

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020620\
 Data File : BM024773.D
 Acq On : 07 Feb 2020 22:17
 Operator : CG/JU
 Sample : L1399-18
 Misc :
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CB6T3

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-BM020620MA.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	3.016	19	22	27	rVB	55068	63387	1.07%	0.074%
2	3.628	121	126	132	rBV2	19447	31779	0.54%	0.037%
3	3.710	136	140	145	rVB2	15281	21041	0.35%	0.025%
4	3.928	174	177	184	rVB2	13841	20965	0.35%	0.025%
5	4.063	194	200	206	rVB10	10557	21418	0.36%	0.025%
6	4.328	242	245	252	rVB3	9841	14655	0.25%	0.017%
7	4.593	286	290	297	rBV	26136	41928	0.71%	0.049%
8	5.440	428	434	439	rBV6	11383	18626	0.31%	0.022%
9	5.516	444	447	454	rVB6	9725	14848	0.25%	0.017%
10	6.604	620	632	642	rBV	768409	1234994	20.81%	1.449%
11	6.757	652	658	667	rBV	716874	1088209	18.34%	1.277%
12	6.946	683	690	701	rBV	924252	1407449	23.72%	1.651%
13	7.122	716	720	726	rVB6	9758	14566	0.25%	0.017%
14	7.404	761	768	776	rBV	1089523	1636472	27.58%	1.920%
15	7.493	780	783	788	rVB4	12870	18182	0.31%	0.021%
16	8.122	882	890	902	rBV	1047552	1671656	28.17%	1.961%
17	8.228	902	908	912	rVB6	11685	23483	0.40%	0.028%
18	8.545	951	962	976	rBV	839680	1398517	23.57%	1.641%
19	8.669	976	983	986	rVV5	8761	17617	0.30%	0.021%
20	8.734	988	994	999	rVB2	44728	68203	1.15%	0.080%
21	9.040	1041	1046	1054	rVB2	37165	55419	0.93%	0.065%
22	9.257	1076	1083	1094	rBV	723734	1213098	20.44%	1.423%
23	9.798	1168	1175	1188	rVV	1118373	1885138	31.77%	2.212%
24	10.163	1230	1237	1244	rBV	1459075	2327561	39.23%	2.731%
25	10.304	1254	1261	1281	rBV	996745	1763831	29.73%	2.069%
26	11.528	1465	1469	1475	rBV5	6531	12152	0.20%	0.014%
27	11.639	1485	1488	1493	rVB2	17679	26141	0.44%	0.031%
28	11.763	1503	1509	1517	rBV2	23909	43757	0.74%	0.051%
29	12.622	1650	1655	1659	rVB5	8772	15039	0.25%	0.018%
30	12.916	1701	1705	1710	rBV	28342	40422	0.68%	0.047%
31	12.957	1710	1712	1717	rVB3	12132	11790	0.20%	0.014%
32	13.375	1779	1783	1788	rBV6	7327	13152	0.22%	0.015%
33	13.480	1795	1801	1807	rVV	2257253	3215594	54.19%	3.773%
34	13.533	1807	1810	1814	rVB	63925	82670	1.39%	0.097%

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35	13.745	1839	1846	1858	rBV	2479075	3534946	59.57%	4.147%
36	14.010	1887	1891	1893	rBV	25193	29208	0.49%	0.034%
37	14.057	1893	1899	1908	rVB	2320132	3388849	57.11%	3.976%
38	14.280	1931	1937	1957	rBV	677180	1206321	20.33%	1.415%
39	14.504	1974	1975	1981	rVB6	11052	12847	0.22%	0.015%
40	14.698	2004	2008	2012	rBV6	8960	11398	0.19%	0.013%
41	14.774	2018	2021	2027	rVB7	9692	12066	0.20%	0.014%
42	14.910	2040	2044	2049	rVB4	10207	12255	0.21%	0.014%
43	14.969	2049	2054	2059	rVB6	16371	22165	0.37%	0.026%
44	15.063	2061	2070	2076	rBV	3352280	4635359	78.12%	5.438%
45	15.110	2076	2078	2087	rVV7	21471	35159	0.59%	0.041%
46	15.192	2087	2092	2105	rVV	998524	1336645	22.53%	1.568%
47	15.304	2107	2111	2116	rVB2	41197	50250	0.85%	0.059%
48	15.533	2146	2150	2154	rBV5	7494	14453	0.24%	0.017%
49	15.674	2171	2174	2179	rVB3	33813	45208	0.76%	0.053%
50	15.721	2179	2182	2185	rBV3	9392	11963	0.20%	0.014%
51	15.804	2190	2196	2199	rBV8	11048	20925	0.35%	0.025%
52	15.839	2199	2202	2203	rBV2	16447	17718	0.30%	0.021%
53	15.951	2212	2221	2224	rVB9	5475	13031	0.22%	0.015%
54	15.992	2224	2228	2233	rBV6	13069	24859	0.42%	0.029%
55	16.192	2256	2262	2265	rBV4	12249	20988	0.35%	0.025%
56	16.380	2290	2294	2296	rBV3	12267	16088	0.27%	0.019%
57	16.504	2311	2315	2319	rVB6	15711	24616	0.41%	0.029%
58	16.627	2333	2336	2343	rVB3	34776	47948	0.81%	0.056%
59	16.815	2360	2368	2372	rBV	2927728	4090195	68.93%	4.799%
60	16.857	2372	2375	2379	rVV	174581	234770	3.96%	0.275%
61	16.910	2379	2384	2390	rVV	3297596	4689891	79.04%	5.502%
62	16.951	2390	2391	2399	rVB2	106629	115224	1.94%	0.135%
63	17.086	2412	2414	2419	rBV5	15975	23532	0.40%	0.028%
64	17.139	2419	2423	2428	rVB	26444	34740	0.59%	0.041%
65	17.233	2434	2439	2451	rBV9	53817	107488	1.81%	0.126%
66	17.392	2464	2466	2474	rVB8	14562	25006	0.42%	0.029%
67	17.686	2512	2516	2521	rBV3	46329	79501	1.34%	0.093%
68	17.739	2521	2525	2534	rVB2	55996	101628	1.71%	0.119%
69	17.815	2535	2538	2543	rBV4	29640	37973	0.64%	0.045%
70	17.880	2544	2549	2554	rVV3	56260	100208	1.69%	0.118%
71	17.921	2554	2556	2560	rVB	29116	35518	0.60%	0.042%

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72	18.198	2598	2603	2608	rBV2	64345	94682	1.60%	0.111%
73	18.280	2614	2617	2622	rVB2	29304	34658	0.58%	0.041%
74	18.468	2644	2649	2653	rVV	73047	104562	1.76%	0.123%
75	18.498	2653	2654	2658	rVB4	21008	19751	0.33%	0.023%
76	18.627	2671	2676	2681	rBV	59032	93908	1.58%	0.110%
77	18.680	2681	2685	2686	rBV4	24499	36034	0.61%	0.042%
78	18.762	2696	2699	2700	rBV2	27811	26791	0.45%	0.031%
79	18.851	2711	2714	2715	rBV	61241	59887	1.01%	0.070%
80	18.880	2715	2719	2726	rVB	448183	639608	10.78%	0.750%
81	19.221	2771	2777	2786	rBV	3970243	5933790	100.00%	6.962%
82	19.715	2859	2861	2862	rBV2	37560	33320	0.56%	0.039%
83	19.827	2878	2880	2883	rBV4	40242	39395	0.66%	0.046%
84	20.780	3039	3042	3053	rBV2	1111817	1697291	28.60%	1.991%
85	21.027	3078	3084	3088	rBV	3765485	4827175	81.35%	5.663%
86	21.062	3088	3090	3099	rVB	291819	344141	5.80%	0.404%
87	21.233	3116	3119	3122	rBV	173358	183234	3.09%	0.215%
88	21.656	3187	3191	3196	rBV2	515038	777303	13.10%	0.912%
89	22.086	3261	3264	3271	rBV	310025	406789	6.86%	0.477%
90	22.297	3296	3300	3308	rVB	1983627	2471535	41.65%	2.900%
91	22.515	3334	3337	3341	rBV	208212	335136	5.65%	0.393%
92	22.562	3341	3345	3347	rVV2	860562	1171190	19.74%	1.374%
93	22.597	3347	3351	3361	rVB	3701815	5373764	90.56%	6.305%
94	23.003	3414	3420	3426	rBV	2806308	4578672	77.16%	5.372%
95	23.086	3431	3434	3437	rVV	387497	599369	10.10%	0.703%
96	23.133	3437	3442	3449	rVB	2537325	4425697	74.58%	5.192%
97	23.374	3478	3483	3490	rVB	722970	1204182	20.29%	1.413%
98	23.686	3531	3536	3542	rVB	1290148	2196823	37.02%	2.577%
99	23.756	3543	3548	3559	rVB	941176	1885223	31.77%	2.212%
100	25.168	3782	3788	3799	rVB3	751283	1887431	31.81%	2.214%

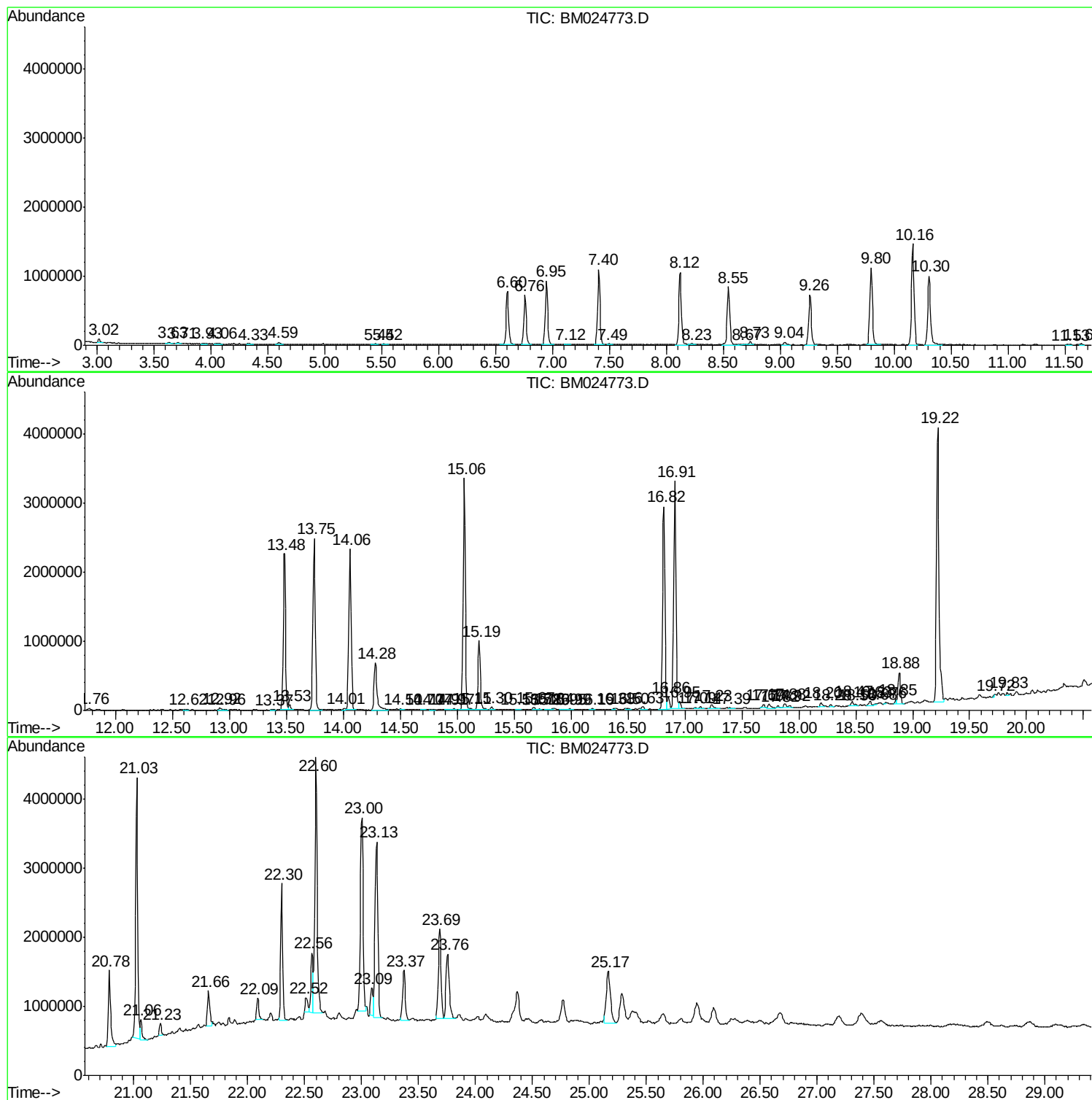
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Quant Title : SVOA CALIBRATION

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



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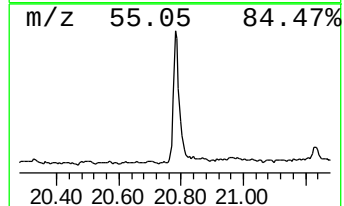
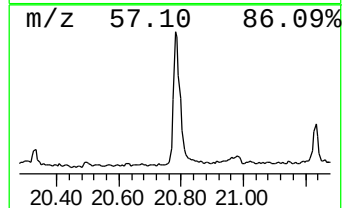
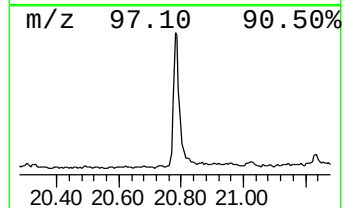
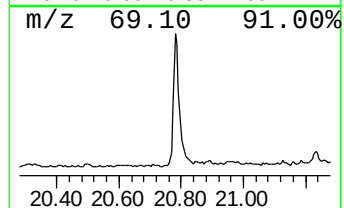
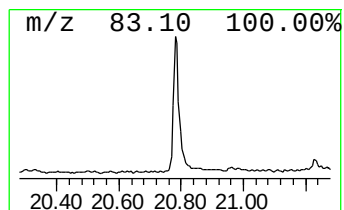
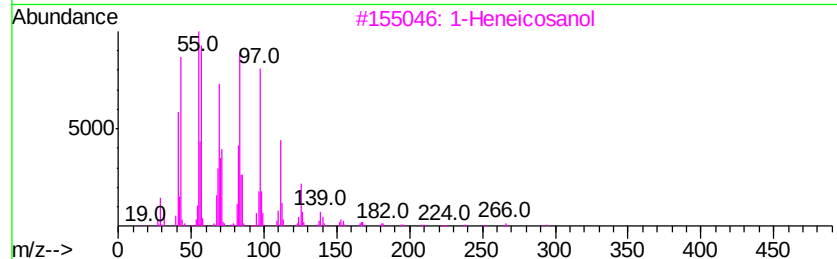
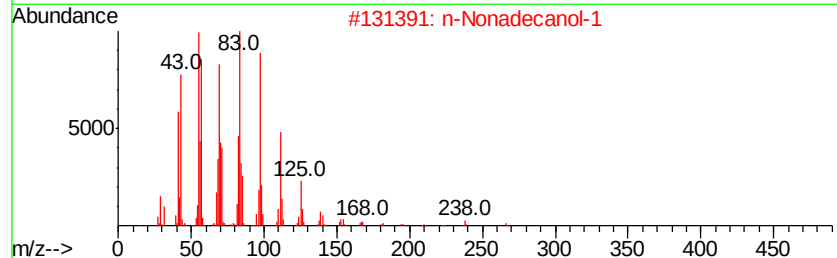
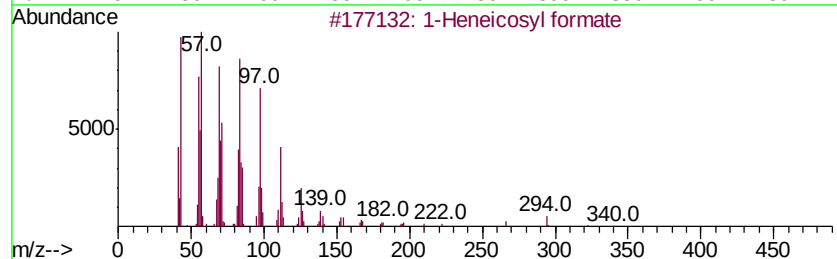
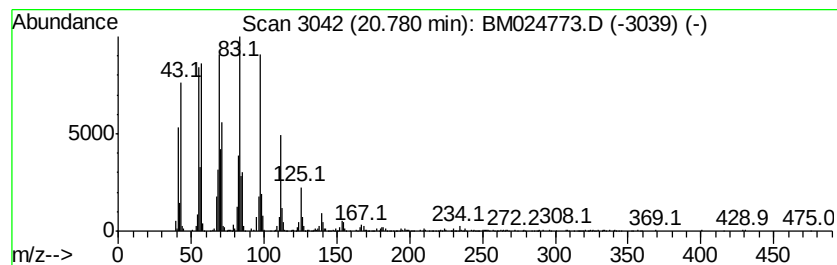
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM020620MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	7.03 ng/ul	1697290	Chrysene-d12	21.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosyl formate	340 C22H44O2	077899-03-7 97
2		n-Nonadecanol-1	284 C19H40O	001454-84-8 94
3		1-Heneicosanol	312 C21H44O	015594-90-8 94
4		1-Heptacosanol	396 C27H56O	002004-39-9 93
5		3-Eicosene, (E)-	280 C20H40	074685-33-9 91



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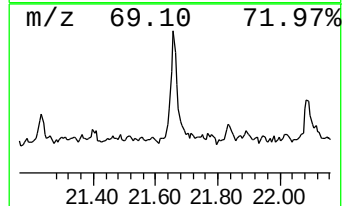
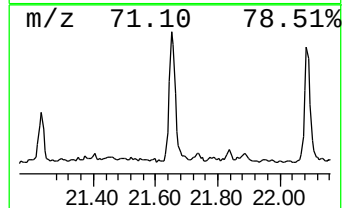
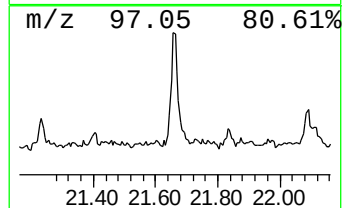
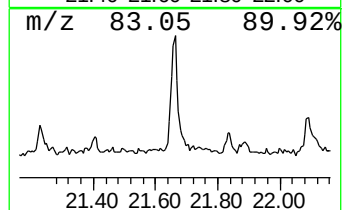
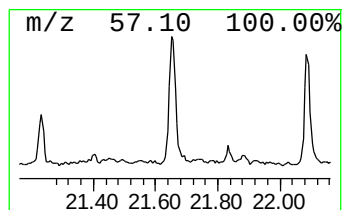
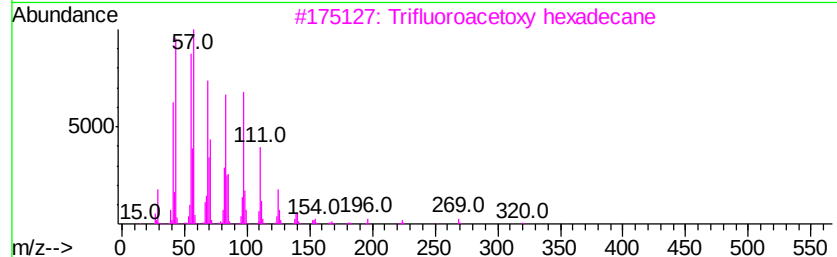
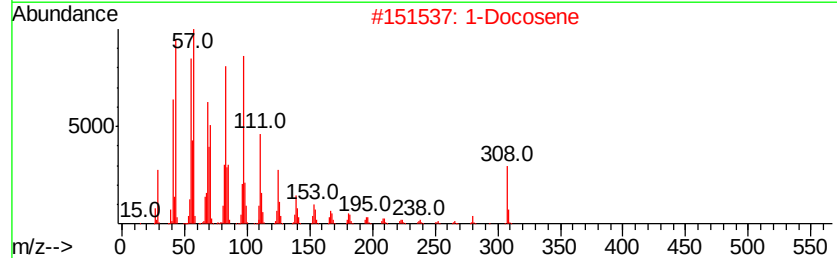
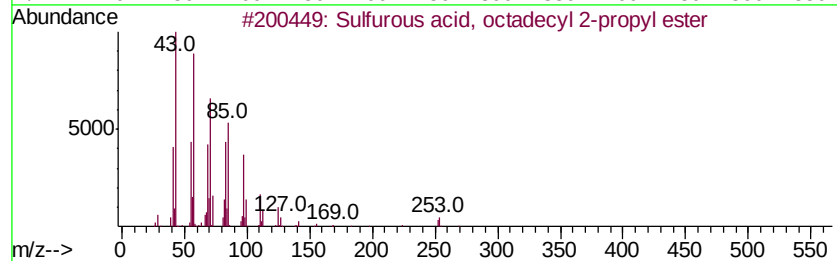
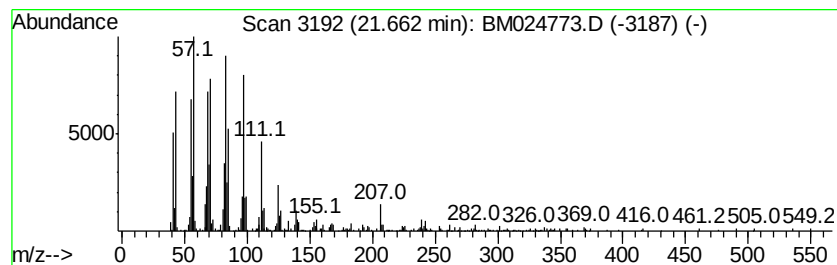
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Sulfurous acid, octadecyl 2... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.66	3.22 ng/ul	777303	Chrysene-d12	21.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	90
2		1-Docosene	308	C22H44	001599-67-3	87
3		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
4		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
5		Hexadecane	226	C16H34	000544-76-3	86



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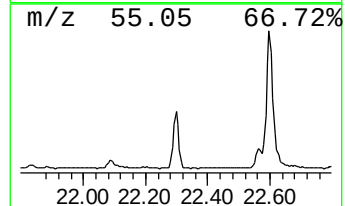
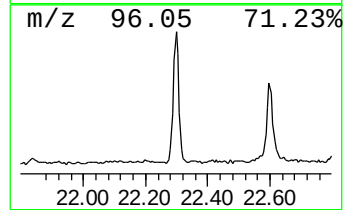
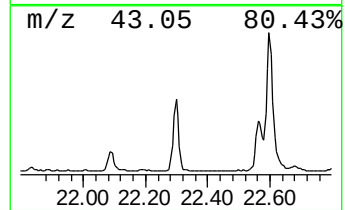
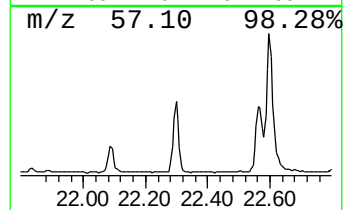
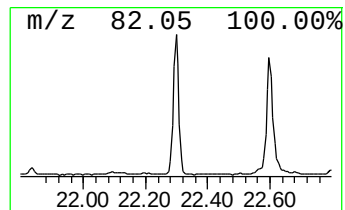
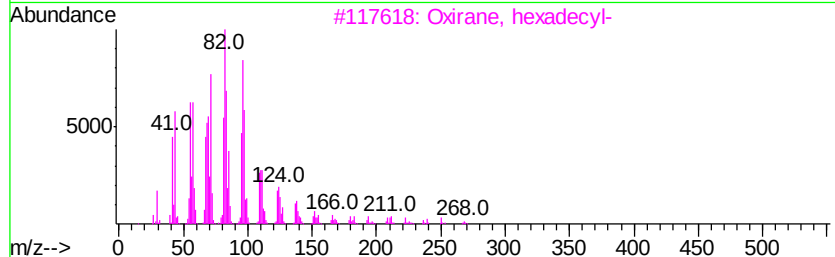
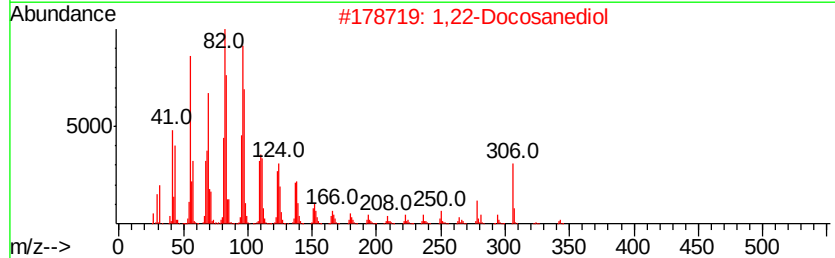
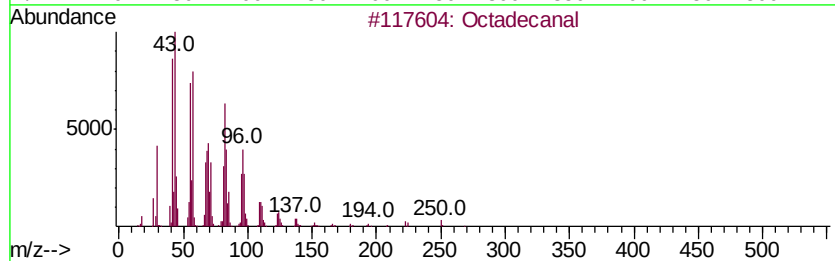
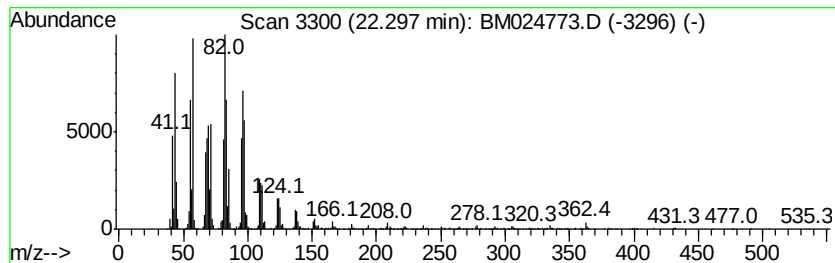
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Peak Number 3 Octadecanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.30	11.17 ng/ul	2471540	Perylene-d12	23.13
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecanal	268 C18H36O	000638-66-4	96
2	1,22-Docosanediol	342 C22H46O2	022513-81-1	95
3	Oxirane, hexadecyl-	268 C18H36O	007390-81-0	94
4	Hexadecanal	240 C16H32O	000629-80-1	91
5	Octadecanal	268 C18H36O	000638-66-4	91



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Data File : BM024773.D
Acq On : 07 Feb 2020 22:17
Operator : CG/JU
Sample : L1399-18
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB6T3

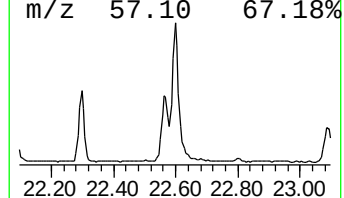
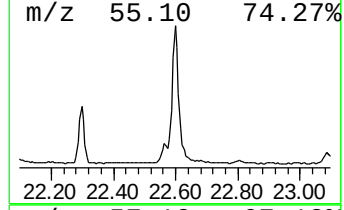
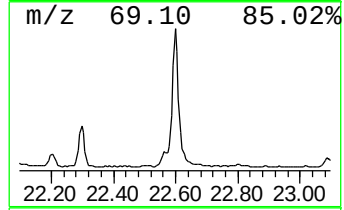
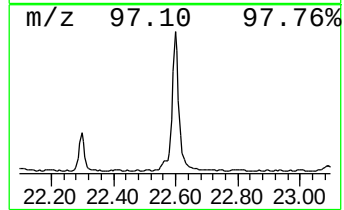
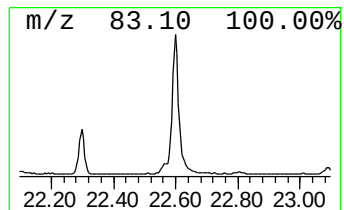
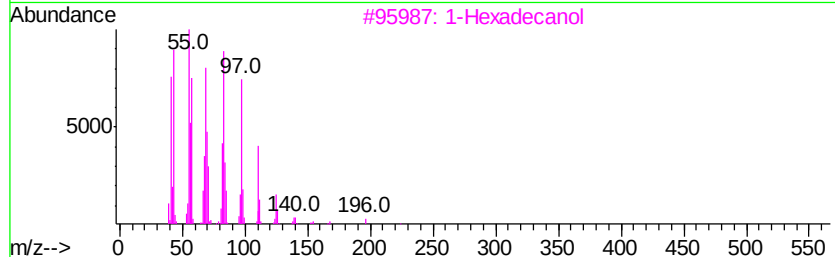
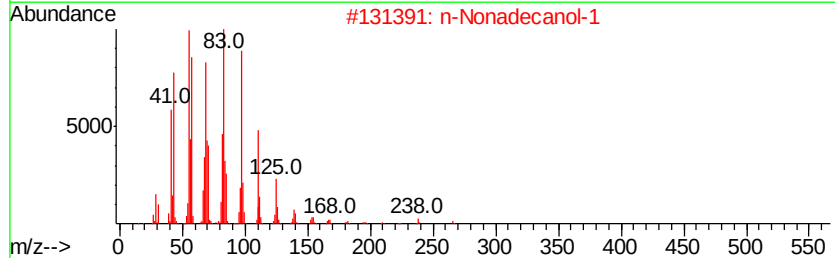
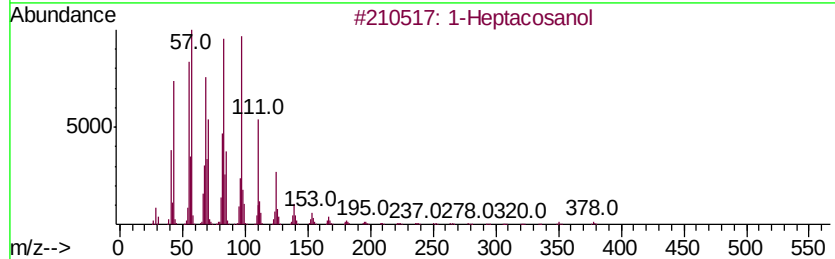
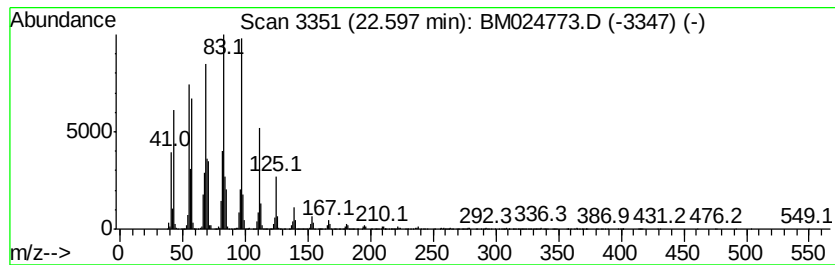
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 1-Heptacosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.60	24.28 ng/ul	5373760	Perylene-d12	23.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3		1-Hexadecanol	242	C16H34O	036653-82-4	91
4		1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	90
5		2-Butenedioic acid (Z)-, monodod...	284	C16H28O4	002424-61-5	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020620\
Data File : BM024773.D
Acq On : 07 Feb 2020 22:17
Operator : CG/JU
Sample : L1399-18
Misc :
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Instrument :
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ClientSampleId :
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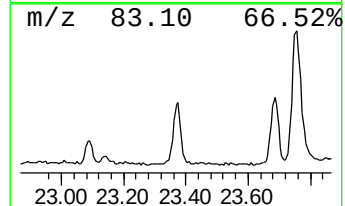
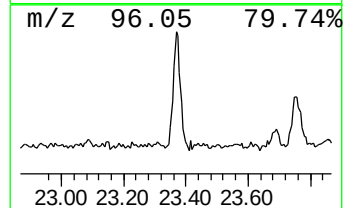
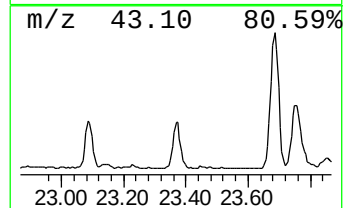
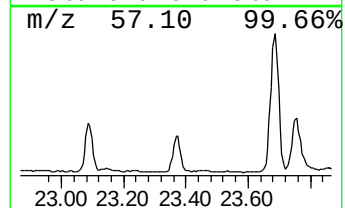
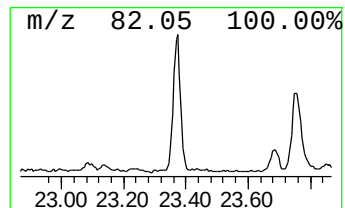
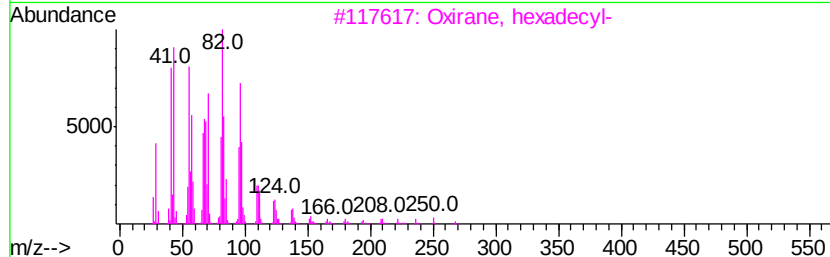
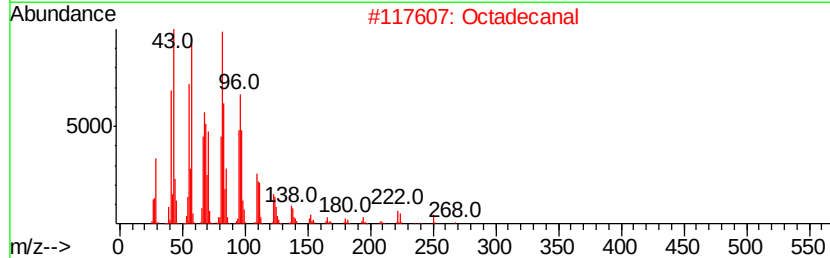
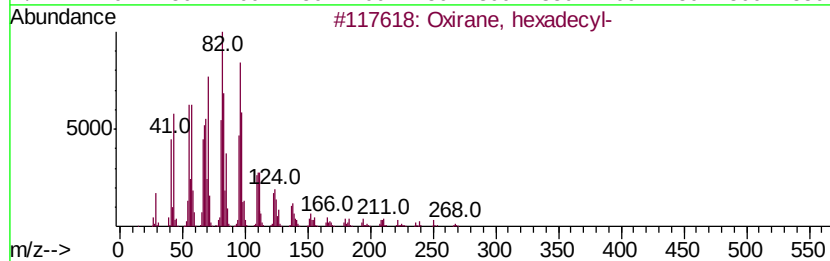
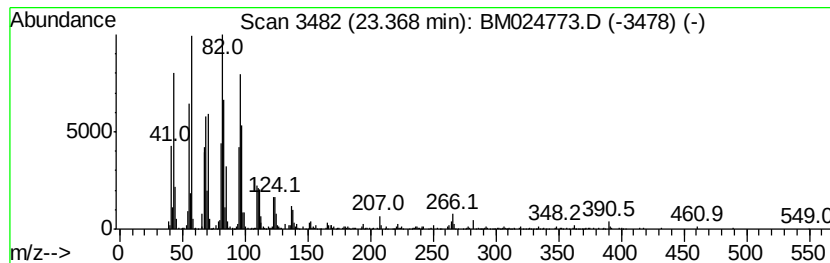
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.37	5.44 ng/ul	1204180	Perylene-d12	23.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94	
2	Octadecanal	268	C18H36O	000638-66-4	93	
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91	
4	Octadecanal	268	C18H36O	000638-66-4	91	
5	Tetracosanal	352	C24H48O	057866-08-7	91	



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020620\
Data File : BM024773.D
Acq On : 07 Feb 2020 22:17
Operator : CG/JU
Sample : L1399-18
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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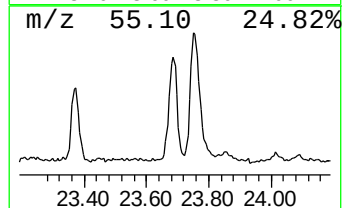
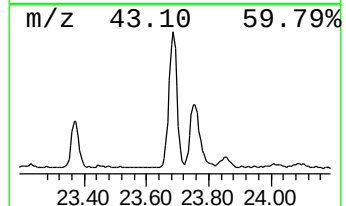
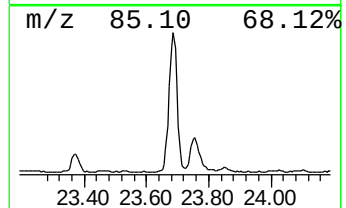
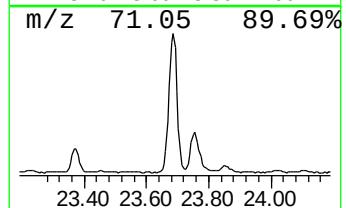
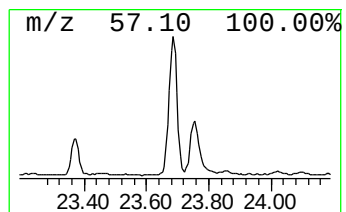
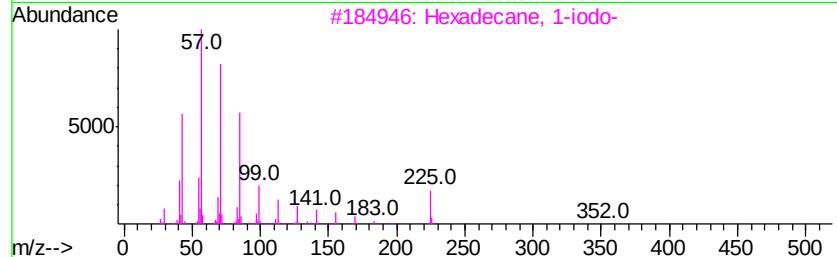
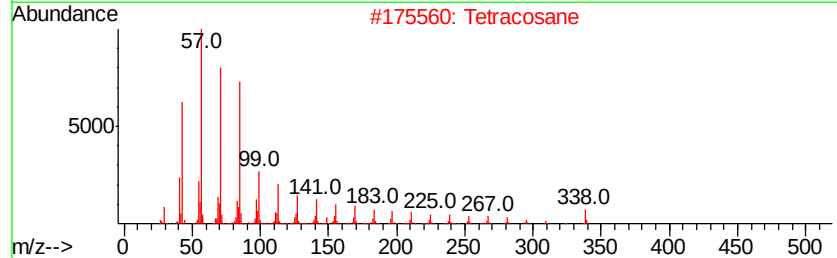
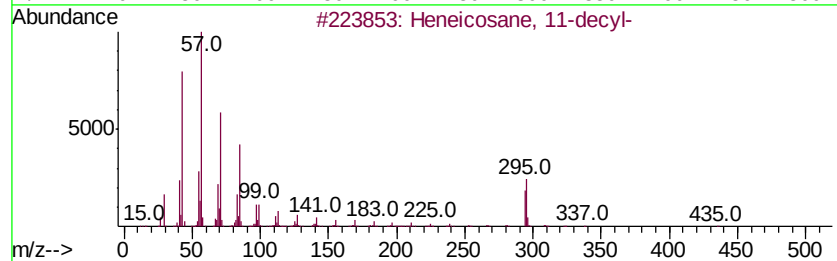
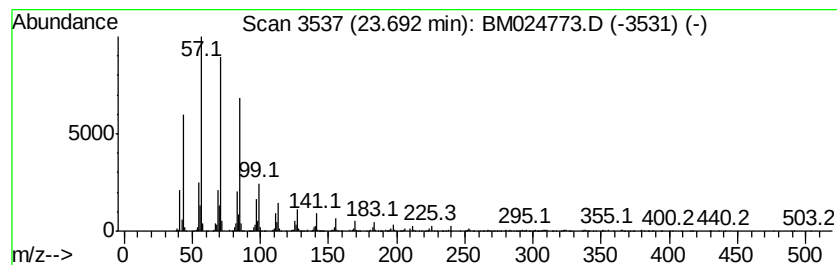
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.69	9.93 ng/ul	2196820	Perylene-d12	23.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	93
2		Tetracosane	338	C24H50	000646-31-1	91
3		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Heptadecane	240	C17H36	000629-78-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020620\
Data File : BM024773.D
Acq On : 07 Feb 2020 22:17
Operator : CG/JU
Sample : L1399-18
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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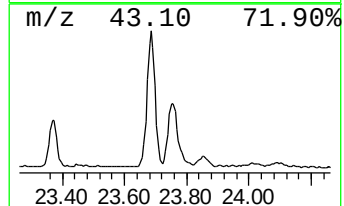
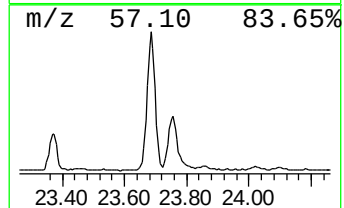
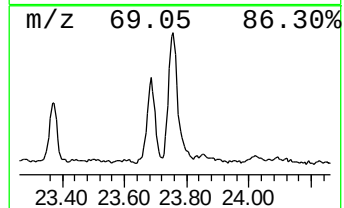
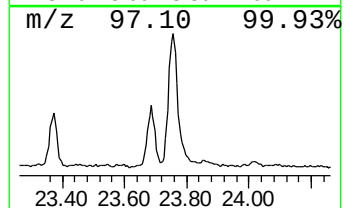
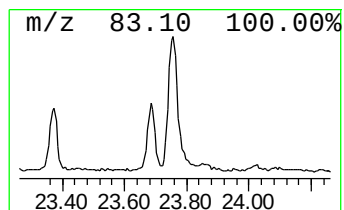
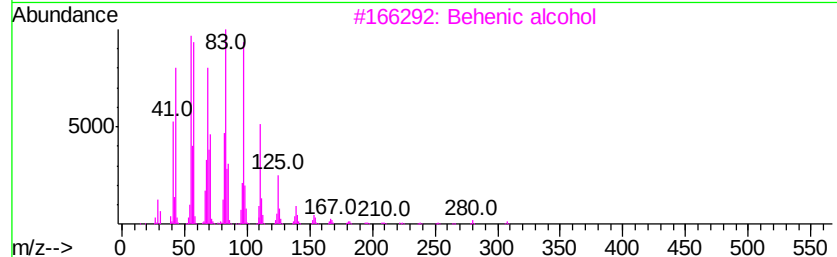
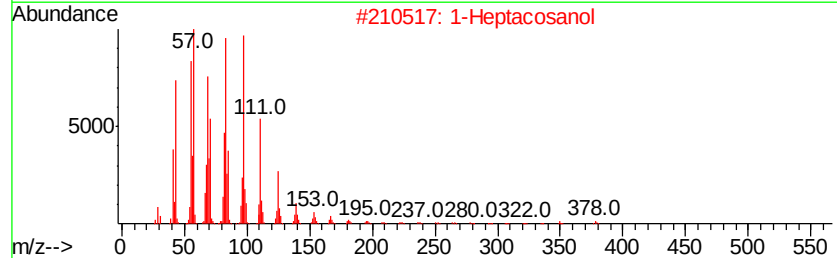
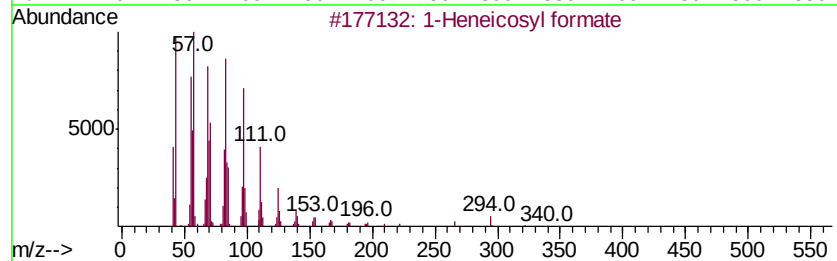
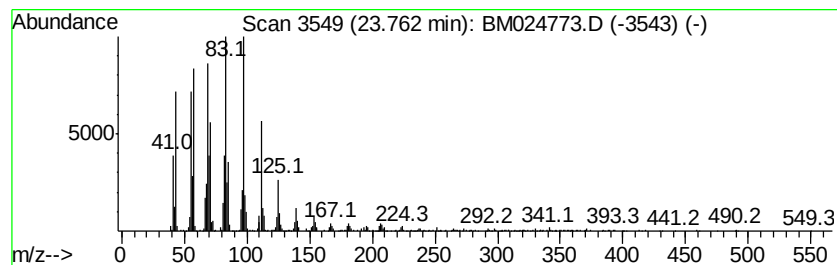
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1-Heneicosyl formate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.76	8.52 ng/ul	1885220	Perylene-d12	23.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate		340	C22H44O2	077899-03-7	94
2	1-Heptacosanol		396	C27H56O	002004-39-9	94
3	Behenic alcohol		326	C22H46O	000661-19-8	93
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	93
5	1-Hexacosene		364	C26H52	018835-33-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM020620\
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ALS Vial : 52 Sample Multiplier: 1

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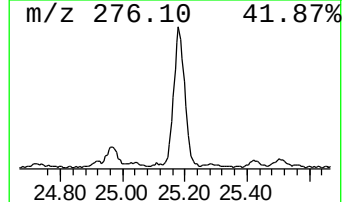
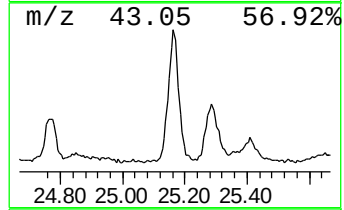
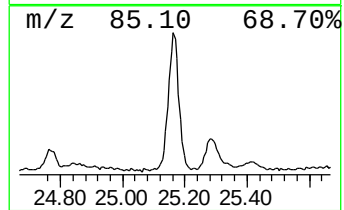
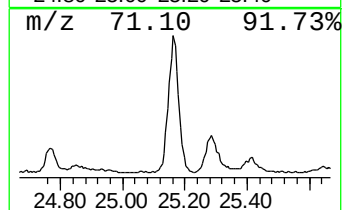
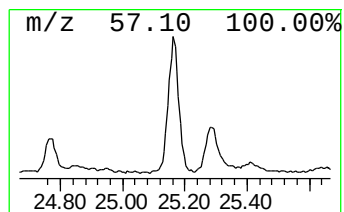
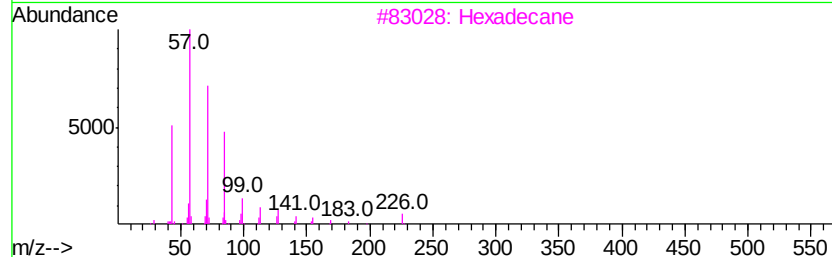
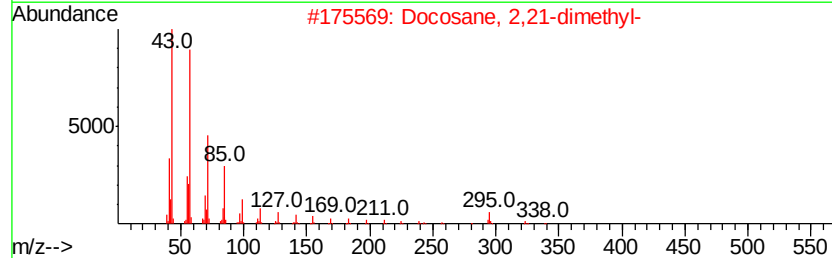
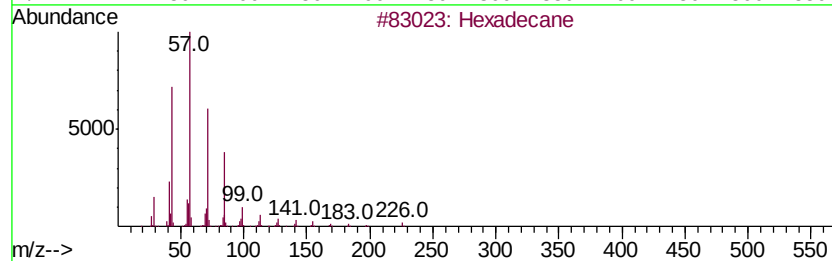
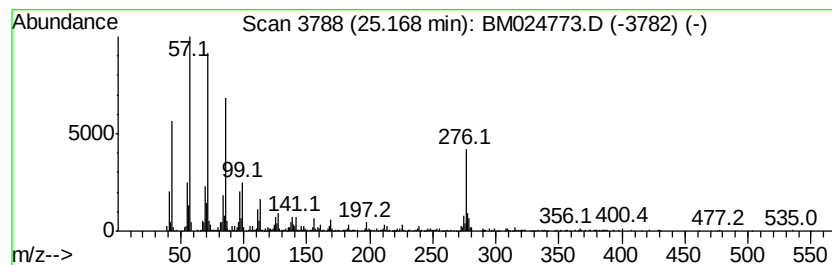
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.17	8.53 ng/ul	1887430	Perylene-d12	23.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Docosane, 2,21-dimethyl-	338	C24H50	077536-31-3	83
3		Hexadecane	226	C16H34	000544-76-3	70
4		Tetratetracontane	619	C44H90	007098-22-8	64
5		Octacosane	394	C28H58	000630-02-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM020620\
Data File : BM024773.D
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Operator : CG/JU
Sample : L1399-18
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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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Sulfurous acid, o...	21.66	3.2	ng/ul	777303	5	21.03	4827180	20.0
Octadecanal	22.30	11.2	ng/ul	2471540	6	23.13	4425700	20.0
1-Heptacosanol	22.60	24.3	ng/ul	5373760	6	23.13	4425700	20.0
Oxirane, hexadecyl-	23.37	5.4	ng/ul	1204180	6	23.13	4425700	20.0
(DEL) Alkane: Str...	23.69	9.9	ng/ul	2196820	6	23.13	4425700	20.0
1-Heneicosyl formate	23.76	8.5	ng/ul	1885220	6	23.13	4425700	20.0
(DEL) Alkane: Str...	25.17	8.5	ng/ul	1887430	6	23.13	4425700	20.0