

SUPPORTING INFORMATION:

**Bioengineering Silicon Quantum Dot Theranostics using a Network Analysis of Metabolomic and Proteomic Data in Cardiac Ischaemia**

*Translating Biomarkers to Theranostics*

<sup>1</sup>Folarin Erogbogbo, <sup>1</sup>Jasmine May, <sup>1</sup>Mark Swihart, <sup>1</sup>Paras N. Prasad, <sup>2</sup>Katie Smart, <sup>3</sup>Seif El Jack, <sup>4</sup>Dariusz Korcyk, <sup>5</sup>Mark Webster, <sup>5</sup>Ralph Stewart, <sup>6</sup>Irene Zeng, <sup>7</sup>Mia Jullig, <sup>8</sup>Katherine Bakeev, <sup>9</sup>Michelle Jamieson, <sup>9</sup>Nikolas Kasabov, <sup>10</sup>Banu Gopalan, <sup>9</sup>Linda Liang, <sup>9</sup>Raphael Hu, <sup>9</sup>Stefan Schliebs, <sup>7</sup>Silas Villas-Boas, <sup>3</sup>Patrick Gladding

<sup>1</sup>University at Buffalo, New York

<sup>2</sup>Lanzatech, Auckland

<sup>3</sup>North Shore Hospital, Auckland

<sup>4</sup>Princess Alexandra hospital, Brisbane

<sup>5</sup>Green Lane Cardiovascular Service, Auckland

<sup>6</sup>CCRep, Middlemore hospital, Auckland

<sup>7</sup>School of Biological Science, Auckland

<sup>8</sup>CAMO Software, New Jersey

<sup>9</sup>KEDRI, Auckland University of Technology

<sup>10</sup>Lerner Research Institute, Cleveland

Corresponding Author:

Patrick Gladding,

Address: Northshore Hospital

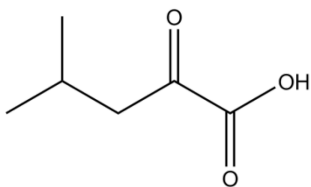
Waitemata DHB

Email: [patrickg@theranosticslab.com](mailto:patrickg@theranosticslab.com)

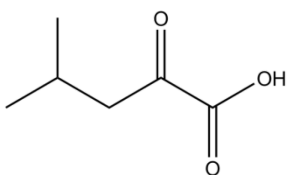
**Table S1. Potential biomarkers: common five metabolites identified by bioinformatic analysis of aortic blood and cross-referenced with coronary sinus data**

**Metabolite**

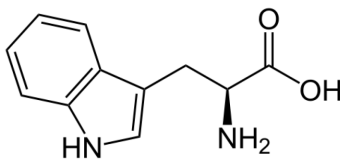
Methyl-2-oxopentanoicacid



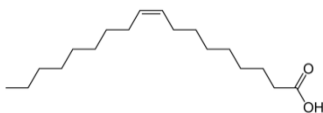
Serine



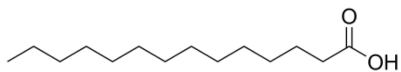
Tryptophan



Oleic acid



\*Myristic acid



**Table S2 Differences between silica and silicon nanostructures**

Silica in nanostructures	Silicon nanocrystals
Formula – SiO <sub>2</sub>	Formula - Si
Used to encapsulate active materials e.g gold	Used as Active Material e.g. optical imaging
Amorphous	Crystalline
Non-Luminescent	Luminescent
Well studied	New and novel material
Generally used as a Controllable Coating	Never used as coating
Never used for size controlled emission	Used for sized tunable emission
Not the main focus of studies (other materials, such as gold, quantum dots, drugs, )	The main focus of its' studies ( how can it be used for imaging, how does it interact)

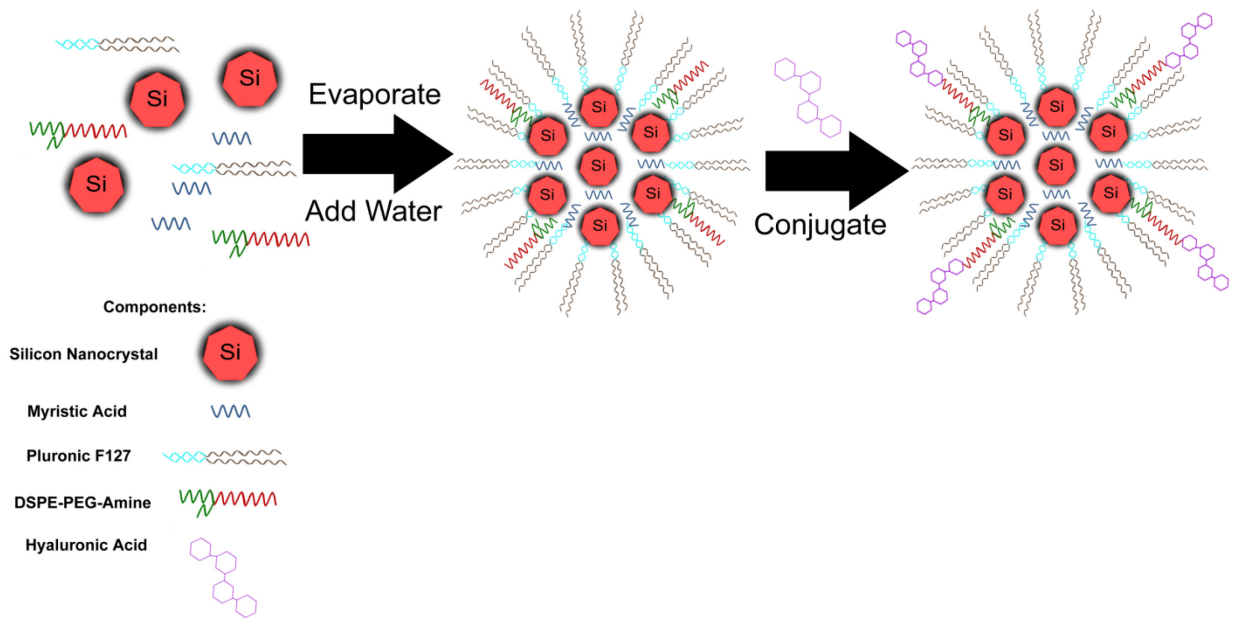


Figure S1. Depiction of an encapsulation process for silicon and myristic acid.

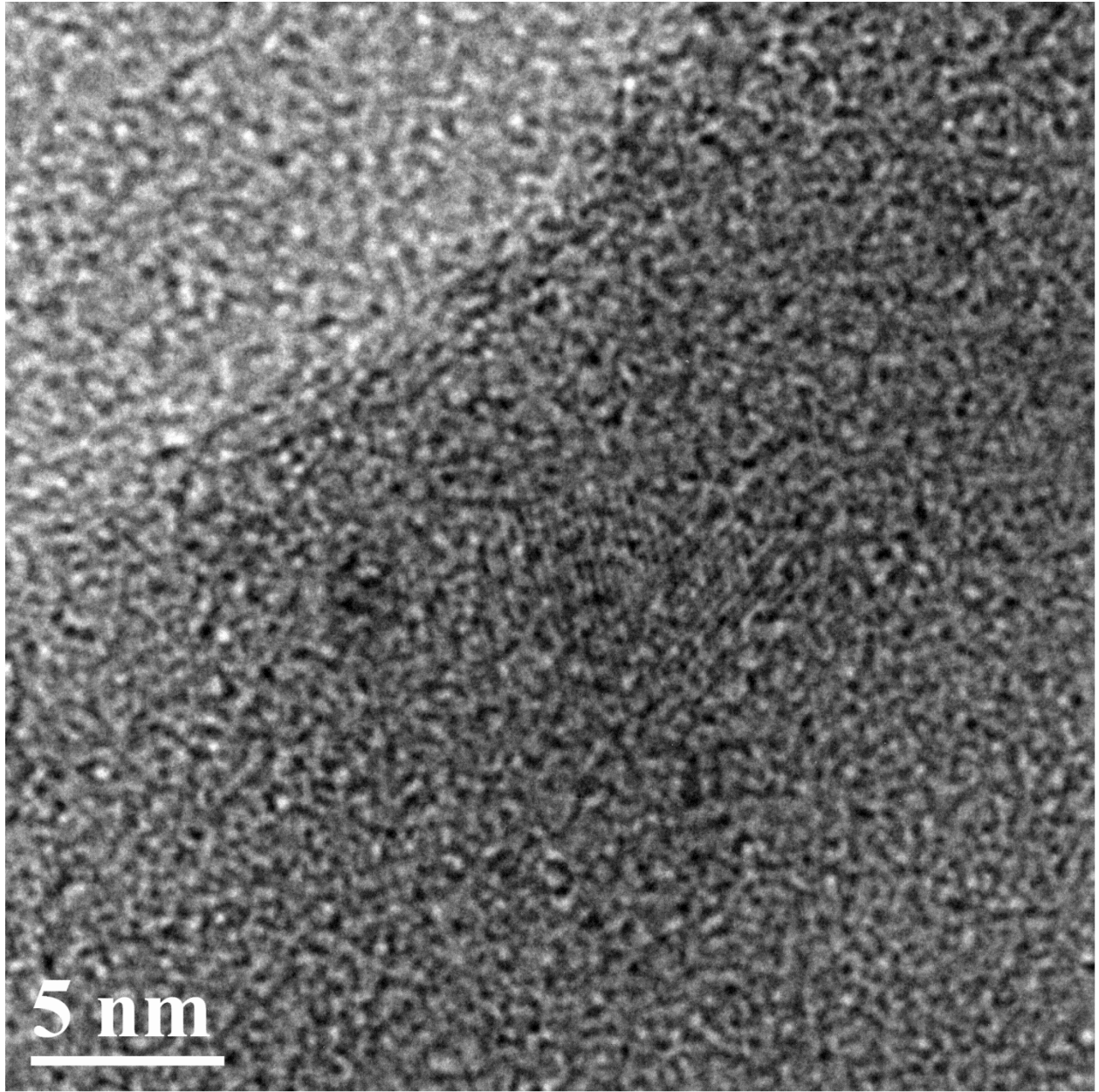
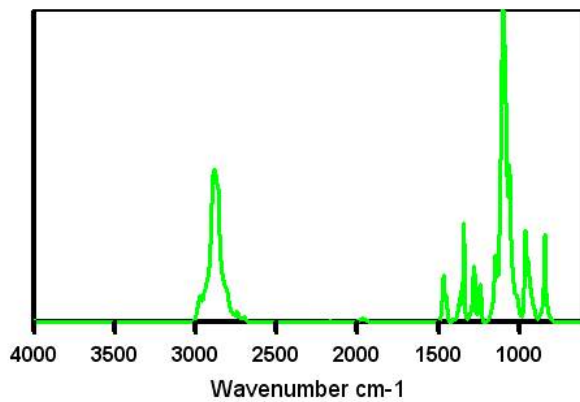


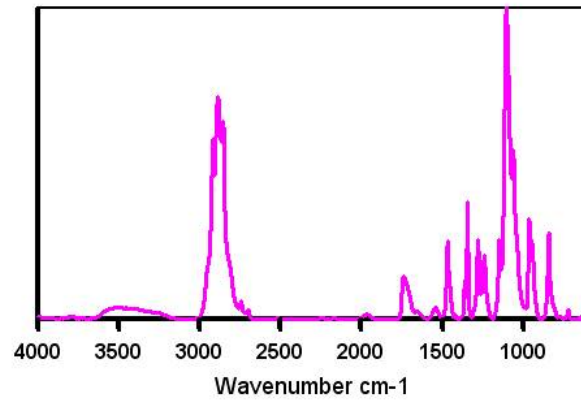
Figure S2. Larger image of TEM in Figure 5c.

Characterization data from components related to the nanostructure are depicted below.

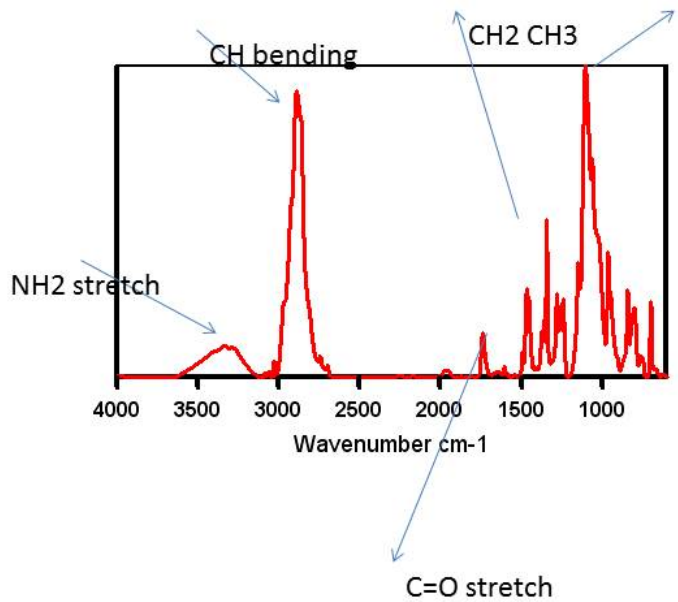
# F127



# Dspe/peg/amine

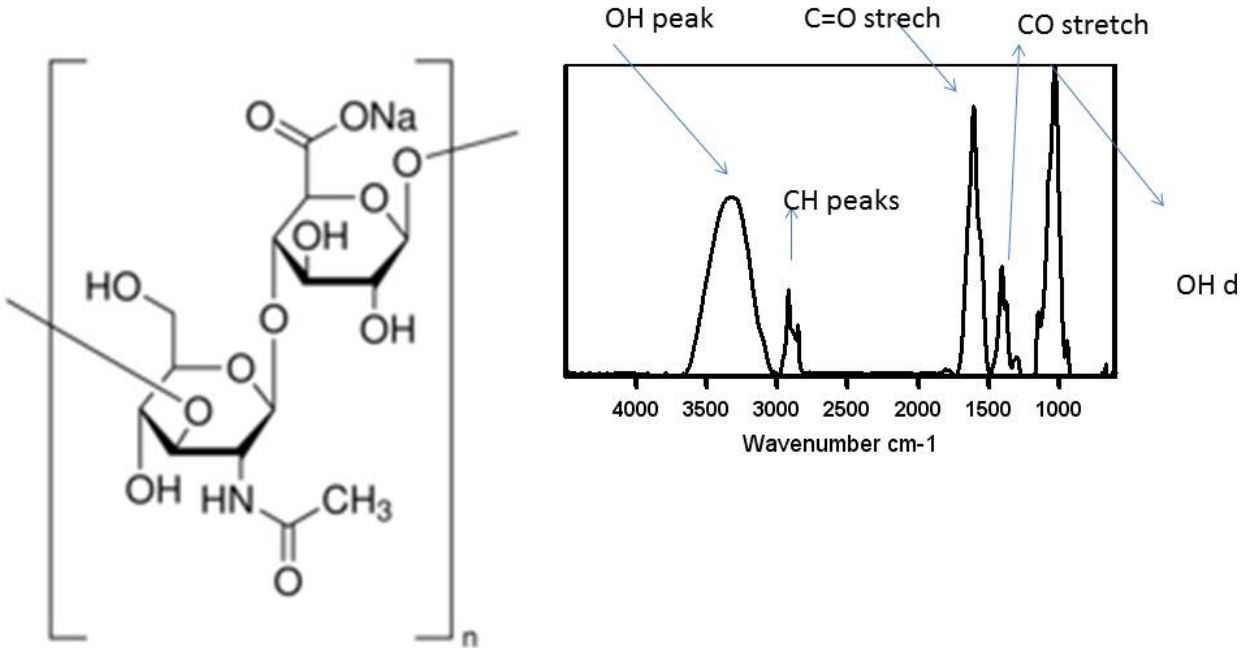


# Msi(f127+Dspepegamine)

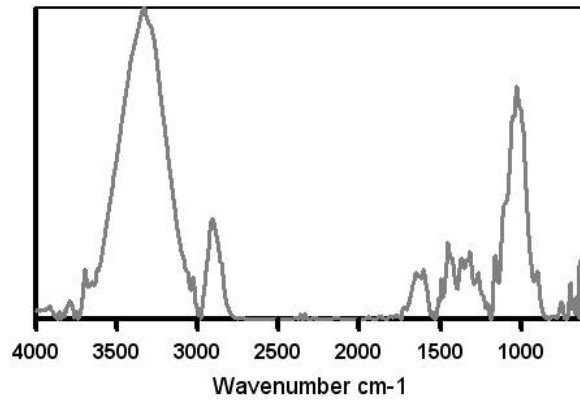


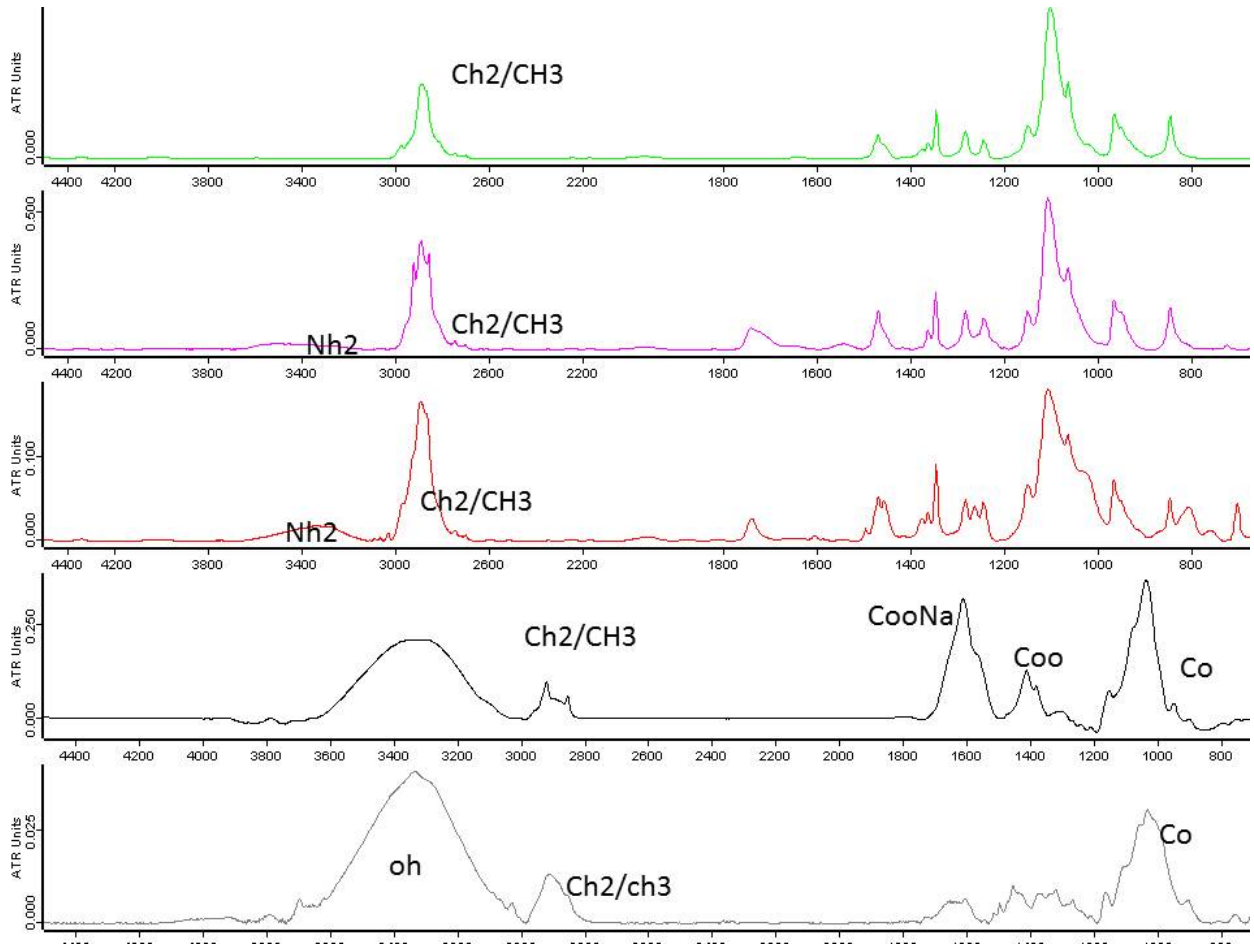


# Hyaluronic Acid Sodium salt

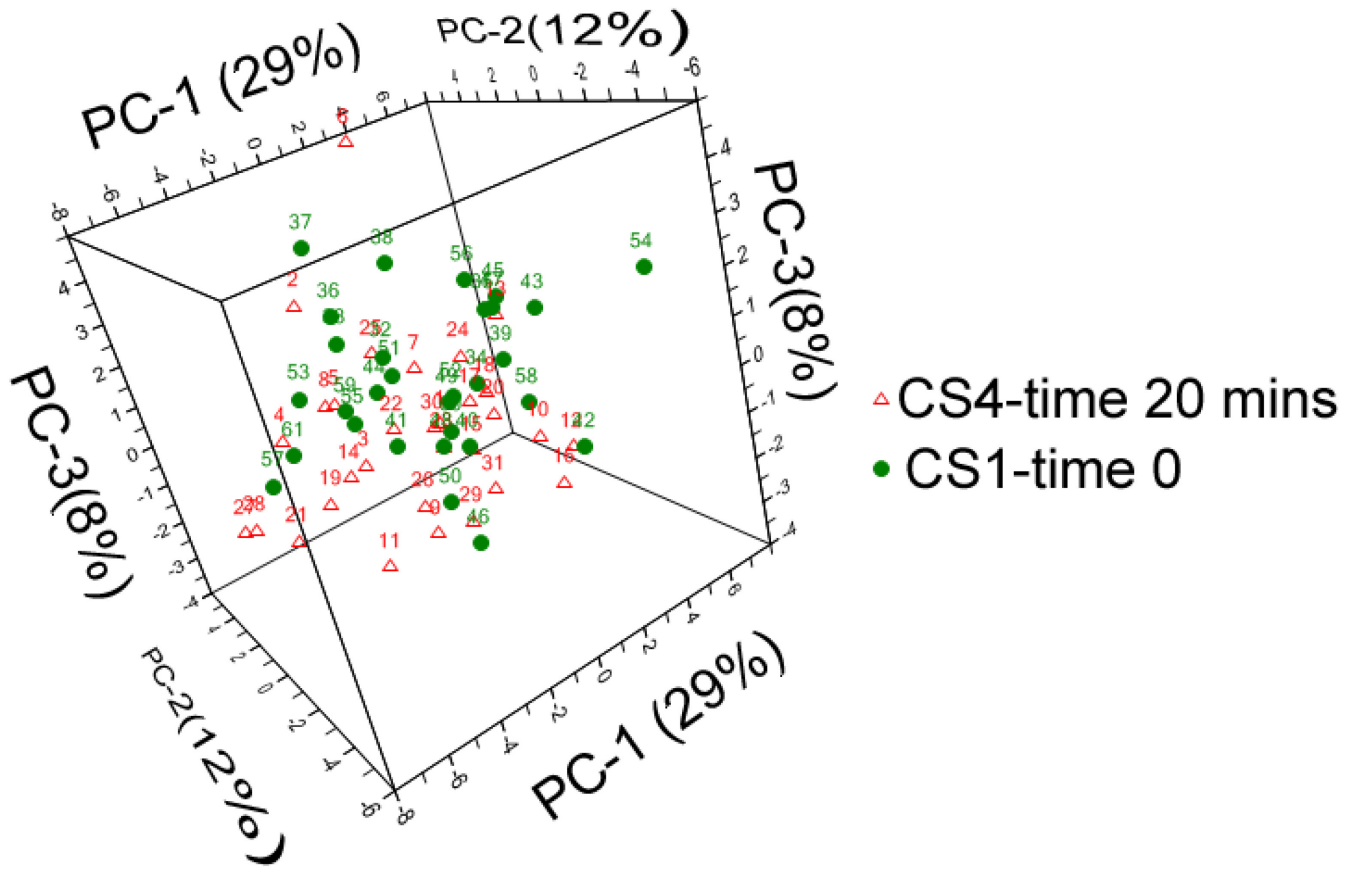


# Hyaluronic Acid conjugated Si

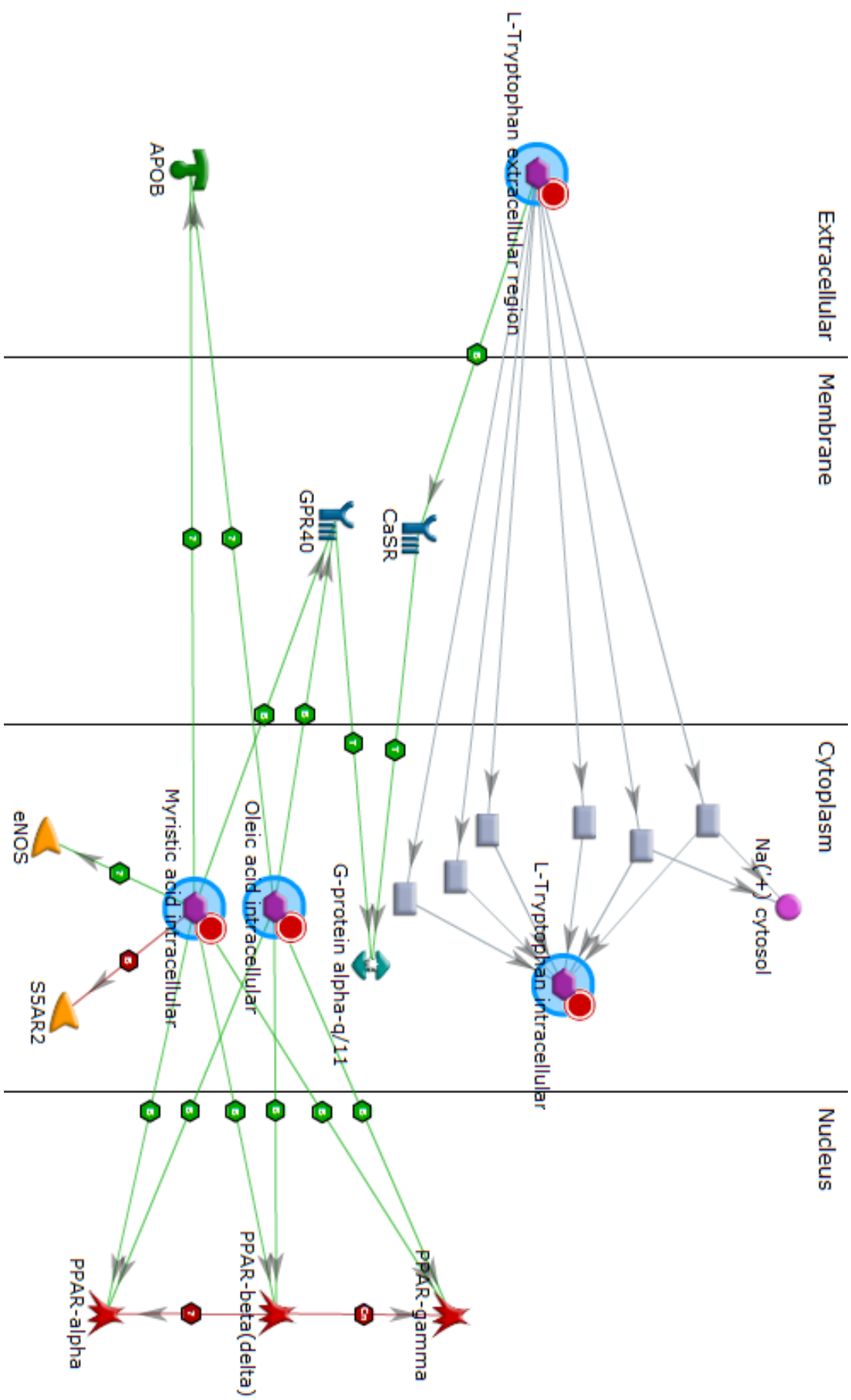


































# 3-D scores for CS1/CS 4 Samples



Enlarged Figure 1



Enlarged Figure 2.

Enzymes		Generic classes	
	Generic enzyme		Receptor ligand
KINASE		PHOSPHATASE	
	Generic kinase		Generic phosphatase
	Protein kinase		Protein phosphatase
	Lipid kinase		Lipid phosphatase
PHOSPHOLIPASE			
	Generic phospholipase		
PROTEASE		GTPase	
	Generic protease		G-alpha
	Metalloprotease		RAS - superfamily
Channels/Transporters		Receptors	
	Generic channel		Generic receptor
	Ligand-gated ion channel		GPCR
	Voltage-gated ion channel		Receptors with enzyme activity
		G protein adaptor/regulators	
			G beta/gamma
			Reaction
			Transcription factor
			Protein
			Cell membrane glycoprotein
			Compound
			Predicted metabolite or user's structure
			Inorganic ion
			DNA
			RNA
			Generic binding protein

Enlarged Figure 2 legend.