

Supporting Information

Using nano-QSAR to determine the most responsible factor(s) in gold nanoparticles exocytosis

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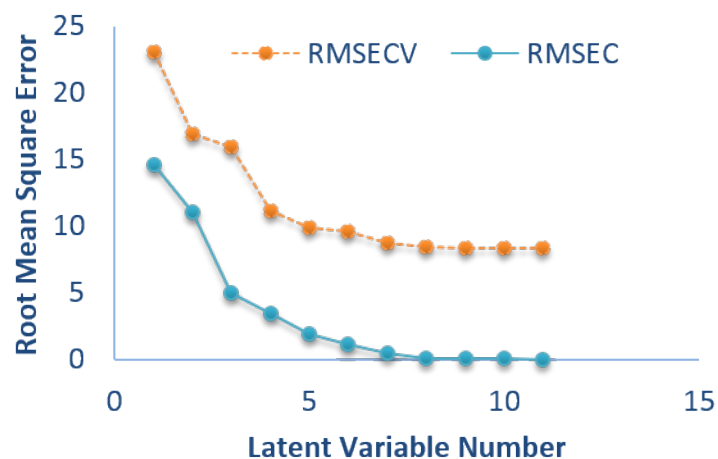


Figure S1. Variance captured by each LV and statistics of RMSEC (filled) and RMSECV (dashed) vs LV number. To avoid overfitting, four latent variables were chosen.

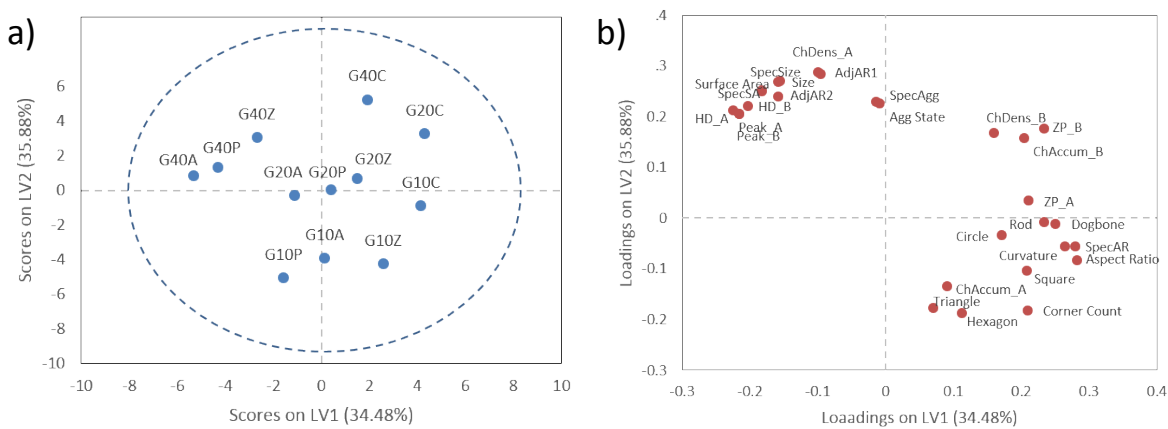


Figure S2. a) Score plot and b) loading plots of PLS regression model.

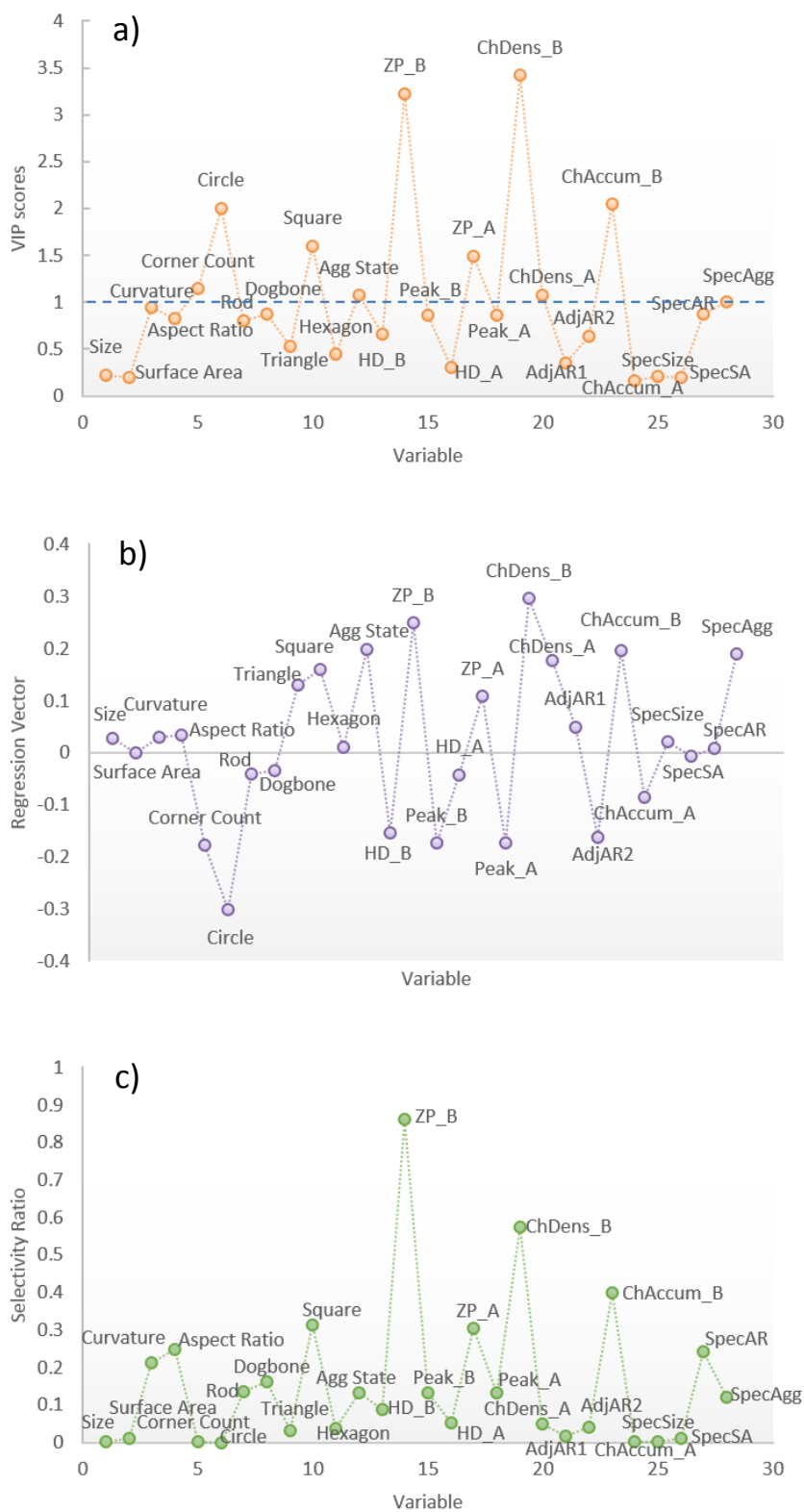


Figure S3. Important variables selected by a) VIP scores, b) selectivity ratio and c) regression vector of the applied PLS model

Table S1. Summarized list of essential attributes for the exocytosis of GNPs indicated by VIP scores, SR and regression vectors

VIP Scores	Important selected variables								
	ChDensB	ZP_B	ChAccumB	Circle	Square	ZP_A	Corner Count	Agg State	ChDensA
Selectivity Ratio	ZP_B	ChDensB	ChAccumB	Square	ZP_A				
Regression Vector	ChDensB	ZP_B	ChAccumB	Agg State	ChDensA	SpecAgg	Square	Triangle	ZP_A