

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082520\
 Data File : BM027240.D
 Acq On : 26 Aug 2020 08:49
 Operator : JU/CG
 Sample : L3613-16
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DBFR5

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_M\METHODS\SOM-EPA-BM082520MA.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	3.158	26	29	38	rVB	23199	34919	0.66%	0.073%
2	3.563	95	98	102	rVB2	8255	11170	0.21%	0.023%
3	3.658	109	114	121	rVB	39027	55113	1.03%	0.115%
4	3.722	122	125	130	rVB3	6481	9328	0.18%	0.019%
5	3.787	130	136	140	rBV	26825	41216	0.77%	0.086%
6	3.869	147	150	154	rVB	15206	18535	0.35%	0.039%
7	4.763	297	302	308	rBV	21546	31151	0.58%	0.065%
8	6.310	559	565	571	rBV2	14645	23388	0.44%	0.049%
9	6.781	638	645	660	rVB	437487	717020	13.46%	1.491%
10	6.940	664	672	683	rVV	344060	539922	10.14%	1.123%
11	7.034	683	688	695	rVB4	15178	26338	0.49%	0.055%
12	7.134	695	705	714	rBV	469470	731894	13.74%	1.522%
13	7.228	718	721	730	rBV3	12808	25848	0.49%	0.054%
14	7.598	776	784	794	rBV	718780	1154764	21.68%	2.402%
15	8.304	897	904	916	rBV	361928	578056	10.85%	1.202%
16	8.410	918	922	930	rVB2	10861	19846	0.37%	0.041%
17	8.734	968	977	986	rBV	425377	715619	13.43%	1.488%
18	9.457	1093	1100	1109	rBV	368321	612067	11.49%	1.273%
19	9.992	1184	1191	1201	rBV	597901	988487	18.56%	2.056%
20	10.363	1246	1254	1264	rBV	1015727	1699041	31.90%	3.534%
21	10.504	1270	1278	1295	rBV	326130	599751	11.26%	1.247%
22	11.963	1521	1526	1534	rVB3	10022	18035	0.34%	0.038%
23	13.128	1719	1724	1734	rVB5	18050	40291	0.76%	0.084%
24	13.569	1794	1799	1804	rVV6	14608	23670	0.44%	0.049%
25	13.651	1807	1813	1817	rVV	1227132	1623118	30.47%	3.376%
26	13.698	1817	1821	1827	rVV	323392	435203	8.17%	0.905%
27	13.757	1827	1831	1838	rVV3	11136	18116	0.34%	0.038%
28	13.827	1838	1843	1847	rVB3	11481	15026	0.28%	0.031%
29	13.922	1853	1859	1865	rBV	1229580	1798512	33.76%	3.741%
30	13.980	1865	1869	1878	rVB5	32736	68729	1.29%	0.143%
31	14.233	1904	1912	1920	rBV	1705885	2519124	47.29%	5.239%
32	14.310	1920	1925	1926	rVV4	13106	20282	0.38%	0.042%
33	14.369	1929	1935	1939	rVV6	22224	48282	0.91%	0.100%
34	14.439	1941	1947	1956	rVV	450484	701822	13.17%	1.460%

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35	14.498	1956	1957	1964	rVV5	21868	37754	0.71%	0.079%
36	14.569	1964	1969	1978	rVV	65675	126469	2.37%	0.263%
37	14.680	1982	1988	1992	rVV8	7003	16452	0.31%	0.034%
38	14.804	2004	2009	2016	rBV7	8659	15262	0.29%	0.032%
39	15.069	2050	2054	2058	rVB3	6202	8921	0.17%	0.019%
40	15.121	2058	2063	2065	rBV5	5595	8366	0.16%	0.017%
41	15.163	2067	2070	2074	rVB4	15097	20996	0.39%	0.044%
42	15.233	2075	2082	2089	rBV	1654093	2340156	43.93%	4.867%
43	15.298	2089	2093	2096	rVB3	8398	14468	0.27%	0.030%
44	15.351	2096	2102	2110	rBV	466579	670752	12.59%	1.395%
45	15.474	2116	2123	2131	rVB2	20062	40857	0.77%	0.085%
46	15.868	2187	2190	2195	rBV6	11151	17999	0.34%	0.037%
47	15.968	2203	2207	2209	rBV5	7003	9200	0.17%	0.019%
48	16.010	2211	2214	2223	rVB8	15071	31277	0.59%	0.065%
49	16.121	2223	2233	2234	rBV6	5240	12278	0.23%	0.026%
50	16.210	2245	2248	2251	rBV5	7690	8615	0.16%	0.018%
51	16.427	2279	2285	2292	rBV10	10886	26202	0.49%	0.054%
52	16.504	2293	2298	2300	rBV4	7996	11749	0.22%	0.024%
53	16.533	2300	2303	2308	rBV	35330	48230	0.91%	0.100%
54	16.768	2340	2343	2346	rBV3	10693	14015	0.26%	0.029%
55	16.980	2372	2379	2384	rBV	2226325	3082565	57.87%	6.411%
56	17.021	2384	2386	2390	rVV	159930	181266	3.40%	0.377%
57	17.080	2390	2396	2406	rVV	1737043	2516565	47.24%	5.234%
58	17.157	2406	2409	2410	rVV3	11540	13076	0.25%	0.027%
59	17.186	2410	2414	2421	rVB3	69758	105319	1.98%	0.219%
60	17.345	2437	2441	2442	rBV3	7244	8529	0.16%	0.018%
61	17.386	2443	2448	2452	rVB2	23045	41494	0.78%	0.086%
62	17.510	2464	2469	2472	rBV7	8338	12255	0.23%	0.025%
63	17.557	2474	2477	2482	rVV7	7258	12495	0.23%	0.026%
64	17.780	2513	2515	2521	rVB7	14695	18943	0.36%	0.039%
65	17.857	2522	2528	2531	rBV4	18176	29289	0.55%	0.061%
66	17.904	2531	2536	2547	rBV	388600	560010	10.51%	1.165%
67	18.051	2557	2561	2565	rBV2	29785	39911	0.75%	0.083%
68	18.210	2584	2588	2596	rVB2	13569	26075	0.49%	0.054%
69	18.298	2596	2603	2607	rBV2	24898	44817	0.84%	0.093%
70	18.362	2611	2614	2617	rVV2	24784	32775	0.62%	0.068%
71	18.398	2617	2620	2624	rVB2	33771	42263	0.79%	0.088%

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72	18.574	2647	2650	2652	rBV4	8551	10216	0.19%	0.021%
73	18.615	2654	2657	2662	rBV5	17456	33308	0.63%	0.069%
74	18.780	2681	2685	2691	rBV8	29852	47767	0.90%	0.099%
75	18.927	2705	2710	2719	rBV5	28169	65067	1.22%	0.135%
76	19.045	2725	2730	2737	rVB	528308	696563	13.08%	1.449%
77	19.115	2738	2742	2747	rBV	72718	87293	1.64%	0.182%
78	19.192	2751	2755	2760	rBV2	115001	161939	3.04%	0.337%
79	19.256	2762	2766	2770	rVB2	22533	43044	0.81%	0.090%
80	19.380	2782	2787	2791	rBV	2489260	3372803	63.32%	7.015%
81	19.745	2844	2849	2854	rBV5	22150	52447	0.98%	0.109%
82	19.909	2875	2877	2883	rVB3	44807	72657	1.36%	0.151%
83	19.962	2884	2886	2890	rVB2	41585	45341	0.85%	0.094%
84	20.009	2892	2894	2898	rVB2	38342	37582	0.71%	0.078%
85	20.227	2928	2931	2933	rVB	45891	44826	0.84%	0.093%
86	20.286	2939	2941	2945	rVB	43999	44853	0.84%	0.093%
87	20.462	2969	2971	2975	rBV5	30818	32367	0.61%	0.067%
88	20.568	2986	2989	2995	rVB5	64484	97669	1.83%	0.203%
89	20.745	3016	3019	3024	rVB3	44664	62756	1.18%	0.131%
90	20.915	3044	3048	3059	rVB4	561166	851126	15.98%	1.770%
91	21.139	3081	3086	3088	rBV2	267630	366050	6.87%	0.761%
92	21.180	3088	3093	3107	rVB2	3224202	5326943	100.00%	11.079%
93	21.798	3193	3198	3209	rVB2	651897	1032089	19.37%	2.147%
94	22.739	3350	3358	3363	rBV2	842921	1526142	28.65%	3.174%
95	23.221	3435	3440	3446	rBV	1200712	2045145	38.39%	4.254%
96	23.362	3458	3464	3475	rVB2	1394355	2516720	47.25%	5.234%
97	23.592	3499	3503	3512	rVB	280012	448930	8.43%	0.934%
98	23.921	3553	3559	3565	rVB	713010	1283496	24.09%	2.669%
99	23.997	3568	3572	3580	rVB2	261055	506611	9.51%	1.054%
100	26.333	3963	3969	3978	rVB4	372922	957405	17.97%	1.991%

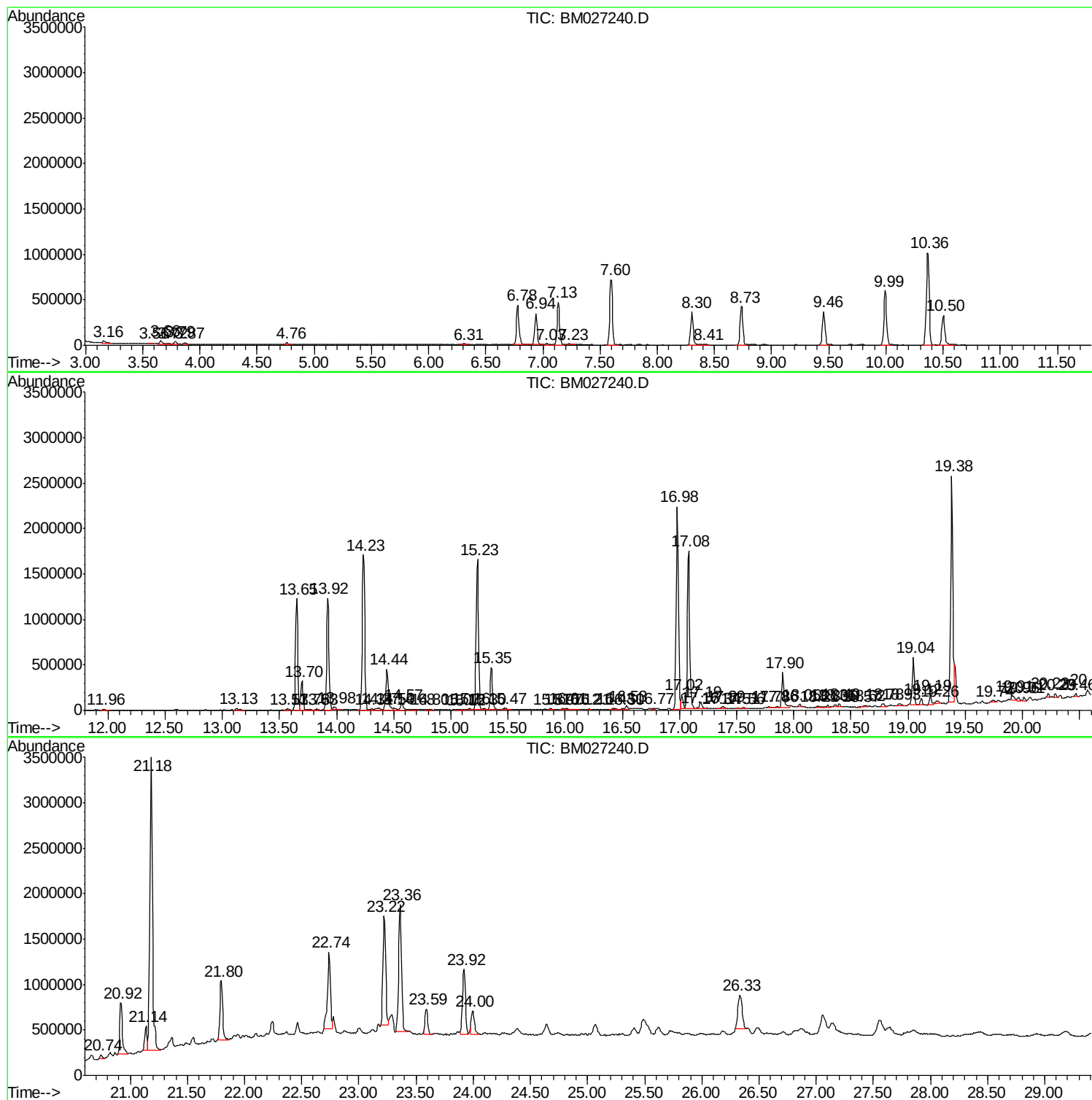
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Quant Title : SVOA CALIBRATION

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



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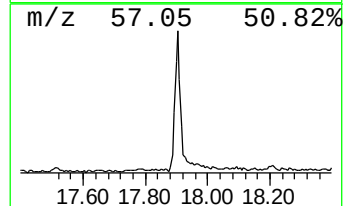
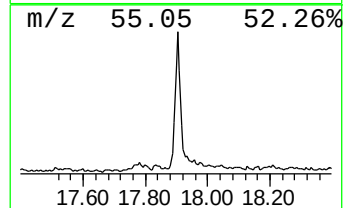
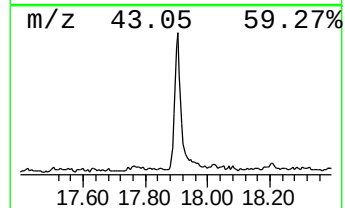
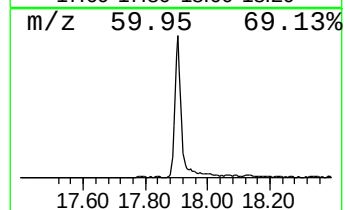
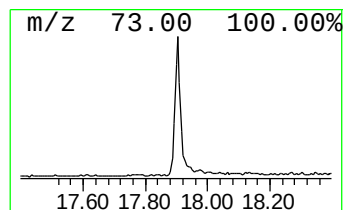
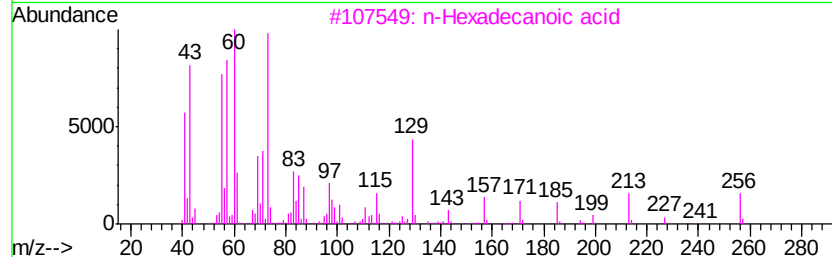
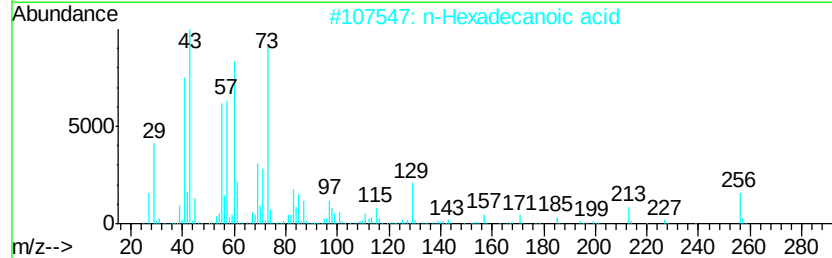
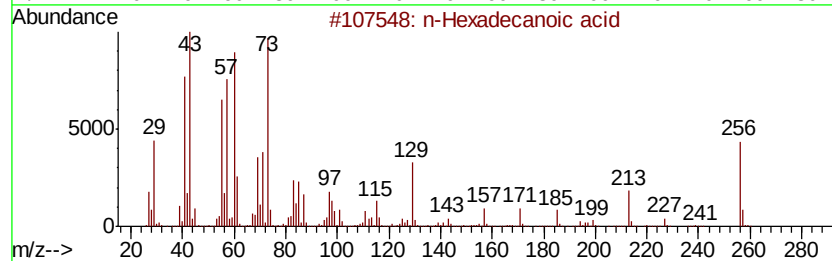
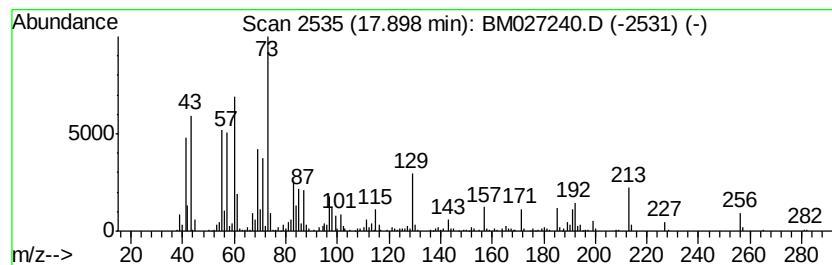
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM082520MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.90	3.63 ng/ul	560010	Phenanthrene-d10		16.98
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53



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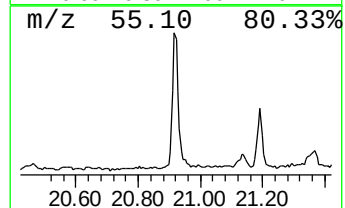
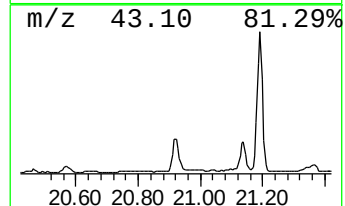
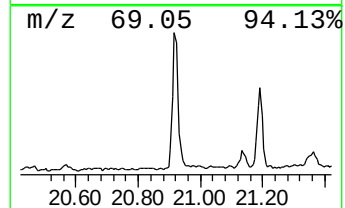
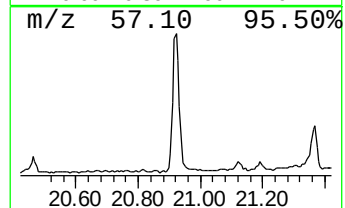
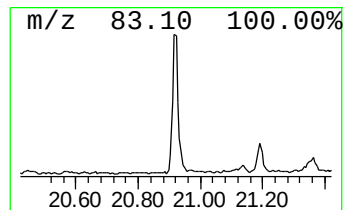
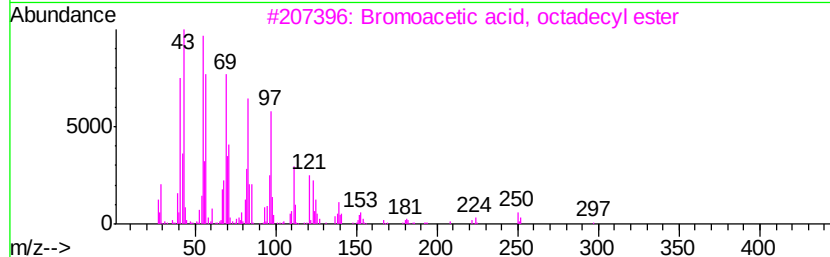
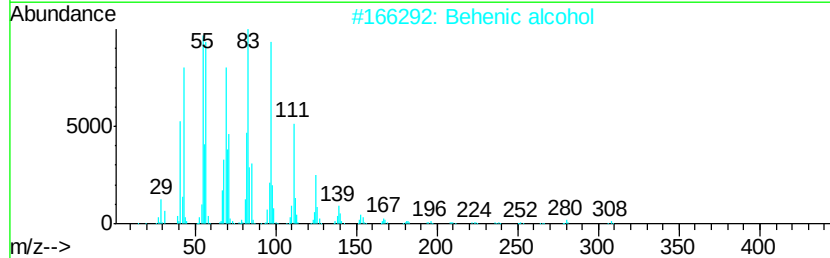
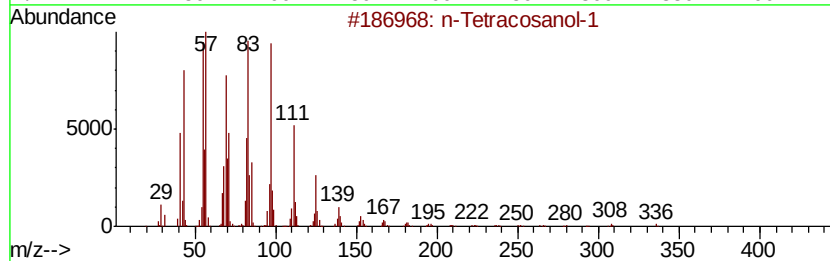
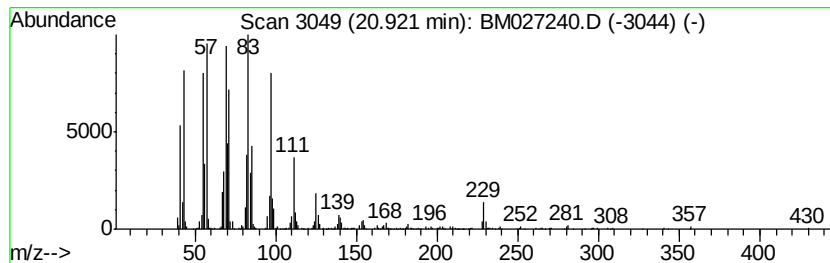
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Tetracosanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.92	3.20 ng/ul	851126	Chrysene-d12	21.18	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



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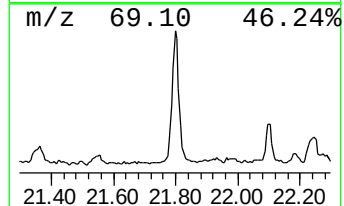
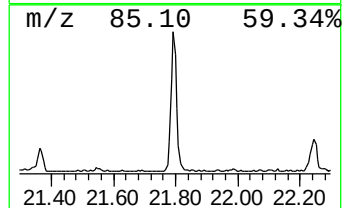
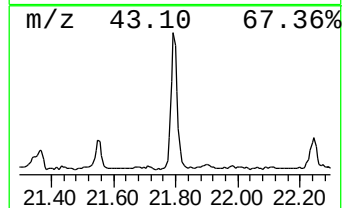
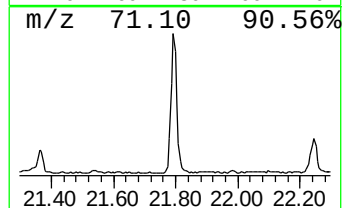
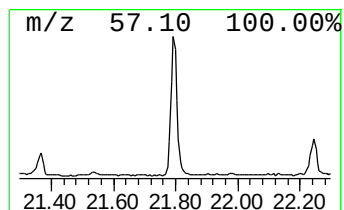
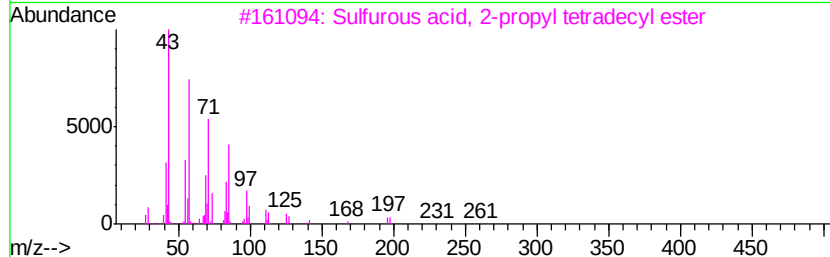
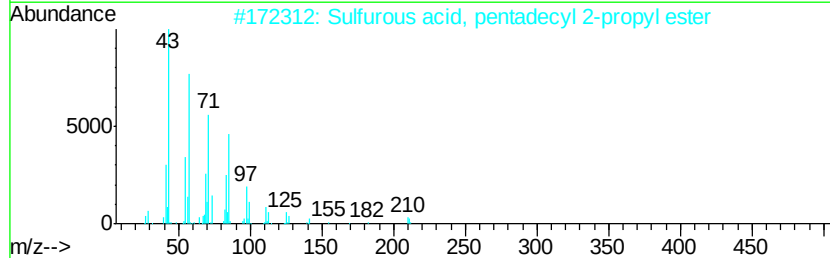
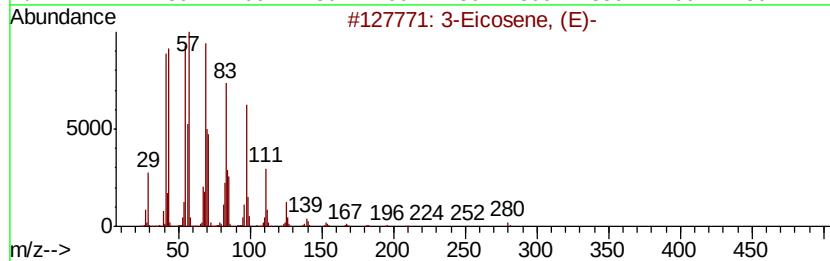
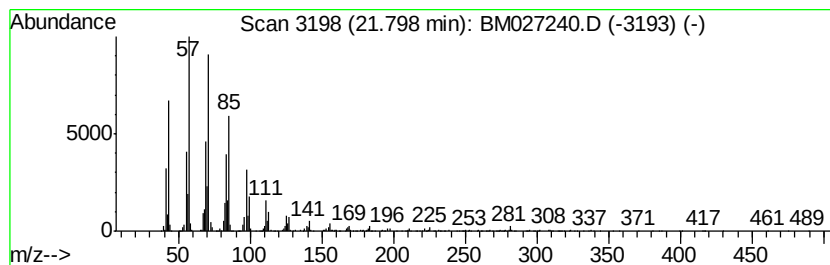
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Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.80	3.87 ng/ul	1032090	Chrysene-d12	21.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91
3		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	91
4		Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	86
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	74



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Data File : BM027240.D
Acq On : 26 Aug 2020 08:49
Operator : JU/CG
Sample : L3613-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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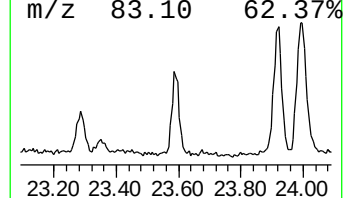
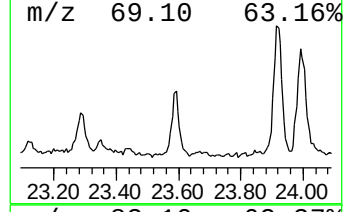
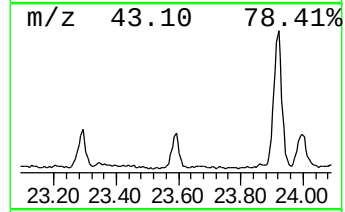
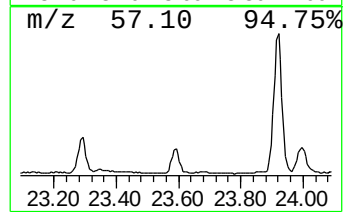
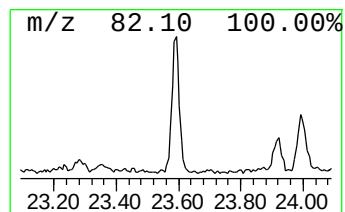
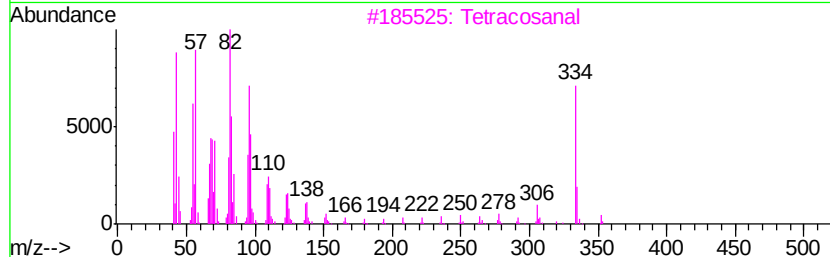
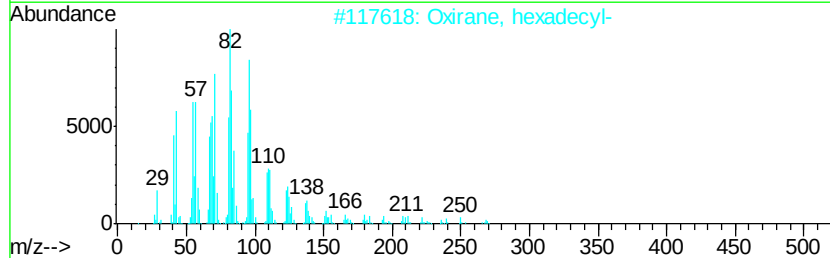
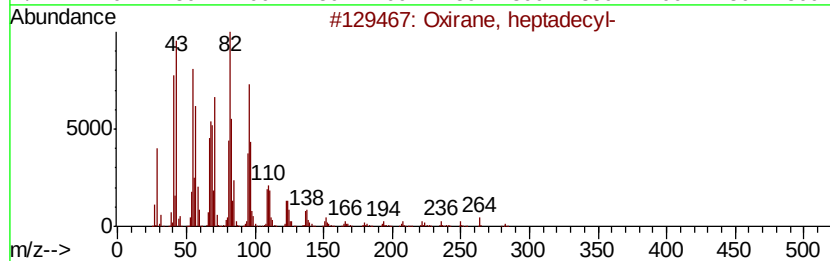
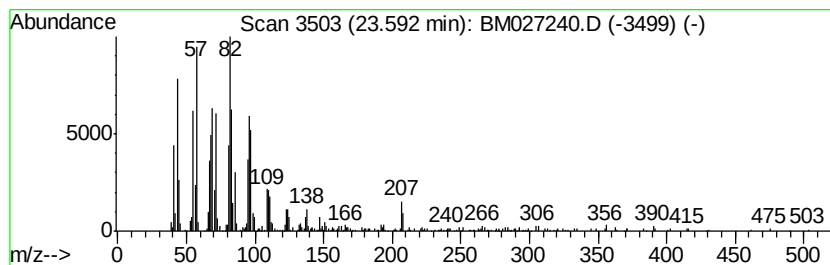
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Oxirane, heptadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.59	3.57 ng/ul	448930	Perylene-d12	23.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95	
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91	
3	Tetracosanal	352	C24H48O	057866-08-7	91	
4	Octadecanal	268	C18H36O	000638-66-4	90	
5	Octadecanal	268	C18H36O	000638-66-4	90	



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082520\
Data File : BM027240.D
Acq On : 26 Aug 2020 08:49
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Sample : L3613-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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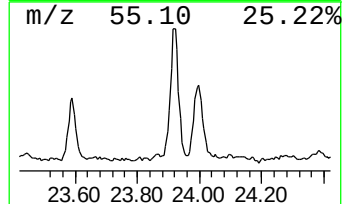
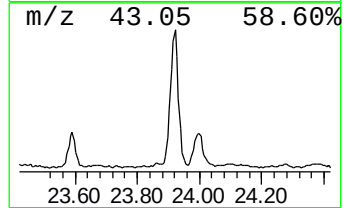
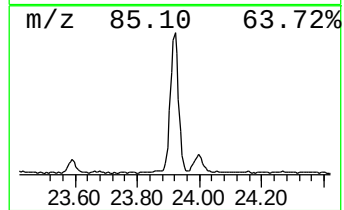
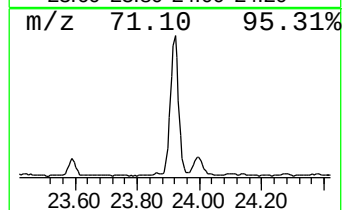
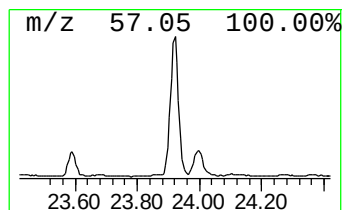
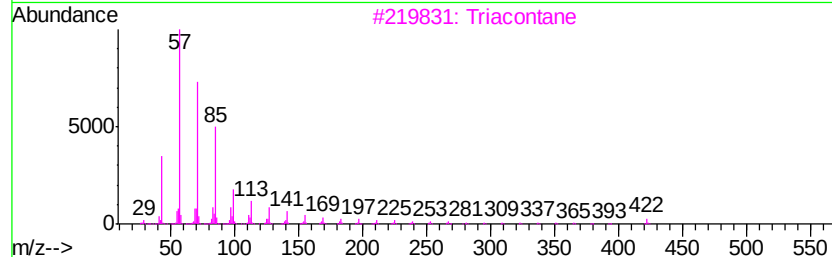
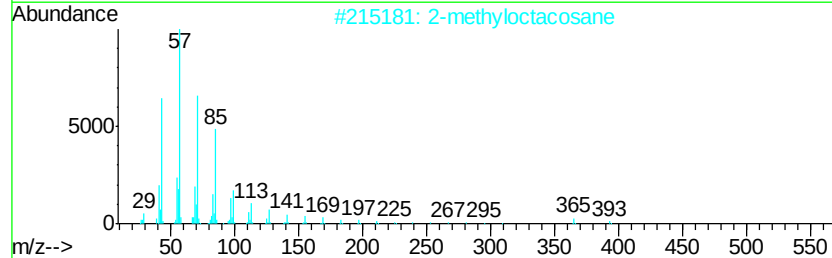
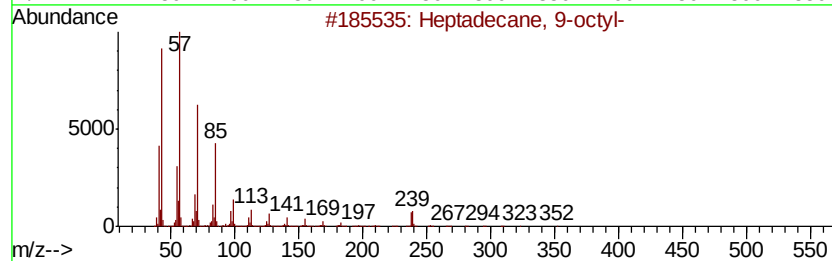
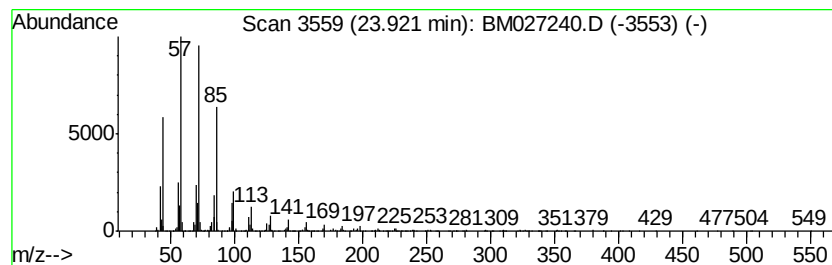
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	10.20 ng/ul	1283500	Perylene-d12	23.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		triacontane	422	C30H62	000638-68-6	91
4		Heneicosane	296	C21H44	000629-94-7	90
5		Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082520\
Data File : BM027240.D
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Operator : JU/CG
Sample : L3613-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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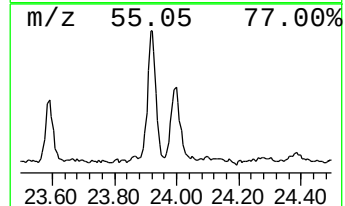
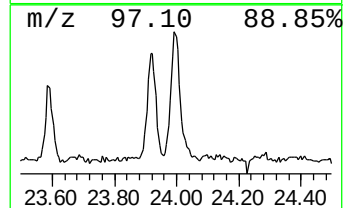
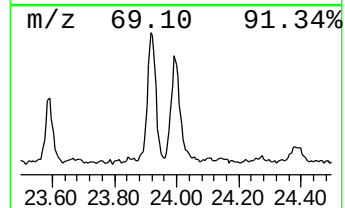
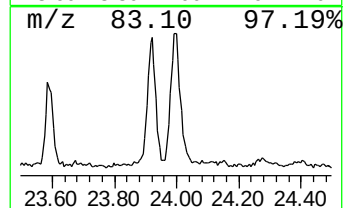
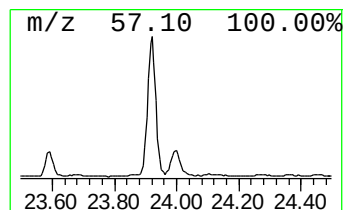
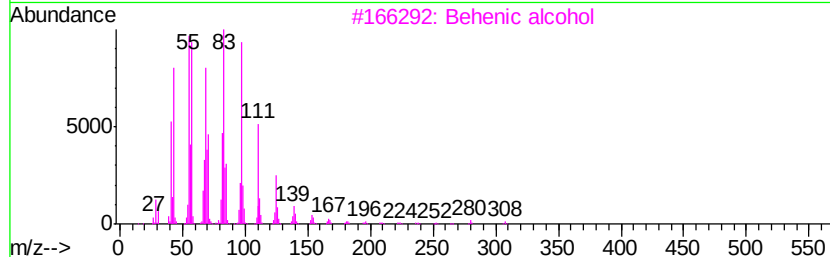
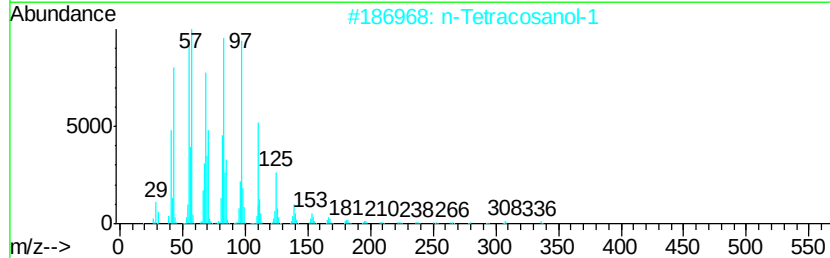
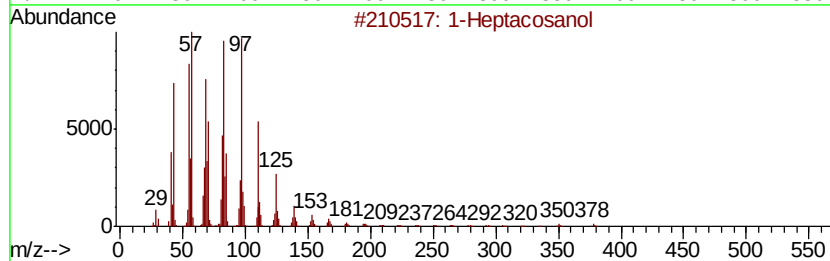
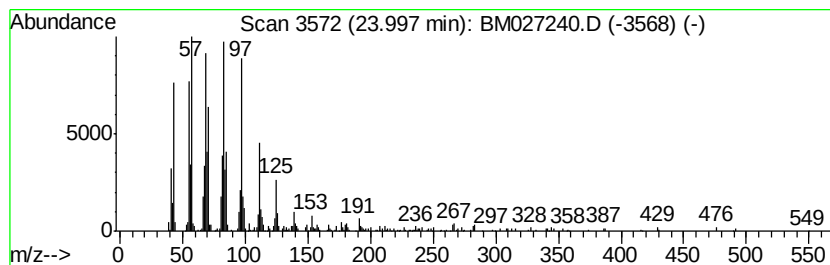
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.00	4.03 ng/ul	506611	Perylene-d12	23.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol		396	C27H56O	002004-39-9	95
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	94
3	Behenic alcohol		326	C22H46O	000661-19-8	94
4	Nonadecyl trifluoroacetate		380	C21H39F3O2	1000351-76-3	93
5	1-Heneicosyl formate		340	C22H44O2	077899-03-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082520\
Data File : BM027240.D
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Operator : JU/CG
Sample : L3613-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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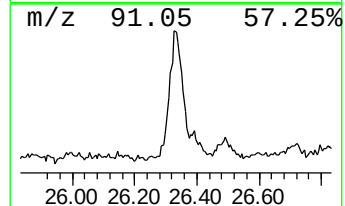
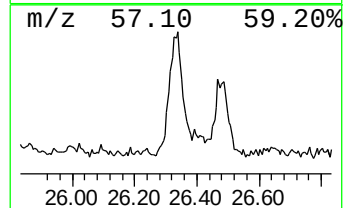
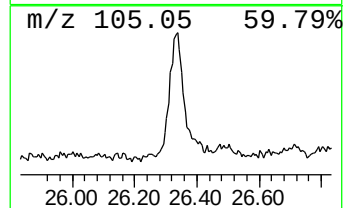
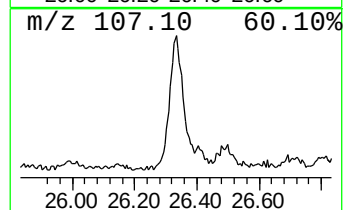
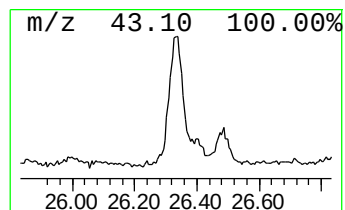
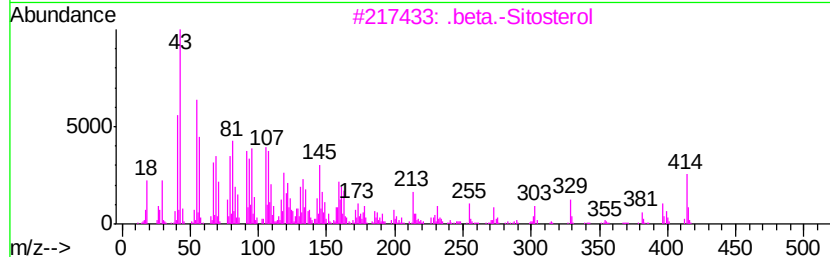
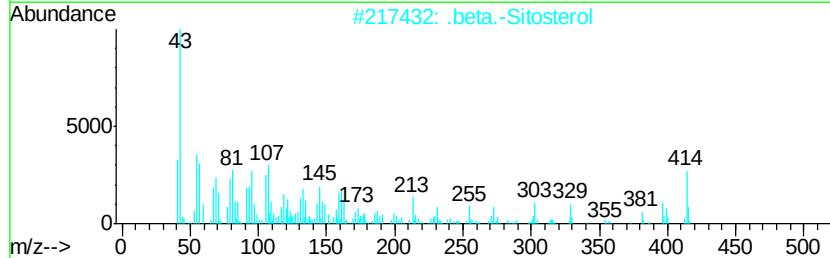
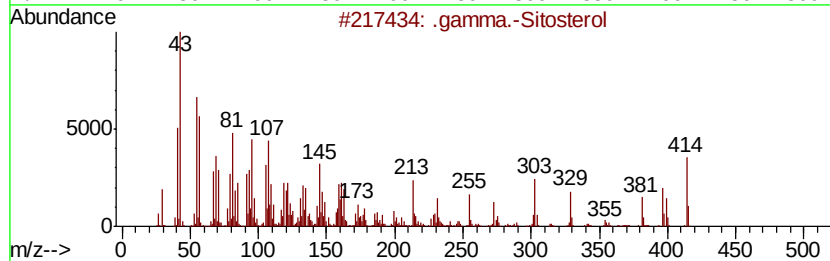
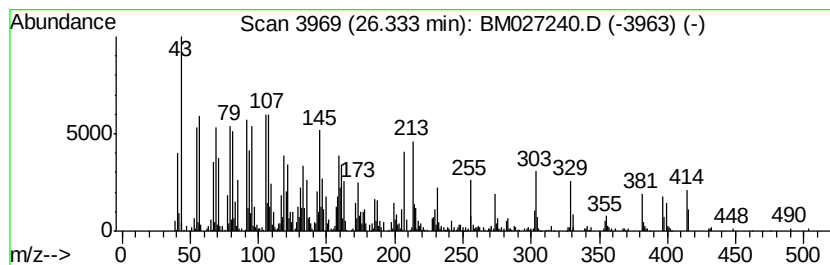
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.33	7.61 ng/ul	957405	Perylene-d12	23.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3		.beta.-Sitosterol	414	C29H50O	000083-46-5	95
4		.gamma.-Sitosterol	414	C29H50O	000083-47-6	41
5		Cyclopentanecarboxylic acid, 1-p...	273	C14H15N3OS	1000311-03-5	11



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM082520\
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Sample : L3613-16
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM082520MA.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
n-Hexadecanoic acid	17.90	3.6	ng/ul	560010	4	16.98	3082570	20.0
n-Tetracosanol-1	20.92	3.2	ng/ul	851126	5	21.18	5326940	20.0
(DEL) Alkane: Str...	21.80	3.9	ng/ul	1032090	5	21.18	5326940	20.0
Oxirane, heptadecyl-	23.59	3.6	ng/ul	448930	6	23.36	2516720	20.0
(DEL) Alkane: Str...	23.92	10.2	ng/ul	1283500	6	23.36	2516720	20.0
1-Heptacosanol	24.00	4.0	ng/ul	506611	6	23.36	2516720	20.0
.gamma.-Sitosterol	26.33	7.6	ng/ul	957405	6	23.36	2516720	20.0