

compound name		relative response ratio	ionization mode	nominal molecular mass (Da)	pseudomolecular ion formulation	nominal parent ion (Da)	nominal daughter ion (Da)	capillary (kV)	cone (V)	collision (eV)	standard source
5-(hydroxymethyl)-2'-deoxycytidine	quantifier	0.033	ESI+	257	[M+H] ⁺	258	124	1.2	15	10	Berry & Associates, Dexter, MI, USA
	qualifier		ESI+	257	[M+H] ⁺	258	142	1.2	15	10	
[D ₃]-5-(hydroxymethyl)-2'-deoxycytidine	quantifier	0.031	ESI+	260	[(M+3)+H] ⁺	261	127	1.2	15	10	Toronto Research Chemicals, Toronto, Canada
	qualifier		ESI+	260	[(M+3)+H] ⁺	261	145	1.2	15	10	
5-formyl-2'-deoxycytidine	quantifier	0.182	ESI-	255	[M-H] ⁻	254	121	3.5	28	18	Berry & Associates, Dexter, MI, USA
	qualifier		ESI-	255	[M-H] ⁻	254	138	3.5	28	18	
[¹³ C ₁₀ , ¹⁵ N ₂]-5-formyl-2'-deoxycytidine	quantifier	0.178	ESI-	267	[(M+12)-H] ⁻	266	128	3.5	28	18	own synthesis, see M&M section
	qualifier		ESI-	267	[(M+12)-H] ⁻	266	145	3.5	28	18	
5-carboxy-2'-deoxycytidine	quantifier	0.318	ESI-	271	[M-H] ⁻	270	110	3.5	20	20	Berry & Associates, Dexter, MI, USA
	qualifier		ESI-	271	[M-H] ⁻	270	93	3.5	20	20	
[¹³ C ₁₀ , ¹⁵ N ₂]-5-carboxy-2'-deoxycytidine	quantifier	0.300	ESI-	283	[(M+12)-H] ⁻	282	116	3.5	20	20	own synthesis, see M&M section
	qualifier		ESI-	283	[(M+12)-H] ⁻	282	99	3.5	20	20	
5-(hydroxymethyl)-2'-deoxyuridine	quantifier	1.092	ESI-	258	[M-H] ⁻	257	124	3.5	20	15	Berry & Associates, Dexter, MI, USA
	qualifier		ESI-	258	[M-H] ⁻	257	214	3.5	20	10	
[¹³ C ₁₀ , ¹⁵ N ₂]-5-(hydroxymethyl)-2'-deoxyuridine	quantifier	1.233	ESI-	270	[(M+12)-H] ⁻	269	131	3.5	20	15	own synthesis, see M&M section
	qualifier		ESI-	270	[(M+12)-H] ⁻	269	224	3.5	20	10	
8-oxo-2'-deoxyguanosine	quantifier	0.280	ESI+	283	[M+H] ⁺	284	168	1.2	20	15	Sigma-Aldrich, St. Louis, MO, USA
	qualifier		ESI+	283	[M+H] ⁺	284	140	1.2	20	30	
[¹⁵ N ₅]-8-oxo-2'-deoxyguanosine	quantifier	0.292	ESI+	288	[(M+5)+H] ⁺	289	173	1.2	20	15	Cambridge Isotope Laboratories, Tewksbury, MA, USA
	qualifier		ESI+	288	[(M+5)+H] ⁺	289	145	1.2	20	30	

Table. S2. Transition patterns specific detector settings and sources of standards for analysed compounds (relative response ratio=area under the peak of qualifier ion/ area under the peak of quantifier ion)