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Integracides: Tetracyclic Triterpenoids from *Fusarium* sp. – Their 5-Lipoxygenase Inhibitory Potential and Structure-activity Relation Using In Vitro and Molecular Docking Studies

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Integracide B (**2**): ^{1}H NMR (DMSO-d_6, 850 MHz): δ_H 2.26 (dd, J = 12.8, 4.3 Hz, H1), 3.74 (td, J = 10.2, 4.3 Hz, H2), 3.57 (d, J = 10.2 Hz, H3), 1.07 (dd, 12.7, 2.6 Hz, H5), 1.67 (m, H6A), 1.56 (m, H6B), 2.30 (m, H7A), 2.19 (m, H7B), 4.07 (d, J = 2.6 Hz, H11), 4.95 (brs, H12), 5.50 (brs, H15), 2.33 (m, H16A), 1.99 (m, H16B), 1.84 (dt, J = 11.1, 8.5 Hz, H17), 1.19 (s, H18), 0.99 (s, H19), 1.58 (m, H20), 0.84 (d, J = 6.0 Hz, H21), 1.51 (m, H22A), 1.10 (m, H22B), 2.05 (m, H23A), 1.87 (m, H23B), 2.18 (m, H25), 0.97 (d, J = 6.6 Hz, H26), 0.97 (d, J = 6.6 Hz, H27), 4.70 (brs, H28A), 4.65 (brs, H28B), 0.75 (s, H29), 0.95 (s, H30), 2.00 (s, H32), 5.31 (brs, 2OH), 5.39 (d d, J = 6.0 Hz, 11OH); ^{13}C NMR (DMSO-d_6, 214 MHz): δ_C 43.4 (C1), 66.8 (C2), 88.0 (C3), 39.5 (C4), 50.3 (C5), 17.7 (C6), 26.2 (C7), 123.8 (C8), 139.4 (C9), 37.2 (C10), 67.4 (C11), 77.7 (C12), 46.4 (C13), 147.0 (C14), 120.2 (C15), 34.8 (C16), 48.5 (C17), 22.6 (C18), 16.6 (C19), 32.7 (C20), 17.9 (C21), 33.9 (C22), 30.4 (C23), 155.7 (C24), 33.1 (C25), 21.8 (C26), 21.7 (C27), 106.5 (C28), 17.4 (C29), 28.6 (C30), 169.8 (C31), 21.0 (C32).

Integracide F (**3**): ^{1}H NMR ($CDCl_3$, 850 MHz): δ_H 2.23 (m, H1), 3.76 (ddd, J = 11.4, 10.1, 4.0 Hz, H2, H2), 3.59 (d, J = 10.1 Hz, H3), 1.70 (dd, J = 11.9, 3.1 Hz, H5), 1.69 (m, H6A), 1.60 (m, H6B), 2.32 (m, H7A), 2.20 (m, H7B), 4.09 (brs. H11), 4.97 (d, J = 2.1 Hz, H12), 5.52 (brt, J = 2.5 Hz, H15), 2.39 (m, H16A), 2.00 (m, H16B), 1.83 (dt, J = 10.3, 7.3 Hz, H17), 1.21(s, H18), 0.98 (s, H19), 1.60 (m, H20), 0.86 (d, J = 6.2 Hz, H21), 1.54 (m, H22A), 1.14 (m, H22B), 2.05 (m, H23A), 1.88 (m, H23B), 2.19 (m, H25), 0.99 (d, J = 6.5 Hz, H26), 1.00 (d, J = 6.5 Hz, H27), 4.71 (brs, H28A), 4.66 (brs, H28B), 0.78 (s, H29), 0.96 (s, H30), 2.05 (s, H32), 2.01 (s, H34), 5.32 (brs, 2OH), 5.38 (brs, 11OH); ^{13}C NMR ($CDCl_3$, 214 MHz): δ_C 43.8 (C1), 67.3 (C2), 88.5 (C3), 39.5 (C4), 50.7 (C5), 18.2 (C6), 26.6 (C7), 124.2 (C8), 139.9 (C9), 37.7 (C10), 67.9 (C11), 78.2 (C12), 46.9 (C13), 147.5 (C14), 120.7 (C15),

35.3 (C16), 49.0 (C17), 23.1 (C18), 17.0 (C19), 33.2 (C20), 18.3 (C21), 34.4 (C22), 30.9 (C23), 156.2 (C24), 33.5 (C25), 22.2 (C26), 22.1 (C27), 107.0 (C28), 17.9 (C29), 29.1 (C30), 170.5 (C31), 21.4 (C32), 170.3 (C33), 21.4 (C34).

Integracide G (**4**): ^{1}H NMR ($CDCl_3$, 850 MHz): δ_H 2.27 (m, H1A), 1.06 (m, H1B), 3.76 (ddd, *J* = 11.2, 10.0, 4.0 Hz, H2), 3.59 (d, *J* = 9.5 Hz, H3), 1.12 (dd, *J* = 11.6, 3.2 Hz, H5), 1.69 (m, H6A), 1.60 (m, H6B), 2.32 (m, 7A), 2.08 (m, H7B), 4.10 (brs, H11), 4.98 (brd, *J* = 2.0 Hz, H12), 5.52 (brt, *J* = 2.0 Hz, H15), 2.35 (m, H16A), 2.02 (m, H16B), 1.87 (dt, *J* = 10.6, 7.5 Hz, H17), 1.21 (s, H18), 0.98 (s, H19), 1.61 (m, H20), 0.86 (d, *J* = 6.3 Hz, H21), 1.52 (m, H22A), 1.15 (m, H22B), 2.08 (m, H23A), 1.89 (m, H23B),2.18 (m, H25), 0.99 (d, *J* = 6.5 Hz, H26), 1.00 (d, *J* = 6.5 Hz, H27), 4.72 (brs, H28A), 4.67 (brs, H28B), 0.78 (s, H29), 0.95 (s, H30), 1.98 (s, H32), 2.32 (t, J = 7.2 Hz, H34), 1.17 (m, H35), 1.26–1.22 (m, H36-39), 1.61 (m, H40), 1.25 (m, H41), 3.35 (t, J = 6.8 Hz, H42), 5.33 (brs, 2OH), 5.38 (brs, 11OH); ^{13}C NMR ($CDCl_3$, 214 MHz): δ_C 43.8 (C1), 67.3 (C2), 88.4 (C3), 39.4 (C4), 50.8 (C5), 18.1 (C6), 26.6 (C7), 124.7 (C8), 139.6 (C9), 37.7 (C10), 67.8 (C11), 78.4 (C12), 46.6 (C13), 147.1 (C14), 120.6 (C15), 35.4 (C16), 49.1 (C17), 23.1 (C18), 17.0 (C19), 33.4 (C20), 18.3 (C21), 34.4 (C22), 31.7 (C23), 156.5 (C24), 33.6 (C25), 22.2 (C26), 22.1 (C27), 107.0 (C28), 17.9 (C29), 29.1 (C30), 170.3 (C31), 21.4 (C32), 170.6 (C33), 34.0 (C34), 23.7 (C35), 29.5–29.1 (C36-39), 24.8 (C40), 30.9 (C41), 63.1 (C42).

Integracide H (**5**): ^{1}H NMR (DMSO-d_6, 850 MHz): δ_H 5.50 (brs, H15), 4.95 (brs, H12), 4.70 (brs, H28A), 4.65 (brs, H28B), 4.08 (brs, H11), 3.86 (td, *J* = 10.6, 4.3 Hz, H2), 3.58 (d, *J* = 10.6 Hz, H3), 2.35 (m, H16A), 2.28 (m, H1A), 2.32 (m, H7A), 2.21 (m, H7B), 2.20 (m, H25), 2.08 (m, H23A), 2.00 (m, H16B), 1.95 (s, H32), 1.89 (s, H34), 1.89 (s, H36), 1.87 (m, H23B), 1.85 (dt, *J* = 11.6, 8.5 Hz, H17), 1.82 (m, H6A), 1.63 (m, H-6B), 1.58 (m, H20), 1.51 (m, H22A), 1.20 (s, H18), 1.11 (dd, *J* = 12.6, 2.8 Hz, H5), 1.02 (m, H22B), 1.01 (m, H1B), 0.98 (s, H19), 0.97 (d, *J* = 6.4 Hz, H27), 0.96 (d, *J* = 6.4 Hz, H26), 0.95 (s, H30), 0.84 (d, *J* = 6.4 Hz, H21), 0.74 (s, H29); ^{13}C NMR (DMSO-d_6, 214 MHz): δ_C 43.4 (C1), 66.8 (C2), 88.1 (C3), 39.5 (C4), 50.2 (C5), 17.8 (C6), 26.4 (C7), 123.9 (C8), 139.4 (C9), 39.9 (C10), 67.7 (C11), 77.8 (C12), 46.4 (C13), 147.1 (C14), 120.3 (C15), 35.0 (C16), 48.6 (C17), 22.7 (C18), 16.6 (C19), 32.8 (C20), 17.9 (C21), 33.9 (C22), 30.4 (C23), 155.3 (C24), 172.1 (C33,35), 169.9 (C31), 33.1 (C25), 21.8 (C26), 21.7 (C27), 106.6 (C28), 17.5 (C29), 28.5 (C30), 21.0 (C32), 21.1 (C34,36).

Integracide J (**6**): ^{1}H NMR (DMSO-d_6, 850 MHz): δ_H 2.26 (m, H1A), 1.06 (m, H1B), 3.74 (td, *J* = 10.4, 4.3 Hz, H2), 3.57 (d, *J* = 10.4 Hz, H3), 1.11 (dd, *J* = 12.8, 2.8 Hz, H5), 1.68 (m, H6A), 1.60 (m, H6B), 2.32 (m, H7A), 2.21 (m, H7B), 4.07 (d, *J* = 2.4 Hz, H11), 4.95 (d, *J* = 1.7 Hz, H12), 5.50 (brs, H15), 2.38 (m, H16A), 2.01 (m, H16B), 1.85 (dt, *J* = 11.4, 8.5 Hz, H17), 1.19 (s, H18), 0.98 (s, H19), 1.58 (m, H20), 0.84 (d, *J* = 6.4 Hz, H21), 1.65 (m, H22A), 1.12 (m, H22B), 2.07 (m, H23A), 1.88 (m, H23B), 2.21 (m, H25), 0.96 (d, *J* = 6.6 Hz, H26), 0.99 (d, *J* = 6.6 Hz, H27), 4.70 (d, *J* = 0.9 Hz, H28A), 4.65 (d, *J* = 0.9 Hz, H28B), 0.75 (s, H29), 0.95 (s, H30), 1.96 (s, H32), 7.00 (d, *J* = 8.5 Hz, H35,39), 6.61 (d, *J* = 8.5 Hz, H36,38), 5.31 (s, 2OH), 5.39 (d, *J* = 6.0 Hz, 11OH), 9.13 (s, 37OH); ^{13}C NMR (DMSO-d_6, 214 MHz): δ_C 43.3 (C1), 66.8 (C2), 88.0 (C3), 39.5 (C4), 50.2 (C5), 17.7 (C6), 26.2 (C7), 123.8 (C8), 139.4 (C9), 37.2 (C10), 67.4 (C11), 77.7 (C12), 46.4 (C13), 147.0 (C14), 120.2 (C15), 34.8 (C16), 48.5 (C17), 22.6 (C18), 16.5 (C19), 32.7 (C20), 17.9 (C21), 33.9 (C22), 31.3 (C23), 155.7 (C24), 33.1 (C25), 21.8 (C26), 21.7 (C27), 106.5 (C28), 17.4 (C29), 28.5 (C30), 169.8 (C31), 21.0 (C32), 170.1 (C33), 127.9 (C34), 130.1 (C35,39), 114.8 (C36,38), 155.7 (C39).