Supporting Information for: Chemometric Approaches for Developing Infrared Nanosensors to Image Anthracyclines

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SUPPLEMENTARY METHODS AND RESULTS

ANALYSIS OF SIMULATED NANOSENSOR FLUORESCENCE DATA

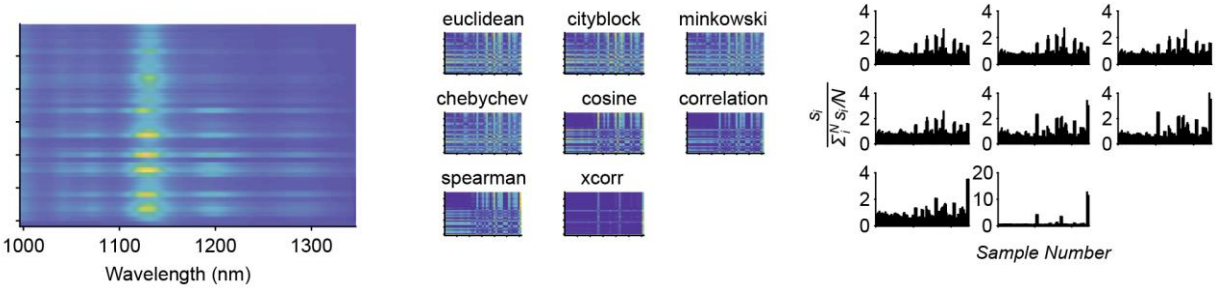
Commonly used pairwise distance matrices are calculated using the following metrics: Euclidean, Cityblock, Chebyshev, Minkowski (order $p=5$), cosine, correlation, Spearman, and cross correlation. Here, SWNT wavelengths and their corresponding intensities are treated as variables and values, respectively, while different analytes correspond to sample elements. We found that certain analytes were highlighted differently depending on the distance metric. We created a signal metric, s, by calculating the mean pairwise distance for each analyte, s_i, and normalizing by the mean signal for all analytes, $\sum_i^N s_i/N$. Of the nanosensor responses simulated, the response with a significant increase of fluorescence intensity (*Response 3*) yielded a large pairwise distance using the Minkowski metric family (Euclidean, Cityblock, and Chebyshev). Using the Chebyshev distance (Minkowski of order $p=\infty$) as a signal metric, all responses, except for *Response 5*, produced a signal above a detection limit of $3\sigma_{SD}$, where the larger the fluorescence difference, the greater the distance metric value. Alternatively, using cosine, correlation, or Spearman distance for signal metrics, only *Response 2, 4, 6* and *8* were above the detection limit, with *Response 4* producing the largest signal. For these analyses, the magnitude of the fluorescence change dictated the strength of the calculated signal response. *Response 5*, which experiences a modest solvatochromic shift, failed to produce a signal above noise using any of the above distance

metrics. Solvatochromic shifts are often preferred signals for use in complex biological media, since the wavelength shift readout can be more selective than a fluorescence intensity modulation. To overcome this limitation of identifying solvatochromic signals, we constructed a metric sensitive to wavelength shifts by calculating pairwise cross correlations between spectra in a shifting reference frame (XCorr) to determine the wavelength offset. Using this metric, we obtained signals above noise for *Response 4* and *Response 5*, the only two simulated signals which corresponded to solvatochromic fluorescence shifts. Thus, results from our simulated nanosensor response libraries suggest that proper selection of a pairwise metric can be employed to readily screen for and quantify modulations in complex fluorescence emission spectra.

SUPPORTING FIGURES

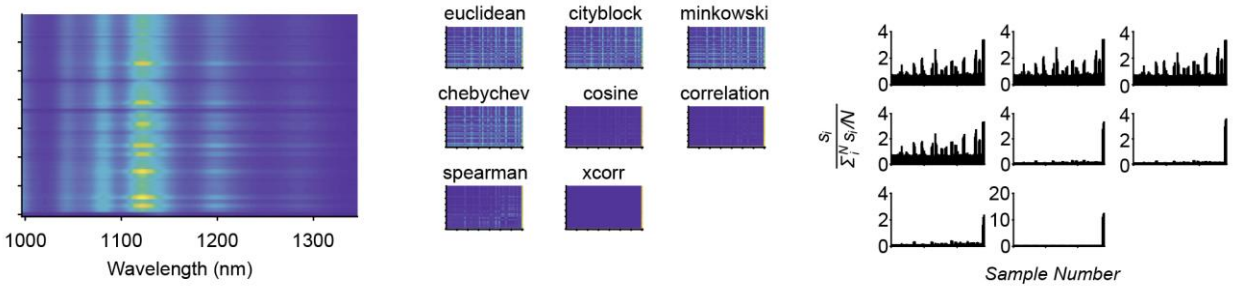
Figure S1. Results from the analysis of screening data from each candidate SWNT nanosensor. (Left) Emission spectra heatmaps collected from chemical screens of SWNT nanosensor candidates against a panel of analytes. Each analyte-nanosensor sample was prepared in at least triplicate. Analytes/samples names for each screen are provided in torder from top to bottom in the file supporting information file "SI_File2_sample-IDs.xlsx". (Center) Pair-wise distance matrices calculated from the fluorescence emission spectra of each analyte sample using different metrics. (Right) Signal response, *s*, calculated for each analyte sample using the corresponding distance metric shown in the pair-wise distance plots. (Bottom) List of all analyte "hits" with signal responses, *s*, above noise. Hits were pooled across all distance metrics calculations.

Corona: DNA $(TTA)_4TT$



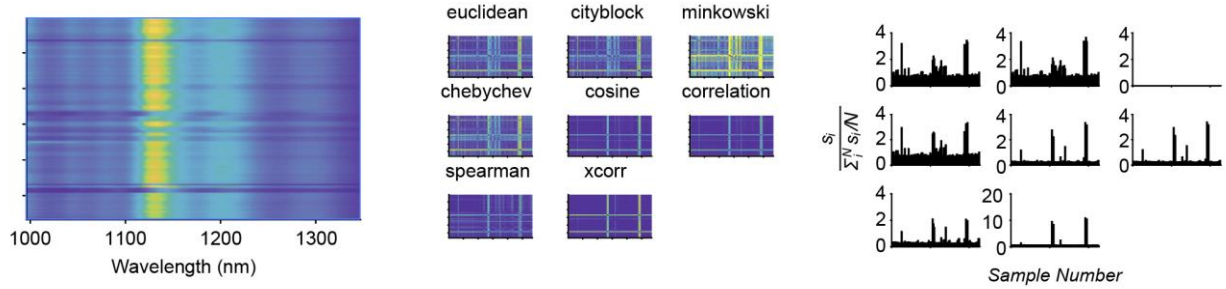
Analyte	Hits
17-beta-estradiol	2
acetylcholine chloride	5
ascorbic acid	21
creatine	3
d-mannitol	2
dopac	18
dopamine	21
dox	24
epinephrine	11
l-cysteine	21
l-dopa	24
l-tyrosine	3
nadh	2
norepinephrine	21
oxytocin	9
riboflavin	1
serotonin	19

Corona: DNA $(TAT)_4$



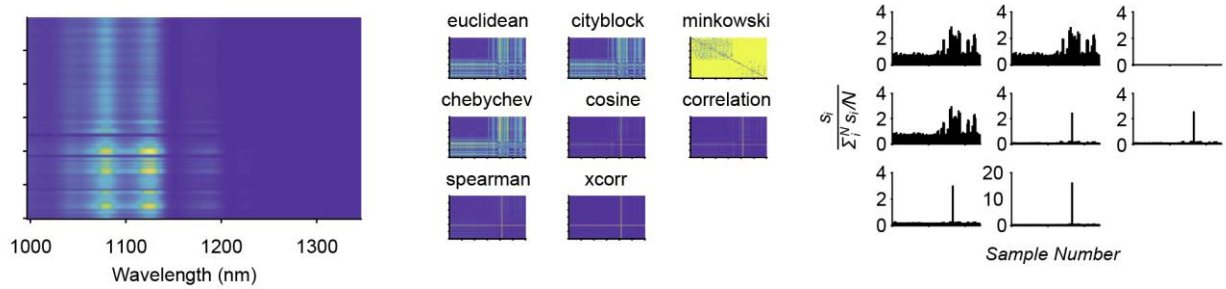
Analyte	Hits
amp	2
ascorbic acid	15
aspartic acid	1
control	1
cysteine	12
cytidine	4
dopamine	27
dox	24
epinephrine	12
guanosine	12
l-dopa	14
l-thyroxine	12
norepinephrine	11
riboflavin	8
serotonin	6

Corona: RITC-PEG-RITC



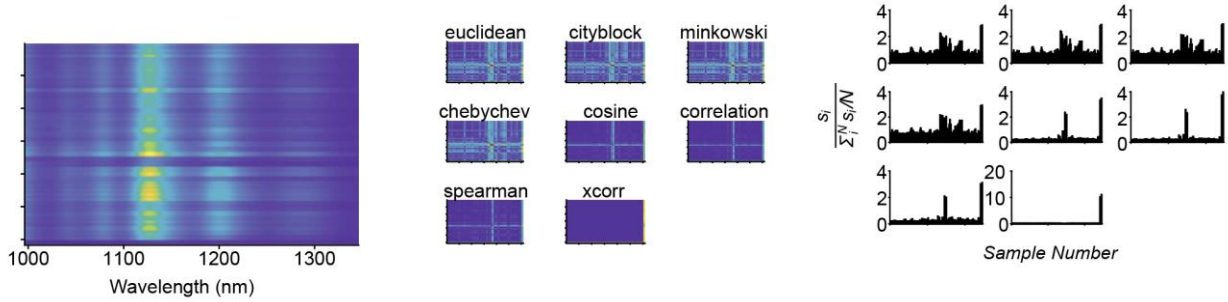
Analyte	Hits
adenosine	2
ampicillin	6
camp	6
d-aspartic acid	3
d-mannose	3
dox	21
epinephrine	2
estradiol	10
norepniephrine	2
oxytocin	8
riboflavin	7
serotonin	6
thyroxine	21
tyrosine	8

Corona: DNA $(GT)_{15}$



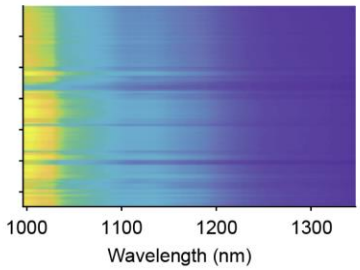
Analyte	Hits
ampicillin	8
ascorbic acid	15
creatine	7
dopac	6
dopamine	3
epinephrine	15
l-cysteine	9
nadh	6
norepinephrine	9
riboflavin	6
serotonin	9

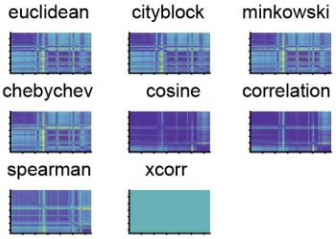
Corona: DNA GTAGTCGAGTGTGTGTGTGTGT

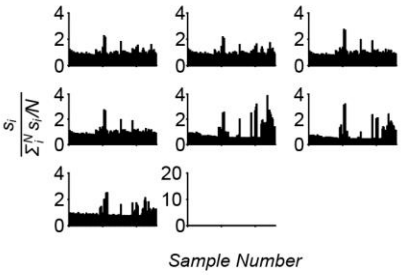


Analyte	Hits
17-beta-estradiol	21
ampicillin	3
ascorbic acid	12
d-glucose	6
dopac	4
dopamine	7
dox	24
epinephrine	10
glutamic acid	10
guanosine	4
melatonin	2
riboflavin	16
serotonin	12

Corona: Phospholipid DTTE-PEG2k

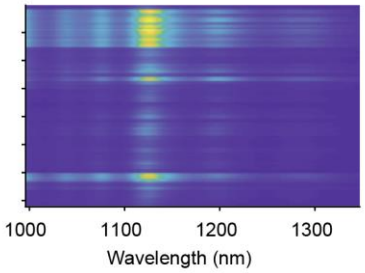


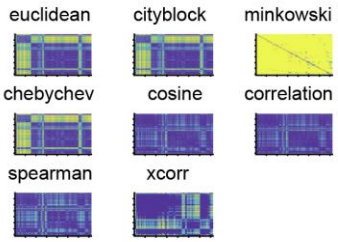


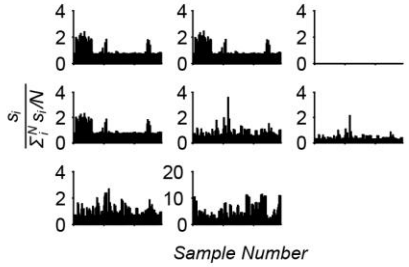


Analyte	Hits
2,4 dinitrophenol	4
acetylcholine	2
control	15
dopac	3
dox	21
epinephrine	7
estradiol	9
glutamic acid	10
glycine	3
l-dopa	8
melatonin	36
norepinephrine	7
oxytocin	8
riboflavin	17
serotonin	15
thyroxine	27
tyrosine	15

Corona: DNA $(CCA)_{10}$



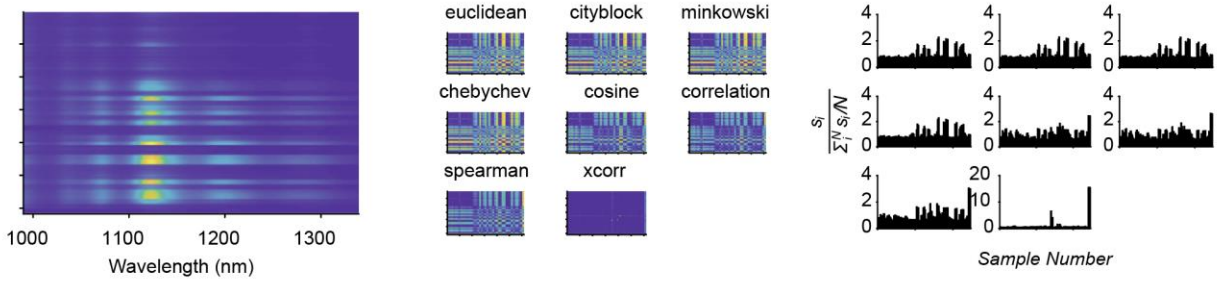




Analyte	Hits
17-beta-estradiol	2
adenosine	6
ascorbic acid	4
atp	2
camp	5
creatine	9
cytidine	2
d-fructose	2
d-galactose	2
d-mannitol	4
dopamine	12
epinephrine	14
gaba	7
glutamic acid	4
glycine	4
guanosine	9
homovanillic acid	10
l-citrulline	6
l-cysteine	6
l-dopa	15
l-thyroxine	8
melatonin	4
norepinephrine	12
oxytocin	12
riboflavin	17
serotonin	1

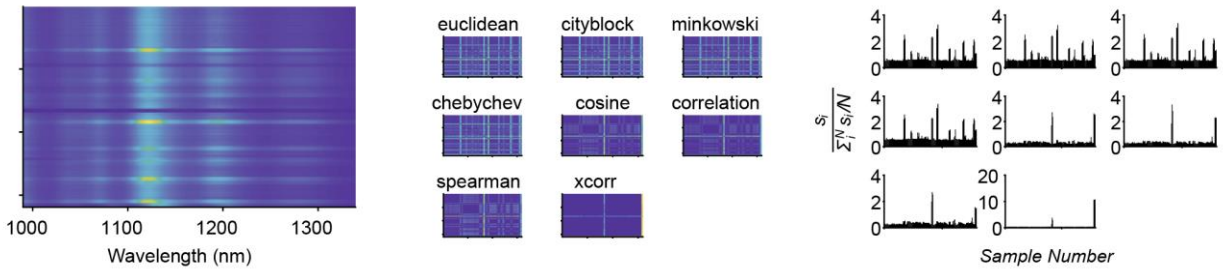
urea 3

Corona: DNA CB14 (CCCCCCCCACCGGCGTTTCCCCCCCC)



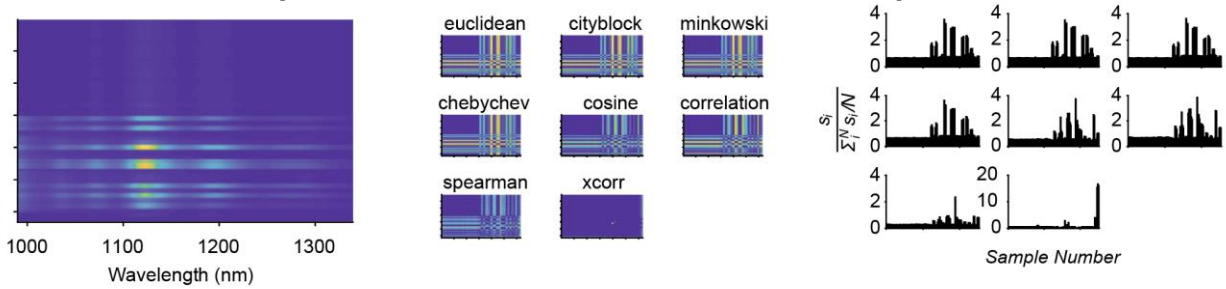
Analyte	Hits
acetylcholine chloride	3
adenosine	4
ascorbic acid	21
camp	2
creatine	7
d-fructose	4
d-galactose	2
dopac (control)	5
dopamine	21
dox	12
epinephrine	21
l-cysteine	21
l-dopa	21
l-tyrosine	21
nadh	15
norepinephrine	21
riboflavin	8
serotonin	16
urea	4

Corona: DNA CB13 (CCCCCCCCAGAATTACTTCCCCCCCC)



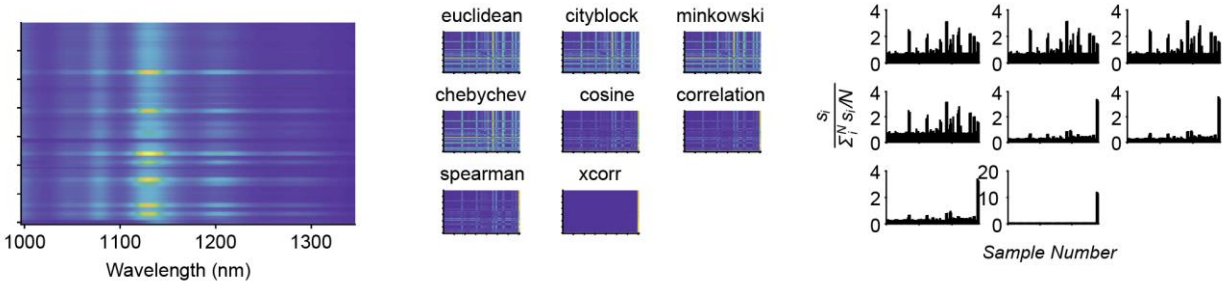
Analyte	Hits
ascorbic acid	15
control	3
d-mannose	1
dopamine	26
dox	24
epinephrine	12
gmp	3
guanosine	12
l-cysteine	12
l-dopa	8
nadh	1
norepinephrine	6
riboflavin	24

Corona: DNA CB4 (CCCCCCCCCCCAGGCGGGGCCCCCCCC)



Analyte	Hits
17-beta-estradiol	9
ascorbic acid	13
control	3
creatine	10
dopac (control)	9
dopamine	12
dox	12
epinephrine	12
glutamic acid	9
glycine	9
l-aspartic acid	9
l-cysteine	12
l-tyrosine	12
melatonin	9
nadh	12
oxytocin	12
riboflavin	6
serotonin	12
urea	6

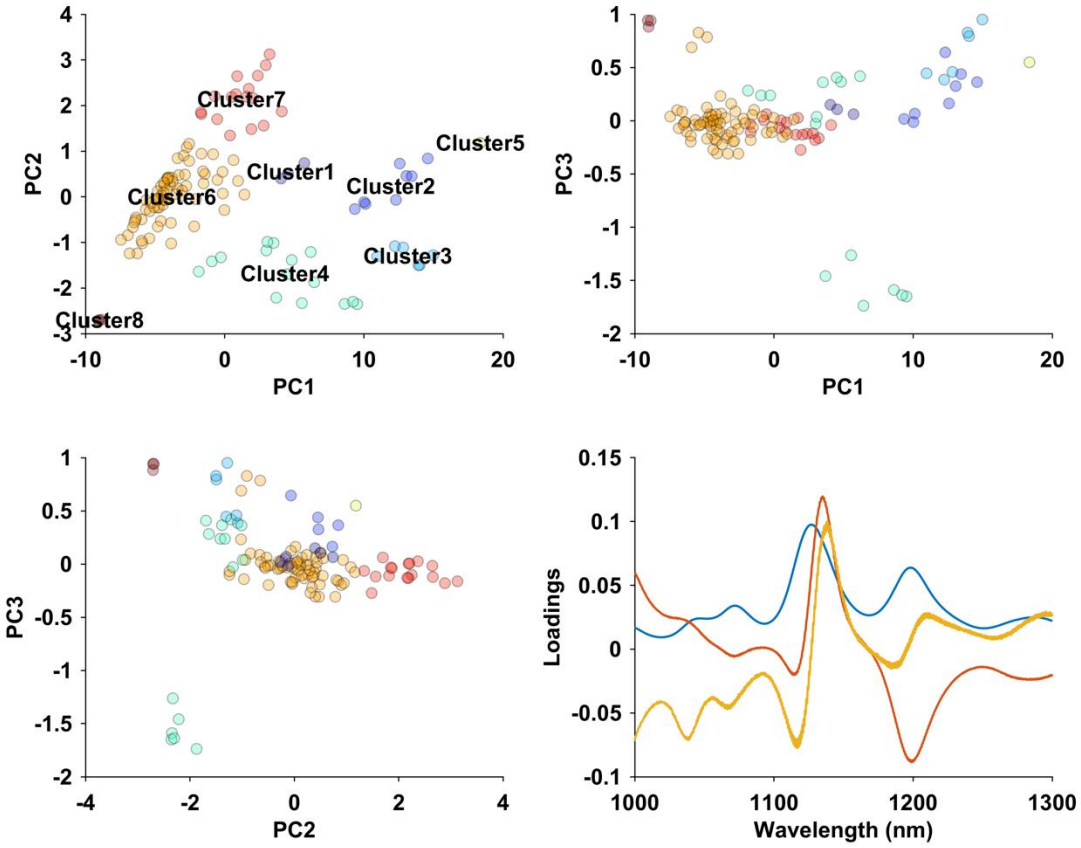
Corona: DNA CB3 (CCCCCCCCCCTCCGCAAGTCCCCCCCC)



Analyte	Hits
ascorbic acid	21
cysteine	21
dopamine	33
dox	24
epinephrine	20
glutamic acid	4
l-dopa	21
nadh	12
norepinephrine	21
riboflavin	12

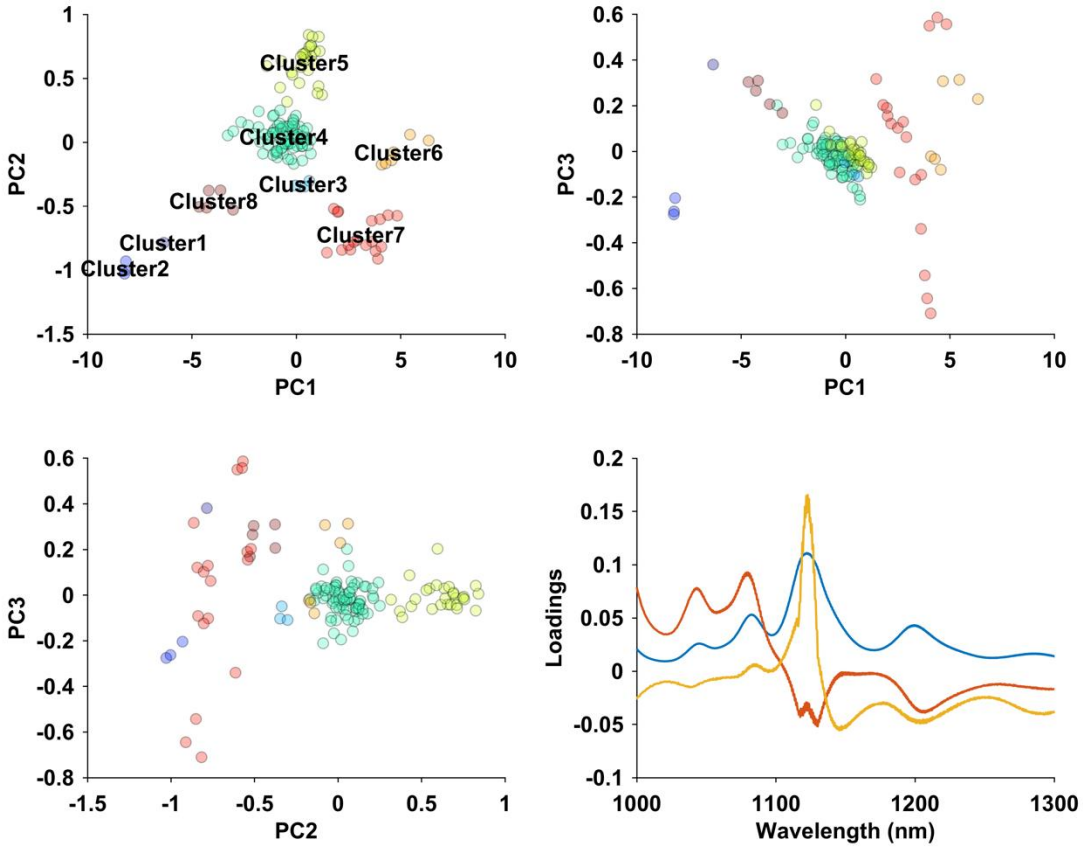
Figure S2. Principal component analysis for the analytes screened against different SWNT-nanosensor candidates. Each dataset is plotted using the first 3 principal component coordinates. Clusters, indicated by colors, were generated by hierarchical clustering with normalized PC coordinates and cluster centroid distances calculated using the Euclidean distance. A plot of the loadings shows the spectral characteristic of each principal component.

Corona: DNA $(TTA)_4TT$



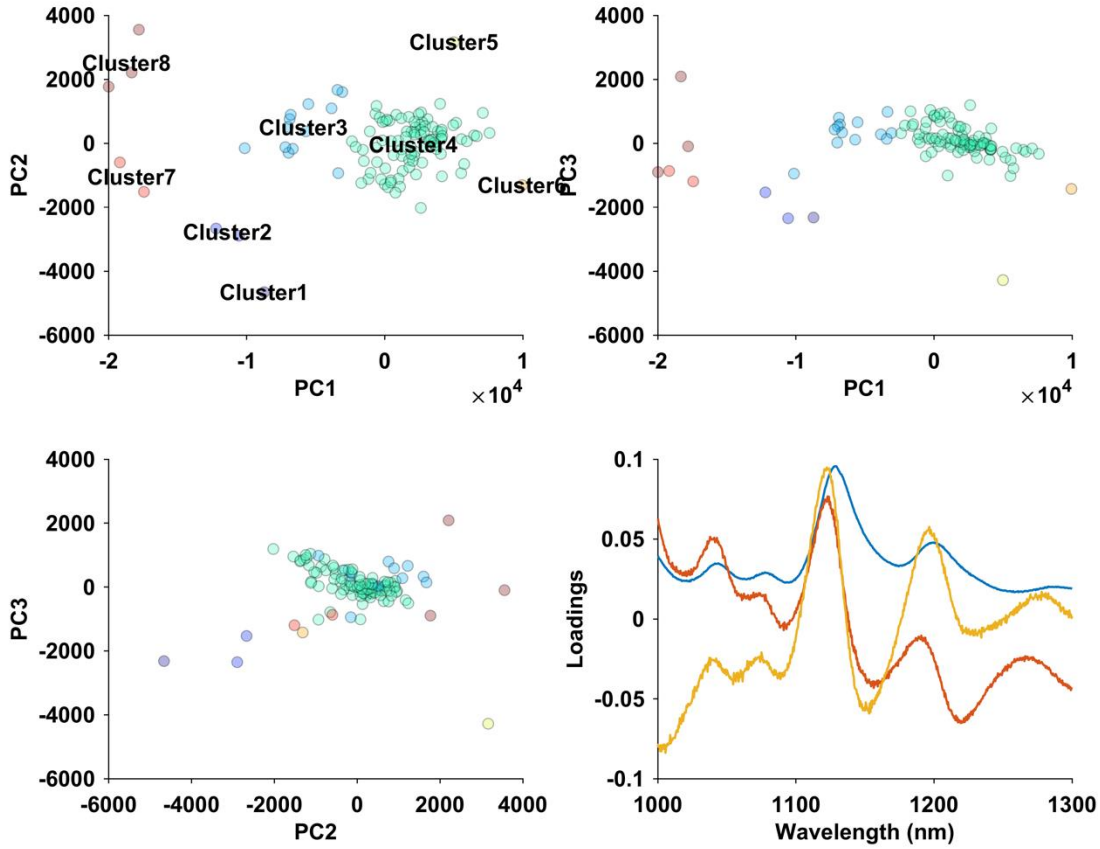
Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
NADH	1	Oxytocin	4	D-Glucose	6	Creatine	6	Homovanillic acid	7
NADH	1	Oxytocin	4	Guanosine	6	Glutamic acid	6	Melatonin	7
NADH	1	Oxytocin	4	Guanosine	6	Glutamic acid	6	Melatonin	7
Serotonin	2	Dopamine	5	Guanosine	6	Glutamic acid	6	Melatonin	7
Serotonin	2	2,4-dinitrophenol	6	Histamine	6	Glycine	6	DOX	8
Serotonin	2	2,4-dinitrophenol	6	Histamine	6	Glycine	6	DOX	8
Dopamine	2	2,4-dinitrophenol	6	Histamine	6	Glycine	6	DOX	8
Dopamine	2	Acetylcholine Chloride	6	Homovanillic acid	6	L-Aspartic acid	6		
Norepinephrine	2	Acetylcholine Chloride	6	Homovanillic acid	6	L-Aspartic acid	6		
Norepinephrine	2	Acetylcholine Chloride	6	L-Citrulline	6	L-Aspartic acid	6		
Norepinephrine	2	Adenosine	6	L-Citrulline	6	L-Histidine	6		
Ascorbic acid	3	Adenosine	6	L-Citrulline	6	L-Histidine	6		
Ascorbic acid	3	Adenosine	6	L-Phenylalanine	6	L-Histidine	6		
Ascorbic acid	3	ATP	6	L-Phenylalanine	6	Urea	6		
L-Cysteine	3	ATP	6	L-Phenylalanine	6	Urea	6		
L-Cysteine	3	ATP	6	L-Thyroxine	6	Urea	6		
L-Cysteine	3	cAMP	6	L-Thyroxine	6	Cytidine	7		
L-Dopa	4	cAMP	6	L-Thyroxine	6	Cytidine	7		
L-Dopa	4	cAMP	6	Riboflavin	6	Cytidine	7		
L-Dopa	4	D-Aspartic acid	6	Riboflavin	6	D-Galactose	7		
L-Tyrosine	4	D-Aspartic acid	6	Riboflavin	6	D-Mannitol	7		
L-Tyrosine	4	D-Aspartic acid	6	17-beta-estradiol	6	D-Mannitol	7		
L-Tyrosine	4	D-Fructose	6	17-beta-estradiol	6	D-Mannitol	7		
DOPAC	4	D-Fructose	6	17-beta-estradiol	6	D-Mannose	7		
DOPAC	4	D-Fructose	6	Ampicillin	6	D-Mannose	7		
DOPAC	4	D-Galactose	6	Ampicillin	6	D-Mannose	7		
Epinephrine	4	D-Galactose	6	Ampicillin	6	GABA	7		
Epinephrine	4	D-Glucose	6	Creatine	6	GABA	7		
Epinephrine	4	D-Glucose	6	Creatine	6	GABA	7		

Corona: DNA $(TAT)_4$



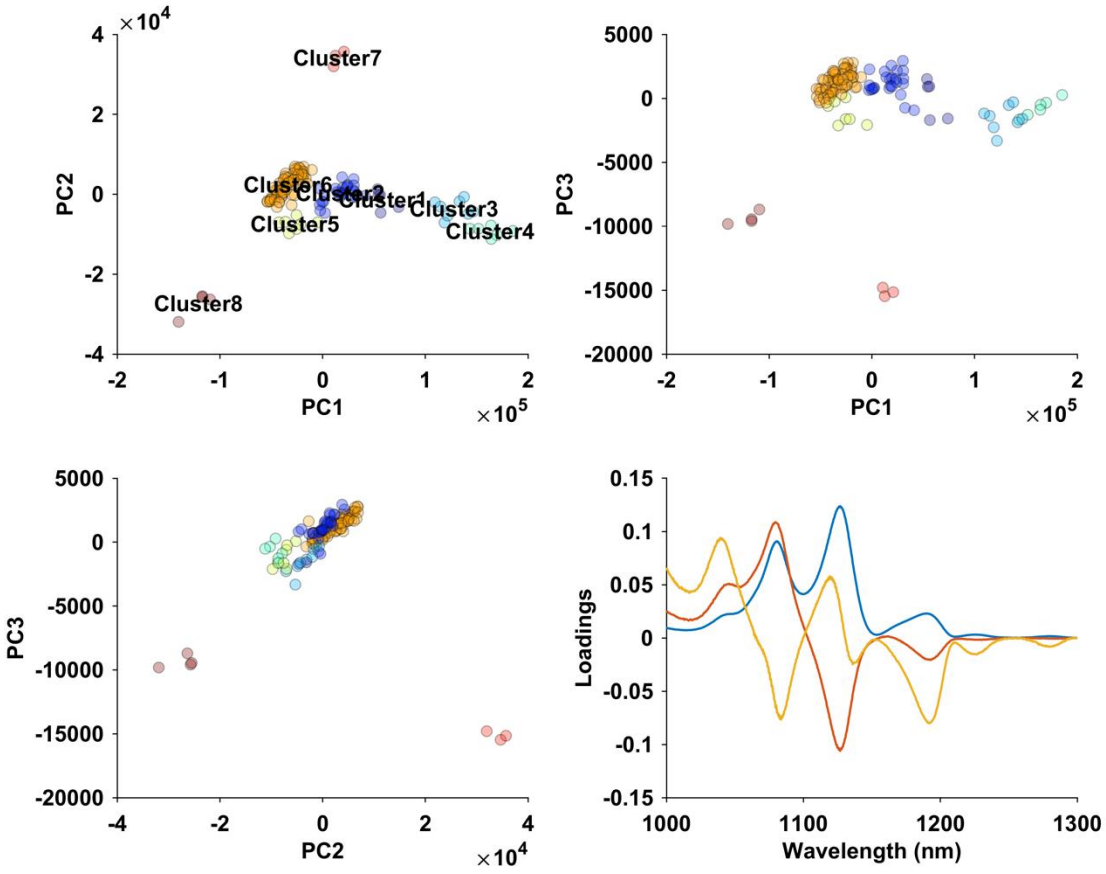
Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
L-thyroxine	1	D-fructose	4	L-citruline	4	Control	5	Cysteine	6
DOX	2	D-fructose	4	L-citruline	4	Glycine	5	Cysteine	6
DOX	2	D-galactose	4	L-phenylalanine	4	Glycine	5	dopamine	7
DOX	2	D-galactose	4	L-phenylalanine	4	Glycine	5	dopamine	7
L-tyrosine	3	D-galactose	4	L-phenylalanine	4	NADH	5	dopamine	7
L-tyrosine	3	D-glucose	4	Melotonin	4	NADH	5	L-DOPA	7
L-tyrosine	3	D-glucose	4	Melotonin	4	NADH	5	L-DOPA	7
control	4	D-glucose	4	Melotonin	4	AMP	5	L-DOPA	7
control	4	GABA	4	Oxytocin	4	AMP	5	Serotonin	7
control	4	GABA	4	Oxytocin	4	AMP	5	Serotonin	7
2,4 dinitrophenol	4	GABA	4	Oxytocin	4	CMP	5	Serotonin	7
2,4 dinitrophenol	4	adenosine	4	Riboflavin	4	CMP	5	Ascorbic acid	7
2,4 dinitrophenol	4	adenosine	4	Riboflavin	4	CMP	5	Ascorbic acid	7
acetylcholine	4	D-mannitol	4	Riboflavin	4	GMP	5	Ascorbic acid	7
acetylcholine	4	D-mannitol	4	Estradiol	4	GMP	5	Norepinephrine	7
acetylcholine	4	D-mannitol	4	Estradiol	4	GMP	5	Norepinephrine	7
ATP	4	D-mannose	4	Estradiol	4	TMP	5	Norepinephrine	7
ATP	4	D-mannose	4	Ampicillin	4	TMP	5	Epinephrine	7
ATP	4	D-mannose	4	Ampicillin	4	TMP	5	Epinephrine	7
cAMP	4	Histamine	4	Ampicillin	4	Aspartic acid	5	Epinephrine	7
cAMP	4	Histamine	4	Creatine	4	Aspartic acid	5	Guanosine	8
cAMP	4	Histamine	4	Creatine	4	Aspartic acid	5	Guanosine	8
cytidine	4	control	4	Creatine	4	Histamine	5	Guanosine	8
cytidine	4	control	4	Glutamic acid	4	Histamine	5	L-thyroxine	8
cytidine	4	control	4	Glutamic acid	4	Histamine	5	L-thyroxine	8
D-aspartic acid	4	Homovanillic acid	4	Glutamic acid	4	Dopamine	6		
D-aspartic acid	4	Homovanillic acid	4	adenosine	5	Dopamine	6		
D-aspartic acid	4	Homovanillic acid	4	Control	5	Dopamine	6		
D-fructose	4	L-citruline	4	Control	5	Cysteine	6		

Corona: RITC-PEG-RITC



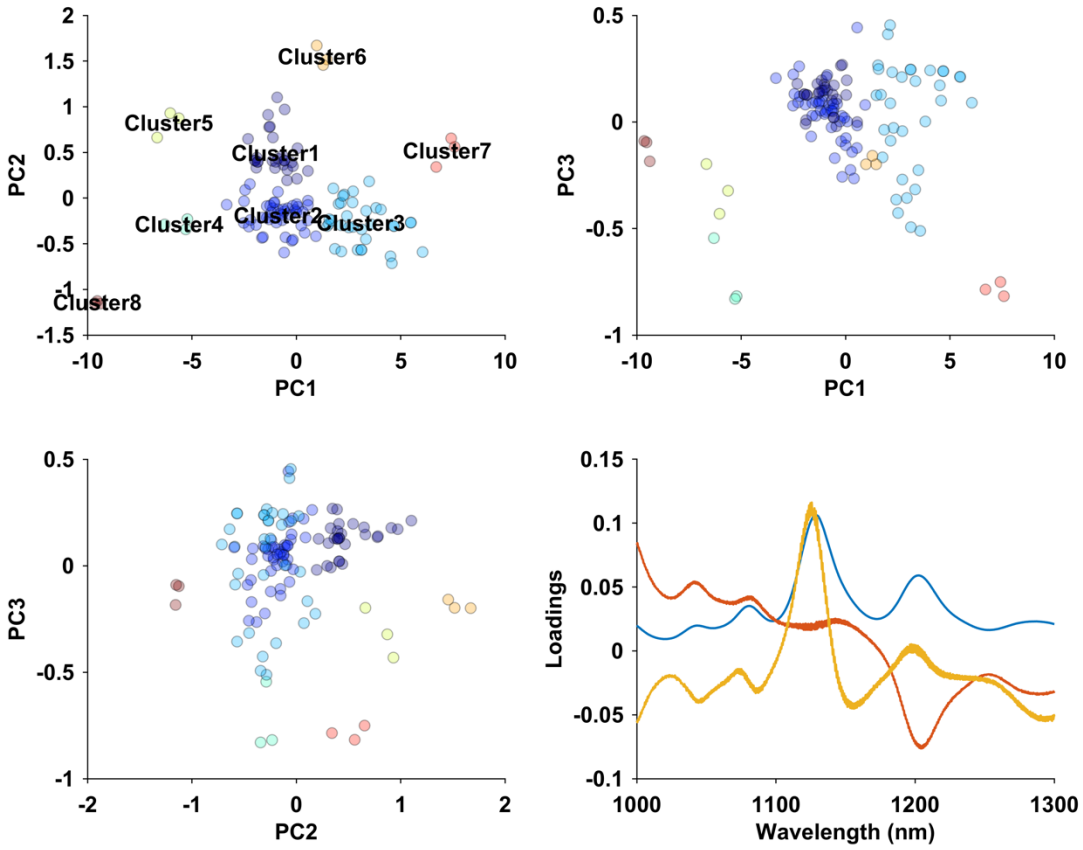
Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
thyroxine	1	cytidine	4	l-dopa	4	glutamic acid	4
thyroxine	2	cytidine	4	l-dopa	4	glutamic acid	4
thyroxine	2	d-mannose	4	l-dopa	4	glycine	4
guanosine	3	d-mannose	4	phenylalanine	4	glycine	4
guanosine	3	d-mannose	4	phenylalanine	4	glycine	4
guanosine	3	d-aspartic acid	4	phenylalanine	4	l-cysteine	4
tyrosine	3	d-aspartic acid	4	melatonin	4	l-cysteine	4
tyrosine	3	d-aspartic acid	4	melatonin	4	l-cysteine	4
tyrosine	3	d-fructose	4	melatonin	4	control	4
serotonin	3	d-fructose	4	riboflavin	4	control	4
serotonin	3	d-fructose	4	riboflavin	4	control	4
riboflavin	3	d-galactose	4	ampicillin	4	histidine	4
estradiol	3	d-galactose	4	ampicillin	4	histidine	4
estradiol	3	d-galactose	4	ascorbic acid	4	histidine	4
estradiol	3	glucose	4	ascorbic acid	4	NADH	4
norepniephrine	3	glucose	4	ascorbic acid	4	NADH	4
2,4 dinitrophenol	4	glucose	4	urea	4	NADH	4
2,4 dinitrophenol	4	mannitol	4	urea	4	norepniephrine	4
2,4 dinitrophenol	4	mannitol	4	urea	4	norepniephrine	4
acetylcholine	4	mannitol	4	DOPAC	4	ampicillin	5
acetylcholine	4	GABA	4	DOPAC	4	oxytocin	6
acetylcholine	4	GABA	4	DOPAC	4	DOX	7
adenosine	4	GABA	4	dopamine	4	DOX	7
adenosine	4	histamine	4	dopamine	4	cAMP	8
ATP	4	histamine	4	dopamine	4	oxytocin	8
ATP	4	histamine	4	epinephrine	4	DOX	8
cAMP	4	citruline	4	epinephrine	4		
cAMP	4	citruline	4	epinephrine	4		
cytidine	4	citruline	4	glutamic acid	4		

Corona: DNA $(GT)_{15}$



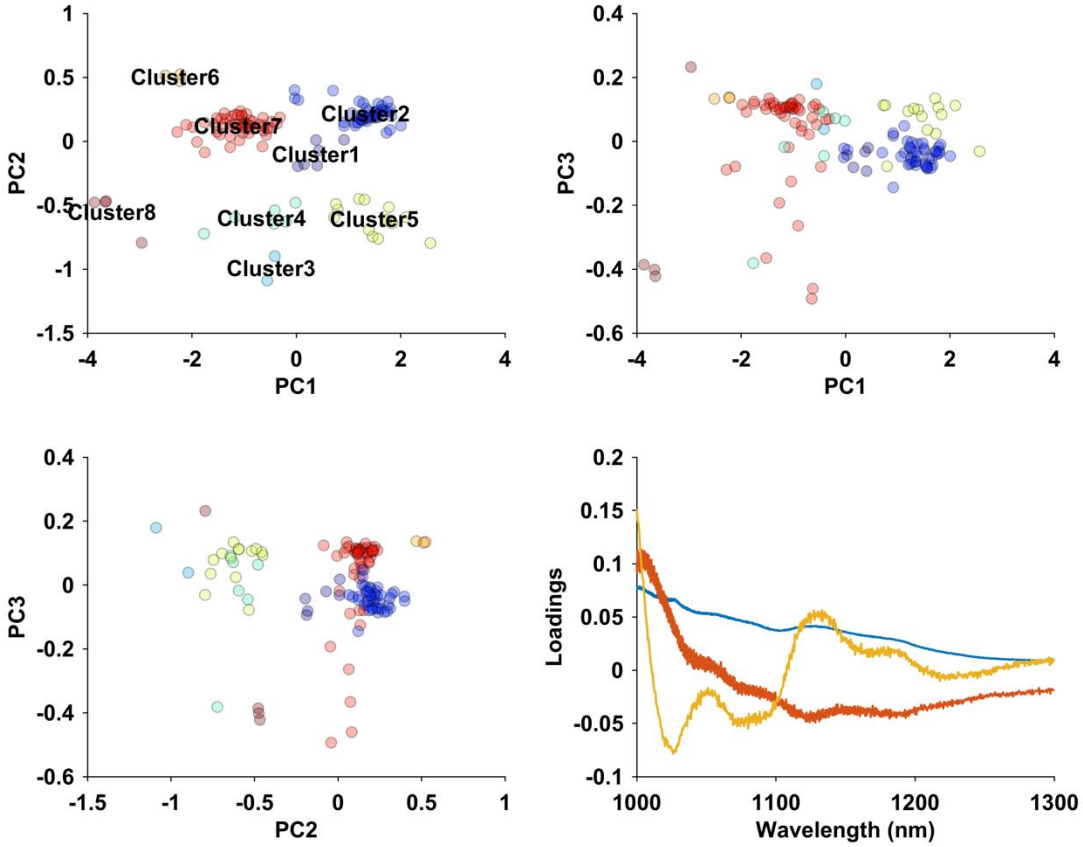
Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
Ampicillin	1	Urea	2	Adenosine	6	GABA	6	Riboflavin	8
Ampicillin	1	DOPAC	3	ATP	6	Guanosine	6	Riboflavin	8
Ampicillin	1	DOPAC	3	ATP	6	Guanosine	6	Creatine	8
NADH	1	Dopamine	3	cAMP	6	Guanosine	6	L-Cysteine	8
NADH	1	L-Cysteine	3	cAMP	6	Histamine	6		
L-Tyrosine	2	L-Cysteine	3	cAMP	6	Histamine	6		
L-Tyrosine	2	Norepinephrine	3	Cytidine	6	Histamine	6		
Riboflavin	2	Norepinephrine	3	Cytidine	6	Homovanillic acid	6		
17-beta-estradiol	2	Norepinephrine	3	Cytidine	6	Homovanillic acid	6		
17-beta-estradiol	2	Ascorbic acid	4	D-Aspartic acid	6	Homovanillic acid	6		
Creatine	2	Ascorbic acid	4	D-Aspartic acid	6	L-Citrulline	6		
Creatine	2	Ascorbic acid	4	D-Aspartic acid	6	L-Citrulline	6		
Dopamine	2	Epinephrine	4	D-Fructose	6	L-Citrulline	6		
Dopamine	2	Epinephrine	4	D-Fructose	6	L-Dopa	6		
Glutamic acid	2	Epinephrine	4	D-Fructose	6	L-Dopa	6		
Glutamic acid	2	2,4-dinitrophenol	5	D-Galactose	6	L-Dopa	6		
Glutamic acid	2	ATP	5	D-Galactose	6	L-Phenylalanine	6		
Glycine	2	17-beta-estradiol	5	D-Galactose	6	L-Phenylalanine	6		
Glycine	2	DOPAC	5	D-Glucose	6	L-Phenylalanine	6		
Glycine	2	Oxytocin	5	D-Glucose	6	L-Thyroxine	6		
L-Aspartic acid	2	Urea	5	D-Glucose	6	L-Thyroxine	6		
L-Aspartic acid	2	Urea	5	D-Mannitol	6	L-Thyroxine	6		
L-Aspartic acid	2	2,4-dinitrophenol	6	D-Mannitol	6	L-Tyrosine	6		
L-Histidine	2	2,4-dinitrophenol	6	D-Mannitol	6	Melatonin	6		
L-Histidine	2	Acetylcholine Chloride	6	D-Mannose	6	Melatonin	6		
L-Histidine	2	Acetylcholine Chloride	6	D-Mannose	6	Melatonin	6		
NADH	2	Acetylcholine Chloride	6	D-Mannose	6	Serotonin	7		
Oxytocin	2	Adenosine	6	GABA	6	Serotonin	7		
Oxytocin	2	Adenosine	6	GABA	6	Serotonin	7		

Corona: DNA GTAGTCGAGTGTGTGTGTGTGT



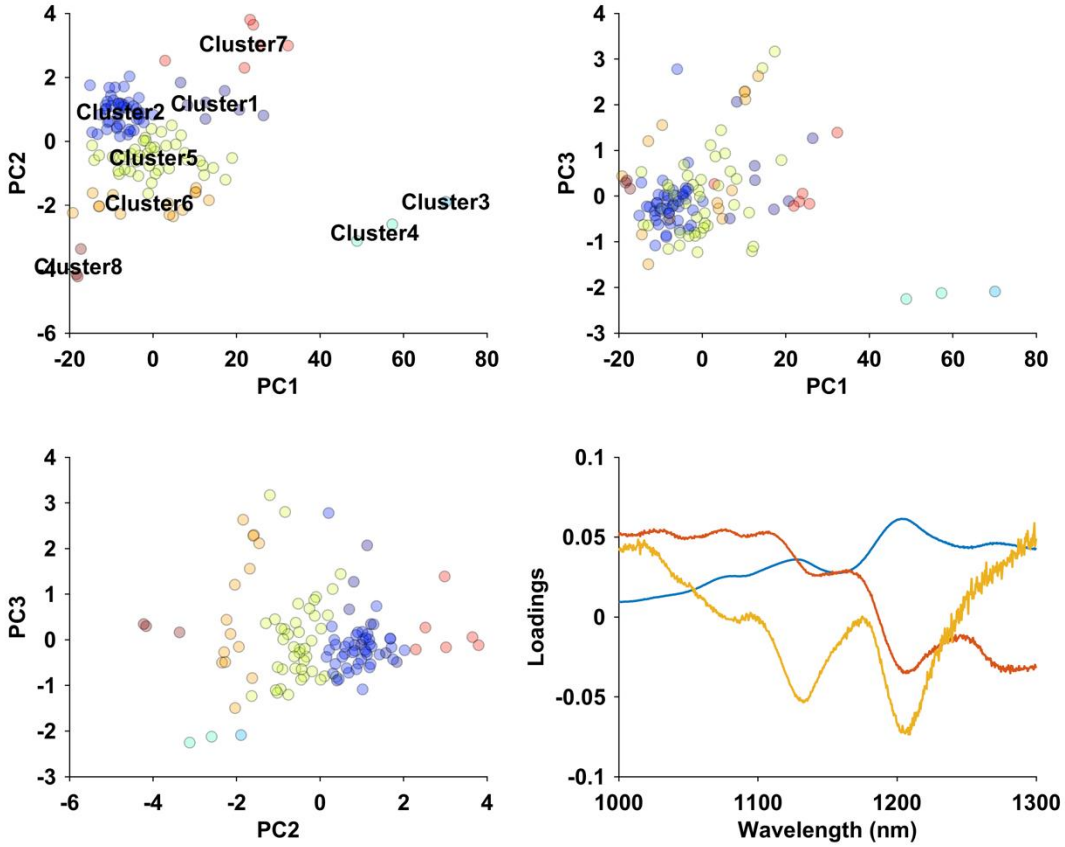
Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
D-Aspartic acid	1	2,4-dinitrophenol	2	GABA	2	Ascorbic acid	3	Melatonin	6
D-Aspartic acid	1	2,4-dinitrophenol	2	GABA	2	Ascorbic acid	3	Serotonin	7
D-Aspartic acid	1	Acetylcholine Chloride	2	Guanosine	2	DOPAC	3	Serotonin	7
Histamine	1	Acetylcholine Chloride	2	Guanosine	2	DOPAC	3	Serotonin	7
Histamine	1	Acetylcholine Chloride	2	Guanosine	2	DOPAC	3	DOX	8
Histamine	1	Adenosine	2	L-Dopa	2	Dopamine	3	DOX	8
Homovanillic acid	1	Adenosine	2	L-Thyroxine	2	Dopamine	3	DOX	8
Homovanillic acid	1	ATP	2	L-Thyroxine	2	Dopamine	3		
Homovanillic acid	1	ATP	2	L-Histidine	2	Epinephrine	3		
L-Citrulline	1	ATP	2	L-Histidine	2	Epinephrine	3		
L-Citrulline	1	cAMP	2	L-Histidine	2	Epinephrine	3		
L-Citrulline	1	cAMP	2	NADH	2	Glutamic acid	3		
L-Phenylalanine	1	cAMP	2	NADH	2	Glutamic acid	3		
L-Phenylalanine	1	Cytidine	2	Oxytocin	2	Glutamic acid	3		
L-Phenylalanine	1	Cytidine	2	Oxytocin	2	L-Cysteine	3		
L-Thyroxine	1	Cytidine	2	Oxytocin	2	L-Cysteine	3		
Creatine	1	D-Fructose	2	Adenosine	3	L-Cysteine	3		
Creatine	1	D-Fructose	2	D-Glucose	3	NADH	3		
Creatine	1	D-Fructose	2	D-Glucose	3	Norepinephrine	3		
Glycine	1	D-Galactose	2	D-Glucose	3	Norepinephrine	3		
Glycine	1	D-Galactose	2	L-Dopa	3	Norepinephrine	3		
Glycine	1	D-Galactose	2	L-Dopa	3	Riboflavin	4		
L-Aspartic acid	1	D-Mannitol	2	L-Tyrosine	3	Riboflavin	4		
L-Aspartic acid	1	D-Mannitol	2	L-Tyrosine	3	Riboflavin	4		
L-Aspartic acid	1	D-Mannitol	2	L-Tyrosine	3	17-beta-estradiol	5		
Urea	1	D-Mannose	2	Ampicillin	3	17-beta-estradiol	5		
Urea	1	D-Mannose	2	Ampicillin	3	17-beta-estradiol	5		
Urea	1	D-Mannose	2	Ampicillin	3	Melatonin	6		
2,4-dinitrophenol	2	GABA	2	Ascorbic acid	3	Melatonin	6		

Corona: Phospholipid DTTE-PEG2k



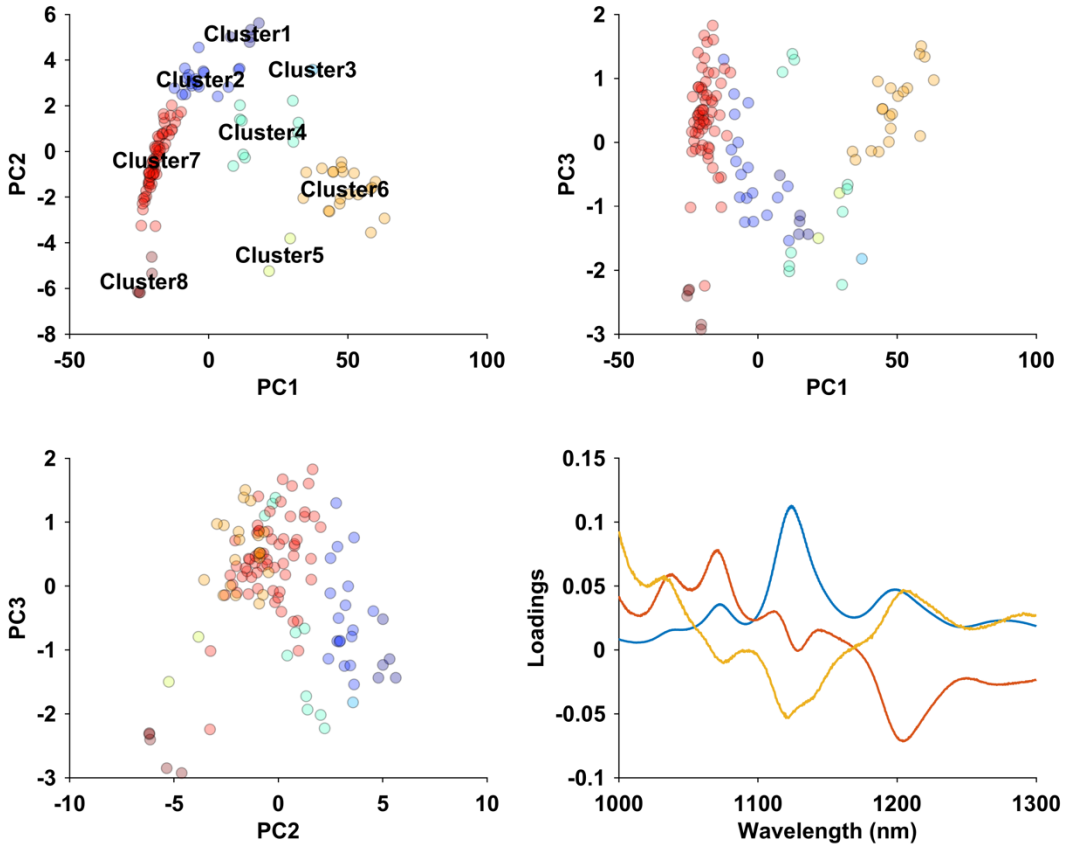
Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
ascorbic acid	1	glycine	2	control	5	cAMP	7	l-dopa	7
dopamine	1	glycine	2	control	5	cAMP	7	thyroxine	7
dopamine	1	glycine	2	control	5	cAMP	7	thyroxine	7
dopamine	1	l-cysteine	2	thyroxine	5	cytidine	7	thyroxine	7
norepinephrine	1	l-cysteine	2	melatonin	5	cytidine	7	tyrosine	7
norepinephrine	1	l-cysteine	2	melatonin	5	cytidine	7	tyrosine	7
l-phenylalanine	2	l-histidine	2	serotonin	5	d-aspartic acid	7	tyrosine	7
l-phenylalanine	2	l-histidine	2	serotonin	5	d-aspartic acid	7	riboflavin	7
l-phenylalanine	2	l-histidine	2	riboflavin	5	d-aspartic acid	7	riboflavin	7
riboflavin	2	NADH	2	riboflavin	5	d-galactose	7	melatonin	8
estradiol	2	NADH	2	riboflavin	5	d-galactose	7	melatonin	8
estradiol	2	NADH	2	estradiol	5	d-galactose	7	melatonin	8
estradiol	2	oxytocin	2	estradiol	5	d-glucose	7	epinephrine	8
amphicilin	2	oxytocin	2	estradiol	5	d-glucose	7		
amphicilin	2	oxytocin	2	DOX	6	d-glucose	7		
amphicilin	2	control	2	DOX	6	d-mannitol	7		
ascorbic acid	2	control	2	DOX	6	d-mannitol	7		
ascorbic acid	2	control	2	2,4 dinitrophenol	7	d-mannitol	7		
creatine	2	control	2	2,4 dinitrophenol	7	d-mannose	7		
creatine	2	control	2	2,4 dinitrophenol	7	d-mannose	7		
creatine	2	control	2	acetylcholine	7	d-mannose	7		
DOPAC	2	melatonin	3	acetylcholine	7	GABA	7		
DOPAC	2	serotonin	3	acetylcholine	7	GABA	7		
DOPAC	2	norepinephrine	4	adenosine	7	GABA	7		
epinephrine	2	thyroxine	4	adenosine	7	l-citruline	7		
epinephrine	2	thyroxine	4	adenosine	7	l-citruline	7		
glutamic acid	2	tyrosine	4	ATP	7	l-citruline	7		
glutamic acid	2	tyrosine	4	ATP	7	l-dopa	7		
glutamic acid	2	tyrosine	4	ATP	7	l-dopa	7		

Corona: DNA $(CCA)_{10}$



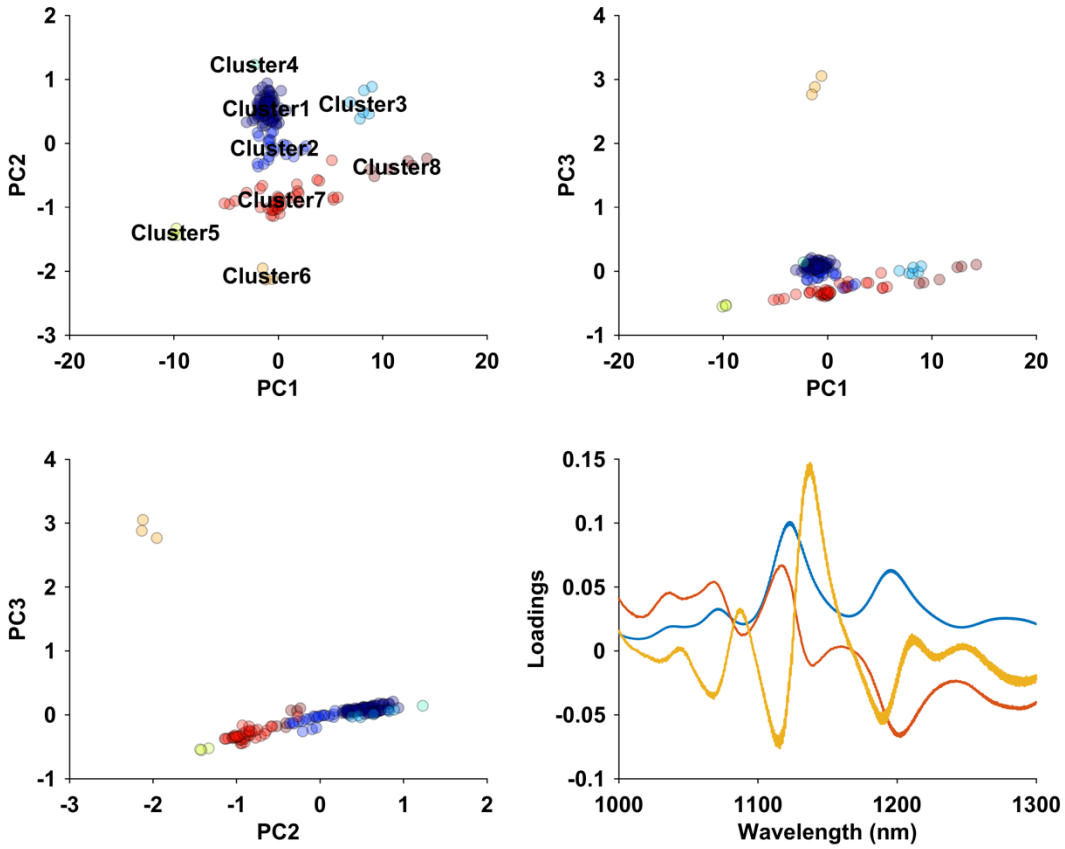
Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
2,4-dinitrophenol	1	L-Phenylalanine	2	Acetylcholine Chloride	5	L-Aspartic acid	5	Epinephrine	7
D-Mannitol	1	Melatonin	2	Acetylcholine Chloride	5	L-Aspartic acid	5	Riboflavin	8
Ascorbic acid	1	Melatonin	2	Cytidine	5	L-Aspartic acid	5	Riboflavin	8
Ascorbic acid	1	Melatonin	2	Cytidine	5	L-Cysteine	5	Riboflavin	8
Dopamine	1	Serotonin	2	D-Aspartic acid	5	L-Histidine	5		
Epinephrine	1	Ampicillin	2	D-Aspartic acid	5	L-Histidine	5		
Norepinephrine	1	Ampicillin	2	D-Aspartic acid	5	L-Histidine	5		
Adenosine	2	Ampicillin	2	D-Fructose	5	Norepinephrine	5		
Adenosine	2	Creatine	2	D-Mannitol	5	Norepinephrine	5		
Adenosine	2	Creatine	2	D-Mannose	5	Oxytocin	5		
cAMP	2	Creatine	2	D-Mannose	5	ATP	6		
cAMP	2	Glutamic acid	2	GABA	5	ATP	6		
Cytidine	2	Glutamic acid	2	Histamine	5	ATP	6		
D-Fructose	2	Glutamic acid	2	Histamine	5	cAMP	6		
D-Fructose	2	Glycine	2	Homovanillic acid	5	L-Thyroxine	6		
D-Galactose	2	Glycine	2	Homovanillic acid	5	L-Thyroxine	6		
D-Galactose	2	Glycine	2	L-Citrulline	5	L-Thyroxine	6		
D-Galactose	2	NADH	2	L-Citrulline	5	L-Tyrosine	6		
D-Glucose	2	NADH	2	L-Phenylalanine	5	L-Tyrosine	6		
D-Glucose	2	NADH	2	L-Phenylalanine	5	17-beta-estradiol	6		
D-Glucose	2	Urea	2	L-Tyrosine	5	L-Cysteine	6		
D-Mannitol	2	Urea	2	Serotonin	5	L-Cysteine	6		
D-Mannose	2	Urea	2	Serotonin	5	Oxytocin	6		
GABA	2	L-Dopa	3	17-beta-estradiol	5	Oxytocin	6		
GABA	2	L-Dopa	4	17-beta-estradiol	5	Histamine	7		
Guanosine	2	L-Dopa	4	Ascorbic acid	5	Homovanillic acid	7		
Guanosine	2	2,4-dinitrophenol	5	DOPAC	5	Dopamine	7		
Guanosine	2	2,4-dinitrophenol	5	DOPAC	5	Dopamine	7		
L-Citrulline	2	Acetylcholine Chloride	5	DOPAC	5	Epinephrine	7		

Corona: DNA CB14 (CCCCCCCCACCGGCGTTTCCCCCCCC)



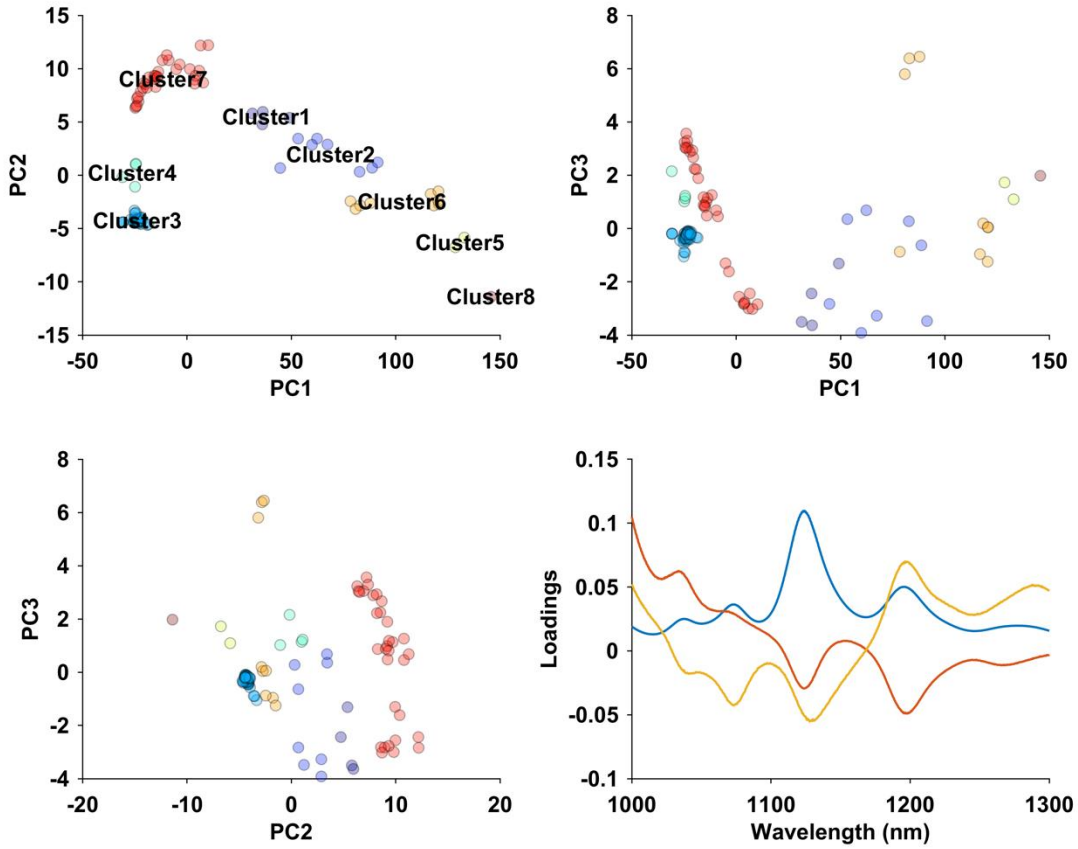
Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
Homovanillic acid	1	Serotonin	4	2,4-dinitrophenol	7	D-Mannose	7	Urea	7
Homovanillic acid	1	Ampicillin	4	Acetylcholine Chloride	7	D-Mannose	7	Urea	7
Oxytocin	1	Ampicillin	4	Acetylcholine Chloride	7	GABA	7	Riboflavin	8
Oxytocin	1	Ampicillin	4	Acetylcholine Chloride	7	GABA	7	Riboflavin	8
Oxytocin	1	NADH	4	Adenosine	7	GABA	7	DOX	8
D-Aspartic acid	2	L-Dopa	5	Adenosine	7	Guanosine	7	DOX	8
D-Aspartic acid	2	Ascorbic acid	5	Adenosine	7	Guanosine	7	DOX	8
D-Mannose	2	L-Dopa	6	ATP	7	L-Citrulline	7		
Guanosine	2	L-Dopa	6	ATP	7	L-Citrulline	7		
Histamine	2	L-Tyrosine	6	ATP	7	L-Citrulline	7		
Histamine	2	L-Tyrosine	6	cAMP	7	Melatonin	7		
Histamine	2	L-Tyrosine	6	cAMP	7	Melatonin	7		
Homovanillic acid	2	Ascorbic acid	6	cAMP	7	Riboflavin	7		
L-Phenylalanine	2	Ascorbic acid	6	Cytidine	7	17-beta-estradiol	7		
L-Phenylalanine	2	Dopamine	6	Cytidine	7	17-beta-estradiol	7		
L-Phenylalanine	2	Dopamine	6	Cytidine	7	17-beta-estradiol	7		
Melatonin	2	Dopamine	6	D-Aspartic acid	7	Creatine	7		
L-Aspartic acid	2	Epinephrine	6	D-Fructose	7	Creatine	7		
L-Aspartic acid	2	Epinephrine	6	D-Fructose	7	Creatine	7		
L-Aspartic acid	2	Epinephrine	6	D-Fructose	7	DOPAC (control)	7		
L-Histidine	2	L-Cysteine	6	D-Galactose	7	DOPAC (control)	7		
L-Histidine	2	L-Cysteine	6	D-Galactose	7	DOPAC (control)	7		
L-Histidine	2	L-Cysteine	6	D-Galactose	7	Glutamic acid	7		
NADH	3	NADH	6	D-Glucose	7	Glutamic acid	7		
L-Thyroxine	4	Norepinephrine	6	D-Glucose	7	Glutamic acid	7		
L-Thyroxine	4	Norepinephrine	6	D-Glucose	7	Glycine	7		
L-Thyroxine	4	Norepinephrine	6	D-Mannitol	7	Glycine	7		
Serotonin	4	2,4-dinitrophenol	7	D-Mannitol	7	Glycine	7		
Serotonin	4	2,4-dinitrophenol	7	D-Mannitol	7	Urea	7		

Corona: DNA CB13 (CCCCCCCCAGAATTACTTCCCCCCCC)



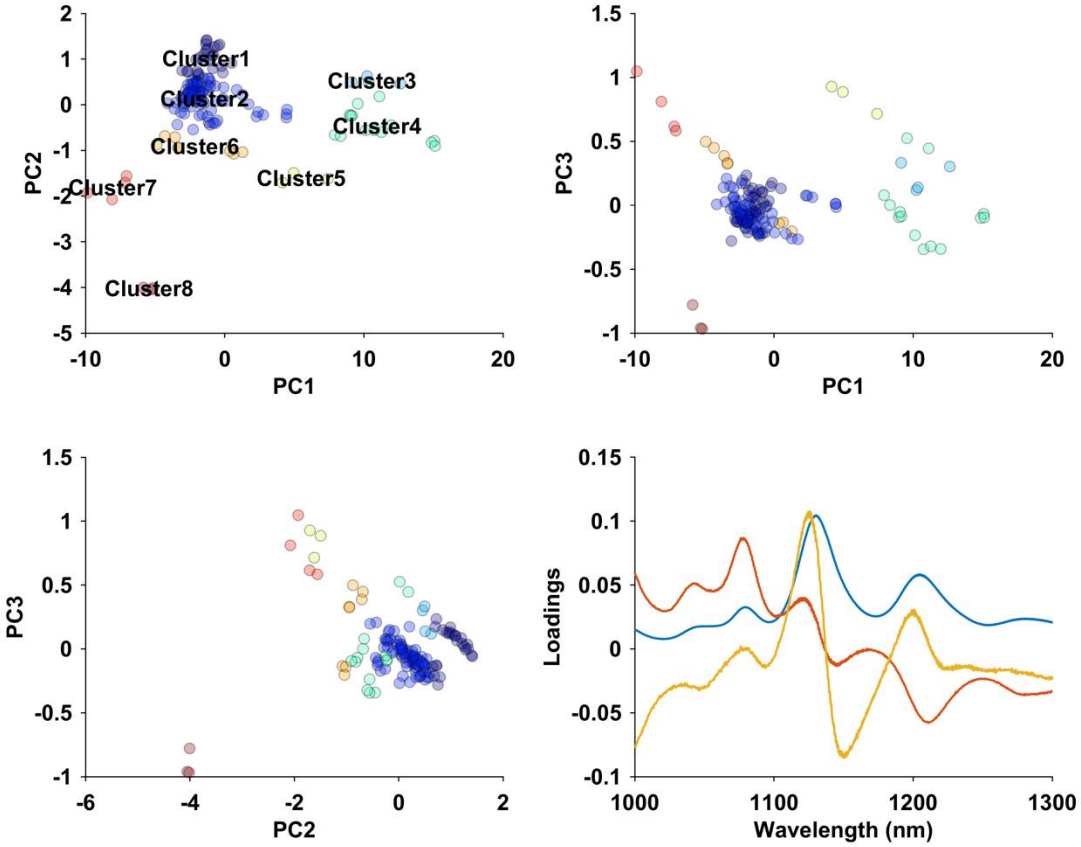
Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
2,4 dinitrophenol	1	GABA	1	control	1	b-estradiol	2	Control	7	Melatonin	7
2,4 dinitrophenol	1	GABA	1	control	1	b-estradiol	2	D-Mannose	7	Melatonin	7
2,4 dinitrophenol	1	control	1	urea	1	l-aspartic acid	2	D-Mannose	7	l-cysteine	7
acetylcholine chloride	1	control	1	urea	1	l-aspartic acid	2	D-Mannose	7	l-cysteine	7
acetylcholine chloride	1	control	1	urea	1	l-histidine	2	Guanosine	7	l-cysteine	7
acetylcholine chloride	1	control	1	Control	1	l-histidine	2	Guanosine	7	norepinephrine	7
adenosine	1	control	1	Control	1	l-histidine	2	Guanosine	7	norepinephrine	7
adenosine	1	D-mannitol	1	Control	1	control	2	Histamine	7	norepinephrine	7
ATP	1	D-mannitol	1	Control	1	oxytocin	2	Histamine	7	dopamine	8
ATP	1	D-mannitol	1	Control	1	oxytocin	2	Histamine	7	dopamine	8
ATP	1	ampicilllin	1	Control	1	oxytocin	2	Homovanillic acid	7	dopamine	8
cAMP	1	ampicilllin	1	AMP	1	NADH	2	Homovanillic acid	7	ascorbic acid	8
cAMP	1	ampicilllin	1	AMP	1	NADH	2	Homovanillic acid	7	ascorbic acid	8
cAMP	1	creatine	1	AMP	1	NADH	2	L-Citrulline	7	ascorbic acid	8
cytidine	1	creatine	1	CMP	1	Epinephrine	3	L-Citrulline	7		
cytidine	1	creatine	1	CMP	1	Epinephrine	3	L-Citrulline	7		
cytidine	1	control	1	CMP	1	Epinephrine	3	L-Dopa	7		
D-aspartic acid	1	control	1	TMP	1	Dopamine	3	L-Dopa	7		
D-aspartic acid	1	control	1	TMP	1	Dopamine	3	L-Dopa	7		
D-fructose	1	control	1	TMP	1	Dopamine	3	L-Phenylalanine	7		
D-fructose	1	control	1	GMP	1	GMP	4	L-Phenylalanine	7		
D-fructose	1	control	1	GMP	1	riboflavin	5	L-Phenylalanine	7		
D-galactose	1	glutamic acid	1	adenosine	2	riboflavin	5	L-Thyroxine	7		
D-galactose	1	glutamic acid	1	D-aspartic acid	2	riboflavin	5	L-Thyroxine	7		
D-galactose	1	glutamic acid	1	control	2	DOX	6	L-Thyroxine	7		
D-glucose	1	glycine	1	serotonin	2	DOX	6	L-Tyrosine	7		
D-glucose	1	glycine	1	serotonin	2	DOX	6	L-Tyrosine	7		
D-glucose	1	glycine	1	serotonin	2	Control	7	L-Tyrosine	7		
GABA	1	l-aspartic acid	1	b-estradiol	2	Control	7	Melatonin	7		

Corona: DNA CB4 (CCCCCCCCCCAGGCGGGGCCCCCCCC)



Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
L-Tyrosine	1	Cytidine	3	Homovanillic acid	3	Epinephrine	6	L-Histidine	7
Oxytocin	1	D-Aspartic acid	3	Homovanillic acid	3	Epinephrine	6	L-Histidine	7
Oxytocin	1	D-Aspartic acid	3	L-Citrulline	3	Epinephrine	6	L-Histidine	7
Oxytocin	1	D-Aspartic acid	3	L-Citrulline	3	L-Cysteine	6	Norepinephrine	7
L-Tyrosine	2	D-Fructose	3	L-Citrulline	3	L-Cysteine	6	Norepinephrine	7
L-Tyrosine	2	D-Fructose	3	L-Dopa	3	L-Cysteine	6	Norepinephrine	7
Serotonin	2	D-Fructose	3	L-Dopa	3	Melatonin	7	Urea	7
Serotonin	2	D-Galactose	3	L-Dopa	3	Melatonin	7	Urea	7
Serotonin	2	D-Galactose	3	L-Phenylalanine	3	Melatonin	7	Urea	7
NADH	2	D-Galactose	3	L-Phenylalanine	3	17-beta-estradiol	7	Ascorbic acid	8
NADH	2	D-Glucose	3	L-Phenylalanine	3	17-beta-estradiol	7		
NADH	2	D-Glucose	3	L-Thyroxine	3	17-beta-estradiol	7		
2,4-dinitrophenol	3	D-Glucose	3	L-Thyroxine	3	Ampicillin	7		
2,4-dinitrophenol	3	D-Mannitol	3	L-Thyroxine	3	Ampicillin	7		
2,4-dinitrophenol	3	D-Mannitol	3	control	3	Ampicillin	7		
Acetylcholine Chloride	3	D-Mannitol	3	control	3	Creatine	7		
Acetylcholine Chloride	3	D-Mannose	3	control	3	Creatine	7		
Acetylcholine Chloride	3	D-Mannose	3	DOX	3	Creatine	7		
Adenosine	3	D-Mannose	3	DOX	3	DOPAC (control)	7		
Adenosine	3	GABA	3	DOX	3	DOPAC (control)	7		
Adenosine	3	GABA	3	Riboflavin	4	DOPAC (control)	7		
ATP	3	GABA	3	Riboflavin	4	Glutamic acid	7		
ATP	3	Guanosine	3	Riboflavin	4	Glutamic acid	7		
ATP	3	Guanosine	3	Glutamic acid	4	Glycine	7		
cAMP	3	Guanosine	3	Ascorbic acid	5	Glycine	7		
cAMP	3	Histamine	3	Ascorbic acid	5	Glycine	7		
cAMP	3	Histamine	3	Dopamine	6	L-Aspartic acid	7		
Cytidine	3	Histamine	3	Dopamine	6	L-Aspartic acid	7		
Cytidine	3	Homovanillic acid	3	Dopamine	6	L-Aspartic acid	7		

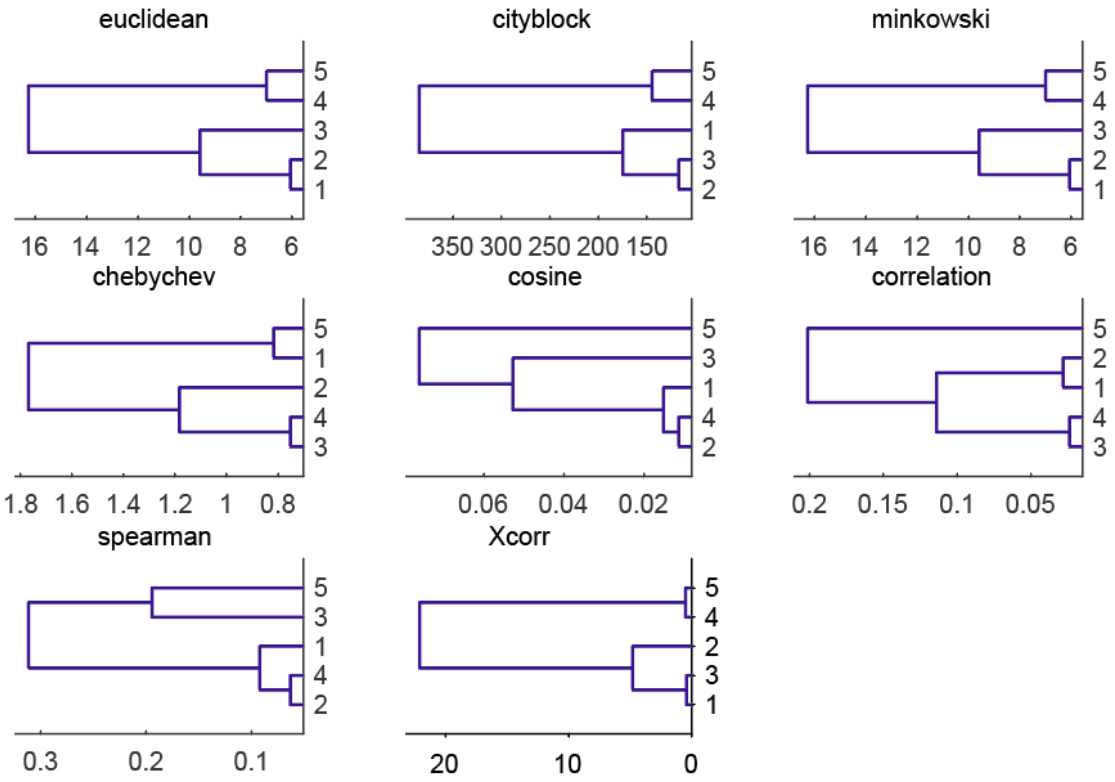
Corona: DNA CB3 (CCCCCCCCCTCCGCAAGTCCCCCCCC)

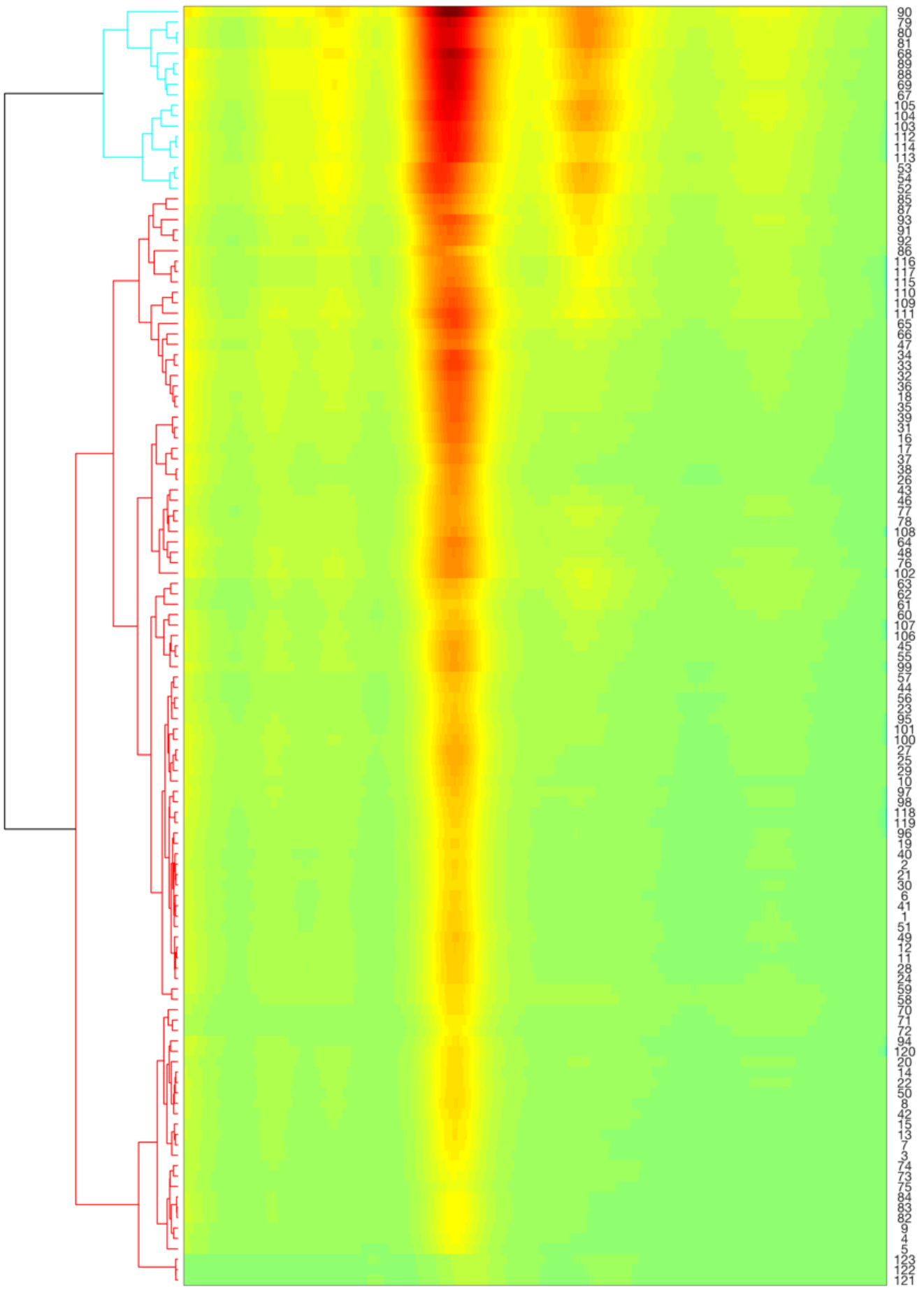


Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster	Analyte	Cluster
GABA	1	2,4 dinitrophenol	2	adenosine	2	Serotonin	2	Ascorbic acid	4
Glutamic acid	1	2,4 dinitrophenol	2	adenosine	2	Oxytocin	2	Ascorbic acid	4
Control	1	acetylcholine	2	D-mannitol	2	Oxytocin	2	Epinephrine	4
Control	1	acetylcholine	2	D-mannitol	2	Oxytocin	2	Epinephrine	4
Control	1	acetylcholine	2	D-mannitol	2	Estradiol	2	Cysteine	4
Glycine	1	ATP	2	D-mannose	2	Estradiol	2	Cysteine	4
Glycine	1	ATP	2	D-mannose	2	Estradiol	2	Cysteine	4
AMP	1	ATP	2	D-mannose	2	Ampicillin	2	Norepinephrine	5
AMP	1	cAMP	2	Histamine	2	Ampicillin	2	Norepinephrine	5
AMP	1	cAMP	2	Histamine	2	Ampicillin	2	Norepinephrine	5
CMP	1	cAMP	2	Histamine	2	Creatine	2	Guanosine	6
CMP	1	cytidine	2	control	2	Creatine	2	Guanosine	6
CMP	1	cytidine	2	control	2	Creatine	2	Guanosine	6
GMP	1	cytidine	2	control	2	Glutamic acid	2	L-thyroxine	6
GMP	1	D-aspartic acid	2	Homovanillic acid	2	Glycine	2	L-thyroxine	6
GMP	1	D-aspartic acid	2	Homovanillic acid	2	NADH	2	L-tyrosine	6
TMP	1	D-aspartic acid	2	Homovanillic acid	2	NADH	2	L-tyrosine	6
TMP	1	D-fructose	2	L-citruline	2	NADH	2	L-tyrosine	6
TMP	1	D-fructose	2	L-citruline	2	Epinephrine	3	Riboflavin	7
Aspartic acid	1	D-fructose	2	L-citruline	2	Dopamine	3	Riboflavin	7
Aspartic acid	1	D-galactose	2	L-phenylalanine	2	Dopamine	3	Riboflavin	7
Aspartic acid	1	D-galactose	2	L-phenylalanine	2	Dopamine	3	Glutamic acid	7
Histamine	1	D-galactose	2	L-phenylalanine	2	dopamine	4	DOX	8
Histamine	1	D-glucose	2	L-thyroxine	2	dopamine	4	DOX	8
Histamine	1	D-glucose	2	Melotonin	2	dopamine	4	DOX	8
control	2	D-glucose	2	Melotonin	2	L-DOPA	4		
control	2	GABA	2	Melotonin	2	L-DOPA	4		
control	2	GABA	2	Serotonin	2	L-DOPA	4		
2,4 dinitrophenol	2	adenosine	2	Serotonin	2	Ascorbic acid	4		

Figure S3. Hierarchical clustering dendrograms generated using different distance metrics for library data acquired for the DNA-wrapped SWNT nanosensors. Analytes contained within each cluster are listed in "SI_File3_dendrograms.zip". A full dendrogram using weighted linkages and cosine distance is displayed alongside a heatmap of the fluorescence emission spectrum for all samples with 990-1340 nm emission indicated by the horizontal axis. Sample IDs can be found in the file "SI_File2_sample-IDs.xlsx". Dendrogram colors indicate a group nodes whose linkage is less than 3.

Corona: DNA $(TTA)_4TT$

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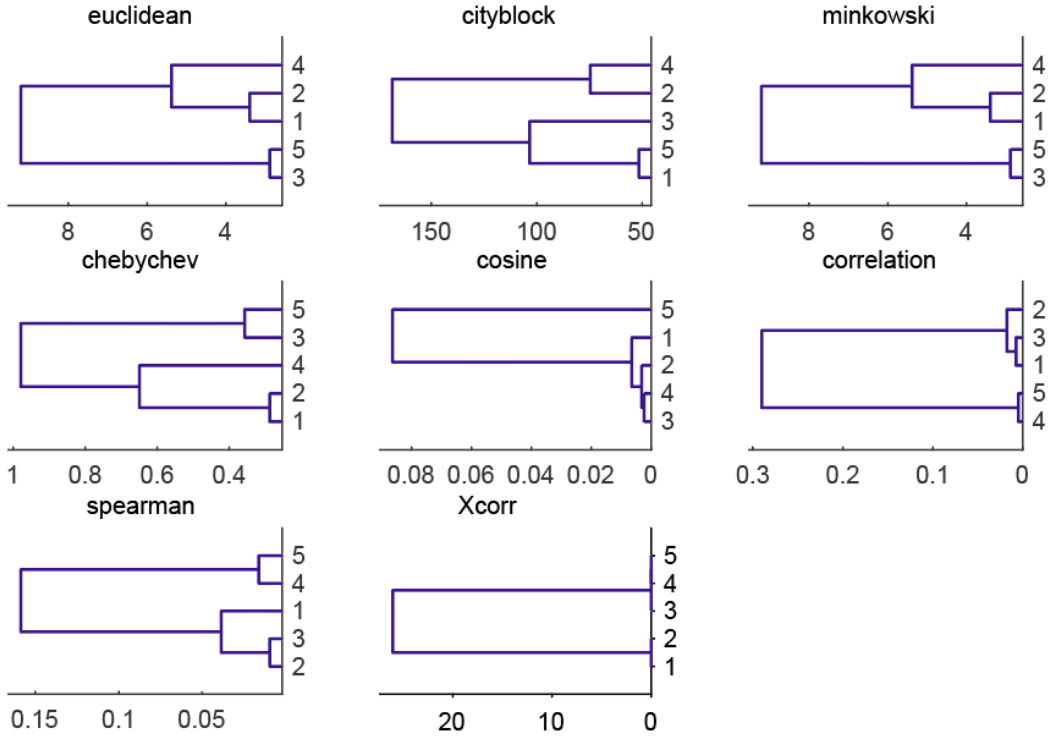
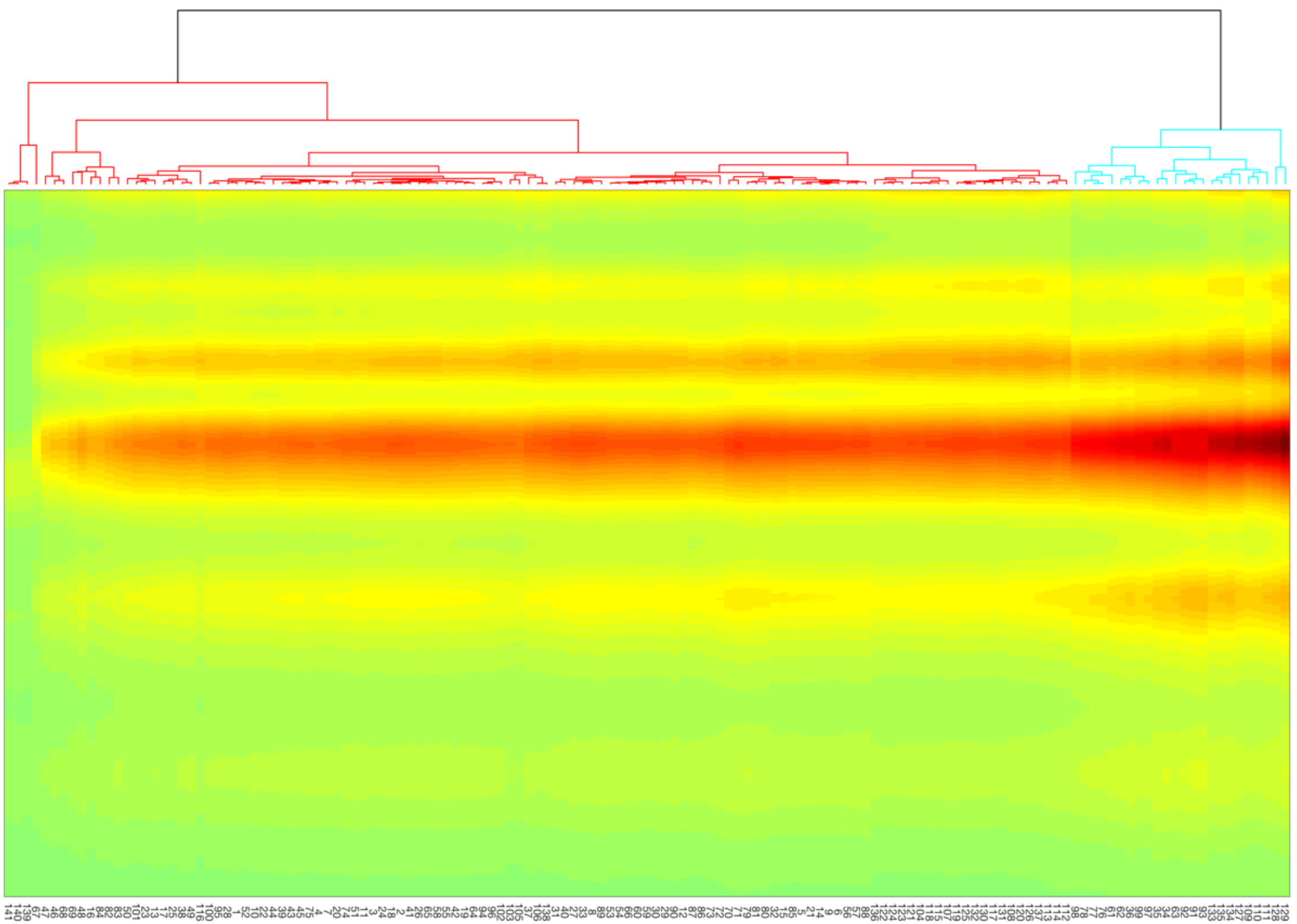
Corona: DNA $(TAT)_4$





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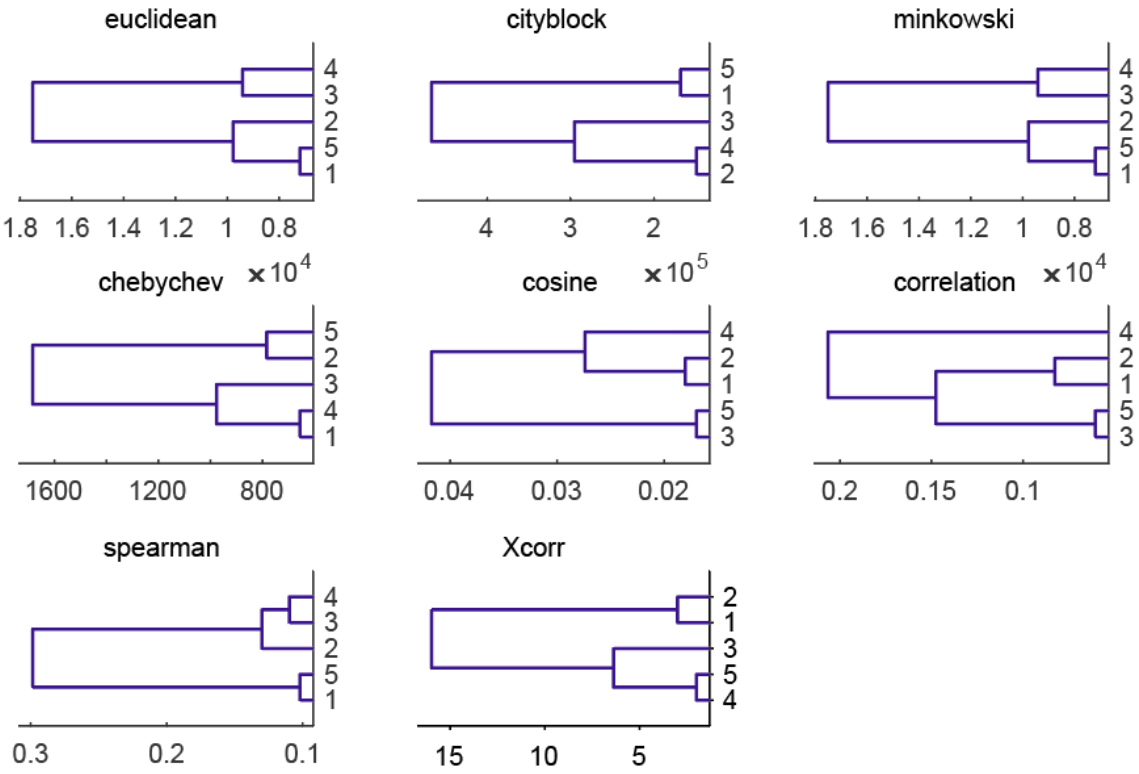

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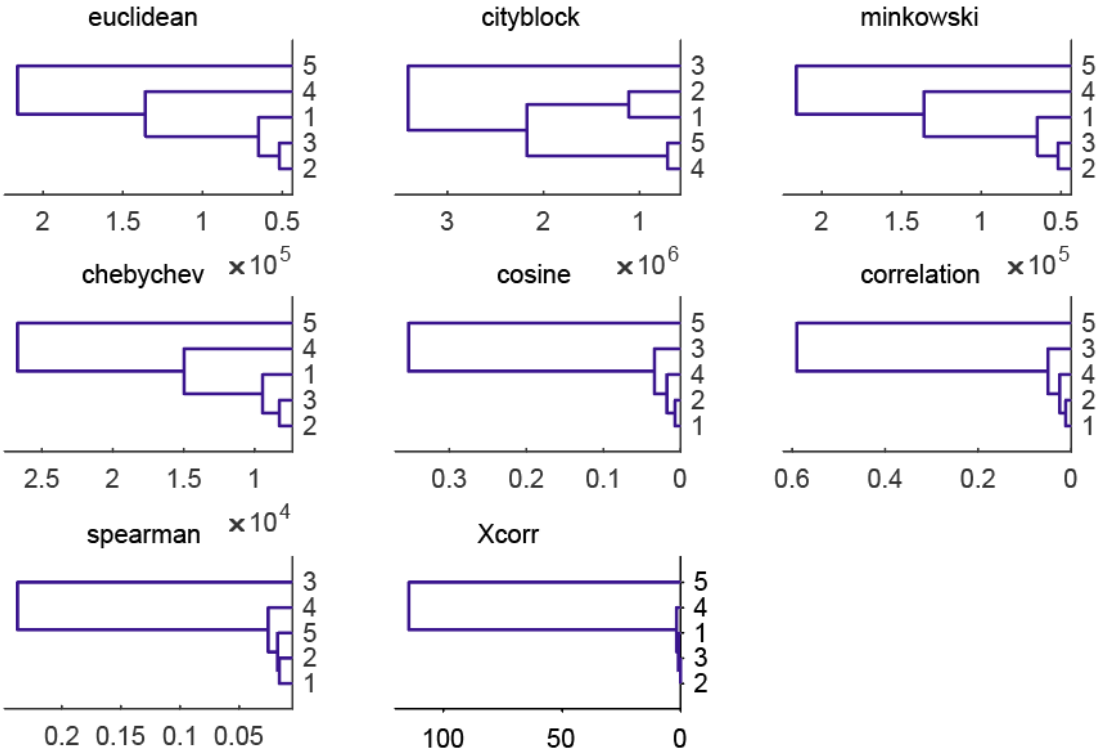
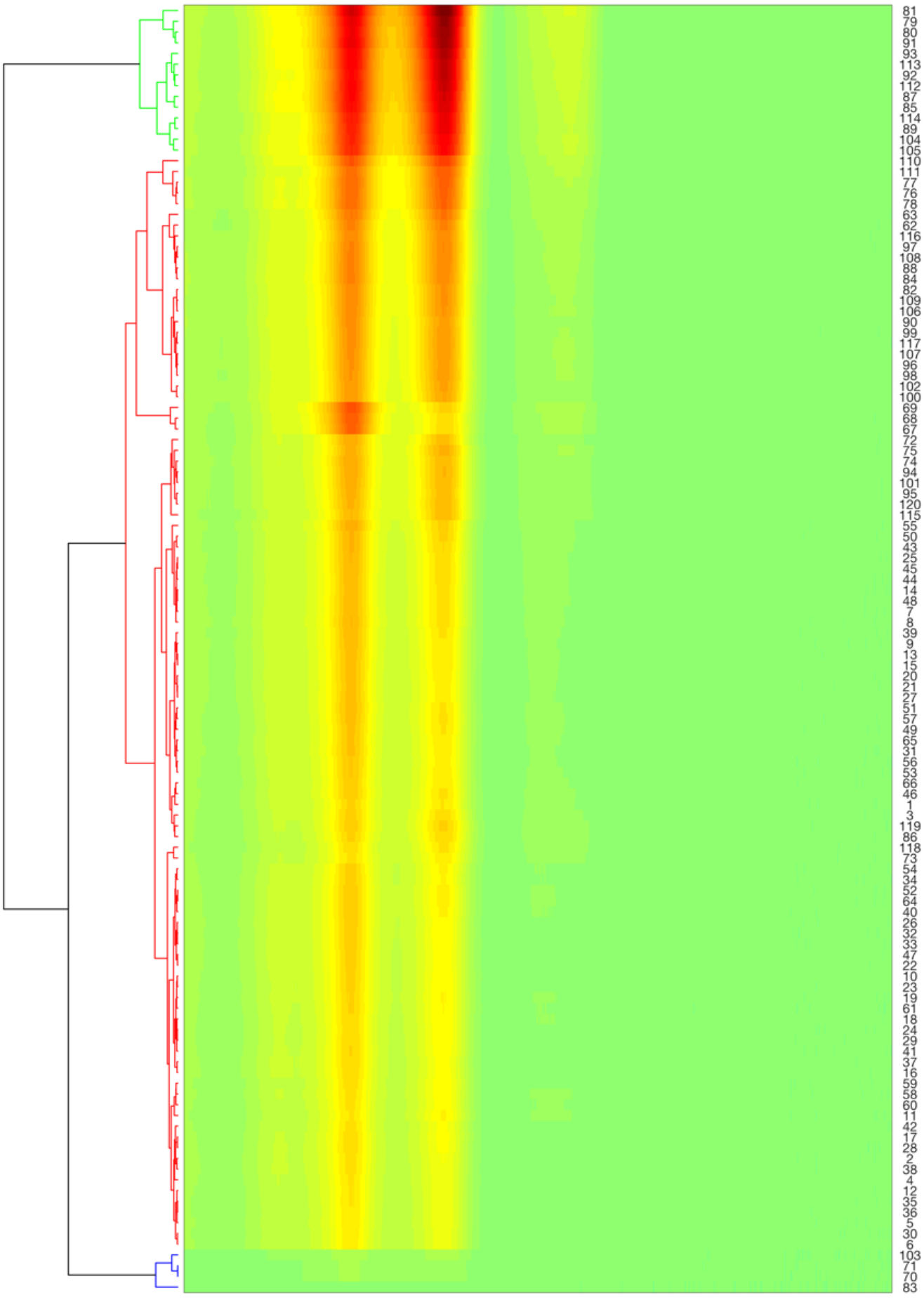
Corona: DNA $(GT)_{15}$

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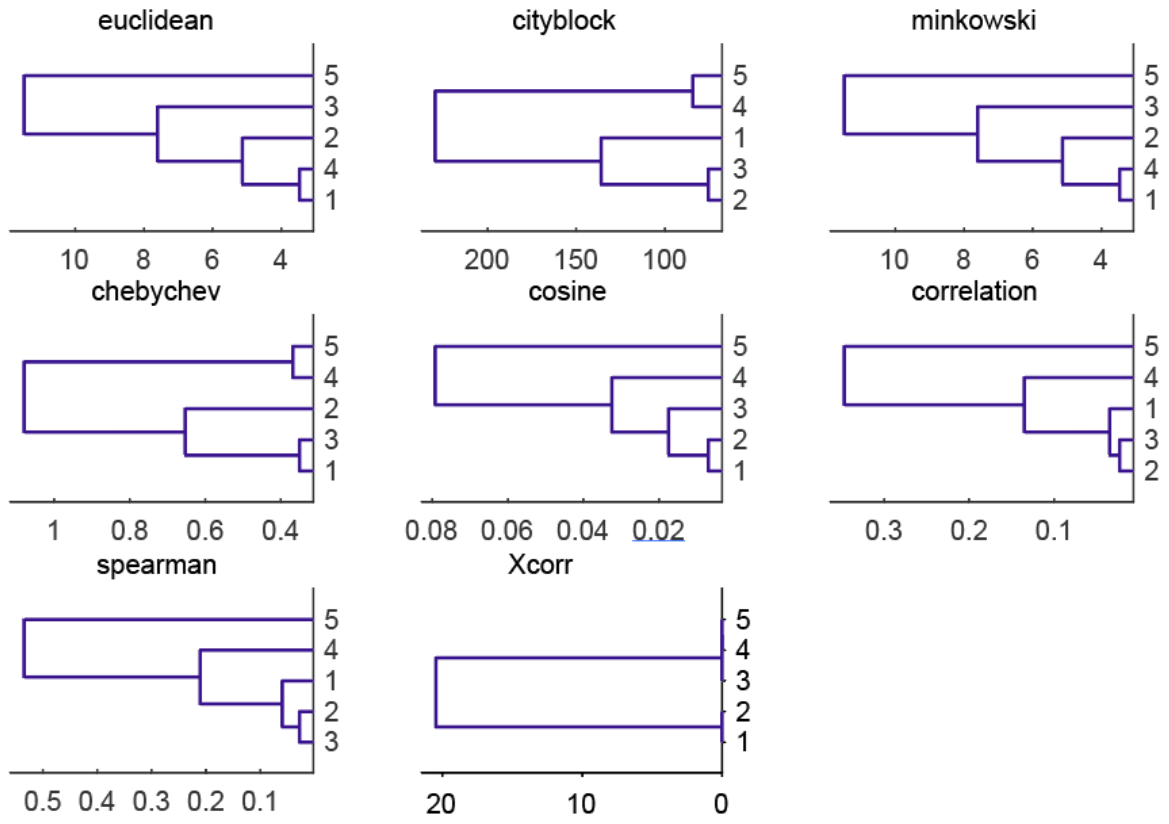
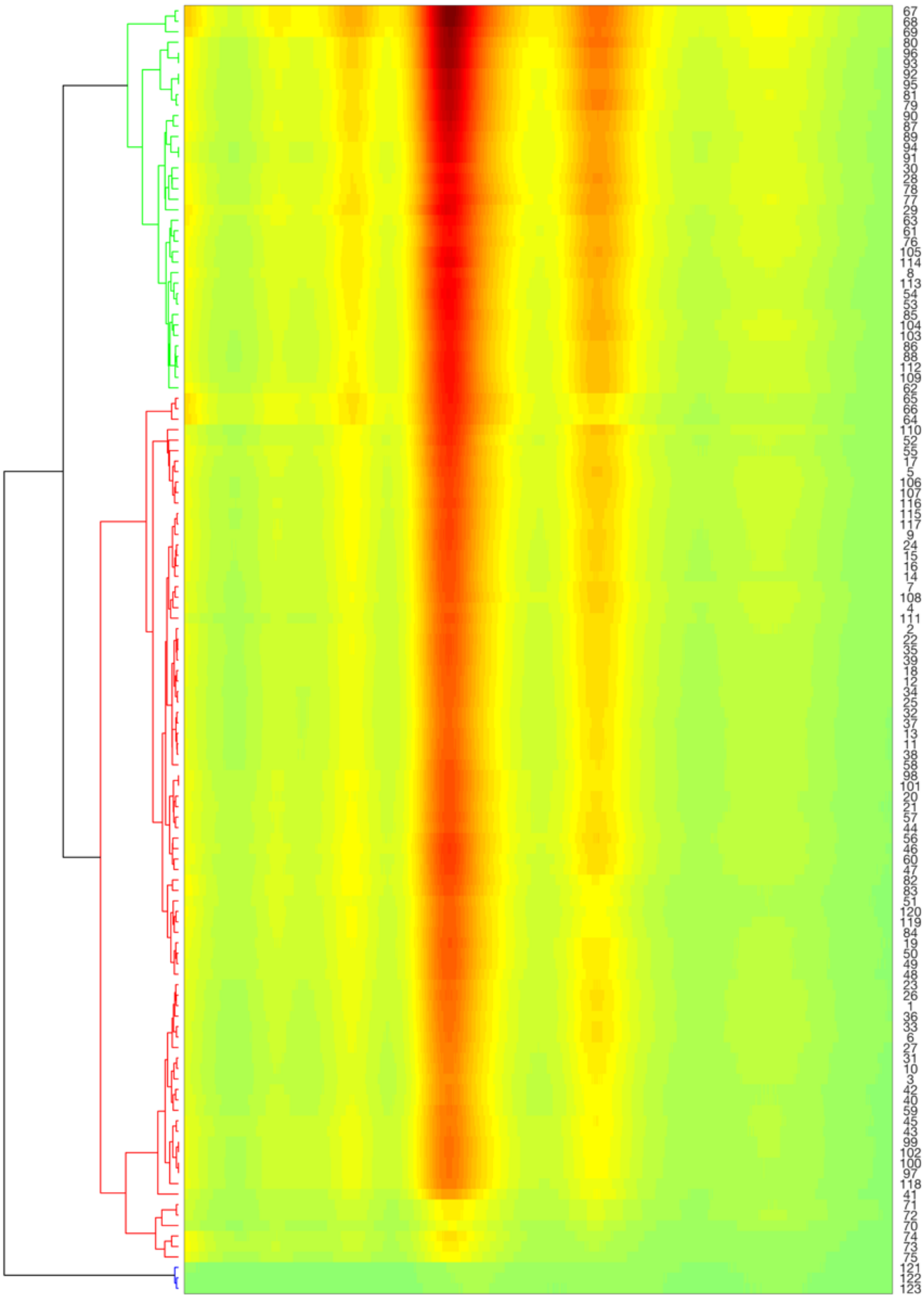
Corona: DNA GTAGTCGAGTGTGTGTGTGTGT

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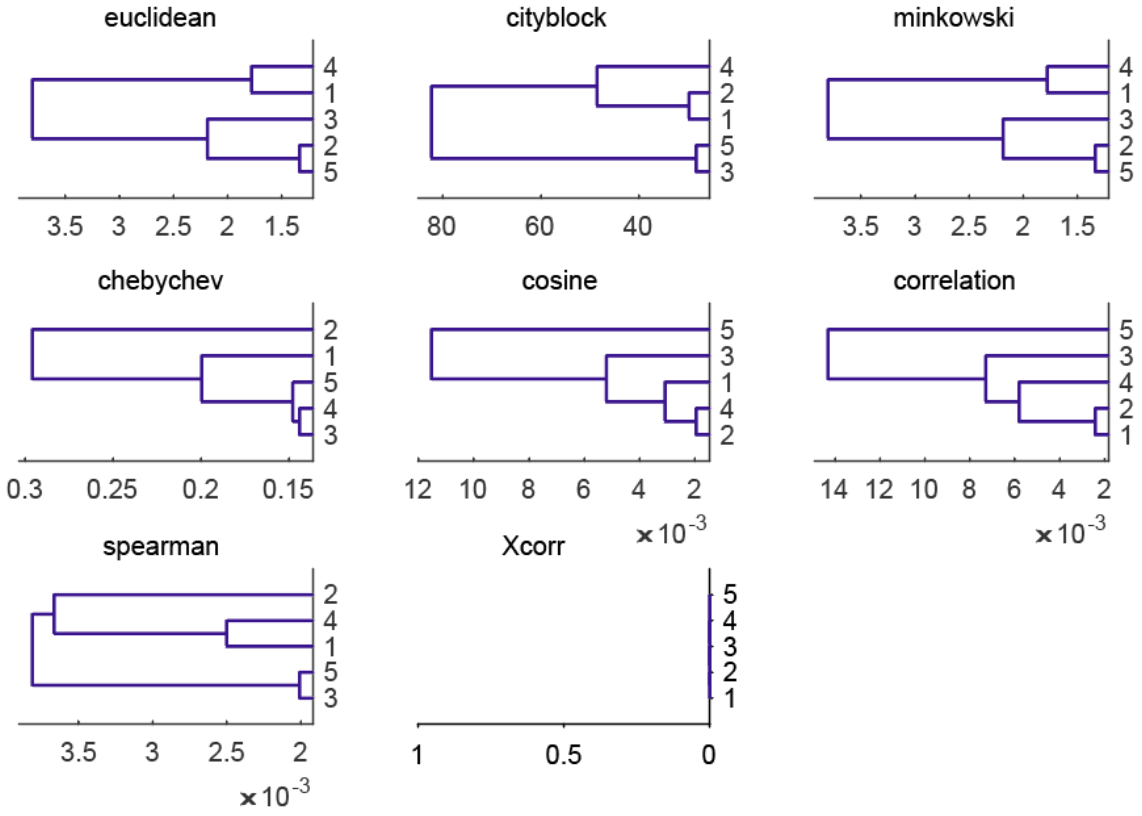
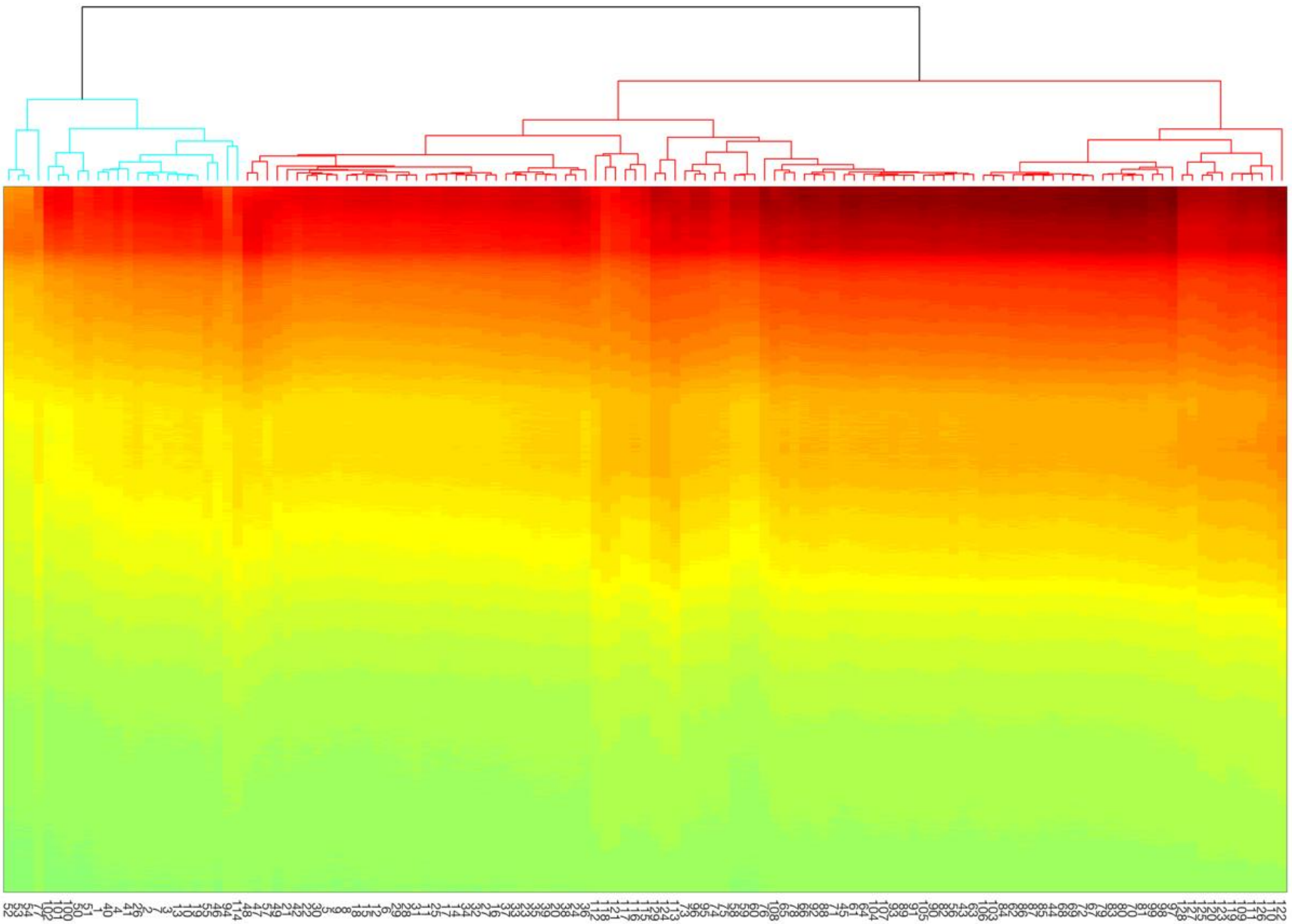
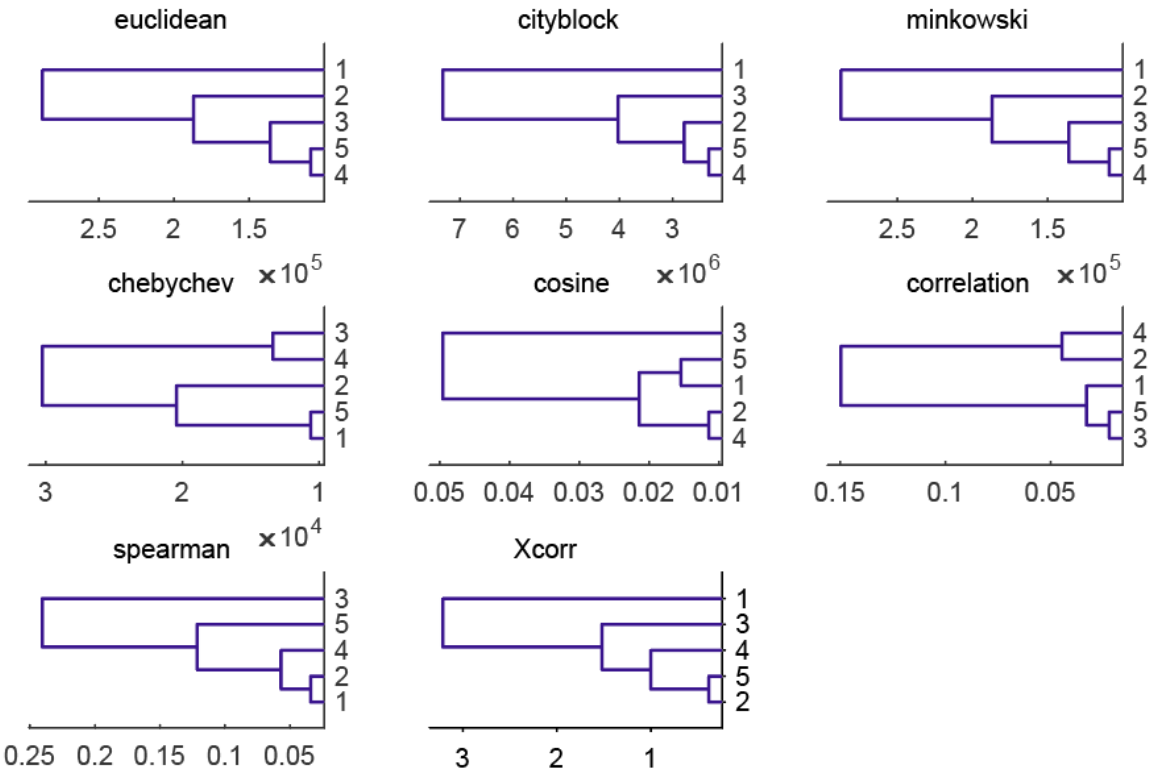
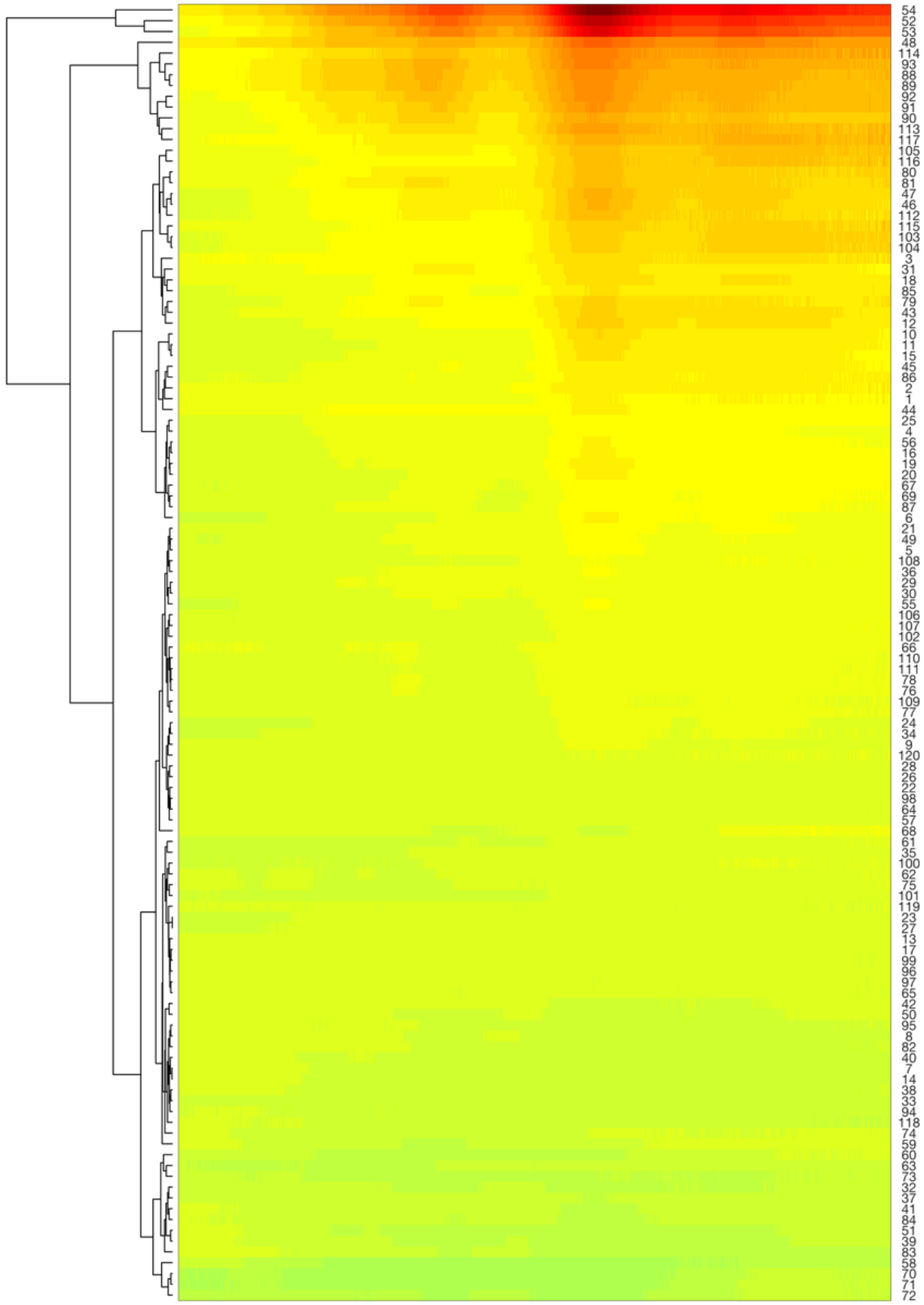
Corona: Phospholipid DTTE-PEG2k





Corona: DNA $(CCA)_{10}$

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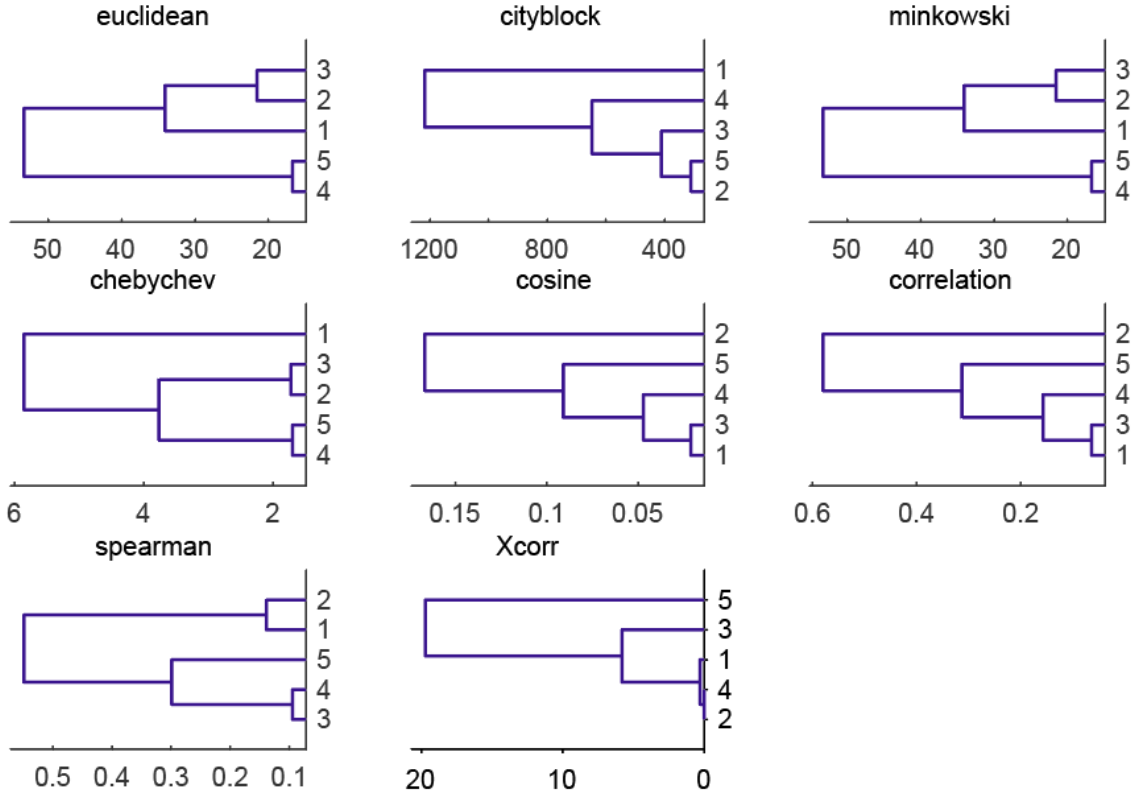
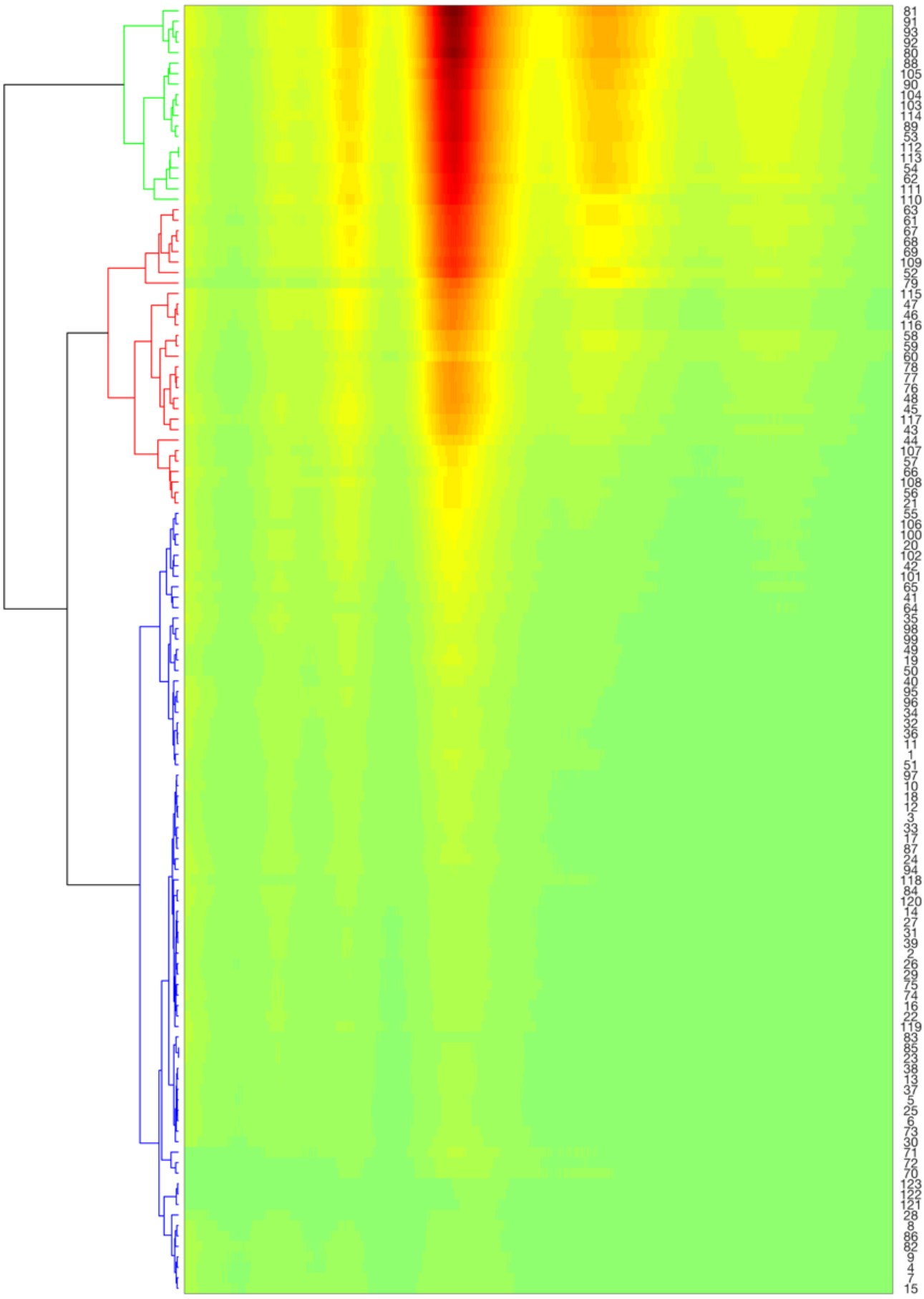
Corona: DNA CB14 (CCCCCCCCCACCGGCGTTTCCCCCCCC)

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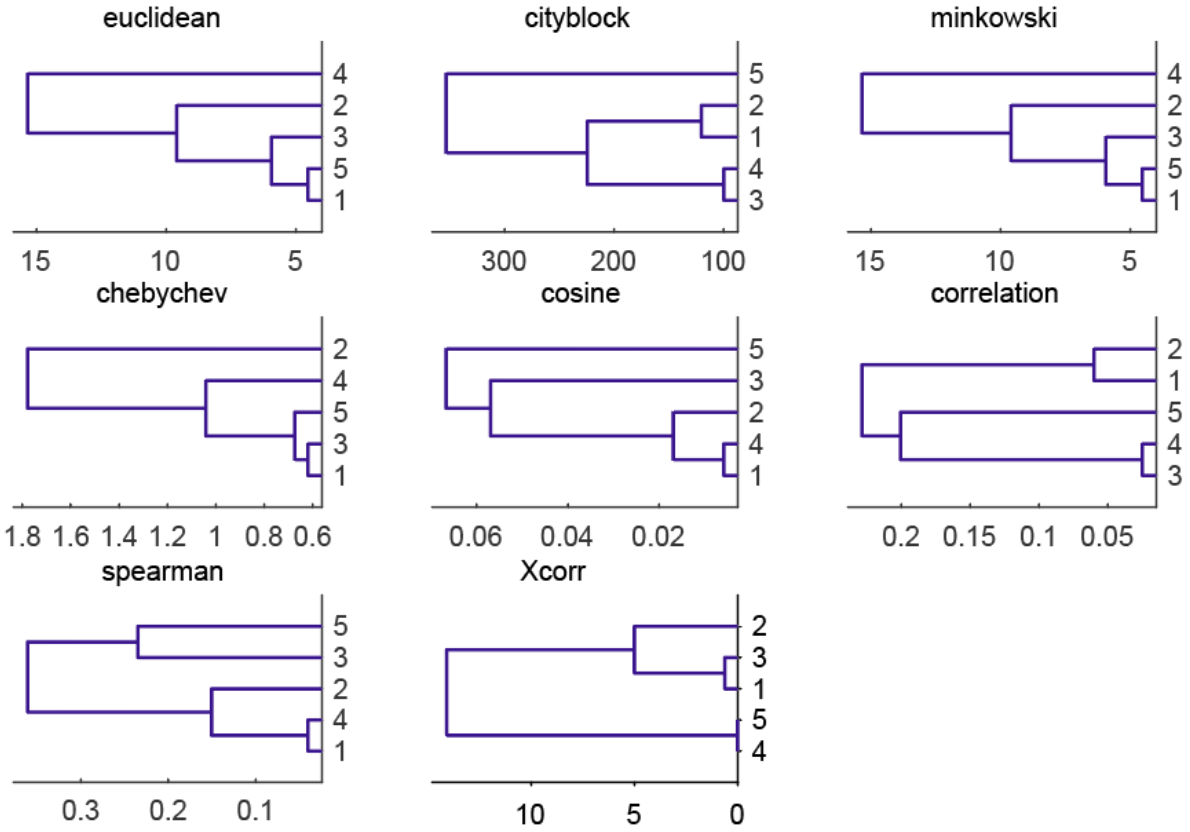
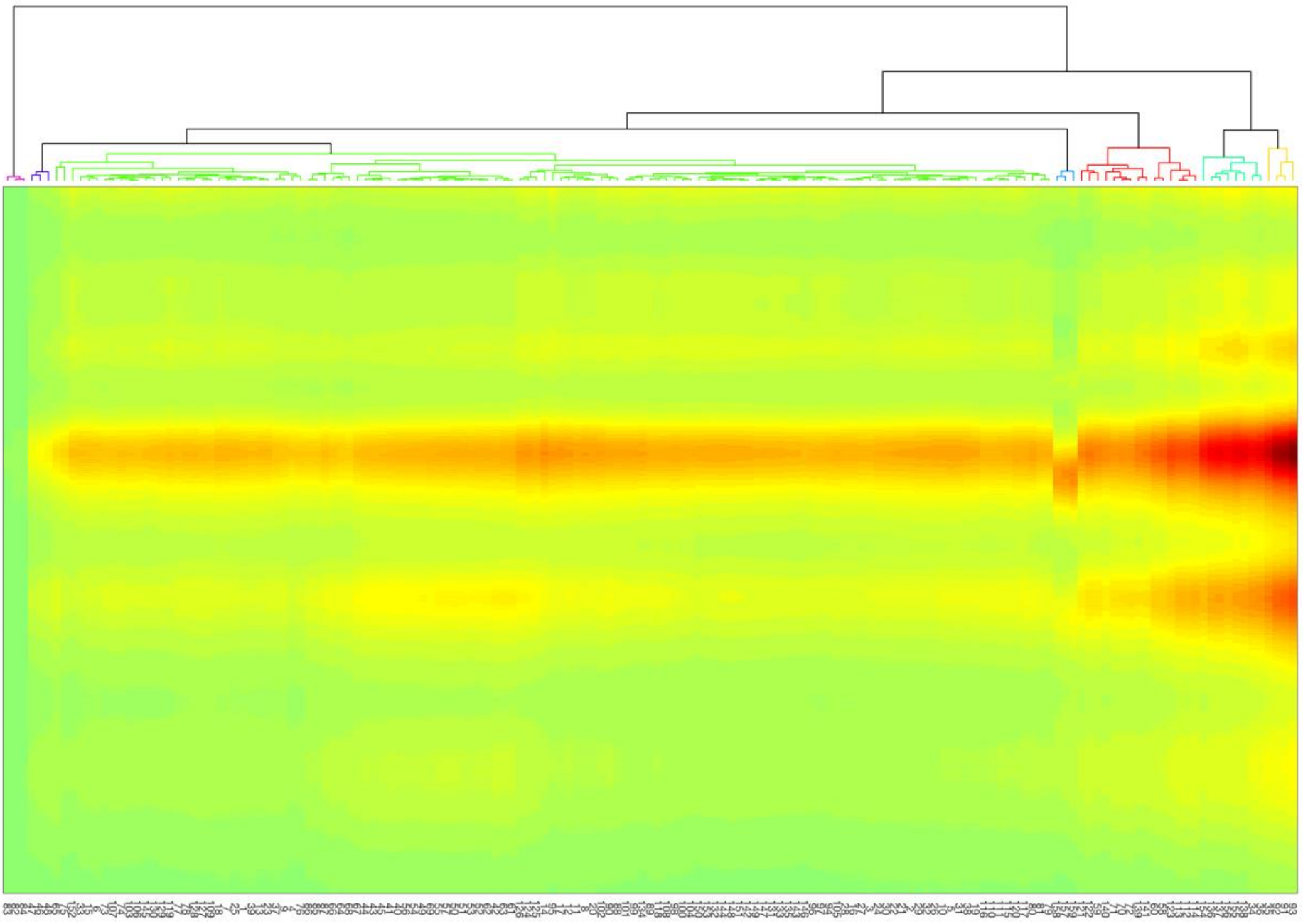
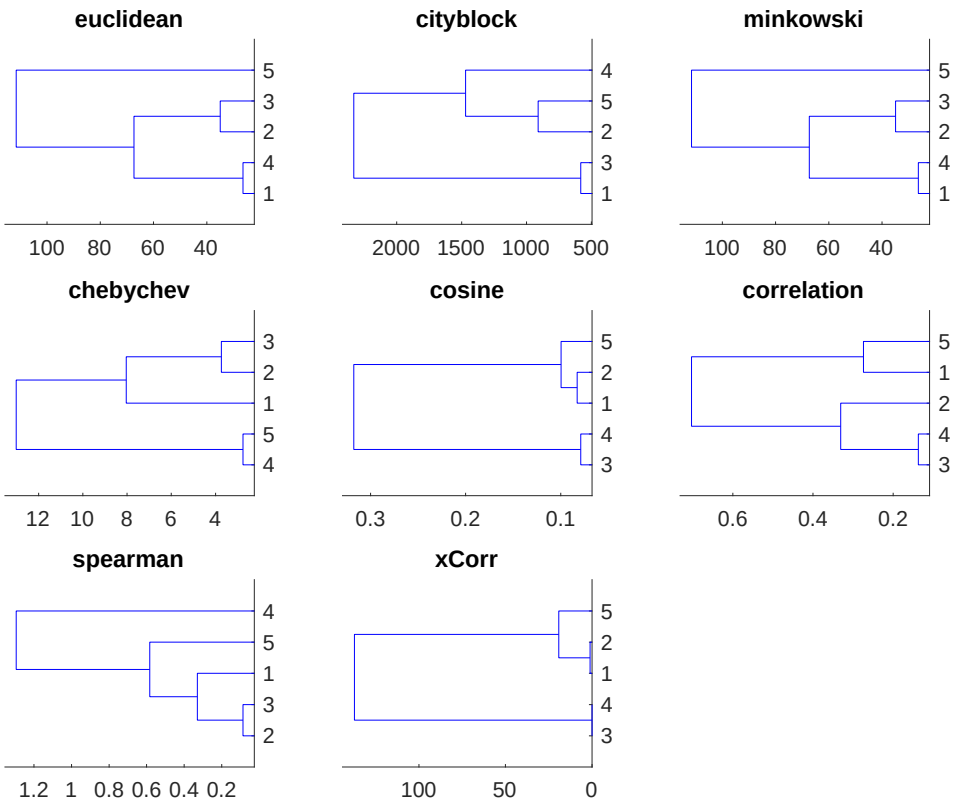
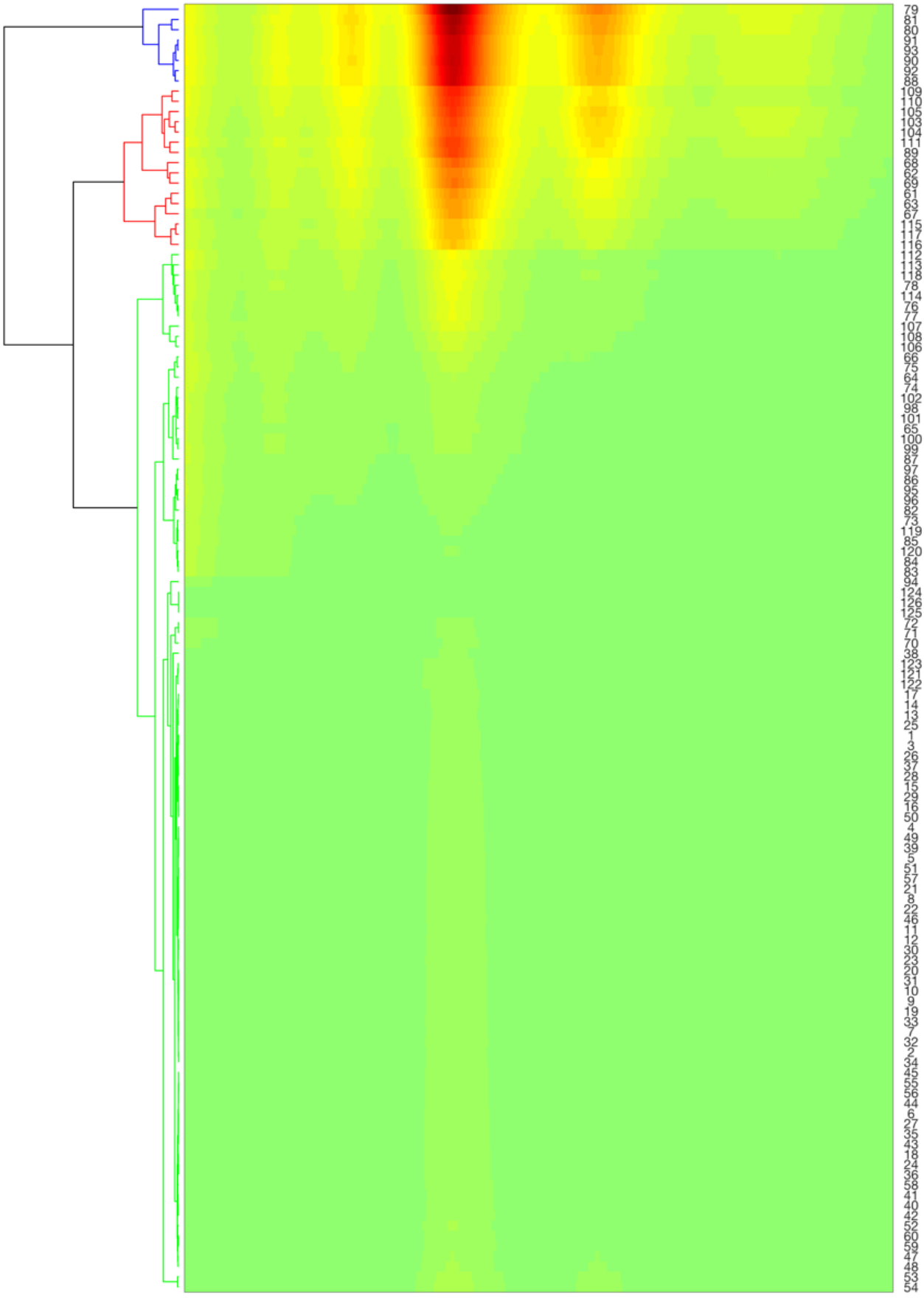
Corona: DNA CB13 (CCCCCCCCCAGAATTACTTCCCCCCCC)





Corona: DNA CB4 (CCCCCCCCCCCAGGCGGGGCCCCCCCC)

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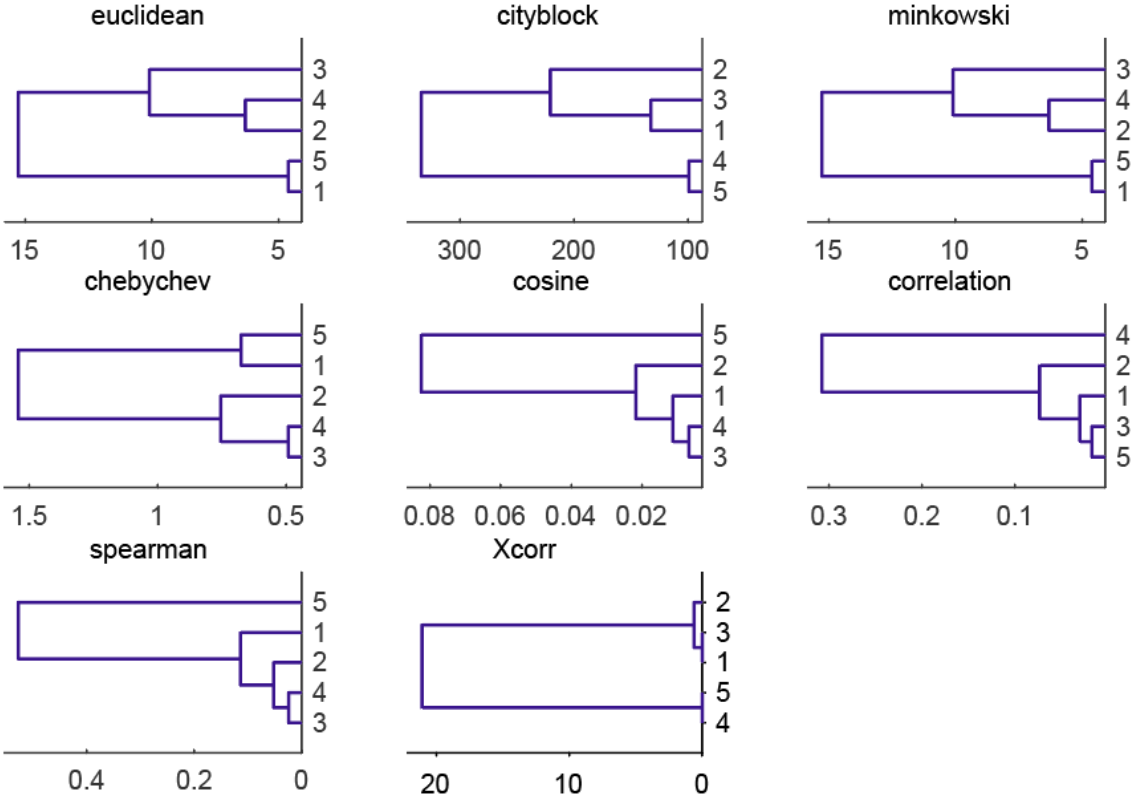
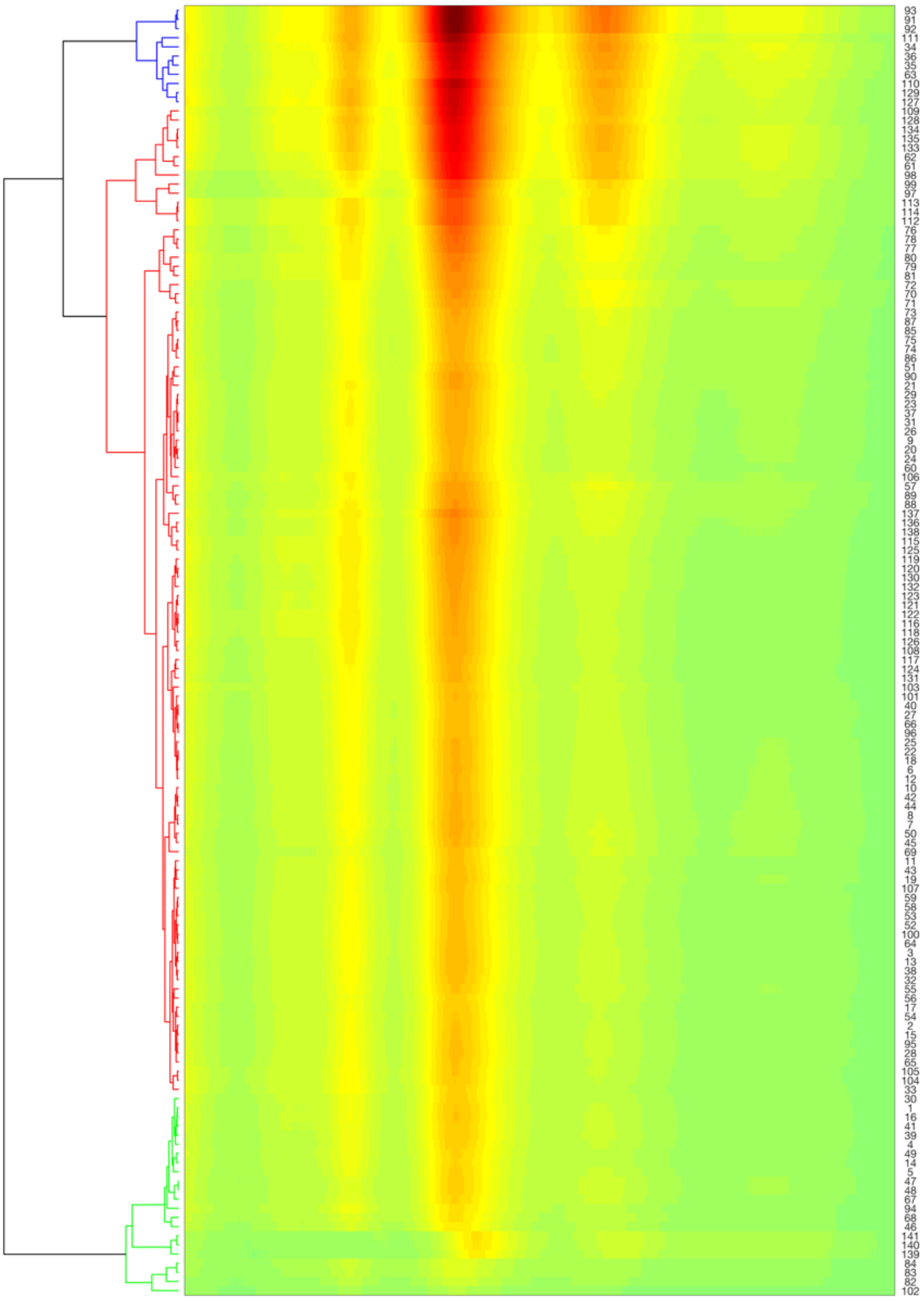
Corona: DNA CB3 (CCCCCCCCCCTCCGCAAGTCCCCCCCC)

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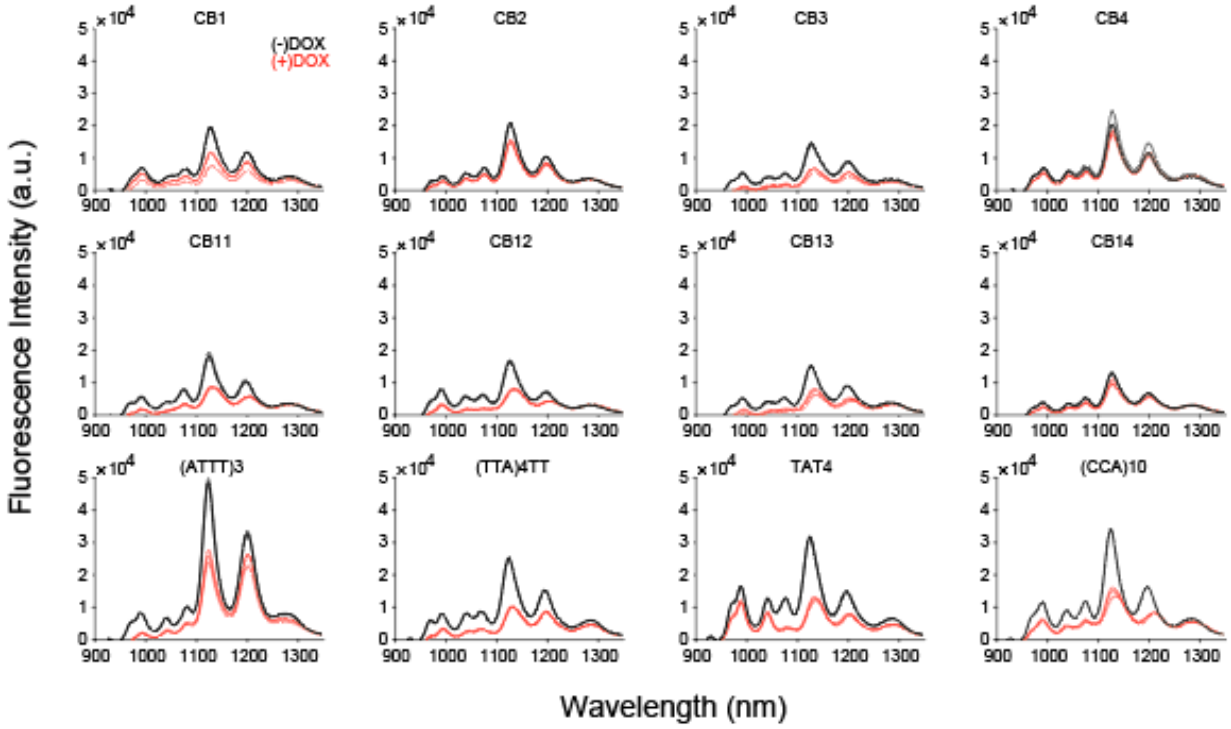

Figure S4. Fluorescence emission spectra for 12 different DNA-wrapped SWNTs (10 µg/mL in 1X PBS) before and after addition of 100 µM doxorubicin. Spectra were collected from 3 technical replicates.

	A	T	C	G	%AT	%CG	length	A632nm	quench	shift
CB1	1	2	18	5	0.115385	0.884615	26	0.2709	yes	no
CB2	3	2	17	4	0.192308	0.807692	26	0.2681	no	no
CB3	2	2	20	2	0.153846	0.846154	26	0.2117	yes	no
CB4	1	0	19	6	0.038462	0.961538	26	0.2954	no	no
CB11	5	4	17	0	0.346154	0.653846	26	0.232	yes	yes
CB12	0	6	18	2	0.230769	0.769231	26	0.2848	yes	yes
CB13	4	4	17	1	0.307692	0.692308	26	0.2242	yes	yes
CB14	1	3	19	3	0.153846	0.846154	26	0.1691	no	no
ATTT3	3	9	0	0	1	0	12	0.3483	yes	no
TTA4TT	4	10	0	0	1	0	14	0.3879	yes	yes
TAT4	4	8	0	0	1	0	12	0.4774	yes	yes
CCA10	10	0	20	0	0.333333	0.666667	30	0.4824	yes	yes

Table S1. Properties of 12 different DNA-wrapped SWNTs preparations.

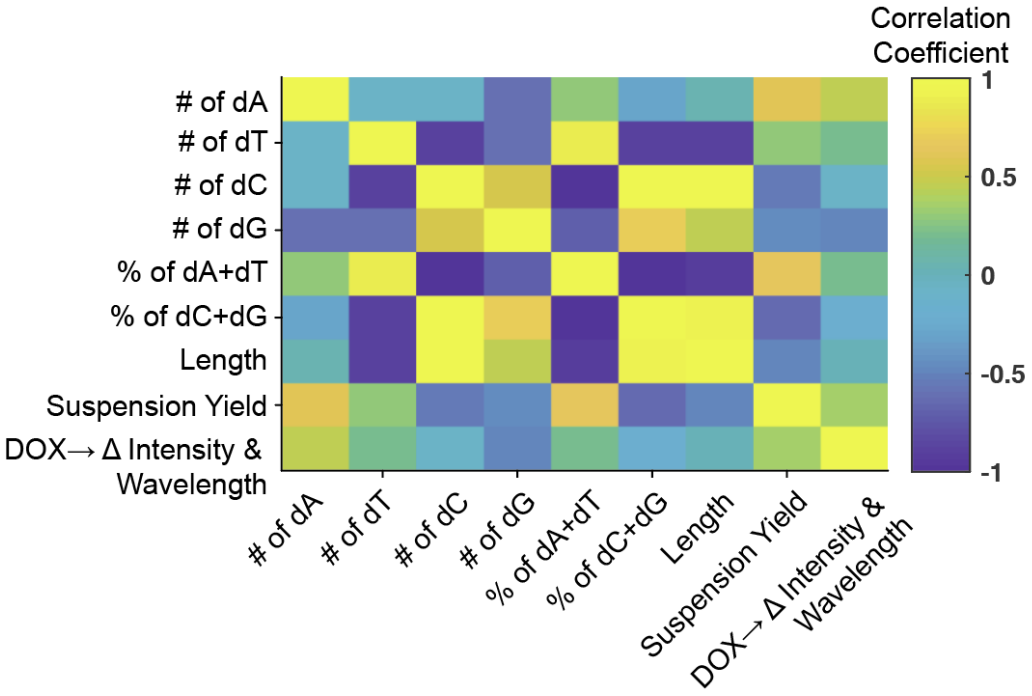

Figure S5. Correlation analysis of DNA-SWNT nanosensor properties and impact on doxorubicin response.

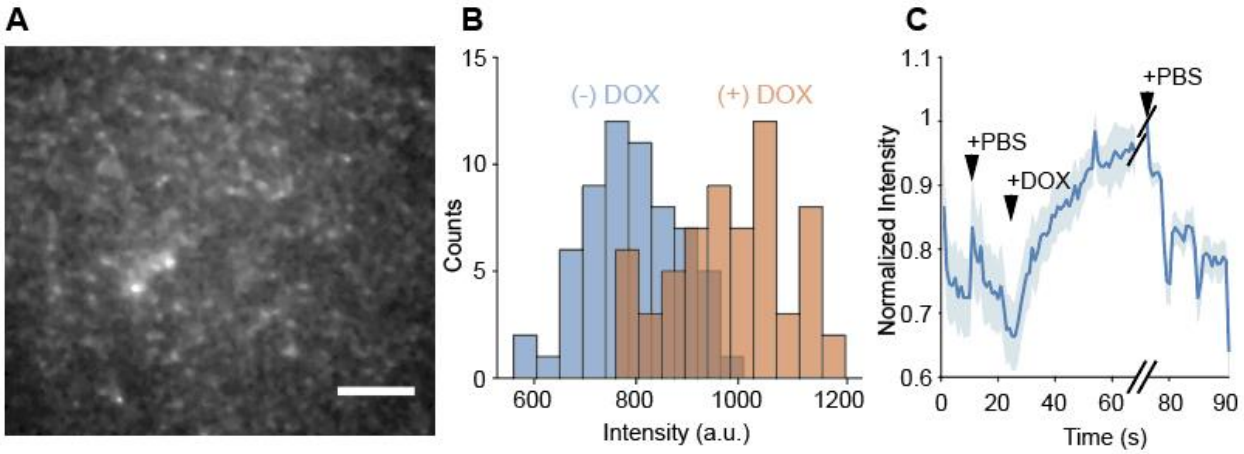

Figure S6. (A) Single molecule measurements of CB13-DNA-SWNT nanosensors adsorbed onto a glass slide. **(B)** Histogram showing fluorescence intensity of individual nanosensors before and after addition of 100 µM doxorubicin. **(C)** Washing of 1X PBS induced negligible fluorescence intensity increase, while addition of 100 µM DOX produced a transient increase in fluorescence. Washing away DOX with PBS reduced fluorescence intensity back to initial levels. Diagonal bars in **(C)** represent a time gap and change in field of view prior to beginning PBS washes. Intensity were collected from between 20-50 single sensors, averaged, and normalized to the peak intensity in time. The shaded region represents the standard deviation between individual SWNTs. Scale bar is 10 µM.

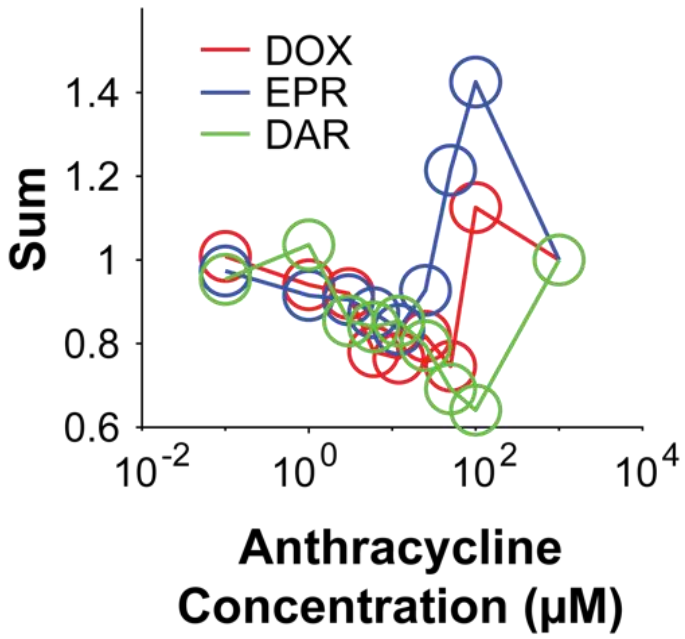

Figure S7. Sum of fitting parameters ($\alpha + \beta$) for anthracycline titrations.