Supplementary Information

Rapid *in-situ* analysis of tobacco chemical composition via ultrasonic nebulization extraction coupled with atmospheric pressure photoionization mass spectrometry

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Figure S1. The HCD MS/MS spectra of nicotine from tobacco in positive ion mode.

Figure S2. The HCD MS/MS spectra of nornicotine from tobacco in positive ion mode.

Figure S3. The HCD MS/MS spectra of cotinine from tobacco in positive ion mode.

Figure S4. The HCD MS/MS spectra of proline from tobacco in positive ion mode.

Figure S5. The HCD MS/MS spectra of malic acid from tobacco in negative ion mode.

Figure S6. The HCD MS/MS spectra of salicylic acid from tobacco in negative ion mode.

Figure S7. The HCD MS/MS spectra of esculetin from tobacco in negative ion mode.

Figure S8. The HCD MS/MS spectra of quinic acid from tobacco in negative ion mode.

Figure S9. The HCD MS/MS spectra of nicotyrine from tobacco in positive ion mode.

Figure S10. The HCD MS/MS spectra of nicotine N-oxide from tobacco in positive ion mode.

Table S1. Precursor and product ions of ten tobacco constituents in MS/MS analysis.

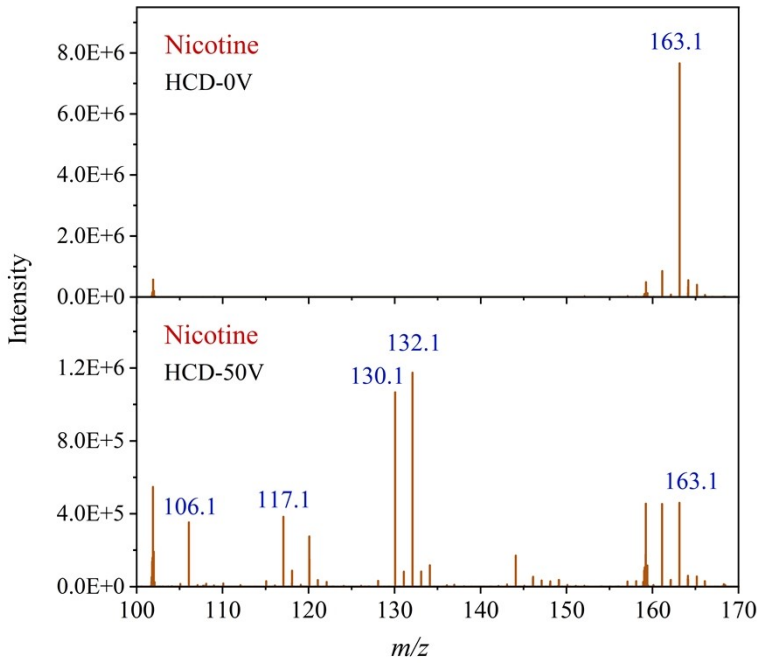

Figure S1. The HCD MS/MS spectra of nicotine from tobacco in positive ion mode.

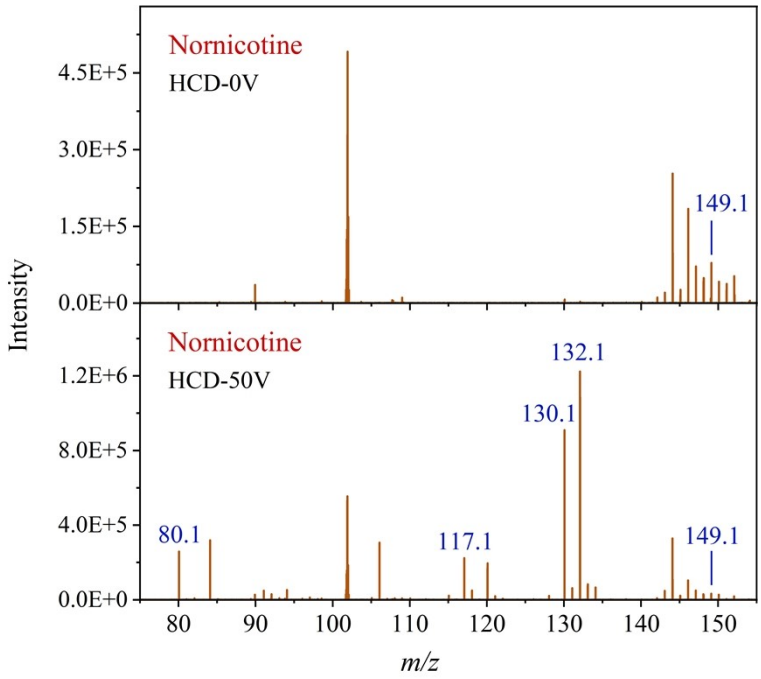

Figure S2. The HCD MS/MS spectra of nornicotine from tobacco in positive ion mode.

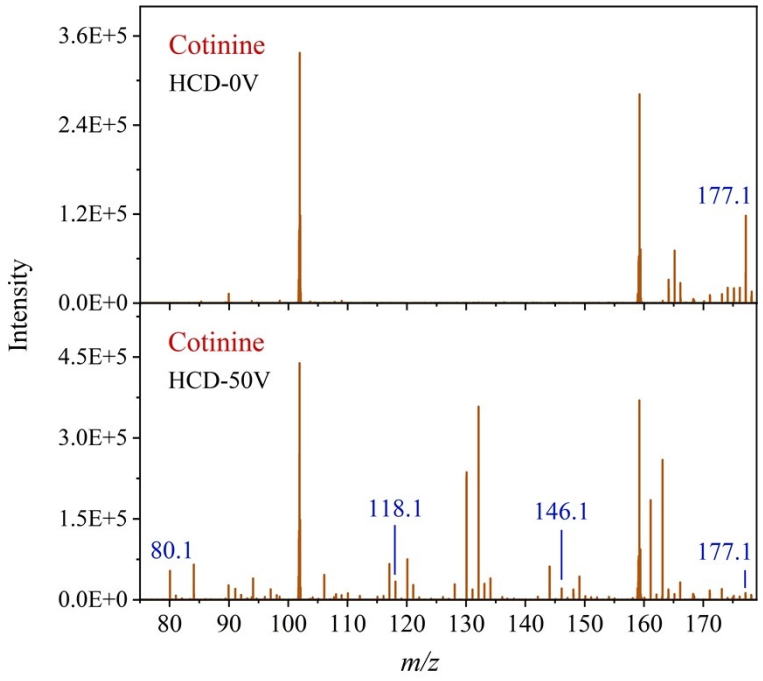

Figure S3. The HCD MS/MS spectra of cotinine from tobacco in positive ion mode.

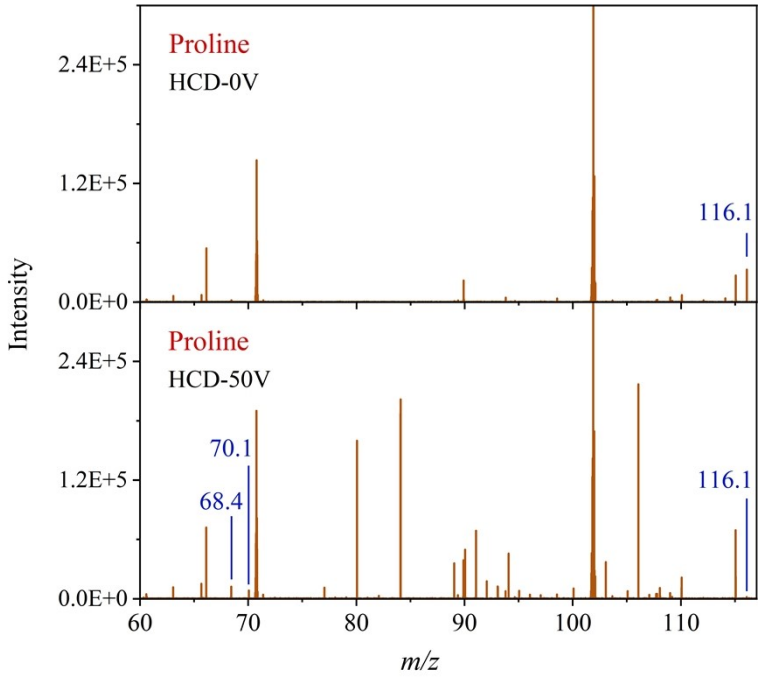

Figure S4. The HCD MS/MS spectra of proline from tobacco in positive ion mode.

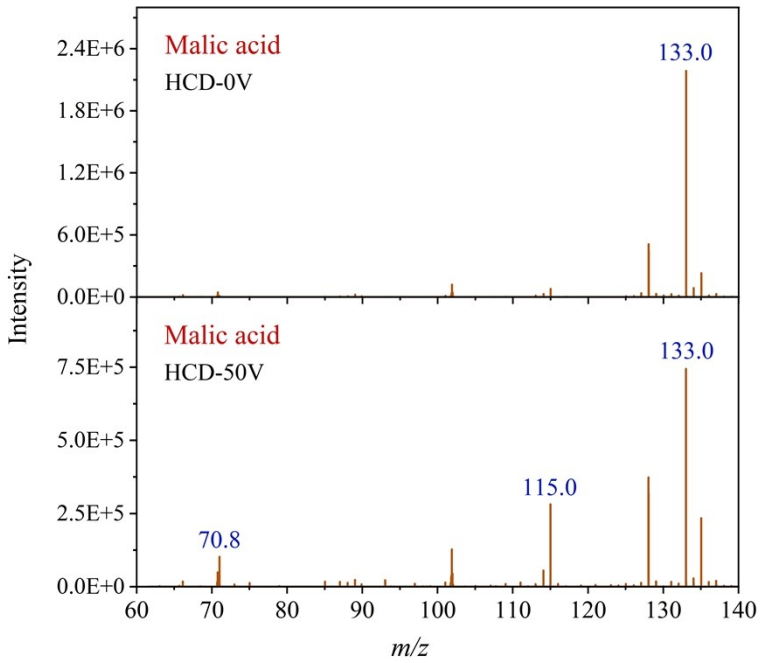

Figure S5. The HCD MS/MS spectra of malic acid from tobacco in negative ion mode.

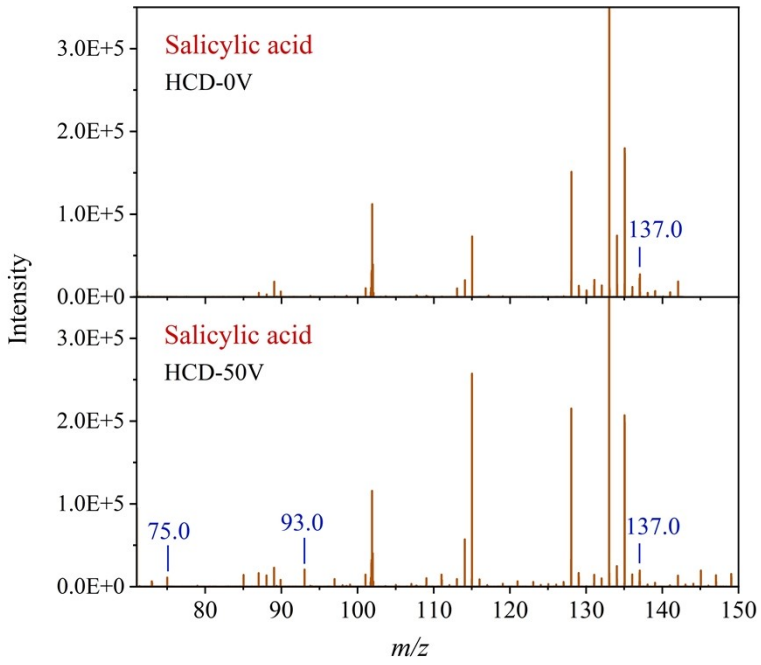

Figure S6. The HCD MS/MS spectra of salicylic acid from tobacco in negative ion mode.

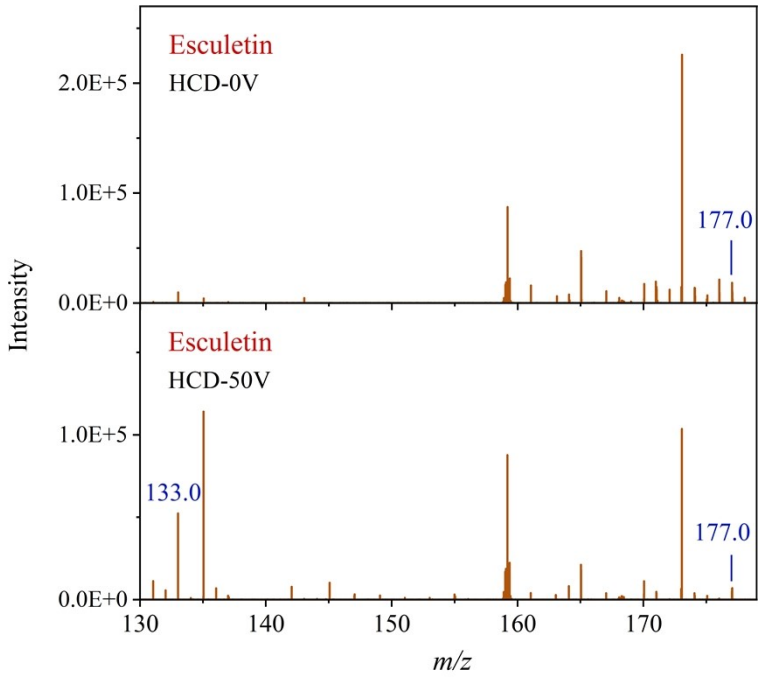

Figure S7. The HCD MS/MS spectra of esculetin from tobacco in negative ion mode.

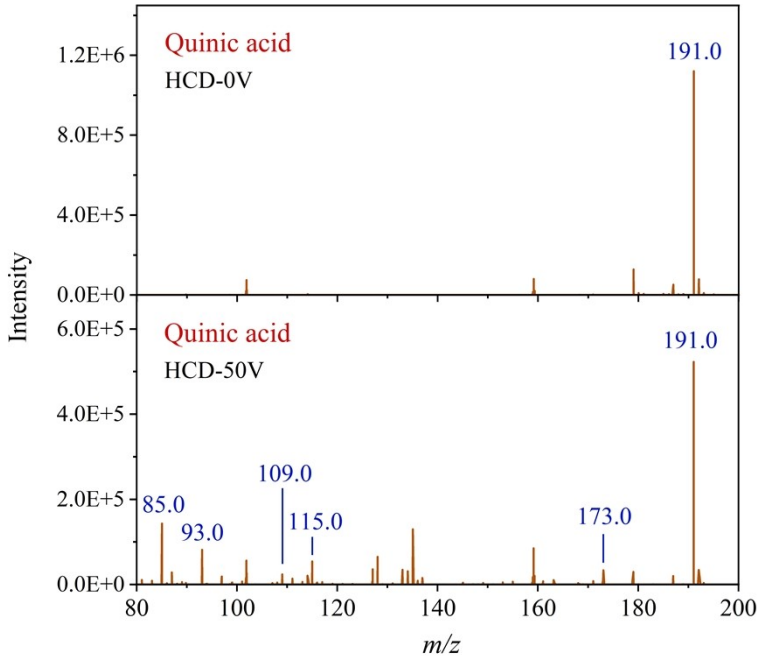

Figure S8. The HCD MS/MS spectra of quinic acid from tobacco in negative ion mode.

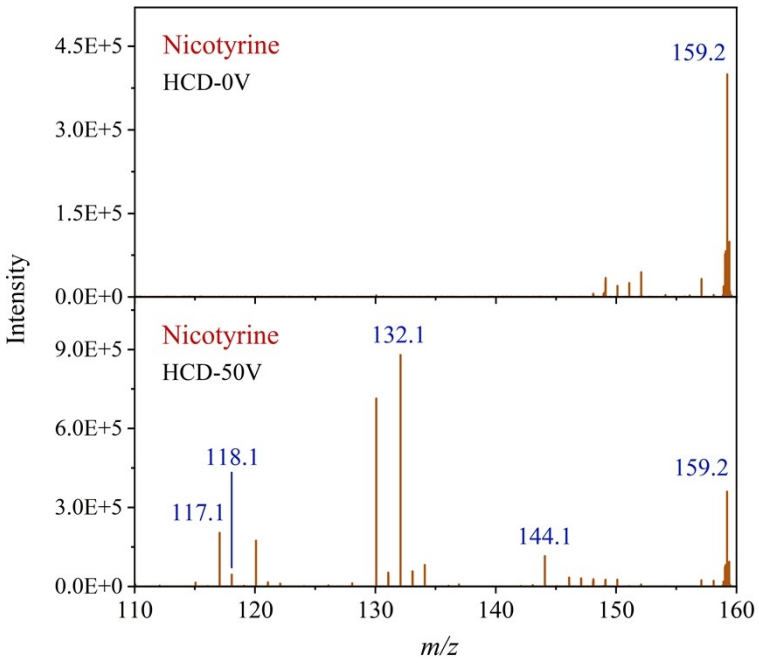

Figure S9. The HCD MS/MS spectra of nicotyrine from tobacco in positive ion mode.

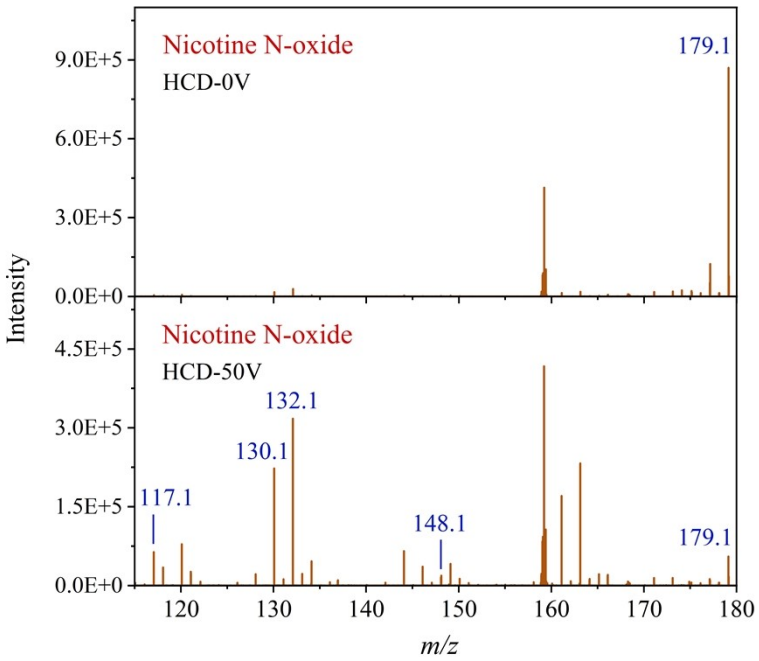

Figure S10. The HCD MS/MS spectra of nicotine N-oxide from tobacco in positive ion mode.

Table S1. Precursor and product ions of ten tobacco constituents in MS/MS analysis.

Components	Precursor ions (*m/z*)	Product ions (*m/z*)	References
Nicotine	163.1	132.1	1-3
		130.1	1, 4
		117.1	1, 5
		106.1	3
Nornicotine	149.1	132.1	3
		130.1	6, 7
		117.1	7
		80.1	2, 4, 6, 7
Cotinine	177.1	146.1	1, 3
		118.1	7
		80.0	1-7
Proline	116.1	70.1	8, 9
		68.4	8
Malic acid	133.0	115.0	10, 11
		70.8	10, 11
Salicylic acid	137.0	93.0	12-15
		75.0	16
Esculetin	177.0	133.0	17, 18
Quinic acid	191.1	173.0	19
		115.0	20
		109.0	19
		93.0	21
		85.0	19, 21, 22
Nicotyrine	159.2	144.1	3, 7, 23
		132.1	3, 7
		118.1	3
		117.1	23
Nicotine N-oxide	179.1	148.1	3, 7
		132.1	2-4, 6, 7
		130.1	6, 7
		117.1	2

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