

Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN082418\
 Data File : BN002525.D
 Acq On : 25 Aug 2018 05:33
 Operator : JU/SJ
 Sample : J4628-19
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 DB3G4

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 1 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN081318MA.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.852	652	657	669	rVB2	143939	264264	4.29%	0.519%
2	7.011	679	684	695	rVB	512284	799724	12.98%	1.572%
3	7.205	712	717	730	rVB	518679	863306	14.01%	1.696%
4	7.669	790	796	807	rVB	425333	689700	11.19%	1.355%
5	8.375	910	916	927	rVB	411969	697600	11.32%	1.371%
6	8.816	985	991	1003	rVB	705310	1175803	19.08%	2.311%
7	9.534	1106	1113	1129	rVB	546613	951688	15.45%	1.870%
8	9.805	1152	1159	1175	rVB	135798	285369	4.63%	0.561%
9	10.069	1198	1204	1222	rVB	726261	1364578	22.15%	2.681%
10	10.440	1260	1267	1276	rVB	634682	1068092	17.34%	2.099%
11	10.951	1349	1354	1365	rBV	28399	77690	1.26%	0.153%
12	12.587	1627	1632	1646	rBV	69405	129143	2.10%	0.254%
13	13.716	1817	1824	1832	rBV	1654040	2354198	38.21%	4.626%
14	13.993	1864	1871	1878	rBV	1880773	2787792	45.25%	5.478%
15	14.298	1917	1923	1932	rBV2	992066	1510562	24.52%	2.968%
16	14.522	1957	1961	1977	rBV	88439	198206	3.22%	0.389%
17	14.745	1991	1999	2011	rBV	400283	645856	10.48%	1.269%
18	15.298	2086	2093	2101	rVB	2433135	3519680	57.13%	6.916%
19	15.428	2109	2115	2128	rBV	780194	1139194	18.49%	2.239%
20	15.869	2185	2190	2195	rBV	250803	303946	4.93%	0.597%
21	15.922	2195	2199	2204	rVB	500417	610096	9.90%	1.199%
22	16.863	2353	2359	2372	rBV2	115872	256970	4.17%	0.505%
23	17.045	2384	2390	2399	rBV2	1301194	1923440	31.22%	3.780%
24	17.145	2400	2407	2415	rVV2	2776712	4026968	65.36%	7.913%
25	17.345	2436	2441	2445	rBV	885822	1079960	17.53%	2.122%
26	17.392	2445	2449	2459	rVB	1881091	2233252	36.25%	4.388%
27	19.451	2792	2799	2808	rBV	3556251	4949224	80.33%	9.726%
28	19.833	2861	2864	2868	rVB	78949	84427	1.37%	0.166%
29	20.775	3020	3024	3027	rBV	133261	155013	2.52%	0.305%
30	20.810	3027	3030	3043	rVB	371941	425619	6.91%	0.836%
31	21.245	3099	3104	3113	rVB	2082390	2619330	42.51%	5.147%
32	21.645	3168	3172	3174	rBV	186666	204228	3.31%	0.401%
33	21.680	3174	3178	3184	rVB	430743	516520	8.38%	1.015%
34	22.257	3272	3276	3279	rBV	97540	119695	1.94%	0.235%

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35	22.298	3279	3283	3288	rVB	78447	99252	1.61%	0.195%
36	22.569	3324	3329	3331	rBV	214103	292487	4.75%	0.575%
37	22.604	3331	3335	3343	rVB	499561	694101	11.27%	1.364%
38	22.798	3364	3368	3373	rVB2	107322	152269	2.47%	0.299%
39	23.327	3450	3458	3469	rVB	3251841	6161230	100.00%	12.107%
40	23.463	3474	3481	3490	rVB2	1518604	2798396	45.42%	5.499%
41	23.980	3564	3569	3575	rBV	118614	224389	3.64%	0.441%
42	24.710	3687	3693	3703	rVB2	127201	282001	4.58%	0.554%
43	25.562	3833	3838	3846	rVB3	64365	153685	2.49%	0.302%

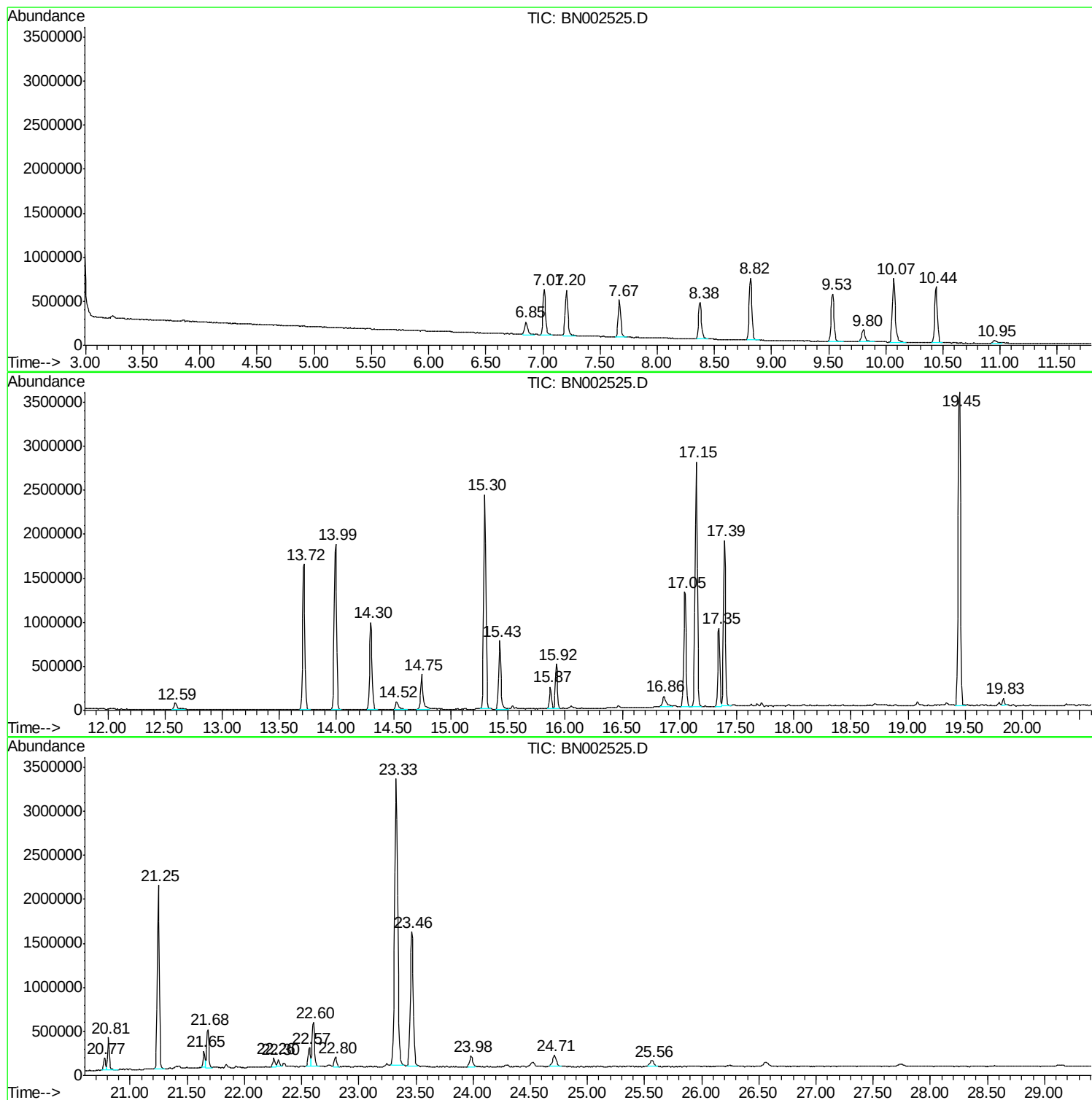
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Quant Title : SVOA CALIBRATION

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



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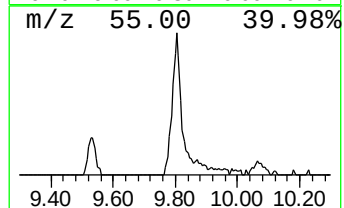
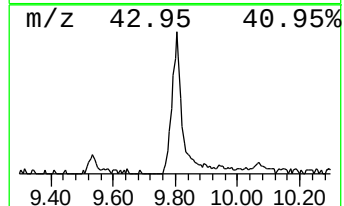
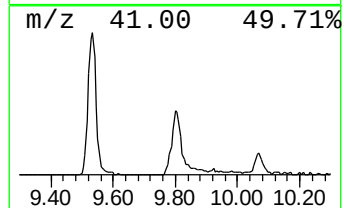
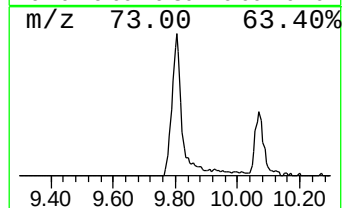
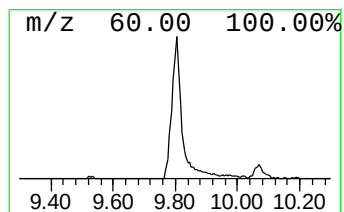
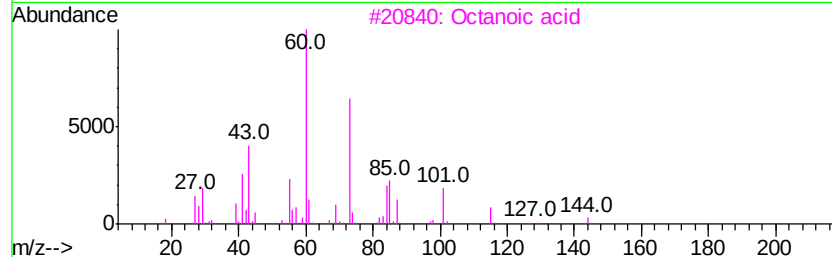
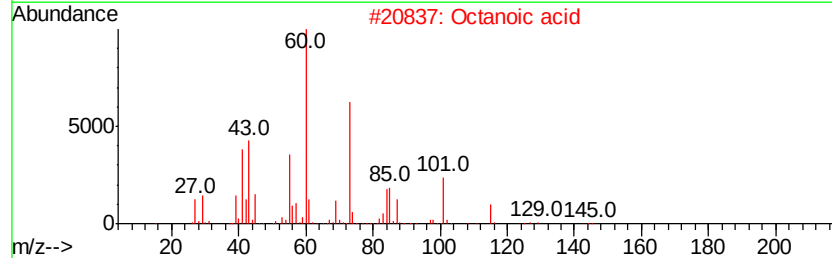
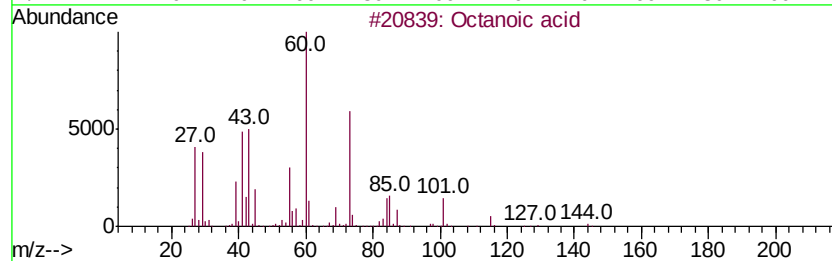
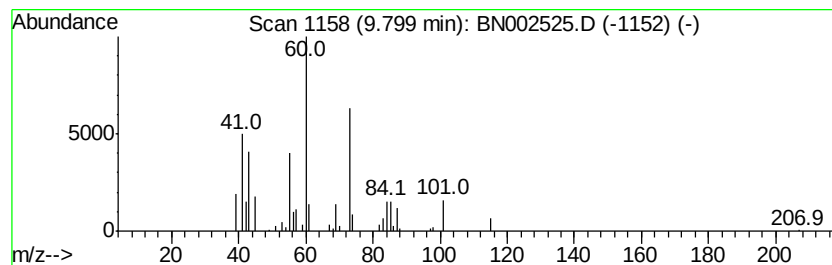
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN081318MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Octanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.80	5.34 ng/ul	285369	Napthalene-d8	10.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanoic acid	144	C8H16O2	000124-07-2	90
2		Octanoic acid	144	C8H16O2	000124-07-2	86
3		Octanoic acid	144	C8H16O2	000124-07-2	86
4		Hexanoic acid	116	C6H12O2	000142-62-1	64
5		Hexanoic acid	116	C6H12O2	000142-62-1	59



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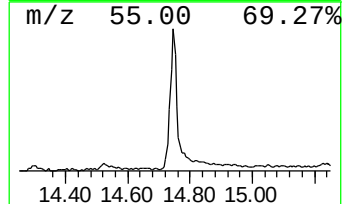
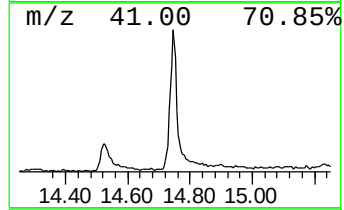
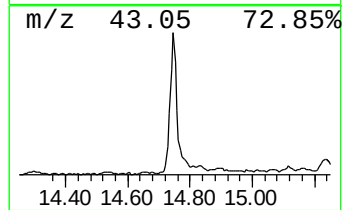
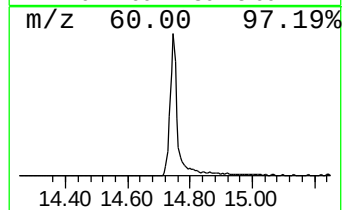
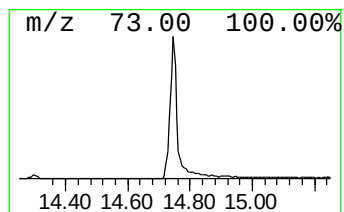
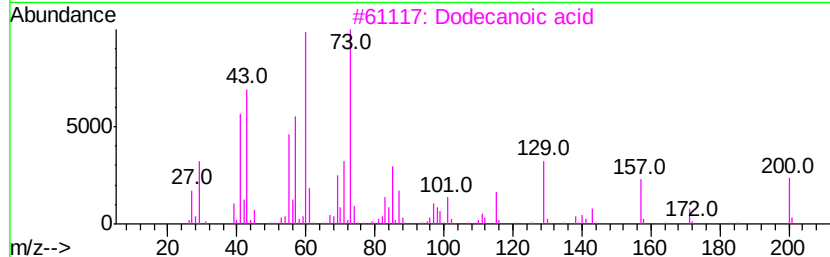
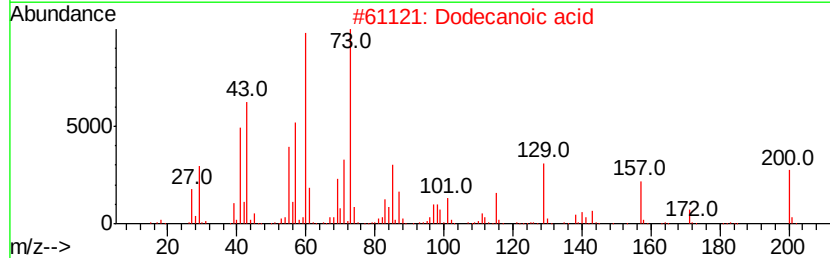
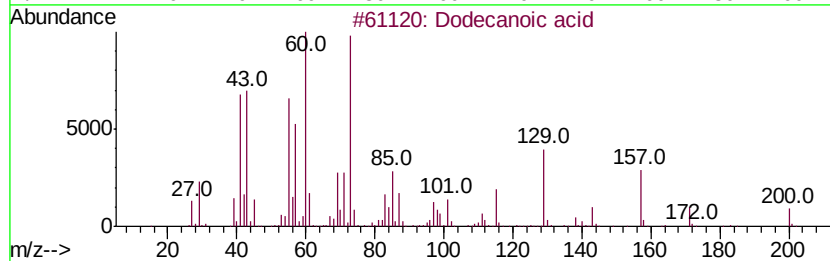
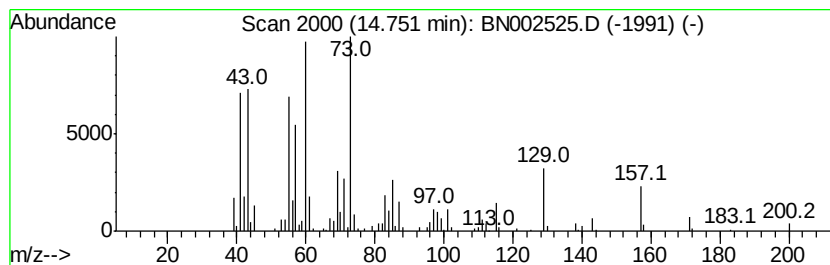
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TIC Library : C:\Database\NIST11.L
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Peak Number 2 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	8.55 ng/ul	645856	Acenaphthene-d10	14.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	98
2		Dodecanoic acid	200	C12H24O2	000143-07-7	91
3		Dodecanoic acid	200	C12H24O2	000143-07-7	90
4		Undecanoic acid	186	C11H22O2	000112-37-8	86
5		Dodecanoic acid	200	C12H24O2	000143-07-7	76



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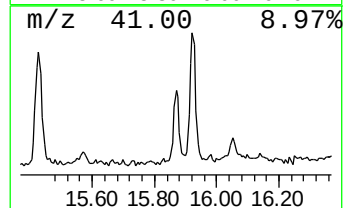
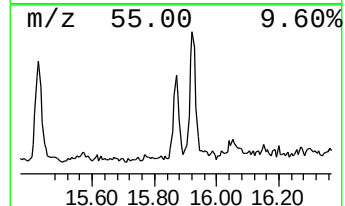
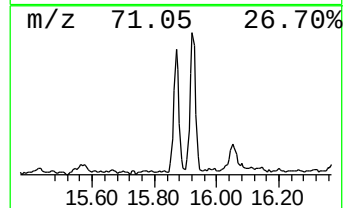
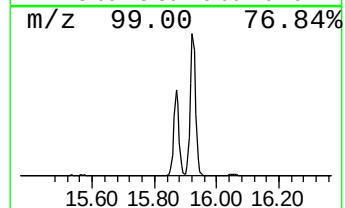
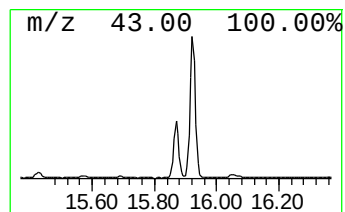
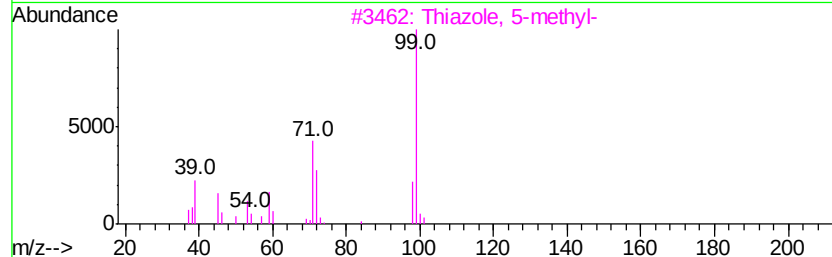
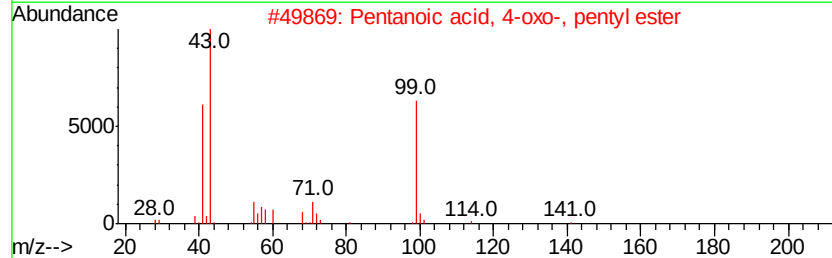
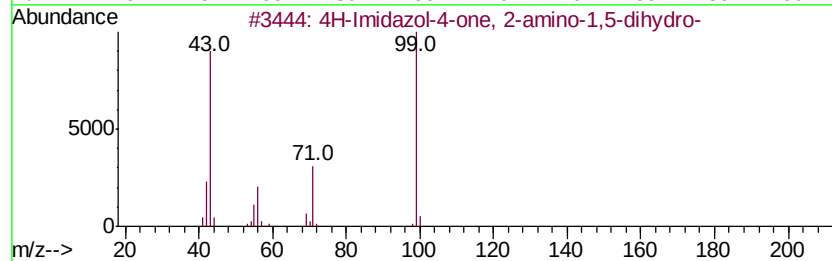
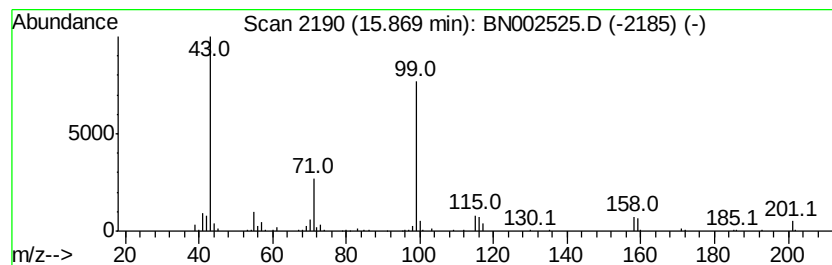
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Imidazol-4-one, 2-amino-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	3.16 ng/ul	303946	Phenanthrene-d10	17.05
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	4H-Imidazol-4-one, 2-amino-1,5-d...	99 C3H5N3O	000503-86-6	64
2	Pentanoic acid, 4-oxo-, pentyl e...	186 C10H18O3	020279-49-6	64
3	Thiazole, 5-methyl-	99 C4H5NS	003581-89-3	50
4	1H-1,2,3,4-Tetrazol-5-amine, 1-m...	99 C2H5N5	1000338-04-0	50
5	Furan, 2,5-dihydro-2,5-dimethoxy-	130 C6H10O3	000332-77-4	50



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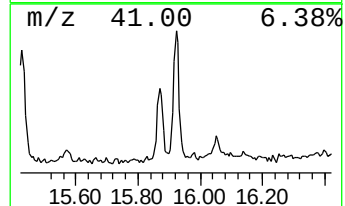
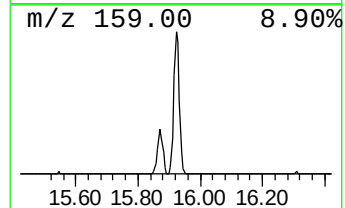
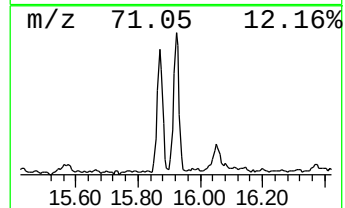
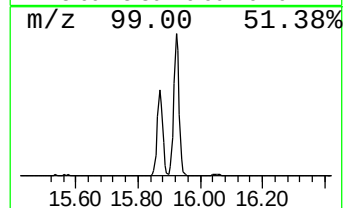
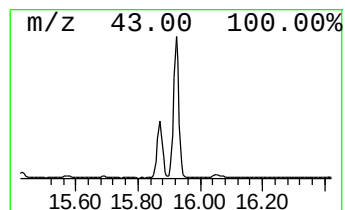
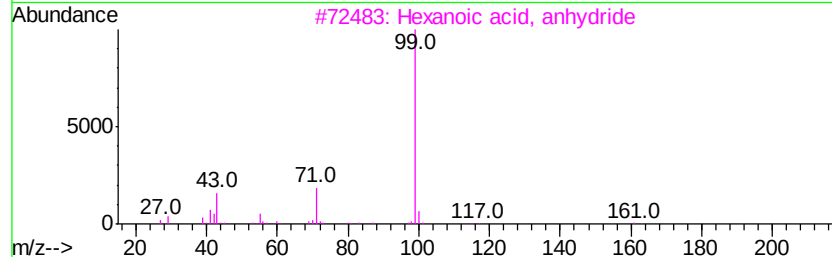
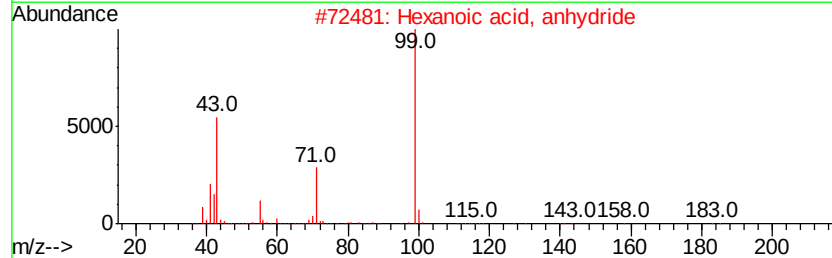
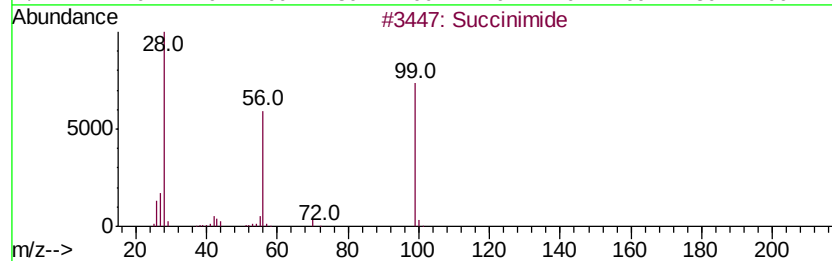
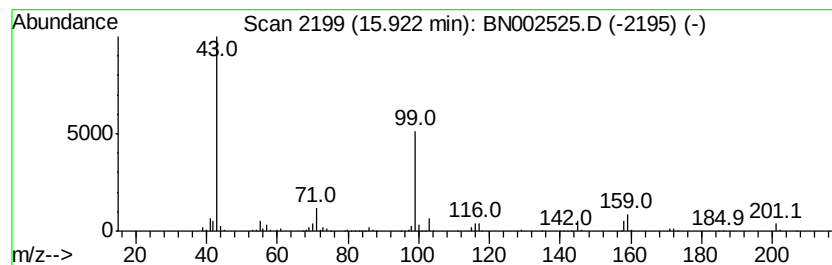
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Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.92	6.34 ng/ul	610096	Phenanthrene-d10	17.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinimide	99	C4H5NO2	000123-56-8	43
2	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	43
3	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	43
4	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	43
5	Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	40



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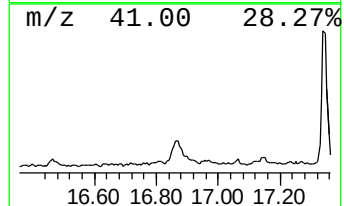
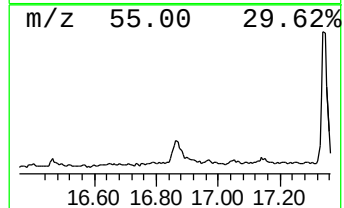
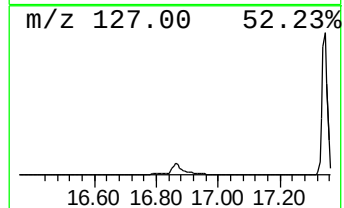
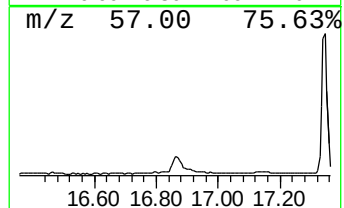
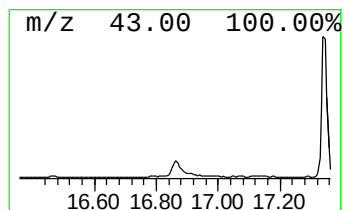
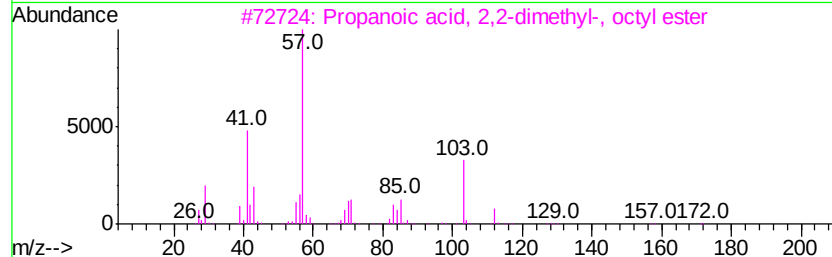
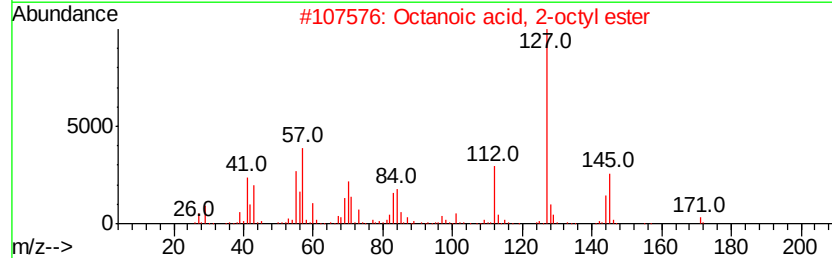
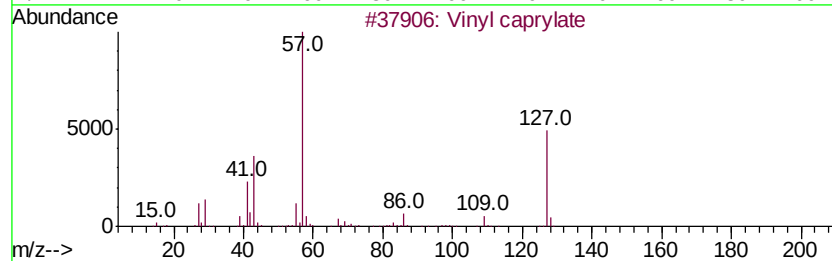
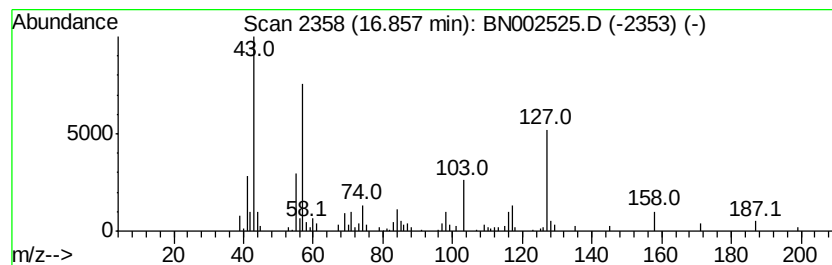
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Peak Number 5 unknown-02 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	2.67 ng/ul	256970	Phenanthrene-d10	17.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Vinyl caprylate	170	C10H18O2	000818-44-0	35
2		Octanoic acid, 2-octyl ester	256	C16H32O2	055193-33-4	32
3		Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	25
4		2,2-Dimethylpropionic acid, dode...	270	C17H34O2	131141-69-0	22
5		2,5-Pyrrolidinedione, 3-ethyl-1,...	155	C8H13NO2	013861-99-9	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN082418\
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Acq On : 25 Aug 2018 05:33
Operator : JU/SJ
Sample : J4628-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

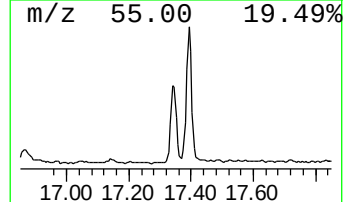
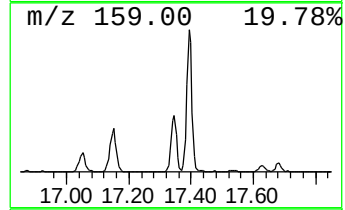
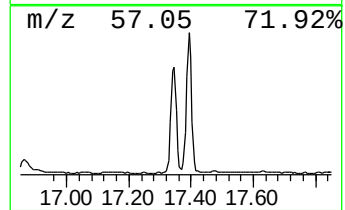
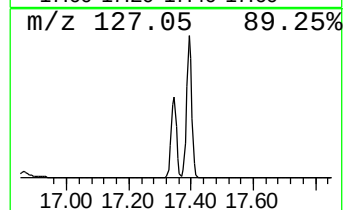
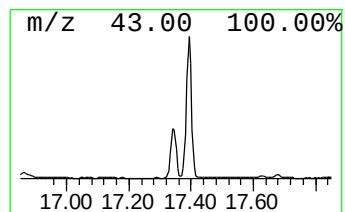
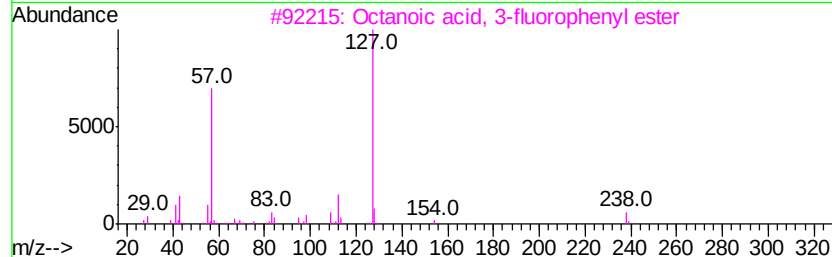
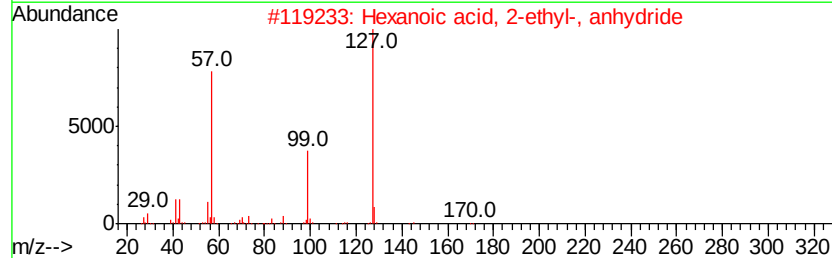
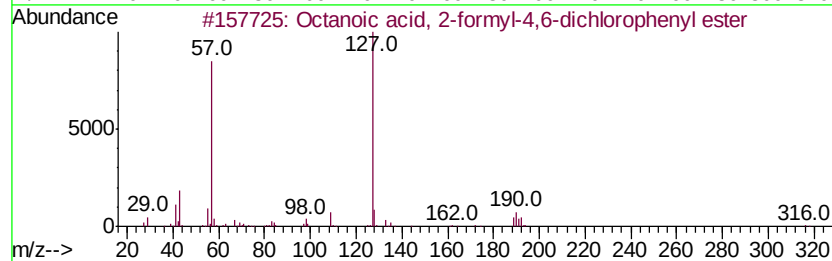
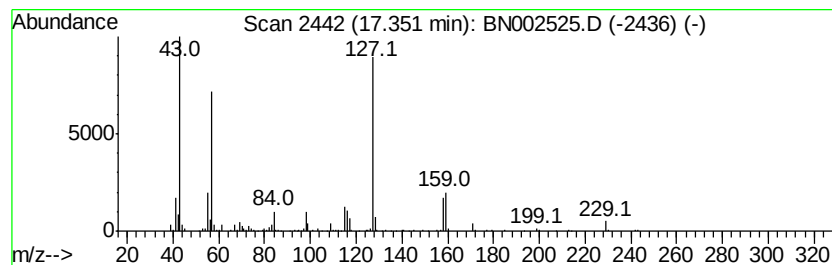
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.35	11.23 ng/ul	1079960	Phenanthrene-d10	17.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid, 2-formyl-4,6-dich...	316	C15H18Cl2O3	1000330-95-4	43
2	Hexanoic acid, 2-ethyl-, anhydride	270	C16H30O3	036765-89-6	43
3	Octanoic acid, 3-fluorophenyl ester	238	C14H19FO2	1000330-94-7	43
4	Octanethioic acid, S-hexyl ester	244	C14H28OS	055590-85-7	40
5	Phosphonofluoridic acid, (1-meth...	224	C10H22FO2P	333416-33-4	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN082418\
Data File : BN002525.D
Acq On : 25 Aug 2018 05:33
Operator : JU/SJ
Sample : J4628-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

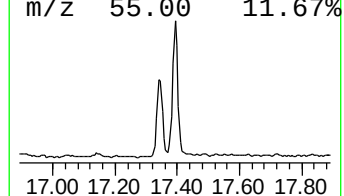
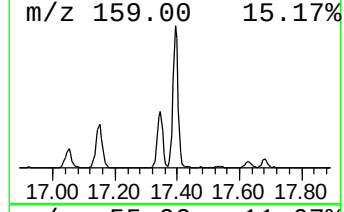
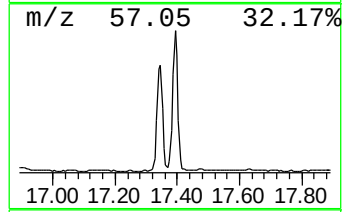
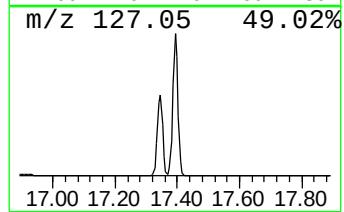
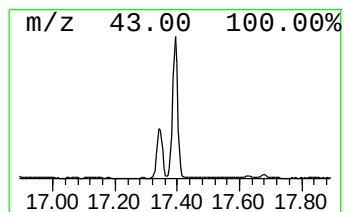
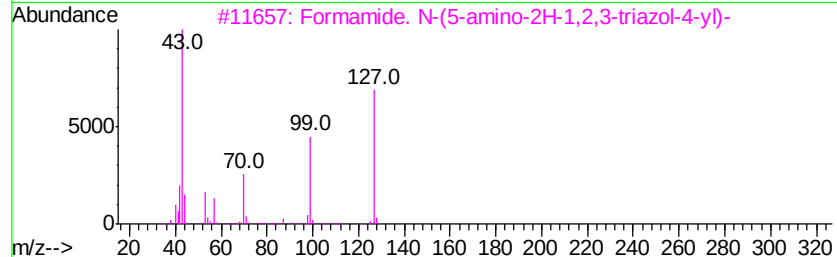
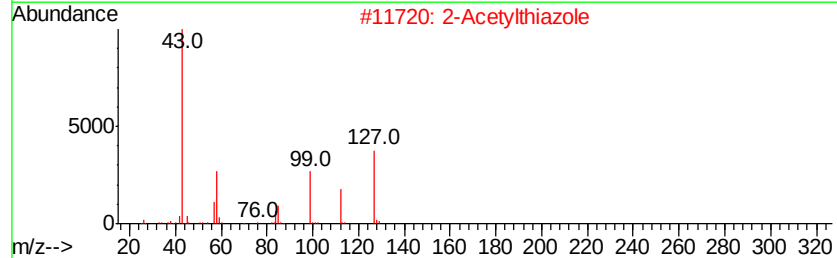
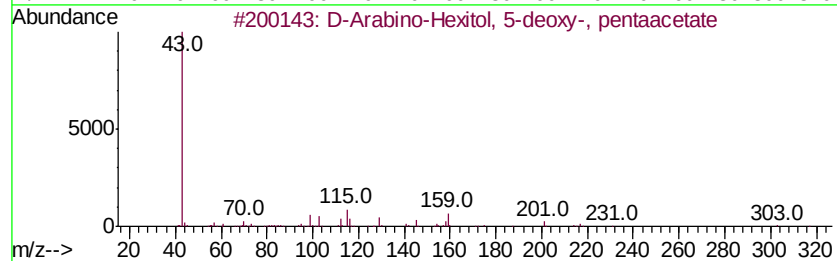
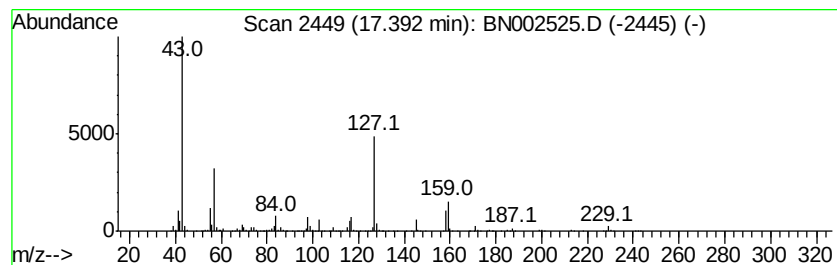
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN081318MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.39	23.22 ng/ul	2233250	Phenanthrene-d10	17.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Arabino-Hexitol, 5-deoxy-, pen...	376	C16H24O10	049560-35-2	10
2	2-Acetylthiazole	127	C5H5NOS	024295-03-2	9
3	Formamide. N-(5-amino-2H-1,2,3-t...	127	C3H5N5O	328977-78-2	9
4	N-Acetylpyrrolidone	127	C6H9NO2	000932-17-2	9
5	1-Deoxy-2,3,4,5-tetraacetyl-d-xy...	304	C13H20O8	007226-55-3	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN082418\
Data File : BN002525.D
Acq On : 25 Aug 2018 05:33
Operator : JU/SJ
Sample : J4628-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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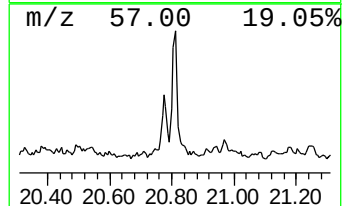
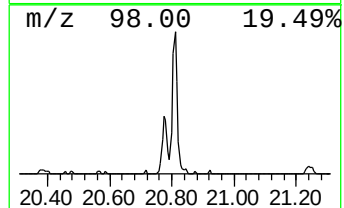
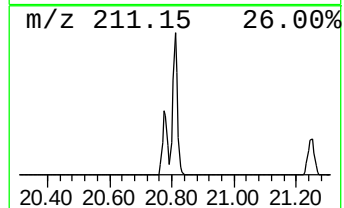
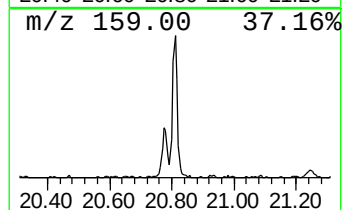
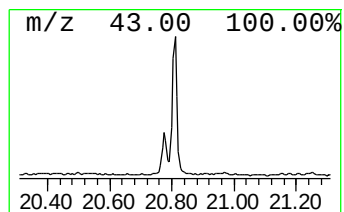
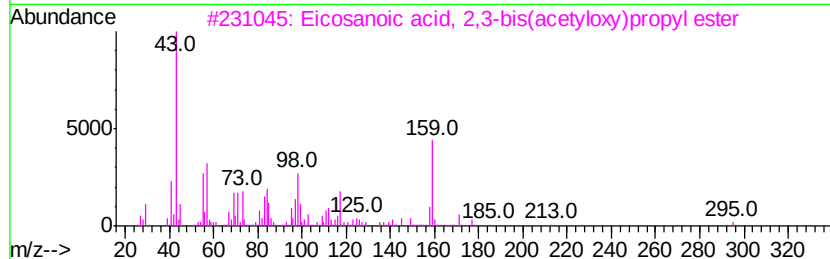
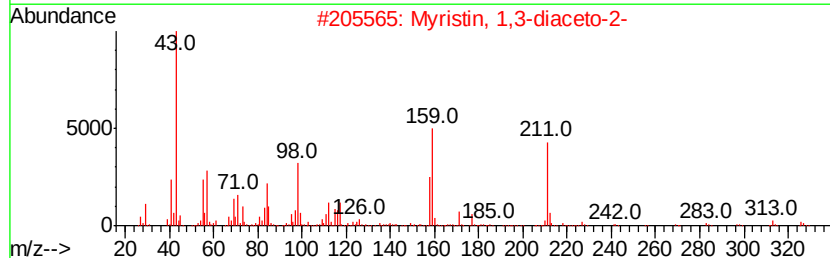
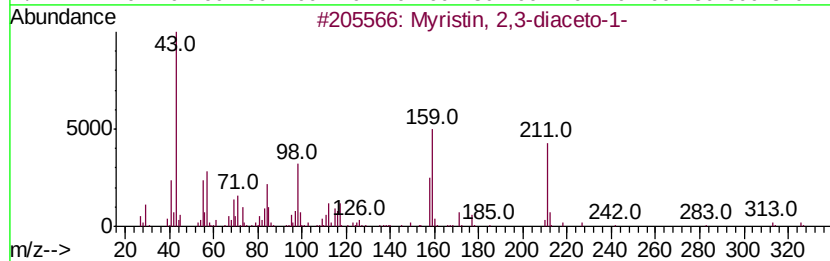
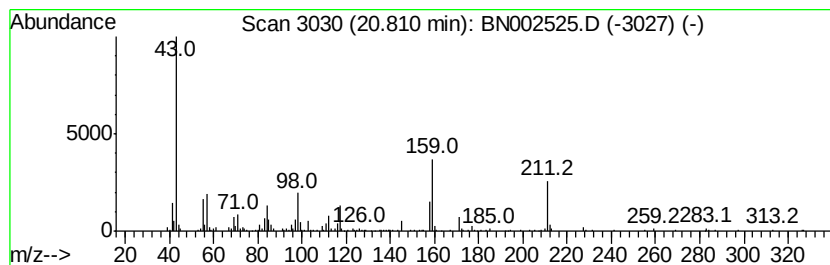
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 Myristin, 2,3-diaceto-1- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.81	3.25 ng/ul	425619	Chrysene-d12	21.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	78
2		Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	78
3		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	43
4		Tetradecanoic acid, 2-hydroxy-1-...	302	C17H34O4	003443-83-2	35
5		Tetradecanoic acid, 2,3-dihydrox...	302	C17H34O4	000589-68-4	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN082418\
Data File : BN002525.D
Acq On : 25 Aug 2018 05:33
Operator : JU/SJ
Sample : J4628-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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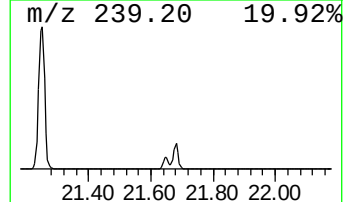
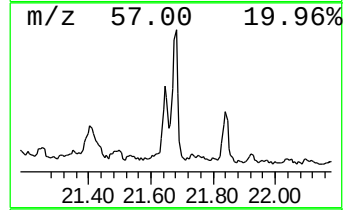
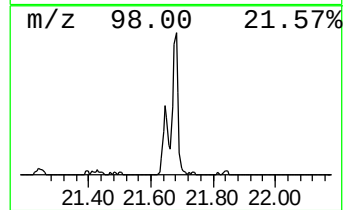
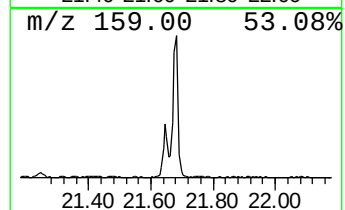
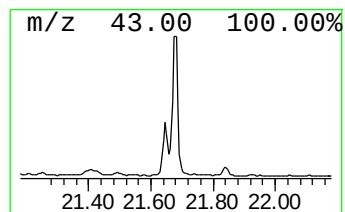
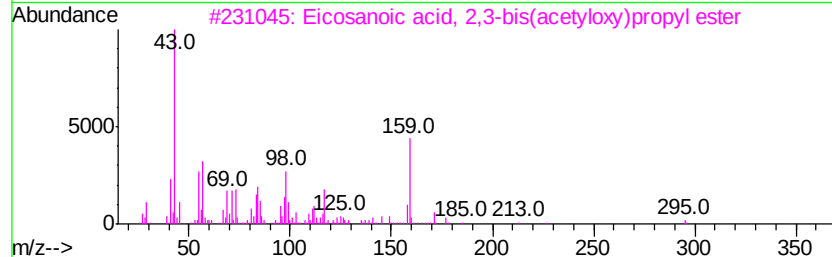
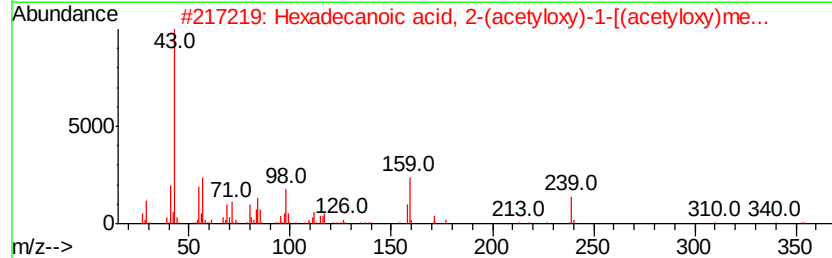
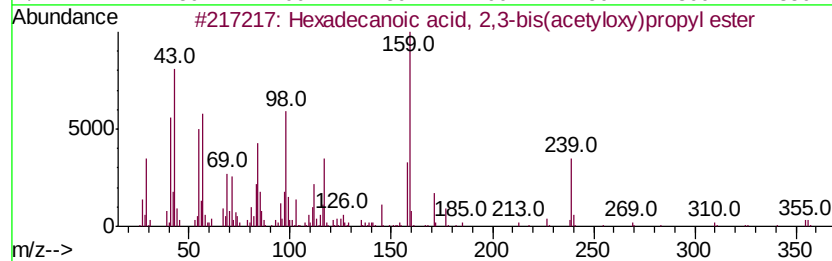
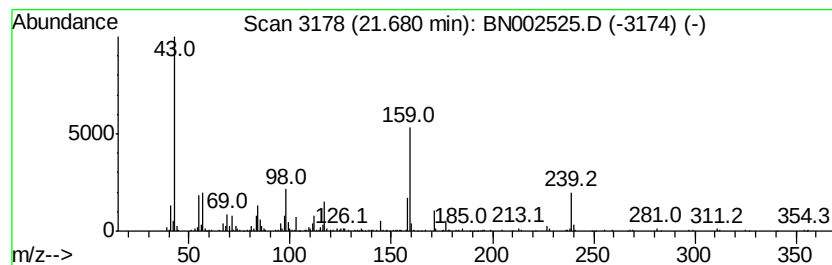
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Hexadecanoic acid, 2,3-bis(...) Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.68	3.94 ng/ul	516520	Chrysene-d12	21.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 2,3-bis(acety...	414	C23H42O6	055268-70-7	91
2		Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	47
3		Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	38
4		Benzenesulfonamide, 2,4-dichloro...	239	C7H7Cl2N02S	1000277-29-3	38
5		2,5-Difluorobenzoic acid, decyl ...	298	C17H24F2O2	1000338-80-9	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN082418\
Data File : BN002525.D
Acq On : 25 Aug 2018 05:33
Operator : JU/SJ
Sample : J4628-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

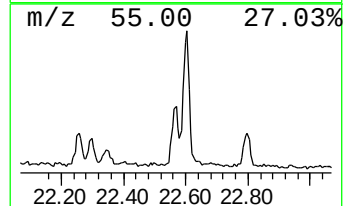
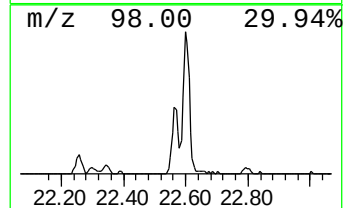
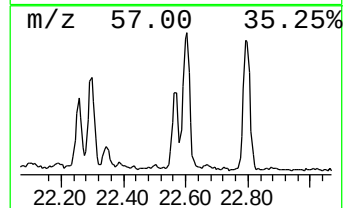
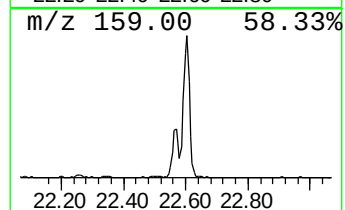
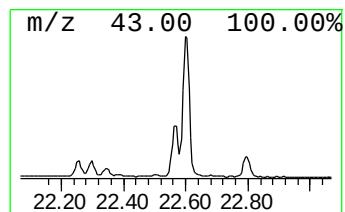
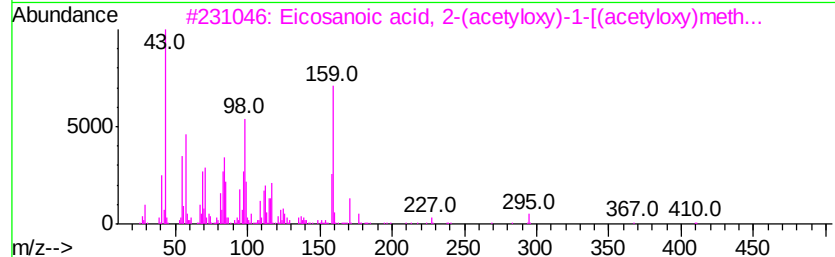
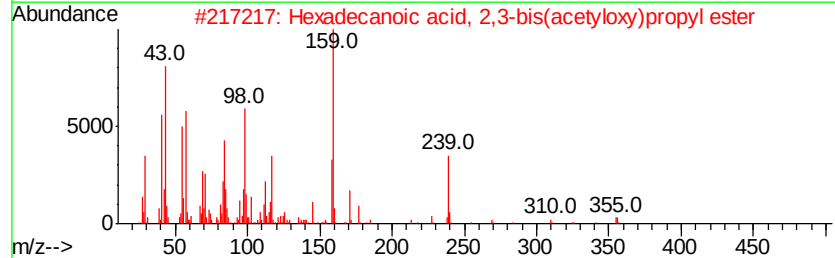
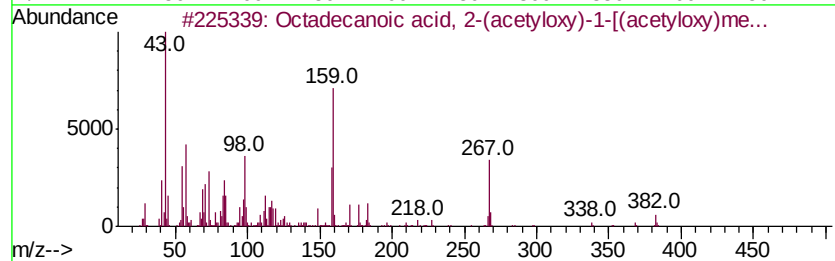
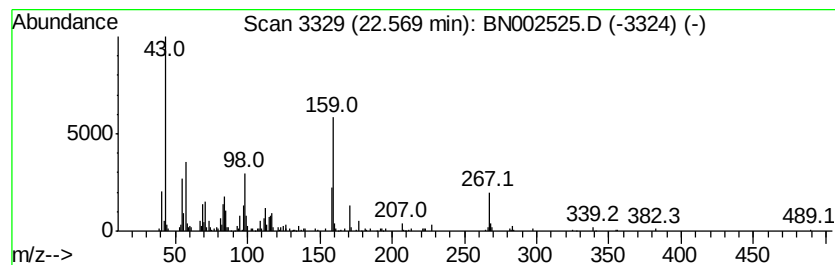
Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN081318MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 10 Octadecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl] ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.57	2.09 ng/ul	292487	Perylene-d12	23.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl] ester	442 C25H46O6	055401-62-2	72
2	Hexadecanoic acid, 2,3-bis(acetyloxy)propyl ester	414 C23H42O6	055268-70-7	64
3	Eicosanoic acid, 2-(acetyloxy)-1-[(acetyloxy)methyl] ester	470 C27H50O6	055429-68-0	58
4	Eicosanoic acid, 2,3-bis(acetyloxy)propyl ester	470 C27H50O6	055429-67-9	35
5	2,3,4-Trifluorobenzoic acid, 4-t-butyl ester	372 C21H31F3O2	1000280-62-0	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN082418\
Data File : BN002525.D
Acq On : 25 Aug 2018 05:33
Operator : JU/SJ
Sample : J4628-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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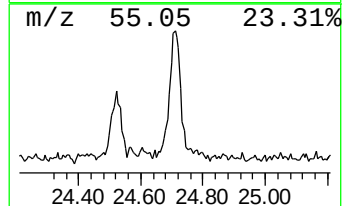
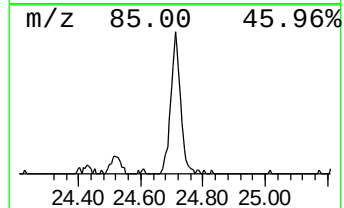
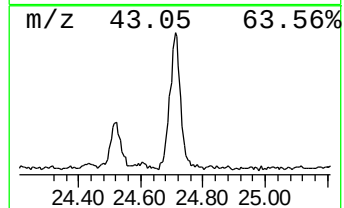
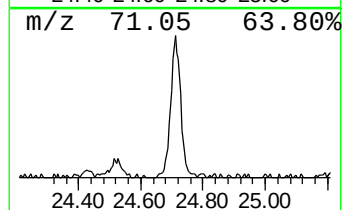
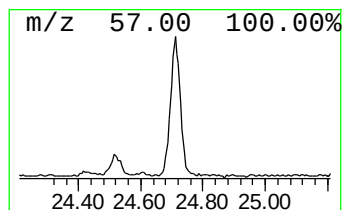
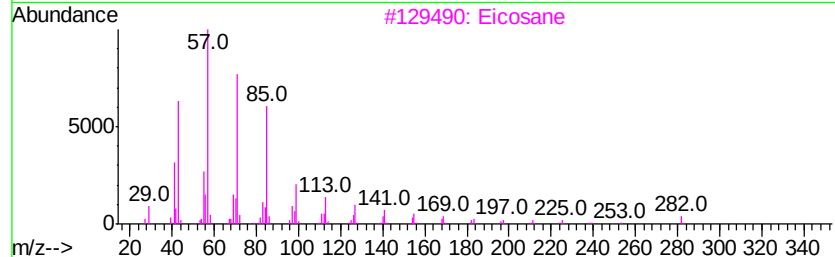
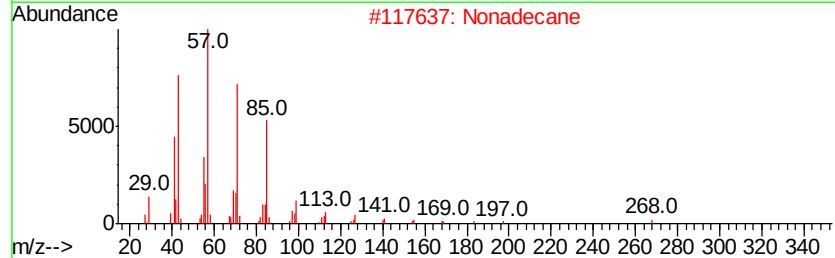
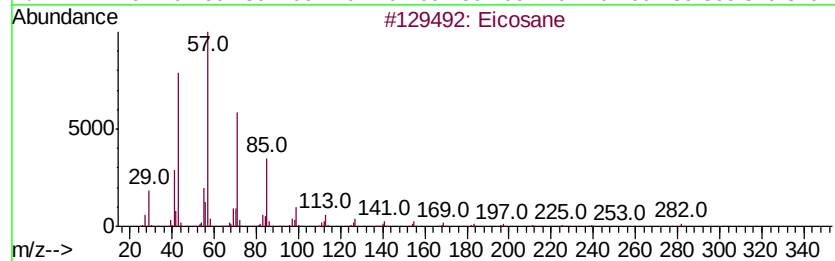
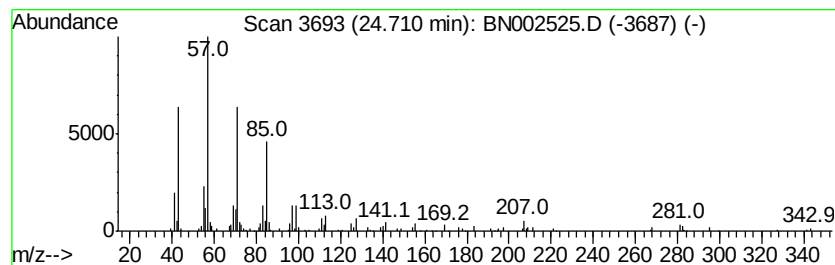
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.71	2.02 ng/ul	282001	Perylene-d12	23.46

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Nonadecane	268	C19H40	000629-92-5	91
3			Eicosane	282	C20H42	000112-95-8	91
4			Nonadecane	268	C19H40	000629-92-5	91
5			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_N\DATA\BN082418\
Data File : BN002525.D
Acq On : 25 Aug 2018 05:33
Operator : JU/SJ
Sample : J4628-19
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
DB3G4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN081318MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octanoic acid	9.80	5.3	ng/ul	285369	2	10.44	1068090	20.0
Dodecanoic acid	14.75	8.6	ng/ul	645856	3	14.30	1510560	20.0
4H-Imidazol-4-one...	15.87	3.2	ng/ul	303946	4	17.05	1923440	20.0
unknown-01	15.92	6.3	ng/ul	610096	4	17.05	1923440	20.0
unknown-02	16.86	2.7	ng/ul	256970	4	17.05	1923440	20.0
unknown-03	17.35	11.2	ng/ul	1079960	4	17.05	1923440	20.0
unknown-04	17.39	23.2	ng/ul	2233250	4	17.05	1923440	20.0
Myristin, 2,3-dia...	20.81	3.3	ng/ul	425619	5	21.25	2619330	20.0
Hexadecanoic acid...	21.68	3.9	ng/ul	516520	5	21.25	2619330	20.0
Octadecanoic acid...	22.57	2.1	ng/ul	292487	6	23.46	2798400	20.0
(DEL) Alkane: Str...	24.71	2.0	ng/ul	282001	6	23.46	2798400	20.0