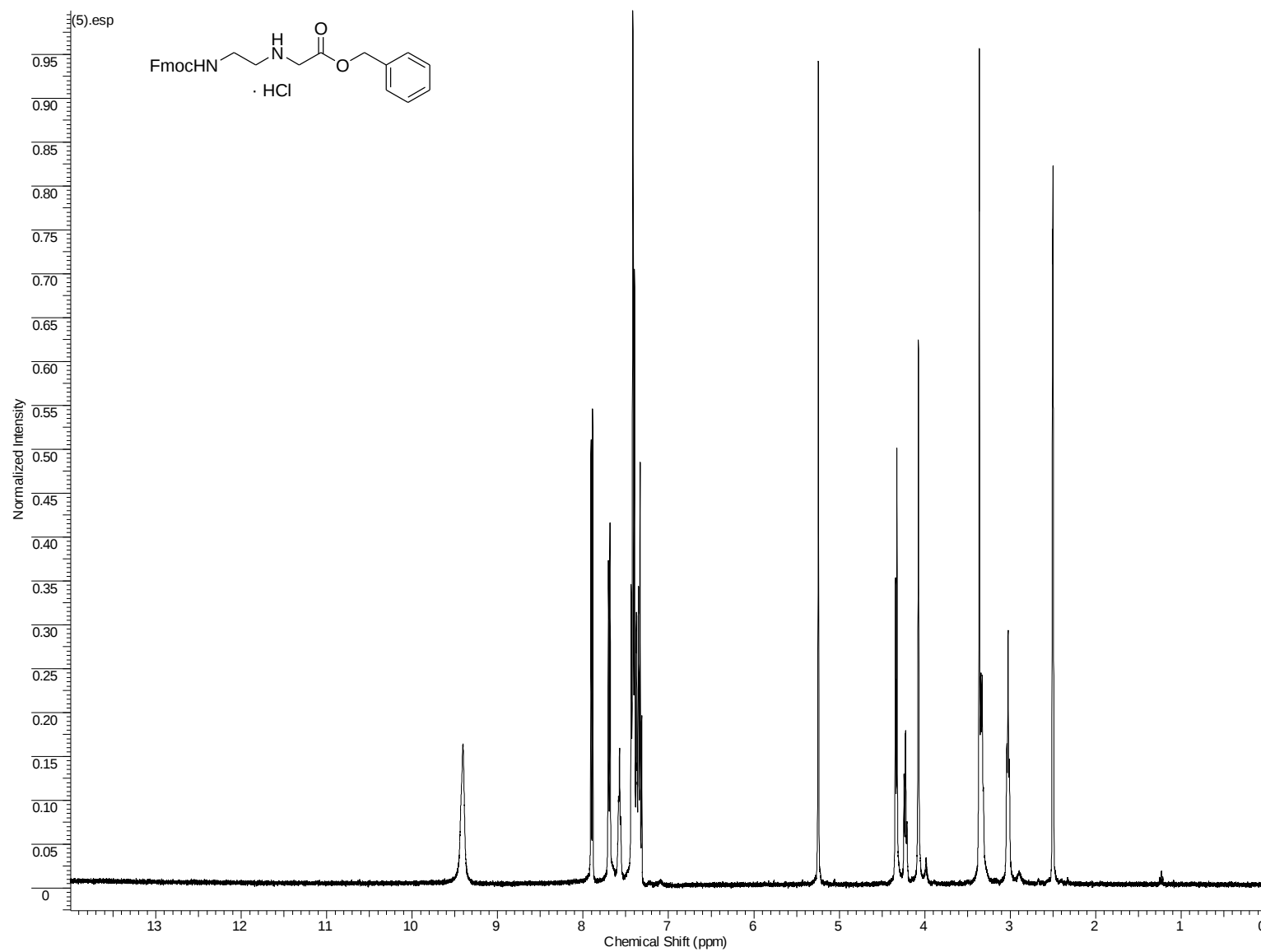
^1H NMR (400 MHz, D_2O) of **4**, 4-Nitrobenzyl *N*-(2-aminoethyl)glycinate $\cdot$ 2 TsOH



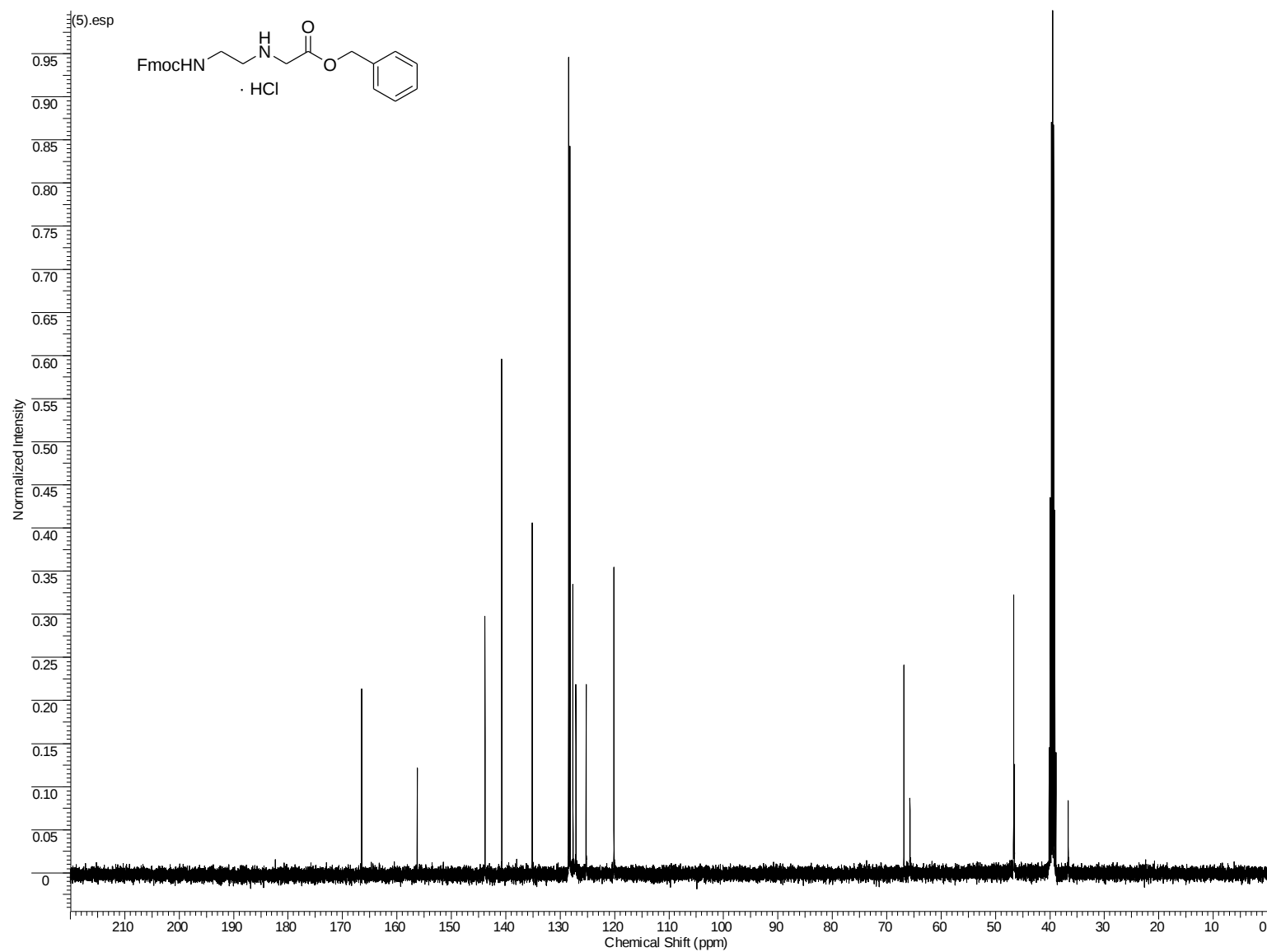
^{13}C NMR (100 MHz, DMSO- d_6) of **4**, 4-Nitrobenzyl *N*-(2-aminoethyl)glycinate $\cdot$ 2 TsOH



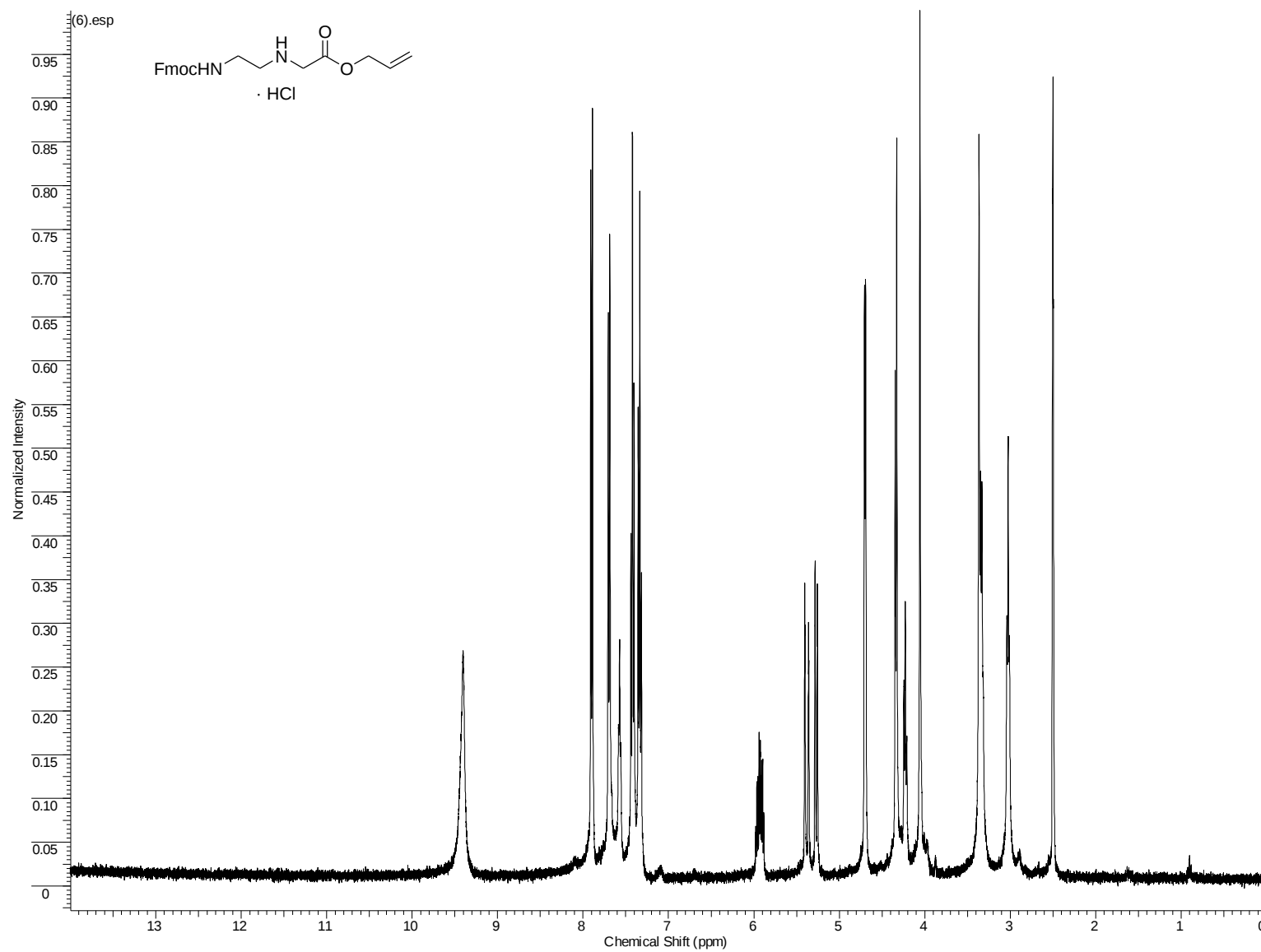
^1H NMR (400 MHz, DMSO- d_6) of 5·HCl, Benzyl *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]glycinate hydrochloride



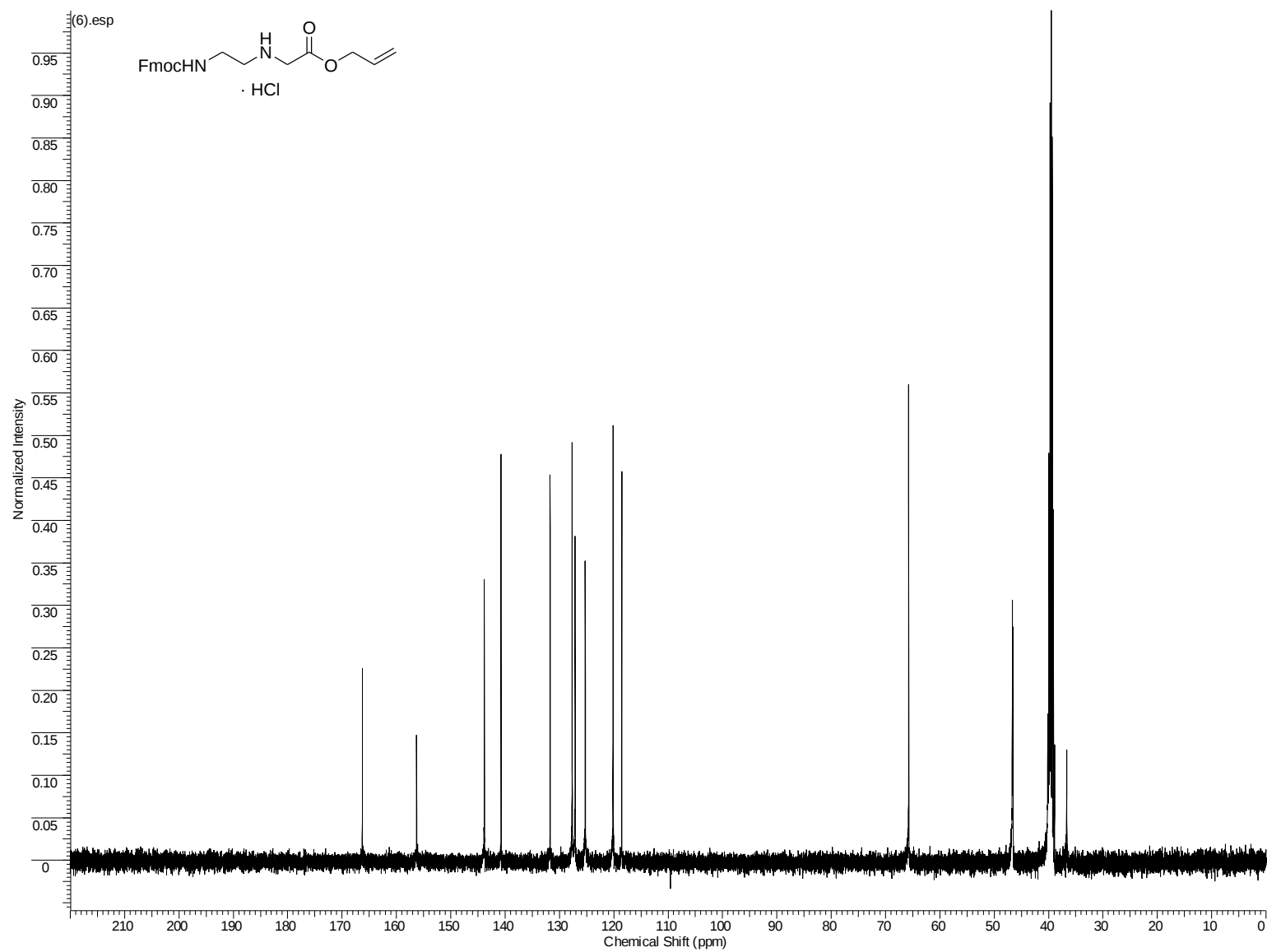
^{13}C NMR (100 MHz, DMSO-d_6) of 5·HCl, Benzyl N-[2-(fluorenylmethoxycarbonyl)aminoethyl]glycinate hydrochloride



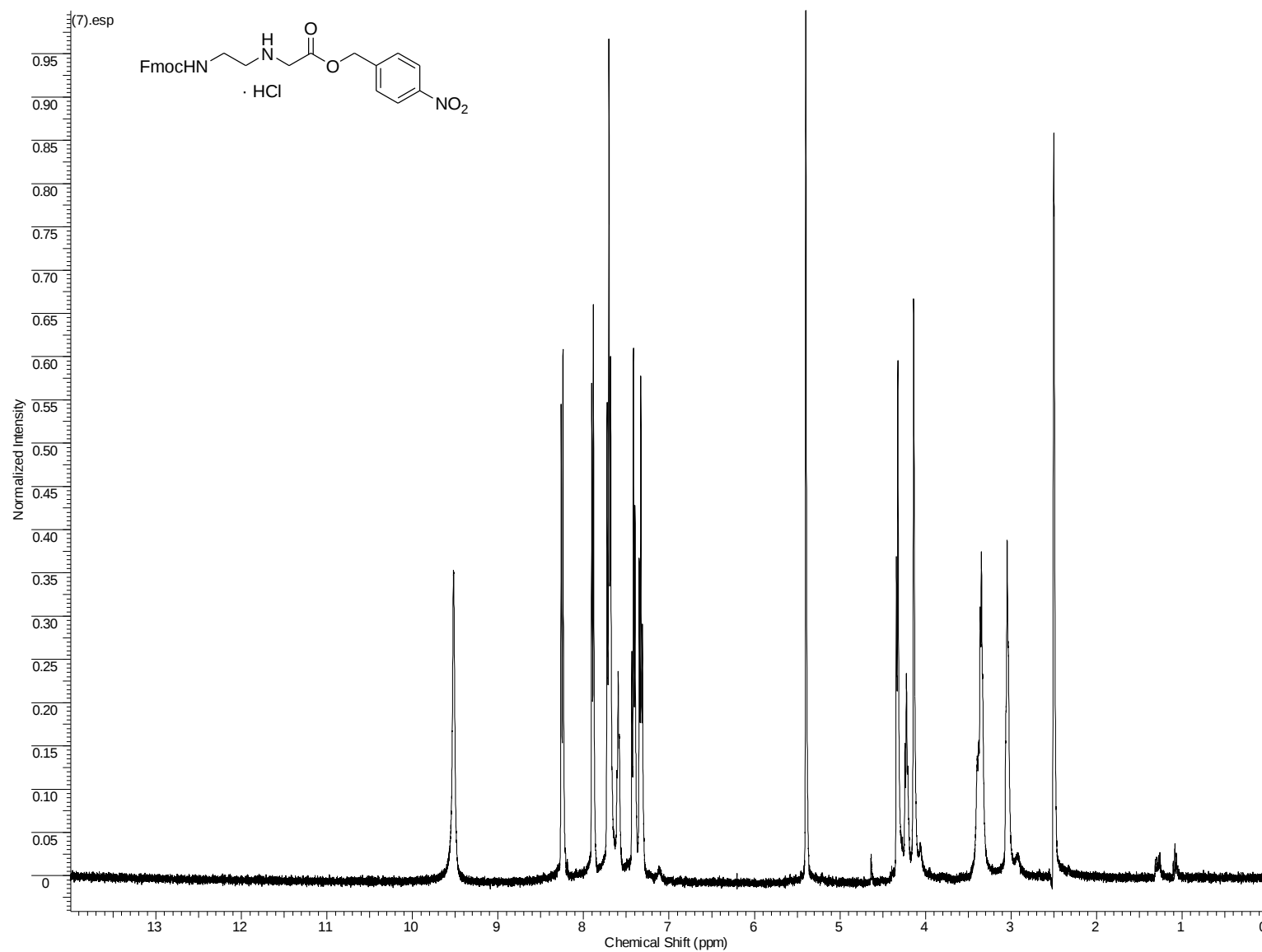
^1H NMR (400 MHz, DMSO- d_6) of **6**·HCl, Allyl *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]glycinate hydrochloride



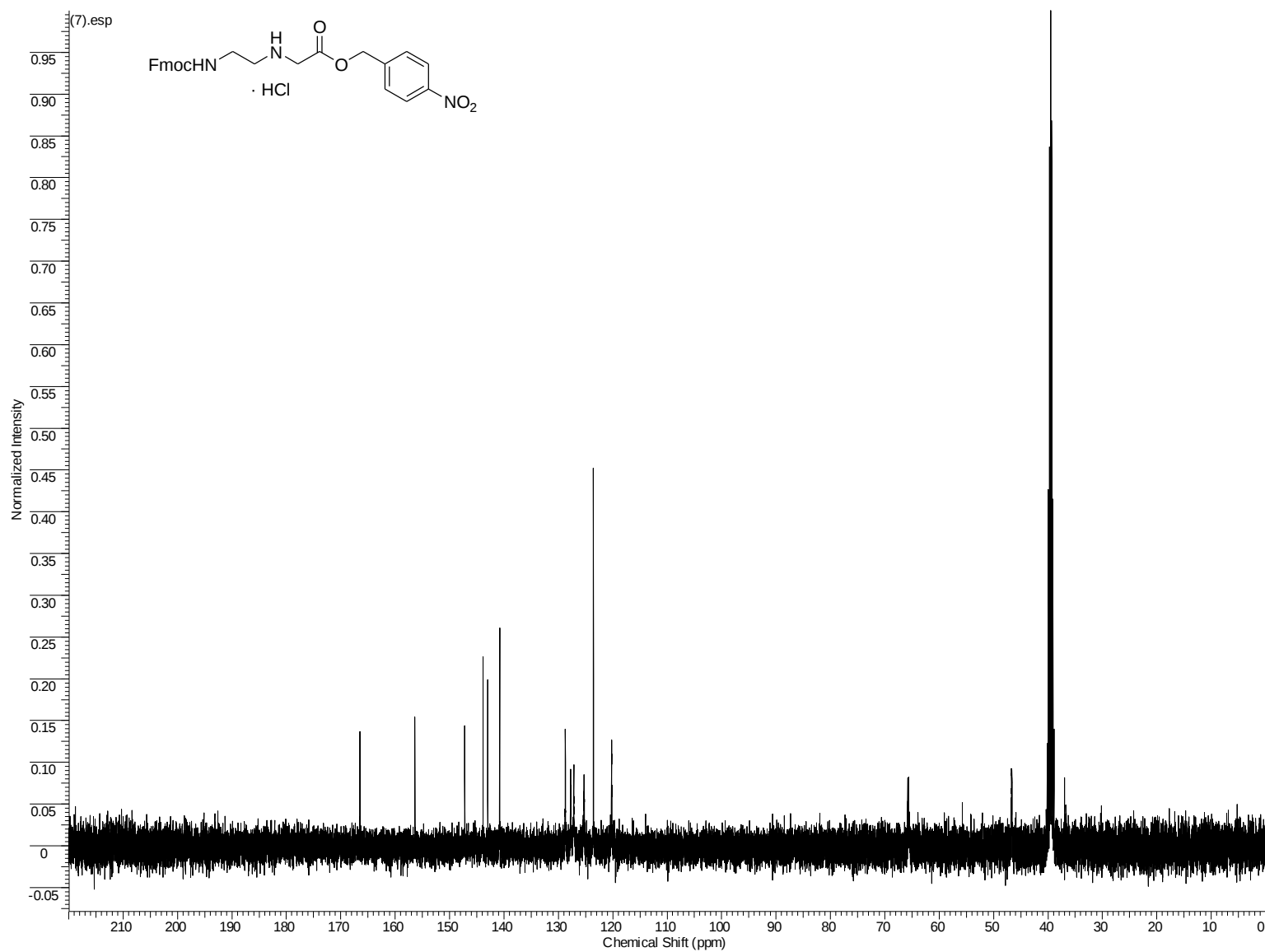
^{13}C NMR (100 MHz, DMSO- d_6) of **6**·HCl, Allyl *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]glycinate hydrochloride



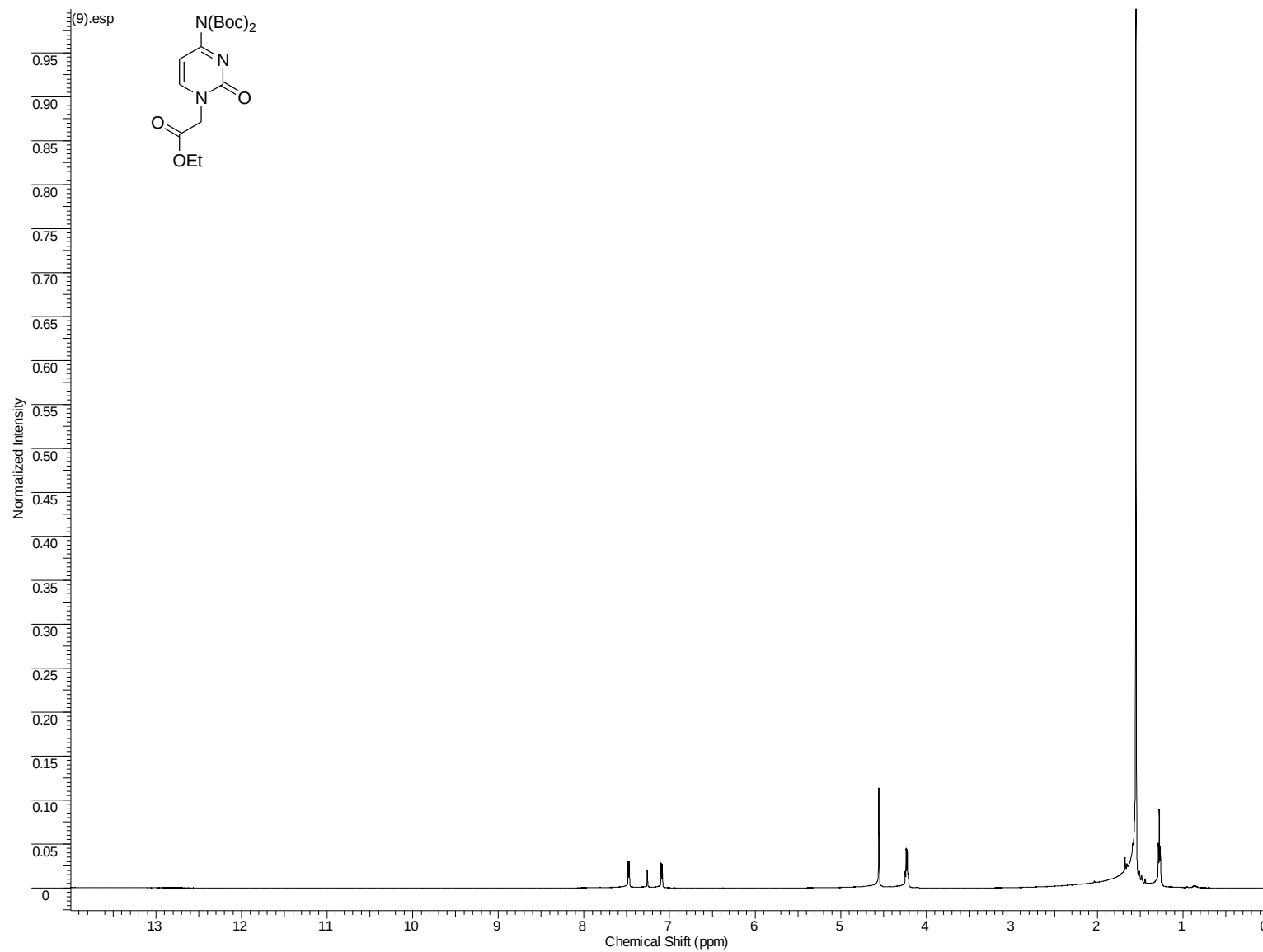
^1H NMR (400 MHz, DMSO- d_6) of 7·HCl, 4-Nitrobenzyl *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]glycinate hydrochloride



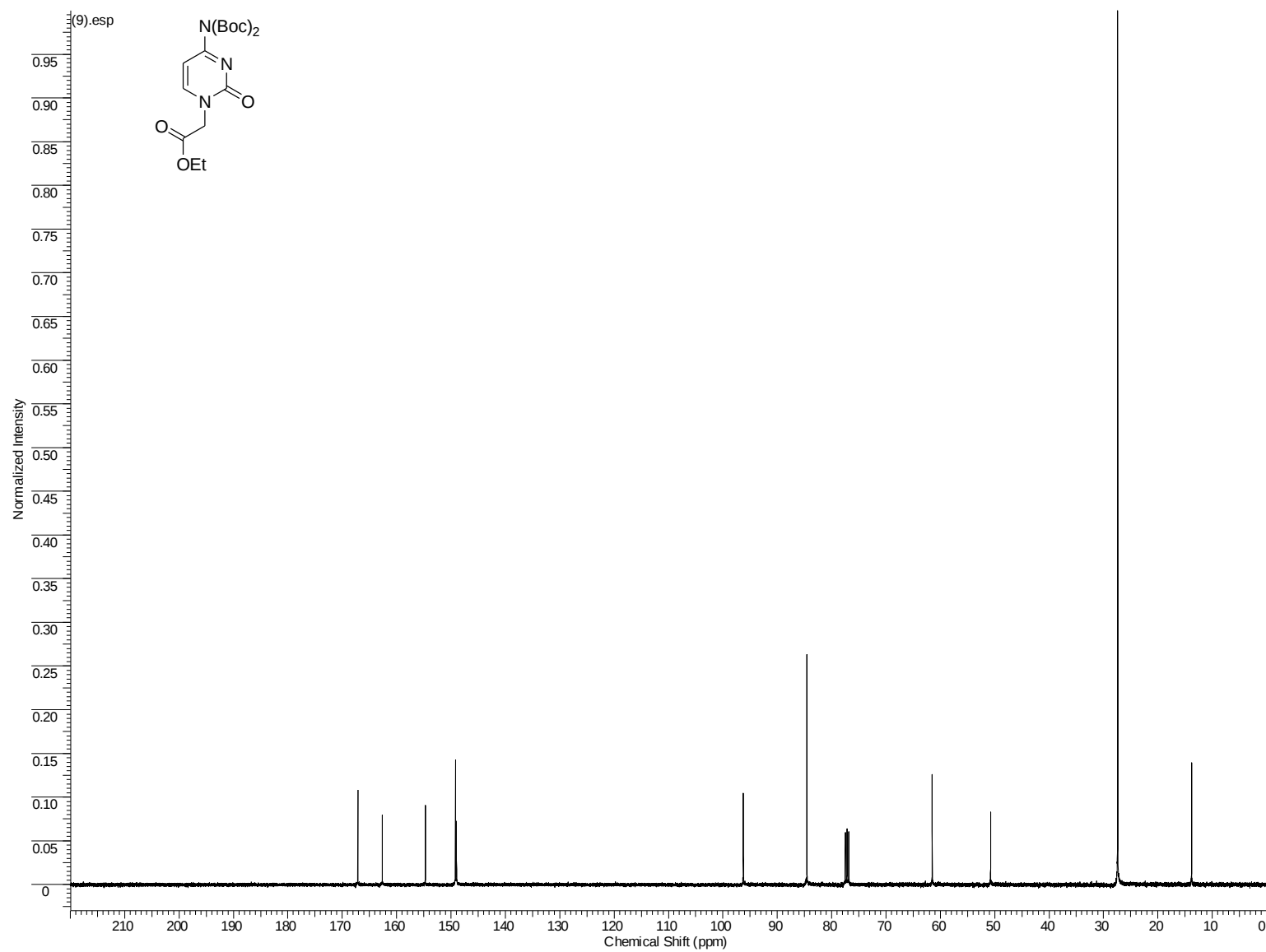
^{13}C NMR (100 MHz, DMSO- d_6) of 7·HCl, 4-Nitrobenzyl *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]glycinate hydrochloride



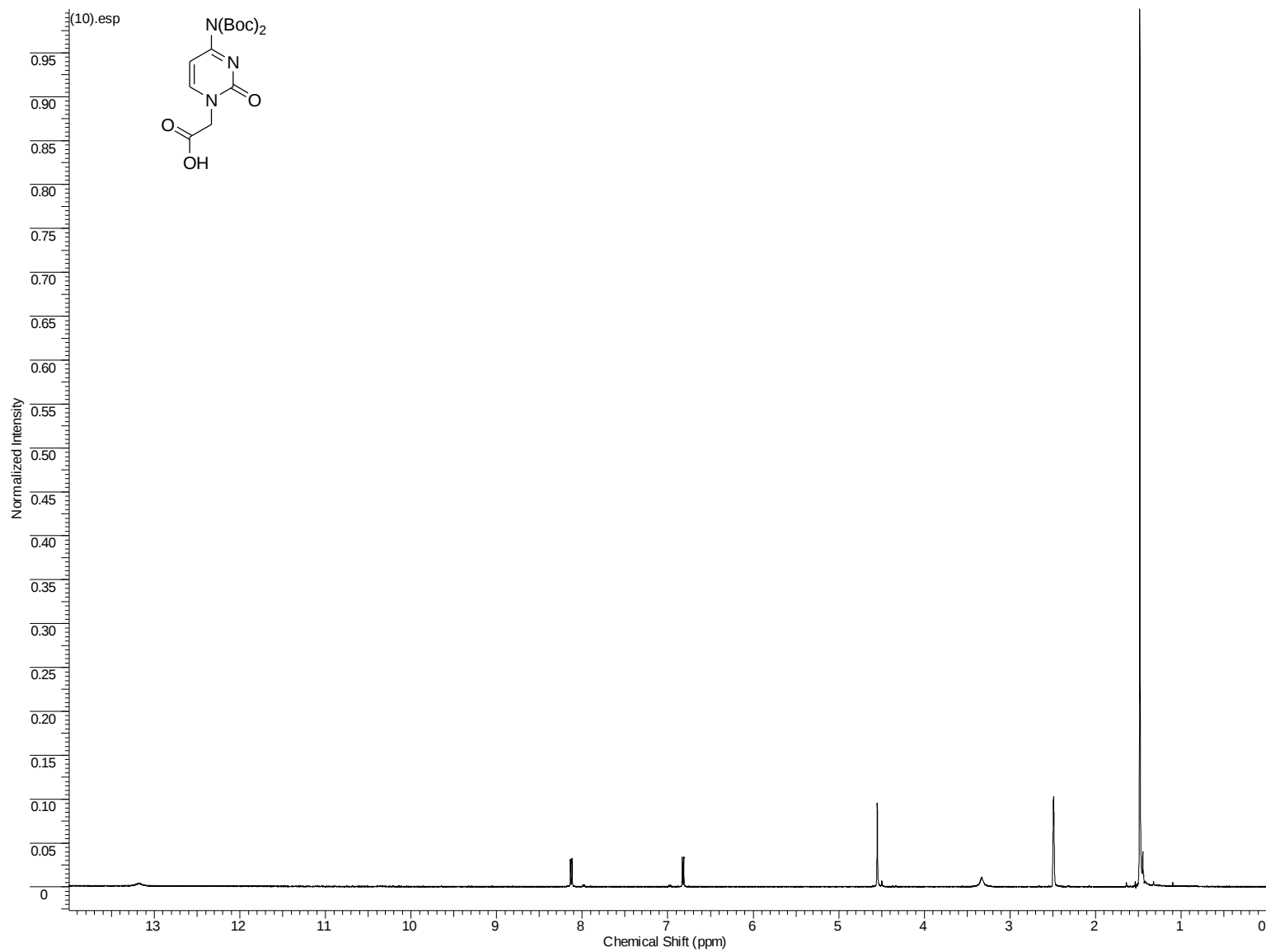
^1H NMR (400 MHz, CDCl_3) of **9**, Ethyl [N^4, N^4 -bis(*tert*-butoxycarbonyl)cytosin-1-yl]acetate



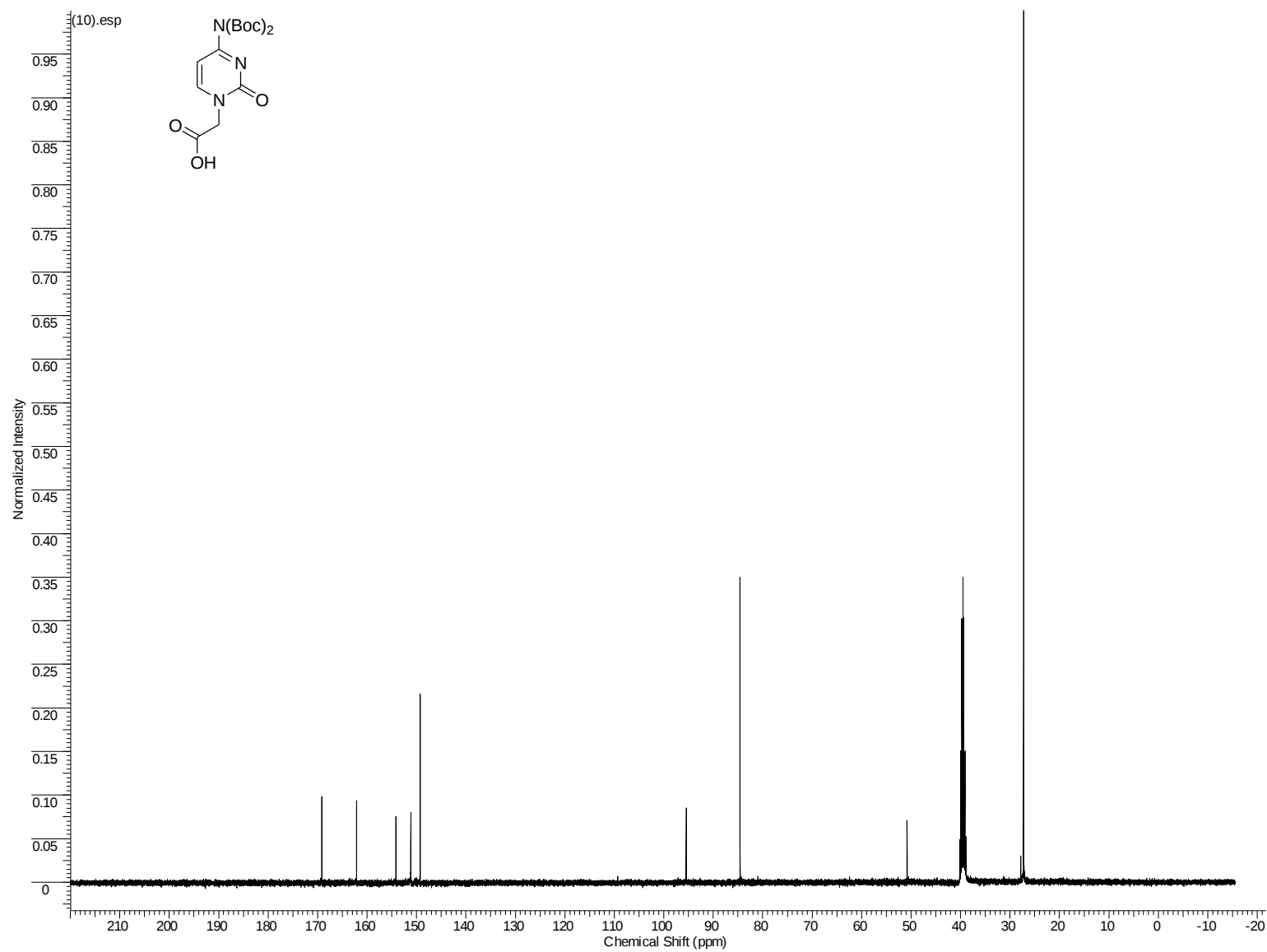
^{13}C NMR (100 MHz, CDCl_3) of **9**, Ethyl [N^4, N^4 -bis(*tert*-butoxycarbonyl)cytosin-1-yl]acetate



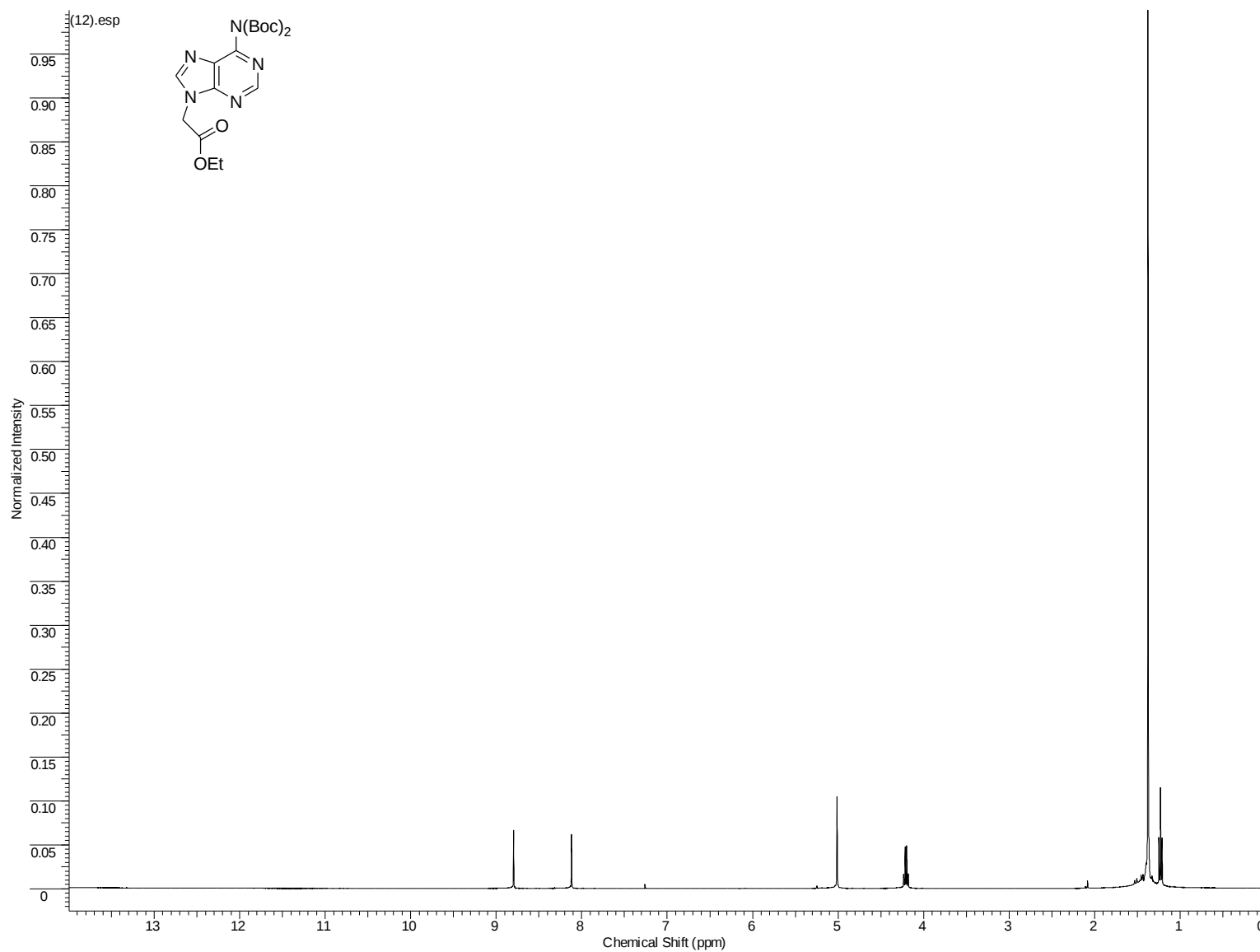
^1H NMR (400 MHz, CDCl_3) of **10**, [N^4, N^4 -bis(*tert*-Butoxycarbonyl)cytosin-1-yl]acetic acid



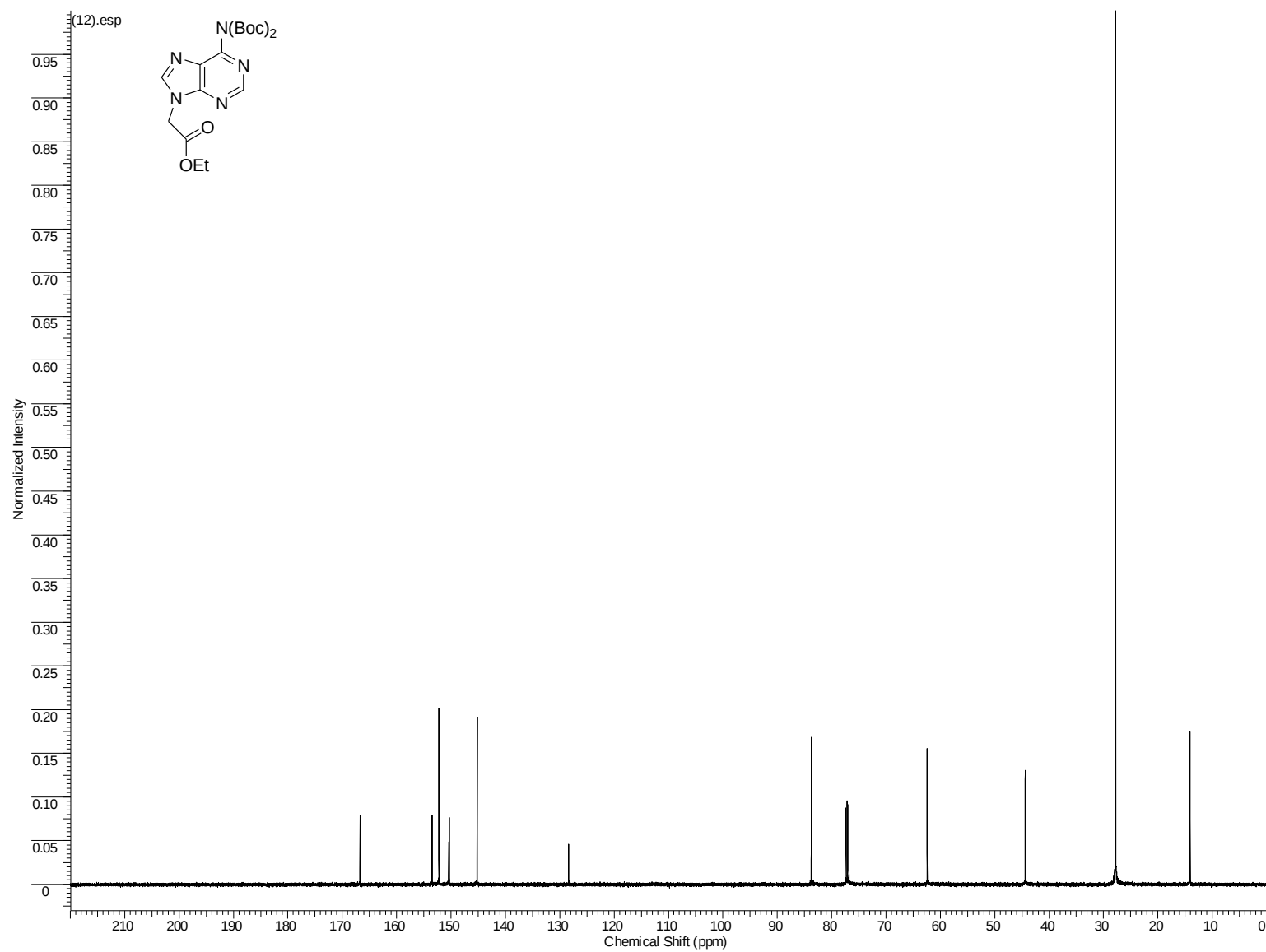
^{13}C NMR (100 MHz, CDCl_3) of **10**, [N^4,N^4 -bis(*tert*-Butoxycarbonyl)cytosin-1-yl]acetic acid



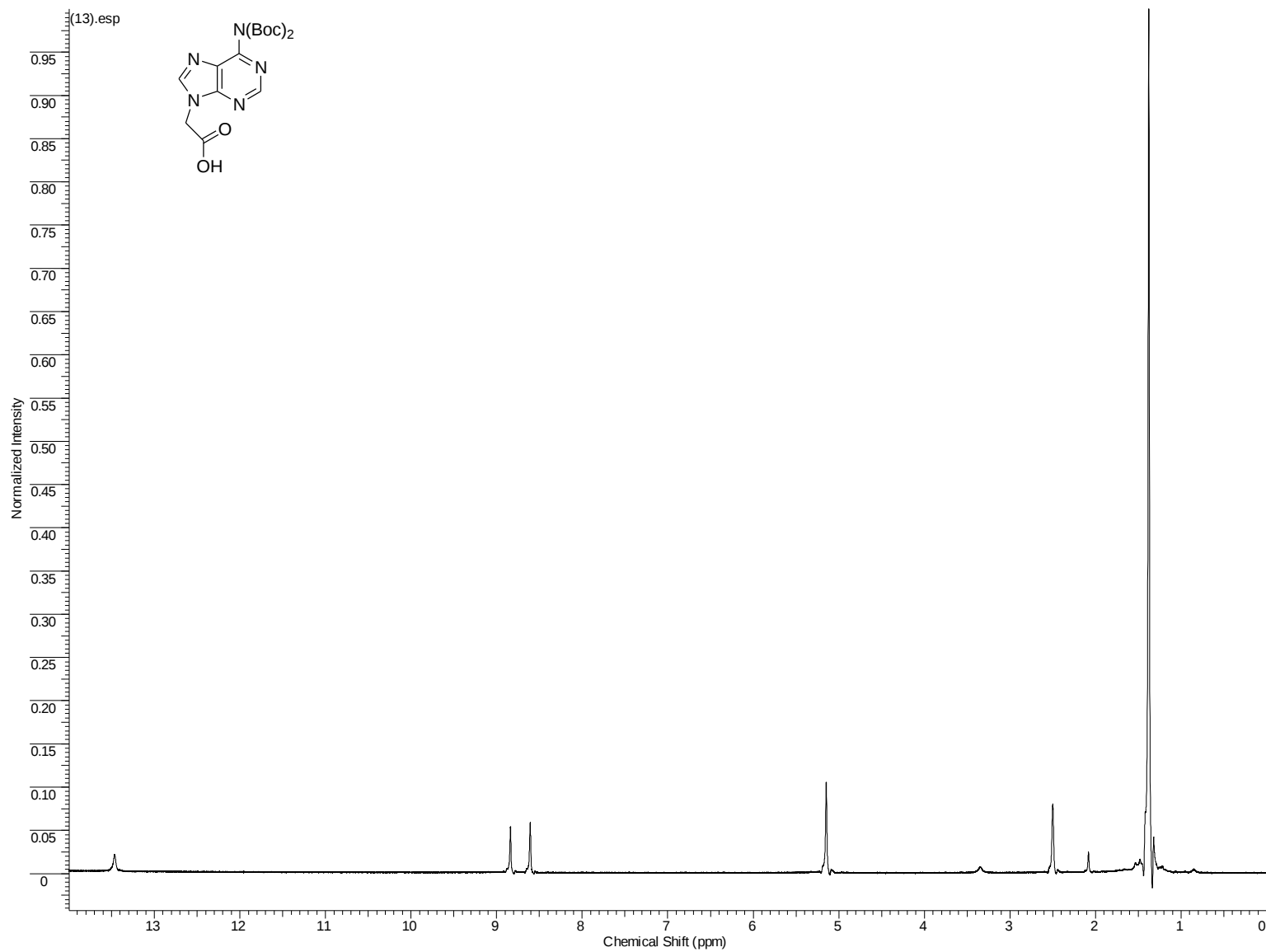
^1H NMR (400 MHz, CDCl_3) of **12**, Ethyl [N^6,N^6 -bis(*tert*-butoxycarbonyl)adenin-9-yl]acetate



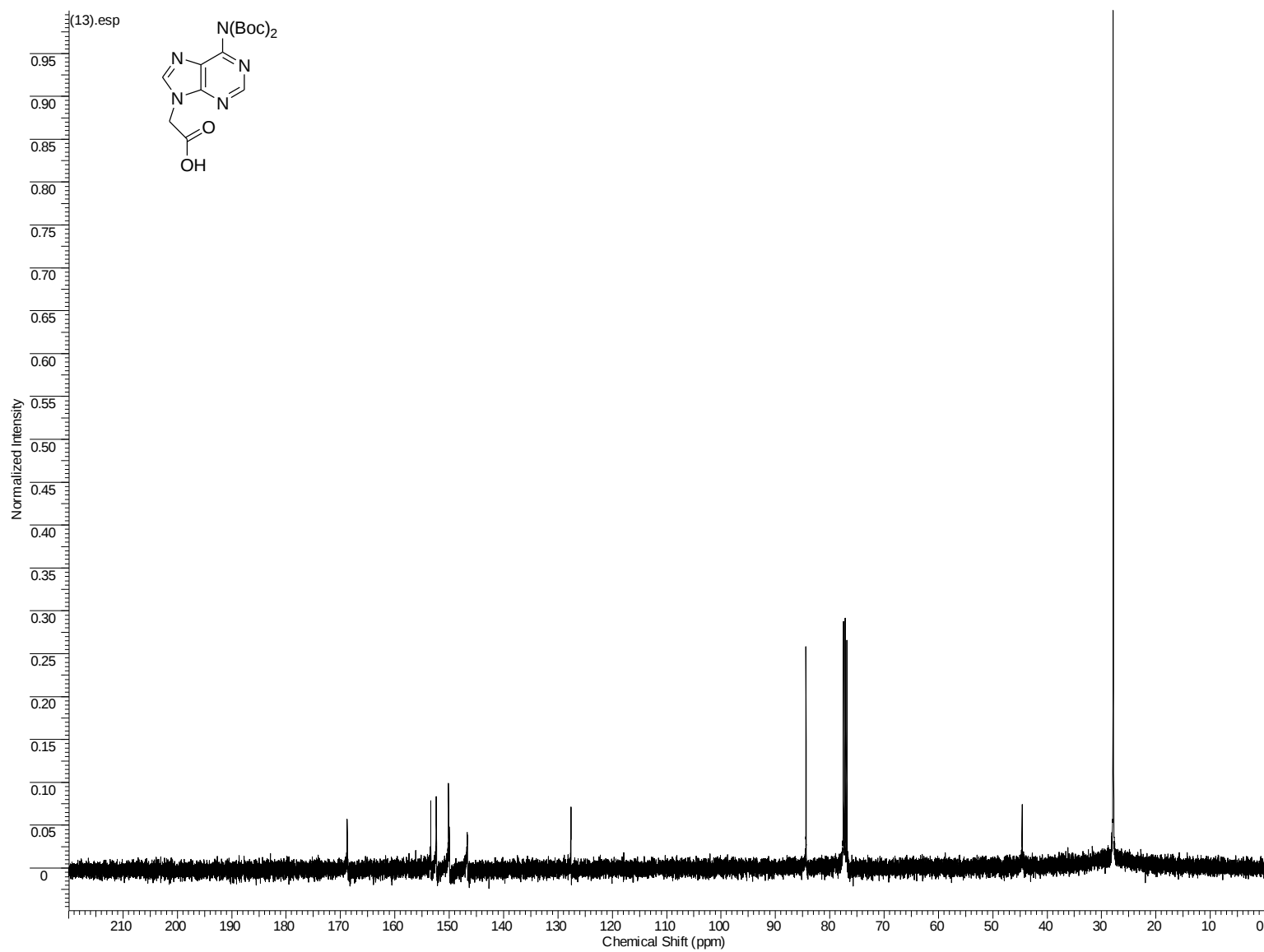
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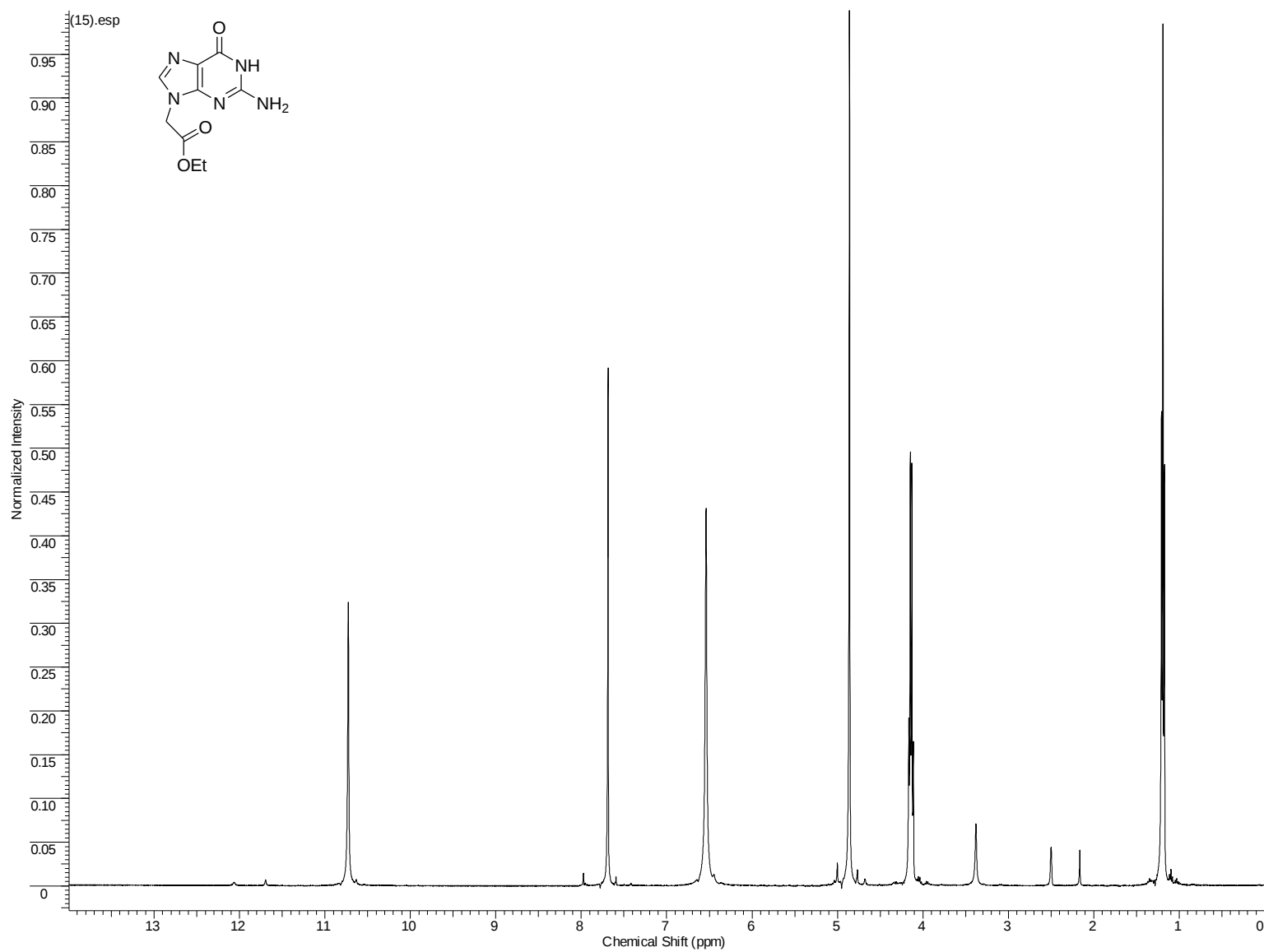
^1H NMR (400 MHz, CDCl_3) of **13**, [N^6,N^6 -bis(*tert*-Butoxycarbonyl)adenin-9-yl]acetic acid



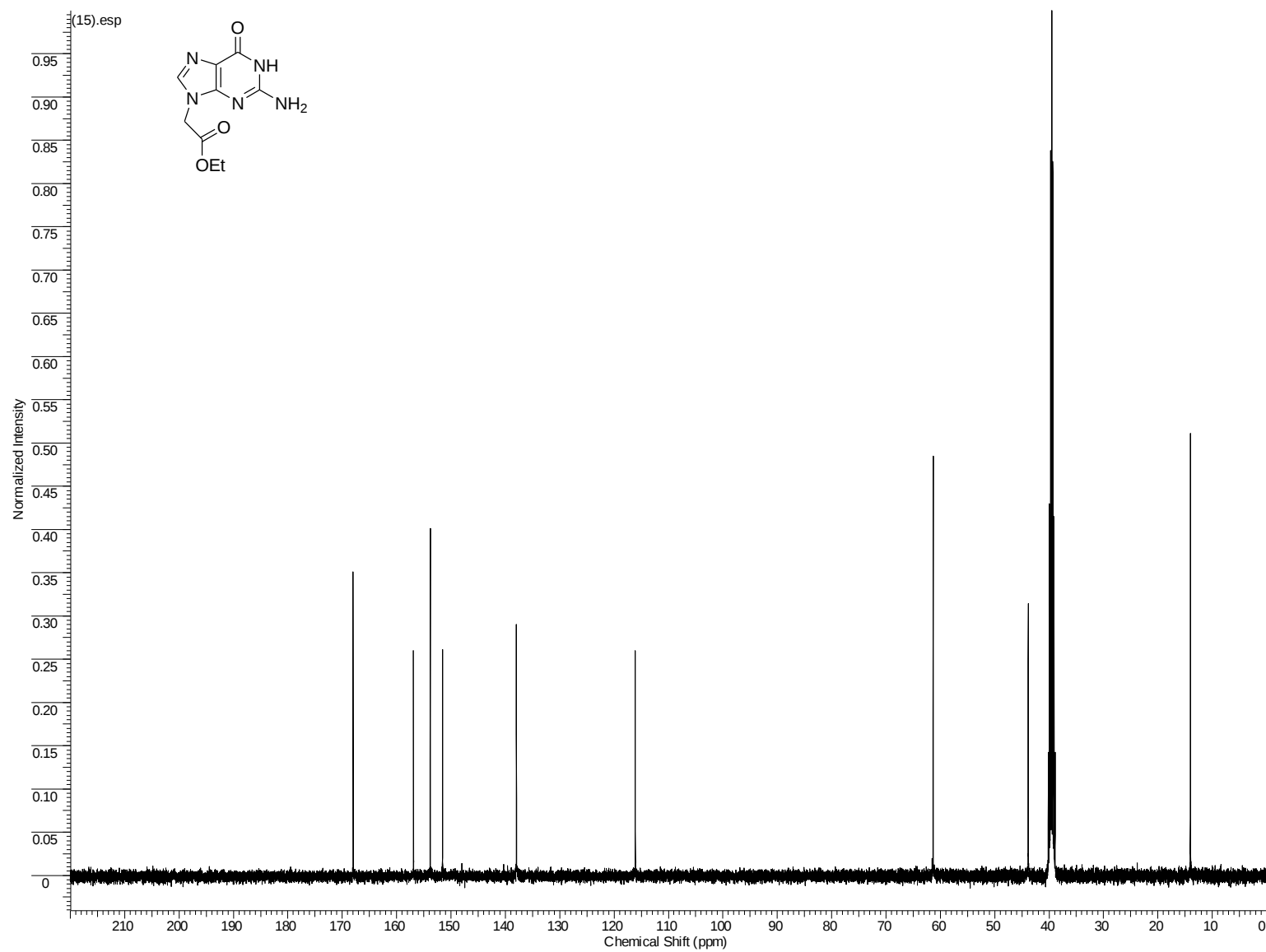
^{13}C NMR (100 MHz, CDCl_3) of **13**, [N^6,N^6 -bis(*tert*-Butoxycarbonyl)adenin-9-yl]acetic acid



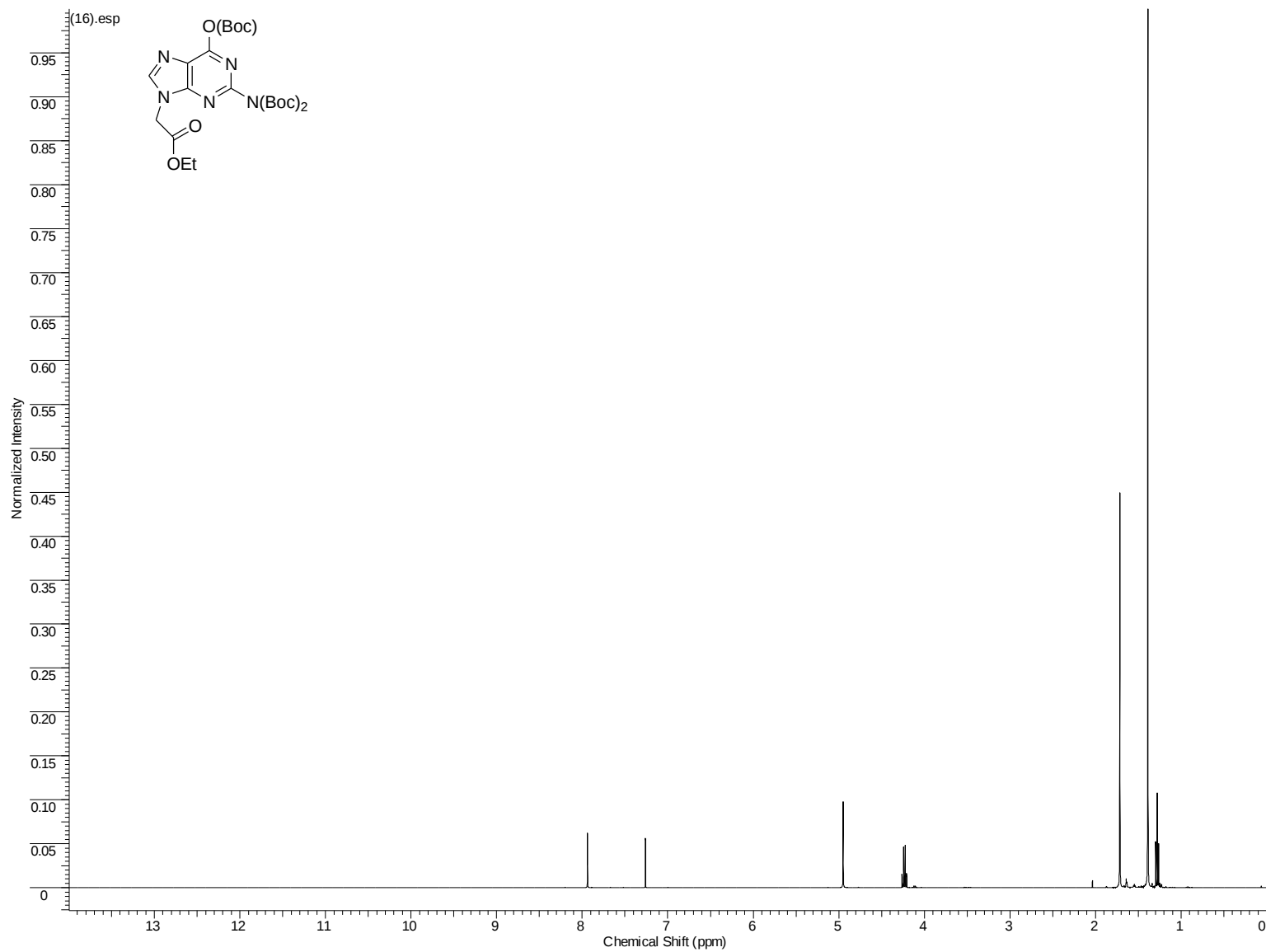
^1H NMR (400 MHz, DMSO- d_6) of **15**, Ethyl guanin-9-ylacetate



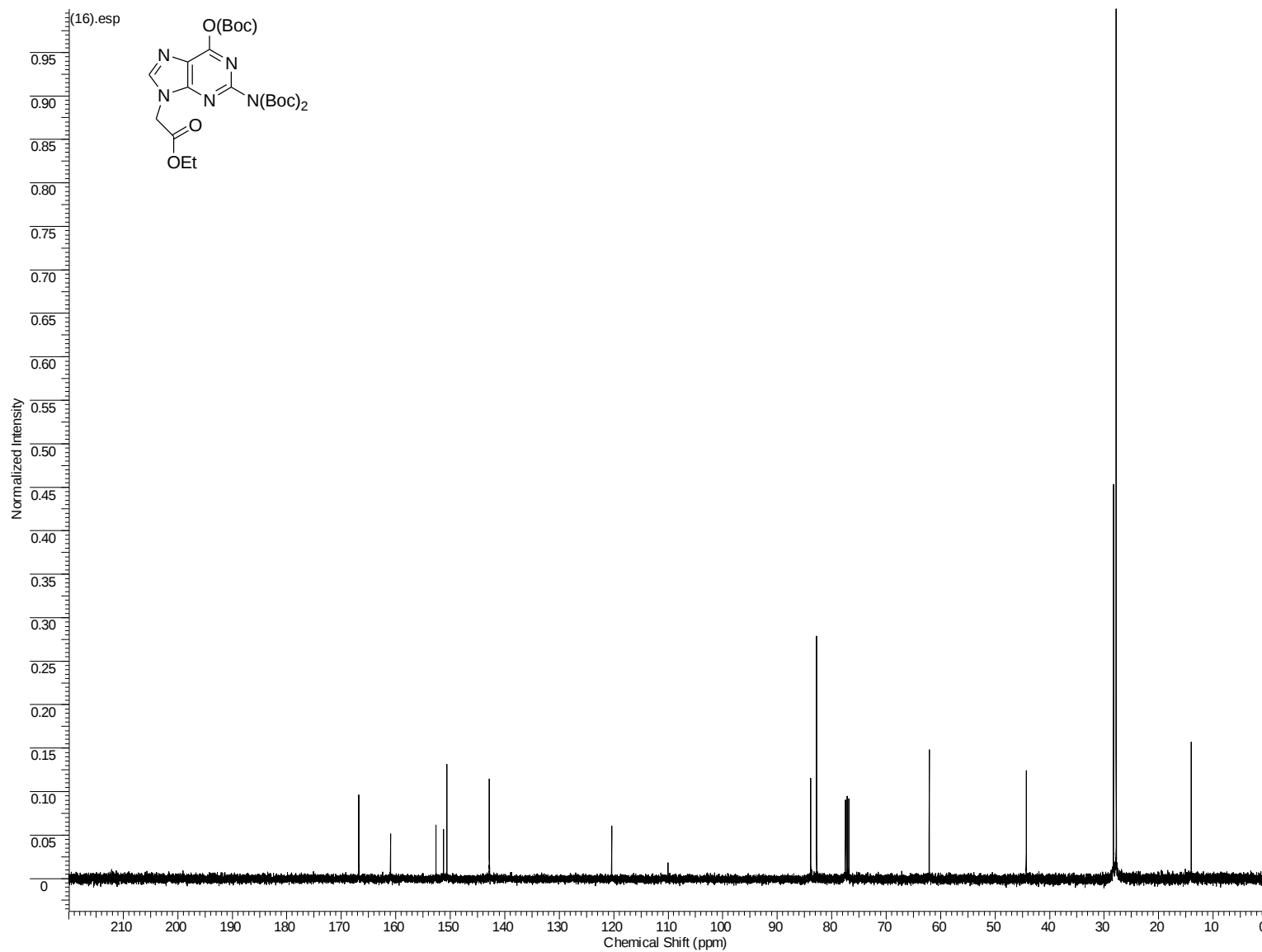
^{13}C NMR (100 MHz, DMSO- d_6) of **15**, Ethyl guanin-9-ylacetate



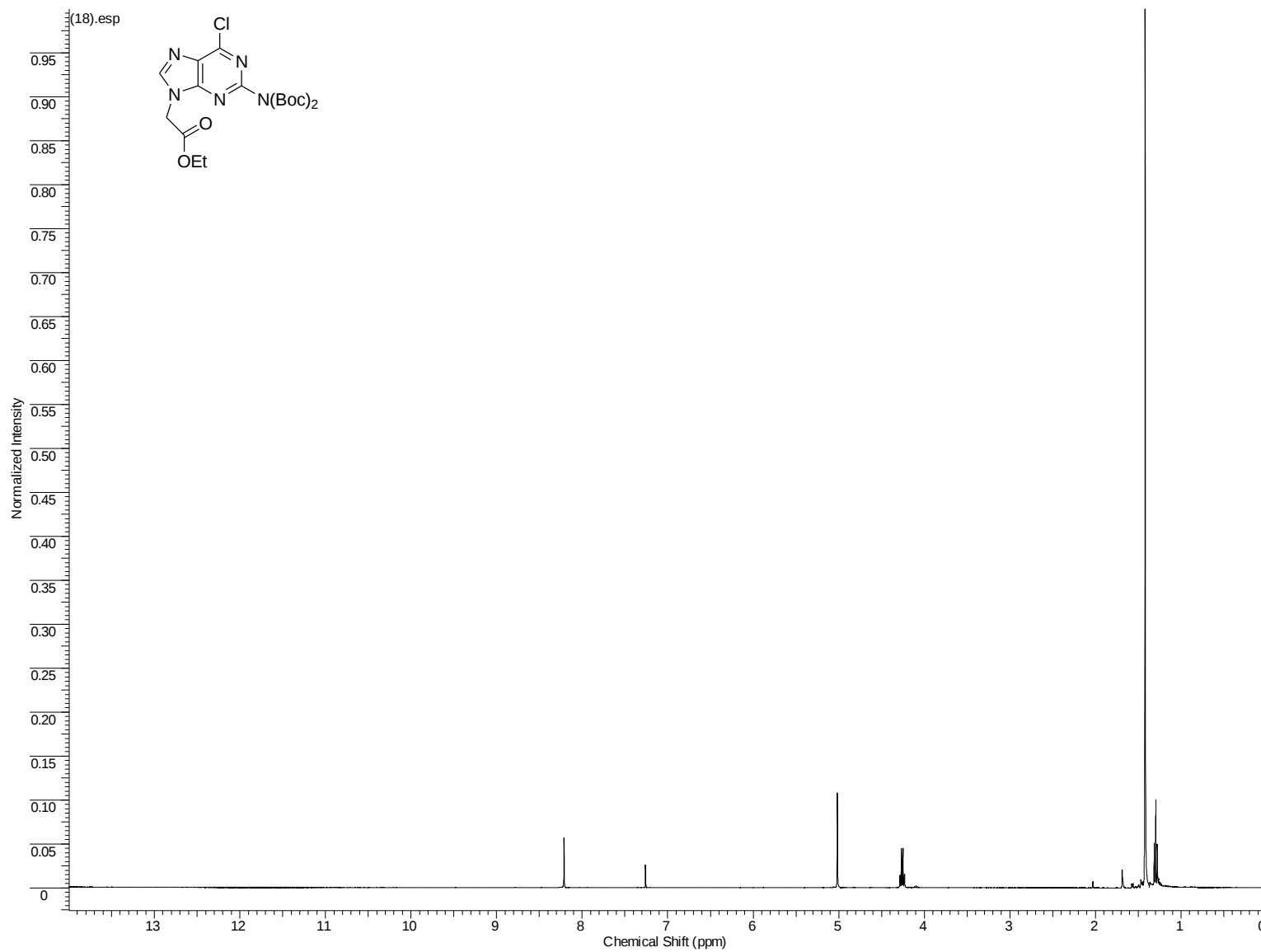
^1H NMR (400 MHz, CDCl_3) of **16**, Ethyl [N^2,N^2 -bis(*tert*-butoxycarbonyl)- O^6 -(*tert*-butoxycarbonyl)guanine-9-yl]acetate



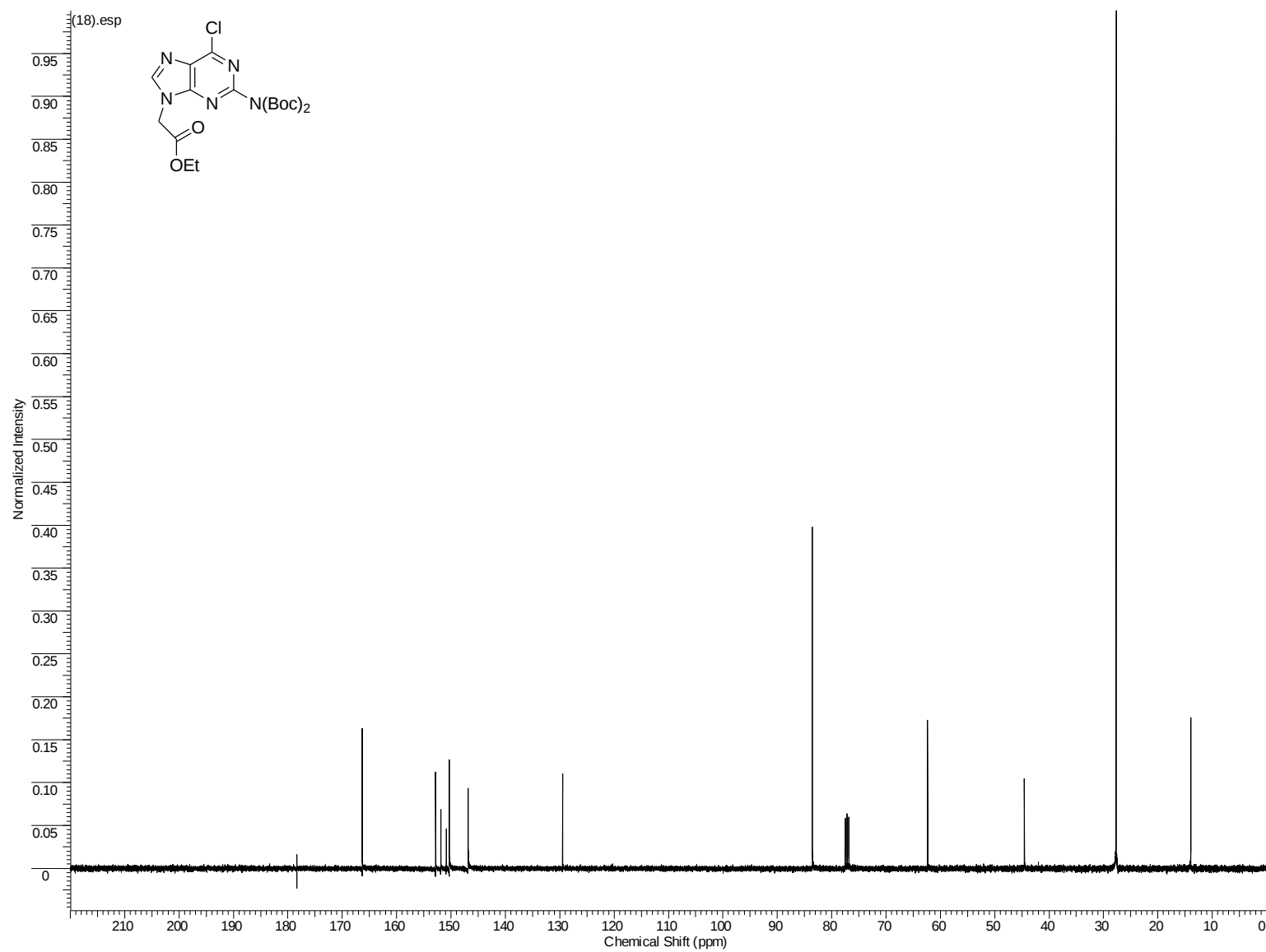
^{13}C NMR (100 MHz, CDCl_3) of **16**, Ethyl [N^2,N^2 -bis(*tert*-butoxycarbonyl)- O^6 -(*tert*-butoxycarbonyl)guanine-9-yl]acetate



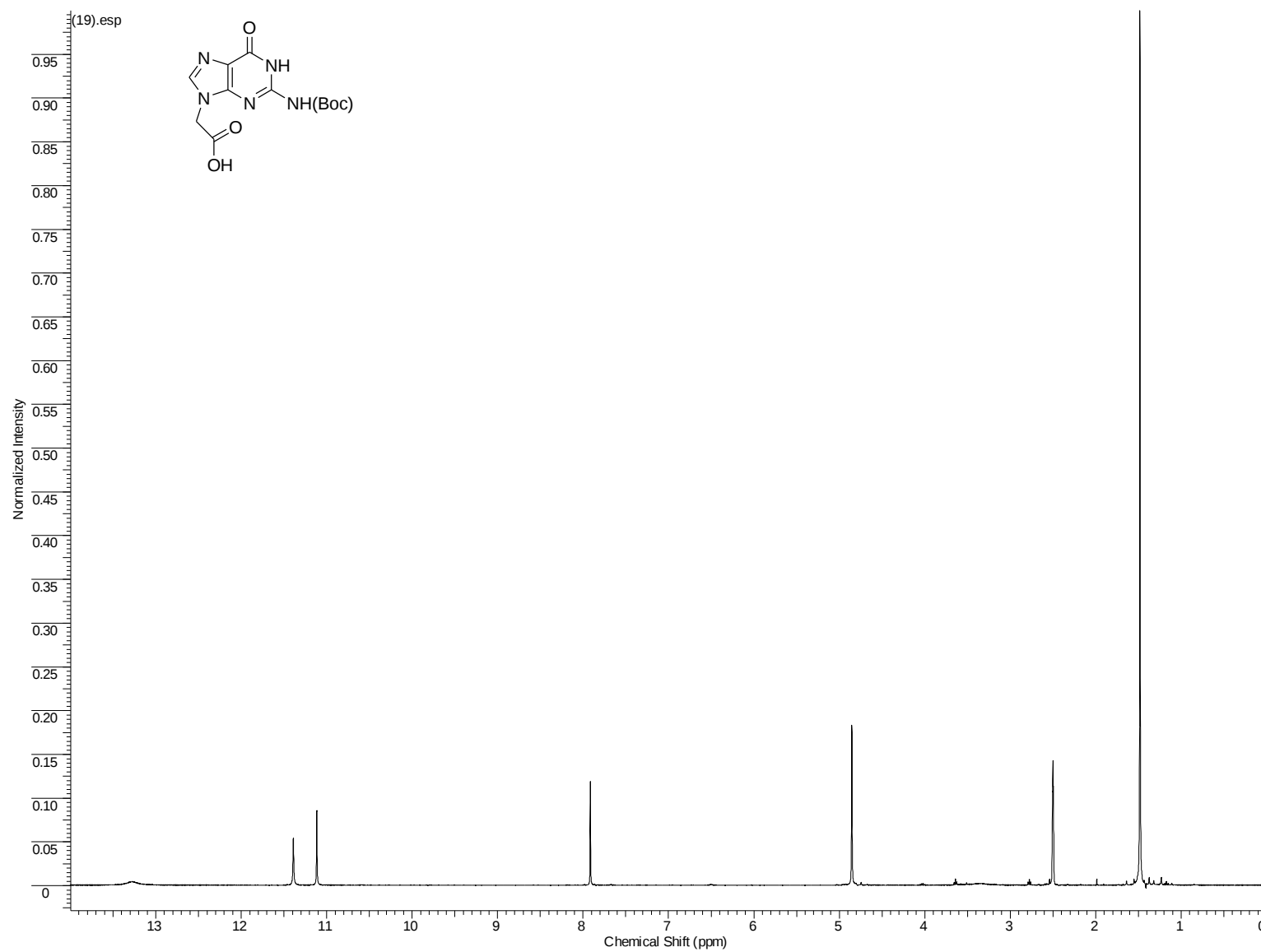
^1H NMR (400 MHz, CDCl_3) of **18**, Ethyl [N^2,N^2 -(bis(*tert*-butoxycarbonyl)amino)-6-chloropurin-9-yl]acetate



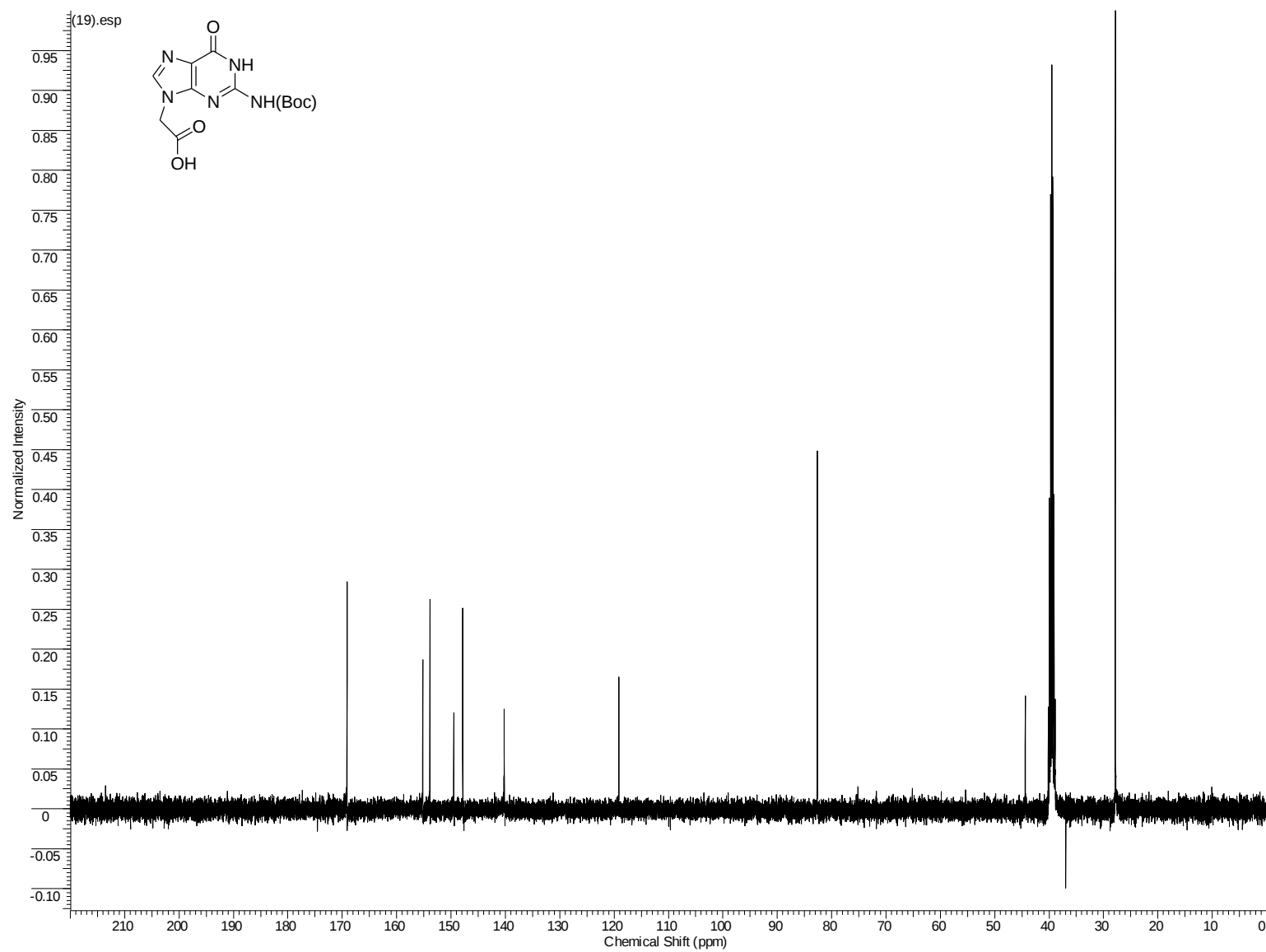
^{13}C NMR (100 MHz, CDCl_3) of **18**, Ethyl [N^2,N^2 -(bis(*tert*-butoxycarbonyl)amino)-6-chloropurin-9-yl]acetate



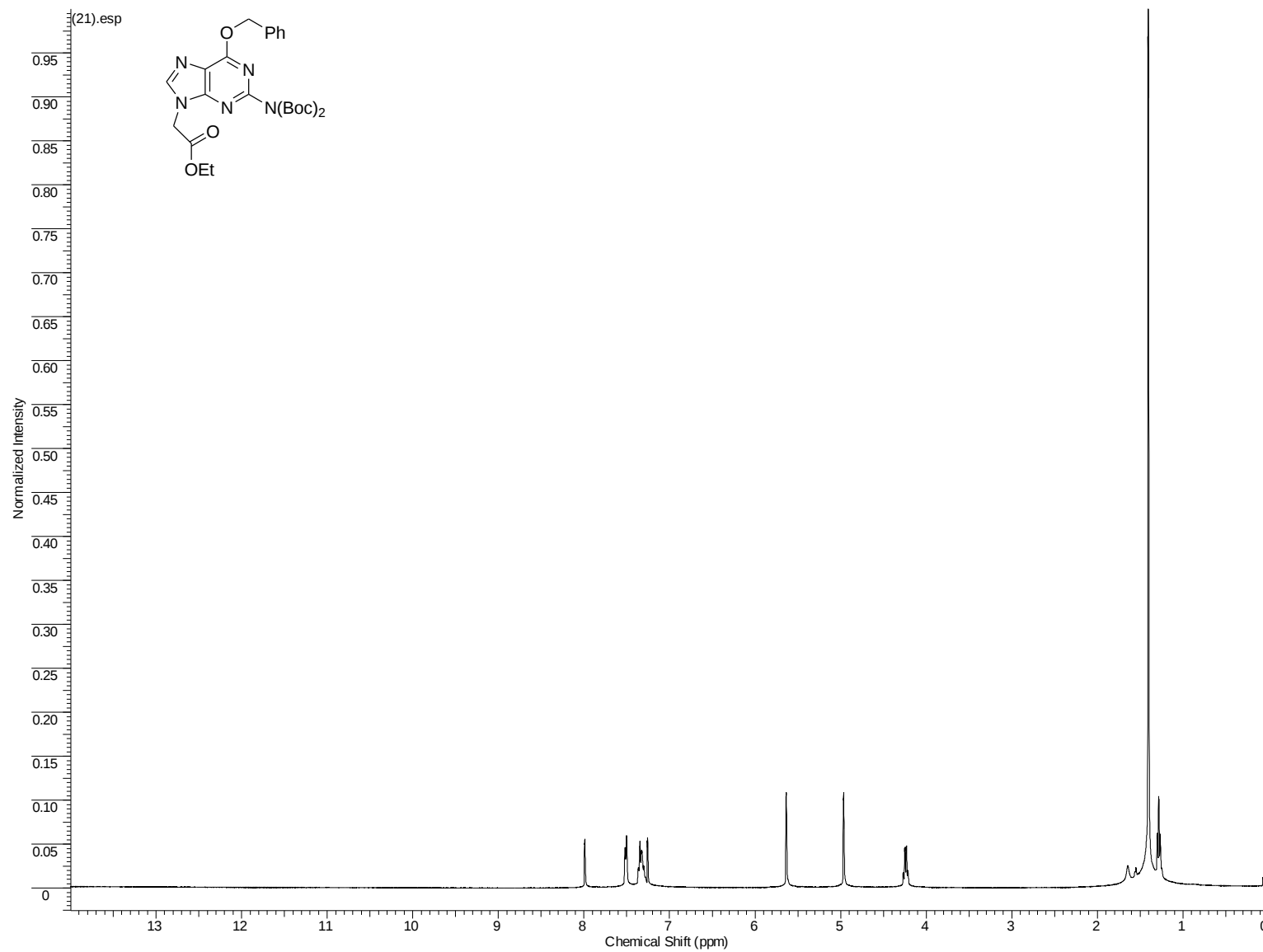
^1H NMR (400 MHz, DMSO- d_6) of **19**, [N²-(*tert*-butoxycarbonyl)guanine-9-yl]acetic acid



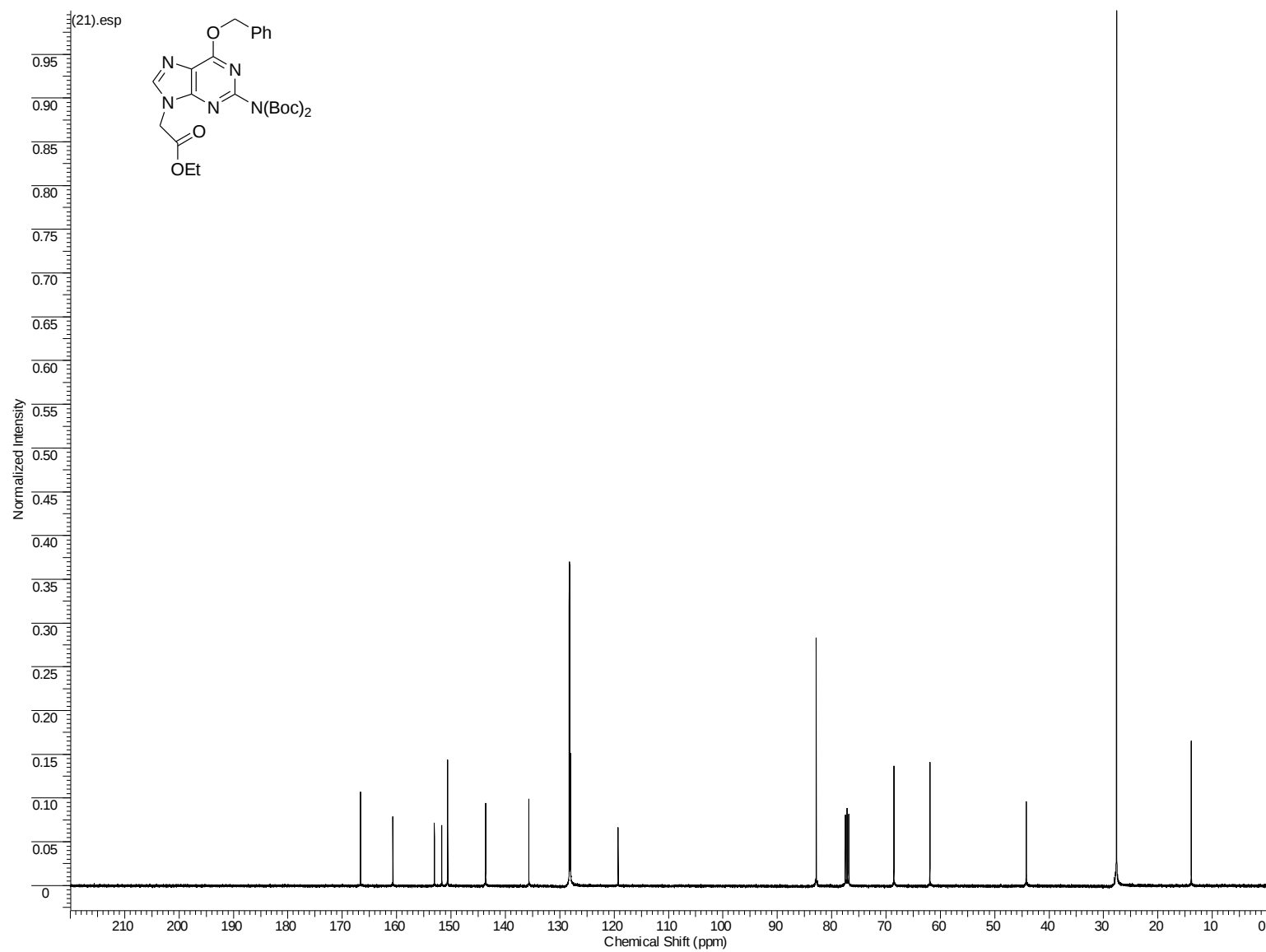
^{13}C NMR (100 MHz, DMSO- d_6) of **19**, [N²-(*tert*-butoxycarbonyl)guanin-9-yl]acetic acid



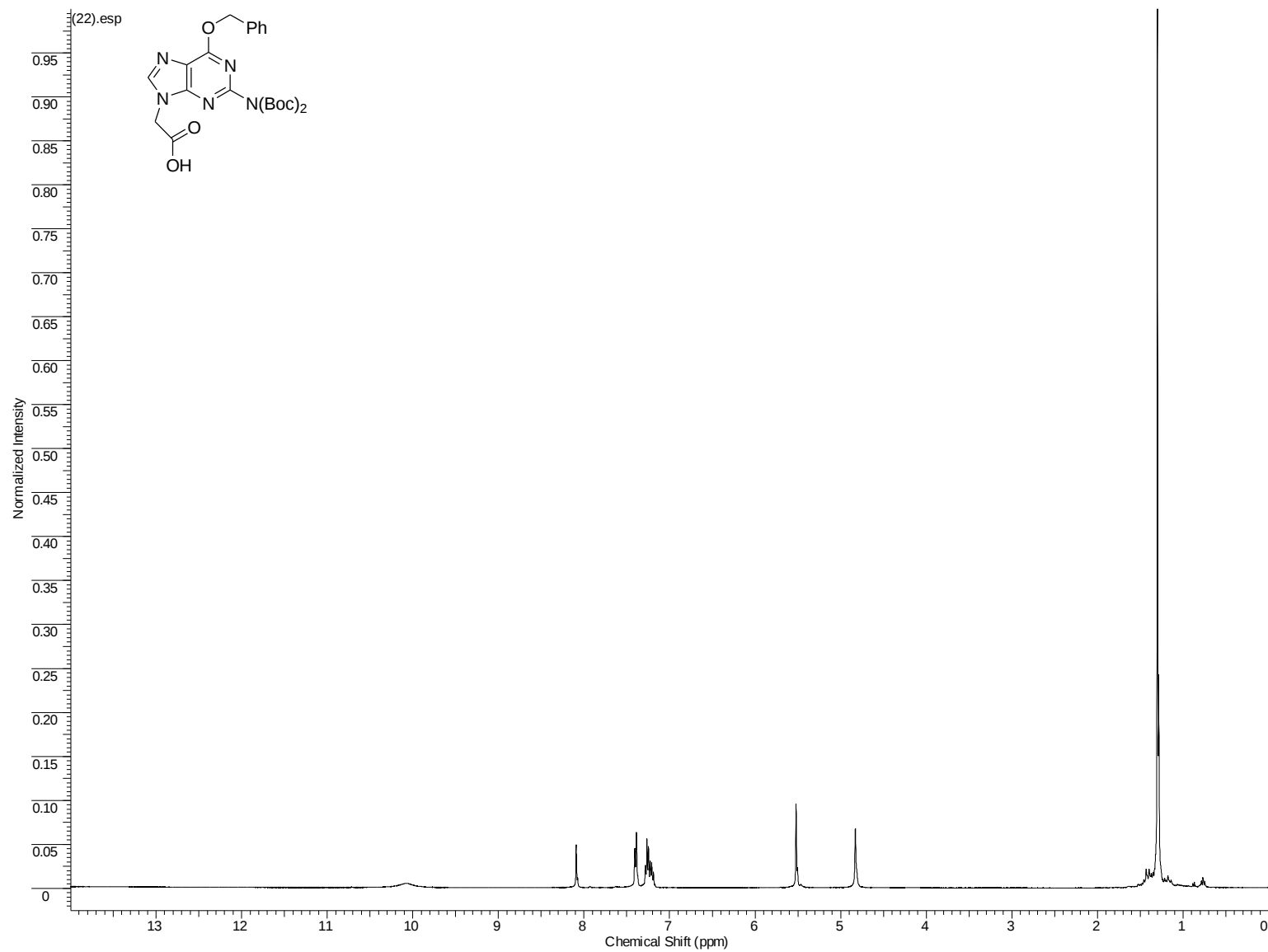
^1H NMR (400 MHz, CDCl_3) of **21**, Ethyl [N^2,N^2 -bis(*tert*-butoxycarbonyl)- O^6 -benzylguanine-9-yl]acetate



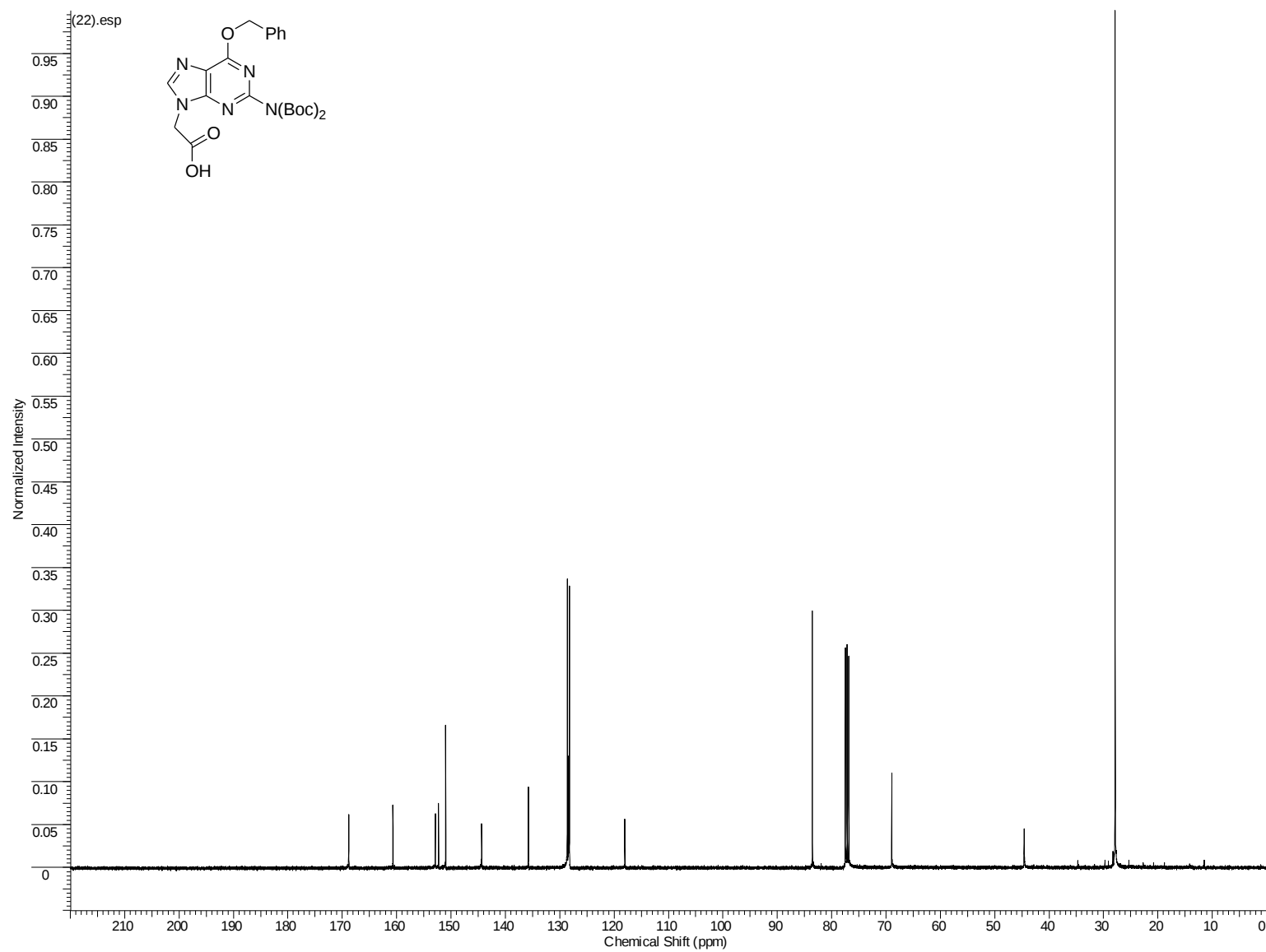
^{13}C NMR (100 MHz, CDCl_3) of **21**, Ethyl [N^2, N^2 -bis(*tert*-butoxycarbonyl)- O^6 -benzylguanine-9-yl]acetate



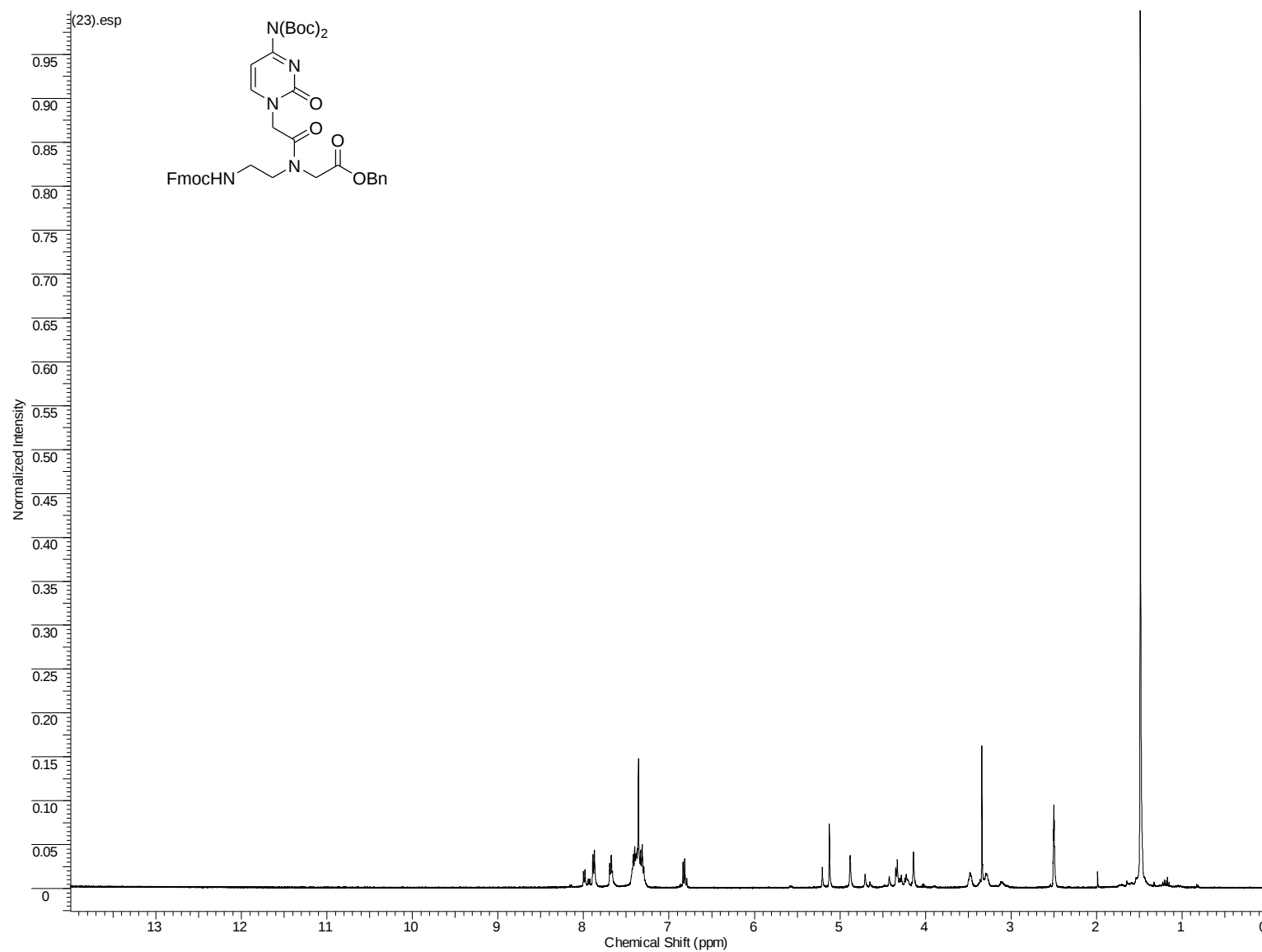
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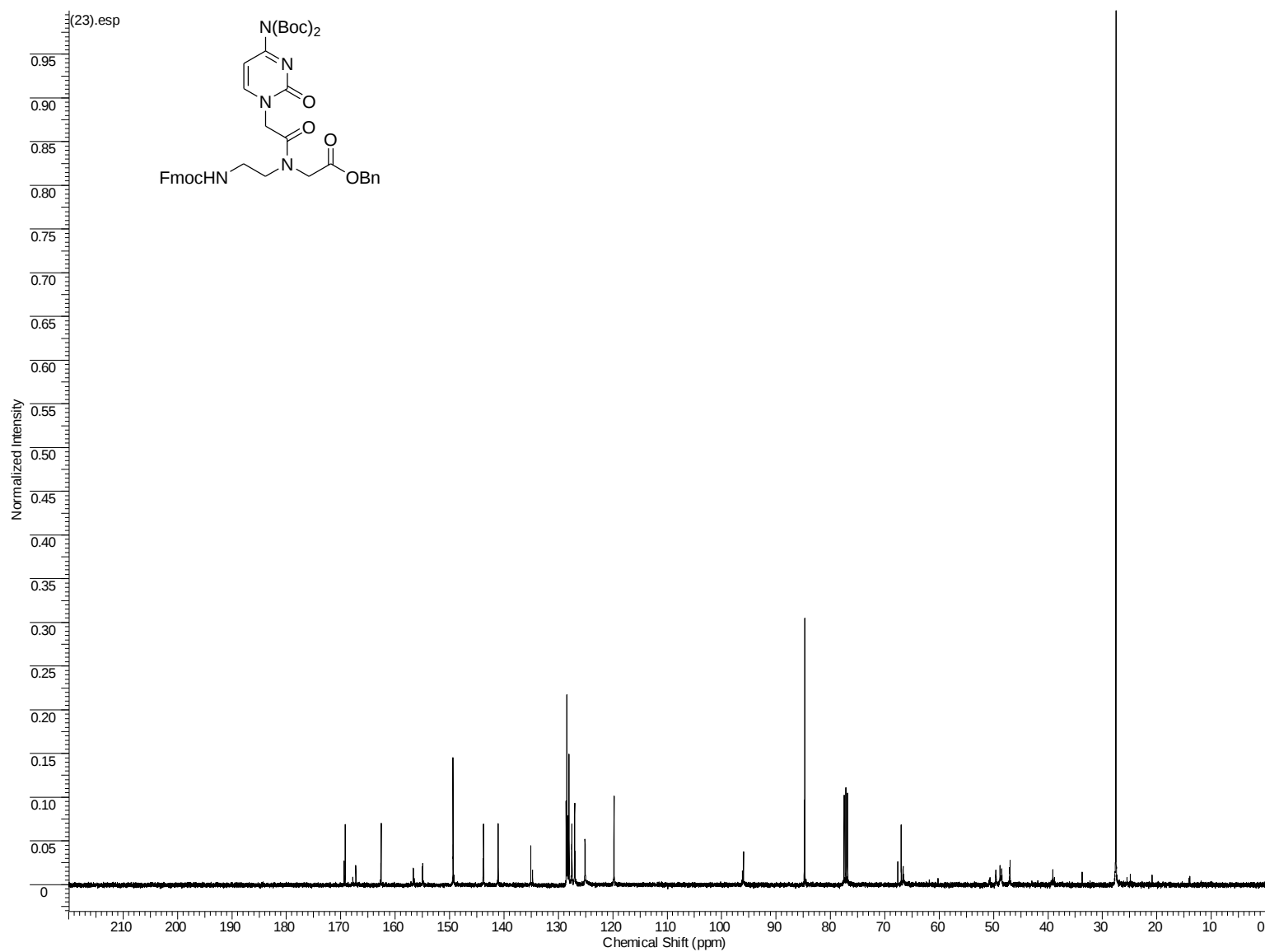
^{13}C NMR (100 MHz, CDCl_3) of **22**, [N^2,N^2 -bis(*tert*-butoxycarbonyl)- O^6 -benzylguanine-9-yl]acetic acid



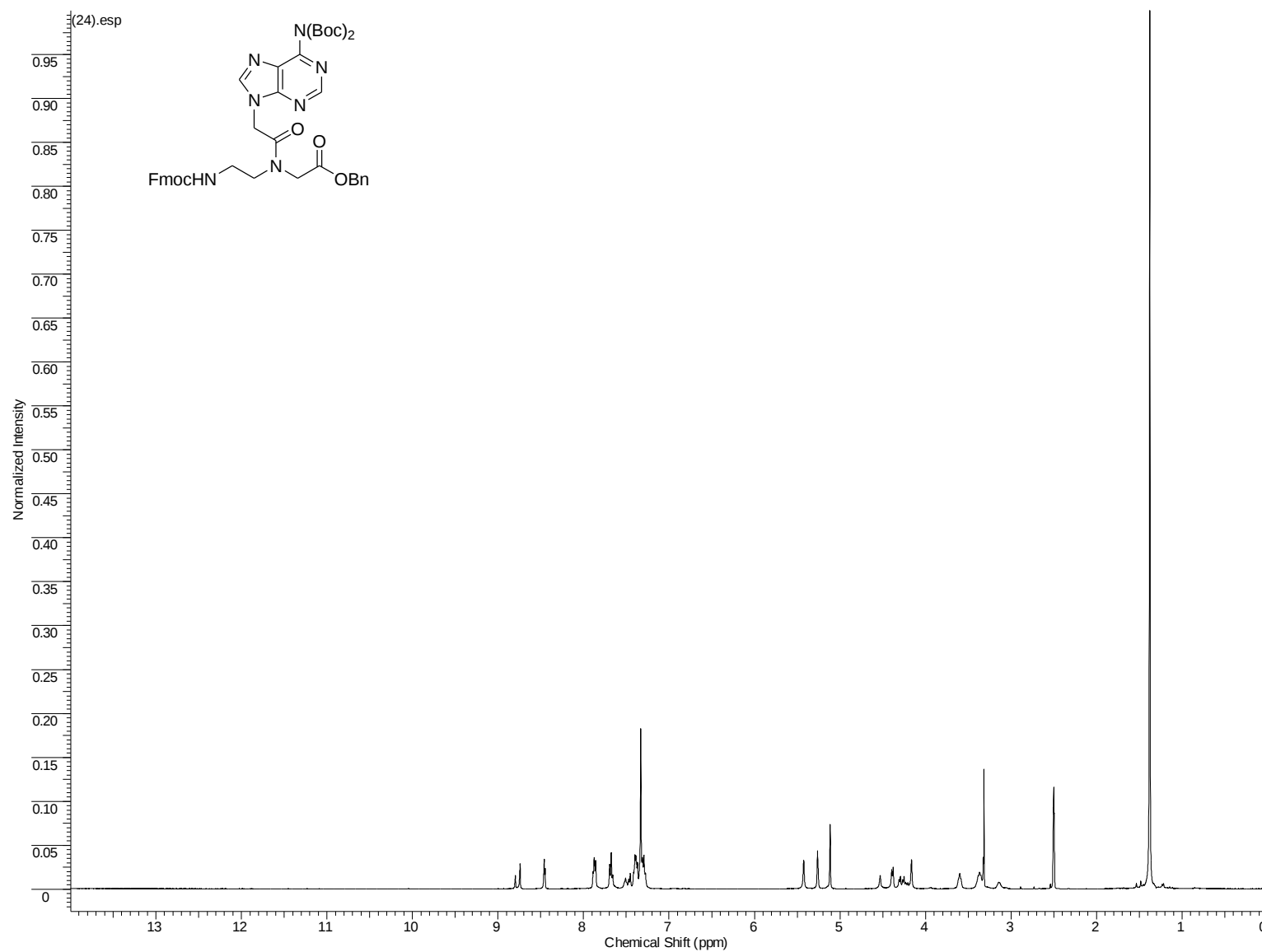
^1H NMR (400 MHz, DMSO- d_6) of **23**, Benzyl *N*-[2-(*N*-9-fluorenylmethoxycarbonyl)aminoethyl]-*N*-[(*N*⁴,*N*⁴-bis(*tert*-butoxycarbonyl)-cytosin-1-yl)acetyl]glycinate



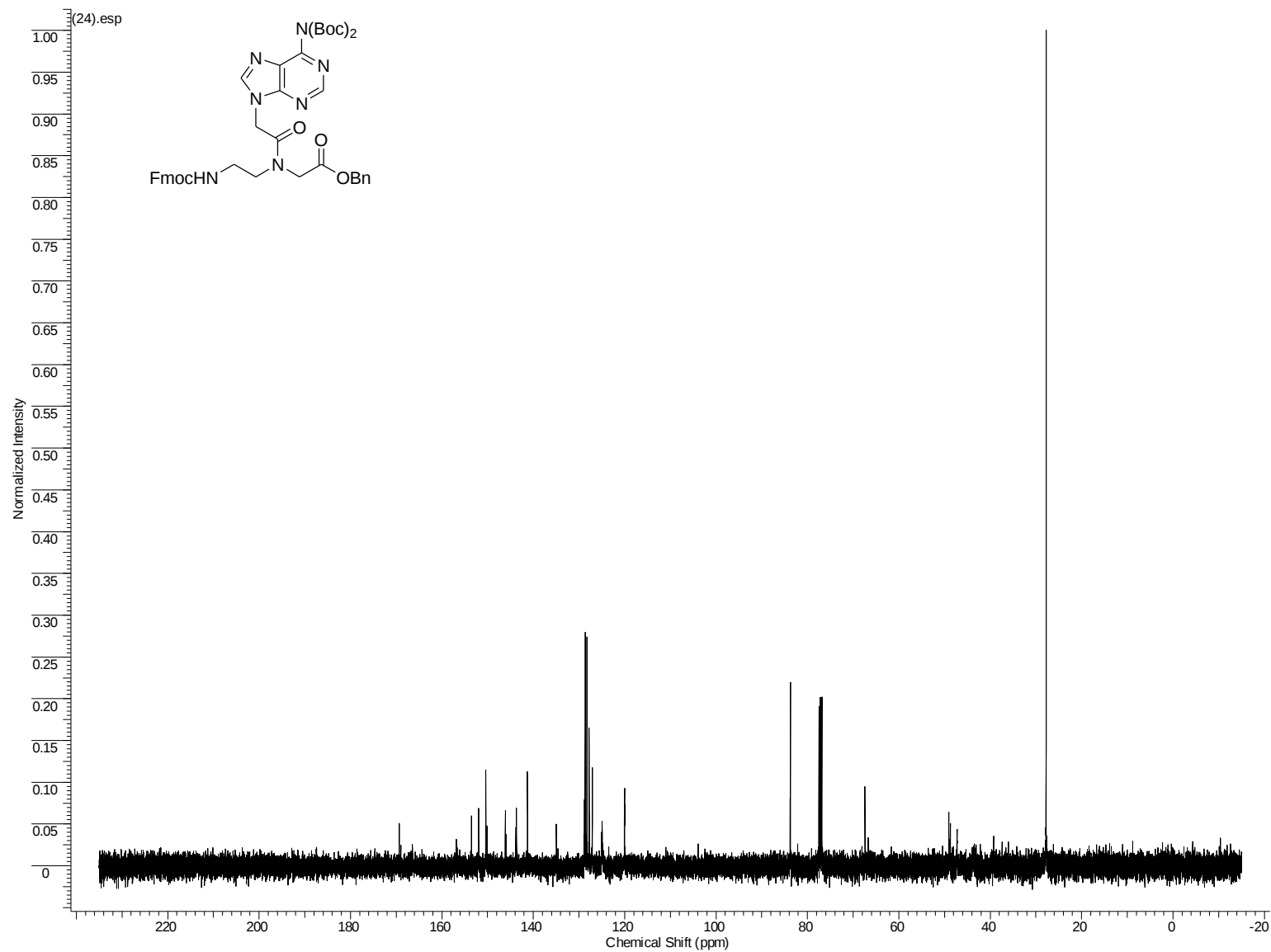
^{13}C NMR (100 MHz, CDCl_3) of **23**, Benzyl *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]-*N*-[N^4,N^4 -bis(*tert*-butoxycarbonyl)cytosin-1-yl]acetyl]glycinate



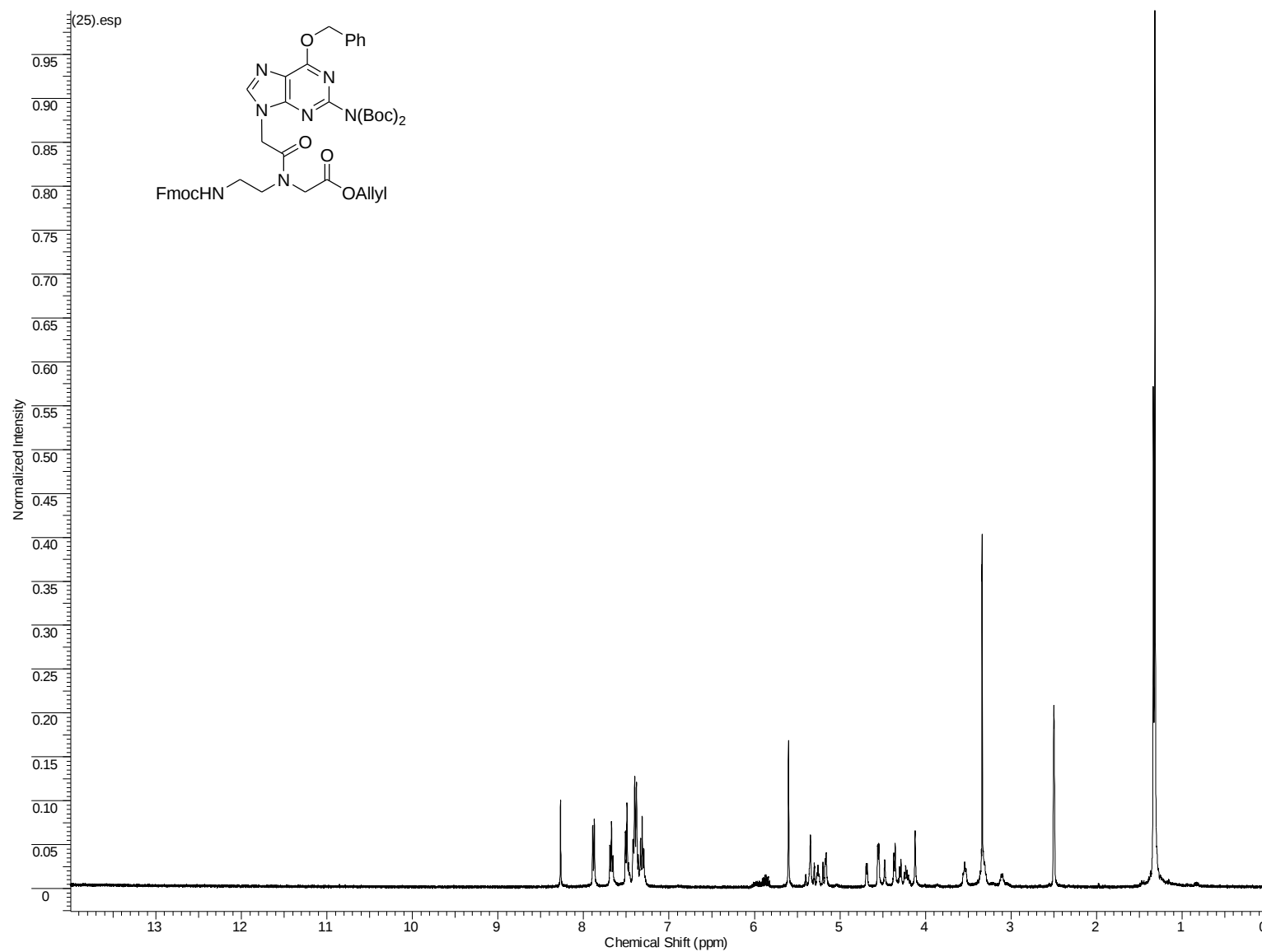
^1H NMR (400 MHz, DMSO- d_6) of **24**, Benzyl *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]-*N*-[(N^6,N^6 -bis(*tert*-butoxycarbonyl)-adenin-9-yl)acetyl]glycinate



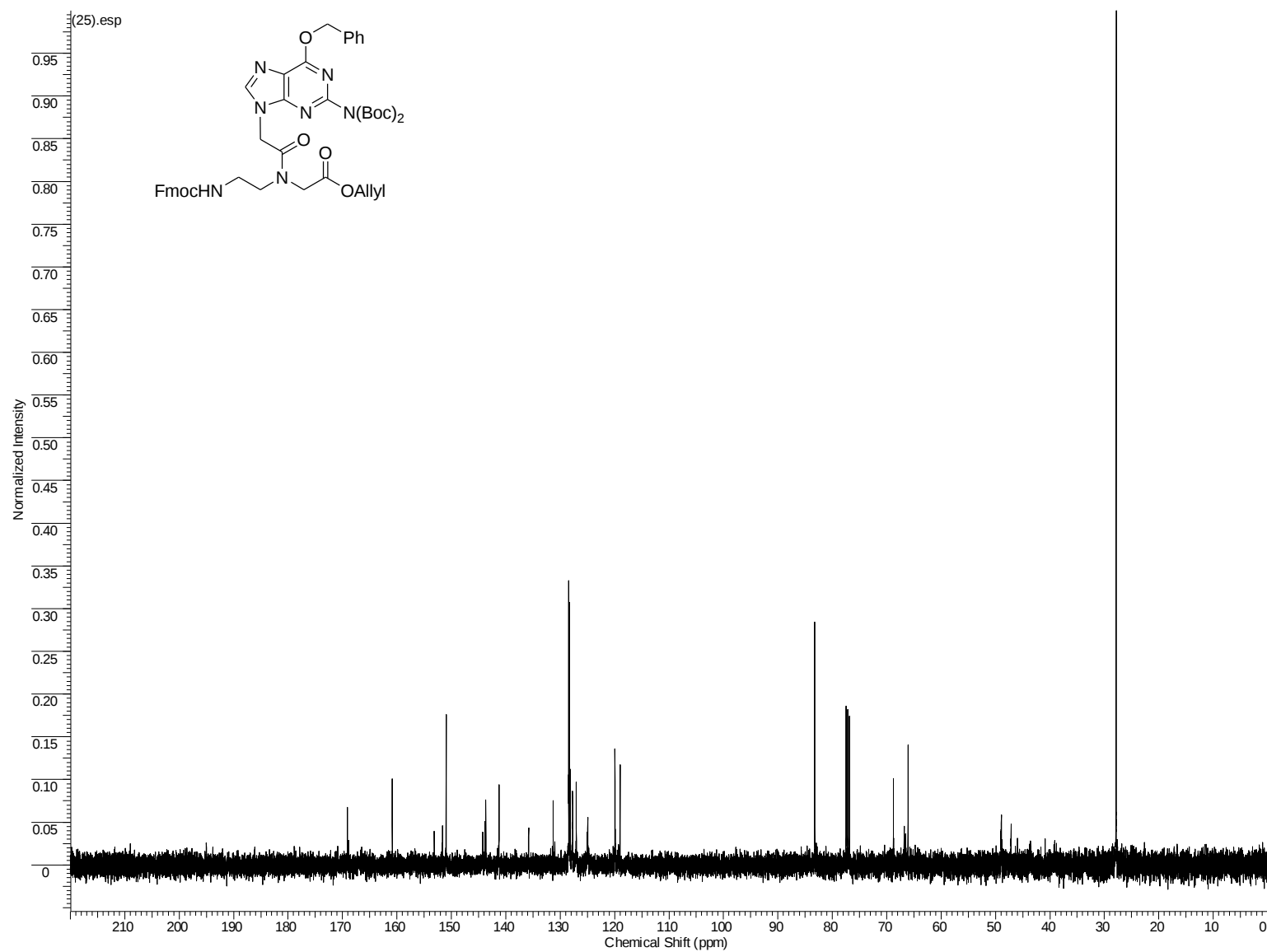
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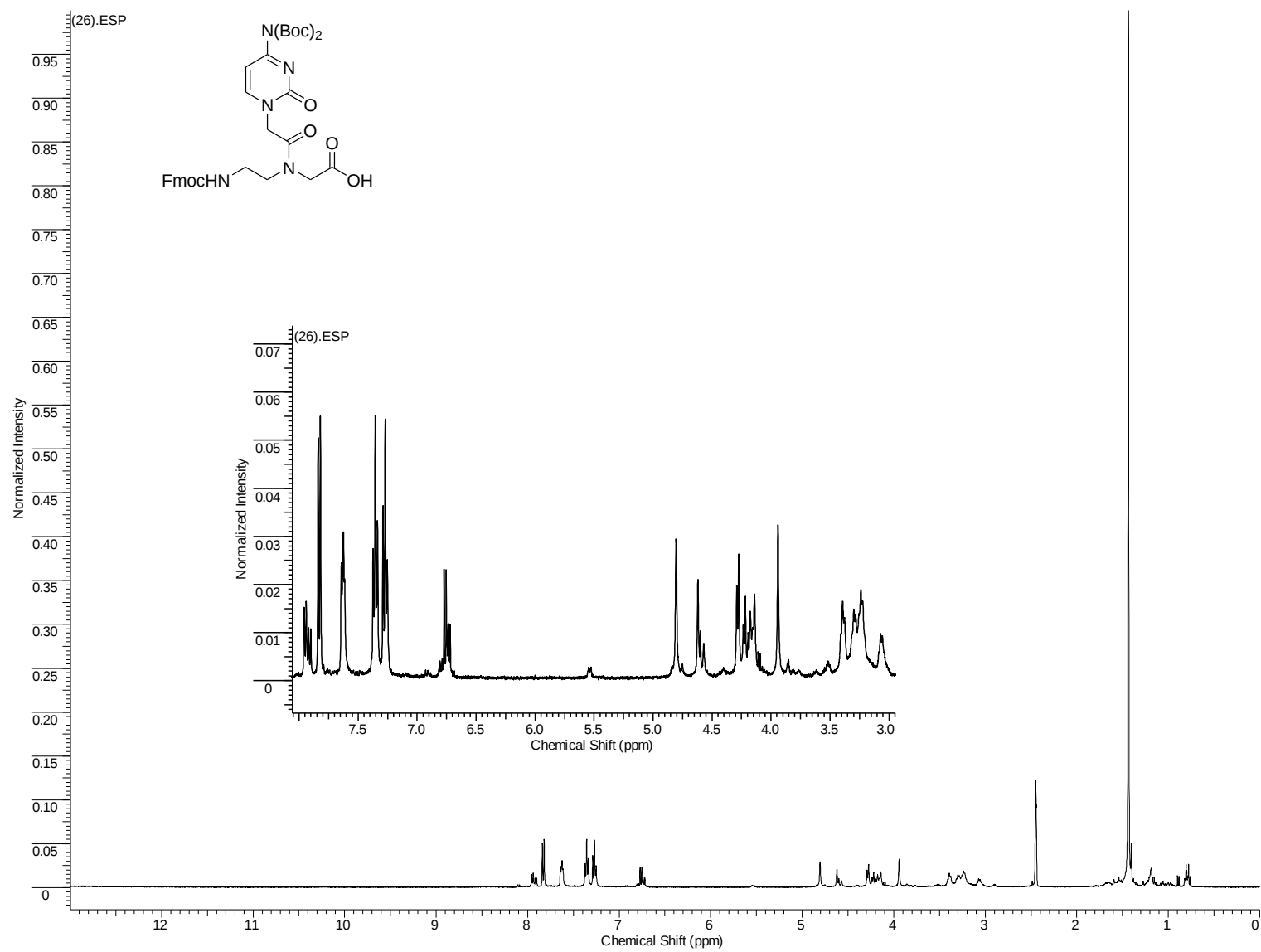
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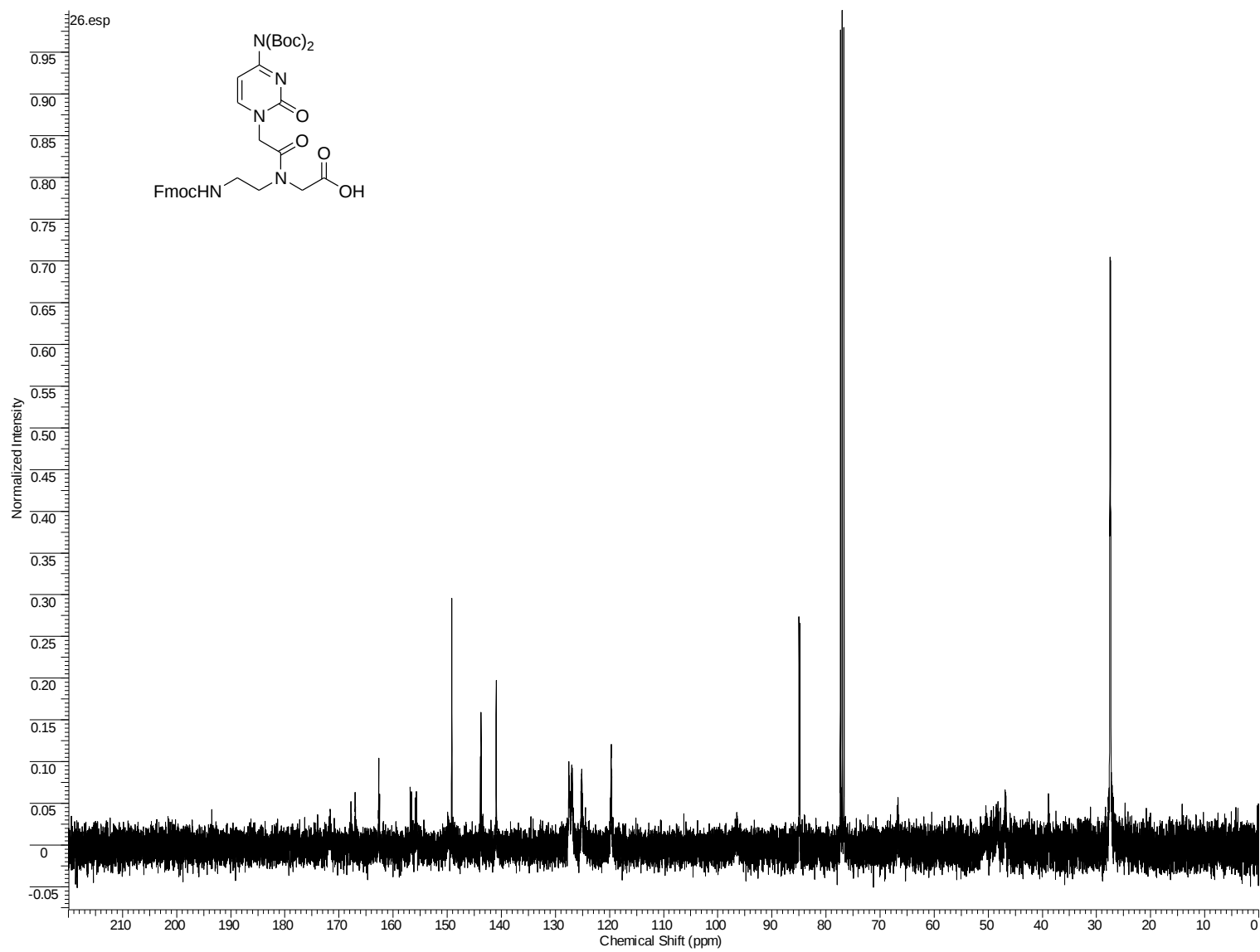
^{13}C NMR (100 MHz, CDCl_3) of **25**, Allyl *N*-[2-(fluorenylmethoxycarbonyl)-aminoethyl]-*N*-[N^2,N^2 -bis(*tert*-butoxycarbonyl)- O^6 -benzylguanine-9-yl]acetyl]glycinate



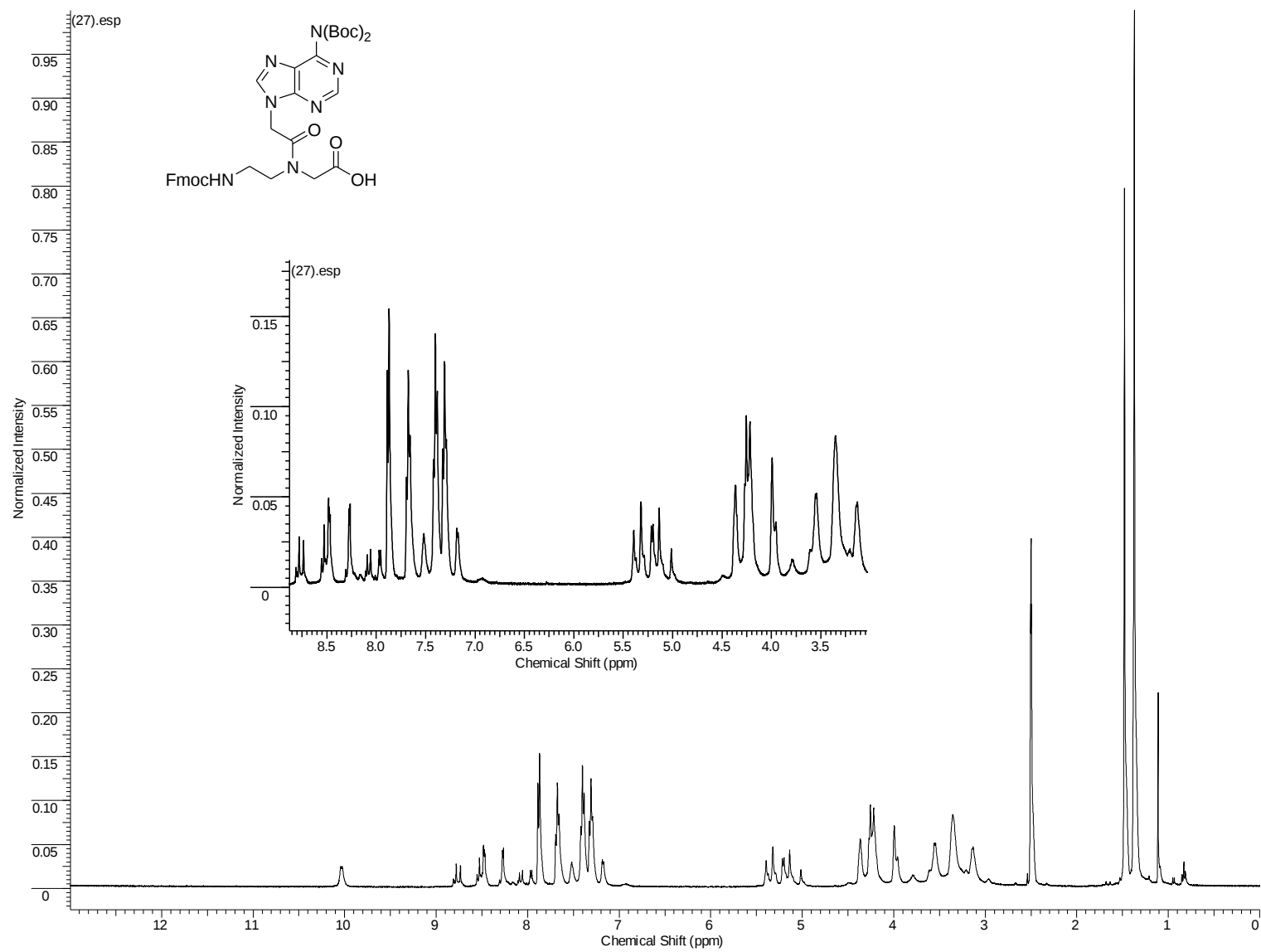
^1H NMR (400 MHz, DMSO- d_6) of **26**, *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]-*N*-[$(N^4,N^4$ -bis(*tert*-butoxycarbonyl)cytosin-1-yl)acetyl]glycine



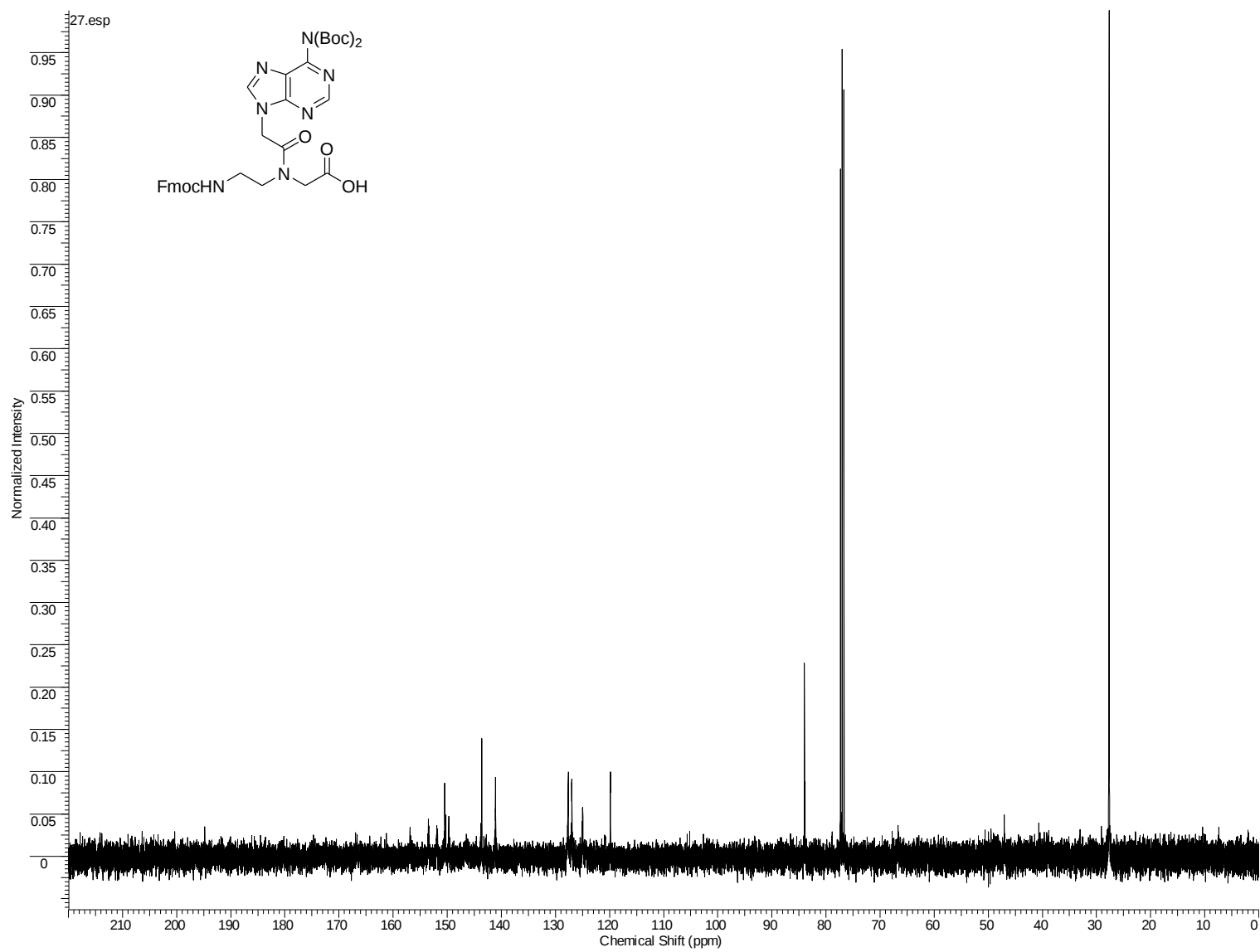
^{13}C NMR (100 MHz, CDCl_3) of **26**, *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]-*N*-[(N^4,N^4 -bis(*tert*-butoxycarbonyl)cytosin-1-yl)acetyl]glycine



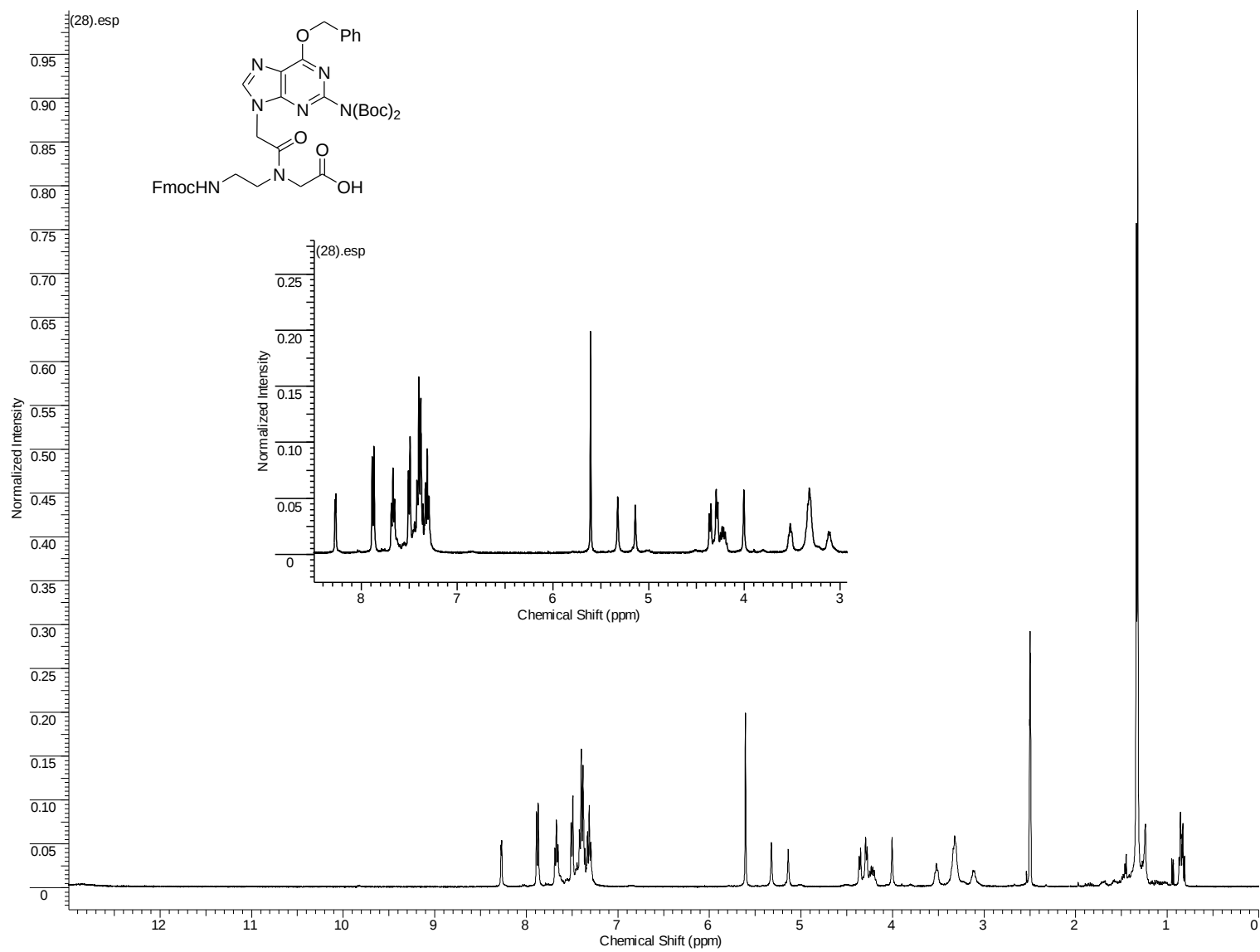
^1H NMR (400 MHz, DMSO- d_6) of **27**, *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]-*N*-[N^6,N^6 -bis(*tert*-butoxycarbonyl)adenin-9-yl]acetyl]glycine



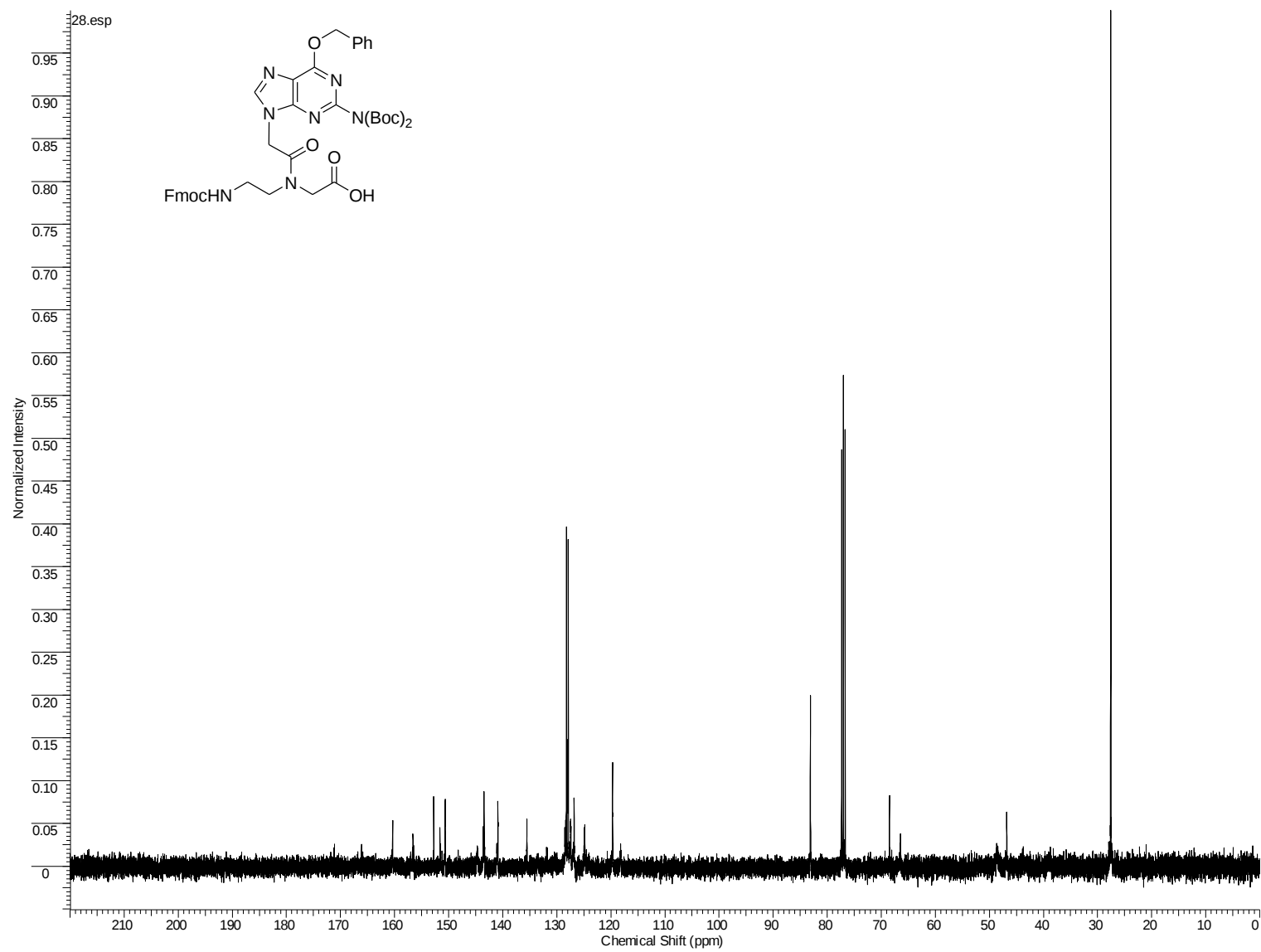
^{13}C NMR (100 MHz, CDCl_3) of **27**, *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]-*N*-[(N^6,N^6 -bis(*tert*-butoxycarbonyl)adenin-9-yl)acetyl]glycine



^1H NMR (400 MHz, DMSO- d_6) of **28**, *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]-*N*-[N^2,N^2 -bis(*tert*-butoxycarbonyl)- O^6 -benzylguanine-9-yl]acetyl]glycine



^{13}C NMR (100 MHz, CDCl_3) of **28**, *N*-[2-(fluorenylmethoxycarbonyl)aminoethyl]-*N*-[N^2,N^2 -bis(*tert*-butoxycarbonyl)- O^6 -benzylguanine-9-yl]acetyl]glycine



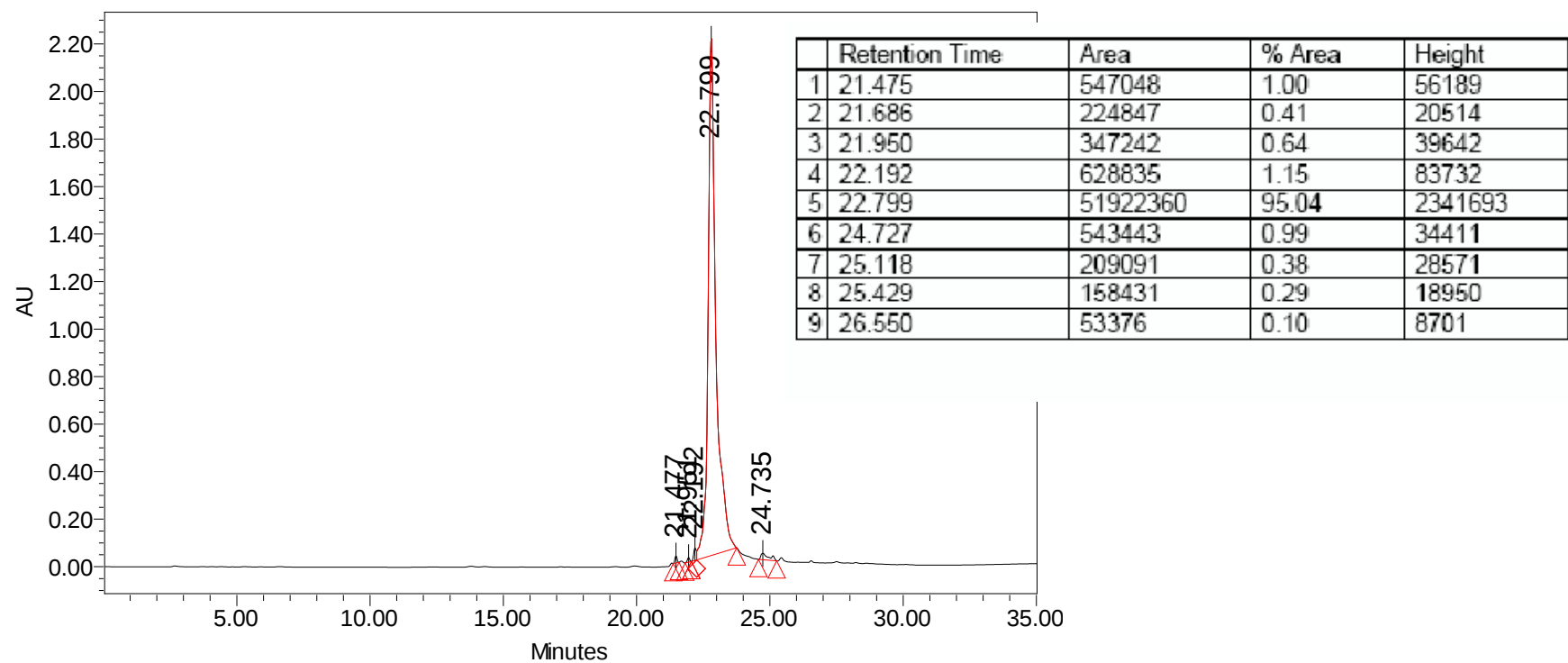


Fig. S1. HPLC chromatogram H-GTA GAT CAC T-Lys-NH₂