

Supplementary methods for: (Suppl S1)

Plumbagin structure

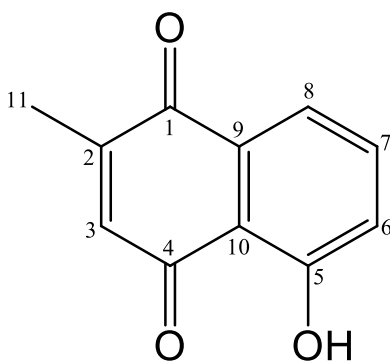


Figure S1: Plumbagin structure

NMR Spectroscopy

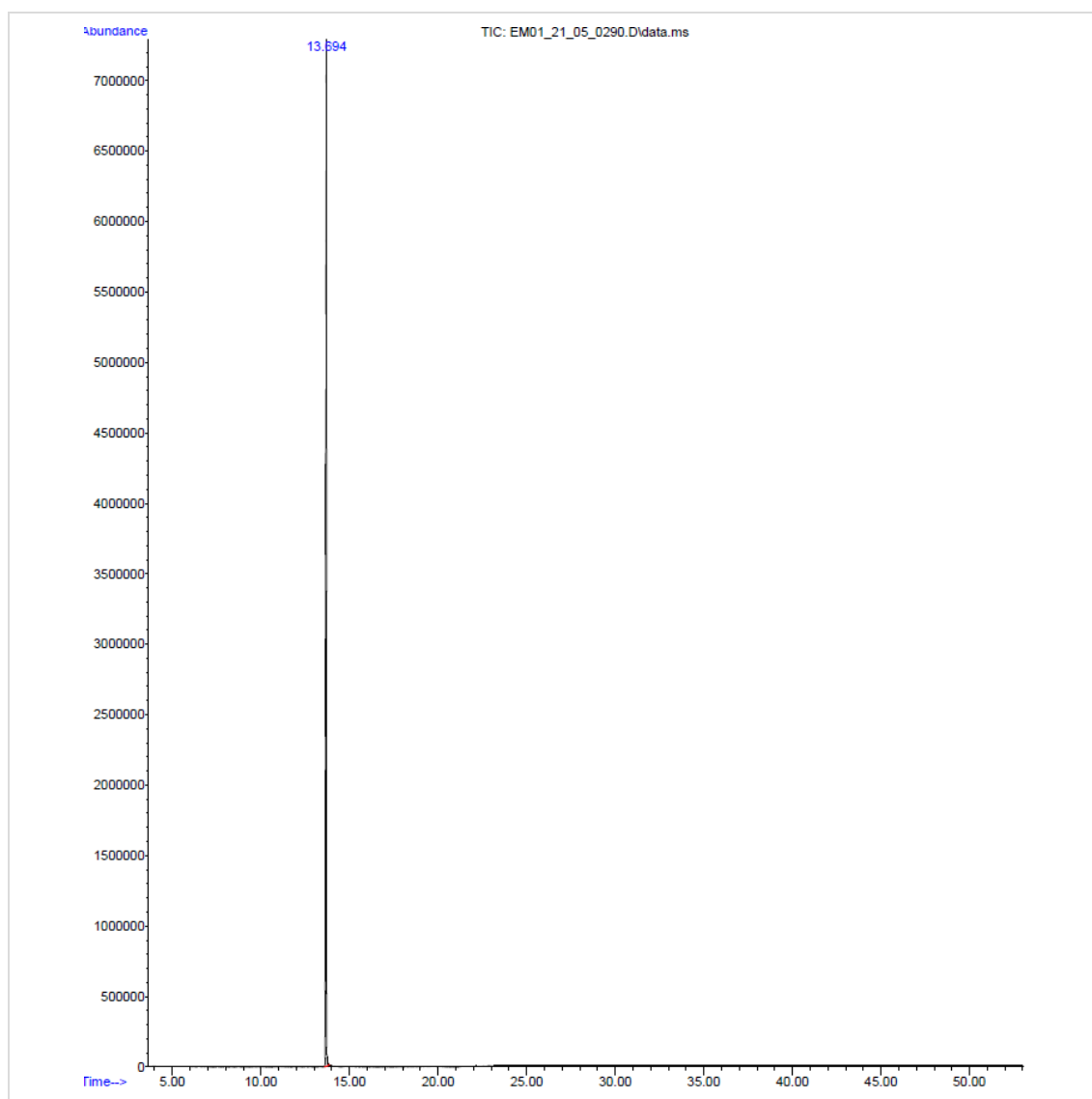


Figure S2: GC-MS for Plumbagin

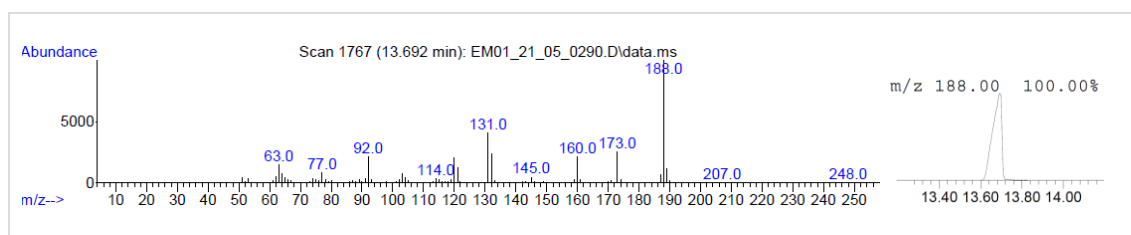


Figure S3: GC-MS for Plumbagin (CG-EM m/z 188 $[M]^+$ (100), 131 (41), 173 $[M - CH_3]$ (25), 132 (24), 160 (21)).

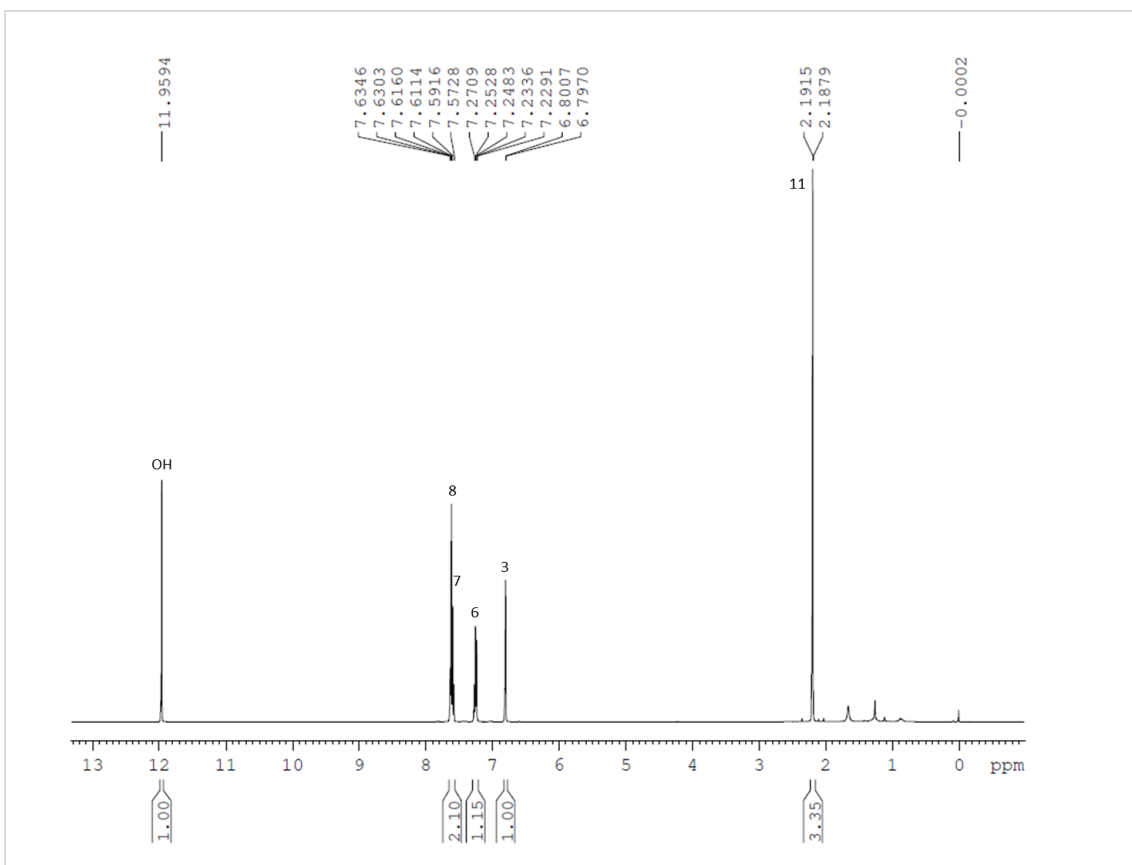


Figure S4: ¹H NMR spectrum for Plumbagin

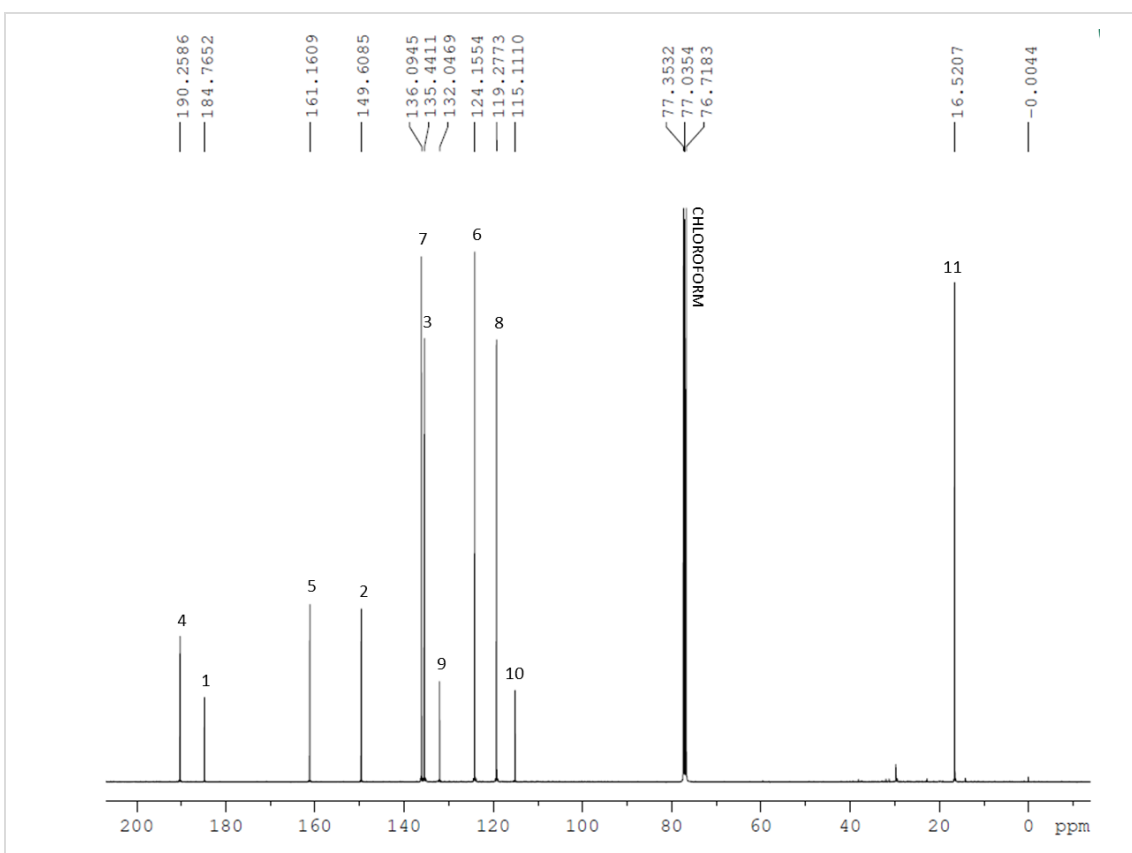
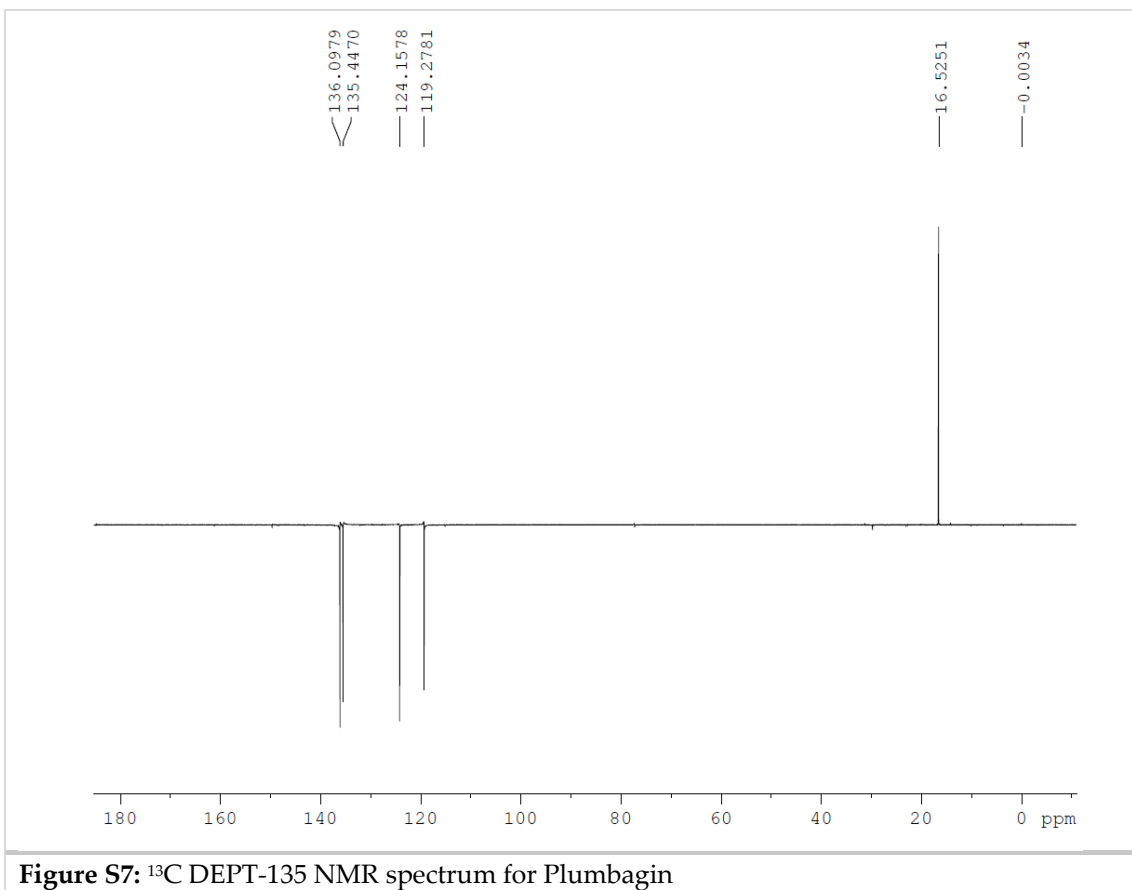
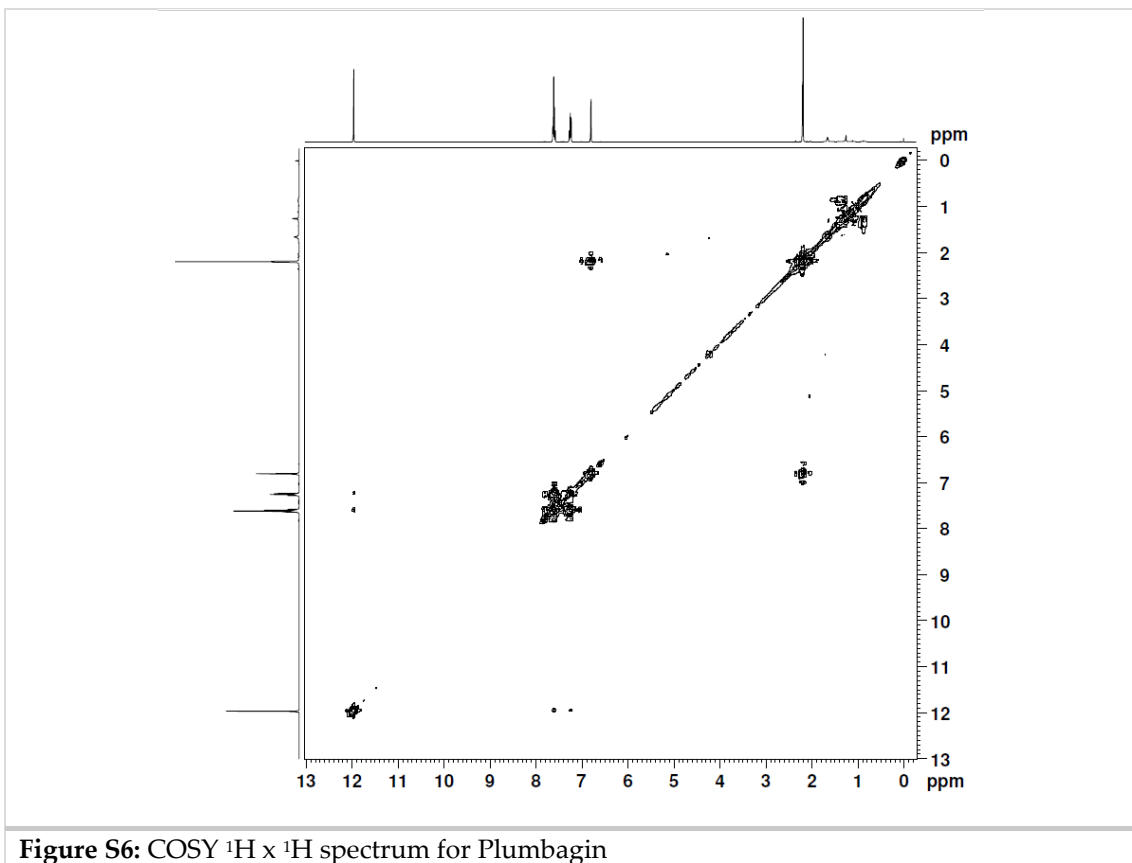


Figure S5: ¹³C NMR spectrum for Plumbagin



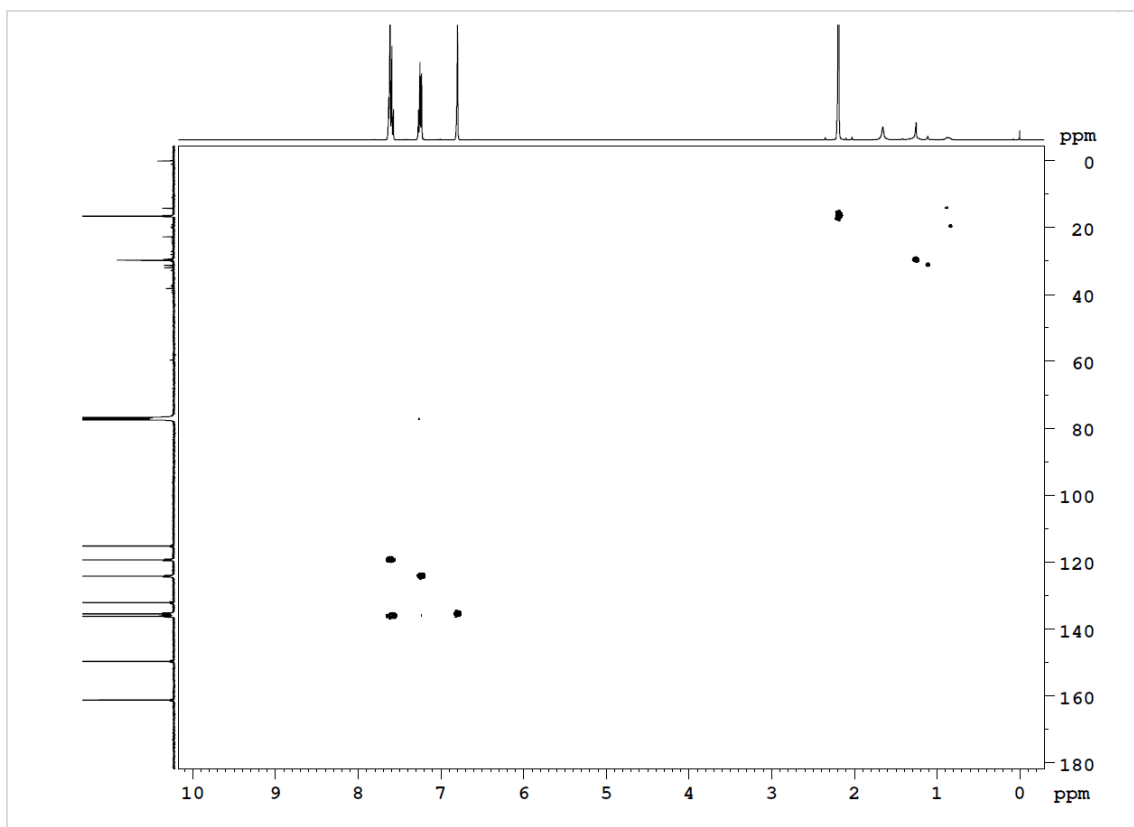


Figure S8: HSQC $^1\text{H} \times ^{13}\text{C}$ spectrum for Plumbagin

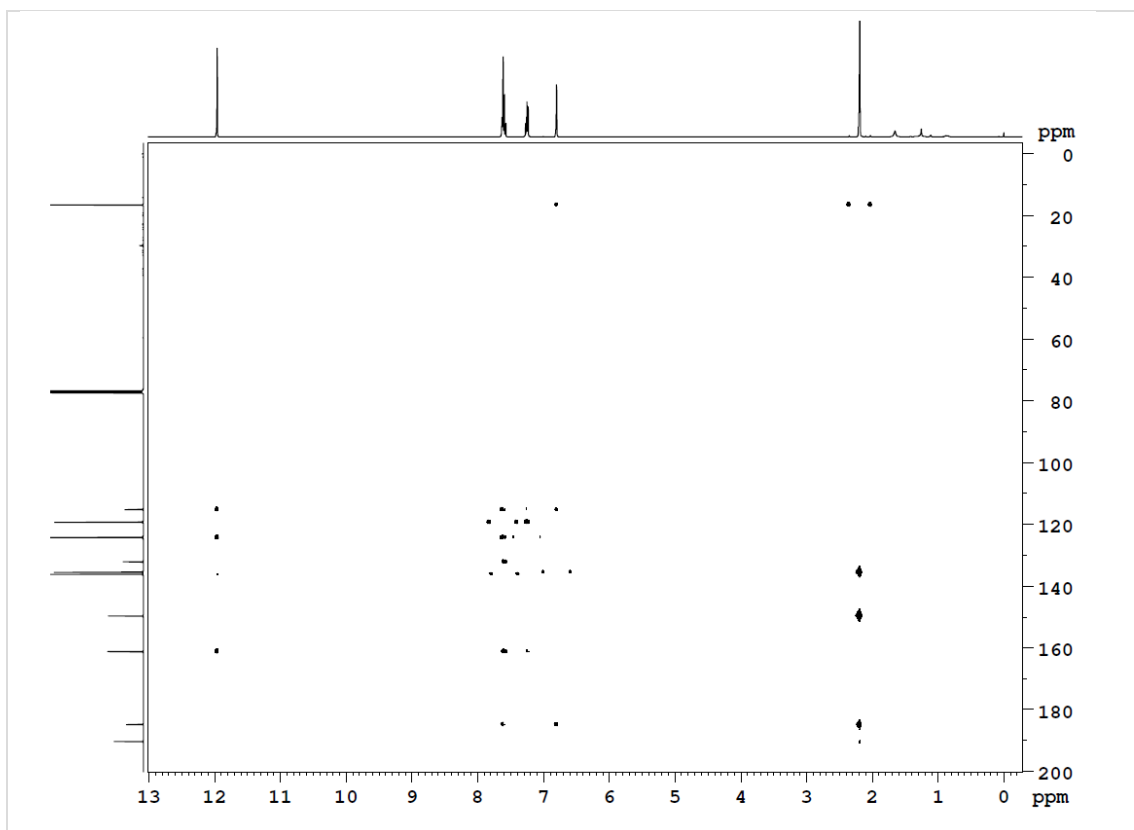


Figure S9: $^1\text{H} \times ^{13}\text{C}$ -HMBC spectrum for Plumbagin

Table S1: NMR data of the isolated plumbagin

| Position | The isolated plumbagin ^a | | The reported plumbagin ^a | | The reported plumbagin ^a | |
|----------|---|---------------------|-------------------------------------|---------------------|--------------------------------------|---------------------|
| | ¹ H NMR | ¹³ C NMR | ¹ H NMR | ¹³ C NMR | ¹ H NMR | ¹³ C NMR |
| 1 | | 184.4 | | 184.7 | | 184.7 |
| 2 | | 149.6 | | 149.5 | | 149.6 |
| 3 | 6.80 (<i>d</i> , H3; <i>J</i> =1.48) | 135.4 | 6.8 (<i>d</i> , H3) | 135.4 | 6.7 (<i>s</i> , H-3) | 136.0 |
| 4 | | 190.2 | | 190.2 | | 190.2 |
| 5 | | 161.1 | | 161.1 | | 161.1 |
| 6 | 7.24 (<i>dd</i> , H6; <i>J</i> ₁ =7.68, <i>J</i> ₂ =1.80) | 124.1 | 7.23 (<i>m</i> , H6) | 124.1 | 7.22 – 7.20 (<i>m</i> , H-6) | 124.1 |
| 7 | 7.59 (<i>t</i> , H7; <i>J</i> =7.52) | 136.0 | 7.60 (<i>m</i> , H7) | 136.0 | 7.59 (<i>m</i> , H7) | 135.4 |
| 8 | 7.62 (<i>dd</i> , H8; <i>J</i> ₁ =7.56, <i>J</i> ₂ =1.72) | 119.2 | 7.60 (<i>m</i> , H8) | 119.0 | 7.55 (<i>m</i> , H8) | 119.2 |
| 9 | | 132.0 | | 132.0 | | 132.0 |
| 10 | | 115.1 | | 115.0 | | 115.2 |
| 11 | 2.19 (<i>d</i> , CH ₃ ; <i>J</i> = 1.44) | 16.5 | 2.18 (<i>d</i> , H11) | 16.5 | 2.16 (<i>s</i> , -CH ₃) | 16.1 |
| -OH | 11.96 (<i>s</i> , OH) | | 11.95 | | 11.94 (<i>brs</i> , - OH) | |

^a Measured in CDCl₃