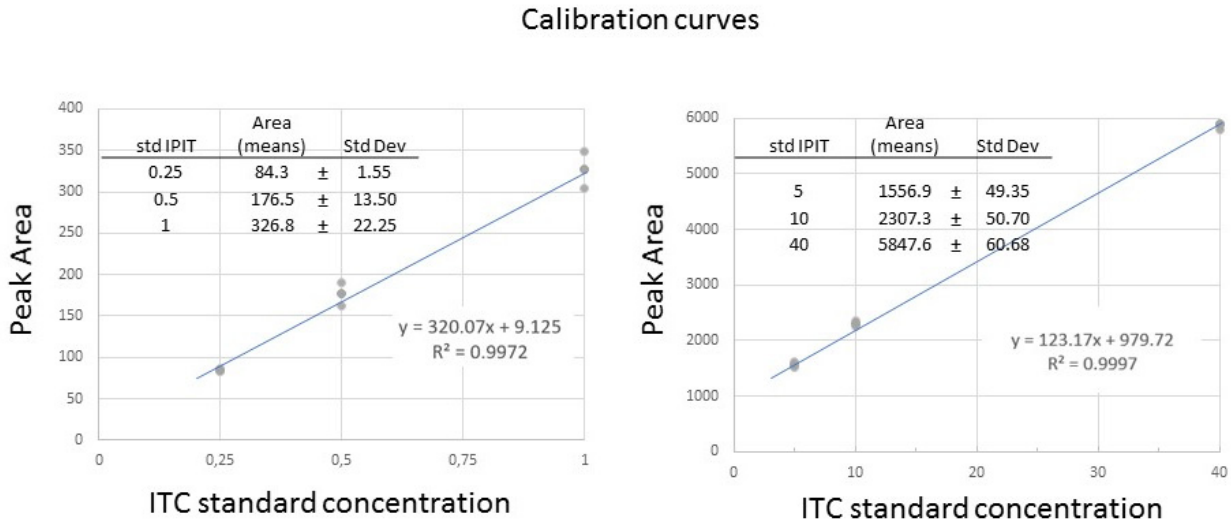
SUPPLEMENTARY MATERIAL

Figure S1. Calibration curves for ITCS. (**a**) concentration range: 0.25-1 ppm; (**b**) concentration range: 5-40 ppm.



(a) (b)

Figure S2: operative conditions for GCMS

```
Oven
Equilibration Time                          0.25 min
Oven Program                                On
    40 °C for 2 min
    then 15 °C/min to 90 °C for 0 min
    then 15 °C/min to 170 °C for 0 min
    then 15 °C/min to 240 °C for 4 min
Run Time                                    19.333 min


No Injectors


Front SS Inlet He
Mode                                        Split
Heater                                      On    200 °C
Pressure                                    On    7.7626 psi
Total Flow                                  On    9 mL/min
Septum Purge Flow                           On    3 mL/min
Gas Saver                                   On    15 mL/min After 6 min
Split Ratio                                 5 :1
Split Flow                                  5 mL/min


Thermal Aux 2 {MSD Transfer Line}
Heater                                      Off
Temperature Program                         Off
    230 °C for 0 min
Run Time                                    19.333 min
Column #1
DB-5: 1479.69599
DB-5
325 °C: 30 m x 250 µm x 0.25 µm
In: Front SS Inlet He
Out: Vacuum

(Initial)                                   40 °C
Pressure                                    7.7626 psi
Flow                                        1 mL/min
Average Velocity                            35.143 cm/sec
Holdup Time                                 1.4227 min
Flow Program                                On
    1 mL/min for 0 min
Run Time                                    19.333 min
```

Figura

Figura 2.5: Condizioni gascromatografiche impiegate

```
Solvent Delay           : 0.50 min

EMV Mode                : Relative
Relative Voltage        : 0
Resulting EM Voltage    : 1812

[Scan Parameters]

Low Mass                : 40.0
High Mass               : 300.0
Threshold               : 150
Sample #                : 2       A/D Samples    4

[MSZones]

MS Source               : 250 C   maximum 250 C
MS Quad                 : 150 C   maximum 200 C
```

Figura 2.6: Parametri di acquisizione ms

Figure S3: Operative conditions for autosampling

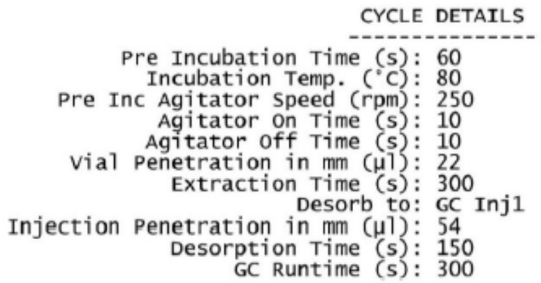


Figura 2.7: Impostazioni di microestrazione utilizzate per i campioni infusi

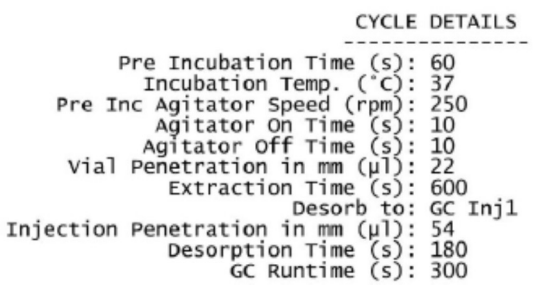


Figura 2.8: Impostazioni di microestrazione utilizzate per i campioni non infusi

Figure S4: Spectrum of IPITC

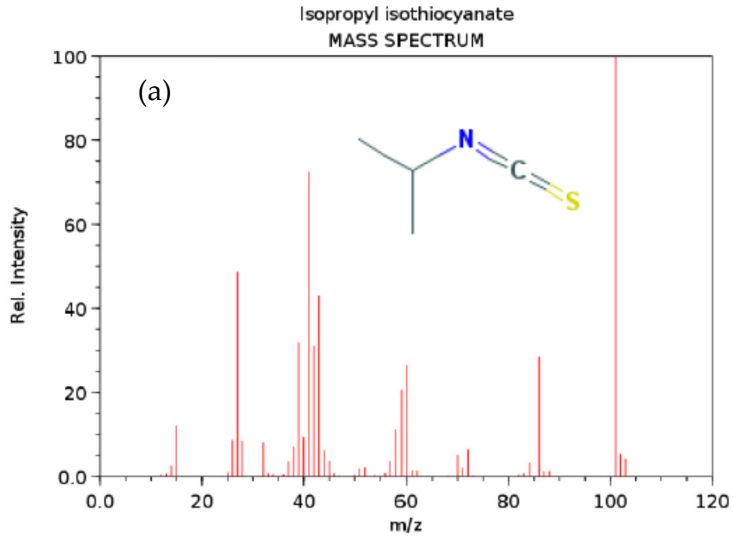
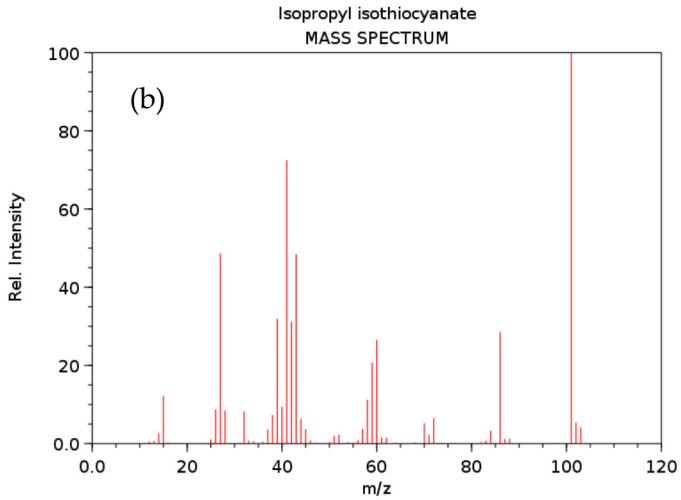
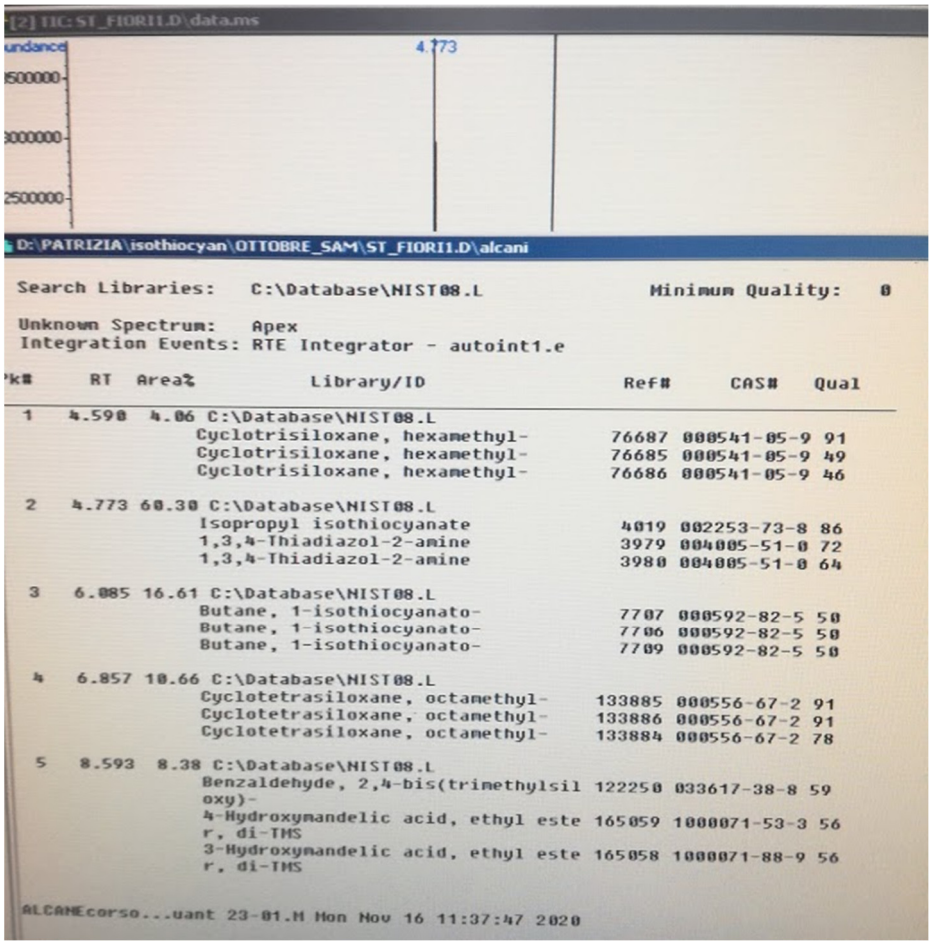


Figura 3.6: Spettro di massa di Isopropil-Isotiocianato

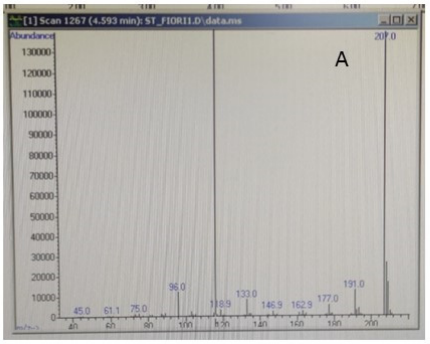


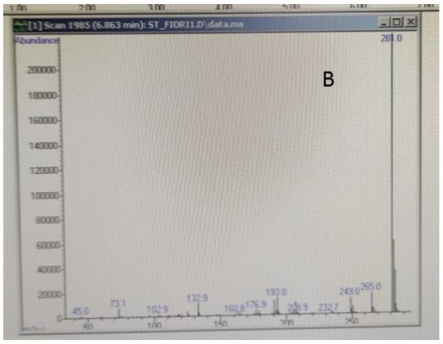
Comparison, Mass spectrum of iPITC (a) from NIST (b)

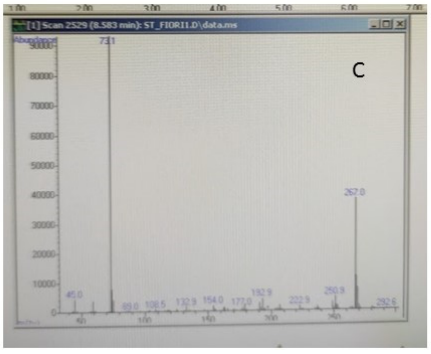
Figure S5: Identification (a) and spectra (b) of unknown peaks



(a)







GCMS spectra of peaks at 4.59, 6.86 and 8.58 min of TIC shown in **Figure 2** correspond to some impurity (silyl derivatives compounds)

(b)

Table S1: additional data to Table 1

sample	**Total ITCs (μg/g)**
S1/1	0.002 ± 0.00018
S1/2	0.804 ± 0.07
S1/3	0.126 ± 0.01
S1/4	0.140 ± 0.09
S1/5	0.150 ± 0.01

Data are the means of 3 replicates ± SD