Electronic Supplementary Material (ESI) for Analyst.

Electronic Supporting Information

Real-world carbon nanoparticle exposures induce brain and gonadal alterations in zebrafish (*Danio rerio*) as determined by biospectroscopy techniques

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Abbreviations:
C_{60}, fullerene
CNTs, carbon nanotubes
Control, vehicle control
F, female
Long, long MWCNTs
M, male
MWCNTs, multi-walled carbon nanotubes
Short, short MWCNTs
Single, single-walled CNTs

Figure S1 Scanning electron microscopy (SEM) images of **(a)** C_{60} fullerene; **(b)** long MWCNTs; **(c)** short MWCNTs; and, **(d)** single-walled CNTs. For characterization, corresponding Raman spectra are also shown.

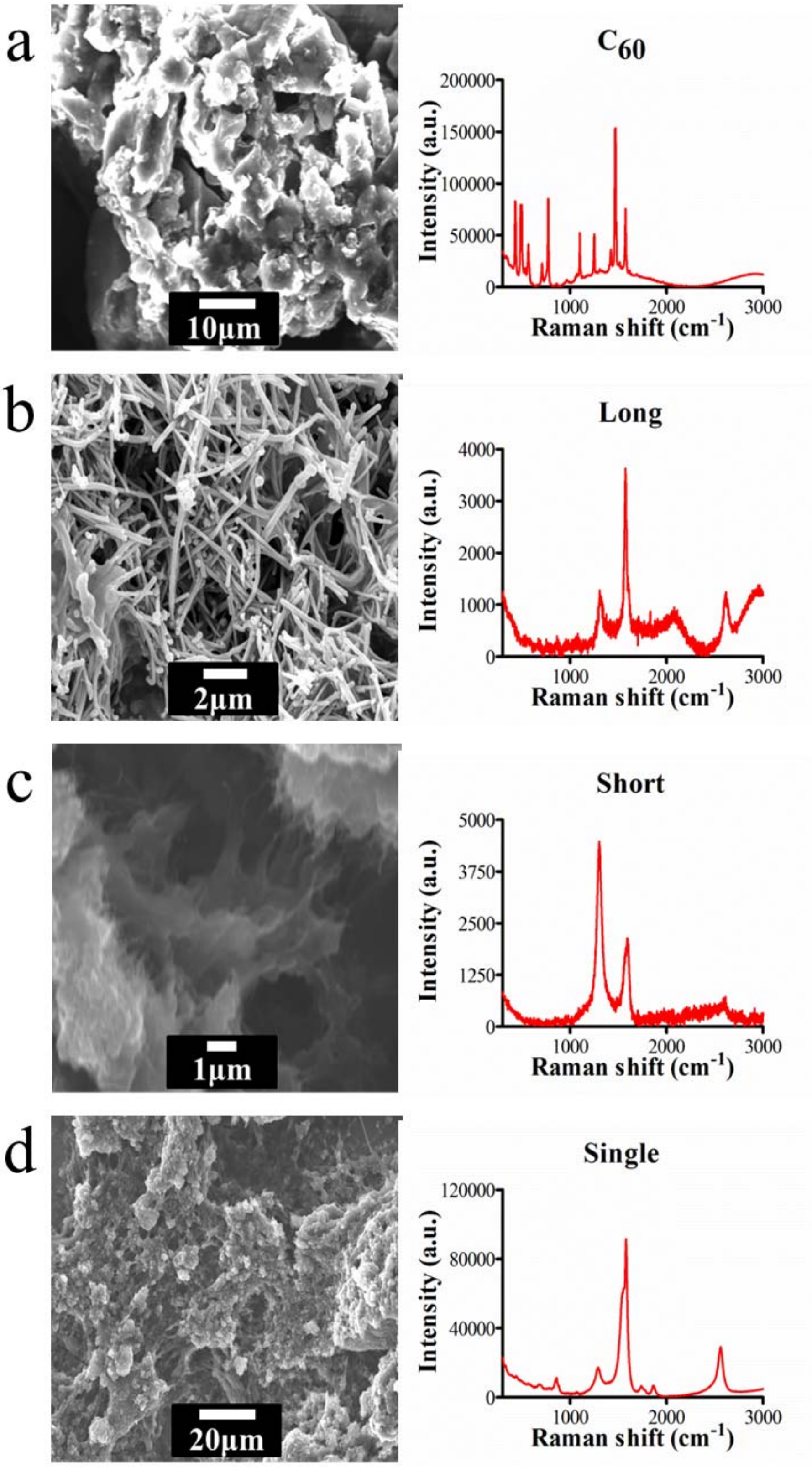
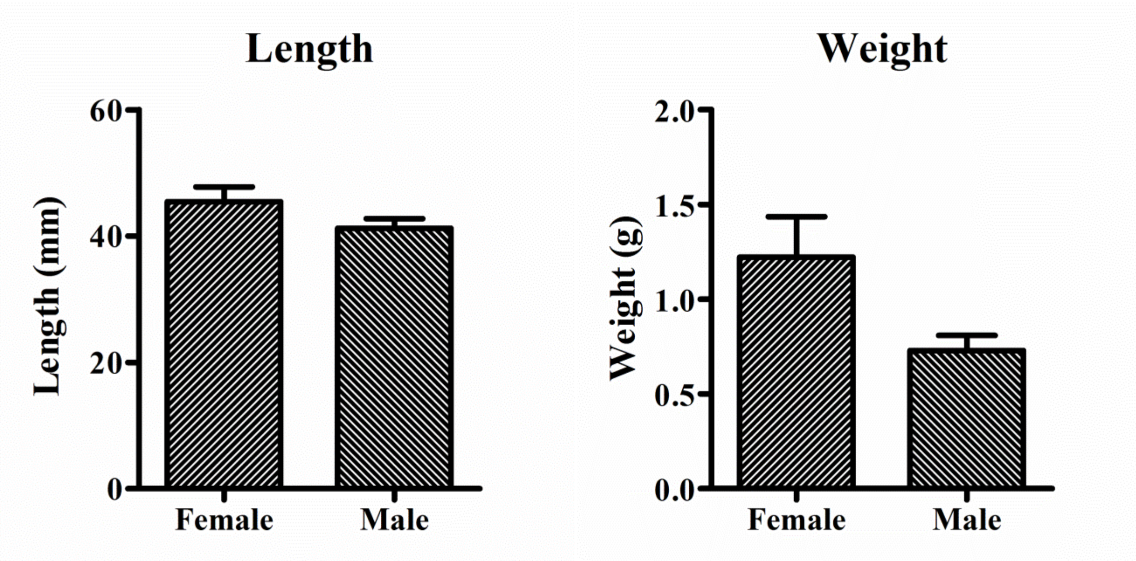


Figure S2 The wet body weight and length of zebrafish.



	Female		Male	
	Weight (g)	Length (mm)	Weight (g)	Length (mm)
Mean	1.221	45.431	0.782	41.225
SD	0.214	2.342	0.081	1.533

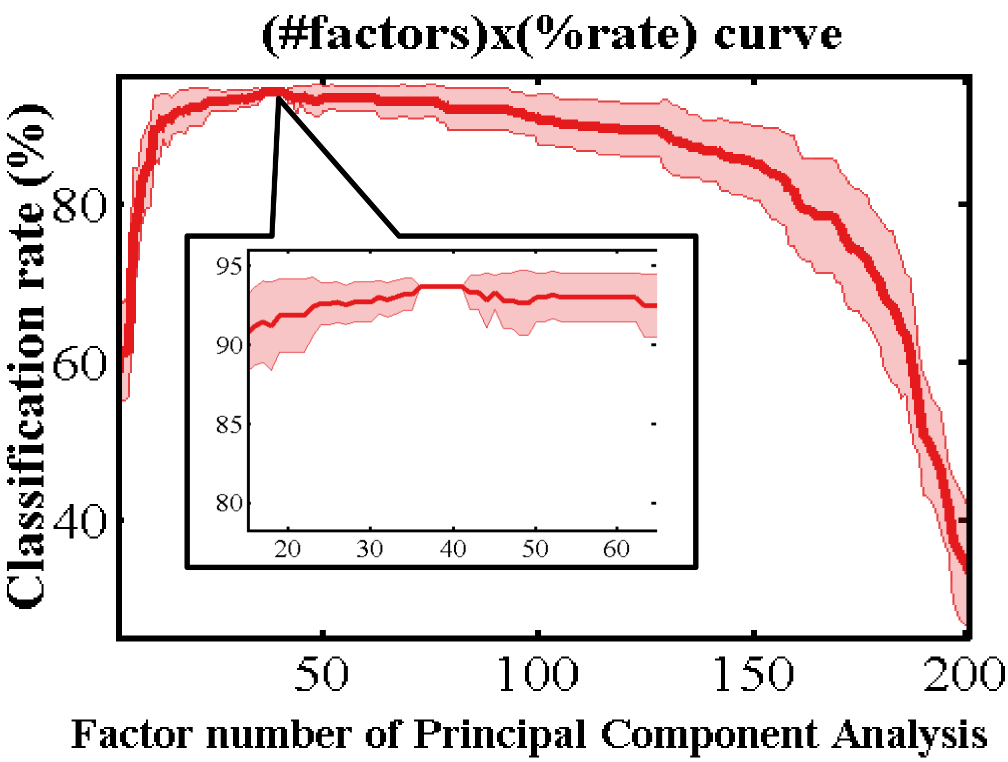


Figure S3. Illustration of optimization of number of principal components (PCs) to use in PCA-LDA. The dataset in this illustration was the NP-8 dataset (refer to Table S1). This procedure was repeated similarly with all the other seven datasets. The optimization searches for the optimal number of PCs for the PCA stage of a PCA-LDC classifier [(PCA as feature extraction, followed by a linear discriminant classifier (LDC)]. The search space is from 1 to 199 PCs and the number of PCs with highest average classification rate is selected for PCA-LDA. Classification rates were obtained through 10-fold cross-validation. The thick line is the average classification rate, and the hachured area represents the ± standard deviation range.

A step-by-step protocol is available at http://irootlab.googlecode.com, allowing for reproduction of the PCA-LDC optimization on a different dataset.

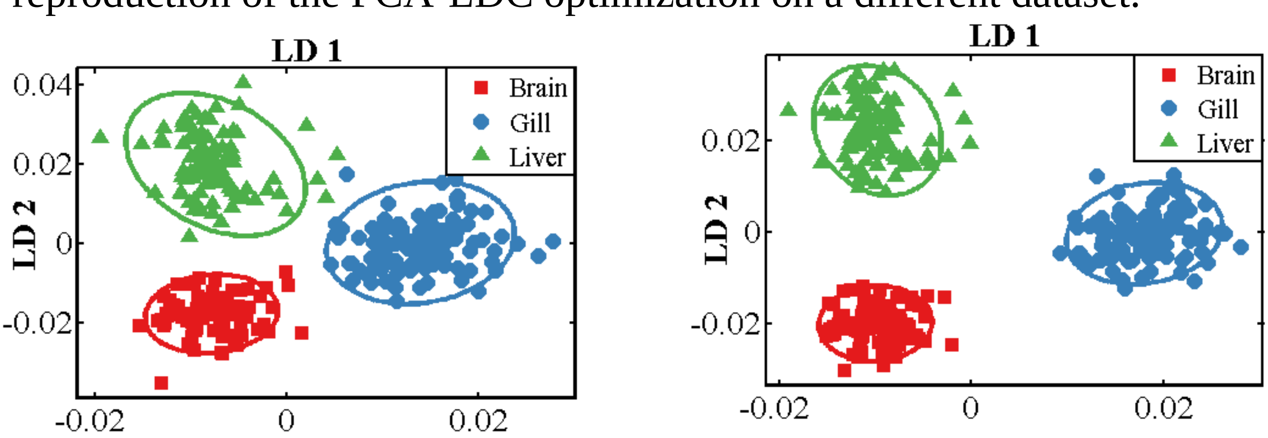


Figure S4 Two-dimensional **cross-calculated PCA-LDA** scores plot (*90% confidence ellipsoids*) derived from zebrafish tissues exposed to **C_{60}** interrogated by **ATR-FTIR spectroscopy**.

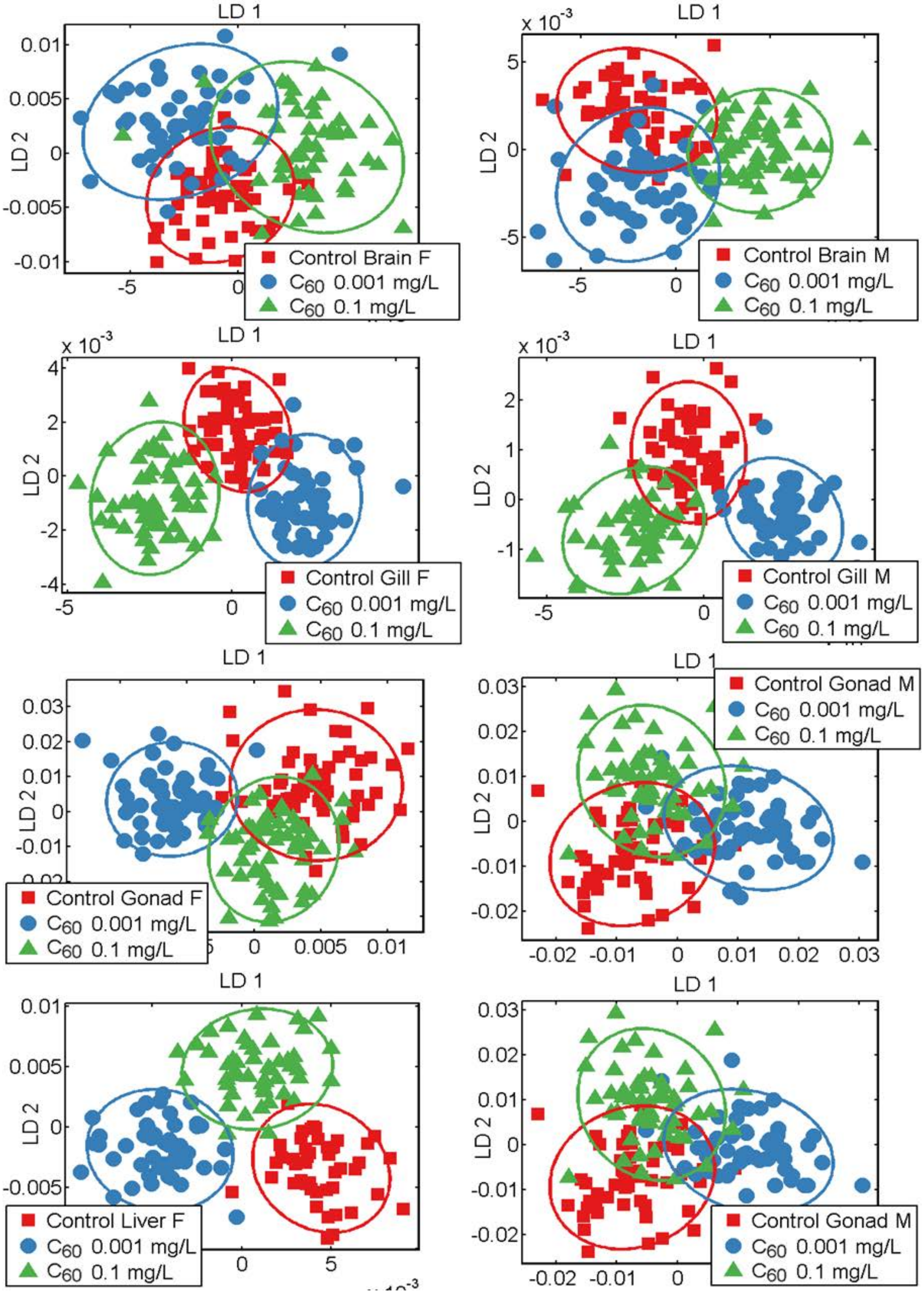


Figure S5 Two-dimensional **cross-calculated PCA-LDA** scores plot (*90% confidence ellipsoids*) derived from zebrafish tissues exposed to **long MWCNTs** interrogated by **ATR-FTIR spectroscopy**.

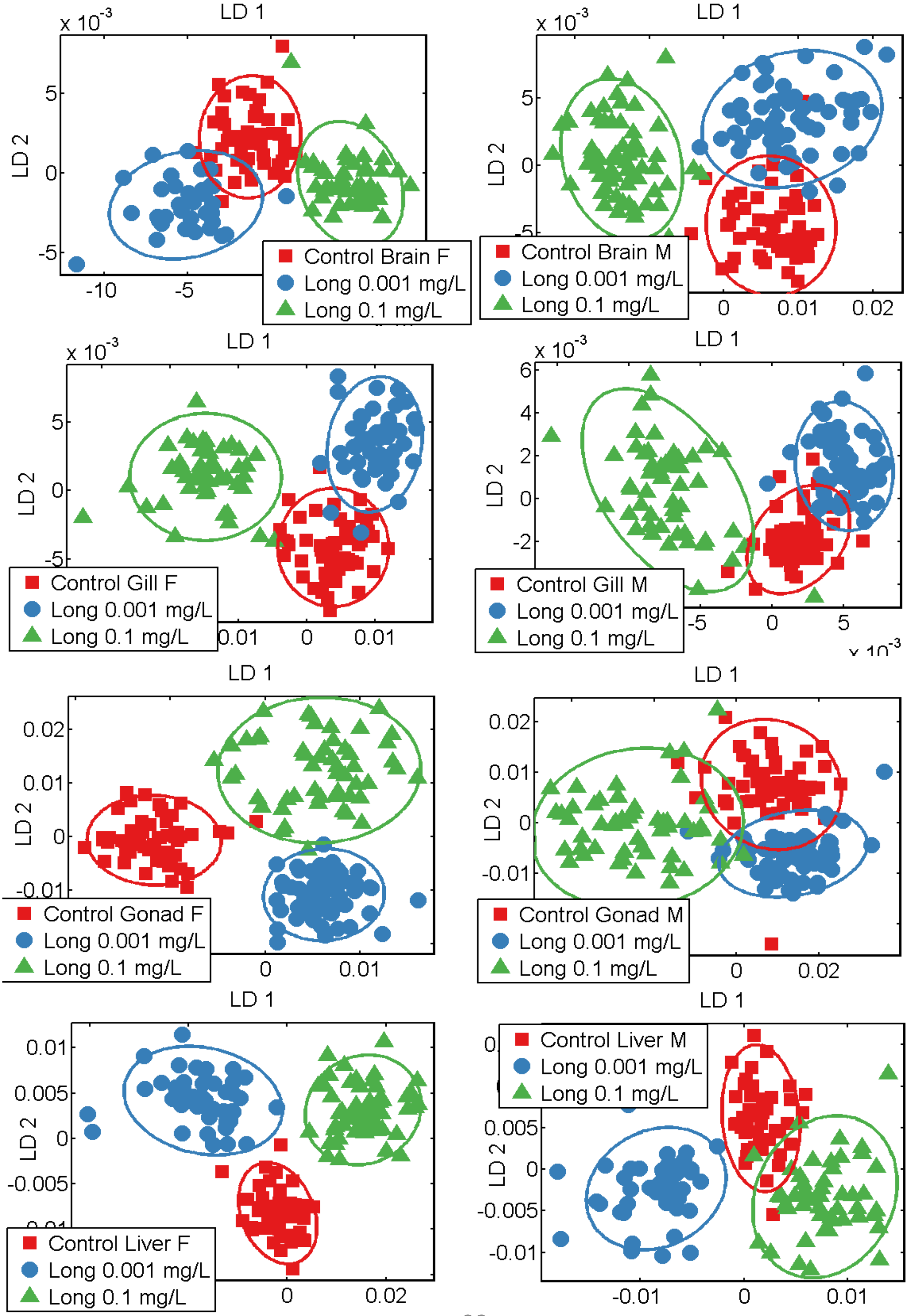


Figure S6 Two-dimensional **cross-calculated PCA-LDA** scores plot (*90% confidence ellipsoids*) derived from zebrafish tissues exposed to **short MWCNTs** interrogated by **ATR-FTIR spectroscopy**.

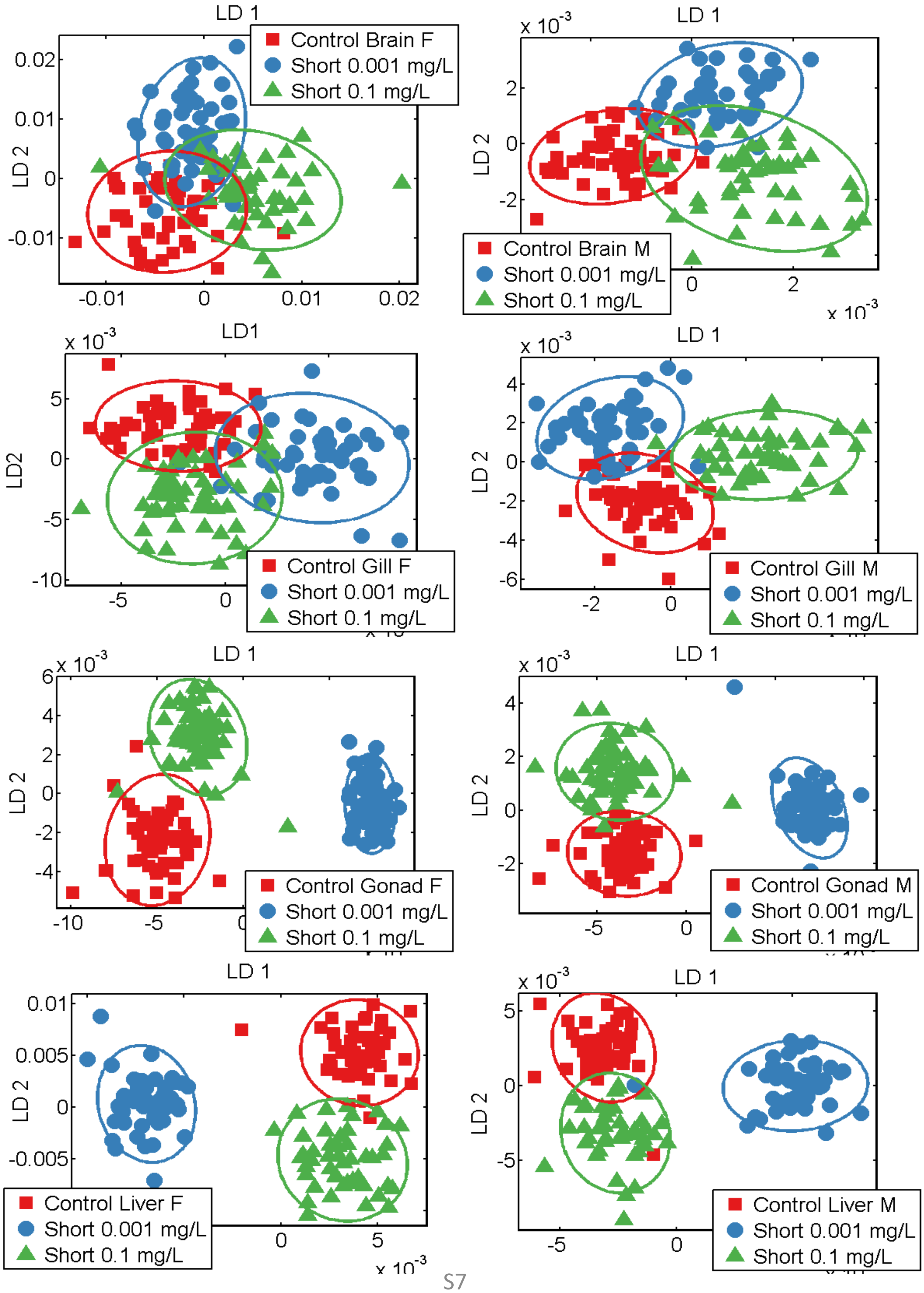


Figure S7 Two-dimensional **cross-calculated PCA-LDA** scores plot (*90% confidence ellipsoids*) derived from zebrafish tissues exposed to **single-walled CNTs** interrogated by **ATR-FTIR spectroscopy**.

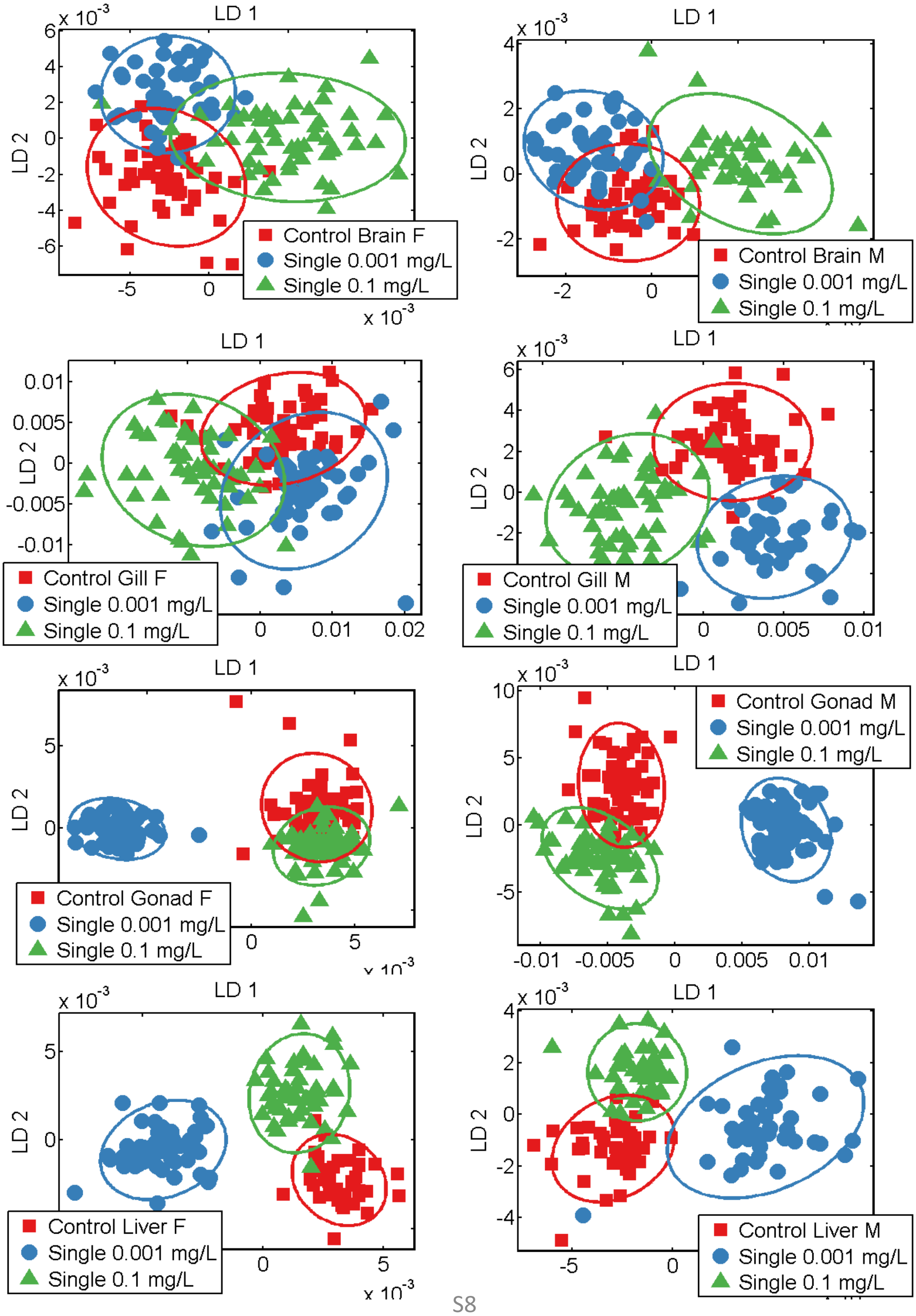


Figure S8 Cross-calculated PCA-LDA cluster vectors plots responsible for the wavenumber basis for segregation of zebrafish **brain, gill, gonads** and **liver** exposed to **C_{60}** or **long MWCNTs** by **ATR-FTIR spectroscopy**. Each treatment was compared to the control. The size of the marker symbol is proportional to the height of corresponding cluster vectors peak.

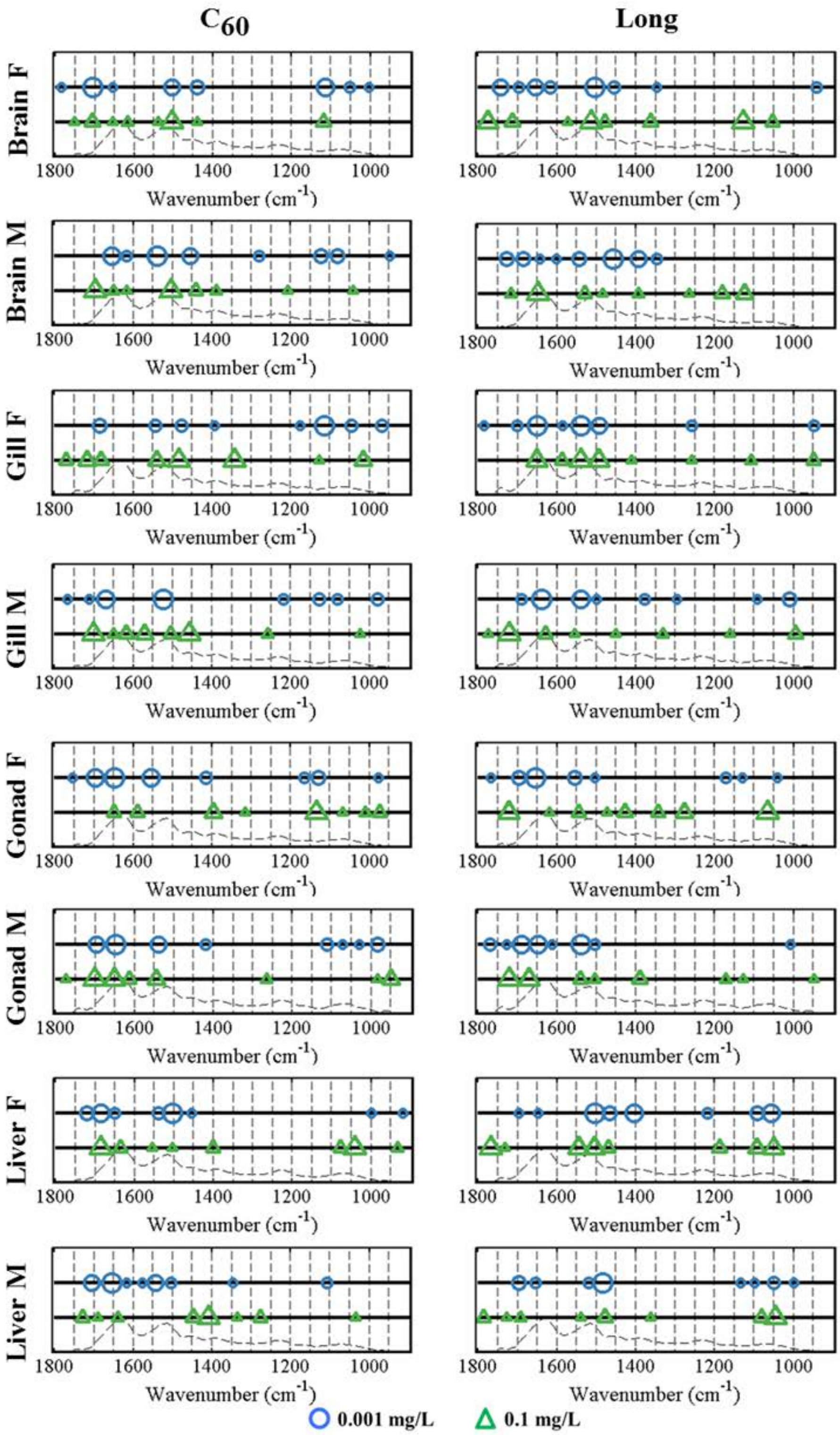


Figure S9 Cross-calculated PCA-LDA cluster vectors plots responsible for the wavenumber basis for segregation of zebrafish **brain, gill, gonads** and **liver** exposed to **short MWCNTs** or **single-walled CNTs** by **ATR-FTIR spectroscopy**. Each treatment was compared to the control. The size of the marker symbol is proportional to the height of corresponding cluster vectors peak.

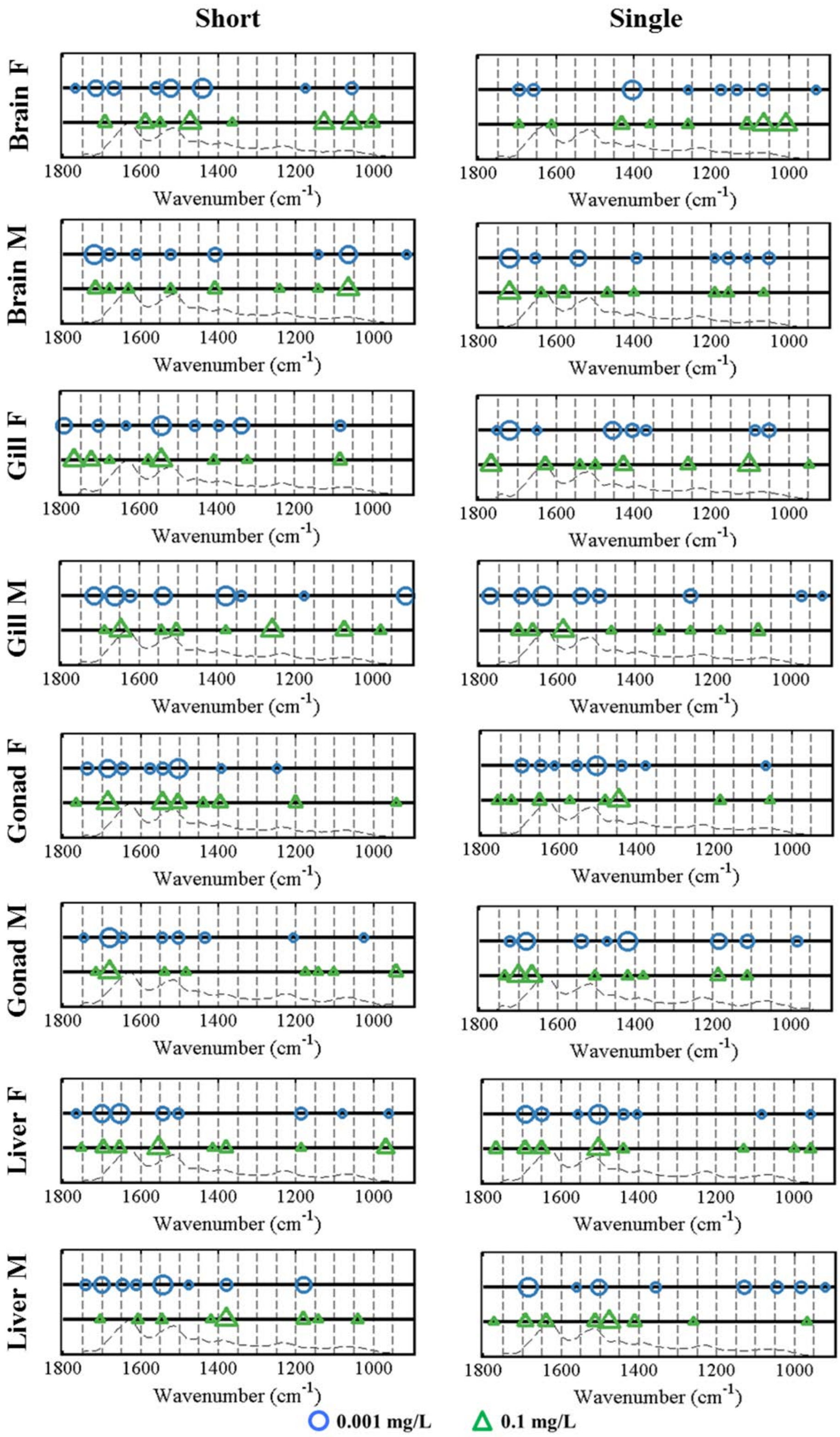


Figure S10 Cross-calculated PCA-LDA cluster vectors plots indicating the wavenumber basis for segregation of zebrafish tissues exposed to **C_{60}** by **ATR-FTIR spectroscopy**. Each treatment was compared to the control. The height of the cluster vectors peak is proportional to the extent of biochemical alteration compared to the vehicle control.

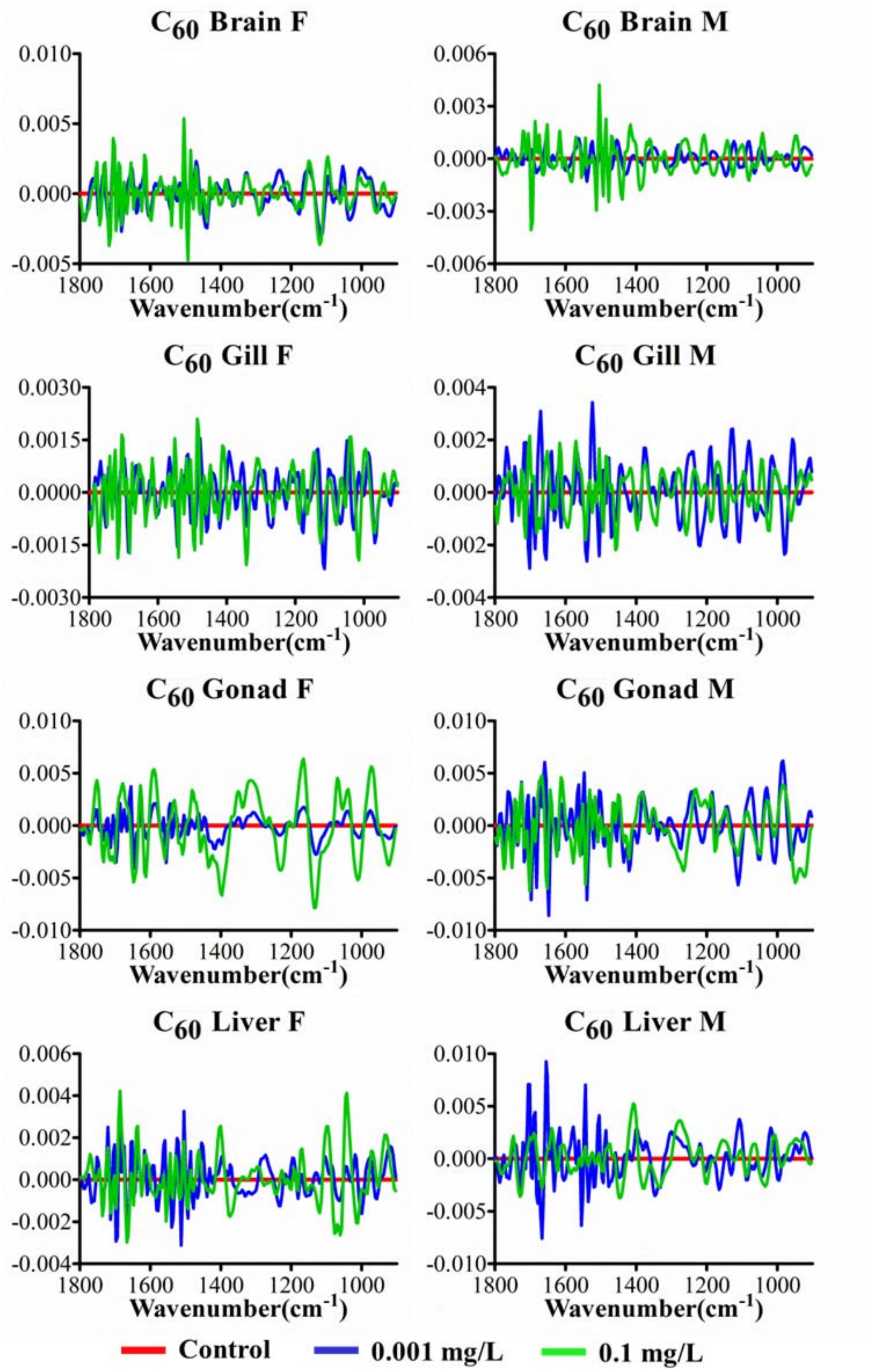


Figure S11 Cross-calculated PCA-LDA cluster vectors plots indicating the wavenumber basis for segregation of zebrafish tissues exposed to **long MWCNTs** by **ATR-FTIR spectroscopy**. Each treatment was compared to the control. The height of the cluster vectors peak is proportional to the extent of biochemical alteration compared to the vehicle control.

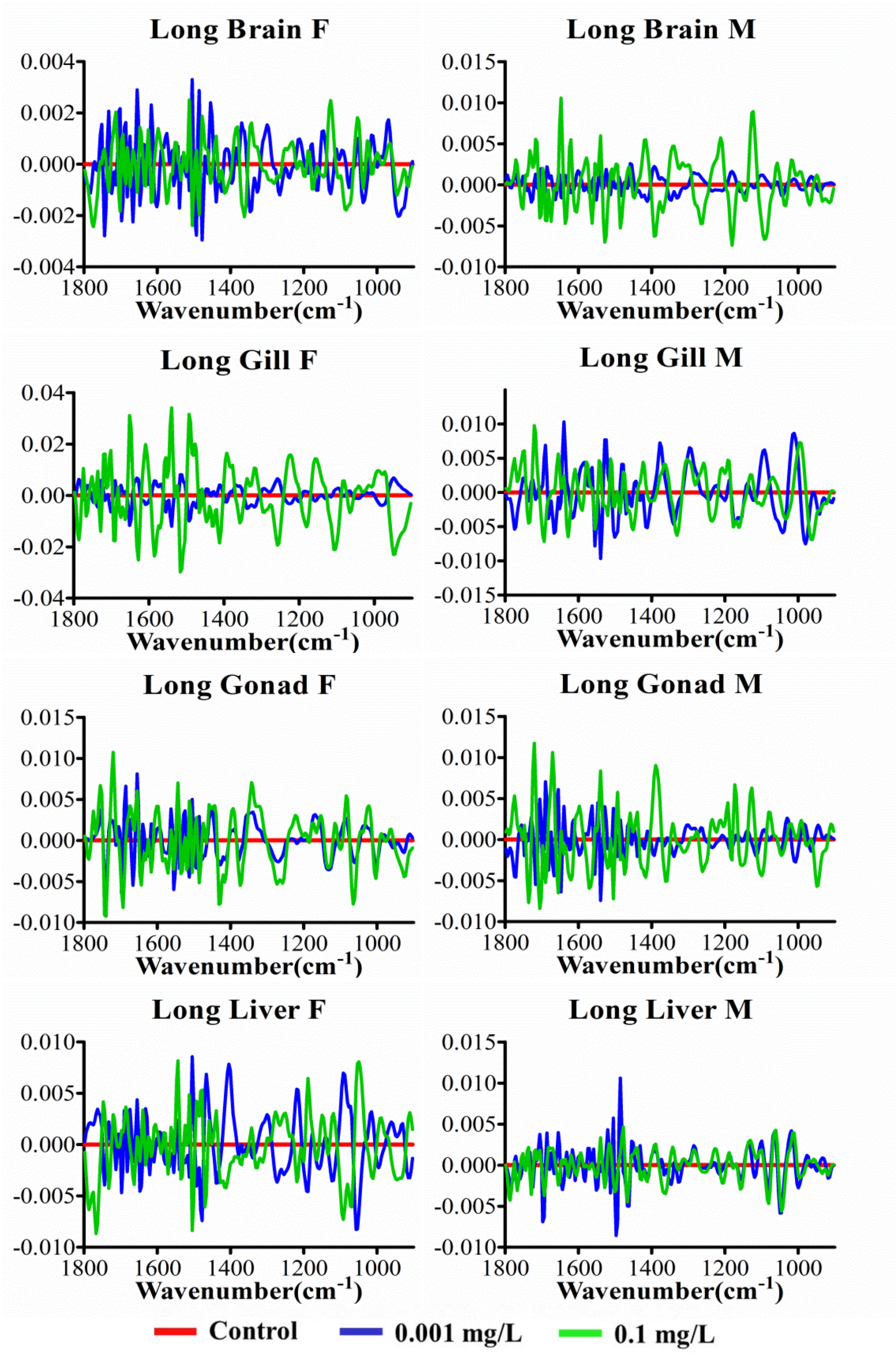


Figure S12 Cross-calculated PCA-LDA cluster vectors plots indicating the wavenumber basis for segregation of zebrafish tissues exposed to **short MWCNTs** by **ATR-FTIR spectroscopy**. Each treatment was compared to the control. The height of the cluster vectors peak is proportional to the extent of biochemical alteration compared to the vehicle control.

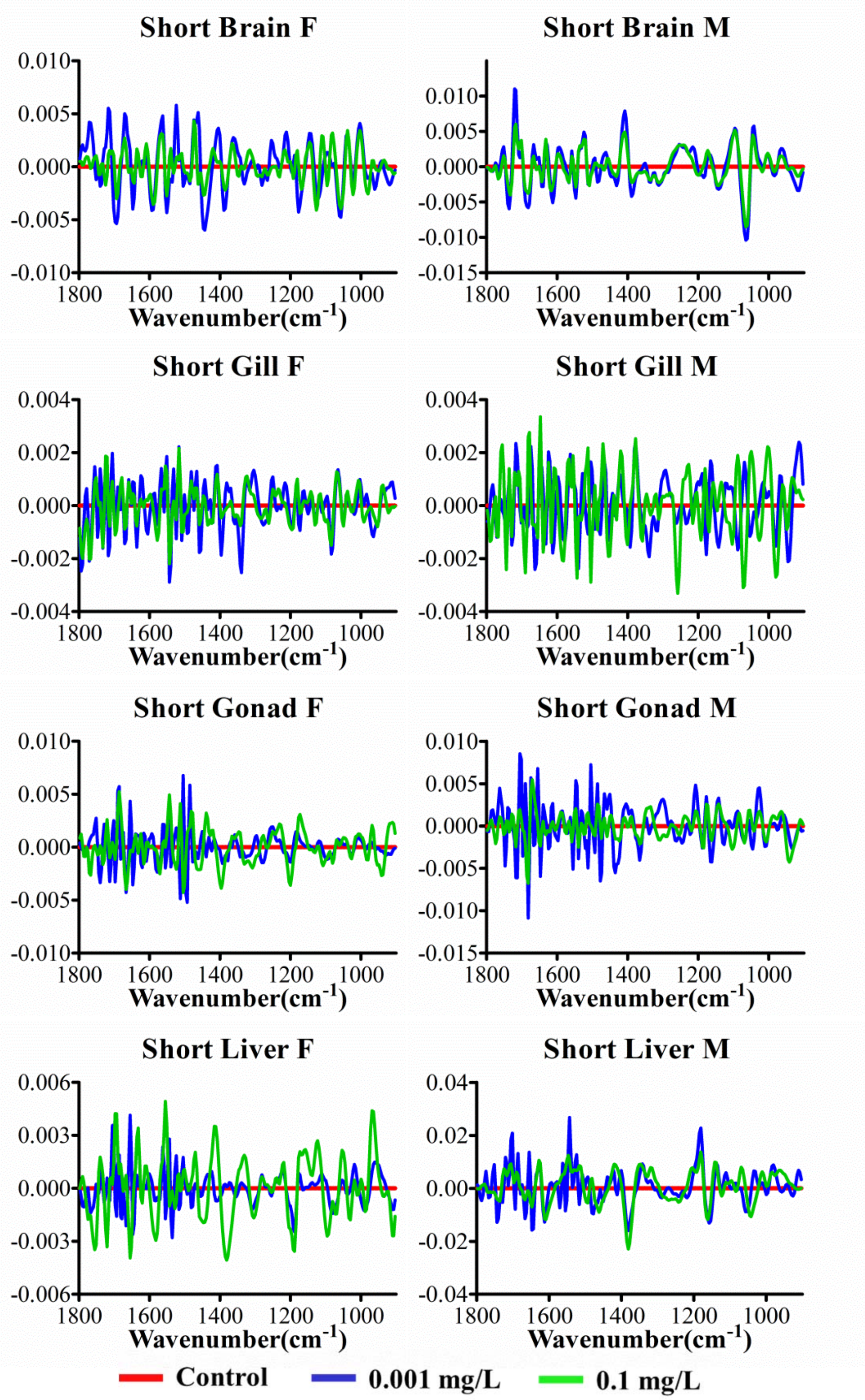


Figure S13 Cross-calculated PCA-LDA cluster vectors plots indicating the wavenumber basis for segregation of zebrafish tissues exposed to **single-walled CNTs** by **ATR-FTIR spectroscopy**. Each treatment was compared to the control. The height of the cluster vectors peak is proportional to the extent of biochemical alteration compared to the vehicle control.

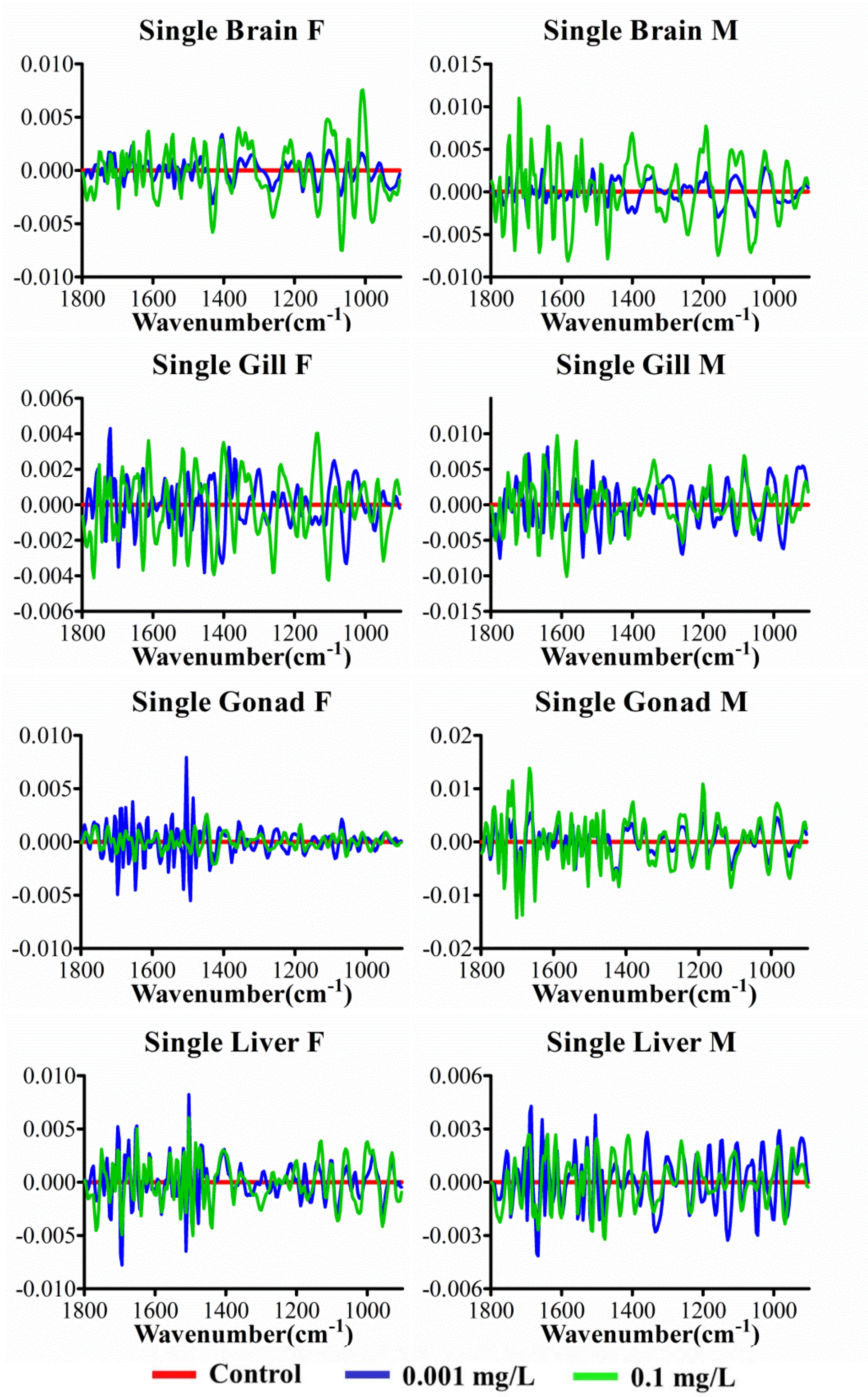


Figure S14 Cross-calculated PCA-LDA cluster vectors plots indicating the wavenumber basis for segregation of zebrafish tissues exposed to **CNPs** by **ATR-FTIR spectroscopy**. Each treatment was compared to the control. The height of the cluster vectors peak is proportional to the extent of biochemical alterations compared to the vehicle control.

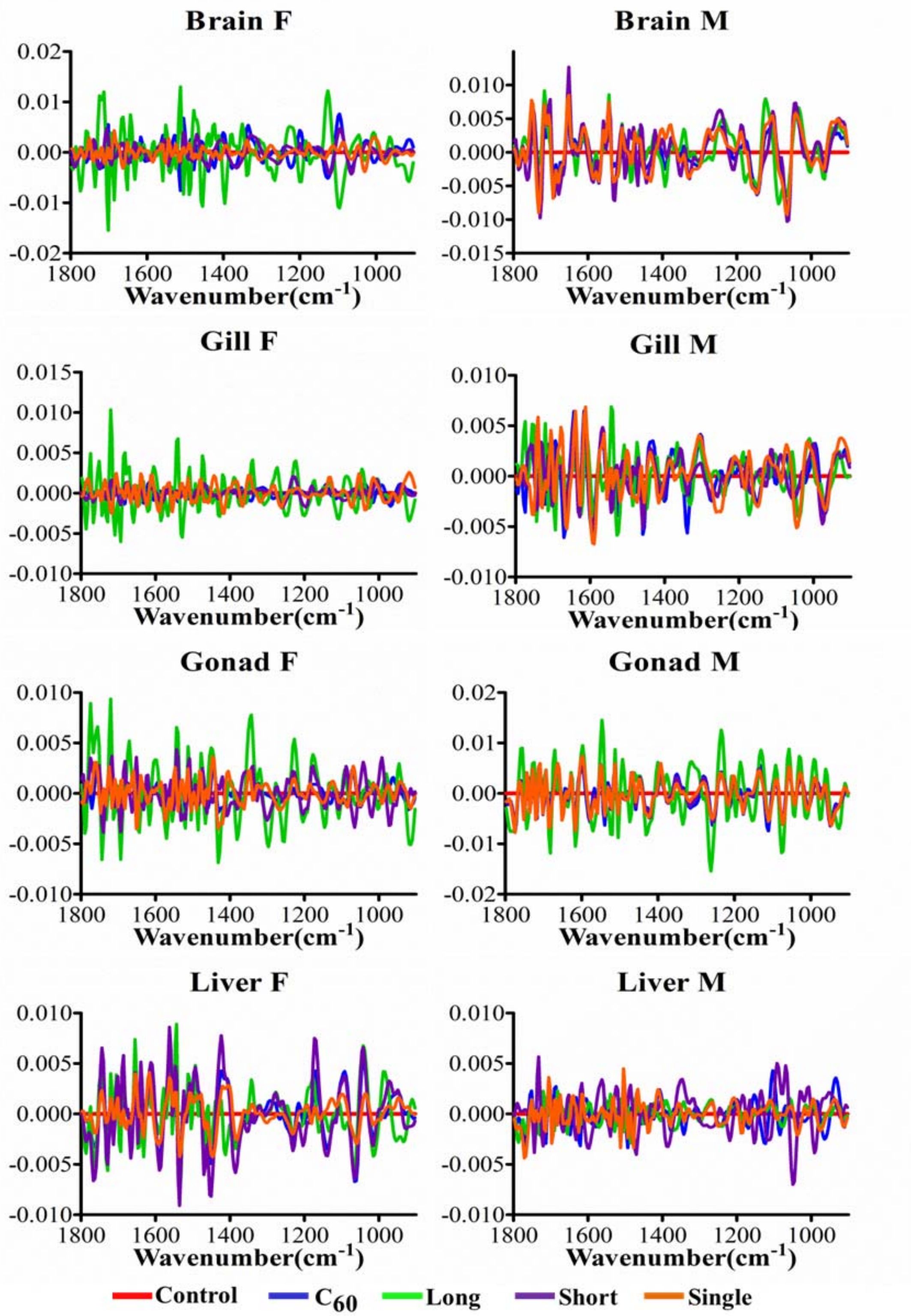


Figure S15 Two-dimension **cross-calculated PCA-LDA** scores plot (*90% confidence ellipsoids*) derived from zebrafish **brain** and **gonad** exposed to **CNPs** at concentration of 0.1 mg/L interrogated by **Raman spectroscopy**.

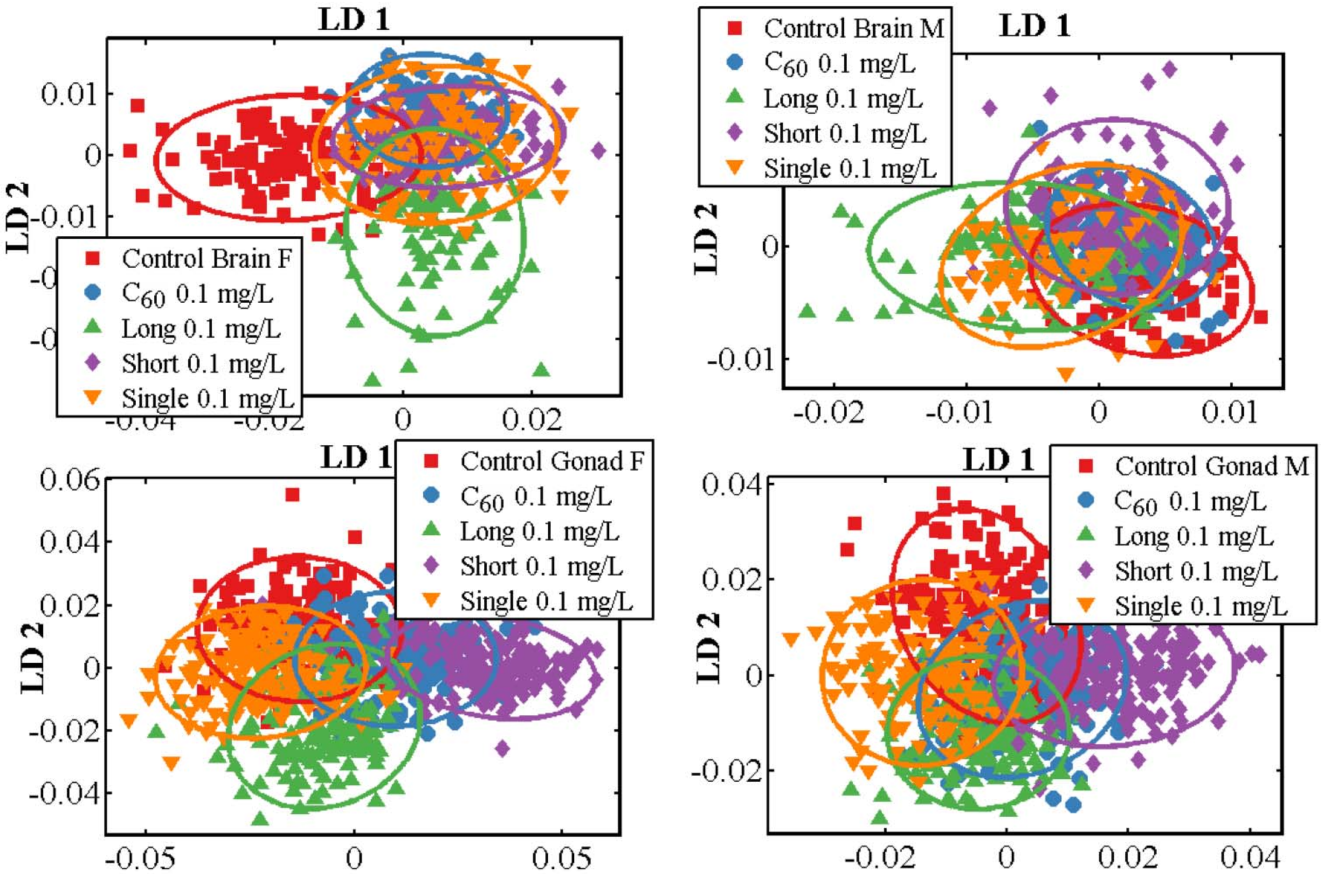


Figure S16 Cross-calculated PCA-LDA cluster vectors plots indicating the wavenumber basis for segregation of zebrafish tissues exposed to **CNPs** at concentration of 0.1 mg/L by **Raman spectroscopy**. Each treatment was compared to the control. The height of the cluster vectors peak is proportional to the extent of biochemical alterations compared to the vehicle control.

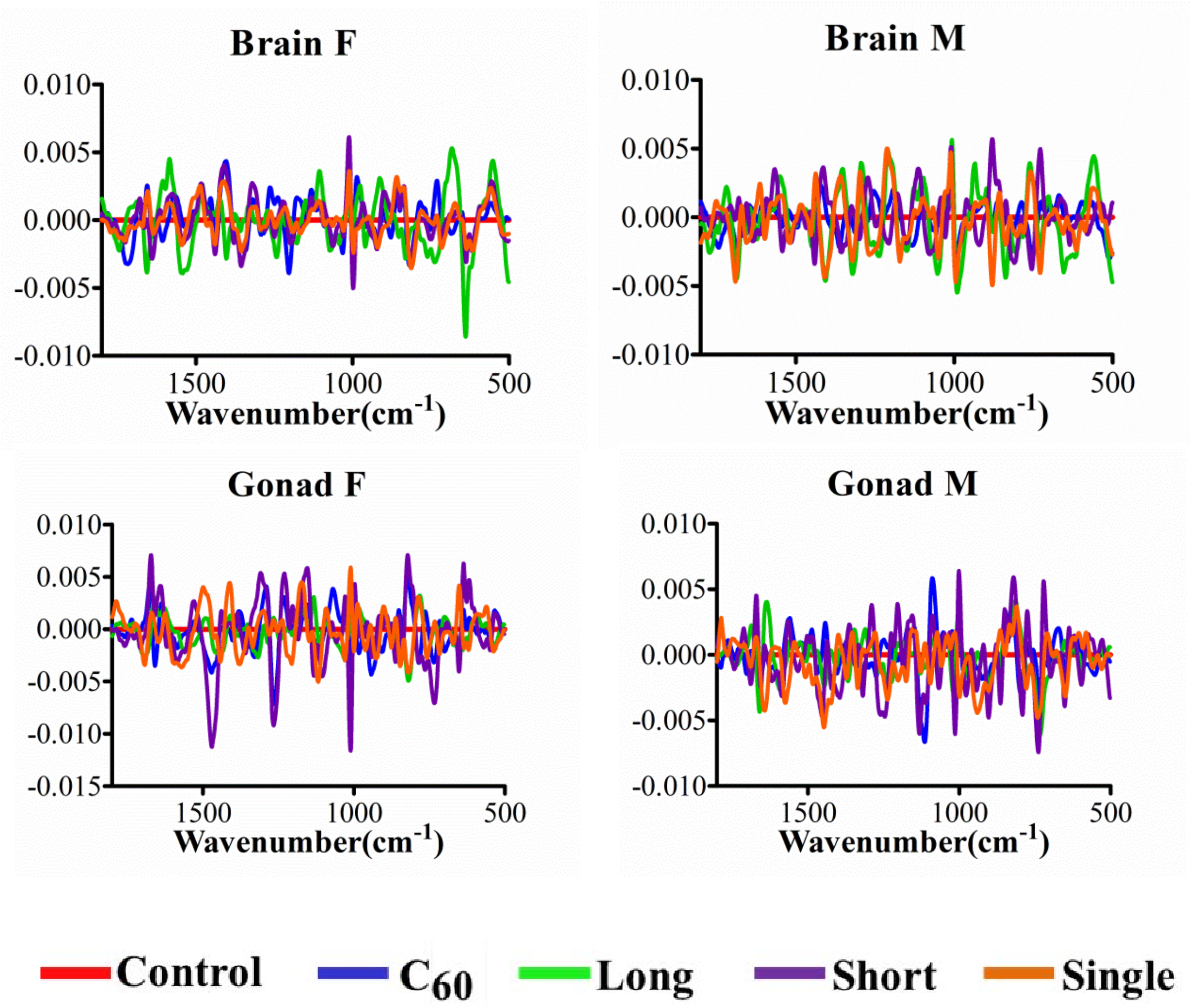


Figure S17 Cross-calculated PCA-LDA cluster vectors plots responsible for the wavenumber basis for segregation of zebrafish **brain** and **gonads** exposed to **CNPs** at concentration of 0.1 mg/L by **Raman spectroscopy**. Each treatment was compared to the control. The size of the marker symbol is proportional to the height of corresponding cluster vectors peak.

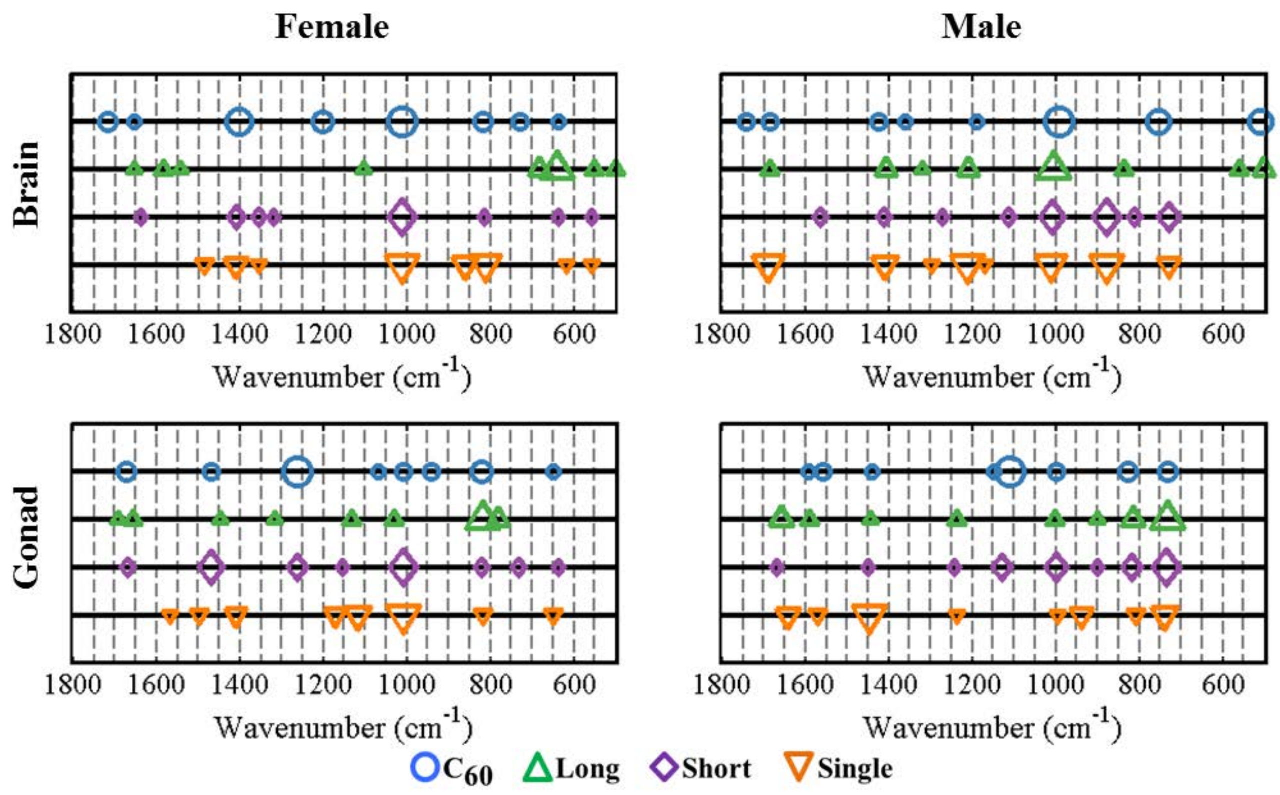


Table S1 *P-value* for each dimension calculated by one-way ANOVA with Dunnett's post-hoc test for 2-D cross-calculated PCA-LDA scores plots.

Tissues of zebrafish exposed to C_{60} (by cross-calculated PCA-LDA) by ATR-FTIR spectroscopy					
One-way ANOVA with Dunnett's Multiple Comparison Test		**Female**		**Male**	
		LD1	LD2	LD1	LD2
Brain	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* >0.05	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
Gill	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
Gonad	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.01	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.01	*P* <0.0001
Liver	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.001	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001

Tissues of zebrafish exposed to **Long MWCNTs** (by cross-calculated PCA-LDA) by ATR-FTIR spectroscopy					
One-way ANOVA with Dunnett's Multiple Comparison Test		**Female**		**Male**	
		LD1	LD2	LD1	LD2
Brain	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
Gill	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
Gonad	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
Liver	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001

Table S2 *P-value* for each dimension calculated by one-way ANOVA with Dunnett's post-hoc test for 2-D cross-calculated PCA-LDA scores plots.

Tissues of zebrafish exposed to **Short MWCNTs** (cross-calculated PCA-LDA) by ATR-FTIR spectroscopy					
One-way ANOVA with Dunnett's Multiple Comparison Test		**Female**		**Male**	
		LD1	LD2	LD1	LD2
Brain	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
Gill	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.01	*P* <0.0001	*P* <0.0001	*P* <0.0001
Gonad	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.0001	*P* <0.0001	*P* >0.05	*P* <0.0001
Liver	Control *vs.* 0.001 mg/L	*P* <0.0001	*P* <0.0001	*P* <0.0001	*P* <0.0001
	Control *vs.* 0.1 mg/L	*P* <0.001	*P* <0.0001	*P* <0.01	*P* <0.0001

Tissues of Zebrafish exposed to **single-walled CNTs** (cross-calculated PCA-LDA) by ATR-FTIR spectroscopy					
One-way ANOVA with Dunnett's Multiple Comparison Test		**Female**		**Male**	
		LD1	LD2	LD1	LD2
Brain	Control *vs.* 0.001 mg/L	*P* > 0.05	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001
	Control *vs.* 0.1 mg/L	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001
Gill	Control *vs.* 0.001 mg/L	*P* < 0.01	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001
	Control *vs.* 0.1 mg/L	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001
Gonad	Control *vs.* 0.001 mg/L	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001
	Control *vs.* 0.1 mg/L	*P* > 0.05	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001
Liver	Control *vs.* 0.001 mg/L	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001
	Control *vs.* 0.1 mg/L	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001	*P* < 0.0001

Table S3 *P-value* for each dimension calculated by one-way ANOVA with Dunnett's post-hoc test for 2-D cross-calculated PCA-LDA scores plots.

Tissues of zebrafish exposed to CNPs (by cross-calculated PCA-LDA) interrogated by **ATR-FTIR spectroscopy**					
One-way ANOVA with Dunnett's Multiple Comparison Test		Female		Male	
		LD1	LD2	LD1	LD2
Brain	Control *vs.* C_{60} 0.1 mg/L	*P <0.0001*	*P <0.001*	*P <0.001*	*P >0.05*
	Control *vs.* Long 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.001*
	Control *vs.* Short 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P >0.05*	*P <0.0001*
	Control *vs.* Single 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.001*
Gill	Control *vs.* C_{60} 0.1 mg/L	*P <0.0001*	*P <0.001*	*P <0.001*	*P >0.05*
	Control *vs.* Long 0.1 mg/L	*P <0.0001*	*P <0.001*	*P <0.0001*	*P >0.05*
	Control *vs.* Short 0.1 mg/L	*P <0.0001*	*P <0.001*	*P <0.0001*	*P <0.0001*
	Control *vs.* Single 0.1 mg/L	*P <0.001*	*P <0.0001*	*P <0.0001*	*P <0.0001*
Gonad	Control *vs.* C_{60} 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P >0.05*	*P <0.0001*
	Control *vs.* Long 0.1 mg/L	*P <0.0001*	*P >0.05*	*P <0.0001*	*P <0.0001*
	Control *vs.* Short 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.01*	*P <0.0001*
	Control *vs.* Single 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.01*	*P <0.0001*
Liver	Control *vs.* C_{60} 0.1 mg/L	*P <0.001*	*P <0.0001*	*P <0.0001*	*P >0.05*
	Control *vs.* Long 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.01*
	Control *vs.* Short 0.1 mg/L	*P >0.05*	*P <0.0001*	*P <0.0001*	*P <0.0001*
	Control *vs.* Single 0.1 mg/L	*P >0.05*	*P <0.0001*	*P <0.0001*	*P <0.01*

Table S4 *P-value* for each dimension calculated by one-way ANOVA with Dunnett's post-hoc test for 2-D cross-calculated PCA-LDA scores plots.

Tissues of zebrafish exposed to CNPs (by cross-calculated PCA-LDA) interrogated by **Raman spectroscopy**					
One-way ANOVA with Dunnett's Multiple Comparison Test		Female		Male	
		LD1	LD2	LD1	LD2
Brain	Control *vs.* C_{60} 0.1 mg/L	*P <0.0001*	*P <0.001*	*P >0.05*	*P <0.0001*
	Control *vs.* Long 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.0001*
	Control *vs.* Short 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.001*	*P <0.0001*
	Control *vs.* Single 0.1 mg/L	*P <0.0001*	*P <0.001*	*P <0.0001*	*P <0.0001*
Gonad	Control *vs.* C_{60} 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.0001*
	Control *vs.* Long 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P >0.05*	*P <0.0001*
	Control *vs.* Short 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.0001*
	Control *vs.* Single 0.1 mg/L	*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.0001*

Table S5 *P-value* for each dimension calculated by one-way ANOVA with Dunnett's post-hoc test for lipid-to-protein ratios derived from **IR** spectra.

Lipid-to-protein ratios derived from IR spectra following ATR-FTIR spectroscopy			
One-way ANOVA with Dunnett's Multiple Comparison Test		**Female**	**Male**
Brain	Control *vs.* C_{60} 0.1 mg/L	*P <0.01*	*P <0.01*
	Control *vs.* Long 0.1 mg/L	*P >0.05*	*P >0.05*
	Control *vs.* Short 0.1 mg/L	*P <0.001*	*P <0.01*
	Control *vs.* Single 0.1 mg/L	*P <0.0001*	*P <0.001*
Gill	Control *vs.* C_{60} 0.1 mg/L	*P >0.05*	*P >0.05*
	Control *vs.* Long 0.1 mg/L	*P <0.0001*	*P <0.0001*
	Control *vs.* Short 0.1 mg/L	*P <0.001*	*P <0.0001*
	Control *vs.* Single 0.1 mg/L	*P <0.0001*	*P <0.0001*
Gonads	Control *vs.* C_{60} 0.1 mg/L	*P >0.05*	*P <0.001*
	Control *vs.* Long 0.1 mg/L	*P <0.0001*	*P <0.0001*
	Control *vs.* Short 0.1 mg/L	*P <0.0001*	*P >0.05*
	Control *vs.* Single 0.1 mg/L	*P <0.0001*	*P <0.01*
Liver	Control *vs.* C_{60} 0.1 mg/L	*P <0.01*	*P >0.05*
	Control *vs.* Long 0.1 mg/L	*P <0.001*	*P <0.01*
	Control *vs.* Short 0.1 mg/L	*P <0.01*	*P >0.05*
	Control *vs.* Single 0.1 mg/L	*P >0.05*	*P <0.01*

Table S6 *P-value* for each dimension calculated by one-way ANOVA with Newman-Keuls' post-hoc test for lipid-to-protein ratios in different tissues derived from **IR** spectra.

Lipid-to-protein ratios derived from IR spectra following ATR-FTIR spectroscopy								
	Brain F	**Brain M**	**Gill F**	**Gill M**	**Gonads F**	**Gonads M**	**Liver F**	**Liver M**
Brain F		*P <0.0001*	*P <0.0001*	*P >0.05*	*P >0.05*	*P <0.0001*	*P <0.0001*	*P <0.01*
Brain M	*P <0.0001*		*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.0001*	*P <0.01*
Gill F	*P <0.0001*	*P <0.0001*		*P <0.0001*	*P <0.0001*	*P <0.001*	*P <0.01*	*P <0.0001*
Gill M	*P >0.05*	*P <0.0001*	*P <0.0001*		*P >0.05*	*P <0.0001*	*P <0.0001*	*P <0.01*
Gonads F	*P >0.05*	*P <0.0001*	*P <0.0001*	*P >0.05*		*P <0.0001*	*P <0.0001*	*P <0.0001*
Gonads M	*P <0.0001*	*P <0.0001*	*P <0.001*	*P <0.0001*	*P <0.0001*		*P <0.0001*	*P <0.0001*
Liver F	*P <0.0001*	*P <0.0001*	*P <0.01*	*P <0.0001*	*P <0.0001*	*P <0.0001*		*P <0.0001*
Liver M	*P <0.01*	*P <0.01*	*P <0.0001*	*P <0.01*	*P <0.001*	*P <0.0001*	*P <0.0001*	

Table S7 *P-value* for each dimension calculated by one-way ANOVA with post-hoc test for $C=C/CH_2$ ratios derived from **Raman** spectra.

Ratio of $C=C/CH_2$ derived from Raman spectra			
One-way ANOVA with Dunnett's Multiple Comparison Test		**Female**	**Male**
Brain	Control *vs.* C_{60} 0.1 mg/L	*P* <0.0001	*P* <0.001
	Control *vs.* Long 0.1 mg/L	*P* <0.0001	*P* >0.05
	Control *vs.* Short 0.1 mg/L	*P* <0.01	*P* >0.05
	Control *vs.* Single 0.1 mg/L	*P* <0.0001	*P* <0.001
Gonad	Control *vs.* C_{60} 0.1 mg/L	*P* >0.05	*P* <0.01
	Control *vs.* Long 0.1 mg/L	*P* <0.0001	*P* <0.0001
	Control *vs.* Short 0.1 mg/L	*P* <0.01	*P* <0.0001
	Control *vs.* Single 0.1 mg/L	*P* >0.05	*P* <0.01

Ratio of $C=C/CH_2$ derived from Raman spectra	
One-way ANOVA with Newman-Keuls' Multiple Comparison Test	***P*-value**
Brain F *vs.* Gonad M	*P* <0.0001
Brain F *vs.* Gonad F	*P* <0.0001
Brain F *vs.* Brain M	*P* <0.0001
Brain M *vs.* Gonad M	*P* <0.0001
Brain M *vs.* Gonad F	*P* <0.0001
Gonad F *vs.* Gonad M	*P* <0.0001

Cluster vectors plots for zebrafish brain tissues derived from IR spectra by cross-calculated PCA-LDA

	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
C_{60}	1740	Lipid, v(C=O)	1065	$v_sPO_2^-$
	1220	$v_{as}PO_2^-$	1543	Amide II
	1065	$v_sPO_2^-$	1145	Carbohydrates, v(C-O)
	1508	Amide II	1710	Lipid, v(C=O)
	1130	Carbohydrates, v(C-O)	1655	Amide I
	960	Protein phosphorylation	1750	Lipid, v(C=O)
	1450	Proteins, $v_{as}CH_3$	1103	$v_sPO_2^-$
	1312	Amide III	1245	$v_{as}PO_2^-$
Long MWCNTs	1616	Amide I	1650	Amide II
	1747	Lipid, v(C=O)	1716	$v_sPO_2^-$
	1180	Carbohydrates, v(C-O)	1543	Amide II
	1454	Proteins, $v_{as}CH_3$	1122	Carbohydrates, v(C-O)
	1265	Amide III	1087	$v_sPO_2^-$
	1000	Protein phosphorylation	1038	Glycogen
	1582	Amide II	1392	$v(COO^-)$
	1320	Amide III	1238	$v_{as}PO_2^-$
Short MWCNTs	1740	Lipid, v(C=O)	1650	Amide I
	1530	Amide II	1065	$v_sPO_2^-$
	1045	Glycogen	1728	Lipid, v(C=O)
	1130	Carbohydrates, v(C-O)	1543	Amide II
	1616	Amide I	1680	Amide I
	960	Protein phosphorylation	1245	Amide III
	1412	Proteins, $v_{as}CH_3$	1103	$v_sPO_2^-$
	1447	Proteins, $v_{as}CH_3$	1145	Carbohydrates, v(C-O)
Single-walled CNTs	1528	Amide II	1065	$v_sPO_2^-$
	1658	Amide I	1732	Lipid, v(C=O)
	1045	Glycogen	1650	Amide I
	1477	Proteins, $v_{as}CH_3$	1543	Amide II
	1744	Lipid, v(C=O)	1690	Amide I
	1226	$v_{as}PO_2^-$	1145	Carbohydrates, v(C-O)
	964	Protein phosphorylation	1103	$v_sPO_2^-$
	1427	Proteins, $v_{as}CH_3$	930	Protein phosphorylation

Cluster vectors plots for zebrafish gill tissues derived from IR spectra by cross-calculated PCA-LDA

	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
C_{60}	1647	Amide I	1616	Amide I
	1504	Amide II	1690	Amide I
	1573	Amide II	1496	Amide II
	1710	Lipid, v(C=O)	1554	Amide II
	1049	Glycogen	1118	Carbohydrates, v(C-O)
	1462	Proteins, $v_{as}CH_3$	1369	$v(COO^-)$
	964	Protein phosphorylation	1199	$v_{as}PO_2^-$
	1750	Lipid, v(C=O)	1743	Lipid, v(C=O)
Long MWCNTs	1647	Amide I	1539	Amide II
	1528	Amide II	1647	Amide I
	1747	Lipid, v(C=O)	1477	Proteins, $v_{as}CH_3$
	1469	Proteins, $v_{as}CH_3$	1700	Lipid, v(C=O)
	1180	Carbohydrates, v(C-O)	1207	$v_{as}PO_2^-$
	1705	Lipid, v(C=O)	1303	Amide III
	1080	$v_sPO_2^-$	1597	Amide I
	1373	$v(COO^-)$	1747	Lipid, v(C=O)
Short MWCNTs	1710	Lipid, v(C=O)	1539	Amide II
	1550	Amide II	1492	Proteins, $v_{as}CH_3$
	1470	Proteins, $v_{as}CH_3$	1650	Amide I
	1211	$v_{as}PO_2^-$	1616	Amide I
	1392	$v(COO^-)$	952	Protein phosphorylation
	1612	Amide I	995	Protein phosphorylation
	1064	$v_sPO_2^-$	1199	$v_{as}PO_2^-$
	987	Protein phosphorylation	1122	Carbohydrates, v(C-O)
Single-walled CNTs	1647	Amide I	1535	Amide II
	1708	Lipid, v(C=O)	1651	Amide II
	1465	Proteins, $v_{as}CH_3$	1447	Proteins, $v_{as}CH_3$
	1550	Amide II	1296	Amide III
	1392	$v(COO^-)$	995	Amide III
	1018	Glycogen	1050	Glycogen
	1211	$v_{as}PO_2^-$	1728	Lipid, v(C=O)
	1311	Amide III	1200	$v_{as}PO_2^-$

Cluster vectors plots for zebrafish gonad tissues derived from IR spectra by cross-calculated PCA-LDA

	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
C_{60}	1724	Lipid, v(C=O)	1774	Lipid, v(C=O)
	1442	Proteins, $v_{as}CH_3$	1110	$v_sPO_2^-$
	1068	$v_sPO_2^-$	948	Protein phosphorylation
	1647	Amide I	1254	Amide III
	1346	$v(COO^-)$	1540	Amide II
	1512	Amide II	1076	$v_sPO_2^-$
	922	Protein phosphorylation	1477	Amide II
	960	Protein phosphorylation	1708	Lipid, v(C=O)
Long MWCNTs	1720	Lipid, v(C=O)	1261	Amide III
	1774	Lipid, v(C=O)	1546	Amide II
	1342	$v(COO^-)$	1681	Amide I
	1430	Proteins, $v_{as}CH_3$	1076	$v_sPO_2^-$
	1543	Amide II	1616	Amide I
	1226	$v_{as}PO_2^-$	1755	Lipid, v(C=O)
	1296	Amide III	1504	Amide II
	1670	Amide I	1130	Carbohydrates, v(C-O)
Short MWCNTs	1543	Amide II	948	Protein phosphorylation
	1740	Lipid, v(C=O)	1774	Lipid, v(C=O)
	1690	Amide I	1685	Amide I
	1651	Amide I	1597	Amide I
	991	Protein phosphorylation	1512	Amide II
	1774	Lipid, v(C=O)	1253	Amide III
	1508	Amide II	1550	Amide II
	1064	$v_sPO_2^-$	1110	$v_sPO_2^-$
Single-walled CNTs	1446	Proteins, $v_{as}CH_3$	1774	Lipid, v(C=O)
	1651	Amide I	1616	Amide I
	1760	Lipid, v(C=O)	1685	Amide I
	1573	Amide II	945	Protein phosphorylation
	1068	$v_sPO_2^-$	1072	$v_sPO_2^-$
	1724	Lipid, v(C=O)	1392	$v(COO^-)$
	1512	Amide II	1512	Amide II
	1346	$v(COO^-)$	1550	Amide II

Cluster vectors plots for zebrafish liver tissues derived from IR spectra by cross-calculated PCA-LDA

	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
C_{60}	1064	$\nu_s PO_2^-$	1103	$\nu_s PO_2^-$
	1535	Amide II	1504	Amide II
	1450	Proteins, $\nu_{as}CH_3$	933	Protein phosphorylation
	1743	Lipid, ν(C=O)	1705	Lipid, ν(C=O)
	1168	Carbohydrates, ν(C-O)	1770	Lipid, ν(C=O)
	1589	Amide I	1620	Amide I
	1408	$\nu(COO^-)$	1408	$\nu(COO^-)$
	1685	Amide I	1342	$\nu(COO^-)$
Long MWCNTs	1543	Amide II	1485	Proteins, $\nu_{as}CH_3$
	1654	Amide I	1786	Lipid, ν(C=O)
	1041	Glycogen	1681	Amide I
	1728	Lipid, ν(C=O)	1720	Lipid, ν(C=O)
	1766	Lipid, ν(C=O)	1037	Glycogen
	1492	Proteins, $\nu_{as}CH_3$	1539	Amide II
	987	Protein phosphorylation	1369	$\nu(COO^-)$
	1411	Proteins, $\nu_{as}CH_3$	1269	Amide III
Short MWCNTs	1535	Amide II	1049	Glycogen
	1450	Proteins, $\nu_{as}CH_3$	1732	Lipid, ν(C=O)
	1172	Carbohydrates, ν(C-O)	1092	$\nu_s PO_2^-$
	1766	Lipid, ν(C=O)	1469	Proteins, $\nu_{as}CH_3$
	1041	Glycogen	991	Protein phosphorylation
	1384	$\nu(COO^-)$	1346	$\nu(COO^-)$
	1685	Amide I	1562	Amide II
	1589	Amide I	1597	Amide I
Single-walled CNTs	1446	Proteins, $\nu_{as}CH_3$	1504	Amide II
	1535	Amide II	1770	Lipid, ν(C=O)
	1616	Amide I	1705	Lipid, ν(C=O)
	1654	Amide I	1465	Proteins, $\nu_{as}CH_3$
	1060	$\nu_s PO_2^-$	1411	Proteins, $\nu_{as}CH_3$
	1404	$\nu(COO^-)$	1037	Glycogen
	1743	Lipid, ν(C=O)	1616	Amide I
	1230	$\nu_{as} PO_2^-$	1188	Carbohydrates, ν(C-O)

Cluster vectors plots for zebrafish brain tissues derived from Raman spectra by cross-calculated PCA-LDA

	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
C_{60}	1008	Phenylalanine	994	Phenylalanine
	1402	Lipid, CH_2	510	Collagen, S-S stretching
	1202	Amide III	753	DNA, nucleic acid
	817	DNA/RNA, phosphodiester	1424	Lipid, CH_2
	1716	Lipid, C=O	1685	Lipid, C=C
	730	DNA, nucleic acid	1743	Lipid, C=O
	635	Protein, v(C-S)	1361	Lipid/protein, CH_3/CH_2
	1655	Lipid, C=C	1190	Protein
Long MWCNTs	638	Protein, v(C-S)	1006	Phenylalanine
	681	DNA, ring breathing modes	1207	Amide III
	505	Collagen, S-S stretching	506	Collagen, S-S stretching
	1584	Phenylalanine, C=C	1406	Lipid, CH_2
	552	v(S-S)	558	v(S-S)
	1542	Amide II	1685	Lipid, C=C
	1655	Lipid, C=C	837	Protein
	1105	Carbohydrates	1320	Lipid/protein, CH_3/CH_2
Short MWCNTs	1010	Phenylalanine	879	Protein
	1409	Lipid, CH_2	1009	Phenylalanine
	1354	Lipid/protein, CH_3/CH_2	727	DNA, nucleic acid
	637	Protein, v(C-S)	1413	Lipid, CH_2
	814	DNA/RNA, phosphodiester	1112	Carbohydrates
	556	v(S-S)	1565	Amide II
	1638	Amide I	810	DNA/RNA, phosphodiester
	1319	Lipid/protein, CH_3/CH_2	1271	Amide III
Single-walled CNTs	1010	Phenylalanine	1211	Amide III
	812	Collagen, C-C stretching	879	Protein
	858	Collagen, C-C stretching	1010	Phenylalanine
	1410	Lipid	1690	Lipid, C=C
	1486	Lipid	1409	Lipid, CH_2
	557	v(S-S)	727	DNA, nucleic acid
	1354	Lipid/protein, CH_3/CH_2	1297	Lipid
	616	Protein, v(C-S)	1171	Protein

Cluster vectors plots for zebrafish Gonad tissues derived from Raman spectra by cross-calculated PCA-LDA

	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
C_{60}	1263	Amide III	1111	Carbohydrates
	821	DNA/RNA, phosphodiester	732	DNA, nucleic acid
	1673	Lipid, C=C	826	DNA/RNA, phosphodiester
	940	Protein	998	Phenylalanine
	1469	Lipid, CH_2	1557	Amide II
	1007	Phenylalanine	1593	Phenylalanine
	1068	Carbohydrates	1441	Lipid, CH_2
	650	Protein, *v*(C-S)	1147	Protein
Long MWCNTs	818	DNA/RNA, phosphodiester	732	DNA, nucleic acid
	780	DNA, nucleic acid	1656	Lipid, C=C
	1131	Protein	813	DNA/RNA, phosphodiester
	1658	Lipid, C=C	1002	Phenylalanine
	1030	Phenylalanine	1235	Amide III
	1315	Lipid/protein, CH_3/CH_2	1589	Phenylalanine
	1693	Lipid, C=C	1444	Lipid, CH_2
	1447	Lipid, CH_2	901	Protein
Short MWCNTs	1009	Phenylalanine	736	DNA, nucleic acid
	1469	Lipid, CH_2	1000	Phenylalanine
	1263	Amide III	1129	Carbohydrates
	820	DNA/RNA, phosphodiester	819	DNA/RNA, phosphodiester
	732	DNA, nucleic acid	901	Protein
	1669	Lipid, C=C	1244	Amide III
	635	Protein, *v*(C-S)	1451	Lipid, CH_2
	1153	Protein	1669	Lipid, C=C
Single-walled CNTs	1009	Phenylalanine	1445	Lipid, CH_2
	1117	Carbohydrates	739	DNA, nucleic acid
	1171	Protein	937	Protein
	1409	Lipid, CH_2	1639	Lipid, C=C
	649	Protein, *v*(C-S)	809	DNA/RNA, phosphodiester
	819	DNA/RNA, phosphodiester	1571	Phenylalanine
	1497	Lipid, CH_2	1235	Amide III
	1568	Amide II	996	Phenylalanine

Cluster vectors plots for zebrafish brain exposed to C_{60} at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	**Female**		**Male**	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1705	Lipid, v(C=O)	1539	Amide II
	1114	Carbohydrates, v(C-O)	1654	Amide I
	1504	Amide II	1454	Proteins, $v_{as}CH_3$
	1438	Proteins, $v_{as}CH_3$	1080	$v_sPO_2^-$
	1053	Glycogen	1122	Carbohydrates, v(C-O)
	1786	Lipid, v(C=O)	1280	Amide III
	1003	Glycogen	1616	Amide I
	1654	Amide I	950	Protein phosphorylation
0.1	1504	Amide II	1504	Amide II
	1705	Lipid, v(C=O)	1700	Lipid, v(C=O)
	1118	Carbohydrates, v(C-O)	1438	Proteins, $v_{as}CH_3$
	1616	Amide I	1650	Amide I
	1539	Amide II	1388	$v(COO^-)$
	1750	Lipid, v(C=O)	1616	Amide I
	1654	Amide I	1041	Glycogen
	1438	Proteins, $v_{as}CH_3$	1207	$v_{as}PO_2^-$

Cluster vectors plots for zebrafish gill exposed to C_{60} at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	**Female**		**Male**	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1114	Carbohydrates, ν(C-O)	1523	Amide II
	1685	Amide I	1670	Amide I
	1543	Amide II	1126	Carbohydrates, ν(C-O)
	1477	Proteins, $\nu_{as}CH_3$	980	Protein phosphorylation
	1045	Glycogen	1218	$\nu_{as}PO_2^-$
	968	Protein phosphorylation	1080	$\nu_sPO_2^-$
	1392	$\nu(COO^-)$	1712	Lipid, ν(C=O)
	1176	Carbohydrates, ν(C-O)	1766	Lipid, ν(C=O)
0.1	1485	Proteins, $\nu_{as}CH_3$	1458	Proteins, $\nu_{as}CH_3$
	1342	$\nu(COO^-)$	1701	Lipid, ν(C=O)
	1014	Glycogen	1570	Amide II
	1716	Lipid, ν(C=O)	1616	Amide I
	1539	Amide II	1504	Amide II
	1681	Amide I	1257	Amide III
	1770	Lipid, ν(C=O)	1651	Amide I
	1126	Carbohydrates, ν(C-O)	1022	Glycogen

Cluster vectors plots for zebrafish gonads exposed to C_{60} at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	**Female**		**Male**	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1647	Amide I	1647	Amide I
	1554	Amide II	1697	Lipid, v(C=O)
	1697	Lipid, v(C=O)	1539	Amide II
	1130	Carbohydrates, v(C-O)	983	Protein phosphorylation
	1415	Proteins, $v_{as}CH_3$	1110	$v_sPO_2^-$
	1164	Carbohydrates, v(C-O)	1419	Proteins, $v_{as}CH_3$
	1755	Lipid, v(C=O)	1029	Glycogen
	975	Protein phosphorylation	1072	$v_sPO_2^-$
0.1	1134	Carbohydrates, v(C-O)	1701	Lipid, v(C=O)
	1396	$v(COO^-)$	1651	Amide I
	972	Protein phosphorylation	1543	Amide II
	1647	Amide I	950	Protein phosphorylation
	1589	Amide I	1612	Amide I
	1010	Glycogen	1265	Amide III
	1068	$v_sPO_2^-$	1774	Lipid, v(C=O)
	1315	Amide III	983	Protein phosphorylation

Cluster vector plots for zebrafish liver exposed to C_{60} at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1504	Amide II	1654	Amide I
	1685	Amide I	1705	Lipid, v(C=O)
	1720	Lipid, v(C=O)	1543	Amide II
	1539	Amide II	1504	Amide II
	1651	Amide I	1107	$v_sPO_2^-$
	1454	Proteins, $v_{as}CH_3$	1346	$v(COO^-)$
	1000	Protein phosphorylation	1577	Amide II
	920	Protein phosphorylation	1616	Amide I
0.1	1685	Amide I	1408	$v(COO^-)$
	1041	Glycogen	1446	Proteins, $v_{as}CH_3$
	1076	$v_sPO_2^-$	1276	Amide III
	1635	Amide I	1728	Lipid, v(C=O)
	1400	$v(COO^-)$	1639	Amide I
	933	Protein phosphorylation	1334	$v(COO^-)$
	1554	Amide II	1033	Glycogen
	1504	Amide II	1689	Amide I

Cluster vectors plots for zebrafish brain exposed to long MWCNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	**Female**		**Male**	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1504	Amide II	1458	Proteins, $\nu_{as}CH_3$
	1654	Amide I	1392	$\nu(COO^-)$
	1743	Lipid, $\nu(C=O)$	1543	Amide II
	1454	Proteins, $\nu_{as}CH_3$	1685	Amide I
	1616	Amide I	1728	Lipid, $\nu(C=O)$
	1697	Lipid, $\nu(C=O)$	1346	$\nu(COO^-)$
	941	Protein phosphorylation	1600	Amide I
	1346	$\nu(COO^-)$	1643	Amide I
0.1	1512	Amide II	1647	Amide I
	1126	Carbohydrates, $\nu(C\text{-}O)$	1122	Carbohydrates, $\nu(C\text{-}O)$
	1774	Lipid, $\nu(C=O)$	1180	Carbohydrates, $\nu(C\text{-}O)$
	1361	$\nu(COO^-)$	1527	Amide II
	1712	Lipid, $\nu(C=O)$	1392	$\nu(COO^-)$
	1477	Proteins, $\nu_{as}CH_3$	1716	Lipid, $\nu(C=O)$
	1053	Glycogen	1485	Proteins, $\nu_{as}CH_3$
	1573	Amide II	1265	Amide III

Cluster vectors plots for zebrafish gill exposed to Long MWCNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1539	Amide II	1639	Amide I
	1651	Amide I	1539	Amide II
	1492	Proteins, $v_{as}CH_3$	1010	Glycogen
	948	Protein phosphorylation	1377	$v(COO^-)$
	1257	Amide III	1689	Amide I
	1701	Lipid, v(C=O)	1296	Amide III
	1789	Lipid, v(C=O)	1500	Amide II
	1585	Amide I	1091	$v_sPO_2^-$
0.1	1539	Amide II	1720	Lipid, v(C=O)
	1492	Proteins, $v_{as}CH_3$	995	Protein phosphorylation
	1651	Amide I	1627	Amide I
	1584	Amide I	1330	$v(COO^-)$
	948	Protein phosphorylation	1450	Proteins, $v_{as}CH_3$
	1107	$v_sPO_2^-$	1554	Amide II
	1257	Amide III	1161	Carbohydrates, v(C-O)
	1411	Proteins, $v_{as}CH_3$	1774	Lipid, v(C=O)

Cluster vectors plots for zebrafish gonads exposed to long MWCNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	**Female**		**Male**	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1654	Amide I	1539	Amide II
	1700	Lipid, ν(C=O)	1689	Amide I
	1554	Amide II	1647	Amide I
	1172	Carbohydrates, ν(C-O)	1770	Lipid, ν(C=O)
	1504	Amide II	1504	Amide II
	1130	Carbohydrates, ν(C-O)	1006	Glycogen
	1766	Lipid, ν(C=O)	1728	Lipid, ν(C=O)
	1041	Glycogen	1612	Amide I
0.1	1064	$\nu_s PO_2^-$	1720	Lipid, ν(C=O)
	1720	Lipid, ν(C=O)	1670	Amide I
	1276	Amide III	1388	$\nu(COO^-)$
	1427	Proteins, $\nu_{as}CH_3$	1539	Amide II
	1342	$\nu(COO^-)$	1504	Amide II
	1543	Amide II	1172	Carbohydrates, ν(C-O)
	1473	Proteins, $\nu_{as}CH_3$	1126	Carbohydrates, ν(C-O)
	1620	Amide I	948	Protein phosphorylation

Cluster vectors plots for zebrafish liver exposed to long MWCNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	**Female**		**Male**	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1504	Amide II	1485	Proteins, $\nu_{as}CH_3$
	1056	$\nu_s PO_2^-$	1697	Lipid, $\nu(C{=}O)$
	1404	$\nu(COO^-)$	1049	Glycogen
	1091	$\nu_s PO_2^-$	1519	Amide II
	1465	Proteins, $\nu_{as}CH_3$	1654	Amide I
	1218	$\nu_{as} PO_2^-$	1099	$\nu_s PO_2^-$
	1697	Lipid, $\nu(C{=}O)$	1000	Protein phosphorylation
	1647	Amide I	1134	Carbohydrates, $\nu(C\text{-}O)$
0.1	1766	Lipid, $\nu(C{=}O)$	1054	Glycogen
	1504	Amide II	1080	$\nu_s PO_2^-$
	1543	Amide II	1477	Proteins, $\nu_{as}CH_3$
	1049	Glycogen	1786	Lipid, $\nu(C{=}O)$
	1091	$\nu_s PO_2^-$	1690	Amide I
	1188	Carbohydrates, $\nu(C\text{-}O)$	1728	Lipid, $\nu(C{=}O)$
	1469	Proteins, $\nu_{as}CH_3$	1361	$\nu(COO^-)$
	1732	Lipid, $\nu(C{=}O)$	1539	Amide II

Cluster vectors plots for zebrafish brain exposed to short MWCNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1442	Proteins, $v_{as}CH_3$	1720	Lipid, v(C=O)
	1523	Amide II	1064	$v_sPO_2^-$
	1716	Lipid, v(C=O)	1408	$v(COO^-)$
	1670	Amide I	1681	Amide I
	1562	Amide II	1612	Amide I
	1056	$v_sPO_2^-$	1523	Amide II
	1176	Carbohydrates, v(C-O)	914	Protein phosphorylation
	1770	Lipid, v(C=O)	1141	Carbohydrates, v(C-O)
0.1	1473	Proteins, $v_{as}CH_3$	1064	$v_sPO_2^-$
	1126	Carbohydrates, v(C-O)	1716	Lipid, v(C=O)
	1056	$v_sPO_2^-$	1408	$v(COO^-)$
	1589	Amide I	1523	Amide II
	1002	Glycogen	1631	Amide I
	1693	Amide I	1681	Amide I
	1550	Amide II	1242	$v_{as}PO_2^-$
	1365	$v(COO^-)$	1141	Carbohydrates, v(C-O)

Cluster vectors plots for zebrafish gill exposed to short MWCNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1543	Amide II	1377	$v(COO^-)$
	1338	$v(COO^-)$	1662	Amide I
	1790	Lipid, v(C=O)	914	Protein phosphorylation
	1705	Lipid, v(C=O)	1539	Amide II
	1396	$v(COO^-)$	1716	Lipid, v(C=O)
	1083	$v_sPO_2^-$	1624	Amide I
	1458	Proteins, $v_{as}CH_3$	1338	$v(COO^-)$
	1635	Amide I	1176	Carbohydrates, v(C-O)
0.1	1543	Amide II	1647	Amide I
	1766	Lipid, v(C=O)	1257	Amide III
	1724	Lipid, v(C=O)	1072	$v_sPO_2^-$
	1083	$v_sPO_2^-$	1504	Amide II
	1577	Amide II	1543	Amide II
	1408	$v(COO^-)$	979	Protein phosphorylation
	1323	Amide III	1689	Amide I
	1678	Amide I	1377	$v(COO^-)$

Cluster vectors plots for zebrafish gonads exposed to short MWCNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1504	Amide II	1681	Amide I
	1685	Amide I	1504	Amide II
	1647	Amide I	1647	Amide I
	1739	Lipid, v(C=O)	1435	Proteins, $v_{as}CH_3$
	1543	Amide II	1546	Amide II
	1577	Amide II	1207	$v_{as}PO_2^-$
	1249	Amide III	1747	Lipid, v(C=O)
	1392	$v(COO^-)$	1026	Glycogen
0.1	1685	Amide I	1681	Amide I
	1543	Amide II	941	Protein phosphorylation
	1504	Amide II	1103	$v_sPO_2^-$
	1396	$v(COO^-)$	1141	Carbohydrates, v(C-O)
	1199	$v_{as}PO_2^-$	1485	Proteins, $v_{as}CH_3$
	1438	Proteins, $v_{as}CH_3$	1176	Carbohydrates, v(C-O)
	941	Protein phosphorylation	1539	Amide II
	1766	Lipid, v(C=O)	1716	Lipid, v(C=O)

Cluster vectors plots for zebrafish liver exposed to short MWCNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1654	Amide I	1543	Amide II
	1701	Lipid, v(C=O)	1180	Carbohydrates, v(C-O)
	1543	Amide II	1701	Lipid, v(C=O)
	1188	Carbohydrates, v(C-O)	1381	$v(COO^-)$
	1504	Amide II	1647	Amide I
	960	Protein phosphorylation	1743	Lipid, v(C=O)
	1080	$v_sPO_2^-$	1612	Amide I
	1766	Lipid, v(C=O)	1477	Proteins, $v_{as}CH_3$
0.1	1554	Amide II	1381	$v(COO^-)$
	968	Protein phosphorylation	1180	Carbohydrates, v(C-O)
	1697	Lipid, v(C=O)	1546	Amide II
	1381	$v(COO^-)$	1608	Amide I
	1654	Amide I	1041	Glycogen
	1188	Carbohydrates, v(C-O)	1141	Carbohydrates, v(C-O)
	1415	Proteins, $v_{as}CH_3$	1705	Lipid, v(C=O)
	1755	Lipid, v(C=O)	1419	Proteins, $v_{as}CH_3$

Cluster vectors plots for zebrafish brain exposed to single-walled CNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	**Female**		**Male**	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1404	$v(COO^-)$	1720	Lipid, $v(C{=}O)$
	1068	$v_sPO_2^-$	1543	Amide II
	1658	Amide I	1157	Carbohydrates, $v(C\text{-}O)$
	1697	Lipid, $v(C{=}O)$	1053	Glycogen
	1134	Carbohydrates, $v(C\text{-}O)$	1654	Amide I
	1176	Carbohydrates, $v(C\text{-}O)$	1392	$v(COO^-)$
	1261	Amide III	1191	$v_{as}PO_2^-$
	929	Protein phosphorylation	1107	$v_sPO_2^-$
0.1	1006	Glycogen	1720	Lipid, $v(C{=}O)$
	1064	$v_sPO_2^-$	1581	Amide II
	1431	Proteins, $v_{as}CH_3$	1469	Proteins, $v_{as}CH_3$
	1107	$v_sPO_2^-$	1191	$v_{as}PO_2^-$
	1261	Amide III	1639	Amide I
	1357	$v(COO^-)$	1157	Carbohydrates, $v(C\text{-}O)$
	1612	Amide I	1064	$v_sPO_2^-$
	1697	Lipid, $v(C{=}O)$	1400	$v(COO^-)$

Cluster vectors plots for zebrafish gill exposed to single-walled CNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	**Female**		**Male**	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1720	Lipid, v(C=O)	1639	Amide I
	1454	Proteins, $v_{as}CH_3$	1774	Lipid, v(C=O)
	1053	Glycogen	1539	Amide II
	1404	$v(COO^-)$	1693	Amide I
	1369	$v(COO^-)$	1257	Amide III
	1087	$v_sPO_2^-$	1492	Proteins, $v_{as}CH_3$
	1651	Amide I	972	Protein phosphorylation
	1755	Lipid, v(C=O)	918	Protein phosphorylation
0.1	1103	$v_sPO_2^-$	1585	Amide I
	1766	Lipid, v(C=O)	1662	Amide I
	1427	Proteins, $v_{as}CH_3$	1701	Lipid, v(C=O)
	1261	Amide III	1083	$v_sPO_2^-$
	1627	Amide I	1338	$v(COO^-)$
	1500	Amide II	1180	Carbohydrates, v(C-O)
	1539	Amide II	1462	Proteins, $v_{as}CH_3$
	948	Protein phosphorylation	1257	Amide III

Cluster vectors plots for zebrafish gonads exposed to single-walled CNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1504	Amide II	1419	Proteins, $v_{as}CH_3$
	1697	Lipid, *v*(C=O)	1681	Amide I
	1647	Amide I	1184	Carbohydrates, *v*(C-O)
	1554	Amide II	1110	$v_sPO_2^-$
	1438	Proteins, $v_{as}CH_3$	1539	Amide II
	1612	Amide I	983	Protein phosphorylation
	1068	$v_sPO_2^-$	1724	Lipid, *v*(C=O)
	1377	$v(COO^-)$	1473	Proteins, $v_{as}CH_3$
0.1	1446	Proteins, $v_{as}CH_3$	1701	Lipid, *v*(C=O)
	1651	Amide I	1666	Amide I
	1184	Carbohydrates, *v*(C-O)	1188	Carbohydrates, *v*(C-O)
	1759	Lipid, *v*(C=O)	1735	Lipid, *v*(C=O)
	1481	Proteins, $v_{as}CH_3$	1110	$v_sPO_2^-$
	1724	Lipid, *v*(C=O)	1419	Proteins, $v_{as}CH_3$
	1056	$v_sPO_2^-$	1504	Amide II
	1573	Amide II	1381	$v(COO^-)$

Cluster vectors plots for zebrafish liver exposed to single-walled CNTs at two doses: derived from IR spectra by cross-calculated PCA-LDA

Dose (mg/L)	Female		Male	
	Wavenumber (cm^{-1})	Tentative assignments	Wavenumber (cm^{-1})	Tentative assignments
0.001	1504	Amide II	1685	Amide I
	1693	Amide I	1504	Amide II
	1651	Amide I	1130	$\nu(COO^-)$
	1438	Proteins, $\nu_{as}CH_3$	1045	Glycogen
	956	Protein phosphorylation	983	Protein phosphorylation
	1558	Amide II	1357	$\nu(COO^-)$
	1404	$\nu(COO^-)$	921	Protein phosphorylation
	1083	$\nu_sPO_2^-$	1562	Amide II
0.1	1504	Amide II	1477	Proteins, $\nu_{as}CH_3$
	1651	Amide I	1512	Amide II
	1693	Amide I	1639	Amide I
	1766	Lipid, $\nu(C{=}O)$	1693	Amide I
	1438	Proteins, $\nu_{as}CH_3$	1411	Proteins, $\nu_{as}CH_3$
	956	Protein phosphorylation	968	Protein phosphorylation
	1130	Carbohydrates, $\nu(C\text{-}O)$	1261	Amide III
	999	Protein phosphorylation	1774	Lipid, $\nu(C{=}O)$