

Supporting information for

Ellagitannins of *Davidaia involucrata*. I. Structure of Davicratinic Acid A, and Effects of *Davidaia* Tannins on Drug-resistant Bacteria and Human Oral Squamous Cell Carcinoma.

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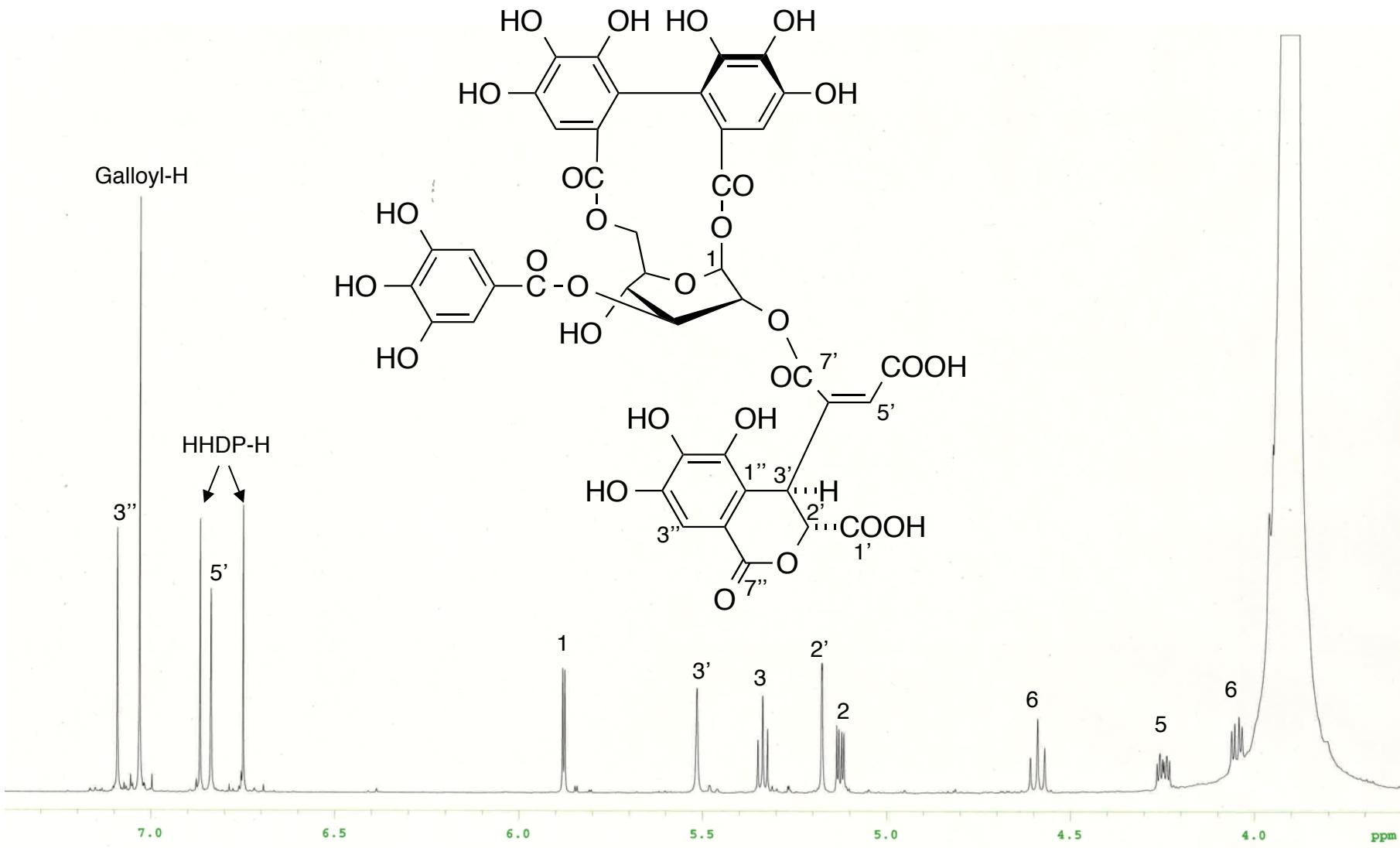
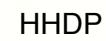
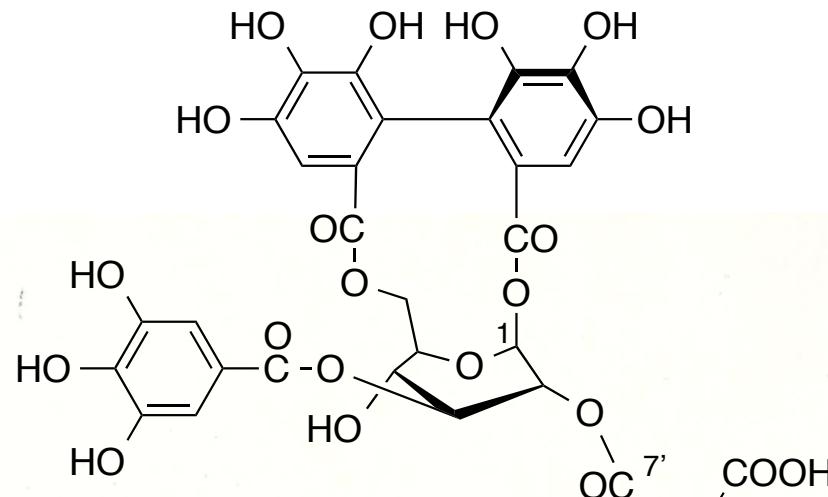


Figure S1. ^1H NMR spectrum of davicratinic acid A (**5**) in acetone- d_6 /D₂O=9/1.



Carbonyl carbons

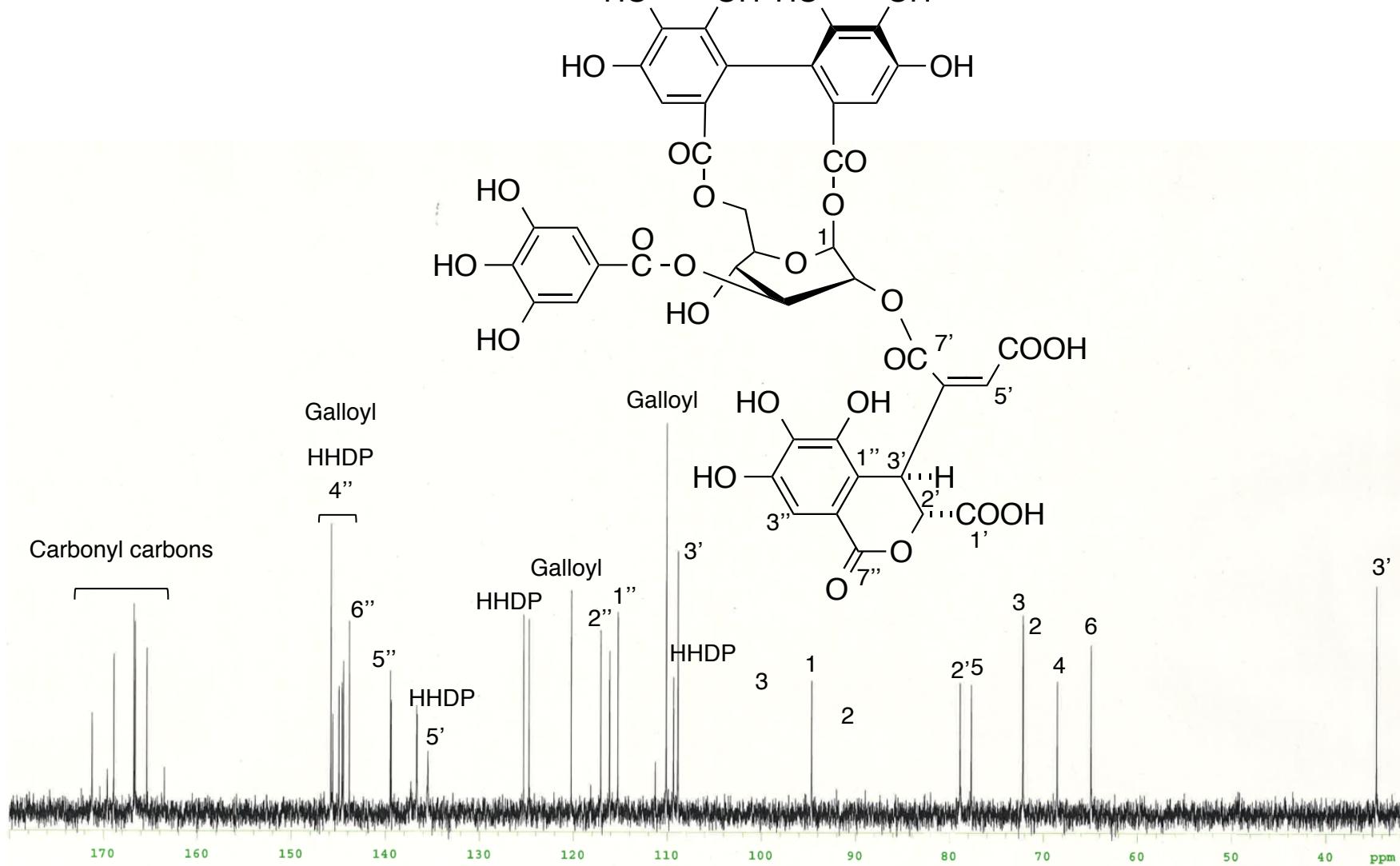


Figure S2. ^{13}C NMR spectrum of davicratinic acid A (**5**) in acetone- d_6 /D₂O=9/1.

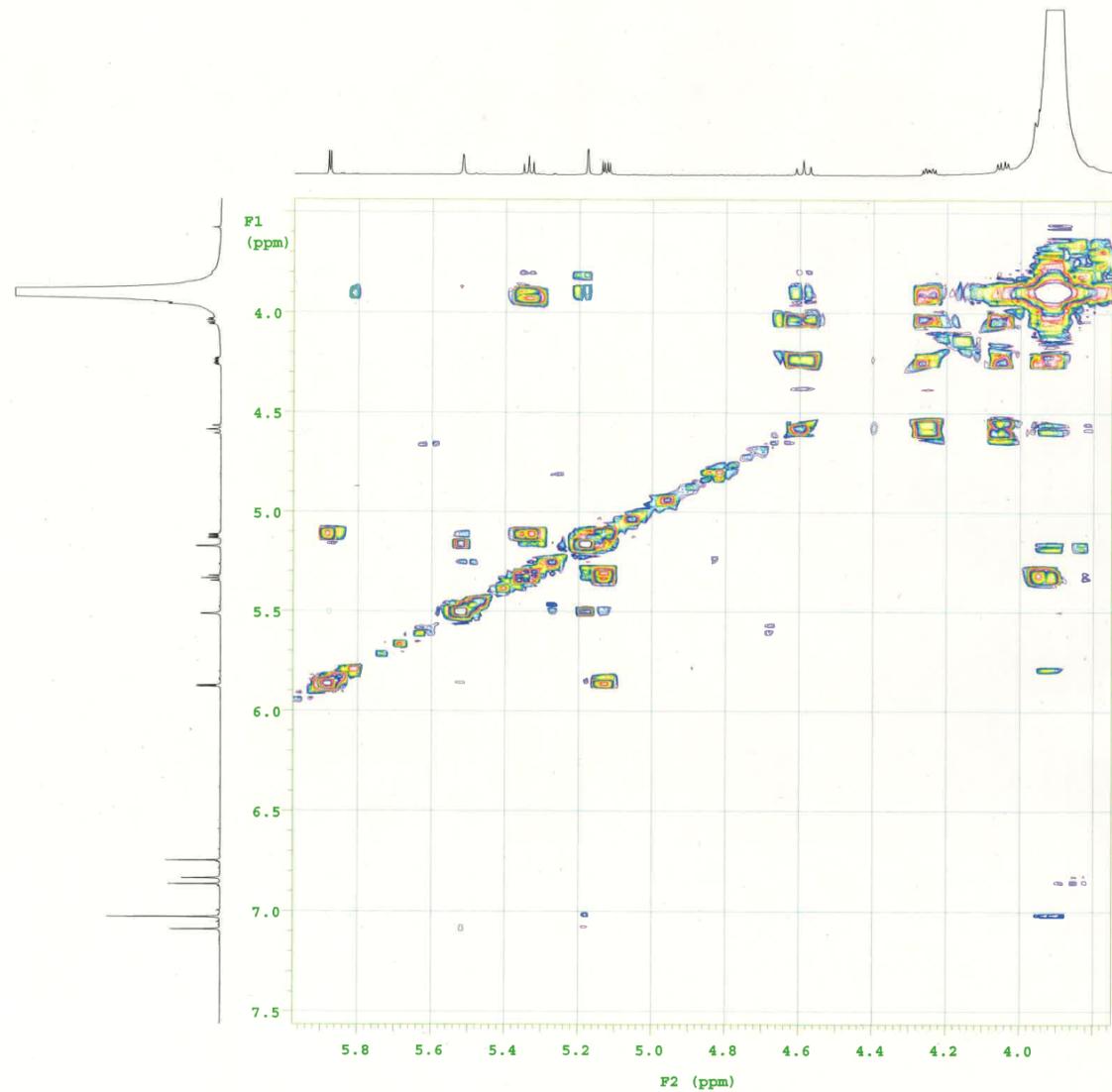


Figure S3. ^1H - ^1H COSY spectrum of davicratinic acid A (**5**) in acetone- d_6 /D₂O=9/1.

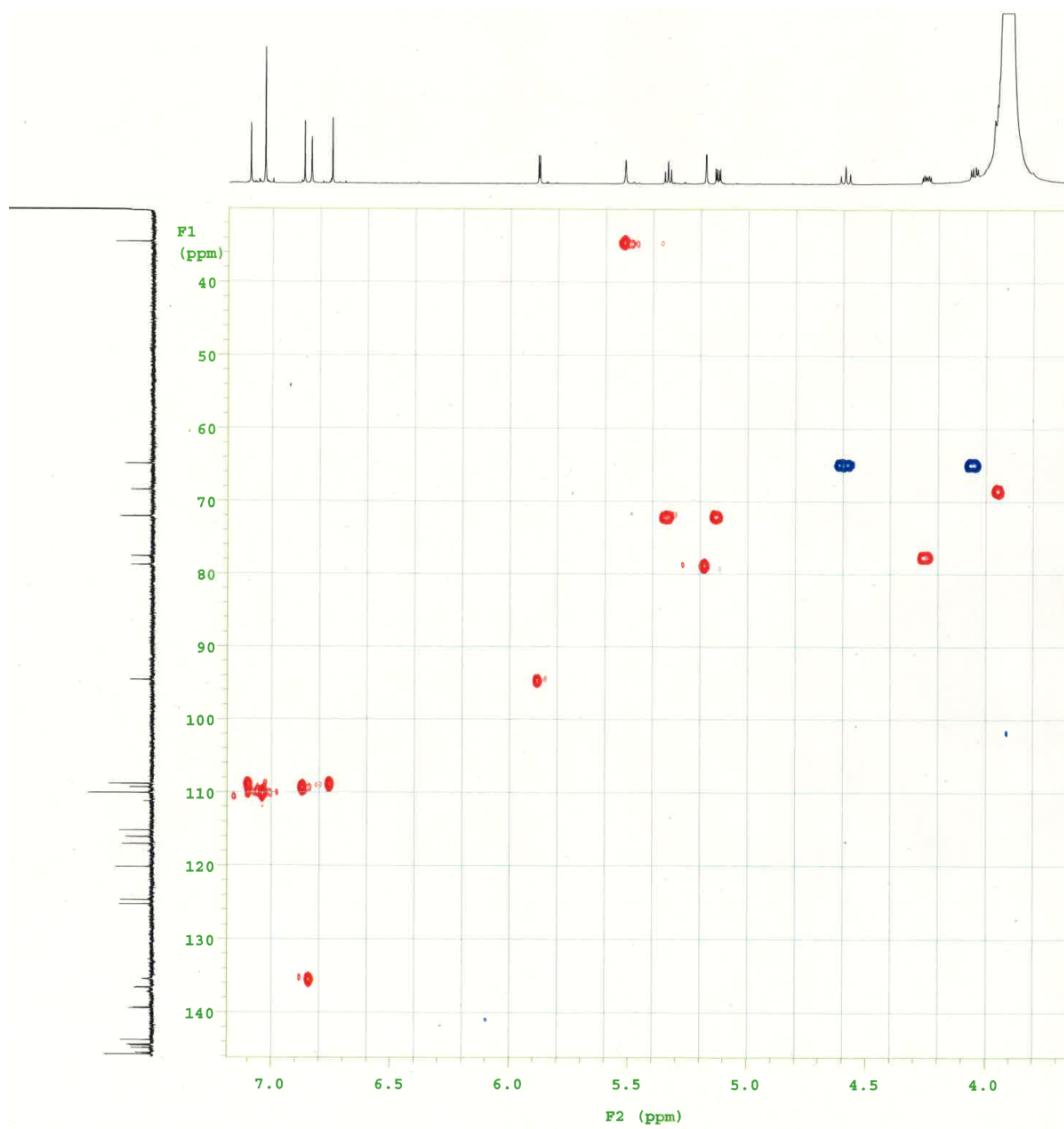


Figure S4. HSQC spectrum of davicratinic acid A (**5**) in acetone-*d*₆/D₂O=9/1.

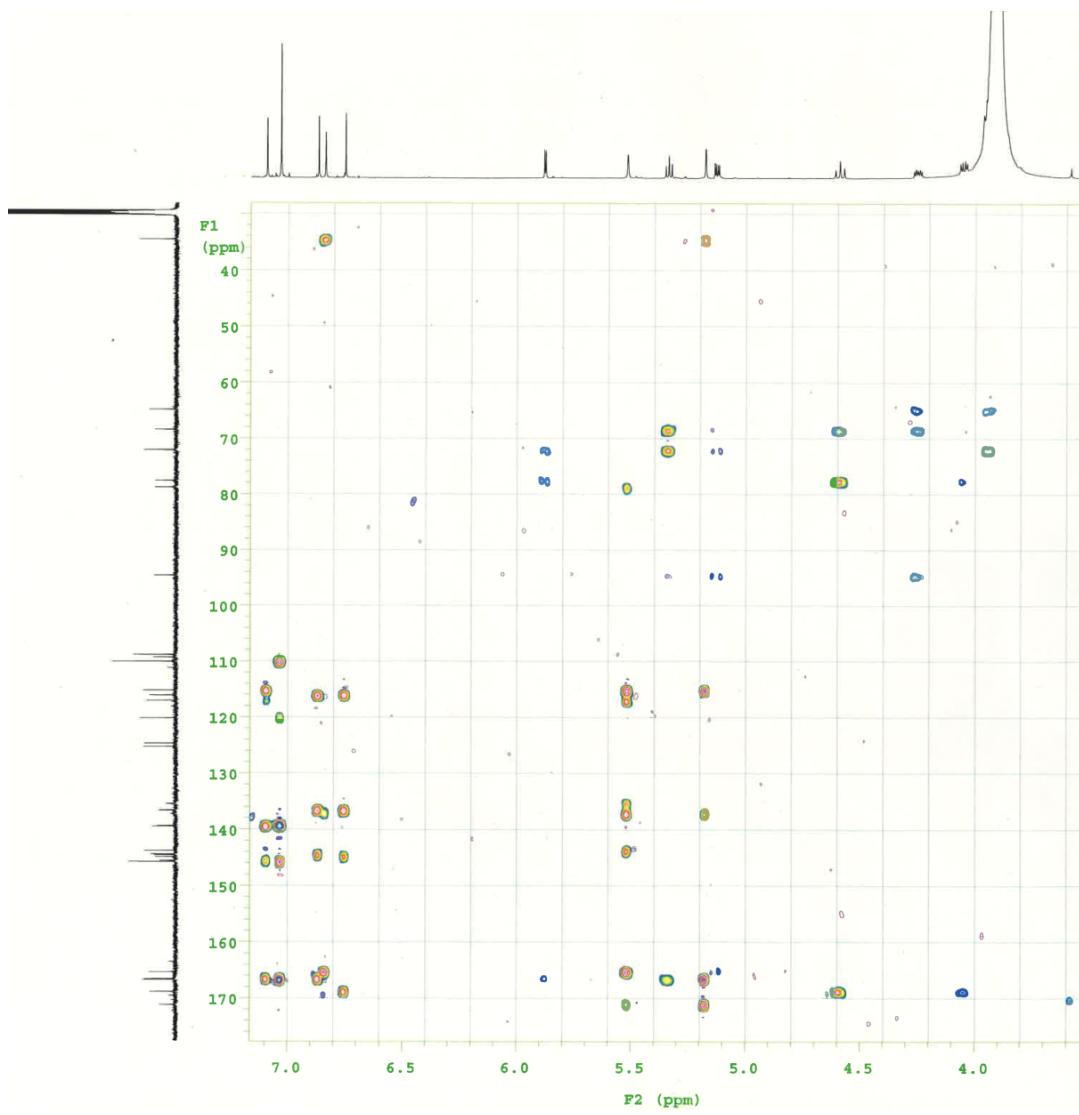


Figure S5. HMBC spectrum of davicratinic acid A (**5**) in acetone-*d*₆/D₂O=9/1.

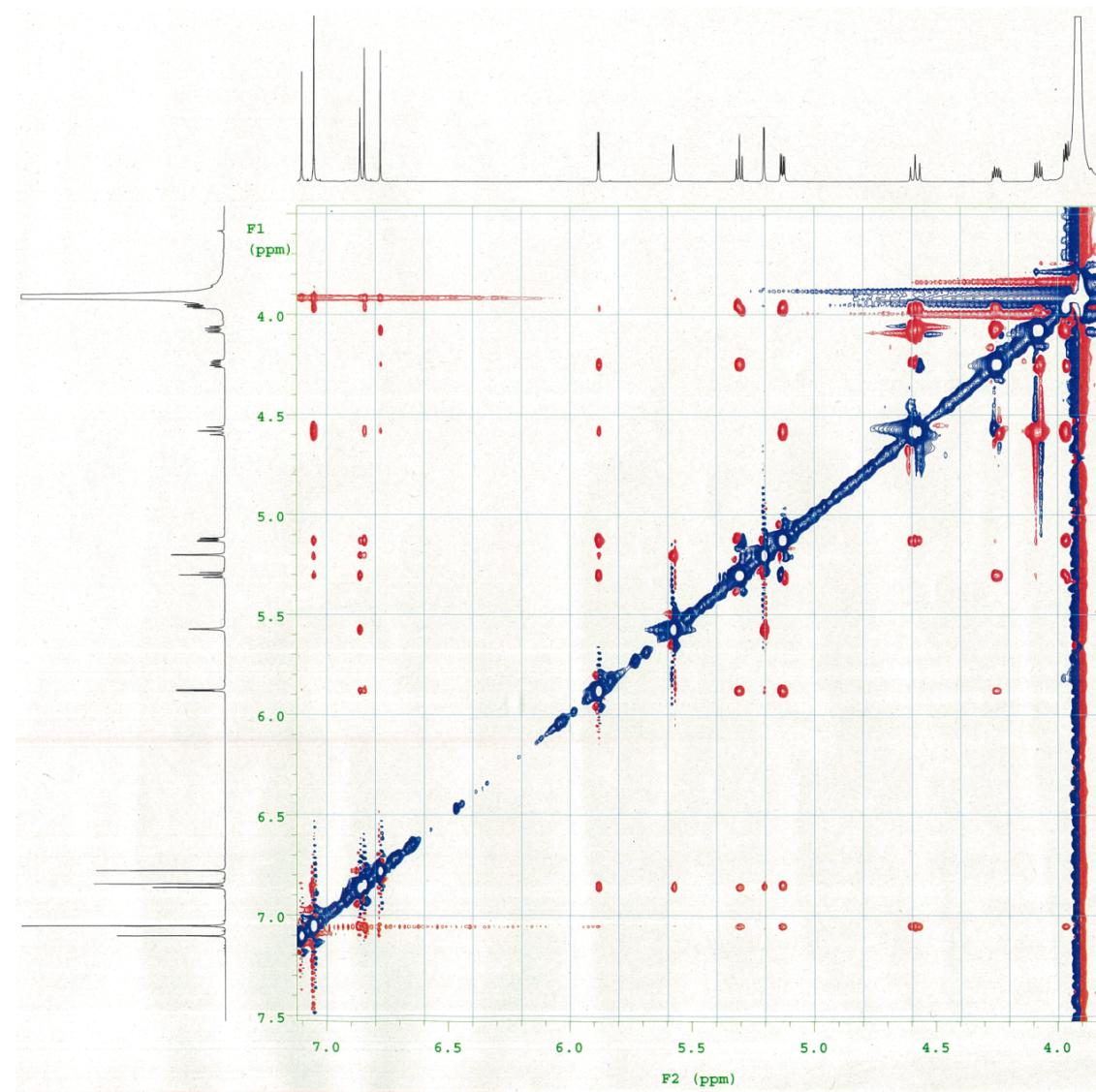


Figure S6. ROESY spectrum of davicratinic acid A (**5**) in acetone-*d*₆/D₂O=9/1.

| | | | | | | | |
|----------|---------------|-------------|--|------------|--------------|--------------------|---------------------|
| サンプル名 | DW-2 | 位置 | | 機器名 | Instrument 1 | ユーザ名 | |
| 注入量 | -1 | InjPosition | | SampleType | Sample | IRM キャリブレーションステータス | Success |
| データファイル名 | 150220-DW-2.d | 測定メソッド | | Comment | | 測定時間 | 2015/02/20 15:05:08 |

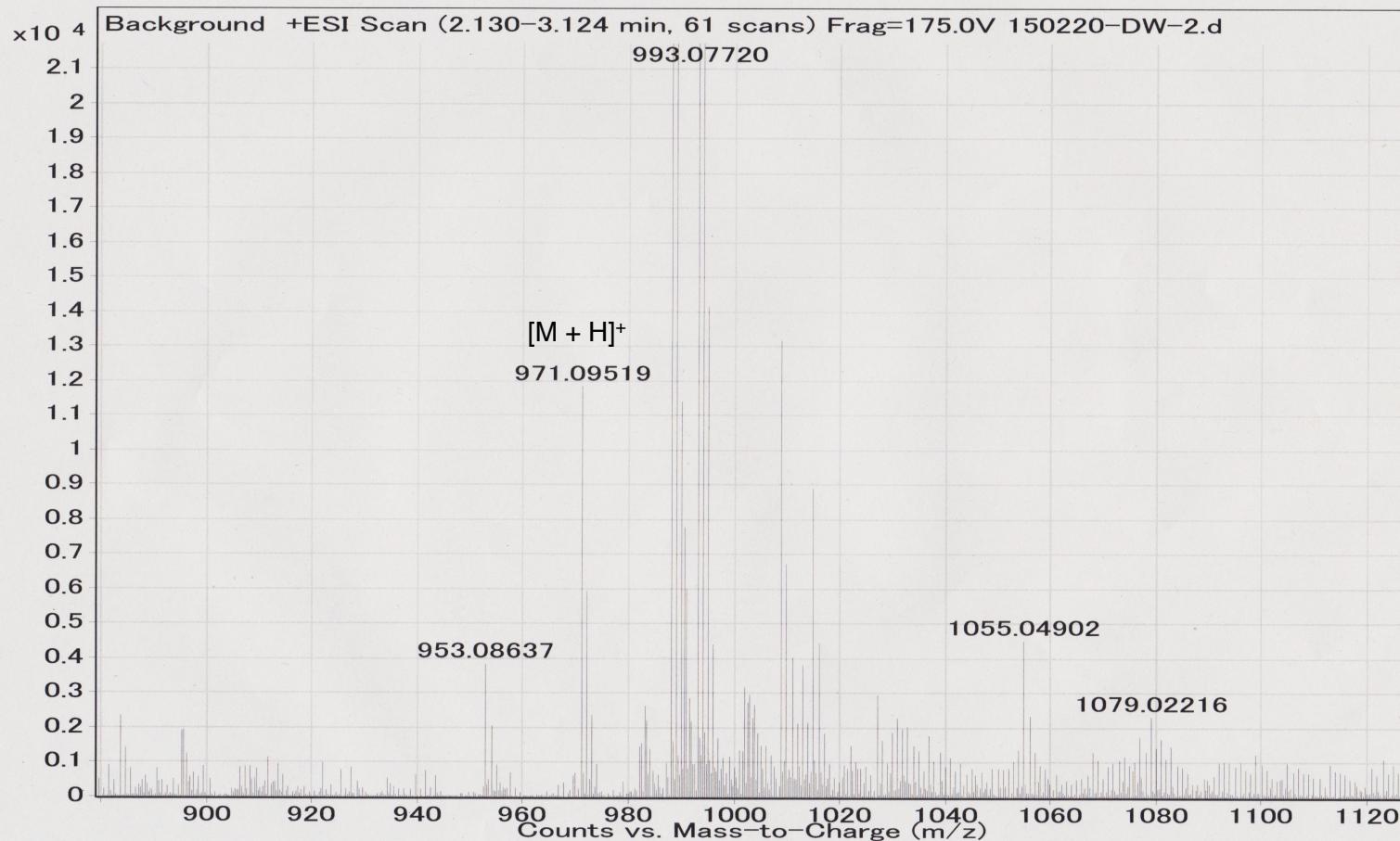


Figure S7. (+)-HR-ESI-MS spectrum of davicrinic acid A (**5**).

Table S1. Cytotoxicity of *Davidaia* tannins.

| 1 Ca9-22 | | | | |
|------------------|-----------------------------------|-----|-----|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | 99 | 89 | 93 | |
| 100 | 77 | 69 | 64 | |
| 200 | 18 | 23 | 17 | |
| 400 | 21 | 15 | 15 | |
| CC ₅₀ | 146 | 144 | 130 | 140 |

| 4 Ca9-22 | | | | |
|------------------|-----------------------------------|----|----|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | 87 | 91 | 78 | |
| 50 | 82 | 75 | 69 | |
| 100 | 53 | 49 | 44 | |
| 200 | 6 | 6 | 4 | |
| 400 | | | | |
| CC ₅₀ | 106 | 98 | 88 | 97.3 |

| Resveratrol Ca9-22 | | | | |
|--------------------|-----------------------------------|-----|-----|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | 64 | 65 | 63 | |
| 100 | 54 | 50 | 52 | |
| 200 | 21 | 17 | 19 | |
| 400 | | | | |
| CC ₅₀ | 112 | 100 | 106 | 106 |

| 1 HSC-2 | | | | |
|------------------|-----------------------------------|-----|-----|-------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | 86 | 83 | 78 | |
| 100 | 57 | 54 | 50 | |
| 200 | 25 | 27 | 24 | |
| 400 | 9 | 8 | 7 | |
| CC ₅₀ | 122 | 115 | 100 | 112.3 |

| 4 HSC-2 | | | | |
|------------------|-----------------------------------|-----|-----|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | 84 | 77 | 80 | |
| 100 | 57 | 54 | 54 | |
| 200 | 10 | 11 | 11 | |
| 400 | | | | |
| CC ₅₀ | 115 | 109 | 109 | 111 |

| Resveratrol HSC-2 | | | | |
|-------------------|-----------------------------------|------|------|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | 92 | 91 | 90 | |
| 50 | 69 | 69 | 70 | |
| 100 | 23 | 23 | 23 | |
| 200 | 6 | 5 | 5 | |
| 400 | | | | |
| CC ₅₀ | 71 | 70.6 | 71.3 | 71 |

| 1 HSC-3 | | | | |
|------------------|-----------------------------------|------|-----|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | 105 | 93 | 88 | |
| 50 | 79 | 59 | 72 | |
| 100 | 52 | 48 | 50 | |
| 200 | 28 | 29 | 28 | |
| 400 | 9 | 11 | 12 | |
| CC ₅₀ | 108 | 90.9 | 100 | 99.6 |

| 4 HSC-3 | | | | |
|------------------|-----------------------------------|-----|-----|-------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | 82 | 80 | 82 | |
| 100 | 62 | 50 | 56 | |
| 200 | 20 | 18 | 17 | |
| 400 | 7 | 11 | 10 | |
| CC ₅₀ | 129 | 100 | 115 | 114.7 |

| Resveratrol HSC-3 | | | | |
|-------------------|-----------------------------------|------|------|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | 90 | 89 | 89 | |
| 50 | 65 | 65 | 67 | |
| 100 | 19 | 25 | 23 | |
| 200 | 3 | 4 | 5 | |
| 400 | | | | |
| CC ₅₀ | 66.3 | 68.8 | 67.9 | 67.7 |

| 1 HSC-4 | | | | |
|------------------|-----------------------------------|-----|-----|-------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | 84 | 89 | 85 | |
| 100 | 75 | 68 | 69 | |
| 200 | 38 | 25 | 29 | |
| 400 | 9 | 32 | 23 | |
| CC ₅₀ | 168 | 142 | 148 | 152.7 |

| 4 HSC-4 | | | | |
|------------------|-----------------------------------|----|----|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | 92 | 83 | 77 | |
| 50 | 81 | 65 | 68 | |
| 100 | 60 | 43 | 39 | |
| 200 | 13 | 8 | 6 | |
| 400 | | | | |
| CC ₅₀ | 121 | 84 | 81 | 95.3 |

| Resveratrol HSC-4 | | | | |
|-------------------|-----------------------------------|------|------|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | 66 | 73 | 72 | |
| 50 | 36 | 51 | 49 | |
| 100 | 7 | 11 | 4 | |
| 200 | | | | |
| 400 | | | | |
| CC ₅₀ | 38.3 | 51.3 | 48.9 | 46.2 |

| 1 HGF | | | | |
|------------------|-----------------------------------|-----|-----|-------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | | | | |
| 100 | 97 | 81 | 84 | |
| 200 | 70 | 54 | 62 | |
| 400 | 9 | 32 | 23 | |
| CC ₅₀ | 266 | 236 | 262 | 254.5 |

| 4 HGF | | | | |
|------------------|-----------------------------------|-----|-----|-------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | | | | |
| 100 | 80 | 78 | 81 | |
| 200 | 72 | 66 | 67 | |
| 400 | 5 | 5 | 4 | |
| CC ₅₀ | 133 | 126 | 127 | 128.7 |

| Resveratrol HGF | | | | |
|------------------|-----------------------------------|-----|-----|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | 66 | 62 | 65 | |
| 50 | 66 | 60 | 59 | |
| 100 | 61 | 58 | 48 | |
| 200 | 0 | 0 | | |
| 400 | | | | |
| CC ₅₀ | 236 | 228 | 181 | 215 |

| 1 HPLF | | | | |
|------------------|-----------------------------------|-----|-----|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | | | | |
| 100 | 88 | 87 | 102 | |
| 200 | 75 | 75 | 79 | |
| 400 | 24 | 28 | 32 | |
| CC ₅₀ | 298 | 306 | 323 | 309 |

| 4 HPLF | | | | |
|------------------|-----------------------------------|-----|-----|------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | | | | |
| 50 | | | | |
| 100 | 101 | 100 | 93 | |
| 200 | 78 | 86 | 80 | |
| 400 | 12 | 29 | 30 | |
| CC ₅₀ | 142 | 163 | 160 | 155 |

| Resveratrol HPLF | | | | |
|------------------|-----------------------------------|-----|-----|-------|
| μM | Viable cell number (% of control) | | | mean |
| 25 | 83 | 84 | 83 | |
| 50 | 74 | 70 | 71 | |
| 100 | 56 | 47 | 46 | |
| 200 | 5 | 1 | 5 | |
| 400 | | | | |
| CC ₅₀ | 224 | 187 | 184 | 198.3 |

| 1 HPC | | | | |
| --- | --- | --- | --- | --- |
| μM | Viable cell number (% of control) | | | mean |

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