Supplementary Material

Development and validation of an LC-MS/MS/MS method for the sensitive quantification of trace β-agonists in complex animal-derived food matrices

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Fig. S1. The stability of NH_2-UiO-66 after treatment with water, 0.1 M HCl, and 0.1 M NaOH for 24 h.

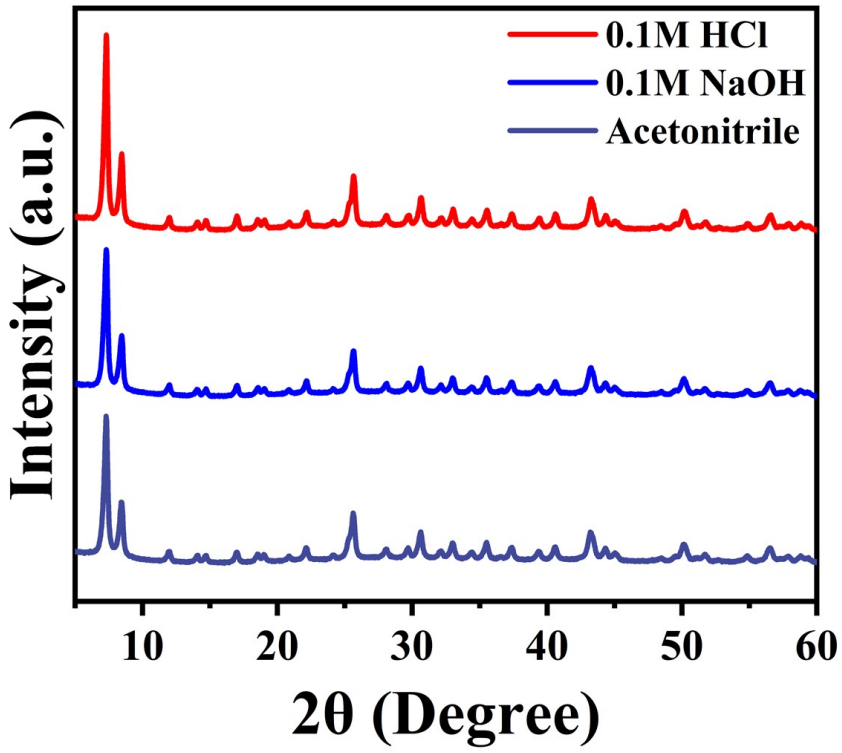

Fig. S2. XRD spectra of NH_2-UiO-66 in different solvents.

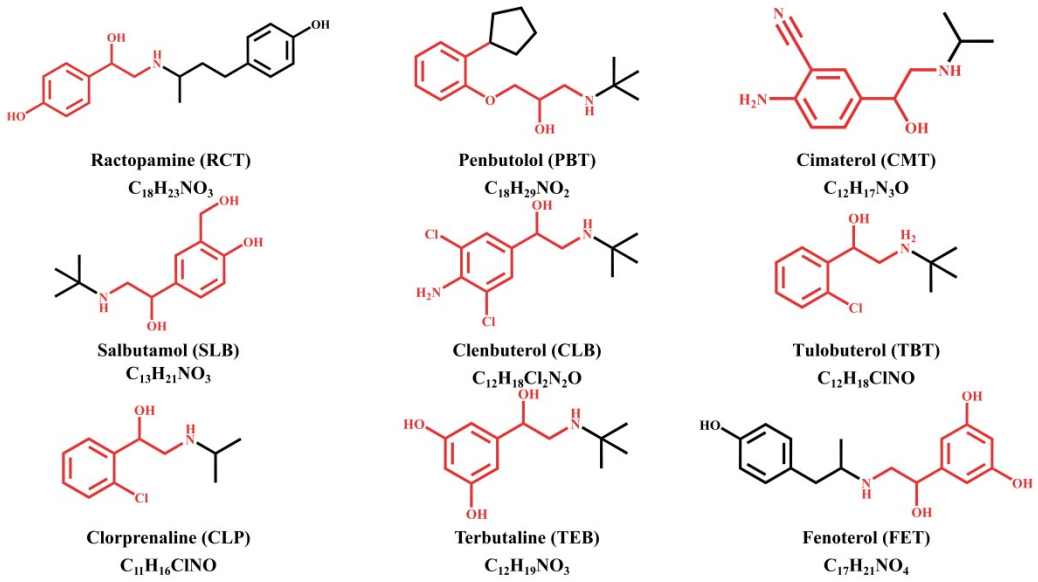

Fig. S3. Structures of the β-agonists.

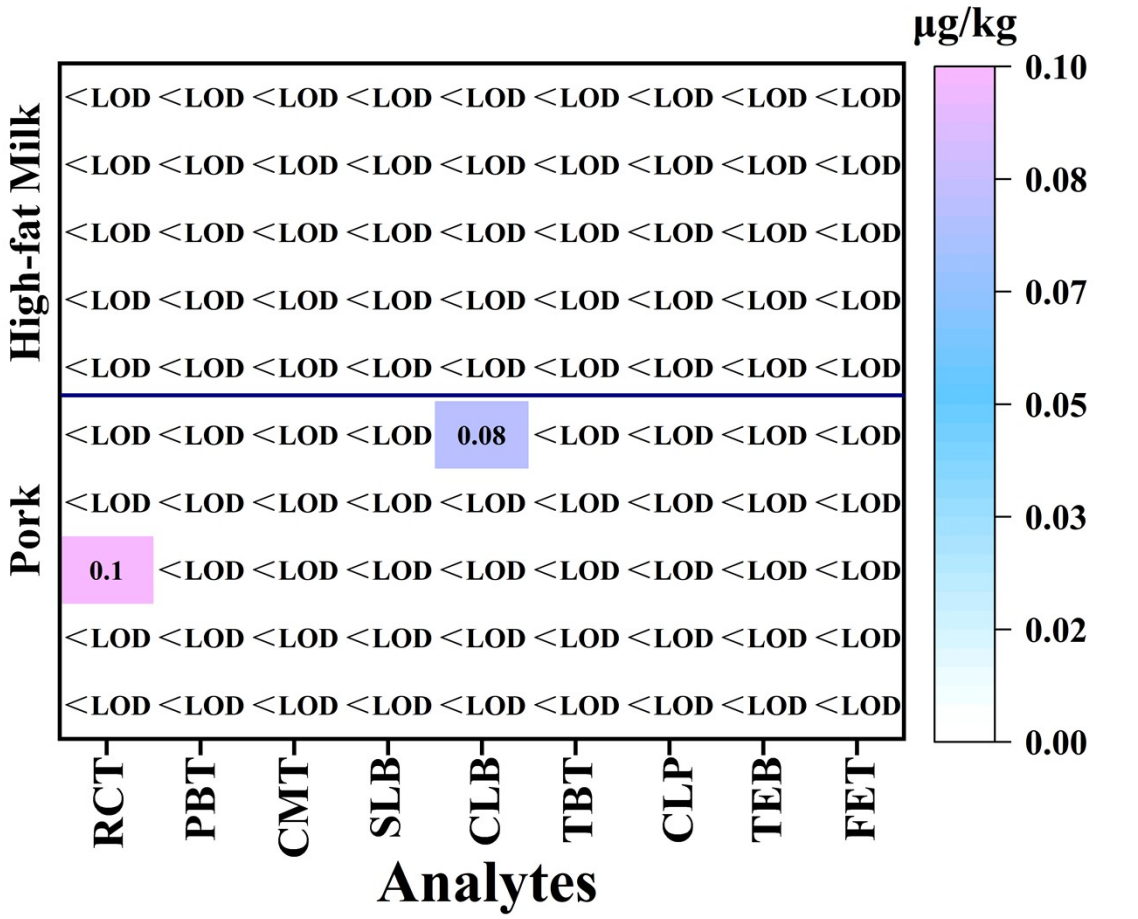

Fig. S4. The determination of β-agonists in real sample matrices.

Table S1 The basic information of β-agonists.

Analytes	Abbreviation	CAS	Molecular formula
Ractopamine	RCT	97825-25-7	$C_{18}H_{23}NO_3$
Penbutolol	PBT	38363-40-5	$C_{18}H_{29}NO_2$
Cimaterol	CMT	54239-37-1	$C_{12}H_{17}N_3O$
Salbutamol	SLB	18559-94-9	$C_{13}H_{21}NO_3$
Clenbuterol	CLB	37148-27-9	$C_{12}H_{18}Cl_2N_2O$
Tulobuterol	TBT	41570-61-0	$C_{12}H_{18}ClNO$
Clorprenaline	CLP	3811-25-4	$C_{11}H_{16}ClNO$
Terbutaline	TEB	23031-25-6	$C_{12}H_{19}NO_3$
Fenoterol	FET	13392-18-2	$C_{17}H_{21}NO_4$

Table S2 MRM and MRM^3 parameters for nine β-agonists tested in ESI^+ mode.

β-agonists	MRM					MRM^3				
	Transition P→F (m/z)	DP (V)	EP (V)	CE (V)	CXP (V)	F' (m/z)	AF2 (V)	Excitation time (ms)	LIT time (ms)	Q0 trapping
RCT	302.1→164.2	56	7	23	9	121.0	0.06	25	15	Yes
	302.1→107.1	47	8	49	10	79.1	0.10	25	15	Yes
PBT	292.1→236.2	74	10	24	13	201.1	0.07	25	20	Yes
	292.1→201.1	117	6	29	18	133.1	0.06	25	20	Yes
CMT	220.1→202.2	27	11	16.	11	160.1	0.06	25	10	Yes
	220.1→160.1	19	10	24	8	143.1	0.06	25	15	Yes
SLB	240.2→222.2	78	7	16	15	148.1	0.04	25	25	Yes

	240.2→148.1	36	10	27	12	133.1	0.03	25	25	Yes
CLB	277.1→259.1	78	9	16	36	203.1	0.07	25	10	Yes
	277.1→203.1	31	9	23	11	132.1	0.06	25	20	Yes
TBT	228.1→172.0	20	9	17	9	154.1	0.06	25	15	Yes
	228.1→154.1	39	11	25	13	118.1	0.06	25	15	Yes
CLP	214.1→196.1	38	3	18	12	154.1	0.05	25	5	Yes
	214.1→154.1	39	2	25	9	118.1	0.05	25	5	Yes
TEB	226.1→152.1	39	10	23	8	125.1	0.04	25	25	Yes
	226.1→125.1	48	7	34	11	107.1	0.05	25	25	Yes
FET	304.1→135.1	30	11	25	14	107.0	0.05	25	20	Yes

	304.1→107.0	28	10	32	35	79.0	0.07	25	25	Yes

Table S3 The ion ratios of nine β-agonists in MRM and MRM^3 modes

Analytes	MRM		MRM^3	
	Ion ratio	Ion ratio (RSD, %)	Ion ratio	Ion ratio (RSD, %)
RCT	0.56	1.92	0.02	4.66
PBT	0.14	2.84	0.31	1.21
CMT	0.66	3.93	0.88	1.49
SLB	0.50	1.68	0.09	4.56
CLB	0.62	1.25	0.74	1.14
TBT	0.24	1.25	0.13	2.86
CLP	0.94	0.34	0.91	1.10
TEB	0.29	3.15	0.55	1.19
FET	0.89	2.11	0.17	2.35