

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM060921\
 Data File : BM030340.D
 Acq On : 09 Jun 2021 13:38
 Operator : CG/JU
 Sample : M2613-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 18-B12(110-114)

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_M\Methods\8270-BM060921.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM030340.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	391	398	411	rBV	3505276	5265551	31.07%	8.231%
2	7.010	657	667	679	rBV	3669868	5777754	34.10%	9.032%
3	7.851	802	810	816	rBV	577175	929154	5.48%	1.453%
4	9.004	998	1006	1015	rBV	2112981	3469797	20.48%	5.424%
5	10.639	1276	1284	1293	rVB	808520	1352912	7.98%	2.115%
6	13.098	1694	1702	1713	rBV	5751420	8459670	49.92%	13.225%
7	14.469	1928	1935	1943	rBV	1287765	1982013	11.70%	3.098%
8	15.957	2179	2188	2206	rBV	4898860	7227275	42.65%	11.298%
9	17.204	2392	2400	2411	rBV	1863131	2695714	15.91%	4.214%
10	18.092	2545	2551	2561	rBV	312063	502752	2.97%	0.786%
11	19.251	2739	2748	2763	rBV2	312828	1037292	6.12%	1.622%
12	19.368	2764	2768	2779	rVB	212173	355527	2.10%	0.556%
13	19.821	2839	2845	2854	rBV	13891310	16945069	100.00%	26.489%
14	21.086	3056	3060	3071	rBV4	114868	287201	1.69%	0.449%
15	21.368	3103	3108	3117	rBV	2938847	3686322	21.75%	5.763%
16	22.562	3307	3311	3317	rVB	314151	416166	2.46%	0.651%
17	23.650	3489	3496	3510	rVB2	1813663	3579045	21.12%	5.595%

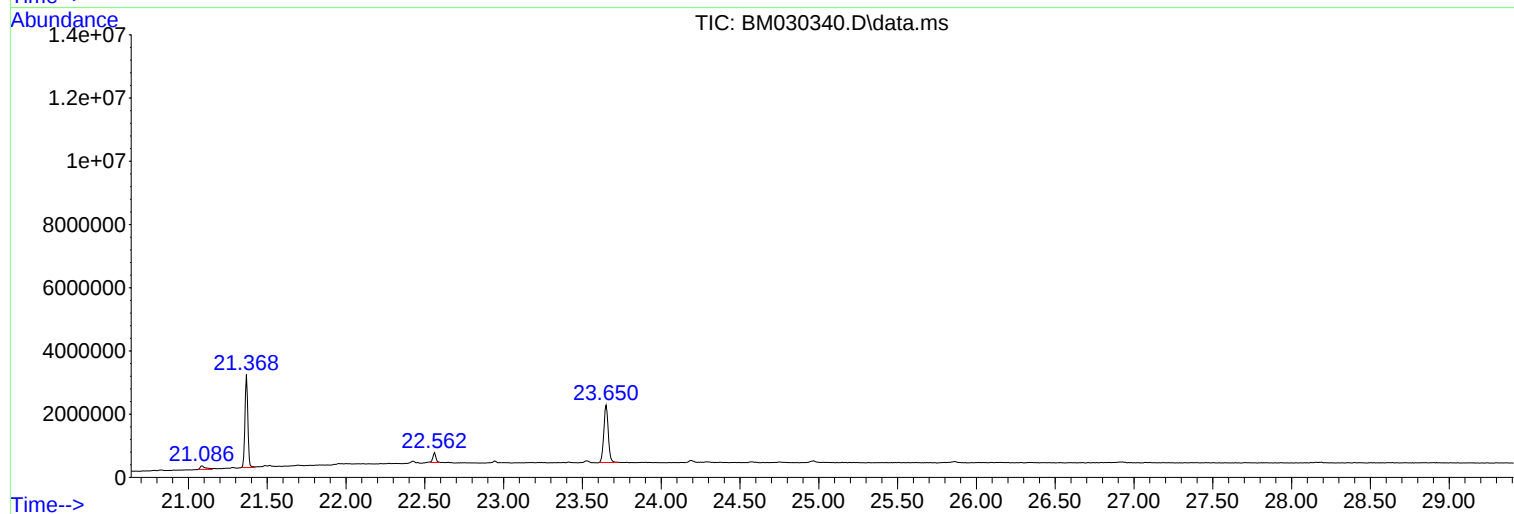
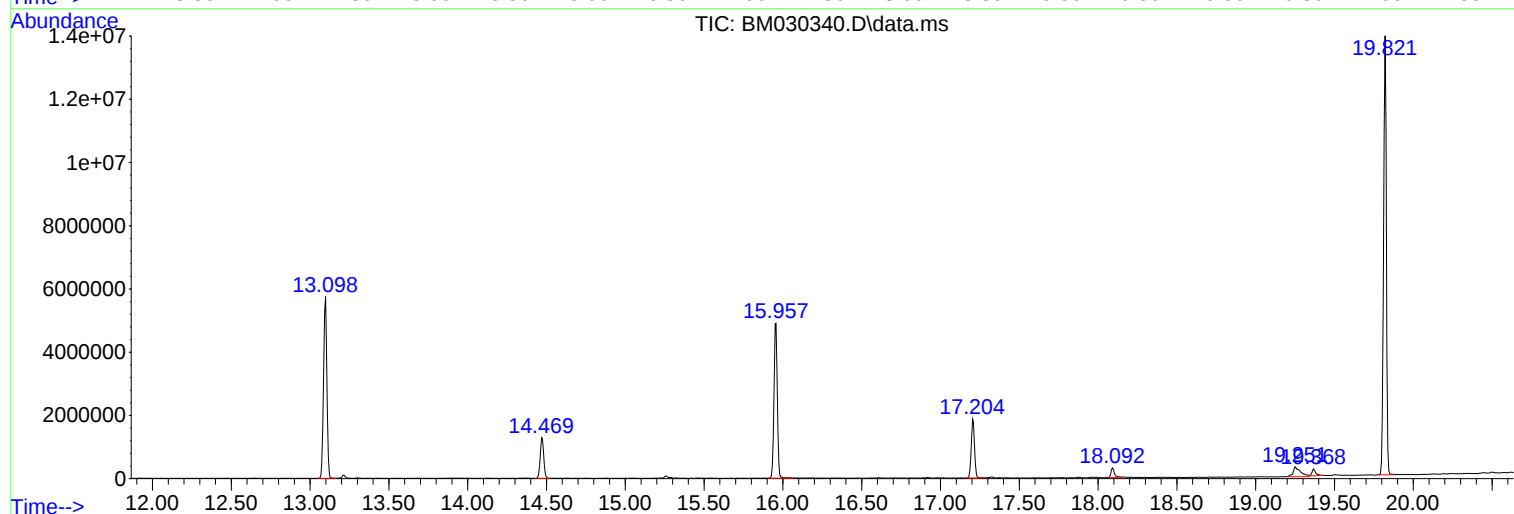
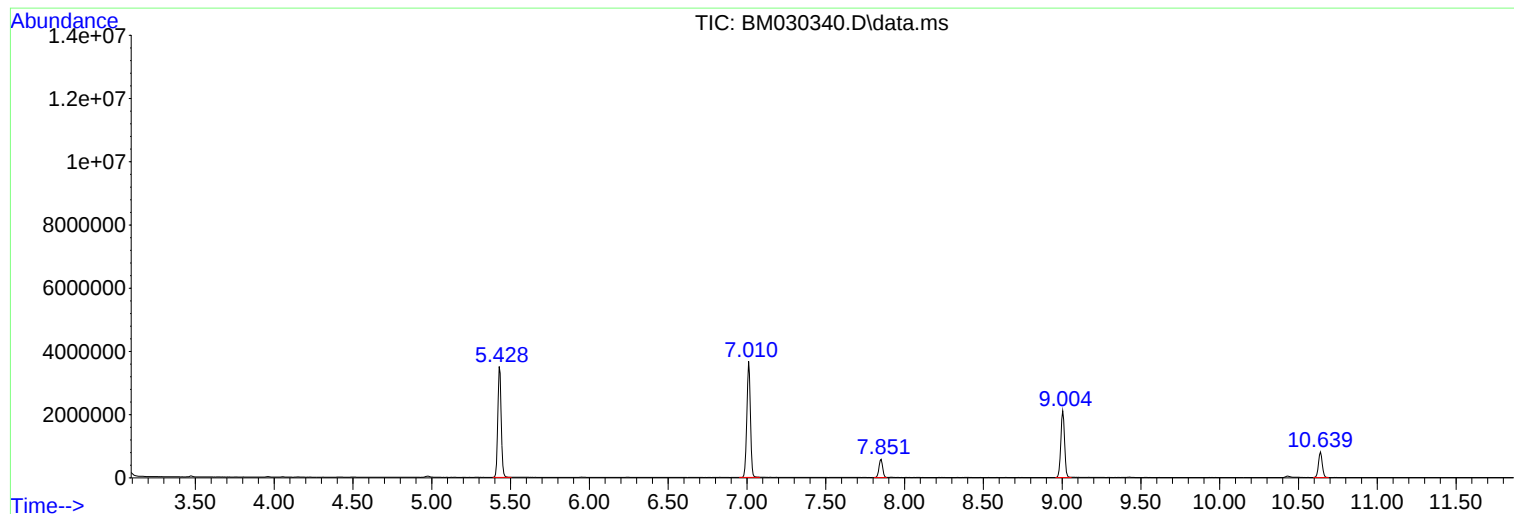
Sum of corrected areas: 63969214

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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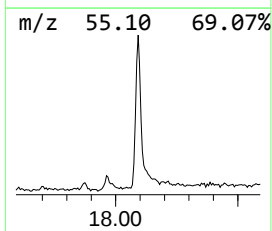
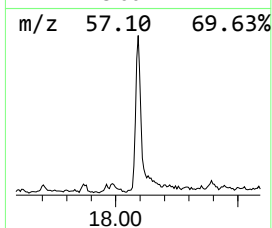
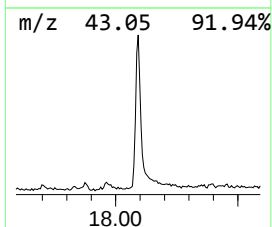
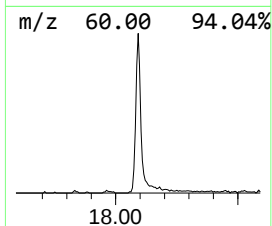
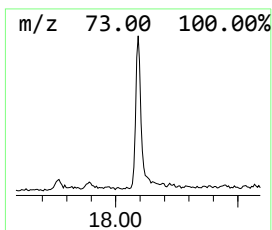
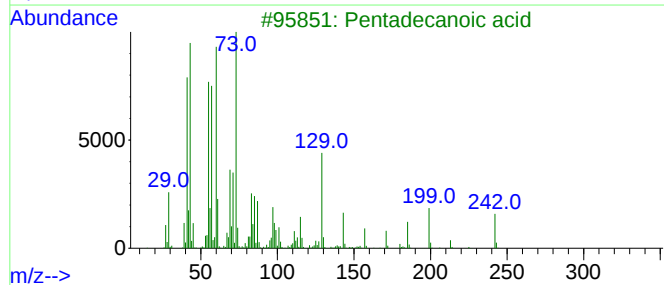
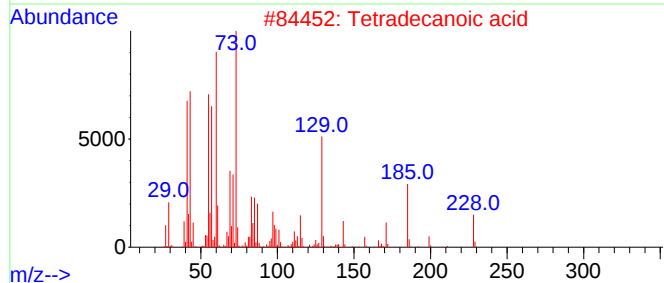
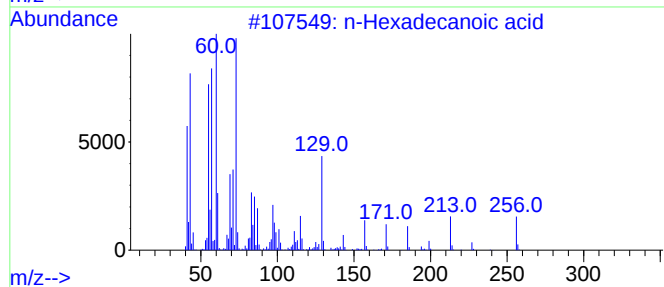
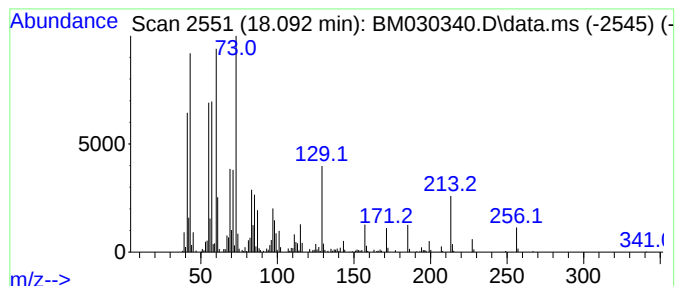
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	3.73 ng	502752	Phenanthrene-d10	17.204

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	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		n-Decanoic acid	172	C10H20O2	000334-48-5	83
5		Tridecanoic acid	214	C13H26O2	000638-53-9	81



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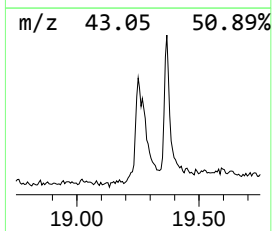
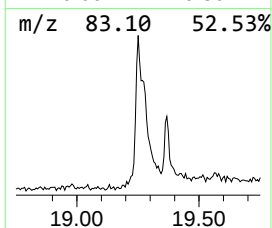
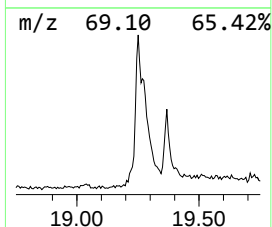
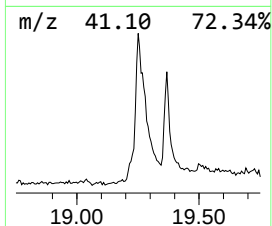
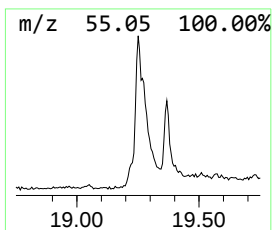
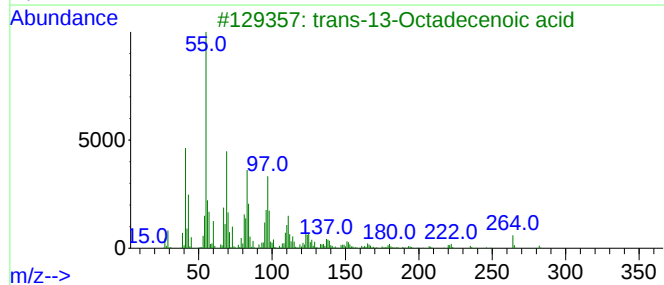
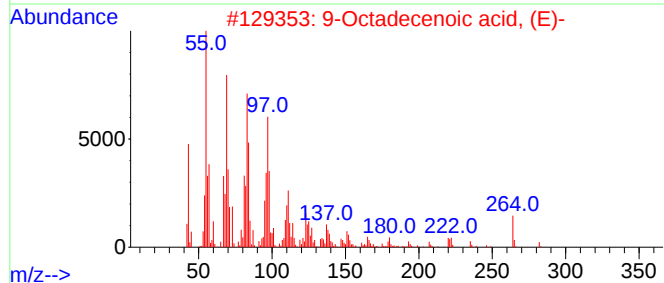
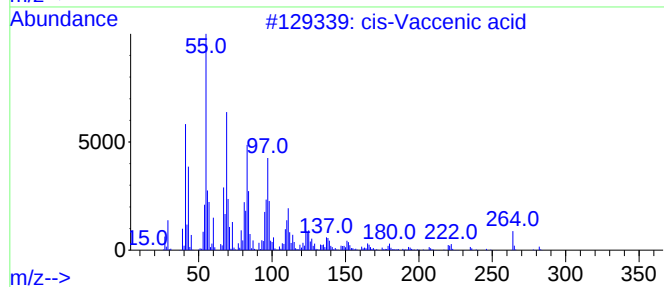
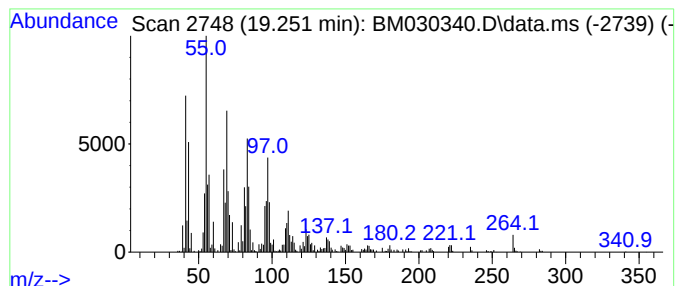
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Peak Number 2 cis-Vaccenic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.251	7.70 ng	1037290	Phenanthrene-d10	17.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	99
2			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	99
3			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	99
4			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	99
5			Oleic Acid	282	C18H34O2	000112-80-1	99



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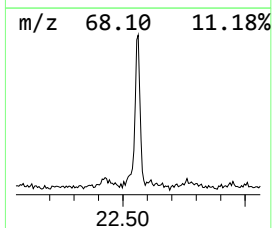
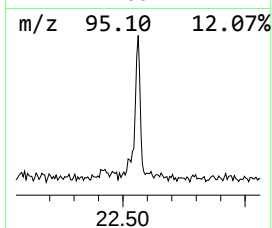
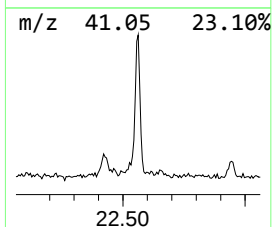
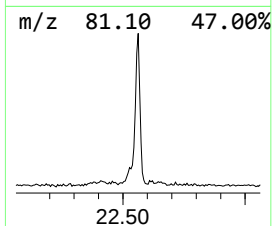
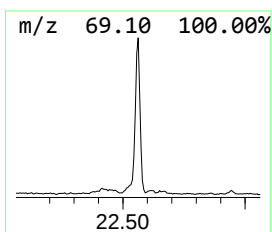
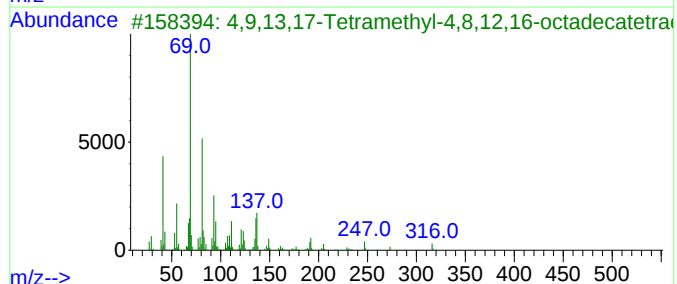
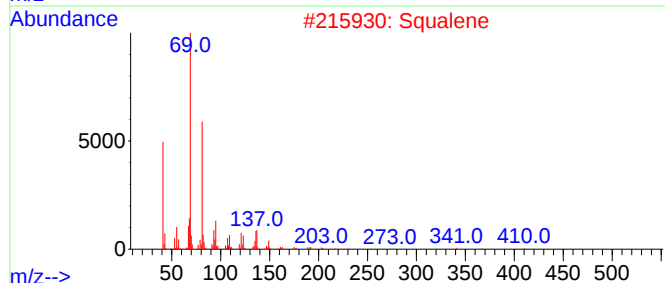
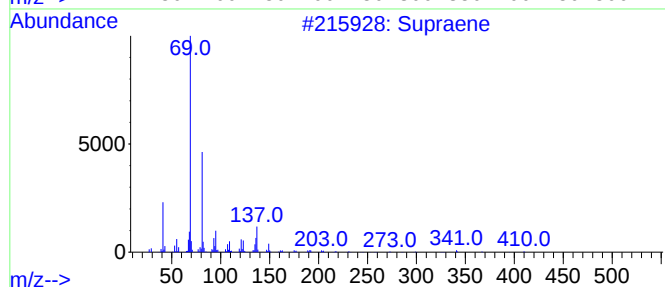
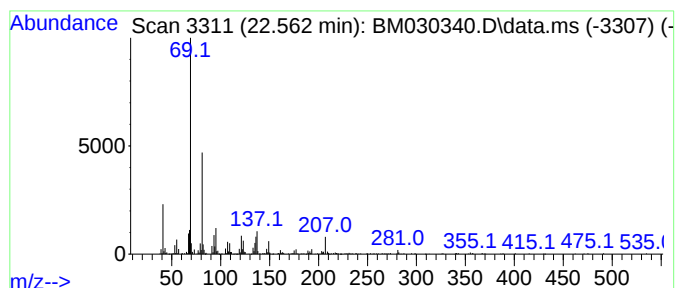
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Peak Number 3 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.562	2.33 ng	416166	Perylene-d12	23.650

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	81
2			Squalene	410	C30H50	000111-02-4	81
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	64
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.092	3.7	ng	502752	4	17.204	2695710	20.0
cis-Vaccenic acid	19.251	7.7	ng	1037290	4	17.204	2695710	20.0
Supraene	22.562	2.3	ng	416166	6	23.650	3579050	20.0