Supplementary Information

Synthesis and Antileishmanial Activity of Some Functionalized Peptoids

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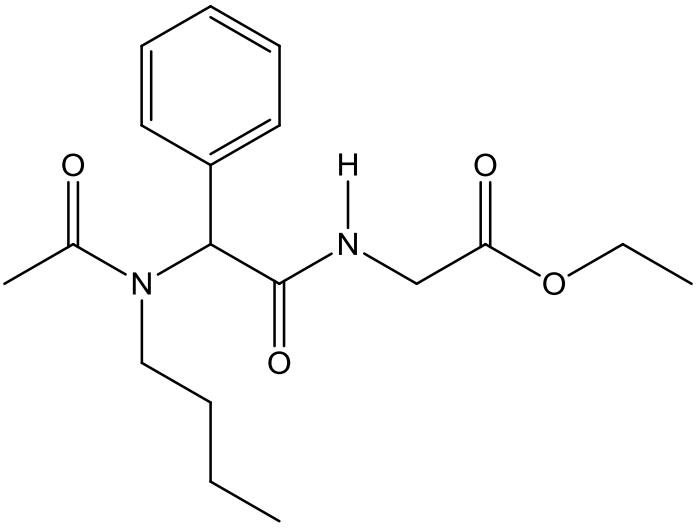
Spectroscopic data for peptoids (**5a**-**m**)

Compound **5a**



Ethyl 2-(2-(*N*-butylacetamido)-2-phenylacetamido)acetate (**5a**)

Yellow oil, yield 71%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40-7.27 (m, 5H), 6.66 (s, 1H), 5.94 (s, 1H), 4.21 (q, 2H, *J* 8.6 Hz), 4.03 (d, 1H, *J* 6.1 Hz), 4.02 (d, 1H, *J* 5.6 Hz), 3.30-3.25 (m, 2H), 2.16 (s, 3H), 1.44-1.35 (m, 2H), 1.26 (t, 3H, *J* 7.1 Hz), 1.12-1.03 (m, 2H), 0.72 (t, 2H, *J* 7.3 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.8 (C), 170.3 (C), 169.8 (C), 135.2 (C), 129.7 (2 CH), 128.8 (2 CH), 128.6 (CH), 62.6 (CH_2), 61.5 (CH), 47.8 (CH_2), 41.6 (CH_2), 31.6 (CH_2), 21.8 (CH_2), 20.1 (CH_3), 14.2 (CH_3), 13.5 (CH_3); FTIR (KBr) ν / cm^{-1} 3231 (N–H), 2947 (C–H), 1750 (C=O, ester), 1641 (C=O, amide), 1190 and 1026 (C–O, ester), 740 and 705 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{18}H_{26}N_2NaO_4$ $[M + Na]^+$: 357.1790; found: 357.1784.

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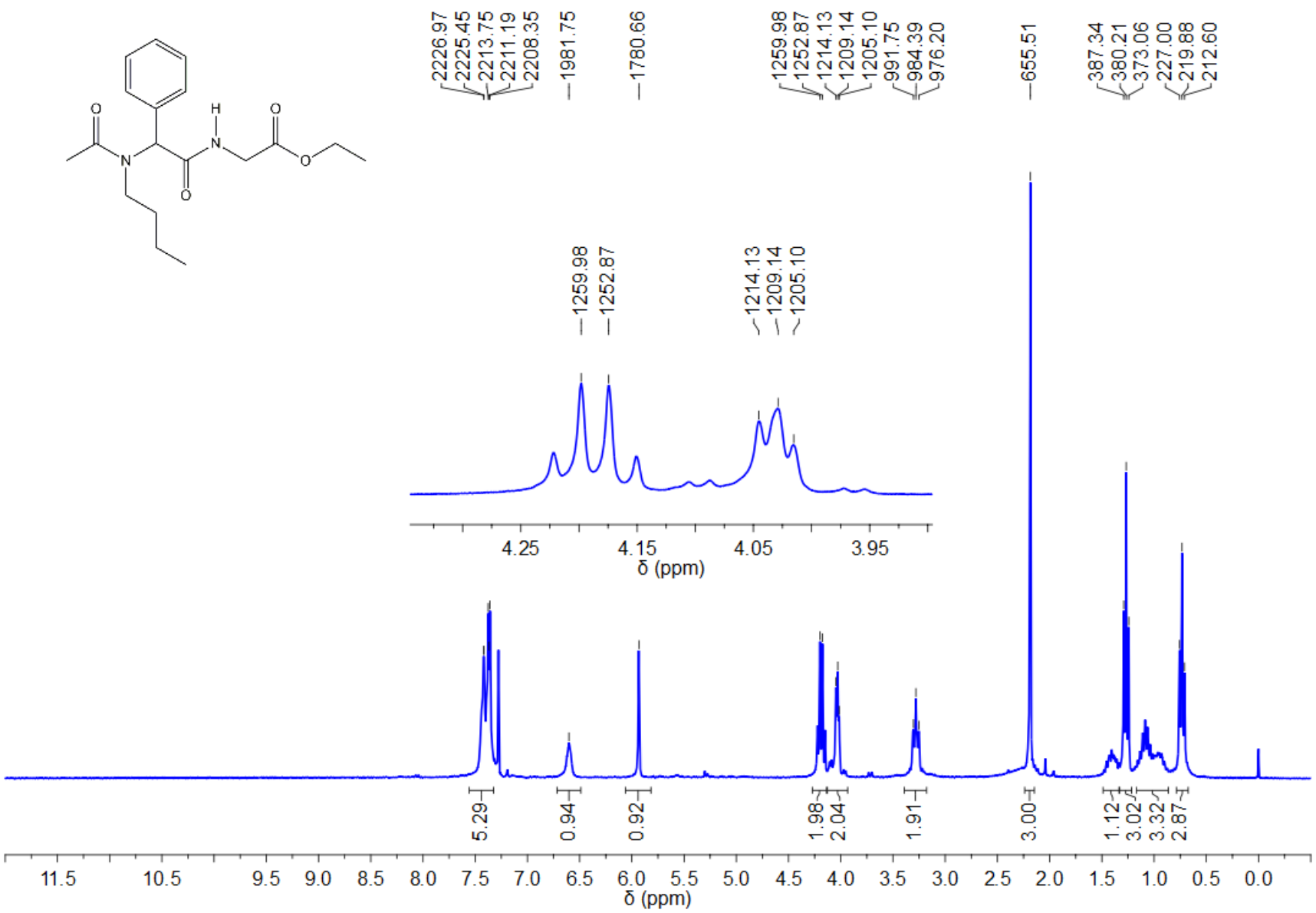


Figure S1. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **5a**.

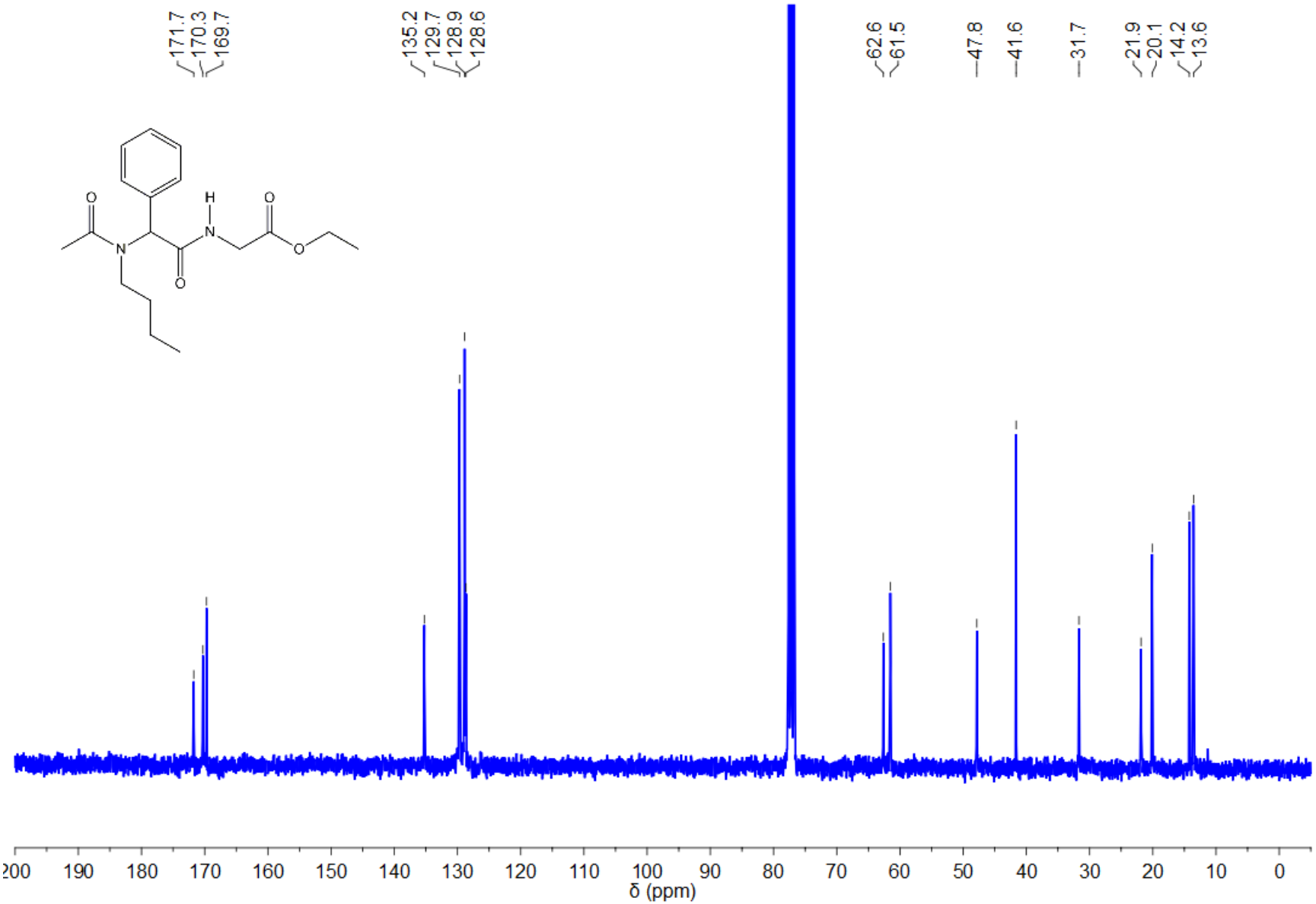


Figure S2. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **5a**.

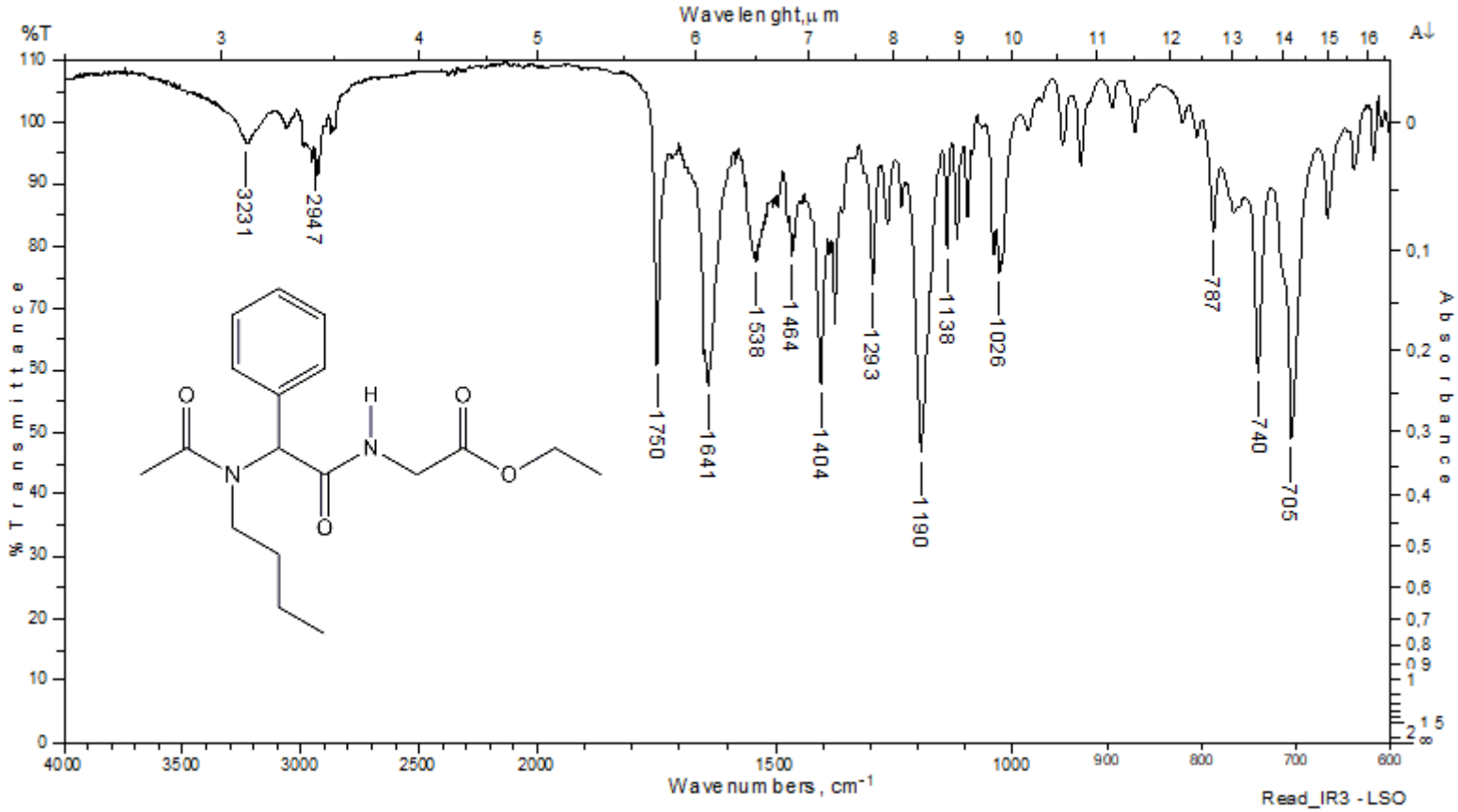


Figure S3. FTIR (KBr) spectrum of compound **5a**.

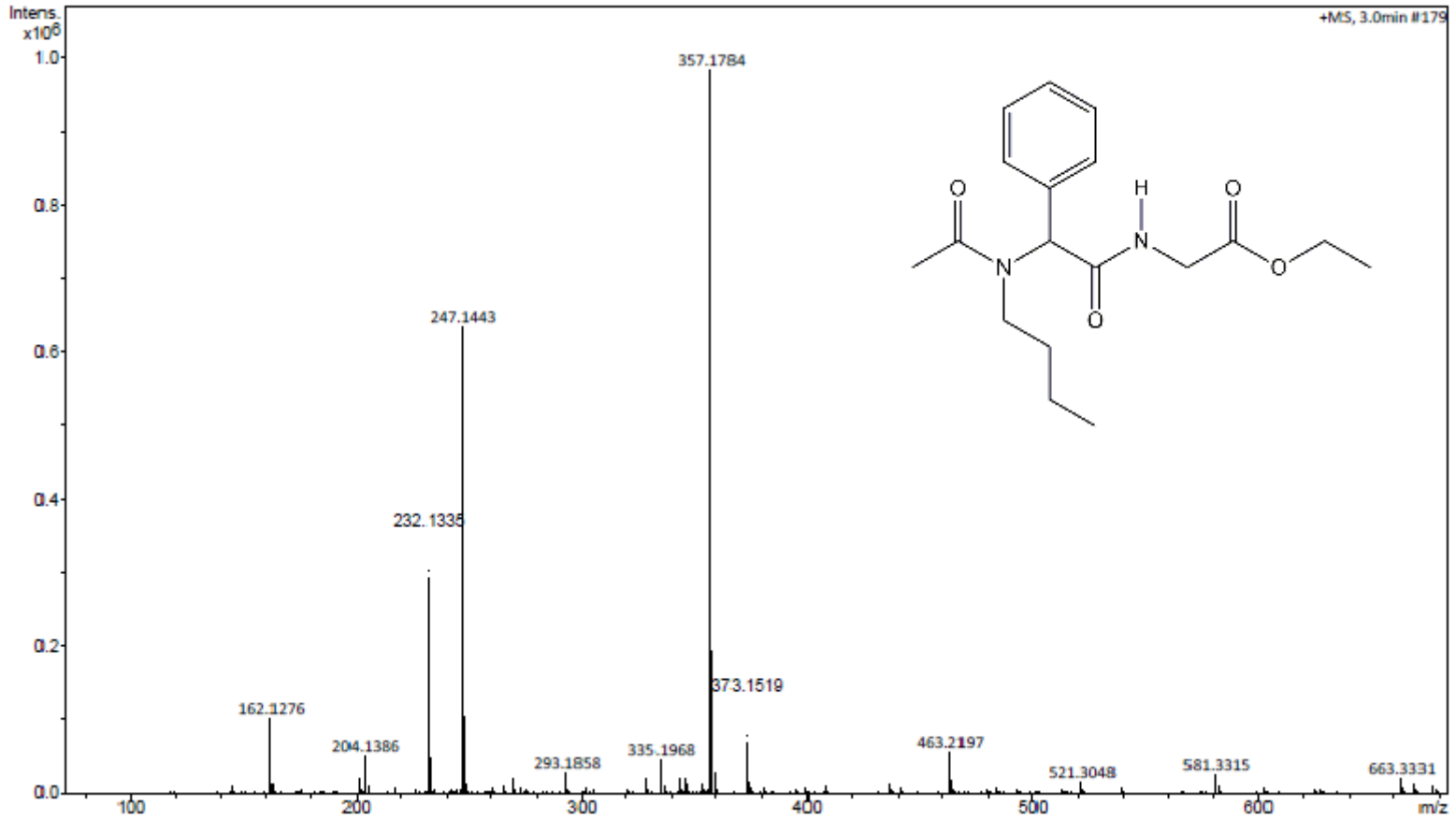
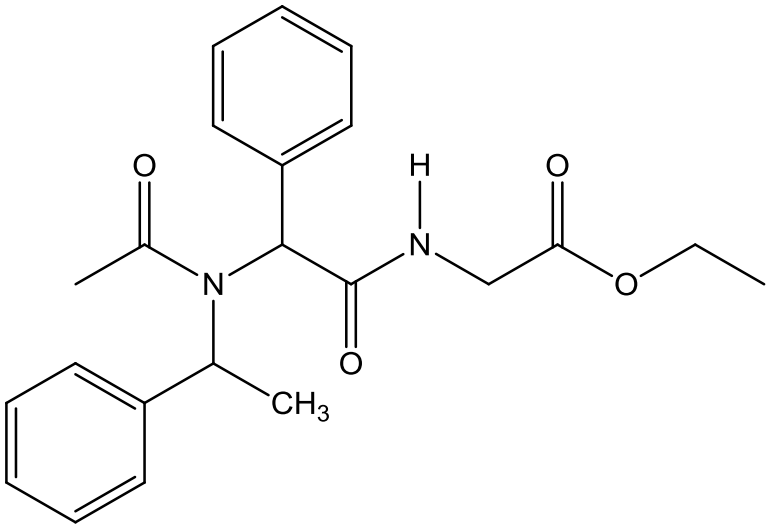


Figure S4. Mass spectrum of compound **5a**.

Compound **5b**



Ethyl 2-(2-phenyl-2-(*N*-(1-phenylethylacetamido)acetamido)acetate (**5b**)

Yellow oil, yield 78%; diastereoisomeric mixture (53:47); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58-6.94 (m, 20H), 6.62 (s, 1H), 6.35 (s, 1H), 5.24 (q, 1H, *J* 7.0 Hz), 5.23 (q, 1H, *J* 6.8 Hz), 4.73 (s, 1H), 4.66 (s, 1H), 4.20-3.90 (m, 8H), 2.35 (s, 3H), 2.28 (s, 3H), 1.80 (d, 3H, *J* 6.8 Hz), 1.42 (d, 3H, *J* 7.0 Hz), 1.24 (t, 3H, *J* 7.1 Hz), 1.22 (t, 3H, *J* 6.9 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.3 (2 C), 170.8 (C), 169.7 (2 C), 139.0 (C), 138.9 (C), 136.1 (2 C), 128.8 (2 CH), 128.6 (2 CH), 128.4 (4 CH), 128.3 (4 CH), 128.1 (2 CH), 128.0 (2 CH), 127.9 (2 CH), 127.8 (2 CH), 63.6 (2 CH), 61.4 (2 CH_2), 57.5 (2 CH), 41.7 (2 CH_2), 23.1 (2 CH_3), 17.3 (2 CH_3), 14.2 (2 CH_3); FTIR (KBr) ν / cm^{-1} 3277 (N–H), 2981 (C–H), 1748 (C=O, ester), 1680 (C=O, amide), 1197 and 1027 (C–O, ester), 760 and 697 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{22}H_{26}N_2NaO_4$ $[M + Na]^+$: 405.1790; found: 405.1784.

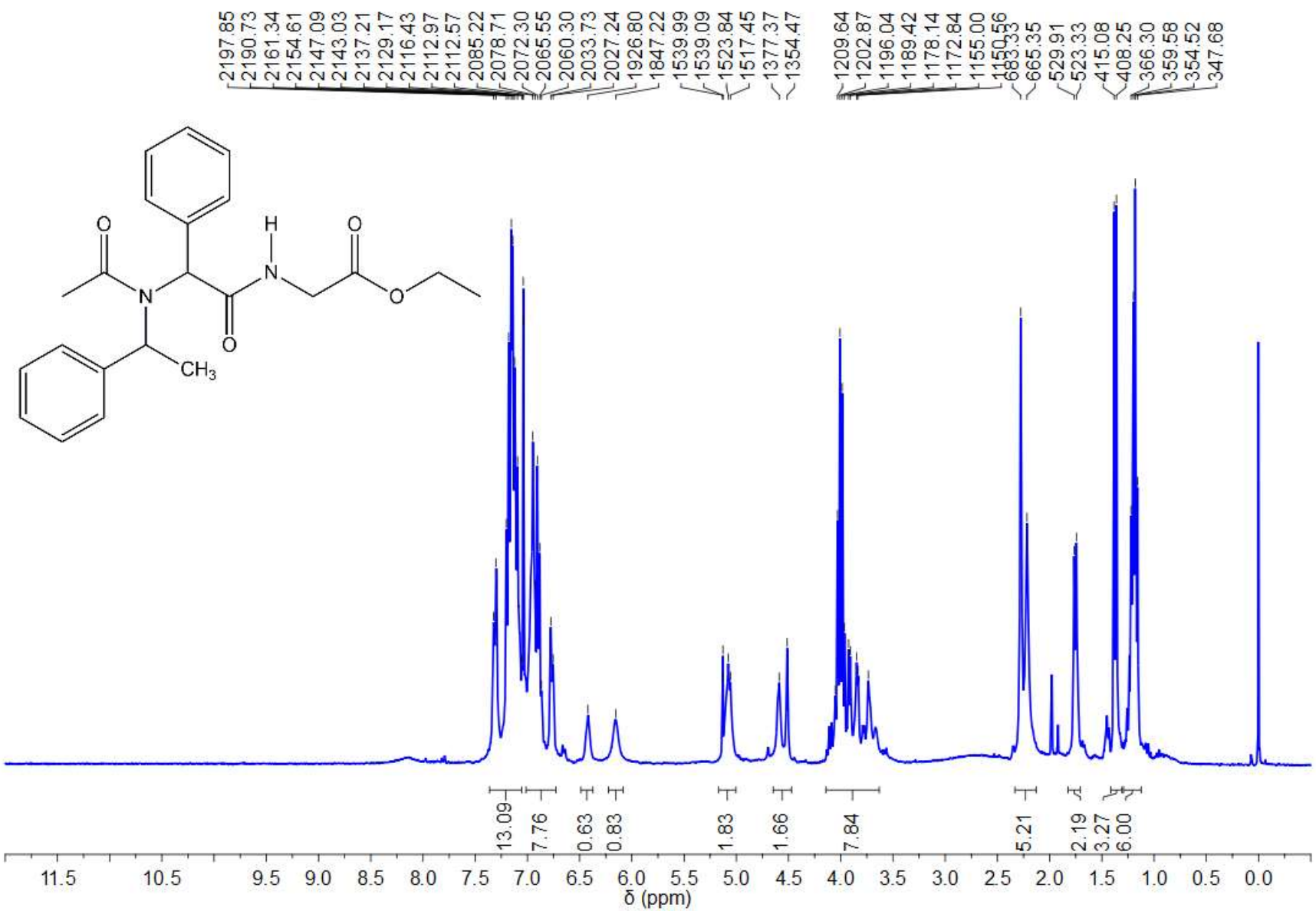


Figure S5. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **5b**.

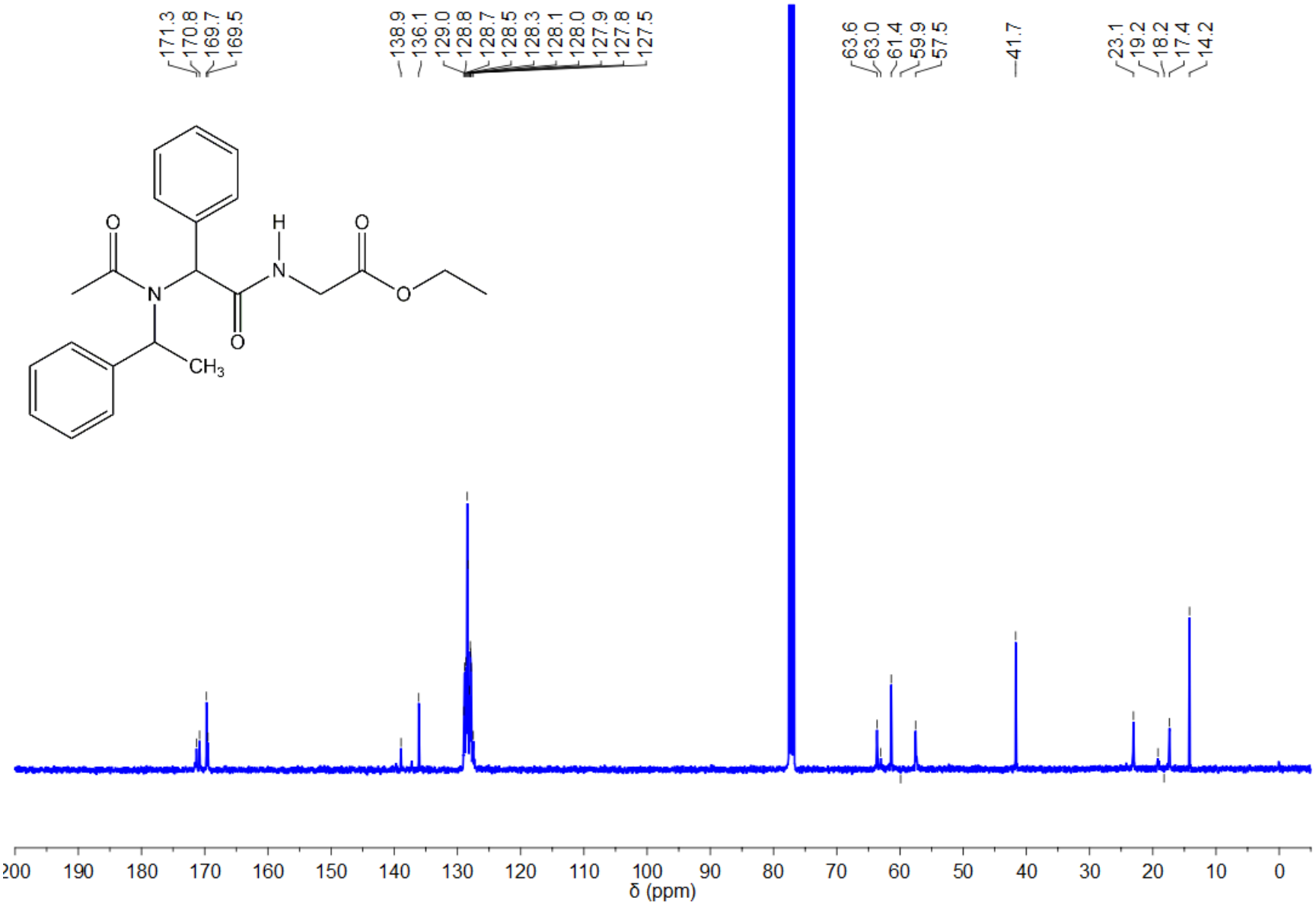


Figure S6. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **5b**.

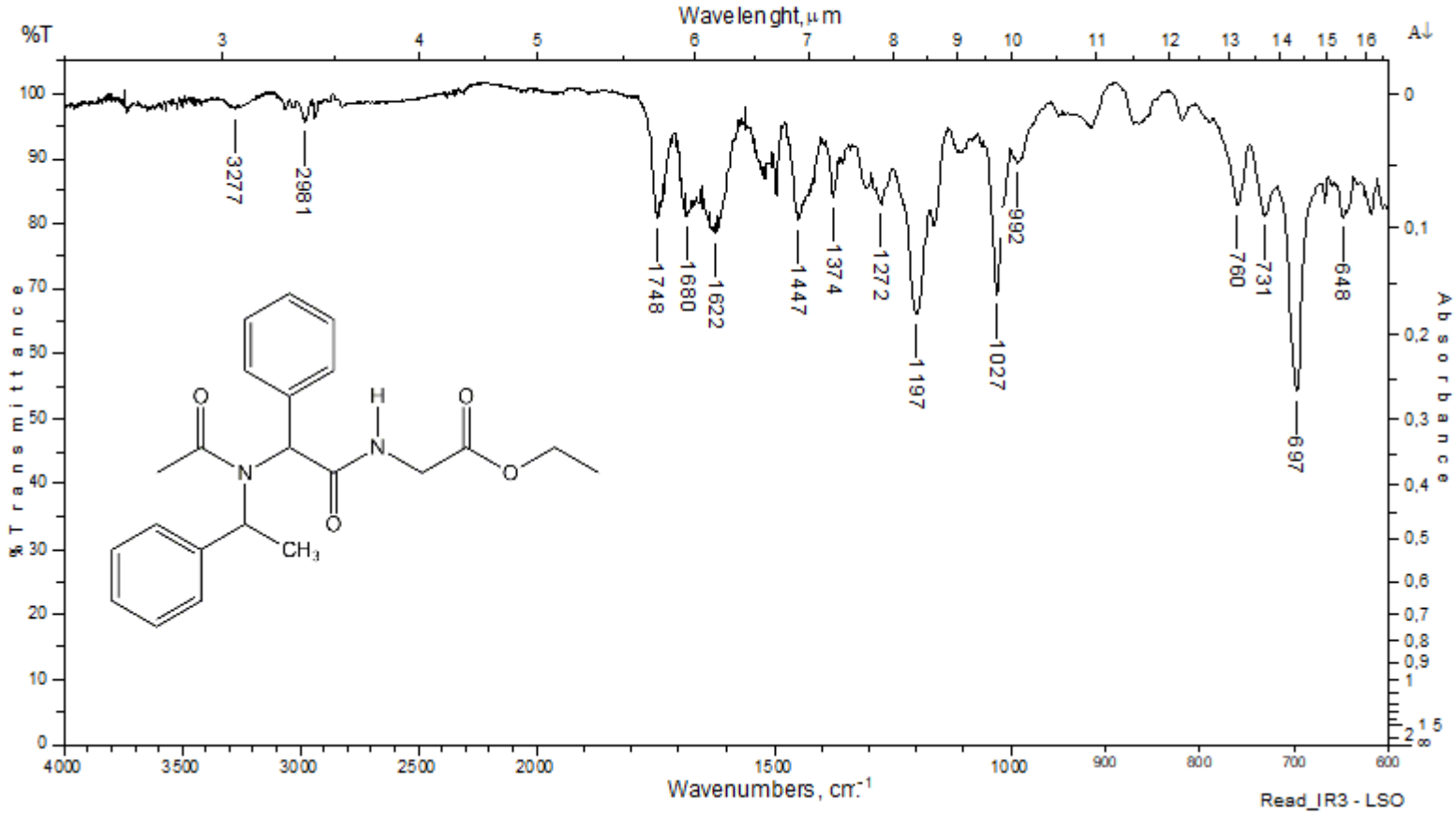


Figure S7. FTIR (KBr) spectrum of compound **5b**.

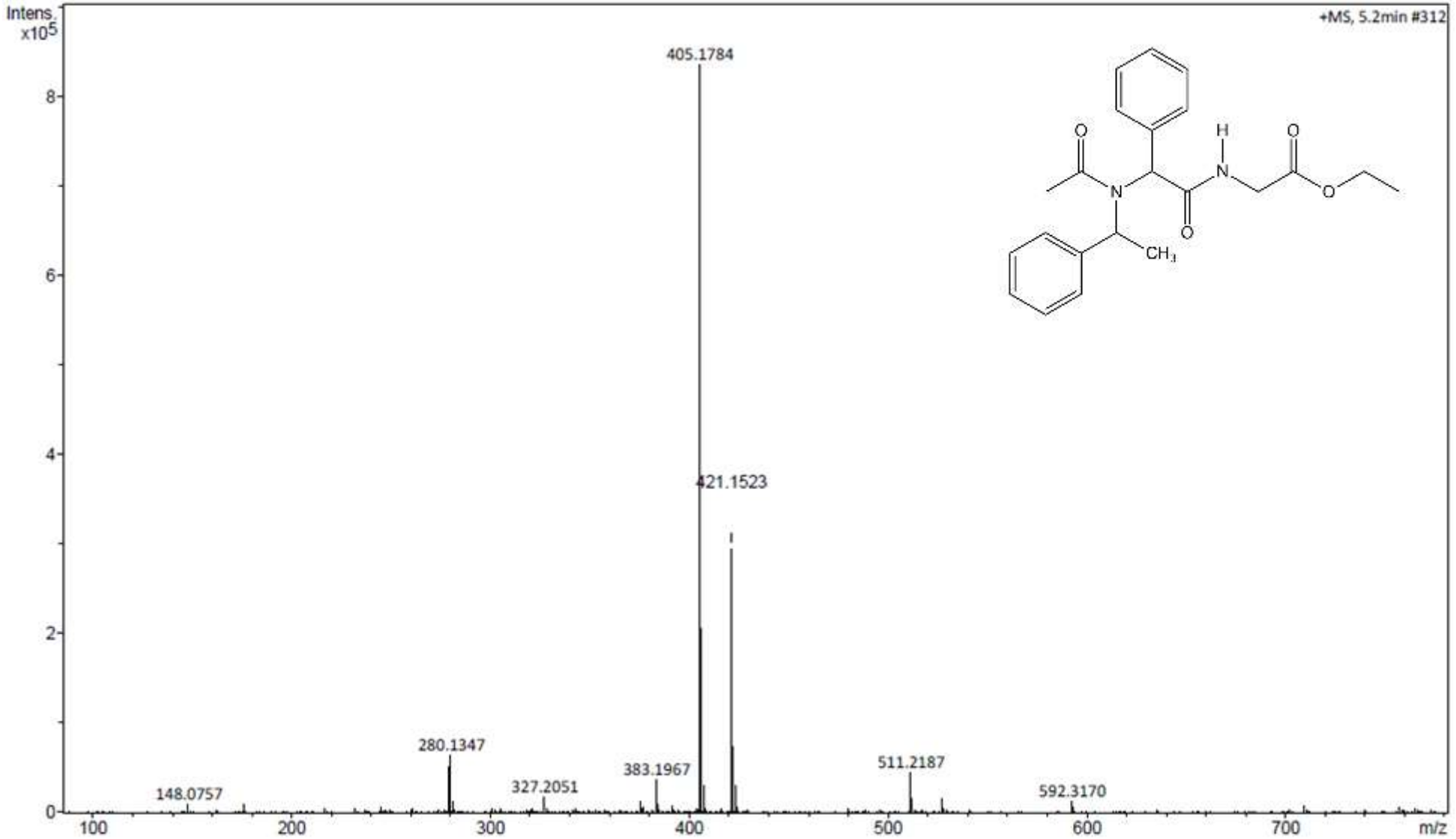
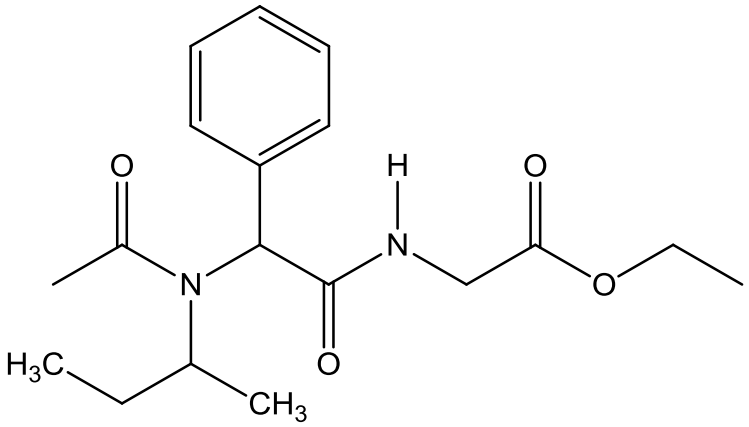


Figure S8. Mass spectrum of compound **5b**.

Compound **5c**



Ethyl 2-(2-(*N*-(*sec*-butyl)acetamido)-2-phenylacetamido)acetate (**5c**)

Yellow oil, yield 58%; diastereoisomeric mixture (53:47); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.7-7.27 (m, 10H), 7.12 (s, 1H), 6.57 (s, 1H), 4.82 (s, 1H), 4.76 (s, 1H), 4.21-4.05 (m, 6H), 3.94-3.80 (m, 4H), 2.23 (s, 3H), 2.21 (s, 3H), 1.92-1.80 (m, 1H), 1.68-1.56 (m, 1H), 1.45-1.35 (m, 2H), 1.40 (d, 3H, *J* 6.6 Hz), 1.26 (t, 3H, *J* 7.1 Hz), 1.24 (t, 3H, *J* 7.1 Hz), 1.12 (d, 3H, *J* 6.7 Hz), 1.05 (t, 3H, *J* 7.4 Hz), 0.72 (t, 3H, *J* 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5 (C), 171.4 (C), 170.9 (C), 170.6 (C), 169.7 (C), 169.6 (C), 136.8 (C), 136.7 (C), 128.8 (2 CH), 128.7 (2 CH), 128.6 (2 CH), 128.2 (CH), 127.9 (CH), 127.5 (2 CH), 62.4 (CH), 62.2 (CH), 61.4 (2 CH_2), 57.5 (CH), 57.4 (CH), 41.7 (CH_2), 41.3 (CH_2), 23.0 (CH_3), 22.9 (CH_3), 19.5 (CH_3), 18.9 (CH_3), 14.1 (2 CH_3), 11.4 (CH_3), 11.3 (CH_3); FTIR (KBr) ν / cm^{-1} 3286 (N–H), 2979 (C–H), 1747 (C=O, ester), 1683 (C=O, amide), 1194 and 1029 (C–O, ester), 729 and 698 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{18}H_{26}N_2NaO_4$ $[M + Na]^+$: 357.1790, found: 357.1785.

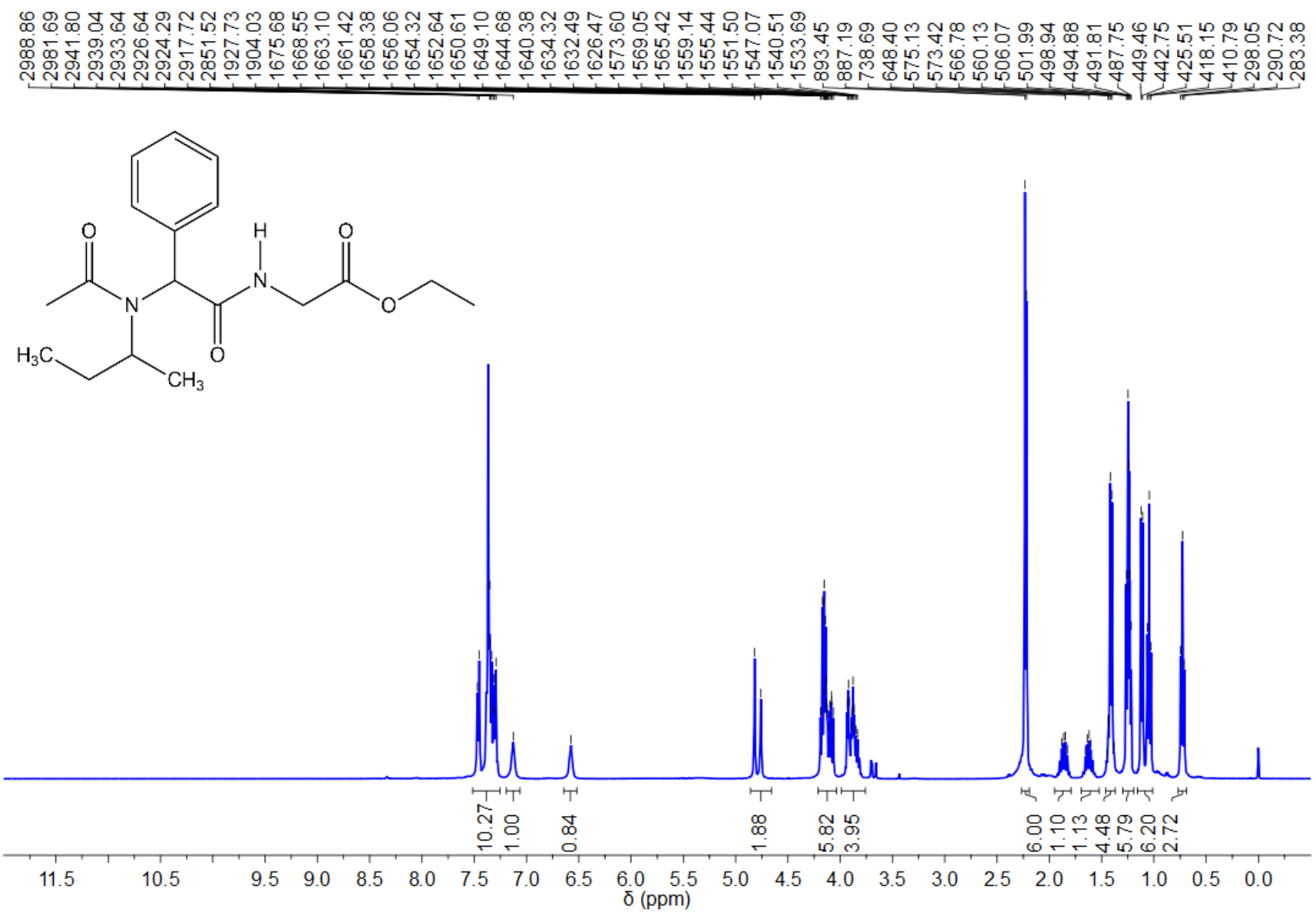


Figure S9. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **5c**.

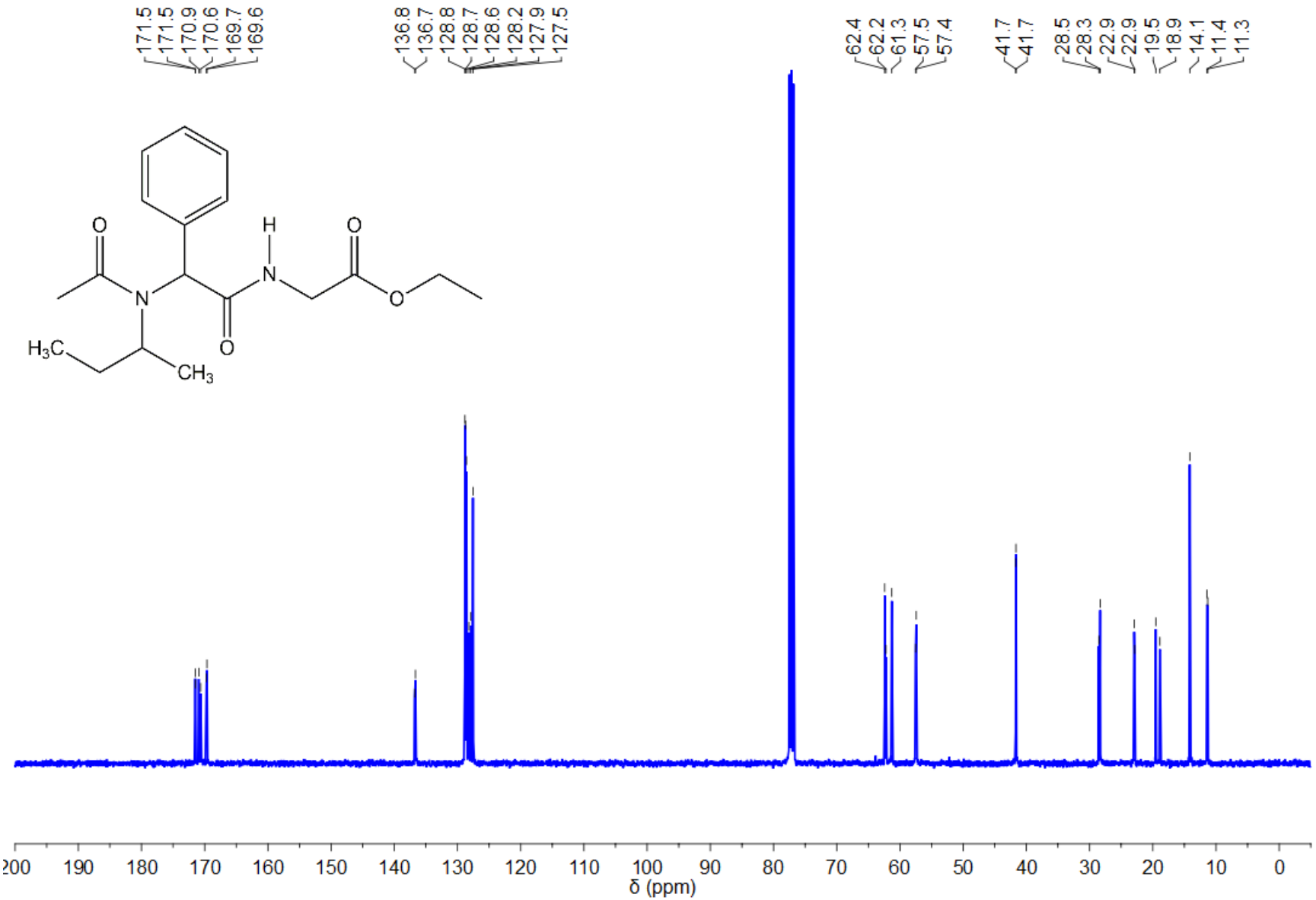


Figure S10. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **5c**.

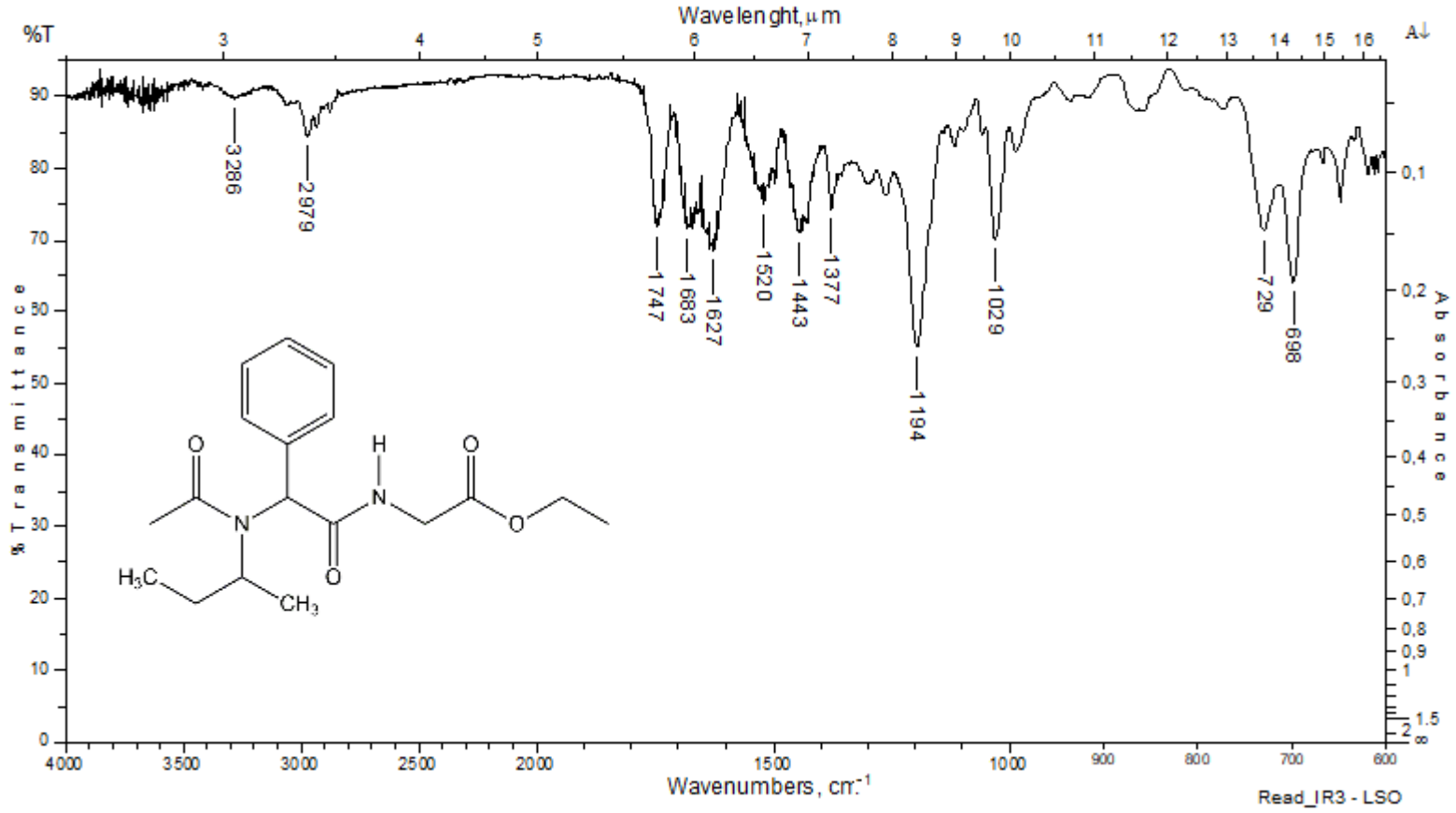


Figure S11. FTIR (KBr) spectrum of compound **5c**.

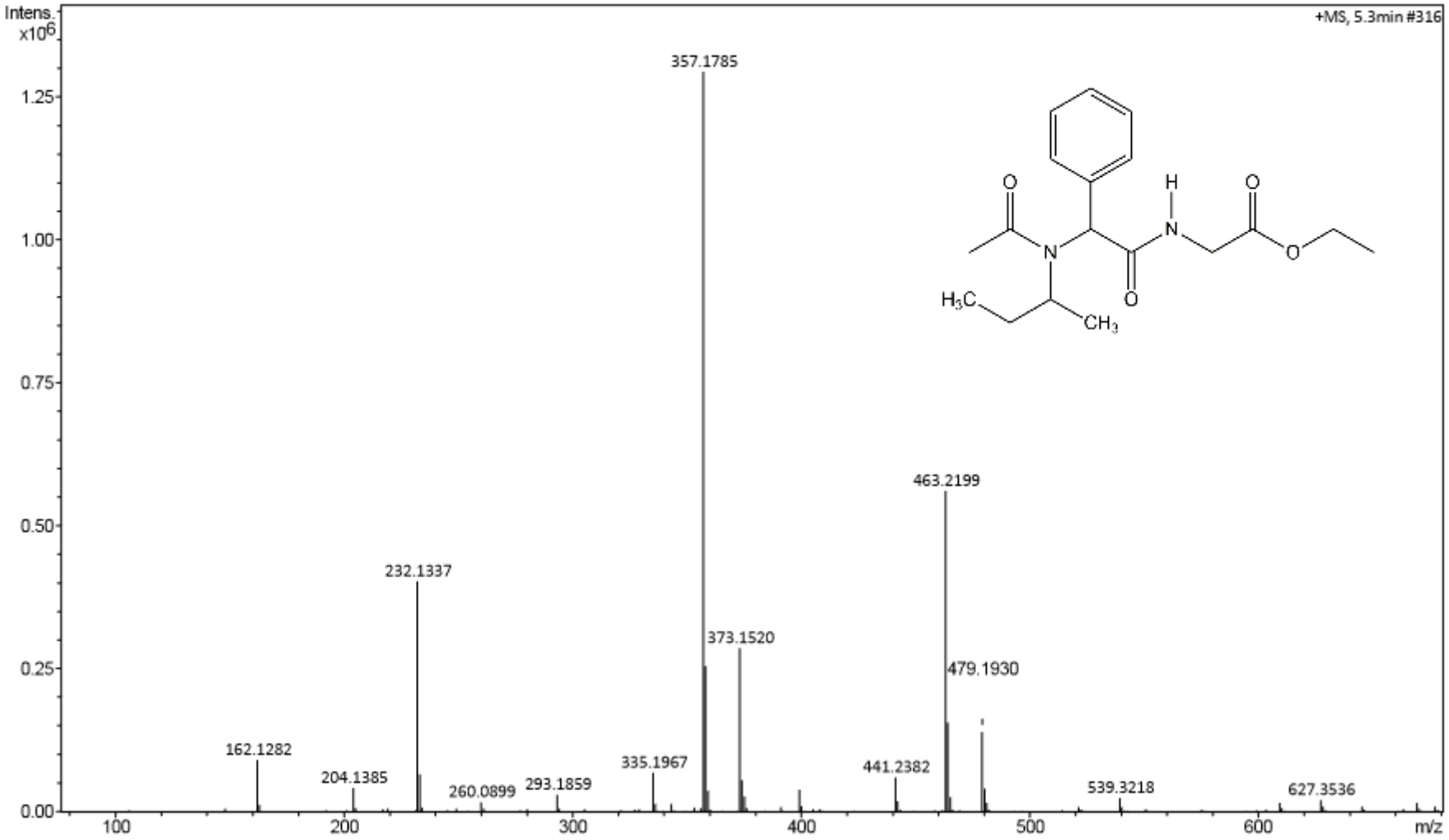
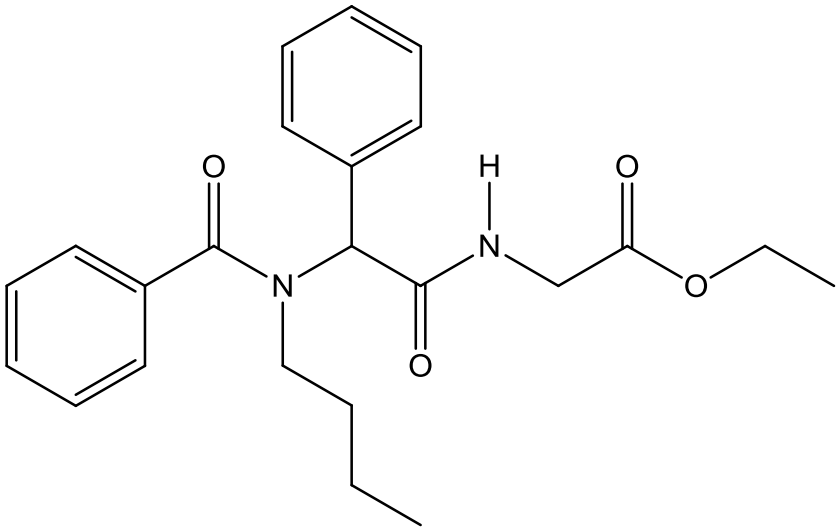


Figure S12. Mass spectrum of compound **5c**.

Compound **5d**



Ethyl 2-(2-(*N*-butylbenzamido)-2-phenylacetamido)acetate (**5d**)

Yellow oil, yield 77%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49-7.38 (m, 11H), 5.82 (s, 1H), 4.24-4.17 (m, 2H), 4.13-4.02 (m, 2H), 3.27-3.20 (m, 2H), 1.28 (t, 3H, *J* 7.1 Hz), 0.95-0.90 (m, 4H), 0.59 (t, 3H, *J* 7.1 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 173.0 (C), 170.2 (C), 169.6 (C), 136.6 (C), 135.1 (C), 133.5 (CH), 130.2 (2 CH), 129.5 (2 CH), 128.5 (CH), 126.7 (2 CH), 61.6 (CH_2), 52.4 (CH), 41.7 (CH_2), 41.5 (CH_2), 31.2 (CH_2), 19.9 (CH_2), 14.2 (CH_3), 13.4 (CH_3); FTIR (KBr) ν / cm^{-1} 3413 (N–H), 2969 (C–H), 1747 (C=O, ester), 1714 (C=O, amide), 1223 and 1093 (C–O, ester), 738 and 704 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{23}H_{28}N_2NaO_4$ $[M + Na]^+$: 419.1947, found: 419.1945.

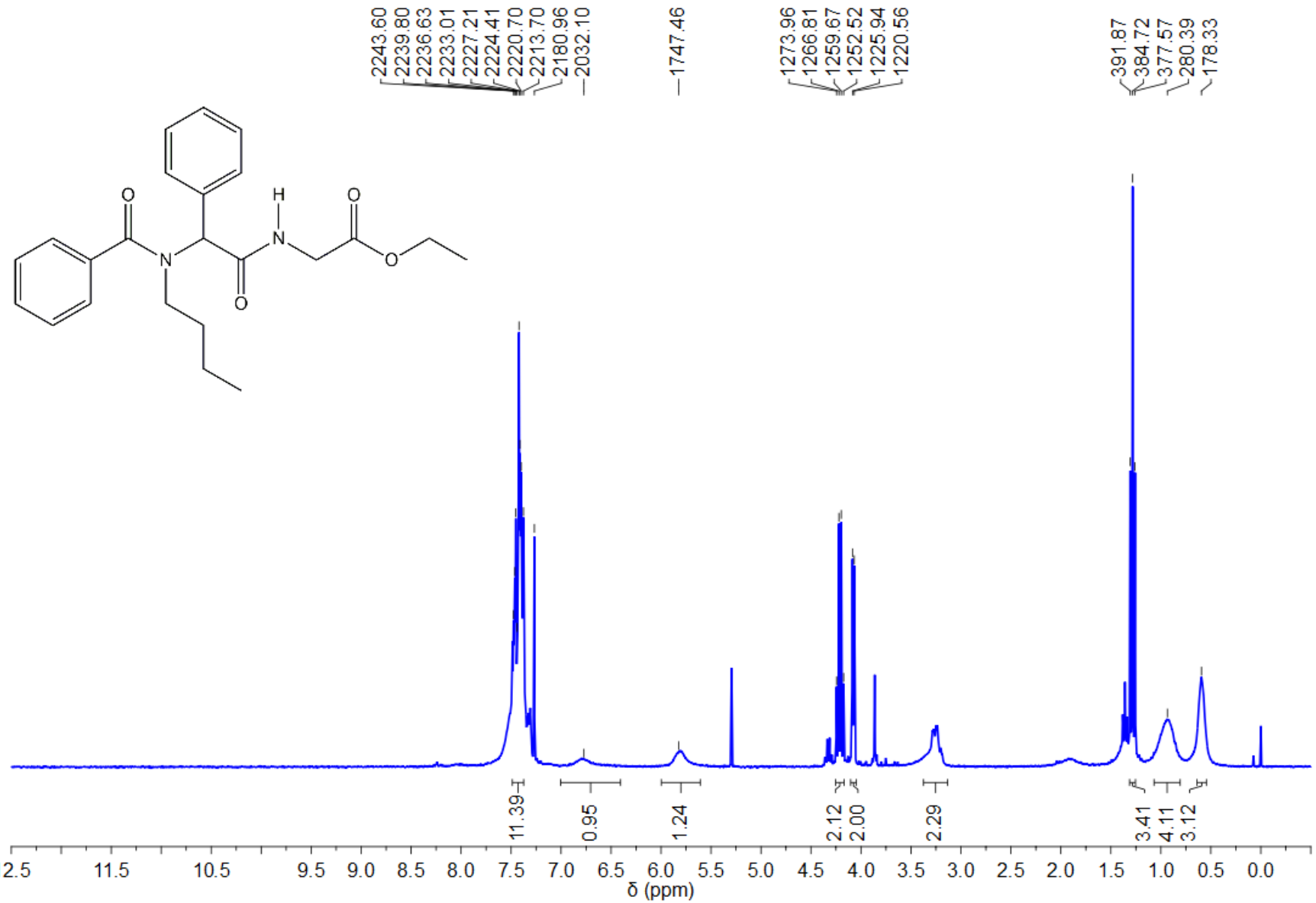


Figure S13. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **5d**.

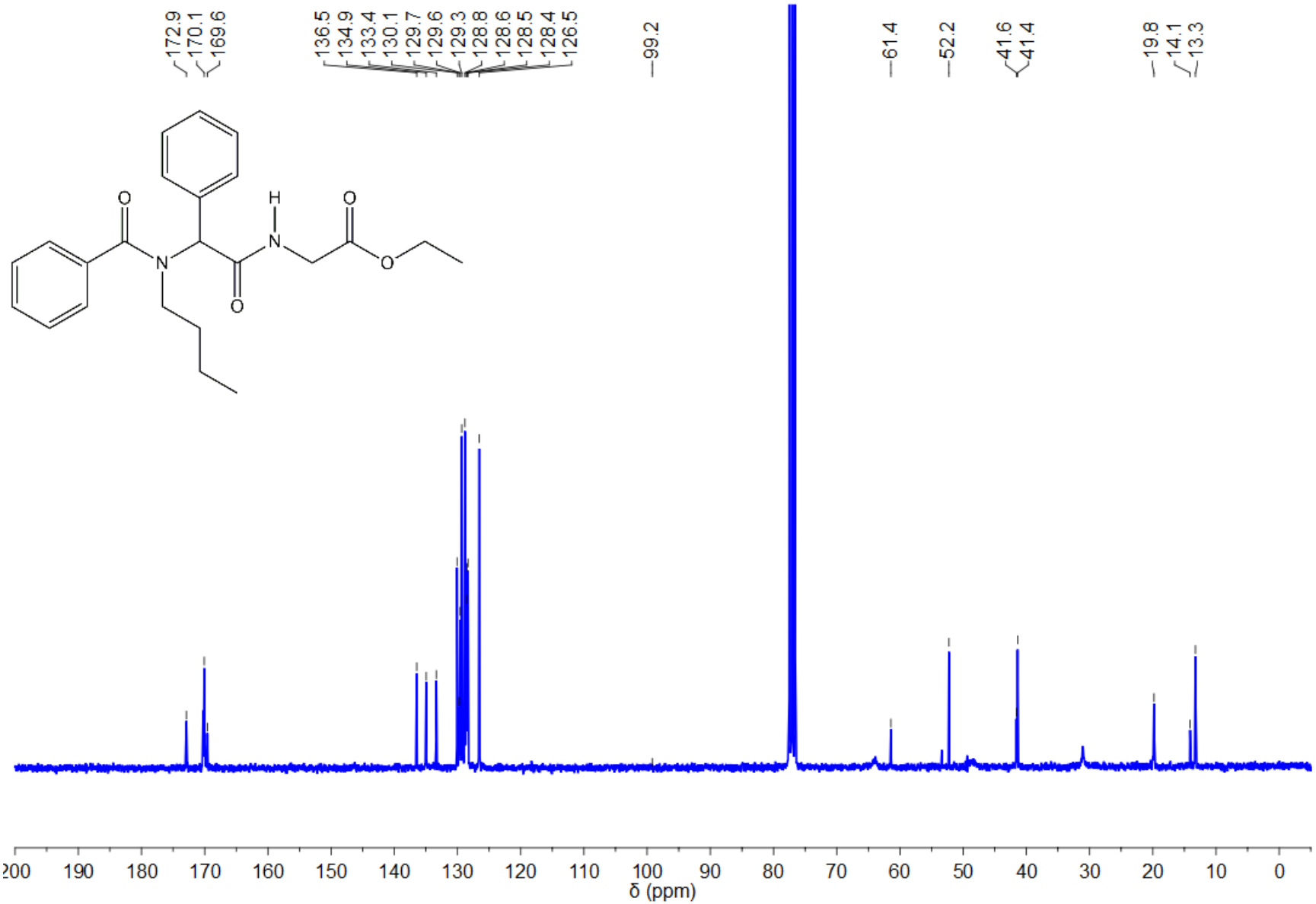


Figure S14. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **5d**.

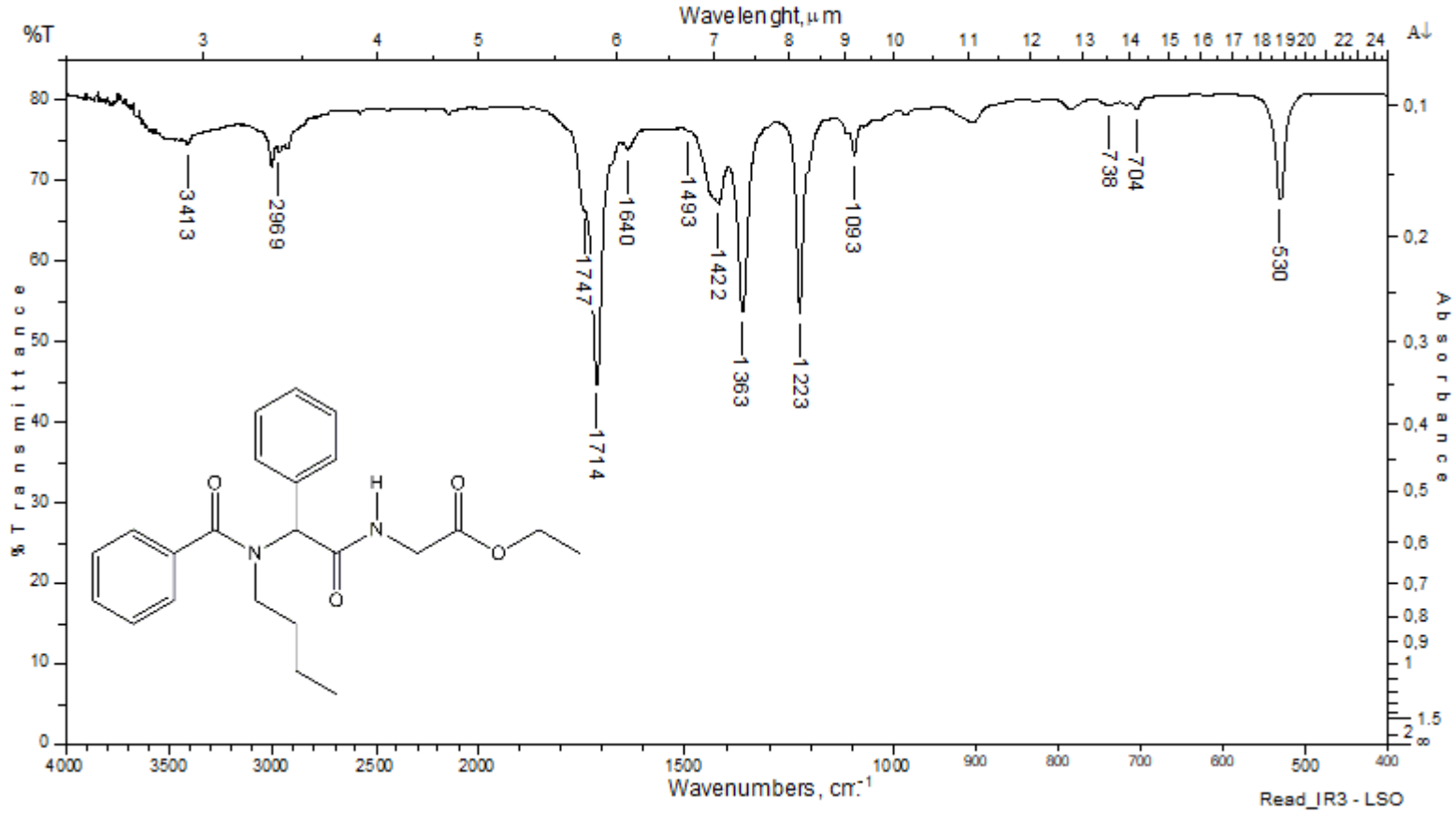


Figure S15. FTIR (KBr) spectrum of compound **5d**.

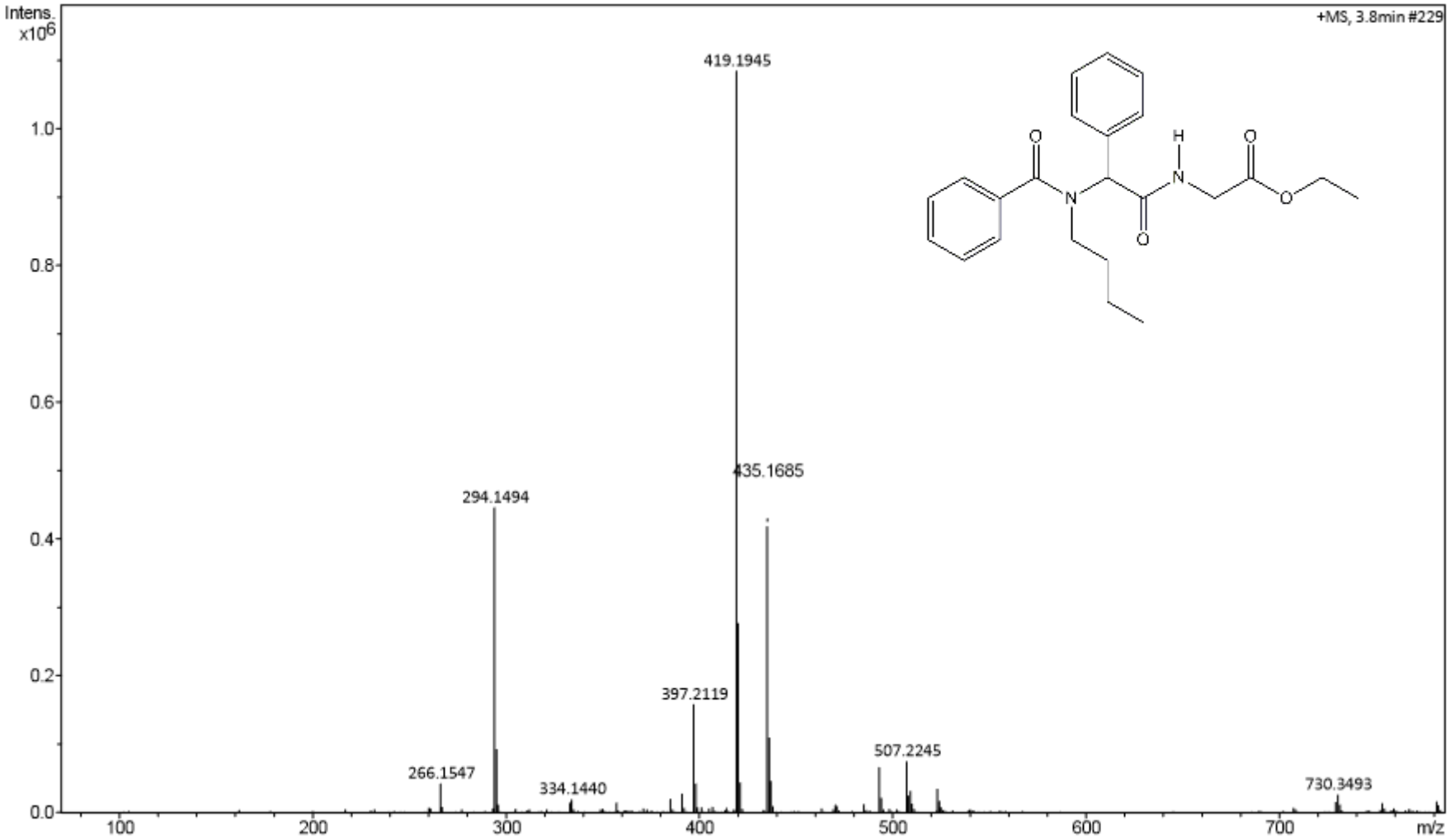
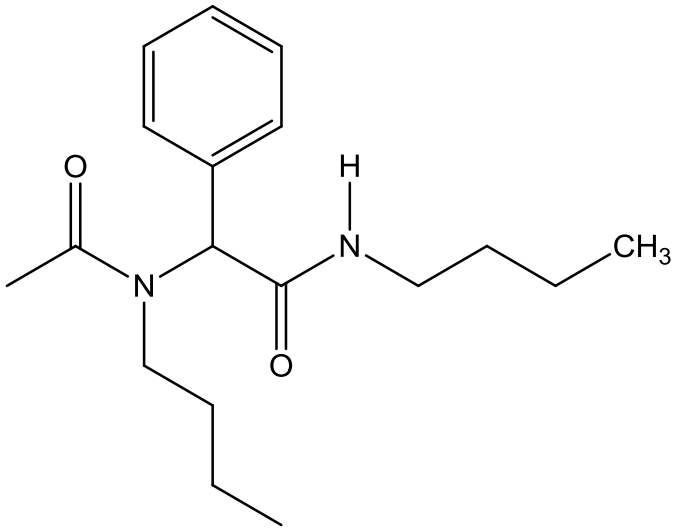


Figure S16. Mass spectrum of compound **5d**.

Compound **5e**



N-Butyl-2-(*N*-butylacetamido)-2-phenylacetamide (**5e**)

White solid, yield 80%, melting point 115-119 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.35 (m, 5H), 6.04 (s, 1H), 5.84 (s, 1H), 3.33-3.27 (m, 4H), 2.20 (s, 3H), 1.49-1.43 (m, 4H), 1.33-1.25 (m, 2H), 1.14-1.06 (m, 2H), 0.89 (t, 3H, *J* 7.3 Hz), 0.75 (t, 3H, *J* 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8 (C), 170.0 (C), 135.6 (C), 129.5 (2 CH), 128.9 (2 CH), 128.6 (CH), 62.9 (CH), 48.1 (CH_2), 39.6 (CH_2), 31.7 (CH_2), 31.5 (CH_2), 22.0 (CH_3), 20.2 (CH_2), 20.1 (CH_2), 13.9 (CH_3), 13.6 (CH_3); FTIR (KBr) ν / cm^{-1} 3278 (N–H), 2959 (C–H), 1678 (C=O, amide), 746 and 703 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{18}H_{28}N_2NaO_2$ $[M + Na]^+$: 327.2047, found: 327.2047.

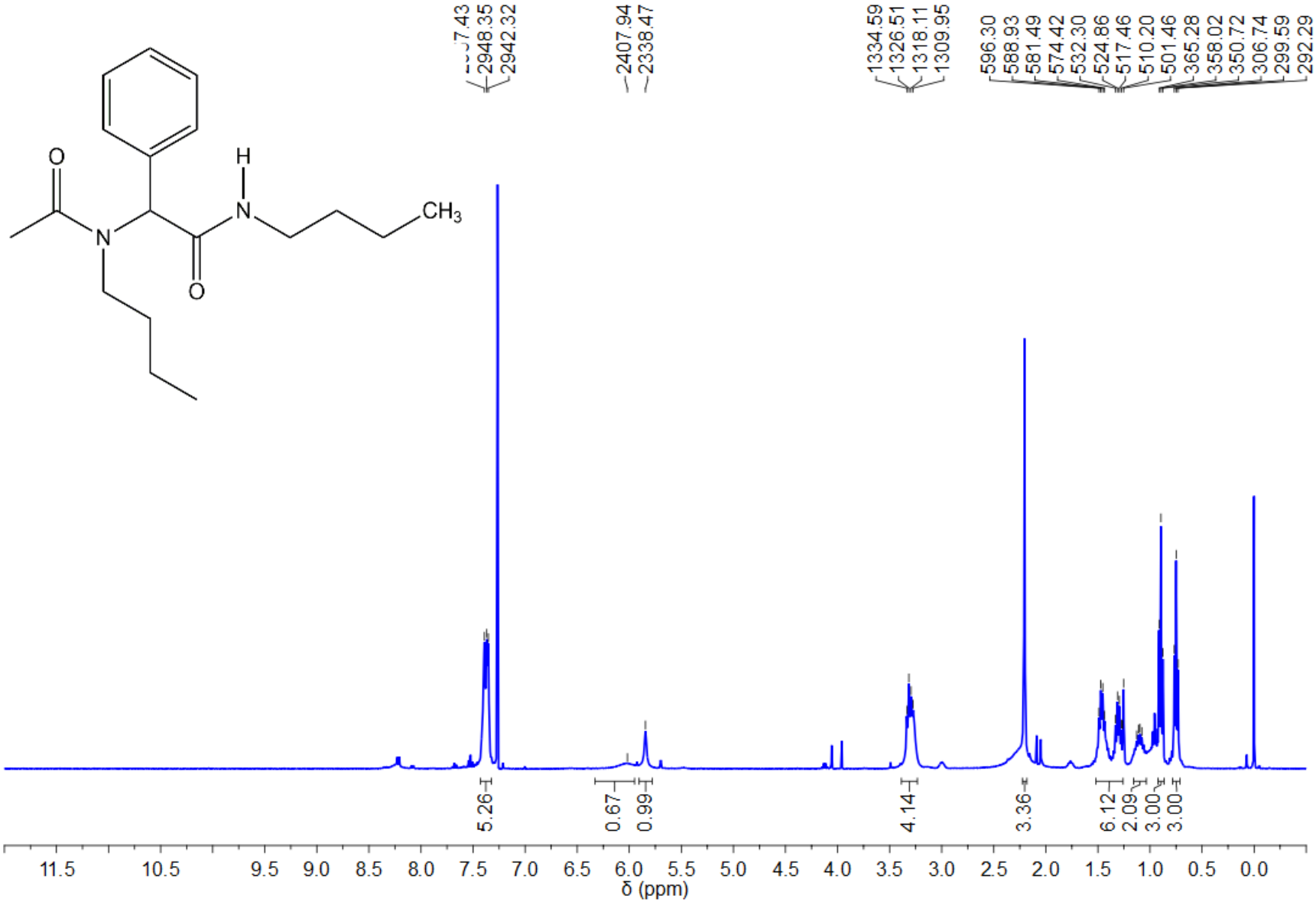


Figure S17. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **5e**.

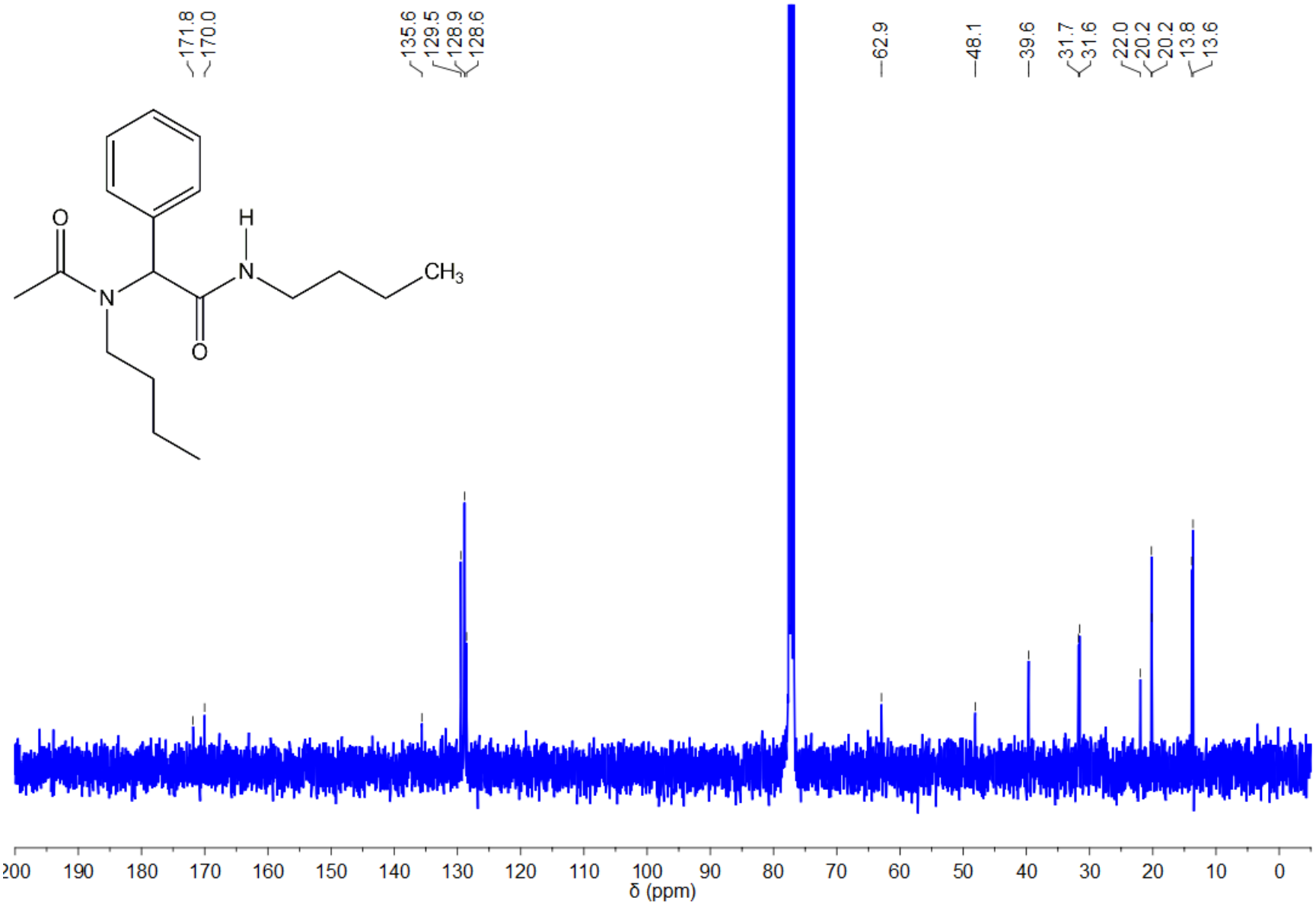


Figure S18. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **5e**.

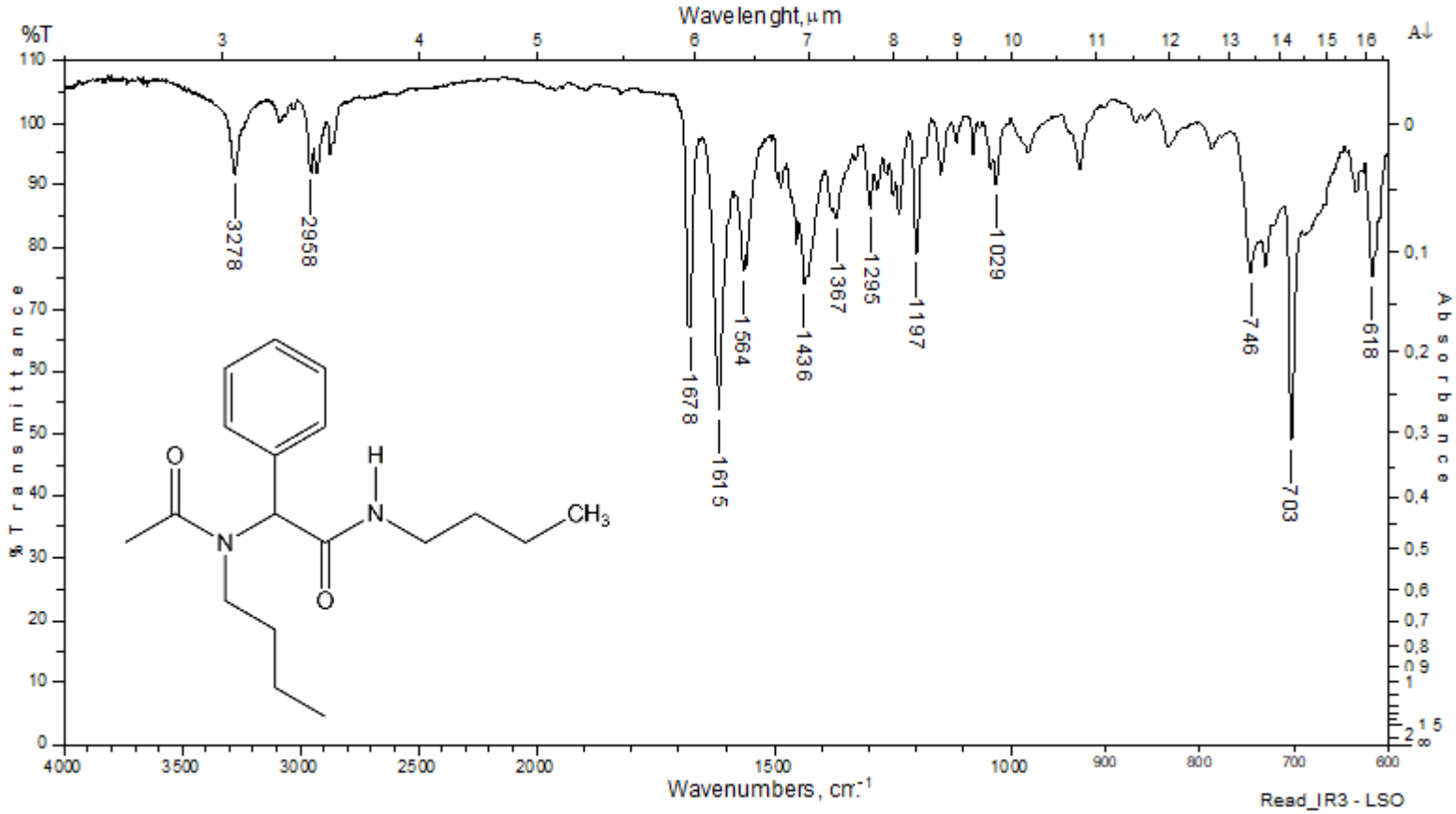


Figure S19. FTIR (KBr) spectrum of compound **5e**.

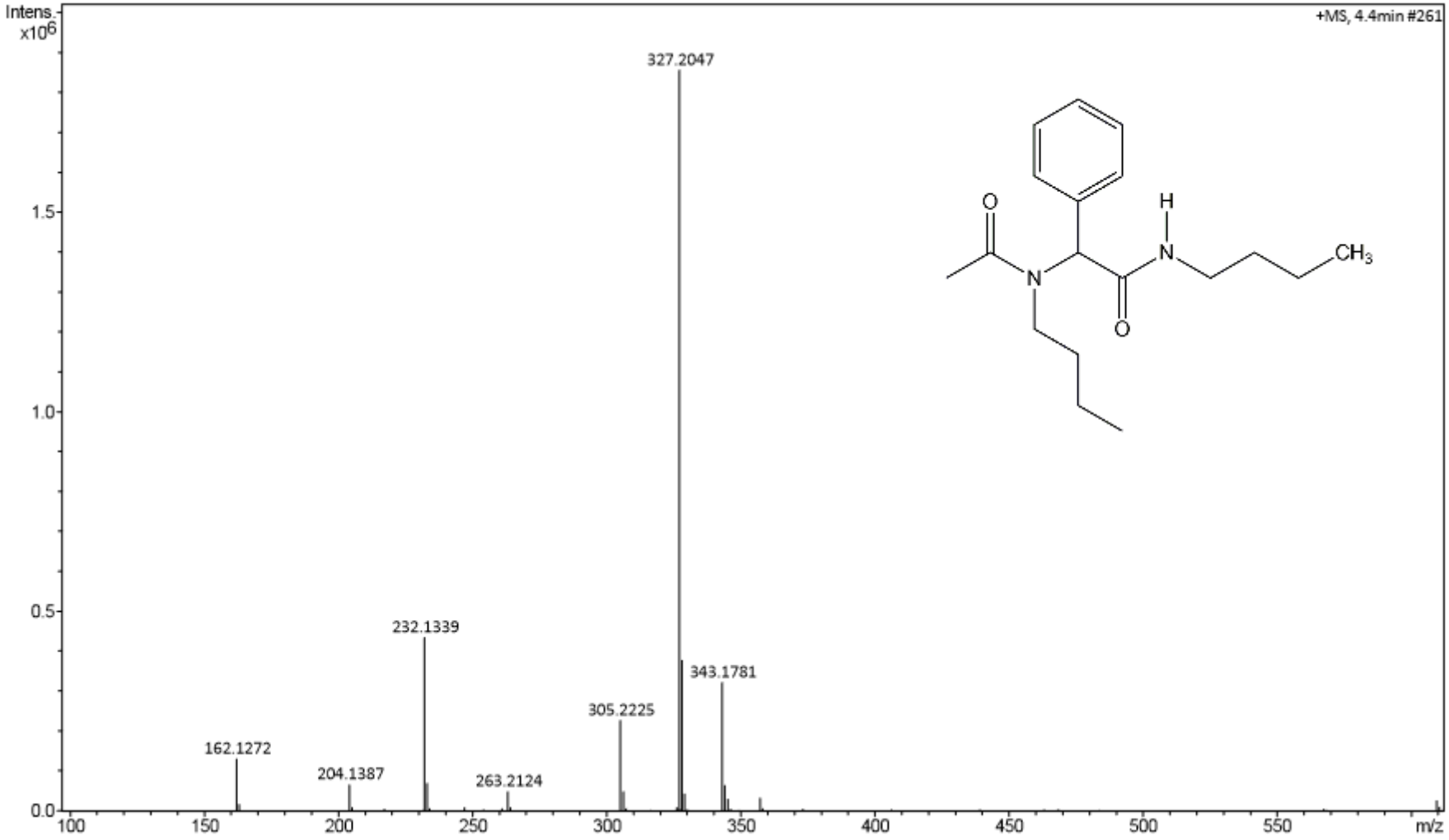
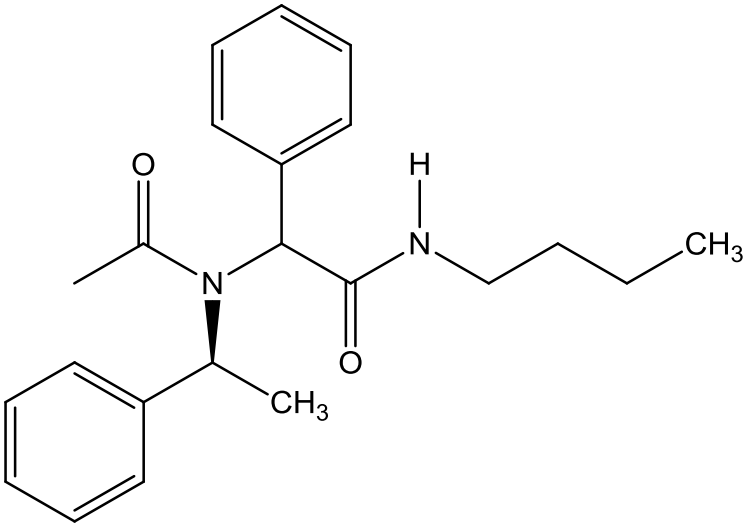


Figure S20. Mass spectrum of compound **5e**.

Compounds **5f** and **5g**

Compounds **5f** and **5g** were obtained as diastereoisomeric mixtures (54:46) and possess the same spectral data (^{1}H NMR, ^{13}C NMR, FTIR and HRMS), then only the spectral data for the diastereoisomers of compound **5g** are presented here. The diastereoisomers **5g-1** and **5g-2** were purified by HPLC (column C18, methanol/water, 70:30, v/v), however, their relative configurations could not be determined by NOE NMR experiments.



N-Butyl-2-phenyl-2-(*N*-((*S*)-1-phenylethyl)acetamido)acetamide (**5g**)

Yield 77%.

Compound **5g-1**

White solid, melting point 120-122 °C; specific optical rotation $[\alpha]_D^{27^\circ}$ = –73.9° (chloroform); retention time (HPLC) 12.6 min; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56-7.31 (m, 10H), 5.88 (s, 1H), 5.24 (d, 1H, *J* 6.8 Hz), 4.76 (s, 1H), 3.18-3.05 (m, 2H), 2.27 (s, 3H), 1.41 (d, 3H, *J* 6.8 Hz), 1.36-1.35 (m, 2H), 1.23-1.18 (m, 2H), 0.84 (t, 3H, *J* 7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5 (C), 169.5 (C), 139.9 (C), 137.7 (C), 128.9 (4 CH), 128.4 (2 CH), 128.2 (2 CH), 127.4 (2 CH), 63.4 (CH), 57.3 (CH), 39.6 (CH_2), 31.3 (CH_2), 23.2 (CH_3), 20.1 (CH_2), 19.2 (CH_3), 13.8 (CH_3); FTIR (KBr) ν / cm^{-1} 3294 (N–H), 2958 (C–H), 1684 (C=O, amide), 728 and 694 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{22}H_{28}N_2NaO_2$ $[M + Na]^+$: 375.2048, found: 375.2042.

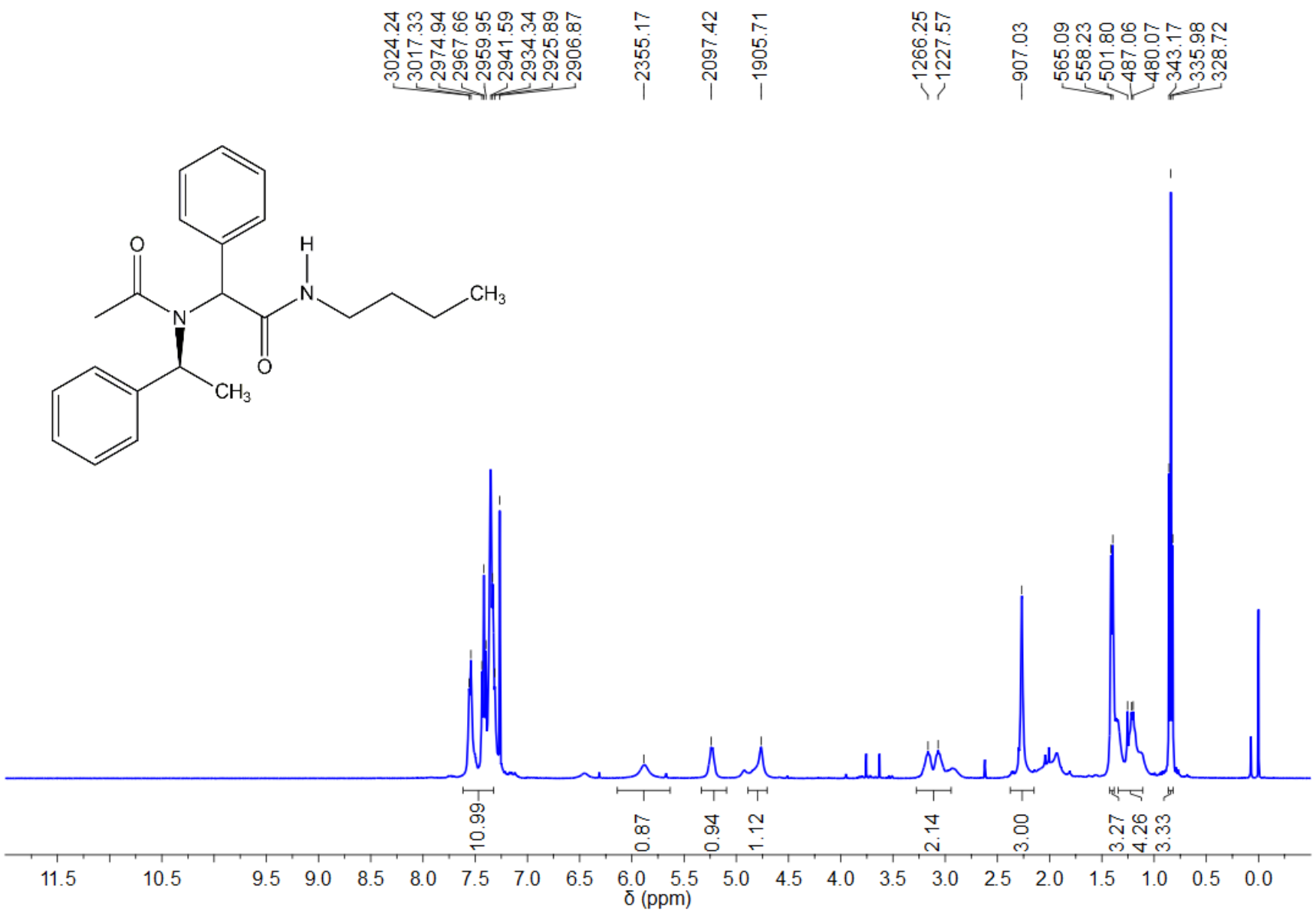


Figure S21. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **5g-1**.

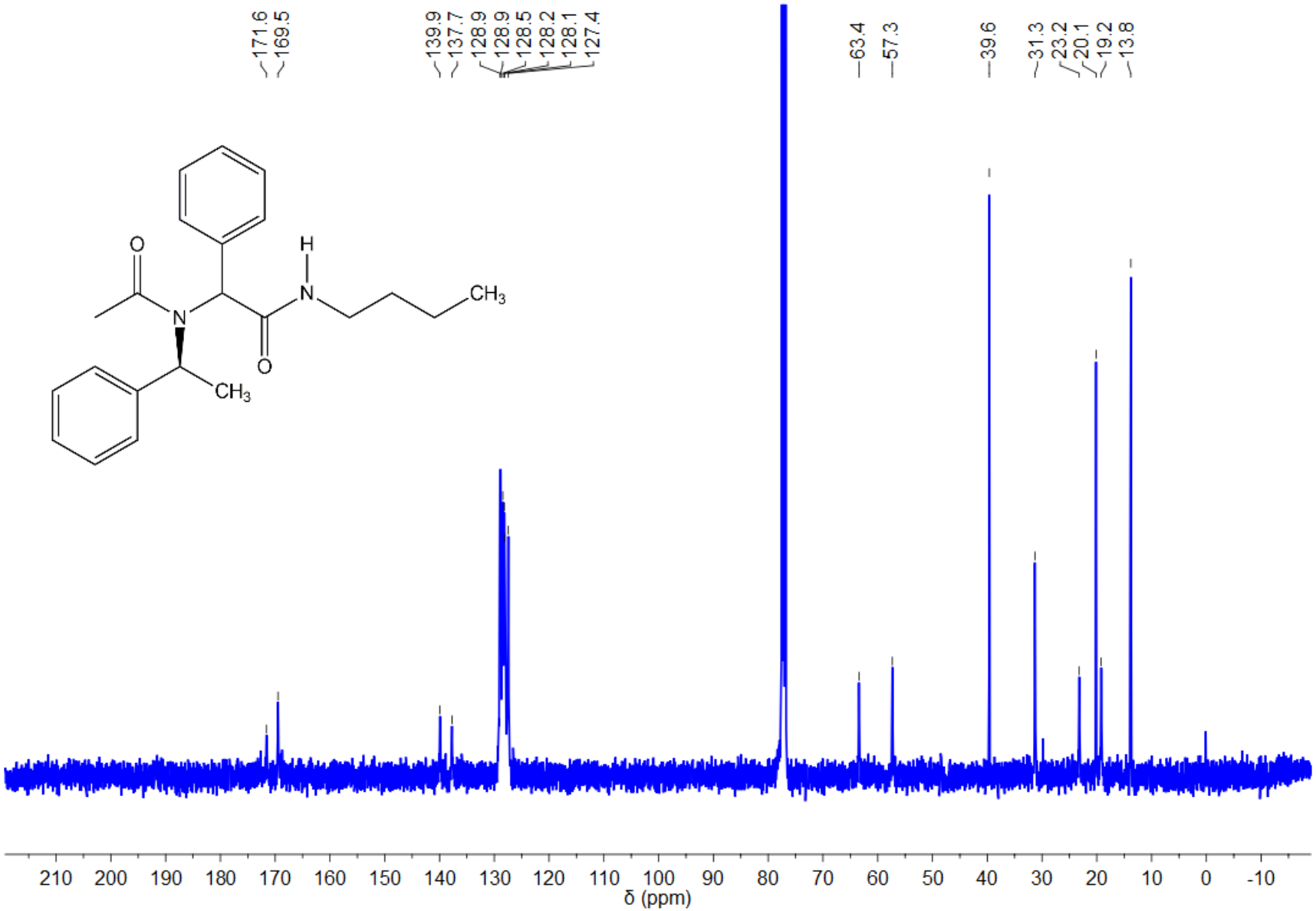


Figure S22. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **5g-1**.

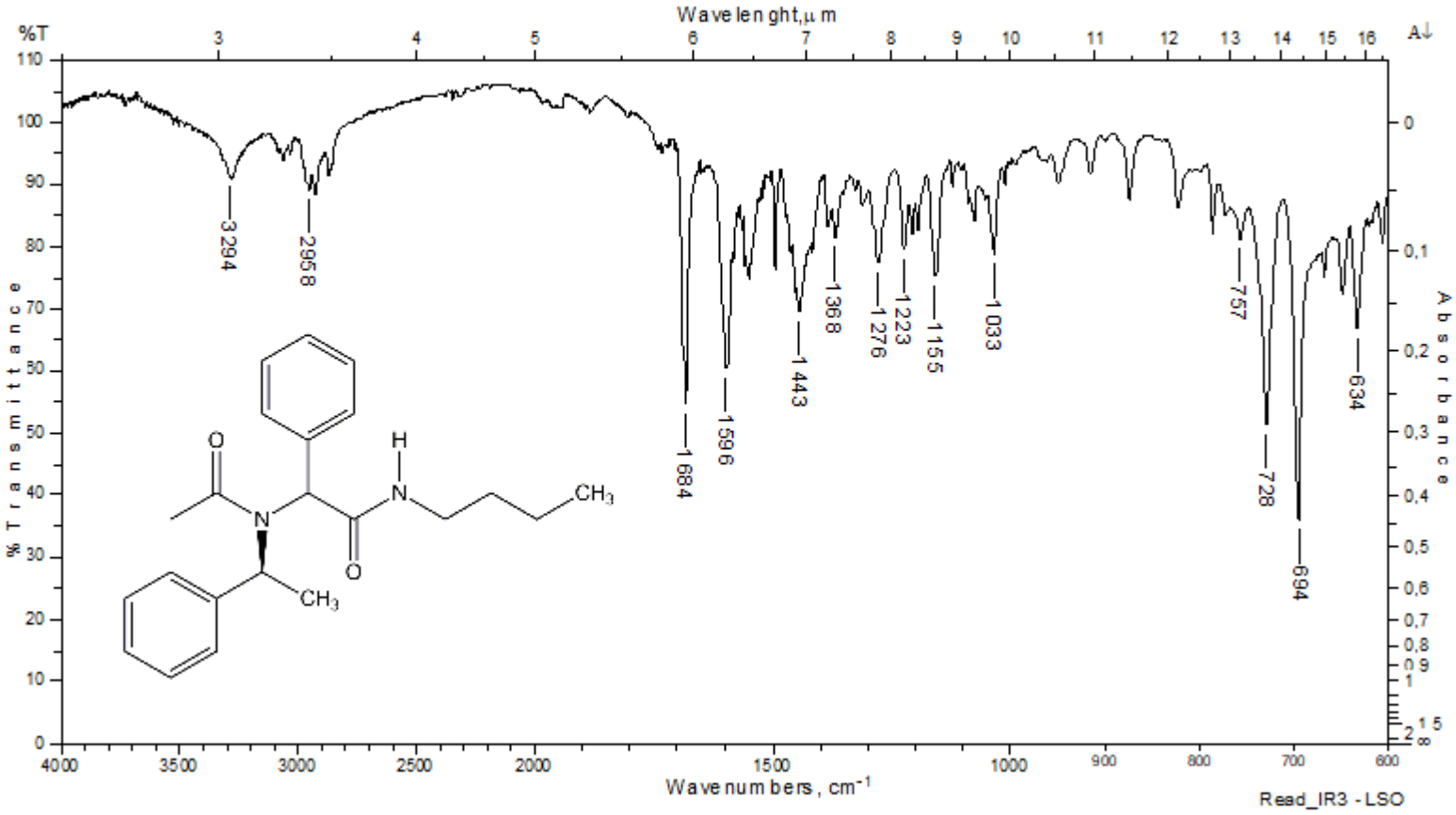


Figure S23. FTIR (KBr) spectrum of compound **5g-1**.

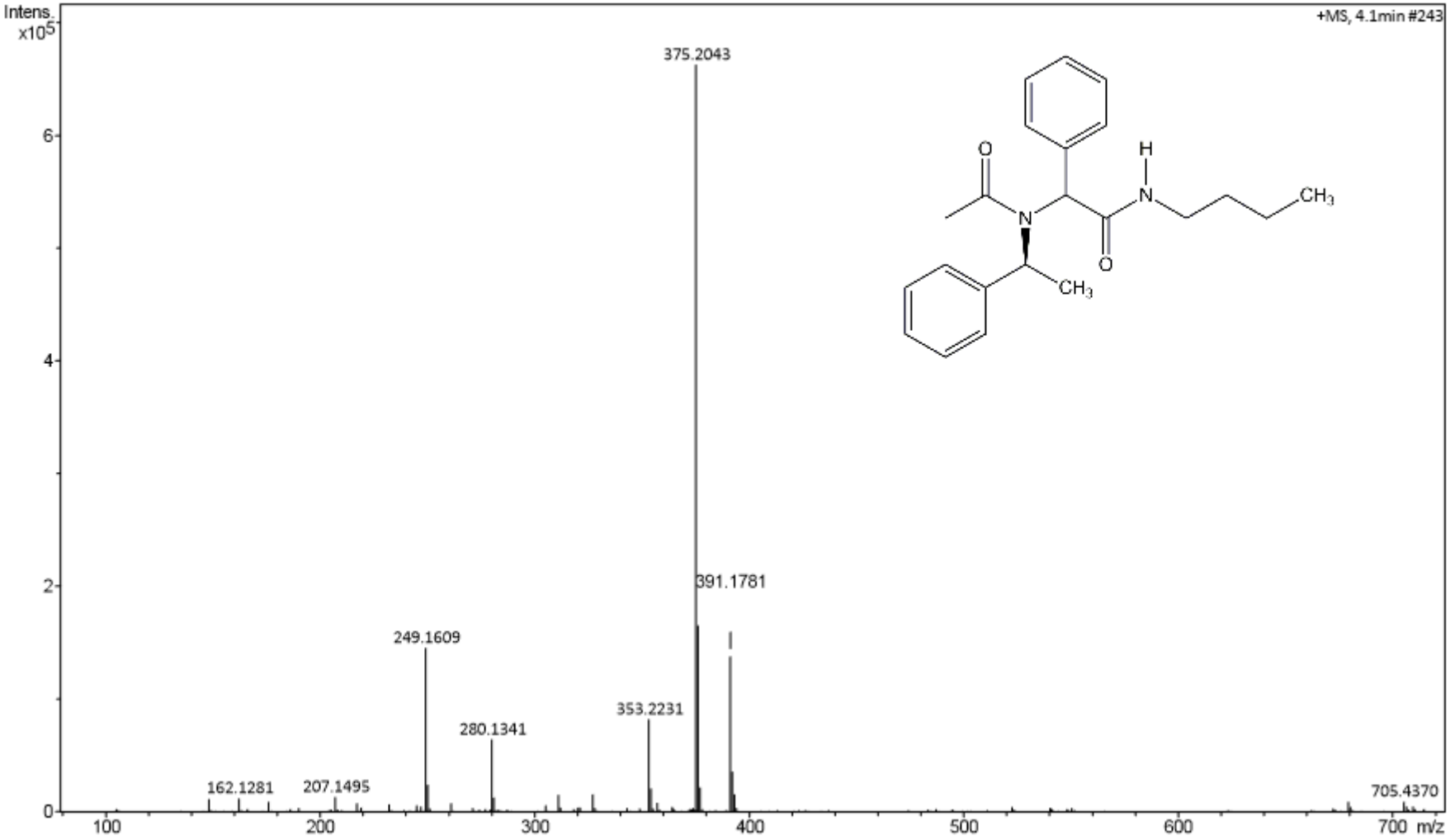


Figure S24. Mass spectrum of compound **5g-1**.

Compound **5g-2**

White solid, melting point 99-101 °C; specific optical rotation $[\alpha]_D^{27^\circ}$ = +6.4° (chloroform); retention time (HPLC) 14.0 min; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.95-6.72 (m, 10H), 5.88 (s, 1H), 5.05 (q, 1H, *J* 6.7 Hz), 4.44 (s, 1H), 3.18-3.03 (m, 2H), 2.26 (s, 3H), 1.75 (d, 3H, *J* 6.7 Hz), 1.39-1.32 (m, 2H), 1.27-1.15 (m, 2H), 0.83 (t, 3H, *J* 6.7 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.2 (C), 170.5 (C), 139.1 (C), 136.7 (C), 128.6 (2 CH), 128.4 (2 CH), 128.3 (2 CH), 127.9 (2 CH), 127.6 (2 CH), 64.0 (CH), 57.5 (CH), 39.6 (CH_2), 31.4 (CH_2), 23.1 (CH_3), 20.1 (CH_2), 17.4 (CH_3), 13.8 (CH_3); FTIR (KBr) ν / cm^{-1} 3282 (N–H), 2958 (C–H), 1683 (C=O, amide), 727 and 696 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{22}H_{28}N_2NaO_2$ $[M + Na]^+$: 375.2048, found: 375.2044.

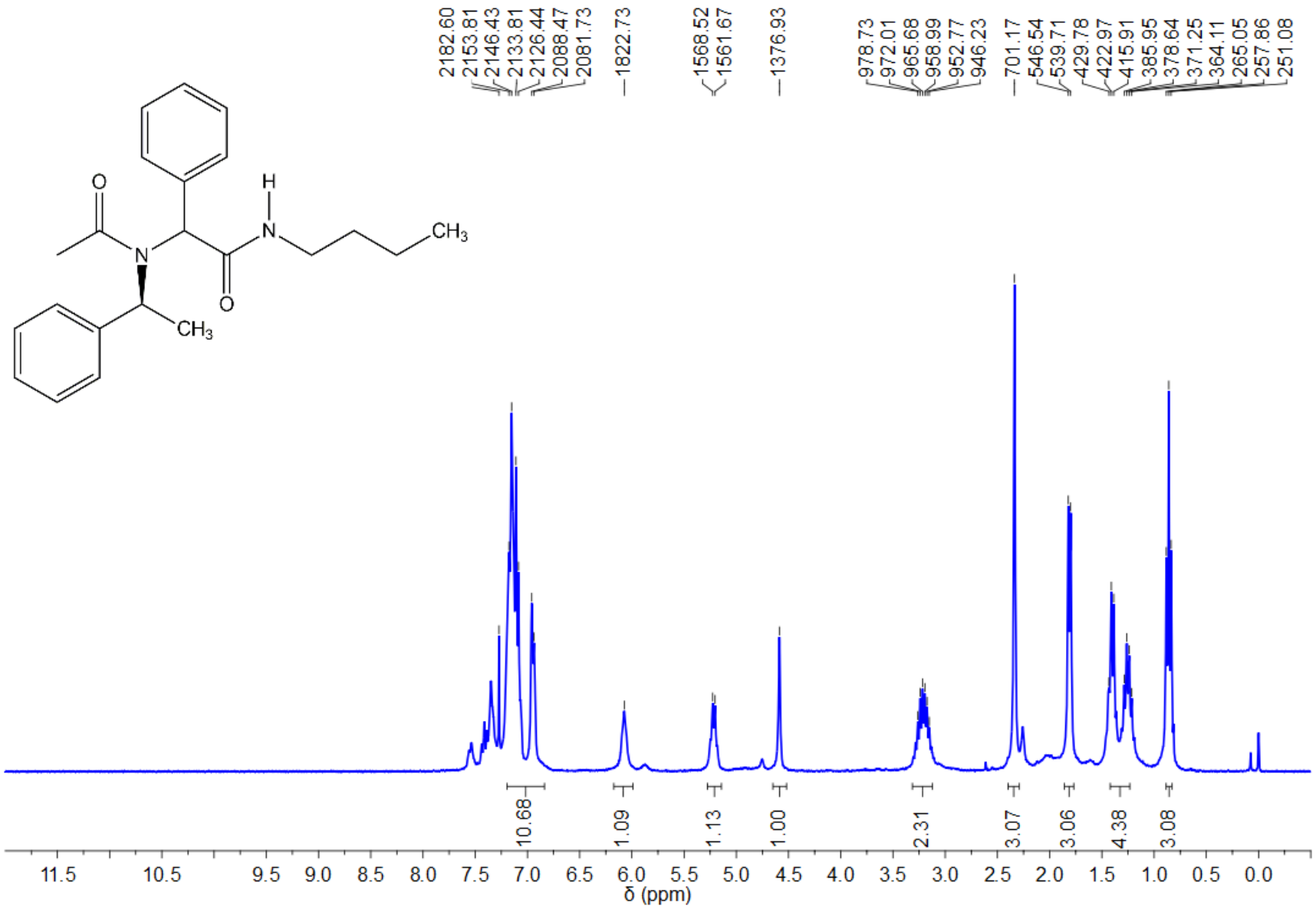


Figure S25. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **5g-2**.

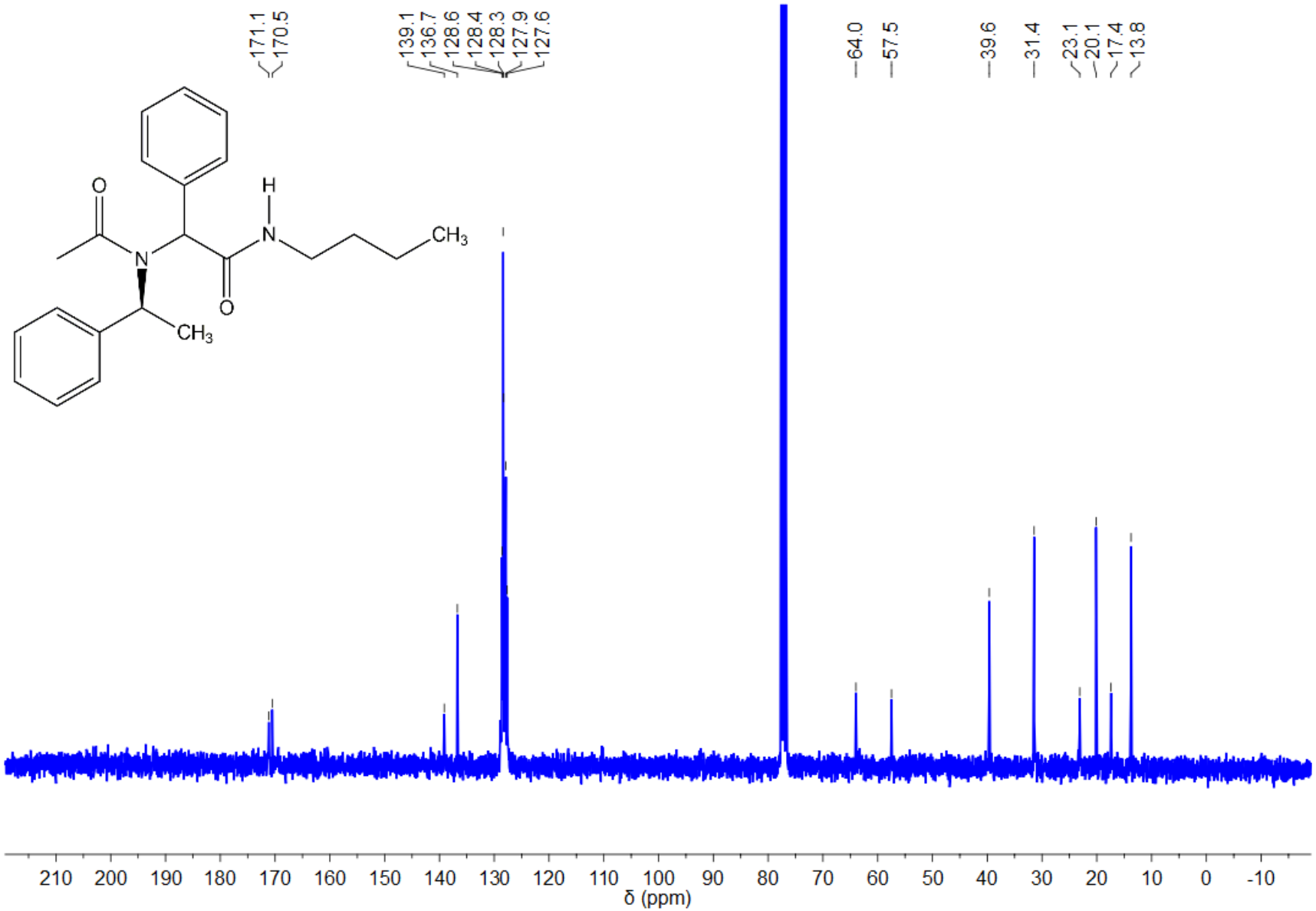


Figure S26. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **5g-2**.

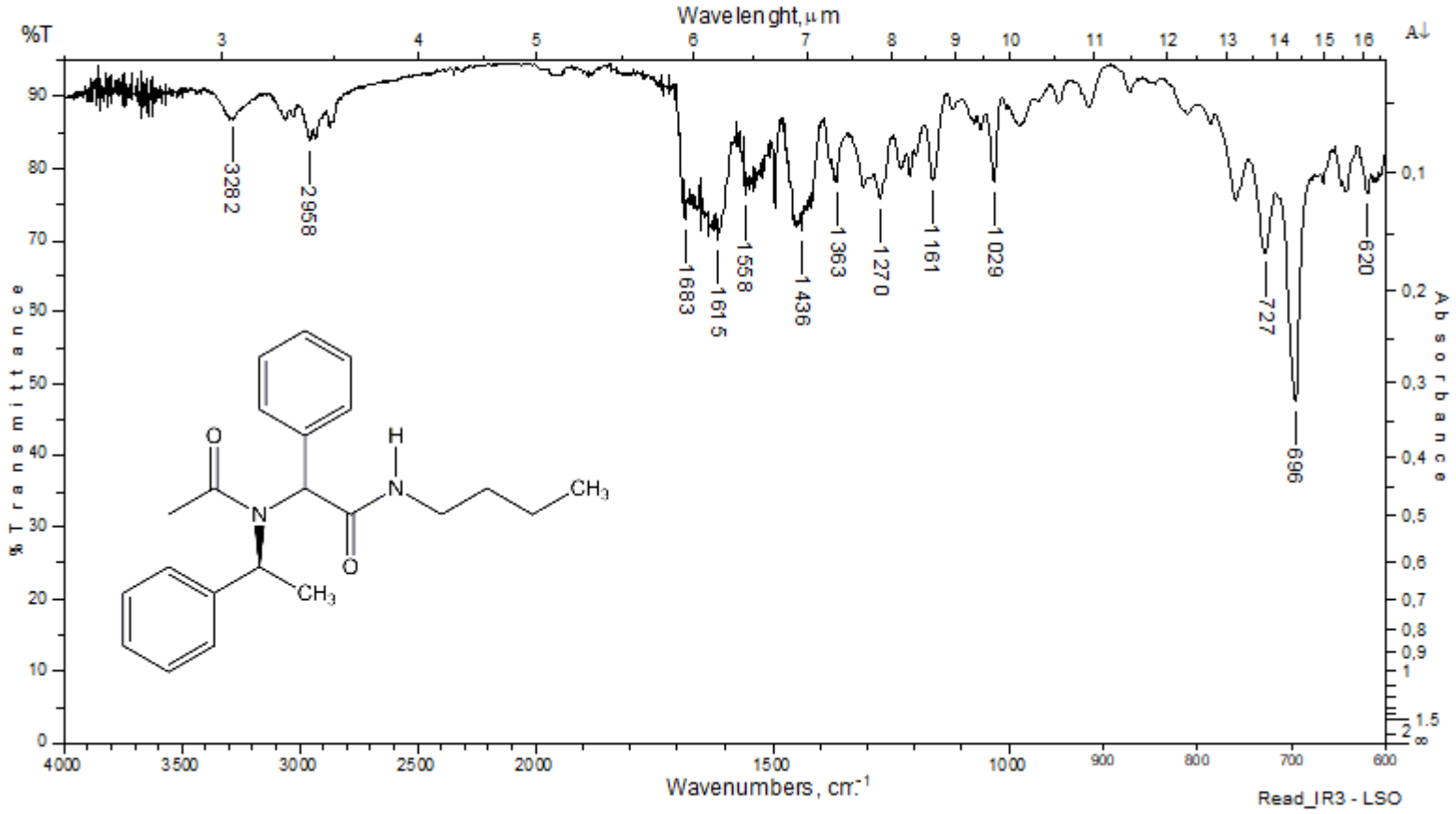


Figure S27. FTIR (KBr) spectrum of compound **5g-2**.

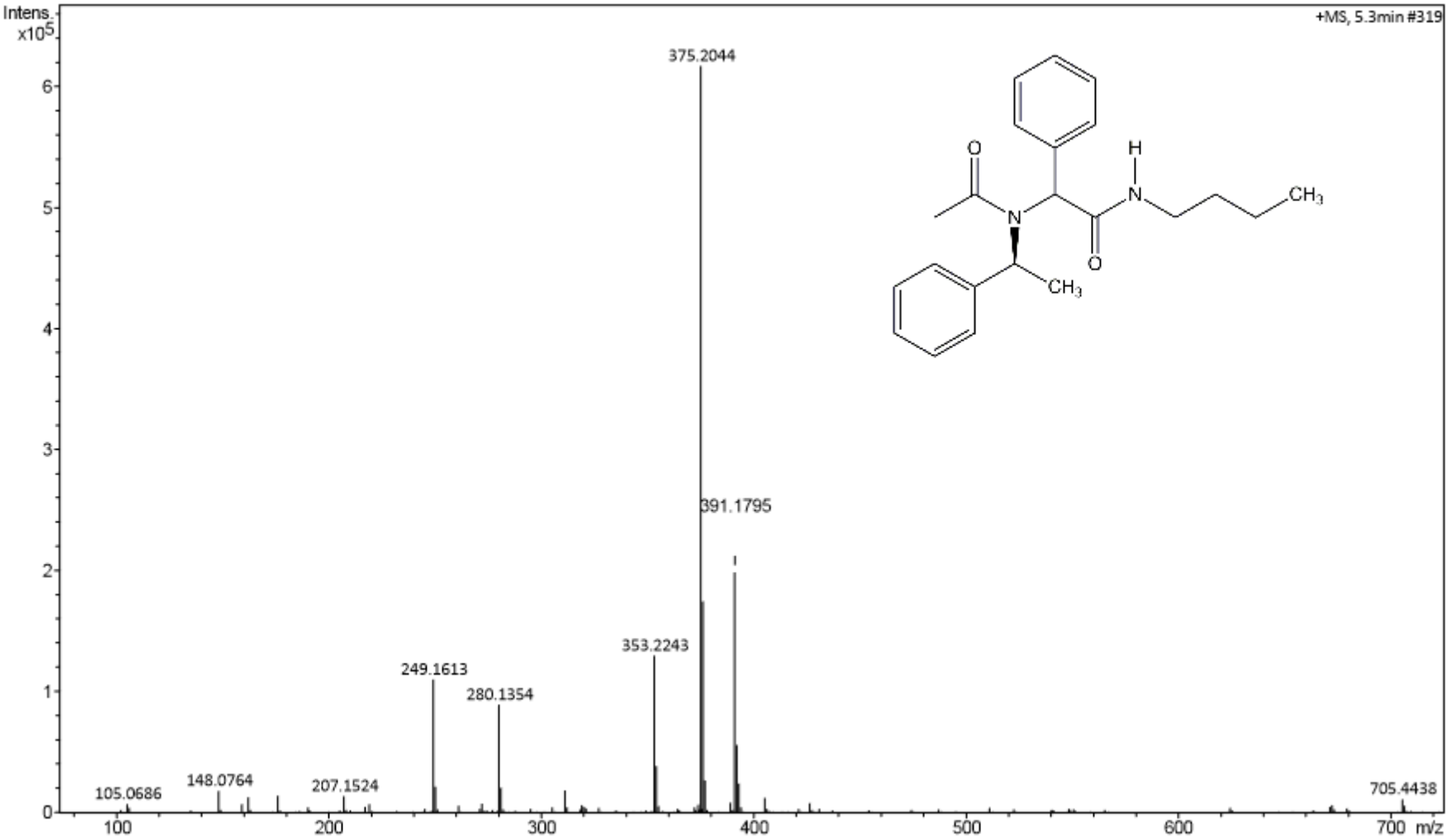
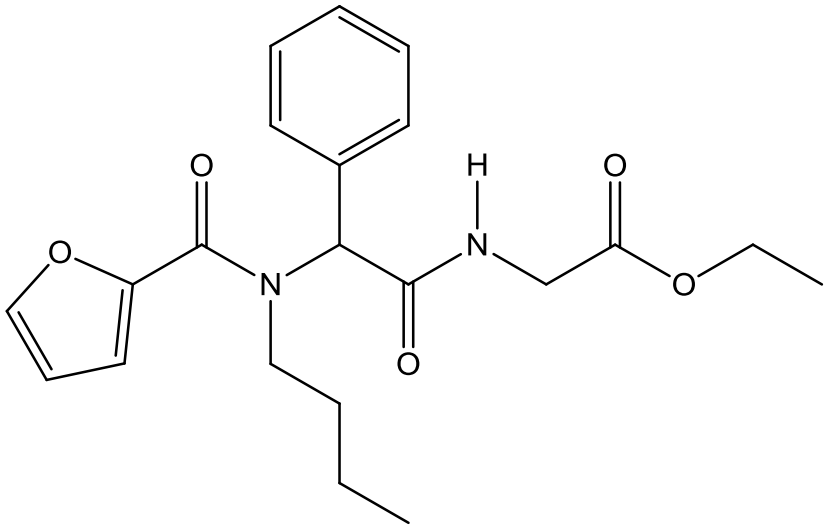


Figure S28. Mass spectrum of compound **5g-2**.

Compound **5h**



Ethyl 2-(2-(*N*-butylfuran-2-carboxamido)-2-phenylacetamido)acetate (**5h**)

Yellow oil, yield 70%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50-7.36 (m, 7H), 7.13-7.12 (m, 1H), 6.51-6.49 (m, 1H), 5.94 (s, 1H), 4.23-4.16 (m, 2H), 4.09-4.07 (m, 2H), 3.75-3.46 (m, 2H), 1.59-1.32 (m, 2H), 1.27 (t, 3H, *J* 7.2 Hz), 1.17-1.10 (m, 2H), 0.75 (t, 3H, *J* 7.2 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.0 (C), 169.6 (C), 161.0 (C), 148.2 (C), 144.2 (CH), 135.0 (C), 129.6 (2 CH), 128.9 (2 CH), 128.7 (CH), 117.6 (CH), 111.7 (CH), 64.5 (CH), 61.6 (CH_2), 48.0 (CH_2), 41.7 (CH_2), 31.7 (CH_2), 20.1 (CH_2), 14.2 (CH_3), 13.3 (CH_3); FTIR (KBr) ν / cm^{-1} 3326 (N–H), 2960 (C–H), 1746 (C=O, ester), 1674 (C=O, amide), 728 and 696 (=C–H aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{21}H_{26}N_2NaO_5$ $[M + Na]^+$: 409.1739, found: 409.1733.

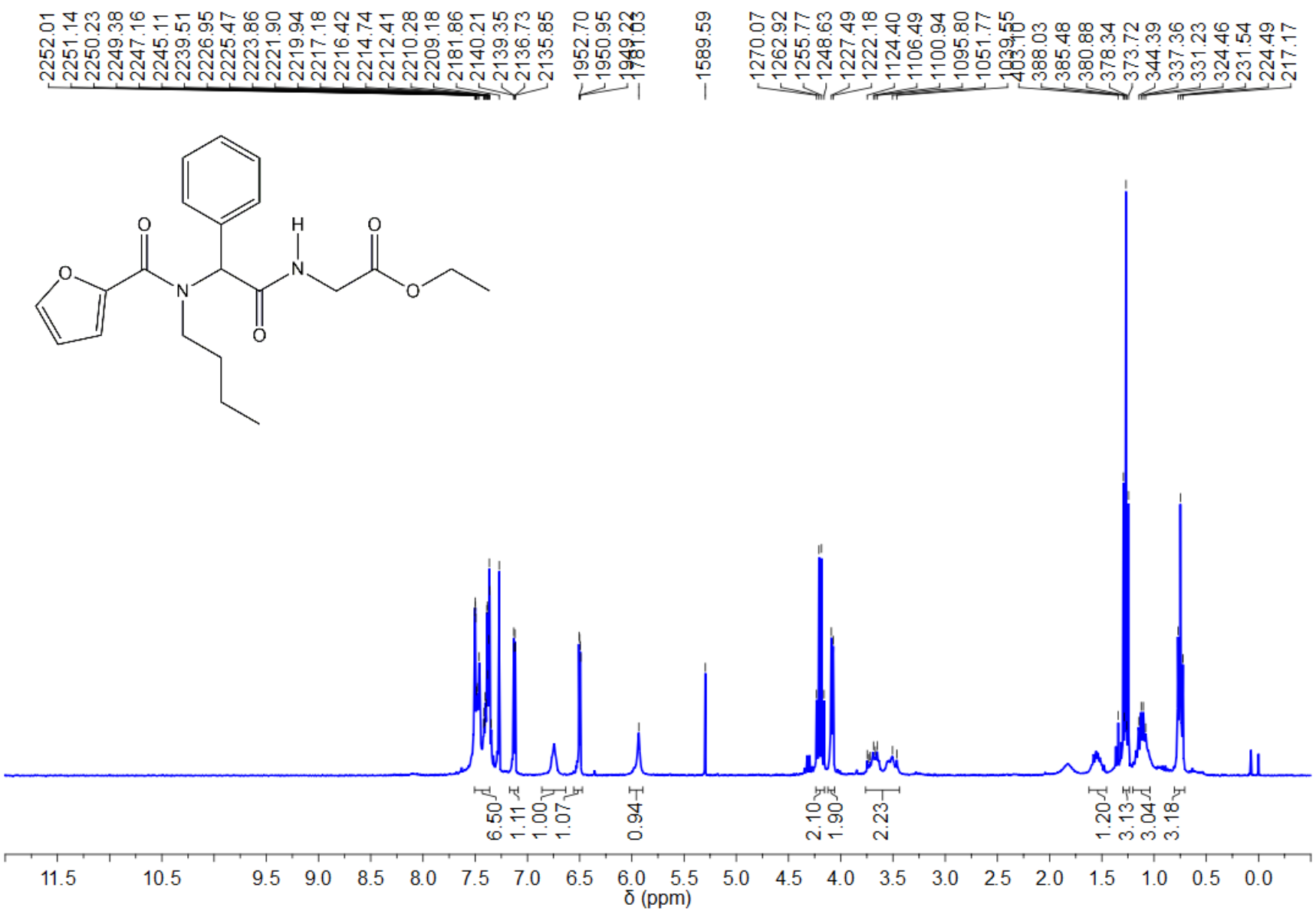


Figure S29. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **5h**.

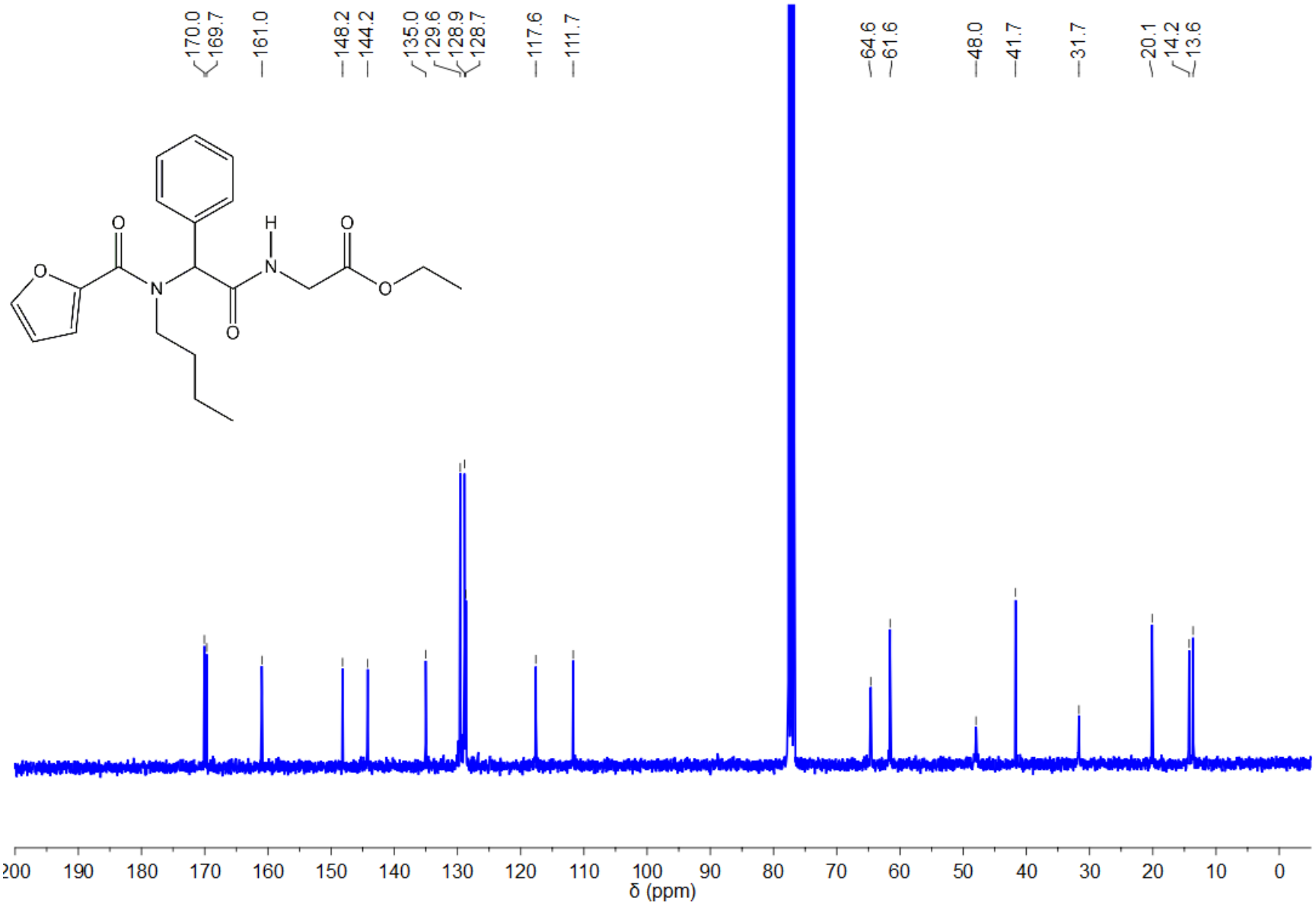


Figure S30. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **5h**.

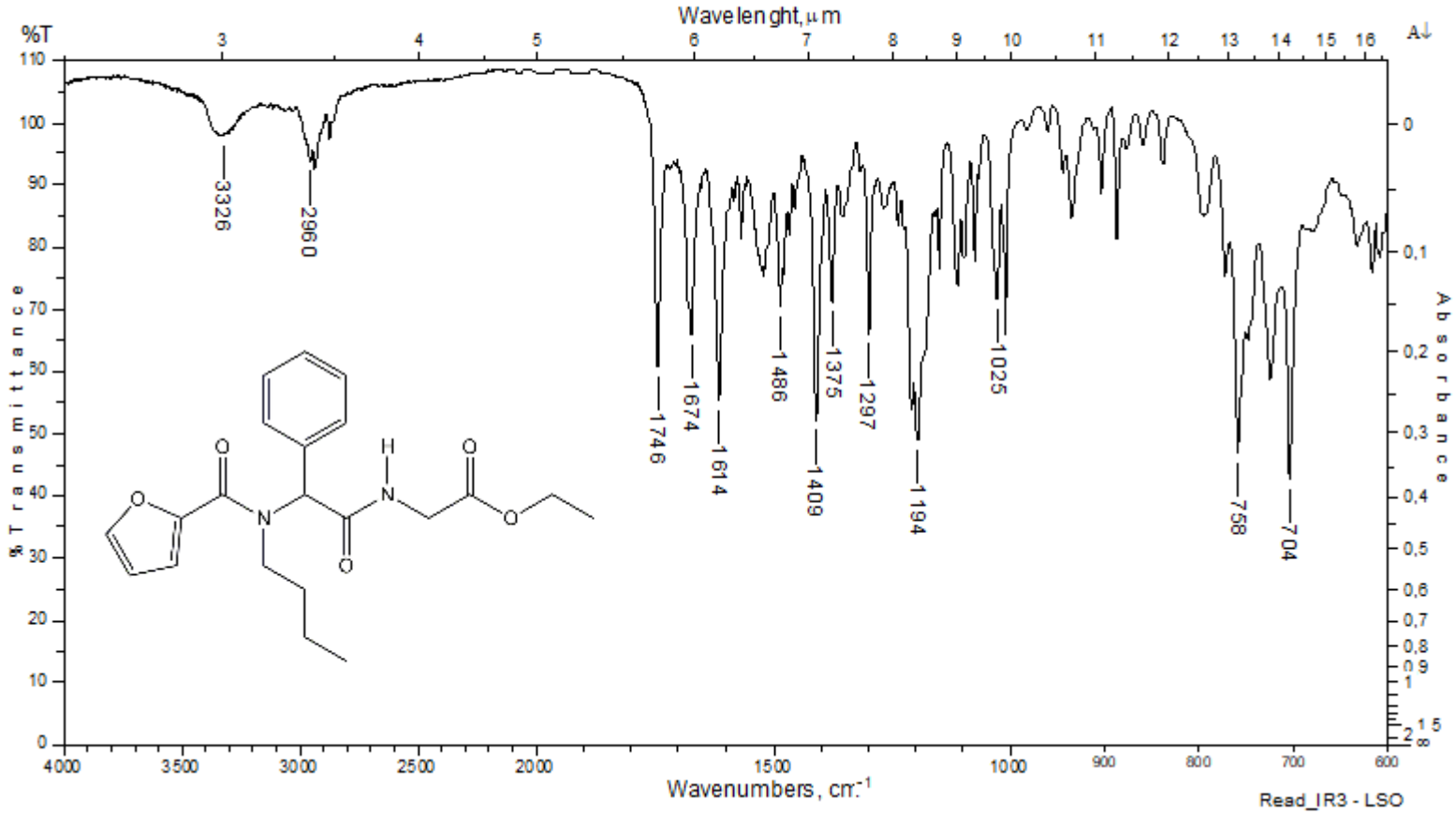


Figure S31. FTIR (KBr) spectrum of compound **5h**.

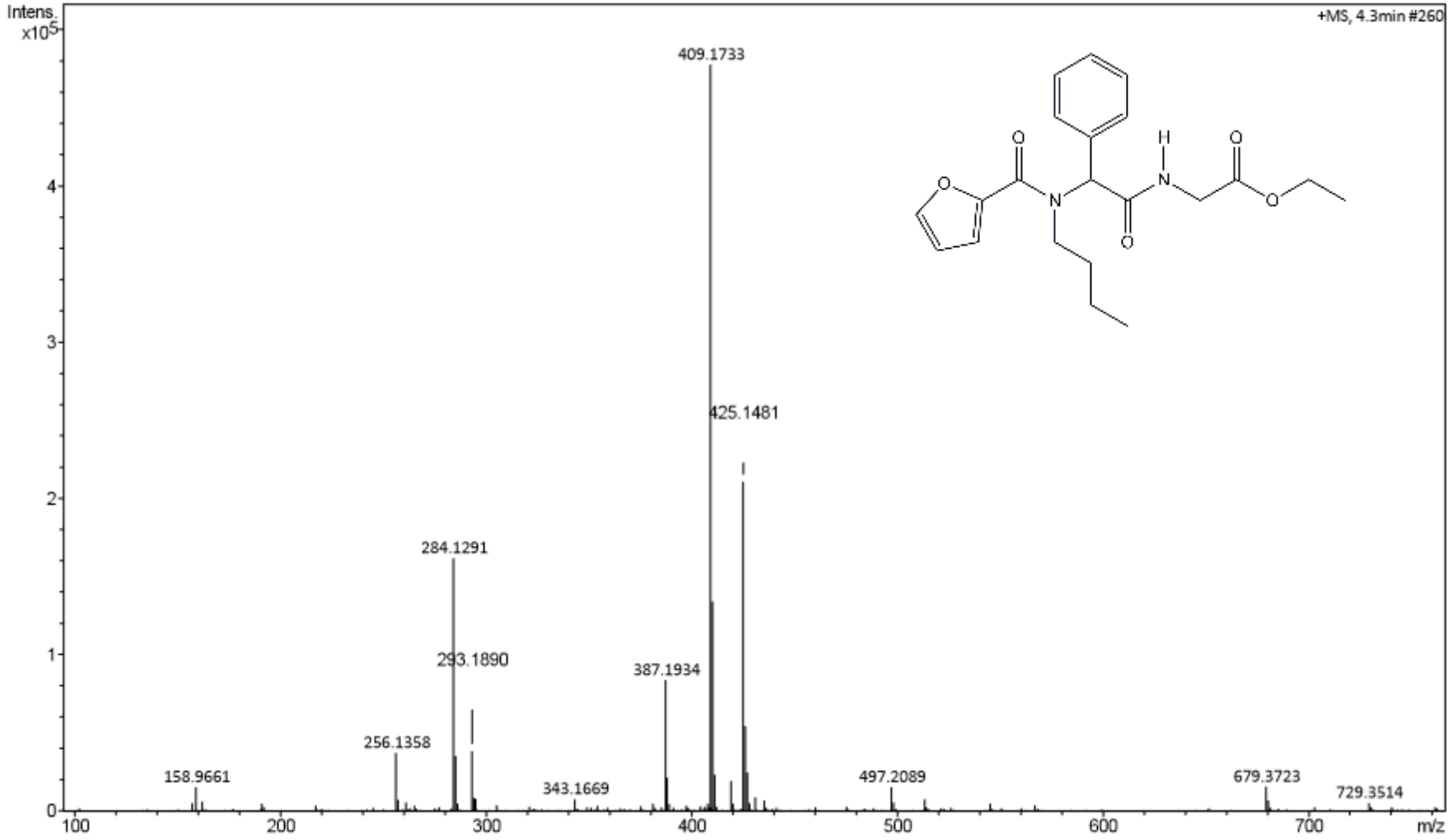
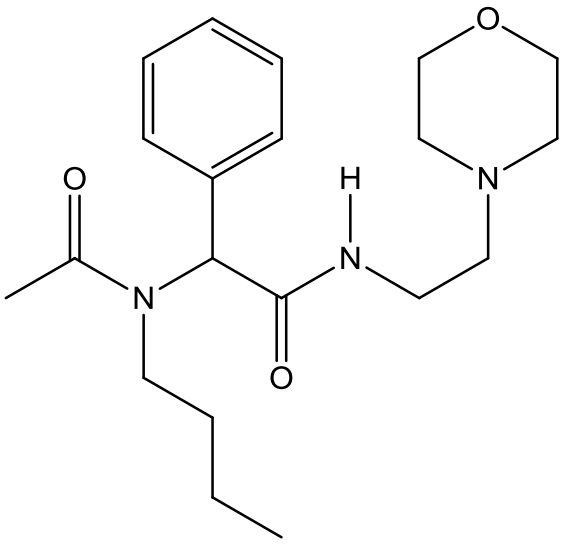


Figure S32. Mass spectrum of compound **5h**.

Compound **5i**



2-(*N*-Butylacetamido)-*N*-(2-morpholinoethyl)-2-phenylacetamide (**5i**)

Yellow oil, yield 55%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41-7.35 (m, 6H), 6.49 (s, 1H), 3.60-3.57 (m, 2H), 3.38-3.26 (m, 4H), 2.47-2.37 (m, 8H), 2.18 (s, 3H), 1.50-1.32 (m, 2H), 1.15-1.05 (m, 2H), 0.74 (t, 3H, *J* 7.2 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.3 (C), 169.8 (C), 135.8 (C), 129.6 (CH), 128.7 (CH), 128.4 (CH), 66.8 (CH_2), 63.0 (2 CH), 56.7 (2 CH_2), 53.2 (CH_2), 47.9 (CH_2), 35.9 (CH_2), 31.6 (CH_2), 21.8 (CH_3), 20.0 (CH_2), 13.5 (CH_3); FTIR (KBr) ν / cm^{-1} 3310 (N–H), 2960 (C–H), 1650 (C=O, amide), 742 and 702 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{20}H_{32}N_3O_3$ $[M + H]^+$: 362.2444, found: 362.2437.

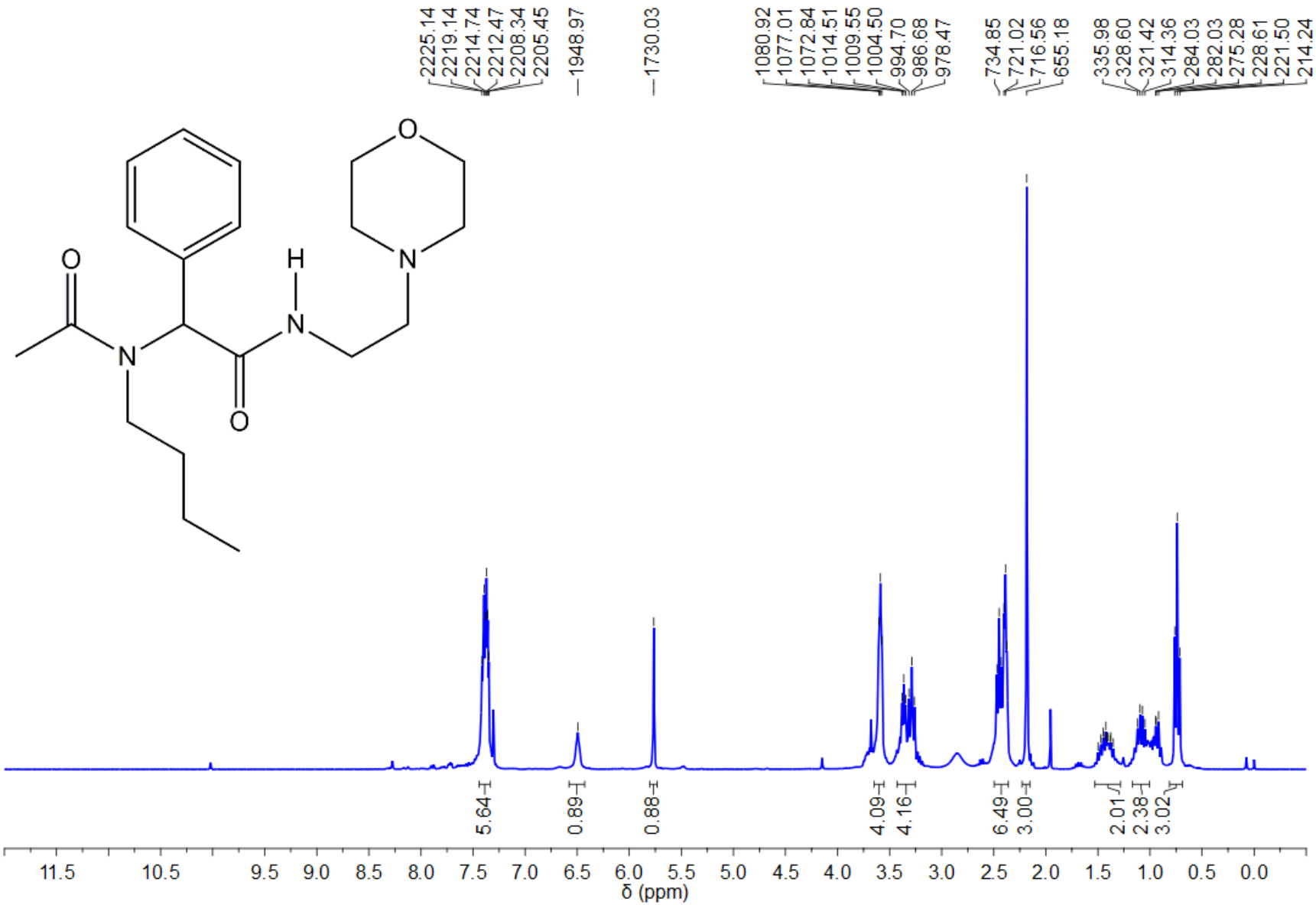


Figure S33. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **5i**.

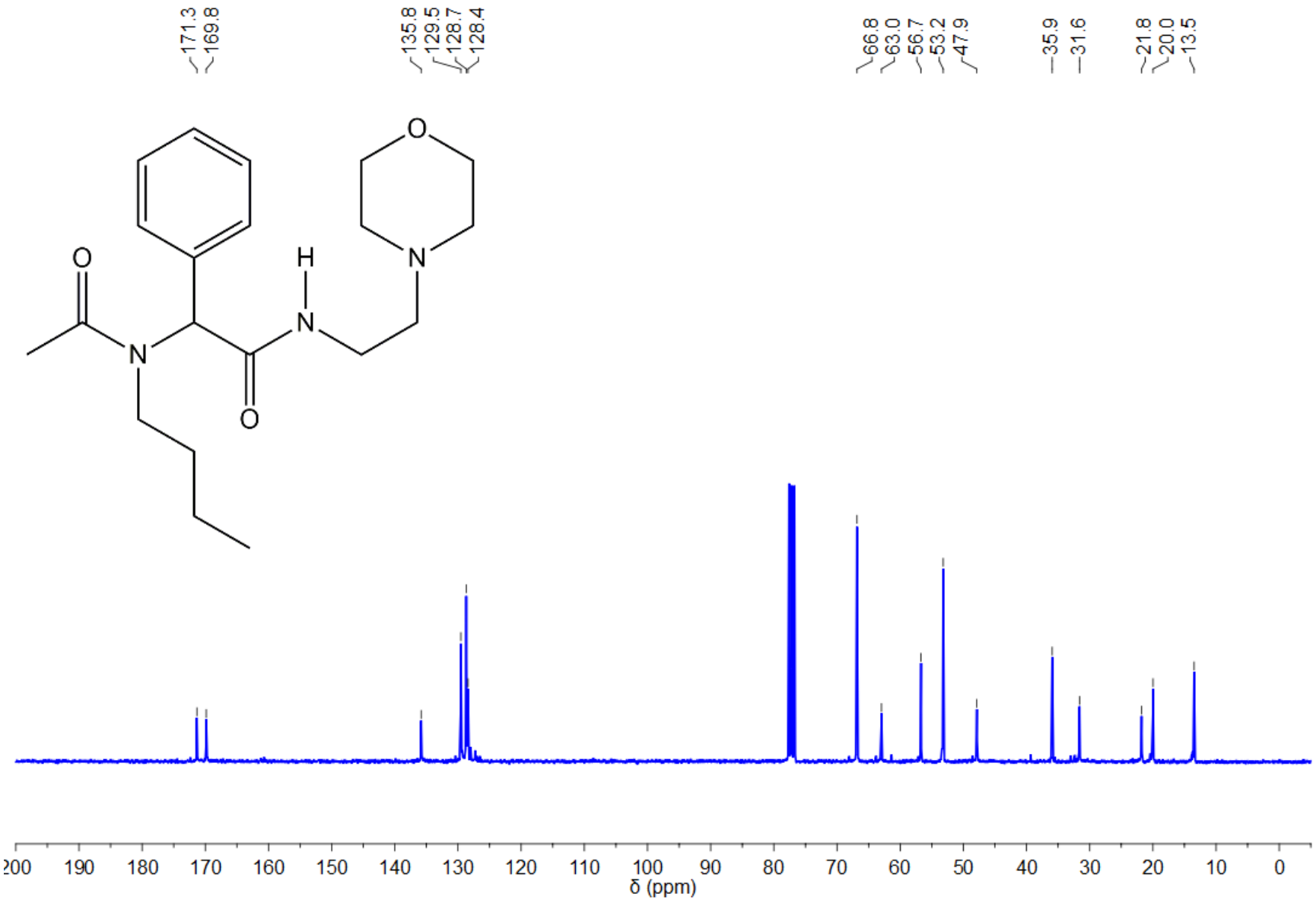


Figure S34. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **5i**.

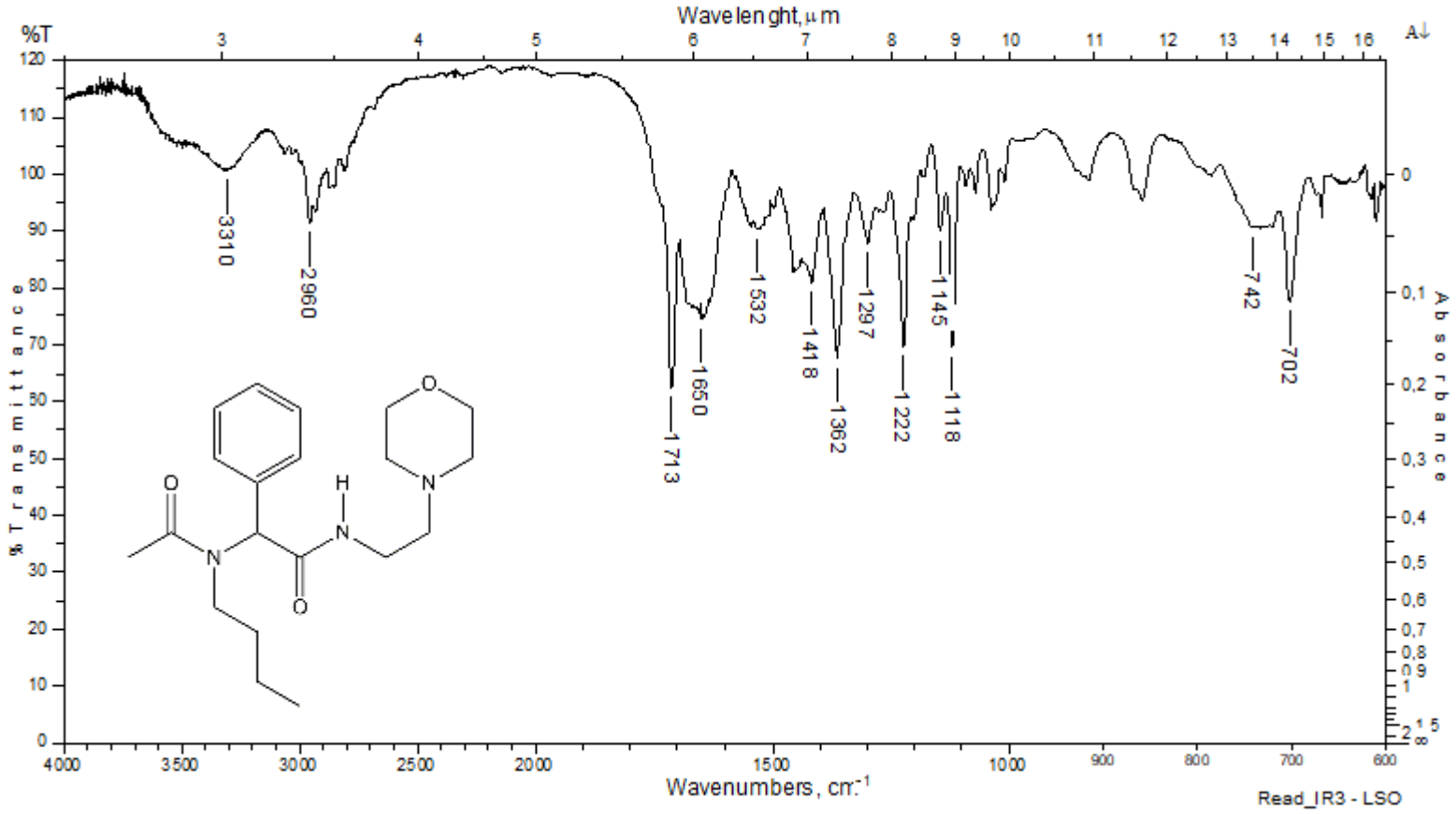


Figure S35. FTIR (KBr) spectrum of compound **5i**.

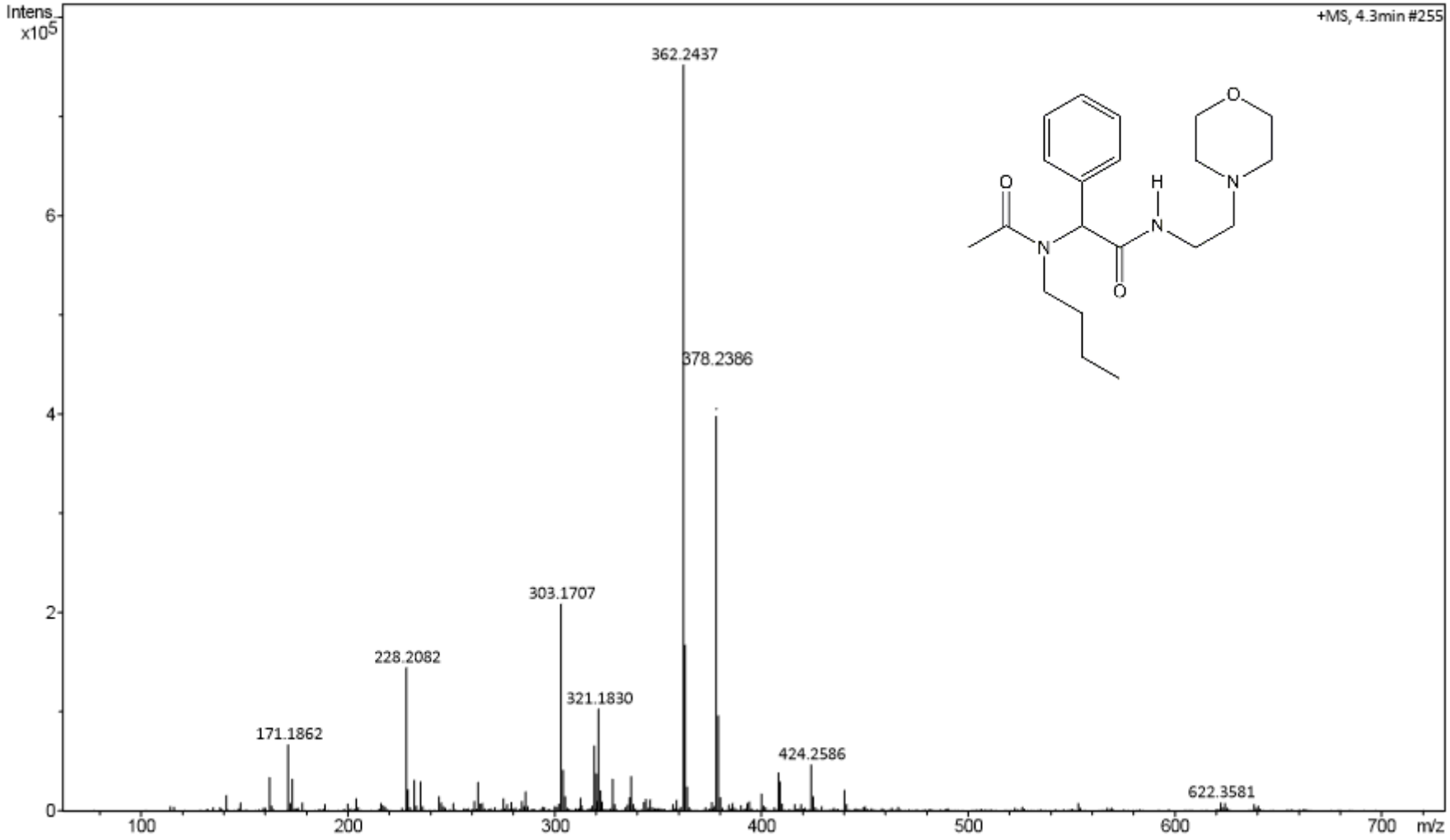
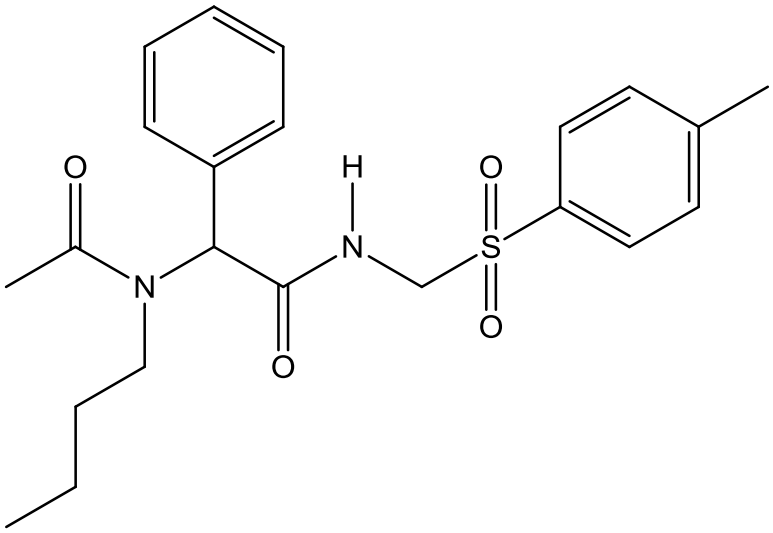


Figure S36. Mass spectrum of compound **5i**.

Compound **5j**



2-(*N*-Butylacetamido)-2-phenyl-*N*-(tosylmethyl)acetamide (**5j**)

Yellow oil, yield 57%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.72-7.66 (m, 3H), 7.42-7.32 (m, 7H), 5.98 (s, 1H), 3.96 (t, 2H, *J* 7.4 Hz), 2.43 (s, 2H), 2.13 (s, 2H), 2.07 (s, 2H), 0.83 (t, 6H, *J* 7.3 Hz), 0.68 (t, 3H, *J* 7.3 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.7 (C), 170.0 (C), 145.1 (C), 137.9 (CH_3), 134.4 (CH), 133.1 (CH), 129.9 (2 CH), 129.0 (2 CH), 128.8 (2 CH), 128.2 (2 CH), 127.2 (CH), 62.0 (CH), 60.6 (CH_2), 45.3 (CH_2), 32.9 (CH_2), 19.7 (CH_2), 13.4 (2 CH_3); FTIR (KBr) ν / cm^{-1} 3219 (N–H), 2960 (C–H), 1698 (S=O), 1650 (C=O, amide), 765 and 700 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{22}H_{28}N_2NaO_4S$ $[M + Na]^+$: 439.1667, found: 439.1662.

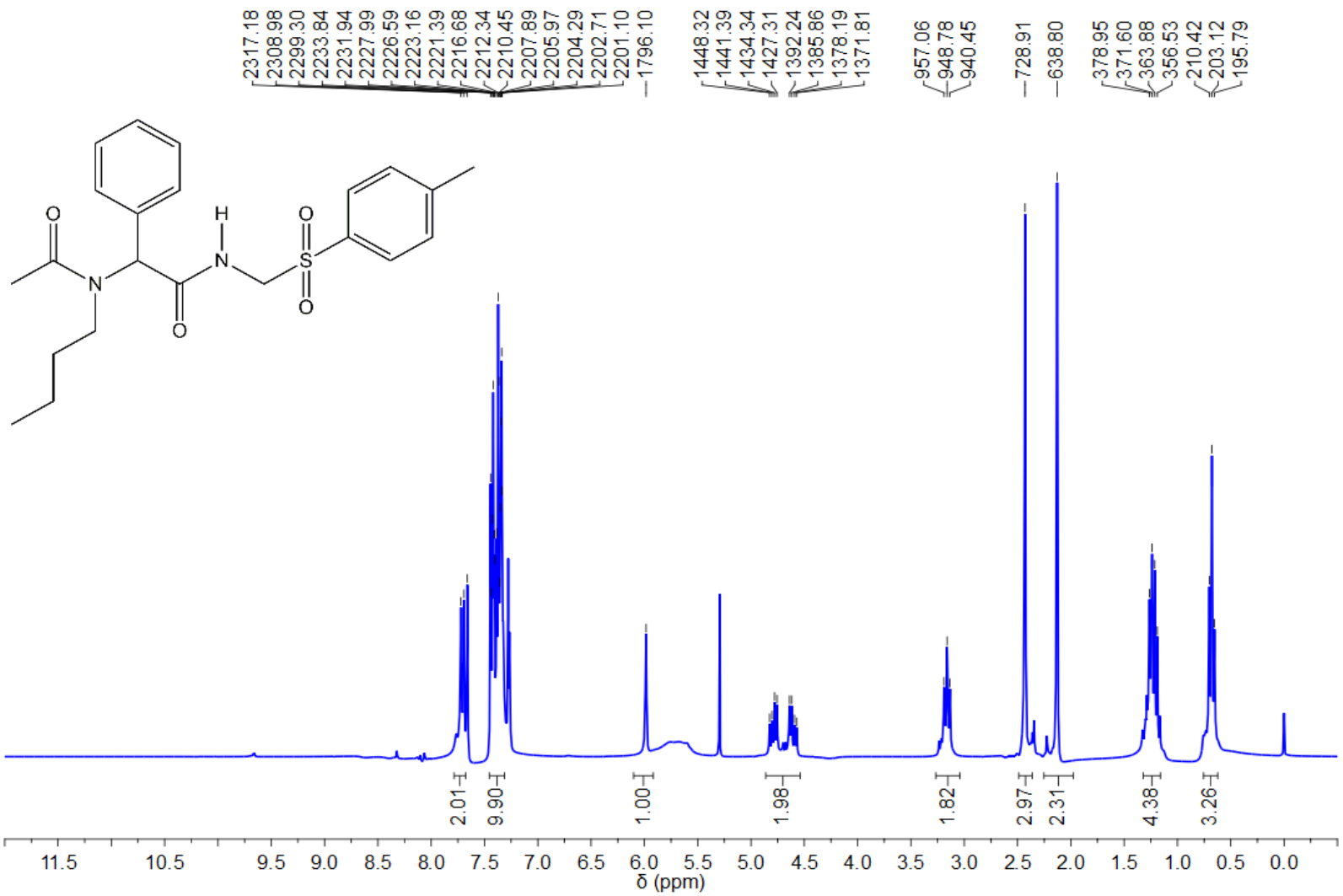


Figure S37. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **5j**.

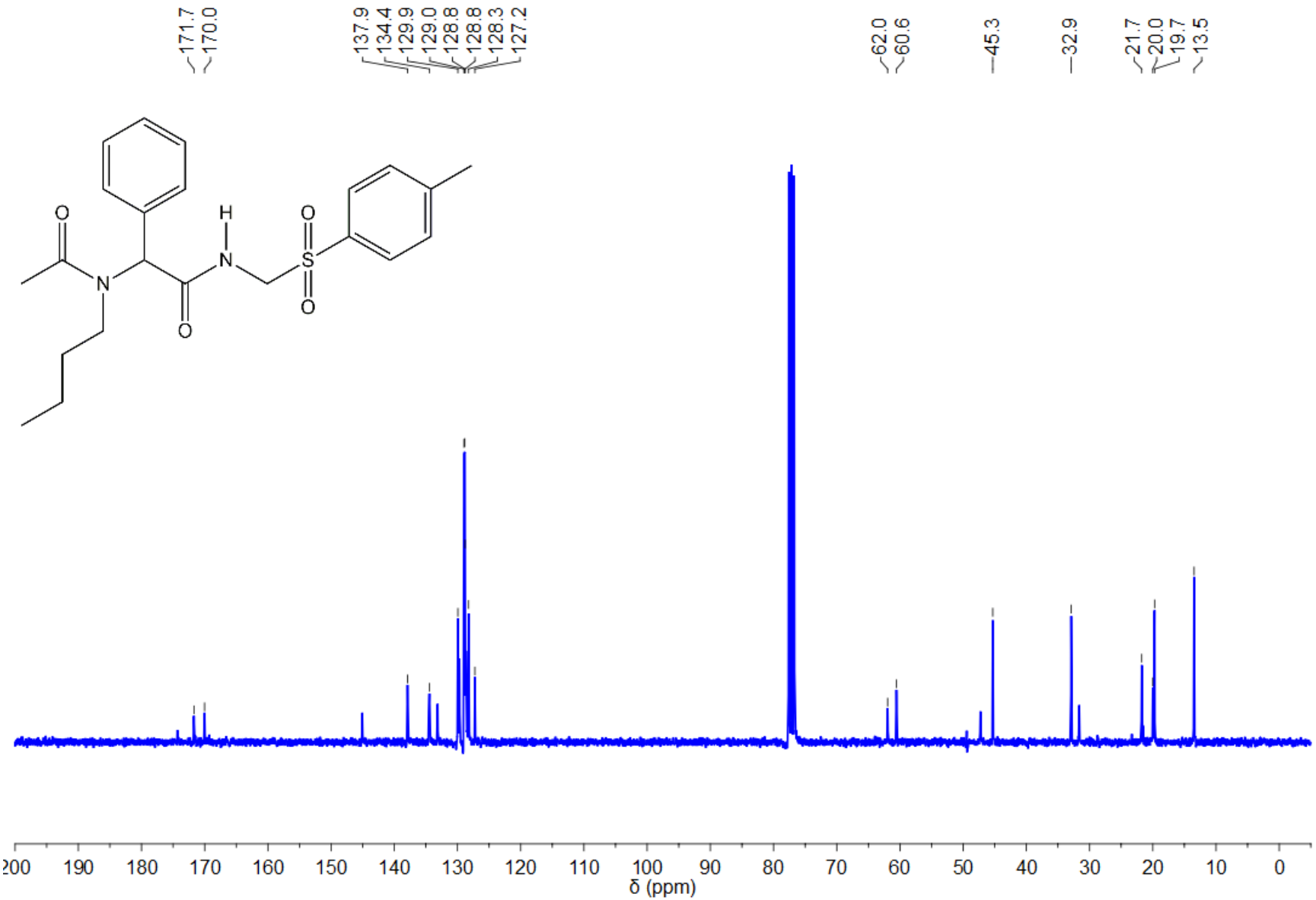


Figure S38. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **5j**.

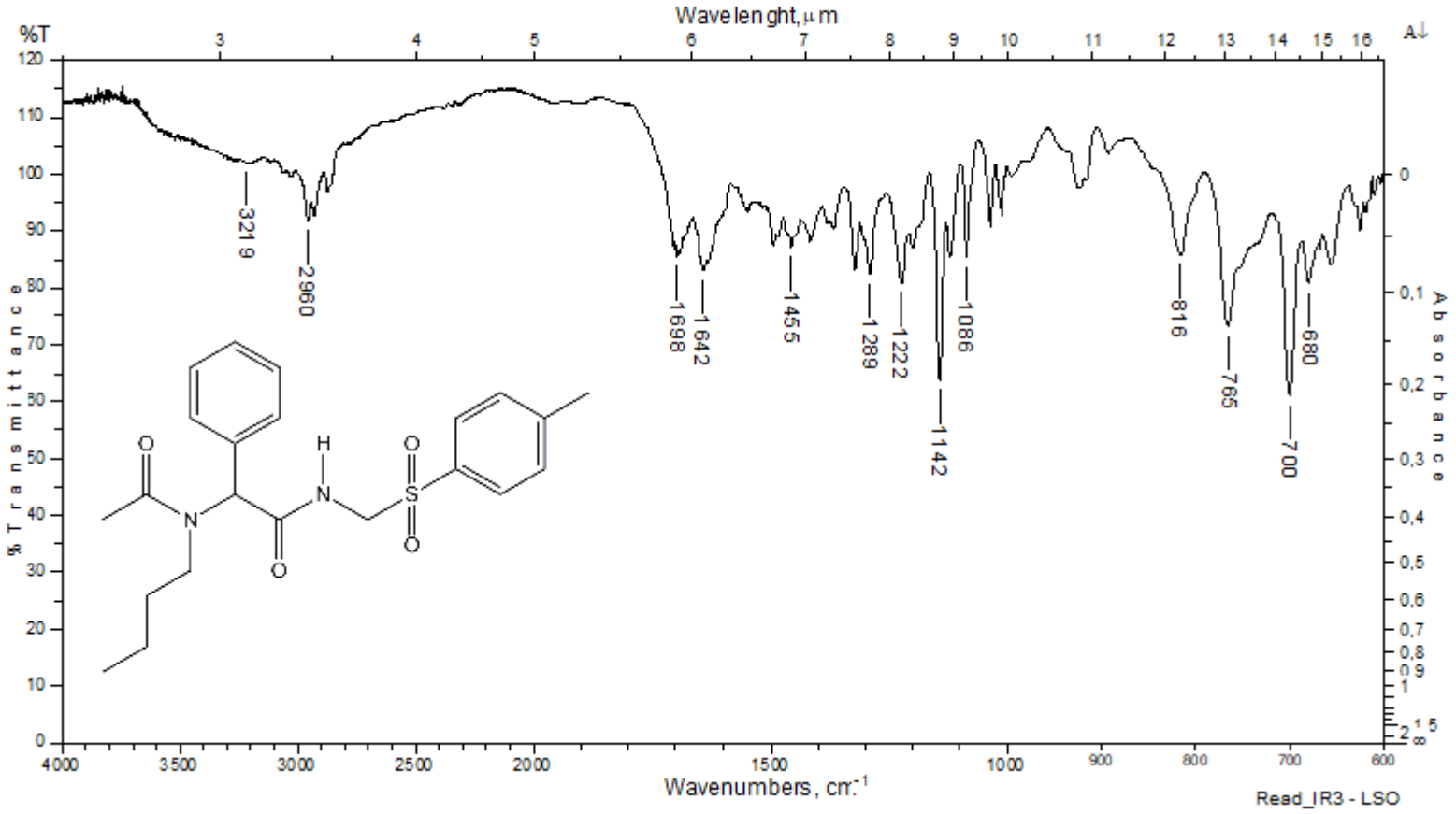


Figure S39. FTIR (KBr) spectrum of compound **5j**.

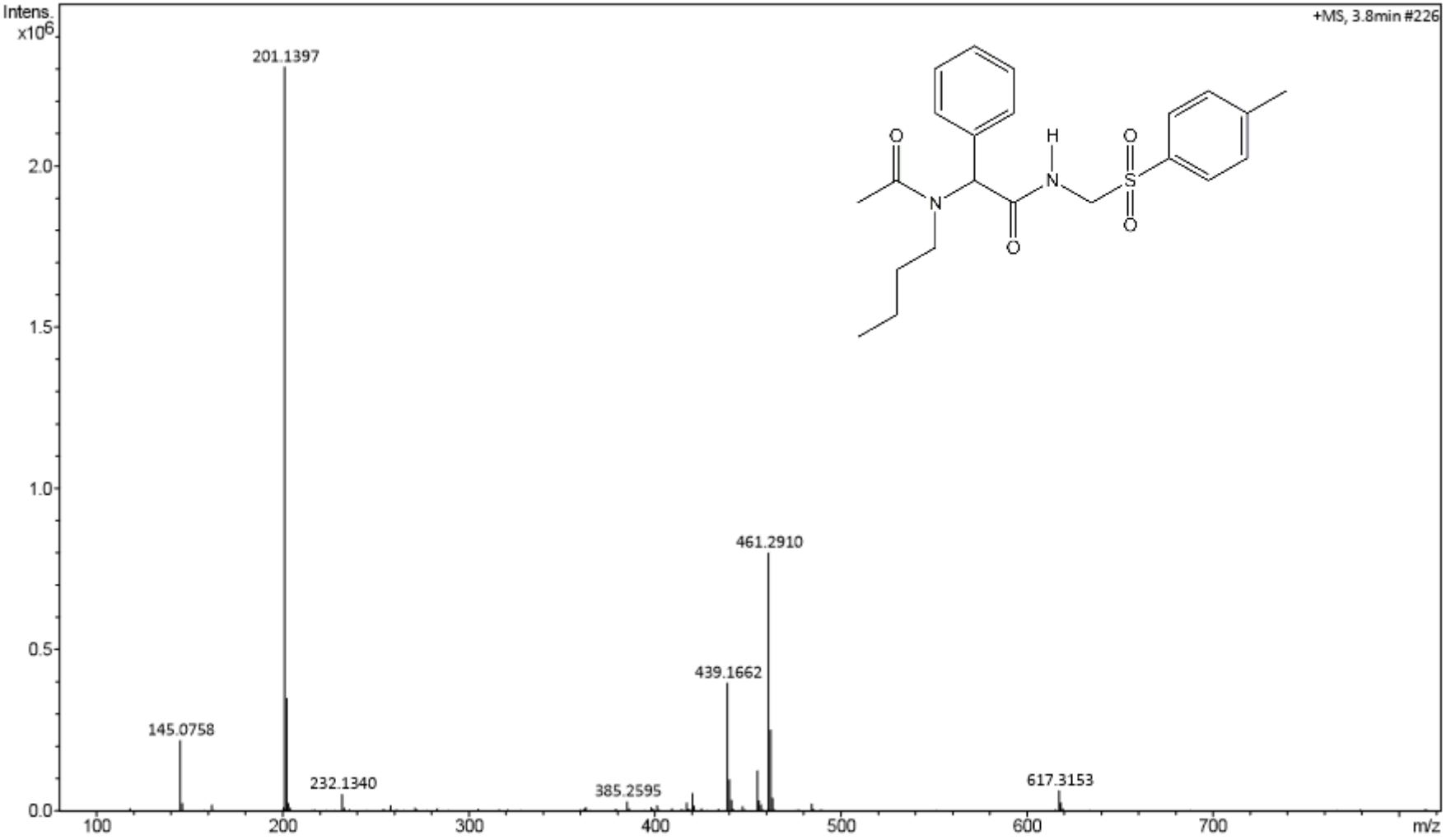
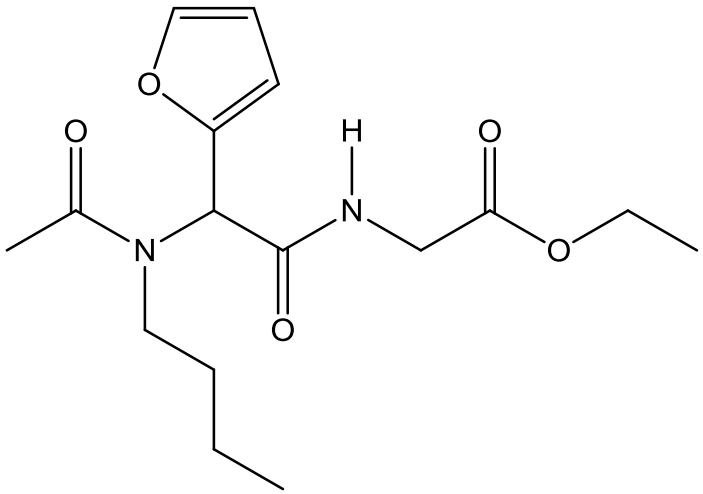


Figure S40. Mass spectrum of compound **5j**.

Compound **5k**



Ethyl 2-(2-(*N*-butylacetamido)-2-(furan-2-yl)acetamido)acetate (**5k**)

Brown oil, yield 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, 1H, *J* 1.8 Hz), 6.74 (s, 1H), 6.64 (d, 1H, *J* 3.2 Hz), 6.33 (dd, 1H, *J* 1.8 Hz), 6.06 (s, 1H), 4.15-4.10 (m, 2H), 3.96-3.94 (m, 2H), 3.25-3.17 (m, 2H), 2.11 (s, 3H), 1.22-1.16 (m, 5H), 1.10-1.04 (m, 2H), 0.73 (t, 3H, *J* 7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7 (C), 169.6 (C), 168.3 (C), 148.2 (C), 142.9 (CH), 112.1 (CH), 111.0 (CH), 61.6 (CH_2), 55.6 (CH), 47.4 (CH_2), 41.6 (CH_2), 31.2 (CH_2), 21.6 (CH_3), 20.1 (CH_2), 14.2 (CH_3), 13.6 (CH_3); FTIR (KBr) ν / cm^{-1} 3412 (N–H), 2960 (C–H), 1714 (C=O, ester), 1679 (C=O, amide), 1222 and 1093 (C–O, ester), 530 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{16}H_{24}N_2NaO_5$ $[M + Na]^+$: 347.1583, found: 347.1577.

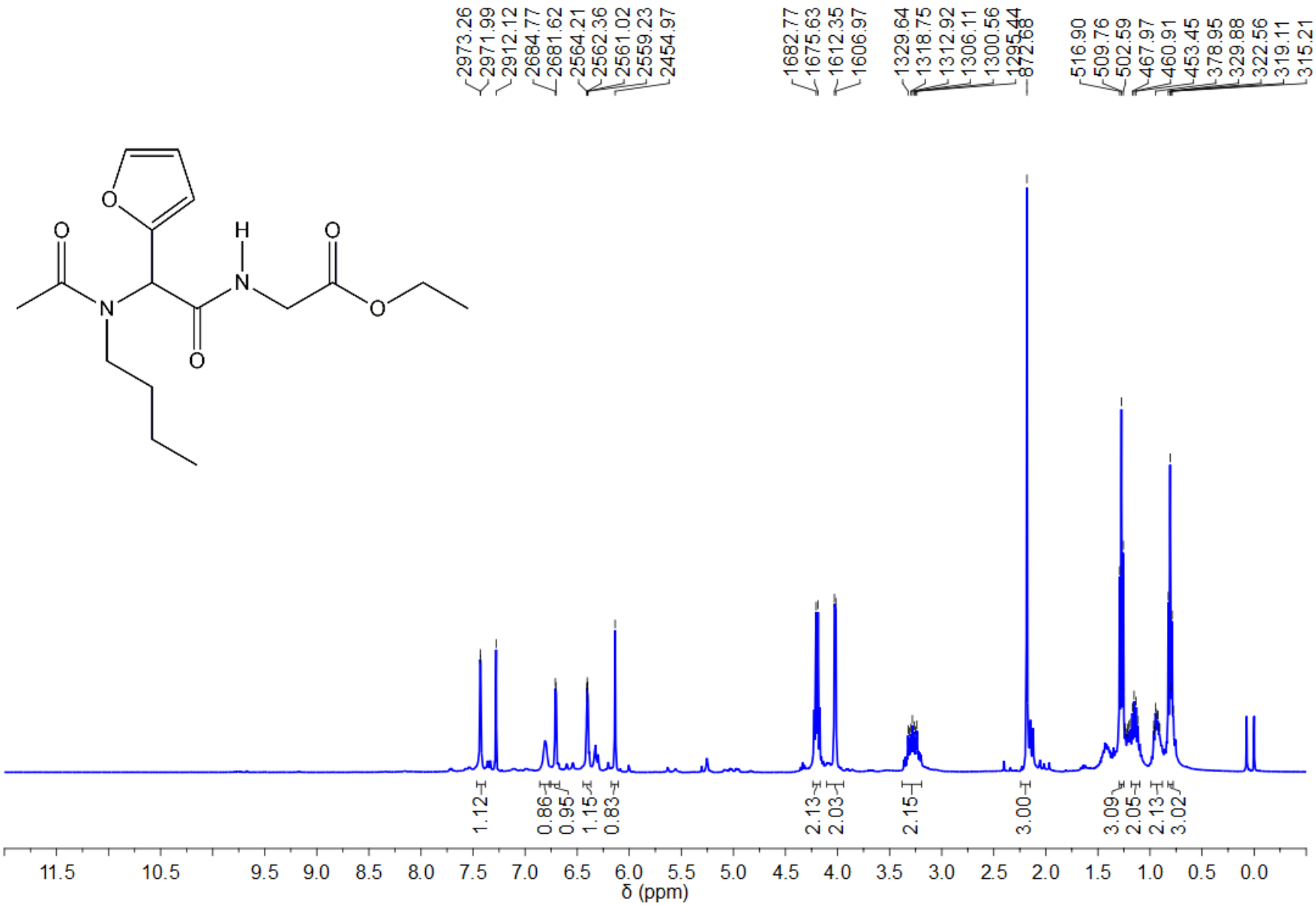


Figure S41. ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **5k**.

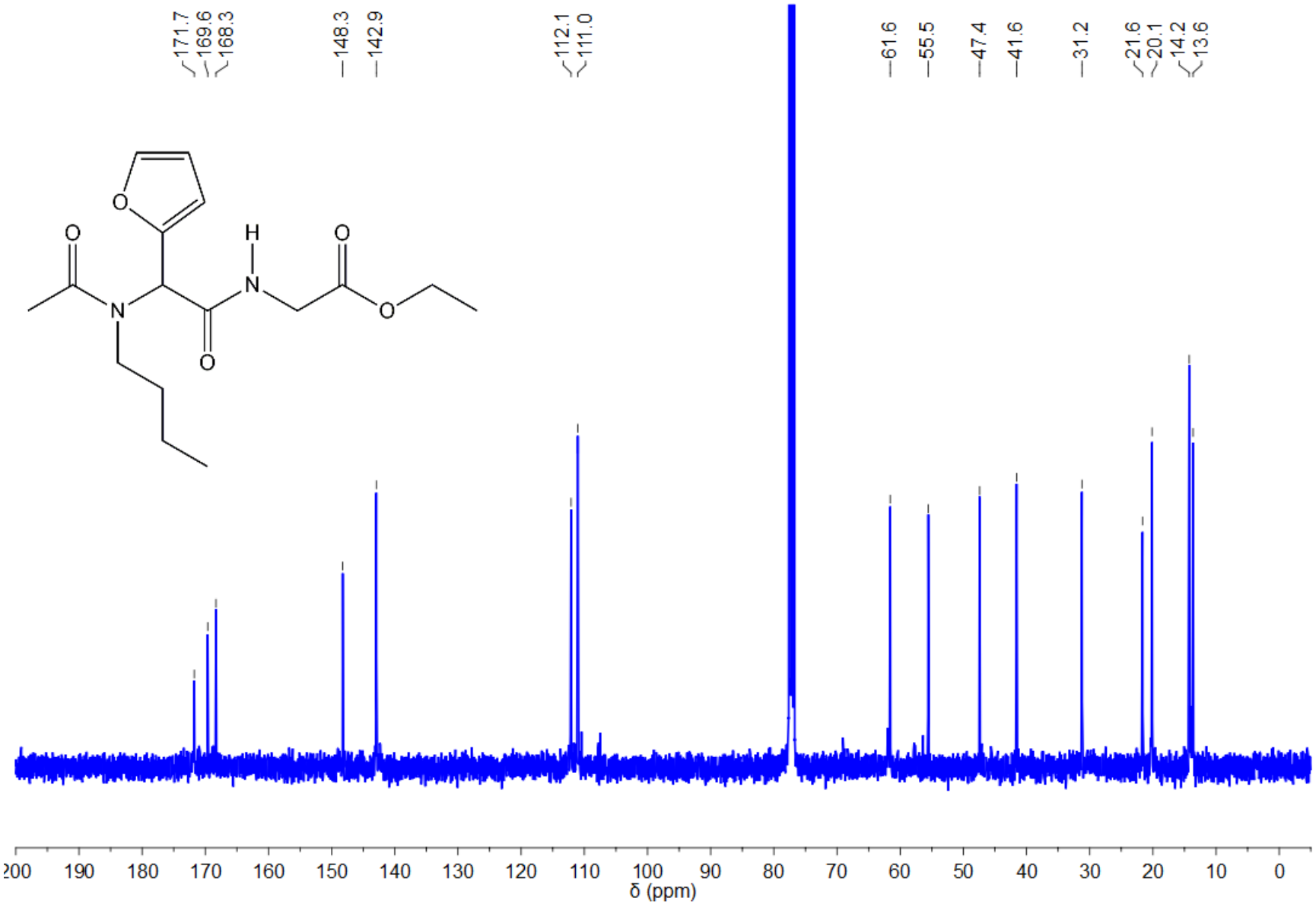


Figure S42. ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **5k**.

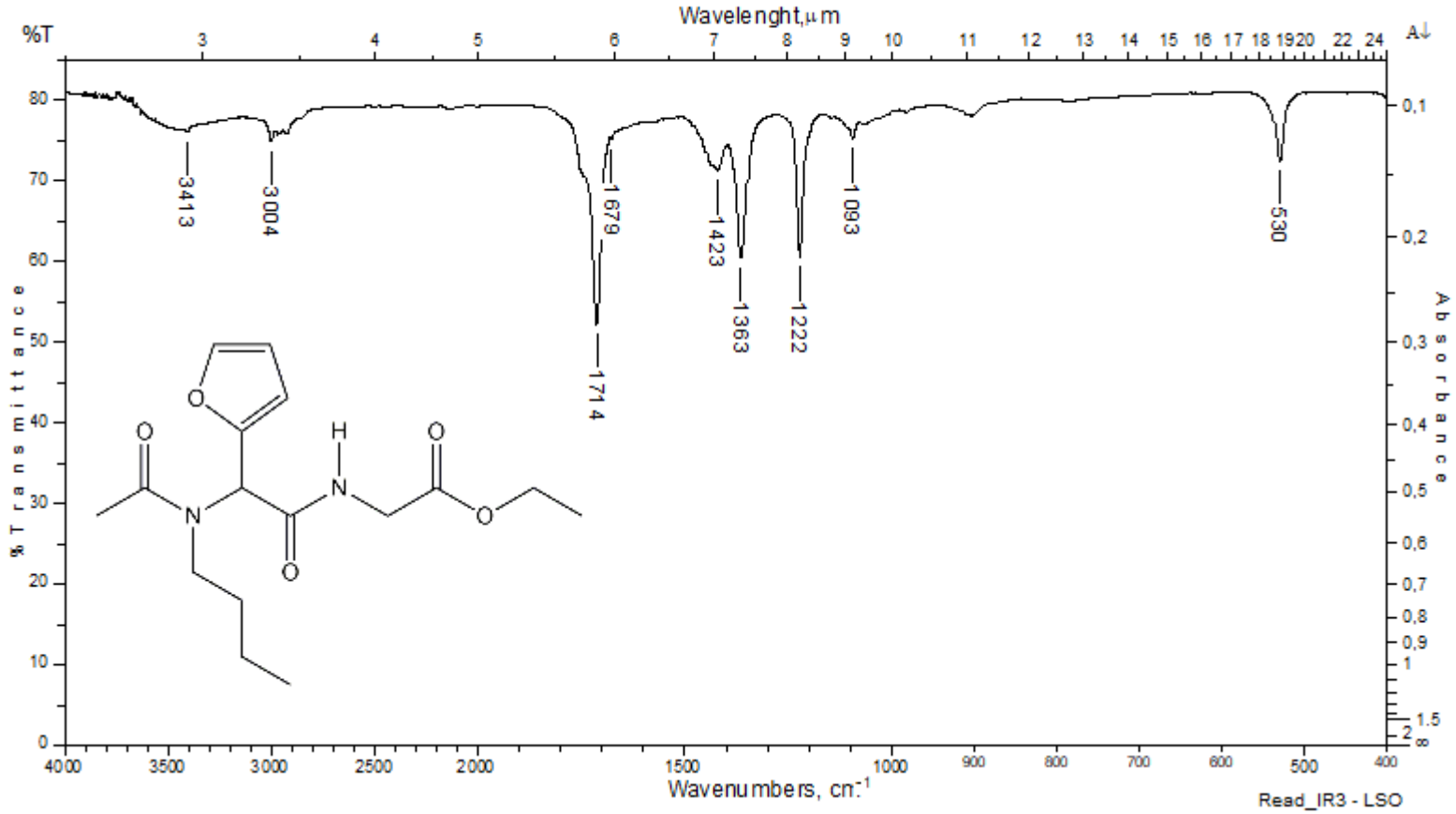


Figure S43. FTIR (KBr) spectrum of compound **5k**.

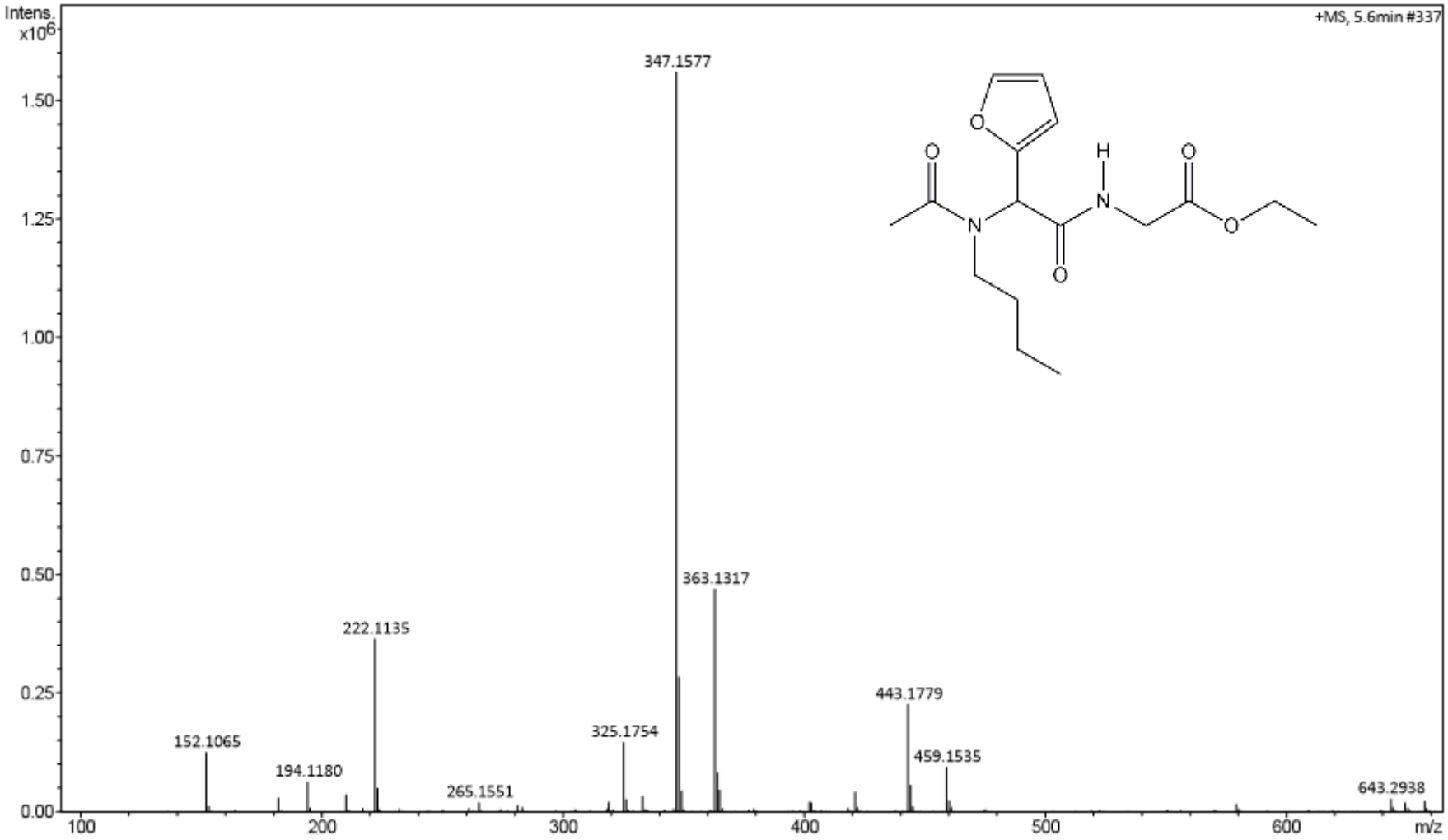
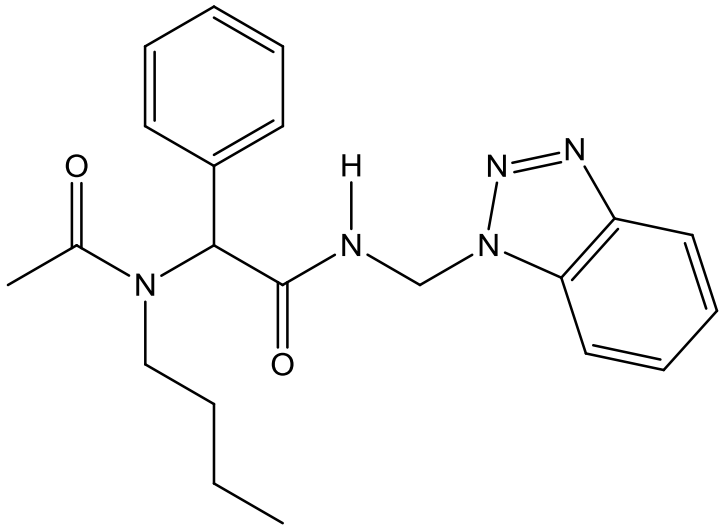


Figure S44. Mass spectrum of compound **5k**.

Compound **5l**



N-((1*H*-Benzo[*d*][1,2,3]triazol-1-yl)methyl)-2-(*N*-butylacetamido)-2-phenylacetamide (**5l**)

Yellow oil, yield 68%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.00-7.93 (m, 3H), 7.43-7.36 (m, 2H), 7.15-7.17 (m, 5H), 6.10-6.06 (m, 2H), 5.86 (s, 1H), 3.30-3.18 (m, 2H), 2.14 (s, 3H), 1.05-0.95 (m, 2H), 0.93-0.76 (m, 2H), 0.65 (t, 3H, *J* 7.2 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.0 (C), 171.1 (C), 134.4 (C), 132.6 (C), 129.5 (C), 129.0 (2 CH), 128.0 (2 CH), 125.9 (CH), 124.4 (CH), 119.7 (CH), 111.0 (CH), 62.9 (CH), 51.3 (CH_2), 47.8 (CH_2), 31.6 (CH_2), 21.8 (CH_3), 20.0 (CH_2), 13.5 (CH_3); FTIR (KBr) ν / cm^{-1} 3261 (N–H), 2957 (C–H), 1699 (C=O, amide), 749 and 702 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{21}H_{25}N_5NaO_2$ $[M + Na]^+$: 402.1906, found: 402.1903.

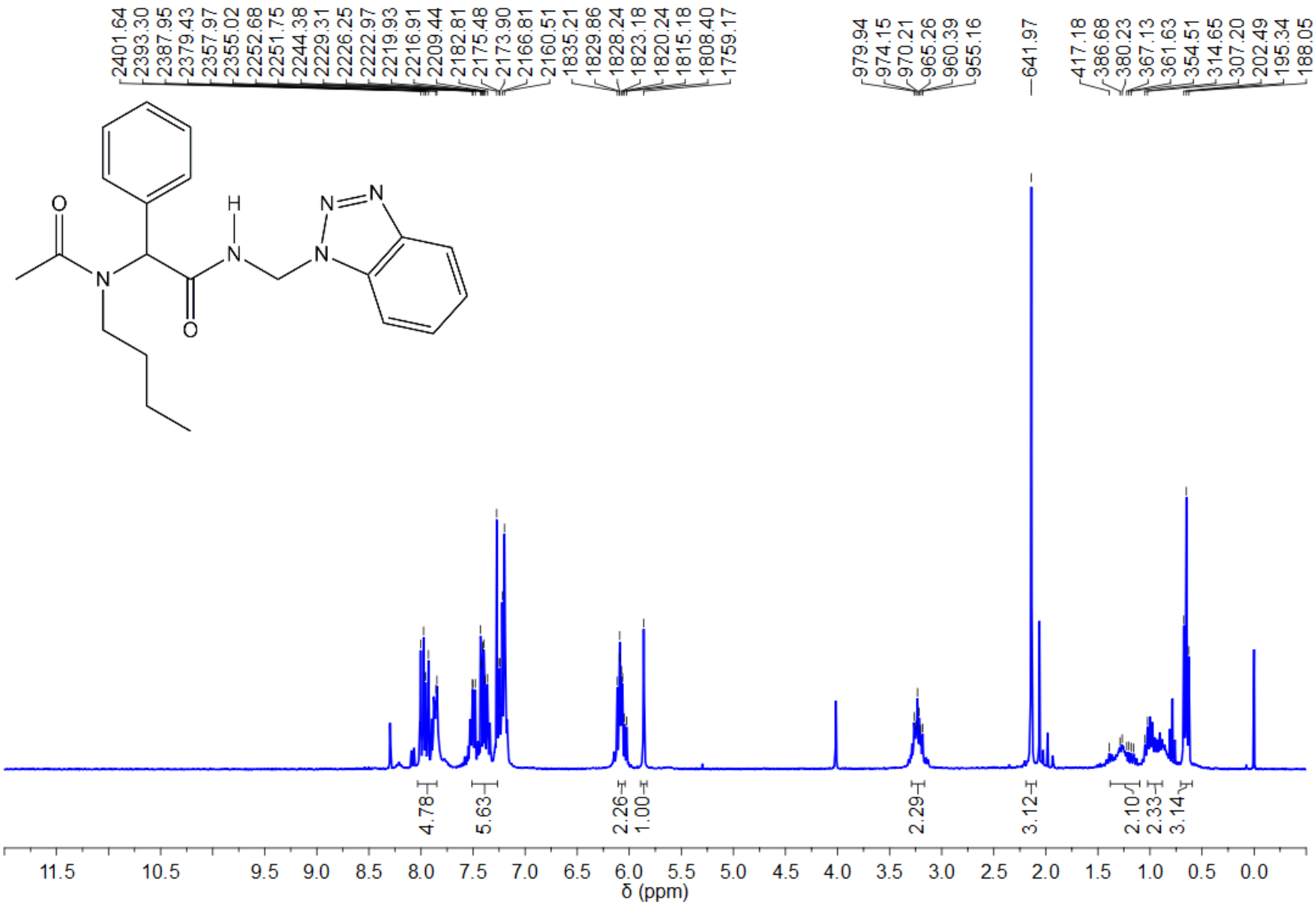


Figure S45. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **5l**.

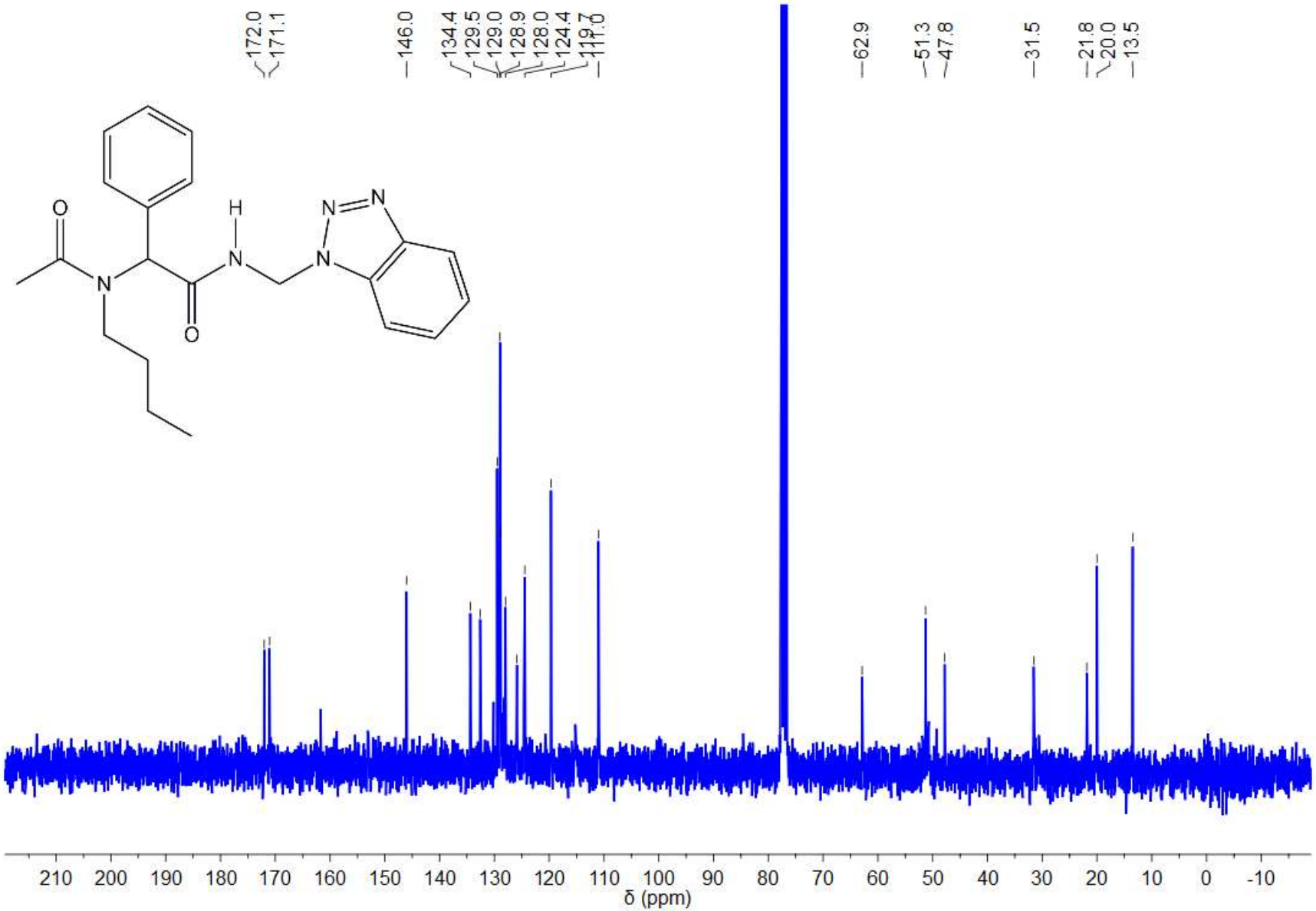


Figure S46. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **5l**.

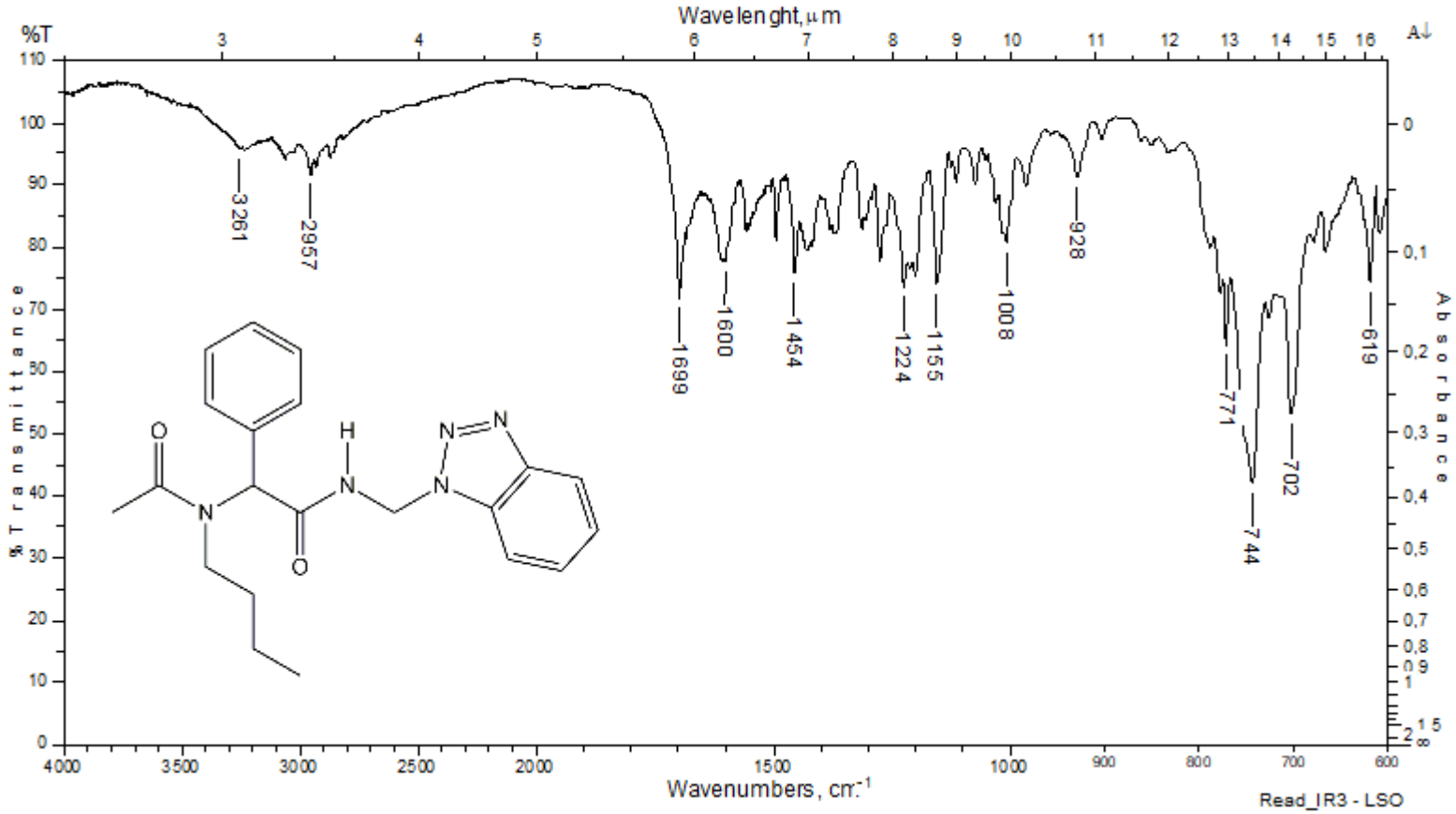


Figure S47. FTIR (KBr) spectrum of compound **5l**.

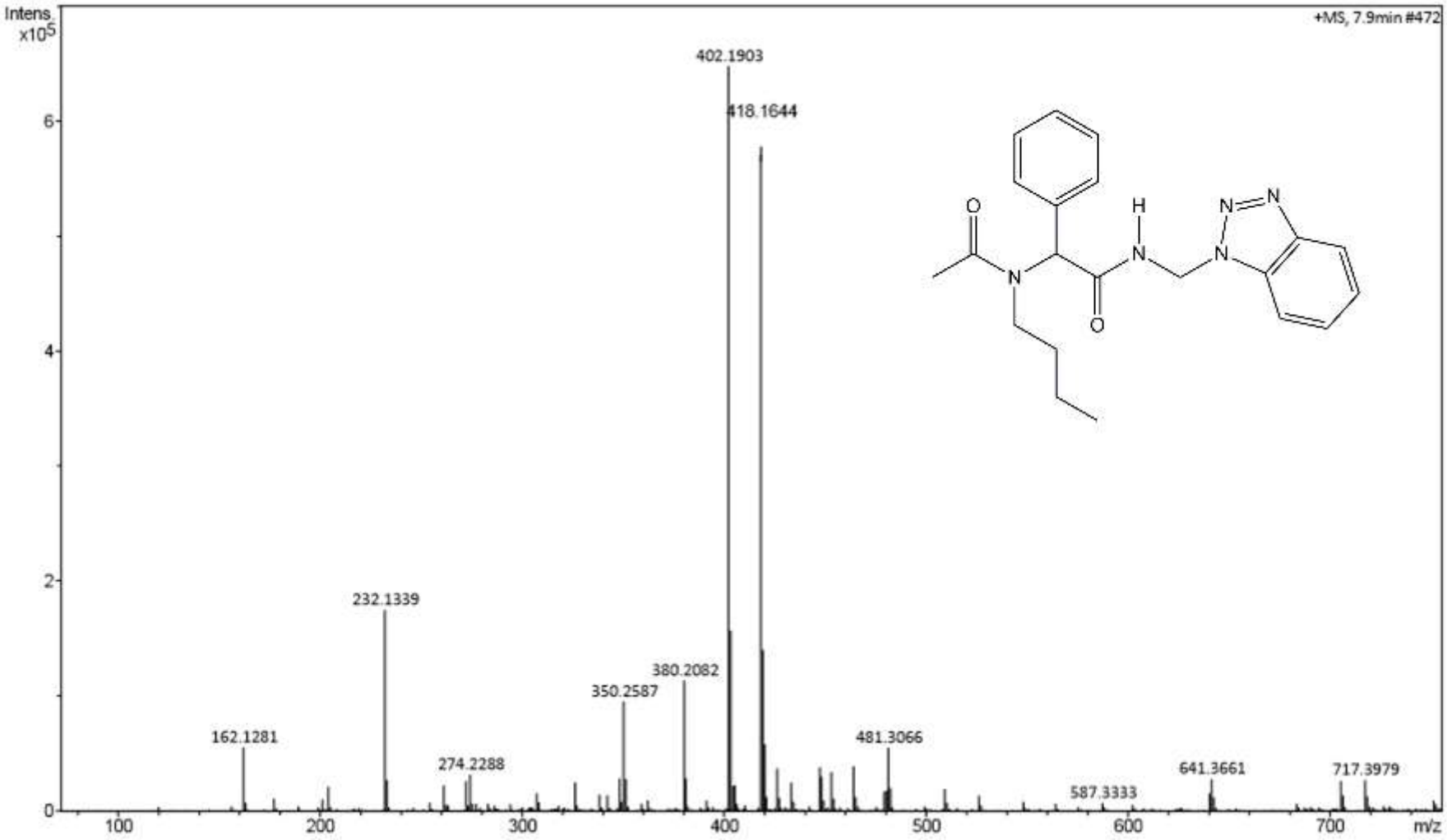
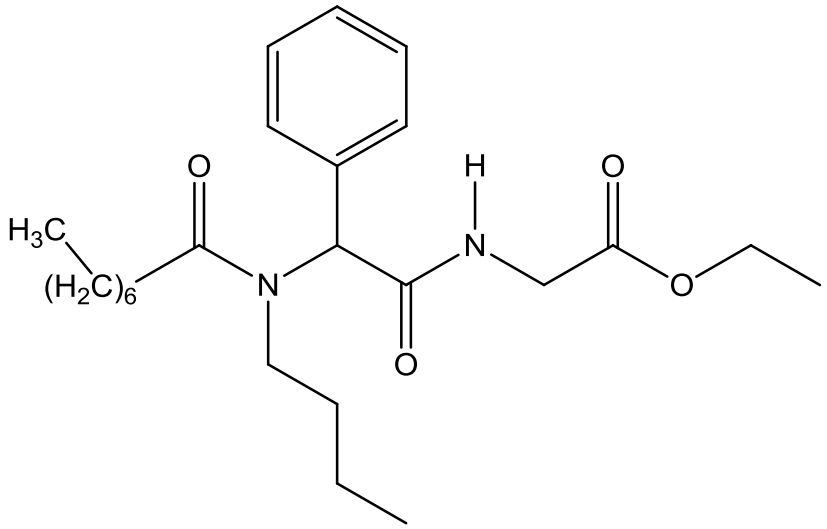


Figure S48. Mass spectrum of compound **5l**.

Compound **5m**



Ethyl 2-(2-(*N*-butyloctanamido)-2-phenylacetamido)acetate (**5m**)

Yellow oil, yield 55%; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37-7.35 (m, 5H), 6.63 (s, 1H), 5.91 (s, 1H), 4.22-4.15 (m, 2H), 4.08-4.02 (m, 2H), 3.31-3.24 (m, 2H), 2.40-2.34 (m, 2H), 1.31-1.28 (m, 14H), 0.90-0.86 (m, 6H), 0.74 (t, 3H, *J* 7.1 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 174.5 (C), 170.4 (C), 169.8 (C), 135.4 (C), 129.7 (CH), 128.8 (CH), 128.6 (CH), 63.0 (CH), 61.5 (CH_2), 47.2 (CH_2), 41.7 (CH_2), 34.0 (CH_2), 33.7 (CH_2), 31.8 (CH_2), 29.5 (CH_2), 29.2 (CH_2), 25.5 (CH_2), 24.9 (CH_2), 22.7 (CH_2), 20.2 (CH_3), 14.2 (CH_3), 13.6 (CH_3); FTIR (KBr) ν / cm^{-1} 3328 (N–H), 2959 (C–H), 1738 (C=O, ester), 1714 (C=O, amide), 1220 and 1029 (C–O, ester), 739 and 701 (=C–H, aromatic); HRMS (ESI+) *m/z*, calcd. for $C_{24}H_{38}N_2NaO_4$ $[M + Na]^+$: 441.2729, found: 441.2723.

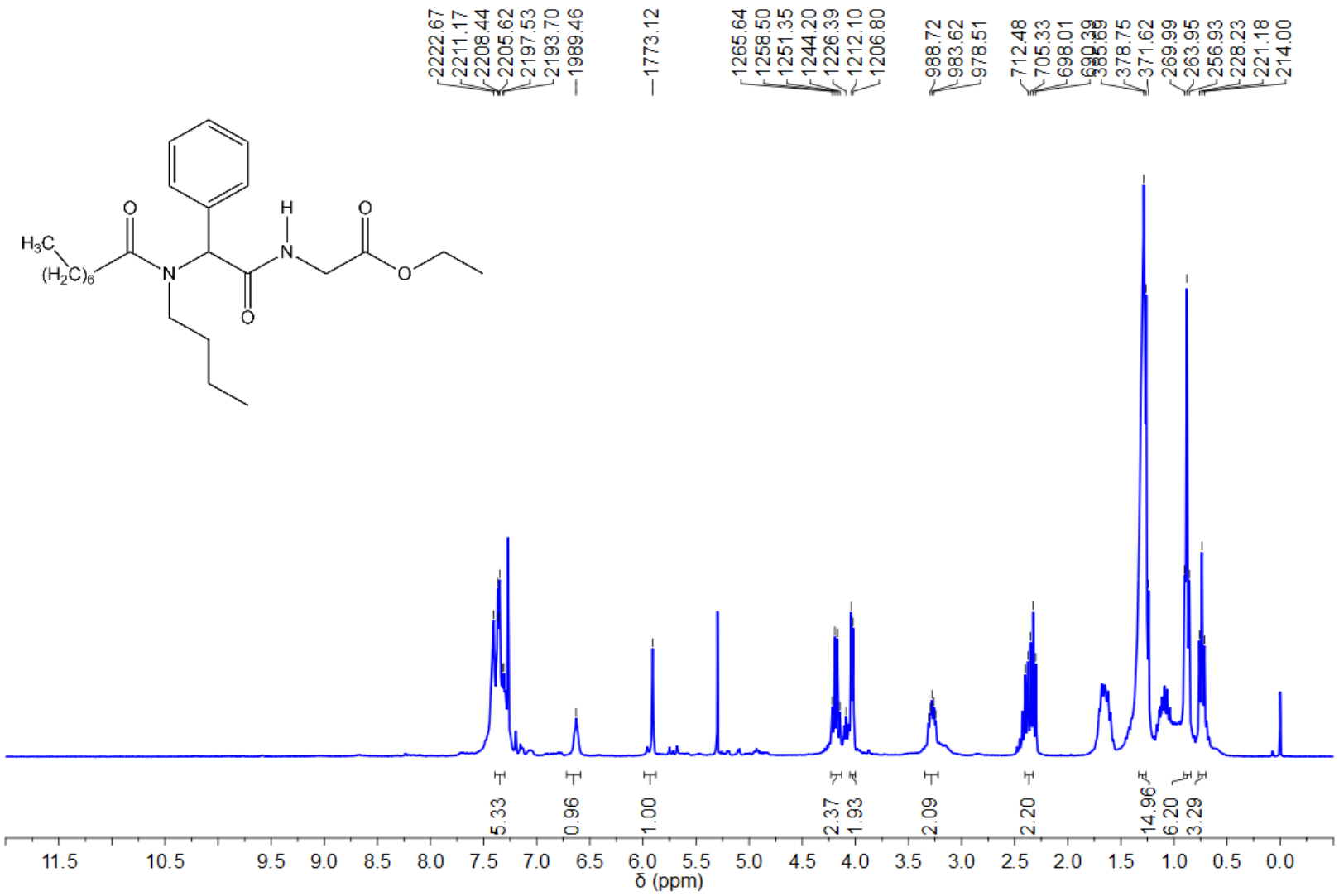


Figure S49. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **5m**.

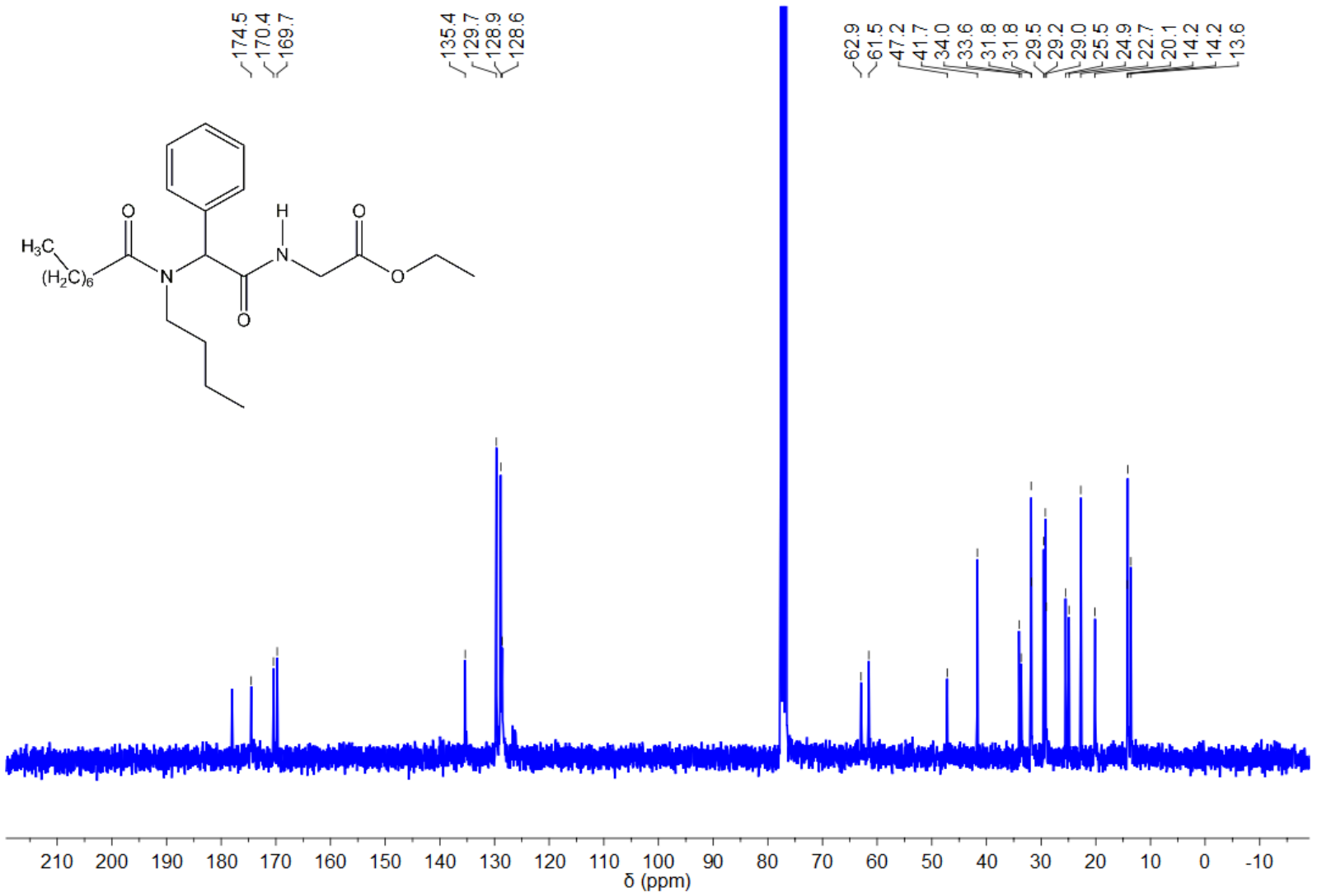


Figure S50. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **5m**.

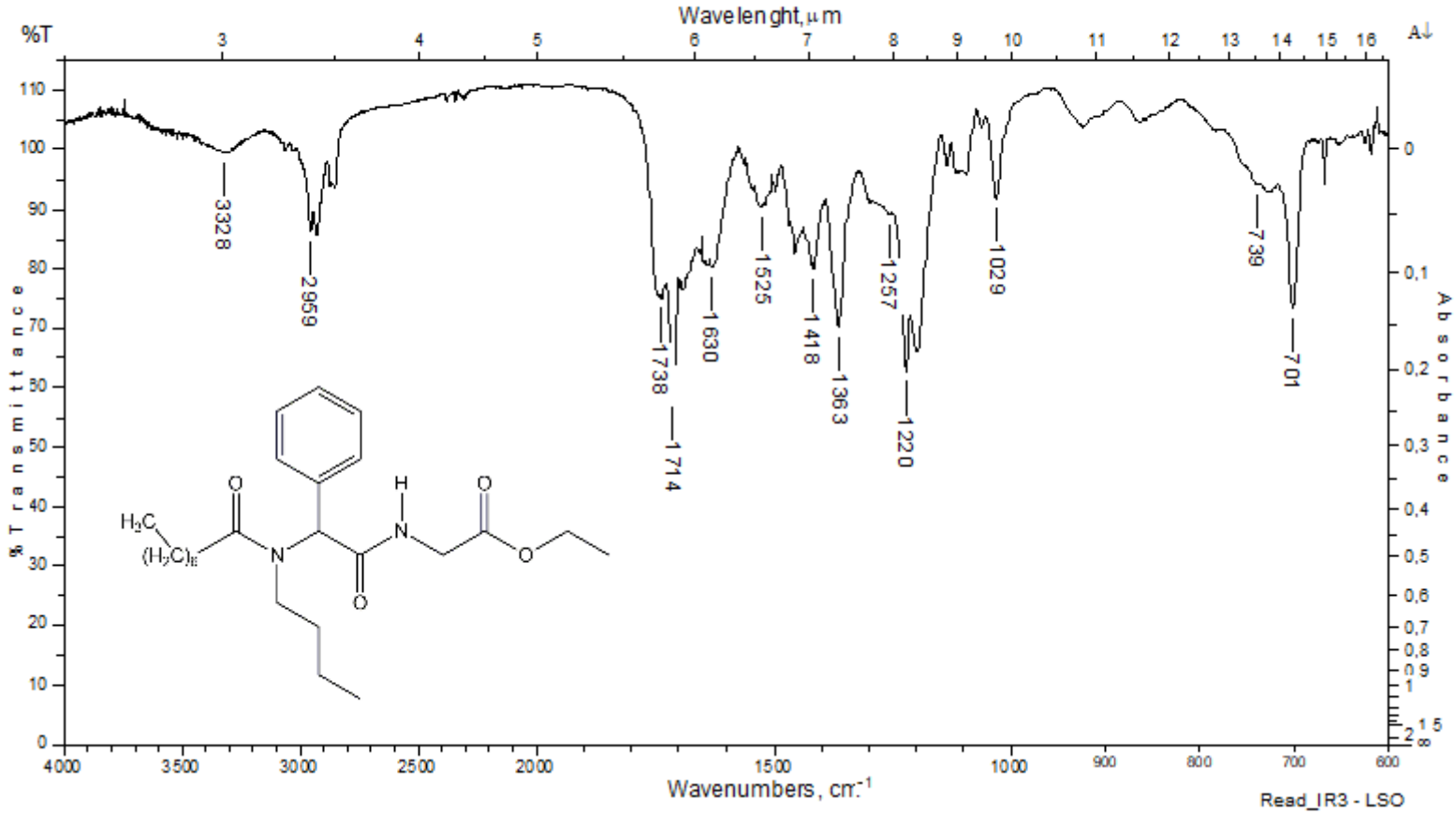


Figure S51. FTIR (KBr) spectrum of compound **5m**.

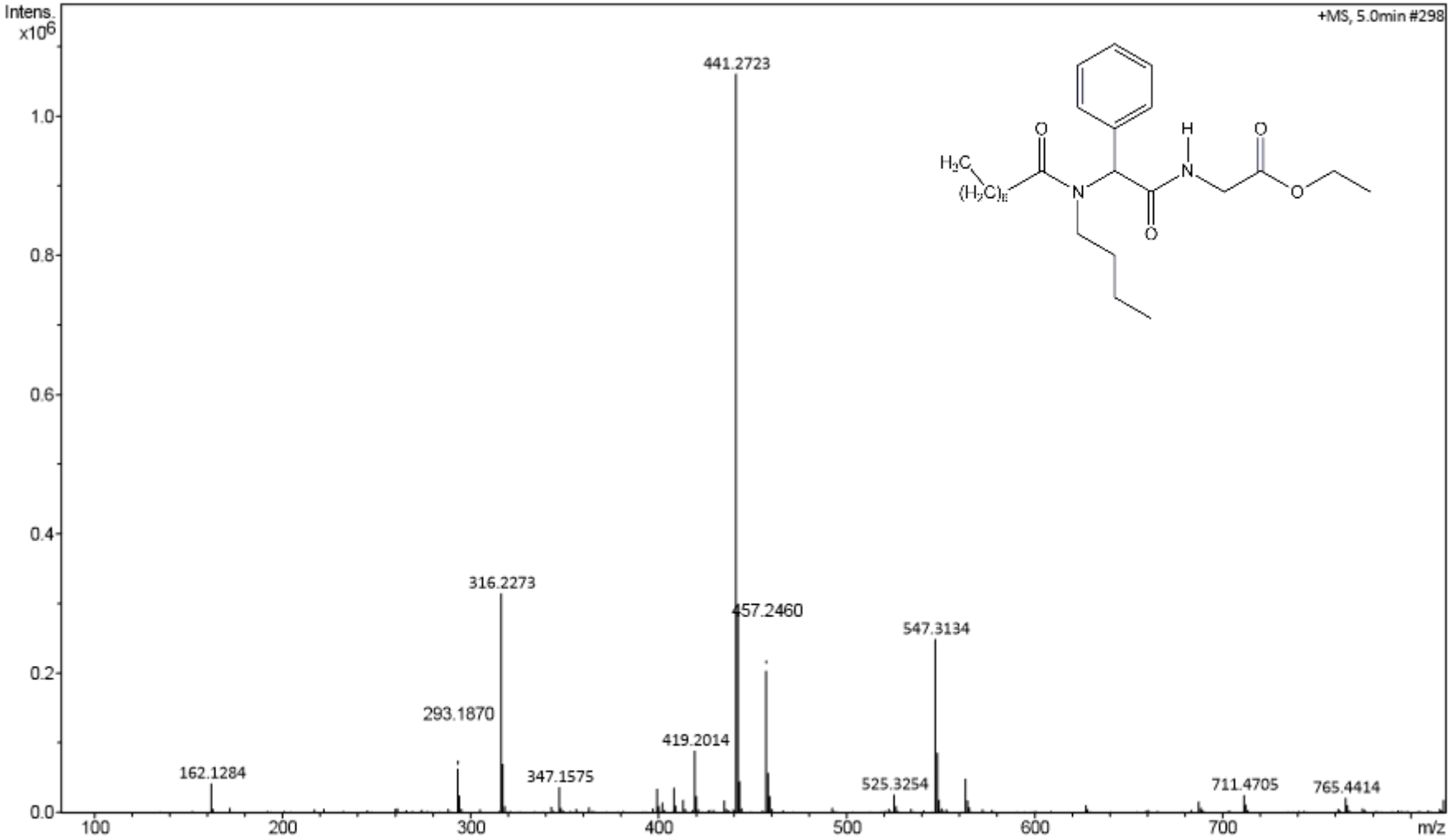


Figure S52. Mass spectrum of compound **5m**.

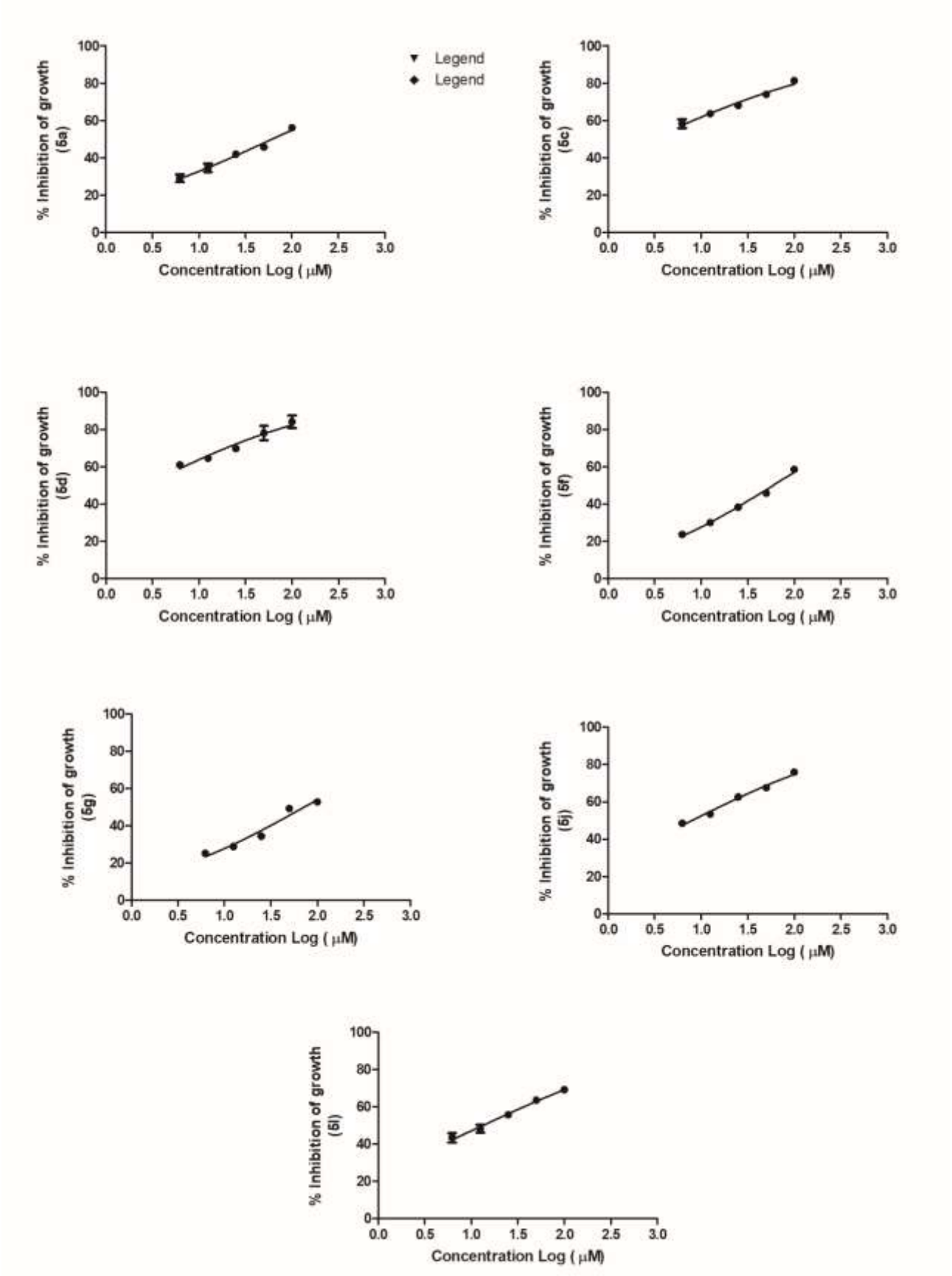


Figure S53. Curves used to calculate the IC_{50} values of compounds **5a**, **5c**, **5d**, **5f**, **5g**, **5j** and **5l**.