

Supplementary Materials for

Investigating the in-solution photo-degradation pathway of Diamond Green G by chromatography and mass spectrometry

Running title: in-solution degradation of Diamond Green

Francesca Sabatini^a

^a University of Pisa, Department of Chemistry and Industrial Chemistry

Via Moruzzi, 13, I-56126 Pisa (Italy)

f.sabatini4@gmail.com

<https://orcid.org/0000-0002-3204-218X>

Ilaria Degano^a

^a University of Pisa, Department of Chemistry and Industrial Chemistry

Via Moruzzi, 13, I-56126 Pisa (Italy)

ilaria.degano@unipi.it

Maarten Van Bommel^{b, c}

^b University of Amsterdam, Faculty of Science, van 't Hoff Institute for Molecular Sciences

Science Park 904, 1098 XH, Amsterdam (The Netherlands)

^c University of Amsterdam, Faculty of Humanities, Amsterdam School for Heritage, Memory and Material

Culture, P. O. Box 94552 | 1090 GN, Amsterdam (The Netherlands)

M.R.vanBommel@uva.nl

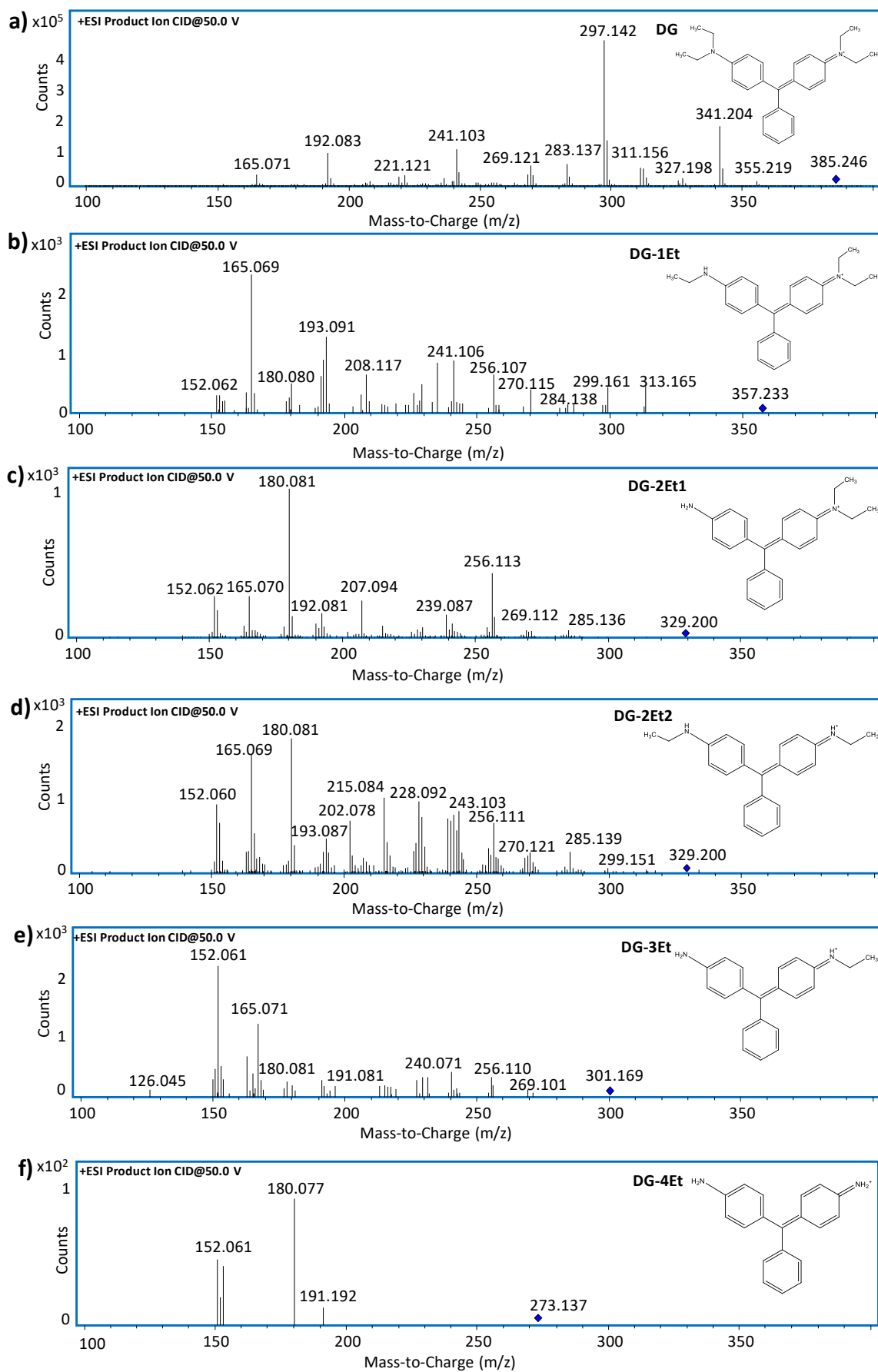


Figure S1: Product-ion mass spectra of **a)** DG; **b)** DG-1Et; **c)** DG-2Et1; **d)** DG-2Et2; **e)** DG-3Et; **f)** DG-4Et. Positive mode, CID at 50.0 V. Precursor-ions are indicated with a blue diamond.

Table S1: Fragments identified in MS/MS spectra of DG and its seven degradation products with triarylmethane structure.

Label/MW	[M] ⁺	[M-Et] ⁺	[M-Et-Me] ⁺	[M-2Et] ⁺	[M-2Et-Me] ⁺	[M-3Et] ⁺ / [M-2Et-2Me] ⁺	[M-Et-(Et) ₂ N] ⁺	[M-4Et] ⁺
DG (385.264)	385.264	355.217	341.204	327.187	311.156	297.142	283.136	269.12
MeDG (371.248)	371.248	341.201	327.187	311.153	297.140	284.142	269.119	
2MeDG (357.233)	357.233	327.185	313.171	299.163	284.138	270.127		
DG-1Et (357.233)	357.233		313.165	299.161	284.138	270.115		
MeDG-1Et (343.217)	343.217		299.137	284.115	269.115			
DG-2Et1 (329.201)	329.201	299.151	285.139	269.112	256.113			
DG-2Et2 (329.201)	329.201	299.151	285.139	269.112	256.111			
DG-3Et (301.170)	301.17	271.12						
DG-4Et (303.186)	273.137							

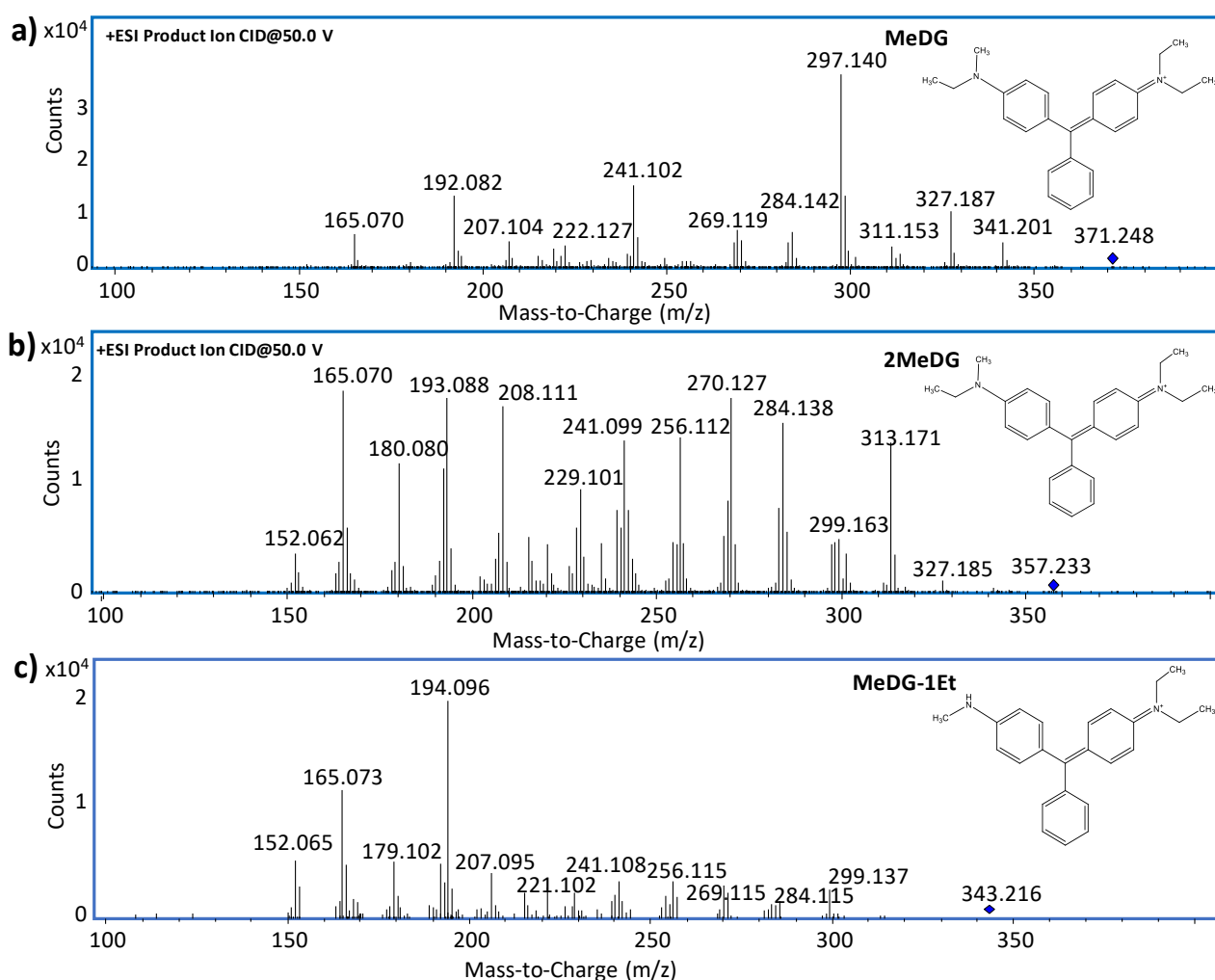


Figure S2: Product-ion mass spectra of a) MeDG; b) 2MeDG; c) MeDG-1Et. Positive mode, CID at 50.0 V.

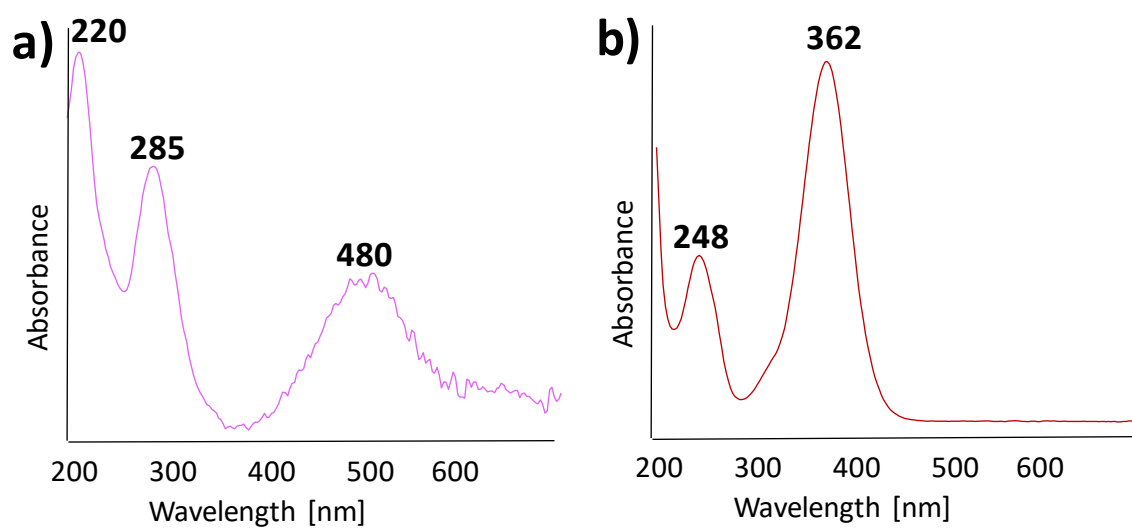


Figure S3: UV-Vis spectra of **a)** Unk and **b)** Carb.