

Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
 Data File : BN003252.D
 Acq On : 22 Oct 2018 22:43
 Operator : MJ/SJ
 Sample : J5568-13
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 C0AK8

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-BN101918MA.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	6.810	645	650	668	rBV2	163094	434370	8.91%	1.635%
2	6.952	668	674	686	rVB	101755	165345	3.39%	0.622%
3	7.152	702	708	718	rBV	141762	245314	5.03%	0.923%
4	7.604	779	785	795	rBV	293081	490934	10.07%	1.847%
5	8.334	903	909	923	rBV	190228	382500	7.84%	1.439%
6	8.763	976	982	997	rBV	107023	203926	4.18%	0.767%
7	9.481	1099	1104	1116	rBV	92720	168485	3.46%	0.634%
8	10.034	1191	1198	1215	rBV	109015	283292	5.81%	1.066%
9	10.369	1246	1255	1264	rBV	480905	836099	17.15%	3.146%
10	10.534	1277	1283	1299	rBV	107906	263421	5.40%	0.991%
11	13.663	1808	1815	1820	rBV	196386	286644	5.88%	1.079%
12	13.710	1820	1823	1831	rVB	49994	73965	1.52%	0.278%
13	13.934	1855	1861	1871	rBV	305488	479220	9.83%	1.803%
14	14.245	1906	1914	1925	rVB2	800800	1205492	24.72%	4.536%
15	14.534	1957	1963	1985	rBV2	74718	279648	5.74%	1.052%
16	15.186	2066	2074	2079	rBV3	25578	75466	1.55%	0.284%
17	15.245	2079	2084	2095	rVB	386968	635527	13.03%	2.392%
18	15.410	2107	2112	2126	rBV	105772	209488	4.30%	0.788%
19	16.422	2276	2284	2296	rBV	158472	248830	5.10%	0.936%
20	16.998	2376	2382	2390	rBV2	1048010	1482228	30.40%	5.578%
21	17.104	2394	2400	2409	rVB2	426096	662181	13.58%	2.492%
22	17.180	2409	2413	2423	rBV2	40905	67056	1.38%	0.252%
23	17.786	2509	2516	2526	rBV	157670	339437	6.96%	1.277%
24	17.922	2531	2539	2578	rVV	2709266	4875900	100.00%	18.349%
25	18.580	2647	2651	2660	rBV3	63816	103605	2.12%	0.390%
26	19.016	2721	2725	2728	rBV	74520	107388	2.20%	0.404%
27	19.051	2728	2731	2732	rVV2	107569	129538	2.66%	0.487%
28	19.086	2732	2737	2752	rVV2	459950	1193276	24.47%	4.490%
29	19.198	2752	2756	2771	rVB	225726	401656	8.24%	1.511%
30	19.404	2786	2791	2804	rVB	541394	812737	16.67%	3.058%
31	20.051	2897	2901	2905	rBV2	86528	132849	2.72%	0.500%
32	20.180	2920	2923	2925	rBV4	36081	49731	1.02%	0.187%
33	20.204	2925	2927	2937	rVB3	64994	105292	2.16%	0.396%
34	20.957	3051	3055	3057	rBV3	60351	93424	1.92%	0.352%

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35	21.210	3093	3098	3109	rVB	1414912	1942415	39.84%	7.310%
36	21.357	3120	3123	3127	rVB	49057	50759	1.04%	0.191%
37	21.786	3192	3196	3199	rVB2	68871	85059	1.74%	0.320%
38	22.233	3269	3272	3277	rVB	119605	143344	2.94%	0.539%
39	22.357	3288	3293	3301	rVB	539294	710204	14.57%	2.673%
40	22.727	3351	3356	3361	rVB	155571	231016	4.74%	0.869%
41	23.274	3443	3449	3460	rVB	629680	1141380	23.41%	4.295%
42	23.415	3466	3473	3489	rBV	1010097	2117060	43.42%	7.967%
43	23.892	3549	3554	3562	rVB	159969	304668	6.25%	1.147%
44	24.645	3671	3682	3704	rBV5	331553	1604125	32.90%	6.037%
45	24.980	3732	3739	3760	rBV9	147945	719069	14.75%	2.706%

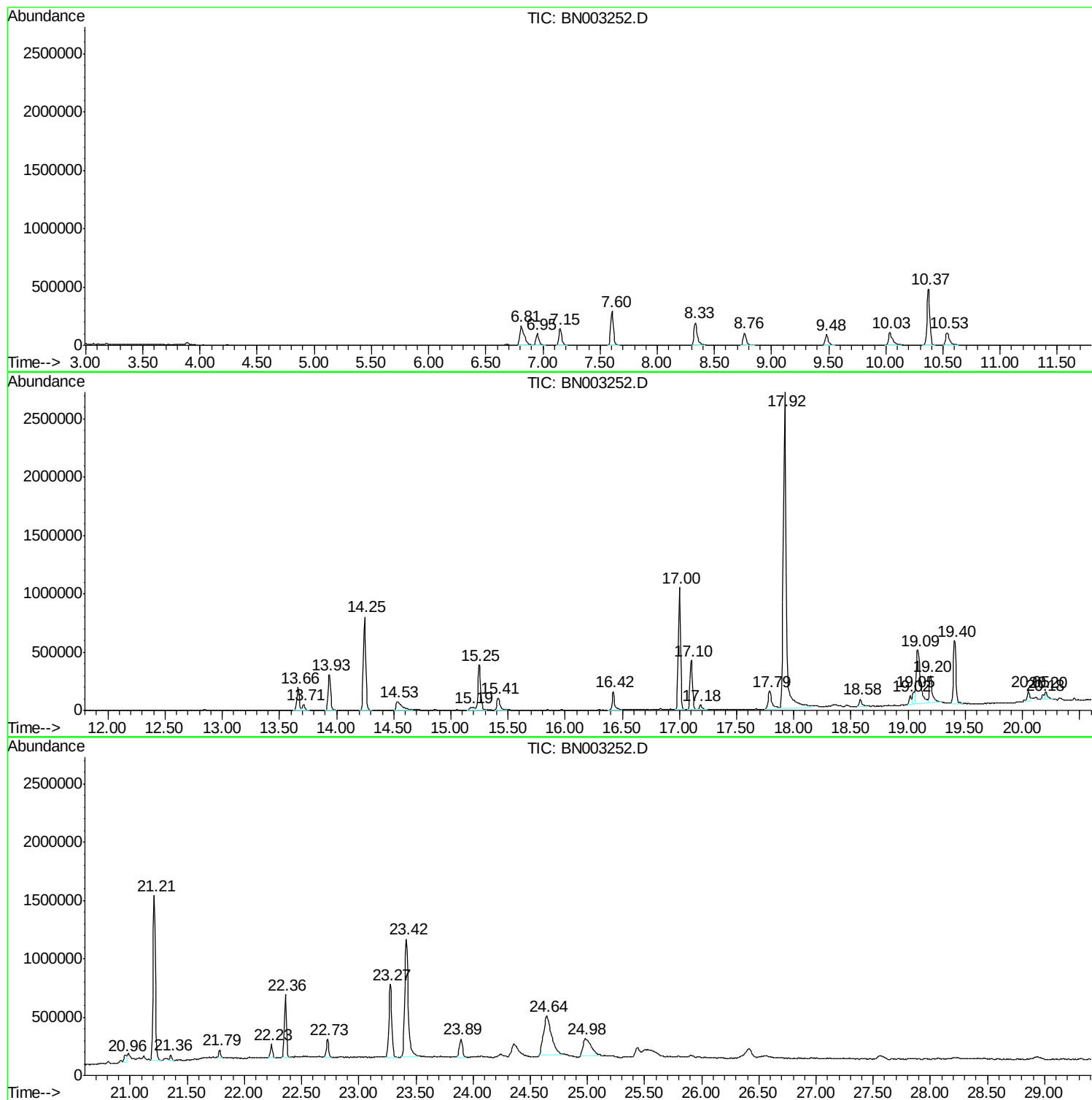
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN101918MA.M
Quant Title : SVOA CALIBRATION

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



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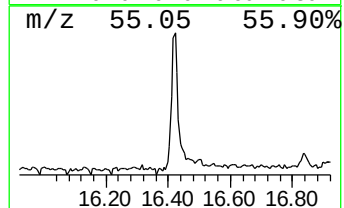
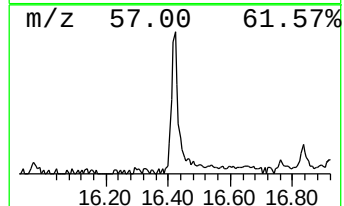
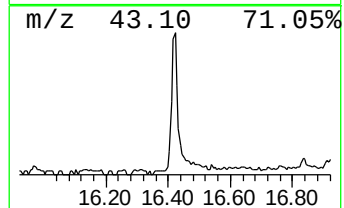
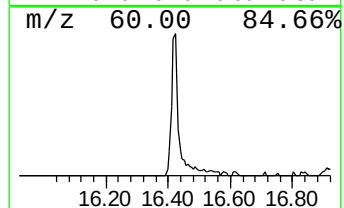
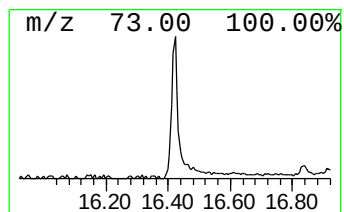
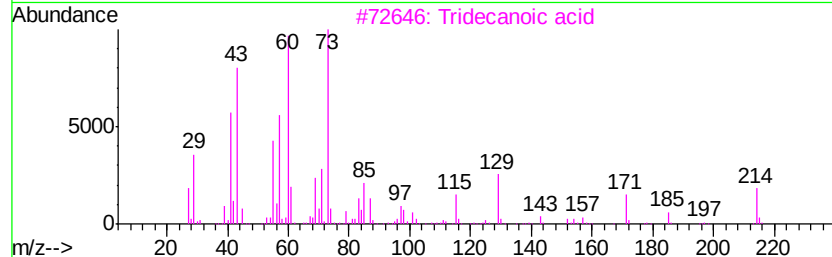
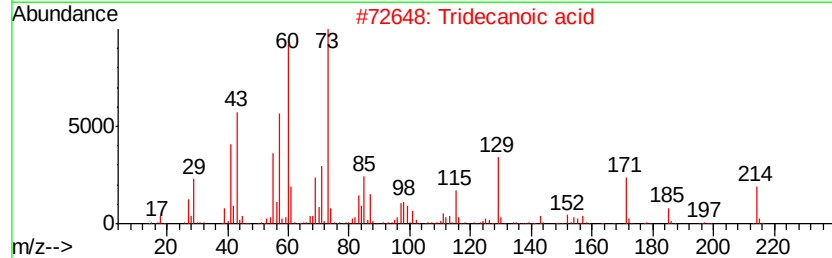
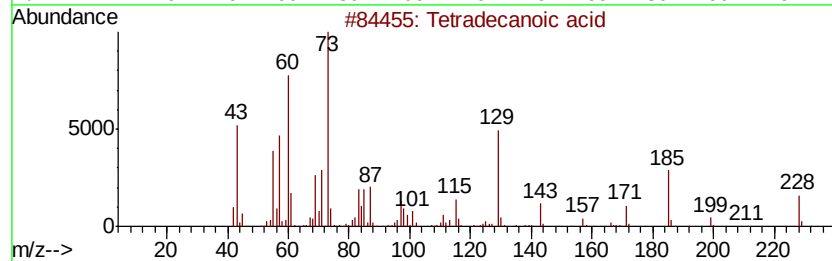
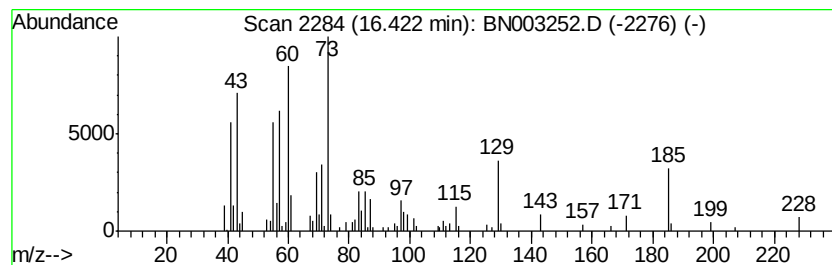
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.42	3.36 ng/ul	248830	Phenanthrene-d10		17.00	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2		Tridecanoic acid	214	C13H26O2	000638-53-9	86
3		Tridecanoic acid	214	C13H26O2	000638-53-9	86
4		Dodecanoic acid	200	C12H24O2	000143-07-7	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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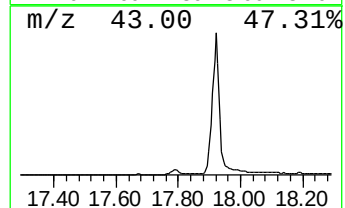
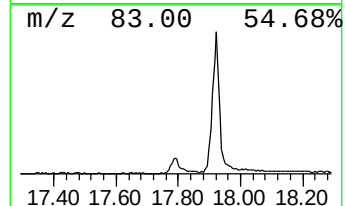
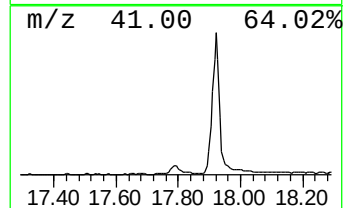
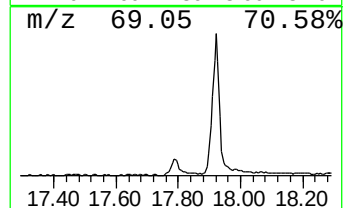
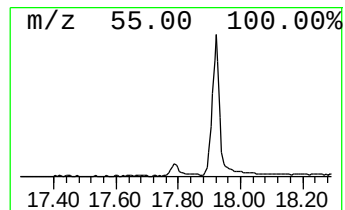
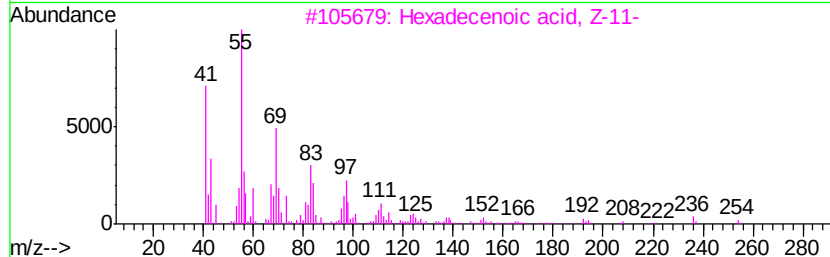
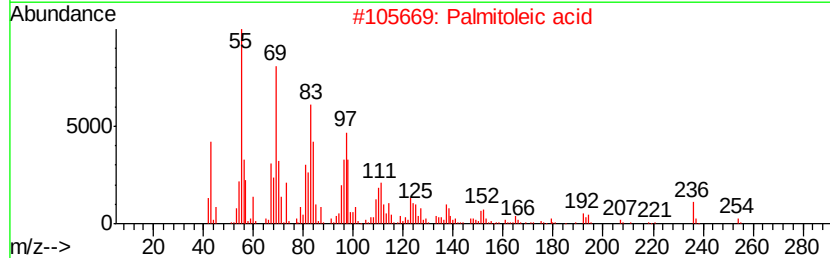
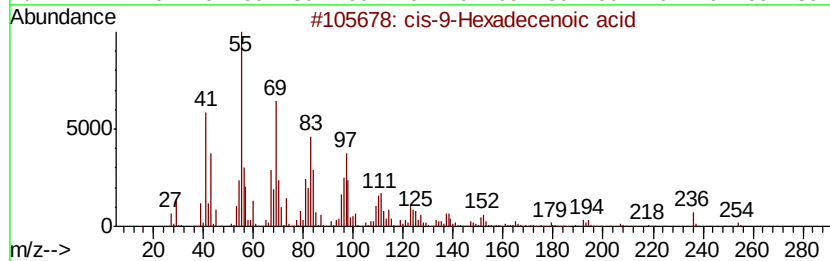
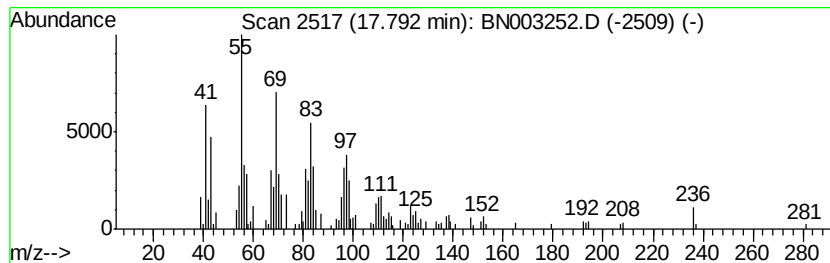
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Peak Number 2 cis-9-Hexadecenoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.79	4.58 ng/ul	339437	Phenanthrene-d10	17.00		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	93
2		Palmitoleic acid	254	C16H30O2	000373-49-9	91
3		Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	87
4		Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	86
5		Oxacyclotetradecane-2,11-dione, ...	240	C14H24O3	074685-36-2	81



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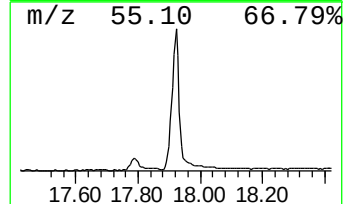
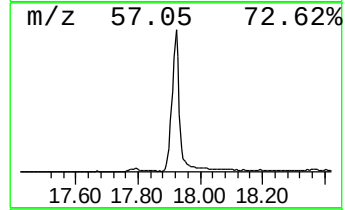
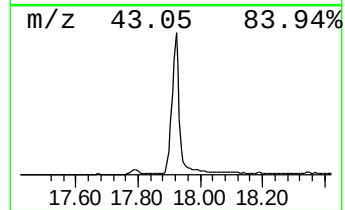
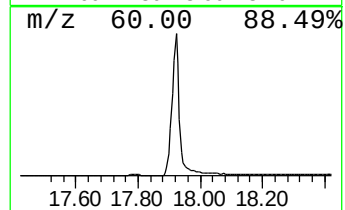
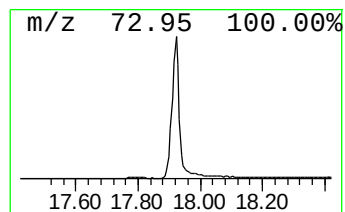
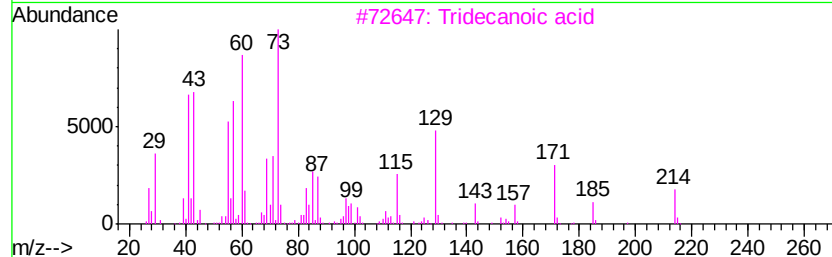
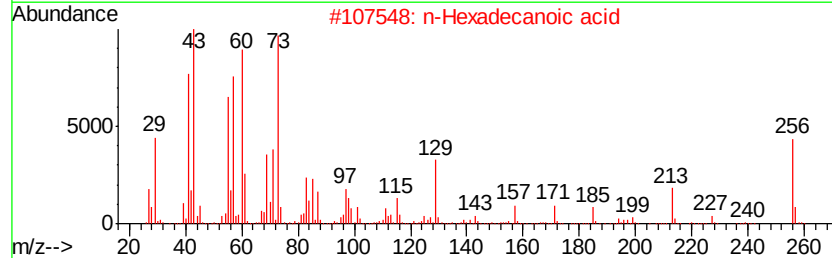
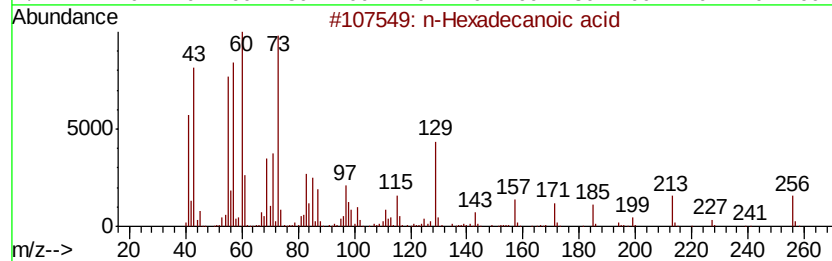
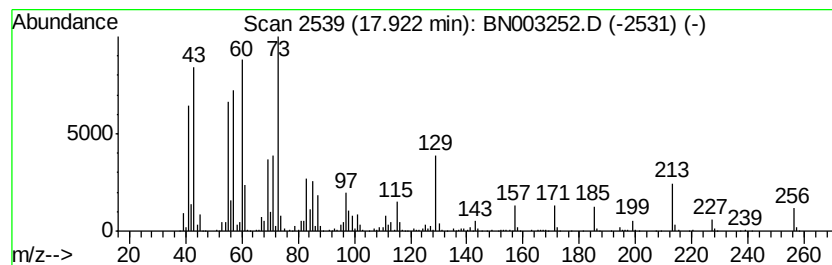
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.92	65.79 ng/ul	4875900	Phenanthrene-d10	17.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3		Tridecanoic acid	214	C13H26O2	000638-53-9	95
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	91



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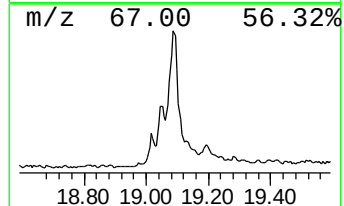
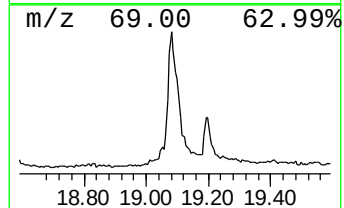
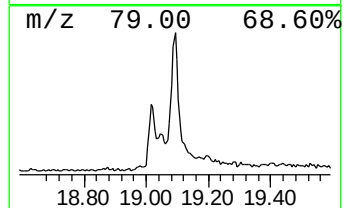
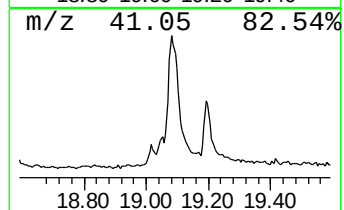
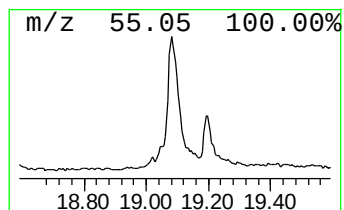
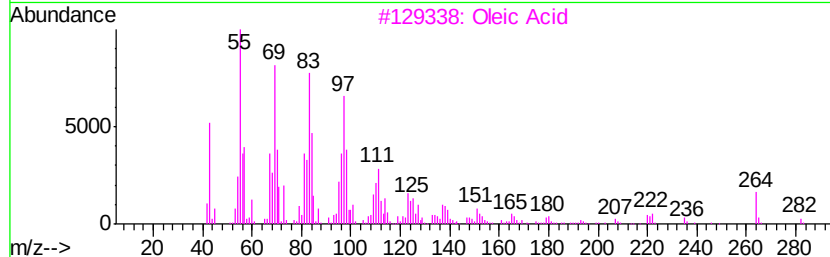
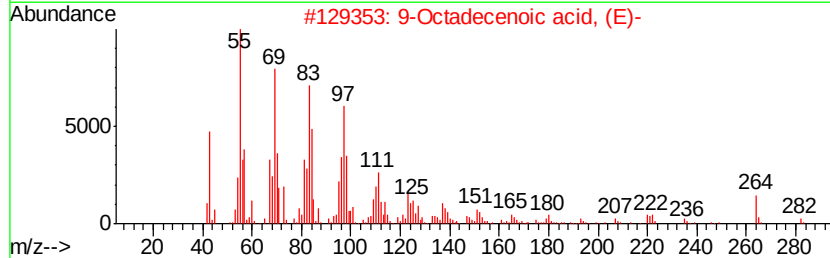
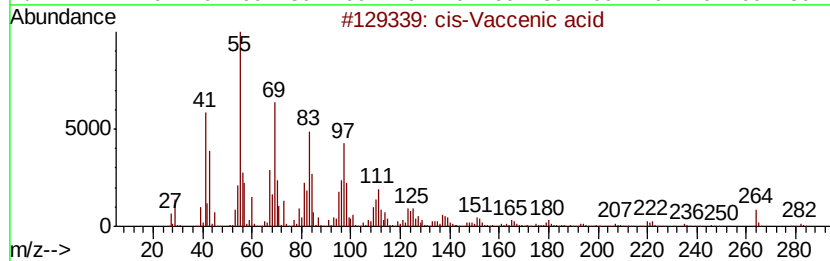
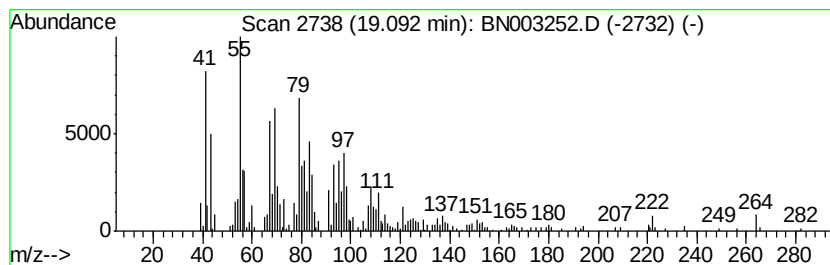
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Peak Number 4 cis-Vaccenic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.09	16.10 ng/ul	1193280	Phenanthrene-d10	17.00		
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		Oleic Acid	282	C18H34O2	000112-80-1	98
4		trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	95
5		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	93



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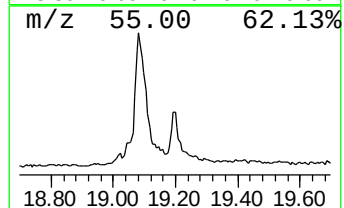
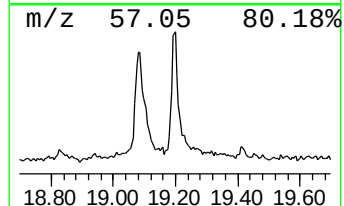
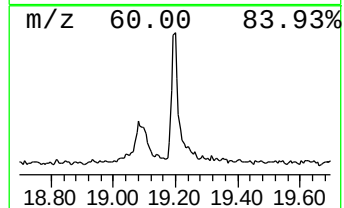
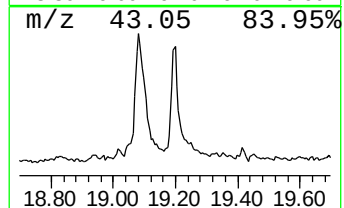
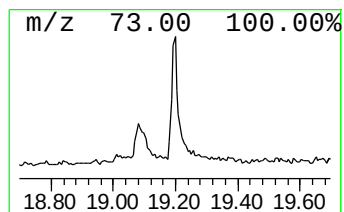
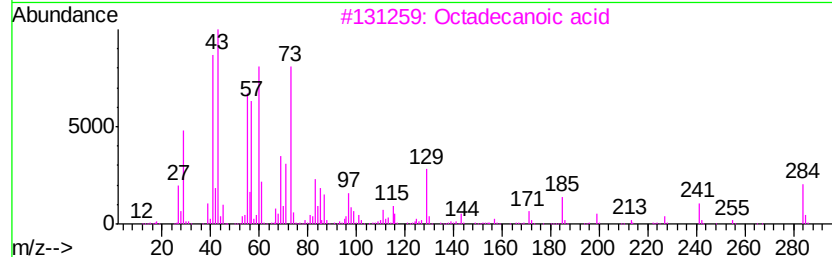
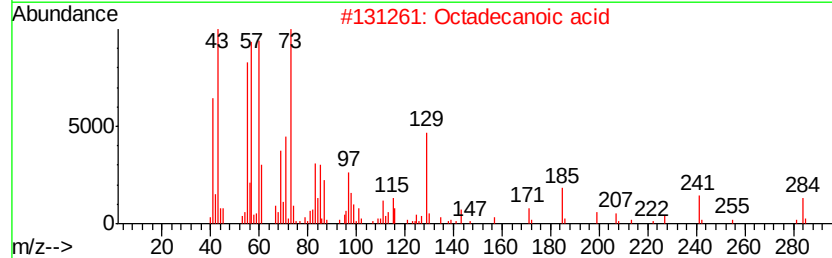
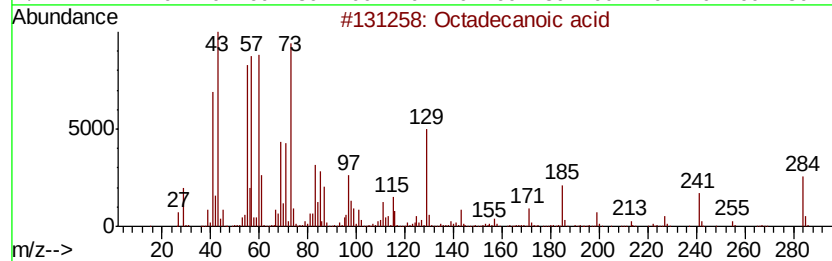
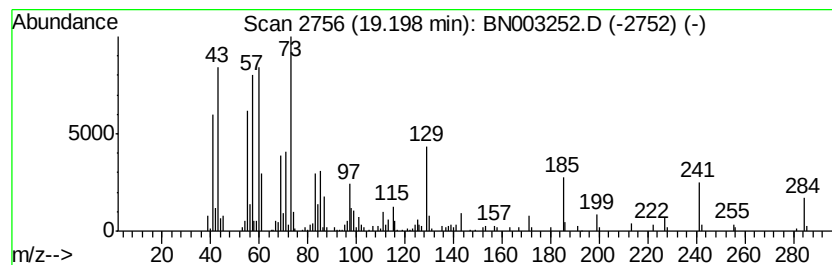
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Quant Title : SVOA CALIBRATION

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Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.20	4.14 ng/ul	401656	Chrysene-d12	21.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99	
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99	
3	Octadecanoic acid	284	C18H36O2	000057-11-4	95	
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93	
5	Octadecanoic acid	284	C18H36O2	000057-11-4	92	



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Acq On : 22 Oct 2018 22:43
Operator : MJ/SJ
Sample : J5568-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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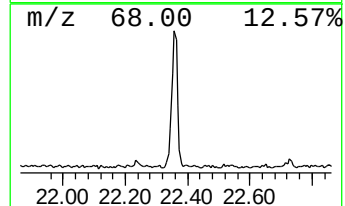
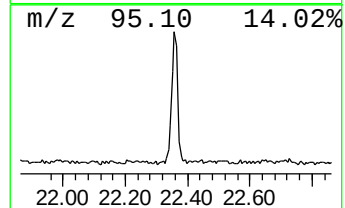
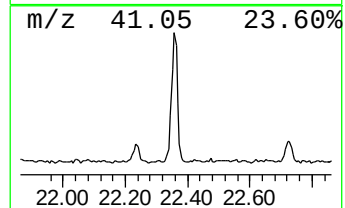
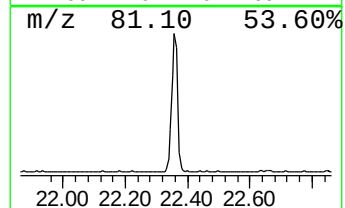
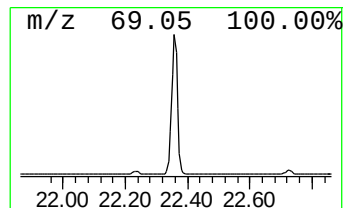
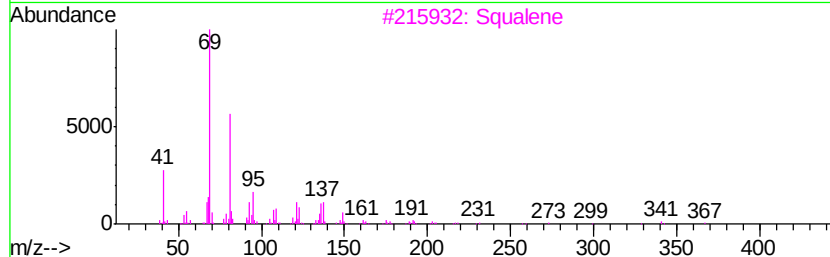
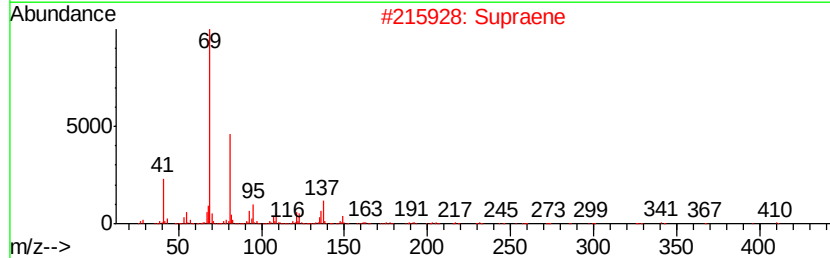
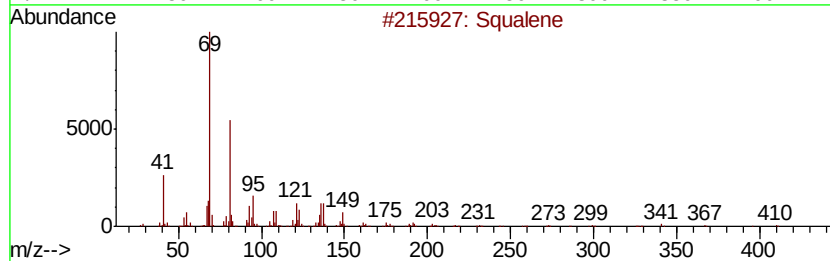
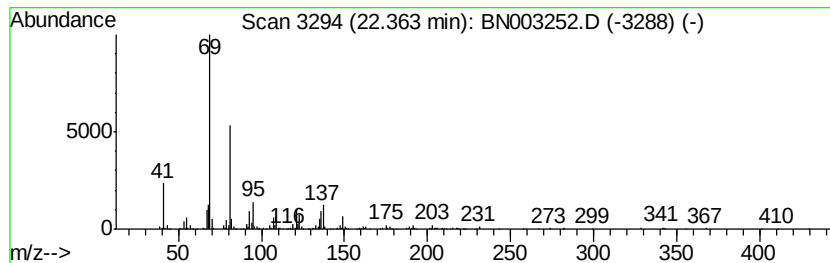
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.36	6.71 ng/ul	710204	Perylene-d12	23.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		Squalene	410	C30H50	000111-02-4	91
4		Squalene	410	C30H50	000111-02-4	91
5		Squalene	410	C30H50	000111-02-4	91



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Acq On : 22 Oct 2018 22:43
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Sample : J5568-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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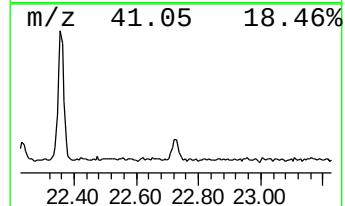
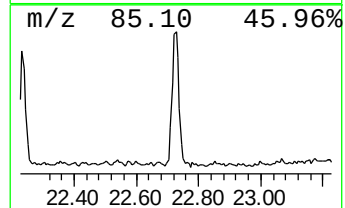
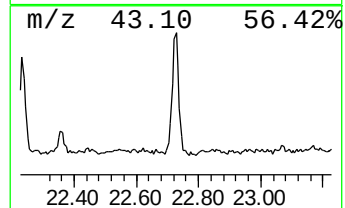
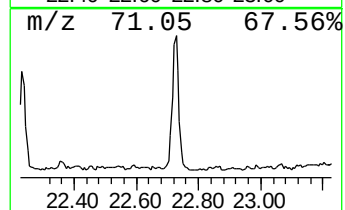
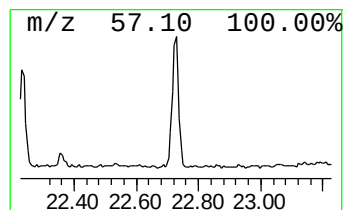
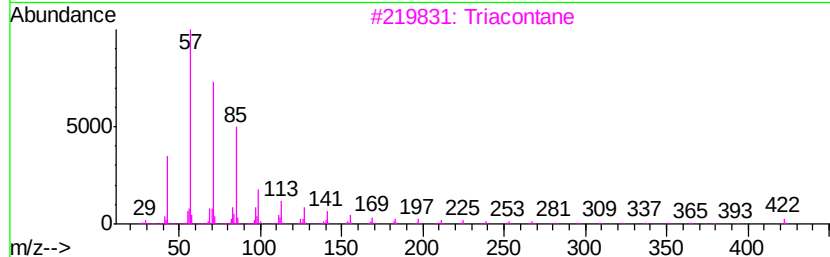
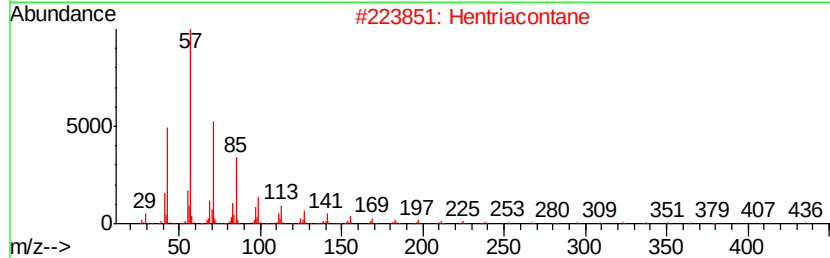
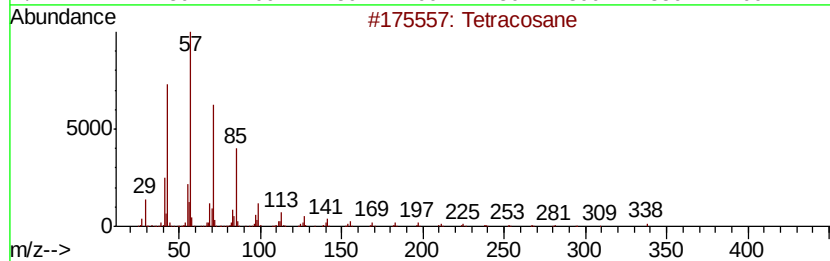
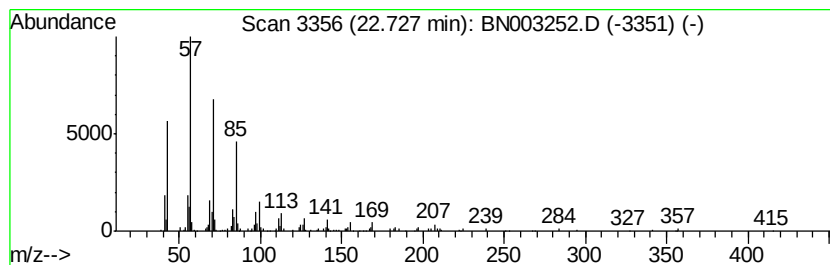
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.73	2.18 ng/ul	231016	Perylene-d12	23.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	90
2		Hentriacontane	437	C31H64	000630-04-6	90
3		Triacontane	422	C30H62	000638-68-6	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	90
5		Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
Data File : BN003252.D
Acq On : 22 Oct 2018 22:43
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Sample : J5568-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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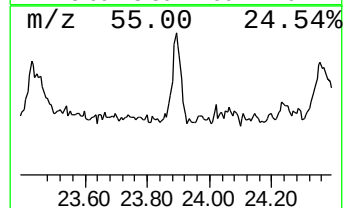
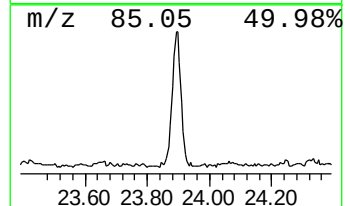
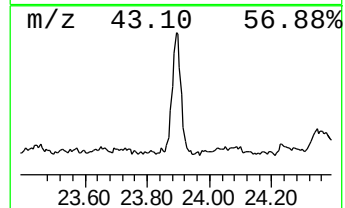
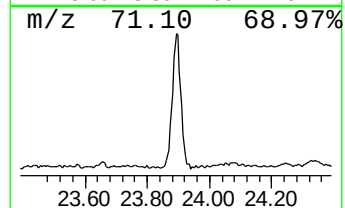
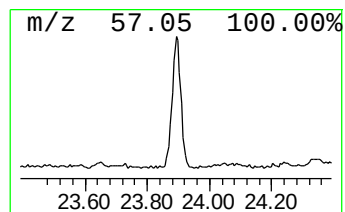
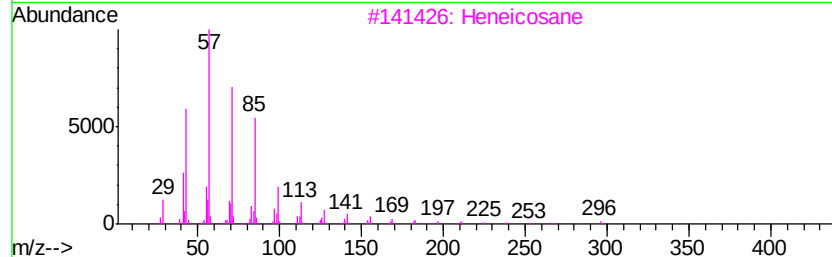
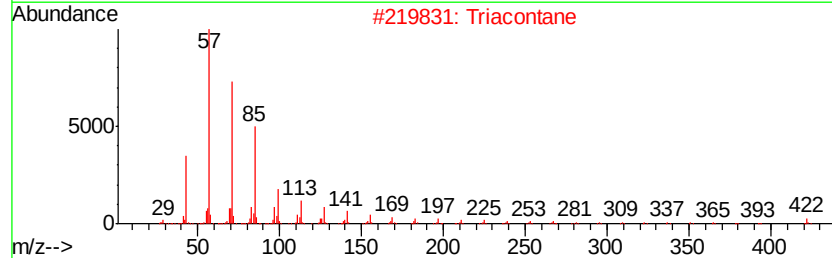
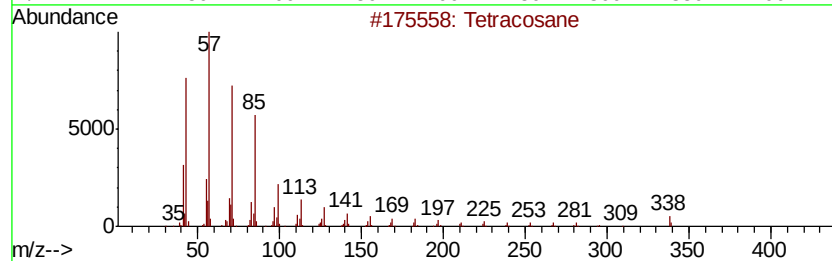
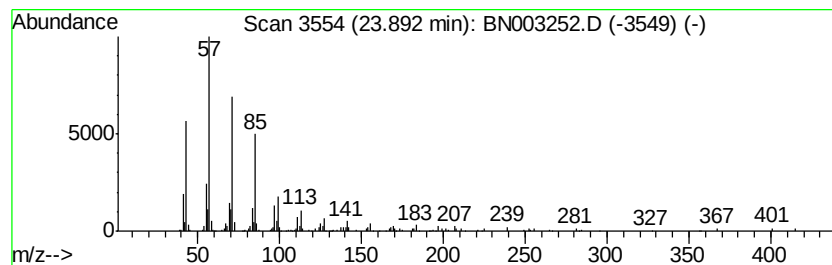
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.89	2.88 ng/ul	304668	Perylene-d12	23.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		triacontane	422	C30H62	000638-68-6	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
Data File : BN003252.D
Acq On : 22 Oct 2018 22:43
Operator : MJ/SJ
Sample : J5568-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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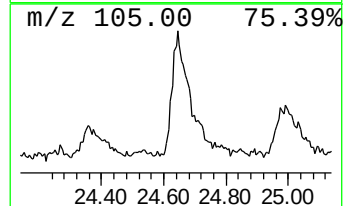
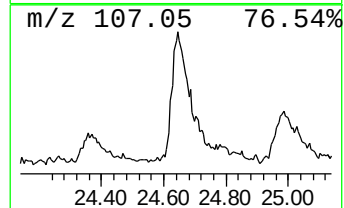
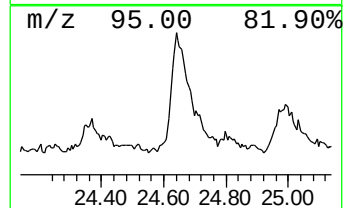
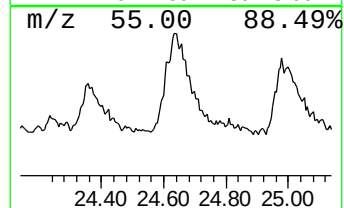
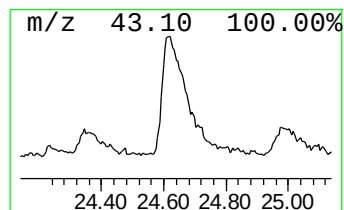
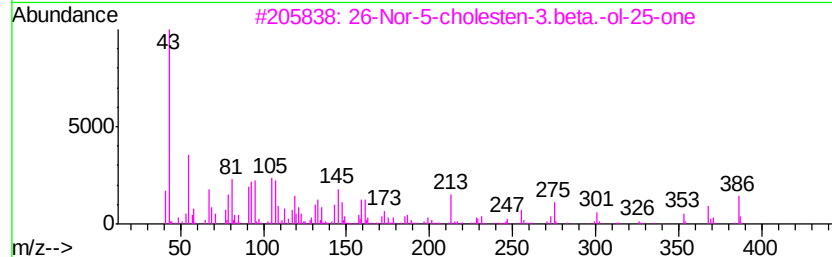
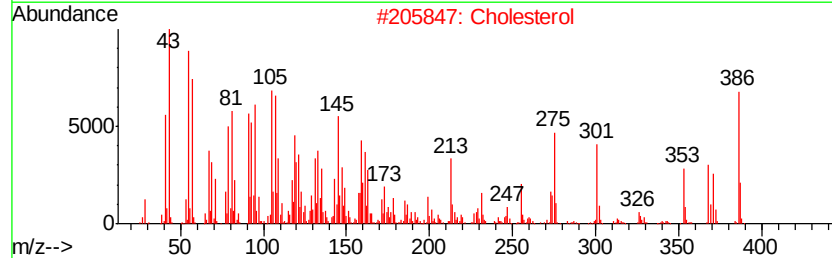
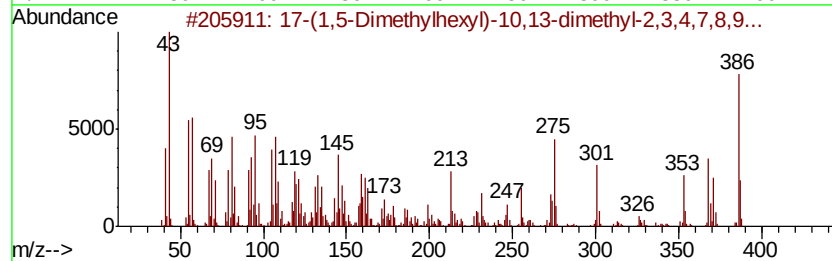
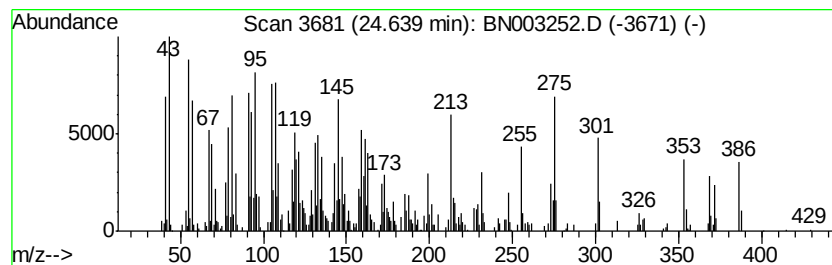
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 17-(1,5-Dimethylhexyl)-10,1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.64	15.15 ng/ul	1604130	Perylene-d12	23.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	99
2		Cholesterol	386	C27H46O	000057-88-5	99
3		26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
4		26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
5		Cholesterol	386	C27H46O	000057-88-5	96



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
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Sample : J5568-13
Misc :
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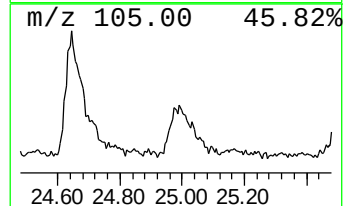
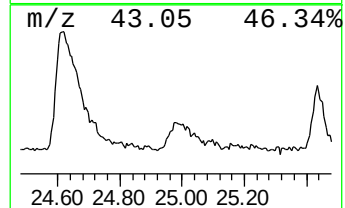
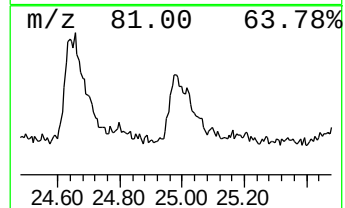
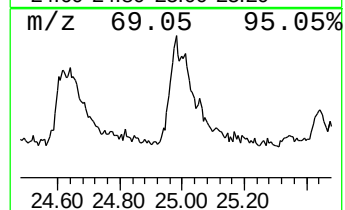
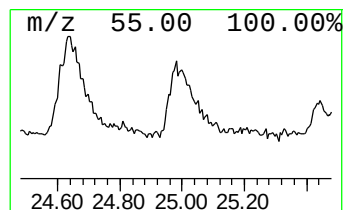
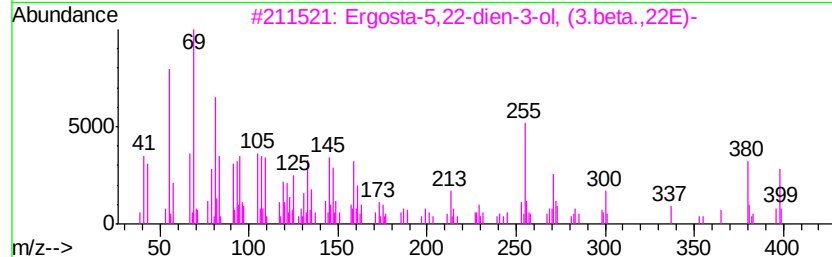
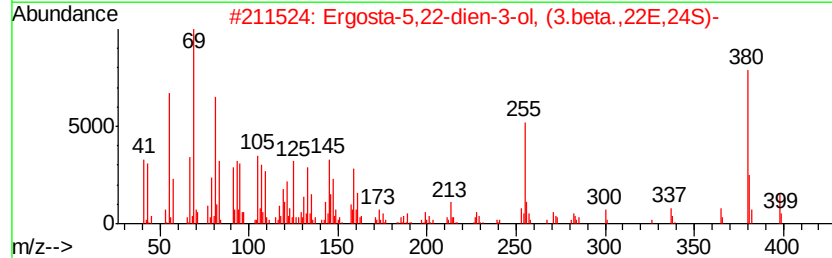
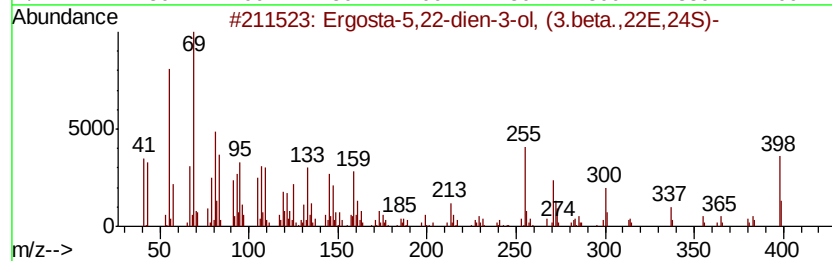
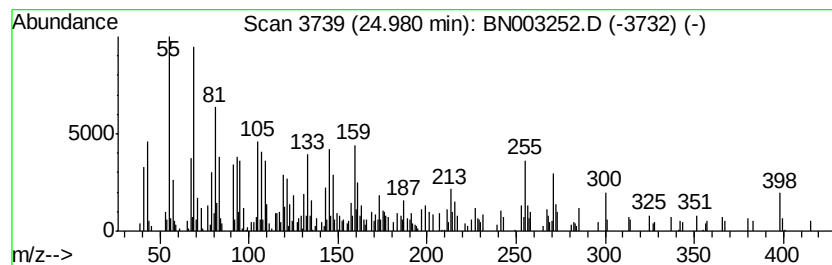
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 Ergosta-5,22-dien-3-ol, (3.... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
24.98	6.79 ng/ul	719069	Perylene-d12	23.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergosta-5,22-dien-3-ol, (3.beta....	398	C28H46O	017472-78-5	92	
2	Ergosta-5,22-dien-3-ol, (3.beta....	398	C28H46O	017472-78-5	83	
3	Ergosta-5,22-dien-3-ol, (3.beta....	398	C28H46O	000474-67-9	78	
4	8(14),22-Ergostadienol	398	C28H46O	051502-42-2	55	
5	Ergost-22-en-3-one, (5.beta.,22E)-	398	C28H46O	018865-44-6	45	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_N\DATA\BN102218\
Data File : BN003252.D
Acq On : 22 Oct 2018 22:43
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Sample : J5568-13
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN101918MA.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
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cis-9-Hexadecenoic acid	17.79	4.6	ng/ul	339437	4	17.00	1482230	20.0
n-Hexadecanoic acid	17.92	65.8	ng/ul	4875900	4	17.00	1482230	20.0
cis-Vaccenic acid	19.09	16.1	ng/ul	1193280	4	17.00	1482230	20.0
Octadecanoic acid	19.20	4.1	ng/ul	401656	5	21.21	1942420	20.0
Squalene	22.36	6.7	ng/ul	710204	6	23.42	2117060	20.0
(DEL) Alkane: Str...	22.73	2.2	ng/ul	231016	6	23.42	2117060	20.0
(DEL) Alkane: Str...	23.89	2.9	ng/ul	304668	6	23.42	2117060	20.0
17-(1,5-Dimethylh...	24.64	15.2	ng/ul	1604130	6	23.42	2117060	20.0
Ergosta-5,22-dien...	24.98	6.8	ng/ul	719069	6	23.42	2117060	20.0