Supplementary Material (ESI) for Analyst

Transmission-Mode Direct Analysis in Real Time and Desorption Electrospray Ionization Mass Spectrometry of Insecticide-Treated Bednets for Malaria Control

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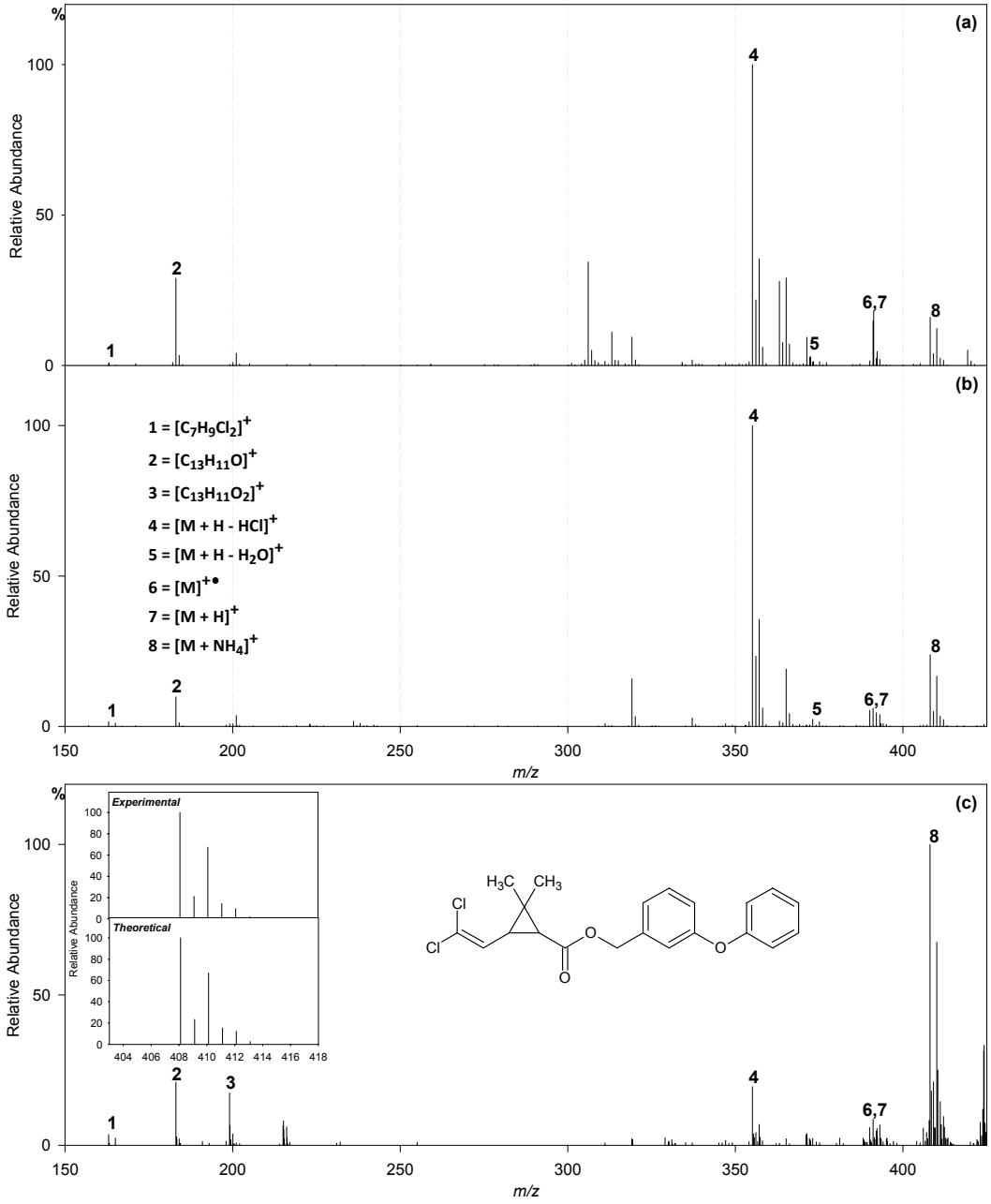

Fig. S1 He-induced DART-TOF MS spectra of a neat permethrin standard obtained at (a) 225°C and (b) 150°C with 1.5 L min^{-1} gas flow rate. Significant fragmentation was observed when He was used as the ionizing gas, increasing only slightly with increasing temperature. The N_2-induced (225°C, 7.0 L min^{-1}) mass spectrum (c) resulted in an abundant $[M+NH_4]^+$ ion but also considerable fragmentation compared to that of deltamethrin (see Fig. 2). Insets in panel (c) show the chemical and isotopic (experi-mental and theoretical) structures of the permethrin pesticide. The inset showing the isotopic distribution corresponds to the $[M+NH_4]^+$ ion of the nitrogen-induced spectra. Spectral peak assignments and mass accuracies are listed in Table S-1.

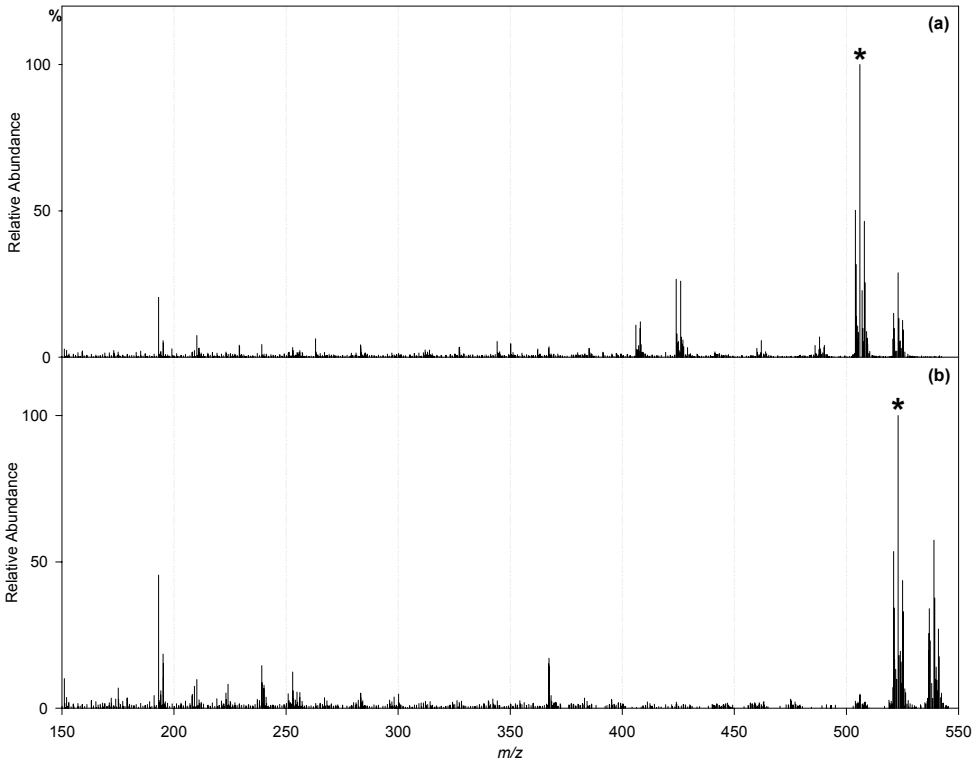

Fig. S2 He- and N_2-induced TM-DART spectra of a 55 mg m^{-2} deltamethrin-impregnated PermaNet® 2.0 net. (a) Helium spectrum obtained at 150°C and 2 L min^{-1}; (b) N_2 spectrum obtained at 150°C and 7 L min^{-1}. Asterisks indicate the $[M+H]^+$ and $[M+NH_4]^+$ for the He and N_2 spectra, respectively.

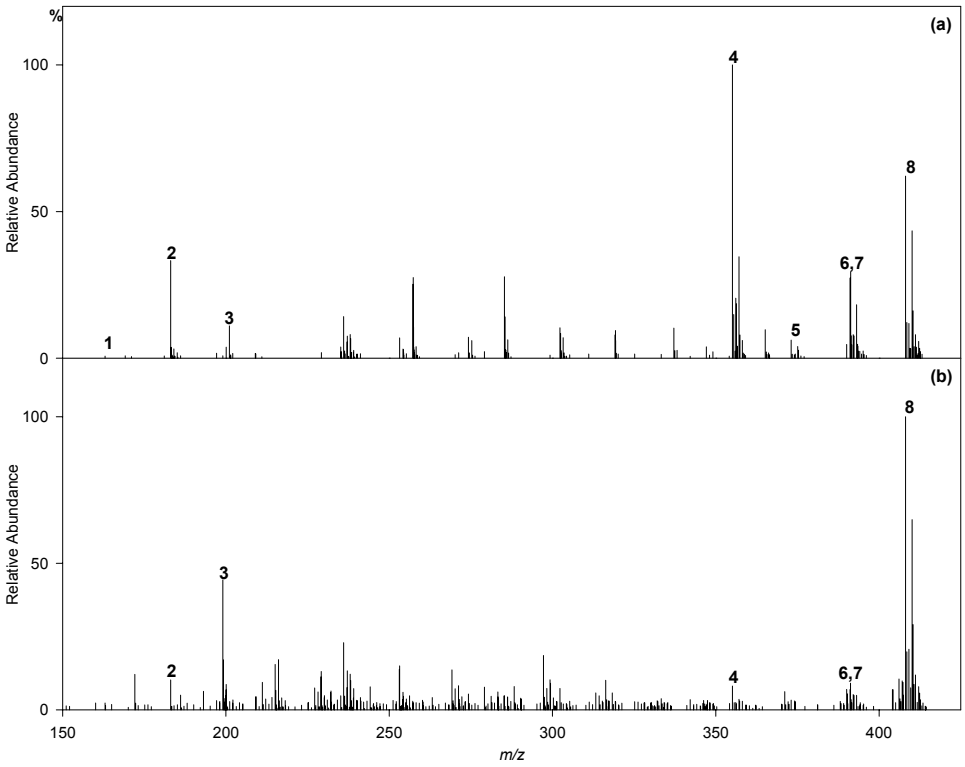

Fig. S3 He- and N_2-induced TM-DART spectra of a 1000 mg m^{-2} permethrin-impregnated Olyset® net. (a) He spectrum obtained at 150 °C and 2 L min^{-1}; (b) N_2 spectrum obtained at 150 °C and 7 L min^{-1}. Spectral peak assignments are consistent with those identified in Figure S-1 and listed in Table S-1.

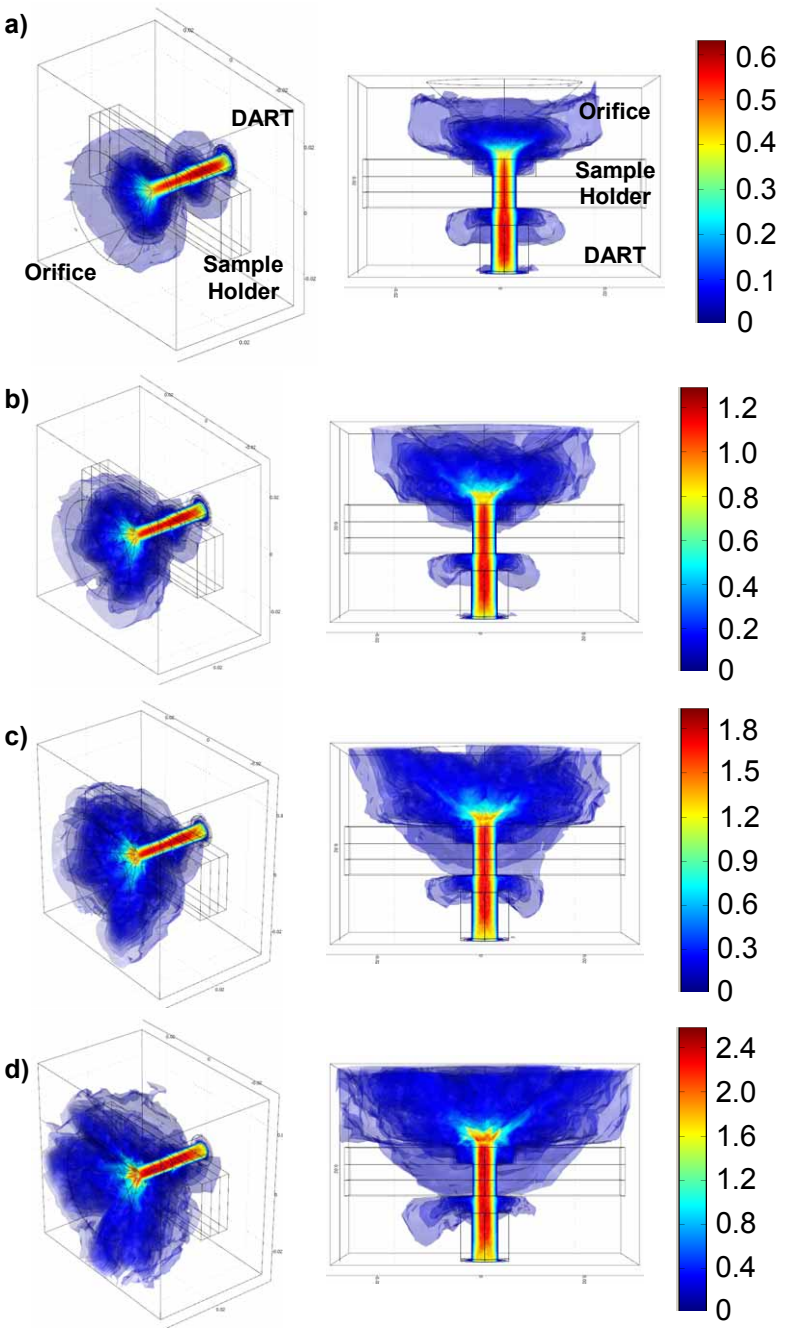

Fig. S4 CFD simulations at a) 0.5, b) 1.0, c) 1.5 and d) 2.0 L min^{-1} He at 150 ºC when the DART gas nozzle is positioned 4 mm away from the sample holder. The images on the left show a 3D perspective of the system, the middle images show the gas flow from above, and the heat map scales on the right are the gas velocities in m s^{-1}.

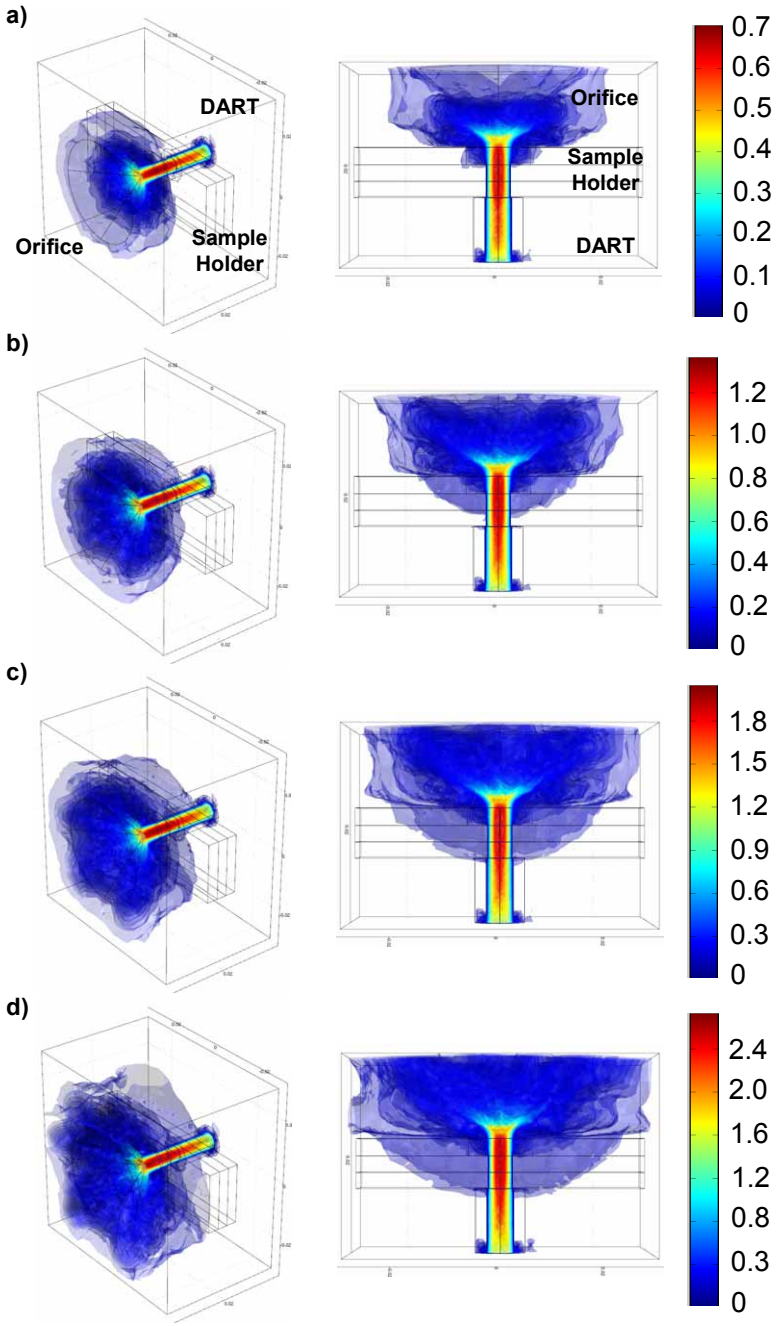

Fig. S5 CFD simulations at a) 0.5, b) 1.0, c) 1.5 and d) 2.0 L min^{-1} He at 150 ºC when the DART gas nozzle is positioned in contact with sample holder. The images on the left show a 3D perspective of the system, the middle images show the gas flow from above, and the heat map scales on the right are the gas velocities in m s^{-1}.

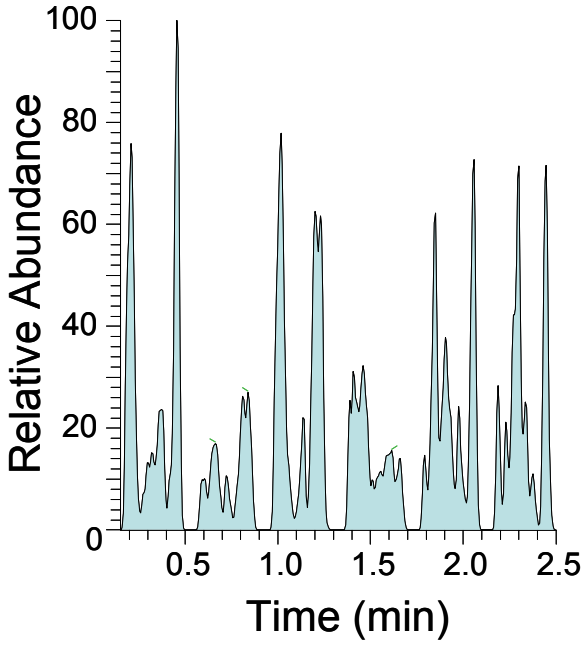

Fig. S-6 TM-DESI MS analysis of a sample composed of three offset layers of a conventionally-treated bednet coated with 16 mg m^{-2} of deltamethrin. Responses for individual strands that were observed in the single-layer sample are no longer observed; however, the greater sample density results in increased response relative to a single-layer sample.

Table S1 Identified peaks in the DART-TOF MS spectra of the permethrin standard

Peak	Formula	Theoretical Mass	Experimental Mass	Δm (mmu)
1	$[C_7H_9Cl_2]^+$	163.0076	163.0131	5.5
		165.0046	165.0107	6.1
		167.0017	167.0020	0.3
2	$[C_{13}H_{11}O]^+$	183.0804	183.0809	0.4
3	$[C_{13}H_{11}O_2]^+$	199.0754	199.0761	0.8
4	$[M+H-HCl]^+$	355.1095	355.1097	0.2
		357.1066	357.1080	1.4
5	$[M+H-H_2O]^+$	373.0757	373.0798	4.1
		375.0727	375.0845	11.8
		377.0698	377.0828	13.0
6	$[M+H]^+$	391.0862	391.0865	0.3
		393.0833	393.0855	2.3
		395.0803	395.0911	10.8
7	$[M]^{+\bullet}$	390.0784	390.0842	5.8
		392.0755	392.0866	11.1
		394.0725	394.0872	14.7
8	$[M+NH_4]^+$	408.1128	408.1126	0.1
		410.1098	410.1107	0.9
		412.1069	412.1149	8.1