Supporting Information

Acrylate-Based Poly-High Internal Phase Emulsions for Effective Enzymes Immobilization and Activity Retention: from Computationally-Assisted Synthesis to Pharmaceutical Applications

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Table SI1. Factors, experimental domain, and concentration levels considered for the polymerization.

Factor	Units	Low level	High level
A: BA + GMA	% w/w	0.7	0.8
B: Surfactant	% w/w	0.05	0.2
C: TMPT	% w/w	0.09	0.15

Constraint: A+B+C = 1

Table SI2. Throats and void diameters of each polyHIPEs expressed as average values ± SD (n=25)

polyHIPE	*Throats diameter (µm)*	*Voids diameter (µm)*
1	1.5 ± 0.5	3.9 ± 1.5
2	0.4 ± 0.1	1.5 ± 0.3
4	1.4 ± 0.3	3.9 ± 1.0
5	0.7 ± 0.2	2.1 ± 0.8
6	0.7 ± 0.2	2.4 ± 0.7
8	1.7 ± 0.3	7.7 ± 3.8

Table SI3. Throats and void diameter of polyHIPEs 11.a, 11.b, 11.c and 11.d expressed as average values ± SD (n=25).

polyHIPE	*Throats diameter (µm)*	*Voids diameter (µm)*
11.a	1.2 ± 0.1	4.7 ± 0.5
11.b	1.1 ± 0.1	4.7 ± 0.5
11.c	1.2 ± 0.1	4.6 ± 0.4
11.d	1.2 ± 0.1	4.7 ± 0.5

Table SI4. Weight loss and swelling in water and THF and semiquantitative analysis by ATR-FTIR of epoxy groups hydrolysis of the obtained materials (11a-11d). The values were expressed as average values ± SD (n=3).

Sample	*WL in H2O*	*WL in THF*	*SW in H2O*	*SW in THF*	*Peak area rate A/B**
11.a	8.10 % ± 2.56 %	6.77 % ± 6.74 %	4.42 ± 0.16	7.42 ± 0.70	0.110/0.213
11.b	8.46 % ± 5.66 %	4.92 % ± 0.68 %	3.86 ± 0.28	6.47 ± 0.25	0.112/0.195
11.c	6.35 % ± 1.54 %	5.75 % ± 2.64 %	4.85 ± 0.58	6.56 ± 0.45	0.130/0.220
11.d	6.97 % ± 2.08 %	6.25 % ± 0.98 %	4.11 ± 0.83	6.37 ± 0.35	0.121/0.206

**The ATR-FTIR semiquantitative analysis was performed by calculating the rate of the areas epoxy/ester 908/1720 cm^{-1} (A) and 847/1720 cm^{-1} (B), these values are adimensional and to higher values corresponds a lower hydrolysis.*

Table SI5. Results of the validation of the models. The coordinates of the point selected for the validation experiments were: BA+GMA: 0.788%, Surfactant: 0.062%, TMPT: 0.15%. These coordinates correspond to coded upper level-bound pseudocomponents: u_1: 0.08; u_2: 0.92; u_3: 0.00.

Response	**Value measured** **Mean ± SD**, (n)	**Value predicted by the model** **value computed ± CI(95%)**	**Relative error** **(%)**
SWaq (%)	4.3 ± 0.6 (2)	4.9 ± 0.3	14
SWthf (%)	6.7 ± 0.6 (2)	7 ± 1	4
WLaq (%)	9 ± 5 (2)	11 ± 3 (median 9.6)§	22
WLthf (%)	6 ± 3 (2)	10 ± 7	67
PID (µm)	1.2 ± 0.1 (4)	1.5 ± 0.4	26
VD (µm)	4.7 ± 0.1 (4)	5 ± 2	12

Responses abbrevations: SWaq, swelling of the polymer in water; SWthf, swelling of the polymer in THF; WLaq, weight loss after polymer wetting with water; and WLthf, weight loss after polymer wetting with THF; PID, polymer throats internal diameter; VD, polymer voids diameter are measured in µm.

§ The WLaq response is computed as mean and median and compared with the data obtained in the validation experiments.

CI(95%), confidence interval computed at the 95% of probability level.

n, number of replicate measurements carried out independently from those used to build the model.

Relative error % = 100* (Value predicted – Value measured)/Value measured.

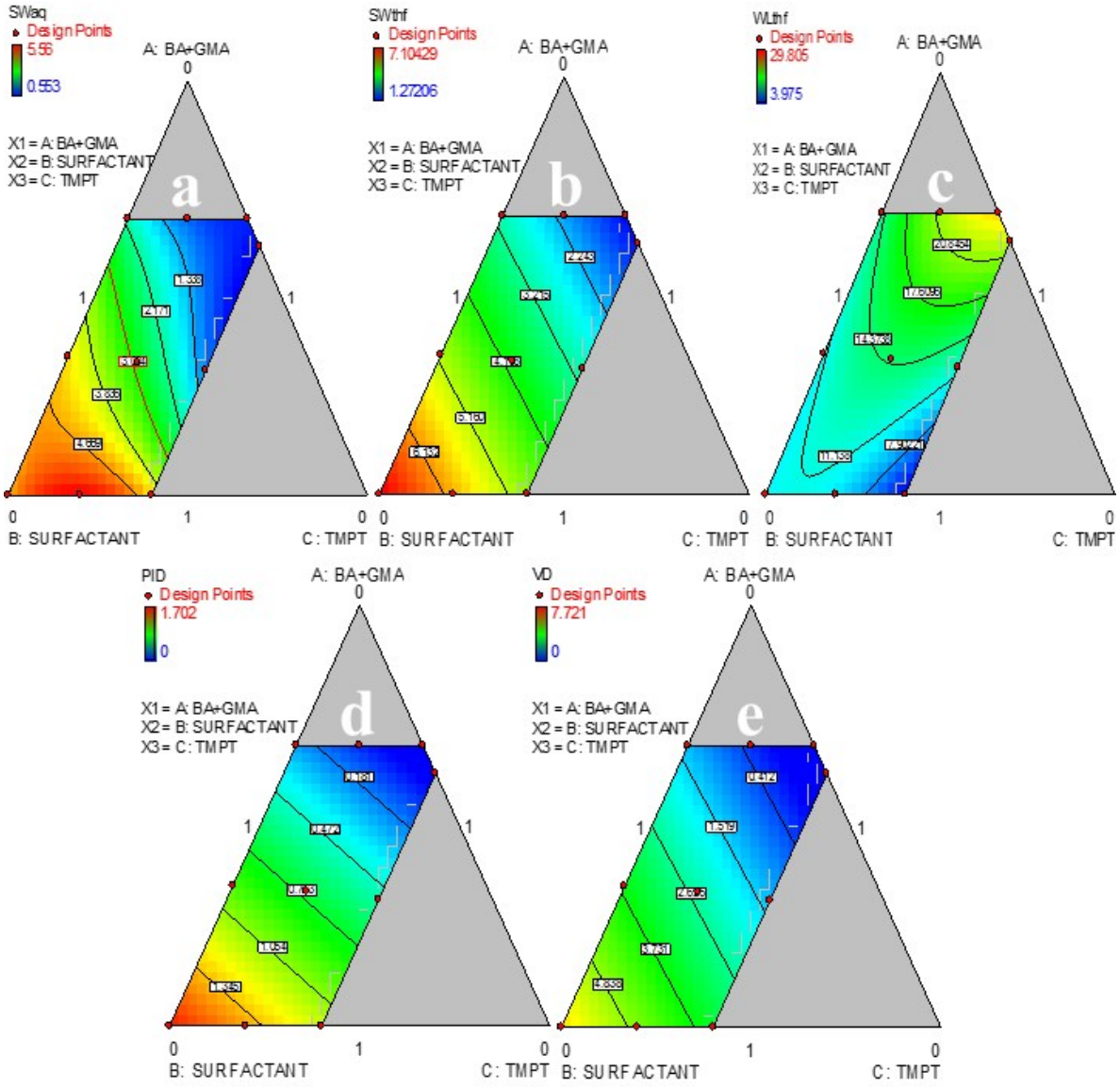

Figure SI1. Response surfaces for the five statistically significant models computed and validated: 4a) Swelling in water (SWaq%), 4b) Swelling in THF (SWthf%), 4c) Weight loss in THF (SWthf%), 4d) Throats internal diameter (PID, µm), and 4e) Voids diameter (VD, µm).

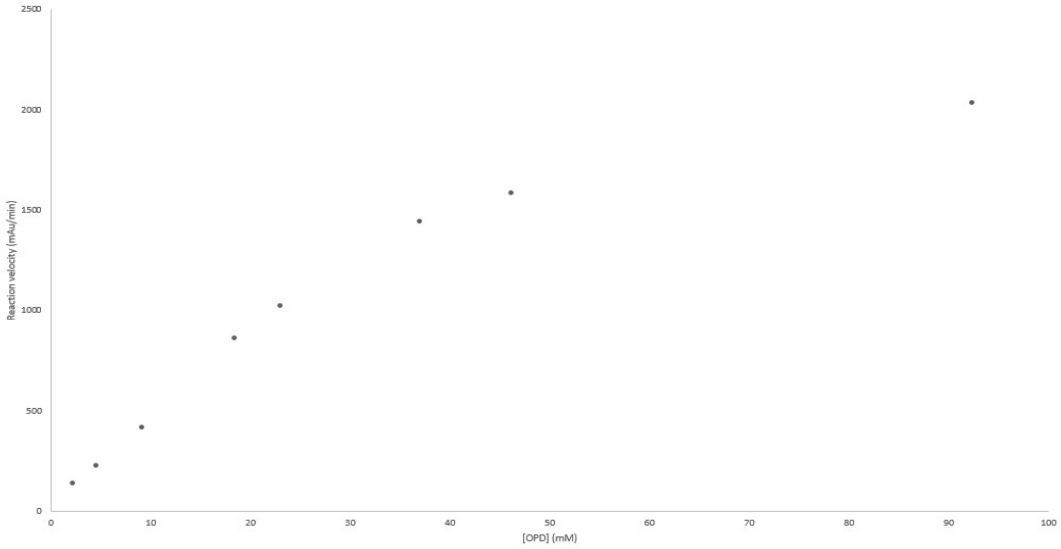

Figure SI2. Relation between OPD concentration and reaction velocity. OPD concentrations were expressed as mM.

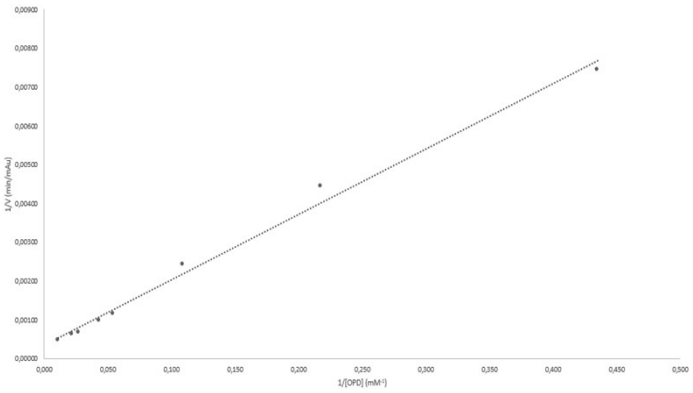

Figure SI3. Double reciprocal plot of relation between OPD concentration (mM) and reaction velocity