

## Supplementary Materials

### Synthesis of Novel 1-(4-Substituted pyridine-3-sulfonyl)-3-phenylureas with Potential Anticancer Activity

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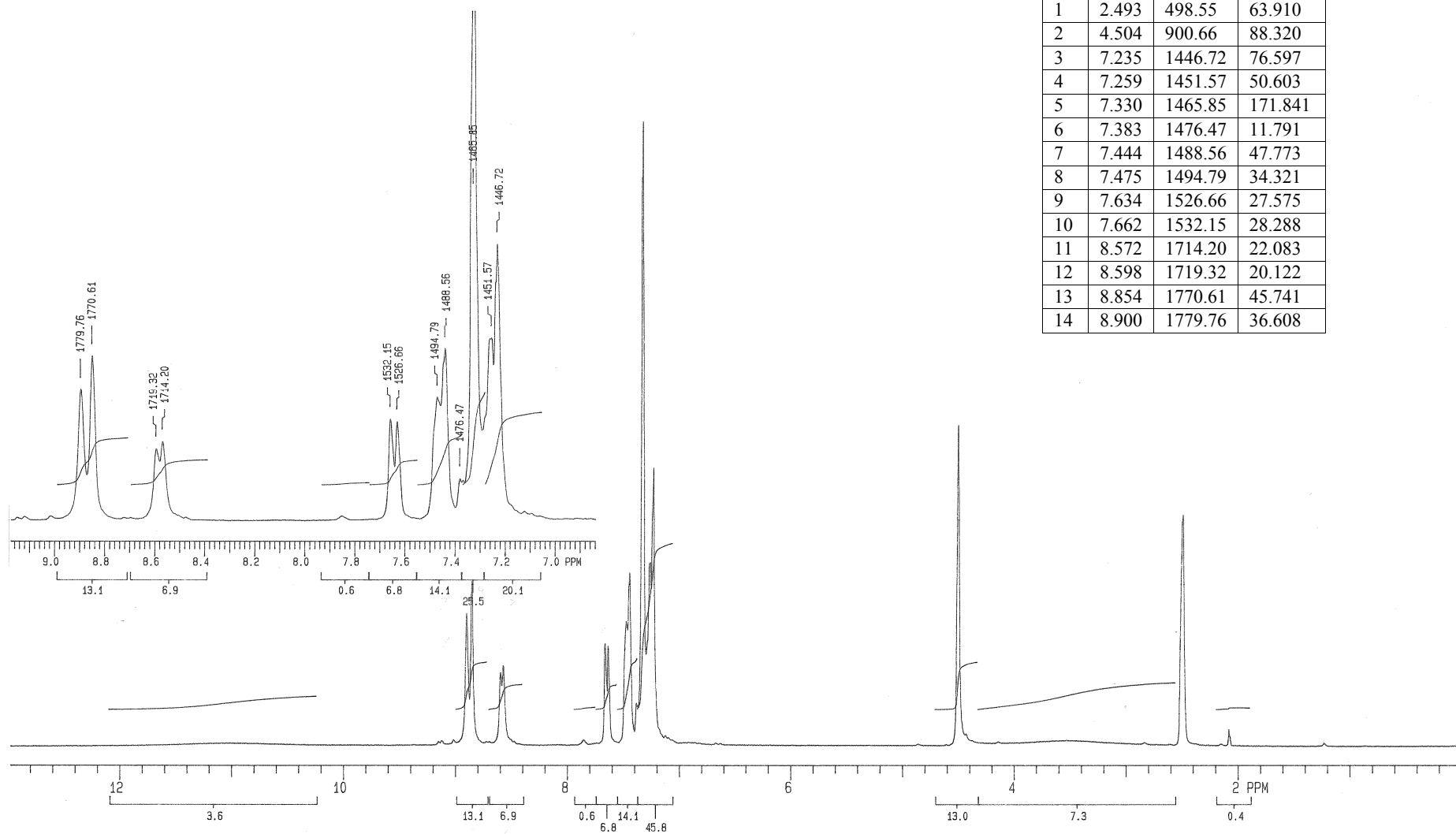
**Table S1.** Inhibition growth percent (IGP [%]) for tested compounds (**11**, **12**, **14–21**, **24–26**) against NCI-60 cancer cell lines at single concentration  $10^{-5}$  M, and anticancer *in vitro* data for compound **21** (right three columns: GI<sub>50</sub>, TGI and LC<sub>50</sub> [ $\mu$ M])<sup>a</sup>.

|                 | IGP [%] of Compound |    |    |    |    |    |    |    |    |     |    |    |    | GI <sub>50</sub> <sup>b</sup> | TGI <sup>c</sup> | LC <sub>50</sub> <sup>d</sup> |
|-----------------|---------------------|----|----|----|----|----|----|----|----|-----|----|----|----|-------------------------------|------------------|-------------------------------|
| Panel/Cell Line | 11                  | 12 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21  | 24 | 25 | 26 | 21                            |                  |                               |
| Leukemia        |                     |    |    |    |    |    |    |    |    |     |    |    |    |                               |                  |                               |
| CCRF-CEM        | 1                   | 4  | 27 | 30 | 7  | NT | 2  | 11 | *  | 85  | 27 | 19 | NT | 8.2                           | 43.6             | >100                          |
| HL-60(TB)       | 3                   | 17 | NT | 26 | NT | *  | 4  | 9  | 8  | 120 | 19 | 22 | *  | 24                            | 69.7             | >100                          |
| K-562           | 6                   | 67 | NT | 45 | NT | 7  | 12 | 70 | 20 | 95  | 42 | 72 | *  | 3                             | >100             | >100                          |
| MOLT-4          | 7                   | 21 | NT | 27 | NT | 6  | 5  | 18 | 9  | 85  | 9  | 20 | 8  | 19.9                          | 68.1             | >100                          |
| RPMI-8226       | *                   | *  | NT | 70 | NT | *  | 1  | 7  | *  | 93  | 72 | 10 | *  | 14.7                          | 54.2             | >100                          |
| SR              | NT                  | 15 | NT | 16 | NT | 12 | NT | NT | NT | 95  | 1  | 29 | 19 | 11.8                          | 51.6             | >100                          |
| NSCLC           |                     |    |    |    |    |    |    |    |    |     |    |    |    |                               |                  |                               |
| A-549/ATCC      | *                   | 16 | 13 | 16 | 2  | *  | 2  | 14 | 0  | 94  | NT | 17 | *  | 14.7                          | 62.8             | >100                          |
| EKVX            | NT                  | NT | 11 | NT | 6  | NT | NT | NT | NT | NT  | NT | *  | NT | NT                            | NT               | NT                            |
| HOP-62          | *                   | *  | 6  | 10 | 10 | *  | 1  | 1  | *  | 82  | 7  | *  | *  | 18.8                          | 43.5             | >100                          |
| HOP-92          | *                   | *  | NT | 53 | NT | *  | *  | 2  | *  | 131 | 28 | *  | NT | NT                            | NT               | NT                            |
| NCI-H226        | 4                   | *  | *  | 13 | *  | *  | 4  | 1  | 10 | 84  | 6  | *  | *  | 13.4                          | 57.9             | >100                          |
| NCI-H23         | *                   | *  | *  | 8  | *  | *  | *  | *  | *  | 98  | 6  | 5  | *  | 19.9                          | 51.9             | >100                          |
| NCI-H322M       | 5                   | 14 | 2  | 8  | 6  | 11 | 2  | 8  | 2  | 123 | 0  | 1  | *  | 18.3                          | >100             | >100                          |
| NCI-H460        | *                   | 3  | 10 | 17 | *  | *  | *  | 2  | *  | 93  | 17 | 5  | *  | 17.2                          | 69.4             | >100                          |
| NCI-H522        | 7                   | 25 | *  | 43 | *  | 8  | 9  | 19 | 5  | 110 | 28 | 12 | 8  | 14.1                          | 49.4             | >100                          |
| Colon cancer    |                     |    |    |    |    |    |    |    |    |     |    |    |    |                               |                  |                               |
| COLO 205        | *                   | *  | *  | 15 | *  | *  | *  | *  | *  | 157 | 16 | *  | *  | 16.8                          | 33               | 65.0                          |
| HCC-2998        | 11                  | 1  | *  | 1  | *  | *  | 11 | 9  | 2  | 73  | *  | 2  | *  | 15.5                          | 31.6             | 64.3                          |
| HCT-116         | 1                   | 9  | 27 | 21 | 17 | *  | *  | 17 | 6  | 92  | 21 | 19 | *  | 15.1                          | 34.4             | 78.2                          |
| HCT-15          | *                   | 39 | 37 | *  | 31 | 9  | *  | 28 | *  | 41  | *  | 53 | 4  | 6.4                           | 68.3             | >100                          |
| HT29            | *                   | 8  | *  | 32 | *  | *  | *  | 7  | *  | 104 | 19 | 8  | *  | 15.9                          | 45.7             | >100                          |
| KM12            | *                   | 43 | *  | 25 | 4  | 7  | NT | 24 | 14 | 89  | 27 | 49 | *  | 13                            | >100             | >100                          |
| SW-620          | *                   | 24 | 30 | 10 | 21 | *  | *  | 30 | *  | 82  | 12 | 40 | *  | 14.4                          | >100             | >100                          |
| CNS cancer      |                     |    |    |    |    |    |    |    |    |     |    |    |    |                               |                  |                               |
| SF-268          | *                   | 18 | 3  | 1  | 6  | *  | *  | 19 | 6  | 71  | *  | 26 | *  | 23.6                          | >100             | >100                          |
| SF-295          | 11                  | 13 | 6  | 43 | 13 | 10 | *  | 10 | NT | 147 | 48 | *  | 1  | 12.2                          | 37.9             | >100                          |
| SF-539          | *                   | 12 | *  | *  | 8  | 4  | 5  | 3  | 1  | 65  | 3  | 5  | *  | 13.1                          | 29               | 64.4                          |
| SNB-19          | *                   | 11 | *  | 14 | 0  | *  | 1  | *  | *  | 81  | 7  | 5  | 0  | 19.1                          | 57.6             | >100                          |
| SNB-75          | 16                  | 8  | 12 | 11 | 8  | NT | 24 | 14 | 22 | 81  | 5  | 12 | NT | 25.6                          | 72.1             | >100                          |
| U251            | 4                   | 4  | 11 | 34 | 7  | *  | 7  | 10 | 3  | 93  | NT | 2  | *  | 13                            | 36.5             | >100                          |
| Melanoma        |                     |    |    |    |    |    |    |    |    |     |    |    |    |                               |                  |                               |
| LOX IMVI        | 7                   | NT | 59 | 10 | 56 | NT | 3  | 47 | 4  | 96  | 10 | 59 | NT | NT                            | NT               | NT                            |
| MALME-3M        | 9                   | 1  | *  | 58 | *  | 3  | 6  | 6  | 5  | 101 | 44 | 2  | *  | 20.3                          | 61.9             | >100                          |
| M14             | *                   | 17 | 16 | 27 | 17 | *  | *  | 9  | 0  | 77  | 25 | 29 | *  | 8.9                           | 53.4             | >100                          |

Table S1. *Cont.*

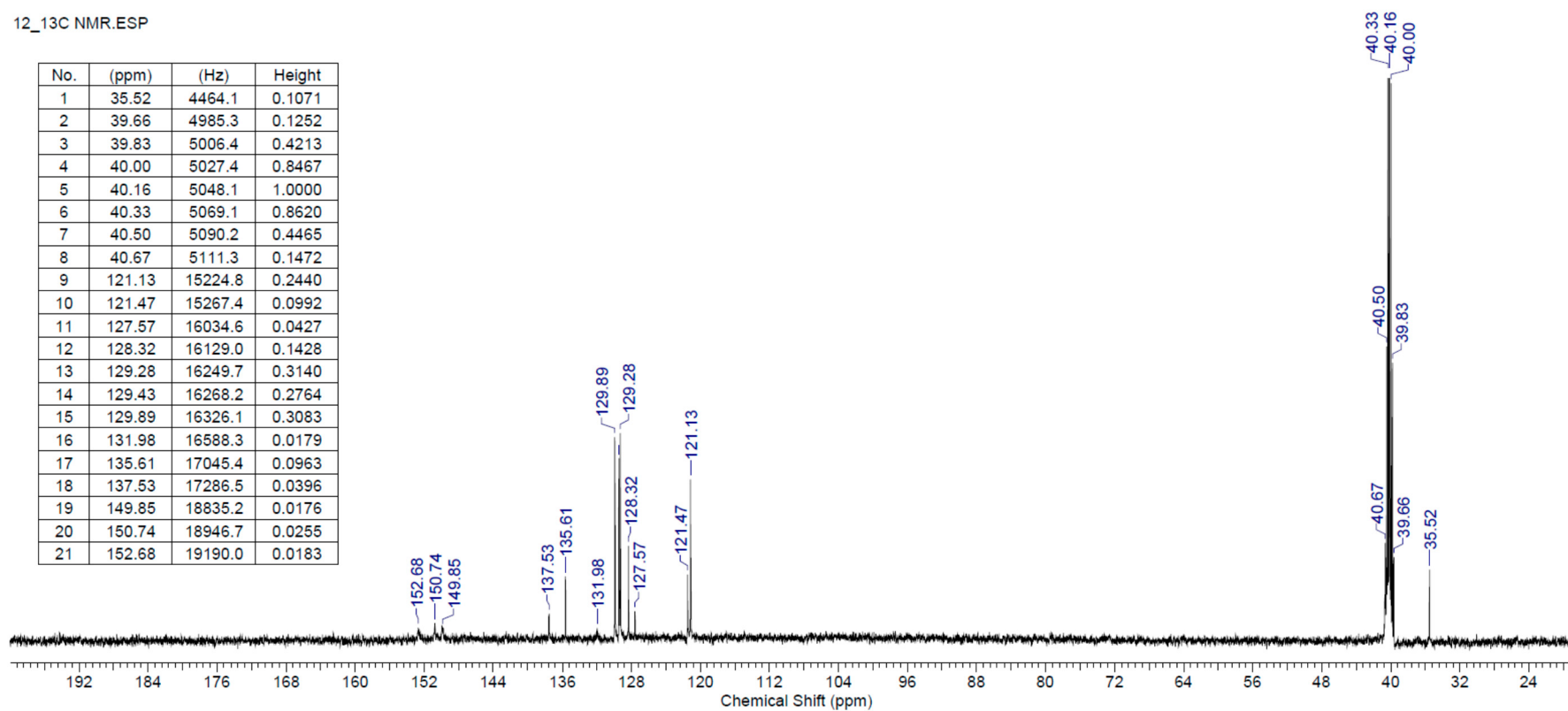
| Panel/Cell Line        | IGP [%] of Compound |    |    |    |    |    |    |    |    |     |    |    |    | GI <sub>50</sub> <sup>b</sup> | TGI <sup>c</sup> | LC <sub>50</sub> <sup>d</sup> |
|------------------------|---------------------|----|----|----|----|----|----|----|----|-----|----|----|----|-------------------------------|------------------|-------------------------------|
|                        | 11                  | 12 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21  | 24 | 25 | 26 | 21                            |                  |                               |
| MDA-MB-435             | *                   | 9  | 16 | 11 | 12 | *  | *  | *  | *  | 93  | 15 | 23 | *  | 18.9                          | >100             | >100                          |
| SK-MEL-2               | NT                  | 2  | *  | 14 | *  | *  | *  | *  | *  | 114 | 4  | *  | *  | NT                            | NT               | NT                            |
| SK-MEL-28              | *                   | 1  | *  | 15 | *  | *  | *  | *  | *  | 41  | 14 | *  | 4  | 20.7                          | 43.1             | 89.9                          |
| SK-MEL-5               | *                   | 21 | 15 | 31 | 15 | 4  | *  | 12 | 2  | 141 | 27 | 15 | 4  | 10.9                          | 36.7             | >100                          |
| UACC-257               | *                   | *  | 3  | 20 | *  | *  | 2  | 3  | *  | 122 | NT | 2  | *  | 23.1                          | 79.8             | >100                          |
| UACC-62                | *                   | 57 | 51 | 33 | 38 | *  | *  | 32 | *  | 73  | 31 | 42 | 10 | 1.5                           | 15.5             | >100                          |
| <i>Ovarian cancer</i>  |                     |    |    |    |    |    |    |    |    |     |    |    |    |                               |                  |                               |
| IGROV1                 | 2                   | 16 | *  | 13 | *  | 8  | *  | 7  | *  | 104 | 11 | 1  | *  | 16.3                          | 68.1             | >100                          |
| OVCAR-3                | *                   | *  | *  | 42 | *  | *  | *  | *  | *  | 75  | 50 | *  | *  | 16.6                          | 36.7             | 81.1                          |
| OVCAR-4                | *                   | *  | 9  | 27 | *  | *  | 1  | *  | *  | 82  | 17 | *  | *  | 22.5                          | 90.8             | >100                          |
| OVCAR-5                | *                   | 29 | 21 | 2  | 10 | 1  | *  | *  | *  | 69  | 3  | 29 | *  | 26.4                          | >100             | >100                          |
| OVCAR-8                | 2                   | 3  | *  | 29 | *  | *  | 4  | *  | 1  | 89  | NT | 5  | *  | 18.6                          | >100             | >100                          |
| NCI/ADR-RES            | *                   | 10 | 12 | *  | 9  | *  | *  | 15 | *  | 31  | *  | 24 | *  | 18.4                          | >100             | >100                          |
| SK-OV-3                | 2                   | *  | 0  | 6  | 4  | *  | *  | *  | *  | 105 | *  | *  | 4  | 35.9                          | 97.2             | >100                          |
| <i>Renal cancer</i>    |                     |    |    |    |    |    |    |    |    |     |    |    |    |                               |                  |                               |
| 786-0                  | *                   | 2  | 1  | 6  | 2  | *  | 2  | 9  | 4  | 76  | 3  | 12 | *  | 16.1                          | 43.7             | >100                          |
| A498                   | 15                  | 19 | 33 | 4  | 42 | 5  | 17 | 13 | 12 | 80  | 7  | 6  | 0  | 15.2                          | 63.1             | >100                          |
| ACHN                   | *                   | 31 | 22 | 25 | 21 | *  | *  | 24 | *  | 93  | 26 | 25 | *  | 11.6                          | >100             | >100                          |
| CAKI-1                 | 2                   | 33 | 29 | *  | 28 | 11 | *  | 23 | *  | 65  | 5  | 17 | 2  | 6.3                           | >100             | >100                          |
| RXF-393                | *                   | *  | *  | 1  | *  | *  | *  | *  | *  | 62  | *  | *  | *  | 20.6                          | 55.1             | >100                          |
| SN12C                  | *                   | 15 | 1  | 21 | 3  | *  | *  | *  | 1  | 92  | 19 | *  | *  | 18.4                          | >100             | >100                          |
| TK-10                  | 9                   | 4  | *  | 13 | *  | *  | 6  | 7  | 8  | 72  | 0  | 2  | *  | 33.1                          | >100             | >100                          |
| UO-31                  | 12                  | 18 | 17 | 27 | 19 | 9  | 5  | 21 | 10 | 110 | 20 | 29 | 16 | 9.8                           | 27.3             | 75.0                          |
| <i>Prostate cancer</i> |                     |    |    |    |    |    |    |    |    |     |    |    |    |                               |                  |                               |
| PC-3                   | 11                  | 6  | 14 | 54 | 17 | *  | 6  | 21 | 16 | 101 | 51 | 12 | *  | 14.4                          | 71.1             | >100                          |
| DU-145                 | *                   | 16 | 5  | *  | 7  | *  | *  | 18 | *  | 67  | 1  | 32 | *  | 17.3                          | 55.7             | >100                          |
| <i>Breast cancer</i>   |                     |    |    |    |    |    |    |    |    |     |    |    |    |                               |                  |                               |
| MCF7                   | 3                   | 5  | 5  | 28 | 5  | 3  | 5  | 7  | 9  | 88  | 18 | *  | 6  | 19.7                          | 97.4             | >100                          |
| MDA-MB-231/ATCC        | *                   | 9  | 1  | *  | 3  | *  | 6  | *  | *  | 100 | *  | *  | *  | 14.6                          | 63.3             | >100                          |
| HS578T                 | *                   | 2  | 9  | NT | *  | 1  | *  | *  | *  | 64  | 12 | 6  | *  | 24                            | 98.1             | >100                          |
| BT-549                 | *                   | 16 | 16 | 2  | 14 | *  | 8  | 12 | 6  | 85  | 4  | 23 | *  | 16.1                          | 44.7             | >100                          |
| T-47D                  | 2                   | 20 | 21 | 33 | 17 | 6  | 10 | 27 | 9  | 92  | 26 | 18 | 7  | 13.9                          | 87.6             | >100                          |
| MDA-MB-468             | *                   | 7  | NT | 59 | NT | 3  | *  | *  | *  | 109 | 57 | *  | *  | 18.9                          | >100             | >100                          |

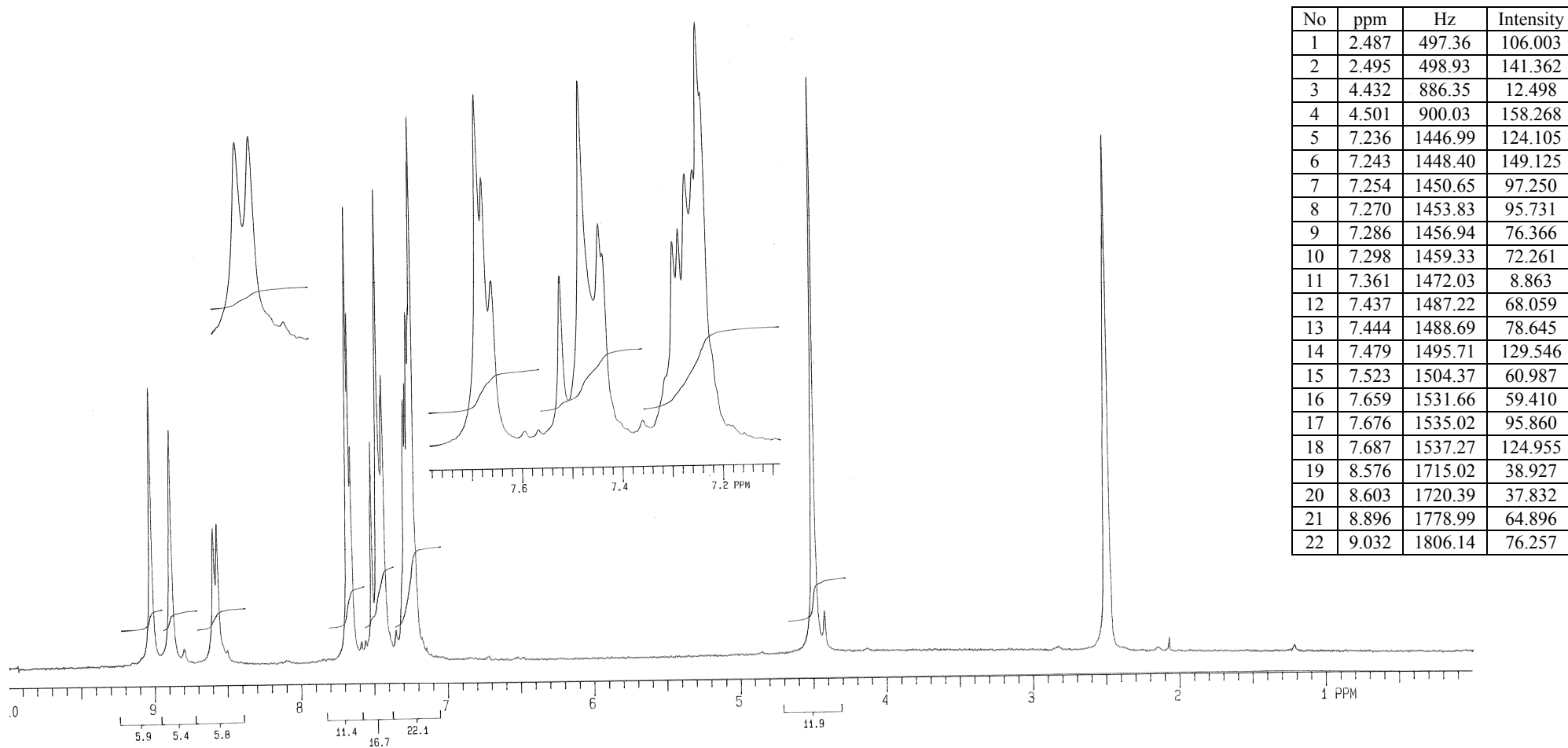
<sup>a</sup> Data obtained from NCI-60 DTP human tumor cell line screening [1–5]; <sup>b</sup> GI<sub>50</sub>: molar concentration that inhibits 50% net cell growth; <sup>c</sup> TGI: molar concentration giving total growth inhibition; <sup>d</sup> LC<sub>50</sub>: molar concentration causing 50% net cell death; NT – not tested; \* IGP ≤ 0%.



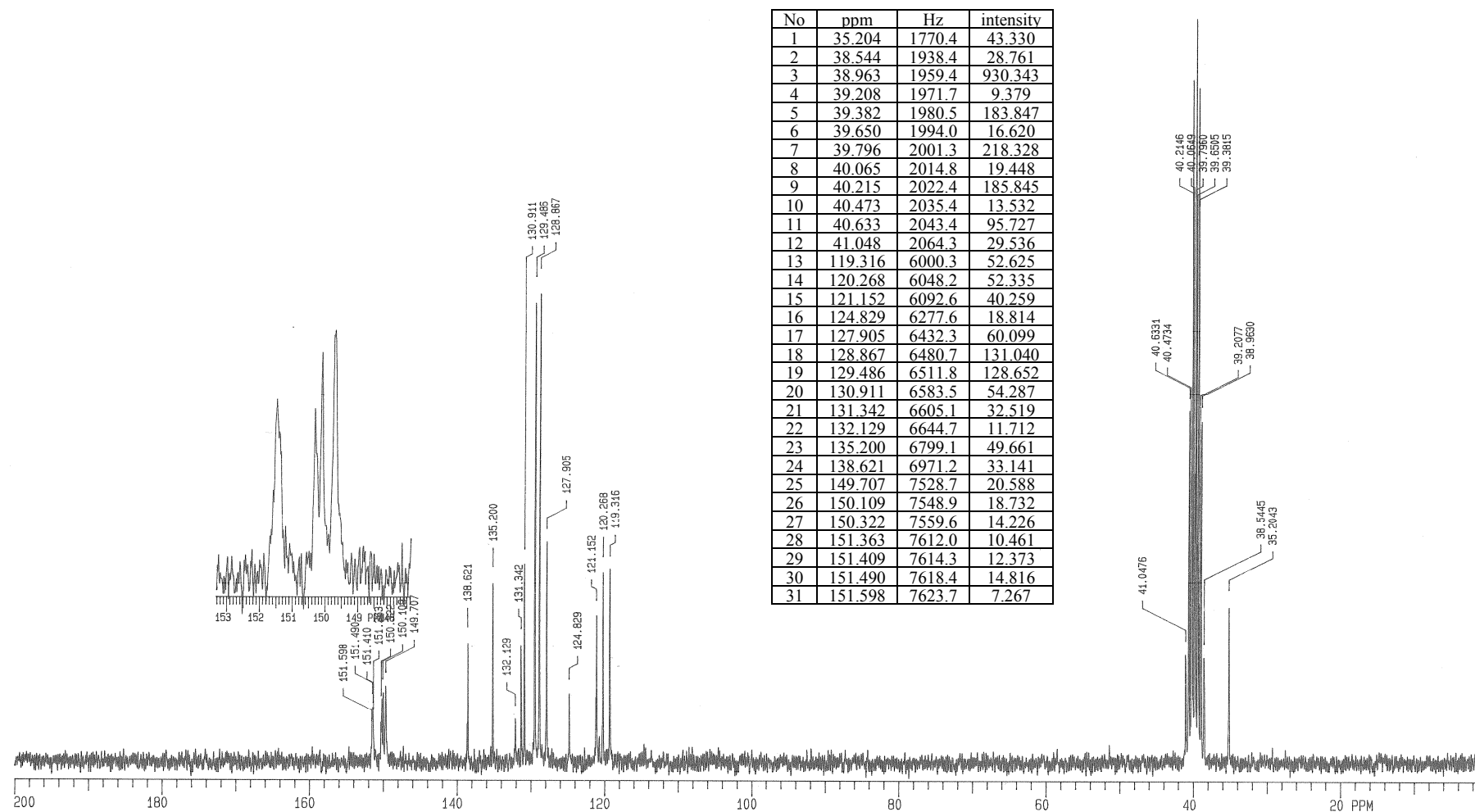
**Spectrum S1.**  $^1\text{H}$ -NMR of compound **12** (200 MHz,  $\text{DMSO}-d_6$ ).

12\_13C NMR.ESP

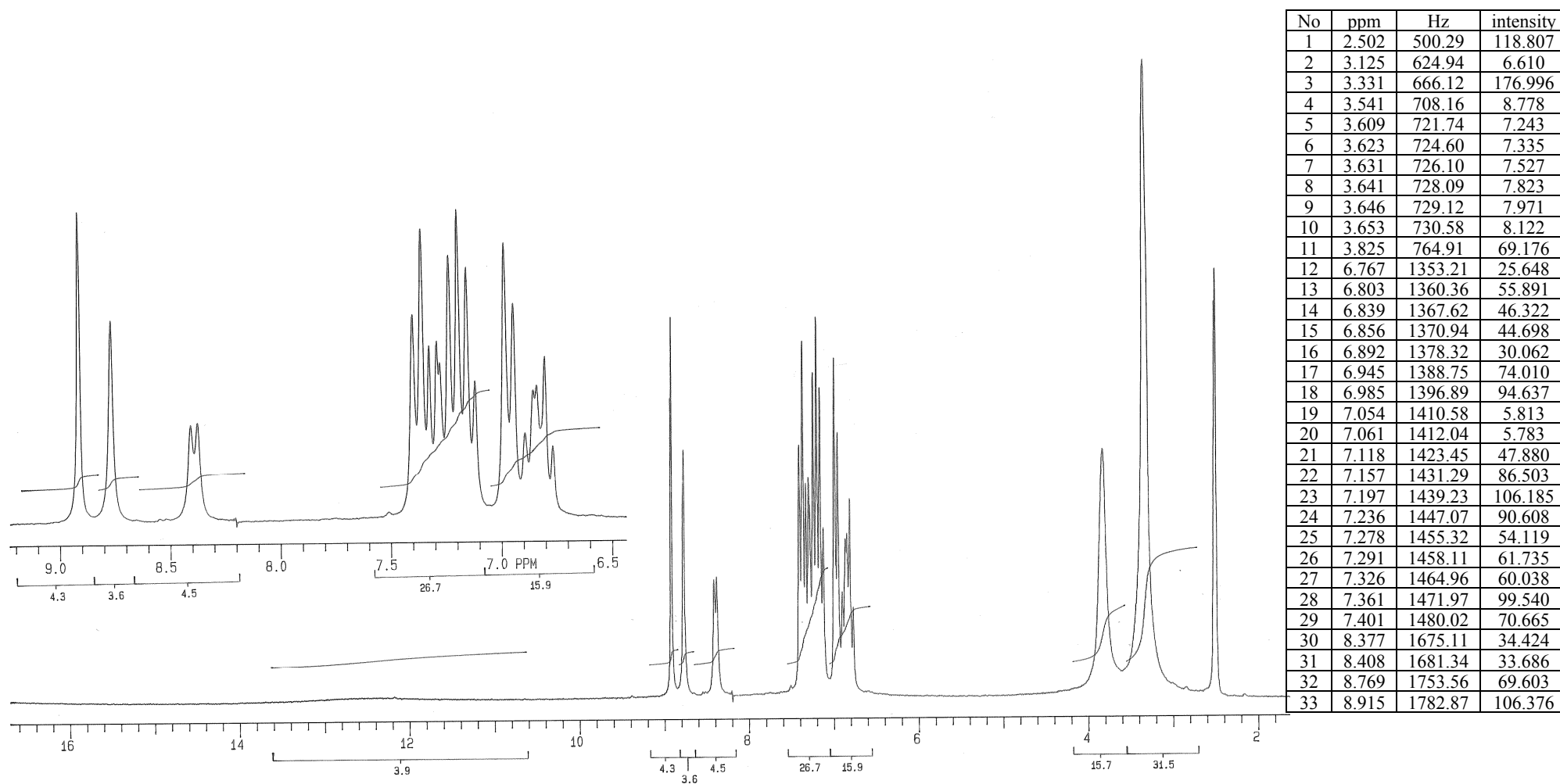
Spectrum S2.  $^{13}\text{C}$ -NMR of compound **12** (125 MHz,  $\text{DMSO-}d_6$ ).



**Spectrum S3.**  $^1\text{H}$ -NMR of compound **13** (200 MHz,  $\text{DMSO}-d_6$ ).

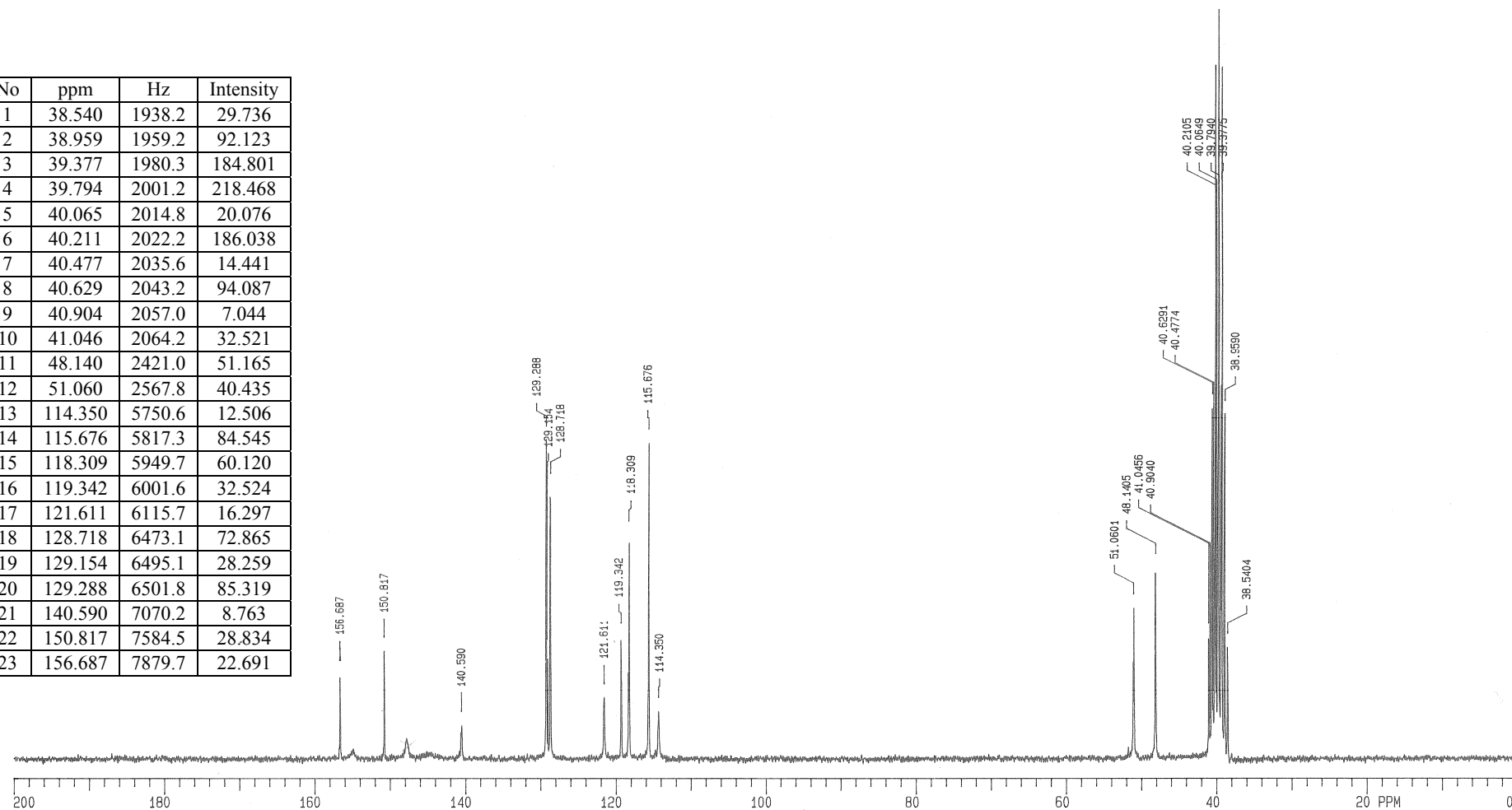


**Spectrum S4.**  $^{13}\text{C}$ -NMR of compound **13** (50 MHz,  $\text{DMSO}-d_6$ ).

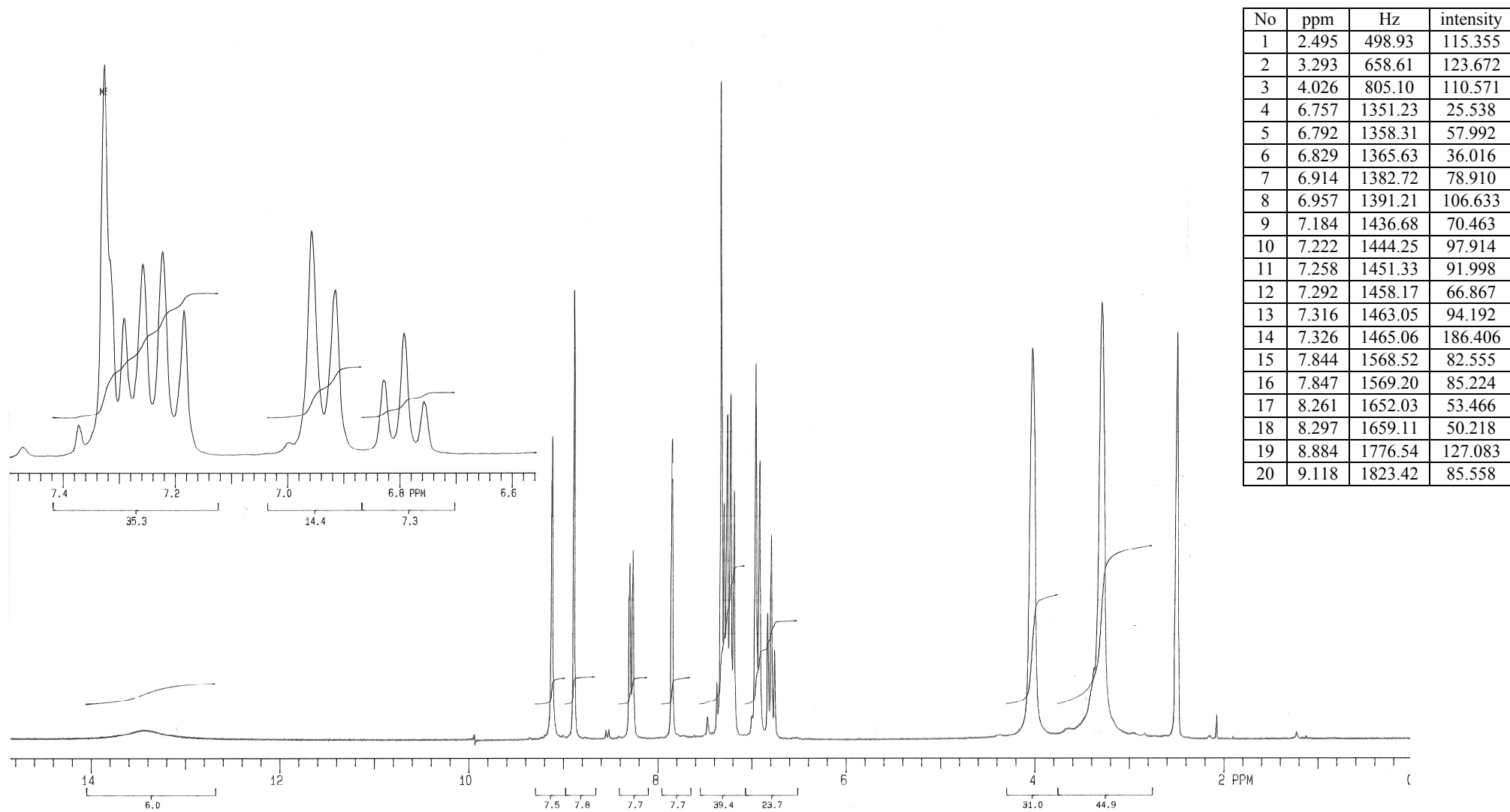


**Spectrum S5.**  $^1\text{H}$ -NMR of compound **15** (200 MHz,  $\text{DMSO}-d_6$ ).

| No | ppm     | Hz     | Intensity |
|----|---------|--------|-----------|
| 1  | 38.540  | 1938.2 | 29.736    |
| 2  | 38.959  | 1959.2 | 92.123    |
| 3  | 39.377  | 1980.3 | 184.801   |
| 4  | 39.794  | 2001.2 | 218.468   |
| 5  | 40.065  | 2014.8 | 20.076    |
| 6  | 40.211  | 2022.2 | 186.038   |
| 7  | 40.477  | 2035.6 | 14.441    |
| 8  | 40.629  | 2043.2 | 94.087    |
| 9  | 40.904  | 2057.0 | 7.044     |
| 10 | 41.046  | 2064.2 | 32.521    |
| 11 | 48.140  | 2421.0 | 51.165    |
| 12 | 51.060  | 2567.8 | 40.435    |
| 13 | 114.350 | 5750.6 | 12.506    |
| 14 | 115.676 | 5817.3 | 84.545    |
| 15 | 118.309 | 5949.7 | 60.120    |
| 16 | 119.342 | 6001.6 | 32.524    |
| 17 | 121.611 | 6115.7 | 16.297    |
| 18 | 128.718 | 6473.1 | 72.865    |
| 19 | 129.154 | 6495.1 | 28.259    |
| 20 | 129.288 | 6501.8 | 85.319    |
| 21 | 140.590 | 7070.2 | 8.763     |
| 22 | 150.817 | 7584.5 | 28.834    |
| 23 | 156.687 | 7879.7 | 22.691    |

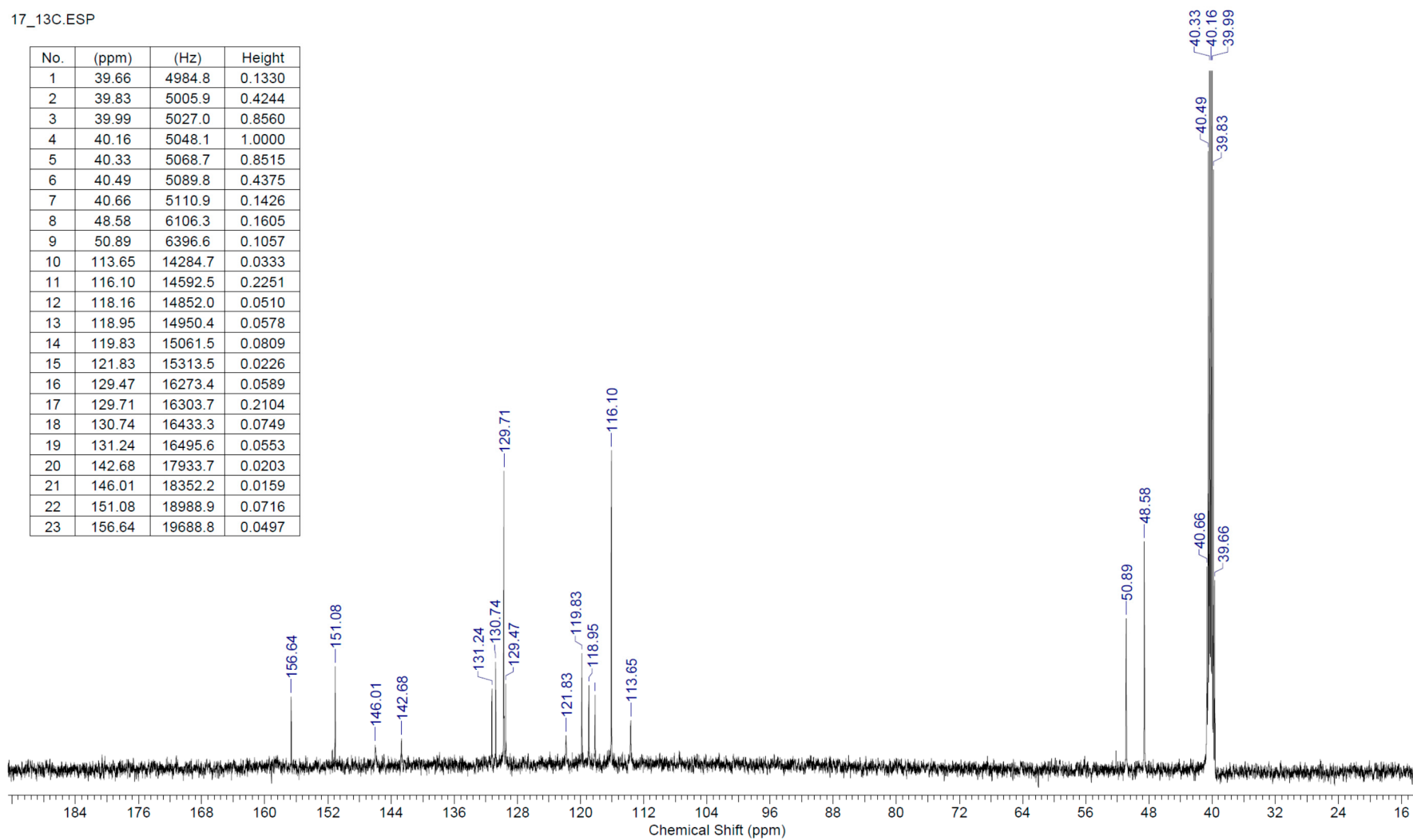


**Spectrum S6.**  $^{13}\text{C}$ -NMR of compound **15** (50 MHz,  $\text{DMSO}-d_6$ ).

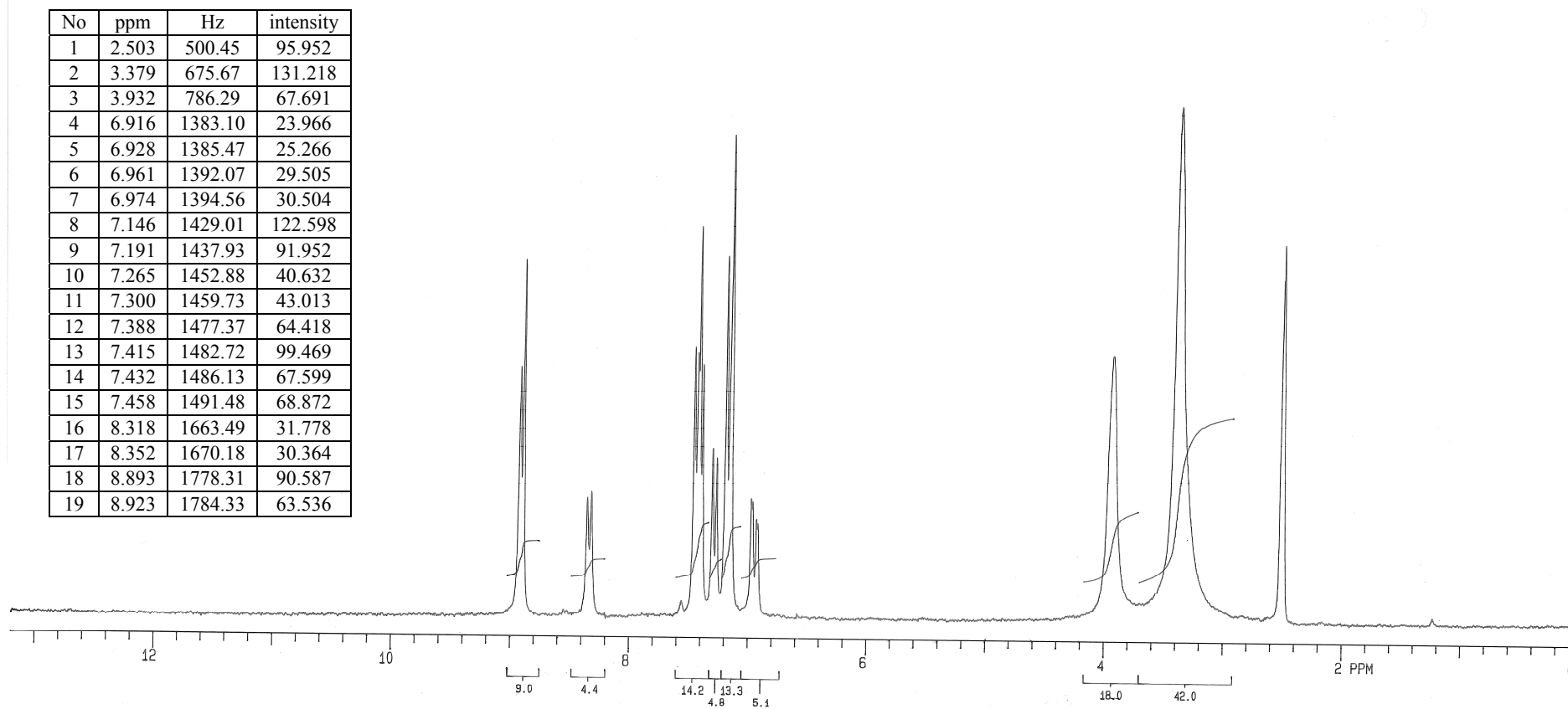


**Spectrum S7.**  $^1\text{H}$ -NMR of compound 17 (200 MHz,  $\text{DMSO}-d_6$ ).

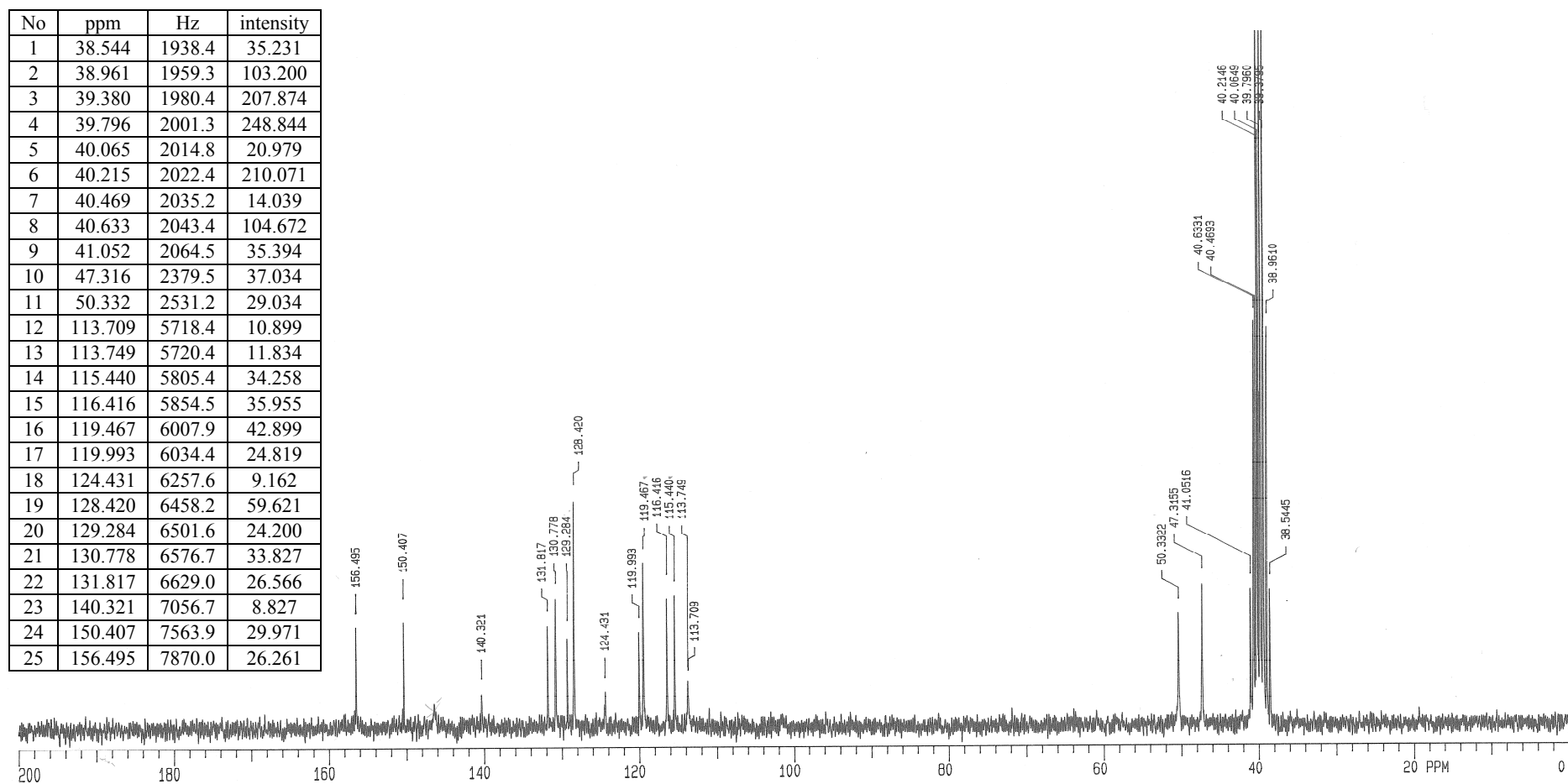
17\_13C.ESP



**Spectrum S8.**  $^{13}\text{C}$ -NMR of compound **17** (125 MHz,  $\text{DMSO-}d_6$ ).

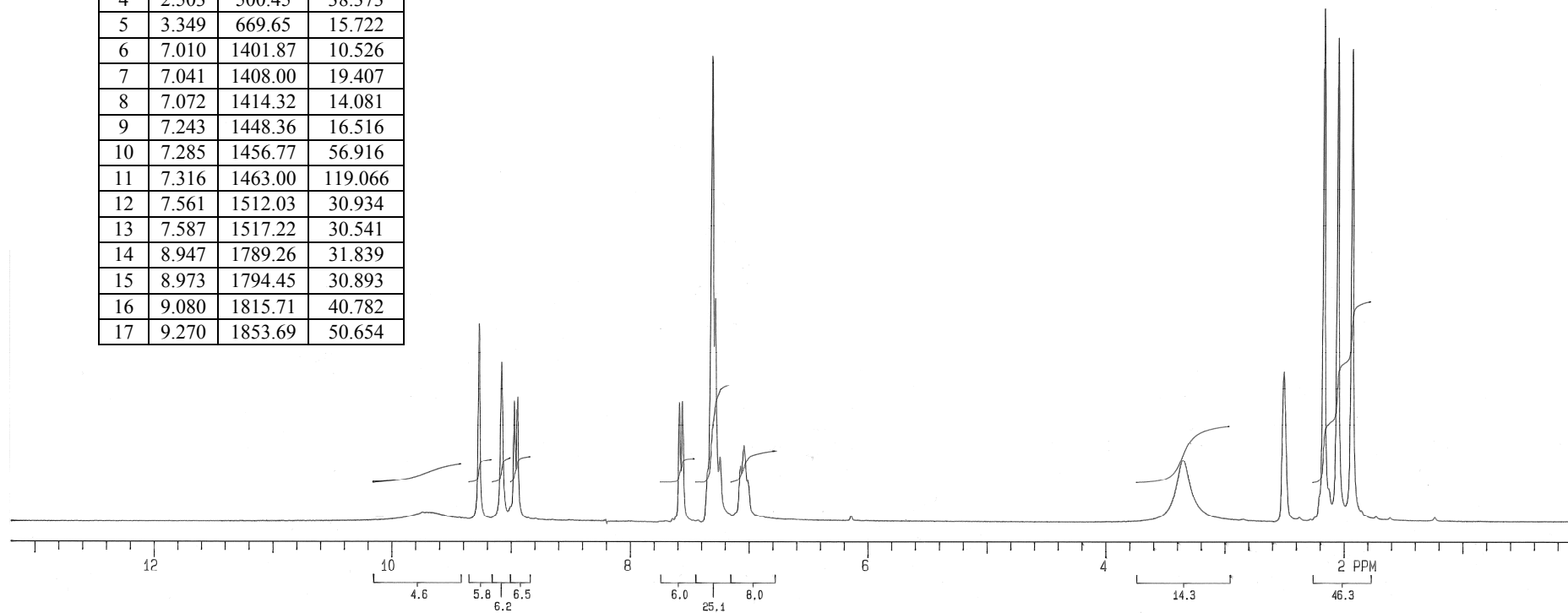


**Spectrum S9.**  $^1\text{H}$ -NMR of compound **21** (200 MHz,  $\text{DMSO}-d_6$ ).



**Spectrum S10.**  $^{13}\text{C}$ -NMR of compound **21** (50 MHz,  $\text{DMSO}-d_6$ ).

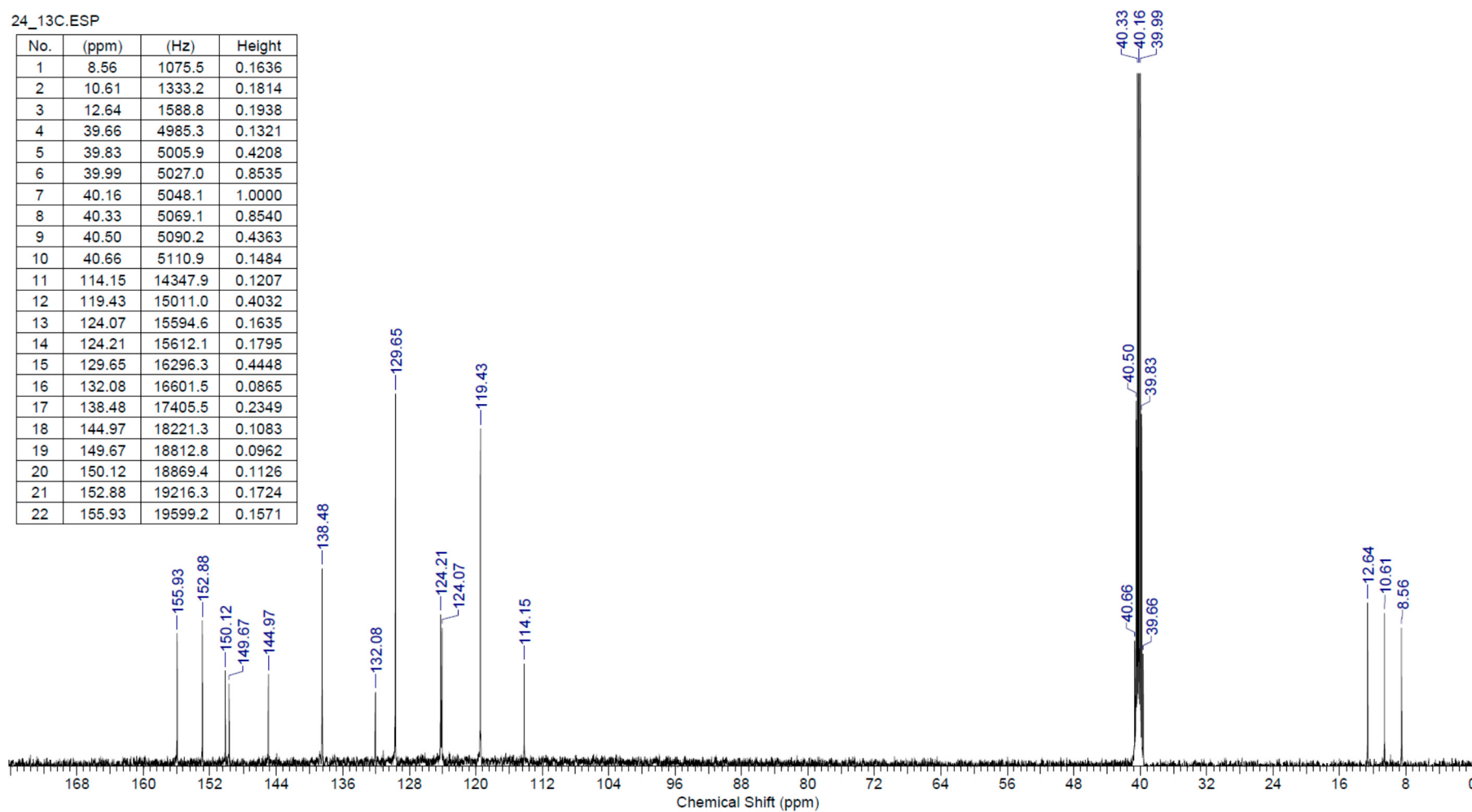
| No | ppm   | Hz      | Intensity |
|----|-------|---------|-----------|
| 1  | 1.931 | 386.10  | 120.803   |
| 2  | 2.052 | 410.38  | 123.727   |
| 3  | 2.168 | 433.63  | 131.093   |
| 4  | 2.503 | 500.45  | 38.373    |
| 5  | 3.349 | 669.65  | 15.722    |
| 6  | 7.010 | 1401.87 | 10.526    |
| 7  | 7.041 | 1408.00 | 19.407    |
| 8  | 7.072 | 1414.32 | 14.081    |
| 9  | 7.243 | 1448.36 | 16.516    |
| 10 | 7.285 | 1456.77 | 56.916    |
| 11 | 7.316 | 1463.00 | 119.066   |
| 12 | 7.561 | 1512.03 | 30.934    |
| 13 | 7.587 | 1517.22 | 30.541    |
| 14 | 8.947 | 1789.26 | 31.839    |
| 15 | 8.973 | 1794.45 | 30.893    |
| 16 | 9.080 | 1815.71 | 40.782    |
| 17 | 9.270 | 1853.69 | 50.654    |



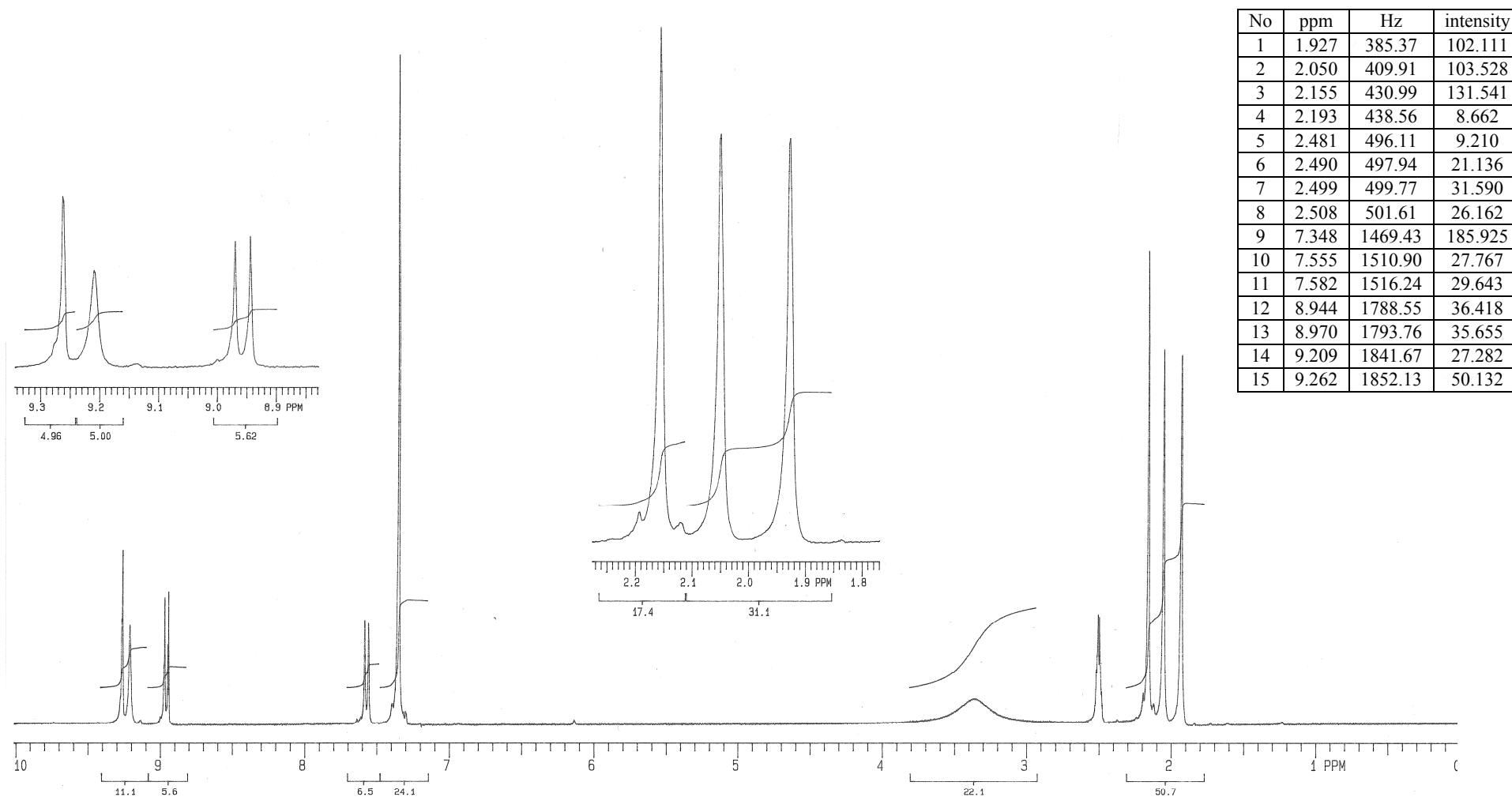
**Spectrum S11.** <sup>1</sup>H-NMR of compound **24** (200 MHz, DMSO-*d*<sub>6</sub>).

24\_13C.ESP

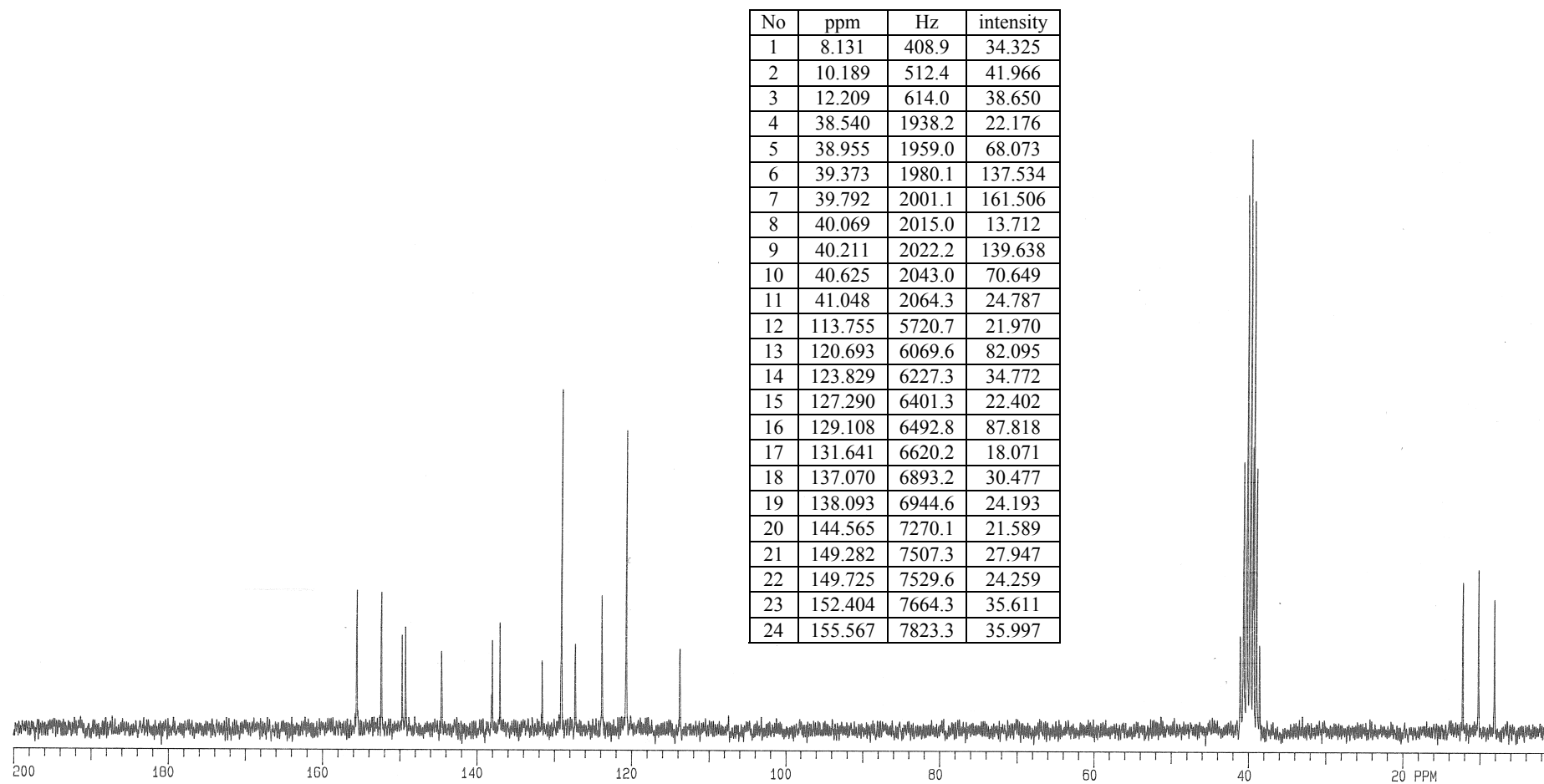
| No. | (ppm)  | (Hz)    | Height |
|-----|--------|---------|--------|
| 1   | 8.56   | 1075.5  | 0.1636 |
| 2   | 10.61  | 1333.2  | 0.1814 |
| 3   | 12.64  | 1588.8  | 0.1938 |
| 4   | 39.66  | 4985.3  | 0.1321 |
| 5   | 39.83  | 5005.9  | 0.4208 |
| 6   | 39.99  | 5027.0  | 0.8535 |
| 7   | 40.16  | 5048.1  | 1.0000 |
| 8   | 40.33  | 5069.1  | 0.8540 |
| 9   | 40.50  | 5090.2  | 0.4363 |
| 10  | 40.66  | 5110.9  | 0.1484 |
| 11  | 114.15 | 14347.9 | 0.1207 |
| 12  | 119.43 | 15011.0 | 0.4032 |
| 13  | 124.07 | 15594.6 | 0.1635 |
| 14  | 124.21 | 15612.1 | 0.1795 |
| 15  | 129.65 | 16296.3 | 0.4448 |
| 16  | 132.08 | 16601.5 | 0.0865 |
| 17  | 138.48 | 17405.5 | 0.2349 |
| 18  | 144.97 | 18221.3 | 0.1083 |
| 19  | 149.67 | 18812.8 | 0.0962 |
| 20  | 150.12 | 18869.4 | 0.1126 |
| 21  | 152.88 | 19216.3 | 0.1724 |
| 22  | 155.93 | 19599.2 | 0.1571 |



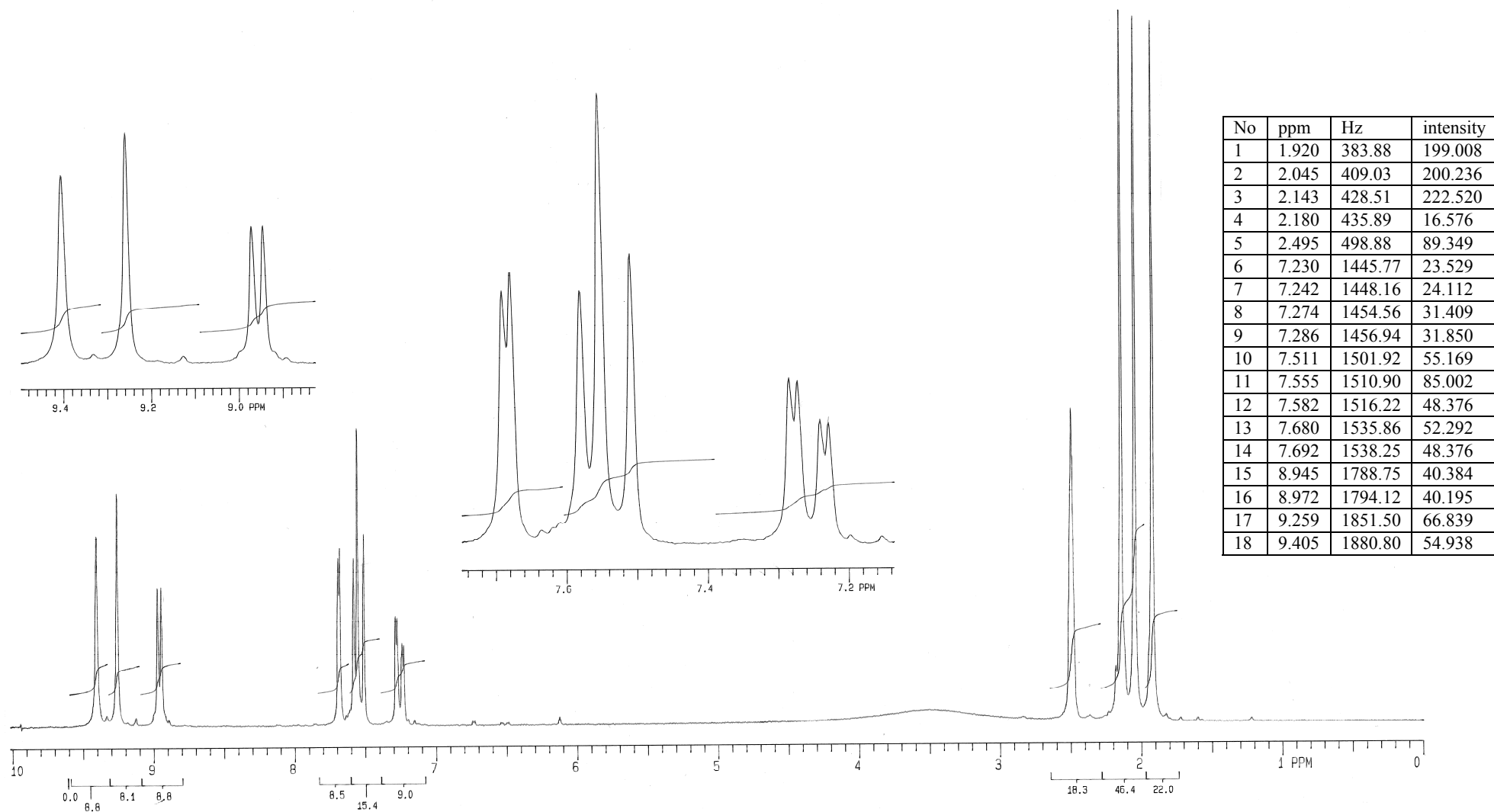
**Spectrum S12.**  $^{13}\text{C}$ -NMR of compound **24** (125 MHz,  $\text{DMSO-}d_6$ ).



**Spectrum S13.**  $^1\text{H}$ -NMR of compound **25** (200 MHz,  $\text{DMSO}-d_6$ ).

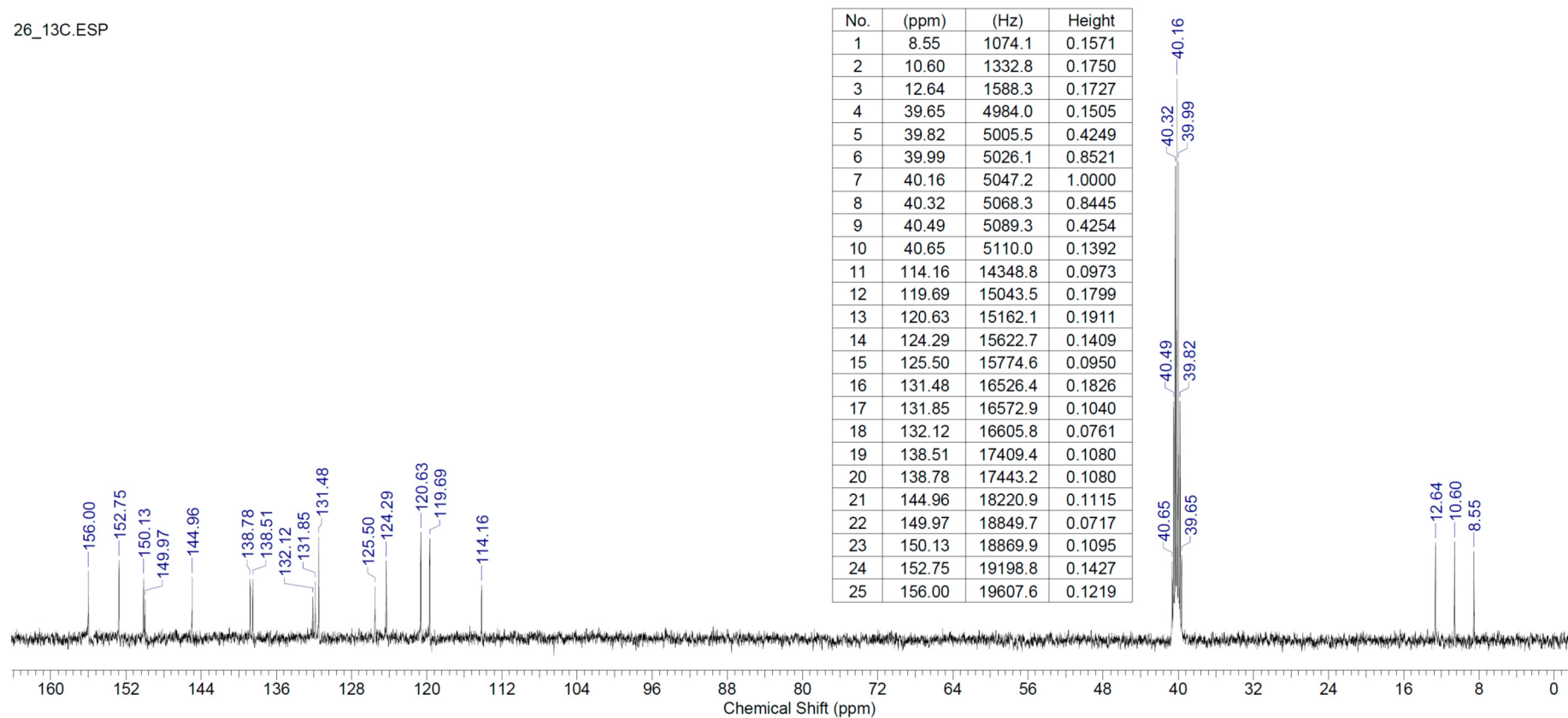


**Spectrum S14.**  $^{13}\text{C}$ -NMR of compound **25** (50 MHz,  $\text{DMSO}-d_6$ ).



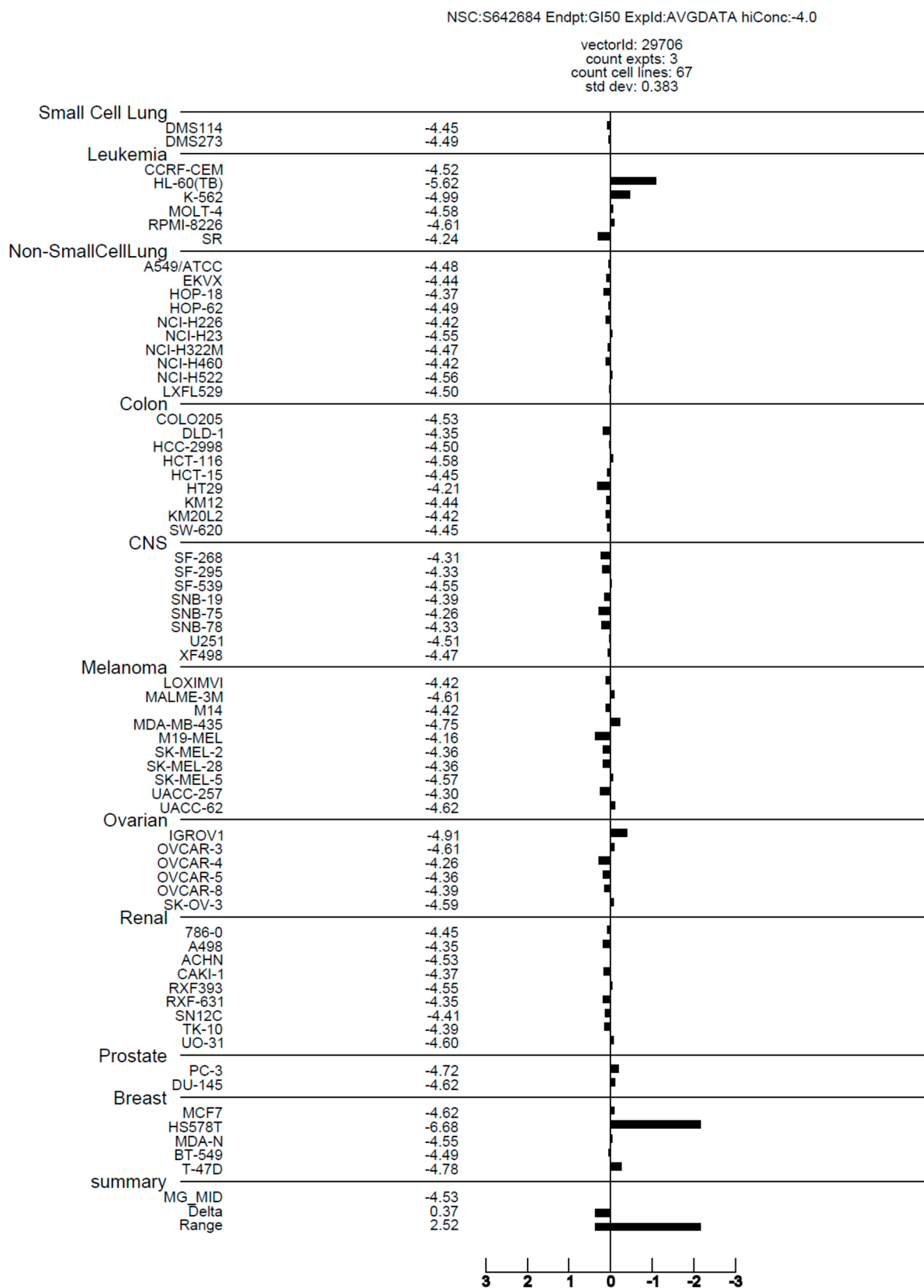
**Spectrum S15.**  $^1\text{H}$ -NMR of compound 26 (200 MHz,  $\text{DMSO}-d_6$ ).

26\_13C.ESP



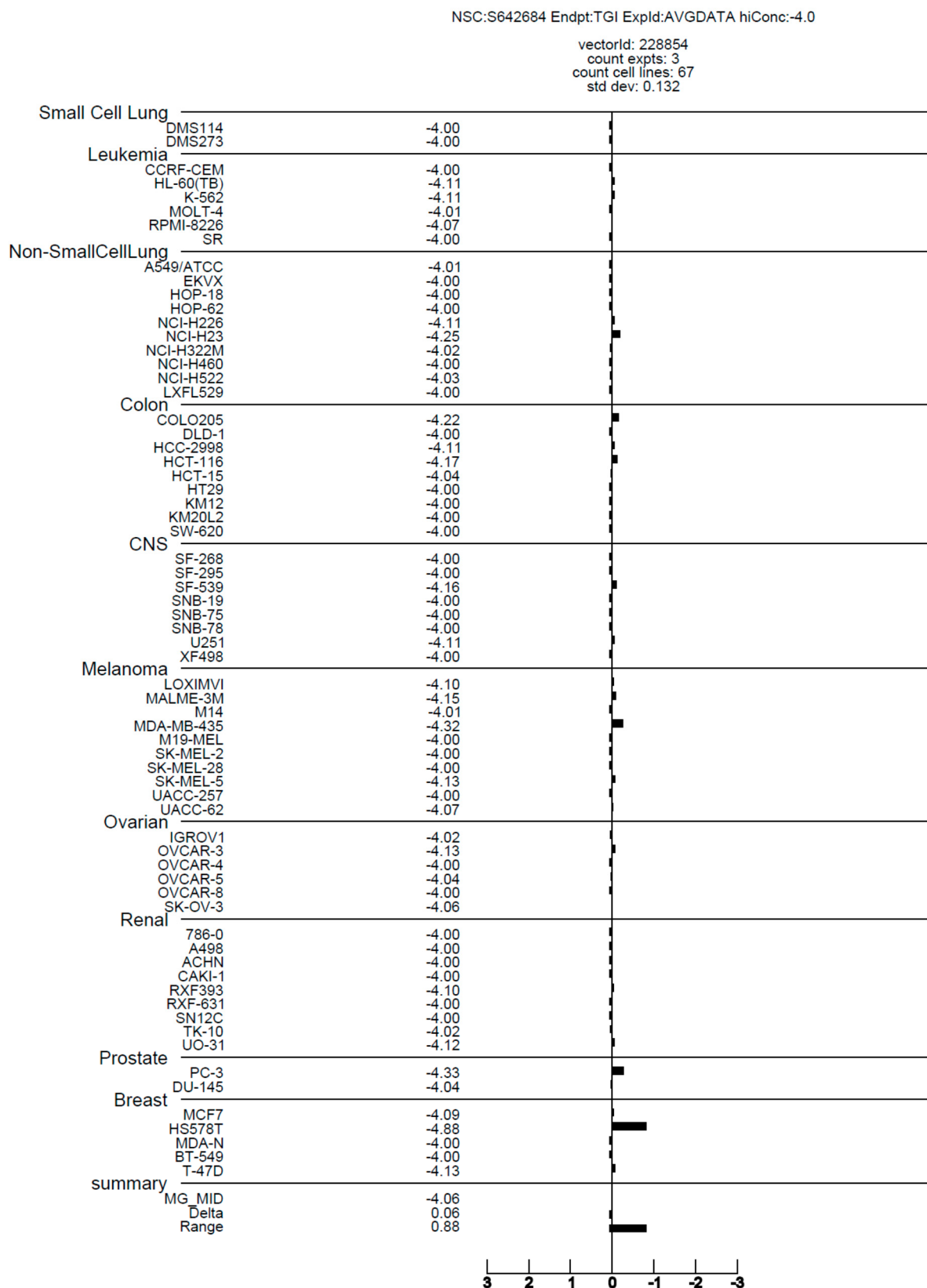
**Spectrum S16.**  $^{13}\text{C}$ -NMR of compound **26** (125 MHz,  $\text{DMSO-}d_6$ ).

Developmental Therapeutics Program Mean Graph  
Selected Data Vectors



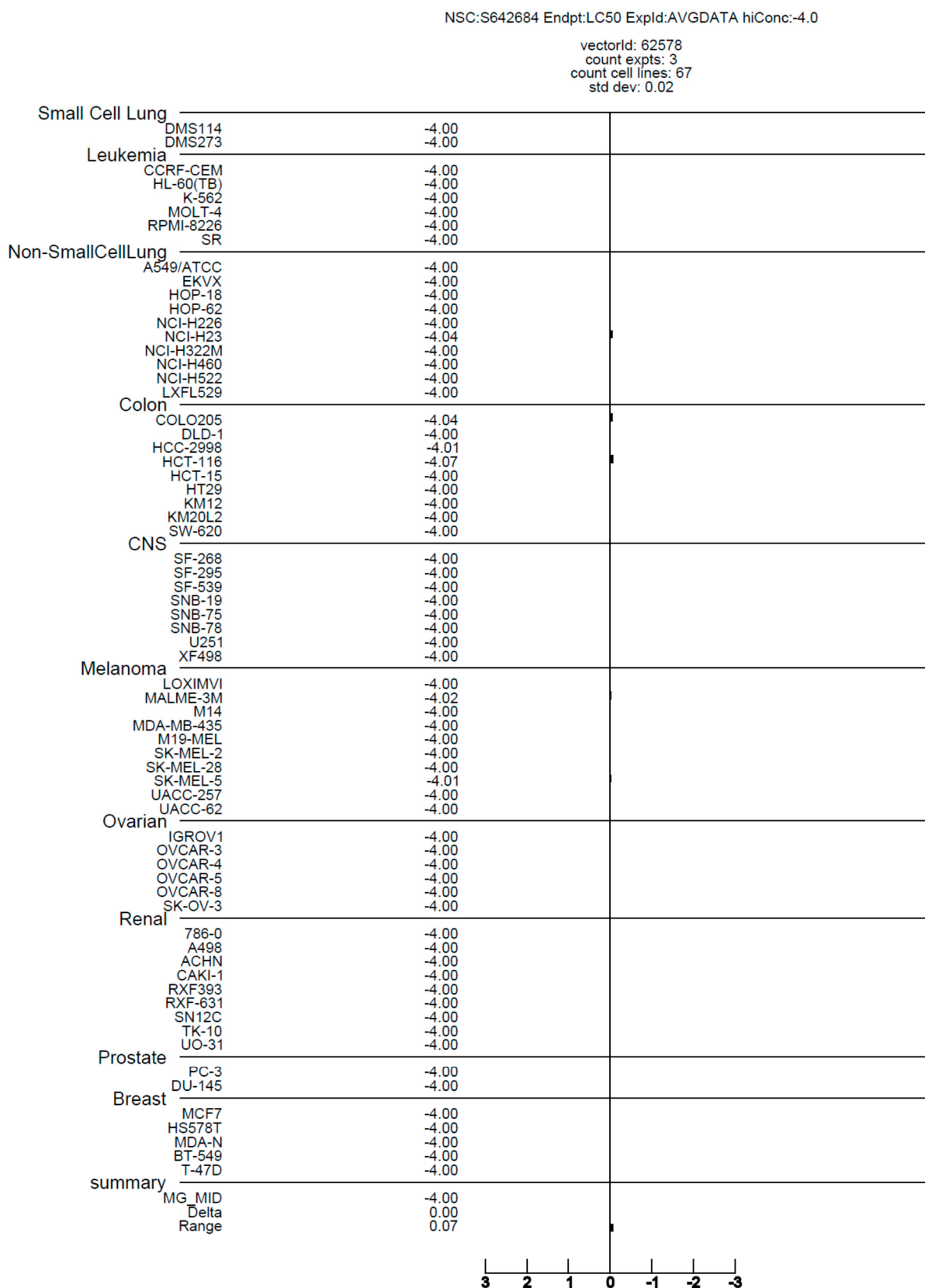
**Graph S1. NCI Cancer Screen Current Data—DTP 60 cell/5 dose for Sulofenur (NSC-642684)—GI<sub>50</sub> [log<sub>10</sub>(M)].**

Developmental Therapeutics Program Mean Graph  
Selected Data Vectors



**Graph S2. NCI Cancer Screen Current Data—DTP 60 cell/5 dose for Sulofenur (NSC-642684)—TGI [log10(M)].**

Developmental Therapeutics Program Mean Graph  
Selected Data Vectors



**Graph S3. NCI Cancer Screen Current Data**—DTP 60 cell/5 dose for Sulofenur (NSC-642684)—LC<sub>50</sub> [log<sub>10</sub>(M)].

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