Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Green tea polyphenol-reduced graphene oxide: Derivatisation, reduction efficiency, reduction mechanism and cytotoxicity

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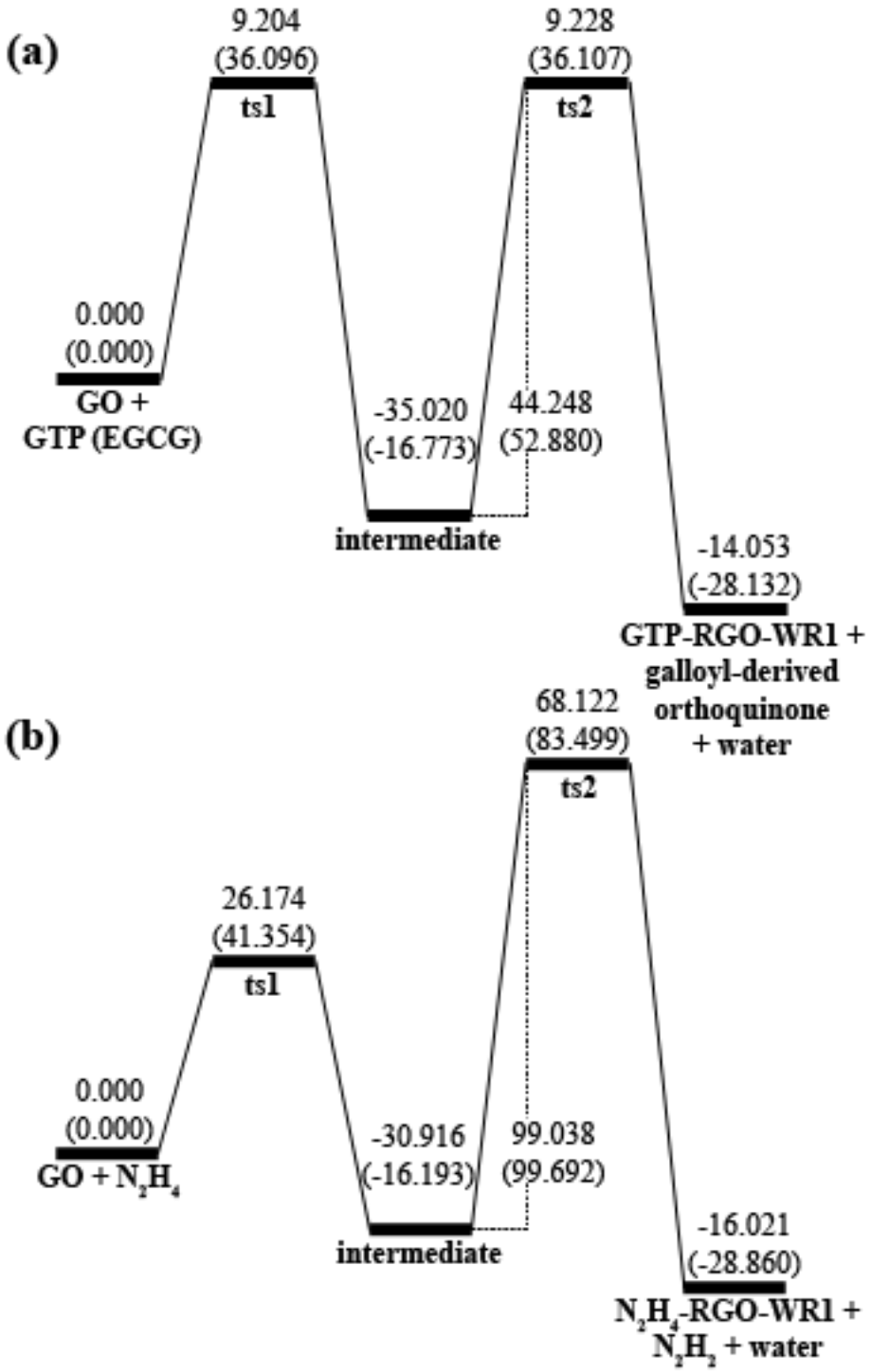

Fig. S1. Reaction energy profiles for the GO reduction using (a) GTP and (b) N_2H_4 calculated at the functional theory level of B3LYP/3-21G. The values of ΔH (kcal/mol) and ΔG (kcal/mol) at 90ºC were shown in normal typefaces without and with parentheses, respectively.

Table S1. Calculated total energies (E_{total}), entropies (S), Gibbs free energies (G), enthalpies (H) and zero-point energies (ZPE) for species investigated in this study at the functional theory level of B3LYP/3-21G.

	Species		E_{total}l (a.u.)	S (cal.mol^{-1}K^{-1})	G (a.u.)	H (a.u.)	ZPE (a.u.)
GO + GTP (EGCG)	reactant	GO + epoxide	-305.5824	78.4650	-305.6267	-305.5813	0.1041
		EGCG	-1666.9518	215.0720	-1667.0751	-1666.9506	0.3773
	ts1		-1972.5184	219.4850	-1972.6443	-1972.5172	0.4703
	intermediate		-1972.5889	243.2910	-1972.7285	-1972.5877	0.4869
	ts2		-1972.5183	219.5220	-1972.6442	-1972.5172	0.4704
	product	GTP-RGO-WR1	-230.8678	72.8740	-230.9088	-230.8667	0.1017
		galloyl-derived orthoquinone	-1665.7392	212.5490	-1665.8610	-1665.7380	0.3547
		water	-75.9507	46.8830	-75.9767	-75.9496	0.0198
GO + N_2H_4	reactant	GO + epoxide	-305.5824	78.4650	-305.6267	-305.5813	0.1041
		N_2H_4	-111.1723	59.9340	-111.2058	-111.1711	0.0517
	ts1		-416.7119	96.5980	-416.7666	-416.7107	0.1574
	intermediate		-416.8029	97.8570	-416.8583	-416.8017	0.1596
	ts2		-416.6450	96.0560	-416.6995	-416.6439	0.1477
	product	N_2H_4-RGO-WR1	-230.8678	72.8740	-230.9088	-230.8667	0.1017
		N_2H_2	-109.9629	53.9950	-109.9930	-109.9617	0.0258
		water	-75.9507	46.8830	-75.9767	-75.9496	0.0198

*1 a.u. = 627.5 kcal/mol