

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010224\
 Data File : BF136891.D
 Acq On : 03 Jan 2024 01:38
 Operator : CG\JU
 Sample : 06016-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MR-322-0-2

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_F\Methods\8270-BF122023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136891.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	495	499	510	rVB	108269	128521	7.27%	1.149%
2	5.428	564	568	584	rBV	1583424	1415084	80.03%	12.655%
3	6.428	734	738	741	rBV	1571087	1444190	81.67%	12.915%
4	6.781	794	798	801	rBV	510962	408433	23.10%	3.653%
5	7.345	889	894	897	rBV	961676	967012	54.69%	8.648%
6	8.057	1011	1015	1018	rBV	648108	528578	29.89%	4.727%
7	9.133	1193	1198	1201	rBV	2133944	1768219	100.00%	15.813%
8	9.810	1310	1313	1323	rBV	648988	576358	32.60%	5.154%
9	10.604	1444	1448	1460	rBV	967042	905655	51.22%	8.099%
10	11.304	1563	1567	1571	rBV	689614	559801	31.66%	5.006%
11	11.839	1654	1658	1669	rBV	112362	137527	7.78%	1.230%
12	12.086	1697	1700	1704	rVB2	35226	30522	1.73%	0.273%
13	12.563	1772	1781	1784	rBV5	16773	34049	1.93%	0.304%
14	12.627	1789	1792	1800	rVV3	16675	25990	1.47%	0.232%
15	12.898	1834	1838	1842	rBV	1540644	1445571	81.75%	12.928%
16	13.957	2015	2018	2027	rVB	358483	360508	20.39%	3.224%
17	15.215	2220	2232	2239	rBV10	23335	88440	5.00%	0.791%
18	15.439	2265	2270	2278	rBV	278466	357576	20.22%	3.198%

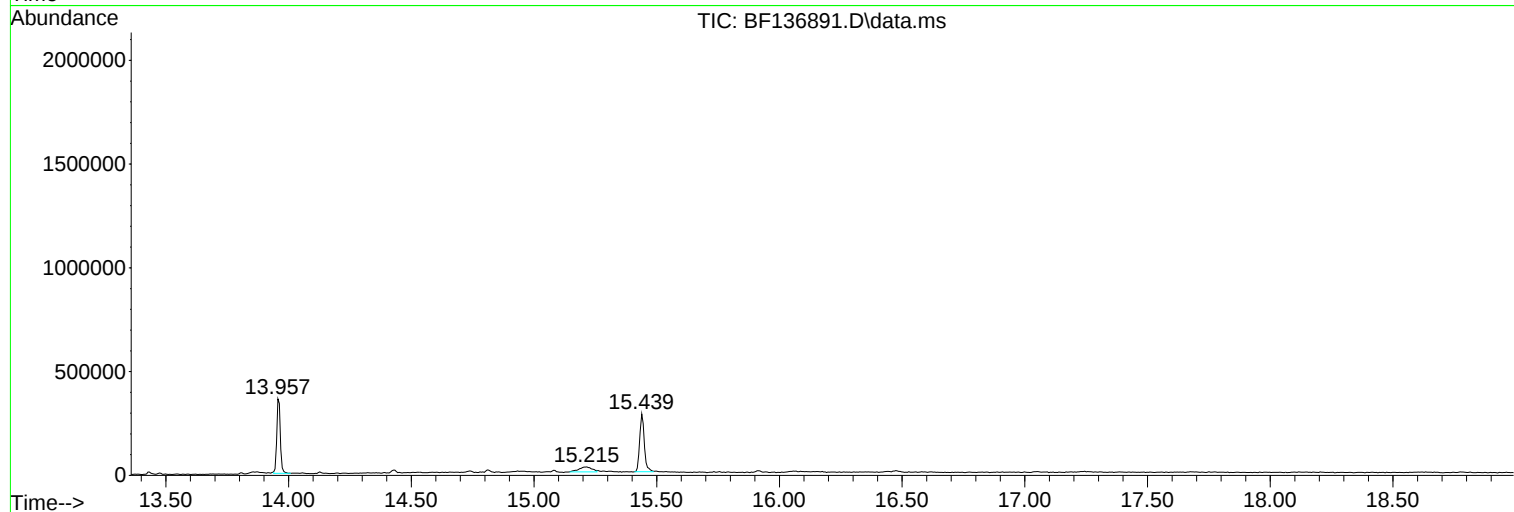
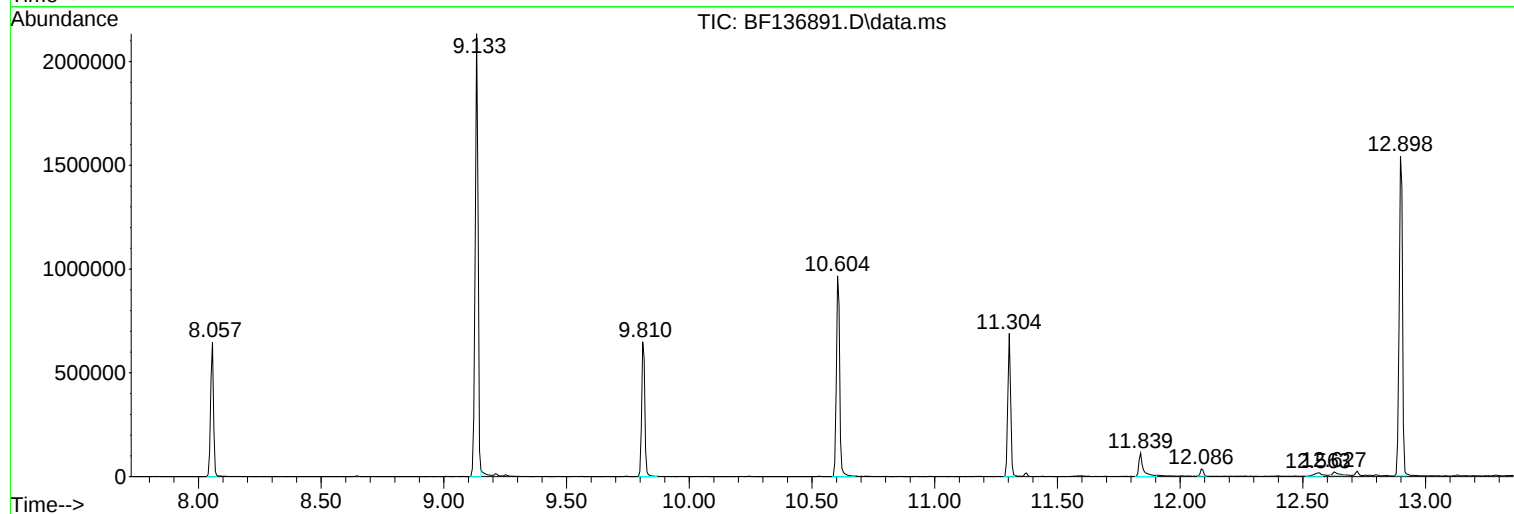
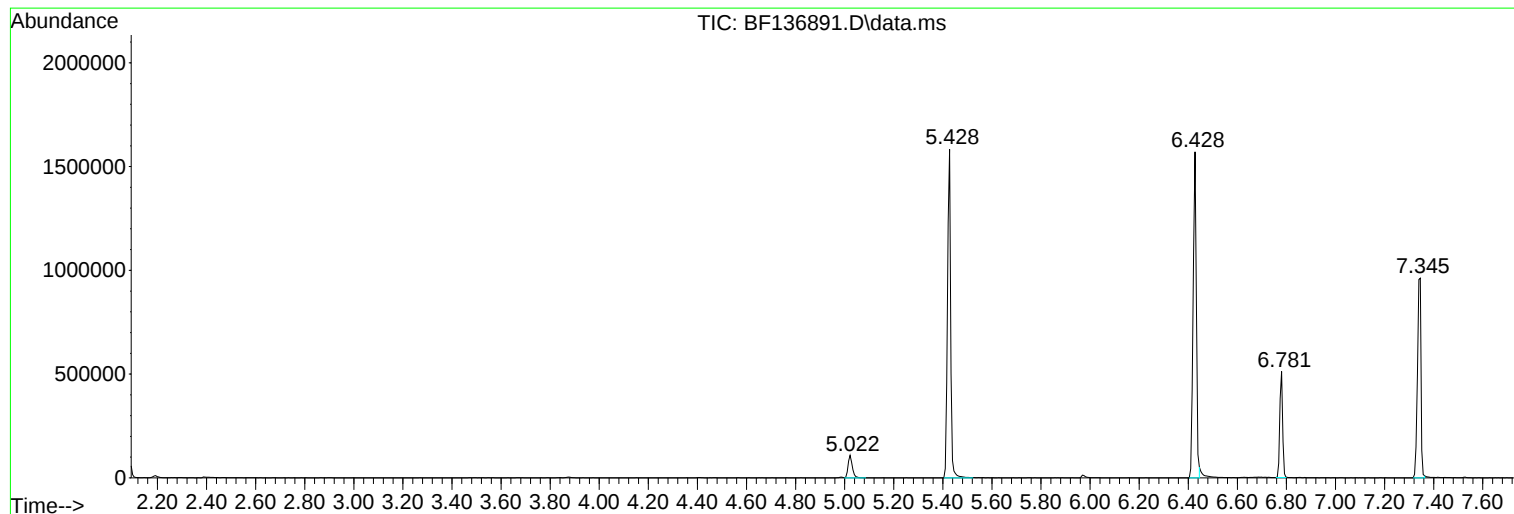
Sum of corrected areas: 11182034

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



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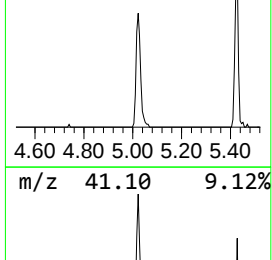
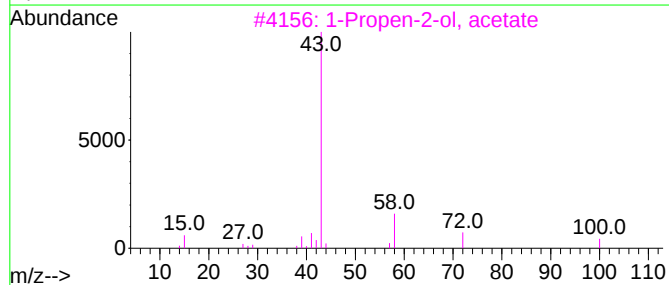
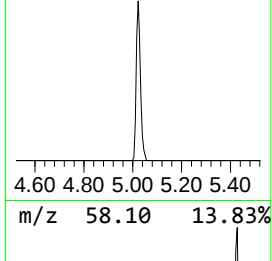
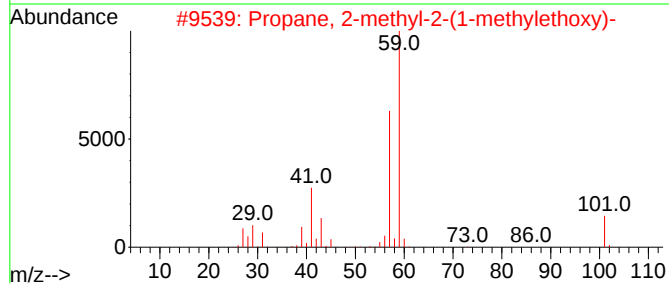
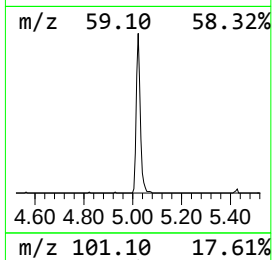
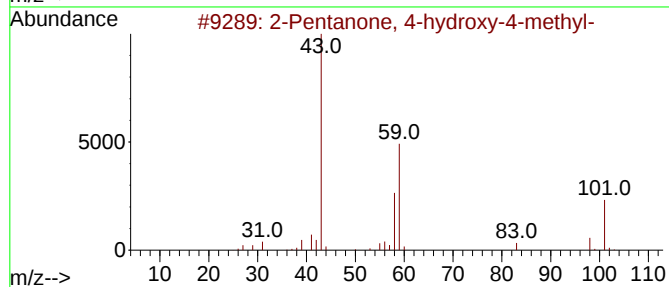
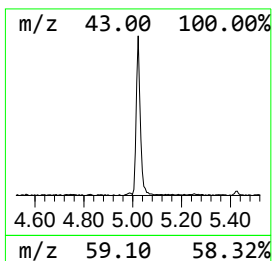
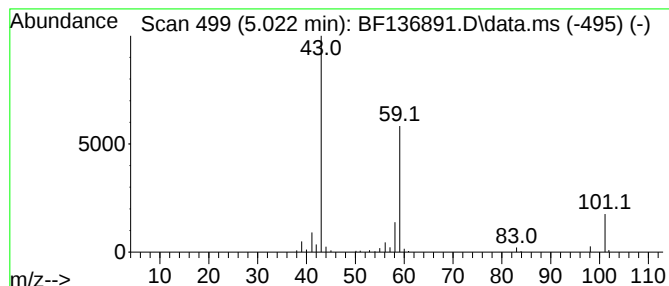
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Peak Number 1 unknown5.022 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	6.29 ng	128521	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9		



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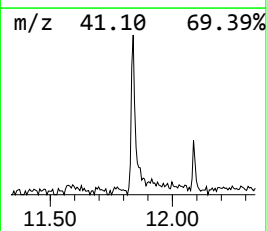
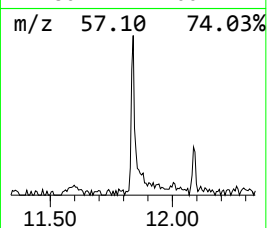
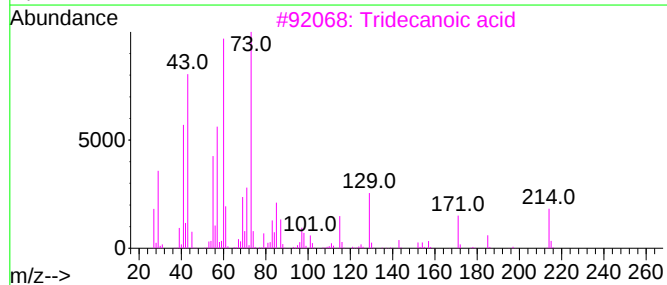
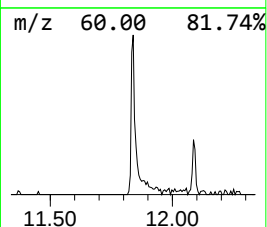
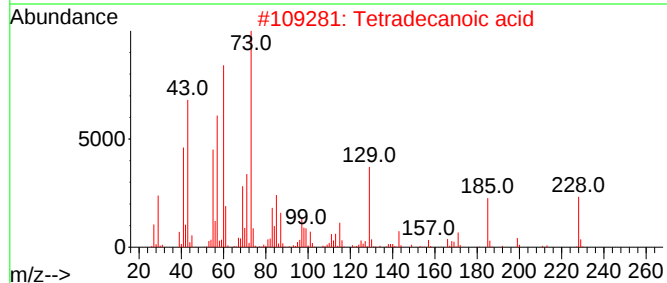
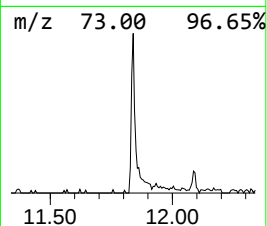
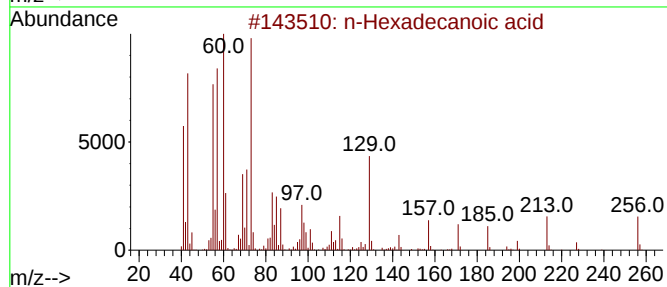
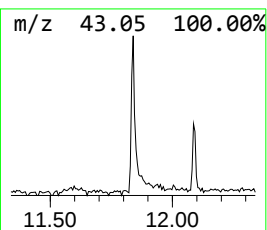
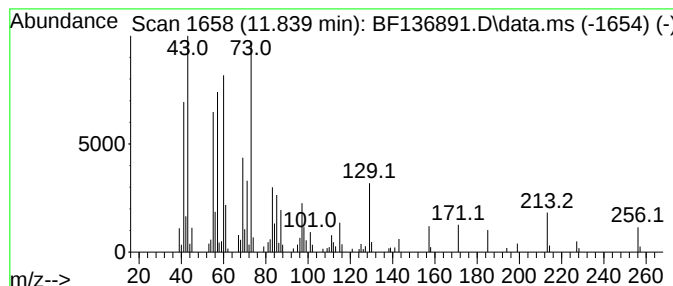
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	4.91 ng	137527	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	43



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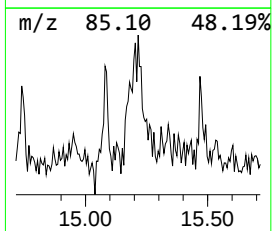
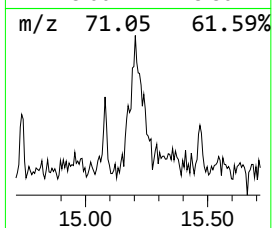
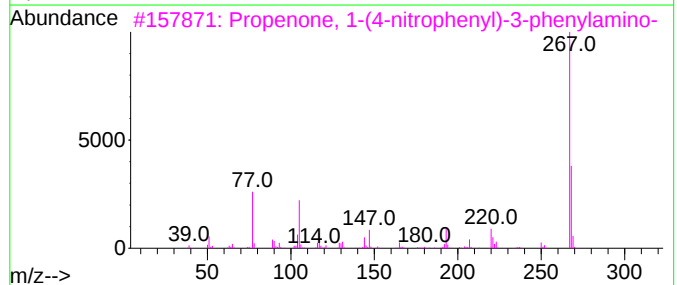
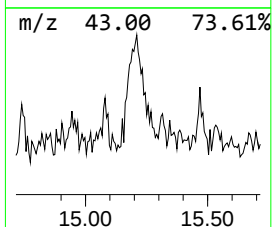
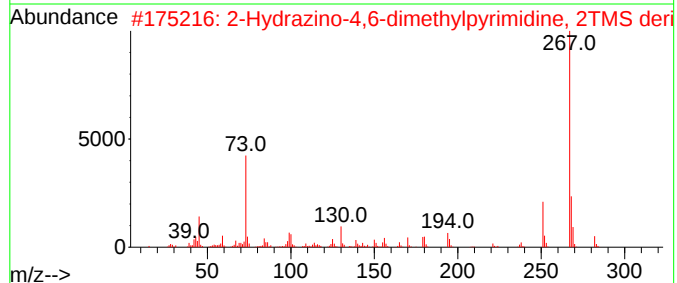
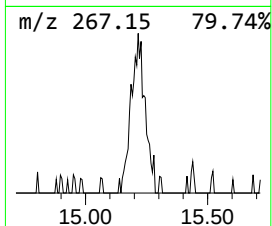
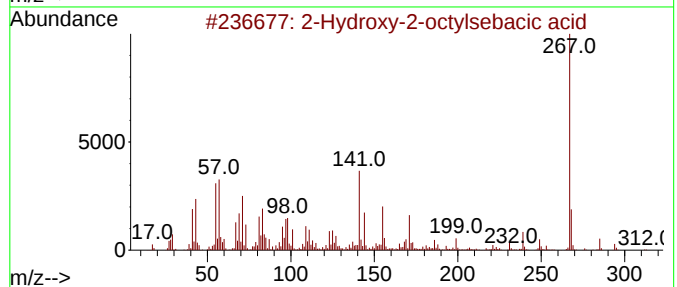
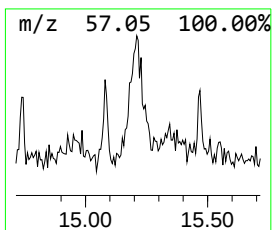
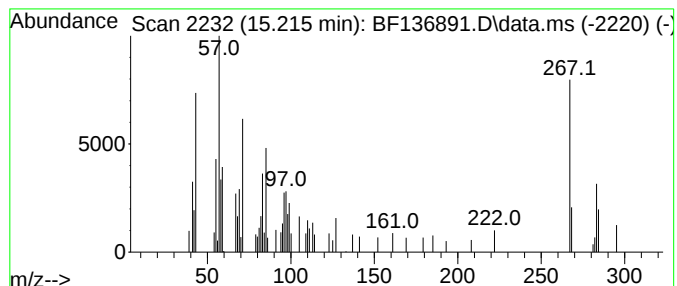
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Peak Number 3 unknown15.215 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.215	4.95 ng	88440	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hydroxy-2-octylsebacic acid	330	C18H34O5	101885-38-5	27
2			2-Hydrazino-4,6-dimethylpyrimidi...	282	C12H26N4Si2	1000332-01-7	25
3			Propenone, 1-(4-nitrophenyl)-3-p...	268	C15H12N2O3	1000302-96-9	22
4			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	22
5			2-(4-chlorophenyl)-4,8-dimethylq...	267	C17H14ClN	1000451-82-4	22



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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
unknown5.022	5.022	6.3	ng	128521	1	6.781	408433	20.0
n-Hexadecanoic ...	11.839	4.9	ng	137527	4	11.304	559801	20.0
unknown15.215	15.215	5.0	ng	88440	6	15.439	357576	20.0