

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121523\
 Data File : BG060037.D
 Acq On : 15 Dec 2023 15:51
 Operator : MA/JU
 Sample : 05791-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-1B-K-T

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060037.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.144	4	9	26	rVB	490070	919641	10.43%	3.362%
2	3.667	93	98	106	rVB	224459	306117	3.47%	1.119%
3	5.523	408	414	428	rBV	520963	873730	9.91%	3.194%
4	7.110	677	684	693	rBV	348307	560677	6.36%	2.050%
5	7.956	821	828	834	rBV	202269	352644	4.00%	1.289%
6	9.119	1017	1026	1035	rBV	757462	1315452	14.92%	4.809%
7	10.764	1299	1306	1313	rBV	294082	513836	5.83%	1.878%
8	13.220	1715	1724	1732	rBV	2527423	3883311	44.06%	14.196%
9	14.595	1951	1958	1966	rVB	564098	836756	9.49%	3.059%
10	16.081	2204	2211	2220	rBV	2764418	4055021	46.01%	14.824%
11	17.345	2416	2426	2431	rBV	879762	1347151	15.28%	4.925%
12	18.232	2573	2577	2582	rBV3	107921	140308	1.59%	0.513%
13	19.507	2791	2794	2798	rBV6	58153	88947	1.01%	0.325%
14	19.965	2866	2872	2878	rBV	6787338	8813964	100.00%	32.221%
15	21.610	3147	3152	3158	rBV2	1050184	1675115	19.01%	6.124%
16	24.806	3689	3696	3704	rVB	638886	1671906	18.97%	6.112%

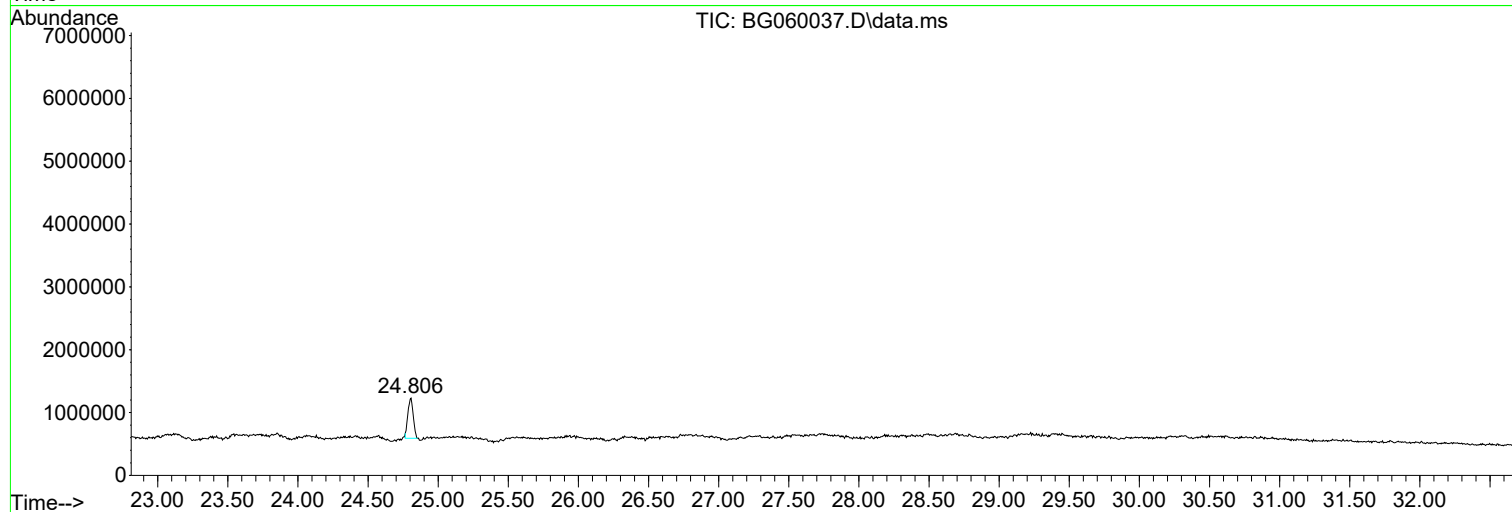
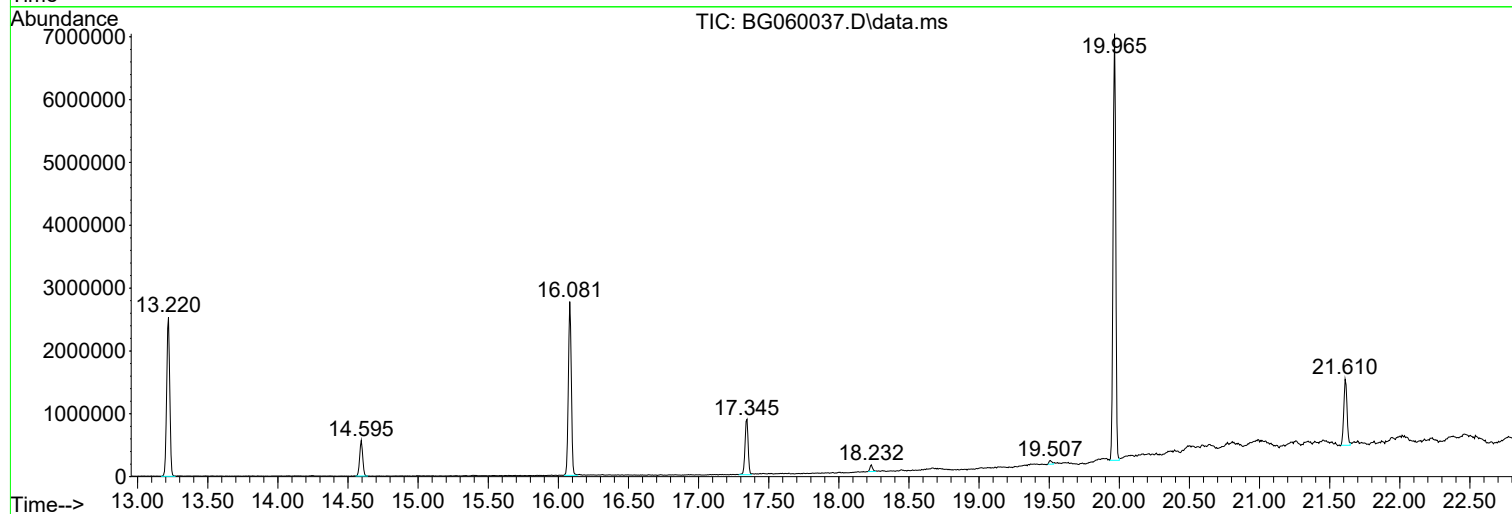
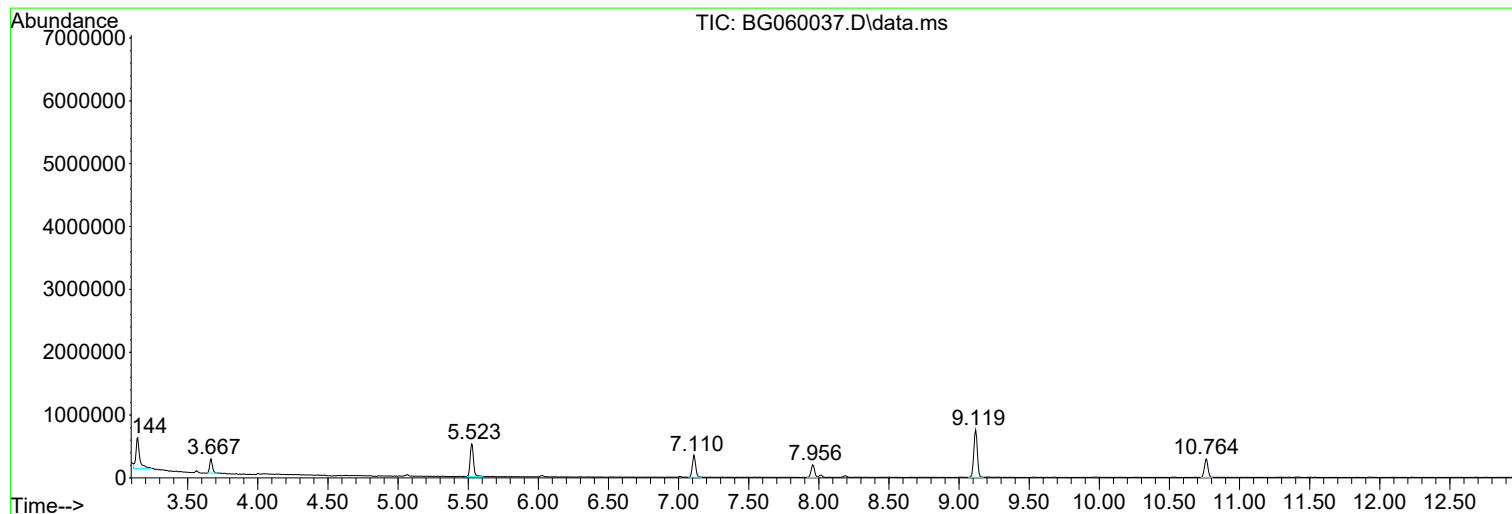
Sum of corrected areas: 27354576

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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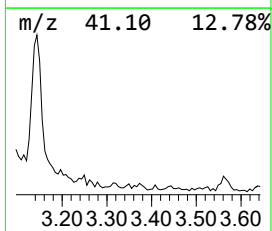
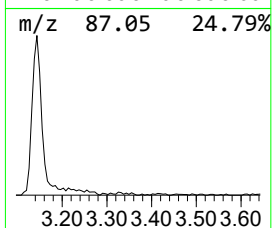
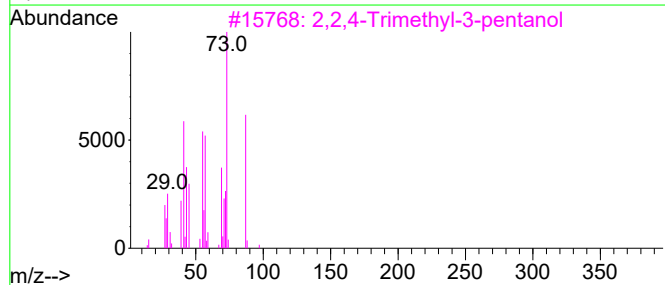
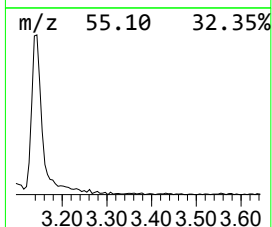
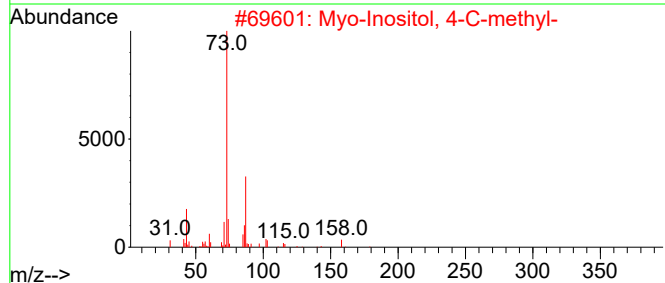
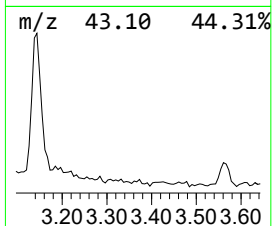
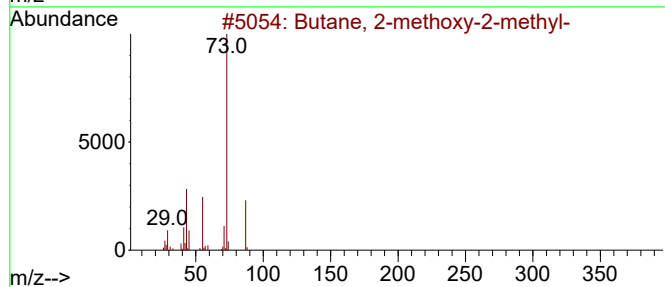
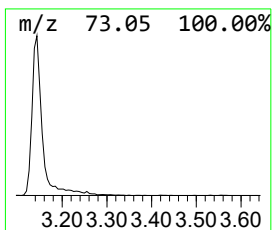
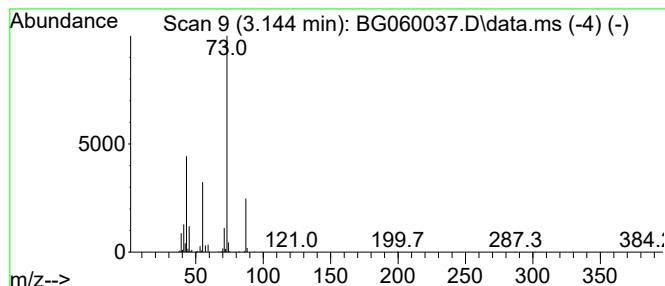
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.144	52.16 ng	919641	1,4-Dichlorobenzene-d4	7.956

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	42
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Myo-Inositol, 2-C-methyl-	194	C7H14O6	000472-96-8	36
5			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36



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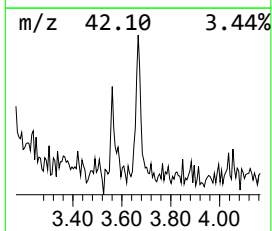
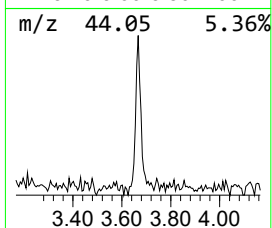
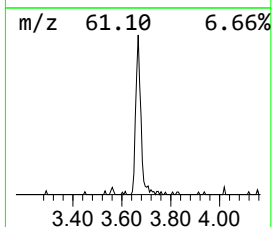
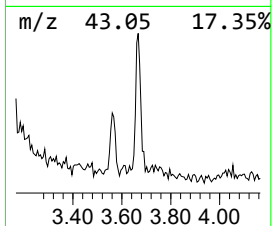
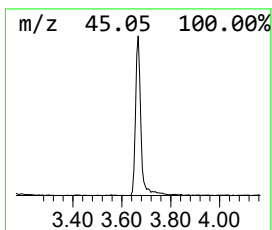
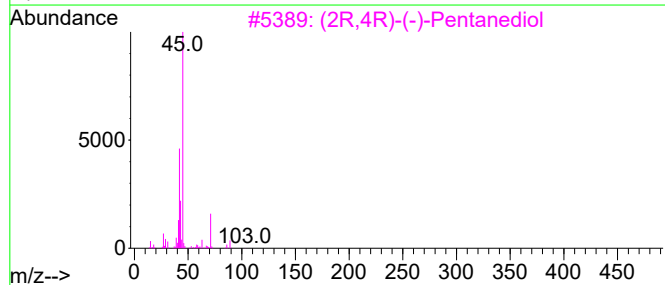
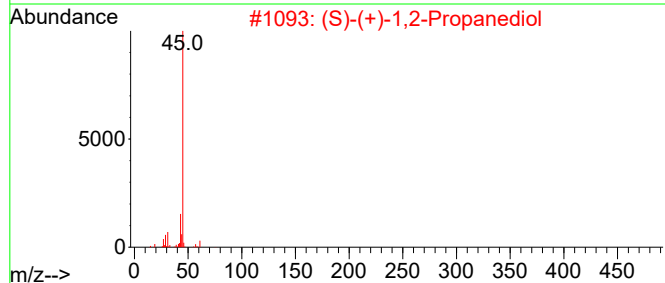
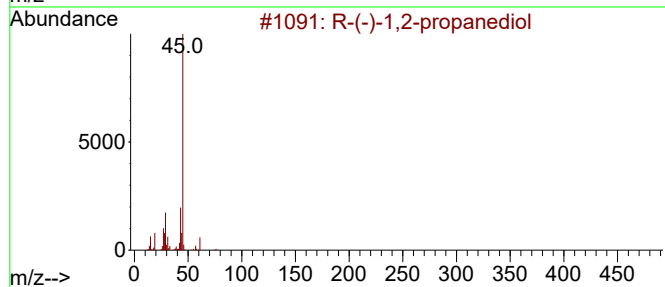
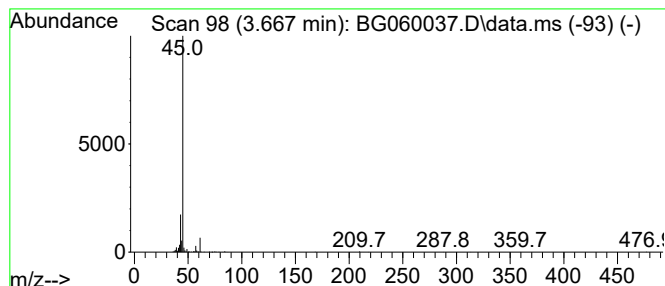
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Peak Number 2 unknown3.667 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.667	17.36 ng	306117	1,4-Dichlorobenzene-d4	7.956

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	40
2	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	9
3	(2R,4R)-(-)-Pentanediol			104	C5H12O2	042075-32-1	9
4	Propylene Glycol			76	C3H8O2	000057-55-6	9
5	2,4-Pentanediol			104	C5H12O2	000625-69-4	9



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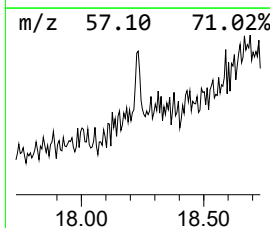
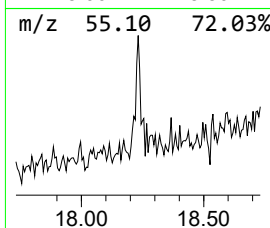
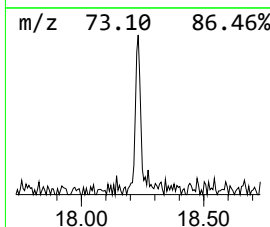
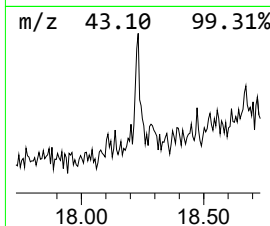
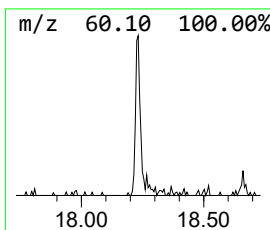
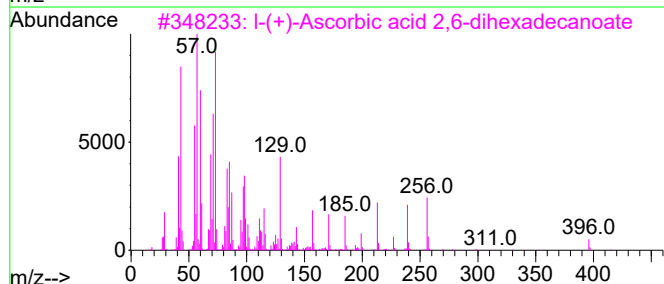
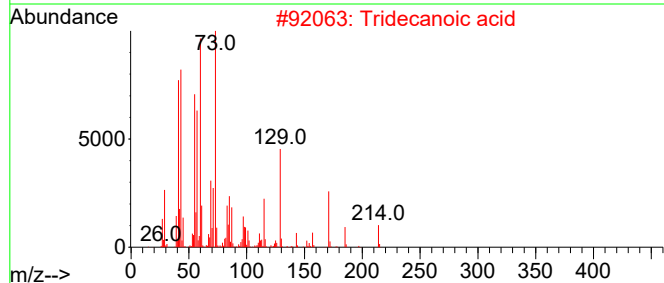
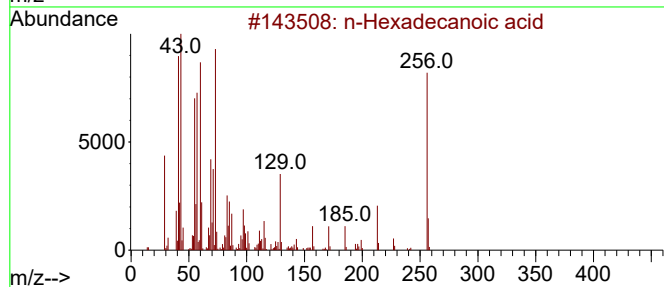
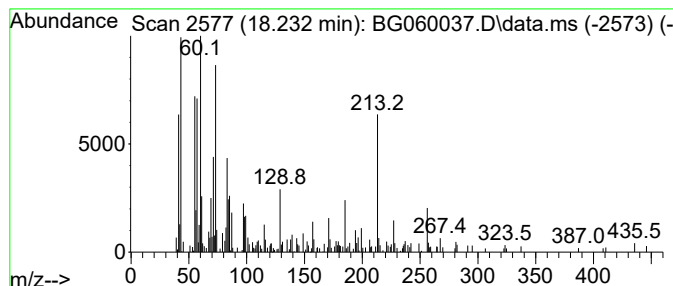
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.232	2.08 ng	140308	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	46
3			l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	46
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5			n-Decanoic acid	172	C10H20O2	000334-48-5	42



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.144	52.2	ng	919641	1	7.956	352644	20.0
unknown3.667	3.667	17.4	ng	306117	1	7.956	352644	20.0
n-Hexadecanoic ...	18.232	2.1	ng	140308	4	17.345	1347150	20.0