## IR, $^{1}$H NMR, $^{13}$C NMR and Mass spectra of all products

**6** *N*-(2-nitro-1-phenylethyl)aniline

Table 1.1: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **6** | 242 | 1 | 241.03 | 20 | 92.04 | 56 | ES- |
| | | 2 | 242.07 | 30 | 72.98 | 24 | ES+ |
| | | 3 | 242.07 | 30 | 94.06 | 26 | ES+ |
| | | 4 | 242.07 | 30 | 86.98 | 24 | ES+ |
| | | 5 | 242.07 | 30 | 122.03 | 24 | ES+ |

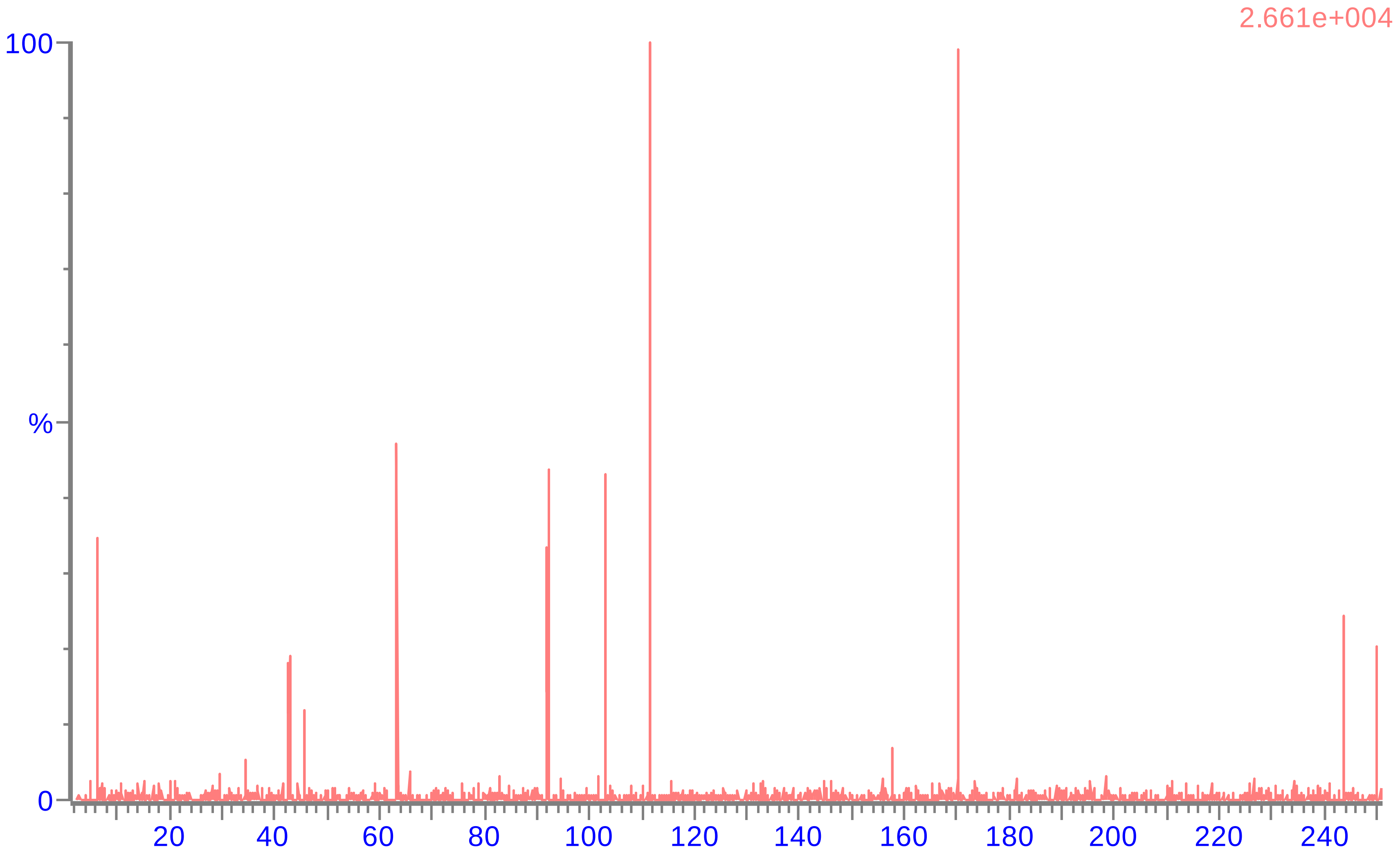

Figure 1.1: Mass spectrum for daughter fragment peak ES+, m/z 241.03 -> 92.04.

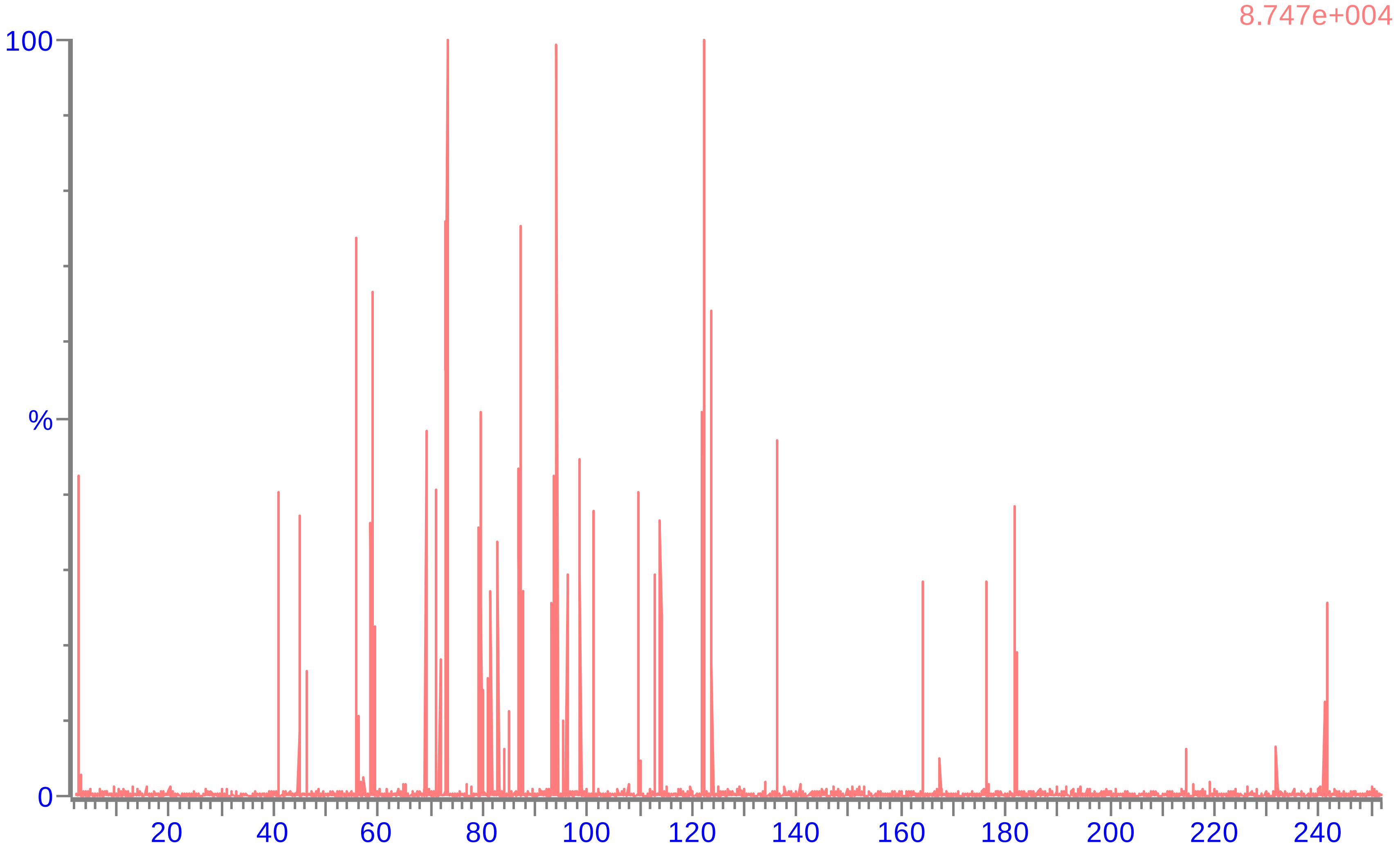

Figure 1.2: Mass spectrum for daughter fragment peak ES+, m/z 241.03 -> 72.98.

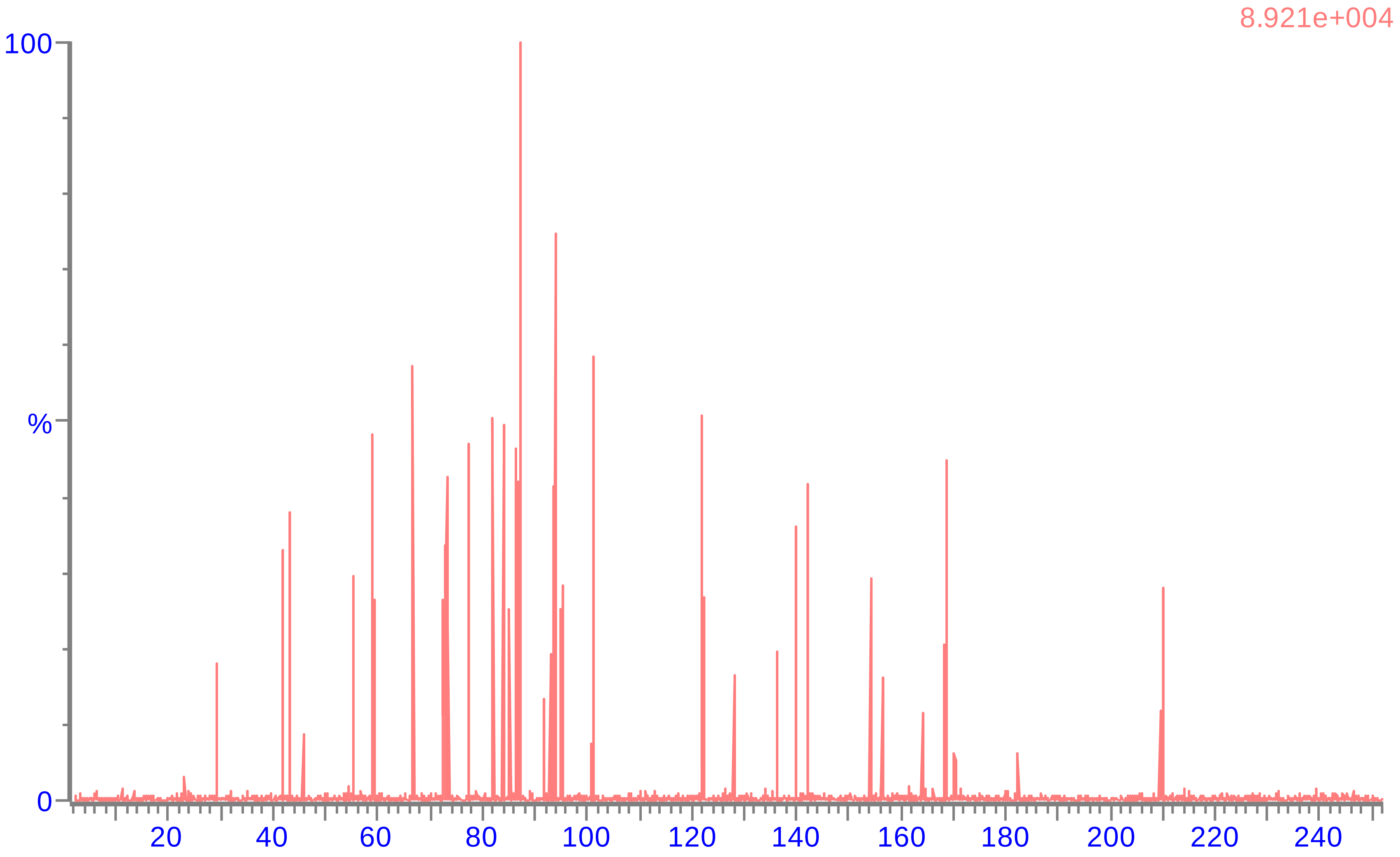

Figure 1.3: Mass spectrum for daughter fragment peak ES+, m/z 241.03 -> 94.06.

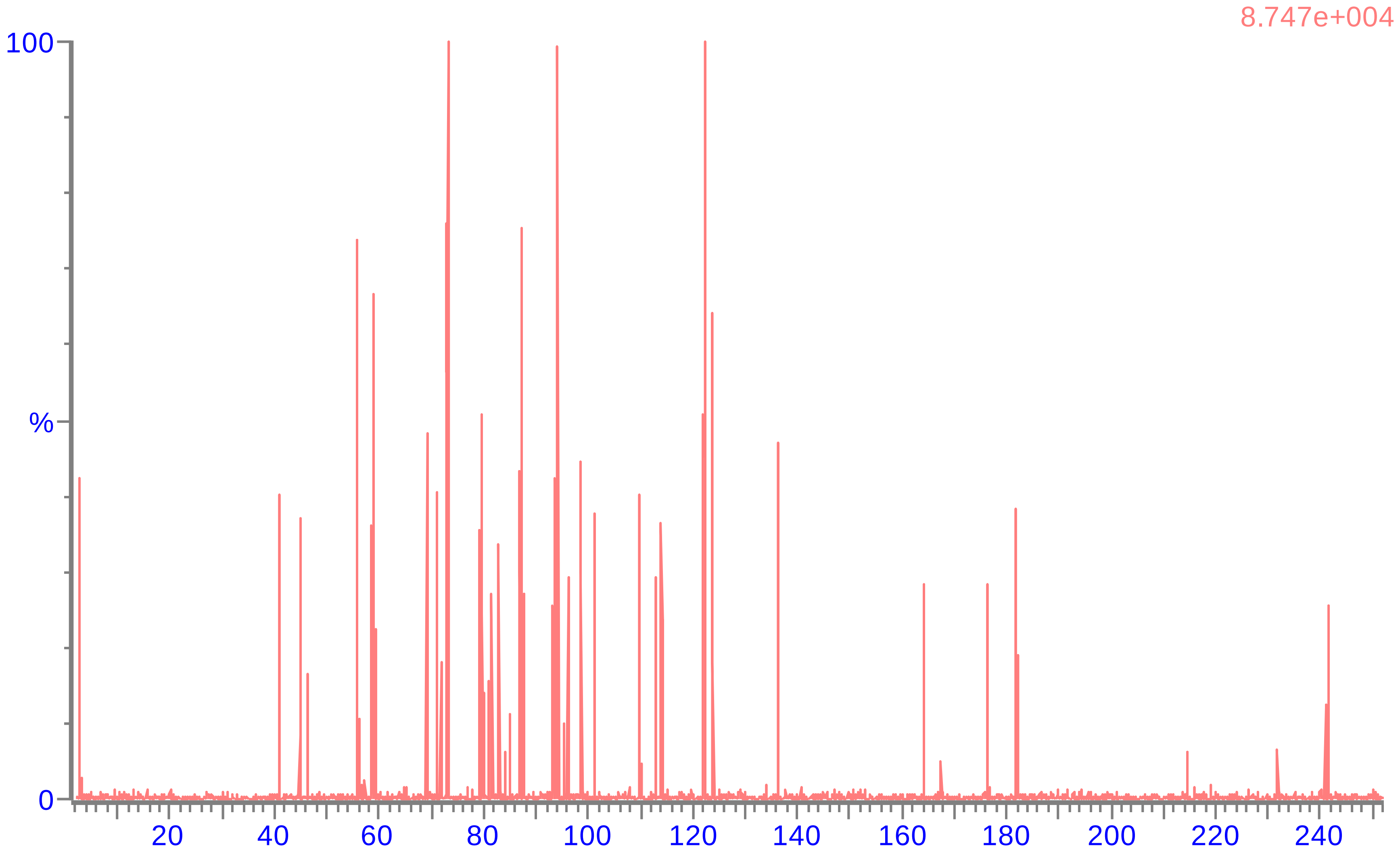

Figure 1.4: Mass spectrum for daughter fragment peak ES+, m/z 241.03 -> 86.98.

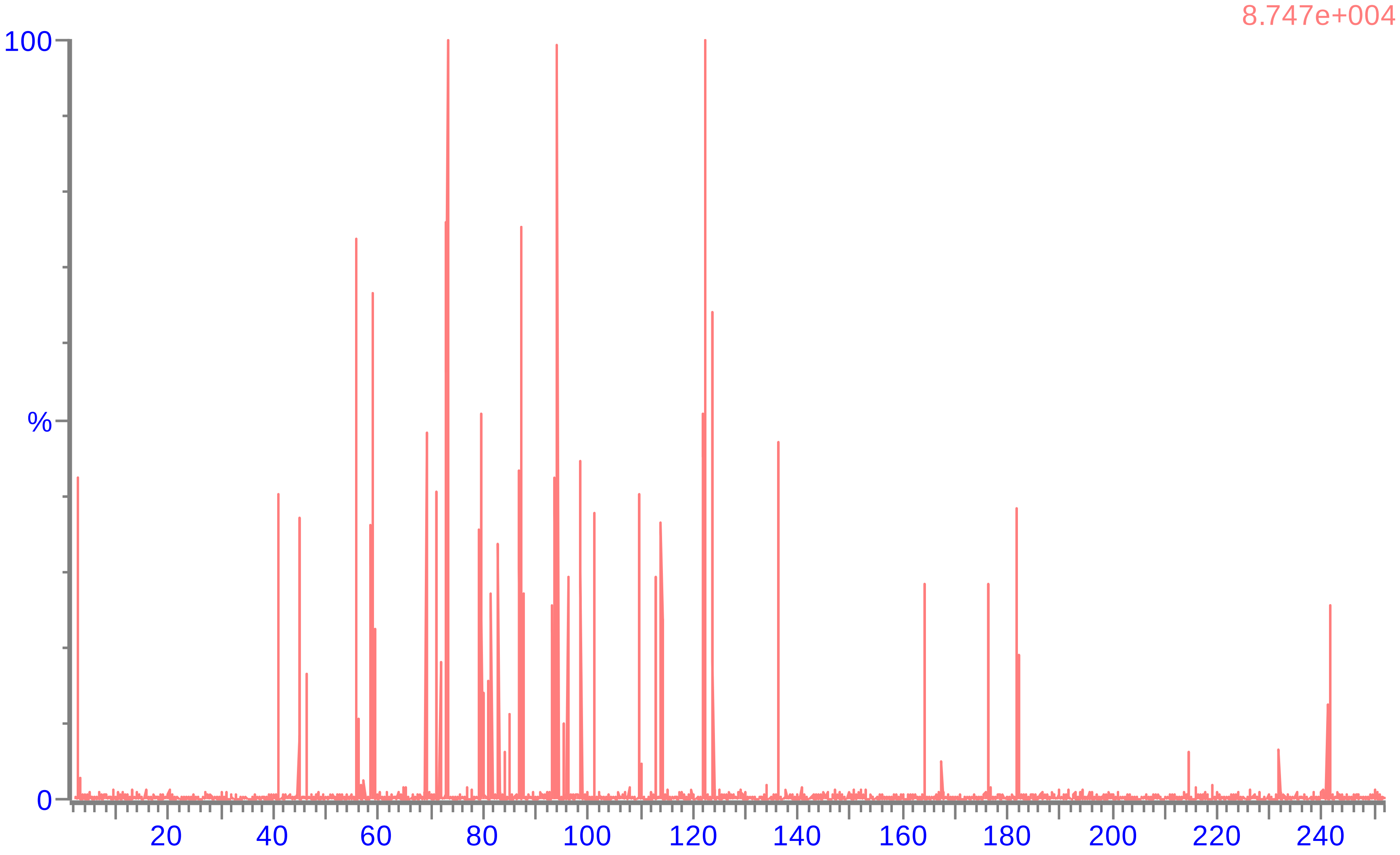

Figure 1.5: Mass spectrum for daughter fragment peak ES+, m/z 241.03 -> 122.03.

**7a** *N*-(2-nitro-1-(*p*-tolyl)ethyl)aniline

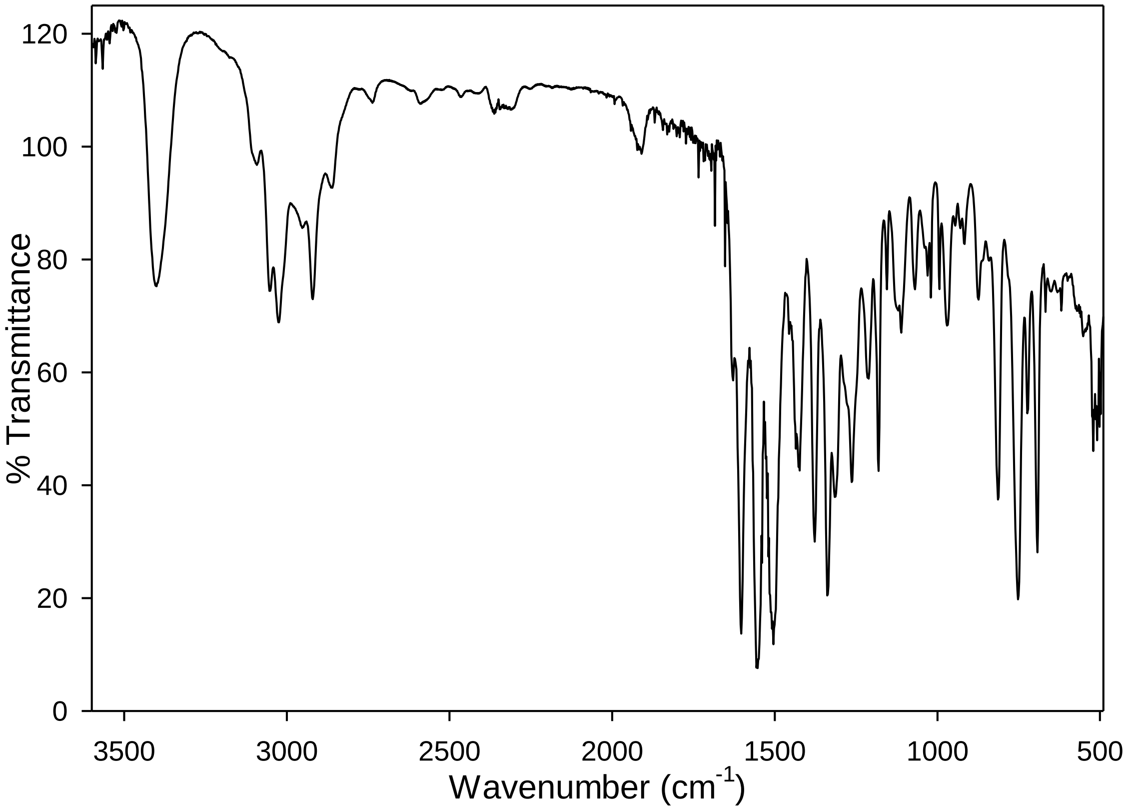

Figure 1.6: IR spectrum of **7a** *N*-(2-nitro-1-(*p*-tolyl)ethyl)aniline.

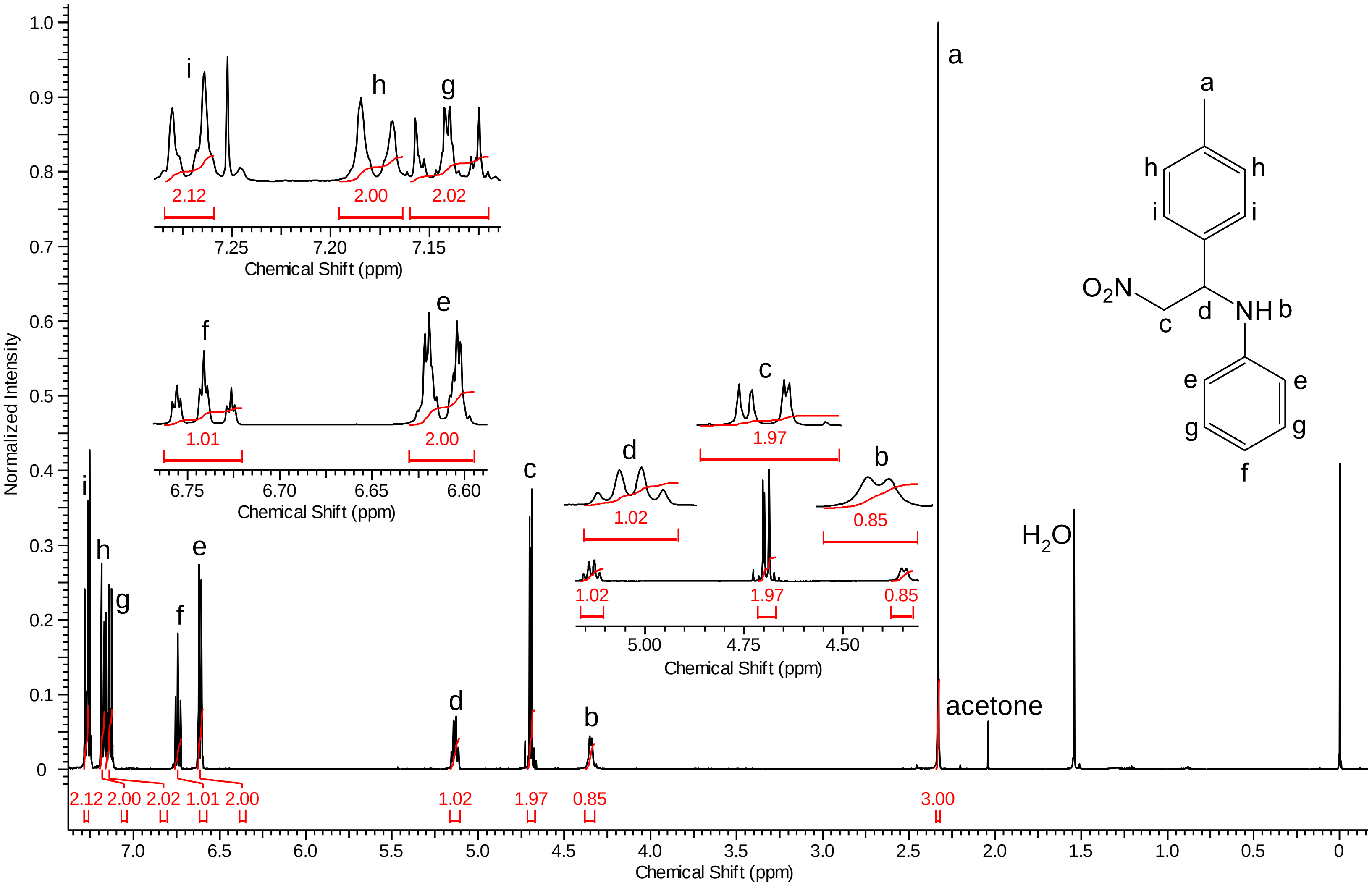

Figure 1.7: $^1$H NMR spectrum of **7a** *N*-(2-nitro-1-(*p*-tolyl)ethyl)aniline.

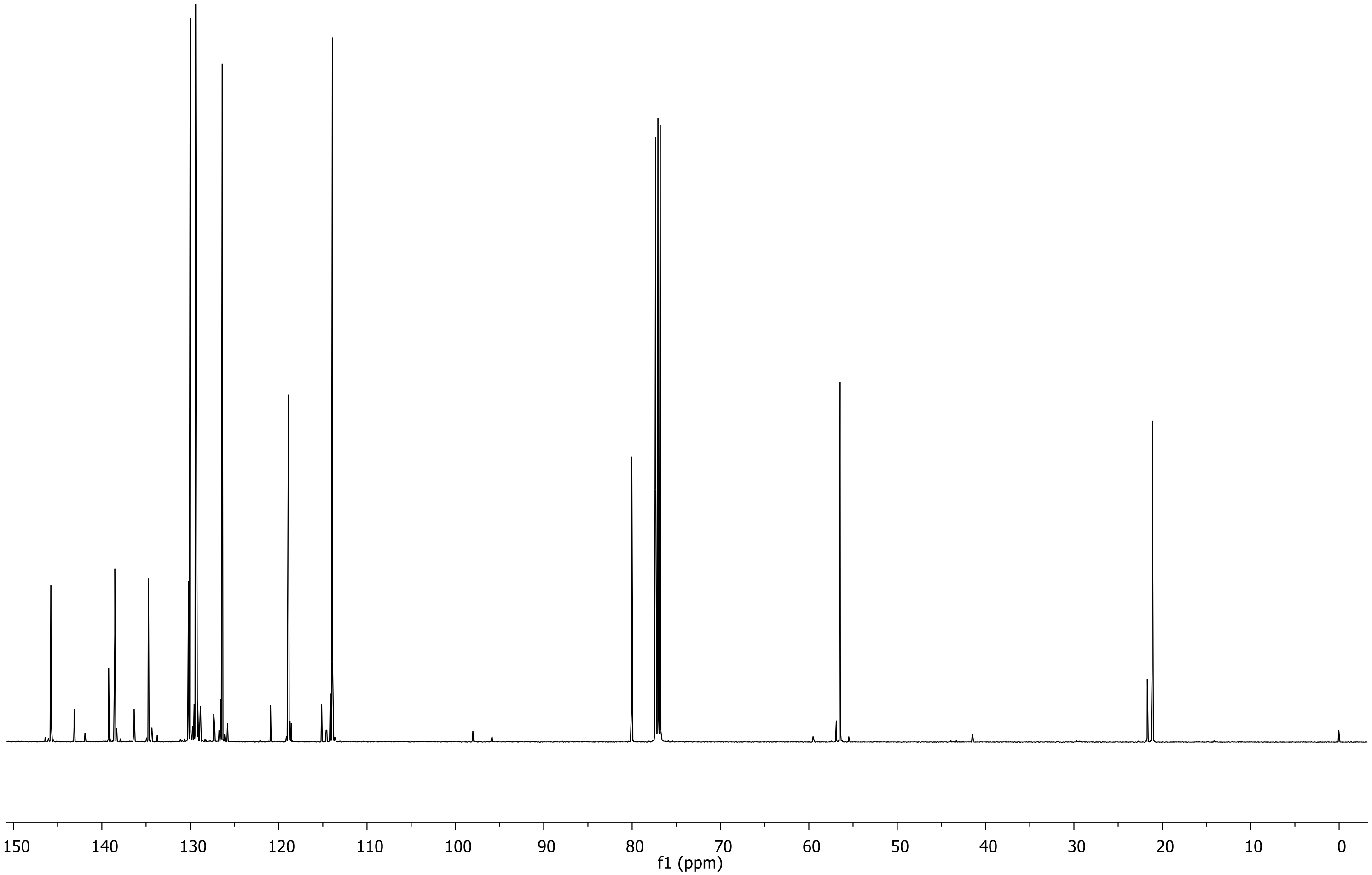

Figure 1.8: $^{13}$C NMR spectrum of **7a** *N*-(2-nitro-1-(*p*-tolyl)ethyl)aniline.

Table 1.2: MS data

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **7a** | 256 | 1 | 257.10 | 16 | 118.06 | 18 | ES+ |
| | | 2 | 257.10 | 16 | 94.06 | 10 | ES+ |
| | | 3 | 257.10 | 16 | 164.05 | 10 | ES+ |
| | | 4 | 257.10 | 16 | 196.12 | 8 | ES+ |
| | | 5 | 257.10 | 16 | 91.07 | 52 | ES+ |

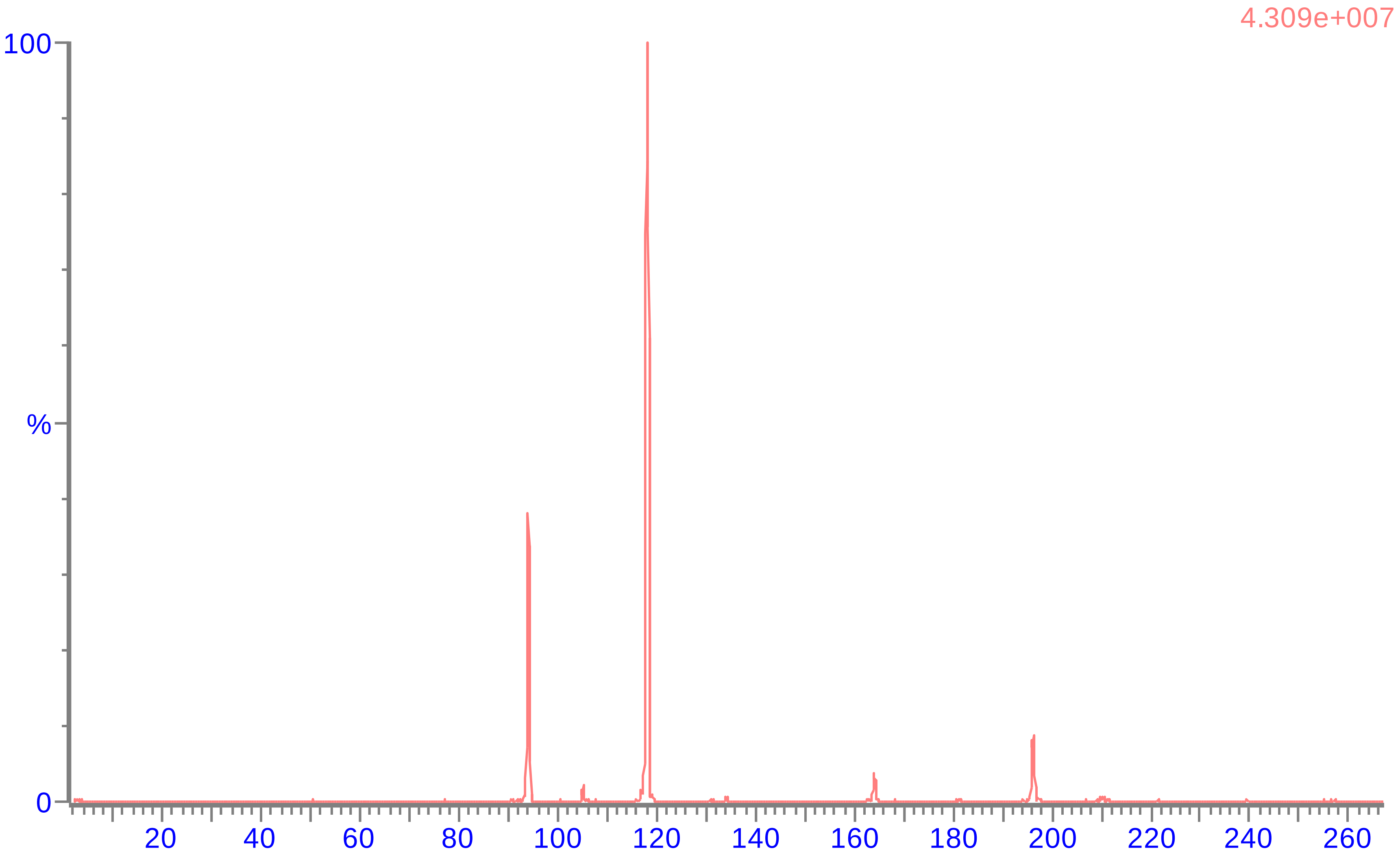

Figure 1.9: Mass spectrum for daughter fragment peak ES+, m/z 257.10 -> 118.06.

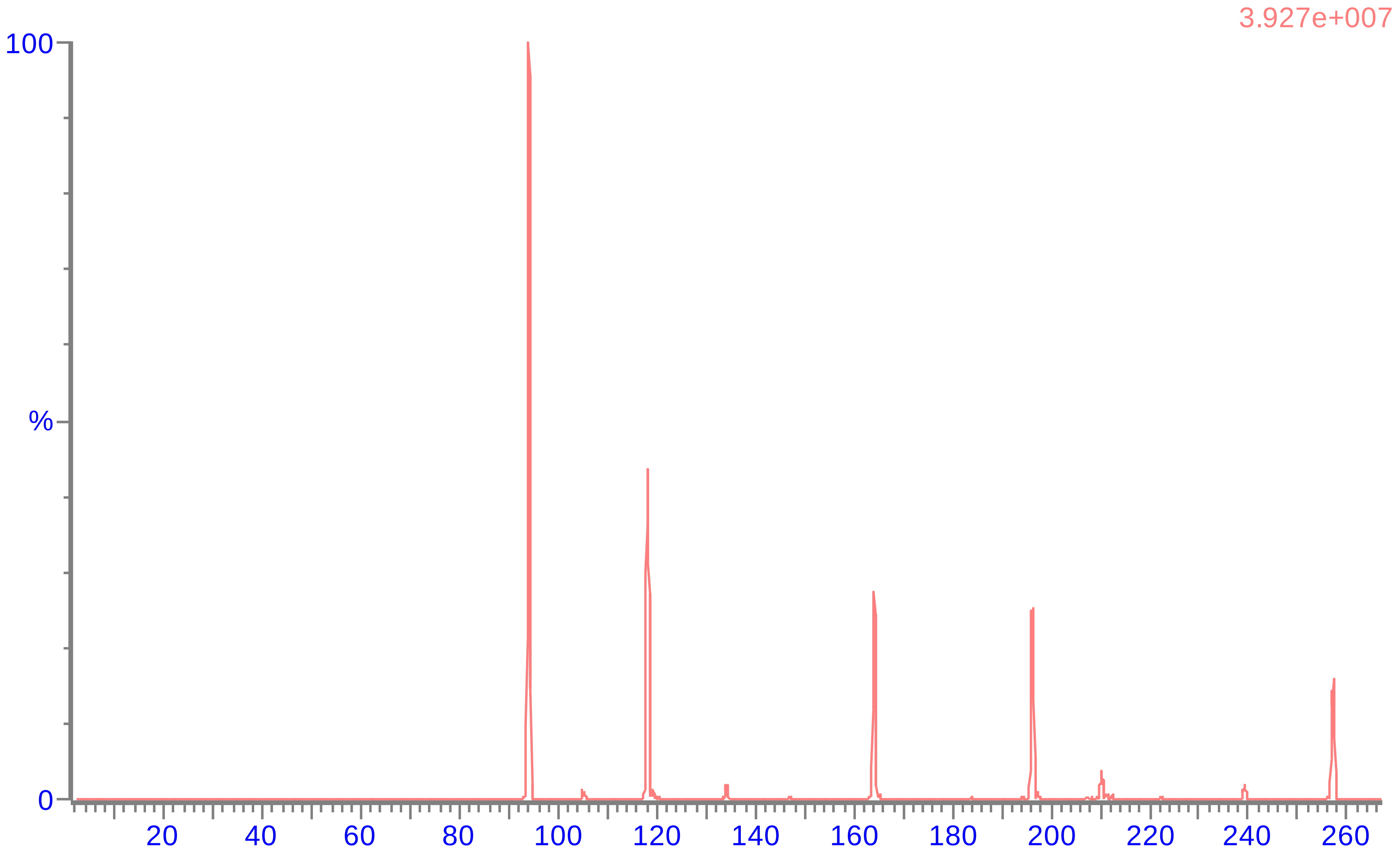

Figure 1.10: Mass spectrum for daughter fragment peak ES+, m/z 257.10 -> 94.06.

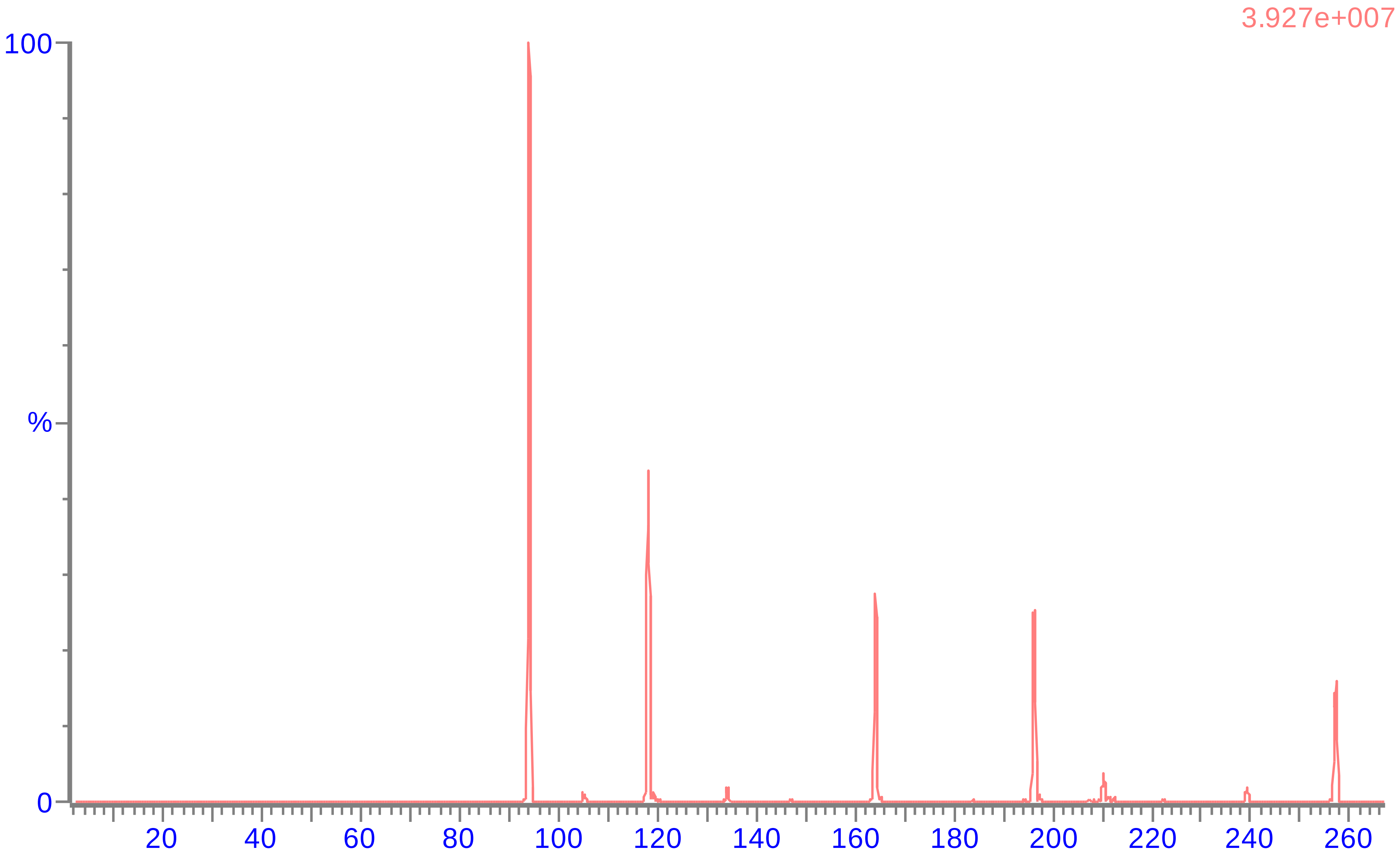

Figure 1.11: Mass spectrum for daughter fragment peak ES+, m/z 257.10 -> 164.05.

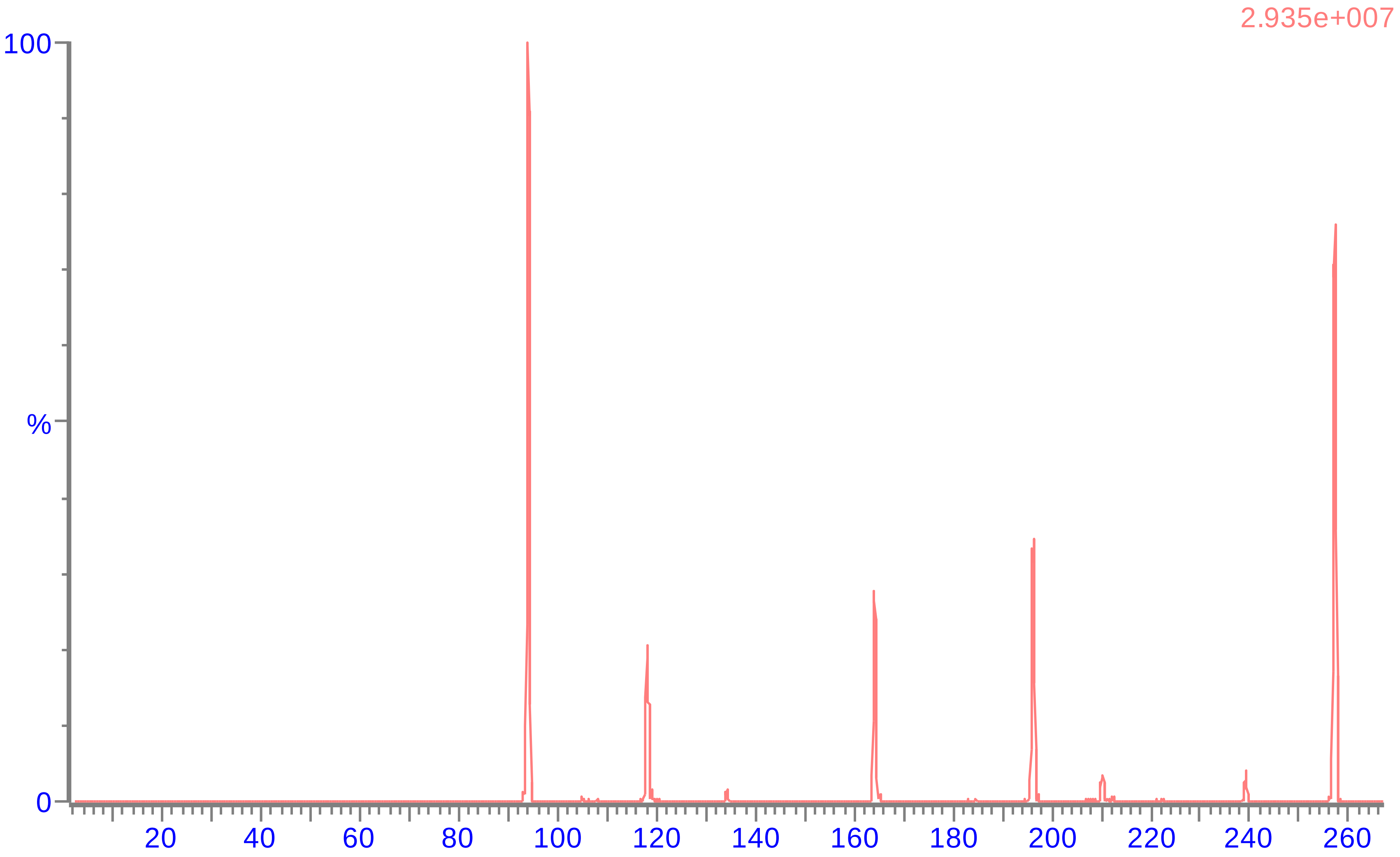

Figure 1.12: Mass spectrum for daughter fragment peak ES+, m/z 257.10 -> 196.12.

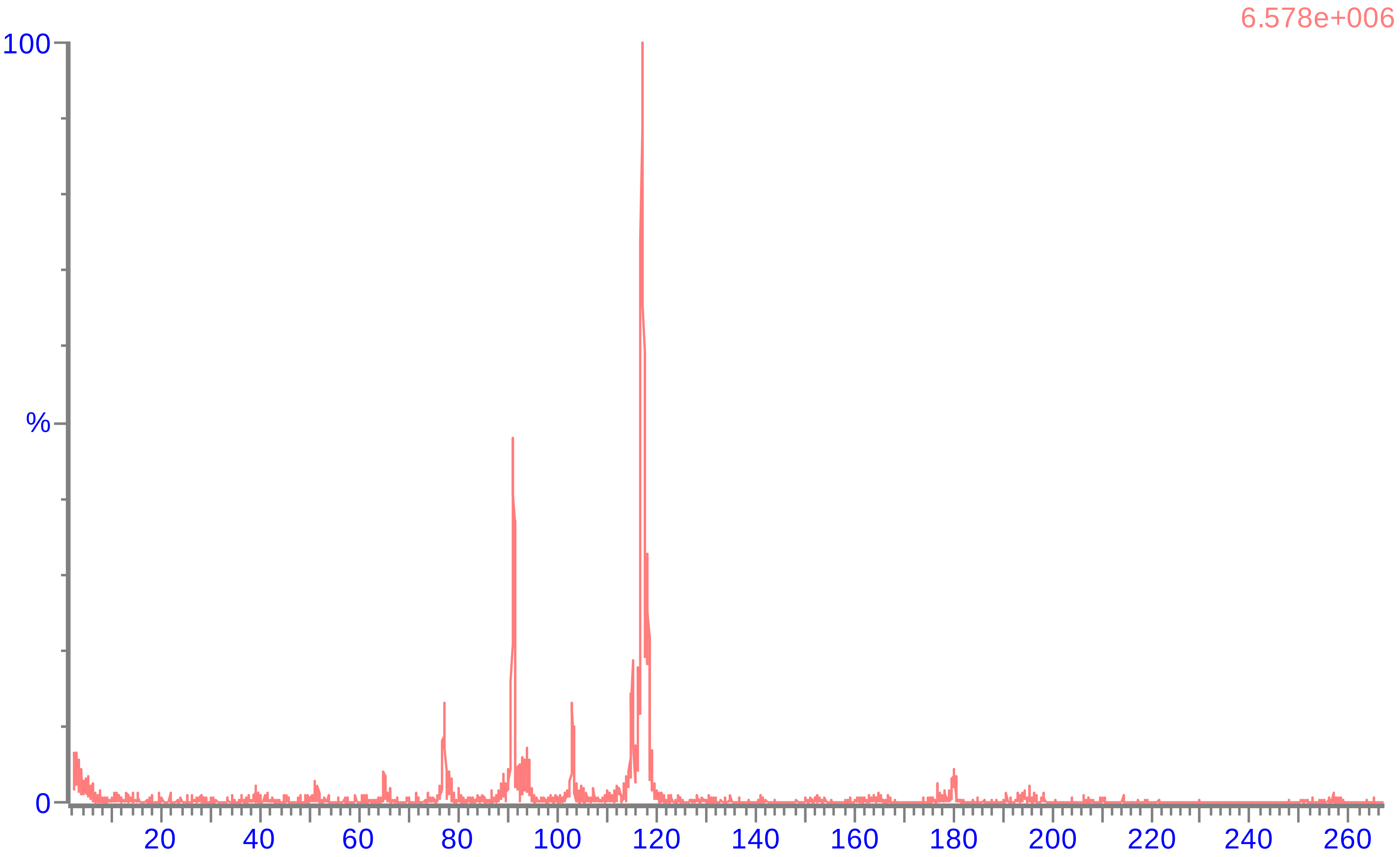

Figure 1.13: Mass spectrum for daughter fragment peak ES+, m/z 257.10 -> 91.07.

**7b** *N*-(1-(4-methoxyphenyl)-2-nitroethyl)aniline

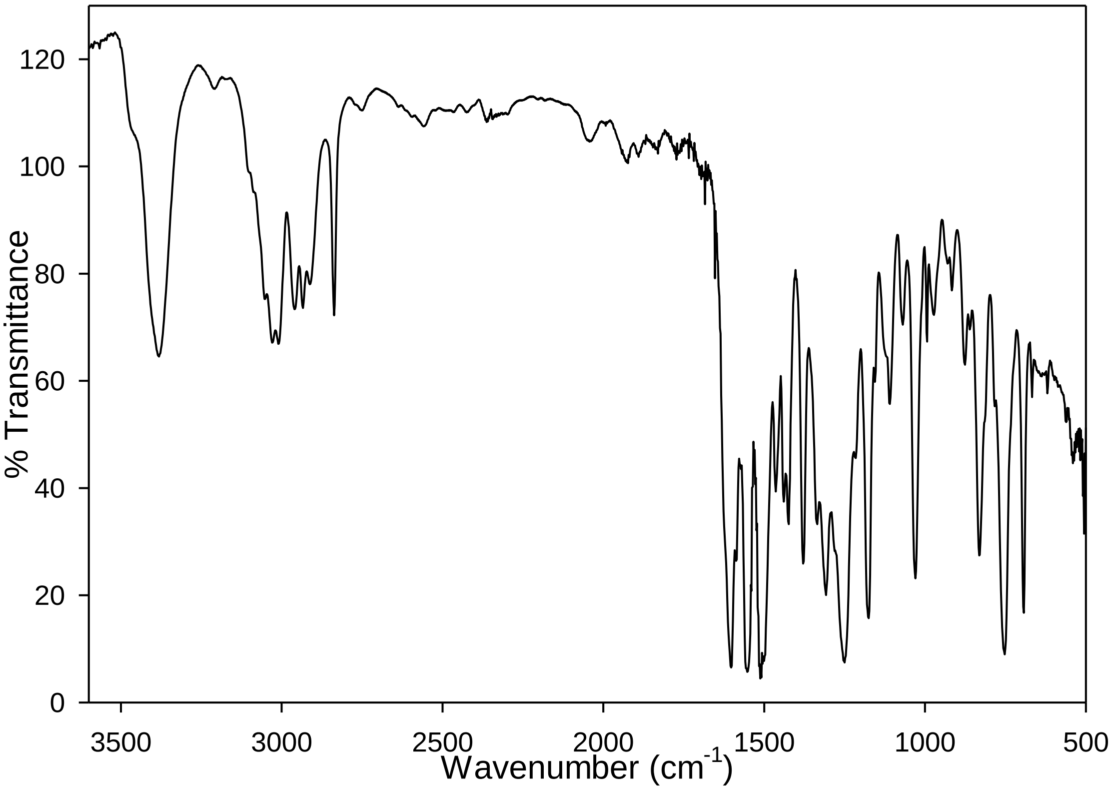

Figure 1.14: IR spectrum of **7b** *N*-(1-(4-methoxyphenyl)-2-nitroethyl)aniline.

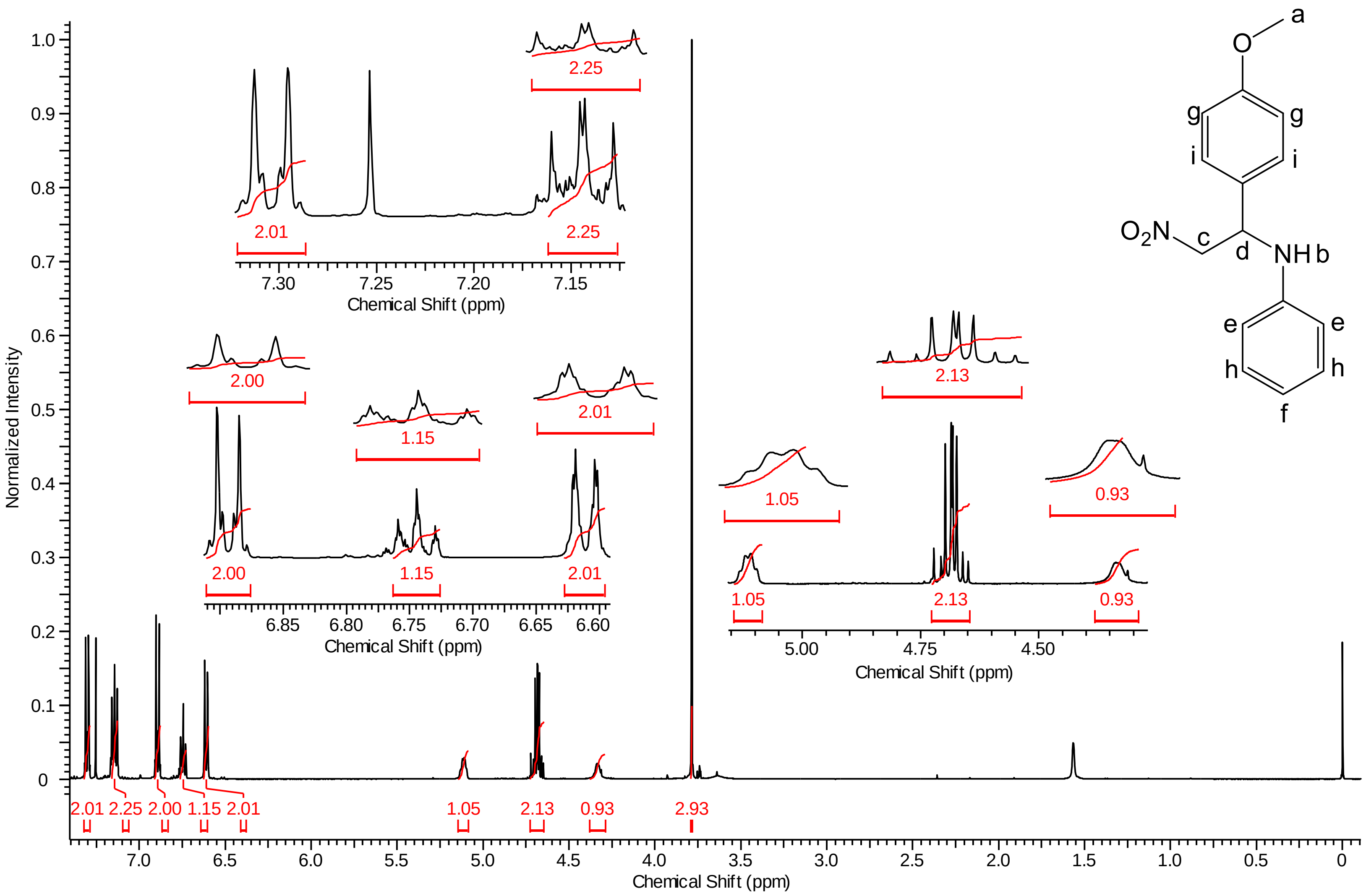

Figure 1.15: $^1$H NMR spectrum of **7b** *N*-(1-(4-methoxyphenyl)-2-nitroethyl)aniline.

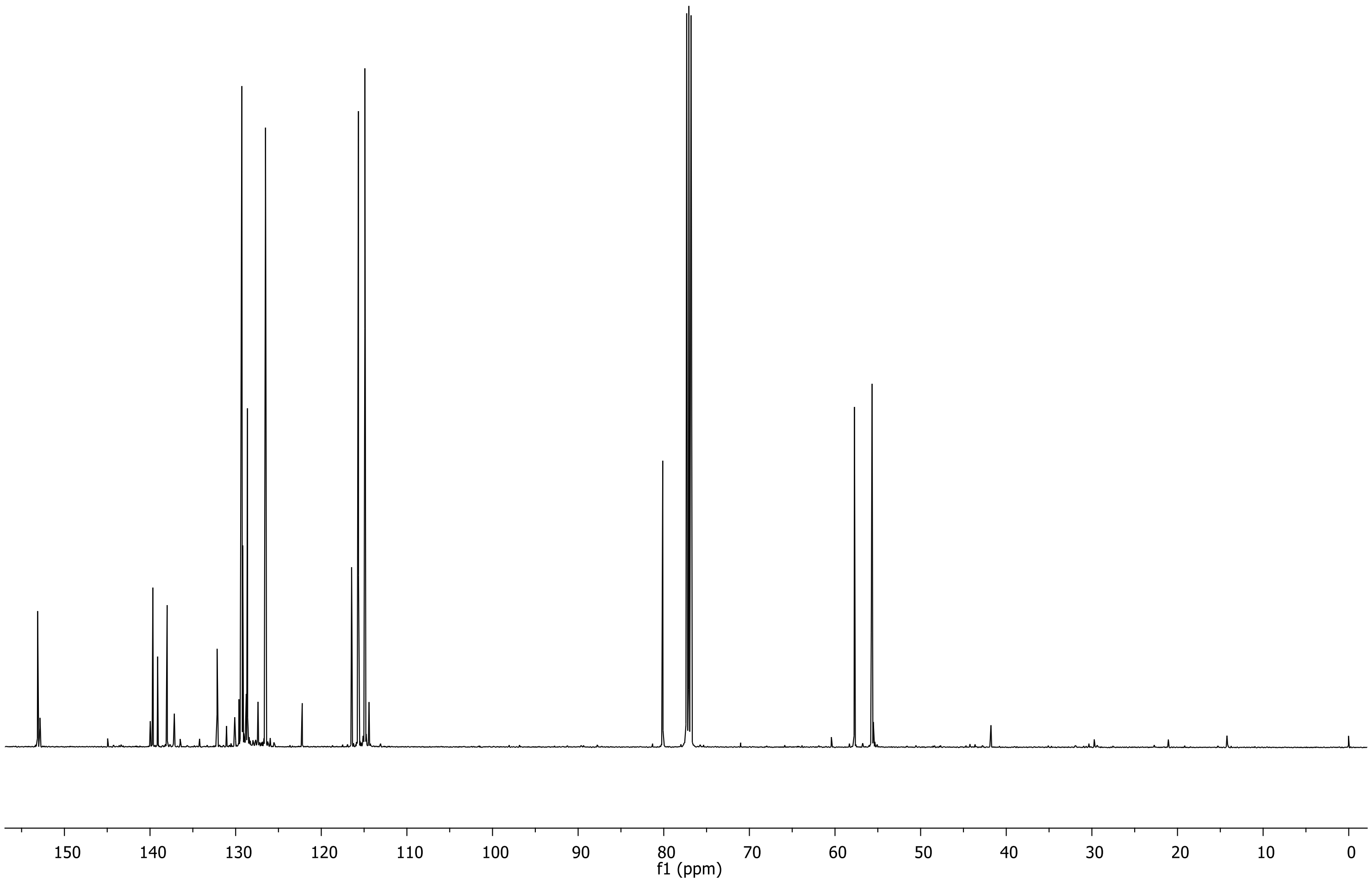

Figure 1.16: $^{13}$C NMR spectrum of **7b** *N*-(1-(4-methoxyphenyl)-2-nitroethyl)aniline.

Table 1.3: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **7b** | 272 | 1 | 273.10 | 22 | 123.05 | 14 | ES+ |
| | | 2 | 273.10 | 22 | 108.02 | 34 | ES+ |
| | | 3 | 273.10 | 22 | 212.14 | 12 | ES+ |
| | | 4 | 273.10 | 22 | 80.06 | 62 | ES+ |
| | | 5 | 273.10 | 22 | 104.06 | 32 | ES+ |

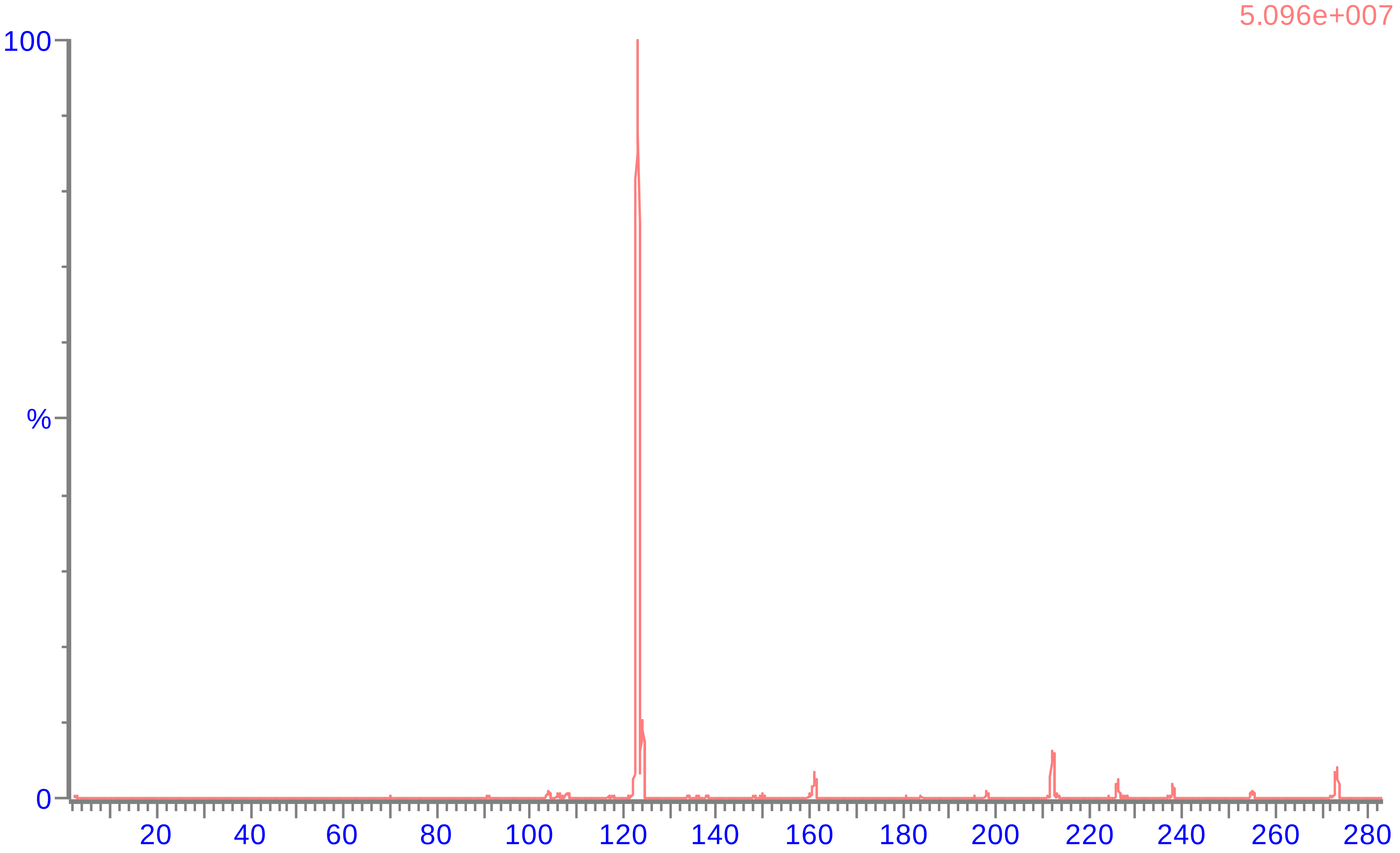

Figure 1.17: Mass spectrum for daughter fragment peak ES+, m/z 273.10 -> 123.05.

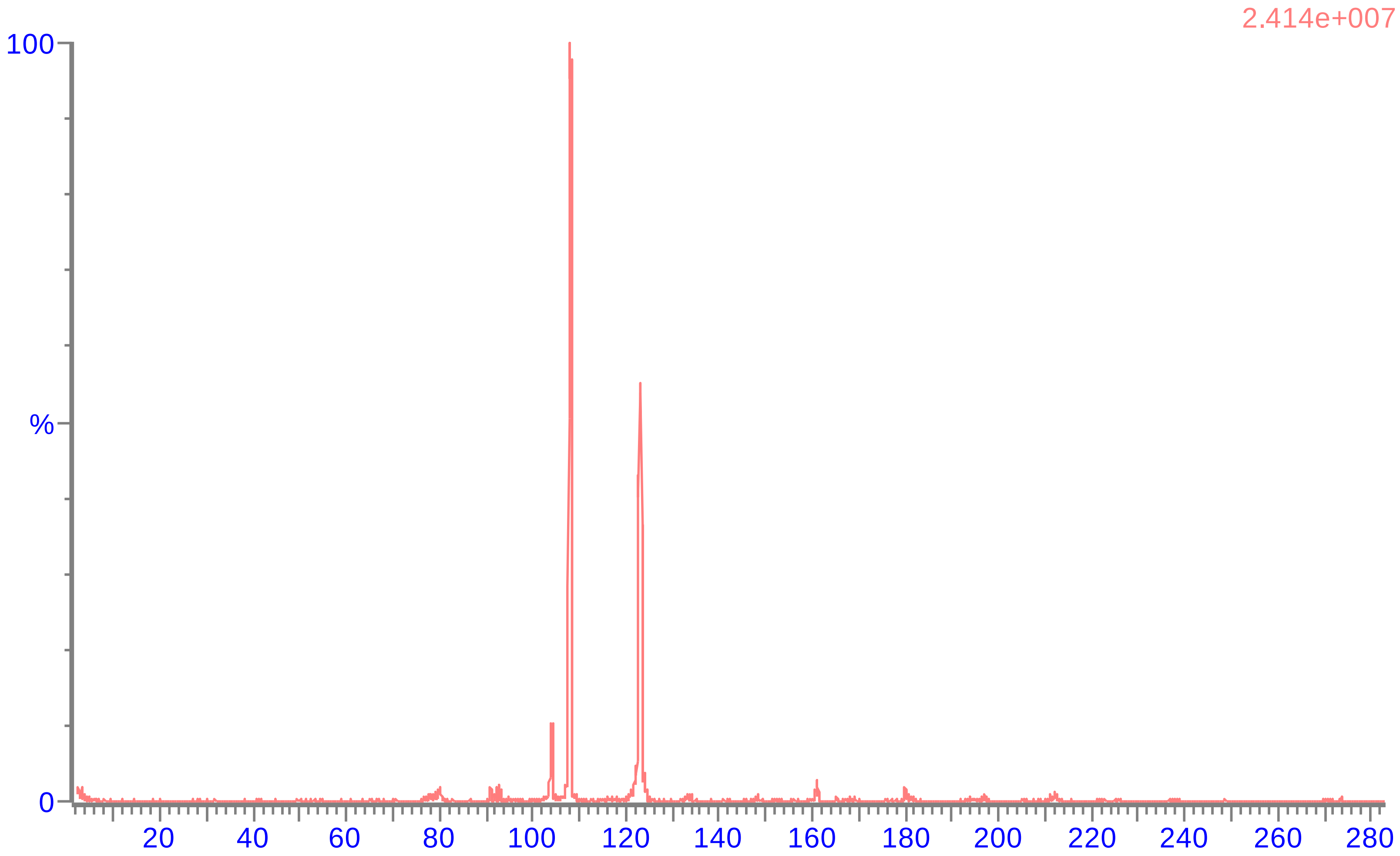

Figure 1.18: Mass spectrum for daughter fragment peak ES+, m/z 273.10 -> 108.02.

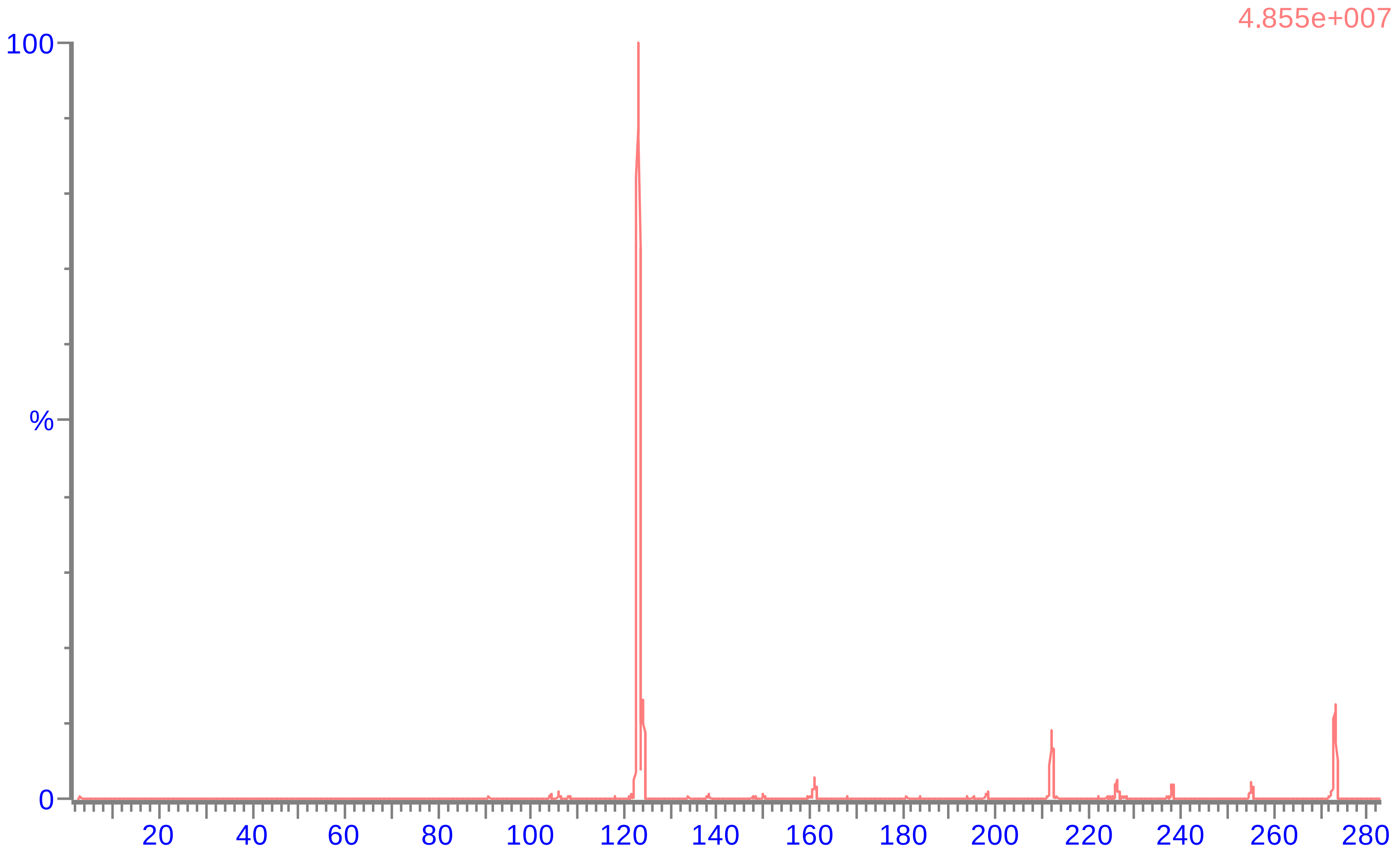

Figure 1.19: Mass spectrum for daughter fragment peak ES+, m/z 273.10 -> 212.14.

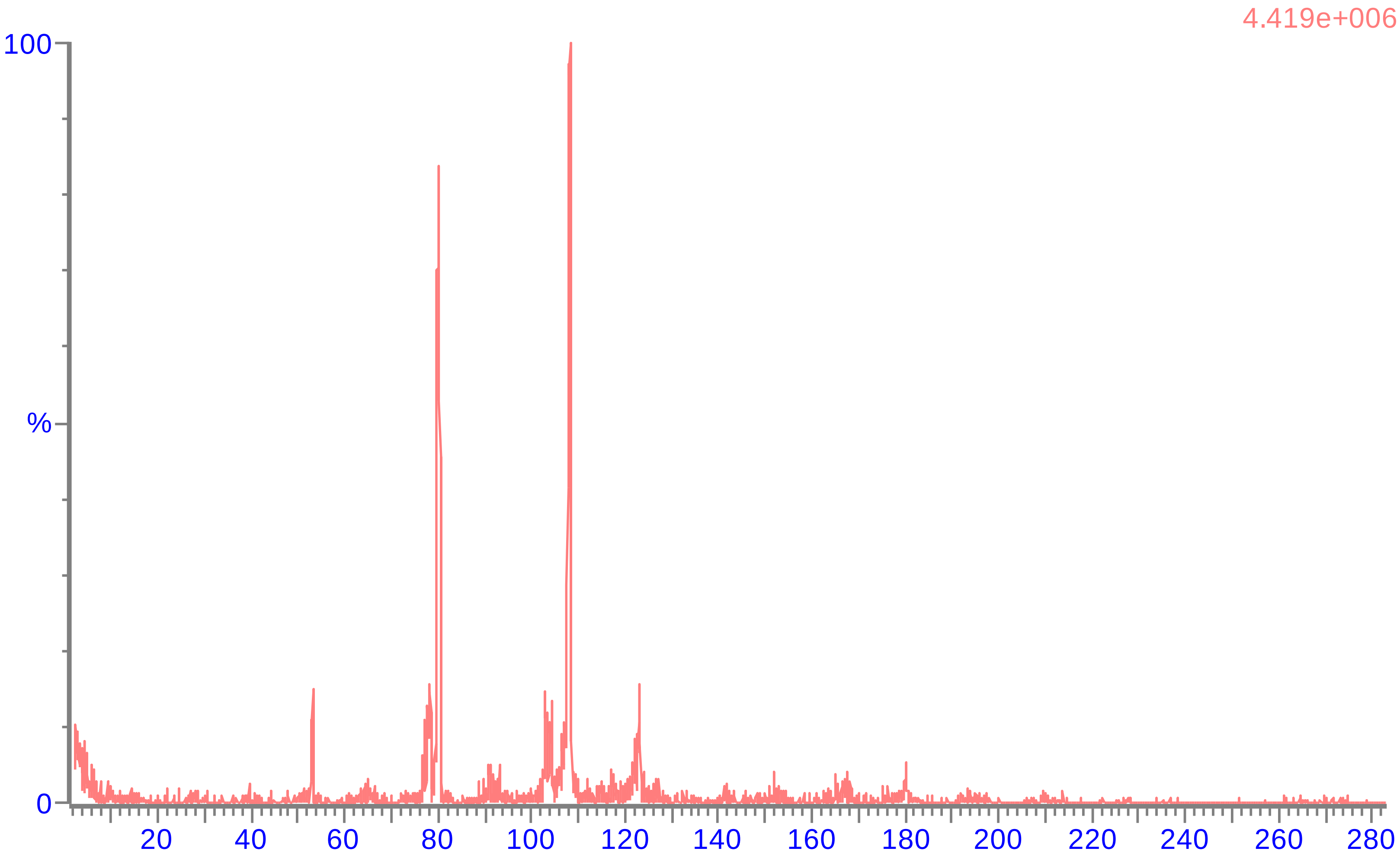

Figure 1.20: Mass spectrum for daughter fragment peak ES+, m/z 273.10 -> 80.06.

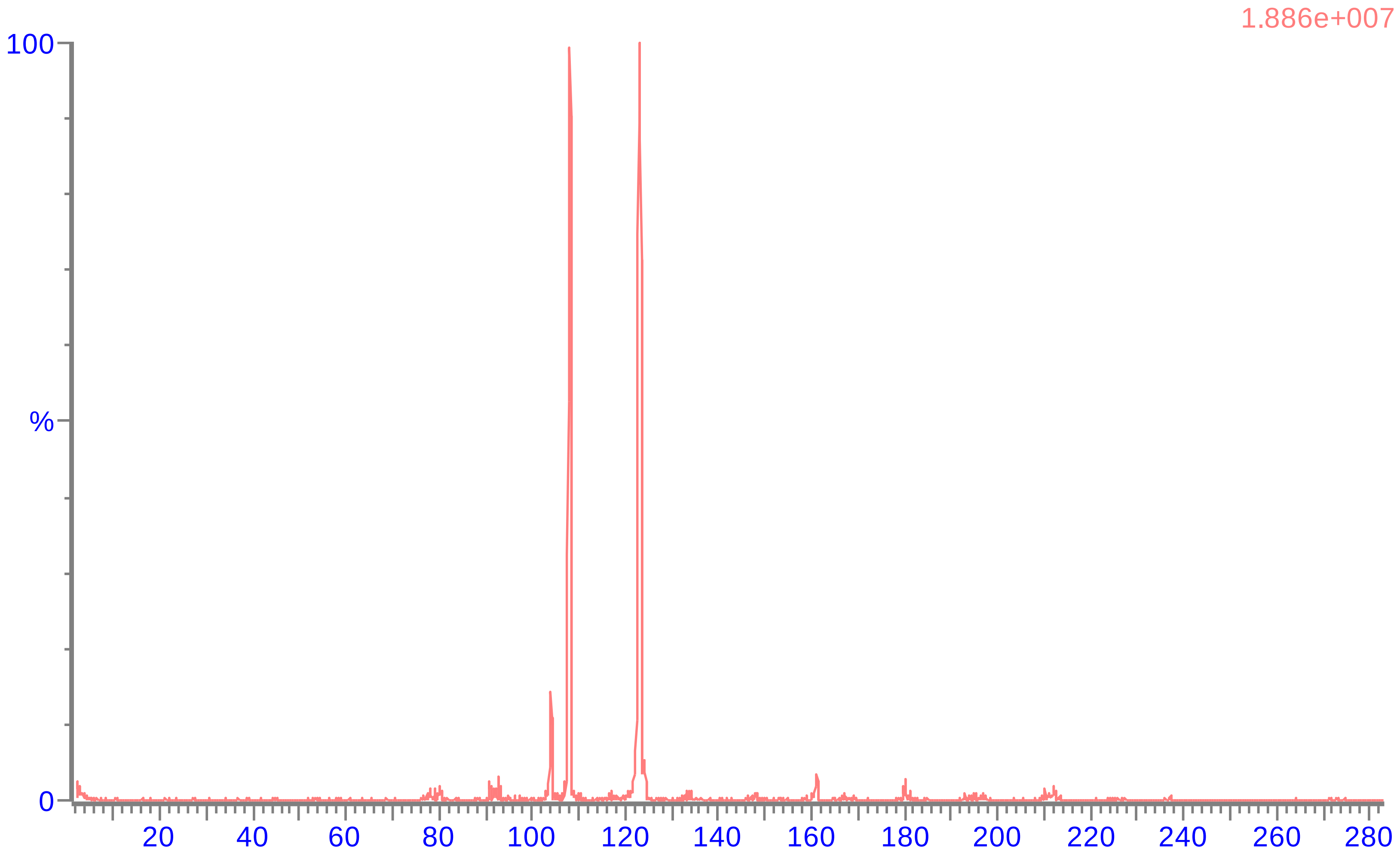

Figure 1.21: Mass spectrum for daughter fragment peak ES+, m/z 273.10 -> 104.06.

**7c** *N*-(1-(4-bromophenyl)-2-nitroethyl)aniline

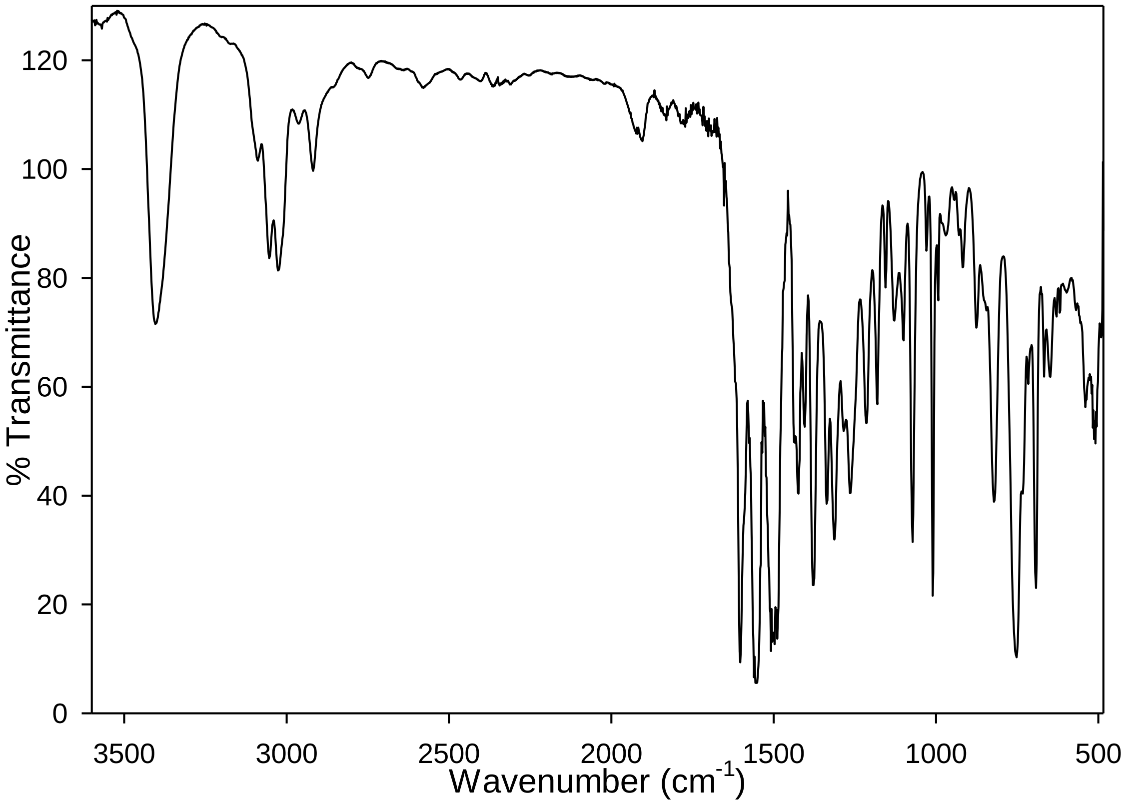

Figure19.22: IR spectrum of **7c** *N*-(1-(4-bromophenyl)-2-nitroethyl)aniline.

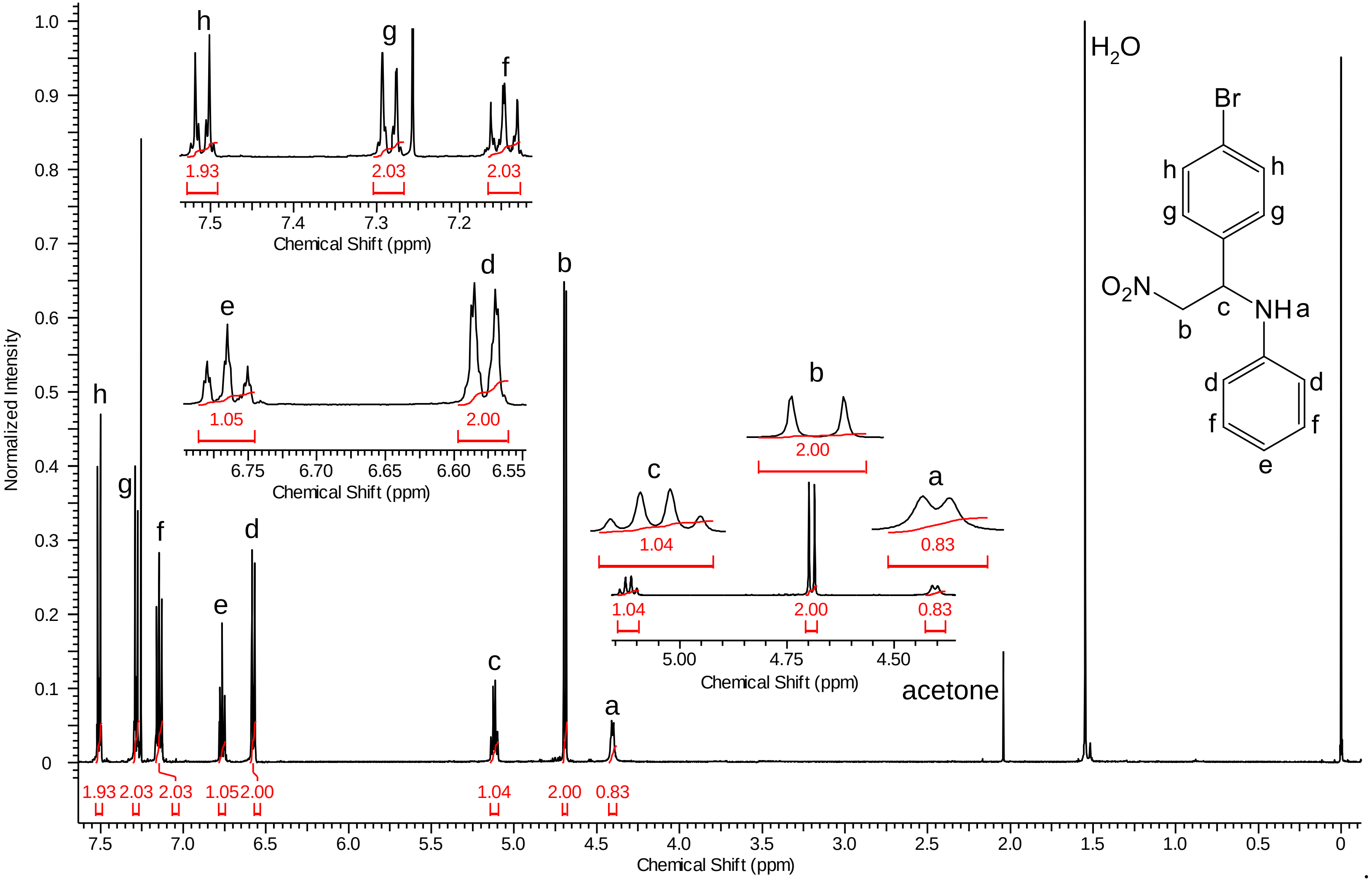

Figure 1.23: $^1$H NMR spectrum of **7c** *N*-(1-(4-bromophenyl)-2-nitroethyl)aniline.

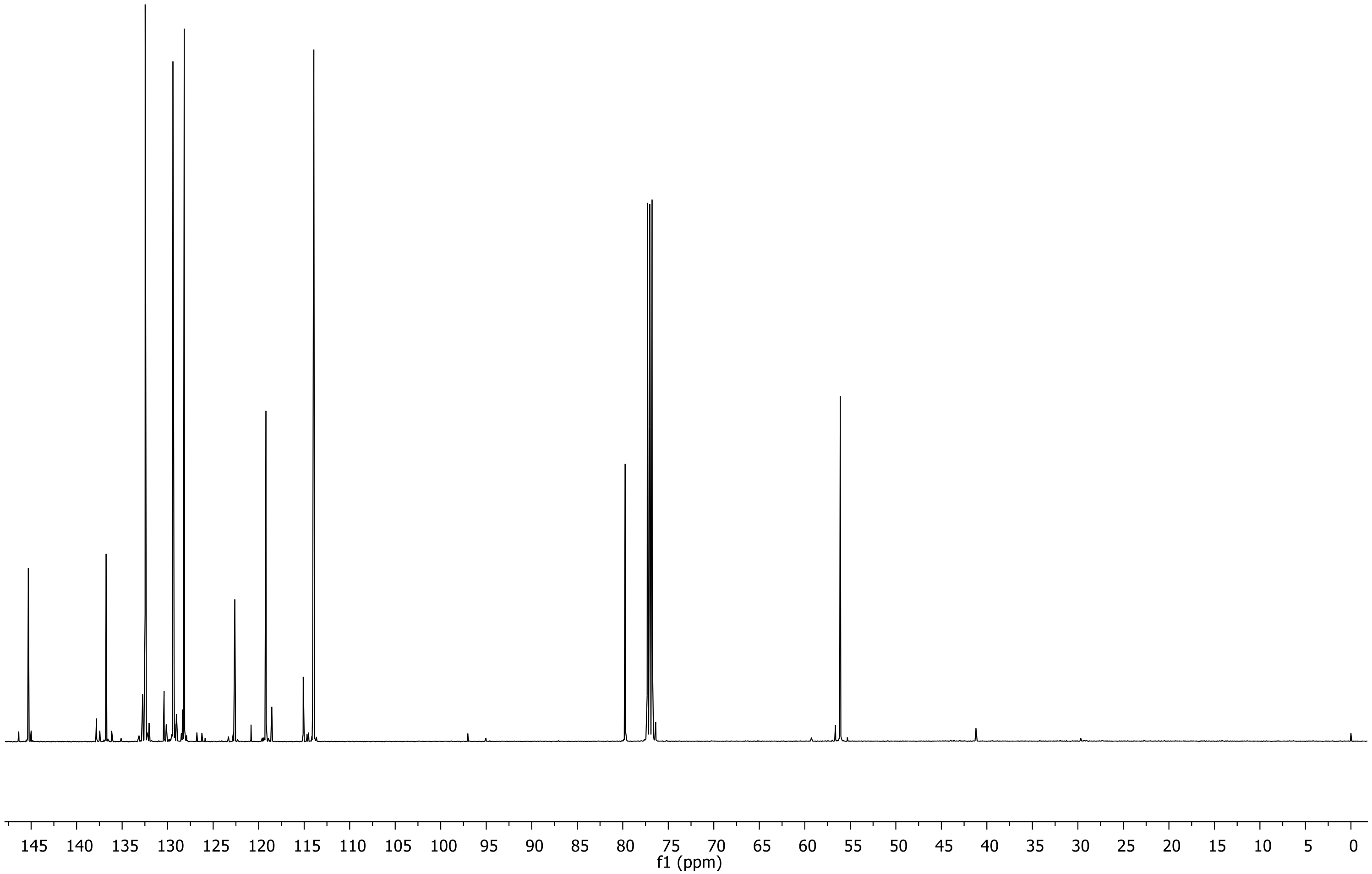

Figure 1.24: $^{13}$C NMR spectrum of **7c** *N*-(1-(4-bromophenyl)-2-nitroethyl)aniline.

Table 1.4: MS data.

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **7c** | 321.5 | 1 | 323.04 | 18 | 93.98 | 14 | ES+ |
| | | 2 | 323.04 | 18 | 183.99 | 28 | ES+ |
| | | 3 | 323.04 | 18 | 262.04 | 16 | ES+ |
| | | 4 | 323.04 | 18 | 103.02 | 50 | ES+ |
| | | 5 | 323.04 | 18 | 77.01 | 62 | ES+ |

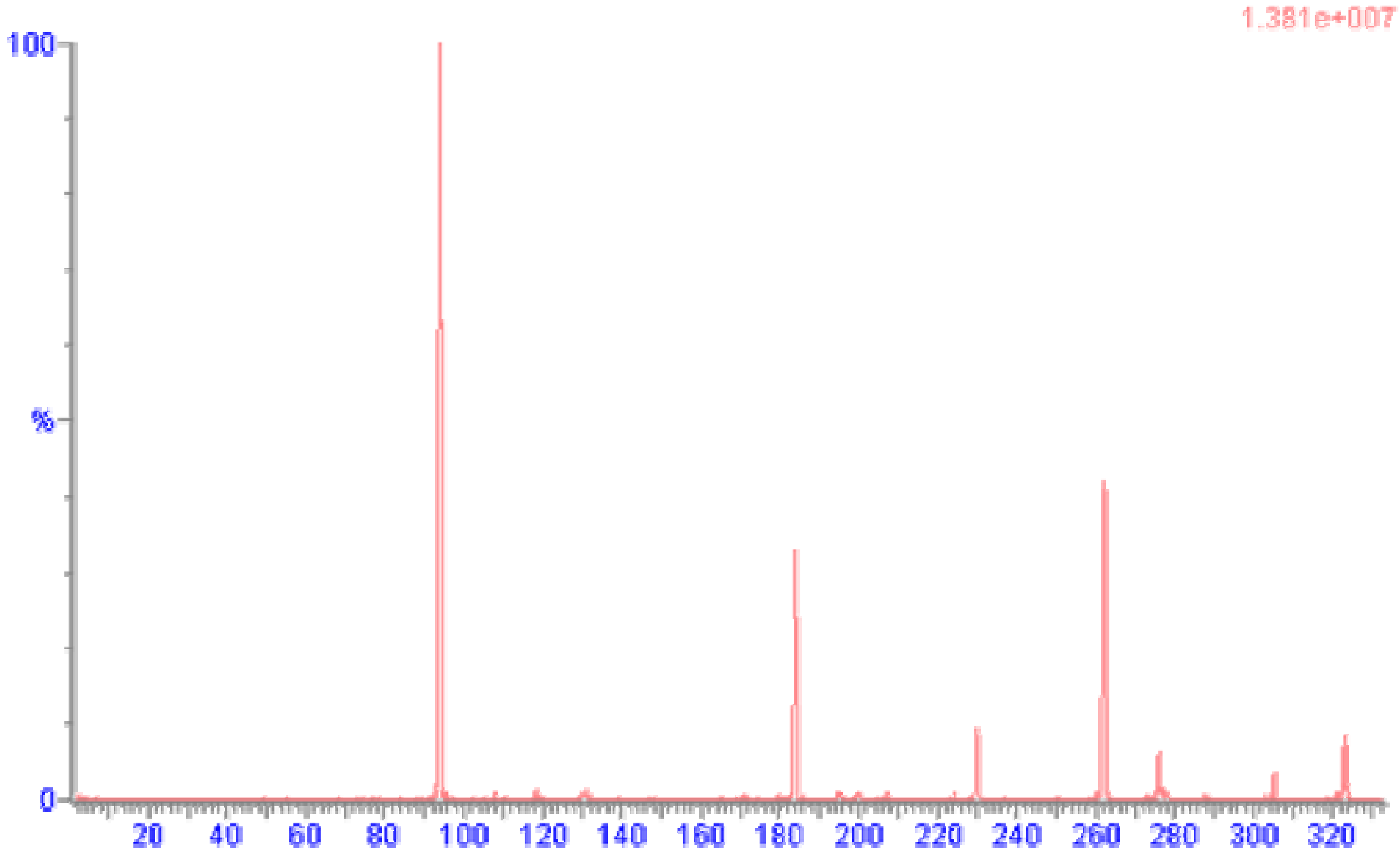

Figure 1.25: Mass spectrum for daughter fragment peak ES+, m/z 323.04 -> 93.98.

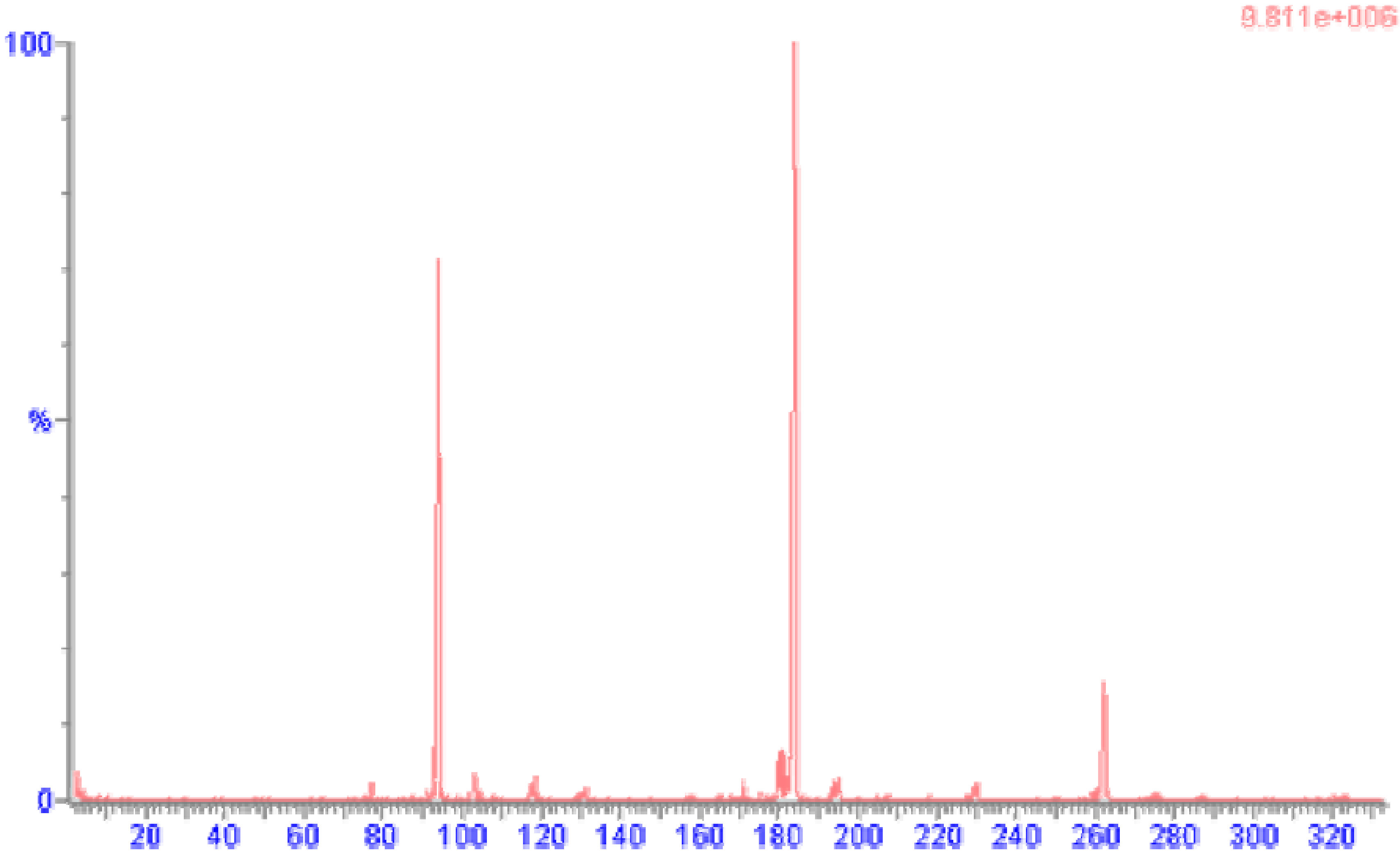

Figure 1.26: Mass spectrum for daughter fragment peak ES+, m/z 323.04 -> 183.99.

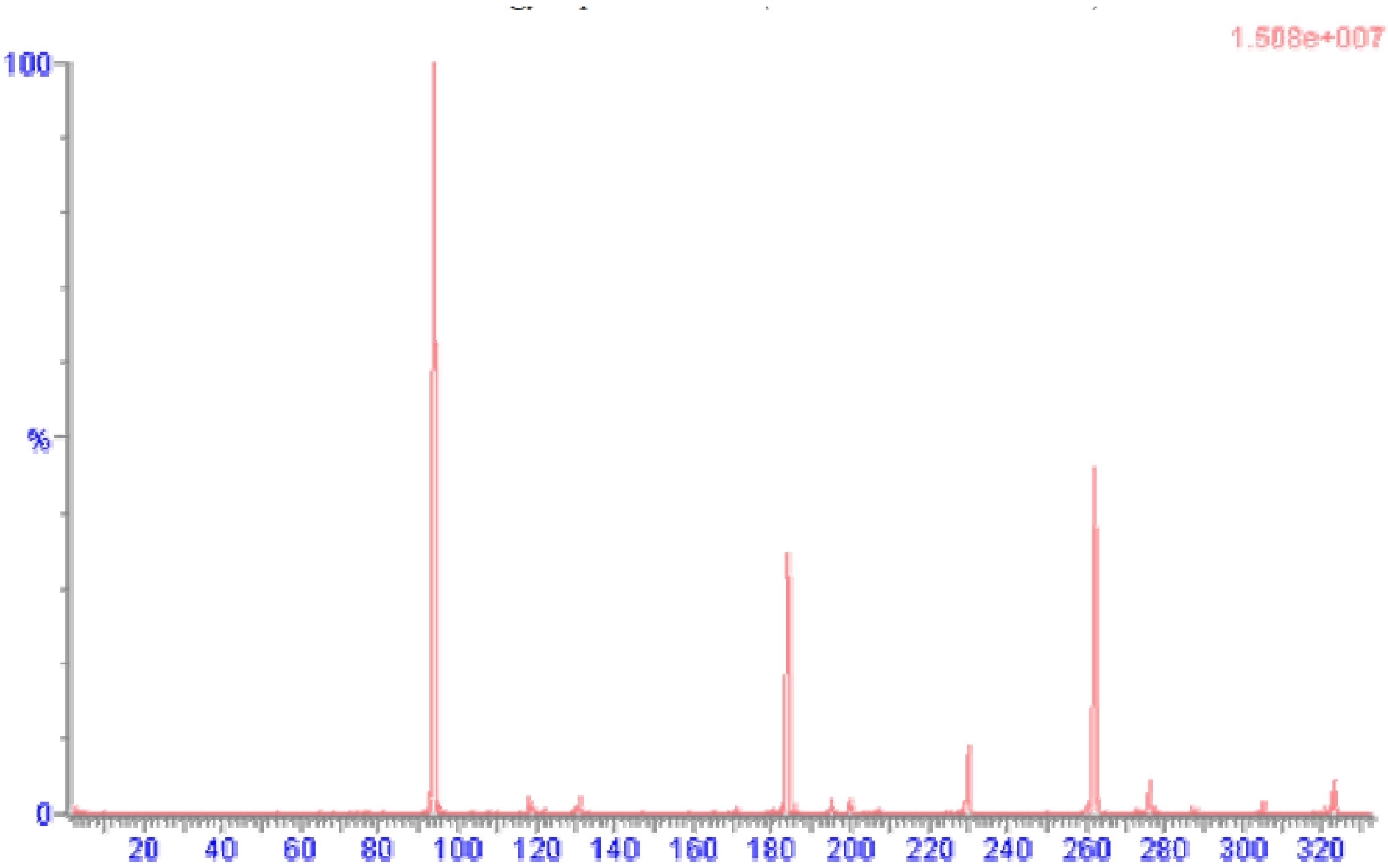

Figure 1.27: Mass spectrum for daughter fragment peak ES+, m/z 323.04 -> 262.04.

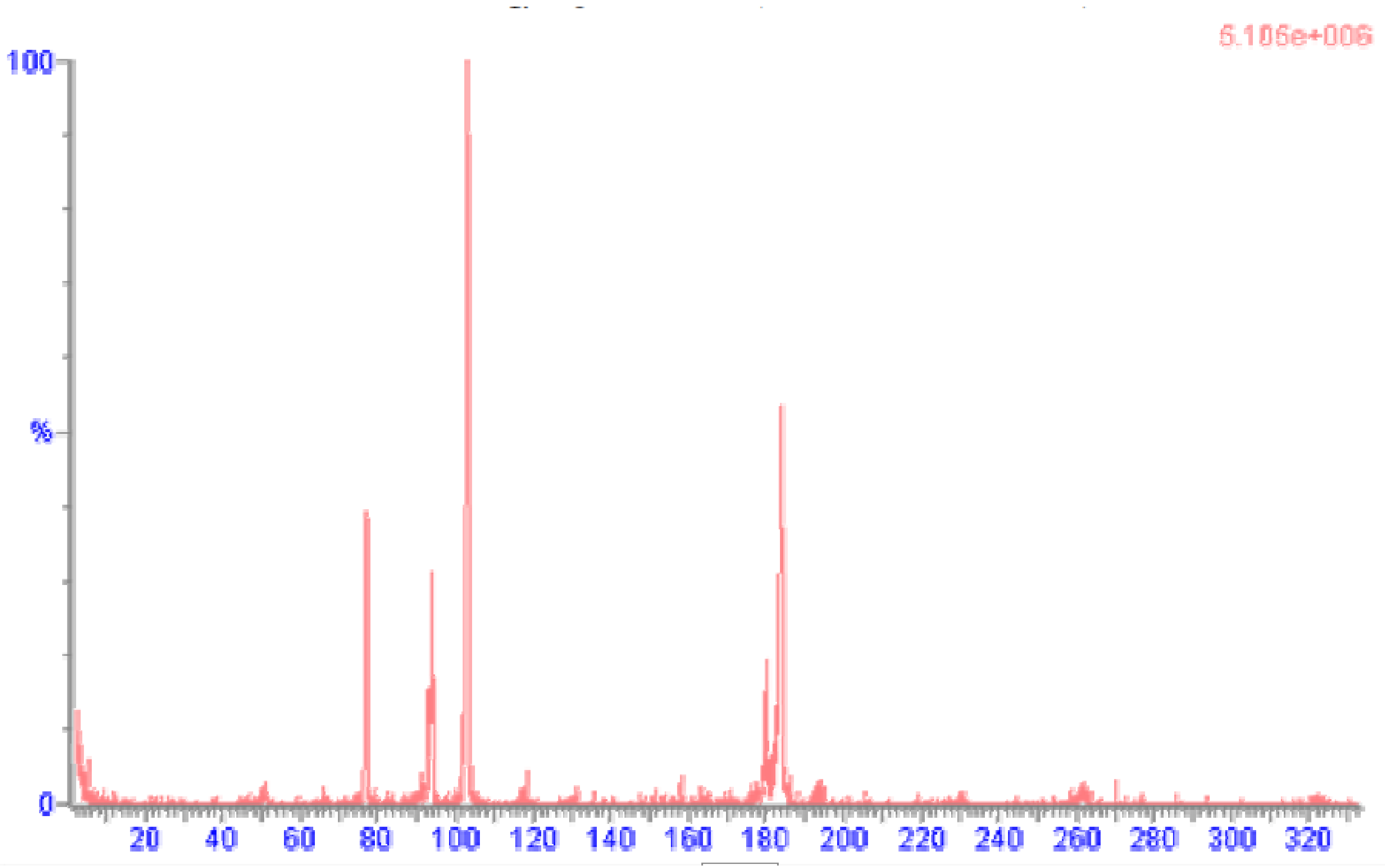

Figure 1.28: Mass spectrum for daughter fragment peak ES+, m/z 323.04 -> 103.02.

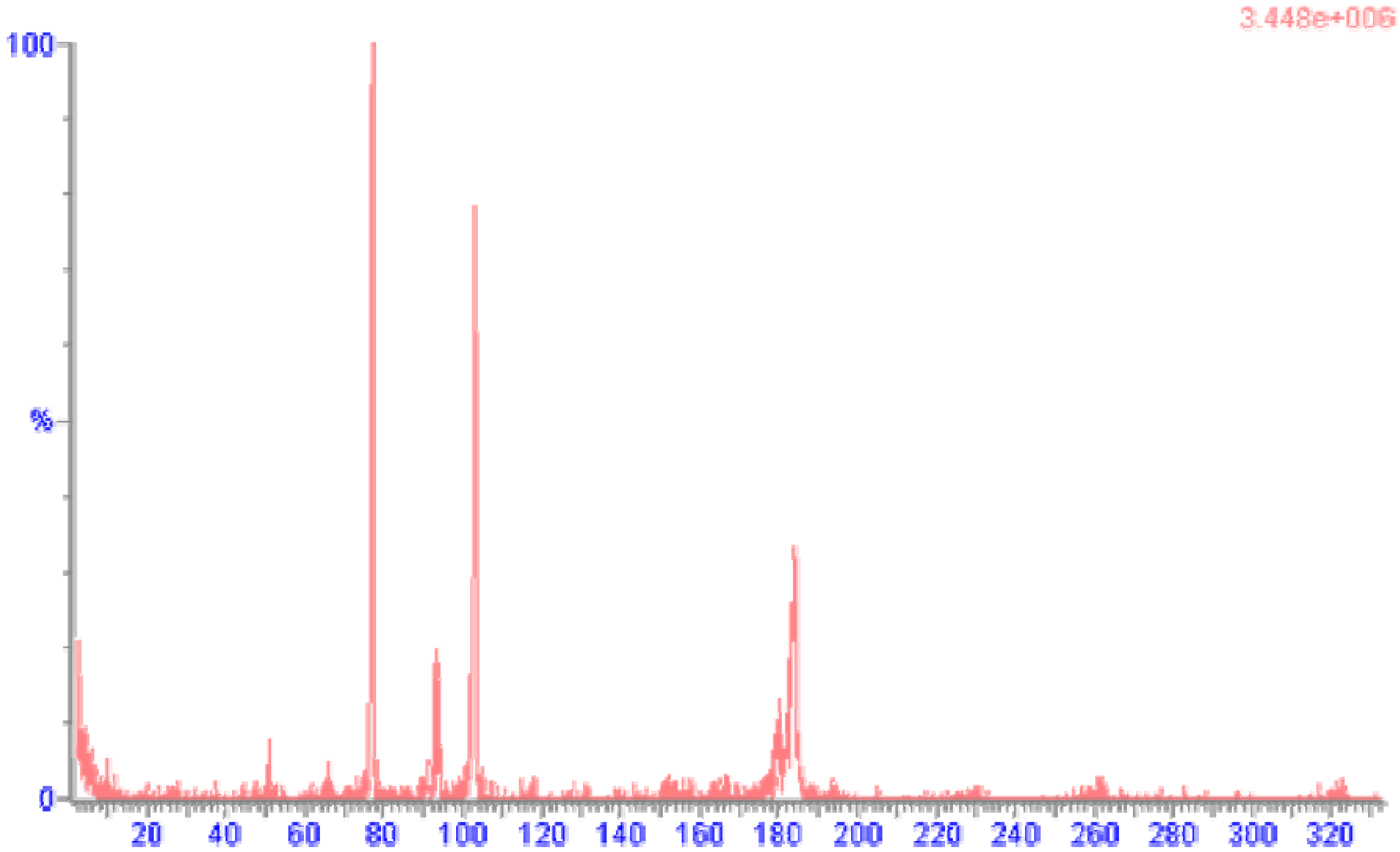

Figure 1.29: Mass spectrum for daughter fragment peak ES+, m/z 323.04 -> 77.01.

**122d** *N*-(2-nitro-1-(2-nitrophenyl)ethyl)aniline

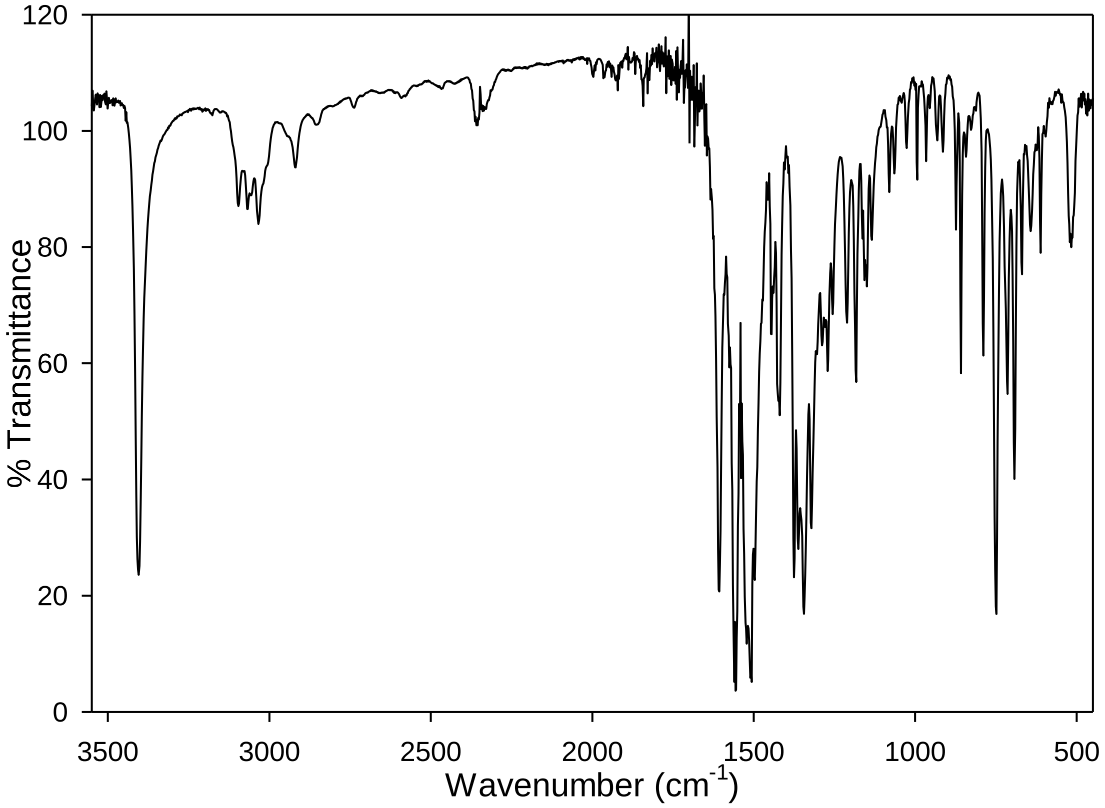

Figure 1.30: IR spectrum of **7d** *N*-(2-nitro-1-(2-nitrophenyl)ethyl)aniline.

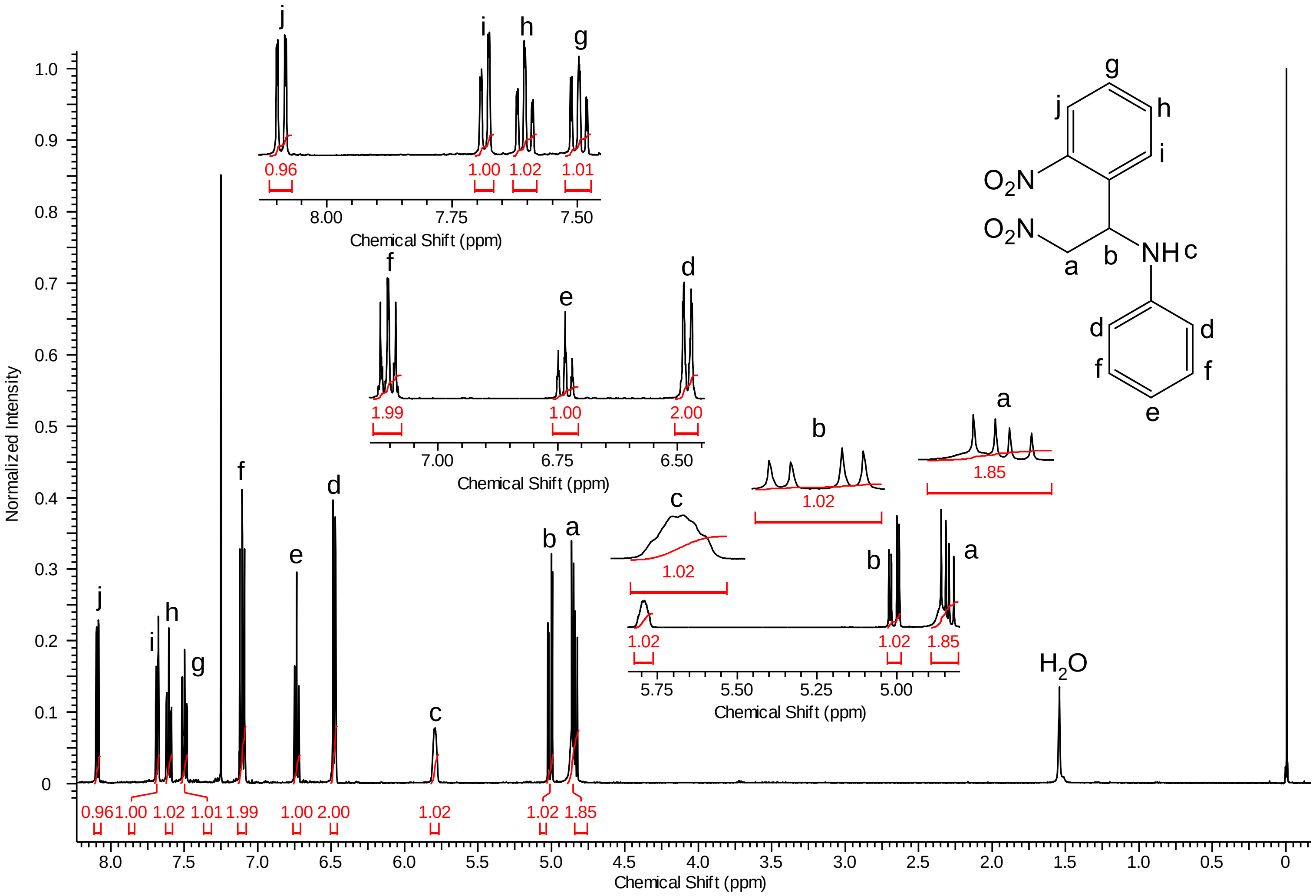

Figure 1.31: $^1$H NMR spectrum of **7d** *N*-(2-nitro-1-(2-nitrophenyl)ethyl)aniline.

**7e** 3-(2-nitro-1-(phenylamino)ethyl)phenol

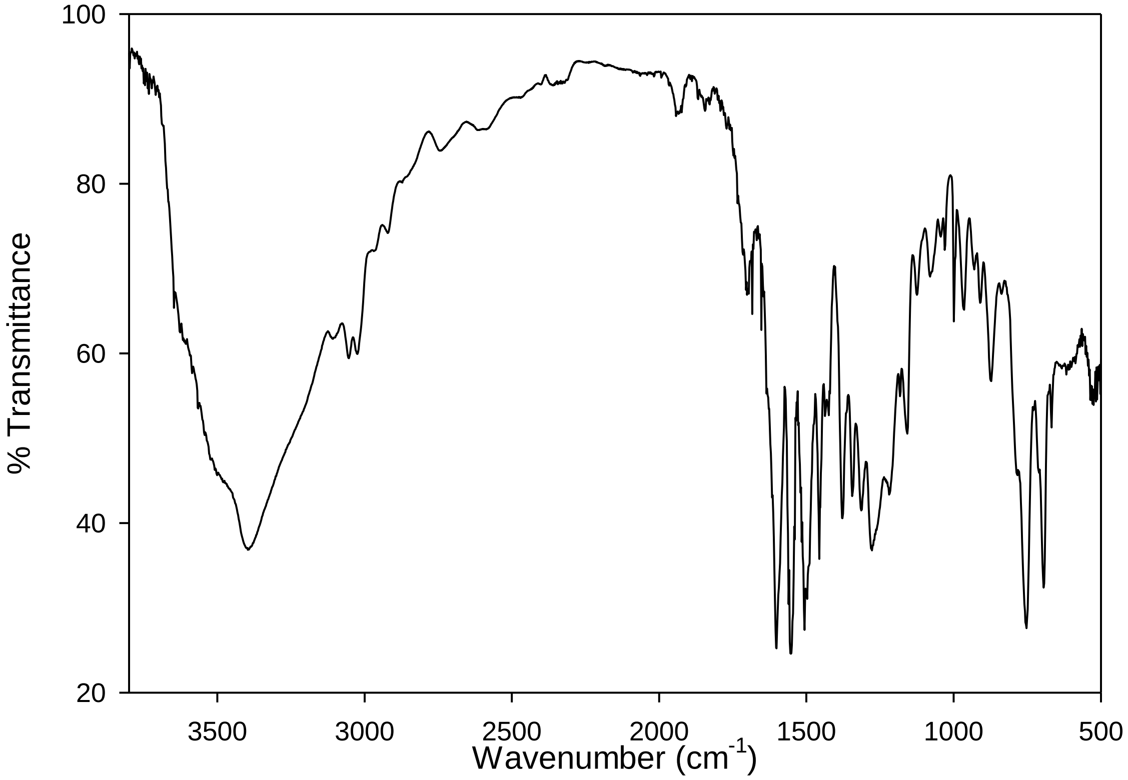

Figure 1.32: IR spectrum of **7e** 3-(2-nitro-1-(phenylamino)ethyl)phenol.

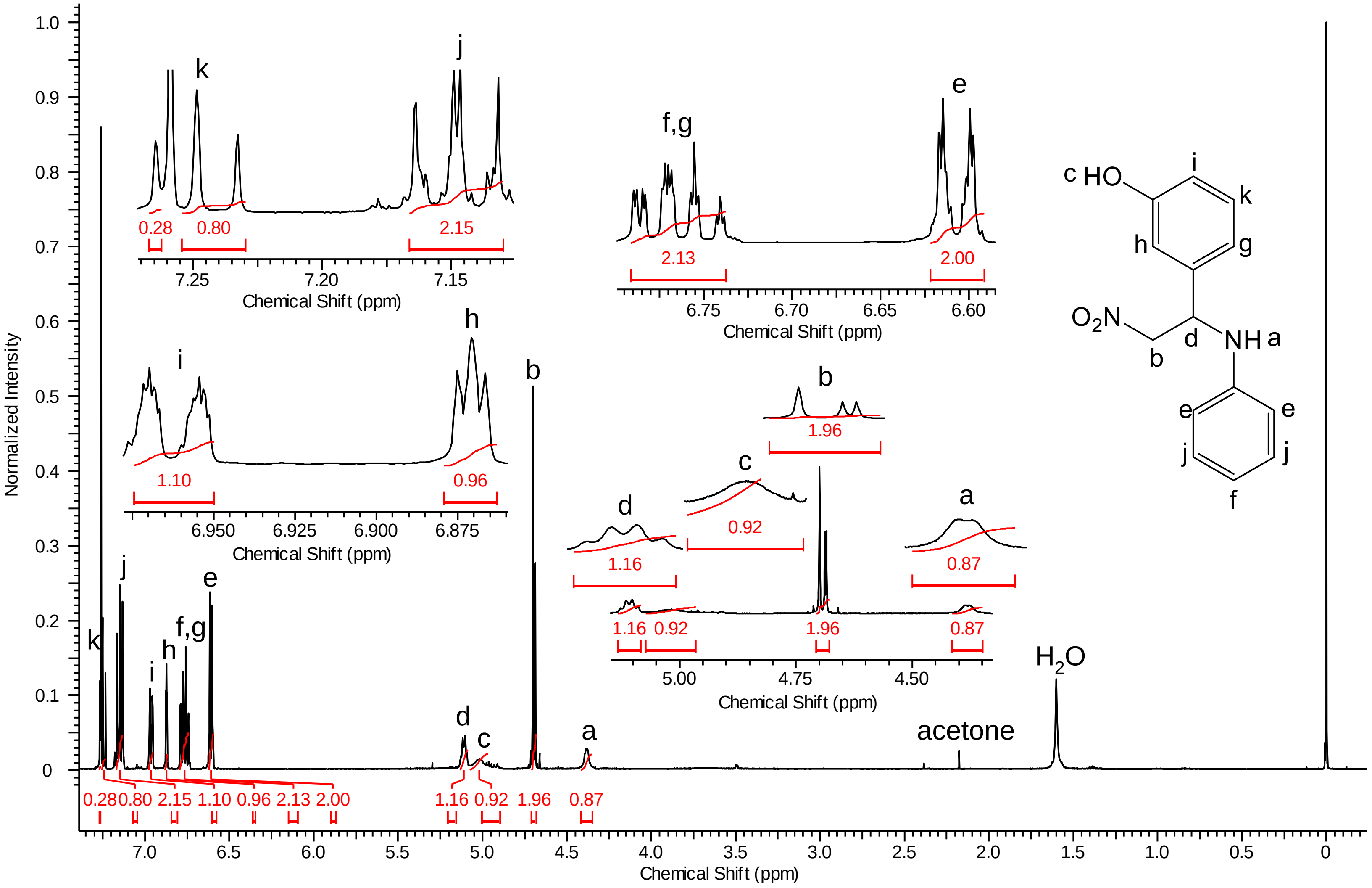

Figure 1.33: $^{1}$H NMR spectrum of **7e** 3-(2-nitro-1-(phenylamino)ethyl)phenol.

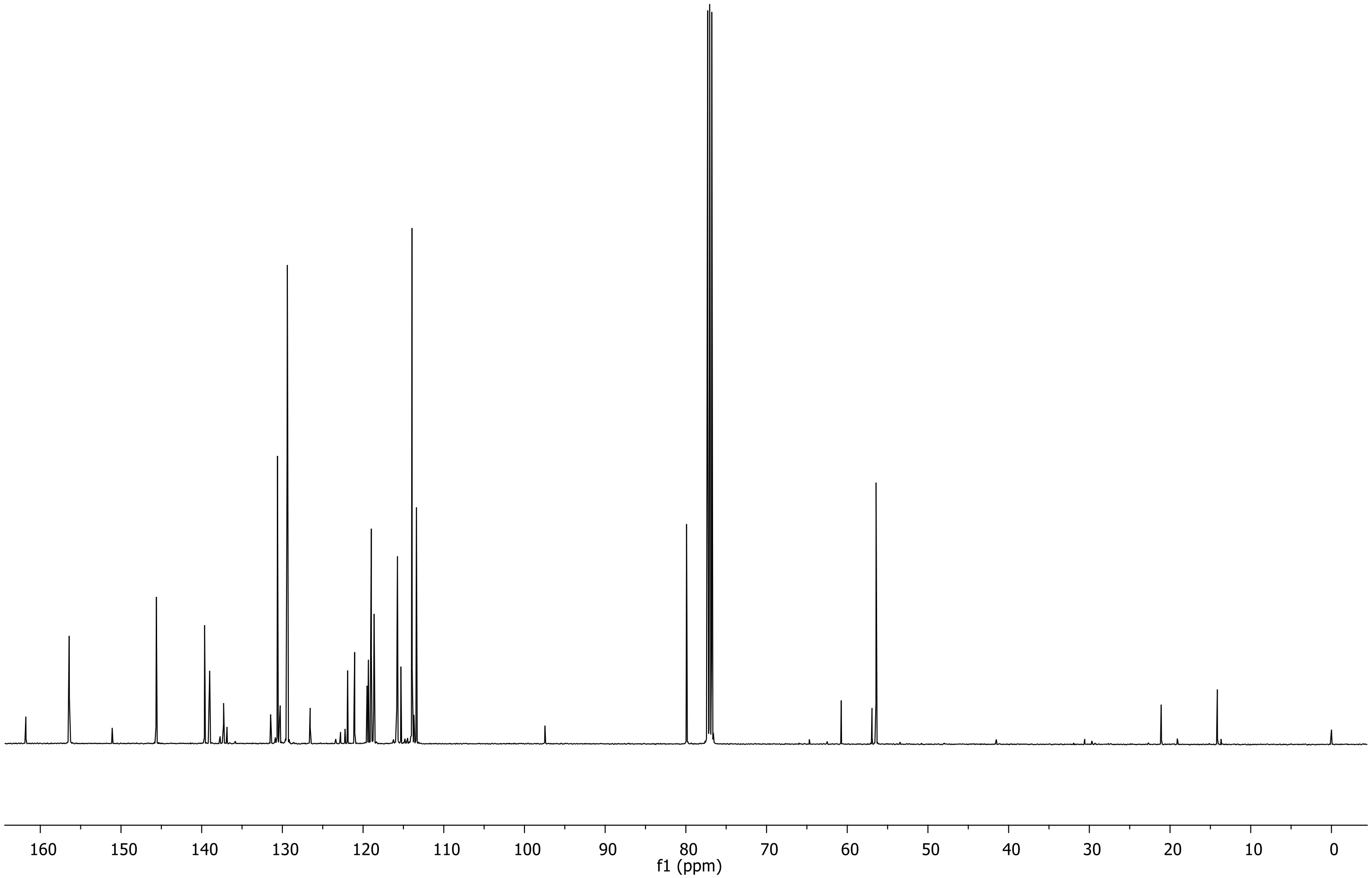

Figure 1.34: $^{13}$C NMR spectrum of **7e** 3-(2-nitro-1-(phenylamino)ethyl)phenol.

Table 1.5: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **7e** | 258 | 1 | 259.10 | 22 | 120.07 | 18 | ES+ |
| | | 2 | 259.10 | 22 | 94.05 | 14 | ES+ |
| | | 3 | 259.10 | 22 | 198.06 | 12 | ES+ |
| | | 4 | 259.10 | 22 | 212.17 | 12 | ES+ |
| | | 5 | 259.10 | 22 | 166.06 | 10 | ES+ |

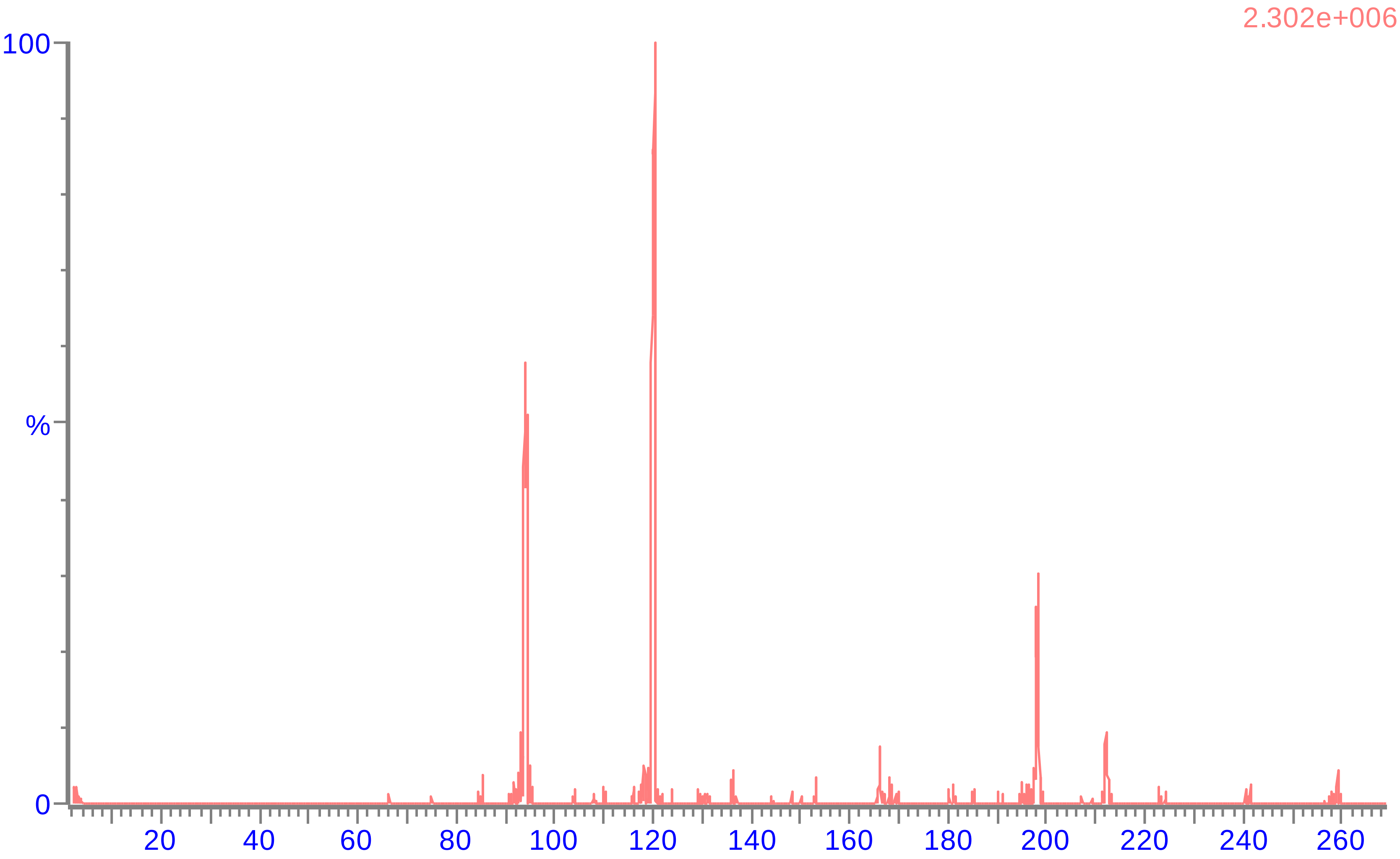

Figure 1.35: Mass spectrum for daughter fragment peak ES+, m/z 259.10 -> 120.07.

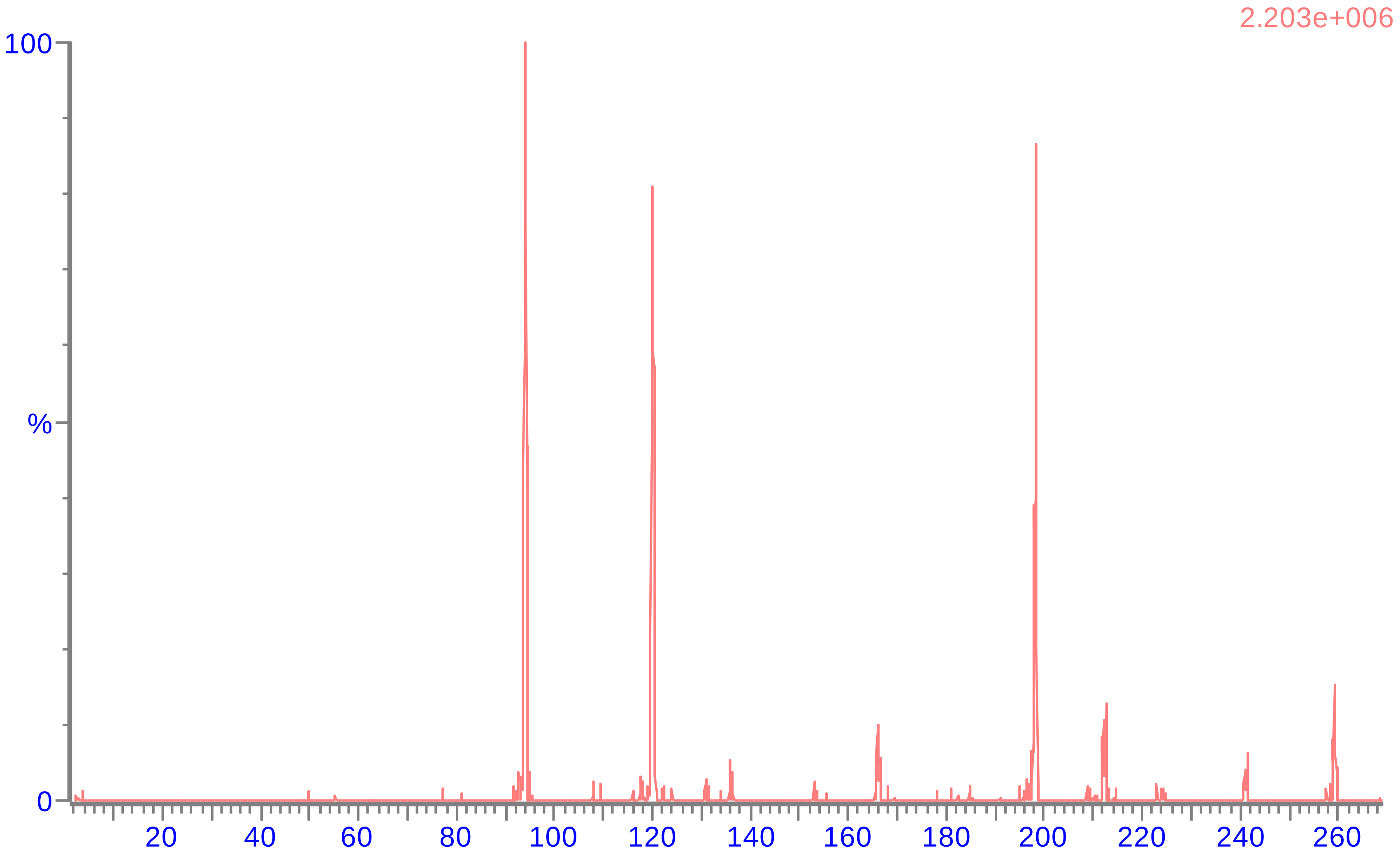

Figure 1.36: Mass spectrum for daughter fragment peak ES+, m/z 259.10 -> 94.05.

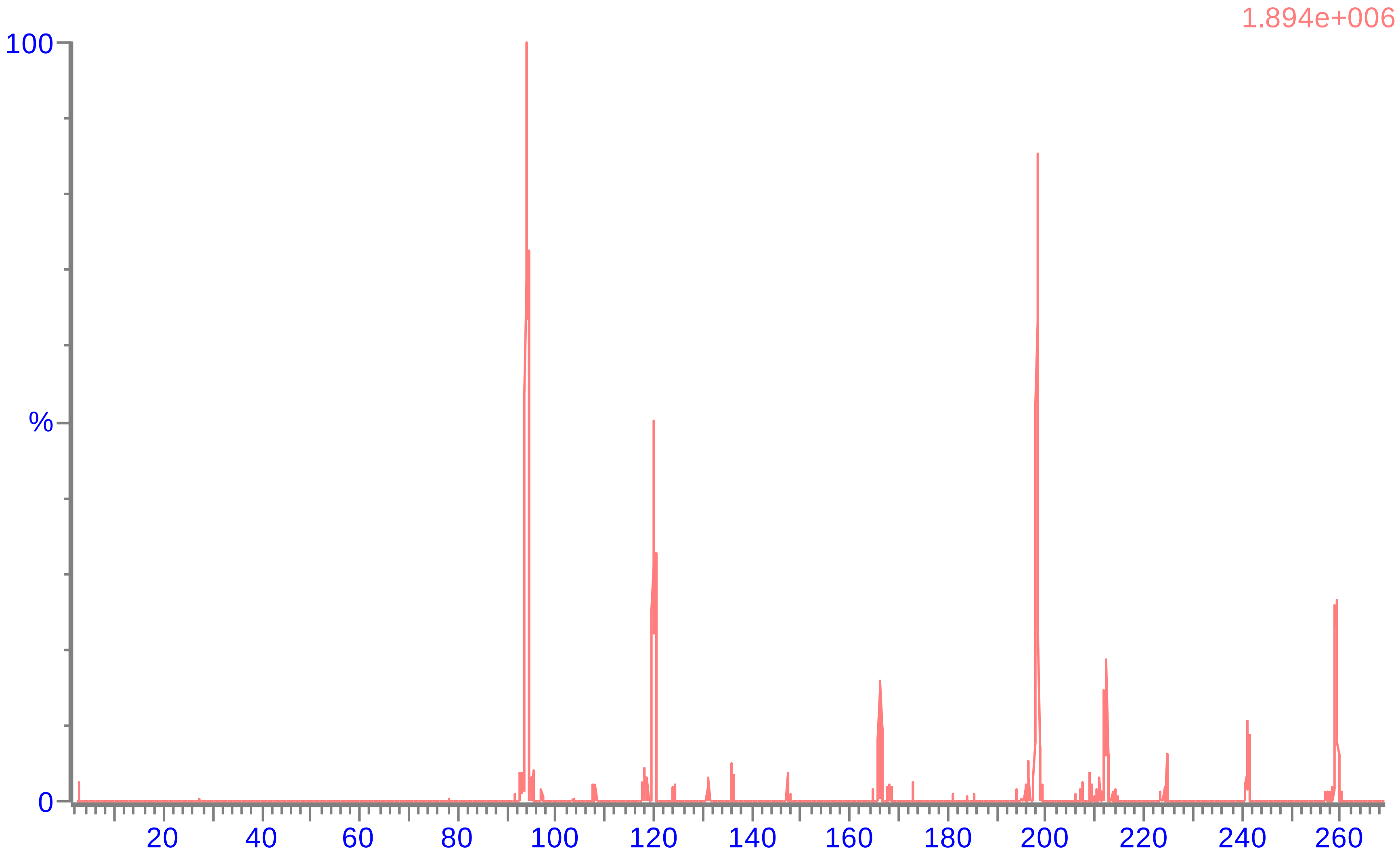

Figure 1.37: Mass spectrum for daughter fragment peak ES+, m/z 259.10 -> 198.06.

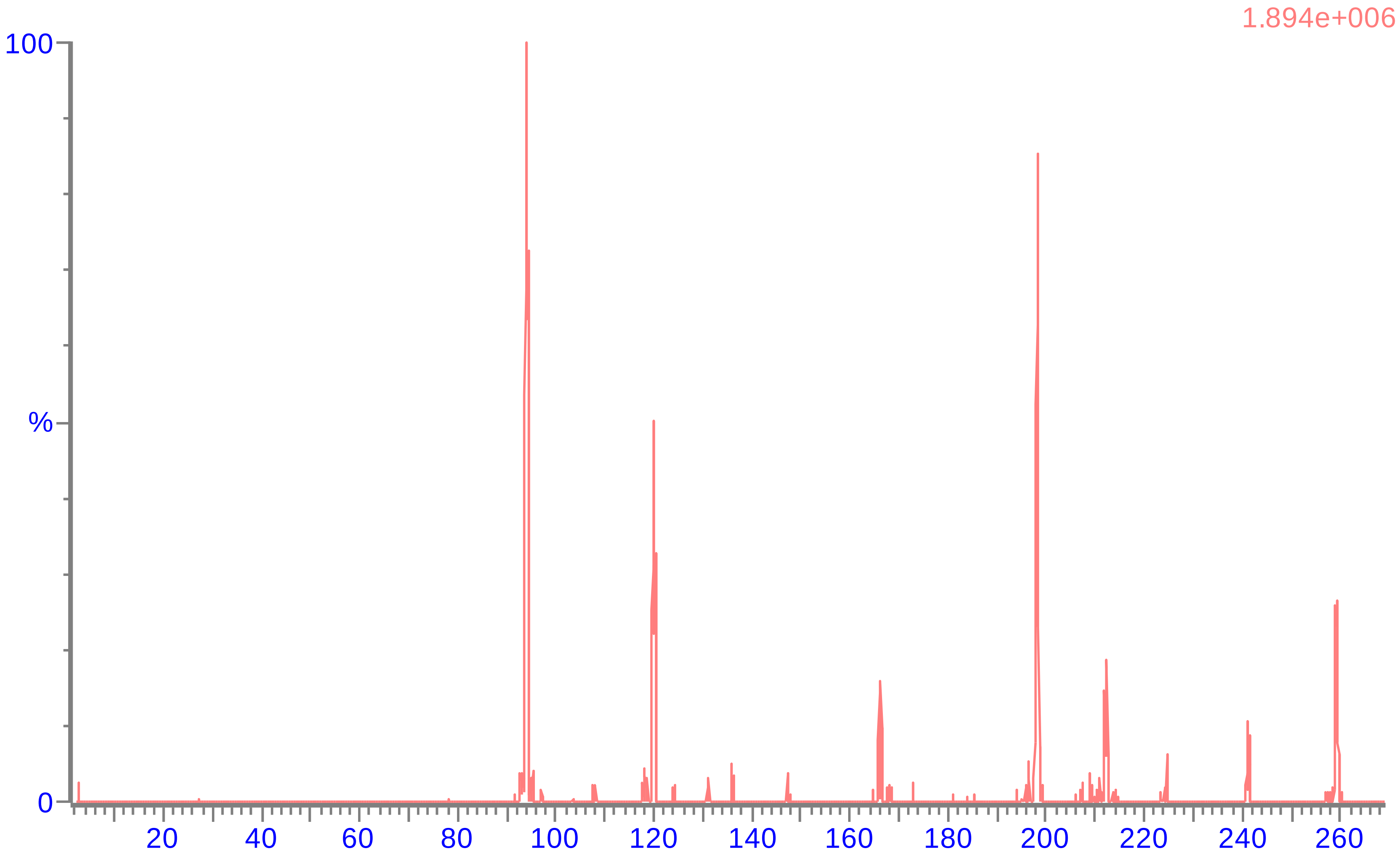

Figure 1.38: Mass spectrum for daughter fragment peak ES+, m/z 259.10 -> 212.17.

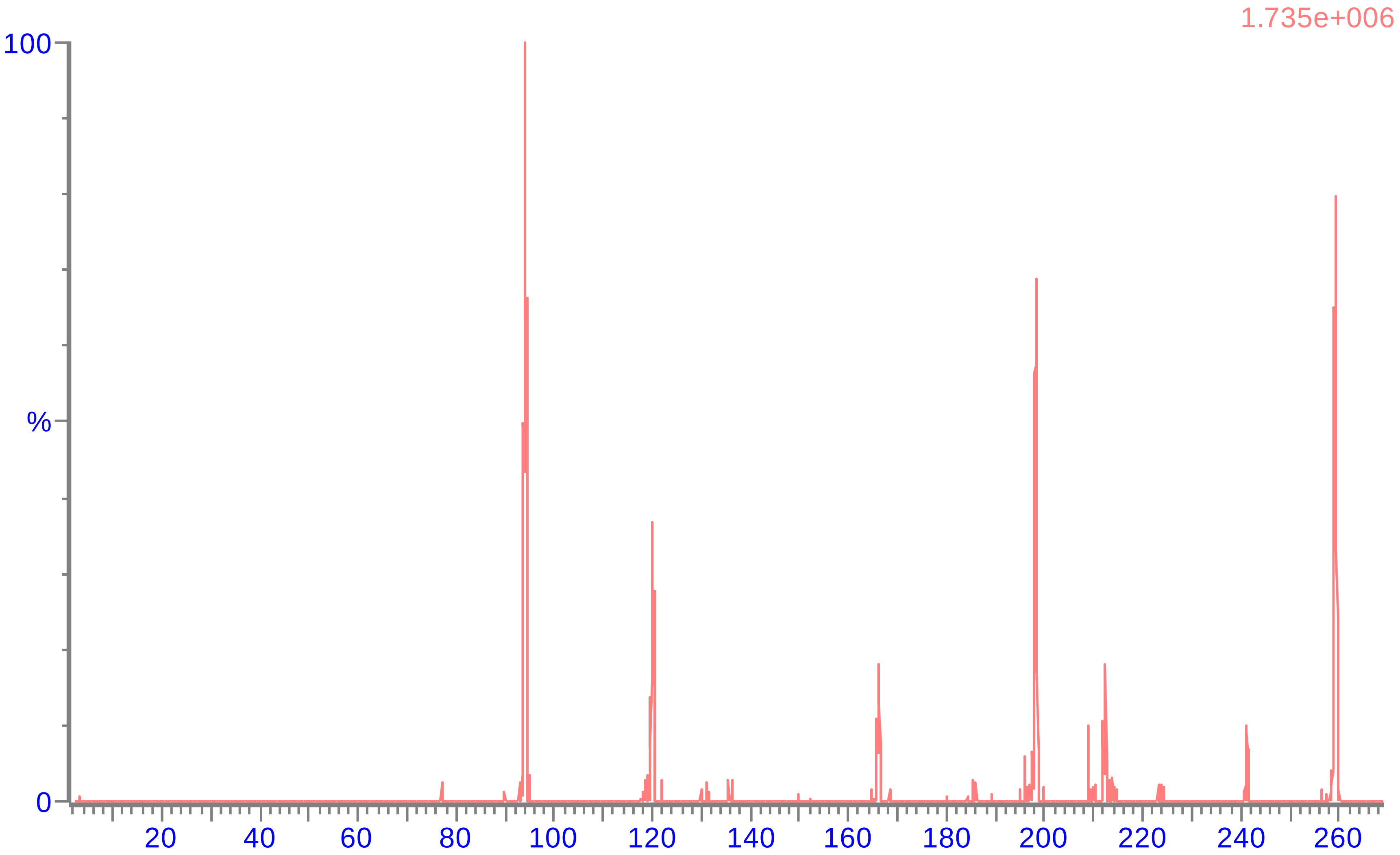

Figure 1.39: Mass spectrum for daughter fragment peak ES+, m/z 259.10 -> 166.06.

**7f** *N*-(1-(naphthalene-1-yl)-2-nitroethyl)aniline

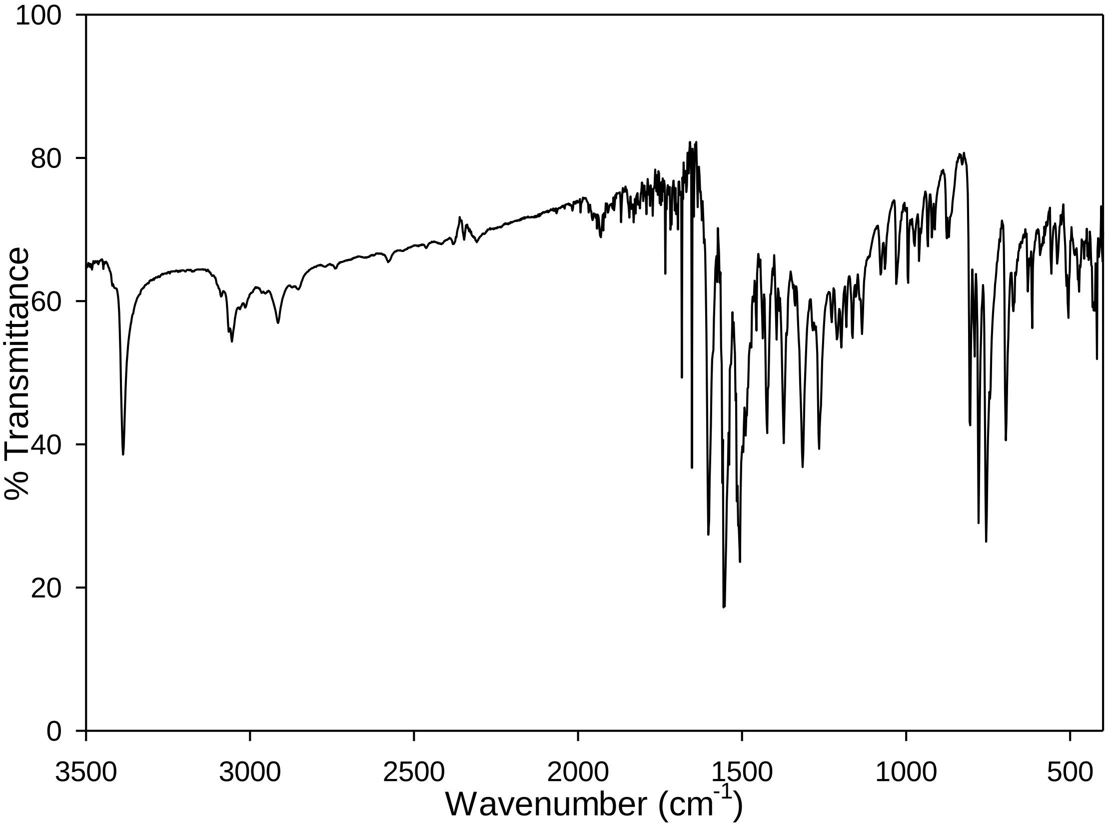

Figure 1.40: IR spectrum of **7f** *N*-(1-(naphthalene-1-yl)-2-nitroethyl)aniline.

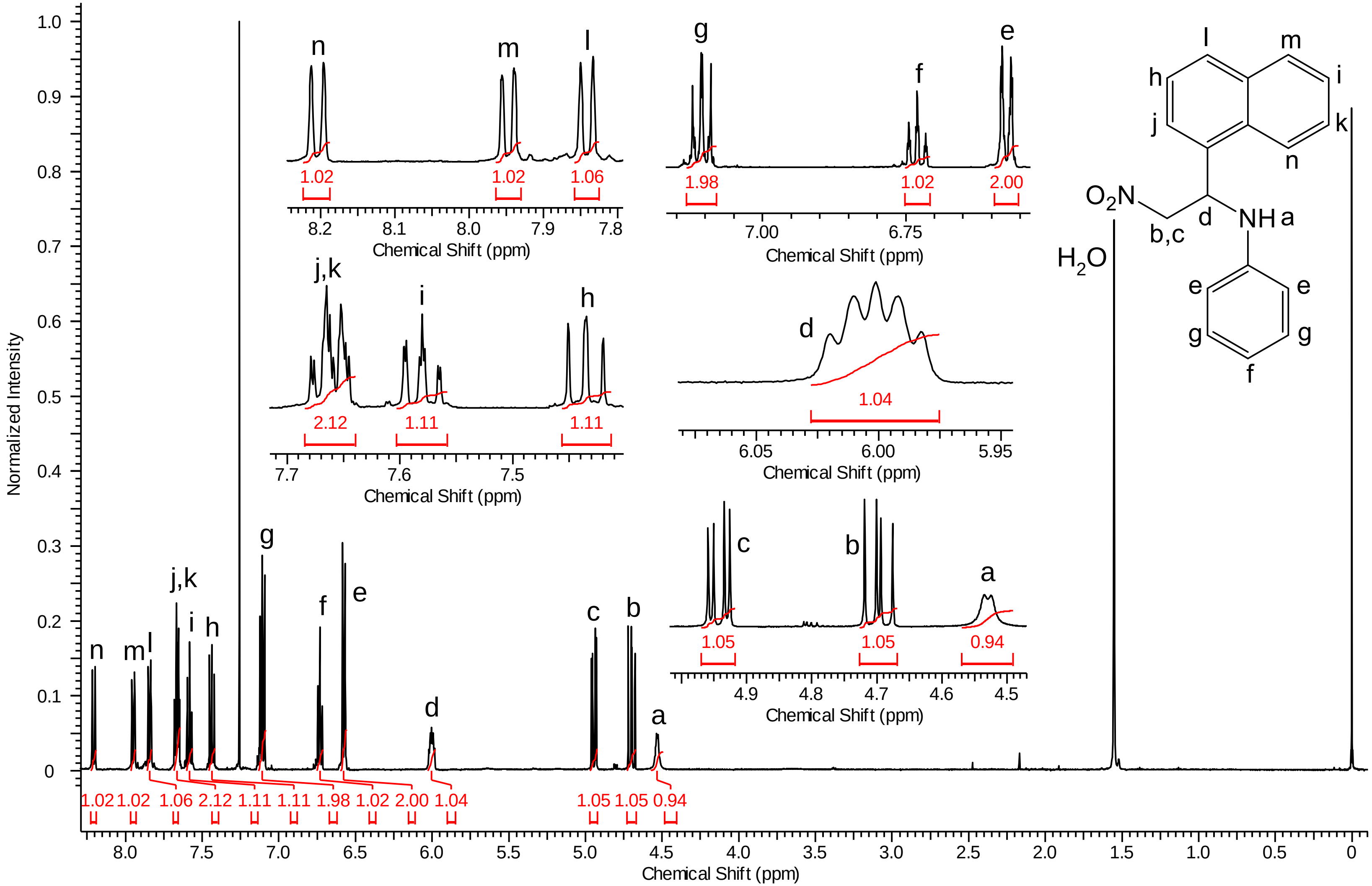

Figure 1.41: $^1$H NMR spectrum of **7f** *N*-(1-(naphthalene-1-yl)-2-nitroethyl)aniline.

Table 1.6: MS data.

| Compound | Formula/Mass |  | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **7f** | 292 | 1 | 293.10 | 16 | 154.02 | 14 | ES+ |
|  |  | 2 | 293.10 | 16 | 93.99 | 8 | ES+ |
|  |  | 3 | 293.10 | 16 | 200.07 | 8 | ES+ |
|  |  | 4 | 291.10 | 16 | 198.07 | 8 | ES- |
|  |  | 5 | 293.10 | 16 | 119.03 | 16 | ES+ |

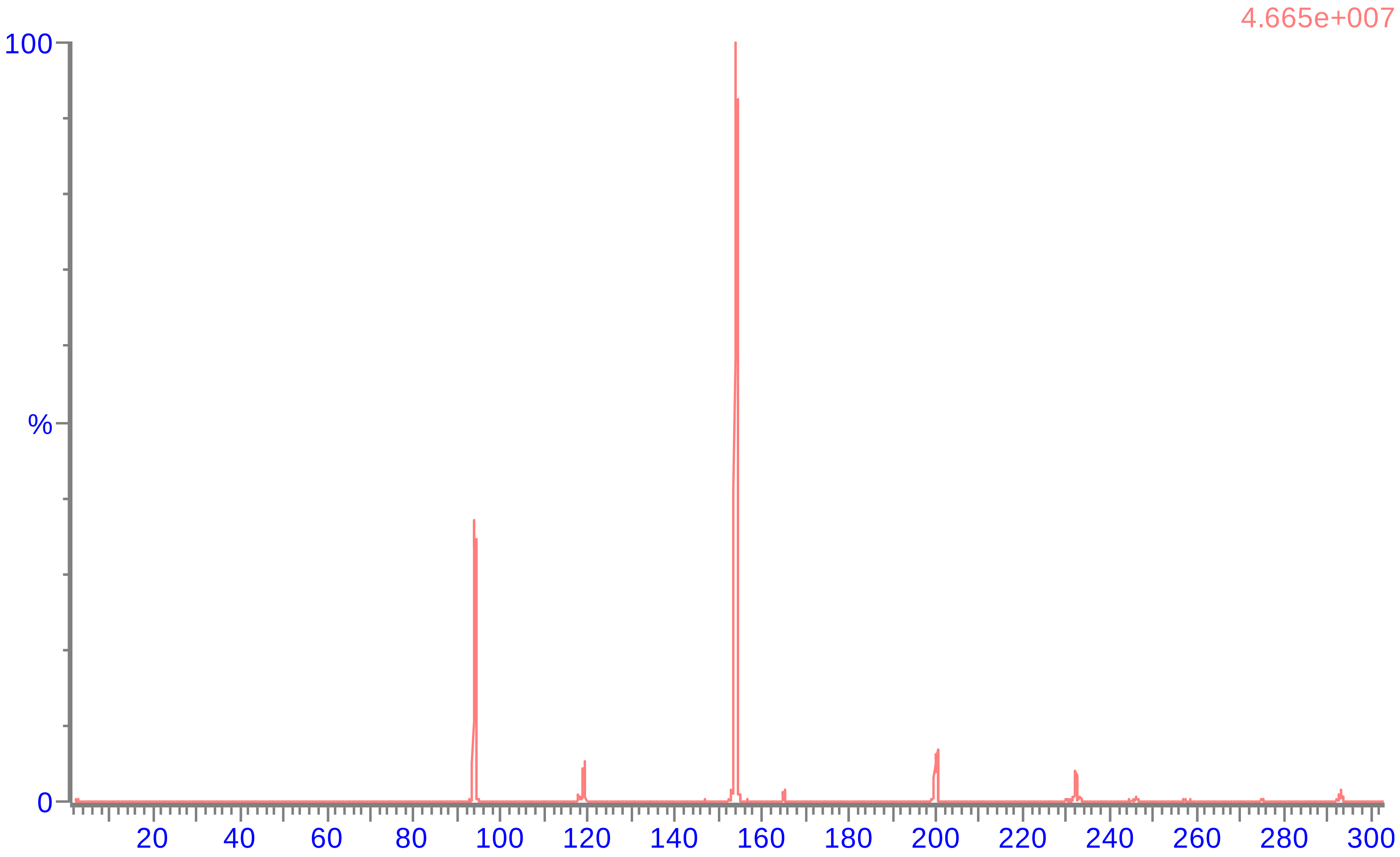

Figure 1.42: Mass spectrum for daughter fragment peak ES+, m/z 293.10 -> 154.02.

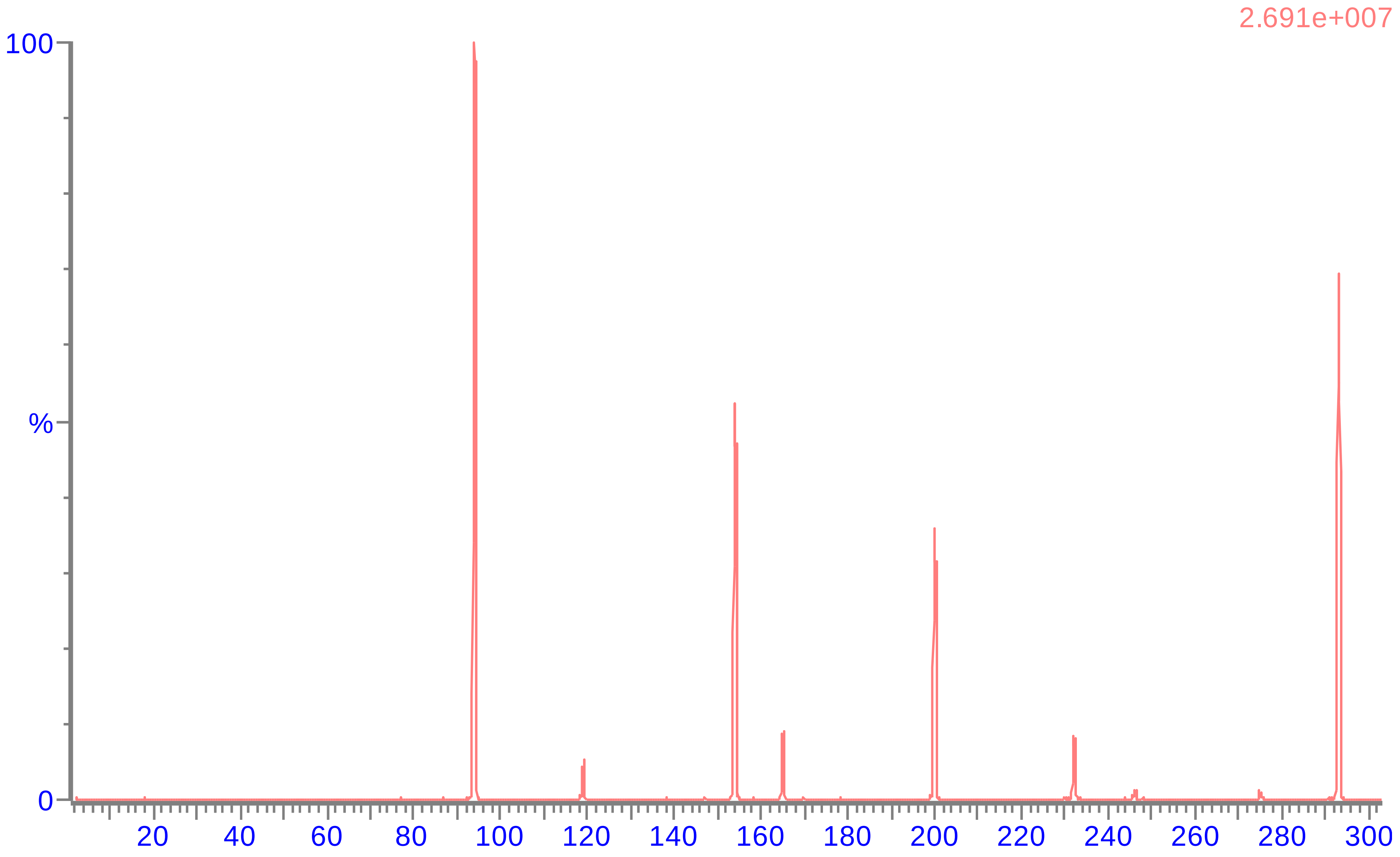

Figure 1.43: Mass spectrum for daughter fragment peak ES+, m/z 293.10 -> 93.99.

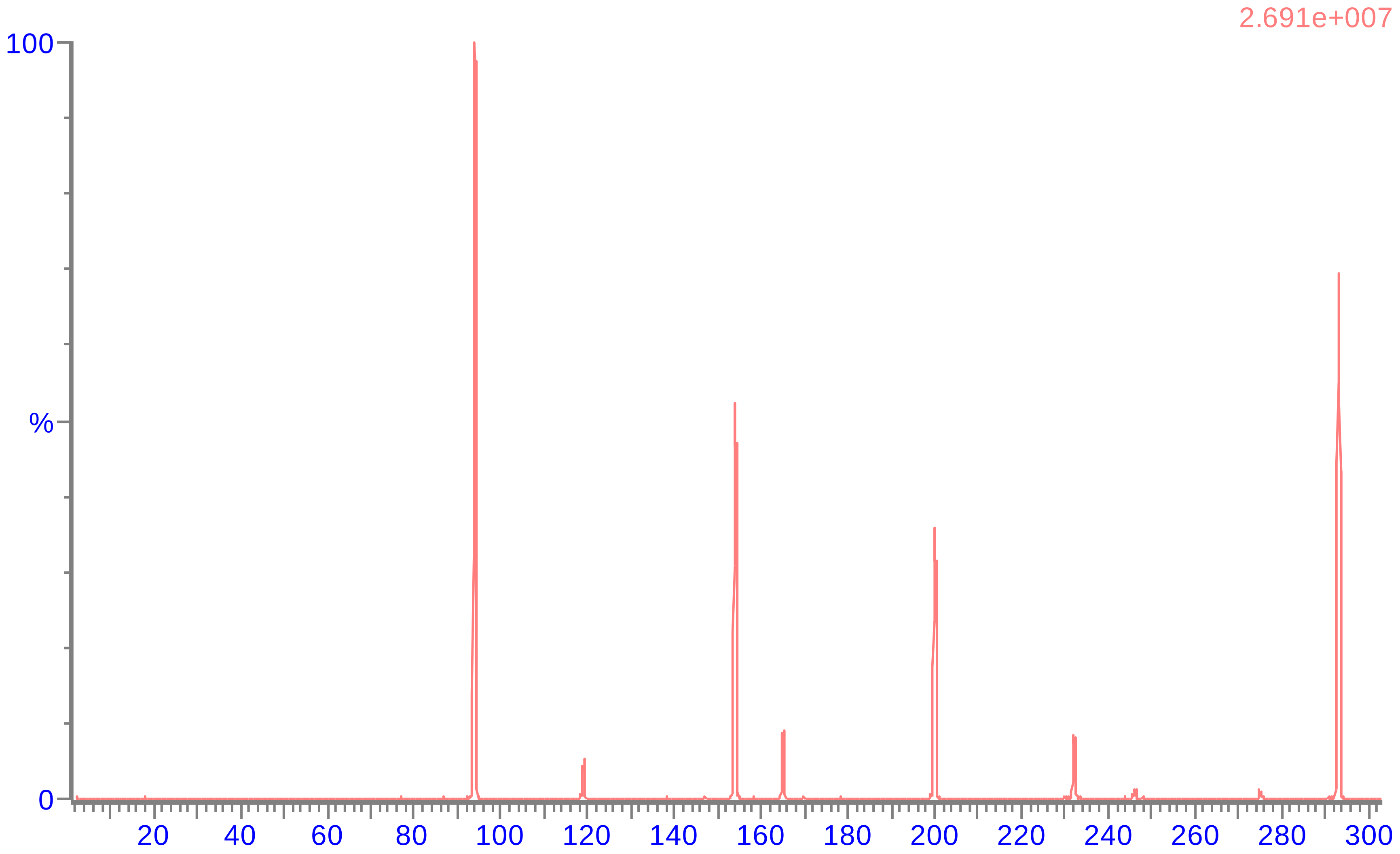

Figure 1.44: Mass spectrum for daughter fragment peak ES+, m/z 293.10 -> 200.07.

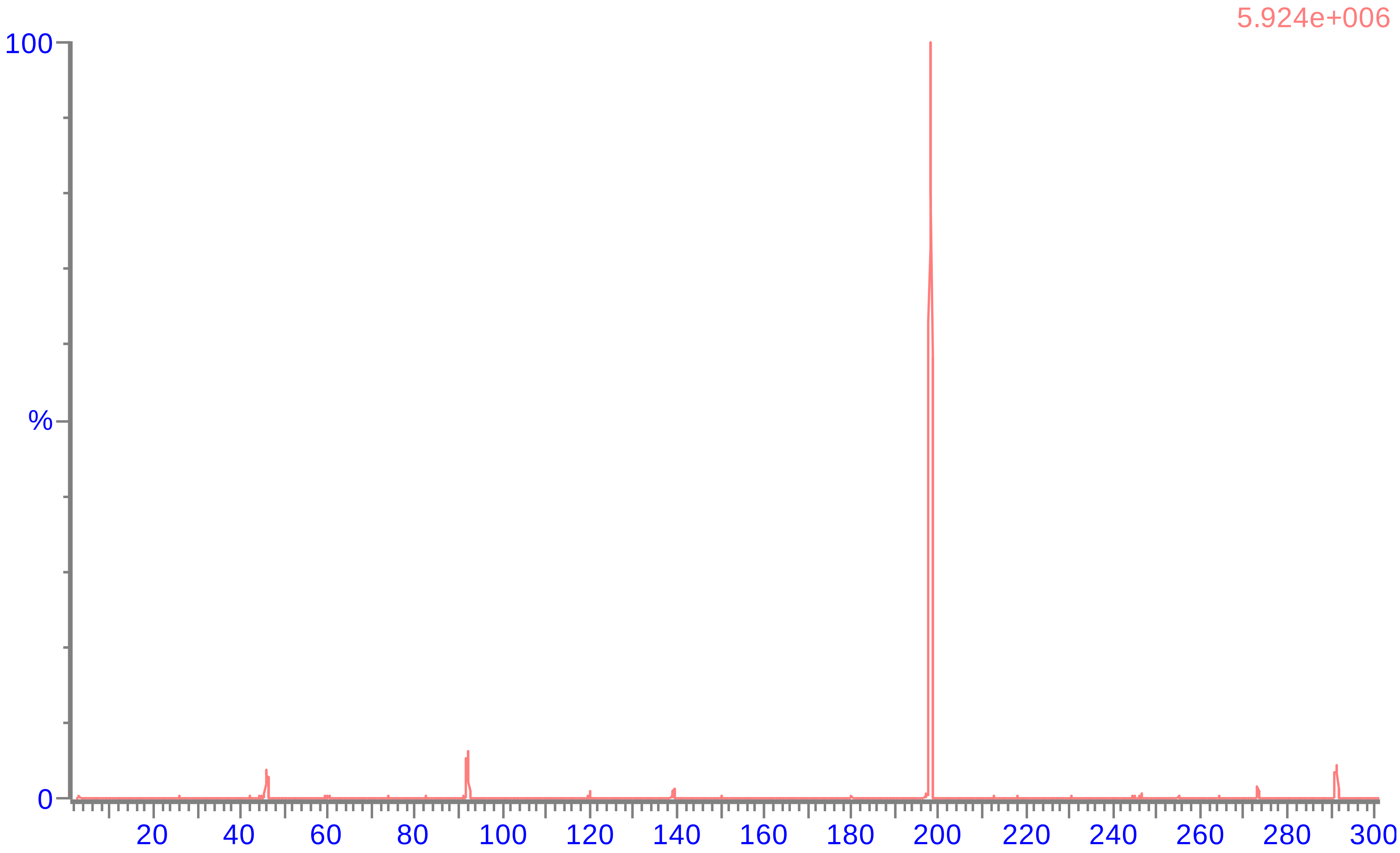

Figure 1.45: Mass spectrum for daughter fragment peak ES+, m/z 293.10 -> 198.07.

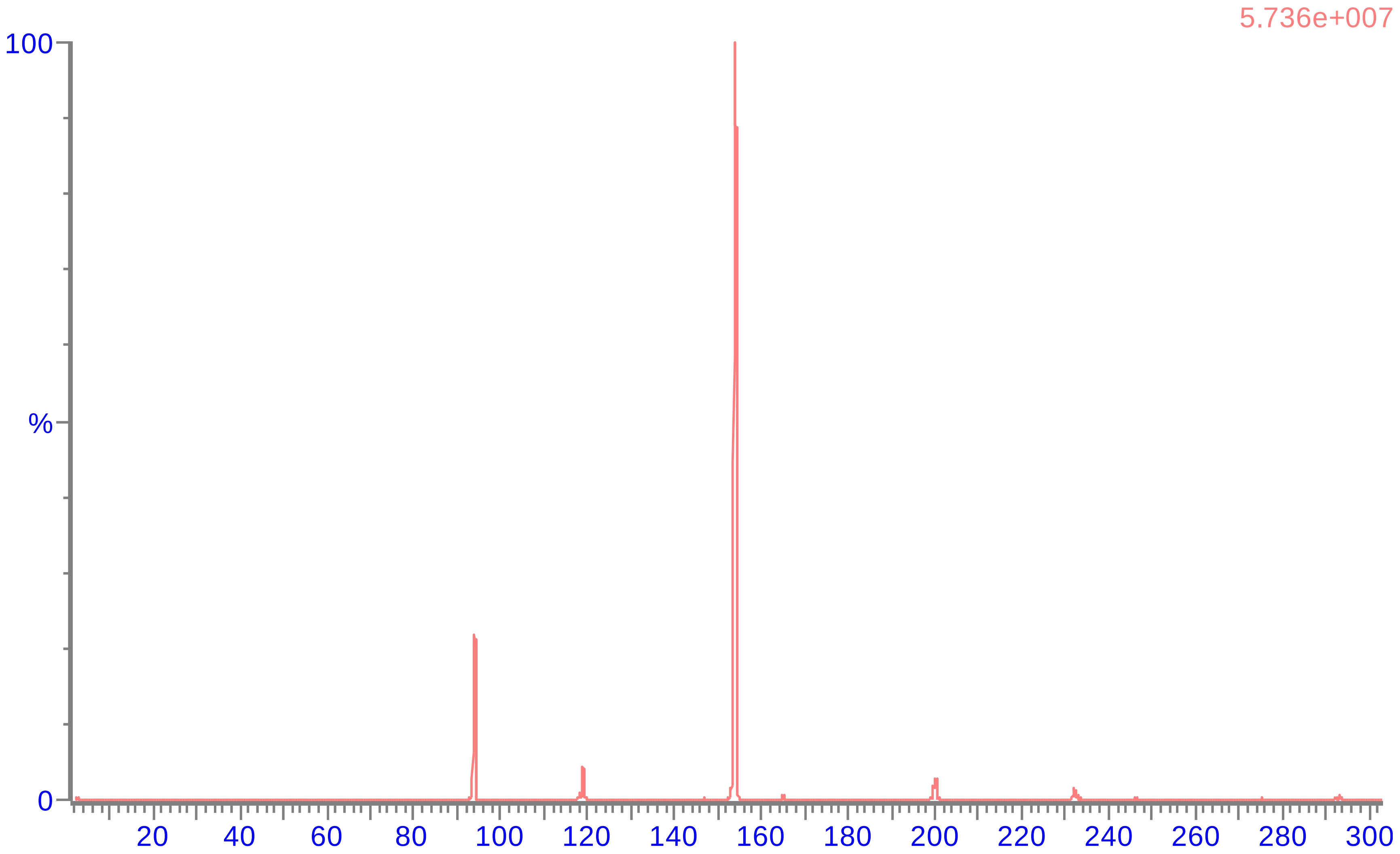

Figure 1.46: Mass spectrum for daughter fragment peak ES+, m/z 293.10 -> 119.03.

**7g** *N*-(1-([1,1-biphenyl]-4-yl)-2-nitroethyl)aniline

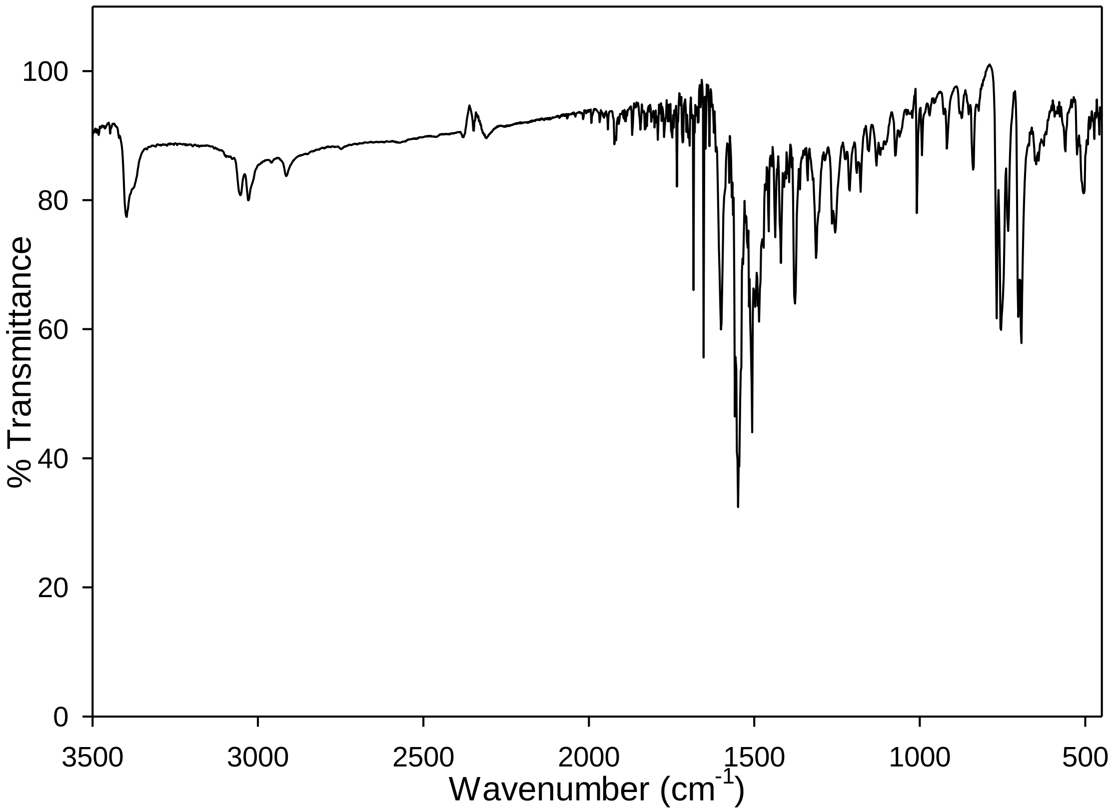

Figure 1.47: IR spectrum of **7g** *N*-(1-([1,1-biphenyl]-4-yl)-2-nitroethyl)aniline.

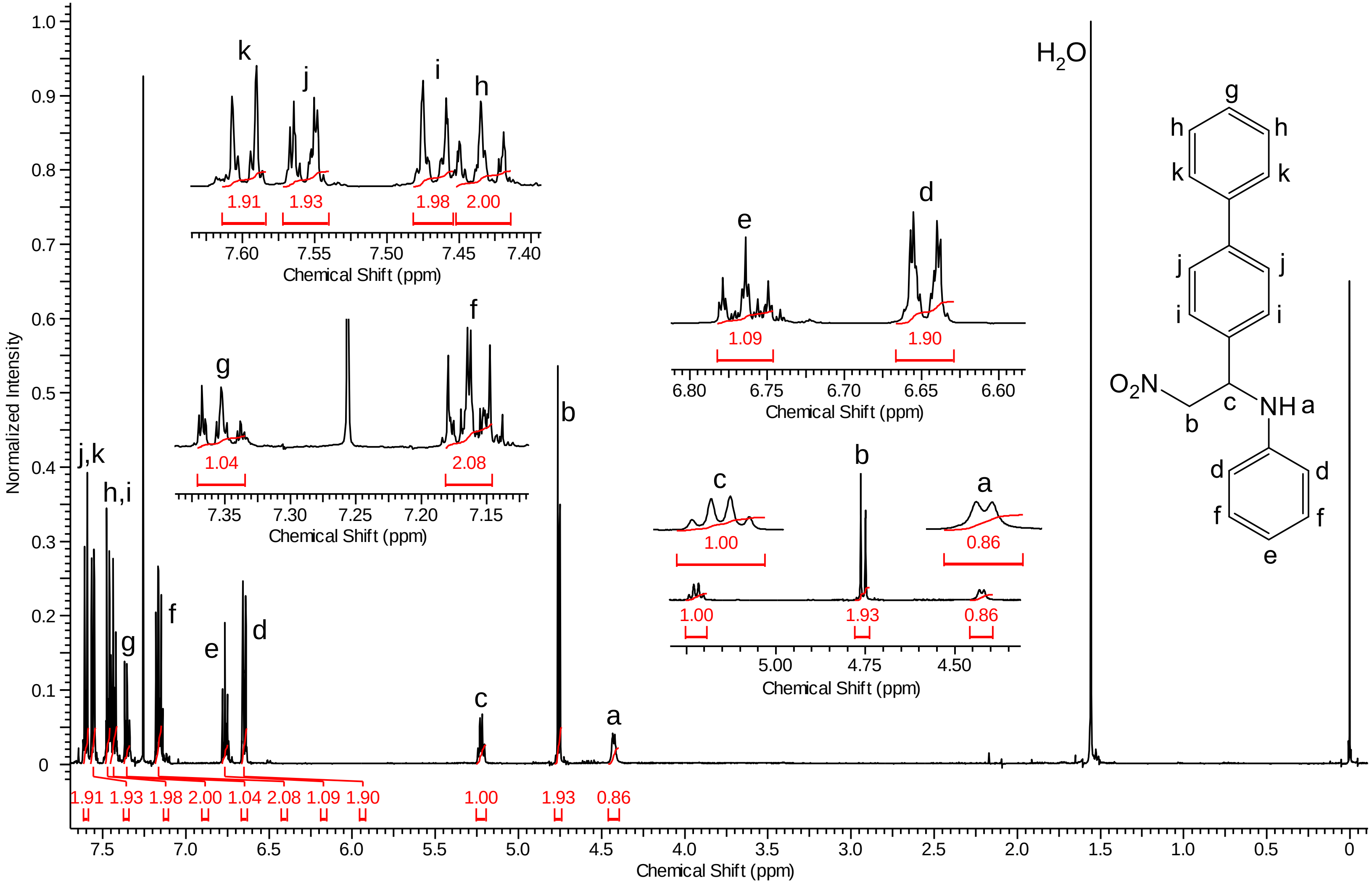

Figure 1.48: $^1$H NMR spectrum of **7g** *N*-(1-([1,1-biphenyl]-4-yl)-2-nitroethyl)aniline.

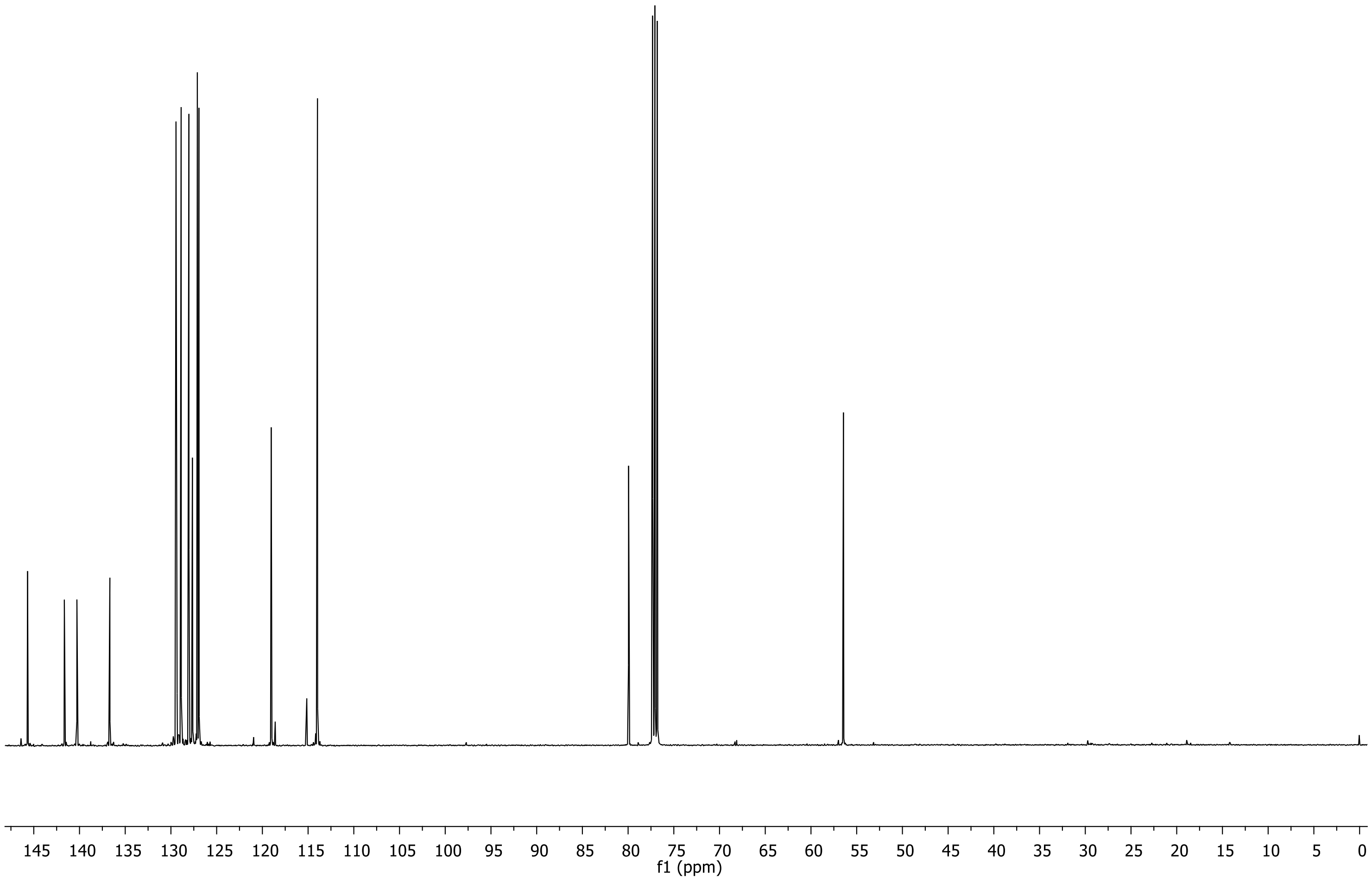

Figure 1.49: ${}^{13}$C NMR spectrum of **7g** *N*-(1-([1,1-biphenyl]-4-yl)-2-nitroethyl)aniline.

Table 1.7 MS data.

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **7g** | 328 | 1 | 327.03 | 16 | 80.91 | 50 | ES- |

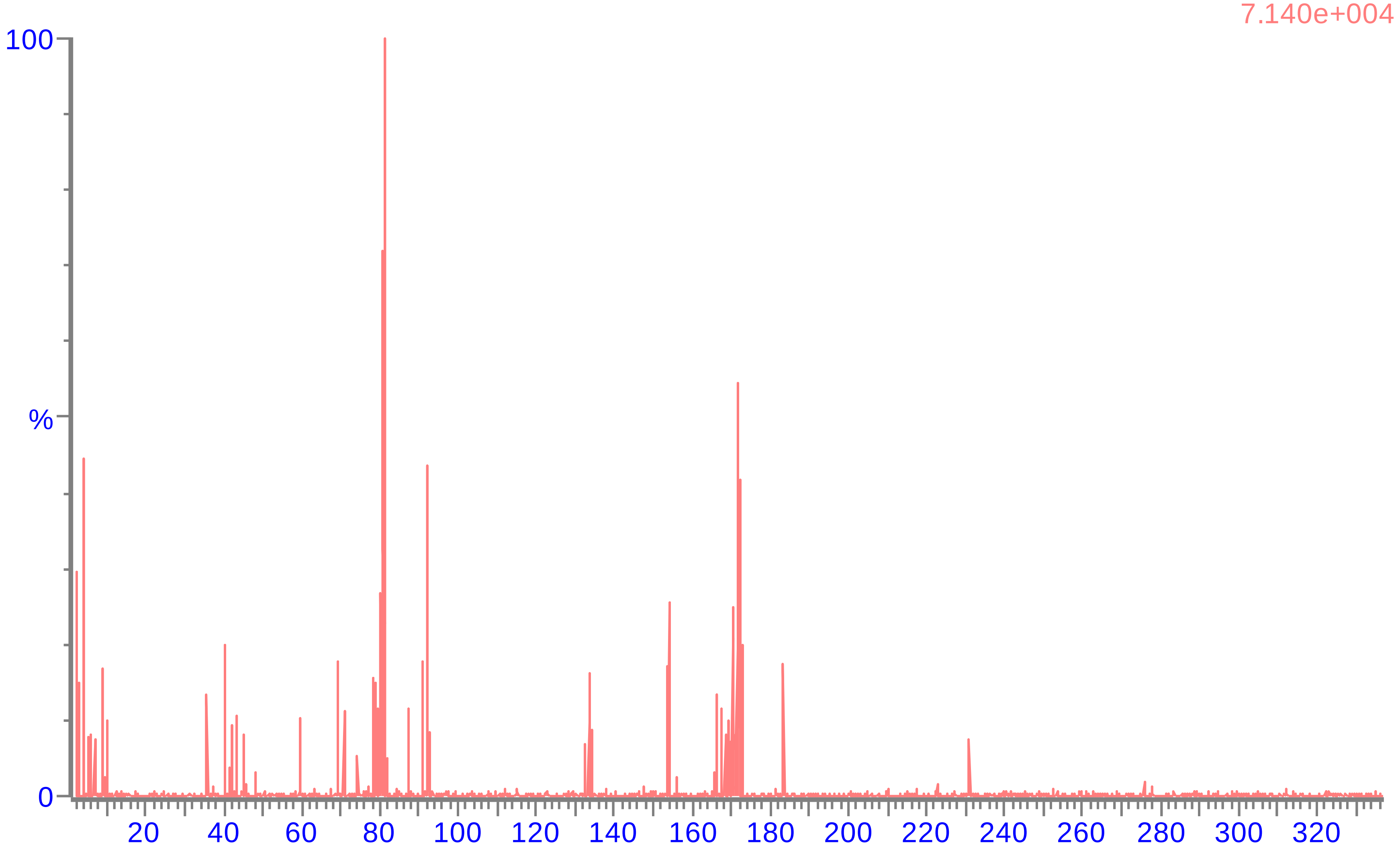

Figure 1.50: Mass spectrum for daughter fragment peak ES+, m/z 327.03 -> 80.91.

**7h** *N*-(1-(3,4-dichlorophenyl)-2-nitroethyl)aniline

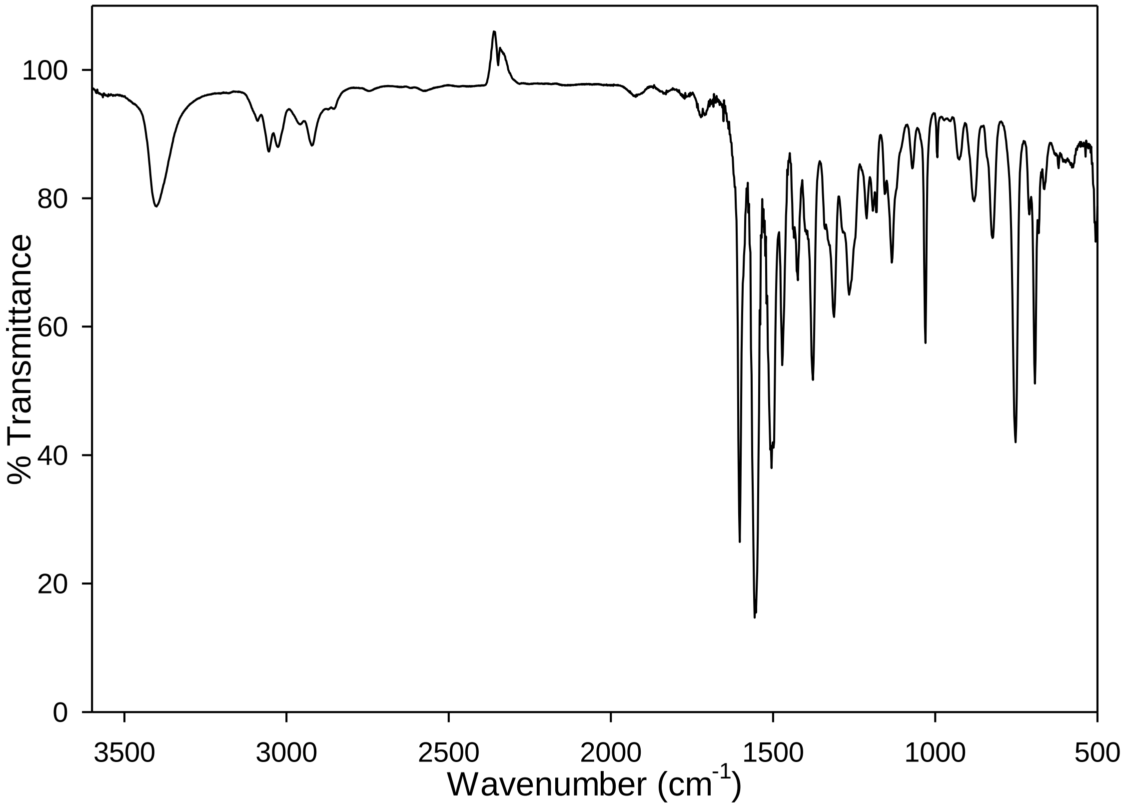

Figure 1.51: IR spectrum of **7h** *N*-(1-(3,4-dichlorophenyl)-2-nitroethyl)aniline.

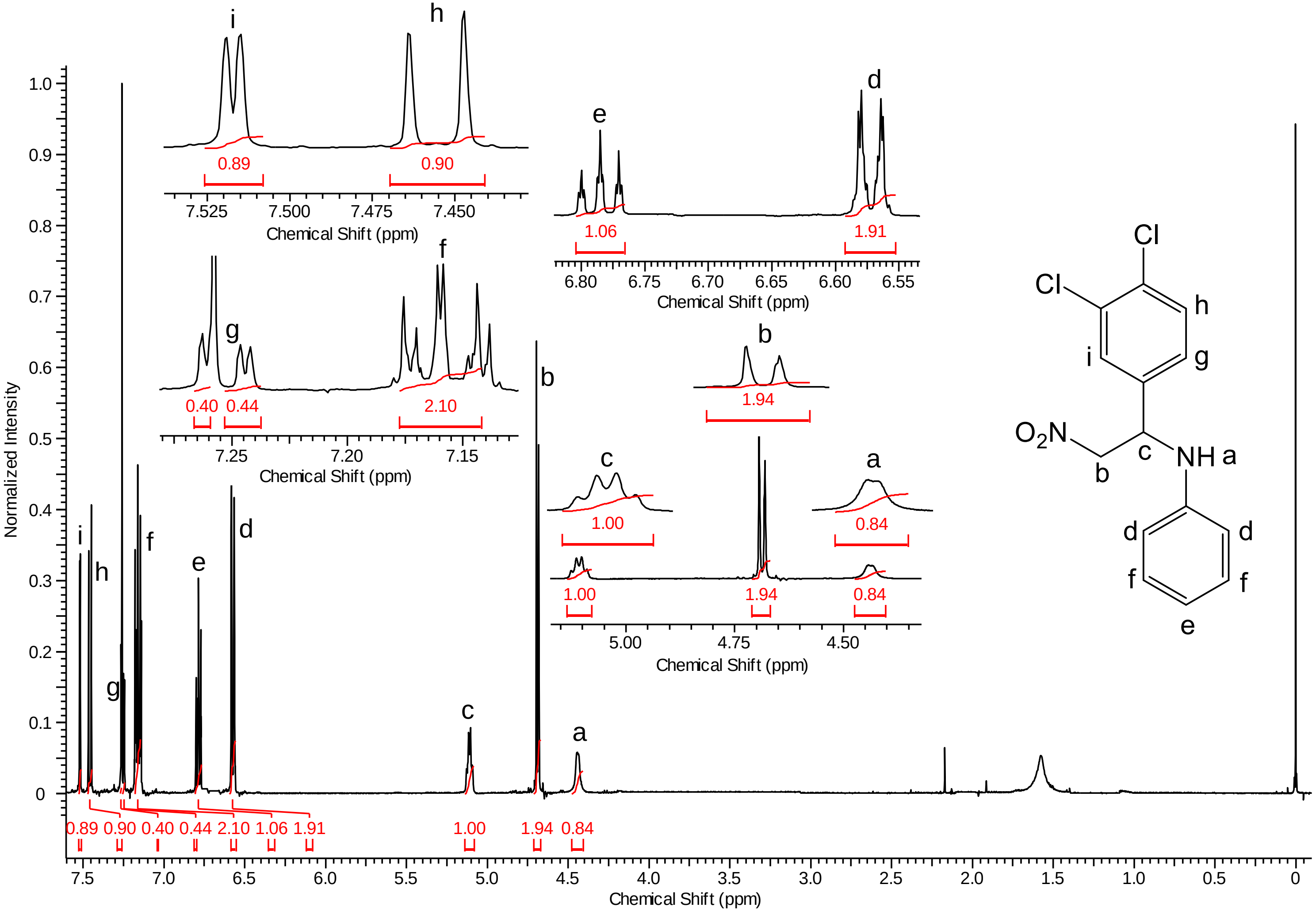

Figure 1.52: $^1$H NMR spectrum of **7h** *N*-(1-(3,4-dichlorophenyl)-2-nitroethyl)aniline.

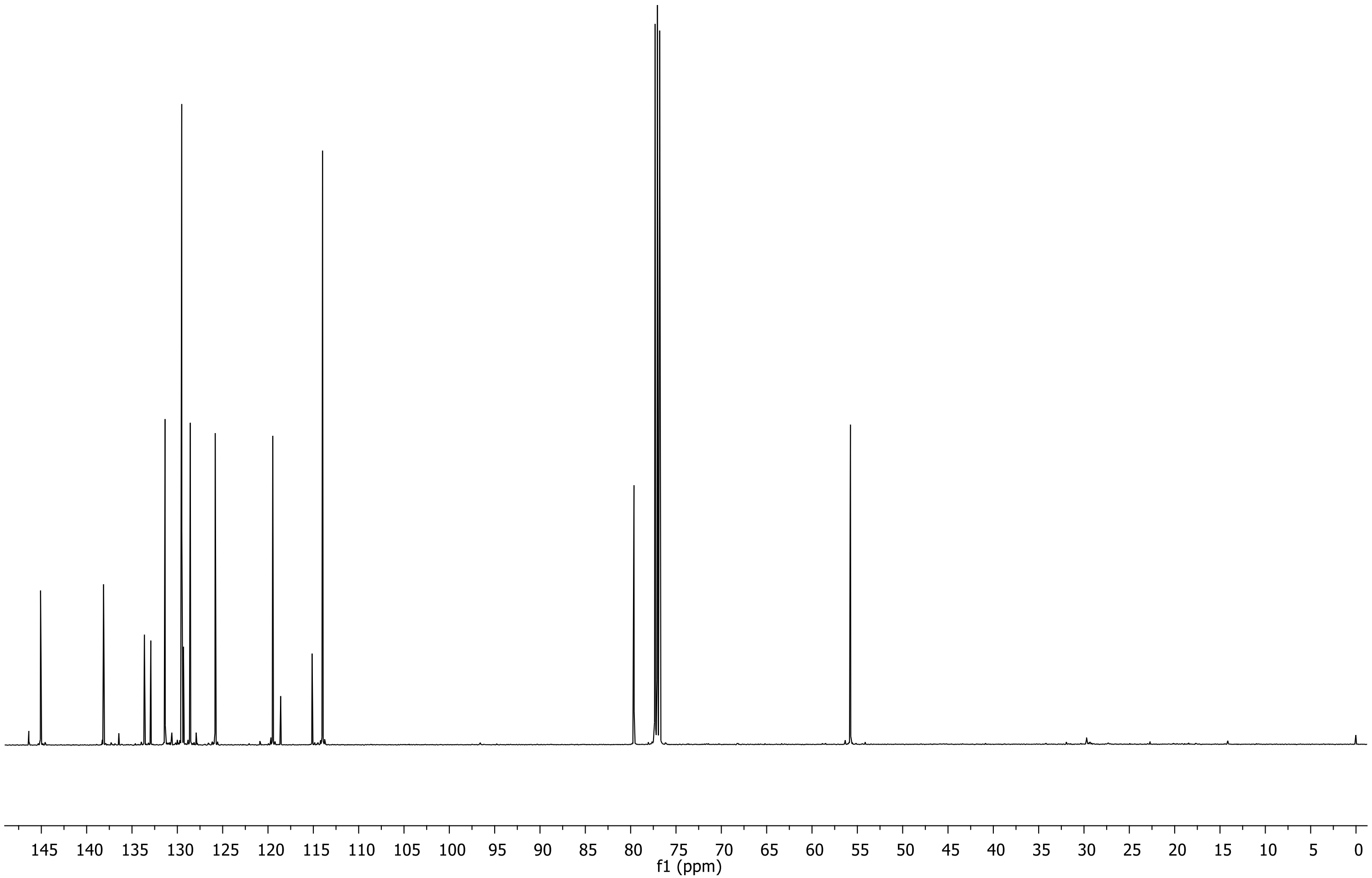

Figure 1.53: $^{13}$C NMR spectrum of **7h** *N*-(1-(3,4-dichlorophenyl)-2-nitroethyl)aniline.

Table 1.8: MS data.

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **7h** | 312 | 1 | 312.97 | 16 | 93.98 | 12 | ES+ |
| | | 2 | 312.97 | 18 | 217.96 | 8 | ES- |
| | | 3 | 312.97 | 16 | 252.02 | 12 | ES+ |
| | | 4 | 312.97 | 16 | 173.91 | 26 | ES+ |
| | | 5 | 312.97 | 16 | 101.73 | 58 | ES+ |

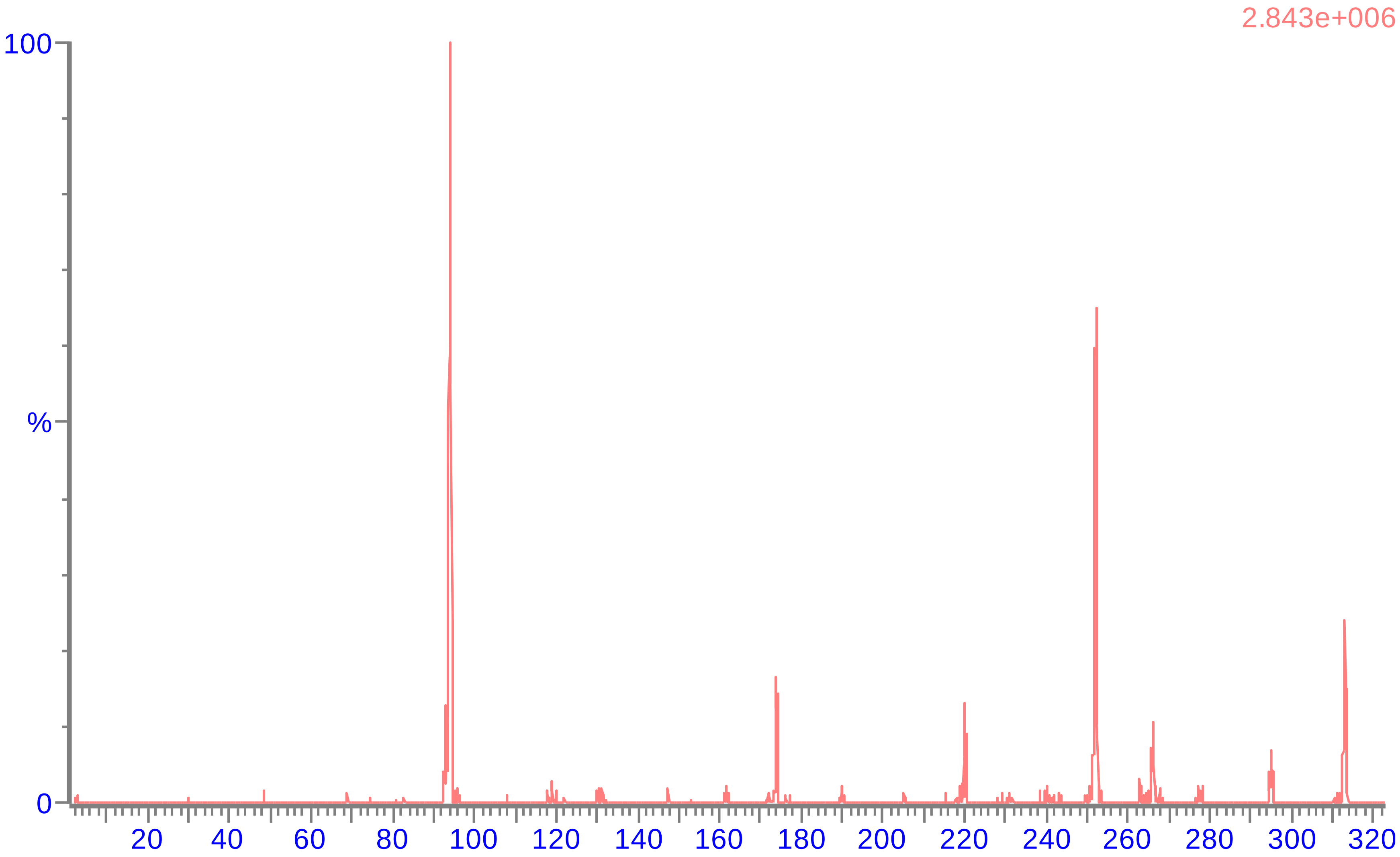

Figure 1.54: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 93.98.

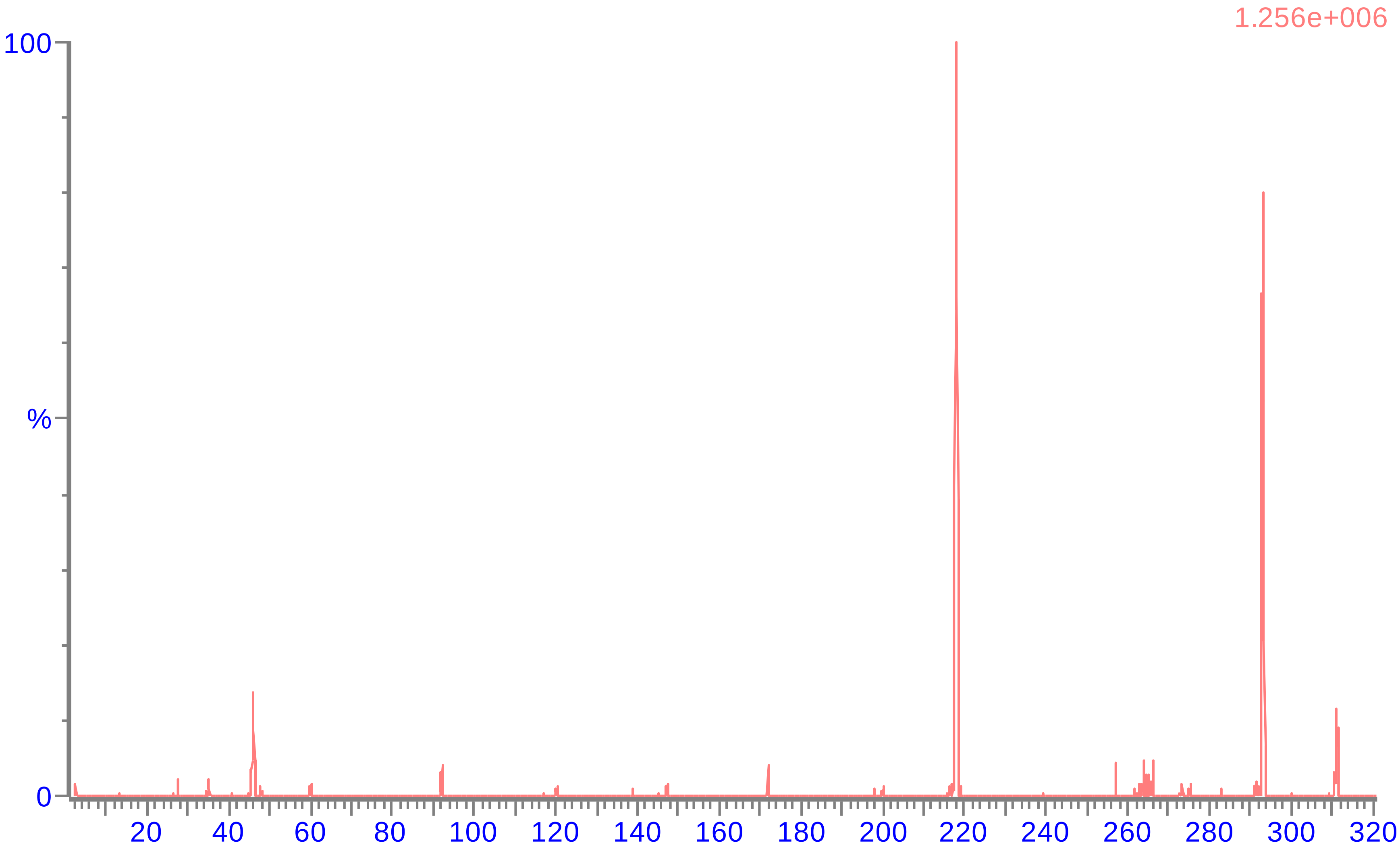

Figure 1.55: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 217.96.

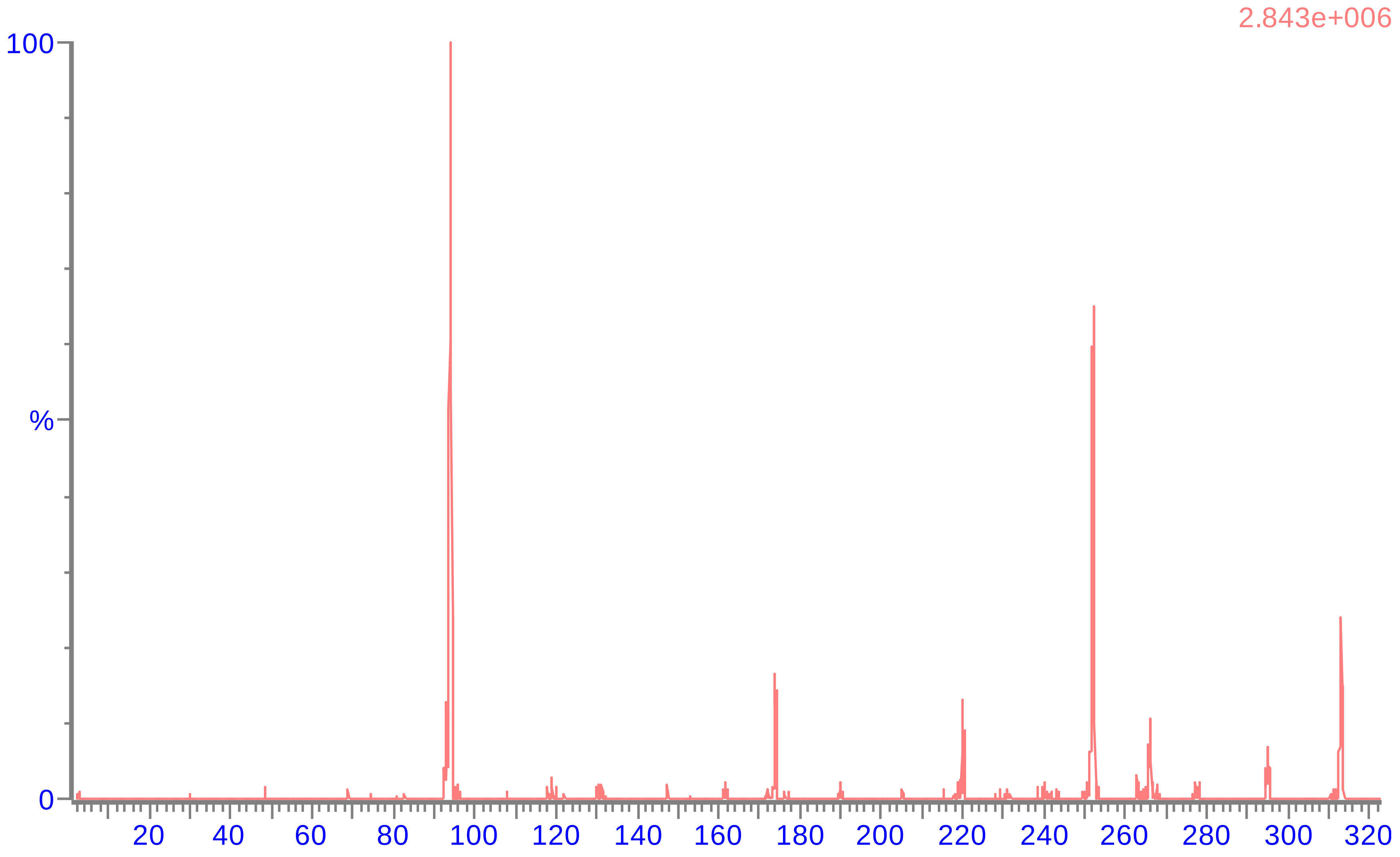

Figure 1.56: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 252.02.

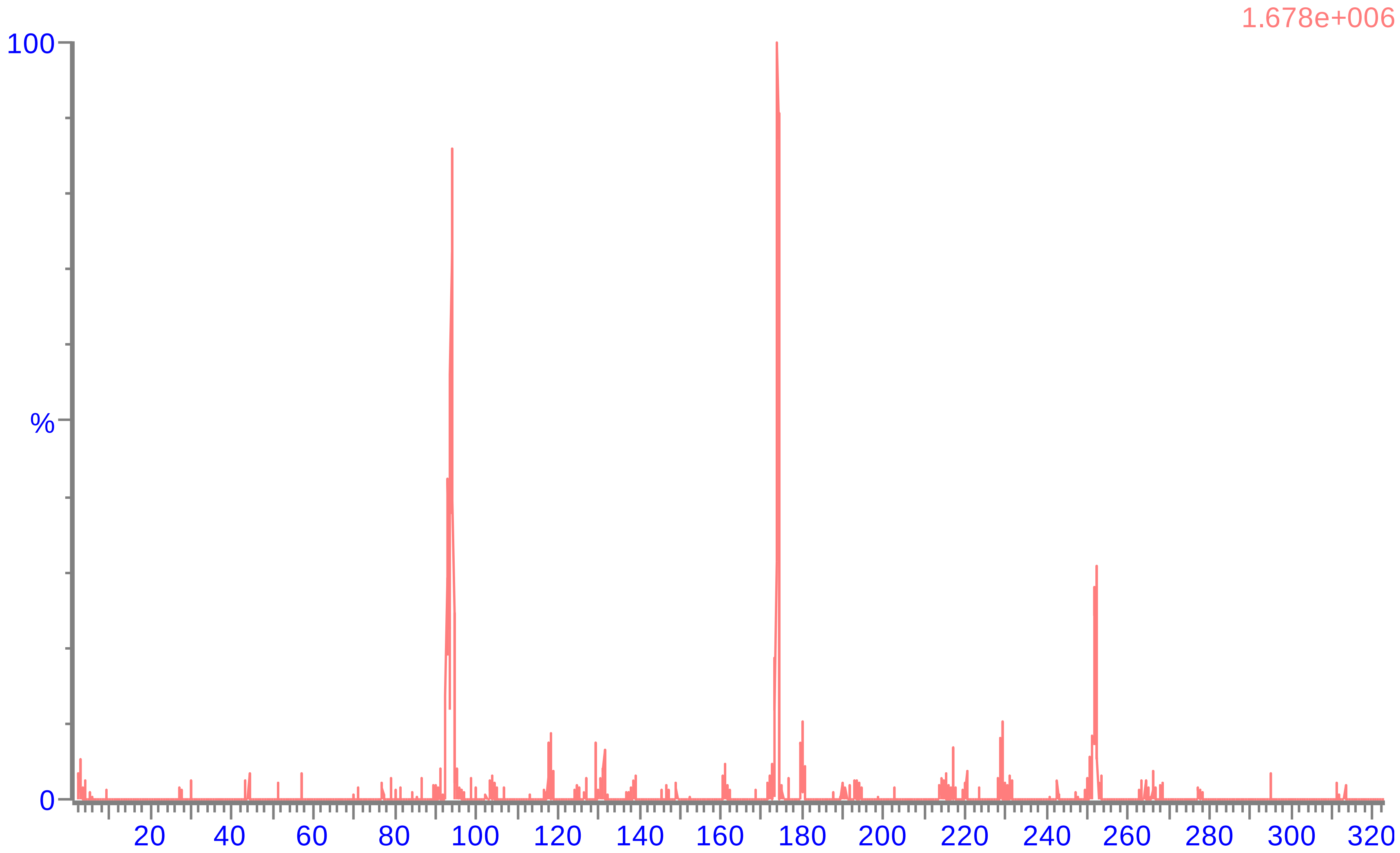

Figure 1.57: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 173.91.

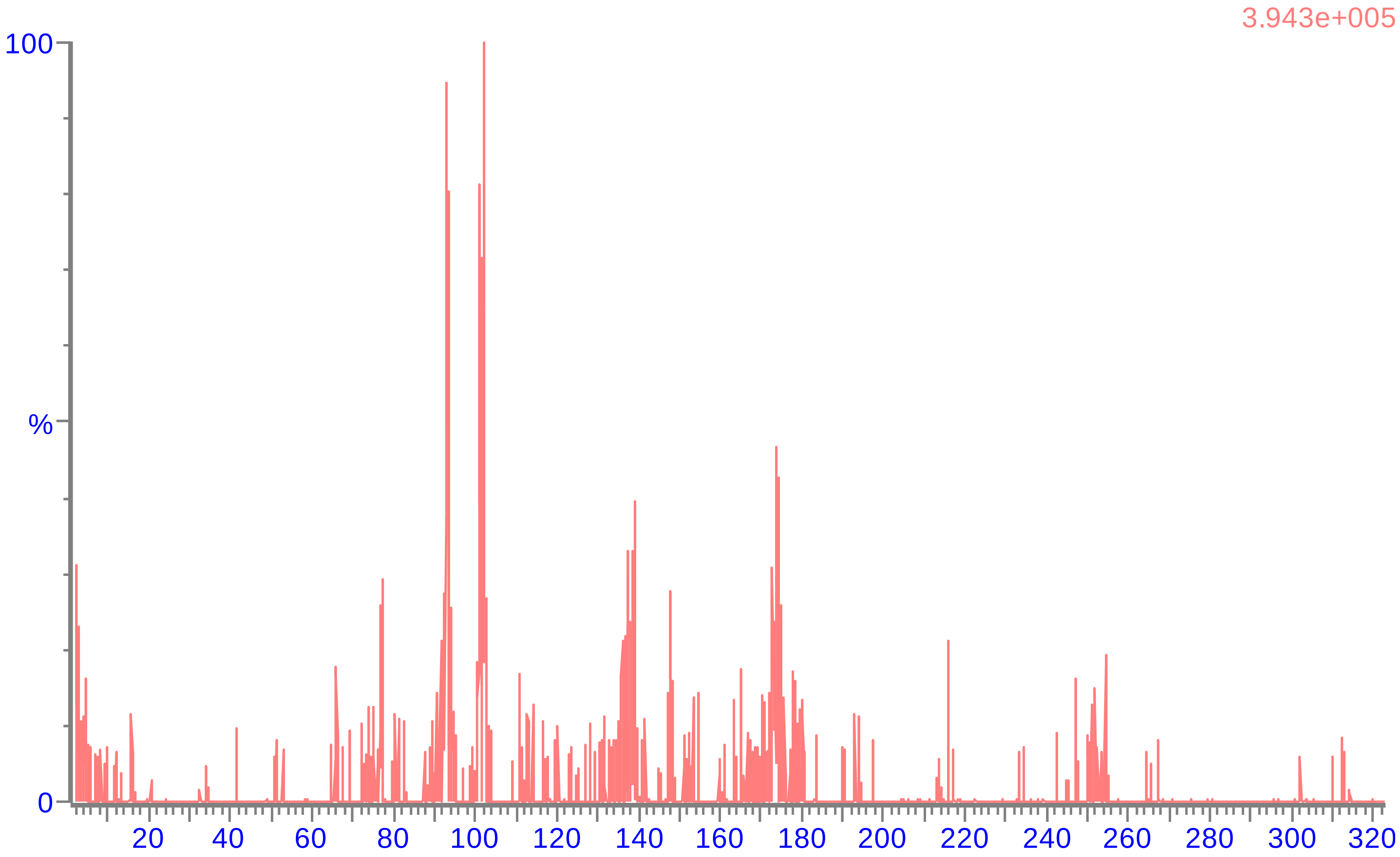

Figure 1.58: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 101.73.

**7i** *N*-(1-(2,6-dichlorophenyl)-2-nitroethyl)aniline.

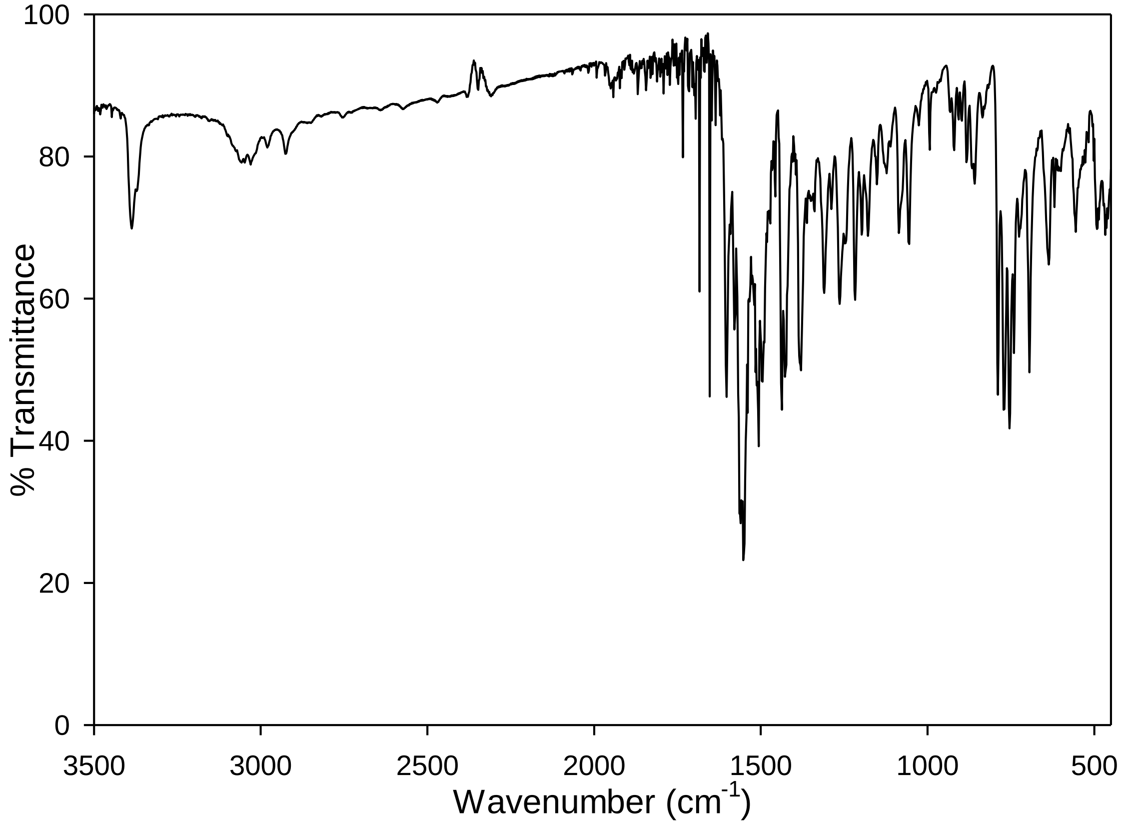

Figure 1.57: IR spectrum of **7i** *N*-(1-(2,6-dichlorophenyl)-2-nitroethyl)aniline.

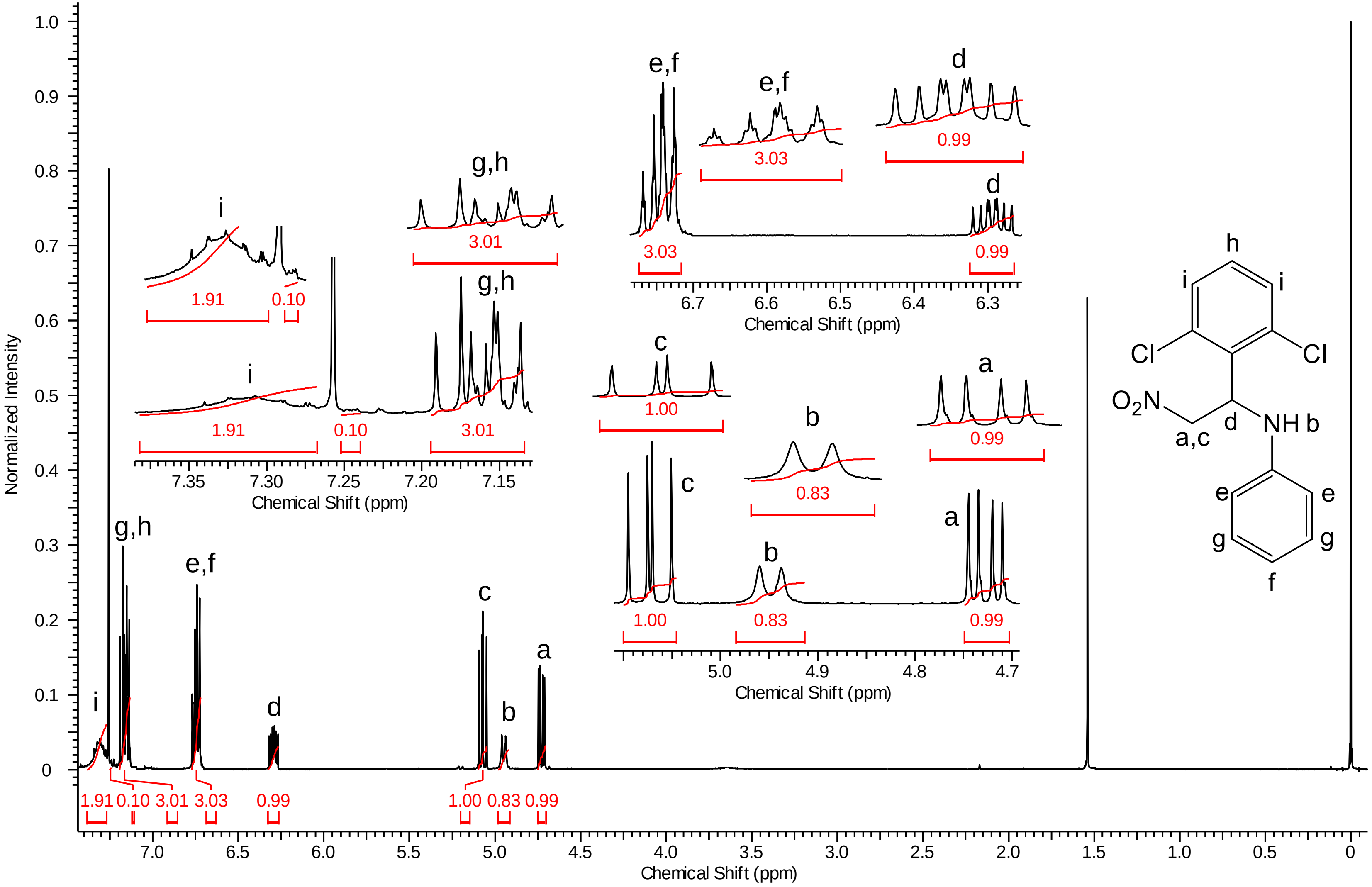

Figure 1.60: $^1$H NMR spectrum of **7i** *N*-(1-(2,6-dichlorophenyl)-2-nitroethyl)aniline.

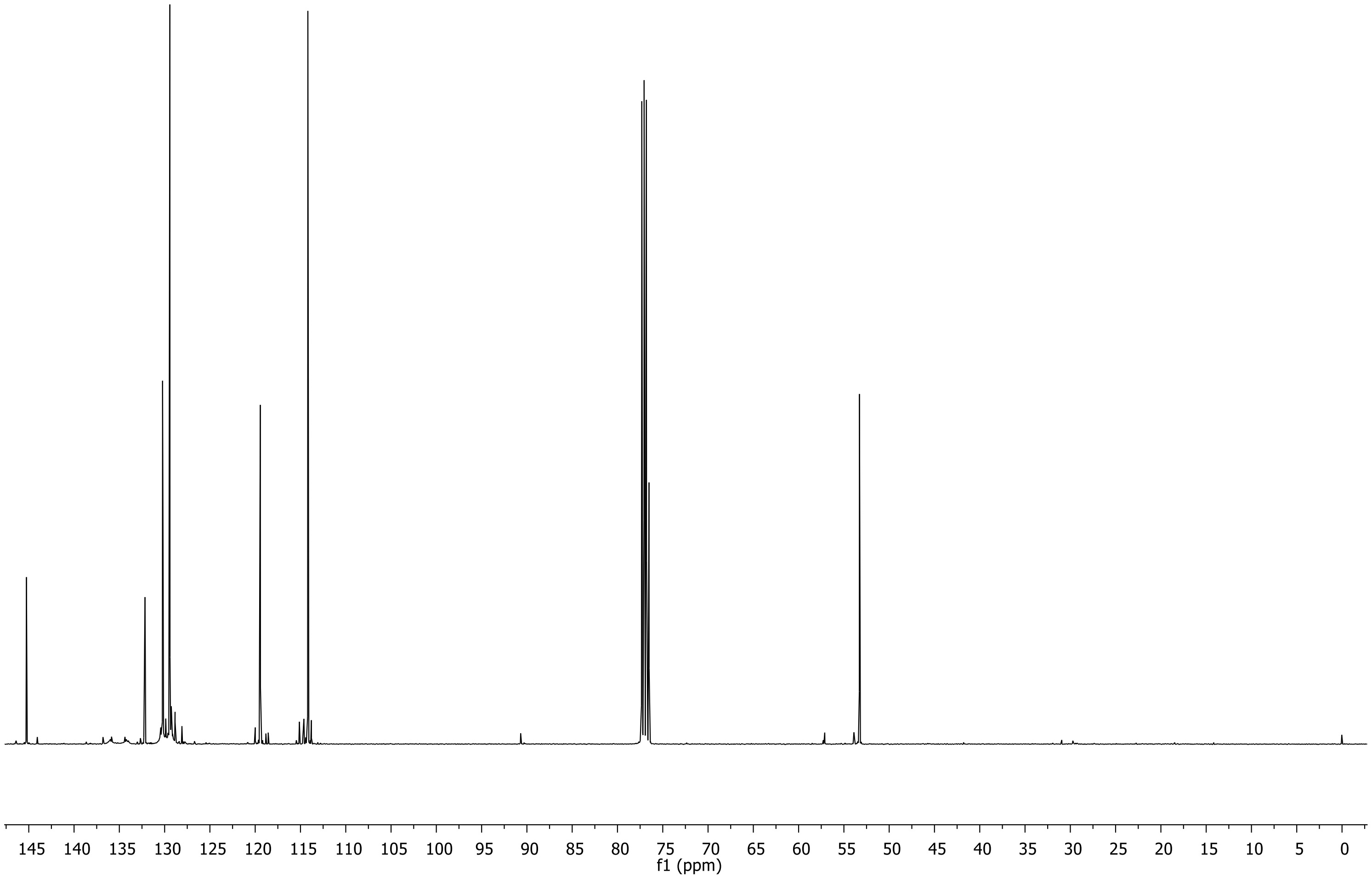

Figure 1.61: $^{13}$C NMR spectrum of **7i** *N*-(1-(2,6-dichlorophenyl)-2-nitroethyl)aniline.

Table 1.9: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **7i** | 310 | 1 | 310.97 | 24 | 93.33 | 22 | ES+ |
| | | 2 | 310.97 | 24 | 250.02 | 12 | ES+ |
| | | 3 | 310.97 | 24 | 136.98 | 44 | ES+ |
| | | 4 | 310.97 | 24 | 124.95 | 34 | ES+ |

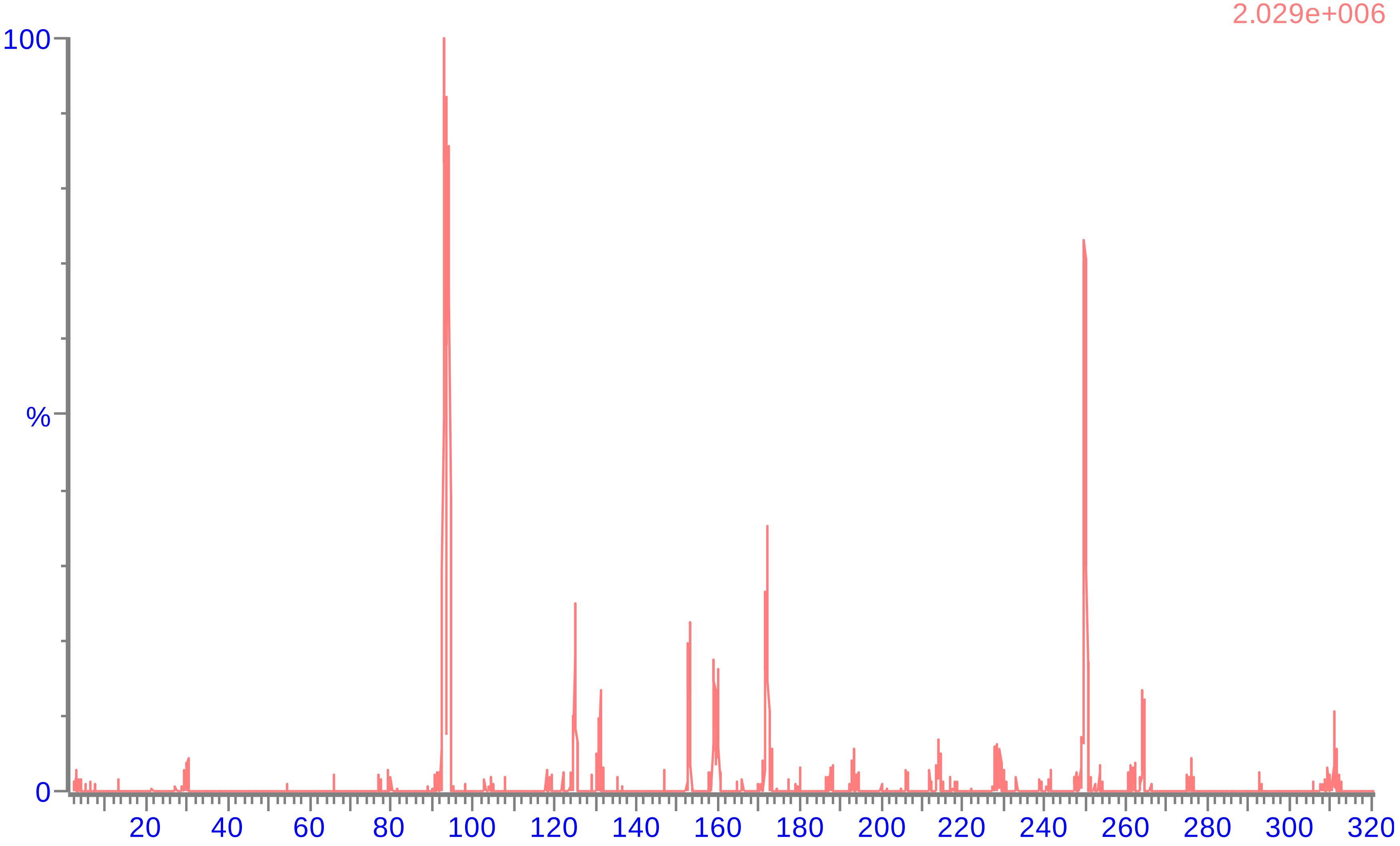

Figure 1.62: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 93.33.

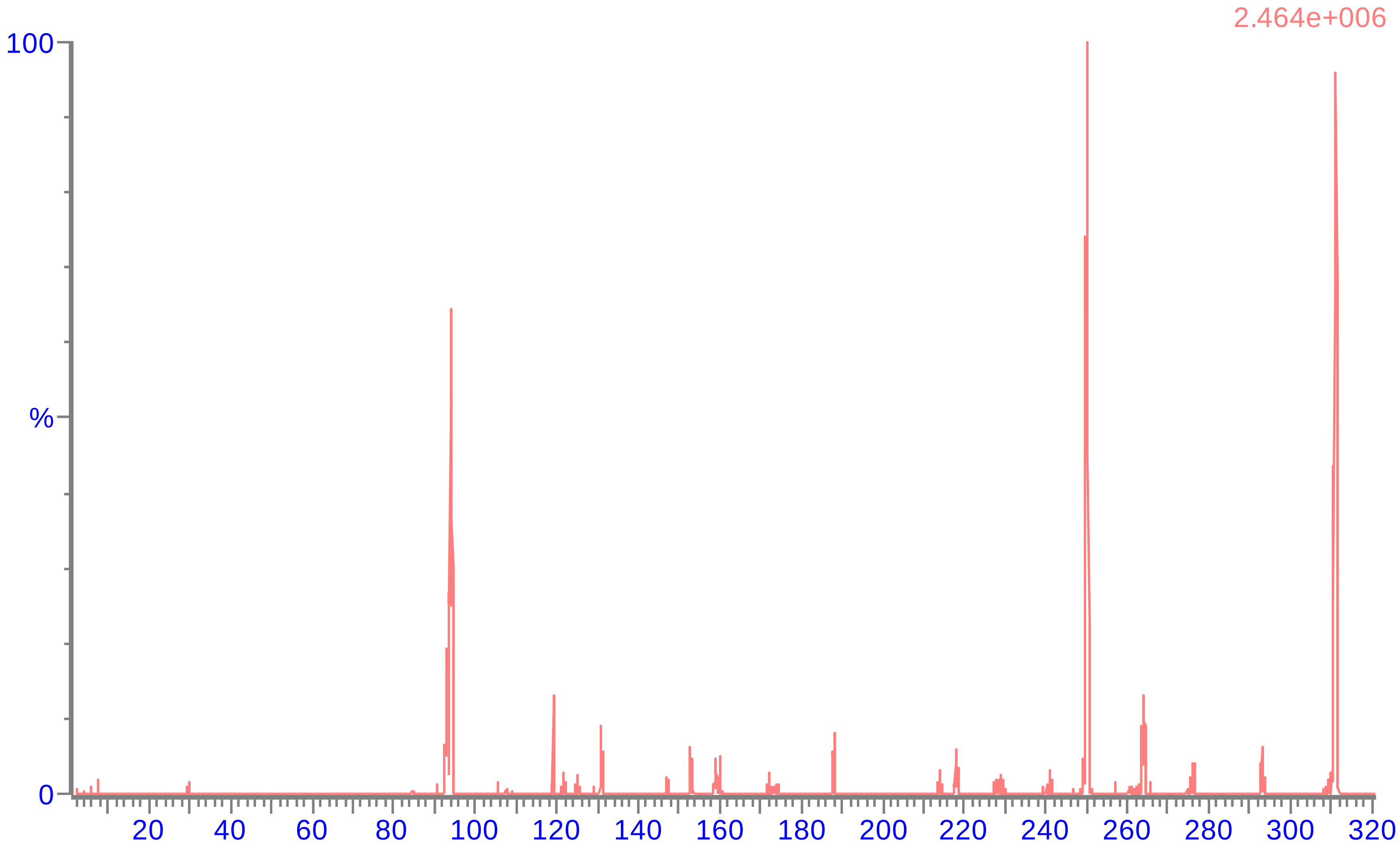

Figure 1.63: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 250.02.

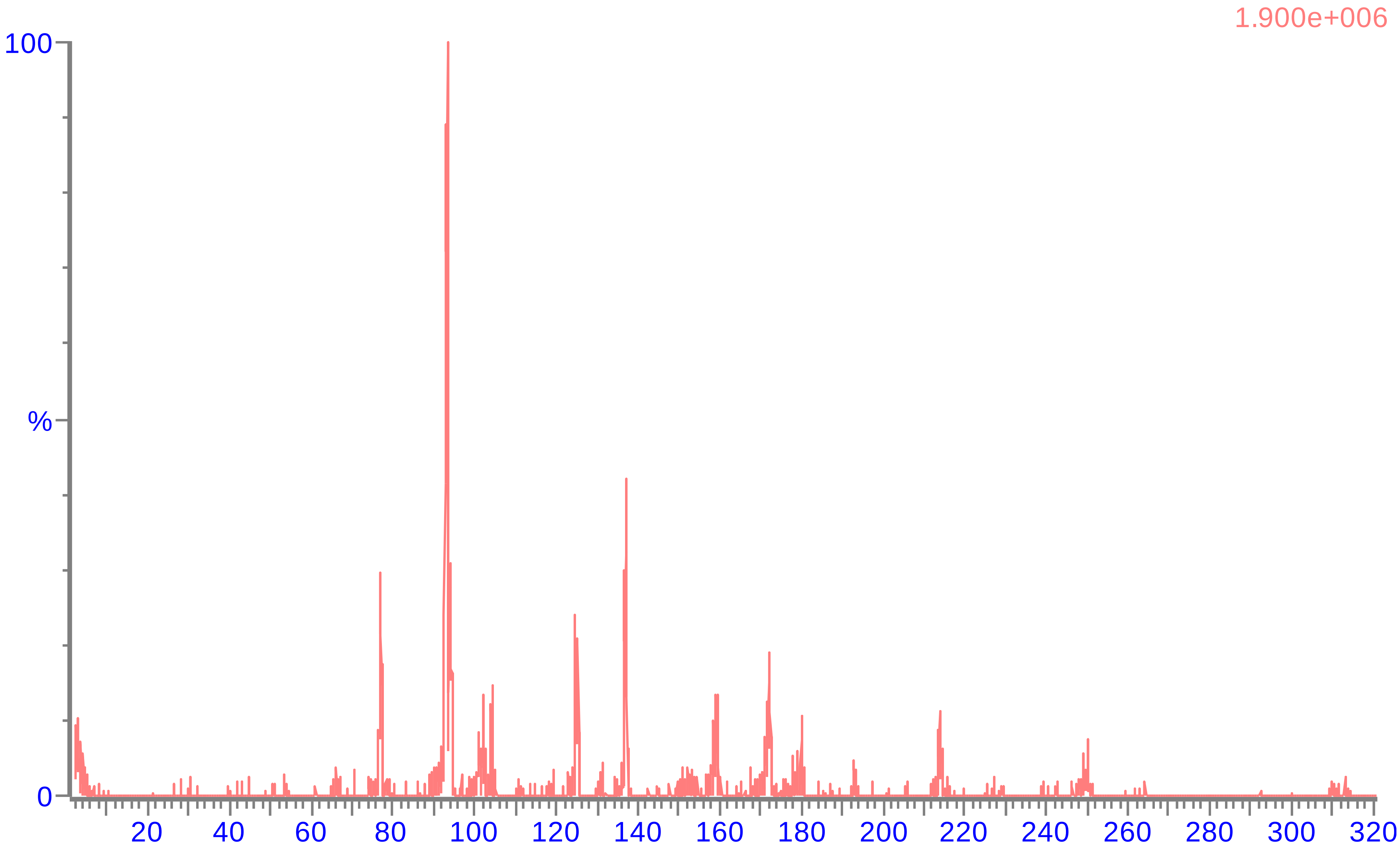

Figure 1.64: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 136.98.

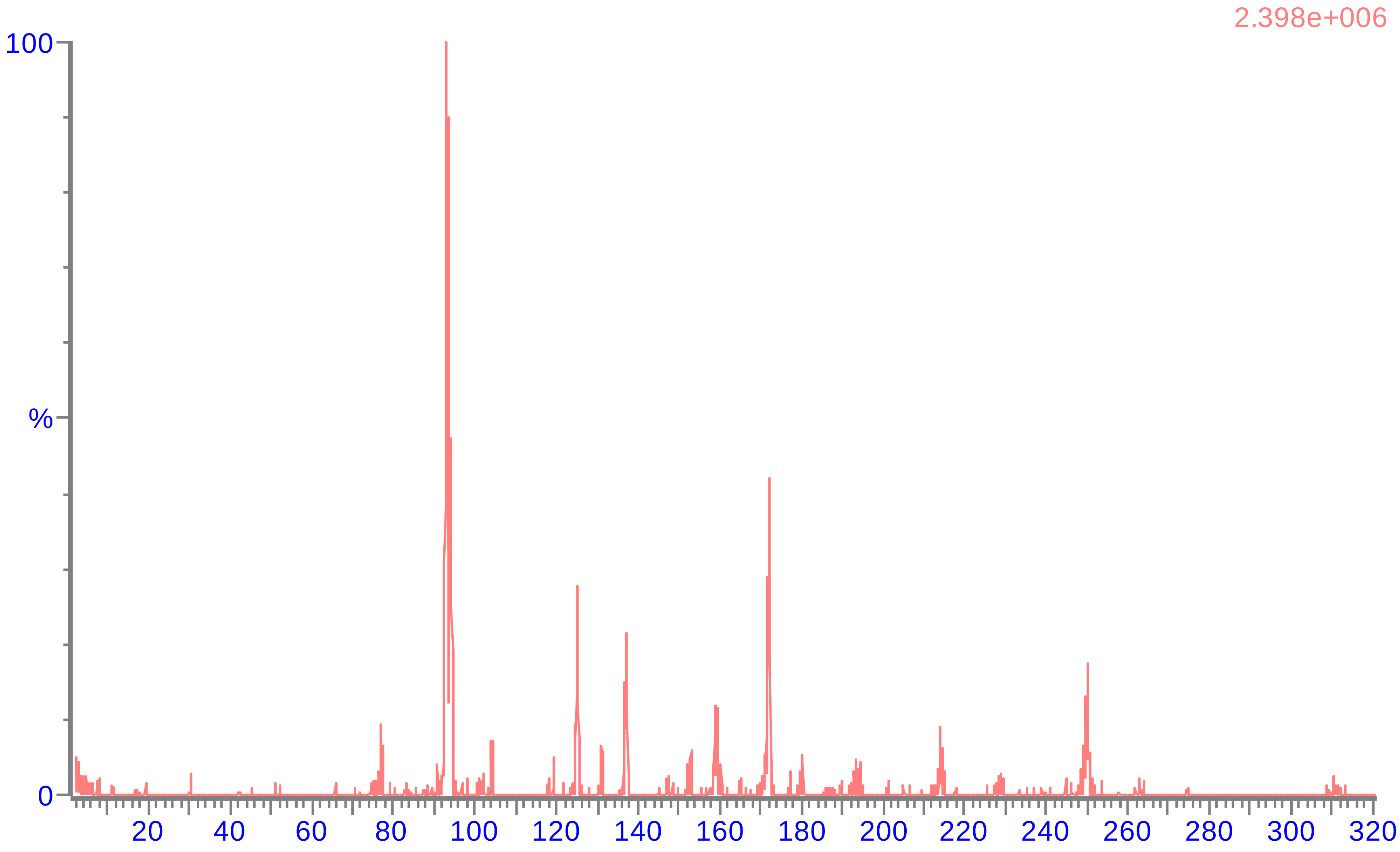

Figure 1.65: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 124.95.

**7j** *N*-(1-(benzo[*d*][1,3]dioxol-5-yl)-2-nitroethyl)aniline

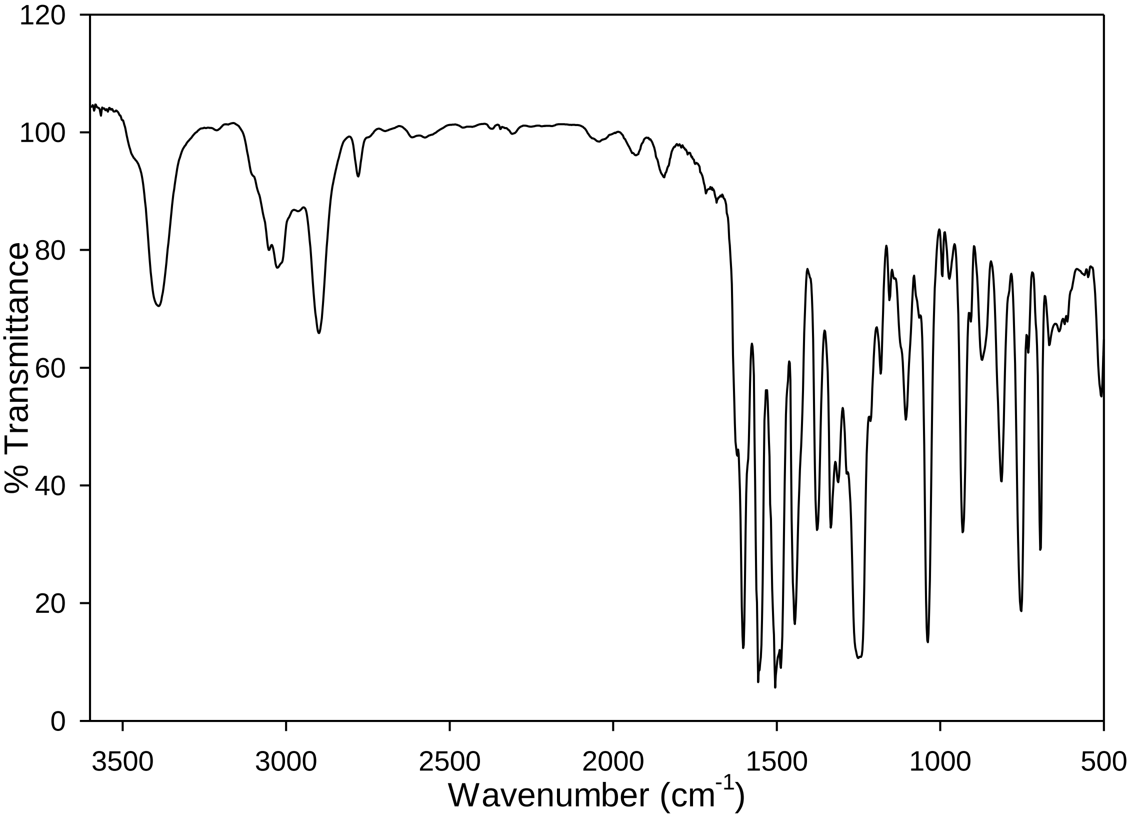

Figure 1.66: IR spectrum of **7j** *N*-(1-(benzo[*d*][1,3]dioxol-5-yl)-2-nitroethyl)aniline.

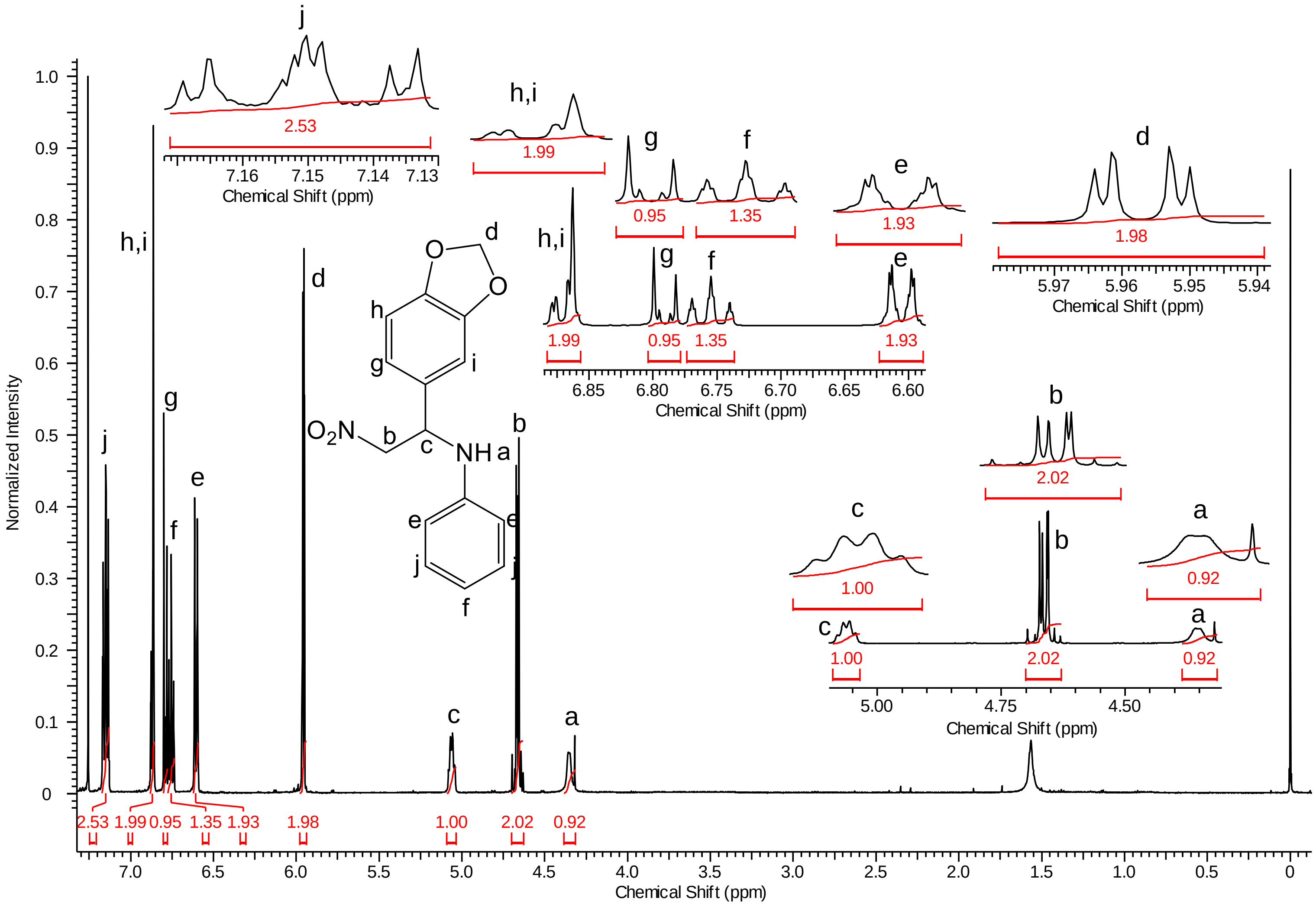

Figure 1.67: $^1$H NMR spectrum of **7j** *N*-(1-(benzo[*d*][1,3]dioxol-5-yl)-2-nitroethyl)aniline.

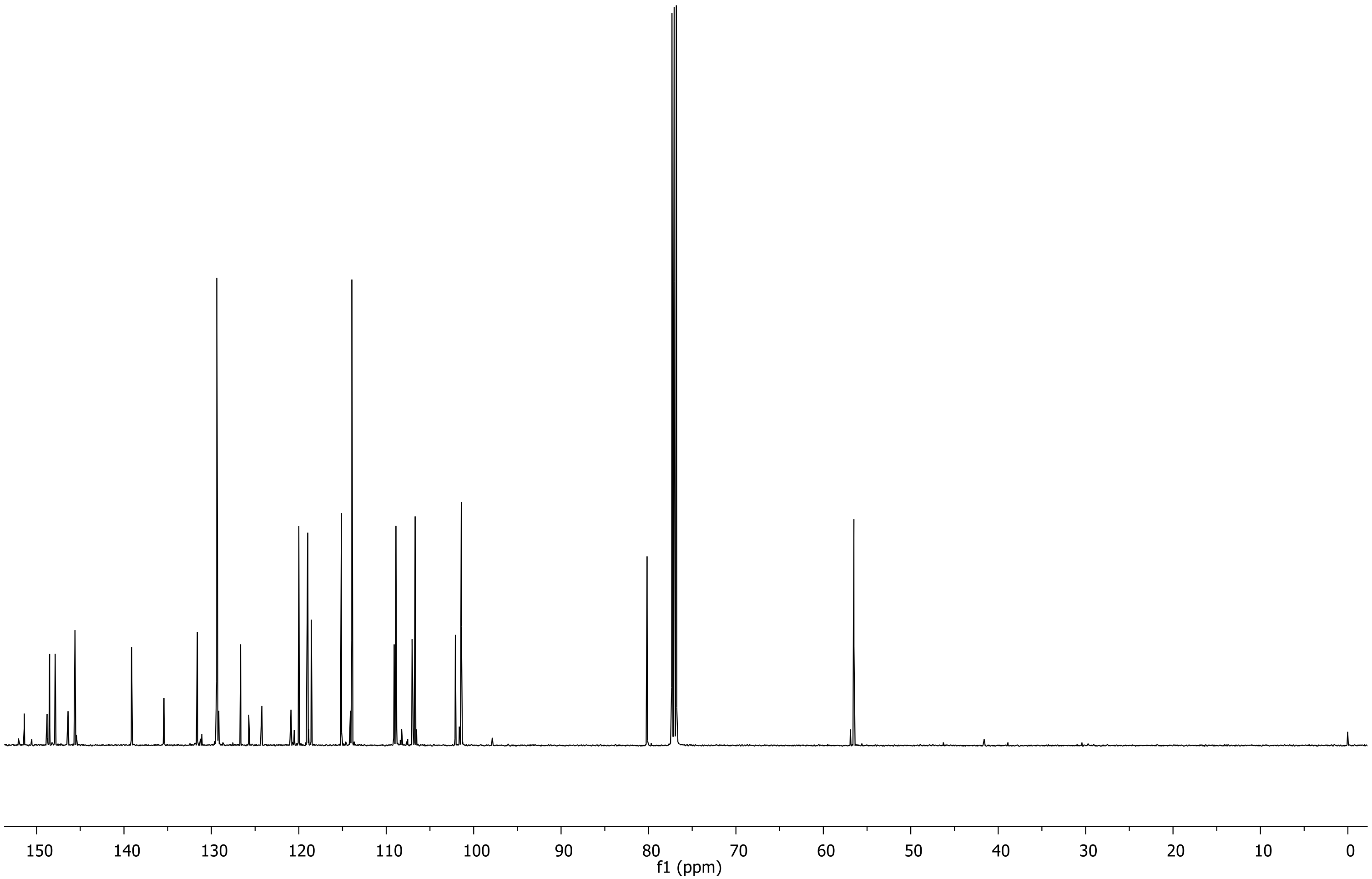

Figure 1.68: $^{13}$C NMR spectrum of **7j** *N*-(1-(benzo[*d*][1,3]dioxol-5-yl)-2-nitroethyl)aniline.

Table 1.10: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **7j** | 286 | 1 | 287.10 | 14 | 148.03 | 14 | ES+ |
| | | 2 | 287.10 | 14 | 94.05 | 6 | ES+ |
| | | 3 | 287.10 | 14 | 194.02 | 8 | ES+ |
| | | 4 | 287.10 | 14 | 91.64 | 64 | ES+ |
| | | 5 | 287.10 | 14 | 90.99 | 56 | ES+ |

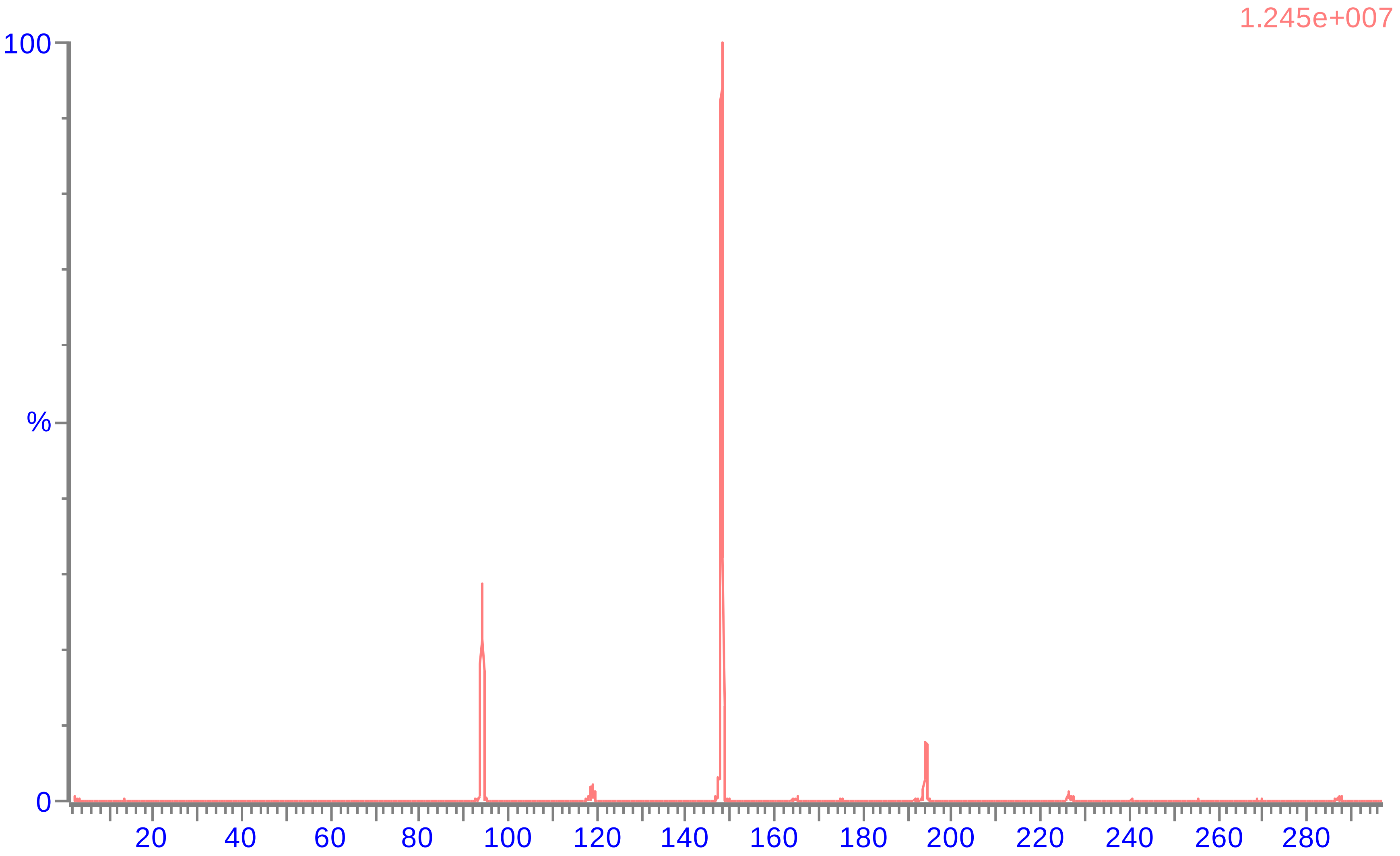

Figure 1.69: Mass spectrum for daughter fragment peak ES+, m/z 287.10 -> 148.03.

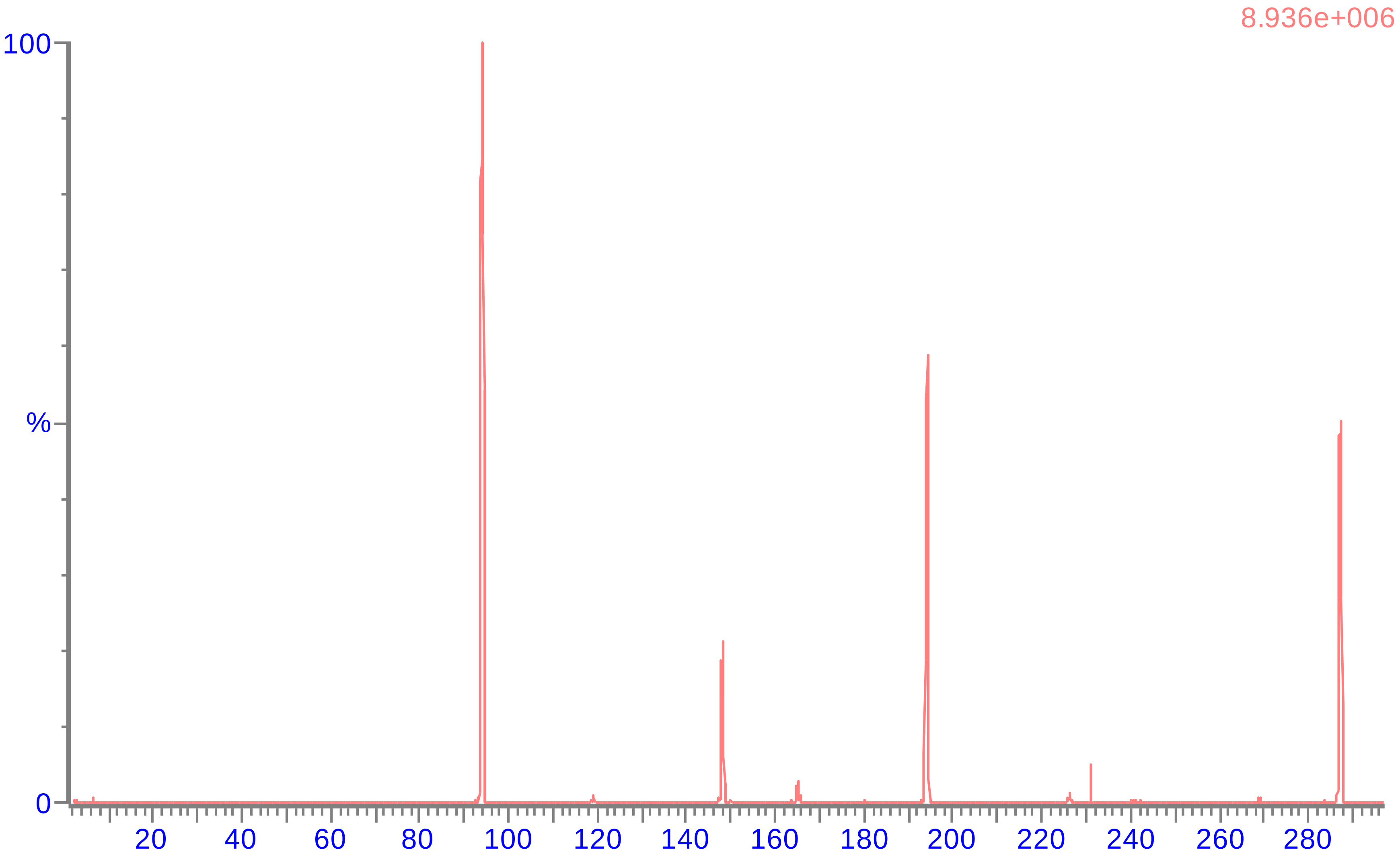

Figure18.70: Mass spectrum for daughter fragment peak ES+, m/z 287.10 -> 94.05.

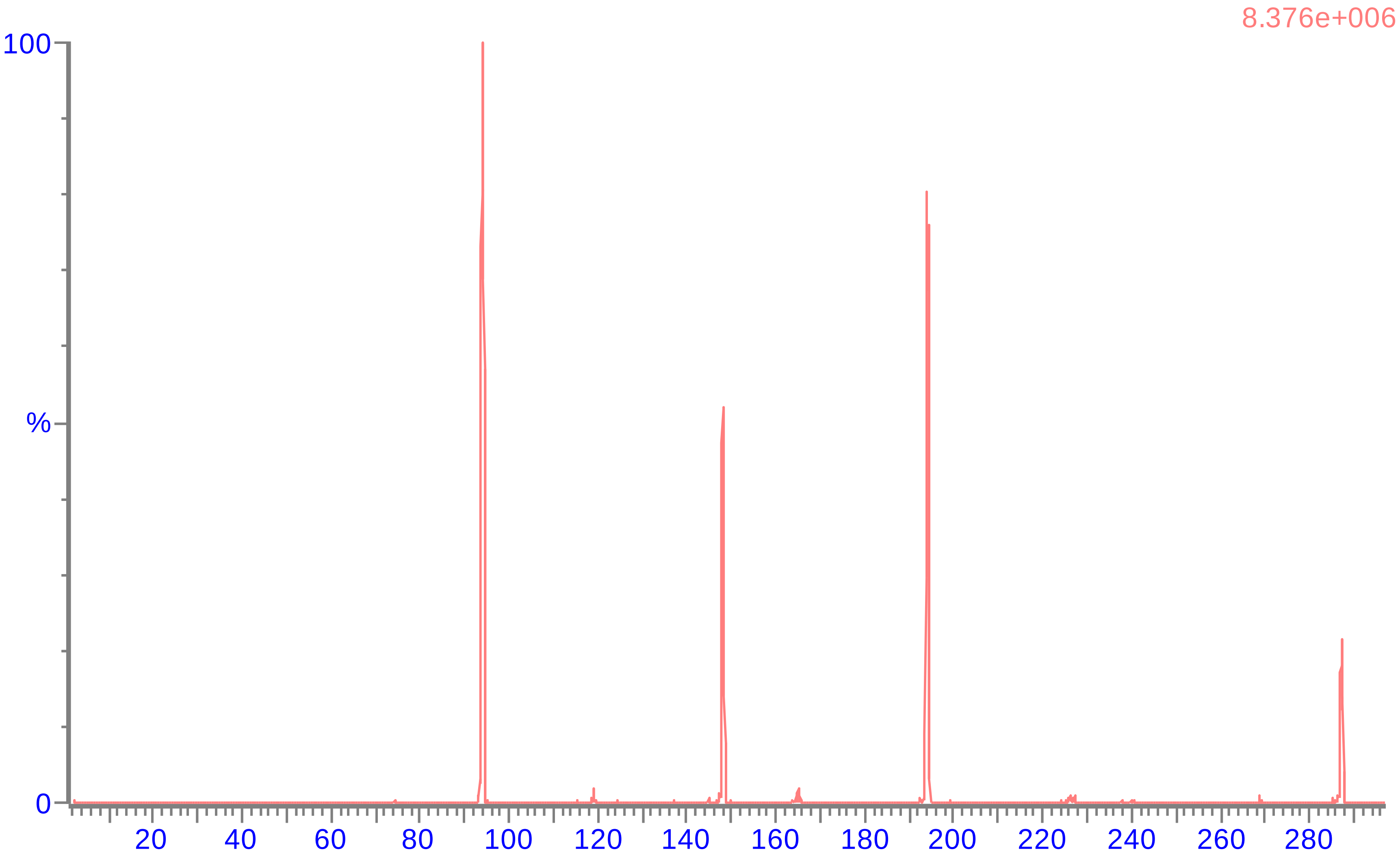

Figure 1.71: Mass spectrum for daughter fragment peak ES+, m/z 287.10 -> 194.02.

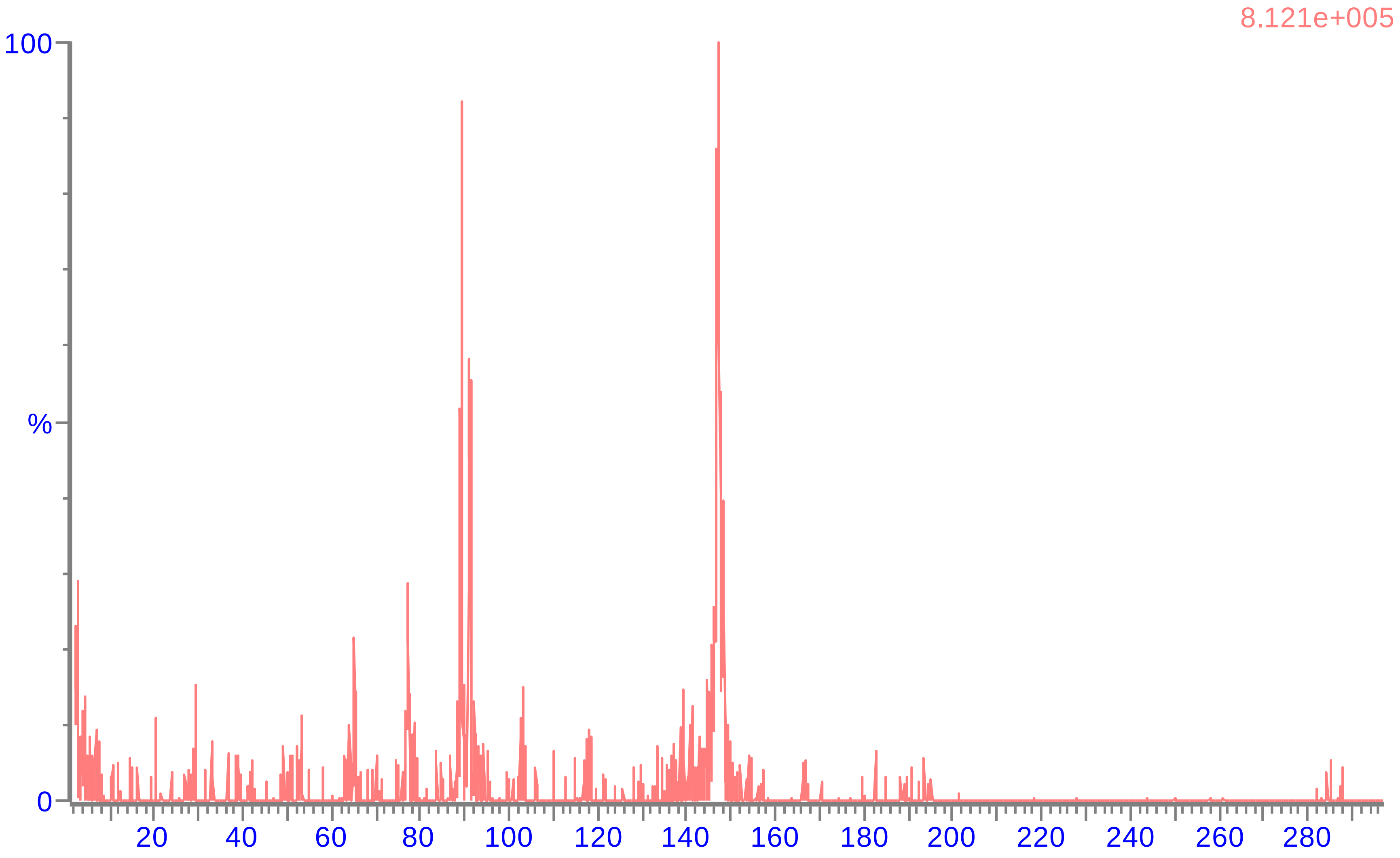

Figure1.72: Mass spectrum for daughter fragment peak ES+, m/z 287.10 -> 91.64.

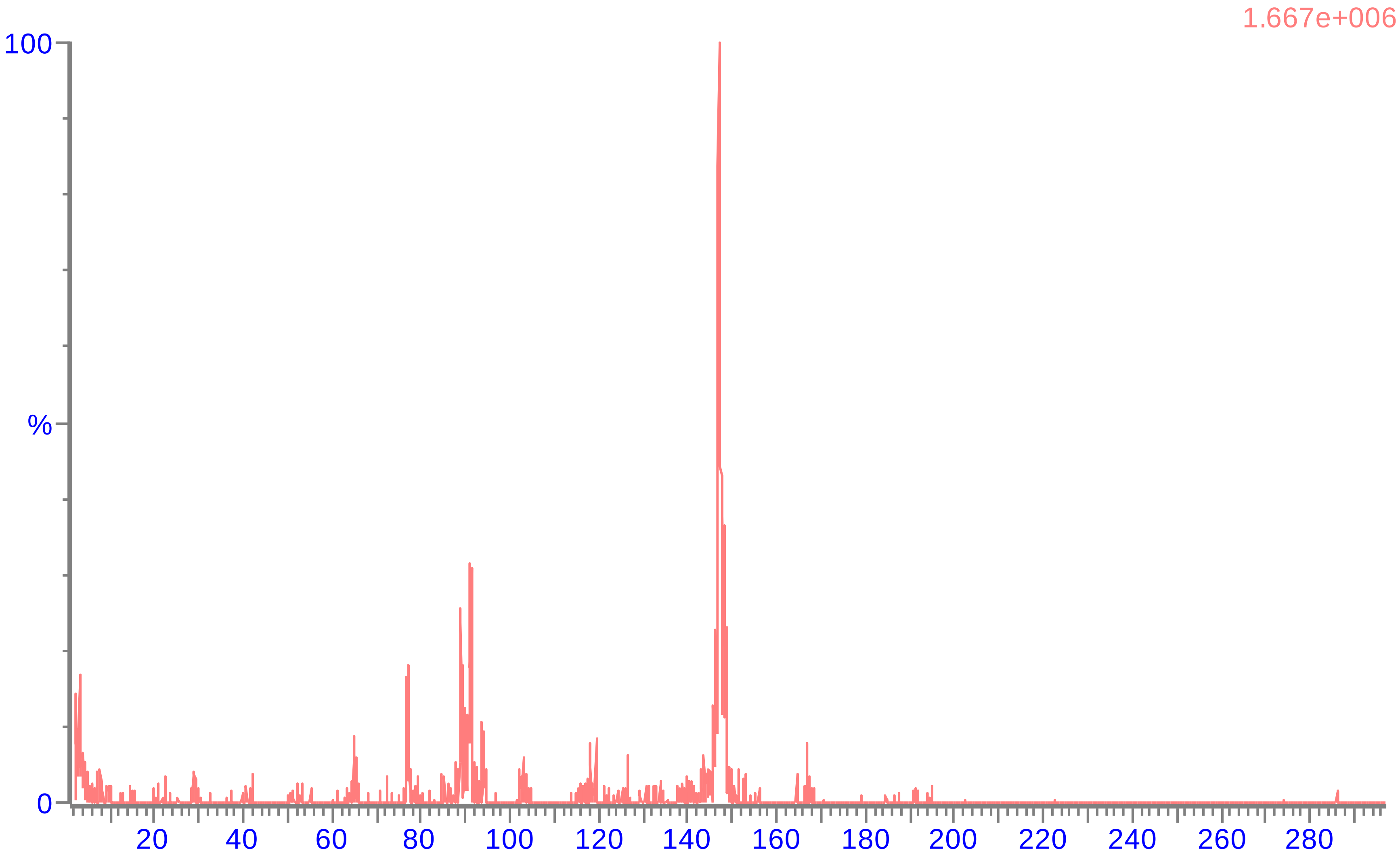

Figure 1.73: Mass spectrum for daughter fragment peak ES+, m/z 287.10 -> 90.99.

**7k** *N*-(1-nitropentan-2-yl)aniline.

Table 1.11: MS data.

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **7k** | 208 | 1 | 209.10 | 26 | 148.11 | 12 | ES+ |
| | | 2 | 209.10 | 26 | 106.02 | 28 | ES+ |
| | | 3 | 209.10 | 26 | 93.08 | 32 | ES+ |
| | | 4 | 209.10 | 26 | 118.25 | 36 | ES+ |
| | | 5 | 209.10 | 26 | 40.98 | 28 | ES+ |

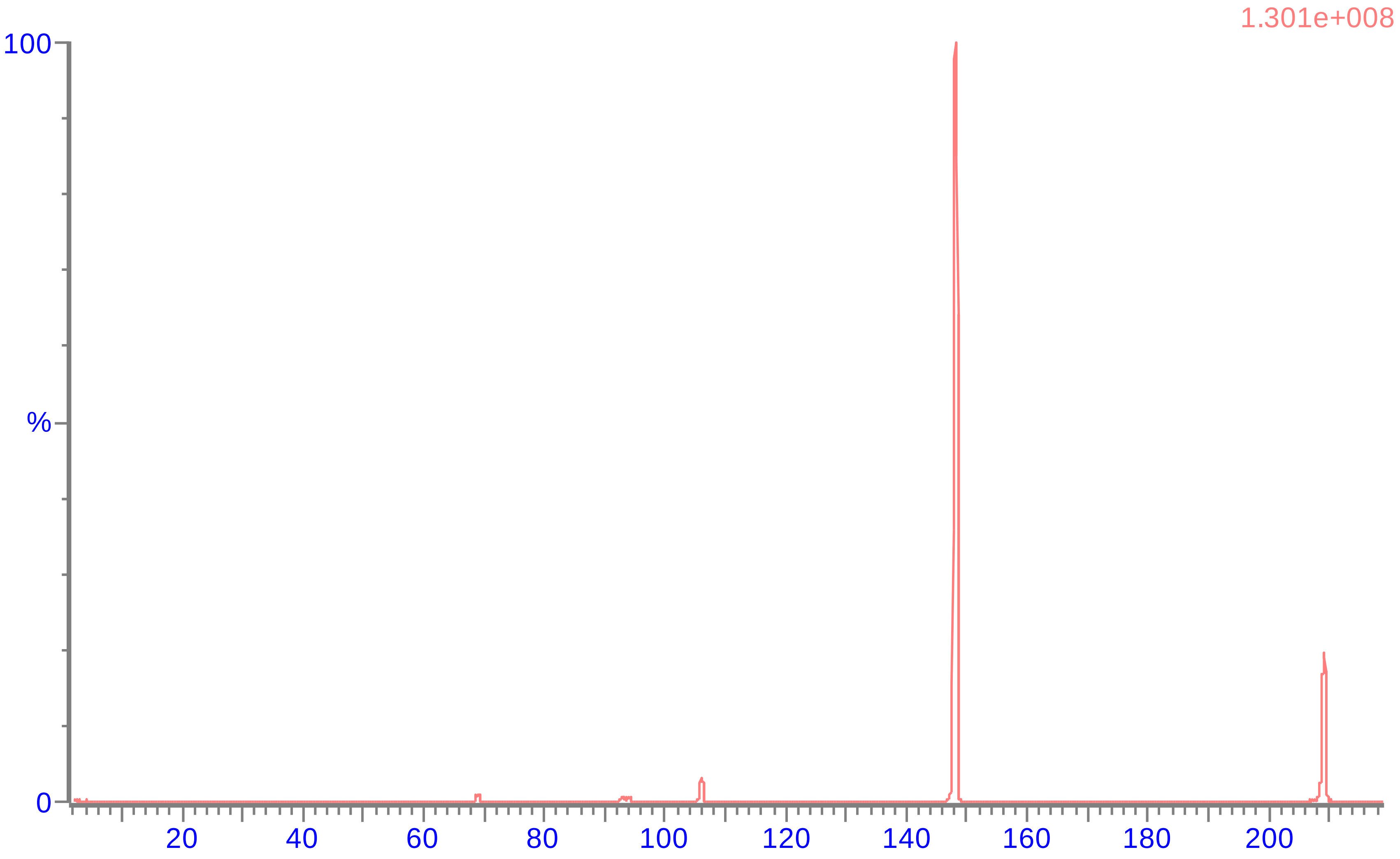

Figure 1.74: Mass spectrum for daughter fragment peak ES+, m/z 209.10 -> 148.11.

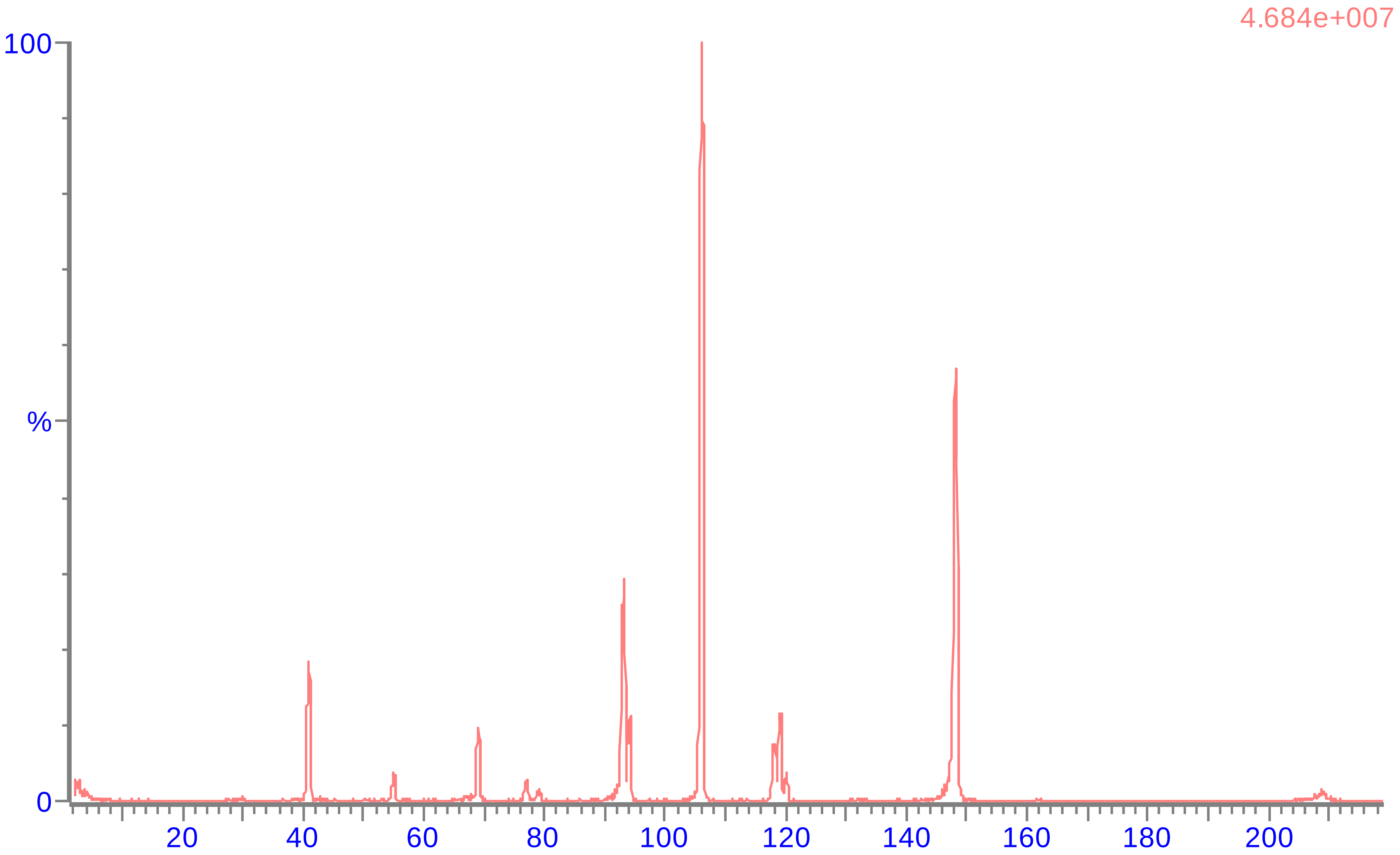

Figure 1.75: Mass spectrum for daughter fragment peak ES+, m/z 209.10 -> 106.02.

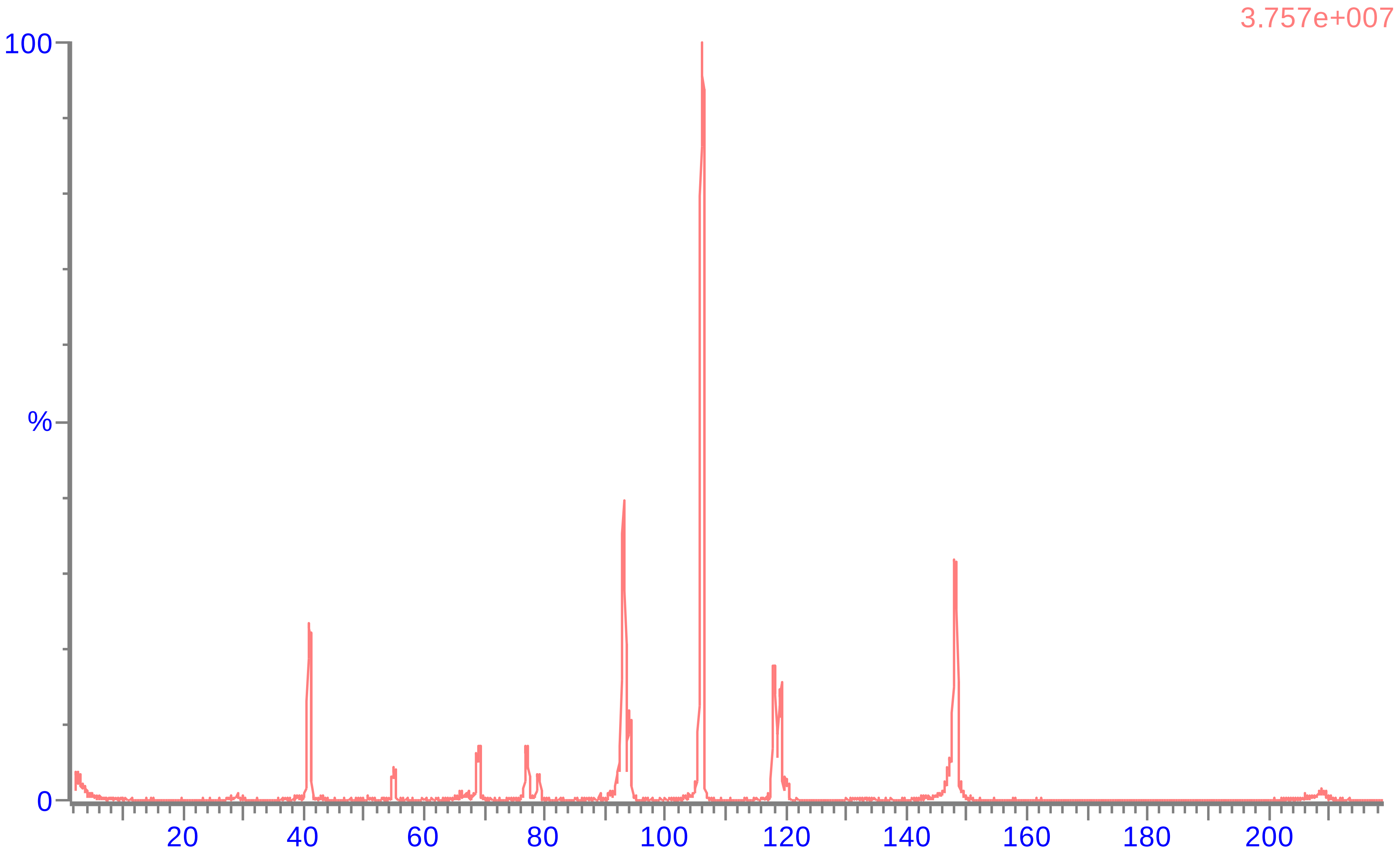

Figure 1.76: Mass spectrum for daughter fragment peak ES+, m/z 209.10 -> 93.08.

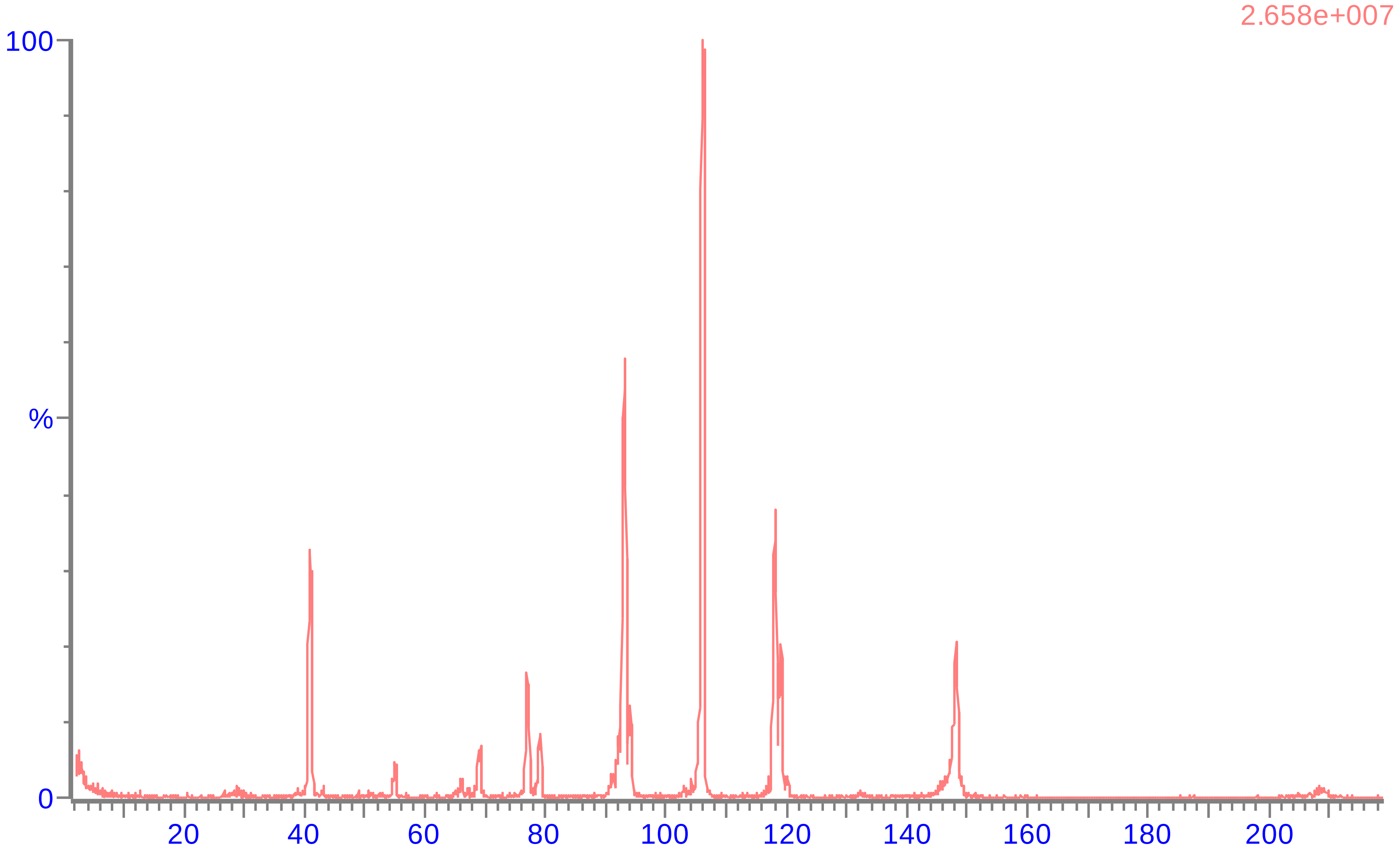

Figure 1.77: Mass spectrum for daughter fragment peak ES+, m/z 209.10 -> 118.25.

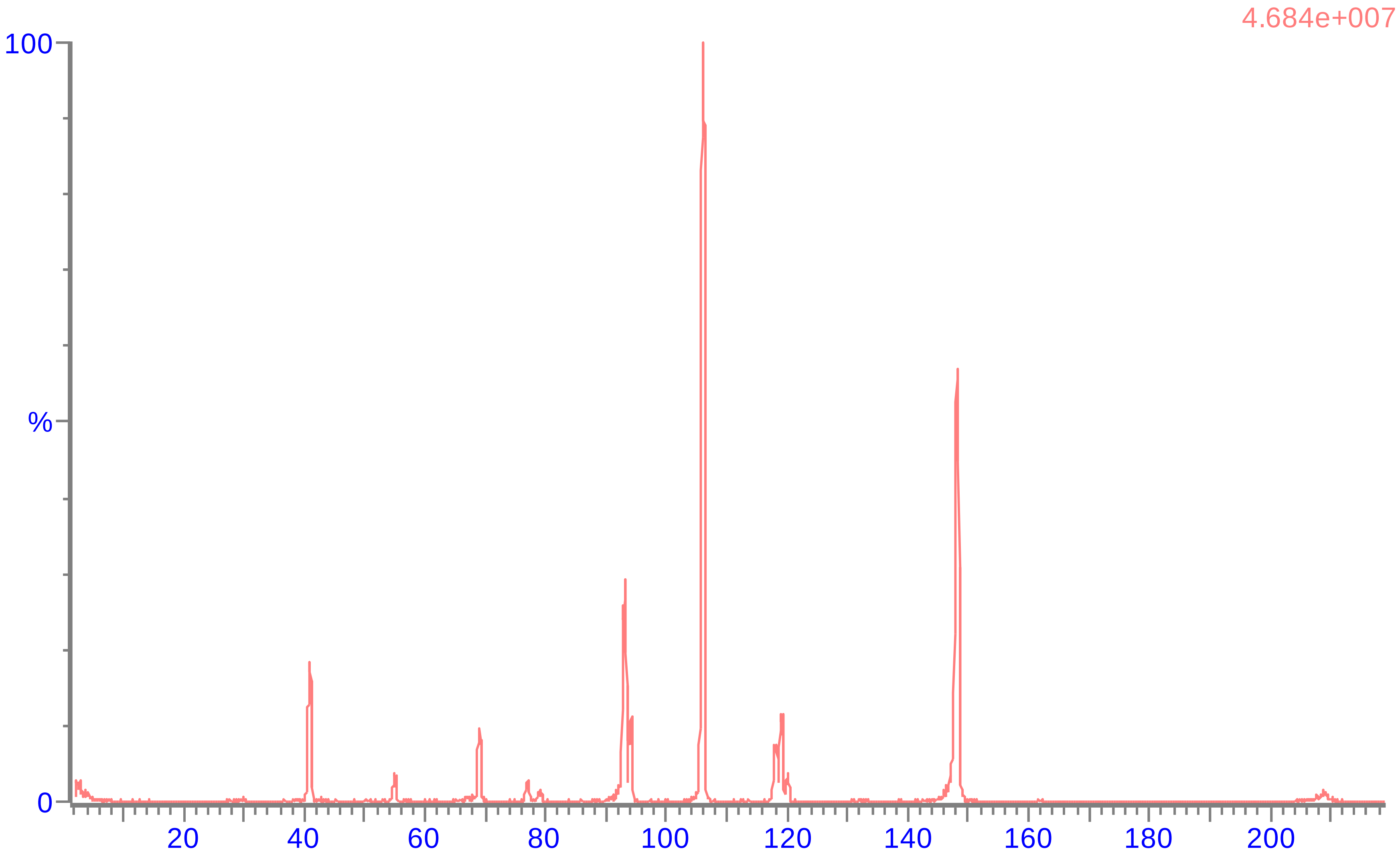

Figure 1.78: Mass spectrum for daughter fragment peak ES+, m/z 209.10 -> 40.98.

**7l** *N*-(1-cyclohexyl-2-nitroethyl)aniline

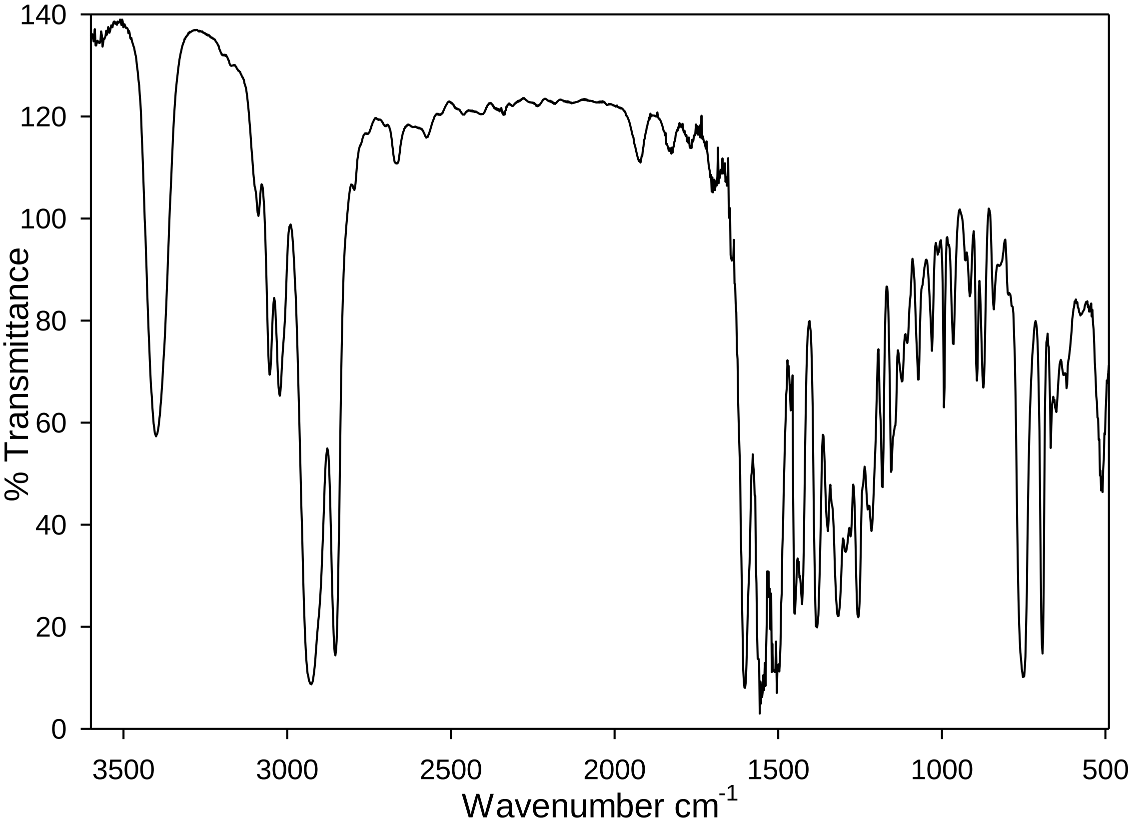

Figure 1.79: IR spectrum of **7l** *N*-(1-cyclohexyl-2-nitroethyl)aniline.

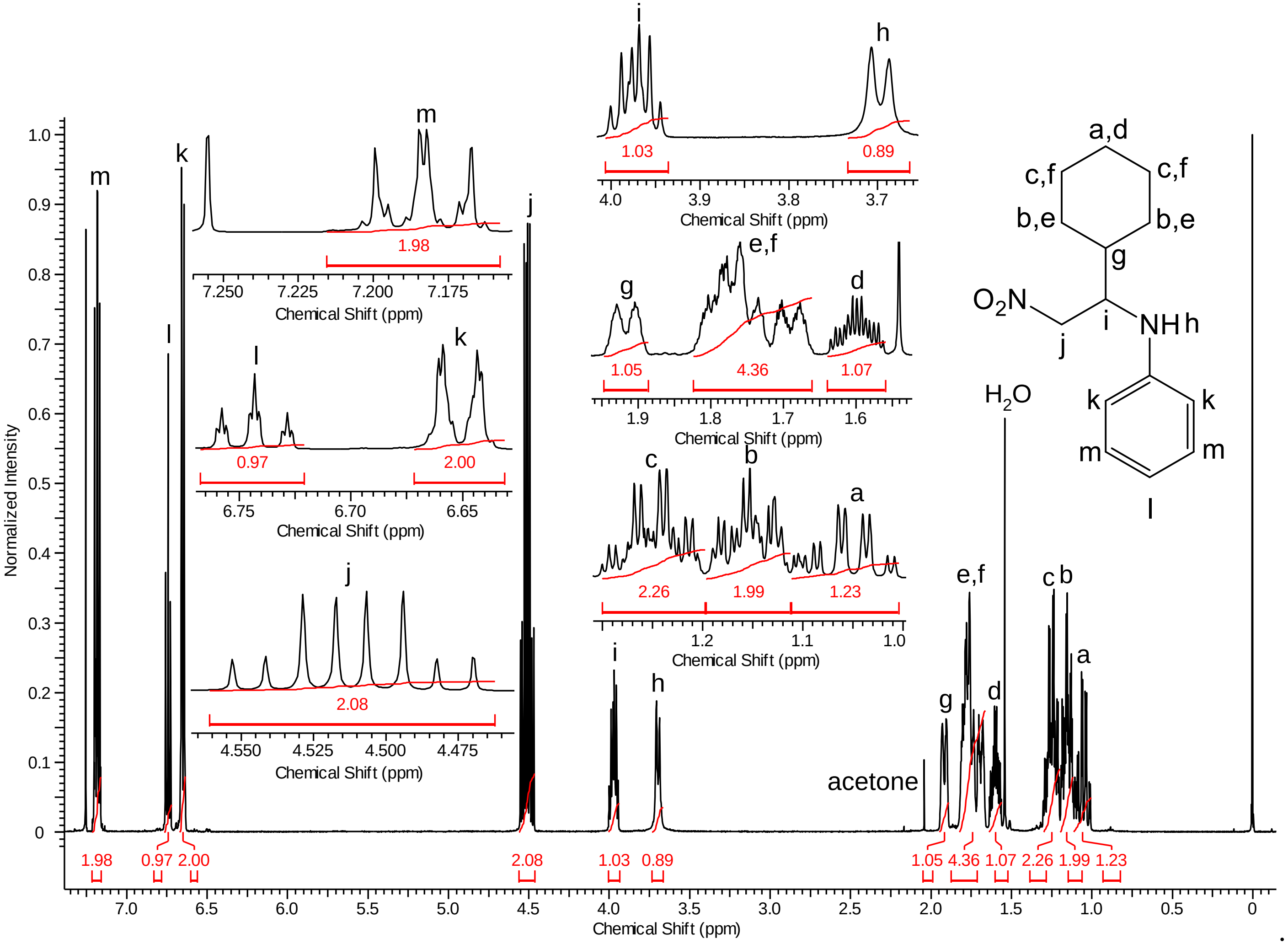

Figure 1.80: $^1$H NMR spectrum of **7l** *N*-(1-cyclohexyl-2-nitroethyl)aniline.

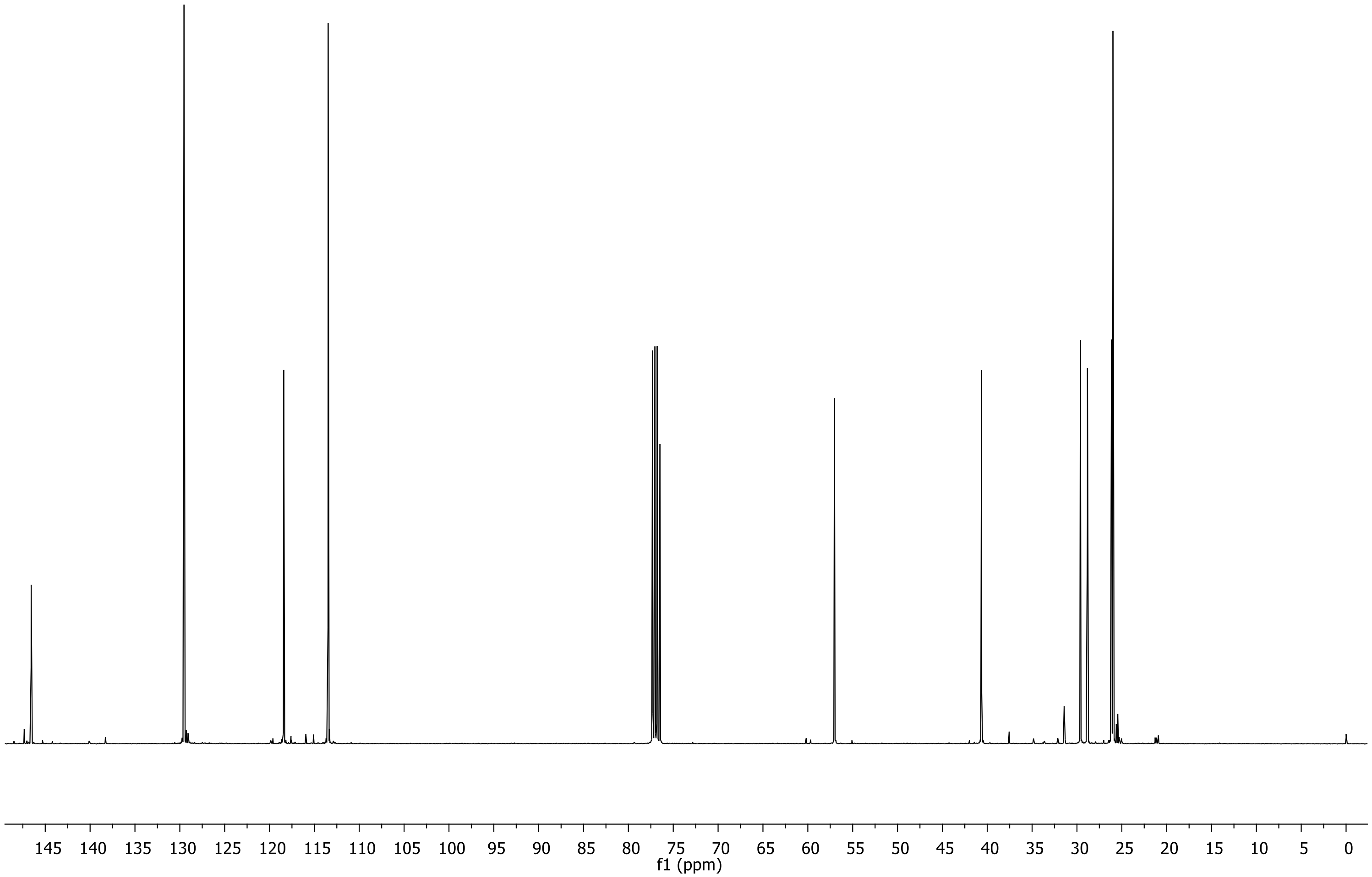

Figure 1.81: $^{13}$C NMR spectrum of **7l** *N*-(1-cyclohexyl-2-nitroethyl)aniline.

Table 1.12: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **7l** | 248.3 | 1 | 249.14 | 14 | 188.17 | 18 | ES+ |
| | | 2 | 249.14 | 14 | 106.02 | 28 | ES+ |
| | | 3 | 249.14 | 14 | 67.06 | 34 | ES+ |
| | | 4 | 249.14 | 14 | 94.71 | 28 | ES+ |
| | | 5 | 249.14 | 14 | 109.08 | 20 | ES+ |

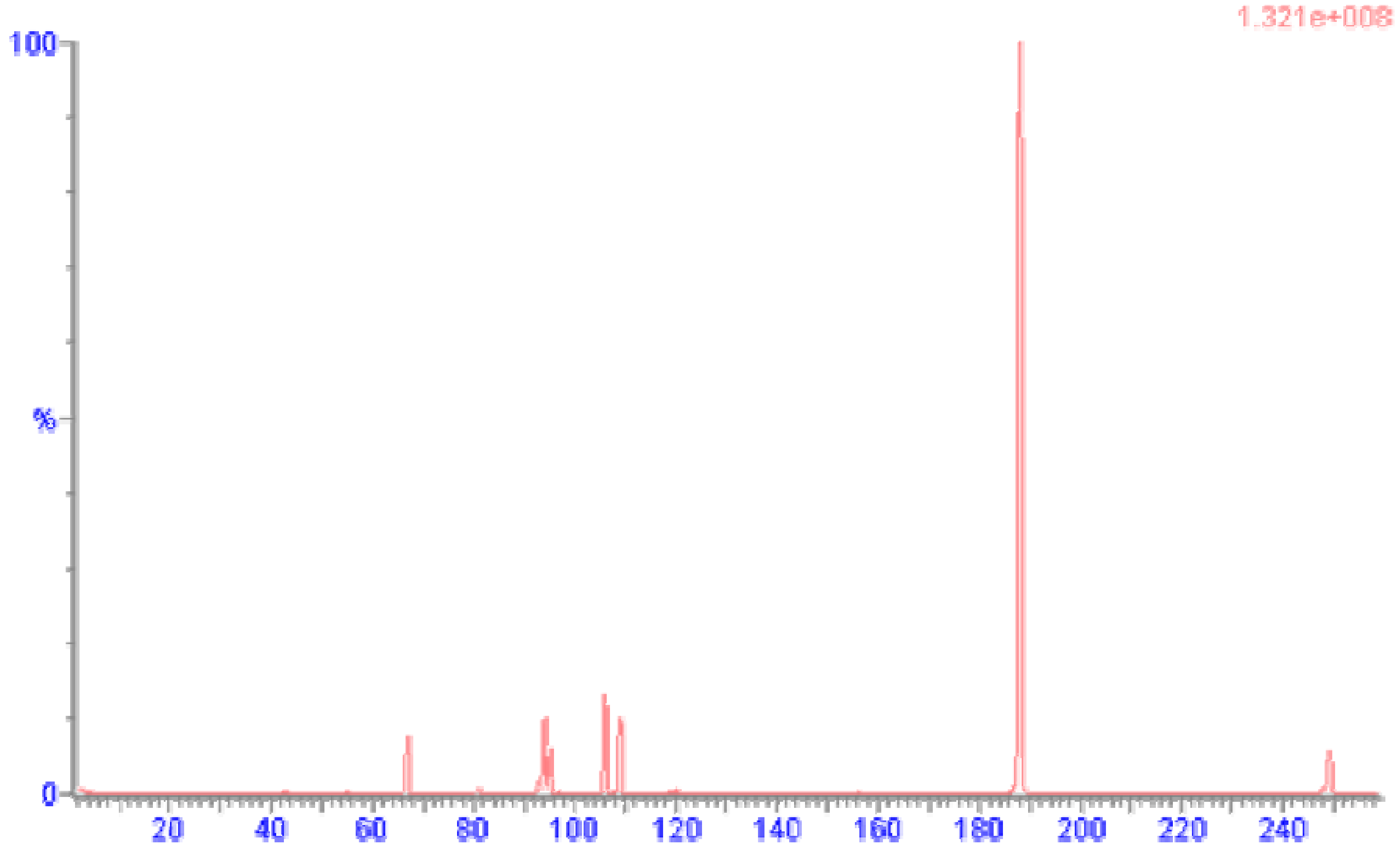

Figure 1.82: Mass spectrum for daughter fragment peak ES+, m/z 249.14 -> 188.17.

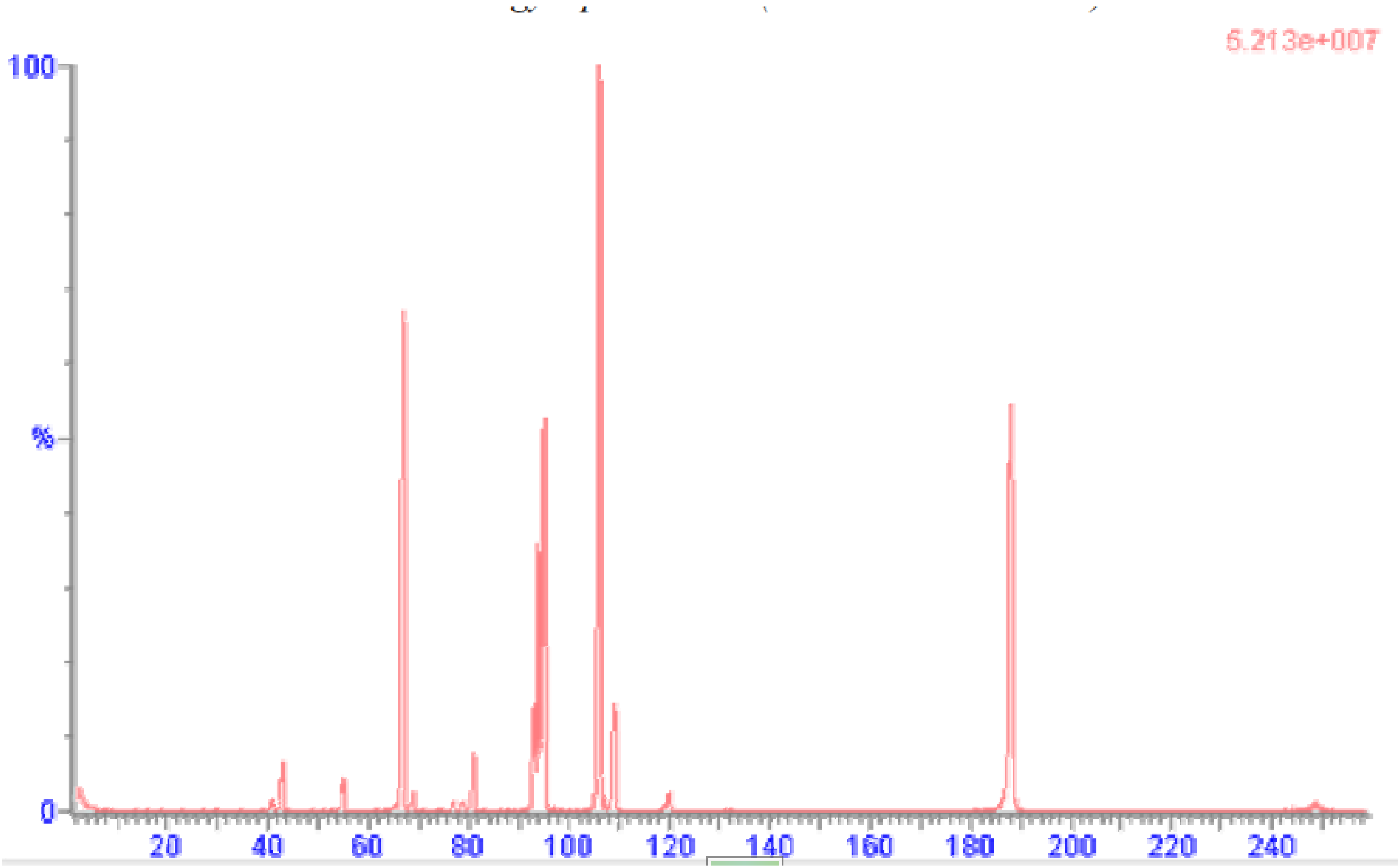

Figure 1.83: Mass spectrum for daughter fragment peak ES+, m/z 249.14 -> 106.02.

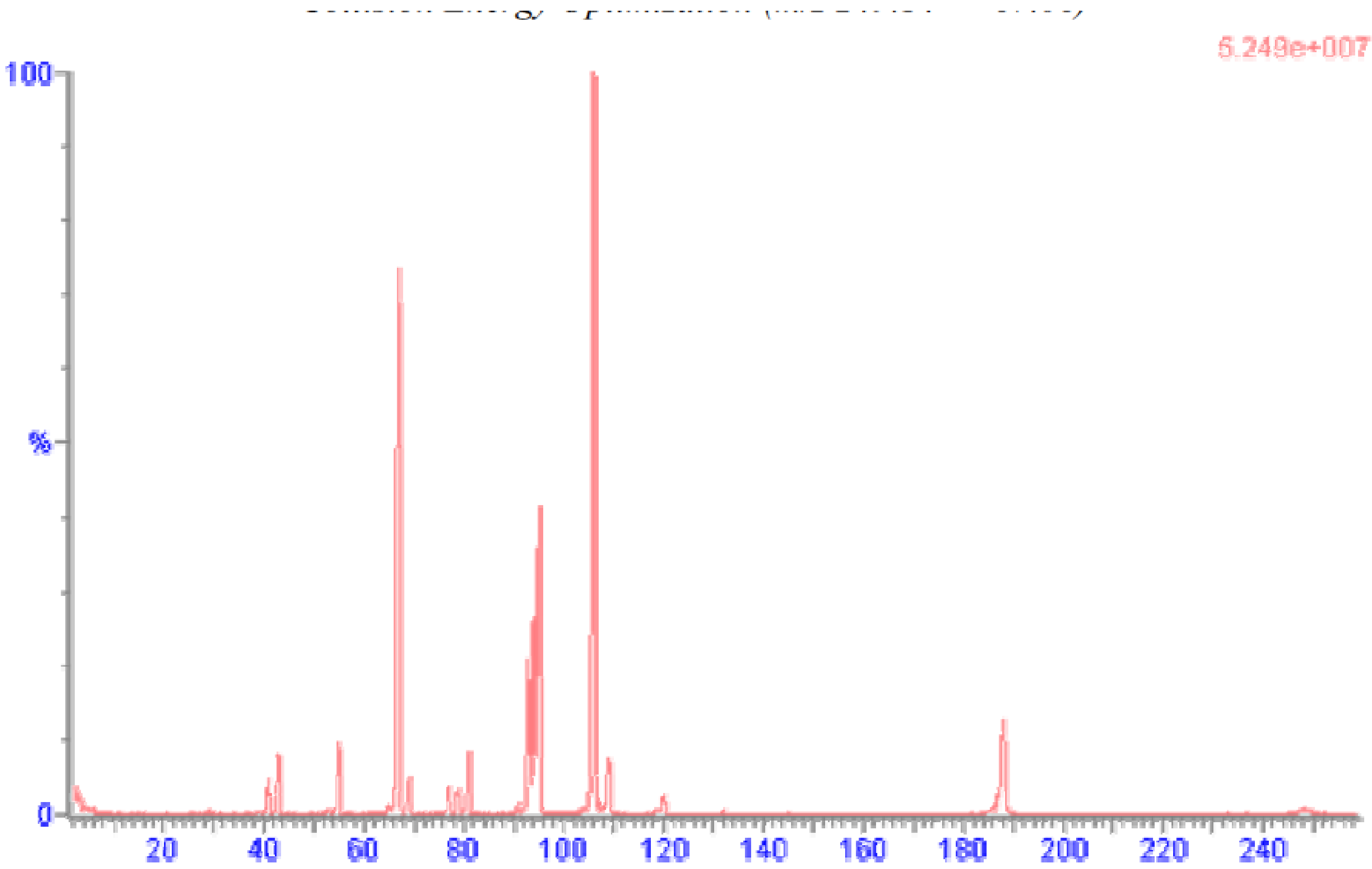

Figure 1.84: Mass spectrum for daughter fragment peak ES+, m/z 249.14 -> 67.06.

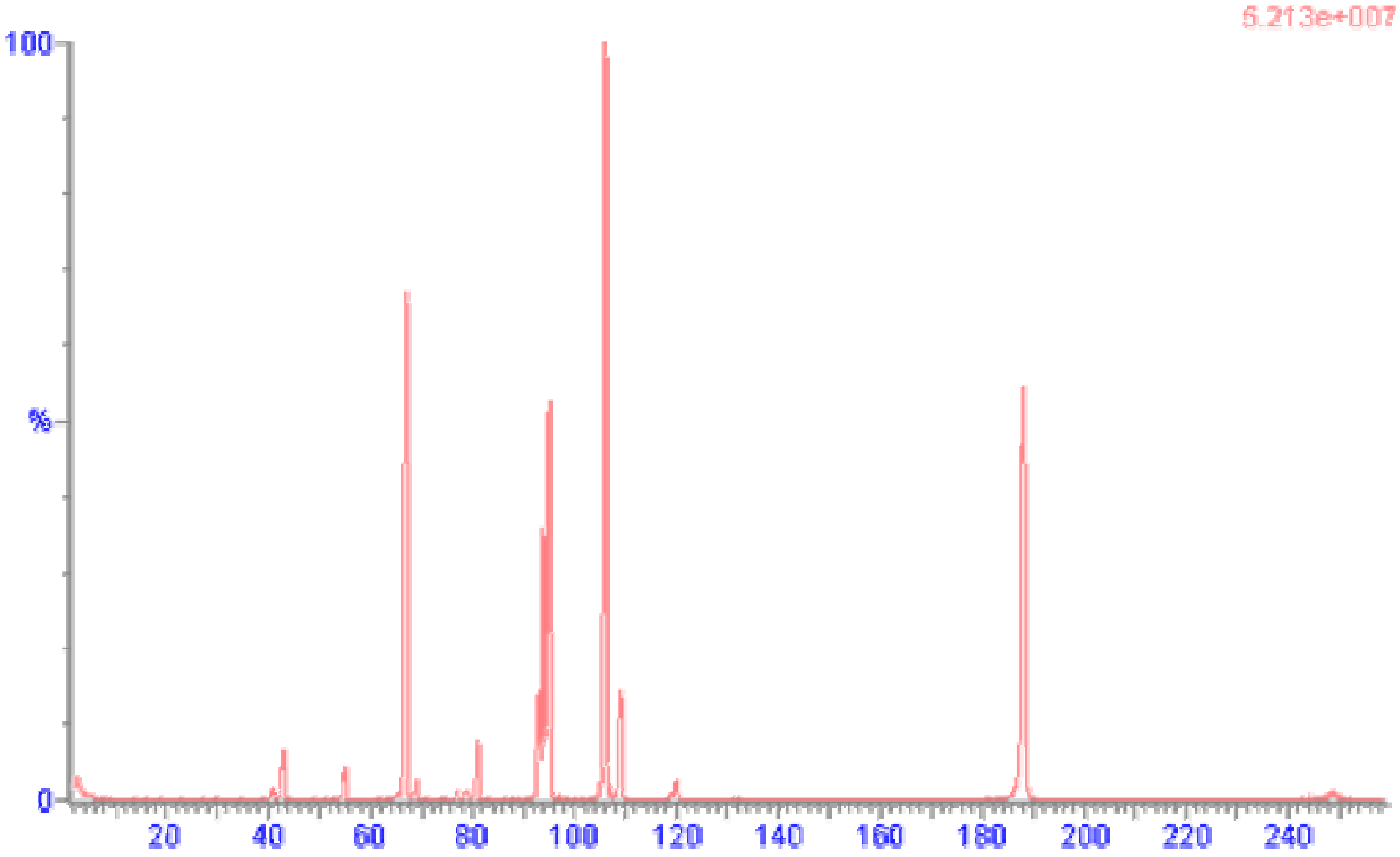

Figure 1.85: Mass spectrum for daughter fragment peak ES+, m/z 249.14 -> 94.71.

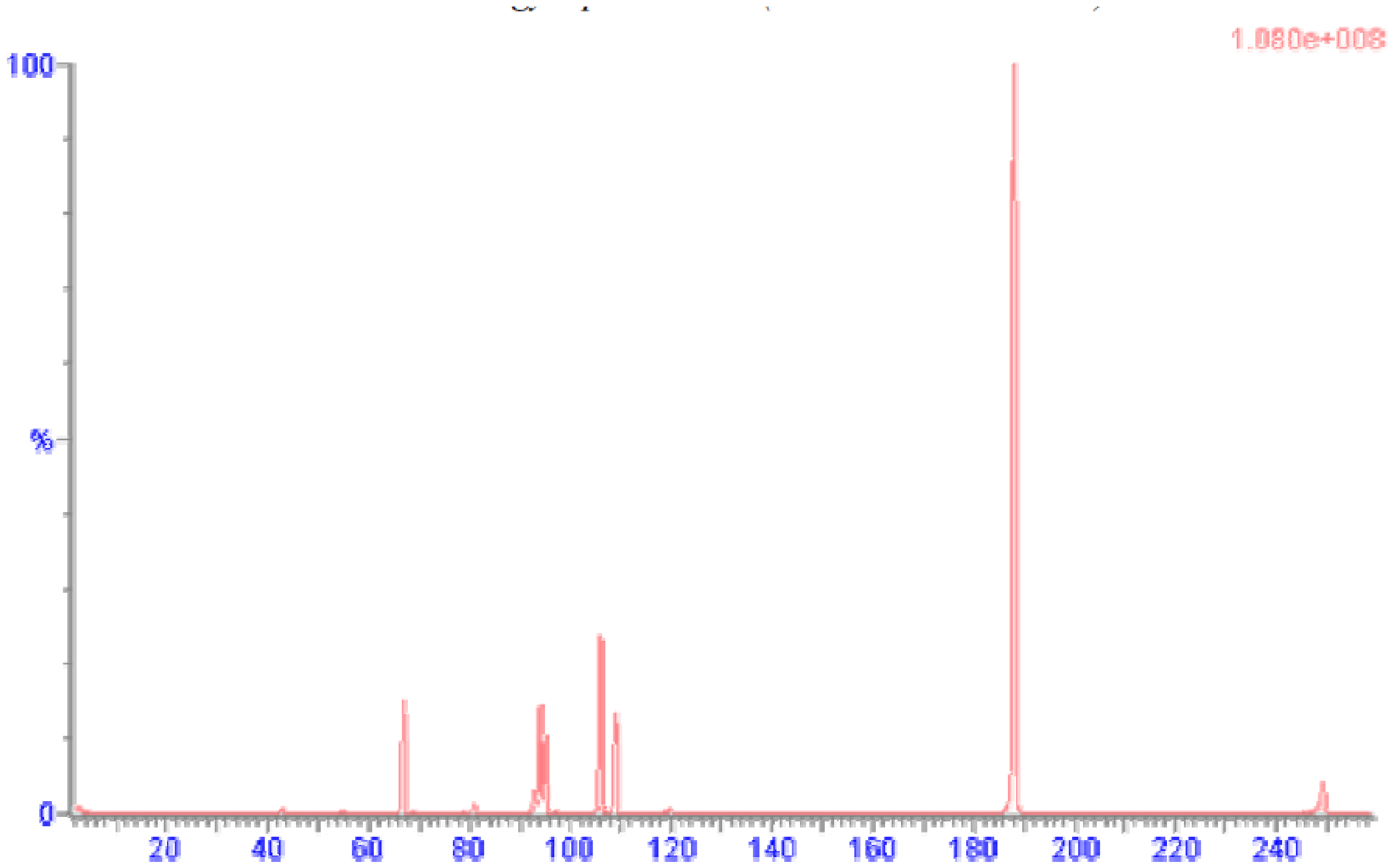

Figure 1.86: Mass spectrum for daughter fragment peak ES+, m/z 249.14 -> 109.08.

**7m** ethyl 3-nitro-2-(phenylamino)propanoate

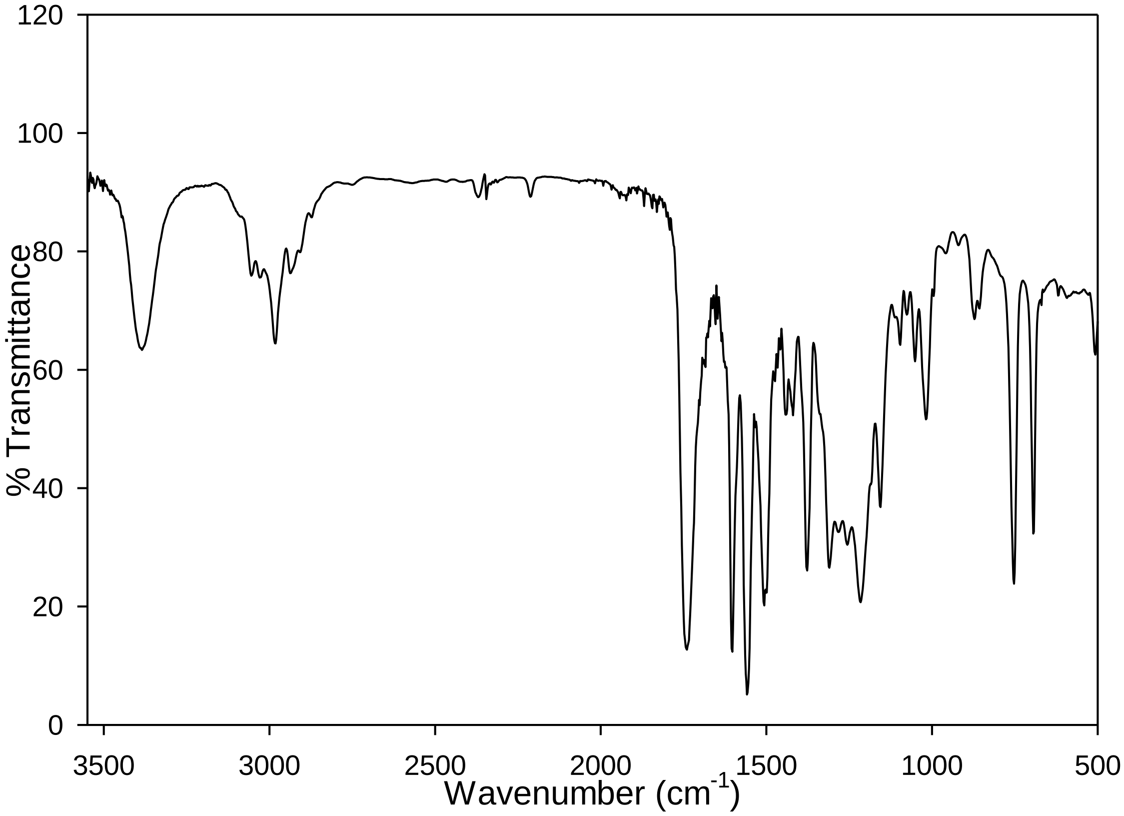

Figure 1.87: IR spectrum of **7m** ethyl 3-nitro-2-(phenylamino)propanoate.

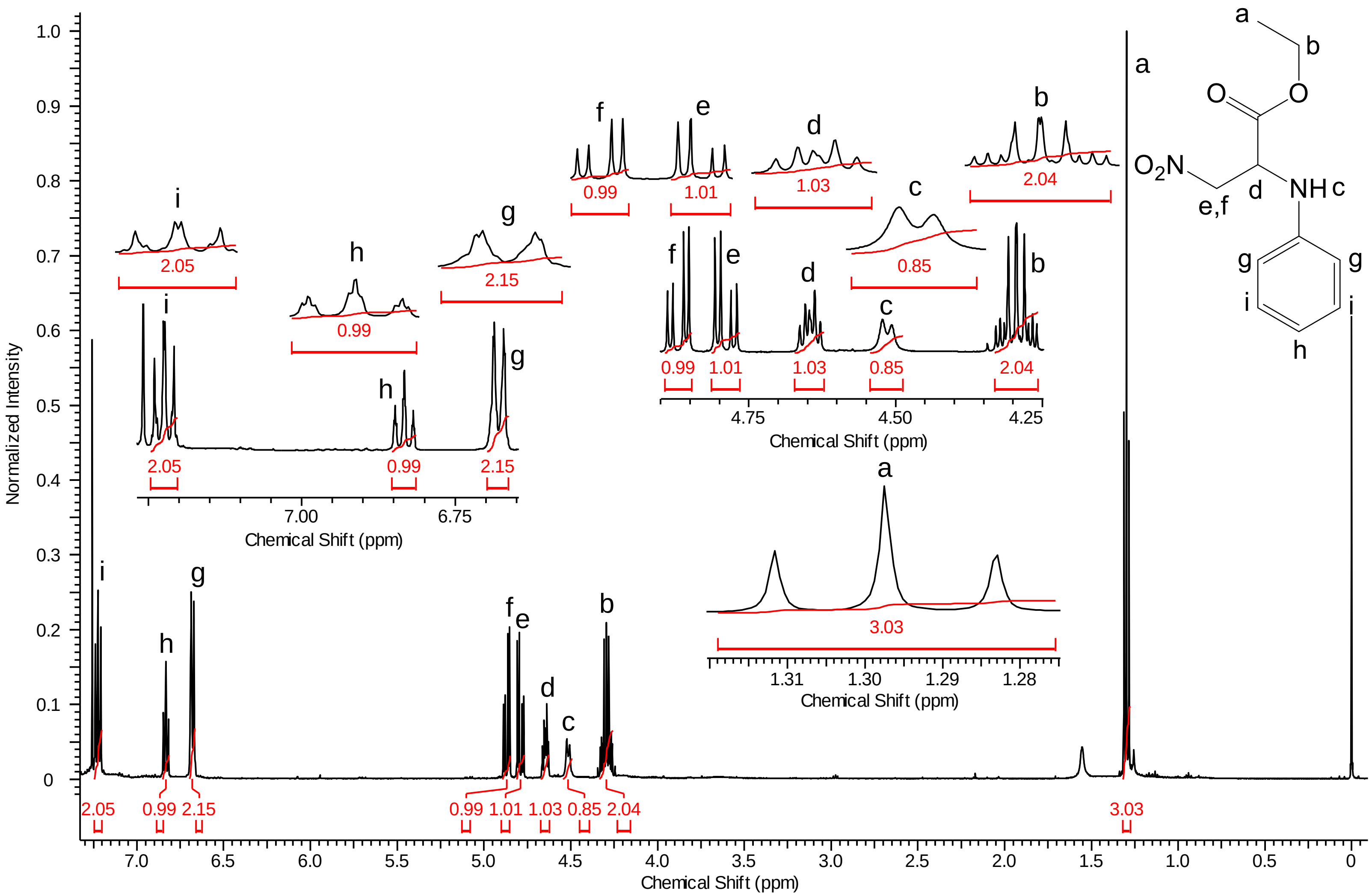

Figure 1.88: $^1$H NMR spectrum of **7m** ethyl 3-nitro-2-(phenylamino)propanoate.

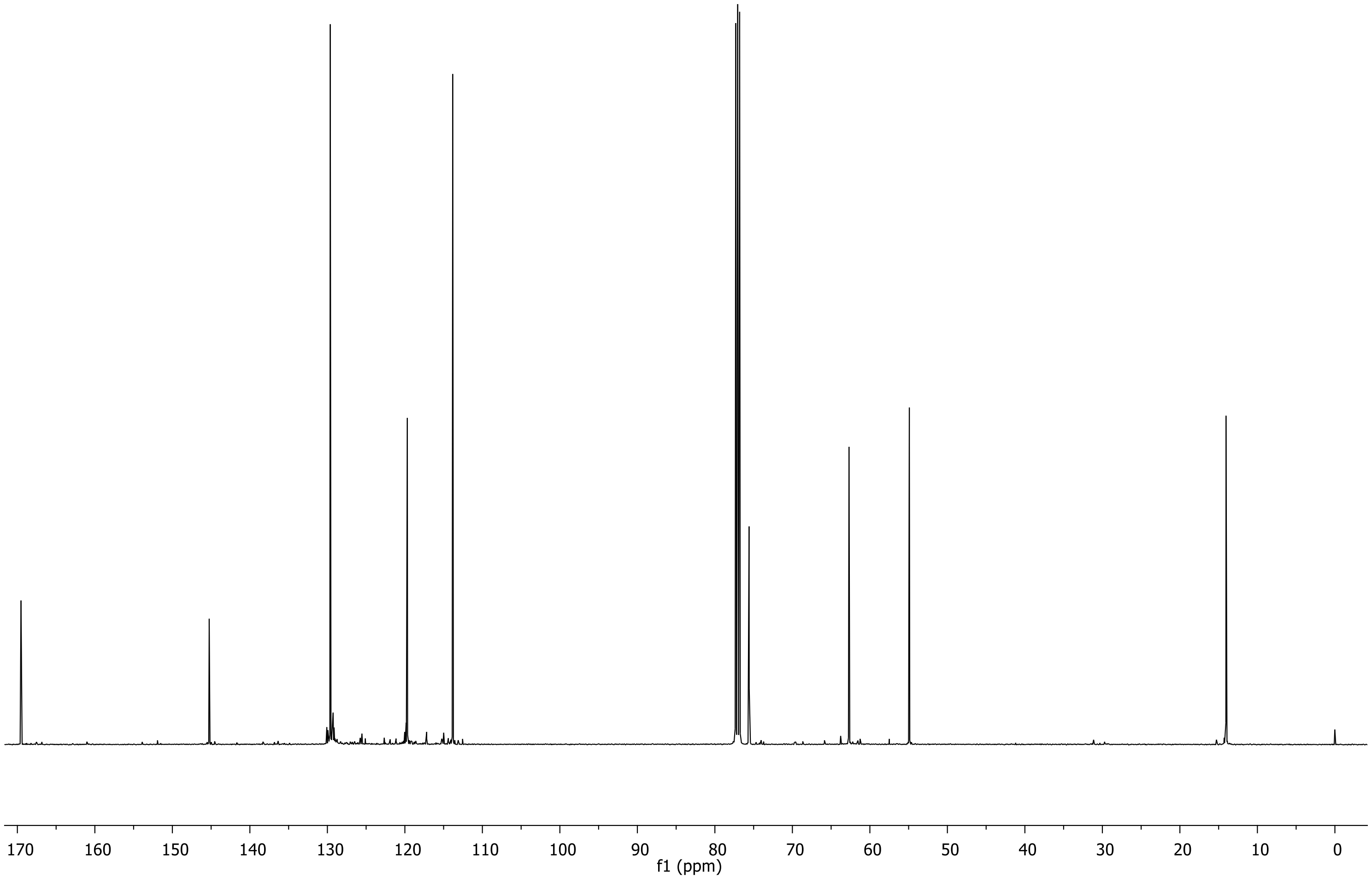

Figure 1.89: $^{13}$C NMR spectrum of **7m** ethyl 3-nitro-2-(phenylamino)propanoate.

Table 1.13: MS data.

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **7m** | 238 | 1 | 239.10 | 20 | 178.11 | 10 | ES+ |
| | | 2 | 239.10 | 20 | 104.02 | 26 | ES+ |
| | | 3 | 239.10 | 20 | 77.02 | 40 | ES+ |
| | | 4 | 239.10 | 20 | 93.02 | 38 | ES+ |
| | | 5 | 239.10 | 20 | 150.07 | 18 | ES+ |

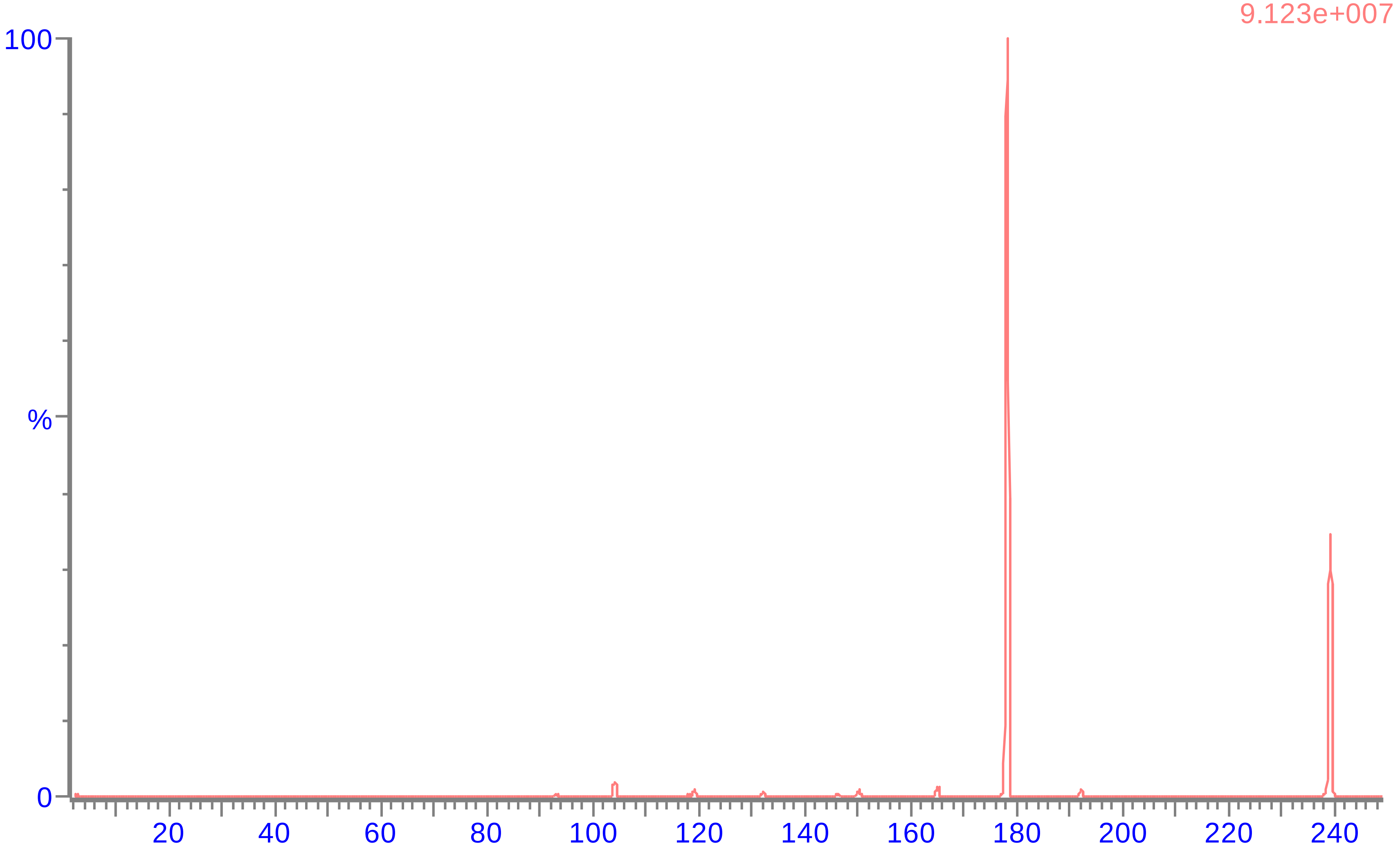

Figure 1.90: Mass spectrum for daughter fragment peak ES+, m/z 239.10 -> 178.11.

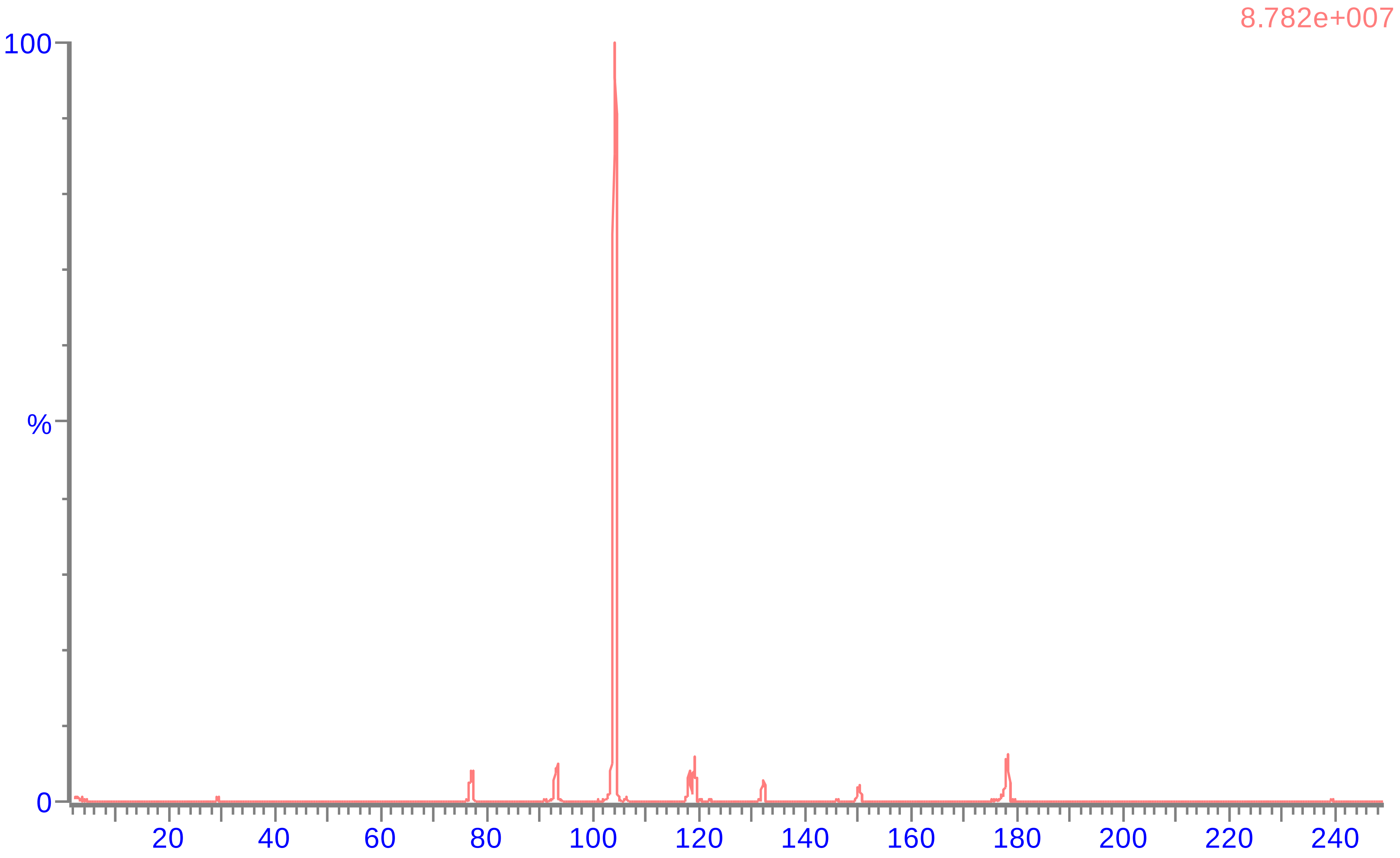

Figure 1.91: Mass spectrum for daughter fragment peak ES+, m/z 239.10 -> 104.02.

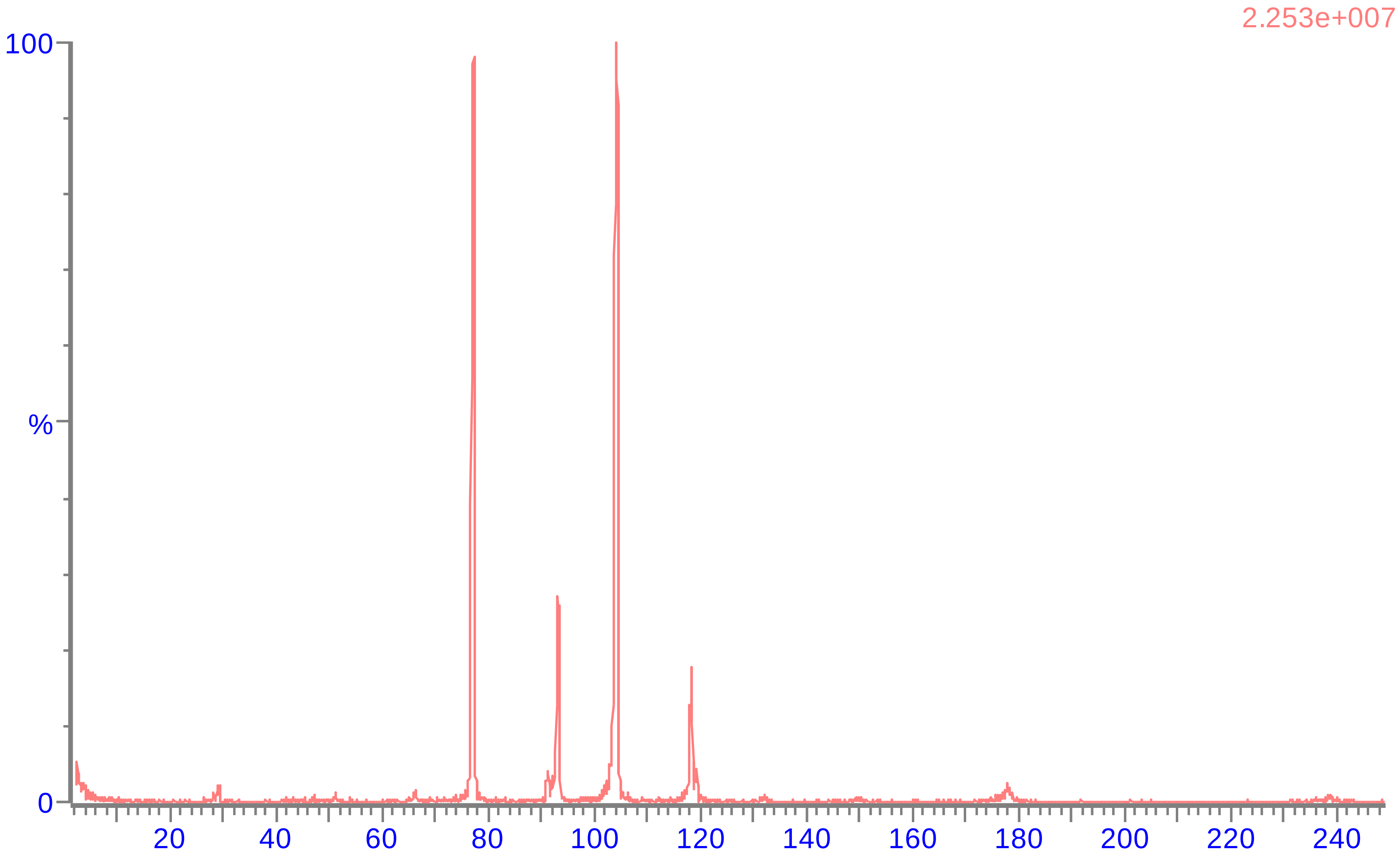

Figure 1.92: Mass spectrum for daughter fragment peak ES+, m/z 239.10 -> 77.02.

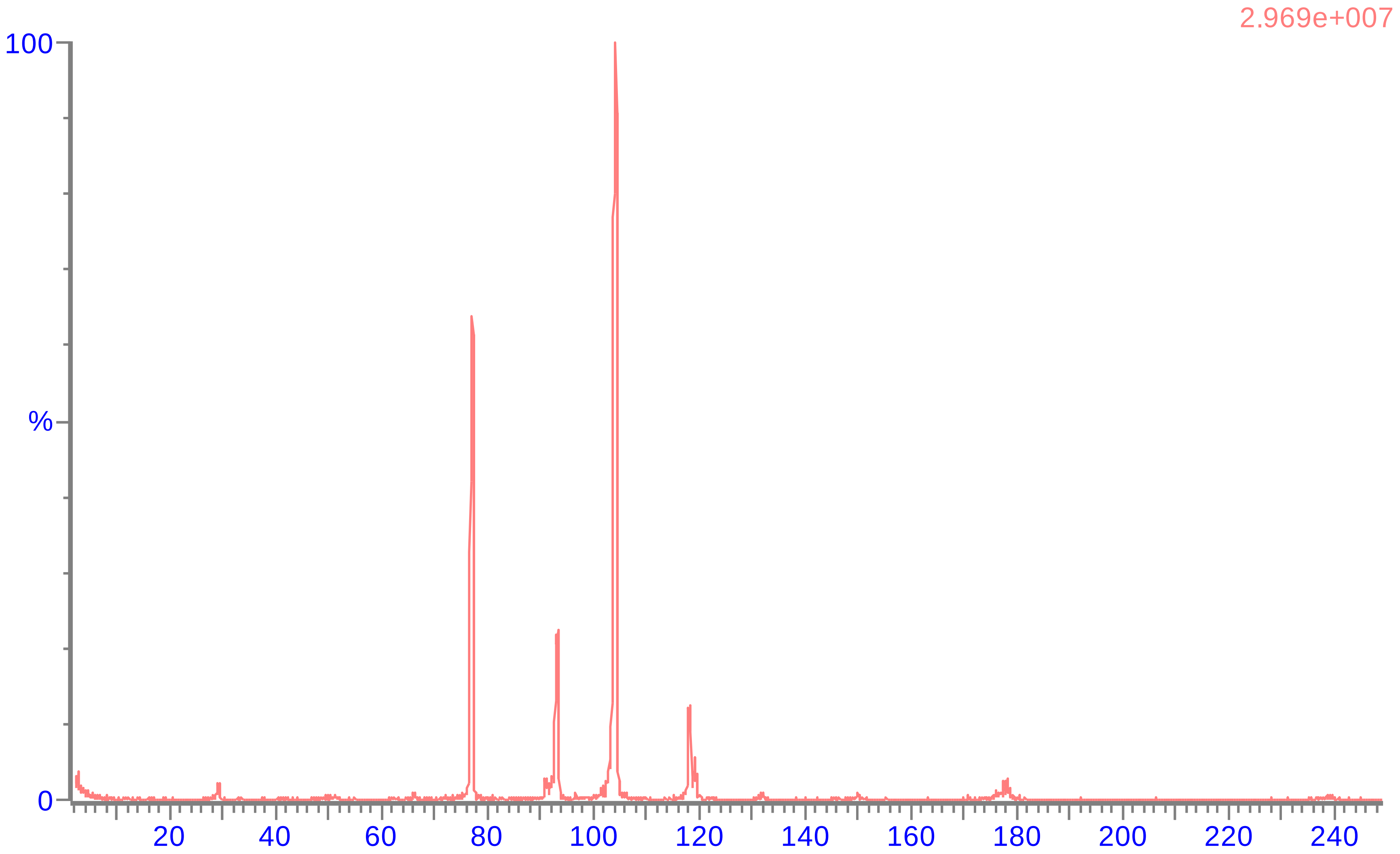

Figure 1.93: Mass spectrum for daughter fragment peak ES+, m/z 239.10 -> 93.02.

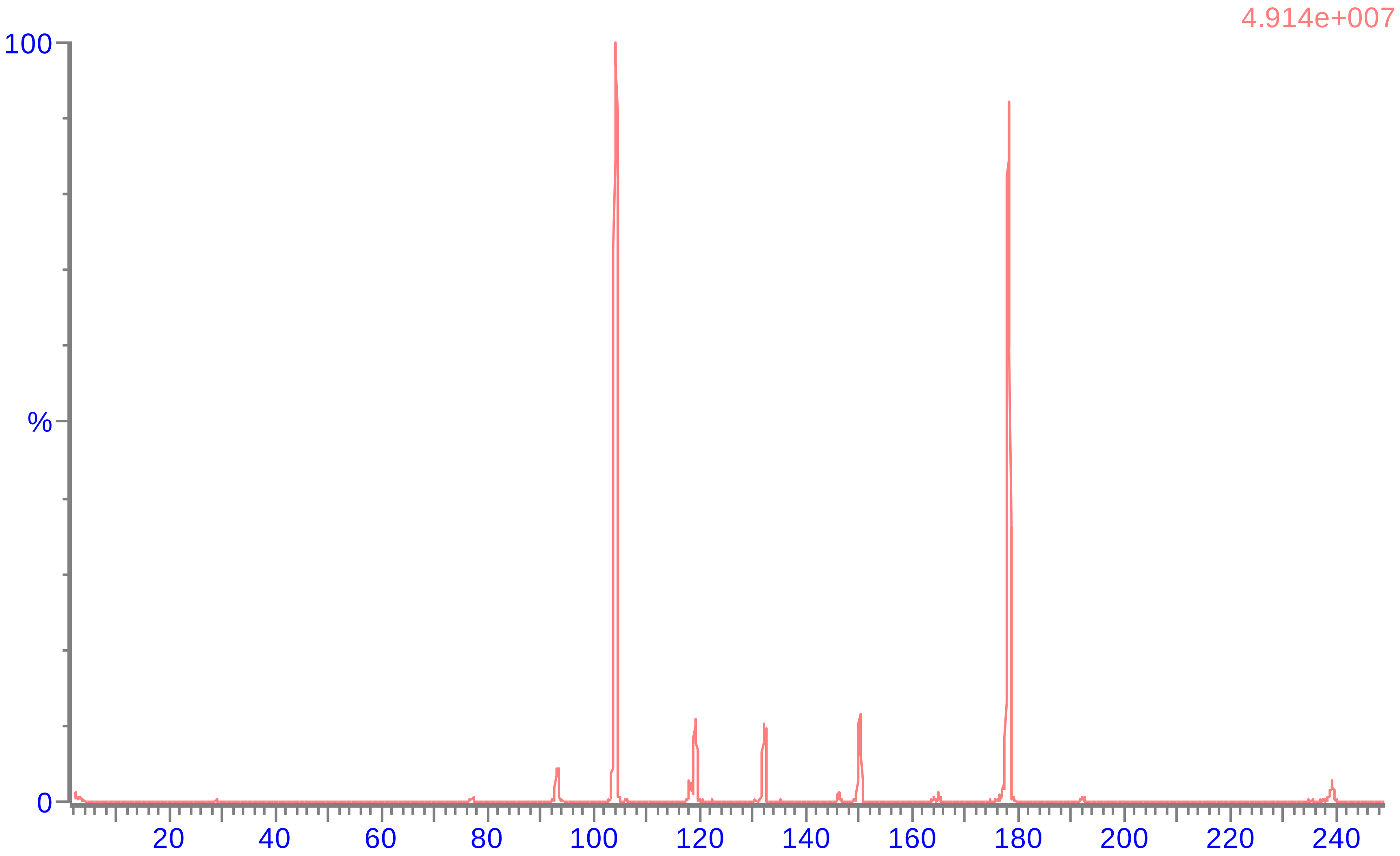

Figure 1.94: Mass spectrum for daughter fragment peak ES+, m/z 239.10 -> 150.07.

**8a** 4-methoxy-*N*-(2-nitro-1-phenylethyl)aniline

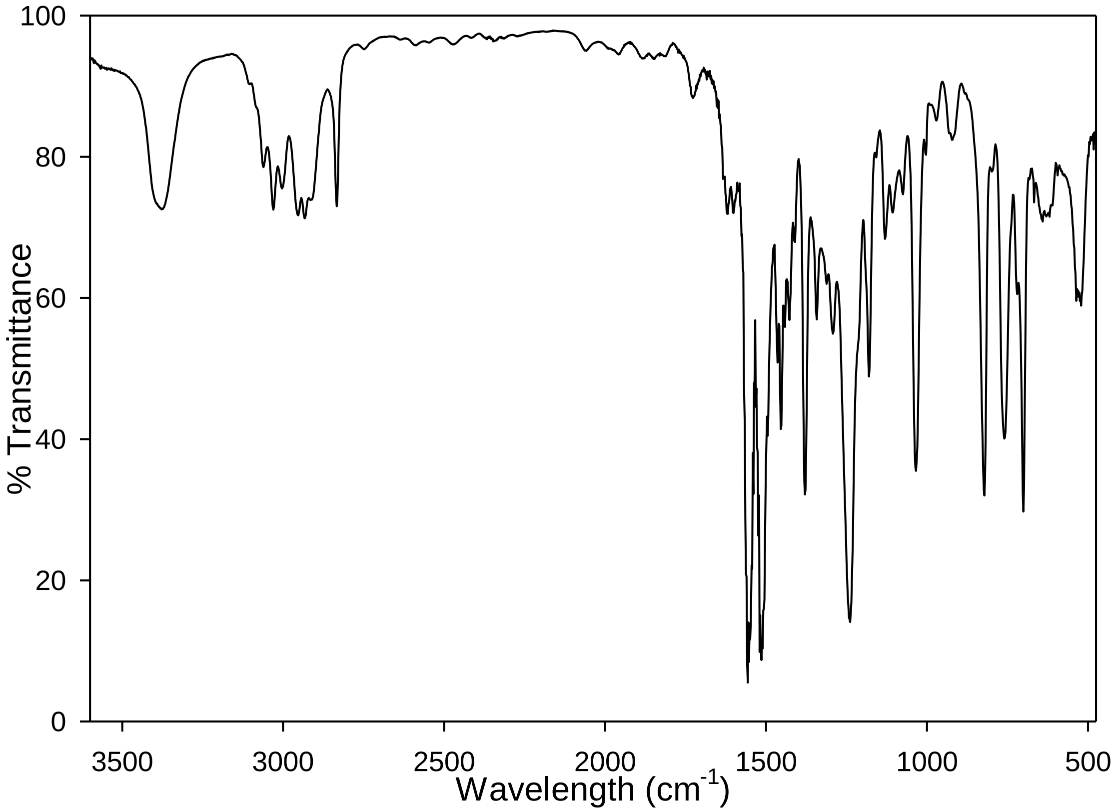

Figure 1.95: IR spectrum of **8a** 4-methoxy-*N*-(2-nitro-1-phenylethyl)aniline.

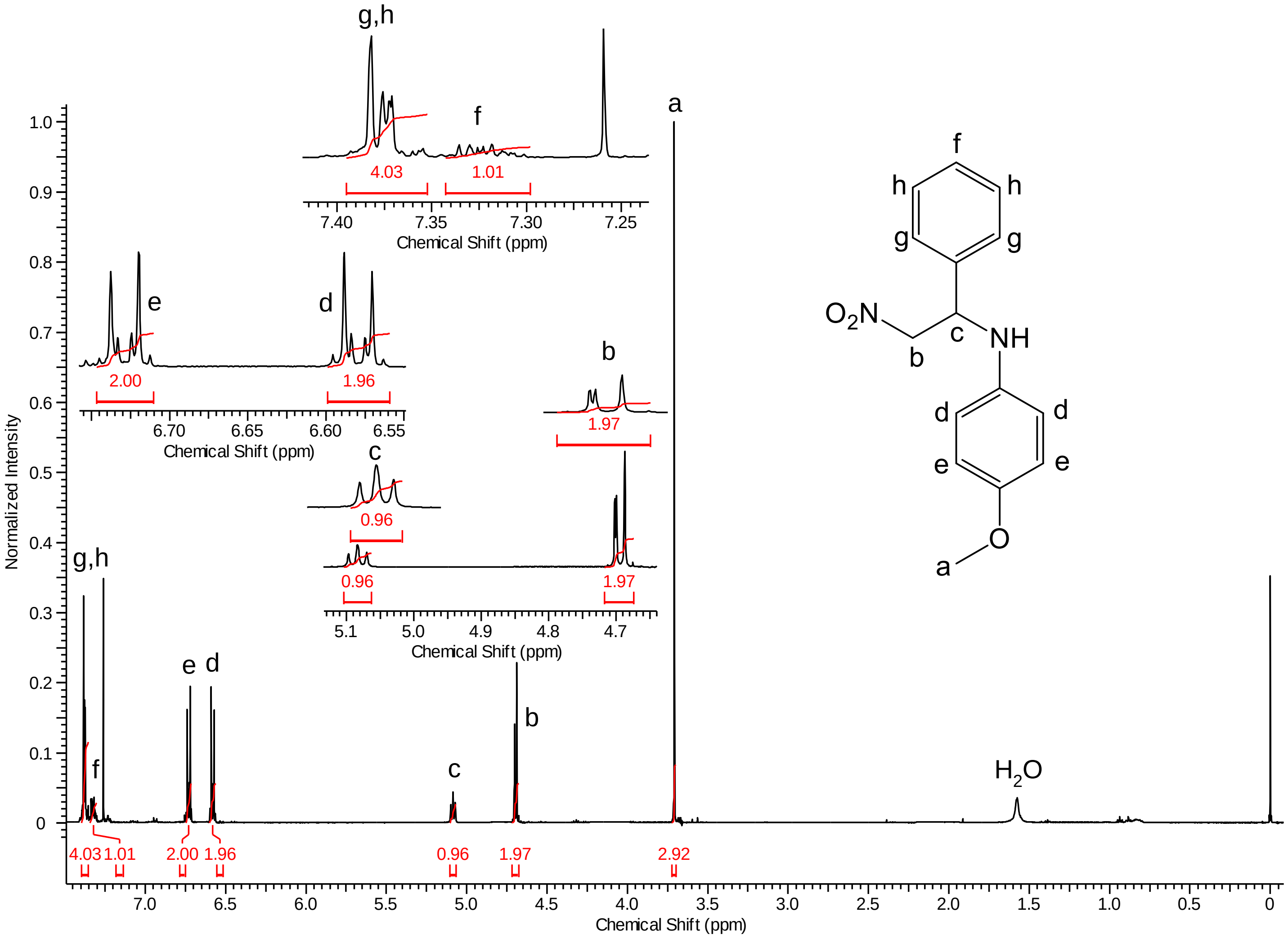

Figure 1.96: $^1$H NMR spectrum of **8a** 4-methoxy-*N*-(2-nitro-1-phenylethyl)aniline.

**8b** 4-methyl-*N*-(2-nitro-1-phenylethyl)aniline

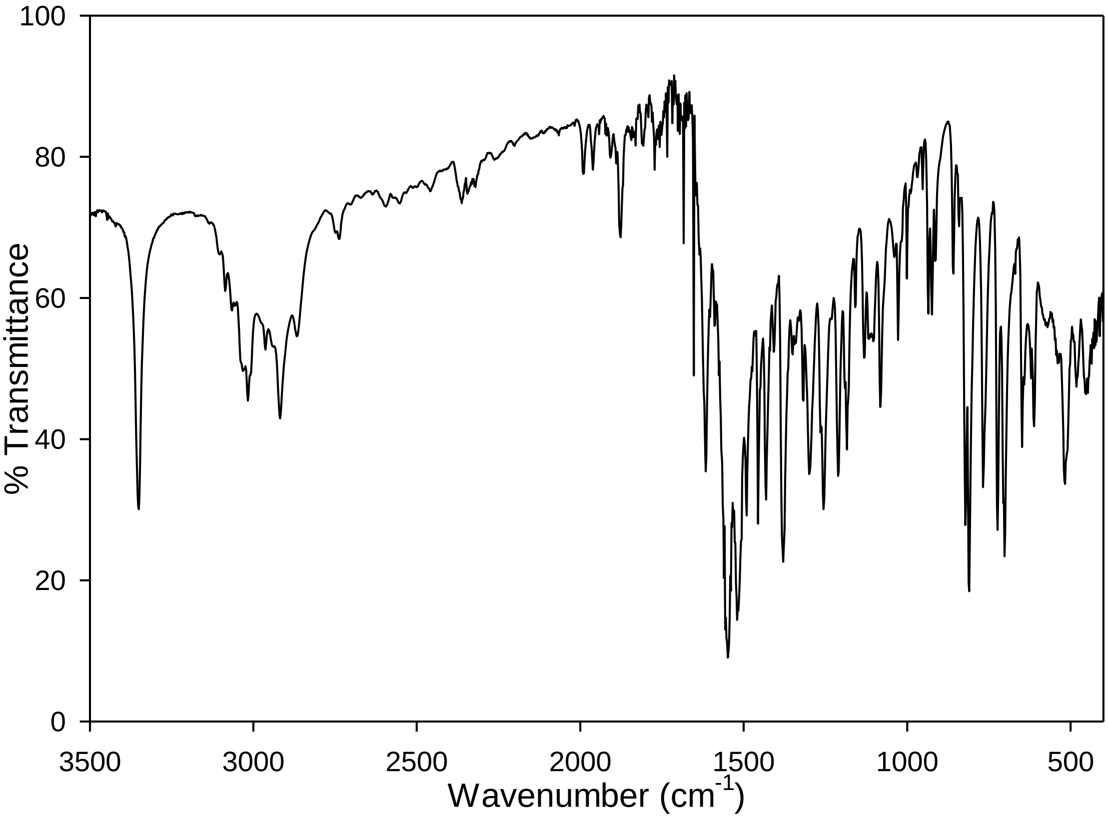

Figure 1.97: IR spectrum of **8b** 4-methyl-*N*-(2-nitro-1-phenylethyl)aniline.

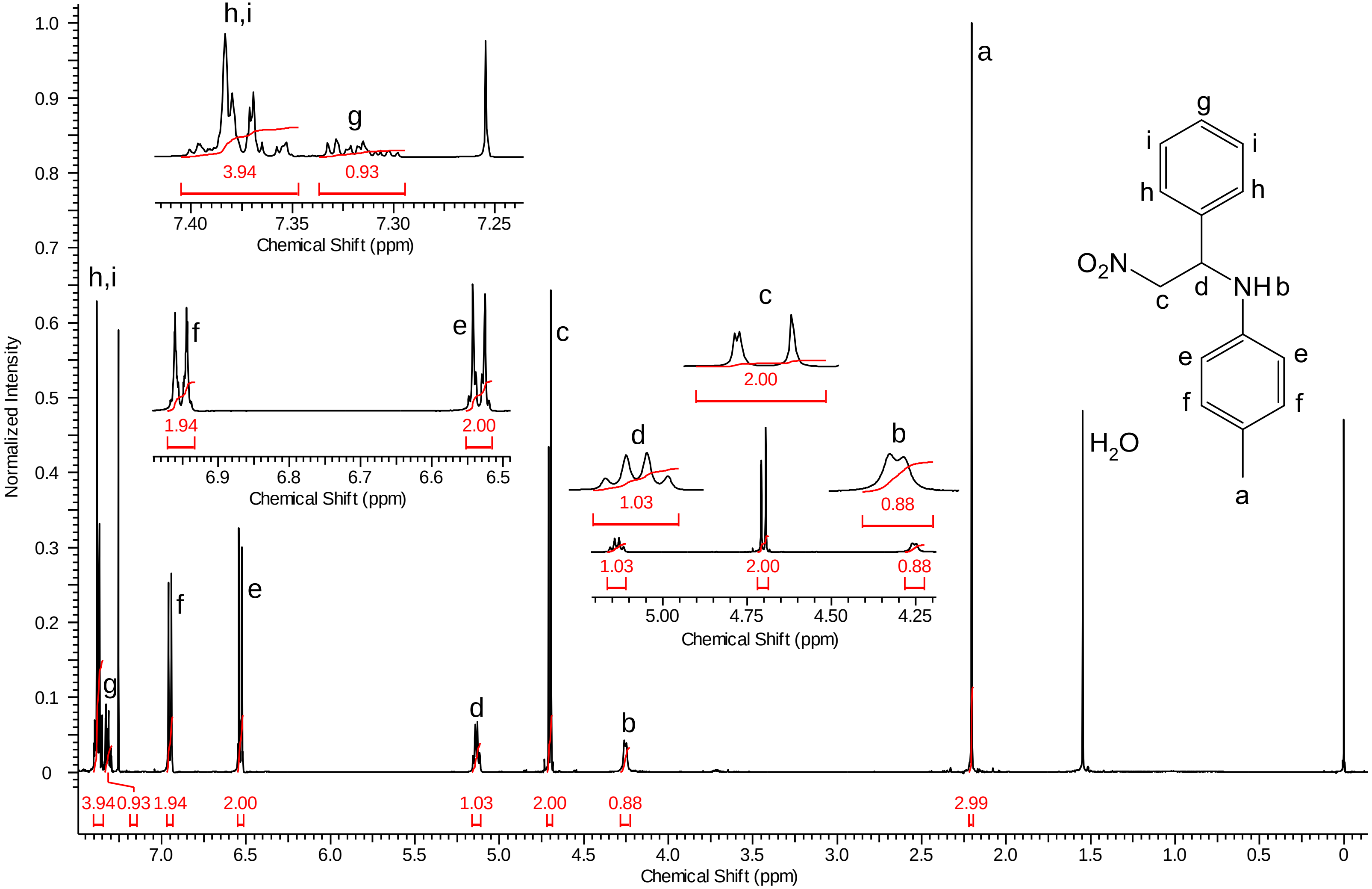

Figure 1.98: ${}^1$H NMR spectrum of **8b** 4-methyl-*N*-(2-nitro-1-phenylethyl)aniline.

**8c** 3-methyl-*N*-(2-nitro-1-phenylethyl)aniline

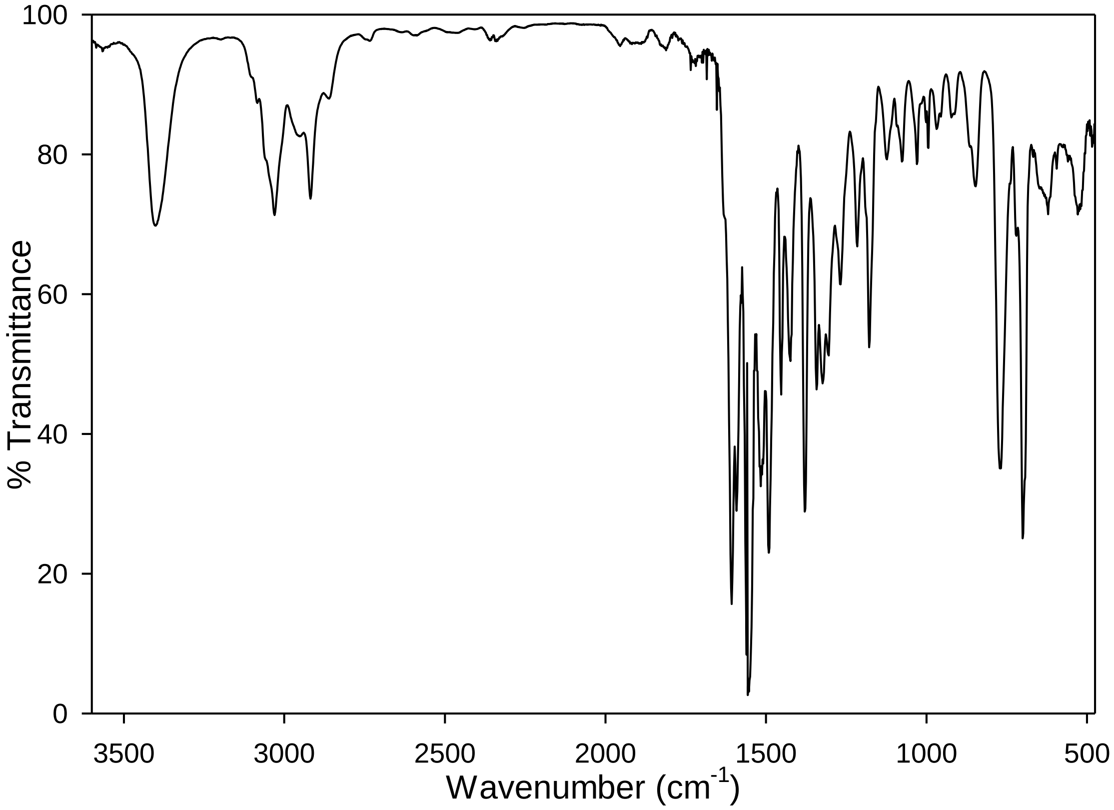

Figure 1.99: IR spectrum of **8c** 3-methyl-*N*-(2-nitro-1-phenylethyl)aniline.

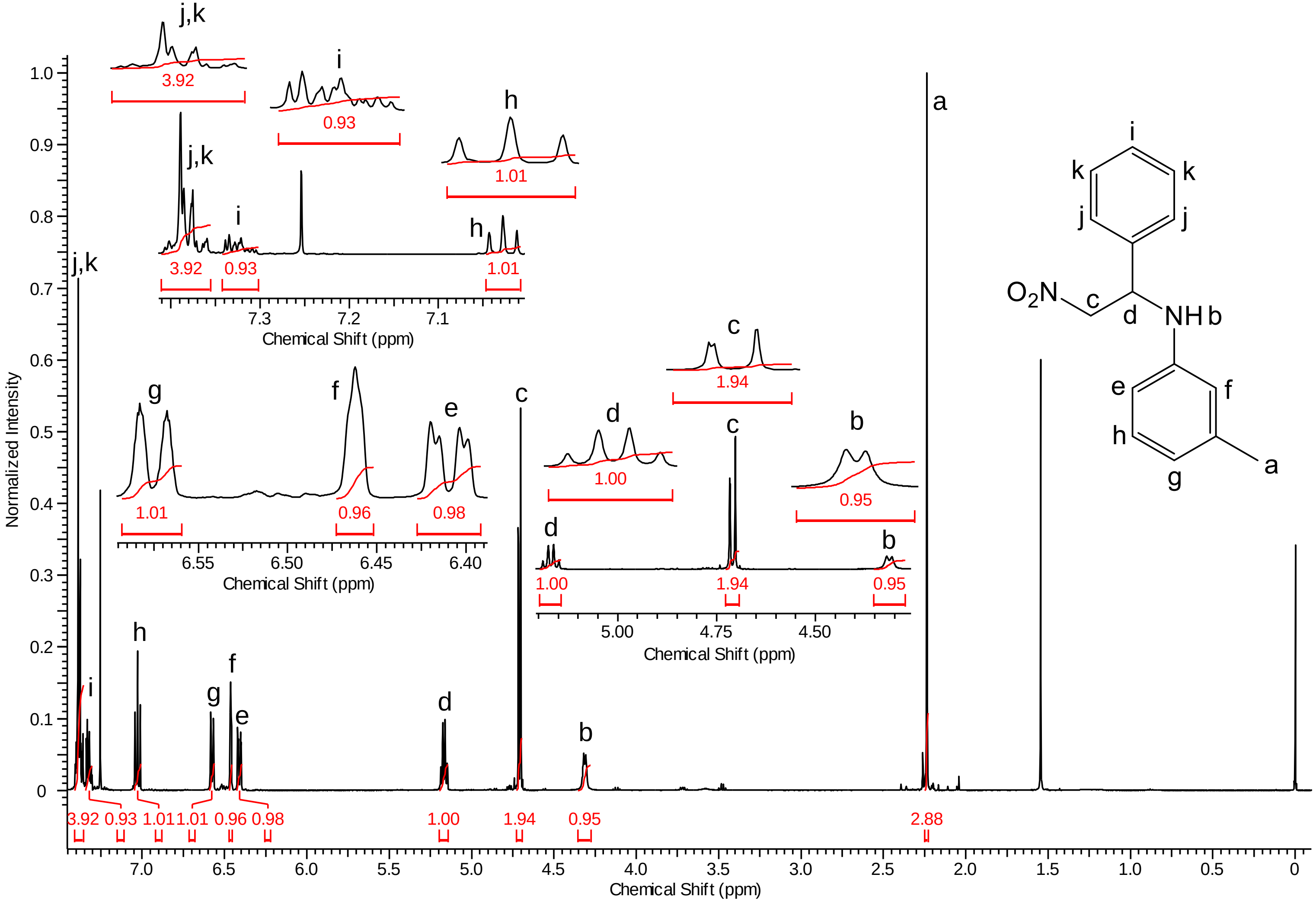

Figure 1.100: $^1$H NMR spectrum of **8c** 3-methyl-*N*-(2-nitro-1-phenylethyl)aniline.

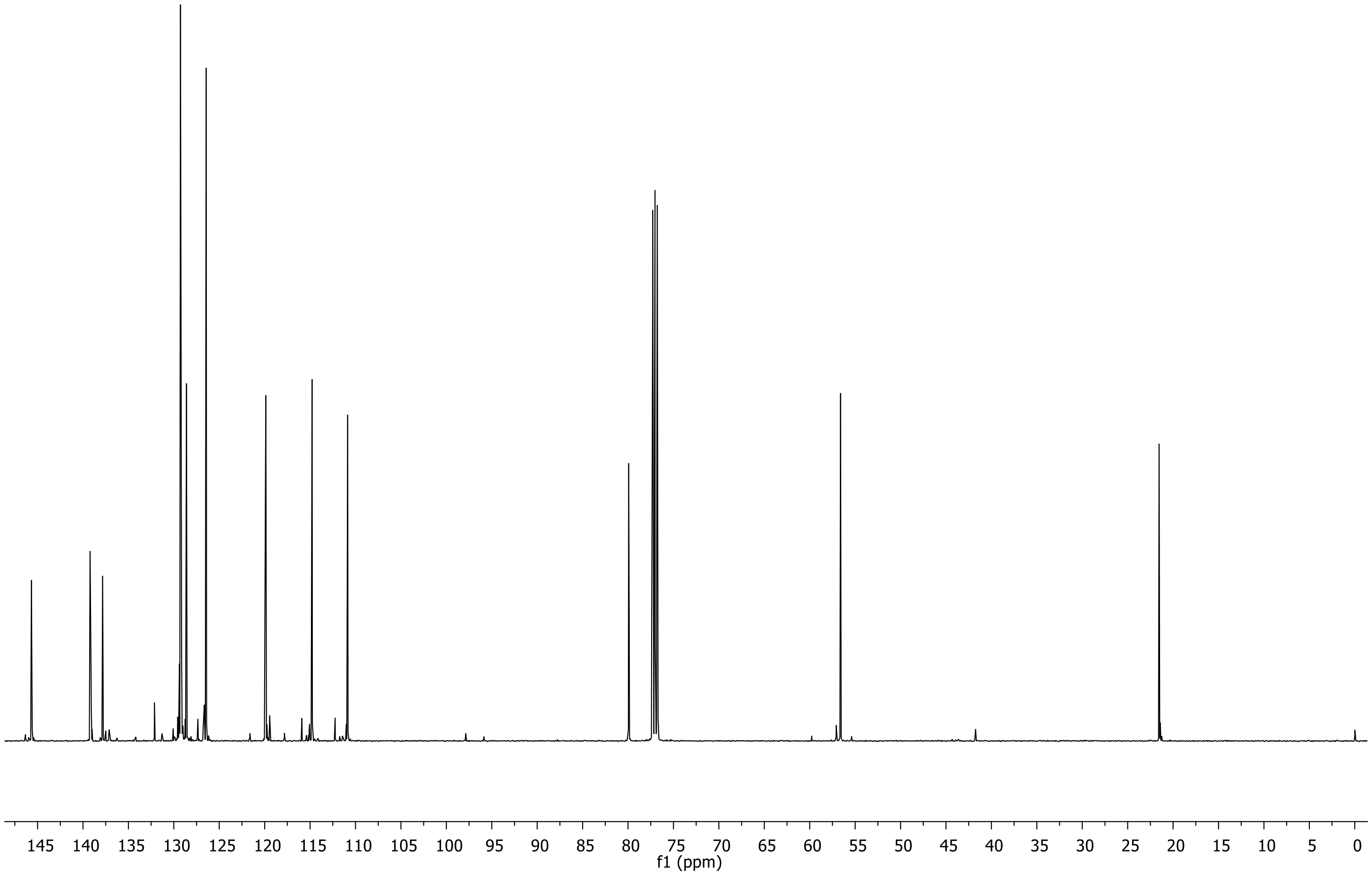

Figure 1.101: $^{13}$C NMR spectrum of **8c** 3-methyl-*N*-(2-nitro-1-phenylethyl)aniline.

Table 1.14: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **8c** | 256.3 | 1 | 257.08 | 20 | 107.98 | 14 | ES+ |
| | | 2 | 257.08 | 20 | 104.07 | 18 | ES+ |
| | | 3 | 257.08 | 20 | 196.11 | 12 | ES+ |
| | | 4 | 257.08 | 20 | 149.99 | 12 | ES+ |
| | | 5 | 257.08 | 20 | 78.05 | 50 | ES+ |

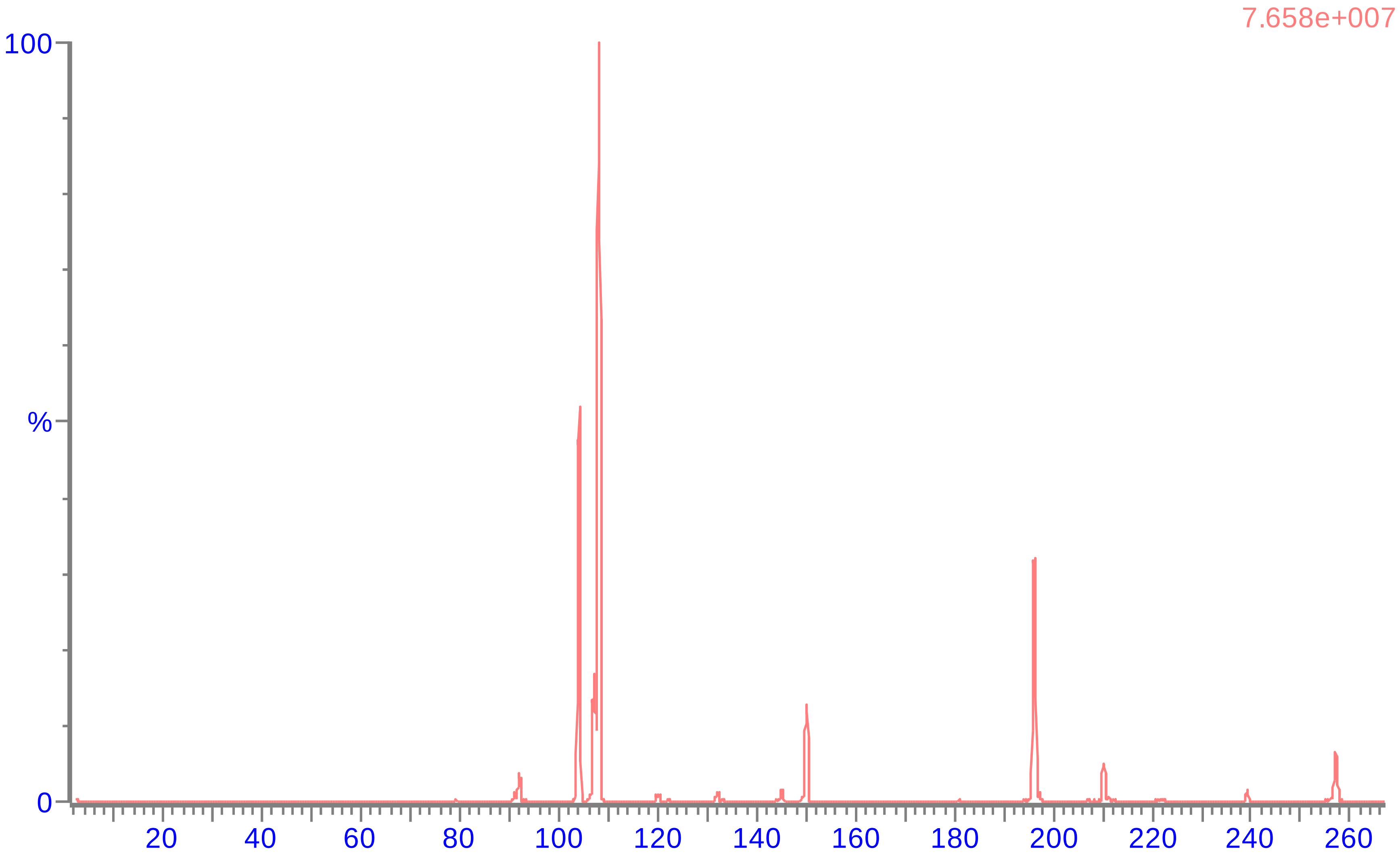

Figure 1.102: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 107.98.

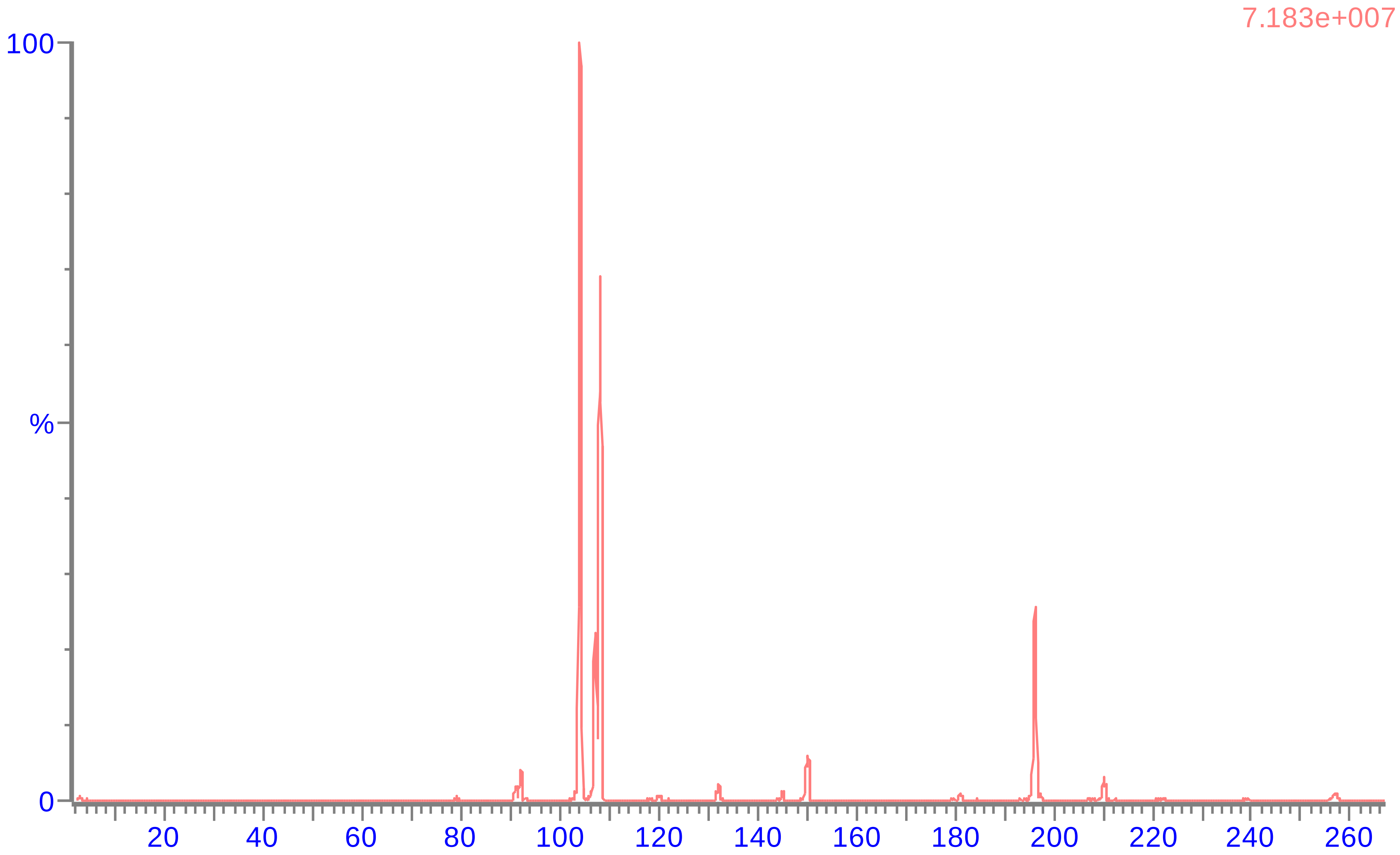

Figure 1.103: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 104.07.

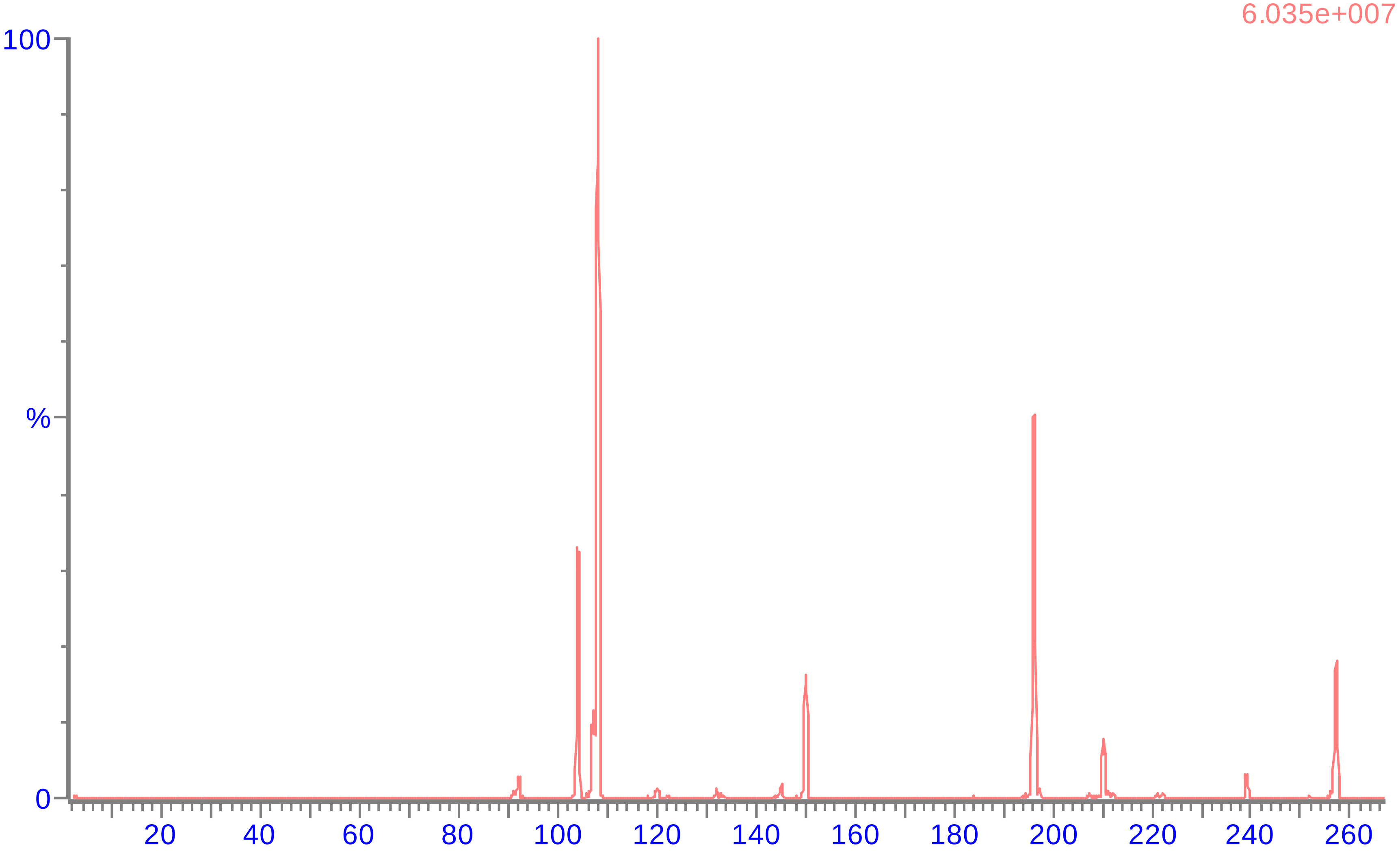

Figure 1.104: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 196.11.

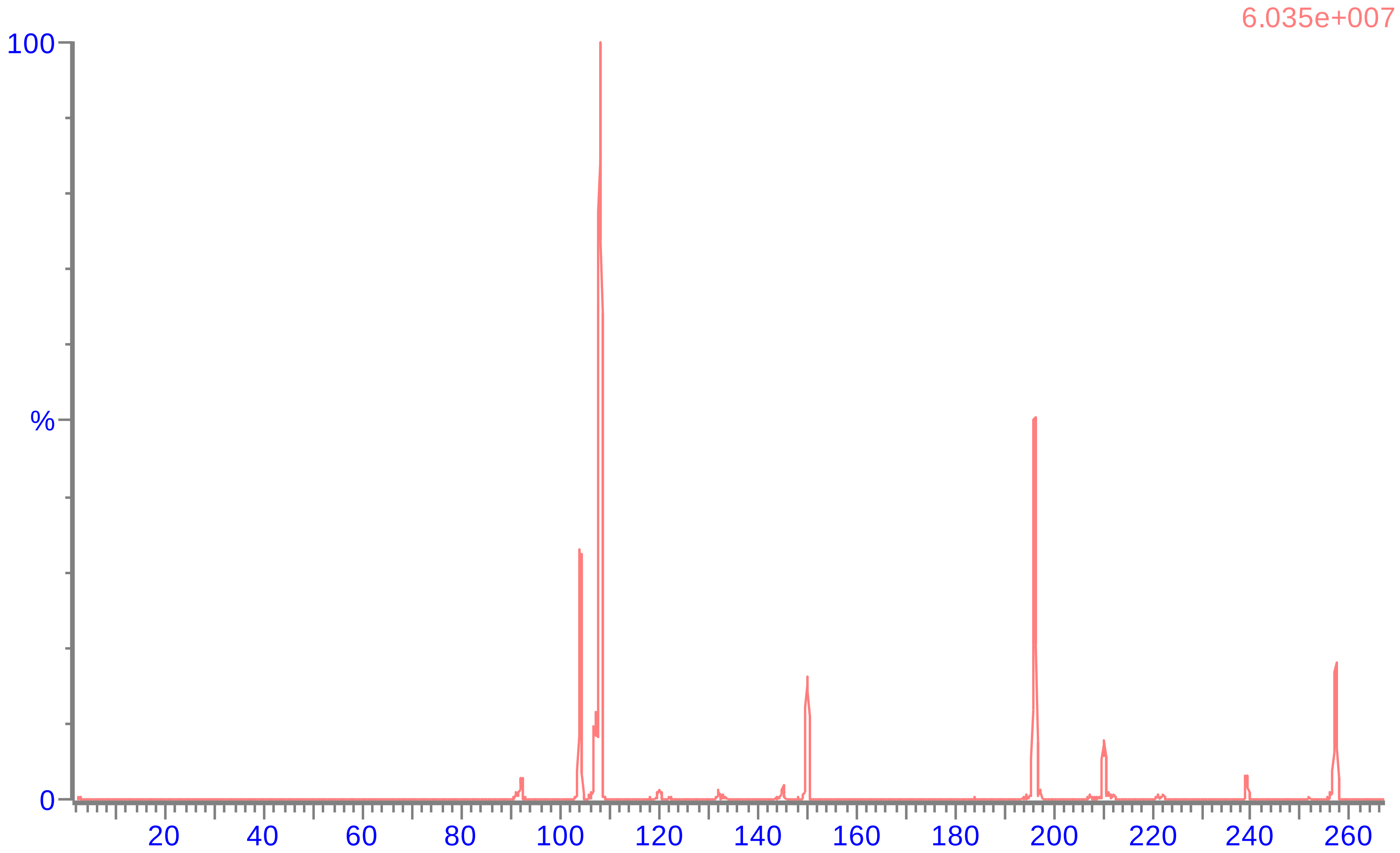

Figure 1.105: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 149.99.

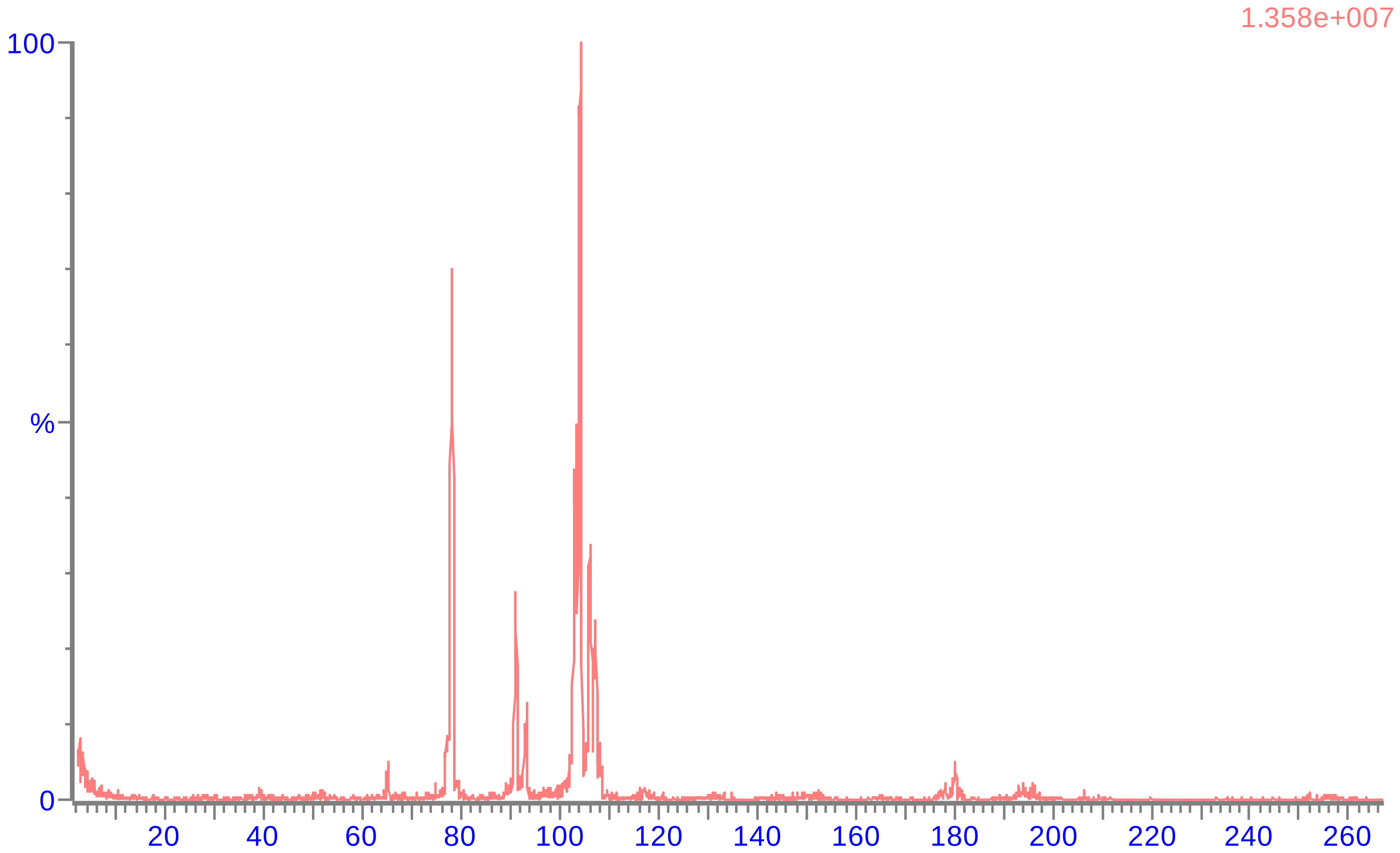

Figure 1.106: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 78.05.

**8d** 2-methyl-*N*-(2-nitro-1-phenylethyl)aniline

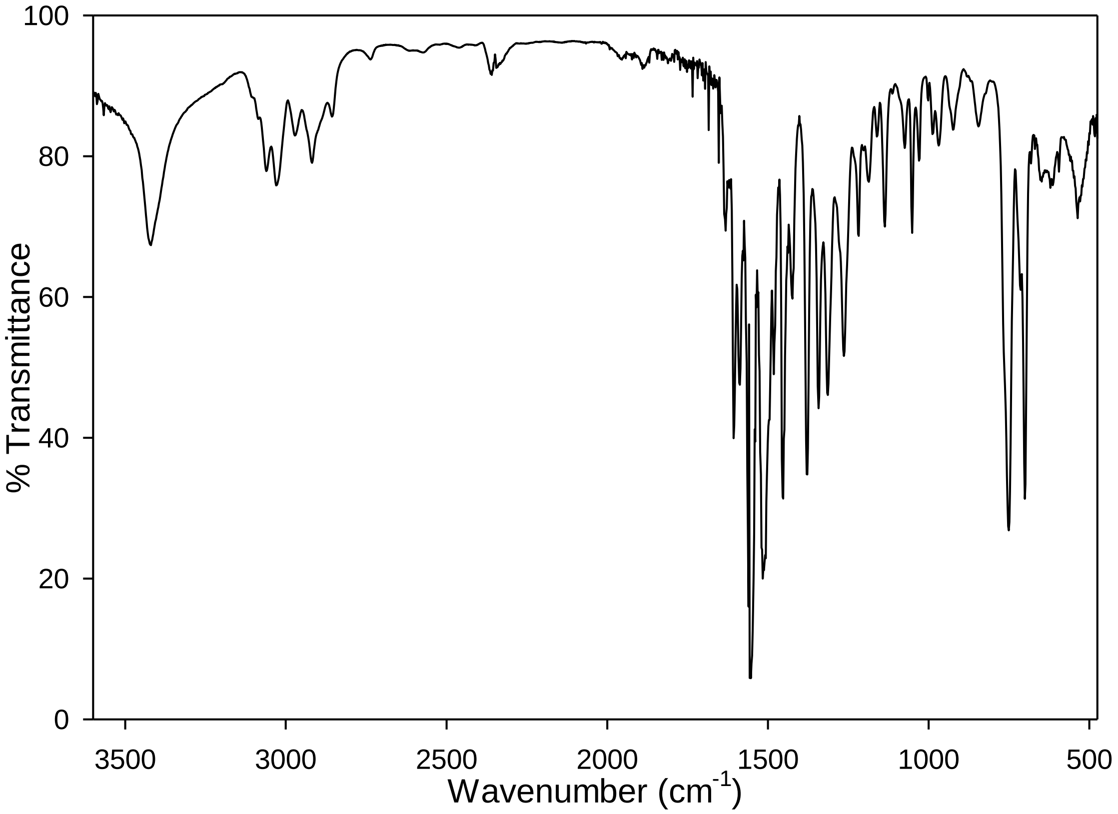

Figure 1.107: IR spectrum of **8d** 2-methyl-*N*-(2-nitro-1-phenylethyl)aniline

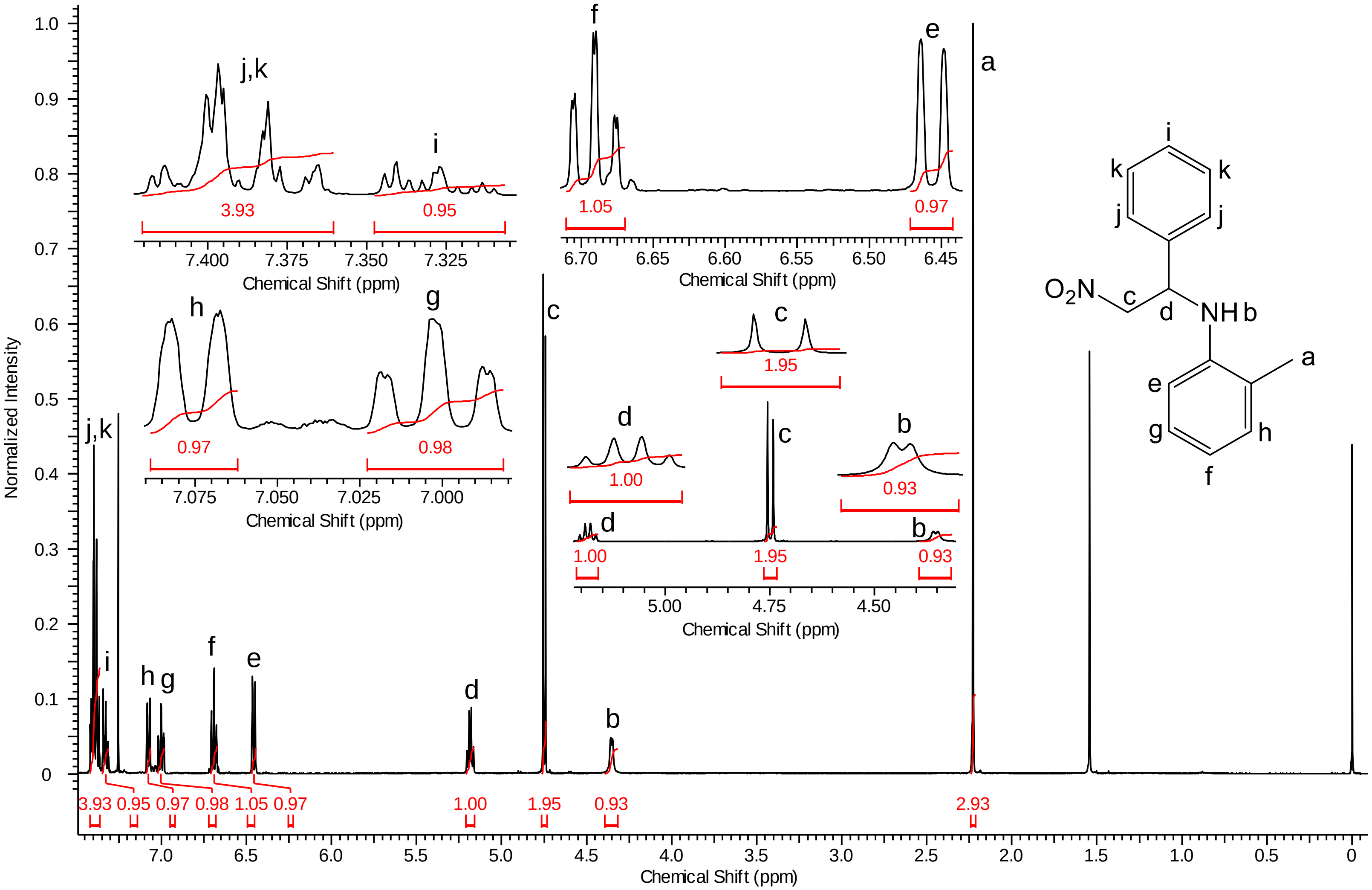

Figure 1.108: $^1$H NMR spectrum of **8d** 2-methyl-*N*-(2-nitro-1-phenylethyl)aniline.

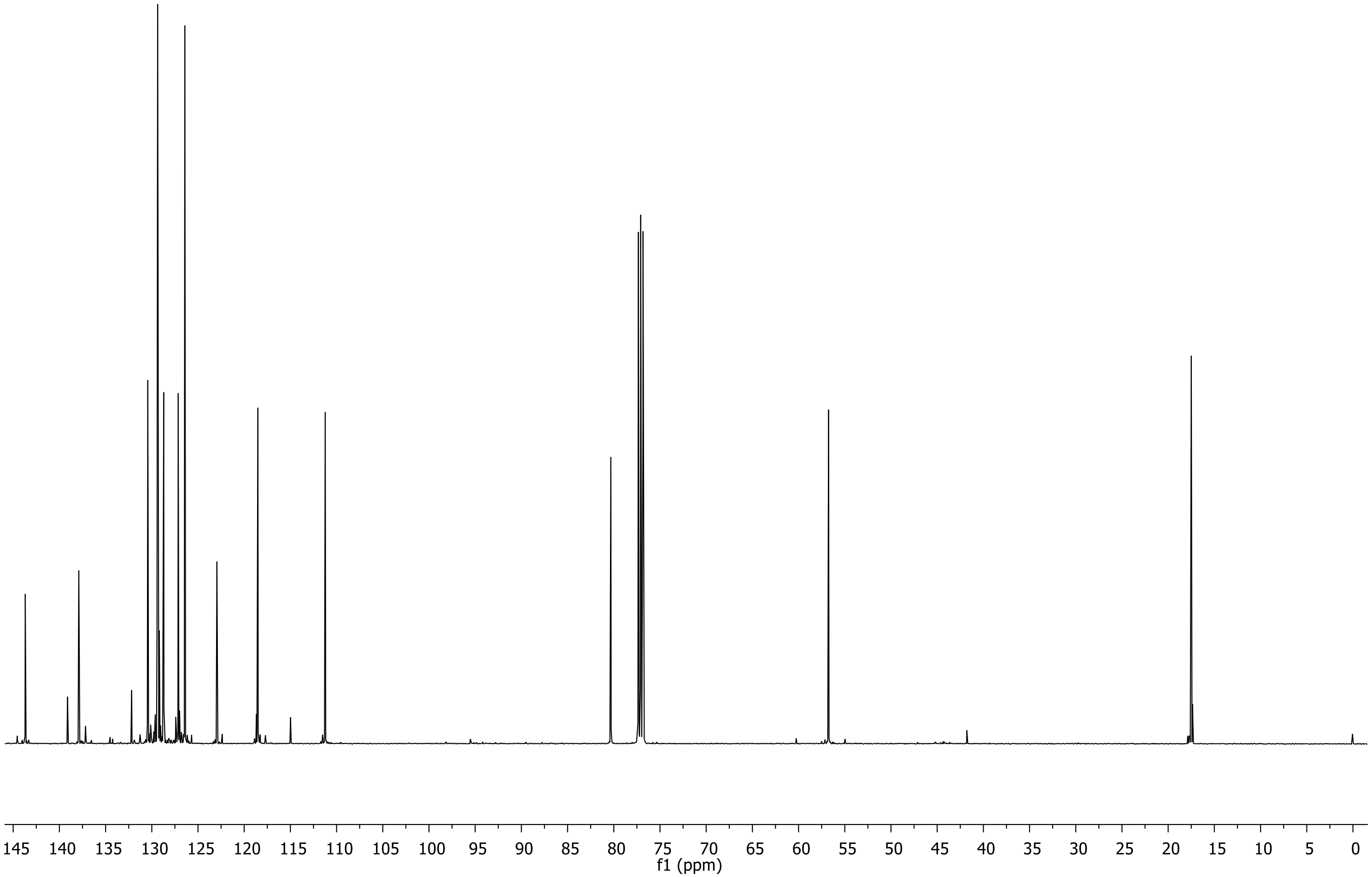

Figure 1.109: $^{13}$C NMR spectrum of **8d** 2-methyl-*N*-(2-nitro-1-phenylethyl)aniline.

Table 1.15: MS data.

| **Compound** | **Formula/Mass** |  | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **8d** | 256.3 | 1 | 257.08 | 20 | 104.07 | 22 | ES+ |
|  |  | 2 | 257.08 | 20 | 196.11 | 10 | ES+ |
|  |  | 3 | 257.08 | 20 | 107.98 | 14 | ES+ |
|  |  | 4 | 257.08 | 20 | 149.99 | 12 | ES+ |
|  |  | 5 | 257.08 | 20 | 77.99 | 50 | ES+ |

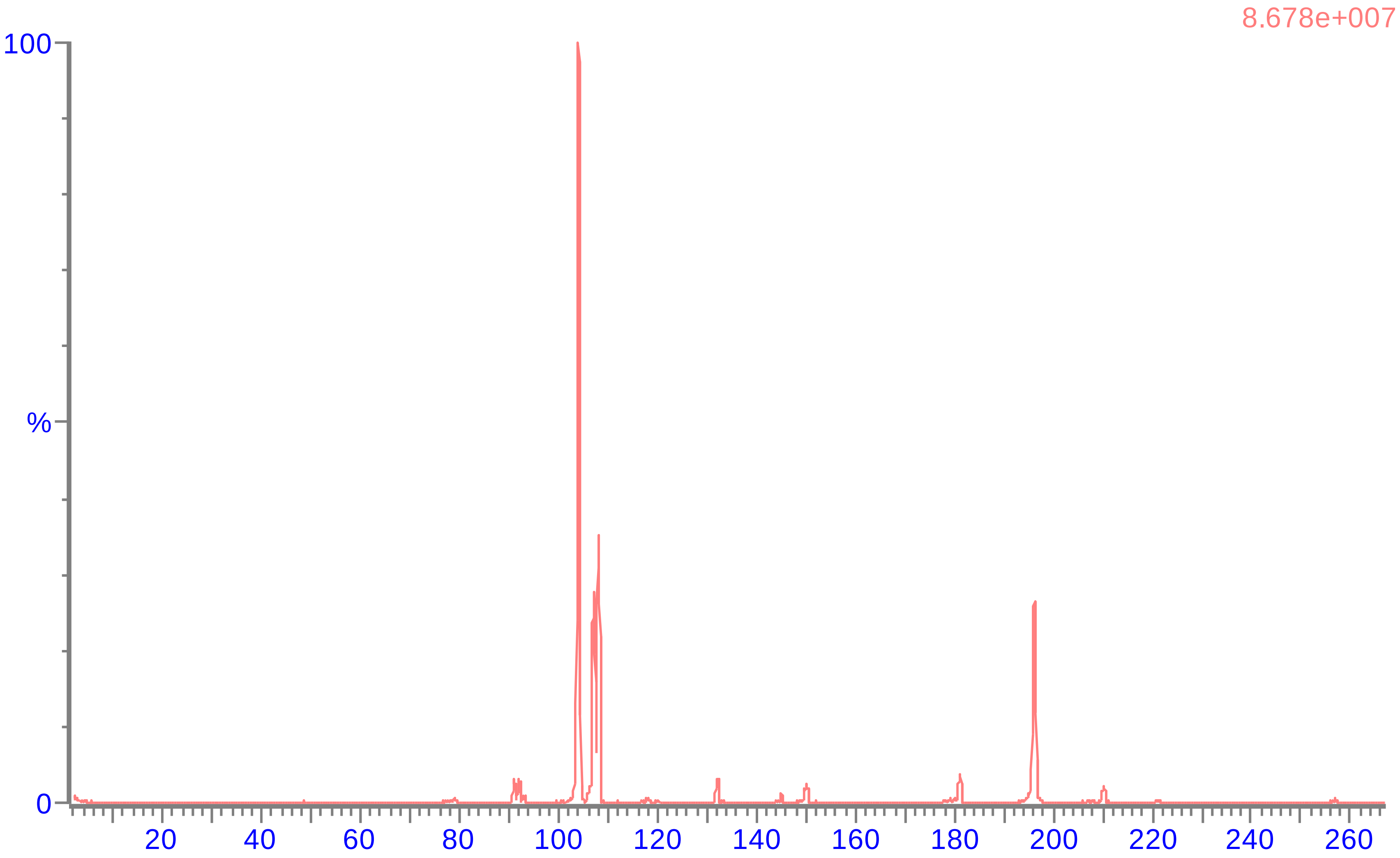

Figure 1.110: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 104.07.

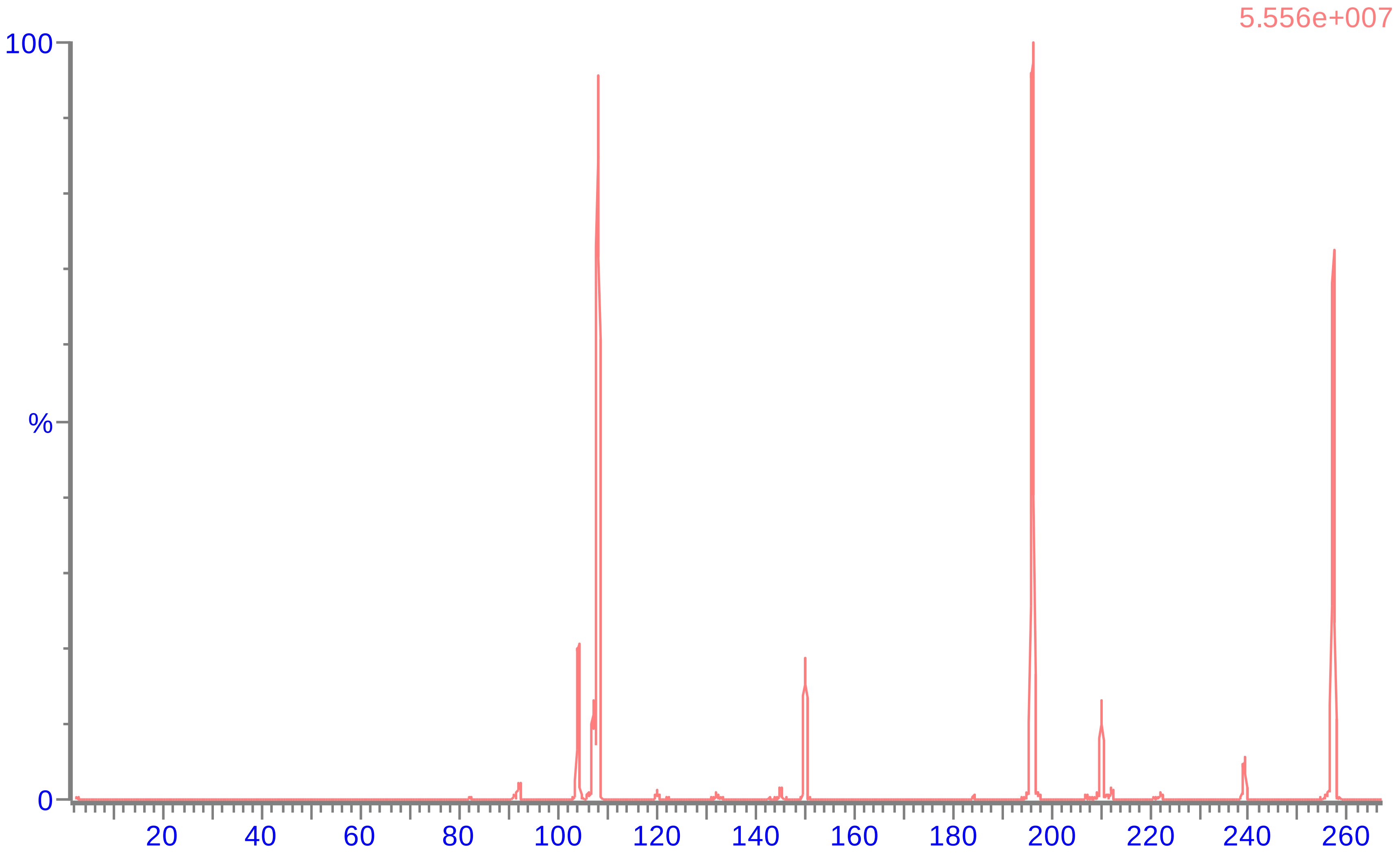

Figure 1.111: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 196.11.

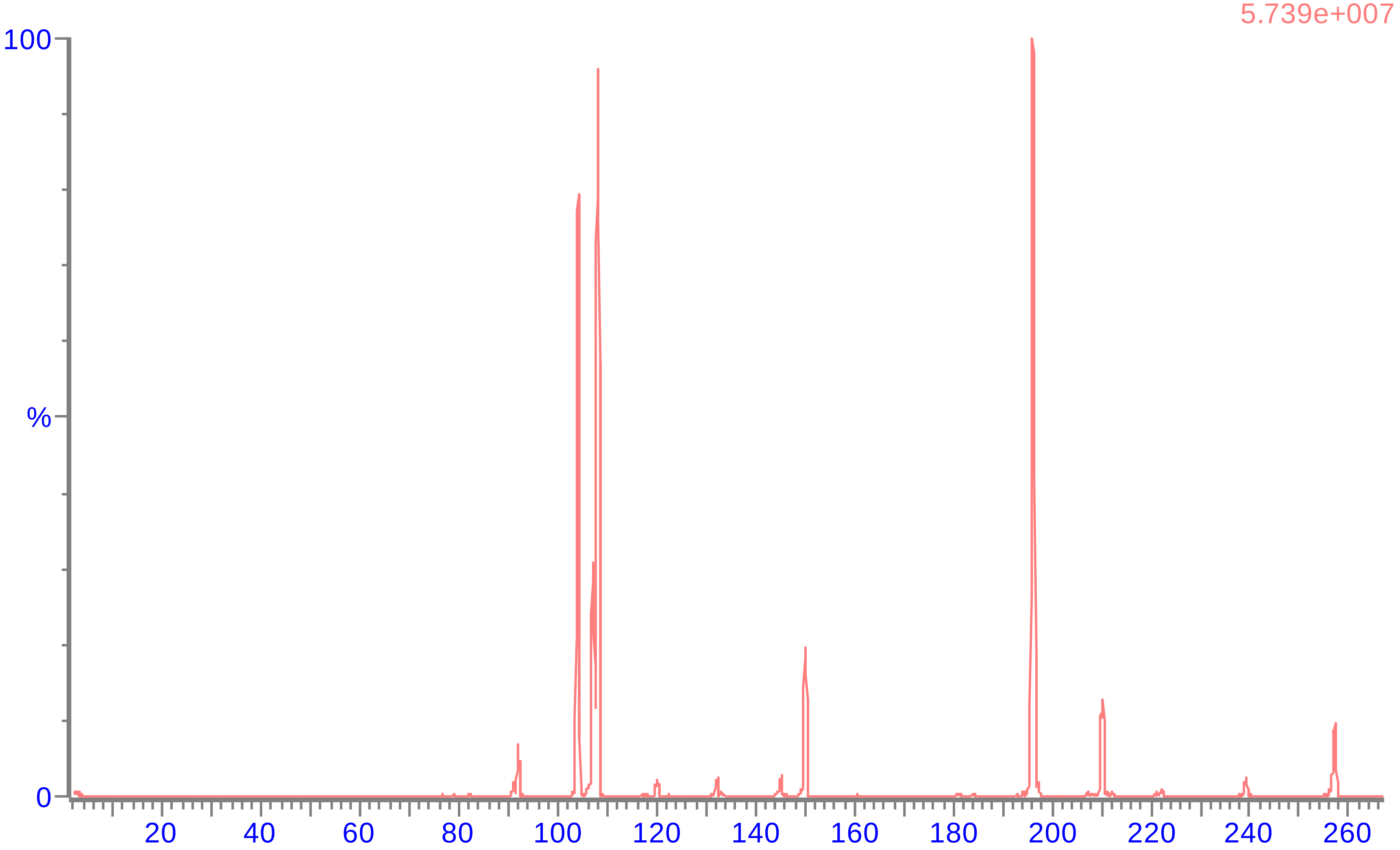

Figure 1.112: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 107.98.

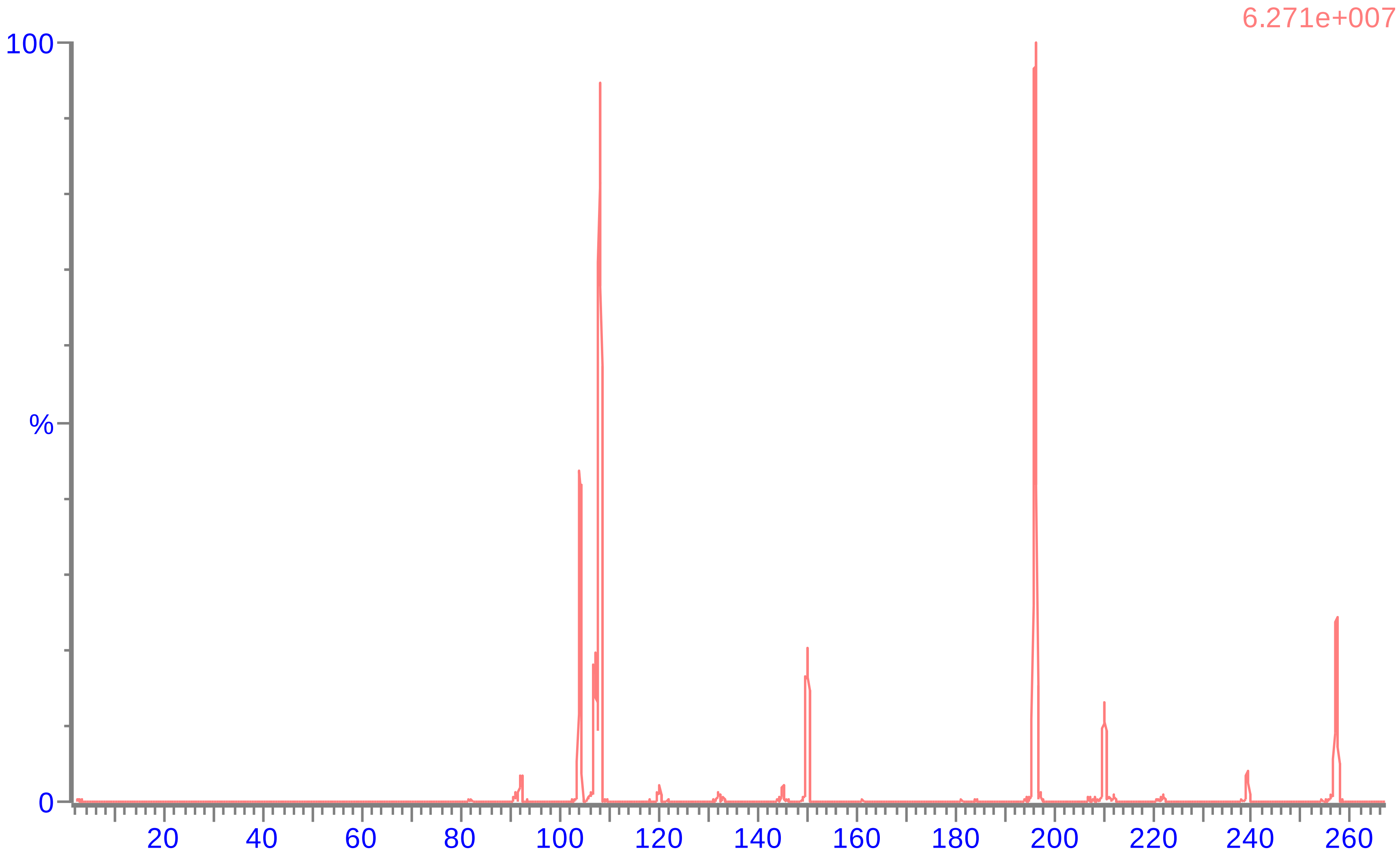

Figure 1.113: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 149.99.

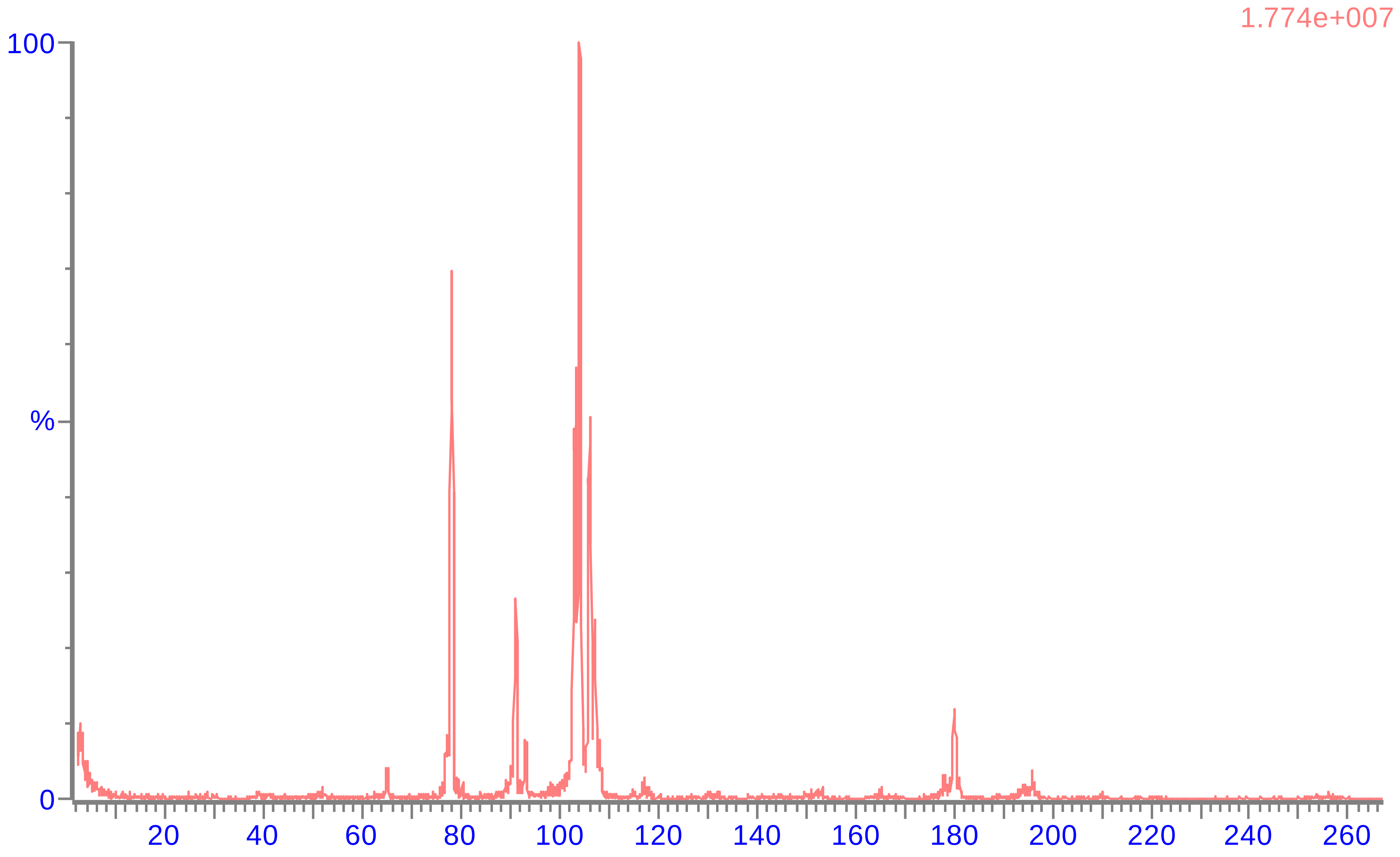

Figure 1.114: Mass spectrum for daughter fragment peak ES+, m/z 257.08 -> 77.99.

**8e** 4-ethyl-*N*-(2-nitro-1-phenylethyl)aniline

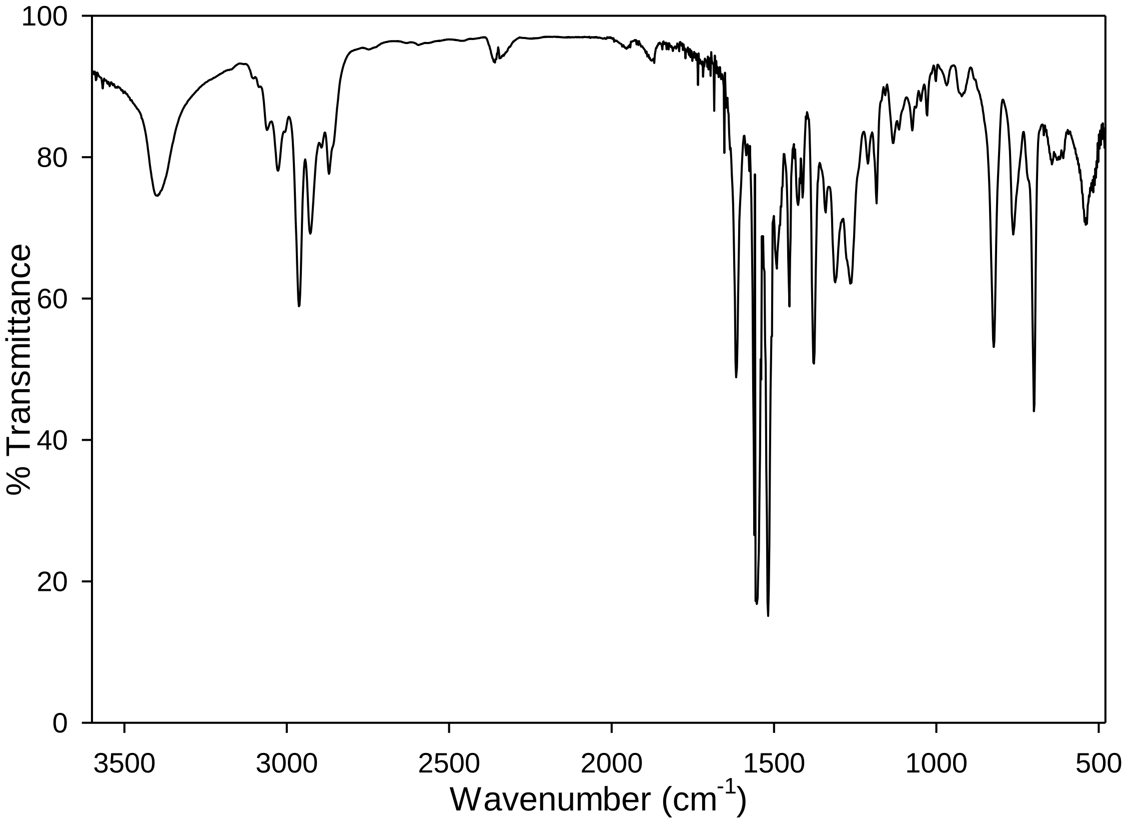

Figure 1.115: IR spectrum of **8e** 4-ethyl-*N*-(2-nitro-1-phenylethyl)aniline.

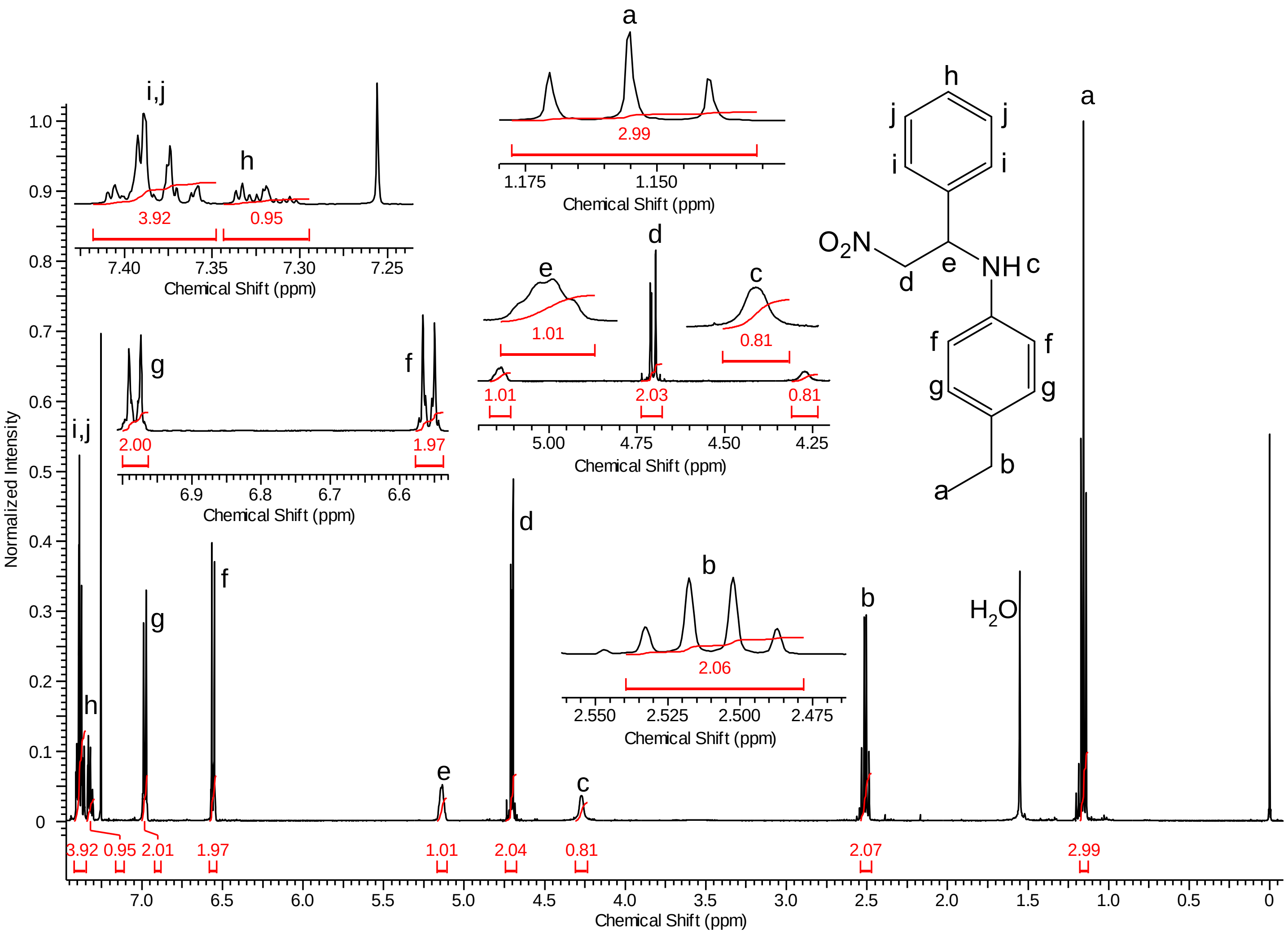

Figure 1.116: $^1$H NMR spectrum of **8e** 4-ethyl-*N*-(2-nitro-1-phenylethyl)aniline.

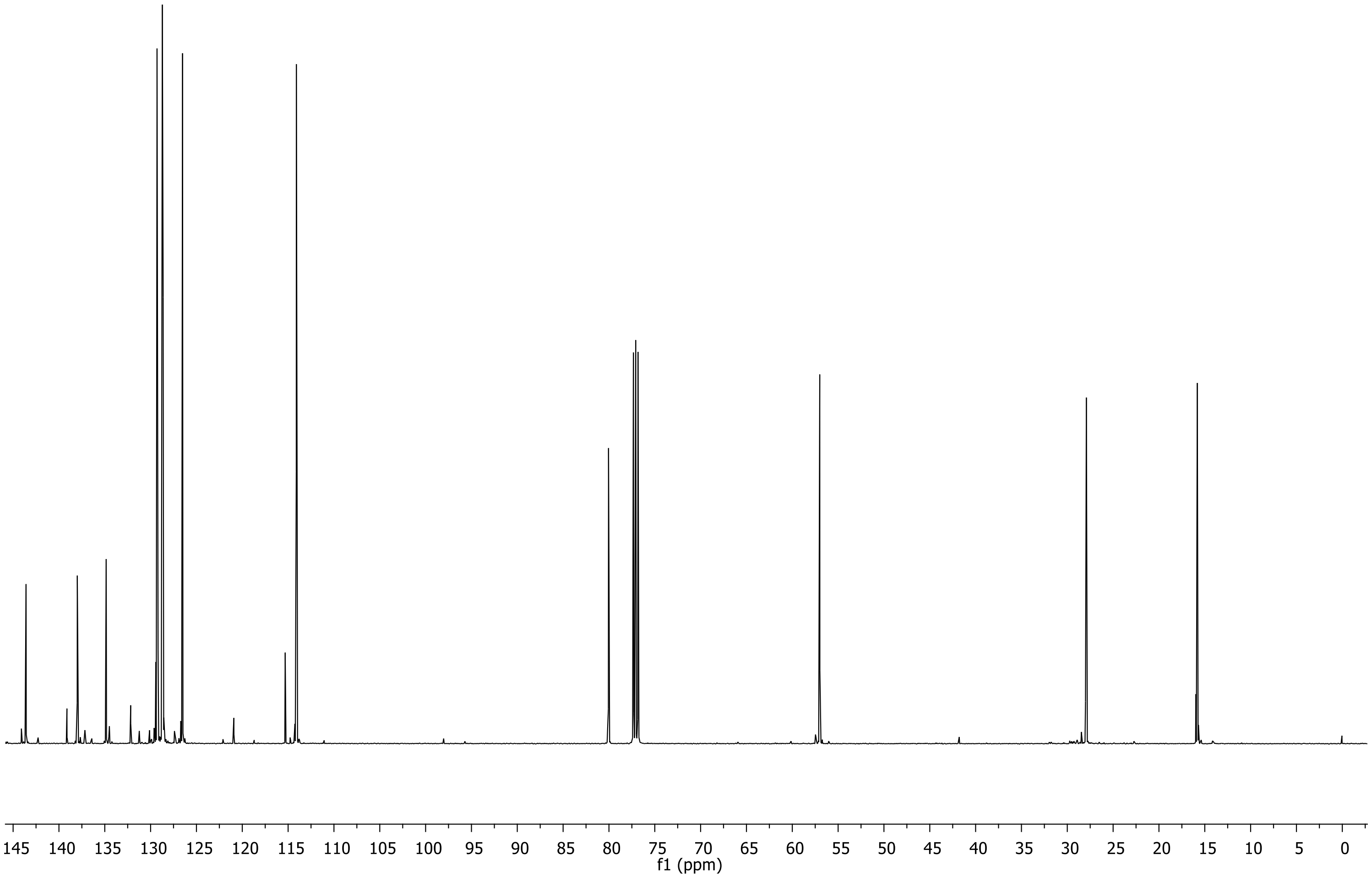

Figure 1.117: $^{13}$C NMR spectrum of **8e** 4-ethyl-*N*-(2-nitro-1-phenylethyl)aniline.

Table 1.16: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **8e** | 270.3 | 1 | 271.08 | 20 | 121.37 | 16 | ES+ |
| | | 2 | 271.08 | 20 | 103.69 | 32 | ES+ |
| | | 3 | 271.08 | 20 | 104.01 | 26 | ES+ |
| | | 4 | 271.08 | 20 | 210.11 | 10 | ES+ |
| | | 5 | 271.08 | 20 | 78.06 | 50 | ES+ |

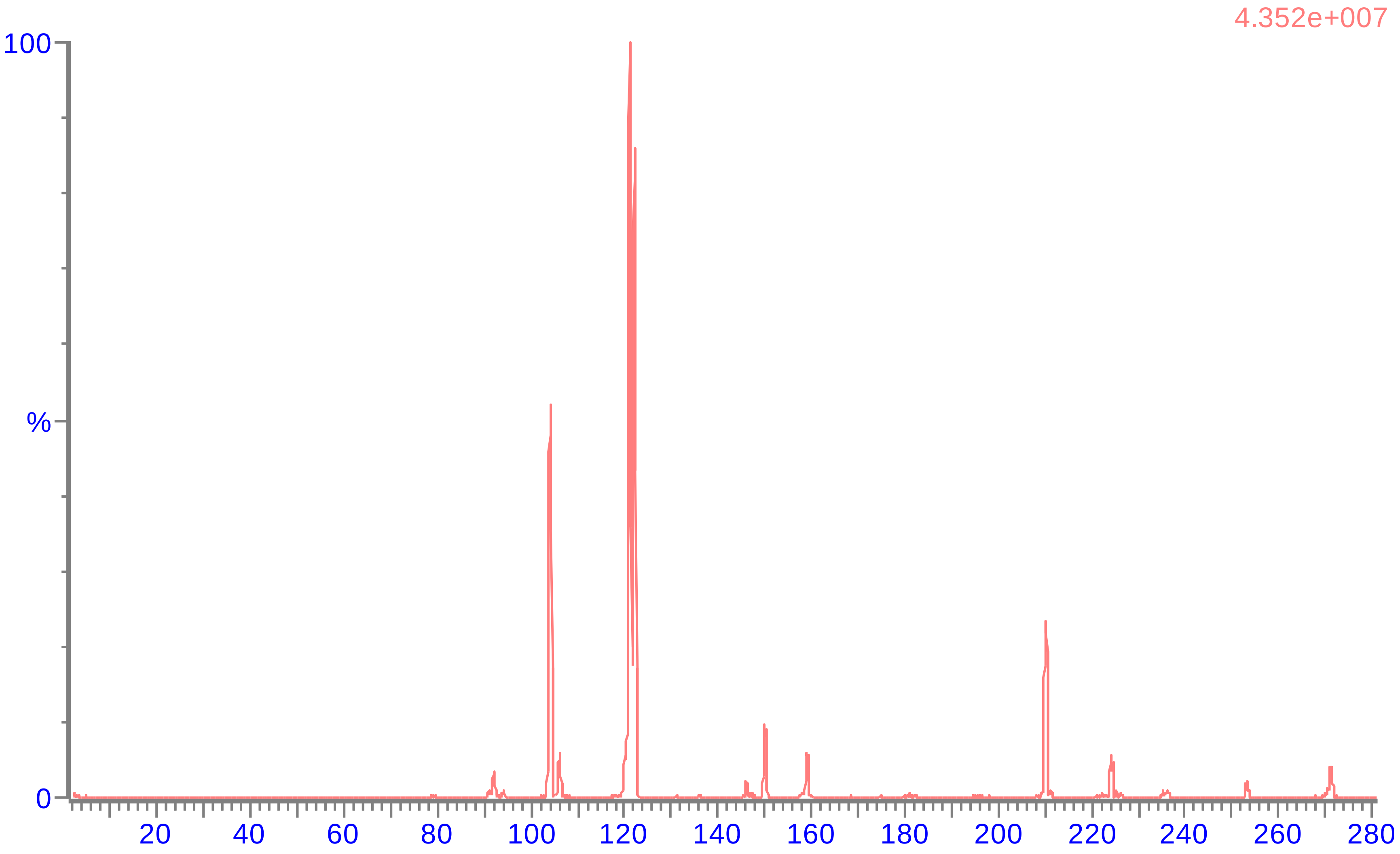

Figure 1.118: Mass spectrum for daughter fragment peak ES+, m/z 271.08 -> 121.37.

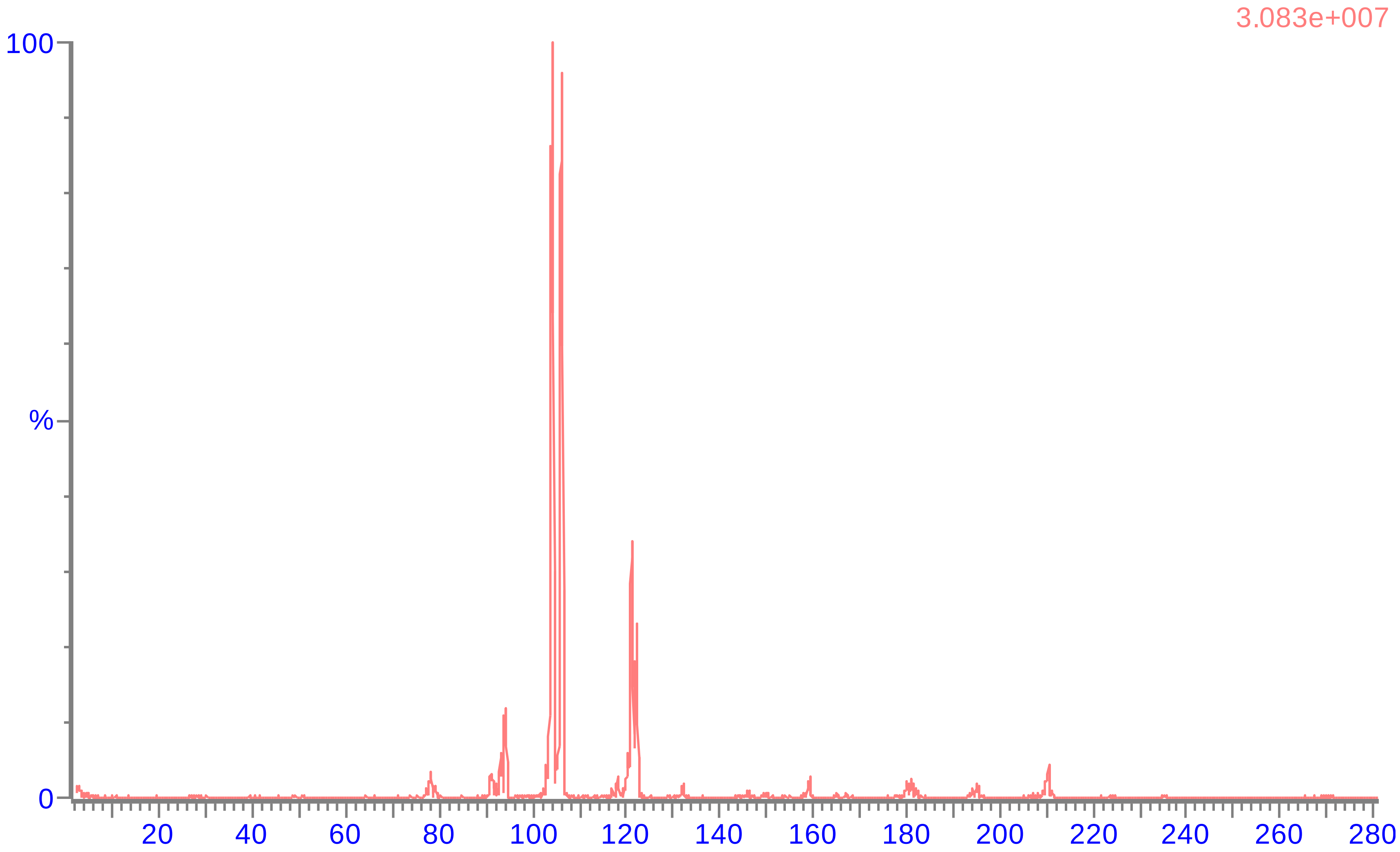

Figure 1.119: Mass spectrum for daughter fragment peak ES+, m/z 271.08 -> 103.69.

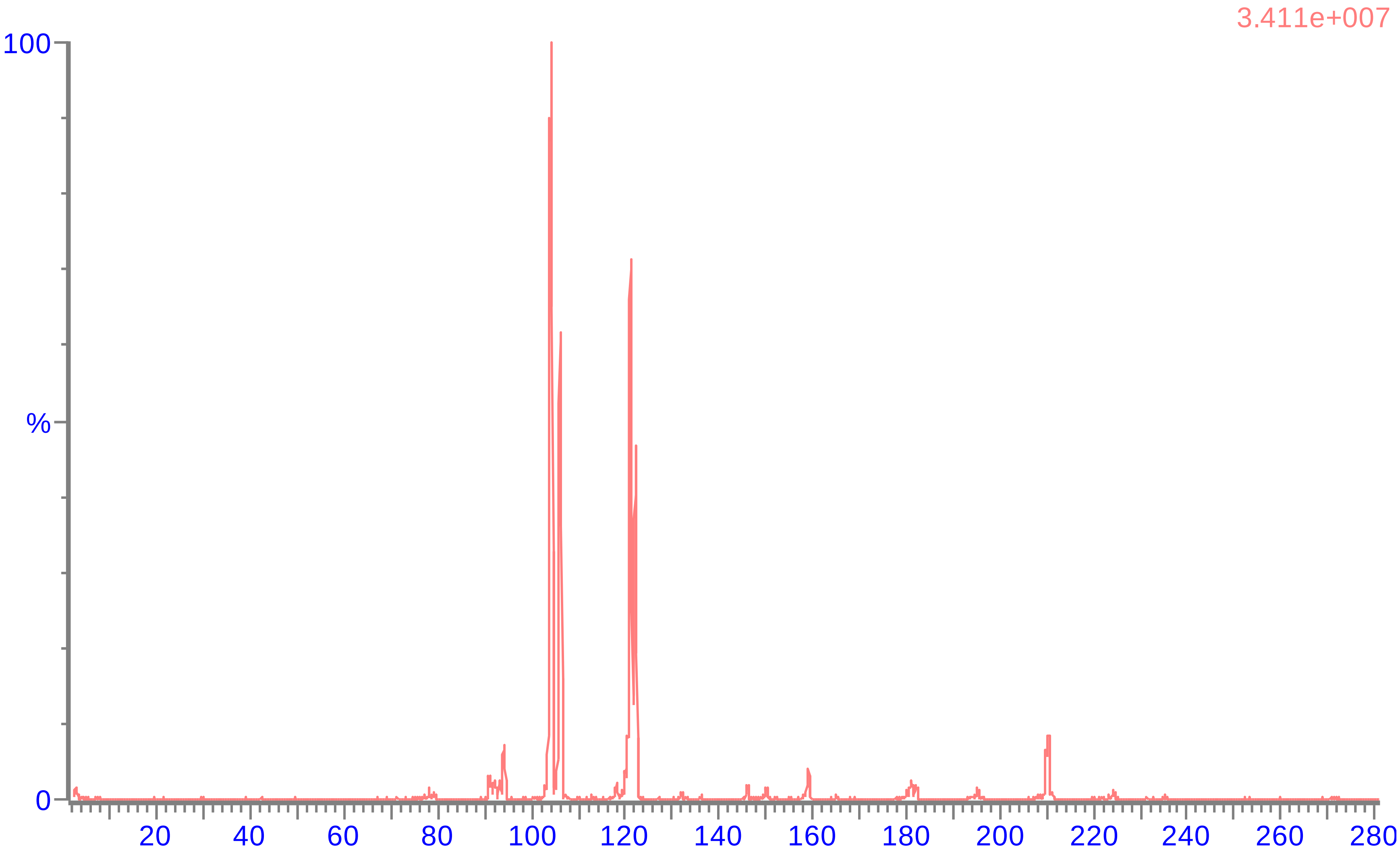

Figure 1.120: Mass spectrum for daughter fragment peak ES+, m/z 271.08 -> 104.01.

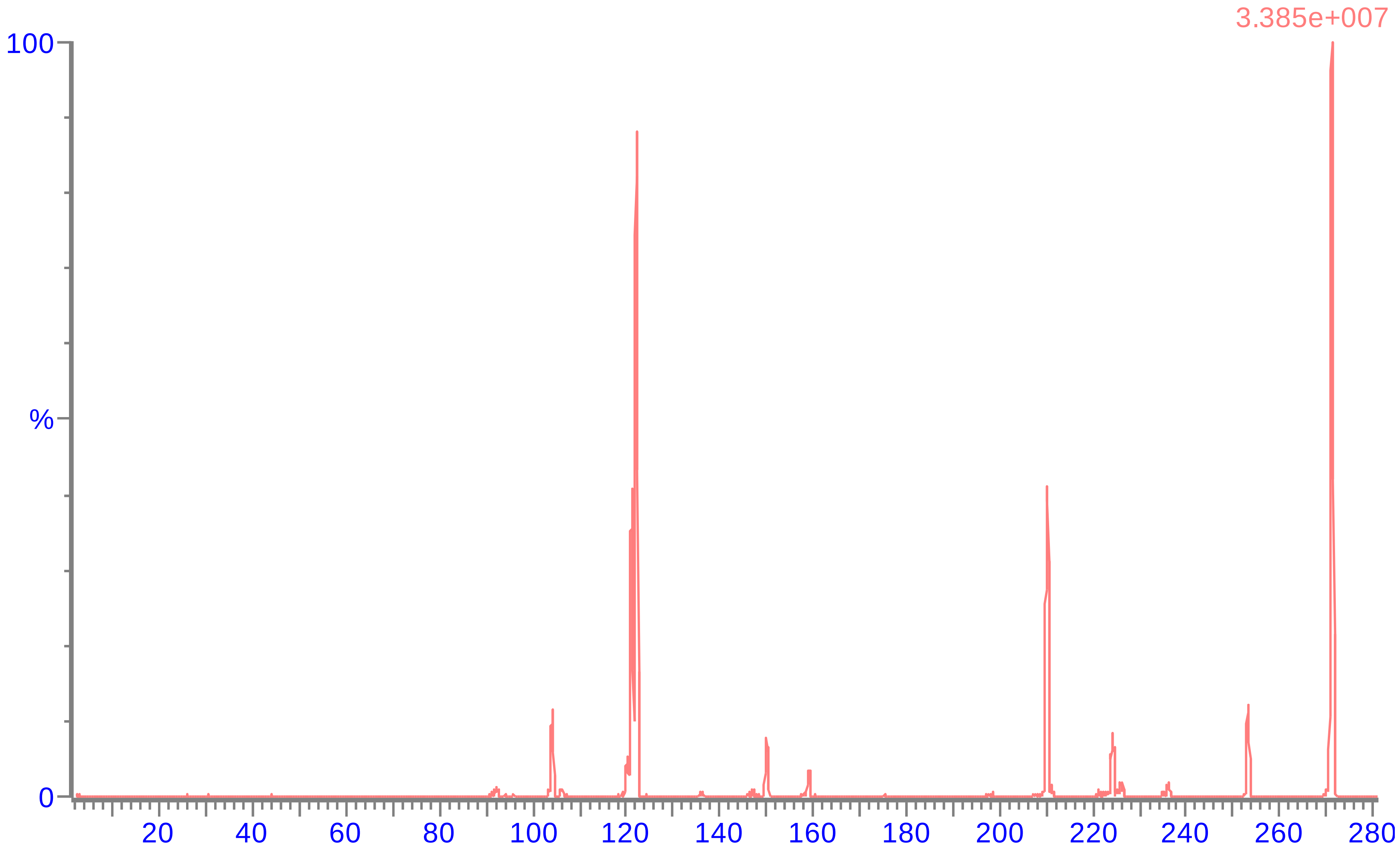

Figure 1.121: Mass spectrum for daughter fragment peak ES+, m/z 271.08 -> 210.11.

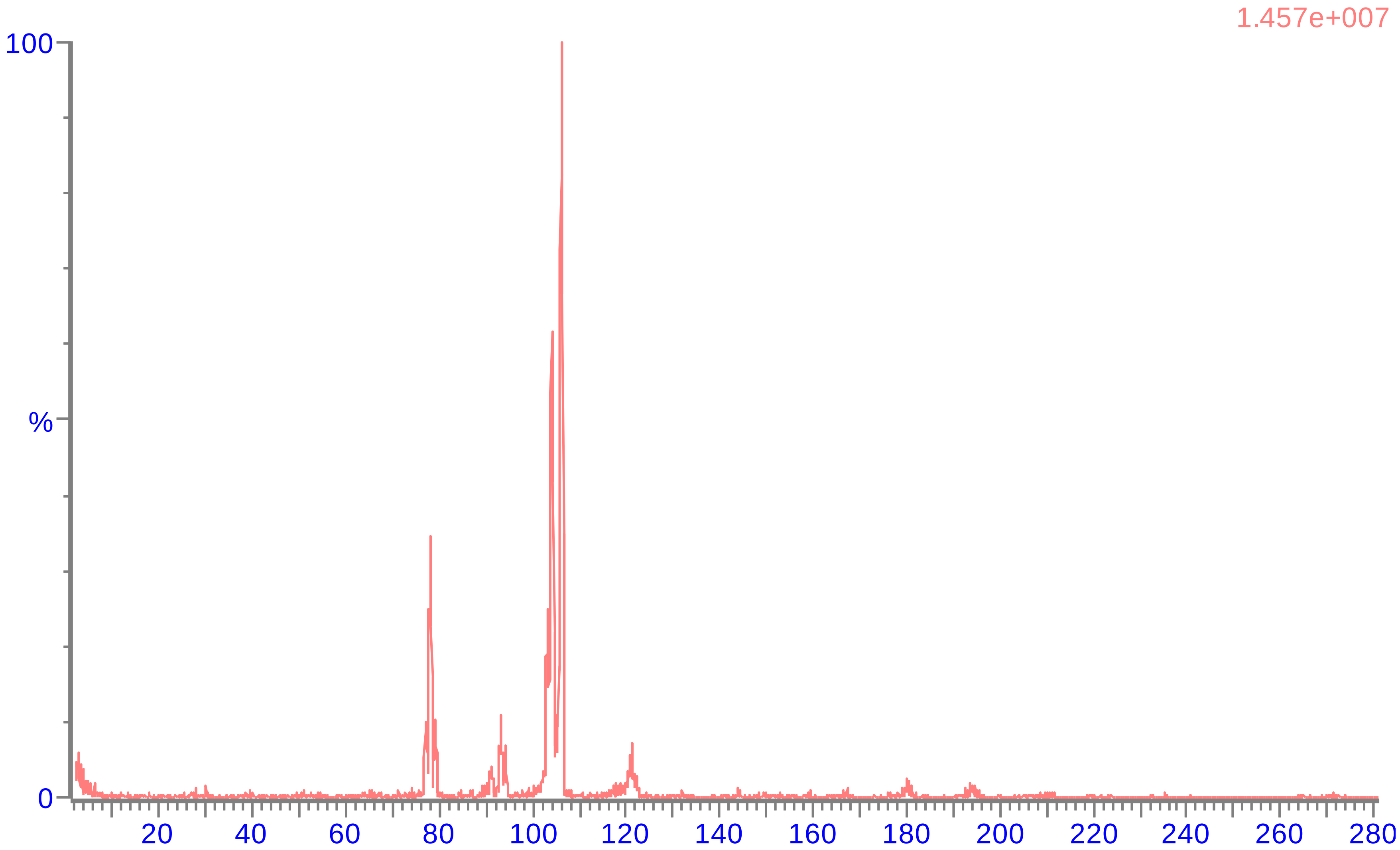

Figure 1.122: Mass spectrum for daughter fragment peak ES+, m/z 271.08 -> 78.06.

**8f** 4-bromo-*N*-(2-nitro-1-phenylethyl)aniline

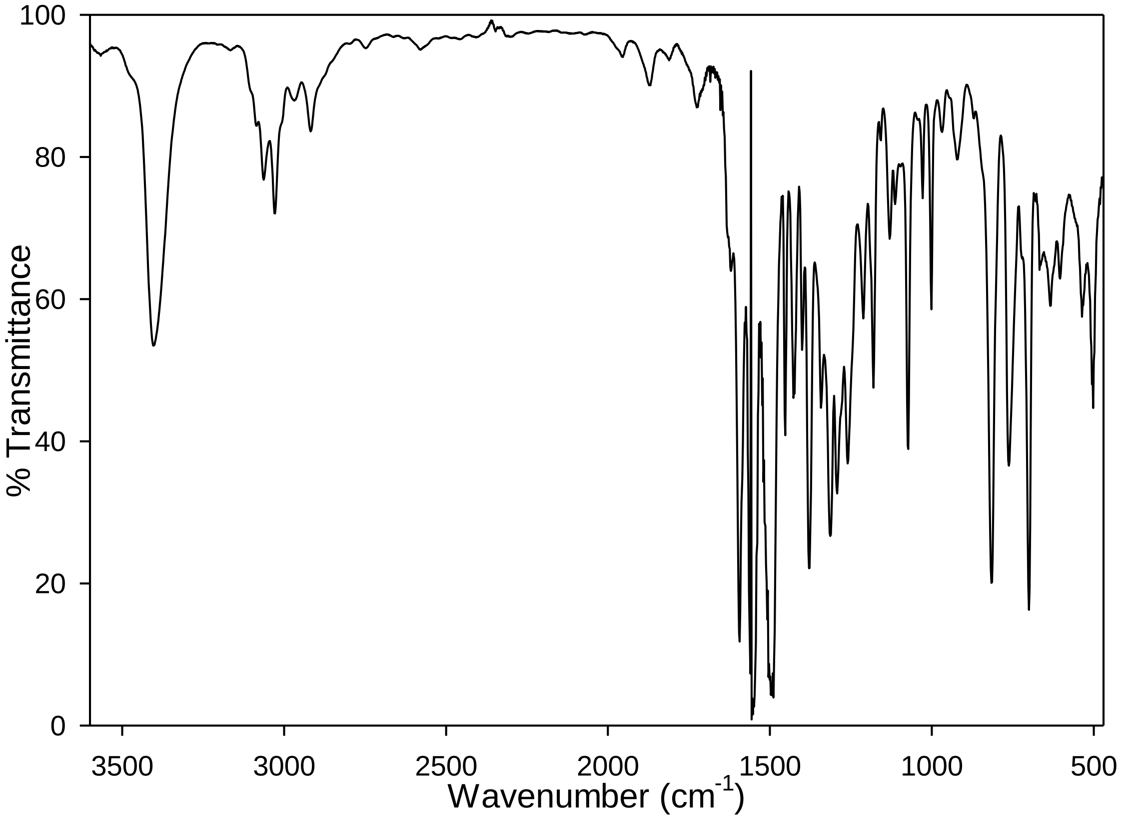

Figure 1.123: IR spectrum of **8f** 4-bromo-*N*-(2-nitro-1-phenylethyl)aniline.

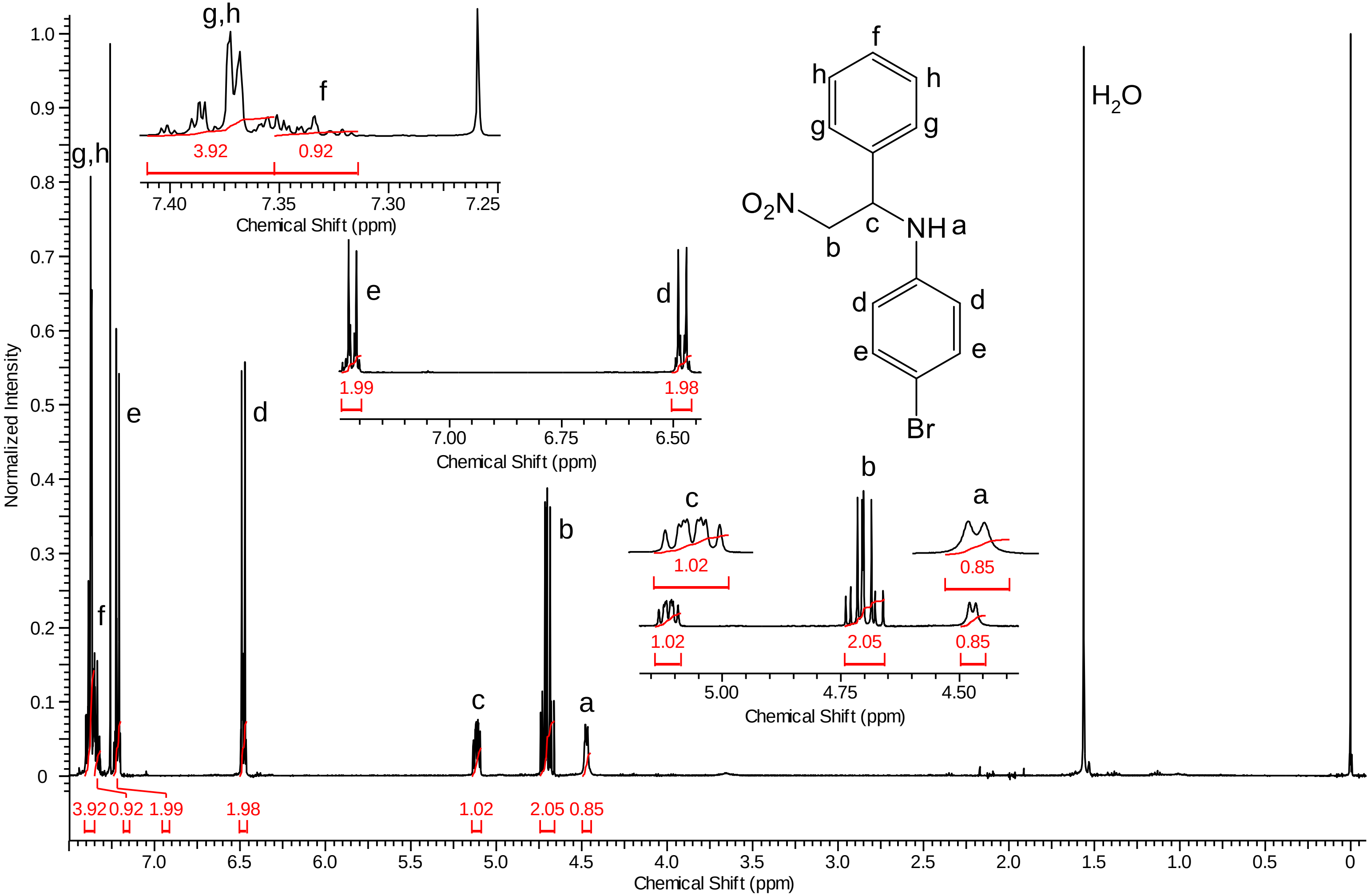

Figure 1.124: $^1$H NMR spectrum of **8f** 4-bromo-*N*-(2-nitro-1-phenylethyl)aniline.

Table 1.17: MS data.

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **8f** | 320 | 1 | 321.03 | 22 | 104.06 | 22 | ES+ |
| | | 2 | 321.03 | 22 | 171.96 | 10 | ES+ |
| | | 3 | 321.03 | 22 | 150.05 | 14 | ES+ |
| | | 4 | 321.03 | 22 | 77.98 | 60 | ES+ |
| | | 5 | 321.03 | 22 | 260.03 | 12 | ES+ |

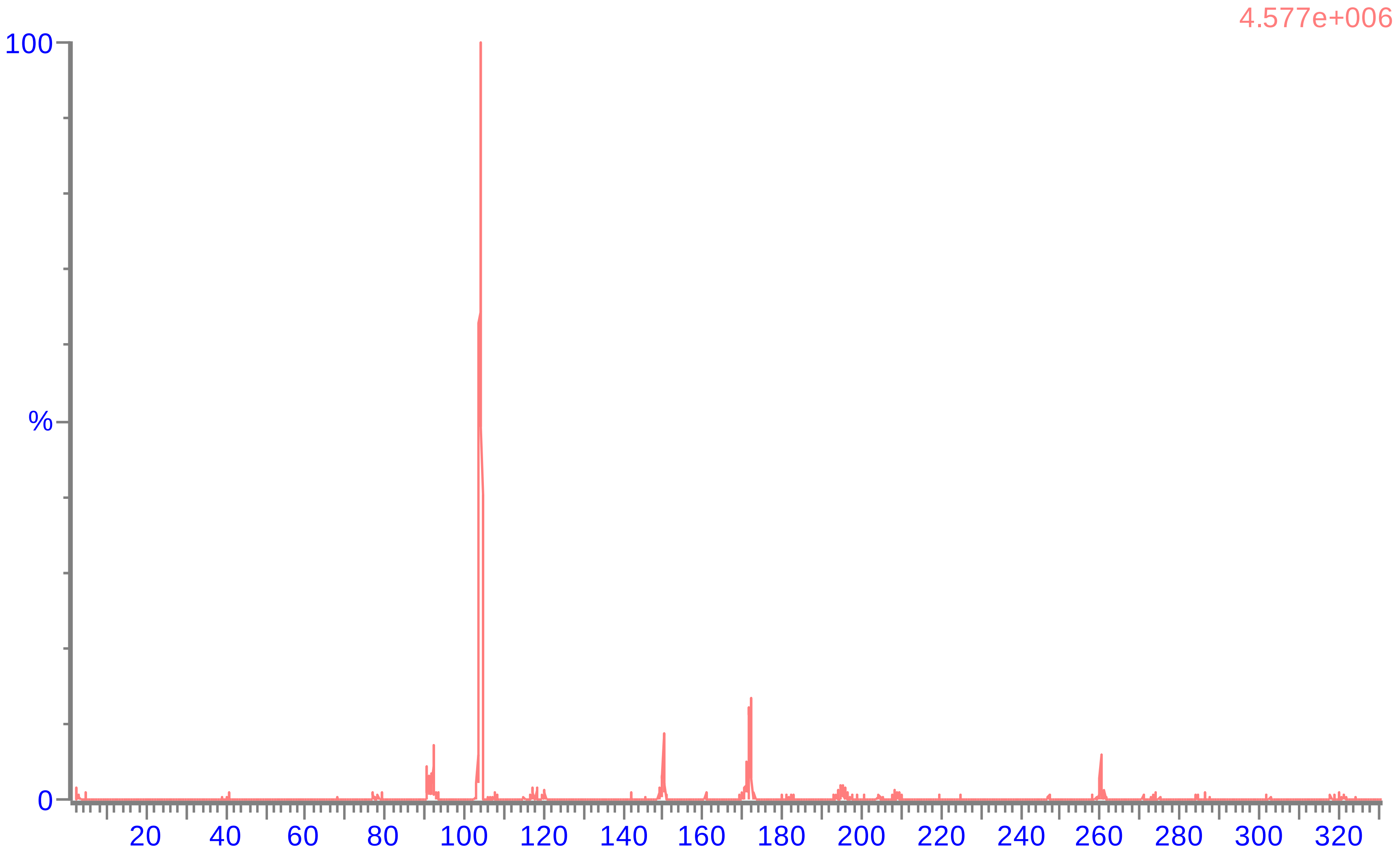

Figure 1.125: Mass spectrum for daughter fragment peak ES+, m/z 321.03 -> 104.06.

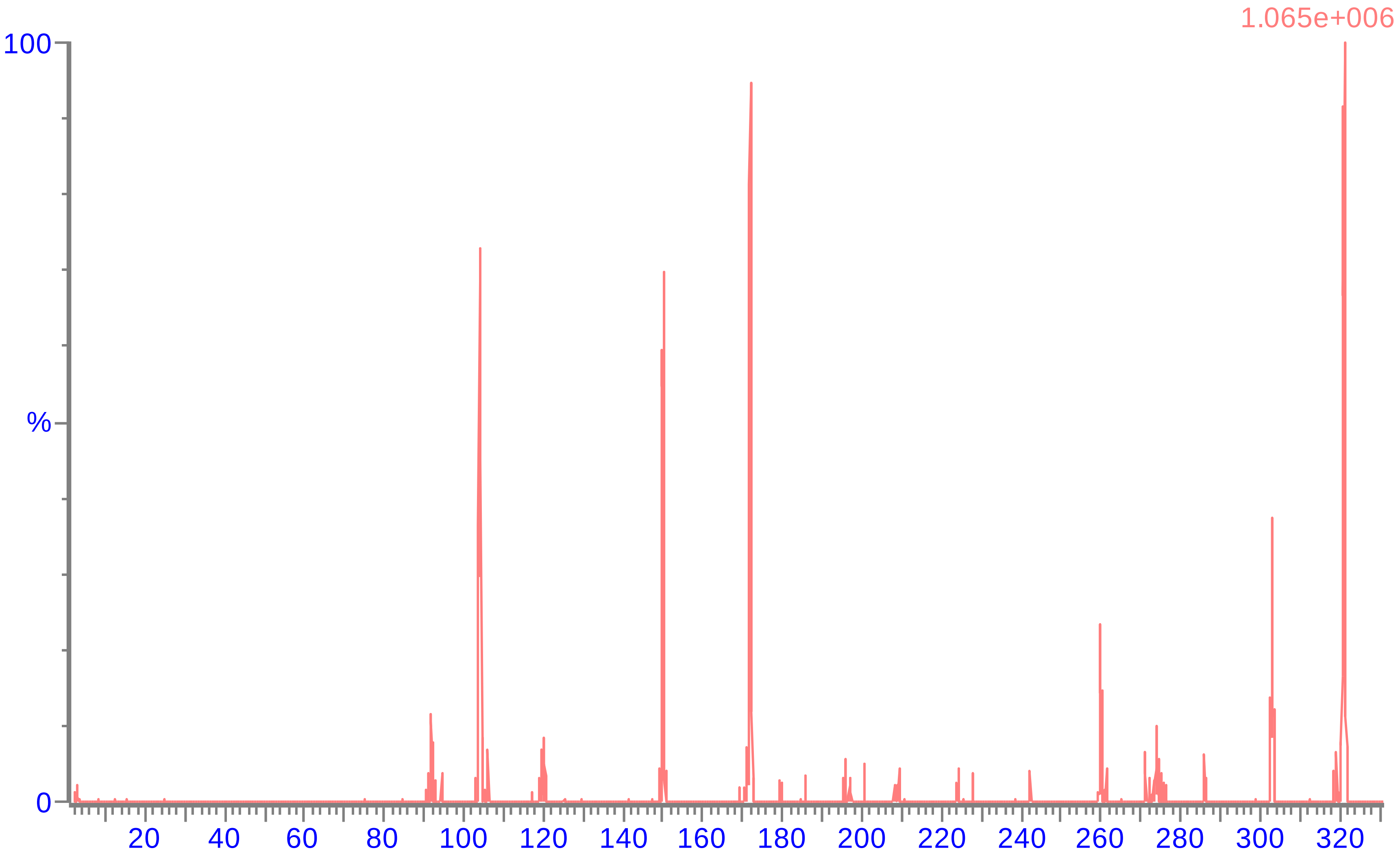

Figure 1.126: Mass spectrum for daughter fragment peak ES+, m/z 321.03 -> 171.96.

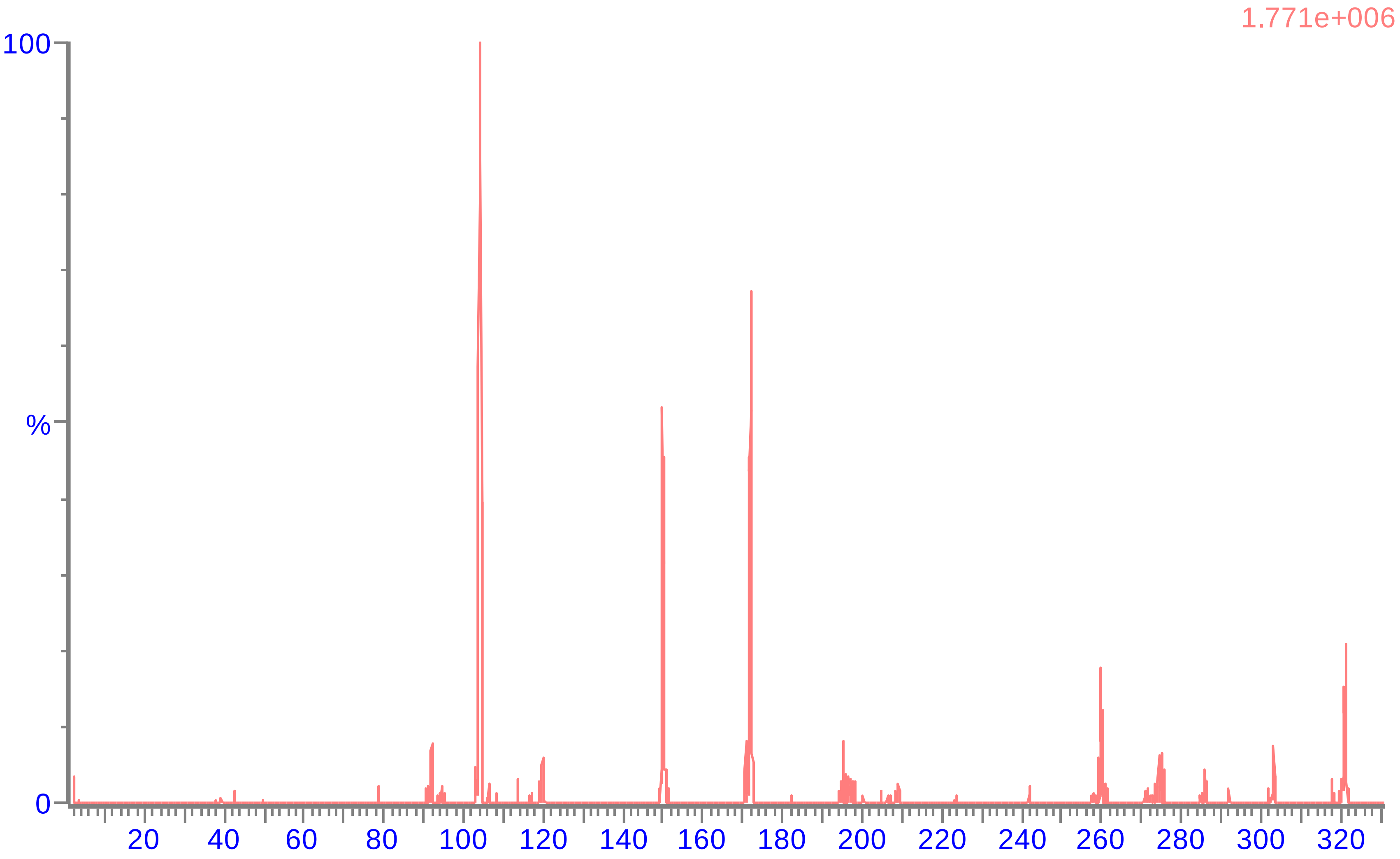

Figure 1.127: Mass spectrum for daughter fragment peak ES+, m/z 321.03 -> 150.05.

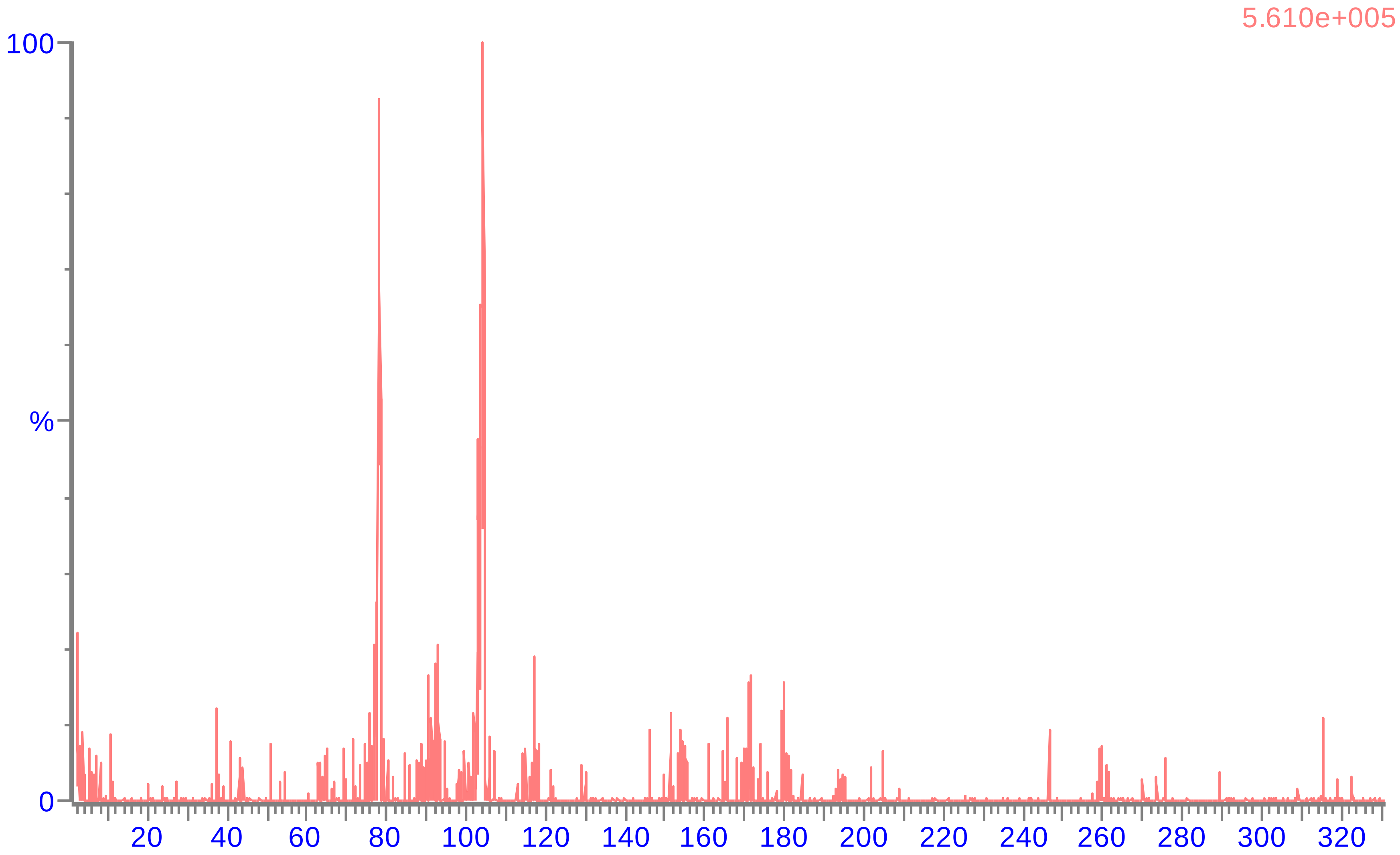

Figure 1.128: Mass spectrum for daughter fragment peak ES+, m/z 321.03 -> 77.98.

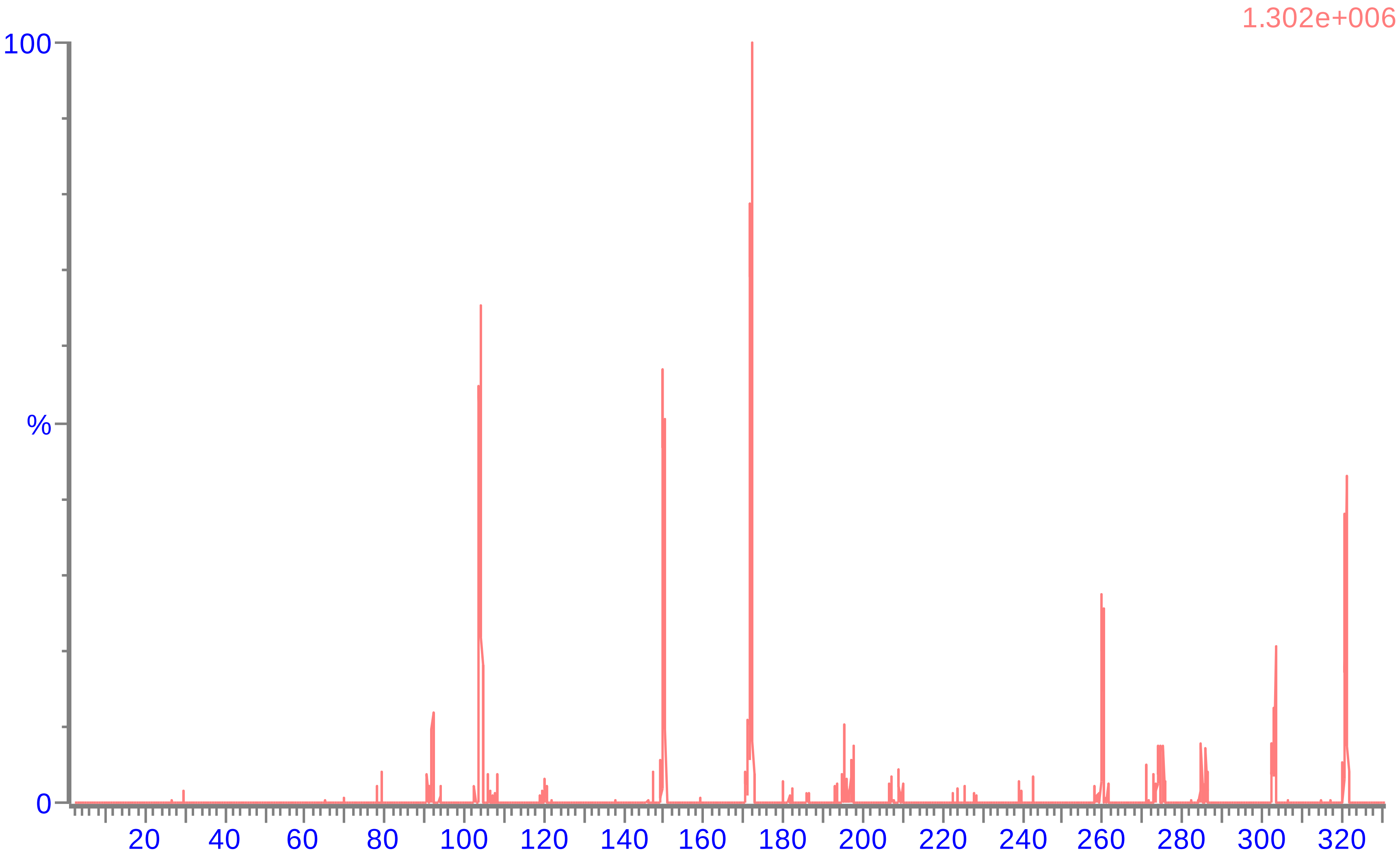

Figure 1.129: Mass spectrum for daughter fragment peak ES+, m/z 321.03 -> 260.03.

**8g** 4-chloro-*N*-(2-nitro-1-phenylethyl)aniline

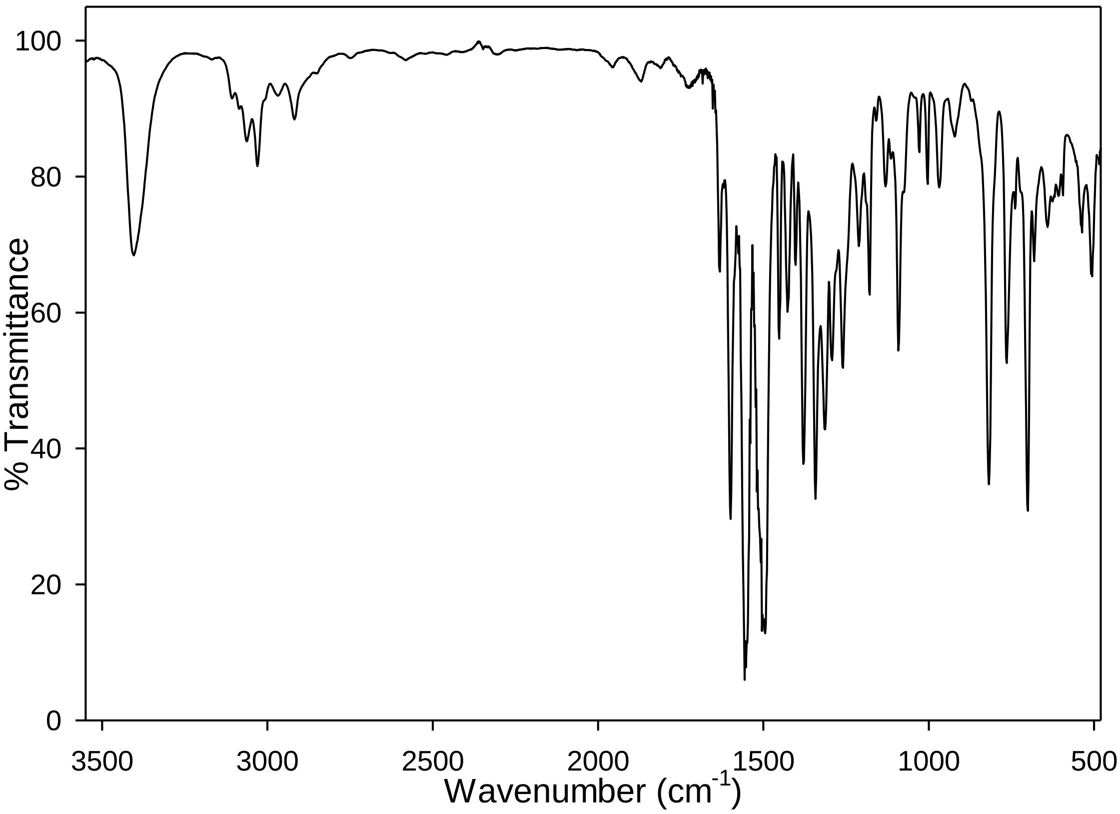

Figure 1.130: IR spectrum of **8g** 4-chloro-*N*-(2-nitro-1-phenylethyl)aniline.

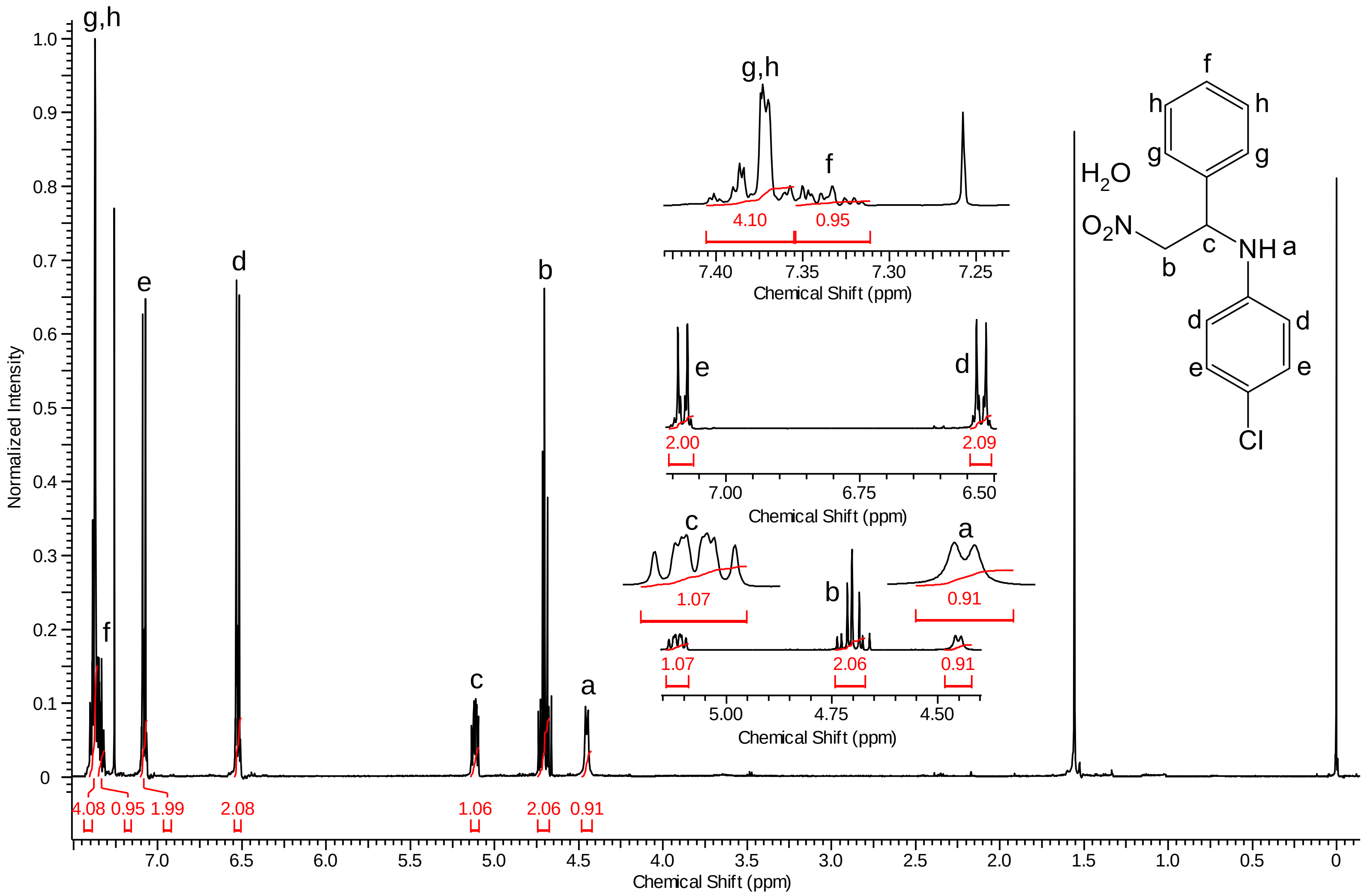

Figure 1.131: $^1$H NMR spectrum of **8g** 4-chloro-*N*-(2-nitro-1-phenylethyl)aniline.

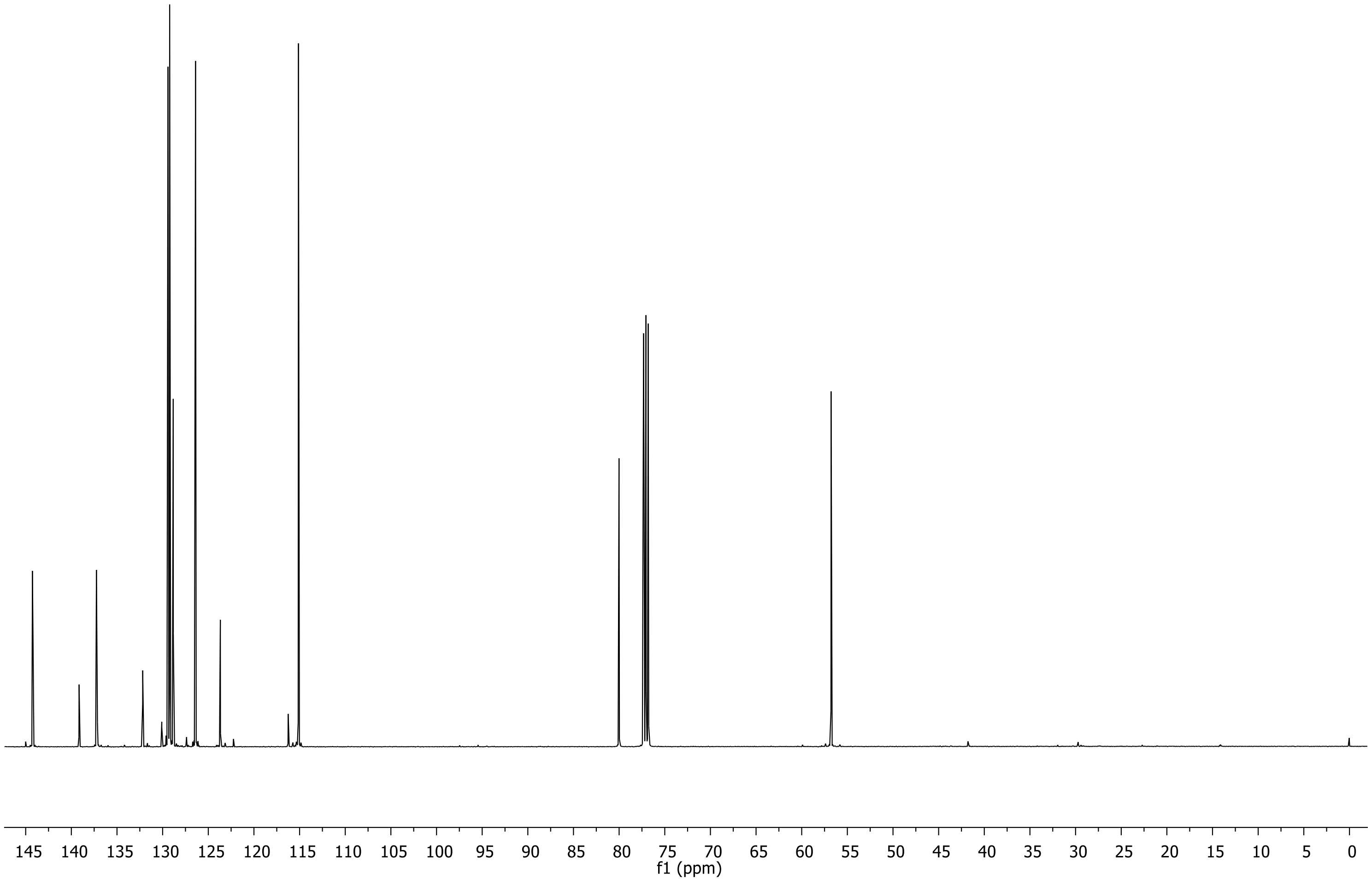

Figure 1.132: $^1$H NMR spectrum of **8g** 4-chloro-*N*-(2-nitro-1-phenylethyl)aniline.

Table 1.18: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **8g** | 276.8 | 1 | 277.07 | 24 | 128.02 | 12 | ES+ |
| | | 2 | 277.07 | 24 | 216.05 | 10 | ES+ |

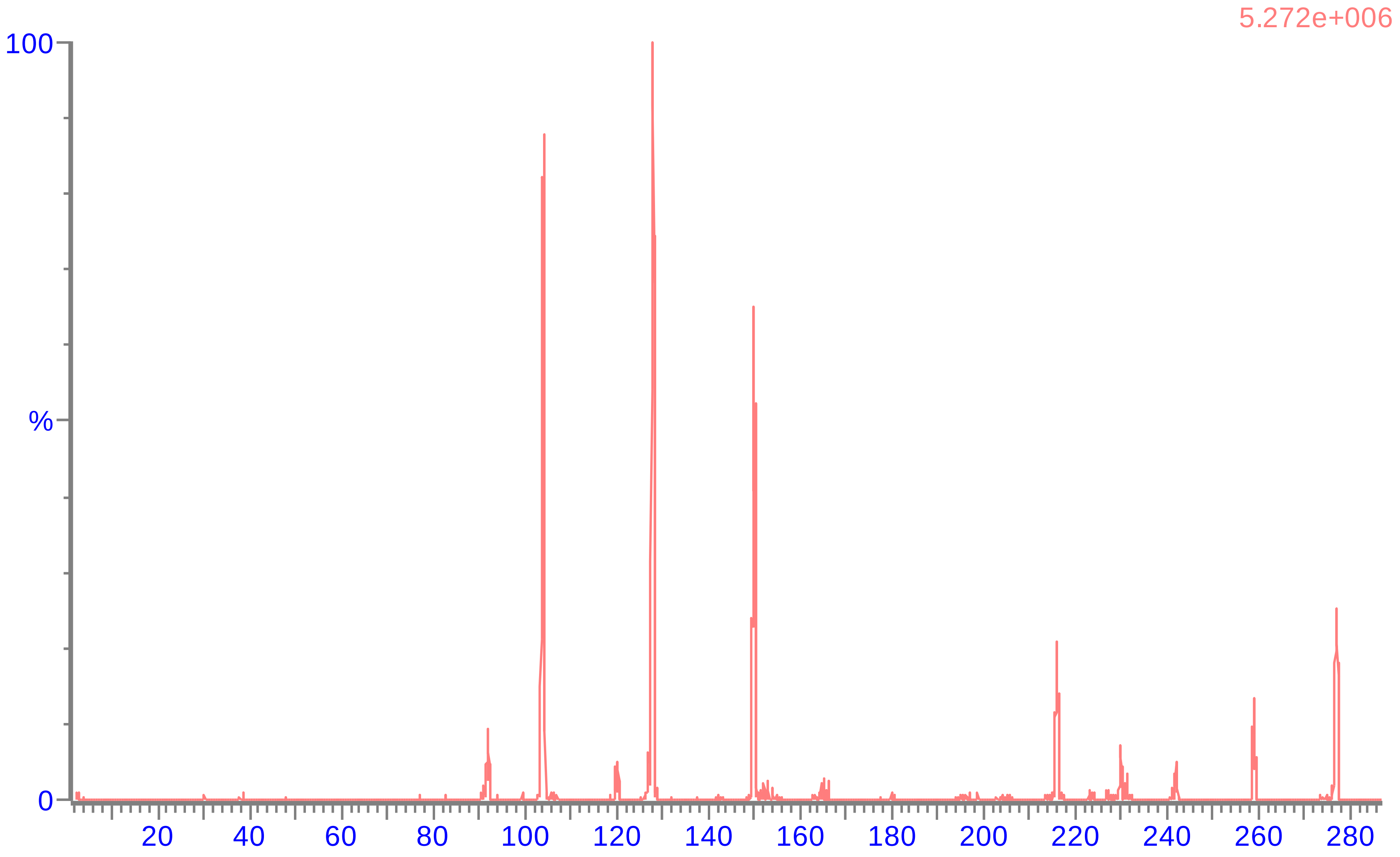

Figure 1.133: Mass spectrum for daughter fragment peak ES+, m/z 277.07 -> 128.02.

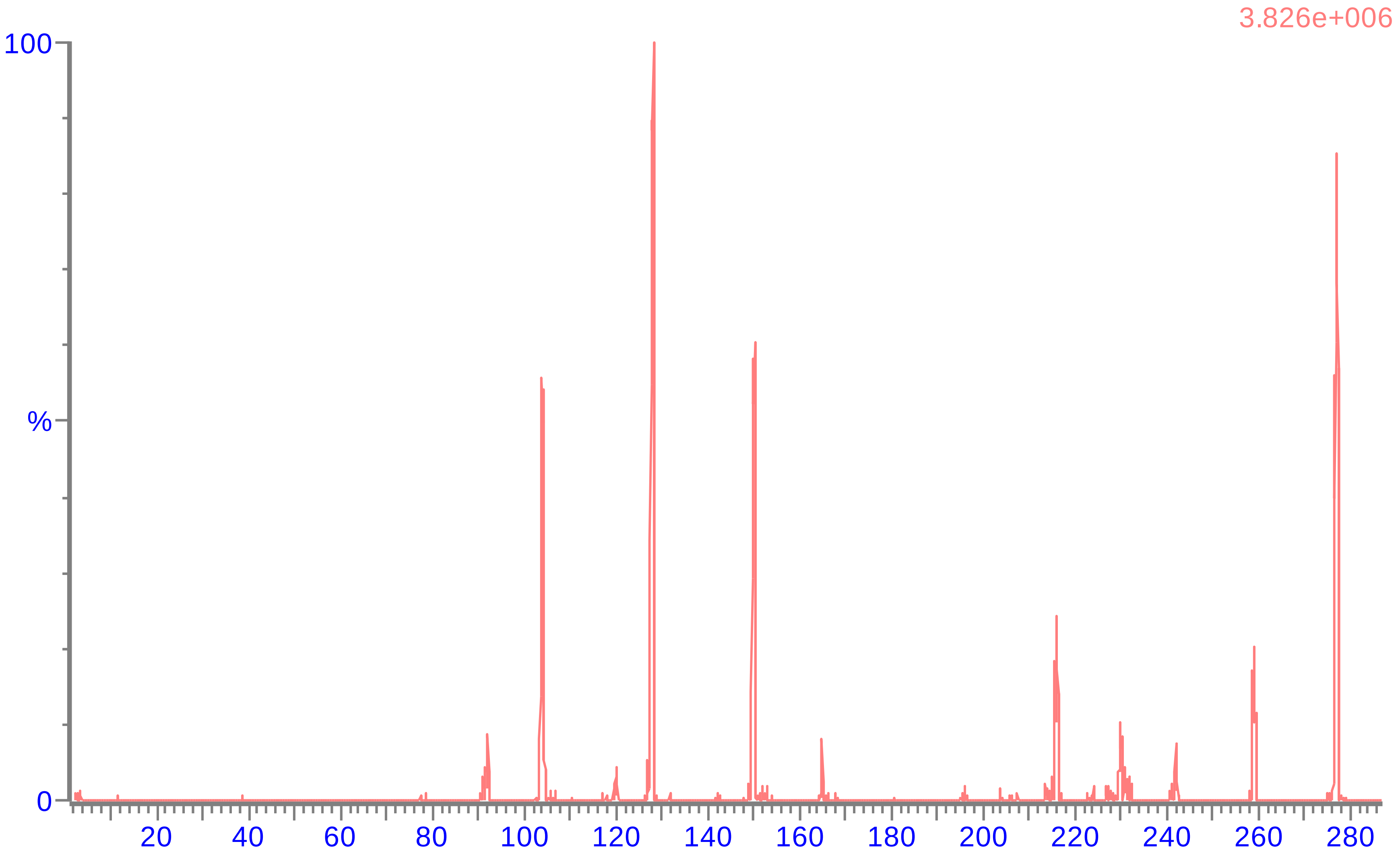

Figure 1.134: Mass spectrum for daughter fragment peak ES+, m/z 277.07 -> 216.05.

**8h** 1-(4-((2-nitro-1-phenylethyl)amino)phenyl)ethanone

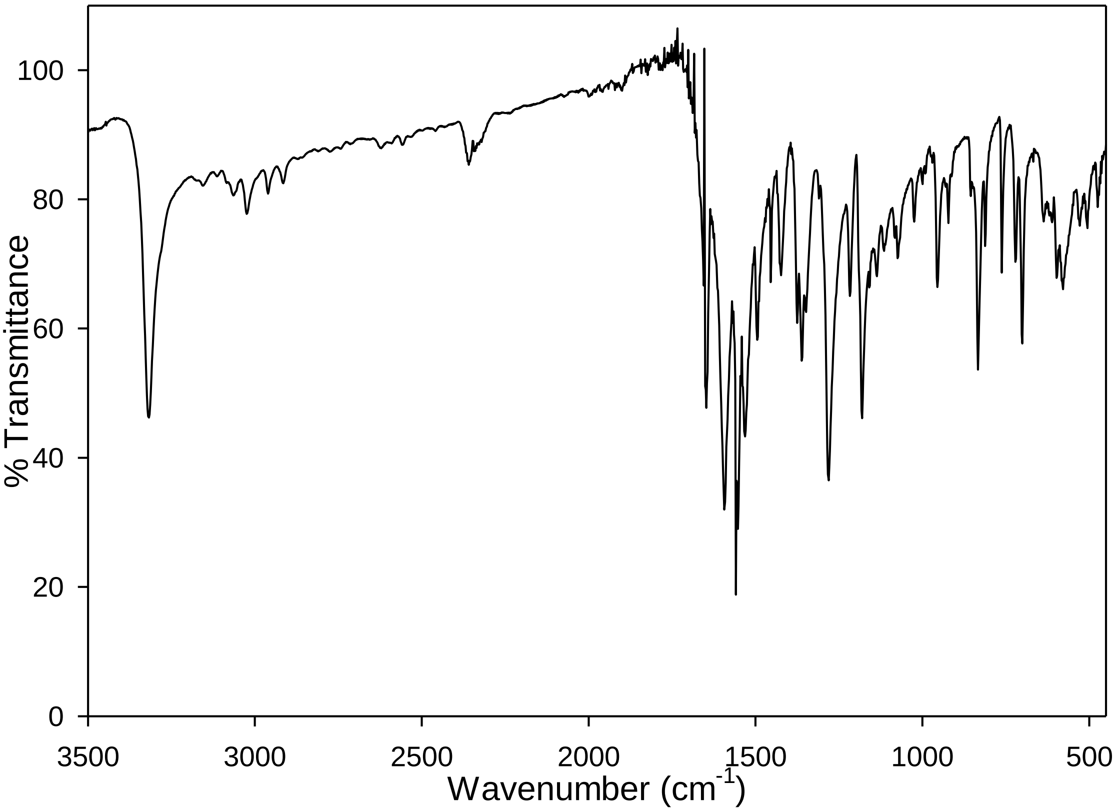

Figure 1.135: IR spectrum of **8h**
1-(4-((2-nitro-1-phenylethyl)amino)phenyl)ethanone.

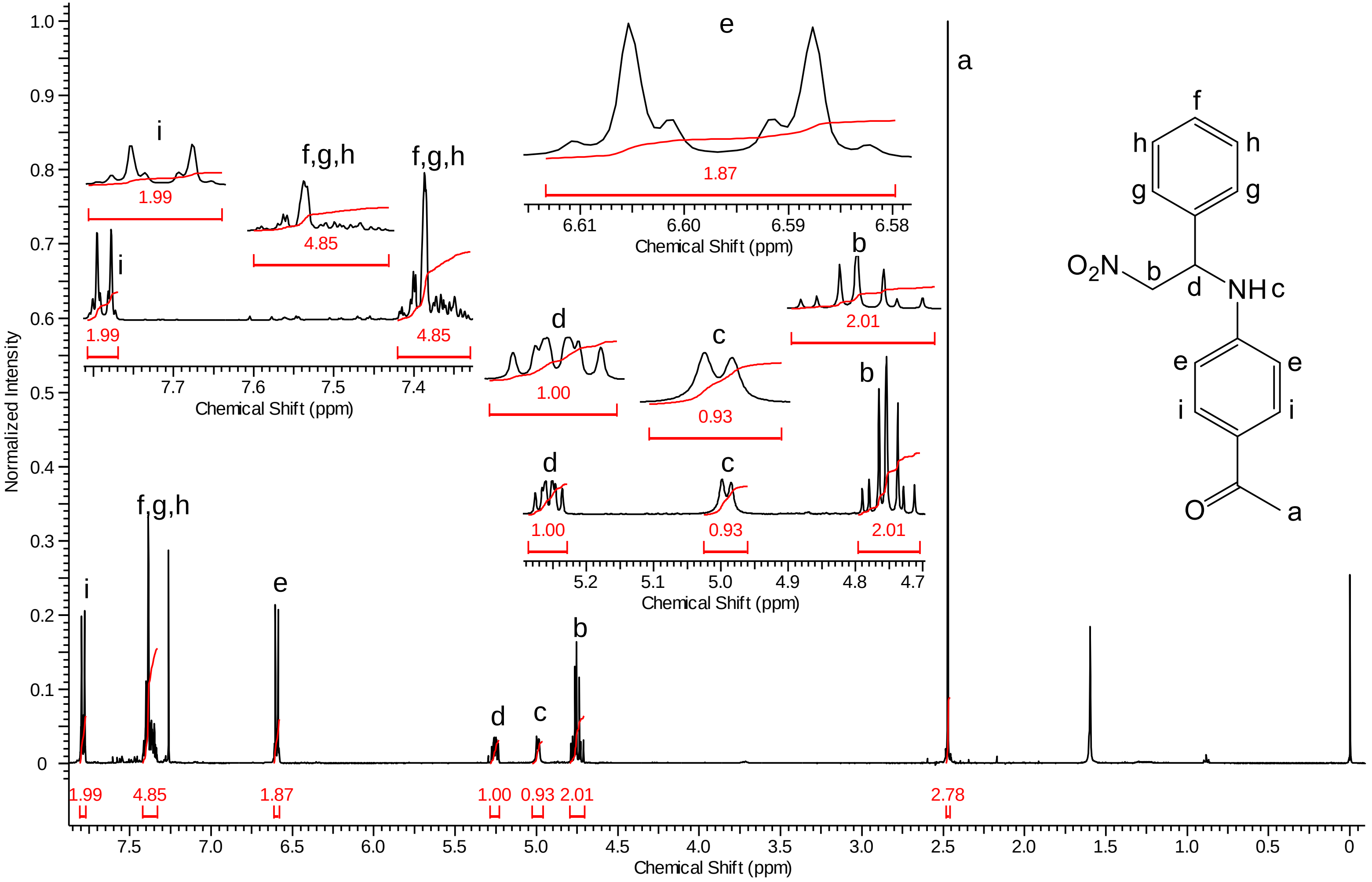

Figure 1.136: $^1$H NMR spectrum of **8h** 1-(4-((2-nitro-1-phenylethyl)amino)phenyl)ethanone.

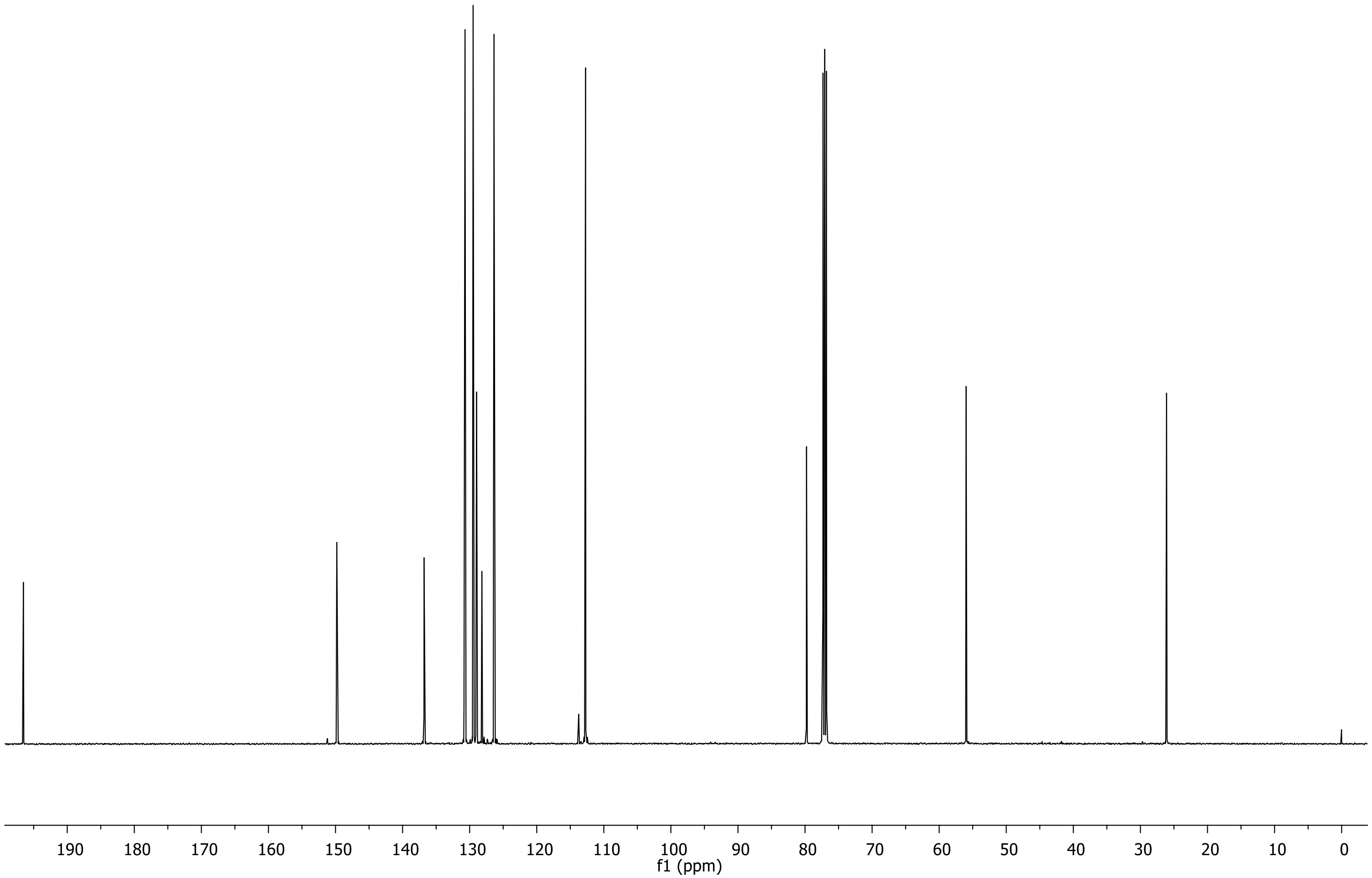

Figure 1.137: $^{13}$C NMR spectrum of **8h** 1-(4-((2-nitro-1-phenylethyl)amino)phenyl)ethanone.

Table 1.19: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **8h** | 284 | 1 | 285.10 | 34 | 135.09 | 22 | ES+ |
| | | 2 | 285.10 | 34 | 224.14 | 16 | ES+ |
| | | 3 | 285.10 | 34 | 42.99 | 48 | ES+ |
| | | 4 | 285.10 | 34 | 93.08 | 40 | ES+ |
| | | 5 | 285.10 | 34 | 104.07 | 32 | ES+ |

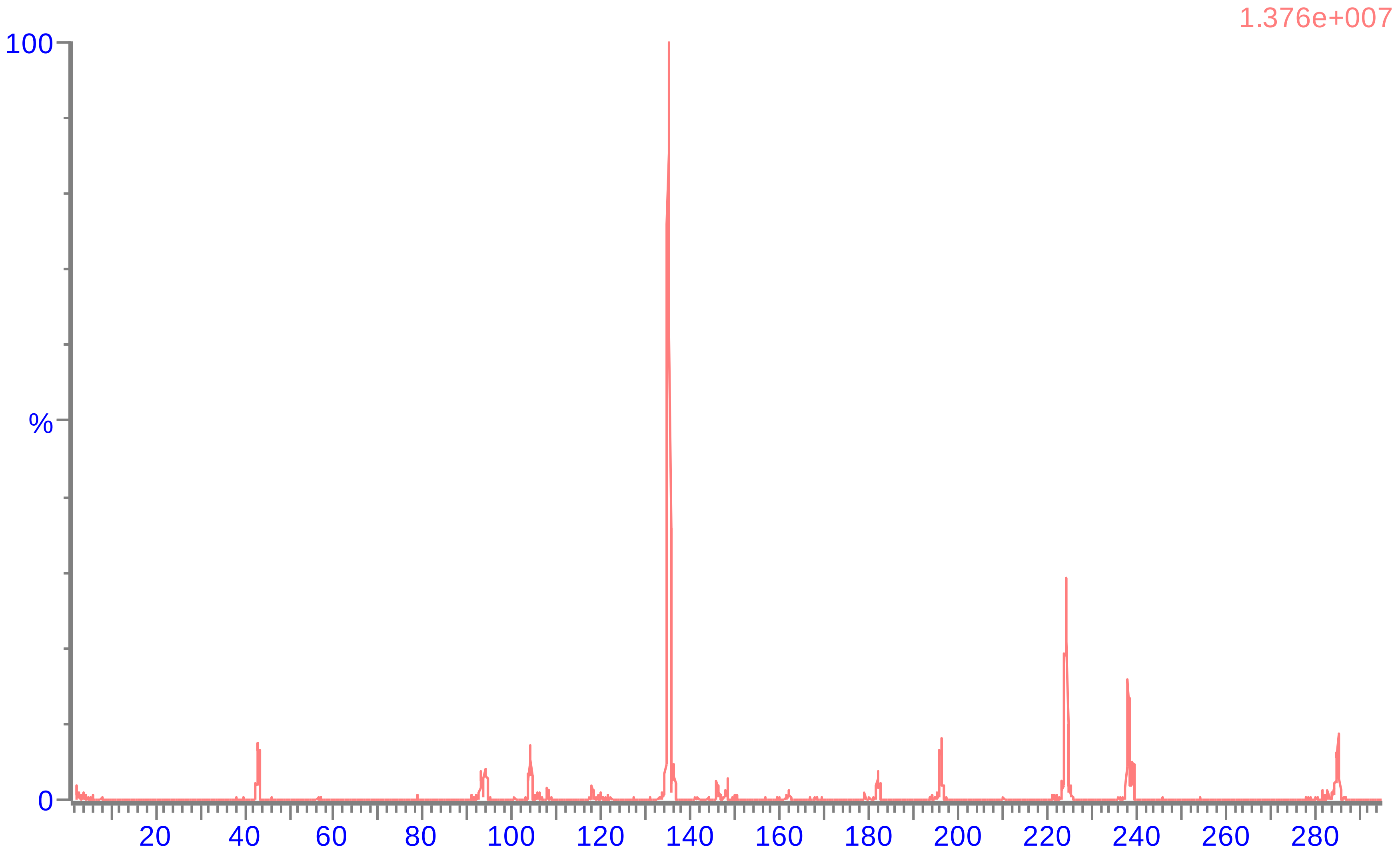

Figure 1.138: Mass spectrum for daughter fragment peak ES+, m/z 285.10 -> 135.09.

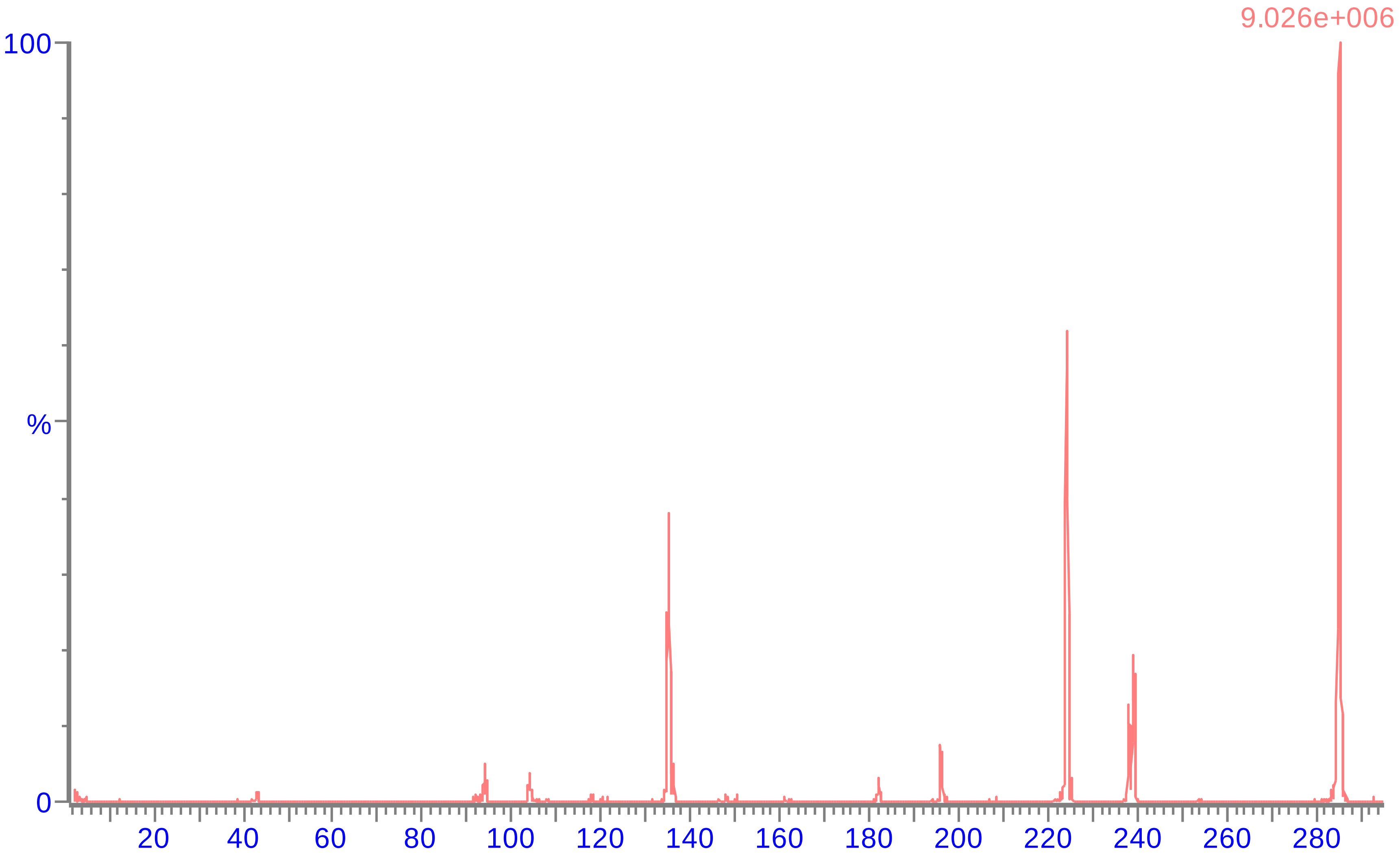

Figure 1.139: Mass spectrum for daughter fragment peak ES+, m/z 285.10 -> 224.14.

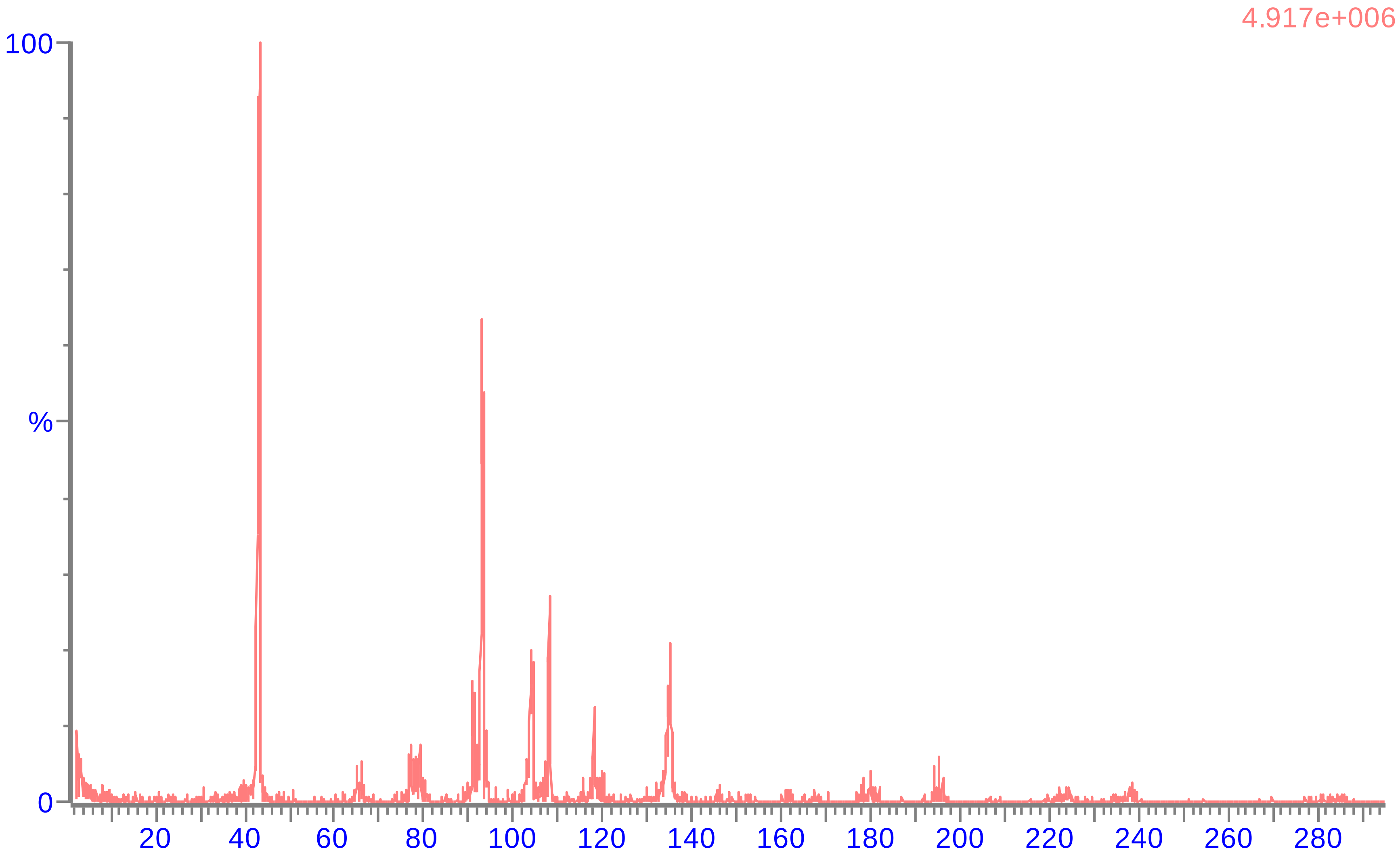

Figure 1.140: Mass spectrum for daughter fragment peak ES+, m/z 285.10 -> 42.99.

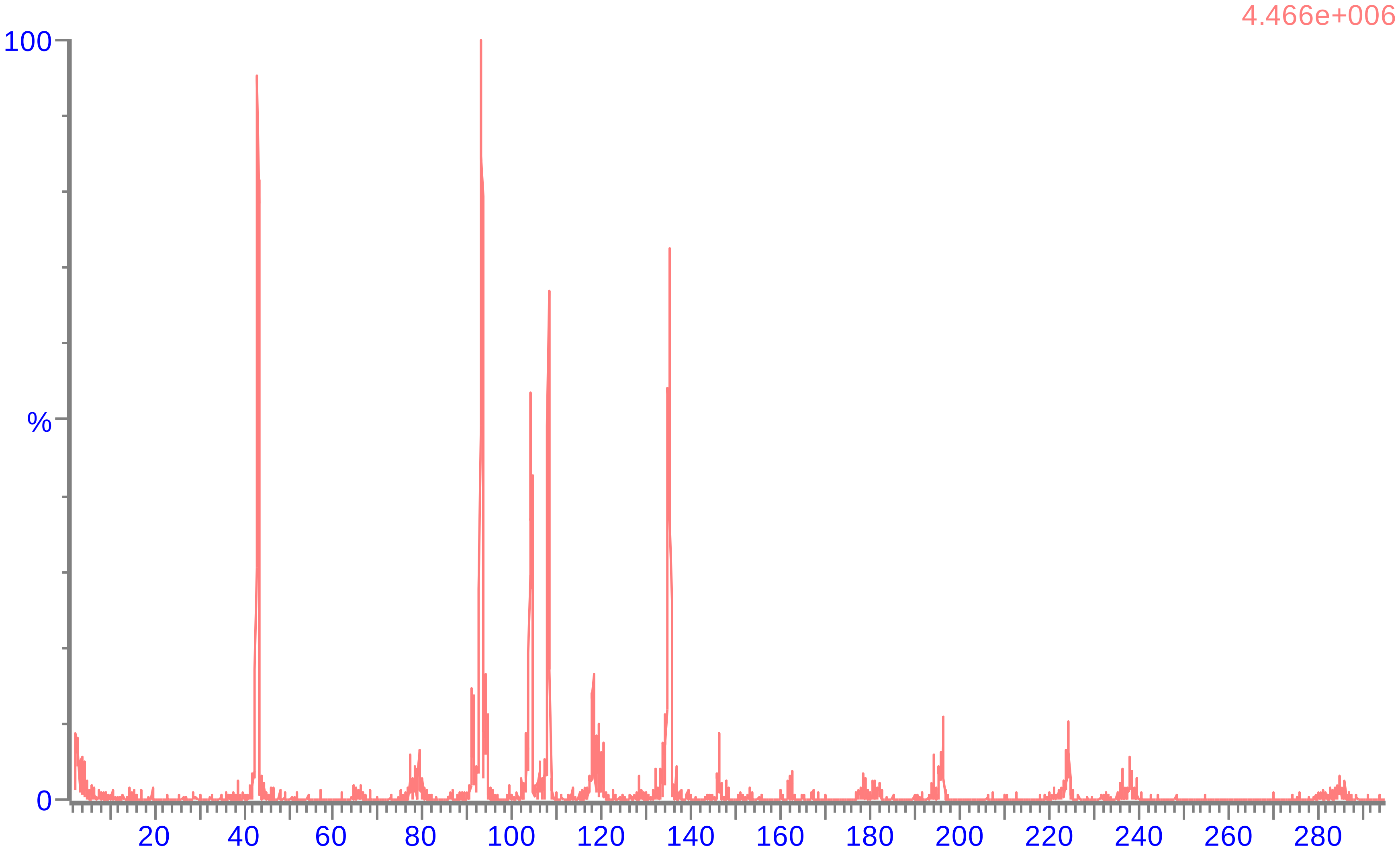

Figure 1.141: Mass spectrum for daughter fragment peak ES+, m/z 285.10 -> 93.08.

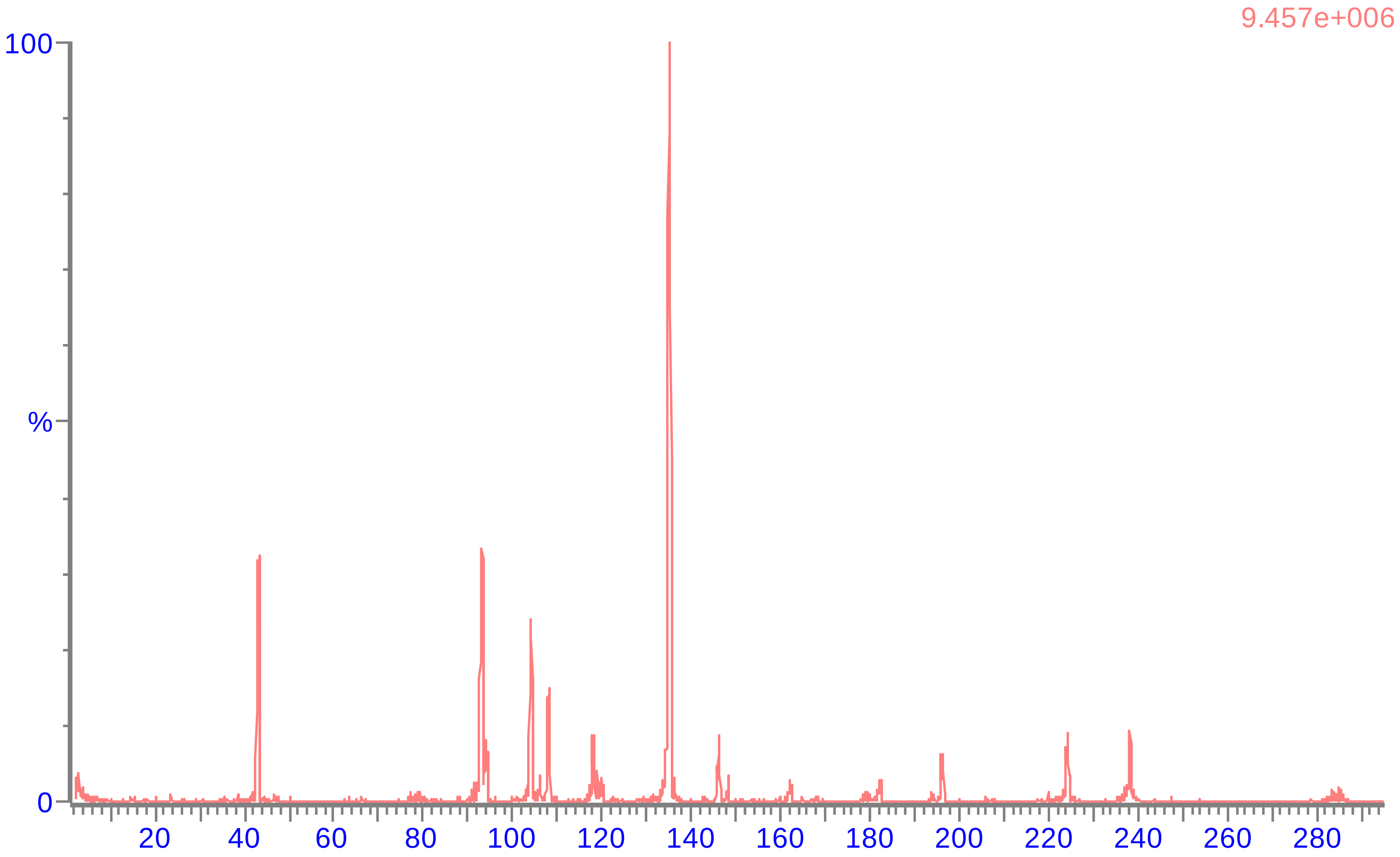

Figure 1.142: Mass spectrum for daughter fragment peak ES+, m/z 285.10 -> 104.07.

**8i** 4-((2-nitro-1-phenylethyl)amino)benzonitrile

Table 1.20: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **8i** | 267 | 1 | 268.10 | 38 | 118.10 | 26 | ES+ |
| | | 2 | 268.10 | 38 | 221.12 | 24 | ES+ |
| | | 3 | 268.10 | 38 | 91.05 | 46 | ES+ |
| | | 4 | 268.10 | 38 | 143.08 | 36 | ES+ |

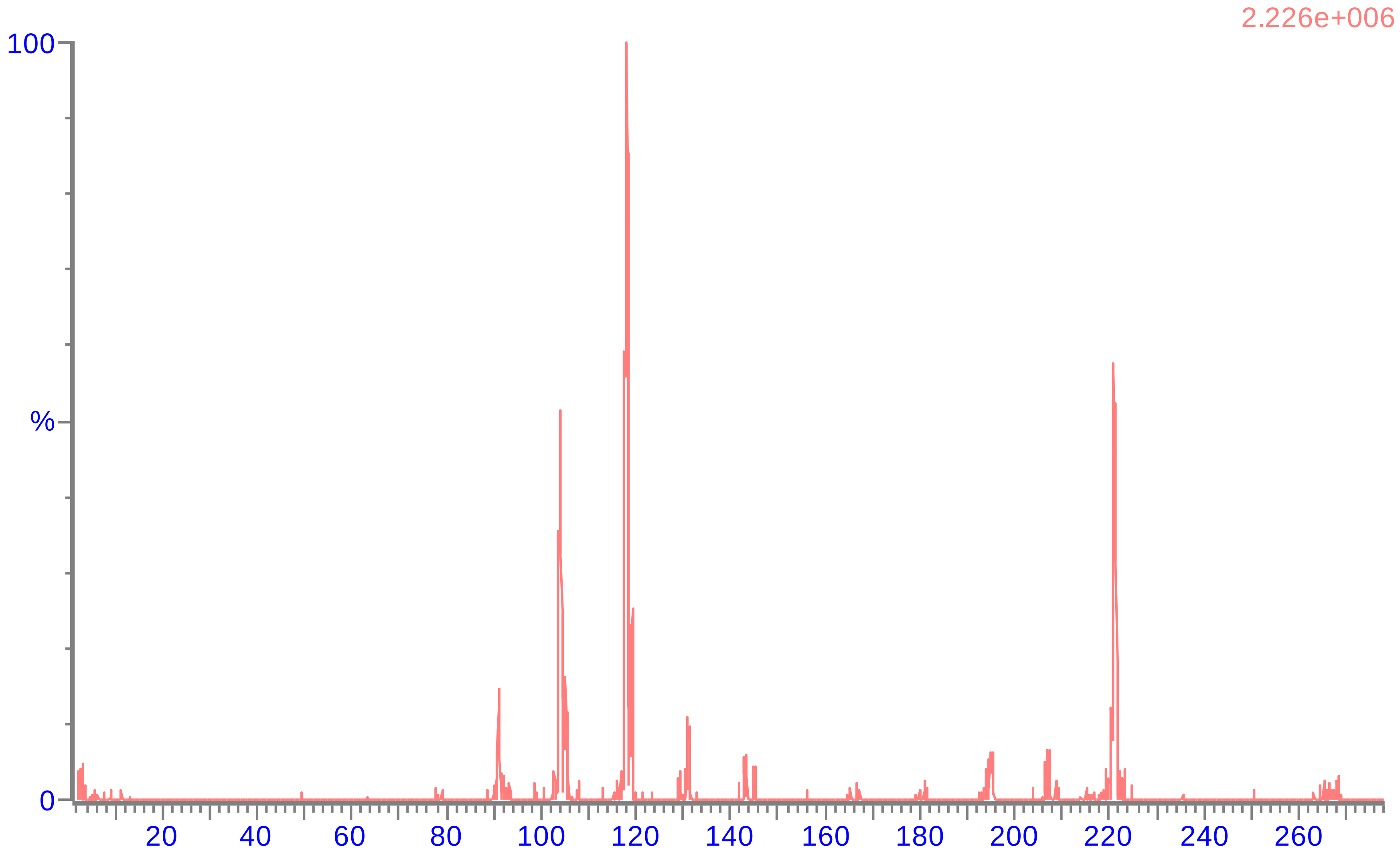

Figure 1.143: Mass spectrum for daughter fragment peak ES+, m/z 268.10 -> 118.10.

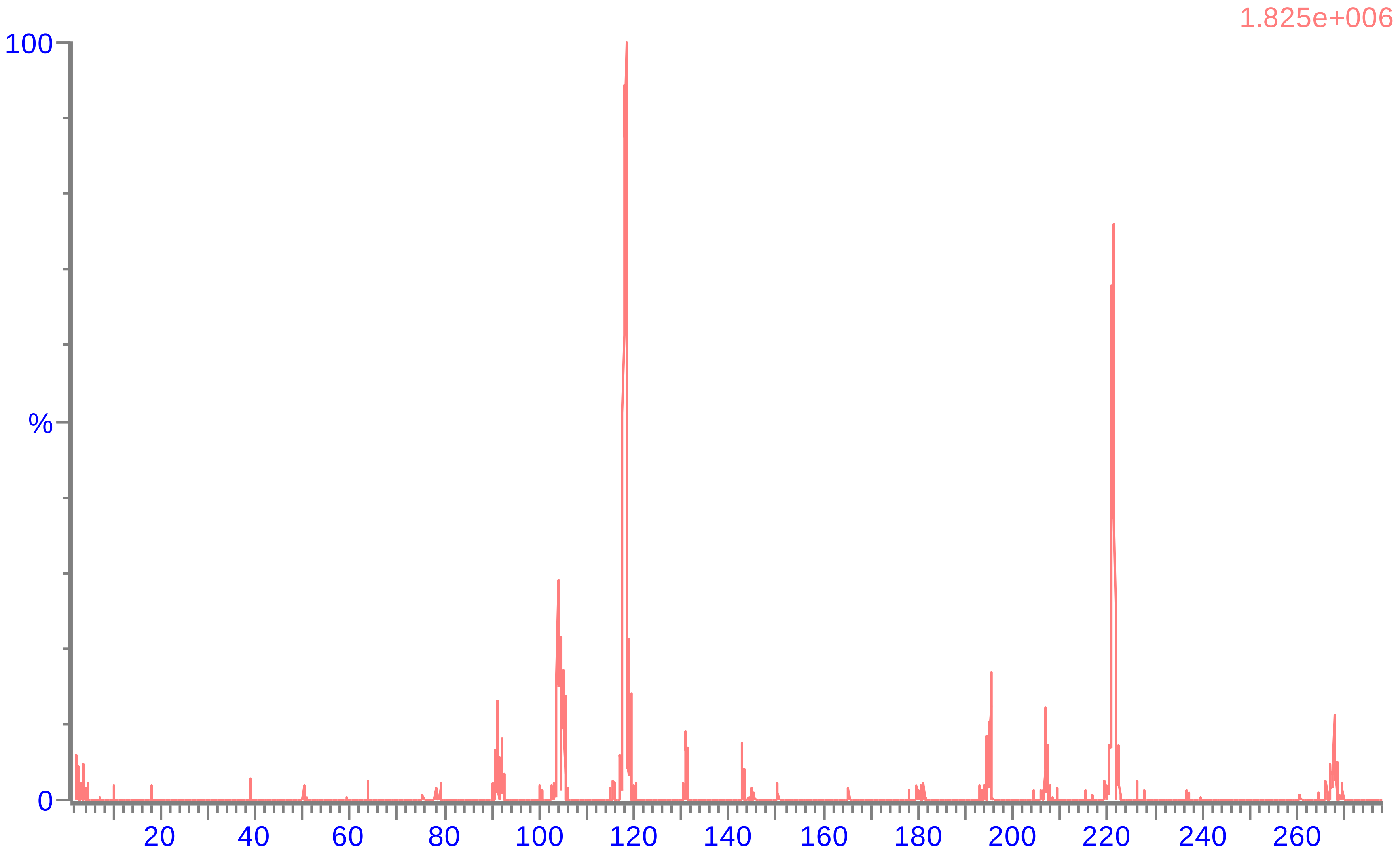

Figure 1.144: Mass spectrum for daughter fragment peak ES+, m/z 268.10 -> 221.12.

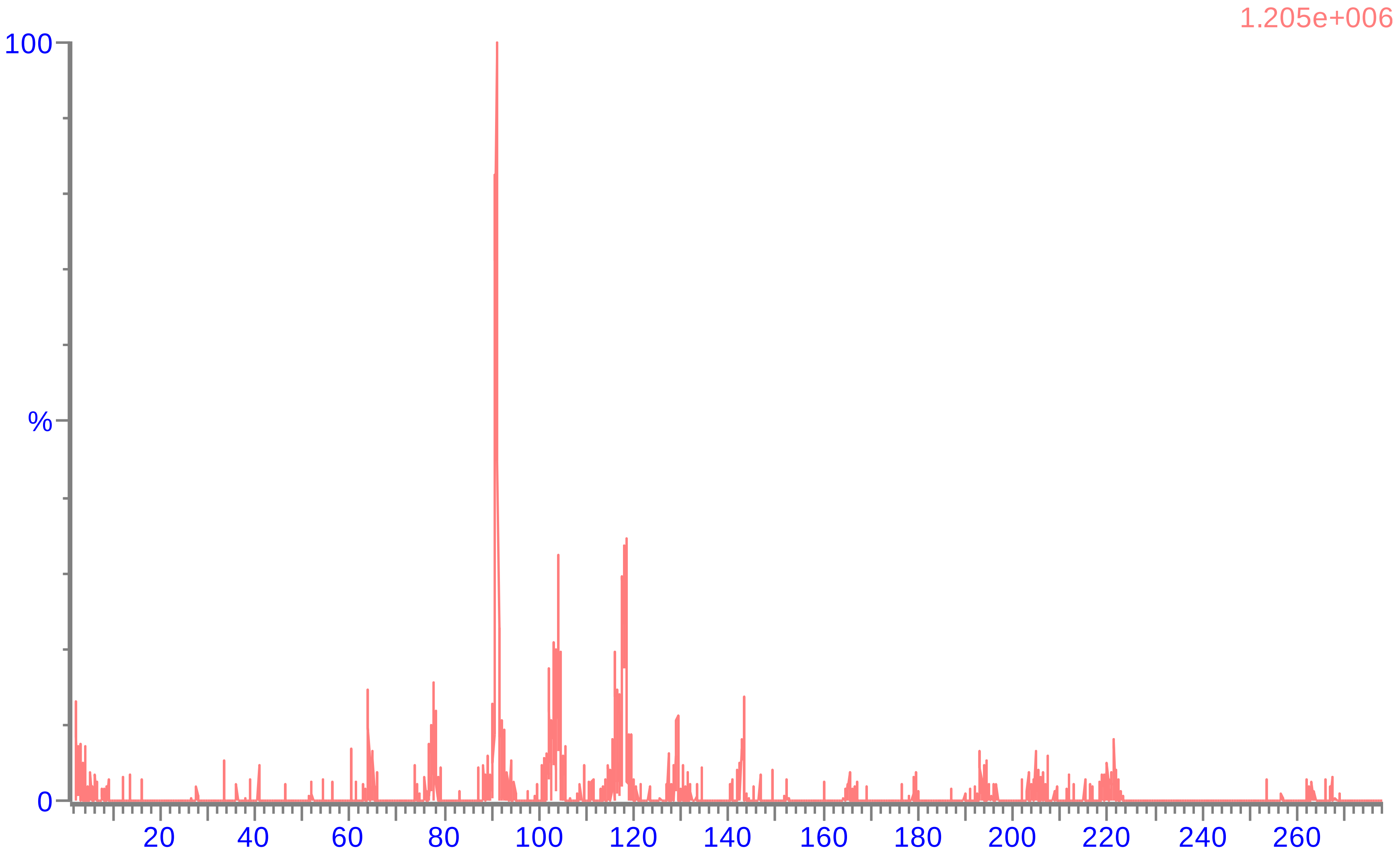

Figure 1.145: Mass spectrum for daughter fragment peak ES+, m/z 268.10 -> 91.05.

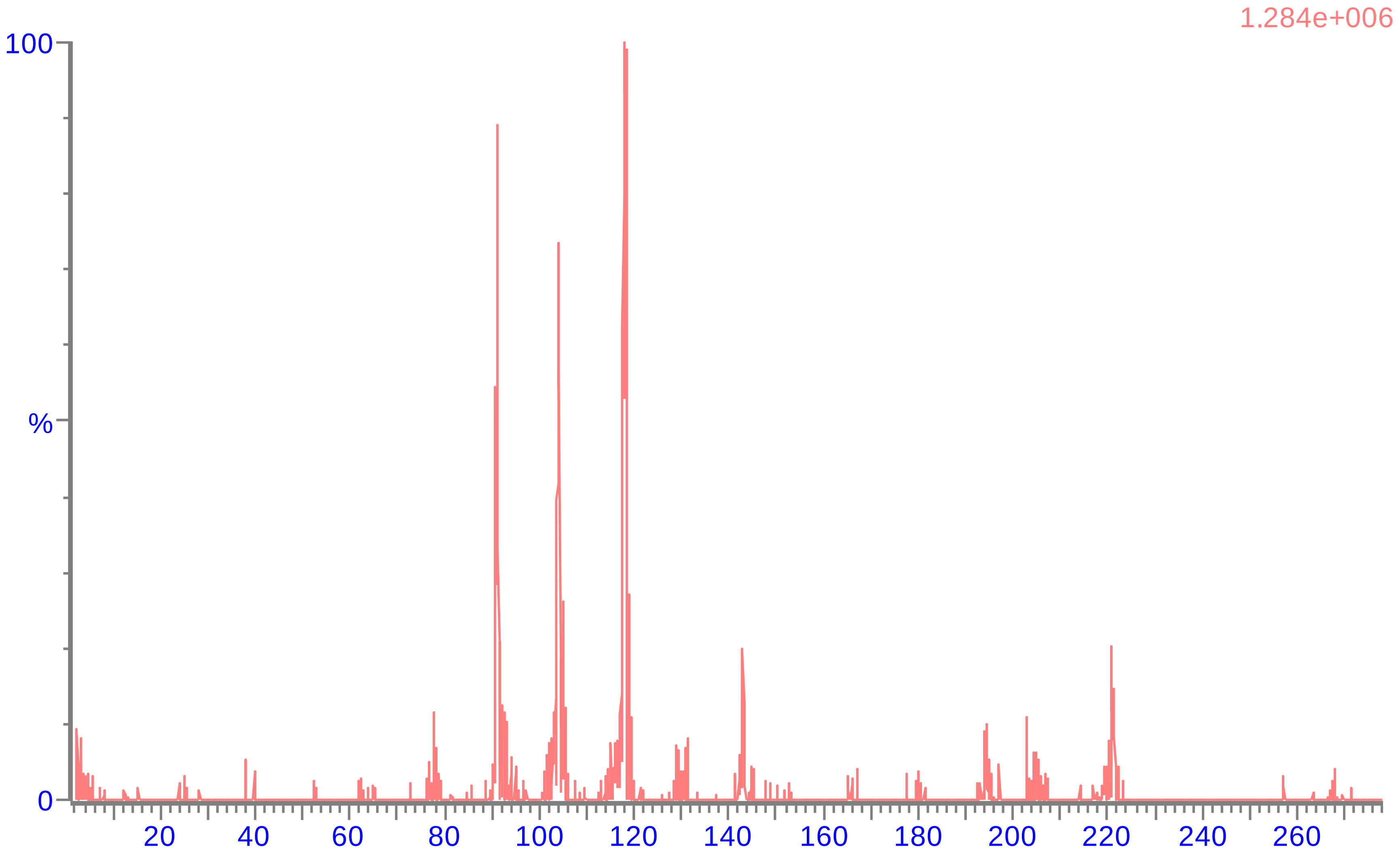

Figure 1.146: Mass spectrum for daughter fragment peak ES+, m/z 268.10 -> 143.08.

**8j** 3-nitro-*N*-(2-nitro-1-phenylethyl)aniline

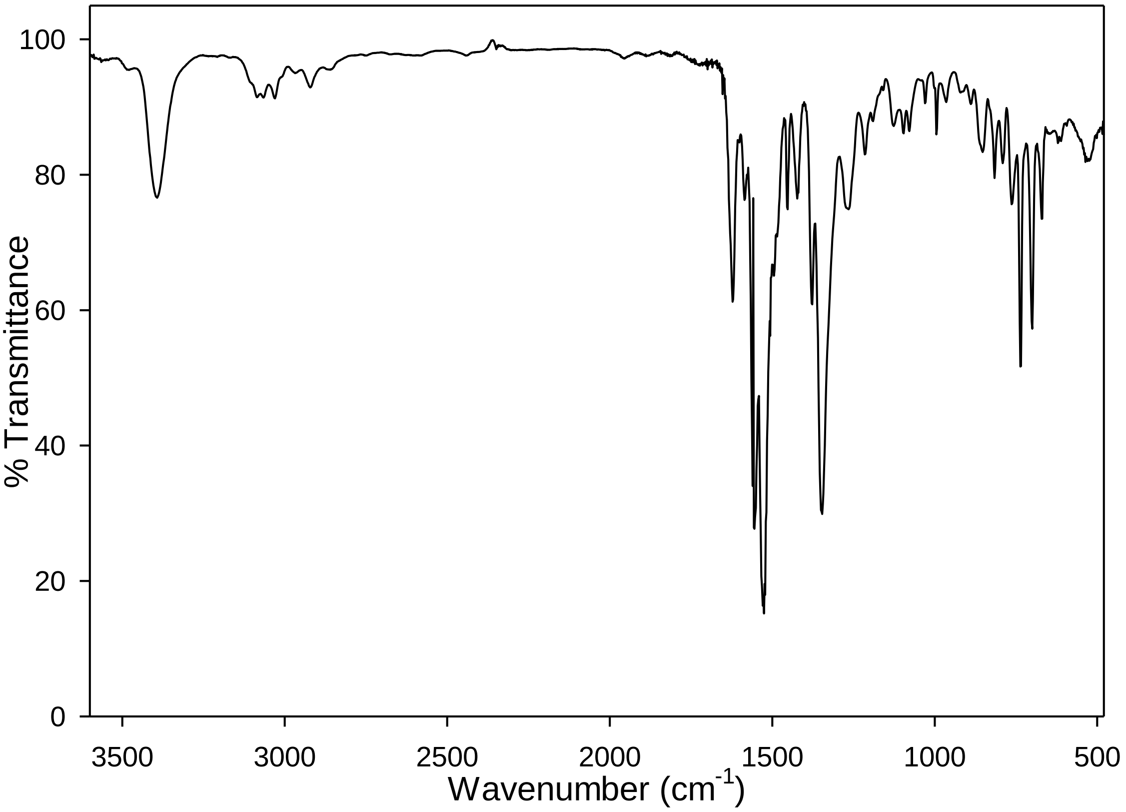

Figure 1.147: IR spectrum of **8j** 3-nitro-*N*-(2-nitro-1-phenylethyl)aniline.

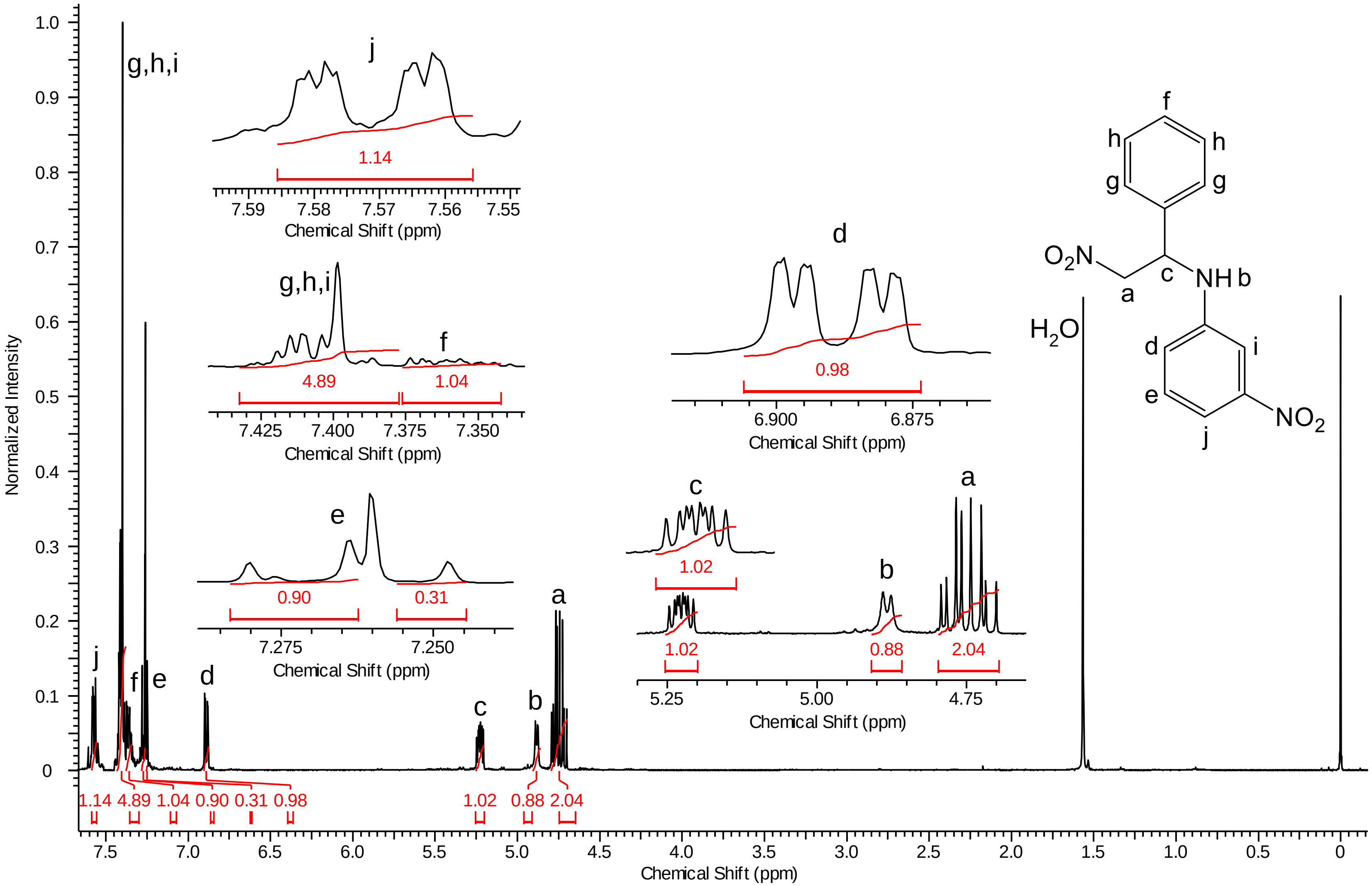

Figure 1.148: $^1$H NMR spectrum of **8j** 3-nitro-*N*-(2-nitro-1-phenylethyl)aniline.

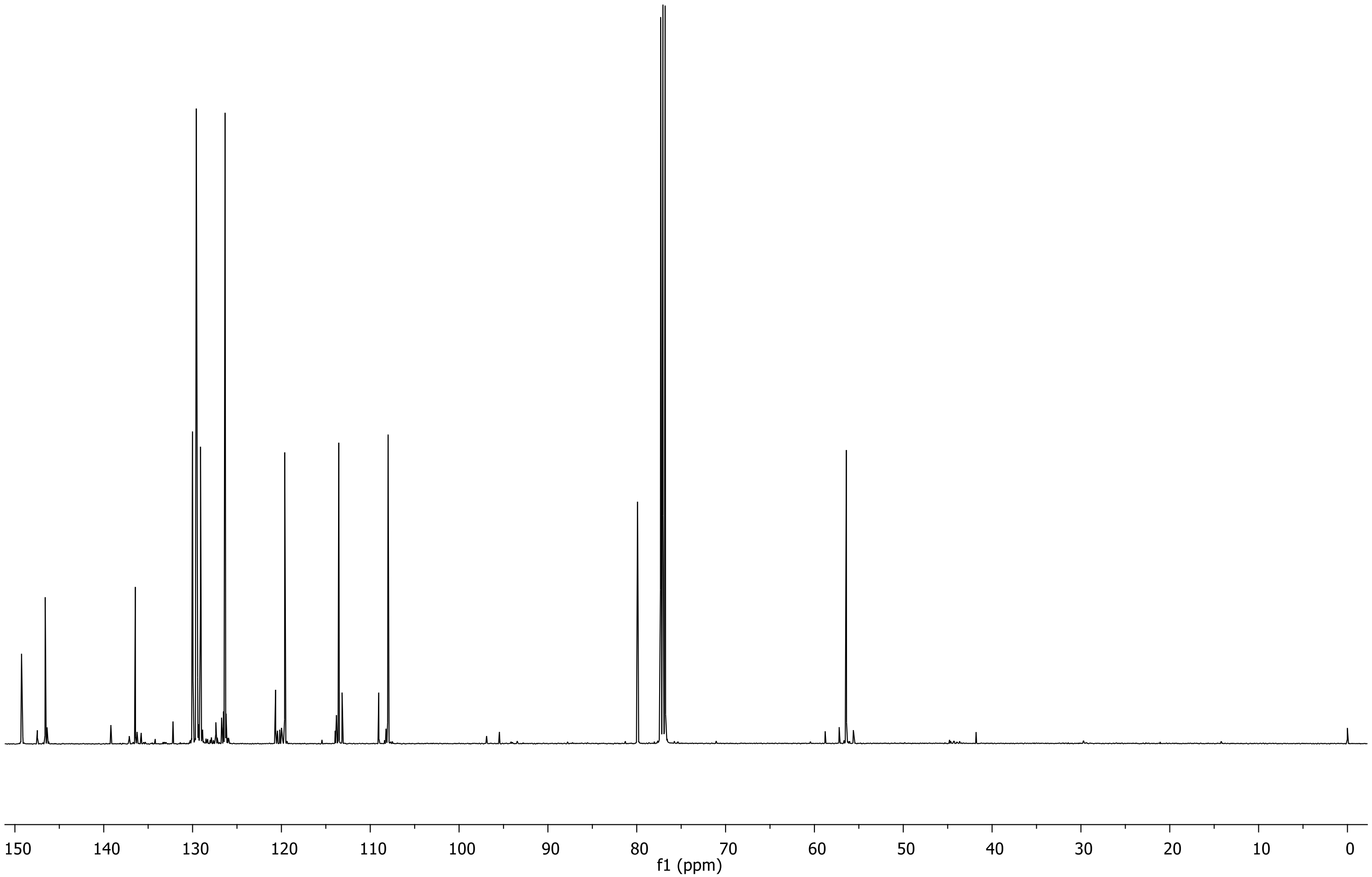

Figure 1.149: $^{13}$C NMR spectrum of **8j** 3-nitro-*N*-(2-nitro-1-phenylethyl)aniline.

Table 1.21: MS data.

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **8j** | 287.3 | 1 | 288.08 | 18 | 104.06 | 28 | ES+ |
| | | 2 | 288.08 | 18 | 150.05 | 8 | ES+ |
| | | 3 | 288.08 | 18 | 138.99 | 8 | ES+ |
| | | 4 | 288.08 | 18 | 77.99 | 48 | ES+ |
| | | 5 | 288.08 | 18 | 91.97 | 14 | ES+ |

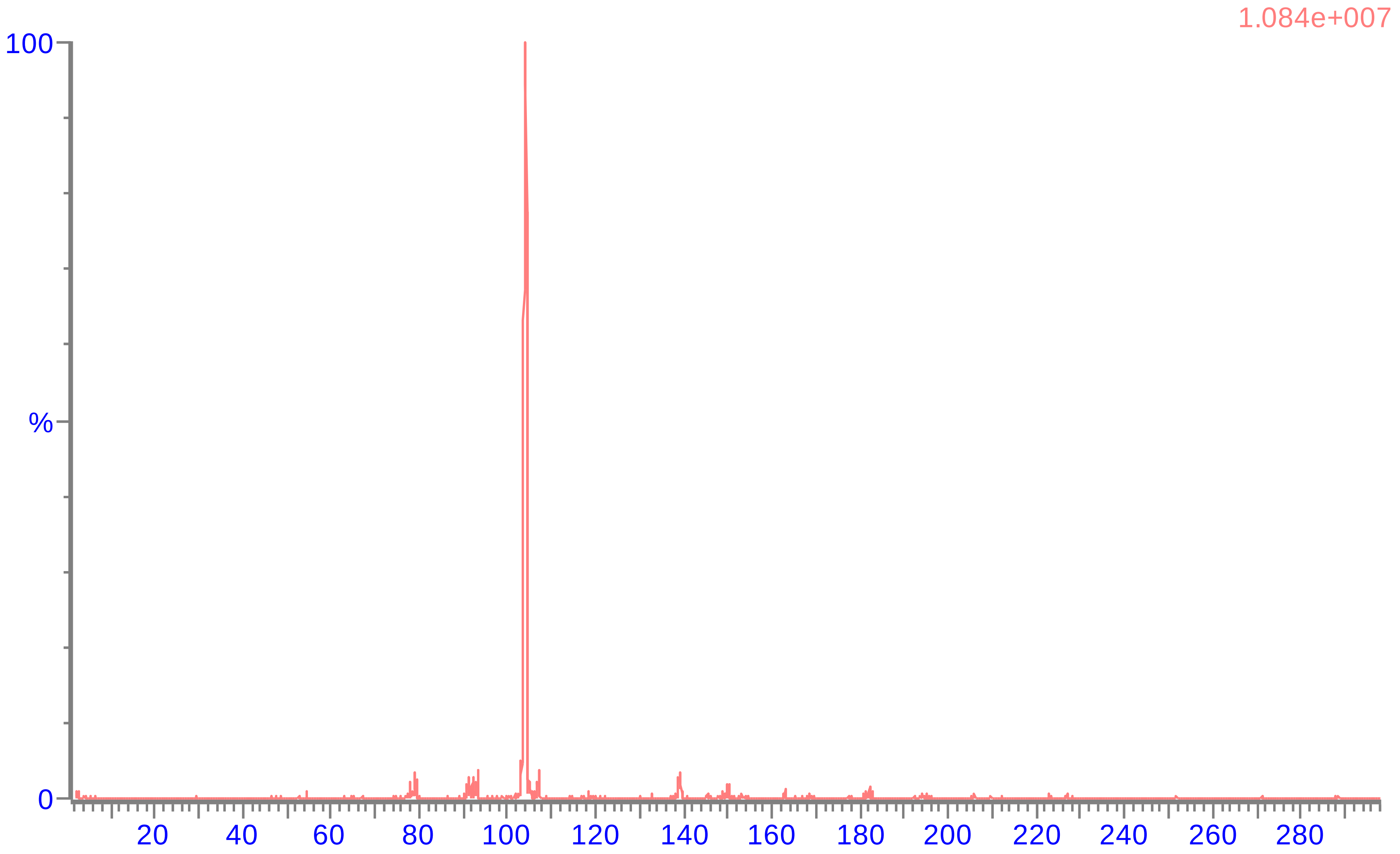

Figure 1.150: Mass spectrum for daughter fragment peak ES+, m/z 288.08 -> 104.06.

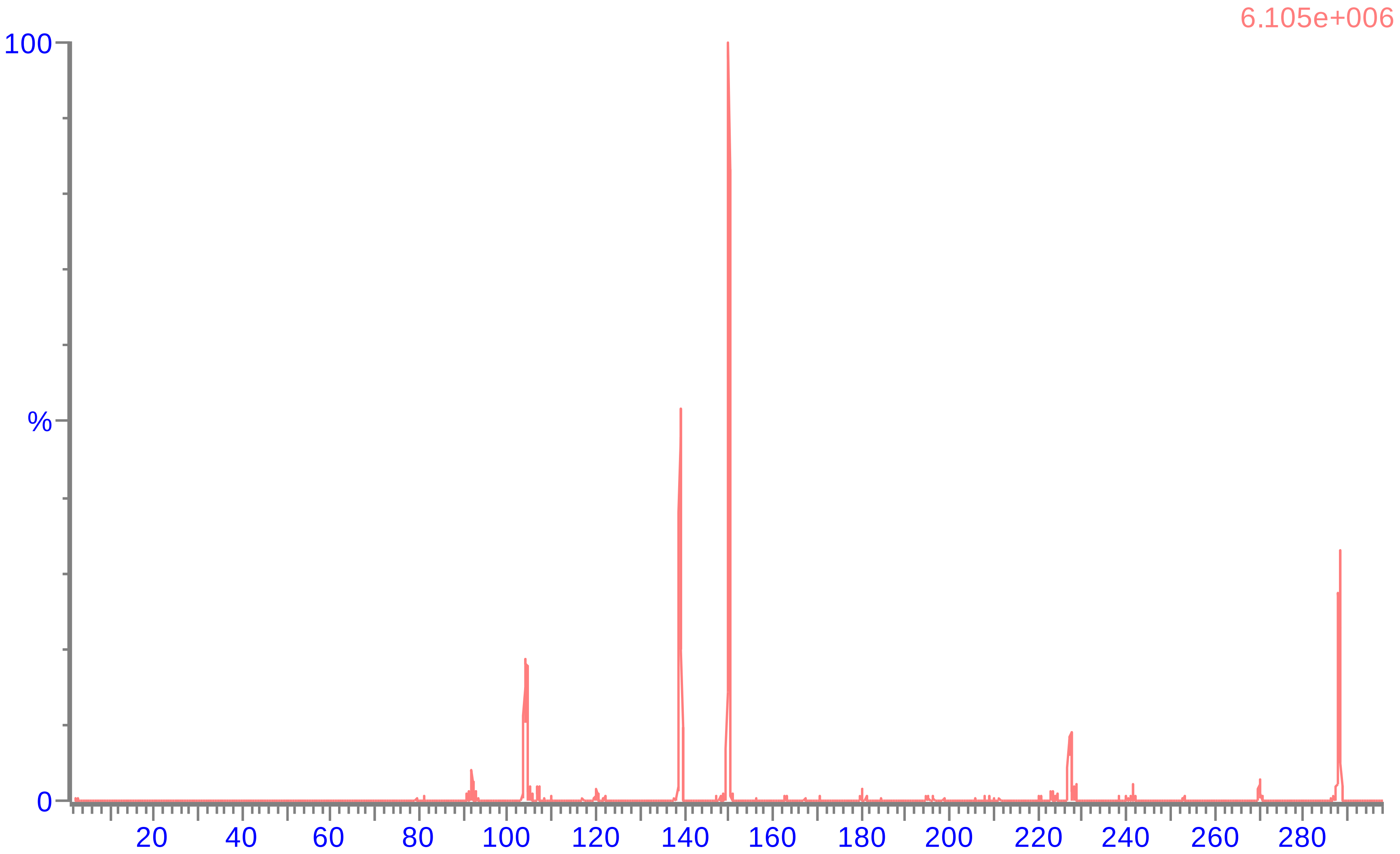

Figure 1.151: Mass spectrum for daughter fragment peak ES+, m/z 288.08 -> 150.05.

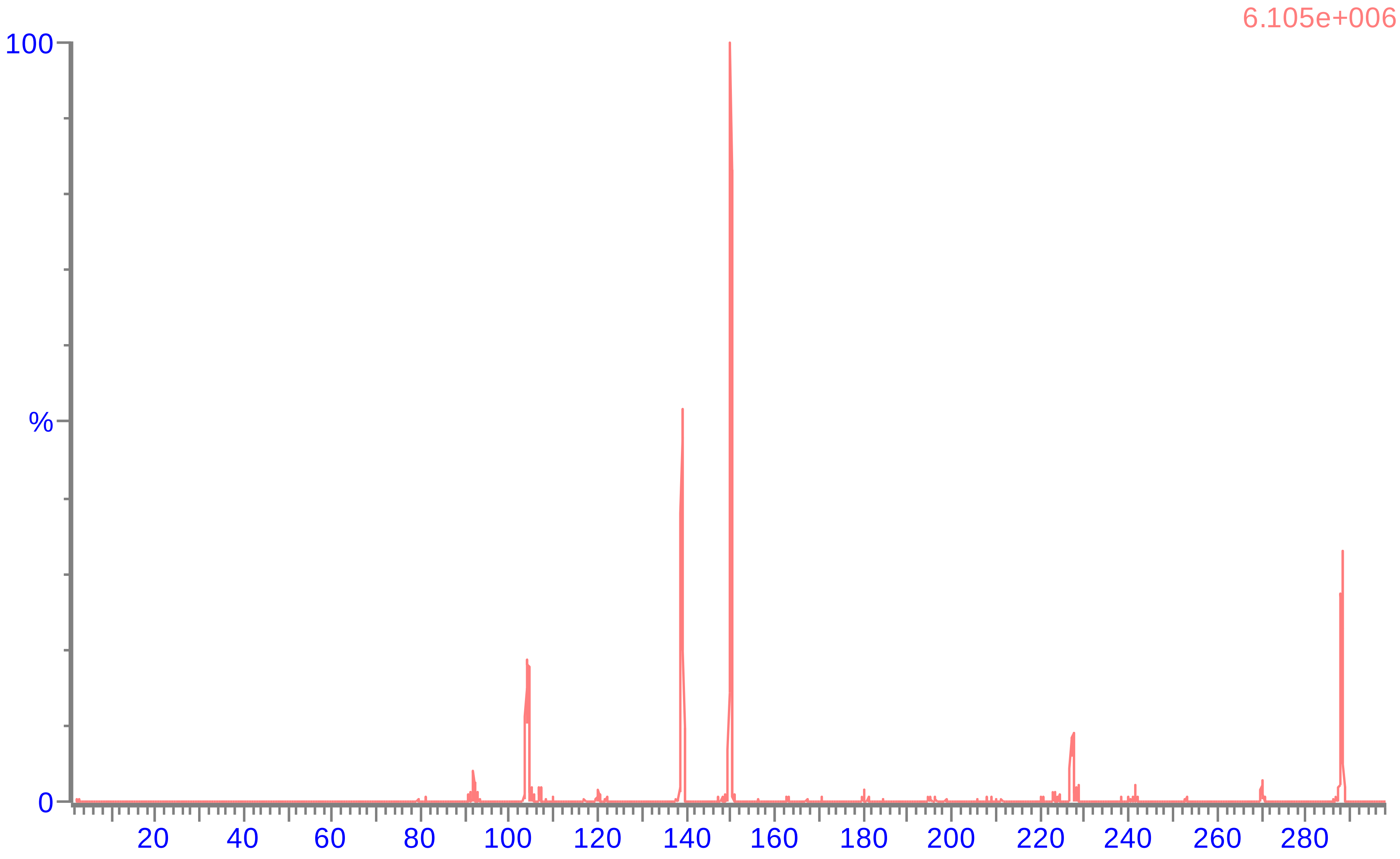

Figure 1.152: Mass spectrum for daughter fragment peak ES+, m/z 288.08 -> 138.99.

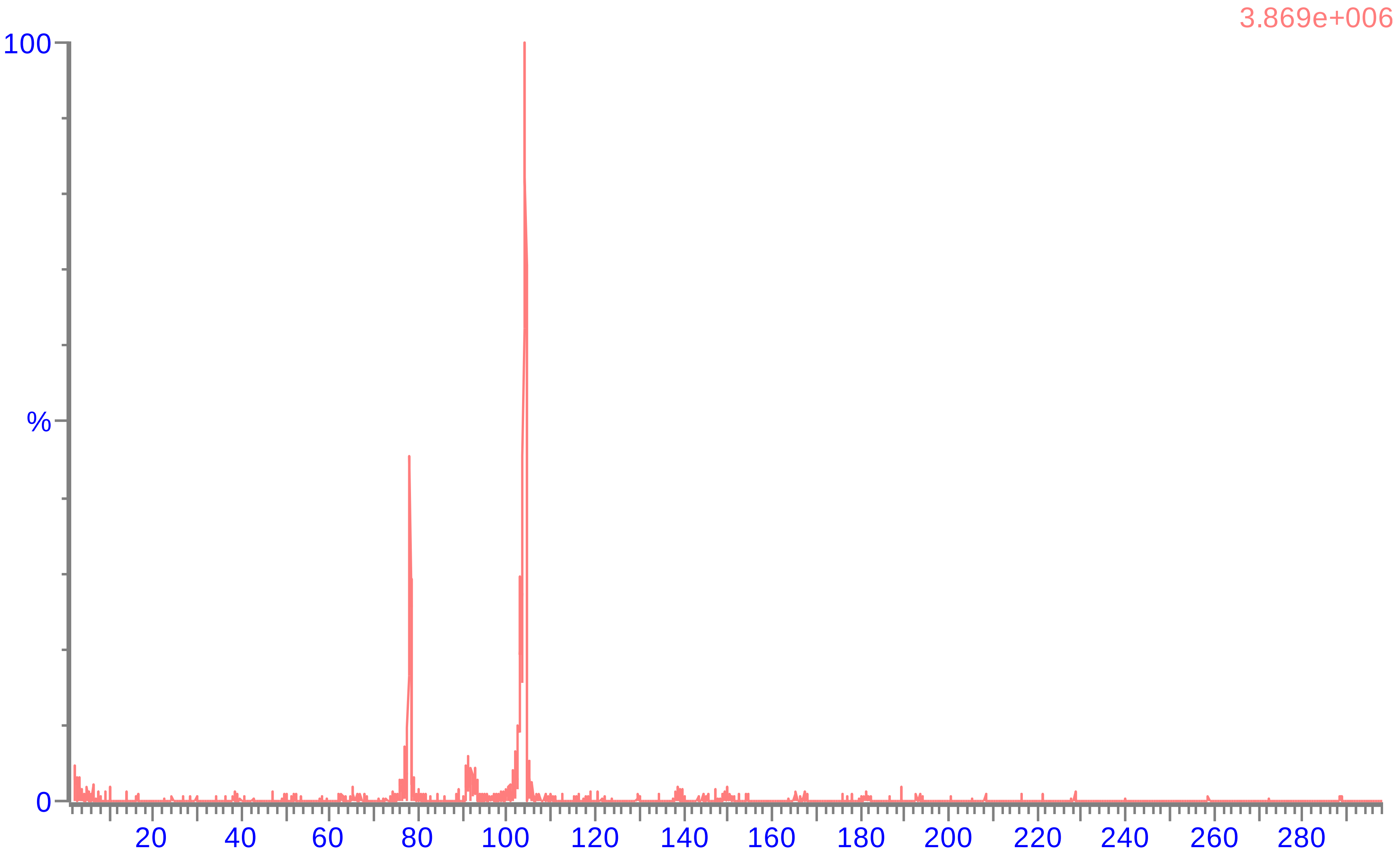

Figure 1.153: Mass spectrum for daughter fragment peak ES+, m/z 288.08 -> 77.99.

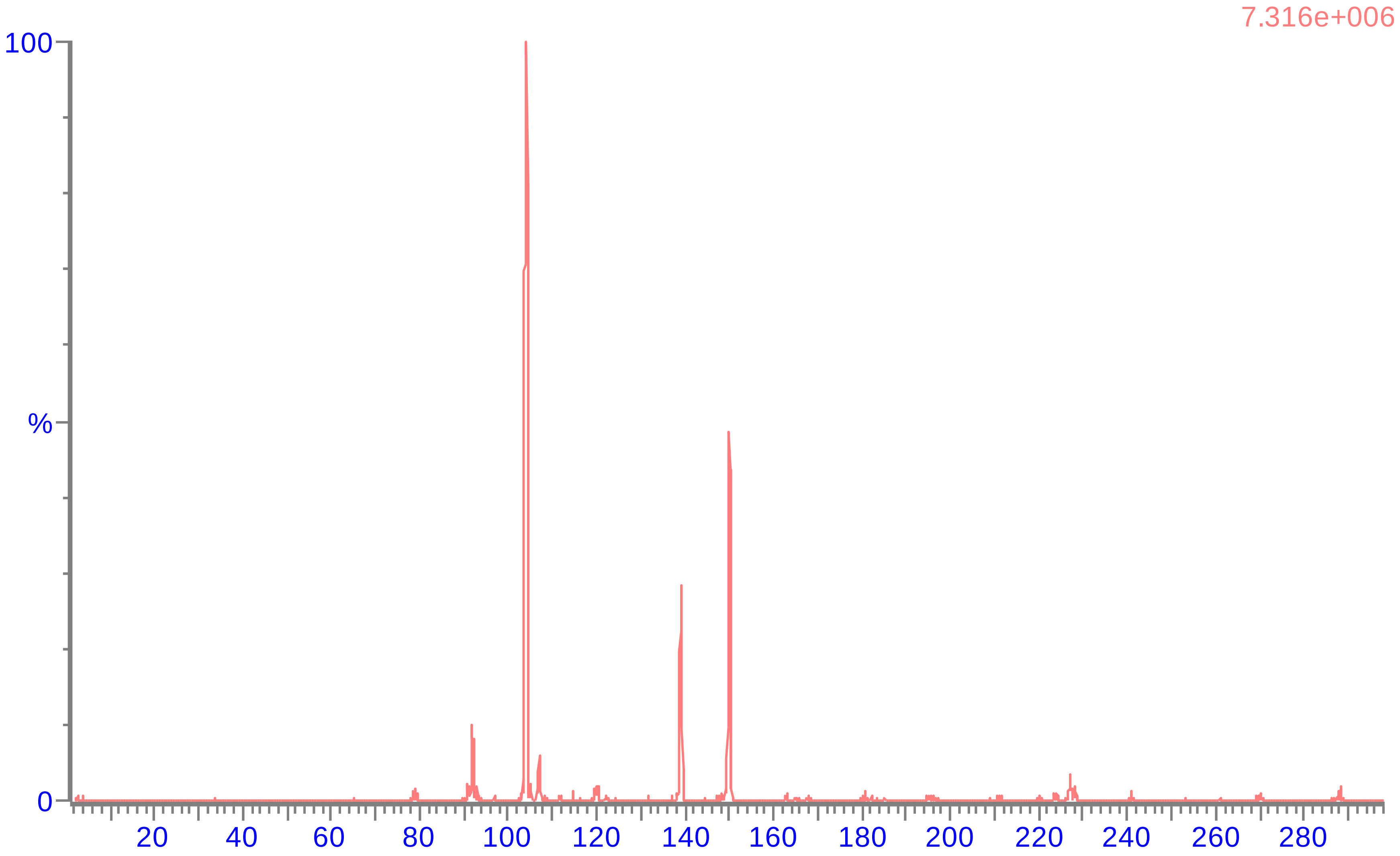

Figure 1.154: Mass spectrum for daughter fragment peak ES+, m/z 288.08 -> 91.97.

**8k** 2,5-dichloro-*N*-(2-nitro-1-phenylethyl)aniline

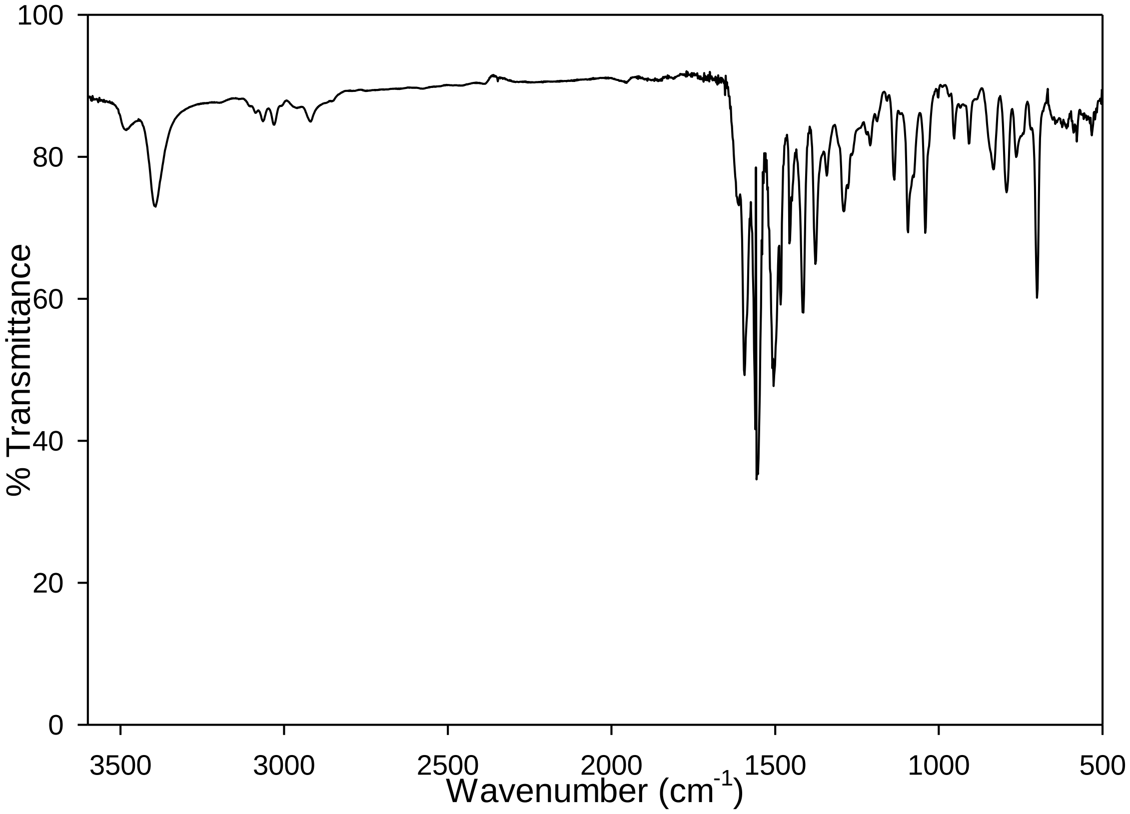

Figure 1.155: IR spectrum of **8k** 2,5-dichloro-*N*-(2-nitro-1-phenylethyl)aniline.

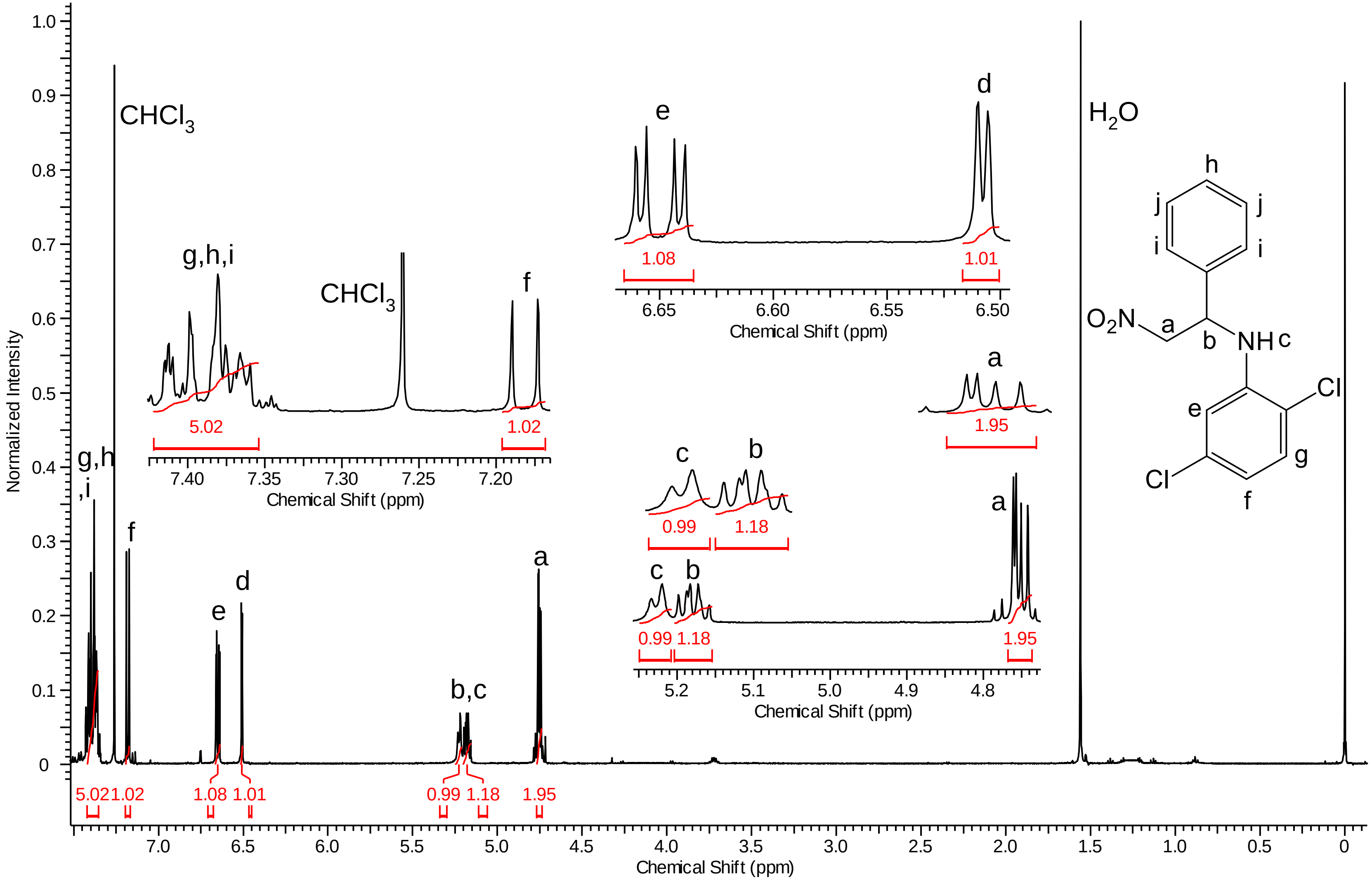

Figure 1.156: $^1$H NMR spectrum of **8k** 2,5-dichloro-*N*-(2-nitro-1-phenylethyl)aniline.

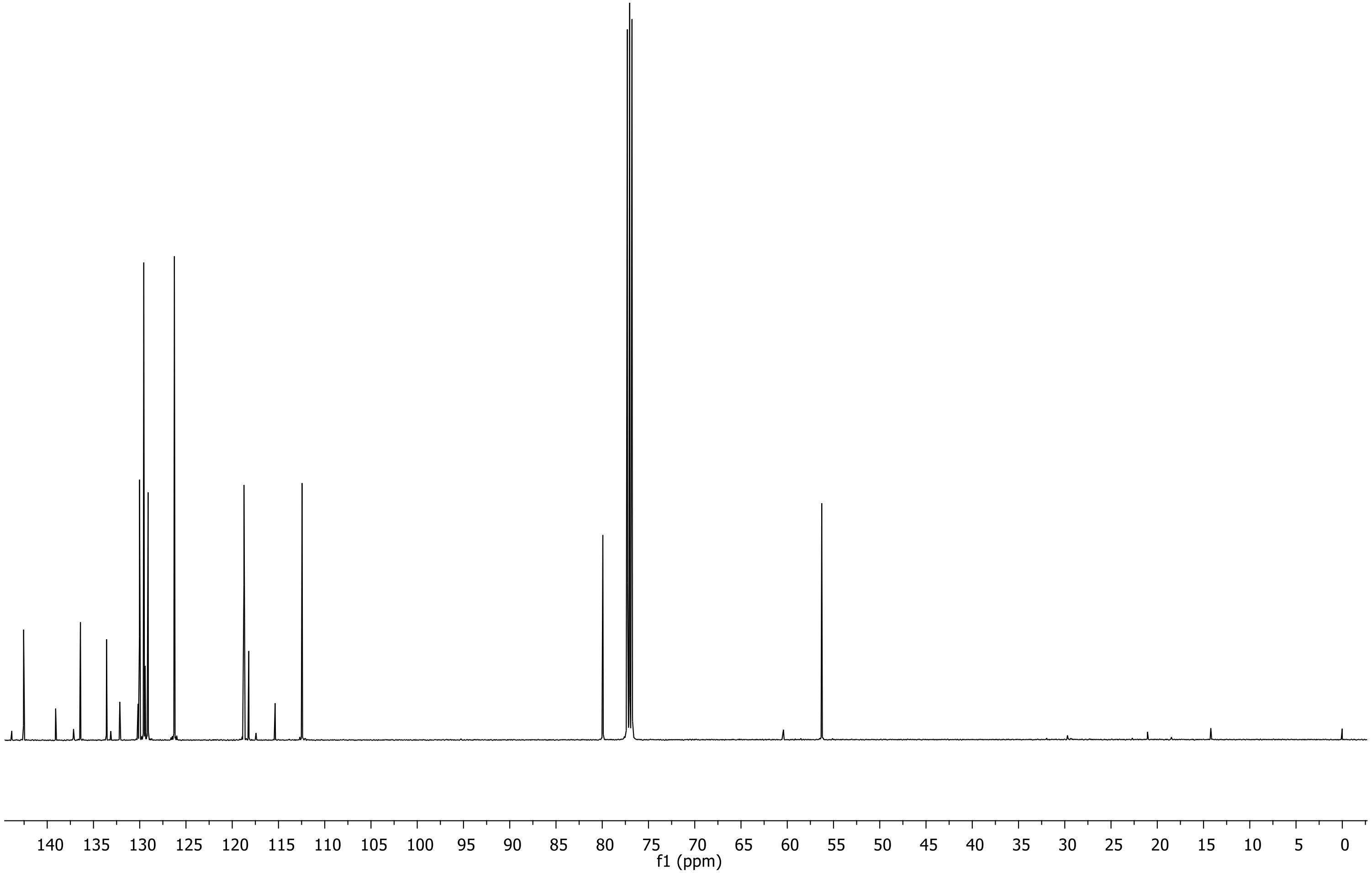

Figure 1.157: $^{13}$C NMR spectrum of **8k** 2,5-dichloro-*N*-(2-nitro-1-phenylethyl)aniline.

Table 1.22: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **8k** | 312 | 1 | 312.97 | 16 | 93.98 | 12 | ES+ |
| | | 2 | 312.97 | 18 | 217.96 | 8 | ES- |
| | | 3 | 312.97 | 16 | 252.02 | 12 | ES+ |
| | | 4 | 312.97 | 16 | 173.91 | 26 | ES+ |
| | | 5 | 312.97 | 16 | 101.73 | 58 | ES+ |

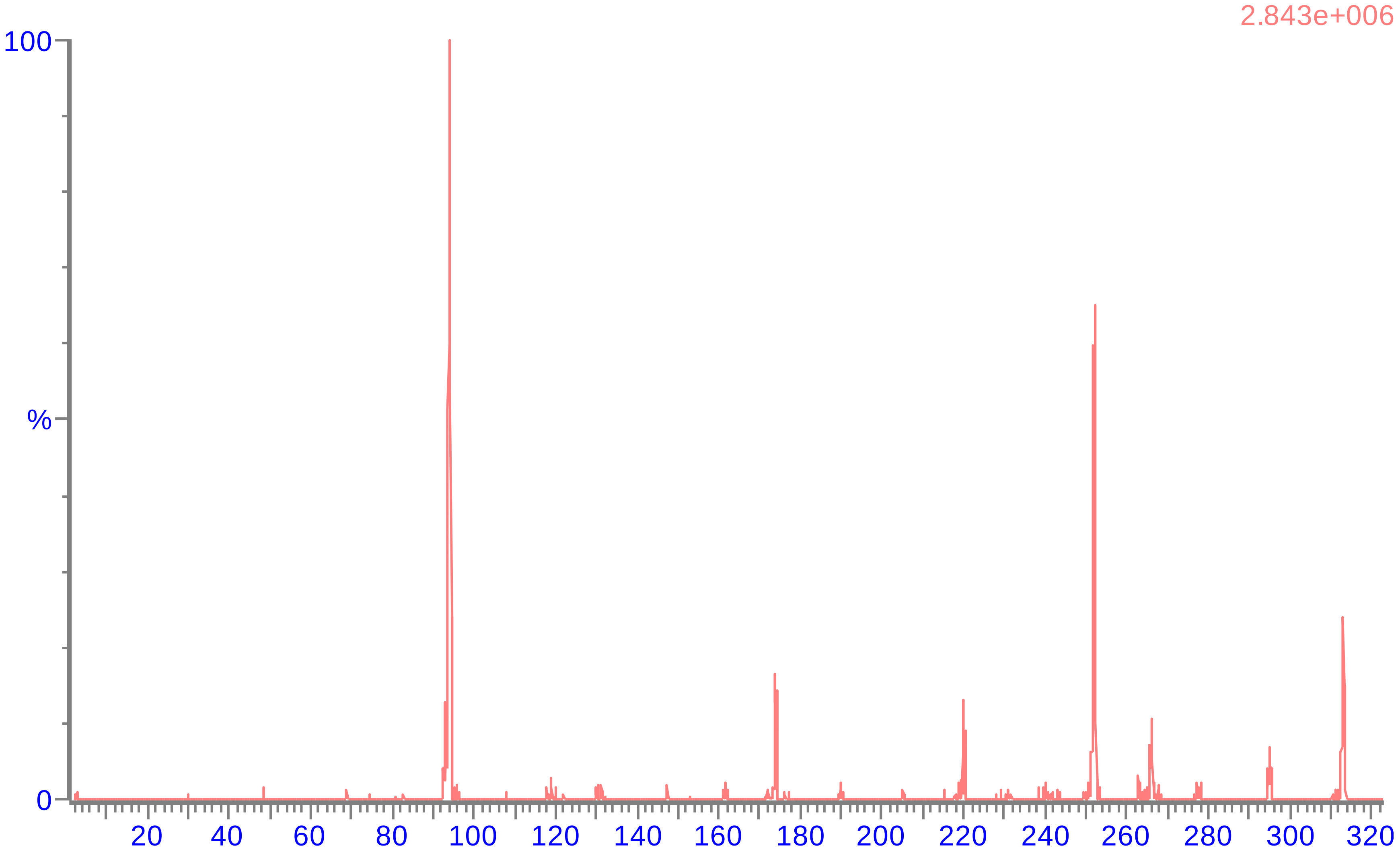

Figure 1.158: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 93.98.

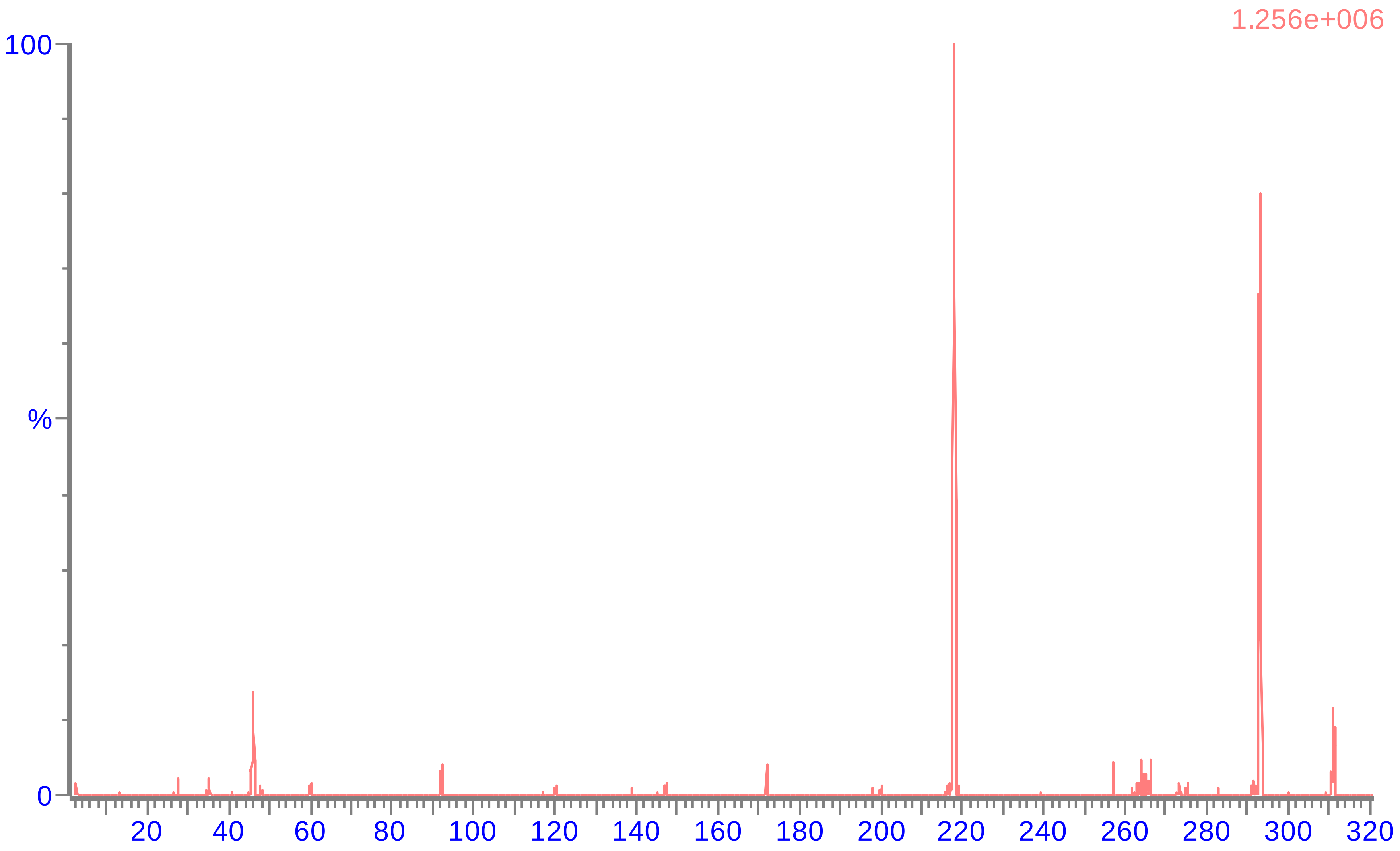

Figure 1.159: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 217.96.

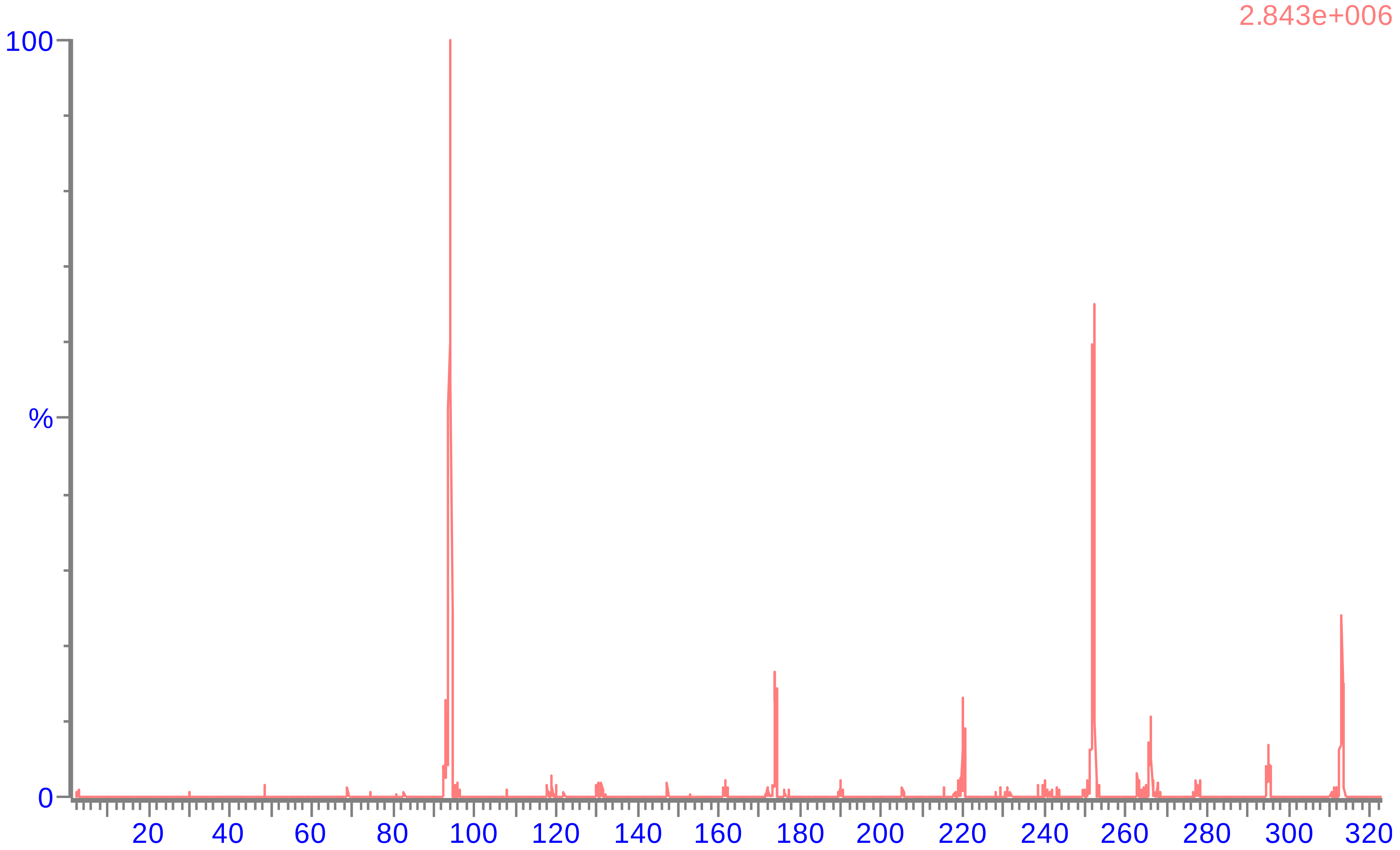

Figure 1.160: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 252.02.

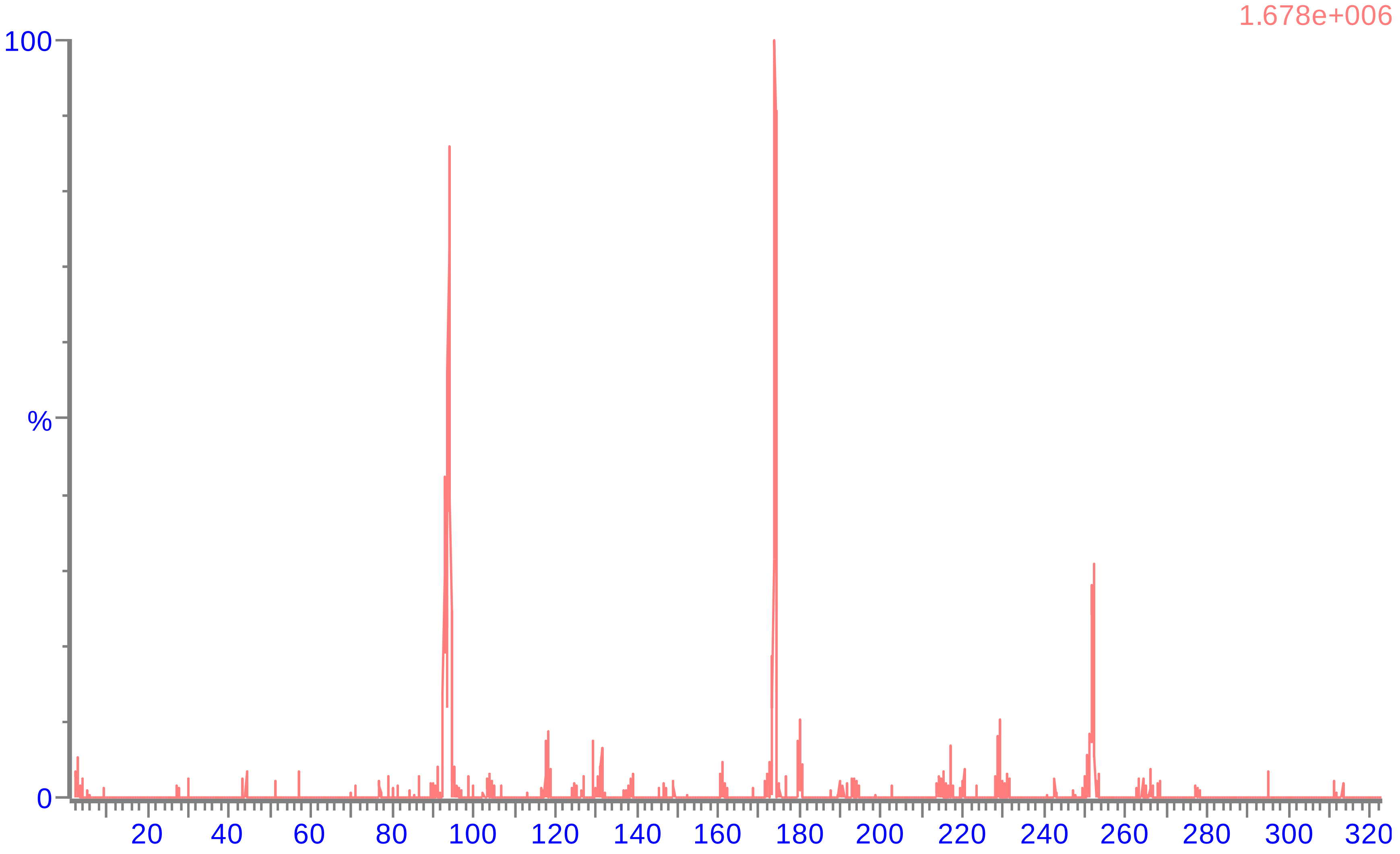

Figure 1.161: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 173.91.

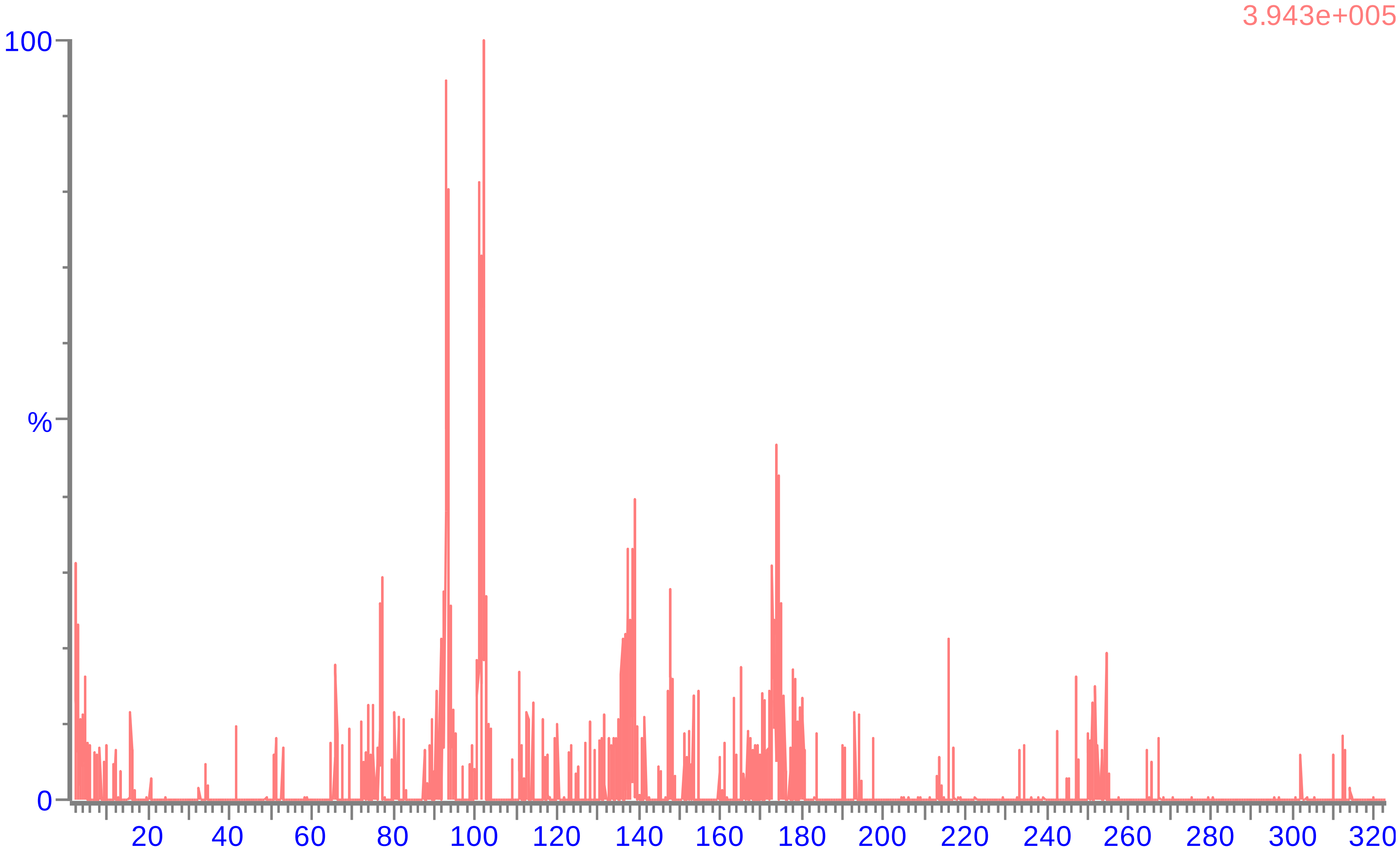

Figure 1.162: Mass spectrum for daughter fragment peak ES+, m/z 312.97 -> 101.73.

**8l** (*E*)-*N*-(2-nitro-1-phenylethyl)-4-(phenyldiazenyl)aniline

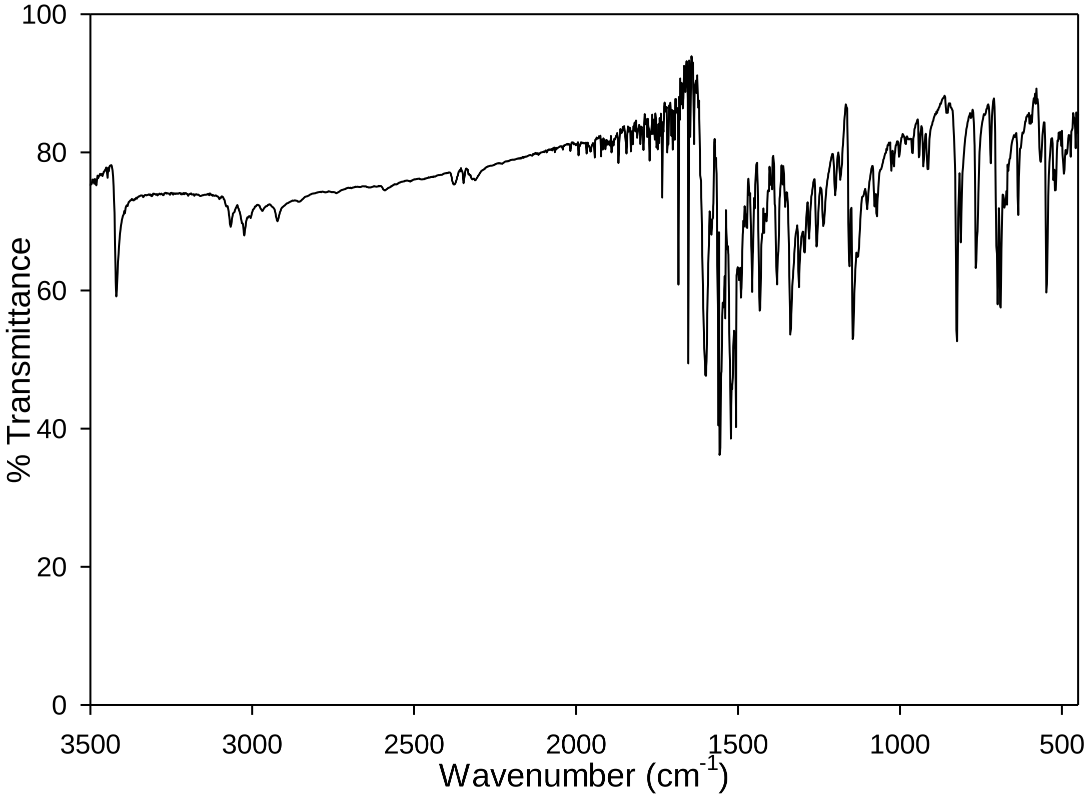

Figure 1.163: IR spectrum of **8l** (*E*)-*N*-(2-nitro-1-phenylethyl)-4-(phenyldiazenyl)aniline.

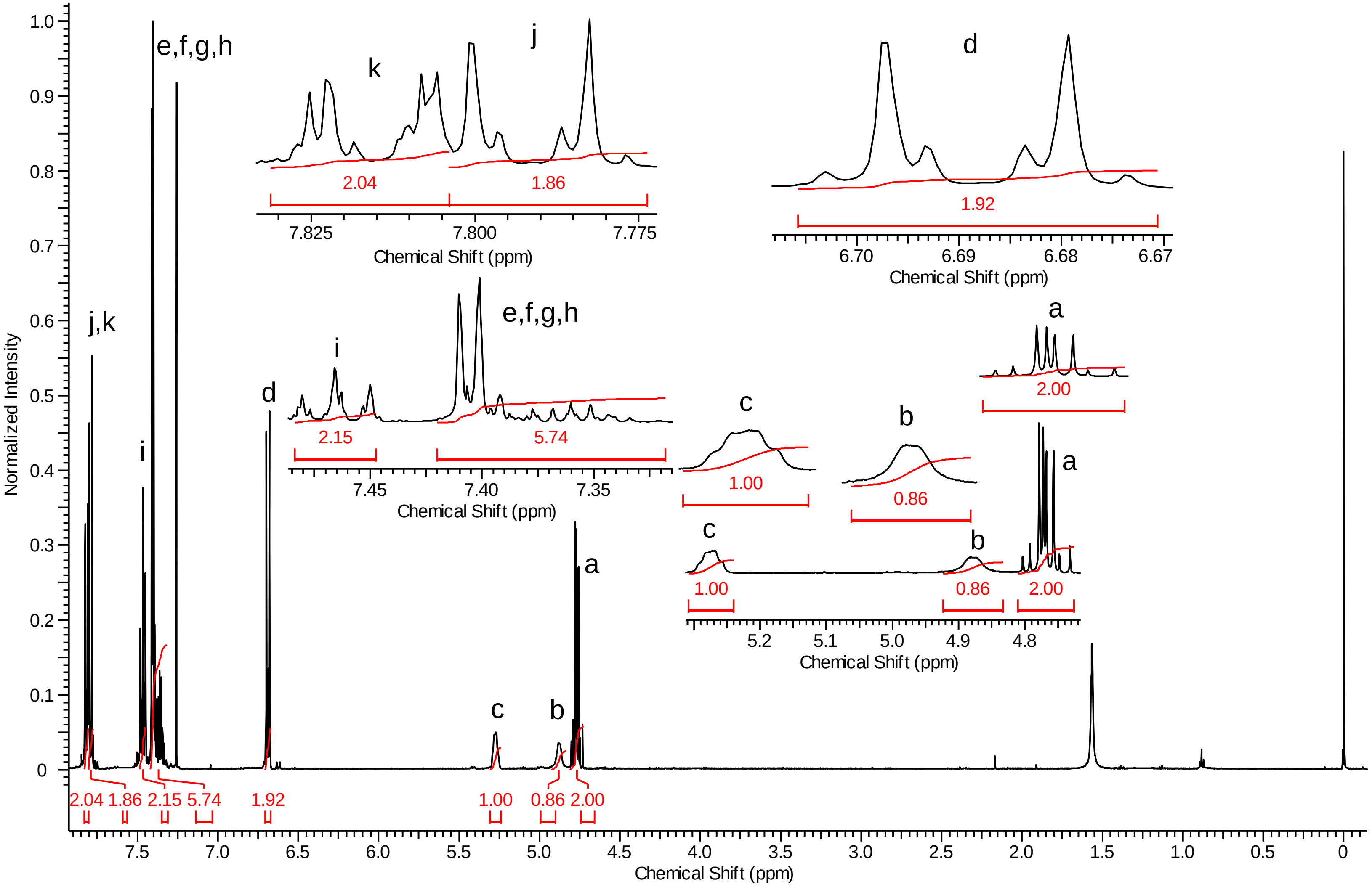

Figure 1.164: $^1$H NMR spectrum of **8l** (*E*)-*N*-(2-nitro-1-phenylethyl)-4-(phenyldiazenyl)aniline.

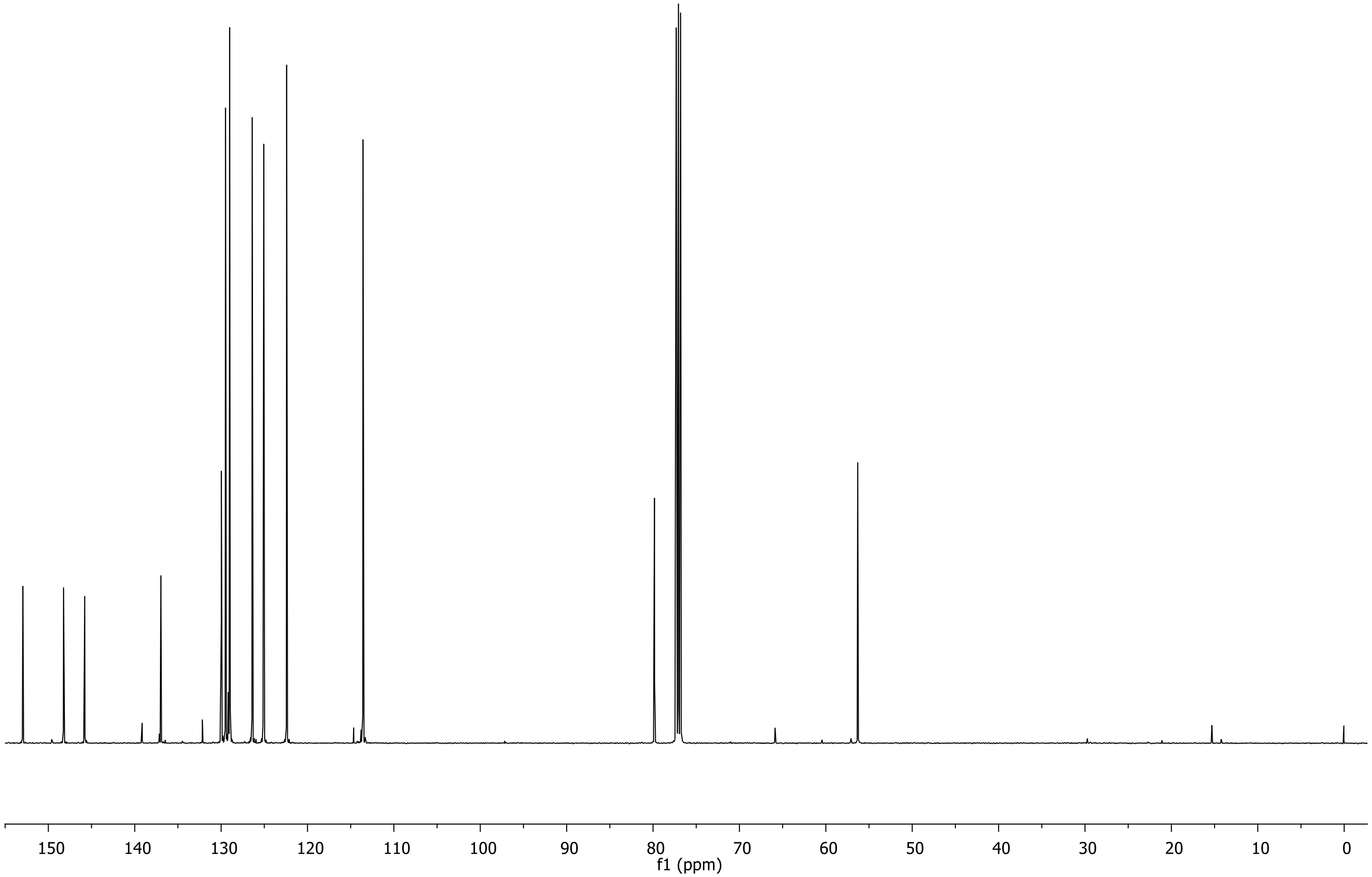

Figure 1.165: $^{13}$C NMR spectrum of **8l** (*E*)-*N*-(2-nitro-1-phenylethyl)-4-(phenyldiazenyl)aniline.

Table 1.23: MS data

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **8l** | 346 | 1 | 347.16 | 40 | 197.07 | 26 | ES+ |
| | | 2 | 347.16 | 40 | 77.07 | 44 | ES+ |
| | | 3 | 347.16 | 40 | 91.97 | 54 | ES+ |
| | | 4 | 347.16 | 40 | 65.04 | 64 | ES+ |
| | | 5 | 347.16 | 40 | 104.13 | 32 | ES+ |

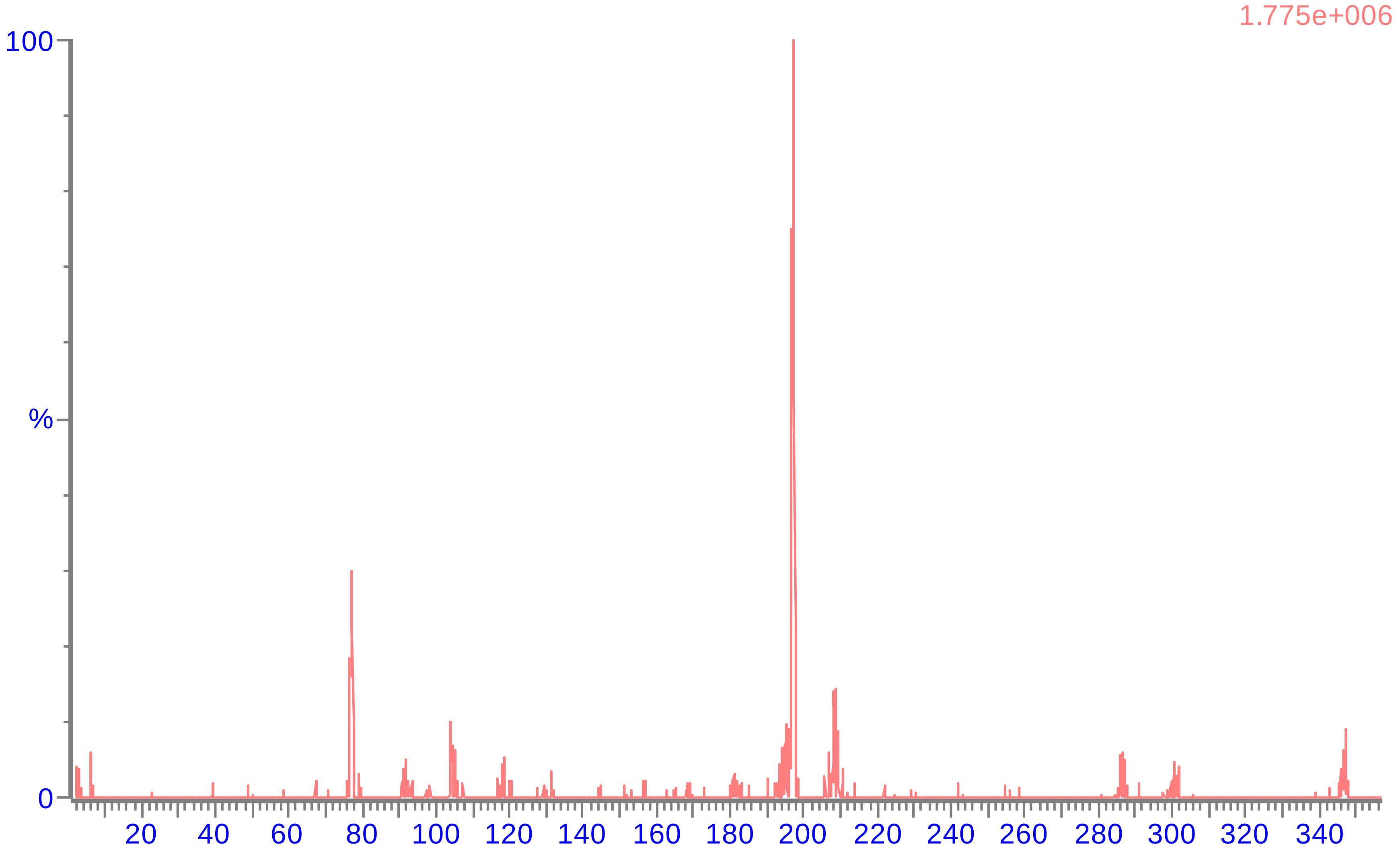

Figure 1.166: Mass spectrum for daughter fragment peak ES+, m/z 347.16 -> 197.07.

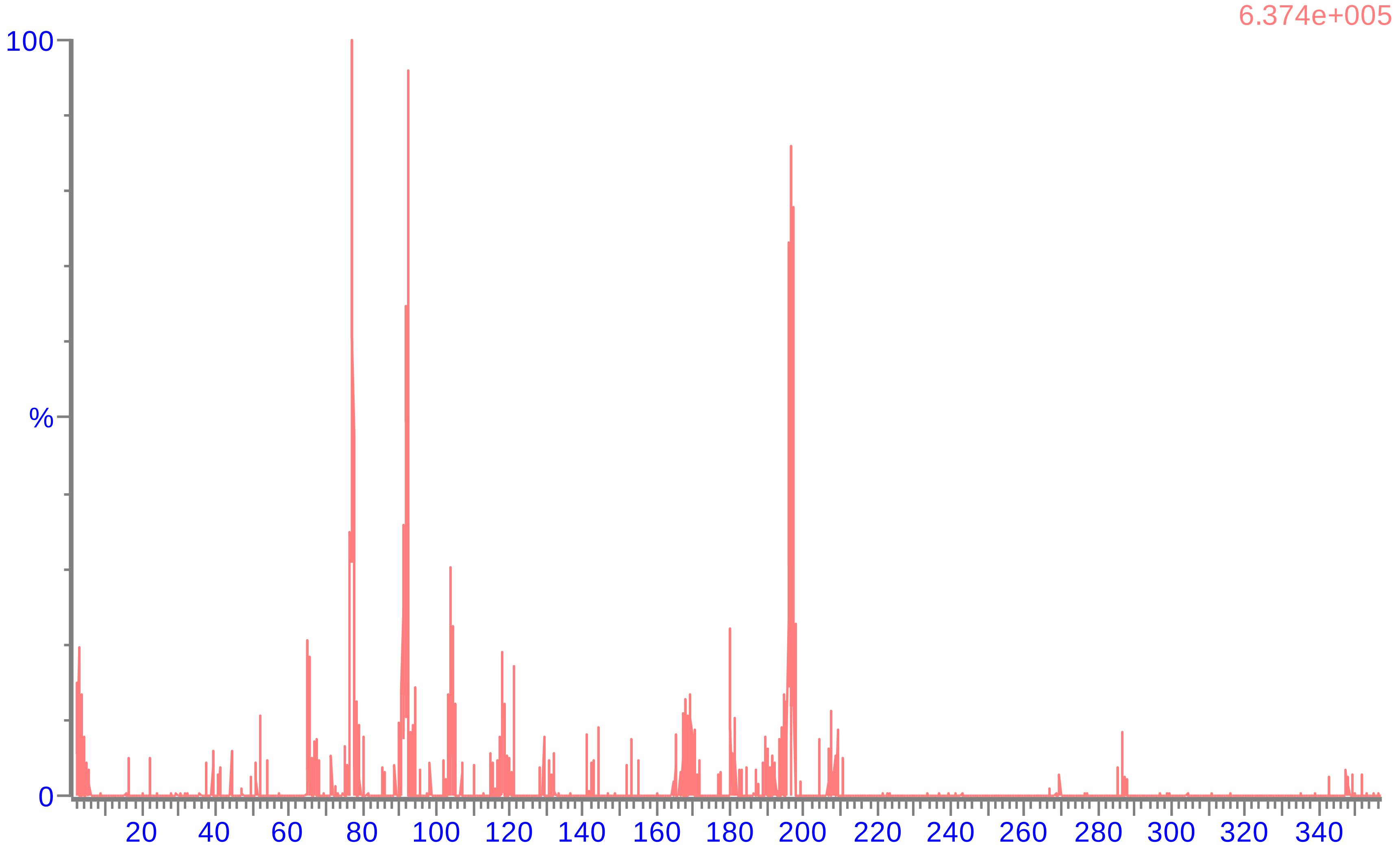

Figure 1.167: Mass spectrum for daughter fragment peak ES+, m/z 347.16 -> 77.07.

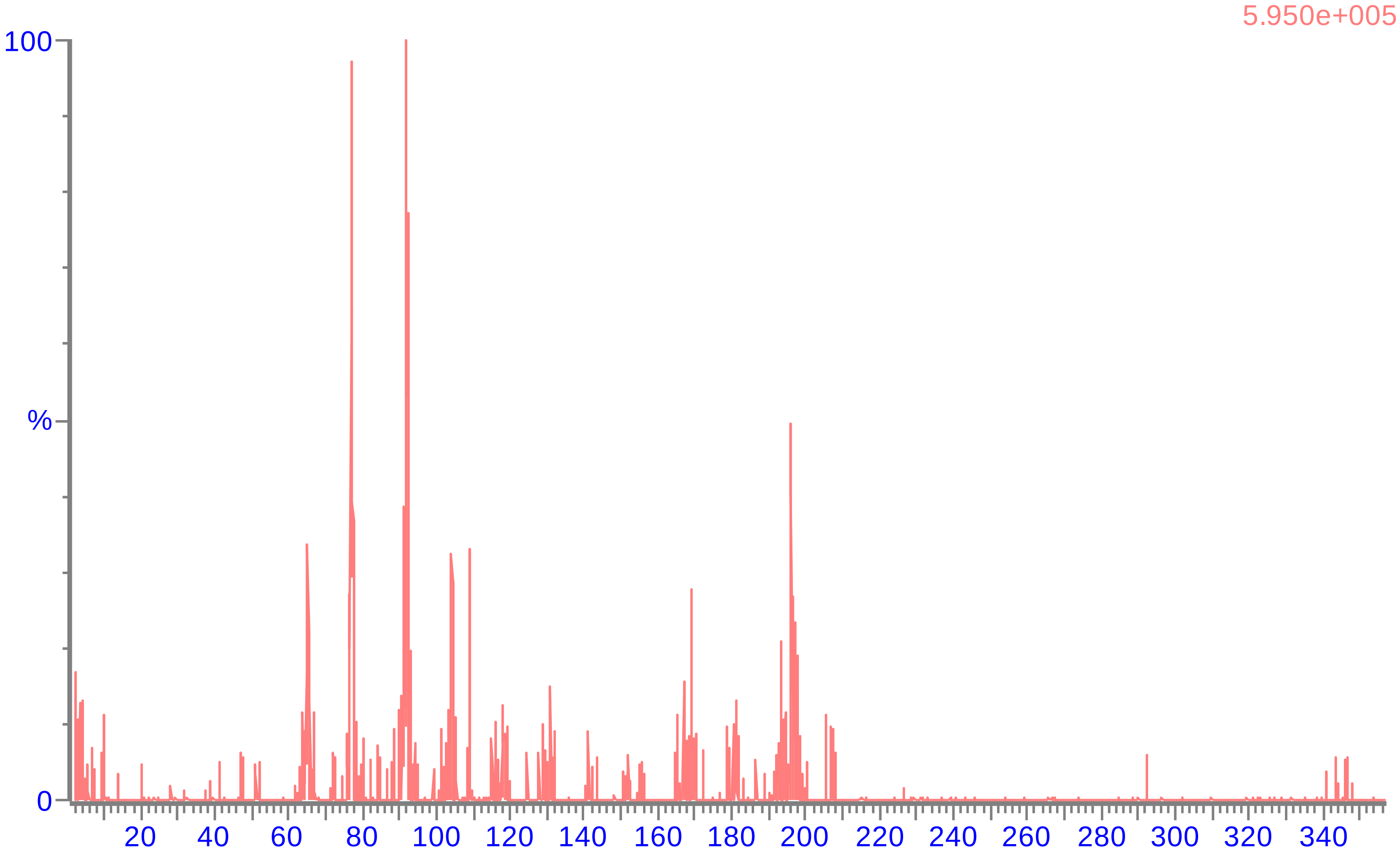

Figure 1.168: Mass spectrum for daughter fragment peak ES+, m/z 347.16 -> 91.97.

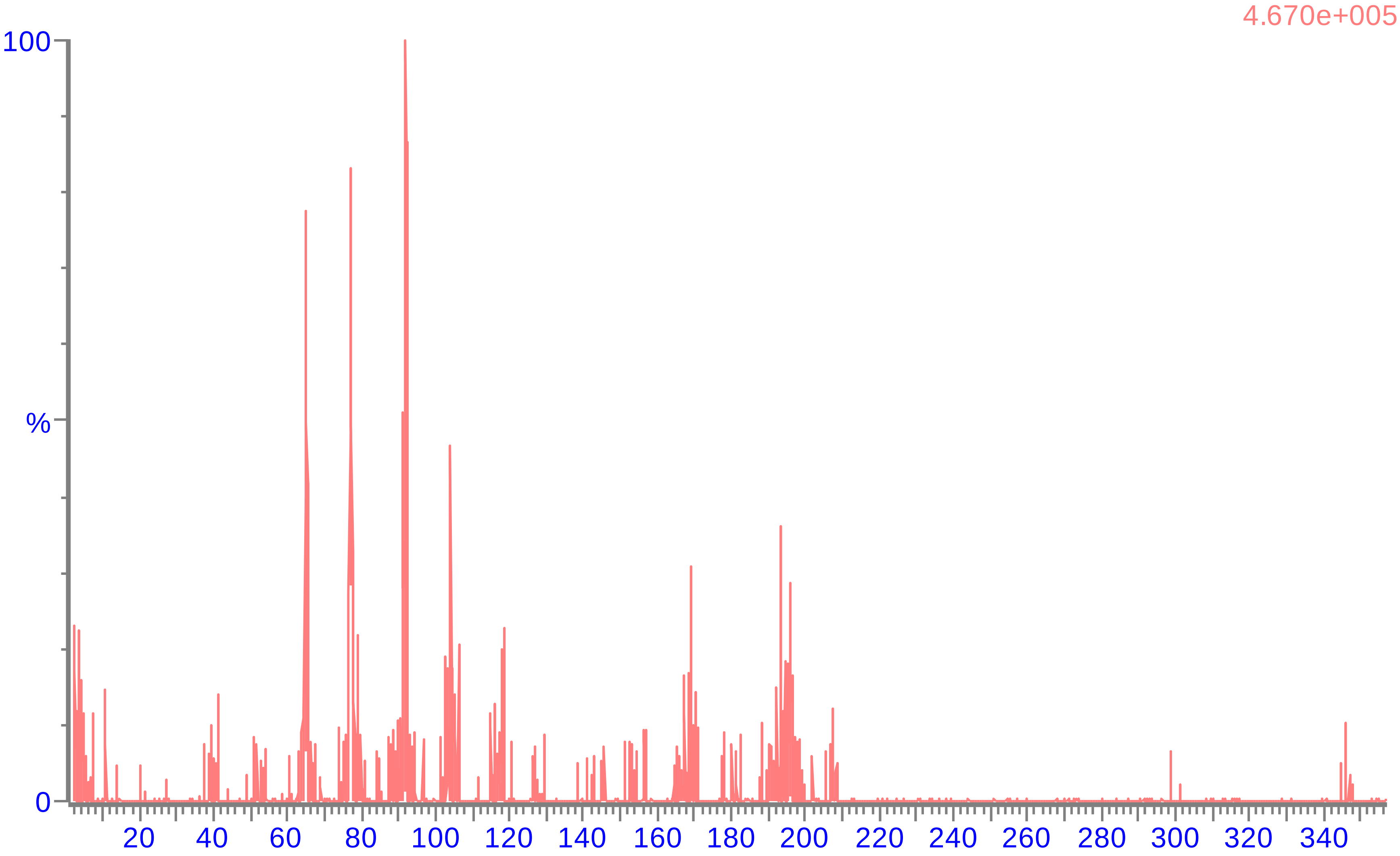

Figure 1.169: Mass spectrum for daughter fragment peak ES+, m/z 347.16 -> 65.04.

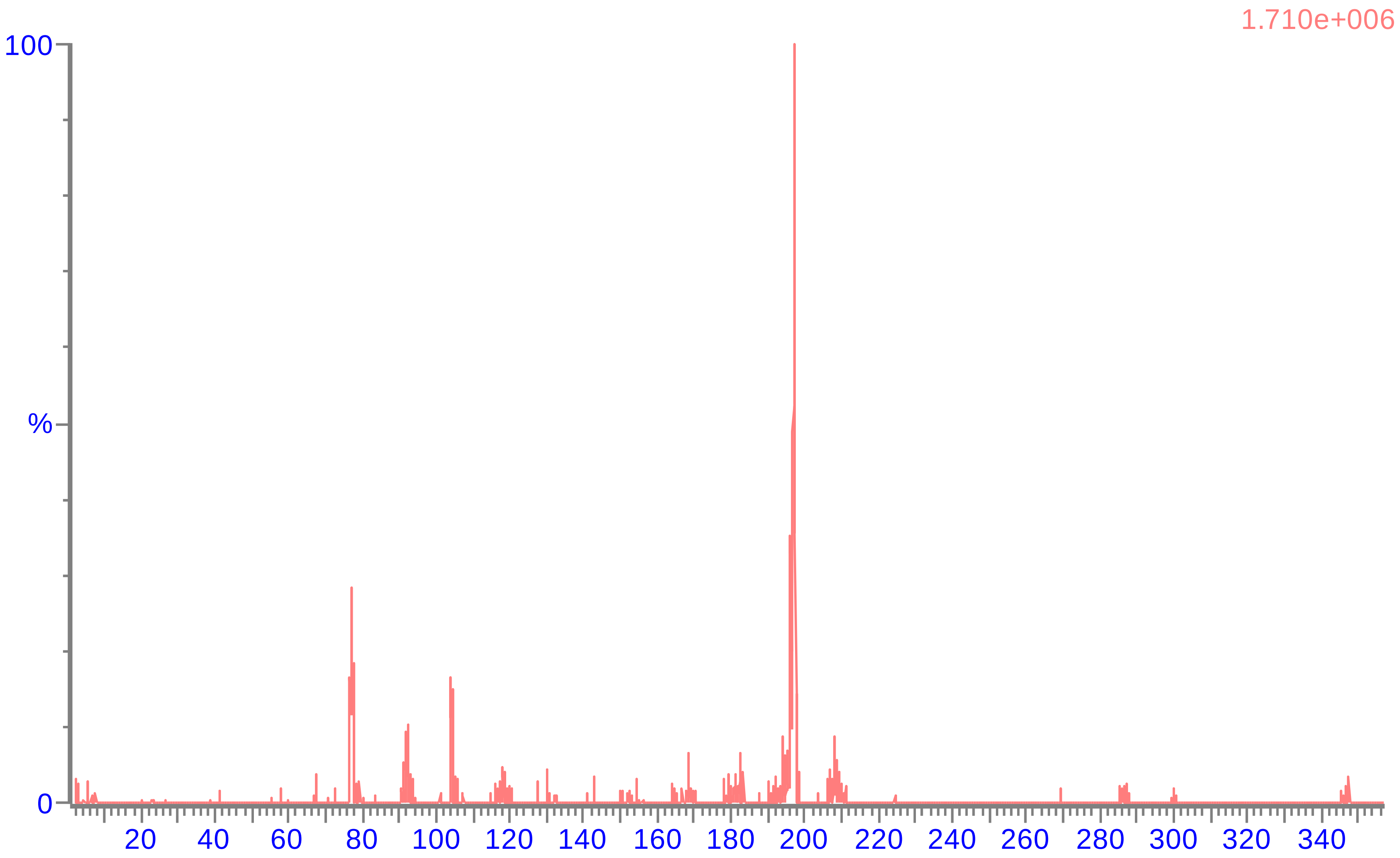

Figure 1.170: Mass spectrum for daughter fragment peak ES+, m/z 347.16 -> 104.13.

**9a** *N*-(2-nitro-1-phenylpropyl)aniline.

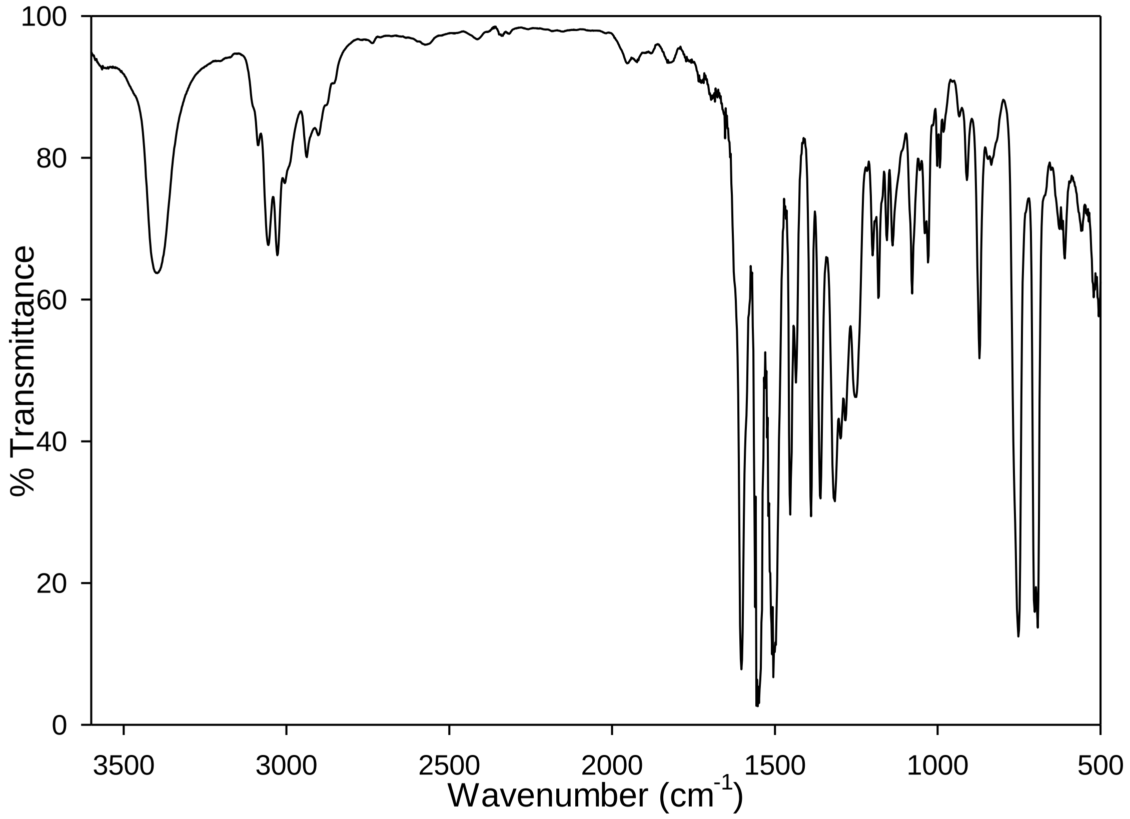

Figure 1.171: IR spectrum of **9a** *N*-(2-nitro-1-phenylpropyl)aniline.

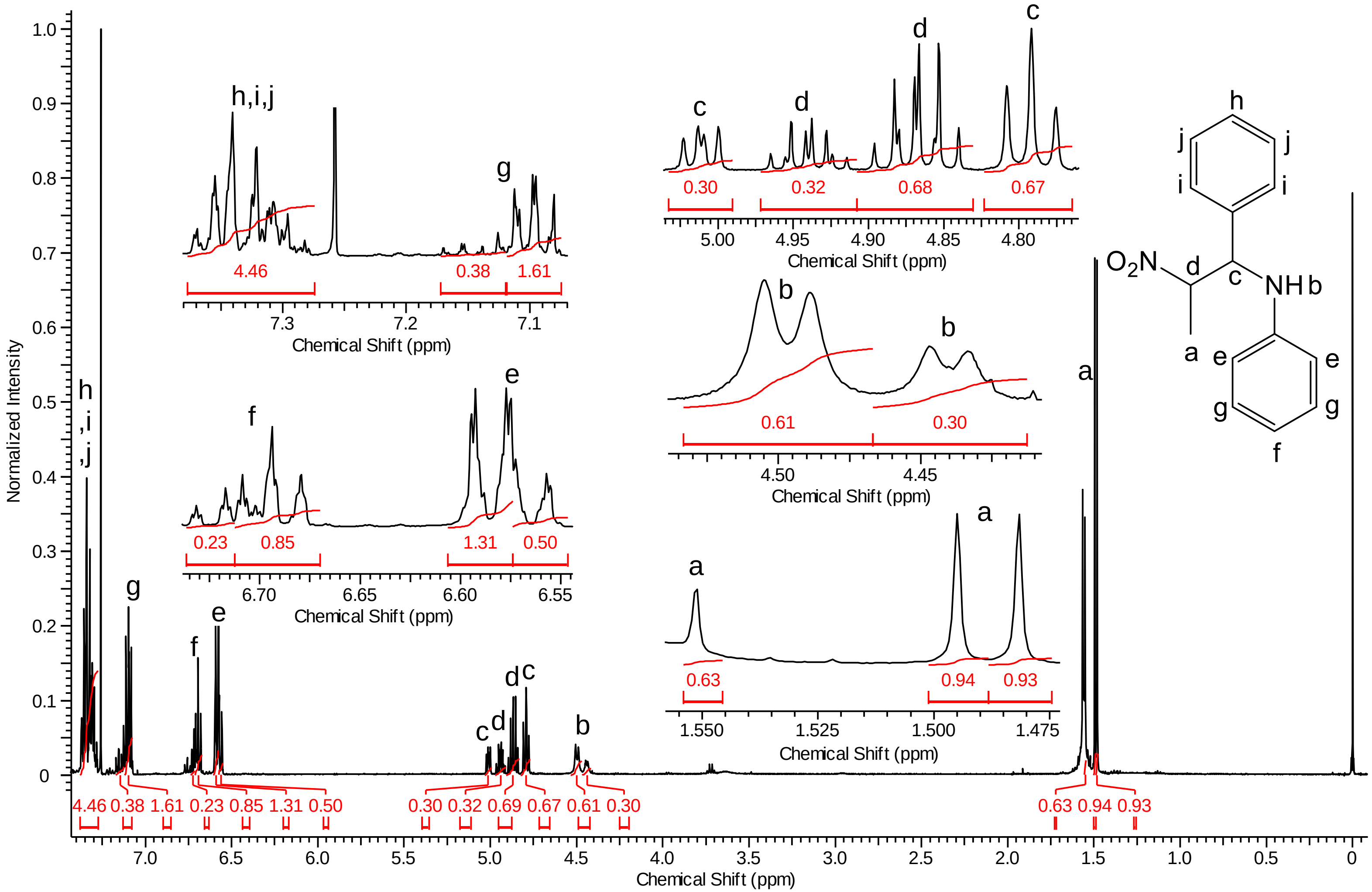

Figure 1.172: $^1$H NMR spectrum of **9a** *N*-(2-nitro-1-phenylpropyl)aniline (two pairs of diastereomers).

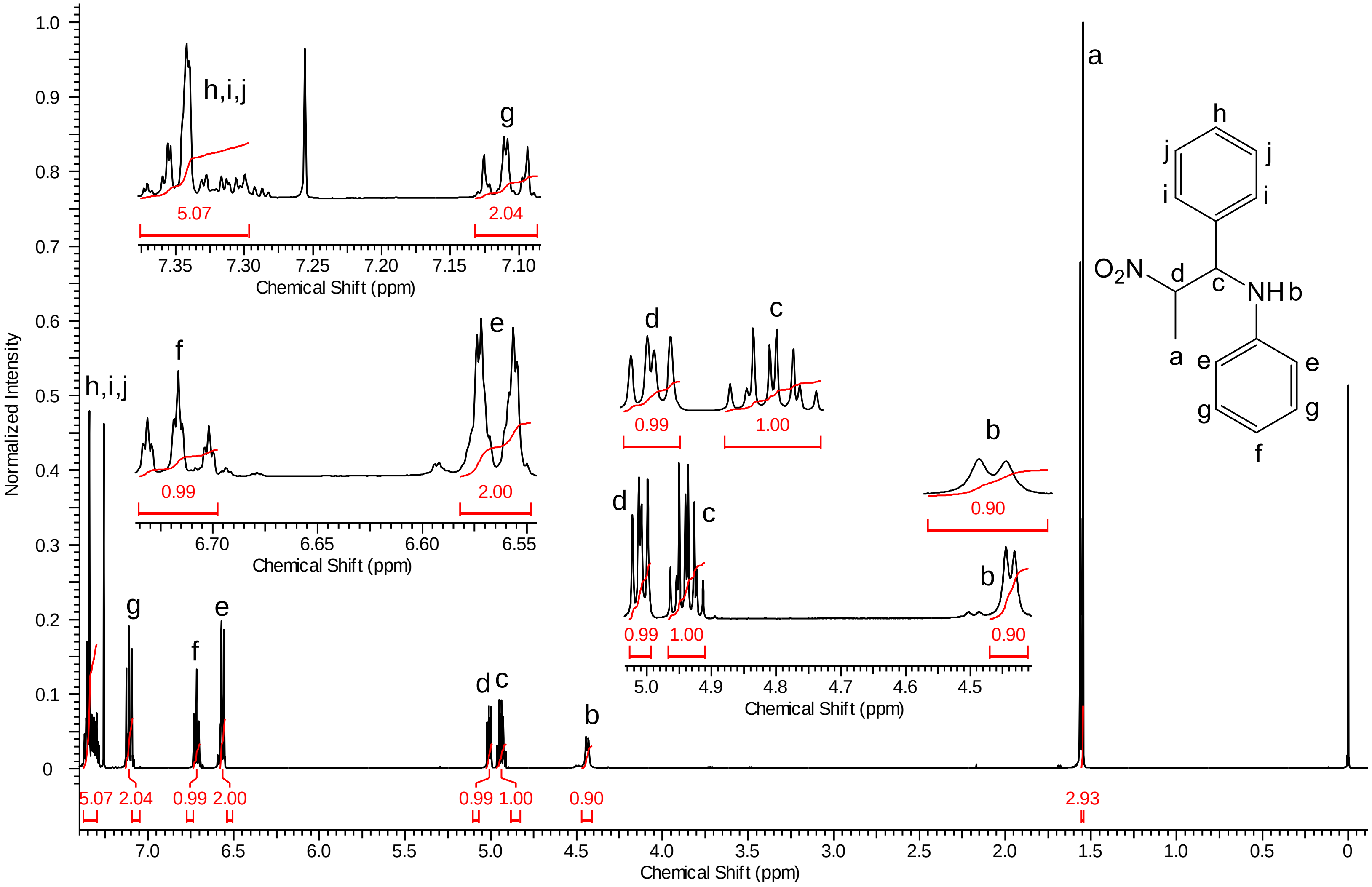

Figure 1.173: $^1$H NMR spectrum of **9a** *N*-(2-nitro-1-phenylpropyl)aniline (one pair of diastereomers).

**9b** *N*-(2-nitro-1-phenylbutyl)aniline

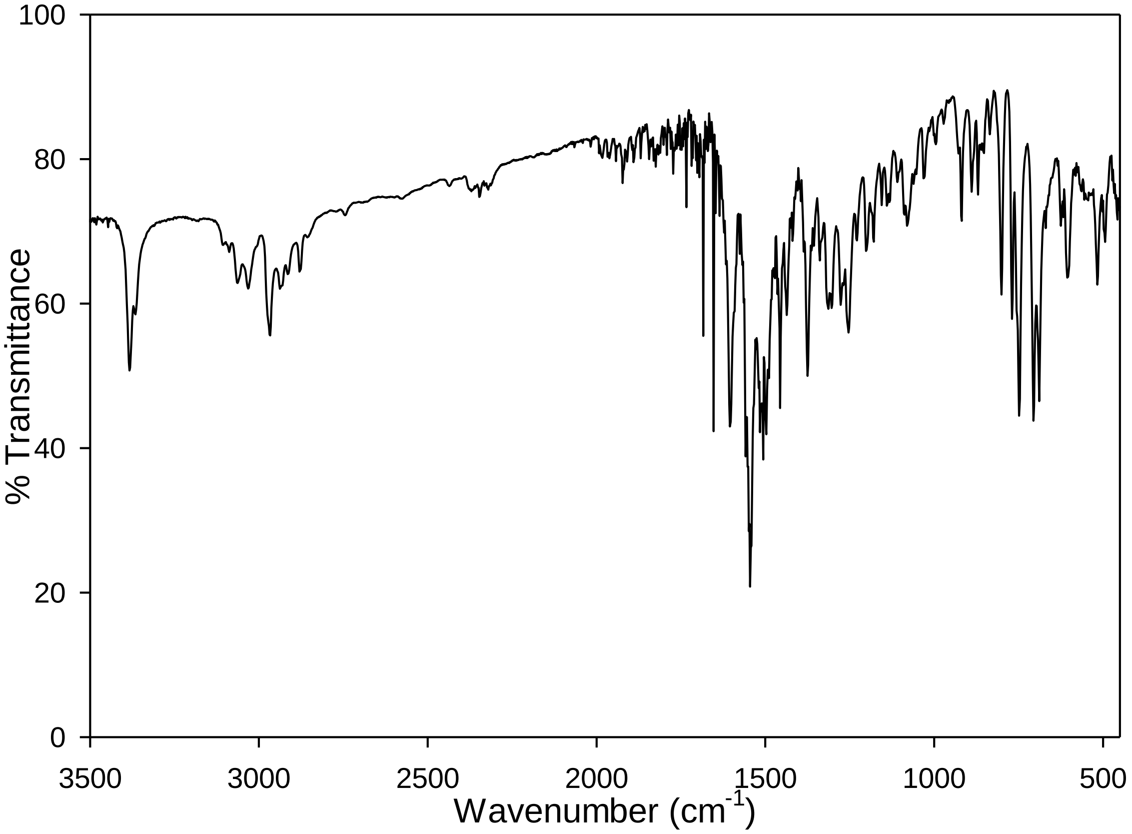

Figure 1.174: IR spectrum of **9b** *N*-(2-nitro-1-phenylbutyl)aniline.

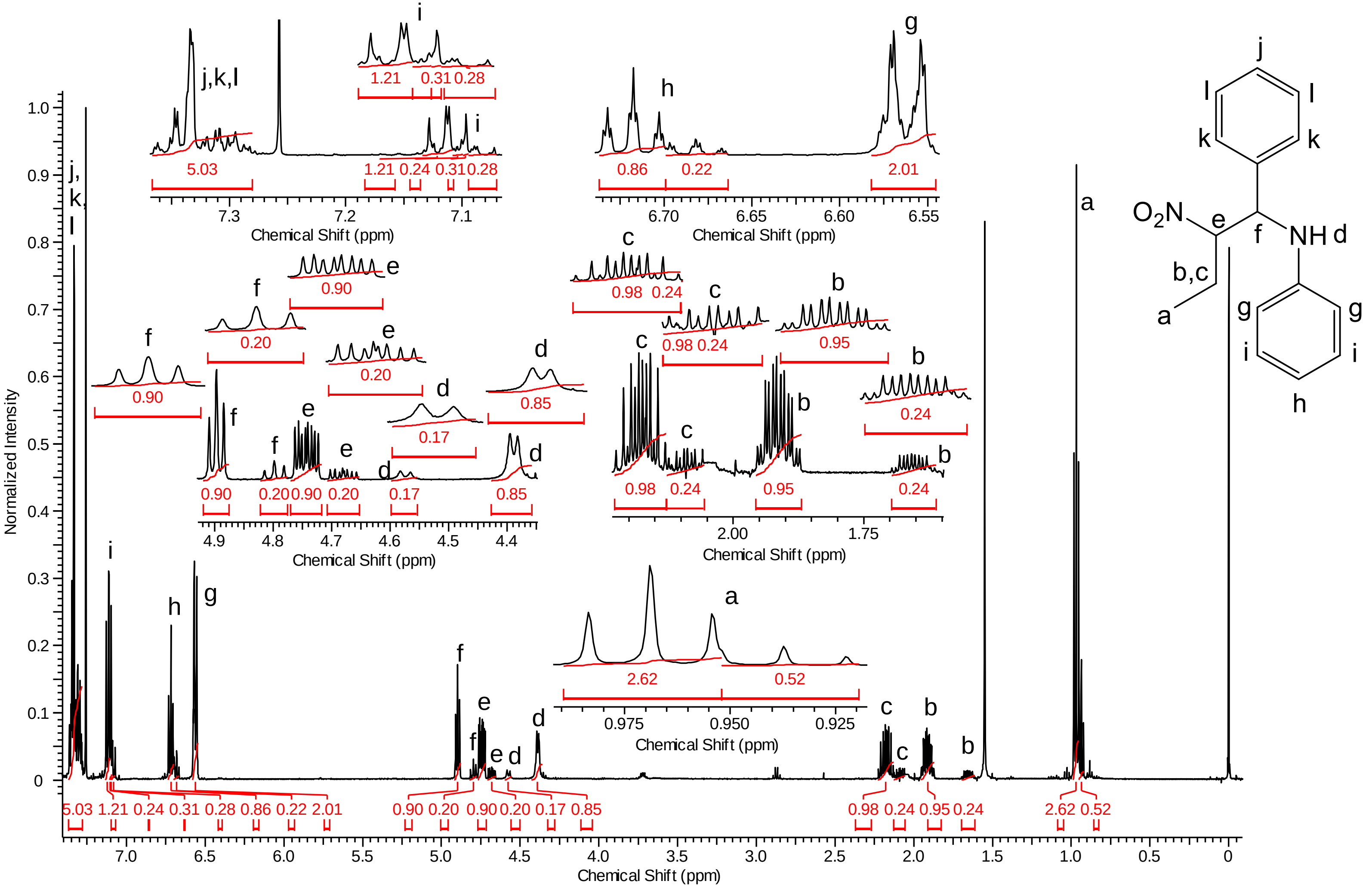

Figure 1.175: $^1$H NMR spectrum of **9b** *N*-(2-nitro-1-phenylbutyl)aniline (two pairs of diastereomers).

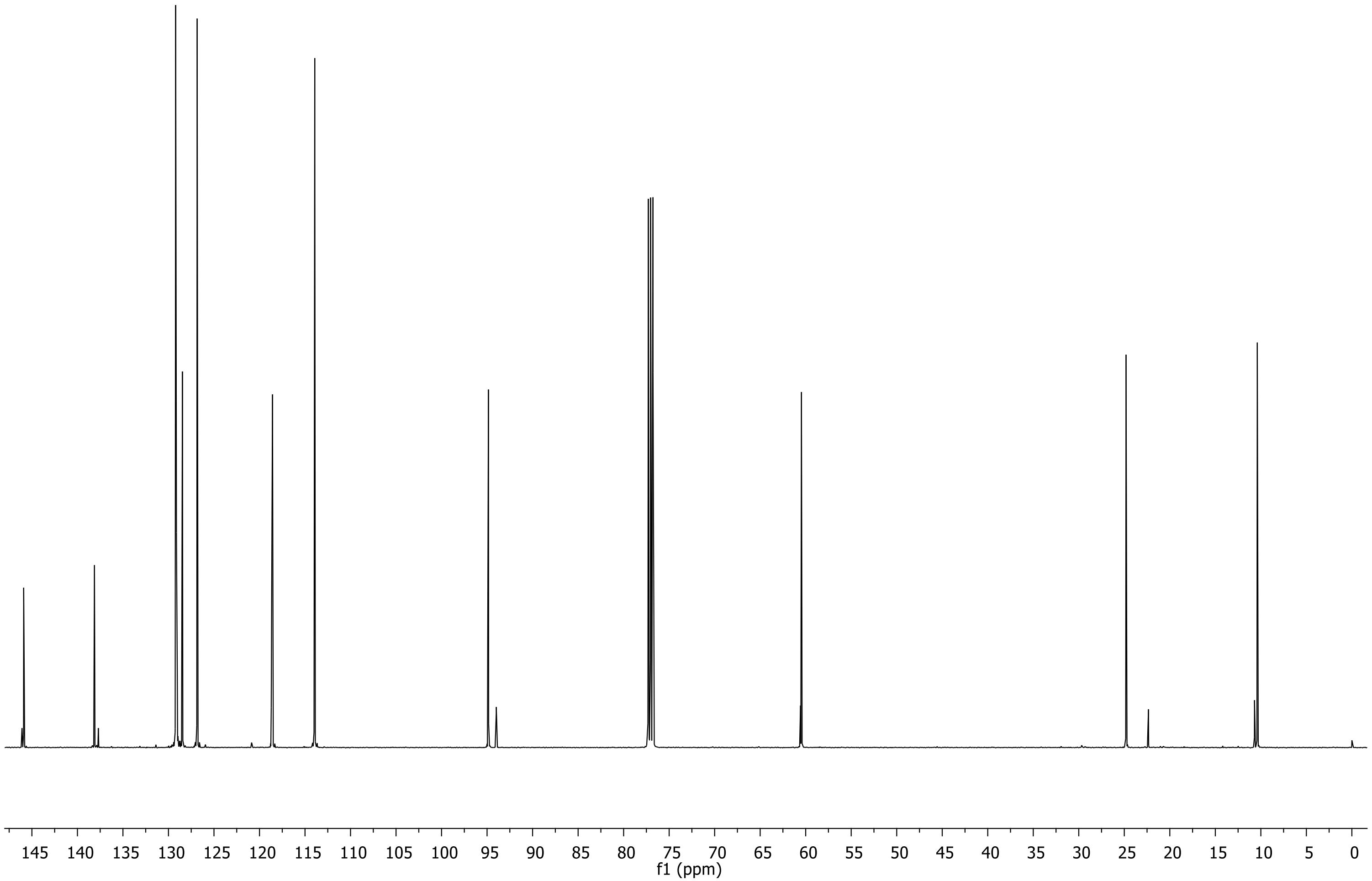

Figure 1.176: $^{13}$C NMR spectrum of **9b** *N*-(2-nitro-1-phenylbutyl)aniline (two pairs of diastereomers).

Table 1.24: MS data.

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **9b** | 270 | 1 | 271.16 | 24 | 148.03 | 16 | ES+ |
| | | 2 | 271.16 | 24 | 77.07 | 56 | ES+ |
| | | 3 | 271.16 | 24 | 56.19 | 22 | ES+ |

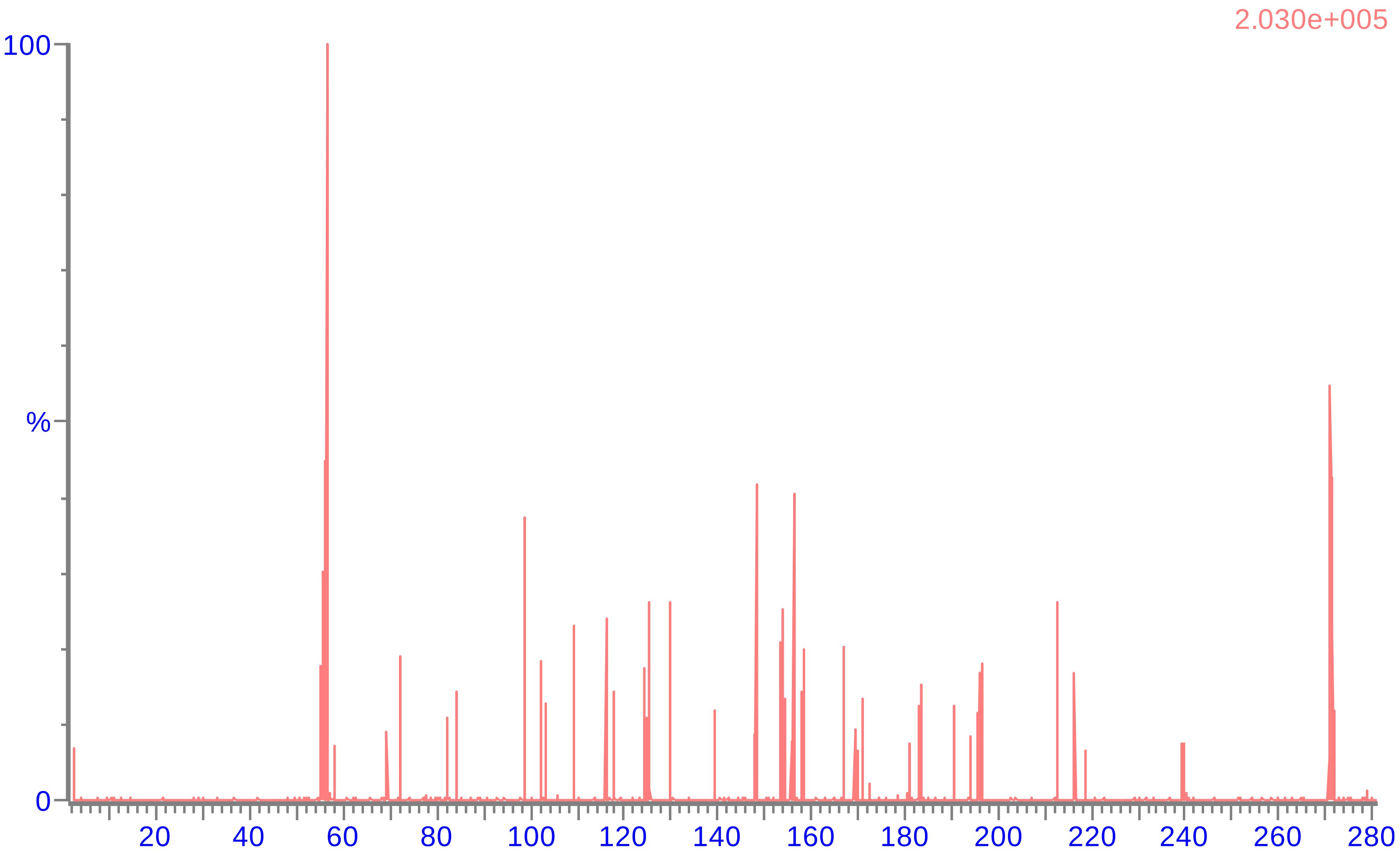

Figure 1.177: Mass spectrum for daughter fragment peak ES+, m/z 276.16 -> 148.03.

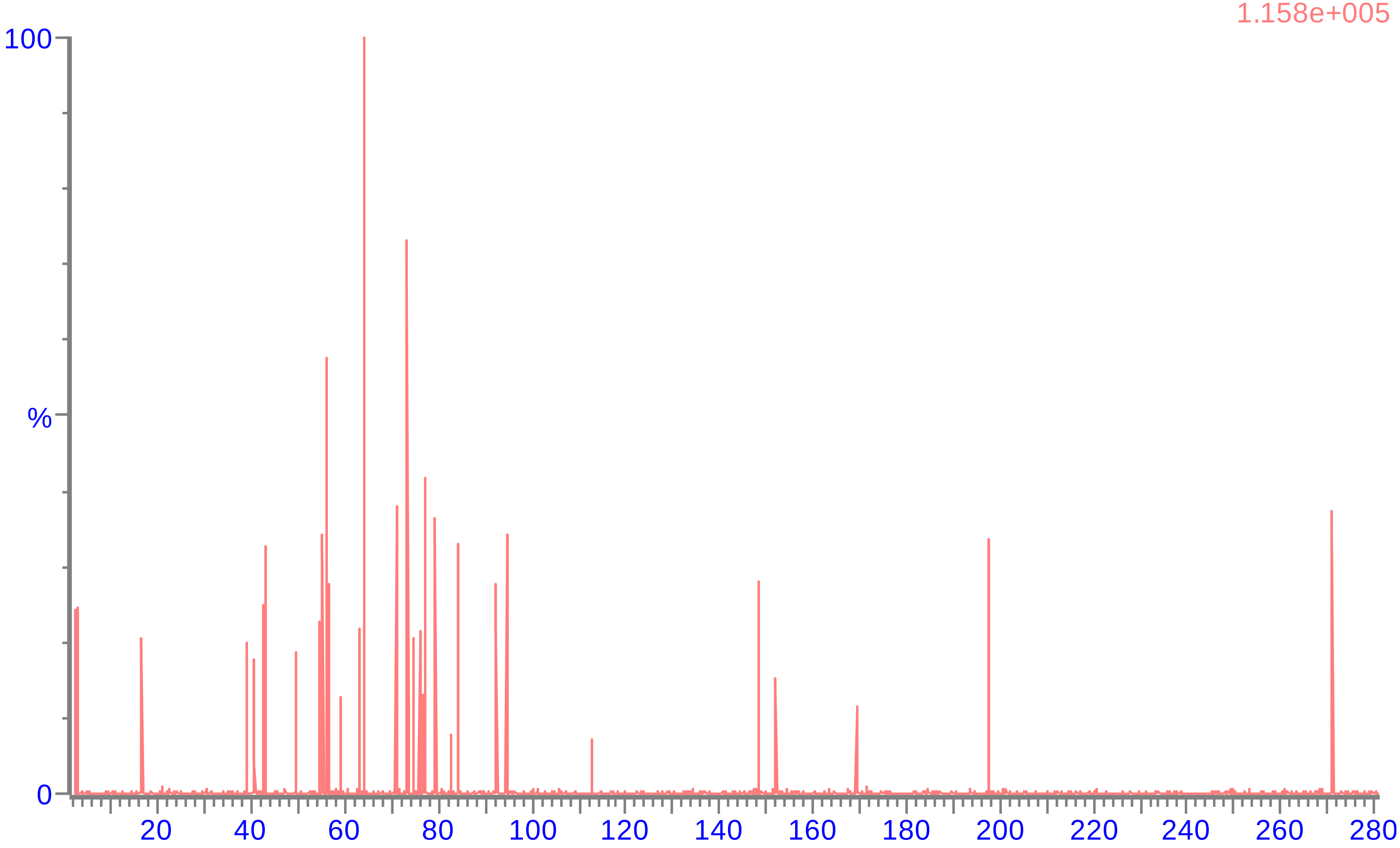

Figure 1.178: Mass spectrum for daughter fragment peak ES+, m/z 276.16 -> 77.07.

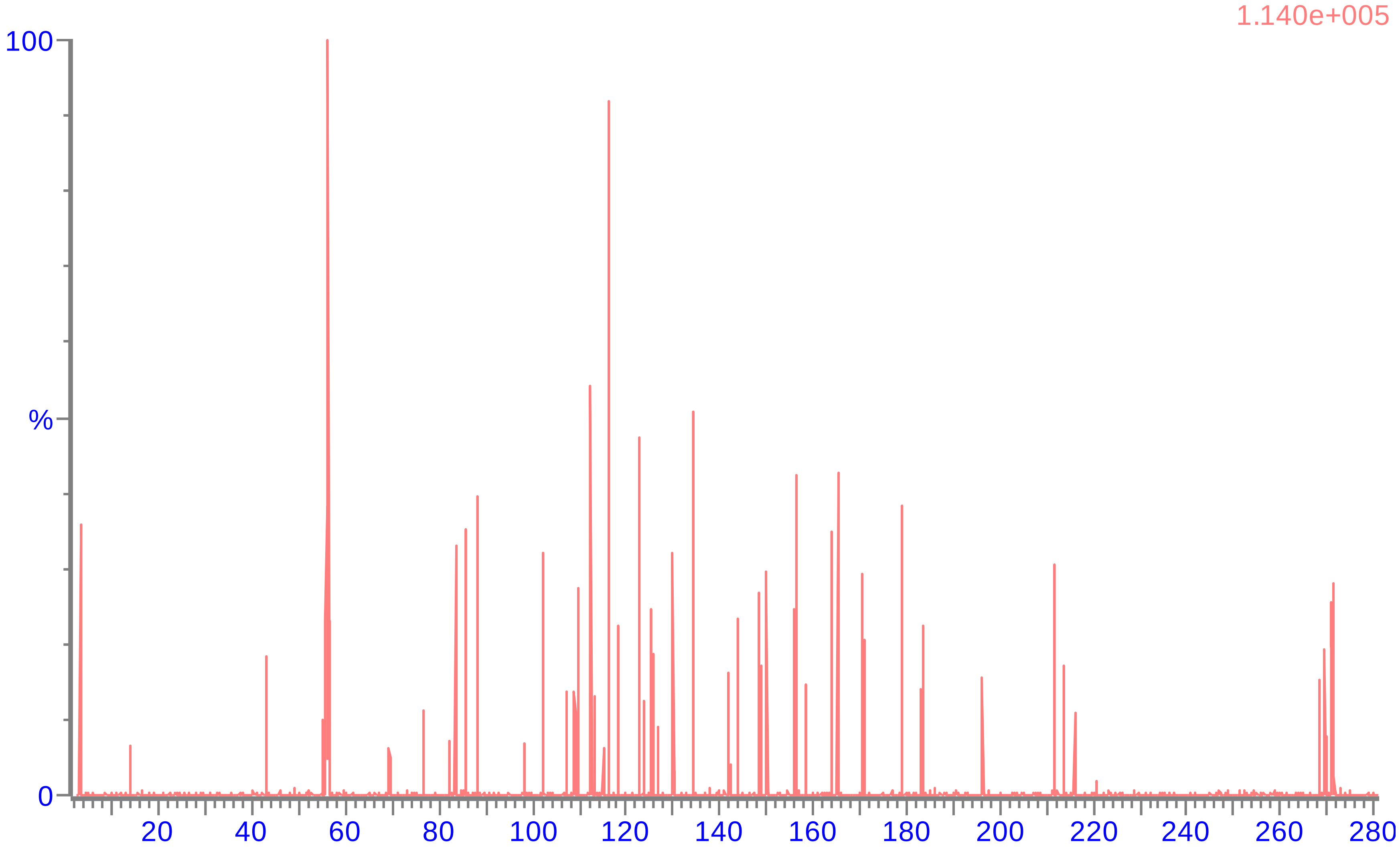

Figure 1.179: Mass spectrum for daughter fragment peak ES+, m/z 276.16 -> 56.19.

**4a** 3-nitro-*N*-(2-nitro-1-(*p*-tolyl)ethyl)aniline

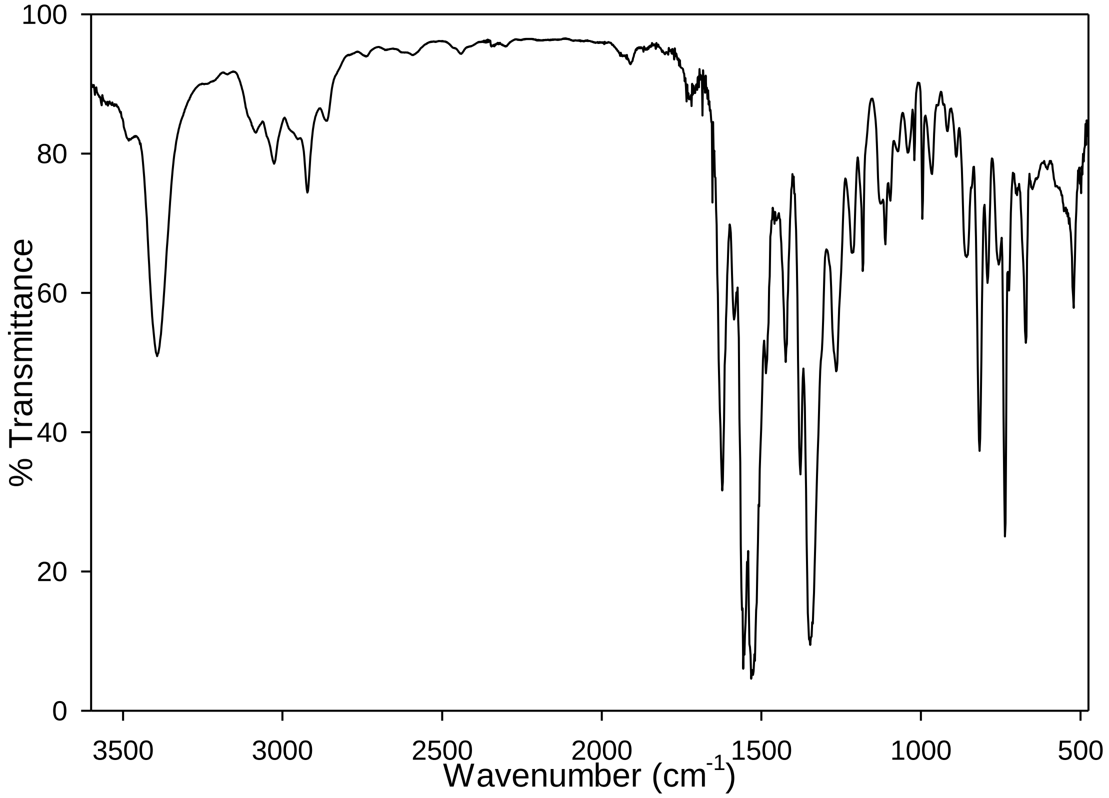

Figure 1.180: IR spectrum of **4a** 3-nitro-*N*-(2-nitro-1-(*p*-tolyl)ethyl)aniline.

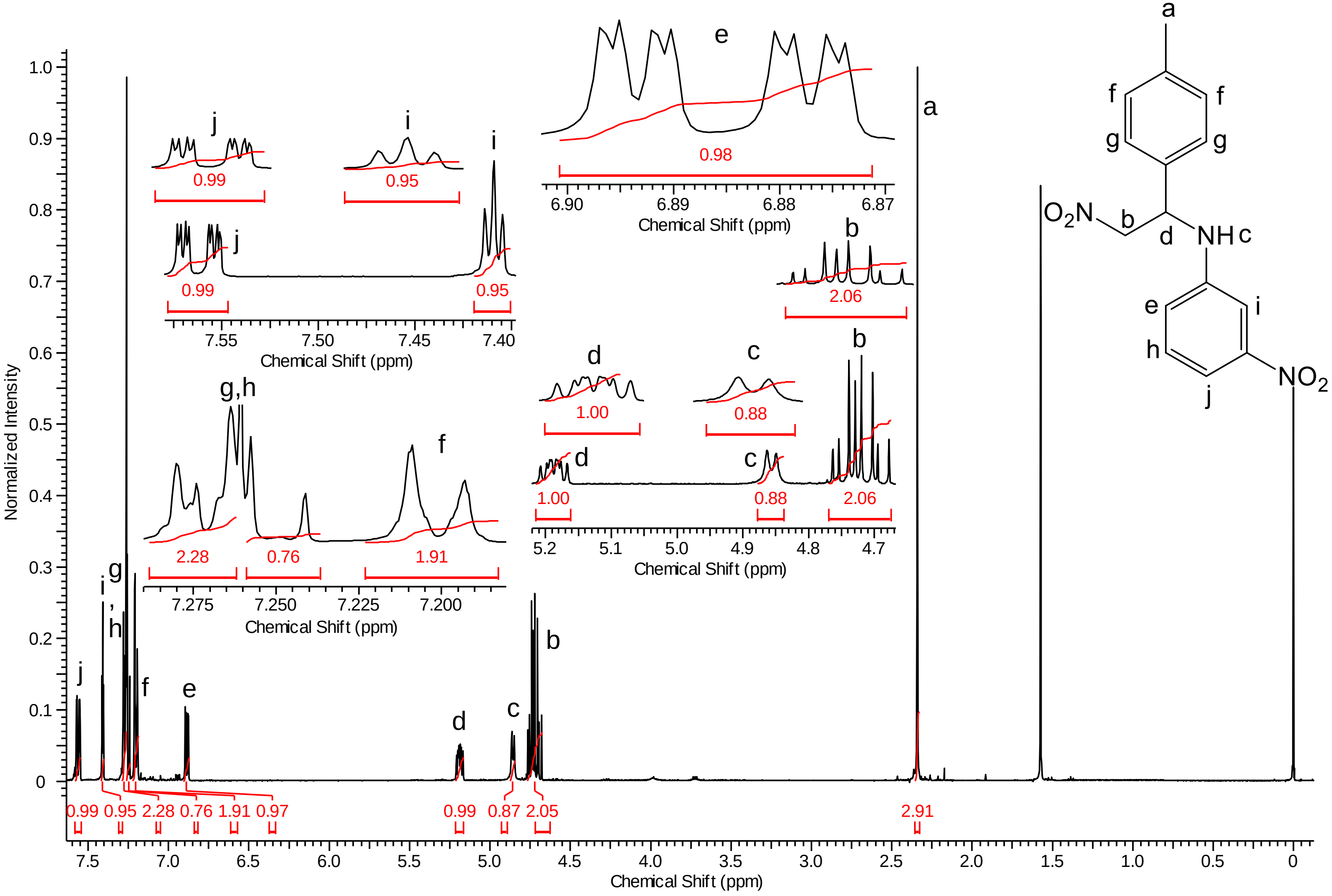

Figure 1.181: $^1$H NMR spectrum of **4a** 3-nitro-*N*-(2-nitro-1-(*p*-tolyl)ethyl)aniline.

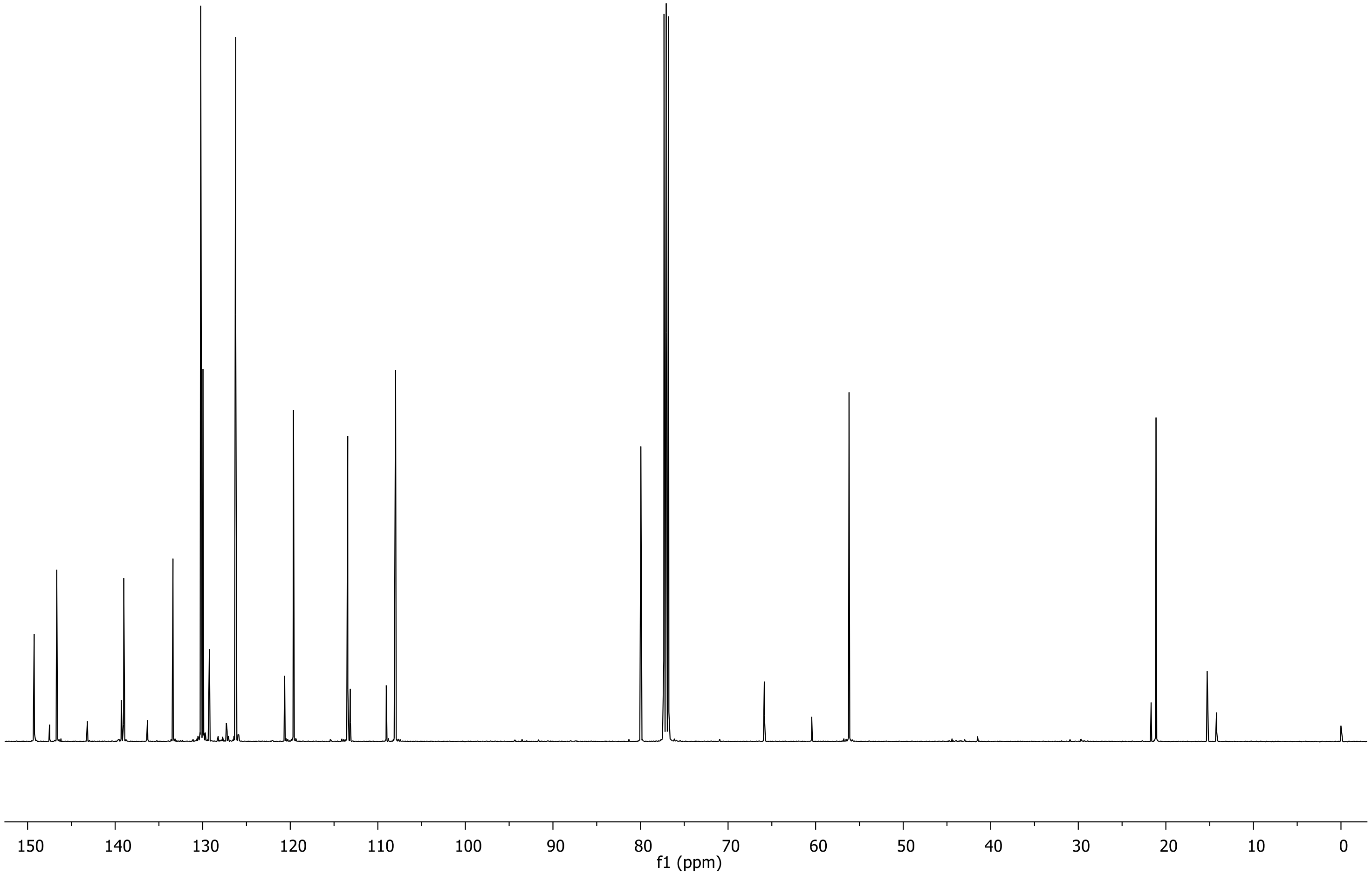

Figure 1.182: $^{13}$C NMR spectrum of **4a** 3-nitro-*N*-(2-nitro-1-(*p*-tolyl)ethyl)aniline.

Table 1.25: MS data

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **4a** | 301 | 1 | 302.10 | 14 | 164.08 | 8 | ES+ |
| | | 2 | 302.10 | 14 | 118.10 | 16 | ES+ |
| | | 3 | 302.10 | 14 | 117.71 | 58 | ES+ |
| | | 4 | 302.10 | 14 | 91.05 | 58 | ES+ |
| | | 5 | 302.10 | 14 | 121.03 | 20 | ES+ |

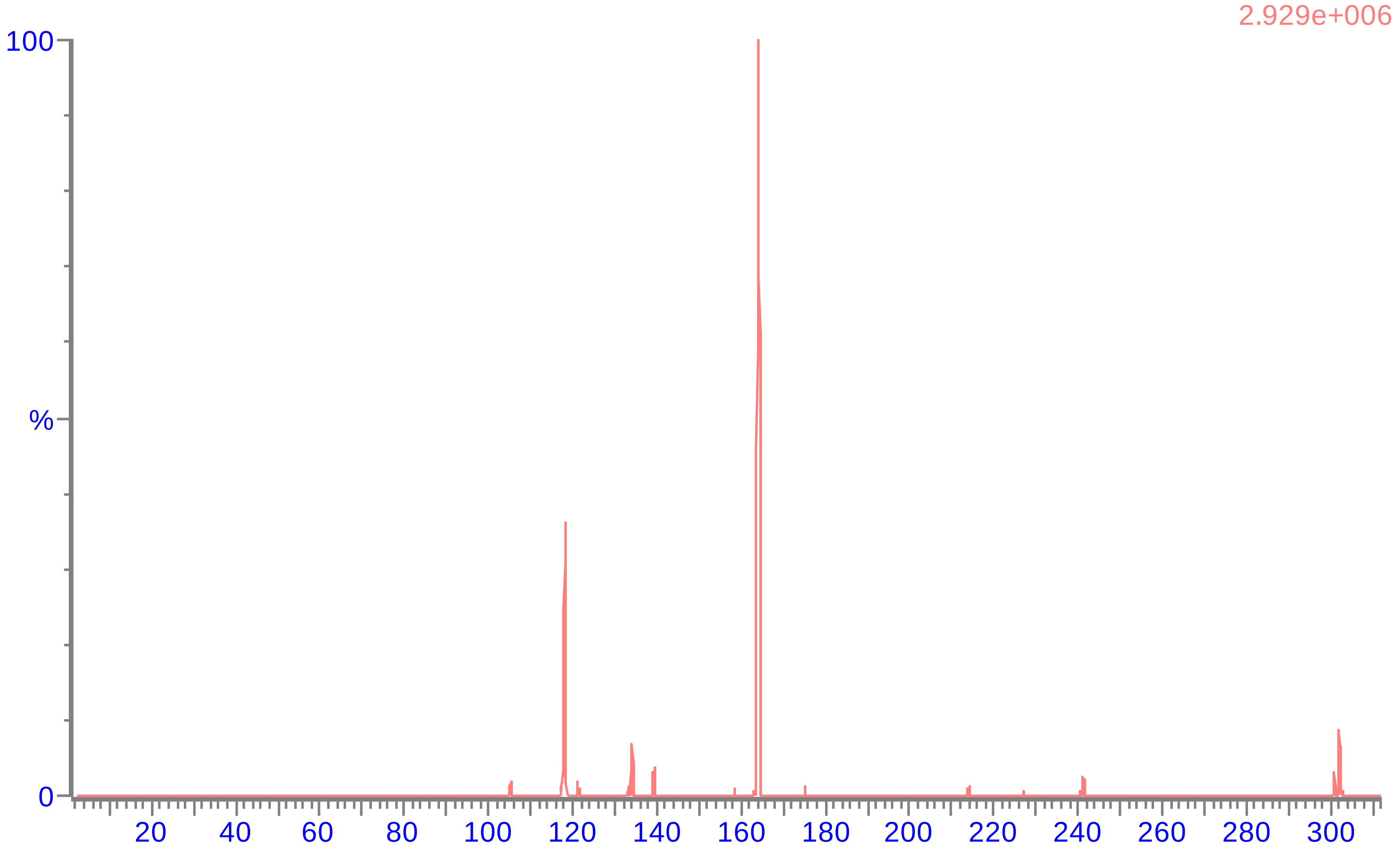

Figure 1.183: Mass spectrum for daughter fragment peak ES+, m/z 302.10 -> 164.08.

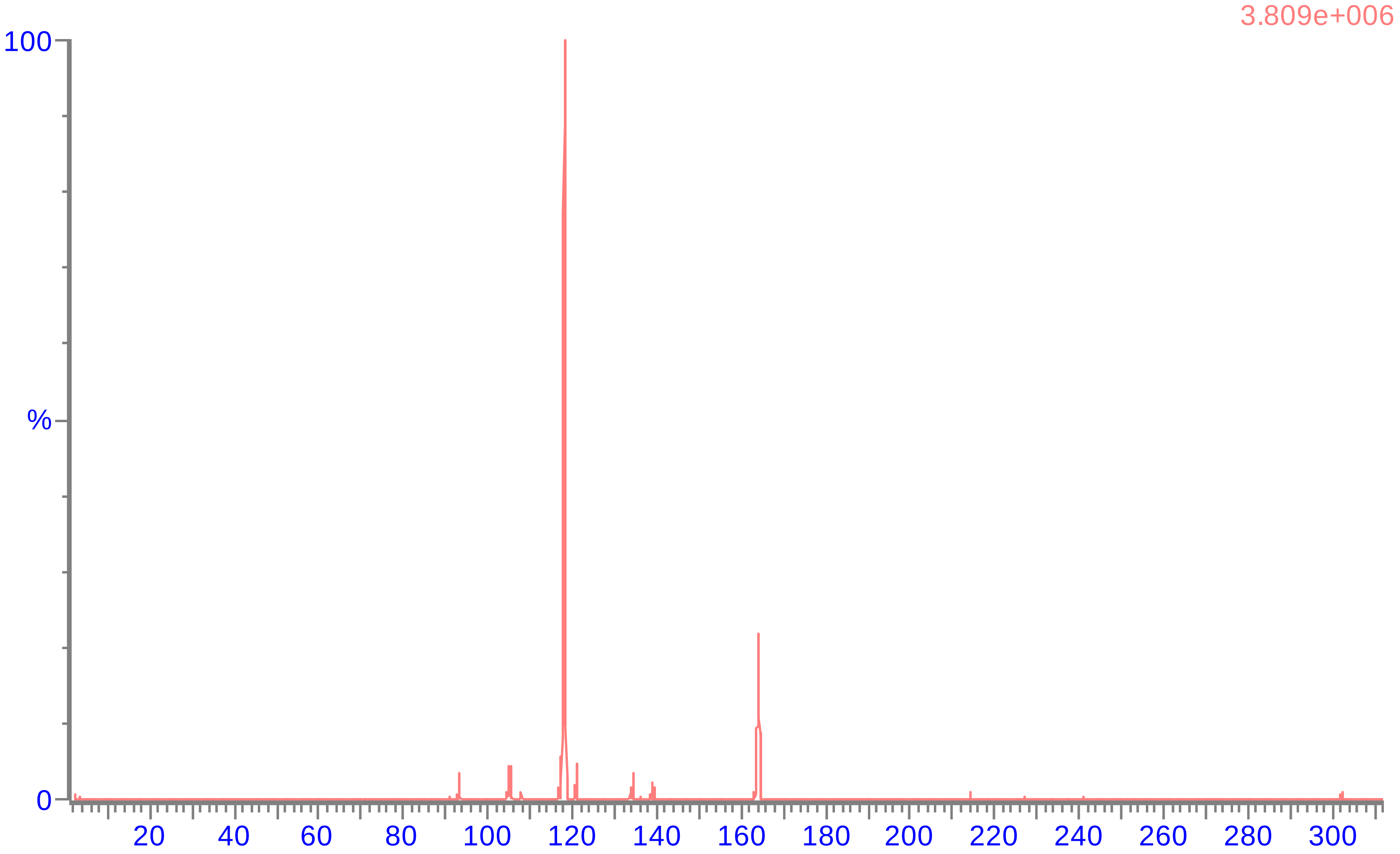

Figure 1.184: Mass spectrum for daughter fragment peak ES+, m/z 302.10 -> 118.10.

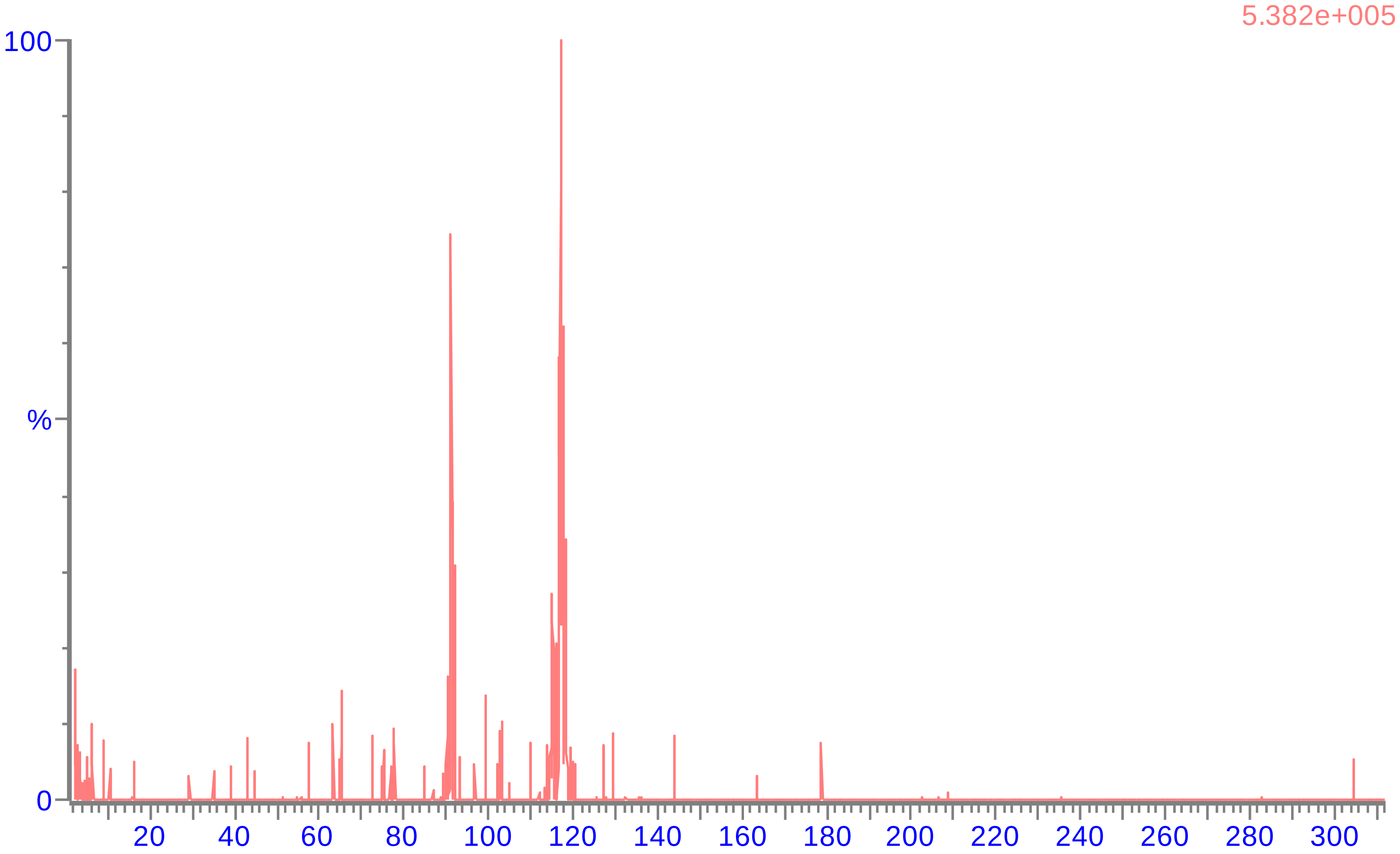

Figure 1.185: Mass spectrum for daughter fragment peak ES+, m/z 302.10 -> 117.71.

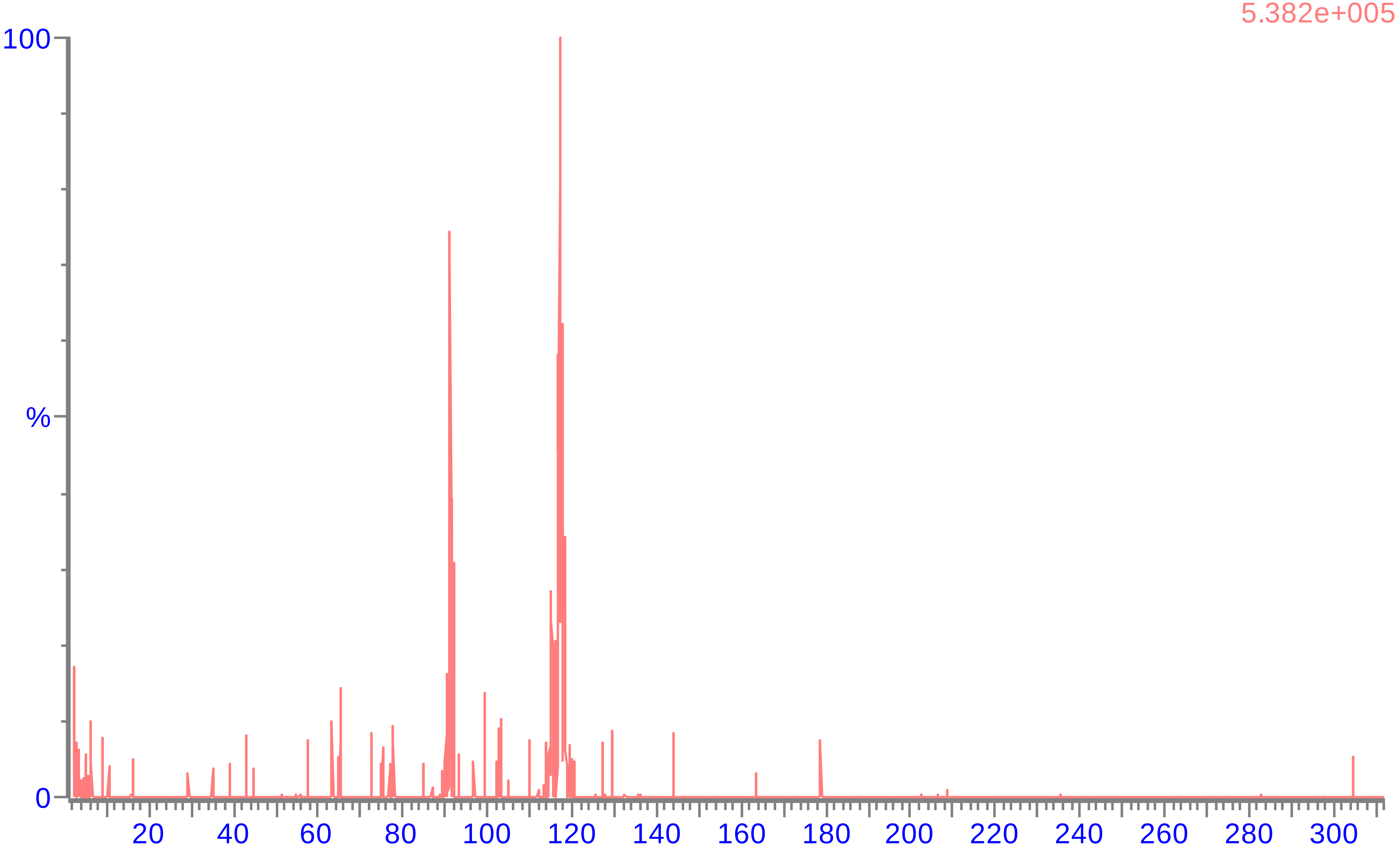

Figure 1.186: Mass spectrum for daughter fragment peak ES+, m/z 302.10 -> 91.05.

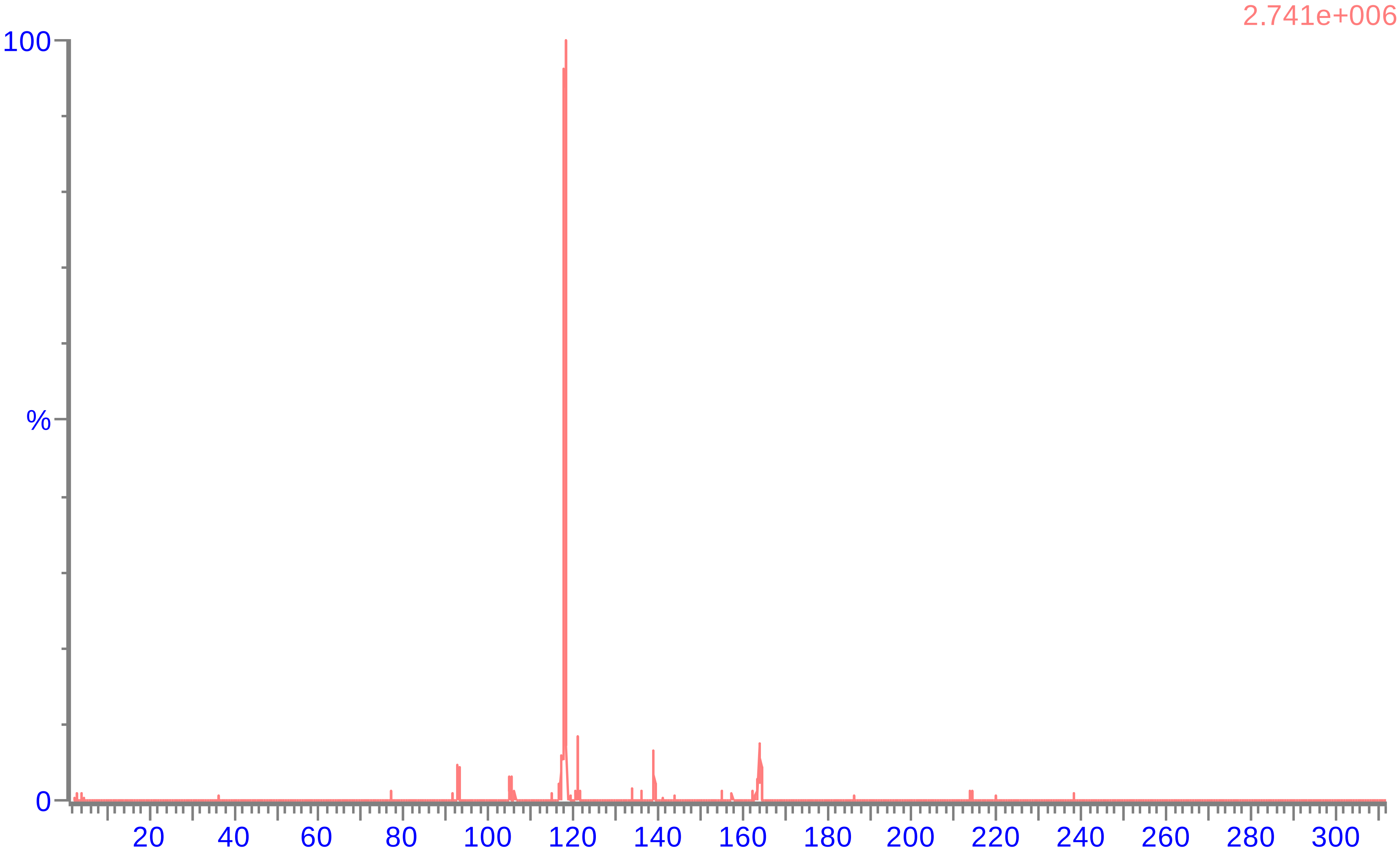

Figure 1.187: Mass spectrum for daughter fragment peak ES+, m/z 302.10 -> 121.03.

**4b** 4-chloro-*N*-(1-(4-methoxyphenyl)-2-nitroethyl)aniline

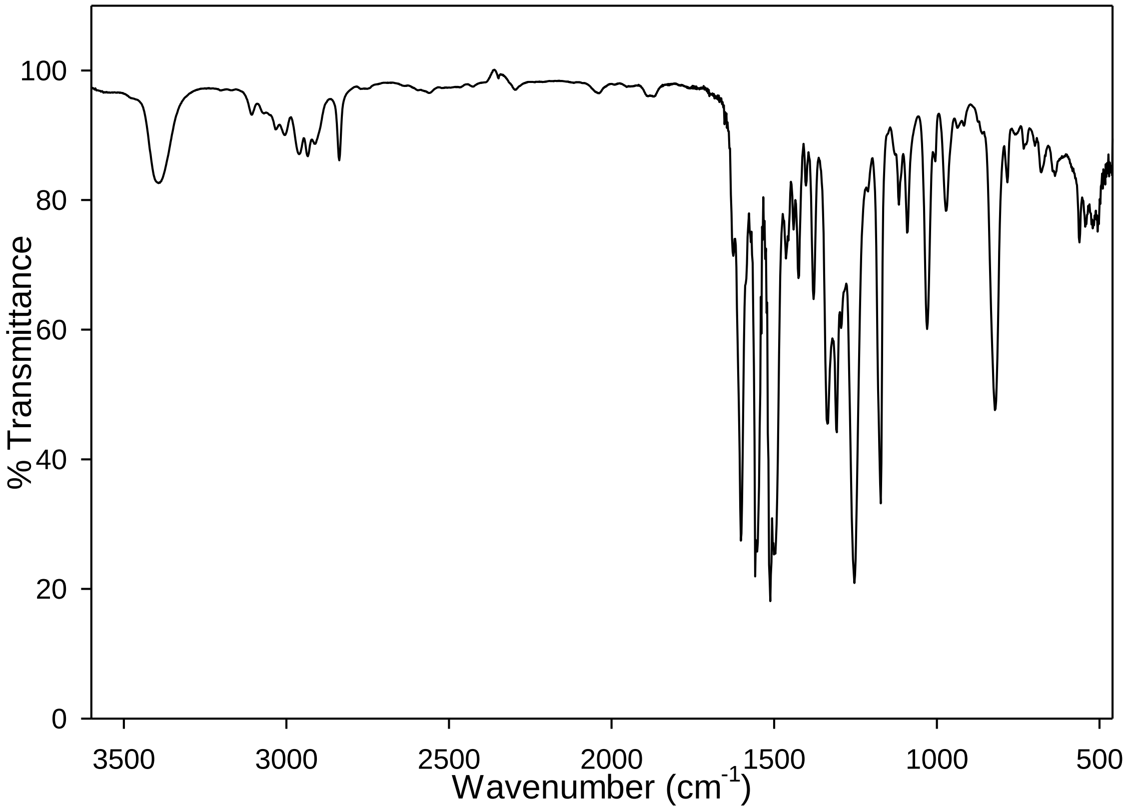

Figure 1.188: IR spectrum of **4b** 4-chloro-*N*-(1-(4-methoxyphenyl)-2-nitroethyl)aniline.

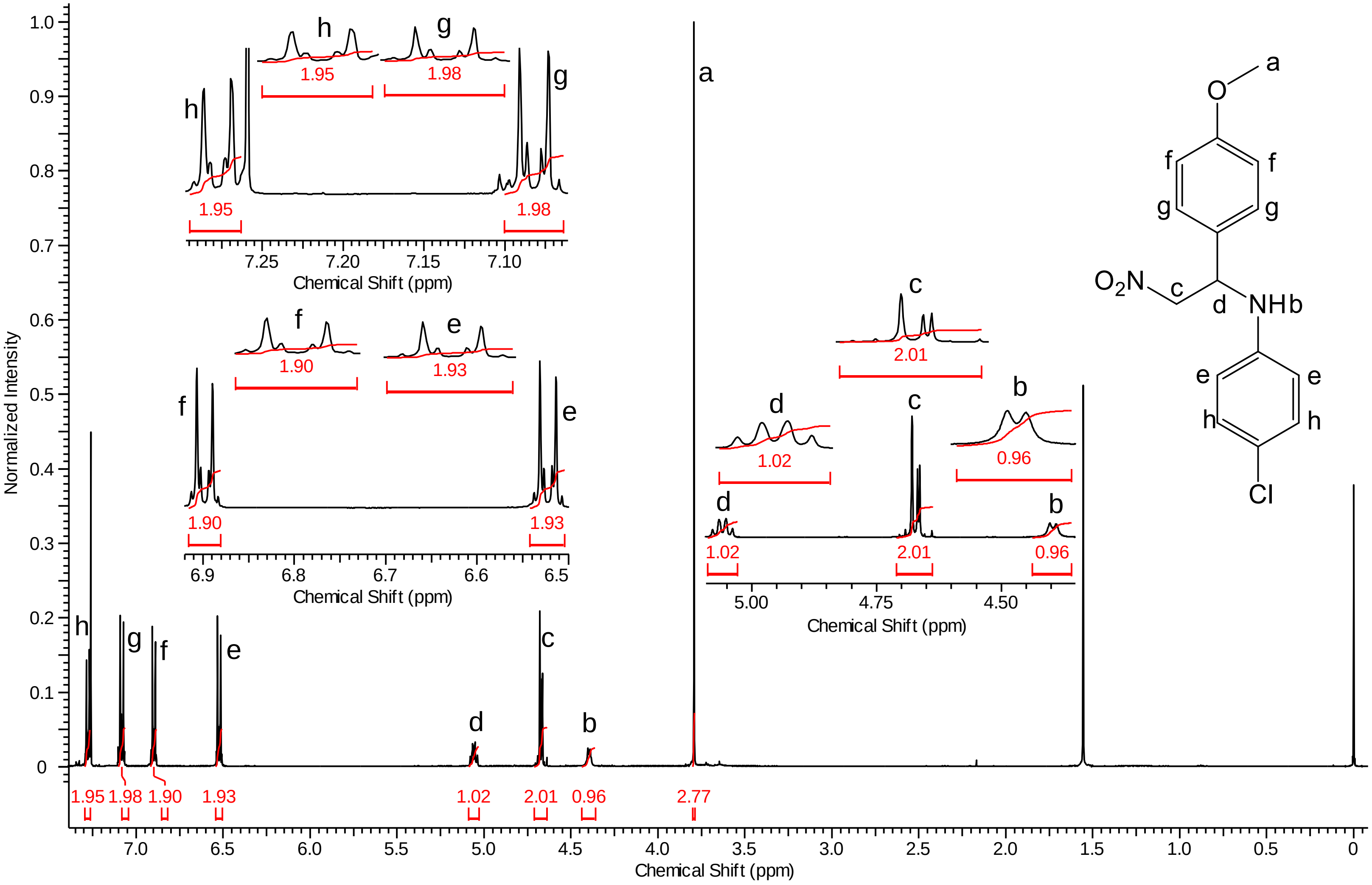

Figure 1.189: $^1$H NMR spectrum of **4b** 4-chloro-*N*-(1-(4-methoxyphenyl)-2-nitroethyl)aniline.

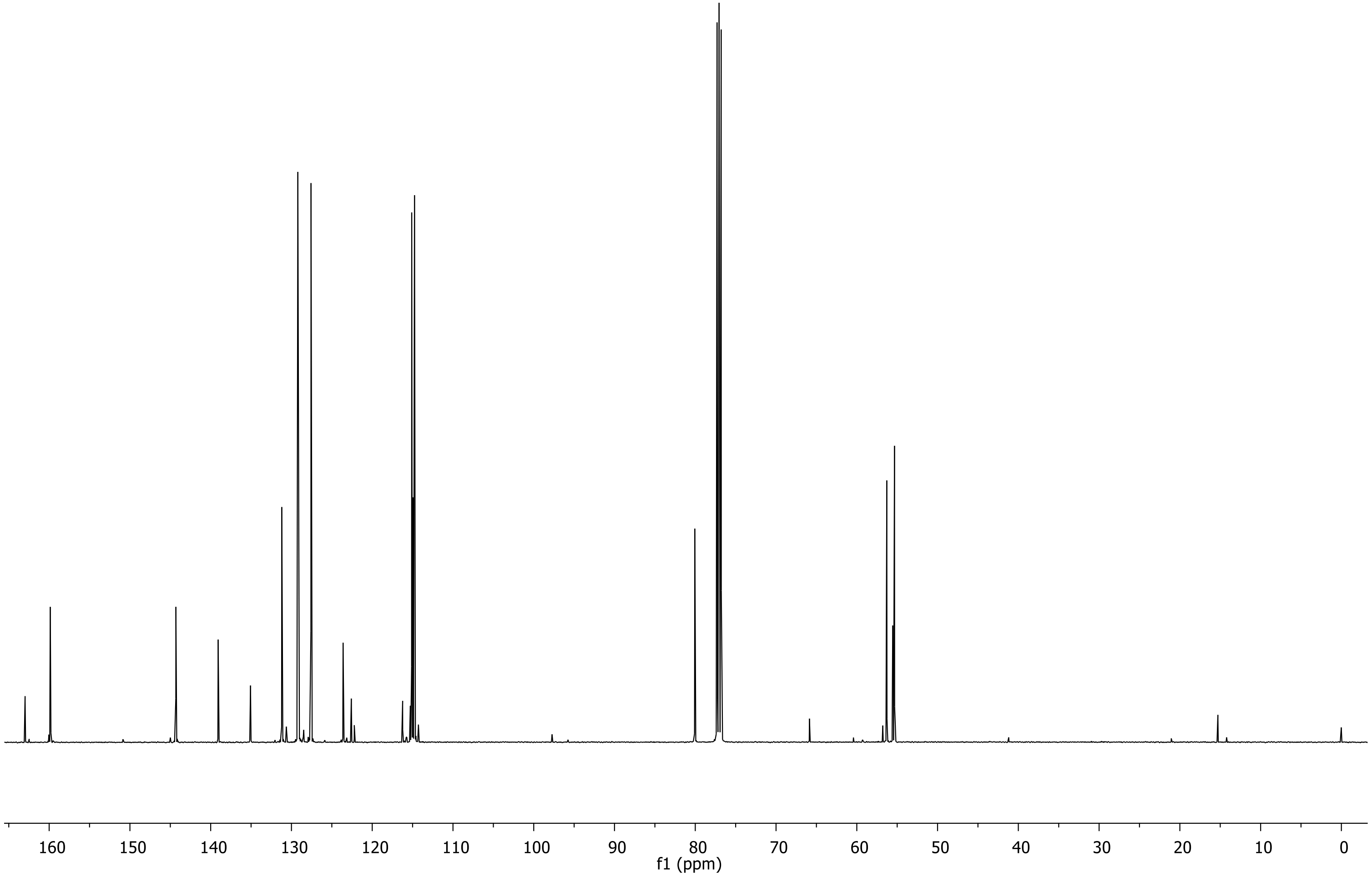

Figure 1.190: $^{13}$C NMR spectrum of **4b** 4-chloro-*N*-(1-(4-methoxyphenyl)-2-nitroethyl)aniline.

Table 1.26: MS data

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **4b** | 305.8 | 1 | 307.09 | 12 | 180.05 | 6 | ES+ |
| | | 2 | 307.09 | 12 | 91.06 | 52 | ES+ |
| | | 3 | 307.09 | 12 | 119.04 | 40 | ES+ |

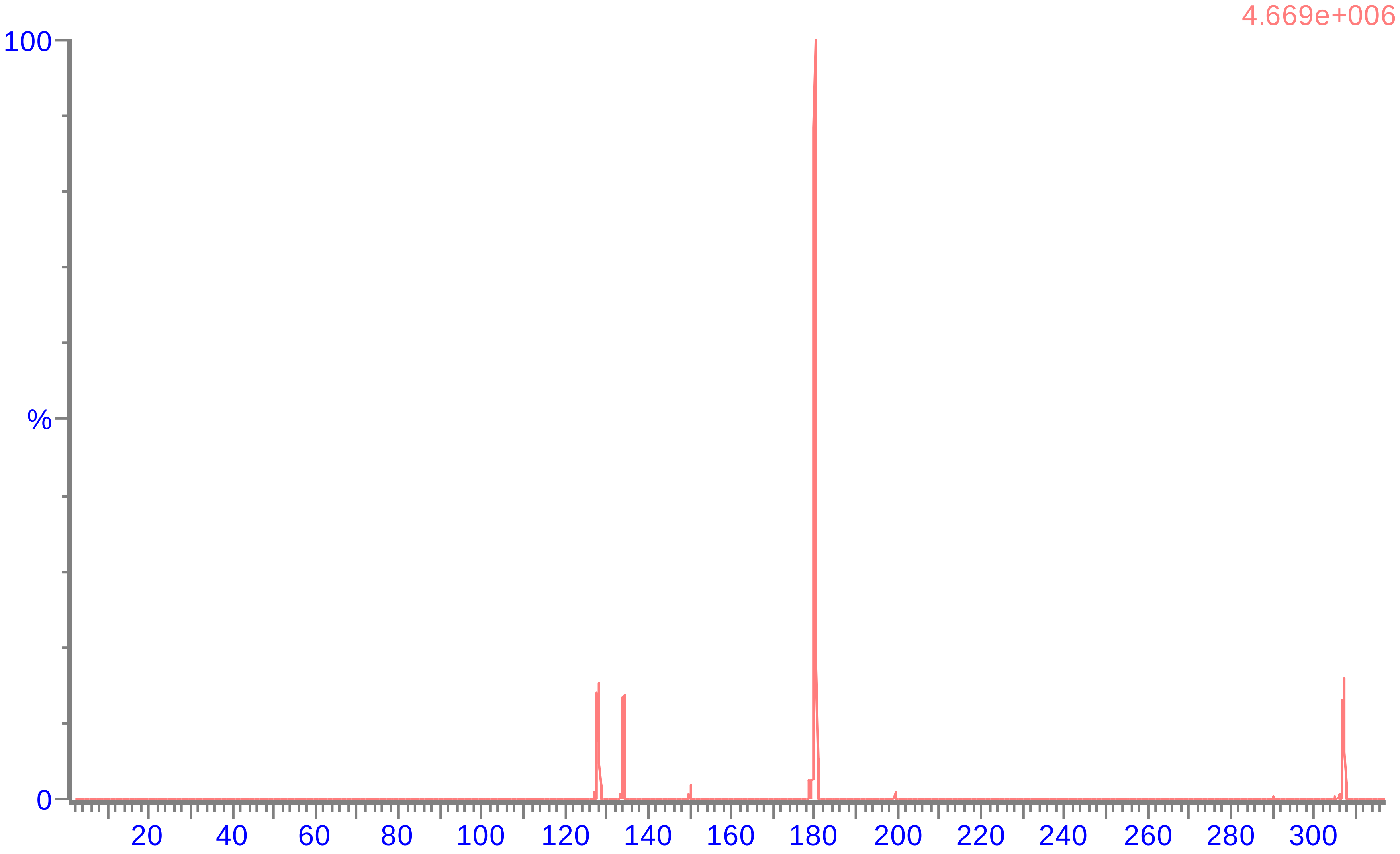

Figure 1.191: Mass spectrum for daughter fragment peak ES+, m/z 307.09 -> 180.05.

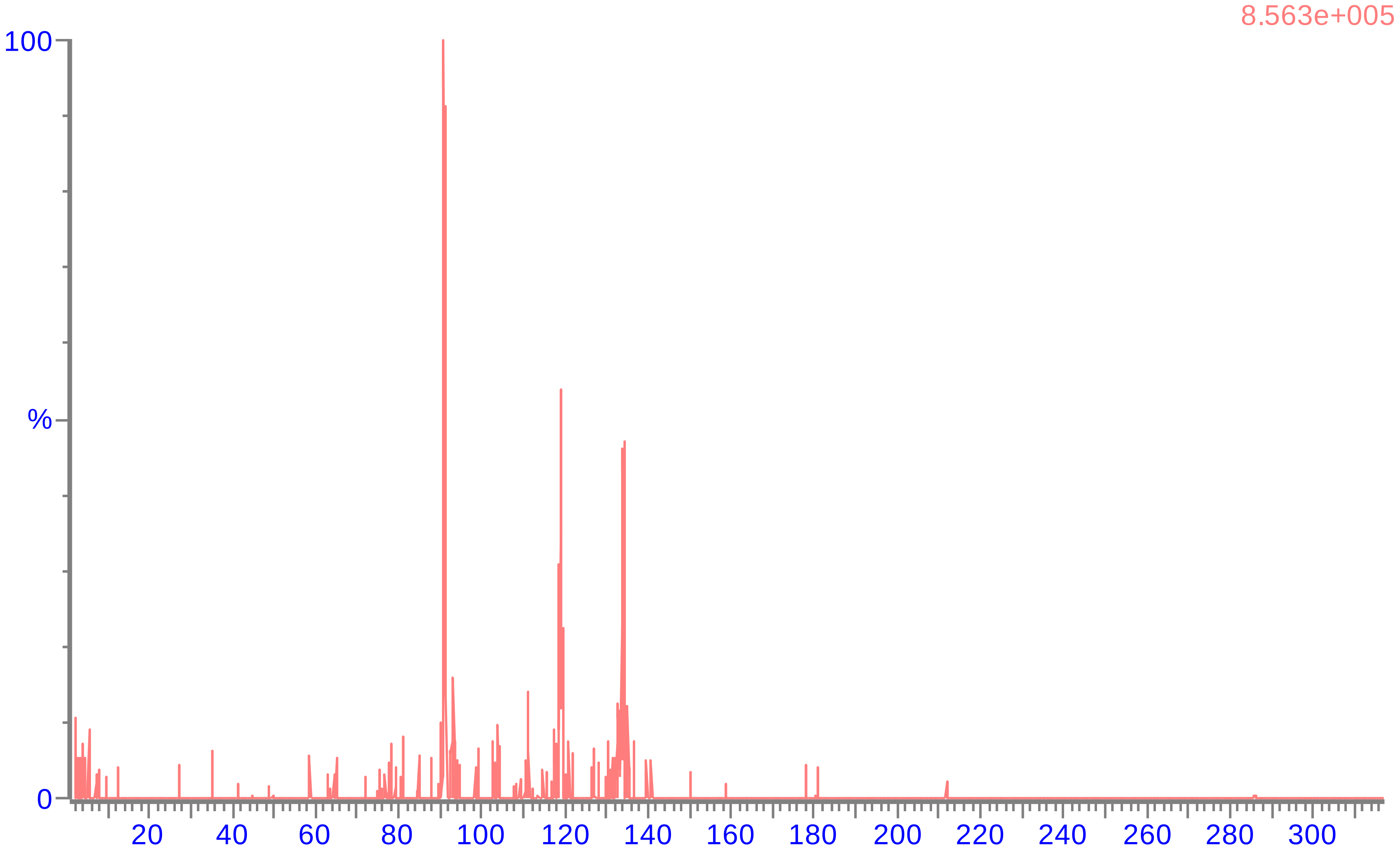

Figure 1.192: Mass spectrum for daughter fragment peak ES+, m/z 307.09 -> 91.06.

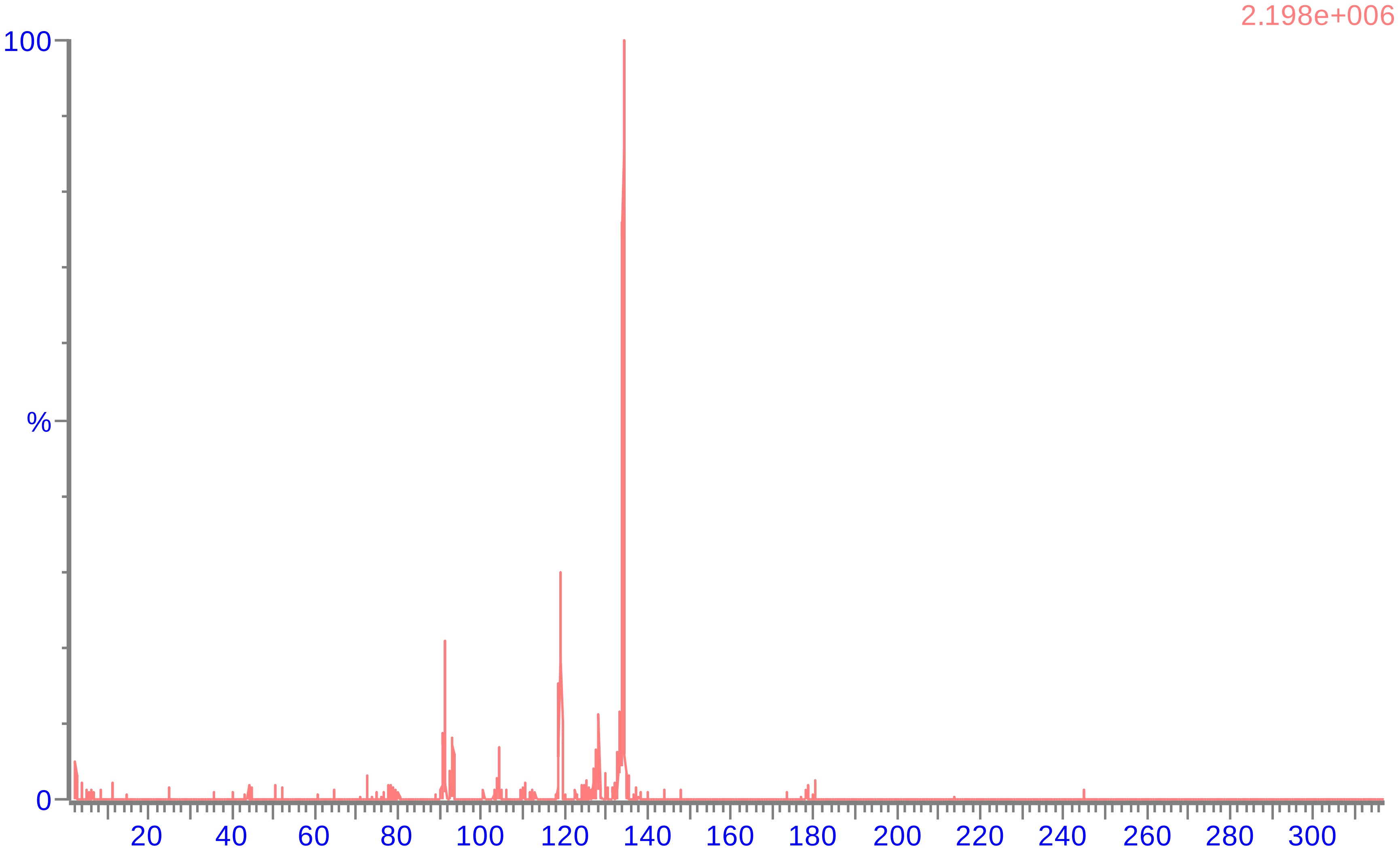

Figure 1.193: Mass spectrum for daughter fragment peak ES+, m/z 307.09 -> 119.04.

**4c** 3-(1-((4-methoxyphenyl)amino)-2-nitroethyl)phenol

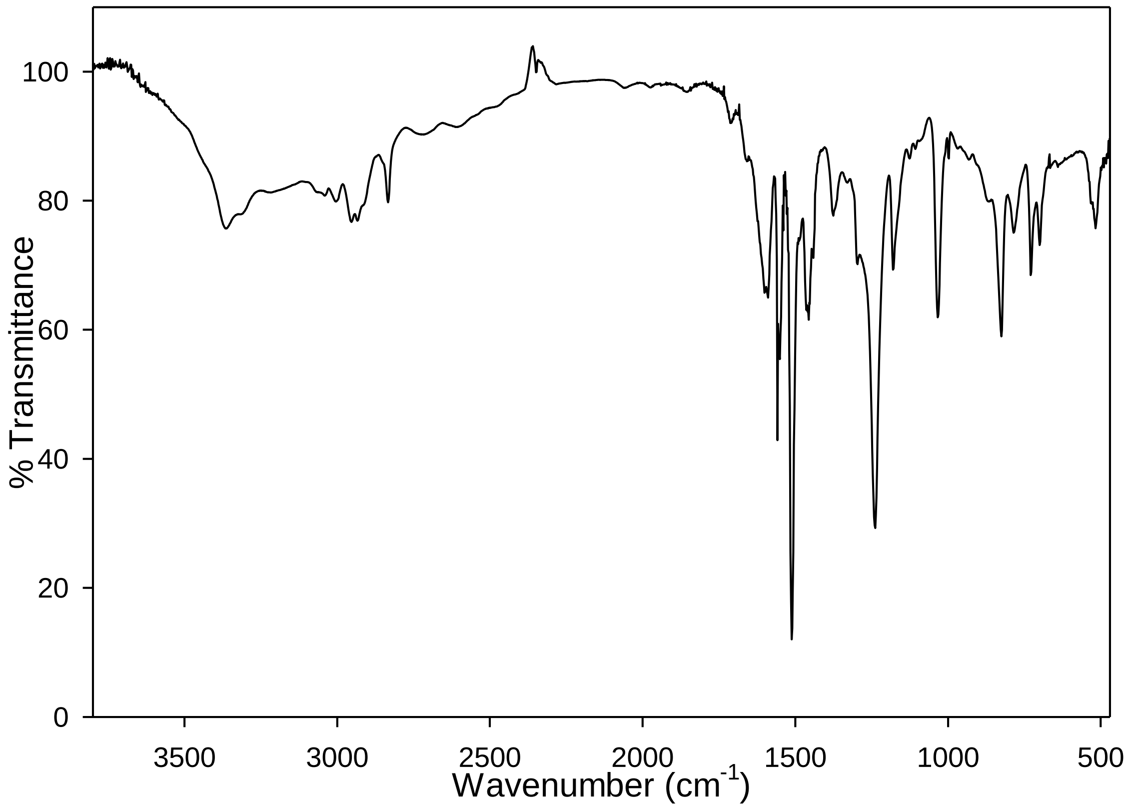

Figure 1.194: IR spectrum of **4c** 3-(1-((4-methoxyphenyl)amino)-2-nitroethyl)phenol.

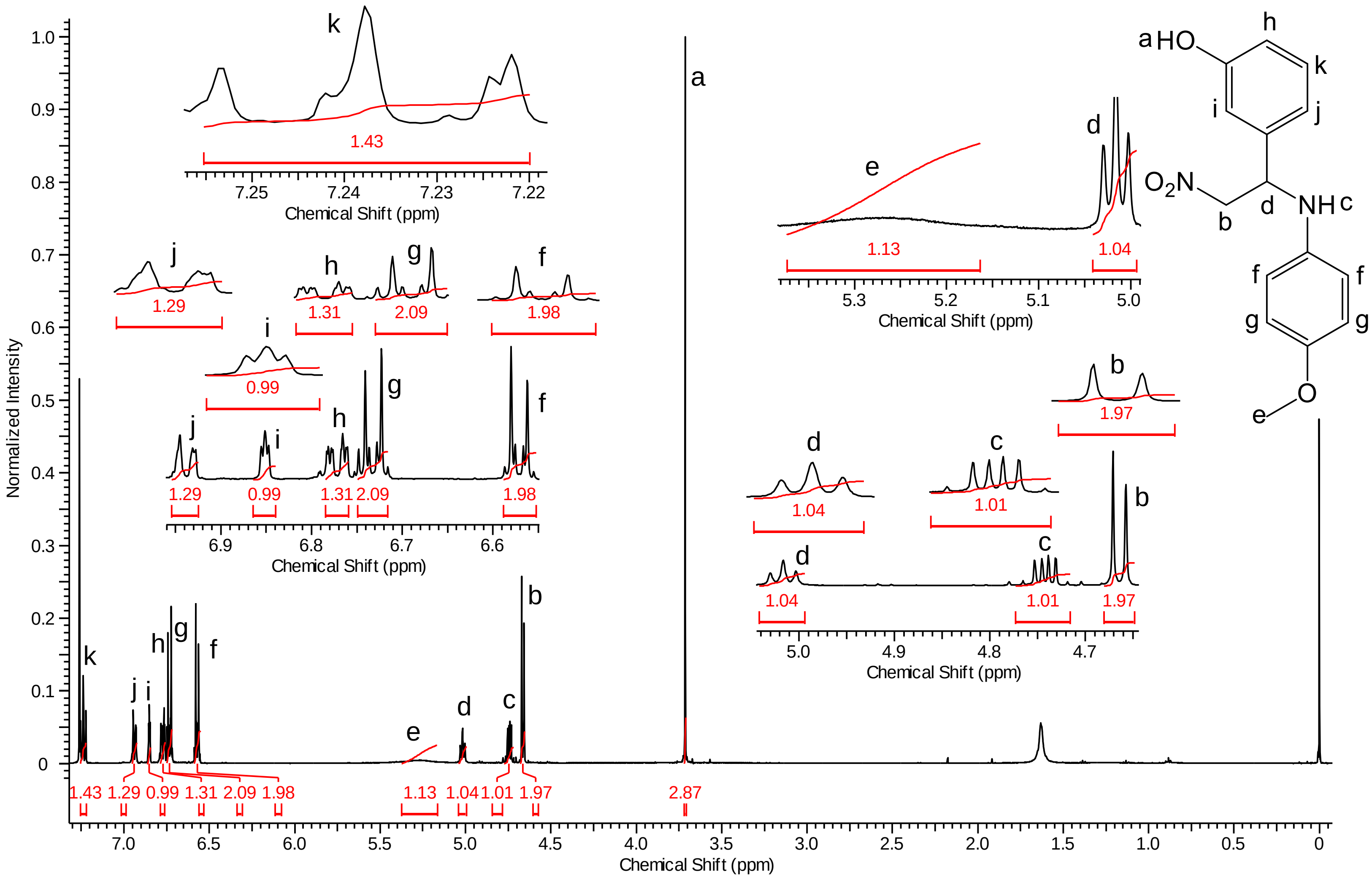

Figure 1.195: $^1$H NMR spectrum of **4c** 3-(1-((4-methoxyphenyl)amino)-2-nitroethyl)phenol.

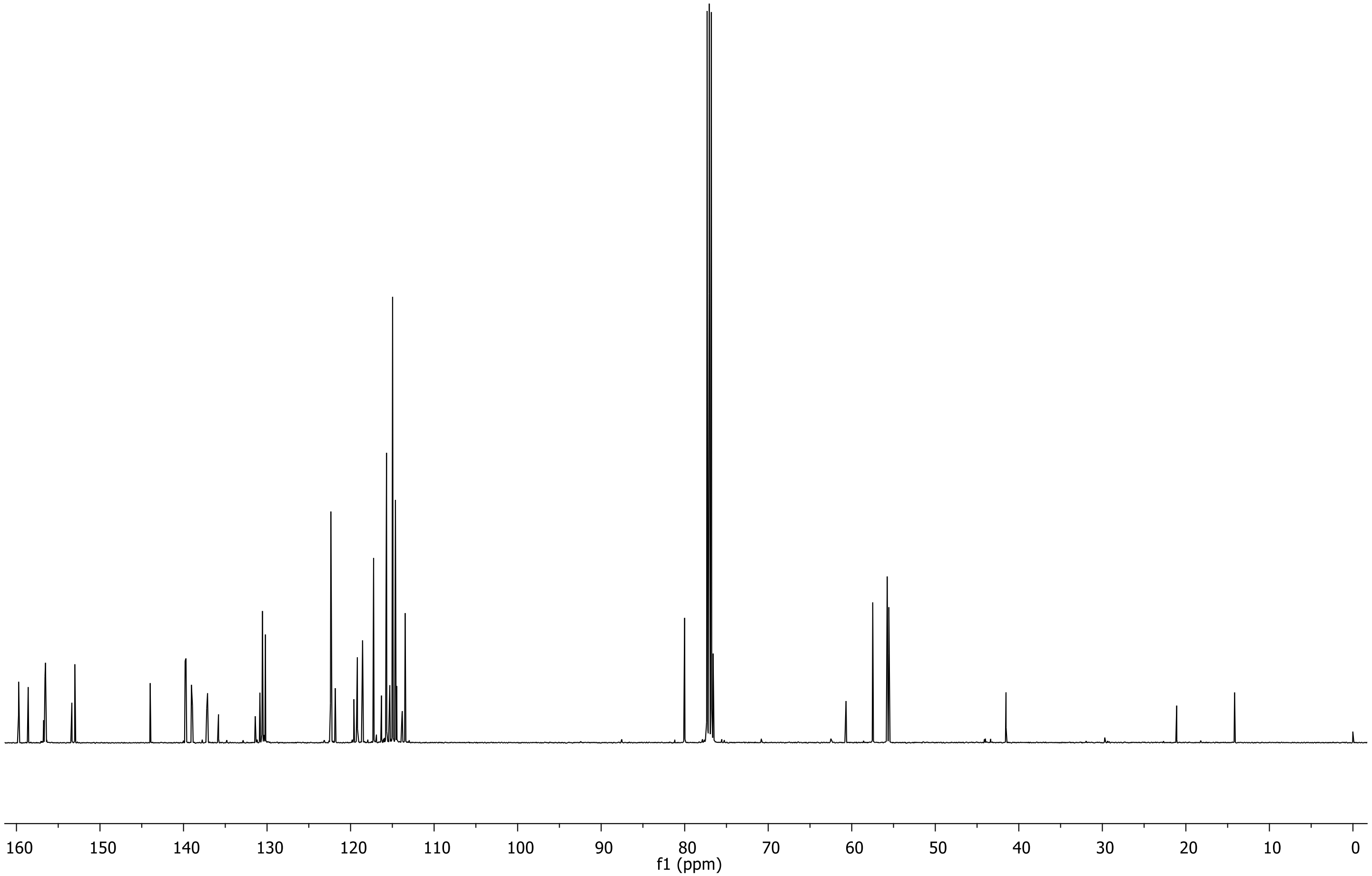

Figure 1.196: $^{13}$C NMR spectrum of **4c** 3-(1-((4-methoxyphenyl)amino)-2-nitroethyl)phenol.

Table 1.27: MS data

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **4c** | 288 | 1 | 289.07 | 14 | 166.06 | 8 | ES+ |
| | | 2 | 289.07 | 14 | 123.92 | 14 | ES+ |
| | | 3 | 289.07 | 38 | 200.15 | 14 | ES+ |

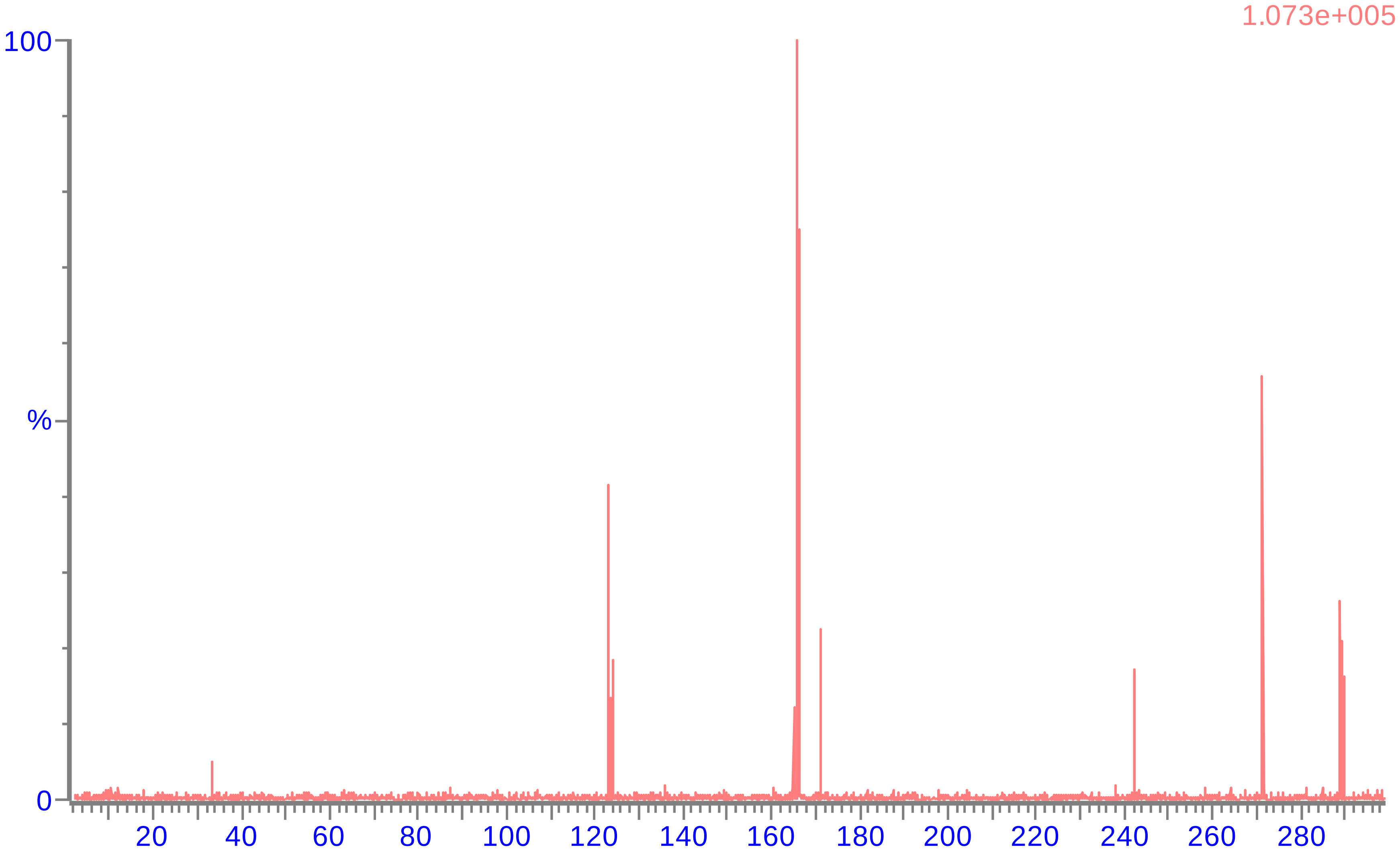

Figure 1.197: Mass spectrum for daughter fragment peak ES+, m/z 289.07 -> 166.06.

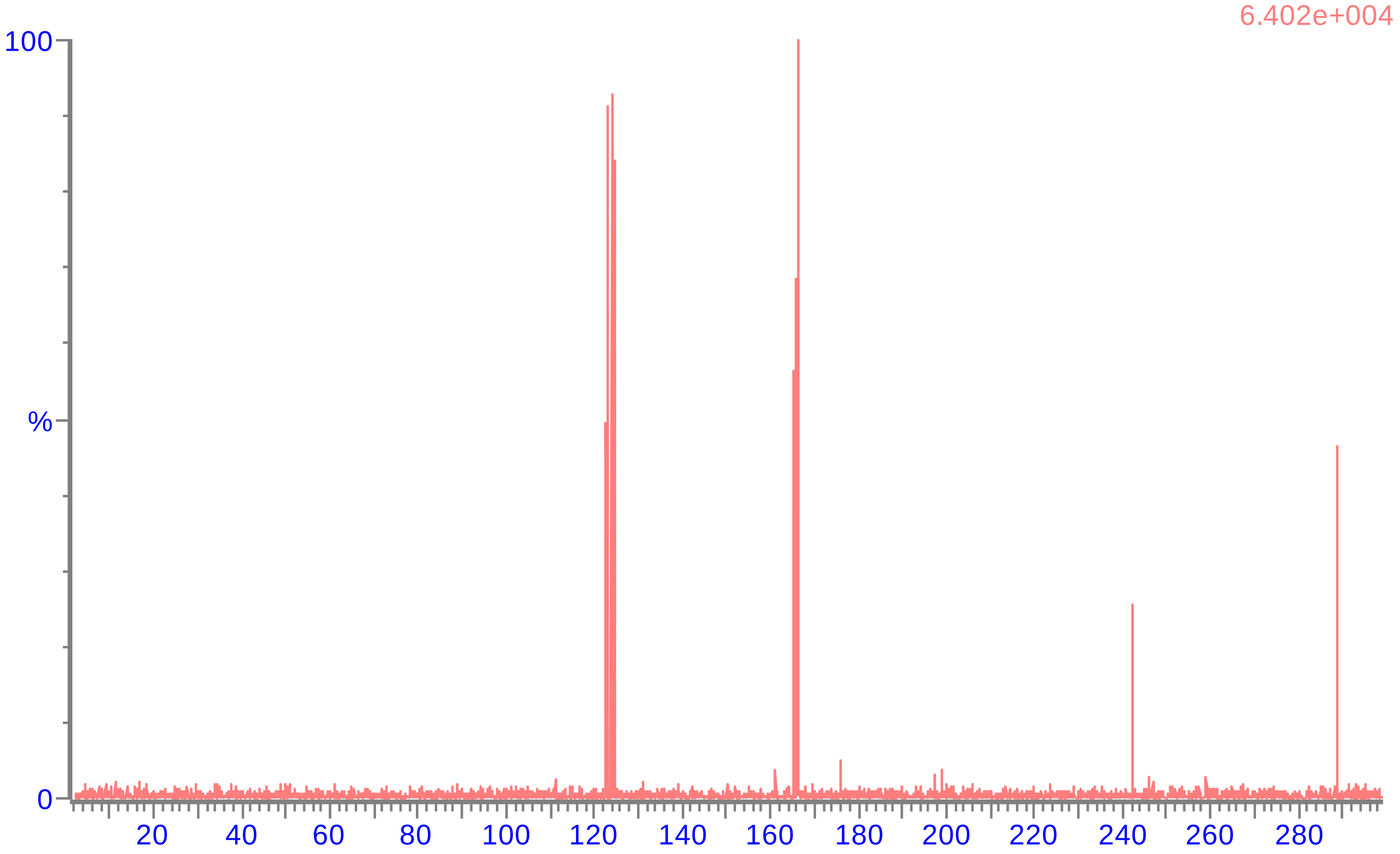

Figure 1.198: Mass spectrum for daughter fragment peak ES+, m/z 289.07 -> 123.92.

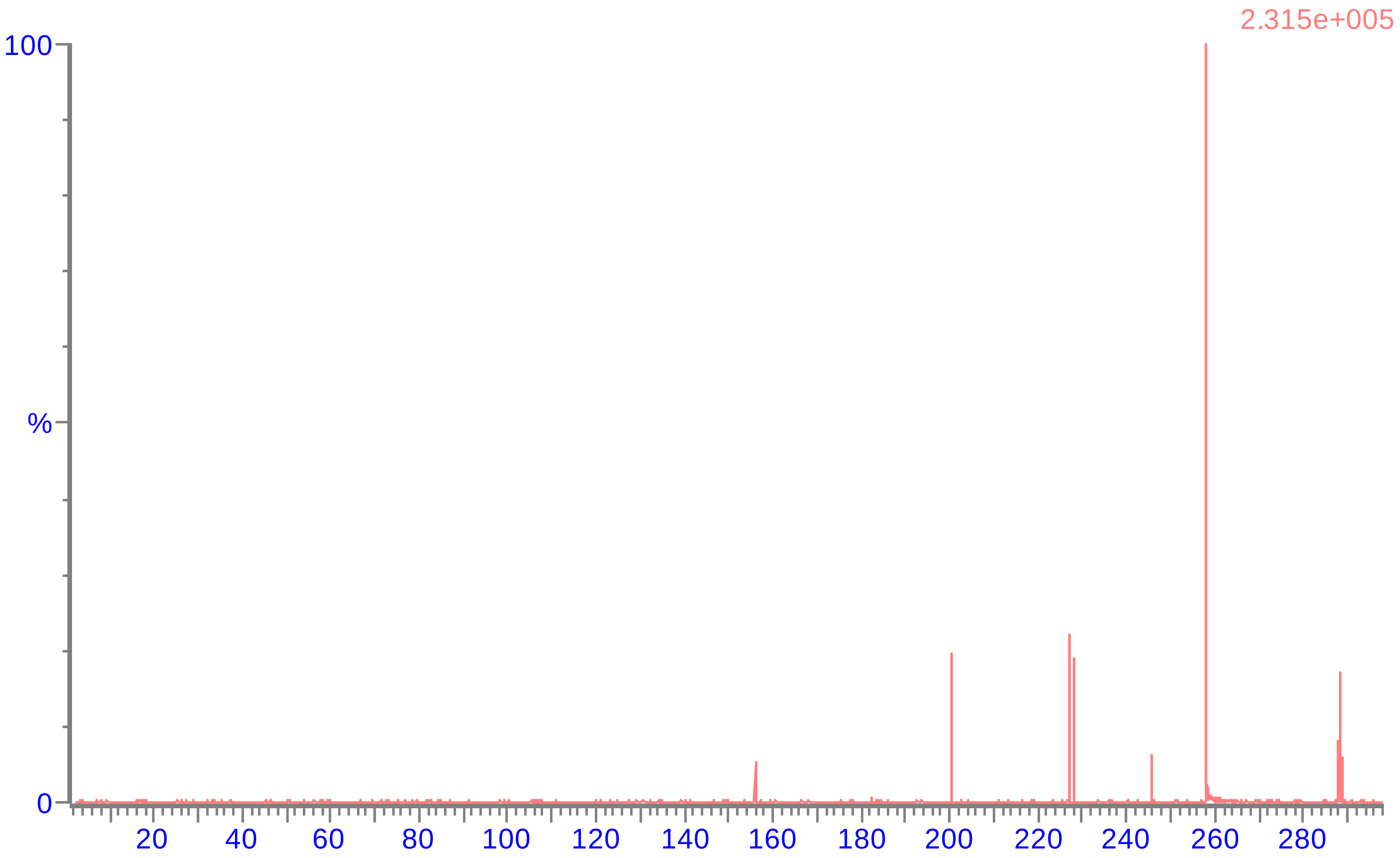

Figure 1.199: Mass spectrum for daughter fragment peak ES+, m/z 289.07 -> 200.15.

**4d** 4-bromo-*N*-(1-cyclohexyl-2-nitroethyl)aniline

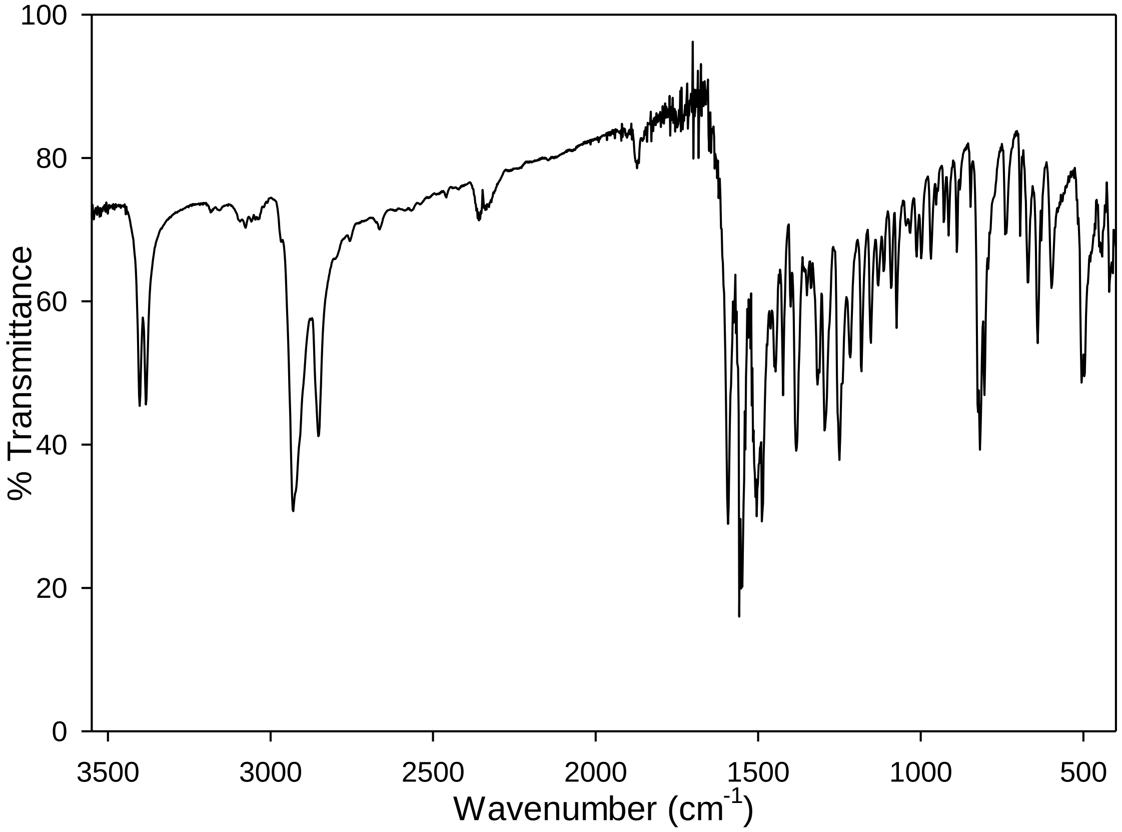

Figure 1.200: IR spectrum of **4d** 4-bromo-*N*-(1-cyclohexyl-2-nitroethyl)aniline.

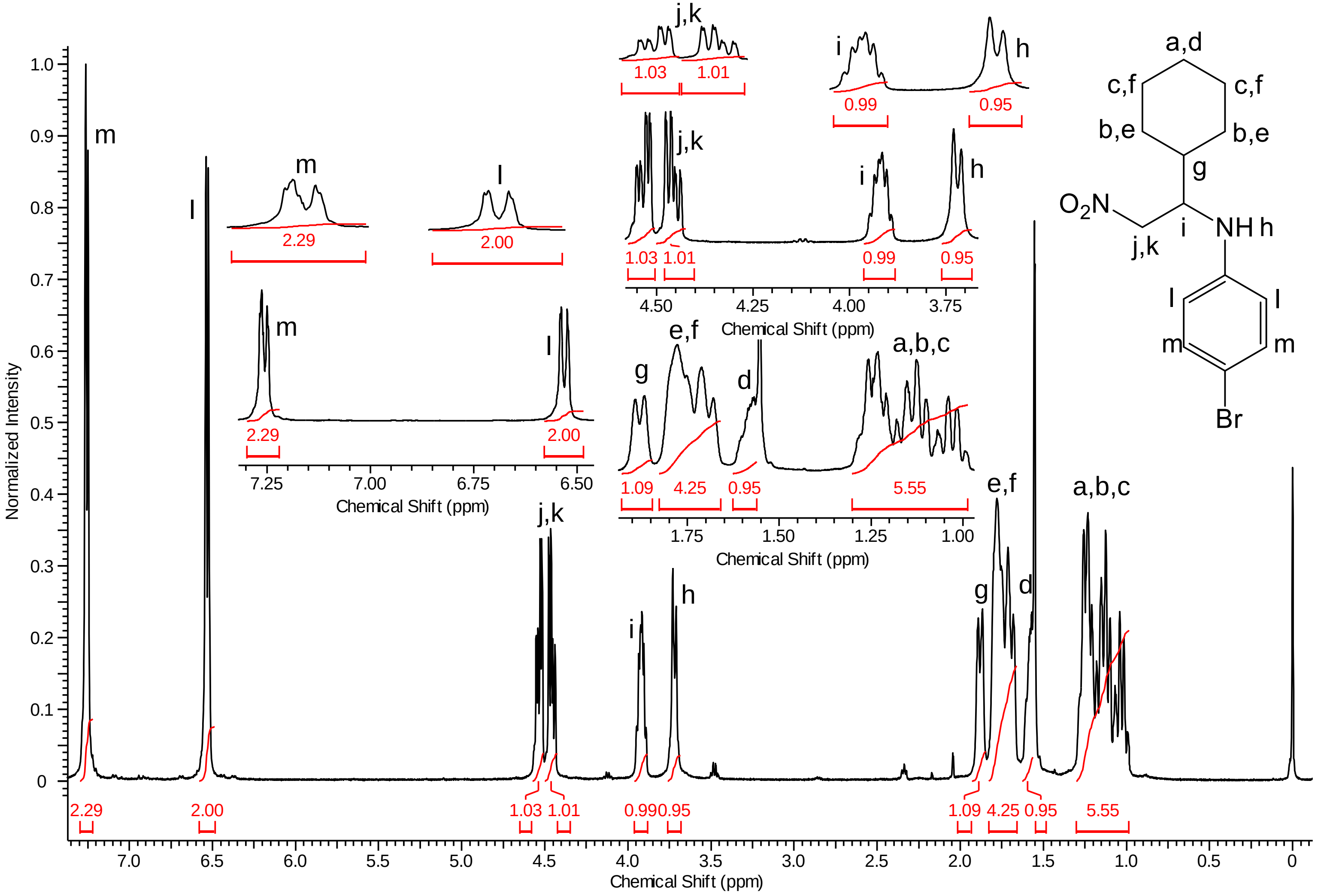

Figure 1.201: $^1$H NMR spectrum of **4d** 4-bromo-*N*-(1-cyclohexyl-2-nitroethyl)aniline.

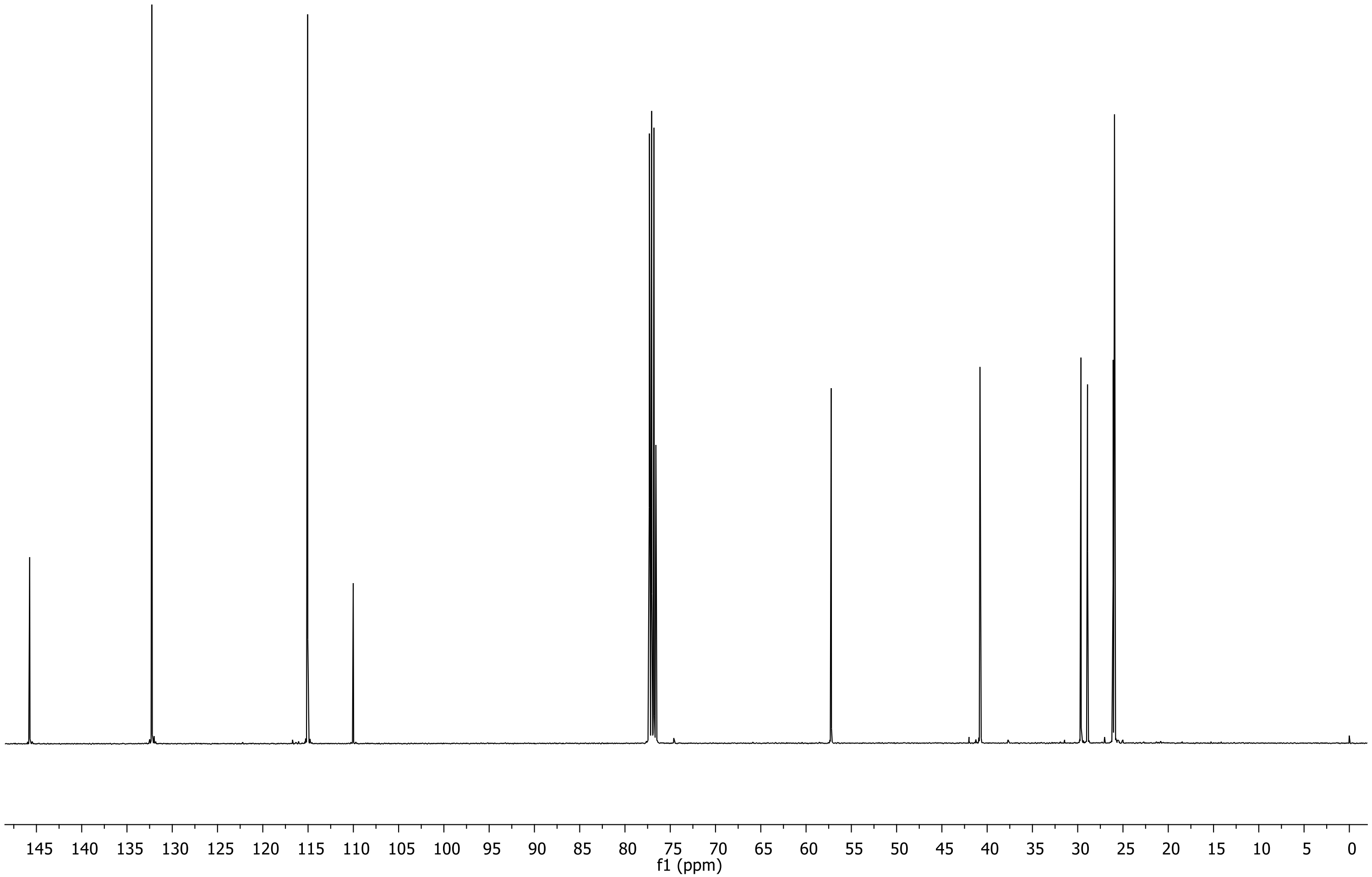

Figure 1.202: $^{13}$C NMR spectrum of **4d** 4-bromo-*N*-(1-cyclohexyl-2-nitroethyl)aniline.

Table 1.28: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **4d** | 326 | 1 | 325.03 | 18 | 154.07 | 6 | ES- |
| | | 2 | 325.03 | 18 | 169.93 | 12 | ES- |
| | | 3 | 325.03 | 18 | 78.89 | 28 | ES- |
| | | 4 | 325.03 | 18 | 136.05 | 18 | ES- |
| | | 5 | 325.03 | 18 | 60.02 | 12 | ES- |

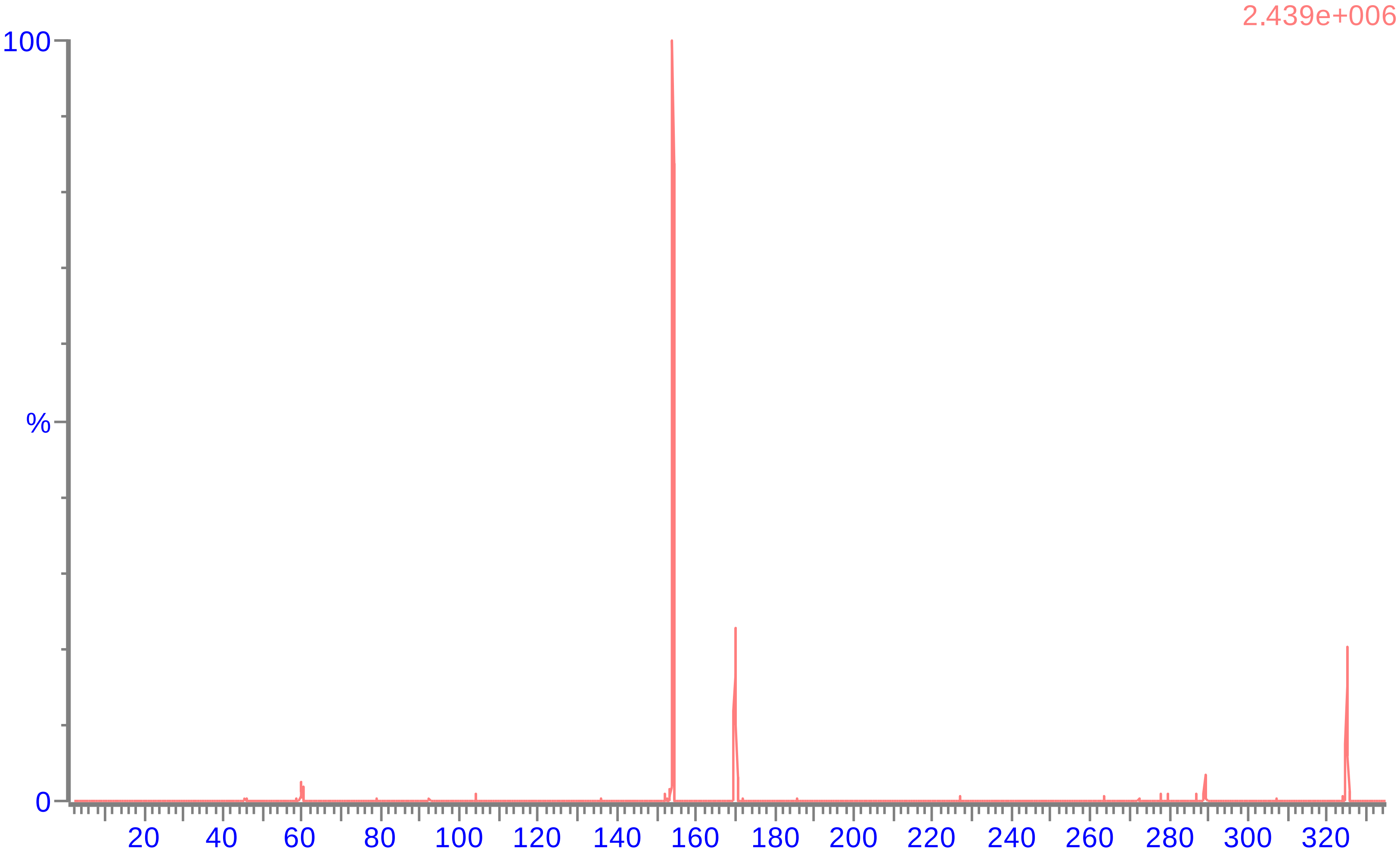

Figure 1.203: Mass spectrum for daughter fragment peak ES+, m/z 325.03 -> 154.07.

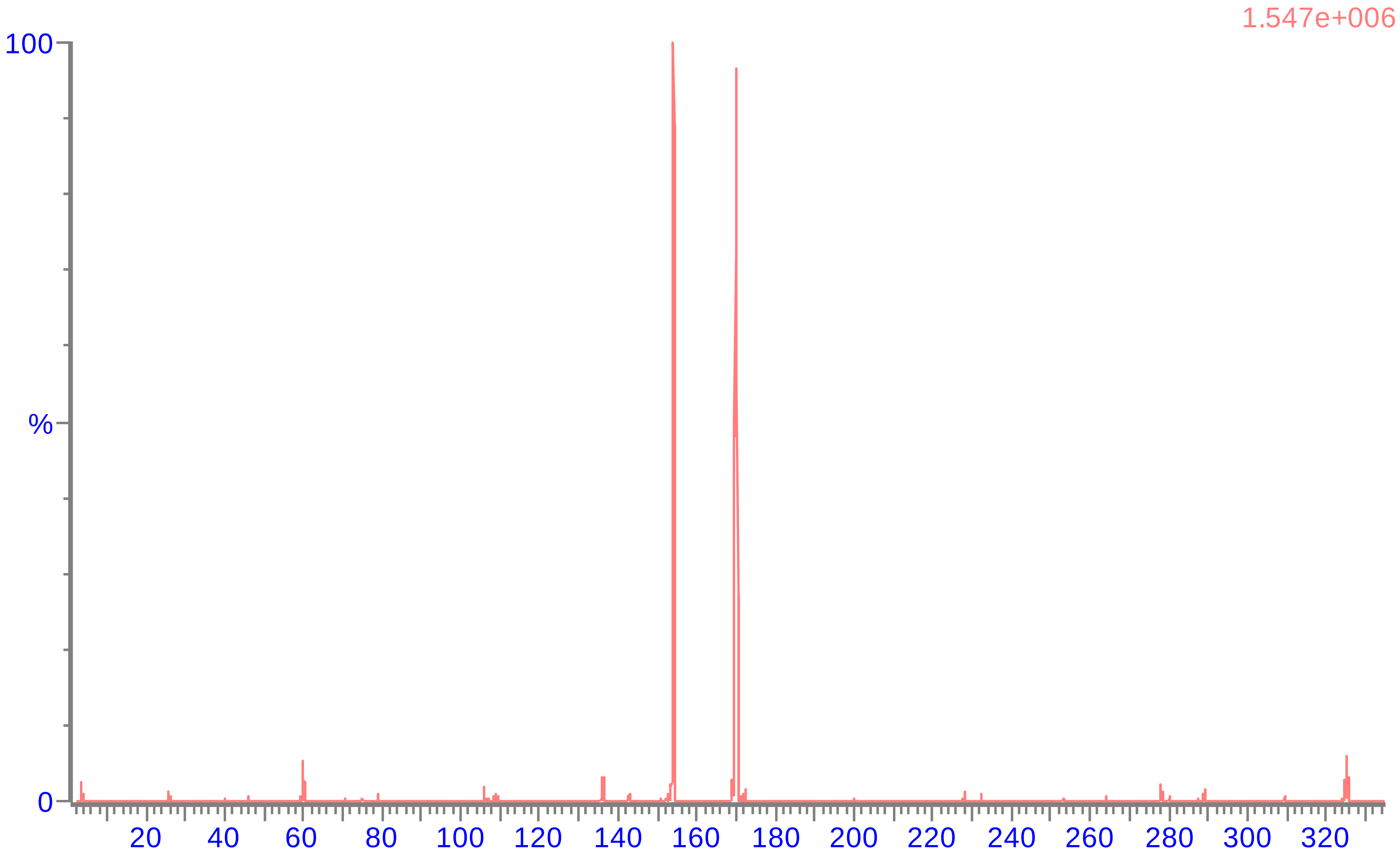

Figure 1.204: Mass spectrum for daughter fragment peak ES+, m/z 325.03 -> 169.93.

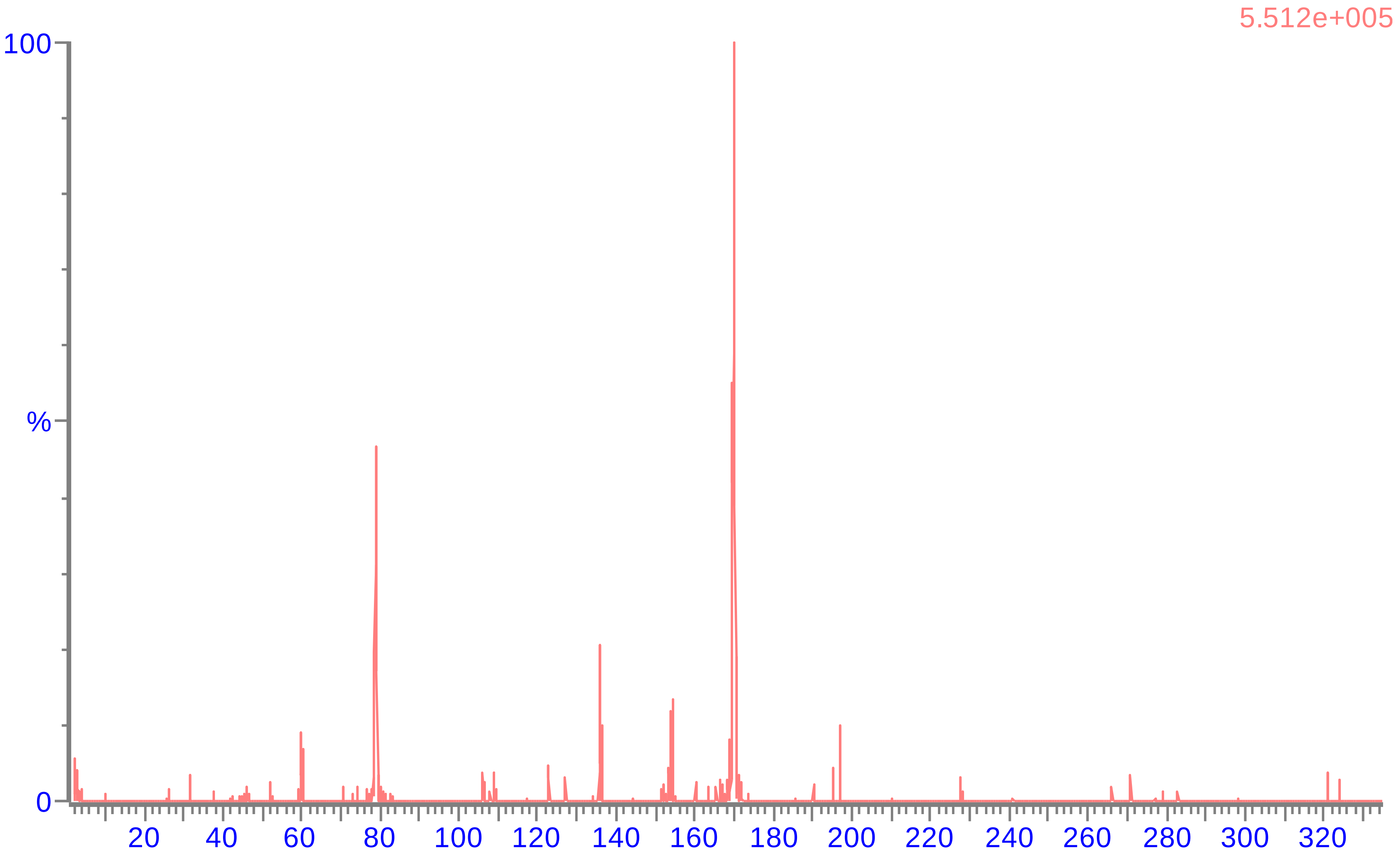

Figure 1.205: Mass spectrum for daughter fragment peak ES+, m/z 325.03 -> 78.89.

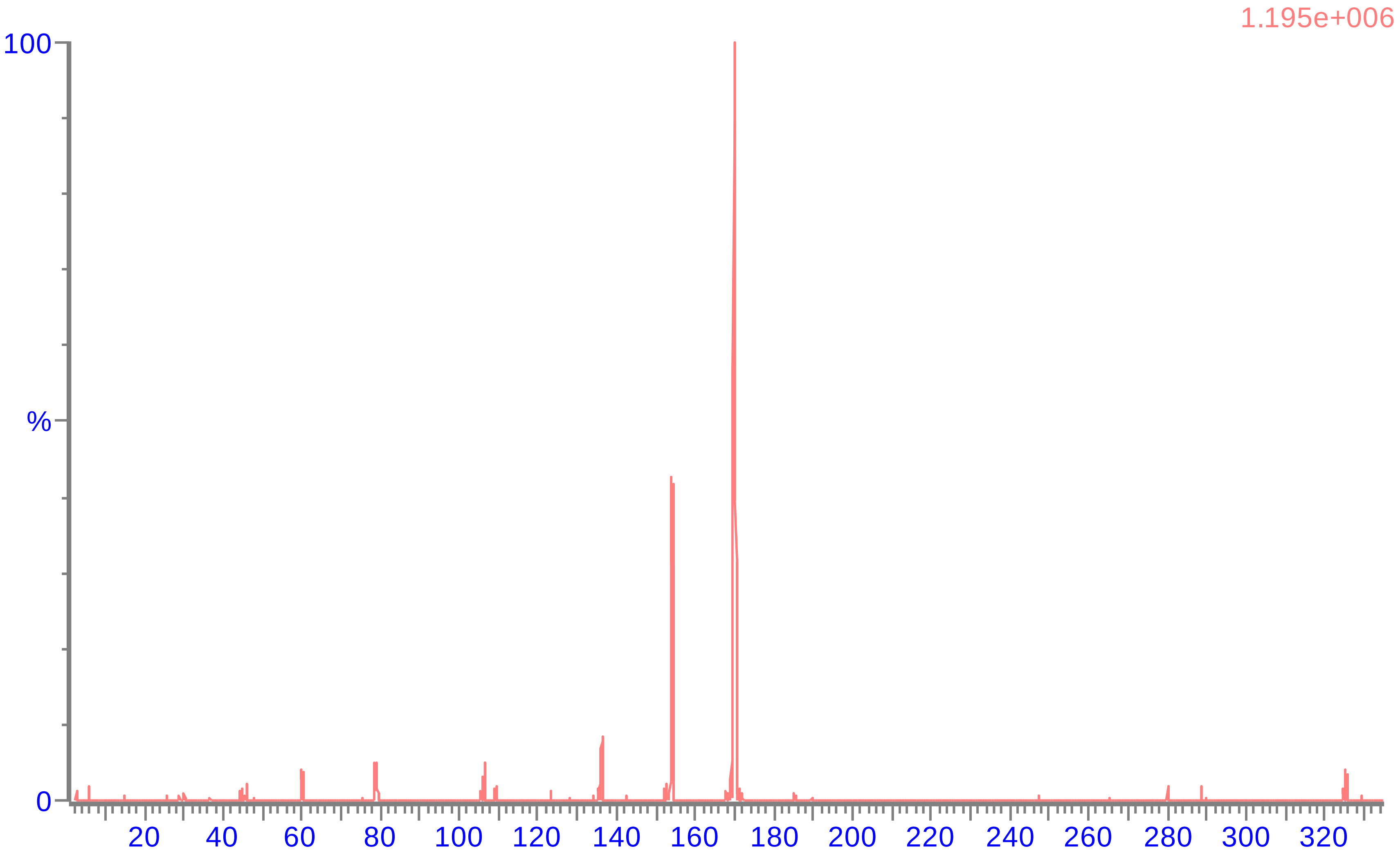

Figure 1.206: Mass spectrum for daughter fragment peak ES+, m/z 325.03 -> 136.05.

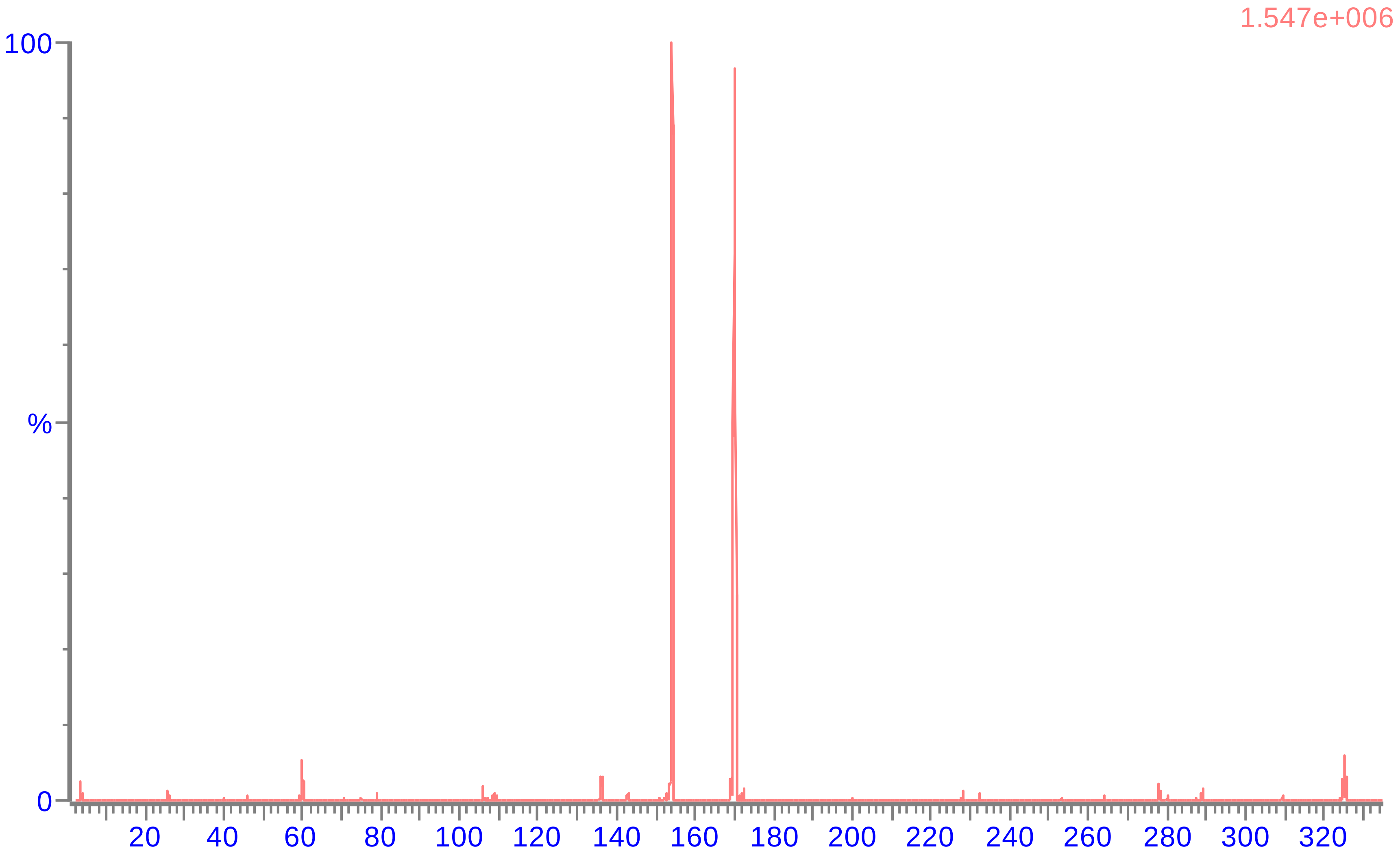

Figure 1.207: Mass spectrum for daughter fragment peak ES+, m/z 325.03 -> 60.02.

**4e** 4-methyl-*N*-(2-nitro-1-(2-nitrophenyl)ethyl)aniline

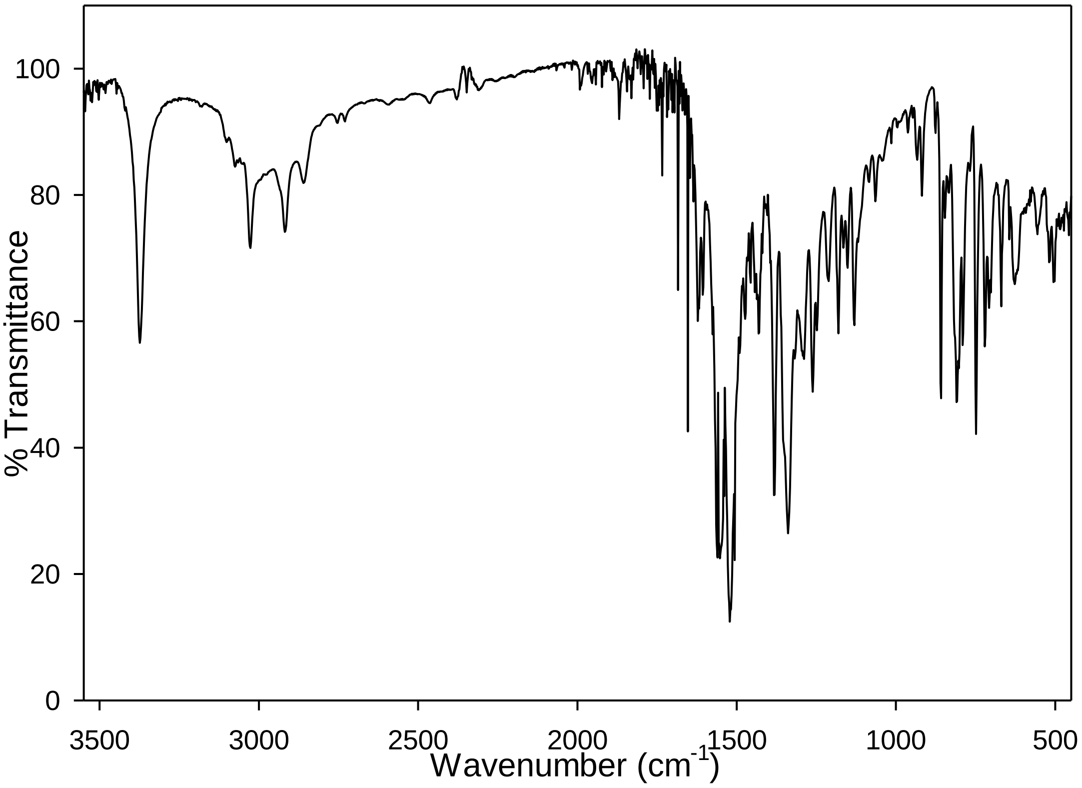

Figure 1.208: IR spectrum of **4e** 4-methyl-*N*-(2-nitro-1-(2-nitrophenyl)ethyl)aniline.

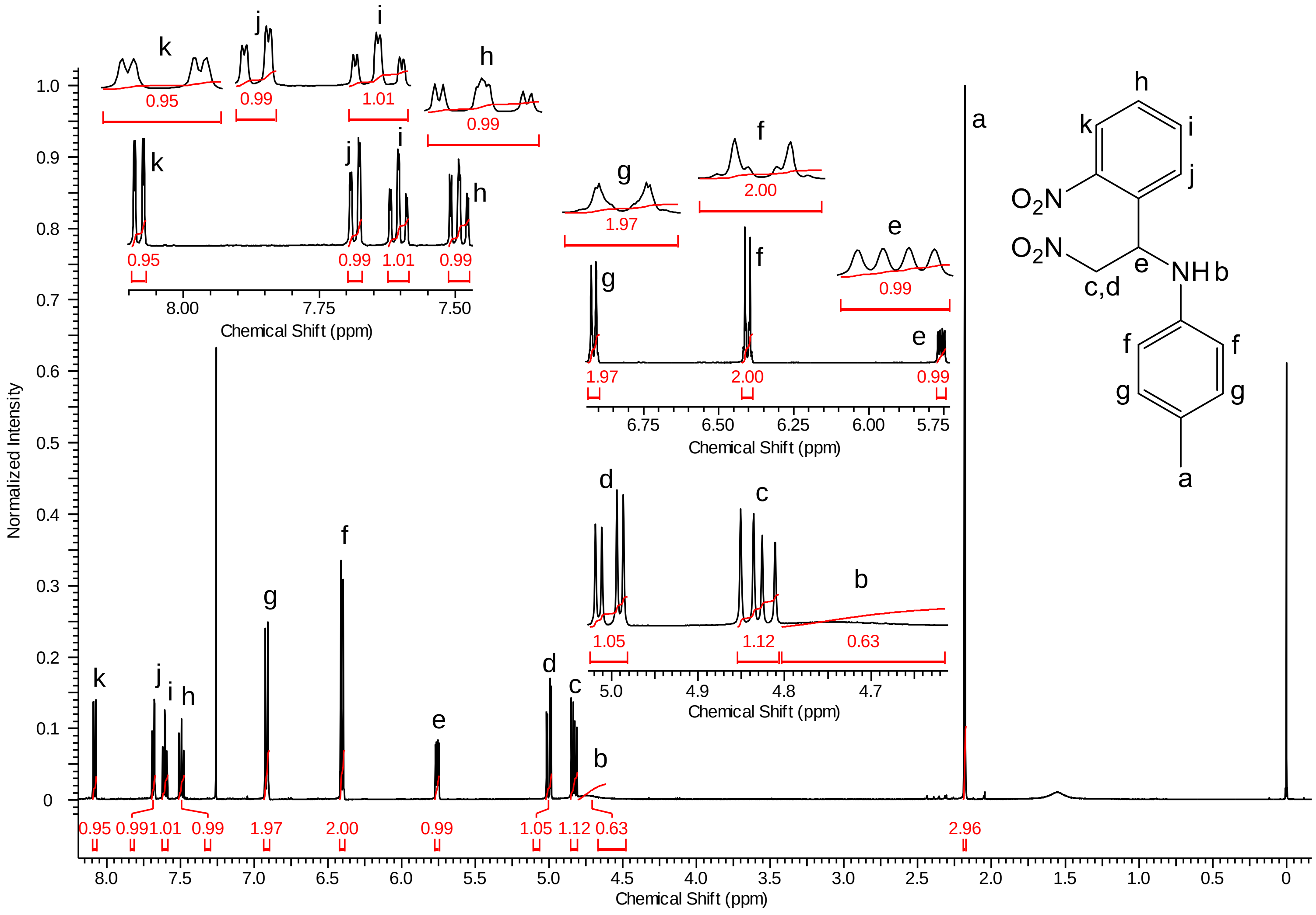

Figure 1.209: ${}^{1}$H NMR spectrum of **4e** 4-methyl-*N*-(2-nitro-1-(2-nitrophenyl)ethyl)aniline.

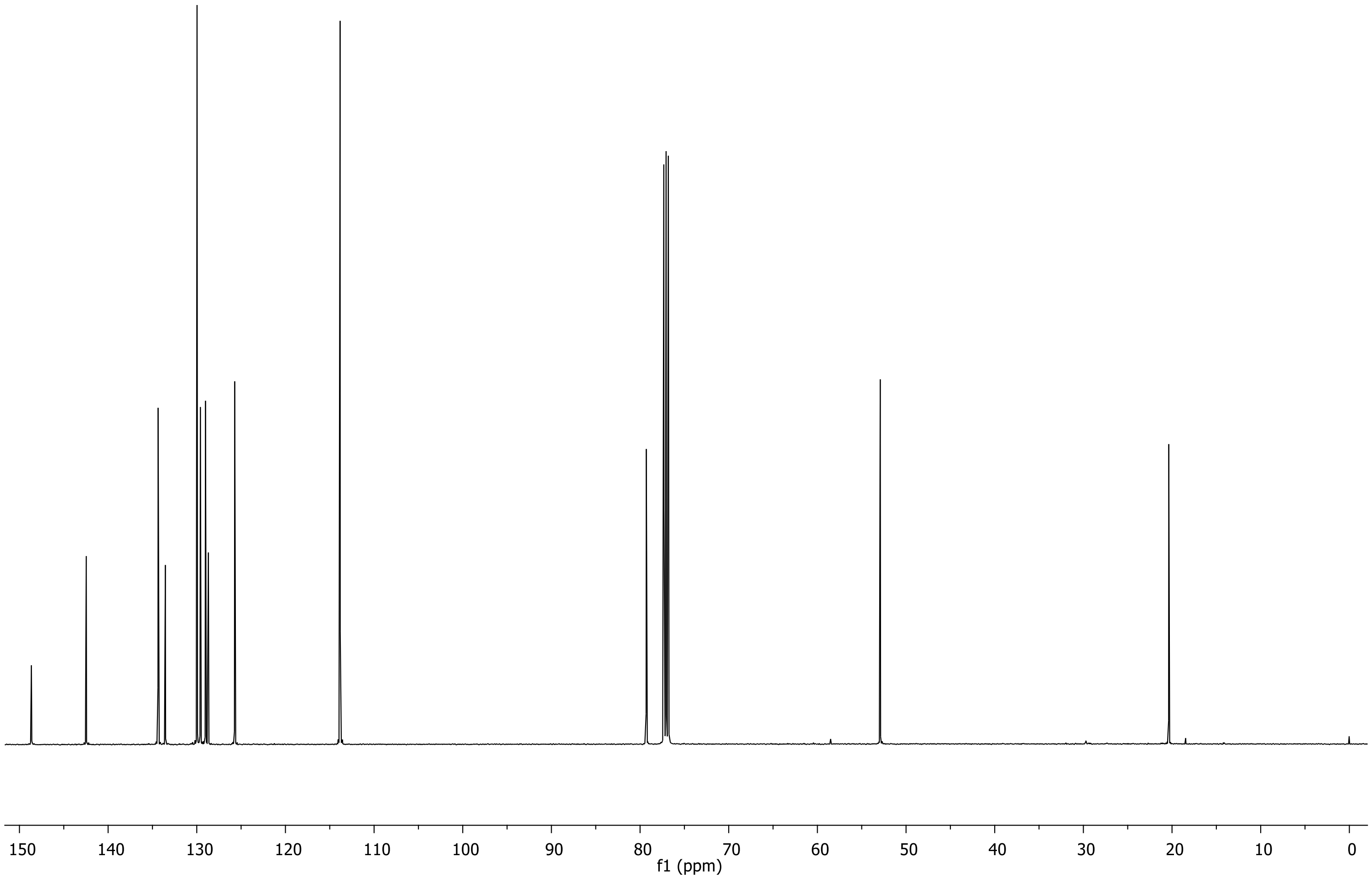

Figure 1.210: $^{13}$C NMR spectrum of **4e** 4-methyl-*N*-(2-nitro-1-(2-nitrophenyl)ethyl)aniline.

Table 1.29: MS data.

| **Compound** | **Formula/Mass** | | **Parent m/z** | **Cone Voltage** | **Daughters** | **Collision Energy** | **Ion Mode** |
|---|---|---|---|---|---|---|---|
| **4e** | 301 | 1 | 302.10 | 24 | 107.05 | 16 | ES+ |
| | | 2 | 302.10 | 24 | 241.15 | 14 | ES+ |
| | | 3 | 302.10 | 24 | 119.73 | 14 | ES+ |
| | | 4 | 302.10 | 24 | 120.05 | 12 | ES+ |

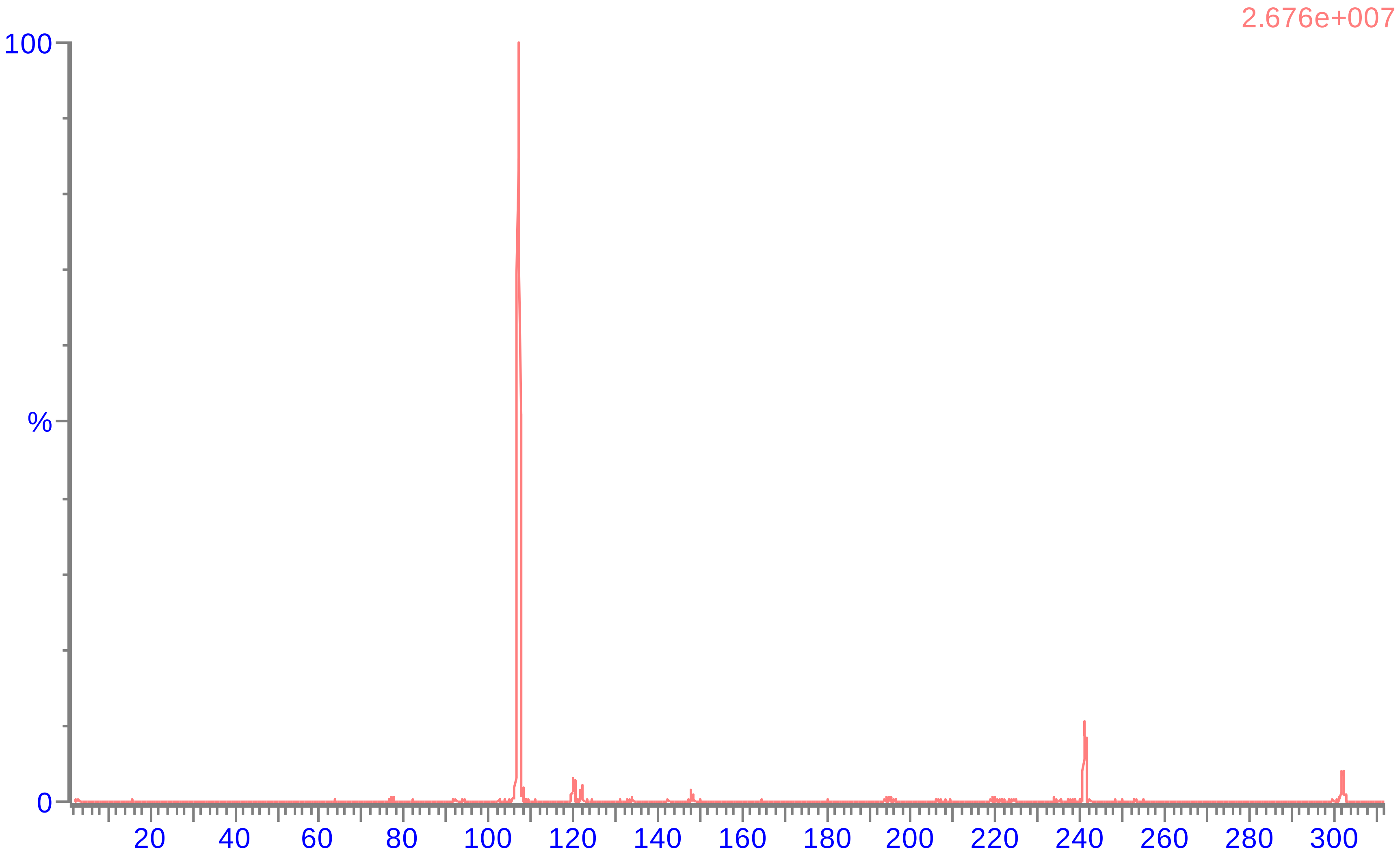

Figure 1.211: Mass spectrum for daughter fragment peak ES+, m/z 302.10 -> 107.05.

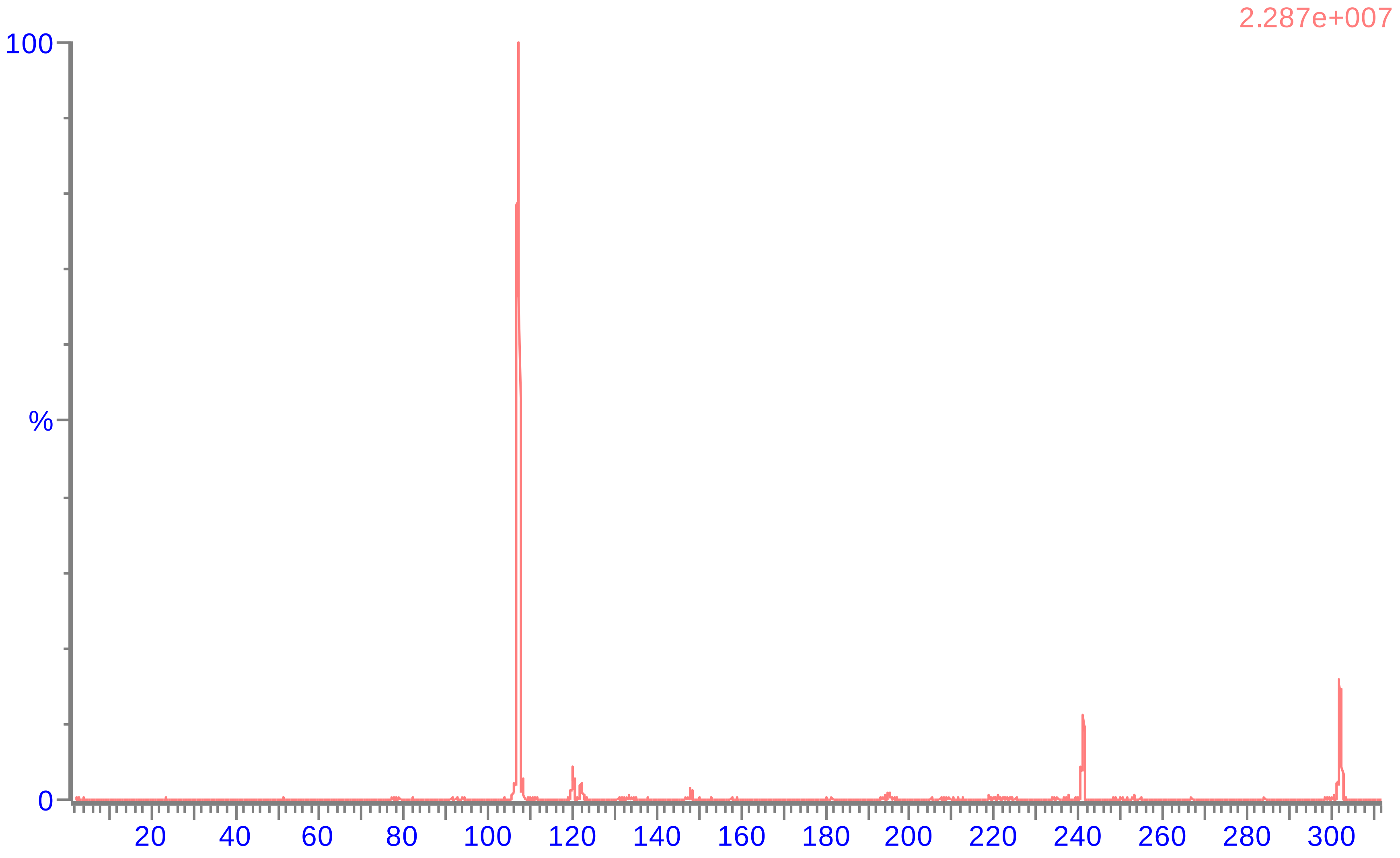

Figure 1.212: Mass spectrum for daughter fragment peak ES+, m/z 302.10 -> 241.15.

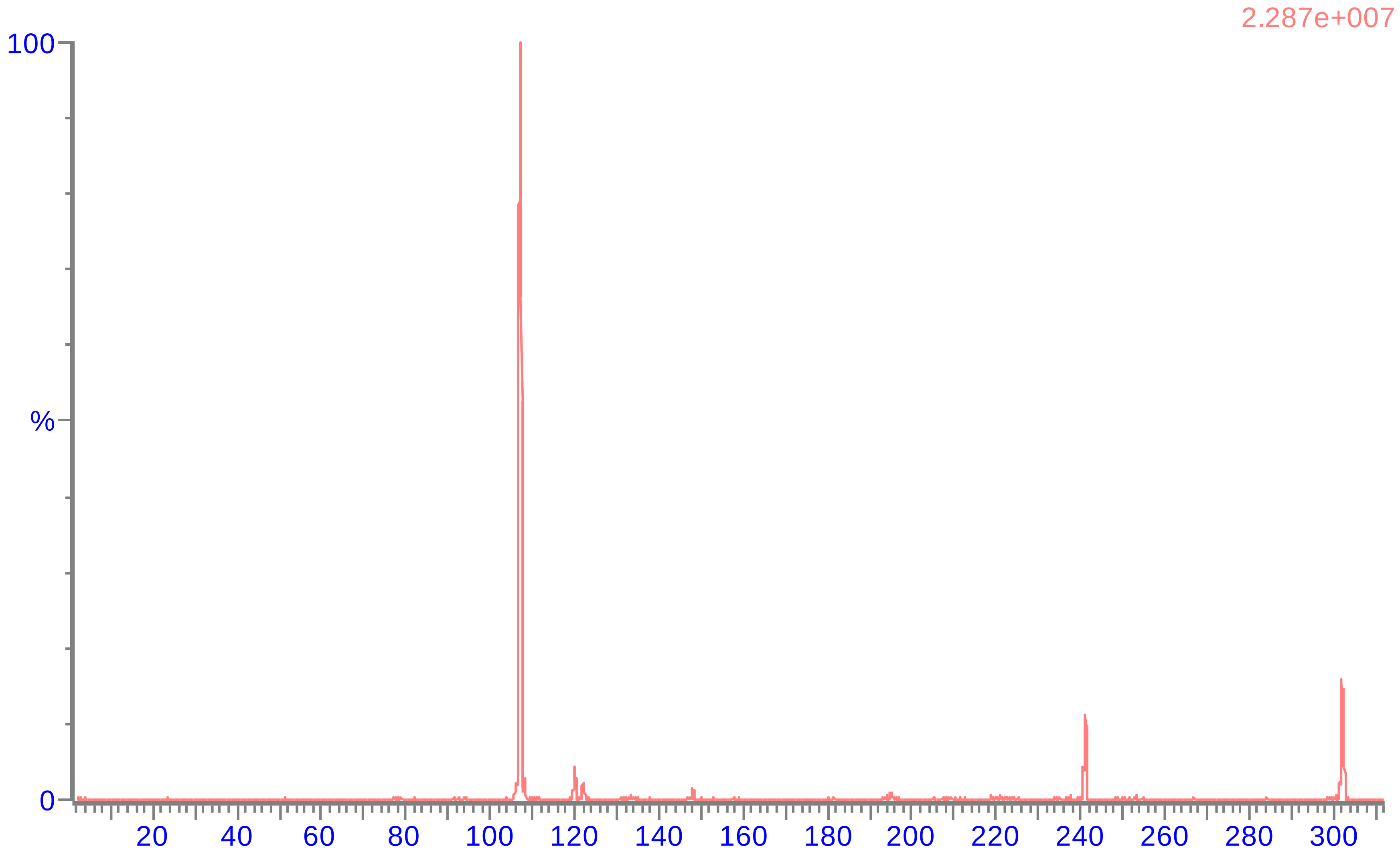

Figure 1.213: Mass spectrum for daughter fragment peak ES+, m/z 302.10 -> 119.73.

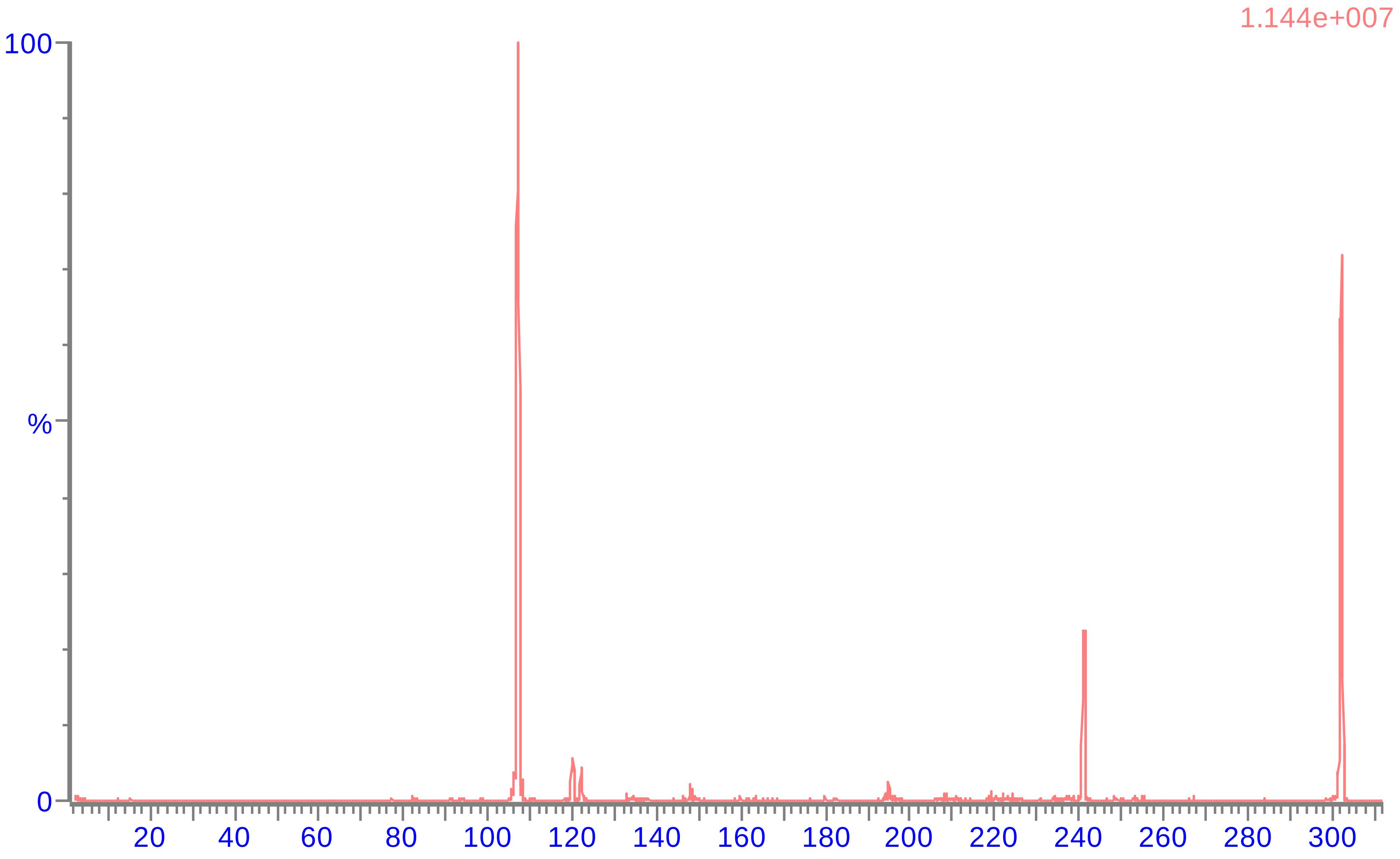

Figure 1.214: Mass spectrum for daughter fragment peak ES+, m/z 302.10 -> 120.05.

**4g** *N*-(1-(4-bromophenyl)-2-nitroethyl)-4-ethylaniline

Table 1.30: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **4g** | 350 | 1 | 351.03 | 92 | 90.98 | 36 | ES+ |
| | | 2 | 351.03 | 92 | 64.97 | 66 | ES+ |
| | | 3 | 351.03 | 92 | 335.77 | 36 | ES+ |
| | | 4 | 351.03 | 92 | 180.26 | 46 | ES+ |

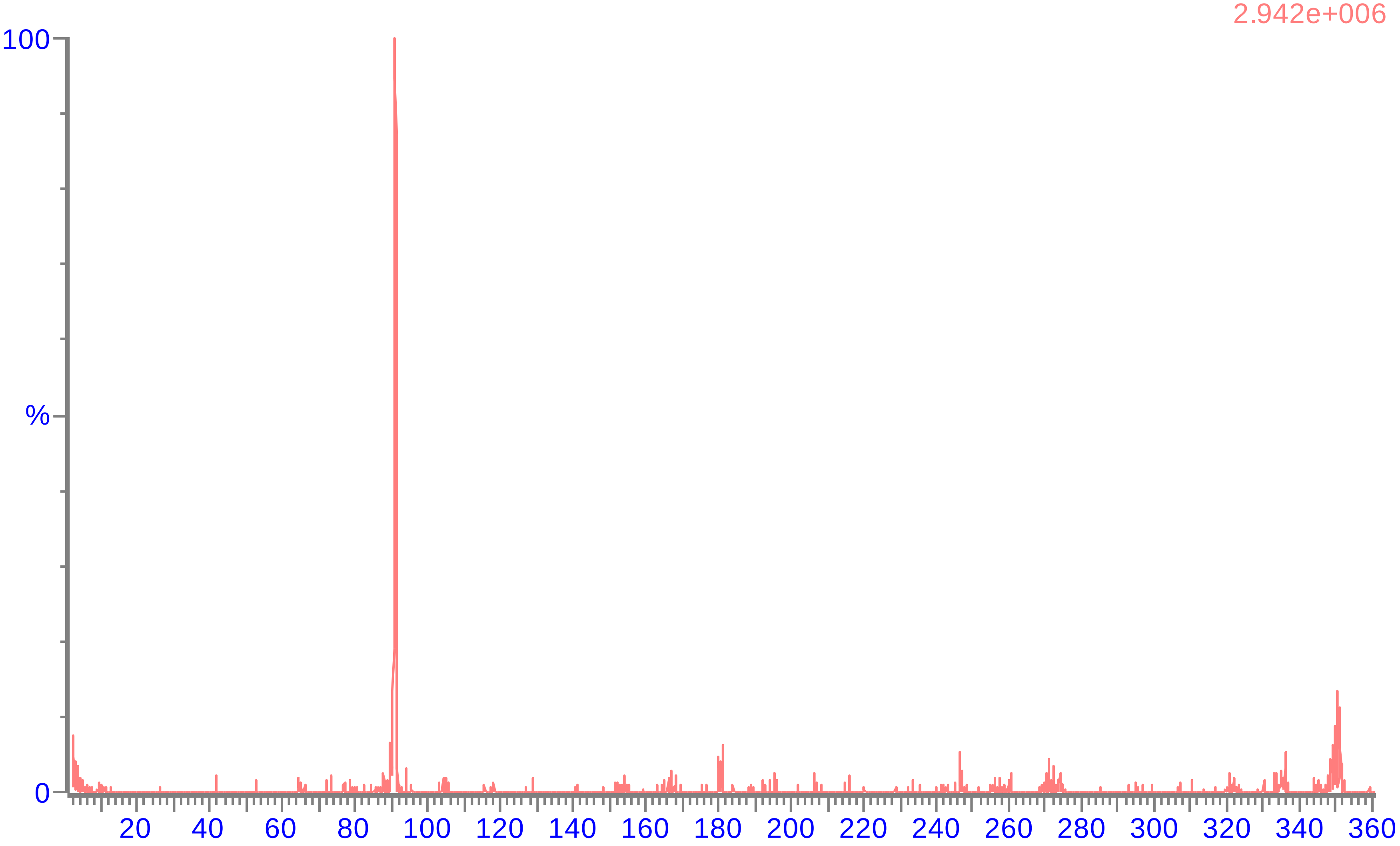

Figure 1.215: Mass spectrum for daughter fragment peak ES+, m/z 351.03 -> 90.98.

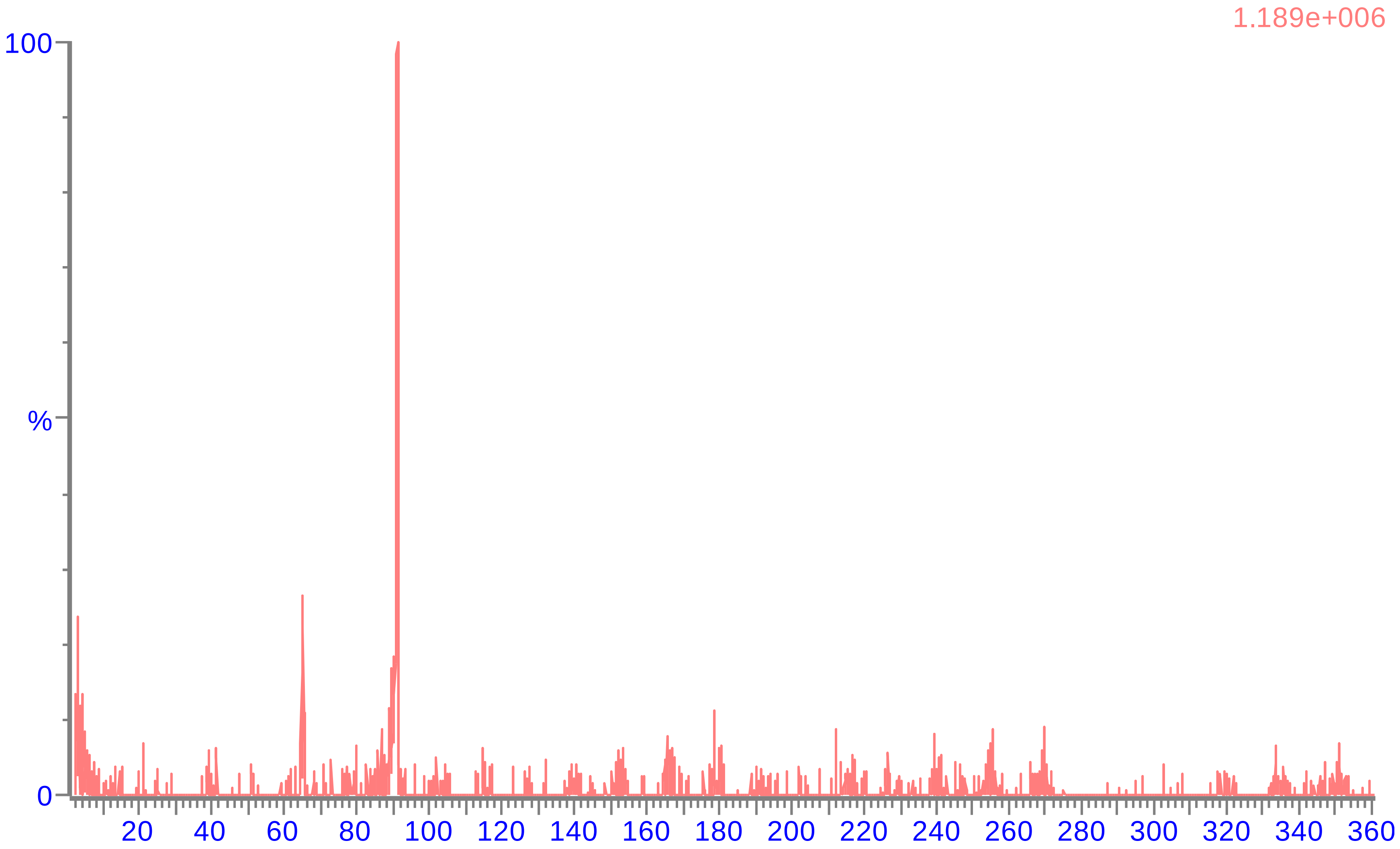

Figure 1.216: Mass spectrum for daughter fragment peak ES+, m/z 351.03 -> 64.97.

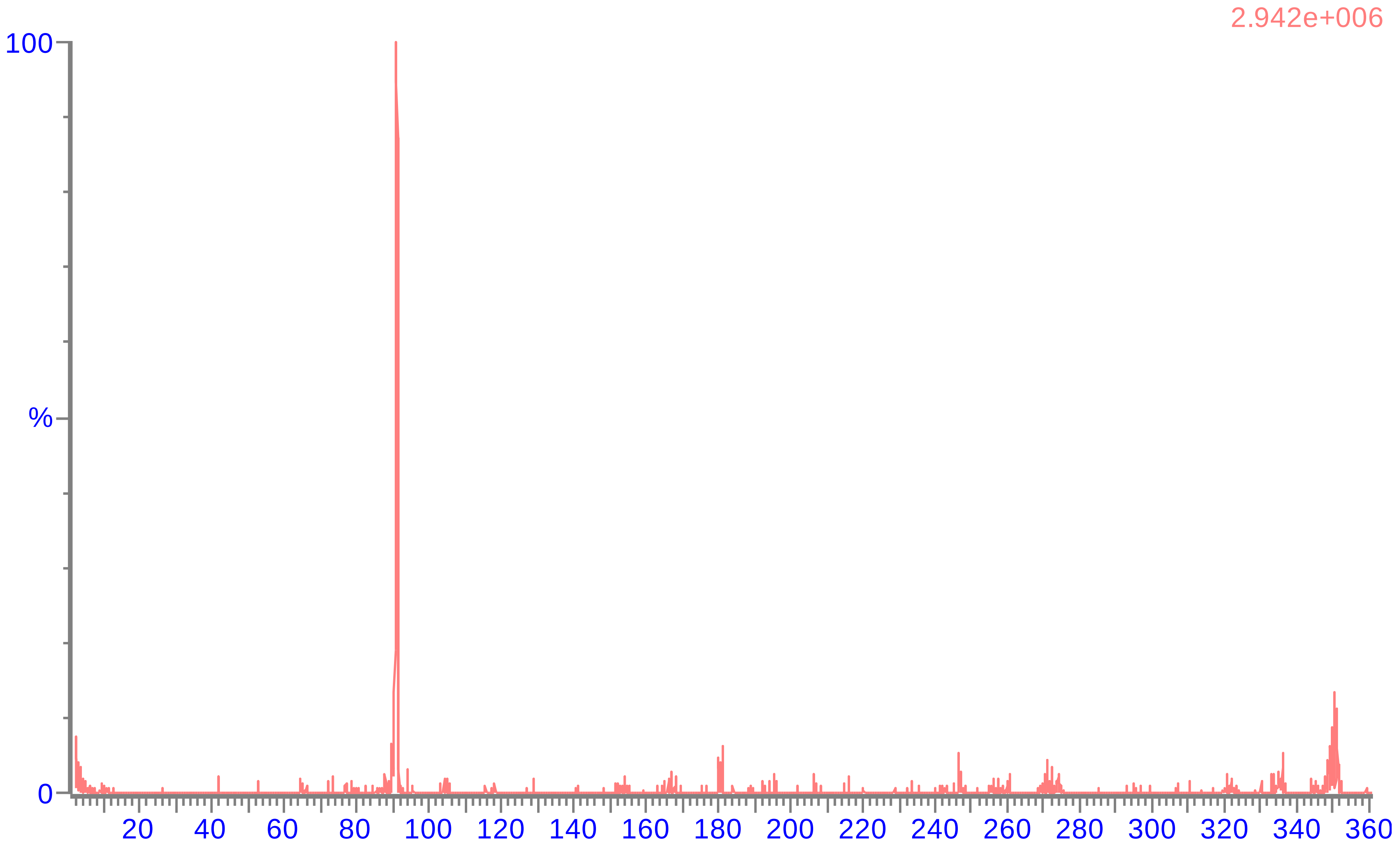

Figure 1.217: Mass spectrum for daughter fragment peak ES+, m/z 351.03 -> 335.77.

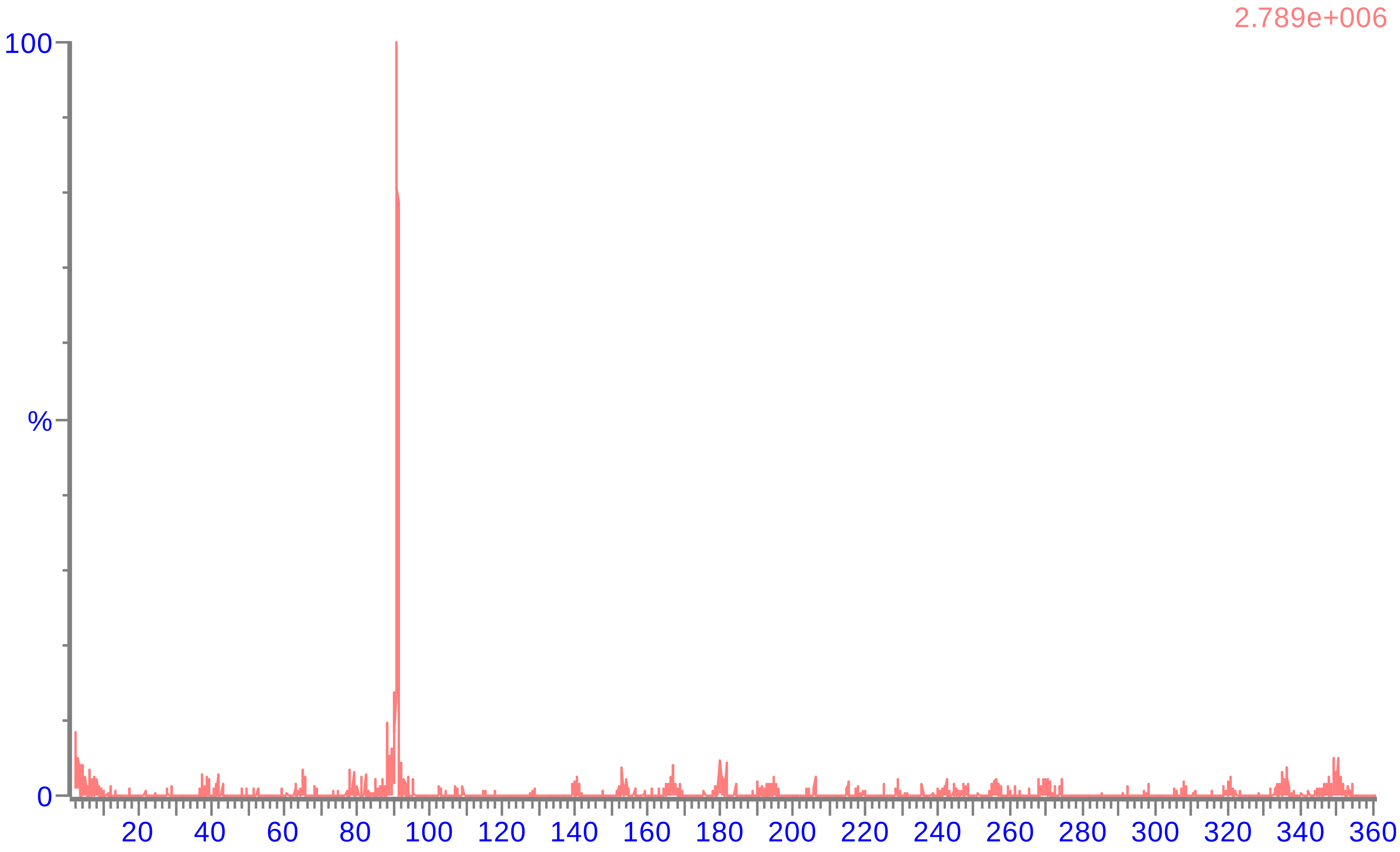

Figure 1.218: Mass spectrum for daughter fragment peak ES+, m/z 351.03 -> 180.26.

**4h** 4-methyl-N-(1-nitropentan-2-yl)aniline

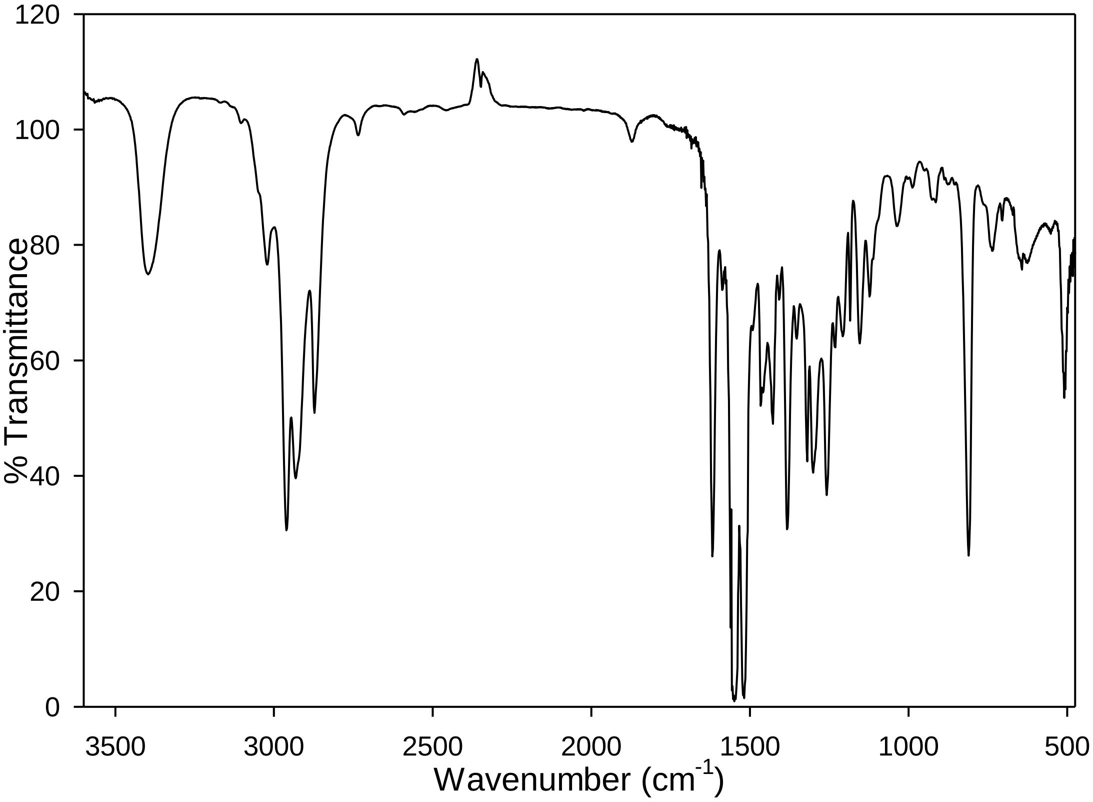

Figure 1.219: IR spectrum of **4h** 4-methyl-N-(1-nitropentan-2-yl)aniline.

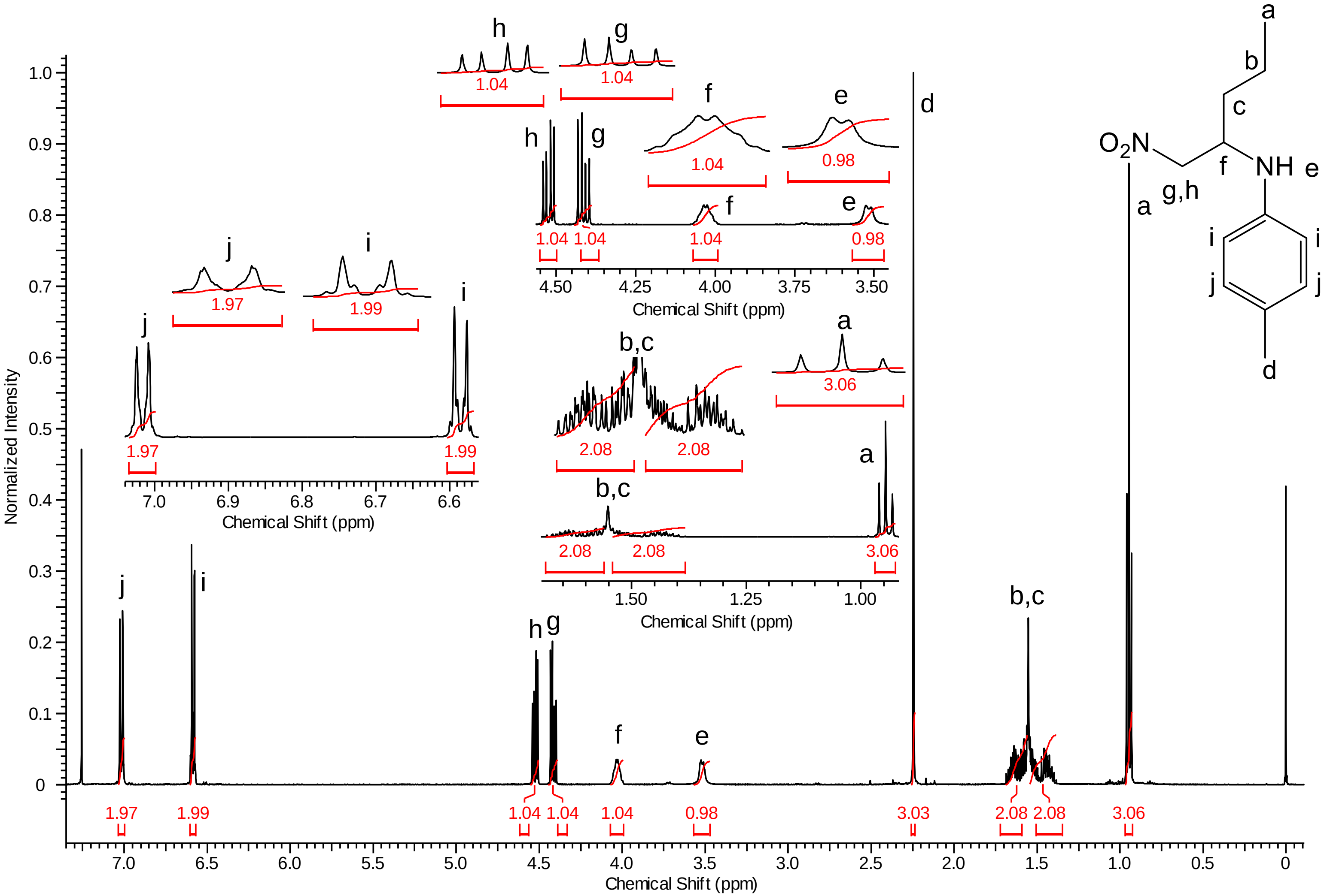

Figure 1.220: $^1$H NMR spectrum of **4h** 4-methyl-N-(1-nitropentan-2-yl)aniline.

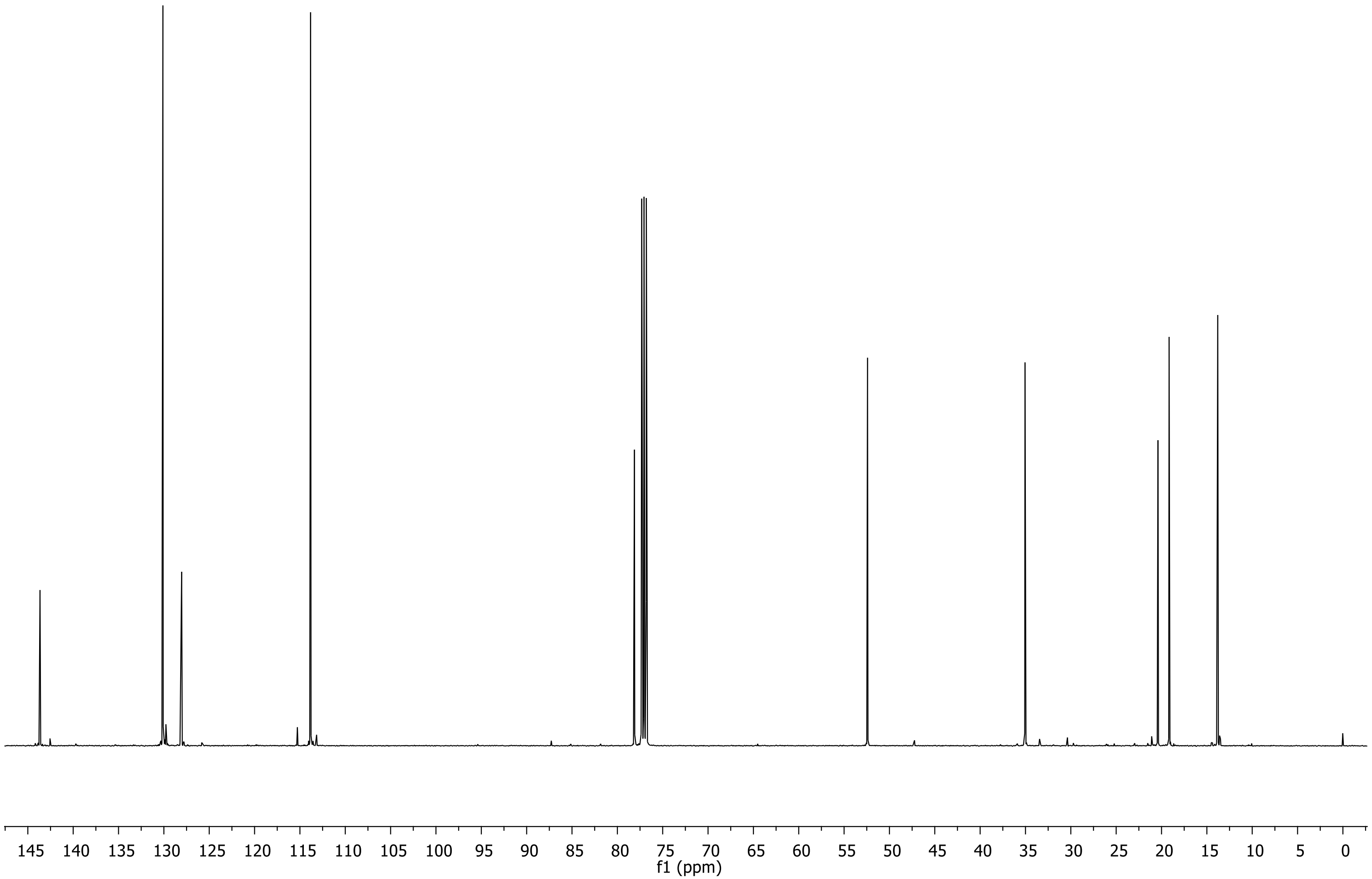

Figure 1.221: $^{13}$C NMR spectrum of **4h** 4-methyl-N-(1-nitropentan-2-yl)aniline.

Table 1.31: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **4h** | 229 | 1 | 229.07 | 58 | 199.24 | 26 | ES+ |
| | | 2 | 229.07 | 58 | 91.06 | 40 | ES+ |
| | | 3 | 229.07 | 58 | 118.00 | 28 | ES+ |
| | | 4 | 229.07 | 58 | 184.74 | 32 | ES+ |

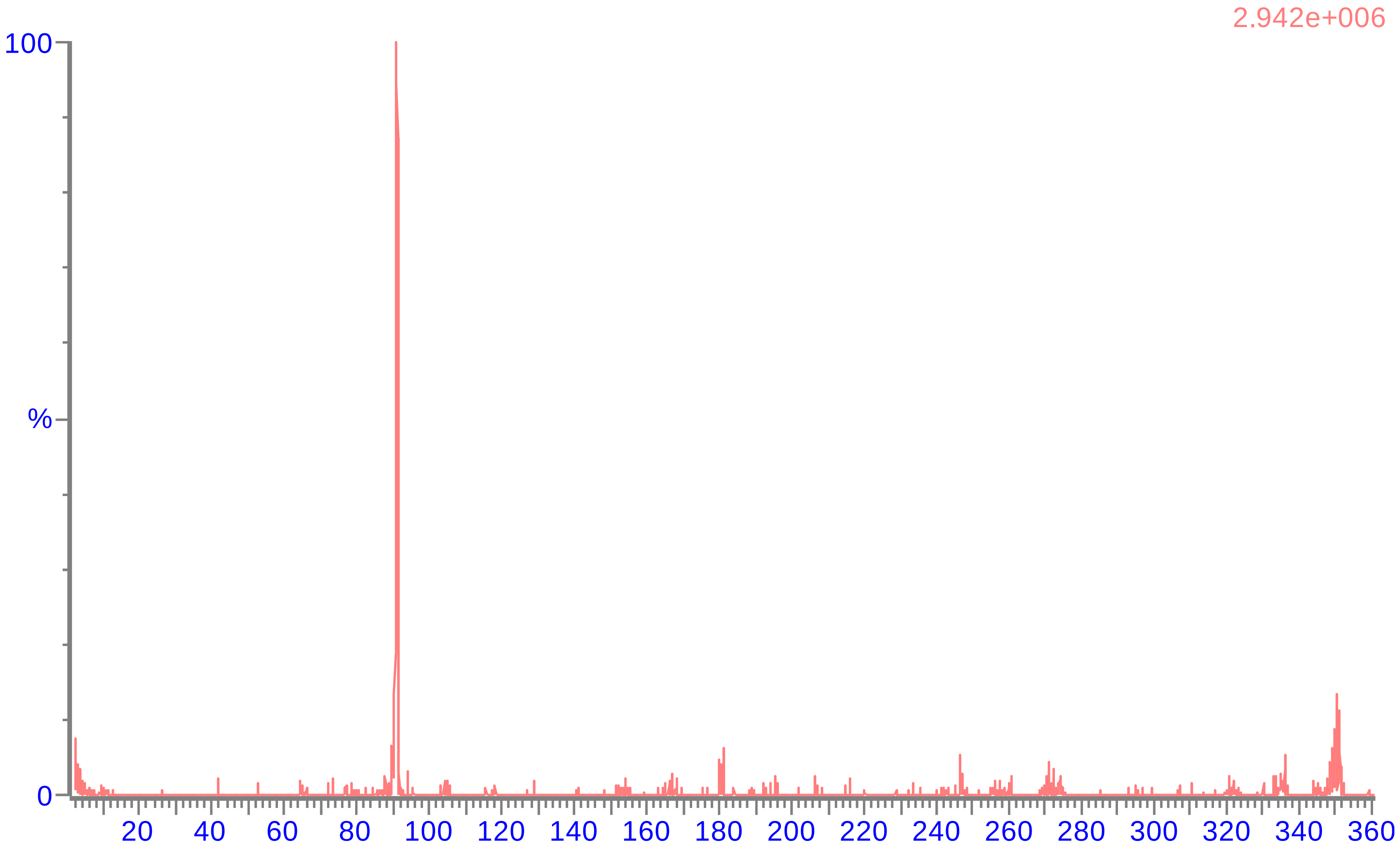

Figure 1.222: Mass spectrum for daughter fragment peak ES+, m/z 229.07 -> 199.24.

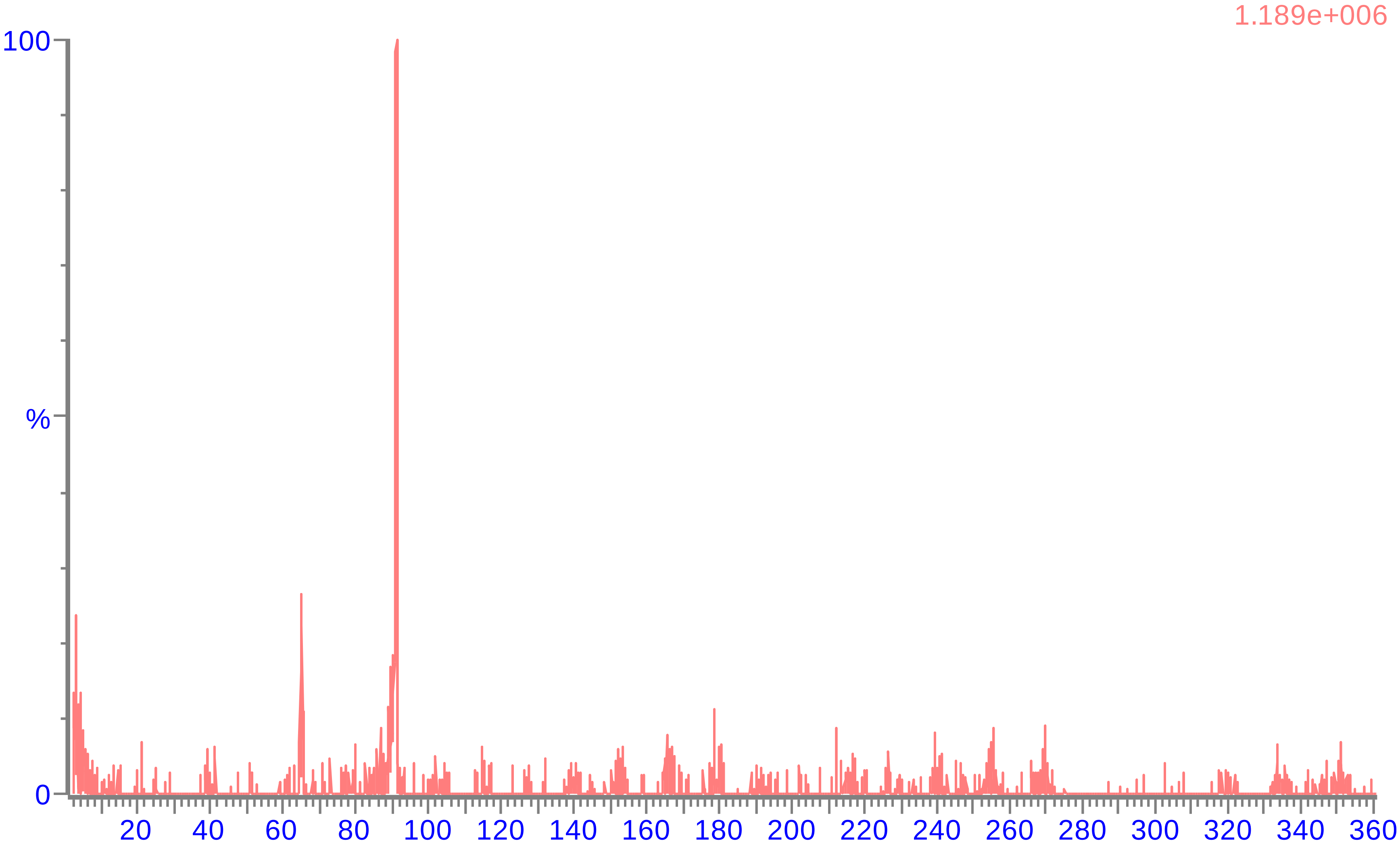

Figure 1.223: Mass spectrum for daughter fragment peak ES+, m/z 229.07 -> 64.97.

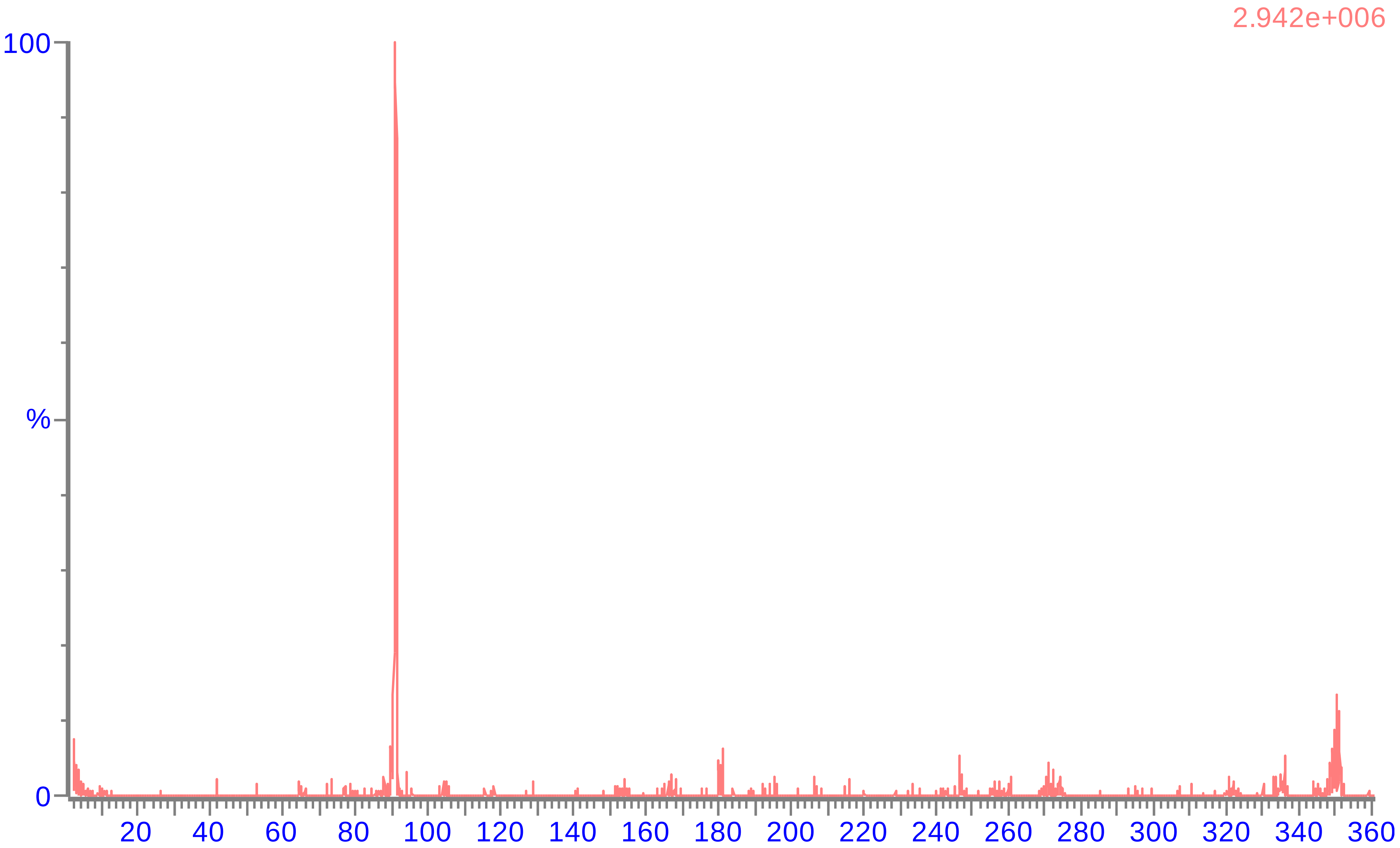

Figure 1.224: Mass spectrum for daughter fragment peak ES+, m/z 229.07 -> 335.77.

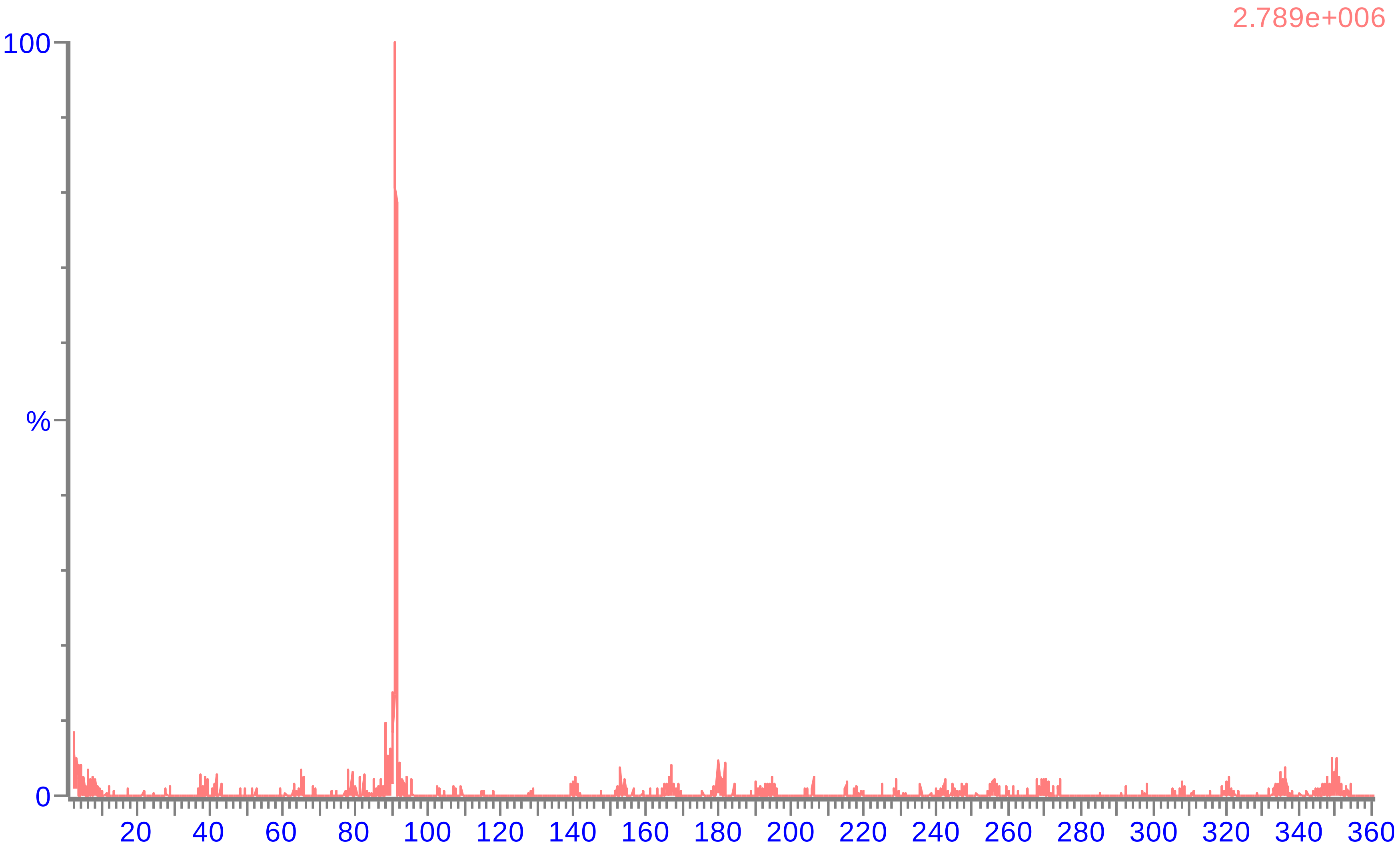

Figure 1.225: Mass spectrum for daughter fragment peak ES+, m/z 229.07 -> 180.26.

**4i** (*E*)-*N*-(2-nitro-1-(*p*-tolyl)ethyl)-4-(phenyldiazenyl)aniline

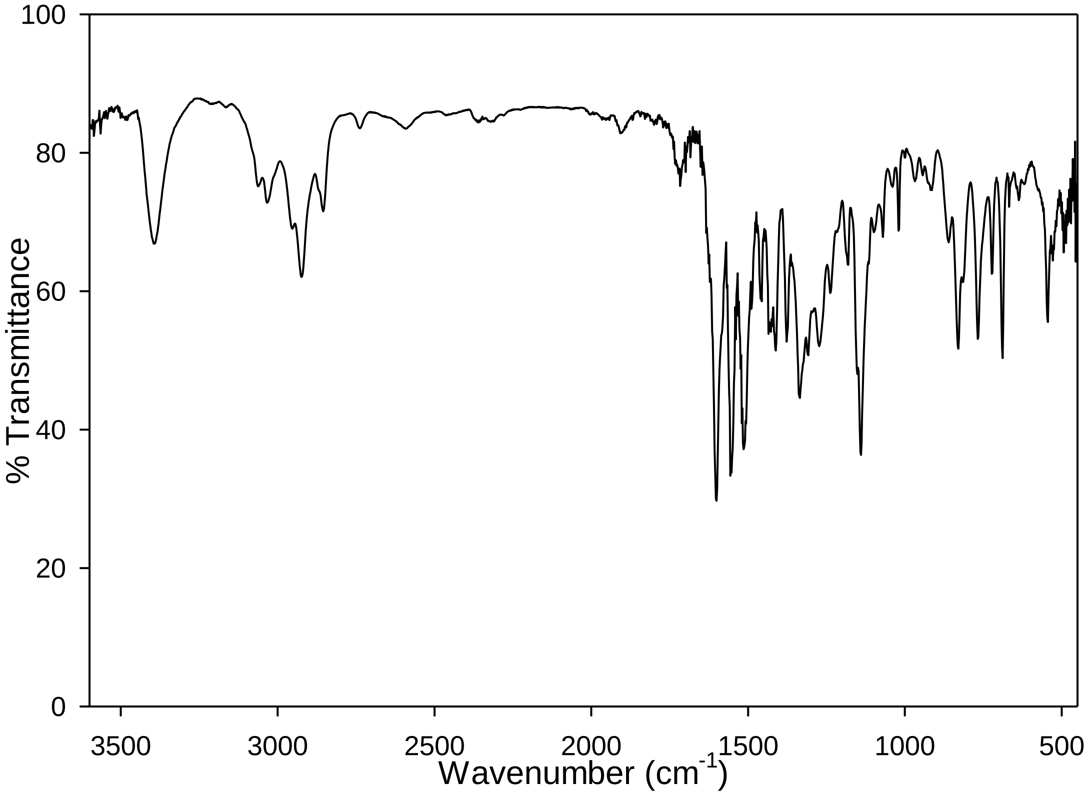

Figure 1.226: IR spectrum of **4i** (*E*)-*N*-(2-nitro-1-(*p*-tolyl)ethyl)-4-(phenyldiazenyl)aniline.

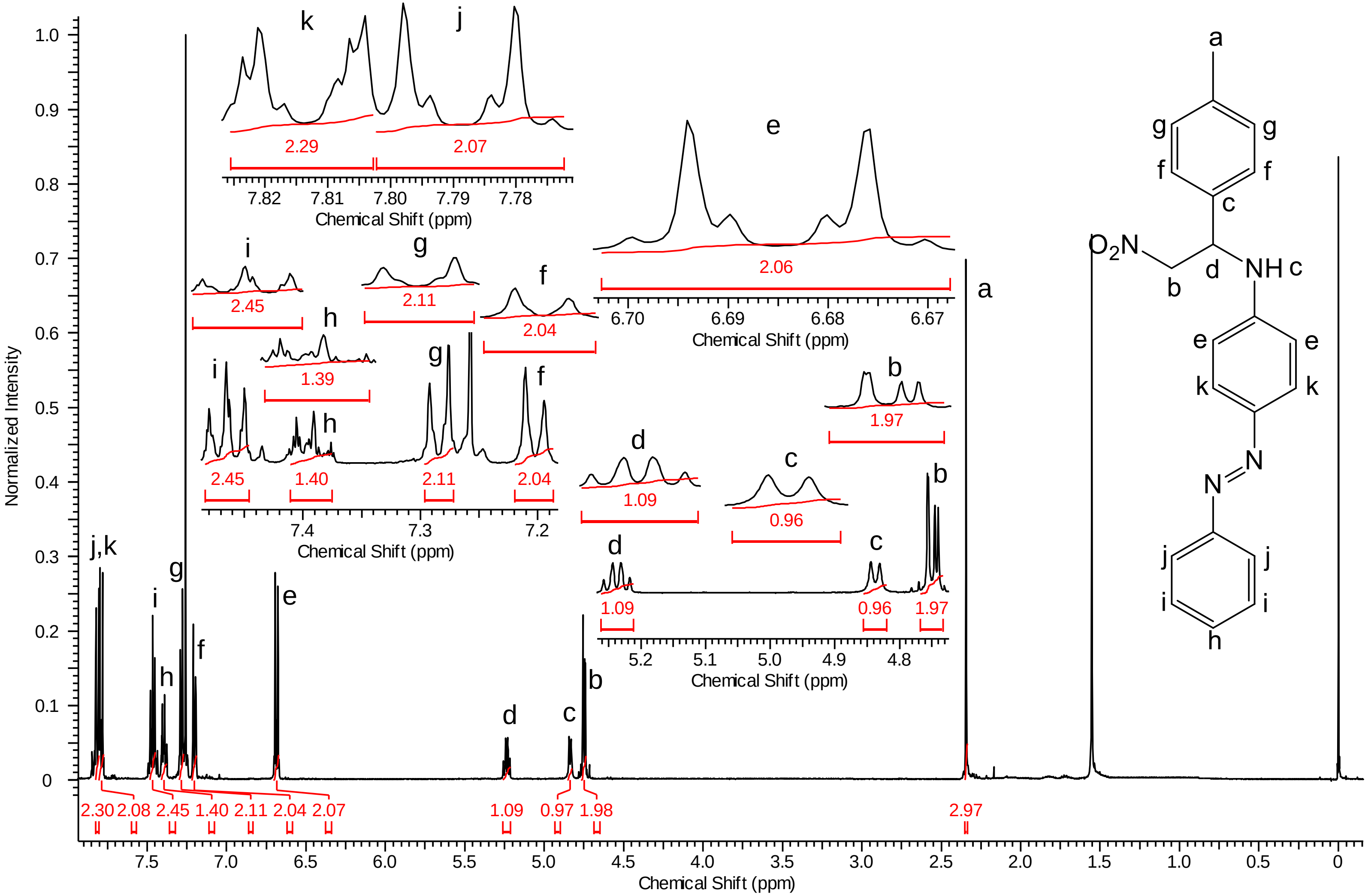

Figure 1.227: $^1$H NMR spectrum of **4i** (*E*)-*N*-(2-nitro-1-(*p*-tolyl)ethyl)-4-(phenyldiazenyl)aniline.

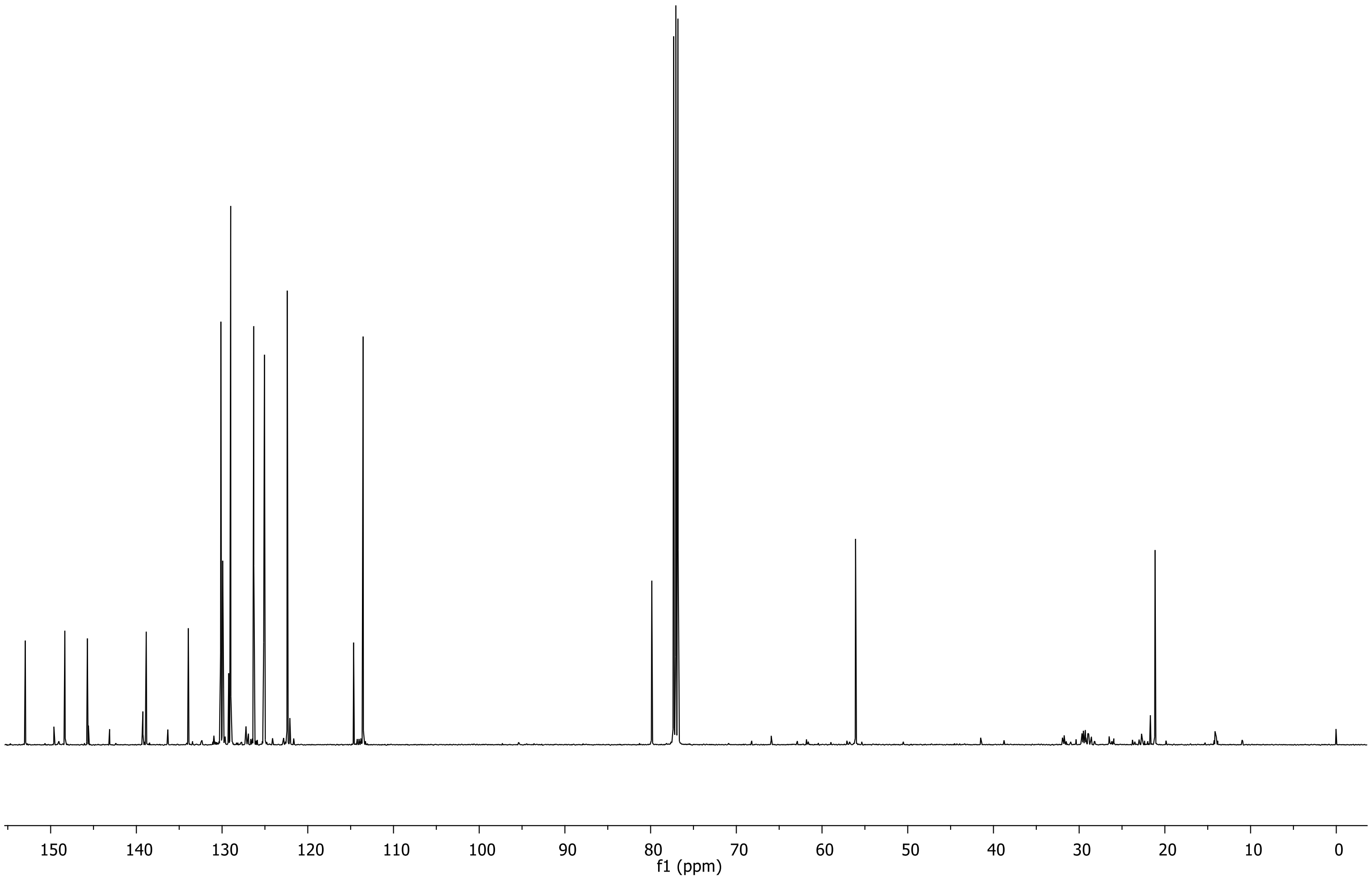

Figure 1.228: $^{13}$C NMR spectrum of **4i** (*E*)-*N*-(2-nitro-1-(*p*-tolyl)ethyl)-4-(phenyldiazenyl)aniline.

Table 1.32: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **4i** | 360.4 | 1 | 361.18 | 40 | 197.18 | 24 | ES+ |
| | | 2 | 361.18 | 40 | 118.04 | 34 | ES+ |
| | | 3 | 361.18 | 40 | 77.00 | 40 | ES+ |
| | | 4 | 361.18 | 40 | 91.90 | 50 | ES+ |
| | | 5 | 361.18 | 40 | 64.97 | 70 | ES+ |

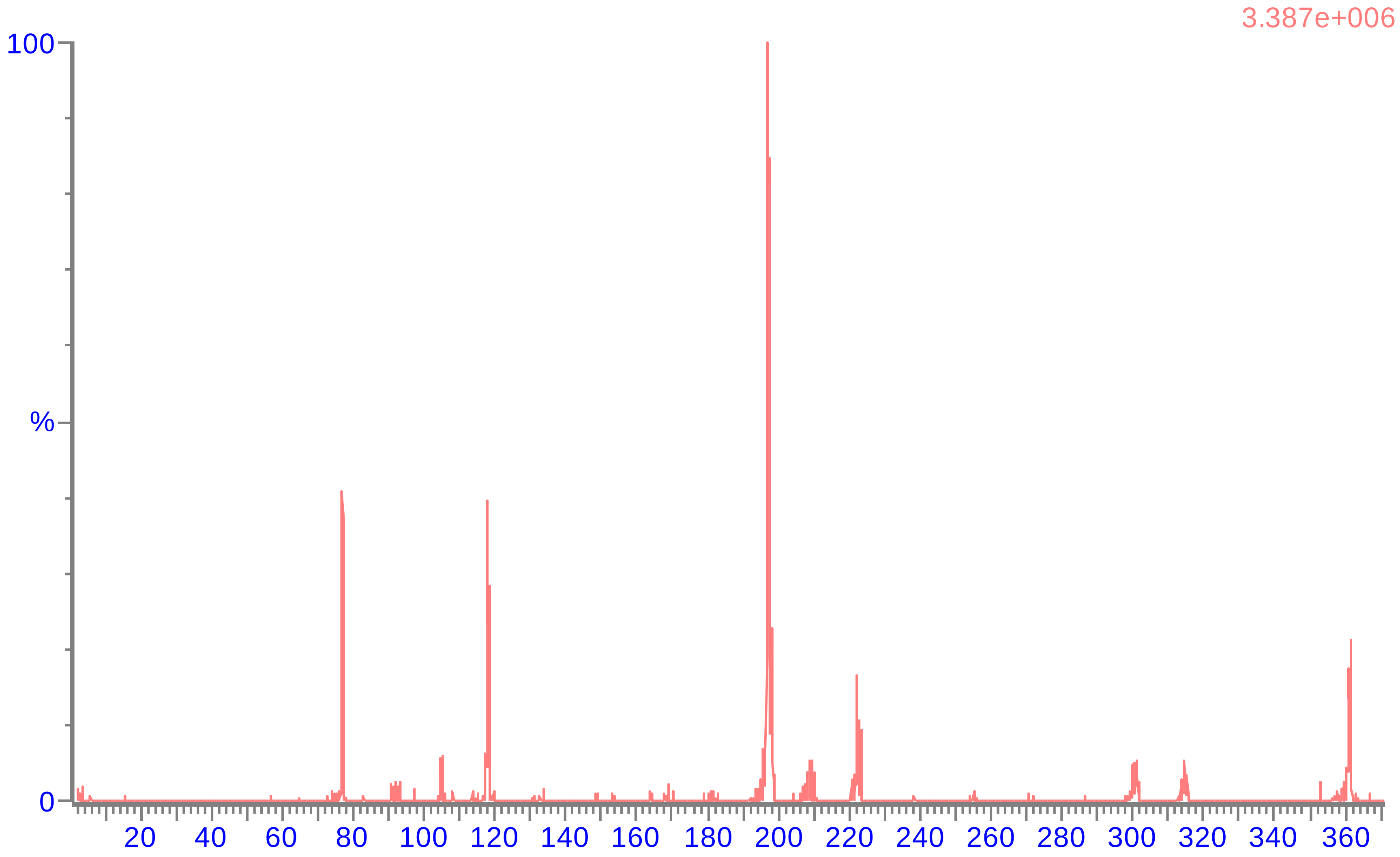

Figure 1.229: Mass spectrum for daughter fragment peak ES+, m/z 361.18 -> 197.18.

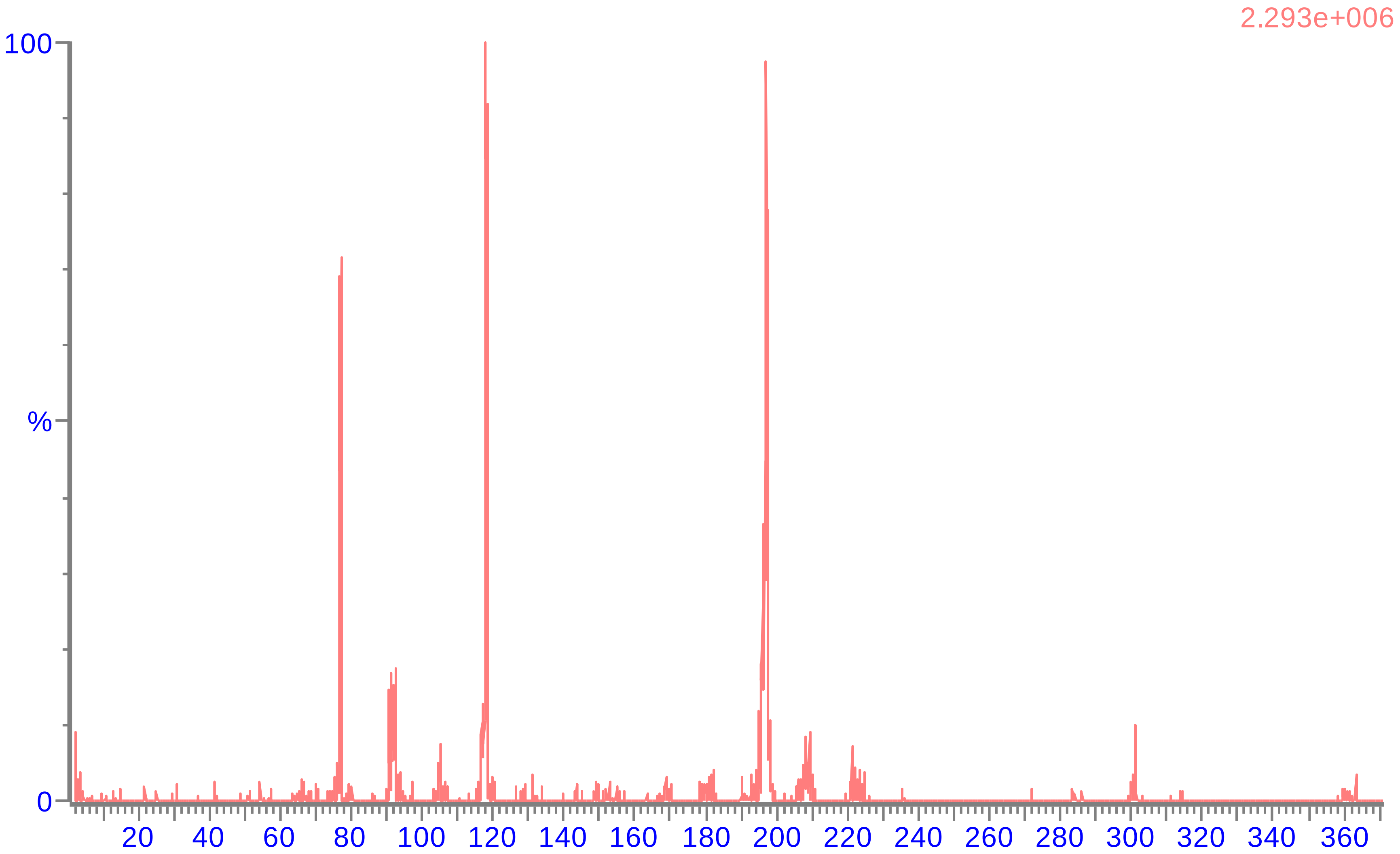

Figure 1.230: Mass spectrum for daughter fragment peak ES+, m/z 361.18 -> 118.04.

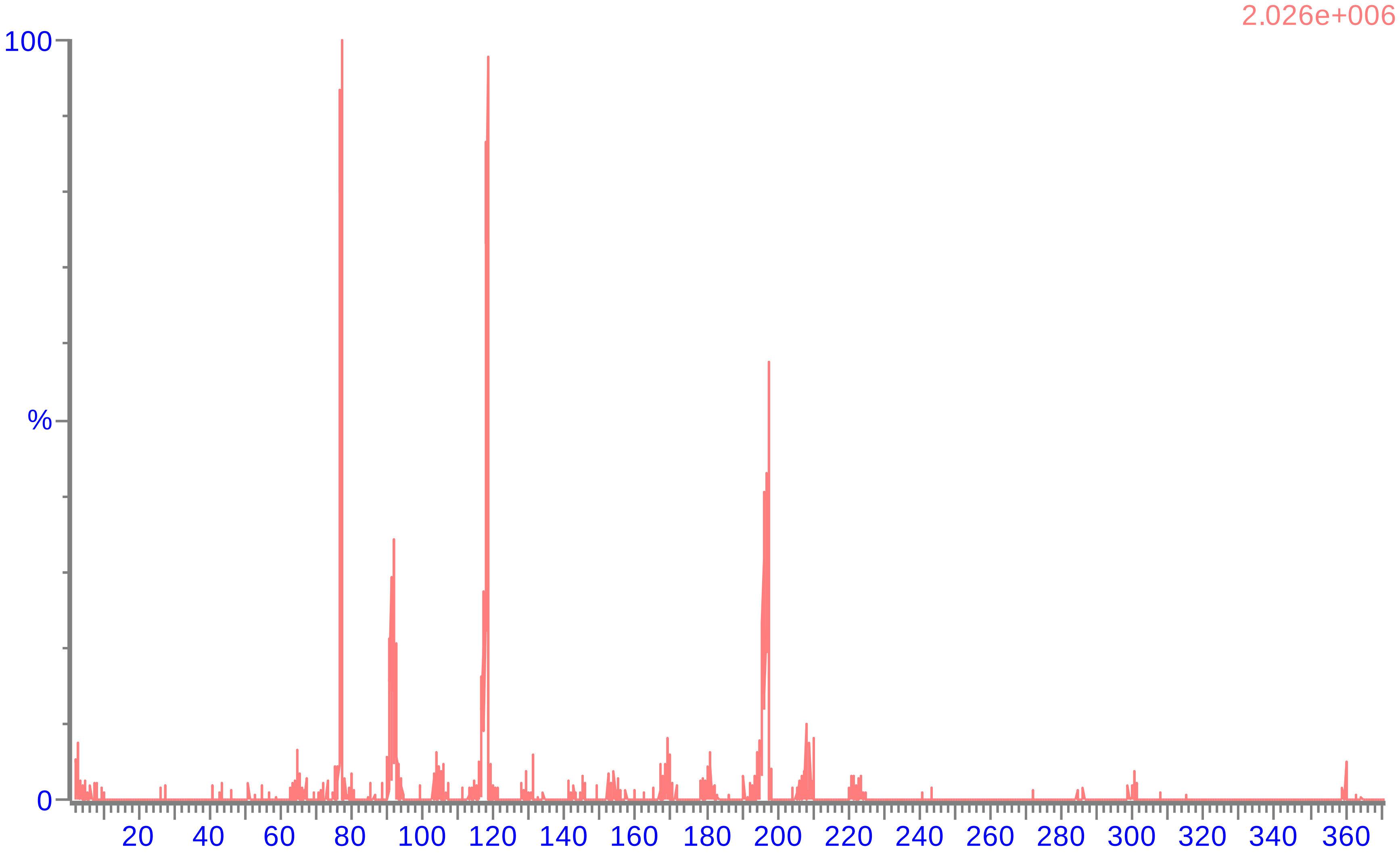

Figure 1.231: Mass spectrum for daughter fragment peak ES+, m/z 361.18 -> 77.00.

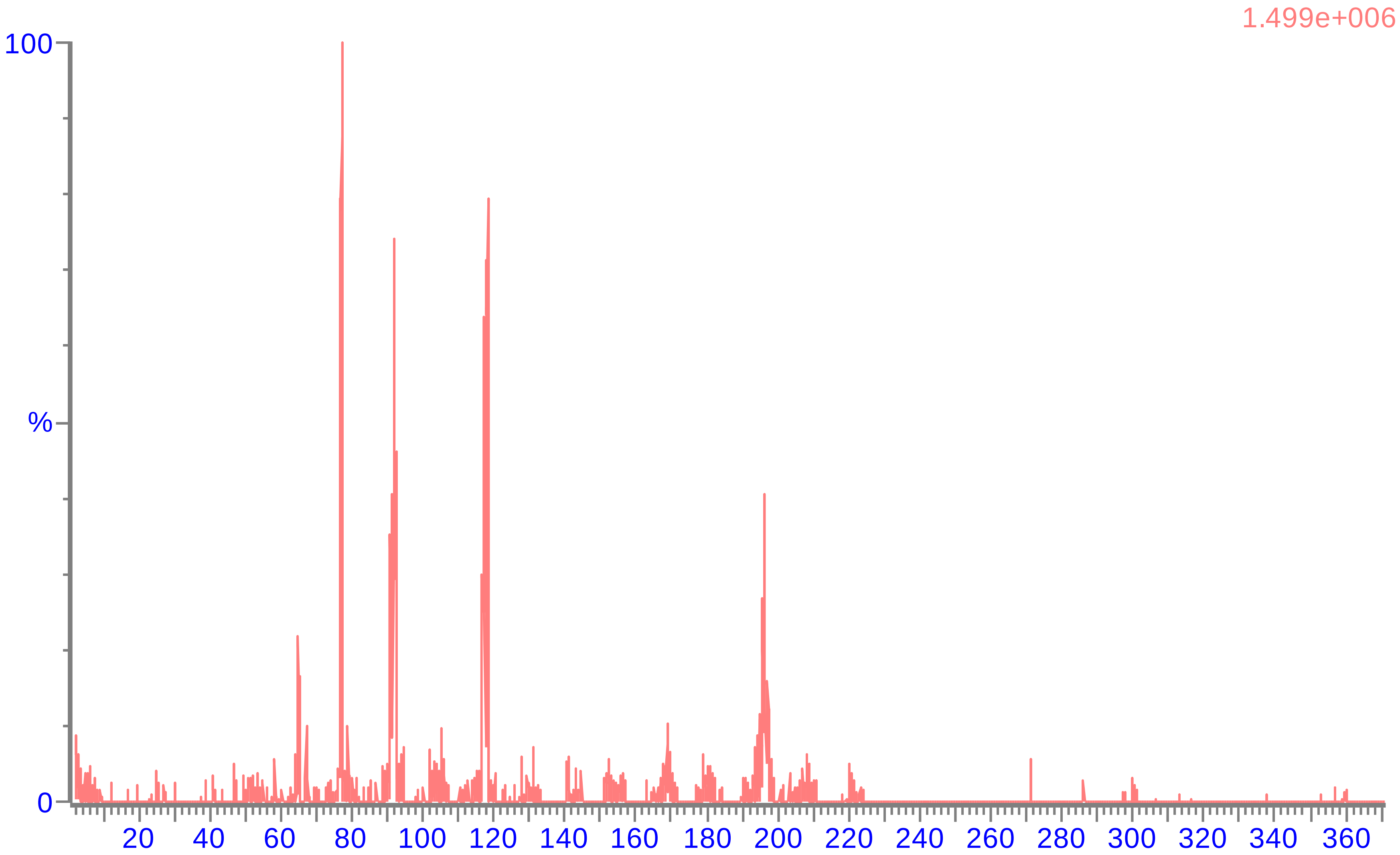

Figure 1.232: Mass spectrum for daughter fragment peak ES+, m/z 361.18 -> 91.90.

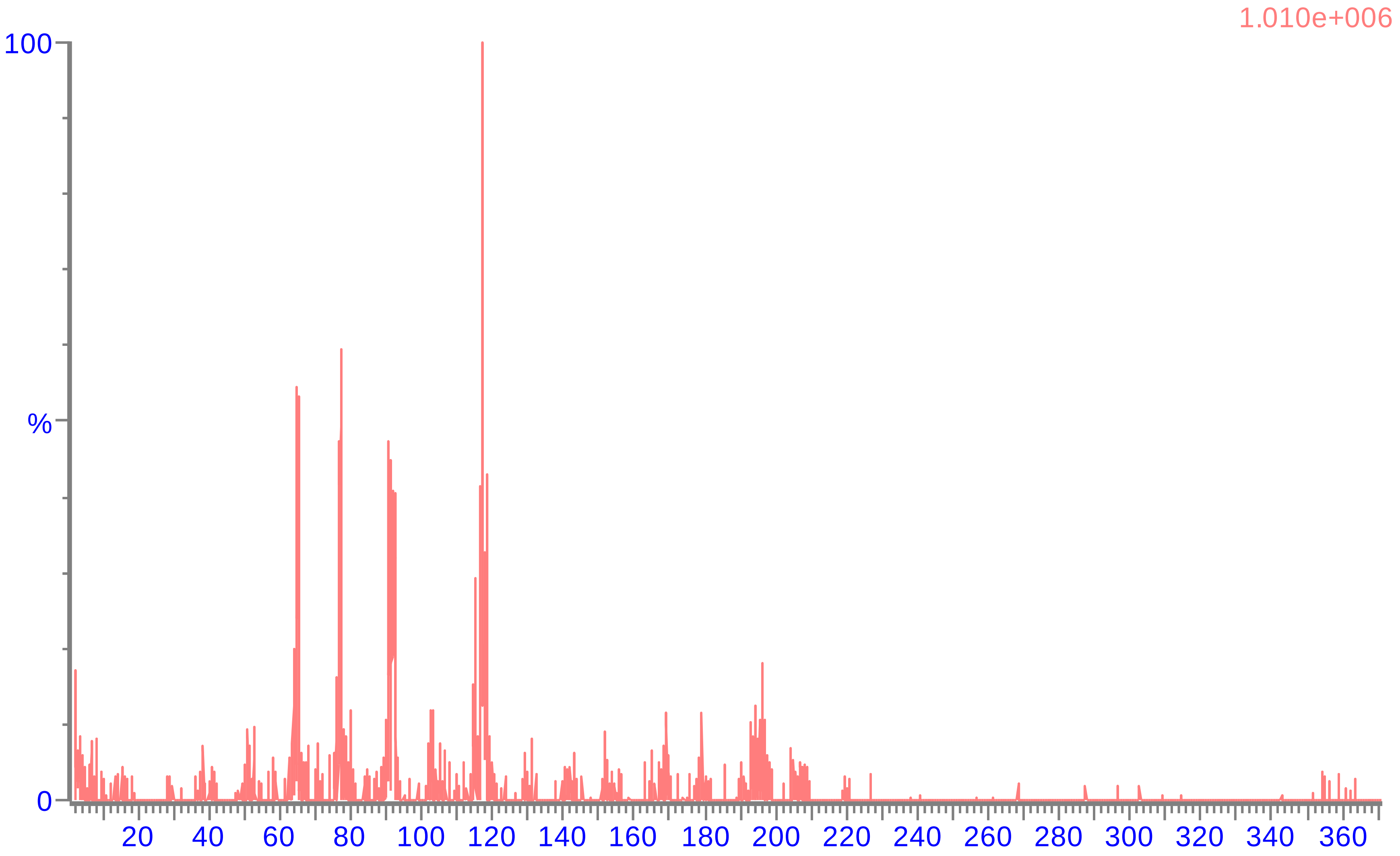

Figure 1.233: Mass spectrum for daughter fragment peak ES+, m/z 361.18 -> 64.97.

**4j** 1-(4-((1-(4-methoxyphenyl)-2-nitropropyl)amino)phenyl)ethanone

Table 1.33: MS data.

| Compound | Formula/Mass | | Parent m/z | Cone Voltage | Daughters | Collision Energy | Ion Mode |
|---|---|---|---|---|---|---|---|
| **4j** | 328 | 1 | 329.10 | 34 | 148.03 | 24 | ES+ |
| | | 2 | 329.10 | 34 | 136.00 | 20 | ES+ |
| | | 3 | 329.10 | 34 | 254.11 | 18 | ES+ |
| | | 4 | 329.10 | 34 | 117.01 | 44 | ES+ |
| | | 5 | 329.10 | 34 | 105.04 | 56 | ES+ |

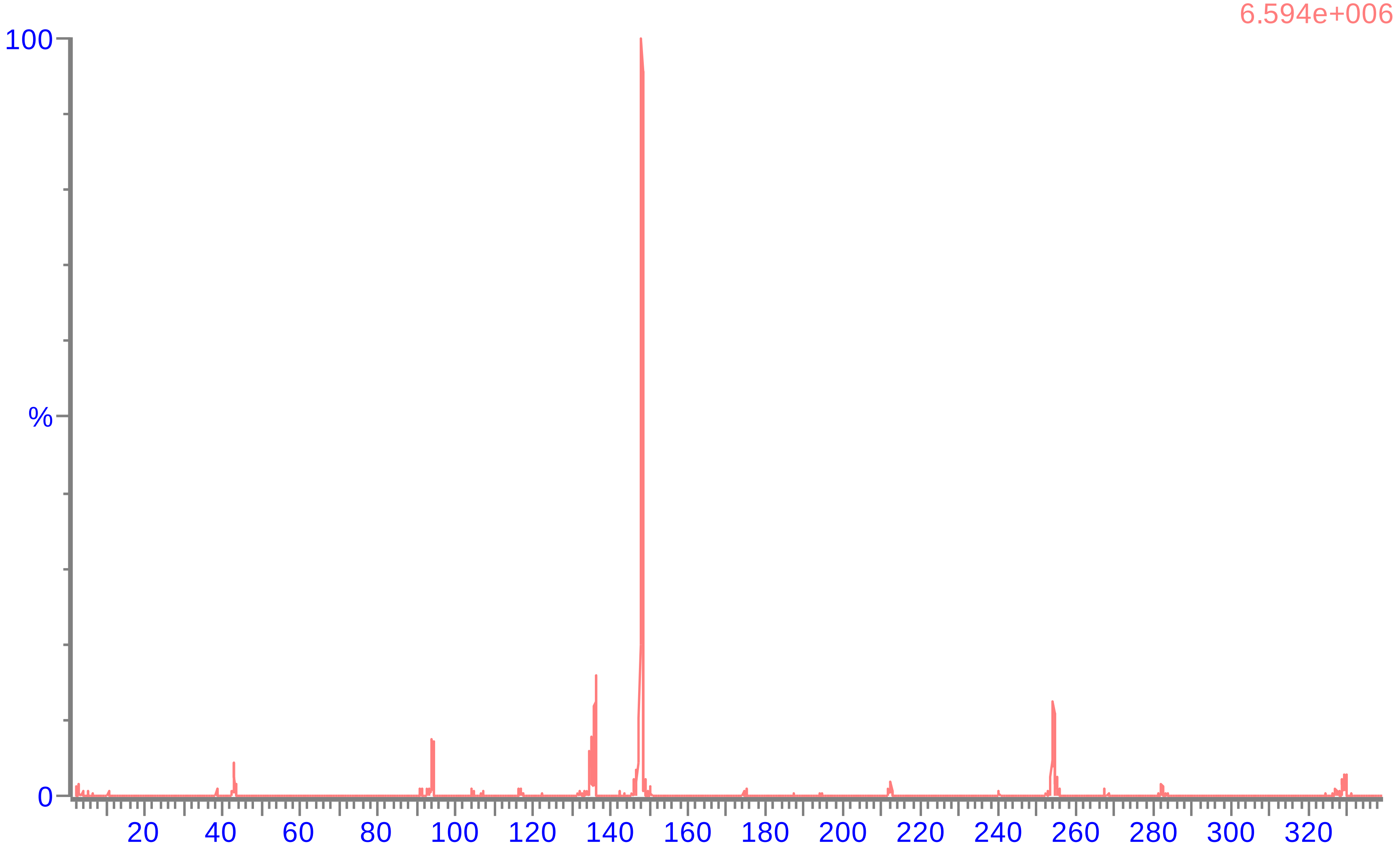

Figure 1.234: Mass spectrum for daughter fragment peak ES+, m/z 329.10 -> 148.03.

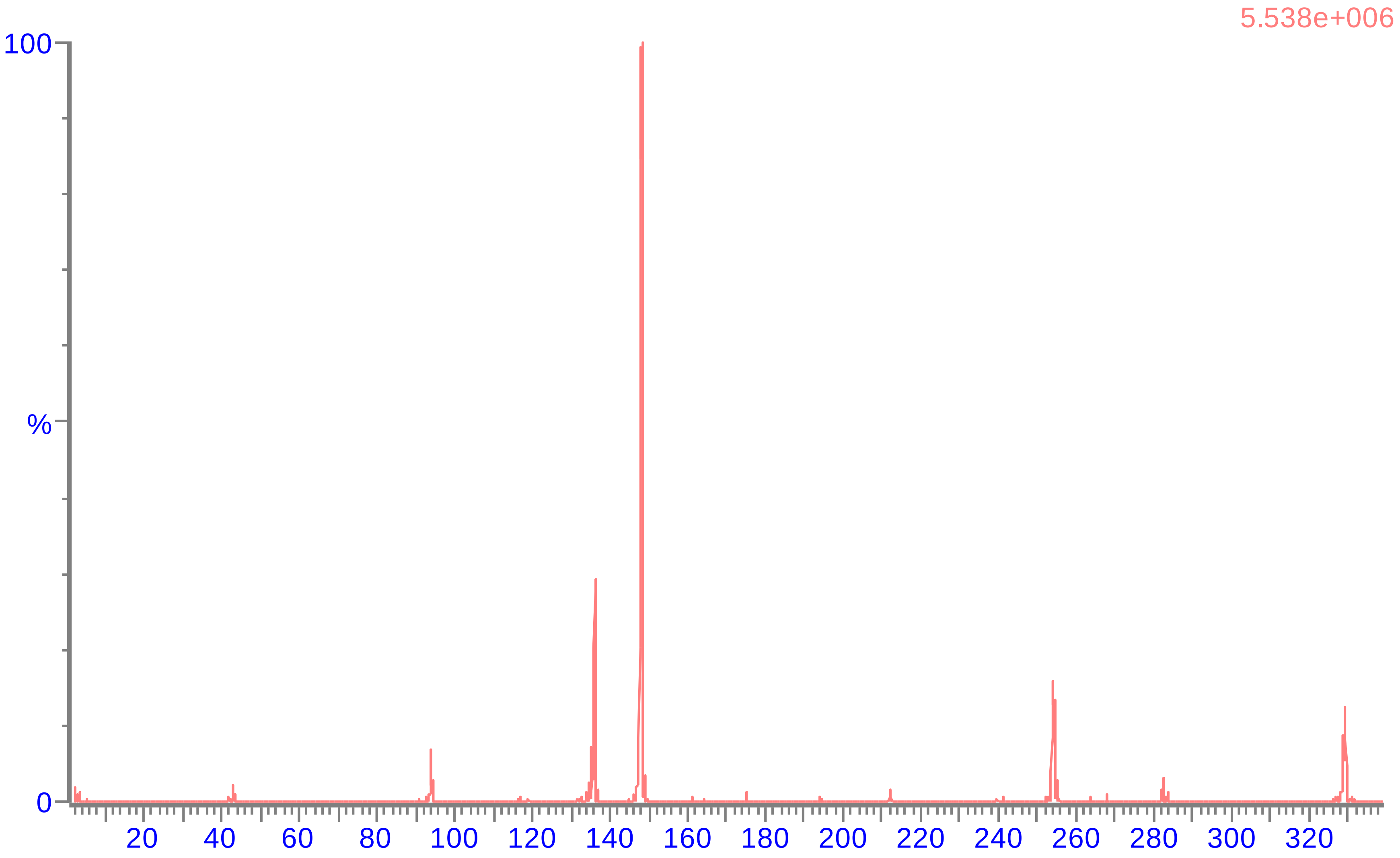

Figure 1.235: Mass spectrum for daughter fragment peak ES+, m/z 329.10 -> 136.00.

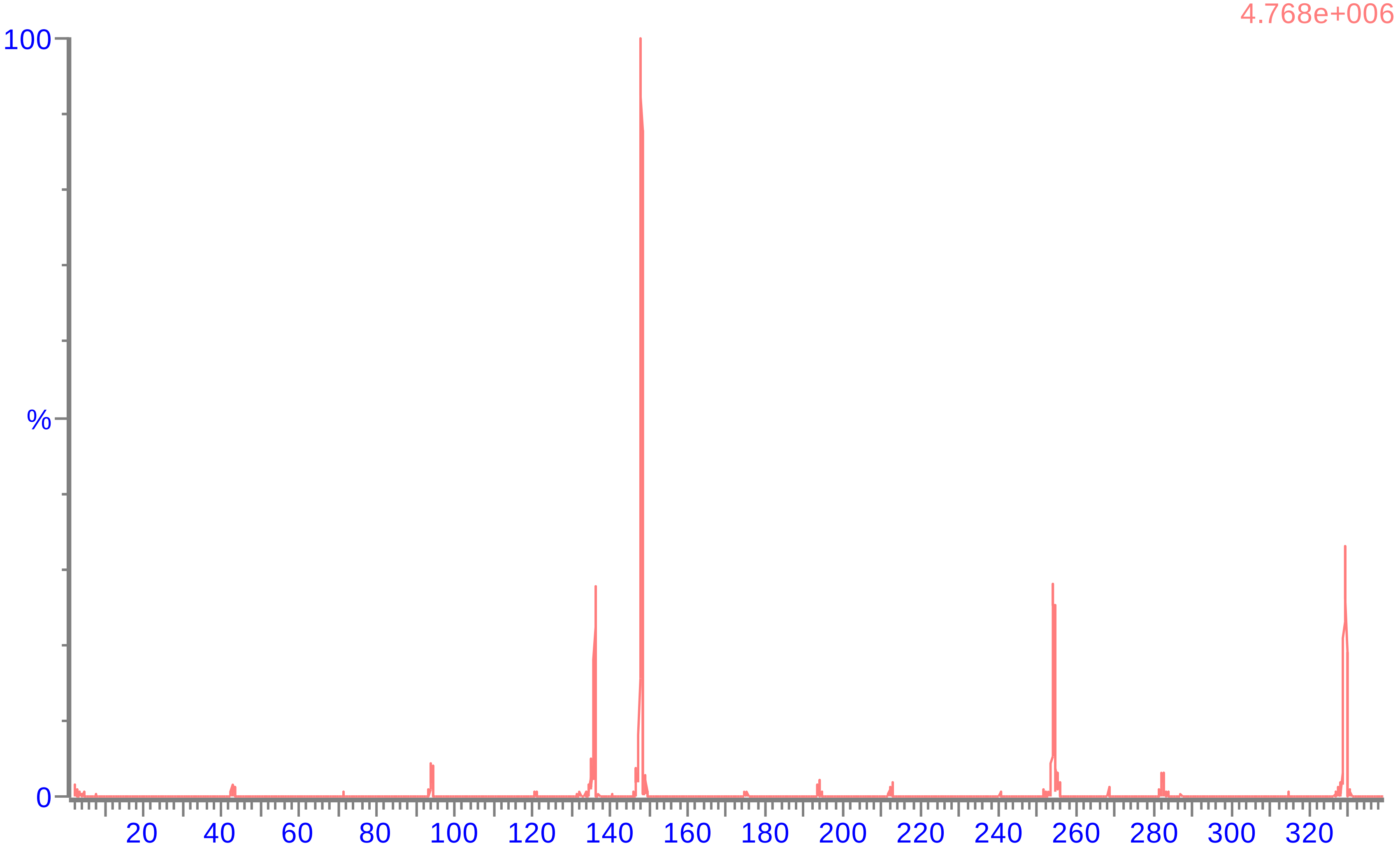

Figure 1.236: Mass spectrum for daughter fragment peak ES+, m/z 329.10 -> 254.11.

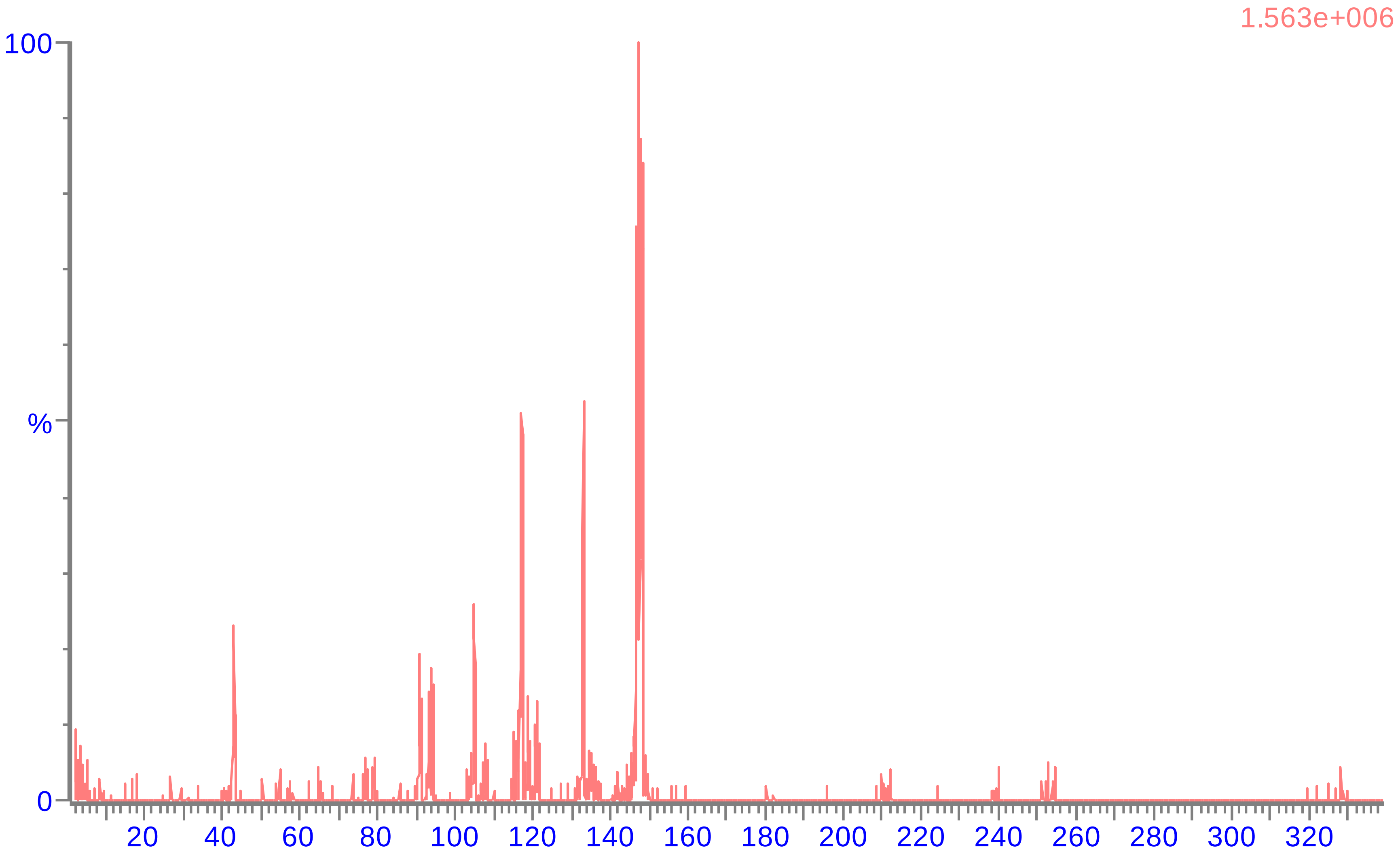

Figure 1.237: Mass spectrum for daughter fragment peak ES+, m/z 329.10 -> 117.01.

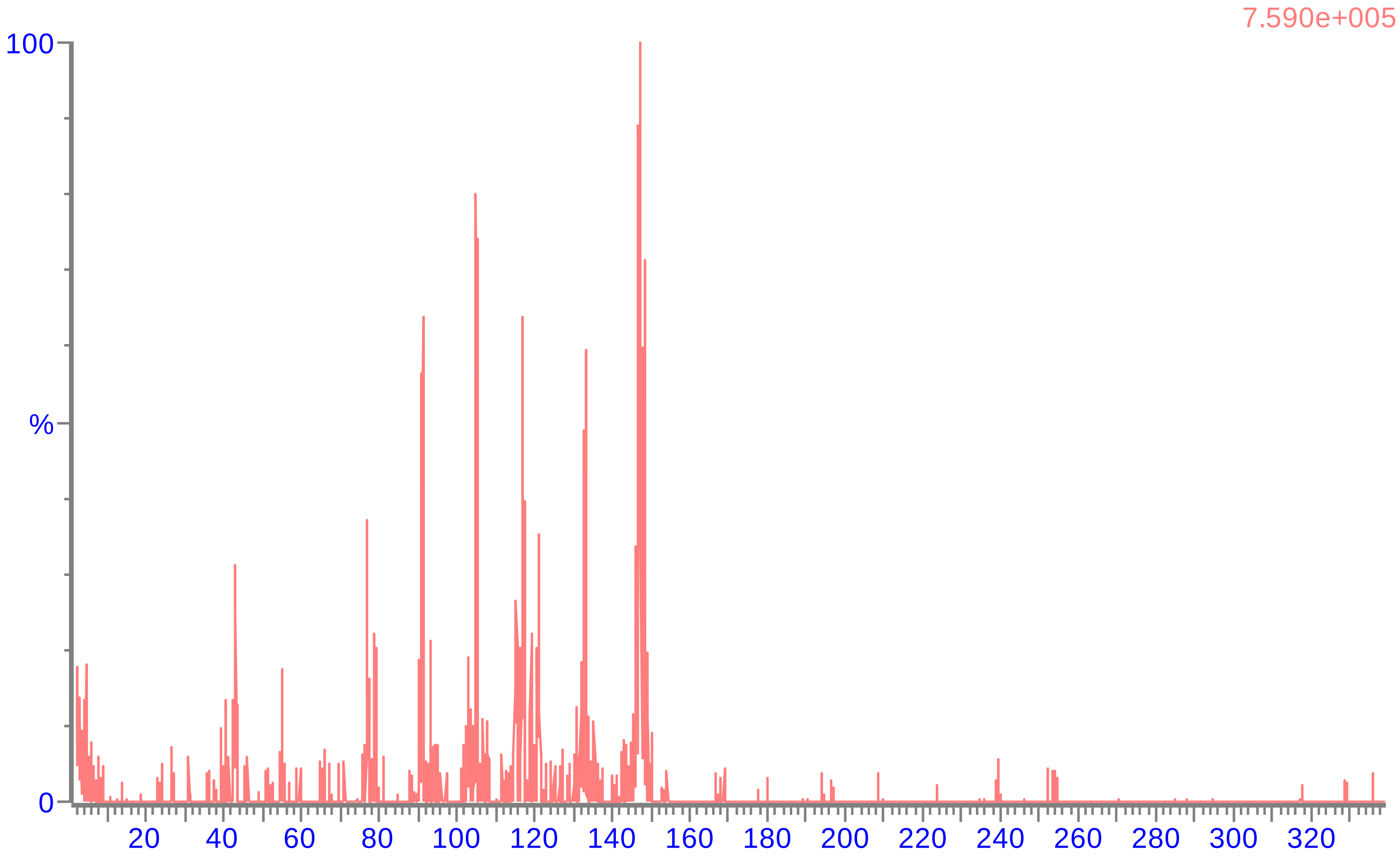

Figure 1.238: Mass spectrum for daughter fragment peak ES+, m/z 329.10 -> 105.04.

**4k** 4-methyl-*N*-(2-nitro-1-(2-nitrophenyl)butyl)aniline

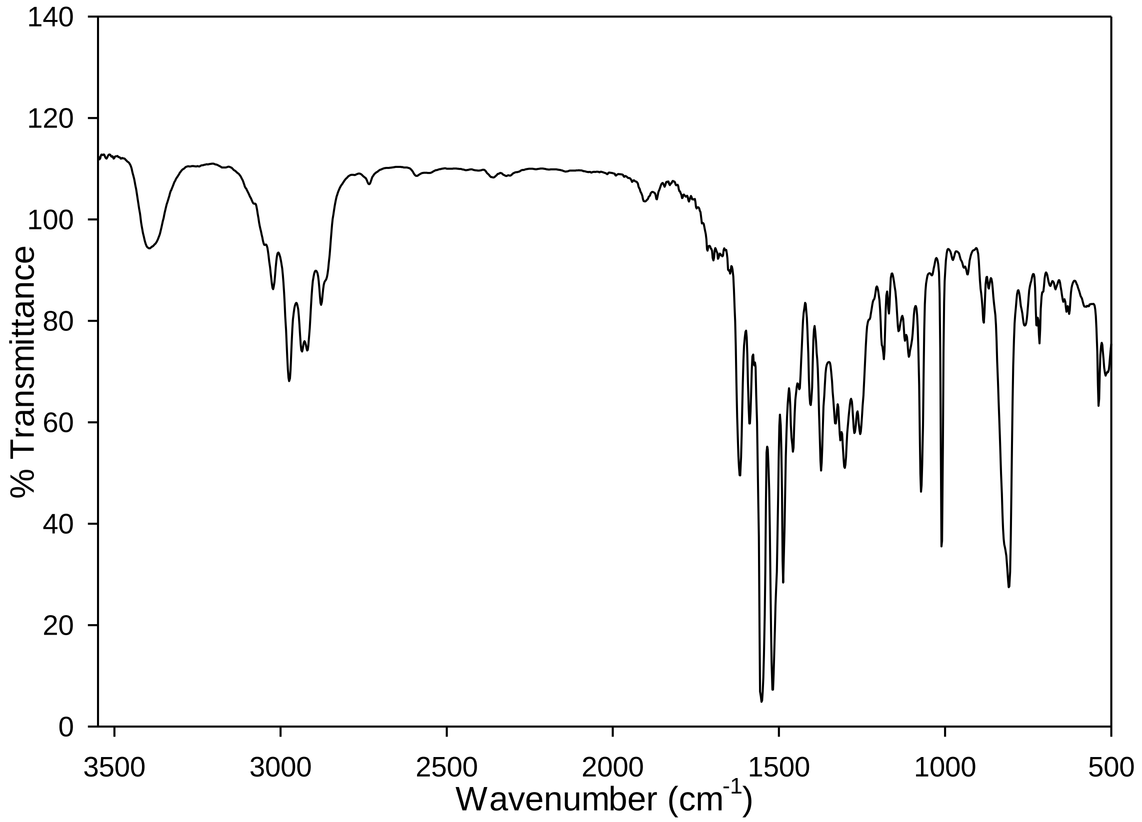

Figure 1.239: IR spectrum of **4k** 4-methyl-*N*-(2-nitro-1-(2-nitrophenyl)butyl)aniline.

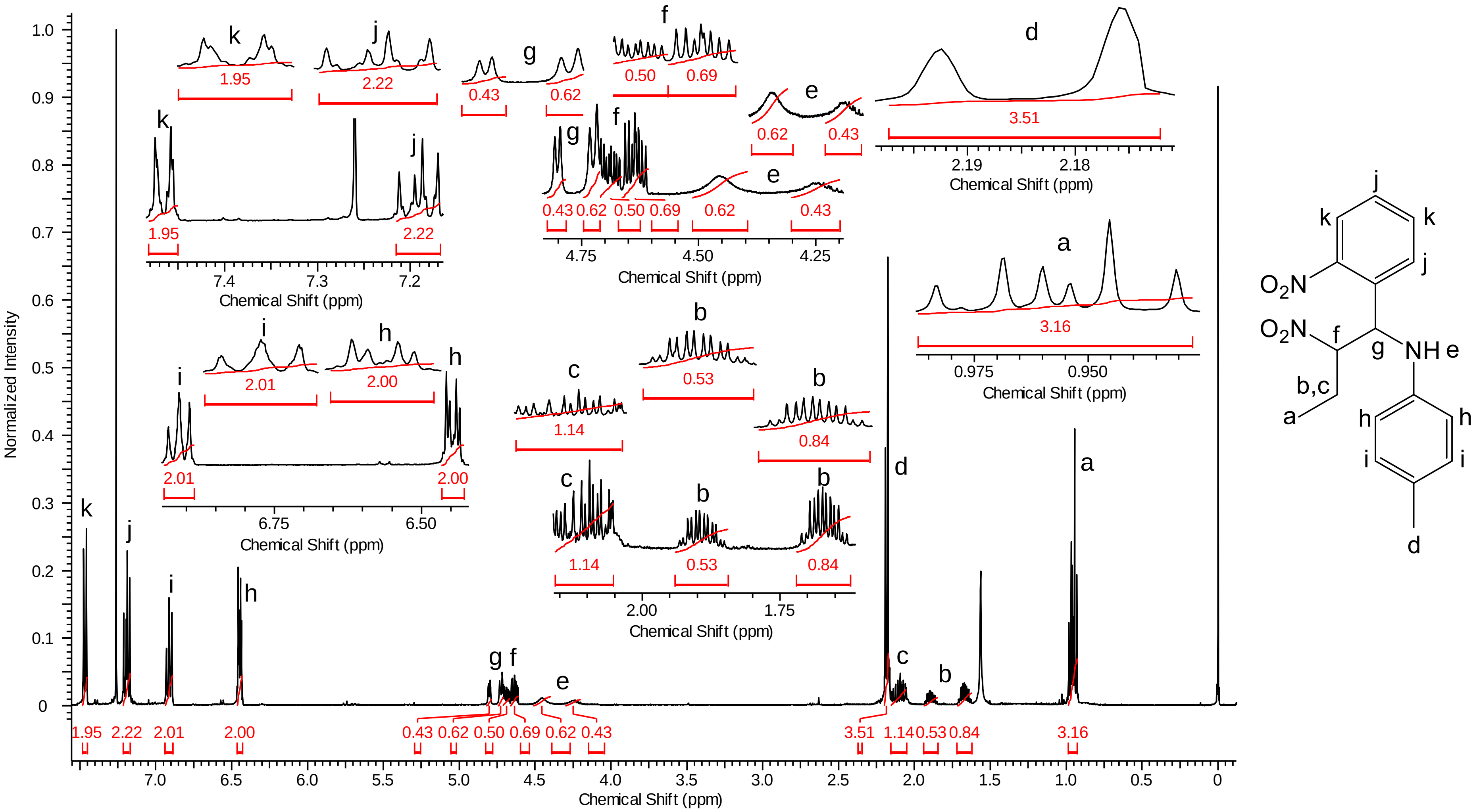

Figure 1.240: $^1$H NMR spectrum of **4k** 4-methyl-*N*-(2-nitro-1-(2-nitrophenyl)butyl)aniline.

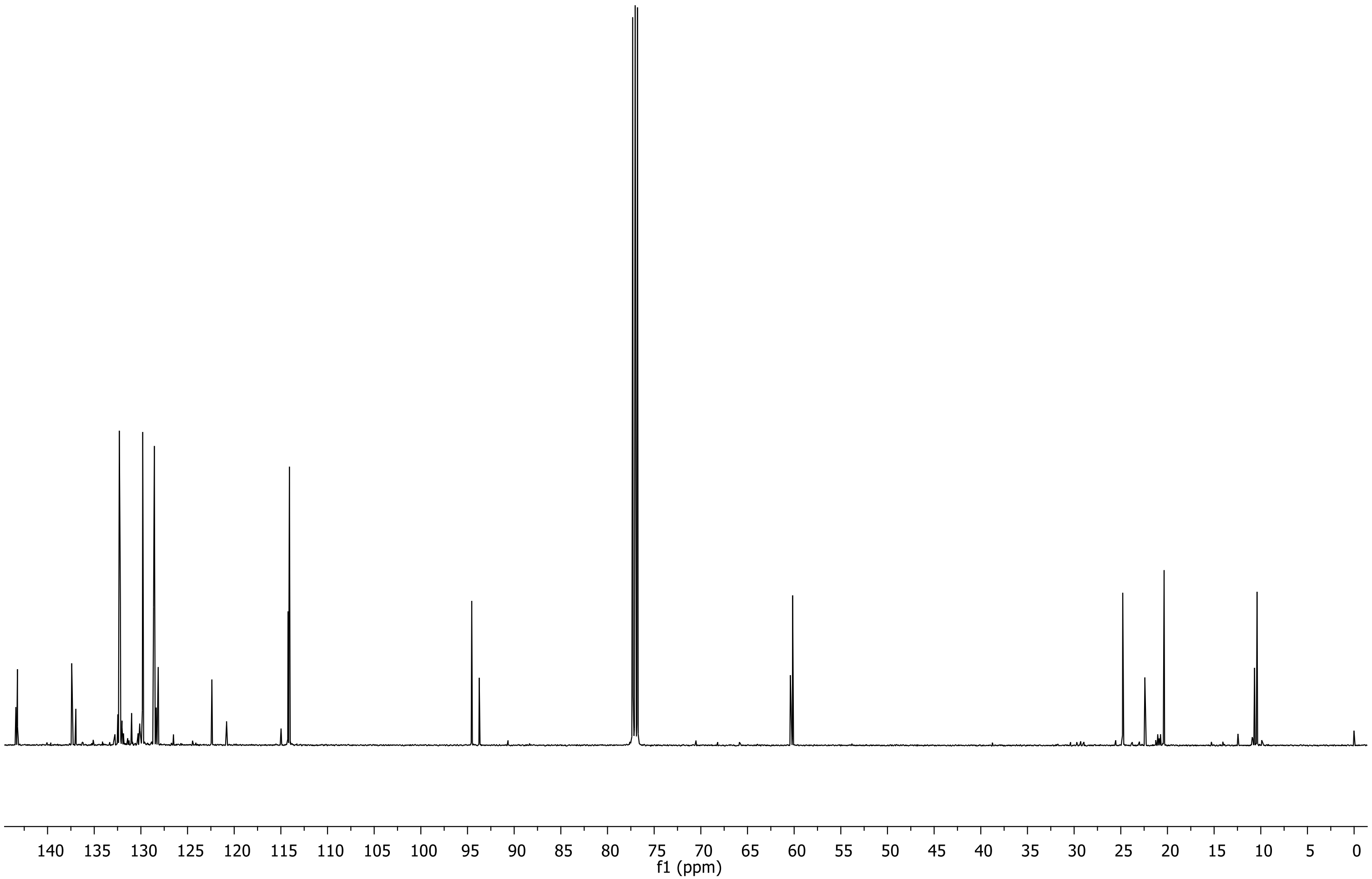

Figure 1.241: $^{13}$C NMR spectrum of **4k** 4-methyl-*N*-(2-nitro-1-(2-nitrophenyl)butyl)aniline.

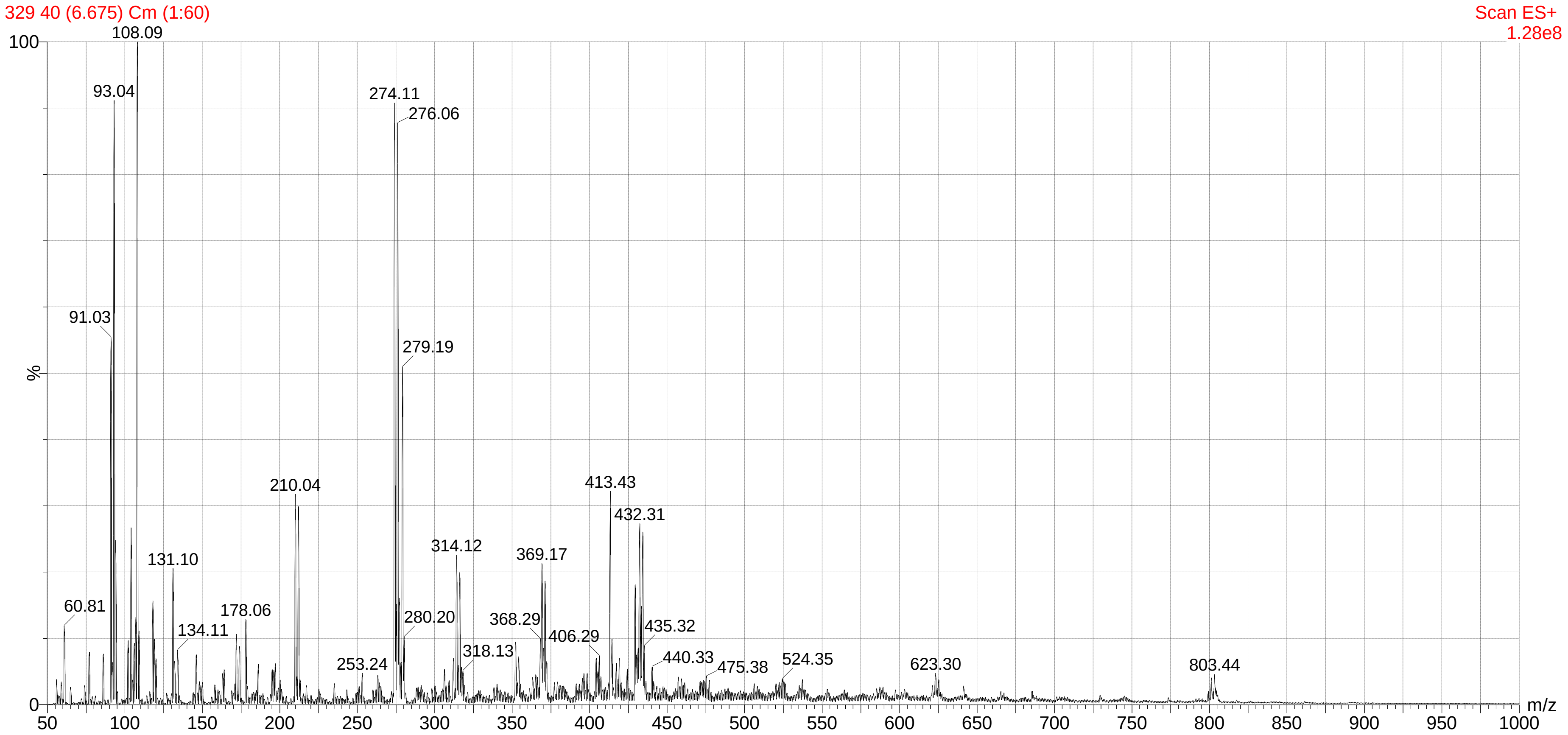

Figure 1.242: Mass spectrum of **4k** 4-methyl-*N*-(2-nitro-1-(2-nitrophenyl)butyl)aniline.