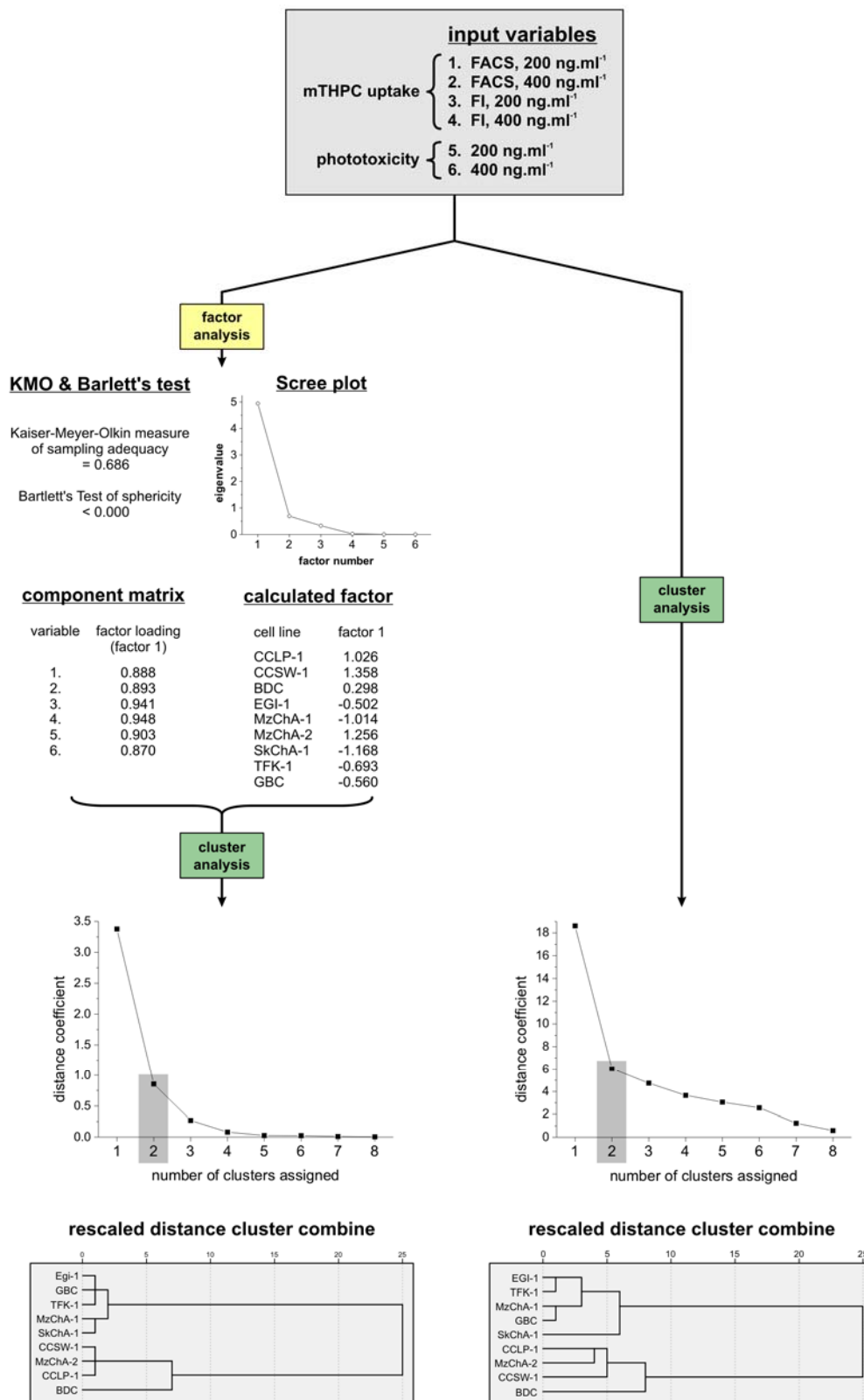


**Supplementary Figure 1. Details on Factor analysis and classification by hierarchical cluster analysis.**

PDT-related variables (uptake and phototoxicity) are subjected to factor analysis in order to identify a representative factor summarising these variables. This calculated factor or the raw data (uptake of mTHPC and phototoxicity) was subsequently used for hierarchical cluster analysis. The eigenvalue associated with each factor represents the variance explained by that particular linear component. The scree plot of the eigenvalue shows that the one factor most reliably represents all input variables (eigenvalue > 1). The factor loadings in the component matrix are a measure of correlation of the calculated factor with each variable and shows very high loadings for all variables ( $\geq 0.870$ ). The distance coefficients extracted from the agglomeration schedule gives the value of the distance statistic used to form the cluster(s). For both approaches, the two cluster solution is most suitable to describe the case's cluster assignment.





**Supplementary Table 2. Raw data on histological characterisation.** (adopted from Ref. <sup>22</sup>)

	<b>Ck19<sup>a</sup></b>	<b>Ck7<sup>a</sup></b>	<b>Ck8/18<sup>a</sup></b>	<b>E-Cadherin<sup>a</sup></b>	<b>Vimentin<sup>a</sup></b>	<b>Cyclin D1<sup>a</sup></b>	<b>Ki67<sup>a</sup></b>	<b>Morphology<sup>b</sup></b>	<b>PAS<sup>c</sup></b>	<b>CAB<sup>d</sup></b>
<b>CCLP-1</b>	0	0	1	0	12	6	12	3	0	1
<b>CCSW-1</b>	1	1	6	0	8	12	8	n.d.	n.d.	n.d.
<b>BDC</b>	12	12	12	4	12	6	12	2	0	2
<b>EGI-1</b>	8	0	12	12	0	6	12	1	1	1
<b>MzChA-1</b>	12	6	8	2	0	0	4	2	1	2
<b>MzChA-2</b>	0	0	8	1	8	4	12	3	0	1
<b>SkChA-1</b>	12	8	12	2	3	4	4	2	1	2
<b>TFK-1</b>	4	8	8	8	1	1	4	2	1	2
<b>GBC</b>	12	12	12	8	1	0	6	1	1	1

<sup>a</sup>...semiquantitative immunocytochemistry on cell blocks  
(quickscore method, range 0-12)

<sup>b</sup>...tumour xenograft growth type:  
ductal = 1, mixed (ductal / solid) = 2, solid = 3

<sup>c</sup>...epithelial mucopolysaccharides in xenograft tumours, PAS reaction  
(score 0 = negative, 3 = strong (>50%) reaction)

<sup>d</sup>...extracellular collagen content in xenograft tumours, chromotrope-aniline blue staining  
(score 0-3 for negative to strong staining)