Supplementary documents

Effect of Alkyl Chain Length on the Inclusion of Carboxylated Nitroxide Radicals in β- and γ-Cyclodextrins: An EPR Study.

Muhammed ALKALI [a], Alexandru Gabriel BUCUR [a], Adrian FIFERE [b], Ioana MOLEAVIN TURIN [b], Florenta Daniella SAVONEA [a], Victorita TECUCEANU [c] and Gabriela IONITA [a*]

[a] Institute of Physical Chemistry - Ilie Murgulescu, Splaiul Independenței 202, Bucharest, 060021, Romania.

[b] "Petru Poni" Institute of Macromolecular Chemistry, Alea Grigore Ghica Voda 41-A, 700487 Iasi, Romania

[c] "Costin D. Nenițescu" Institute of Organic and Supramolecular Chemistry of the Roumanian Academy, 202B Splaiul Independentei, 060023 Bucharest, Roumania

*Corresponding author: gabi2ionita@yahoo.com

Contents

Pages

1. Figures S1(A-F) Mass spectrometry spectra. 2-4

2. Figure S2 Trends of a_N variation relative to carbon chain length. 5

3. Figure S3 a_N modification upon the formation of an inclusion complex with cyclodextrin. 5

4. Table S1 Complete EPR parameters for all CD concentrations studied. 6

5. Table S2 a_N values for the spin probes in water and in cyclodextrin. 7

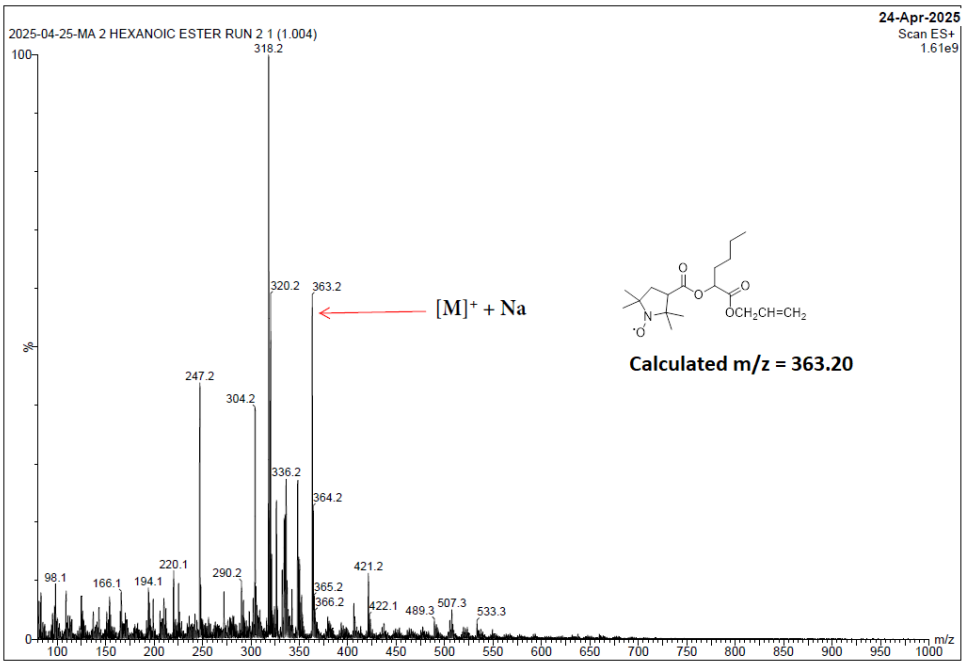

Figure S1A: Mass spectra for the intermediate of compound **1.**

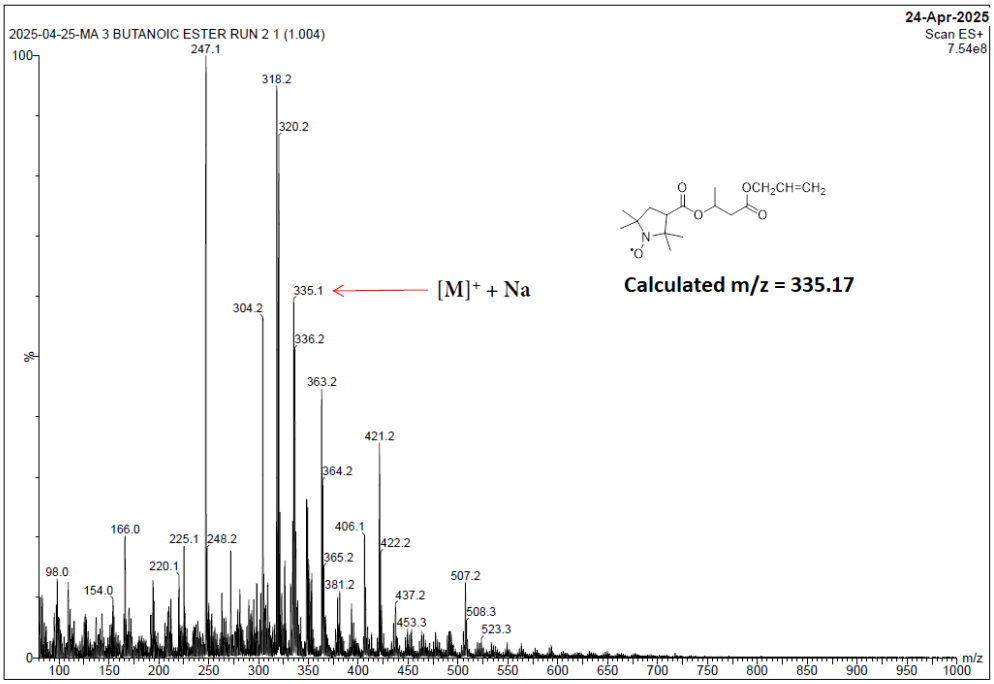

Figure S1B: Mass spectra for the intermediate of compound **2.**

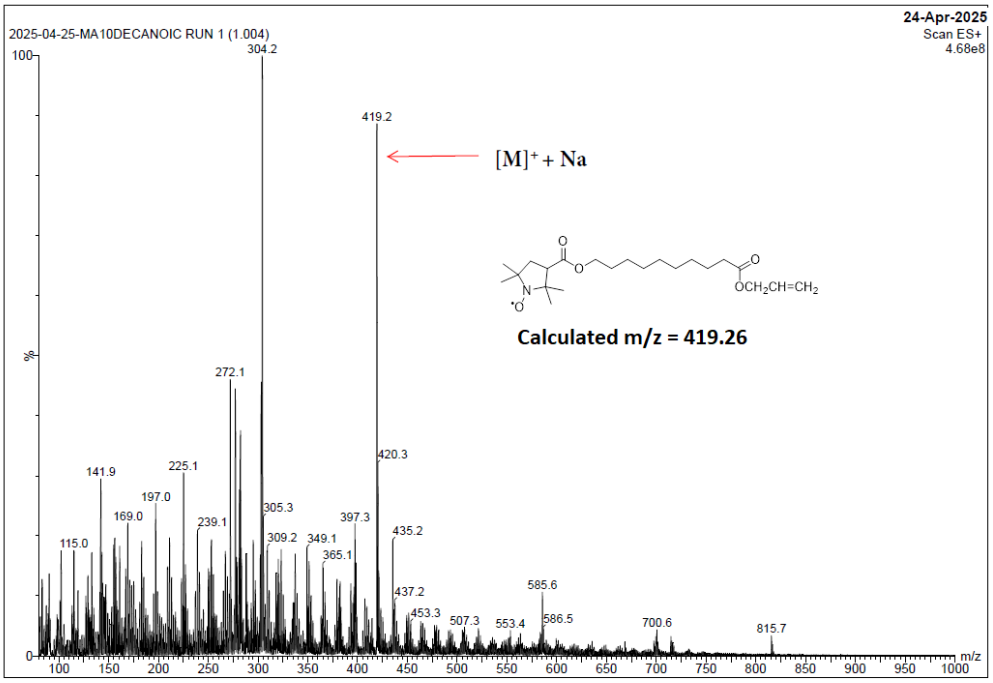

Figure S1C: Mass spectra for the intermediate of compound **3.**

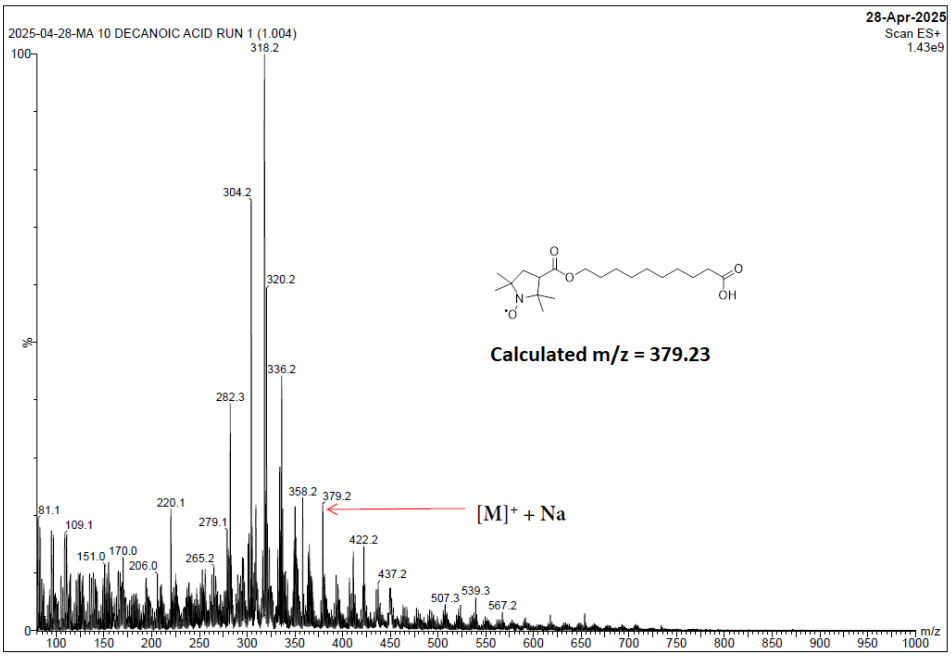

Figure S1D: Mass spectra for compound **3.**

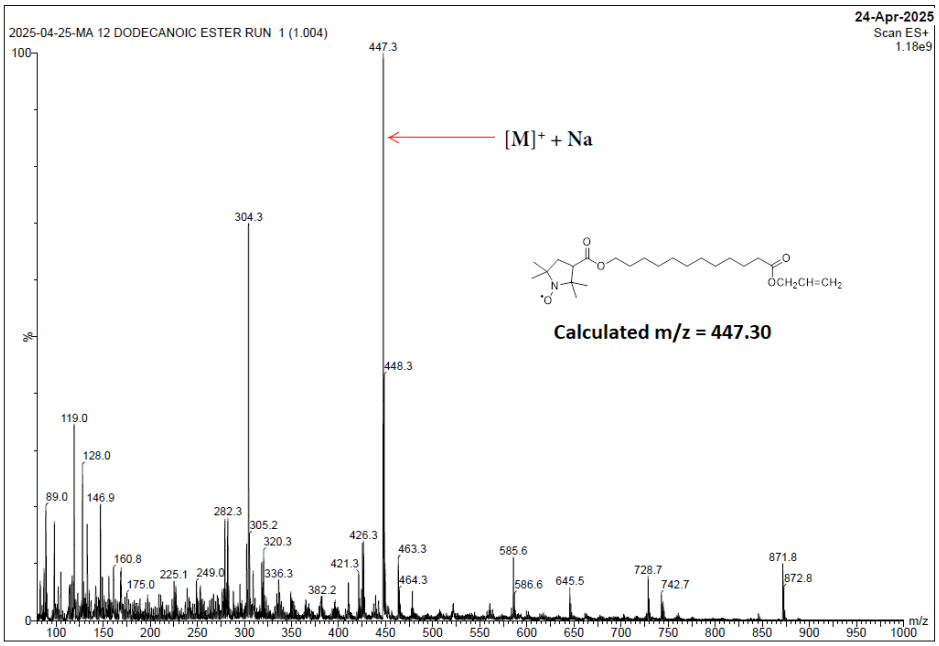

Figure S1E: Mass spectra for the intermediate of compound **4.**

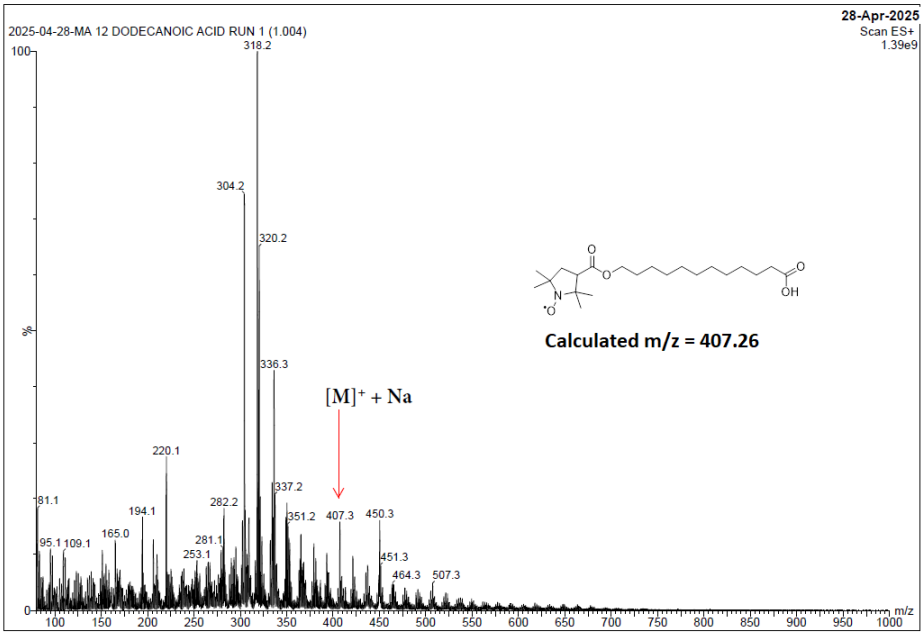

Figure S1F: Mass spectra for compound **4.**

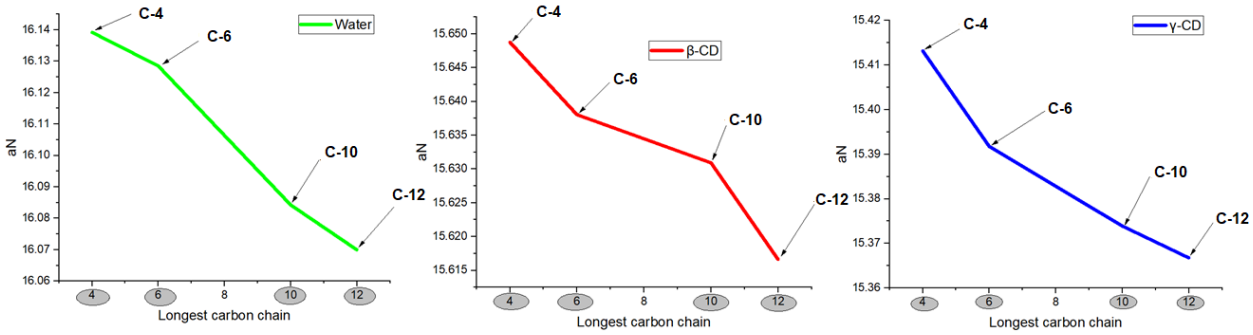

Figure S2: Trends of a_N variation relative to carbon chain length.

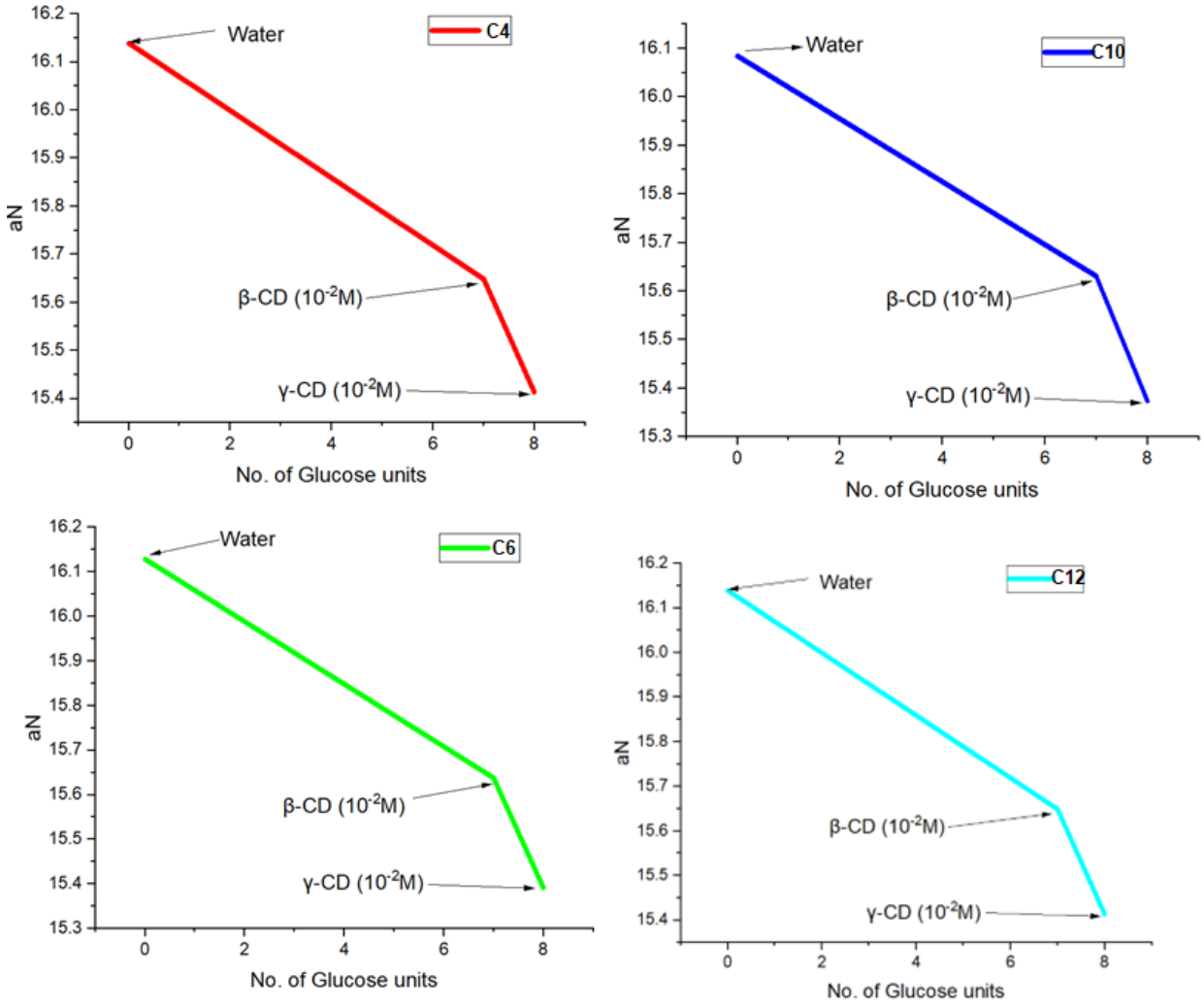

Figure S3: a_N modification upon the formation of an inclusion complex with cyclodextrin.

Table S1: Hyperfine splitting constants values and complexed species proportions obtained from EPR spectra simulations.

		β-CD		γ-CD	
Radical	CD concentration	% complexed species	a_N [G] (complex)	% complexed species	a_N [G] (complex)
C4	10^{-2} M	70.41	15.65	74.83	15.41
	$7x10^{-3}$ M	61.85	15.66	67.26	15.40
	$3x10^{-3}$ M	41.38	15.64	46.82	15.41
	10^{-3} M	18.72	15.65	22.71	15.42
	$5x10^{-4}$ M	10.51	15.65	12.34	15.42
C6	10^{-2} M	70.92	15.64	75.14	15.39
	$7x10^{-3}$ M	62.31	15.64	67.71	15.39
	$3x10^{-3}$ M	41.68	15.65	46.95	15.38
	10^{-3} M	19.12	15.64	22.68	15.39
	$5x10^{-4}$ M	10.71	15.66	12.79	15.39
C10	10^{-2} M	71.32	15.63	75.84	15.37
	$7x10^{-3}$ M	63.14	15.62	68.32	15.37
	$3x10^{-3}$ M	42.31	15.62	47.85	15.38
	10^{-3} M	19.64	15.64	23.07	15.37
	$5x10^{-4}$ M	10.92	15.63	13.11	15.37
C12	10^{-2} M	71.64	15.62	76.19	15.37
	$7x10^{-3}$ M	63.87	15.61	68.85	15.36
	$3x10^{-3}$ M	42.92	15.62	48.23	15.36
	10^{-3} M	19.86	15.62	23.62	15.37
	$5x10^{-4}$ M	11.03	15.62	13.28	15.37

Table S2: Nitrogen hyperfine splitting constant (a_N) values for the spin probes in water and in cyclodextrin.

Radical	**Water (free)**	**β-CD (complexed)**	**γ-CD (complexed)**
C-4	16.14	15.65	15.41
C-6	16.13	15.64	15.39
C-10	16.08	15.63	15.37
C-12	16.07	15.62	15.36