Supplementary Material

for

Development of a Single Aptamer-based Surface Enhanced Raman Scattering Method for Rapid Detection of Multiple Pesticides

Shintaro Pang,[a] Theodore P. Labuza[b] and Lili He*[a]

[a] Department of Food Science, University of Massachusetts, Amherst, MA 01003, USA

[b] Department of Food Science and Nutrition, University of Minnesota, St. Paul, MN 55108, USA

* Corresponding Author

Telephone: (413)-545-5847. Fax: (413)-545-1262. Email: lilihe@foodsci.umass.edu.

Abstract for Supplementary Data

The supplementary materials presented here provide details of some of the secondary steps that were taken into account in order to develop the single aptamer based SERS method for detecting multiple pesticides.

Supporting Figures

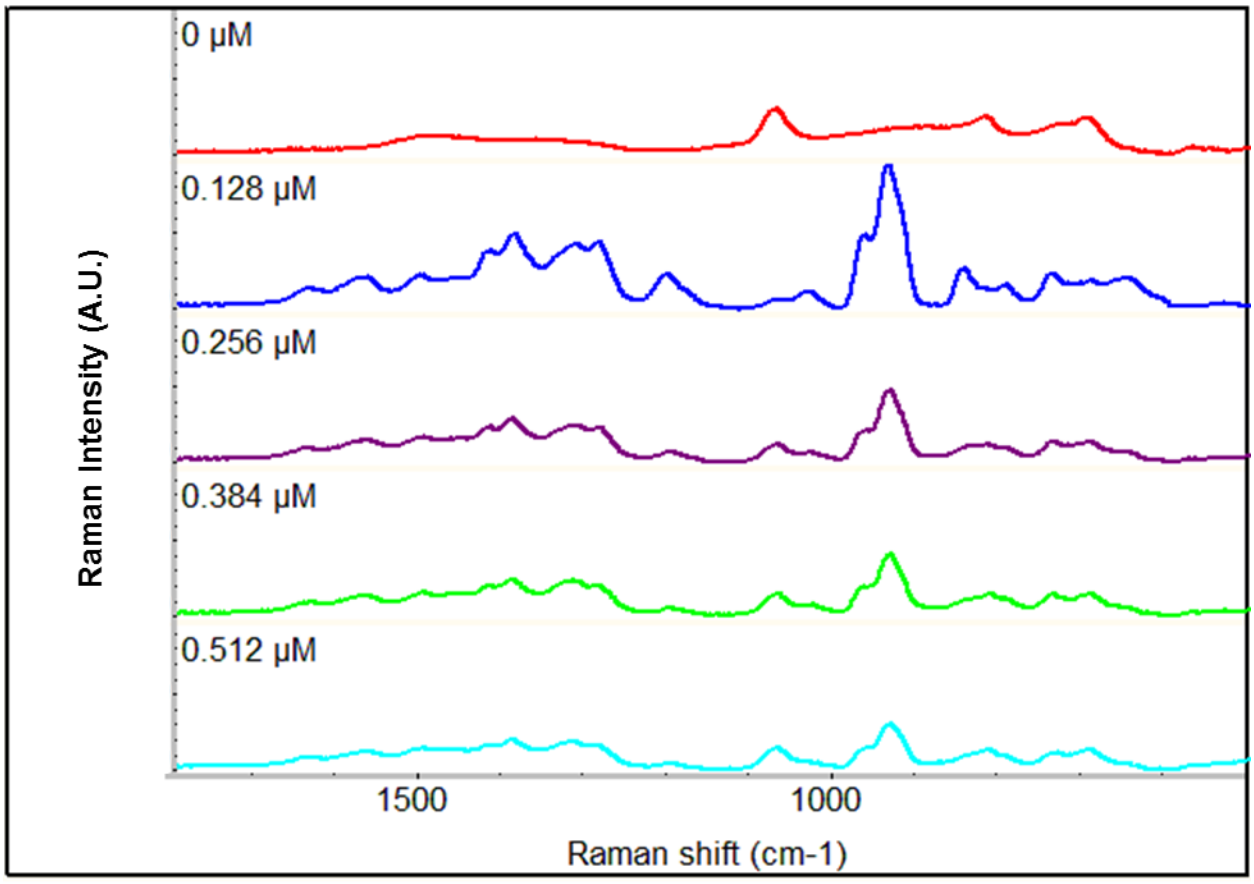

Fig. S1 Raman spectra of various concentrations of thiolated aptamer (S2-55) mixed with Ag dendrites in double distilled water. The largest peak intensities were produced at the smallest concentration (0.128 µM). As the thiolated aptamer concentration introduced was increased, the Raman peaks kept falling, suggesting a mechanism that was making less aptamer have access to the surface of the Ag dendrites.

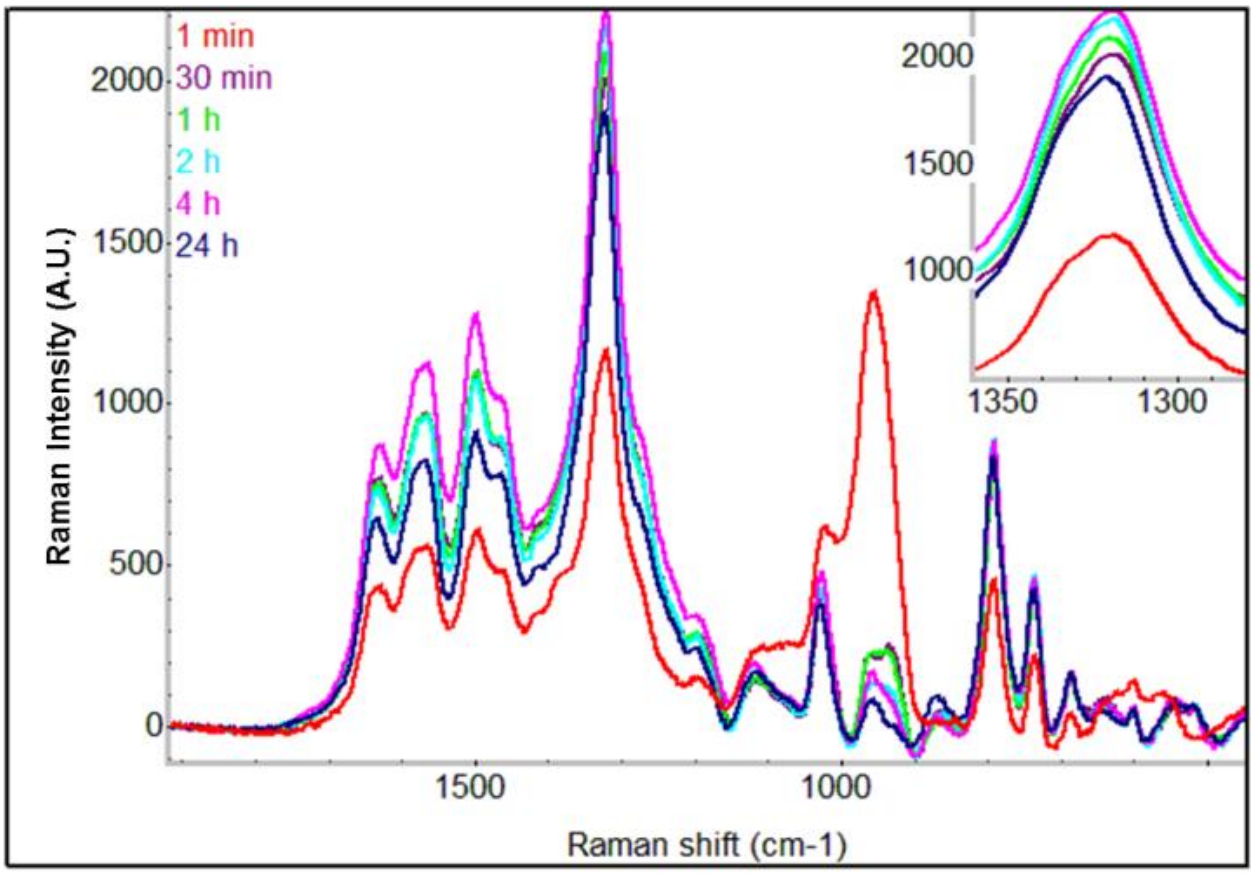

Fig. S2 Raman spectra of silver-aptamer complex (Ag-Ap) with various incubation times to assess the binding time optimization of thiolated aptamer (5 µM) onto Ag. The aptamer capture peaks, such as the one in 1330 cm^{-1} was maximized after four hours incubation, which was the incubation time used for further analysis.

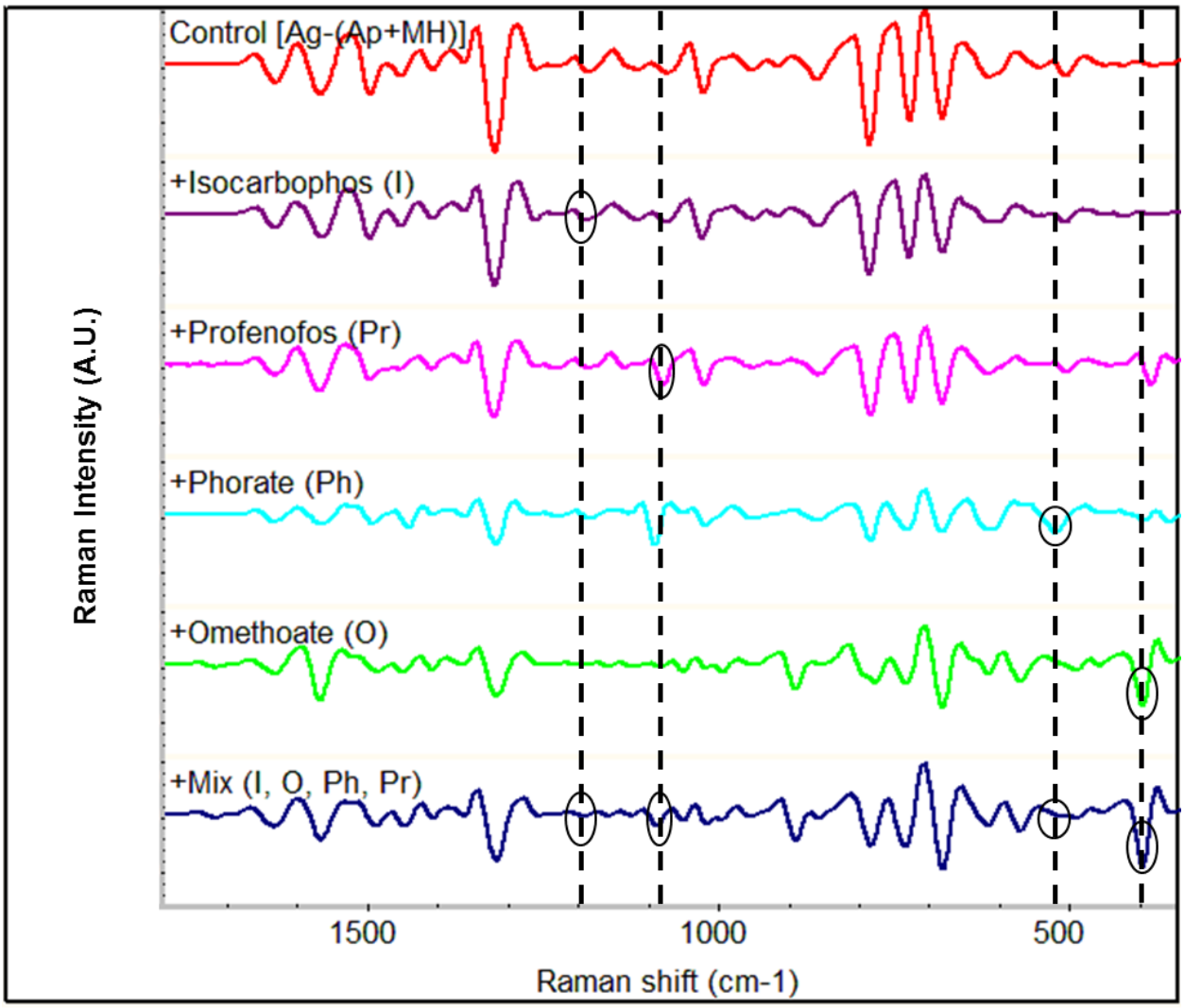

Fig. S3 Second derivative Raman spectra of modified nanoparticles [Ag-(Ap+MH)] with iscarbophos, omethoate, phorate and profenofos respectively and the four pesticides mixed together at even concentrations. Total pesticide concentration for each sample was 0.5 mM. The distinct Raman peaks produced by each pesticide at different Raman shifts allows for simultaneous detection of the four specific pesticide.

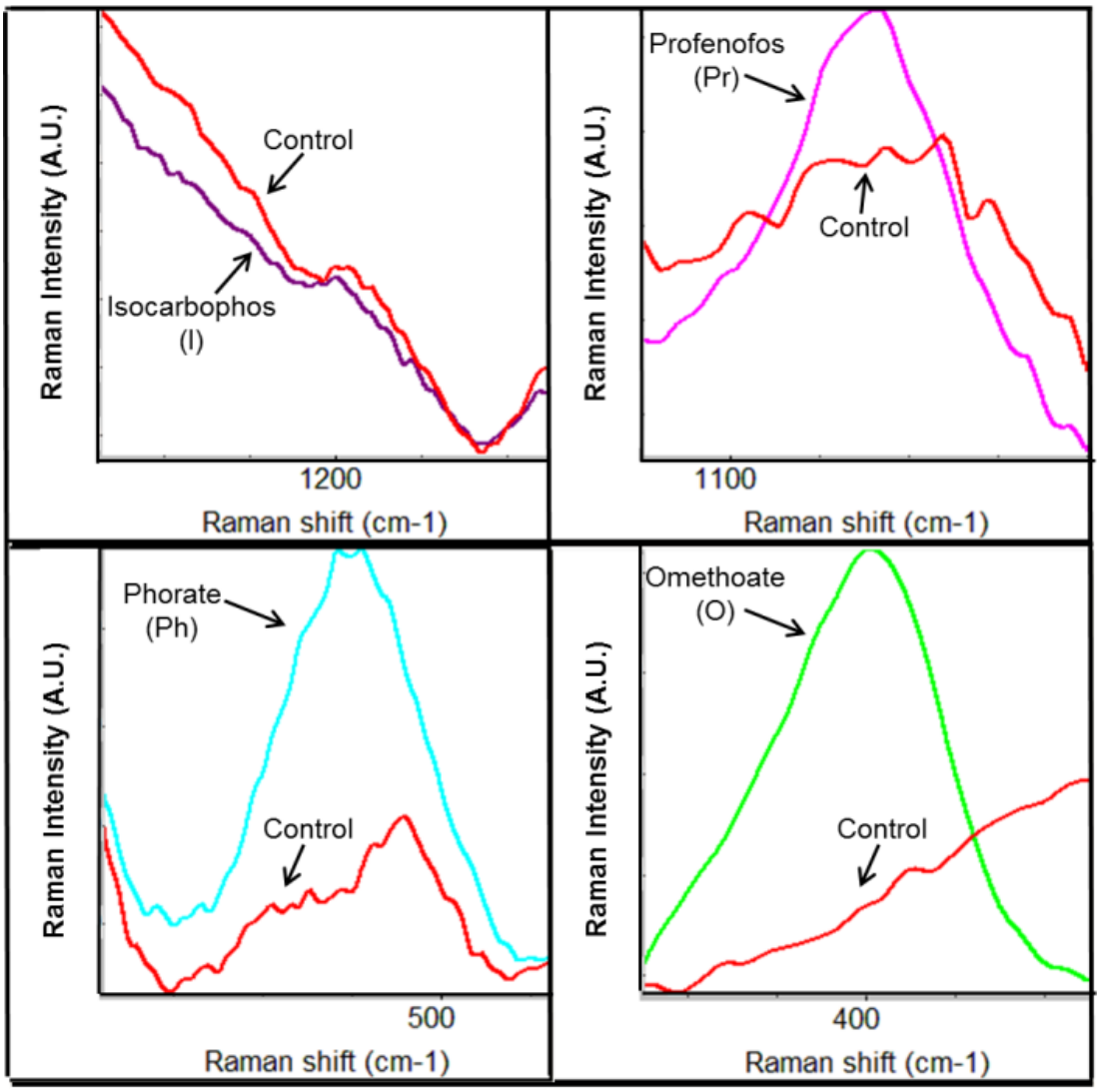

Fig. S4 Raw (real) Raman spectra of an isocarbophos capture peak and the control between 1270-1140 cm^{-1}; a profenofos capture peak and the control between 1110-1060 cm^{-1}; a phorate capture peak and the control between 600-470 cm^{-1}; an omethoate capture peak and the control between 425-375 cm^{-1}. The control was the modified Ag dendrites [Ag-(Ap+MH)]. The spiked concentration for the four pesticides was 0.5 mM. All samples were conducted in a capture buffer with a 20 min incubation period. The second derivative Raman spectra yielded similar trends.

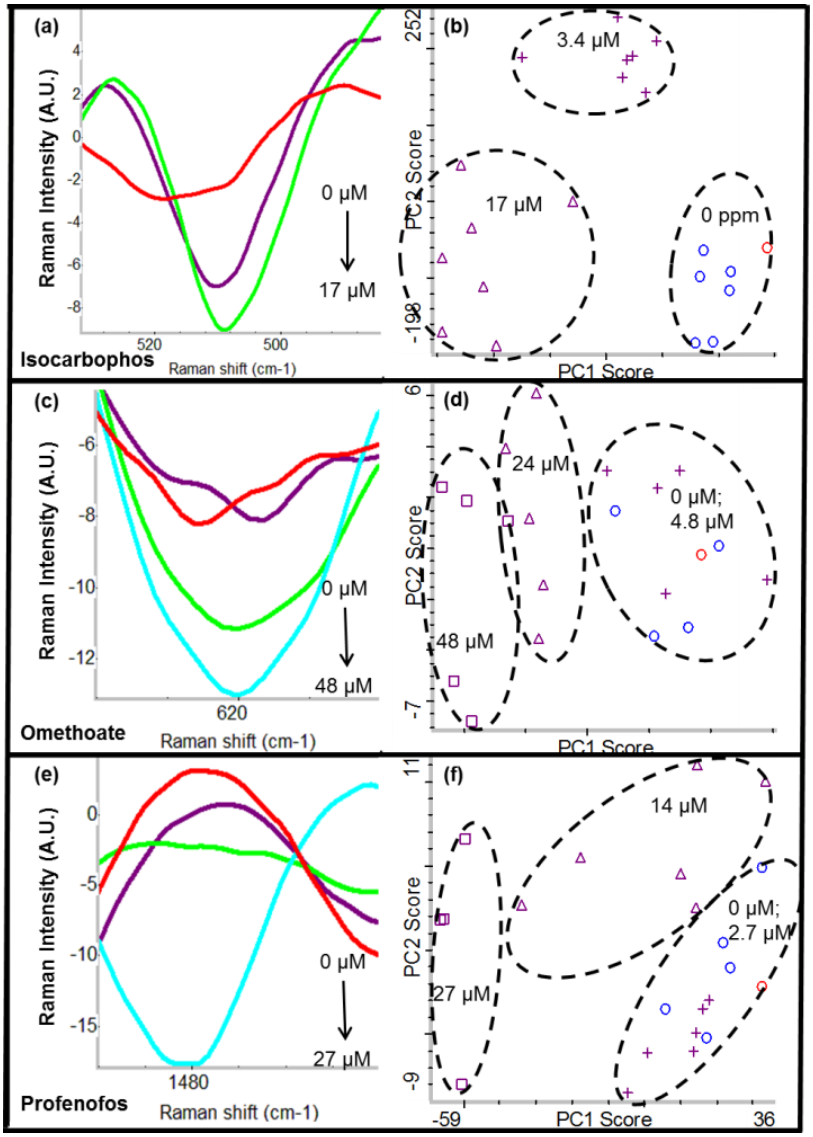

Fig. S5 (a) Second derivative Raman spectra and (b) PCA plot of isocarbophos between 530-480 cm^{-1} for 0 µM, 3.4 µM (1 ppm) and 17 µM (5 ppm); (c) Second derivative Raman spectra and (d) PCA plot of omethoate between 630-610 cm^{-1} for 0 µM, 4.8 µM (1 ppm), 24 µM (5 ppm) and 48 µM (10 ppm); (e) Second derivative Raman spectra and (f) PCA plot of profenofos between 1490-1460 cm^{-1} for 0 µM, 2.7 µM (1 ppm) , 14 µM (5ppm) and 27 µM (10 ppm). A gradual increase in Raman peak intensities was seen when the spiked pesticide was introduced at increasing concentrations. Significant difference against the control (0 µM) was seen at 3.4 µM (1 ppm) for isocarbophos, 24 µM (5 ppm) for omethoate, and 14 µM (5 ppm) for profenofos.

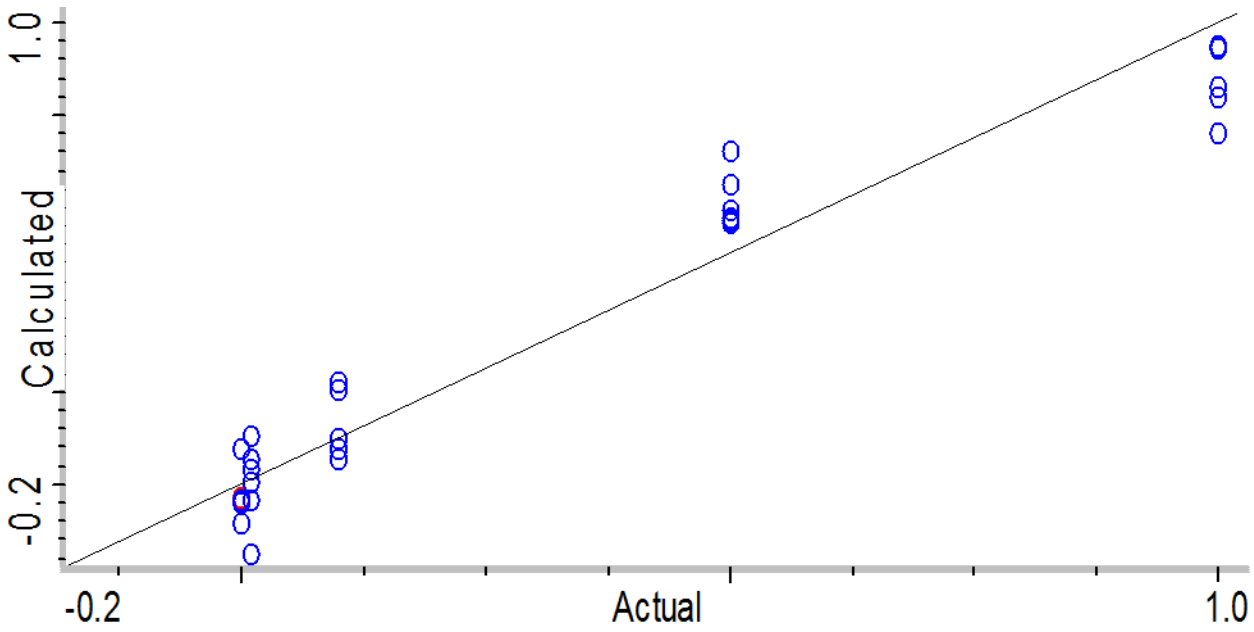

Fig. S6 Partial Least Square analysis (PLS) of phorate spiked at 0 µM, 0.04 µM (0.01 ppm), 0.4 µM (0.1 ppm), 2 µM (0.5 ppm), 4 µM (1 ppm). This result shows a linear relationship between the spectral peak intensities (i.e. calculated value) and the actual phorate concentration. Quantitative analysis of phorate was possible within this range. The root mean square error calibration (RMSEC) was 0.101 and the correlation coefficient was 0.9628.

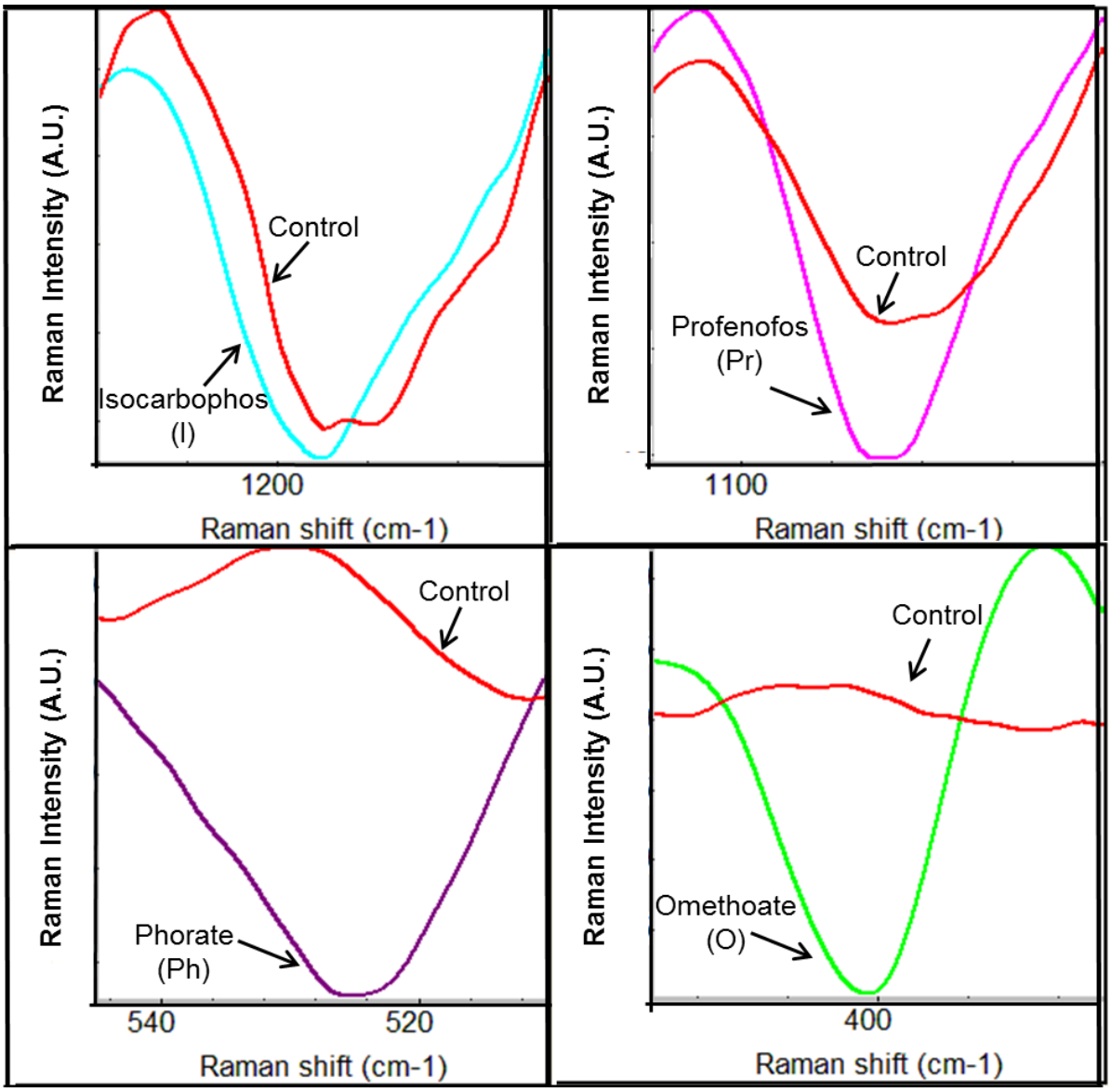

Fig. S7 Second derivative transformation of the Raman spectra of an isocarbophos capture peak and the control between 1220-1170 cm^{-1} in apple juice (diluted 1:10) (AJ); a profenofos capture peak and the control between 1110-1060 cm^{-1} in AJ; a phorate capture peak and the control between 545-510 cm^{-1} in AJ; an omethoate capture peak and the control between 425-375 cm^{-1} in AJ. The control was the modified Ag dendrites [Ag-(Ap+MH)]. The spiked concentration for the four pesticides was 0.5 mM. All samples were conducted in a capture buffer with a 20 min incubation period.