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Supporting Information

Characterization of the Interaction of a Novel Anticancer Molecule with PMMA, PCL, and PLGA Polymers via Computational Chemistry

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Table S1. Structural and electronic properties of PMMA, PCL, and PLGA with 1, 3, and 6 units, including molecular weight, solvation energy, dipole moment, HOMO-LUMO energies, PSA, log P, HBD/HBA counts, and polarizability, highlighting hydrophobicity trends and interaction profiles.

	PMMA			**PCL**			**PLGA**		
	1 U	**3 U**	**6U**	**1 U**	**3 U**	**6U**	**1 U**	**3 U**	**6U**
Weight (amu)	100.117	302.367	630.722	144.214	400.556	700.907	148.114	408.312	782.610
Solvation Energy (kJ/mol)	-5.57	-25.89	- - - -	-5.44	-59.22	- - - - -	-64.65	-71.98	-82.15
Dipole (Debye)	1.76	2.00	6.54	1.70	7.23	2.97	6.63	6.62	14.01
HOMO energy (eV)	-7.60	-7.45	-7.37	-7.70	-6.59	-7.02	-8.12	-7.79	-7.53
LUMO energy (eV)	-1.52	-0.18	-0.36	-0.29	-0.67	-0.91	-1.27	-0.97	-0.75
PSA (Å^2)	19.858	56.482	115.159	20.734	65.017	124.564	71.624	154.338	254.494
log P	0.99	3.11	7.14	2.28	2.96	5.18	-0.98	-1.88	-2.53
HBD count	0	0	0	0	0	0	2	2	0

HBA count	1	3	0	1	6	7	3	7	0
Polarizability (10^{-30} m^3)	49.20	65.74	93.52	53.69	76.99	102.04	50.70	69.47	96.75
Calculated quantum chemical parameters for the compounds studied in this work, ranging from 1 to 6 repeating units of each polymer.									
Gap energy (ΔE) (eV)	6.08	7.27	**7.01**	7.41	6.00	**6.11**	6.85	6.82	**6.78**
Ionization energy (I) (eV)	7.60	7.45	**7.37**	7.70	6.59	**7.02**	8.12	7.79	**7.53**
Electron affinity (A)	1.52	0.18	**0.36**	0.29	0.59	**0.91**	1.27	0.97	**0.75**
Electronegativity (x)	4.56	3.82	**3.86**	3.995	3.59	**3.97**	4.695	4.38	**4.14**
Chemical potential (μ)	-4.56	-3.82	**-3.86**	-3.995	-3.59	**-3.97**	-4.695	-4.38	-4.14
Global electrophilicity (GE)	3.42	2.00	**2.12**	2.155	3.00	**2.58**	3.425	2.81	**3.39**
Hardness (η)	3.04	3.64	**3.51**	3.705	2.15	**3.06**	3.22	3.41	**6.11**

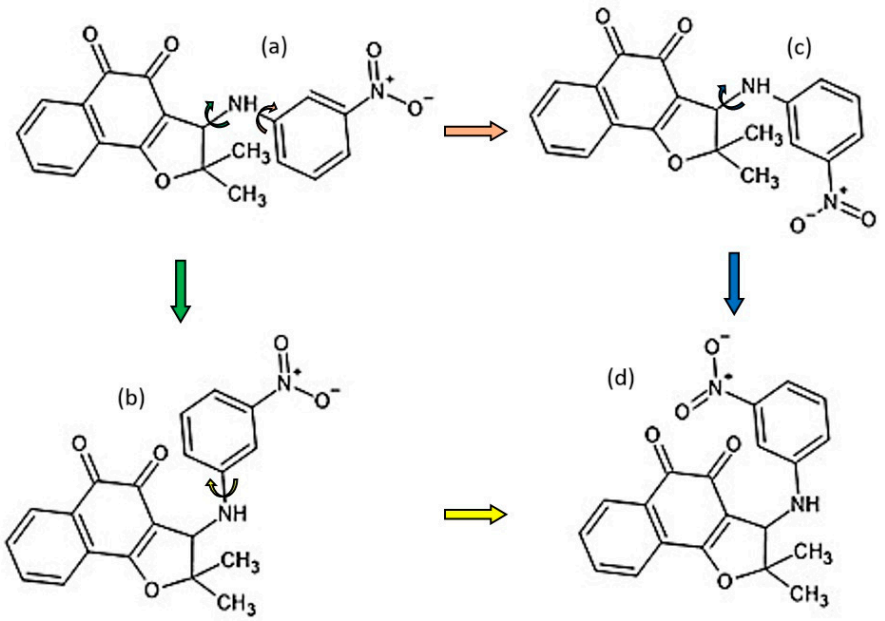


Figure S1. Several configurations of the $QPhNO_2$ molecule as result of rotation in one of the ligations C-NH-C, as indicated by curved arrows. (a) – (d) identify different configurations, not necessarily the most energetically stable.

Study of the properties of the PMMA polymer with 1, 3, and 6 repeating units.

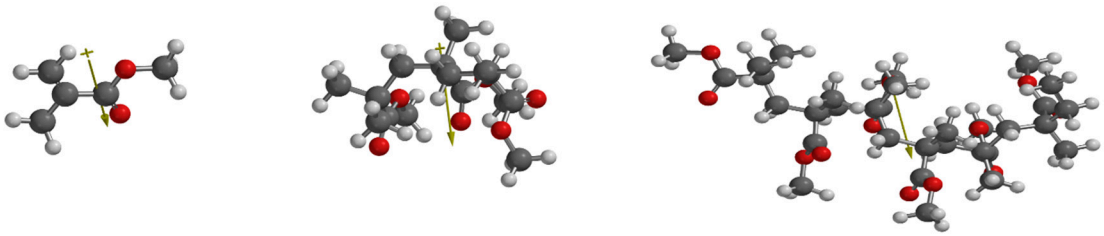


Figure S2. 3D molecular structures of polymethyl methacrylate (PMMA) with single (1U, left), three (3U, middle), and six repeating units (6U, right), showcasing the progression from monomeric configuration to extended polymer chains.

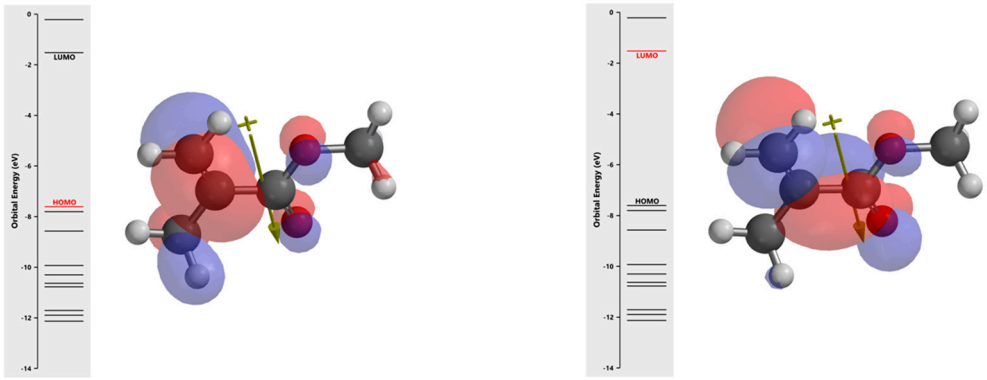


Figure S3. HOMO and LUMO analysis of PMMA (1U): HOMO (left) shows electron density in the highest occupied orbital, and LUMO (right) represents the lowest unoccupied orbital.

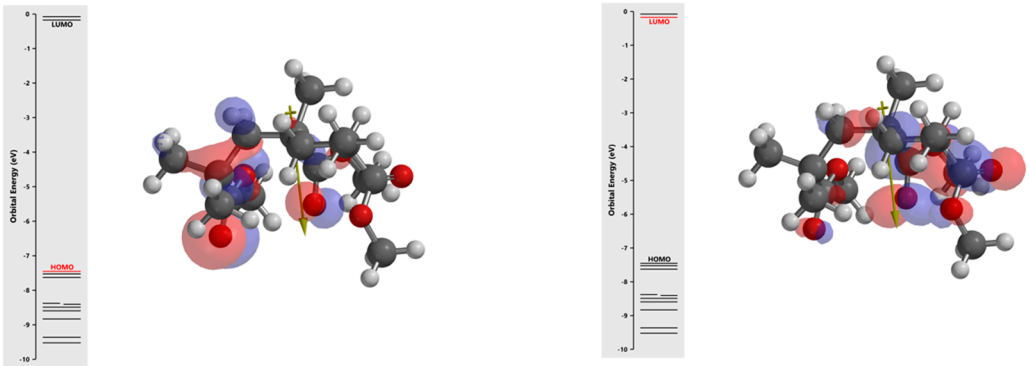


Figure S4. HOMO and LUMO analysis of PMMA (3U): HOMO (left) highlights electron density in the highest occupied state, and LUMO (right) shows the lowest unoccupied orbital.

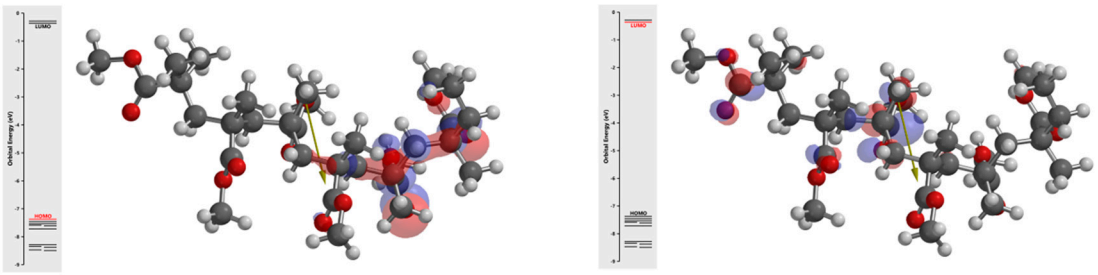


Figure S51. HOMO and LUMO analysis of PMMA (6U): HOMO (left) shows electron density in the highest occupied state, and LUMO (right) represents the lowest unoccupied orbital.

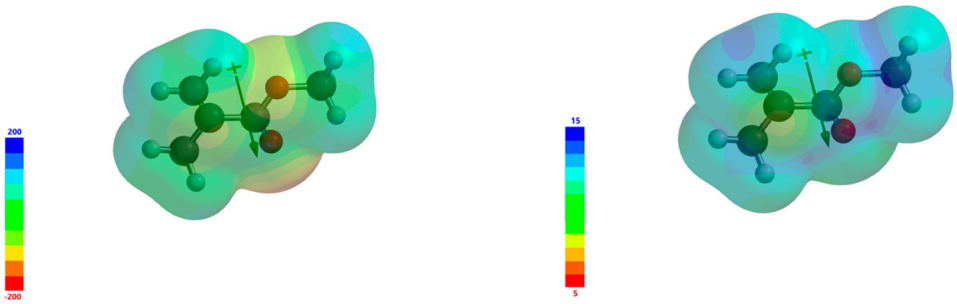


Figure S6. Electrostatic potential (left) and local ionization potential (right) maps for PMMA (1U), highlighting reactive sites with color-coded potential distributions.

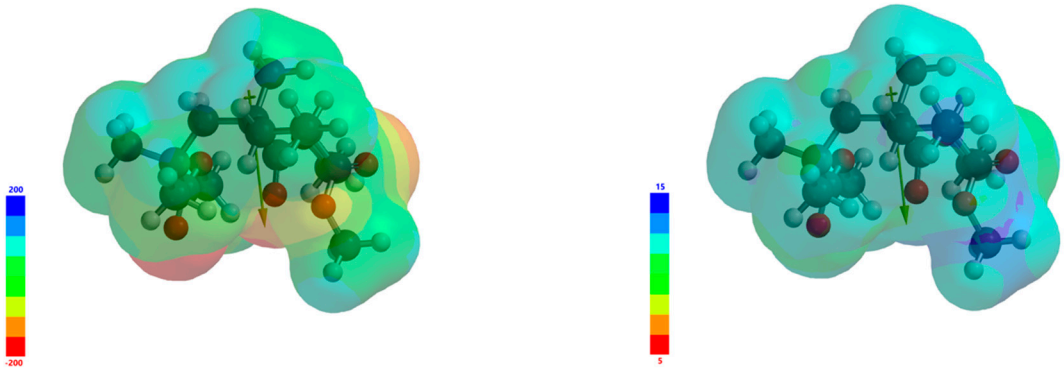


Figure S7. Electrostatic potential (left) and local ionization potential (right) maps for PMMA (3U), highlighting potential distribution and interaction sites.

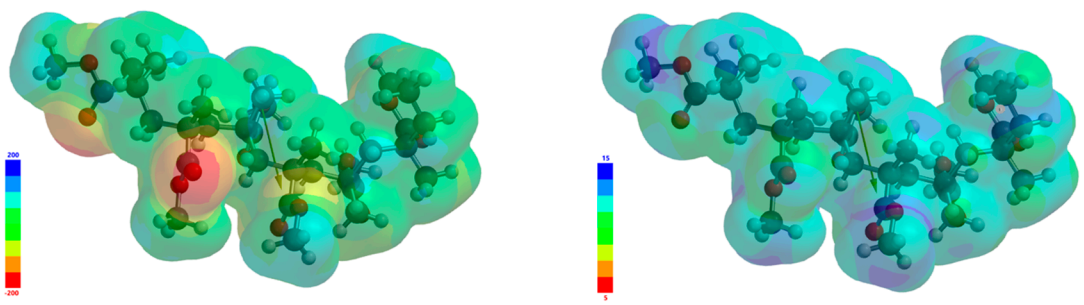


Figure S8. Electrostatic potential (left) and local ionization potential (right) maps for PMMA (6U), highlighting regions of electrostatic variation and interaction sites along the polymer chain.

Study of the properties of the PCL polymer with 1, 3, and 6 repeating units.

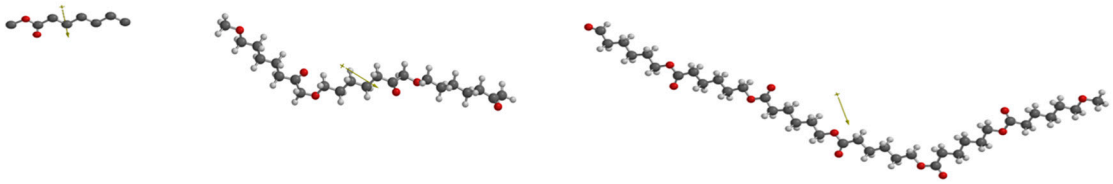


Figure S2. 3D molecular structures of polycaprolactone (PCL) with a single unit (left), three units (center), and six units (right), illustrating the progression from monomer to extended polymer chain.

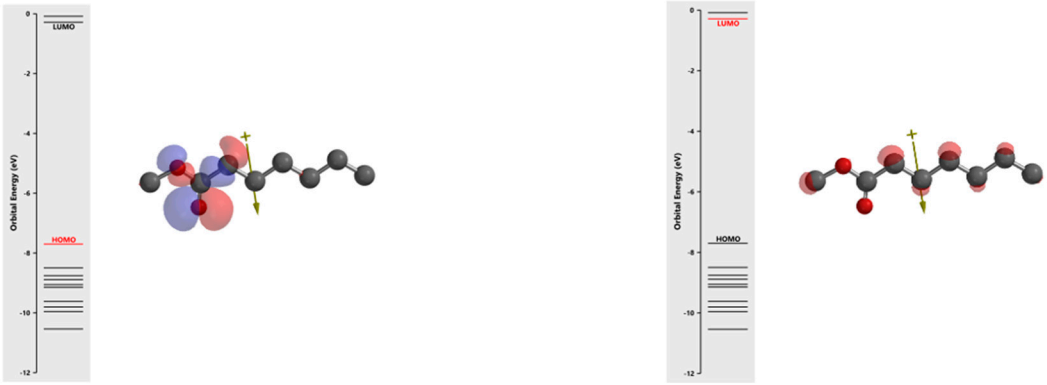


Figure S10. HOMO and LUMO analysis for a single unit (1U) of polycaprolactone (PCL). (Left) Highest Occupied Molecular Orbital (HOMO). (Right) Lowest Unoccupied Molecular Orbital (LUMO).

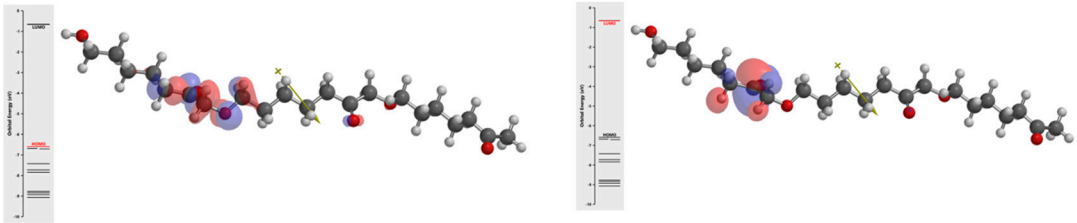


Figure S31. HOMO and LUMO analysis for three units (3U) of polycaprolactone (PCL). (Left) Highest Occupied Molecular Orbital (HOMO). (Right) Lowest Unoccupied Molecular Orbital (LUMO)

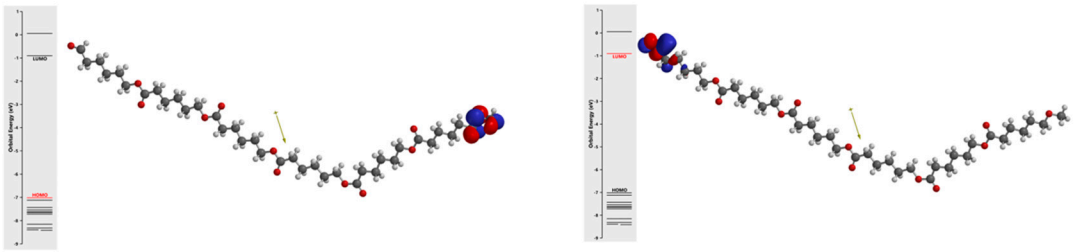


Figure S12. HOMO and LUMO analysis for six units (6U) of polycaprolactone (PCL). (Left) Highest Occupied Molecular Orbital (HOMO). (Right) Lowest Unoccupied Molecular Orbital (LUMO).

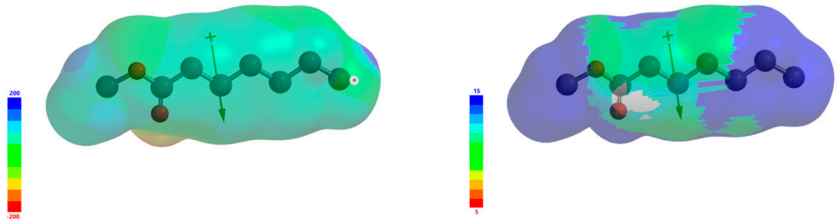


Figure S43. Electrostatic potential (left) and local ionization potential (right) maps for PCL (1U), highlighting charge distribution and reactivity regions.

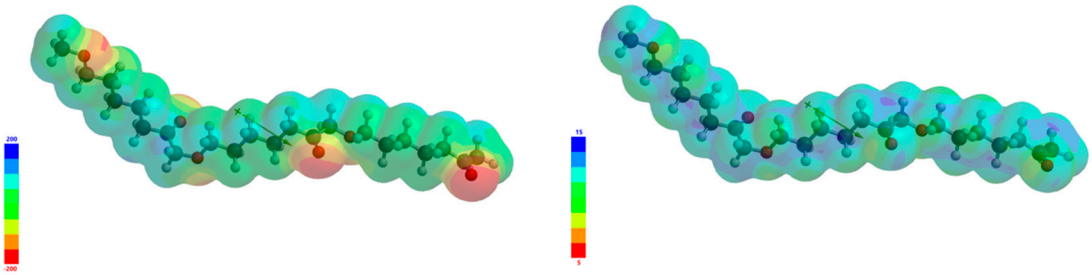


Figure S54. Electrostatic potential (left) and local ionization potential (right) maps for PCL (3U), showing charge distribution and reactivity regions.

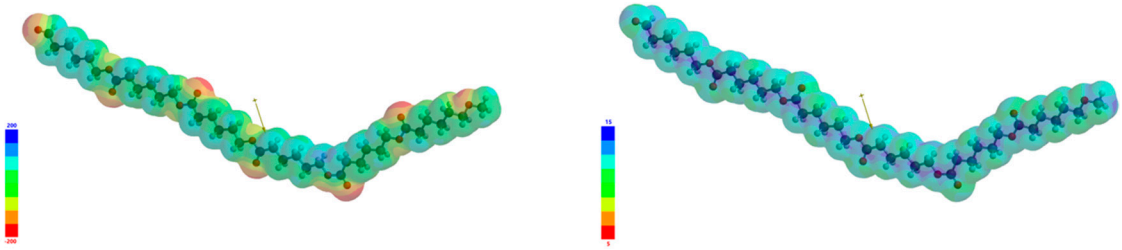


Figure S15. Electrostatic potential (left) and local ionization potential (right) maps for PCL (6U), highlighting charge distribution and reactivity regions.

Study of the properties of the PCL polymer with 1, 3, and 6 repeating units.

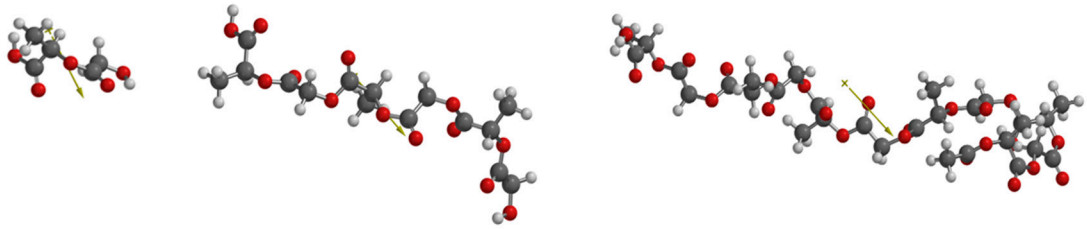


Figure S16. 3D molecular structures of PLGA with a single unit (left), three units (center), and six units (right), illustrating the progression from monomer to extended polymer chain.

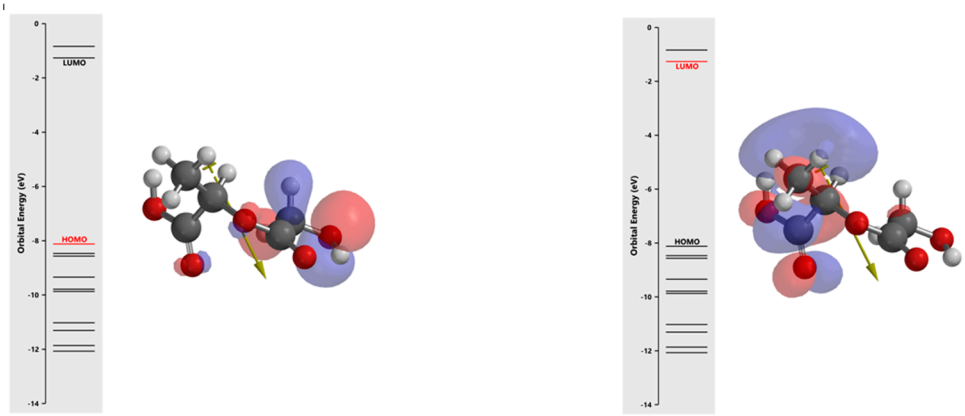


Figure S17. HOMO (left) and LUMO (right) analysis for PLGA (1U), showing electron density in the highest occupied and lowest unoccupied states to assess electronic properties and reactivity.

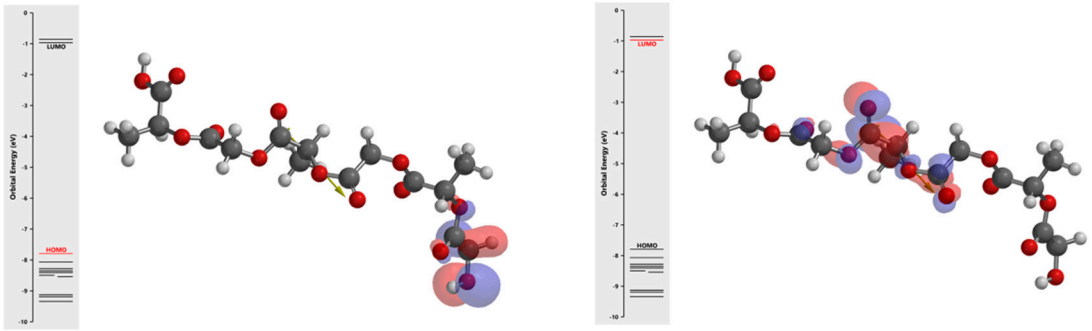


Figure S18. HOMO (left) and LUMO (right) analysis for PLGA (3U), highlighting electron density in the highest occupied and lowest unoccupied states for electronic structure and reactivity insights.

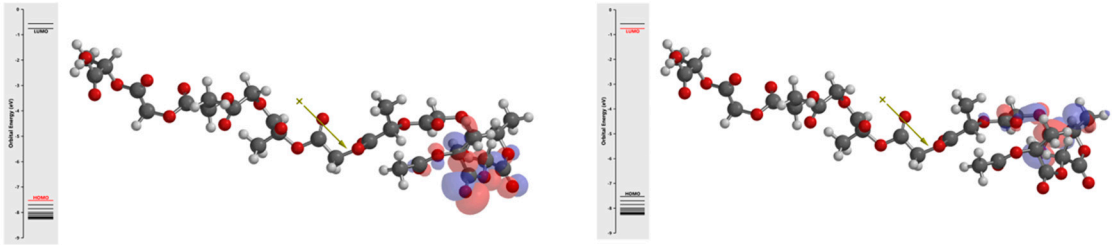


Figure S19. HOMO (left) and LUMO (right) analysis for PLGA (6U), showing electron density distribution and interaction regions, with energy levels in eV.



Figure S20. Electrostatic potential (left) and local ionization potential (right) maps for PLGA (1U), showing charge distribution and ionization energy variations.

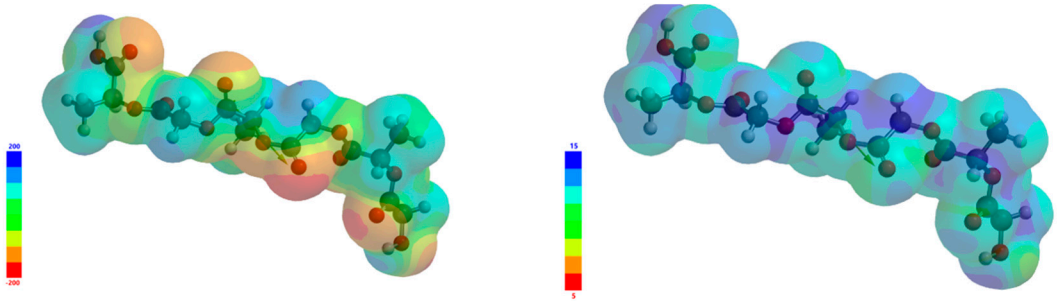


Figure S21. Electrostatic potential (left) and local ionization potential (right) maps for PLGA (3U), showing charge distribution and ionization energy variations.

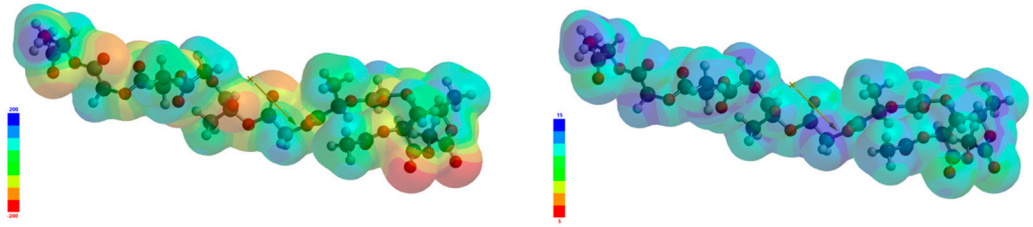


Figure S22. Electrostatic potential (left) and local ionization potential (right) maps for PLGA (6U) , showing charge distribution and ionization energy levels