

Table 3. Exact mass, molecular formula and adducts obtained using SIRIUS 4.0.1, and results obtained using METLIN and LIPID MAPS databases

Monoisotopic mass	Molecular Formula	Adduct	Potential METLIN assignement	Potential LIPID MAPS assignement
219.1471	$C_{10}H_{21}NO_4$	[M+H] ⁺	NA	NA
415.3086	$C_{26}H_{41}NO_3$	[M+H] ⁺	NA	N-linoleoyl dopamine
431.3036	$C_{26}H_{41}NO_4$	[M+H] ⁺	NA	NA
443.3036	$C_{27}H_{41}NO_4$	[M+H] ⁺	17-phenyl trinor PGF2 α diethyl amide	NA
596.3309	$C_{30}H_{48}N_2O_{10}$	[M+H] ⁺	NA	NA
420.2988	$C_{24}H_{40}N_2O_4$	[M+H] ⁺	NA	NA