Supplementary Information (SI) for Analyst.

Supporting Information:

Monte Carlo-like peaks assignment using Time-Resolved in-situ NMR approach for complex reaction monitoring. A case of photodegradation of Retinyl Acetate.

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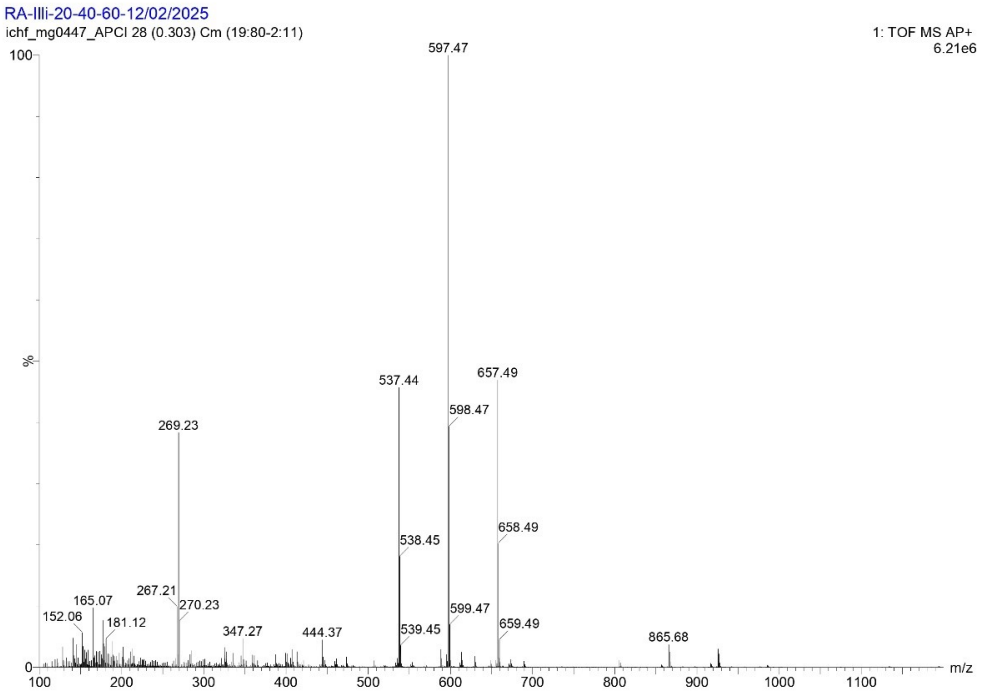

Fig. S1. Mass spectrum overview of sample mixture (positive mode) after 44 hours of illumination showing m/z of 267, 536, 597, and 656 as a major product.

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Entry	Compound Name	Molecular Mass (g/mol)
1.	Retinyl acetate (RA)	328.49
2.	Anhydro retinol (AR)	268
3.	Homodimer of AR	537
4.	Homodimer of RA	656
5.	Dimer of AR with RA	596

Table S1. List of all the reactants of the studied photodegradation process.

Entry	Compound Name	Molecular mass(M) (g/mol)	Diffusion coefficient (D) (m/s^2)
1.	Retinoic Acid	300.44	3.63E-10
2.	Retinyl Acetate	328.49	3.40 E-10
3.	Reaction mixture at the end of illumination	545	1.78E-10

Table S2. The Reference compound used to determine the scaling coefficient k=3.97e-7 and α=-1.22.