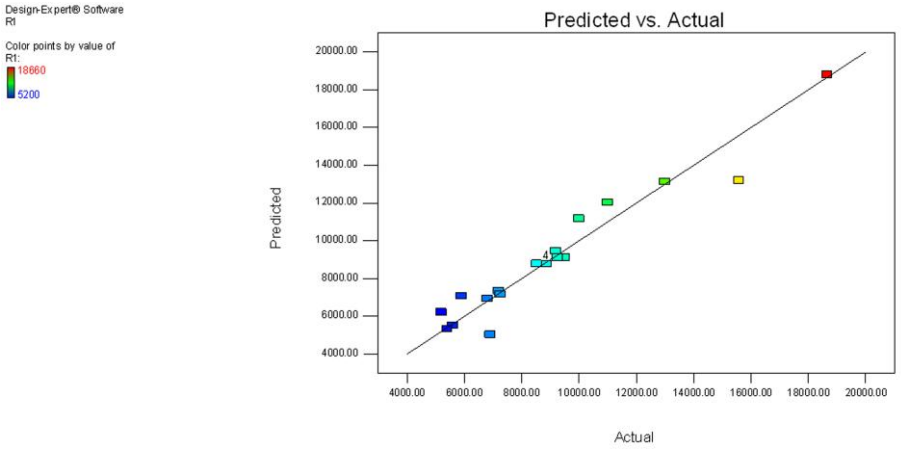

Fig. A: the actual versus predicted values for the Y_1

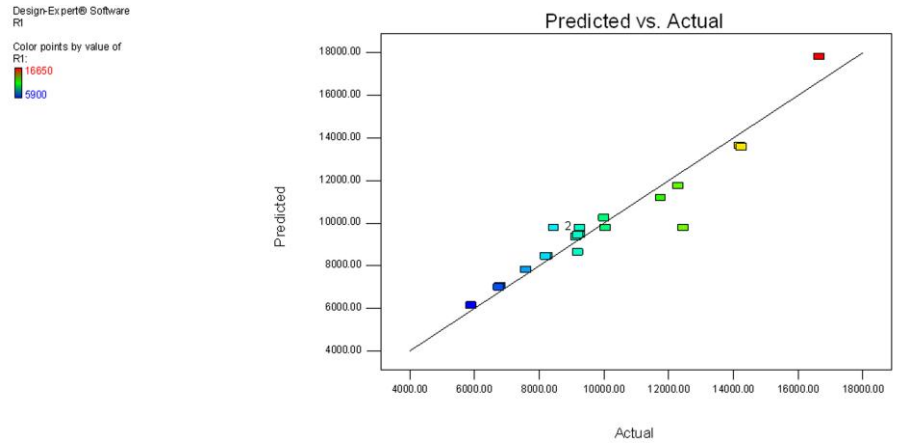

Fig. B: relation between actual and predicted values (Parity plot) for Y_2

Table A: Effective factors and factor levels for Synthesis of MePEC.

Factors	unit	Levels				
		Lowest -1.62	low -1	Center 0	high 1	Highest 1.62
A)Time	hour	1.95	4	7	10	12.05
B) Temperature	^{0}C	109.66	125	147.50	170	185.34
C)MePEG/Cl ratio	%wt	24.77	35	50	65	75.23
D) amount of Sn(OCT)2	mg	0.16	0.25	0.38	0.50	0.59

The estimated quadratic model in terms of coded factors (for GPC) is:

$$Y_1 = +9121.95 + 1218.94 * X_1 + 1724.35 * X_2 - 2427.32 * X_3 - 200.38 * X_4 + 632.12 * X_1 * X_2 - 532.50 * X_1 * X_3 - 1120.65 * X_1 * X_4 - 1570.00 * X_2 * X_3 + 236.44 * X_2 * X_4 + 482.50 * X_3 * X_4 \quad \text{(eq. 1)}$$

and in terms of actual factors (for GPC) is:

$$Y_1 = -23483.71373 + 737.33258 * \text{Time} + 212.15237 * \text{Temperature} + 510.66016 * \text{MePEG/Cl} - 5950.74624 * \text{Sn(Oct)}_2 + 9.36472 * \text{Time} * \text{Temperature} - 11.83333 * \text{Time} * \text{MePEG/Cl} - 2988.39916 * \text{Time} * \text{Sn(Oct)}_2 - 4.65185 * \text{Temperature} * \text{PEG/Cl} + 84.06659 * \text{Temperature} * \text{Sn(Oct)}_2 + 257.33333 * \text{PEG/Cl} * \text{Sn(Oct)}_2$$

The estimated quadratic model in terms of coded factors (for NMR) is:

$$Y_2 = +9775.71 + 951.37 * X_1 + 431.09 * X_2 - 1262.10 * X_3 - 981.10 * X_4 - 356.10 * X_1 * X_2 - 237.50 * X_1 * X_3 + 418.59 * X_1 * X_4 + 175.00 * X_2 * X_3 + 76.37 * X_2 * X_4 + 762.50 * X_3 * X_4 - 400.16 * X_1^2 - 727.20 * X_2^2 + 2092.39 * X_3^2 - 700.68 * X_4^2 \quad \text{(eq. 2)}$$

final equation in terms of actual factors (for NMR):

$$Y_2 = +3979.27570 + 1563.03506 * \text{Time} + 443.73118 * \text{Temperature} - 1206.12719 * \text{PEG/Cl} - 367.86891 * \text{Sn(OCT)}_2 - 5.27549 * \text{Time} * \text{Temperature} - 5.27778 * \text{Time} * \text{PEG/Cl} + 1116.23354 * \text{Time} * \text{Sn(OCT)}_2 + 0.51852 * \text{Temperature} * \text{PEG/Cl} + 27.15225 * \text{Temperature} * \text{Sn(OCT)}_2 + 406.66667 * \text{PEG/Cl} * \text{Sn(OCT)}_2 - 44.46260 * \text{Time}^2 - 1.43645 * \text{Temperature}^2 + 9.29950 * \text{PEG/Cl}^2 - 44843.76331 * \text{Sn(OCT)}_2^2$$

Table B: Results of calibration and validation of the PLS models on the raw spectra and spectra with various pretreatments.

Pretreatment process	PLS factors	Calibration		Cross-validation		SD
		R^2	RMSEC[a]	R^2	RMSECV[b]	
Raw spectra	8	0.1352	37.7300	0.1352	37.7780	1190.2879
Mean centering	8	0.14943	34.3589	0.14939	34.2584	1070.2888
Auto scaling	7	0.25236	1.3258	0.25936	1.3324	503.3395
Auto net analysis signal	3	0.88373	0.3248	0.84445	0.5625	49.2371

[a]Root-mean-square error of calibration.
[b]Root-mean-square error of cross-validation.

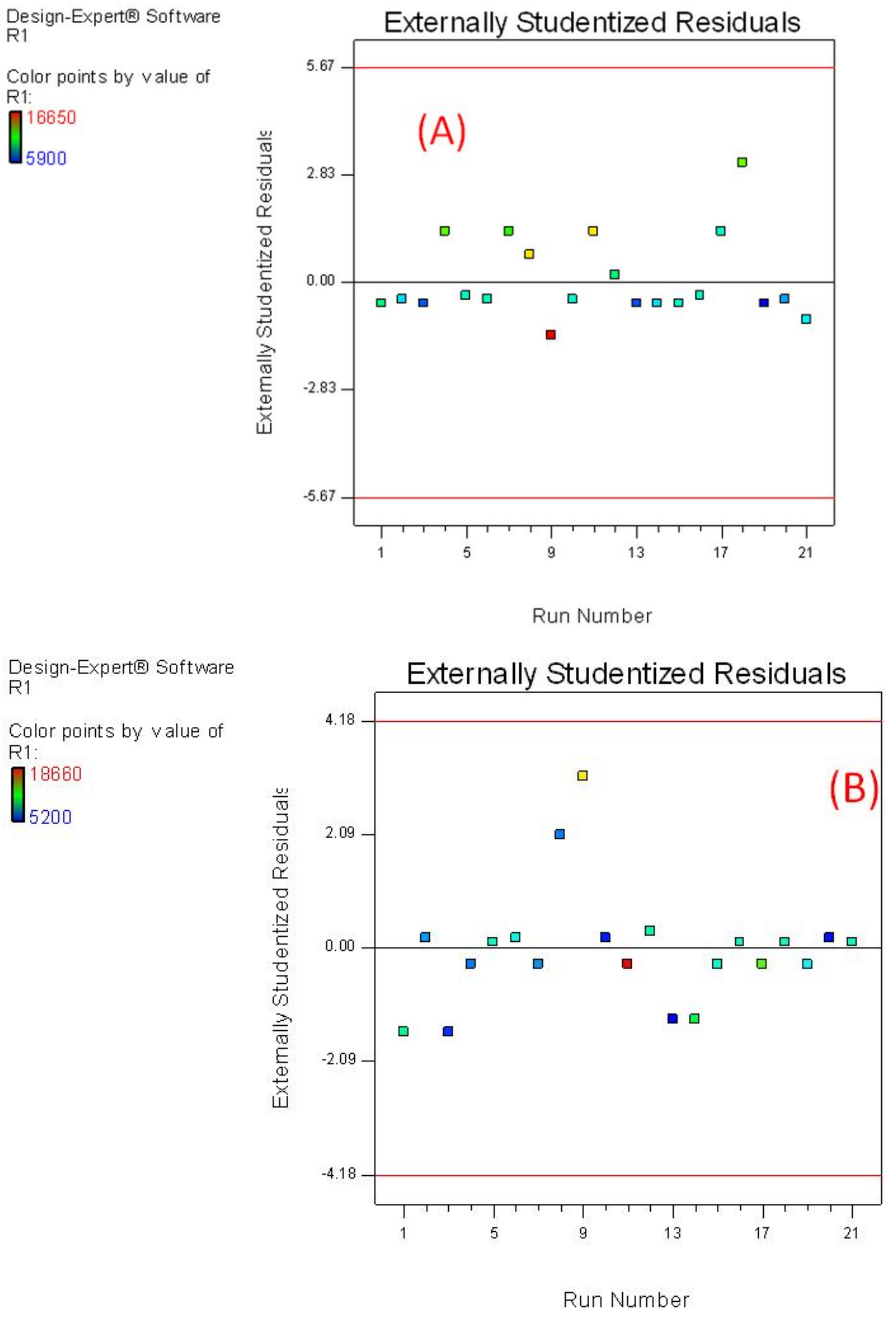

Fig. C: The externally studentized residuals plot determined for A) Y_1 response, B) Y_2 response.

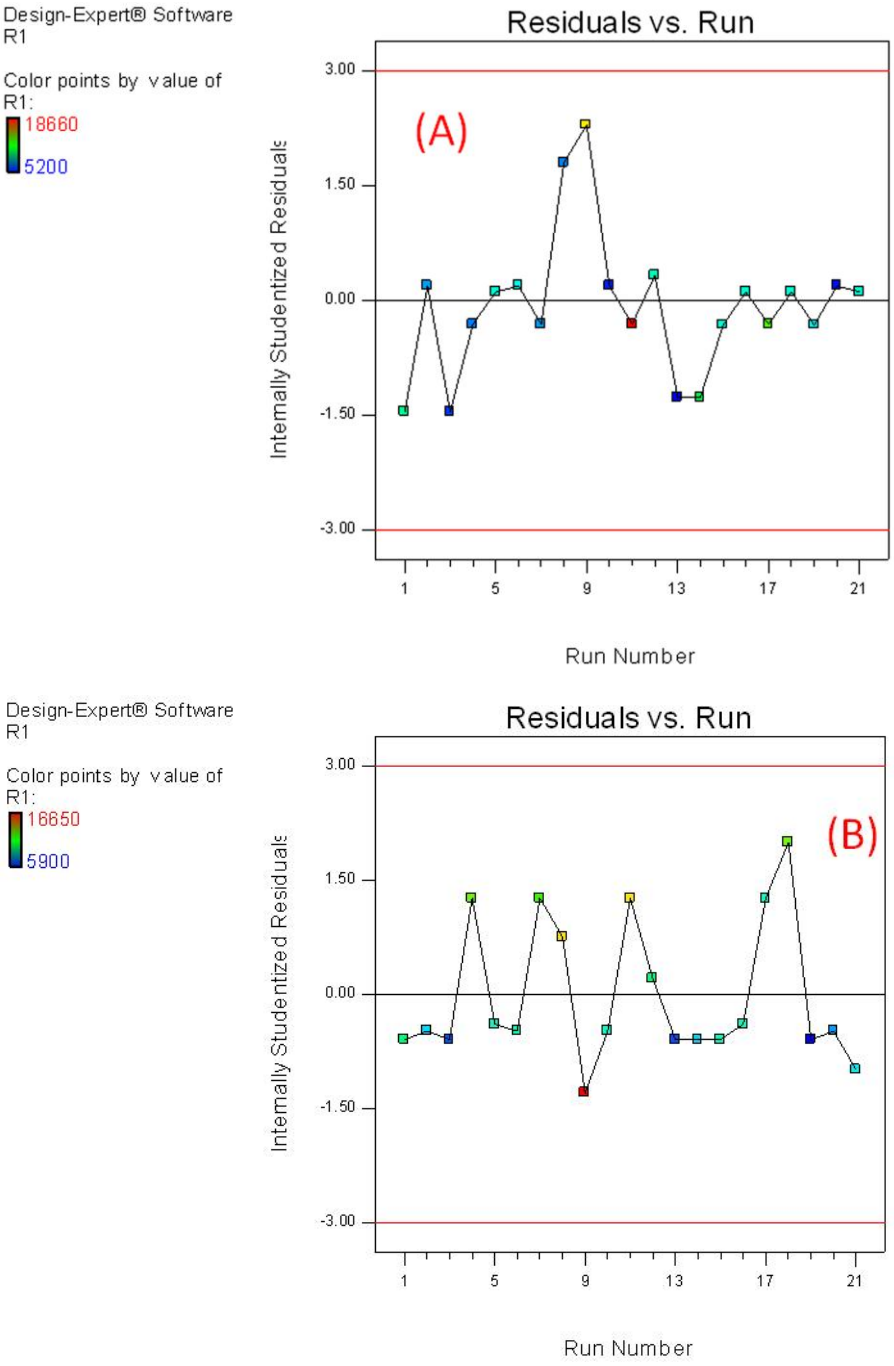

Fig. D: The internally studentized residuals plot determined for A) Y_1 response, B) Y_2 response.