

Table S1 Detailed information for bile acid standards

Name	Source	Product code
Taurolithocholic acid-3-sulfate	TRC	CDDM-T009115
Dehydrolithocholic acid	Zzstandard	ZS-20089
Isoallolithocholic acid	Zzstandard	ZS-20054
Isolithocholic acid	Zzstandard	ZS-20053
Lithocholic acid	ANPEL	CDAA-280500
Nor-deoxycholic acid	Zzstandard	ZS-20171
7-ketolithocholic acid	Zzstandard	ZS-20055
12-ketolithocholic acid	Zzstandard	ZS-20056
3-oxodeoxycholic acid	TRC	ZTR-O856870
Murideoxycholic acid	Zzstandard	ZS-20309
3 β -Ursodeoxycholic acid	TRC	CDDM-U850005
β -Hyodeoxycholic acid	TRC	ZTR-H998105
Ursodeoxycholic acid	ANPEL	CDAA-280296
Hyodeoxycholic acid	ANPEL	CDAA-280059
3 β -deoxycholic acid	Zzstandard	ZS-20121
Chenodeoxycholic acid	ANPEL	CDAA-281174
Deoxycholic acid	ANPEL	CDAA-280597
Isooxycholic acid	Zzstandard	ZS-20193
Norcholic acid	TRC	CDDM-N661440
Dehydrocholic acid	Zzstandard	ZS-20156
7,12-diketolithocholic acid	Zzstandard	ZS-20059
6,7-diketolithocholic acid	Boc Sciences	FB-76
7-Ketodeoxycholic acid	TRC	CDDM-K188480
12-Oxochenodeoxycholic acid	Boc Sciences	FE-55
3-Oxocholic acid	TRC	O856895
Ursocholic acid	TRC	CDDM-U849900
ω -muricholic acid	IsoReag	IR-15786
3 β -Cholic acid	TRC	C432605
α -muricholic acid	Zzstandard	ZS-20001
β -muricholic acid	Zzstandard	ZS-20003
Hyocholic acid	Zzstandard	ZS-20008
Cholic acid	ANPEL	CDAA-263004
Glycolithocholic acid	TRC	CDDM-L469200
Glycoursodeoxycholic acid	ANPEL	CDAA-281118
Glycochenodeoxycholic acid	ANPEL	CDAA-281120
Glycodeoxycholic acid	ANPEL	CDAA-281119
Lithocholic acid-3-sulfate	IsoReag	IR-15705
Glycodehydrocholic acid	Zzstandard	ZS-20161
Glycohyocholic acid	Zzstandard	ZS-20022
Glycocholic acid	IsoReag	IR-15333
Taurolithocholic acid	Zzstandard	ZS-20048
Tauroursodeoxycholic acid	ANPEL	CDAA-280703

Taurochenodeoxycholic acid	Zzstandard	ZS-20036
Taurodeoxycholic acid	Zzstandard	ZS-20147
Taurodehydrocholic acid	Zzstandard	ZS-20160
Glycolithocholic acid-3-sulfate	IsoReag	IR-15691
Tauro- β -muricholic acid	Zzstandard	ZS-20002
Taurohyocholic acid	Zzstandard	ZS-20025
Taurocholic acid	CMASS	CMS-T610030
Chenodeoxycholic acid-3- β -D-glucuronide	TRC	C291920
