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## Electronic Supplementary Information

# Oligostilbenes from *Vatica mangachapoi* with Xanthine Oxidase and Acetylcholinesterase Inhibitory Activities

**Yan Hua Qin, Jie Zhang, Jiang Tao Cui, Zhi Kai Guo, Nan Jiang, Ren Xiang Tan and Hui Ming Ge**

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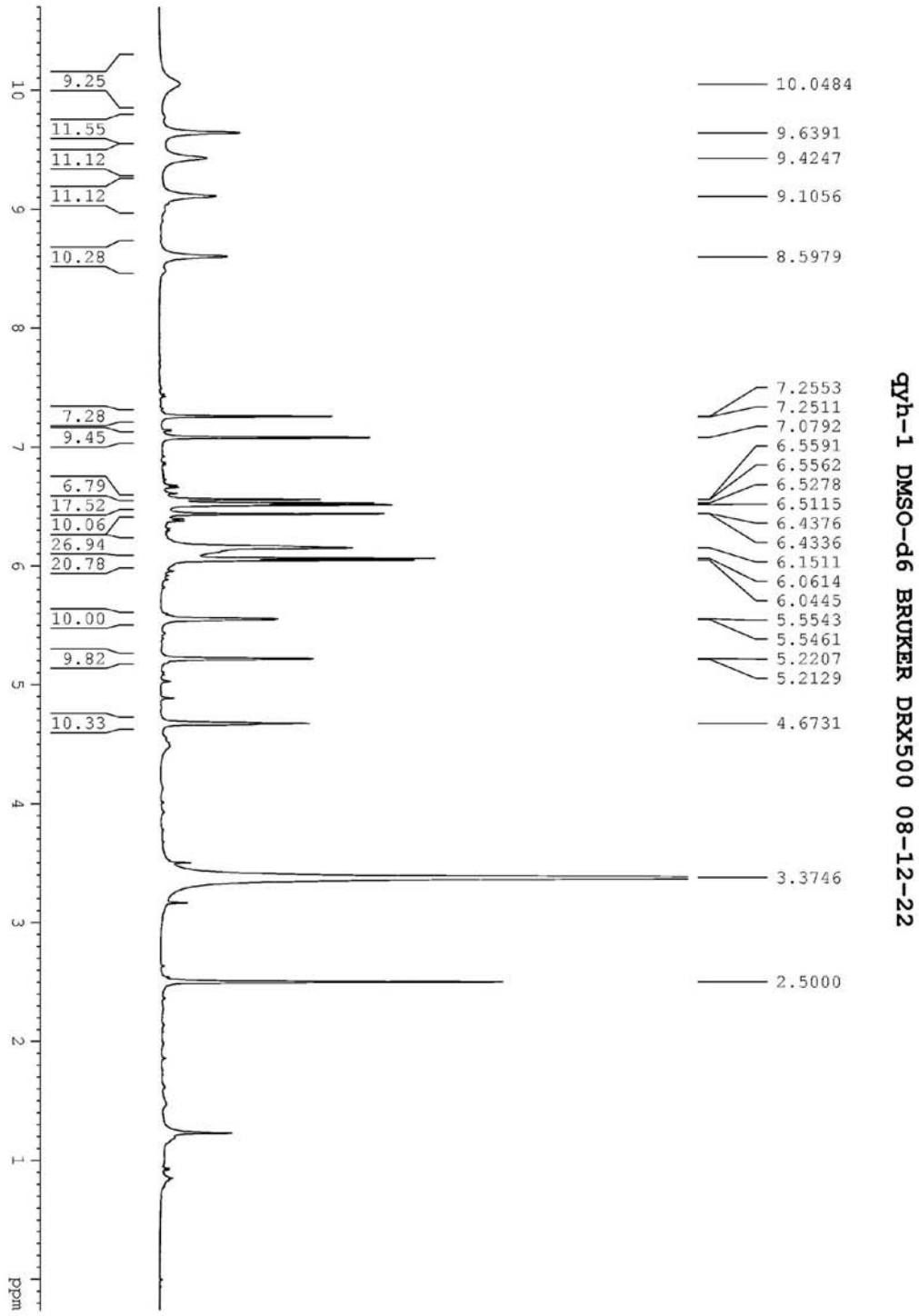


Figure S1 $^{1}$H-NMR spectrum of compound **1** (DMSO-$d_6$)

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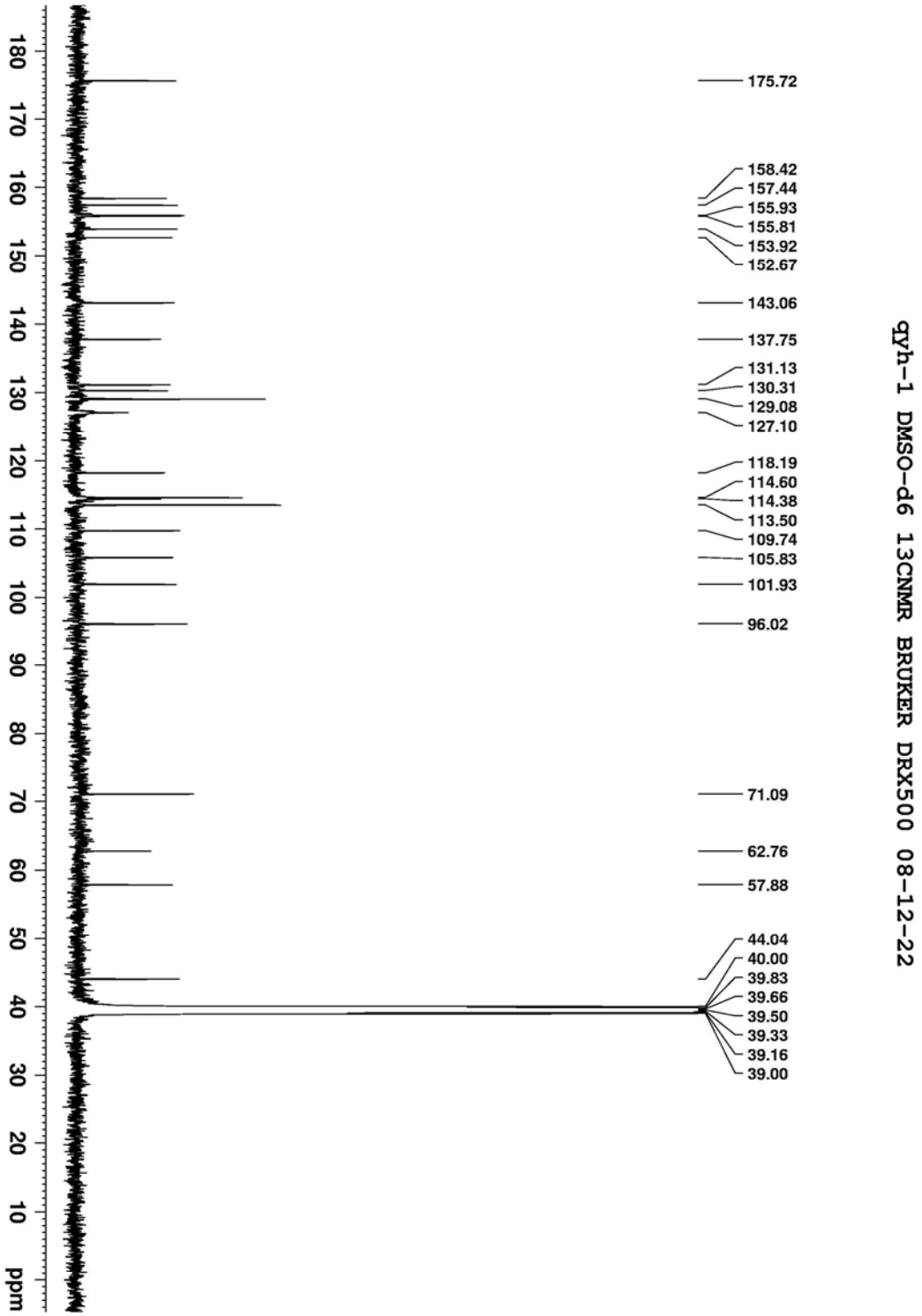


Figure S2 $^{13}$C-NMR spectrum of compound **1** (DMSO-$d_6$)

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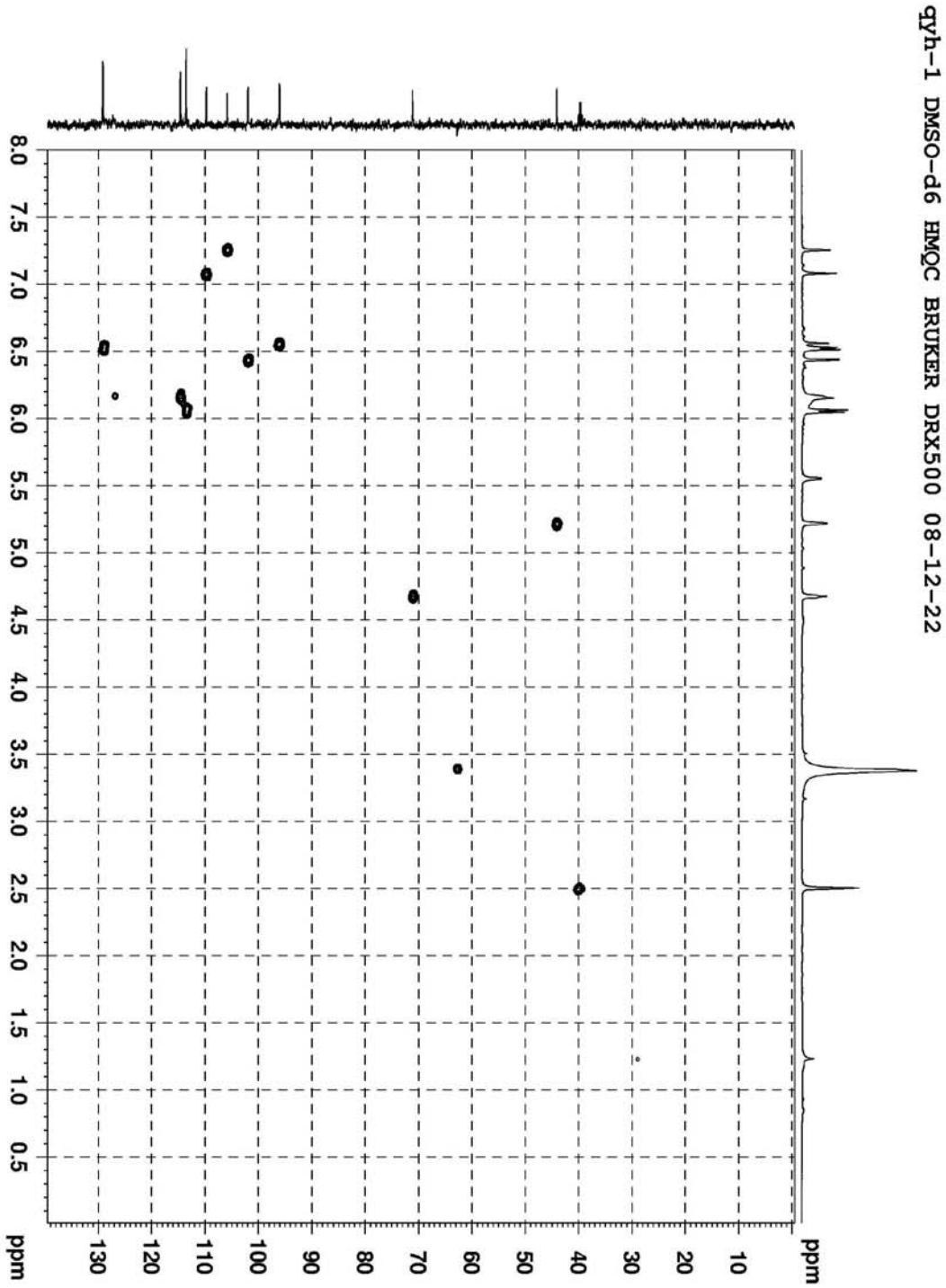


Figure S3 HMQC spectrum of compound **1** (DMSO-$d_6$)

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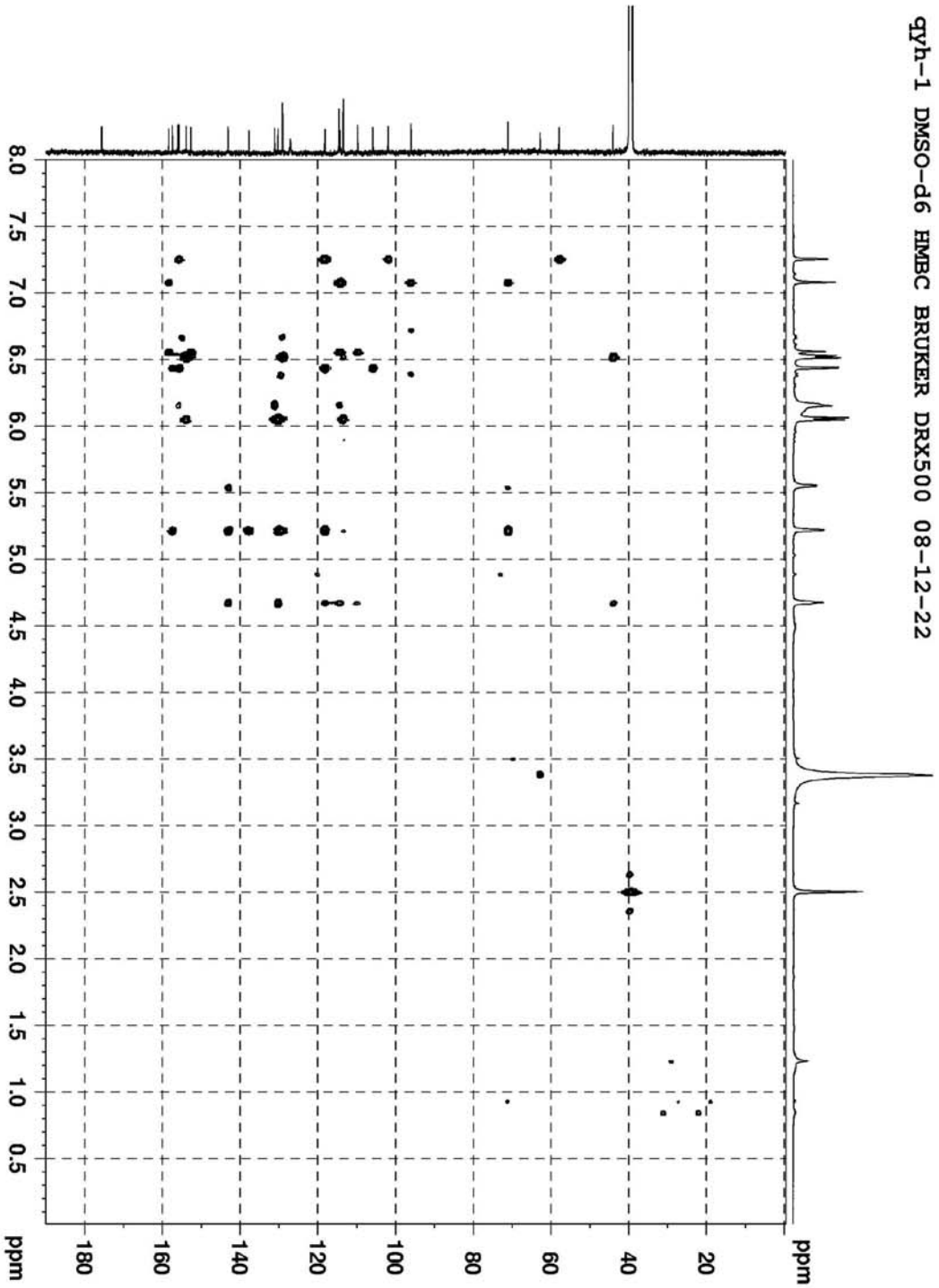


Figure S4 HMBC spectrum of compound **1** (DMSO-$d_6$)

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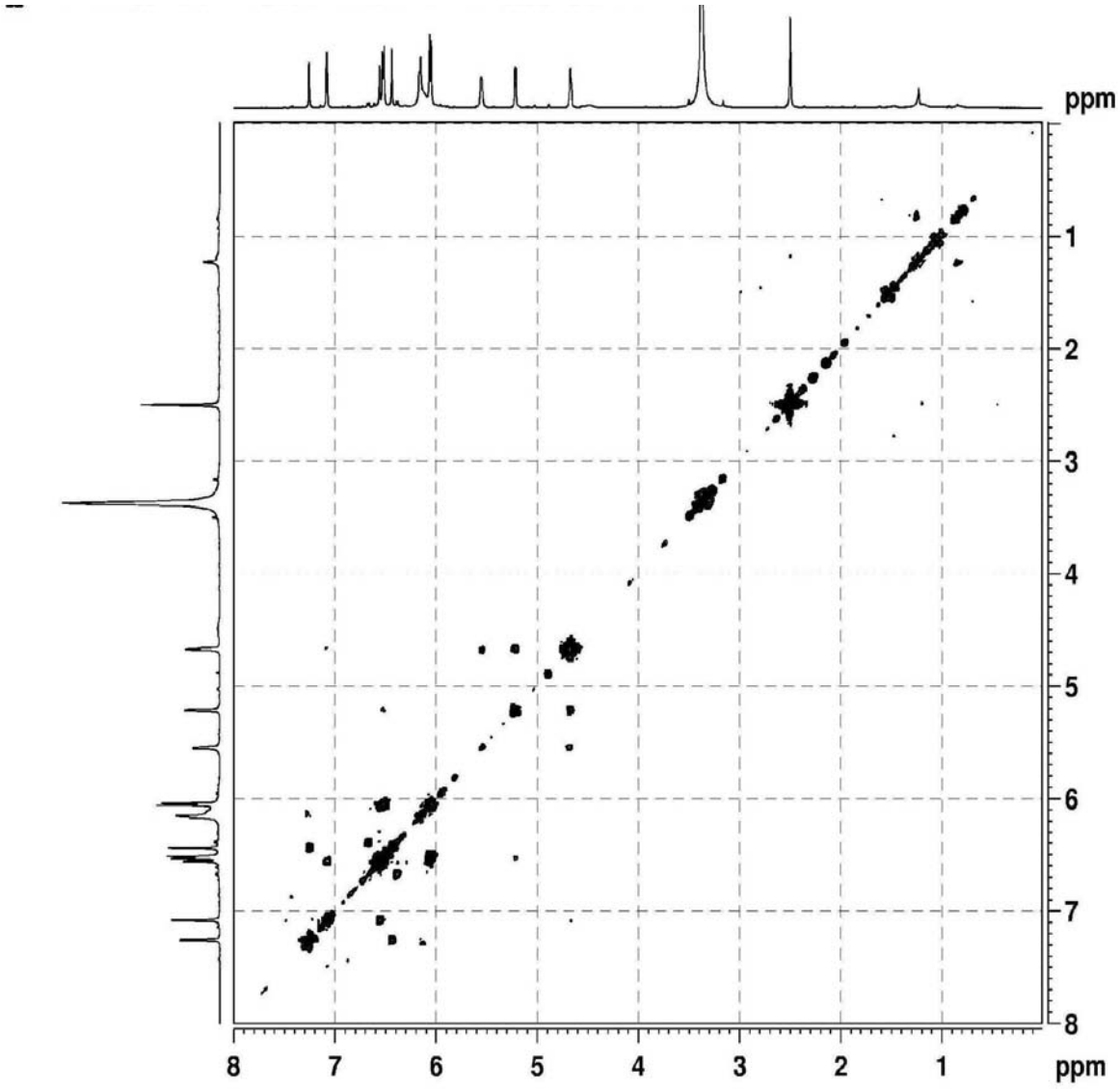


Figure S5 $^{1}$H-$^{1}$H COSY spectrum of compound **1** (DMSO-$d_6$)

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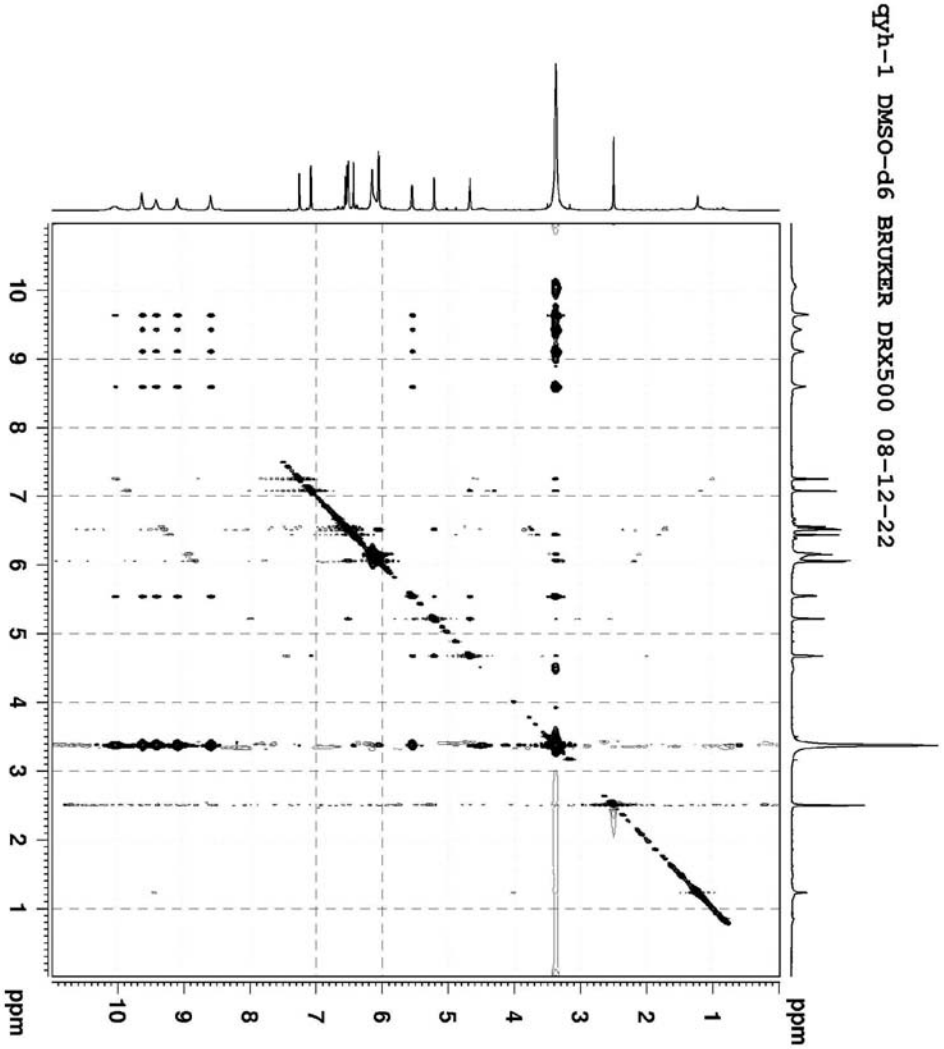


Figure S6 NOESY spectrum of compound **1** (DMSO-$d_6$)

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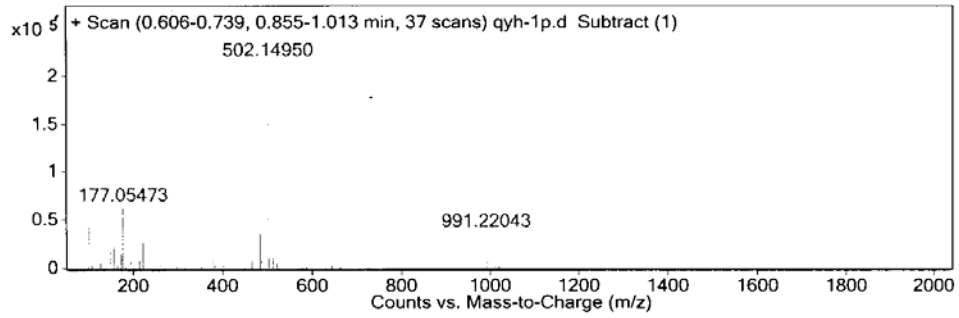
# Qualitative Analysis Report

| | | | |
|---|---|---|---|
| **Data Filename** | qyh-1p.d | **Sample Name** | qyh-1 |
| **Sample Type** | Sample | **Position** | P1-D1 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | positive_2.m | **IRM Calibration Status** | [redacted] |
| **DA Method** | Default.m | **Comment** | |

**User Spectra**

| Spectrum Source | Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|---|
| Peak (1) in "+ EIC(485.12157) Scan" | 160 | 0 | Esi |




Peak List

| m/z | z | Abund. | Formula | Ion |
|---|---|---|---|---|
| 102.12795 | | 42352 | | |
| 149.02351 | | 43355 | | |
| 177.05473 | | 64307 | | |
| 223.09286 | | 26539 | | |
| 245.0785 | | 23818 | | |
| 485.12299 | | 35487 | C28H21O8 | (M+H)+ |
| 502.1495 | 1 | 226394 | | |
| 503.15258 | 1 | 62350 | | |
| 507.10472 | 1 | 55020 | | |
| 991.22043 | 1 | 36900 | | |

--- End Of Report ---



Figure S7 HRESIMS spectrum of compound **1** (positive mode)

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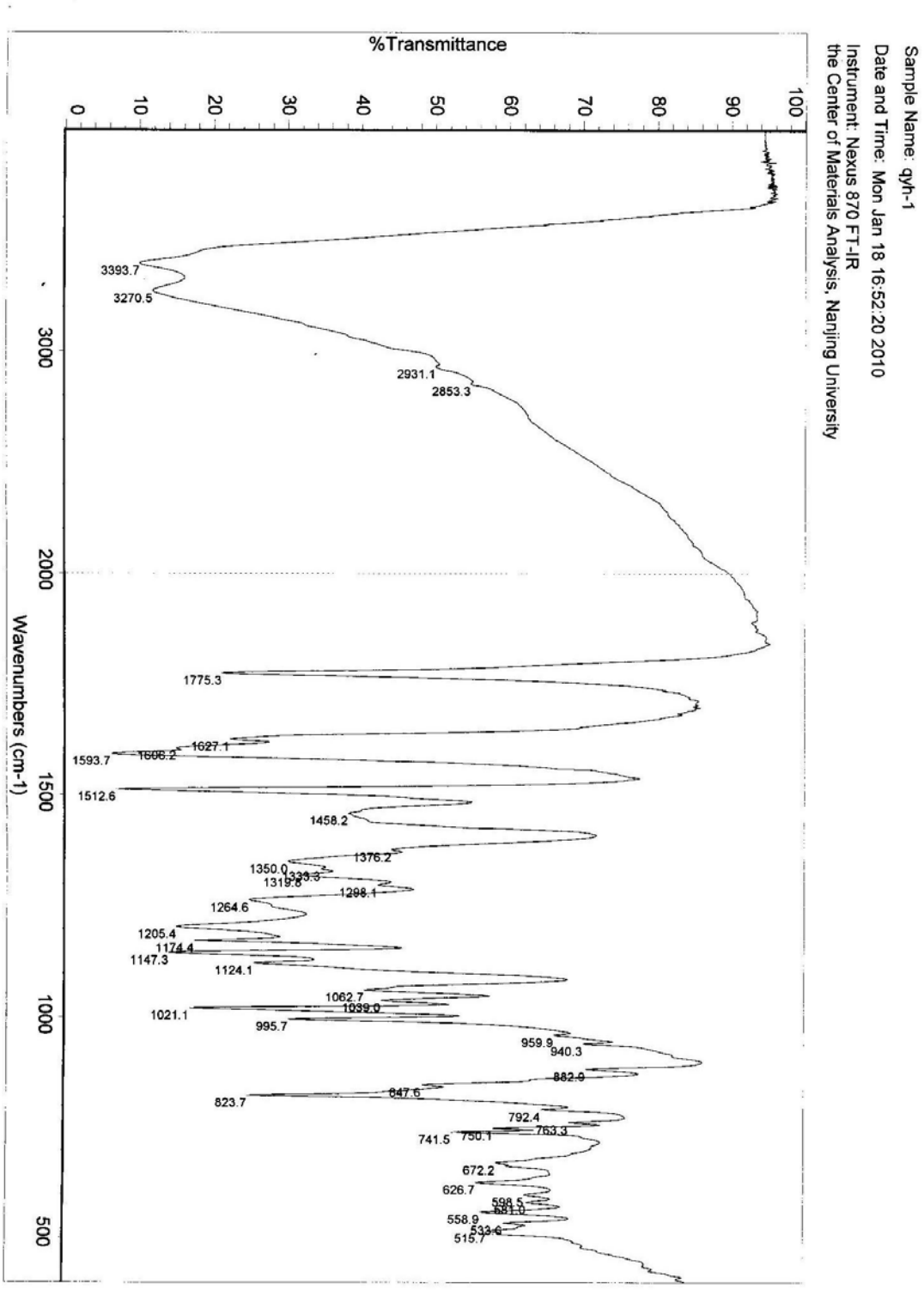


Figure S8 FT-IR spectrum of compound **1** (KBr)

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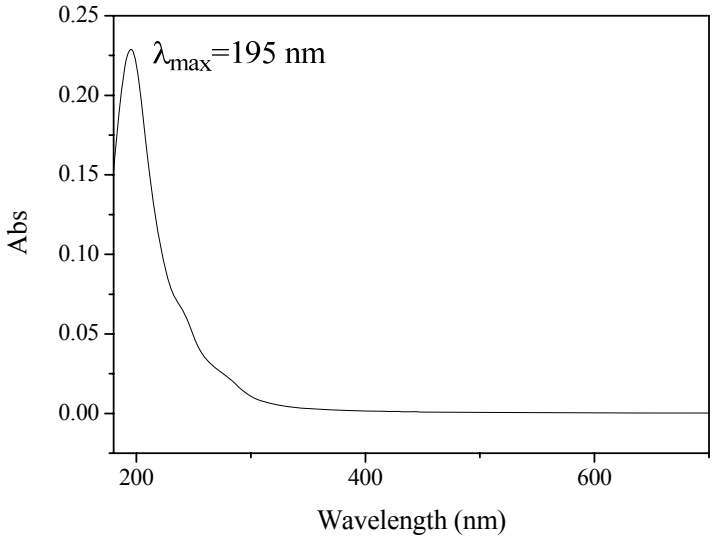


Figure S9 The theoretically predicted UV spectrum for **1**. The calculations are carried out at B3LYP/6−31G(d) level within the polarizable continuum model ($CH_3OH$ solvent: dielectric constant ε = 32.63).

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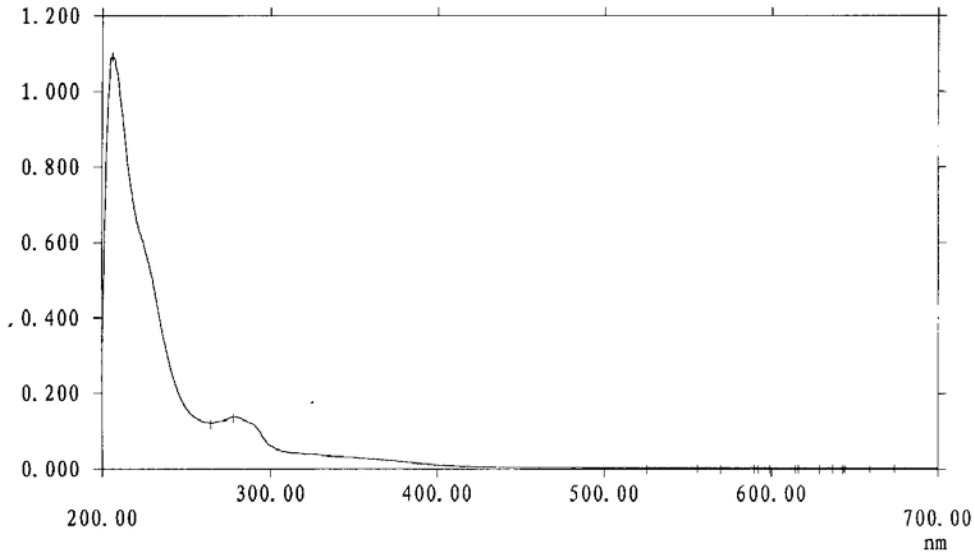


| No. | WL (nm) | Peak (Abs) | No. | WL (nm) | Valley (Abs) |
|---|---|---|---|---|---|
| 1 | 673.50 | 0.004 | 1 | 658.50 | 0.003 |
| 2 | 643.50 | 0.004 | 2 | 642.50 | 0.003 |
| 3 | 636.50 | 0.004 | 3 | 628.50 | 0.003 |
| 4 | 616.00 | 0.004 | 4 | 614.00 | 0.003 |
| 5 | 598.50 | 0.004 | 5 | 592.00 | 0.003 |
| 6 | 589.50 | 0.004 | 6 | 569.50 | 0.003 |
| 7 | 556.00 | 0.004 | 7 | 525.50 | 0.003 |
| 8 | 277.50 | 0.137 | 8 | 264.00 | 0.121 |
| 9 | 206.00 | 1.096 | | | |

Figure S10 UV spectrum of compound **1** ($CH_3OH$)

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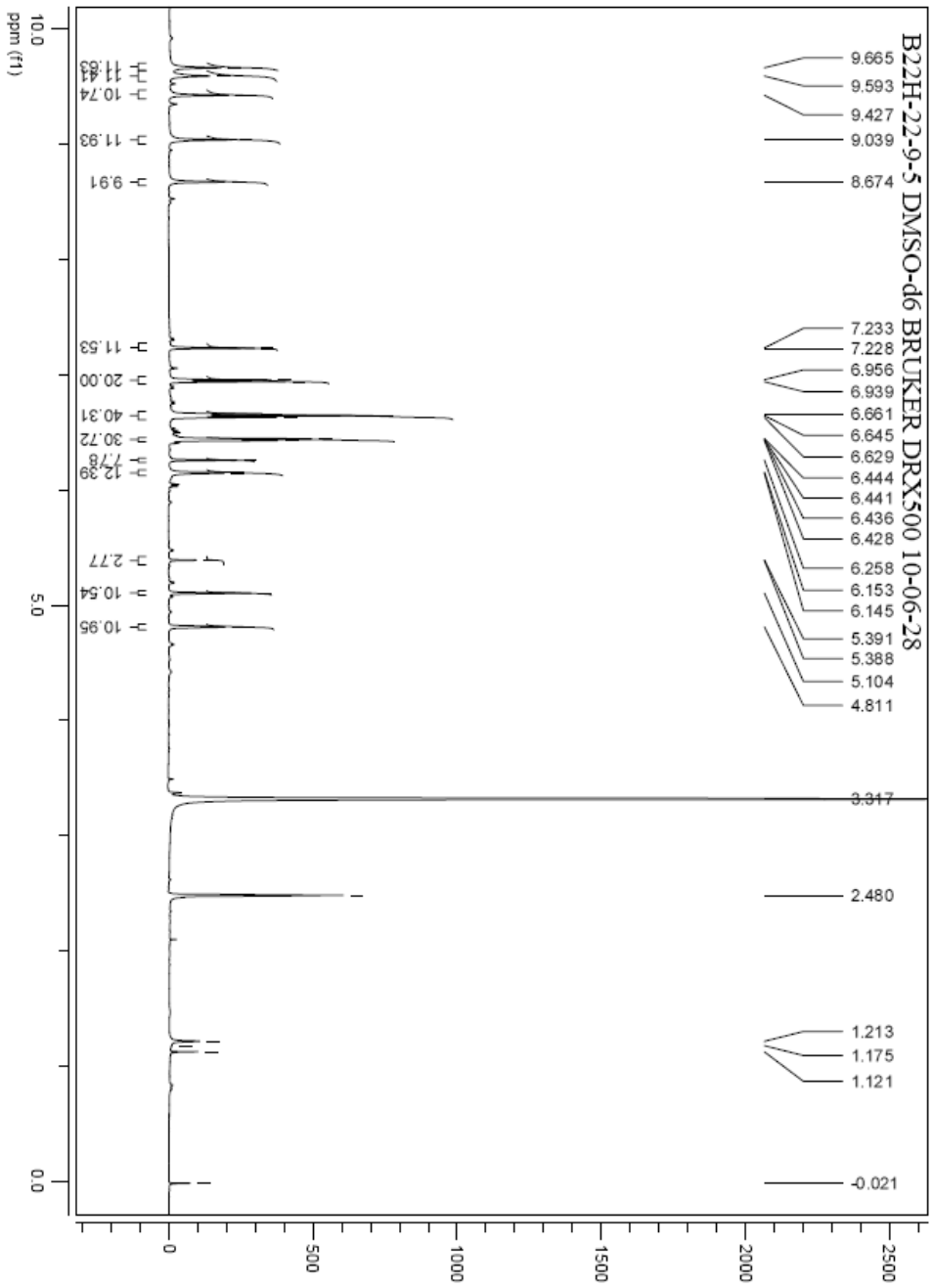


Figure S11 $^{1}$H-NMR spectrum of compound **2** (DMSO-$d_6$)

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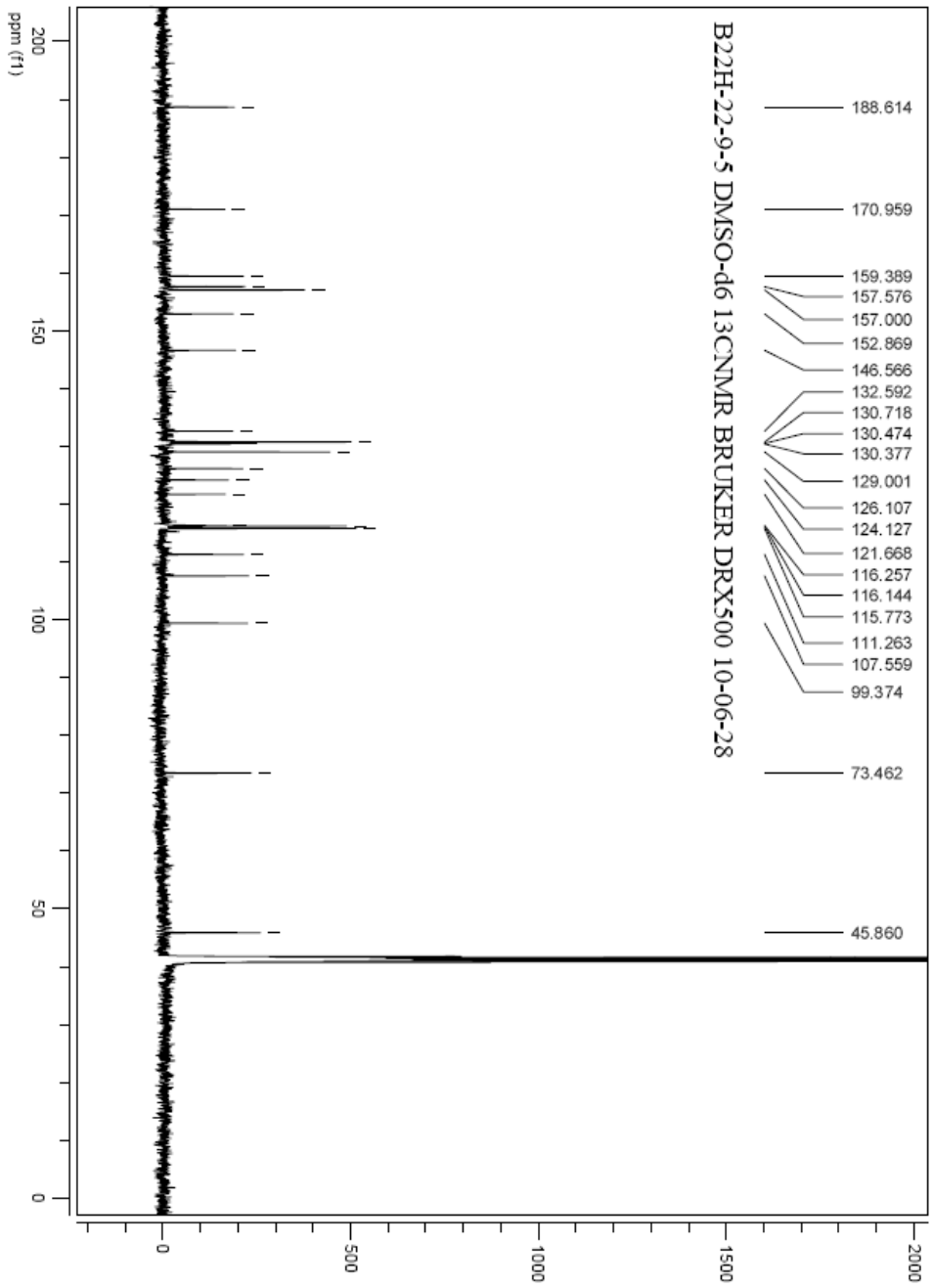


Figure S12 $^{13}$C-NMR spectrum of compound **2** (DMSO-$d_6$)

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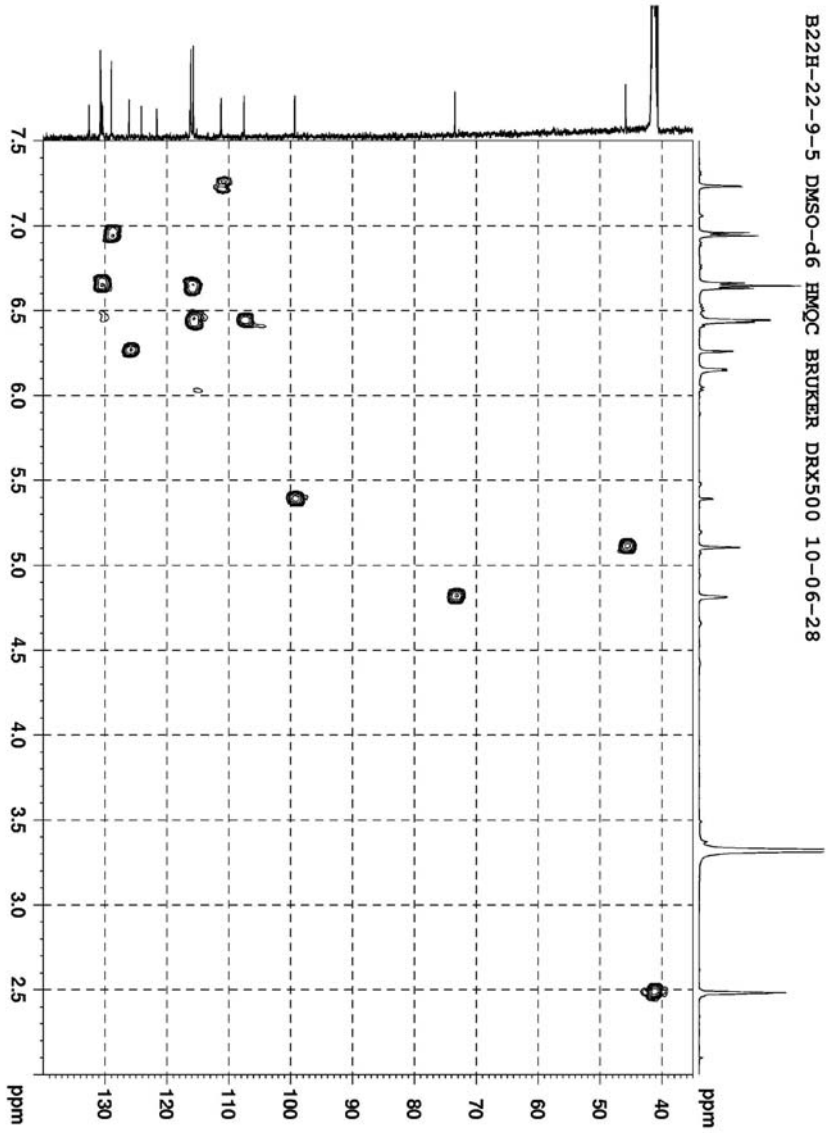


Figure S13 HMQC spectrum of compound **2** (DMSO-$d_6$)

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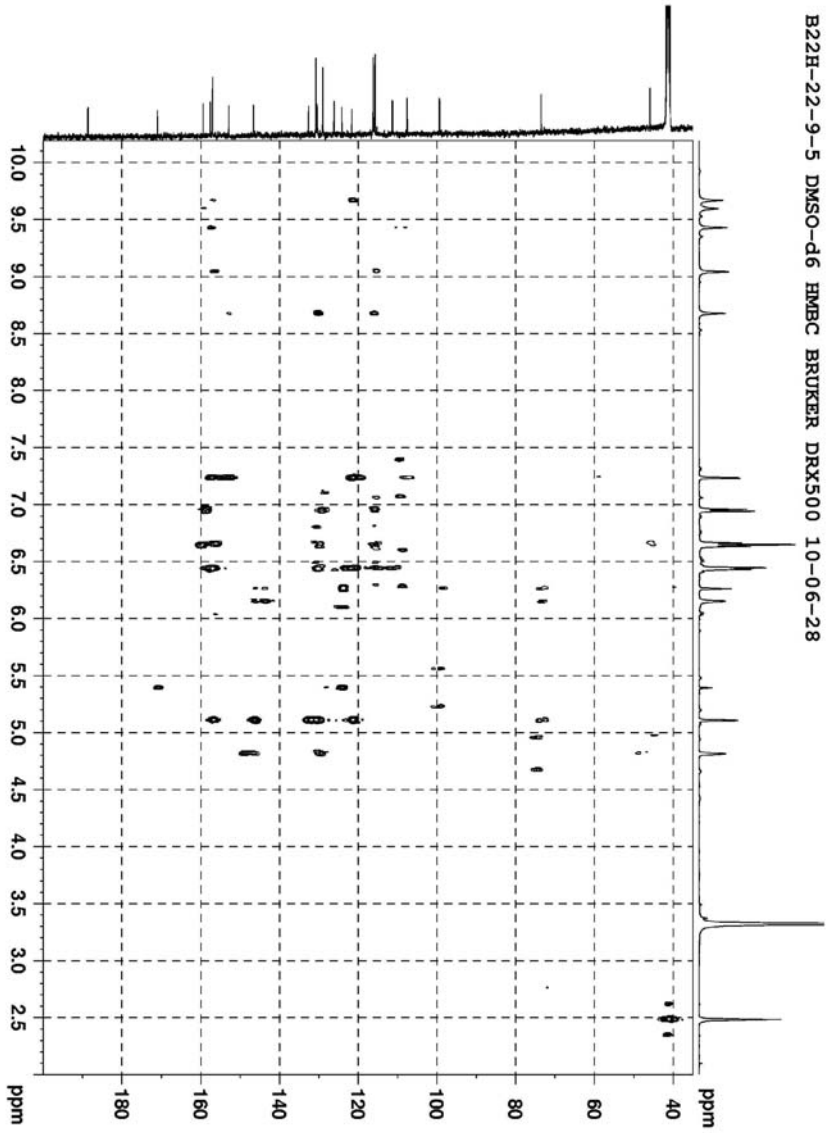


Figure S14 HMBC spectrum of compound **2** (DMSO-$d_6$)

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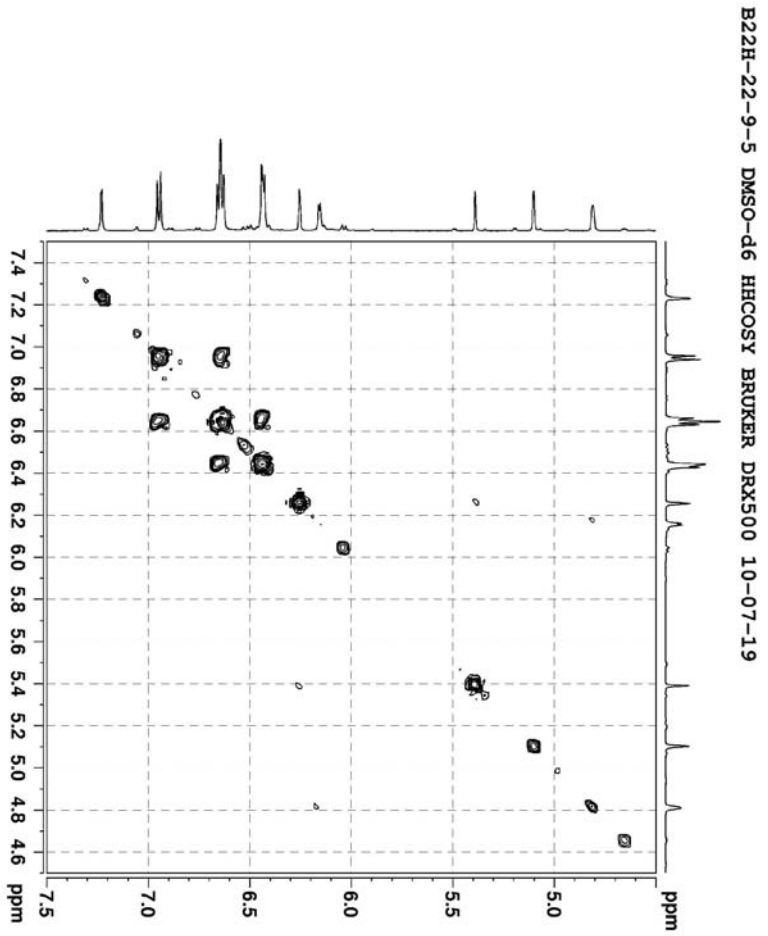


Figure S15 $^{1}$H-$^{1}$H COSY spectrum of compound **2** (DMSO-$d_6$)

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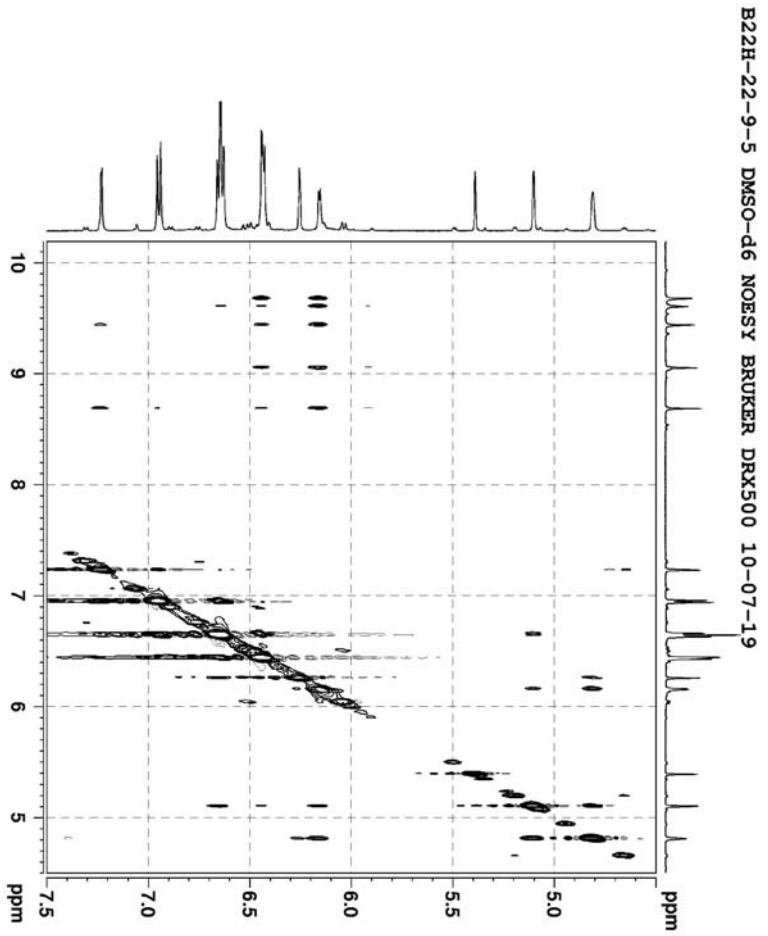


Figure S16 NOESY spectrum of compound **2** (DMSO-$d_6$)

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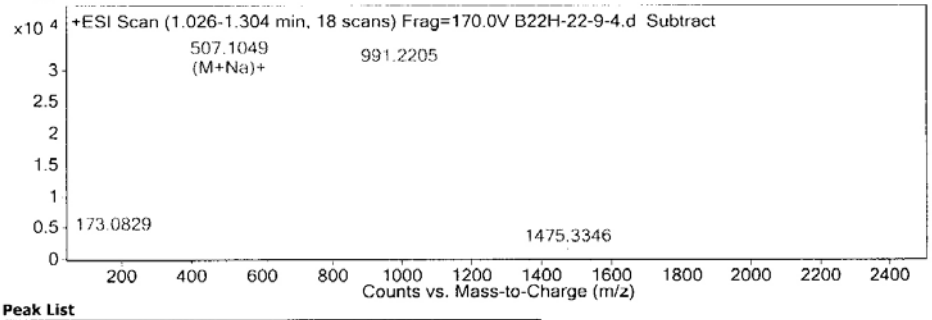
## Qualitative Analysis Report

| | | | |
|---|---|---|---|
| **Data Filename** | B22H-22-9-4.d | **Sample Name** | B22H-22-9-4 |
| **Sample Type** | Sample | **Position** | P1-D5 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | TEMP2.m | **Acquired Time** | 5/5/2010 6:48:07 PM |
| **IRM Calibration Status** | Some Ions Missed | **DA Method** | Default.m |
| **Comment** | | | |

### User Spectra

| Spectrum Source | Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|---|
| Peak (1) in "+ TIC Scan" | 170 | 0 | Esi |




**Peak List**

| *m/z* | z | Abund | Formula | Ion |
|---|---|---|---|---|
| 173.0829 | | 3876 | | |
| 485.1232 | 1 | 15882 | C28 H21 O8 | (M+H)+ |
| 486.1264 | 1 | 4303 | C28 H21 O8 | (M+H)+ |
| 507.1049 | 1 | 33319 | C28 H20 Na O8 | (M+Na)+ |
| 508.1086 | 1 | 8317 | C28 H20 Na O8 | (M+Na)+ |
| 955.2047 | 1 | 8060 | | |
| 956.2079 | 1 | 3540 | | |
| 991.2205 | 1 | 30555 | | |
| 992.2241 | 1 | 16822 | | |
| 993.2264 | 1 | 5094 | | |

--- End Of Report ---

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Figure S17 HRESIMS spectrum of compound **2** (positive mode)

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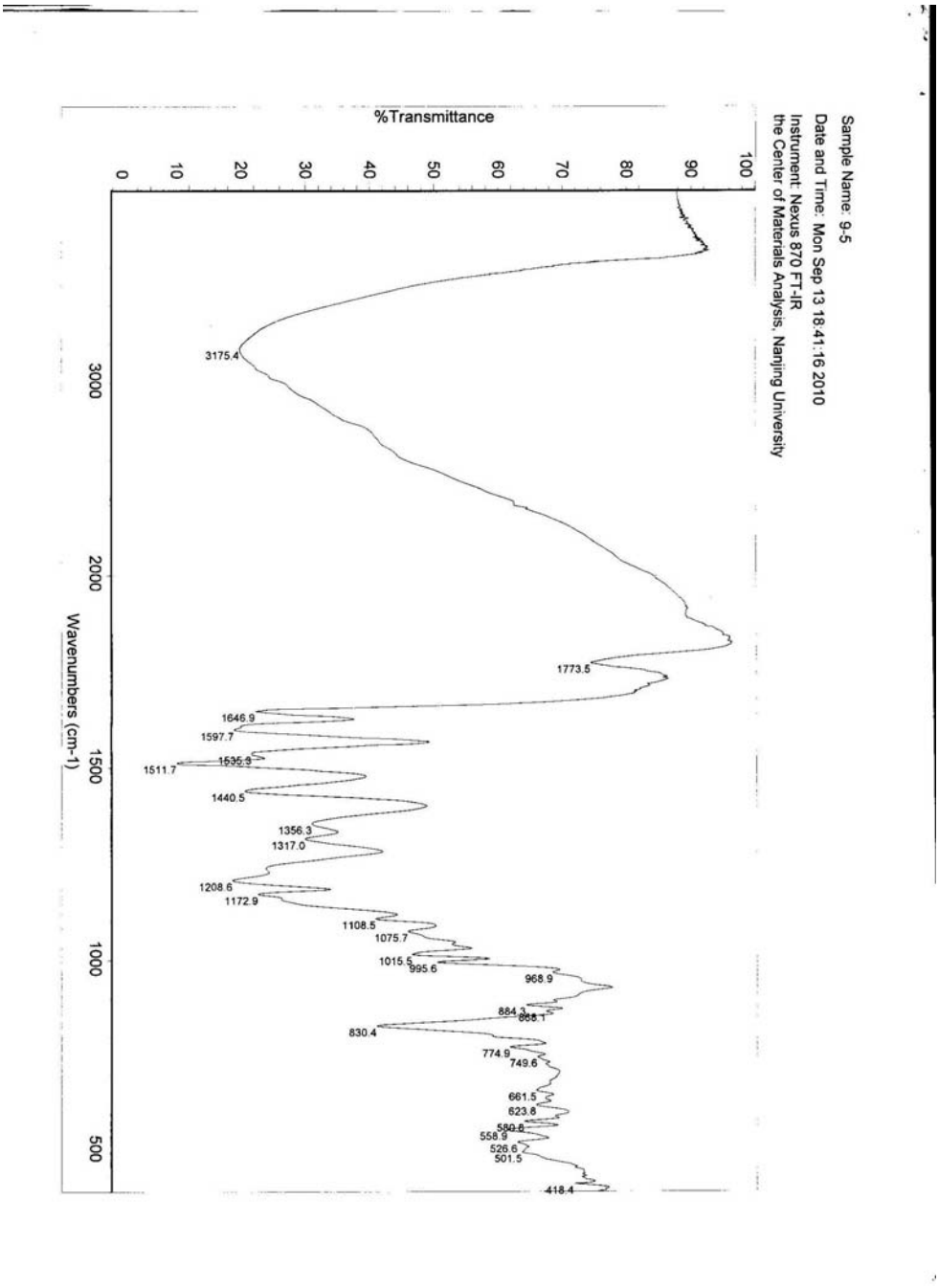


Figure S18 FT-IR spectrum of compound **2** (KBr)

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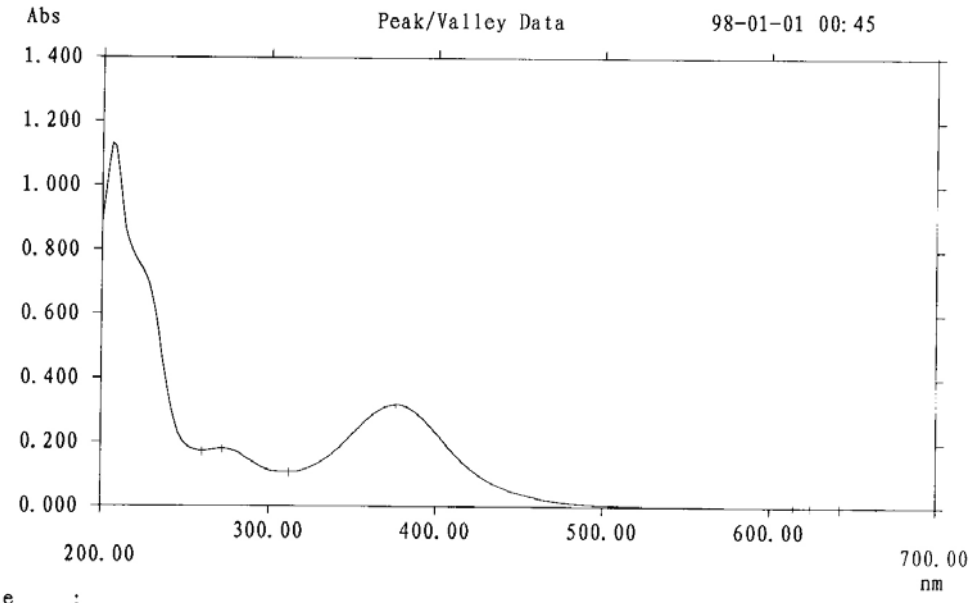


Sample :
Comment :
Scan Speed : 1200 nm/min Slit : 2.0 nm PMT Voltage : Auto Gain
Baseline : User 1 Sampling Interval: Auto

| No. | WL (nm) | Peak (Abs) | No. | WL (nm) | Valley (Abs) |
|---|---|---|---|---|---|
| 1 | 664.00 | 0.000 | 1 | 642.00 | 0.000 |
| 2 | 624.00 | 0.000 | 2 | 614.00 | 0.000 |
| 3 | 376.00 | 0.318 | 3 | 312.00 | 0.108 |
| 4 | 272.00 | 0.180 | 4 | 260.00 | 0.173 |

Figure S19 UV spectrum of compound **2** ($CH_3OH$)

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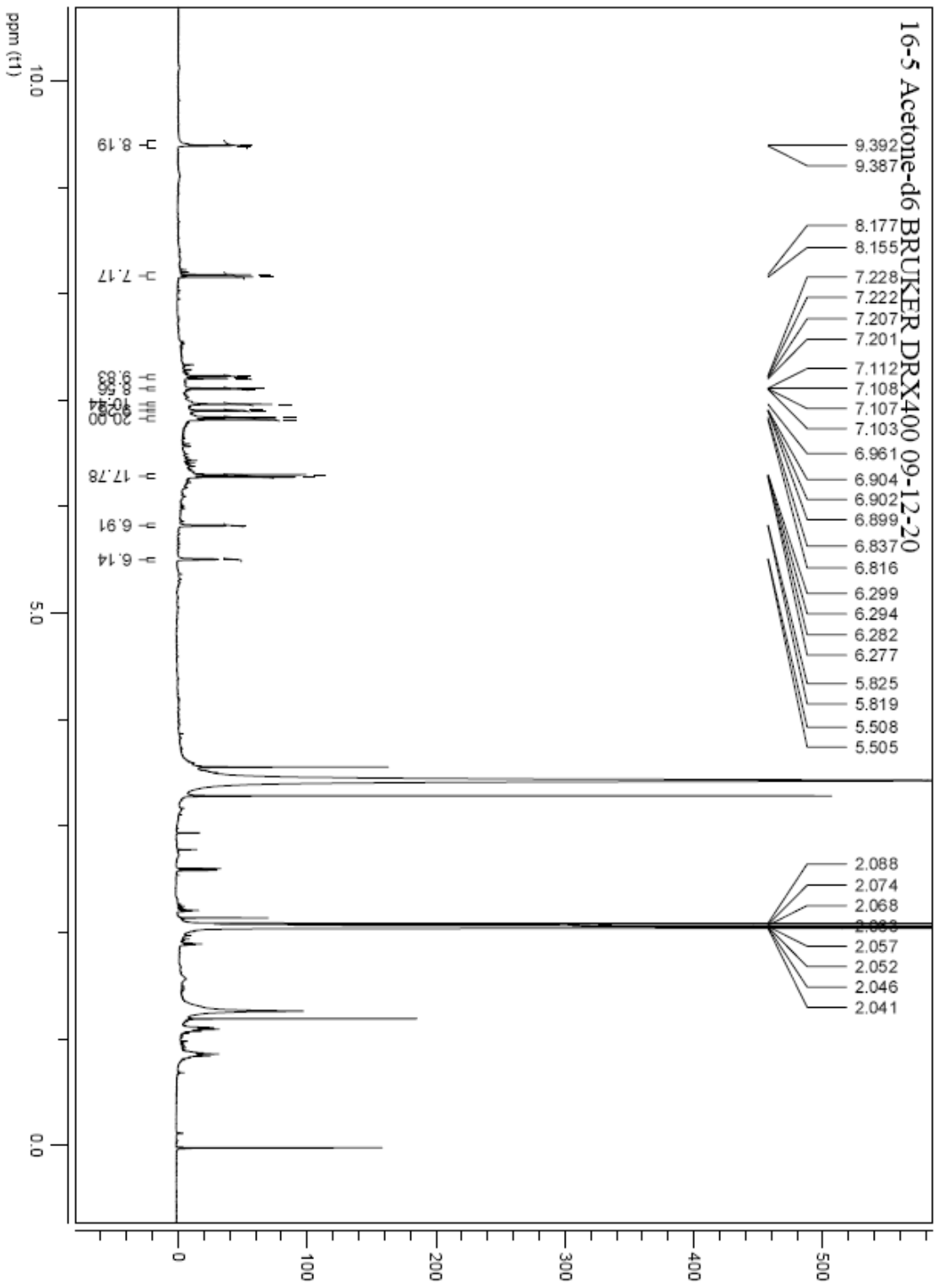


Figure S20 $^{1}$H-NMR spectrum of compound **3** (acetone-$d_6$)

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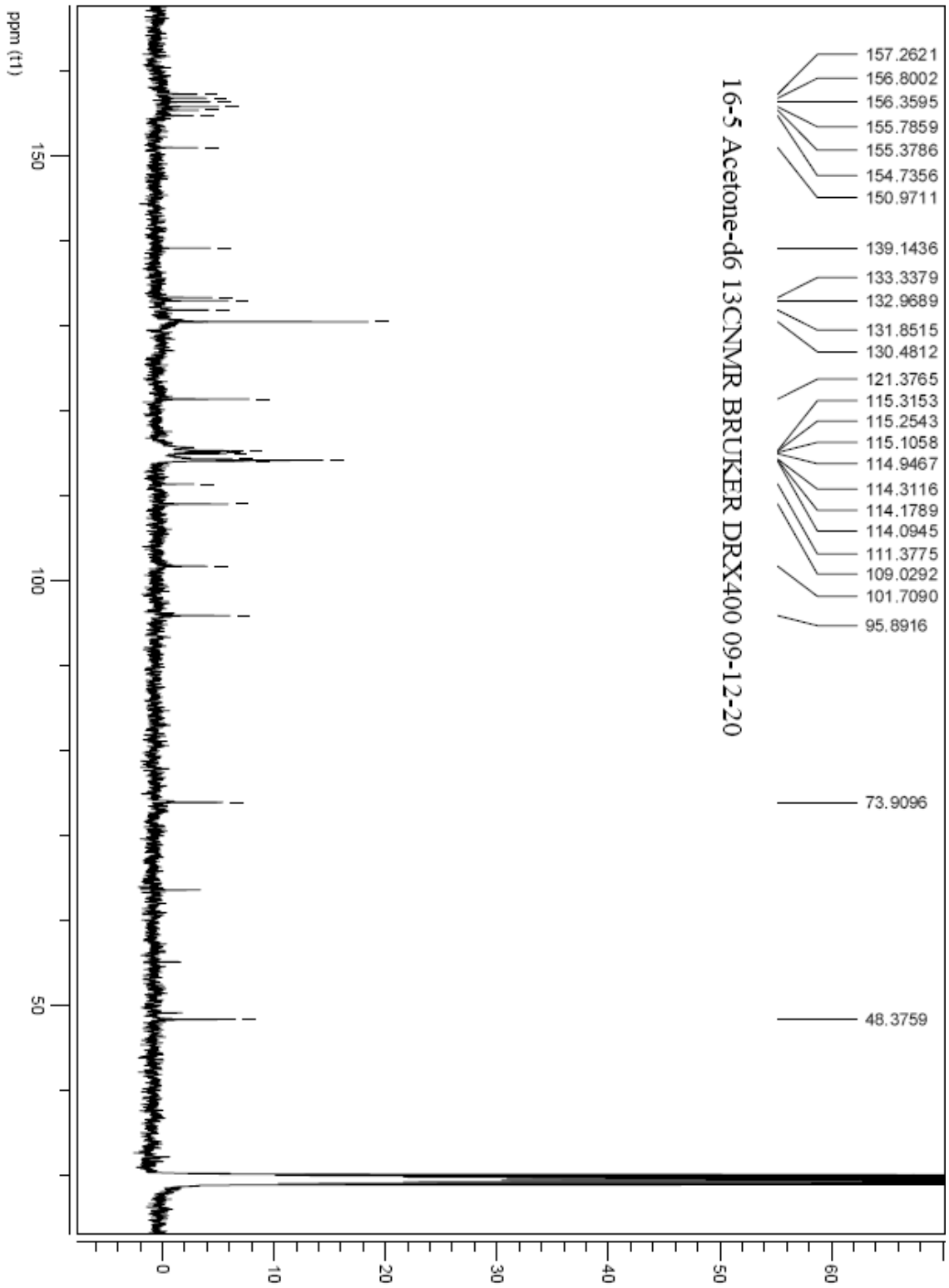


Figure S21 $^{13}$C-NMR spectrum of compound **3** (acetone-$d_6$)

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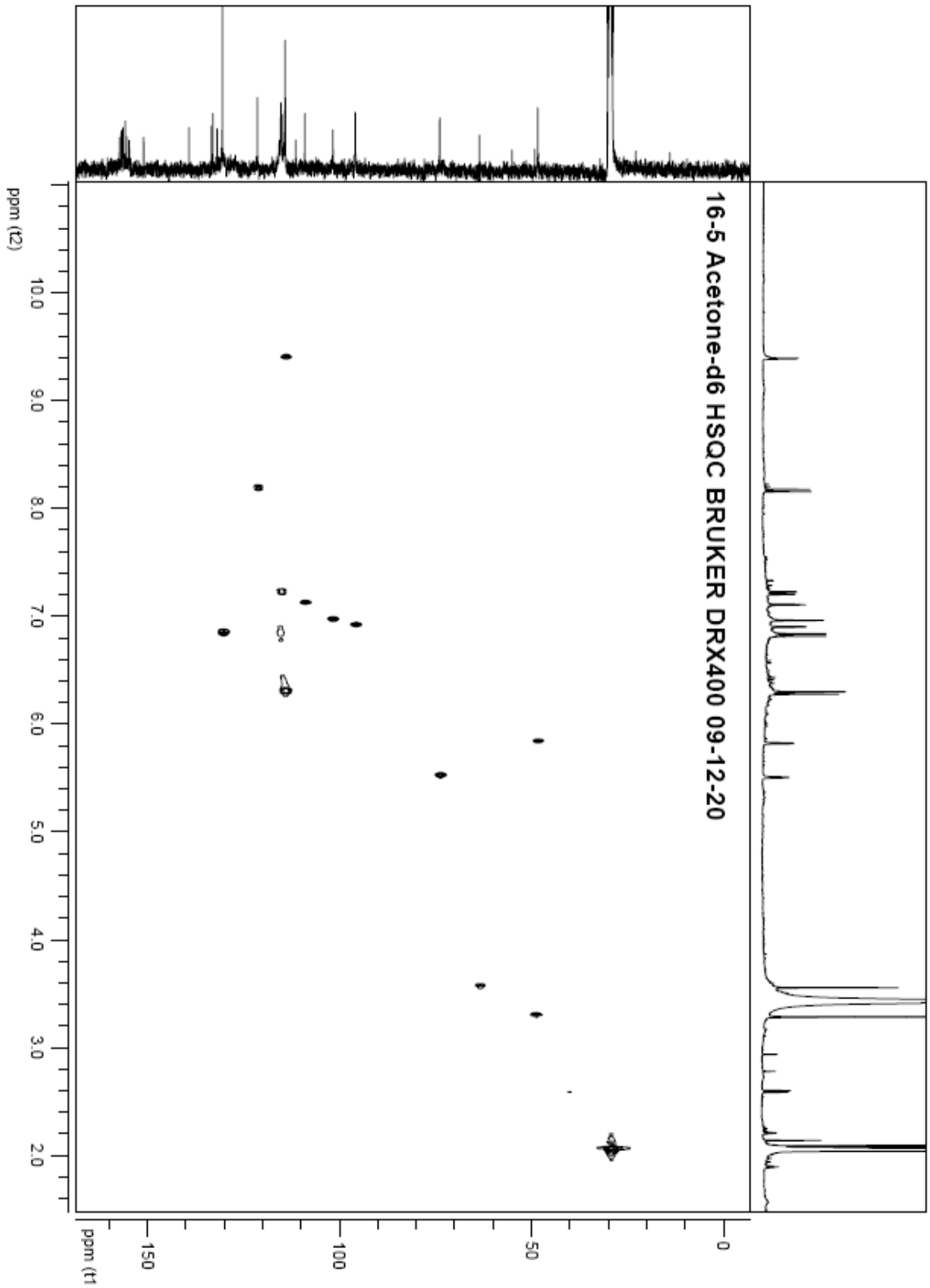


Figure S22 HSQC spectrum of compound **3** (acetone-$d_6$)

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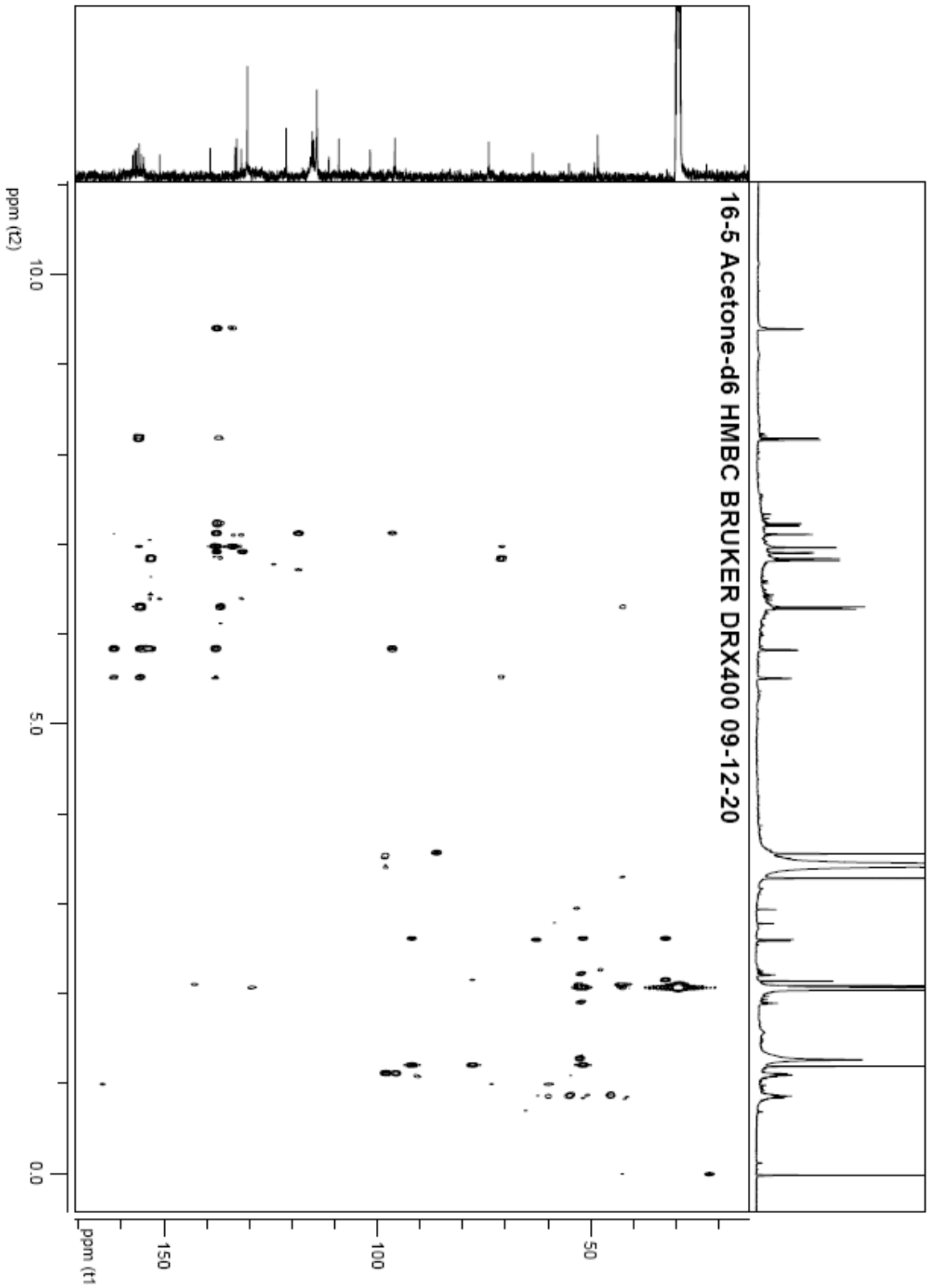


Figure S23 HMBC spectrum of compound **3** (acetone-$d_6$)

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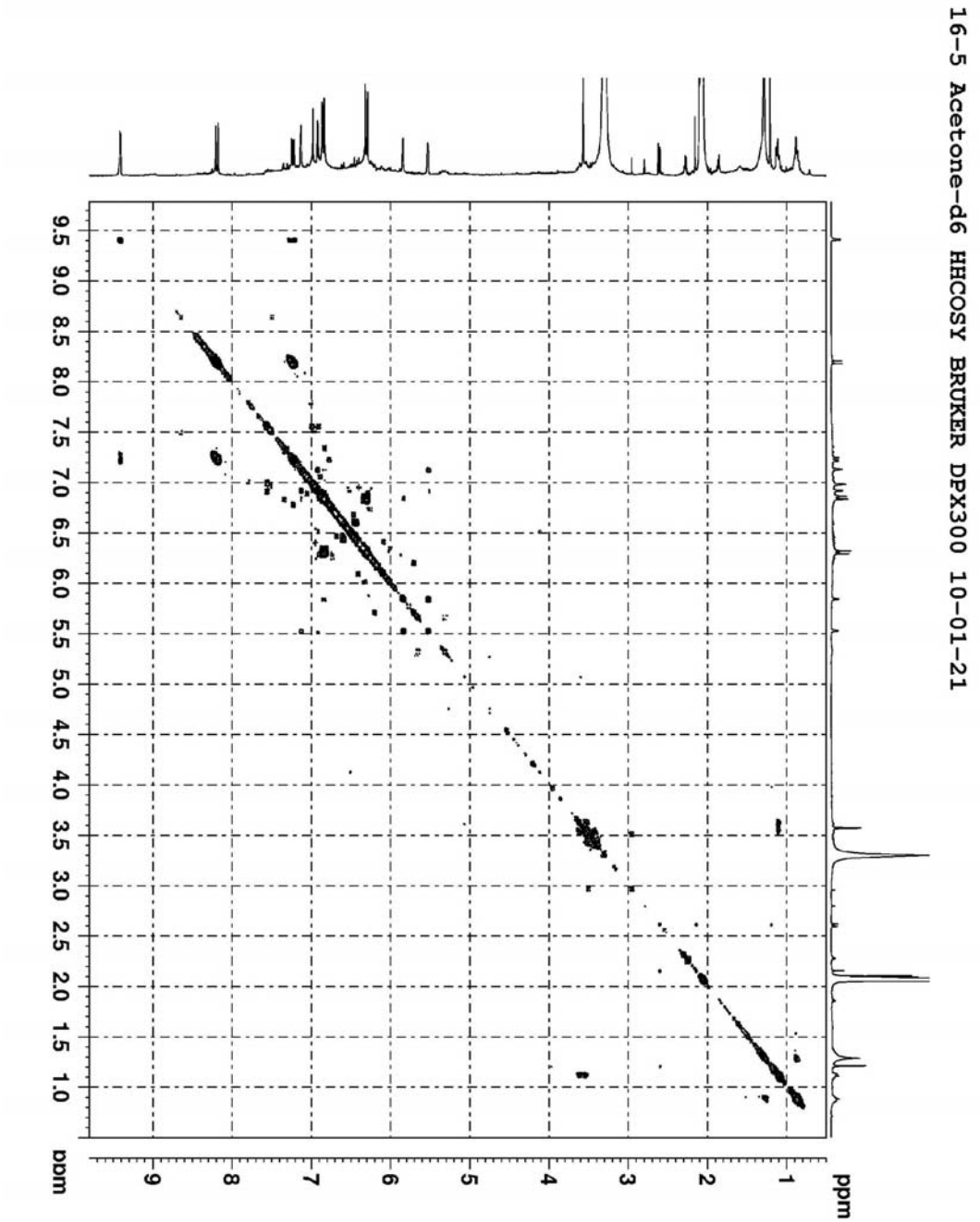


Figure S24 $^{1}$H-$^{1}$H COSY spectrum of compound **3** (acetone-$d_6$)

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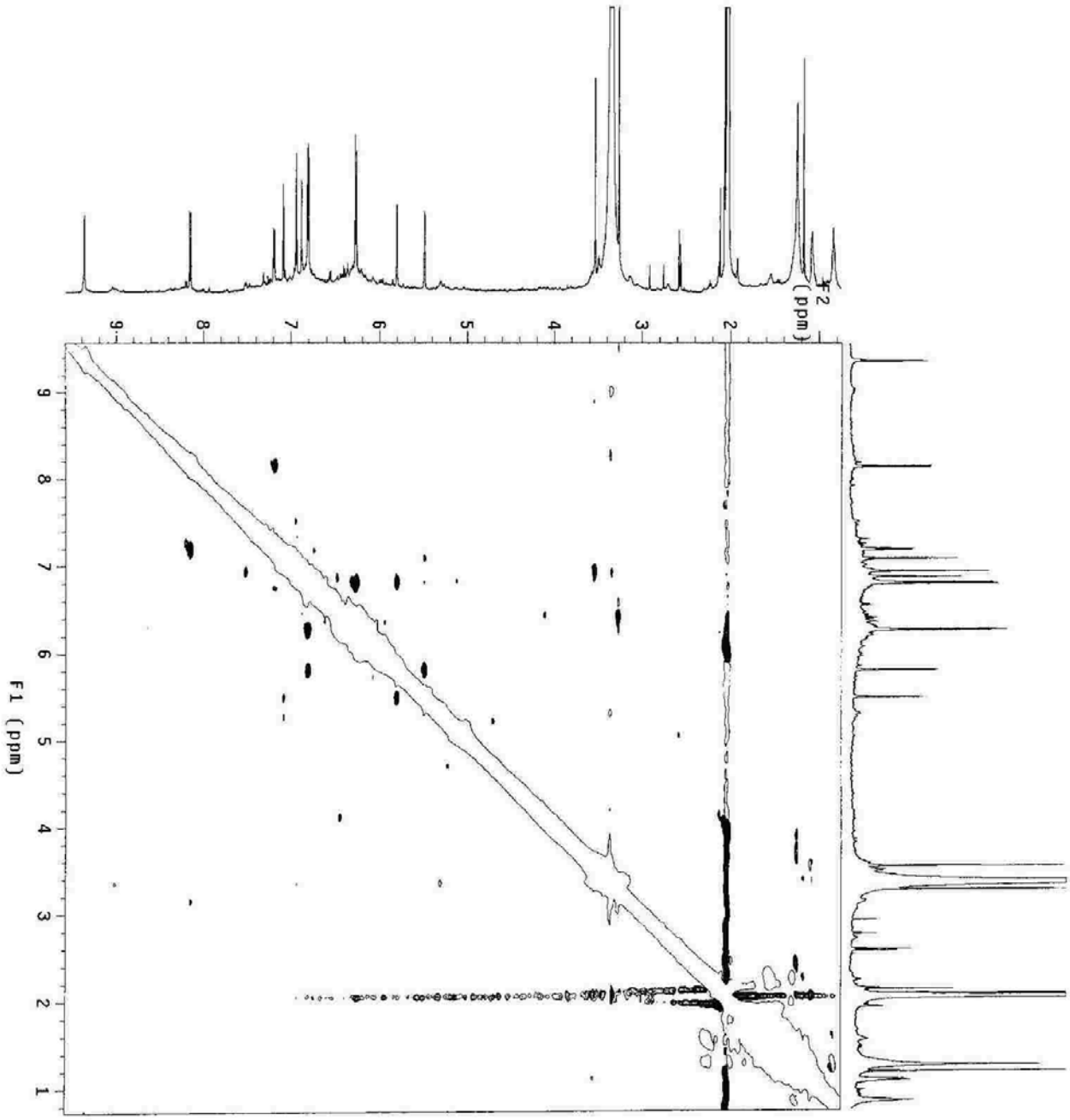


Figure S25 ROESY spectrum of compound **3** (acetone-$d_6$)

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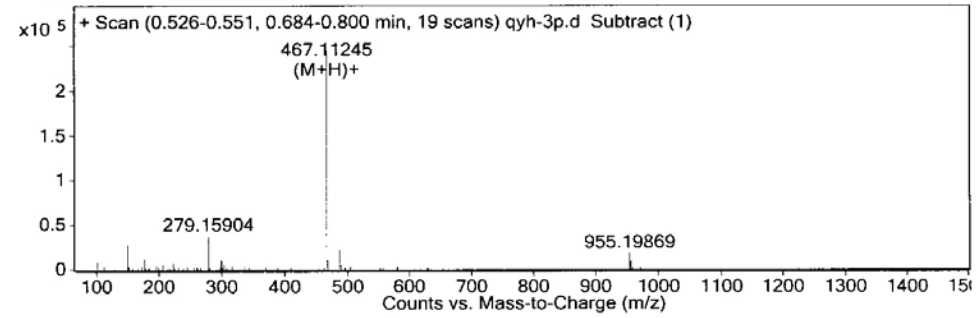
# Qualitative Analysis Report

| | | | |
|---|---|---|---|
| **Data Filename** | qyh-3p.d | **Sample Name** | qyh-3 |
| **Sample Type** | Sample | **Position** | P1-D3 |
| **Instrument Name** | Instrument 1 | **User Name** | |
| **Acq Method** | positive.m | **IRM Calibration Status** | [redacted] |
| **DA Method** | Default.m | **Comment** | |

**User Spectra**

| Spectrum Source | Fragmentor Voltage | Collision Energy | Ionization Mode |
|---|---|---|---|
| Peak (1) in "+ TIC Scan" | 160 | 0 | Esi |




Peak List

| m/z | z | Abund. | Formula | Ion |
|---|---|---|---|---|
| 149.02341 | | 27281 | | |
| 279.15904 | | 37659 | | |
| 467.11245 | 1 | 244253 | C28H19O7 | (M+H)+ |
| 467.37867 | | 15248 | | |
| 468.1153 | 1 | 67709 | C28H19O7 | (M+H)+ |
| 489.09437 | | 22240 | | |
| 955.19869 | | 17157 | | |

--- End Of Report ---

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Figure S26 HRESIMS spectrum of compound **3** (positive mode)

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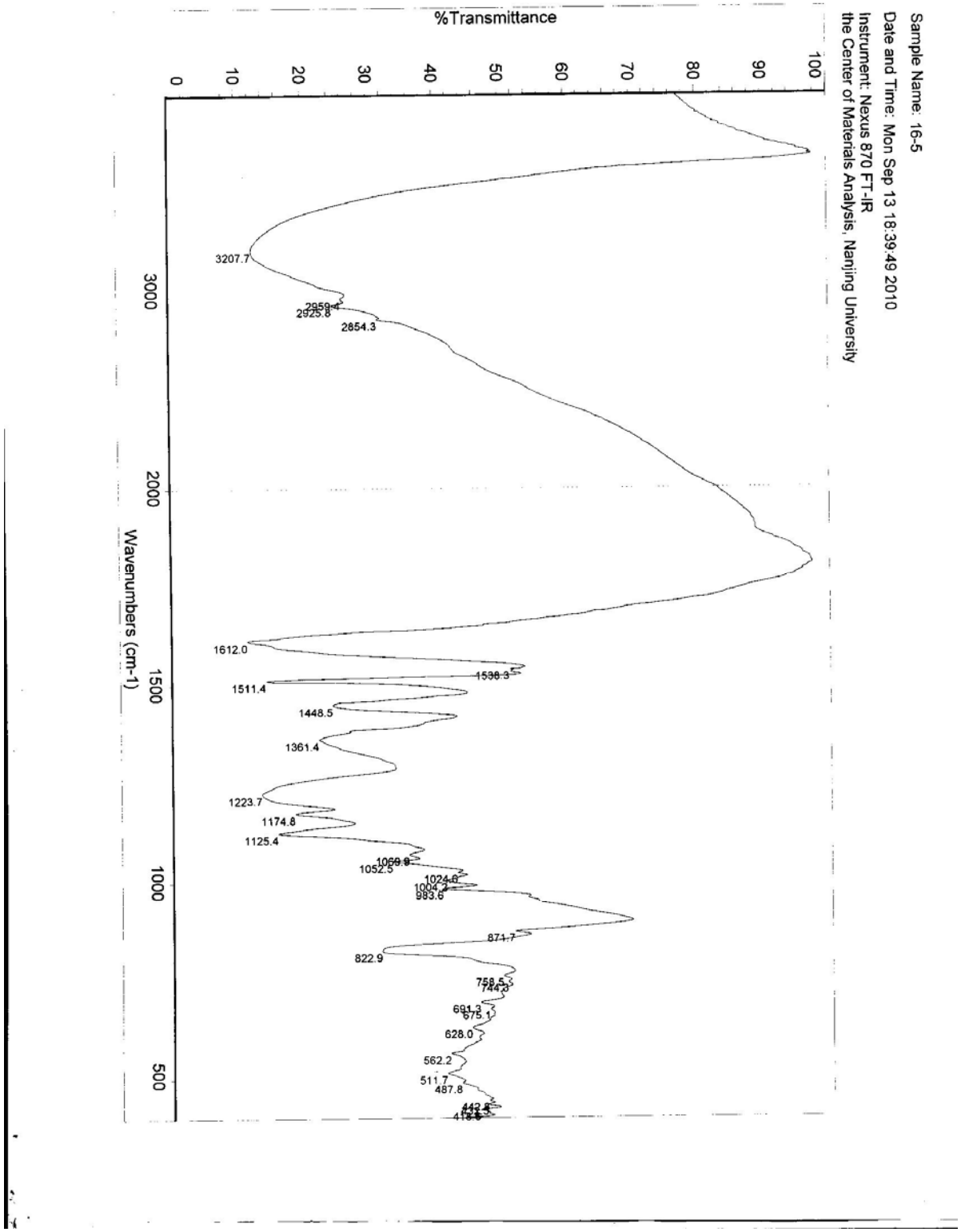


Figure S27 FT-IR spectrum of compound **3** (KBr)

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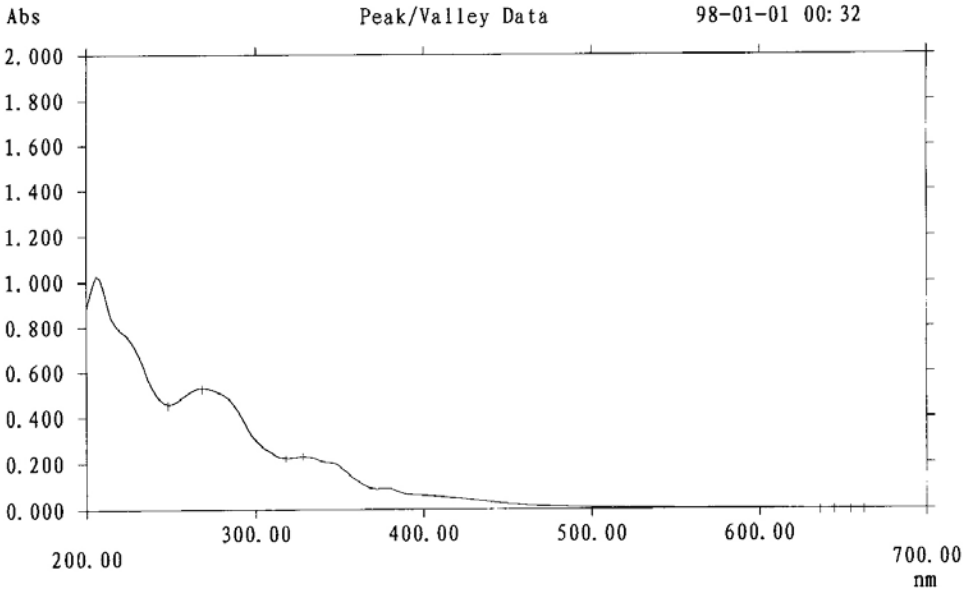


Sample :
Comment :
Scan Speed : 1200 nm/min Slit : 2.0 nm PMT Voltage : Auto Gain
Baseline : User 1 Sampling Interval: Auto

| No. | WL (nm) | Peak (Abs) | No. | WL (nm) | Valley (Abs) |
|---|---|---|---|---|---|
| 1 | 662.00 | 0.001 | 1 | 654.00 | 0.001 |
| 2 | 644.00 | 0.001 | 2 | 636.00 | 0.001 |
| 3 | 328.00 | 0.229 | 3 | 318.00 | 0.222 |
| 4 | 268.00 | 0.530 | 4 | 248.00 | 0.457 |

Figure S28 UV spectrum of compound **3** ($CH_3OH$)

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Table S1 The optimized structural information for **1** within polarizable continuum model ($CH_3OH$ solvent: dielectric constant ε = 32.63) at B3LYP/6−31G(d) level.

| Atoms | Coordinate X | Coordinate Y | Coordinate Z |
|---|---|---|---|
| C | 0.535 | -0.801 | 1.099 |
| C | -0.688 | -0.243 | 1.546 |
| C | -1.103 | -0.357 | 2.874 |
| C | -0.313 | -1.054 | 3.790 |
| C | 0.871 | -1.651 | 3.374 |
| C | 1.280 | -1.537 | 2.039 |
| H | -2.024 | 0.090 | 3.222 |
| H | 1.480 | -2.221 | 4.076 |
| C | -3.313 | -2.085 | -2.505 |
| C | -1.921 | -2.145 | -2.382 |
| C | -4.070 | -1.269 | -1.653 |
| C | -1.230 | -1.390 | -1.421 |
| H | -1.381 | -2.795 | -3.067 |
| C | -3.359 | -0.519 | -0.733 |
| H | -5.154 | -1.225 | -1.697 |
| C | -1.970 | -0.523 | -0.609 |
| C | -1.595 | 0.442 | 0.507 |
| C | -3.010 | 0.815 | 1.041 |
| C | 0.273 | -1.623 | -1.296 |
| H | 0.712 | -1.502 | -2.300 |
| C | 0.977 | -0.624 | -0.359 |
| H | 0.590 | 0.349 | -0.672 |
| C | 2.482 | -0.506 | -0.607 |
| C | 3.119 | 0.696 | -0.278 |
| C | 3.254 | -1.512 | -1.207 |
| C | 4.477 | 0.895 | -0.527 |
| H | 2.543 | 1.499 | 0.177 |
| C | 4.608 | -1.324 | -1.472 |
| H | 2.793 | -2.464 | -1.445 |
| C | 5.226 | -0.118 | -1.130 |
| H | 4.948 | 1.841 | -0.265 |
| H | 5.201 | -2.106 | -1.937 |
| O | 0.529 | -2.950 | -0.824 |
| H | -0.089 | -3.550 | -1.270 |
| O | -3.887 | -2.857 | -3.473 |
| H | -4.847 | -2.724 | -3.461 |
| O | -3.977 | 0.290 | 0.199 |
| O | -3.315 | 1.505 | 1.972 |
| C | -1.044 | 1.811 | 0.029 |
| C | -0.448 | 2.675 | 0.956 |
| C | -1.215 | 2.264 | -1.287 |
| C | -0.012 | 3.942 | 0.577 |
| H | -0.327 | 2.357 | 1.986 |
| C | -0.783 | 3.529 | -1.677 |
| H | -1.683 | 1.619 | -2.024 |

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| | | | |
|---|---|---|---|
| C | -0.177 | 4.375 | -0.744 |
| H | 0.451 | 4.598 | 1.312 |
| H | -0.908 | 3.874 | -2.698 |
| O | 0.231 | 5.605 | -1.176 |
| H | 0.614 | 6.091 | -0.429 |
| O | -0.764 | -1.126 | 5.079 |
| H | -0.133 | -1.639 | 5.607 |
| O | 2.425 | -2.150 | 1.629 |
| H | 2.829 | -2.603 | 2.385 |
| O | 6.562 | 0.014 | -1.411 |
| H | 6.852 | 0.896 | -1.130 |

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Table S2 TDDFT results for the optimized conformer of (7b*S*)-**1** (200nm<λ<400nm). The TDDFT calculations are done at the level of B3LYP/6−31G(*d*) in the polarizable continuum model ($CH_3OH$ solvent: dielectric constant ε = 32.63).

| Transition | Excitation energy[a] (nm) | Rotatory Strength $R^b$ ($10^{-40}$ cgs) | Oscillator Strength $f^b$ | Dominant Contributions[c] | Weight |
|---|---|---|---|---|---|
| 4 | 283.33 | 30.1915 | 0.0550 | 124 →127 | 0.44 |
| 5 | 281.26 | 36.4259 | 0.0259 | 123 →127 | 0.46 |
| 7 | 273.28 | 1.5034 | 0.0621 | 126 →129 | 0.26 |
| 10 | 264.87 | -47.8648 | 0.0117 | 122 →127 | 0.34 |
| 11 | 263.73 | -20.6052 | 0.0078 | 125 →129 | 0.32 |
| 12 | 261.37 | 52.7662 | 0.0296 | 124 →128 | 0.24 |
| 16 | 249.32 | 21.2609 | 0.0362 | 126 →132 | 0.24 |
| 18 | 247.56 | 15.7061 | 0.0346 | 122 →128 | 0.15 |
| 19 | 245.65 | 26.7606 | 0.0456 | 123 →129 | 0.30 |
| 21 | 243.29 | -16.5655 | 0.0549 | 123 →130 | 0.29 |
| 22 | 242.34 | 22.7906 | 0.0298 | 121 → 127 | 0.30 |
| 23 | 240.22 | 76.2092 | 0.0673 | 120 →127 | 0.42 |
| 25 | 235.92 | -40.3156 | 0.0327 | 119 → 127 | 0.24 |
| 26 | 235.41 | -27.1127 | 0.0517 | 126 → 134 | 0.10 |
| 31 | 229.47 | 17.2238 | 0.0408 | 122 → 130 | 0.26 |
| 32 | 228.41 | 31.0249 | 0.0111 | 117 → 127 | 0.48 |
| 36 | 225.01 | 19.4478 | 0.0132 | 124 → 132 | 0.20 |
| 45 | 216.58 | 20.9542 | 0.1103 | 120 → 129<br>126 → 132 | 0.12<br>0.14 |
| 46 | 216.11 | 22.7801 | 0.0669 | 120 → 129<br>123 → 133 | 0.13<br>0.10 |
| 48 | 215.11 | -37.8064 | 0.0617 | 125 → 135 | 0.24 |
| 51 | 212.27 | -27.5234 | 0.0398 | 120 → 130<br>123 → 134 | 0.10<br>0.23 |
| 52 | 210.14 | 95.6042 | 0.2251 | 122 → 132 | 0.15 |
| 53 | 208.12 | -32.6942 | 0.0157 | 119 → 130<br>124 → 135 | 0.17<br>0.17 |
| 55 | 206.53 | 30.5997 | 0.0228 | 119 → 129<br>124 → 135 | 0.11<br>0.11 |
| 56 | 205.11 | -159.092 | 0.1134 | 121 → 132<br>122 → 133 | 0.10<br>0.10 |
| 57 | 204.88 | -220.727 | 0.1386 | 123 → 134 | 0.09 |
| 58 | 204.63 | -31.5183 | 0.0487 | 121→ 132<br>123→ 135 | 0.12<br>0.13 |
| 60 | 202.45 | -72.4806 | 0.1782 | 120 → 131<br>122 → 134 | 0.13<br>0.09 |
| 61 | 202.00 | 228.1845 | 0.2204 | 122 → 134 | 0.19 |
| 62 | 201.12 | 236.9758 | 0.3268 | 120 → 132 | 0.19 |
| 63 | 200.06 | 36.0665 | 0.0614 | 116 → 127 | 0.39 |

[a] Excited states with f < 0.1 and R < ± 16.0 were not presented. All the excitation energies are shifted 11 nm according to the UV correction.
[b] All the strengths were in the velocity representation.
[c] Configurations with weights below 0.10 were not displayed.

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Table S3. The Cartesian coordinates of the optimized structure for **2** within PCM model ($CH_3OH$ solvent: dielectric constant ε=32.63) at B3LYP/6−31G(d) level.

| Atom | X | Y | Z |
|---|---|---|---|
| C | −1.250 | 0.628 | −0.748 |
| C | 1.614 | 0.324 | −0.049 |
| C | 1.711 | 1.792 | −0.550 |
| H | 0.906 | 0.358 | 0.789 |
| H | 2.503 | 2.299 | 0.017 |
| O | 2.048 | 1.772 | −1.938 |
| H | 2.074 | 2.694 | −2.241 |
| C | 2.920 | −0.164 | 0.575 |
| C | 2.872 | −1.034 | 1.667 |
| C | 4.180 | 0.273 | 0.141 |
| C | 4.035 | −1.469 | 2.306 |
| H | 1.909 | −1.384 | 2.033 |
| C | 5.348 | −0.142 | 0.771 |
| H | 4.247 | 0.927 | −0.723 |
| C | 5.279 | −1.020 | 1.859 |
| H | 3.971 | −2.145 | 3.158 |
| H | 6.321 | 0.197 | 0.431 |
| O | 6.460 | −1.397 | 2.443 |
| H | 6.265 | −1.997 | 3.180 |
| C | 0.945 | −0.568 | −1.103 |
| C | −0.446 | −0.436 | −1.363 |
| C | 1.642 | −1.537 | −1.855 |
| C | −1.093 | −1.287 | −2.282 |
| C | 0.993 | −2.380 | −2.761 |
| C | −0.375 | −2.253 | −2.974 |
| H | −2.144 | −1.139 | −2.496 |
| H | 1.552 | −3.124 | −3.322 |
| O | −0.951 | −3.094 | −3.885 |
| H | −1.891 | −2.871 | −3.963 |
| C | 0.424 | 2.544 | −0.277 |
| C | −0.864 | 1.872 | −0.337 |
| C | 0.444 | 3.842 | 0.108 |
| C | −2.042 | 2.609 | 0.097 |
| C | −0.768 | 4.627 | 0.469 |
| H | 1.383 | 4.382 | 0.211 |
| C | −2.041 | 3.907 | 0.470 |
| H | −2.942 | 4.434 | 0.764 |
| O | −0.670 | 5.817 | 0.776 |
| O | −3.133 | 1.803 | 0.074 |
| C | −2.766 | 0.512 | −0.479 |
| O | −3.463 | 0.354 | −1.689 |
| H | −4.410 | 0.349 | −1.468 |
| C | −3.127 | −0.555 | 0.550 |
| C | −2.941 | −0.314 | 1.916 |
| C | −3.624 | −1.804 | 0.155 |
| C | −3.245 | −1.288 | 2.862 |

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| | | | |
|---|---|---|---|
| H | −2.569 | 0.650 | 2.249 |
| C | −3.935 | −2.785 | 1.092 |
| H | −3.773 | −2.015 | −0.899 |
| C | −3.745 | −2.530 | 2.453 |
| H | −3.102 | −1.080 | 3.921 |
| H | −4.325 | −3.751 | 0.786 |
| O | −4.066 | −3.523 | 3.331 |
| H | −3.891 | −3.218 | 4.235 |
| O | 2.990 | −1.654 | −1.696 |
| H | 3.312 | −2.363 | −2.274 |

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Table S4. TDDFT results for the optimized conformer of compound (7a*R*, 8a*R*, 7b*R*)-**2** (200nm<λ<600nm). The TDDFT calculations are done at the level of B3LYP/6−31G(d) in the PCM model ($CH_3OH$ solvent: dielectric constant ε=32.63).

| Transition | Excitation energy[a] (nm) | Rotatory Strength $R$[b] ($10^{-40}$ cgs) | Oscillator Strength $f$[b] | Dominant Contributions[c] | Weight |
|---|---|---|---|---|---|
| 2 | 468.92 | 20.2392 | 0.0151 | 125 → 127<br>126 → 127 | 0.11<br>0.26 |
| 4 | 388.61 | −28.0819 | 0.1250 | 122 → 127<br>124 → 127 | 0.20<br>0.15 |
| 5 | 378.57 | −70.7110 | 0.2493 | 122 → 127<br>124 → 127 | 0.20<br>0.20 |
| 6 | 362.02 | 16.6995 | 0.0739 | 121 → 127 | 0.36 |
| 9 | 296.93 | −21.5154 | 0.0409 | 117 → 127 | 0.36 |
| 10 | 290.56 | −22.1269 | 0.1405 | 117 → 127<br>119 → 127 | 0.13<br>0.22 |
| 24 | 233.72 | −22.6919 | 0.0247 | 114 → 127<br>124 → 130 | 0.13<br>0.19 |
| 33 | 222.26 | −18.2217 | 0.0267 | 124 → 131 | 0.29 |
| 36 | 218.74 | −62.1837 | 0.0633 | 122 → 127 | 0.11 |
| 37 | 218.49 | 19.9538 | 0.0243 | 122 → 129 | 0.12 |
| 38 | 217.54 | 39.8335 | 0.0512 | 123 → 129 | 0.10 |
| 39 | 216.85 | 28.0179 | 0.0145 | 121 → 129<br>122 → 130 | 0.14<br>0.21 |
| 41 | 212.80 | 18.3992 | 0.0415 | 112 → 127 | 0.18 |
| 43 | 211.46 | 49.9723 | 0.0492 | 125 → 134 | 0.06 |
| 44 | 210.98 | −53.7444 | 0.0444 | 121 → 130 | 0.22 |
| 45 | 210.72 | 33.4481 | 0.0130 | 111 → 127 | 0.13 |

[a] Excited states with f < 0.1 and R < ± 15.0 were not presented.
[b] All the strengths were in the velocity representation.
[c] Configurations with weights below 0.10 were not displayed.

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Table S5. The Cartesian coordinates of the optimized structure for **3** within PCM model ($CH_3OH$ solvent: dielectric constant ε=32.63) at B3LYP/6-31G(d) level.

| Atom | X | Y | Z |
|---|---|---|---|
| C | 1.050 | 0.814 | −0.046 |
| C | −1.970 | 1.409 | 0.808 |
| C | −1.796 | 0.118 | −0.048 |
| C | −3.141 | −0.525 | −0.389 |
| C | −4.243 | −0.496 | 0.474 |
| C | −3.316 | −1.124 | −1.643 |
| C | −5.472 | −1.039 | 0.104 |
| H | −4.133 | −0.058 | 1.462 |
| C | −4.534 | −1.682 | −2.029 |
| H | −2.480 | −1.155 | −2.341 |
| C | −5.624 | −1.639 | −1.153 |
| H | −6.318 | −1.005 | 0.791 |
| H | −4.657 | −2.141 | −3.008 |
| O | −6.804 | −2.188 | −1.576 |
| H | −7.482 | −2.092 | −0.872 |
| C | −0.941 | 2.458 | 0.432 |
| C | 0.356 | 2.077 | 0.066 |
| C | −1.245 | 3.821 | 0.427 |
| C | 1.301 | 3.066 | −0.252 |
| C | −0.279 | 4.791 | 0.086 |
| C | 1.029 | 4.424 | −0.261 |
| C | −0.707 | −0.855 | 0.460 |
| C | 0.667 | −0.543 | 0.240 |
| C | −0.977 | −2.107 | 1.024 |
| C | 1.734 | −1.507 | 0.328 |
| C | 0.050 | −3.047 | 1.204 |
| C | 1.358 | −2.787 | 0.832 |
| C | 4.172 | −2.075 | −0.155 |
| C | 5.448 | −1.691 | −0.555 |
| H | 4.020 | −3.113 | 0.093 |
| C | 4.712 | 0.574 | −0.844 |
| C | 5.730 | −0.355 | −0.899 |
| H | 4.904 | 1.611 | −1.107 |
| O | −2.240 | −2.425 | 1.408 |
| H | −2.273 | −3.365 | 1.694 |
| O | 2.301 | −3.760 | 0.988 |
| H | 1.879 | −4.576 | 1.340 |
| H | −0.195 | −4.020 | 1.633 |
| C | 2.348 | 1.135 | −0.368 |
| C | 3.410 | 0.203 | −0.449 |
| C | 3.103 | −1.151 | −0.078 |
| H | 6.735 | −0.068 | −1.206 |
| O | 6.403 | −2.667 | −0.599 |
| H | 7.258 | −2.283 | −0.896 |
| O | 2.524 | 2.495 | −0.529 |

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| | | | |
|---|---|---|---|
| H | −1.414 | 0.471 | −1.016 |
| H | −2.968 | 1.838 | 0.609 |
| O | −1.880 | 1.038 | 2.191 |
| H | −2.119 | 1.828 | 2.720 |
| O | −0.567 | 6.125 | 0.076 |
| H | −1.502 | 6.268 | 0.344 |
| H | 1.773 | 5.173 | −0.515 |
| H | −2.251 | 4.151 | 0.688 |

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Table S6**.** TDDFT results for the optimized conformer of compound (7a*R*, 8a*R*)-**3** (200nm<λ<600nm). The TDDFT calculations are done at the level of B3LYP/6−31G(d) in the PCM model ($CH_3OH$ solvent: dielectric constant ε=32.63).

| Transition | Excitation energy[a] (nm) | Rotatory Strength $R^b$ ($10^{-40}$ cgs) | Oscillator Strength $f^b$ | Dominant Contributions[c] | Weight |
|---|---|---|---|---|---|
| 1 | 357.47 | −23.4709 | 0.3012 | 121 → 122 | 0.36 |
| 2 | 343.16 | −21.2557 | 0.1386 | 121 → 123 | 0.32 |
| 3 | 308.97 | −12.1778 | 0.1331 | 120 → 122 | 0.31 |
| 5 | 287.95 | 22.7403 | 0.0440 | 121 → 124 | 0.41 |
| 6 | 285.12 | −17.2423 | 0.1033 | 118 → 122 | 0.30 |
| 7 | 279.25 | −21.1226 | 0.4884 | 120 → 123 | 0.28 |
| 9 | 271.95 | 17.1501 | 0.2131 | 121 → 125 | 0.26 |
| 11 | 262.49 | 59.0263 | 0.1940 | 118 → 123<br>120 → 124<br>121 → 126 | 0.14<br>0.33<br>0.15 |
| 12 | 255.36 | 0.1334 | 0.1380 | 117 → 122 | 0.34 |
| 13 | 249.96 | 25.8374 | 0.0631 | 120 → 124 | 0.23 |
| 21 | 238.85 | −23.7552 | 0.0146 | 120 → 126 | 0.36 |
| 22 | 232.08 | 21.3873 | 0.0765 | 119 → 125 | 0.39 |
| 23 | 228.91 | −8.8636 | 0.2678 | 118 → 124 | 0.25 |
| 31 | 215.64 | 37.8311 | 0.0254 | 118 → 126 | 0.26 |
| 40 | 203.83 | −15.7421 | 0.0359 | 116 → 124 | 0.31 |

[a] Excited states with f < 0.1 and R < ± 15.0 were not presented.
[b] All the strengths were in the velocity representation.
[c] Configurations with weights below 0.10 were not displayed.