Chemical Constituents and Antimicrobial Activity of Branches and Leaves of *Cordia insignis* (Boraginaceae)

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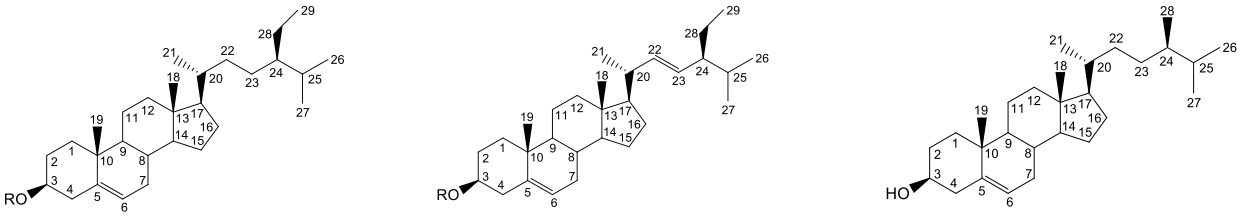
Supplementary Material

List of Figures



(**1**) (**2**) (**3**)

β-sitosterol (**1**): ^{1}H-NMR (400 MHz, $CDCl_3$) *δ*: 3.51-3.57 (1H, *m,* H-3), 5.36 (1H, *sl*, H-6); ^{13}C-NMR (125 MHz, $CDCl_3$) *δ*: 37.2 (C-1), 31.6 (C-2), 71.8 (C-3), 42.3 (C-4), 140.7 (C-5), 121.6 (C-6), 31.6 (C-7,8), 50.2 (C-9), 36.1 (C-10), 21.1 (C-11), 39.7 (C-12), 42.3 (C-13), 56.8 (C-14), 24.2 (C-15), 28.2 (C-16), 56.0 (C-17), 12.1 (C-18), 19.3 (C-19), 40.4 (C-20), 18.7 (C-21), 33.9 (C-22), 26.1 (C-23), 45.9 (C-24), 29.6 (C-25), 19.7 (C-26), 19.0 (C-27), 23.1 (C-28), 11.9 (C-29).

Stigmasterol (**2**): ^{1}H-NMR (400 MHz, $CDCl_3$) *δ*: 3.51-3.57 (1H, *m,* H-3), 5.36 (1H, *sl*, H-6), 5.18 (1H, *dd*, J= 15.2, 8.6 Hz, H-22), 5.05 (1H, *dd*, J= 15.2, 8.6 Hz, H-23); ^{13}C-NMR (125 MHz, $CDCl_3$) *δ*: 37.2 (C-1), 31.6 (C-2), 71.8 (C-3), 42.3 (C-4), 140.7 (C-5), 121.6 (C-6), 31.6 (C-7,8), 50.2 (C-9), 36.1 (C-10), 21.1 (C-11), 39.7 (C-12), 42.3 (C-13), 56.8 (C-14), 24.2 (C-15), 28.2 (C-16), 56.0 (C-17), 12.1 (C-18), 19.3 (C-19), 40.4 (C-20), 20.1 (C-21), 138.2 (C-22), 129.3 (C-23), 50.1 (C-24), 31.9 (C-25), 22.6 (C-26), 19.7 (C-27), 25.3 (C-28), 11.8 (C-29).

Campesterol (**3**): ^{1}H-NMR (400 MHz, $CDCl_3$) *δ*: 3.51-3.57 (1H, *m,* H-3), 5.36 (1H, *sl*, H-6); ^{13}C-NMR (125 MHz, $CDCl_3$) *δ*: 37.2 (C-1), 31.6 (C-2), 71.8 (C-3), 42.3 (C-4), 140.7 (C-5), 121.6 (C-6), 31.6 (C-7,8), 50.2 (C-9), 36.1 (C-10), 21.1 (C-11), 39.7 (C-12), 42.3 (C-13), 56.8 (C-14), 24.2 (C-15), 28.2 (C-16), 56.0 (C-17), 12.1 (C-18), 19.3 (C-19), 40.4 (C-20), 18.7 (C-21), 33.9 (C-22), 26.1 (C-23), 45.9 (C-24), 29.6 (C-25), 19.7 (C-26), 19.0 (C-27), 23.1 (C-28).

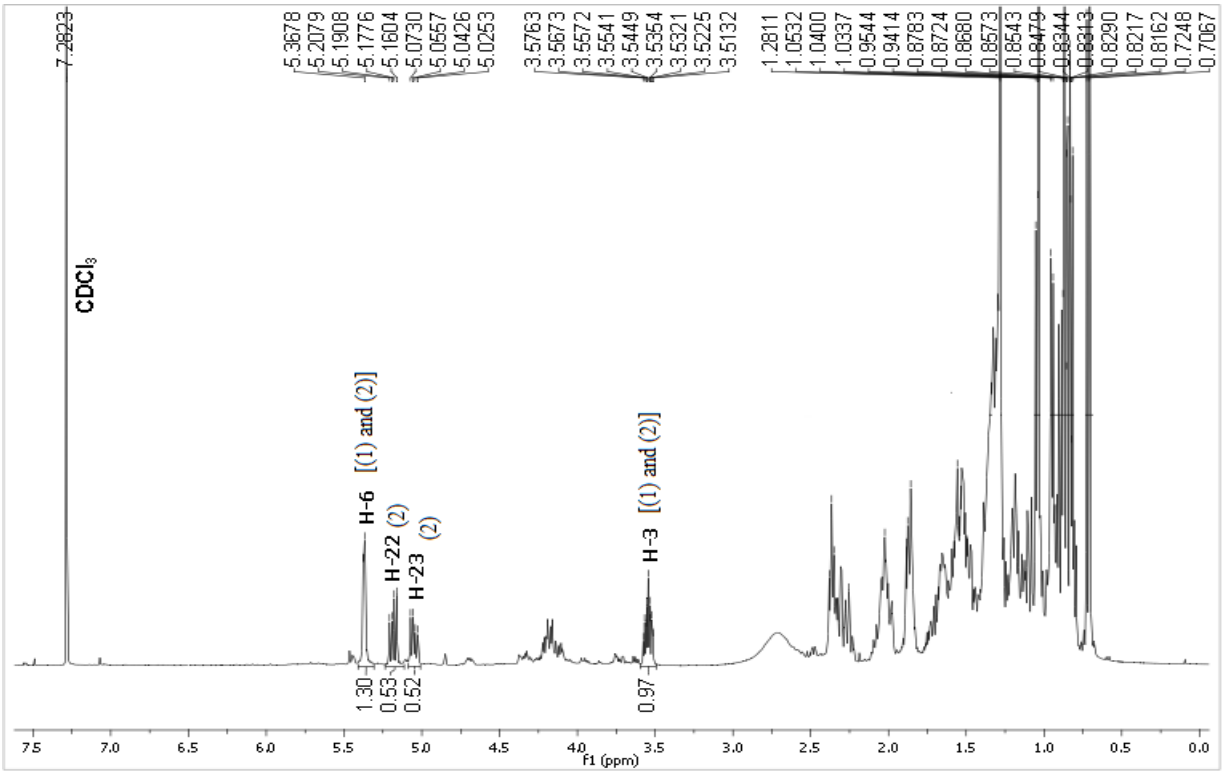


Figure 1. ^{1}H -NMR spectrum ($CDCl_3$, 500 MHz) of the mixture of **1**, **2** and **3**.

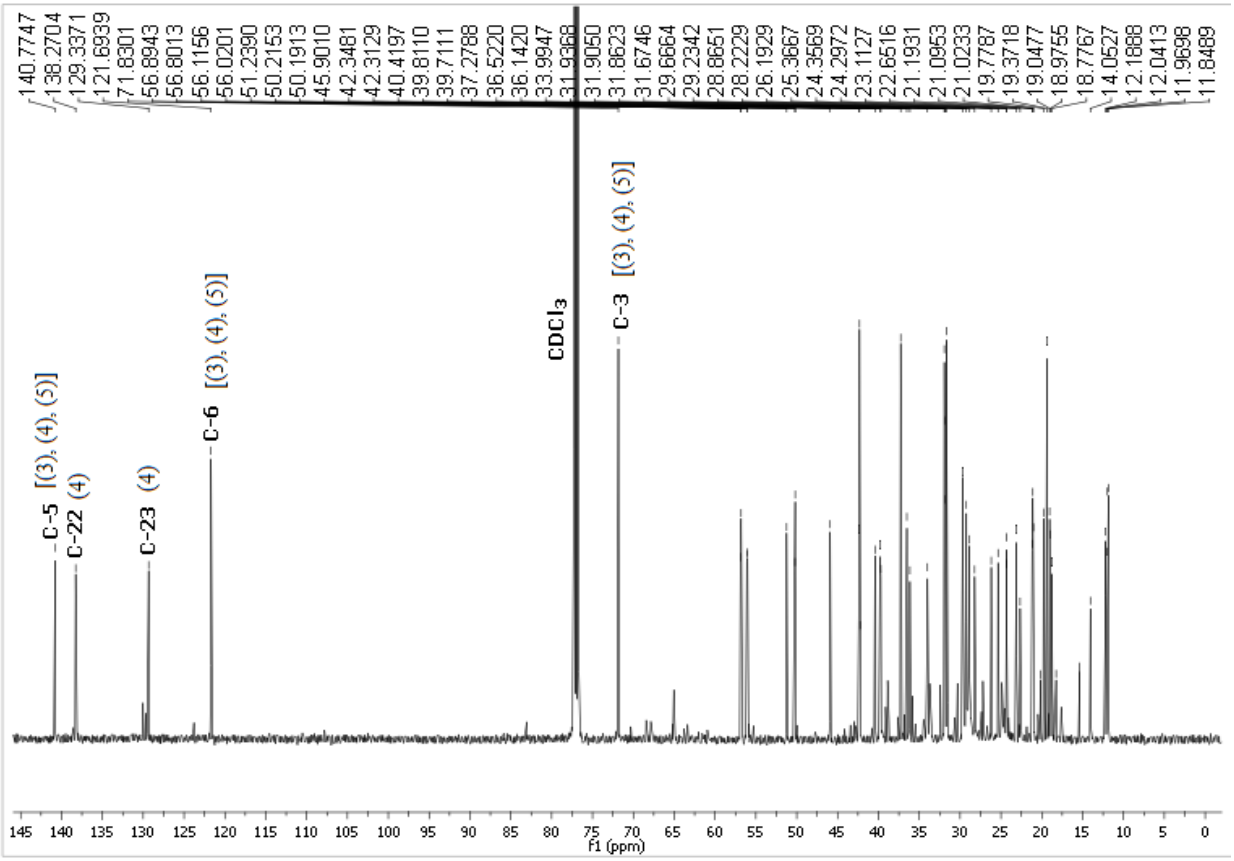


Figure 2. ^{13}C-NMR spectrum ($CDCl_3$, 125 MHz) of the mixture of **1**, **2** and **3**.

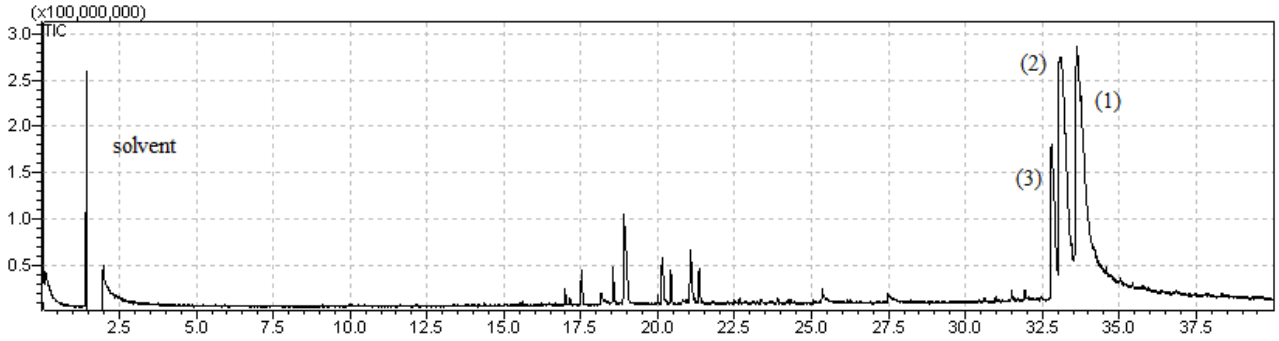


Figure 3. Gas chromatogram of the mixture of **1, 2** and **3**.

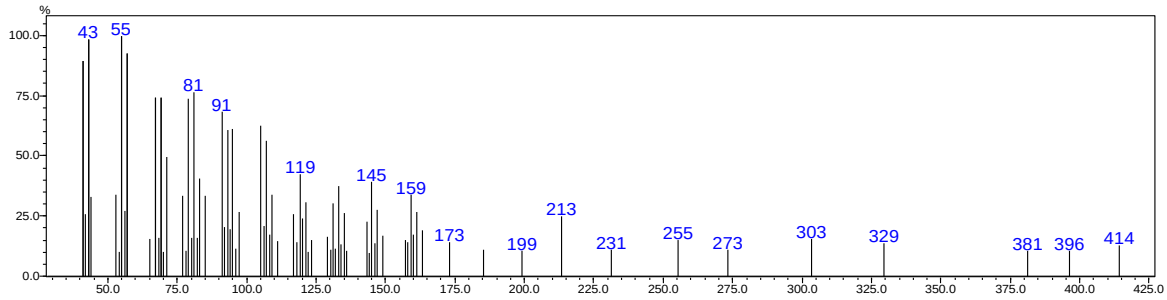


Figure 4. Mass spectrum of **1**.

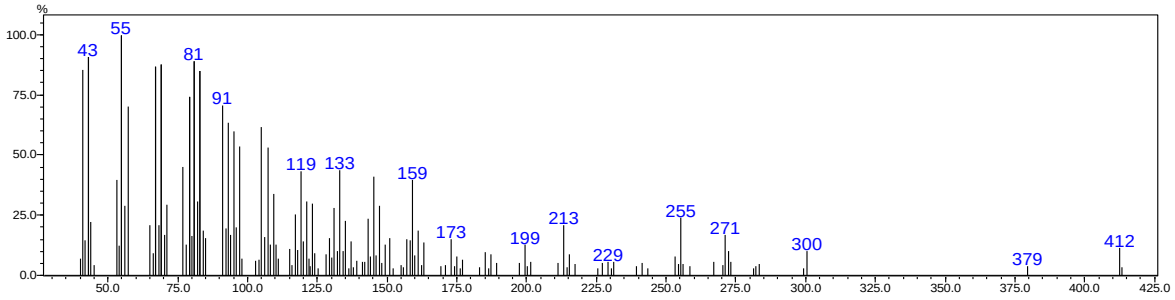


Figure 5. Mass spectrum of **2**.

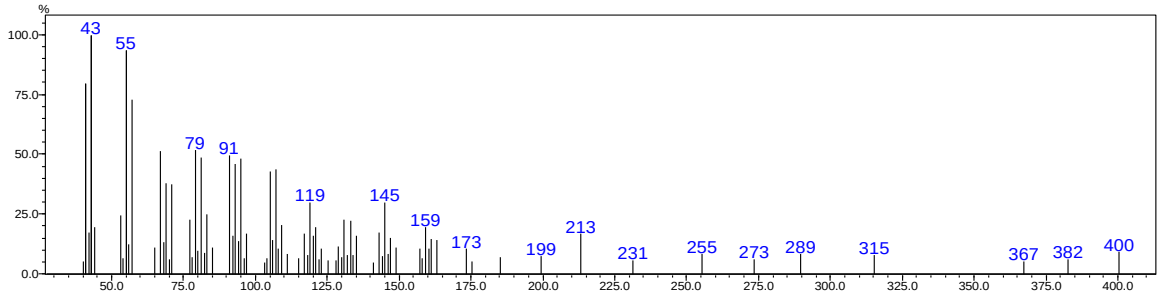
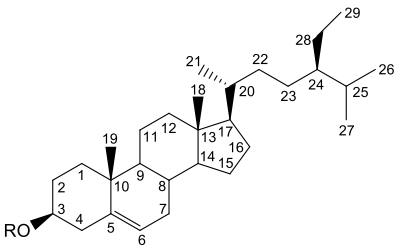
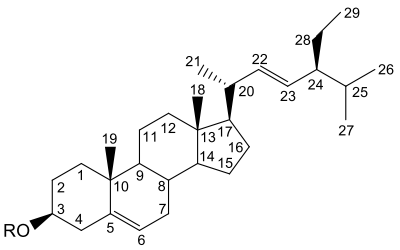


Figure 6. Mass spectrum of **3**.



(**4**) R= *β-D*-glucose



(**5**) R= *β-D*-glucose

3-*O-β-D*- glucopyranosyl sitosterol (**4**): ^{1}H-NMR (400 MHz, C_5D_5N) *δ*: 3.82-3.91 (1H, *m*, H-3), 5.35 (1H, *sl*, H-6), 4.87 (1H, *dl*, J= 7.7 Hz, H-1'), 3.98-4.05 (2H, m, H-2', 3'), 4.32-4.38 (2H, *m*, H-4', 5'), 4.17 (2H, *dd*, J= 11.7, 5.4 Hz); ^{13}C-NMR (125 MHz, C_5D_5N) *δ*: 37.2 (C-1), 30.0 (C-2), 78.2 (C-3), 42.2 (C-4), 140.7 (C-5), 121.7 (C-6), 31.9 (C-7), 31.8 (C-8), 50.1 (C-9), 36.7 (C-10), 21.0 (C-11), 39.1 (C-12), 42.1 (C-13), 56.6 (C-14), 24.2 (C-15), 28.3 (C-16), 56.0 (C-17), 11.7 (C-18), 19.0 (C-19), 36.1 (C-20), 18.8 (C-21), 33.9 (C-22), 26.1 (C-23), 45.8 (C-24), 29.2 (C-25), 19.7 (C-26), 19.2 (C-27), 23.1 (C-28), 11.9 (C-29), 102.3 (C-1'), 75.0 (C-2'), 77.9 (C-3'), 71.4 (C-4'), 78.3 (C-5'), 62.6 (C-6').

3-*O-β-D*- glucopyranosyl stigmasterol (**5**): ^{1}H-NMR (400 MHz, C_5D_5N) *δ*: 3.82-3.91 (1H, *m*, H-3), 5.35 (1H, *sl*, H-6), 5.20 (1H, *dd*, J= 15.1, 8.7 Hz, H-22), 5.05 (1H, *dd*, J= 15.1, 8.7 Hz, H-23), 4.58-3.60 (6H, *m*, H-1',2',3',4',5',6'): ^{13}C-NMR (125 MHz, C_5D_5N) *δ*: 37.2 (C-1), 30.0 (C-2), 78.2 (C-3), 42.2 (C-4), 140.7 (C-5), 121.7 (C-6), 31.9 (C-7), 31.8 (C-8), 50.1 (C-9), 36.7 (C-10), 21.0 (C-11), 39.1 (C-12), 42.1 (C-13), 56.6 (C-14), 24.2 (C-15), 28.3 (C-16), 56.0 (C-17), 11.7 (C-18), 19.0 (C-19), 36.1 (C-20), 18.8 (C-21), 138.6 (C-22), 129.2 (C-23), 45.8 (C-24), 29.2 (C-25), 19.7 (C-26), 19.2 (C-27), 23.1 (C-28), 11.9 (C-29), 102.3 (C-1'), 75.0 (C-2'), 77.9 (C-3'), 71.4 (C-4'), 78.3 (C-5'), 62.6 (C-6').

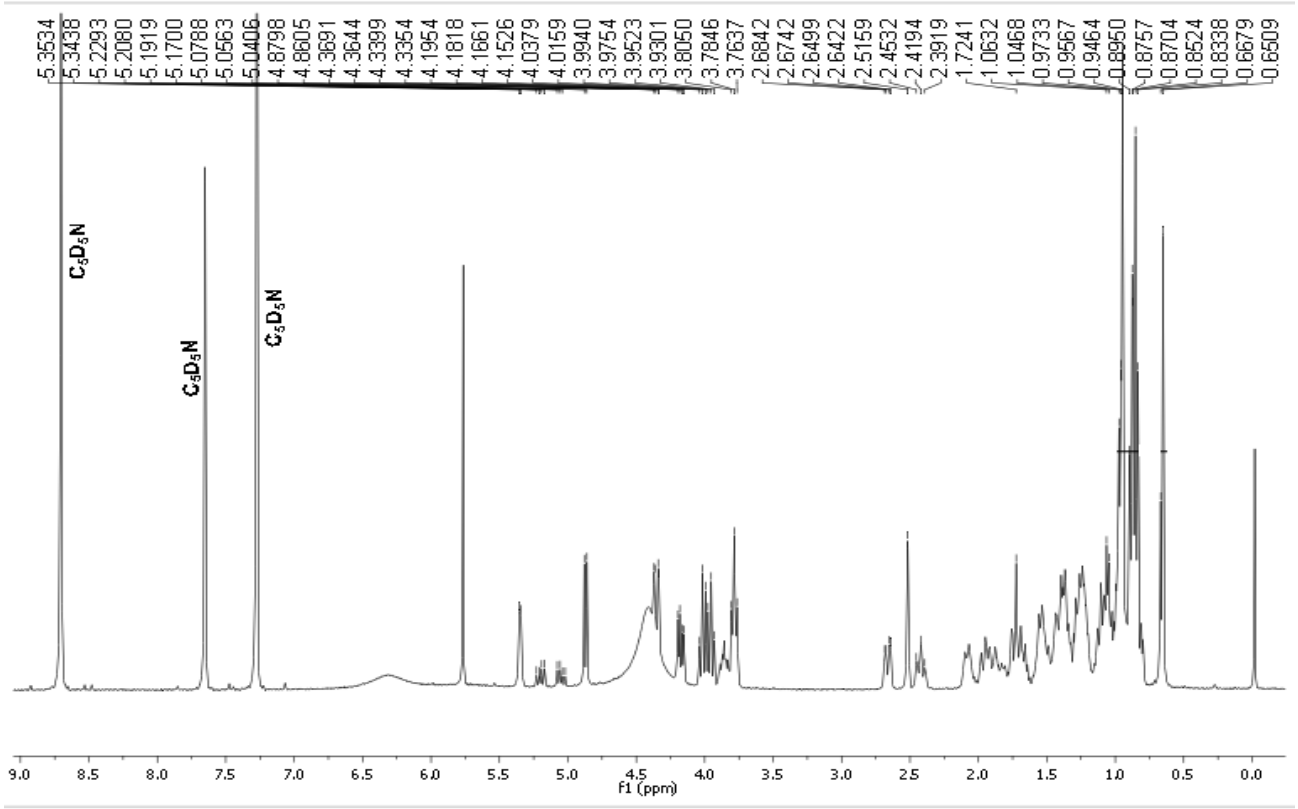


Figure 7. ^{1}H-NMR spectrum (C_5D_5N, 500 MHz) of the mixture of **4** and **5**.

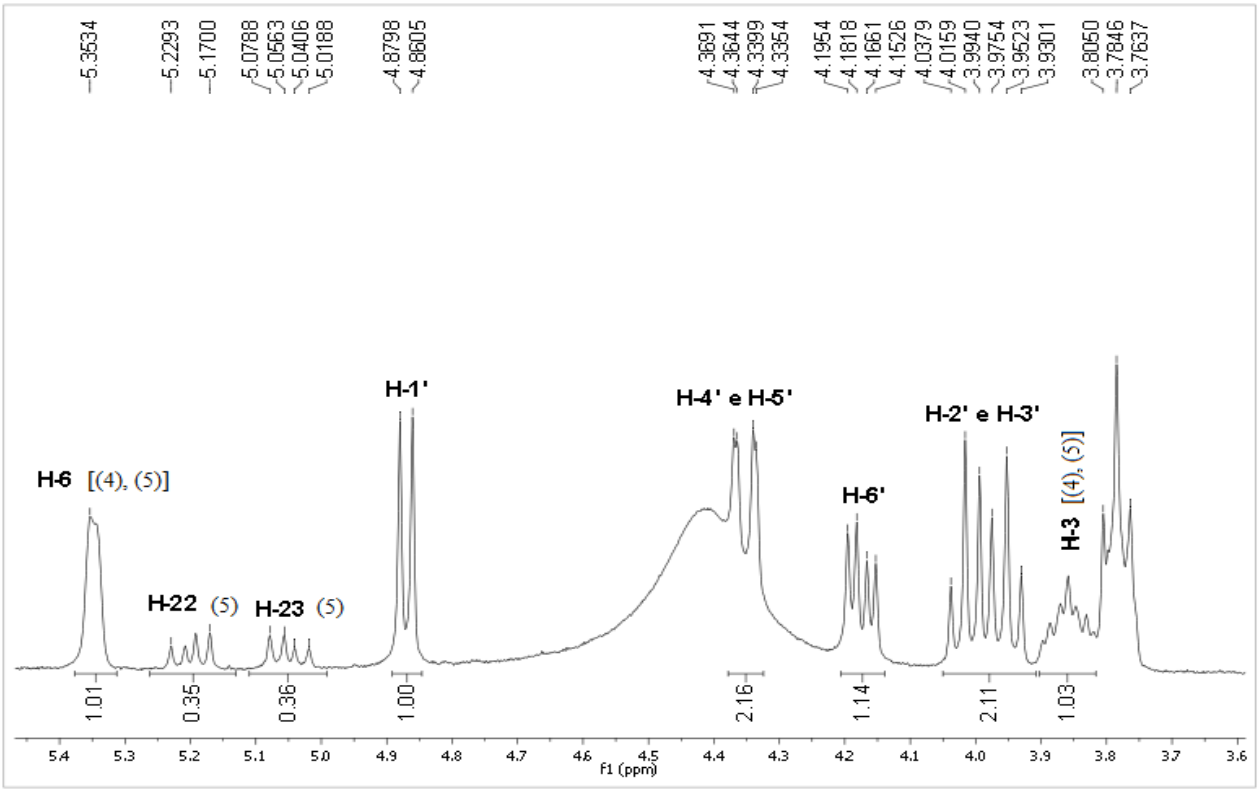


Figure 8. Expansion (δ$_H$ 3.6-5.4 ppm) of ^{1}H-NMR spectrum (C_5D_5N, 500 MHz) of the mixture of **4** and **5**.

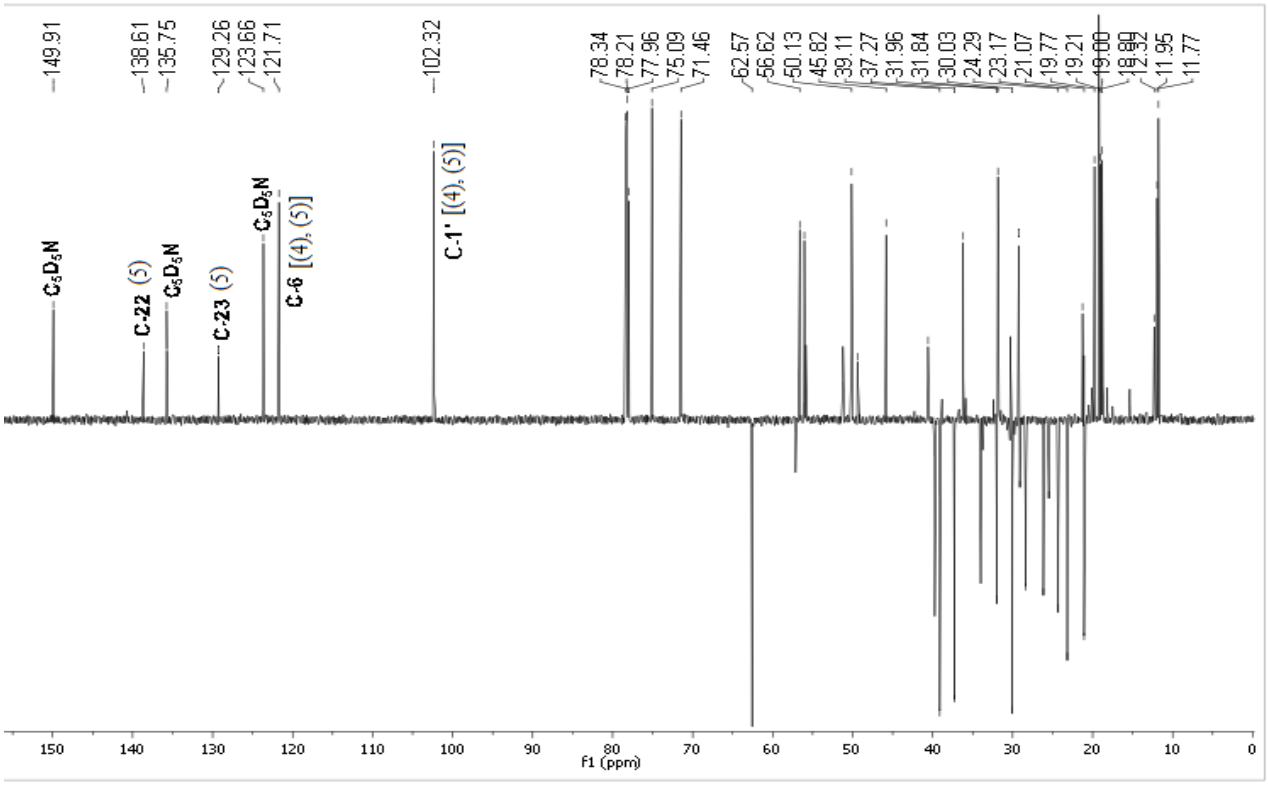


Figure 9. DEPT 135 spectrum (C_5D_5N, 125 MHz) of the mixture of **4** and **5**

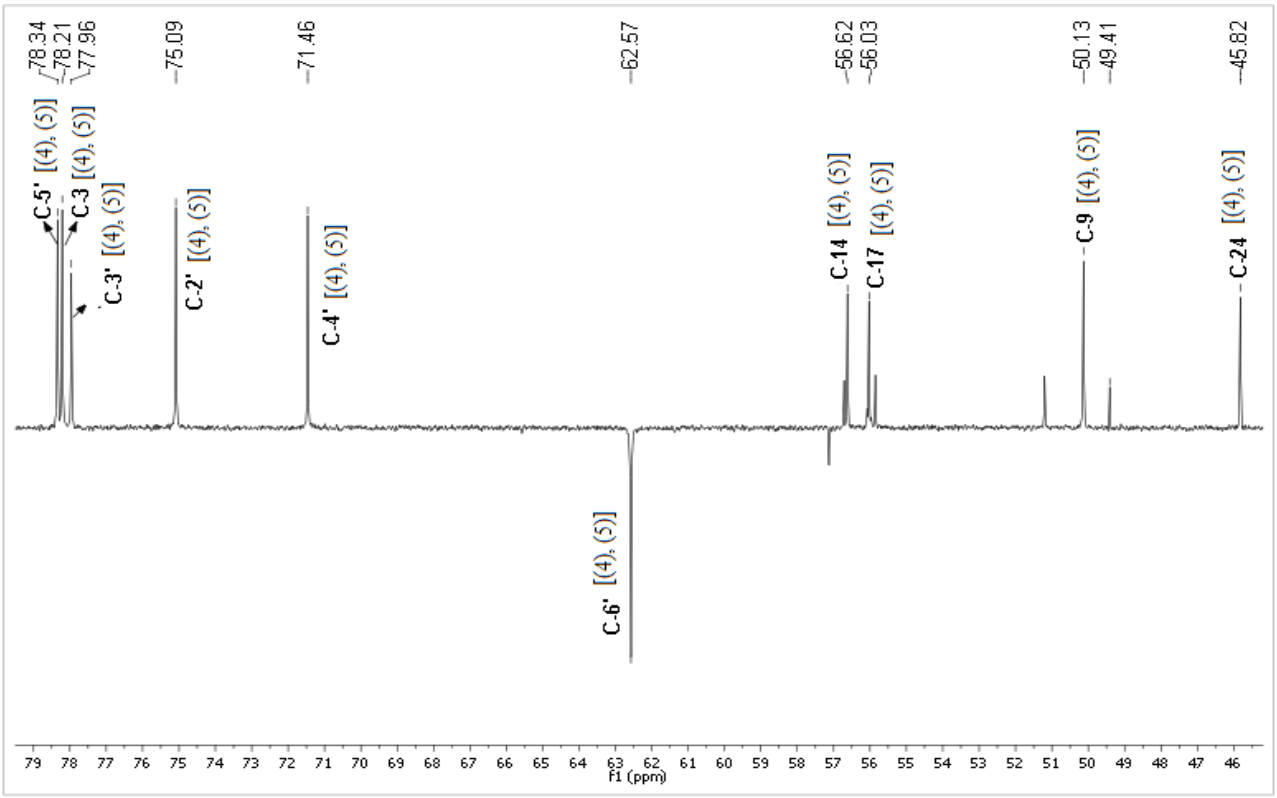


Figure 10. Expansion (δC 46.0-79.0 ppm) DEPT 135 spectrum (C_5D_5N, 125 MHz) of the mixture of **4** and **5**.

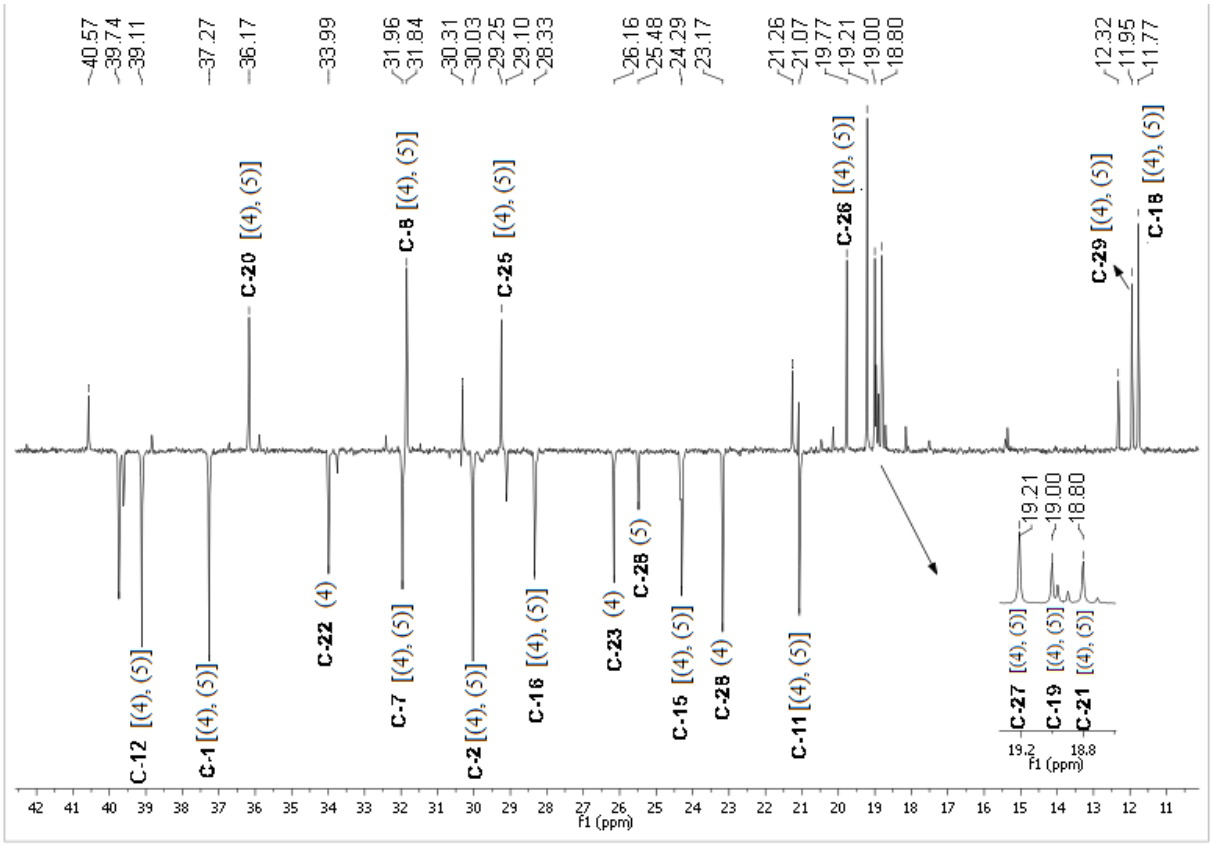
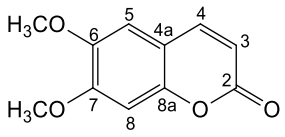


Figure 11. Expansion (δC 11.0-42.0 ppm) DEPT 135 spectrum (C_5D_5N, 125 MHz) of the mixture of **4** and **5**.



(**6**)

Scoparone (**6**): ^{1}H-NMR (500 MHz, $CDCl_3$) δ: 6.32 (1H, *d*, J= 9.45 Hz, H-3), 7.65 (1H, *d*, J= 9.45 Hz, H-4), 6.83 (1H, *s*, H-5), 7.82 (1H, *s*, H-8), 3.95 (3H, *s*, -OCH_3), 3.98 (3H, *s*, -OCH_3); DEPT 135 (125 MHz, $CDCl_3$) δ: 161.4 (C-2), 113.5 (C-3), 143.3 (C-4), 111.4 (C-4a), 107.9 (C-5), 146.3 (C-6), 152.8 (C-7), 100.0 (C-8), 150.0 (C-8a), 56.3 (-OCH_3).

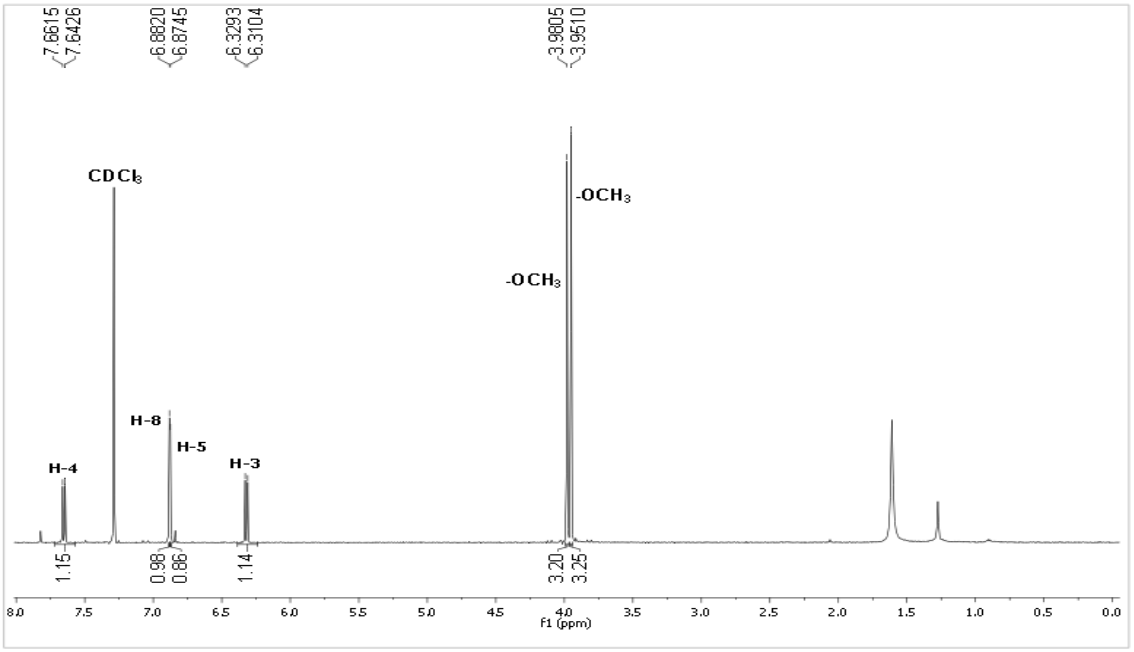


Figure 12. ^{1}H-NMR spectrum ($CDCl_3$, 500 MHz) of **6**.

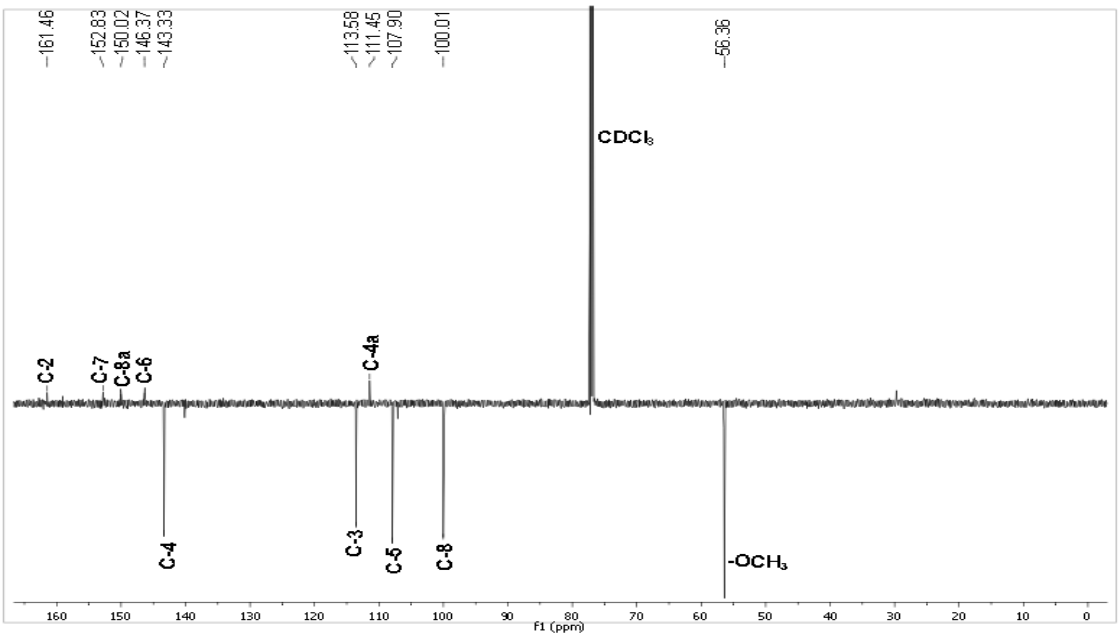
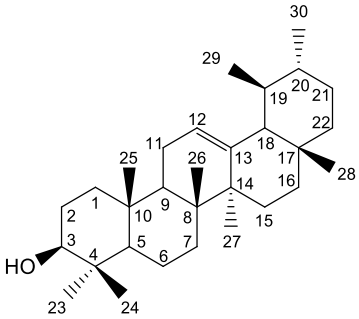
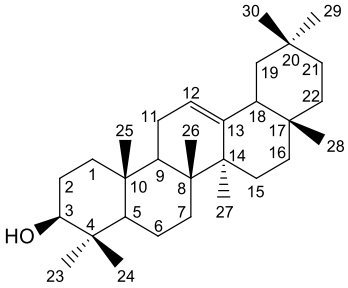


Figure 13. DEPT 135 spectrum ($CDCl_3$, 125 MHz) of **6.**



(**7**)



(**8**)

α-amyrin (**7**): DEPT 135 (125 MHz, CD_3OD) *δ*: 38.4 (C-1), 28.3 (C-2), 78.3 (C-3), 38.9 (C-4), 55.3 (C-5), 18.1 (C-6), 32.4 (C-7), 39.1 (C-8), 48.4 (C-9), 36.7 (C-10), 23.1 (C-11), 125.7 (C-12), 138.5 (C-13), 41.4 (C-14), 26.5 (C-15), 26.4 (C-16), 33.5 (C-17), 55.5 (C-18), 41.3 (C-19, 20), 30.9 (C-21), 41.8 (C-22), 27.3 (C-23), 15.2 (C-24), 15.0 (C-25), 16.3 (C-26), 22.5 (C-27), 27.3 (C-28), 17.1 (C-29), 20.8 (C-30).

β-amyrin (**8**): DEPT 135 (125 MHz, CD_3OD) *δ*: 38.4 (C-1), 27.4 (C-2), 78.2 (C-3), 38.9 (C-4), 55.3 (C-5), 18.0 (C-6), 32.4 (C-7), 39.1 (C-8), 48.4 (C-9), 36.6 (C-10), 23.1 (C-11), 122.2 (C-12), 143.8 (C-13), 41.4 (C-14), 26.1 (C-15, 16), 32.6 (C-17), 46.2 (C-18), 45.8 (C-19), 31.6 (C-20), 34.5 (C-21), 38.7 (C-22), 27.3 (C-23), 14.9 (C-24), 14.4 (C-25), 16.3 (C-26), 24.9 (C-27), 27.3 (C-28), 34.2 (C-29), 22.5 (C-30).

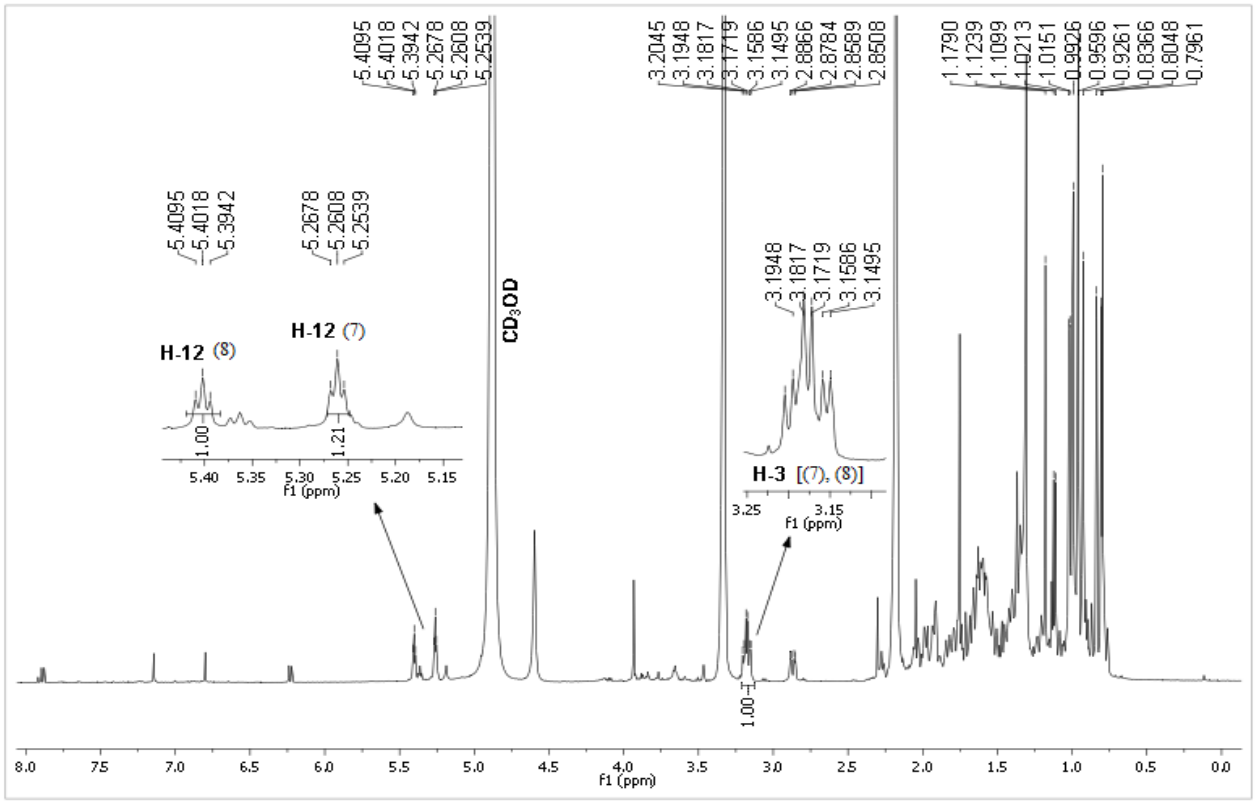


Figure 14: ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of the mixture of **7** and **8**.

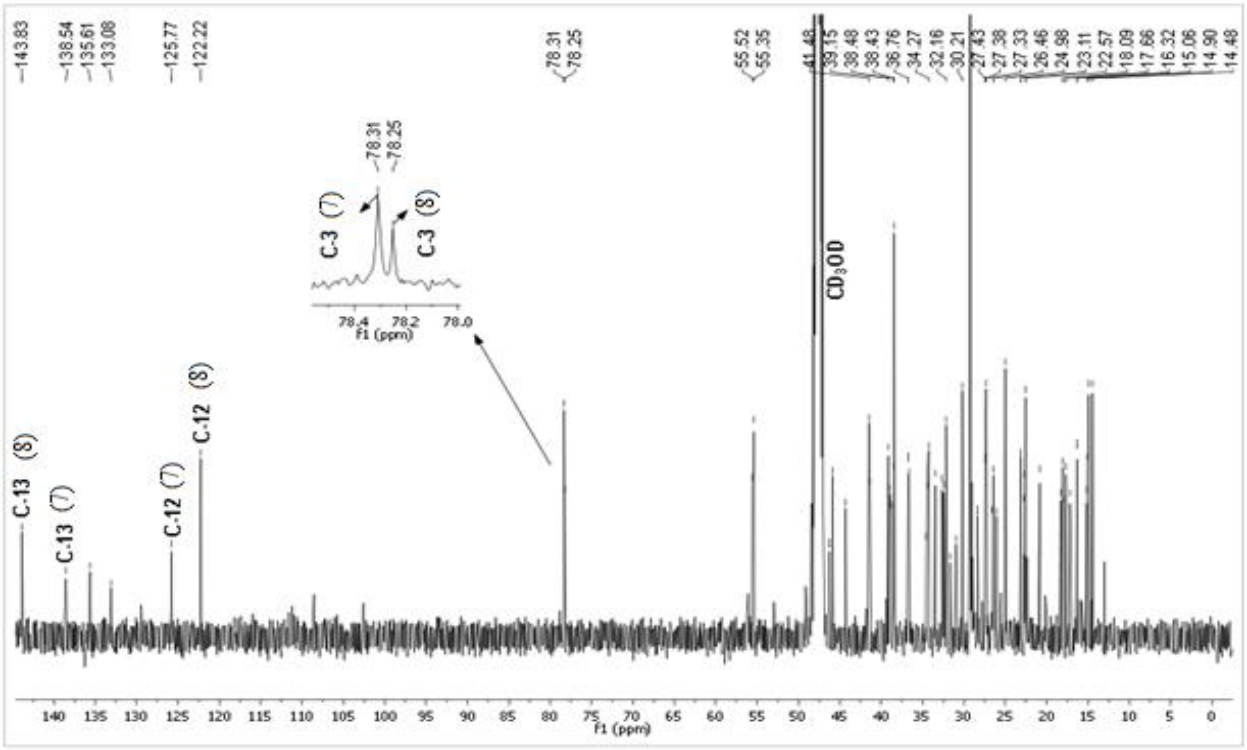


Figure 15: ^{13}C-NMR spectrum (CD_3OD, 125 MHz) of the mixture of **7** and **8**.

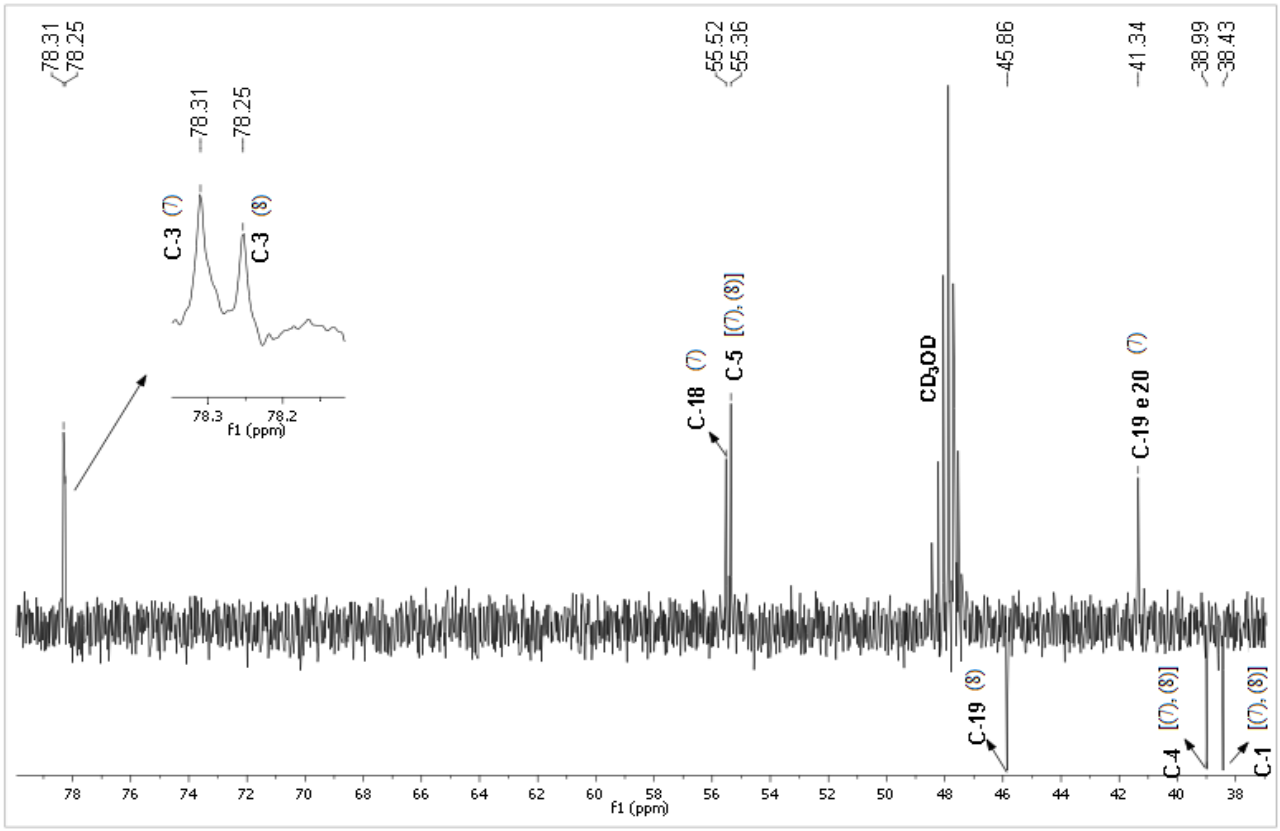


Figure 16. Expansion (δ_C 38.0-78.0 ppm) DEPT 135 spectrum (CD_3OD, 125 MHz) of the mixture of **7** and **8**.

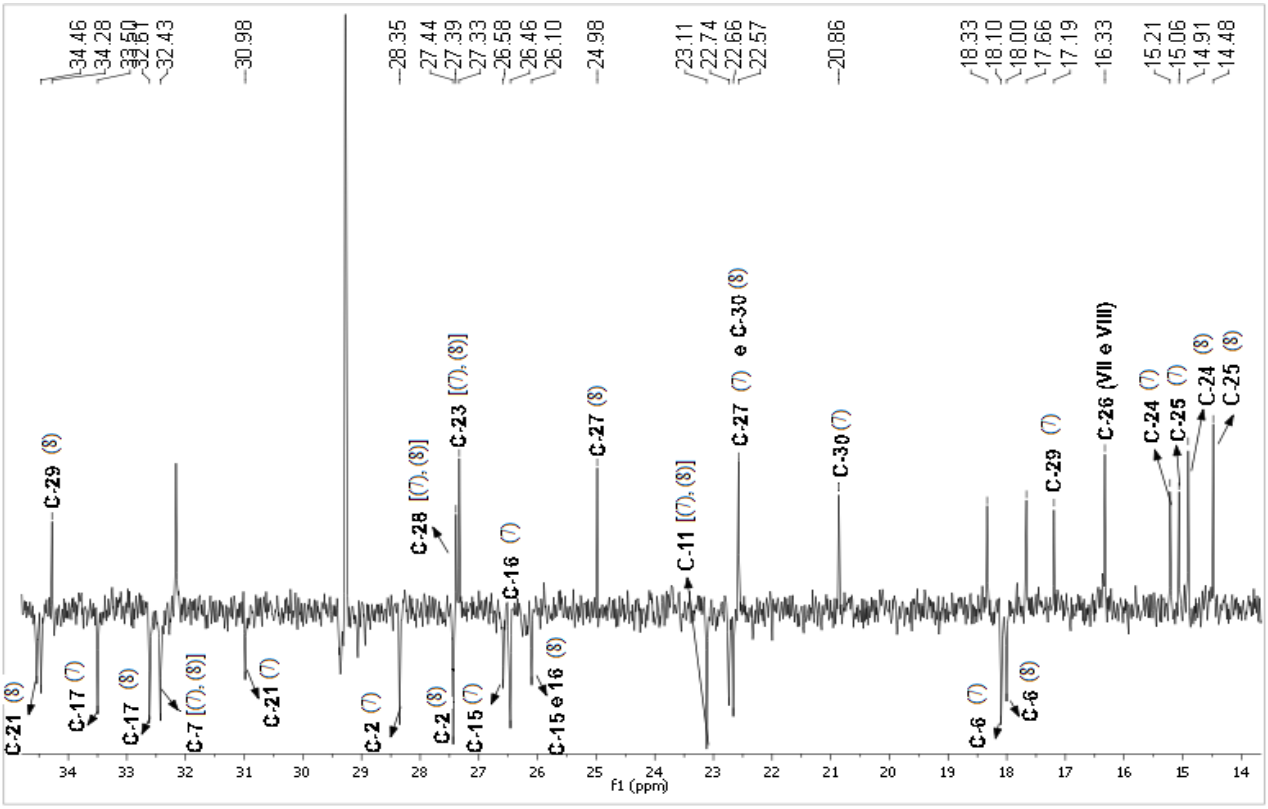
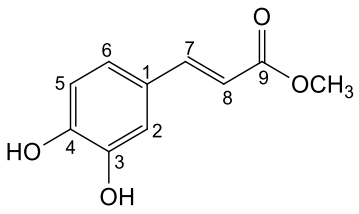


Figure 17. Expansion (δ_C 14.0 – 34.5 ppm) DEPT 135 spectrum (CD_3OD, 125 MHz) of the mixture of **7** and **8**.



(**9**)

Methyl caffeoate (**9**): ^{1}H-NMR (500 MHz, CD_3OD) *δ*: 7.05 (1H, *d*, J= 2.0 Hz, H-2), 6.79 (1H, d, J= 8.2 Hz, H-5), 6.96 (1H, *dd*, J= 2.0, 8.2 Hz, H-6), 7.56 (1H, *d*, J= 15.9 Hz, H-7), 6.28 (1H, *d*, J= 15.9 Hz, H-8), 3.78 (3H, *s*); ^{13}C-NMR (125 MHz, CD_3OD) *δ*: 126.2 (C-1), 115.1 (C-2), 145.6 (C-3), 148.1 (C-4), 113.4 (C-5), 121.6 (C-6), 145.3 (C-7), 113.7 (C-8), 168.5 (C-9), 56.9 (-OCH_3).

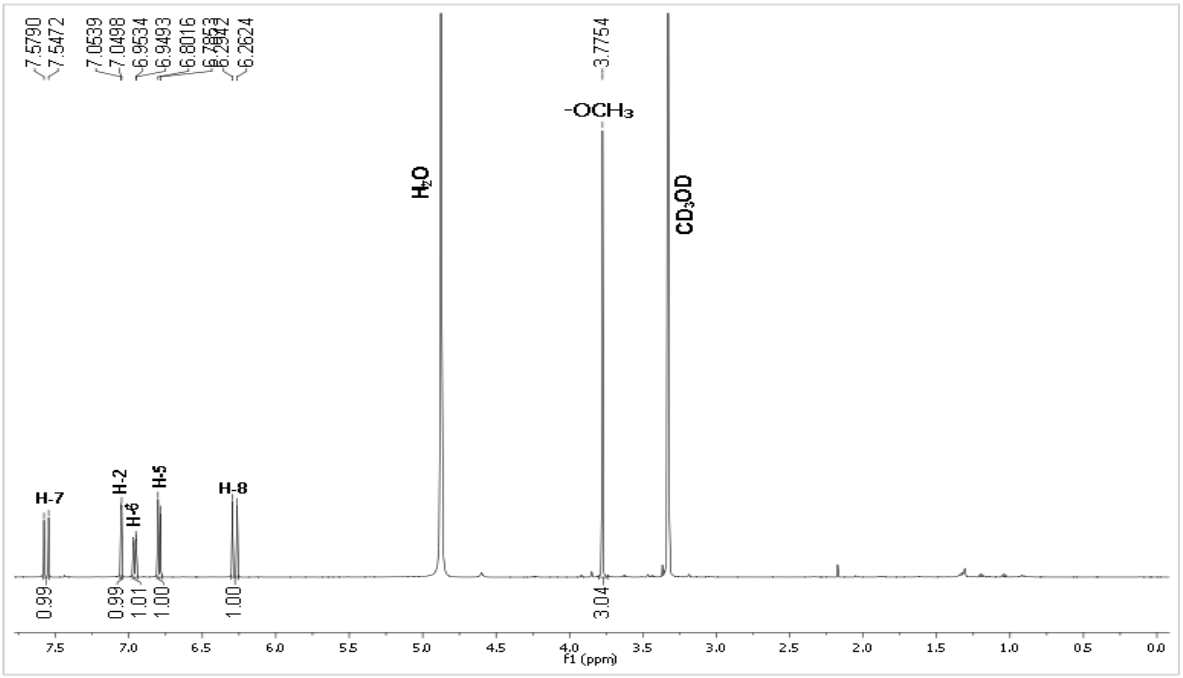


Figure 18. ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of **9**.

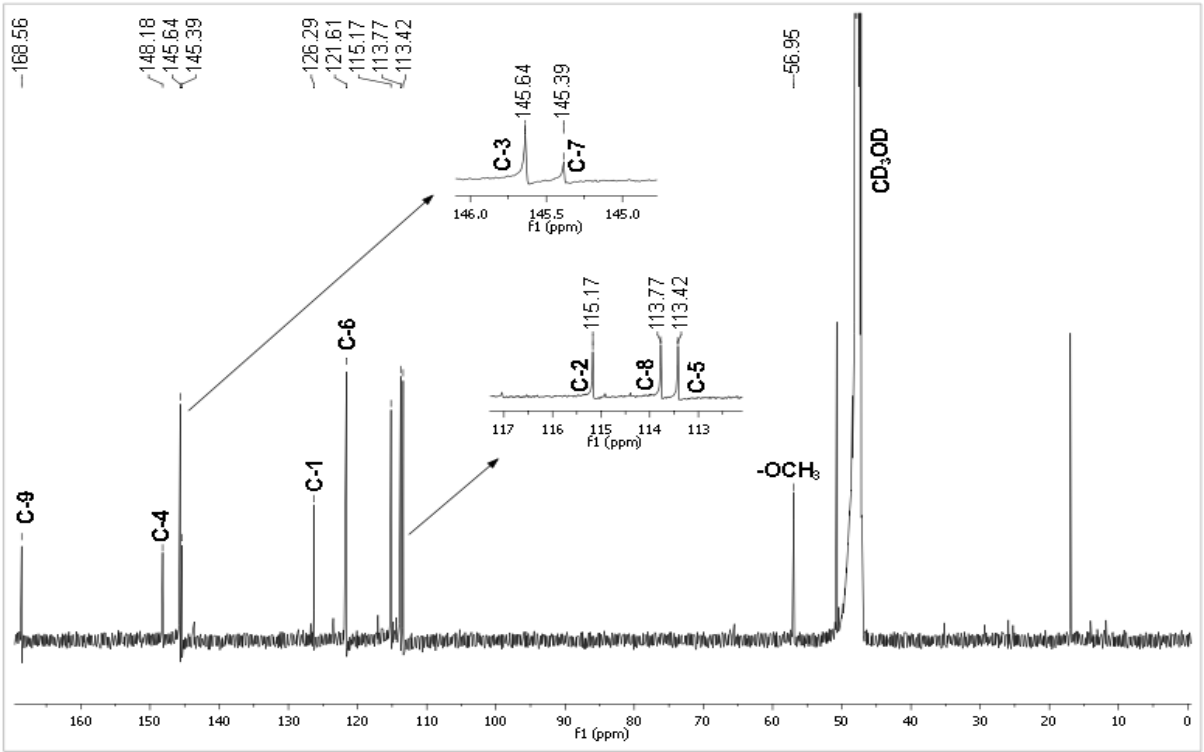
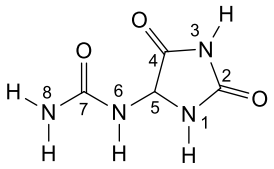


Figure 19. ^{13}C-NMR spectrum (CD_3OD, 125 MHz) of **9**.



(**10**)

Allantoin (**10**): ^{1}H-NMR (500 MHz, DMSO-d_6) δ: 8.04 (1H, *sl*, H-1), 10.53 (1H, *s*, H-3), 5.25 (1H, *d*, J= 8.1 Hz, H-5), 6.89 (1H, *d*, J= 8.1 Hz, H-6), 5.77 (1H, *sl*, H-8); ^{13}C-NMR (125 MHz, DMSO-d_6) δ: 156.8 (C-2), 157.4 (C-4), 62.9 (C-5), 174.1 (C-7).

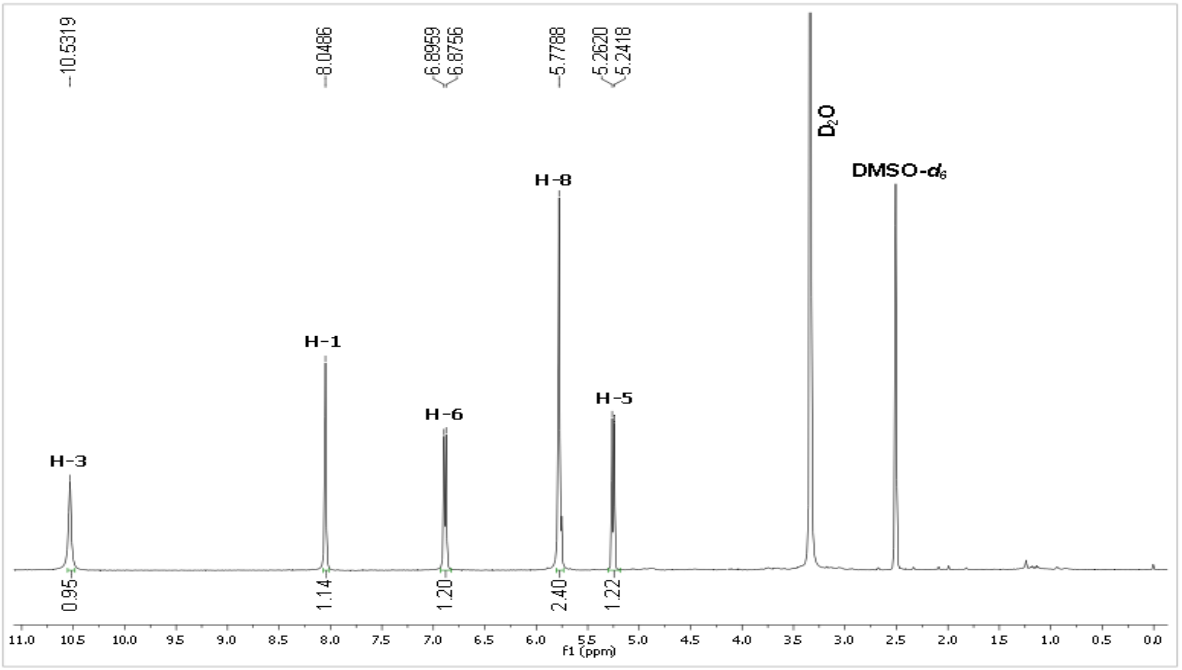


Figure 20. ^{1}H-NMR spectrum (DMSO-d_6, 500 MHz) of **10**.

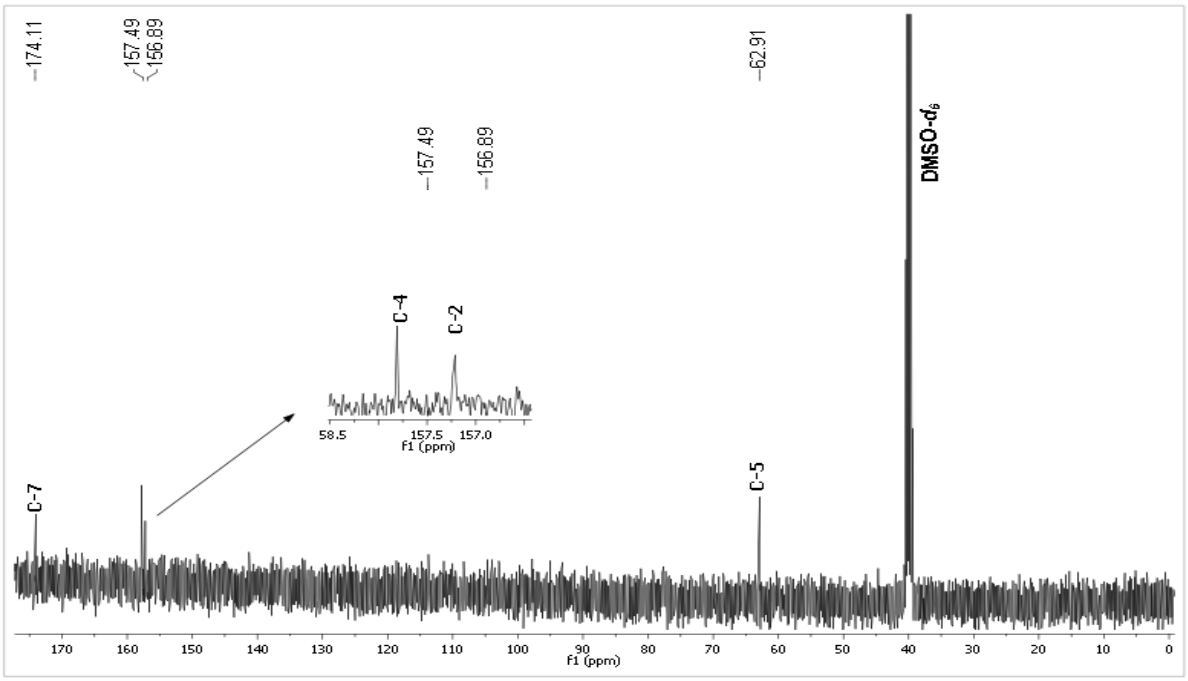
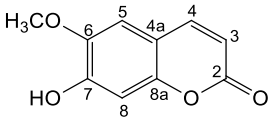


Figure 21. ^{13}C-NMR spectrum (DMSO-d_6, 125 MHz) of **10**.



(11)

Scopoletin (**11**): ^{1}H-NMR (500 MHz, CD_3OD) δ: 6.26 (1H, *d*, J= 9.4 Hz, H-3), 7.84 (1H, *d*, J= 9.4 Hz, H-4), 6.98 (1H, *s*, H-5), 8.50 (1H, *sl*, -OH), 6.99 (1H, *s*, H-8), 3.97 (3H, *s*, $-OCH_3$); ^{13}C-NMR (125 MHz, CD_3OD) δ: 168.8 (C-2), 112.1 (C-3), 143.9 (C-4), 111.5 (C-4a), 104.2 (C-5), 144.4 (C-6), 152.7 (C-7), 99.2 (C-8), 148.9 (C-8a), 55.4 ($-OCH_3$).

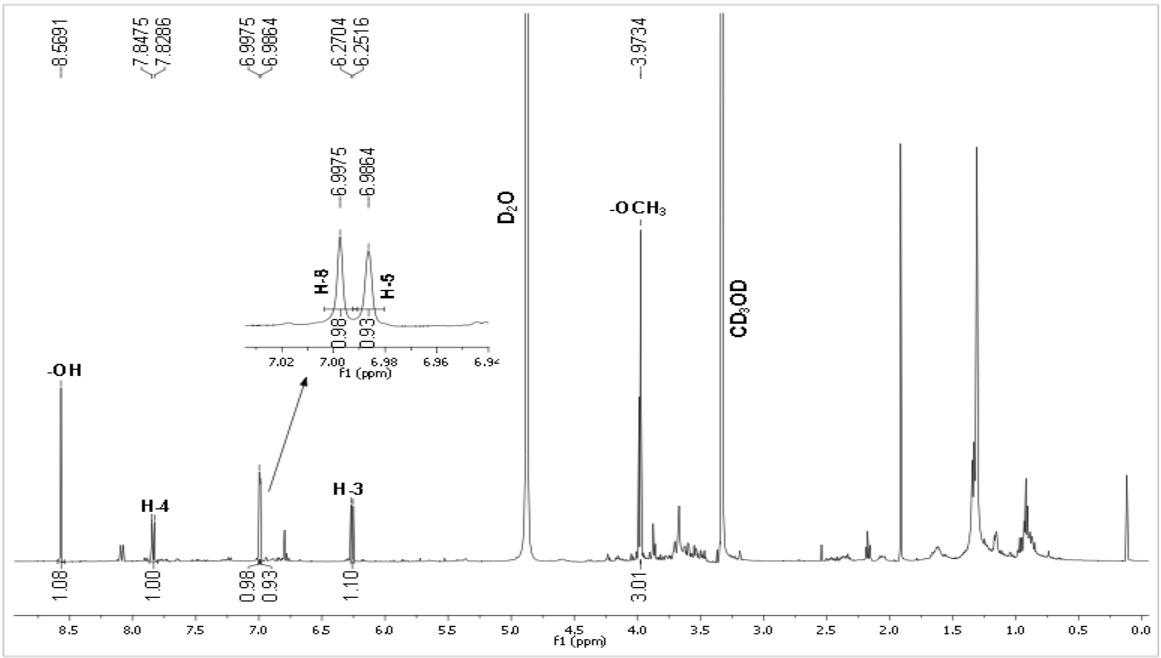


Figure 22. ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of **11**.

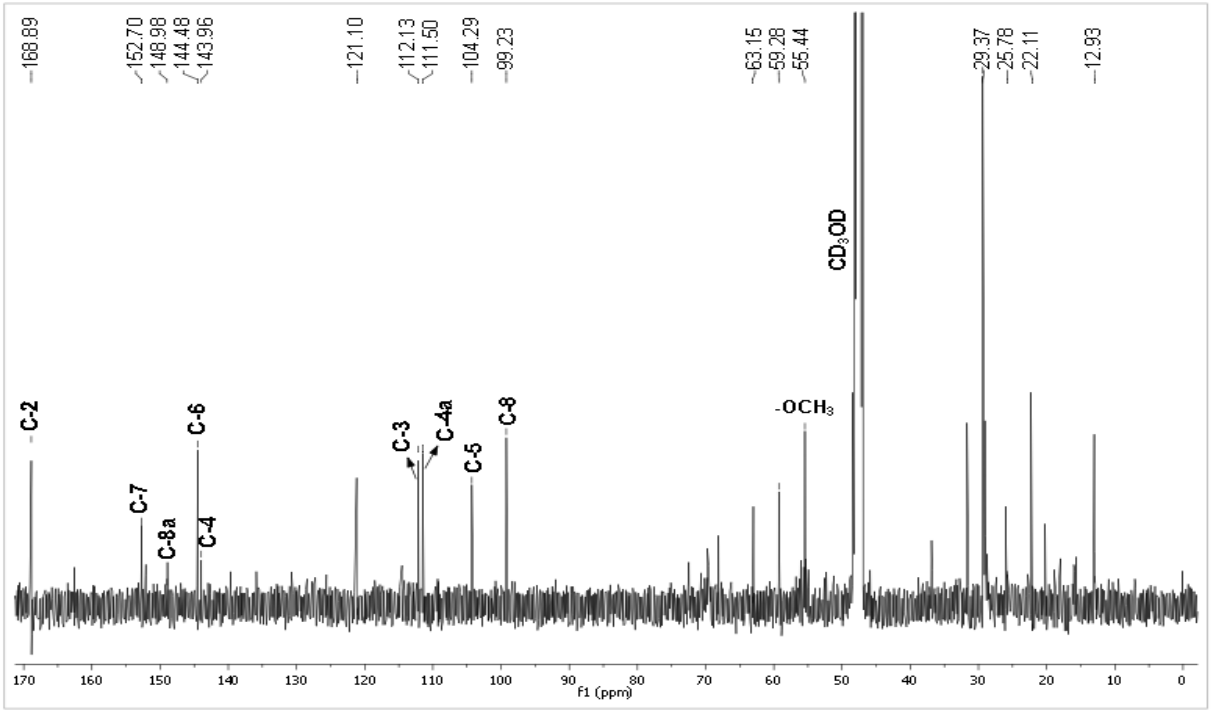
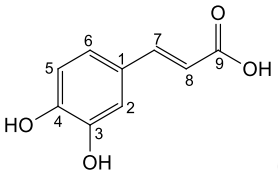


Figure 23. ^{13}C-NMR spectrum (CD_3OD, 125 MHz) of **11**.



(**12**)

Caffeic acid (**12**): ^{1}H-NMR (500 MHz, CD_3OD) *δ*: 7.05 (1H, *d*, J= 2.0 Hz, H-2), 6.79 (1H, *d*, J= 8.2 Hz, H-5), 6.94 (1H, *dd*, J= 8.2, 2.0 Hz, H-6), 7.53 (1H, *d*, J= 15.9 Hz, H-7), 6.24 (1H, *d*, J= 15.9 Hz, H-8); ^{13}C-NMR (125 MHz, CD_3OD) *δ*: 126.5 (C-1), 113.6 (C-2), 145.1 (C-3), 145.3 (C-4), 115.0 (C-5), 121.3 (C-6), 147.9 (C-7), 116.3 (C-8), 170.0 (C-9).

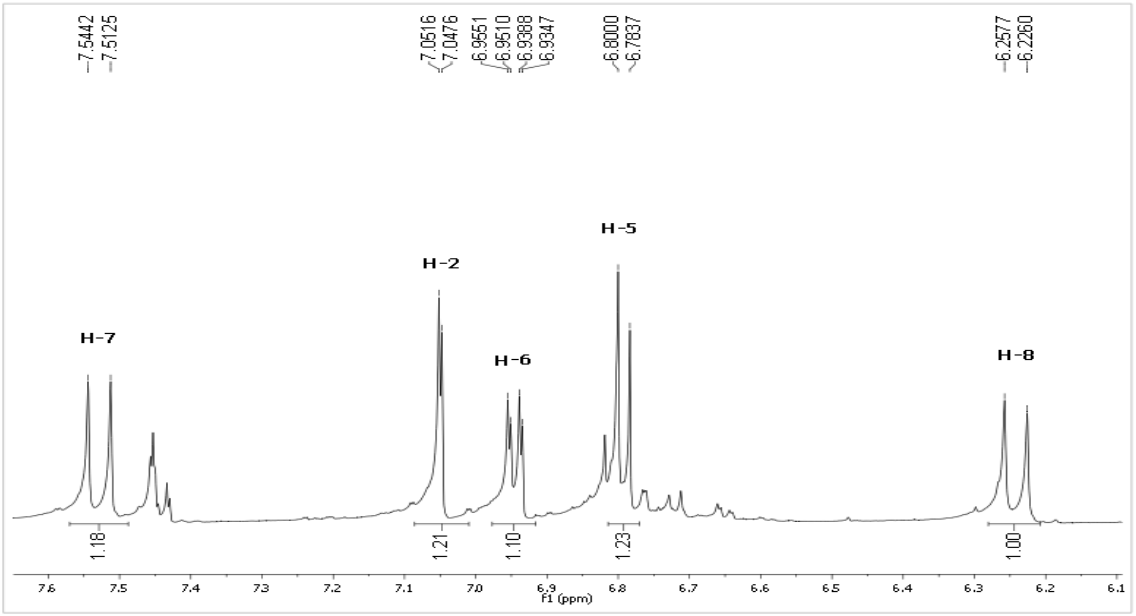


Figure 24. Expansion (δ_H 6.1-7.6 ppm) of ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of **12**.

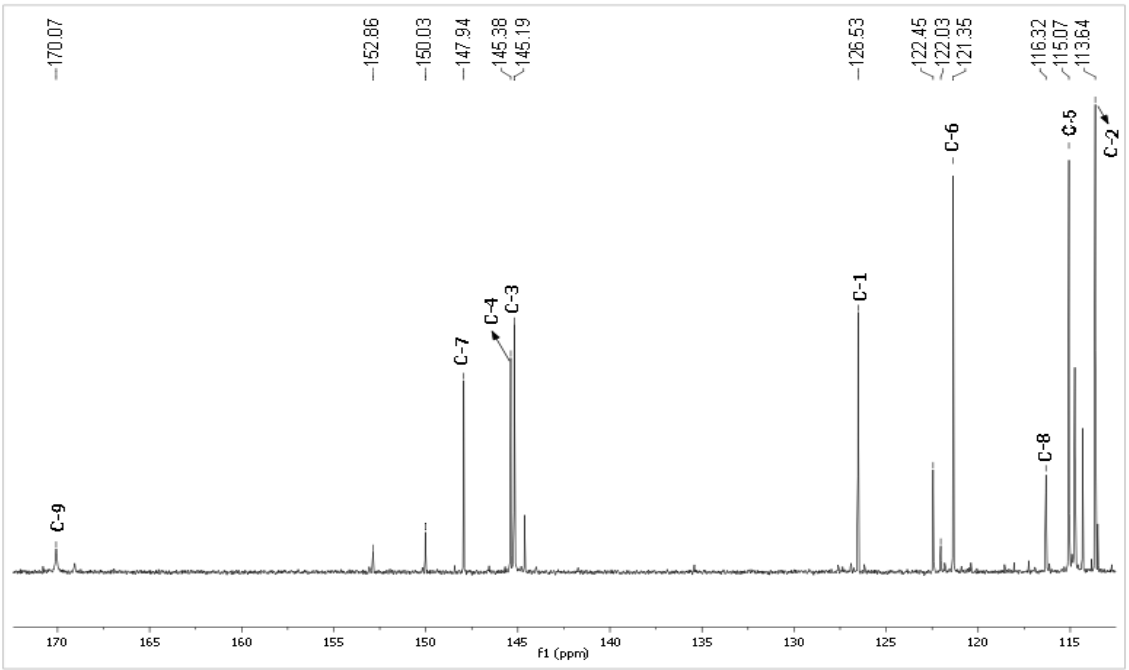
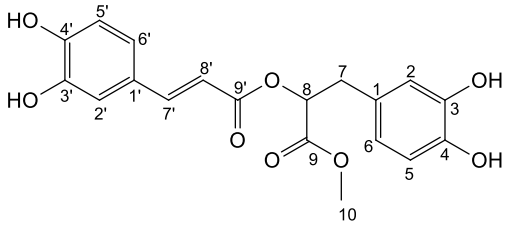


Figure 25. Expansion (δ_C 115.0-170.0 ppm) of ^{13}C-NMR spectrum (CD_3OD, 125 MHz) of **12**.



(**13**)

Methyl rosmarinate (**13**): ^{1}H-NMR (500 MHz, CD_3OD) δ: 7.07 (1H, *d*, J= 2.1 Hz, H-2'), 6.79 (1H, *d*, J= 8.1 Hz, H-5'), 6.98 (1H, *dd*, J= 8.3, 2.0 Hz, H-6'), 7.57 (1H, *d*, J= 15.9 Hz, H-7'), 6.28 (1H, *d*, J= 15.9 Hz, H-8'), 5.21 (2H, *dd*, J= 7.6, 5.5 Hz, H-8), 3.03 (1H, *dd*, J= 14.4, 7.7 Hz, H-7a), 3.08 (1H, *dd*, J= 14.8, 5.8 Hz, H-7b), 6.59 (1H, *dd*, J= 8.1, 2.1 Hz, H-6), 6.72 (1H, *d*, J= 8.1 Hz, H-5), 3.72 (3H, *s*). ^{13}C-NMR (125 MHz, CD_3OD) δ: 126.1 (C-1'), 113.8 (C-2'), 146.5 (C-3'), 145.4 (C-4'), 115.1 (C-5'), 121.8 (C-6'), 148.4 (C-7'), 112.7 (C-8'), 166.9 (C-9'), 170.7 (C-9), 72.2 (C-8), 36.5 (C-7), 120.4 (C-6), 115.0 (C-5), 144.8 (C-4), 143.9 (C-3), 116.1 (C-2), 127.3 (C-1), 51.2 (-OCH_3).

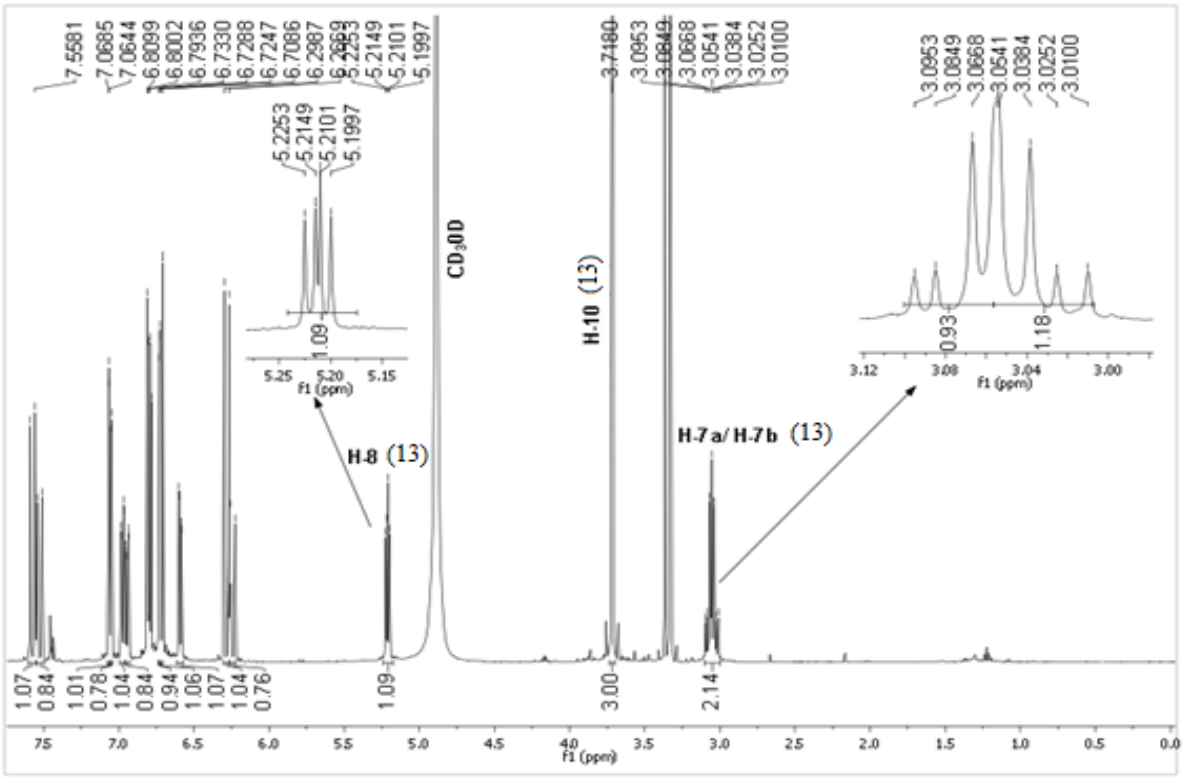


Figure 26. ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of the mixture of **12** and **13**.

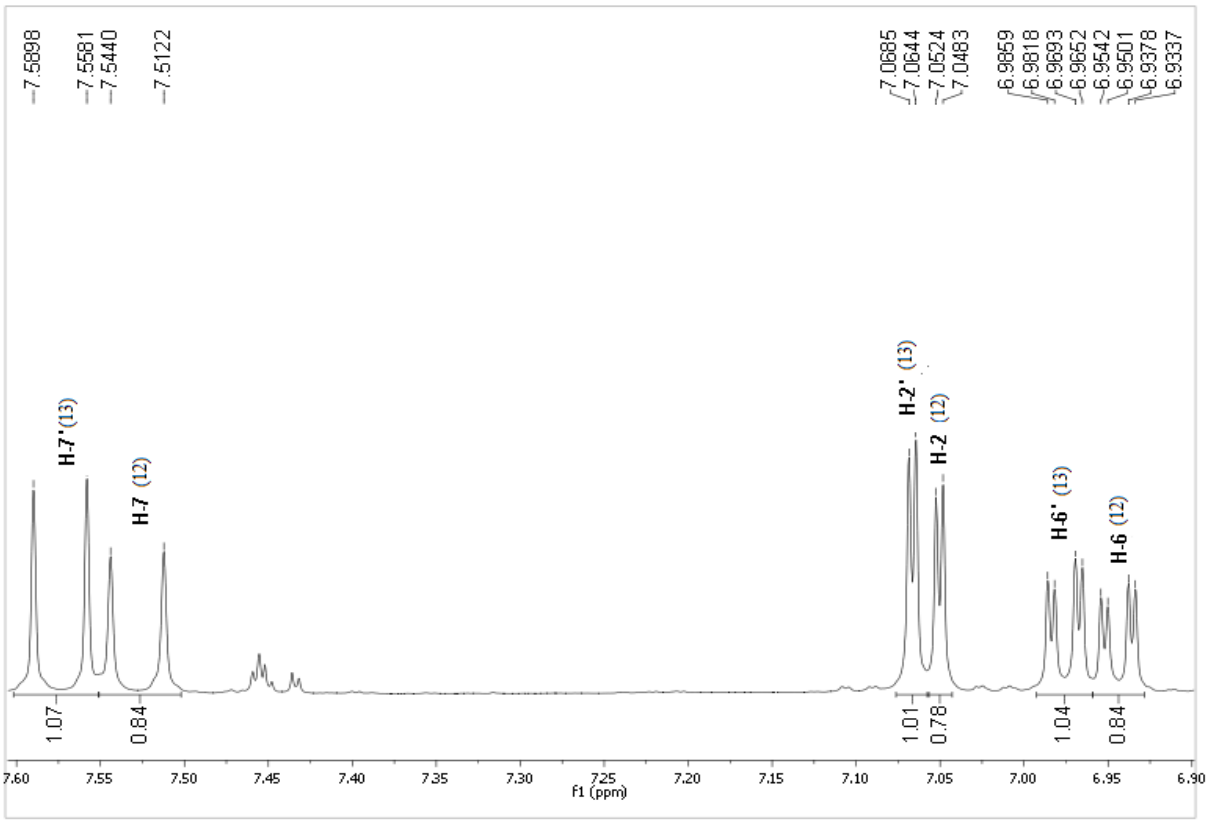


Figure 27. Expansion (δ_H 6.90-7.60 ppm) of ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of the mixture of **12** and **13**.

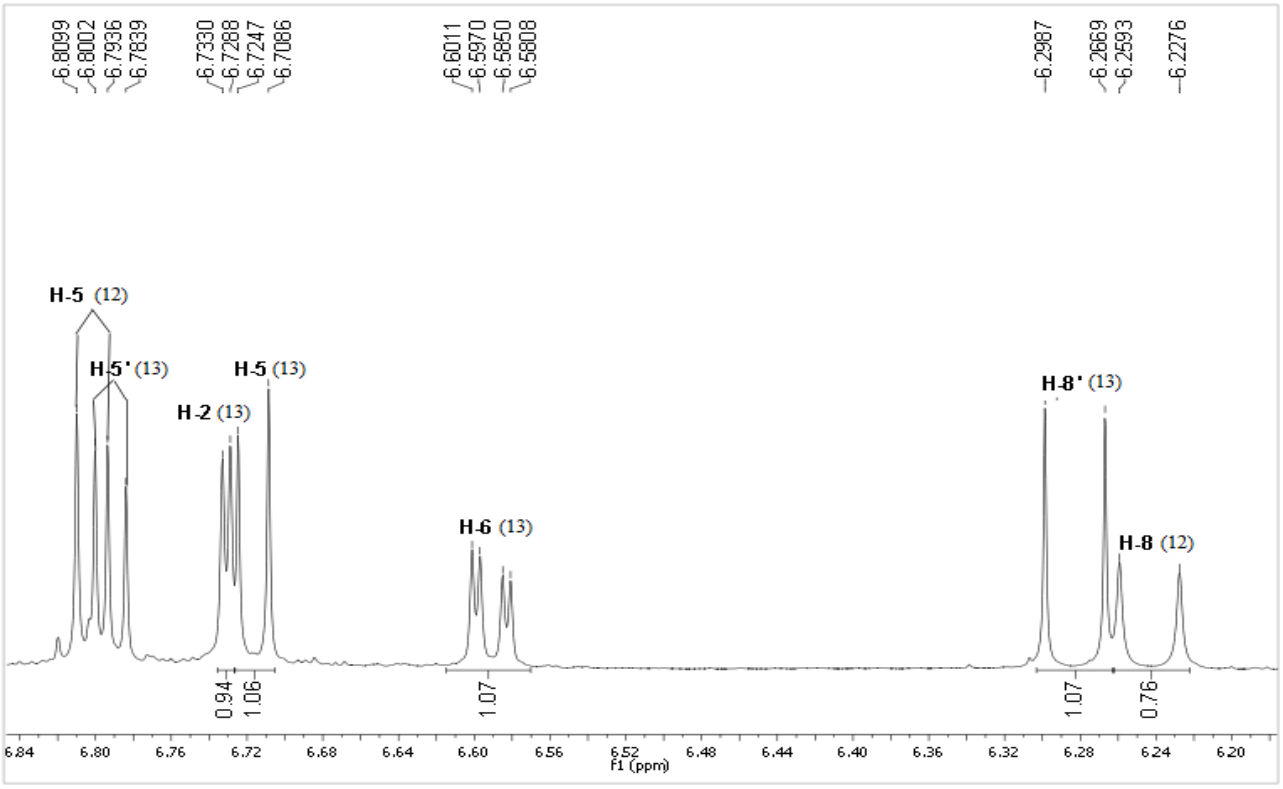


Figure 28. Expansion (δ_H 6.20-6.84 ppm) of ^{1}H-NMR spectrum (CD_3OD, 500 MHz) of the mixture of **12** and **13**.

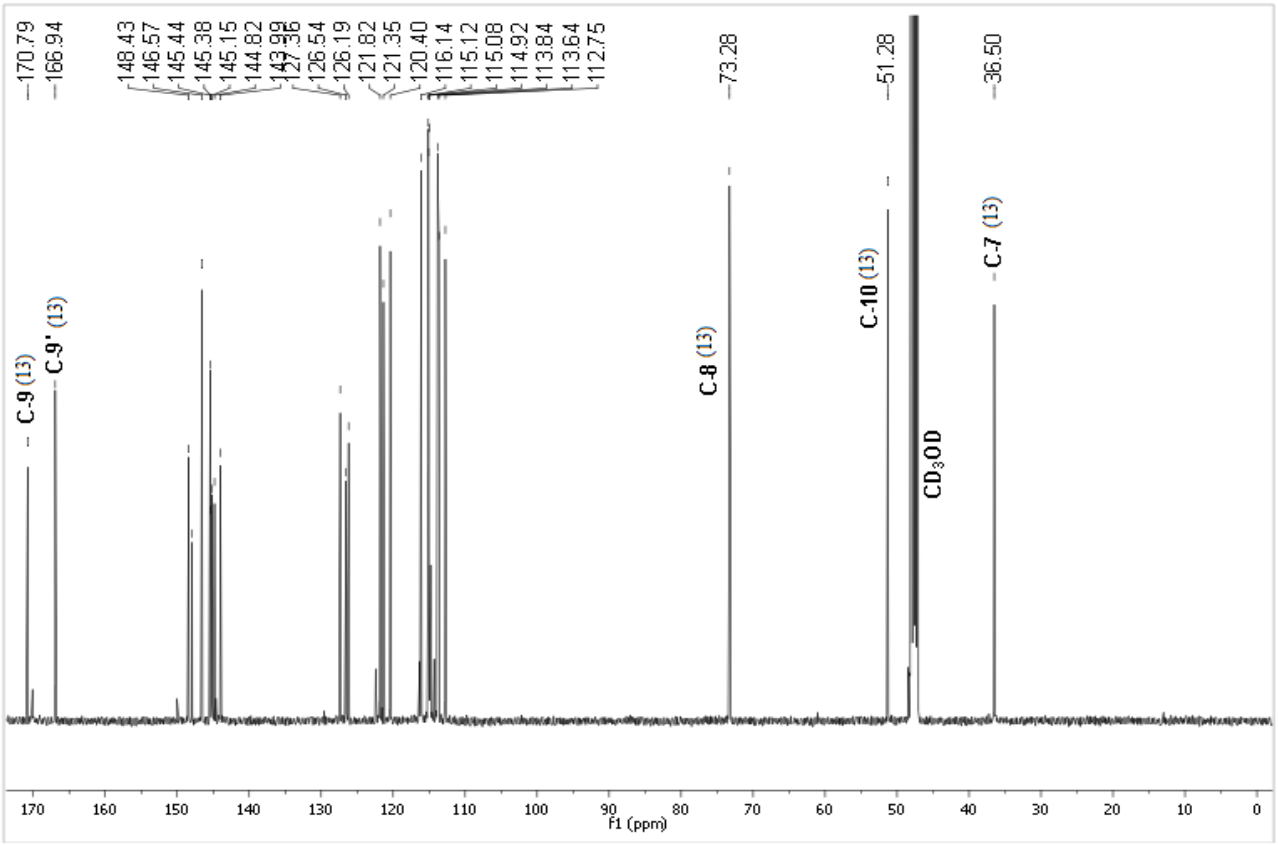


Figure 29. ^{13}C-NMR spectrum (CD_3OD, 125 MHz) of the mixture **12** and **13**.

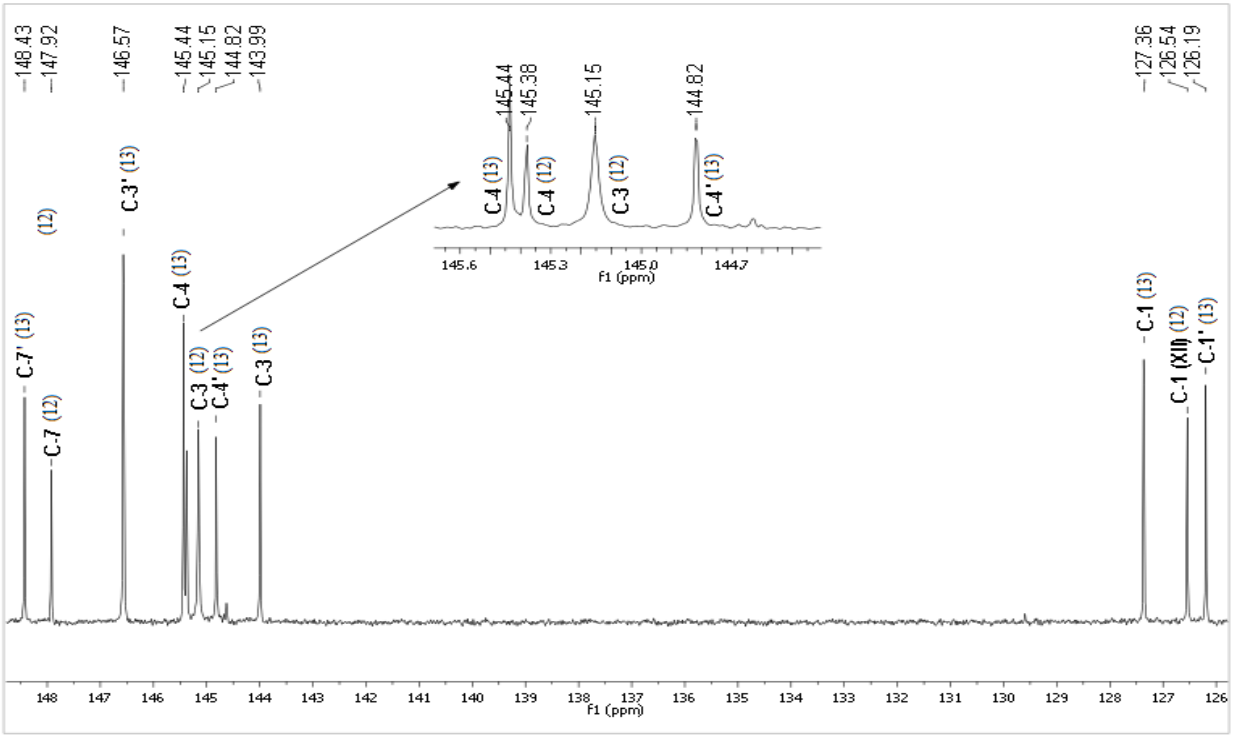


Figure 30. Expansion (δ_C 126.0-149.0 ppm) of ^{13}C-NMR spectrum (CD_3OD, 125 MHz) of the mixture of **12** and **13**.

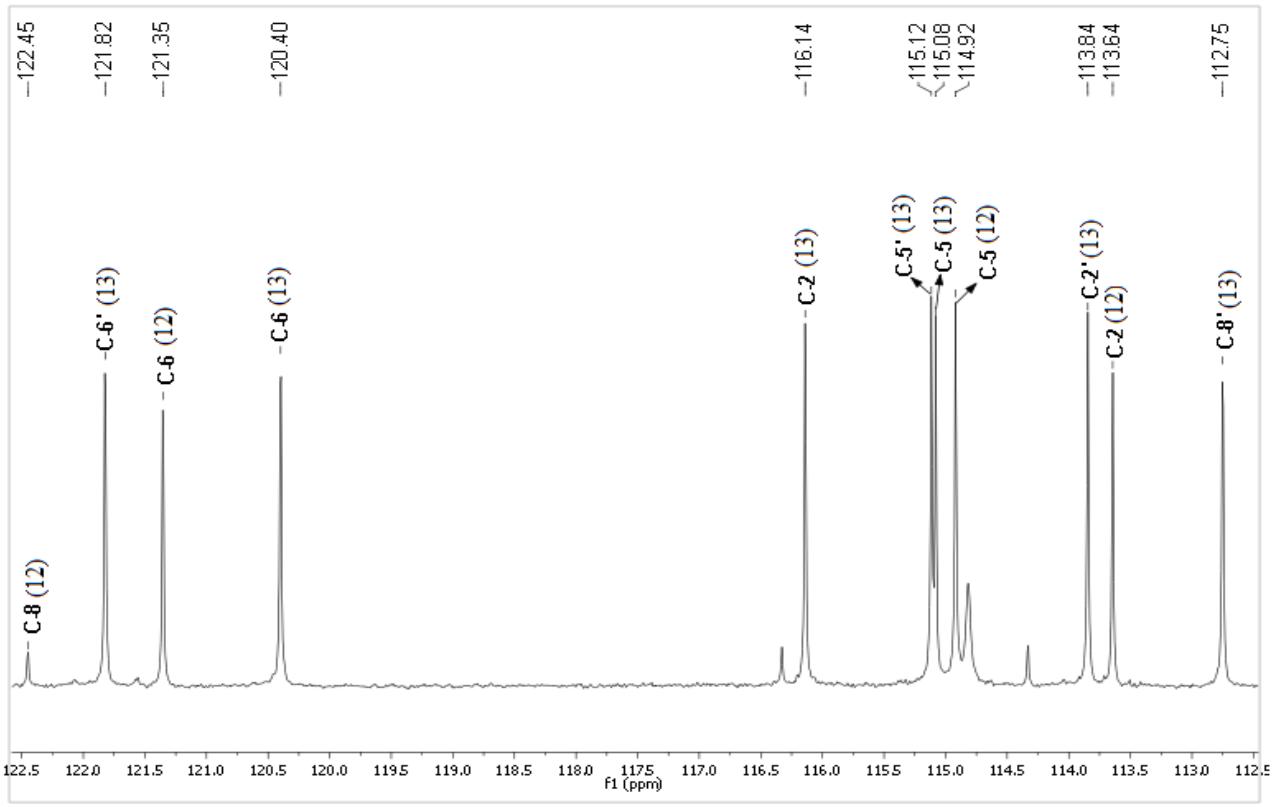


Figure 31. Expansion (δ_C 112.5-122.5 ppm) of ^{13}C-NMR spectrum (CD_3OD, 125 MHz) of the mixture **12** and **13**.

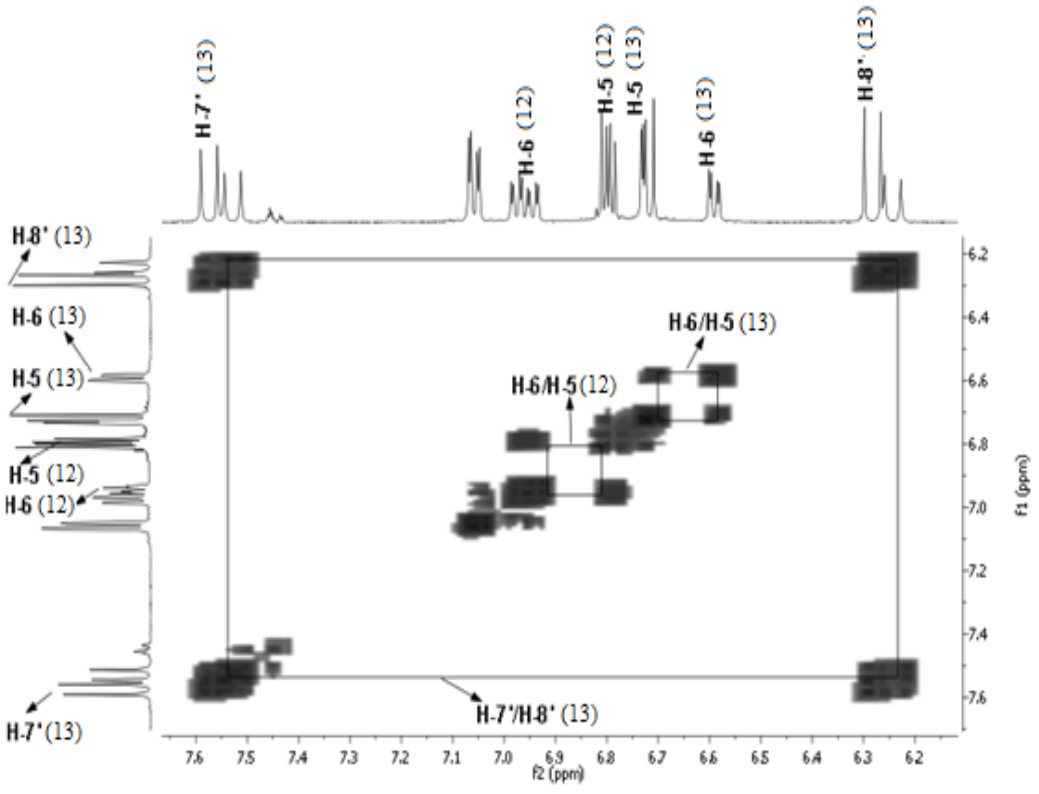


Figure 32. Expansion (δ_H 6.20-7.60 ppm) of COSY spectrum (CD_3OD, 500 MHz) of the mixture **12** and **13**.

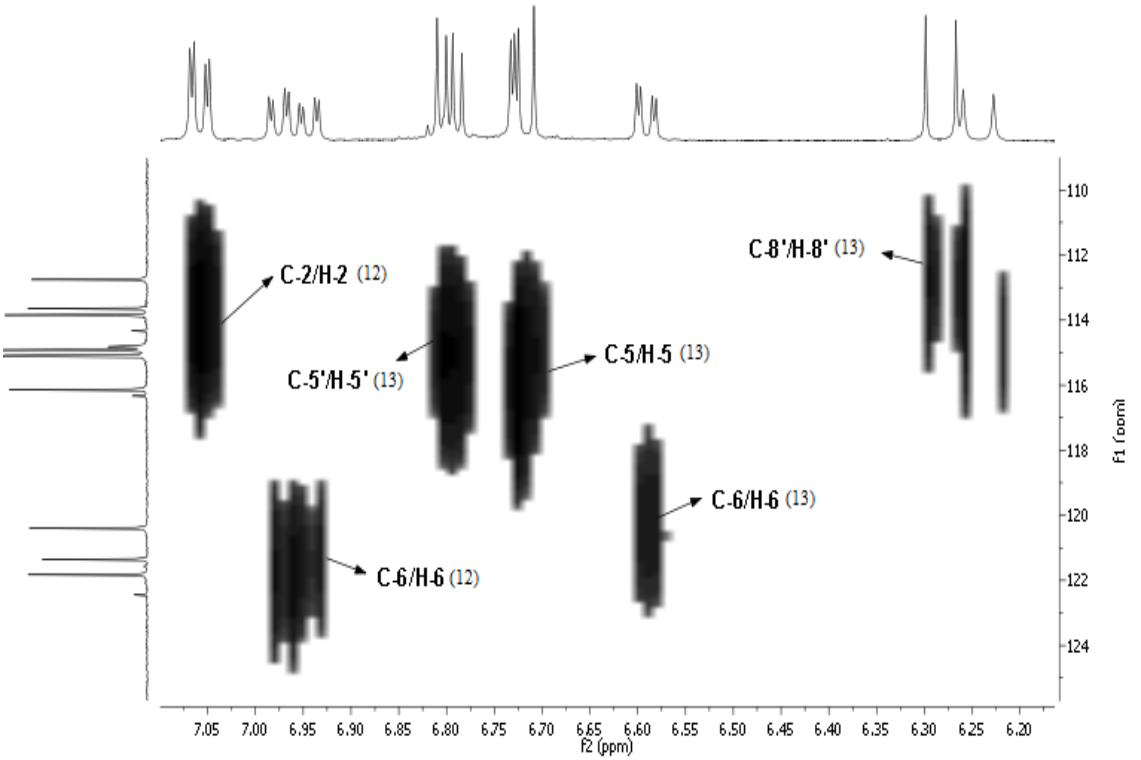


Figure 33: Expansion (δ_H 6.20 – 7.05 and δ_C 110.0 – 124 ppm) of HSQC spectrum (CD_3OD, 500/125 MHz) of the mixture **12** and **13**.

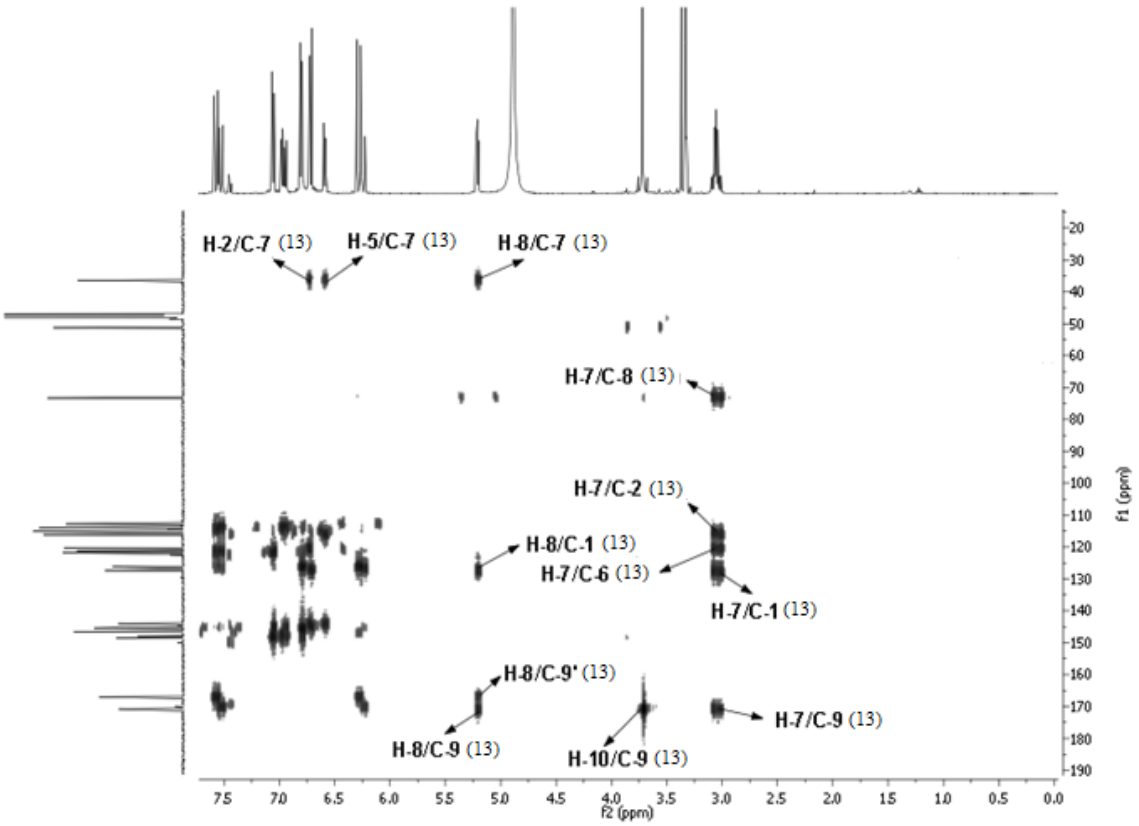


Figure 34. HMBC spectrum (CD_3OD, 500/125 MHz) of the mixture **12** and **13**.

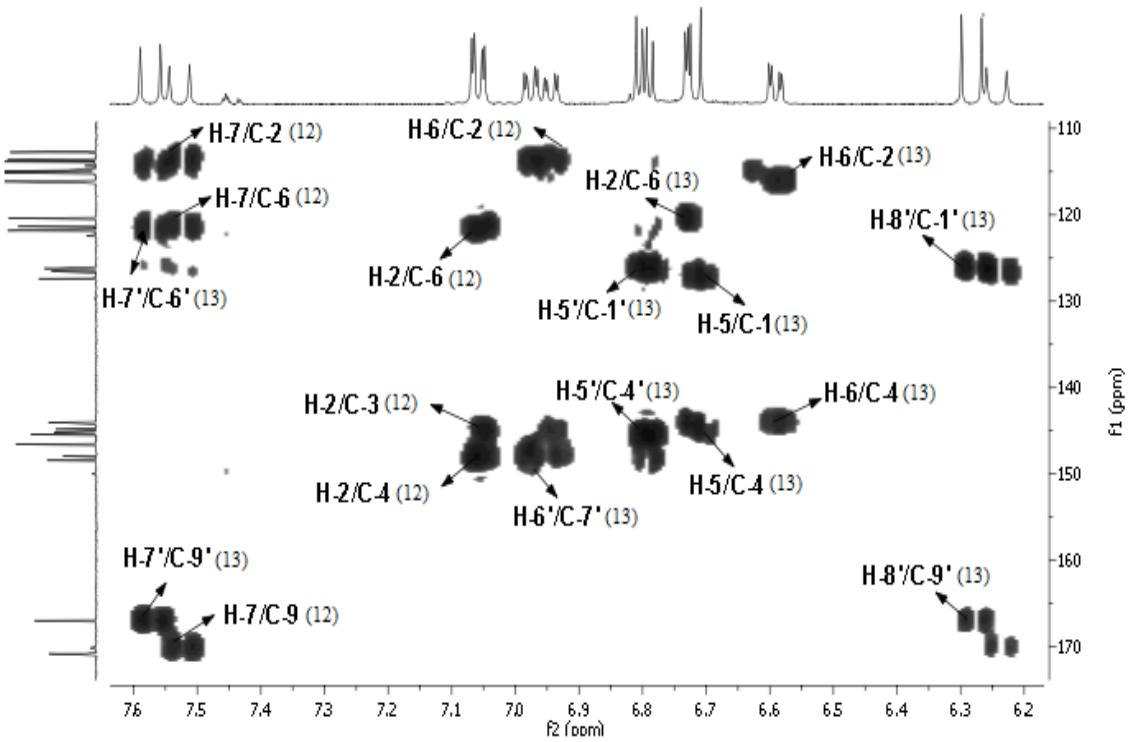


Figure 35. Expansion (δ_H 6.20 – 7.60 and δ_C 110.0 – 170.0 ppm) of HMBC spectrum (CD_3OD, 500/125 MHz) of the mixture **12** and **13**.