

Table S1. List of compounds included in the FooDOxS database, including common name, abbreviations used in the database, IUPAC systematic name and EPA CompTox ID³¹. N/A = CompTox entry not available.

Name	Abbreviation	ACD/IUPAC name	CompTox ID
Cholesterol	cholesterol	(3 β)-Cholest-5-en-3-ol	DTXSID3022401
7-ketocholesterol	7-keto	(3 β)-3-Hydroxycholest-5-en-7-one	DTXSID901033744
25-hydroxycholesterol	25-OH	(3 β)-Cholest-5-ene-3,25-diol	DTXSID5044023
7 α -hydroxycholesterol	7 α -OH	(3 β ,7 α)-Cholest-5-ene-3,7-diol	DTXSID40903965
7 β -hydroxycholesterol	7 β -OH	(3 β ,7 β)-Cholest-5-ene-3,7-diol	DTXSID60862207
5 α ,6 α -epoxycholesterol	5 α ,6 α -epoxy	(3 β ,5 α ,6 α)-5,6-Epoxycholestan-3-ol	DTXSID80921305
5 β ,6 β -epoxycholesterol	5 β ,6 β -epoxy	(3 β ,5 β ,6 β)-5,6-Epoxycholestan-3-ol	DTXSID501314152
6-ketocholestanol	6-keto	(3 β ,5 α)-3-Hydroxycholestan-6-one	DTXSID10922441
20-hydroxycholesterol	20-OH	(3 β)-Cholest-5-ene-3,20-diol	DTXSID70862096
Cholestane-3,5,6-triol	triol	(3 β ,5 α ,6 β)-Cholestane-3,5,6-triol	DTXSID70862612
4 β -hydroxycholesterol	4 β -OH	(3 β ,4 β)-Cholest-5-ene-3,4-diol	N/A
27-hydroxycholesterol	27-OH	(25R)-cholest-5-ene-3 β ,26-diol	DTXSID40864941
22-ketocholesterol	22-keto	(3 β)-3-Hydroxycholest-5-en-22-one	DTXSID70940904
19-hydroxycholesterol	19-OH	(3 β)-Cholest-5-ene-3,19-diol	N/A
3 β ,5-dihydroxy-5 α -cholesten-6-one	cholesten-6-one	(3 β ,5 α)-3,5-Dihydroxycholestan-6-one	DTXSID80926658
4-cholesten-3-one	cholesten-3-one	Cholest-4-en-3-one	DTXSID90872379
4-cholesten-3,6-dione	cholesten-3,6-dione	Cholest-4-ene-3,6-dione	DTXSID20913305
3,5-cholestadien-7-one	cholestadien-7-one	(20R)-Cholesta-3,5-dien-7-one	DTXSID10972143
3-keto-5-cholestene	3-keto-5-cholestene	Cholest-5-en-3-one	DTXSID40208841
β -sitosterol	β -sitosterol	(3 β)-Stigmast-5-en-3-ol	DTXSID5022481
Campesterol	Campesterol	(3 β ,24R)-Ergost-5-en-3-ol	DTXSID801009891
Δ 7-avenasterol	Avenasterol	(3 β ,5 α ,24Z)-Stigmasta-7,24(28)-dien-3-ol	DTXSID10177858
Δ 5-avenasterol	Δ 5-avenasterol	(24Z)-Stigmasta-5,24(28)-dien-3-ol	N/A
Brassicasterol	brassicasterol	(3 β ,22E)-Ergosta-5,22-dien-3-ol	DTXSID80197124
Campestanol	campestanol	(3 β ,5 α ,24R)-Ergostan-3-ol	DTXSID3040988
Stigmasterol	stigmasterol	(3 β ,20R,22E,24S)-Stigmasta-5,22-dien-3-ol	DTXSID801015733
Stigmastanol	stigmastanol	(3 β)-Stigmastan-3-ol	DTXSID8051835
Fucosterol	fucosterol	(3 β ,20R,24E)-Stigmasta-5,24(28)-dien-3-ol	DTXSID701033229
Desmosterol	desmosterol	(3 β)-Cholesta-5,24-dien-3-ol	DTXSID10878676

6 β -hydroxybrassicastanol	6 β -OH-brassicastanol	N/A	N/A
6 β -hydroxycampesterol	6 β -OH-campesterol	N/A	N/A
6 β -hydroxycampestanol	6 β -OH-campestanol	(3 β ,5 α ,6 α ,24R)-Ergostane-3,6-diol	N/A
6 α -hydroxysitostanol	6 α -OH-sitostanol	5 α -Stigmast-3 β ,6 α -diol	N/A
7 α -hydroxycampesterol	7 α -OH-campesterol	(3 β ,7 α ,24R)-Ergost-5-ene-3,7-diol	N/A
7 α -hydroxystigmasterol	7 α -OH-stigmasterol	(3 β ,7 α ,22E)-Stigmasta-5,22-diene-3,7-diol	N/A
7 α -hydroxysitosterol	7 α -OH-sitosterol	(3 β ,7 α)-Stigmast-5-ene-3,7-diol	N/A
7 β -hydroxycampesterol	7 β -OH-campesterol	(3 β ,7 β ,24R)-Ergost-5-ene-3,7-diol	N/A
7 β -hydroxystigmasterol	7 β -OH-stigmasterol	(3 β ,7 β ,22E)-Stigmasta-5,22-diene-3,7-diol	N/A
7 β -hydroxysitosterol	7 β -OH-sitosterol	(3 β ,7 β)-Stigmast-5-ene-3,7-diol	N/A
24-ethylcholest-4-ene-6 β -ol-3-one	24-ethylcholest-4-ene-6 β -ol-3-one	6 β -Hydroxystigmast-4-en-3-one	N/A
24-ethylcholest-4-ene-6 α -ol-3-one	24-ethylcholest-4-ene-6 α -ol-3-one	6 α -Hydroxystigmast-4-en-3-one	N/A
24-hydroxystigmasterol	24-OH-stigmasterol	(3 β ,22E)-Stigmasta-5,22-diene-3,24-diol	N/A
24-hydroxycampesterol	24-OH-campesterol	(3 β ,22S,24R)-Ergost-5-ene-3,22-diol	N/A
24-hydroxysitosterol	24-OH-sitosterol	(3b,24R)-24-Ethylcholest-5-ene-3,24-diol	N/A
25-hydroxysitosterol	25-OH-sitosterol	(3b,24R)-24-Ethylcholest-5-ene-3,25-diol	N/A
Campesterol-5 β ,6 β -epoxide	campesterol-5 β ,6 β -epoxide	(24R)-5 β ,6 β -Epoxy-24-methylcholestan-3 β -ol	N/A
Campesterol-5 α ,6 α -epoxide	campesterol-5 α ,6 α -epoxide	(24R)-5 α ,6 α -Epoxy-24-methylcholestan-3 β -ol	N/A
Stigmasterol-5 α ,6 α -epoxide	stigmasterol-5 α ,6 α -epoxide	(24S)-5 α ,6 α -Epoxy-24-ethylcholest-22-en-3 β -ol	N/A
Stigmasterol-5 β ,6 β -epoxide	stigmasterol-5 β ,6 β -epoxide	(24S)-5 β ,6 β -Epoxy-24-ethylcholest-22-en-3 β -ol	N/A
Sitosterol-5 α ,6 α -epoxide	sitosterol-5 α ,6 α -epoxide	(24R)-5 α ,6 α -Epoxy-24-ethylcholestan-3 β -ol	N/A
Sitosterol-5 β ,6 β -epoxide	sitosterol-5 β ,6 β -epoxide	(24R)-5 β ,6 β -Epoxy-24-ethylcholestan-3 β -ol	N/A
Campestanetriol	campestanetriol	(24R)-Methylcholestan-3 β ,5 α ,6 β -triol	N/A
Stigmastetriol	stigmastetriol	(24S)-Ethylcholest-22-en-3 β ,5 α ,6 β -triol	N/A
Sitostanetriol	sitostanetriol	(24R)-Ethylcholestan-3 β ,5 α ,6 β -triol	N/A
Brassicastanetriol	brassicastanetriol	(24S)-Methylcholest-22-en-3 β ,5 α ,6 β -triol	N/A
7-ketobrassicasterol	7-ketobrassicasterol	(24S)-Methylcholest-5,22-dien-3 β -ol-7-one	N/A
7-ketocampesterol	7-ketocampesterol	(24R)-Methylcholest-5-en-3 β -ol-7-one	N/A
7-ketostigmasterol	7-ketostigmasterol	(24S)-Ethylcholest-5,22-dien-3 β -ol-7-one	N/A
7-ketositosterol	7-ketositosterol	(24R)-Ethylcholest-5-en-3 β -ol-7-one	N/A
6-ketositosterol	6-ketositosterol	(24R)-Ethylcholest-5-en-3 β -ol-6-one	N/A

Table S2. Distribution of analytical techniques for determining DOxS in papers included in the FooDOxS database.

Method	%
Gas-chromatography (FID ^a detector)	39.5
Gas-chromatography (MS ^b detector)	49.1
<i>Total Gas-chromatography</i>	88.6
Liquid-chromatography (DAD ^c detector)	8.8
Liquid-chromatography (MS detector)	1.8
<i>Total Liquid-chromatography</i>	10.5
¹ H-NMR ^d	0.9

^aFlame Ionization Detector, ^bMass-Spectrometer, ^cDiode-Array Detector, ^dNuclear Magnetic Resonance