Electronic Supplementary Information

An improved algorithm for resolving overlapping peaks in ion mobility spectrometry and its application to the separation of glycan isomers

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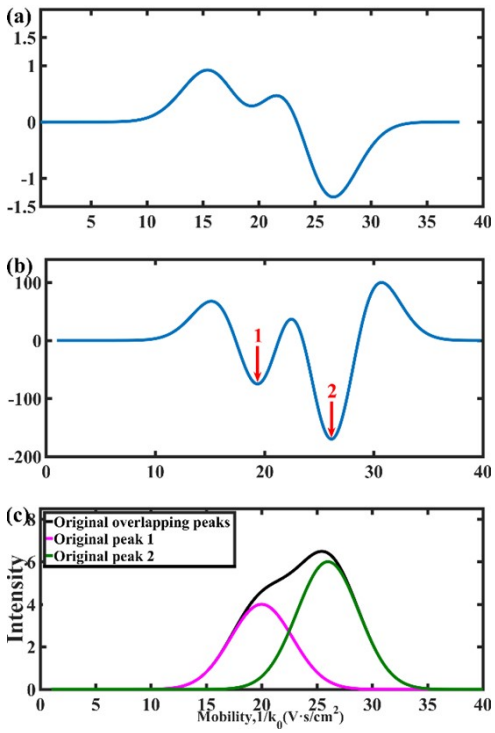


Fig.S1 The first-order differentiation (a) and the second-order differentiation (b) of the simulated overlapping peaks containing two types of components. (c) Overlapping peak an its single peak composition.

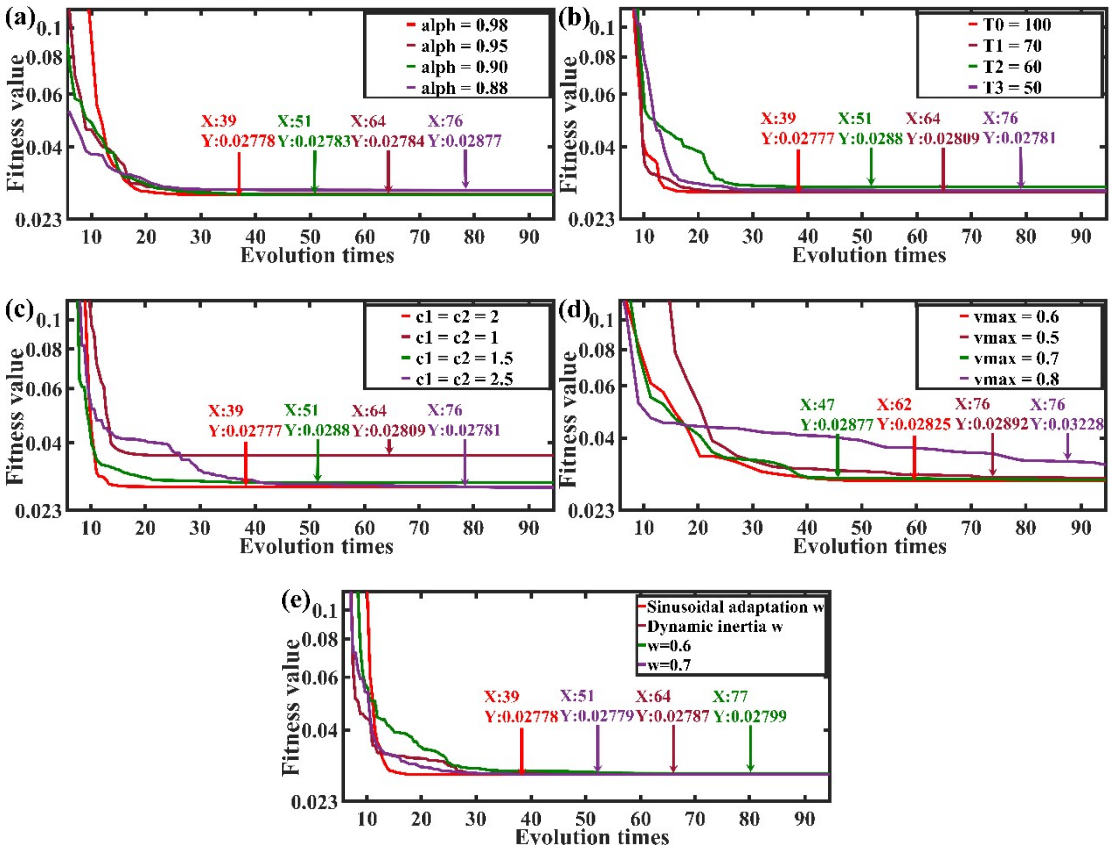


Fig.S2 The effect of different parameters (a).alph, (b).T, (c).c1 and c2, (d).Vmax and (e).w on the DWSA-PSO algorithm.

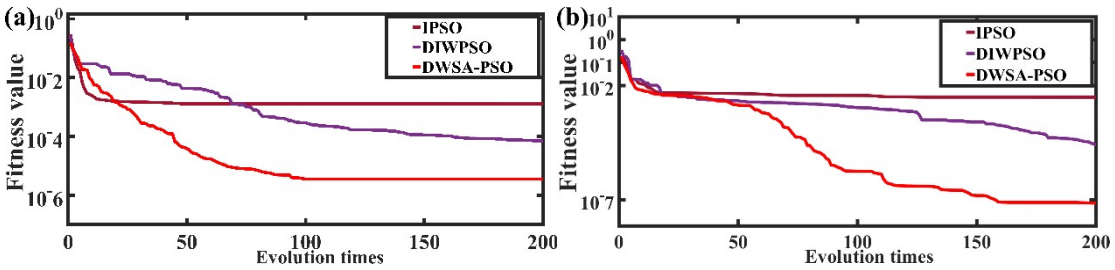


Fig.S3 The variation of fitness value with the number of evolution iterations when analyzing two types of overlapping peaks using three different methods.

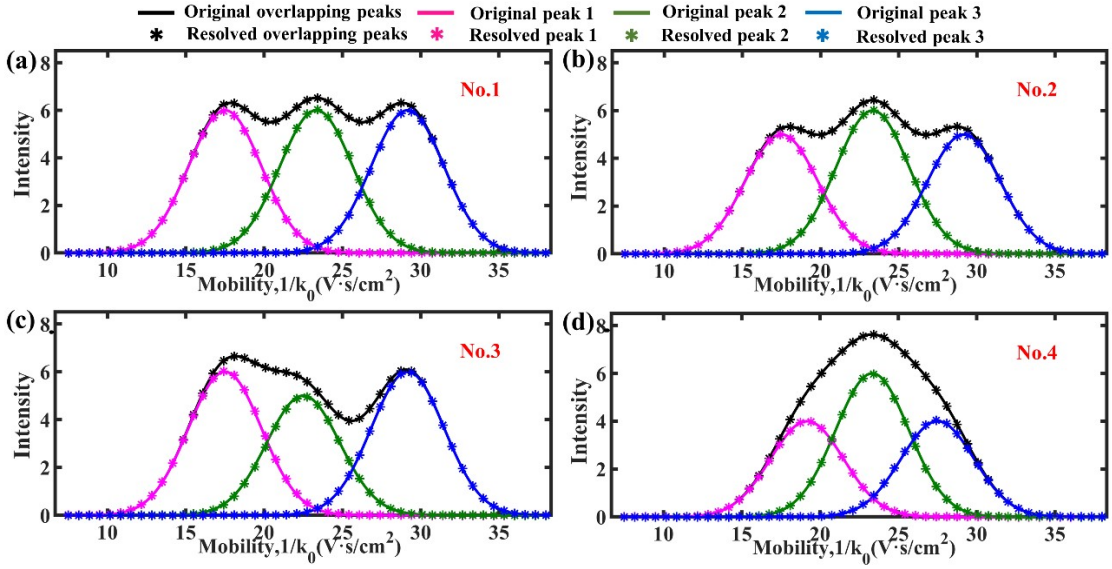
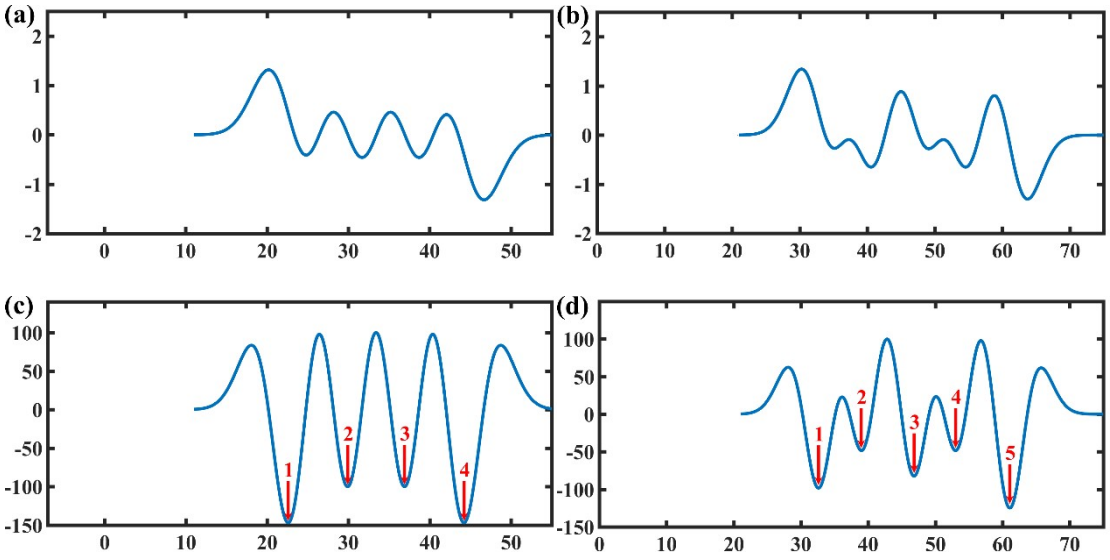


Fig.S4 Separation results of four types of simulated overlapping peaks with different degrees of overlap by using the DWSA-PSO method



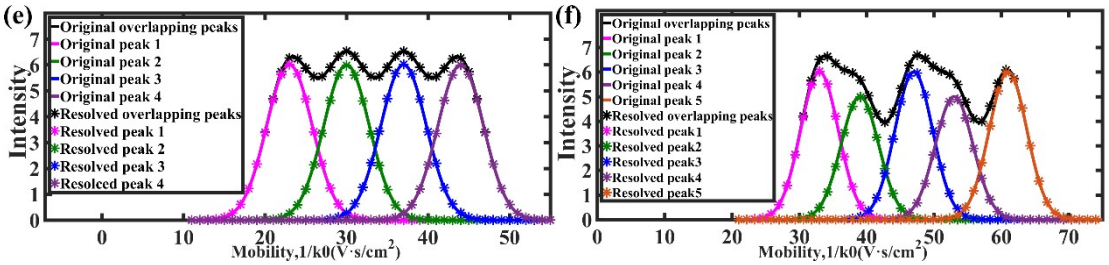


Fig.S5 Separation results of four- and five-component overlapping peaks by using DWSA-PSO: (a-b) The first-order differentiation; (c-d) The second-order differentiation; (e-f) Overlapping peak resolution contours.

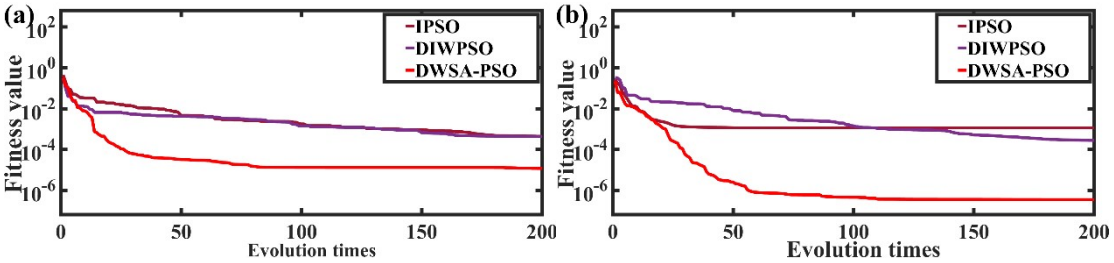


Fig.S6 The variation of fitness value with the number of evolution iterations graph obtained from the analysis of overlapping peaks of four-components (a) and five-components (b) using three different methods.

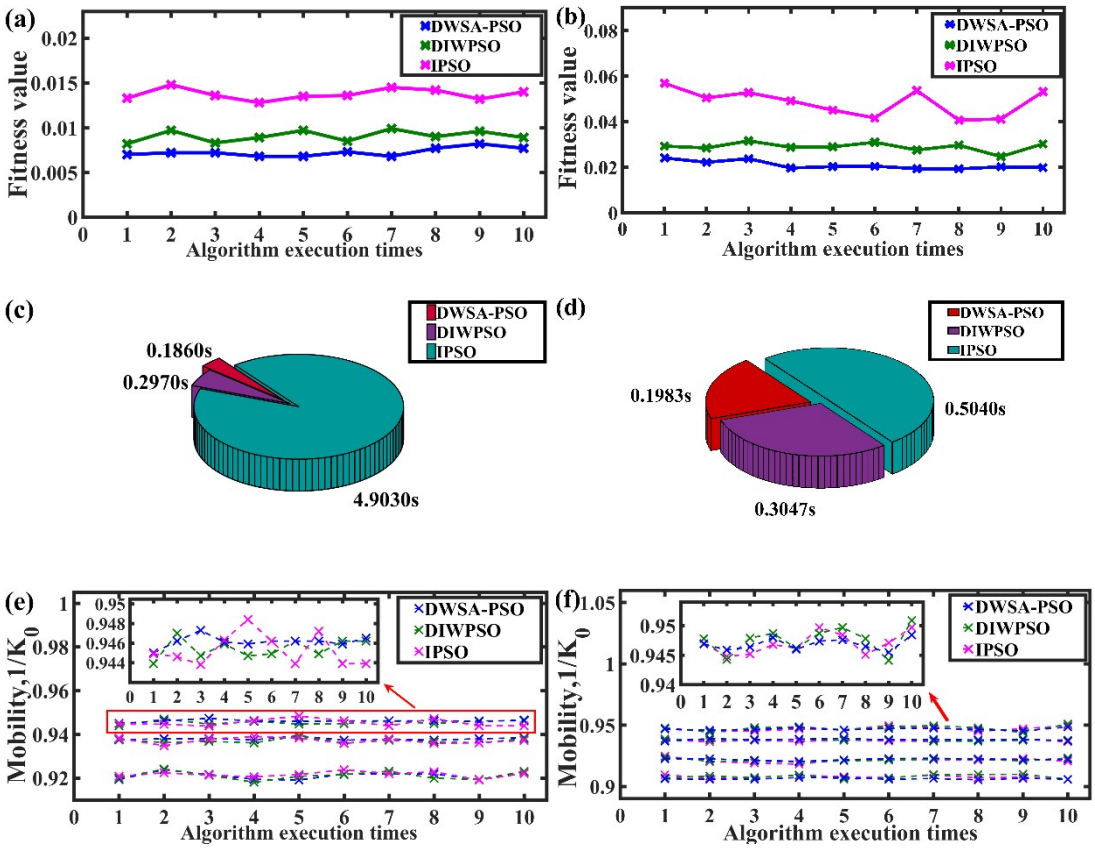


Fig.S7 Parameter values obtained by analyzing overlapping peaks containing three- and four- components 10 times using three methods (a-b) Fitness value; (c-d) Average time; (e-f) Mobility.

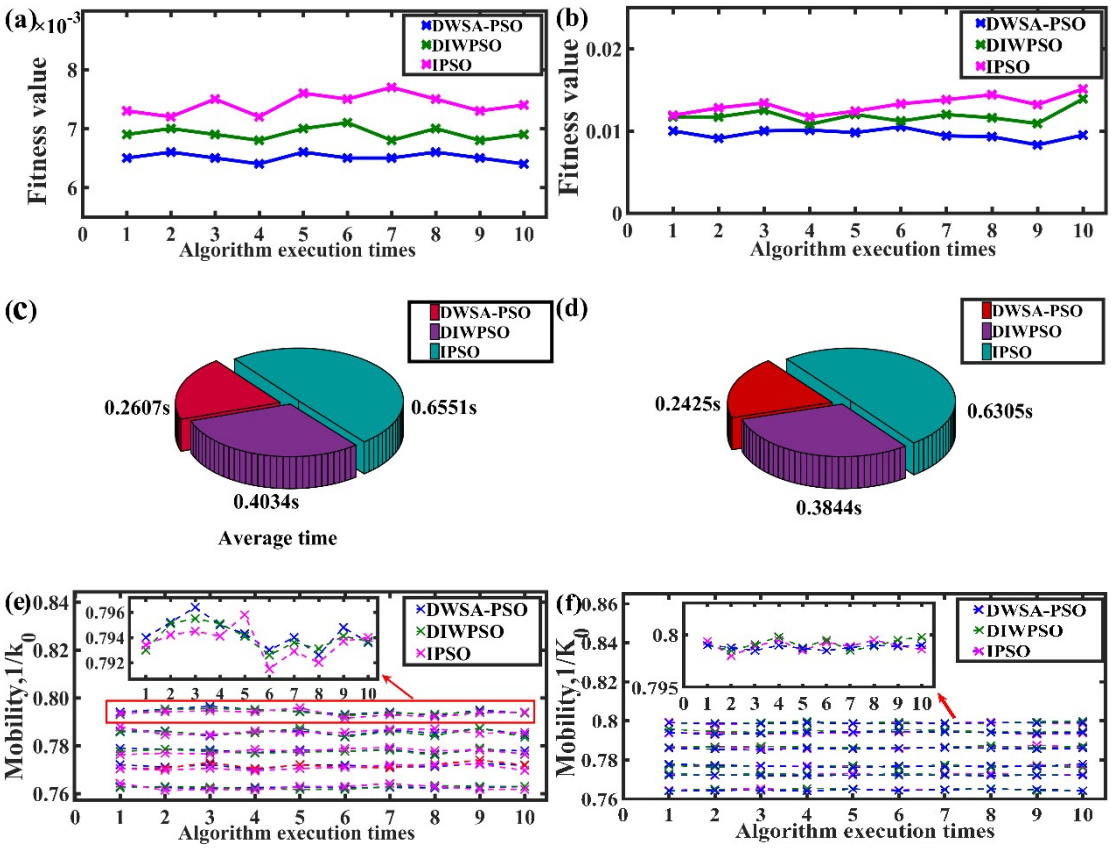


Fig.S8 Parameter values obtained by analyzing overlapping peaks containing five- and six- components 10 times using three methods: (a-b) Fitness value; (c-d) Average time; (e-f) Mobility.

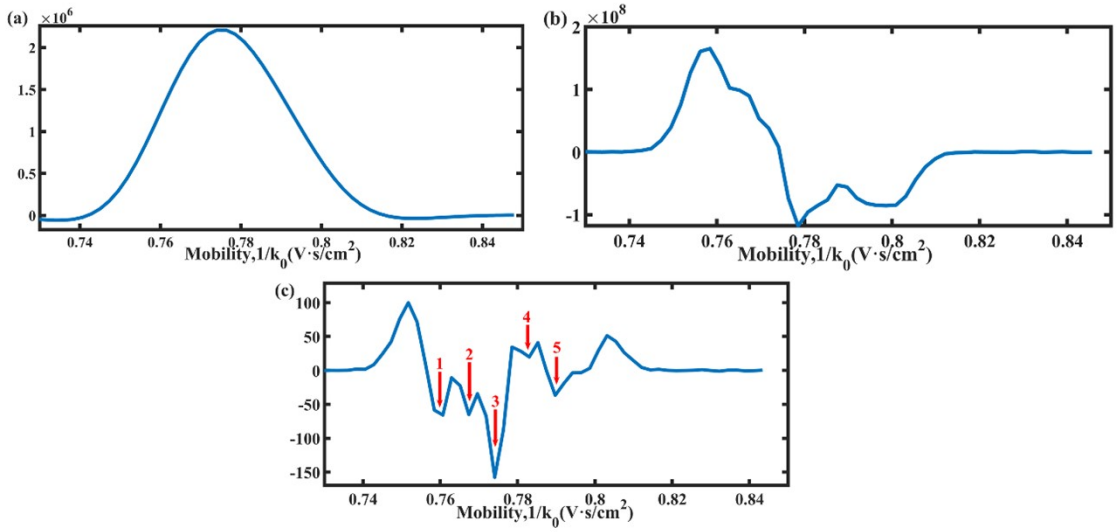


Fig.S9 (a) Original peak shape of the five-component ([SUC+TRE+MEL+LAC+MAL+CL]-) overlapping peaks; (b) The first-order differentiation; (c) The second-order differentiation.

Table S1(a). Separation results of four simulated overlapping peaks with different overlap degree using DWSA-PSO

No.	single peak	Error (100%)		
		Intensity	Position	FWHM
1	1	0.01	0.04	0.01
	2	-0.01	-0.02	0.01
	3	-0.006	-0.01	0.01
2	1	0.44	0.56	0.23
	2	-0.40	-1.25	-0.006
	3	0.47	0.56	-0.11
3	1	0.39	0.12	0.11
	2	-0.24	-0.76	0.03
	3	0.03	0.29	-0.03
4	1	-0.75	-0.58	-0.24
	2	-0.24	-0.32	-0.28
	3	1.53	0.63	-0.20

Abbreviations: No, the type of overlapping peaks; FWHM, full width at half maximum.

Table S1(b). Running times and Fitness value of four simulated overlapping peaks with different overlap degree using DWSA-PSO

No.	Running time	Fitness value
1	0.45	1.35×10^{-7}
2	0.45	1.03×10^{-5}
3	0.49	5.25×10^{-6}
4	0.44	2.62×10^{-6}

Abbreviations: No, the type of overlapping peaks

Table S2(a). Separation results of IPSO, DIWPSO and DWSA-PSO for simulated four- and five-overlapping peaks

C.	Parameters	Error (%)		
		IPSO	DIWPSO	DWSA-PSO
4	I1	-4.27	2.41	-0.37
	I2	3.64	-8.07	-0.05
	I3	-6.55	3.79	-0.26
	I4	2.11	-5.09	-0.11
	P1	-1.46	1.20	-0.11
	P2	0.81	-0.93	-0.02
	P3	0.87	-0.49	0.05
	P4	-0.28	0.66	0.02
	W1	-2.83	3.05	-0.10
	W2	0.14	-10.62	0.80
	W3	-9.32	16.29	0.15
	W4	1.41	-3.46	-0.09
5	I1	-18.17	5.84	-0.28
	I2	8.08	-7.00	0.28
	I3	-1.13	1.66	-0.33
	I4	-3.00	-3.20	0.37
	I5	-0.12	-0.22	-0.02
	P1	-4.00	2.20	-0.09
	P2	-3.22	1.13	-0.03
	P3	1.10	-0.09	-0.03

P4	0.40	0.27	-0.04
P5	-0.02	0.0002	-0.004
W1	-6.87	4.57	-0.18
W2	25.24	-10.59	0.52
W3	-0.65	5.07	-0.45
W4	-2.70	-0.63	0.36
W5	0.58	0.09	-0.03

Abbreviations: C, the number of overlapping peak components; I, Intensity; P, Position; W, full width at half maximum.

Table S2(b). Running times and Fitness value of IPSO, DIWPSO and DWSA-PSO for simulated four- and five-overlapping peaks

C.	Running time (s)			Fitness value		
	IPSO	DIWPSO	DWSA-PSO	IPSO	DIWPSO	DWSA-PSO
4	2.97	1.94	1.24	4.29×10^{-4}	4.29×10^{-4}	1.16×10^{-5}
5	3.18	2.06	2.03	1.13×10^{-3}	2.74×10^{-4}	3.46×10^{-7}

Abbreviations: C, the number of overlapping peak components

Table S3. Mobility, FWHM, and CCS of $[M+Cl]^-$ complexes

Glycan isomers	Ion species	Mobility (V s/cm^2)	FWHM	CCS
Sucrose	$[SUC+Cl]^-$	0.764	0.015	158.5
Trehalose	$[TRE+Cl]^-$	0.772	0.014	160.2
Lactose	$[LAC+Cl]^-$	0.786	0.016	163.1
Melibiose	$[MEL+Cl]^-$	0.778	0.015	161.4
Maltose	$[MAL+Cl]^-$	0.794	0.015	164.7
Cellobiose	$[CEL+Cl]^-$	0.799	0.016	165.8
Maltotriose	$[MAL-3+Cl]^-$	0.946	0.018	194.2
Raffinose	$[RAF-3+Cl]^-$	0.922	0.015	189.3
Isomaltotriose	$[ISO-3+Cl]^-$	0.938	0.017	192.6
Melezitose	$[MEL-3+Cl]^-$	0.905	0.016	185.9