Supplementary File

Myricitrin – a flavonoid isolated from Indian olive tree (*Elaeocarpus floribundus*) inhibits Monoamine oxidase in brain and elevates striatal dopamine levels: therapeutic implications against Parkinson's disease

Chayan Banerjee[1, 3], Sumangal Nandy[1], Joy Chakraborty [1, 3*], Deepak Kumar [2, 3*]

[1]Department of Cell Biology and Physiology, CSIR-Indian Institute of Chemical Biology-TRUE campus, Kolkata, India

[2]Organic and Medicinal Chemistry Division, CSIR-Indian Institute of Chemical Biology, Jadavpur, Kolkata, India

[3]Academy of Scientific and Innovative Research (AcSIR), CSIR- Human Resource Development Centre, Ghaziabad, India.

*Co-corresponding author

joy.chakraborty@iicb.res.in, deepak@iicb.res.in

Spectroscopic characterization

***Myricitrin (1)*:** (myricetin 3-*O*-rhamnoside)

UV, λmax nm 257, 360; *m/z* 319.0539 $[M-146+H]^+$, 465.1073 $[M+H]^+$, 487.0903 $[M+Na]^+$; ^{1}H-NMR (CD_3OD), δ_H 6.91 (2H, s, H-2′, H-6′), 6.32 (1H, *d*, *J* = 1.8 Hz, H-8), 6.16 (1H, d, *J* = 1.8 Hz, H-6), 5.28 (1H, s, H-1″), 4.19 (1H, brs, H-2″), 3.76 (1H, *dd*, 3.0, 9.6 Hz, H-3″), 3.48 (1H, *m*, H-4″), 3.27 (1H, brs, H-5″), 0.93 (3H, *d*, 6 Hz); ^{13}C NMR (CD_3OD): δ_C 179.6 (C-4), 165.8 (C-7), 163.1 (C-5), 159.4 (C-9), 158.4 (C-2), 146.8 (C-3′, C-5′), 137.8 (C-4′), 136.3 (C-3), 121.9 (C-1′), 109.5 (C-2′, C-6′), 105.8 (C-10), 103.6 (C-1″), 99.8 (C-6), 94.7 (C-8), 73.3 (C-4″), 72.1 (C-3″), 72.0 (C-2″), 71.8 (C-5″), 17.6 (C-6″). The compound was identified as myricitrin by comparing the spectroscopic data with those reported in the literature.[1,2]

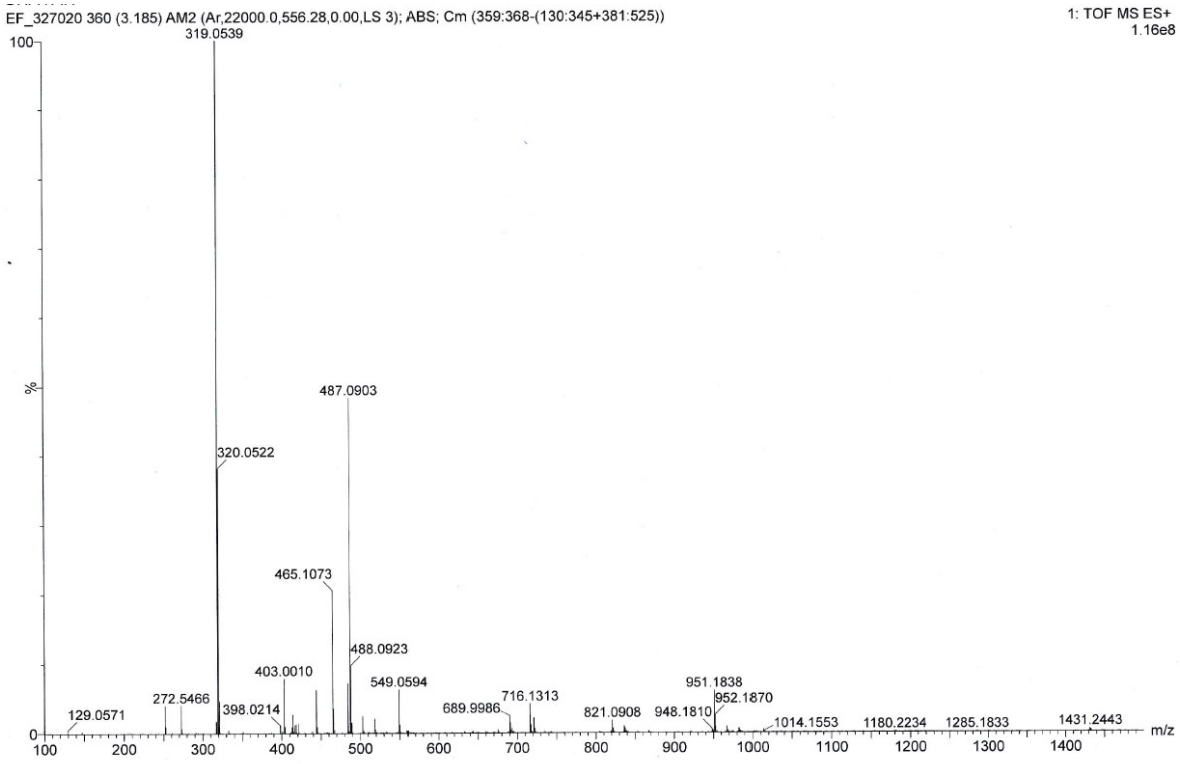

Fig. S1: ESI-MS (+ve) spectrum of myricitrin (**1**).

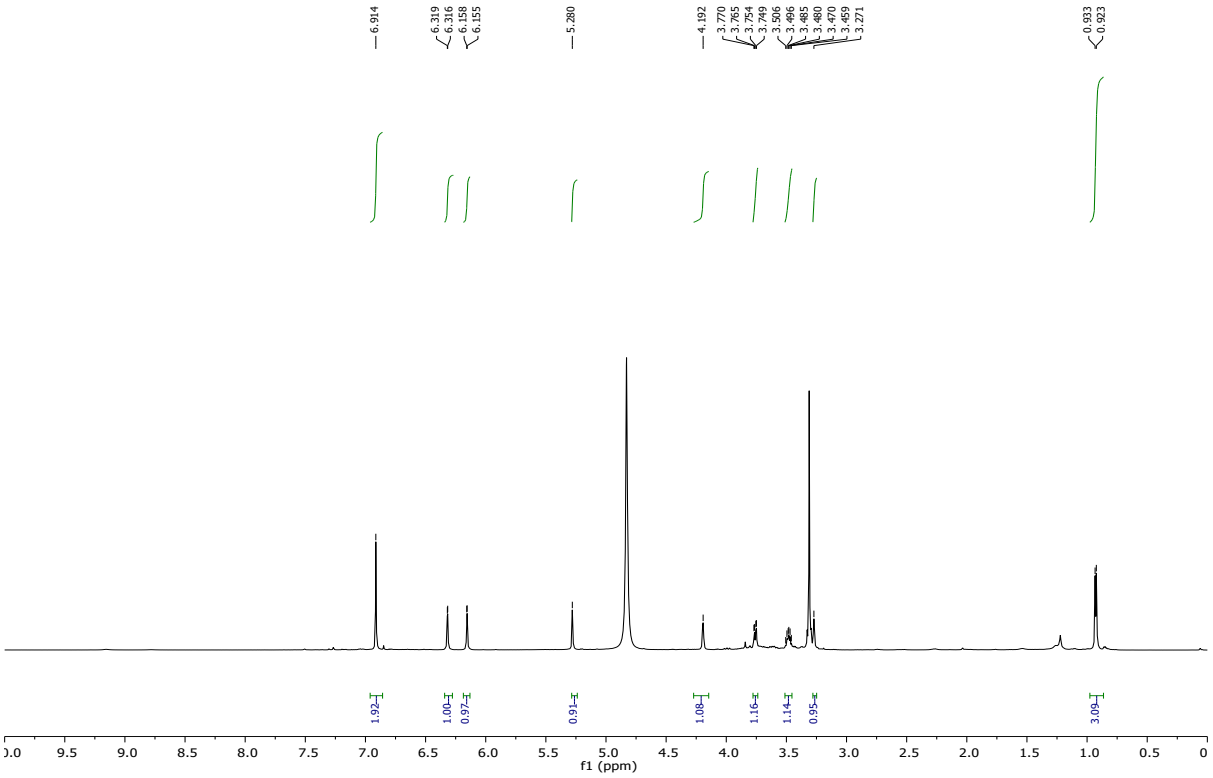

Fig. S2: ^{1}H-NMR of myricitrin (**1**) in MeOD, 600 MHz.

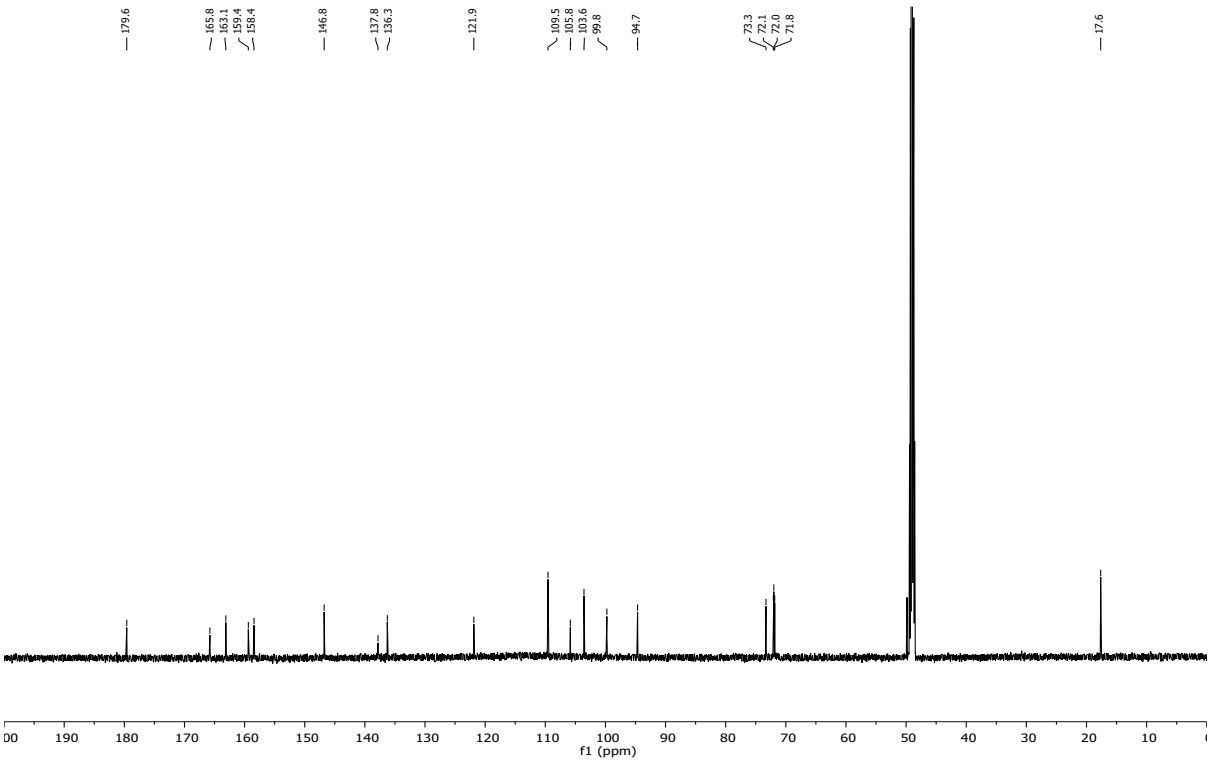

Fig. S3: ^{13}C-NMR of myricitrin (**1**) in MeOD, 150 MHz.

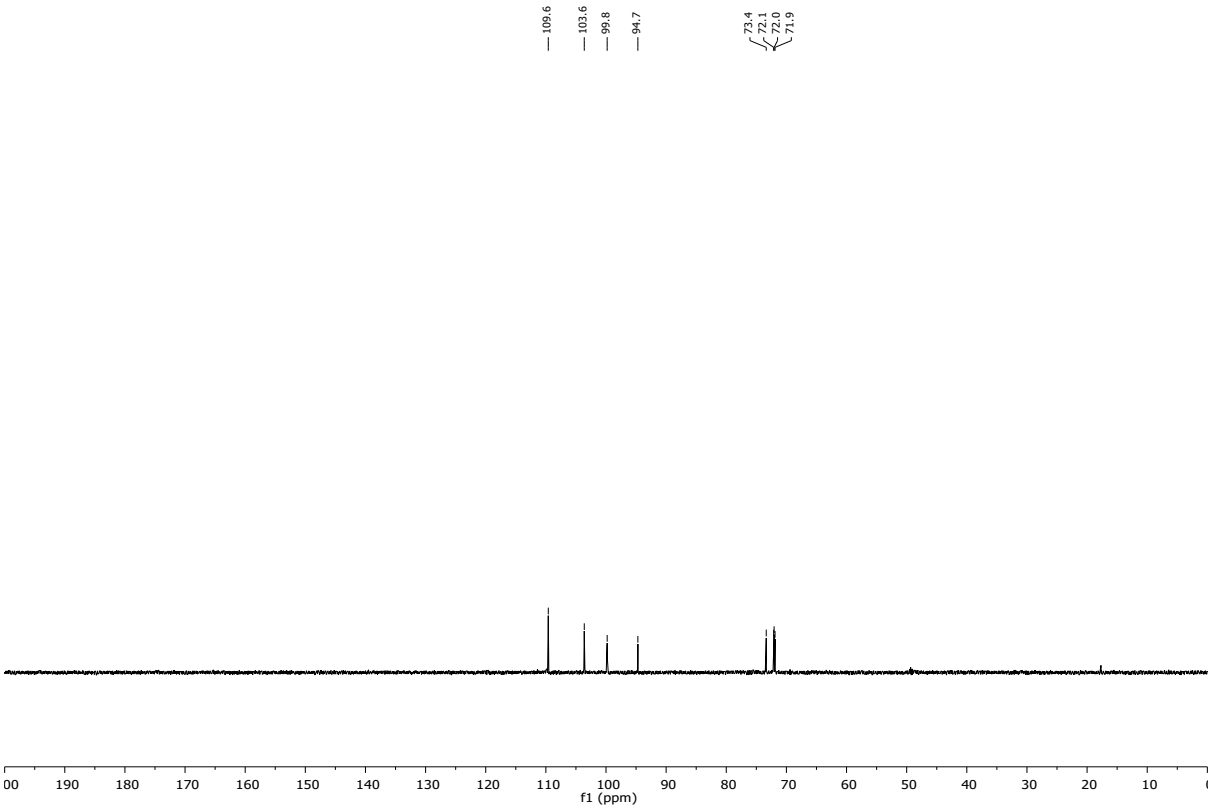

Fig. S4: DEPT-90 of myricitrin (**1**) in MeOD.

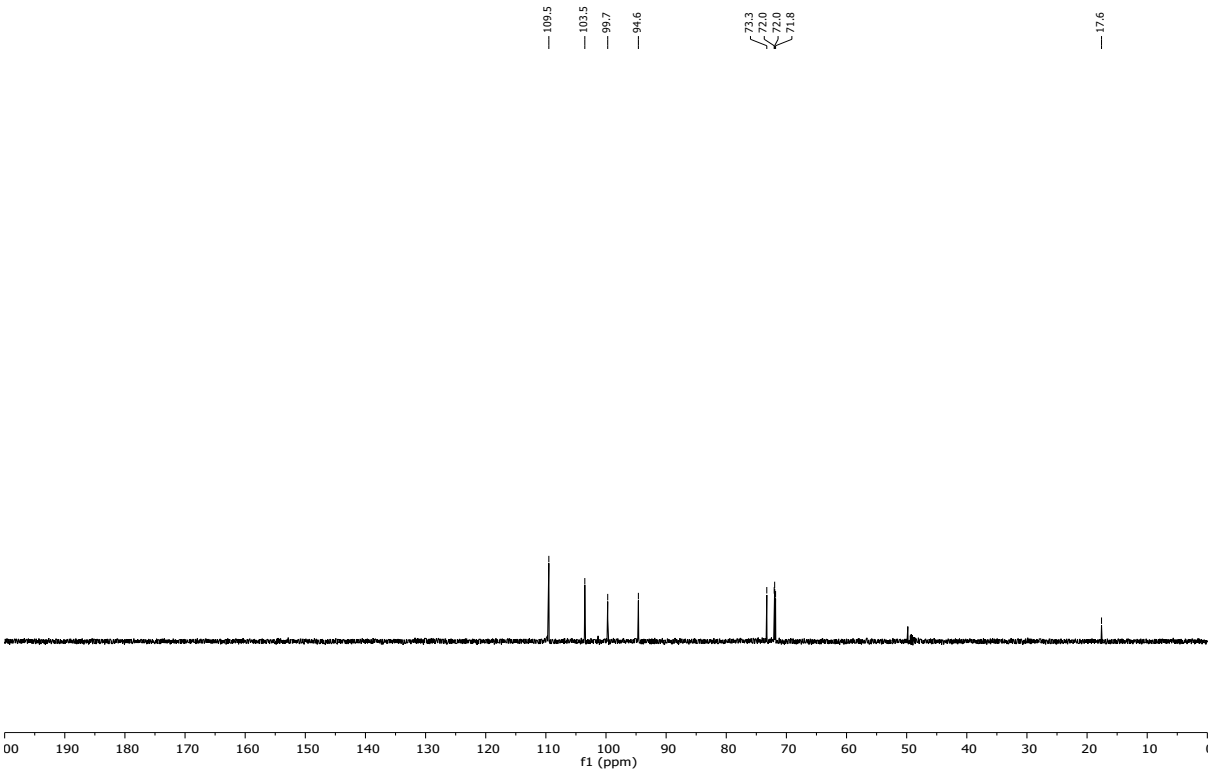

Fig. S5: DEPT-135 of myricitrin (**1**) in MeOD.

***Mearnsitrin (2)*:** (Mearncetin 3-*O*-rhamnoside)

UV, λmax nm 257, 360; *m/z* 333.0818 $[M-146+H]^+$, 479.1370 $[M+H]^+$, 501.1240 $[M+Na]^+$; ^{1}H-NMR (CD_3OD): δ_H 6.87 (2H, *s*, H-2', 6'), 6.37 (1H, *d*, *J* = 1.8 Hz, H-8), 6.21 (1H, *d*, *J* = 1.8 Hz, H-6), 5.31 (1H, *d*, *J* = 1.2 Hz, H-1''), 4.23 (1H, *m*, H-2''), 3.88 (3H, *s*, -O*C*H$_3$), 3.33-3.75 (3H, *m*, H-3'', H-4'', H-5''), 0.95 (3H, *d*, 5.4 Hz, H-6''); ^{13}C NMR (CD_3OD): δ_C 179.6 (C-4), 166.0 (C-7), 163.2 (C-5), 159.0 (C-2), 158.5 (C-9), 151.9 (C-3', 5'), 139.3 (C-4'), 136.7 (C-3), 127.0 (C-1'), 109.8 (C-2', 6'), 106.0 (C-10), 103.7 (C-1''), 99.9 (C-6), 94.7 (C-8), 73.2 (C-4''), 72.1 (C-5''), 72.0 (C-3''), 71.9 (C-2''), 60.9 (4'-O*C*H$_3$), 17.7 (C-6''). The compound was identified as mearnsitrin by comparing the data with those reported in the literature.[3,4]

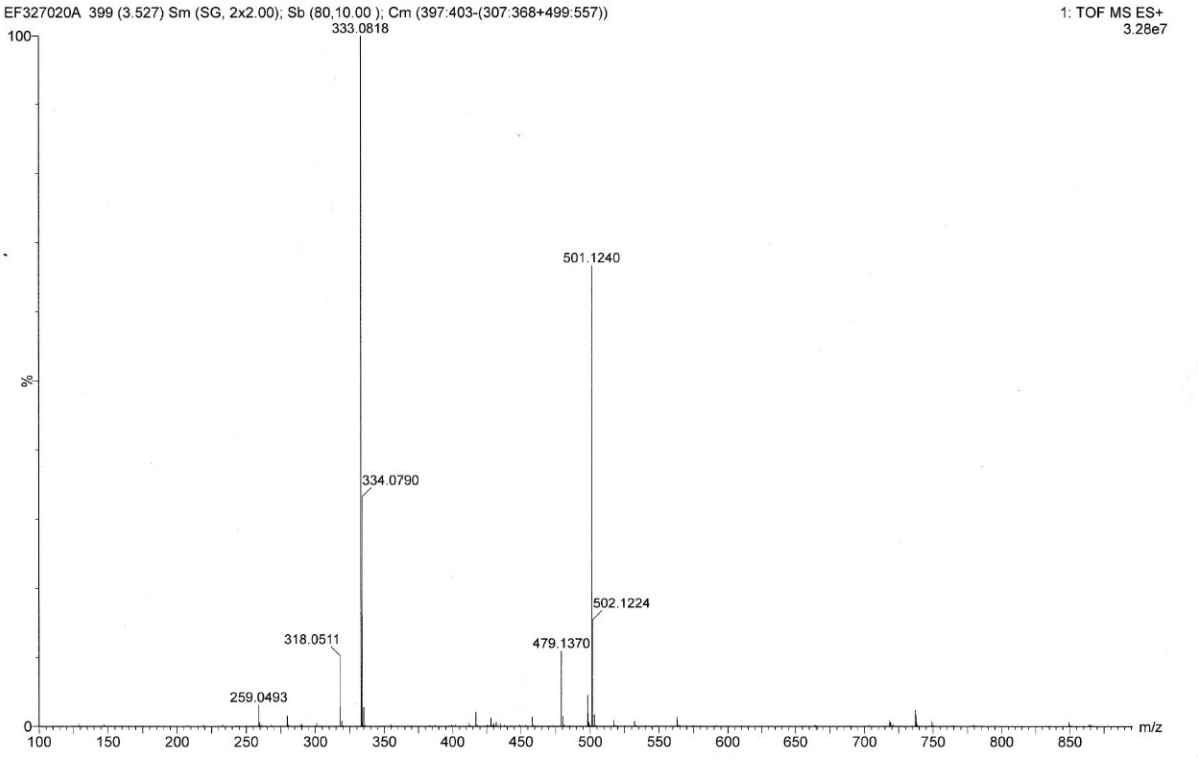

Fig. S6: ESI-MS (+ve) spectrum of mearnsitrin (**2**).

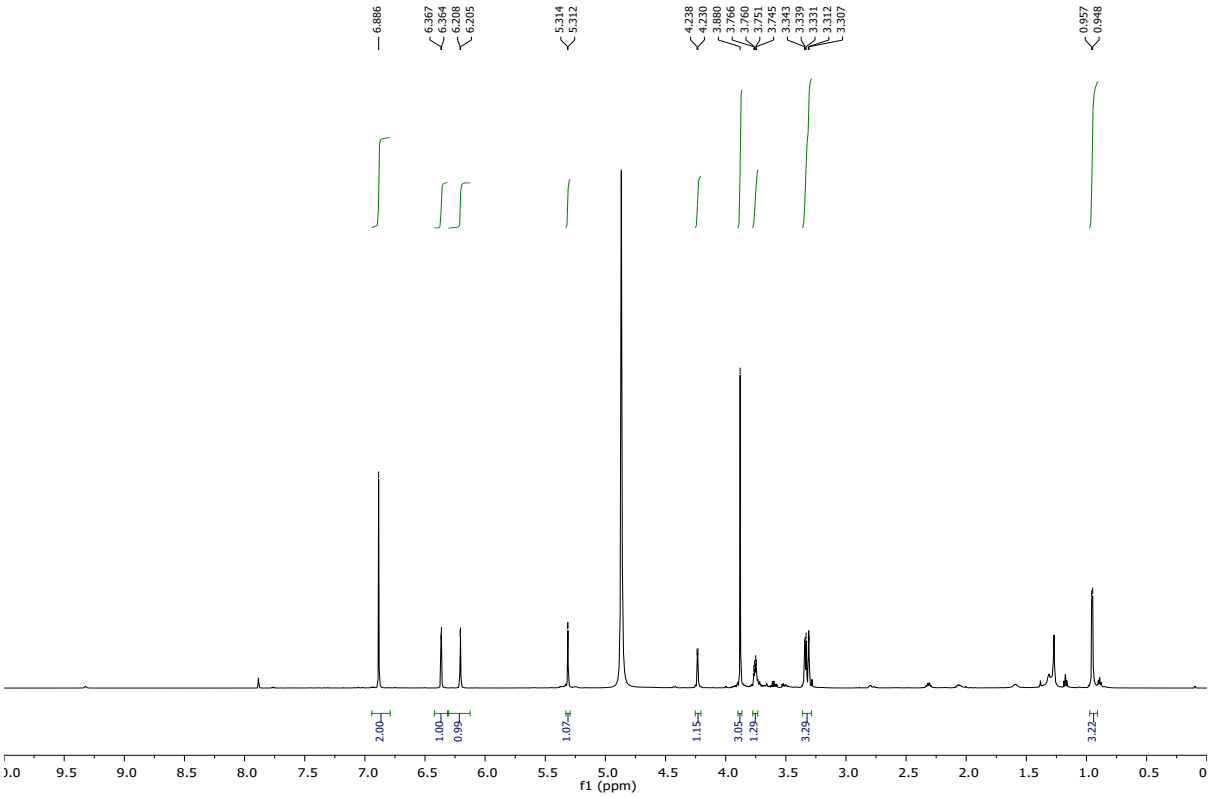

Fig. S7: ^{1}H-NMR of mearnsitrin (**2**) in MeOD, 600 MHz.

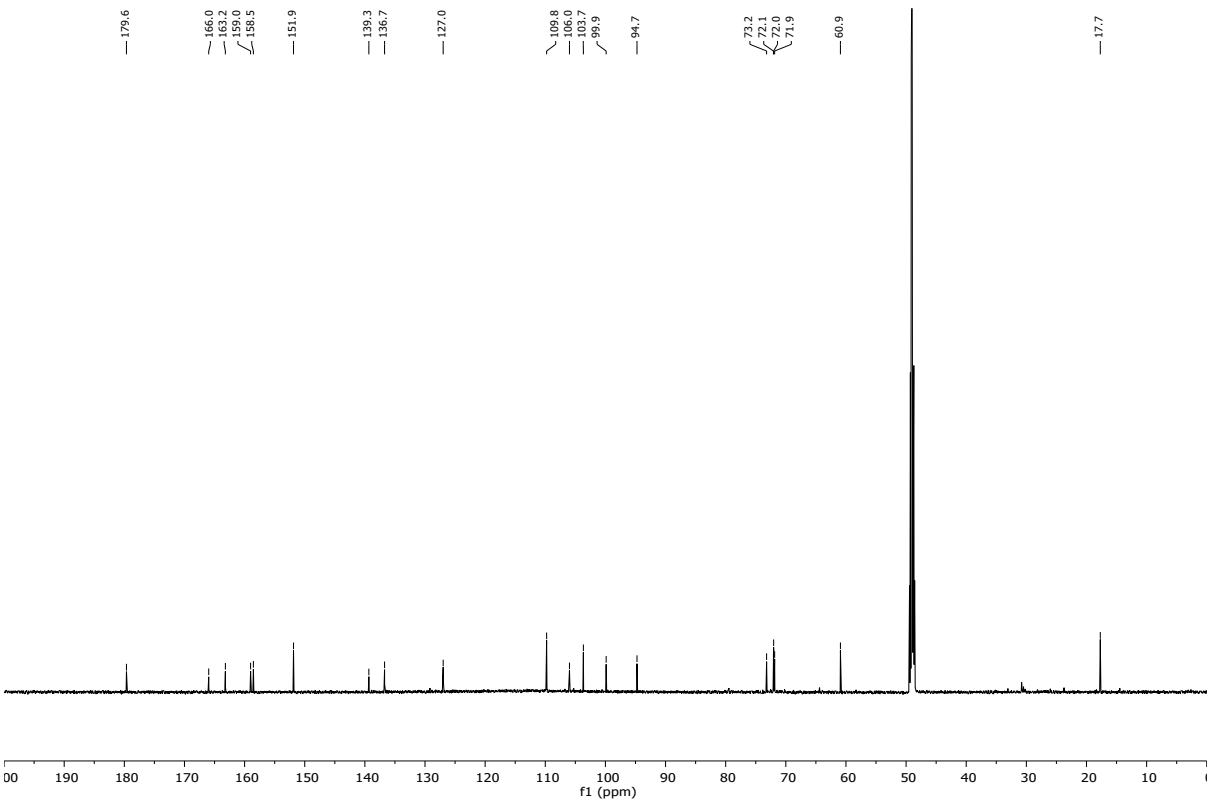

Fig. S8: ^{13}C-NMR of mearnsitrin (**2**) in MeOD, 150 MHz.

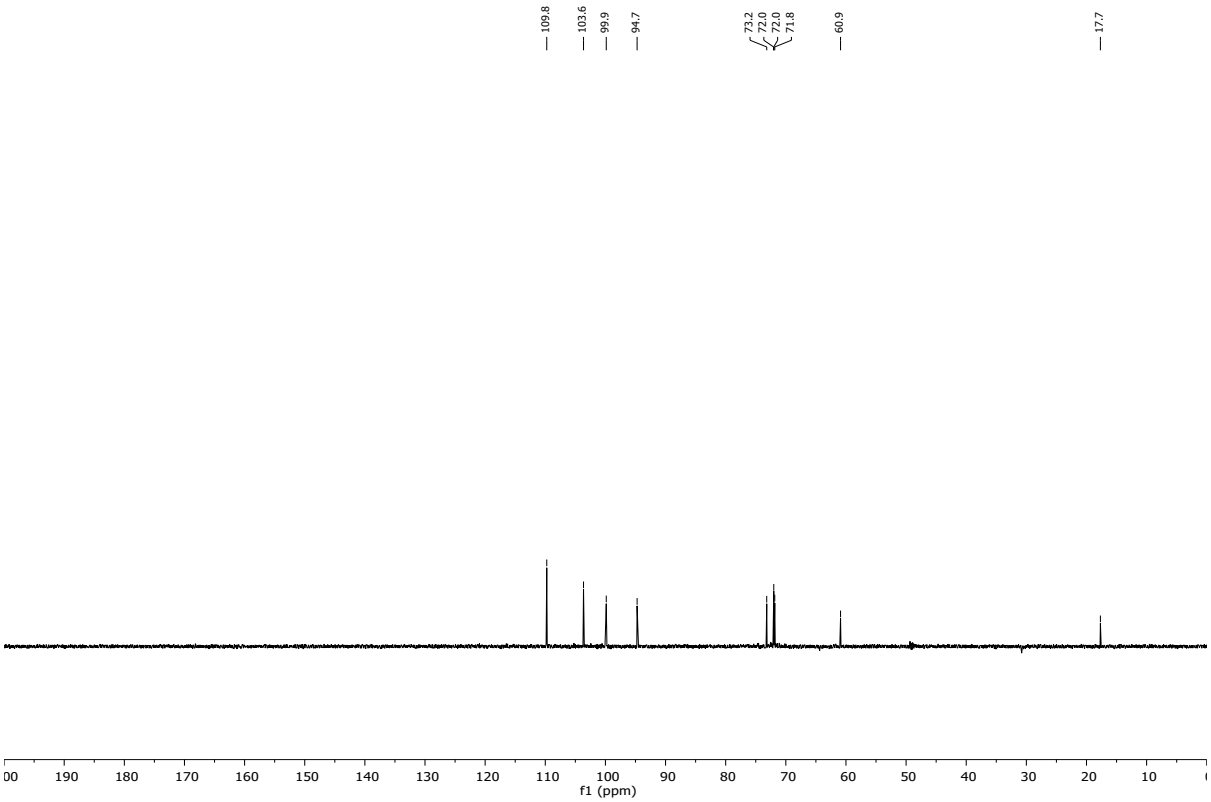

Fig. S9: DEPT-135 of mearnsitrin (**2**) in MeOD.

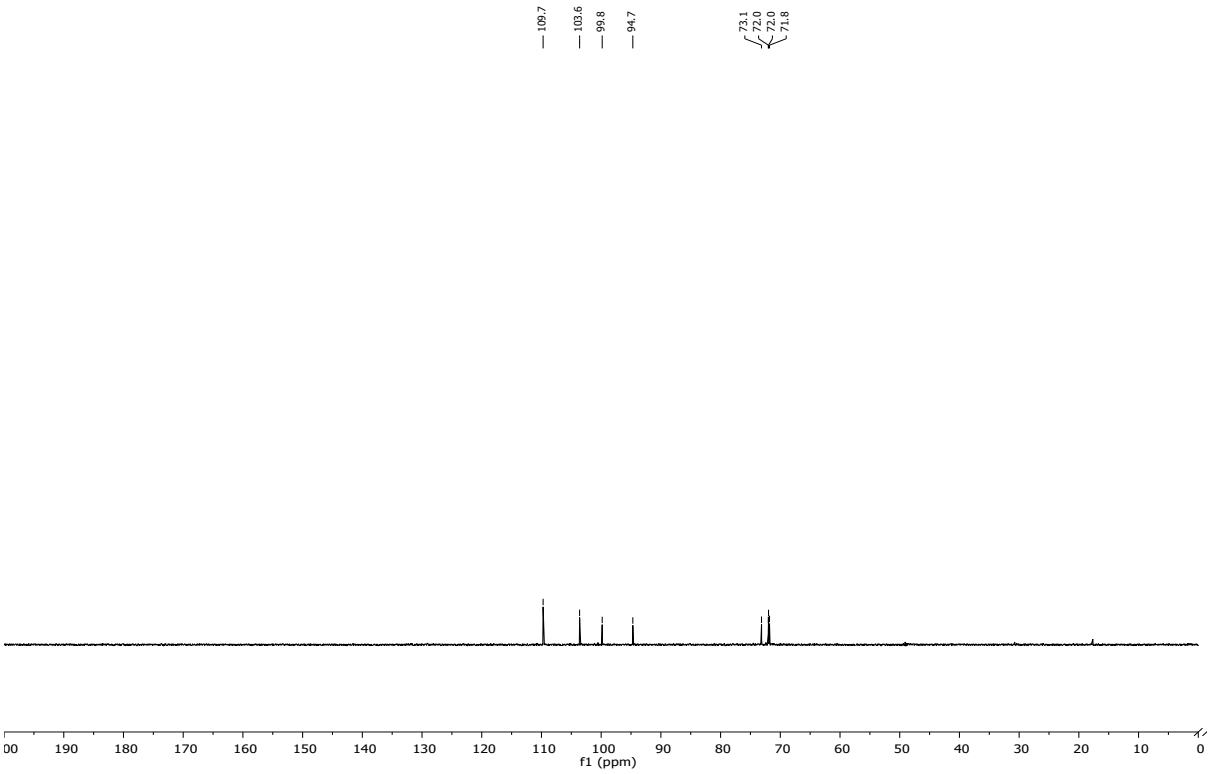

Fig. S10: DEPT-90 of mearnsitrin (**2**) in MeOD.

Mearnsetin (3)

UV, λmax nm 257, 360; *m/z* 333.0615 $[M+H]^+$; ^{1}H-NMR (CD_3OD), δ_H 7.32 (2H, *s*, C-2', 6'), 6.40 (1H, brs, C-8), 6.21 (1H, brs, C-6), 3.90 (3H, *s,* -OCH_3); ^{13}C NMR (CD_3OD): δ_C 177.5 (C-4), 165.8 (C-7), 162.5 (C-5), 158.2 (C-9), 151.6 (C-3', 5'), 147.0 (C-2), 138.5 (C-3), 138.1 (C-4'), 128.0 (C-1'), 108.6 (C-2', 6'), 104.5 (C-10), 99.3 (C-6), 94.4 (C-8), 60.8 (-OCH_3). The compound was identified as mearnsetin by comparing the data with those reported in the literature.[3,5]

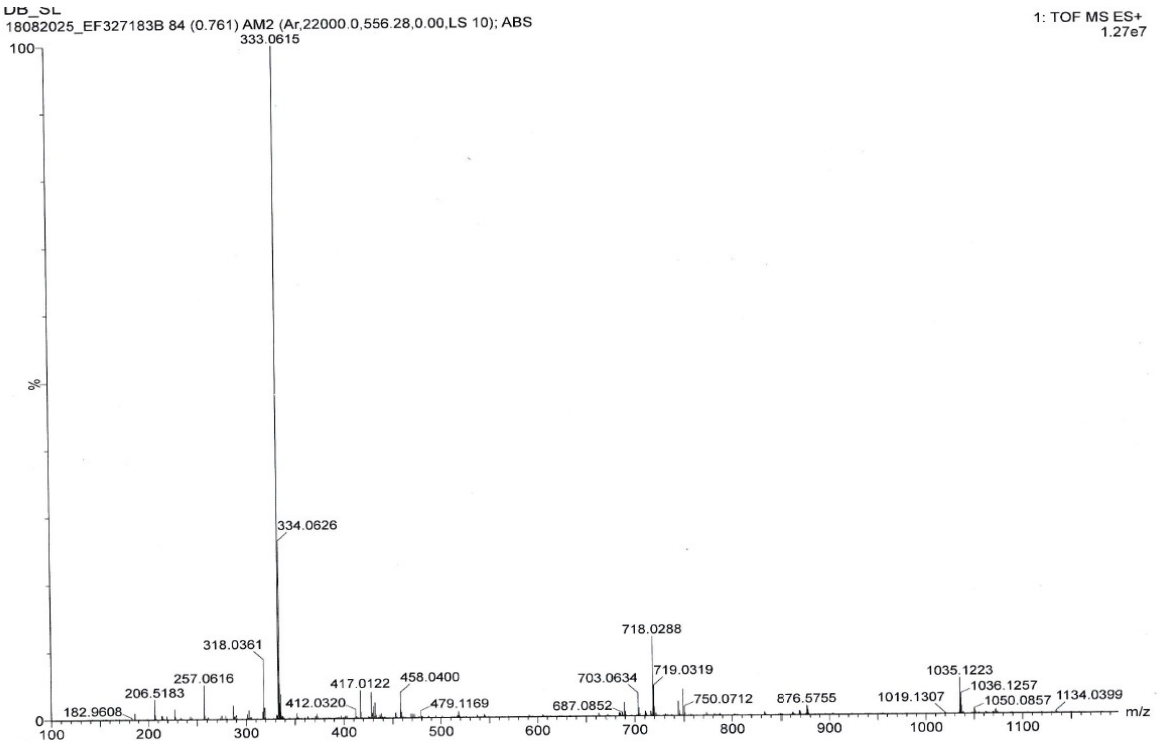

Fig. S11: ESI-MS (+ve) spectrum of mearnsetin (**3**).

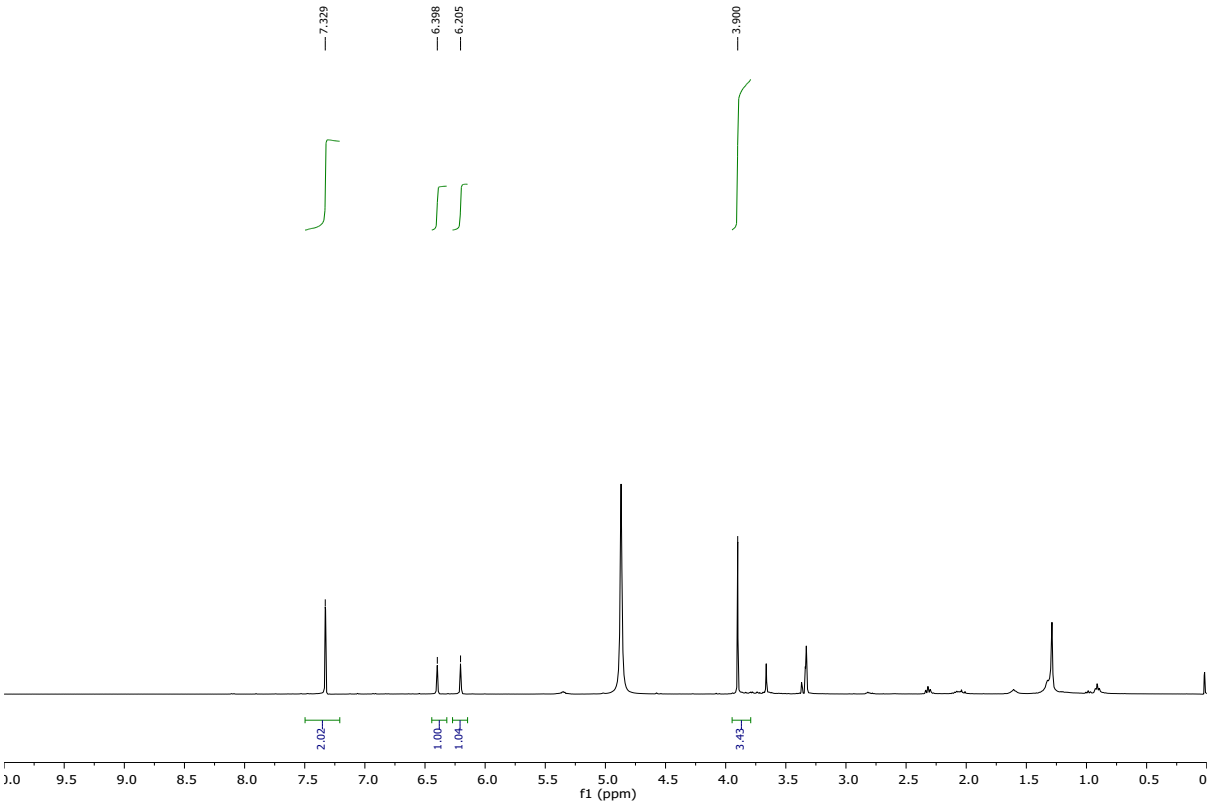

Fig. S12: ^{1}H-NMR of mearnsetin (**3**) in MeOD, 600 MHz.

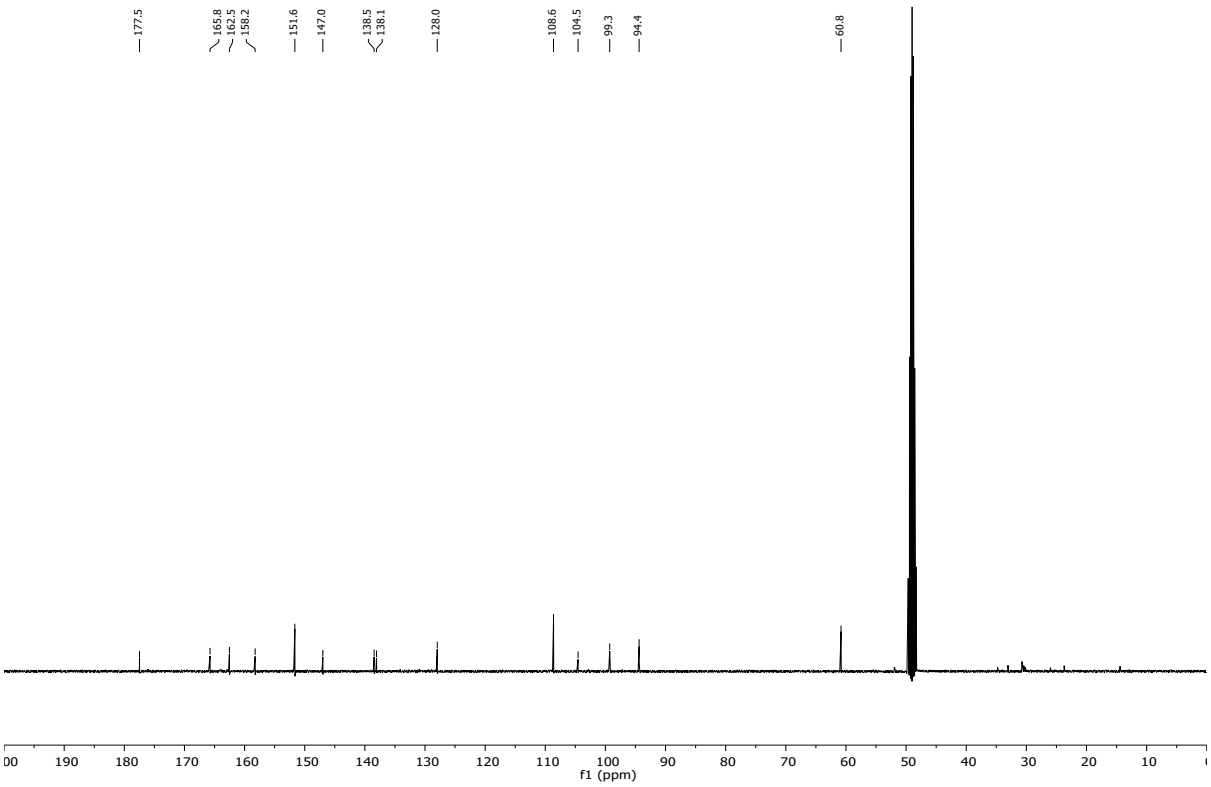

Fig. S13: ^{13}C-NMR of mearnsetin (**3**) in MeOD, 150 MHz.

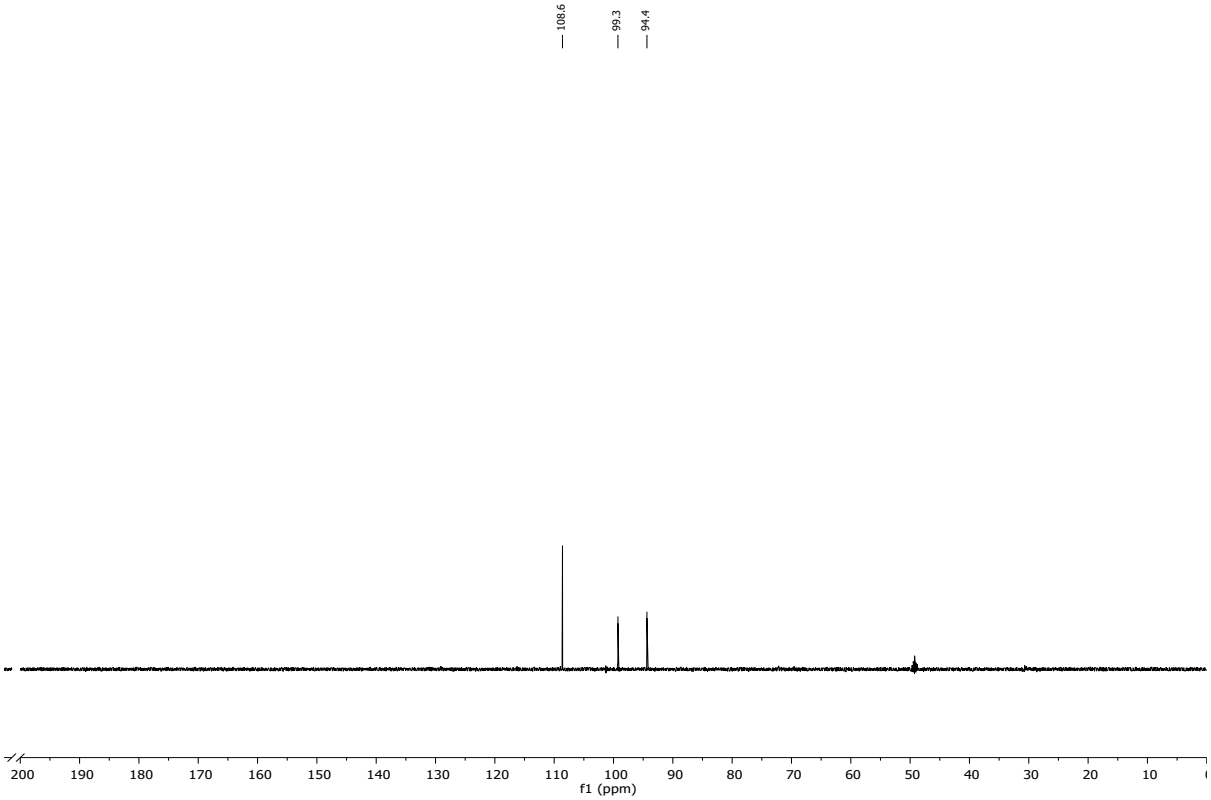

Fig. S14: DEPT-90 of mearnsetin (**3**) in MeOD.

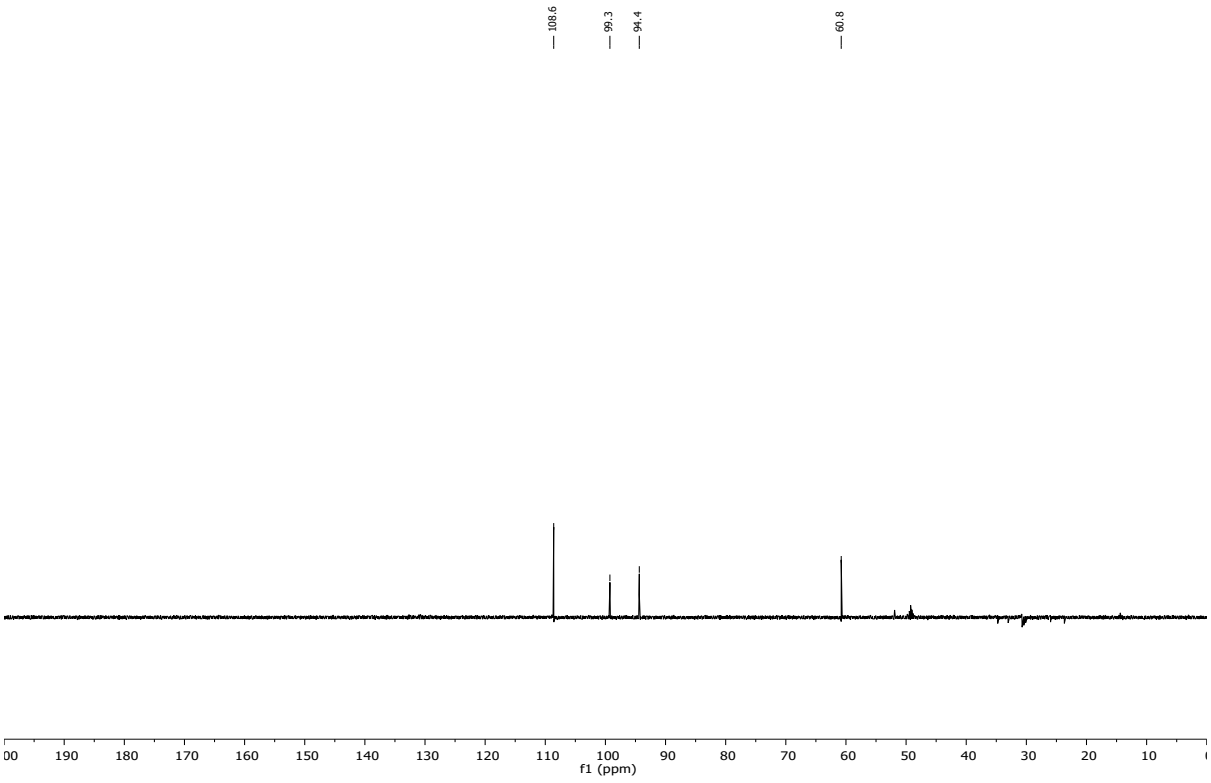

Fig. S15: DEPT-135 of mearnsetin (**3**) in MeOD.

Myricetin (4)

UV, λmax nm 257, 360; *m/z* 319.0426 $[M+H]^+$; ^{1}H-NMR (CD_3OD), δ_H 7.36 (2H, *s*, H-2′, H-6′), 6.39 (1H, *d*, *J* = 2 Hz, H-8), 6.19 (1H, *d*, *J* = 2 Hz, H-6); ^{13}C NMR (CD_3OD): δ_C 177.2 (C-4), 165.5 (C-7), 162.4 (C-5), 158.1 (C-9), 147.9 (C-2), 146.7 (C-3′, C-5′), 137.3 (C-4′), 136.9 (C-3), 123.1 (C-1′), 108.5 (C-2', C-6′), 104.5 (C10), 99.2 (C6), 94.3 (C8). The compound was identified as myricetin by comparing the data with those of reported in the literature.[2]

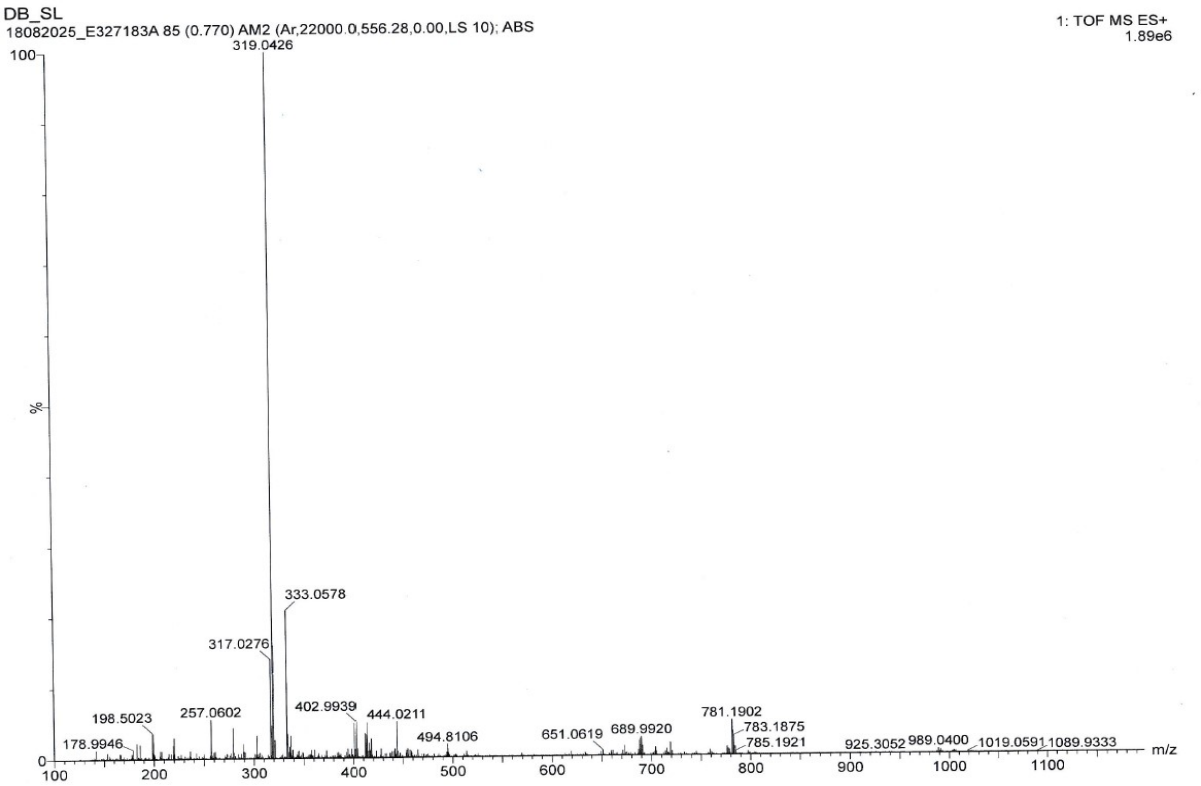

Fig. S16: ESI-MS (+ve) spectrum of myricetin (**4**).

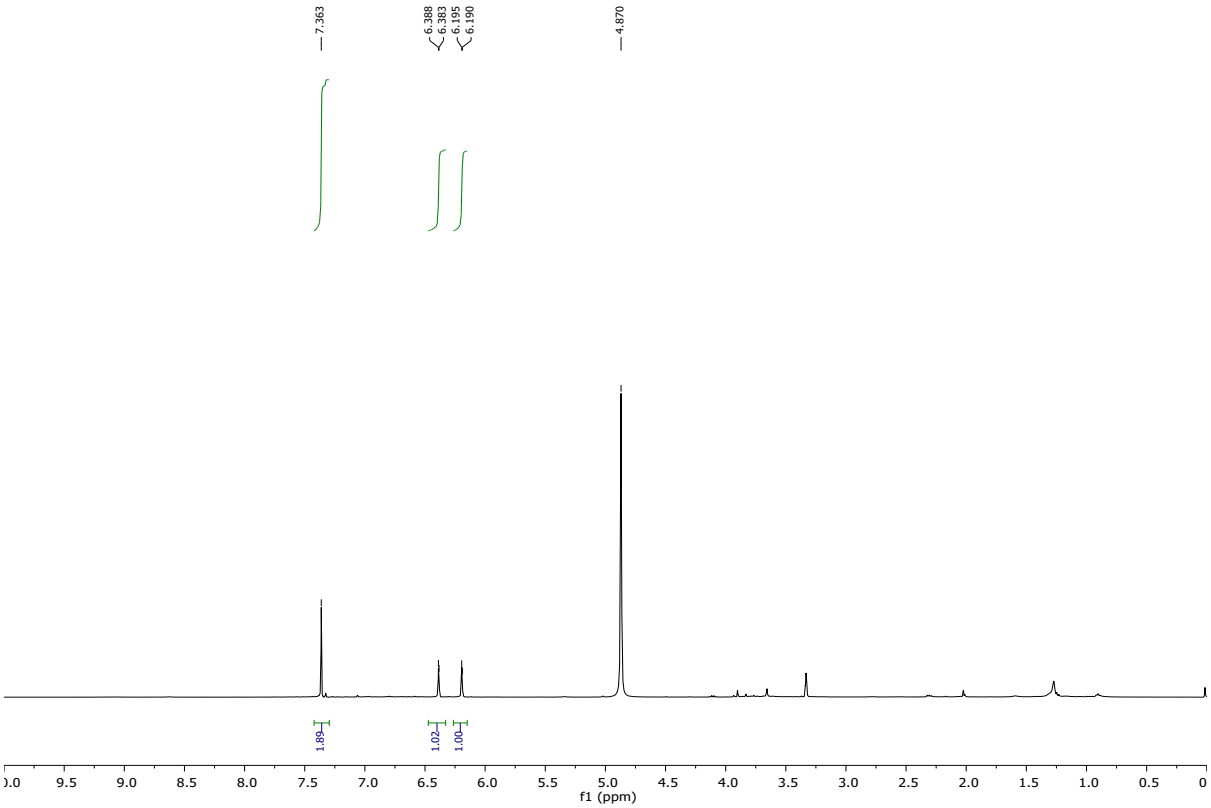

Fig. S17: ^{1}H-NMR of myricetin (**4**) in MeOD, 600 MHz.

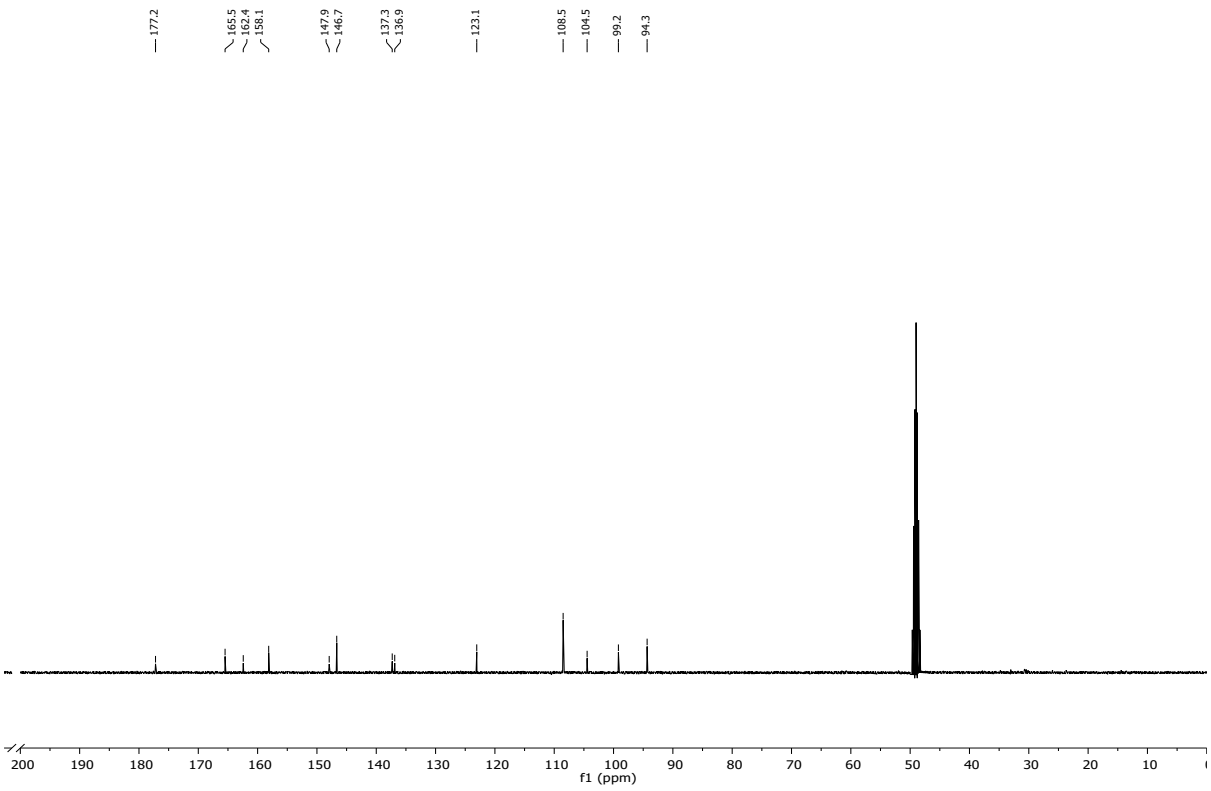

Fig. S18: ^{13}C-NMR of myricetin (**4**) in MeOD, 150 MHz.

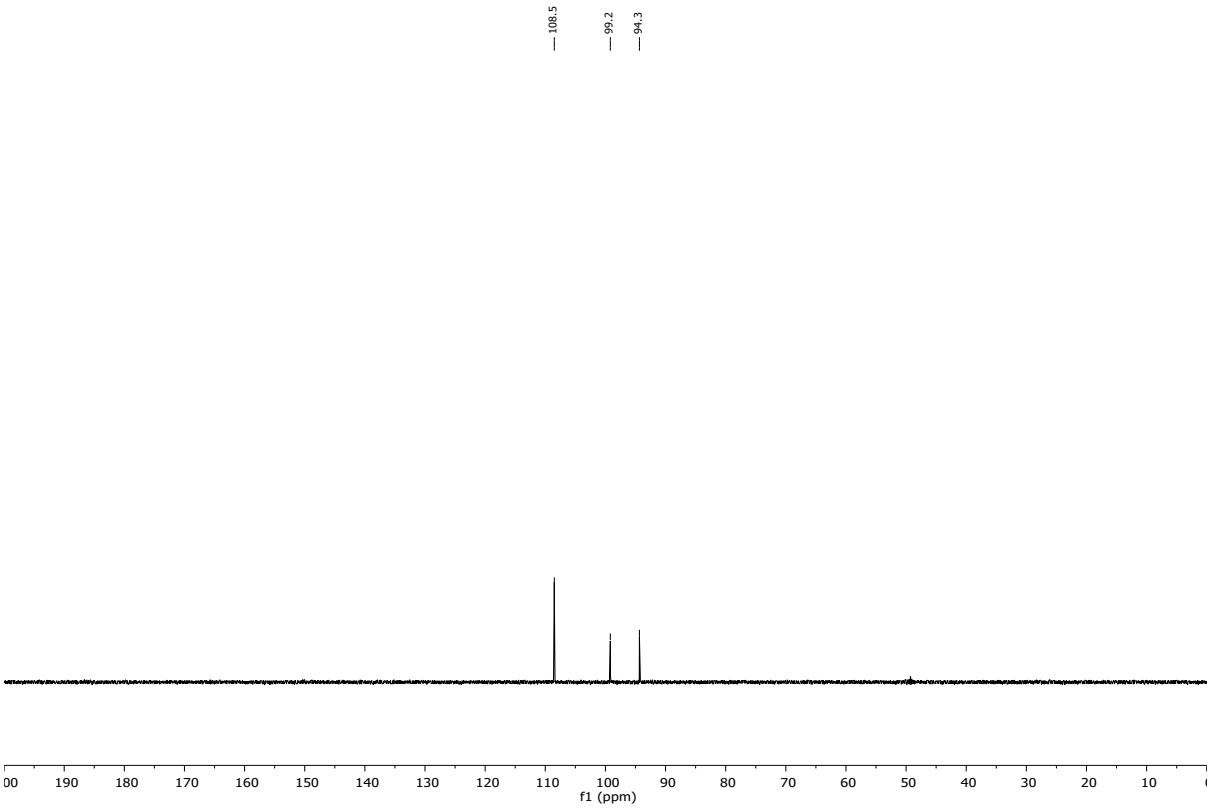

Fig. S19: DEPT-135 of myricetin (**4**) in MeOD.

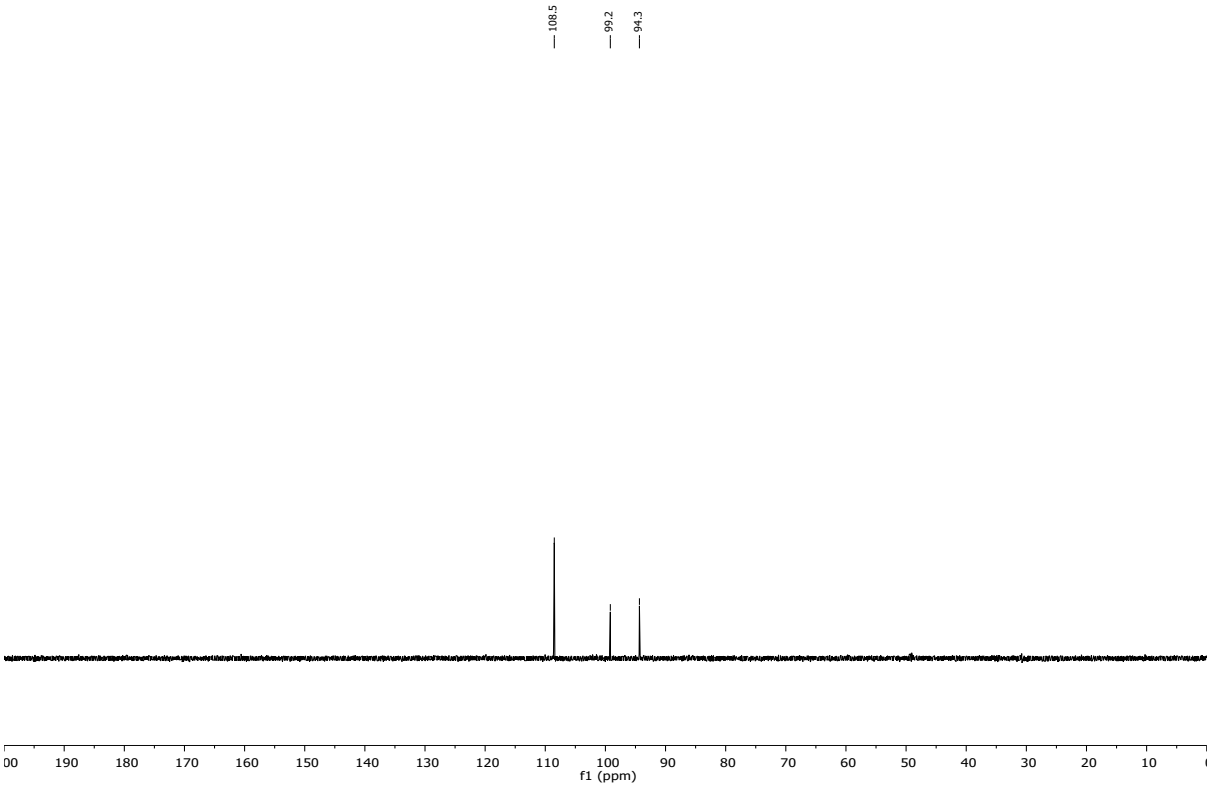

Fig. S20: DEPT-90 of myricetin (**4**) in MeOD.

References

1. I. W. Hwang and S. K. Chung, Isolation and Identification of Myricitrin, an Antioxidant Flavonoid, from *Daebong Persimmon* Peel, *Prev Nutr Food Sci*, 2018, **23**, 341-346.

2. S. Y. Mok and S. Lee, Identification of flavonoids and flavonoid rhamnosides from *Rhododendron mucronulatum* for. albiflorum and their inhibitory activities against aldose reductase, *Food Chem*, 2013, **136**, 969-974.

3. K. Gluchoff-Fiasson, B. Fenet, J. C. Leclerc, J. Reynaud, M. Lussignol and M. Jay, Three new flavonol malonylrhamnosides from *Ribes alpinum*, *Chem Pharm Bull (Tokyo)*, 2001, **49**, 768-770.

4. Y. Noreen, G. Serrano, P. Perera and L. Bohlin, Flavan-3-ols isolated from some medicinal plants inhibiting COX-1 and COX-2 catalysed prostaglandin biosynthesis, *Planta Med*, 1998, **64**, 520-524.

5. A. O. Oladimeji, I. A. Oladosu, M. S. Ali and Z. Ahmed, Flavonoids from the roots of *Dioclea reflexa* (Hook F.), *Bulletin of The Chemical Society of Ethiopia*, 2015, **29**, 441-448.