



**Fig. S7: Evaluation of similarity diagrams**

Shaded “reference” areas, indicate areas covered by data points obtained from modeled spectra ( $\blacktriangle$ ) within a 10 by 10 grid. Percentage of data points from measured spectra ( $\blacklozenge$ ) within the reference areas was evaluated.

Results are given as % (n/m), with m being the total number of data points and n the number of data points within the reference area:

$ANN_{sub}^{HT}$	98.2% (276/281)	$ANN_{sub}^{IPEC}$	80.1% (133/166)
$ANN_{sub}^{HT+EGTA}$	97.3% (109/112)	$ANN_{sub}^{IPEC+EGTA}$	100% (26/26)
$ANN_{epi}^{HT}$	98.2% (276/281)	$ANN_{epi}^{IPEC}$	82.5% (137/166)
$ANN_{epi}^{HT+EGTA}$	95.5% (107/112)	$ANN_{epi}^{IPEC+EGTA}$	96.2% (25/26)

High percentages indicate that modeled spectra used for ANN training appropriately cover physiologically relevant parameter ranges.