A Study of the γ-Radiolysis of Di-dodecyl Di-octyl Diglycolamide (D^3DODGA) Using UHPLC-ESI-MS Analysis.

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Supplementary Material:

Table S1. Source parameters for the Bruker MicrOTOF-QII, optimized for transmission of low *m/z* ions, positive mode.

Parameter	*Value*	*Parameter*	*Value*
Source			
End plate offset	-500 V	Capillary	+4500 V
Nebulizer	0.4 Bar	Dry Gas	9.0 L/min
Dry Temp	220 ^{o}C		
Transfer			
Funnel 1 RF	200 V_{pp}	Funnel 2 RF	200 V_{pp}
ISCID Energy	0 eV	Hexapole RF	100 V_{pp}
Quadrupole			
Ion energy	3 eV	Low mass	100 *m/z*
Collision Cell			
Collision energy	8 eV	Collision RF	100 V_{pp}
Transfer time	70 μs	Pre-pulse storage	50 μs

Table S2: Experimental and theoretical exact mass-to-charge ratio measured using HPLC-APCI-FT-MS for the compounds detected.

Compound	Experimental *m/z* ratio (protonated species)	Detected ion chemical formula	Calculated *m/z* ratio (protonated species)	*m/z* difference [ppm]
$D^3DODGA+H^+$	693.6869	$C_{44}H_{89}N_2O_3^+$	693.6868	0.215
1a	525.4989	$C_{32}H_{65}N_2O_3^+$	525.4990	-0.058
1b	581.5615	$C_{36}H_{73}N_2O_3^+$	581.5616	-0.087
2a	358.2951	$C_{20}H_{40}NO_4^+$	358.2952	-0.349
2b	470.4204	$C_{28}H_{26}NO_4^+$	470.4204	-0.033
3a	242.2842	$C_{16}H_{36}N^+$	242.2842	0.017
3b	354.4094	$C_{24}H_{52}N^+$	354.4094	-0.048
4a	300.2896	$C_{18}H_{38}NO_2^+$	300.2897	-0.453
4b	412.4149	$C_{26}H_{54}NO_2^+$	412.4149	-0.016
5a	284.2948	$C_{18}H_{38}NO^+$	284.2948	-0.075
5b	396.4201	$C_{26}H_{54}NO^+$	396.4200	0.197
6a	270.2791	$C_{17}H_{36}NO^+$	270.2791	-0.190
6b	382.4044	$C_{25}H_{52}NO^+$	382.4043	0.038
2c	526.4831	$C_{32}H_{64}NO_4^+$	526.4830	0.293
2d	386.3265	$C_{22}H_{44}NO_4^+$	386.3265	-0.066
Unknown 1	256.2634	$C_{16}H_{34}NO^+$	256.2635	-0.239
Unknown 2	368.3886	$C_{24}H_{50}NO^+$	368.3887	-0.276

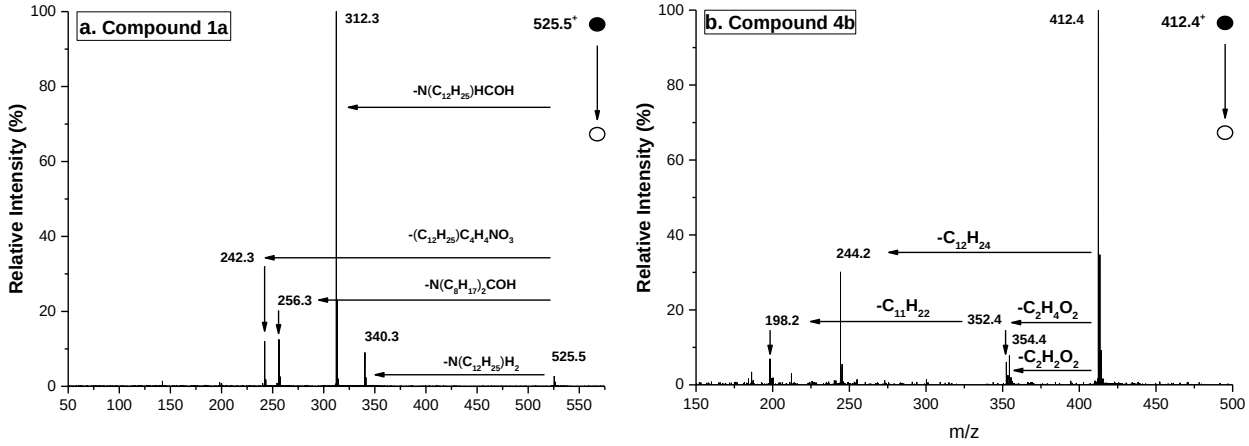


Figure S1: CID spectra of Compounds 1b and 4b.

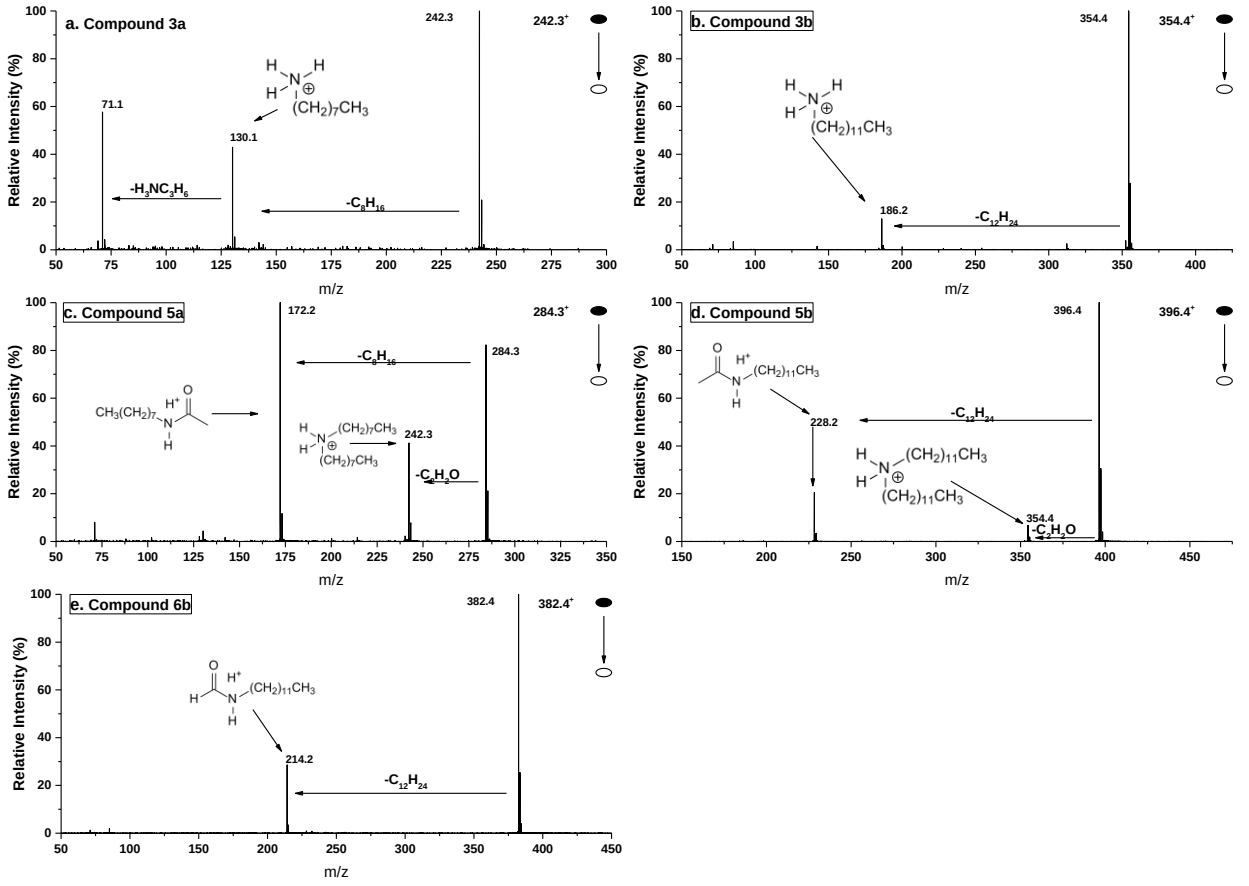
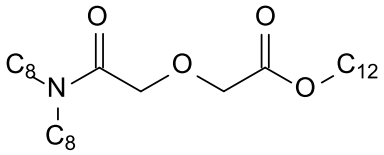
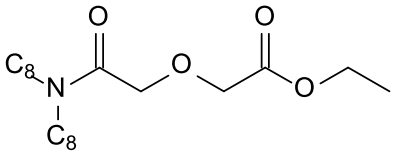


Figure S2: CID spectra of Compounds 3a, 3b, 5a, 5b, and 6b.



Compound 2c
Dodecyl 2-(2-dioctylamino)-2-oxoethoxy) acetate
Monoisotopic MW
525.476



Compound 2d
Ethyl 2-(2-dioctylamino)-2-oxoethoxy) acetate
Monoisotopic MW
385.319

Figure S3: Proposed structures of Compounds 2c and 2d.

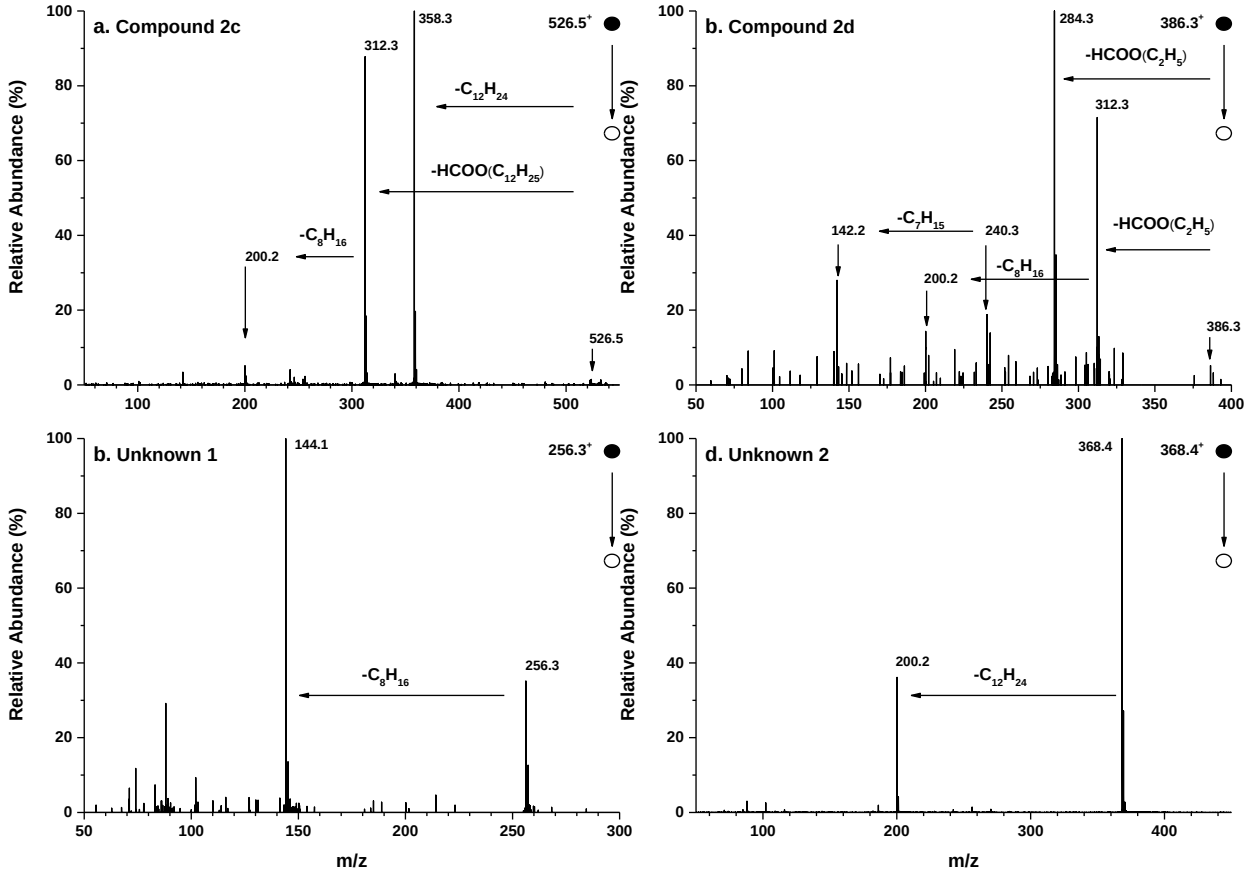


Figure S4: a) CID spectrum of Compound 2c, *m/z* = 526.5; b) CID spectrum of Compound 2d, *m/z* = 386.3; CID spectrum of Unknown 1, *m/z* = 256.3; d) CID spectrum of Unknown 2, *m/z* = 368.4.