

Supplementary Information

Co-precipitation based on layered double hydroxides and anionic surfactants for preconcentration of six benzoylurea insecticides in soft drinks before simultaneous analysis by high-performance liquid chromatography

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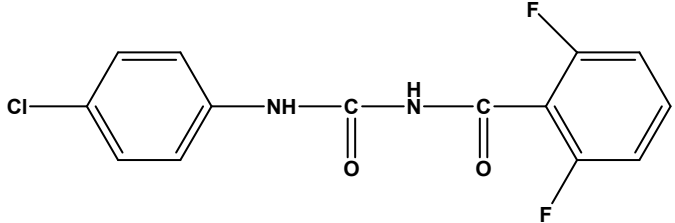
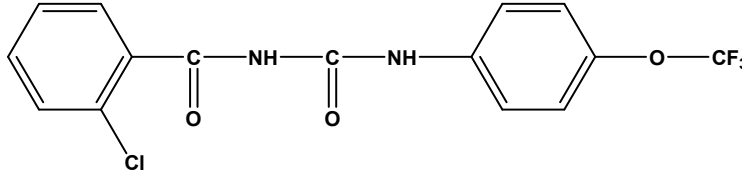
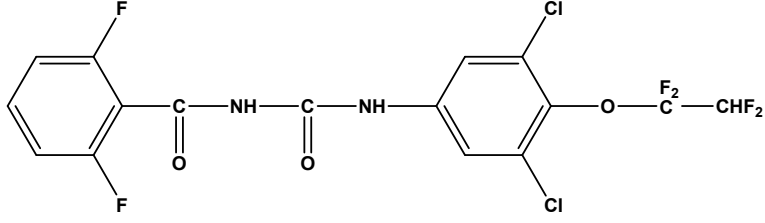
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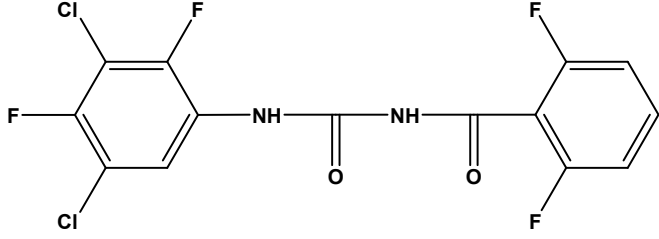
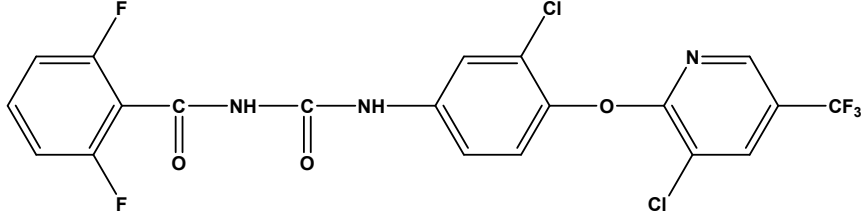
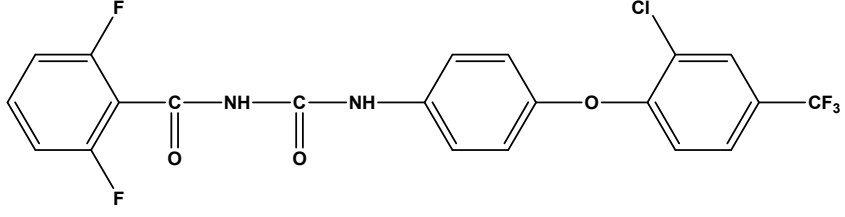
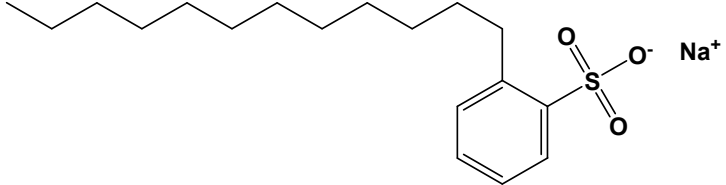
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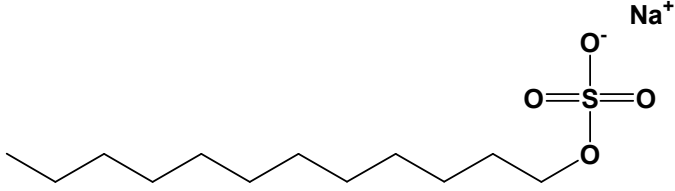
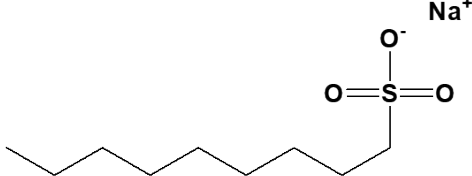
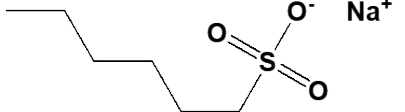
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Table S1 Chemical structures and physicochemical properties of benzoylurea insecticides and surfactants used in this study

Name	Structure/CAS Number	Mw (g/mol)	Aqueous solubility (mg/L)	Log K _{ow}
Diflubenzuron (DFL)	 CAS: 35367-38-5	310.69	5.164 ^a (0.080) ^b	3.59 ^a (3.88) ^b
Triflumuron (TRF)	 CAS: 64628-44-0	358.70	0.352 ^a (0.025) ^b	4.24 ^a (4.91) ^b
Hexaflumuron (HXF)	 CAS: 86479-06-3	461.14	0.018 ^a (0.027) ^b	5.64 ^a (5.68) ^b

<p>Teflubenzuron (TFL)</p>	 <p>CAS: 83121-18-0</p>	<p>381.12</p>	<p>0.511^a (0.019)^b</p>	<p>4.64^a (4.56)^b</p>
<p>Fluazuron (FLU)</p>	 <p>CAS: 86811-58-7</p>	<p>506.21</p>	<p>0.029^a (0.020)^b</p>	<p>5.23^a (5.10)^b</p>
<p>Flufenoxuron (FLF)</p>	 <p>CAS: 101463-69-8</p>	<p>488.77</p>	<p>0.007^a (0.002)^b</p>	<p>5.97^a (Not reported)^b</p>
<p>Sodium dodecylbenzenesulfonate (SDBS)</p>		<p>348.48</p>	<p>134.1^a (800)^b</p>	<p>3.00^a (1.96)^b</p>

	CAS: 25155-30-0			
Sodium dodecylsulfate (SDS)	 CAS: 151-21-3	288.38	616.8 ^a (1×10 ⁵) ^b	1.69 ^a (1.60) ^b
Sodium 1-nonanesulfonate (SNS)	 CAS: 35192-74-6	230.30	Not reported ^a (Not reported) ^b ; Soluble in water	Not reported ^a (Not reported) ^b
Sodium 1-hexanesulfonate (SHS)	 CAS: 2832-45-3; CAS: 207300-91-2 (monohydrate form)	188.22; 206.24 (monohydrate form)	1×10 ⁶ ^a (Not reported) ^b	-2.07 ^a (Not reported) ^b

^a Obtained by calculating using the Estimation Programs Interface (EPI) Suite™ v.4.1 (Environmental Protection Agency, USA)

^b Experimental database match as reported in EPI software

Table S2 The calculation results of XRD reflections obtained for the studied LDH forms

LDH form	XRD reflection series					
	(003)		(006)		(009)	
	2 θ (degree)	d (nm)	2 θ (degree)	d (nm)	2 θ (degree)	d (nm)
LDH-1	11.4255	0.7739	22.5702	0.3936	34.9947	0.2562
SDBS-LDH	10.9189	0.8096	22.3302	0.3978	34.9947	0.2562
BUs-SDBS-LDH	9.1593	0.9647	22.0636	0.4026	35.2346	0.2545
LDH-2	11.0754	0.7982	20.3039	0.4370	34.9947	0.2562
SDS-LDH	11.0256	0.8018	20.0373	0.4428	35.7412	0.2510
BUs-SDS-LDH	10.3590	0.8533	20.0373	0.4428	36.7543	0.2443
LDH-3	11.1589	0.7923	22.8368	0.3891	34.9947	0.2562
SNS-LDH	11.2922	0.7830	22.8368	0.3891	35.2346	0.2545
BUs-SNS-LDH	11.1589	0.7923	22.5702	0.3936	34.9947	0.2562
LDH-4	10.7590	0.8216	22.0636	0.4026	34.728	0.2581
SHS-LDH	11.1589	0.7923	22.5702	0.3936	34.4881	0.2598
BUs-SHS-LDH	11.0256	0.8018	22.3302	0.3978	34.728	0.2581

Note: Bragg's equation; $\lambda = 2d\sin\theta$, where $\lambda=1.5406 \text{ \AA}$ (0.15406 nm)

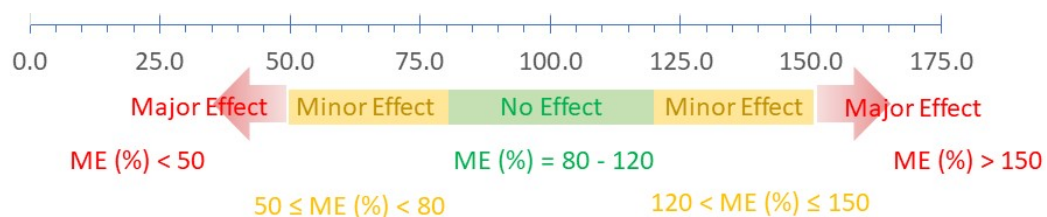
Table S3 Matrix effect (ME, %) data of target BUs in the studied soft drink samples

Sample	Analyte	Sm	Ss	ME (%)	ME level*	R ²	
						Sm	Ss
Bael fruit	DFL	1092	1315	83	No	0.9918	0.9991
	TRF	2367	1984	119	Minor	0.9921	0.9981
	HXF	1000	1340	75	Minor	0.9933	0.9981
	TFL	825	1013	81	No	0.9976	0.9986
	FLU	1124	1245	90	No	0.9971	0.9983
	FLF	1526	1718	89	No	0.9964	0.9979
White tea chrysanthemum	DFL	695	1315	53	Minor	0.9918	0.9991
	TRF	1926	1984	97	No	0.9921	0.9981
	HXF	950	1340	71	Minor	0.9933	0.9981
	TFL	698	1013	69	Minor	0.9976	0.9986
	FLU	907	1245	73	Minor	0.9971	0.9983
	FLF	1278	1718	74	Minor	0.9964	0.9979
Chrysanthemum & chamomile	DFL	796	1315	60	Minor	0.9935	0.9991
	TRF	1583	1984	80	No	0.9978	0.9981
	HXF	1036	1340	77	Minor	0.9971	0.9981
	TFL	811	1013	80	No	0.9933	0.9986
	FLU	1200	1245	96	No	0.9955	0.9983
	FLF	2285	1718	133	Minor	0.9981	0.9979
Jiaogulan & safflower	DFL	499	1315	38	Major	0.9943	0.9991
	TRF	1274	1984	64	Minor	0.9946	0.9981
	HXF	1097	1340	82	No	0.9955	0.9981
	TFL	836	1013	83	No	0.9962	0.9986
	FLU	1151	1245	92	No	0.9966	0.9983
	FLF	2230	1718	130	Minor	0.9951	0.9979

Sm: slope of calibration in sample matrix

Ss: slope of calibration in solvent medium

*Matrix effect level:



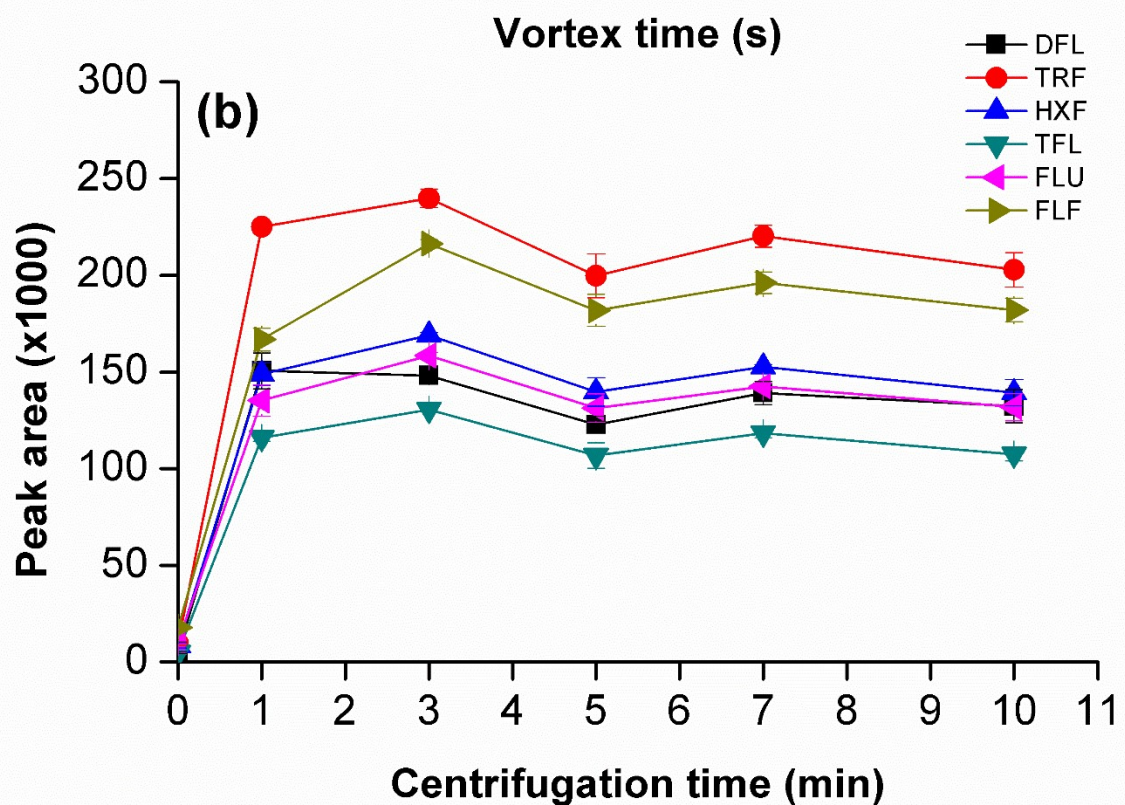
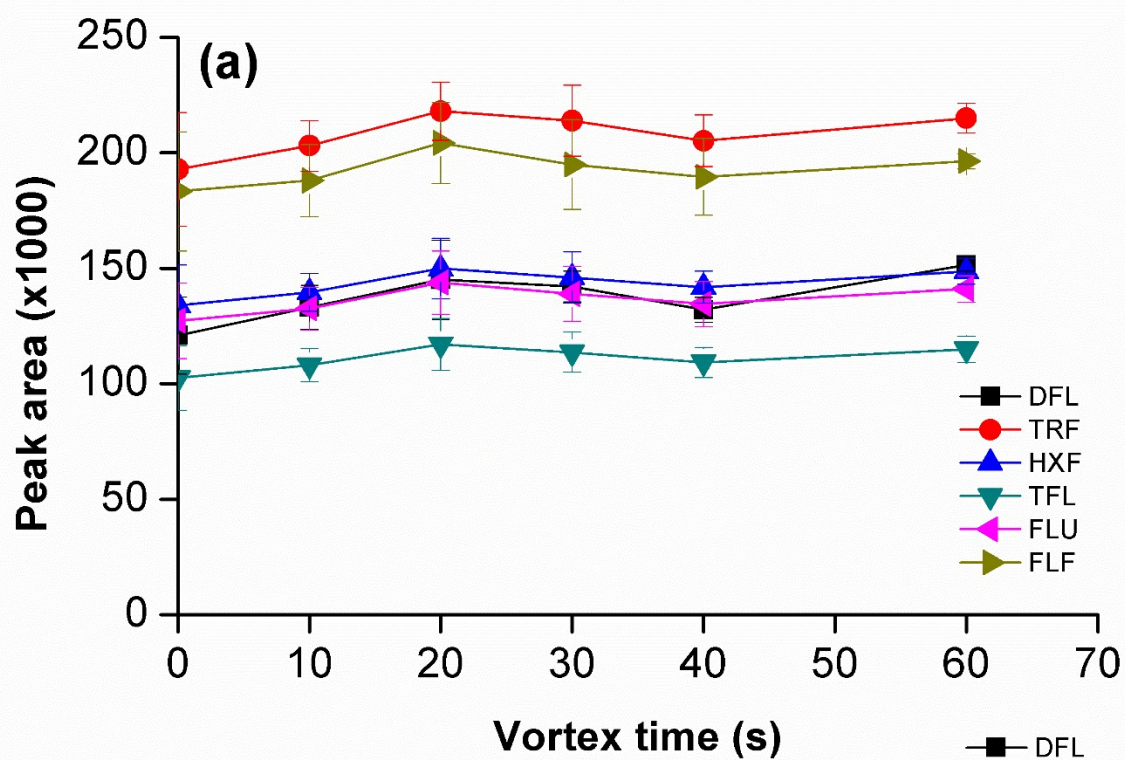


Figure S1 Effect of (a) vortex time and (b) centrifugation time on the extraction performance

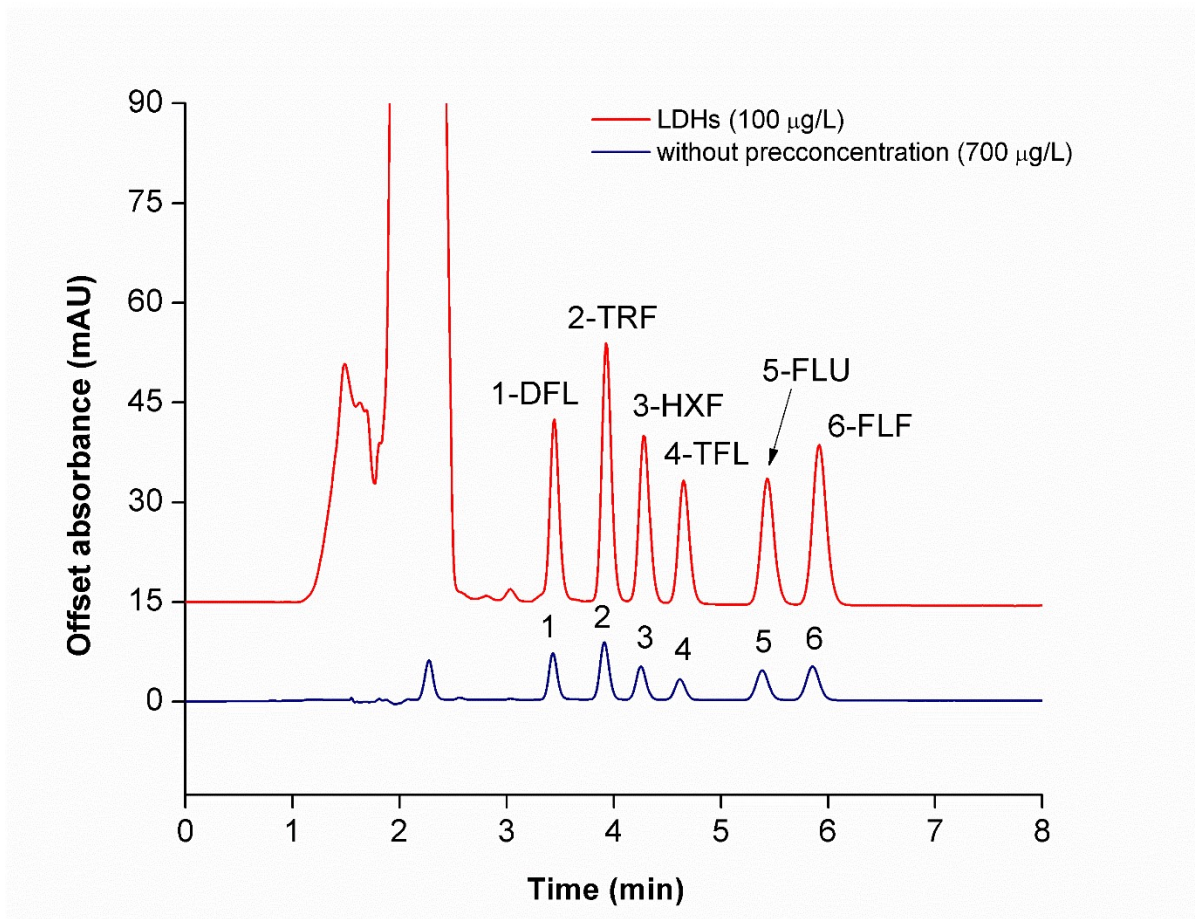


Figure S2 Overlaid chromatograms of target BUs obtained from without preconcentration and preconcentration with LDHs

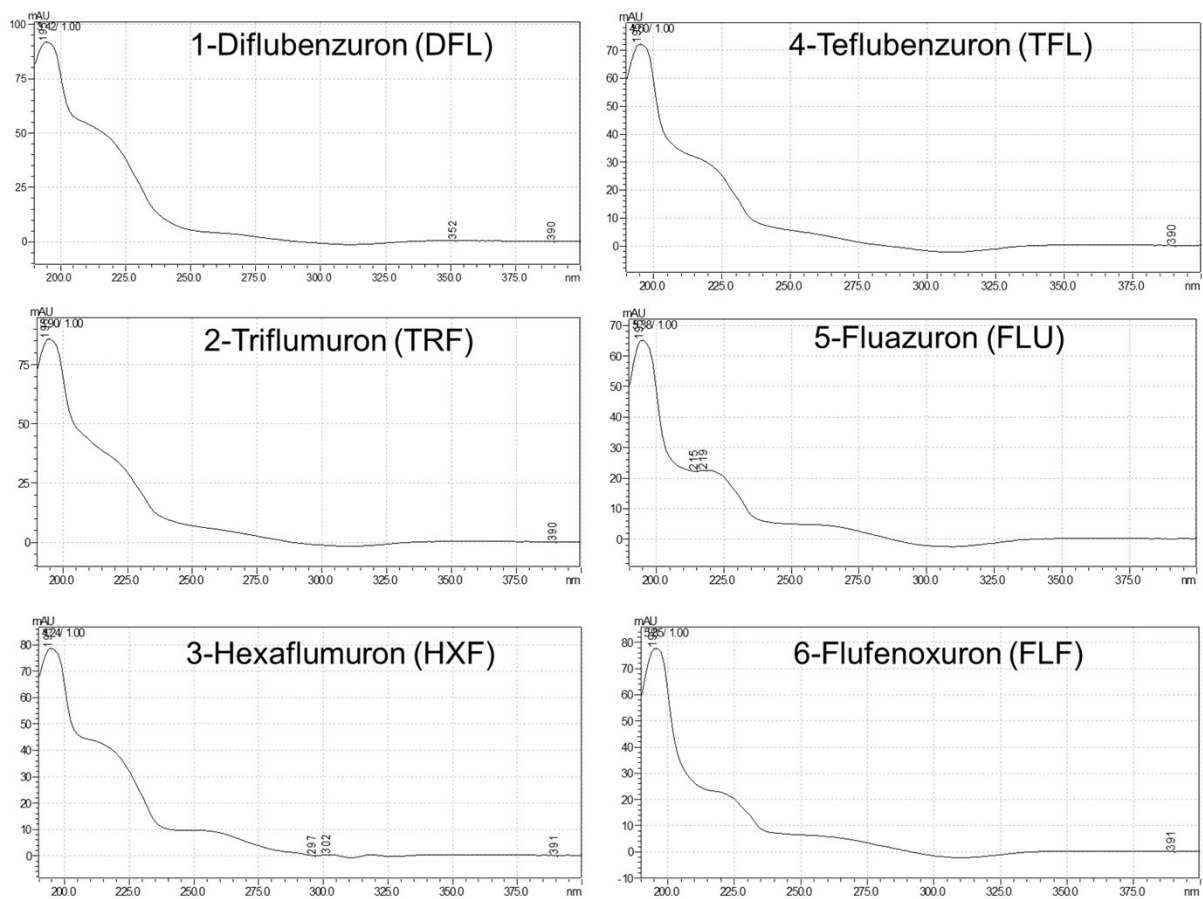


Figure S3 Absorption spectra of six benzoylurea insecticides obtained from HPLC-photo-diode array detector.