

Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
 Data File : BN003253.D
 Acq On : 22 Oct 2018 23:18
 Operator : MJ/SJ
 Sample : J5568-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 C0AK6

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	3.887	148	153	162	rVB	89760	140461	3.47%	0.410%
2	6.675	620	627	638	rBV2	24529	58049	1.43%	0.169%
3	6.810	644	650	665	rBV2	208754	541946	13.40%	1.582%
4	6.951	668	674	685	rVB	186623	302657	7.48%	0.884%
5	7.145	701	707	720	rBV	226389	388998	9.61%	1.136%
6	7.604	779	785	794	rBV	248023	411249	10.16%	1.201%
7	8.328	901	908	921	rBV	283804	531940	13.15%	1.553%
8	8.757	974	981	995	rBV	225506	398400	9.85%	1.163%
9	9.475	1097	1103	1123	rBV	190648	344993	8.53%	1.007%
10	10.022	1190	1196	1219	rBV	256024	558330	13.80%	1.630%
11	10.369	1249	1255	1265	rBV	417457	708712	17.52%	2.069%
12	10.528	1276	1282	1302	rBV	211283	453019	11.20%	1.323%
13	13.657	1808	1814	1819	rBV	639627	905600	22.38%	2.644%
14	13.704	1819	1822	1835	rVB	170970	254887	6.30%	0.744%
15	13.933	1852	1861	1872	rBV	780734	1169211	28.90%	3.414%
16	14.245	1906	1914	1923	rBV2	696489	1072180	26.50%	3.131%
17	14.527	1956	1962	1983	rBV2	106602	367049	9.07%	1.072%
18	14.851	2012	2017	2028	rVB	38051	53166	1.31%	0.155%
19	15.245	2078	2084	2095	rVB	1048299	1509155	37.30%	4.406%
20	15.404	2106	2111	2122	rBV	229917	408270	10.09%	1.192%
21	16.416	2279	2283	2292	rBV2	55926	77857	1.92%	0.227%
22	16.998	2376	2382	2390	rBV	1009618	1372768	33.93%	4.008%
23	17.098	2390	2399	2408	rVB2	1165728	1707710	42.21%	4.986%
24	17.786	2510	2516	2529	rBV	86558	190564	4.71%	0.556%
25	17.910	2530	2537	2564	rVV	1235718	1996532	49.35%	5.829%
26	18.580	2646	2651	2658	rBV3	36923	67147	1.66%	0.196%
27	19.015	2721	2725	2727	rBV3	33952	43599	1.08%	0.127%
28	19.045	2727	2730	2732	rVV2	68861	92233	2.28%	0.269%
29	19.086	2732	2737	2747	rVV4	196604	493420	12.20%	1.441%
30	19.192	2751	2755	2770	rVB	207075	335783	8.30%	0.980%
31	19.404	2785	2791	2798	rBV2	1461814	2071973	51.21%	6.050%
32	19.957	2881	2885	2890	rBV2	37901	54733	1.35%	0.160%
33	20.051	2897	2901	2908	rVV2	67271	112139	2.77%	0.327%
34	20.204	2925	2927	2934	rVB4	37053	50206	1.24%	0.147%

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35	20.451	2965	2969	2973	rBV2	54703	70795	1.75%	0.207%
36	20.915	3045	3048	3051	rBV	57478	65286	1.61%	0.191%
37	20.951	3051	3054	3058	rBV4	47612	85304	2.11%	0.249%
38	21.209	3093	3098	3108	rVB	1346565	1858947	45.95%	5.428%
39	21.357	3119	3123	3128	rVB	91570	103060	2.55%	0.301%
40	21.780	3192	3195	3199	rVB2	115523	138435	3.42%	0.404%
41	22.233	3268	3272	3278	rVB	173495	216040	5.34%	0.631%
42	22.356	3288	3293	3299	rVB	302138	387083	9.57%	1.130%
43	22.721	3351	3355	3361	rVB	188683	270918	6.70%	0.791%
44	23.274	3442	3449	3462	rVB	1448062	2657780	65.69%	7.760%
45	23.415	3466	3473	3489	rVV	994373	2074911	51.29%	6.058%
46	23.892	3549	3554	3562	rVB2	205697	375627	9.28%	1.097%
47	24.356	3627	3633	3653	rVB9	120534	500330	12.37%	1.461%
48	24.633	3670	3680	3701	rBV5	1035516	4045798	100.00%	11.813%
49	24.974	3730	3738	3763	rBV5	465447	2153539	53.23%	6.288%

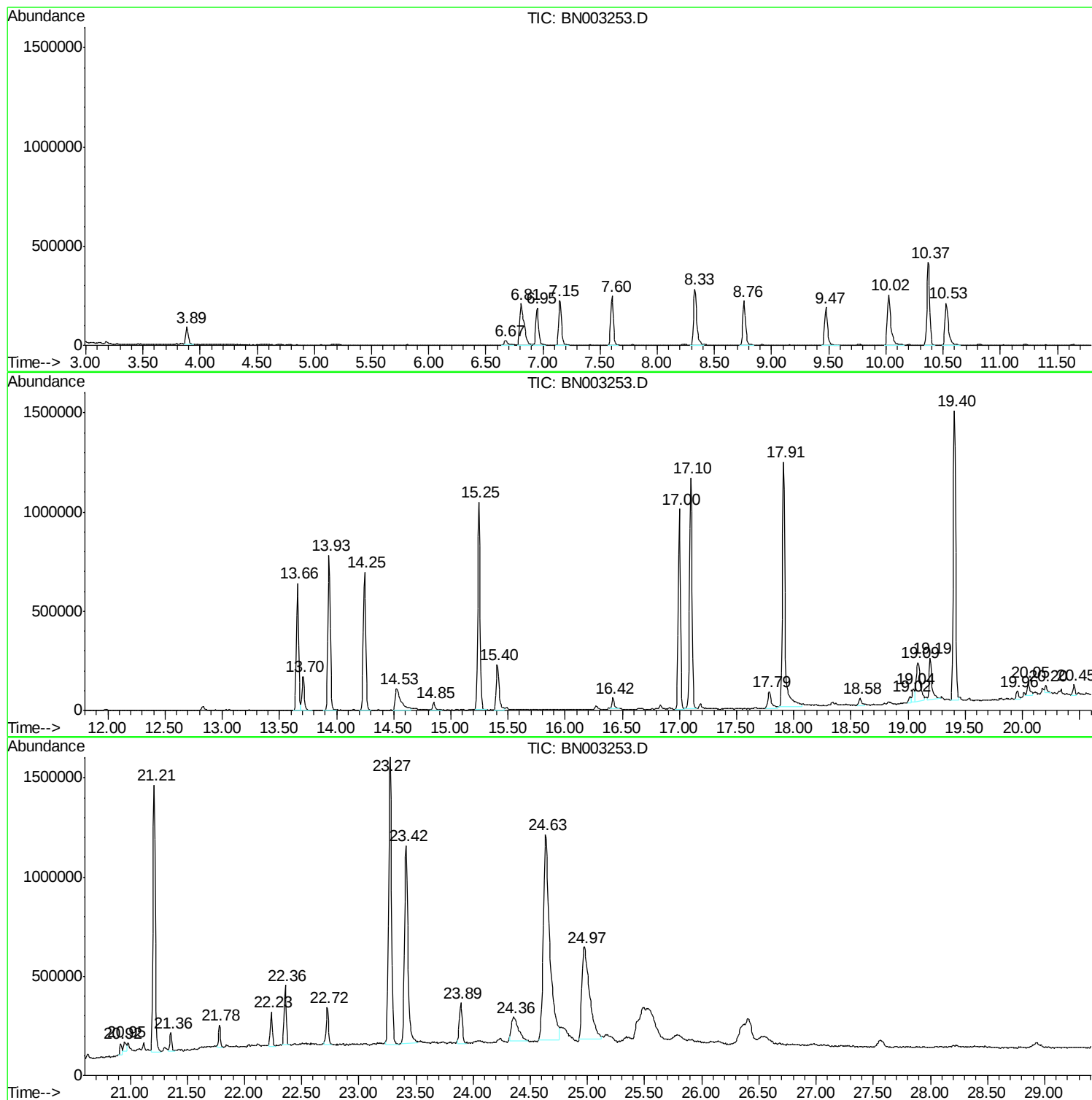
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN101918MA.M
Quant Title : SVOA CALIBRATION

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



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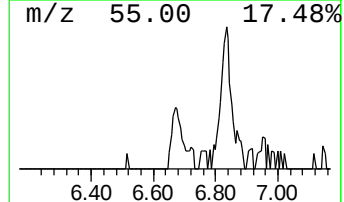
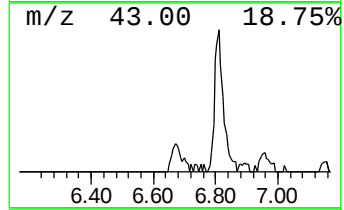
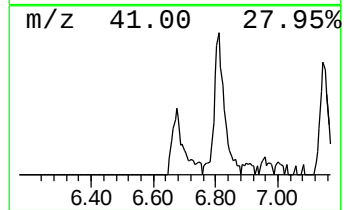
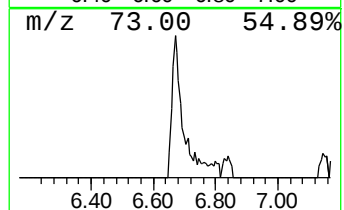
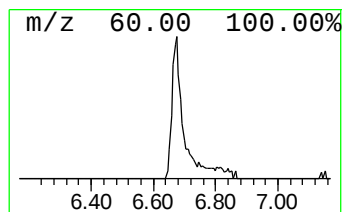
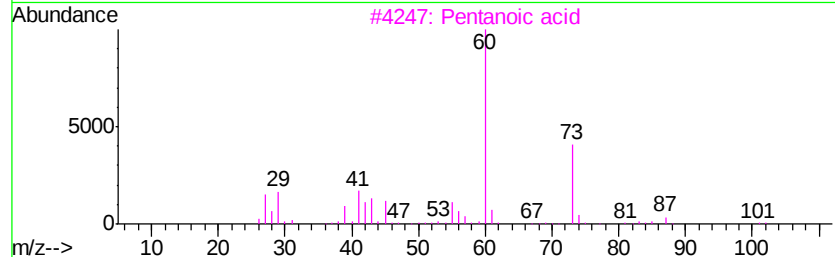
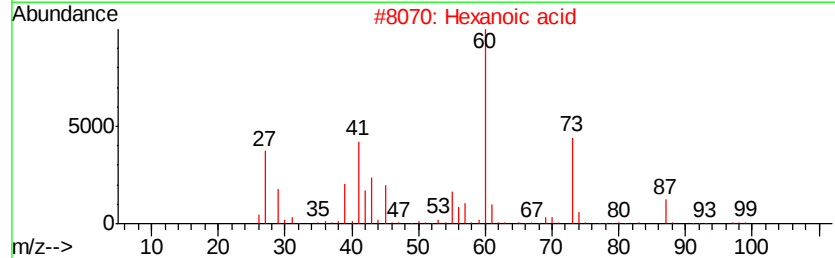
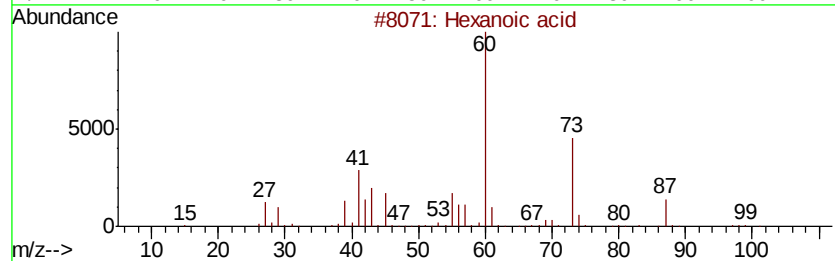
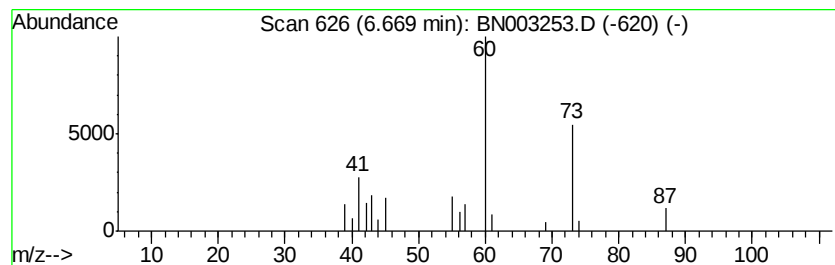
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 Hexanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	2.82 ng/ul	58049	1,4-Dichlorobenzene-d4	7.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	90
3			Pentanoic acid	102	C5H10O2	000109-52-4	78
4			Hexanoic acid	116	C6H12O2	000142-62-1	78
5			Pentanoic acid	102	C5H10O2	000109-52-4	72



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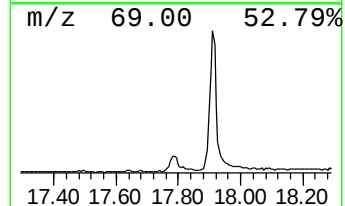
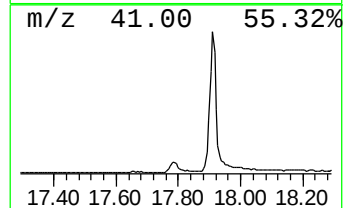
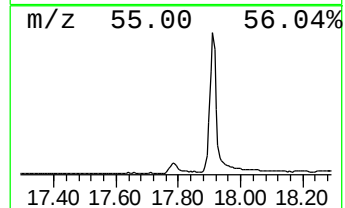
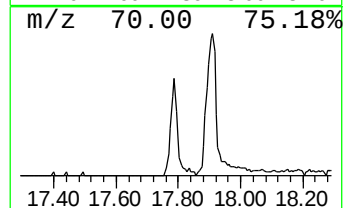
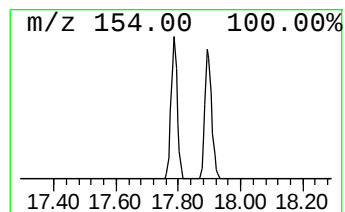
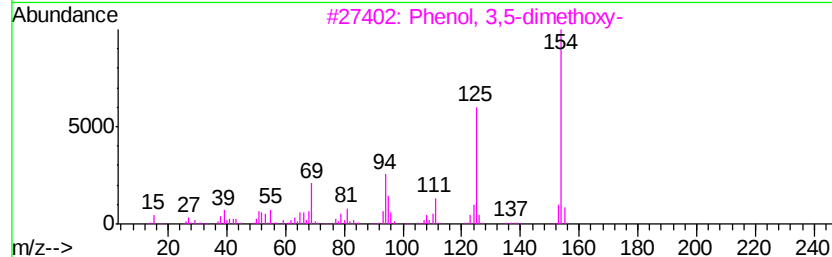
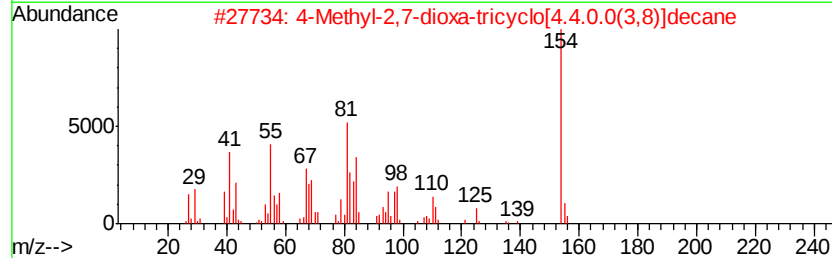
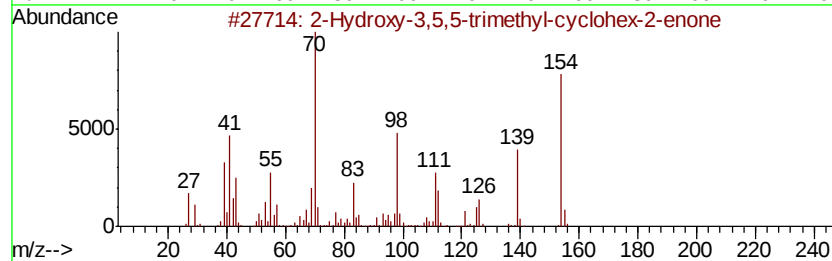
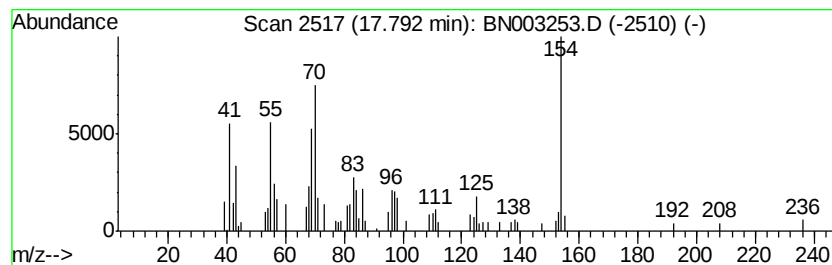
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 2-Hydroxy-3,5,5-trimethyl-c... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.79	2.78 ng/ul	190564	Phenanthrene-d10	17.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-3,5,5-trimethyl-cyclohex-2-enone	154	C9H14O2	004883-60-7	58
2		4-Methyl-2,7-dioxatricyclo[4.4.0.0(3,8)]decane	154	C9H14O2	1000193-48-4	46
3		Phenol, 3,5-dimethoxy-	154	C8H10O3	000500-99-2	30
4		Fumaric acid, monoamide, N-metha...	305	C16H19NO5	1000357-45-9	27
5		2-Undecenal, E-	168	C11H20O	053448-07-0	27



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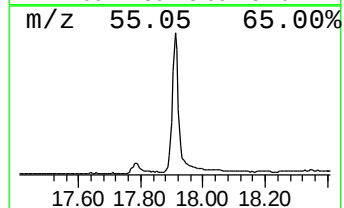
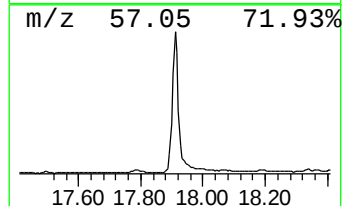
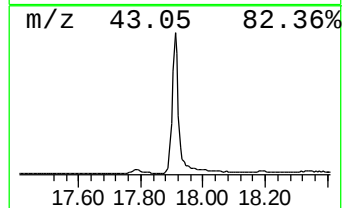
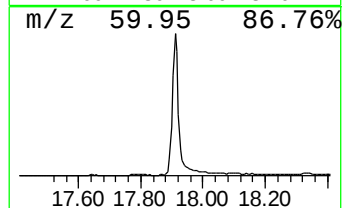
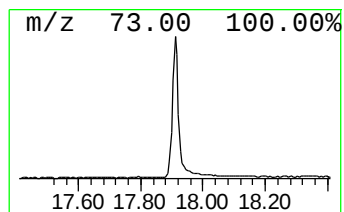
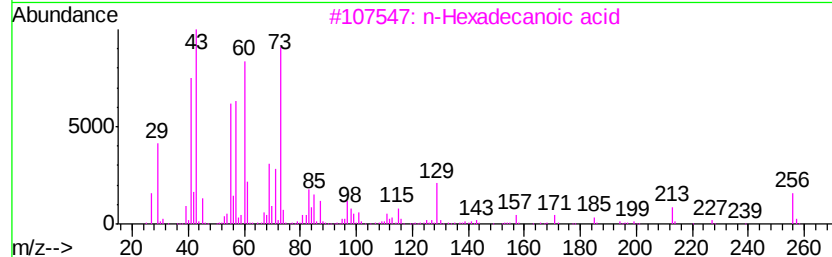
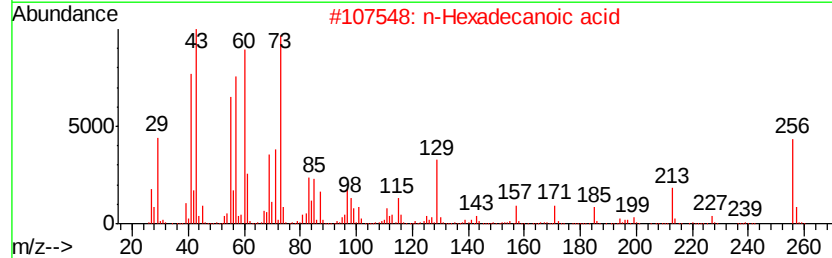
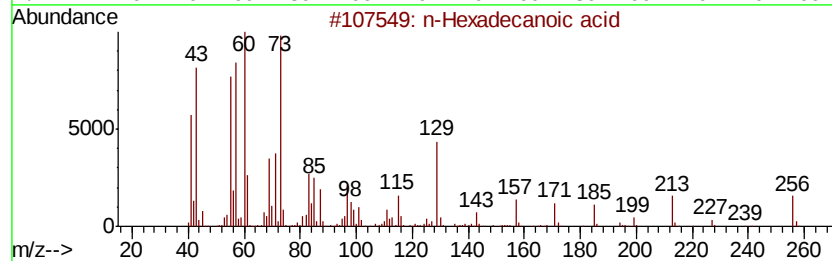
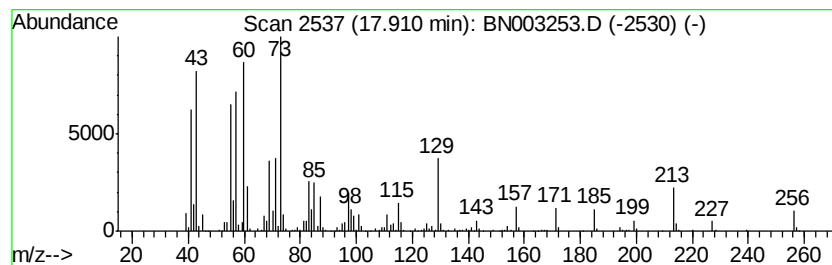
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.91	29.09 ng/ul	1996530	Phenanthrene-d10		17.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99	
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98	
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97	
4	Tridecanoic acid	214	C13H26O2	000638-53-9	95	
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	91	



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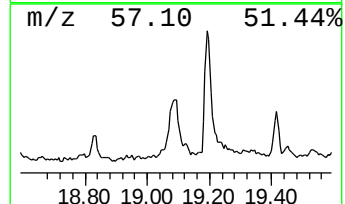
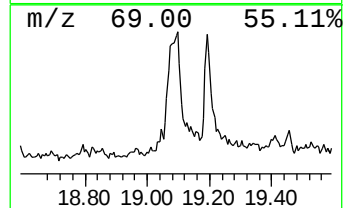
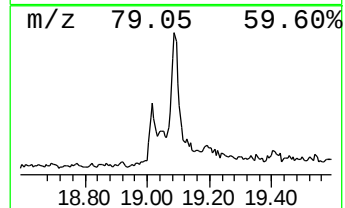
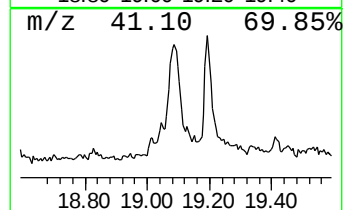
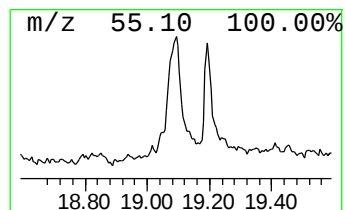
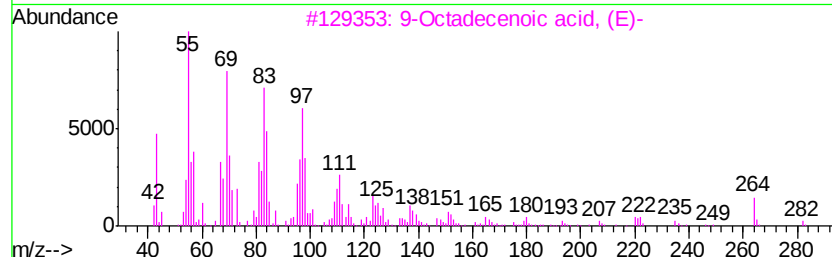
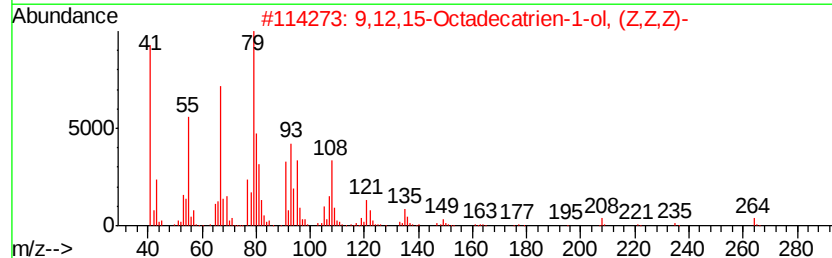
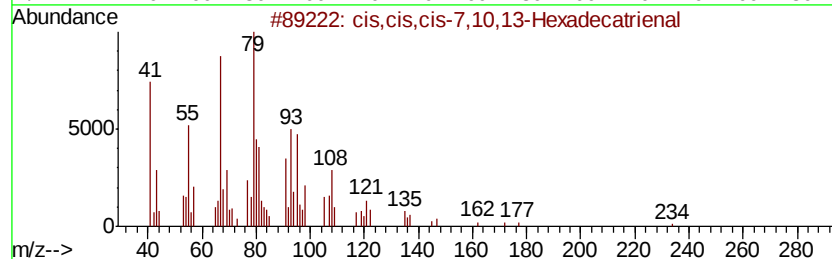
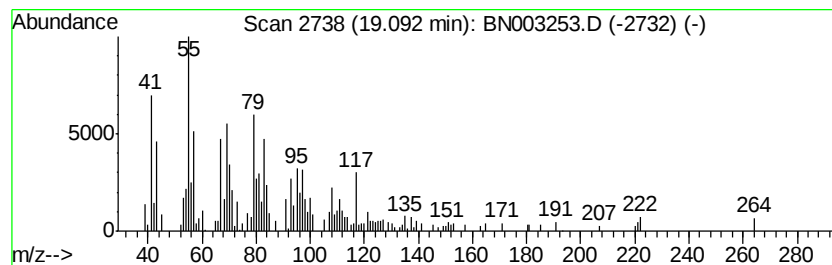
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Peak Number 5 unknown-01 Concentration Rank 4

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19.09	7.19 ng/ul	493420	Phenanthrene-d10	17.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis,cis,cis-7,10,13-Hexadecatrienal	234	C16H26O	056797-43-4	45
2		9,12,15-Octadecatrien-1-ol, (Z,Z...	264	C18H32O	000506-44-5	41
3		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	38
4		cis-Vaccenic acid	282	C18H34O2	000506-17-2	38
5		1-Hexadecanol	242	C16H34O	036653-82-4	35



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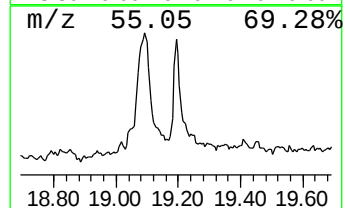
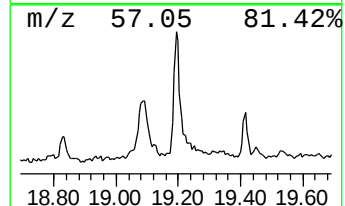
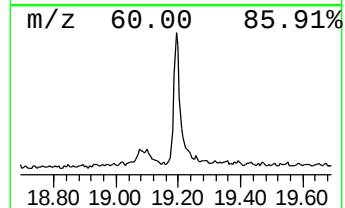
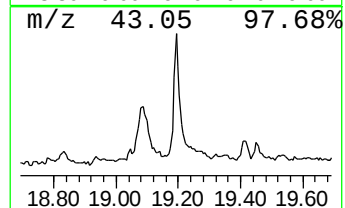
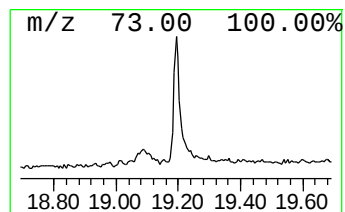
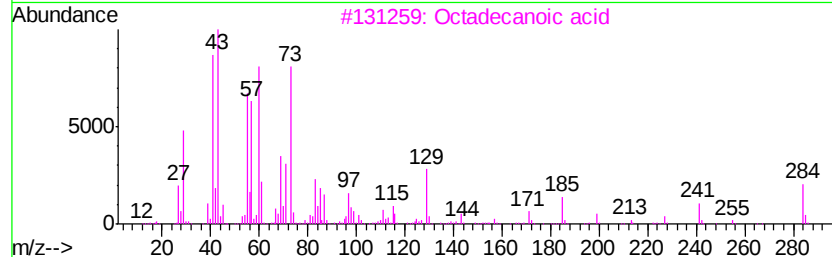
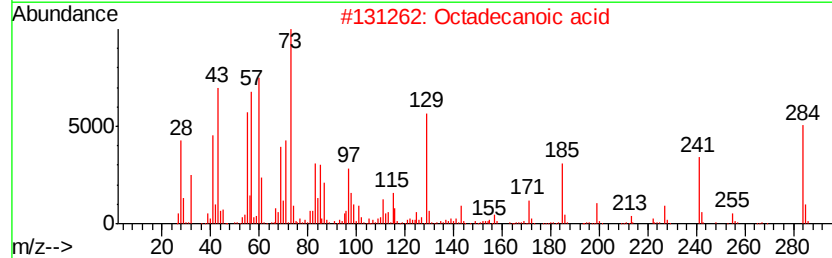
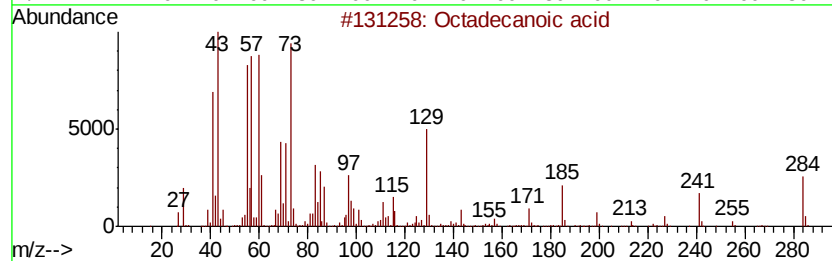
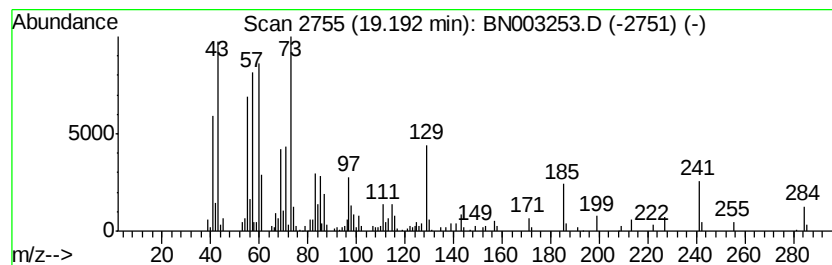
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.		
19.19	3.61 ng/ul	335783	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	98
3			Octadecanoic acid	284	C18H36O2	000057-11-4	98
4			Octadecanoic acid	284	C18H36O2	000057-11-4	95
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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Data File : BN003253.D
Acq On : 22 Oct 2018 23:18
Operator : MJ/SJ
Sample : J5568-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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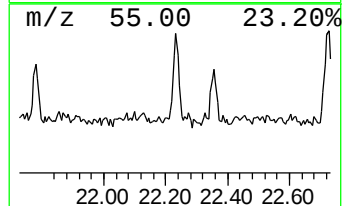
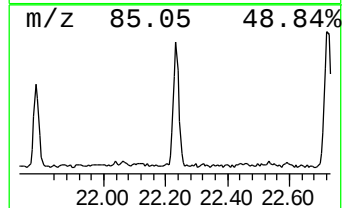
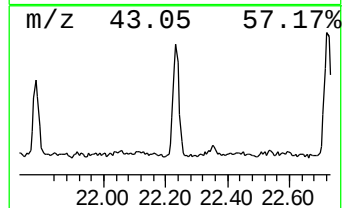
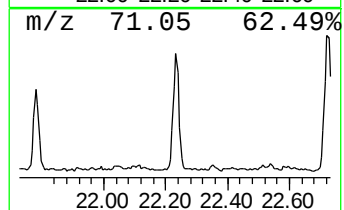
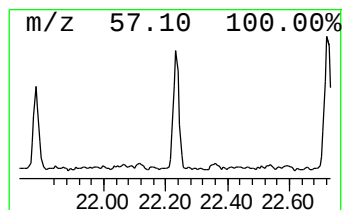
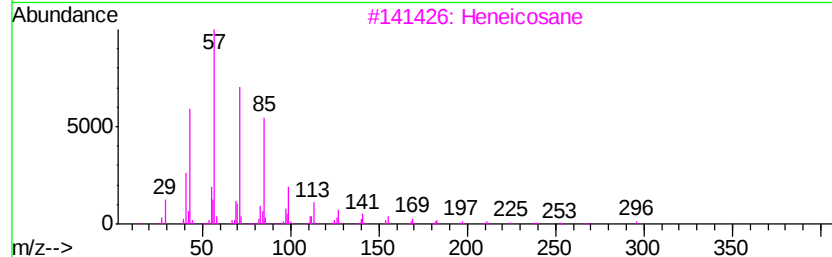
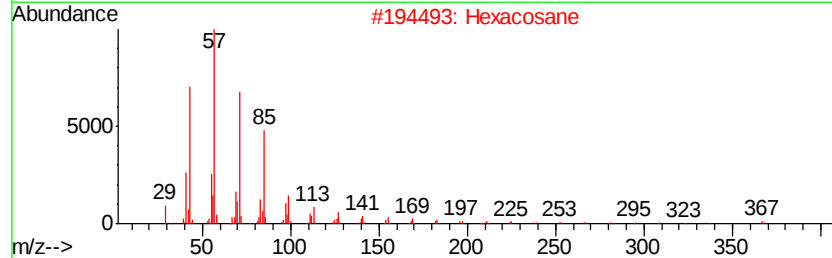
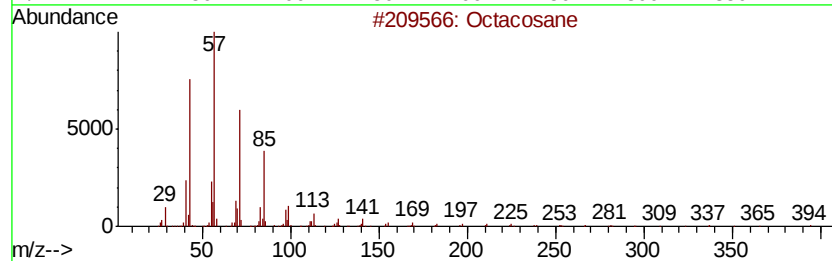
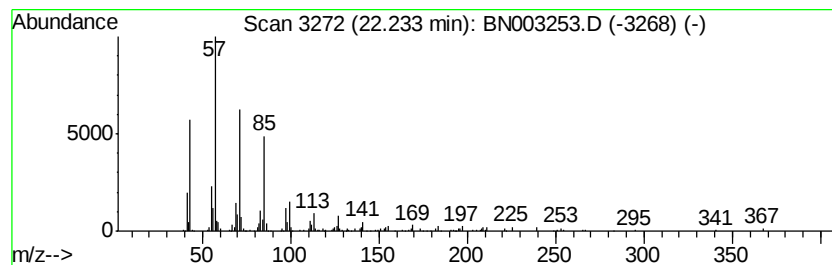
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.23	2.32 ng/ul	216040	Chrysene-d12	21.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
Data File : BN003253.D
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Sample : J5568-11
Misc :
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Instrument :
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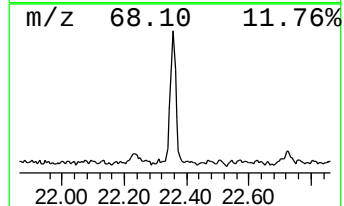
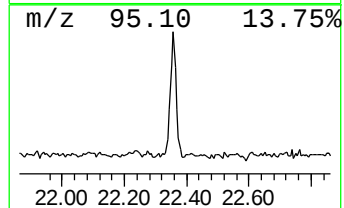
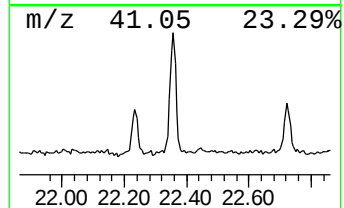
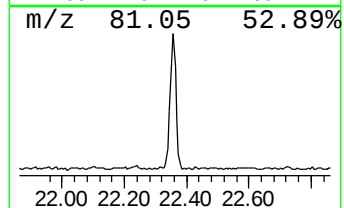
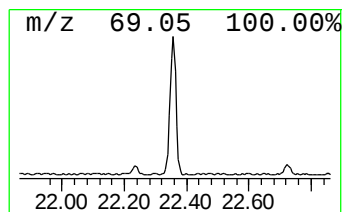
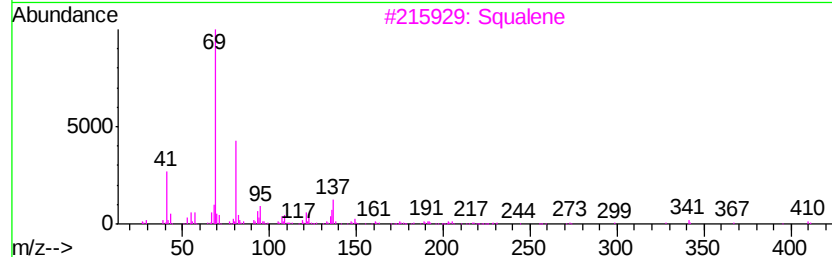
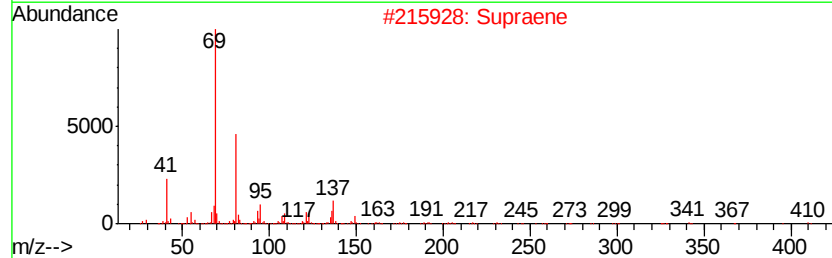
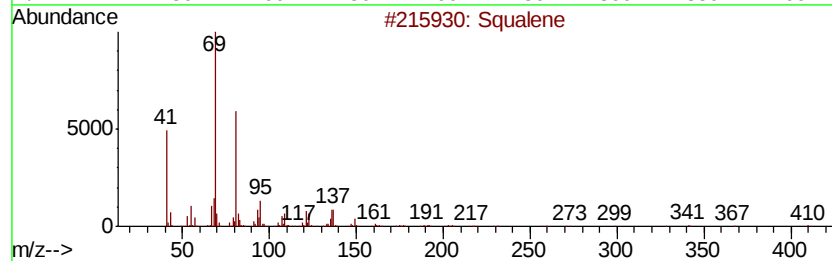
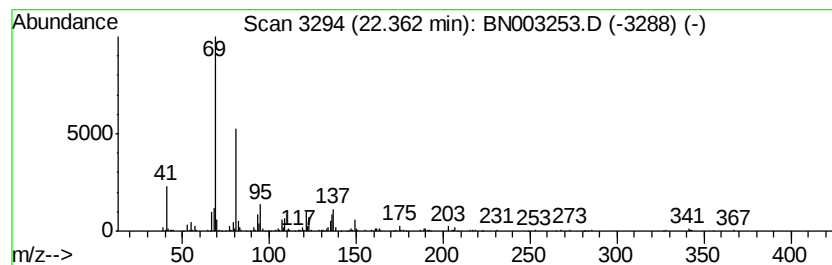
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.36	3.73 ng/ul	387083	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		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
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Sample : J5568-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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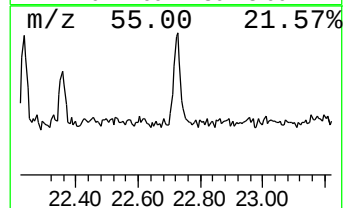
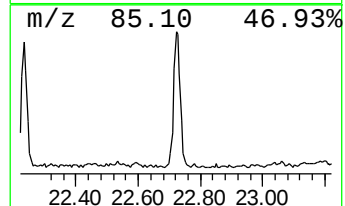
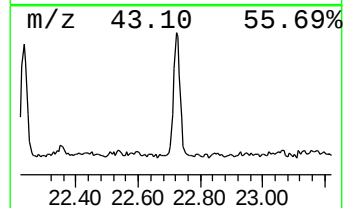
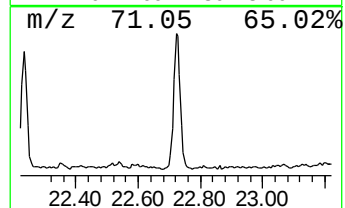
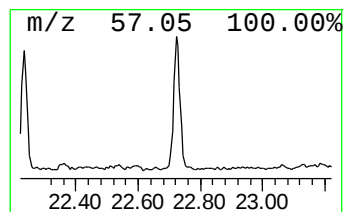
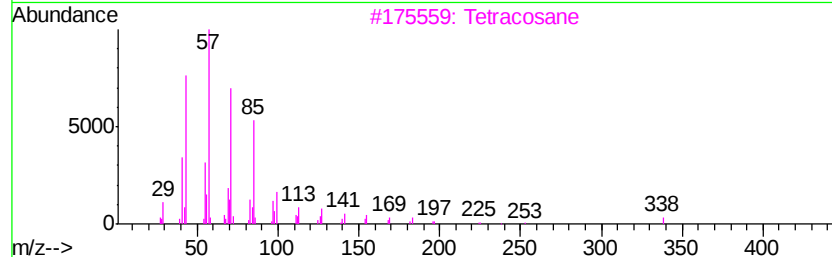
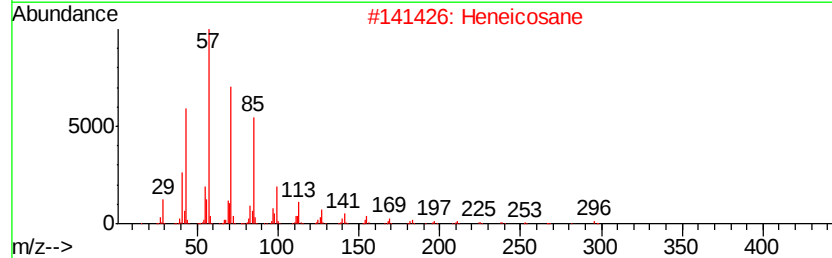
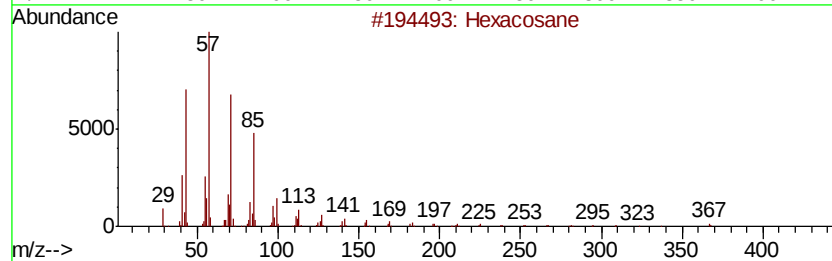
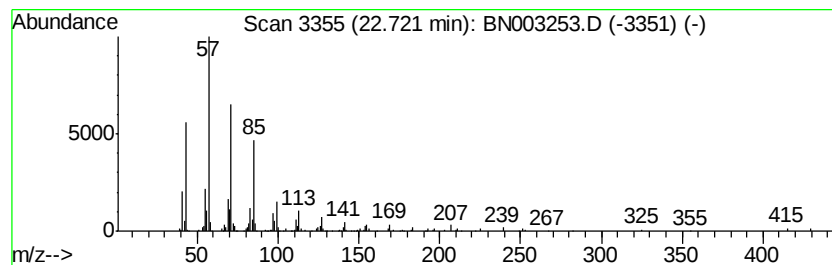
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.72	2.61 ng/ul	270918	Perylene-d12	23.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	93
2		Heneicosane	296	C21H44	000629-94-7	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
5		Docosane	310	C22H46	000629-97-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
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Sample : J5568-11
Misc :
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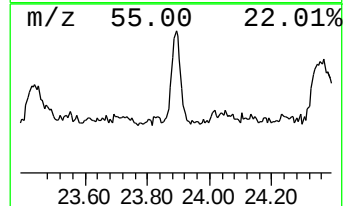
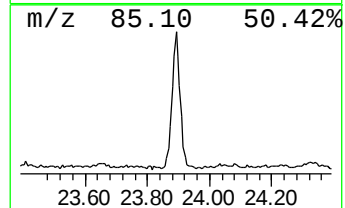
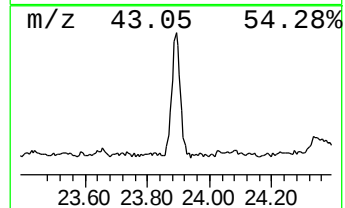
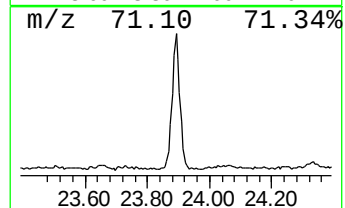
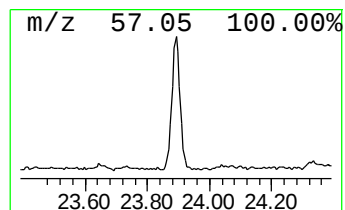
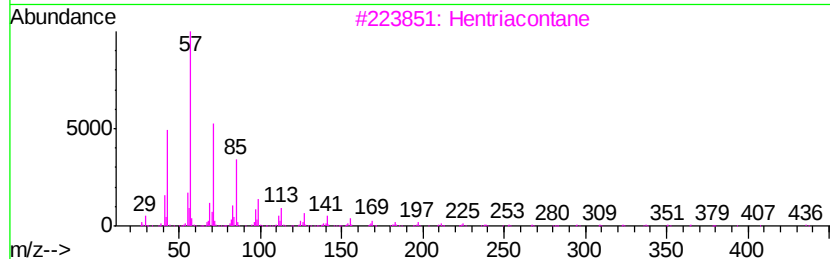
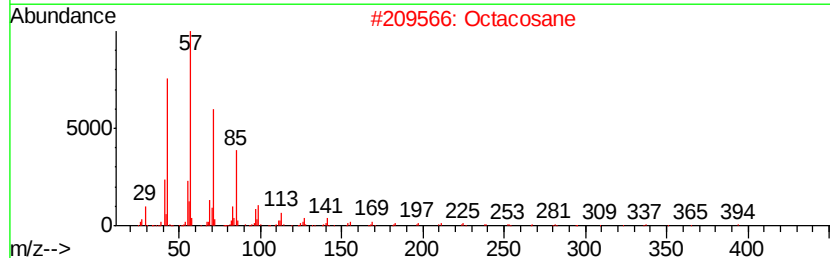
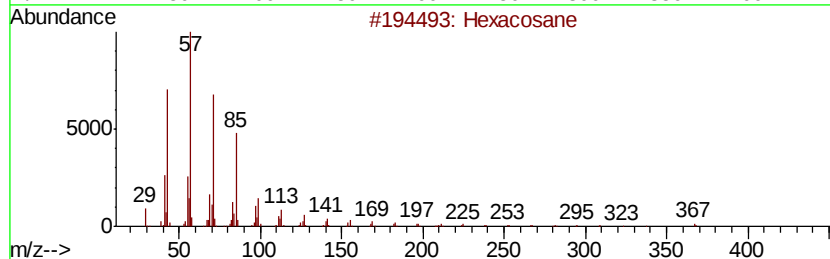
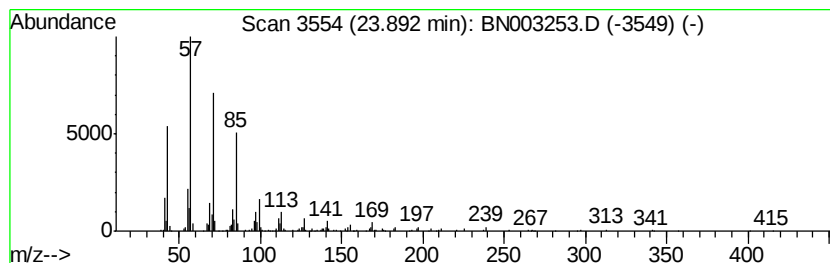
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.89	3.62 ng/ul	375627	Perylene-d12	23.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	93
2			Octacosane	394	C28H58	000630-02-4	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Tetracosane	338	C24H50	000646-31-1	91



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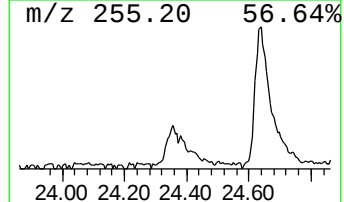
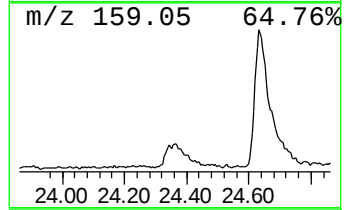
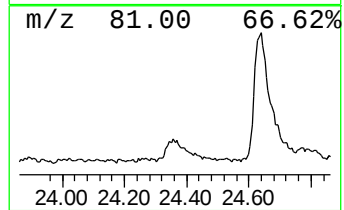
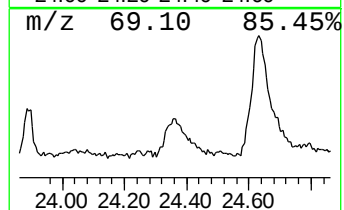
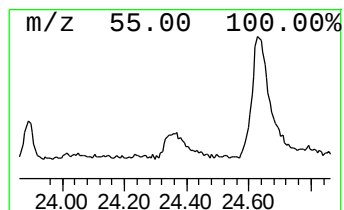
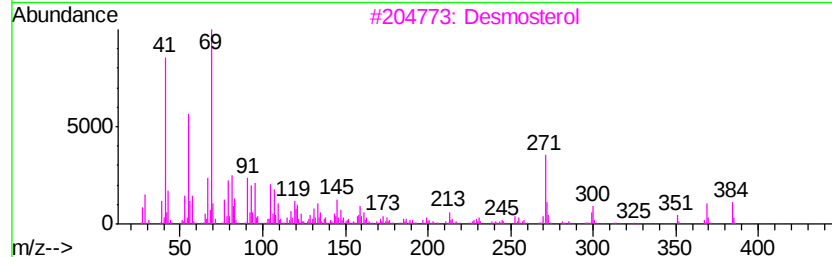
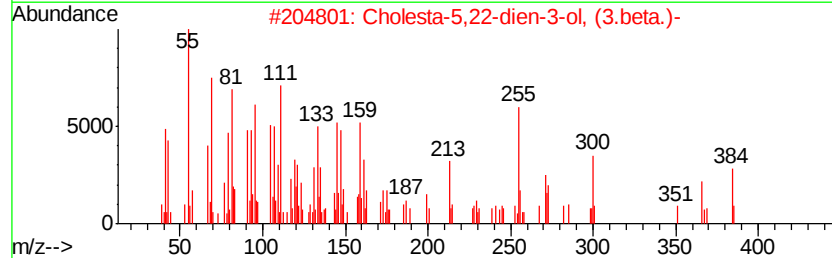
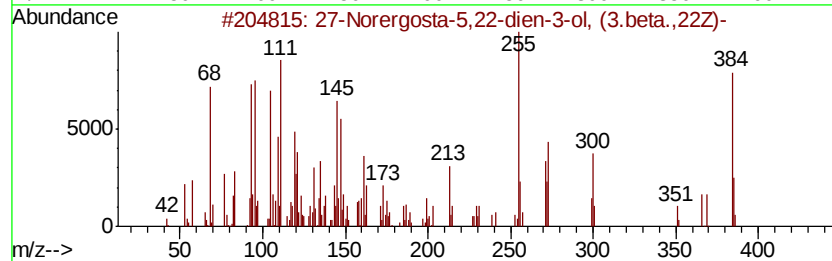
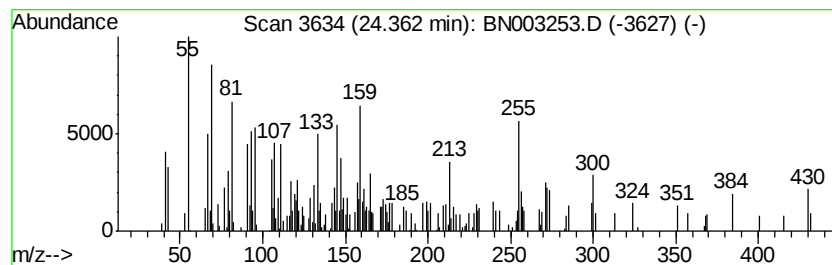
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 27-Norergosta-5,22-dien-3-o... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.36	4.82 ng/ul	500330	Perylene-d12	23.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		27-Norergosta-5,22-dien-3-ol, (3...	384 C27H44O	058072-43-8 86
2		Cholesta-5,22-dien-3-ol, (3.beta.)-	384 C27H44O	092218-20-7 78
3		Desmosterol	384 C27H44O	000313-04-2 25
4		Desmosterol	384 C27H44O	000313-04-2 16
5		Pregna-5,17(20)-dien-3-ol, (3.be...	300 C21H32O	001159-25-7 10



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
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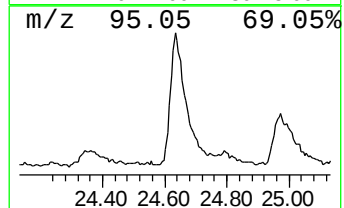
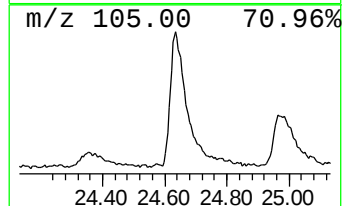
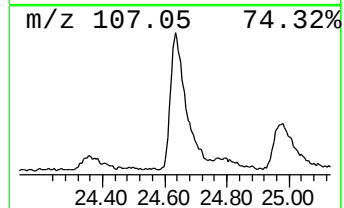
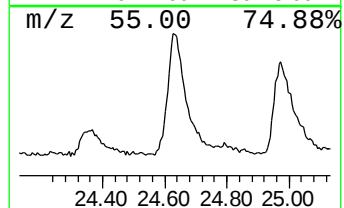
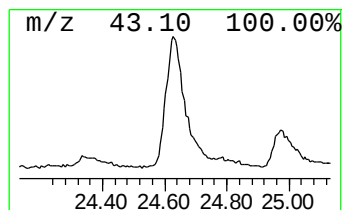
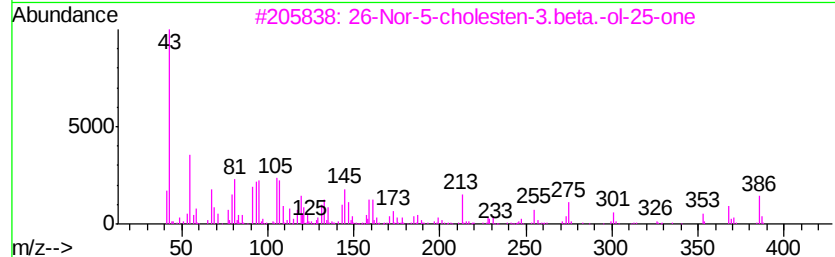
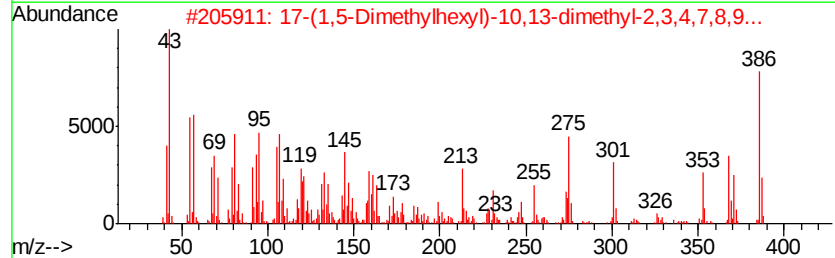
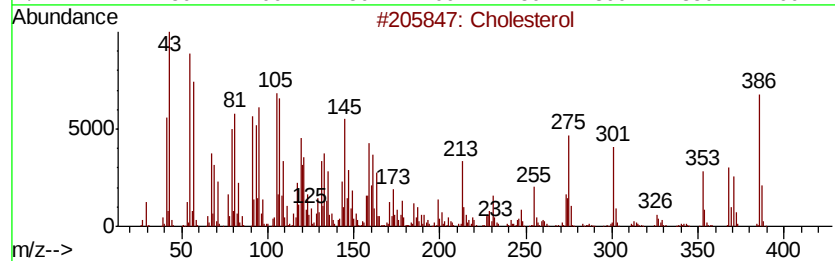
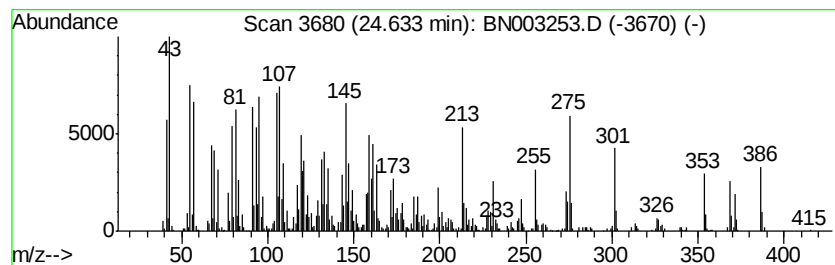
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 Cholesterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.63	39.00 ng/ul	4045800	Perylene-d12	23.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cholesterol		386 C27H46O	000057-88-5 99
2	17-(1,5-Dimethylhexyl)-10,13-dim...		386 C27H46O	1000210-38-4 99
3	26-Nor-5-cholesten-3.beta.-ol-25...		386 C26H42O2	007494-34-0 99
4	Cholesterol		386 C27H46O	000057-88-5 96
5	26-Nor-5-cholesten-3.beta.-ol-25...		386 C26H42O2	007494-34-0 64



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN102218\
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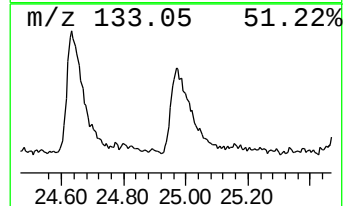
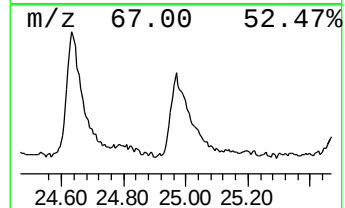
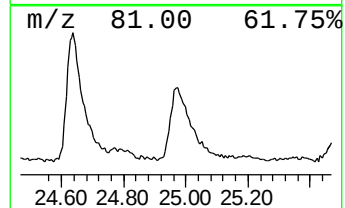
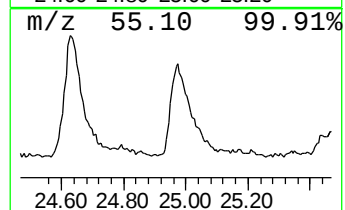
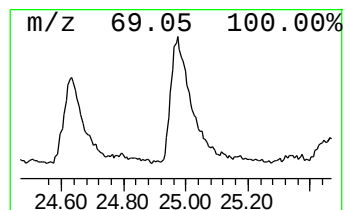
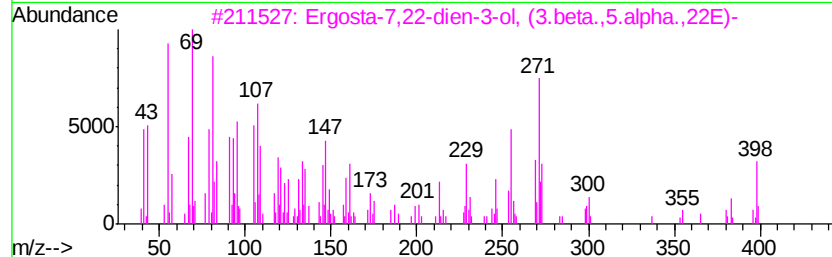
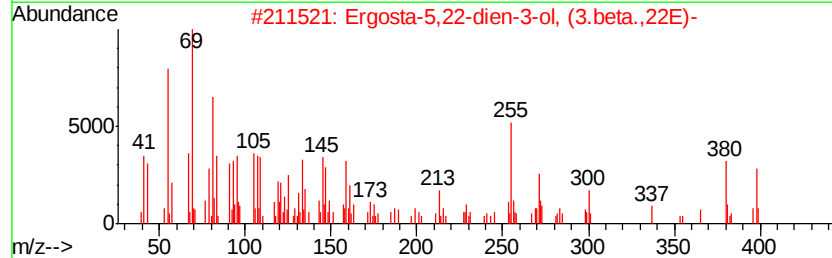
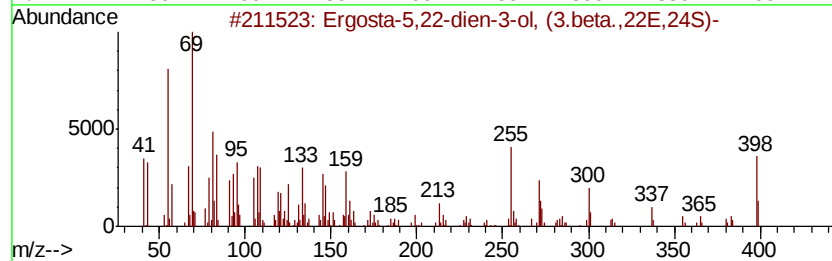
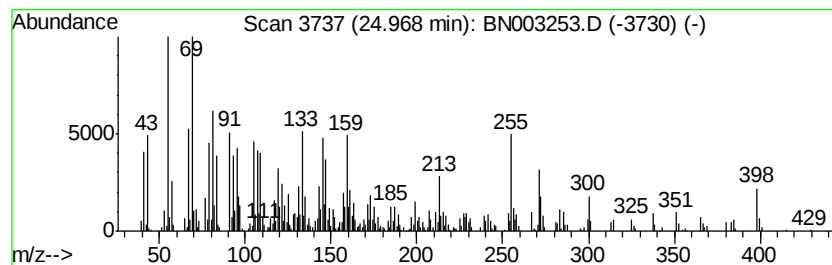
Instrument :
BNA_N
ClientSampleId :
C0AK6

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

Peak Number 13 Ergosta-5,22-dien-3-ol, (3.... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.97	20.76 ng/ul	2153540	Perylene-d12	23.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Ergosta-5,22-dien-3-ol, (3.beta....	398 C28H460	017472-78-5	90
2	Ergosta-5,22-dien-3-ol, (3.beta....	398 C28H460	000474-67-9	90
3	Ergosta-7,22-dien-3-ol, (3.beta....	398 C28H460	002465-11-4	70
4	Ergosta-5,7-dien-3-ol, (3.beta.)-	398 C28H460	000516-79-0	45
5	Ergosta-14,22-dien-3-ol, (3.beta...	398 C28H460	055514-97-1	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_N\DATA\BN102218\
 Data File : BN003253.D
 Acq On : 22 Oct 2018 23:18
 Operator : MJ/SJ
 Sample : J5568-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 C0AK6

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
Hexanoic acid	6.67	2.8	ng/ul	58049	1	7.60	411249	20.0
2-Hydroxy-3,5,5-t...	17.79	2.8	ng/ul	190564	4	17.00	1372770	20.0
n-Hexadecanoic acid	17.91	29.1	ng/ul	1996530	4	17.00	1372770	20.0
unknown-01	19.09	7.2	ng/ul	493420	4	17.00	1372770	20.0
Octadecanoic acid	19.19	3.6	ng/ul	335783	5	21.21	1858950	20.0
(DEL) Alkane: Str...	22.23	2.3	ng/ul	216040	5	21.21	1858950	20.0
Squalene	22.36	3.7	ng/ul	387083	6	23.42	2074910	20.0
(DEL) Alkane: Str...	22.72	2.6	ng/ul	270918	6	23.42	2074910	20.0
(DEL) Alkane: Str...	23.89	3.6	ng/ul	375627	6	23.42	2074910	20.0
27-Norergosta-5,2...	24.36	4.8	ng/ul	500330	6	23.42	2074910	20.0
Cholesterol	24.63	39.0	ng/ul	4045800	6	23.42	2074910	20.0
Ergosta-5,22-dien...	24.97	20.8	ng/ul	2153540	6	23.42	2074910	20.0