

Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN051019\
 Data File : BN005619.D
 Acq On : 11 May 2019 09:30
 Operator : JU/SJ
 Sample : K2613-11
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 BFHD6

Integration Parameters: LSCINT.P

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

Filtering: 5
 Min Area: 0.1 % 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-BN041919MA.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	3.204	34	37	46	rVB2	40337	61916	1.46%	0.109%
2	6.769	637	643	658	rVB	726824	1288641	30.49%	2.268%
3	6.928	664	670	684	rVB	583375	942411	22.30%	1.659%
4	7.122	696	703	717	rVB	793113	1297247	30.69%	2.284%
5	7.581	775	781	790	rBV	774848	1264285	29.91%	2.226%
6	8.287	894	901	916	rVB	956704	1623685	38.42%	2.858%
7	8.728	968	976	987	rBV	767221	1320565	31.24%	2.325%
8	8.892	1000	1004	1012	rVB5	9339	17839	0.42%	0.031%
9	9.157	1043	1049	1055	rVB4	13211	18964	0.45%	0.033%
10	9.439	1088	1097	1111	rBV	670811	1149255	27.19%	2.023%
11	9.975	1181	1188	1207	rBV	935685	1741225	41.20%	3.065%
12	10.339	1244	1250	1264	rVB	1106611	1850489	43.78%	3.258%
13	10.486	1268	1275	1295	rVV	863465	1683730	39.84%	2.964%
14	11.963	1518	1526	1534	rBV2	9694	23738	0.56%	0.042%
15	12.169	1555	1561	1566	rBV3	2133	5001	0.12%	0.009%
16	13.457	1774	1780	1783	rBV2	2417	4290	0.10%	0.008%
17	13.633	1803	1810	1815	rBV	1810092	2516385	59.54%	4.430%
18	13.680	1815	1818	1827	rVB	383363	527411	12.48%	0.928%
19	13.904	1850	1856	1873	rBV	2092051	3145511	74.42%	5.537%
20	14.133	1892	1895	1902	rVB3	2946	4859	0.11%	0.009%
21	14.216	1902	1909	1920	rBV2	1612113	2446817	57.89%	4.307%
22	14.445	1942	1948	1968	rBV	470198	1005737	23.80%	1.770%
23	14.663	1983	1985	1989	rVB4	4698	5263	0.12%	0.009%
24	14.757	1998	2001	2008	rVB4	3346	5343	0.13%	0.009%
25	14.980	2034	2039	2045	rVB3	21367	29215	0.69%	0.051%
26	15.092	2055	2058	2064	rVB3	7306	9373	0.22%	0.016%
27	15.216	2073	2079	2088	rBV	2507114	3736519	88.41%	6.578%
28	15.363	2099	2104	2116	rBV	458064	745584	17.64%	1.312%
29	15.457	2116	2120	2126	rVV	33149	54314	1.29%	0.096%
30	15.504	2126	2128	2132	rVB2	4394	4422	0.10%	0.008%
31	15.910	2193	2197	2201	rVB4	3126	4426	0.10%	0.008%
32	15.957	2201	2205	2207	rBV4	8261	10326	0.24%	0.018%
33	16.010	2210	2214	2219	rVB3	11366	16635	0.39%	0.029%
34	16.127	2227	2234	2239	rVV7	7274	10843	0.26%	0.019%

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35	16.268	2255	2258	2260	rBV3	3606	4715	0.11%	0.008%
36	16.398	2277	2280	2286	rBV3	21626	35266	0.83%	0.062%
37	16.716	2326	2334	2337	rBV5	3501	9465	0.22%	0.017%
38	16.763	2337	2342	2346	rBV5	14036	26556	0.63%	0.047%
39	16.974	2371	2378	2388	rBV2	2040809	2884694	68.25%	5.078%
40	17.074	2388	2395	2408	rVV	2708440	3974060	94.03%	6.996%
41	17.168	2408	2411	2419	rVB7	12353	19722	0.47%	0.035%
42	17.286	2424	2431	2437	rBV9	7140	16212	0.38%	0.029%
43	17.380	2442	2447	2458	rBV6	25640	59071	1.40%	0.104%
44	17.486	2461	2465	2468	rBV4	7973	12130	0.29%	0.021%
45	17.763	2507	2512	2524	rBV5	49144	112142	2.65%	0.197%
46	17.898	2529	2535	2549	rBV	901820	1534303	36.30%	2.701%
47	18.180	2578	2583	2586	rBV5	11639	18907	0.45%	0.033%
48	18.221	2588	2590	2593	rVV4	6563	5363	0.13%	0.009%
49	18.451	2625	2629	2633	rBV7	5584	10685	0.25%	0.019%
50	18.515	2637	2640	2641	rBV3	4756	5343	0.13%	0.009%
51	18.574	2647	2650	2654	rBV6	6103	8875	0.21%	0.016%
52	18.762	2679	2682	2687	rBV4	12576	21997	0.52%	0.039%
53	18.827	2691	2693	2697	rVB4	6523	7265	0.17%	0.013%
54	18.945	2711	2713	2716	rBV4	6255	7557	0.18%	0.013%
55	19.021	2722	2726	2728	rBV	28024	36641	0.87%	0.065%
56	19.068	2729	2734	2743	rVB7	38465	90403	2.14%	0.159%
57	19.192	2751	2755	2764	rBV	293437	523030	12.37%	0.921%
58	19.268	2766	2768	2775	rVB	37150	55361	1.31%	0.097%
59	19.386	2782	2788	2798	rVB	3068139	4226506	100.00%	7.440%
60	20.321	2945	2947	2953	rVB7	28581	44377	1.05%	0.078%
61	20.462	2966	2971	2975	rBV5	33937	60061	1.42%	0.106%
62	20.927	3046	3050	3060	rBV	408036	680860	16.11%	1.199%
63	21.204	3091	3097	3106	rBV	1926874	2608167	61.71%	4.591%
64	21.374	3123	3126	3130	rBV	112883	116726	2.76%	0.205%
65	21.803	3196	3199	3203	rBV	151131	198579	4.70%	0.350%
66	22.256	3271	3276	3287	rVB2	405902	645028	15.26%	1.135%
67	22.386	3293	3298	3305	rVB	1400820	1911255	45.22%	3.364%
68	22.756	3357	3361	3366	rVB	281257	370516	8.77%	0.652%
69	22.921	3385	3389	3396	rVB	318718	471985	11.17%	0.831%
70	23.262	3440	3447	3452	rBV2	1658675	3136626	74.21%	5.522%
71	23.403	3464	3471	3482	rVB	1114747	2230219	52.77%	3.926%

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72	23.933	3556	3561	3568	rVB	211587	395350	9.35%	0.696%
73	24.068	3579	3584	3592	rVB2	405287	794957	18.81%	1.399%
74	24.650	3678	3683	3692	rBV3	161031	349947	8.28%	0.616%
75	25.568	3834	3839	3851	rVB3	176614	513827	12.16%	0.905%

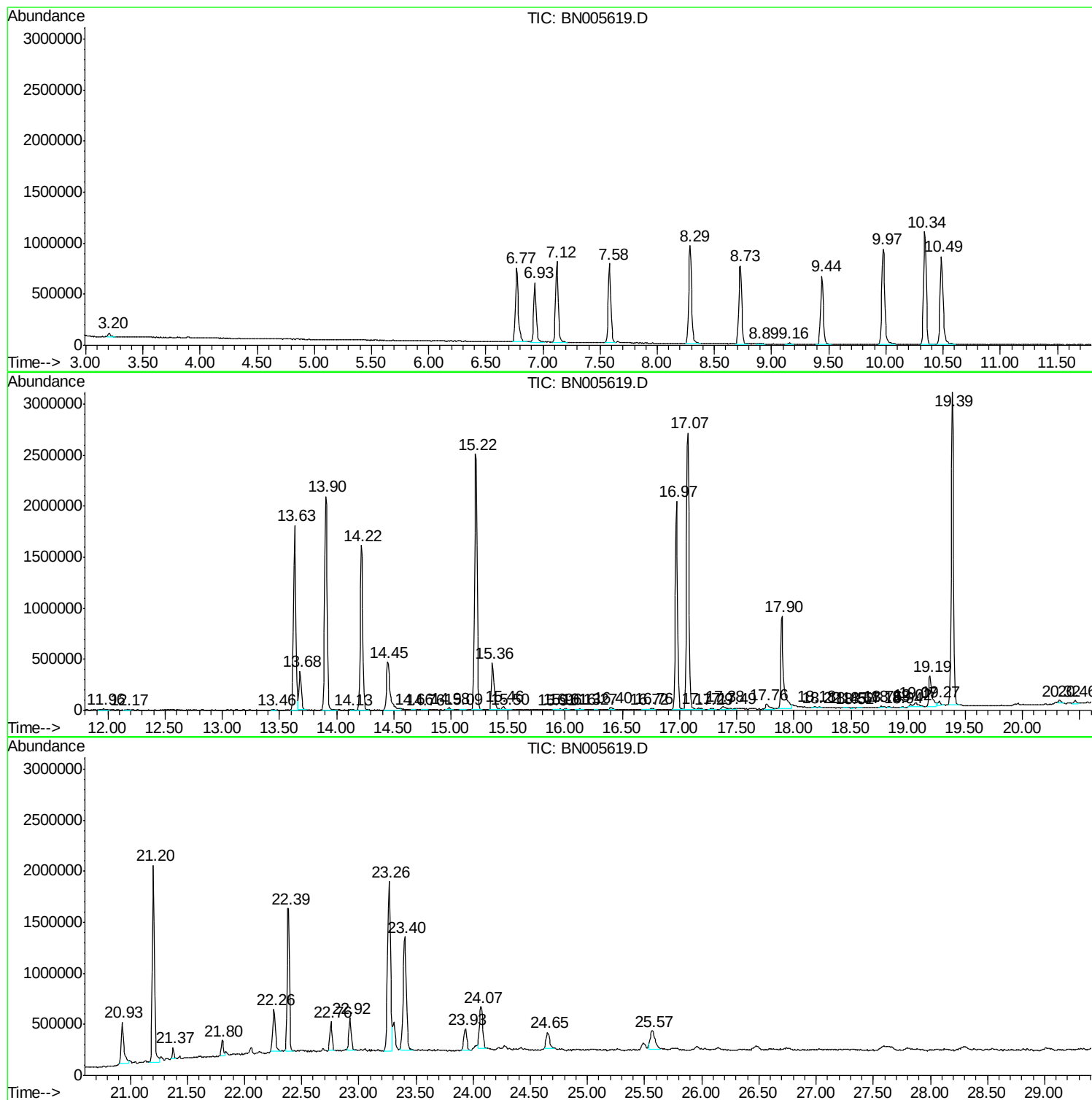
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041919MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN051019\
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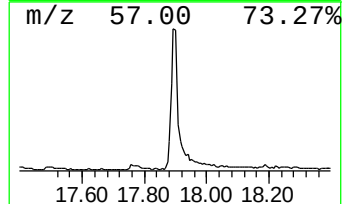
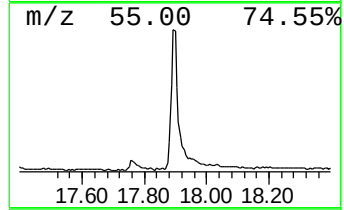
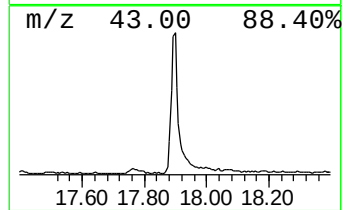
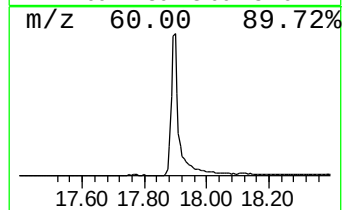
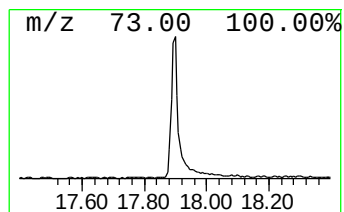
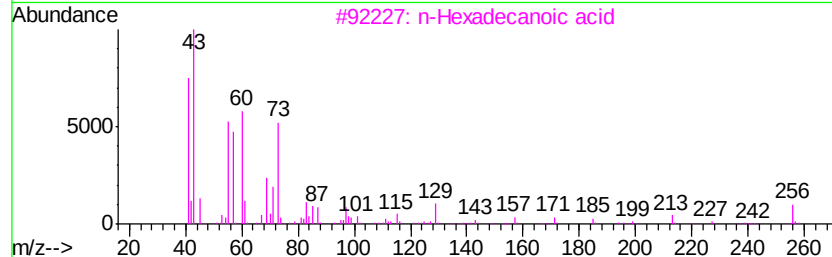
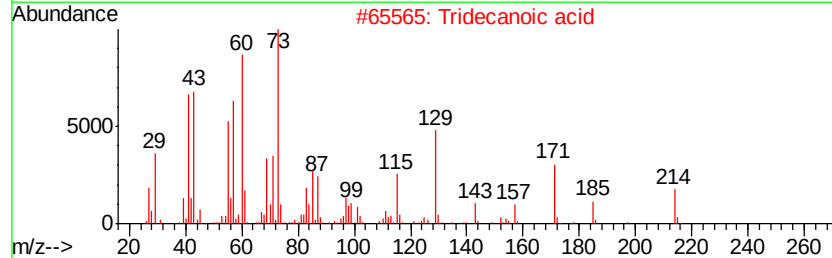
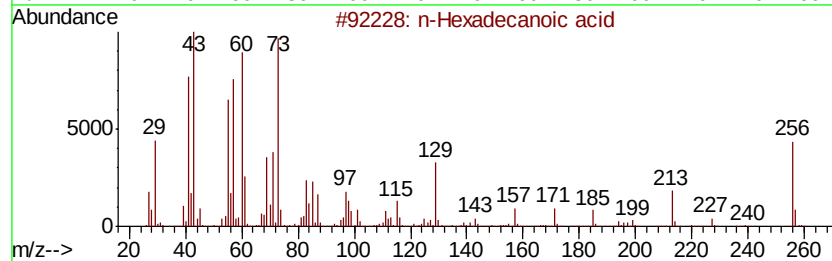
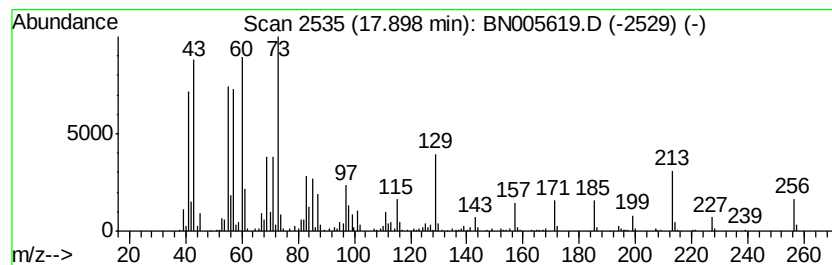
Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041919MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.90	10.64 ng/ul	1534300	Phenanthrene-d10	16.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	96
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
4		Tridecanoic acid	214	C13H26O2	000638-53-9	91
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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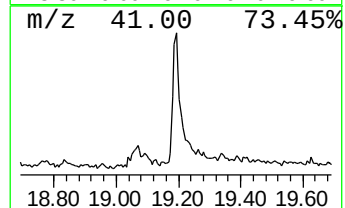
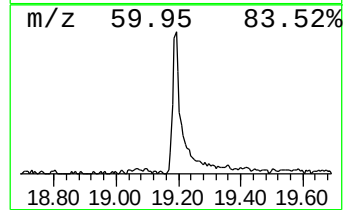
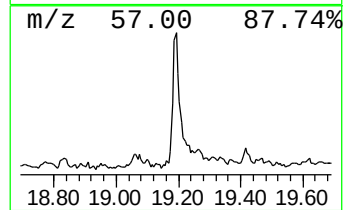
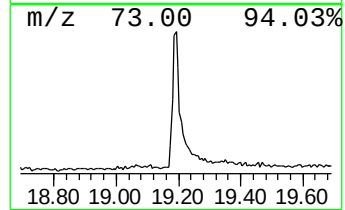
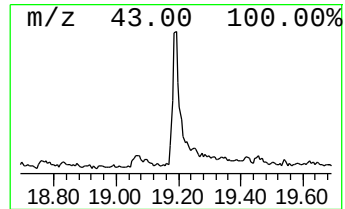
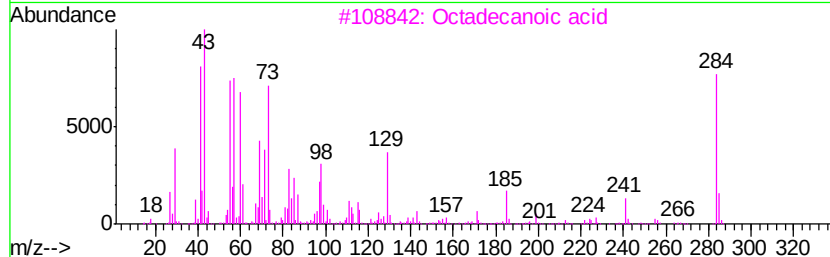
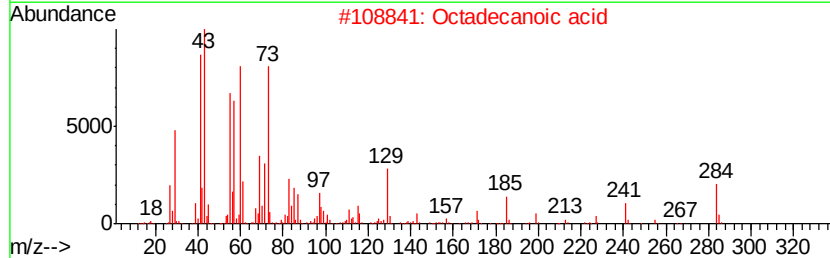
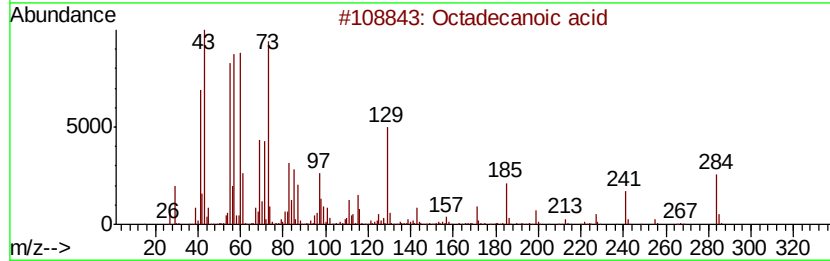
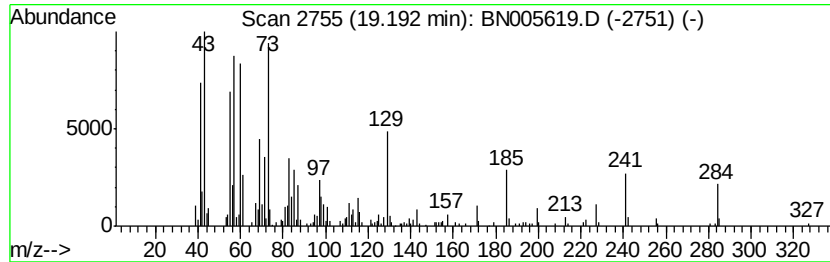
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041919MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.19	4.01 ng/ul	523030	Chrysene-d12	21.20

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	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	95
4			Octadecanoic acid	284	C18H36O2	000057-11-4	94
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	81



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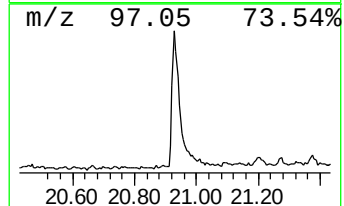
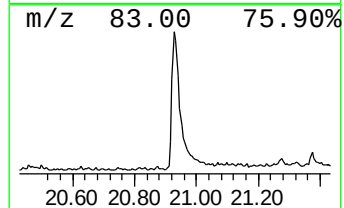
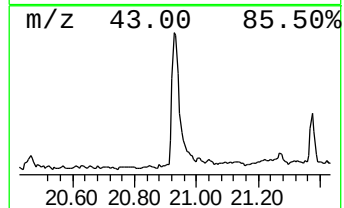
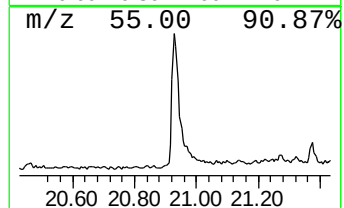
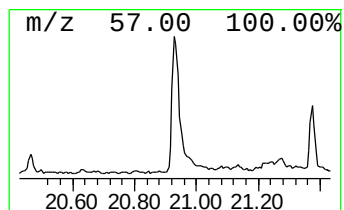
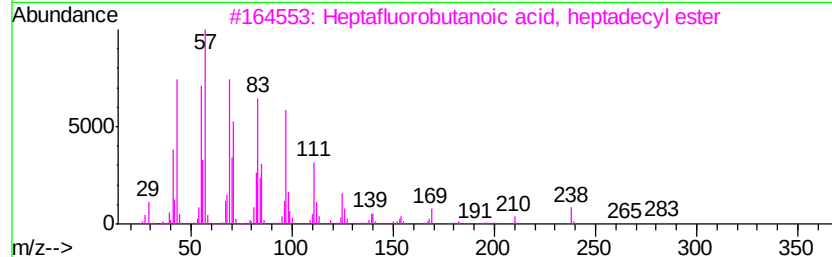
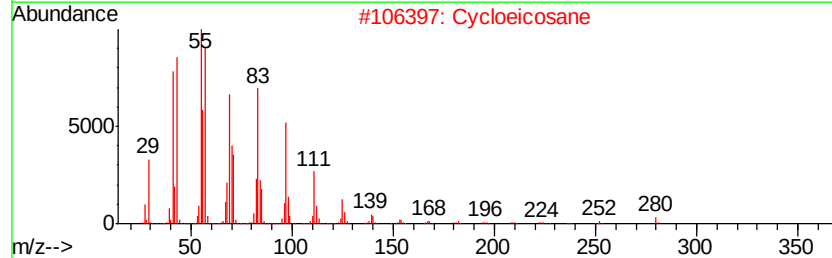
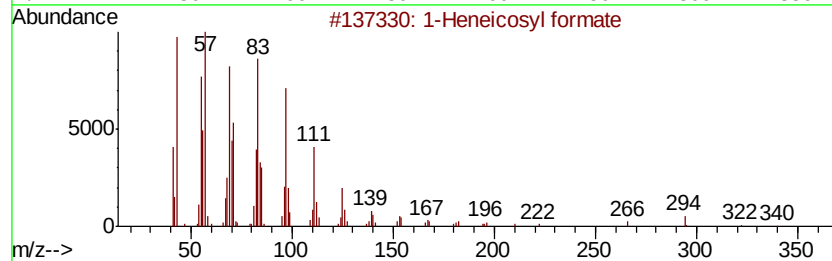
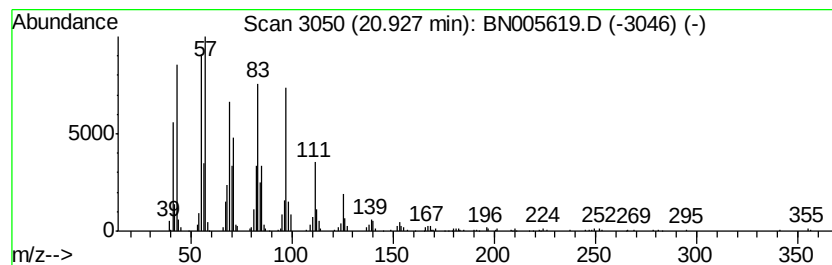
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	5.22 ng/ul	680860	Chrysene-d12	21.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosyl formate	340 C22H44O2	077899-03-7	94
2	Cycloeicosane	280 C20H40	000296-56-0	91
3	Heptafluorobutanoic acid, heptadecyl ester	452 C21H35F7O2	1000282-97-3	91
4	2-Chloropropionic acid, octadecyl ester	360 C21H41ClO2	088104-31-8	91
5	1-Docosene	308 C22H44	001599-67-3	91



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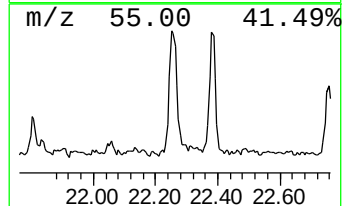
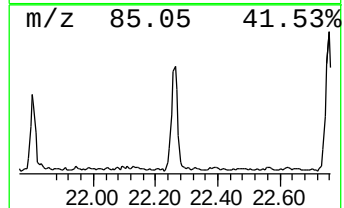
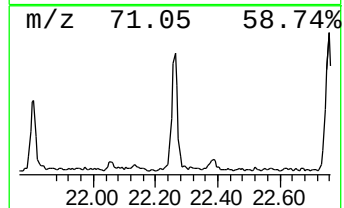
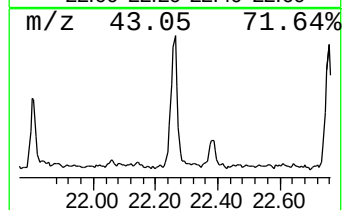
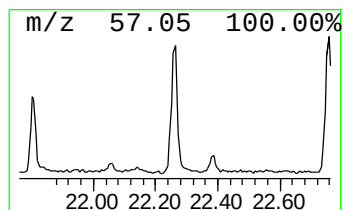
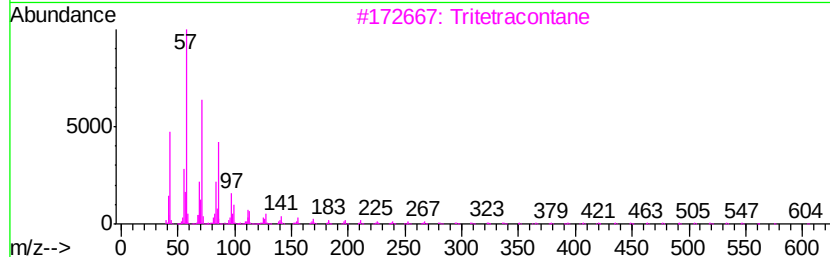
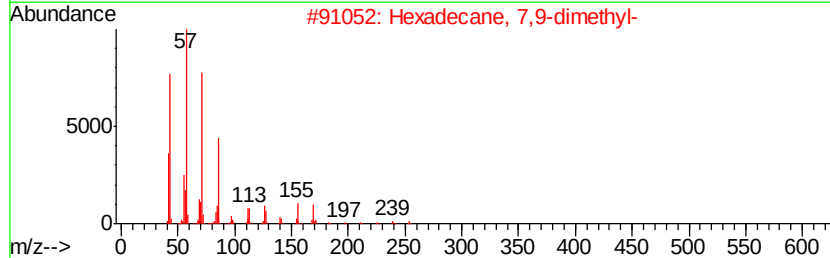
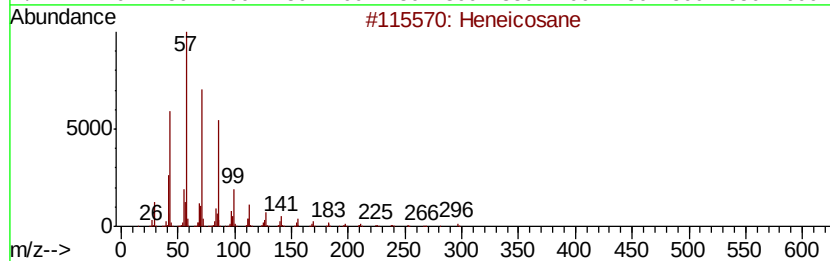
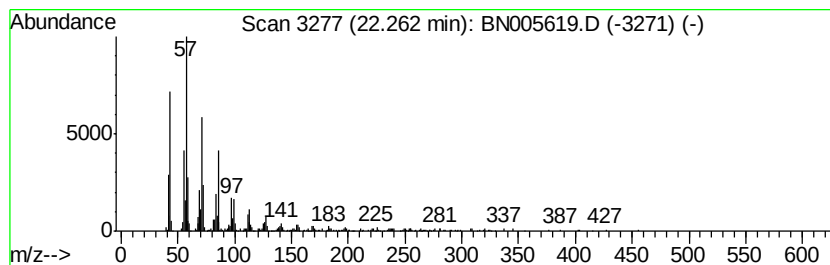
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.26	4.95 ng/ul	645028	Chrysene-d12	21.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	86
2		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	59
3		Tritetracontane	605	C43H88	007098-21-7	53
4		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	53
5		Docosane, 9-octyl-	422	C30H62	055319-83-0	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN051019\
 Data File : BN005619.D
 Acq On : 11 May 2019 09:30
 Operator : JU/SJ
 Sample : K2613-11
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 BFHD6

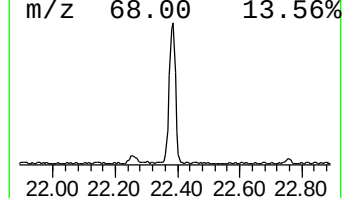
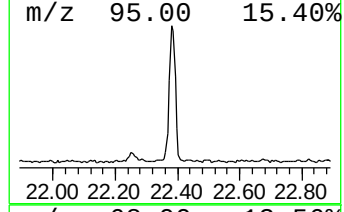
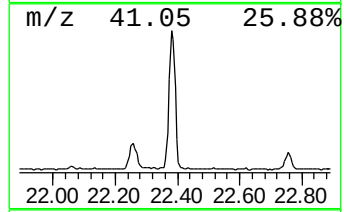
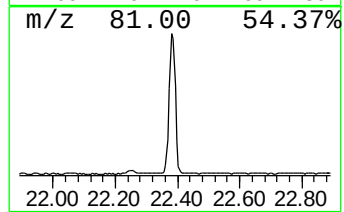
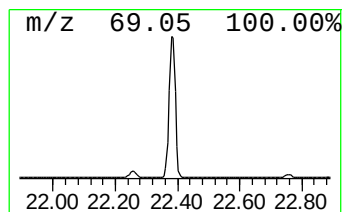
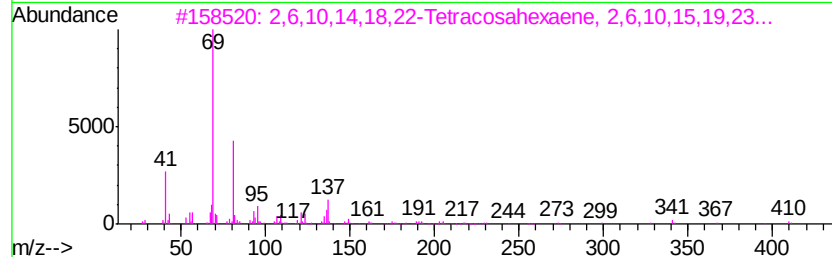
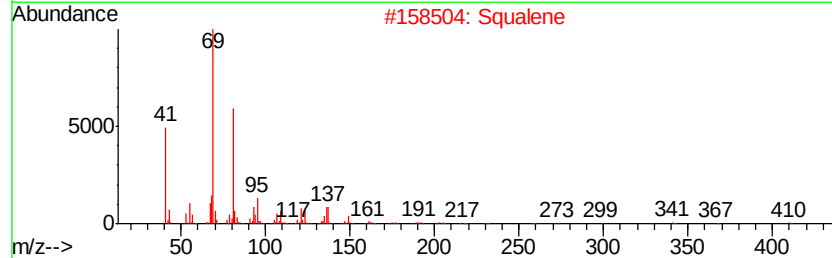
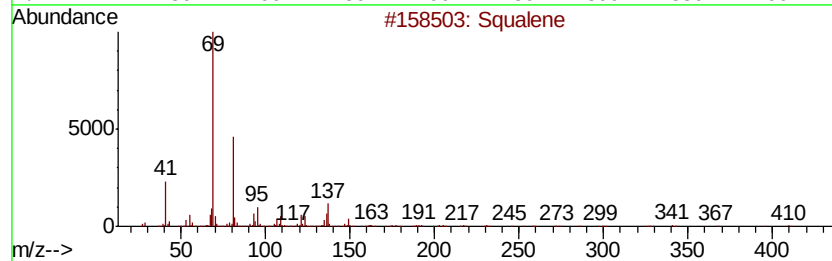
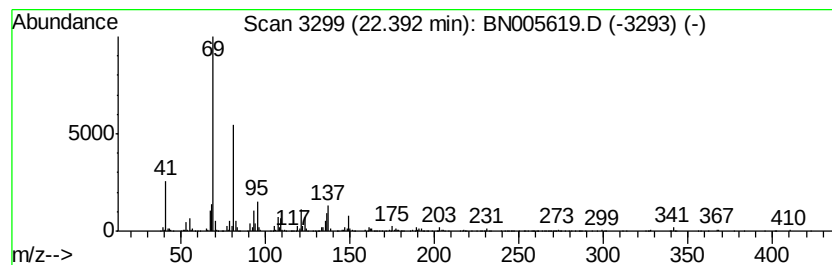
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 Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	17.14 ng/ul	1911260	Perylene-d12	23.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	007683-64-9	91
3		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
4		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	86
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN051019\
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Acq On : 11 May 2019 09:30
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Sample : K2613-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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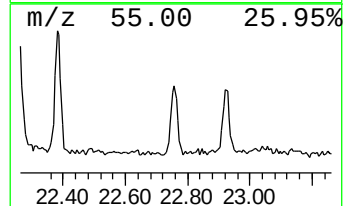
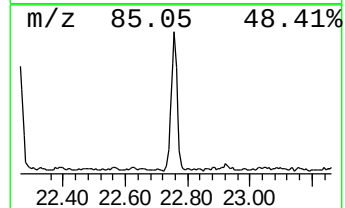
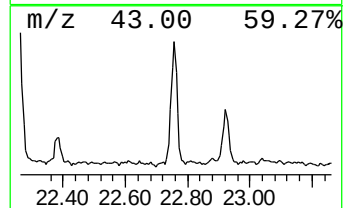
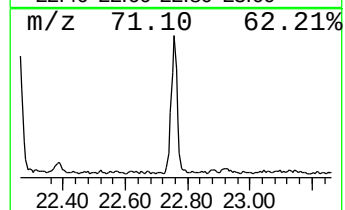
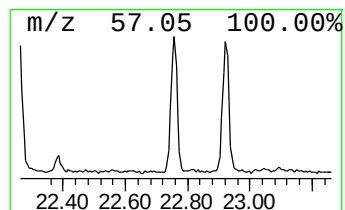
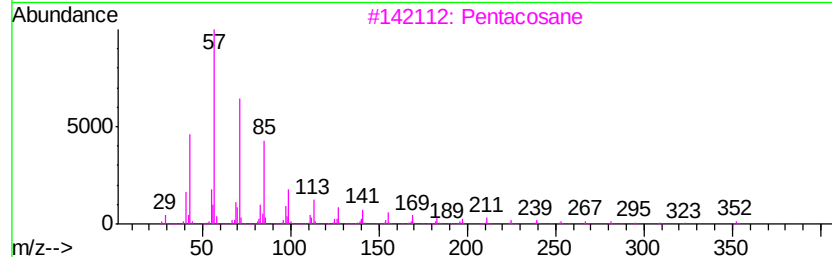
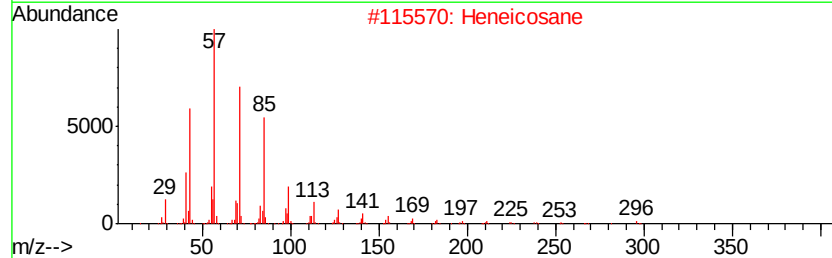
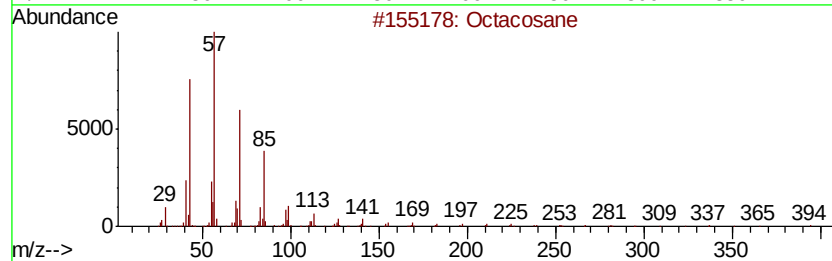
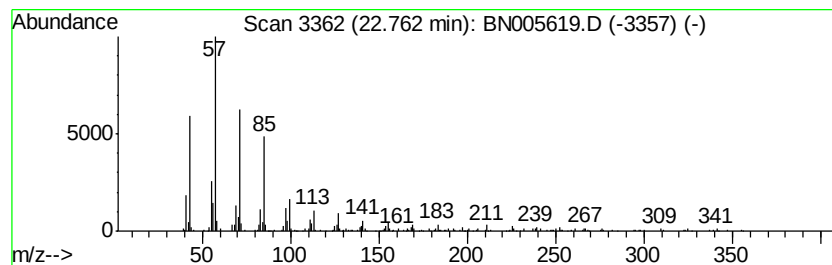
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.76	3.32 ng/ul	370516	Perylene-d12	23.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Pentacosane	352	C25H52	000629-99-2	87
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	87
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN051019\
Data File : BN005619.D
Acq On : 11 May 2019 09:30
Operator : JU/SJ
Sample : K2613-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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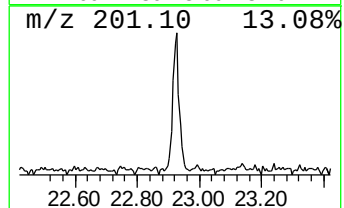
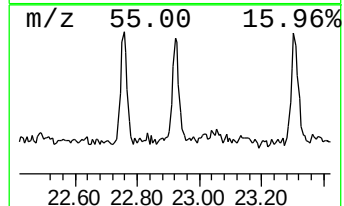
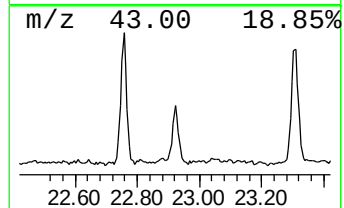
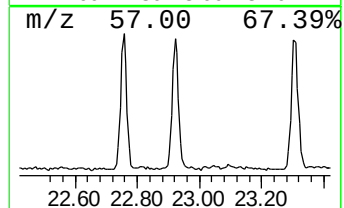
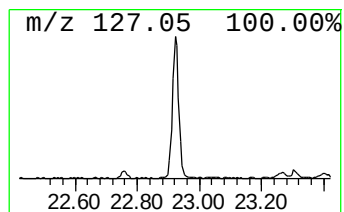
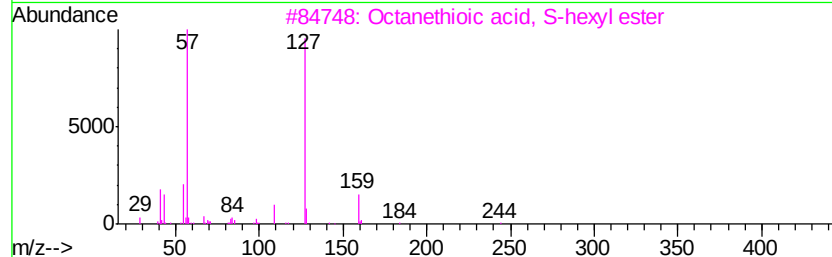
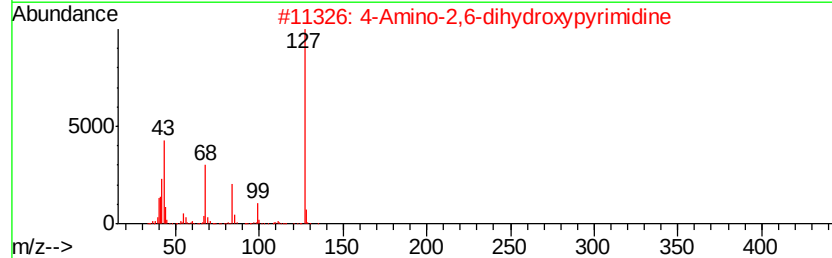
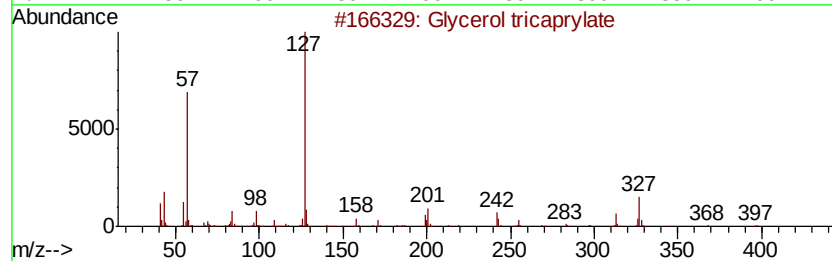
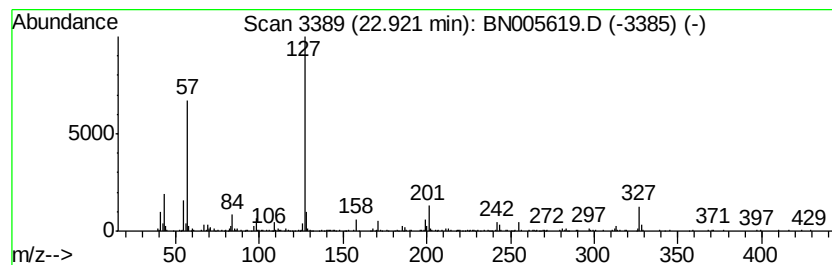
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Glycerol tricaprylate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.92	4.23 ng/ul	471985	Perylene-d12	23.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Glycerol tricaprylate	470	C27H50O6	000538-23-8	90
2		4-Amino-2,6-dihydroxypyrimidine	127	C4H5N3O2	000873-83-6	58
3		Octanethioic acid, S-hexyl ester	244	C14H28OS	055590-85-7	58
4		Ethanediamide, n-dodecyl-N'-(2-t...	339	C17H29N3O2S	296245-21-1	53
5		Piperazine, 1-methyl-4-[2-(p-tol...	282	C14H22N2O2S	016191-68-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN051019\
Data File : BN005619.D
Acq On : 11 May 2019 09:30
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Sample : K2613-11
Misc :
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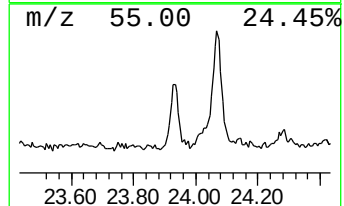
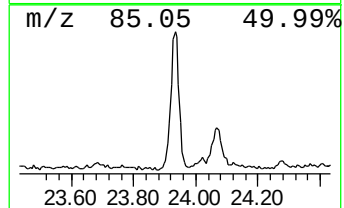
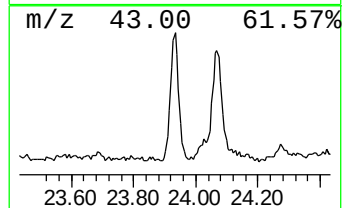
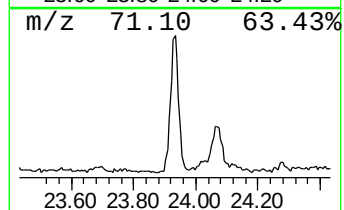
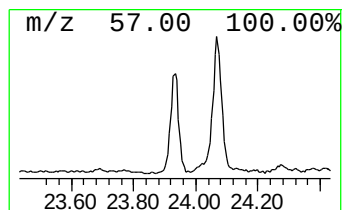
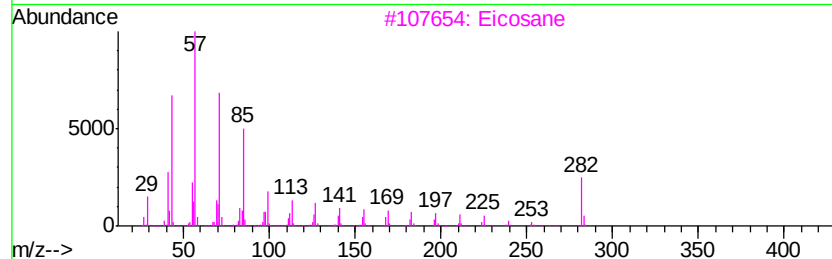
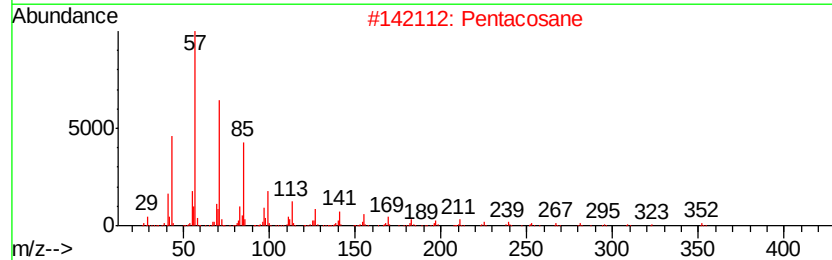
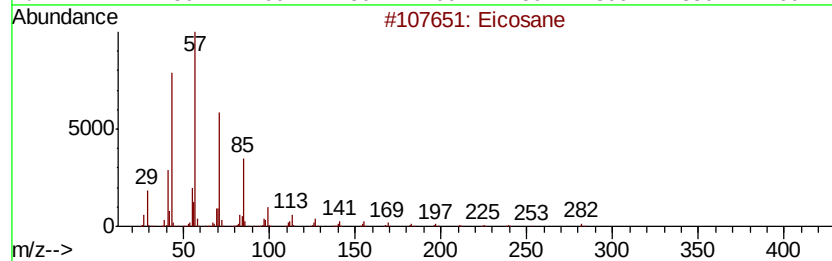
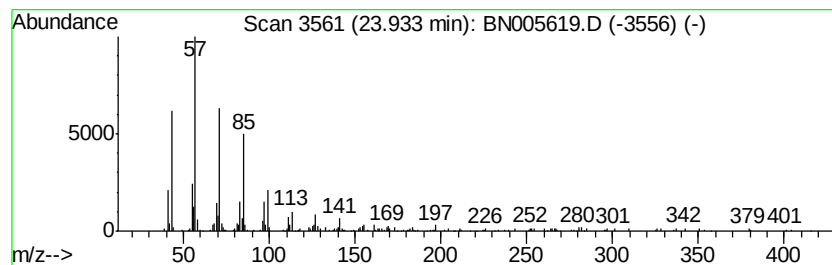
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
23.93	3.55 ng/ul	395350	Perylene-d12	23.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	90
2	Pentacosane			352	C25H52	000629-99-2	87
3	Eicosane			282	C20H42	000112-95-8	87
4	Octacosane			394	C28H58	000630-02-4	83
5	Decane, 3,8-dimethyl-			170	C12H26	017312-55-9	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN051019\
Data File : BN005619.D
Acq On : 11 May 2019 09:30
Operator : JU/SJ
Sample : K2613-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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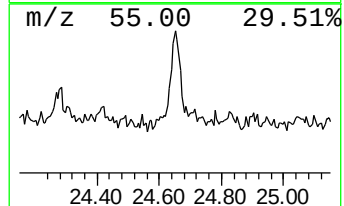
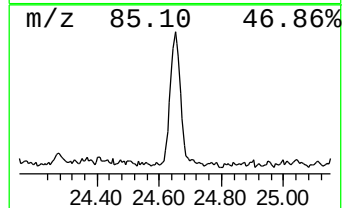
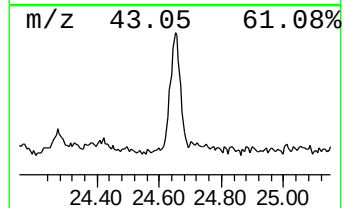
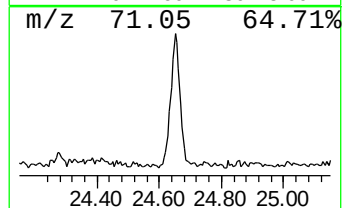
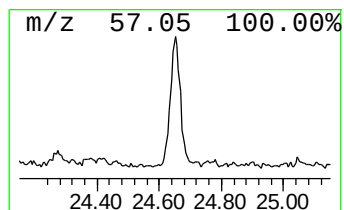
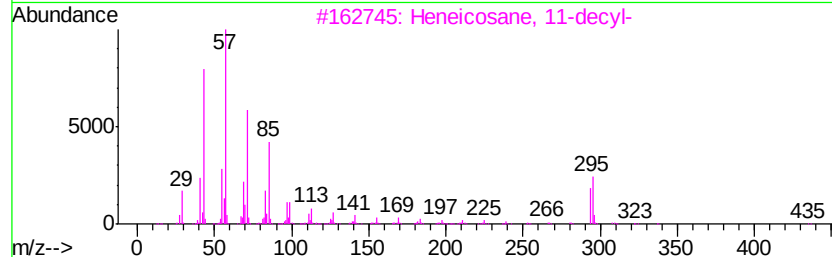
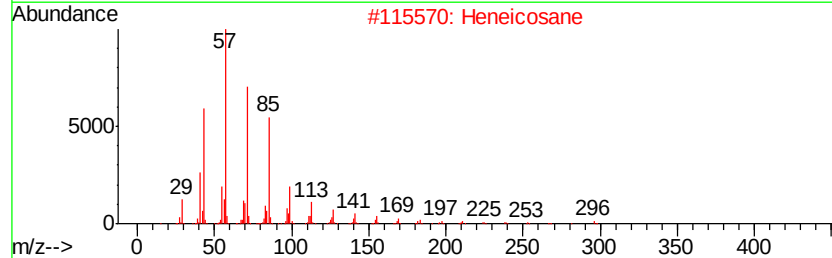
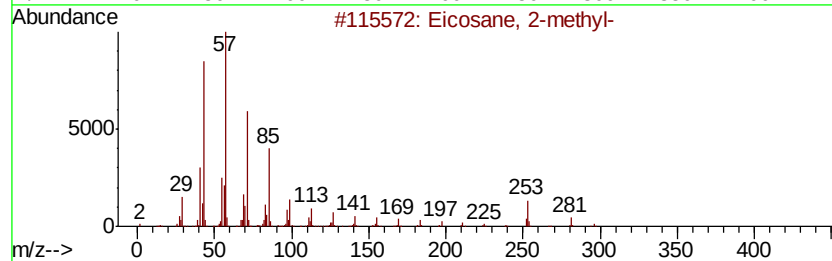
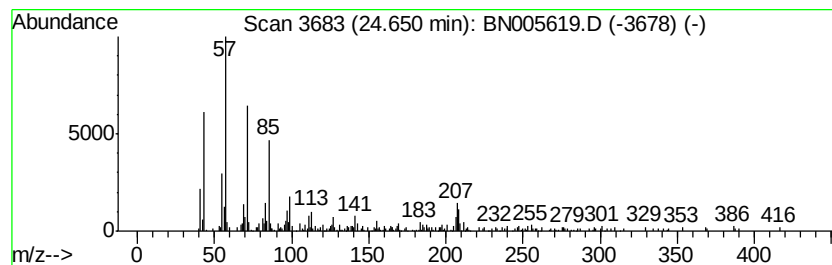
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.65	3.14 ng/ul	349947	Perylene-d12	23.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	93
2		Heneicosane	296	C21H44	000629-94-7	89
3		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	76
4		Octacosane	394	C28H58	000630-02-4	76
5		Pentacosane	352	C25H52	000629-99-2	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN051019\
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Instrument :
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ClientSampleId :
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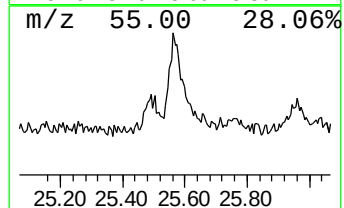
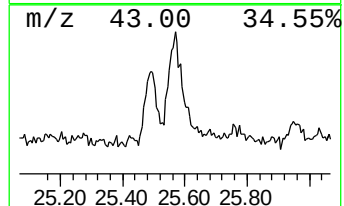
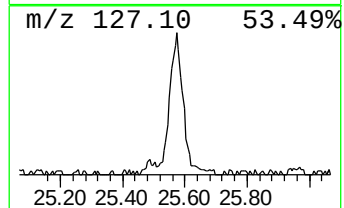
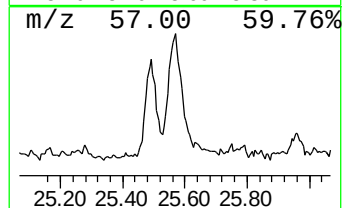
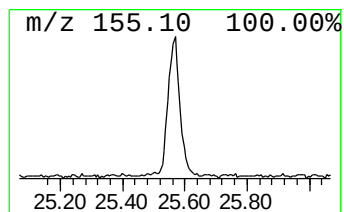
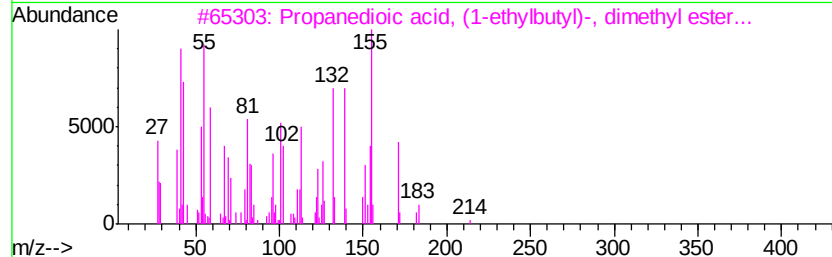
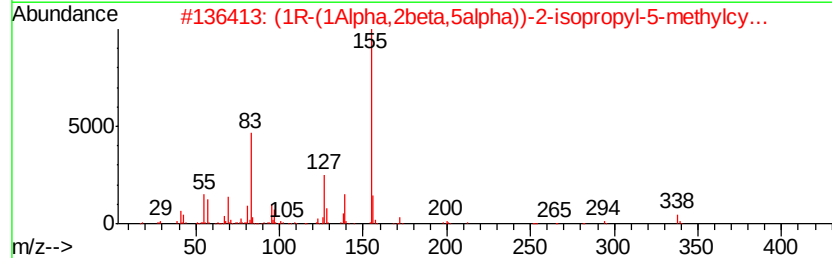
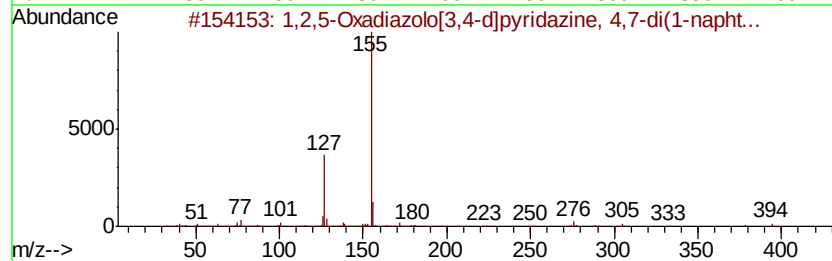
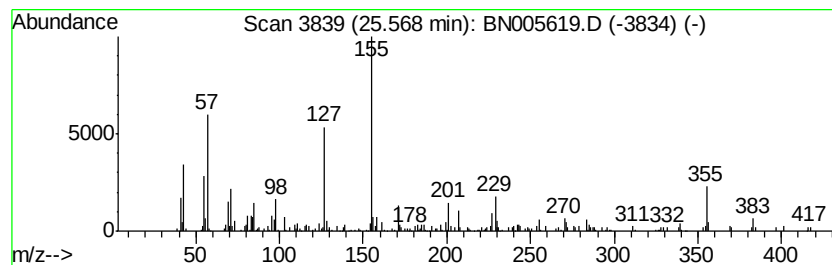
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.57	4.61 ng/ul	513827	Perylene-d12	23.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,5-Oxadiazolo[3,4-d]pyridazin...	390	C24H14N4O2	1000276-89-8	42
2			(1R-(1Alpha,2beta,5alpha))-2-iso...	338	C22H26O3	018434-67-8	37
3			Propanedioic acid, (1-ethylbutyl...	214	C11H18O4	092747-24-5	35
4			2,3,4-Trimethylpentan-2-ol decan...	284	C18H36O2	1000130-74-2	25
5			1-Naphthalenecarboxamide, N-(1-m...	241	C16H19NO	053463-12-0	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA_N\DATA\BN051019\
Data File : BN005619.D
Acq On : 11 May 2019 09:30
Operator : JU/SJ
Sample : K2613-11
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SOM-EPA-BN041919MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic acid	17.90	10.6	ng/ul	1534300	4	16.97	2884690	20.0
Octadecanoic acid	19.19	4.0	ng/ul	523030	5	21.20	2608170	20.0
1-Heneicosyl formate	20.93	5.2	ng/ul	680860	5	21.20	2608170	20.0
(DEL) Alkane: Str...	22.26	5.0	ng/ul	645028	5	21.20	2608170	20.0
Squalene	22.39	17.1	ng/ul	1911260	6	23.40	2230220	20.0
(DEL) Alkane: Str...	22.76	3.3	ng/ul	370516	6	23.40	2230220	20.0
Glycerol tricapry...	22.92	4.2	ng/ul	471985	6	23.40	2230220	20.0
(DEL) Alkane: Str...	23.93	3.5	ng/ul	395350	6	23.40	2230220	20.0
(DEL) Alkane: Str...	24.65	3.1	ng/ul	349947	6	23.40	2230220	20.0
unknown-01	25.57	4.6	ng/ul	513827	6	23.40	2230220	20.0