SI: Part - A

# Supporting Information

## Soluble Polymer Supported Divergent Synthesis of Tetracyclic Benzene-Fused Pyrazino/Diazepino Indoles: An Advanced Synthetic Approach to Bioactive Scaffolds

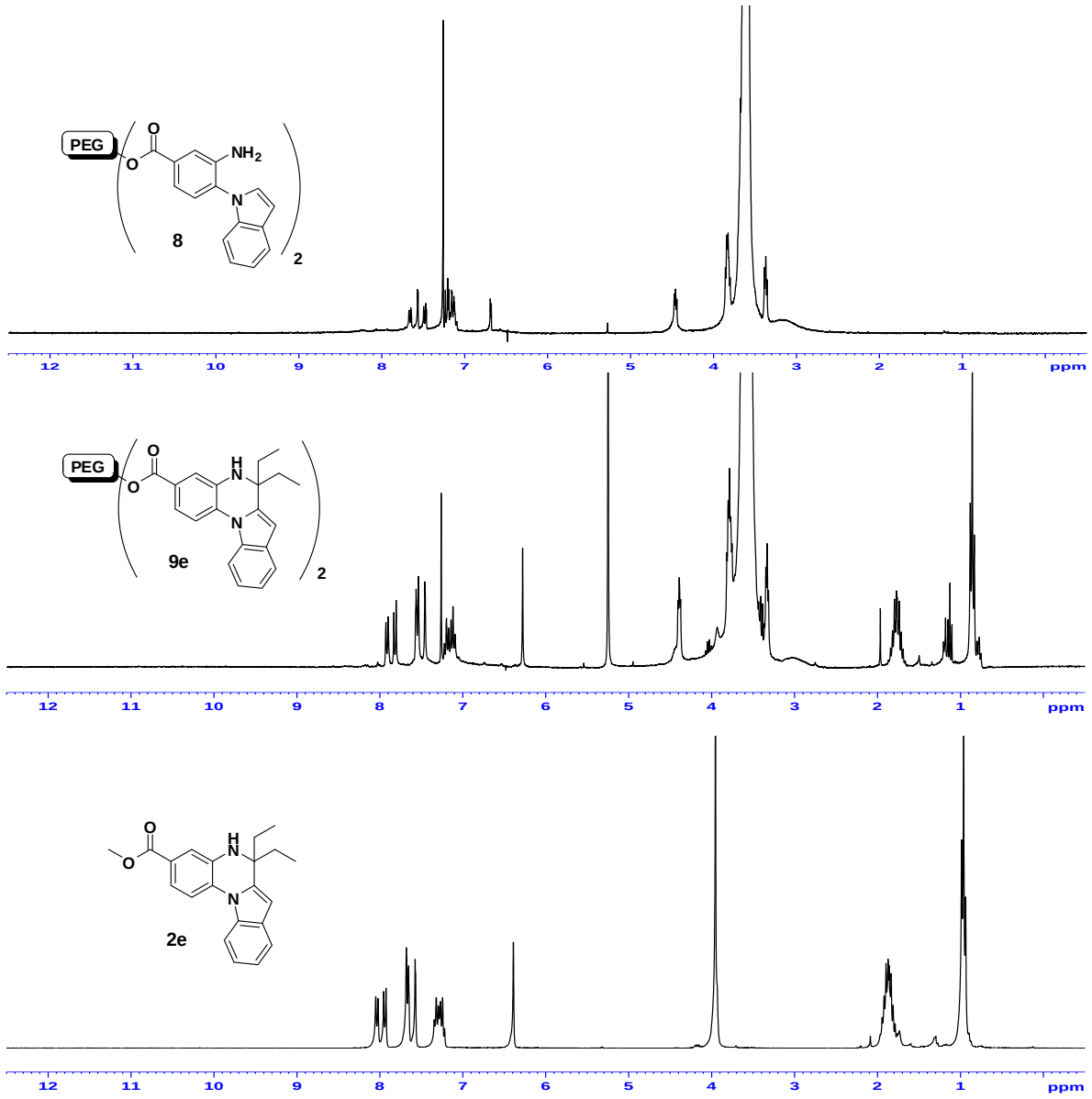
Po-Tsung Lin, Deepak B. Salunke, Li-Hsun Chen and Chung-Ming Sun*

*Department of Applied Chemistry, National Chiao Tung University, Hsinchu 300-10, Taiwan*

*E-mail: cmsun@mail.nctu.edu.tw*

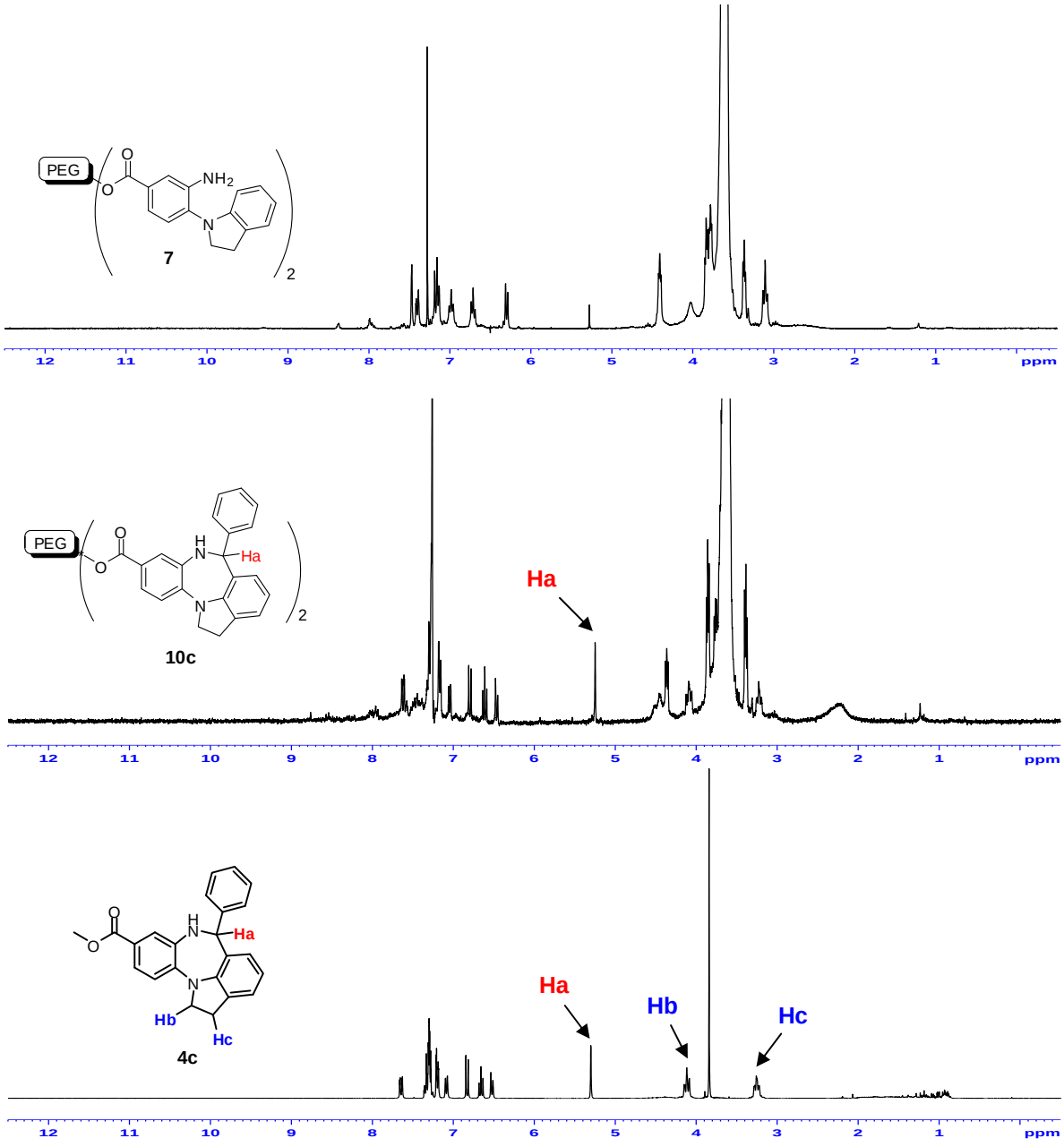
### Contents

## Stepwise $^{1}$H NMR Monitoring on a PEG Support




**SI Figure 1.** The stepwise proton NMR monitoring towards the synthesis of **2e** from **8**.

SI: Part - A




**SI Figure 2.** The stepwise proton NMR monitoring towards the synthesis of **4c** from **7**.

## X-ray crystallographic data (2a)

**SI Table 1.** Crystal data and structure refinement for **2a**.

| | | |
|---|---|---|
| Empirical formula | $C_{38}H_{36}N_4O_4$ | |
| Formula weight | 612.71 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 1 c 1 | |
| Unit cell dimensions | a = 10.1275(4) Å | $\alpha$ = 90° |
| | b = 19.1023(7) Å | $\beta$ = 106.1820(10)° |
| | c = 8.0831(3) Å | $\gamma$ = 90° |
| Volume | 1501.79(10) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.355 $Mg/m^3$ | |
| Absorption coefficient | 0.089 $mm^{-1}$ | |
| F(000) | 648 | |
| Crystal size | 0.25 x 0.25 x 0.15 $mm^3$ | |
| Theta range for data collection | 2.09 to 26.41° | |
| Index ranges | -12<=h<=11, -23<=k<=23, -6<=l<=10 | |
| Reflections collected | 13111 | |
| Independent reflections | 4539 [R(int) = 0.0173] | |
| Completeness to theta = 26.41° | 99.3% | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7454 and 0.7180 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4539 / 2 / 421 | |
| Goodness-of-fit on $F^2$ | 1.150 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0318, wR2 = 0.0912 | |
| R indices (all data) | R1 = 0.0344, wR2 = 0.1044 | |
| Absolute structure parameter | -0.2(8) | |
| Largest diff. peak and hole | 0.431 and -0.467 $e.Å^{-3}$ | |

**SI Table 2.** Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for **2a**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | 3878(2) | 980(1) | -2073(3) | 17(1) |
| C(2) | 2690(2) | 952(1) | -1312(3) | 15(1) |
| C(3) | 1499(2) | 582(1) | -1807(3) | 18(1) |
| C(4) | 697(2) | 757(1) | -673(3) | 18(1) |
| C(5) | -622(2) | 567(1) | -622(3) | 21(1) |
| C(6) | -1180(2) | 874(1) | 574(3) | 24(1) |
| C(7) | -435(2) | 1373(1) | 1726(3) | 23(1) |
| C(8) | 879(2) | 1566(1) | 1724(3) | 19(1) |
| C(9) | 1453(2) | 1253(1) | 530(3) | 15(1) |
| C(10) | 3815(2) | 1798(1) | 913(2) | 15(1) |
| C(11) | 4021(2) | 2096(1) | 2540(3) | 17(1) |
| C(12) | 5115(2) | 2547(1) | 3208(3) | 18(1) |
| C(13) | 6057(2) | 2680(1) | 2270(3) | 16(1) |
| C(14) | 5892(2) | 2363(1) | 681(3) | 16(1) |
| C(15) | 4762(2) | 1936(1) | -39(2) | 15(1) |
| C(16) | 4933(2) | 406(1) | -1298(3) | 23(1) |
| C(17) | 3378(2) | 900(1) | -4024(3) | 21(1) |
| C(18) | 7253(2) | 3151(1) | 2916(3) | 16(1) |
| C(19) | 8347(2) | 3962(1) | 5038(3) | 20(1) |
| C(20) | 1376(2) | 4075(1) | 11691(2) | 15(1) |
| C(21) | 2566(2) | 4110(1) | 10919(2) | 15(1) |
| C(22) | 3751(2) | 4481(1) | 11436(2) | 16(1) |
| C(23) | 4566(2) | 4296(1) | 10304(3) | 16(1) |
| C(24) | 5870(2) | 4510(1) | 10229(3) | 19(1) |
| C(25) | 6380(2) | 4250(1) | 8939(3) | 18(1) |
| C(26) | 5600(2) | 3790(1) | 7701(3) | 18(1) |
| C(27) | 4307(2) | 3567(1) | 7742(3) | 17(1) |
| C(28) | 3807(2) | 3812(1) | 9085(3) | 14(1) |
| C(29) | 1476(2) | 3232(1) | 8753(2) | 14(1) |
| C(30) | 1565(2) | 2704(1) | 7600(2) | 16(1) |
| C(31) | 442(2) | 2284(1) | 6865(3) | 15(1) |
| C(32) | -776(2) | 2370(1) | 7322(2) | 15(1) |

| | | | | |
|---|---|---|---|---|
| C(33) | -848(2) | 2879(1) | 8531(3) | 15(1) |
| C(34) | 253(2) | 3319(1) | 9237(2) | 15(1) |
| C(35) | 1713(2) | 3550(1) | 13186(3) | 23(1) |
| C(36) | 1099(2) | 4797(1) | 12337(3) | 21(1) |
| C(37) | -1987(2) | 1918(1) | 6609(3) | 16(1) |
| C(38) | -2892(2) | 1004(1) | 4675(3) | 23(1) |
| N(1) | 4505(2) | 1678(1) | -1709(2) | 17(1) |
| N(2) | 2702(2) | 1355(1) | 136(2) | 15(1) |
| N(3) | 136(2) | 3863(1) | 10335(2) | 16(1) |
| N(4) | 2574(2) | 3690(1) | 9505(2) | 14(1) |
| O(1) | 8171(2) | 3224(1) | 2243(2) | 23(1) |
| O(2) | 7219(1) | 3495(1) | 4355(2) | 20(1) |
| O(3) | -3033(1) | 1929(1) | 7046(2) | 21(1) |
| O(4) | -1792(1) | 1487(1) | 5384(2) | 20(1) |

**SI Table 3.** Bond lengths [Å] for **2a** (Symmetry transformations used to generate equivalent atoms).

| | | | | | |
|---|---|---|---|---|---|
| C(1)-N(1) | 1.471(2) | C(15)-N(1) | 1.392(2) | C(27)-C(28) | 1.400(3) |
| C(1)-C(2) | 1.497(3) | C(16)-H(16A) | 0.9800 | C(27)-H(27) | 0.9500 |
| C(1)-C(17) | 1.523(3) | C(16)-H(16B) | 0.9800 | C(28)-N(4) | 1.402(2) |
| C(1)-C(16) | 1.538(3) | C(16)-H(16C) | 0.9800 | C(29)-C(30) | 1.393(3) |
| C(2)-C(3) | 1.359(3) | C(17)-H(17A) | 0.9800 | C(29)-C(34) | 1.409(3) |
| C(2)-N(2) | 1.398(3) | C(17)-H(17B) | 0.9800 | C(29)-N(4) | 1.411(2) |
| C(3)-C(4) | 1.425(3) | C(17)-H(17C) | 0.9800 | C(30)-C(31) | 1.383(3) |
| C(3)-H(3) | 0.9500 | C(18)-O(1) | 1.208(2) | C(30)-H(30) | 0.9500 |
| C(4)-C(5) | 1.397(3) | C(18)-O(2) | 1.345(2) | C(31)-C(32) | 1.393(3) |
| C(4)-C(9) | 1.419(3) | C(19)-O(2) | 1.433(2) | C(31)-H(31) | 0.9500 |
| C(5)-C(6) | 1.379(3) | C(19)-H(19A) | 0.9800 | C(32)-C(33) | 1.395(3) |
| C(5)-H(5) | 0.9500 | C(19)-H(19B) | 0.9800 | C(32)-C(37) | 1.479(2) |
| C(6)-C(7) | 1.398(3) | C(19)-H(19C) | 0.9800 | C(33)-C(34) | 1.386(3) |
| C(6)-H(6) | 0.9500 | C(20)-N(3) | 1.474(2) | C(33)-H(33) | 0.9500 |
| C(7)-C(8) | 1.382(3) | C(20)-C(21) | 1.505(3) | C(34)-N(3) | 1.394(2) |
| C(7)-H(7) | 0.9500 | C(20)-C(36) | 1.528(3) | C(35)-H(35A) | 0.9800 |
| C(8)-C(9) | 1.393(3) | C(20)-C(35) | 1.534(3) | C(35)-H(35B) | 0.9800 |
| C(8)-H(8) | 0.9500 | C(21)-C(22) | 1.356(3) | C(35)-H(35C) | 0.9800 |
| C(9)-N(2) | 1.402(2) | C(21)-N(4) | 1.398(2) | C(36)-H(36A) | 0.9800 |
| C(10)-C(11) | 1.394(3) | C(22)-C(23) | 1.437(3) | C(36)-H(36B) | 0.9800 |
| C(10)-N(2) | 1.409(2) | C(22)-H(22) | 0.9500 | C(36)-H(36C) | 0.9800 |
| C(10)-C(15) | 1.412(3) | C(23)-C(24) | 1.401(3) | C(37)-O(3) | 1.207(2) |
| C(11)-C(12) | 1.389(3) | C(23)-C(28) | 1.412(3) | C(37)-O(4) | 1.344(2) |
| C(11)-H(11) | 0.9500 | C(24)-C(25) | 1.378(3) | C(38)-O(4) | 1.437(2) |
| C(12)-C(13) | 1.397(3) | C(24)-H(24) | 0.9500 | C(38)-H(38A) | 0.9800 |
| C(12)-H(12) | 0.9500 | C(25)-C(26) | 1.400(3) | C(38)-H(38B) | 0.9800 |
| C(13)-C(14) | 1.387(3) | C(25)-H(25) | 0.9500 | C(38)-H(38C) | 0.9800 |
| C(13)-C(18) | 1.483(3) | C(26)-C(27) | 1.386(3) | N(1)-H(1) | 0.8800 |
| C(14)-C(15) | 1.394(3) | C(26)-H(26) | 0.9500 | N(3)-H(3A) | 0.8800 |
| C(14)-H(14) | 0.9500 | | | | |

**SI Table 4.** Bond angles [°] for **2a** (Symmetry transformations used to generate equivalent atoms).

| | | | |
|---|---|---|---|
| N(1)-C(1)-C(2) | 107.57(15) | C(12)-C(11)-H(11) | 119.6 |
| N(1)-C(1)-C(17) | 107.38(16) | C(10)-C(11)-H(11) | 119.6 |
| C(2)-C(1)-C(17) | 110.41(16) | C(11)-C(12)-C(13) | 119.53(18) |
| N(1)-C(1)-C(16) | 110.64(16) | C(11)-C(12)-H(12) | 120.2 |
| C(2)-C(1)-C(16) | 110.69(15) | C(13)-C(12)-H(12) | 120.2 |
| C(17)-C(1)-C(16) | 110.07(16) | C(14)-C(13)-C(12) | 119.96(17) |
| C(3)-C(2)-N(2) | 109.47(17) | C(14)-C(13)-C(18) | 117.79(17) |
| C(3)-C(2)-C(1) | 130.25(18) | C(12)-C(13)-C(18) | 122.25(18) |
| N(2)-C(2)-C(1) | 120.28(16) | C(13)-C(14)-C(15) | 120.97(18) |
| C(2)-C(3)-C(4) | 107.83(18) | C(13)-C(14)-H(14) | 119.5 |
| C(2)-C(3)-H(3) | 126.1 | C(15)-C(14)-H(14) | 119.5 |
| C(4)-C(3)-H(3) | 126.1 | N(1)-C(15)-C(14) | 121.45(17) |
| C(5)-C(4)-C(9) | 119.45(19) | N(1)-C(15)-C(10) | 119.42(16) |
| C(5)-C(4)-C(3) | 132.82(19) | C(14)-C(15)-C(10) | 119.01(17) |
| C(9)-C(4)-C(3) | 107.62(17) | C(1)-C(16)-H(16A) | 109.5 |
| C(6)-C(5)-C(4) | 119.46(19) | C(1)-C(16)-H(16B) | 109.5 |
| C(6)-C(5)-H(5) | 120.3 | H(16A)-C(16)-H(16B) | 109.5 |
| C(4)-C(5)-H(5) | 120.3 | C(1)-C(16)-H(16C) | 109.5 |
| C(5)-C(6)-C(7) | 120.46(19) | H(16A)-C(16)-H(16C) | 109.5 |
| C(5)-C(6)-H(6) | 119.8 | H(16B)-C(16)-H(16C) | 109.5 |
| C(7)-C(6)-H(6) | 119.8 | C(1)-C(17)-H(17A) | 109.5 |
| C(8)-C(7)-C(6) | 121.5(2) | C(1)-C(17)-H(17B) | 109.5 |
| C(8)-C(7)-H(7) | 119.3 | H(17A)-C(17)-H(17B) | 109.5 |
| C(6)-C(7)-H(7) | 119.3 | C(1)-C(17)-H(17C) | 109.5 |
| C(7)-C(8)-C(9) | 118.32(19) | H(17A)-C(17)-H(17C) | 109.5 |
| C(7)-C(8)-H(8) | 120.8 | H(17B)-C(17)-H(17C) | 109.5 |
| C(9)-C(8)-H(8) | 120.8 | O(1)-C(18)-O(2) | 122.82(17) |
| C(8)-C(9)-N(2) | 132.49(18) | O(1)-C(18)-C(13) | 124.52(18) |
| C(8)-C(9)-C(4) | 120.79(17) | O(2)-C(18)-C(13) | 112.66(16) |
| N(2)-C(9)-C(4) | 106.59(17) | O(2)-C(19)-H(19A) | 109.5 |
| C(11)-C(10)-N(2) | 123.79(17) | O(2)-C(19)-H(19B) | 109.5 |
| C(11)-C(10)-C(15) | 119.52(16) | H(19A)-C(19)-H(19B) | 109.5 |
| N(2)-C(10)-C(15) | 116.69(17) | O(2)-C(19)-H(19C) | 109.5 |
| C(12)-C(11)-C(10) | 120.89(18) | H(19A)-C(19)-H(19C) | 109.5 |

Continued…

| | | | |
|---|---|---|---|
| H(19B)-C(19)-H(19C) | 109.5 | C(29)-C(30)-H(30) | 119.7 |
| N(3)-C(20)-C(21) | 108.56(15) | C(30)-C(31)-C(32) | 120.03(17) |
| N(3)-C(20)-C(36) | 107.59(15) | C(30)-C(31)-H(31) | 120.0 |
| C(21)-C(20)-C(36) | 110.28(16) | C(32)-C(31)-H(31) | 120.0 |
| N(3)-C(20)-C(35) | 111.26(16) | C(31)-C(32)-C(33) | 119.43(17) |
| C(21)-C(20)-C(35) | 109.09(16) | C(31)-C(32)-C(37) | 121.82(17) |
| C(36)-C(20)-C(35) | 110.02(17) | C(33)-C(32)-C(37) | 118.71(17) |
| C(22)-C(21)-N(4) | 110.23(17) | C(34)-C(33)-C(32) | 121.16(17) |
| C(22)-C(21)-C(20) | 129.60(17) | C(34)-C(33)-H(33) | 119.4 |
| N(4)-C(21)-C(20) | 120.09(16) | C(32)-C(33)-H(33) | 119.4 |
| C(21)-C(22)-C(23) | 106.92(16) | C(33)-C(34)-N(3) | 120.86(17) |
| C(21)-C(22)-H(22) | 126.5 | C(33)-C(34)-C(29) | 118.95(16) |
| C(23)-C(22)-H(22) | 126.5 | N(3)-C(34)-C(29) | 120.09(16) |
| C(24)-C(23)-C(28) | 119.87(18) | C(20)-C(35)-H(35A) | 109.5 |
| C(24)-C(23)-C(22) | 132.19(18) | C(20)-C(35)-H(35B) | 109.5 |
| C(28)-C(23)-C(22) | 107.94(16) | H(35A)-C(35)-H(35B) | 109.5 |
| C(25)-C(24)-C(23) | 118.95(18) | C(20)-C(35)-H(35C) | 109.5 |
| C(25)-C(24)-H(24) | 120.5 | H(35A)-C(35)-H(35C) | 109.5 |
| C(23)-C(24)-H(24) | 120.5 | H(35B)-C(35)-H(35C) | 109.5 |
| C(24)-C(25)-C(26) | 120.77(18) | C(20)-C(36)-H(36A) | 109.5 |
| C(24)-C(25)-H(25) | 119.6 | C(20)-C(36)-H(36B) | 109.5 |
| C(26)-C(25)-H(25) | 119.6 | H(36A)-C(36)-H(36B) | 109.5 |
| C(27)-C(26)-C(25) | 121.62(19) | C(20)-C(36)-H(36C) | 109.5 |
| C(27)-C(26)-H(26) | 119.2 | H(36A)-C(36)-H(36C) | 109.5 |
| C(25)-C(26)-H(26) | 119.2 | H(36B)-C(36)-H(36C) | 109.5 |
| C(26)-C(27)-C(28) | 117.71(18) | O(3)-C(37)-O(4) | 123.25(18) |
| C(26)-C(27)-H(27) | 121.1 | O(3)-C(37)-C(32) | 125.11(18) |
| C(28)-C(27)-H(27) | 121.1 | O(4)-C(37)-C(32) | 111.64(16) |
| C(27)-C(28)-N(4) | 132.21(18) | O(4)-C(38)-H(38A) | 109.5 |
| C(27)-C(28)-C(23) | 120.99(18) | O(4)-C(38)-H(38B) | 109.5 |
| N(4)-C(28)-C(23) | 106.75(16) | H(38A)-C(38)-H(38B) | 109.5 |
| C(30)-C(29)-C(34) | 119.72(17) | O(4)-C(38)-H(38C) | 109.5 |
| C(30)-C(29)-N(4) | 123.15(17) | H(38A)-C(38)-H(38C) | 109.5 |
| C(34)-C(29)-N(4) | 117.12(16) | H(38B)-C(38)-H(38C) | 109.5 |
| C(31)-C(30)-C(29) | 120.62(17) | C(15)-N(1)-C(1) | 117.91(16) |
| C(31)-C(30)-H(30) | 119.7 | C(15)-N(1)-H(1) | 121.0 |

Continued…

| | | | |
|---|---|---|---|
| C(1)-N(1)-H(1) | 121.0 | C(20)-N(3)-H(3A) | 120.9 |
| C(2)-N(2)-C(9) | 108.44(15) | C(21)-N(4)-C(28) | 108.12(15) |
| C(2)-N(2)-C(10) | 121.54(16) | C(21)-N(4)-C(29) | 121.61(16) |
| C(9)-N(2)-C(10) | 129.96(16) | C(28)-N(4)-C(29) | 130.26(16) |
| C(34)-N(3)-C(20) | 118.16(15) | C(18)-O(2)-C(19) | 115.29(15) |
| C(34)-N(3)-H(3A) | 120.9 | C(37)-O(4)-C(38) | 115.47(16) |

**SI Table 5.** Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+...+2hka^*b^*U^{12}]$.

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 16(1) | 17(1) | 19(1) | 0(1) | 6(1) | 0(1) |
| C(2) | 16(1) | 13(1) | 16(1) | 2(1) | 5(1) | 3(1) |
| C(3) | 18(1) | 18(1) | 18(1) | 0(1) | 5(1) | 0(1) |
| C(4) | 16(1) | 18(1) | 18(1) | 3(1) | 4(1) | -1(1) |
| C(5) | 16(1) | 24(1) | 22(1) | 2(1) | 3(1) | -5(1) |
| C(6) | 14(1) | 32(1) | 25(1) | 4(1) | 6(1) | -5(1) |
| C(7) | 17(1) | 31(1) | 22(1) | 2(1) | 8(1) | 1(1) |
| C(8) | 17(1) | 21(1) | 21(1) | 0(1) | 6(1) | -2(1) |
| C(9) | 12(1) | 16(1) | 17(1) | 6(1) | 3(1) | 0(1) |
| C(10) | 12(1) | 14(1) | 18(1) | 3(1) | 2(1) | 1(1) |
| C(11) | 13(1) | 22(1) | 17(1) | 3(1) | 7(1) | 0(1) |
| C(12) | 18(1) | 20(1) | 14(1) | -1(1) | 5(1) | 1(1) |
| C(13) | 14(1) | 16(1) | 17(1) | 3(1) | 4(1) | 1(1) |
| C(14) | 14(1) | 17(1) | 18(1) | 2(1) | 6(1) | 0(1) |
| C(15) | 17(1) | 15(1) | 15(1) | 2(1) | 5(1) | 3(1) |
| C(16) | 21(1) | 20(1) | 29(1) | 4(1) | 10(1) | 4(1) |
| C(17) | 22(1) | 24(1) | 20(1) | -3(1) | 10(1) | -3(1) |
| C(18) | 15(1) | 16(1) | 17(1) | 4(1) | 4(1) | 2(1) |
| C(19) | 19(1) | 19(1) | 22(1) | -3(1) | 5(1) | -4(1) |
| C(20) | 15(1) | 19(1) | 11(1) | -2(1) | 3(1) | 0(1) |
| C(21) | 17(1) | 14(1) | 13(1) | 0(1) | 3(1) | 2(1) |
| C(22) | 16(1) | 17(1) | 16(1) | -2(1) | 4(1) | -1(1) |
| C(23) | 15(1) | 15(1) | 16(1) | 2(1) | 3(1) | 0(1) |
| C(24) | 17(1) | 18(1) | 21(1) | 1(1) | 4(1) | -2(1) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(25) | 13(1) | 19(1) | 21(1) | 3(1) | 4(1) | -1(1) |
| C(26) | 18(1) | 19(1) | 19(1) | 1(1) | 9(1) | 1(1) |
| C(27) | 18(1) | 18(1) | 14(1) | 0(1) | 3(1) | -1(1) |
| C(28) | 13(1) | 14(1) | 16(1) | 3(1) | 5(1) | 1(1) |
| C(29) | 13(1) | 14(1) | 13(1) | 3(1) | 2(1) | 0(1) |
| C(30) | 14(1) | 17(1) | 18(1) | 2(1) | 5(1) | 2(1) |
| C(31) | 17(1) | 14(1) | 15(1) | 0(1) | 5(1) | 2(1) |
| C(32) | 14(1) | 16(1) | 14(1) | 3(1) | 2(1) | 0(1) |
| C(33) | 14(1) | 17(1) | 17(1) | 2(1) | 6(1) | 0(1) |
| C(34) | 15(1) | 16(1) | 12(1) | 1(1) | 4(1) | 2(1) |
| C(35) | 21(1) | 29(1) | 21(1) | 6(1) | 8(1) | 1(1) |
| C(36) | 20(1) | 22(1) | 23(1) | -8(1) | 7(1) | 0(1) |
| C(37) | 16(1) | 17(1) | 16(1) | 2(1) | 4(1) | 1(1) |
| C(38) | 19(1) | 20(1) | 29(1) | -6(1) | 4(1) | -6(1) |
| N(1) | 20(1) | 16(1) | 15(1) | 1(1) | 8(1) | -3(1) |
| N(2) | 13(1) | 17(1) | 15(1) | 1(1) | 5(1) | 0(1) |
| N(3) | 13(1) | 18(1) | 16(1) | -5(1) | 4(1) | 1(1) |
| N(4) | 14(1) | 15(1) | 14(1) | 0(1) | 5(1) | 0(1) |
| O(1) | 19(1) | 28(1) | 23(1) | -3(1) | 8(1) | -5(1) |
| O(2) | 16(1) | 23(1) | 20(1) | -5(1) | 6(1) | -5(1) |
| O(3) | 15(1) | 28(1) | 22(1) | -5(1) | 8(1) | -5(1) |
| O(4) | 16(1) | 20(1) | 23(1) | -8(1) | 6(1) | -5(1) |

**SI Table 6.** Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for **2a**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3) | 1247 | 262 | -2743 | 22 |
| H(5) | -1132 | 228 | -1405 | 26 |
| H(6) | -2076 | 745 | 616 | 29 |
| H(7) | -843 | 1584 | 2529 | 27 |
| H(8) | 1378 | 1904 | 2518 | 23 |
| H(11) | 3405 | 1988 | 3200 | 20 |
| H(12) | 5223 | 2763 | 4296 | 21 |
| H(14) | 6560 | 2439 | 74 | 19 |
| H(16A) | 5729 | 453 | -1754 | 34 |
| H(16B) | 4510 | -55 | -1603 | 34 |
| H(16C) | 5231 | 455 | -41 | 34 |

| | | | | |
|---|---|---|---|---|
| H(17A) | 2689 | 1261 | -4503 | 32 |
| H(17B) | 2967 | 436 | -4312 | 32 |
| H(17C) | 4157 | 953 | -4511 | 32 |
| H(19A) | 9212 | 3700 | 5297 | 30 |
| H(19B) | 8246 | 4178 | 6096 | 30 |
| H(19C) | 8353 | 4327 | 4189 | 30 |
| H(22) | 3996 | 4802 | 12368 | 20 |
| H(24) | 6396 | 4830 | 11054 | 22 |
| H(25) | 7271 | 4385 | 8891 | 21 |
| H(26) | 5966 | 3626 | 6810 | 21 |
| H(27) | 3779 | 3259 | 6888 | 20 |
| H(30) | 2404 | 2632 | 7316 | 19 |
| H(31) | 502 | 1937 | 6048 | 18 |
| H(33) | -1667 | 2925 | 8877 | 18 |
| H(35A) | 921 | 3505 | 13650 | 35 |
| H(35B) | 2510 | 3717 | 14094 | 35 |
| H(35C) | 1925 | 3094 | 12770 | 35 |
| H(36A) | 979 | 5139 | 11402 | 32 |
| H(36B) | 1879 | 4936 | 13303 | 32 |
| H(36C) | 263 | 4779 | 12719 | 32 |
| H(38A) | -3027 | 701 | 5592 | 35 |
| H(38B) | -2660 | 717 | 3790 | 35 |
| H(38C) | -3740 | 1265 | 4157 | 35 |
| H(1) | 4711 | 1925 | -2522 | 20 |
| H(3A) | -656 | 4075 | 10223 | 19 |

## X-ray crystallographic data (4k)

**SI Table 7.** Crystal data and structure refinement for **4k**.

| | | |
|---|---|---|
| Empirical formula | $C_{23}H_{19}N_3O_4$ | |
| Formula weight | 401.41 | |
| Temperature | 100(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Triclinic | |
| Space group | P 1 | |
| Unit cell dimensions | a = 6.7967(2) Å | $\alpha$ = 69.5460(10)° |
| | b = 12.1325(3) Å | $\beta$ = 81.7740(10)° |
| | c = 12.4682(3) Å | $\gamma$ = 85.6650(10)° |
| Volume | 953.04(4) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.399 $Mg/m^3$ | |
| Absorption coefficient | 0.098 $mm^{-1}$ | |
| F(000) | 420 | |
| Crystal size | 0.15 x 0.12 x 0.10 $mm^3$ | |
| Theta range for data collection | 1.76 to 26.43° | |
| Index ranges | -8<=h<=8, -14<=k<=15, -13<=l<=15 | |
| Reflections collected | 15954 | |
| Independent reflections | 3916 [R(int) = 0.0219] | |
| Completeness to theta = 26.43° | 99.6 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7454 and 0.7211 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 3916 / 0 / 272 | |
| Goodness-of-fit on $F^2$ | 1.055 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0440, wR2 = 0.1376 | |
| R indices (all data) | R1 = 0.0547, wR2 = 0.1587 | |
| Largest diff. peak and hole | 0.503 and -0.622 $e.Å^{-3}$ | |

**SI Table 8.** Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2 x\ 10^3$) for **4k**. U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| C(1) | 2217(2) | 6877(1) | 2358(1) | 34(1) |
| C(2) | 1895(2) | 5583(1) | 2681(1) | 34(1) |
| C(3) | 167(3) | 5107(2) | 3393(2) | 44(1) |
| C(4) | -290(3) | 3938(2) | 3693(2) | 52(1) |
| C(5) | 988(3) | 3199(2) | 3276(2) | 47(1) |
| C(6) | 2728(3) | 3636(1) | 2587(1) | 37(1) |
| C(7) | 4332(3) | 3017(2) | 2043(2) | 45(1) |
| C(8) | 5965(3) | 3918(2) | 1539(2) | 42(1) |
| C(9) | 6097(2) | 6073(1) | 1090(1) | 32(1) |
| C(10) | 8127(2) | 6000(2) | 701(2) | 39(1) |
| C(11) | 9219(2) | 6986(2) | 83(2) | 40(1) |
| C(12) | 8330(2) | 8101(2) | -152(1) | 36(1) |
| C(13) | 6347(2) | 8191(1) | 278(1) | 34(1) |
| C(14) | 5203(2) | 7216(1) | 882(1) | 31(1) |
| C(15) | 3191(2) | 4822(1) | 2286(1) | 33(1) |
| C(16) | 3264(2) | 7179(1) | 3217(1) | 34(1) |
| C(17) | 4826(3) | 6496(2) | 3748(2) | 43(1) |
| C(18) | 5744(3) | 6802(2) | 4524(2) | 49(1) |
| C(19) | 5109(3) | 7788(2) | 4801(2) | 46(1) |
| C(20) | 3562(3) | 8451(2) | 4273(2) | 42(1) |
| C(21) | 2645(3) | 8180(1) | 3481(1) | 39(1) |
| C(22) | 9400(3) | 9190(2) | -849(1) | 38(1) |
| C(23) | 12409(3) | 9970(2) | -1962(2) | 56(1) |
| N(1) | 3160(2) | 7389(1) | 1162(1) | 34(1) |
| N(2) | 5042(2) | 5044(1) | 1598(1) | 36(1) |
| N(3) | 2809(3) | 9476(2) | 4586(2) | 64(1) |
| O(1) | 3048(3) | 9488(2) | 5531(2) | 90(1) |
| O(2) | 2003(4) | 10267(2) | 3886(2) | 112(1) |
| O(3) | 8687(2) | 10171(1) | -1034(1) | 51(1) |
| O(4) | 11255(2) | 8968(1) | -1257(1) | 50(1) |

**SI Table 9.** Bond lengths [Å] for **4k** (Symmetry transformations used to generate equivalent atoms).

| | | | |
|---|---|---|---|
| C(1)-N(1) | 1.470(2) | C(12)-C(13) | 1.388(2) |
| C(1)-C(2) | 1.503(2) | C(12)-C(22) | 1.480(2) |
| C(1)-C(16) | 1.523(2) | C(13)-C(14) | 1.386(2) |
| C(1)-H(1) | 1.0000 | C(13)-H(13) | 0.9500 |
| C(2)-C(15) | 1.393(2) | C(14)-N(1) | 1.400(2) |
| C(2)-C(3) | 1.395(2) | C(15)-N(2) | 1.404(2) |
| C(3)-C(4) | 1.382(3) | C(16)-C(21) | 1.388(2) |
| C(3)-H(3) | 0.9500 | C(16)-C(17) | 1.391(2) |
| C(4)-C(5) | 1.381(3) | C(17)-C(18) | 1.387(2) |
| C(4)-H(4) | 0.9500 | C(17)-H(17) | 0.9500 |
| C(5)-C(6) | 1.379(3) | C(18)-C(19) | 1.380(3) |
| C(5)-H(5) | 0.9500 | C(18)-H(18) | 0.9500 |
| C(6)-C(15) | 1.403(2) | C(19)-C(20) | 1.374(3) |
| C(6)-C(7) | 1.494(2) | C(19)-H(19) | 0.9500 |
| C(7)-C(8) | 1.525(3) | C(20)-C(21) | 1.380(2) |
| C(7)-H(7A) | 0.9900 | C(20)-N(3) | 1.464(2) |
| C(7)-H(7B) | 0.9900 | C(21)-H(21) | 0.9500 |
| C(8)-N(2) | 1.481(2) | C(22)-O(3) | 1.208(2) |
| C(8)-H(8A) | 0.9900 | C(22)-O(4) | 1.334(2) |
| C(8)-H(8B) | 0.9900 | C(23)-O(4) | 1.437(2) |
| C(9)-N(2) | 1.389(2) | C(23)-H(23A) | 0.9800 |
| C(9)-C(10) | 1.402(2) | C(23)-H(23B) | 0.9800 |
| C(9)-C(14) | 1.423(2) | C(23)-H(23C) | 0.9800 |
| C(10)-C(11) | 1.380(2) | N(1)-H(1A) | 0.8800 |
| C(10)-H(10) | 0.9500 | N(3)-O(2) | 1.207(3) |
| C(11)-C(12) | 1.389(2) | N(3)-O(1) | 1.216(3) |
| C(11)-H(11) | 0.9500 | | |

**SI Table 10.** Bond angles [°] for **4k** (Symmetry transformations used to generate equivalent atoms).

| | | | |
|---|---|---|---|
| N(1)-C(1)-C(2) | 111.64(12) | N(2)-C(9)-C(14) | 123.34(14) |
| N(1)-C(1)-C(16) | 112.97(13) | C(10)-C(9)-C(14) | 117.59(14) |
| C(2)-C(1)-C(16) | 113.63(13) | C(11)-C(10)-C(9) | 122.10(15) |
| N(1)-C(1)-H(1) | 106.0 | C(11)-C(10)-H(10) | 119.0 |
| C(2)-C(1)-H(1) | 106.0 | C(9)-C(10)-H(10) | 119.0 |
| C(16)-C(1)-H(1) | 106.0 | C(10)-C(11)-C(12) | 120.26(15) |
| C(15)-C(2)-C(3) | 117.20(16) | C(10)-C(11)-H(11) | 119.9 |
| C(15)-C(2)-C(1) | 124.10(14) | C(12)-C(11)-H(11) | 119.9 |
| C(3)-C(2)-C(1) | 118.67(15) | C(13)-C(12)-C(11) | 118.31(15) |
| C(4)-C(3)-C(2) | 122.51(18) | C(13)-C(12)-C(22) | 118.89(15) |
| C(4)-C(3)-H(3) | 118.7 | C(11)-C(12)-C(22) | 122.80(15) |
| C(2)-C(3)-H(3) | 118.7 | C(14)-C(13)-C(12) | 122.72(15) |
| C(5)-C(4)-C(3) | 119.72(17) | C(14)-C(13)-H(13) | 118.6 |
| C(5)-C(4)-H(4) | 120.1 | C(12)-C(13)-H(13) | 118.6 |
| C(3)-C(4)-H(4) | 120.1 | C(13)-C(14)-N(1) | 118.61(14) |
| C(6)-C(5)-C(4) | 119.27(17) | C(13)-C(14)-C(9) | 118.91(14) |
| C(6)-C(5)-H(5) | 120.4 | N(1)-C(14)-C(9) | 122.14(14) |
| C(4)-C(5)-H(5) | 120.4 | C(2)-C(15)-C(6) | 120.36(15) |
| C(5)-C(6)-C(15) | 120.91(16) | C(2)-C(15)-N(2) | 129.59(14) |
| C(5)-C(6)-C(7) | 129.20(16) | C(6)-C(15)-N(2) | 110.05(14) |
| C(15)-C(6)-C(7) | 109.88(15) | C(21)-C(16)-C(17) | 118.28(15) |
| C(6)-C(7)-C(8) | 103.81(14) | C(21)-C(16)-C(1) | 118.82(14) |
| C(6)-C(7)-H(7A) | 111.0 | C(17)-C(16)-C(1) | 122.90(14) |
| C(8)-C(7)-H(7A) | 111.0 | C(18)-C(17)-C(16) | 121.18(17) |
| C(6)-C(7)-H(7B) | 111.0 | C(18)-C(17)-H(17) | 119.4 |
| C(8)-C(7)-H(7B) | 111.0 | C(16)-C(17)-H(17) | 119.4 |
| H(7A)-C(7)-H(7B) | 109.0 | C(19)-C(18)-C(17) | 120.56(17) |
| N(2)-C(8)-C(7) | 105.64(14) | C(19)-C(18)-H(18) | 119.7 |
| N(2)-C(8)-H(8A) | 110.6 | C(17)-C(18)-H(18) | 119.7 |
| C(7)-C(8)-H(8A) | 110.6 | C(20)-C(19)-C(18) | 117.65(16) |
| N(2)-C(8)-H(8B) | 110.6 | C(20)-C(19)-H(19) | 121.2 |
| C(7)-C(8)-H(8B) | 110.6 | C(18)-C(19)-H(19) | 121.2 |
| H(8A)-C(8)-H(8B) | 108.7 | C(19)-C(20)-C(21) | 123.03(16) |
| N(2)-C(9)-C(10) | 118.98(14) | C(19)-C(20)-N(3) | 118.68(17) |

Continued...

| | | | |
|---|---|---|---|
| C(21)-C(20)-N(3) | 118.27(17) | H(23B)-C(23)-H(23C) | 109.5 |
| C(20)-C(21)-C(16) | 119.28(16) | C(14)-N(1)-C(1) | 120.35(12) |
| C(20)-C(21)-H(21) | 120.4 | C(14)-N(1)-H(1A) | 119.8 |
| C(16)-C(21)-H(21) | 120.4 | C(1)-N(1)-H(1A) | 119.8 |
| O(3)-C(22)-O(4) | 123.36(16) | C(9)-N(2)-C(15) | 130.98(13) |
| O(3)-C(22)-C(12) | 124.24(16) | C(9)-N(2)-C(8) | 119.68(13) |
| O(4)-C(22)-C(12) | 112.39(14) | C(15)-N(2)-C(8) | 109.11(13) |
| O(4)-C(23)-H(23A) | 109.5 | O(2)-N(3)-O(1) | 123.7(2) |
| O(4)-C(23)-H(23B) | 109.5 | O(2)-N(3)-C(20) | 117.98(19) |
| H(23A)-C(23)-H(23B) | 109.5 | O(1)-N(3)-C(20) | 118.3(2) |
| O(4)-C(23)-H(23C) | 109.5 | C(22)-O(4)-C(23) | 116.67(15) |
| H(23A)-C(23)-H(23C) | 109.5 | | |

**Table 11.** Anisotropic displacement parameters ($Å^2x10^3$) for **4k**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+...+2hka^*b^*U^{12}]$.

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| C(1) | 31(1) | 36(1) | 35(1) | -16(1) | -4(1) | 5(1) |
| C(2) | 34(1) | 36(1) | 34(1) | -14(1) | -6(1) | 1(1) |
| C(3) | 38(1) | 48(1) | 46(1) | -17(1) | 1(1) | 0(1) |
| C(4) | 44(1) | 50(1) | 54(1) | -11(1) | 4(1) | -9(1) |
| C(5) | 52(1) | 38(1) | 50(1) | -11(1) | -6(1) | -10(1) |
| C(6) | 47(1) | 34(1) | 34(1) | -12(1) | -9(1) | -2(1) |
| C(7) | 62(1) | 34(1) | 41(1) | -18(1) | -3(1) | -3(1) |
| C(8) | 47(1) | 34(1) | 49(1) | -20(1) | -5(1) | 7(1) |
| C(9) | 34(1) | 33(1) | 31(1) | -14(1) | -5(1) | 2(1) |
| C(10) | 37(1) | 33(1) | 48(1) | -16(1) | -4(1) | 6(1) |
| C(11) | 33(1) | 42(1) | 47(1) | -18(1) | -2(1) | 2(1) |
| C(12) | 37(1) | 37(1) | 35(1) | -15(1) | -6(1) | 0(1) |
| C(13) | 40(1) | 31(1) | 34(1) | -15(1) | -8(1) | 5(1) |
| C(14) | 33(1) | 34(1) | 28(1) | -14(1) | -6(1) | 4(1) |
| C(15) | 36(1) | 35(1) | 28(1) | -12(1) | -7(1) | -1(1) |
| C(16) | 36(1) | 33(1) | 31(1) | -12(1) | 0(1) | 0(1) |
| C(17) | 44(1) | 46(1) | 45(1) | -23(1) | -10(1) | 11(1) |
| C(18) | 47(1) | 60(1) | 47(1) | -25(1) | -14(1) | 9(1) |
| C(19) | 51(1) | 52(1) | 41(1) | -22(1) | -6(1) | -7(1) |
| C(20) | 55(1) | 33(1) | 42(1) | -17(1) | 0(1) | -6(1) |
| C(21) | 46(1) | 30(1) | 39(1) | -11(1) | -5(1) | 3(1) |
| C(22) | 42(1) | 38(1) | 34(1) | -14(1) | -7(1) | -2(1) |
| C(23) | 56(1) | 53(1) | 54(1) | -16(1) | 10(1) | -16(1) |
| N(1) | 32(1) | 38(1) | 32(1) | -10(1) | -8(1) | 8(1) |
| N(2) | 39(1) | 30(1) | 40(1) | -16(1) | 0(1) | 3(1) |
| N(3) | 80(1) | 47(1) | 77(1) | -38(1) | -9(1) | 0(1) |
| O(1) | 108(2) | 102(2) | 97(1) | -79(1) | -15(1) | 7(1) |
| O(2) | 178(2) | 53(1) | 126(2) | -49(1) | -57(2) | 42(1) |
| O(3) | 56(1) | 35(1) | 55(1) | -10(1) | -4(1) | 0(1) |
| O(4) | 45(1) | 43(1) | 54(1) | -14(1) | 7(1) | -6(1) |

**SI Table 12.** Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for **4k**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | 861 | 7256 | 2381 | 40 |
| H(3) | -731 | 5606 | 3683 | 53 |
| H(4) | -1478 | 3645 | 4183 | 62 |
| H(5) | 673 | 2399 | 3463 | 57 |
| H(7A) | 3854 | 2802 | 1431 | 53 |
| H(7B) | 4814 | 2296 | 2625 | 53 |
| H(8A) | 7103 | 3685 | 1995 | 51 |
| H(8B) | 6445 | 3990 | 730 | 51 |
| H(10) | 8771 | 5246 | 869 | 47 |
| H(11) | 10584 | 6903 | -183 | 48 |
| H(13) | 5750 | 8952 | 152 | 41 |
| H(17) | 5271 | 5808 | 3576 | 51 |
| H(18) | 6821 | 6329 | 4868 | 59 |
| H(19) | 5720 | 8000 | 5338 | 55 |
| H(21) | 1601 | 8674 | 3121 | 47 |
| H(23A) | 11914 | 10313 | -2713 | 84 |
| H(23B) | 13807 | 9722 | -2073 | 84 |
| H(23C) | 12295 | 10559 | -1580 | 84 |
| H(1A) | 2438 | 7807 | 618 | 41 |

# Supporting Information

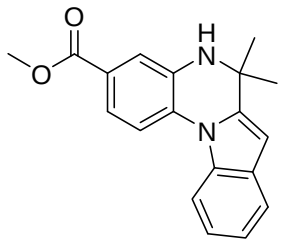
## Soluble Polymer Supported Divergent Synthesis of Tetracyclic Benzene-Fused Pyrazino/Diazepino Indoles: An Advanced Synthetic Approach to Bioactive Scaffolds

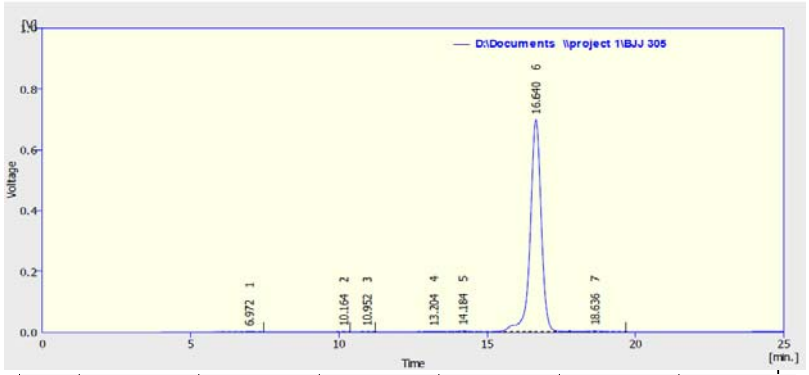
Po-Tsung Lin, Deepak B. Salunke, Li-Hsun Chen and Chung-Ming Sun*

*Department of Applied Chemistry, National Chiao Tung University, Hsinchu, 300-10*, *Taiwan*

*E-mail: cmsun@mail.nctu.edu.tw*

## Contents

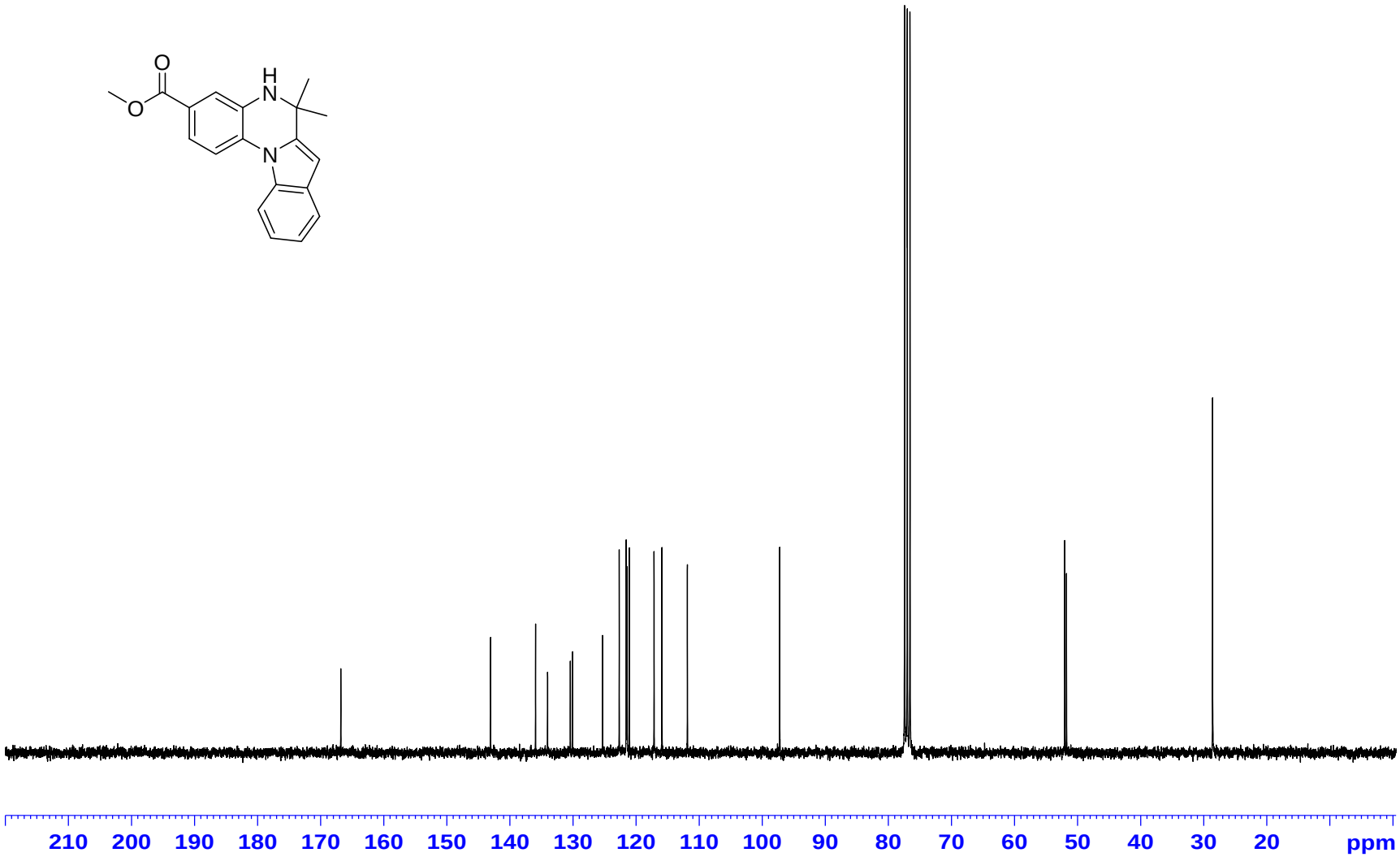


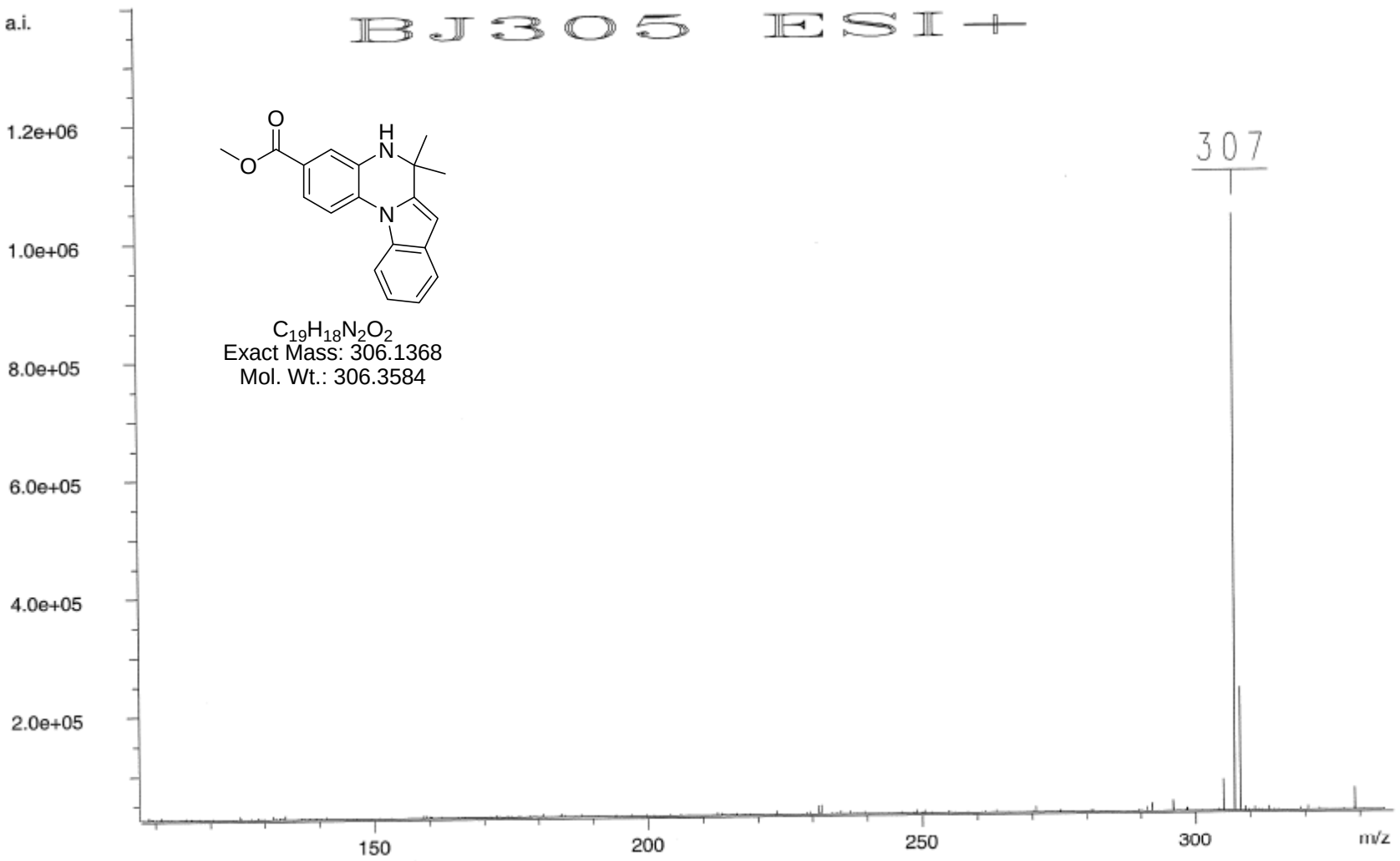

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 6.972 | 23.634 | 0.843 | 0.1 | 0.1 | 0.38 |
| 2 | 10.164 | 3.691 | 0.274 | 0.0 | 0.0 | 0.23 |
| 3 | 10.952 | 2.872 | 0.215 | 0.0 | 0.0 | 0.23 |
| 4 | 13.204 | 38.757 | 1.055 | 0.2 | 0.1 | 0.66 |
| 5 | 14.184 | 64.531 | 2.881 | 0.4 | 0.4 | 0.32 |
| 6 | 16.640 | 18072.867 | 697.657 | 98.7 | 98.9 | 0.38 |
| 7 | 18.636 | 107.490 | 2.582 | 0.6 | 0.4 | 0.47 |
| | Total | 18313.842 | 705.507 | 100.0 | 100.0 | |




HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **2a** in $CDCl_3$

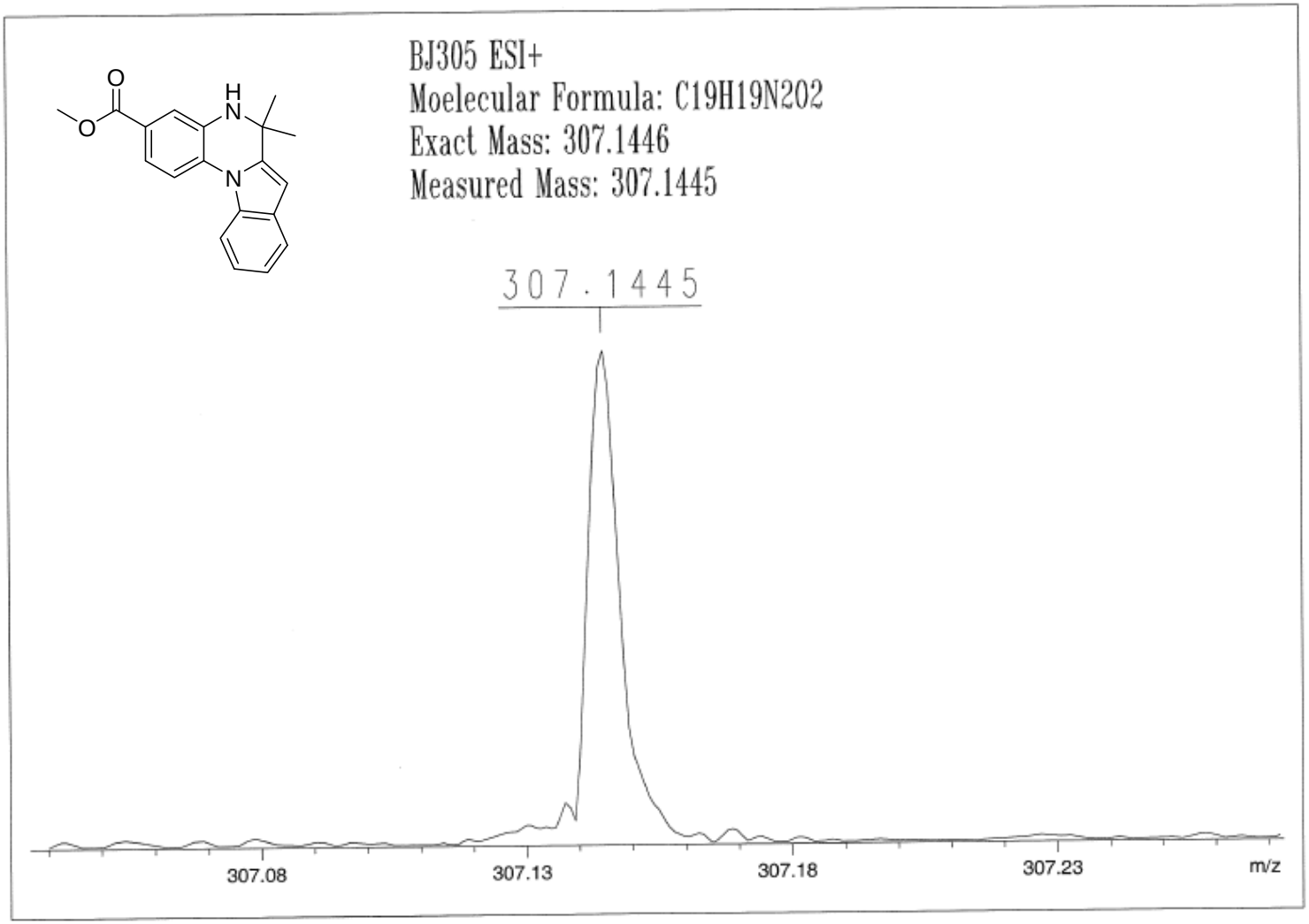



$^{13}$C NMR Spectrum (75 MHz) of compound **2a** in $CDCl_3$

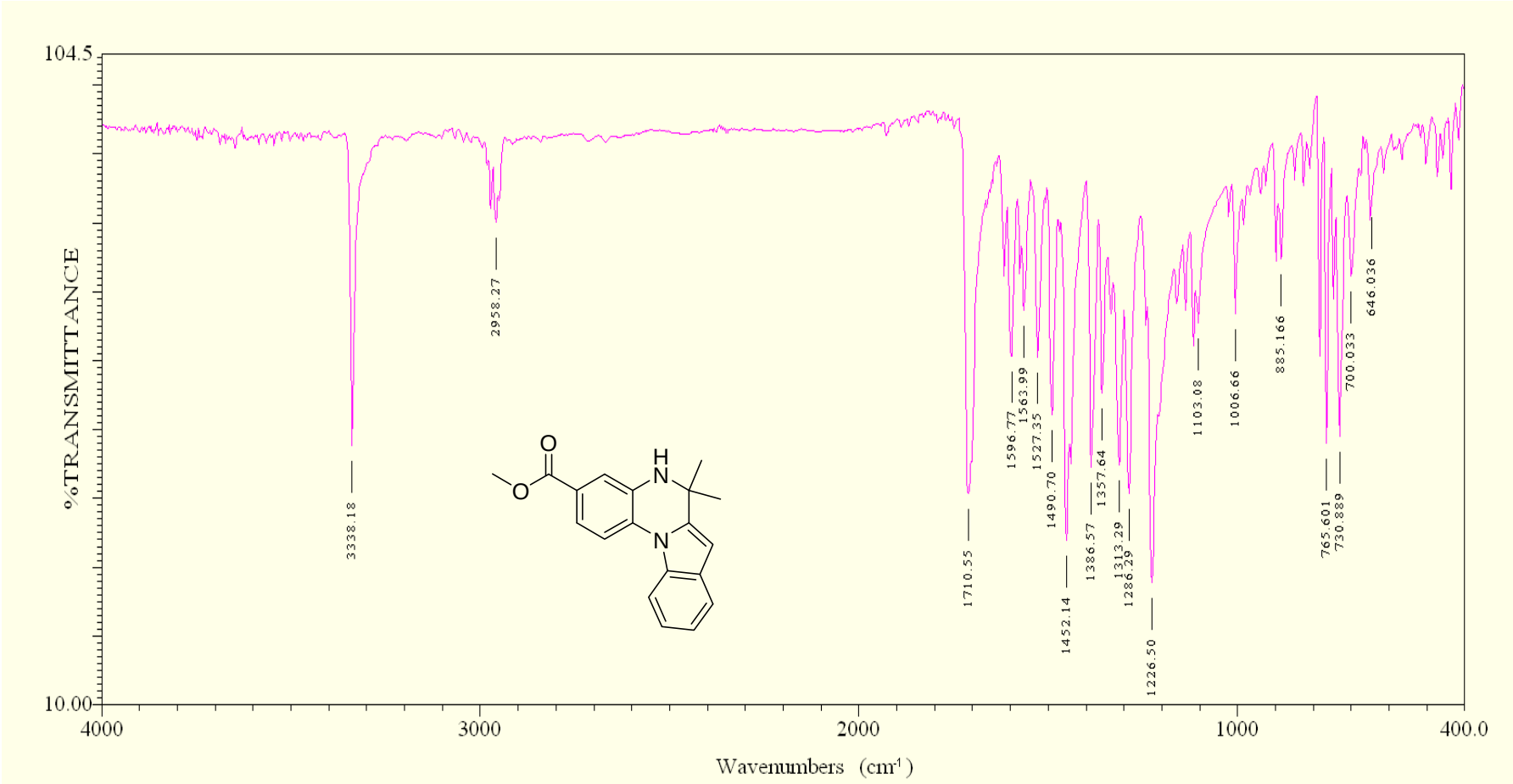



$C_{19}H_{18}N_2O_2$
Exact Mass: 306.1368
Mol. Wt.: 306.3584

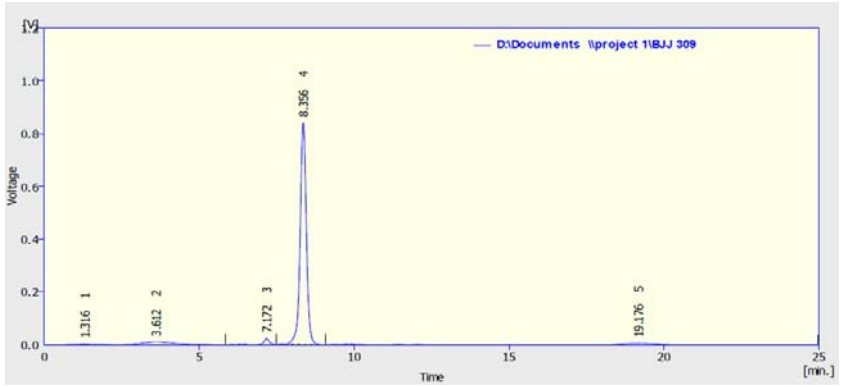
Low Resolution Mass Spectrum (LRMS) of compound **2a**



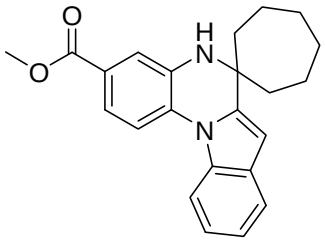

High Resolution Mass Spectrum (HRMS) of compound **2a**

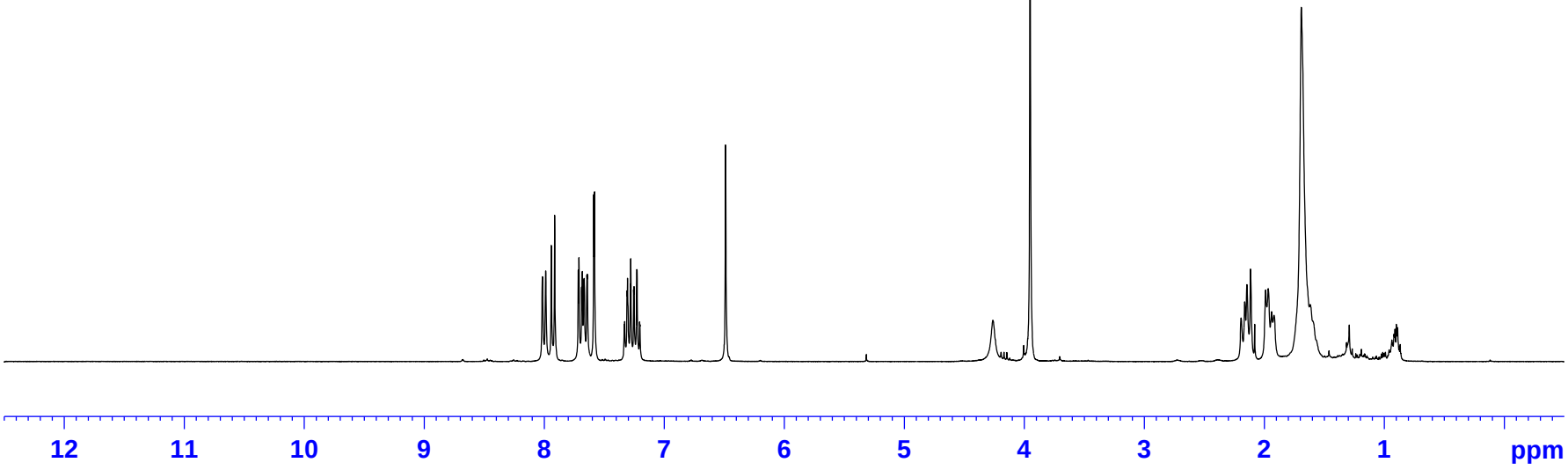



IR Spectrum of compound **2a** (Neat)

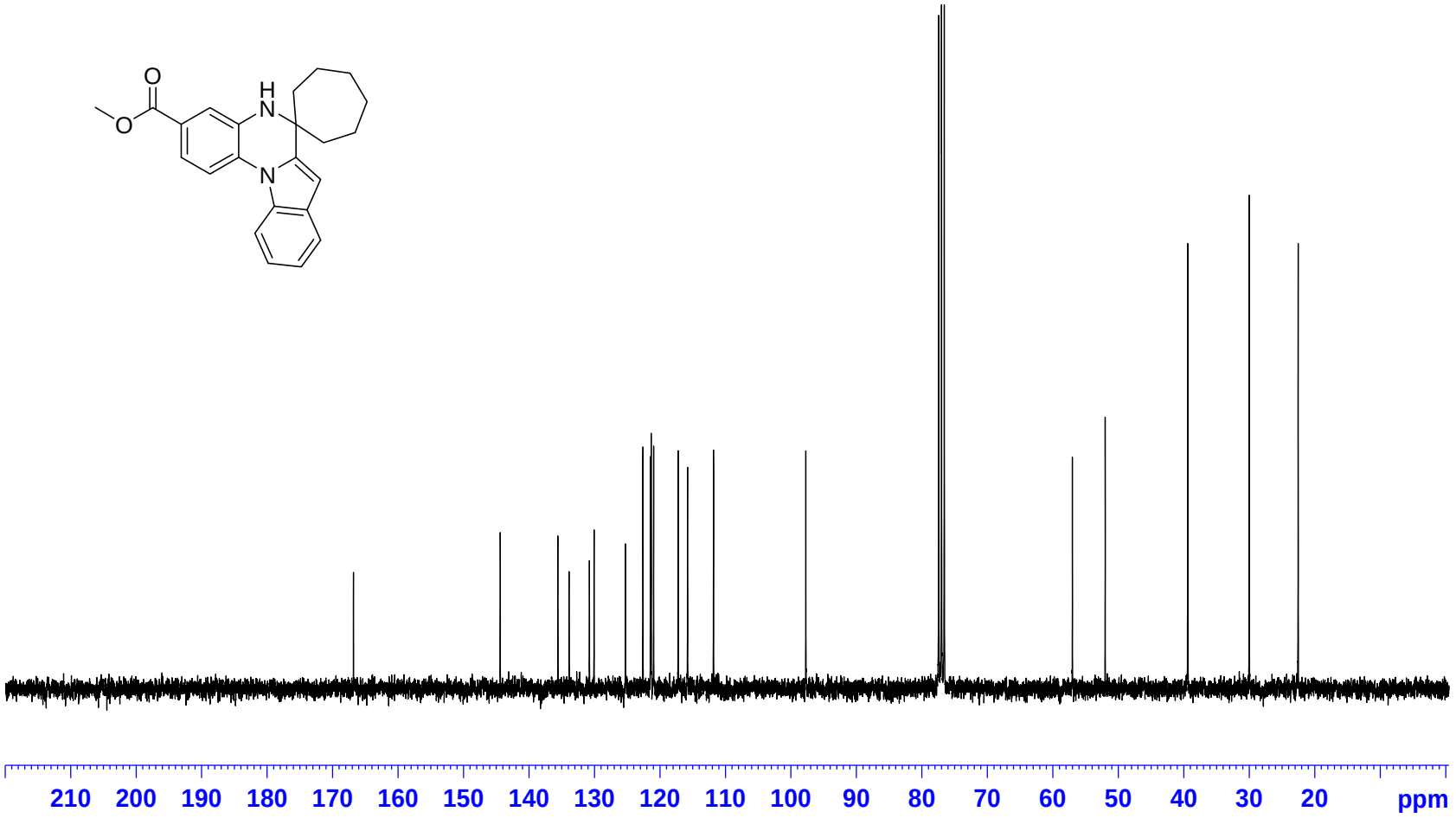



| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 1.316 | 134.411 | 1.887 | 1.0 | 0.2 | 1.15 |
| 2 | 3.612 | 732.502 | 10.066 | 5.5 | 1.1 | 1.05 |
| 3 | 7.172 | 262.953 | 23.121 | 2.0 | 2.6 | 0.16 |
| 4 | 8.356 | 11673.605 | 841.154 | 87.1 | 95.4 | 0.21 |
| 5 | 19.176 | 599.342 | 5.848 | 4.5 | 0.7 | 1.32 |
| | Total | 13402.814 | 882.076 | 100.0 | 100.0 | |

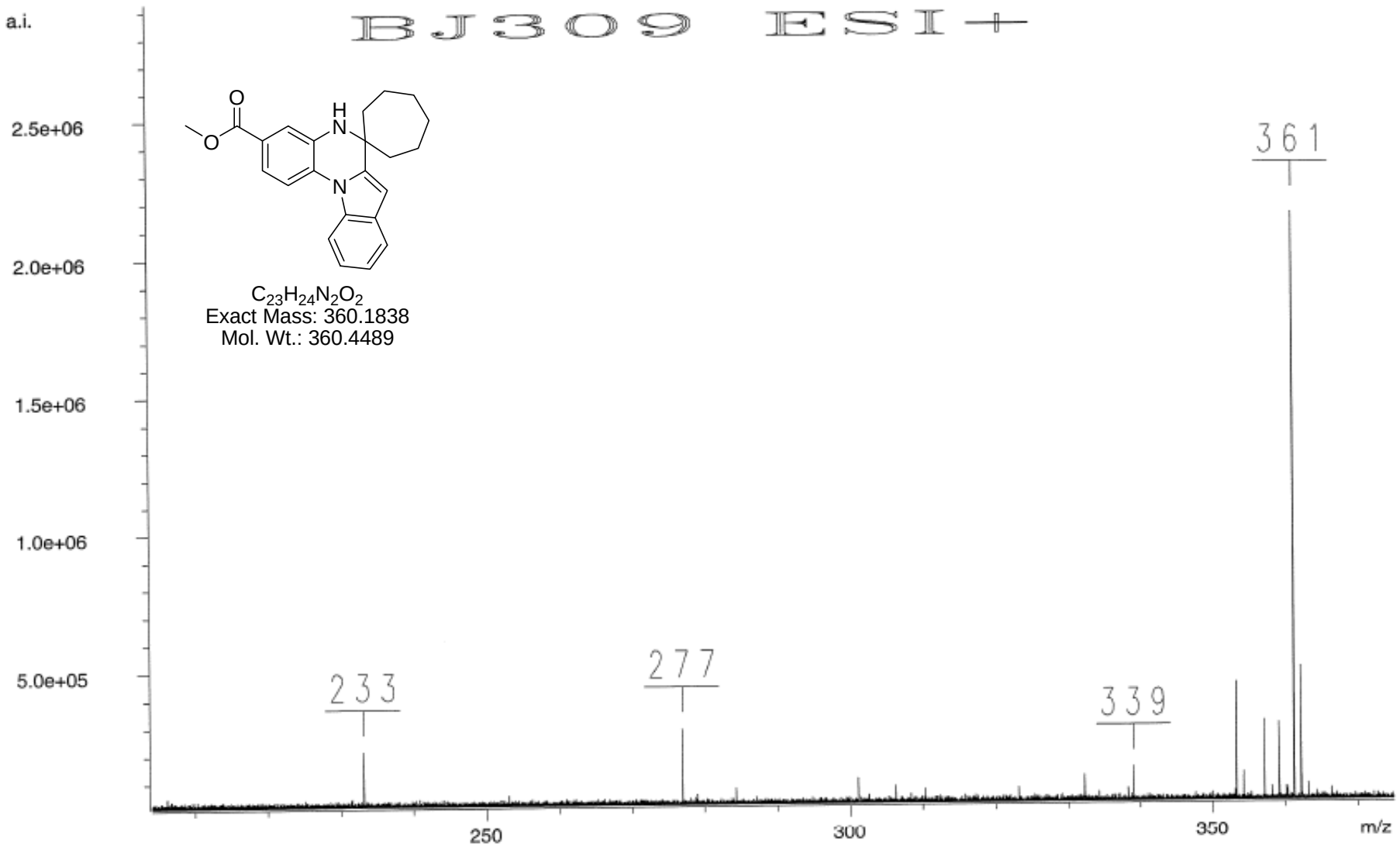


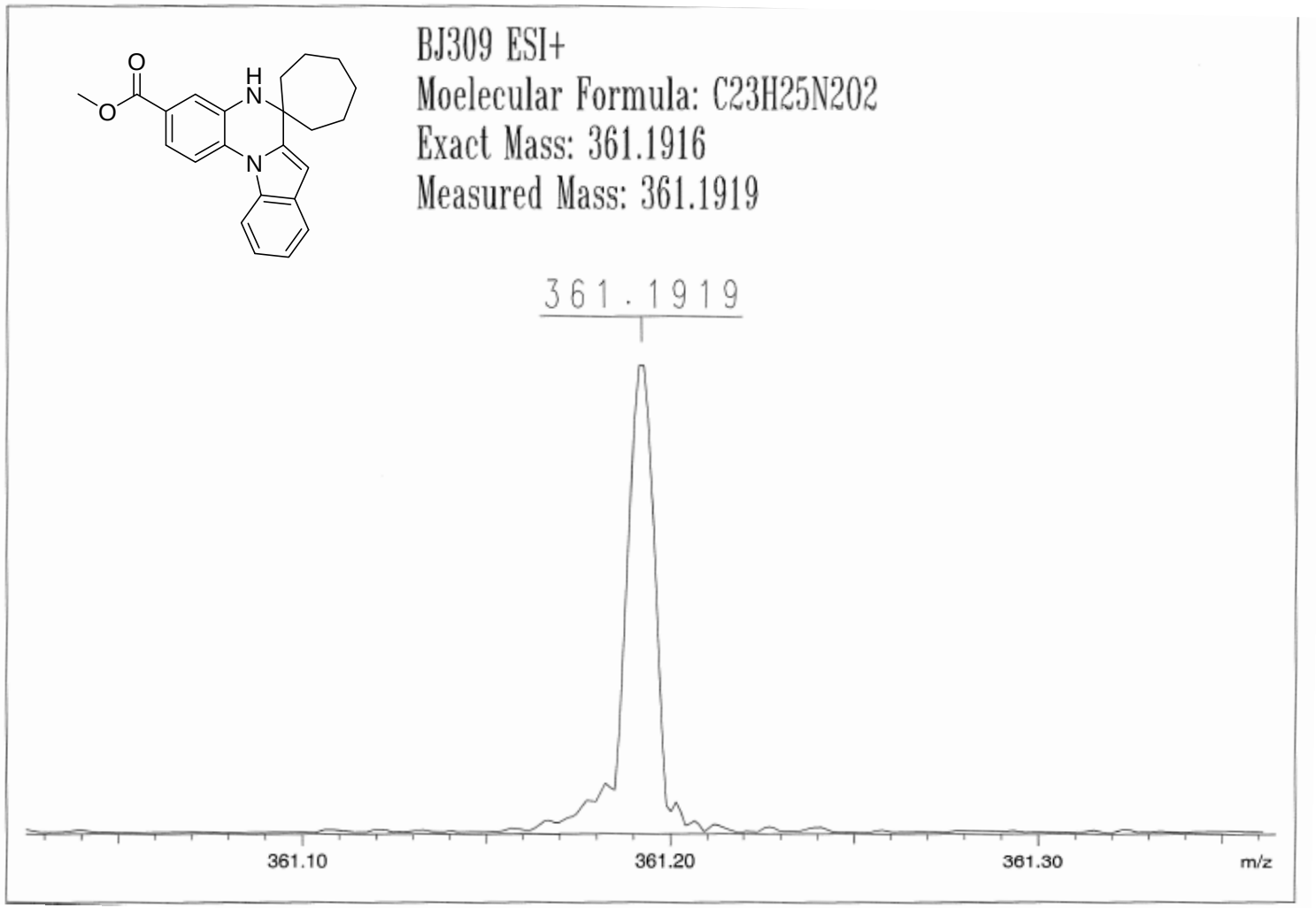

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **2b** in $CDCl_3$



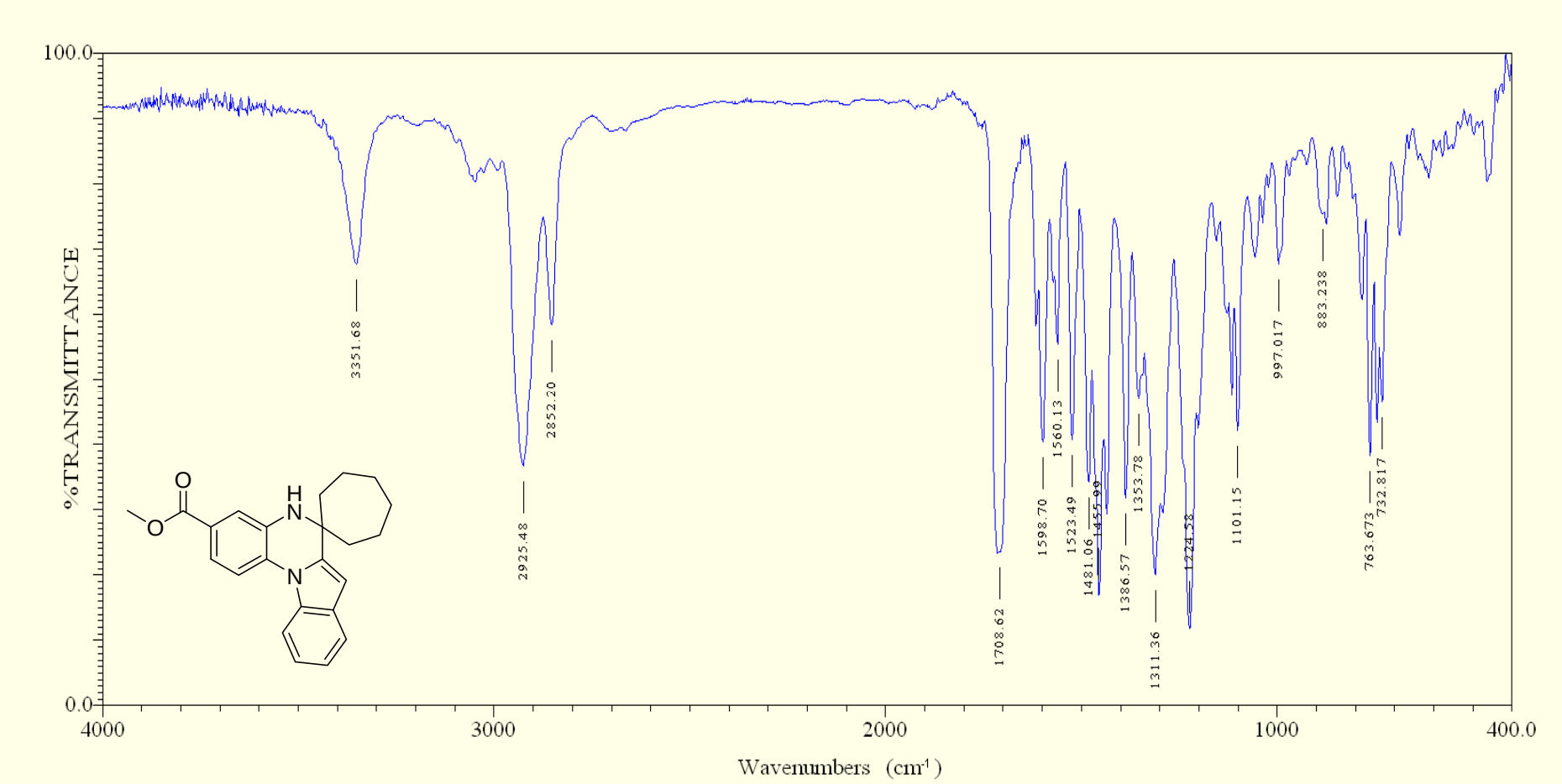

$^{13}$C NMR Spectrum (75 MHz) of compound **2b** in $CDCl_3$



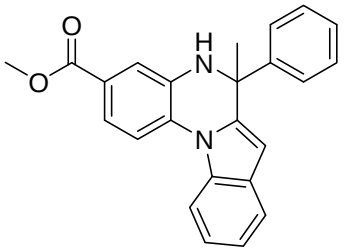

Low Resolution Mass Spectrum (LRMS) of compound **2b**

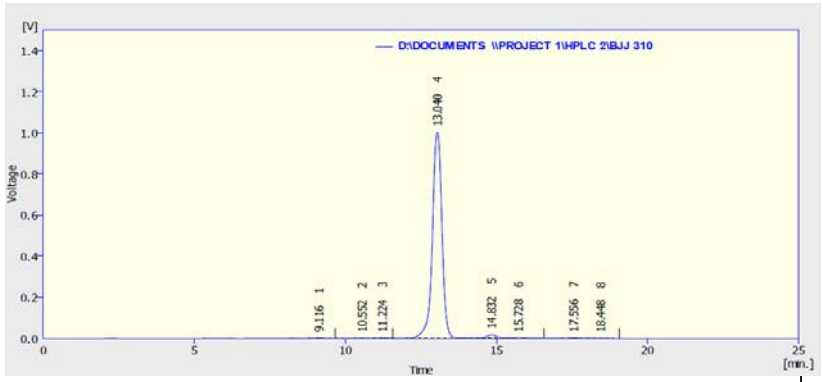



High Resolution Mass Spectrum (HRMS) of compound **2b**

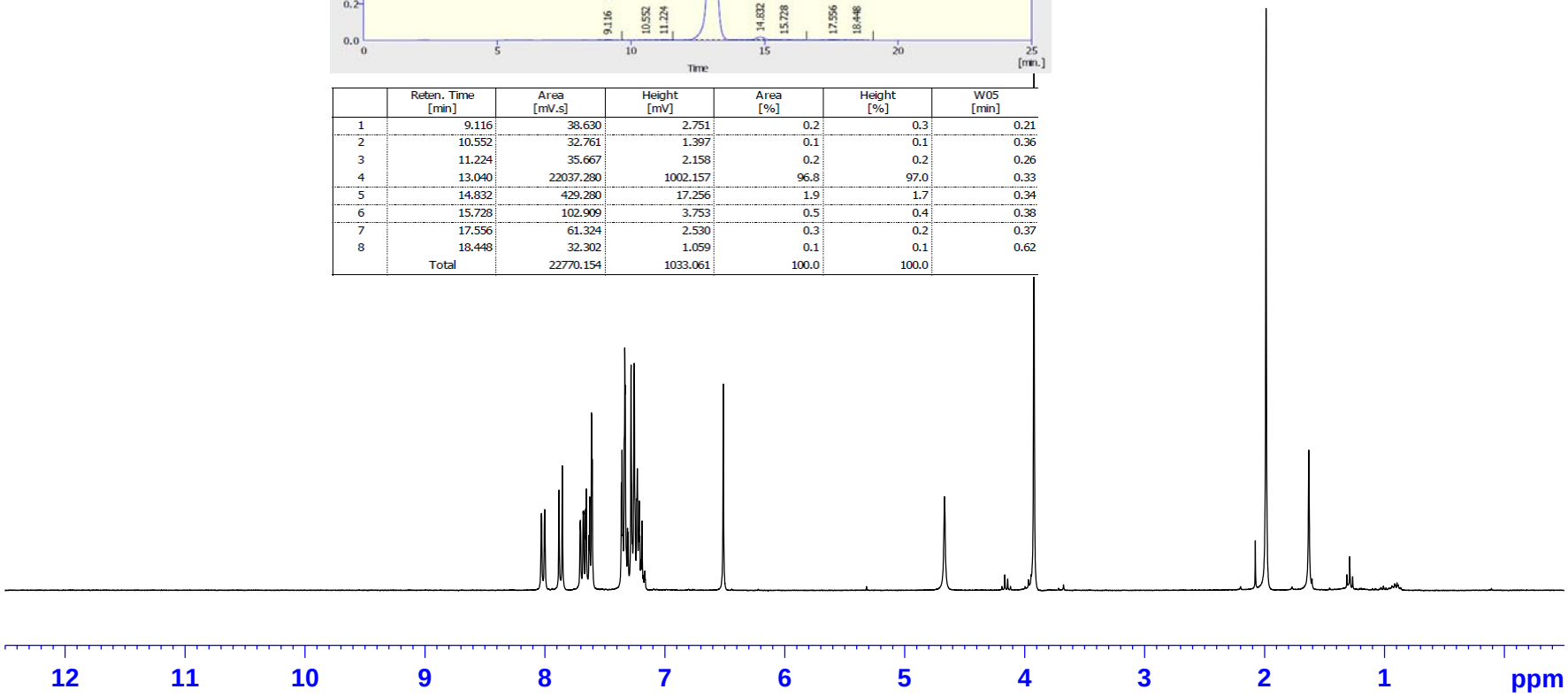



IR Spectrum of compound **2b** (Neat)

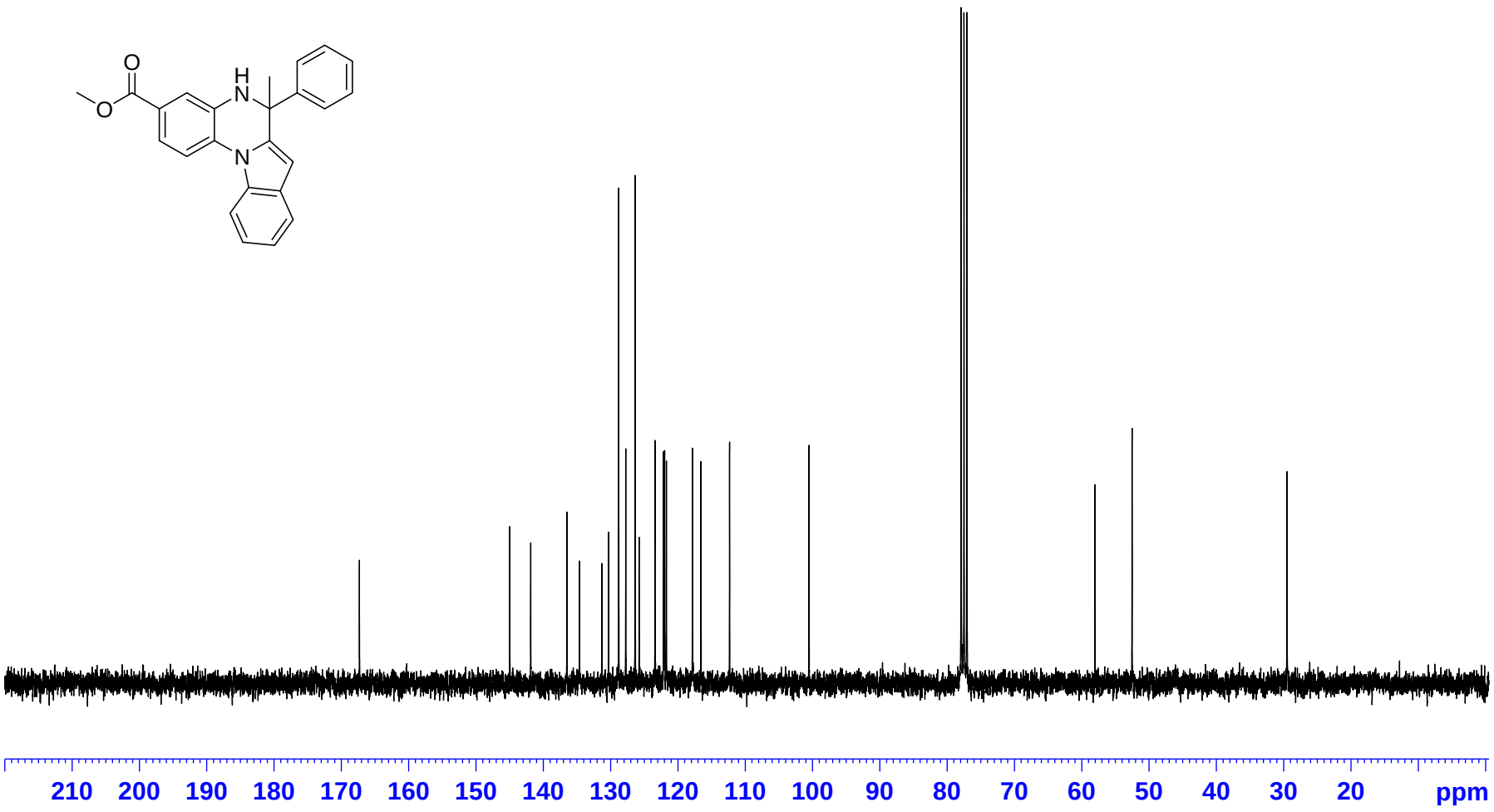


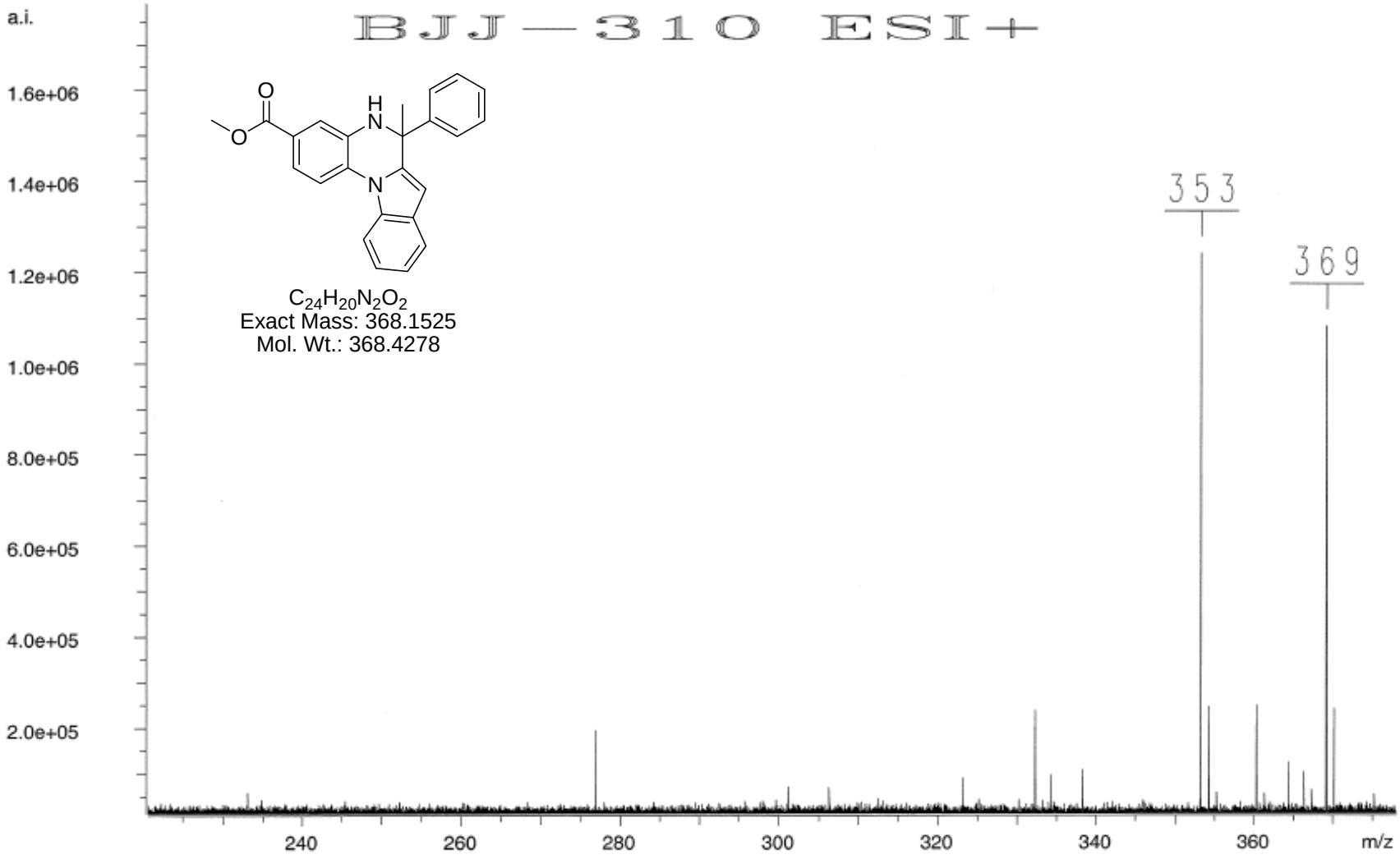

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 9.116 | 38.630 | 2.751 | 0.2 | 0.3 | 0.21 |
| 2 | 10.552 | 32.761 | 1.397 | 0.1 | 0.1 | 0.36 |
| 3 | 11.224 | 35.667 | 2.158 | 0.2 | 0.2 | 0.26 |
| 4 | 13.040 | 22037.280 | 1002.157 | 96.8 | 97.0 | 0.33 |
| 5 | 14.832 | 429.280 | 17.256 | 1.9 | 1.7 | 0.34 |
| 6 | 15.728 | 102.909 | 3.753 | 0.5 | 0.4 | 0.38 |
| 7 | 17.556 | 61.324 | 2.530 | 0.3 | 0.2 | 0.37 |
| 8 | 18.448 | 32.302 | 1.059 | 0.1 | 0.1 | 0.62 |
| | Total | 22770.154 | 1033.061 | 100.0 | 100.0 | |



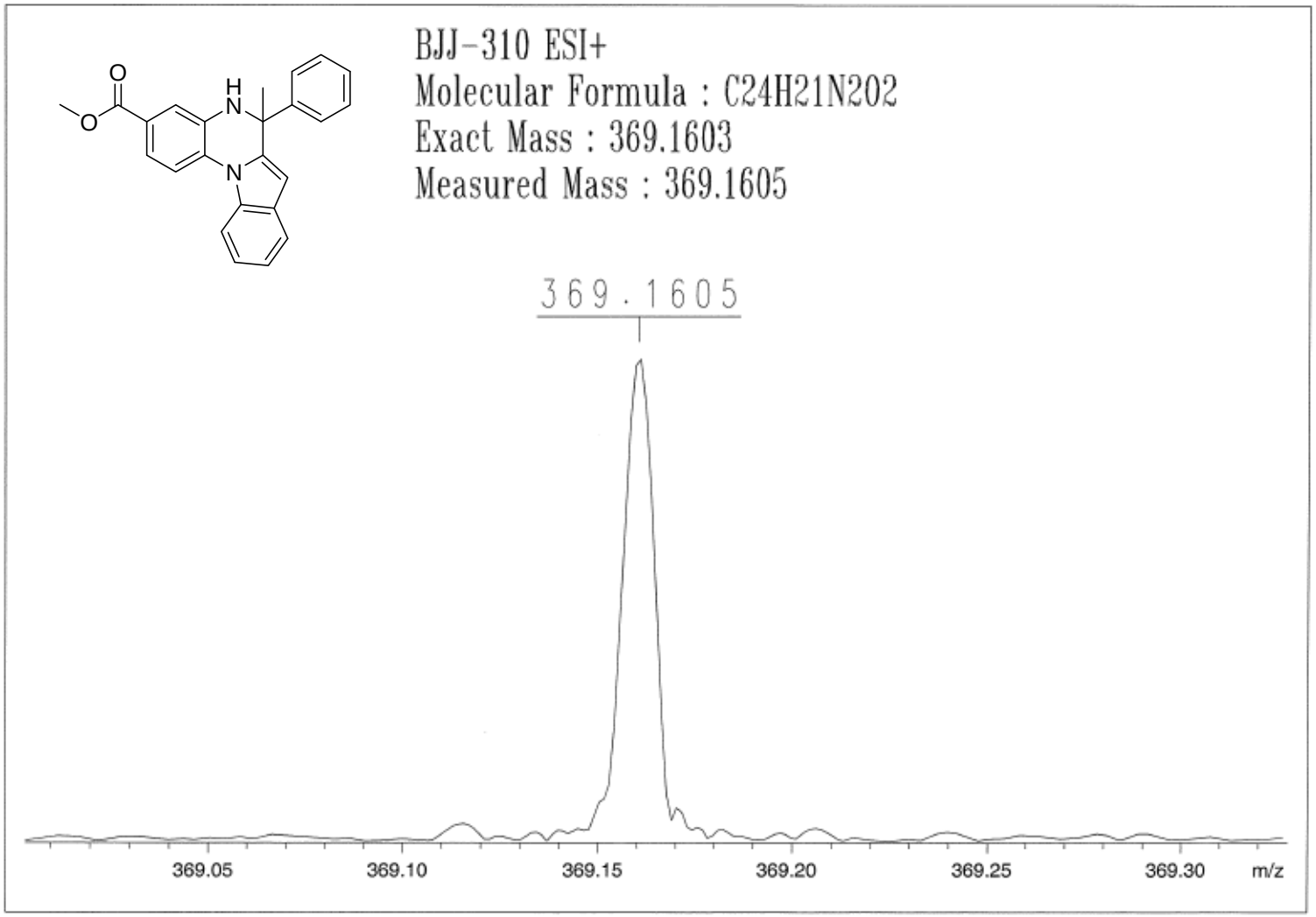

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **2c** in $CDCl_3$



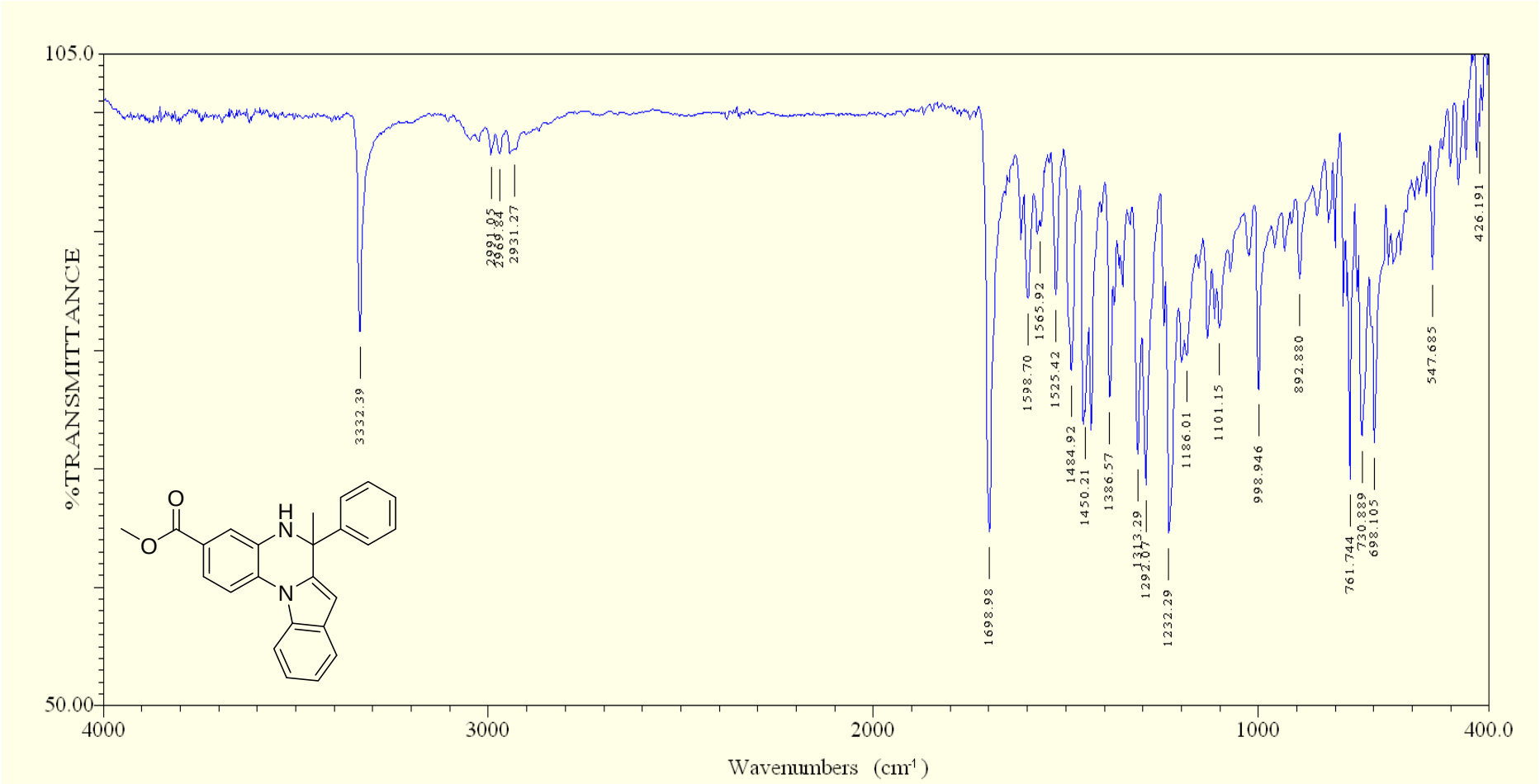

$^{13}C$ NMR Spectrum (75 MHz) of compound **2c** in $CDCl_3$



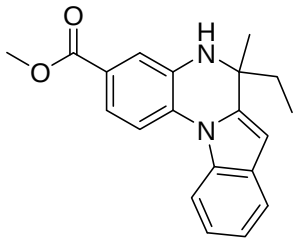

Low Resolution Mass Spectrum (LRMS) of compound **2c**

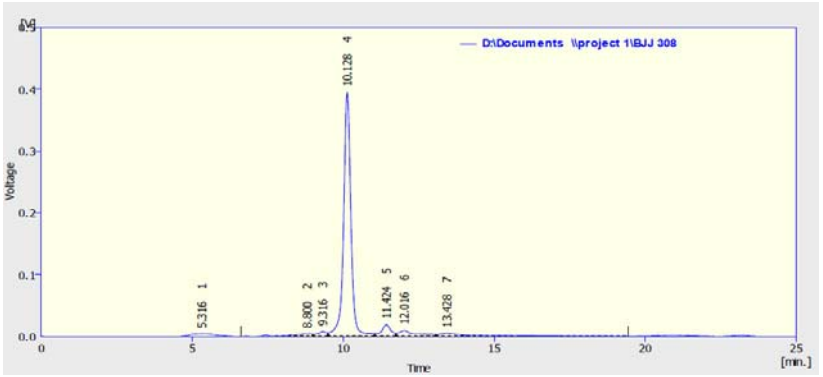



High Resolution Mass Spectrum (HRMS) of compound **2c**




IR Spectrum of compound **2c** (Neat)

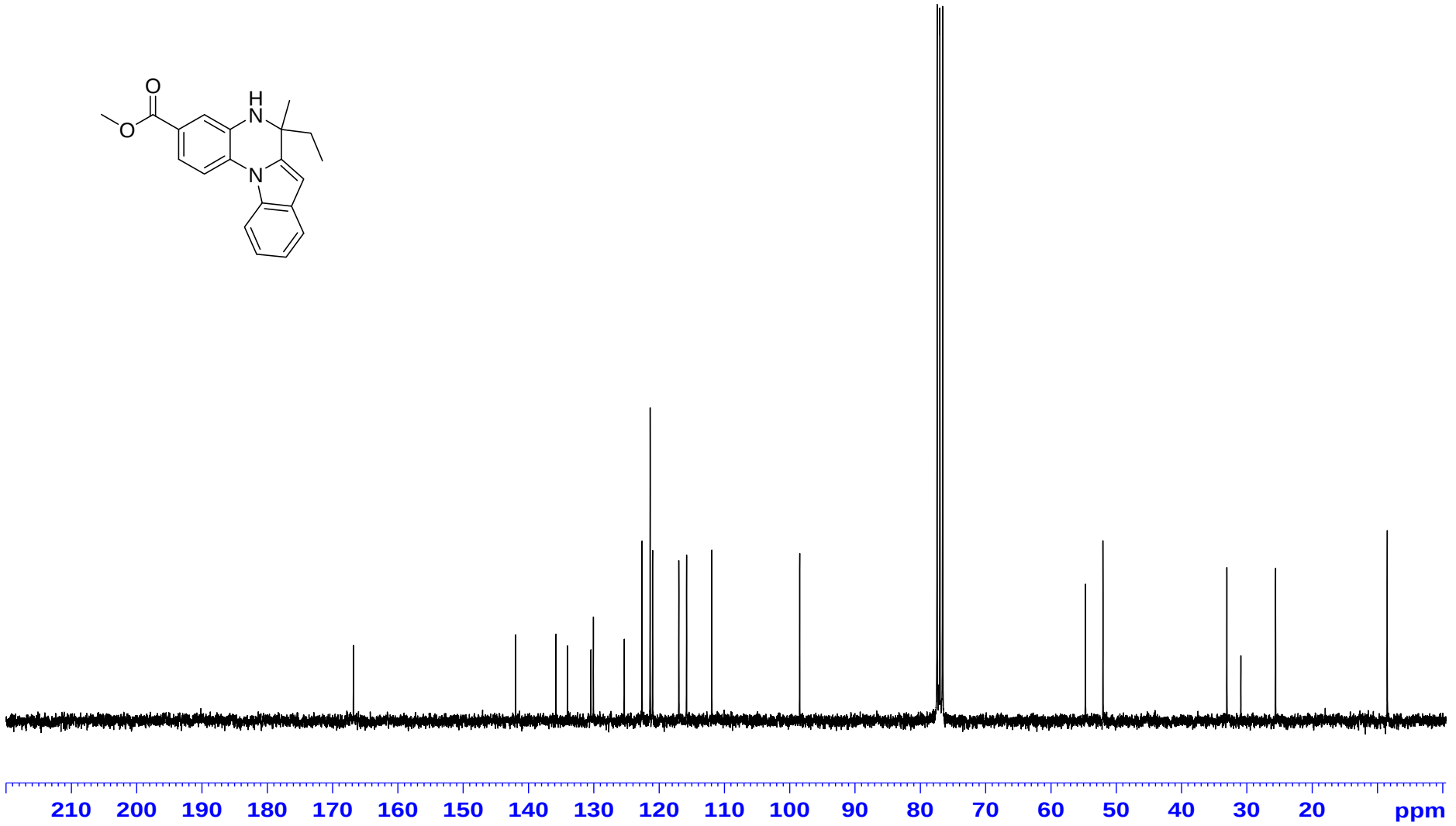


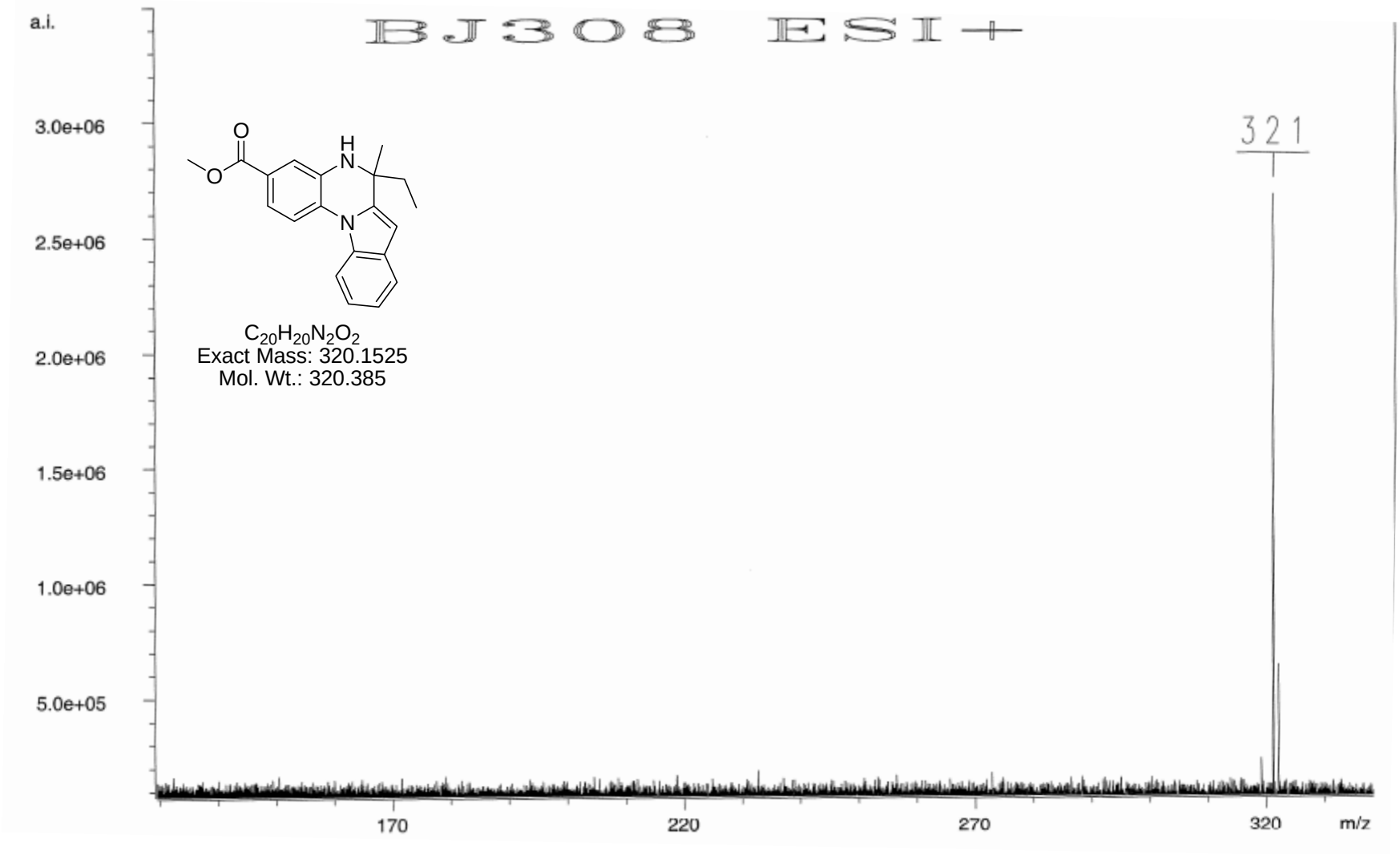

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 5.316 | 283.379 | 4.396 | 3.3 | 1.0 | 1.03 |
| 2 | 8.800 | 157.530 | 3.871 | 1.9 | 0.9 | 0.74 |
| 3 | 9.316 | 161.633 | 7.331 | 1.9 | 1.7 | 0.41 |
| 4 | 10.128 | 6669.596 | 394.886 | 78.6 | 89.0 | 0.24 |
| 5 | 11.424 | 407.687 | 18.796 | 4.8 | 4.2 | 0.30 |
| 6 | 12.016 | 380.713 | 9.275 | 4.5 | 2.1 | 0.48 |
| 7 | 13.428 | 423.097 | 5.165 | 5.0 | 1.2 | 0.73 |
| | Total | 8483.635 | 443.720 | 100.0 | 100.0 | |



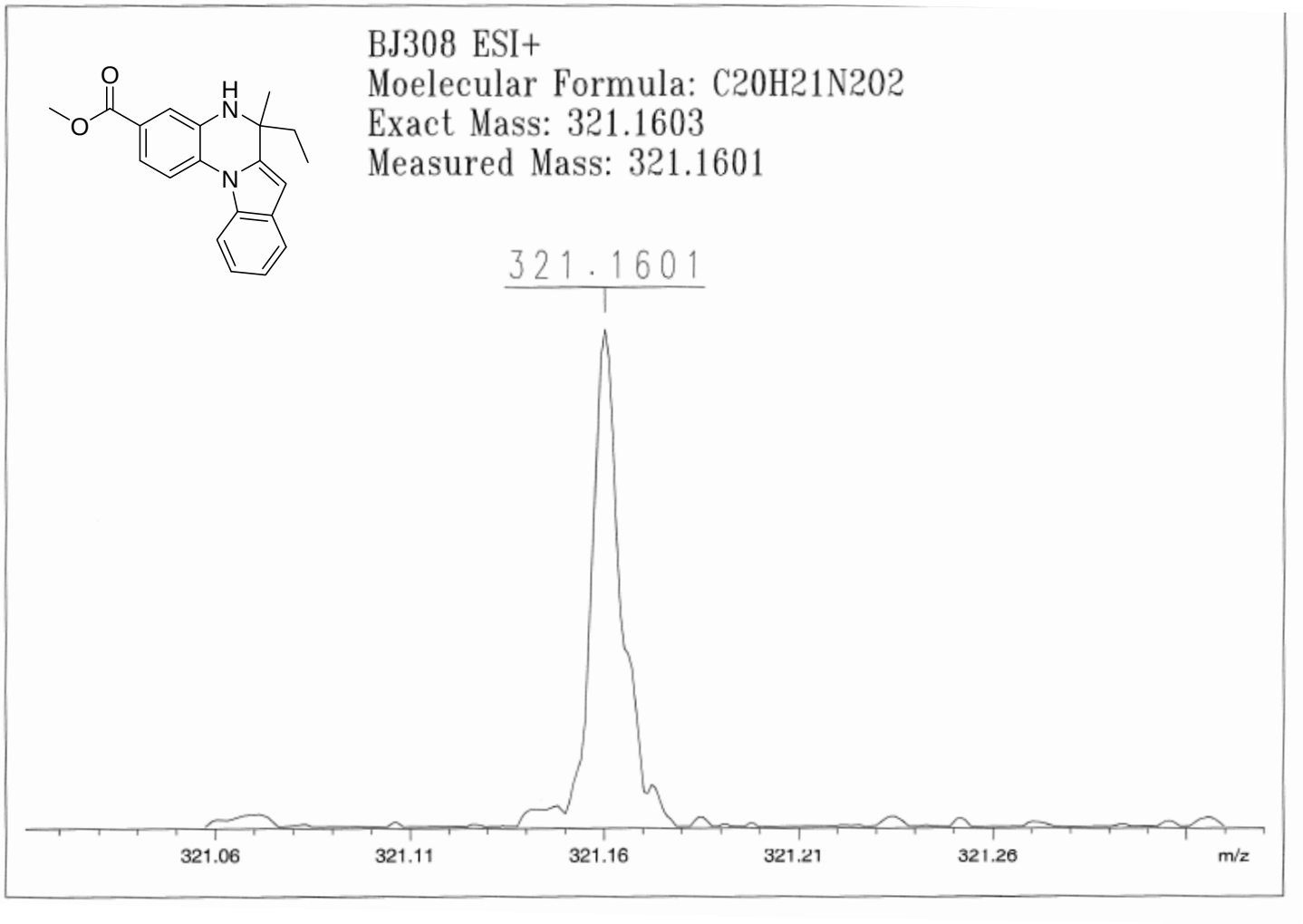

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **2d** in $CDCl_3$



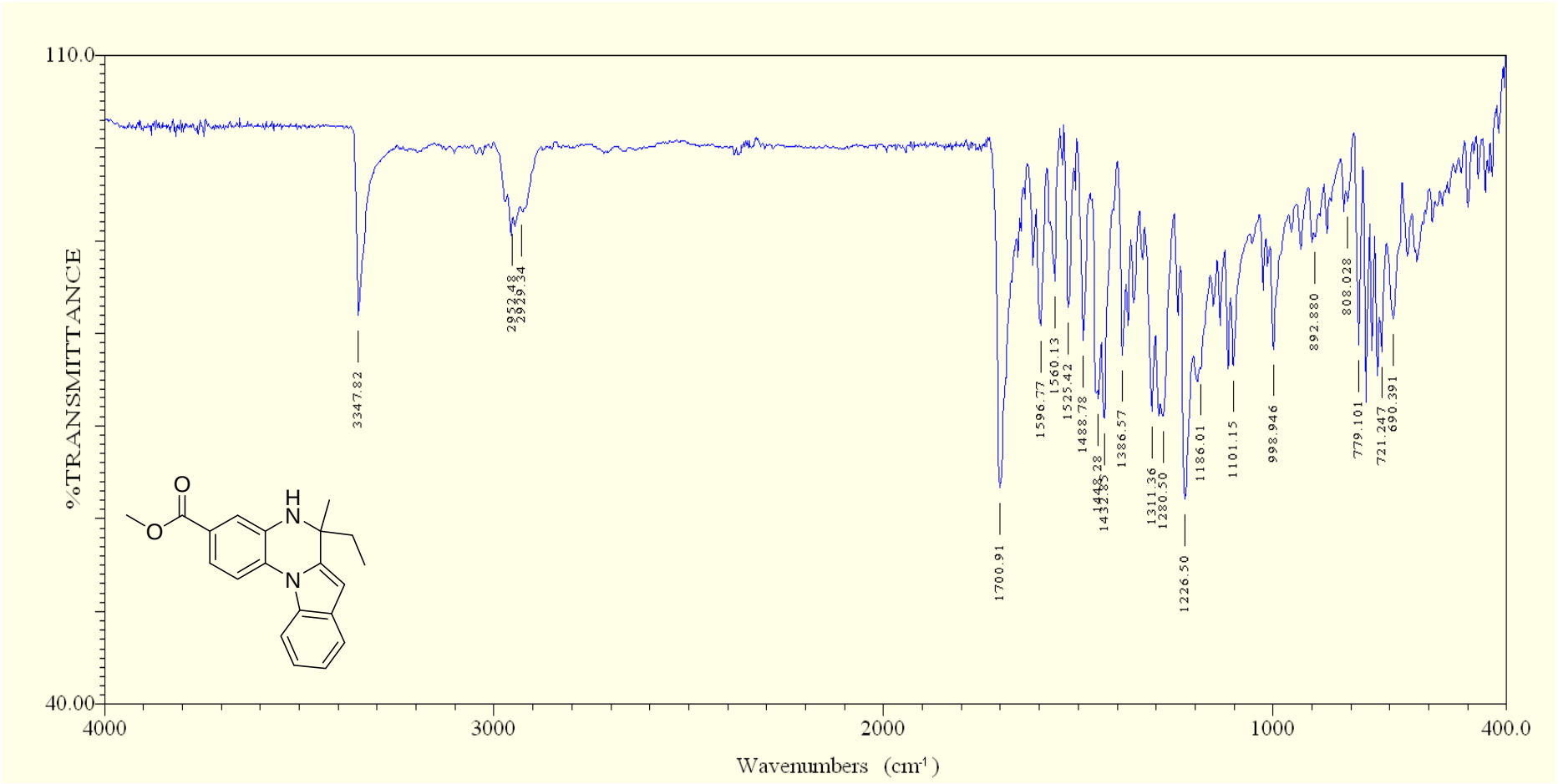

$^{13}C$ NMR Spectrum (75 MHz) of compound **2d** in $CDCl_3$



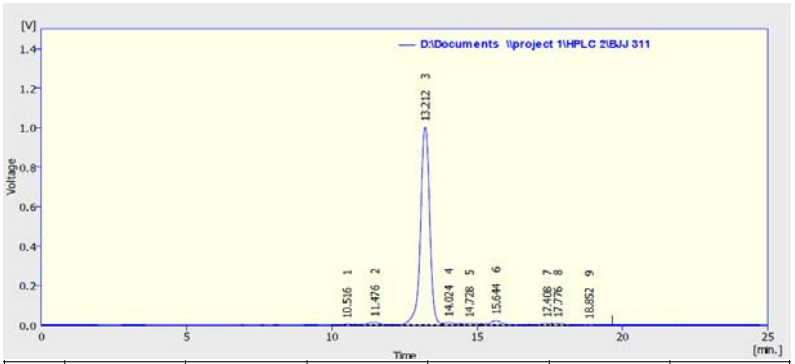

Low Resolution Mass Spectrum (LRMS) of compound **2d**




High Resolution Mass Spectrum (HRMS) of compound **2d**



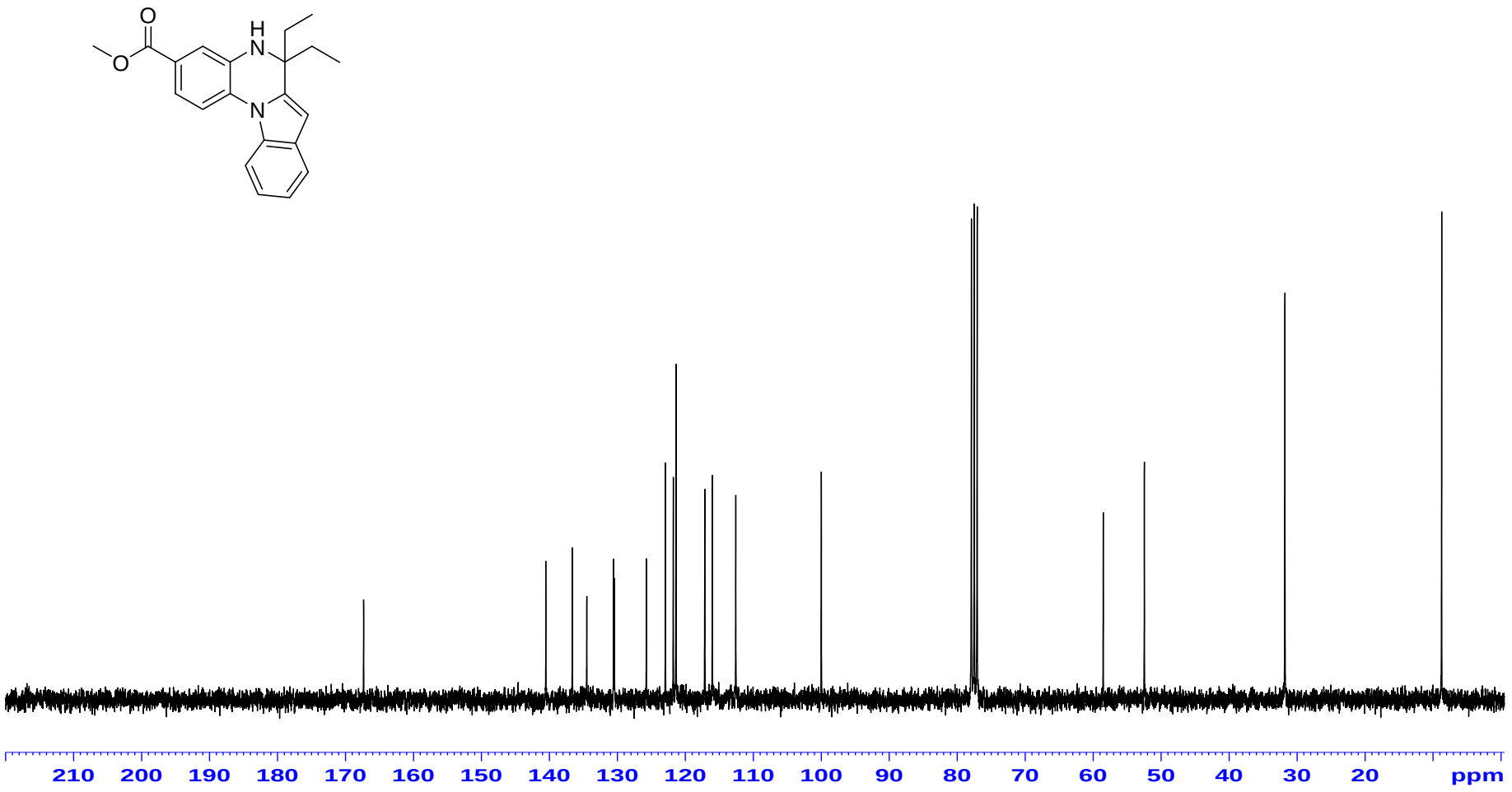

IR Spectrum of compound **2d** (Neat)



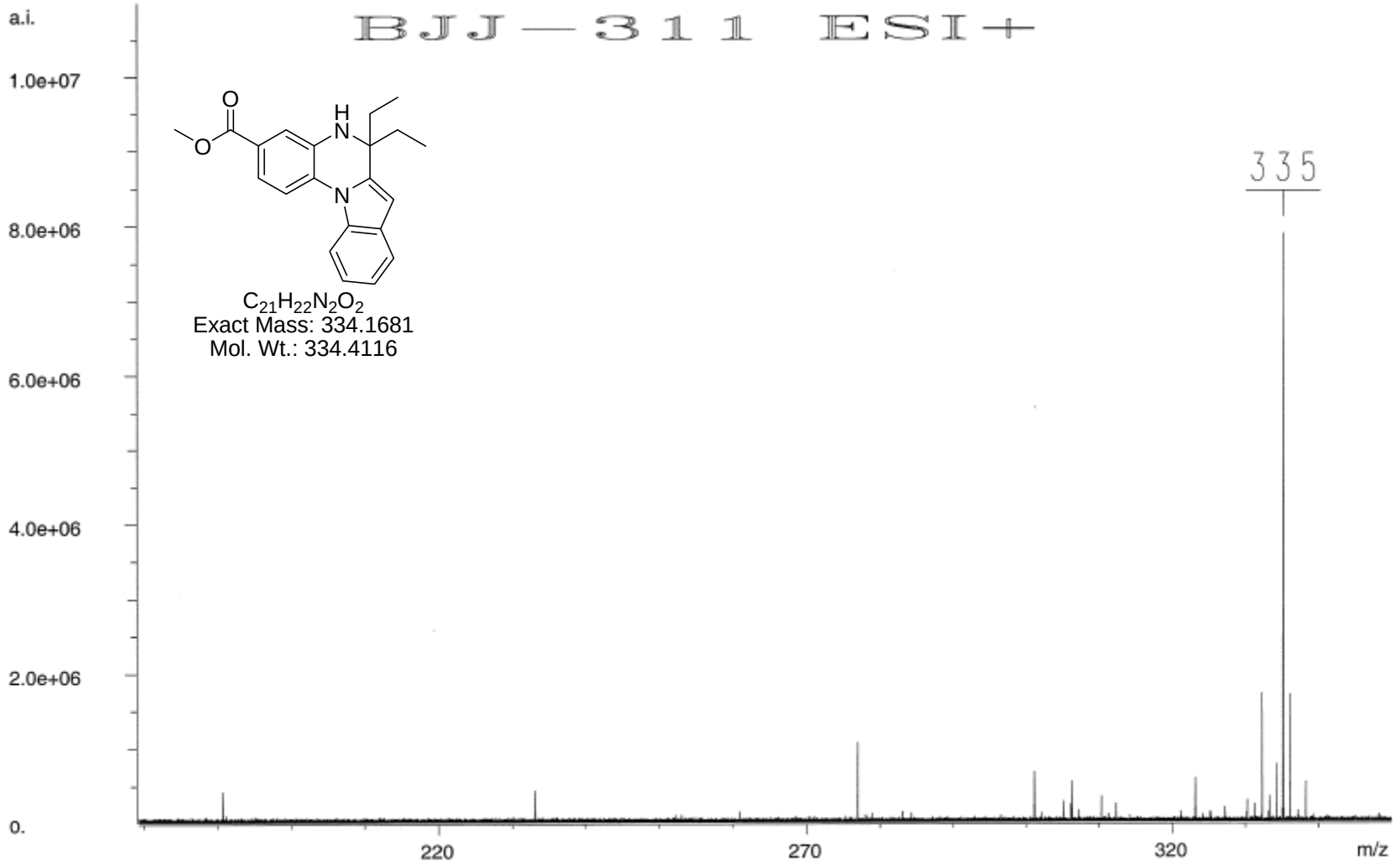

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 10.516 | 78.073 | 4.780 | 0.3 | 0.4 | 0.24 |
| 2 | 11.476 | 413.636 | 13.979 | 1.7 | 1.3 | 0.44 |
| 3 | 13.212 | 22075.517 | 1001.303 | 90.9 | 92.7 | 0.33 |
| 4 | 14.024 | 337.264 | 13.393 | 1.4 | 1.2 | 0.44 |
| 5 | 14.728 | 256.059 | 7.686 | 1.1 | 0.7 | 0.73 |
| 6 | 15.644 | 673.558 | 22.358 | 2.8 | 2.1 | 0.38 |
| 7 | 17.408 | 180.354 | 6.979 | 0.7 | 0.6 | 0.39 |
| 8 | 17.776 | 201.880 | 7.729 | 0.8 | 0.7 | 0.43 |



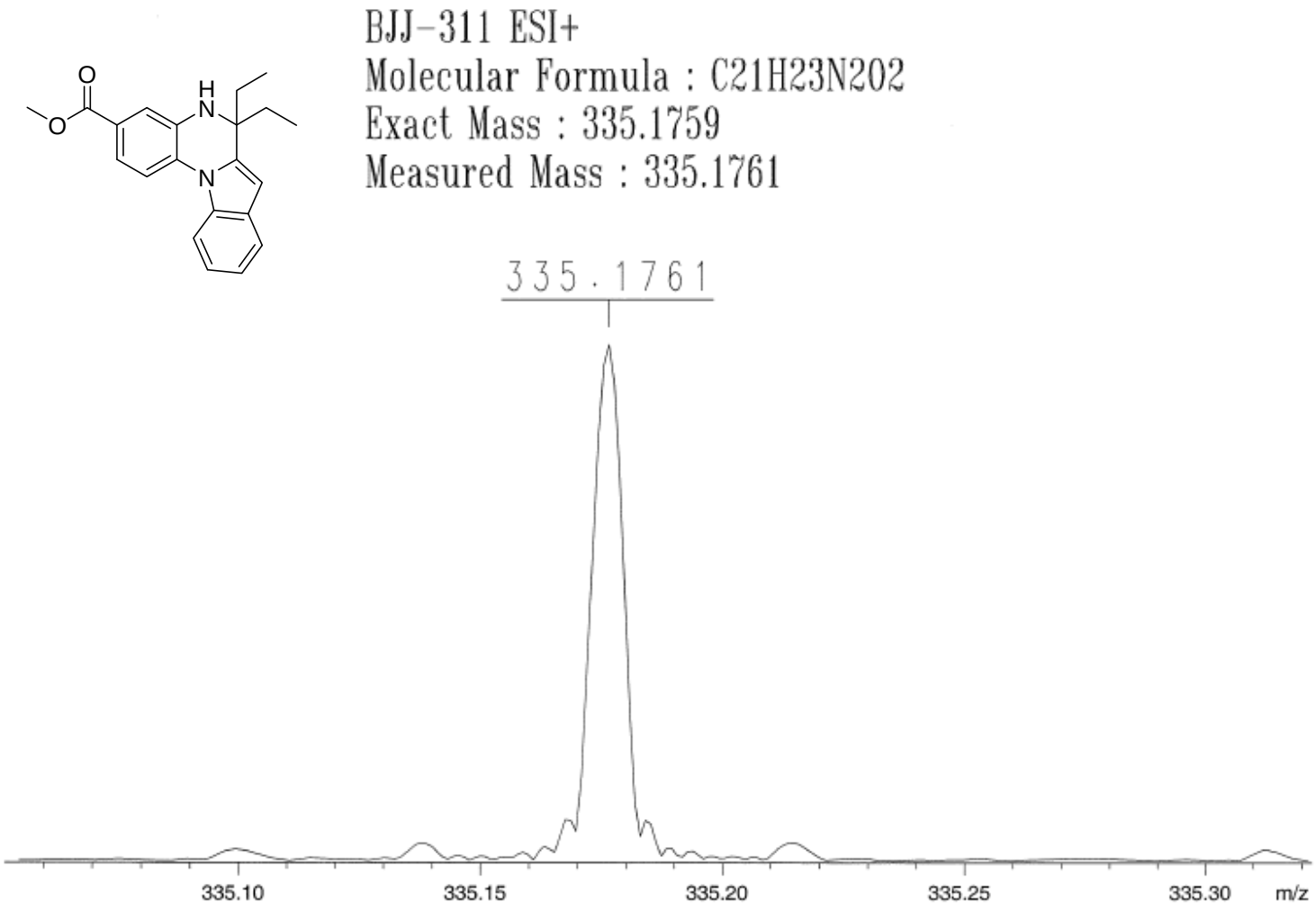

HPLC and $^{1}$H NMR Spectrum (300 MHz) of compound **2e** in $CDCl_3$



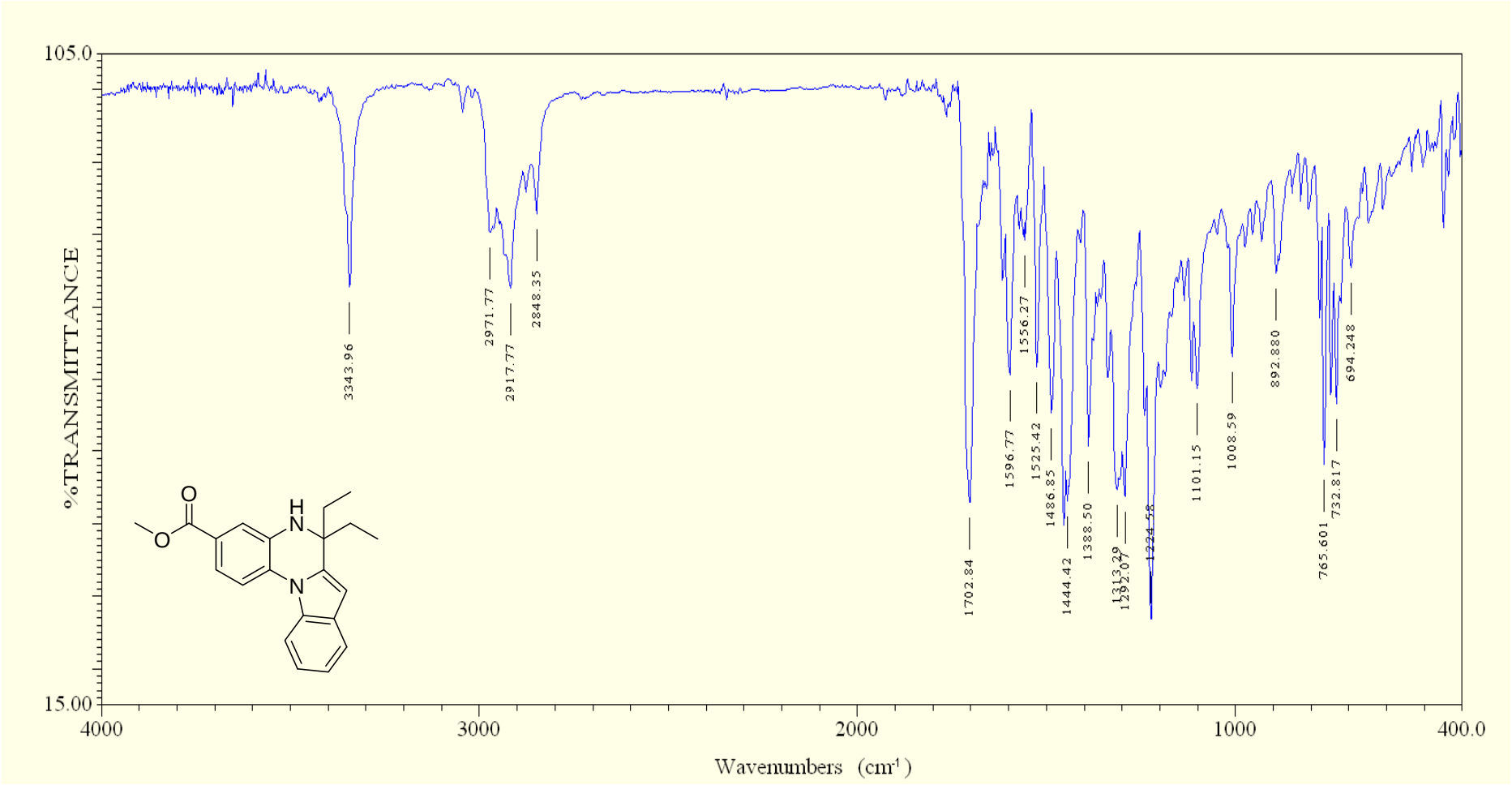

$^{13}$C NMR Spectrum (75 MHz) of compound **2e** in $CDCl_3$



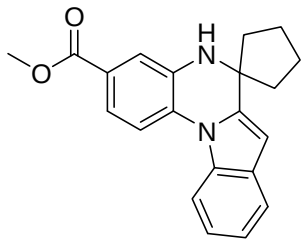

Low Resolution Mass Spectrum (LRMS) of compound **2e**

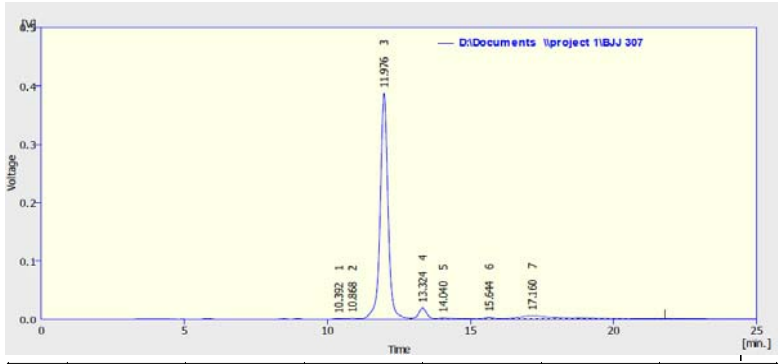



High Resolution Mass Spectrum (HRMS) of compound **2e**

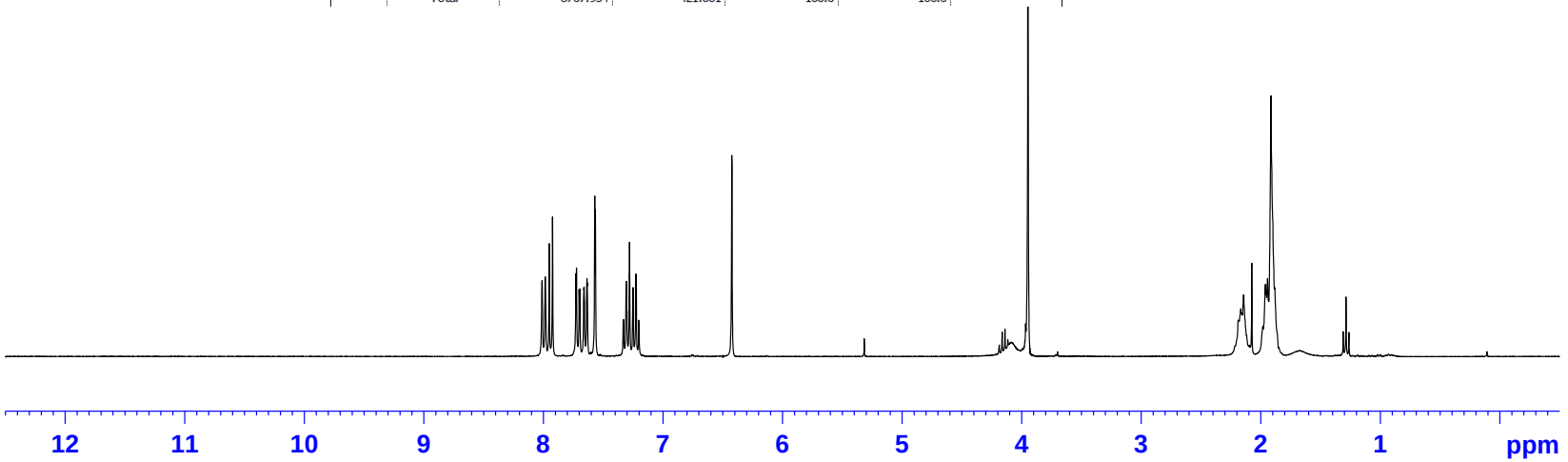



IR Spectrum of compound **2e** (Neat)

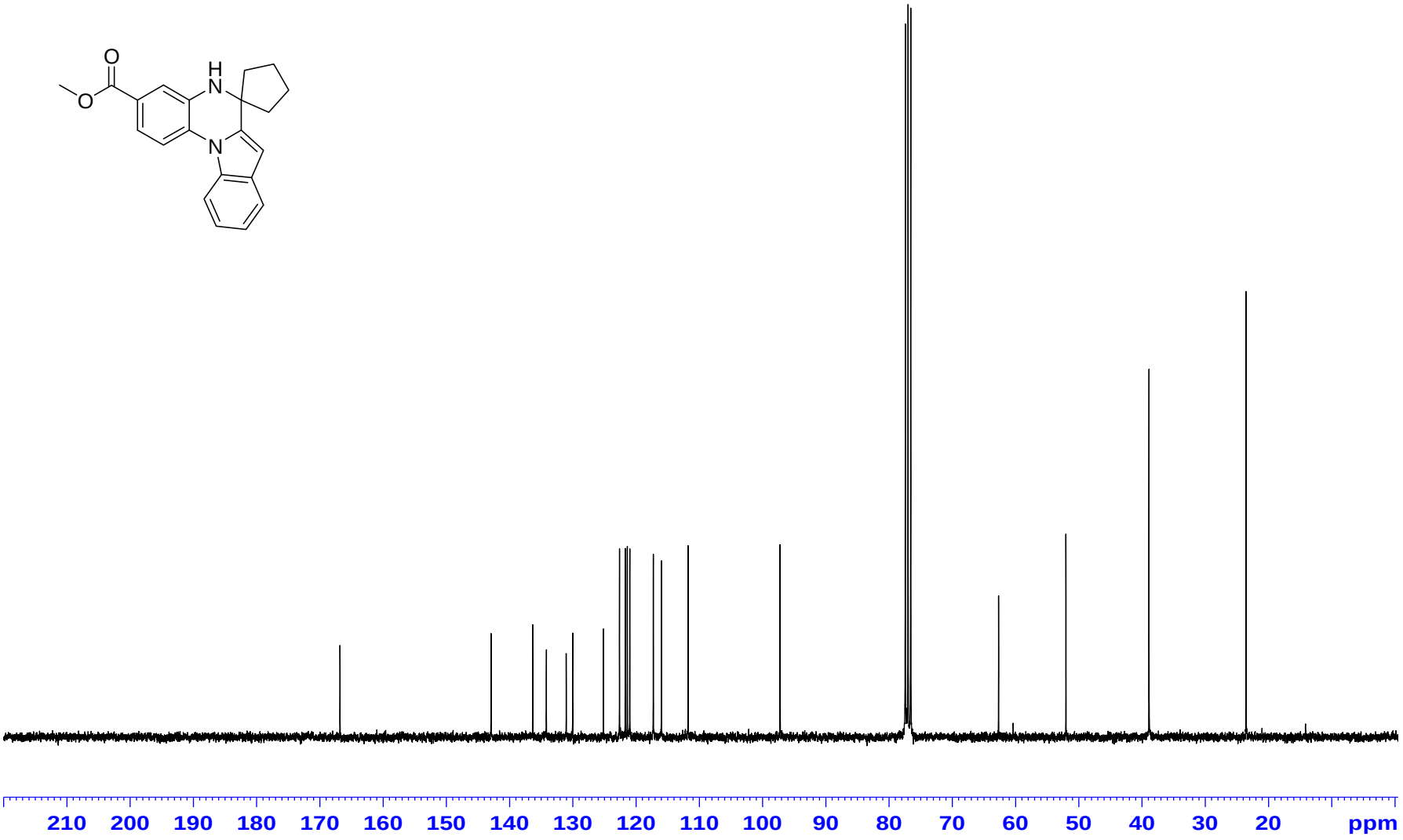


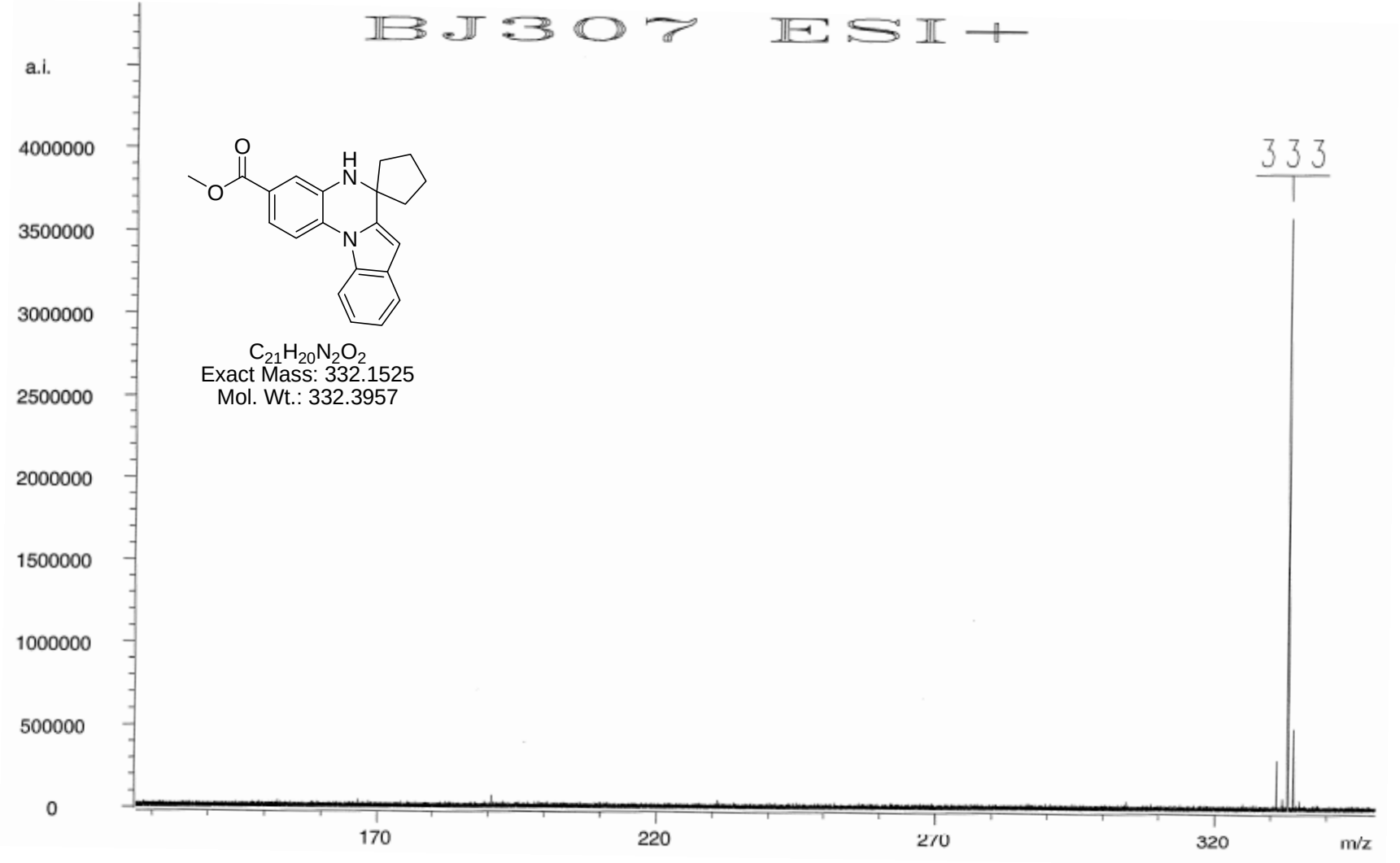

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 10.392 | 34.885 | 1.282 | 0.4 | 0.3 | 0.44 |
| 2 | 10.868 | 40.478 | 2.107 | 0.5 | 0.5 | 0.32 |
| 3 | 11.976 | 7460.768 | 387.678 | 85.7 | 92.1 | 0.27 |
| 4 | 13.324 | 394.352 | 19.227 | 4.5 | 4.6 | 0.30 |
| 5 | 14.040 | 93.224 | 2.248 | 1.1 | 0.5 | 0.64 |
| 6 | 15.644 | 82.636 | 3.257 | 0.9 | 0.8 | 0.37 |
| 7 | 17.160 | 601.610 | 5.262 | 6.9 | 1.2 | 1.50 |
| | Total | 8707.954 | 421.061 | 100.0 | 100.0 | |



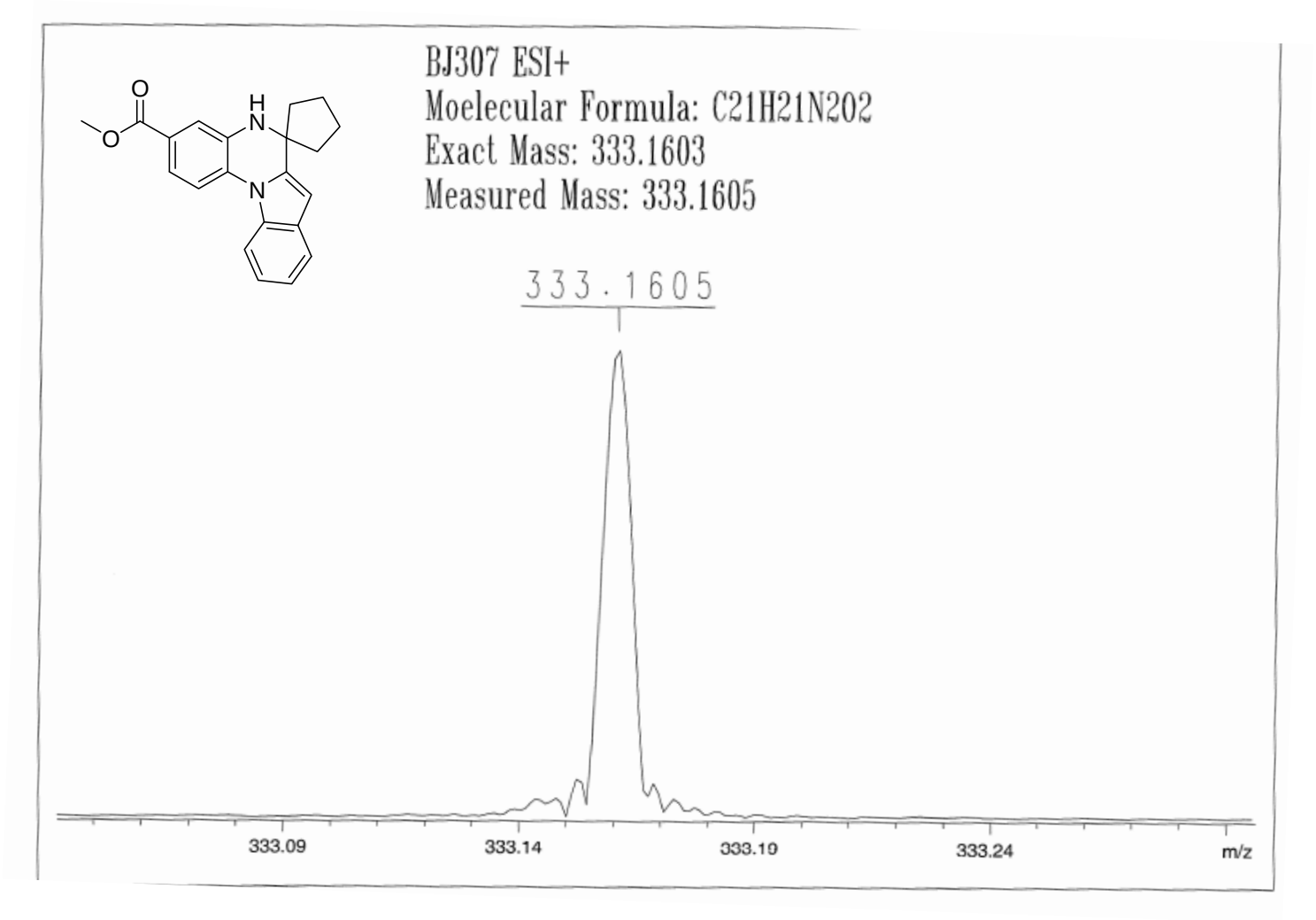

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **2f** in $CDCl_3$



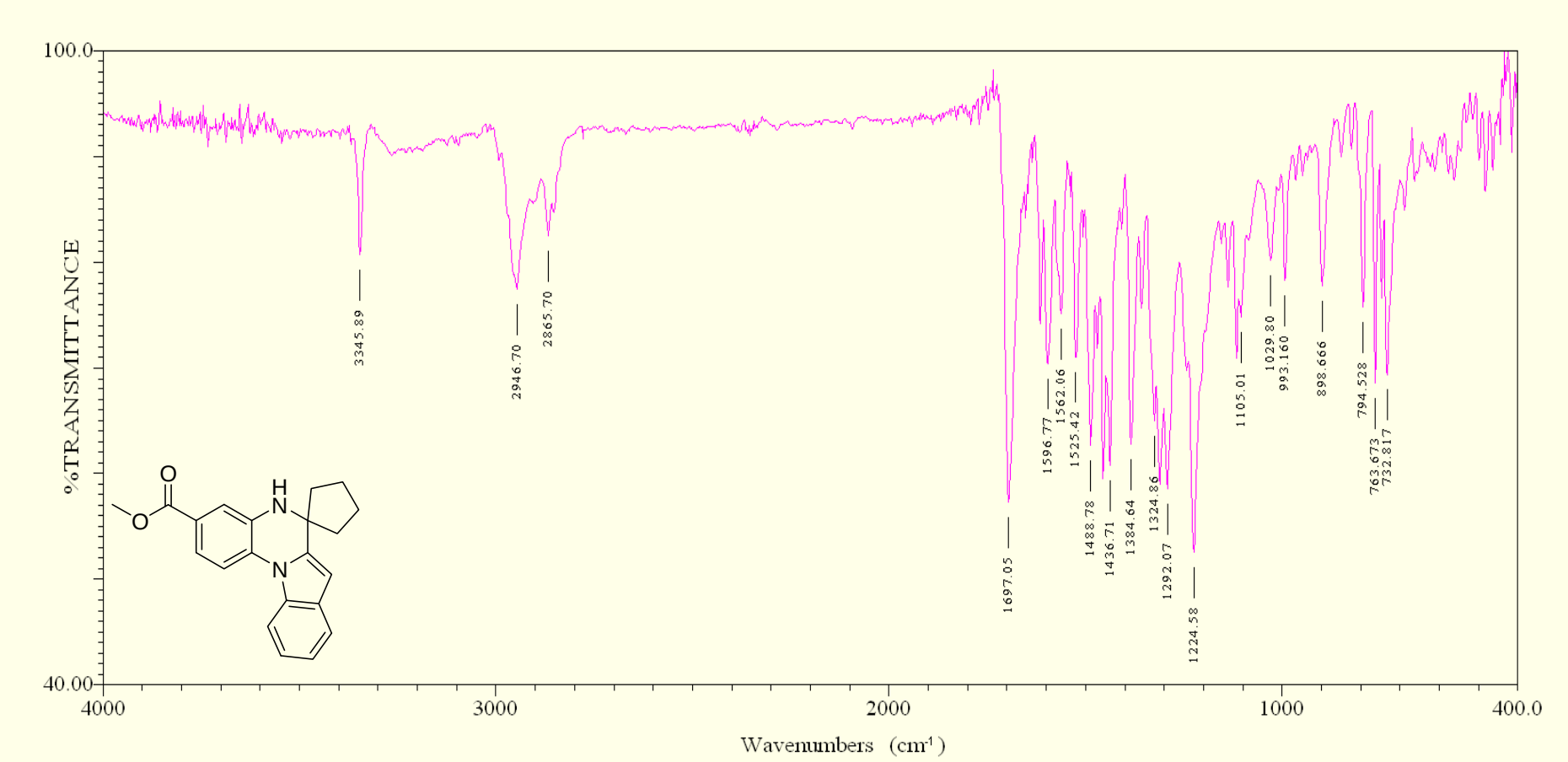

$^{13}C$ NMR Spectrum (75 MHz) of compound **2f** in $CDCl_3$



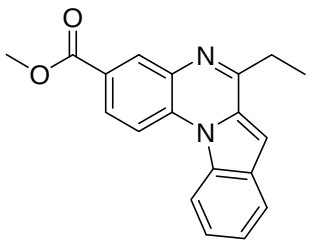

Low Resolution Mass Spectrum (LRMS) of compound **2f**

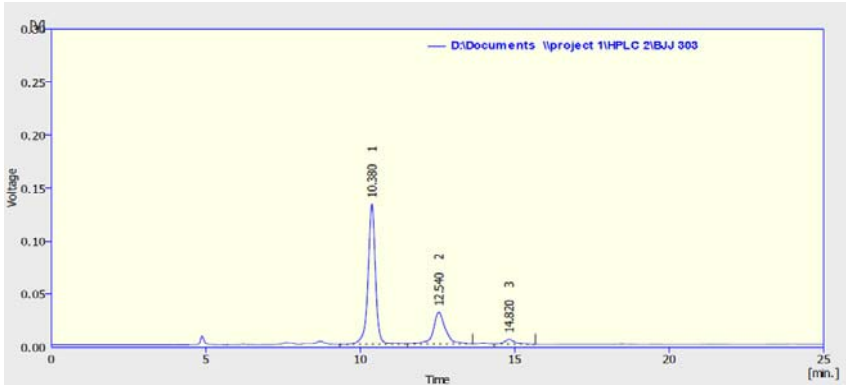



High Resolution Mass Spectrum (HRMS) of compound **2f**

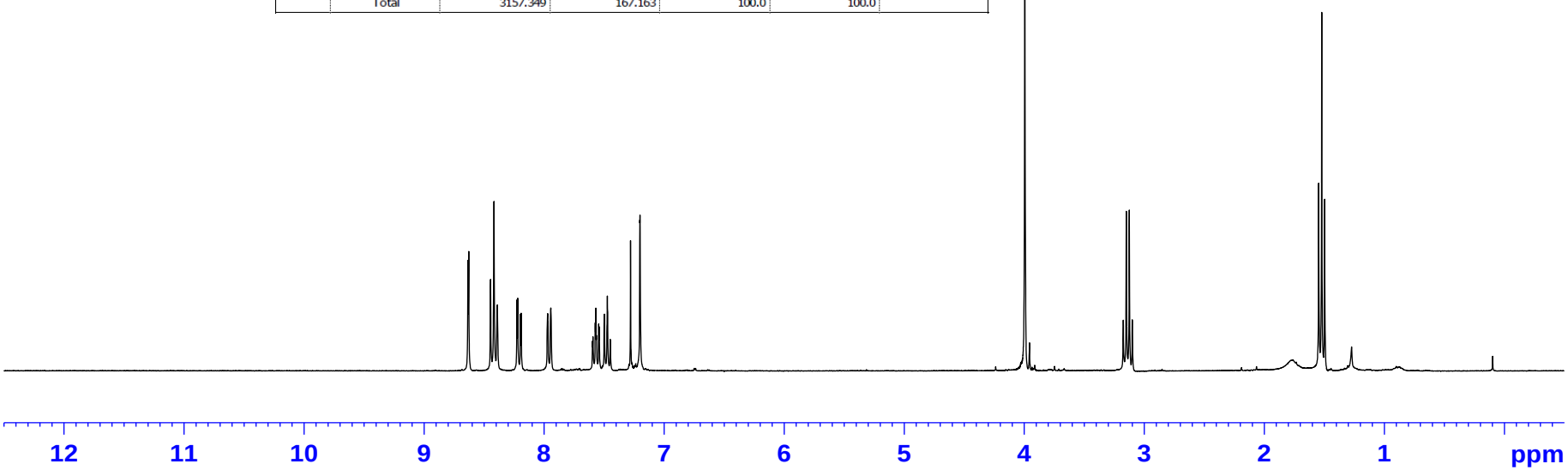



IR Spectrum of compound **2f** (Neat)

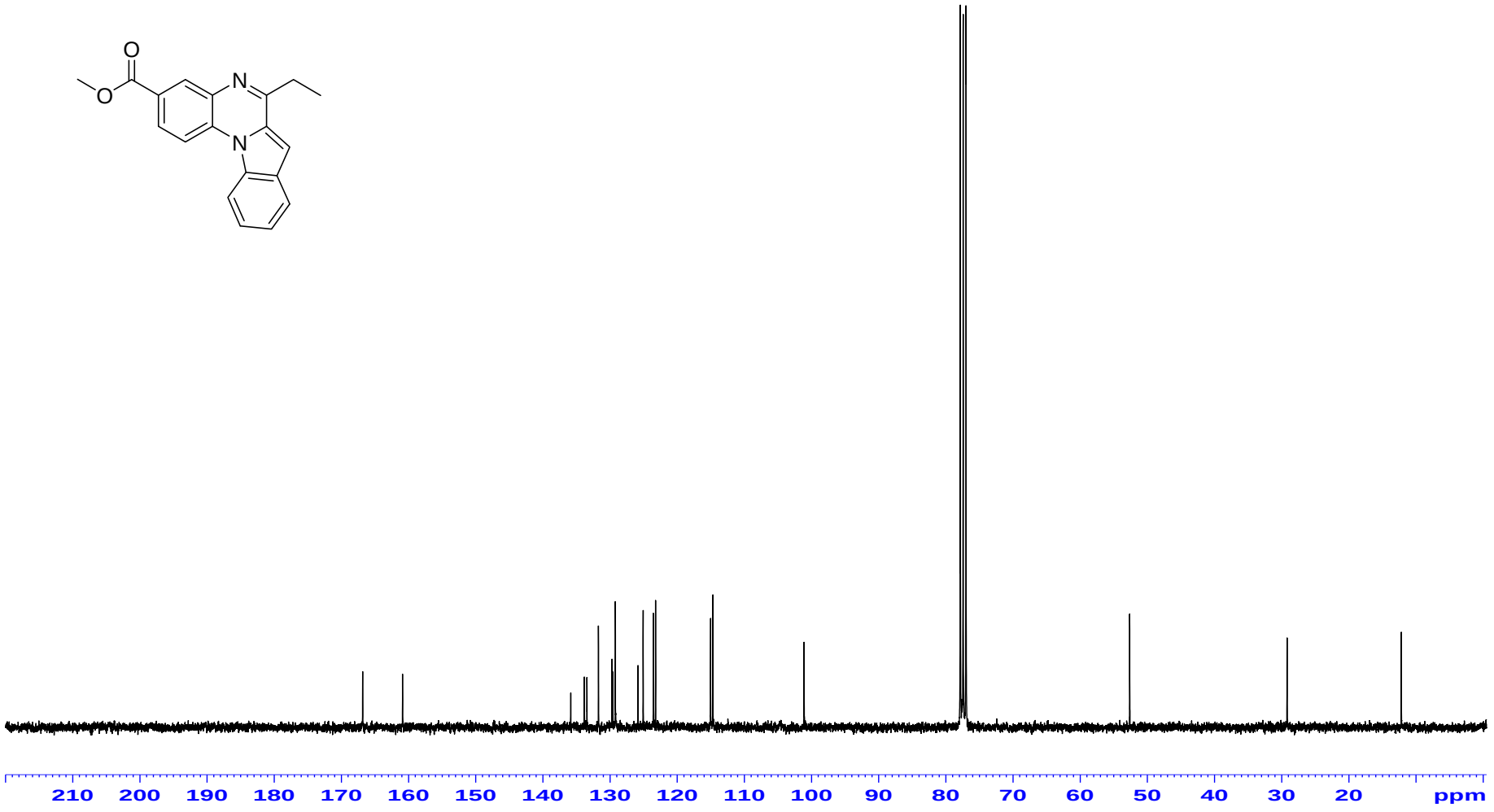


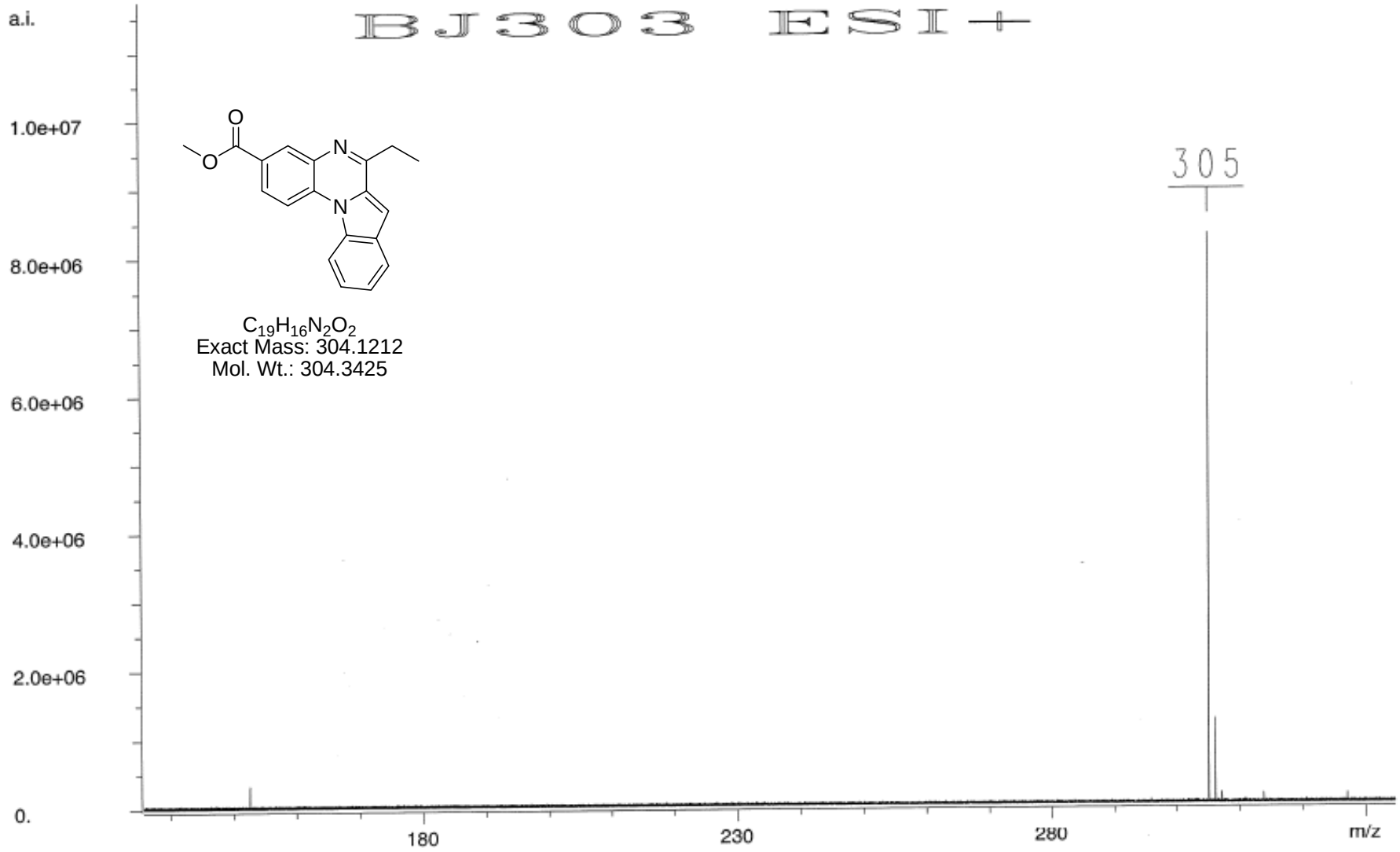

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 10.380 | 2215.581 | 132.418 | 70.2 | 79.2 | 0.24 |
| 2 | 12.540 | 831.541 | 30.217 | 26.3 | 18.1 | 0.37 |
| 3 | 14.820 | 110.227 | 4.528 | 3.5 | 2.7 | 0.34 |
| | Total | 3157.349 | 167.163 | 100.0 | 100.0 | |



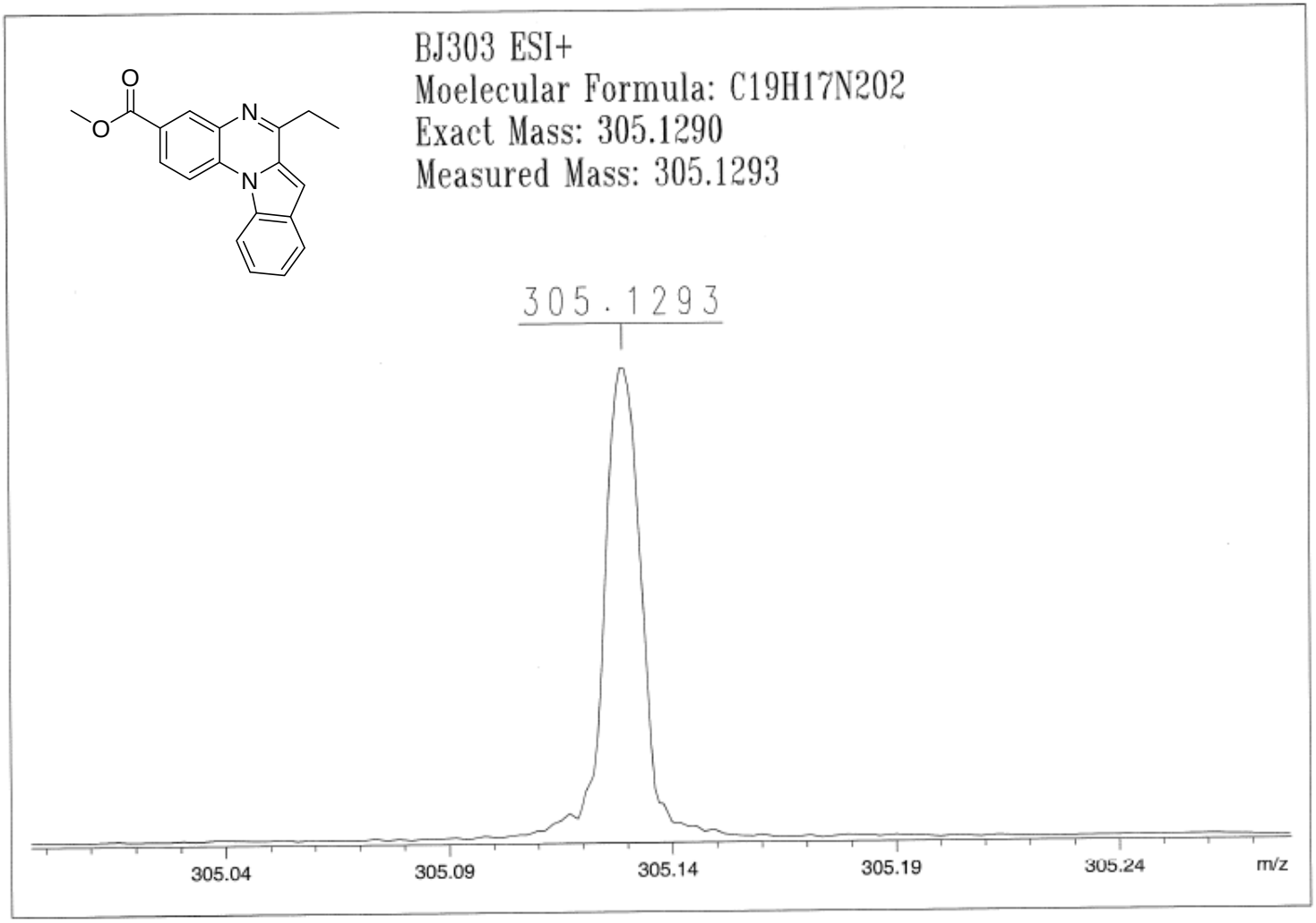

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **3a** in $CDCl_3$



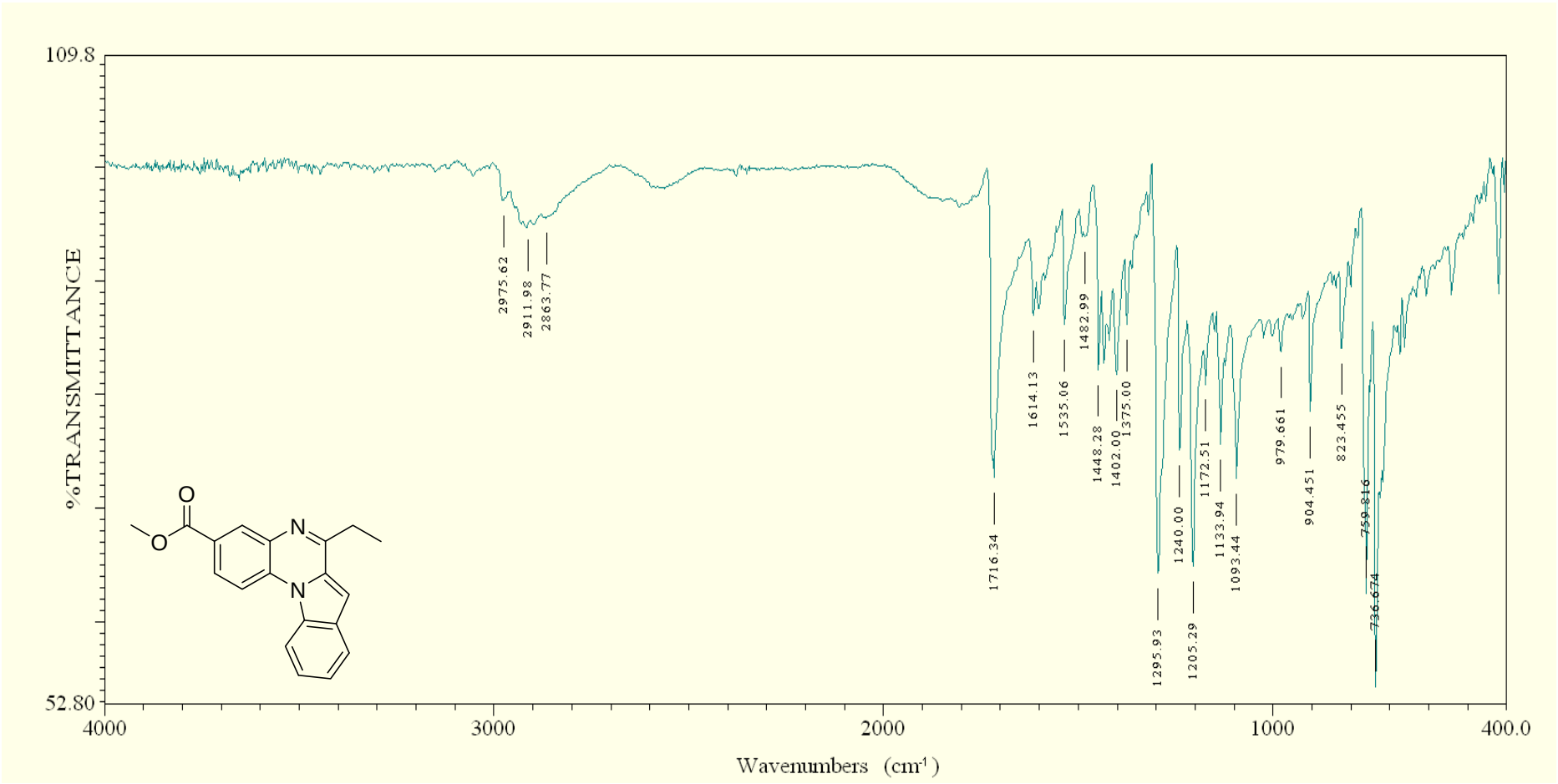

$^{13}$C NMR Spectrum (75 MHz) of compound **3a** in $CDCl_3$



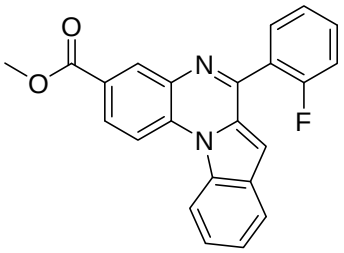

Low Resolution Mass Spectrum (LRMS) of compound **3a**

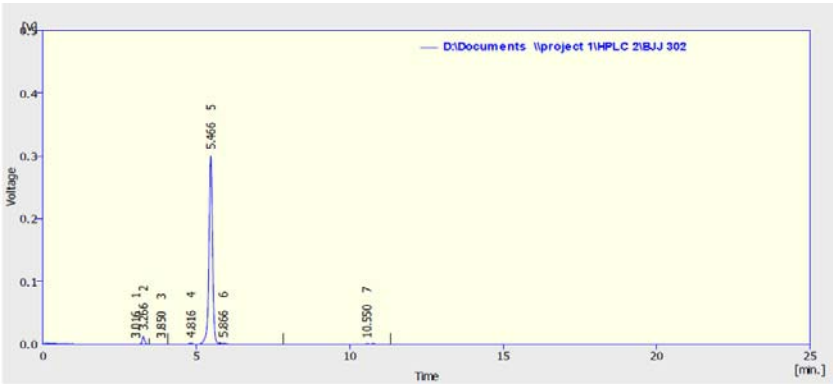



High Resolution Mass Spectrum (HRMS) of compound **3a**

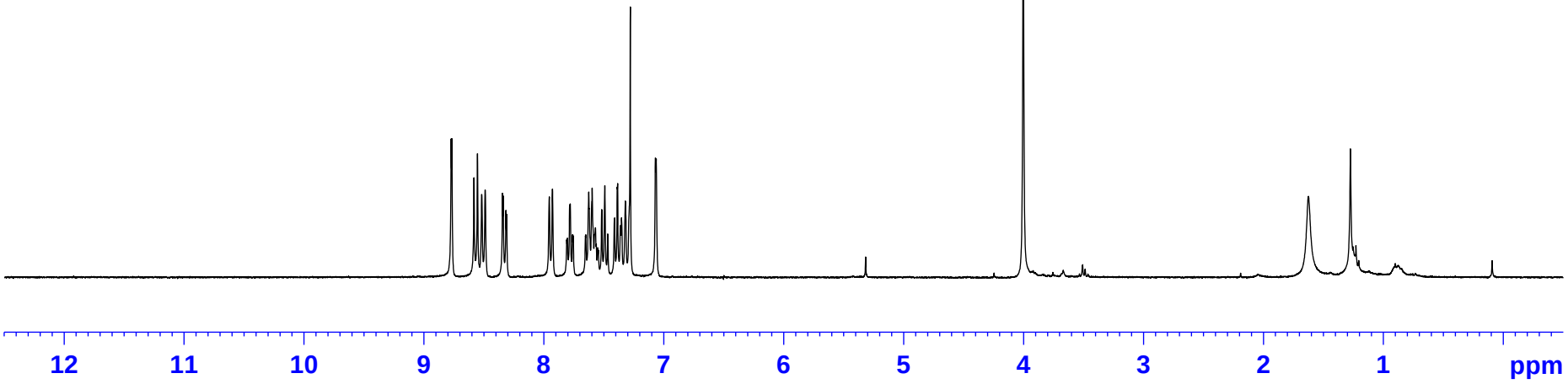



IR Spectrum of compound **3a** (Neat)

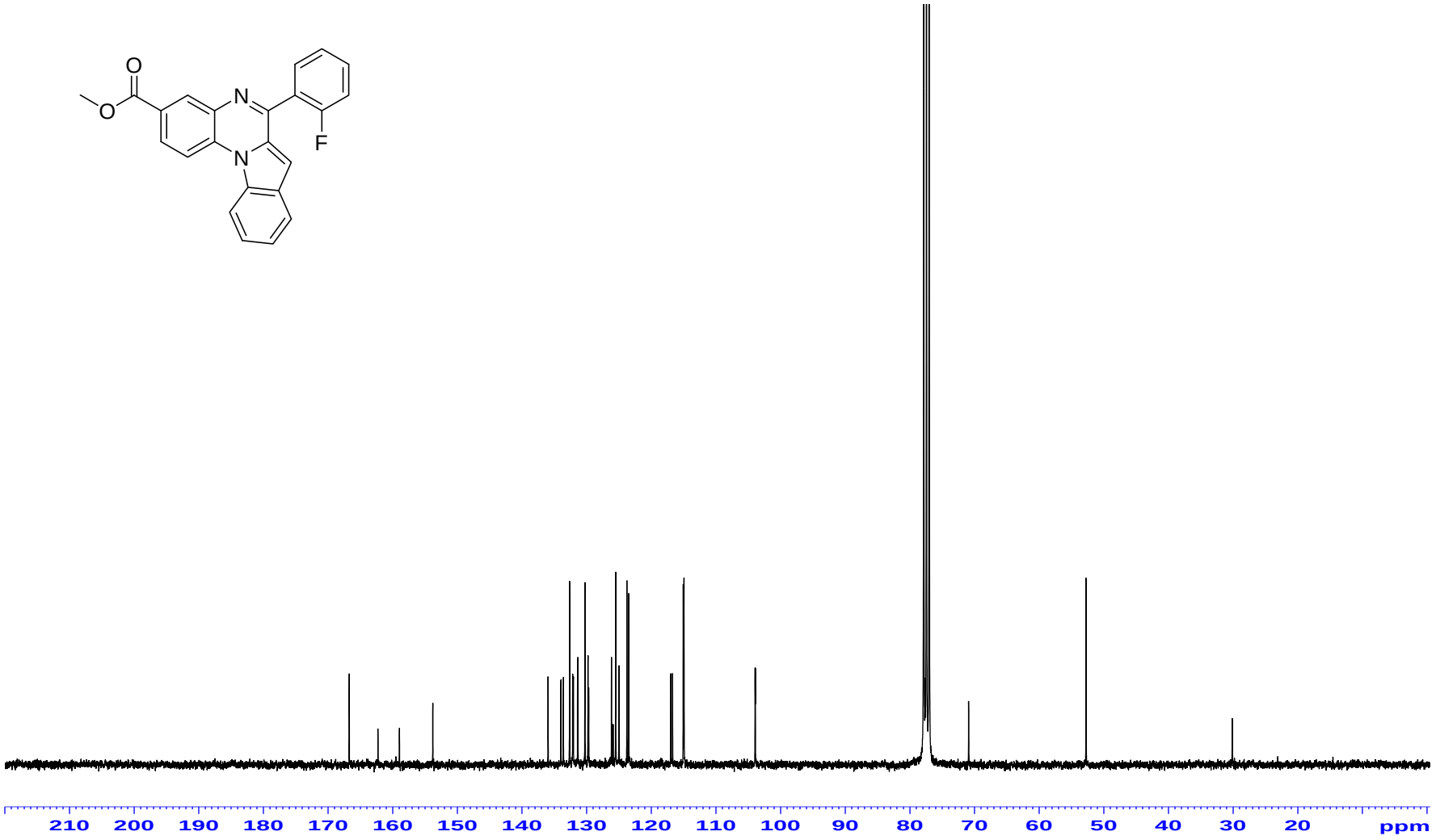


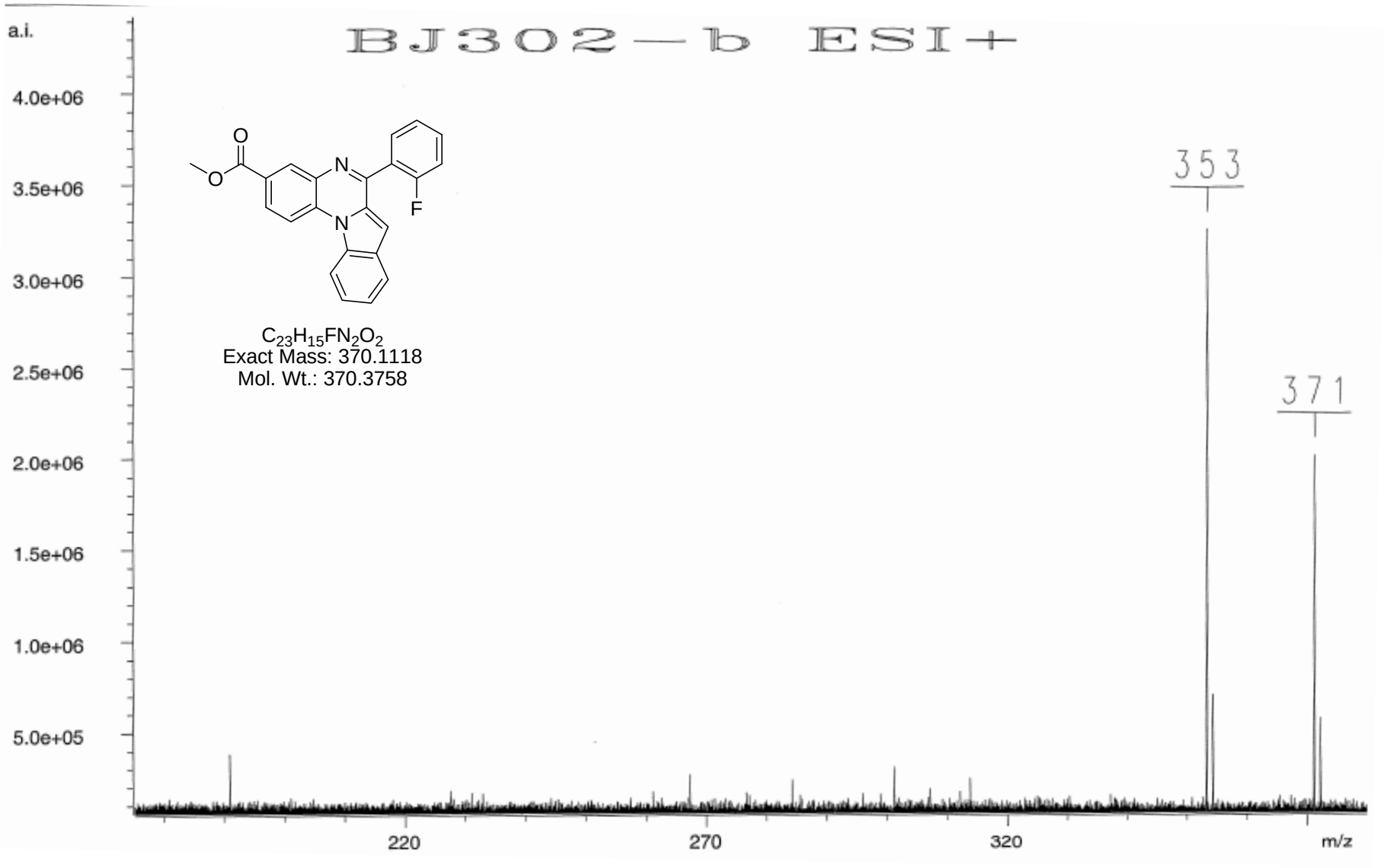

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 6.032 | 20.295 | 1.352 | 0.4 | 0.4 | 0.28 |
| 2 | 6.532 | 335.459 | 17.056 | 6.0 | 5.2 | 0.21 |
| 3 | 7.700 | 223.148 | 3.466 | 4.0 | 1.1 | 0.98 |
| 4 | 9.632 | 25.530 | 1.463 | 0.5 | 0.4 | 0.23 |
| 5 | 10.932 | 4893.142 | 300.932 | 87.8 | 92.3 | 0.24 |
| 6 | 11.732 | 58.911 | 1.493 | 1.1 | 0.5 | 0.37 |
| 7 | 21.100 | 16.927 | 0.261 | 0.3 | 0.1 | 1.01 |
| | Total | 5573.413 | 326.024 | 100.0 | 100.0 | |




HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **3b** in $CDCl_3$

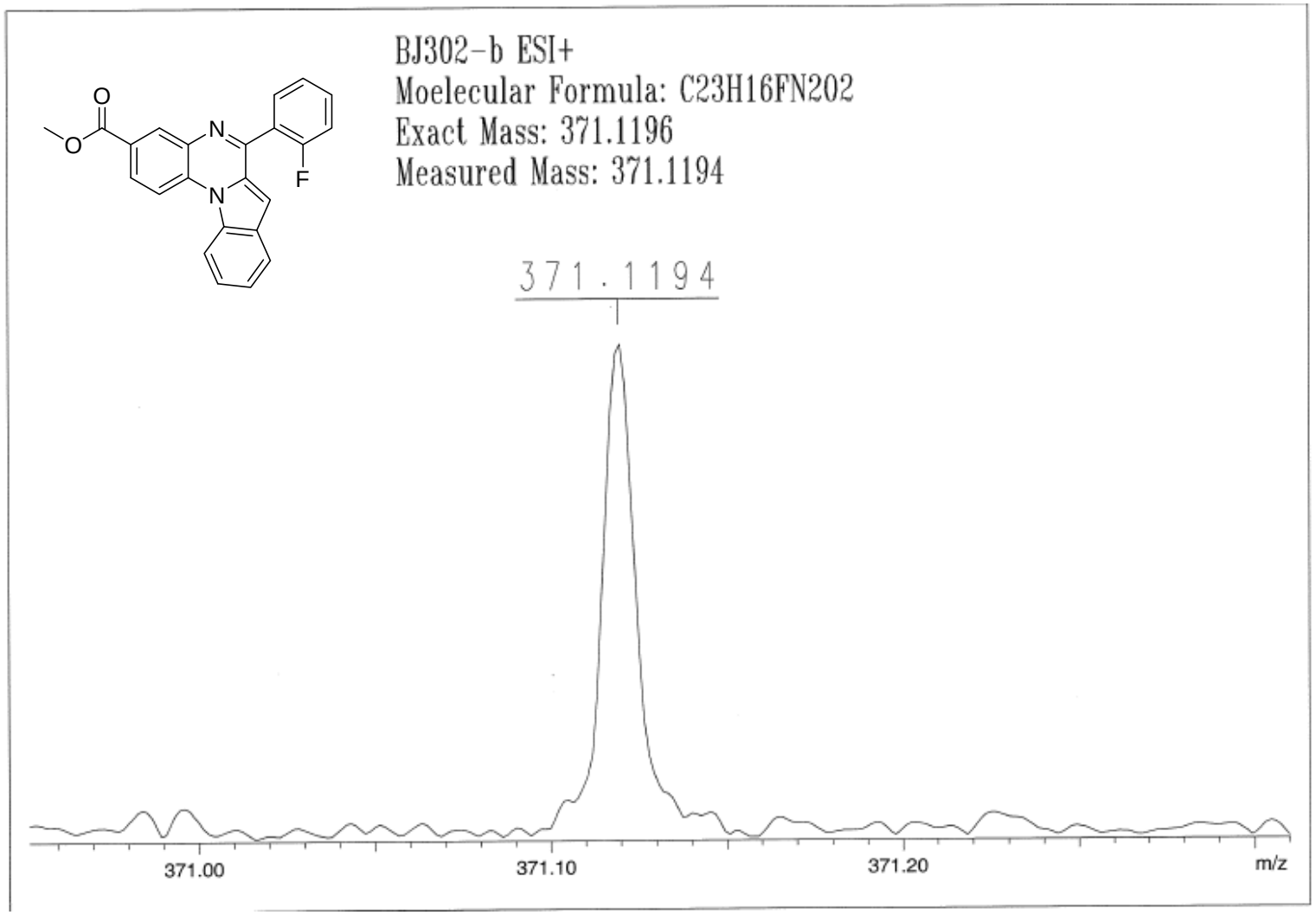



$^{13}C$ NMR Spectrum (75 MHz) of compound **3b** in $CDCl_3$

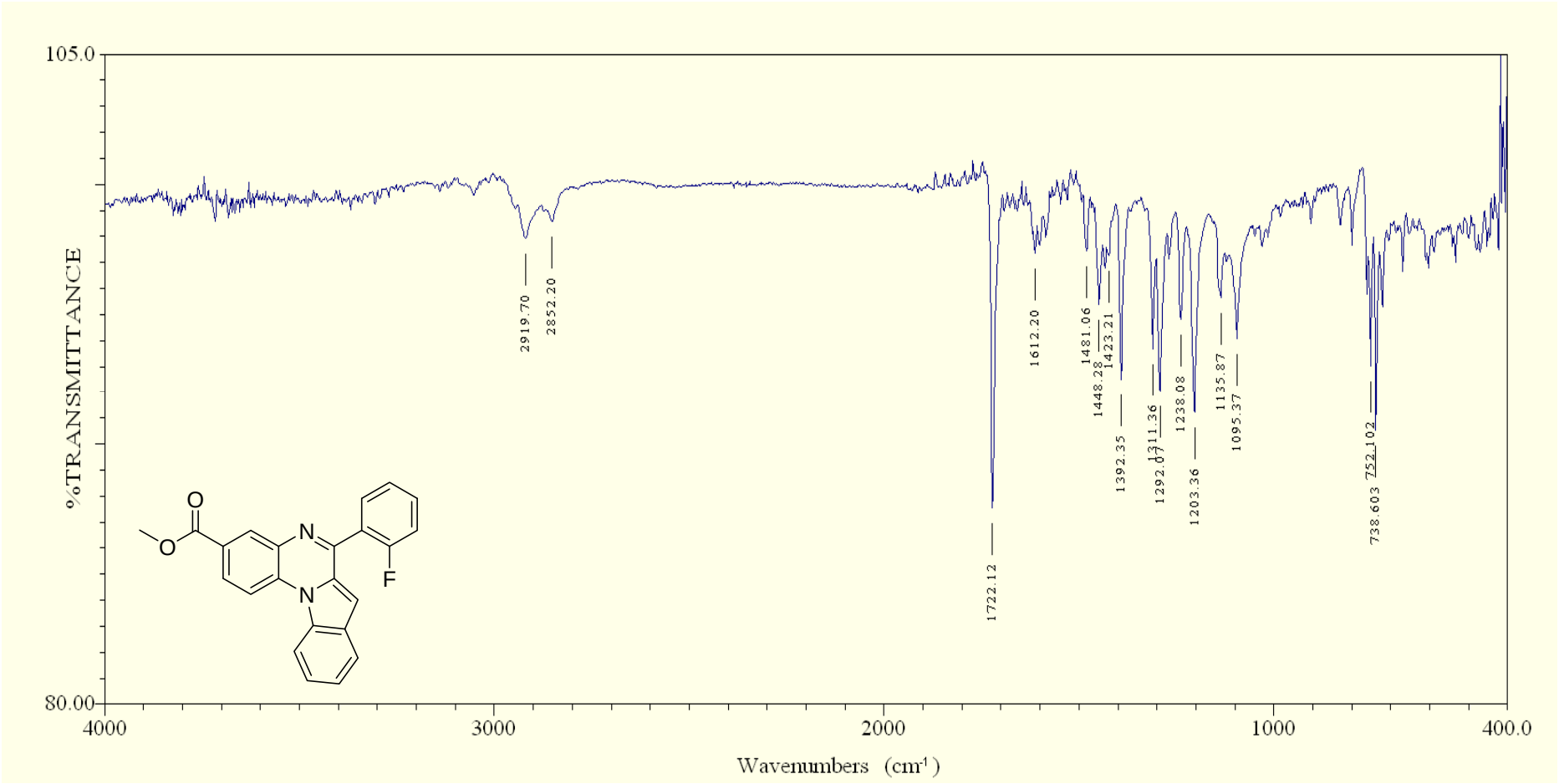



$C_{23}H_{15}FN_2O_2$
Exact Mass: 370.1118
Mol. Wt.: 370.3758

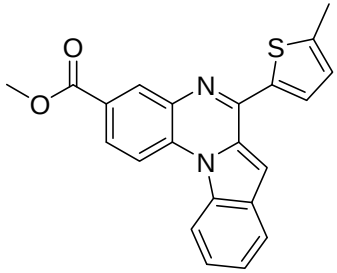
Low Resolution Mass Spectrum (LRMS) of compound **3b**

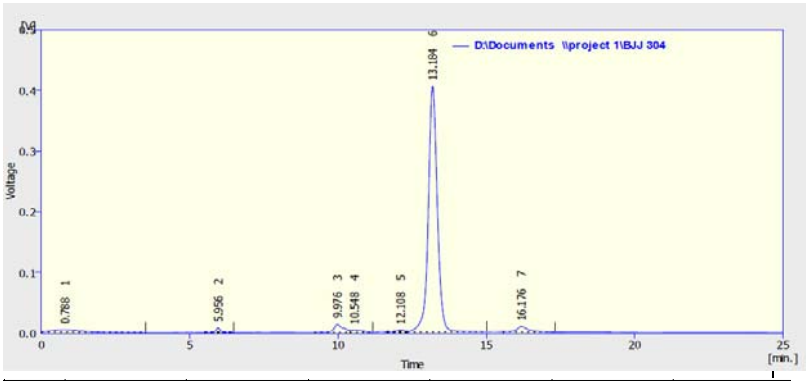



High Resolution Mass Spectrum (HRMS) of compound **3b**




IR Spectrum of compound **3b** (Neat)

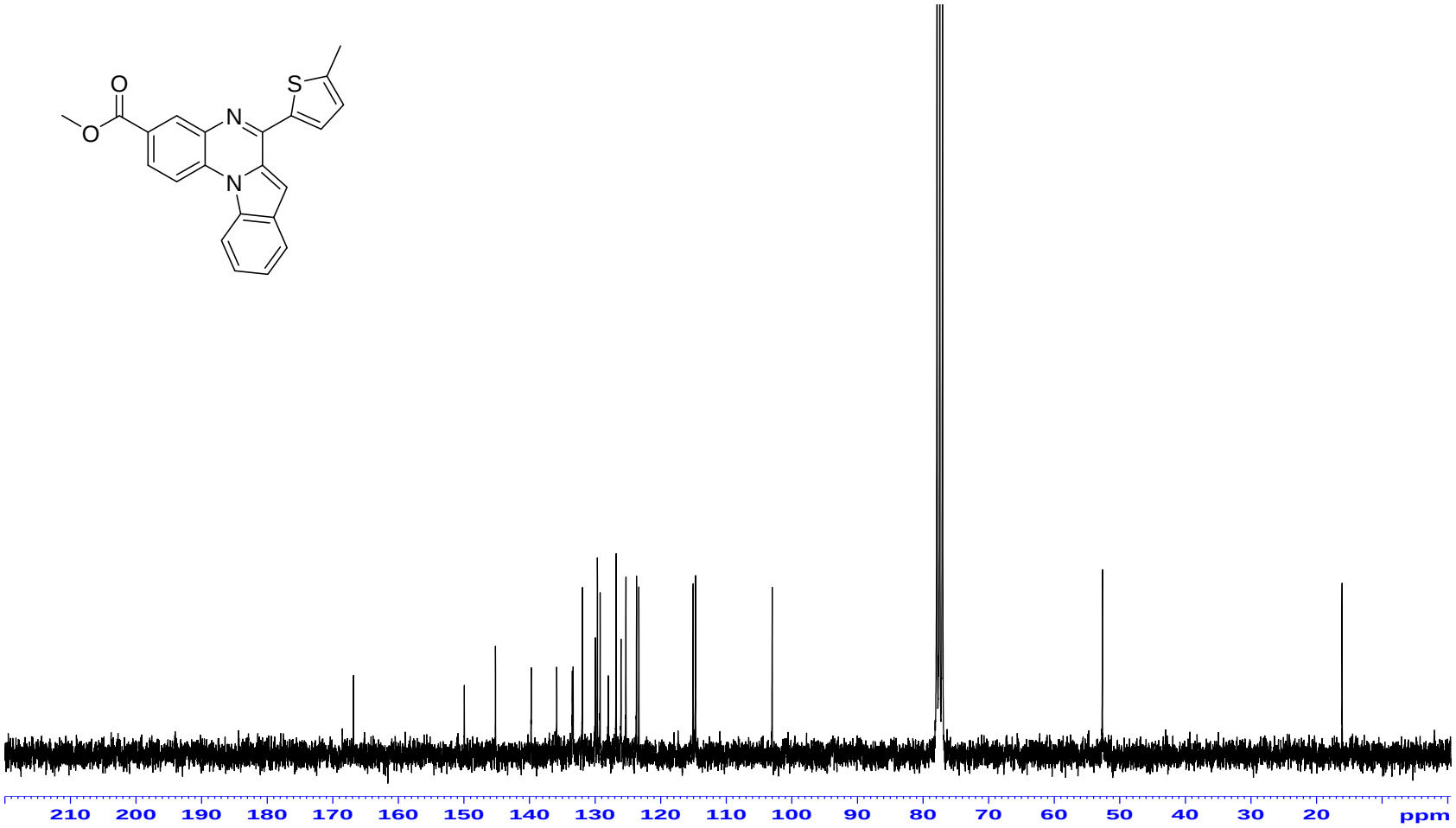


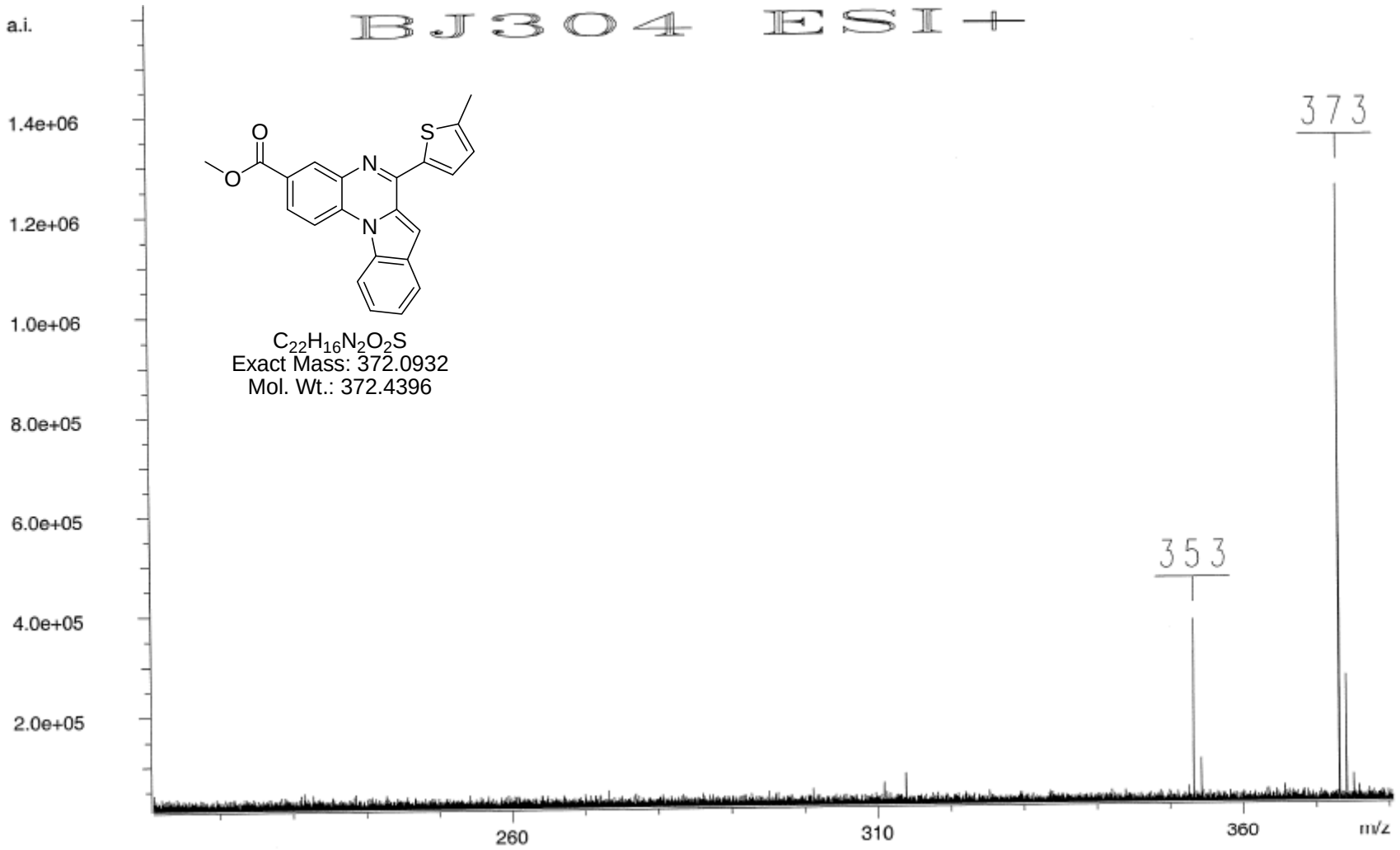

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 0.788 | 227.838 | 3.618 | 2.4 | 0.8 | 0.95 |
| 2 | 5.956 | 71.667 | 7.678 | 0.8 | 1.7 | 0.14 |
| 3 | 9.976 | 281.200 | 13.194 | 3.0 | 3.0 | 0.35 |
| 4 | 10.548 | 91.675 | 3.704 | 1.0 | 0.8 | 0.47 |
| 5 | 12.108 | 51.149 | 2.971 | 0.5 | 0.7 | 0.26 |
| 6 | 13.184 | 8524.755 | 404.894 | 90.0 | 91.0 | 0.31 |
| 7 | 16.176 | 221.562 | 8.716 | 2.3 | 2.0 | 0.34 |
| | Total | 9469.845 | 444.776 | 100.0 | 100.0 | |



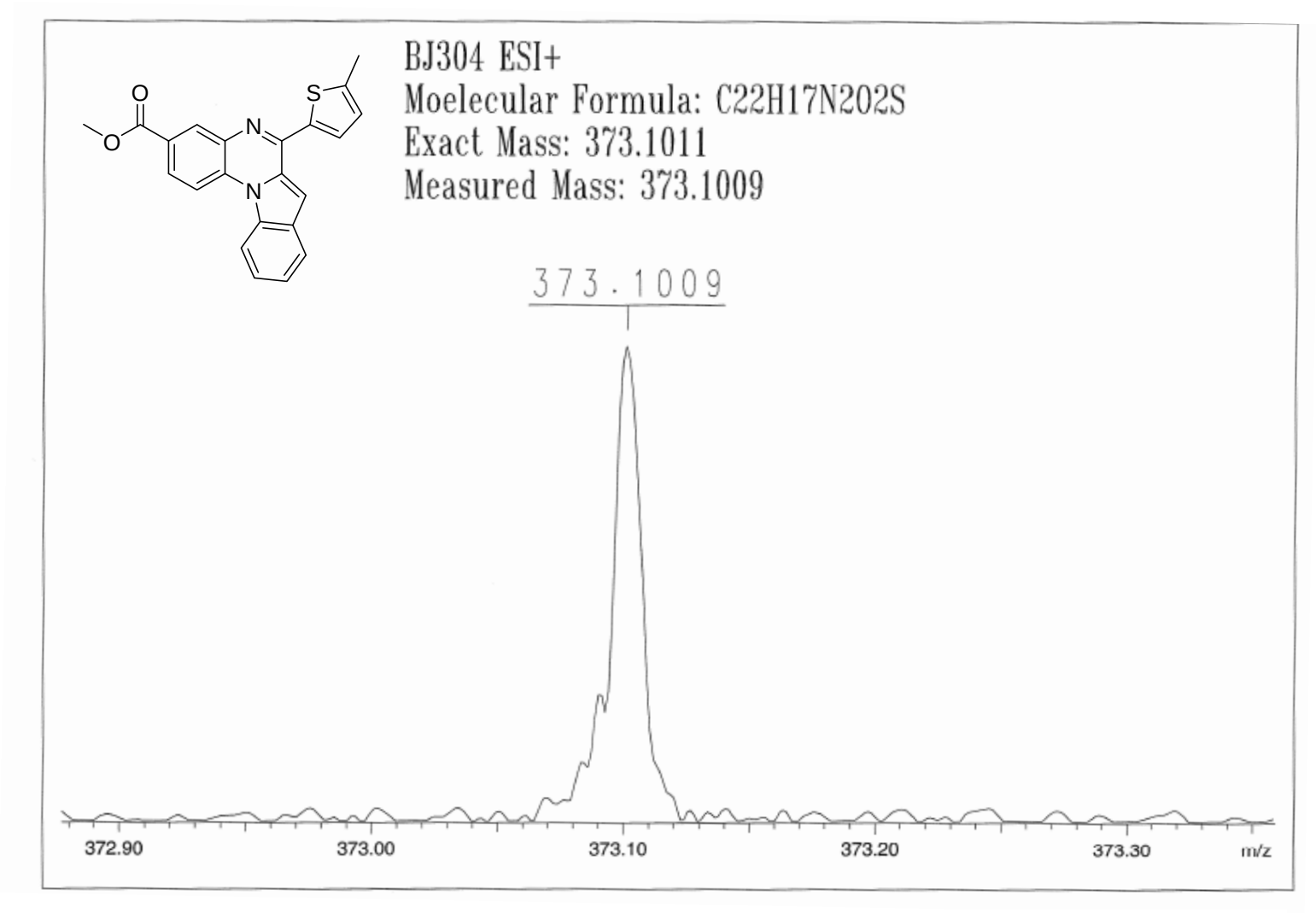

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **3c** in $CDCl_3$



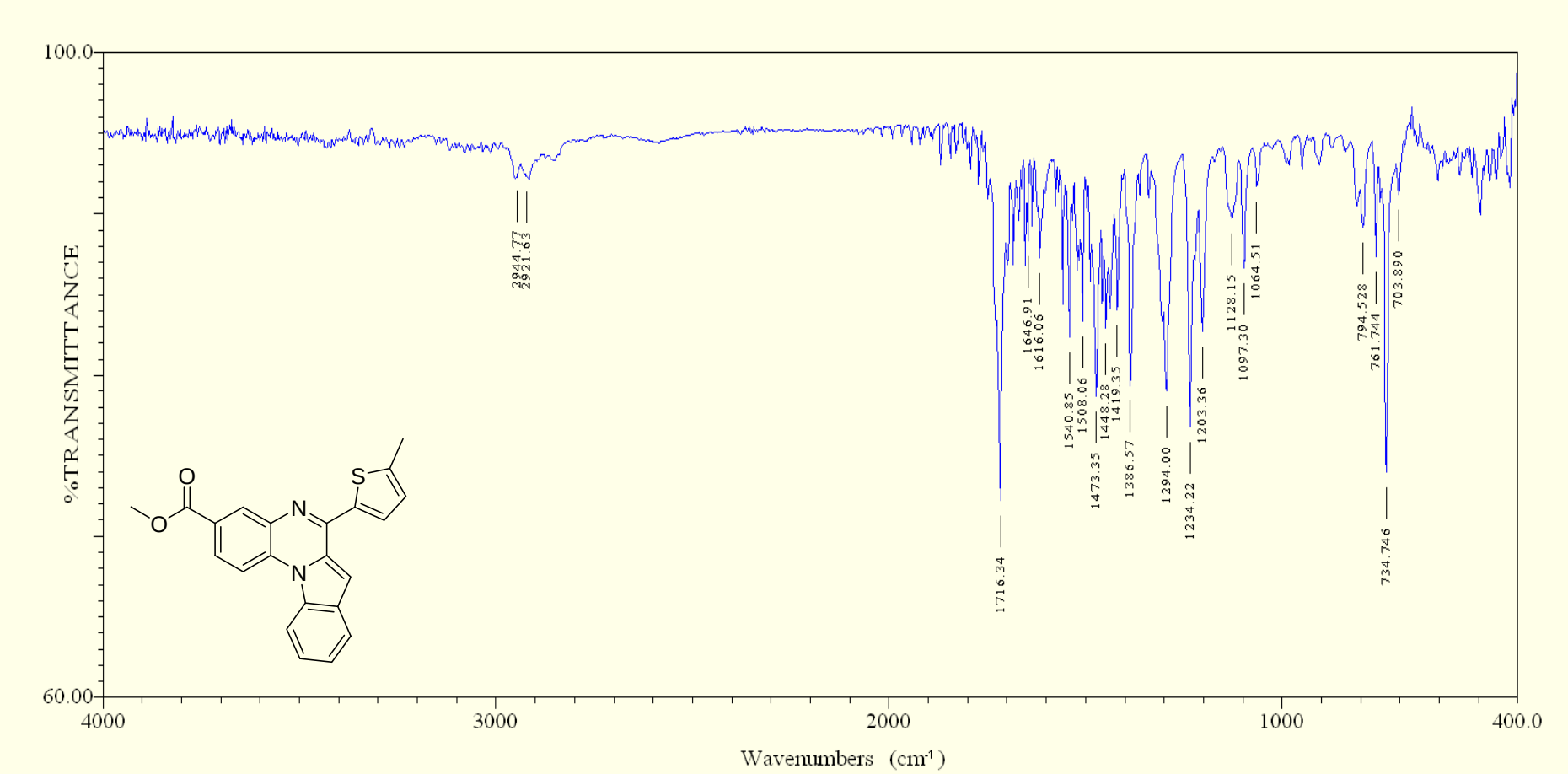

$^{13}C$ NMR Spectrum (75 MHz) of compound **3c** in $CDCl_3$



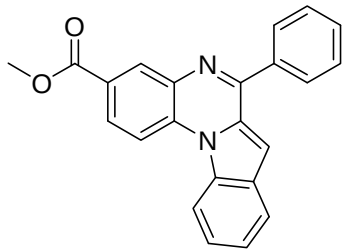

Low Resolution Mass Spectrum (LRMS) of compound **3c**

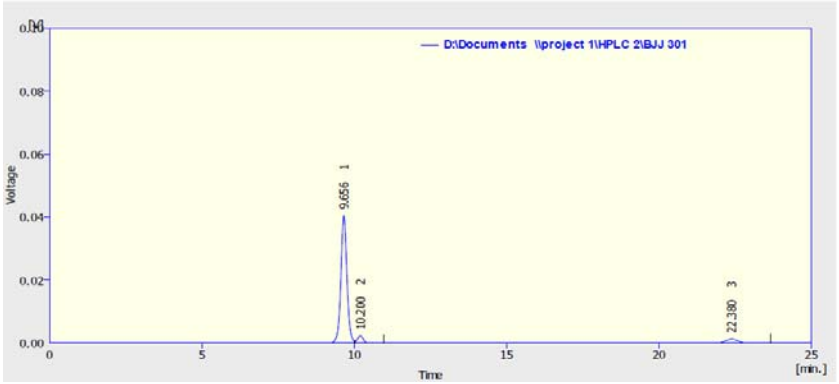



High Resolution Mass Spectrum (HRMS) of compound **3c**

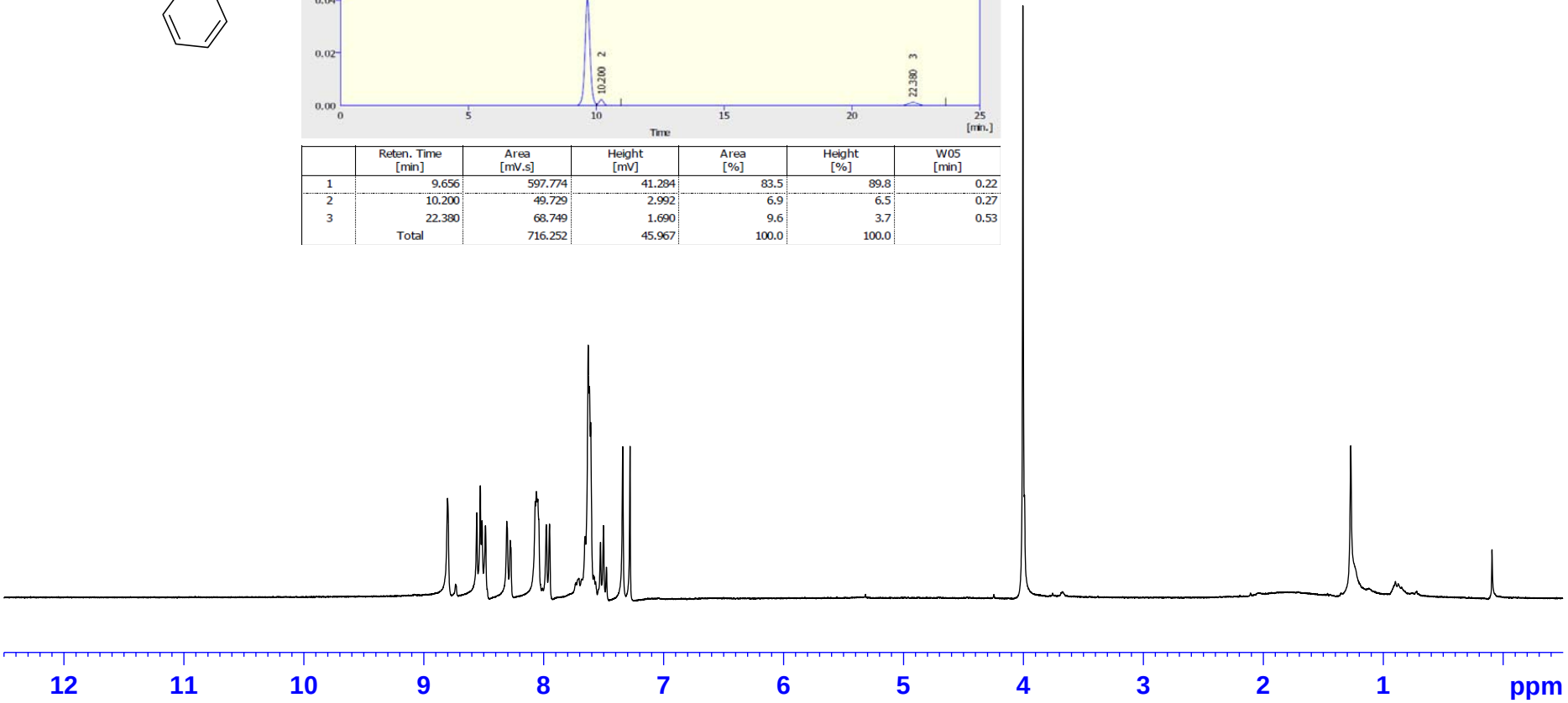



IR Spectrum of compound **3c** (Neat)

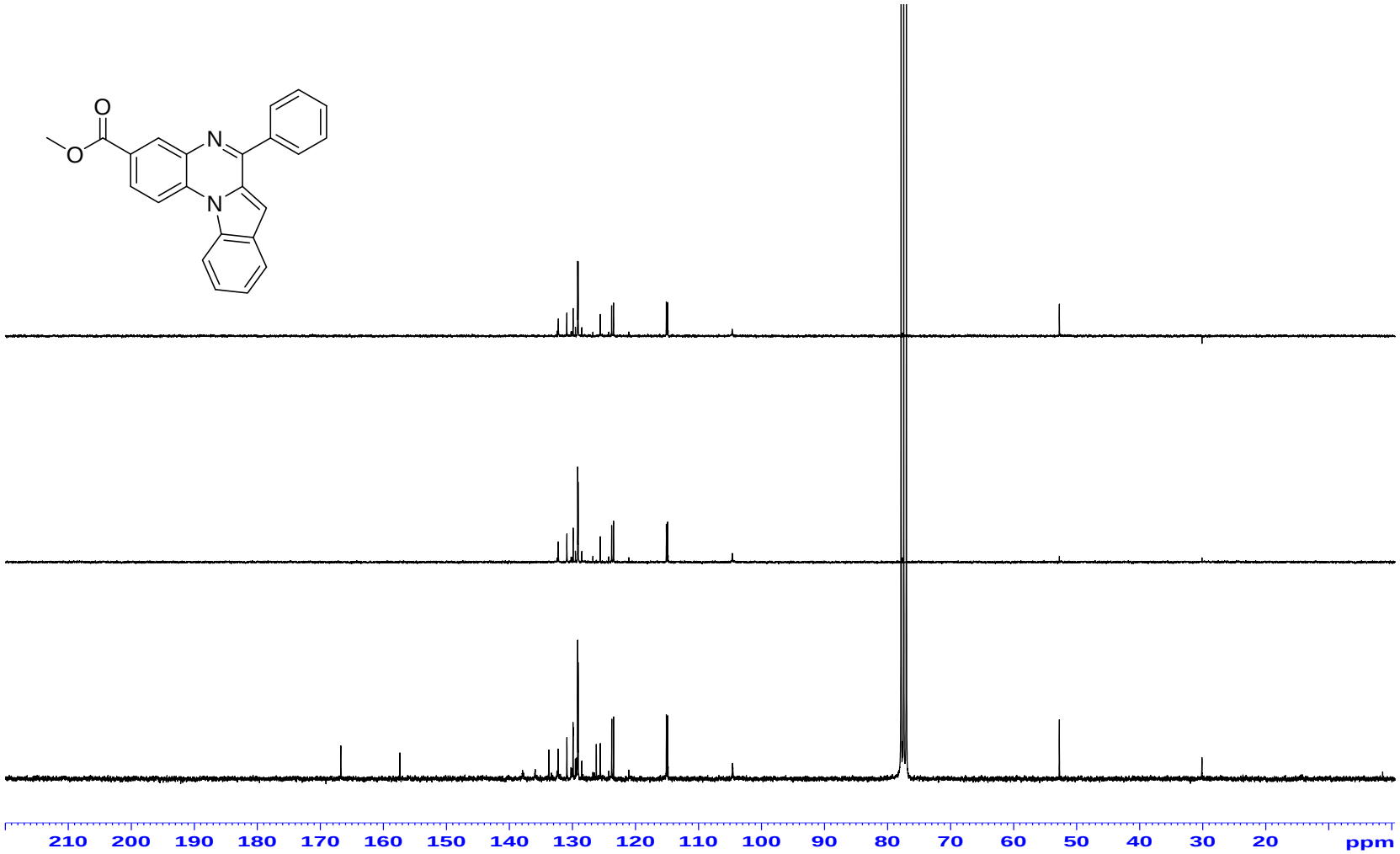


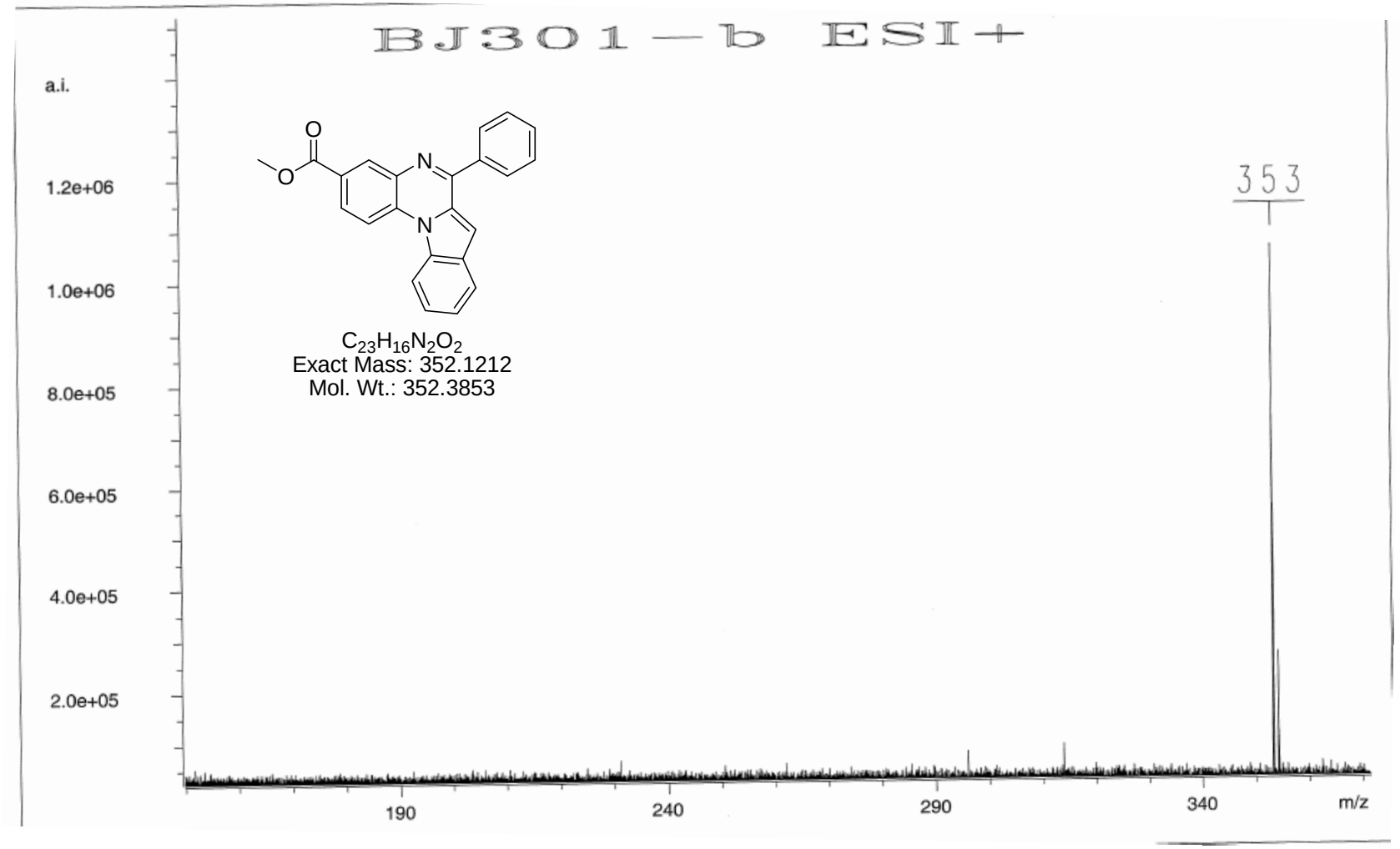

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 9.656 | 597.774 | 41.284 | 83.5 | 89.8 | 0.22 |
| 2 | 10.200 | 49.729 | 2.992 | 6.9 | 6.5 | 0.27 |
| 3 | 22.380 | 68.749 | 1.690 | 9.6 | 3.7 | 0.53 |
| | Total | 716.252 | 45.967 | 100.0 | 100.0 | |



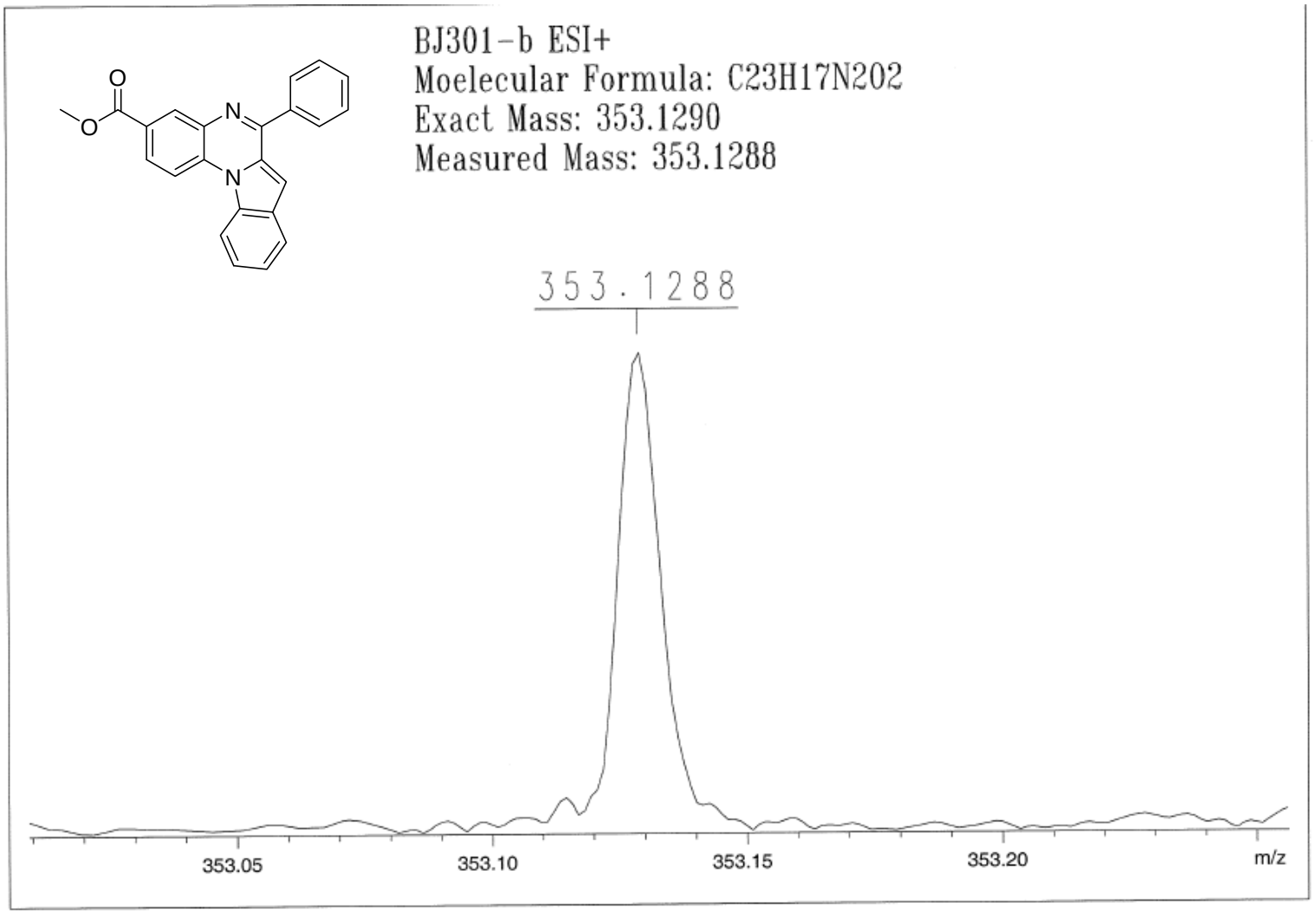

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **3d** in $CDCl_3$



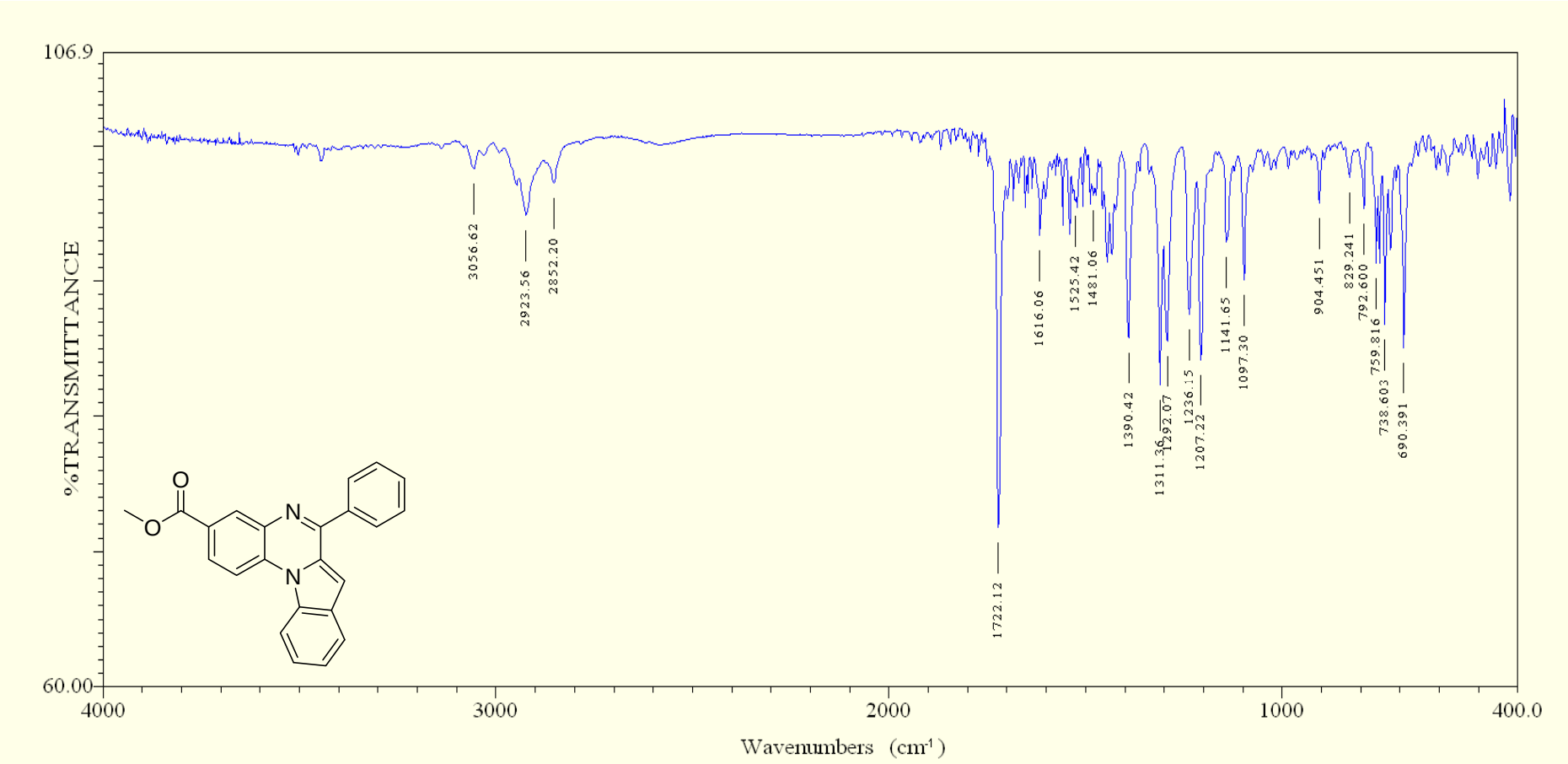

$^{13}C$, DEPT NMR Spectrum (75 MHz) of compound **3d** in $CDCl_3$



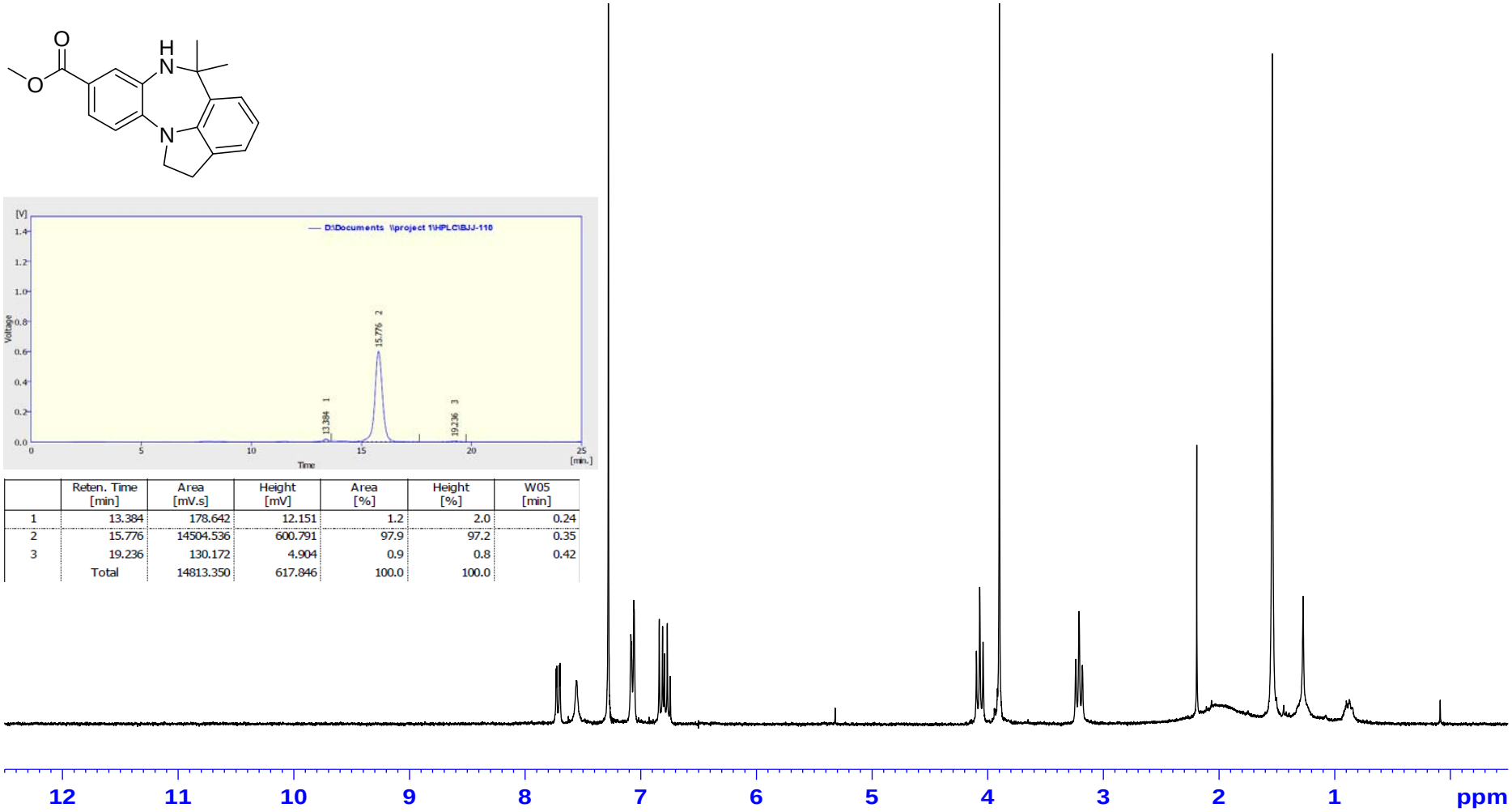

Low Resolution Mass Spectrum (LRMS) of compound **3d**




High Resolution Mass Spectrum (HRMS) of compound **3d**

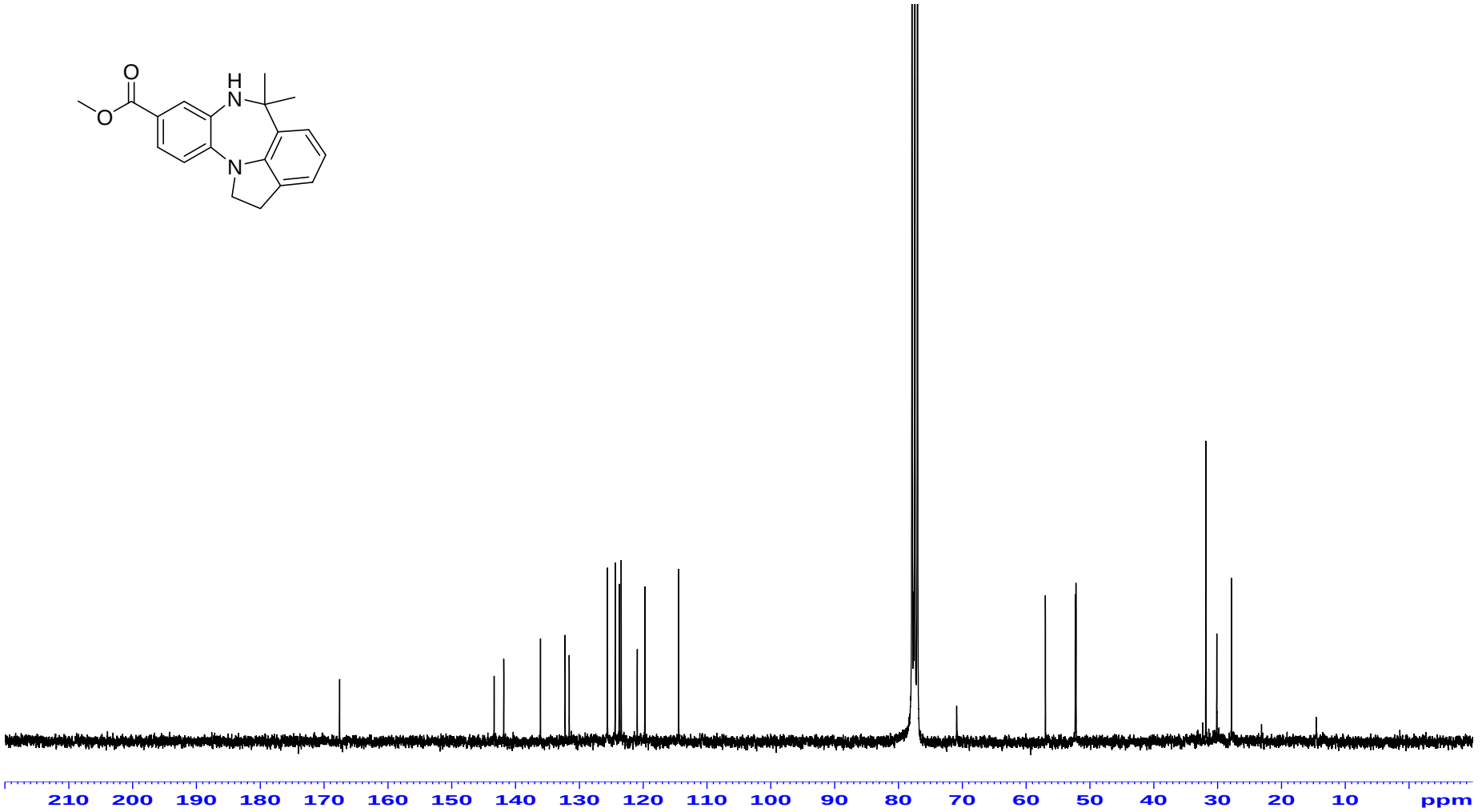



IR Spectrum of compound **3d** (Neat)

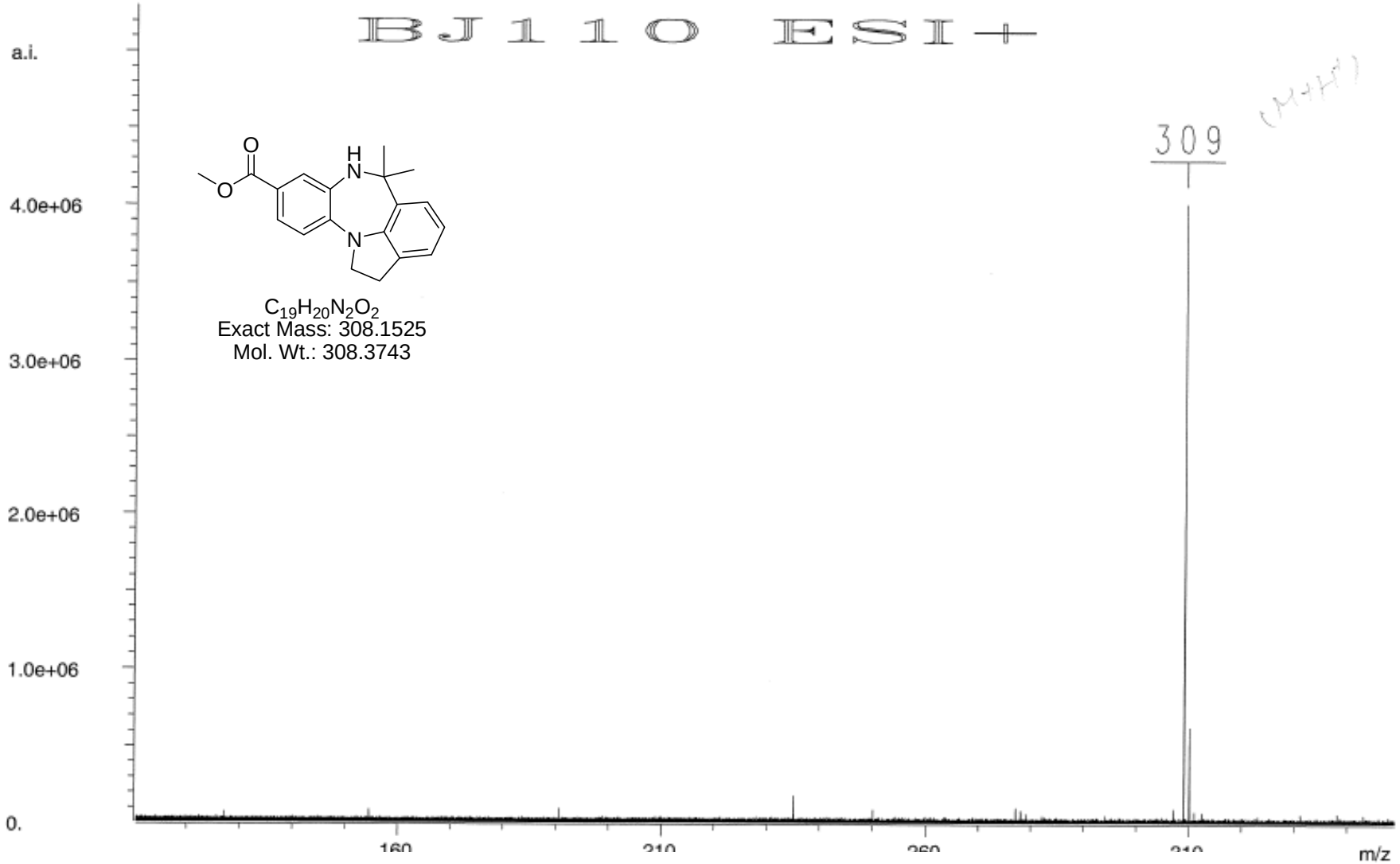



| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 13.384 | 178.642 | 12.151 | 1.2 | 2.0 | 0.24 |
| 2 | 15.776 | 14504.536 | 600.791 | 97.9 | 97.2 | 0.35 |
| 3 | 19.236 | 130.172 | 4.904 | 0.9 | 0.8 | 0.42 |
| | Total | 14813.350 | 617.846 | 100.0 | 100.0 | |

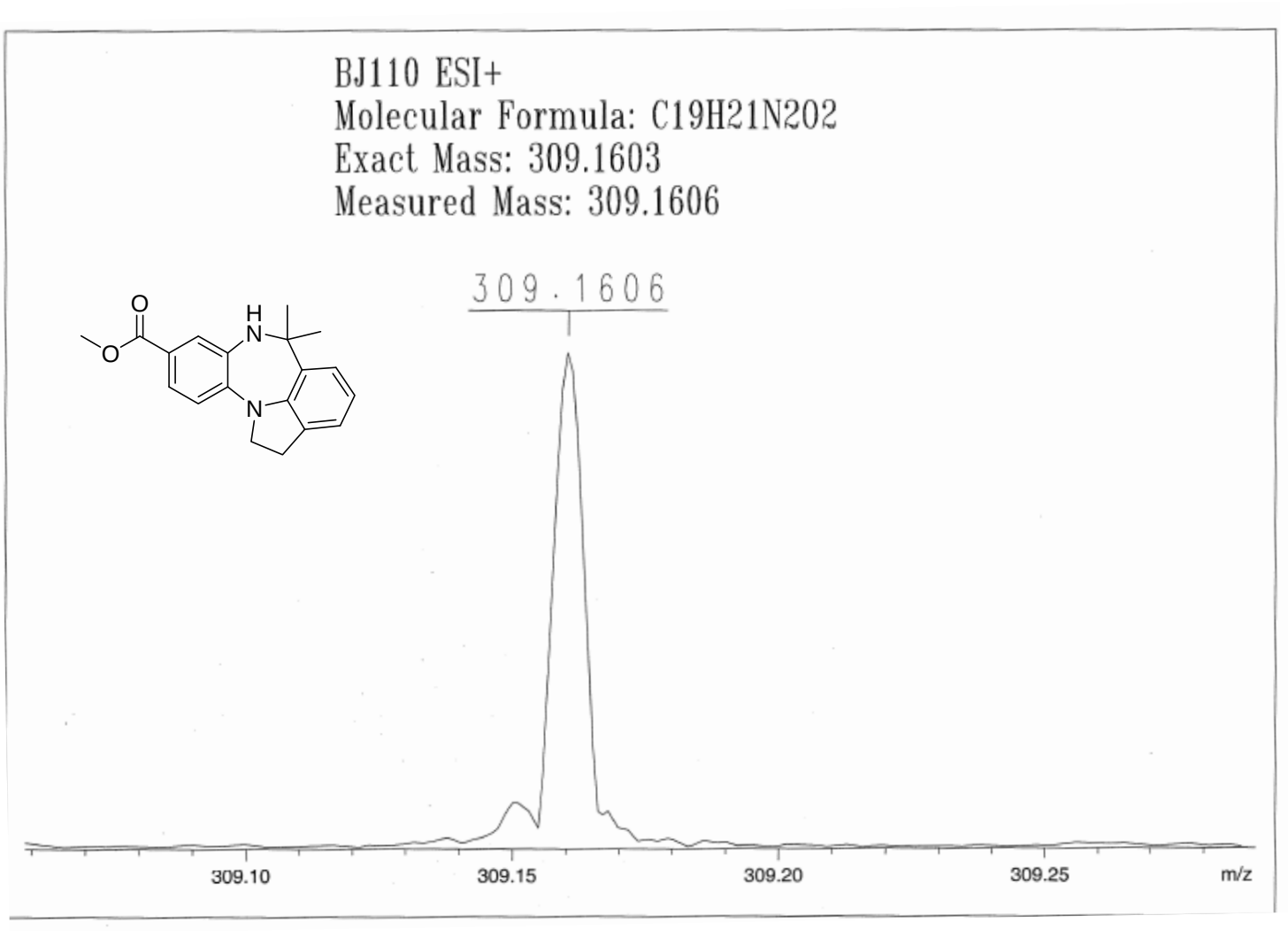
HPLC and $^{1}$H NMR Spectrum (300 MHz) of compound **4a** in $CDCl_3$



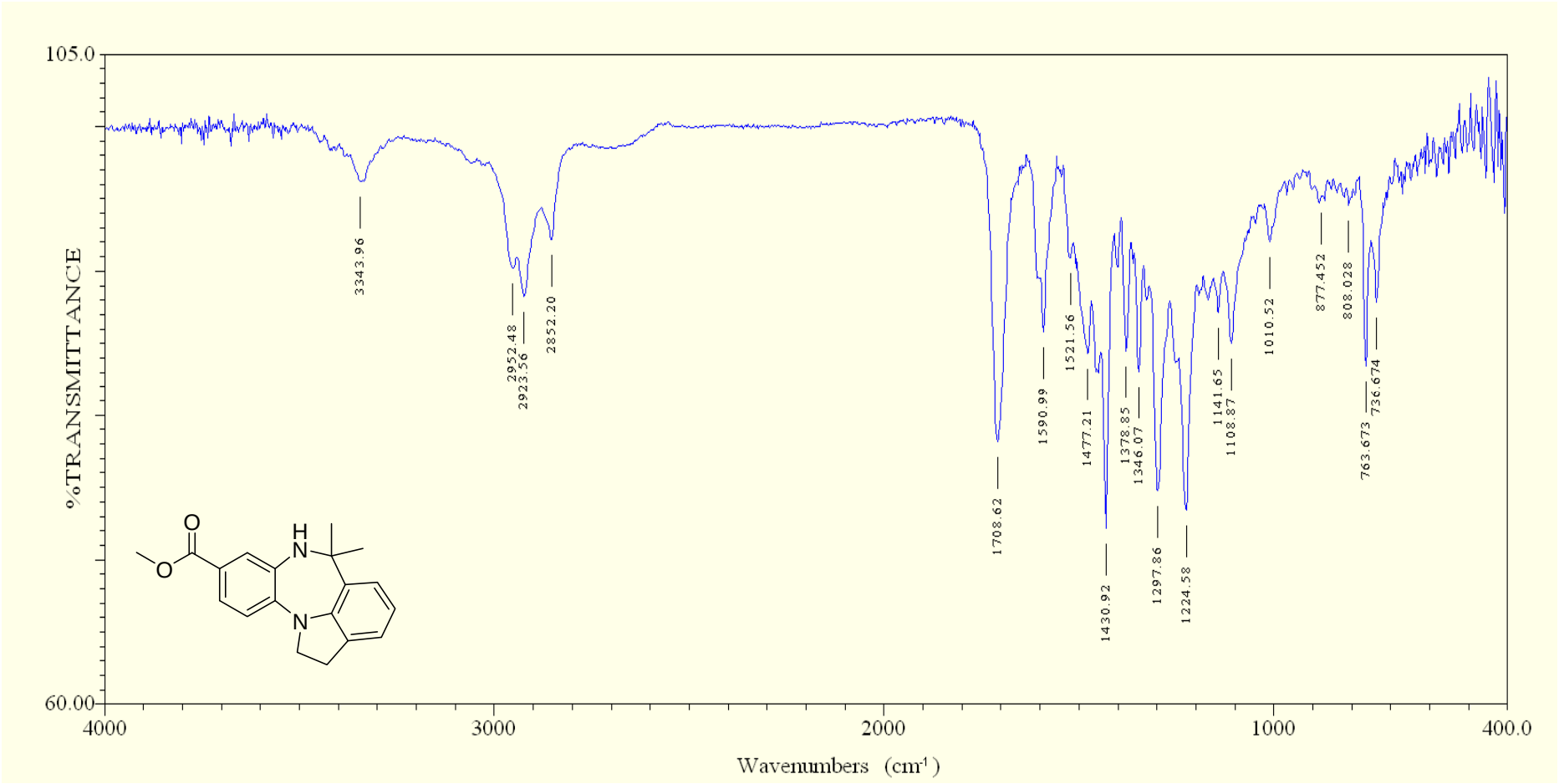

$^{13}$C NMR Spectrum (75 MHz) of compound **4a** in $CDCl_3$



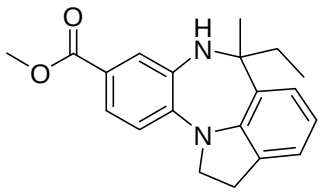

Low Resolution Mass Spectrum (LRMS) of compound **4a**

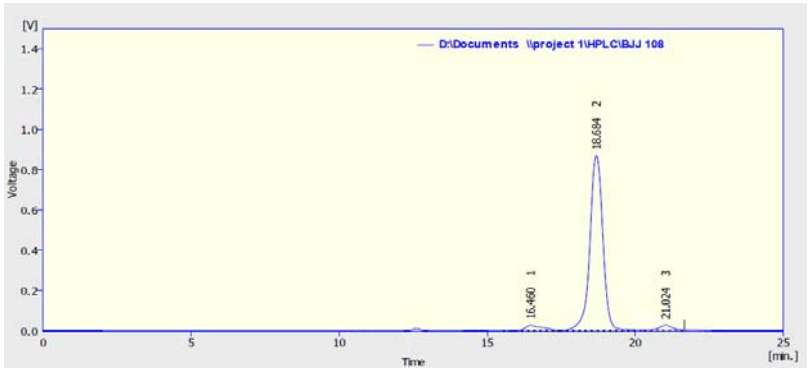



High Resolution Mass Spectrum (HRMS) of compound **4a**




IR Spectrum of compound **4a** (Neat)

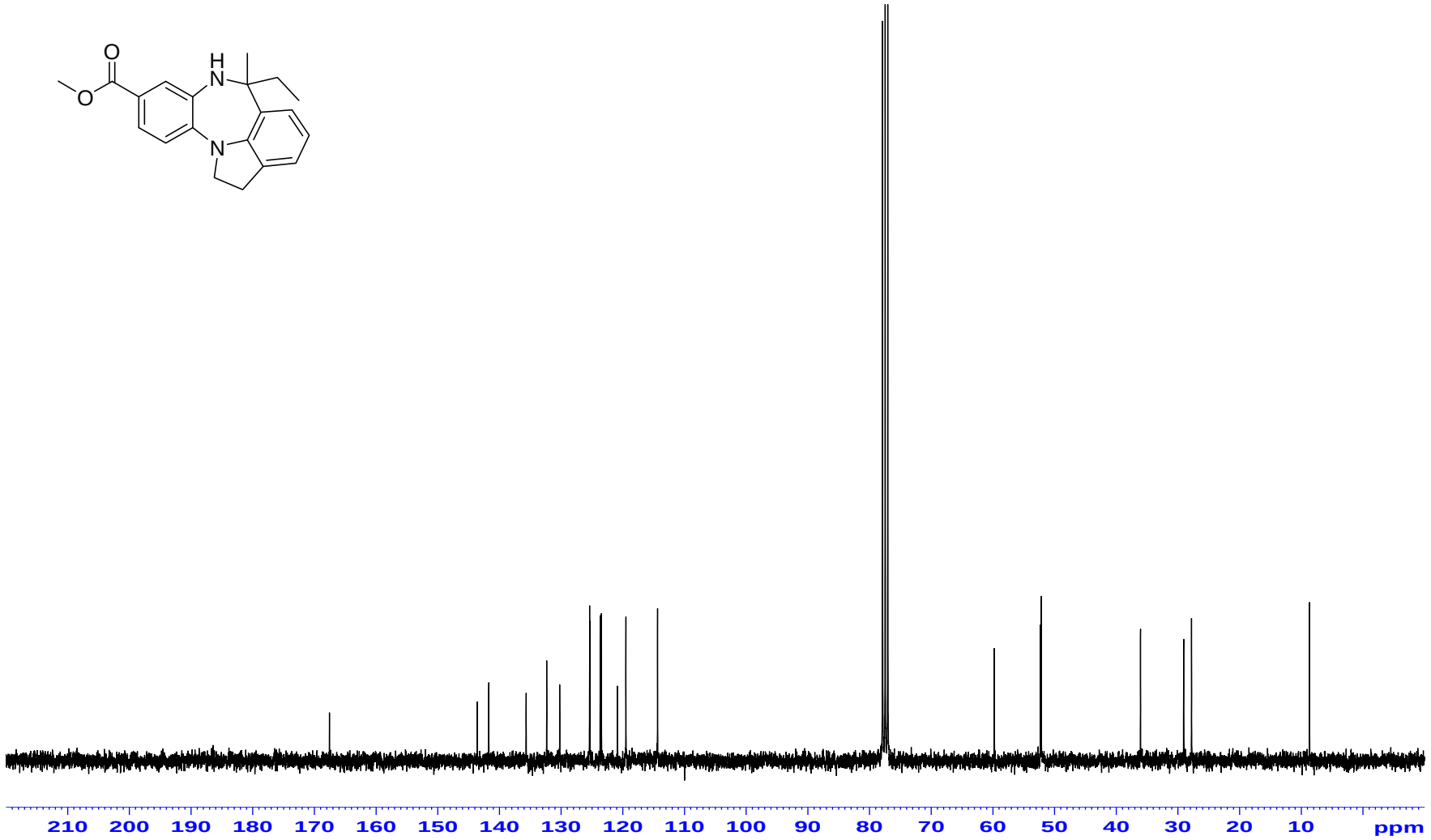


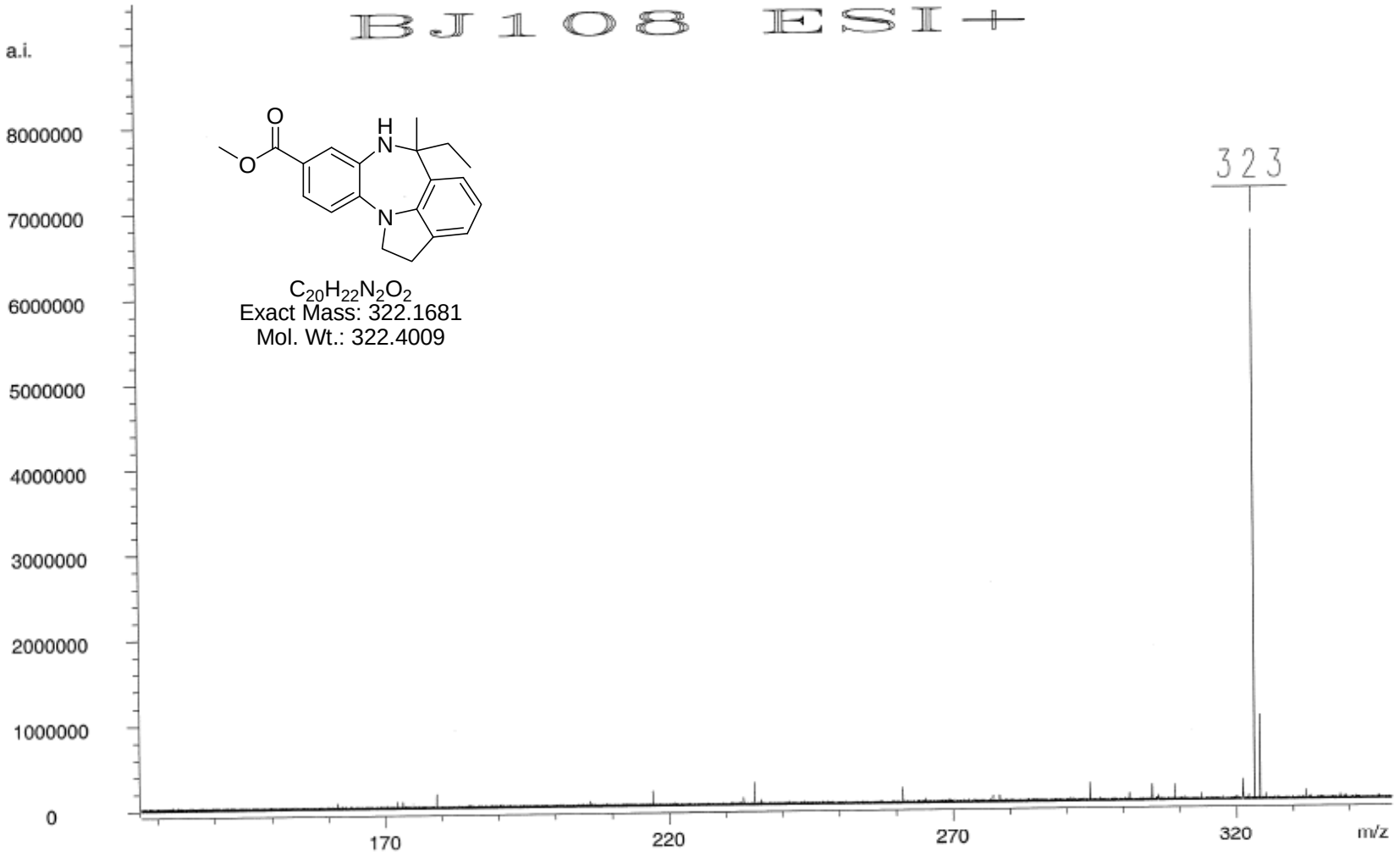

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 16.460 | 1032.831 | 26.128 | 3.7 | 2.8 | 0.68 |
| 2 | 18.684 | 26302.147 | 867.260 | 93.8 | 94.5 | 0.46 |
| 3 | 21.024 | 695.044 | 23.943 | 2.5 | 2.6 | 0.44 |
| | Total | 28030.022 | 917.330 | 100.0 | 100.0 | |



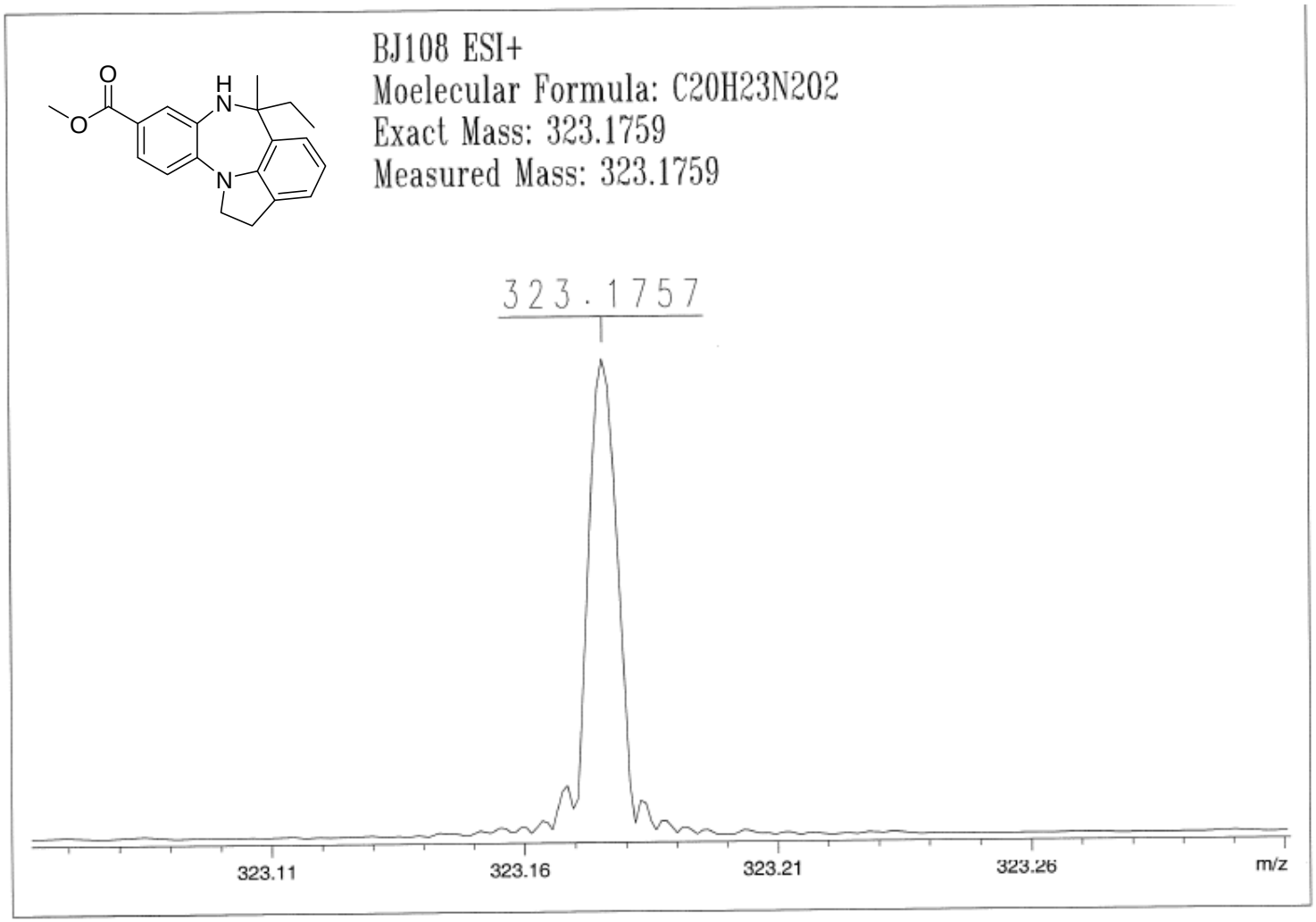

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4b** in $CDCl_3$



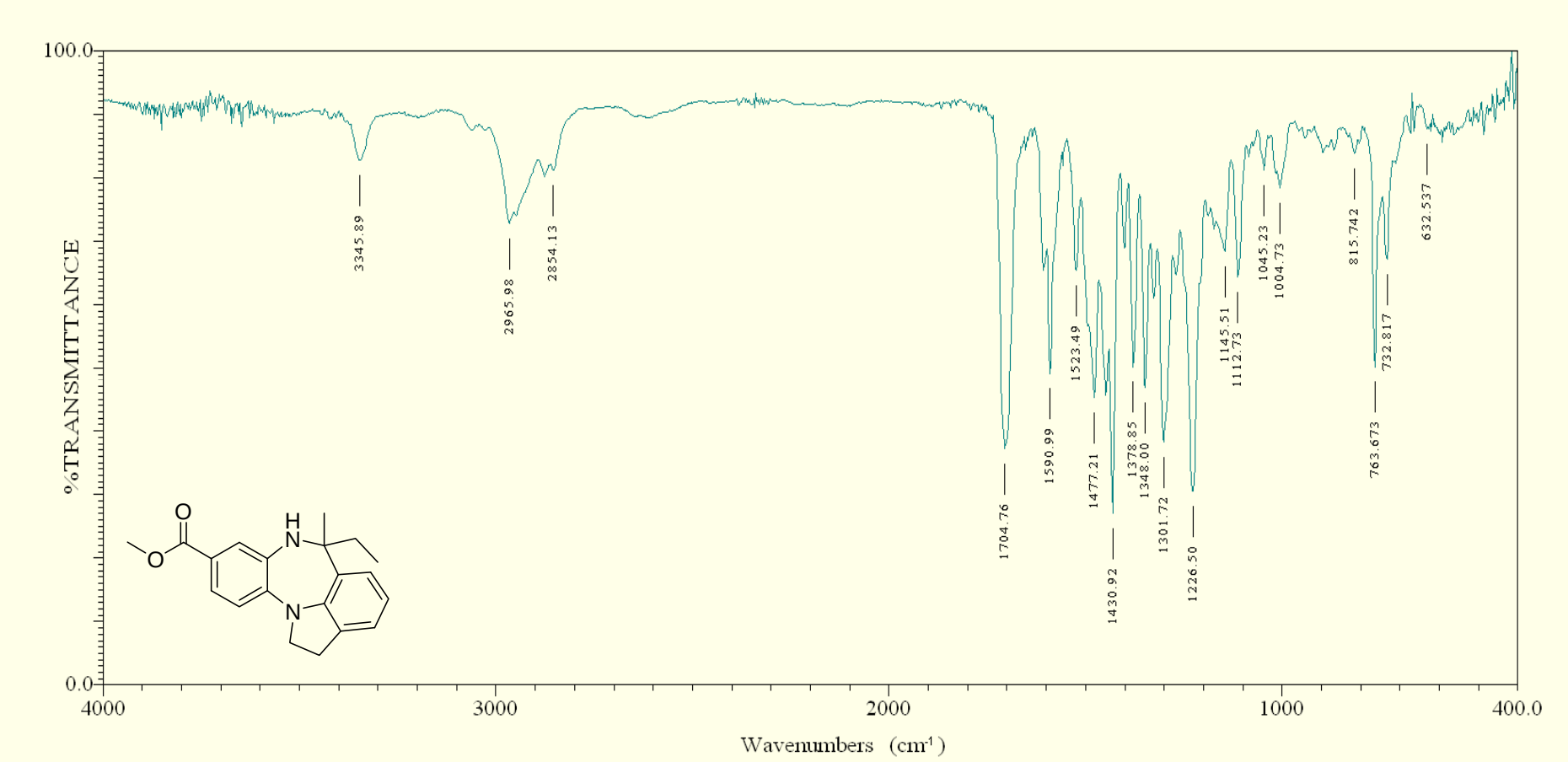

$^{13}$C NMR Spectrum (75 MHz) of compound **4b** in $CDCl_3$



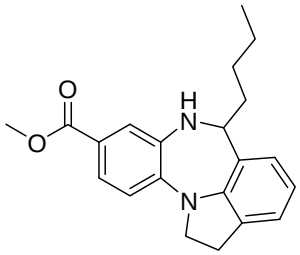

Low Resolution Mass Spectrum (LRMS) of compound **4b**

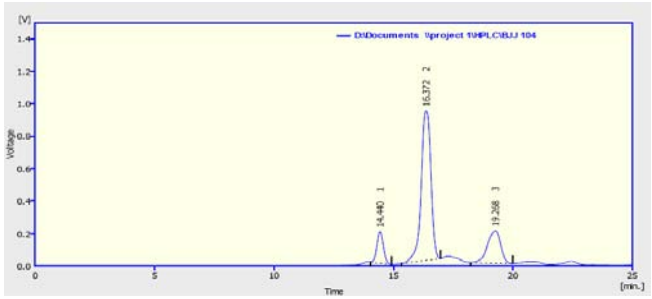



High Resolution Mass Spectrum (HRMS) of compound **4b**




IR Spectrum of compound **4b** (Neat)

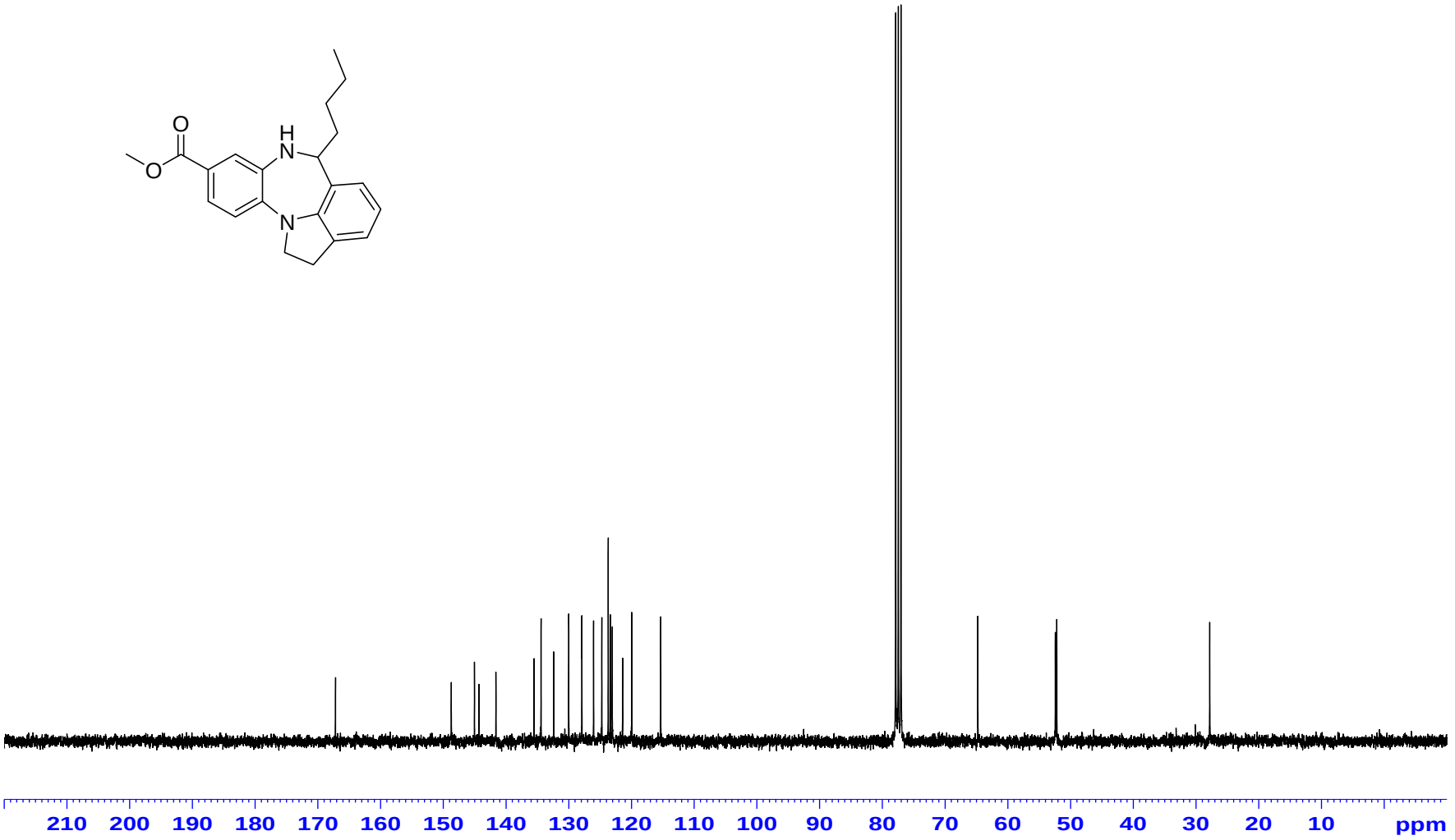


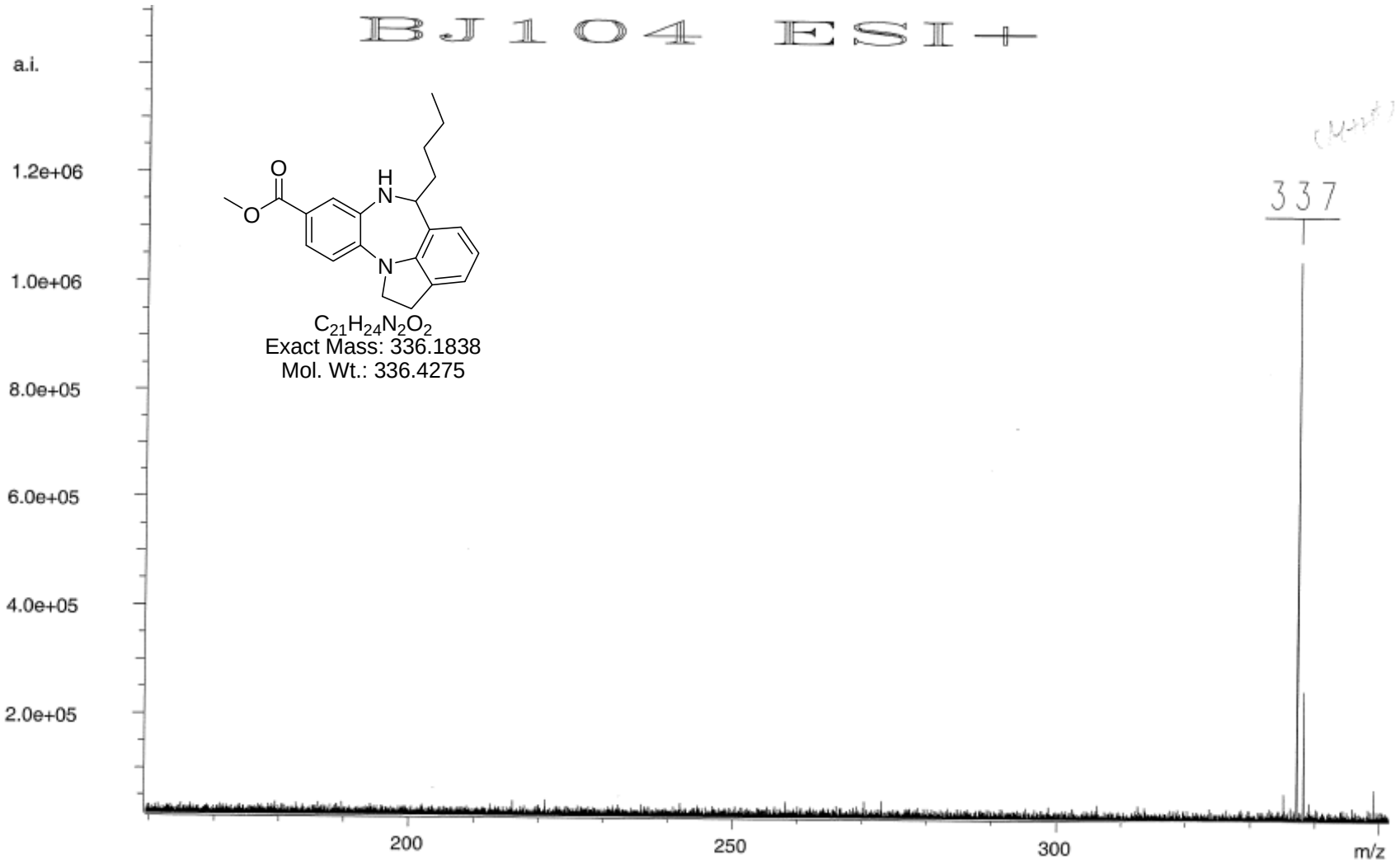

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 14.440 | 3659.877 | 195.095 | 9.8 | 14.8 | 0.30 |
| 2 | 16.372 | 26113.331 | 921.515 | 69.8 | 70.0 | 0.43 |
| 3 | 19.268 | 7644.807 | 199.610 | 20.4 | 15.2 | 0.61 |
| | Total | 37418.015 | 1316.220 | 100.0 | 100.0 | |



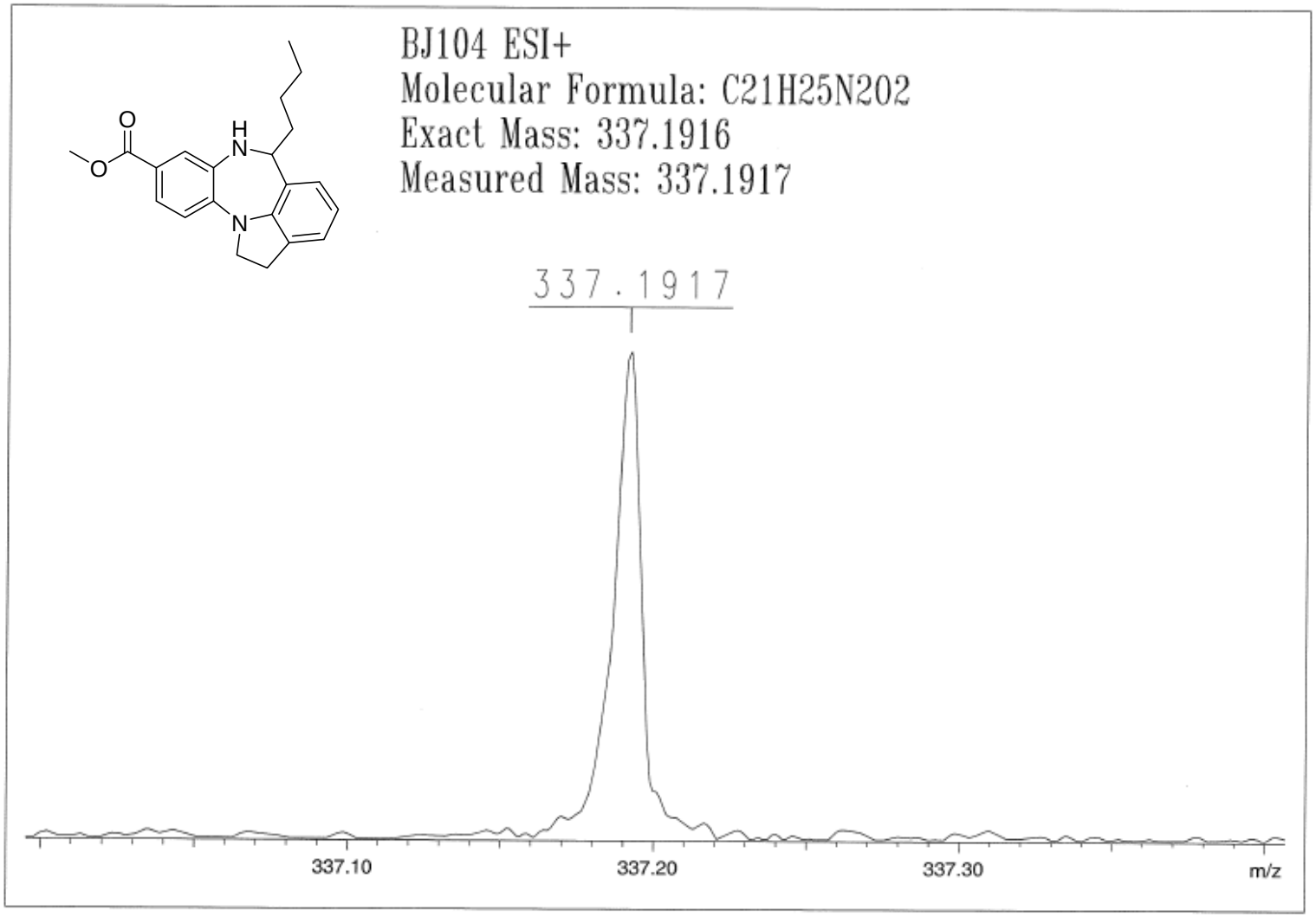

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4c** in $CDCl_3$



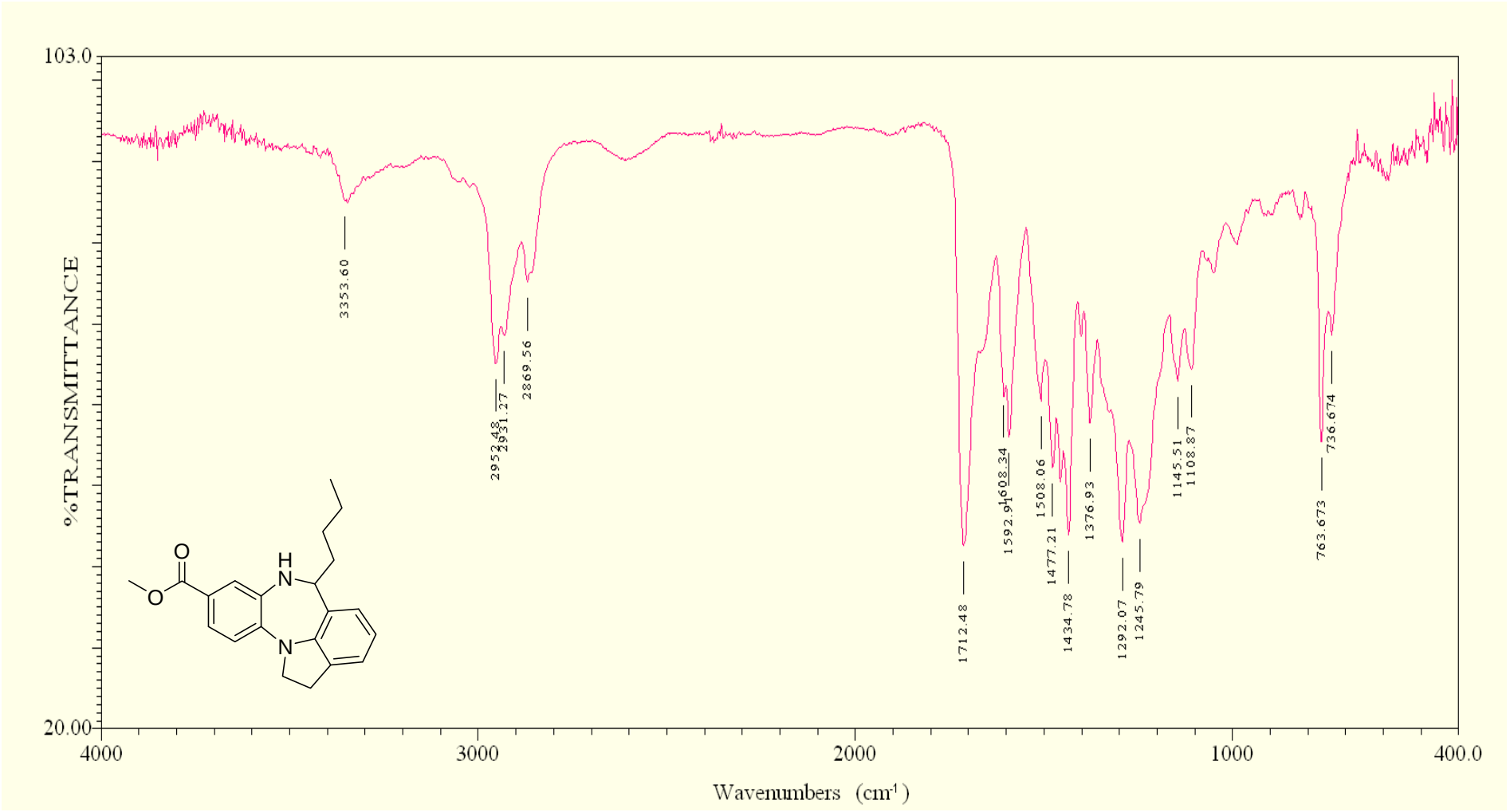

$^{13}C$ NMR Spectrum (75 MHz) of compound **4c** in $CDCl_3$



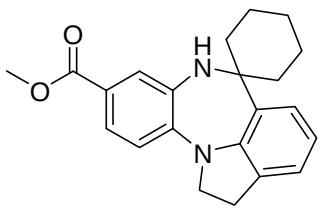

Low Resolution Mass Spectrum (LRMS) of compound **4c**

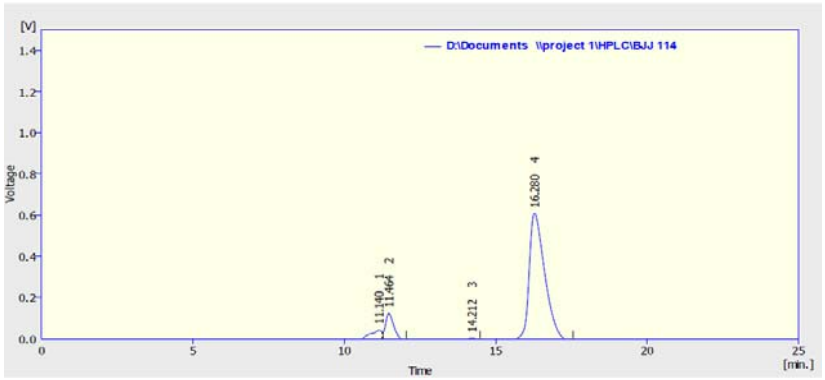



High Resolution Mass Spectrum (HRMS) of compound **4c**




IR Spectrum of compound **4c** (Neat)

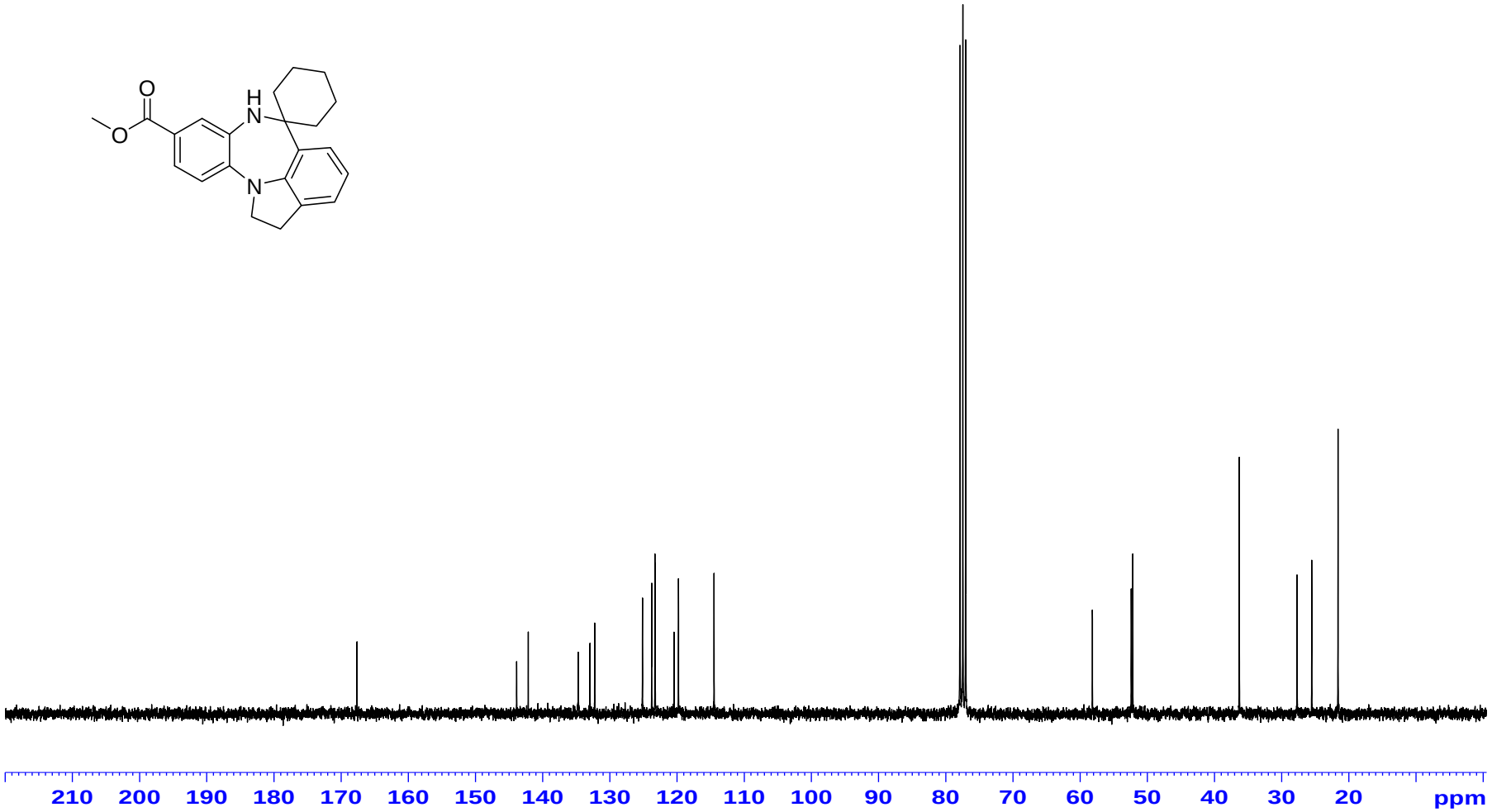


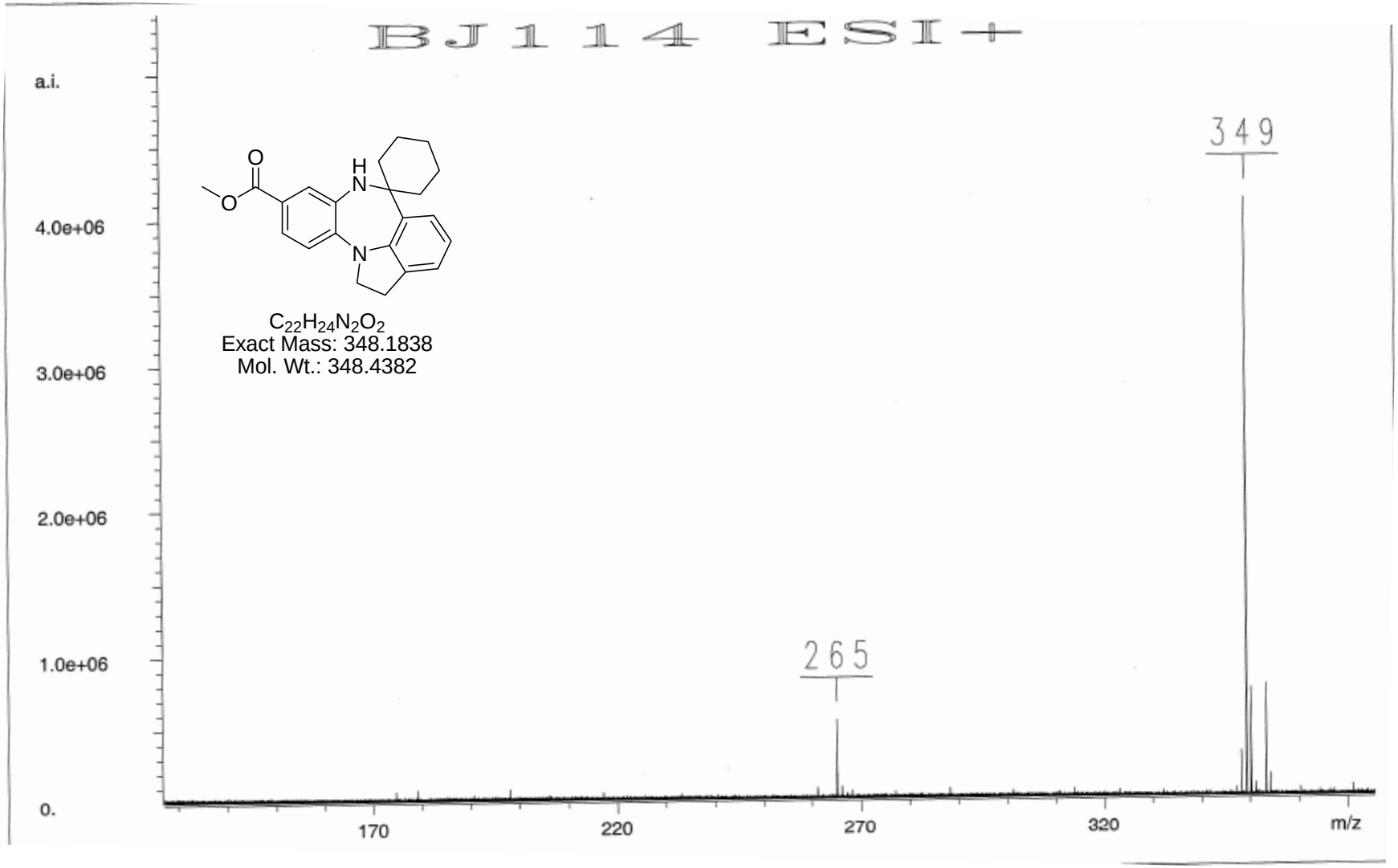

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 11.140 | 1436.848 | 51.650 | 5.4 | 6.3 | 0.54 |
| 2 | 11.464 | 2621.230 | 131.925 | 9.9 | 16.2 | 0.31 |
| 3 | 14.212 | 220.583 | 12.226 | 0.8 | 1.5 | 0.30 |
| 4 | 16.280 | 22218.440 | 619.751 | 83.9 | 76.0 | 0.54 |
| | Total | 26497.102 | 815.553 | 100.0 | 100.0 | |



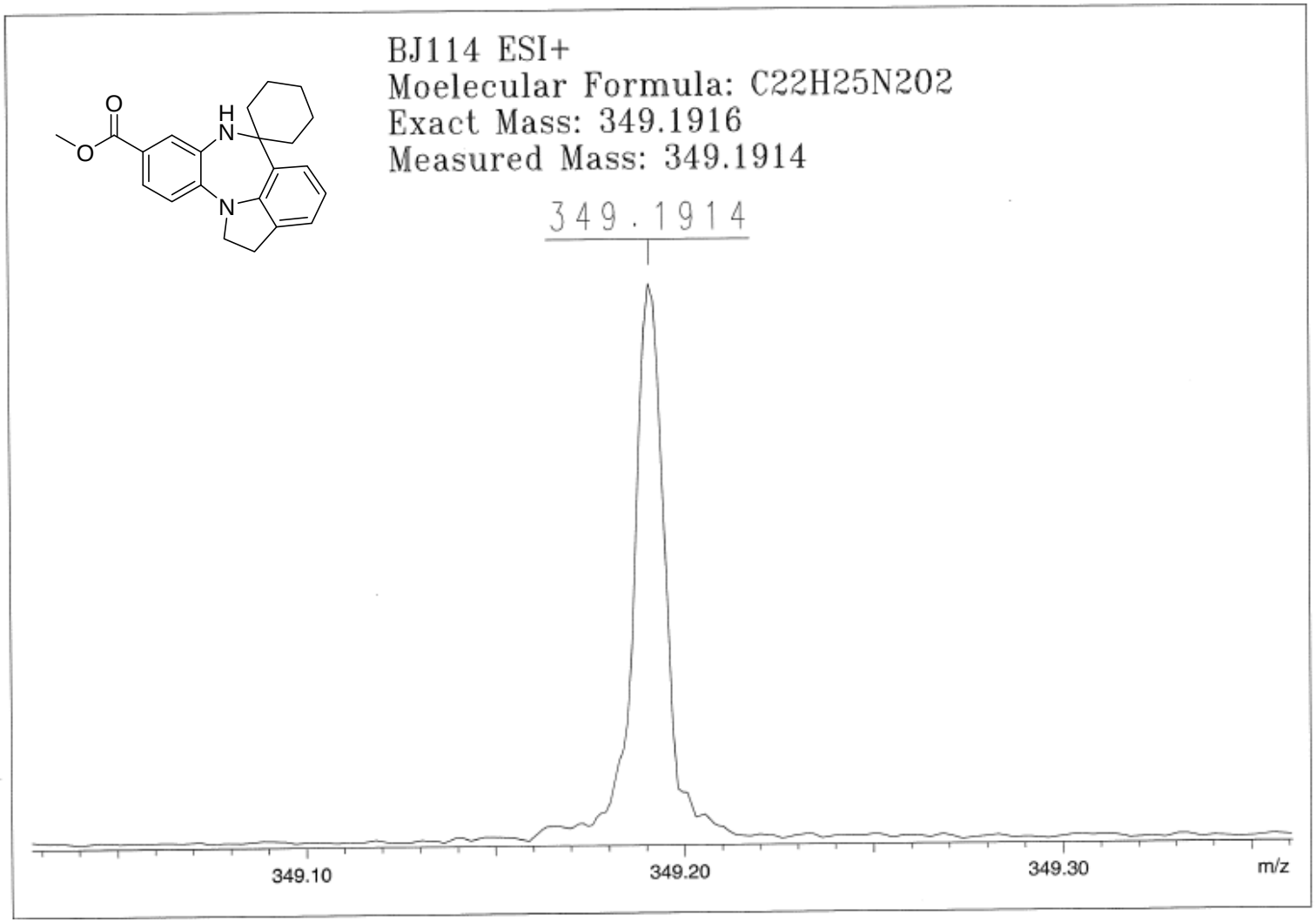

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4d** in $CDCl_3$



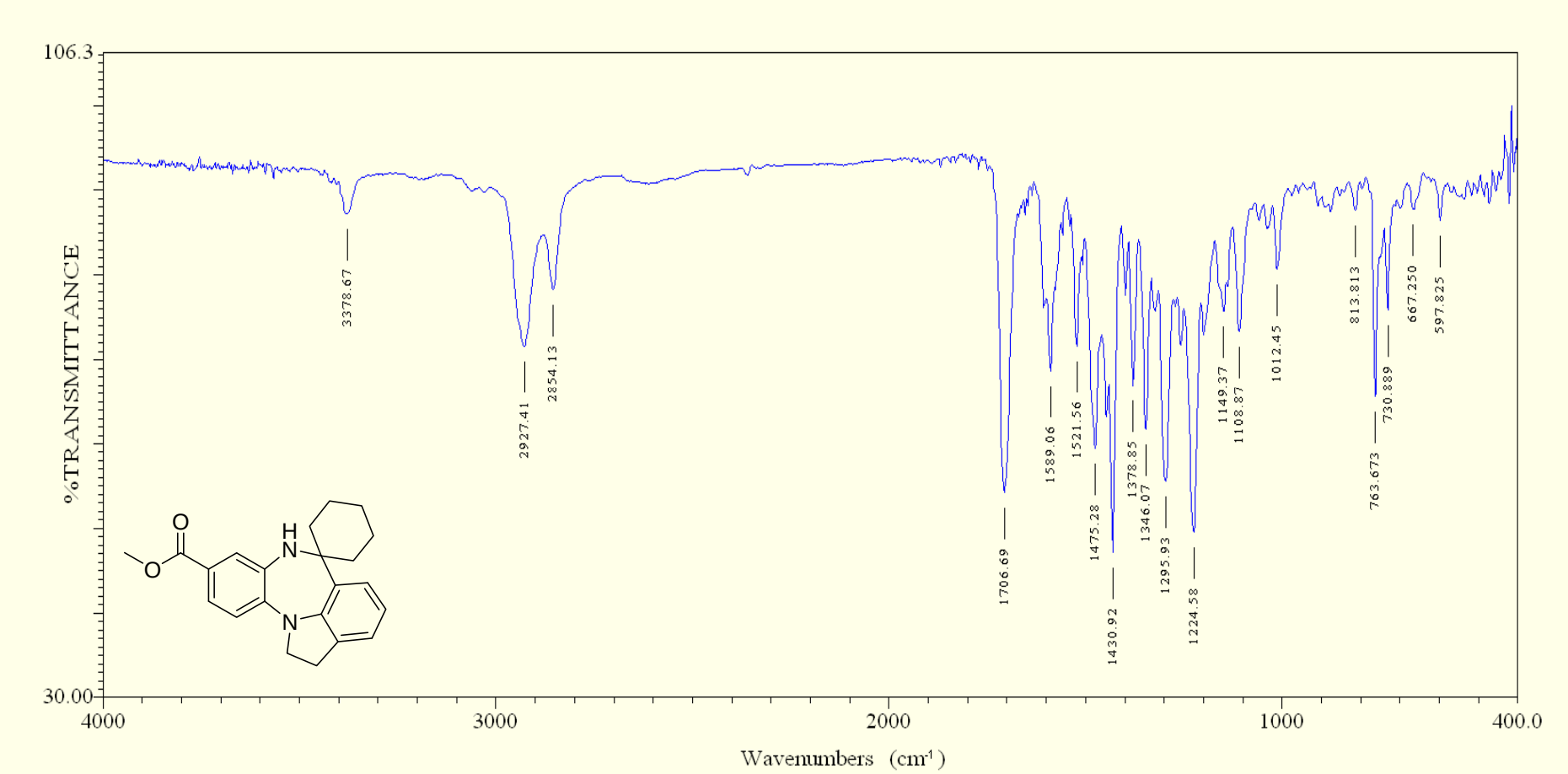

$^{13}$C NMR Spectrum (75 MHz) of compound **4d** in $CDCl_3$



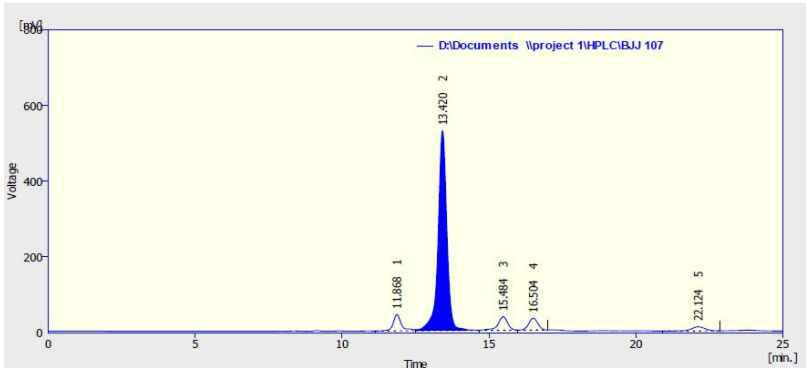

Low Resolution Mass Spectrum (LRMS) of compound **4d**



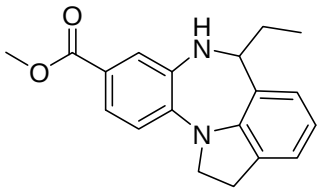

High Resolution Mass Spectrum (HRMS) of compound **4d**




IR Spectrum of compound **4d** (Neat)



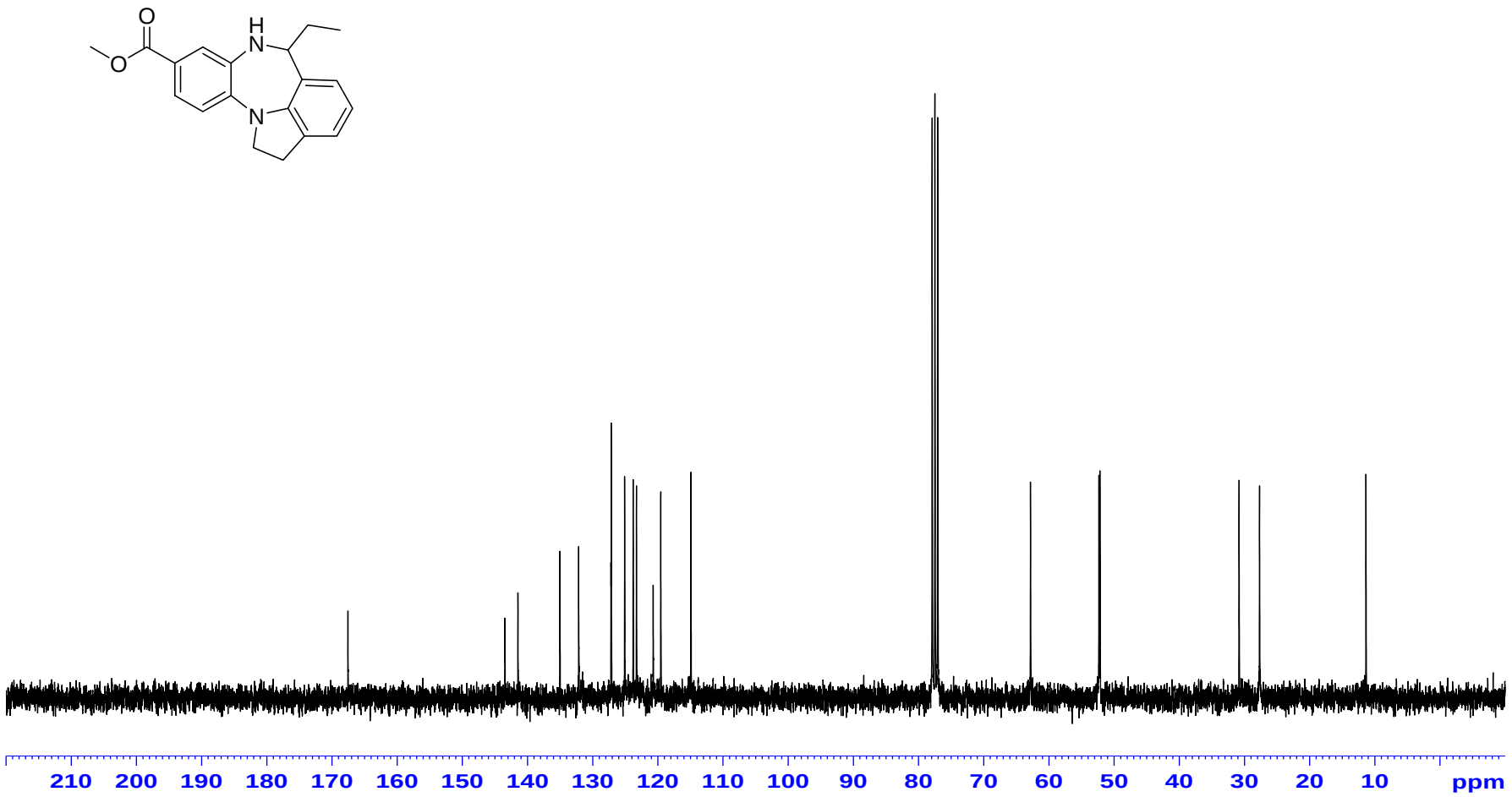

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 11.868 | 845.311 | 43.239 | 6.2 | 6.7 | 0.26 |
| 2 | 13.420 | 10990.925 | 528.279 | 80.2 | 81.3 | 0.30 |
| 3 | 15.484 | 837.078 | 36.017 | 6.1 | 5.5 | 0.33 |
| 4 | 16.504 | 683.093 | 31.525 | 5.0 | 4.8 | 0.34 |
| 5 | 22.124 | 350.833 | 10.997 | 2.6 | 1.7 | 0.49 |
| | Total | 13707.240 | 650.058 | 100.0 | 100.0 | |



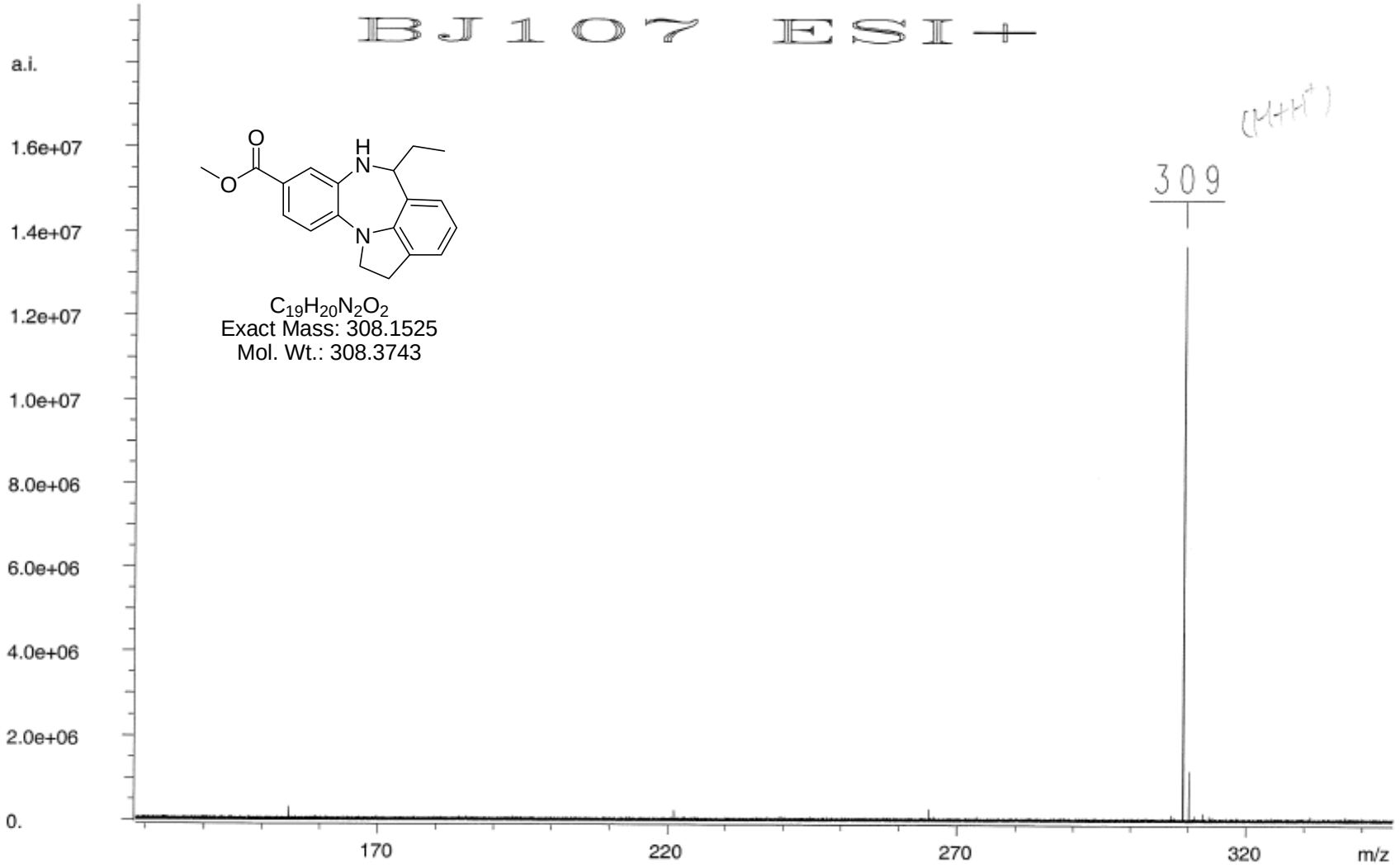




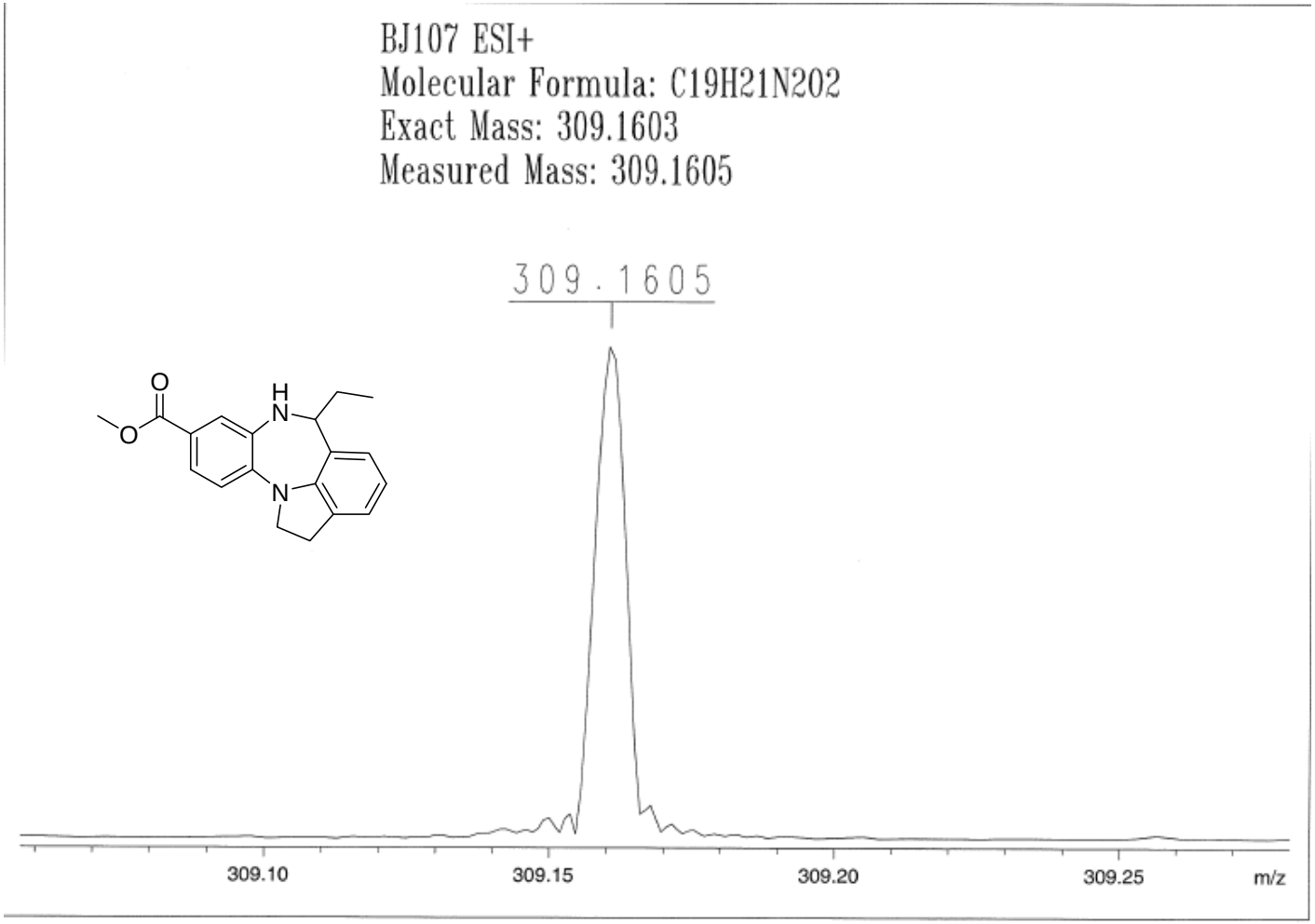
HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4e** in $CDCl_3$



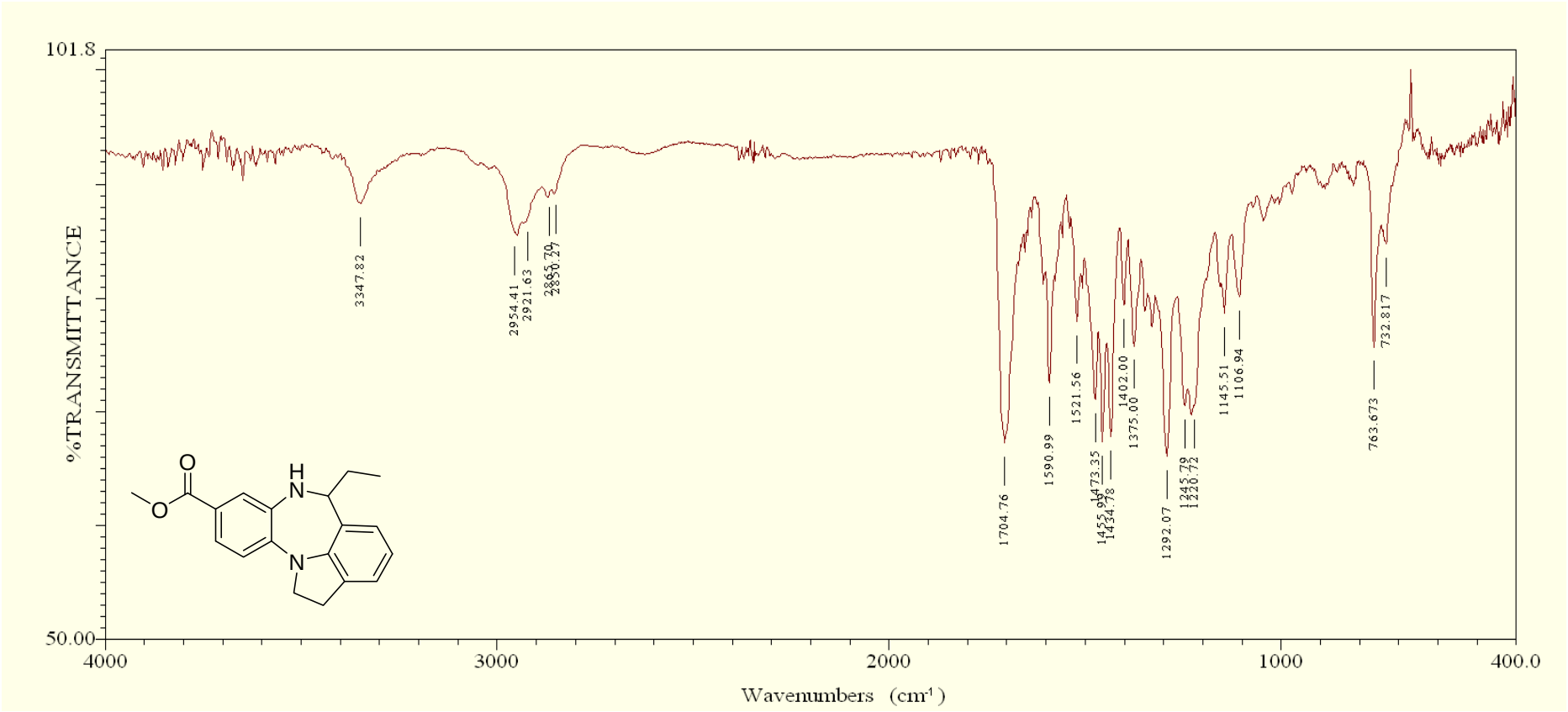

$^{13}C$ NMR Spectrum (75 MHz) of compound **4e** in $CDCl_3$



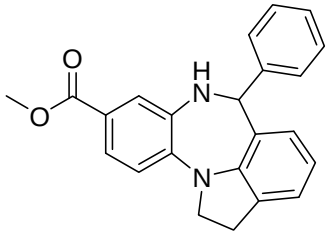

Low Resolution Mass Spectrum (LRMS) of compound **4e**

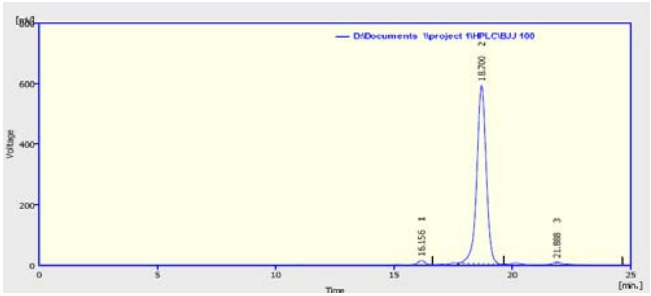



High Resolution Mass Spectrum (HRMS) of compound **4e**




IR Spectrum of compound **4e** (Neat)

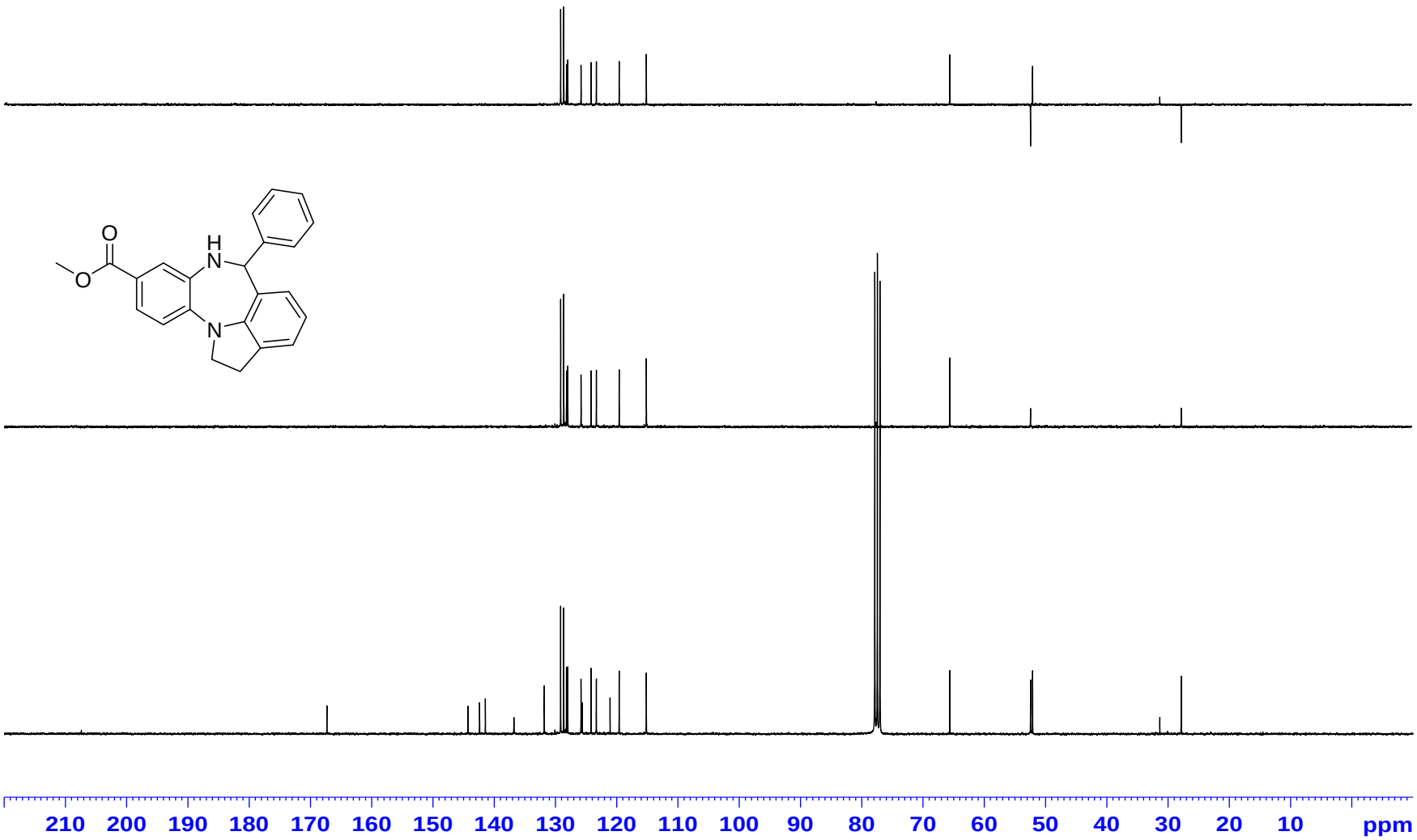


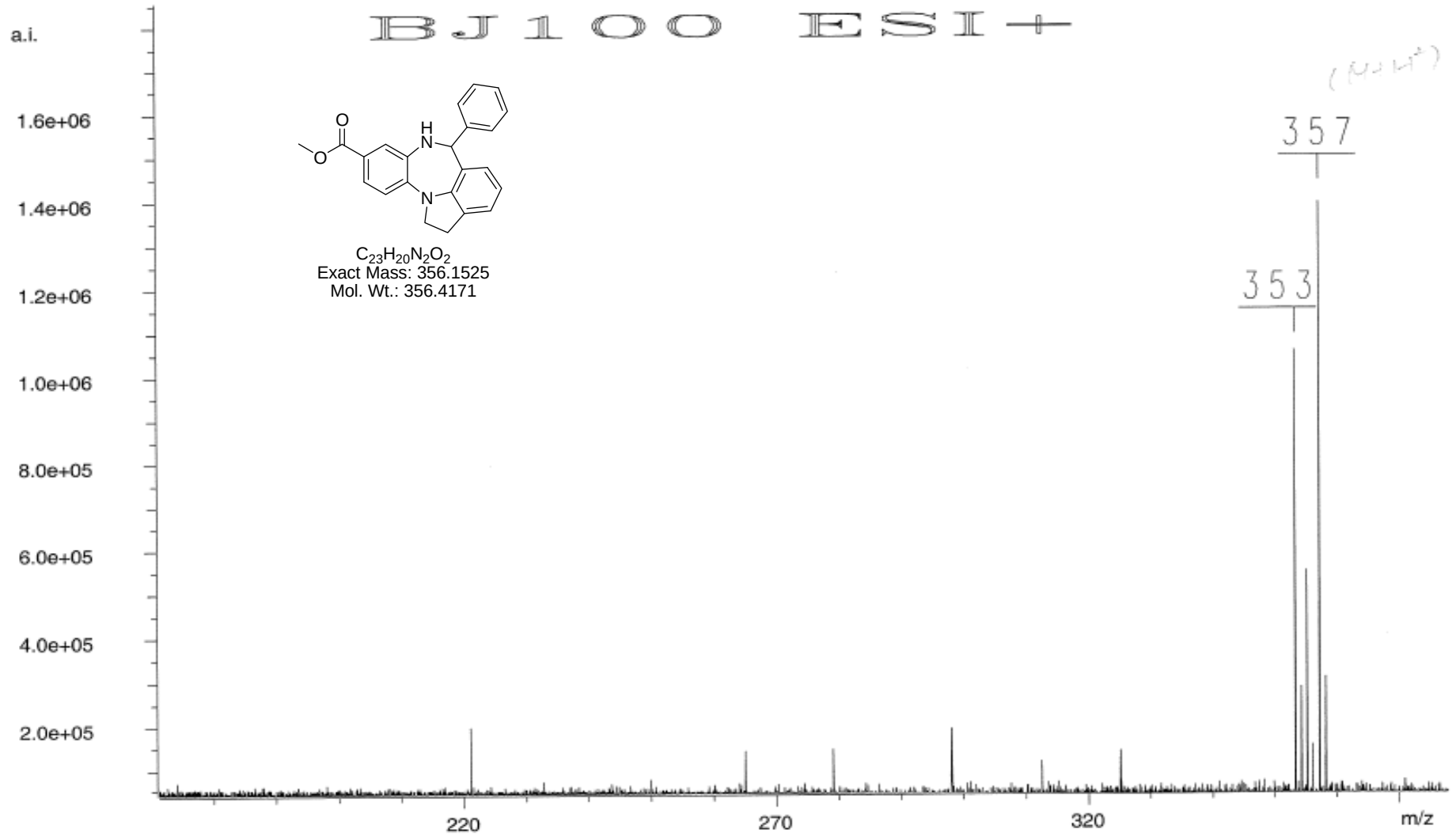

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 16.156 | 298.760 | 13.765 | 1.8 | 2.3 | 0.34 |
| 2 | 18.700 | 16252.775 | 588.165 | 96.2 | 96.4 | 0.42 |
| 3 | 21.888 | 339.144 | 7.886 | 2.0 | 1.3 | 0.52 |
| | Total | 16890.679 | 609.816 | 100.0 | 100.0 | |



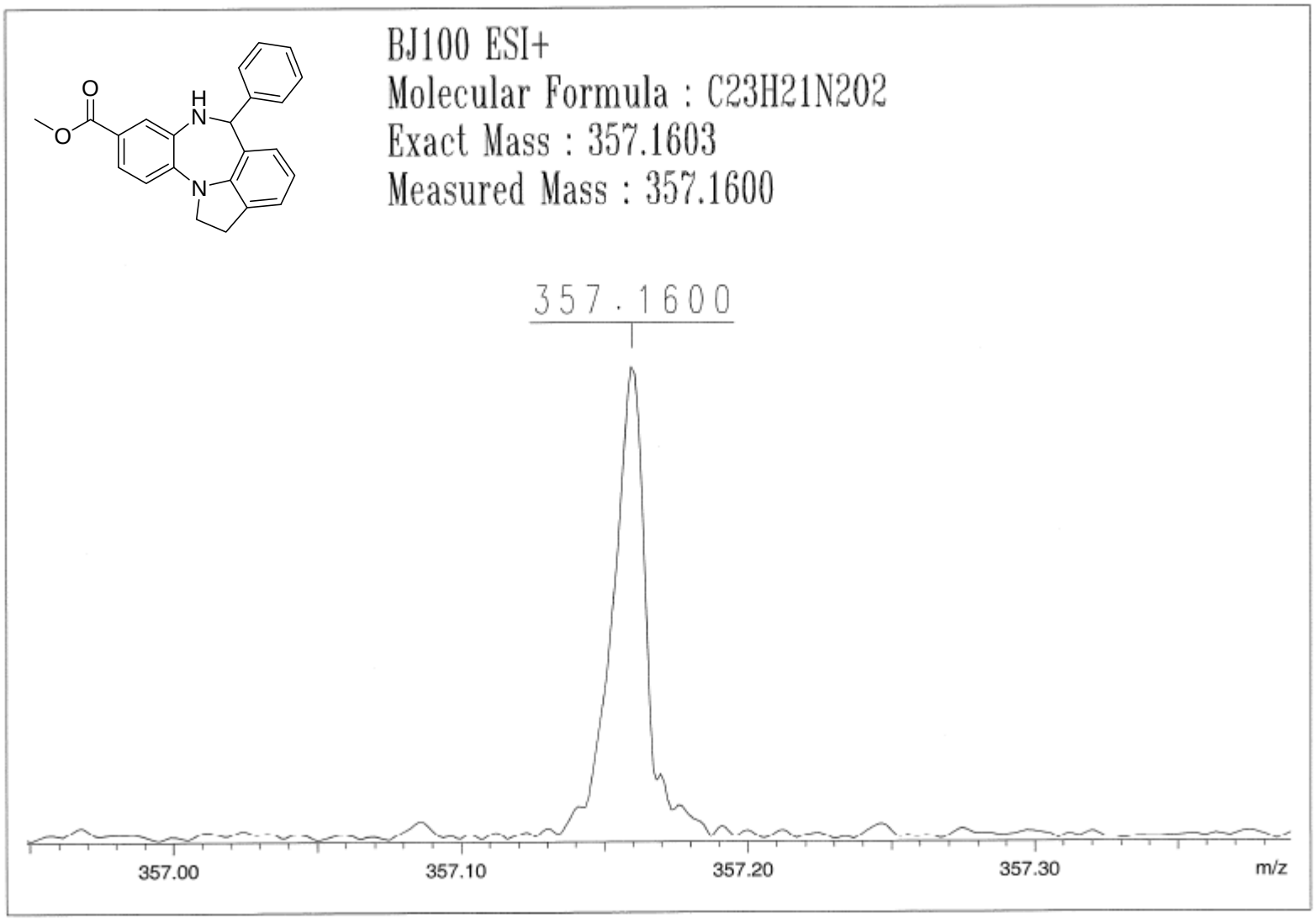

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4f** in $CDCl_3$



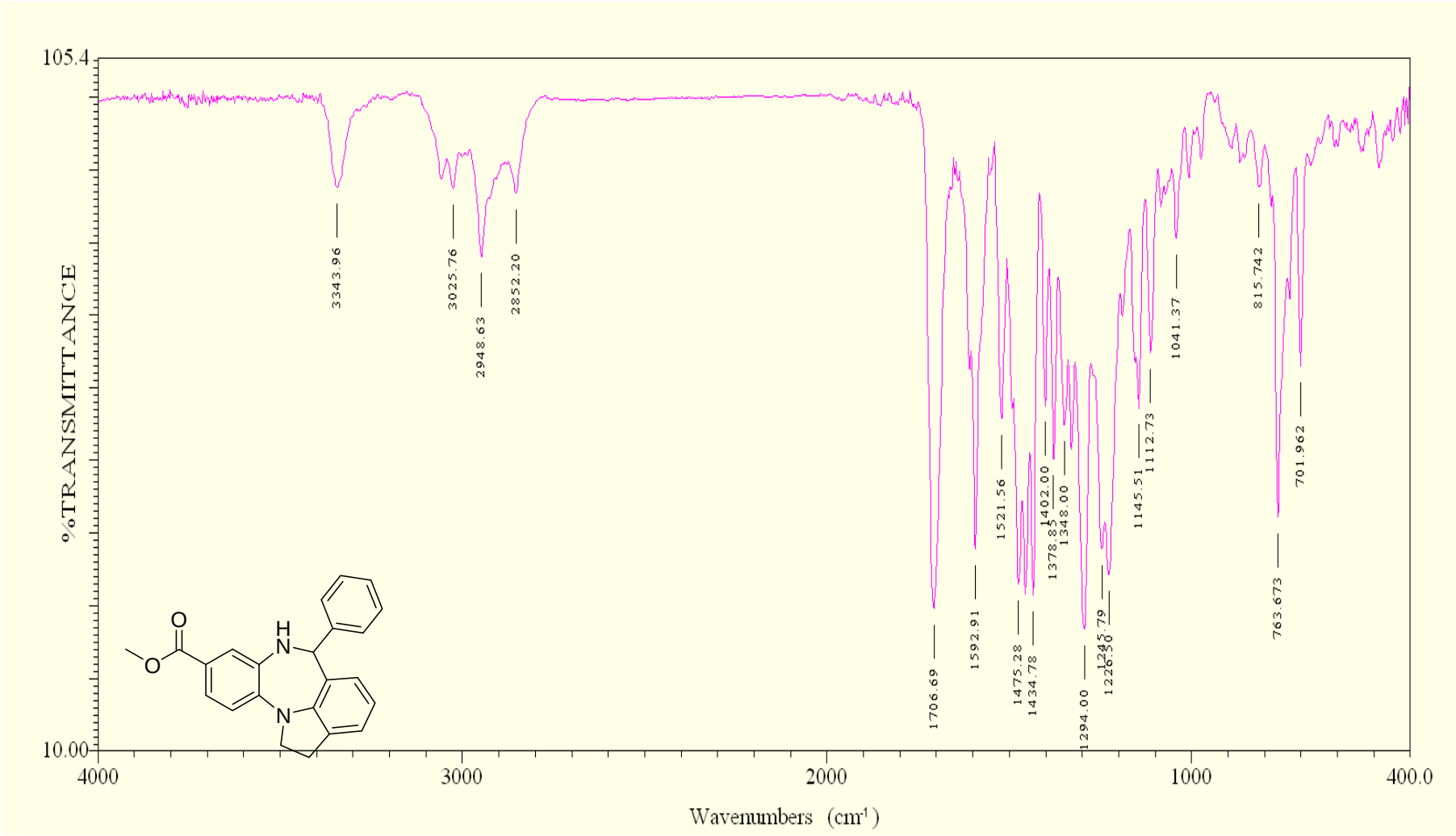

$^{13}C$, DEPT NMR Spectrum (75 MHz) of compound **4f** in $CDCl_3$



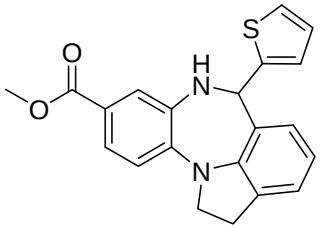

Low Resolution Mass Spectrum (LRMS) of compound **4f**

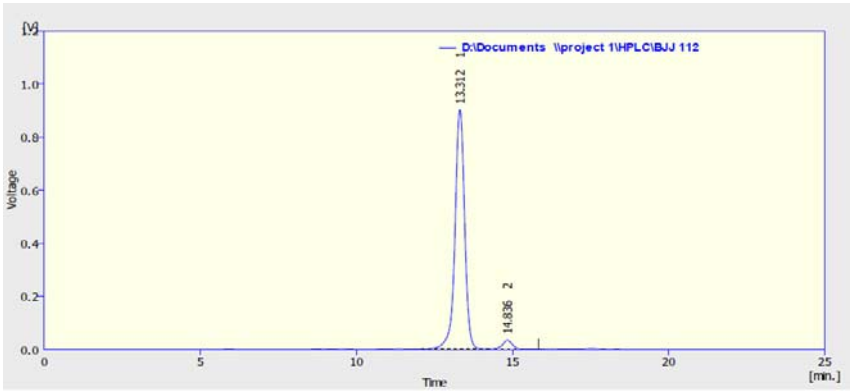



High Resolution Mass Spectrum (HRMS) of compound **4f**




IR Spectrum of compound **4f** (Neat)

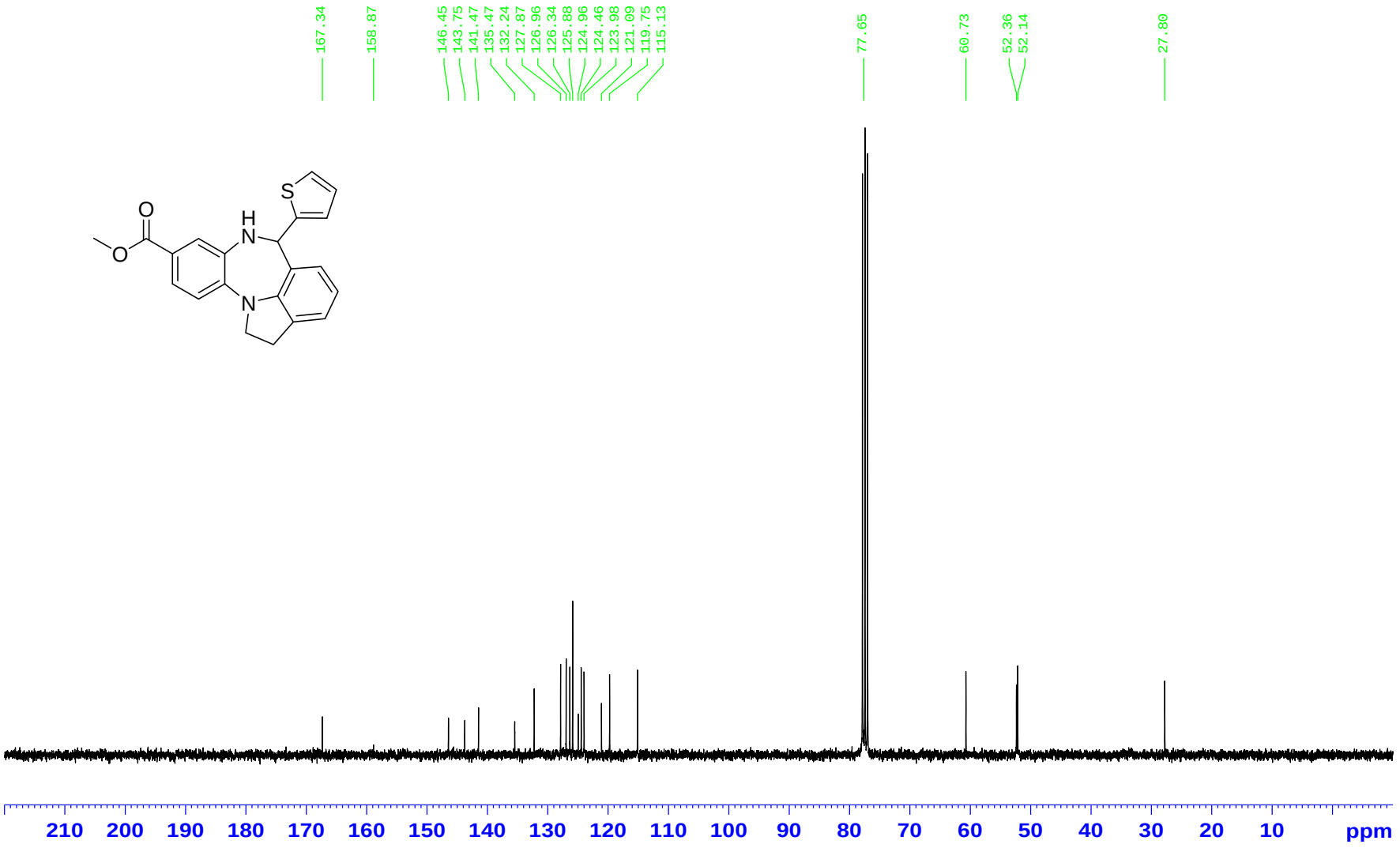


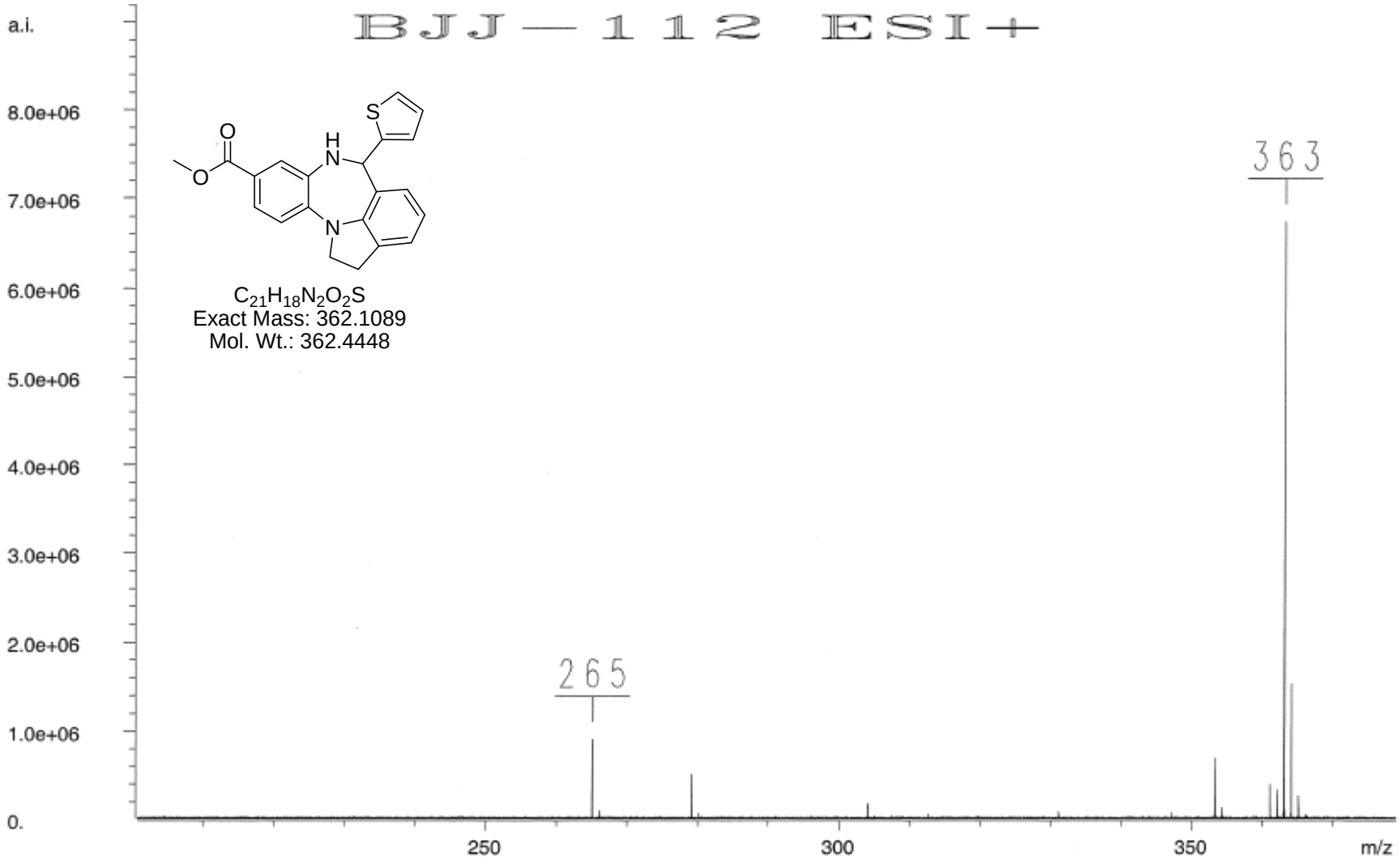

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 13.312 | 19425.827 | 901.979 | 96.3 | 96.5 | 0.32 |
| 2 | 14.836 | 755.886 | 32.924 | 3.7 | 3.5 | 0.34 |
| | Total | 20181.712 | 934.903 | 100.0 | 100.0 | |



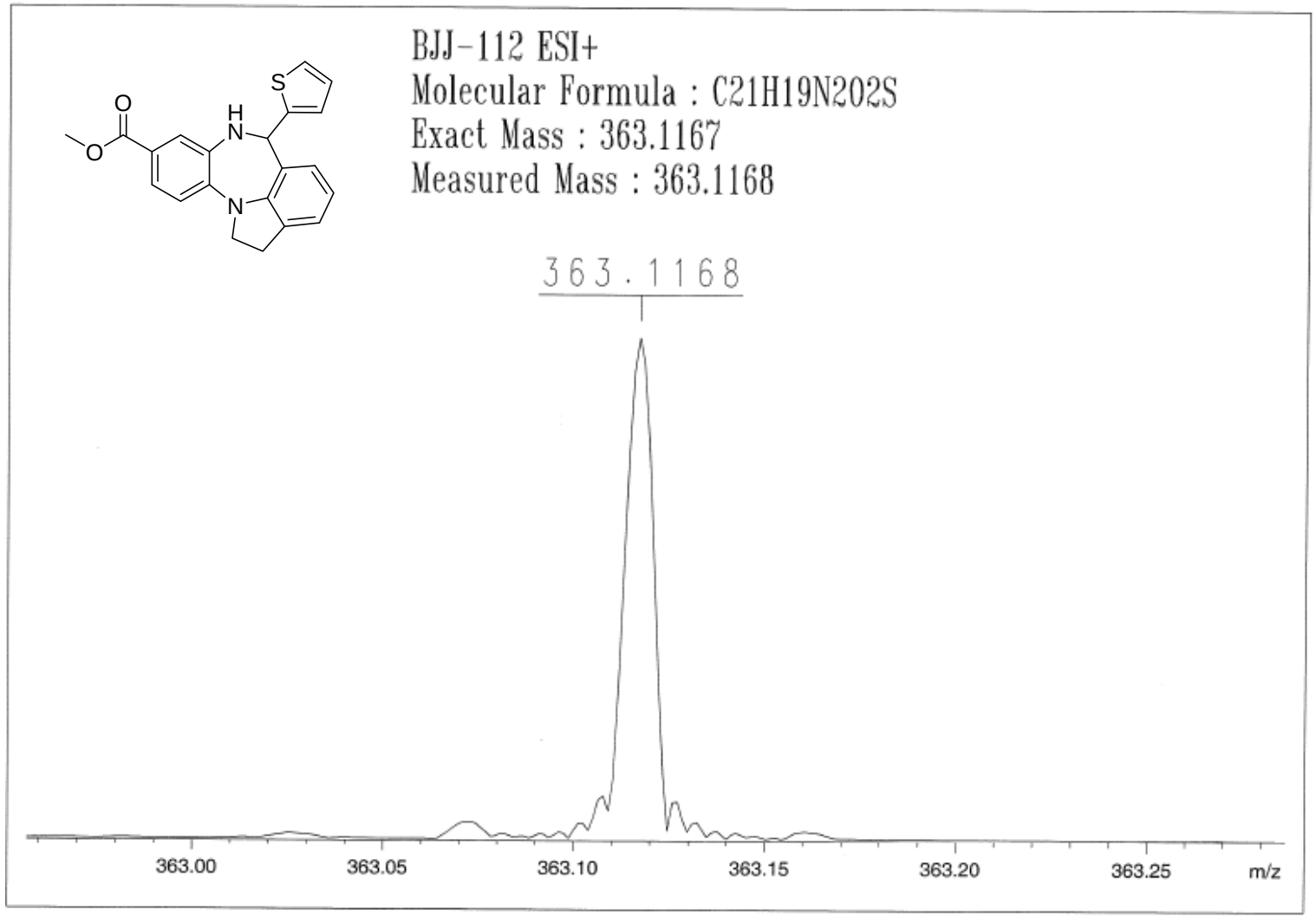

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4g** in $CDCl_3$



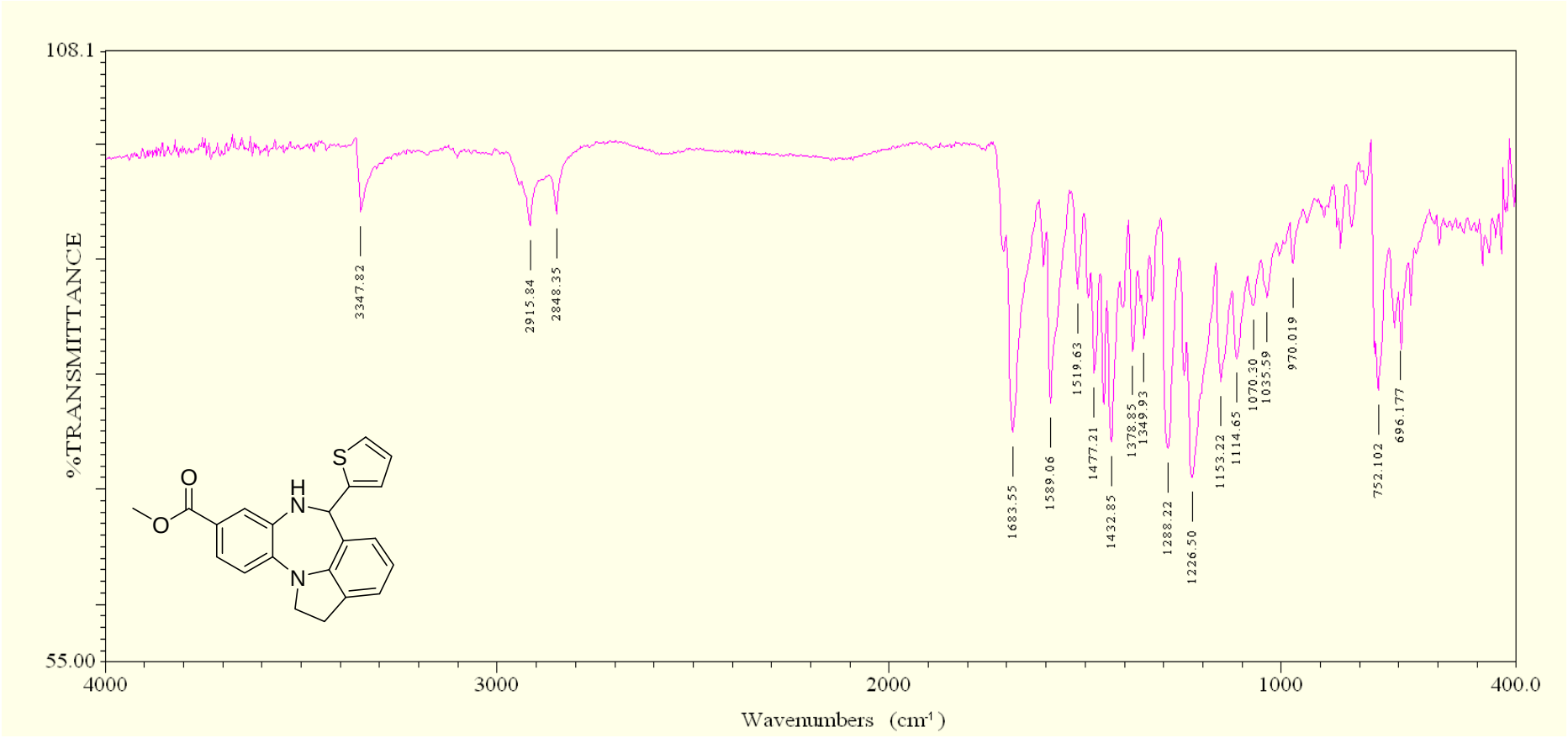

$^{13}$C NMR Spectrum (75 MHz) of compound **4g** in $CDCl_3$



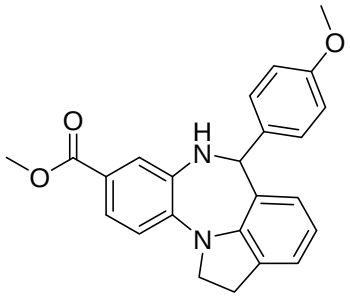

Low Resolution Mass Spectrum (LRMS) of compound **4g**

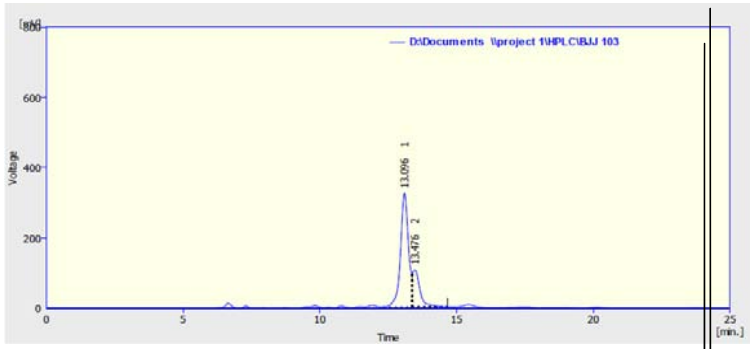



High Resolution Mass Spectrum (HRMS) of compound **4g**

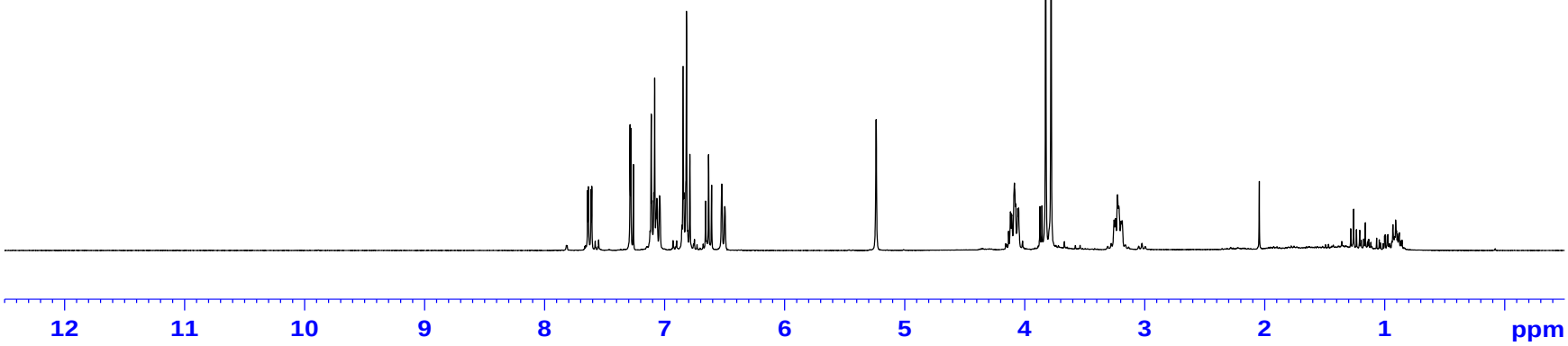



IR Spectrum of compound **4g** (Neat)

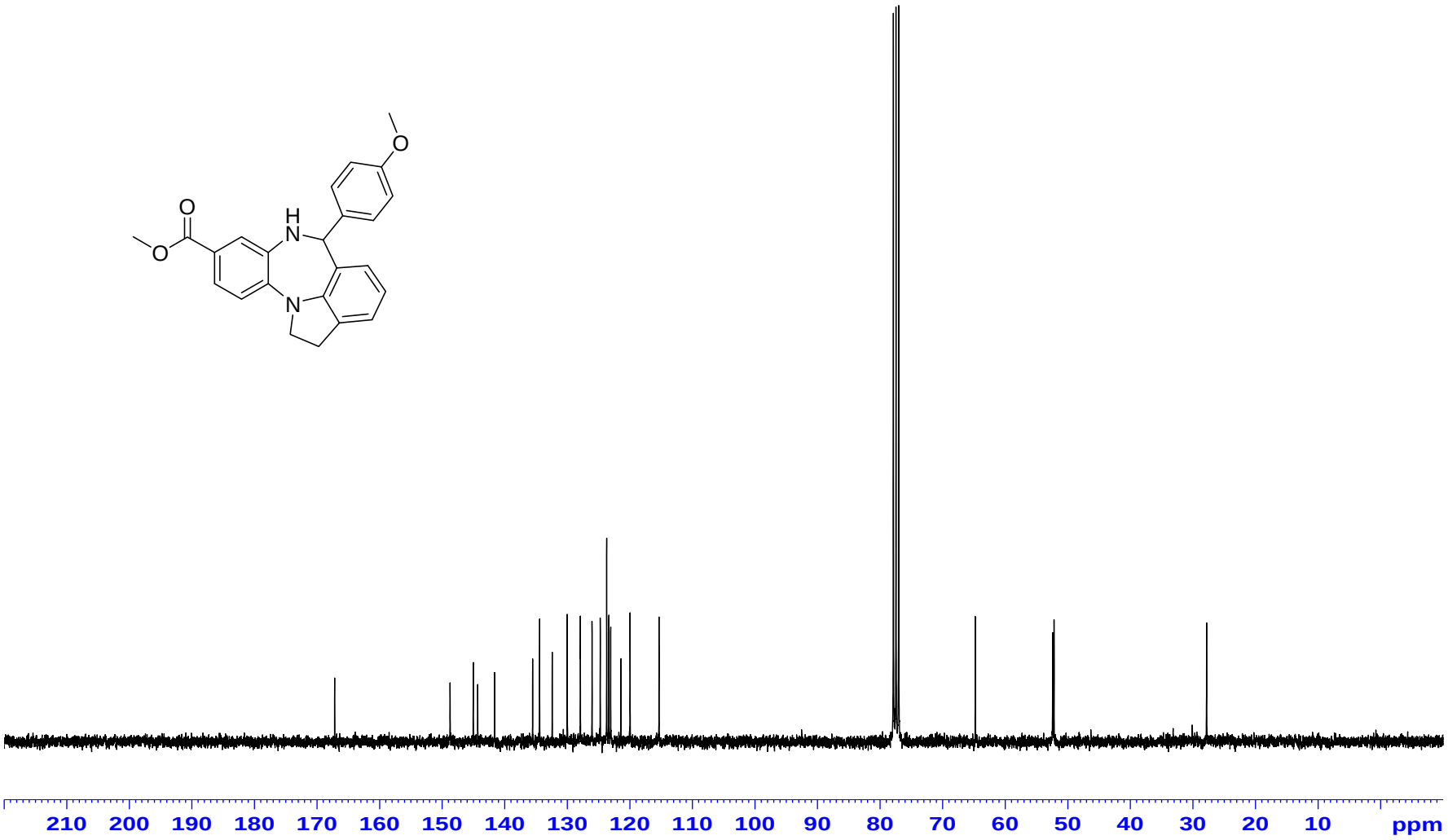


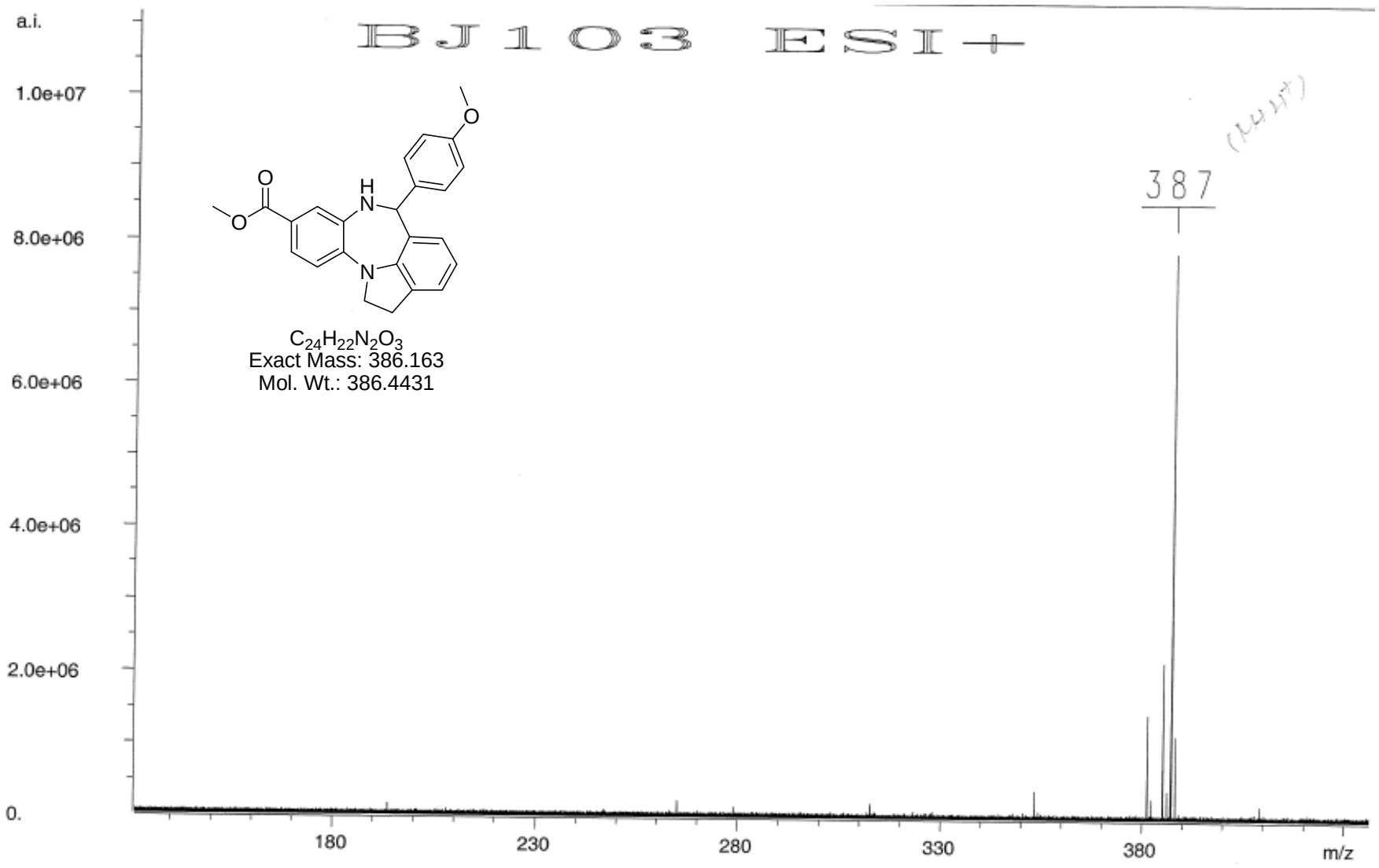

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] | |
|---|---|---|---|---|---|---|---|
| 1 | 13.096 | 6500.595 | 322.711 | 76.7 | 75.4 | | 0.30 |
| 2 | 13.476 | 1979.173 | 105.133 | 23.3 | 24.6 | | 0.28 |
| | Total | 8479.768 | 427.844 | 100.0 | 100.0 | | |



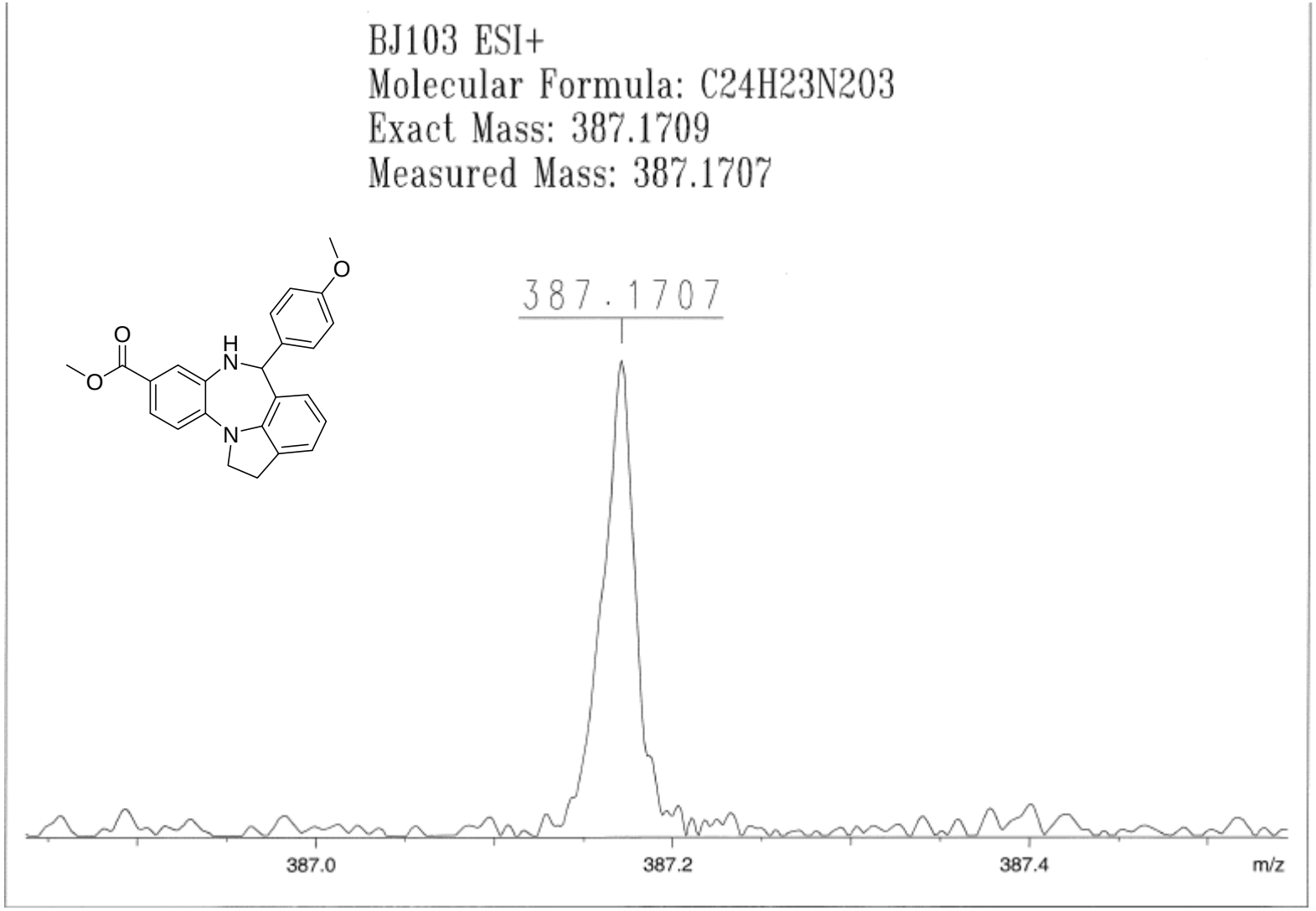

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4h** in $CDCl_3$



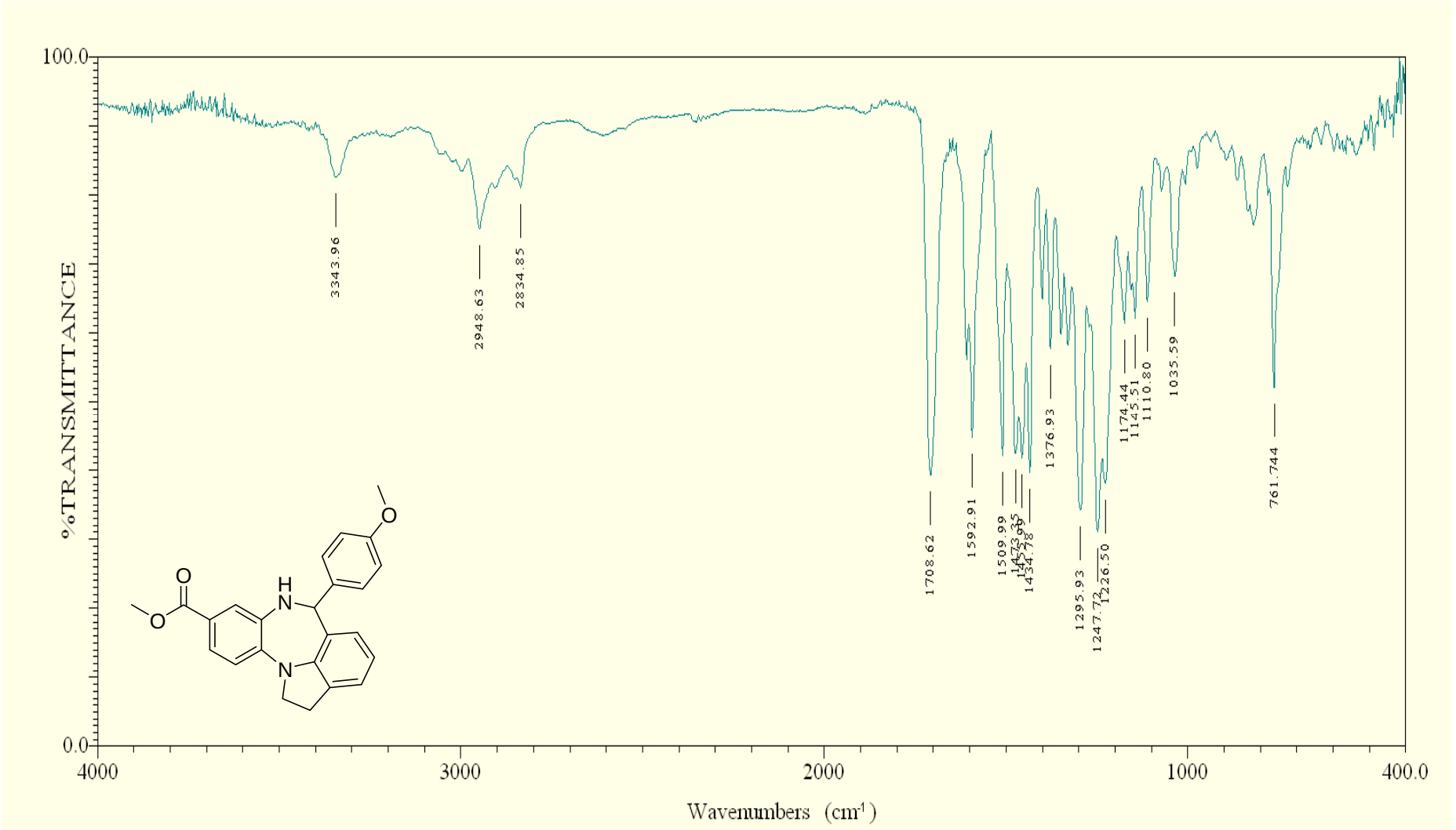

$^{13}C$, DEPT NMR Spectrum (75 MHz) of compound **4h** in $CDCl_3$



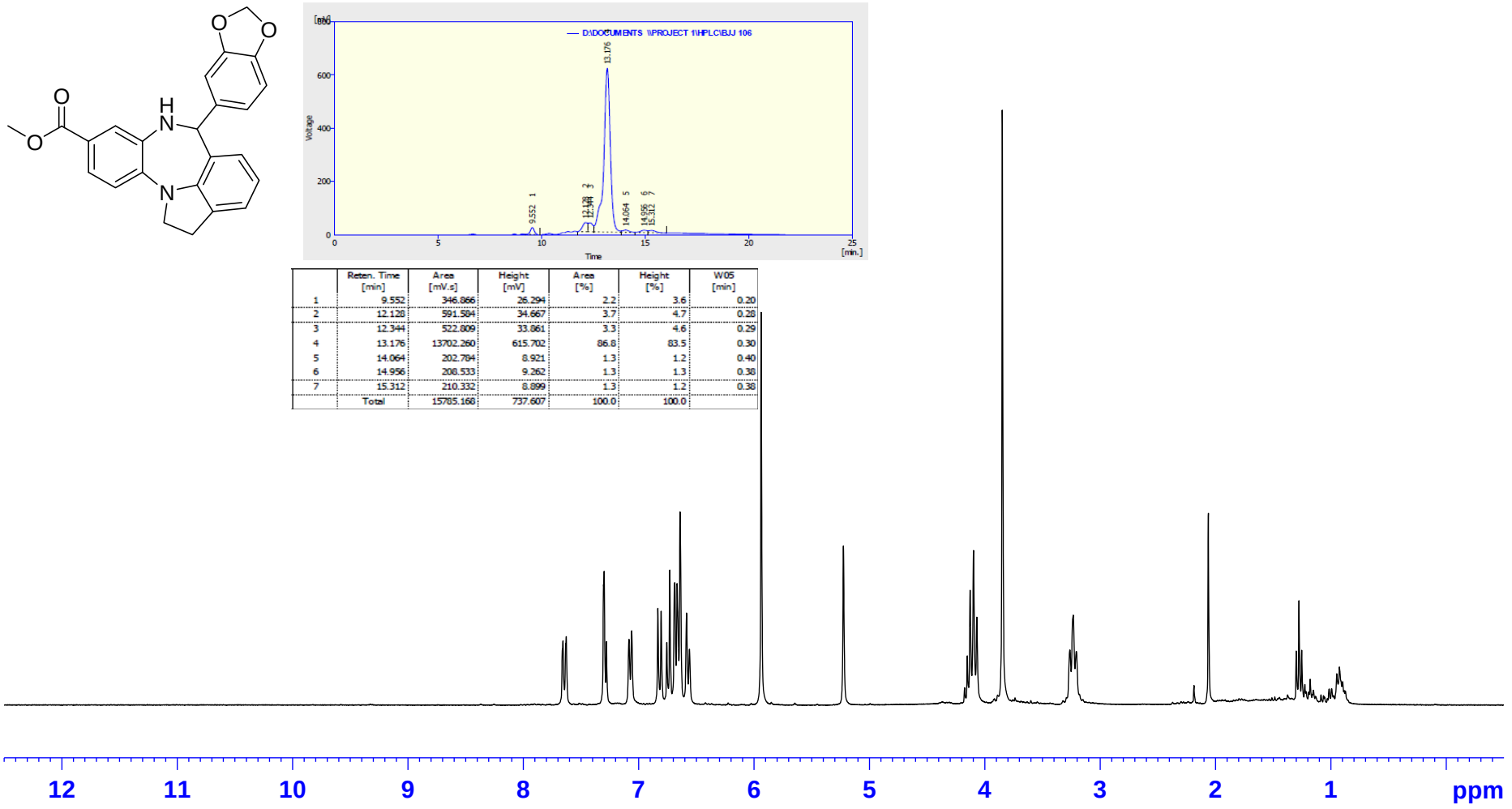

Low Resolution Mass Spectrum (LRMS) of compound **4h**



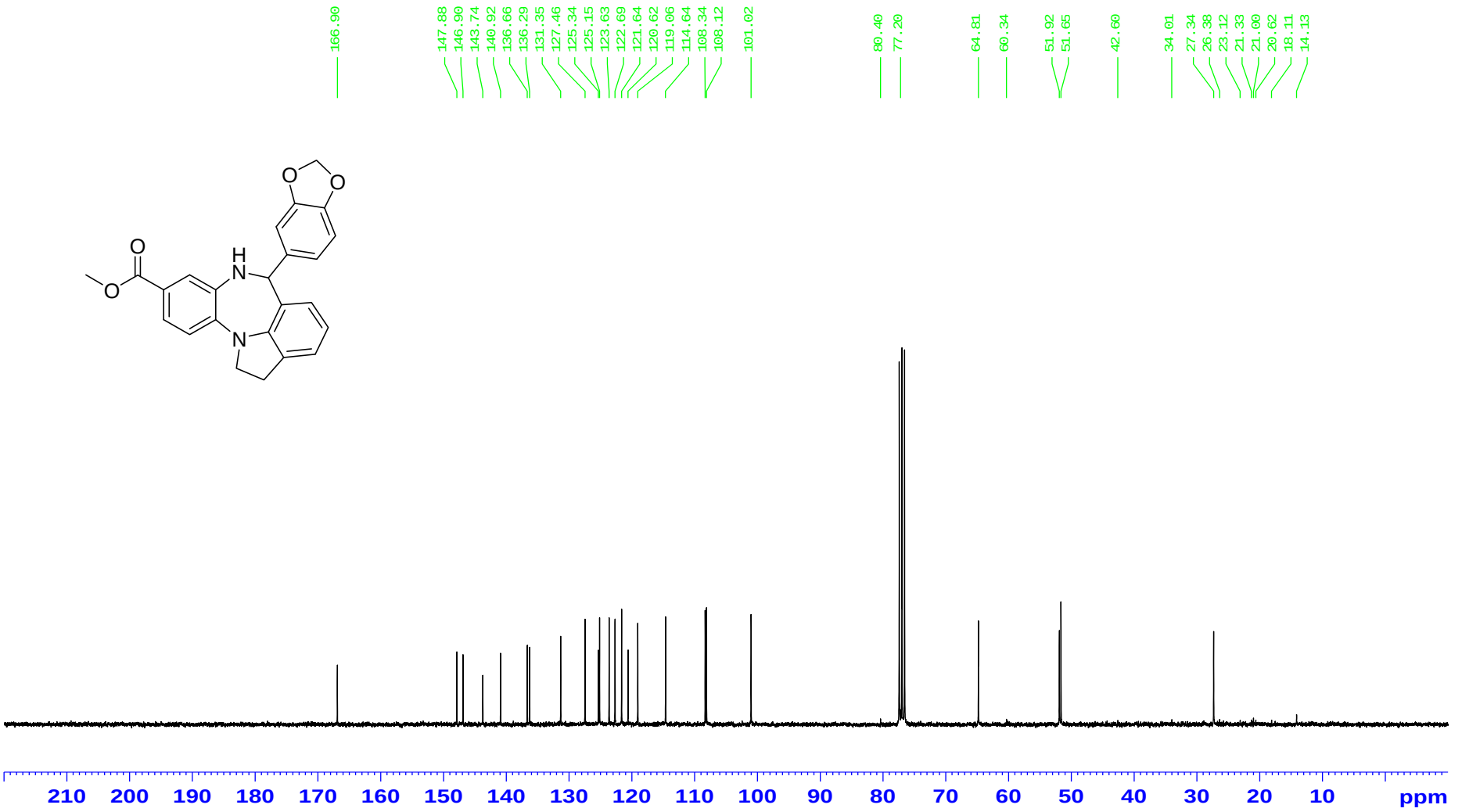

High Resolution Mass Spectrum (HRMS) of compound **4h**



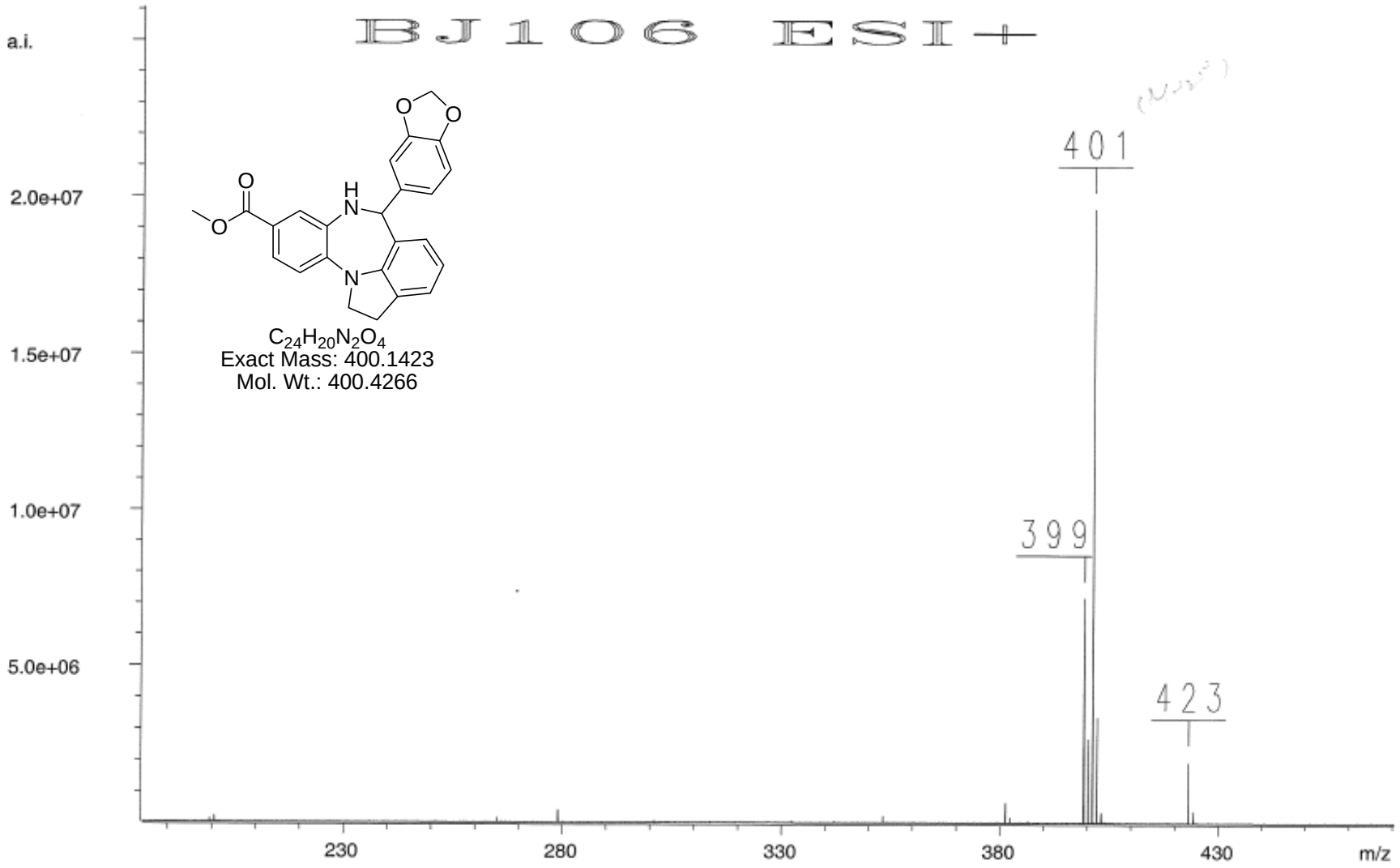

IR Spectrum of compound **4h** (Neat)



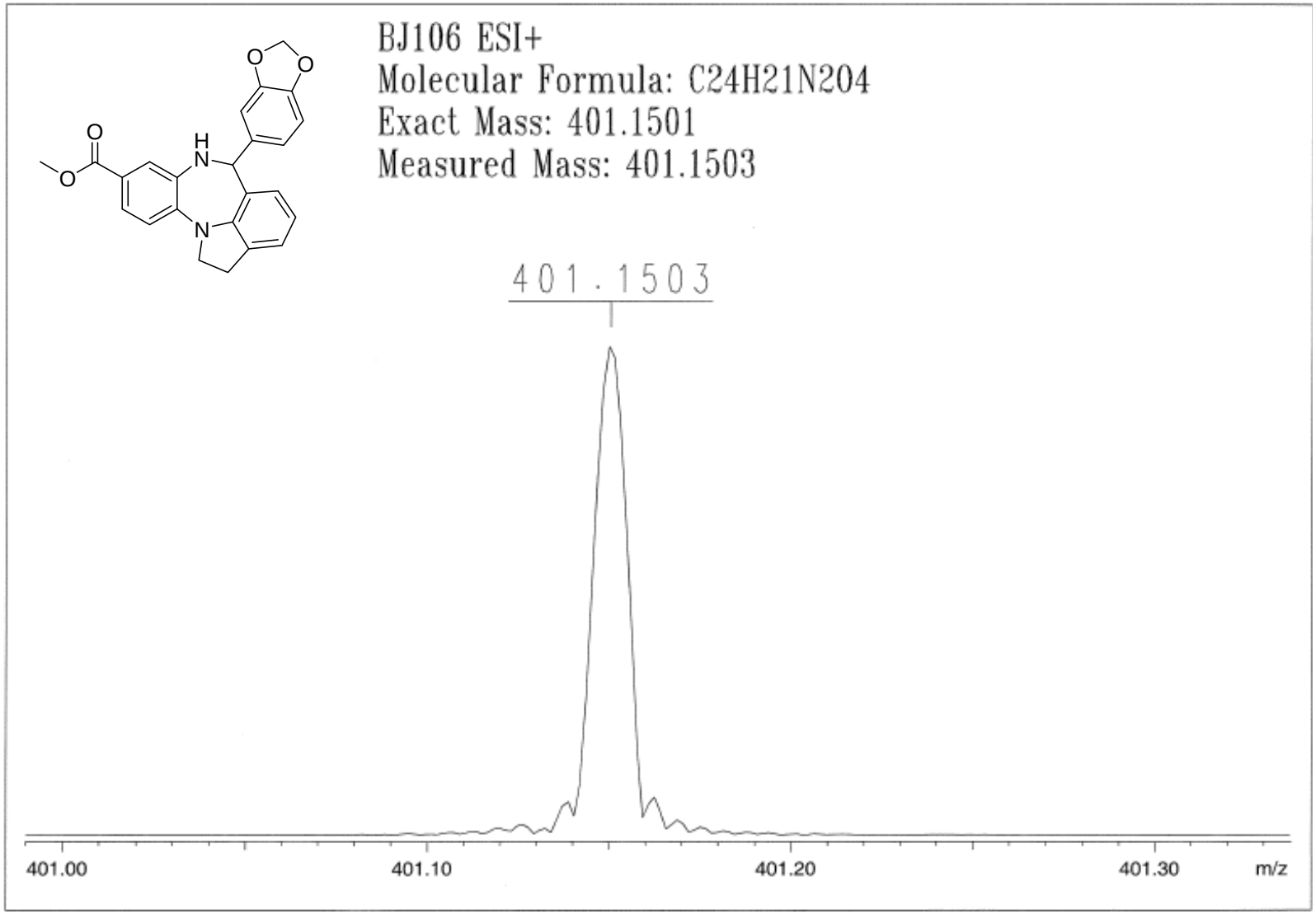

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4i** in $CDCl_3$



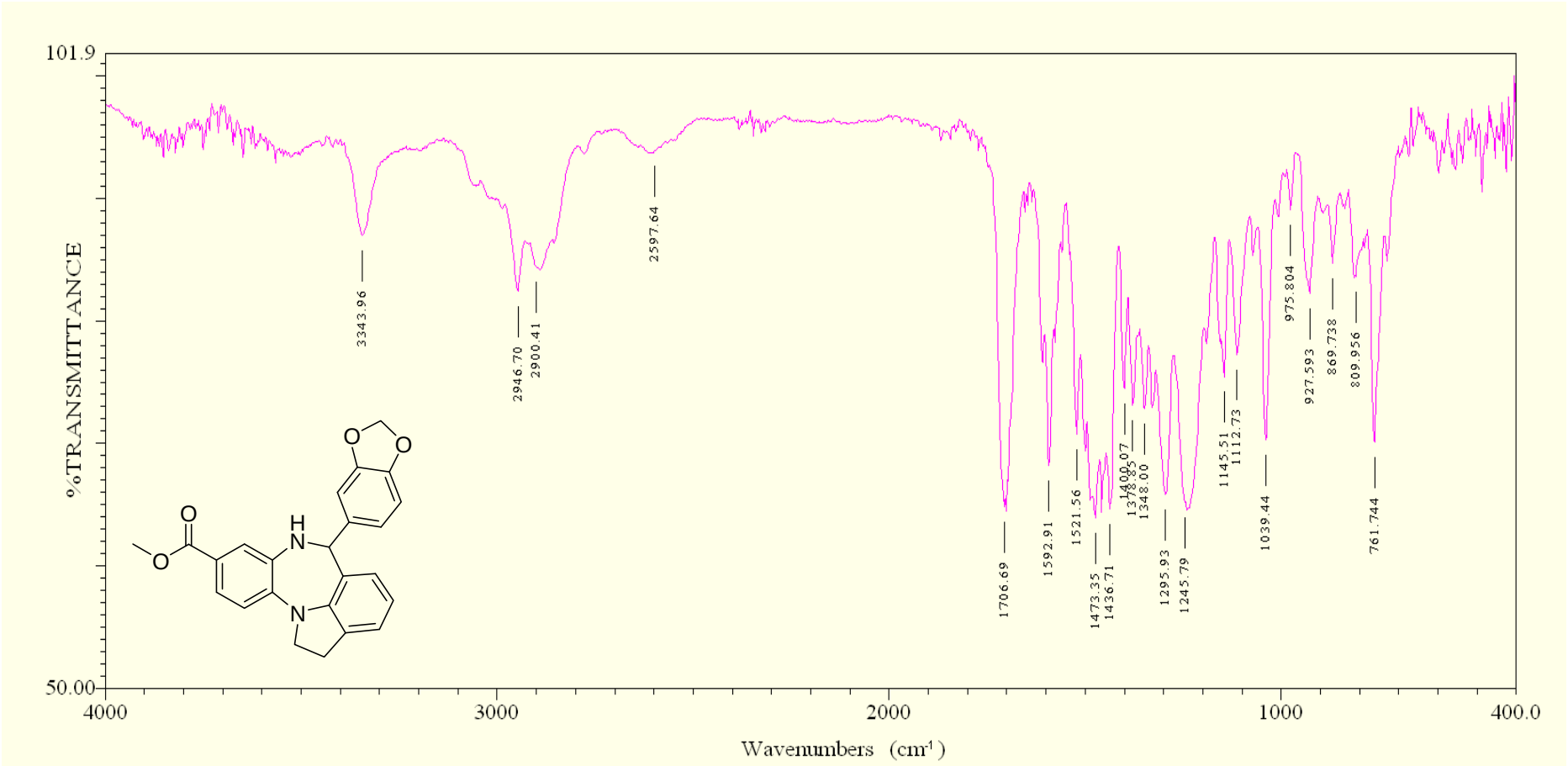

$^{13}$C NMR Spectrum (75 MHz) of compound **4i** in $CDCl_3$



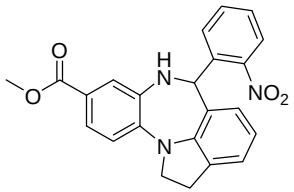

Low Resolution Mass Spectrum (LRMS) of compound **4i**

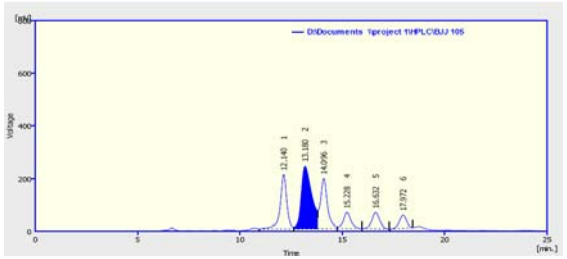



High Resolution Mass Spectrum (HRMS) of compound **4i**




IR Spectrum of compound **4i** (Neat)

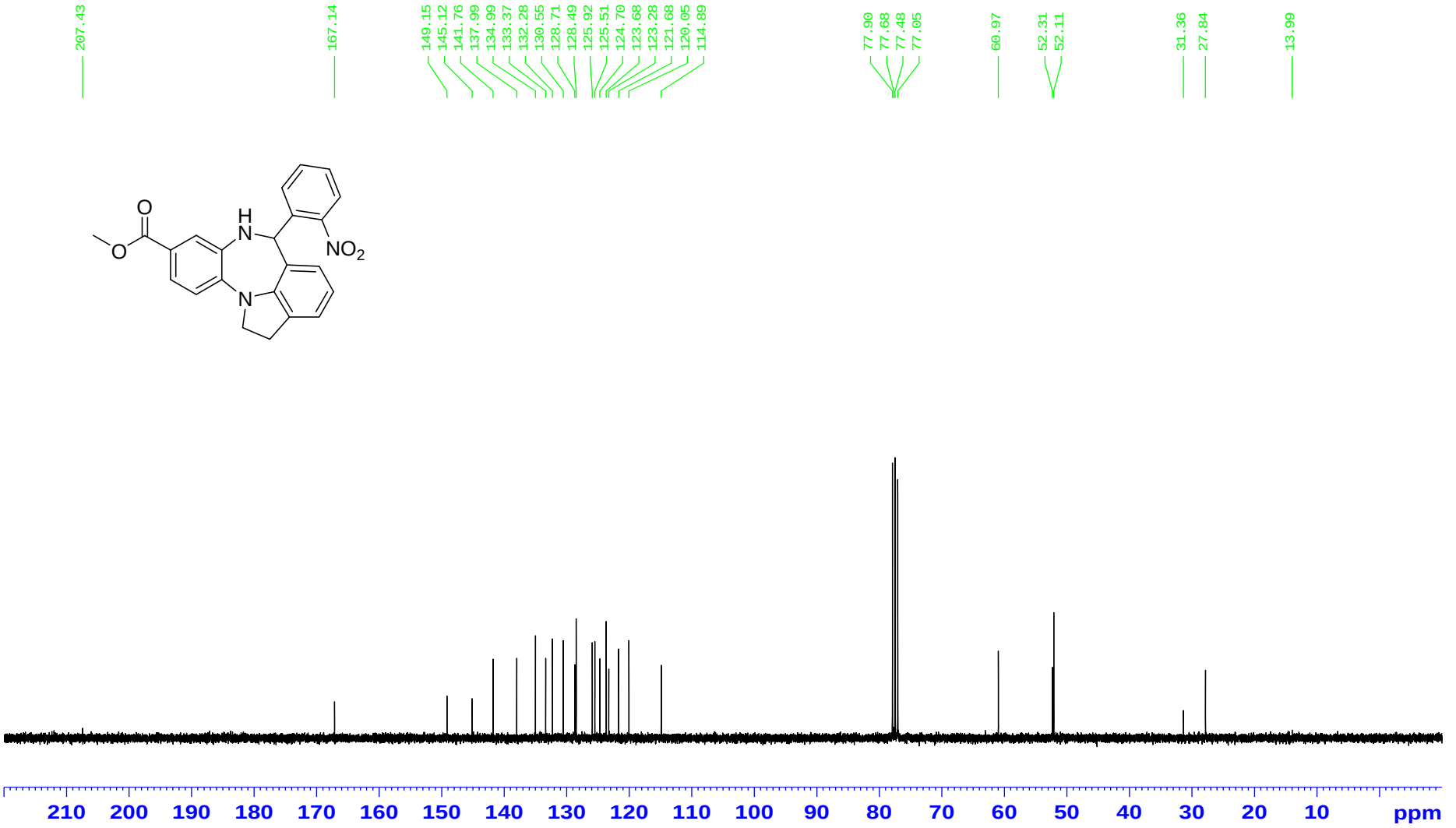


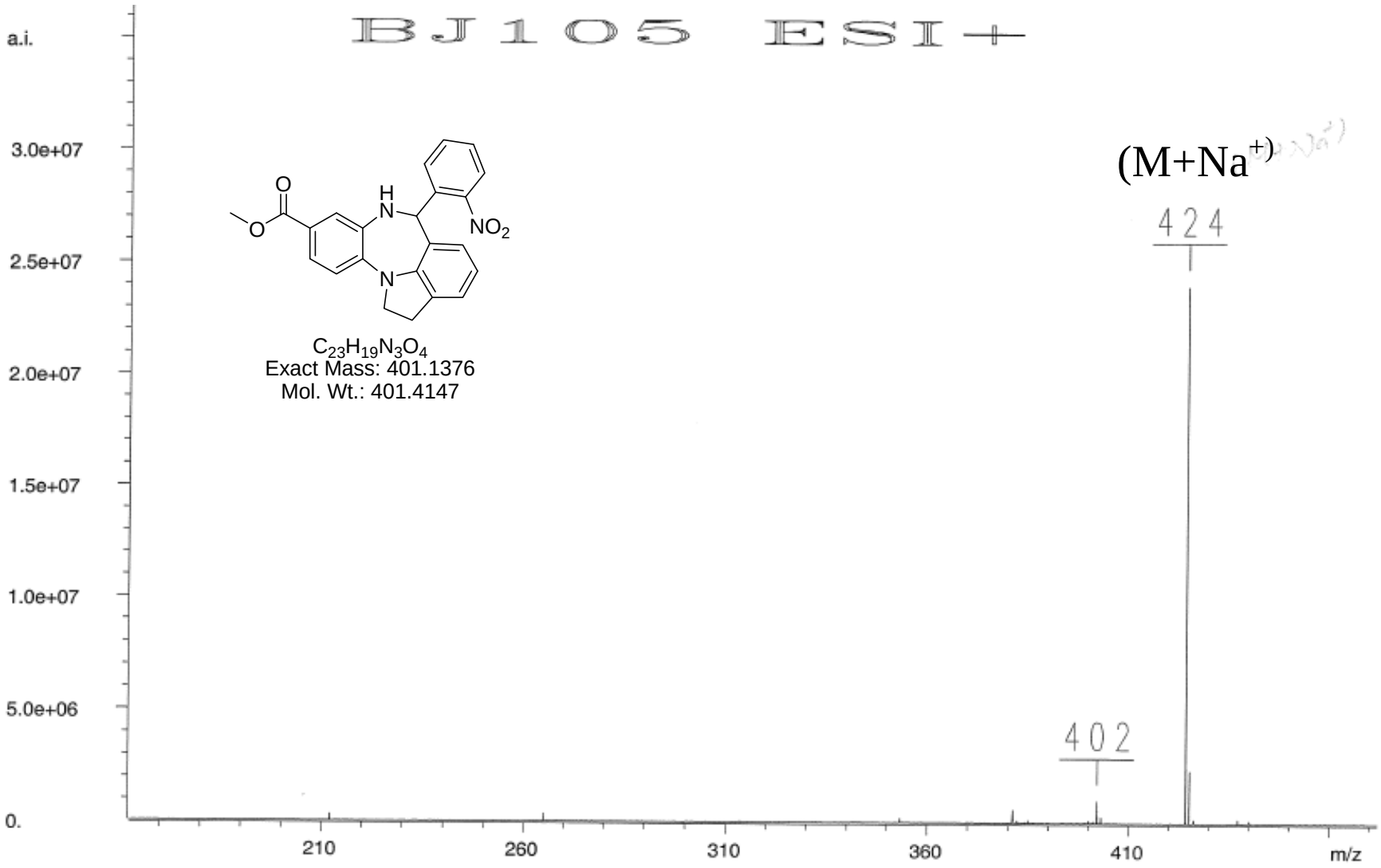

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 12.140 | 4690.873 | 208.240 | 21.1 | 25.7 | 0.31 |
| 2 | 13.180 | 8449.461 | 239.028 | 38.1 | 29.5 | 0.56 |
| 3 | 14.096 | 4640.002 | 191.116 | 20.9 | 23.6 | 0.36 |
| 4 | 15.228 | 1566.813 | 61.040 | 7.1 | 7.5 | 0.37 |
| 5 | 16.632 | 1646.368 | 61.694 | 7.4 | 7.6 | 0.40 |
| 6 | 17.972 | 1196.461 | 49.188 | 5.4 | 6.1 | 0.38 |
| | Total | 22189.980 | 810.307 | 100.0 | 100.0 | |



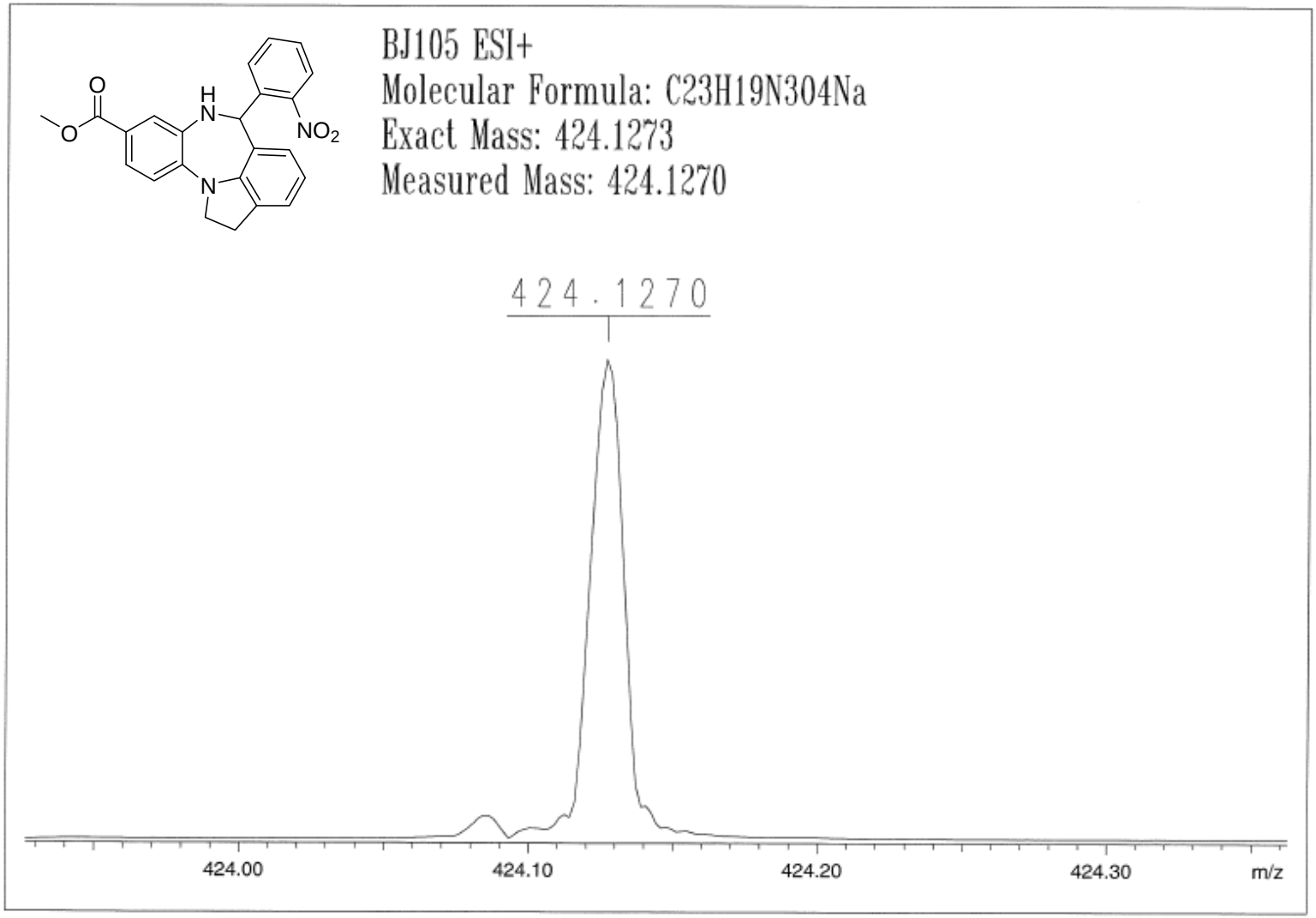

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4j** in $CDCl_3$



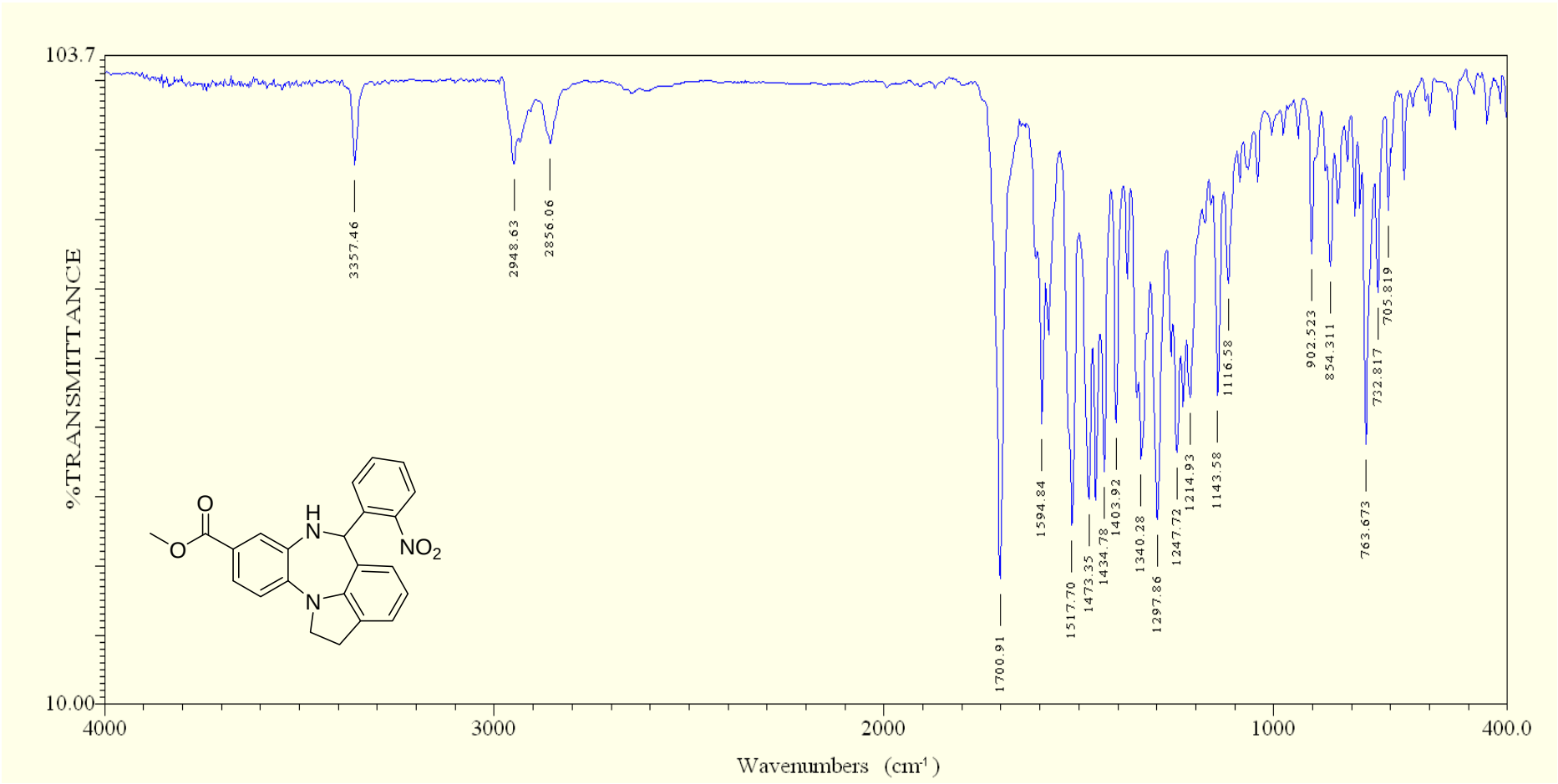

$^{13}$C NMR Spectrum (75 MHz) of compound **4j** in $CDCl_3$



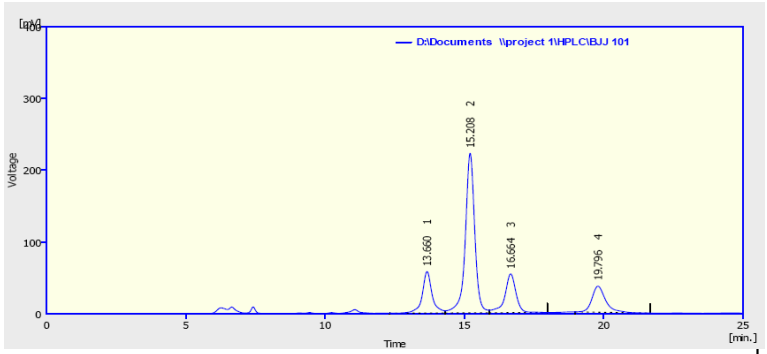

Low Resolution Mass Spectrum (LRMS) of compound **4j**



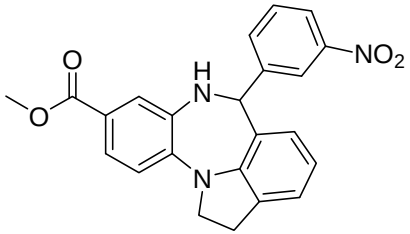

High Resolution Mass Spectrum (HRMS) of compound **4j**

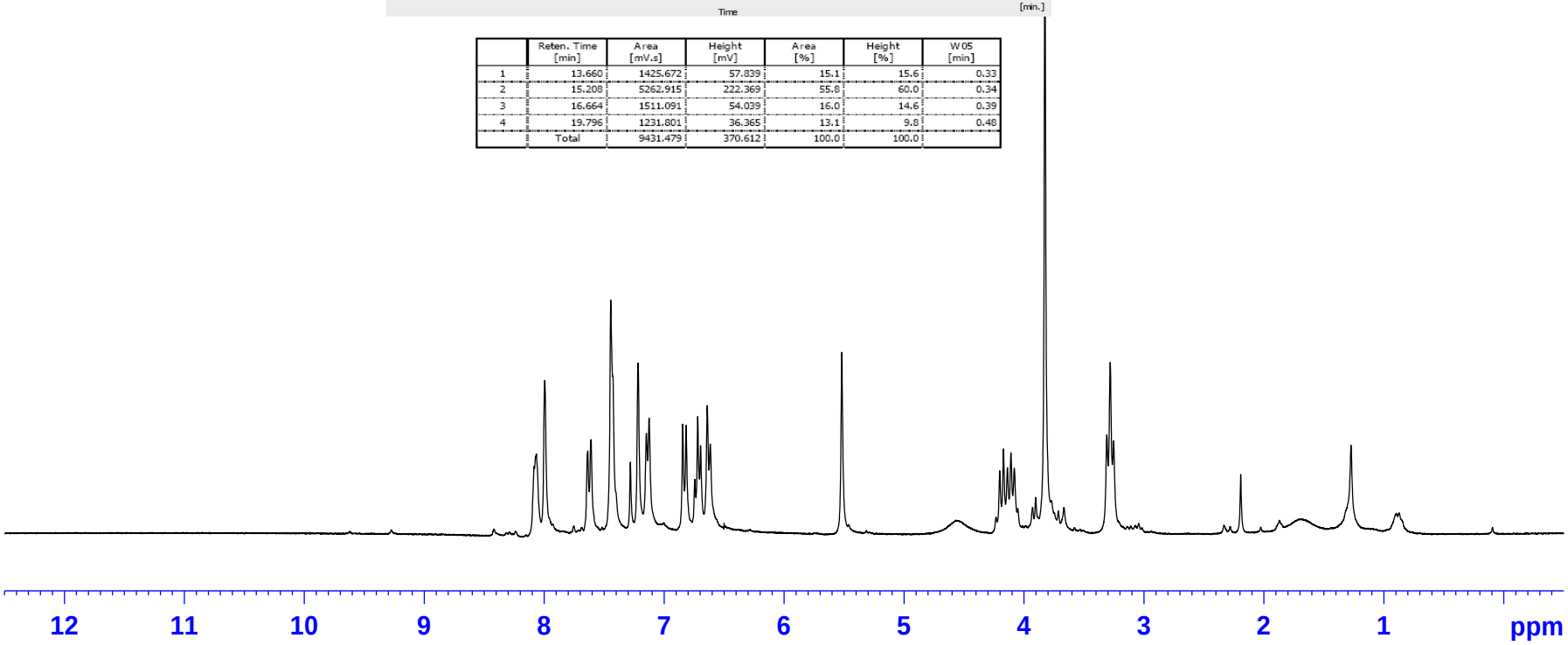



IR Spectrum of compound **4j** (Neat)

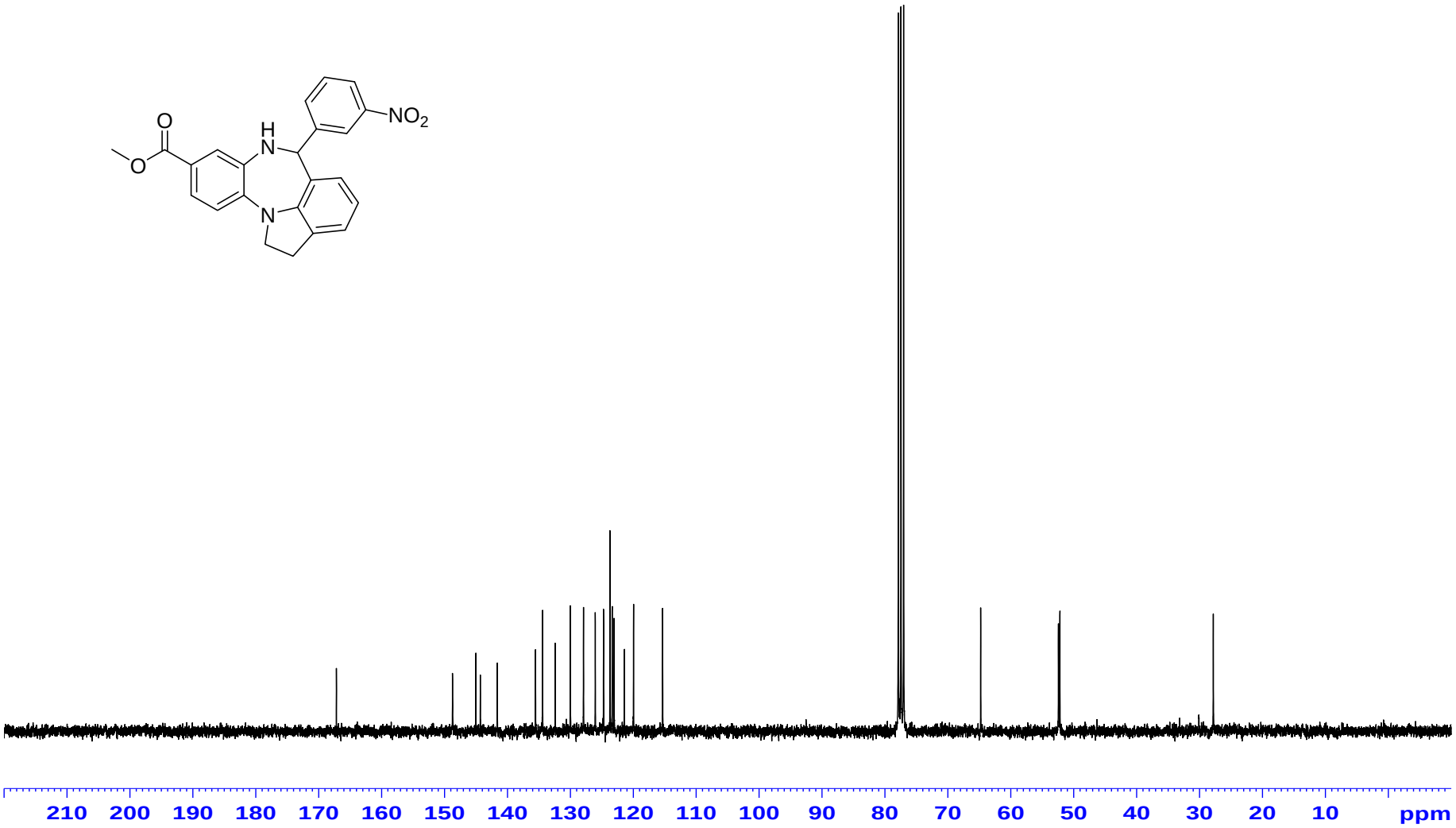



| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 13.660 | 1425.672 | 57.839 | 15.1 | 15.6 | 0.33 |
| 2 | 15.208 | 5262.915 | 222.369 | 55.8 | 60.0 | 0.34 |
| 3 | 16.664 | 1511.091 | 54.039 | 16.0 | 14.6 | 0.39 |
| 4 | 19.796 | 1231.801 | 36.365 | 13.1 | 9.8 | 0.48 |
| | Total | 9431.479 | 370.612 | 100.0 | 100.0 | |

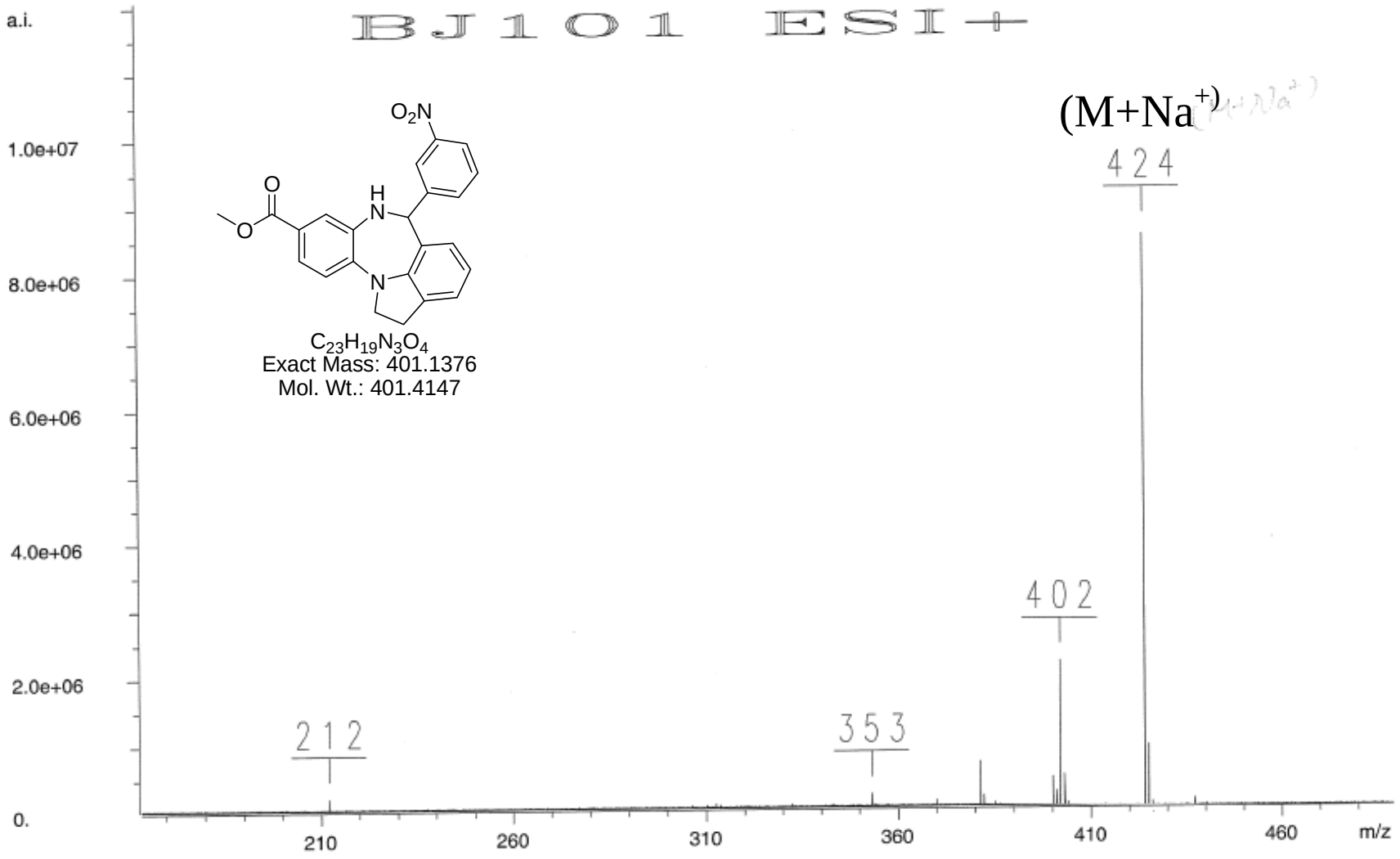


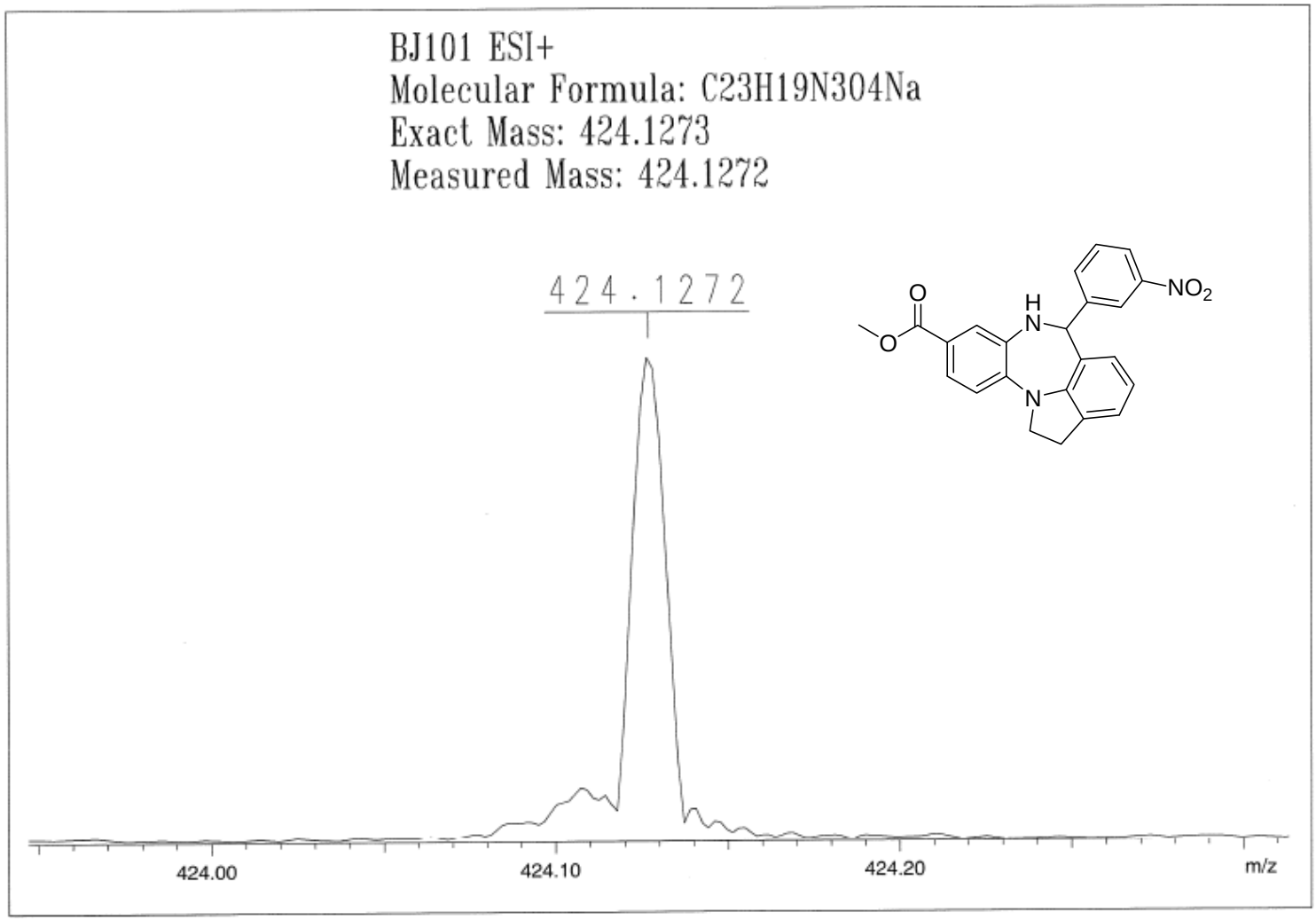

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **4k** in $CDCl_3$



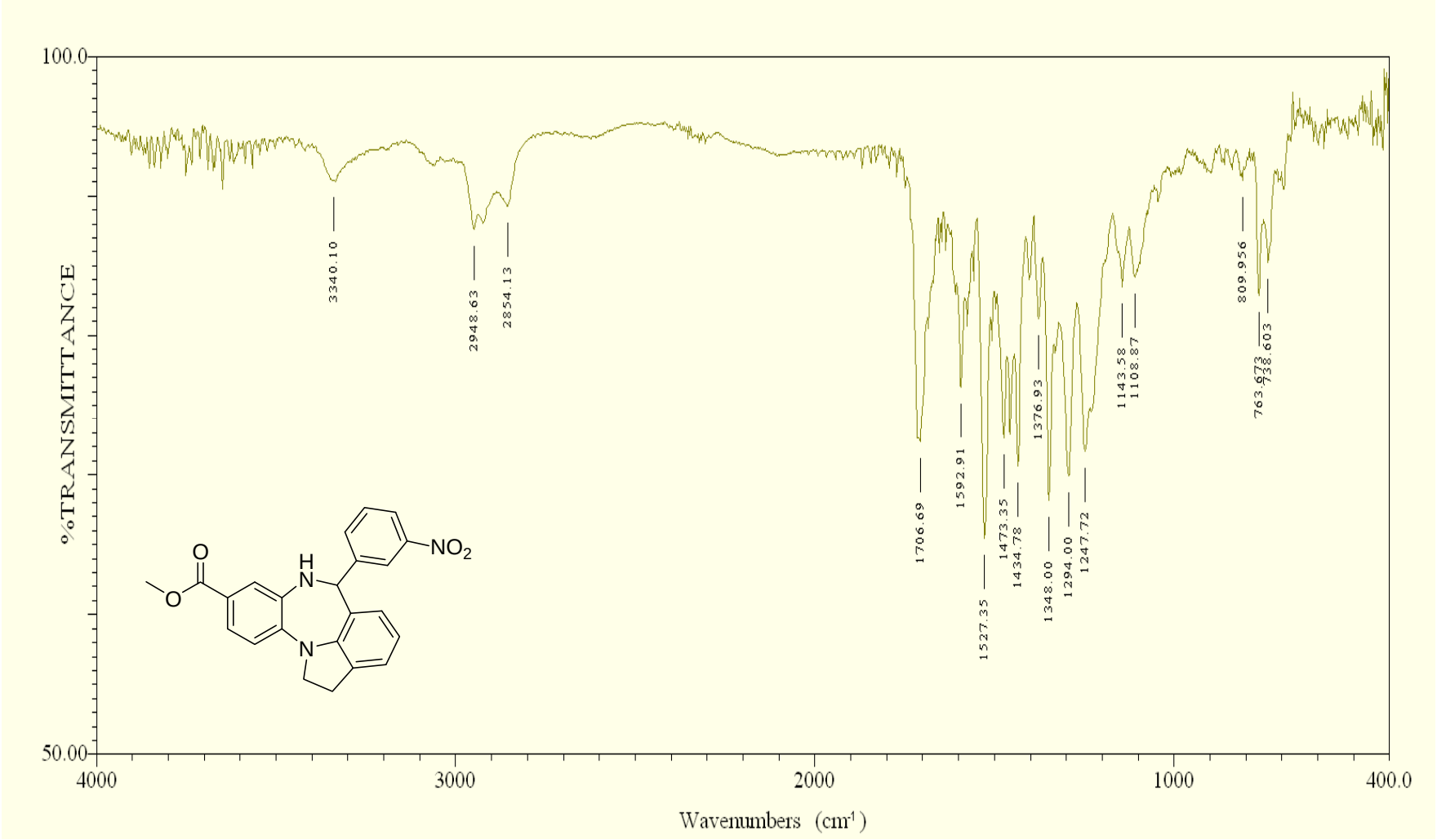

$^{13}$C NMR Spectrum (75 MHz) of compound **4k** in $CDCl_3$



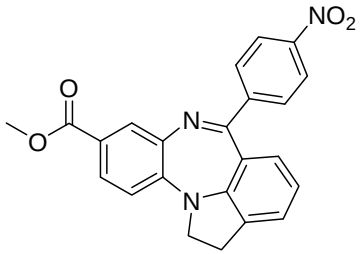

Low Resolution Mass Spectrum (LRMS) of compound **4k**

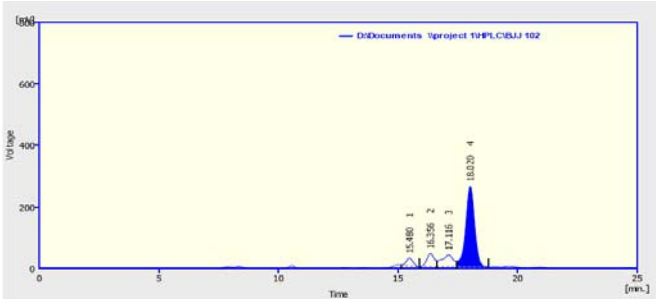



High Resolution Mass Spectrum (HRMS) of compound **4k**




IR Spectrum of compound **4k** (Neat)

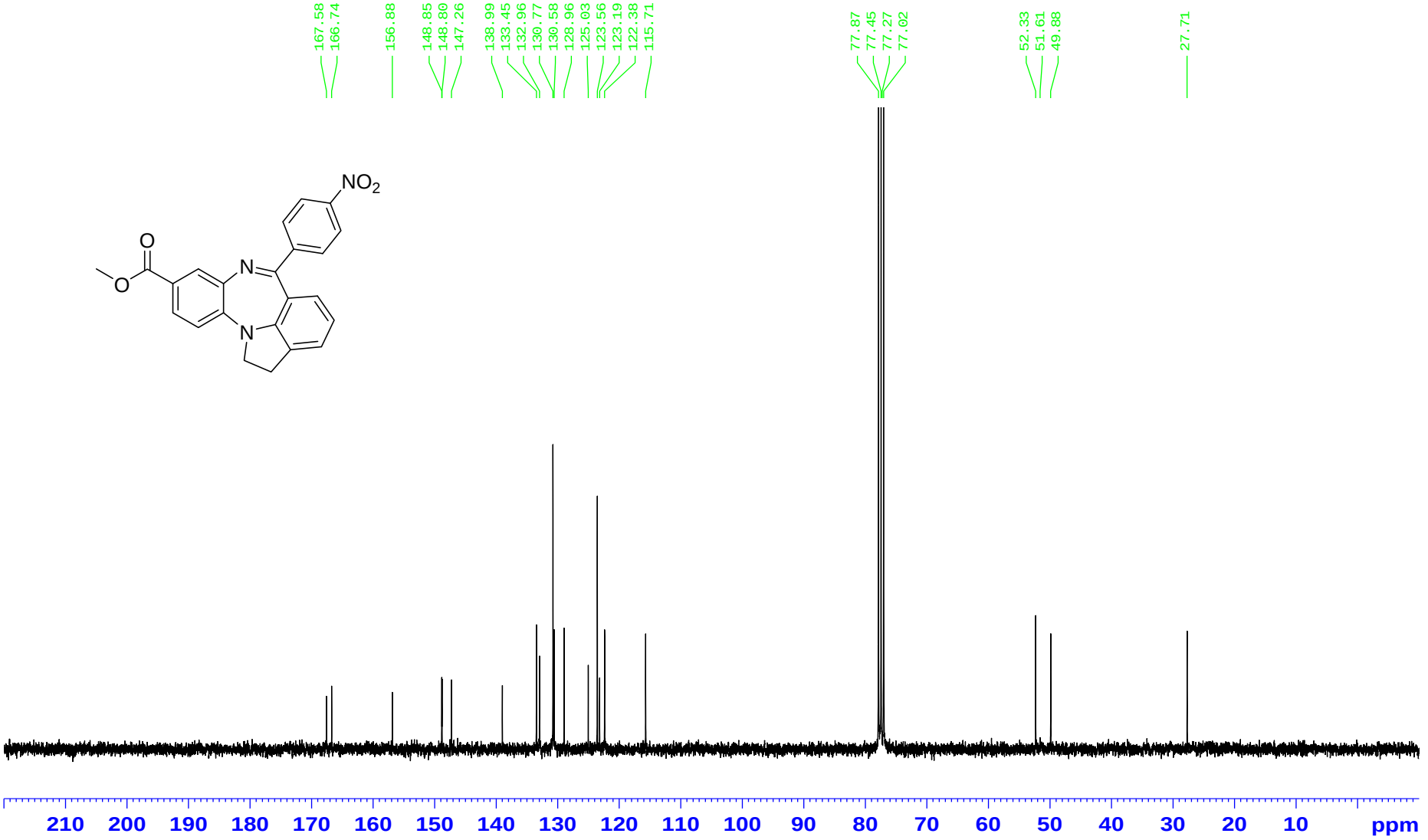


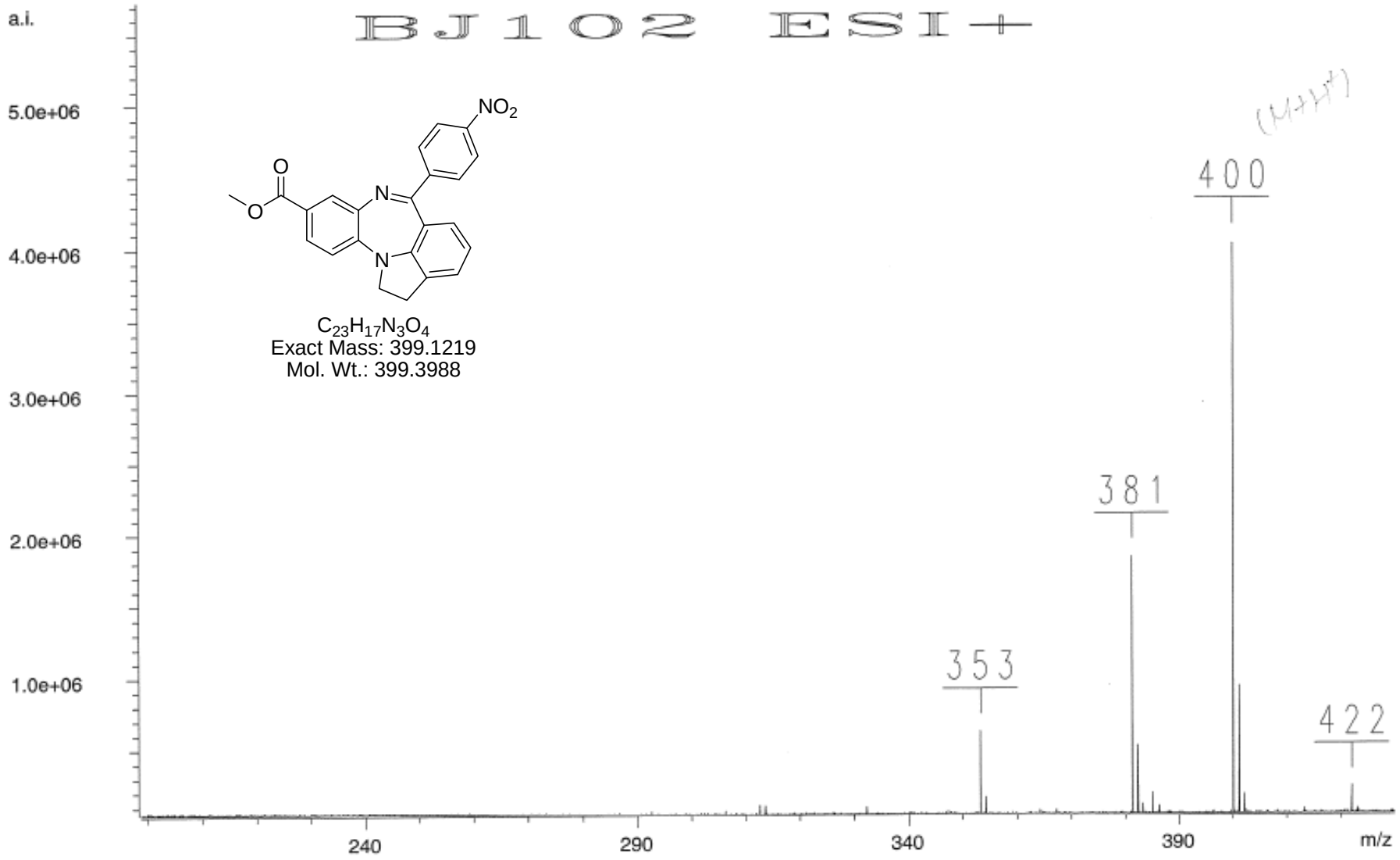

| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] |
|---|---|---|---|---|---|---|
| 1 | 15.480 | 486.677 | 25.549 | 5.1 | 6.9 | 0.30 |
| 2 | 16.356 | 958.940 | 42.938 | 10.0 | 11.6 | 0.38 |
| 3 | 17.116 | 1304.787 | 38.697 | 13.7 | 10.5 | 0.73 |
| 4 | 18.020 | 6806.411 | 262.210 | 71.2 | 71.0 | 0.39 |
| | Total | 9556.815 | 369.394 | 100.0 | 100.0 | |



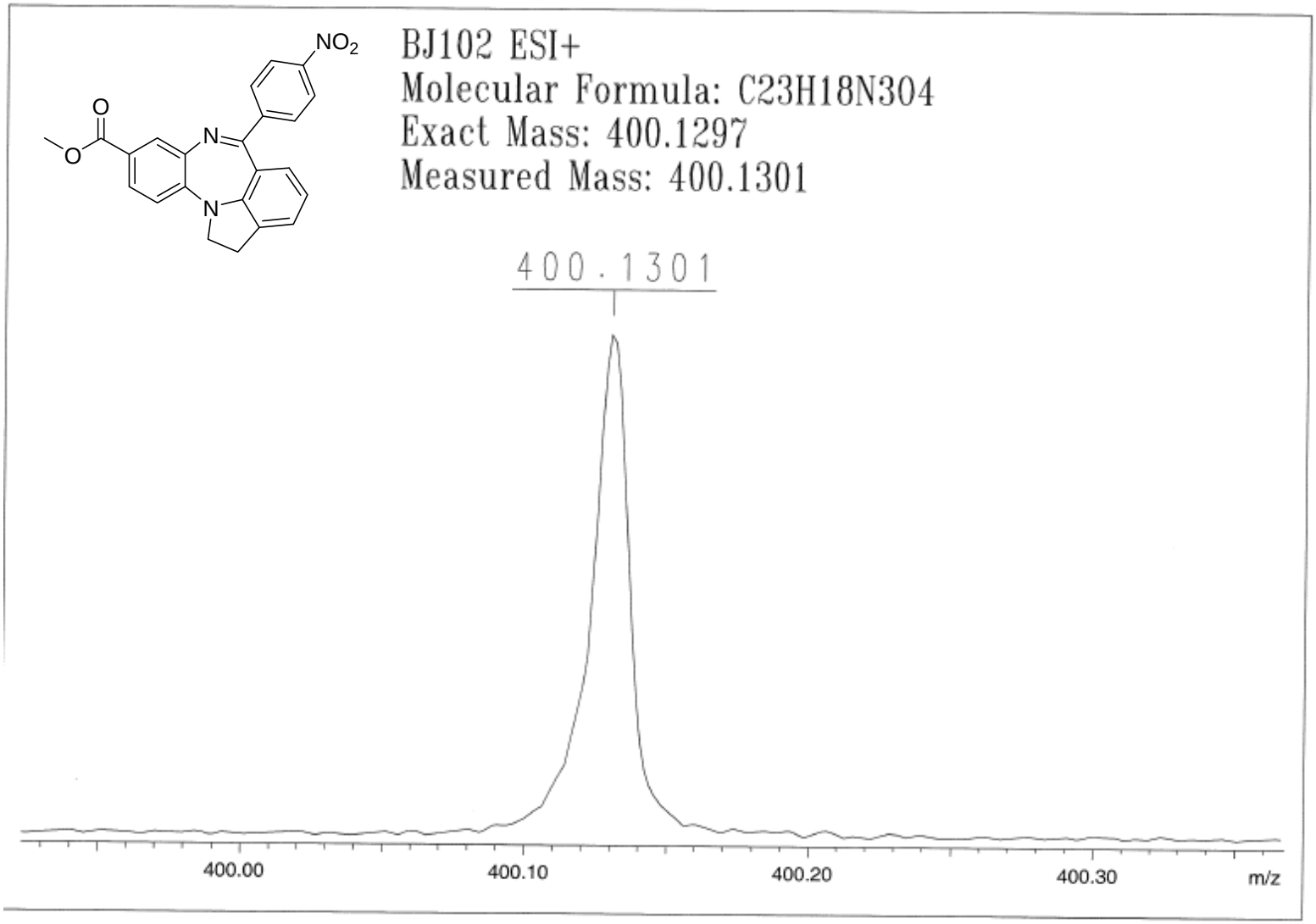

HPLC and $^{1}H$ NMR Spectrum (300 MHz) of compound **5** in $CDCl_3$



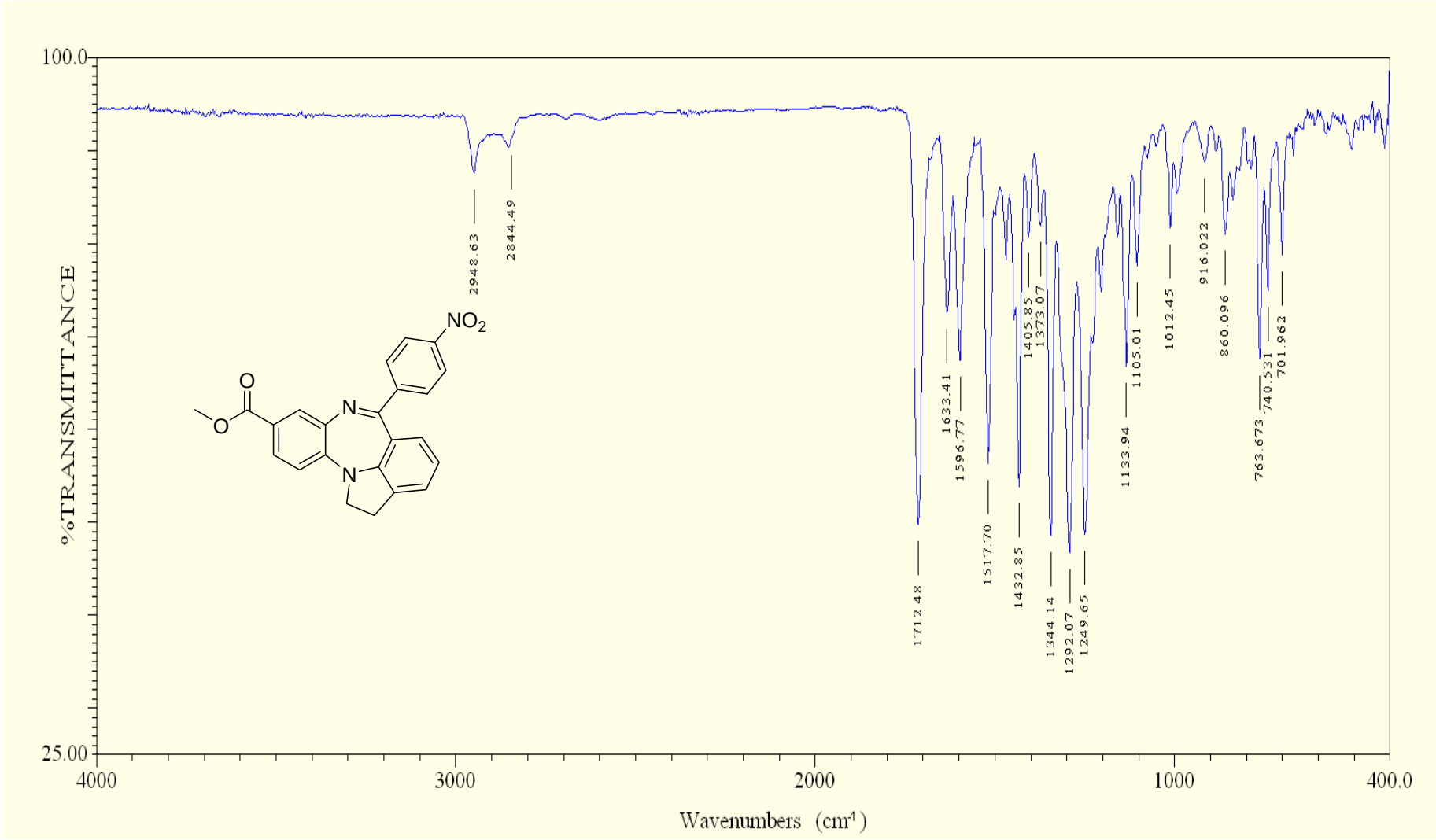

$^{13}$C NMR Spectrum (75 MHz) of compound **5** in $CDCl_3$




Low Resolution Mass Spectrum (LRMS) of compound **5**




High Resolution Mass Spectrum (HRMS) of compound **5**




IR Spectrum of compound **5** (Neat)