Supporting Information

Meliacarpinin-type limonoids from the bark of *Melia toosendan* Yalin Hu^{2†}, Li Heng^{1†}, Rong Xu¹, Junhe Li², Shanshan Wei², Deran Xu², Jun Luo², Yi Li¹*

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Figure S31. The NO inhibition rate and cell viabilities of toosendane B (2) and toosendane C (3) in different concentration





Elemental Composition Calculator

| Target m/z: | 713.2783 | Result type: | Positive ions | Species: | [M+Na] ⁺ | |
|-------------|----------|---|---------------|----------|---------------------|--|
| Elements: | | C (0-80); H (0-120); O (0-30); Na (0-5) | | | | |
| Ion Formula | | Calculated m/z PPM Error | | ror | | |
| C35H46NaO14 | | | 713.2780 | -0.42 | | |

Figure S2. ¹H NMR (500 MHz, CDCl₃) spectrum of Toosendane A (1)





Figure S4. HSQC spectrum of Toosendane A (1)





Figure S6. ROESY spectrum of Toosendane A (1)



Figure S7. IR spectrum (KBr disc) of Toosendane A (1)



Figure S8. ECD spectra of Toosendane A (1) (in MeOH)







Elemental Composition Calculator

| Target m/z: | 929.3177 | Result type: | Positive ions | Species: | [M+Na] ⁺ | |
|---------------|----------|---|---------------|-----------|---------------------|--|
| Elements: | | C (0-80); H (0-120); O (0-30); Na (0-5) | | | | |
| Ion Formula | | Calculated m/z | | PPM Error | | |
| C45H53F3NaO16 | | | 929.3178 | 0.05 | | |











Elemental Composition Calculator

| Target m/z: | 929.3179 | Result type: | Positive ions | Species: | [M+Na] ⁺ | |
|---------------|----------|---|---------------|-----------|---------------------|--|
| Elements: | | C (0-80); H (0-120); O (0-30); Na (0-5) | | | | |
| Ion Formula | | Calculated m/z | | PPM Error | | |
| C45H53F3NaO16 | | | 929.3178 | -0.13 | | |







Figure S15. HRESIMS spectrum of Toosendane B (2)



Elemental Composition Calculator

| Target m/z: | 697.2834 | Result type: | Positive ions | Species: | [M+Na] ⁺ | |
|-------------|----------|---|---------------|----------|---------------------|--|
| Elements: | | C (0-80); H (0-120); O (0-30); Na (0-5) | | | | |
| Ion Formula | | Calculated m/z PPM Error | | ror | | |
| C35H46NaO13 | | | 697.2831 | -0.44 | | |







Figure S18. HSQC spectrum of Toosendane B (2)



Figure S19. HMBC spectrum of Toosendane B (2)



Figure S20. ROESY spectrum of Toosendane B (2)



Figure S21. IR spectrum (KBr disc) of Toosendane B (2)



Figure S22. ECD spectra of Toosendane B (2) (in MeOH)







Elemental Composition Calculator

| Target m/z: | 683.2673 | Result type: | Positive ions | Species: | [M+Na] ⁺ | |
|-------------|----------|---|---------------|----------|---------------------|--|
| Elements: | | C (0-80); H (0-120); O (0-30); Na (0-5) | | | | |
| Ion Formula | | Calculated m/z | | PPM Er | PPM Error | |
| C34H44NaO13 | | | 683.2674 | 0.12 | | |

Figure S24. ¹H NMR (500 MHz, CDCl₃) spectrum of Toosendane C (3)





Figure S26. HSQC spectrum of Toosendane C (3)





Figure S27. HMBC spectrum of Toosendane C (3)

Figure S28. ROESY spectrum of Toosendane C (3)





Figure S29. IR spectrum (KBr disc) of Toosendane C (3)

Figure S30. ECD spectra of Toosendane C (3) (in MeOH)





Figure S31. The NO inhibition rate and cell viabilities of toosendane B (2) and toosendane C (3) in different concentration