Supporting information for

Silk-based Organic Photoresist for Extreme Ultraviolet Lithography: A Multiscale in Silico Study

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1. Supplementary Figures

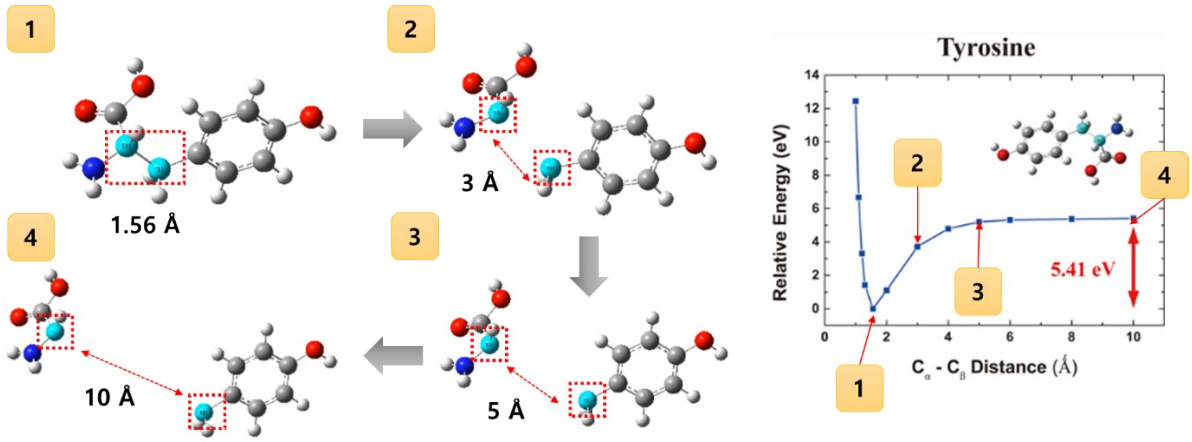

Figure S1. Representation of the dissociation process and dissociation curve.

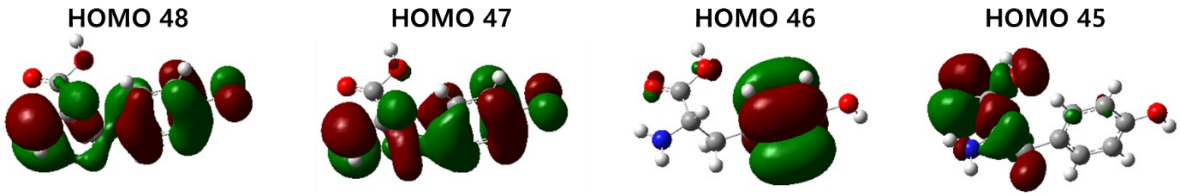

Figure S2. Representation of molecular orbital of HOMO and LUMO states.

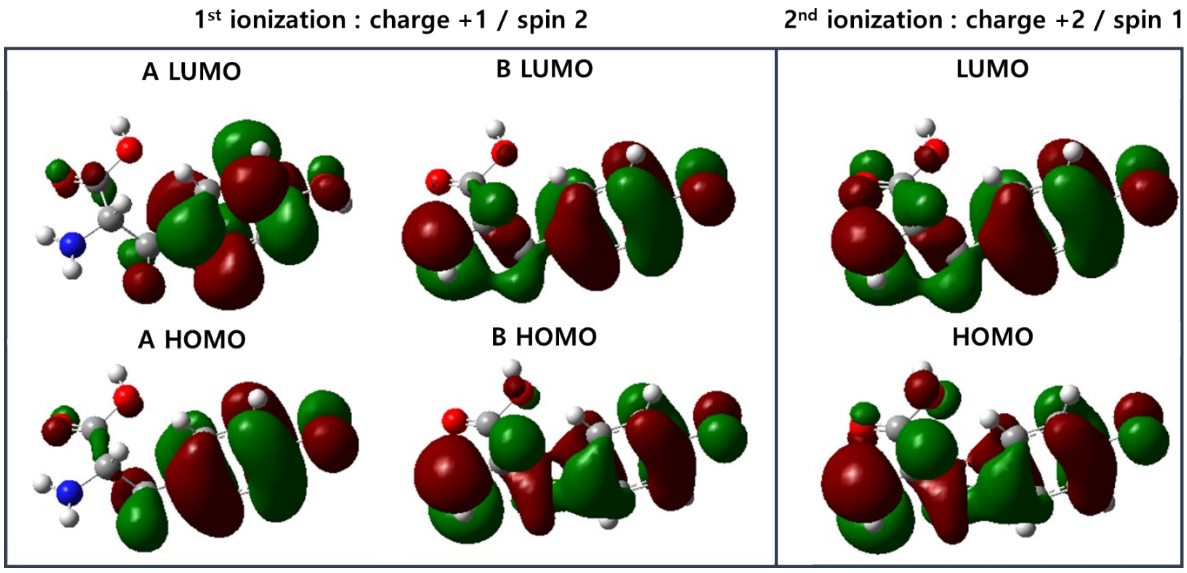

Figure S3. Representation of molecular orbital of HOMO and LUMO states at first and secondary ionization.

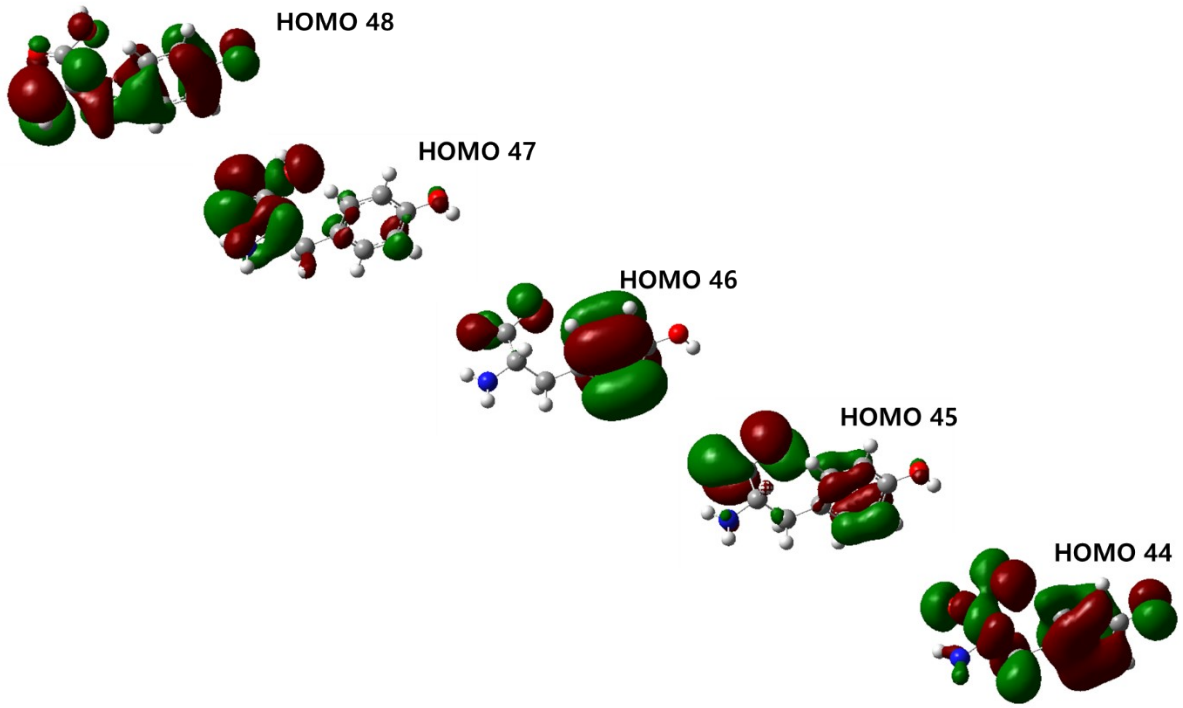

Figure S4. Representation of molecular orbital of secondary electron ionization. HOMO 44 to 48 are represented.

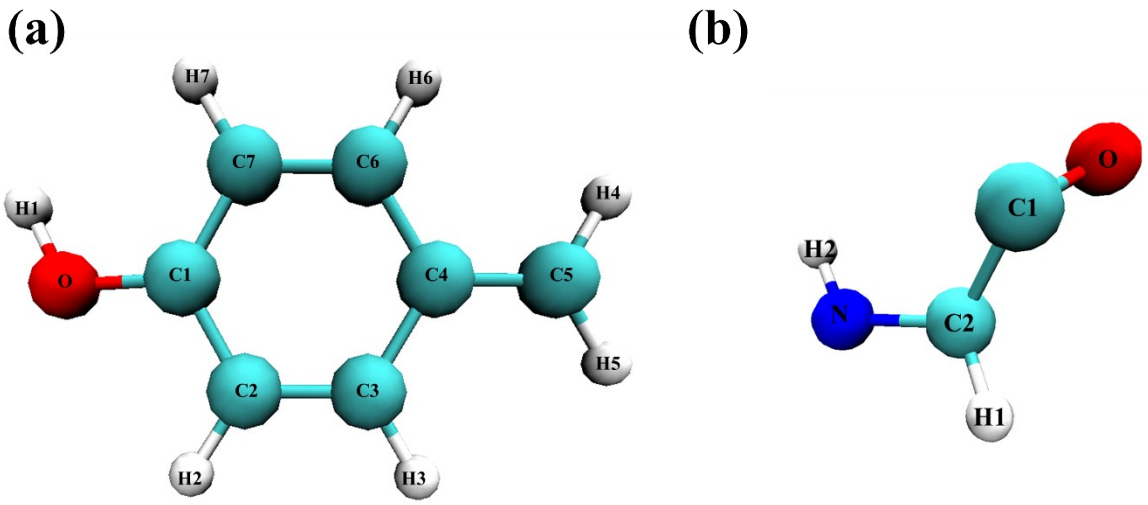

Figure S5. Atom index of dissociated tyrosine. (a) Quinone methide. (b) Glycine

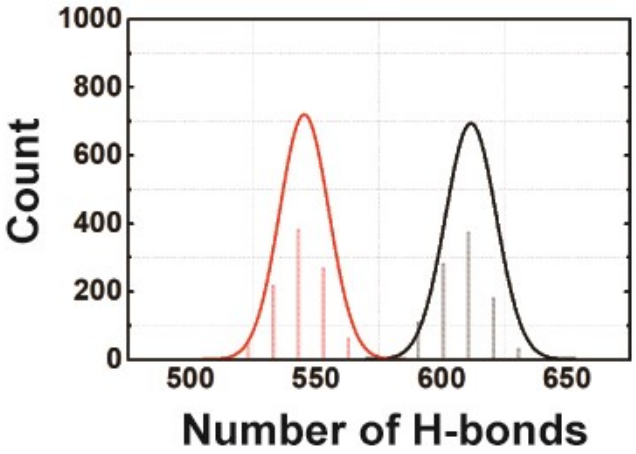

Figure S6. Comparison of the number of the hydrogen bonds before (black line and region) and after(red line and region) photoreaction

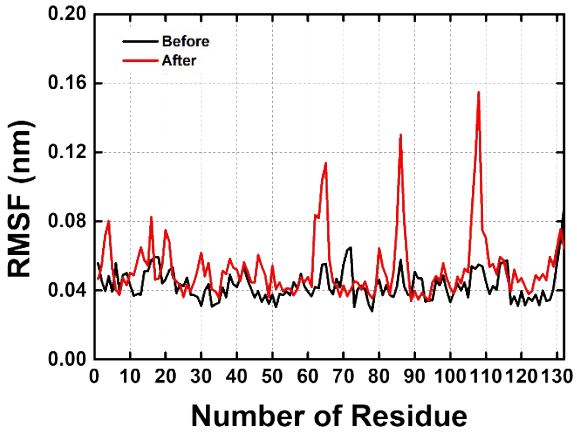

Figure S7. Silk peptide root mean square fluctuation (RMSF) before (black line) and after (red line) photoreaction.

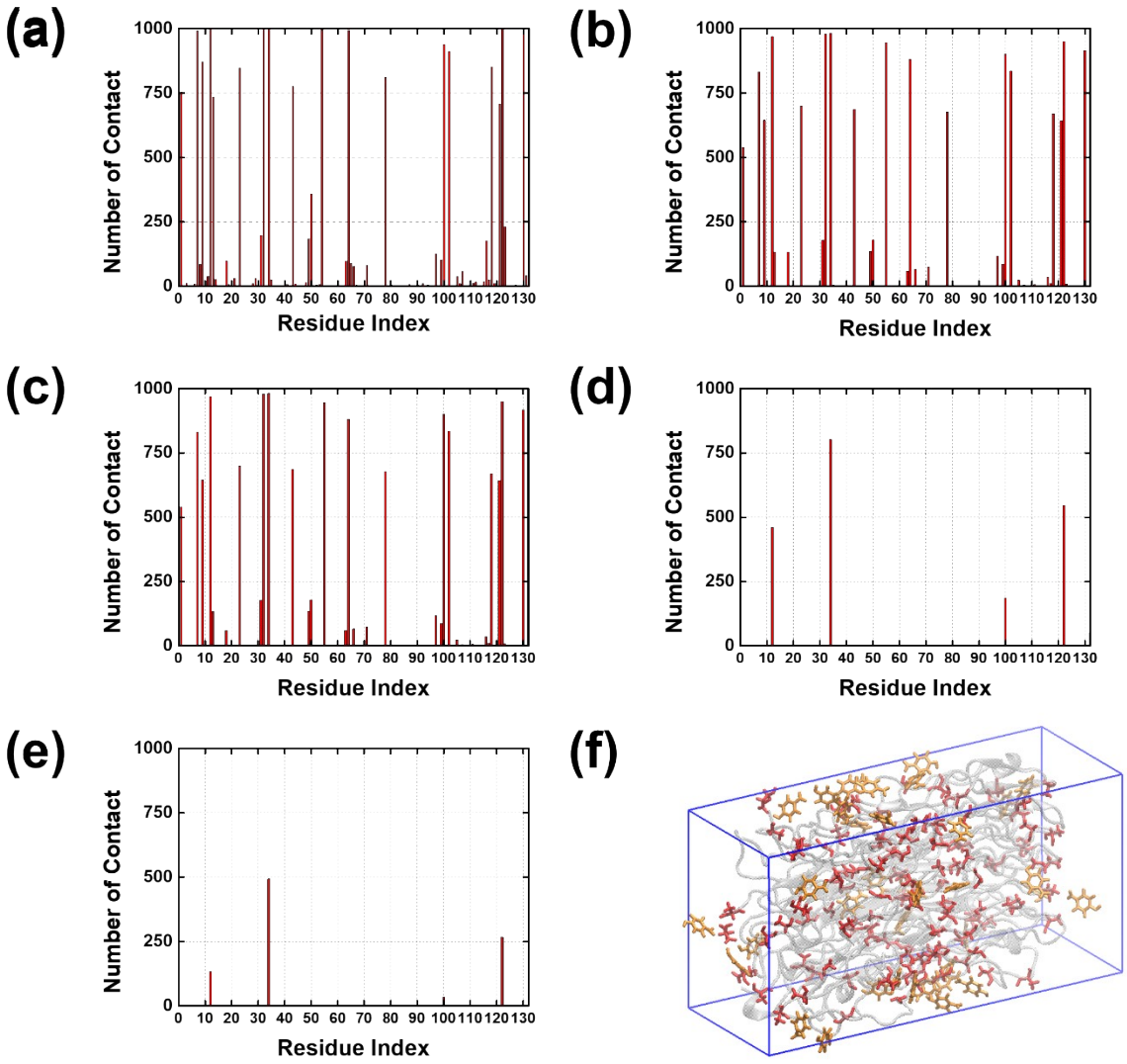

Figure S8. Number of contact atoms of silk peptide residue and quinone methide (QMC) through MD trajectories as a function of the cut-off distance. (a) 2.0 nm, (b) 1.8 nm, (c) 1.6 nm, (d) 1.4 nm, and (e) 1.2 nm cut-off distance. (f) Molecular representation of the binding of silk and quinone methide. Photoionized tyrosine is in red and quinone methides are in yellow.

2. Supplementary Tables

Table S1. Molecular parameters of dissociated tyrosine (glycine part)

Atom index	Atom name	Partial charge
1	N	-0.233
2	H1	0.196
3	C1	0.078
4	H2	0.401
5	C2	0.596
6	O	-0.038

Table S2. Molecular parameters of dissociated tyrosine (quinone methide part)

Atom index	Atom name	Partial charge
1	H1	0.484
2	O	-0.501
3	C1	0.572
4	C2	-0.289
5	H	0.203
6	C3	-0.041
7	H	0.174
8	C4	0.131
9	C5	-0.154
10	H2	0.187
11	H3	0.187
12	C6	-0.041
13	H4	0.174
14	C7	-0.289
15	H5	0.203