Supporting Information for

Two new pyridine derivatives and two new furan derivatives from *Irpex lacteus*

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ABSTRACT

Two undescribed di-substituted pyridine derivatives irpexidines A and B (**1** and **2**) and two undescribed alkylfuran derivatives irpexins K and L (**3** and **4**) were isolated from fermentation broth of *Irpex lacteus*. Their structures were established by extensive spectroscopic methods. The pyridine derivatives from this fungus were reported for the first time. The new compounds were evaluated for their cytotoxicity against Hela cancer cell and inhibitory activity on NO production.

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Section S2. NMR spectra and HRESIMS for compounds **1–4**.

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Figure S15-S21. NMR and MS spectra of irpexin K (**3**).

Figure S22-S28. NMR and MS spectra of irpexin L (**4**).

Section S1. Spectroscopic data for compounds **1–4**.

Irpexidine A (1)

Colorless oil. UV (H_2O) λ_{max} nm (log ε): 210 (3.25), 220 (3.24), 265 (2.92). IR (KBr) ν_{max} cm^{-1}: 1732, 1638, 1607, 1443, 1319, 1217. HRESIMS *m/z* 224.09171 $[M + H]^+$ (calcd for $C_{11}H_{13}NO_4^+$ 224.09173). ^{1}H-NMR (methanol-d_4, 600 MHz): δ_H 8.53 (1H, d, *J* = 5.0 Hz, H-6), 8.03 (1H, d, *J* = 1.7 Hz, H-5), 7.51 (1H, d, *J* = 5.0, 1.7 Hz, H-3), 3.95 (3H, s, OMe-C7), 3.62 (3H, s, OMe-C10), 3.02 (2H, t, *J* = 7.4 Hz, H-8), 2.73 (2H, t, *J* = 7.4 Hz, H-9). ^{13}C-NMR (methanol-d_4, 150 MHz): δ_C 174.3 (C-10, C), 166.6 (C-7, C), 153.9 (C-4, C), 150.5 (C-6, CH), 148.7 (C-2, C), 128.8 (C-3, CH), 126.5 (C-5, CH), 53.2 (OMe-C7, CH_3), 52.2 (OMe-C10, CH_3), 34.7 (C-9, CH_2), 30.9 (C-8, CH_2).

Irpexidine B (2)

Colorless oil. HRESIMS *m/z* 288.12028 $[M + Na]^+$ (calcd for $C_{14}H_{19}NO_4Na^+$ 288.12063). ^{1}H-NMR (methanol-d_4, 600 MHz): δ_H 8.51 (1H, d, *J* = 5.0 Hz, H-6), 8.01 (1H, d, *J* = 1.7 Hz, H-3), 7.49 (1H, dd, *J* = 5.0, 1.7 Hz, H-5), 4.01 (2H, t, *J* = 6.6 Hz, H-1′), 3.93 (3H, s, OMe-C7), 3.01 (2H, t, *J* = 7.4 Hz, H-8), 2.71 (2H, t, *J* = 7.3 Hz, H-9), 1.48-1.54 (2H, m, H-2′), 1.22-1.30 (2H, m, H-3′), 0.85 (3H, t, *J* = 7.5 Hz, H-4′). ^{13}C-NMR (methanol-d_4, 150 MHz): δ_C 173.3 (C-10, C), 166.6 (C-7, C), 154.0 (C-4, C), 150.5 (C-6, CH), 148.7 (C-2, C), 128.8 (C-5, CH), 126.6 (C-3, CH), 65.6 (C-1′, CH_2), 53.2 (OMe-C7, CH_3), 35.0 (C-9, CH_2), 31.8 (C-2′, CH_2), 30.9 (C-8, CH_2), 20.1 (C-3′, CH_2), 14.0 (C-4′, CH_3).

Irpexin K (3)

Colorless oil. UV (H_2O) λ_{max} nm (log ε): 210 (3.27), 255 (3.77). IR (KBr) ν_{max} cm^{-1}: 2959, 1647, 1526, 1018. HRESIMS *m/z* 263.08887 $[M + Na]^+$ (calcd for $C_{12}H_{16}NaO_5^+$ 263.08899). ^{1}H-NMR (DMSO-d_6, 600 MHz): δ_H 7.05 (1H, d, *J* = 3.3 Hz, H-3), 6.28 (1H, d, *J* = 3.3 Hz, H-4), 4.01 (2H, t, *J* = 6.6 Hz, H-1′), 2.92 (2H, t, *J* = 7.3 Hz, H-6), 2.67 (2H, t, *J* = 7.4 Hz, H-7), 1.48-1.55 (2H, m, H-2′), 1.24-1.32 (2H, m, H-3′), 0.86 (3H, t, *J* = 7.4 Hz, H-4′). ^{13}C-NMR (DMSO-d_6, 150 MHz): δ_C 172.1 (C-8, C), 160.0 (C-9, C), 158.5 (C-5, CH), 144.5 (C-2, C), 118.5 (C-3, CH), 108.2 (C-4, CH), 61.4 (C-1′, CH_2), 31.8 (C-7, CH_2), 30.4 (C-2′, CH_2), 23.4 (C-6, CH_2), 18.8 (C-3′, CH_2), 13.8 (C-4′, CH_3).

Irpexin L (4)

Colorless oil. HRESIMS *m/z* 263.12531 $[M + Na]^+$ (calcd for $C_{13}H_{20}O_4Na^+$, 263.12538). ^{1}H-NMR (methanol-d_4, 600 MHz): δ_H 6.22 (1H, d, *J* = 3.1 Hz, H-3), 5.98 (1H, d, *J* = 3.1 Hz, H-4), 3.92-3.95 (1H, m, H-12), 3.91-3.94 (1H, m, H-11), 3.20 (3H, s, OMe-C12), 2.58 (2H, d, *J* = 7.3 Hz, H-6), 2.49 (2H, t, *J* = 7.2 Hz, H-8), 2.08 (3H, s, H-10), 1.80-1.87 (2H, m, H-7), 1.17 (3H, d, *J* = 6.1 Hz, H-13). ^{13}C-NMR (methanol-d_4,150 MHz): δ_C 211.5 (C-9, C), 156.7 (C-5, C), 151.9 (C-2, C), 111.2 (C-3, CH), 106.9 (C-4, CH), 82.8 (C-12, CH), 69.6 (C-11, CH), 57.1 (OMe-C12, CH_3), 43.2 (C-8, CH_2), 29.9 (C-10, CH_3), 28.1 (C-6, CH_2), 23.3 (C-7, CH_2), 19.3 (C-13, CH_3).

Section S2. NMR spectra and HRESIMS for compounds **1–4**.

Figure S1. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of irpexidine A (**1**)

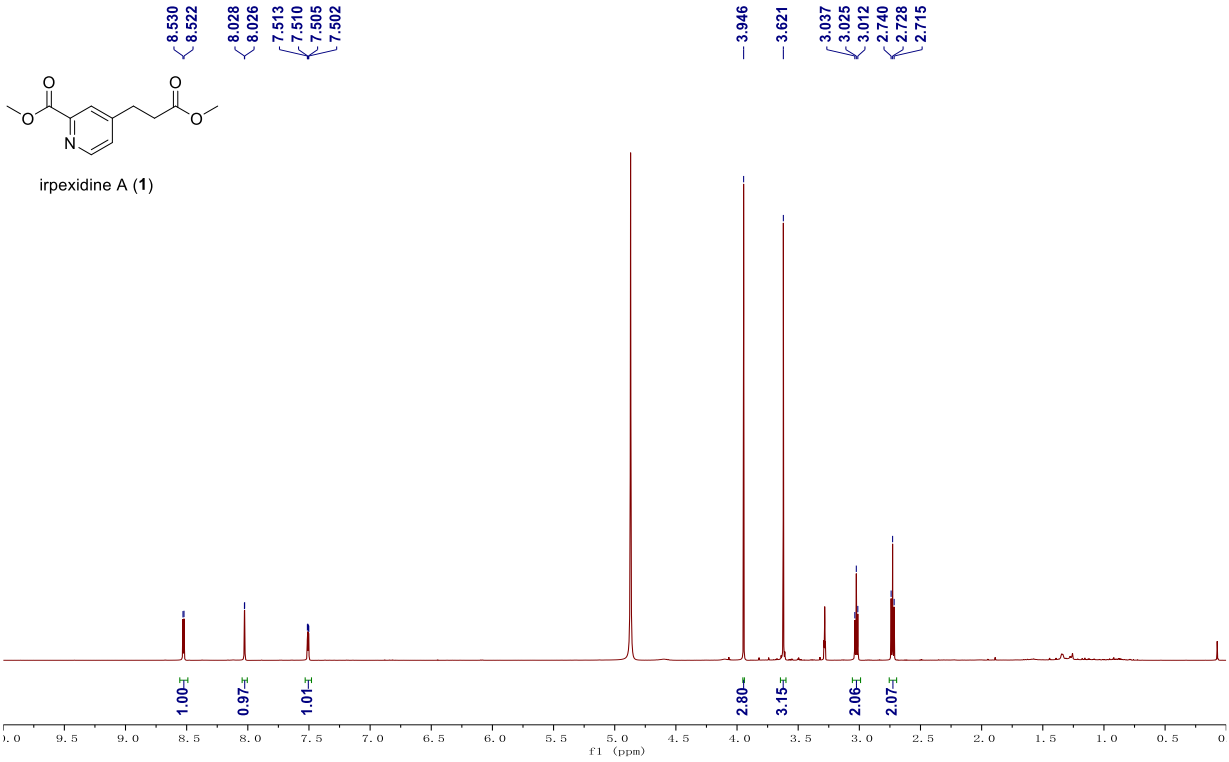

Figure S2. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of irpexidine A (**1**)

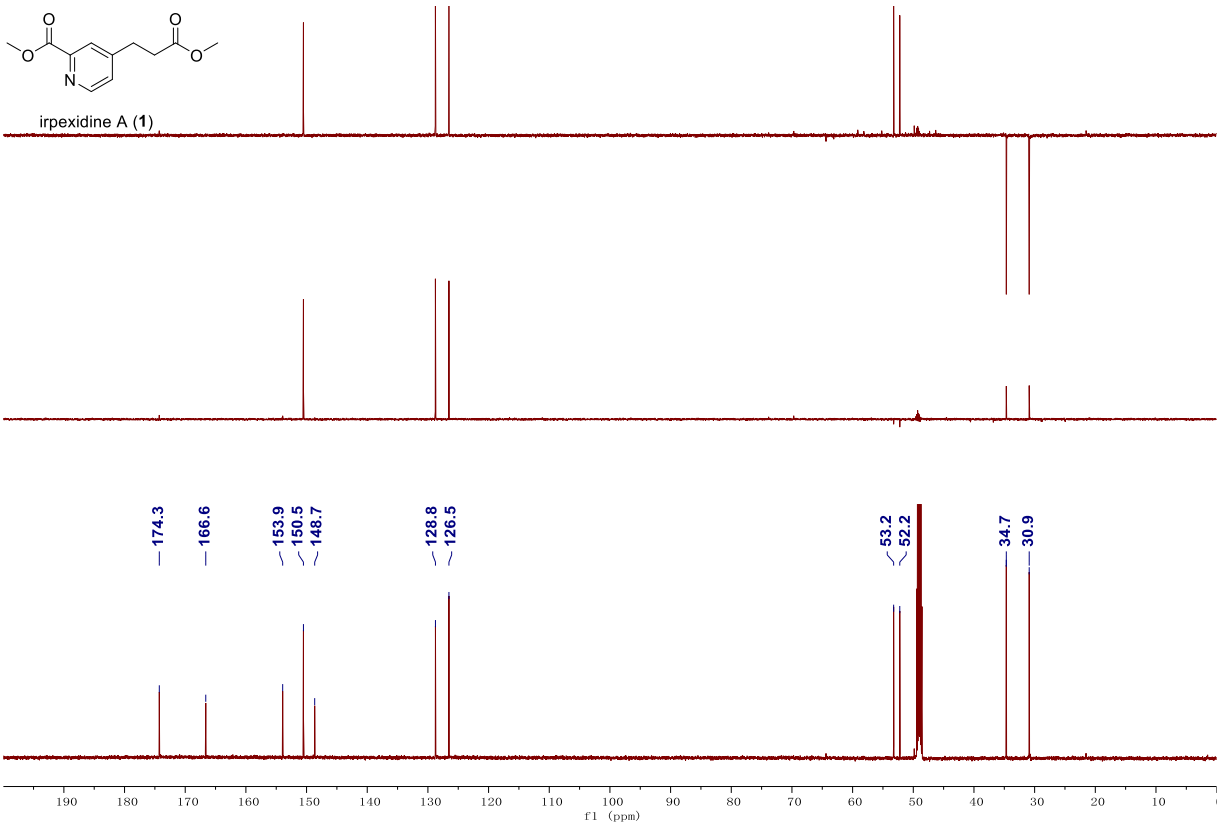

Figure S3. HSQC spectrum of irpexidine A (**1**)

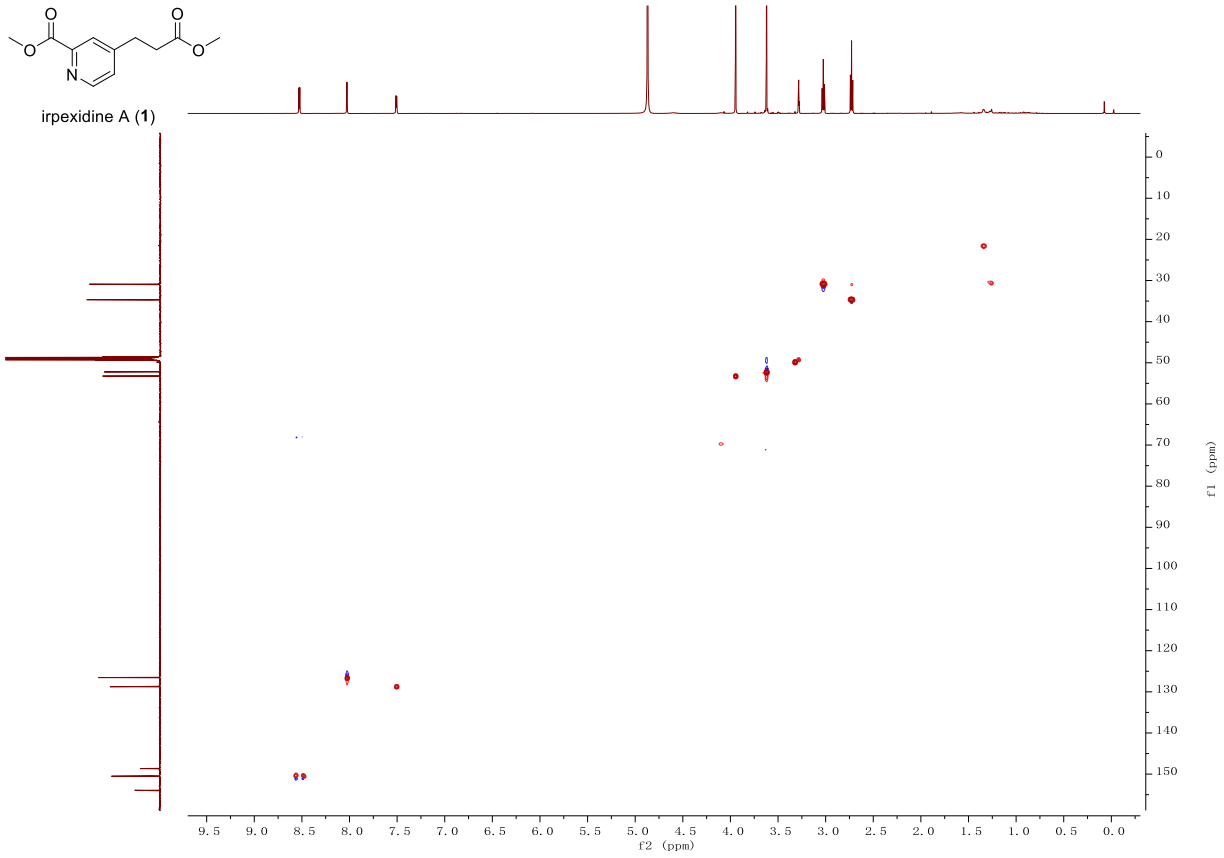

Figure S5. HMBC spectrum of irpexidine A (**1**)

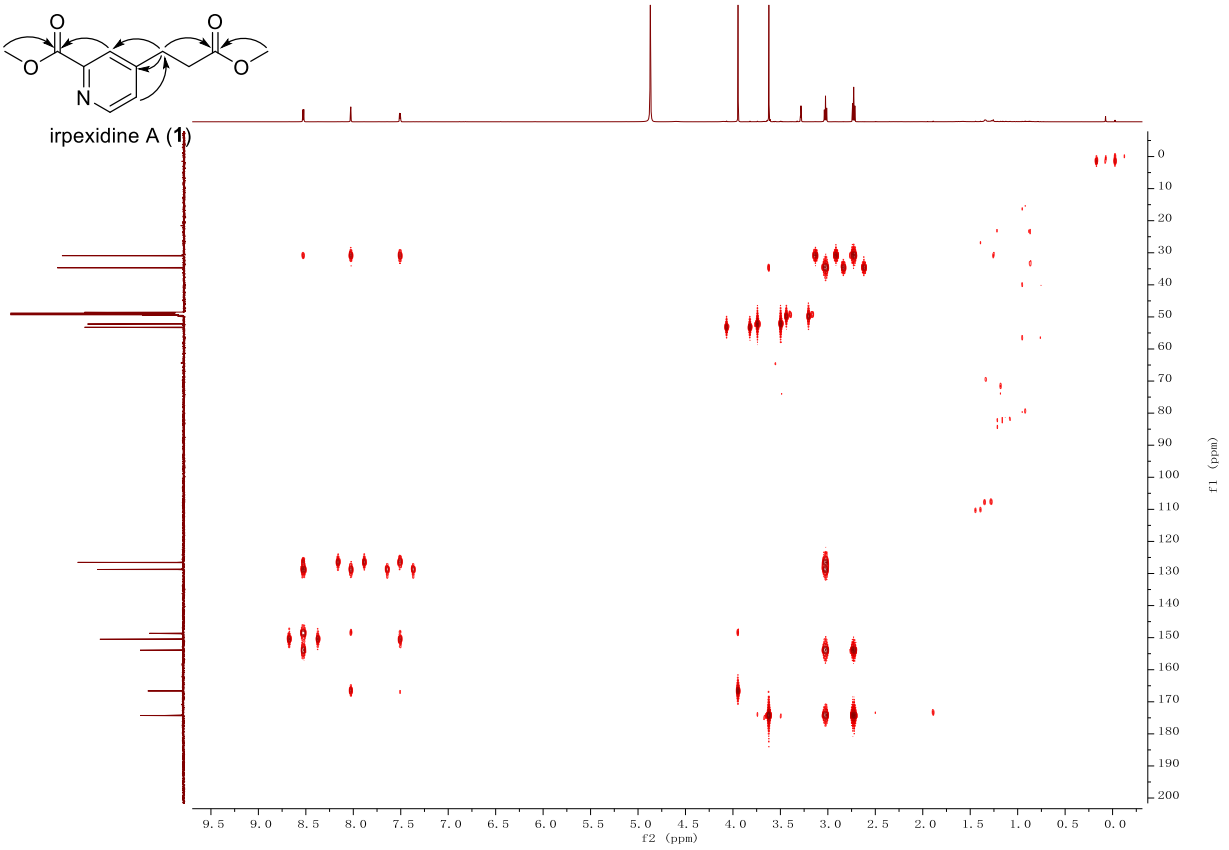

Figure S4. COSY spectrum of irpexidine A (**1**)

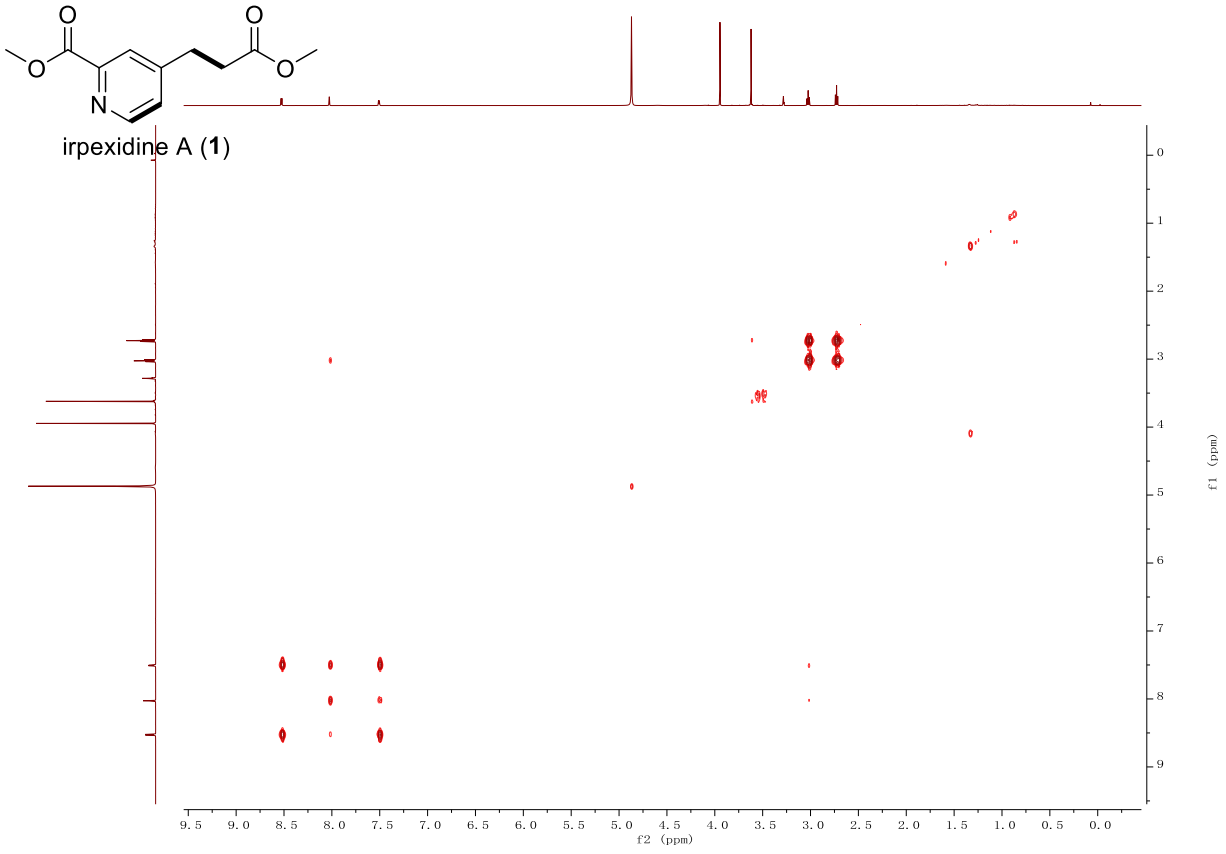

Figure S6. ROESY spectrum of irpexidine A (**1**)

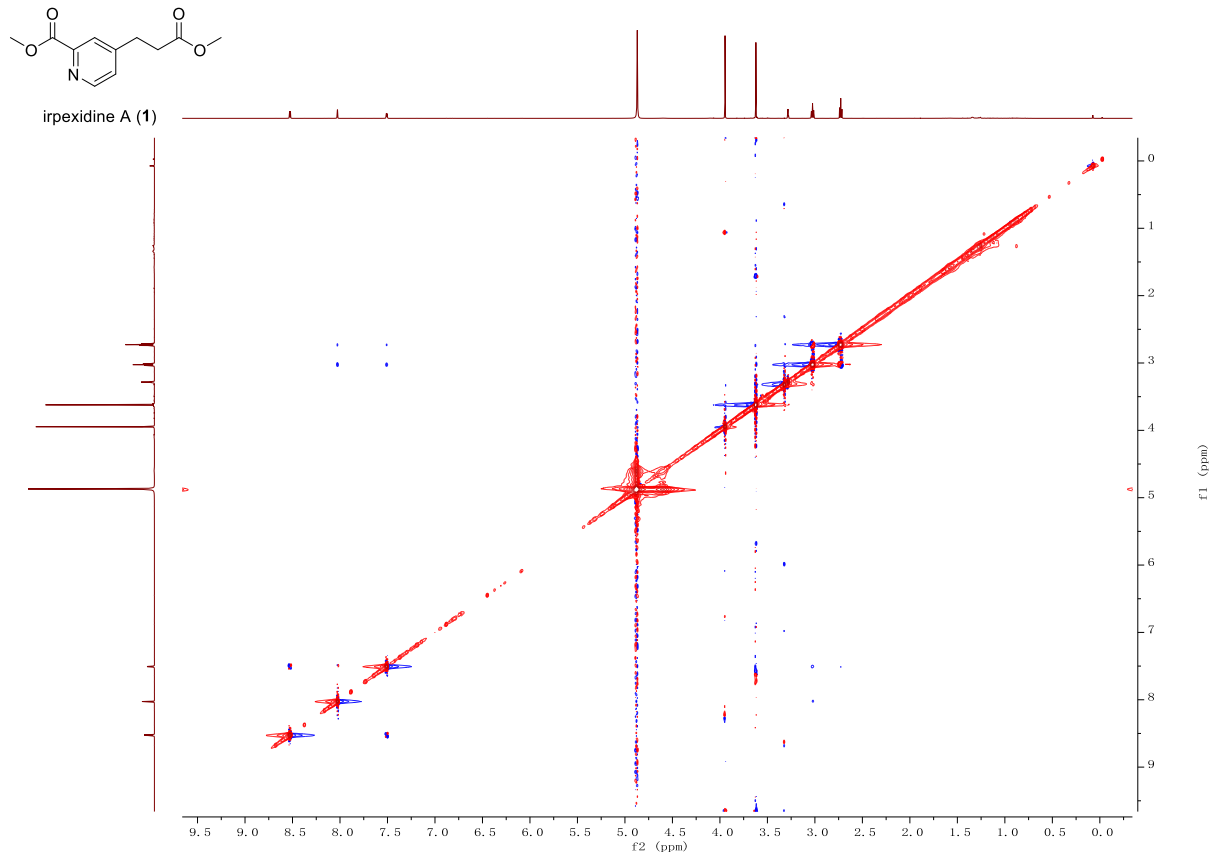

Figure S7. HR-ESI-MS of irpexidine A (**1**)

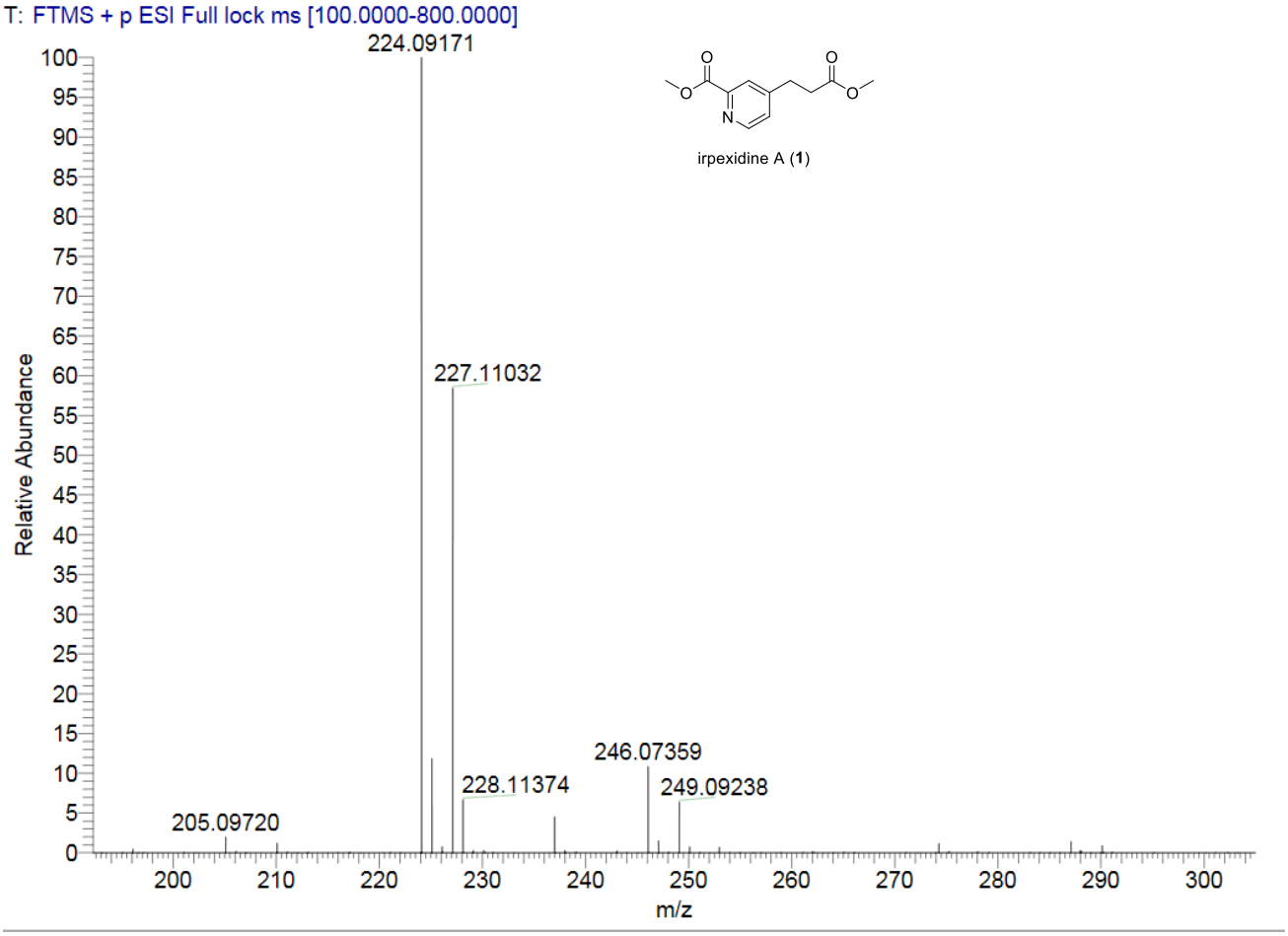

Figure S8. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of irpexidine B (**2**)

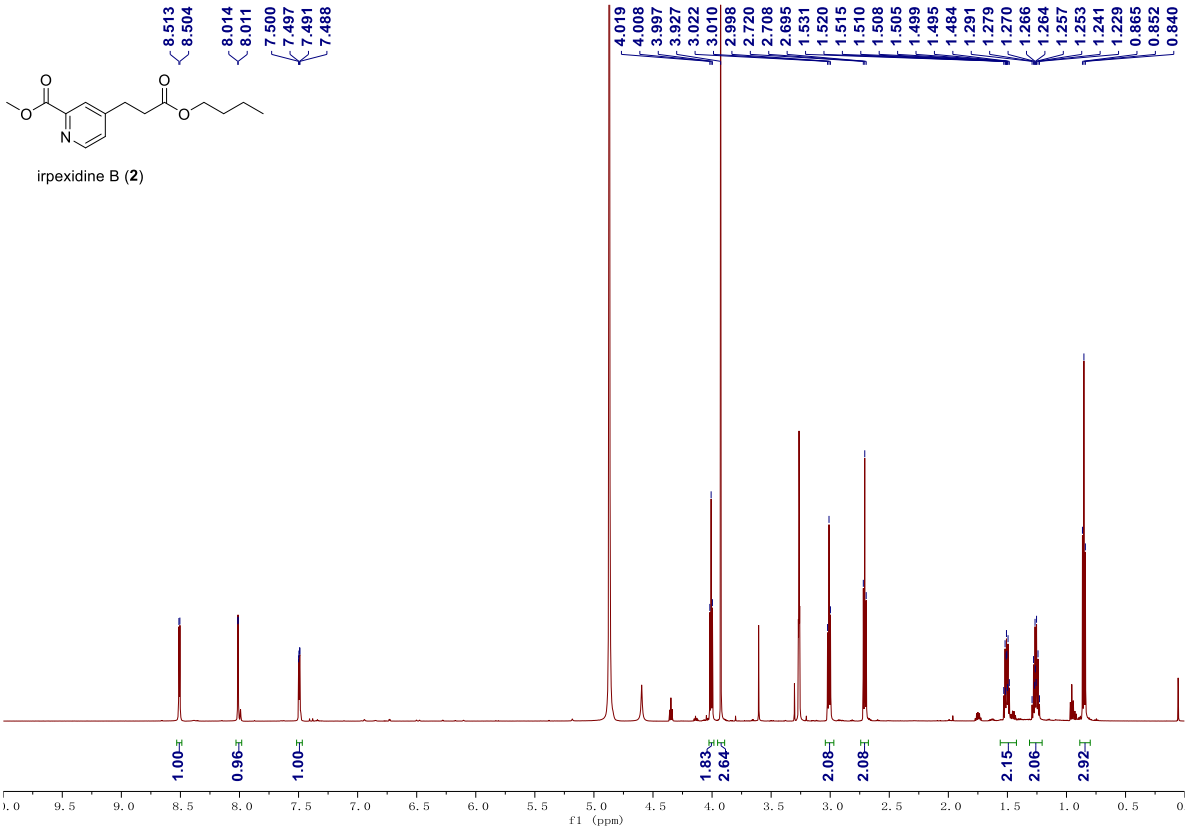

Figure S9. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of irpexidine B (**2**)

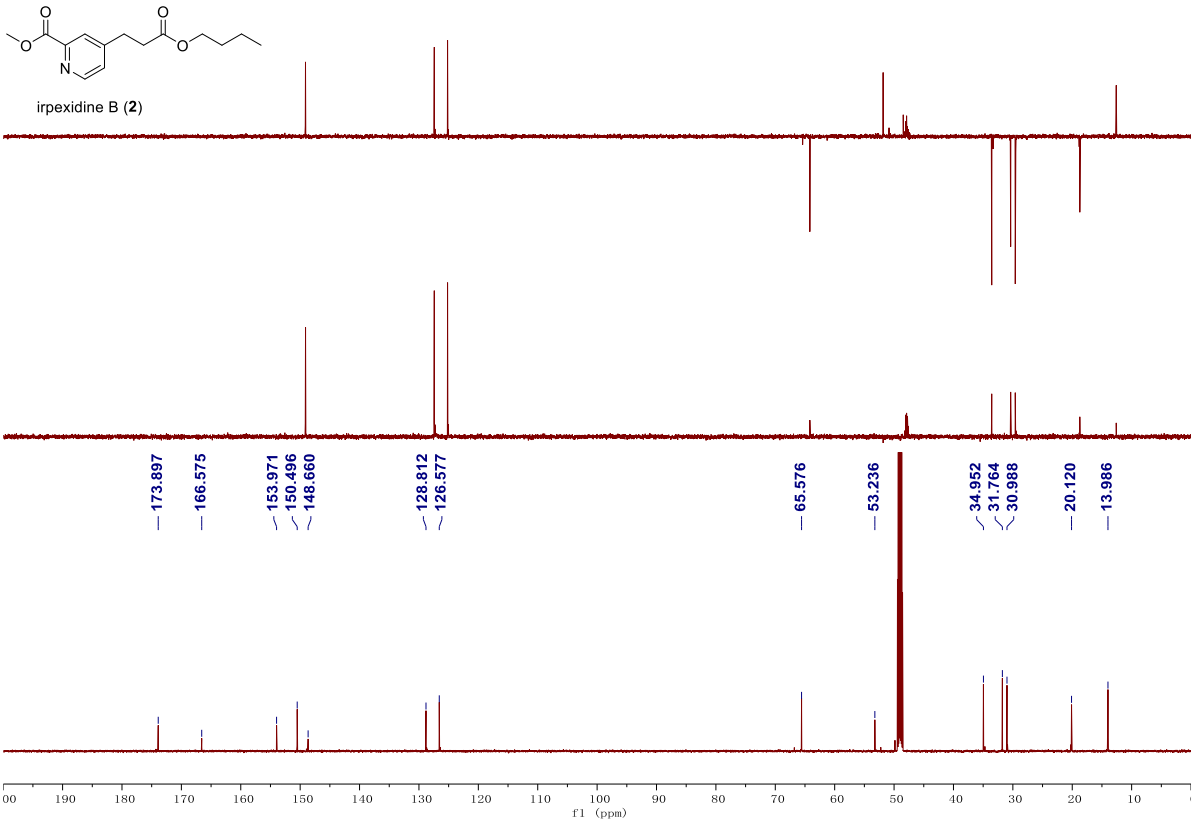

Figure S10. HSQC spectrum of irpexidine B (**2**)

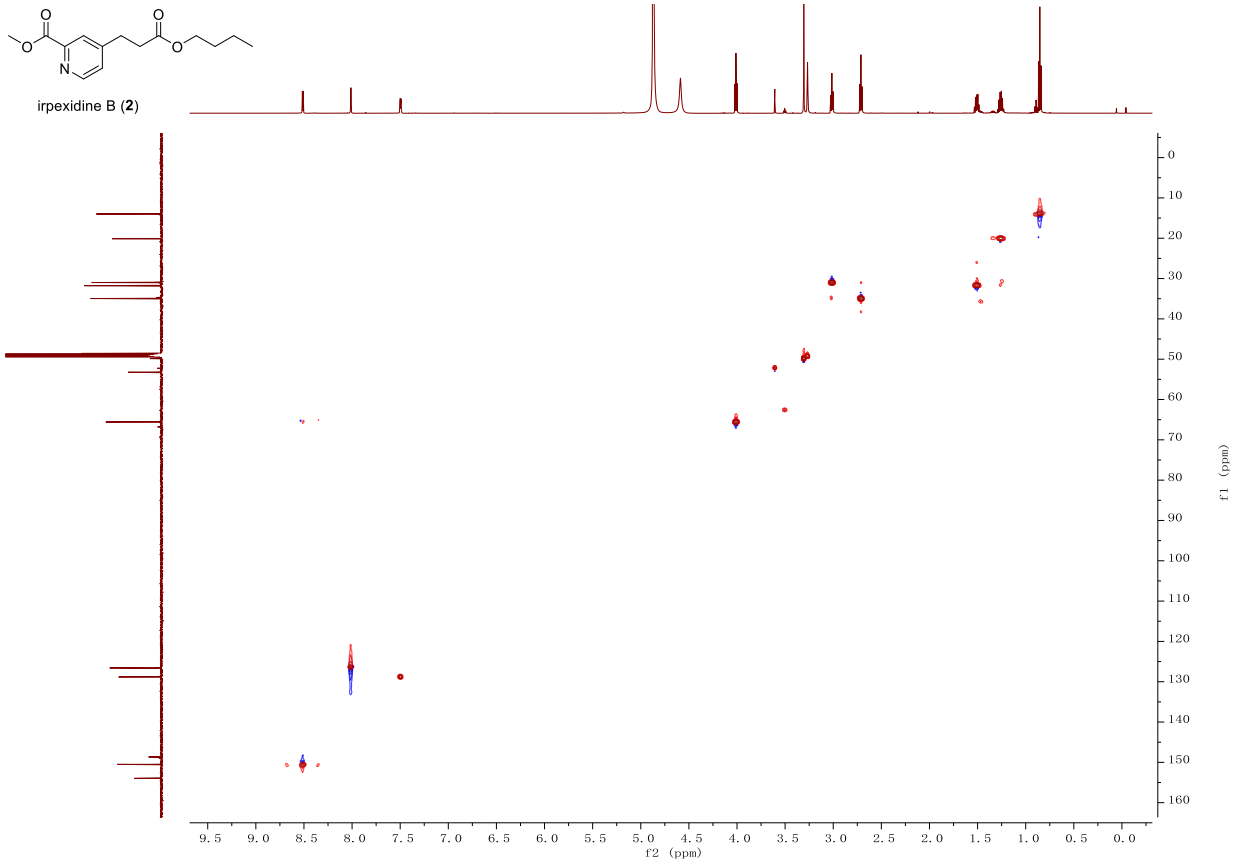

Figure S11. HMBC spectrum of irpexidine B (**2**)

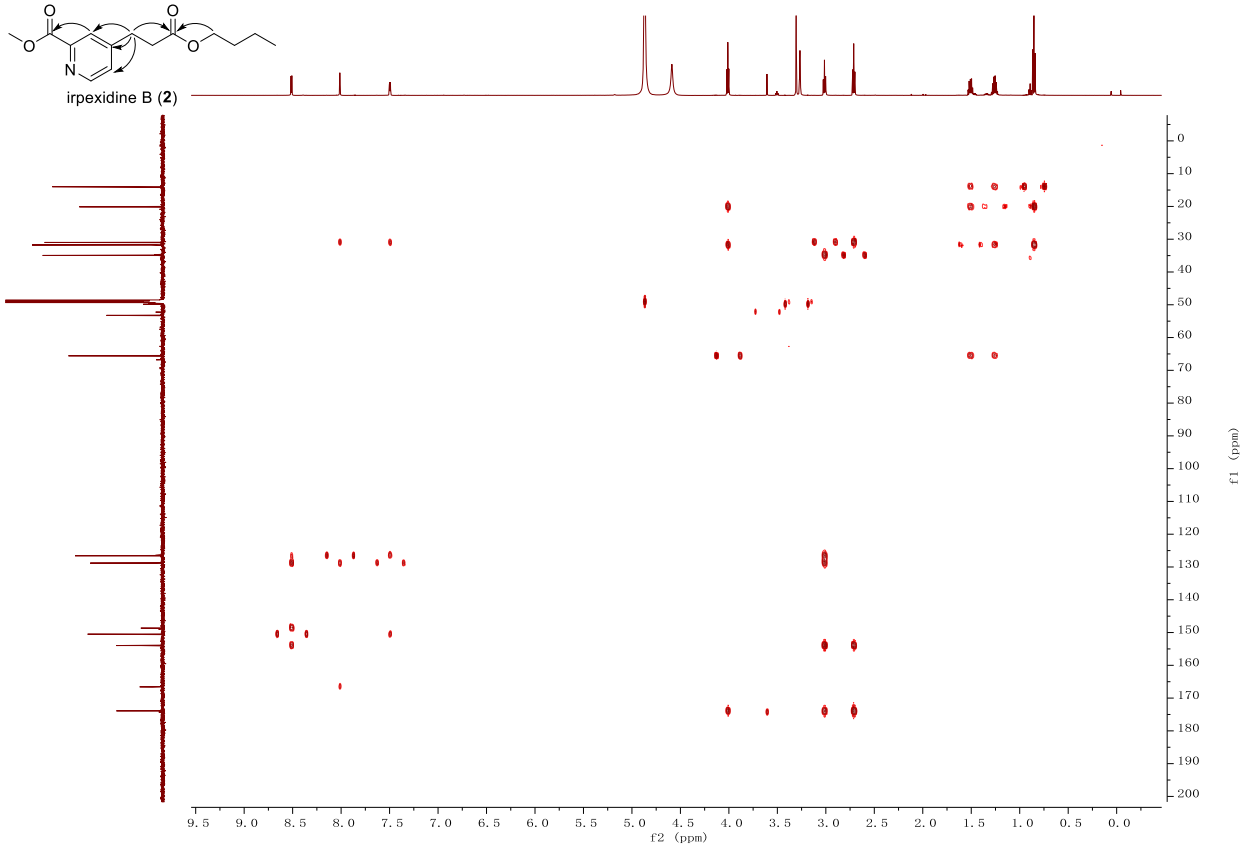

Figure S12. COSY spectrum of irpexidine B (**2**)

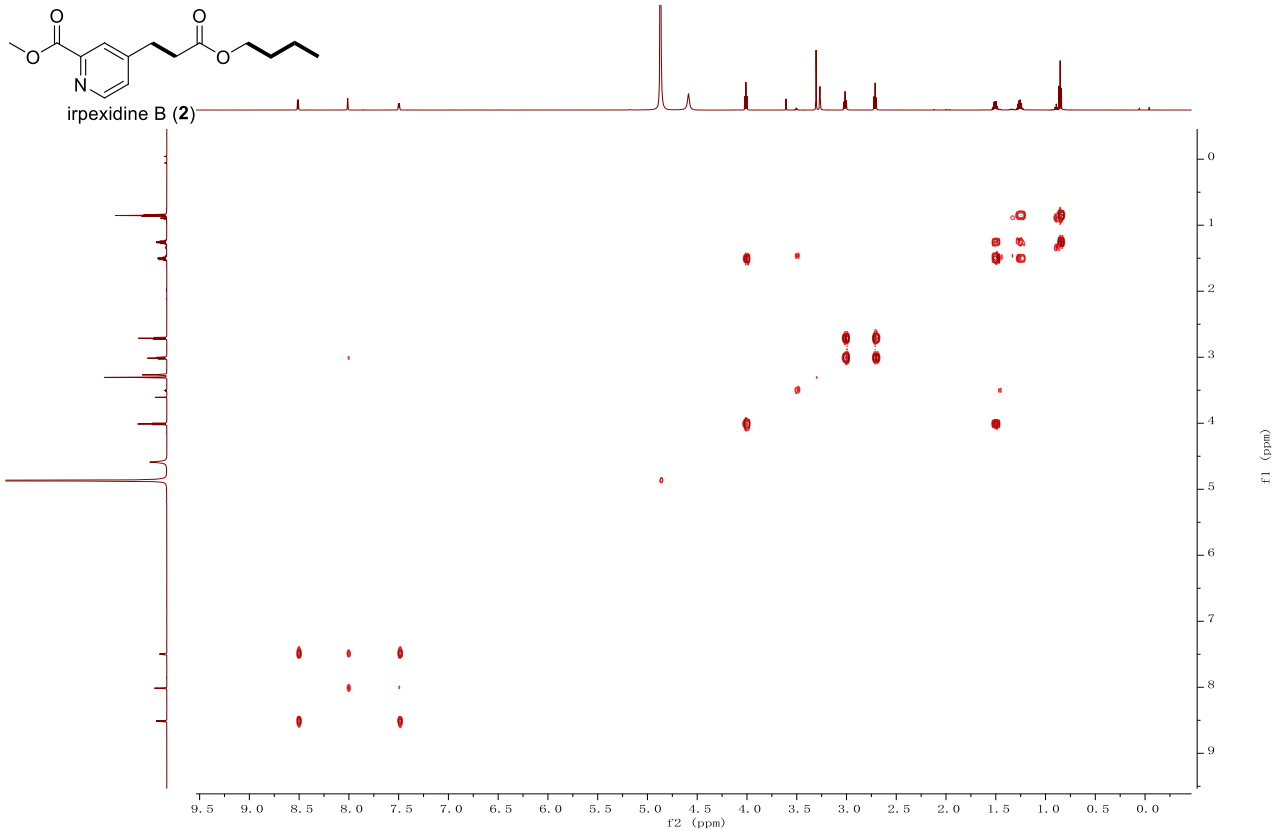

Figure S13. ROESY spectrum of irpexidine B (**2**)

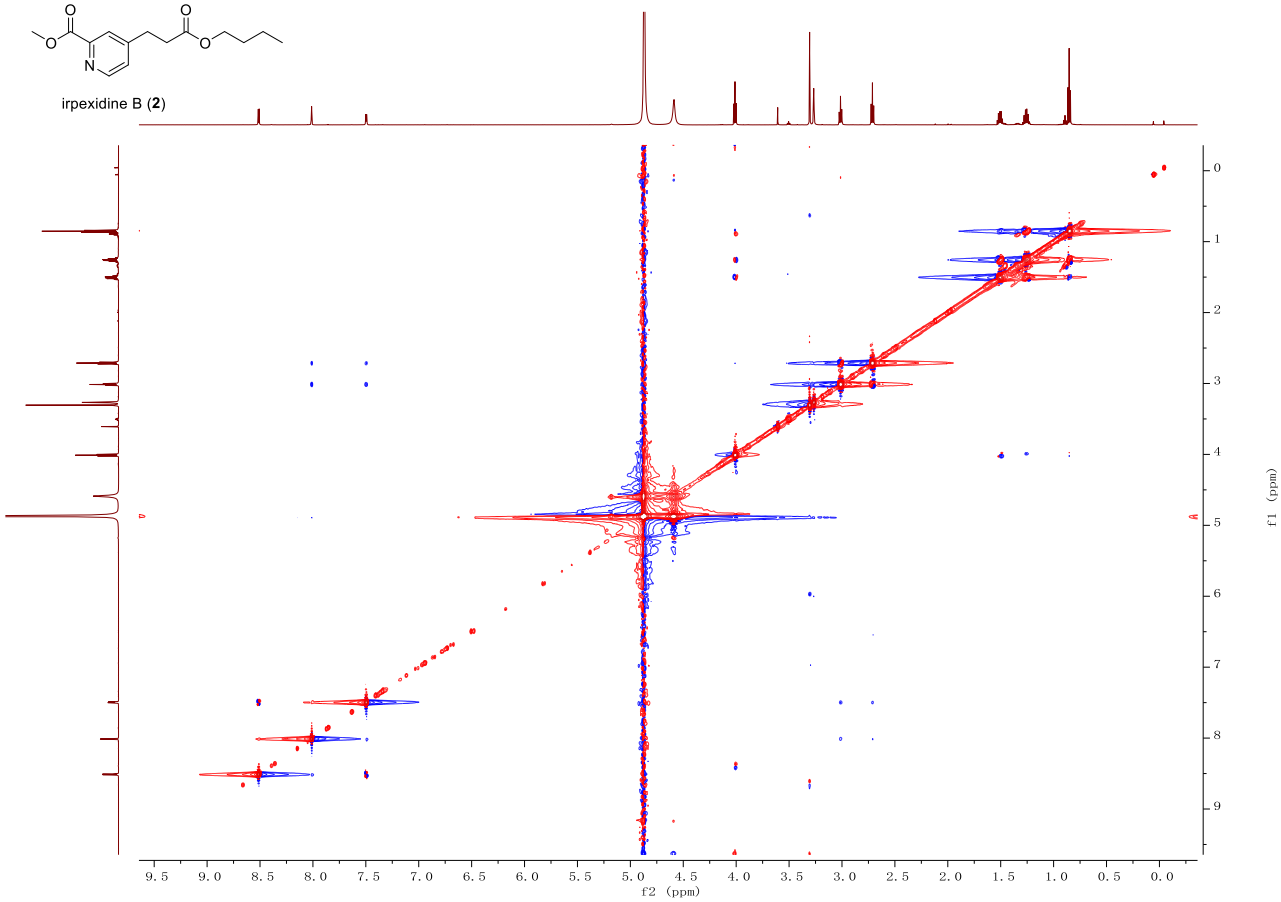

Figure S14. HR-ESI-MS of irpexidine B (**2**)

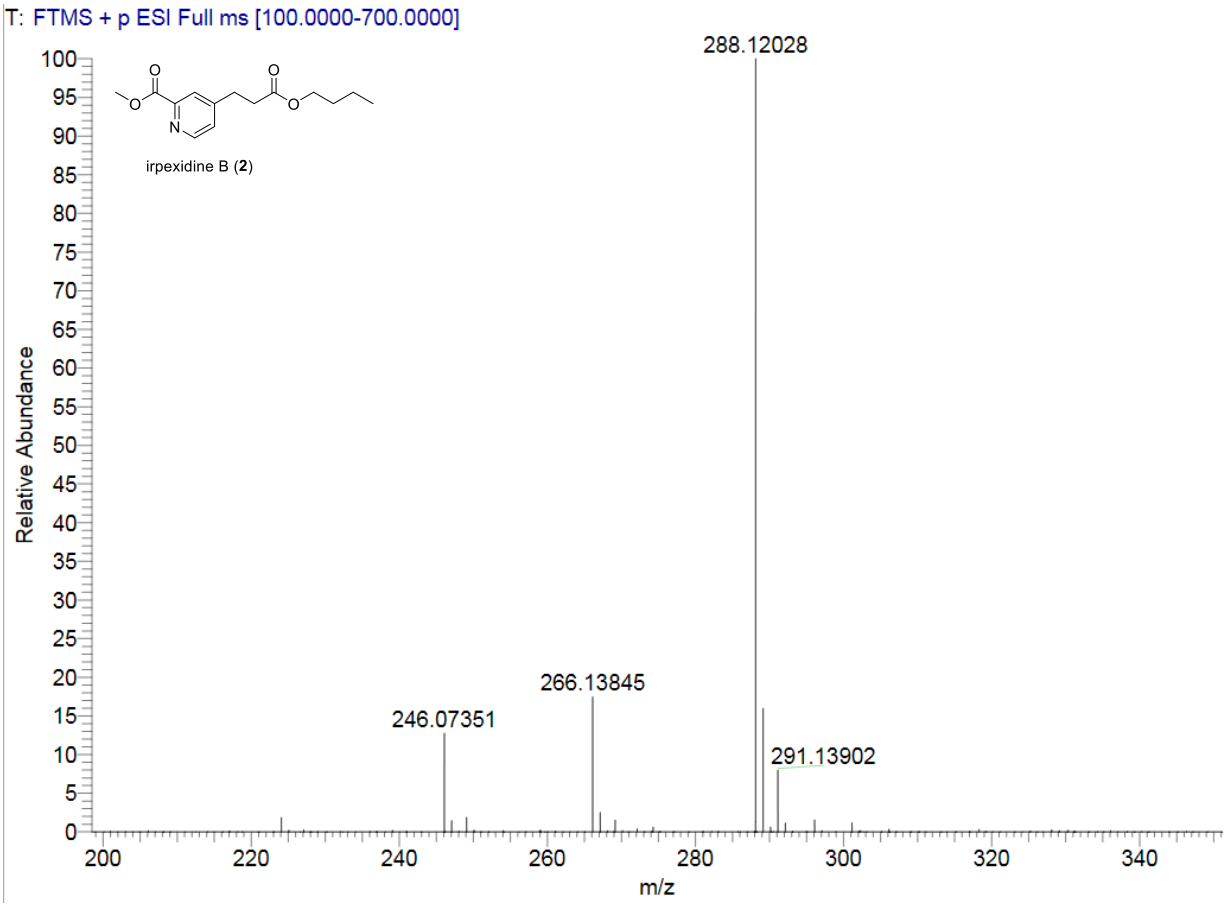

Figure S15. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of irpexin K (**3**)

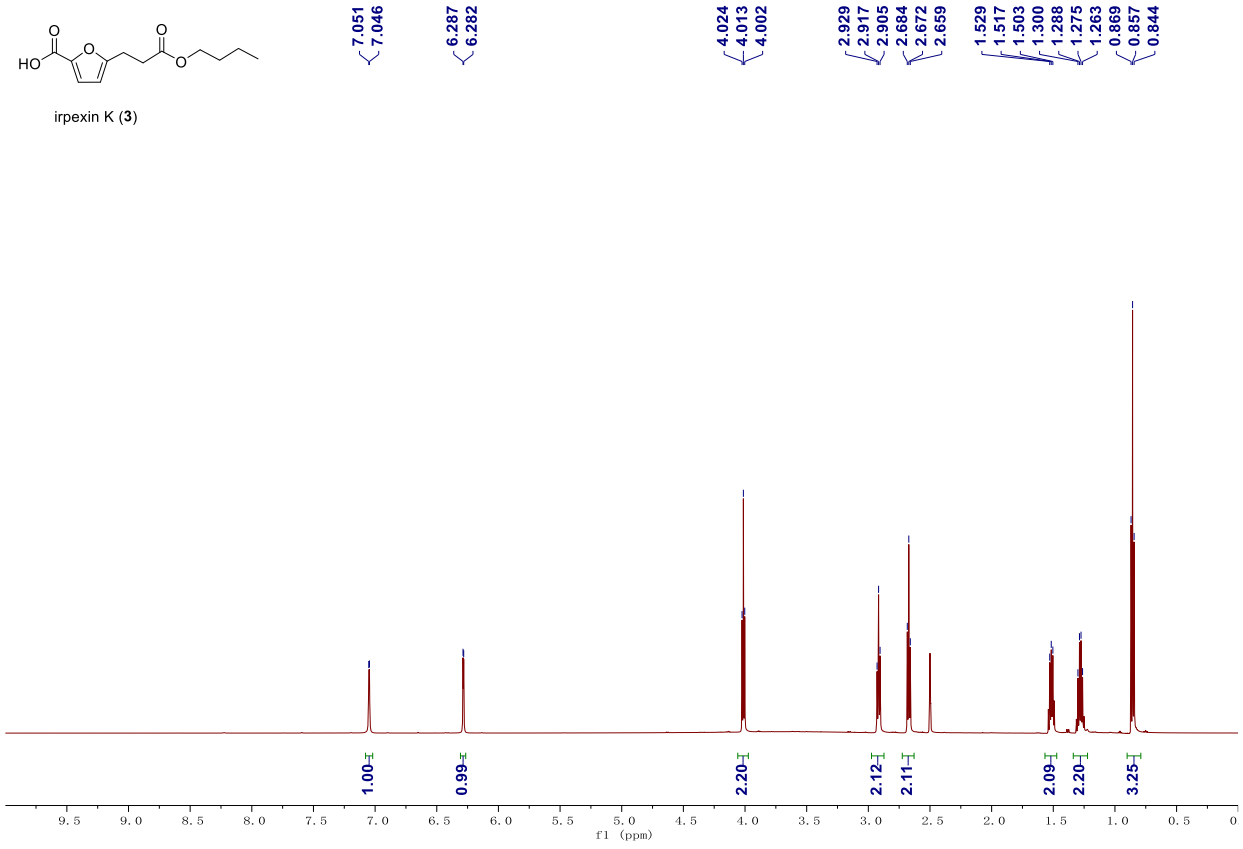

Figure S16. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of irpexin K (**3**)

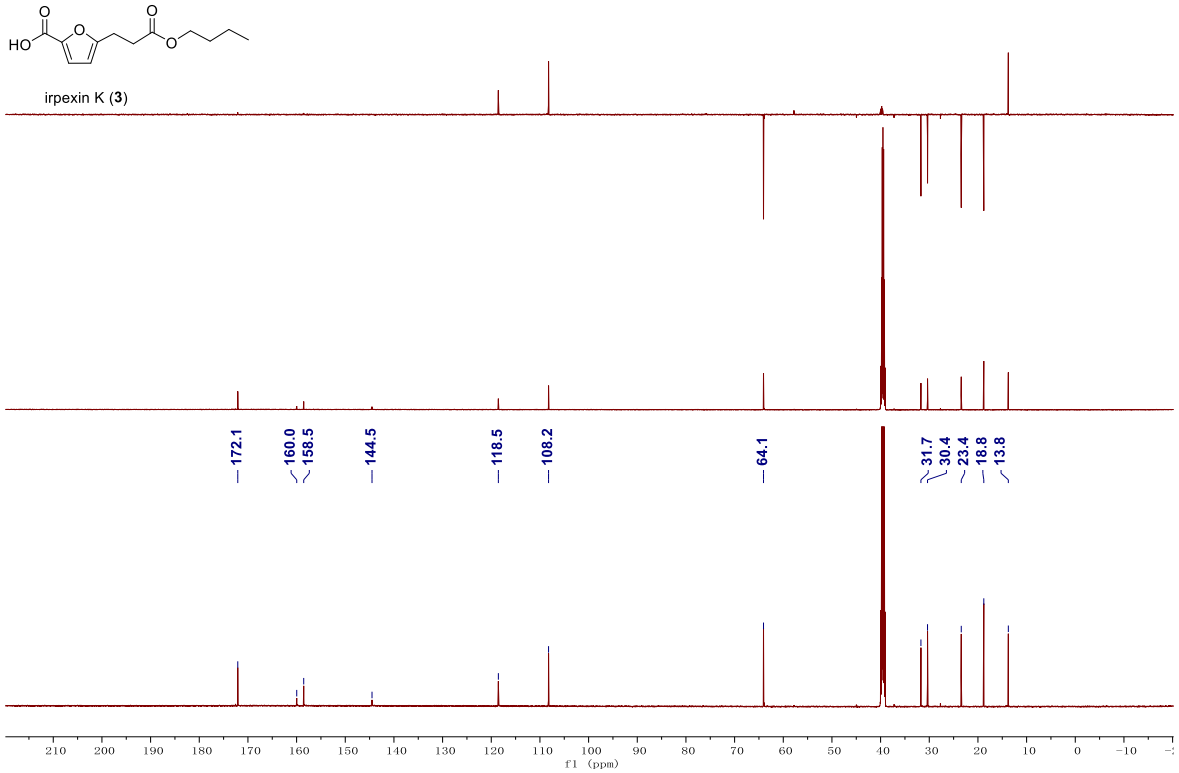

Figure S17. HSQC spectrum of irpexin K (**3**)

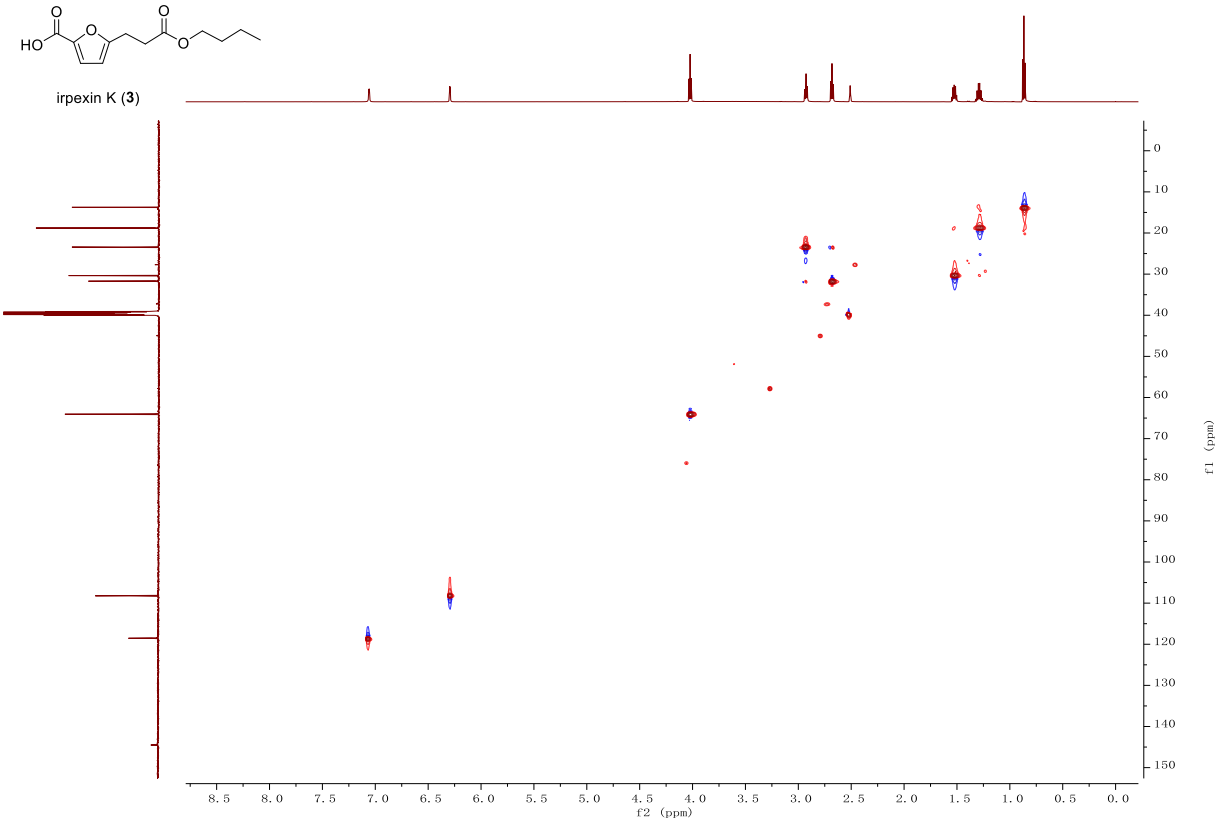

Figure S18. HMBC spectrum of irpexin K (**3**)

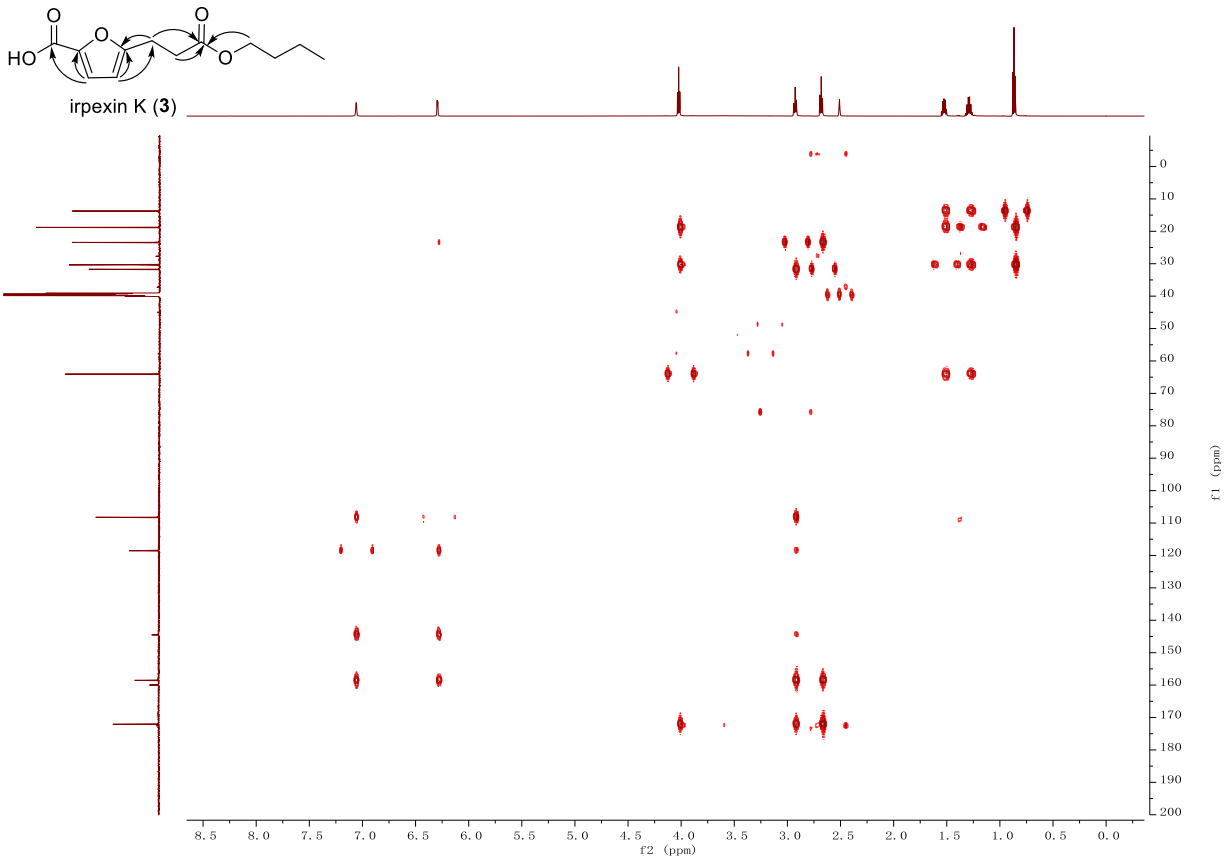

Figure S19. COSY spectrum of irpexin K (**3**)

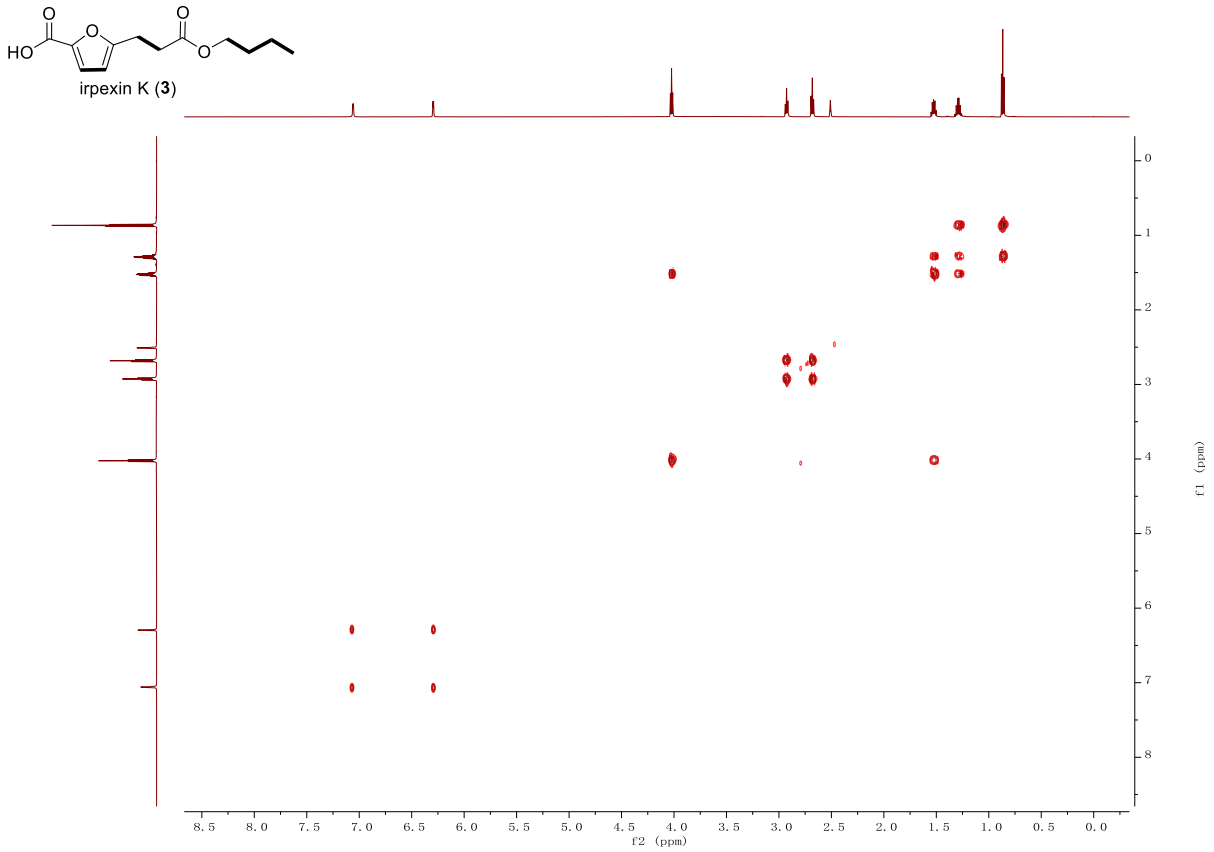

Figure S20. ROESY spectrum of irpexin K (**3**)

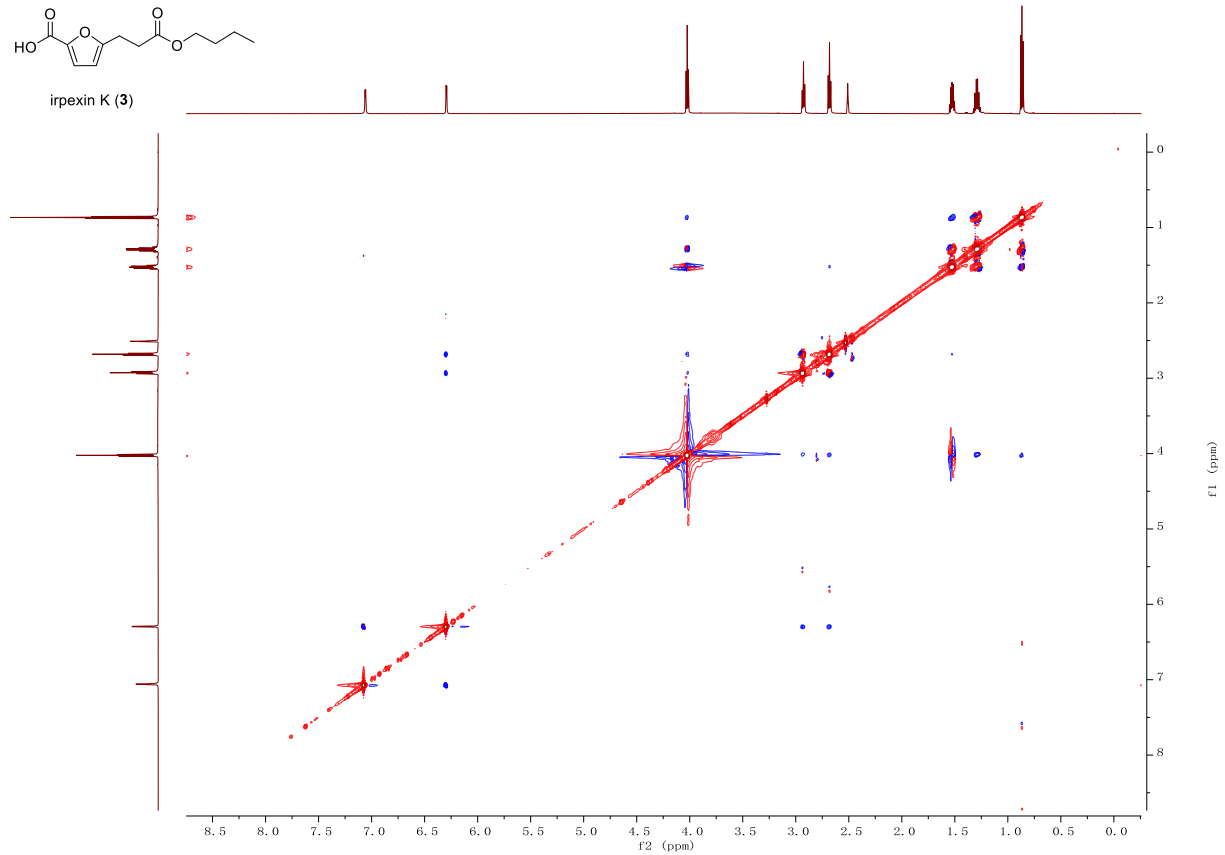

Figure S21. HR-ESI-MS of irpexin K (**3**)

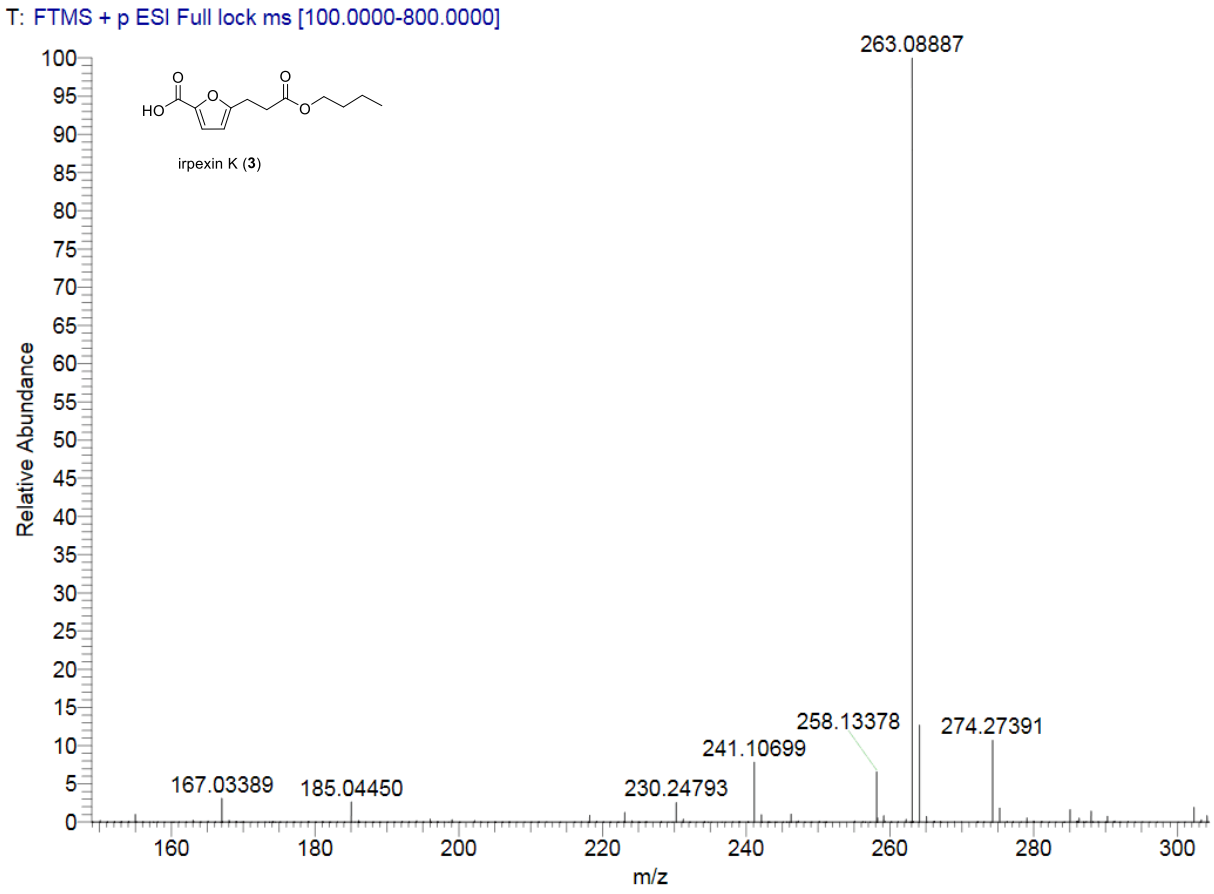

Figure S22. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of irpexin L (**4**)

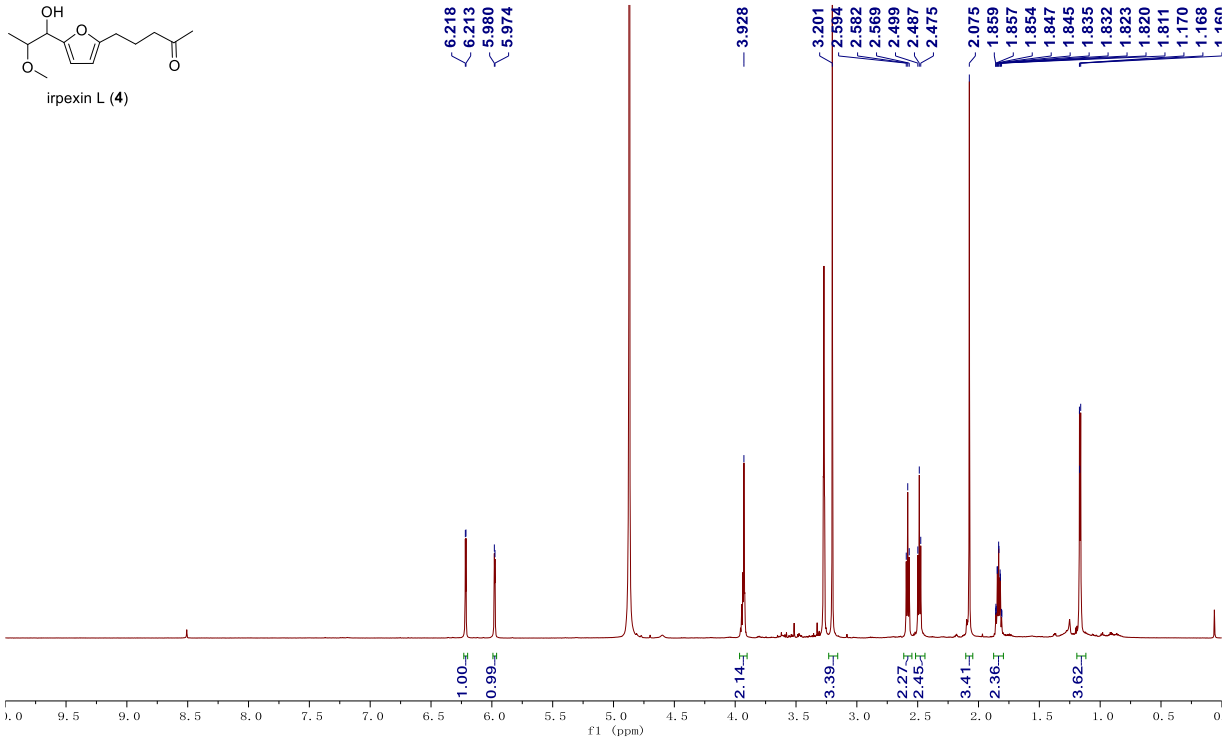

Figure S23. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of irpexin L (**4**)

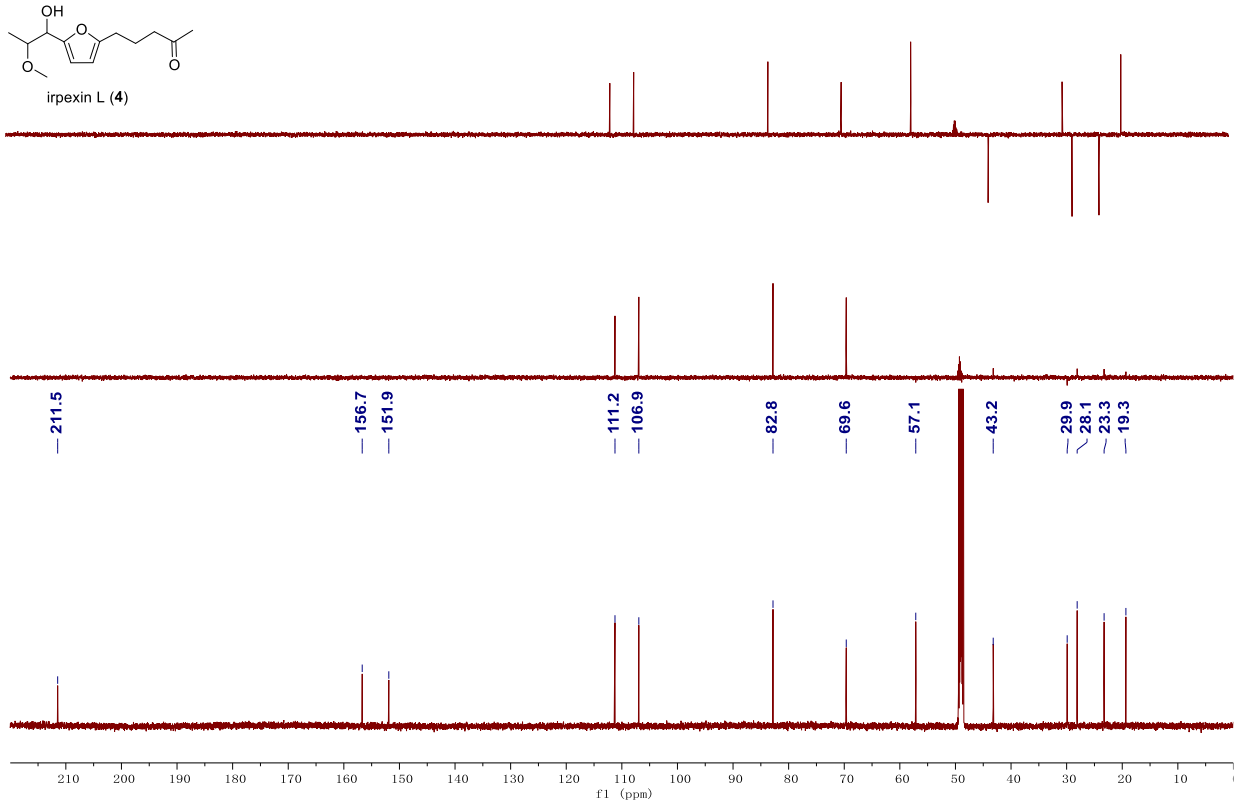

Figure S24. HSQC spectrum of irpexin L (**4**)

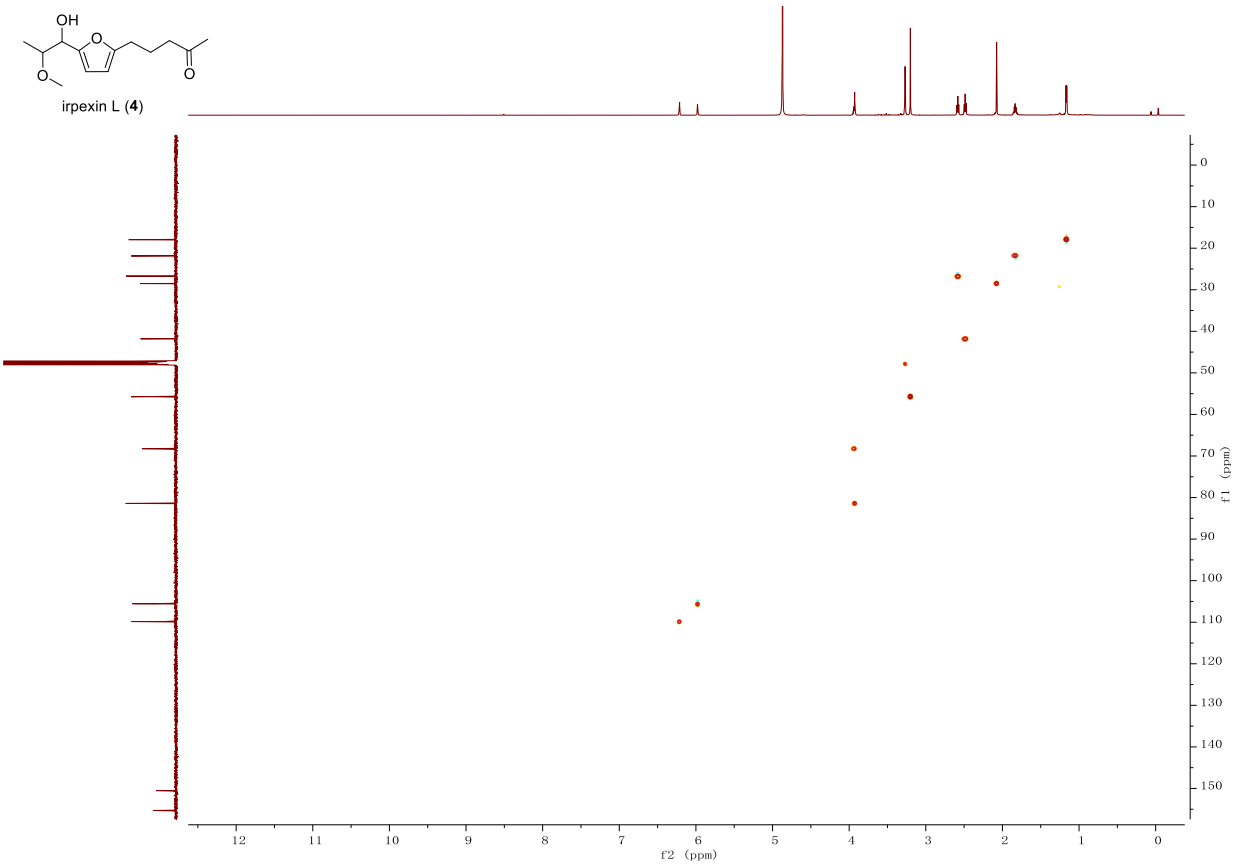

Figure S25. HMBC spectrum of irpexin L (**4**)

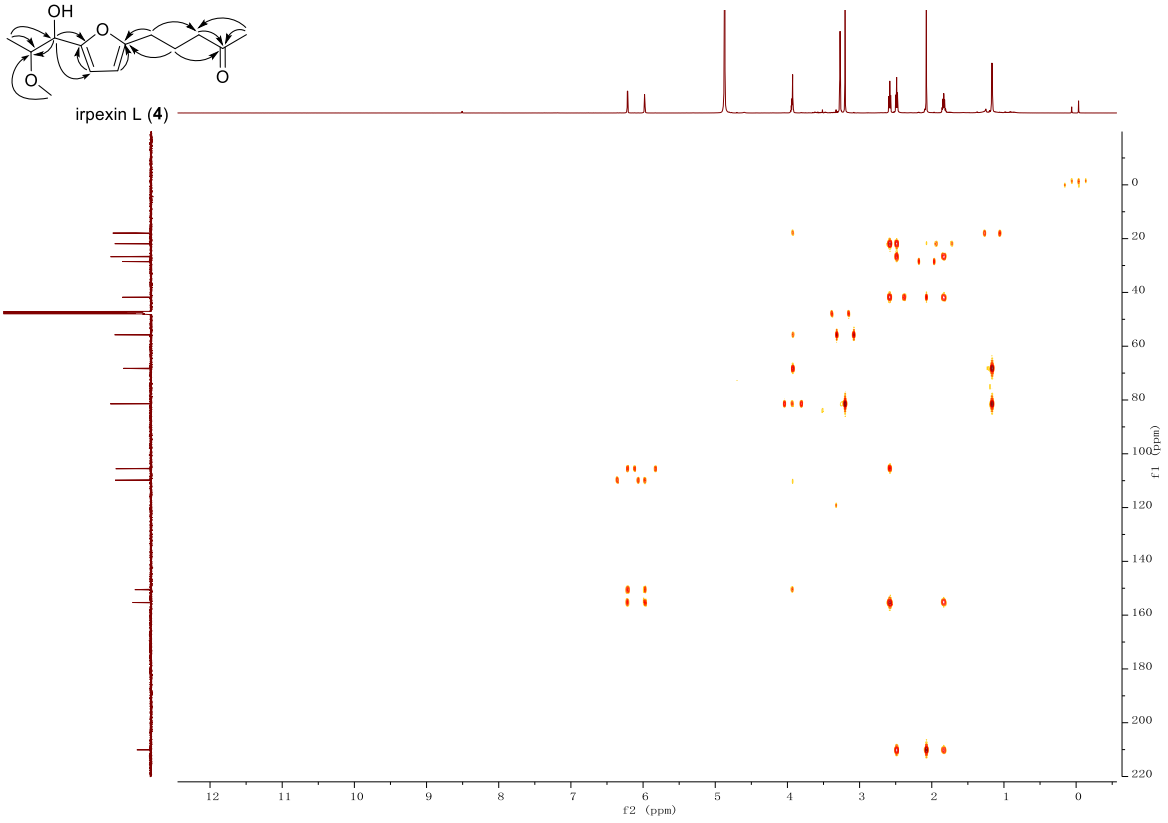

Figure S26. COSY spectrum of irpexin L (**4**)

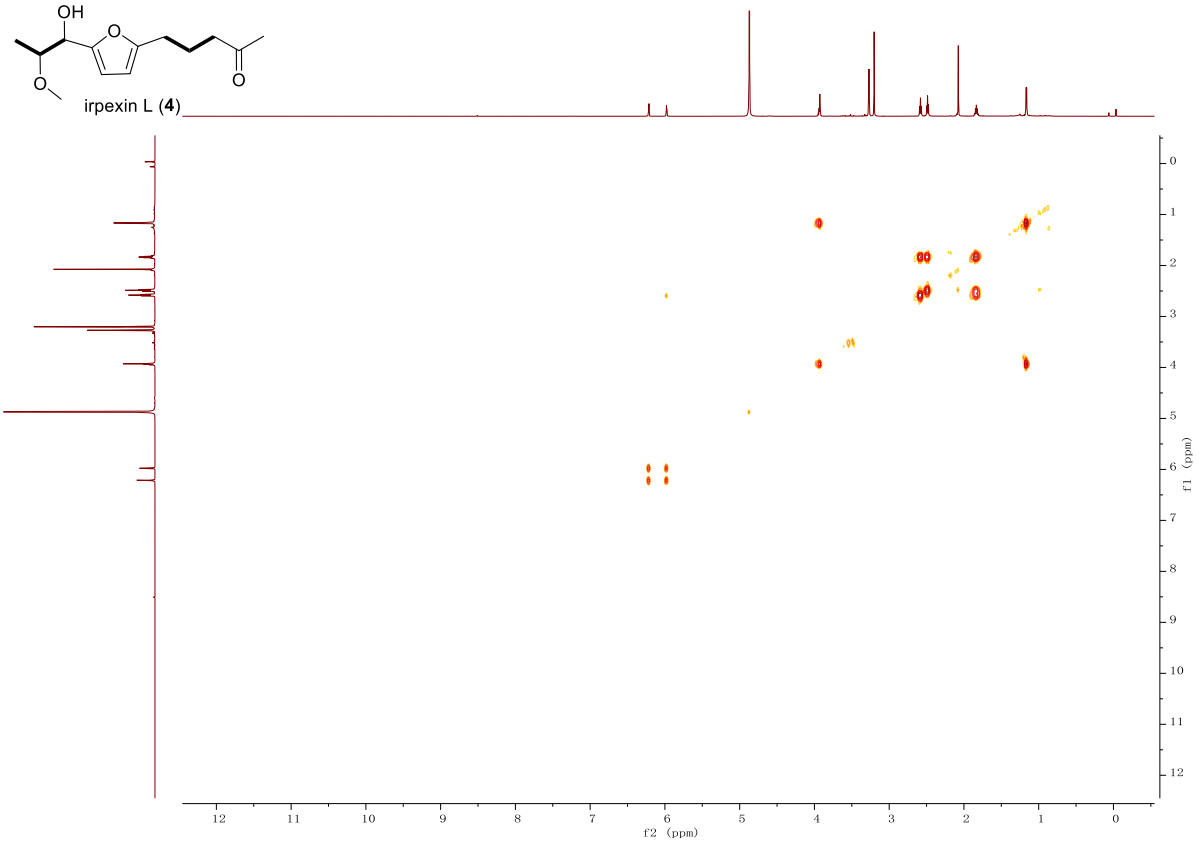

Figure S27. ROESY spectrum of irpexin L (**4**)

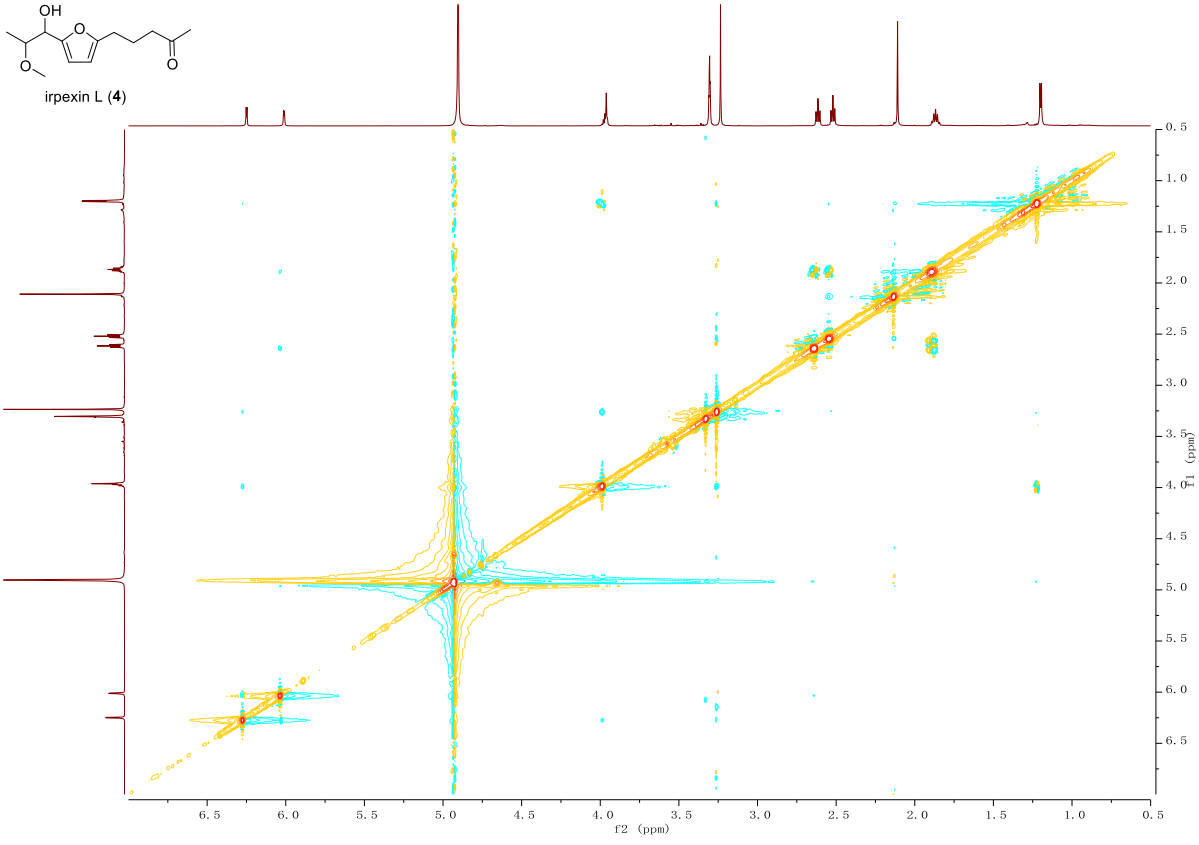

Figure S28. HR-ESI-MS of irpexin L (**4**)\