Computer-aided discovery, validation and mechanistic characterisation of novel neolignan activators of PPARgamma

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Compounds identification

NMR spectra were recorded on a BRUKER Avance300 spectrometer operating at 300MHz (^{1}H) and 75MHz (^{13}C) respectively using $CDCl_3$ as solvent. Chemical shifts are given in δ-values [ppm] referenced to the solvent (δ=7.26 and 77.16 respectively). Assignments are based on HSQC (edited), HMBC and COSY spectra. HRMS data were recorded on a Bruker MicrOTOF QII.

Dieugenol

^{1}H-NMR (300 MHz, $CDCl_3$, δ , ppm): 6.759, 2H, d, J=1.9, H-6; 6.731, 2H, d, J=1.9, H-4; 6.025, 2H, s, HO; 5.987, 2H, m, H-8; 5.118 and 5.071, 4H, m, H_2C(9); 3.371, 6H, s, H_3CO; 3.371, 4H, br d, J=6.7, H_2C(7).

^{13}C-NMR (75 MHz, $CDCl_3$, δ , ppm): 147.3, s, C(3); 141.02, s, C(2); 137.78, d, C(8); 132.05, s, C(5); 124.52, s, C(1); 123.23, d, C(6); 115.86, t, C(9); 110.80, d, C(4); 56.21, q, CH_3O; 40,11, t, C(7) (Ogata et al., 2005).

HR ESIMS (neg. modus): *m/z* 325.15036 $[M-H]^-$ (calculated for $C_{20}H_{21}O_4^-$ 325.14453); (pos. modus): *m/z* 349.13566 $[M+Na^+]^+$ (calculated for $C_{20}H_{22}NaO_4^+$ 349.14103).

Tetrahydrodieugenol

^{1}H-NMR (300 MHz, $CDCl_3$, δ , ppm): 6.754, 2H, d, J=2.0, H-6: 6.730, 2H, d, J=1.9, H-4; 6.026, 2H, s, HO; 3.923, 6H, s, H_3CO; 2.569, 4H, t, J=7.7, H_2C(7); 1.660, 4H, m, H_2C(8); 0.968, 6H, t, J=7.3, H_3C(9).

^{13}C-NMR (75 MHz, $CDCl_3$, δ , ppm): 147.27, s, C(3); 140.68, s, C(2); 134.80, d, C(5); 124.61, s, C(1); 123.13, d, C(6); 110.81, d, C(4); 56.22, q, CH_3O; 38.02, t, C(7); 24.89, t, C(8); 14.02, q, C(9).

HR ESIMS (neg. modus): *m/z* 329.18312 $[M-H]^-$ (calculated for $C_{20}H_{25}O_4^-$ 329.17583); (pos. modus): *m/z* 353.16211 $[M+Na^+]^+$ (calculated for $C_{20}H_{26}NaO_4^+$ 353.17233); *m/z* 683.33093 $[2M+Na^+]^+$ (calculated for $C_{40}H_{52}NaO_8^+$ 683.35544).

Magnolol

^{1}H-NMR (300 MHz, $CDCl_3$, δ , ppm): 7.134, 2H, dd, J=8.2, J=2.1, , H-4; 7.085, 2H, d, J=1.9, H-6; 6.952, 2H, d, J=8.2, H-3; 5.973, 2H, tdd, J=16.8, J=10.0, J=6.7, H-8, 5.557, 2H, s, OH; 5.094, 4H, m, H_2C(9); 3.372, 4H, d, J=6.7, H-7.

^{13}C-NMR (75 MHz, $CDCl_3$, δ , ppm): 151.12, s, C(2); 137.48, s, C(8); 133.21, s, C(5); 131.18, s, C(6); 129.97, s, C(4); 123.70, s, C(1); 116.64, s, C(3); 115.81, s, C(9); 39.32, s, C(7).(Yahara et al., 1991)

HR ESIMS (neg. modus): *m/z* 265.13150 $[M-H]^-$ (calculated for $C_{18}H_{17}O_2^-$ 265.12340); (pos. modus): *m/z* 289.11387 $[M+Na^+]^+$ (calculated for $C_{18}H_{18}NaO_2^+$ 289.11990).

References

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