Chemical constituents and hepatoprotective properties of *Rhododendron simsii* Planch extract in Con A-induced autoimmune hepatitis

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S1. 1H NMR spectrum of quercetin 3-O-α-L-rhamnoside



S2. 13C NMR spectrum of quercetin 3-O-α-L-rhamnoside



S3. 1H NMR spectrum of Tamarixetin 3-rhamnoside



S4. 13C NMR spectrum of Tamarixetin 3-rhamnoside



S5. 1H NMR spectrum of isoquercitrin



S6. 13C NMR spectrum of isoquercitrin



S7. 1H NMR spectrum of hyperoside



S8. 13C NMR spectrum of hyperoside



S9. 1H NMR spectrum of myricetin-3-O-α-L-rhamnopyranoside



S10. 13C NMR spectrum of myricetin-3-O-α-L-rhamnopyranoside



S11. 1H NMR spectrum of afzelin



S12. 13C NMR spectrum of afzelin



S13. 1H NMR spectrum of quercetin-3-O-α-L-arabinofuranoside



S14. 13C NMR spectrum of quercetin-3-O-α-L-arabinofuranoside



S15. 1H NMR spectrum of quercetin-3-O-α-D-arabinopyranoside



S16. 13C NMR spectrum of quercetin-3-O-α-D-arabinopyranoside



S17. 1H NMR spectrum of (+)-catechin



S18. 13C NMR spectrum of (+)-catechin



S19. 1H NMR spectrum of kaempferol



S20. 13C NMR spectrum of kaempferol



S21. 1H NMR spectrum of dihydromyricetin



S22. 13C NMR spectrum of dihydromyricetin



S23. 1H NMR spectrum of quercetin



S24. 13C NMR spectrum of quercetin



S25. 1H NMR spectrum of vanillic acid



S26. 13C NMR spectrum of vanillic acid



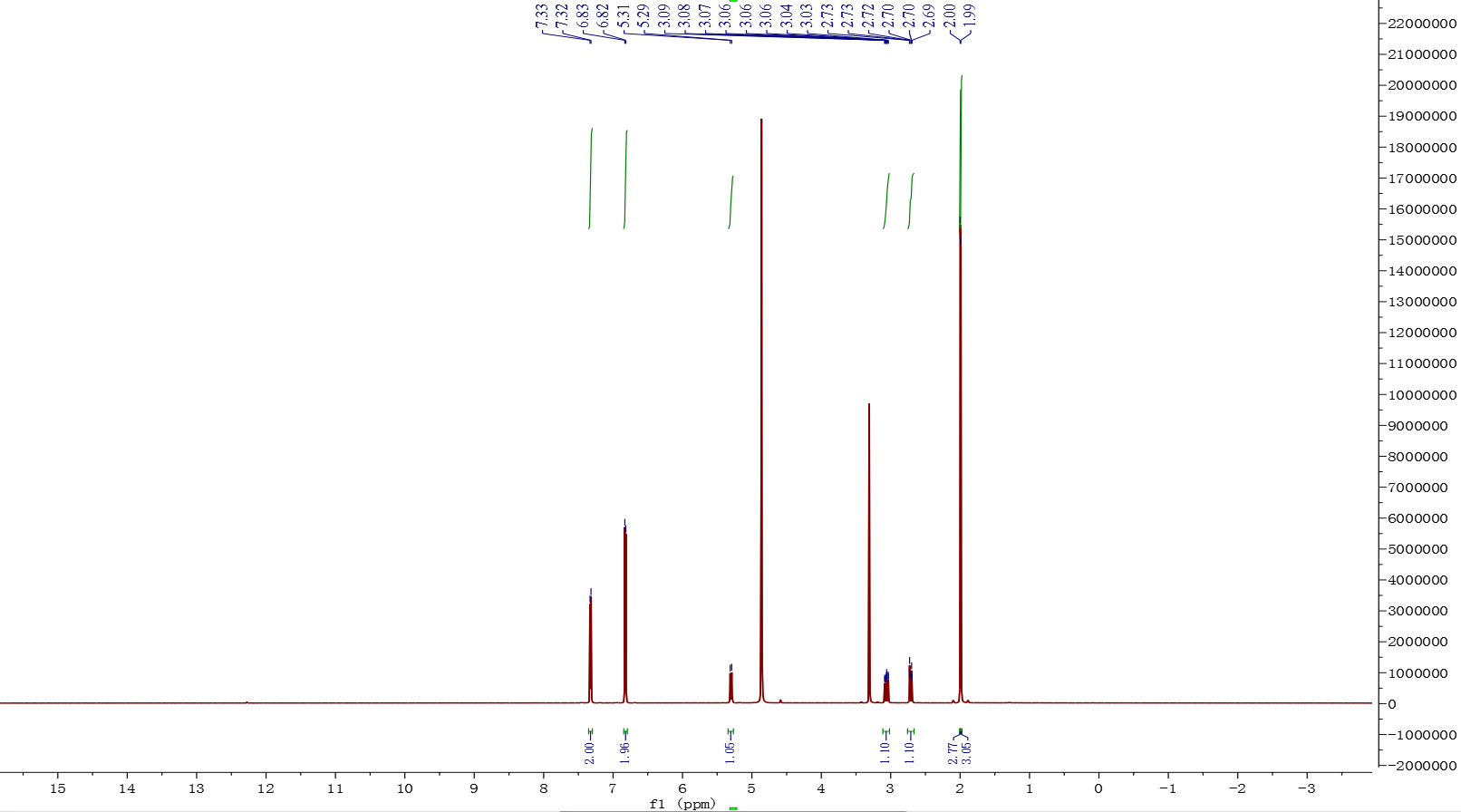
S27. 1H NMR spectrum of Gallic acid



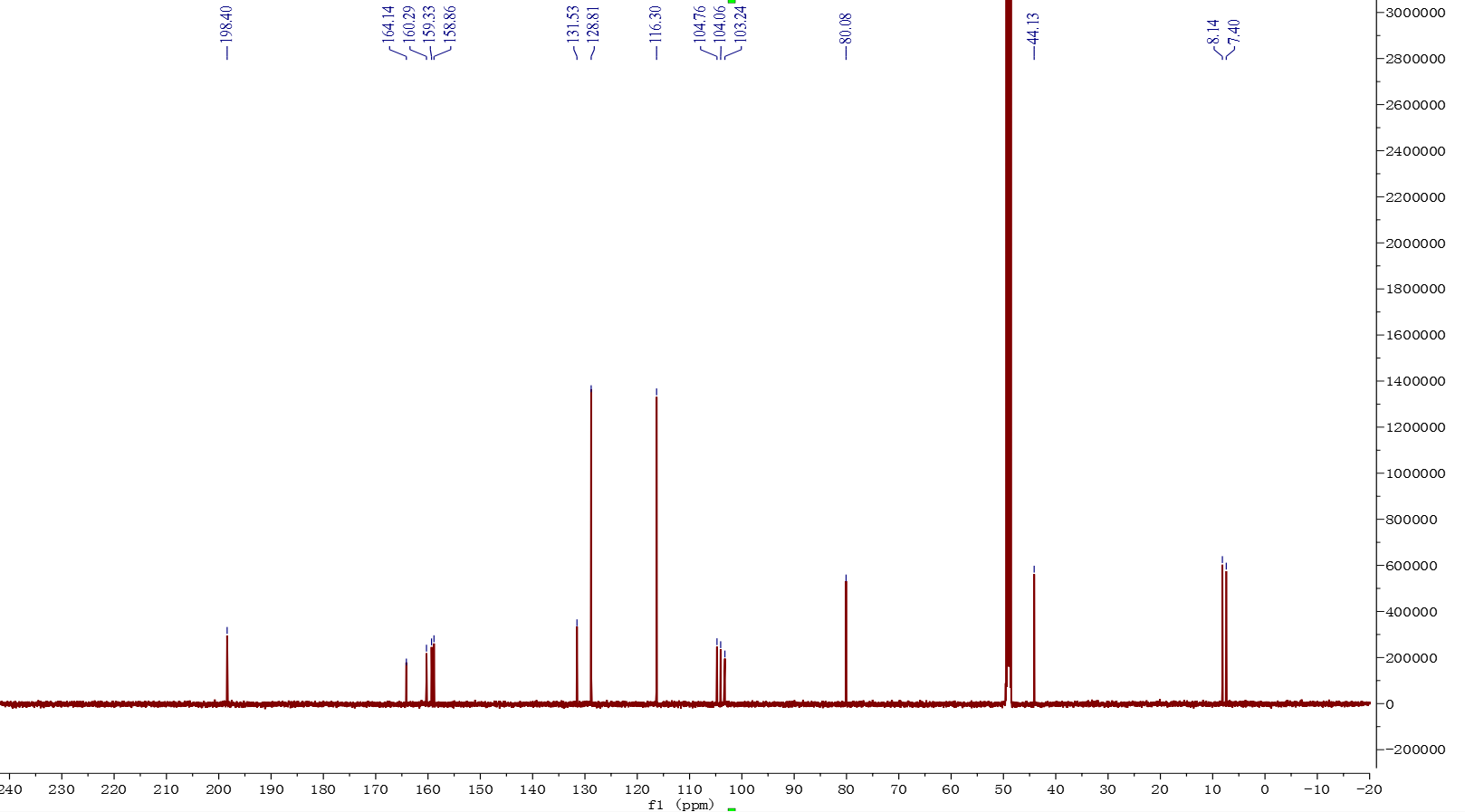
S28. 13C NMR spectrum of Gallic acid



S29. 1H NMR spectrum of Farrerol



S30. 13C NMR spectrum of Farrerol



**Table 2.** 1H NMR data of compounds 1–8 (400 MHz, *J* in Hz)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **no** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** |
| 6 | 6.22 (d, 1.9) | 6.40 (d, 1.8) | 6.21 (d) | 6.23 (d, 1.9) | 6.22 (d, 2.1) | 6.23 (d, 2.0) | 6.20 (d, 2.1) | 6.19 (d, 1.7) |
| 8 | 6.39 (d, 1.9) | 6.23 (d, 1.9) | 6.41 (s) | 6.43 (d, 1.7) | 6.39 (d, 2.1) | 6.41 (d, 1.9) | 6.39 (d, 2.0) | 6.39 (s) |
| 1’ |  |  |  |  |  |  |  |  |
| 2’ | 7.36 (d, 2.0) | 7.36 (d, 2.1) | 7.73 (d, 2.1) | 7.87 (d, 2.0) | 6.97 (s) | 7.79 (d, 8.7) | 7.52 (d, 2.1) | 7.74 (d, 2.1) |
| 3’ |  |  |  |  |  | 6.96 (d, 8.8) |  |  |
| 5’ | 6.93 (d, 8.3) | 7.10 (d, 8.5) | 6.89 (d, 8.5) | 6.89 (d, 8.5) |  | 6.96 (d, 8.8) | 6.89 (d, 8.3) | 6.86 (d, 8.5) |
| 6’ | 7.33 (dd, 8.3, 2.0) | 7.44 (dd, 8.5, 2.1) | 7.61 (dd, 8.5, 2.0) | 7.61 (dd, 8.5, 2.1) | 6.97 (s) | 7.79 (d, 8.7) | 7.49 (dd, 8.3, 2.2) | 7.57 (dd, 8.5, 2.0) |
| 1’’ | 5.37 (d, 1.4) | 5.40 (d, 1.5) | 5.29 (d, 7.5) | 5.19 (d, 7.8) | 5.33 (d, 1.4) | 5.40 (d, 1.6) | 5.46 (s) | 5.15 (d, 6.6) |
| 2’’ | 3.77 (dd, 9.3, 3.3) | 4.24 (dd, 3.2, 1.6) | 3.51 (m) | 3.83 (d, 8.0) | 4.24 (dd, 3.2, 1.7) | 4.24 (dd, 3.3, 1.7) | 4.32 (dd, 3.0, 0.9) | 3.89 (dd, 8.4, 6.7) |
| 3’’ | 3.46 (m) | 3.75 (dd, 9.0, 3.3) | 3.45 (t, 8.8) | 3.58 (m) | 3.81 (dd, 9.5, 3.3) | 3.73 (d, 5.8) | 3.90 (dd, 5.2, 3.0) | 3.64 (dd, 8.4, 3.0) |
| 4’’ | 3.37 (m) | 3.35 (m) | 3.34 (t, 10.0) | 3.88 (d, 3.2) | 3.37 (m) | 3.33 (m) | 3.84 (q, 4.7) | 3.80 (m, overlap) |
| 5’’*a* | 4.24 (dd, 3.1, 1.4) | 3.35 (m) | 3.4 (m) | 3.50 (t, 6.0) | 3.54 (m) | 3.35 (m) | 3.49 (dd, 4.1, 2.0) | 3.82 (m, overlap ) |
| 5’’*b* | 3.44 (m) |
| 6’’*a* | 0.96 (d, 6.1) | 0.95 (d, 5.5) | 3.74 (dd, 11.9, 2.1) | 3.67 (dd, 11.2, 6.0) | 0.98 (d, 6.2) | 0.94 (d, 5.6) |  |  |
| 6’’*b* | 3.60 (dd, 11.9, 5.3) | 3.57 (m) |  |  |

record in CD3OD

**Table 3**. 1H NMR data of compounds 9–15 (400 MHz, *J* in Hz)

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **No** | **9** | **10** | **11** | **12** | **13** | **14** | **15** |
| 2 | 4.58 (d, 7.5) |  | 4.85 (d, 11.4) |  | 7.57 (d, 8.7) | 6.93 (s) | 5.30 (d, 12.8) |
| 3 | 3.99 (td, 7.9, 5.4) |  | 4.48 (d, 11.4) |  | 6.85 (d, 8.7) |  | 3.06 (dd, 16.9, 12.9) |
| 2.71 (dd, 16.9, 2.2) |
| 4*a* | 2.87 (dd, 16.1, 5.4) |  |  |  |  |  |  |
| 4*b* | 2.52 (dd, 16.1, 8.2) |  |  |  |  |  |  |
| 6 | 5.95 (d, 2.3) | 6.20 (d, 1.7) | 5.90 (d, 2.1) | 6.19 (s) | 7.58 (s) | 6.93 (s) |  |
| 8 | 5.87 (d, 2.2) | 6.42 (s) | 5.94 (d, 2.1) | 6.40 (s) |  |  |  |
| 2’ | 6.86 (d, 1.9) | 8.11 (d, 8.6) | 6.54 (s) | 7.76 (s) |  |  | 7.32 (d, 8.2) |
| 3’ |  | 6.93 (d, 8.9) |  |  |  |  | 6.82 (d, 8.6) |
| 5’ | 6.78 (d, 8.1) | 6.93 (d, 8.9) |  | 6.91 (d, 8.5) |  |  | 6.82 (d, 8.6) |
| 6’ | 6.74 (dd, 8.1, 1.9) | 8.11 (d, 8.6) | 6.54 (s) | 7.66 (d, 8.3) |  |  | 7.32 (d, 8.2) |
| 3,5-OH |  |  |  |  |  | 9.22 (s) |  |
| 4-OH |  |  |  |  |  | 8.87 (s) |  |
| 6-Me |  |  |  |  |  |  | 2.00 (s) |
| 8-Me |  |  |  |  |  |  | 1.99 (s) |
| -OMe |  |  |  |  | 3.91 (s) |  |  |
| -COOH |  |  |  |  |  | 12.27 (s) |  |

All except 14 (DMSO-*d6*) are record in CD3OD.

**Table 4**. 13C NMR data of compounds 1–15 (150 MHz)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **no** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** | **11** | **12** | **13** | **14** | **15** |
| 1 |  |  |  |  |  |  |  |  |  |  |  |  | 123.3 | 120.9 |  |
| 2 | 158.5 | 158.9 | 158.6 | 158.8 | 159.9 | 159.4 | 159.5 | 159.0 | 83.0 | 148.2 | 85.4 | 148.1 | 125.4 | 109.2 | 80.1 |
| 3 | 136.2 | 136.4 | 135.7 | 136.0 | 136.4 | 136.4 | 135.0 | 136.2 | 68.9 | 137.4 | 73.8 | 137.3 | 115.9 | 145.8 | 44.1 |
| 4 | 179.6 | 179.6 | 179.6 | 179.8 | 179.8 | 179.8 | 180.1 | 180.0 | 28.7 | 177.6 | 198.4 | 177.4 | 152.8 | 138.4 | 198.4 |
| 5 | 159.3 | 158.6 | 163.2 | 163.3 | 163.4 | 163.4 | 163.2 | 163.6 | 157.9 | 162.6 | 165.5 | 162.6 | 148.8 | 145.8 | 160.3 |
| 6 | 99.8 | 94.7 | 100.0 | 100.3 | 99.9 | 99.9 | 100.0 | 100.5 | 96.4 | 99.4 | 97.4 | 99.5 | 113.9 | 109.2 | 104.8 |
| 7 | 165.9 | 166.0 | 166.2 | 159.1 | 166.1 | 166.1 | 166.2 | 166.7 | 157.7 | 165.7 | 168.8 | 166.2 |  |  | 159.7 |
| 8 | 94.7 | 99.9 | 94.8 | 95.0 | 94.8 | 94.9 | 94.9 | 95.3 | 95.6 | 94.6 | 96.4 | 94.6 |  |  | 103.3 |
| 9 | 163.2 | 163.2 | 159.1 | 159.1 | 158.6 | 158.7 | 158.7 | 159.2 | 157.0 | 158.4 | 164.6 | 158.4 |  |  | 164.1 |
| 10 | 105.9 | 105.9 | 105.8 | 105.9 | 105.9 | 106.1 | 105.7 | 106.1 | 100.9 | 104.7 | 101.9 | 104.5 |  |  | 104.1 |
| 1’ | 122.9 | 124.3 | 123.3 | 123.3 | 122.0 | 122.8 | 123.1 | 123.6 | 132.3 | 123.9 | 129.2 | 124.3 |  |  | 131.5 |
| 2’ | 116.3 | 116.6 | 116.1 | 116.4 | 109.7 | 132.0 | 116.9 | 118.0 | 115.4 | 130.8 | 108.1 | 116.1 |  |  | 128.8 |
| 3’ | 146.4 | 147.7 | 150.0 | 146.1 | 147.0 | 116.7 | 146.5 | 146.5 | 146.4 | 116.4 | 147.0 | 148.9 |  |  | 116.3 |
| 4’ | 149.8 | 151.6 | 146.0 | 150.2 | 138.0 | 161.7 | 150.0 | 150.5 | 146.5 | 160.1 | 135.0 | 146.3 |  |  | 158.9 |
| 5’ | 116.9 | 112.4 | 117.7 | 118.1 | 147.0 | 116.7 | 116.6 | 116.7 | 116.2 | 116.4 | 147.0 | 116.4 |  |  | 116.3 |
| 6’ | 122.8 | 122.7 | 123.2 | 123.2 | 109.7 | 132.0 | 123.2 | 123.4 | 120.2 | 130.8 | 108.1 | 121.8 |  |  | 128.8 |
| 1’’ | 103.5 | 103.5 | 104.4 | 105.7 | 103.8 | 103.6 | 109.6 | 105.2 |  |  |  |  |  |  |  |
| 2’’ | 72.0 | 71.9 | 75.8 | 73.5 | 72.2 | 72.1 | 83.5 | 73.4 |  |  |  |  |  |  |  |
| 3’’ | 72.1 | 72.0 | 78.2 | 75.4 | 72.1 | 72.3 | 78.8 | 74.7 |  |  |  |  |  |  |  |
| 4’’ | 73.2 | 72.1 | 71.3 | 70.3 | 73.5 | 73.3 | 88.1 | 69.7 |  |  |  |  |  |  |  |
| 5’’ | 71.9 | 73.2 | 78.5 | 77.5 | 72.0 | 72.2 | 62.7 | 67.5 |  |  |  |  |  |  |  |
| 6’’ | 17.6 | 17.7 | 62.7 | 62.2 | 17.8 | 17.8 |  |  |  |  |  |  |  |  |  |
| 4’-OMe |  | 56.4 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| 5-OMe |  |  |  |  |  |  |  |  |  |  |  |  | 56.5 |  |  |
| 6-Me |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 8.1 |
| 8-Me |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 7.4 |
| COOH |  |  |  |  |  |  |  |  |  |  |  |  | 170.3 | 167.9 |  |

All except 14 (DMSO-*d6*) are record in CD3OD.