

## SUPPLEMENTARY INFORMATION: Quantitative Carbon Detector (QCD) for Enhanced Detection of Food, Pharmaceuticals, Cosmetics, Flavors, and Fuel

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**1.0 Analyte Preparation.** The supplementary information consists of the methods of preparation of each of the organic compounds analyzed by GC/FID and GC/QCD-FID.

**1.1 Molecule A with Polyarc<sup>TM</sup>: Glucose.** Glucose (10 mg) was silylated using 750 uL of TMSI and 750 uL of pyridine added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc<sup>TM</sup> integrated into the system. The injection size was 0.2 uL with a 0.5 uL syringe with a 10:1 split. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 65 °C for 2 minutes, the oven was ramped to 300 °C at 6 °C/min, and then held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc<sup>TM</sup>, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc<sup>TM</sup> were set to 35 mL/min and 2.5 mL/min respectively. The peak area for glucose was normalized using the pyridine peak for the calculations of the response factor. This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system.

**1.2 Molecule B with Polyarc<sup>TM</sup>: Xylose.** Xylose (15 mg) was silylated using 750 uL of TMSI and 750 uL of pyridine added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc<sup>TM</sup> integrated into the system. The injection size was 0.2 uL with a 0.5 uL syringe with a 10:1 split. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 65 °C for 2 minutes, the oven was ramped to 300 °C at 6 °C/min, and then held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc<sup>TM</sup>, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc<sup>TM</sup> were set to 35 mL/min and 2.5 mL/min respectively. The peak area for xylose was normalized using the pyridine peak for the calculations of the response factor. This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system.

**1.3 Molecule C with Polyarc™: Cellobiose.** Cellobiose (7 mg) was silylated using 750  $\mu$ L of TMSI and 750  $\mu$ L of pyridine added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.2  $\mu$ L with a 0.5  $\mu$ L syringe with a 10:1 split. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 65 °C for 2 minutes, the oven was ramped to 300 °C at 6 °C/min, and then held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for cellobiose was normalized using the pyridine peak for the calculations of the response factor. This was completed six times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system.

**1.4 Molecule D with Polyarc™: 2,5-Furandicarboxylic Acid (FDCA).** FDCA (10 mg) was silylated using 750  $\mu$ L of BSTFA & 1% TMCS, 750  $\mu$ L of pyridine, and 50  $\mu$ L of ethyl acetate added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02  $\mu$ L with a 0.5  $\mu$ L syringe with splitless mode. This was changed from a split ratio of 10:1 to splitless because there was a lower RF than expected. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 65 °C for 2 minutes, the oven was ramped to 300 °C at 6 °C/min, and then held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for FDCA was normalized using the ethyl acetate peak for the calculations of the response factor. This was completed five times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system. A sample of silylated FDCA was injected in a 7890A-5975C Agilent GC-MS, and was confirmed to be disubstituted with the trimethyl silicon groups. The range scanned for the MS using electrical ionization was 44.0 to 550.0.

**1.5 Molecule E with Polyarc™: Terephthalic Acid (TPA).** TPA (10 mg) was silylated using 750  $\mu$ L of BSTFA & 1% TMCS, 750  $\mu$ L of pyridine, and 50  $\mu$ L of ethyl acetate added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After four hours, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02  $\mu$ L with a 0.5  $\mu$ L syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 65 °C for 2 minutes, the oven was ramped to 300 °C at 6 °C/min, and then held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for TPA was normalized using the ethyl acetate peak for the calculations of the response factor.

This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system. A sample of silylated TPA was injected in a 7890A-5975C Agilent GC-MS, and was confirmed to be disubstituted with the trimethyl silicon groups. The range scanned for the MS using electrical ionization was 44.0 to 550.0.

**1.6 Molecule F with Polyarc™: Acetaminophen.** Acetaminophen (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, and 50 uL of ethyl acetate added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 65 °C for 2 minutes, the oven was ramped to 300 °C at 6 °C/min, and then held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for acetaminophen was normalized using the ethyl acetate peak for the calculations of the response factor. This was completed six times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system. A sample of silylated acetaminophen was injected in a 7890A-5975C Agilent GC-MS, and was confirmed to be both monosubstituted and disubstituted with the trimethyl silicon group. Acetaminophen was monosubstituted on only the hydroxyl group, while disubstituted on both the hydroxyl and amine functional groups. The disubstituted acetaminophen eluted earlier than the monosubstituted derivative. The range scanned for the MS using electrical ionization was 44.0 to 550.0.

**1.7 Molecule G with Polyarc™: Ibuprofen.** Ibuprofen (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for ibuprofen was normalized using the tetrahydrofuran peak for the calculations of the response factor. This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system. A sample of silylated ibuprofen was injected in a 7890A-5975C Agilent GC-MS, and was confirmed to be monosubstituted with the trimethyl silicon group. The range scanned for the MS using electrical ionization was 44.0 to 550.0.

**1.8 Molecule H with Polyarc™: Vanillin.** Vanillin (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, and 50 uL of ethyl acetate added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for vanillin was normalized using the ethyl acetate peak for the calculations of the response factor. This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system. A sample of silylated vanillin was injected in a 7890A-5975C Agilent GC-MS, and was confirmed to be monosubstituted with the trimethyl silicon group. The range scanned for the MS using electrical ionization was 44.0 to 550.0.

**1.9 Molecule I with Polyarc™: Cinnamic Acid.** Cinnamic acid (9 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for cinnamic acid was normalized using the heptane peak for the calculations of the response factor. This was repeated four times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system. A sample of silylated cinnamic acid was injected in a 7890A-5975C Agilent GC-MS, and was confirmed to be monosubstituted with the trimethyl silicon group. The range scanned for the MS using electrical ionization was 44.0 to 550.0.

**1.10 Molecule J with Polyarc™: Ascorbic Acid.** Ascorbic acid (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the

makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for ascorbic acid was normalized using the heptane peak for the calculations of the response factor. This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system. A sample of silylated ascorbic acid was injected in a GC-MS 7890A-5975C Agilent GC-MS, and was confirmed to be tetrasubstituted with the trimethyl silicon group. The range scanned for the MS using electrical ionization was 44.0 to 550.0.

**1.11 Molecule K with Polyarc™: Butylparaben.** Butylparaben (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for butylparaben was normalized using the heptane peak for the calculations of the response factor. This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system.

**1.12 Molecule L with Polyarc™: Nonylphenol.** Nonylphenol (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for nonylphenol was normalized using the heptane peak for the calculations of the response factor. This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system.

**1.13 Molecule M with Polyarc™: Dicamba.** Dicamba (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a

plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak area for dicamba was normalized using the heptane peak for the calculations of the response factor. This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system.

**1.14 Complex Mixture with Polyarc™: Molecules G, H, J, K, and M.** Vanillin (4 mg), ibuprofen (10 mg), dicamba (15 mg), butylparaben (45 mg), and ascorbic acid (80 mg) was silylated using 1200 uL of BSTFA & 1% TMCS, 300 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, and put into a water thermal bath at 60 °C for 90 minutes while being sonicated. After 90 minutes the mixture was injected into a 7890A Agilent GC-FID with a Polyarc™ integrated into the system. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 10 mL/min, the air flow was 400 mL/min, and the makeup gas (He) flow was 10 mL/min. For the Polyarc™, the temperature was held constant at 450 °C by setting the Thermal Auxiliary temperature to 293 °C. Flows of H<sub>2</sub> and air to the Polyarc™ were set to 35 mL/min and 2.5 mL/min respectively. The peak areas of the analytes were normalized using the heptane peak for the calculations of the response factor. This was completed three times. The flows of H<sub>2</sub> and air were checked after twelve hours of usage and reset to original flows if there was a change. Before and after each injection, a mixture with known concentrations of heptane, toluene, and isopropanol was tested to confirm there was no change in response factor from the introduction of silicon into the system.

**1.15 Molecule A with FID only: Glucose.** Glucose (10 mg) was silylated using 750 uL of TMSI, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for glucose was normalized using the pyridine peak for the calculations of the response factor. This was completed three times.

**1.16 Molecule B with FID only: Xylose.** Xylose (10 mg) was silylated using 750 uL of TMSI, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID.

The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for xylose was normalized using the pyridine peak for the calculations of the response factor. This was completed three times.

**1.17 Molecule C with FID only: Cellobiose.** Cellobiose (10 mg) was silylated using 750 uL of TMSI, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for cellobiose was normalized using the pyridine peak for the calculations of the response factor. This was completed three times.

**1.18 Molecule D with FID only: 2,5-Furandicarboxylic Acid (FDCA).** FDCA (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, and 50 uL of ethyl acetate added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for FDCA was normalized using the ethyl acetate peak for the calculations of the response factor. This was completed three times.

**1.19 Molecule F with FID only: Terephthalic Acid (TPA).** TPA (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, and 50 uL of ethyl acetate added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After four hours, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for TPA was normalized using the ethyl acetate peak for the calculations of the response factor. This was completed six times.

**1.20 Molecule F with FID only: Acetaminophen.** Acetaminophen (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, and 50 uL of ethyl acetate added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was

heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for acetaminophen was normalized using the ethyl acetate peak for the calculations of the response factor. This was completed three times.

**1.21 Molecule G with FID only: Ibuprofen.** Ibuprofen (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for ibuprofen was normalized using the THF peak for the calculations of the response factor. This was completed three times.

**1.22 Molecule H with FID only: Vanillin.** Vanillin (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, and 50 uL of ethyl acetate added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for vanillin was normalized using the ethyl acetate peak for the calculations of the response factor. This was completed three times.

**1.23 Molecule I with FID only: Cinnamic Acid.** Cinnamic acid (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for cinnamic acid was normalized using the heptane peak for the calculations of the response factor. This was completed three times.

**1.24 Molecule J with FID only: Ascorbic Acid.** Ascorbic acid (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless



mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for ascorbic acid was normalized using the heptane peak for the calculations of the response factor. This was completed three times.

**1.25 Molecule K with FID only: Butylparaben.** Butylparaben (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for butylparaben was normalized using the heptane peak for the calculations of the response factor. This was completed three times.

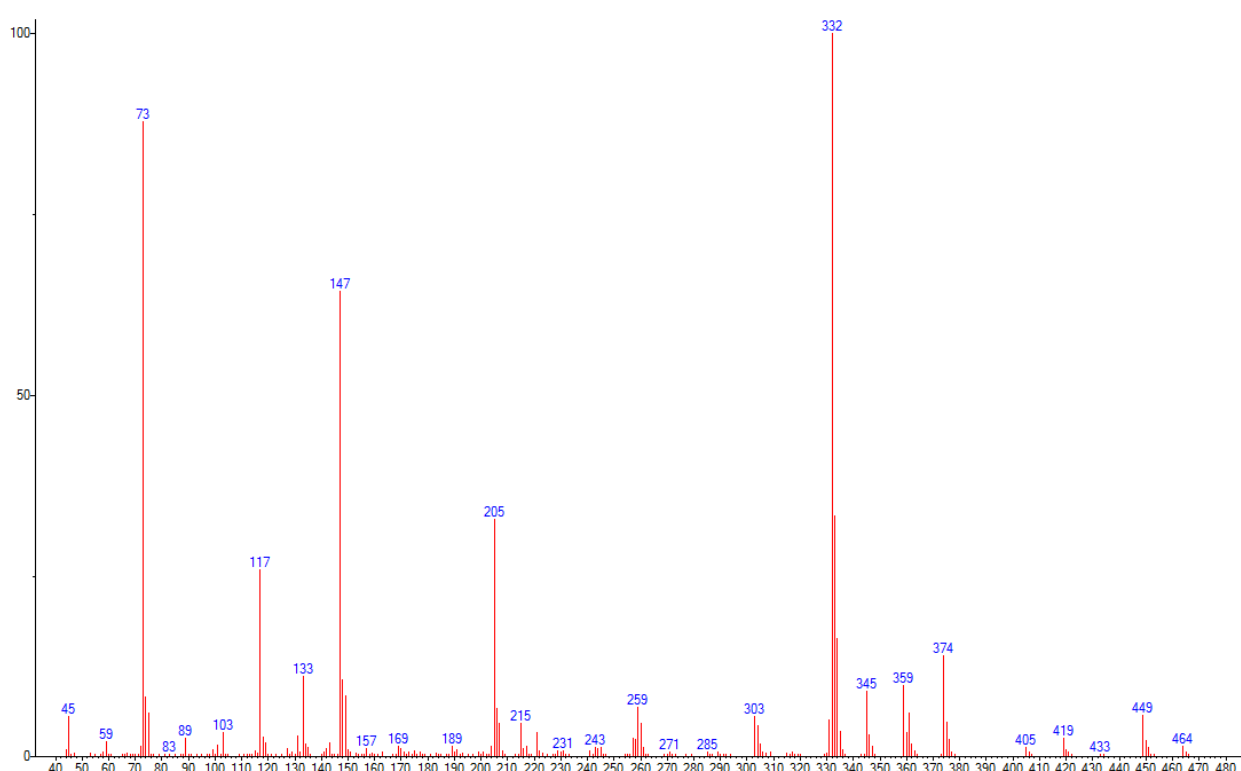
**1.26 Molecule L with FID only: Nonylphenol.** Nonylphenol (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for nonylphenol was normalized using the heptane peak for the calculations of the response factor. This was completed three times.

**1.27 Molecule M with FID only: Dicamba.** Dicamba (10 mg) was silylated using 750 uL of BSTFA & 1% TMCS, 750 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, placed into a plastic bag, and put into a water thermal bath at 60 °C for one hour. After an hour, the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak area for dicamba was normalized using the heptane peak for the calculations of the response factor. This was completed three times.

**1.28 Complex Mixture with FID only: Molecules G, H, J, K, and M.** Vanillin (3 mg), ibuprofen (10 mg), dicamba (15 mg), butylparaben (37 mg), and ascorbic acid (80 mg) was silylated using 1200 uL of BSTFA & 1% TMCS, 300 uL of pyridine, 200 uL of heptane, and 200 uL of tetrahydrofuran added into a 1.5 mL amber screw top vial. For each compound added to the mixture, the mass was taken and used for all calculations. The mixture was shaken for one minute, wrapped in plastic paraffin film, and put into a

water thermal bath at 60 °C for 90 minutes while being sonicated. After 90 minutes the mixture was injected into a 7890A Agilent GC-FID. The injection size was 0.02 uL with a 0.5 uL syringe with splitless mode. The inlet was heated to 280 °C with a septum purge flow of 3 mL/min. Column pressure was kept constant at 14 psi. Starting at 40 °C for 10 minutes, the oven was ramped to 60 °C at 2 °C/min, then 300 °C at 6 °C/min, held constant for 20 minutes. The FID heater was set to 300 °C, while the H<sub>2</sub> flow was 40 mL/min, the air flow was 200 mL/min, and the makeup gas (He) flow was 10 mL/min. The peak areas of the analytes were normalized using the heptane peak for the calculations of the response factor. This was completed three times.

**2.1 Mass Spectrum of Molecule J: Ascorbic Acid.** Shown below as an example is the mass spectrum of ascorbic acid, which was confirmed to be tetra-substituted with MS.



**Figure S1. EI MS spectrum of TMS-derivatized ascorbic acid.**