Supplementary Information

Ligand -controlled Fe_3O_4 nanoparticles as reusable adsorbents for dye removal in the chemical recycling of coloured polyester textiles

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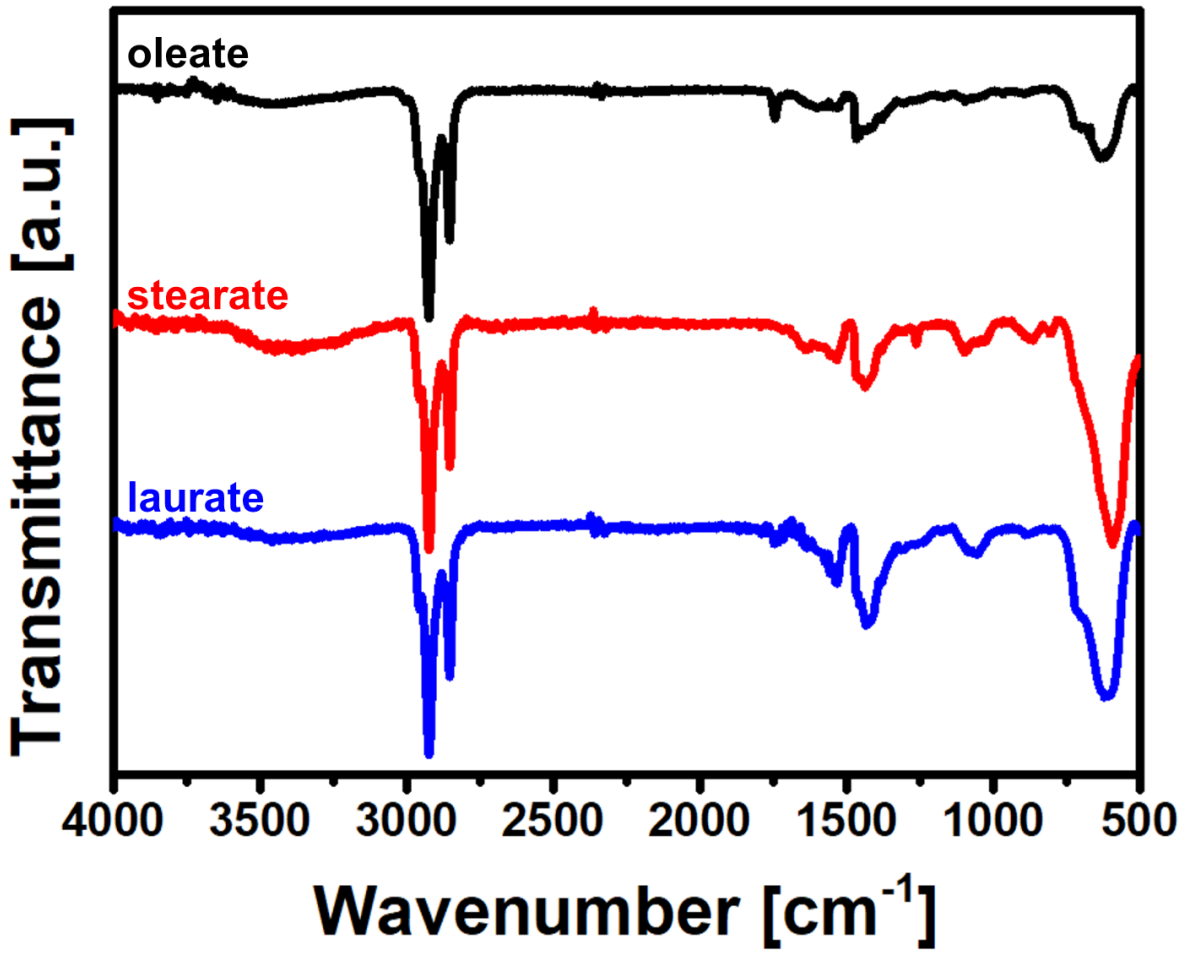


Fig. S1. FT-IR spectra of oleate, stearate and laurate-capped nanoparticles in the range of 500–4000 cm^{-1}.

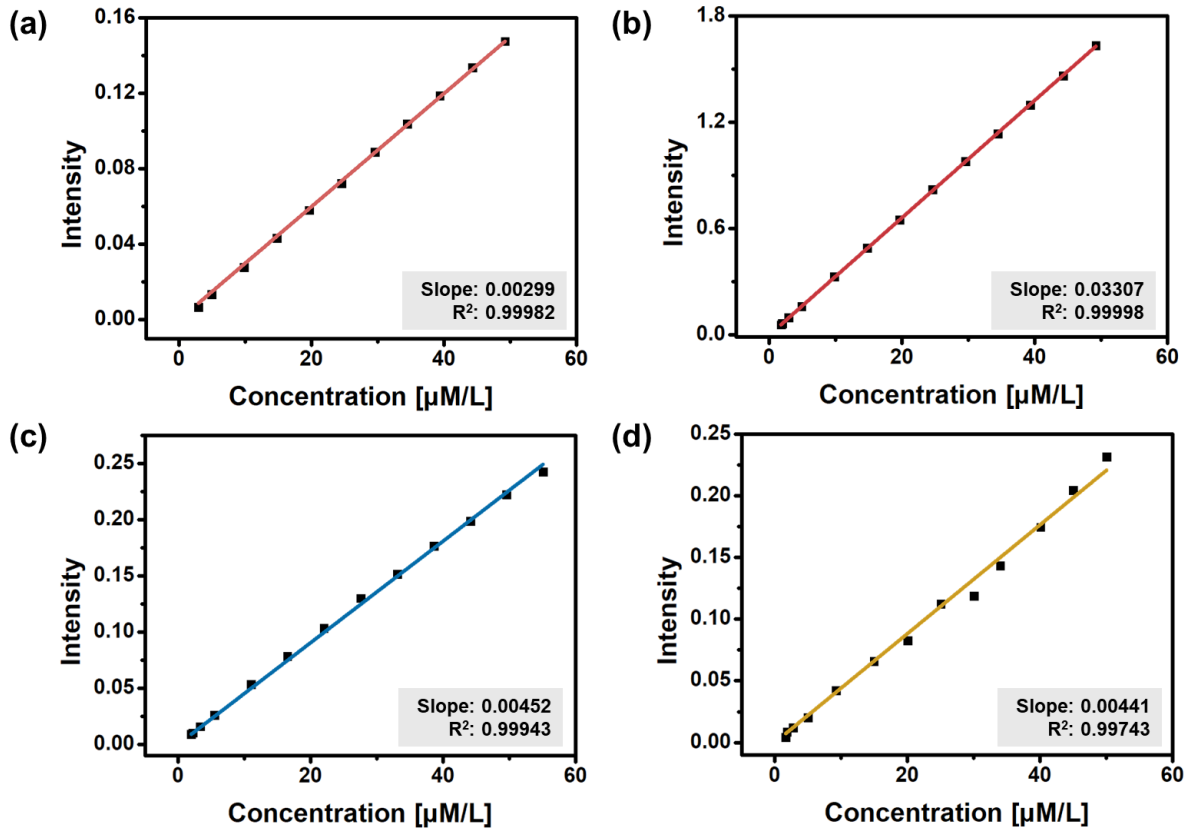


Fig. S2. Calibration curves of four dyes: (a) Disperse Red 60 (DR60), (b) Disperse Red 1 (DR1), (c) Disperse Yellow 54 (DY54), and (d) Disperse Blue 56 (DB56).

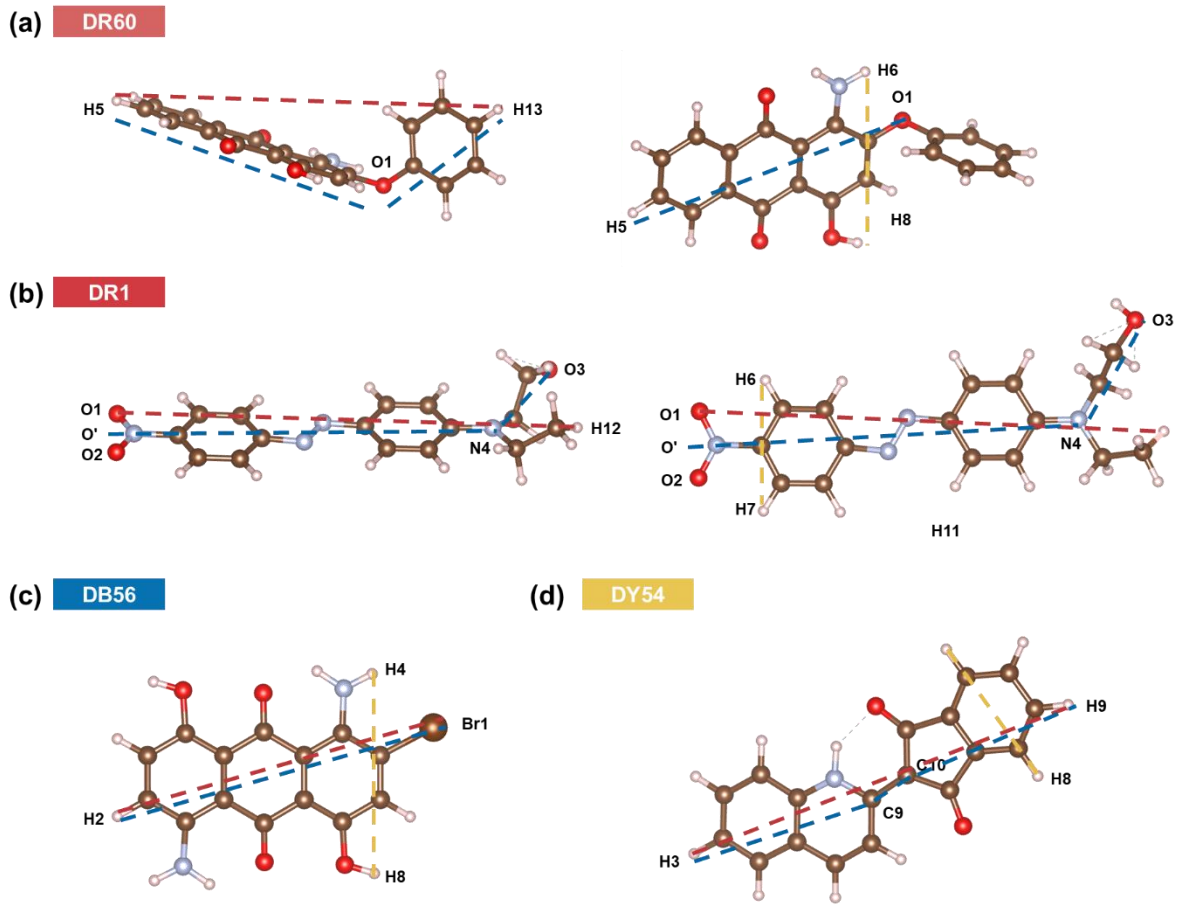


Fig. S3. Defined parameters of dye molecules: red dashed line (end-to-end distance), blue dashed line (contour length), and yellow dashed line (width). (a) DR60, (b) DR1, (c) DB56, and (d) DY54.

Supplementary Text 1.

The three-dimensional molecular structures of DR1 and DY54 were constructed from published atomic coordinate data (N. Wazzan, J. Mol. Struct., 2009, 920, 235–242; G. R. Han, et al., Sci. Rep., 2017, 7, 3863). The structures of DR60 and DB56 were obtained from the MolView database as .mol files. All molecules were imported into VESTA program, from which atomic Cartesian coordinates were exported. Interatomic distances were calculated as Euclidean distances between atomic coordinates.

We report three parameters for each dye: i) end-to-end distance, defined as the maximum separation between any two atoms; ii) contour length, defined by bisecting the molecule at a chemically meaningful pivot and summing the two straight-line segments from the pivot to the two terminal atoms; and iii) width, defined as the maximum lateral separation

For DR60, we explicitly used the following VESTA-derived Cartesian coordinates (Å) for the measurements: H5 (6.70410, 0.72550, −0.91020), O1 (2.84360, −0.71500, 1.13590), H13 (6.72770, 0.42830, −2.18520), H6 (1.66200, −2.78670, 0.93720), and H8 (0.99220, 3.47670, 0.63850). The end-to-end distance corresponds to the H5–H13 separation. The contour length was obtained by bisecting at the ether oxygen (O1) and summing the two straight-line segments, H5–O1 and O1–H13. The width corresponds to the H6–H8 distance.

The same definitions were applied to DR1, DB56, and DY54. For DB56, which is near-planar, the end-to-end distance coincides with the contour length due to the linear topology. For DR1, the contour length was measured by dividing the molecule into two parts at the N1 atom. For the planar DB56 molecule, the end-to-end distance and the contour length were identical. For DY54, the midpoint between atoms C9 and C10 was defined as a pivot point A. The molecule was then divided into two parts (H3-A and A-H9) to calculate the contour length. Measured segments overlaid as dashed guides are shown in Fig. S3.

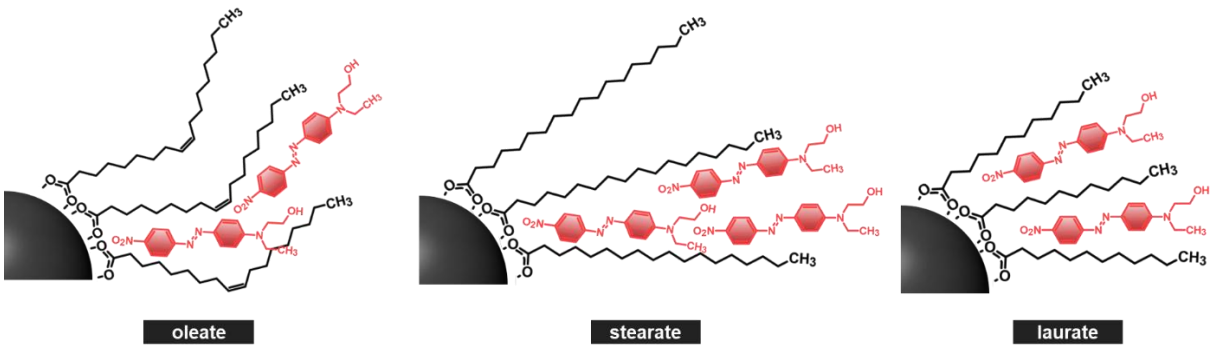


Fig. S4. Schematic representation of the effect of ligand chain length on dye removal efficiency.

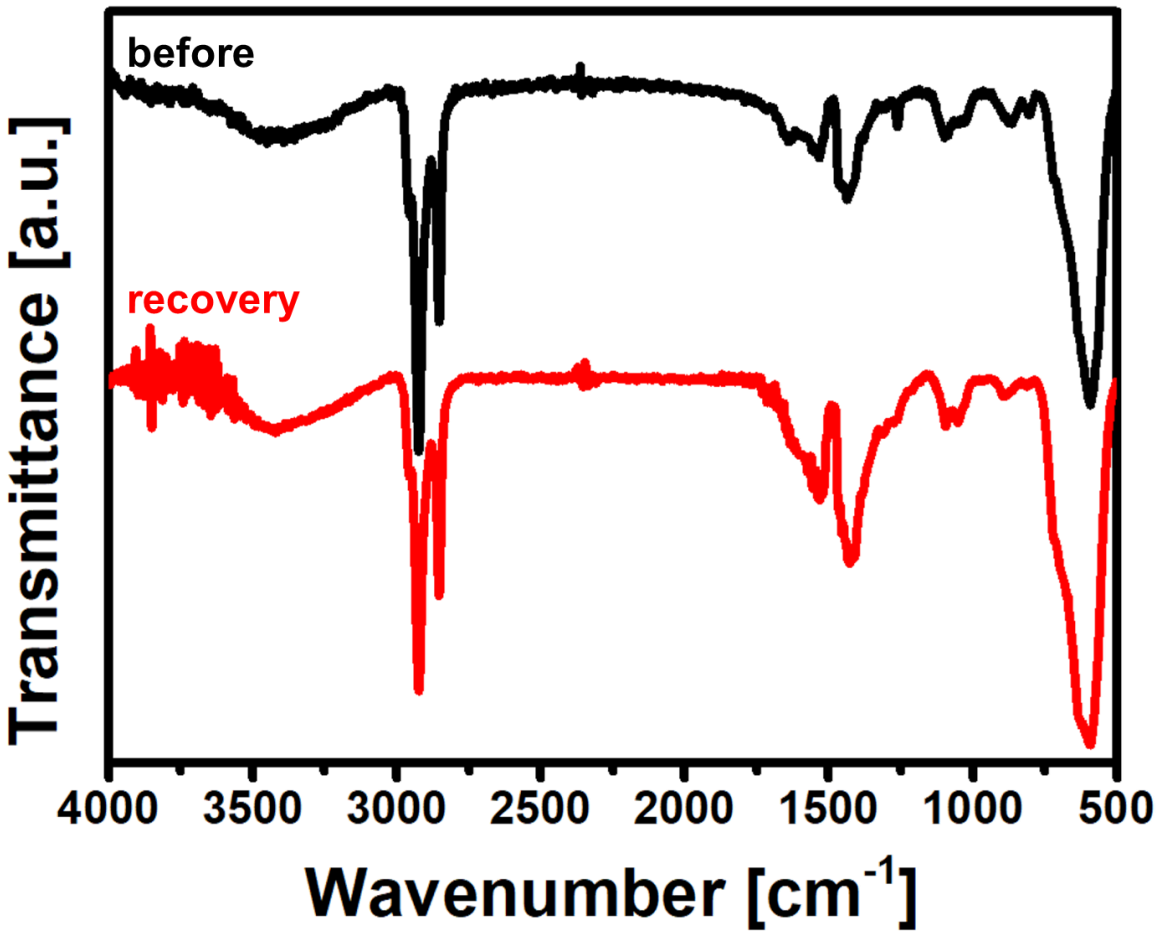
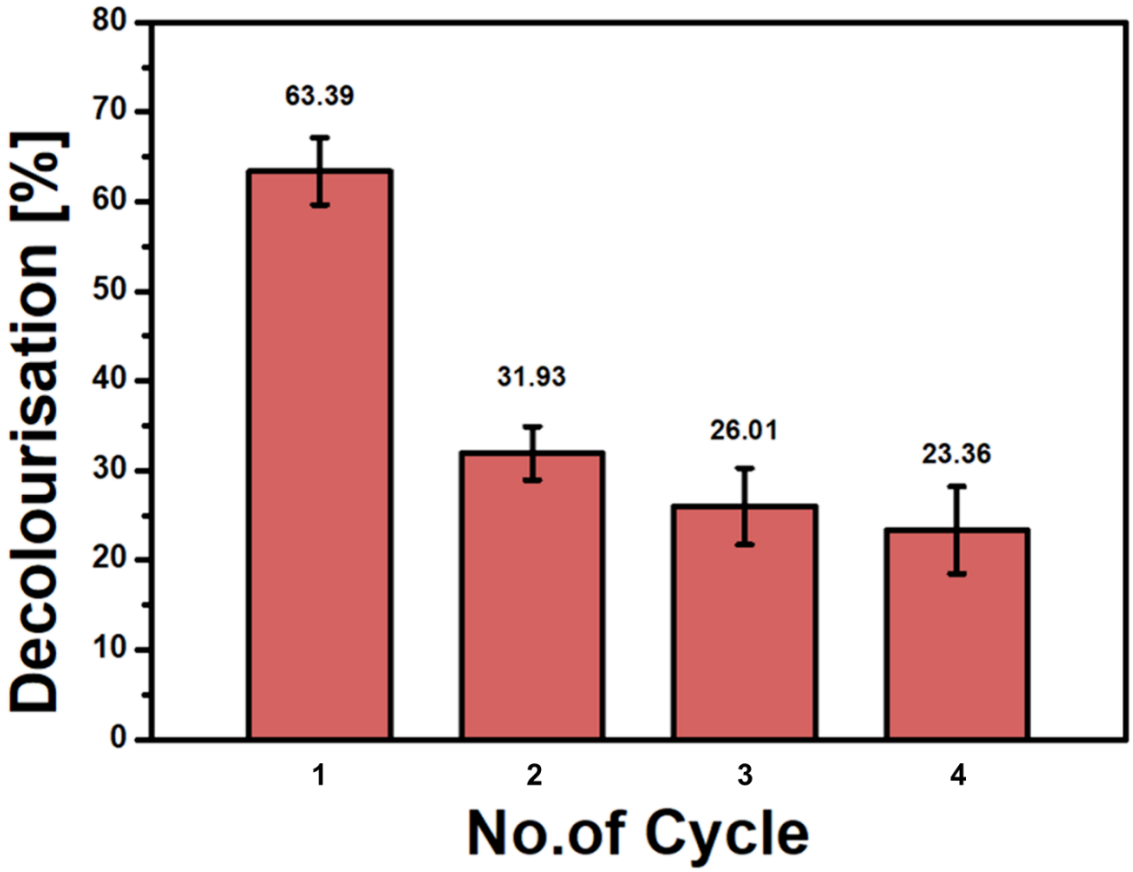


Fig. S5. FT-IR spectra of nanoparticles before dye adsorption and of nanoparticles recovered after dye desorption, recorded in the range of 4000–500 cm^{-1}.



FigS6. Decolorization efficiency of oleate-capped Fe_3O_4 over four adsorption-desorption cycles under PET-glycolysis simulated solution for the removal of DR60.

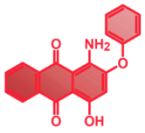
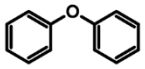
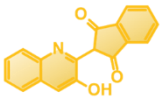
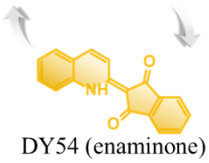
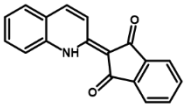
Disperse dye	Molecule	Rotation energy	ref
 DR60	 Diphenyl ether	0.36 kcalmol^{-1}	48
		0.40 kcalmol^{-1}	49
 DY54 (ketoenol)  DY54 (enaminone)	 Quinoline yellow	15.5 kcalmol^{-1}	50

Table. S1. Rotational energies of molecules characterized by bonds similar to DR60 and DY54.