SUPPORTING INFORMATION

Rapid Screening of COVID-19 Disease Directly from Clinical Nasopharyngeal Swabs using the MasSpec Pen Technology

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Supporting Methods

Engineering the lab-built ESI housing and sprayer

The plastic outer cover of the Agilent APCI source was completely removed. Aluminum blocks and rubber gaskets were machined onto the back end Agilent APCI source to create a vacuum seal when interfaced to Thermo mass spectrometers with a Legacy interface, and a metal adapter was machined into the bottom of the aluminum block to connect a vacuum tube attached to an external rough pump (Edwards Vacuum). The corona needle was removed from the source, and the hole was plugged with a stopper to ensure a vacuum seal. Additionally, a ceramic block was engineered and interfaced to the outside of heater using RTV silicone, with the purpose of holding the lab-built ESI sprayer. The lab-built sprayer consists of a metal capillary (7 in, 0.62 in OD, 0.16 in ID, New England Small Tube Corporation) concentric with a ceramic tube (10 in, 0.125 in OD, 0.063 in ID, Omega Engineering, Inc.) through which N\textsubscript{2} gas flows acting as a sheath gas, a plastic union tee (0.25 in, Legris) to which a gas tube is attached, and two neoprene rubber stoppers each machined with a hole to fit the ceramic tube or metal capillary. A 1.5 m polytetrafluoroethylene (PTFE) tubing and silicone were used to connect the PDMS swab sampling port to the metal capillary of the lab-built sprayer.

Handling and storage of transport media and clinical nasal swabs

Various types of transport media from COVID-19 positive and negative clinical nasal samples were obtained from LabCorp and Clinical Pathology Laboratories (CPL). Information regarding the type of media was not provided. All media solution was heat inactivated for 65°C for 30 min prior to use. Following heat inactivation, Bligh and Dyer lipid extracts were performed on media from 35 COVID-19 positive and 35 COVID-19 negative samples.

HydraFlock polyester swabs sterilized by gamma irradiation (Puritan Medical Products) were shipped to Brazil. A permit to import samples from Brazil to UT Austin was received from the Brazilian Health Regulatory Agency (ANVISA) and the Center for Disease Control and Prevention (CDC). Prior to shipment, all swabs were heat-inactivated in Brazil at 65°C for 30 min and kept at -20°C until the shipment
in dry ice. Experiments were performed at the University of Texas at Austin under Biosafety Level 2 conditions. Swabs were handled by the principal investigator in the biosafety cabinet following biosafety protocols and requirements from the institutional biosafety committee.

**ESI of lipid extracts of various types of transport media**

Lipid extracts were performed on aliquots of 60 samples from CPL and 10 samples from LabCorp using the Bligh and Dyer method. Extracts were then directly infused into a QE HF mass spectrometer for ESI in the negative ion mode using a mass range of \( m/z \) 200-2000 and a voltage of 3.5 kV.

**Optimization of MasSpec Pen-ESI MS system for analysis of swabs**

Various swab tip materials were tested using the MasSpec Pen-ESI MS system, including nylon (Copan Diagnostics) and polyester flock (Puritan Medical Products) swabs. Each swab was dipped in a 13 µM standard solution of CL 72:4 and analyzed using the MasSpec Pen-ESI system in the negative ion mode, with the mass spectrum of polyester flock swabs containing minimal interfering ions in the lipid range compared to nylon flock swabs. The interfering ions presented polymer-like distribution and were identified as repeating units of ethylene oxide. Additionally, solvents including methanol, isopropylalcohol, ethanol:ethylacetate (1:1, v/v), CHCl₃:MeOH (1:1, v/v), and CHCl₃:MeOH (2:1, v/v) were tested for compatibility with the MasSpec Pen-ESI MS system.

To evaluate the robustness of the MasSpec Pen-ESI MS system for the detection of lipids from gamma-irradiated polyester flock swabs, swabs dipped in 100 µL of an equimolar (10 µM) lipid standard mixture of PE 36:2 (\( m/z \) 742.540) and PG 36:2 (\( m/z \) 773.539) were analyzed using CHCl₃:MeOH (1:1, v/v) as the solvent, yielding a relative standard deviation of 6.4% (n=10).

To evaluate the effect of heat inactivation of the biological material on the swabs, swabs dipped in a mixture of PG and PE lipid standards were heat-treated for 30 min at 65°C (n=5) to simulate heat-inactivation, while control swabs (n=5) dipped in the same lipid mixture standard were not heat-treated, followed by analysis using the MasSpec Pen-ESI system. To assess the effect of the ionization method on
the mass spectral profile, the MasSpec Pen with ESI (n=4) or solvent assisted inlet ionization (n=4) was employed to analyze a 20 ppm CL 72:4 lipid standard.

**MasSpec Pen-ESI MS analysis of clinical nasal swabs**

Extraction solvent, solvent volume, and swab type were optimized using the ion trap analyzer of an LTQ-Orbitrap XL, while the heat inactivation experiments, reproducibility experiments, and analysis of clinical swabs were performed using the orbitrap mass analyzer of a Q Exactive HF mass spectrometer. MasSpec Pen-ESI MS analysis of swabs was performed in the negative ion mode at a mass range of \( m/z \) 100-1500, resolving power of 120,000, and an inlet temperature of 300°C. A voltage of 3.3 kV was applied to the ESI sprayer, and the nitrogen sheath gas pressure was set to 20 psi. The pressure inside the ESI source was approximately 1.4-1.6 mbar for all analyses and experiments. Selected molecular ions were identified by tandem MS (MS\(^2\)) using higher-energy collisional dissociation (HCD) and high mass accuracy measurements (<5 ppm) acquired during MasSpec Pen-ESI MS analyses of swabs on the Q Exactive. Molecules subjected to MS\(^2\) were identified based on head group and fatty acid chain fragments. Double bond location and SN position were not determined in this study. For the analysis of swabs, chloroform:methanol (CHCl\(_3\):MeOH, 1:1, v/v) was used as the extraction solvent. A new sampling device and tubing and a clean sprayer were used for each analysis to avoid cross-contamination between each analysis.

**Statistical analysis**

The reproducibility of the MasSpec Pen-ESI system for swab analysis was quantified by calculating the relative standard deviation using the ratio of the intensities of lipid standards, \( m/z \) 773.534 (PG 36:2)/\( m/z \) 742.539 (PE 36:2) (n=10). To evaluate the effect of heat inactivation on the stability of lipids, a t-test was performed on the intensities of two lipid standards, \( m/z \) 742.639 and \( m/z \) 773.533, extracted from swabs without heat inactivation (n=5) and swabs heat-inactivated for 30 min at 65°C (n=5) using the MasSpec Pen-ESI system. Lastly, descriptive statistics were also computed for clinical and demographic variables. Categorical variables were expressed as count (percentage), whereas continuous variables were expressed
as median (25–75\textsuperscript{th} percentiles). The chi-square test was used to compare categorical variables proportions, and the Mann–Whitney U-test was used to evaluate continuous data.

\textbf{Supplementary Discussion}

\textbf{Case Studies}

Sample 108 was obtained from a 60-year-old female with preexisting conditions, including obesity and hypertension. She received a PCR negative diagnosis and was classified as positive by our method. Her symptoms included chest CT results suggestive of infection with GGO, consolidations, crazy-paving appearance, and pulmonary commitment (50%), as well as fever and low O\textsubscript{2} saturation levels (<95%). The patient was discharged from the hospital after nine days. Sample 242 was collected from a 28-year-old female who received a PCR negative diagnosis and was also classified by our method as negative for viral infection. The patient was hospitalized for three days with symptoms including coughing, sore throat, and dyspnea, whereas her chest CT results were not indicative of an infection.
**Figure S1.** Representative mass spectrum from the MasSpec Pen-ESI MS analysis of a nylon flock swab dipped in 20 ppm CL 72:4 (m/z 727.510) lipid standard. The doubly charged CL species are labeled in red while the repeating units of ethylene oxide are labeled in black.
Figure S2. Comparison of mass spectra obtained using the MasSpec Pen with ESI or solvent-assisted inlet ionization to analyze a 20 ppm CL 72:4 lipid standard. The top mass spectrum shows the profile obtained using ESI as the ionization mechanism and the bottom spectrum shows the data collected using a solvent-assisted inlet ionization. The singly and doubly charged CL species are labeled in red.
**Figure S3.** Comparison of mass spectra of swabs containing a 10 µM PG 36:2 (m/z 773.533) and PE 36:2 (m/z 742.539) lipid standard mixture with and without heat inactivation. The mass spectrum on top was obtained from the MasSpec Pen-ESI MS analysis of a swab without heat inactivation while the bottom shows the profile for a swab that had been heat-inactivated at 60°C for 30 min. Both insets are a zoom of m/z 720-800 range to show the detection of the lipid standards.
Figure S4. Mass spectrum from the negative ion mode ESI analysis of a lipid extracts of viral transport media of an unknown type. The inset shows a zoom in of the m/z 790-890 region, with lipid species detected labeled in red.
**Table S1.** Demographic and detailed clinical information, including clinical diagnosis, hospitalization, chest CT, and symptom information, for the 26 symptomatic negative patients in the withheld set of samples used in Classifier 1 and in the training set for Classifier 2.

| ID# | Gender | Age | RT-PCR Prediction (Classifier 1) | Hospitalization Days | ICU days | Mechanical Ventilation Days | Outcome |
|-----|--------|-----|---------------------------------|----------------------|----------|----------------------------|---------|
| 20  | M      | 76  | NEG                             | 4                    | 0        | 0                          | Discharged |
| 46  | M      | 58  | NEG                             | 6                    | 0        | 0                          | Discharged |
| 86  | F      | 49  | NEG                             | 7                    | 0        | 0                          | Discharged |
| 267 | F      | 52  | NEG                             | 10                   | 0        | 0                          | Discharged |
| 265 | M      | 84  | NEG                             | 3                    | 0        | 0                          | Discharged |
| 263 | M      | 71  | NEG                             | 3                    | 0        | 0                          | Discharged |
| 262 | M      | 81  | NEG                             | 4                    | 0        | 0                          | Discharged |
| 242 | M      | 68  | NEG                             | 3                    | 0        | 0                          | Discharged |
| 240 | M      | 57  | NEG                             | 6                    | 0        | 0                          | Discharged |
| 236 | M      | 28  | POS                             | 2                    | 0        | 0                          | Discharged |
| 233 | M      | 10  | POS                             | 6                    | 0        | 0                          | Discharged |
| 230 | M      | 7  | POS                             | 3                    | 0        | 0                          | Discharged |
| 229 | M      | 5  | POS                             | 2                    | 0        | 0                          | Discharged |
| 226 | M      | 1  | POS                             | 3                    | 0        | 0                          | Discharged |
| 219 | M      | 13  | POS                             | 3                    | 0        | 0                          | Discharged |
| 218 | M      | 7  | POS                             | 2                    | 0        | 0                          | Discharged |
| 217 | M      | 5  | POS                             | 2                    | 0        | 0                          | Discharged |
| 216 | M      | 1  | POS                             | 3                    | 0        | 0                          | Discharged |
| 214 | M      | 3  | POS                             | 1                    | 0        | 0                          | Discharged |
| 213 | M      | 5  | POS                             | 2                    | 0        | 0                          | Discharged |
| 212 | M      | 3  | POS                             | 1                    | 0        | 0                          | Discharged |

**Demographic and Detailed Clinical Information:**
- **S11**: Symptomatic Negative
- **Symptomatic Negative**: Symptomatic Negative
- **M**: Male
- **F**: Female
- **NEG**: Negative
- **POS**: Positive
- **Discharged**: Discharged
- **Death**: Death
| Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation | Symptomatology Negation |
|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| 0                      | 0                      | 0                      | 0                      | 0                      | 0                      | 0                      | 0                      | 0                      | 0                      | 0                      | 0                      | 0                      |
| 10                     | 10                     | 10                     | 10                     | 10                     | 10                     | 10                     | 10                     | 10                     | 10                     | 10                     | 10                     | 10                     |
| 20                     | 20                     | 20                     | 20                     | 20                     | 20                     | 20                     | 20                     | 20                     | 20                     | 20                     | 20                     | 20                     |
| 30                     | 30                     | 30                     | 30                     | 30                     | 30                     | 30                     | 30                     | 30                     | 30                     | 30                     | 30                     | 30                     |
| 40                     | 40                     | 40                     | 40                     | 40                     | 40                     | 40                     | 40                     | 40                     | 40                     | 40                     | 40                     | 40                     |
| 50                     | 50                     | 50                     | 50                     | 50                     | 50                     | 50                     | 50                     | 50                     | 50                     | 50                     | 50                     | 50                     |
| 60                     | 60                     | 60                     | 60                     | 60                     | 60                     | 60                     | 60                     | 60                     | 60                     | 60                     | 60                     | 60                     |
| 70                     | 70                     | 70                     | 70                     | 70                     | 70                     | 70                     | 70                     | 70                     | 70                     | 70                     | 70                     | 70                     |
| 80                     | 80                     | 80                     | 80                     | 80                     | 80                     | 80                     | 80                     | 80                     | 80                     | 80                     | 80                     | 80                     |
| 90                     | 90                     | 90                     | 90                     | 90                     | 90                     | 90                     | 90                     | 90                     | 90                     | 90                     | 90                     | 90                     |

| Chest CT Findings | Original Class | ID |
|-------------------|----------------|----|
|                   |                |    |
| ID  | Original Class | Fever | Cough | Myalgia | Shortness of Breath | Headache | Diagnoses | Loss of Smell/Taste | Oz Smell/Taste | COPD | Emphysema | Asthma | Ex-smoker | Presence of Other Information | % | Repaired Symptoms |
|-----|----------------|-------|-------|---------|---------------------|----------|-----------|---------------------|--------------|------|-----------|--------|-----------|-----------------------------|---|----------------|
| 27  | Symptomless Negative | NO    | NO    | NO      | YES                 | YES       | NO        | YES                 | YES           | YES  | NO        | NO     | NO        | YES                           |   |                 |
| 26  | Symptomless Negative | YES   | YES   | YES     | YES                 | YES       | YES       | YES                 | YES           | YES  | YES       | YES     | YES        | YES                           |   | YES              |
| 25  | Symptomless Negative | YES   | YES   | YES     | YES                 | YES       | YES       | YES                 | YES           | YES  | YES       | YES     | YES        | YES                           |   | YES              |
| 24  | Symptomless Negative | YES   | YES   | YES     | YES                 | YES       | YES       | YES                 | YES           | YES  | YES       | YES     | YES        | YES                           |   | YES              |
| 23  | Symptomless Negative | YES   | YES   | YES     | YES                 | YES       | YES       | YES                 | YES           | YES  | YES       | YES     | YES        | YES                           |   | YES              |
| 22  | Symptomless Negative | YES   | YES   | YES     | YES                 | YES       | YES       | YES                 | YES           | YES  | YES       | YES     | YES        | YES                           |   | YES              |
| 21  | Symptomless Negative | YES   | YES   | YES     | YES                 | YES       | YES       | YES                 | YES           | YES  | YES       | YES     | YES        | YES                           |   | YES              |
| 20  | Symptomless Negative | YES   | YES   | YES     | YES                 | YES       | YES       | YES                 | YES           | YES  | YES       | YES     | YES        | YES                           |   | YES              |
Table S2. Confusion matrices of the Lasso results for Classifiers 1 and 2.

| Classification Model | Sample Set | PCR Diagnosis | Model Prediction and Performance |
|----------------------|------------|---------------|---------------------------------|
|                      |            | Negative      | Positive                        | Sensitivity (%) | Specificity (%) | Accuracy (%) | NPV (%) | PPV (%) | FNR  | FPR  |
| Classifier 1:        | Training   | Negative      | 58                | 9                      | 7               | 76.7         | 86.6       | 83.5       | 89.2 | 71.9 | 23.3 | 13.4 |
| Asymptomatic         | Validation | Negative      | 29                | 5                      | 0               | 100.0        | 85.3       | 89.6       | 100.0| 73.7 | 0.0  | 14.7 |
| vs Symptomatic       | Withheld Data | Positive    | 17                | 9                      | -               | -            | -          | -          | -    | -    | -    | -    |
| Classifier 2:        | Training   | Negative      | 98                | 29                     | 8               | 81.8         | 77.2       | 78.4       | 92.5 | 65.4 | 18.2 | 22.8 |
| Asymptomatic +       |            | Positive      | 36                |                        |                |              |            |            |      |      |      |      |
| Symptomatic Negative vs Symptomatic Positive |
Table S3. Observed m/z, mass error, and identification for the features selected by Lasso for Classifier 1 and 2. Identifications are based on high mass accuracy and/or tandem MS measurements.

| Lasso Feature | Observed m/z | Theoretical m/z | Mass Error | Attribution | Formula                  |
|---------------|--------------|----------------|------------|-------------|--------------------------|
| 415.23        | 415.226      | 415.2255       | 1.204      | LPA O-18:4  | C21H37O6P [M-H]-         |
| 417.24        | 417.241      | 417.2412       | -0.479     | LPA O-18:3  | C21H39O6P [M-H]-         |
| 418.24        | 418.244      | 418.2445       | -1.195     | Isotope of LPA O-18:3, m/z 417.241 | C21H39O6P [M-H]- |
| 422           | 421.997      | -              | -          | Unidentified | -                        |
| 446.34        | 446.336      | -              | -          | Isotope of m/z 445.333, unidentified | -                        |
| 450.87        | 450.874      | -              | -          | Unidentified | -                        |
| 467.32        | 467.316      | 467.3143       | 3.638      | LPA O-20:0  |                          |
| 506.32        | 506.324      | 506.3252       | -2.370     | LPE 20:1    | C25H50NO7P [M-H]-        |
| 508.34        | 508.341      | 508.3409       | 0.197      | LPE 20:0    | C25H52NO7P [M-H]-        |
| 509.34        | 509.344      | 509.3442       | -0.393     | Isotope of LPE 20:0 | C25H52NO7P [M-H]- |
| 512.28        | 512.283      | 512.2864       | -          | Unidentified | -                        |
| 522.28        | 522.284      | 522.2838       | 0.383      | LPS 18:1    | C24H46NO9P [M-H]-        |
| 556.32        | 556.318      | 556.3176       | 0.719      | LPC 18:1    | C26H52NO7P               |
| 600.51        | 600.514      | 600.5128       | 1.998      | Cer 36:1    | C36H71NO3 [M+Cl]-        |
| 618.52        | 618.524      | 618.5234       | 0.970      | Cer 36:0    | C36H73NO4 [M+Cl]-        |
| 619.29        | 619.289      | 619.2889       | 0.161      | LPI 20:4    | C29H49O12P [M-H]-        |
| 624.52        | 624.522      | -              | -          | Unidentified | -                        |
| 629.49        | 629.492      | 629.4917       | 0.477      | DG 34:1     | C37H70O5 [M+Cl]-         |
| 635.48        | 635.482      | 635.4812       | 1.259      | DG O-36:5   | C39H68O4 [M+Cl]-         |
| 655.51        | 655.508      | 655.5074       | 0.915      | DG 36:2     | C39H72O5 [M+Cl]-         |
| 679.51        | 679.507      | 679.5074       | -0.589     | DG O-38:5   | C41H72O5 [M+Cl]-         |
| 680.58        | 680.576      | 680.5754       | 0.882      | Cer 42:3    | C42H79NO3 [M+Cl]-        |
| 682.59        | 682.591      | 682.5911       | -0.147     | Cer 42:2    | C42H81NO3 [M+Cl]-        |
| 683.59        | 683.594      | 683.5944       | -0.585     | Isotope of m/z 682.591, Cer 42:2 | C42H81NO3 [M+Cl]- |
| 684.59        | 684.588      | 684.5881       | -0.146     | Isotope of m/z 682.591, Cer 42:3 | C42H81NO4 [M+Cl]- |
| 694.59        | 694.592      | 694.5911       | 1.296      | Cer 43:3    | C43H81NO3 [M+Cl]-        |
| 697.61        | 697.61       | -              | -          | Unidentified | -                        |
| Mass  | Mass  | Mass  | Retention Time | Compound Description | Molecular Formula | Mass Accuracy [ppm] |
|-------|-------|-------|----------------|----------------------|-------------------|--------------------|
| 700.59| 700.587| 700.5886| -2.284 | Cer 44:5 | C44H79NO5 [M+Cl]- | -1583.60 |
| 703.51| 703.507| 703.5074| -0.569 | DG 40:6 | C43H72O5 [M+Cl]- | -1549.60 |
| 703.6 | 703.603| - | - | Unidentified | - | - |
| 710.62| 710.623| 710.6224| 0.844 | Cer 44:2 | C44H85NO3 [M+Cl]- | -1719.60 |
| 714.51| 714.508| 714.5079| 0.140 | PE 34:2 | C39H78NO9P [M-H]- | -1768.60 |
| 718.61| 718.613| - | - | Unidentified | - | - |
| 723.98| 723.981| 723.9805| 0.691 | Isotope of m/z 723.479, CL 72:8 | - | - |
| 725.53| 725.533| 725.5362| -4.411 | DG 42:7 | C45H74O7 [M-H]- | -1854.60 |
| 734.53| 734.534| 734.5342| -0.272 | PE 34:0 | C39H78NO9P [M-H]- | -1867.60 |
| 737.54| 737.537| 737.5370| 0.000 | SM 34:1 | - | - |
| 746.51| 746.513| 746.5130| 0.000 | PE O-38:7 | - | - |
| 750.53| 750.528| 750.5292| -1.599 | HexCer 34:1 | C49H77NO9 [M-H]- | -1977.60 |
| 754.55| 754.554| 754.5523| 2.253 | PC O-32:0 | C40H82NO7P [M+Cl]- | -2071.60 |
| 761.53| 761.534| 761.532| 2.626 | Isotope of m/z 760.529, PE O-39:7 | C44H76NO7P [M-H]- | -2165.60 |
| 769.54| 769.535| 769.5389| - | Unidentified | - | - |
| 770.57| 770.570| 770.5705| -0.649 | PE 38:2 | C43H82NO8P [M-H]- | -2257.60 |
| 771.57| 771.573| 771.574| -1.296 | Isotope of m/z 770.570, PE 38:2 | C43H82NO8P [M-H]- | -2290.60 |
| 773.53| 773.534| 773.5338| 0.259 | PG 36:2 | C42H79O10P [M+Cl]- | -2323.60 |
| 776.56| 776.559| 776.5600| -1.288 | PE O-40:6 | C45H80NO7P [M-H]- | -2397.60 |
| 794.51| 794.508| 794.5108| -3.524 | PE 36:2 | C41H78NO9P [M+Cl]- | -2555.60 |
| 794.53| 794.529| - | - | Unidentified | - | - |
| 808.5 | 808.504| 808.5054| -1.732 | PE O-40:8 | C45H76NO7P [M+Cl]- | -2617.60 |
| 845.61| 845.610| 845.611| -1.183 | Isotope of m/z 844.607, PS 40:1 | C46H88NO10P [M-H]- | -2727.60 |
| 847.53| 847.529| 847.5283| 0.826 | PA 48:12 | C51H77O8P [M-H]- | -2787.60 |
| 858.72| 858.723| - | - | Unidentified | - | - |
| 860.64| 860.638| 860.6388| -0.930 | HexCer 42:2 | C48H91NO9 [M+Cl]- | -2835.60 |
| 869.57| 869.569| 869.5662| 3.220 | Isotope of m/z 868.563, PC 40:6 | C48H84NO8P [M+Cl]- | -2895.60 |
| 872.64| 872.638| 872.6386| -0.688 | PS 42:1 | C48H92NO10P [M-H]- | -2955.60 |
| 880.52| 880.519| 880.5195| -0.568 | HexCer 32:3 | C44H79NO14 [M+Cl]- | -2995.60 |
| 910.55| 914.584| 914.5845| -0.547 | Isotope of m/z 913.585, PI 40:4 | C49H87O13P [M-H]- | -3095.60 |
| 976.62| 976.619| 976.6204| -1.434 | PE 50:9 | C55H92NO9P [M+Cl]- | -3195.60 |
