Electronic Supplementary Material (ESI) for RSC Advances.

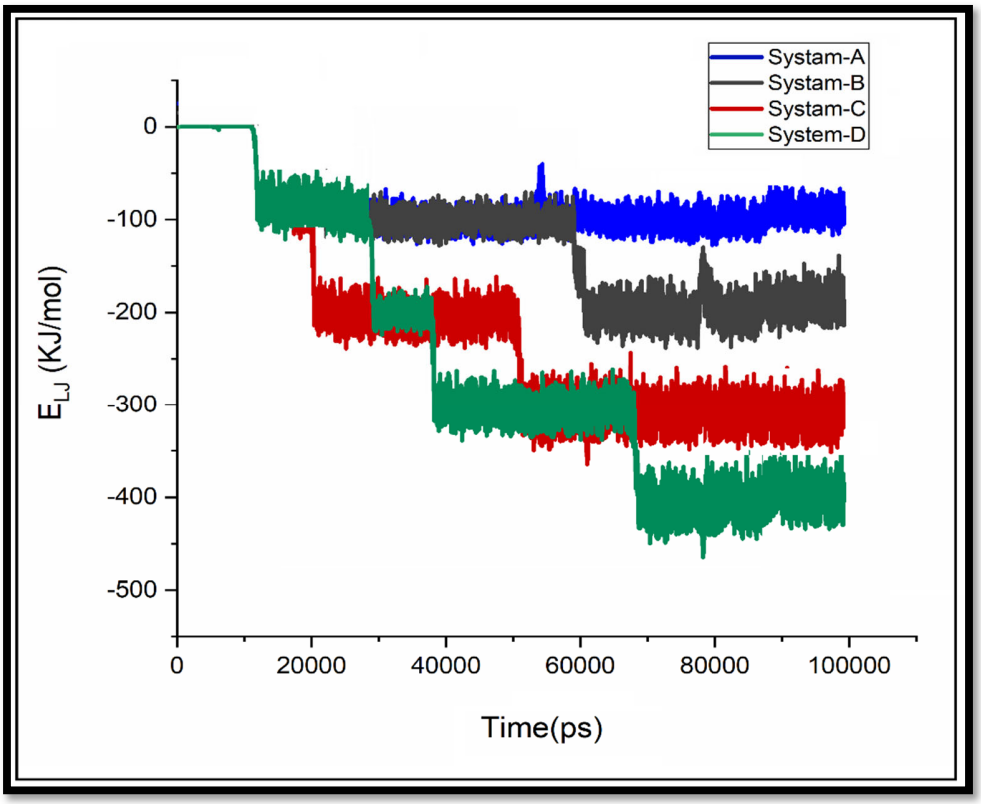

Figure S1. The L-J interaction energy between the pollutant molecules and SNS as a function of simulation time.

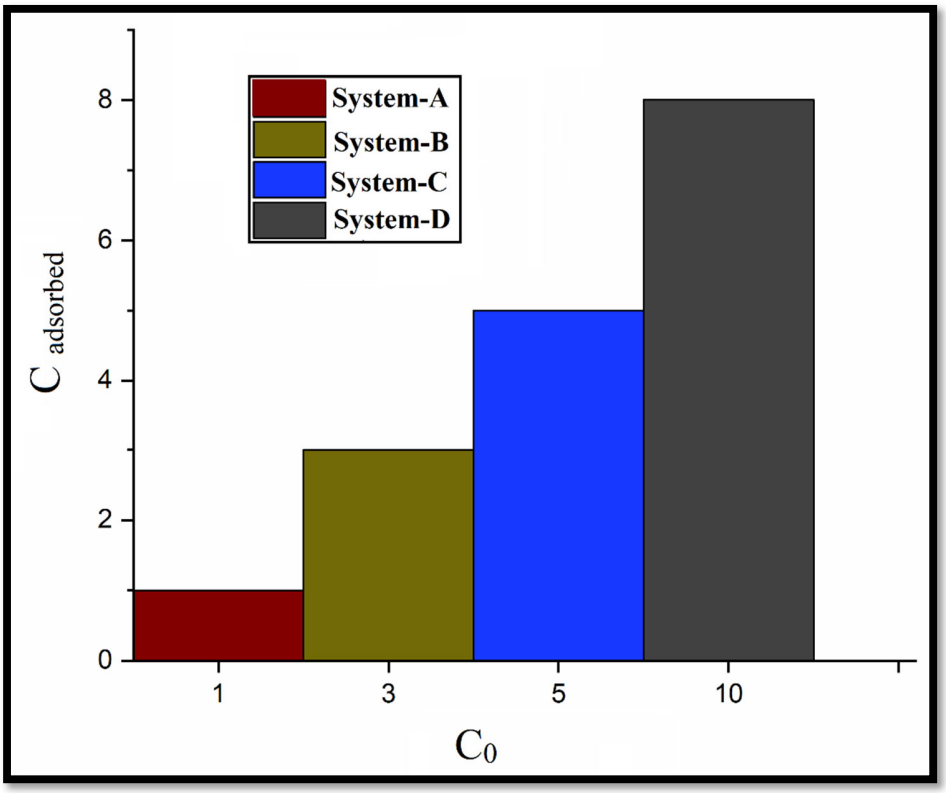

Figure S2. The number of adsorbed GLY molecules on SNS ($C_{adsorbed}$) versus initial concentrations of GLY (C_0)

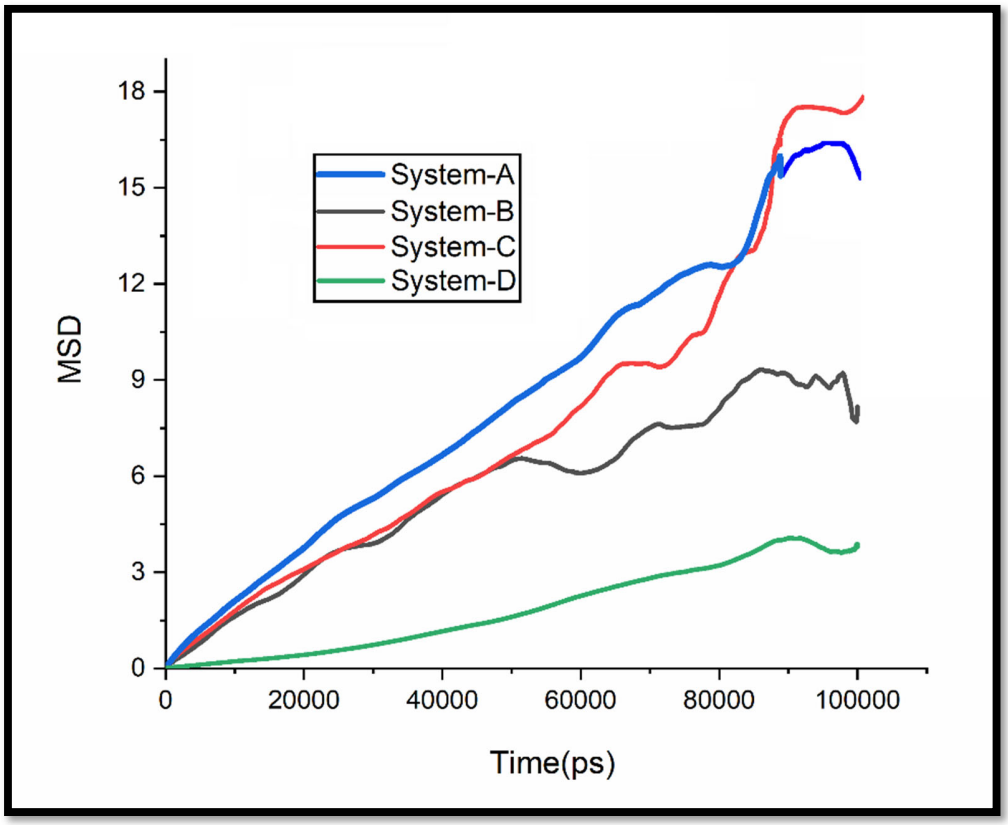

Figure S3. Time evolutions of MSD of GLY in all of the studied complexes.

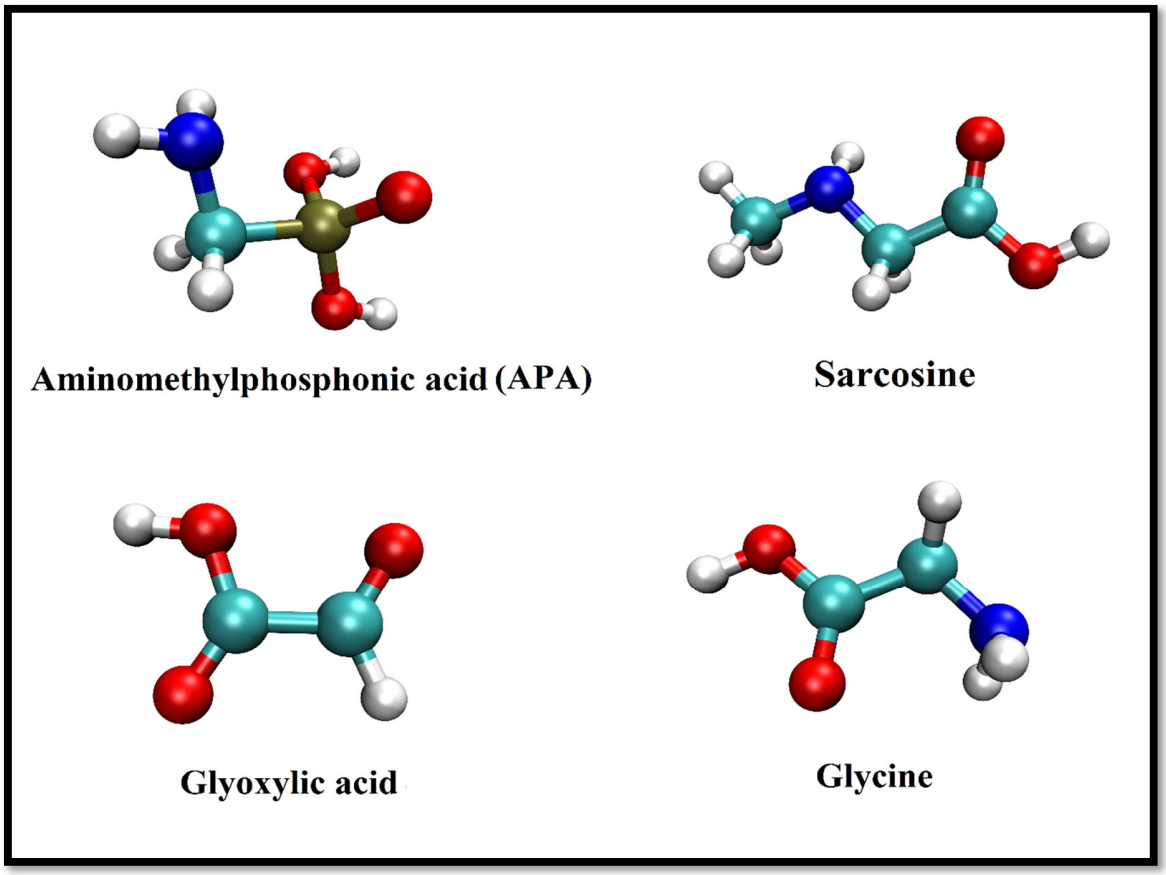

Figure S4. The GLY and the main products of the degradation processes.

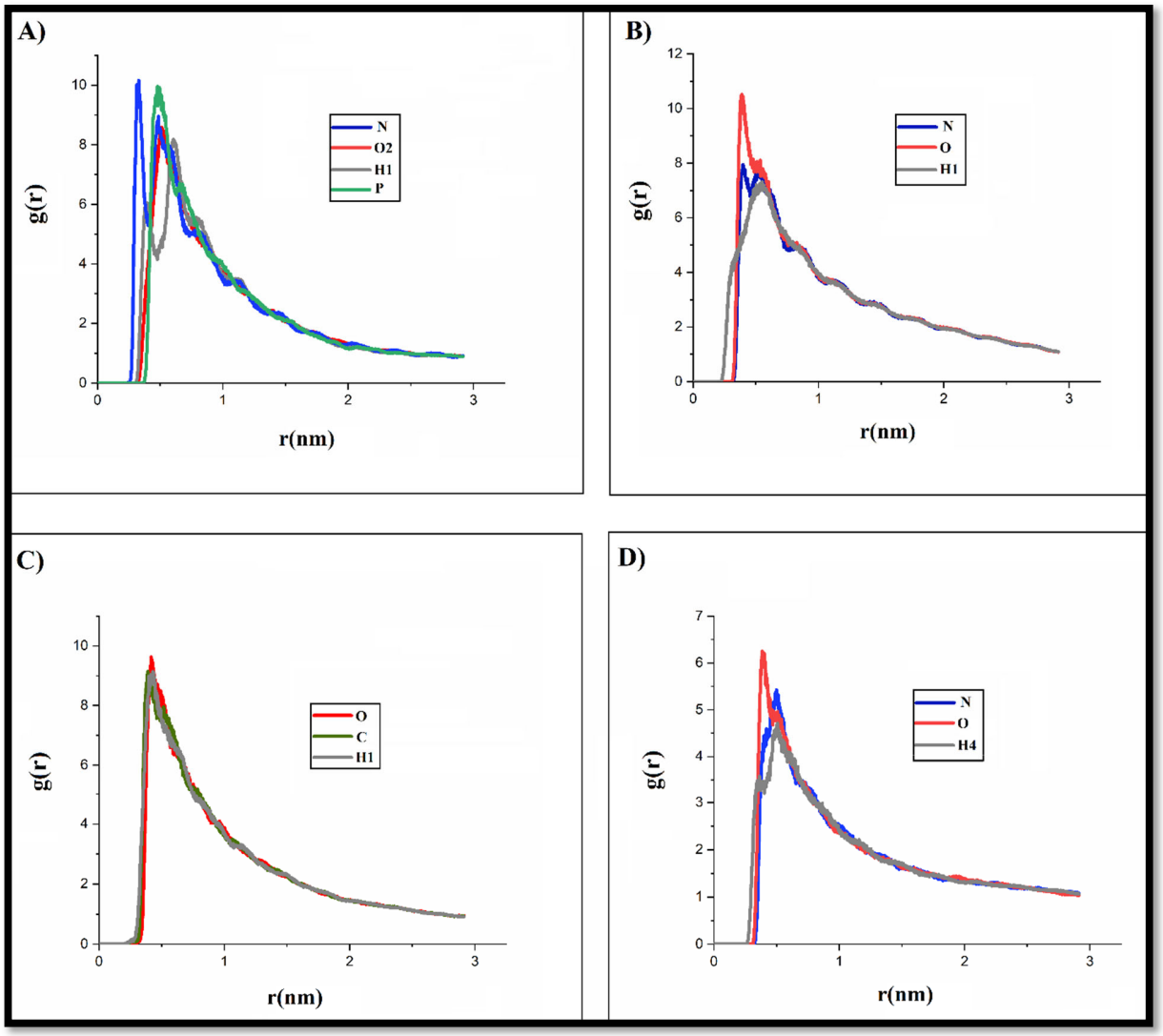

Figure S5. Atomic radial distribution function of the **A)** SNS@APA **B)** SNS@ SAR **C)** SNS@ GLA and **D)** SNS@ GLC complexes.

Table S1. Adsorption energy values for different glyphosate-adsorbent complexes. GOX (Glyphosate oxidoreductase). All energy values are in kJ/mol.

Complexes	ΔE_{ads}(kJ/mol)	Ref.
GOX–glyphosate	-22.68	[3]
C–P-lyase–glyphosate	-18.06	[3]
NU-1000–glyphosate	-37.63	[41]
NiO-67– glyphosate	-17.37	[41]

Table S2. The obtained pair interaction energy between different components of the investigated systems at the first (0 ns) and the last (75 ns) of the MD production. (all in kJ mol^{-1})

	L-J		Coul		Total
Time	**0 ns**	**100 ns**	**0 ns**	**100 ns**	-
System-A	0	-75.95	0	-3.01	-78.96
System-B	0	-175.35	0	-2.11	-177.46
System-C	0	-338.78	0	-4.31	-343.09
System-D	0	-442.08	0	-6.43	-448.51