

Supplementary Information

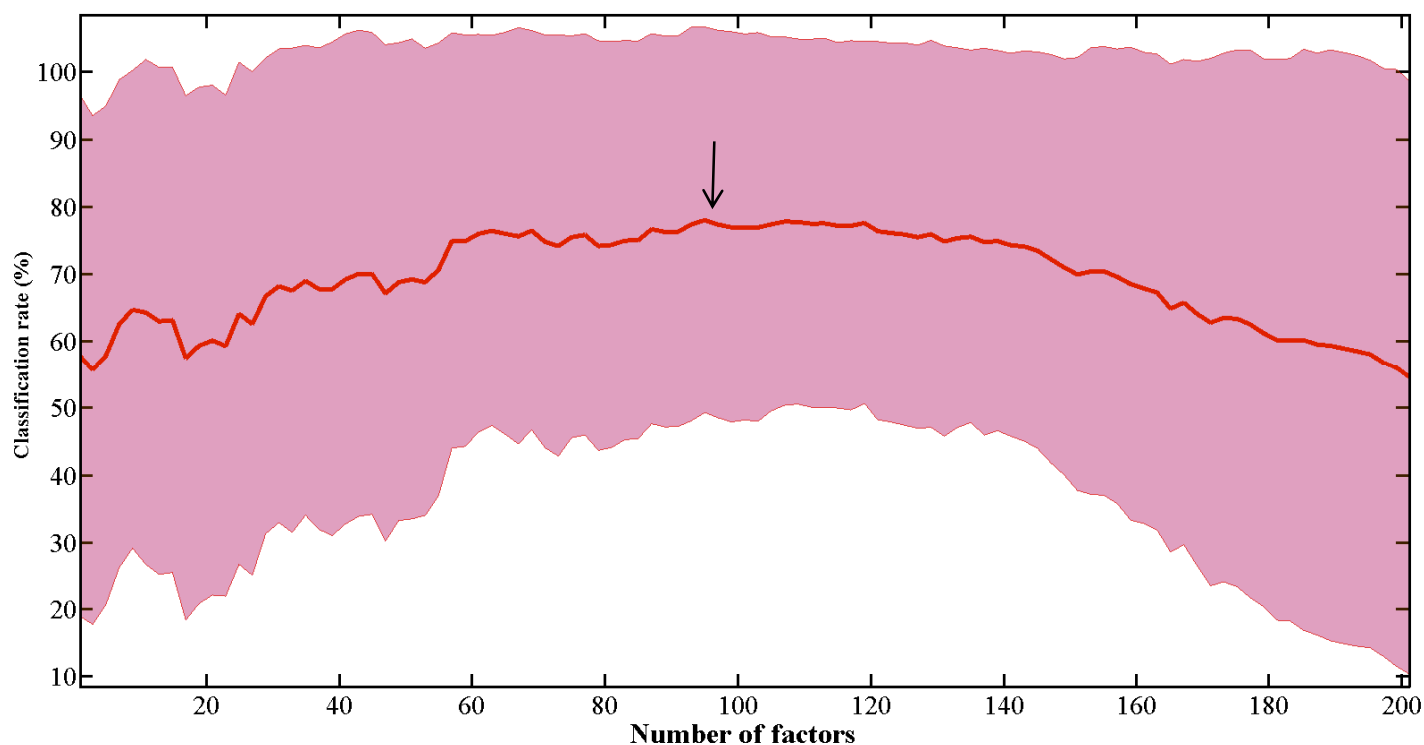


Figure S1 Example of optimisation of the number of principal component (PCs) for use in cross-validated PCA-LDA. Arrow indicates the highest classification rate possible, which gives us the optimum number of PCs.

Table S1 Optimal number of principal component (PCs) used for each dataset.

Dataset	Optimal no. of PCs
<i>P. fluorescens</i>	95
<i>M. vanbaalenii</i>	75
<i>P. fluorescens</i> UV-A positive control	10
<i>M. vanbaalenii</i> UV-A positive control	15

Table S2 Tentative wavenumber assignments for the top five peaks (in order of magnitude) from the cluster vector for *P. fluorescens* treated with 0.01 mg.L⁻¹ CBN as assessed by SR-FTIR spectroscopy.

Short MWCNTs	
Wavenumber (cm ⁻¹)	Assignment
1608	Adenine vibration of DNA
1411	COO- stretching and C-H bending of proteins
1149	C-O stretching of carbohydrate
1500	Amide II
1740	C=O stretching of lipids

C ₆₀ Fullerene	
Wavenumber (cm ⁻¹)	Assignment
1149	C-O stretching of carbohydrate
1612	Amide I
1497	Amide II
1412	Proteins
1739	C=O stretching of lipids

Long MWCNTs	
Wavenumber (cm ⁻¹)	Assignment
1485	Proteins
1411	COO- stretching and C-H bending of proteins
1608	Adenine vibration of DNA
1686	Amide I
1651	Amide I

Fullerene soot	
Wavenumber (cm ⁻¹)	Assignment
1612	Amide I
1651	Amide I
1497	Amide II
1412	Proteins
1149	C-O stretching of carbohydrate

Table S3 Tentative wavenumber assignments for the top five peaks (in order of magnitude) from the cluster vector for *P. fluorescens* treated with 0.01 mg.L⁻¹ CBN as assessed by ATR-FTIR spectroscopy.

Short MWCNTs	
Wavenumber (cm ⁻¹)	Assignment
1065	C-O stretching of DNA
1084	$\nu_s\text{PO}_2^-$
1666	Amide I
1516	Amide II
1794	Lipid

C ₆₀ Fullerene	
Wavenumber (cm ⁻¹)	Assignment
1447	CH ₃ bending of proteins
1639	Amide I
1501	Amide II
1574	Amide II
1115	Carbohydrate

Long MWCNTs	
Wavenumber (cm ⁻¹)	Assignment
1080	$\nu_s\text{PO}_2^-$
1782	Lipid
1142	C-O stretching of carbohydrate
1516	Amide II
1501	Amide II

Fullerene soot	
Wavenumber (cm ⁻¹)	Assignment
1084	$\nu_s\text{PO}_2^-$
1072	C-O vibration of DNA
1516	Amide II
1782	Lipid
1219	$\nu_{as}\text{PO}_2^-$

Table S4 Tentative wavenumber assignments for the top five peaks (in order of magnitude) from the cluster vector for *M. vanbaalenii* treated with 0.01 mg.L⁻¹ CBN as assessed by SR-FTIR spectroscopy.

Short MWCNTs	
Wavenumber (cm ⁻¹)	Assignment
1581	Amide II
1743	C=O stretching of lipids
1616	Amide I
1157	Carbohydrate
1477	Protein

C ₆₀ Fullerene	
Wavenumber (cm ⁻¹)	Assignment
1585	Amide I
1619	Amide I
1742	C=O stretching of lipids
1793	C=O stretching of lipids
1481	Proteins

Long MWCNTs	
Wavenumber (cm ⁻¹)	Assignment
1585	Amide I
1619	Amide I
1743	C=O stretching of lipids
984	Protein phosphorylation
1477	Proteins

Fullerene soot	
Wavenumber (cm ⁻¹)	Assignment
1161	Carbohydrate
1565	Amide II
914	Protein phosphorylation
1199	$\nu_{as}PO_2^-$
1612	Amide I

Table S5 Tentative wavenumber assignments for the top five peaks (in order of magnitude) from the cluster vector for *M. vanbaalenii* treated with 0.01 mg.L⁻¹ CBN as assessed by ATR-FTIR spectroscopy.

Short MWCNTs	
Wavenumber (cm ⁻¹)	Assignment
1003	Carbohydrate
1420	Proteins
1435	Proteins
1060	C-O stretching of DNA
937	DNA

C ₆₀ Fullerene	
Wavenumber (cm ⁻¹)	Assignment
1385	COO- stretching
1018	CO vibration of polysaccharides
1003	Carbohydrate
1234	$\nu_{as}PO_2^-$
1053	C-O stretching and C-O bending of carbohydrate

Long MWCNTs	
Wavenumber (cm ⁻¹)	Assignment
1555	Amide II
1504	Amide II
1130	C-O stretching of carbohydrate
934	DNA
1466	Amide II

Fullerene soot	
Wavenumber (cm ⁻¹)	Assignment
1003	Carbohydrate
1720	C=O stretching of lipid
1558	Amide II
1015	CO vibration of polysaccharides
1466	Amide II