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Sesquiterpenes and lignans from the flower buds of Daphne genkwa and their nitric oxide inhibitory activities

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Abstract: Chemical investigation of the Daphne genkwa has led to the isolation of four sesquiterpenes (1a/1b, 2, and 3), including one pair of sesquiterpene enantiomers (1a/1b). 1a is a new compound (+)-4-Hydroxy-10-epirotundone, and twelve lignans (4–15). Their structures were elucidated by spectroscopic analysis, and the absolute configurations of 1a/1b were determined by CD analysis. All compounds were examined for their inhibitory effects on the nitric oxide (NO) production induced by lipopolysaccharide (LPS) in BV-2 microglial cells, and compounds 7–10 exhibited pronounced inhibition on NO production with IC\textsubscript{50} values in the range of 5.8–10.2 \mu M, being more active than the positive control, quercetin (IC\textsubscript{50} = 17.0 \mu M).

Keywords: Daphne genkwa; Sesquiterpene; Lignan; Nitric Oxide
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T: FTMS + p ESI Full ms [220.00-850.00]
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Figure S19. $^{13}$C NMR (600 MHz, CDCl$_3$) spectrum of 5

- 87.1
- 74.1
- 63.8
- 61.9
- 56.6
- 56.4
Figure S20. $^1$H NMR (150 MHz, CDCl$_3$) spectrum of 6
Figure S21. $^{13}$C NMR (150 MHz, CDCl$_3$) spectrum of 6
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Figure S25. $^1$C NMR (150 MHz, CDCl$_3$) spectrum of 8

90  100  110  120  130  140  150  160  170  180

$\delta$ (ppm)
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Figure S27. $^{13}$C NMR (150 MHz, CDCl$_3$) spectrum of 9.
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Figure S33. $^{13}$C NMR (150 MHz, CDCl$_3$) spectrum of 12

149.0 147.1 135.8 133.6 122.2 119.8 116.2 116.0 113.5 110.7

-84.1 -73.5 -60.5 -56.4 -54.1 -43.9 -33.7

$\delta$ (ppm)
Figure S34. $^1$H NMR (600 MHz, CDCl$_3$) spectrum of 13
Figure S35. $^{13}$C NMR (150 MHz, CDCl$_3$) spectrum of 13
Figure S36. $^1$H NMR (600 MHz, CDCl$_3$) spectrum of 14
Figure S37. $^{13}$C NMR (150 MHz, CDCl$_3$) spectrum of 14

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