**Supplementary Information**

Robust curcumin-mustard oil emulsions for pro to anti-oxidant modulation of graphene oxide

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**Table S1**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| *T*/K | *ρlit/* | *n* | *t* | *ηlit* | *γlit* | *Kη* | *Kγ* |
|  | ×103kg m-3 | | sec | ±10-4 mPa.s | ±10-2mN/m |  |  |
| 298.15 | 0.997044a | 121 | 90.81 | 0.8937d | 71.97c | 0.00987 | 8806.045 |
|  |  | 122 | 90.81 |  |  | 0.00987 | 8806.045 |
|  |  | 122 | 90.82 |  |  | 0.00987 | 8806.045 |
|  |  | 122 | 90.81 |  |  | 0.00987 | 8806.045 |
|  |  | 122 | 90.82 |  |  | 0.00987 | 8806.045 |
|  |  |  |  |  |  |  |  |
| 303.15 | 0.995646a | 125 | 81.75 | 0.8007d | 71.18c | 0.00984 | 8936.086 |
|  |  | 125 | 81.75 |  |  | 0.00984 | 8936.086 |
|  |  | 125 | 81.74 |  |  | 0.00984 | 8936.086 |
|  |  | 125 | 81.75 |  |  | 0.00984 | 8936.086 |
|  |  | 124 | 81.75 |  |  | 0.00984 | 8936.086 |
|  |  |  |  |  |  |  |  |
| 308.15 | 0.994030b | 128 | 75.56 | 0.7225d | 70.38c | 0.00962 | 9061.25 |
|  |  | 128 | 75.57 |  |  | 0.00962 | 9061.25 |
|  |  | 129 | 75.56 |  |  | 0.00962 | 9061.25 |
|  |  | 128 | 75.57 |  |  | 0.00962 | 9061.25 |
|  |  | 128 | 75.56 |  |  | 0.00962 | 9061.25 |

Uncertainties in density, surface tension and viscosity measurements are less than ±1 x 103 kg. m-3, ±10-2mN/m and ±10-4 mPa.s respectively, with temperature uncertainties of ±0.01K.

aReference [1], b Reference [2], c Reference [3], d Reference [4]

[1] Handbook of Chemistry and Physics, 53rd Ed., p. F4, Updated by C.R. Snelling, 6/14/08.

[2] Lange, p. 1199. Due to the old definition of litre used at the time, the data from the Handbook was converted from old g/ml to g/cm3, by multiplying by 0.999973.

[3] Lange, p. 1663. Due to the old definition of litre used at the time, the data from the Handbook was converted from old g/ml to g/cm3, by multiplying by 0.999973.

[4] David R. Lide, CRC Handbook of Chemistry and Physics CRC Press, 2004, p. 6-201, ISBN 0849304857.

**Table S2**

|  |  |  |  |
| --- | --- | --- | --- |
| Ethanol dispersed GO | Oil-curc/ (w/v)% | 1:1 (SDS + DTAB) CLFs | Combined samples |
|  | 0.026 | 5.42 | 3.61 |
|  | 0.052 | 6.36 | 3.53 |
| 1.90 | 0.078 | 6.37 | 3.52 |
|  | 0.104 | 6.55 | 3.46 |
|  | 0.130 | 6.01 | 3.55 |
|  |  |  |  |

curc: curcumin, GO = graphene oxide

|  |  |  |  |
| --- | --- | --- | --- |
| **Sr. No.** | **Fatty Acid** | **Chemical Structure** | **Relative abundance (%)** |
| 1. | Erucic acid |  | 42.16 |
| 2. | Linoleic acid |  | 13.31 |
| 3. | α-Linolenic acid |  | 11.10 |
| 4. | Oleic acid |  | 9.56 |
| 5. | Eicosanoic acid |  | 6.36 |

**Table S3**

**Table S4**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Oil-curc (w/v)% | Particle Size (nm) | PDI | Particle Size (nm) | PDI |
|  | With SDS | | With DTAB | |
| 0.026 | 62.05 | 0.2858 | 1230.00 | 1.347 |
| 0.052 | 37.80 | 1.121 | 681.12 | 2.265 |
| 0.078 | 40.50 | 2.190 | 299.65 | 3.71 |
| 0.104 | 27.37 | 2.483 | 439.63 | 6.98 |
| 0.130 | 48.50 | 2.585 | 261.72 | 2.20 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **T/K** | **298.15** | **303.15** | **308.15** | **298.15** | **303.15** | **308.15** | **298.15** | **303.15** | **308.15** |
| **Property** | *ρo*(g/cm3) | | | *γo* (mN/m) | | | *ηo* (mPa.s) | | |
| SDS | 0.986267 | 0.984550 | 0.979587 | 56.39 | 54.84 | 54.46 | 1.0802 | 0.9698 | 0.8489 |
| DTAB | 0.988262 | 0.986748 | 0.981294 | 54.74 | 53.72 | 53.04 | 0.9414 | 0.9368 | 1.0695 |
|  | **For 1:1 (SDS + DTAB) CLF mixtures** | | | | | | | | |
|  | 0.988384 | 0.986772 | 0.985048 | 42.98 | 43.45 | 38.66 | 1.4596 | 0.9932 | 0.8971 |
|  | **For Combined samples (1:1 (SDS + DTAB) CLF mixtures + ethanol dispersed GO)** | | | | | | | | |
|  | 0.935132 | 0.927190 | 0.913718 | 32.32 | 31.47 | 31.72 | 2.1789 | 1.7571 | 1.4917 |
|  | **For ethanol dispersed GO (individual values)** | | | | | | | | |
|  | 0.790386 | 0.786115 | 0.781879 | 22.19 | 21.65 | 21.28 | 1.1525 | 1.0344 | 0.8936 |

**Table S5**

Standard uncertainties, u are: *u*(*T*) = 0.01 K, *u*(*ρ*) = 2×10-6 g/cm3*, u*(*γ)=* 1× 10-2 mN·m-1 and *u*(*η*) =1× 10-4mPa-s.

**Table S6**

|  |  |  |  |
| --- | --- | --- | --- |
|  | **298.15** | **303.15** | **308.15** |
| SDS | 0.024201 | 0.022353 | 0.020242 |
| DTAB | 0.015203 | 0.018034 | 0.019925 |
|  | **For 1:1 (SDS + DTAB) CLF mixtures** | | |
|  | 0.034201 | 0.022718 | 0.023148 |
|  | **For Combined samples (1:1 (SDS + DTAB) CLF mixtures + ethanol dispersed GO)** | | |
|  | 0.067563 | 0.055448 | 0.047475 |
|  | **For ethanol dispersed GO (individual values)** | | |
|  | 0.051942 | 0.047771 | 0.041993 |

**Table S7**

|  |  |  |  |
| --- | --- | --- | --- |
| Oil + curc /(w/v)% | *ρ*(SDS +DTAB) CLFs/ ( g•cm-3) | *ρ*(GO)/  (g•cm-3) | *ρ*(combined samples)/  ( g•cm-3) |
| **298.15 K** | | | |
| 0.026 | 0.988381 |  | 0.946157 |
| 0.052 | 0.988370 |  | 0.932014 |
| 0.078 | 0.988380 | 0.790386 | 0.947646 |
| 0.104 | 0.988372 |  | 0.948202 |
| 0.130 | 0.988375 |  | 0.931812 |
| **303.15 K** | | | |
| 0.026 | 0.986842 |  | 0.941796 |
| 0.052 | 0.986926 |  | 0.924668 |
| 0.078 | 0.986927 | 0.786115 | 0.944079 |
| 0.104 | 0.986921 |  | 0.944706 |
| 0.130 | 0.986918 |  | 0.923407 |
| **308.15 K** | | | |
| 0.026 | 0.985124 |  | 0.936277 |
| 0.052 | 0.985225 |  | 0.914165 |
| 0.078 | 0.985220 | 0.781879 | 0.940108 |
| 0.104 | 0.985222 |  | 0.941220 |
| 0.130 | 0.985224 |  | 0.908729 |

curc: curcumin. Standard uncertainties: *u*(*ρ*) = 2×10-6 g•cm-3, *u*(*T*) = 0.01 K.

**Table S8**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Oil-curc/(w/v)% | *γ*/(mN•m-1) | *η*/(mPa-s) | | *σ*/ (s•m-1) |
| **298.15 K** | | | | |
| 0.026 | 42.16 | 1.3136 | 0.031161 | |
| 0.052 | 33.41 | 1.1113 | 0.033258 | |
| 0.078 | 42.52 | 1.1298 | 0.026575 | |
| 0.104 | 44.40 | 1.1202 | 0.025228 | |
| 0.130 | 46.25 | 1.1185 | 0.024180 | |
| **303.15 K** | | | | |
| 0.026 | 41.06 | 1.0107 | 0.024612 | |
| 0.052 | 33.43 | 0.9700 | 0.029018 | |
| 0.078 | 39.00 | 1.0255 | 0.026295 | |
| 0.104 | 41.58 | 0.9901 | 0.023815 | |
| 0.130 | 42.82 | 0.9806 | 0.022903 | |
| **308.15 K** | | | | |
| 0.026 | 37.65 | 0.8924 | 0.023705 | |
| 0.052 | 31.01 | 0.8349 | 0.026919 | |
| 0.078 | 36.05 | 0.8893 | 0.024666 | |
| 0.104 | 39.09 | 0.8813 | 0.022544 | |
| 0.130 | 38.65 | 0.8850 | 0.022897 | |

Curc: curcumin. Standard uncertainties, u are: *u*(*T*) = 0.01 K, *u*(*γ)=* 1× 10-2

mN•m-1, *u*(*η*) =1× 10-4mPa-s and *u*(*σ*) = 0.00002 (s·m-1).

**Table S9**

|  |  |  |  |
| --- | --- | --- | --- |
| Oil-curc/(w/v)% | *γ*/(mN•m-1) | *η*/(mPa-s) | *σ*/ (s•m-1) |
| **298.15 K** | | | |
| 0.026 | 33.21 | 2.1486 | 0.064702 |
| 0.052 | 32.82 | 2.1084 | 0.064228 |
| 0.078 | 32.92 | 2.1205 | 0.064418 |
| 0.104 | 33.16 | 2.2024 | 0.066406 |
| 0.130 | 31.29 | 2.2155 | 0.070795 |
| **303.15 K** | | | |
| 0.026 | 32.77 | 1.8241 | 0.055663 |
| 0.052 | 32.62 | 1.7701 | 0.054264 |
| 0.078 | 33.19 | 1.8160 | 0.054715 |
| 0.104 | 33.10 | 1.9766 | 0.059724 |
| 0.130 | 31.92 | 1.8541 | 0.058101 |
| **308.15 K** | | | |
| 0.026 | 32.87 | 1.5410 | 0.046885 |
| 0.052 | 32.64 | 1.4844 | 0.045465 |
| 0.078 | 33.45 | 1.6058 | 0.047996 |
| 0.104 | 32.93 | 1.5364 | 0.046657 |
| 0.130 | 31.37 | 1.5410 | 0.049121 |

Curc: curcumin. Standard uncertainties, u are: *u*(*T*) = 0.01 K, *u*(*γ)=* 1× 10-2

mN•m-1, *u*(*η*) =1× 10-4mPa-s and *u*(*σ*) = 0.00002 (s·m-1).

**Table Captions**

**Table S1** Calibration data: Density, *ρLiterature*, PDN, *nExperimental*, VFT, *tExperimental*, viscosity, *ηLiterature*, surface tension, *γLiterature*, calibration constant for viscosity, *Kη* and surface tension, *Kγ*, at T = (298.15, 303.15 and 308.15) K.

**Table S2** Room temperature (RT) pH values of 1:1 SDS and DTAB CLF mixtures and combined samples having 40% GO, as functions of increasing oil-curc contents.

**Table S3** Fatty acid (FA) profile of mustard oil with relative abundance of major FA. Highest contribution of erucic acid (42.16%) argues a significant hydrophobicity with > 10% contributions of multiple unsaturated linoleic and α-linolenic acid.

**Table S4** Particle size (PS) and PDIs of individual SDS and DTAB CLFs, lower sizes and PDIs for SDS formulations infers a greater curc monodispersion than DTAB.

**Table S5** *ρo*(g/cm3), *γo*(mN/m) and *ηo*(mPa•s) for SDS and DTAB CLFs (separately), 1:1 (SDS and DTAB) CLF mixtures, ethanol dispersed GO and combined samples. Highest *η* and decreasing *ρ*, *γ* for combined samples compared to 1:1 (SDS and DTAB) CLF mixtures infer enhanced curc monodispersion on GO inclusion.

**Table S6** *σo*/(s•m-1) for SDS and DTAB CLFs (separately), 1:1 (SDS and DTAB) CLF mixtures, ethanol dispersed GO and combined samples. (97.55 to 105.09)% increments from 1:1 CLF mixtures to combined samples infer a dispersion supporting role of GO.

**Table S7** Densities (*ρ*, g•cm-3) of ethanol dispersed GO, 1:1 SDS and DTAB CLF mixtures and combined samples, as implicit functions of increasing oil-curc contents.

**Table S8** *γ*/(mN•m-1), *η*/(mPa-s) and *σ*/(s•m-1) of 1:1 SDS and DTAB CLF mixtures at (298.15, 303.15 and 308.15) K, as functions of increasing oil-curc (w/v)%.

**Table S9** *γ*/(mN•m-1), *η*/(mPa-s) and *σ*/(s•m-1) of combined samples having 40% (v/v) GO at (298.15, 303.15 and 308.15) K, as functions of increasing oil-curc (w/v)%.

**Figures**

**Fig.S1**





(a)

K.E. ≠ P.E.



(b)

(c) (d)



(e)



(f)



(g)

**Fig.S2**



**Fig.S3**



**Fig.S4(a)**

Hydrophobicity driven CF increment and decrement

**Fig.S4(b)**

**Micellization**

**Aggregation**

**Fig.S4(c)**

**Oil-curc concentration driven distinctions of SDS and DTAB chemical activities**

**Temperature distinguished SDS and DTAB chemical activities**

**Fig.S4(d)**

Critical concentration for temperature dependent finer (SDS at 303.15 K) and weaker curc dispersion (SDS at 308.15 K and DTAB at 298.15 K)

**Aggregation**

**Micellization**

**Fig.S5(a)**

Higher u with SDS and DTAB at 308.15 K indicates strengthened compactness of formulation ingredients

**Fig.S5(b)**

# Decreased IMFs: finer curc dispersion

Decreasing IMFs: weaker interactions: finer curc dispersion

No significant dispersion

changes with increasing

temperature

**Fig.S6(a)**

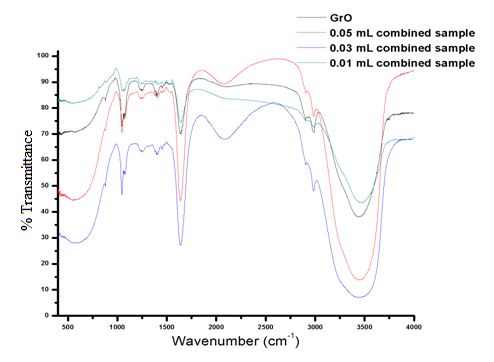
**Fig.S6(b)**

C:\Users\Dell\Desktop\Parth Paper\GO 2.tif

**Fig.S6(c)**

Suppressed C-C and C=C SF of fatty acids and surfactants

Less interactive fingerprint regions of curc biound in oil FA (C-C, C=C, C-H SF)



-C-H SF (alkane group vibration inferring GO structural involvement)

-C=O SF of curc β-diketonic backbone: engages –OH and –COOH functionality in GO, ethanol, glycerol and oil FA

-OH SF (3467 to 3489) cm-1 (Curc interactions with ethanol-glycerol-water bound FFA)

**Figure Captions**

**Fig.S1**Molecular structures of (a) SDS, (b) DTAB, (c) Tw-20, (d) Tw-40, (e) ethanol, (f) glycerol, (g) water, (h) curc (keto form), (i) curc (enol form) and (j) DPPH•. The structural functionalities are key players of vigorous kinetic impacts within nanoemulsion boundaries.

**Fig.S2** Schematic representation of 1:1 SDS and DTAB CLF mixtures and combined samples, as per the speicific polydispersity indices (PDIs). Inclusion of GO has decreased the PDI although the characteristic sizes of oil-dispersed curc droplets have increased.

**Fig.S3** Comparative antioxidant activities of GO (alone) and combined samples (having 40% GO in 1:1 SDS and DTAB CLF mixtures). Vibrant kinetic activities of CLFs catalyze a transition from pro-oxidant (< 50% FRSA) to antioxidant (> 50% FRSA) GO state.

**Fig.S4**(a-d)*ρ*, *γ*, *η* and *σ* variations (respectively) for SDS and DTAB CLFs, as functions of increasing oil-curc hydrophobicities. Instantaneous *γ* increments and decrements for SDS and DTAB, from 0.052 to 0.078 (w/v)% oil-curc contents, alongwith lower values for DTAB formulations infer a finer curc distribution with more hydrophobic DTAB.

**Fig.S5** The sound velocity, *u*(m•s-1)variations with respect to increasing oil-curc contents for(a) SDS, DTAB CLFs and their 1:1 mixtures, and (b) 1:1 CLF mixtures and combined samples. Decrements and increments respectively account for finer and weaker dispersion, owing to the characteristic property of sound to travel fastest in the medium having least intermolecular spaces.

**Fig.S6** FT-IR spectra for (a) mustard oil and its curc mixture, (b) GO and (c) select combined samples. Significant mismatch in oil and oil-curc SF indicates a weaker curc binding in mustard oil. GO has depicted characteristic C=O (~ 1620 cm-1) and C=C (~ 1060 cm-1). All combined samples, displayed ~ 1600 cm-1, 2000 cm-1 and ~ 3500 cm-1 characteristic SF, pointing out at vibrant –C=O, -OH, C-C, C=C, C-H curc and oil FA chemical controls.