**Table S1:** NMR Data of compound **1** ($CD_3OD$, 600 and 150 MHz for $^1H$ and $^{13}C$, respectively)

| **Position** | $\delta_C$ | $\delta_H$ (*J* in Hz) | **COSY** Characteristic correlations | **HMBC** Characteristic correlations |
|---|---|---|---|---|
| **Aglycone (myricetin)** | | | | |
| **2** | **158.0** | | | |
| **3** | **135.3** | | | |
| **4** | **178.9** | | | |
| **5** | **163.1** | | | |
| **6** | **99.7** | **6.15 (d, 2.1)** | | |
| **7** | **165.7** | | | |
| **8** | **94.4** | **6.32 (d, 2.1)** | | |
| **9** | **158.2** | | | |
| **10** | **105.9** | | | |
| **1'** | **122.0** | | | |
| **2'** | **109.8** | **7.27 (s)** | | |
| **3'** | **146.4** | | | |
| **4'** | **137.9** | | | |
| **5'** | **146.4** | | | |
| **6'** | **109.8** | **7.27 (s)** | | |
| **3-*O*-galactopyranoside moiety** | | | | |
| **1''** | **101.4** | **5.78 (d, 8)** | **H-2''** | **3, 5'', 3''** |
| **2''** | **74.6** | **5.45 (dd, 9.9, 8)** | **H-1'', H-3''** | **3'', 1'', 7'''** |
| **3''** | **73.5** | **3.84 (dd, 9.9, 3.4)** | **H-2'', H4''** | |
| **4''** | **70.6** | **3.96 (dd, 3.3, 1.3)** | **H-3'', H-5''** | |
| **5''** | **77.5** | **3.61 (t, 6.3)** | **H-4'', H-6''** | |
| **6'' (2H)** | **62.1** | **3.70 (m)** | **H-5''** | |
| **2''-*O*-galloyl moiety** | | | | |
| **1'''** | **121.7** | **-** | | |
| **2'''** | **110.7** | **7.14 (s)** | | |
| **3'''** | **146.3** | **-** | | |
| **4'''** | **139.9** | **-** | | |
| **5'''** | **146.3** | **-** | | |
| **6'''** | **110.7** | **7.14 (s)** | | |
| **7''' (C=O)** | **168.4** | **-** | | |

**Table S2:** NMR Data of compound **2** ($CD_3OD$, 600 and 150 MHz for $^1H$ and $^{13}C$, respectively)

| **Position** | $\delta_C$ | $\delta_H$ (*J* in Hz) | **COSY** Characteristic correlations |
|---|---|---|---|
| **Aglycone (myricetin)** | | | |
| **2** | **158.6** | | |
| **3** | **135.7** | | |
| **4** | **179.4** | | |
| **5** | **163.3** | | |
| **6** | **99.9** | **6.19 (d, 2.1)** | |
| **7** | **166.0** | | |
| **8** | **94.7** | **6.36 (d, 2.1)** | |
| **9** | **159.5** | | |
| **10** | **105.9** | | |
| **1'** | **121.8** | | |
| **2'** | **110.4** | **7.07 (s)** | |
| **3'** | **146.5** | | |
| **4'** | **138.0** | | |
| **5'** | **146.5** | | |
| **6'** | **110.4** | **7.07 (s)** | |
| **3-*O*-rhamnopyranosyl moiety** | | | |
| **1''** | **100.5** | **5.51 (d, 1.5)** | **H-2''** |
| **2''** | **73.5** | **5.63 (dd, 3.3, 1.7)** | **H-1'', H-3''** |
| **3''** | **70.8** | **4.04 (dd, 9.5, 3.3)** | **H-2''', H-4'''** |
| **4''** | **73.9** | **3.47 (t, 9.7)** | **H-3''', H-5'''** |
| **5''** | **72.3** | **3.49 (dd, 9.7, 6.3)** | **H4''', H-6'''** |
| **6''** | **17.8** | **1.04 (d, 6)** | **H-5'''** |
| **2''-*O*-galloyl moiety** | | | |
| **1'''** | **121.3** | **-** | |
| **2'''** | **109.6** | **6.98 (s)** | |
| **3'''** | **146.9** | **-** | |
| **4'''** | **140.0** | **-** | |
| **5'''** | **146.9** | **-** | |
| **6'''** | **109.6** | **6.98 (s)** | |
| **7''' (C=O)** | **167.5** | **-** | |

**Table S3:** NMR Data of compound **3** ($CD_3OD$, 400 and 100 MHz for $^1H$ and $^{13}C$, respectively)

| Position | $\delta_C$ | $\delta_H$ (*J* in Hz) | COSY Characteristic correlations | HMBC Characteristic correlations |
|---|---|---|---|---|
| **Aglycone (myricetin)** | | | | |
| **2** | **157.1** | | | |
| **3** | **135.0** | | | |
| **4** | **178.2** | | | |
| **5** | **161.8** | | | |
| **6** | **98.4** | **6.20 (d, 1.6)** | | |
| **7** | **164.5** | | | |
| **8** | **93.3** | **6.37 (d, 1.6)** | | |
| **9** | **158.0** | | | |
| **10** | **104.5** | | | |
| **1'** | **120.5** | | | |
| **2'** | **108.2** | **6.99 (s)** | | |
| **3'** | **145.5** | | | |
| **4'** | **136.5** | | | |
| **5'** | **145.5** | | | |
| **6'** | **108.2** | **6.99 (s)** | | |
| **3-*O*-rhamnopyranosyl moiety** | | | | |
| **1''** | **102.3** | **5.28 (d, 1.4)** | **H-2''** | **3, 5'', 3''** |
| **2''** | **70.9** | **4.48 (dd, 3.1, 1.4)** | **H-1'', H-3''** | |
| **3''** | **69.5** | **5.24 (dd, 9.1, 3.1)** | **H-2'', H-4''** | **5'', 7'''** |
| **4''** | **73.9** | **3.69 (m, overlaped)** | **H-3'', H-5''** | |
| **5''** | **68.6** | **3.69 (m, overlaped)** | **H4'', H-6''** | |
| **6''** | **16.3** | **1.0 (d, 5.6)** | **H-5''** | |
| **3''-*O*-galloyl moiety** | | | | |
| **1'''** | **120.2** | **-** | | |
| **2'''** | **109.1** | **7.17 (s)** | | |
| **3'''** | **145.0** | **-** | | |
| **4'''** | **138.5** | **-** | | |
| **5'''** | **145.0** | **-** | | |
| **6'''** | **109.1** | **7.17 (s)** | | |
| **7''' (C=O)** | **167.0** | **-** | | |

**Table S4:** NMR Data of compound **4** ($CD_3OD$, 400 and 100 MHz for $^1H$ and $^{13}C$, respectively)

| Position | $\delta_C$ | $\delta_H$ (*J* in Hz) |
|---|---|---|
| **Gallic acid** | | |
| **1** | **122.3** | **-** |
| **2** | **110.3** | **6.93 (s)** |
| **3** | **146.4** | **-** |
| **4** | **139.5** | **-** |
| **5** | **146.4** | **-** |
| **6** | **110.3** | **6.93 (s)** |
| **7** | **170.6** | **-** |

**Table S5:** NMR Data of compound **5** ($CD_3OD$, 400 and 100 MHz for $^1H$ and $^{13}C$, respectively)

| Position | $\delta_C$ | $\delta_H$ (*J* in Hz) |
|---|---|---|
| **Aglycone (myricetin)** | | |
| **2** | **157.0** | |
| **3** | **134.6** | |
| **4** | **177.9** | |
| **5** | **161.1** | |
| **6** | **98.6** | **6.22 (d, 2)** |
| **7** | **164.2** | |
| **8** | **93.3** | **6.42 (d, 2)** |
| **9** | **157.5** | |
| **10** | **105.9** | |
| **1'** | **121.7** | |
| **2'** | **108.5** | **7.41 (s)** |
| **3'** | **145.0** | |
| **4'** | **137.0** | |
| **5'** | **145.0** | |
| **6'** | **108.5** | **7.41 (s)** |
| **3-*O*-galactopyranoside moiety** | | |
| **1''** | **104.2** | **5.19 (d, 7.8)** |
| **2''** | **71.8** | **3.90 (dd, 9.5, 7.8)** |
| **3''** | **75.8** | **3.70 (dd, 9.5, 3.4)** |
| **4''** | **68.6** | **3.65 (dd, 3.0, 1.5)** |
| **5''** | **73.7** | **3.61 (t, 6.3)** |
| **6''a** | **60.5** | **3.86 (dd, 10.3, 6.0)** |
| **6''b** | | **3.52 (dd, 10.3, 6.7)** |

**Table S6:** NMR Data of compound **6** (DMSO-d6, 600 and 150 MHz for $^{1}H$ and $^{13}C$, respectively)

| Position | $\delta_C$ | $\delta_H$ (*J* in Hz) |
|---|---|---|
| **Aglycone (apigenin)** | | |
| **2** | **165.1** | **-** |
| **3** | **103.8** | **6.59 (s)** |
| **4** | **182.9** | **-** |
| **5** | **162.4** | **-** |
| **6** | **100.1** | **6.12 (d, 2.1)** |
| **7** | **165.2** | **-** |
| **8** | **95.3** | **6.41 (d, 2.1)** |
| **9** | **158.5** | **-** |
| **10** | **104.8** | **-** |
| **1'** | **122.4** | **-** |
| **2'** | **129.6** | **7.79 (d, 8.9)** |
| **3'** | **117.2** | **6.86 (d, 8.9)** |
| **4'** | **162.1** | **-** |
| **5'** | **117.2** | **6.86 (d, 8.9)** |
| **6'** | **129.6** | **7.79 (d, 8.9)** |

**Table S7:** NMR Data of compound **7** ($CD_3OD$, 400 and 100 MHz for $^1H$ and $^{13}C$, respectively)

| Position | $\delta_C$ | $\delta_H$ (*J* in Hz) |
|---|---|---|
| **Aglycone (myricetin)** | | |
| **2** | **146.6** | |
| **3** | **135.9** | |
| **4** | **175.9** | |
| **5** | **161.1** | |
| **6** | **97.8** | **6.20 (d, 2)** |
| **7** | **164.2** | |
| **8** | **92.9** | **6.40 (d, 2)** |
| **9** | **156.8** | |
| **10** | **103.1** | |
| **1'** | **121.7** | |
| **2'** | **107.1** | **7.36 (s)** |
| **3'** | **145.3** | |
| **4'** | **135.5** | |
| **5'** | **145.3** | |
| **6'** | **107.1** | **7.36 (s)** |

**Table S8:** NMR Data of compound **8** ($CD_3OD$, 400 and 100 MHz for $^{1}H$ and $^{13}C$, respectively)

| Position | $\delta_C$ | $\delta_H$ (*J* in Hz) |
|---|---|---|
| **Ethyl gallate** | | |
| **1** | 120.4 | - |
| **2** | 108.9 | 7.07 (s) |
| **3** | 145.1 | - |
| **4** | 138.3 | - |
| **5** | 145.1 | - |
| **6** | 108.9 | 7.07 (s) |
| **7** | 167.6 | - |
| **8** | 60.3 | 4.28 (q, 6.68) |
| **9** | 13.2 | 1.35 (t, 6.44) |

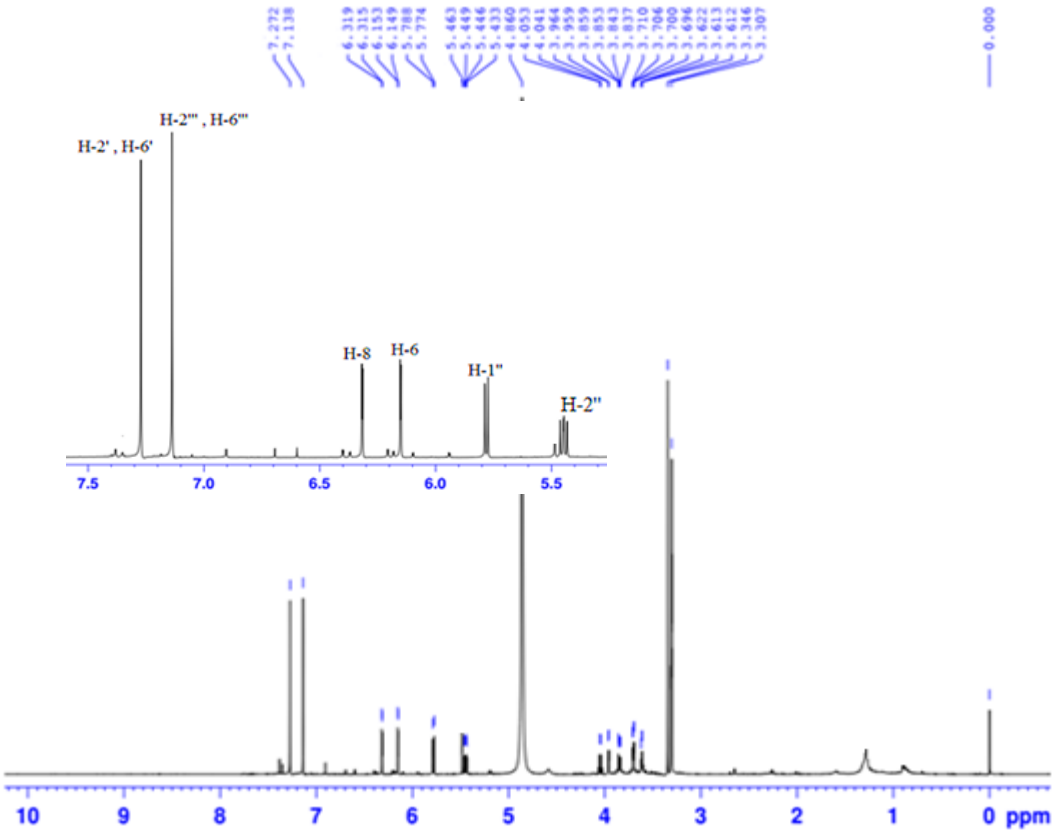



**Fig. S1.** $^{1}$H-NMR spectrum (600 MHz, $CD_3OD$) of compound **1**

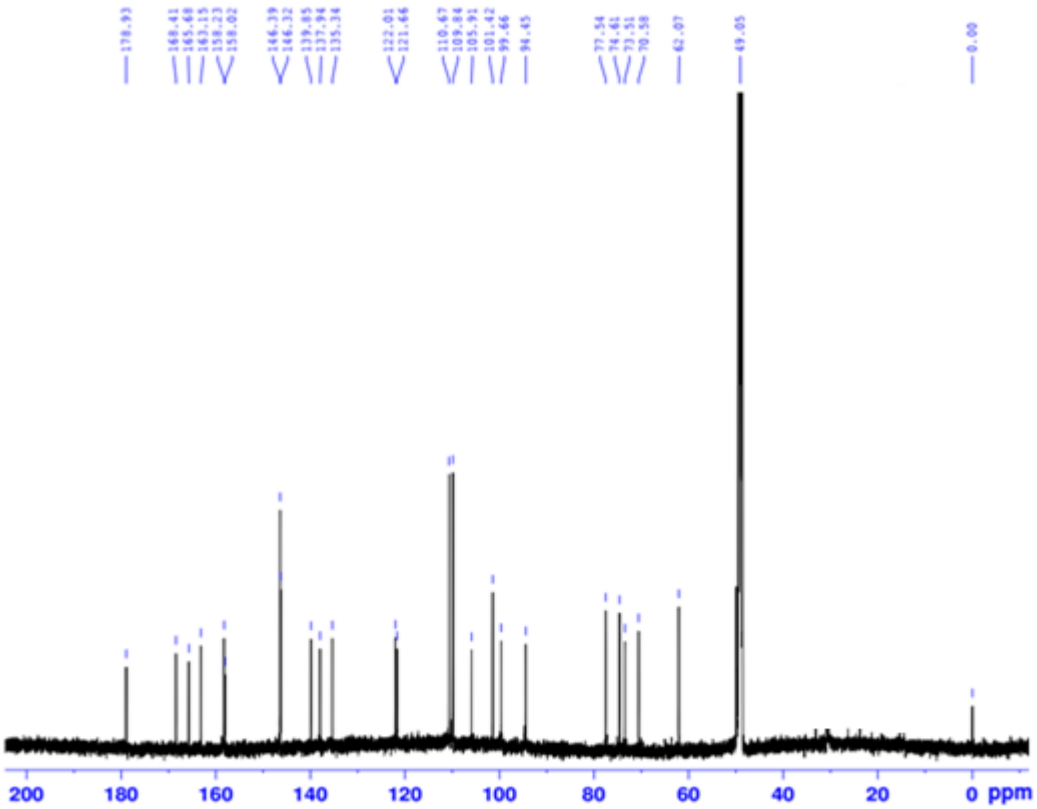



**Fig. S2.** $^{13}$C-NMR spectrum (150 MHz, $CD_3OD$) of compound **1**

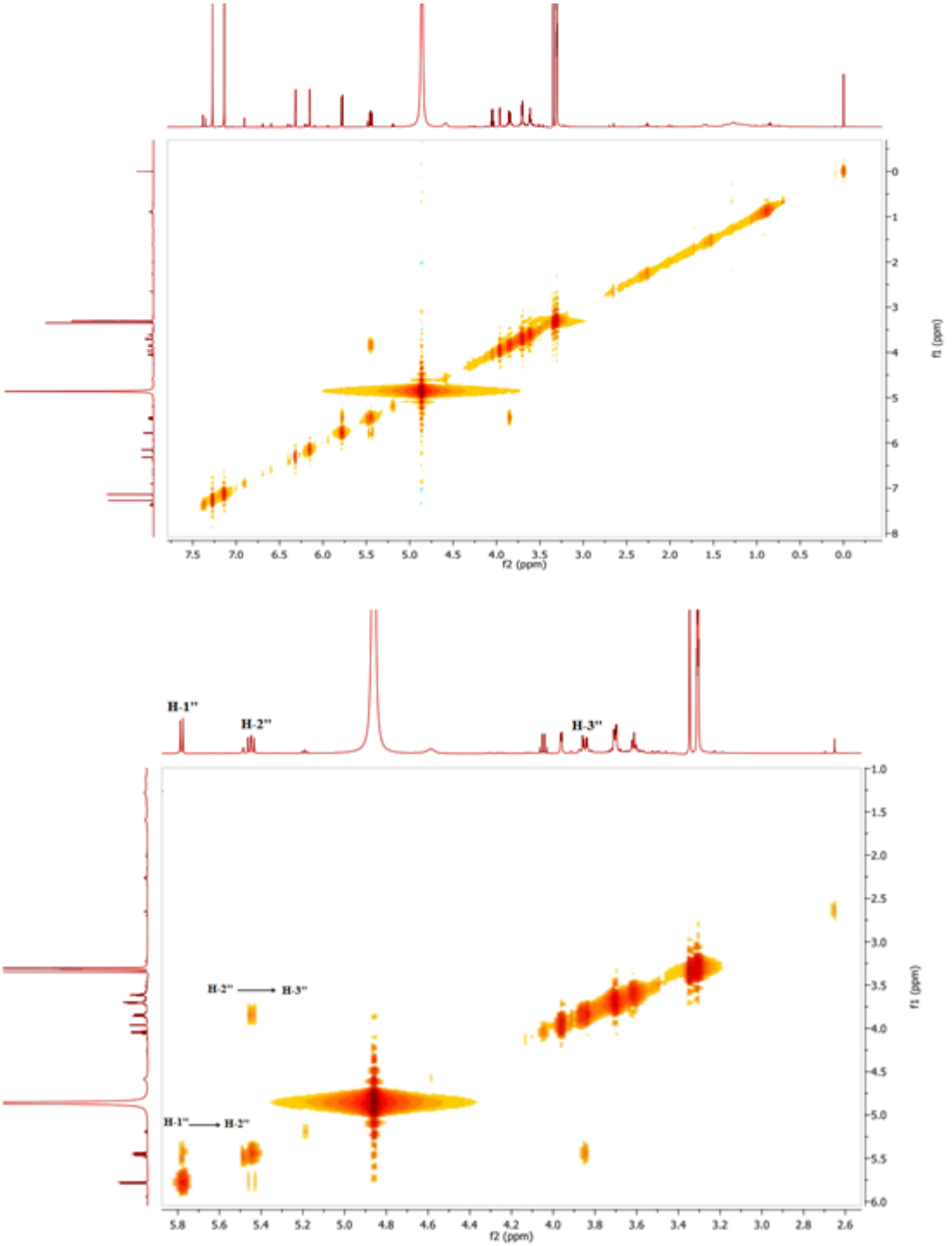



**Fig. S3.** COSY spectrum of compound **1**

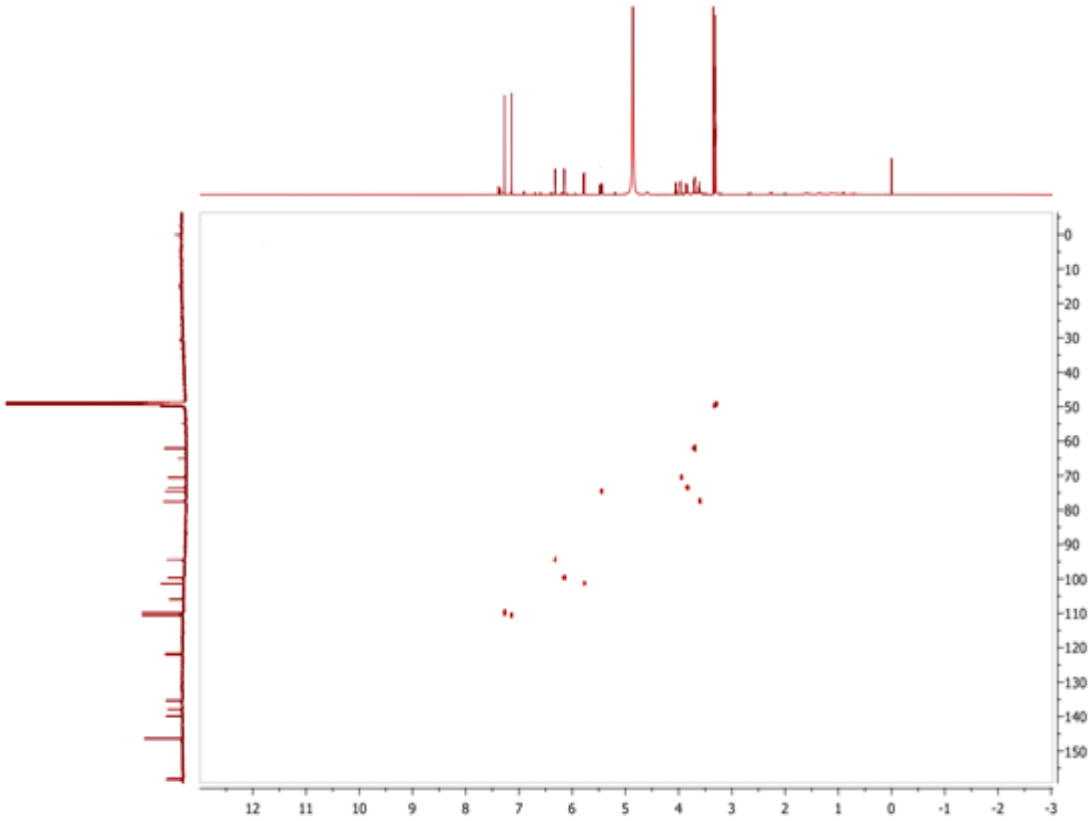



**Fig. S4.** HSQC spectrum of compound **1**

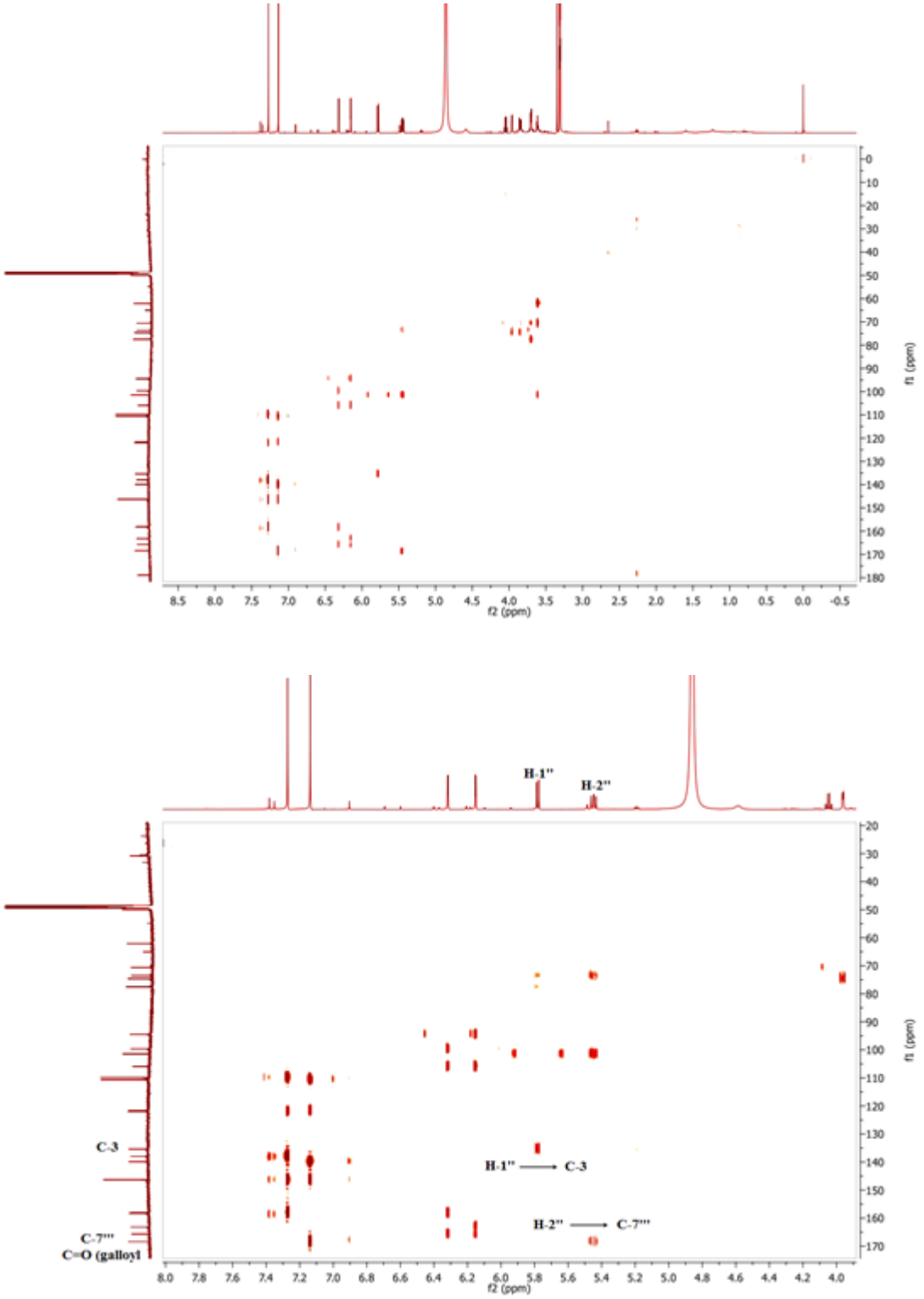



**Fig. S5.** HMBC spectrum of compound **1**

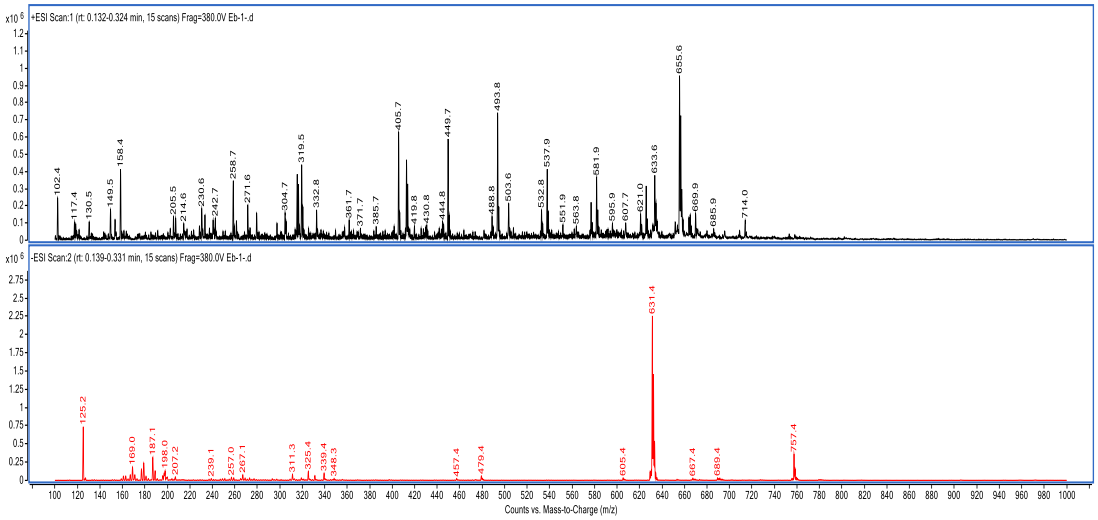



**Fig. S6.** ESI-MS *m/z* of compound **1**

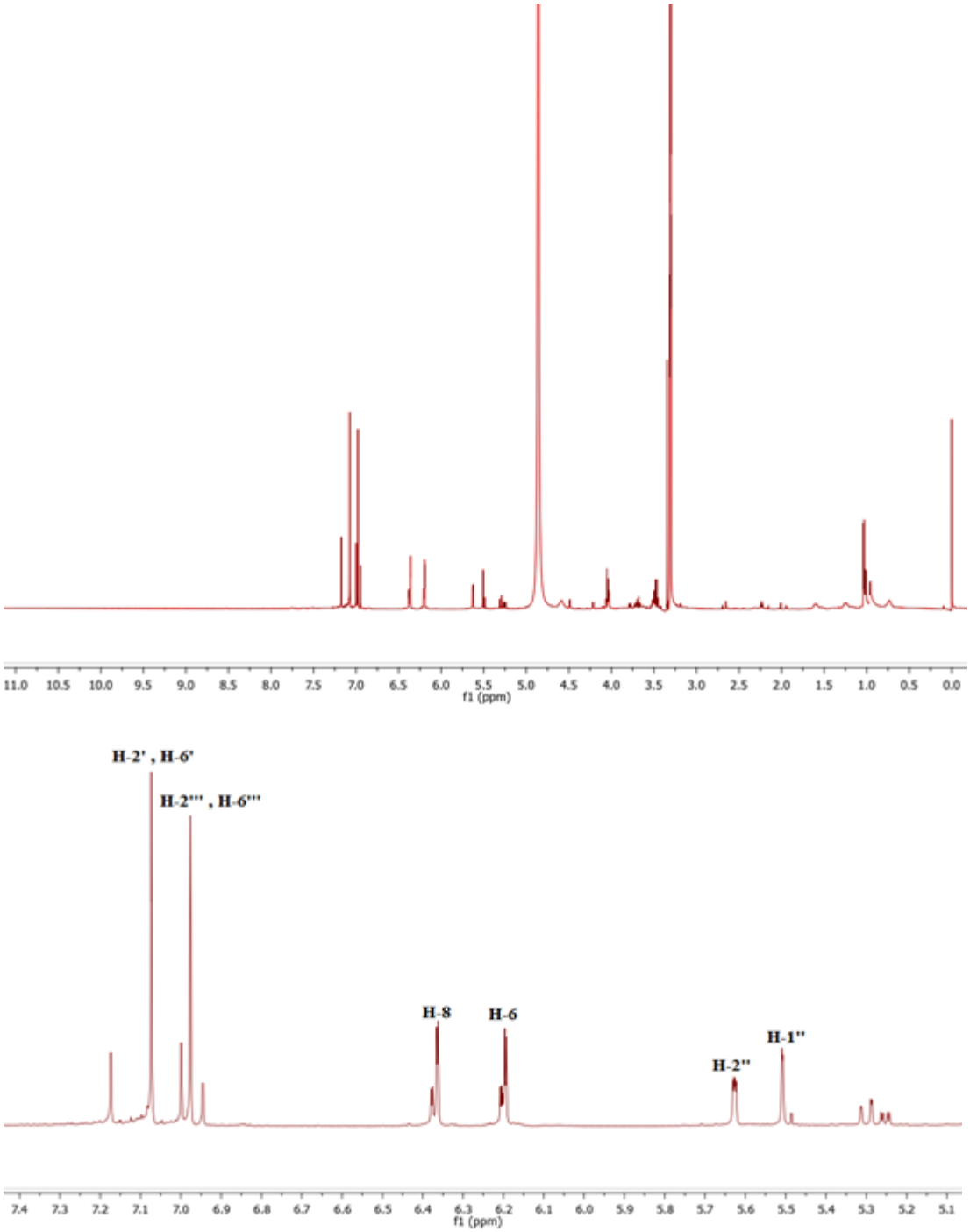



**Fig. S7.** $^{1}$H-NMR spectrum (600 MHz, $CD_3OD$) of compound **2**

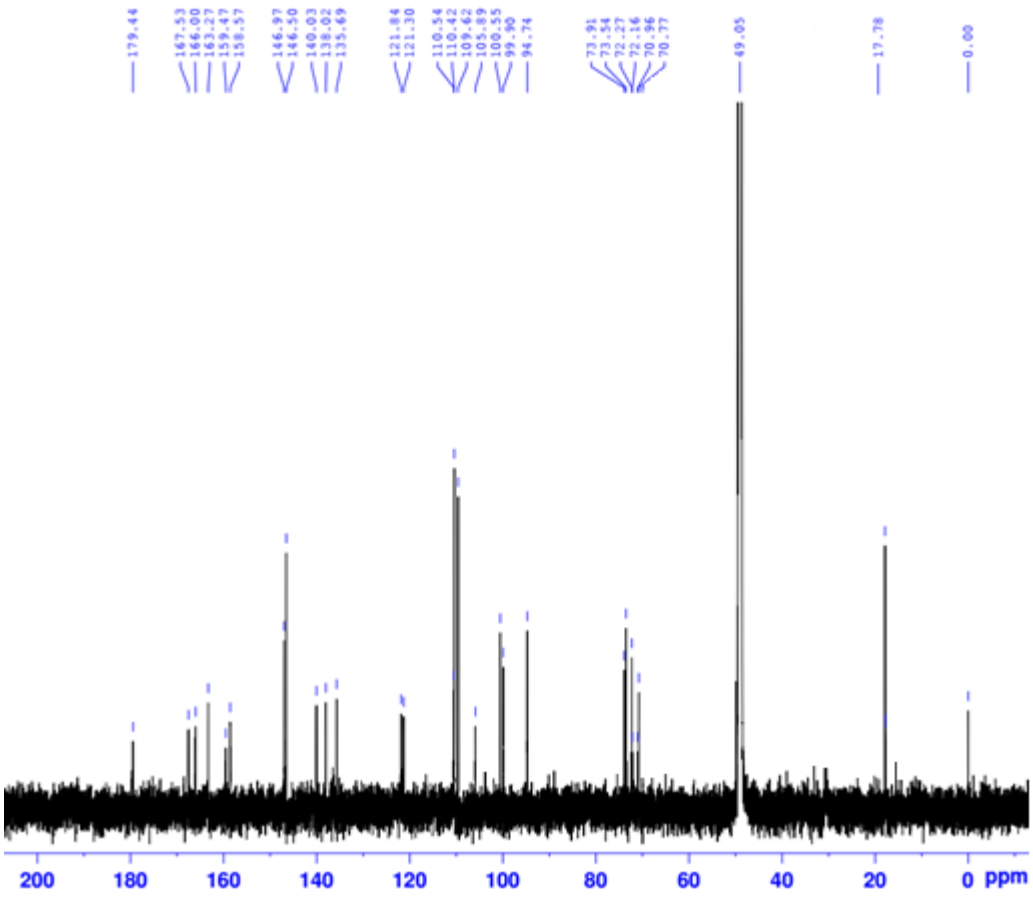



**Fig. S8.** $^{13}$C-NMR spectrum (150 MHz, $CD_3OD$) of compound **2**

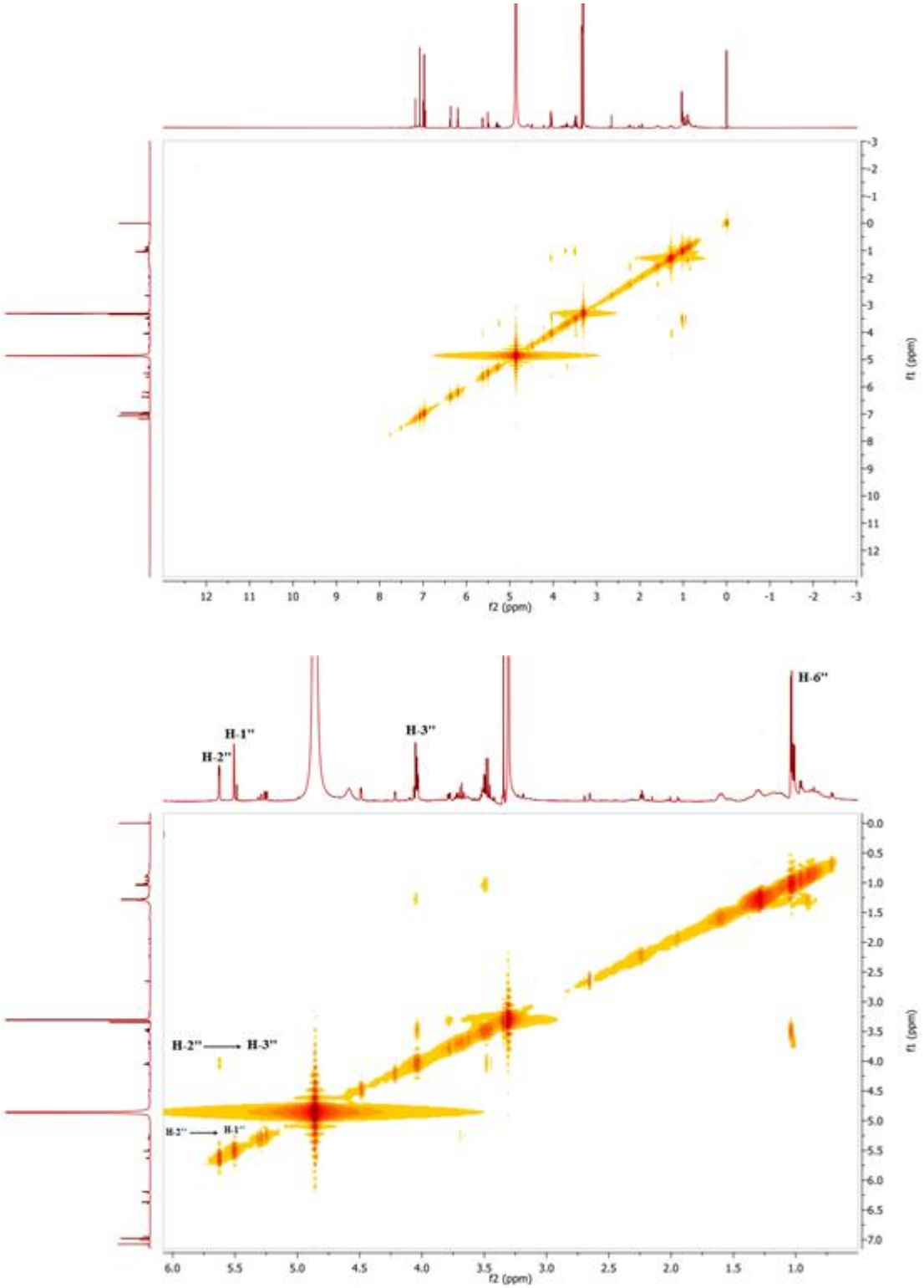



**Fig. S9.** COSY spectrum of compound **2**

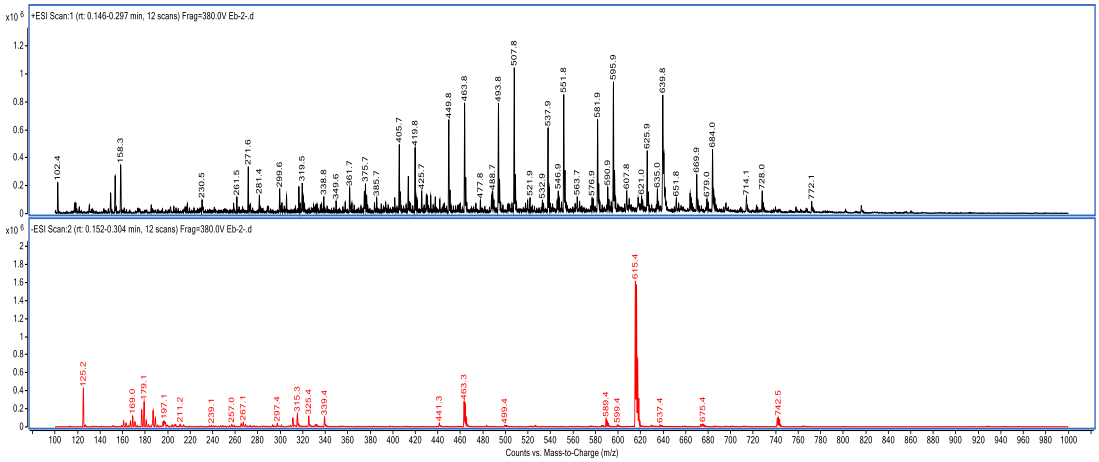



**Fig. S10.** ESI-MS *m/z* of compound **2**

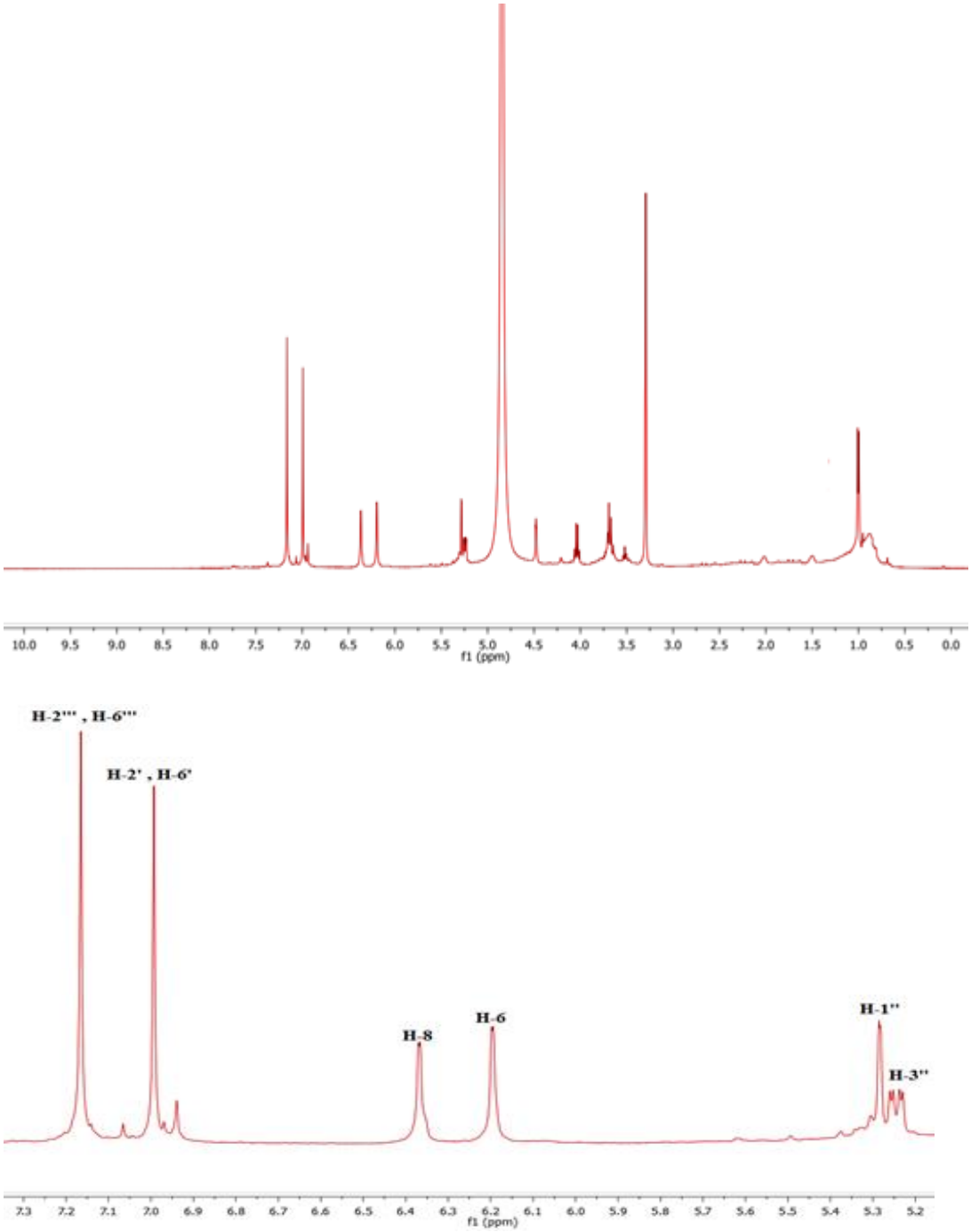



**Fig. S11.** $^{1}$H-NMR spectrum (400 MHz, $CD_3OD$) of compound **3**

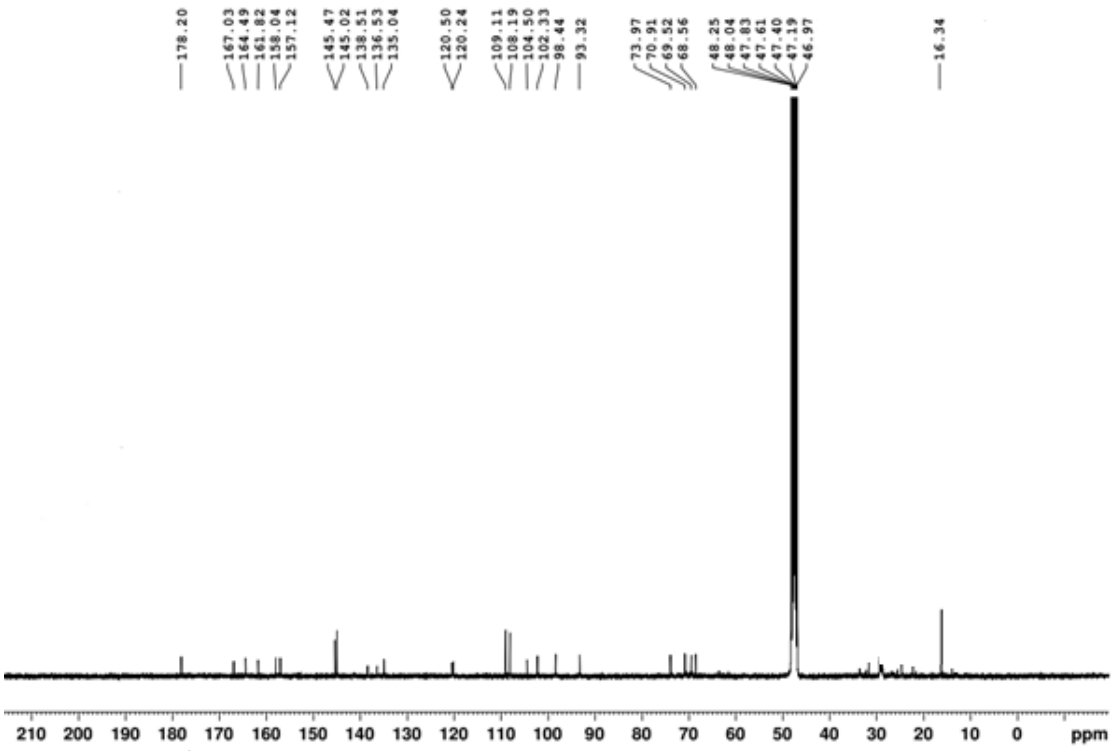



**Fig. S12.** $^{13}$C-NMR spectrum (100 MHz, $CD_3OD$) of compound **3**

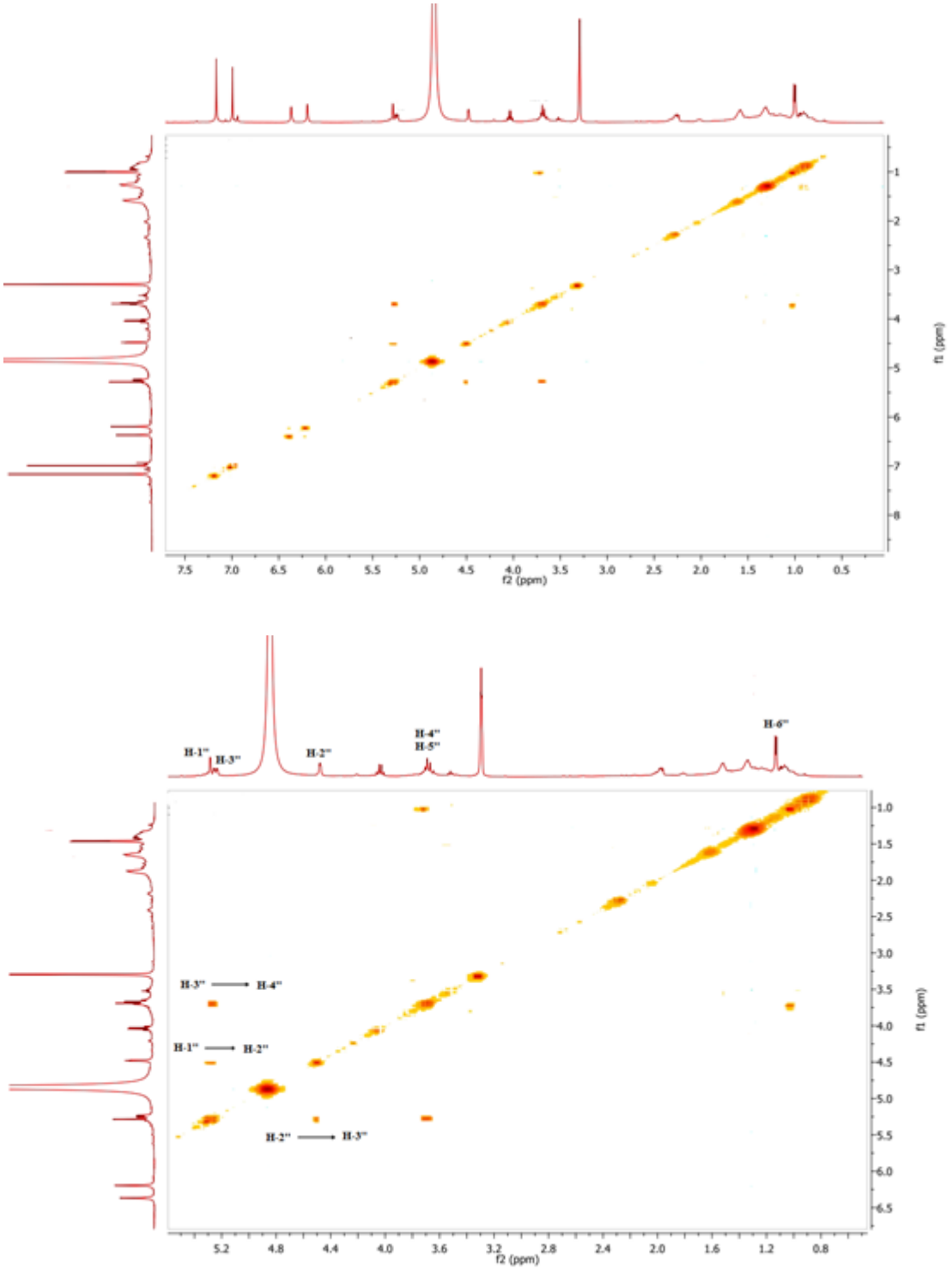



**Fig. S13.** COSY spectrum of compound **3**

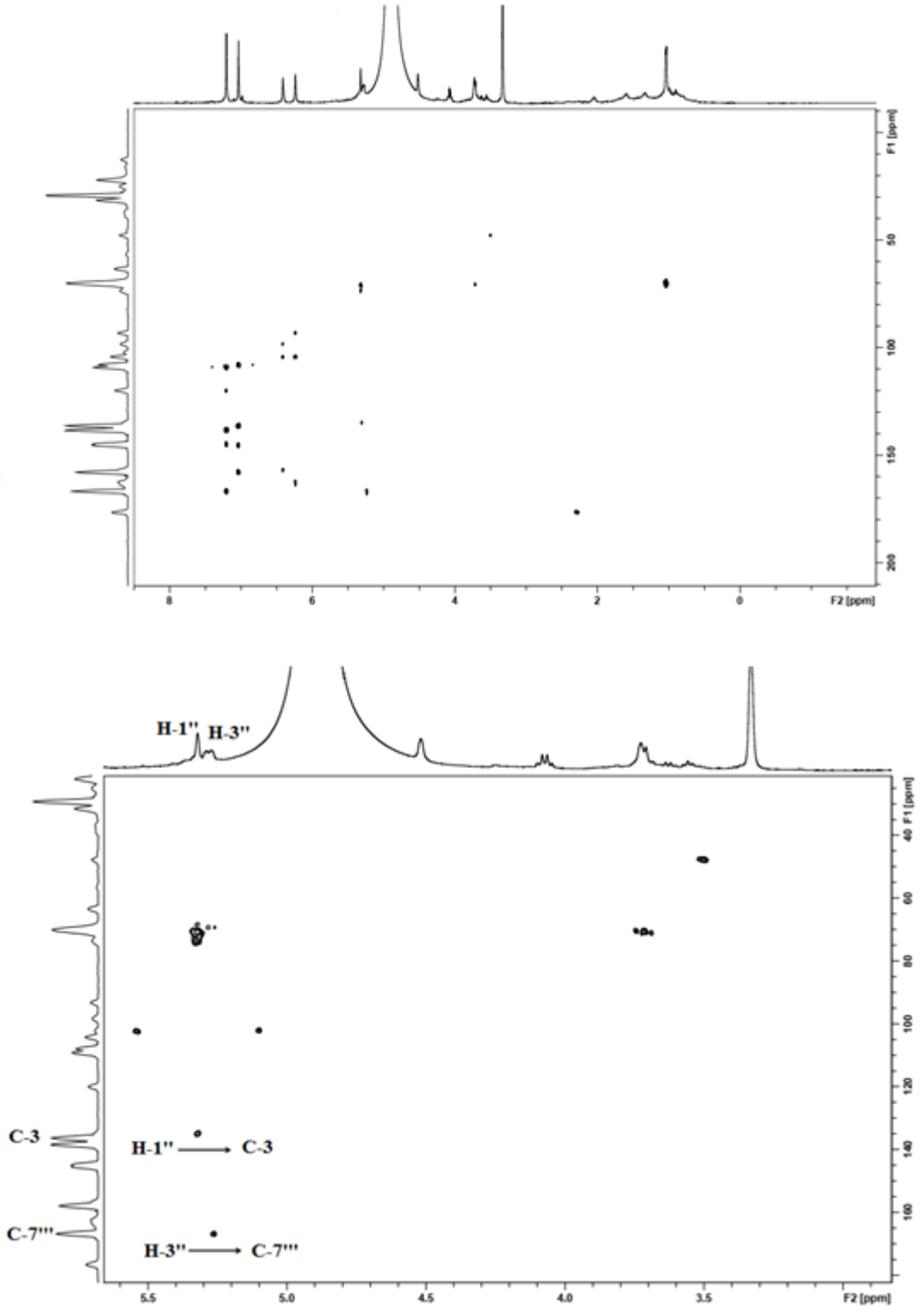



**Fig. S14.** HMBC spectrum of compound **3**

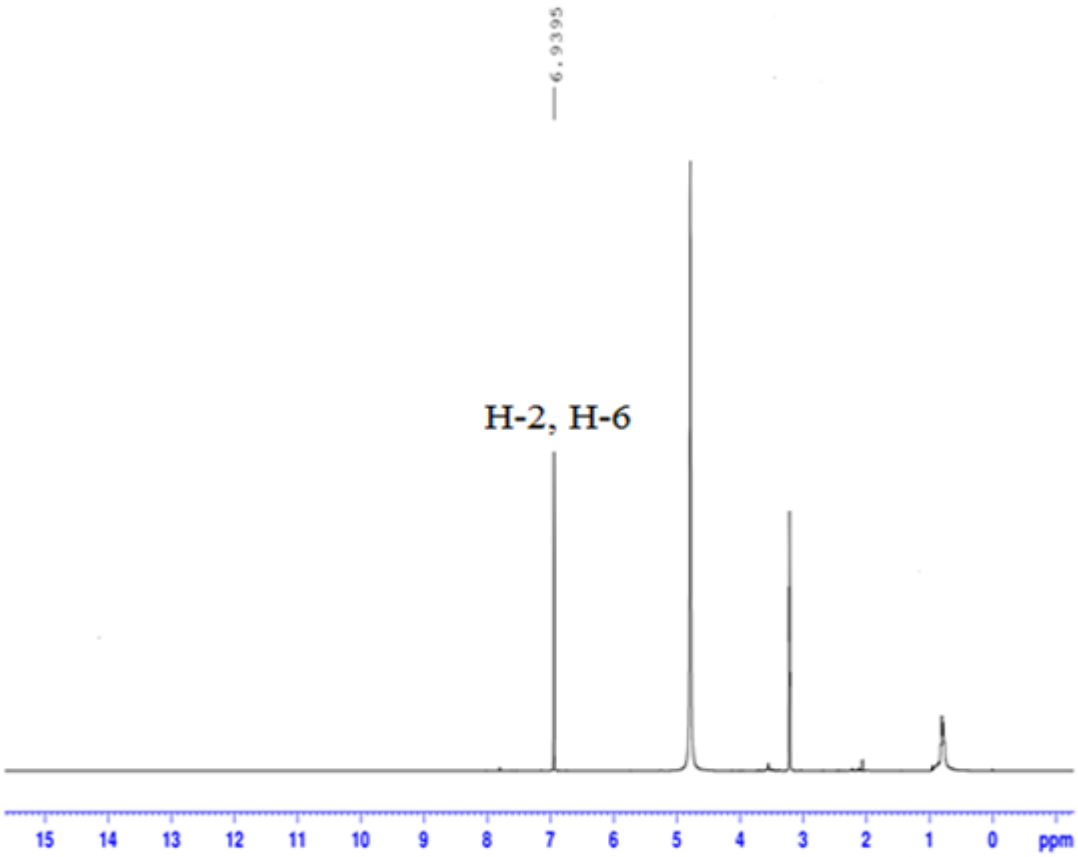



**Fig. S15.** $^{1}$H-NMR spectrum (400 MHz, $CD_3OD$) of compound **4**

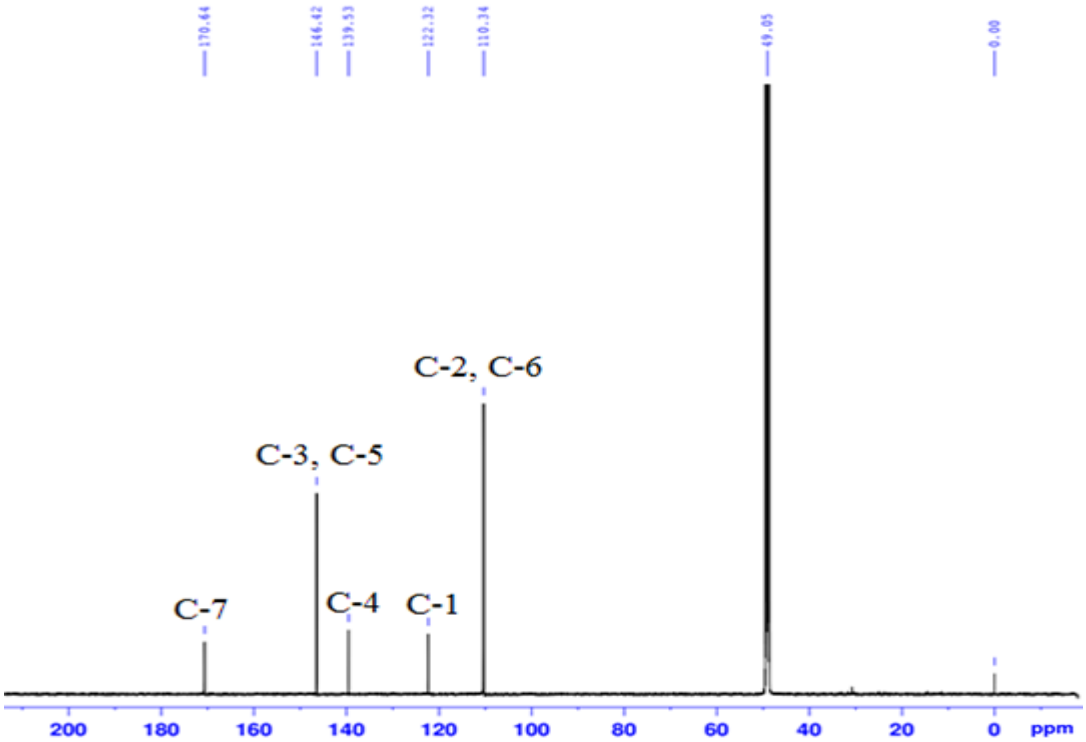



**Fig. S16.** $^{13}$C-NMR spectrum (100 MHz, $CD_3OD$) of compound **4**

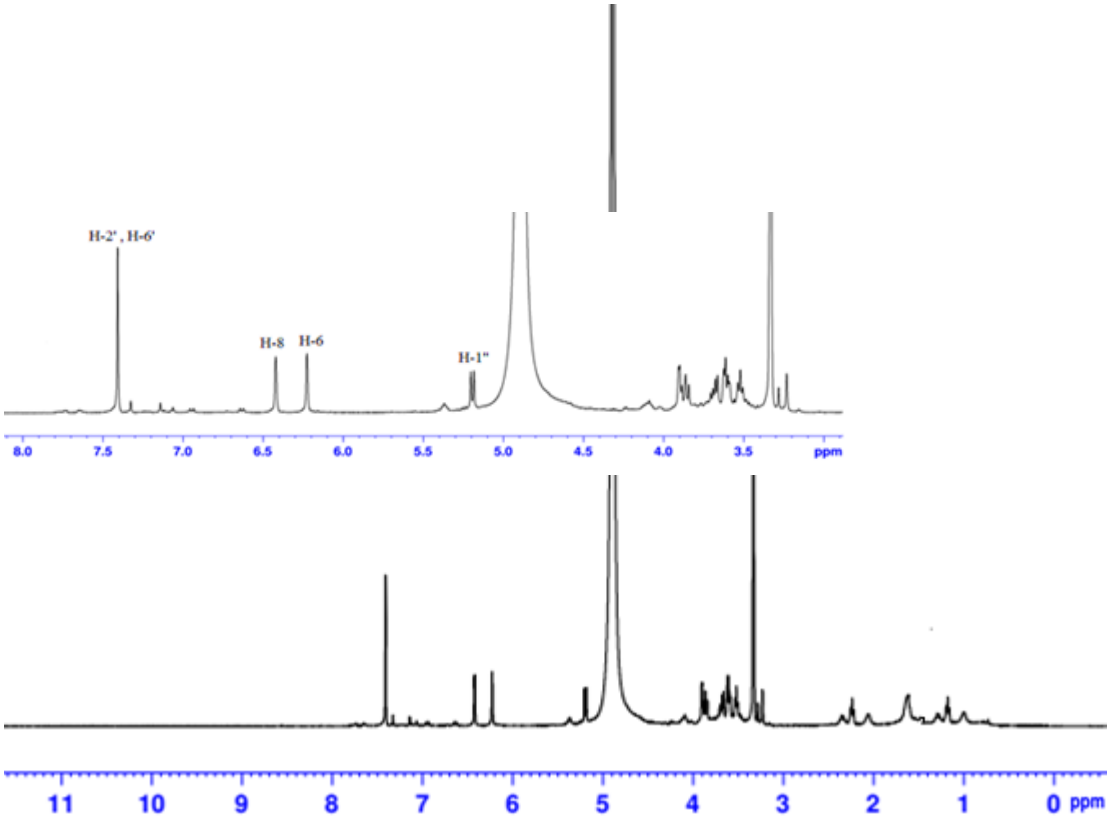



**Fig. S17.** $^{1}$H-NMR spectrum (400 MHz, $CD_3OD$) of compound **5**

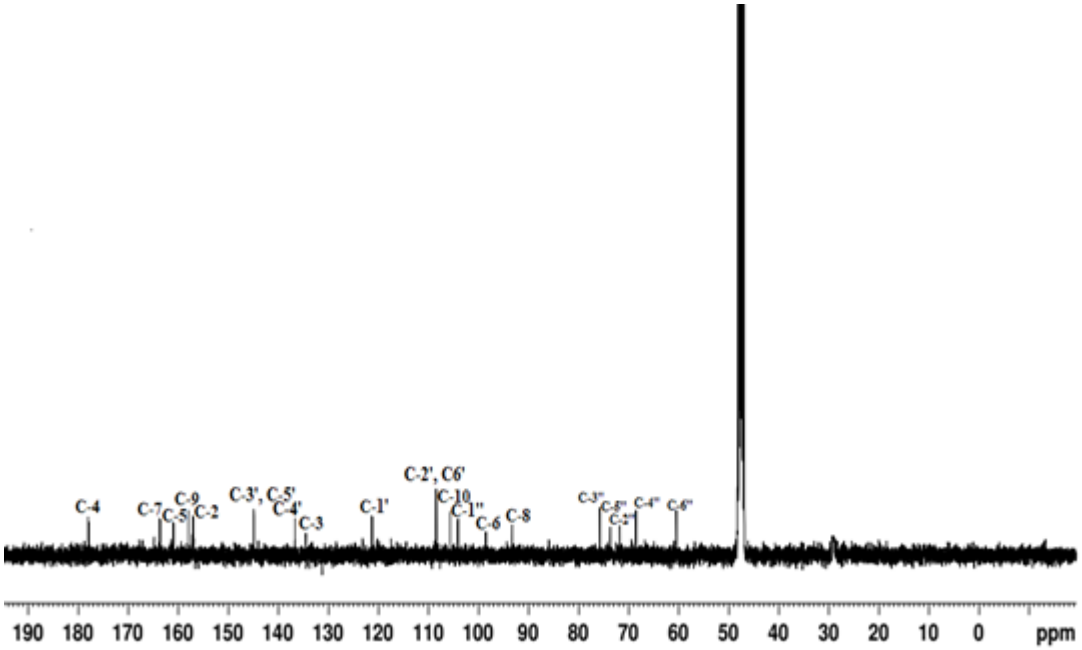



**Fig. S18.** $^{13}$C-NMR spectrum (100 MHz, $CD_3OD$) of compound **5**

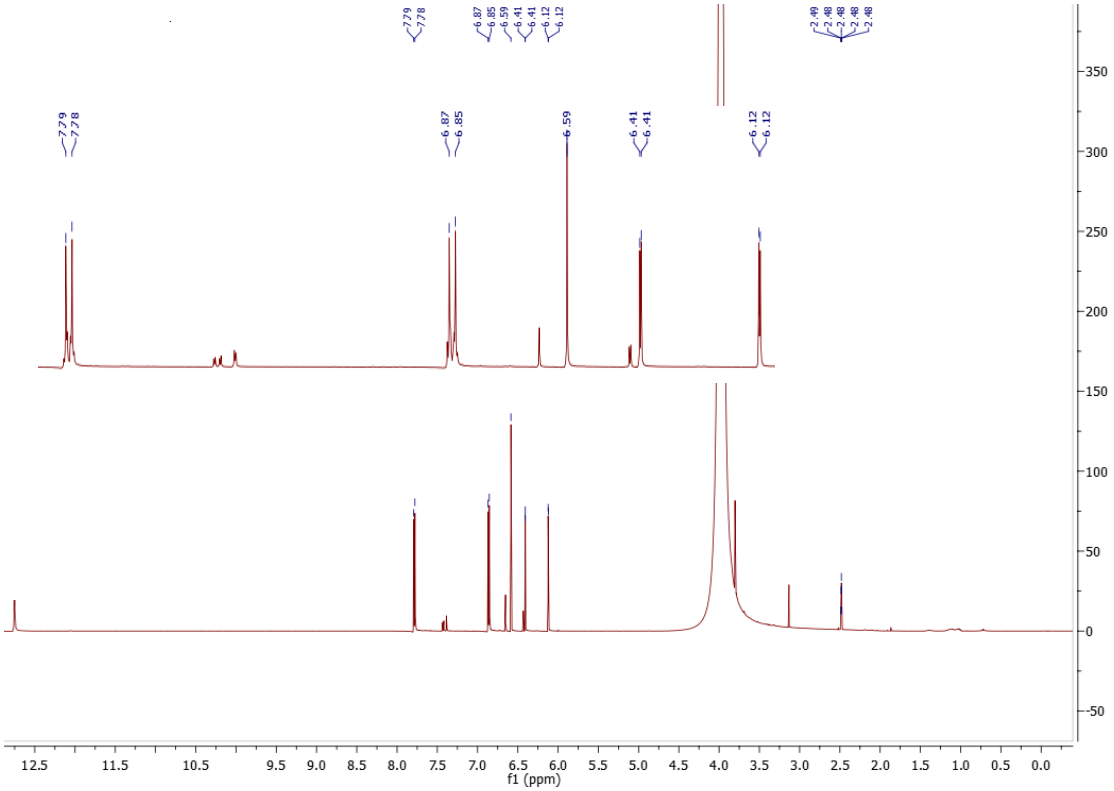



**Fig. S19.** $^{1}$H-NMR spectrum (600 MHz, DMSO-d6) of compound **6**

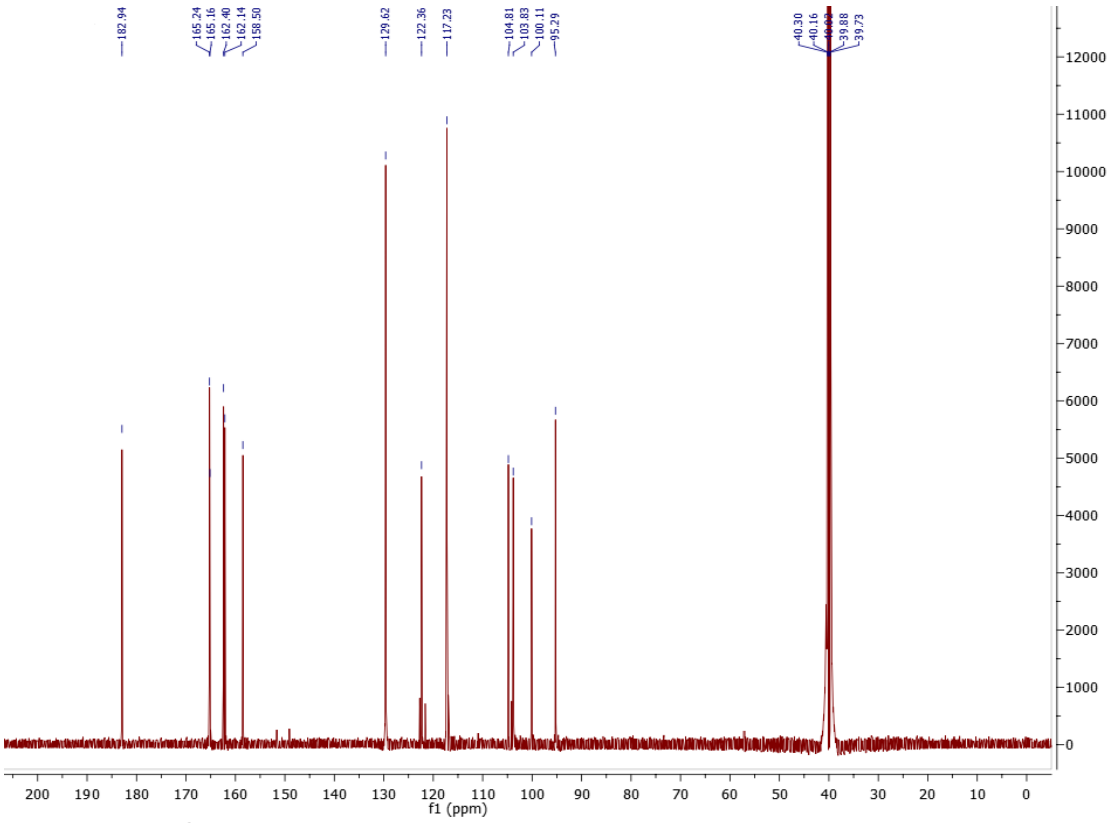



**Fig. S20.** $^{13}$C-NMR spectrum (150 MHz, DMSO-d6) of compound **6**

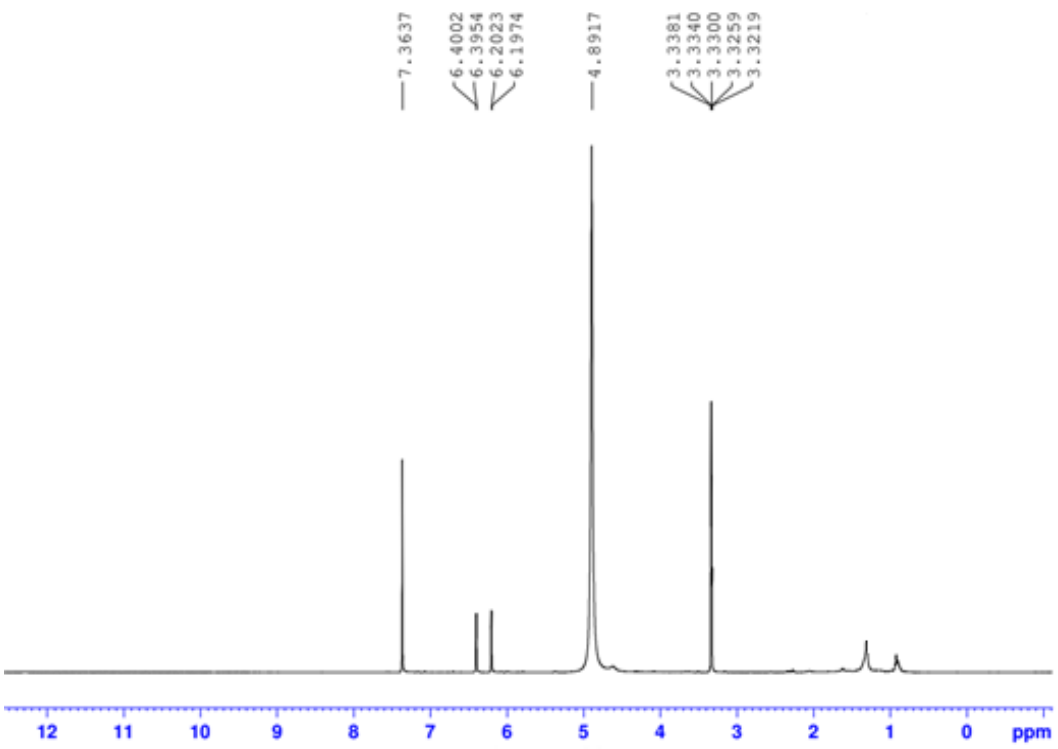



**Fig. S21.** $^{1}$H-NMR spectrum (400 MHz, $CD_3OD$) of compound **7**

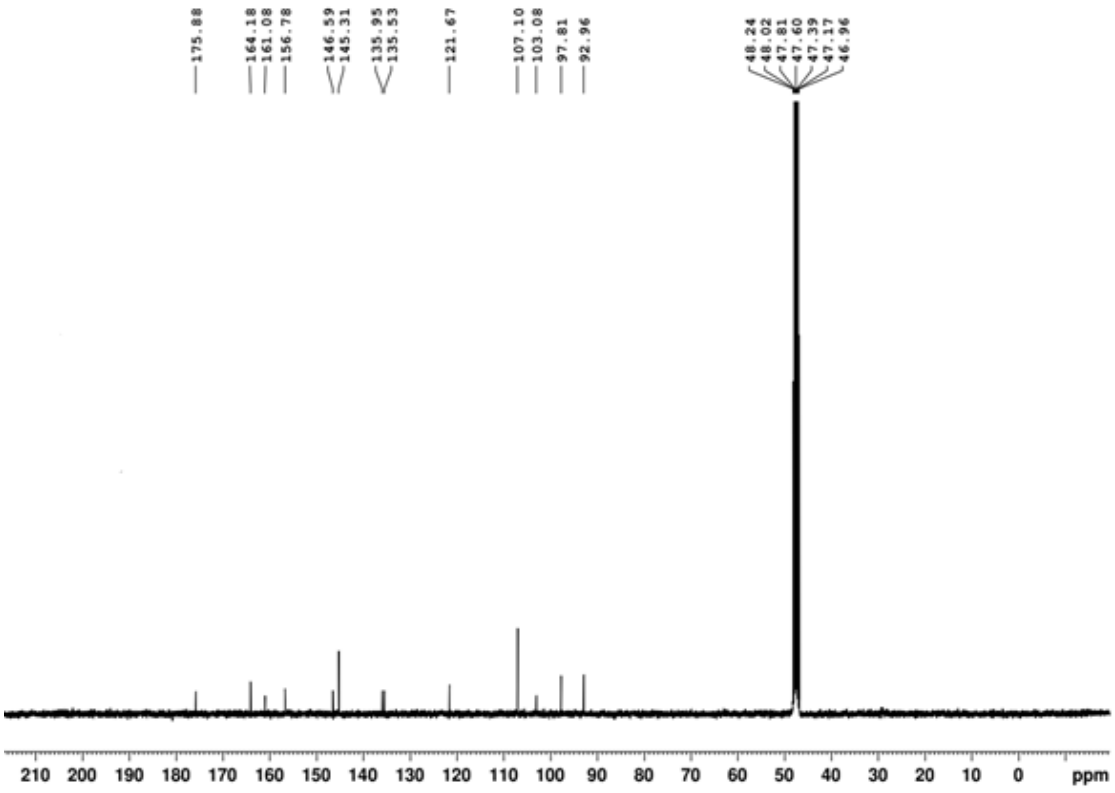



**Fig. S22.** $^{13}$C-NMR spectrum (100 MHz, $CD_3OD$) of compound **7**

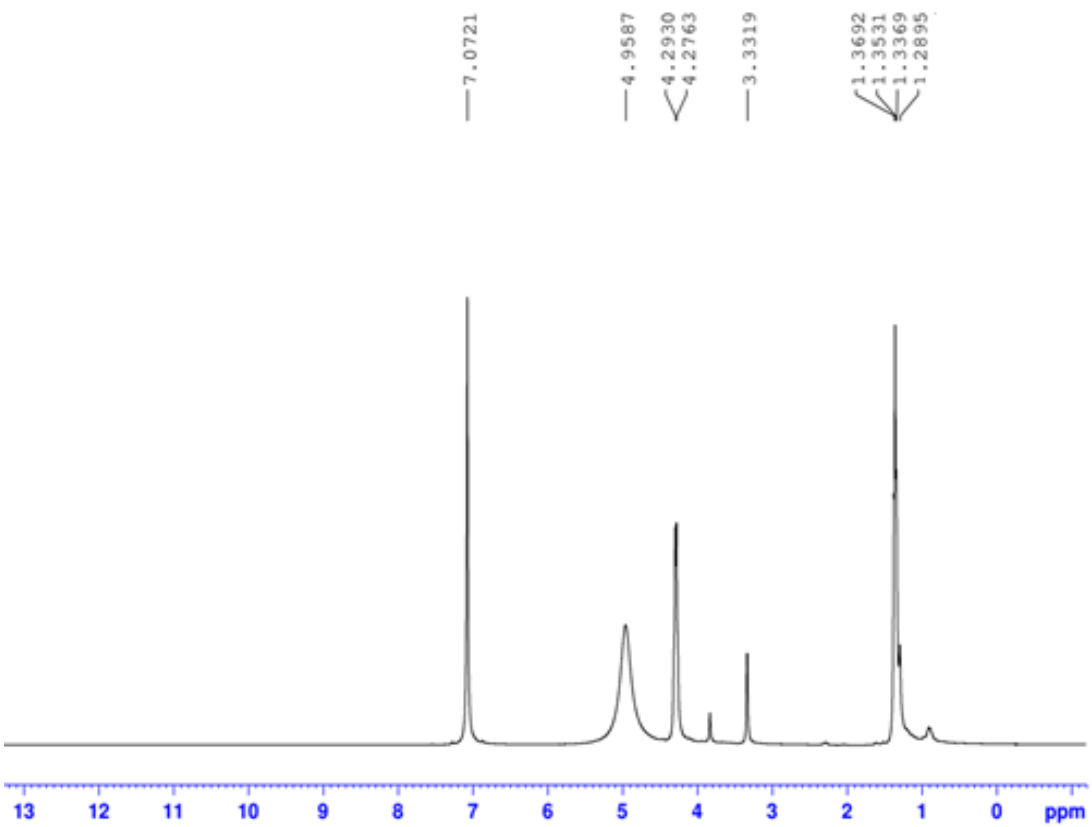



**Fig. S23.** $^{1}$H-NMR spectrum (400 MHz, $CD_3OD$) of compound **8**

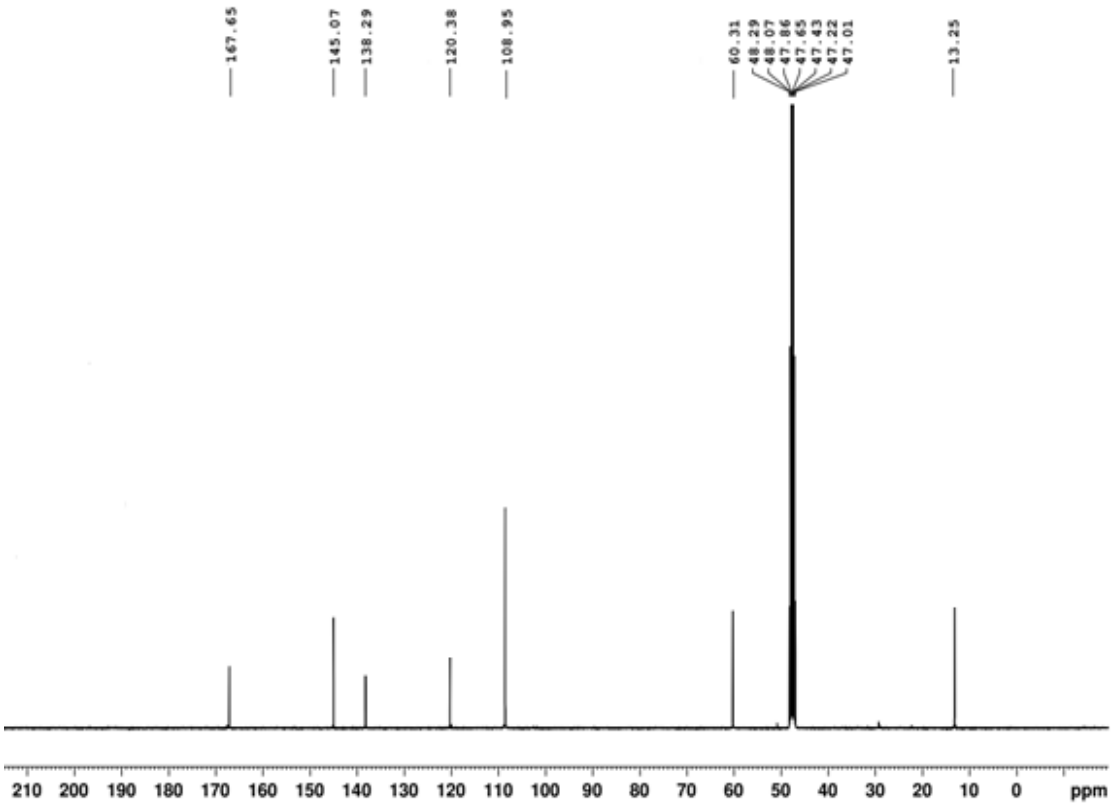



**Fig. S24.** $^{13}$C-NMR spectrum (100 MHz, $CD_3OD$) of compound **8**

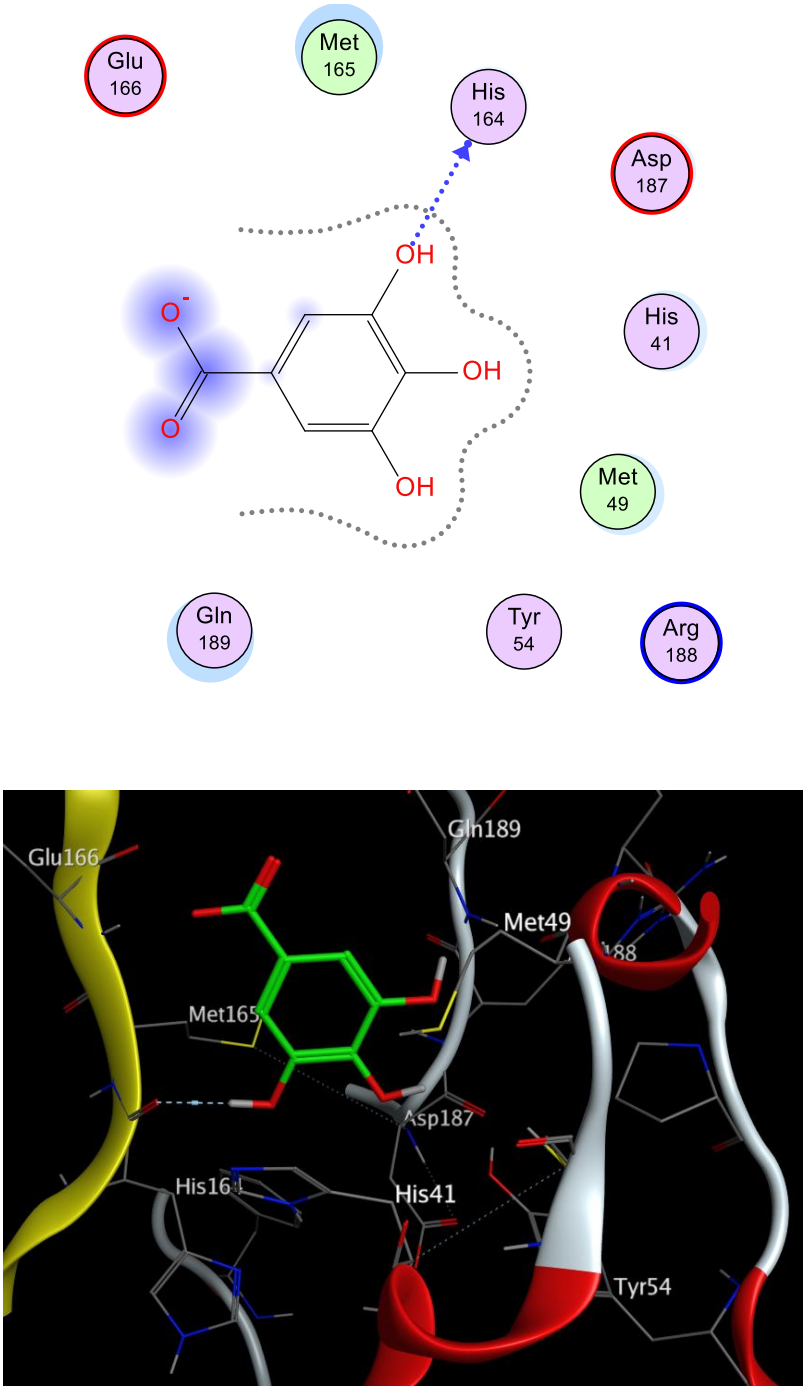



**Fig. S25.** 2D and 3D ligand interactions of compound **4** with main protease receptor

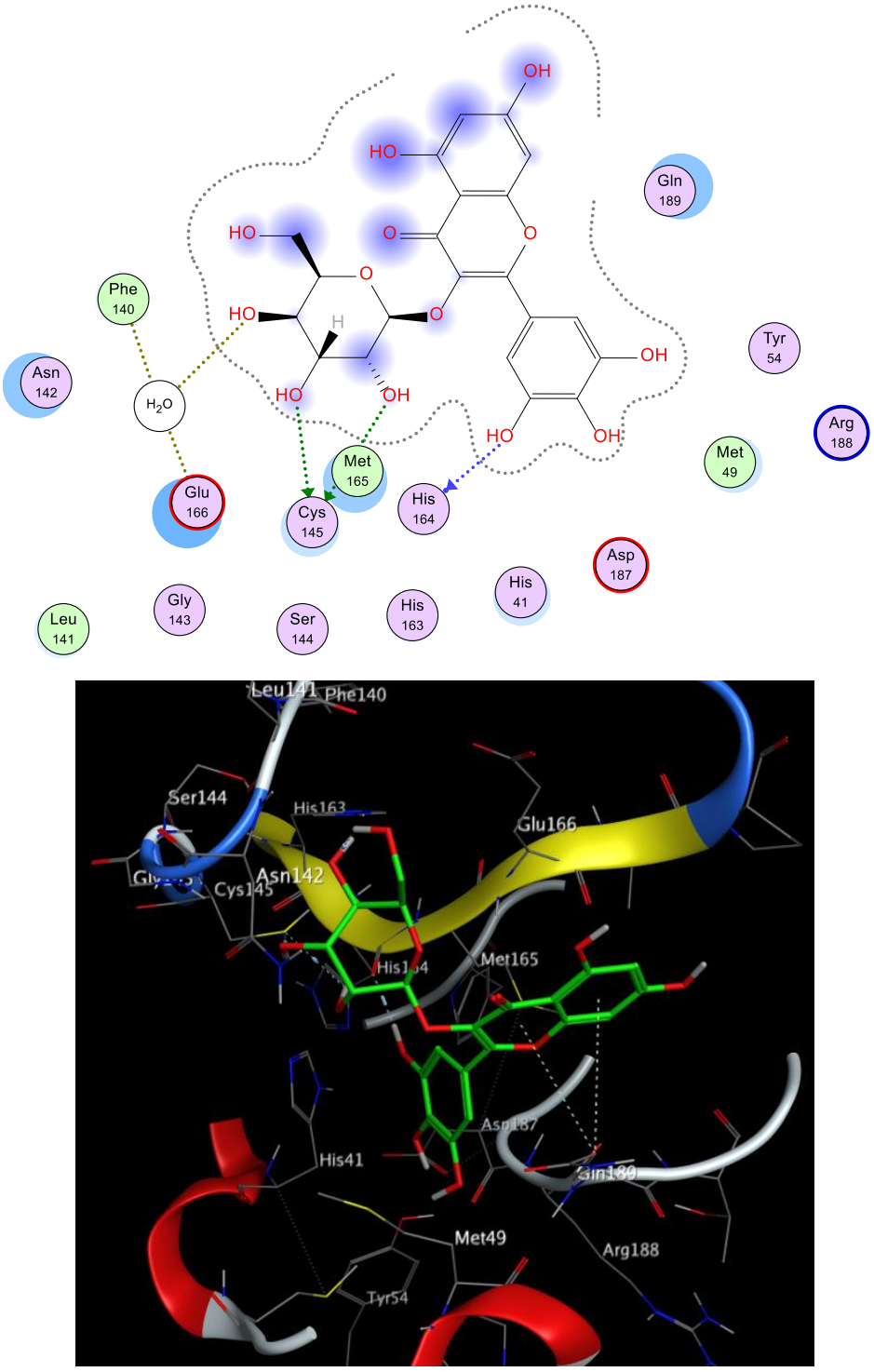



**Fig. S26.** 2D and 3D ligand interactions of compound **5** with main protease receptor

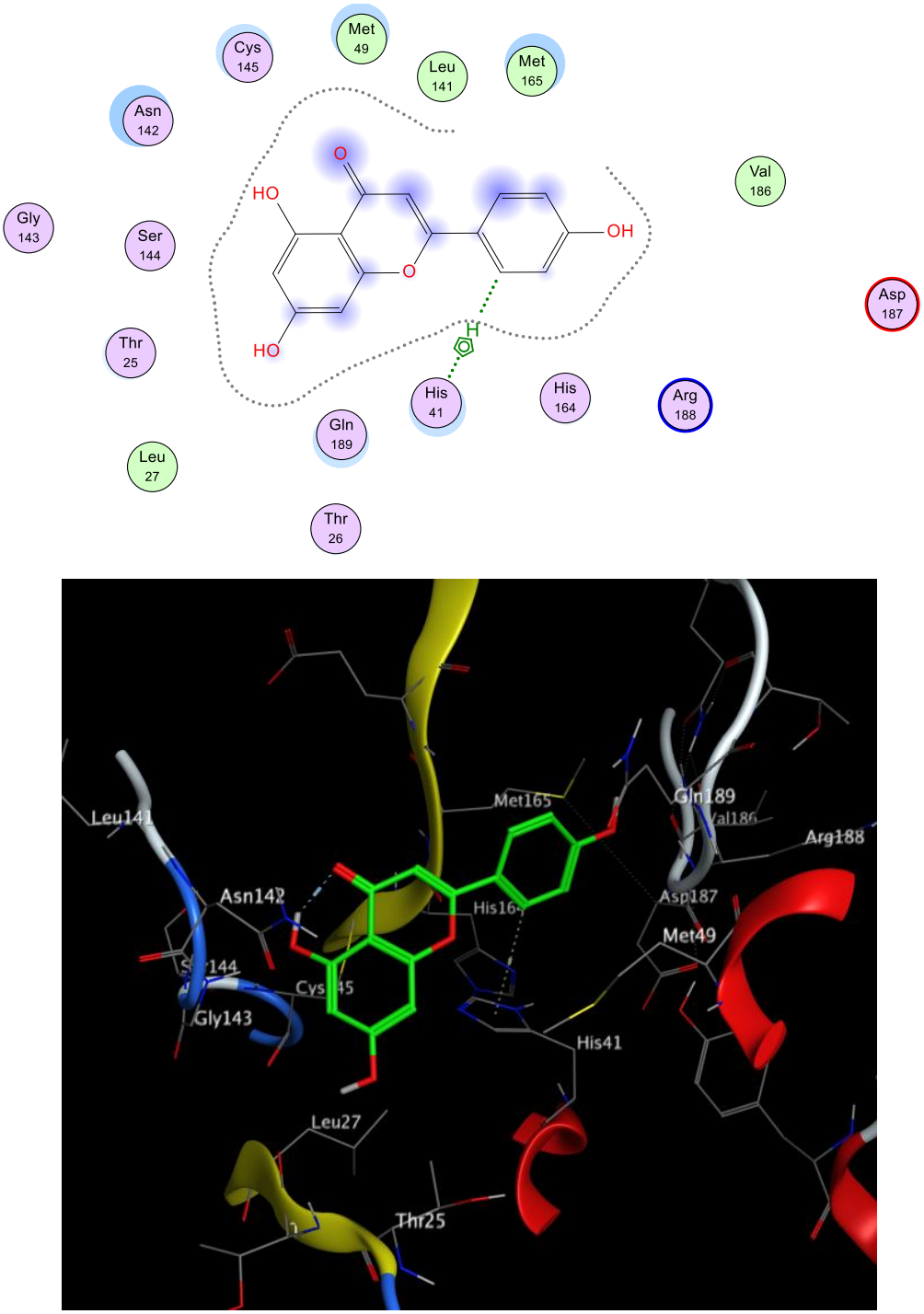



**Fig. S27.** 2D and 3D ligand interactions of compound **6** with main protease receptor

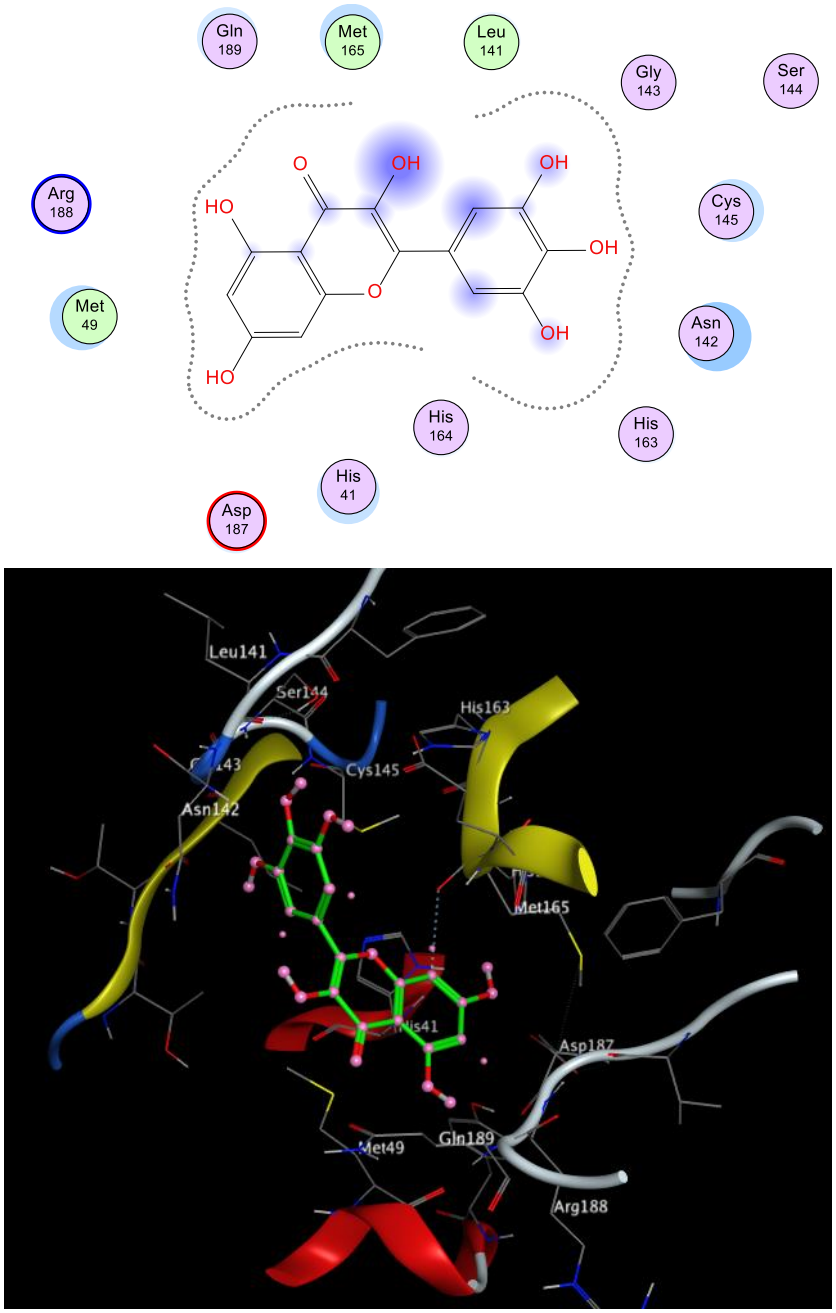



**Fig. S28.** 2D and 3D ligand interactions of compound **7** with main protease receptor

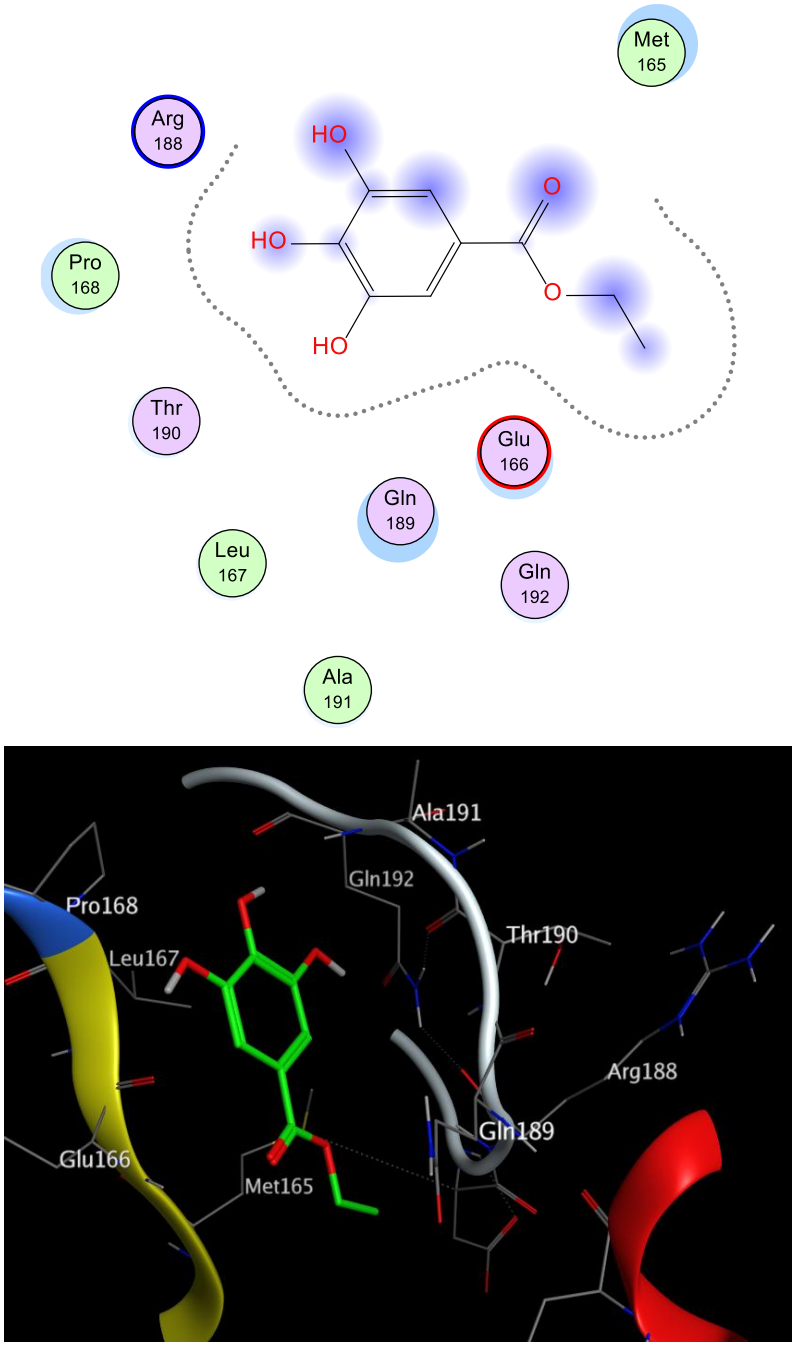



**Fig. S29.** 2D and 3D ligand interactions of compound **8** with main protease receptor

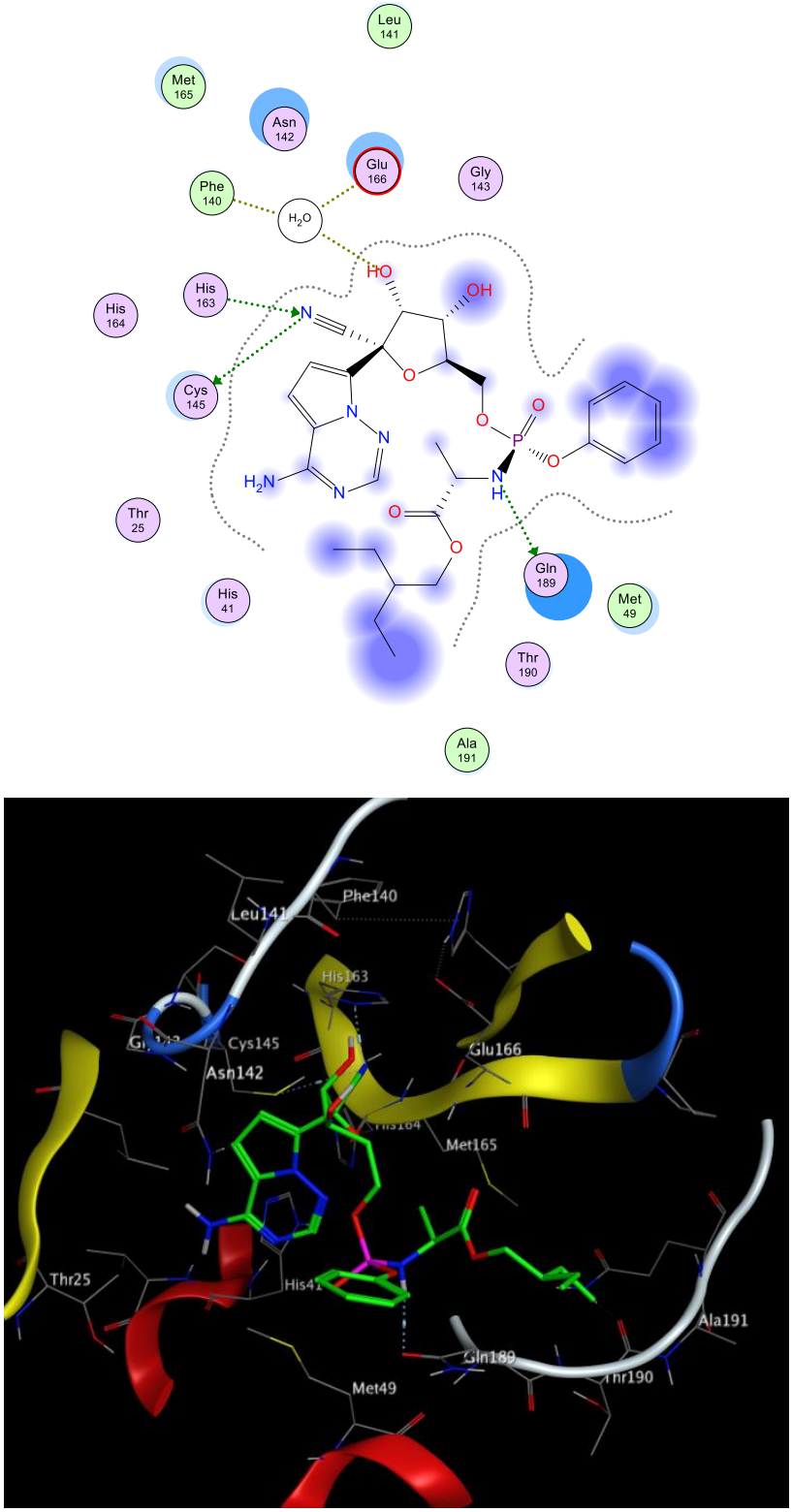



**Fig. S30.** 2D and 3D ligand interactions of compound **Remdesivir** with main protease receptor

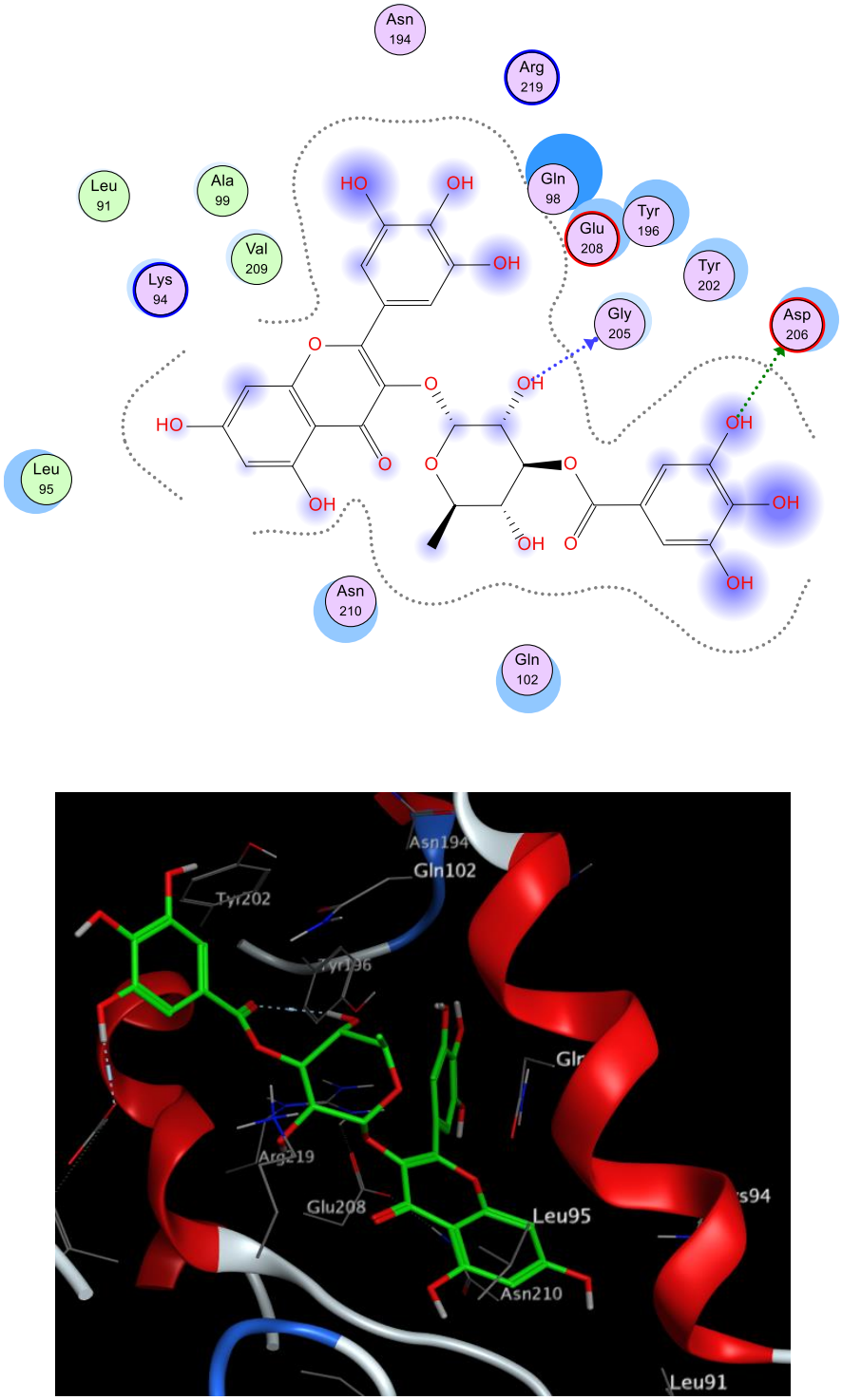
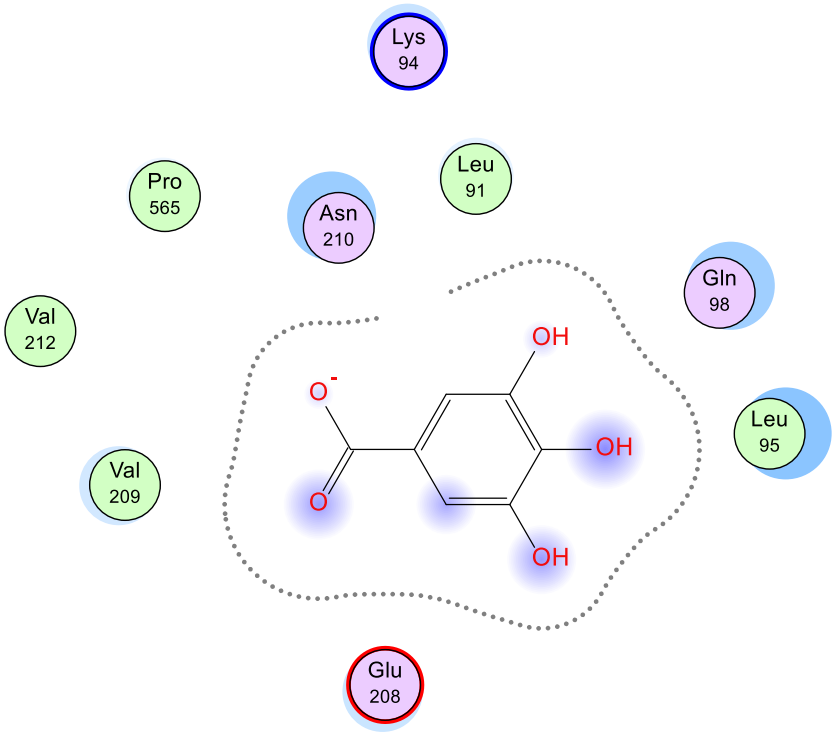



**Fig. 31.** 2D and 3D ligand interactions of compound **3** with spike glycoprotein



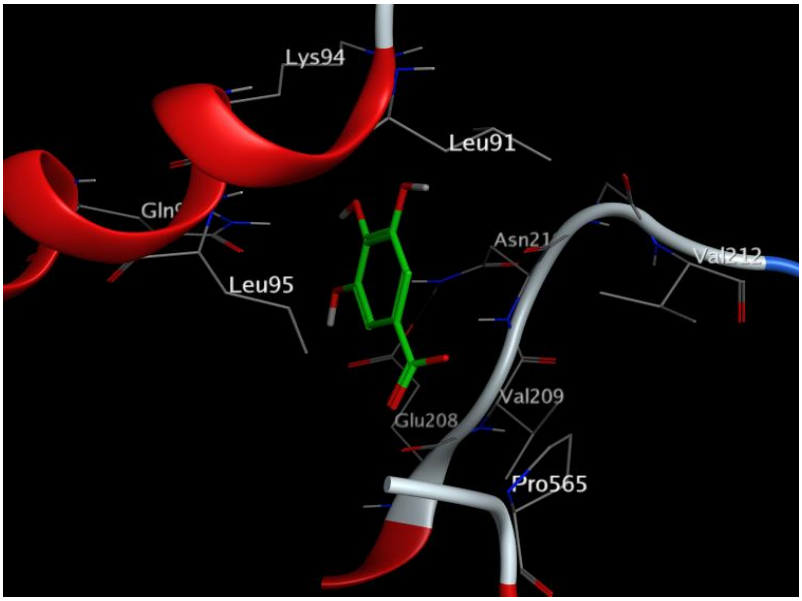




**Fig. S32.** 2D and 3D ligand interactions of compound **4** with spike glycoprotein

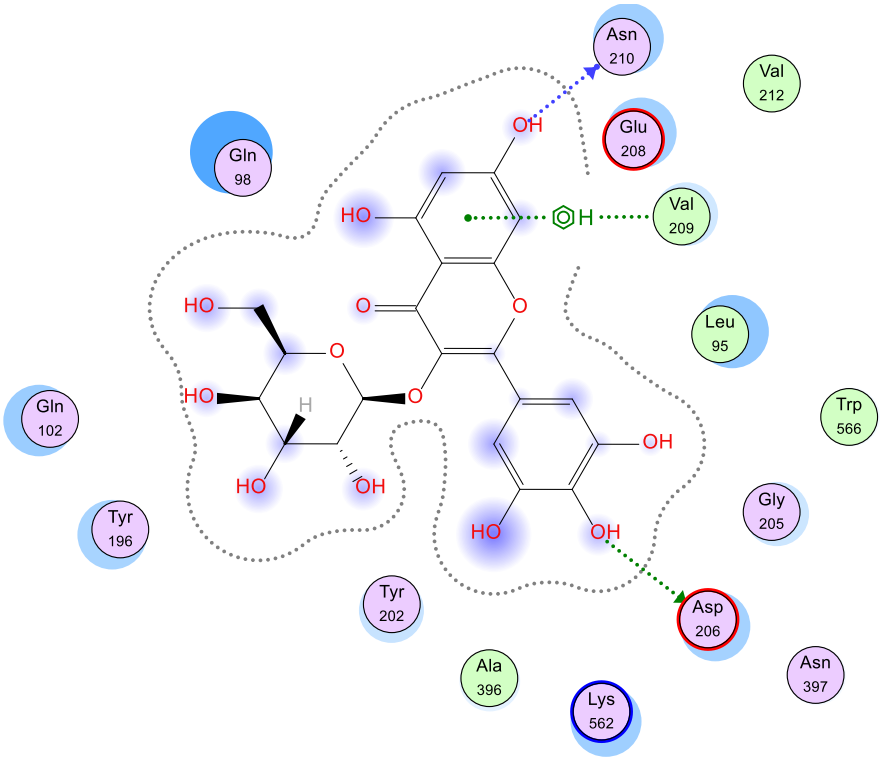



**Fig. S33.** 2D and 3D ligand interactions of compound **5** with spike glycoprotein

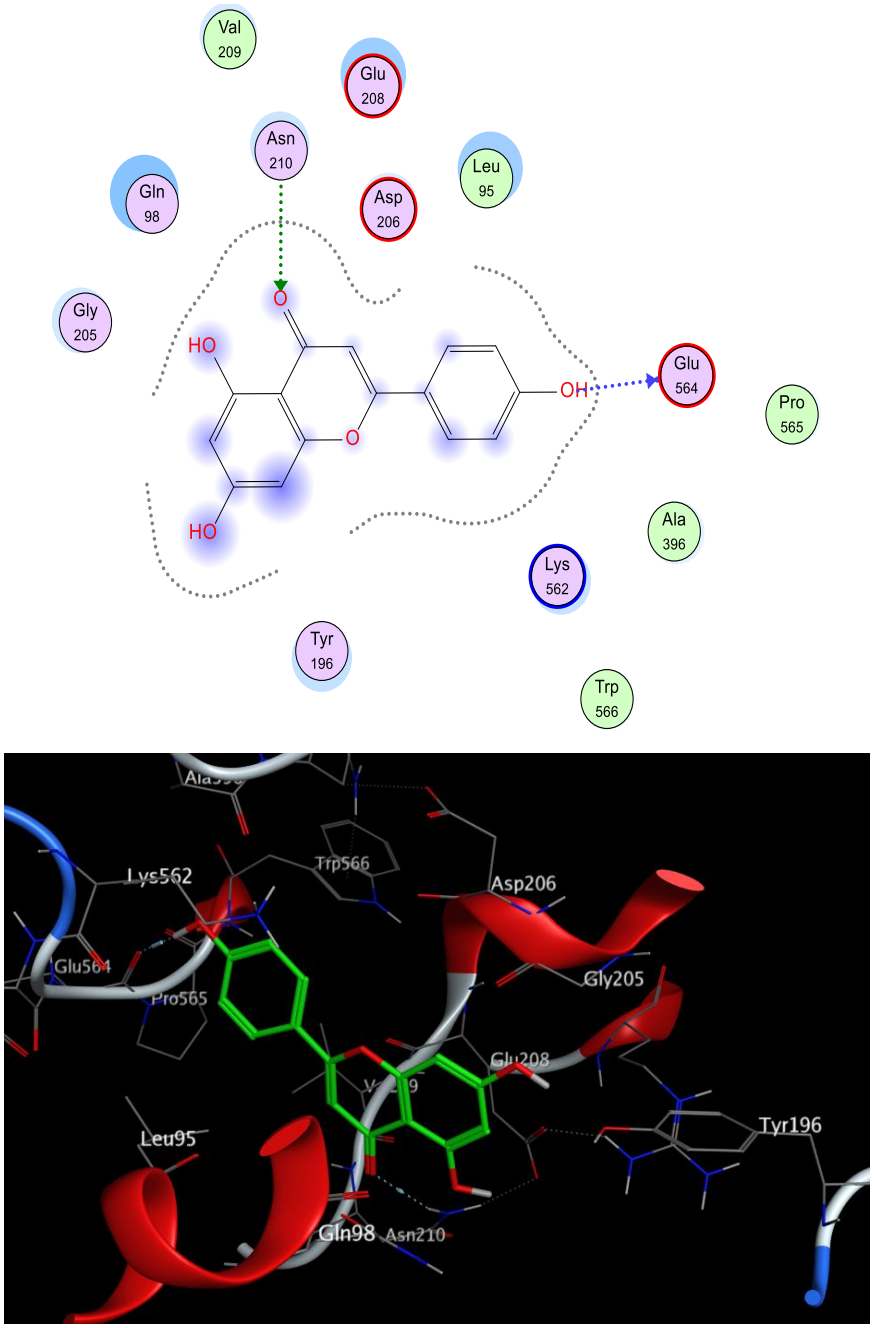



**Fig. S34.** 2D and 3D ligand interactions of compound **6** with spike glycoprotein

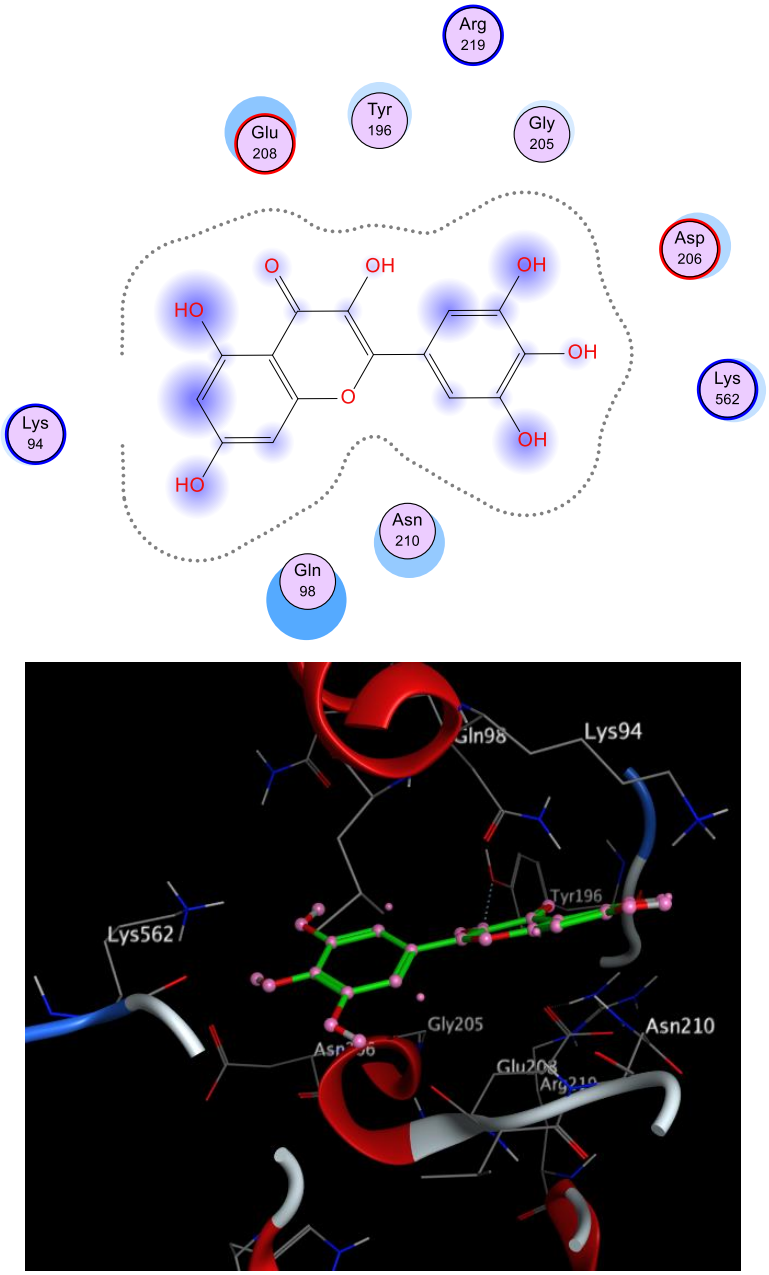
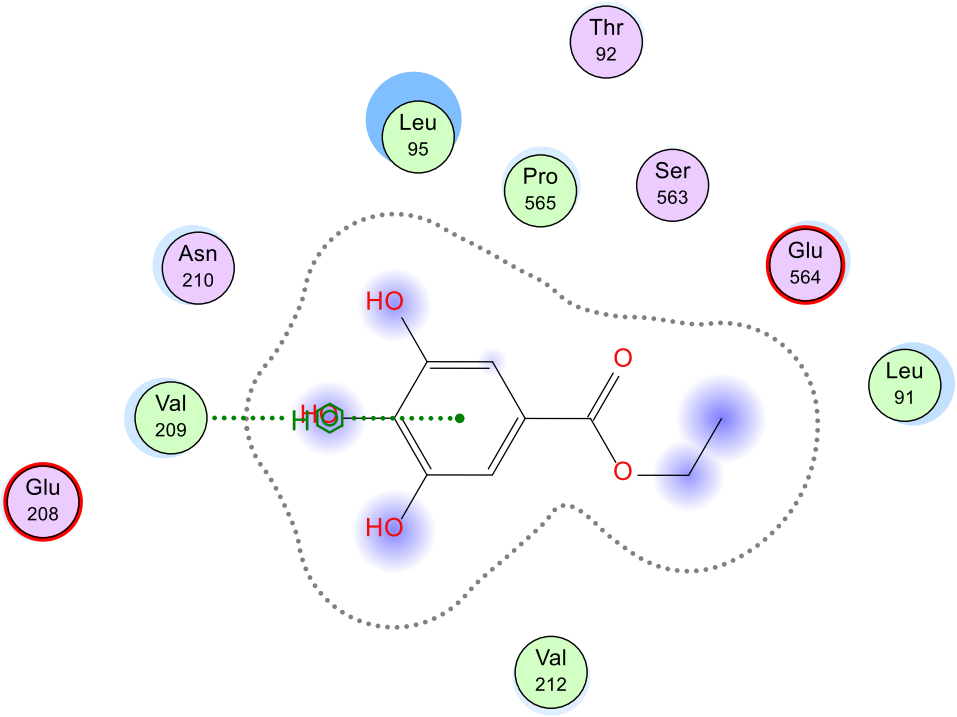



**Fig. S35.** 2D and 3D ligand interactions of compound **7** with spike glycoprotein



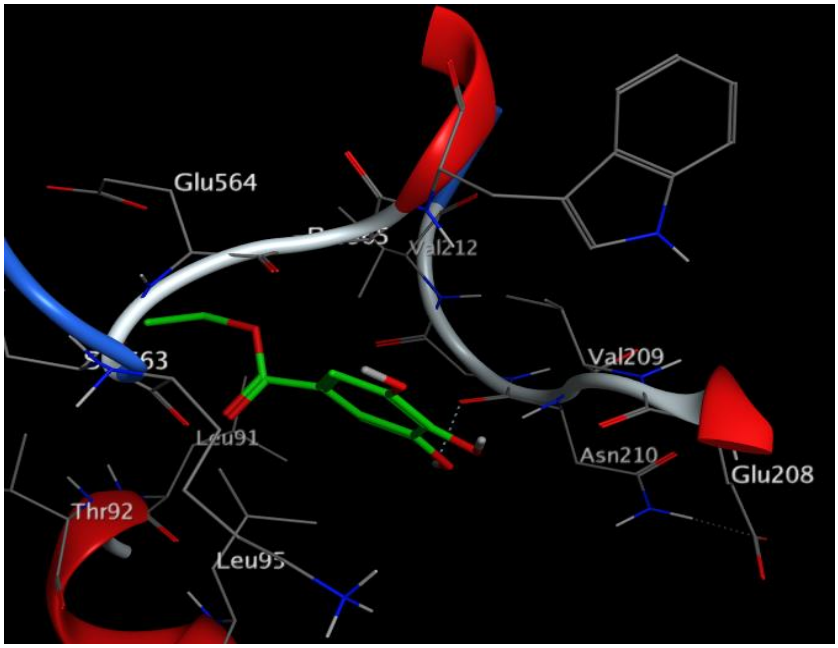




**Fig. S36.** 2D and 3D ligand interactions of compound **8** with spike glycoprotein

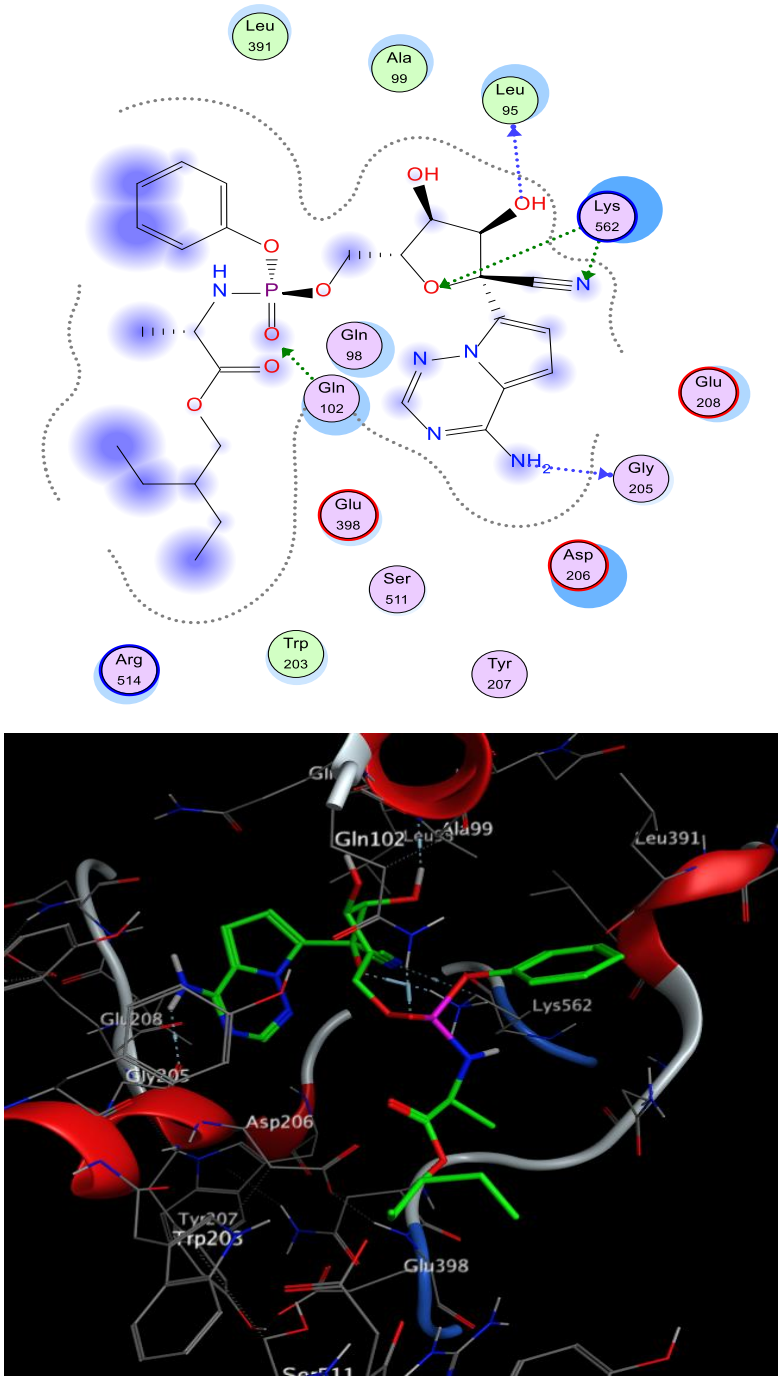



**Fig. S37.** 2D and 3D ligand interactions of compound **remdesivir** with spike glycoprotein

**Fig. S38.** Photo of the aerial parts of *Limonium tubiflorum* (Delile) Kuntze var *tubiflorum*