

## Supplementary Information

### Correlations of elemental and metabolic profiles of the lichen

#### *Dirinaria picta* after road traffic exposure

Xulei Huang<sup>a</sup>, Lei Wang<sup>a</sup>, , Anna Karen Carrasco Laserna<sup>a</sup> and Sam Fong Yau Li<sup>a,b,\*</sup>

<sup>a</sup>*Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore*

<sup>b</sup>*NUS Environmental Research Institute (NERI), #02-01, T-Lab Building (TL), 5A Engineering Drive 1, Singapore 117411, Singapore*

#### **\*Corresponding author**

National University of Singapore, Department of Chemistry, 3 Science Drive 3, Singapore 117543, Singapore.

Phone: +65 6516 2681. Fax: + 65-6779-1691.

E-mail address: chmlifys@nus.edu.sg (S.F.Y. Li).

	Fe	Ni	Co	Cu	Zn	Ga	As	Se	Rb	Y	Cd
Ni	.404**										
Co	<u>.875**</u>	.453**									
Cu	<u>.866**</u>	.470**	<u>.948**</u>								
Zn	<u>.832**</u>	.316**	<u>.889**</u>	<u>.880**</u>							
Ga	<u>.873**</u>	.329**	<u>.909**</u>	<u>.895**</u>	<u>.887**</u>						
As	<u>.873**</u>	.317**	<u>.918**</u>	<u>.903**</u>	<u>.921**</u>	<u>.948**</u>					
Se	.449**	.150	.415**	.423**	.331**	.332**	.266*				
Rb	.465**	-.160	.497**	.505**	.615**	.645**	.619**	.023			
Y	<u>.899**</u>	<u>.371**</u>	<u>.939**</u>	<u>.916**</u>	<u>.919**</u>	<u>.958**</u>	<u>.954**</u>	<u>.320**</u>	<u>.567**</u>		
Cd	<u>.877**</u>	<u>.395**</u>	<u>.928**</u>	<u>.909**</u>	<u>.876**</u>	<u>.871**</u>	<u>.894**</u>	<u>.368**</u>	<u>.568**</u>	<u>.887**</u>	Mn
Li	.553**	-.093	.566**	.583**	.690**	.723**	.699**	.004	<u>.931**</u>	.678**	.610**
Ba	<u>.878**</u>	.249*	<u>.861**</u>	<u>.852**</u>	<u>.878**</u>	<u>.980**</u>	<u>.938**</u>	.270*	.702**	<u>.930**</u>	<u>.858**</u>
Na	<u>.870**</u>	<u>.548**</u>	<u>.905**</u>	<u>.893**</u>	<u>.910**</u>	<u>.950**</u>	<u>.936**</u>	.297*	.565**	<u>.984**</u>	<u>.865**</u>
Mg	<u>.884**</u>	<u>.643**</u>	<u>.925**</u>	<u>.895**</u>	<u>.908**</u>	<u>.955**</u>	<u>.945**</u>	.291*	.562**	<u>.986**</u>	<u>.867**</u>
Ce	<u>.892**</u>	<u>.533**</u>	<u>.908**</u>	<u>.897**</u>	<u>.910**</u>	<u>.946**</u>	<u>.932**</u>	.293*	.572**	<u>.980**</u>	<u>.864**</u>
Kr	<u>.872**</u>	<u>.643**</u>	<u>.909**</u>	<u>.891**</u>	<u>.900**</u>	<u>.949**</u>	<u>.935**</u>	.292*	.568**	<u>.983**</u>	<u>.859**</u>
Ga	<u>.825**</u>	<u>.349**</u>	<u>.913**</u>	<u>.898**</u>	<u>.914**</u>	<u>.954**</u>	<u>.945**</u>	.305**	.564**	<u>.991**</u>	<u>.871**</u>
Se	<u>.839**</u>	<u>.688**</u>	<u>.940**</u>	<u>.899**</u>	<u>.893**</u>	<u>.962**</u>	<u>.947**</u>	.346**	.513**	<u>.975**</u>	<u>.869**</u>
Pb	<u>.898**</u>	<u>.540**</u>	<u>.889**</u>	<u>.870**</u>	<u>.926**</u>	<u>.851**</u>	<u>.892**</u>	.428**	.494**	<u>.898**</u>	<u>.811**</u>
Bi	<u>.878**</u>	<u>.630**</u>	<u>.880**</u>	<u>.902**</u>	<u>.857**</u>	<u>.878**</u>	<u>.880**</u>	<u>.968**</u>	<u>.738**</u>	<u>.890**</u>	<u>.807**</u>
Mn	<u>.869**</u>	<u>.668**</u>	<u>.897**</u>	<u>.948**</u>	<u>.859**</u>	<u>.964**</u>	<u>.887**</u>	<u>.928**</u>	<u>.674**</u>	<u>.893**</u>	<u>.789**</u>
Fr	<u>.820**</u>	<u>.709**</u>	<u>.853**</u>	<u>.875**</u>	<u>.814**</u>	<u>.887**</u>	<u>.801**</u>	<u>.896**</u>	<u>.769**</u>	<u>.891**</u>	<u>.886**</u>
Ni	.382**	.311**	.162	.028	.233	.227	-.188	.415**	.499**	.392**	.357**
Co	.946**	.678**	.585**	.641**	.469**	.588**	.456**	.948**	.762**	.938**	.908**
Cu	.922**	.635**	.576**	.661**	.522**	.633**	.471**	.926**	.771**	.920**	.870**
Zn	.911**	.630**	.629**	.689**	.504**	.632**	.589**	.893**	.659**	.900**	.890**
Ga	.977**	.662**	.566**	.707**	.482**	.615**	.576**	.936**	.654**	.967**	.965**
As	.948**	.633**	.624**	.705**	.516**	.621**	.557**	.940**	.653**	.954**	.948**
Se	.362**	.394**	.204	.162	.150	.258*	.002	.333**	.549**	.333**	.287*
Rb	.610**	.512**	.546**	<u>.853**</u>	.631**	.746**	<u>.817**</u>	.543**	.148	.572**	.587**
Y	.969**	.655**	.599**	.635**	.442**	.545**	.513**	.959**	.701**	.979**	.968**
Cd	.891**	.629**	.602**	.714**	.541**	.632**	.568**	.887**	.667**	.882**	.863**
Cs	.698**	.549**	.581**	<u>.832**</u>	.577**	.670**	<u>.814**</u>	.628**	.250*	.671**	.689**
Ba	.934**	.615**	.596**	.756**	.495**	.612**	.667**	.884**	.568**	.931**	.947**
Nd	.947**	.614**	.591**	.618**	.421**	.525**	.529**	.936**	.680**	.969**	.964**
Sm	.952**	.621**	.589**	.622**	.423**	.526**	.519**	.942**	.680**	.975**	.971**
Ce	.947**	.615**	.607**	.627**	.447**	.548**	.524**	.931**	.692**	.969**	.962**
Pr	.946**	.607**	.592**	.614**	.417**	.527**	.527**	.934**	.679**	.969**	.965**
Gd	.955**	.625**	.593**	.625**	.429**	.528**	.525**	.943**	.682**	.974**	.969**
La	.950**	.666**	.583**	.589**	.414**	.529**	.456**	.945**	.749**	.968**	.961**
Pb	.858**	.568**	.584**	.556**	.401**	.530**	.514**	.850**	.678**	.863**	.845**
Bi	.899**	.639**	.509**	.595**	.482**	.613**	.414**	.912**	.721**	.909**	.853**
U	.904**	.573**	.462**	.603**	.368**	.500**	.516**	.864**	.557**	.896**	.916**
Th	.909**	.573**	.410**	.532**	.350**	.498**	.434**	.929**	.604**	.912**	.873**

Table S1 Pearson correlations of elements in lichens. \* denotes p<0.05, \*\* denotes p<0.01. Correlation values larger than 0.8 are underlined.

	Cs	Ba	Nd	Sm	Ce	Pr	Gd	La	Pb	Bi	U
Ba	.771**										
Nd	.681**	<u>.937**</u>									
Sm	.680**	<u>.941**</u>	<u>.998**</u>								
Ce	.683**	<u>.930**</u>	<u>.995**</u>	<u>.992**</u>							
Pr	.682**	<u>.936**</u>	<u>.999**</u>	<u>.997**</u>	<u>.996**</u>						
Gd	.681**	<u>.938**</u>	<u>.997**</u>	<u>.998**</u>	<u>.992**</u>	<u>.996**</u>					
La	.617**	<u>.903**</u>	<u>.975**</u>	<u>.975**</u>	<u>.977**</u>	<u>.976**</u>	<u>.976**</u>				
Pb	.586**	<u>.834**</u>	<u>.903**</u>	<u>.891**</u>	<u>.903**</u>	<u>.905**</u>	<u>.898**</u>	<u>.887**</u>			
Bi	.601**	<u>.814**</u>	<u>.875**</u>	<u>.876**</u>	<u>.889**</u>	<u>.876**</u>	<u>.877**</u>	<u>.881**</u>	<u>.847**</u>		
U	.663**	<u>.908**</u>	<u>.887**</u>	<u>.901**</u>	<u>.878**</u>	<u>.887**</u>	<u>.899**</u>	<u>.875**</u>	<u>.755**</u>	<u>.734**</u>	
Th	.635**	<u>.851**</u>	<u>.883**</u>	<u>.896**</u>	<u>.881**</u>	<u>.885**</u>	<u>.895**</u>	<u>.875**</u>	<u>.757**</u>	<u>.869**</u>	<u>.878**</u>

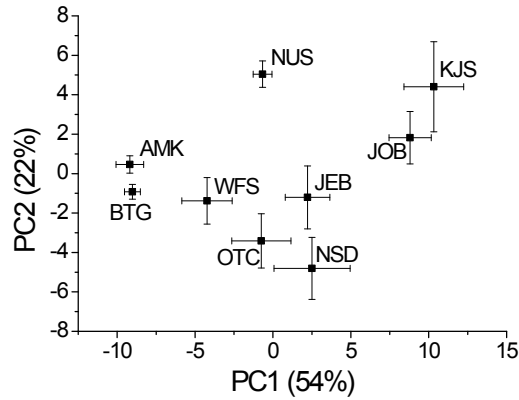


Figure S1 PCA score plot of PC1 (first component) versus PC2 (second component) for the elemental profiles of lichen samples from 9 sites in Singapore. For both PC1 and PC2, data were shown as mean scores and the associated standard errors.

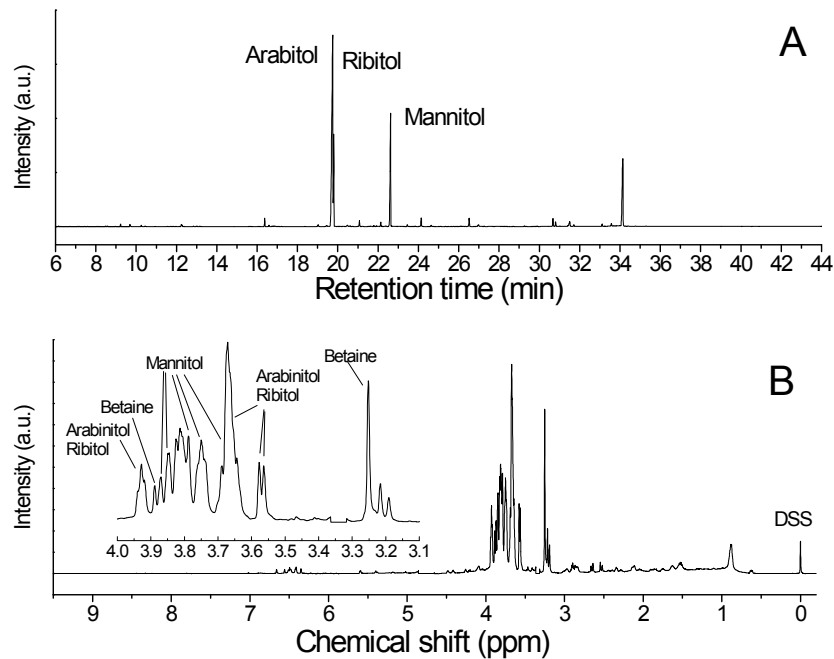


Figure S2 Typical (A) GC-MS and (B) NMR spectrum of lichens extracts. Several major metabolites were annotated in the inset figure.

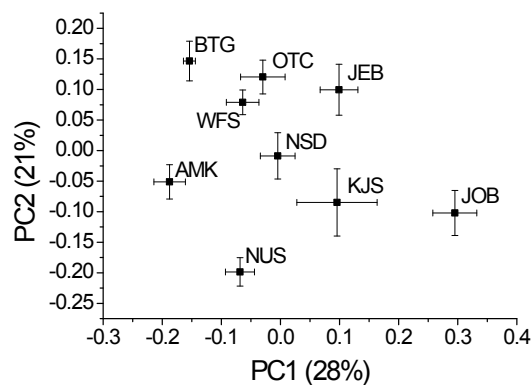


Figure S3 PCA score plot of PC1 (first component) versus PC2 (second component) for the NMR data of lichen extracts from 9 sites in Singapore. For both PC1 and PC2, data were shown as mean scores and the associated standard errors.