

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021920\
 Data File : BM024978.D
 Acq On : 20 Feb 2020 12:14
 Operator : CG/JU
 Sample : L1423-22
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C5B02

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	3.040	21	26	39	rVB	37242	101829	1.77%	0.139%
2	3.428	89	92	97	rBV5	9320	16964	0.30%	0.023%
3	3.516	103	107	115	rBV	44017	82116	1.43%	0.112%
4	3.710	138	140	145	rVB4	12485	19936	0.35%	0.027%
5	4.246	227	231	238	rVB5	10660	16156	0.28%	0.022%
6	4.593	285	290	299	rVB	65320	118592	2.06%	0.162%
7	6.587	618	629	646	rBV	841086	1527843	26.59%	2.084%
8	6.740	648	655	667	rVV	818858	1295244	22.54%	1.767%
9	6.928	680	687	698	rVB	1004838	1669894	29.07%	2.278%
10	7.045	704	707	709	rVB4	6964	6982	0.12%	0.010%
11	7.381	757	764	776	rBV	1227922	2014423	35.06%	2.748%
12	7.475	777	780	784	rVB4	7320	8747	0.15%	0.012%
13	8.098	880	886	897	rBV	709249	1157566	20.15%	1.579%
14	8.204	899	904	910	rVB	39753	64931	1.13%	0.089%
15	8.522	950	958	972	rBV	869938	1475770	25.69%	2.013%
16	9.004	1035	1040	1047	rVB	51274	75237	1.31%	0.103%
17	9.233	1072	1079	1098	rBV	730434	1241574	21.61%	1.694%
18	9.604	1137	1142	1144	rBV5	3905	6191	0.11%	0.008%
19	9.769	1163	1170	1189	rBV	1023192	1972712	34.34%	2.691%
20	10.133	1225	1232	1242	rBV	1633506	2616759	45.55%	3.570%
21	10.280	1248	1257	1272	rBV	550491	1178577	20.51%	1.608%
22	10.410	1277	1279	1285	rVB6	7089	9322	0.16%	0.013%
23	10.992	1370	1378	1380	rBV6	4968	9334	0.16%	0.013%
24	11.739	1493	1505	1512	rBV6	16577	37223	0.65%	0.051%
25	12.957	1707	1712	1717	rBV3	20081	30569	0.53%	0.042%
26	13.457	1789	1797	1802	rBV	2005170	2790953	48.58%	3.807%
27	13.504	1802	1805	1813	rVB	385264	521525	9.08%	0.711%
28	13.716	1833	1841	1855	rBV	2515073	3609544	62.83%	4.924%
29	14.033	1888	1895	1903	rVV	2288105	3438497	59.85%	4.691%
30	14.092	1903	1905	1910	rVB4	5688	6049	0.11%	0.008%
31	14.263	1927	1934	1957	rVV	369912	888958	15.47%	1.213%
32	14.421	1957	1961	1965	rVV7	21339	46756	0.81%	0.064%
33	14.486	1968	1972	1983	rVB7	31048	74477	1.30%	0.102%
34	14.668	1999	2003	2009	rBV6	3603	9339	0.16%	0.013%

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35	14.886	2036	2040	2043	rBV3	10027	14419	0.25%	0.020%
36	14.945	2045	2050	2055	rVB5	8951	11849	0.21%	0.016%
37	15.033	2059	2065	2077	rVV	3112309	4375293	76.15%	5.968%
38	15.115	2077	2079	2083	rVV2	22792	27732	0.48%	0.038%
39	15.168	2083	2088	2102	rVV	551596	838359	14.59%	1.144%
40	15.280	2102	2107	2112	rVB	33381	50110	0.87%	0.068%
41	15.827	2192	2200	2208	rBV8	15710	35908	0.62%	0.049%
42	15.957	2217	2222	2229	rVB10	4194	10289	0.18%	0.014%
43	16.251	2268	2272	2275	rBV5	10085	14417	0.25%	0.020%
44	16.357	2285	2290	2296	rBV	64709	93498	1.63%	0.128%
45	16.462	2307	2308	2313	rVB4	7806	10363	0.18%	0.014%
46	16.574	2321	2327	2330	rBV2	12996	21292	0.37%	0.029%
47	16.609	2330	2333	2336	rVB4	9765	12374	0.22%	0.017%
48	16.739	2350	2355	2357	rBV5	13346	18431	0.32%	0.025%
49	16.786	2357	2363	2368	rVV	2833642	3865251	67.28%	5.273%
50	16.827	2368	2370	2374	rVV	94848	119022	2.07%	0.162%
51	16.886	2374	2380	2393	rVB	3012900	4250717	73.99%	5.799%
52	17.009	2398	2401	2405	rVB6	9942	16645	0.29%	0.023%
53	17.168	2423	2428	2430	rBV6	7069	14056	0.24%	0.019%
54	17.215	2431	2436	2441	rVB9	22504	39182	0.68%	0.053%
55	17.333	2454	2456	2460	rVB5	7321	6676	0.12%	0.009%
56	17.486	2479	2482	2484	rBV4	8785	10161	0.18%	0.014%
57	17.509	2484	2486	2488	rVB3	9667	7981	0.14%	0.011%
58	17.604	2498	2502	2506	rBV7	15825	24170	0.42%	0.033%
59	17.668	2509	2513	2517	rBV3	32202	45854	0.80%	0.063%
60	17.733	2517	2524	2532	rBV2	414793	655129	11.40%	0.894%
61	17.856	2541	2545	2549	rBV4	29879	47695	0.83%	0.065%
62	17.898	2549	2552	2554	rVB3	15600	18220	0.32%	0.025%
63	18.021	2568	2573	2579	rBV6	27348	60005	1.04%	0.082%
64	18.174	2594	2599	2602	rBV5	51406	81783	1.42%	0.112%
65	18.427	2637	2642	2645	rBV7	16812	23141	0.40%	0.032%
66	18.562	2661	2665	2668	rVB6	14374	23590	0.41%	0.032%
67	18.603	2668	2672	2675	rBV4	37257	57670	1.00%	0.079%
68	18.745	2691	2696	2697	rBV5	20387	34710	0.60%	0.047%
69	18.827	2706	2710	2711	rBV2	40879	50116	0.87%	0.068%
70	18.856	2711	2715	2720	rVB	343689	454871	7.92%	0.621%
71	19.027	2740	2744	2750	rBV3	154697	245509	4.27%	0.335%

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72	19.080	2751	2753	2761	rVB2	53369	84525	1.47%	0.115%
73	19.192	2766	2772	2782	rBV	3913069	5745355	100.00%	7.837%
74	19.303	2788	2791	2795	rBV6	26724	37982	0.66%	0.052%
75	20.762	3035	3039	3049	rBV3	646467	1019138	17.74%	1.390%
76	21.003	3074	3080	3084	rBV	3160633	4226968	73.57%	5.766%
77	21.209	3112	3115	3118	rVB	184707	197562	3.44%	0.270%
78	21.627	3183	3186	3199	rVB2	397769	562799	9.80%	0.768%
79	22.062	3256	3260	3264	rVB	519983	626092	10.90%	0.854%
80	22.533	3336	3340	3343	rVB2	700981	855736	14.89%	1.167%
81	22.968	3408	3414	3420	rBV	2705645	4470878	77.82%	6.099%
82	23.050	3425	3428	3431	rVV	390055	575399	10.02%	0.785%
83	23.097	3431	3436	3443	rVB	2377230	3989134	69.43%	5.442%
84	23.644	3524	3529	3535	rVB	707459	1241316	21.61%	1.693%
85	25.521	3842	3848	3854	rBV	914689	2172088	37.81%	2.963%
86	25.591	3855	3860	3869	rVB2	912963	2222306	38.68%	3.032%
87	25.968	3919	3924	3932	rVB2	629458	1452389	25.28%	1.981%

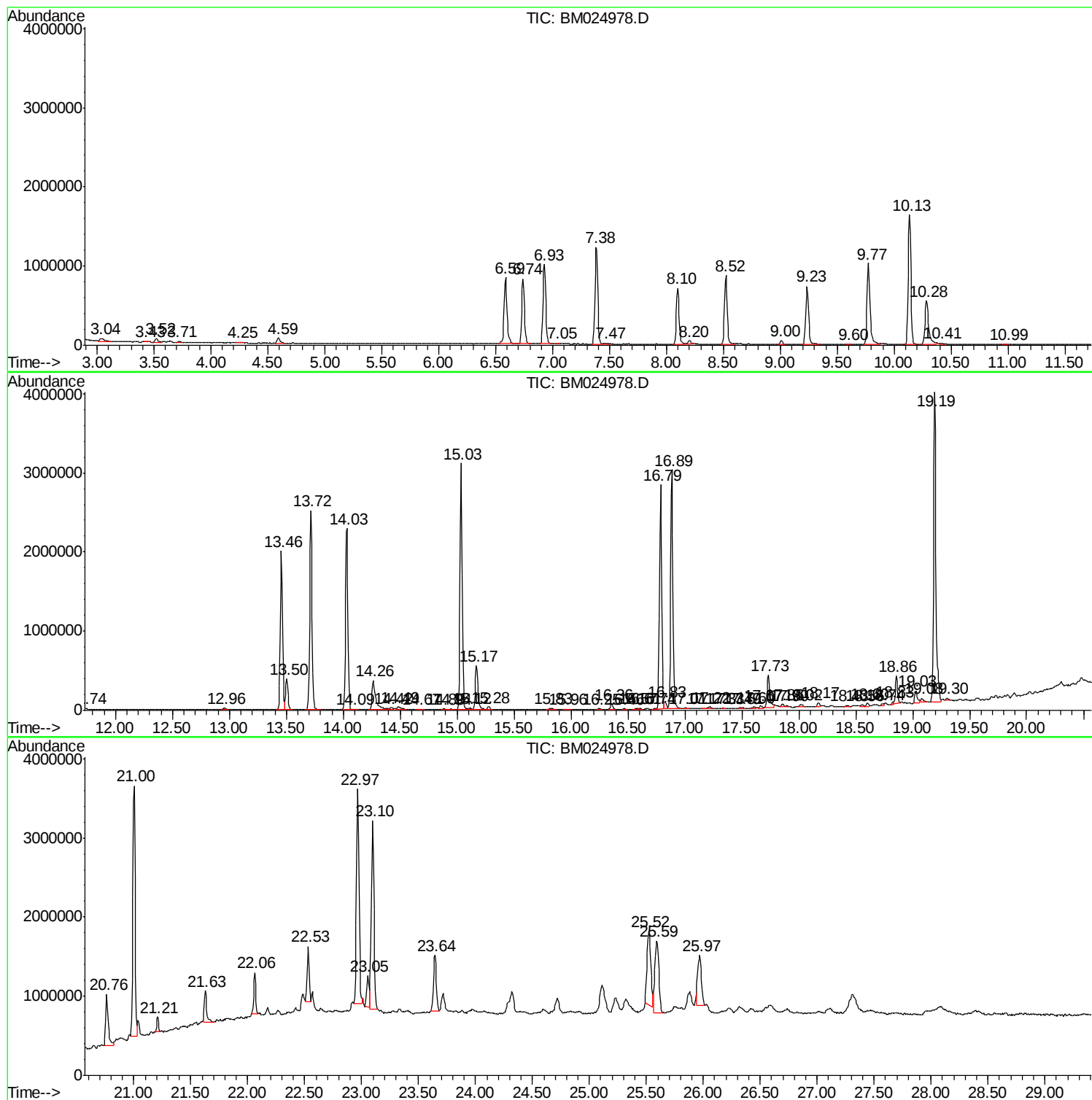
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM020620MA.M
Quant Title : SVOA CALIBRATION

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



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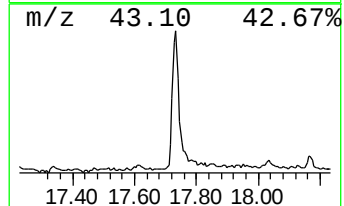
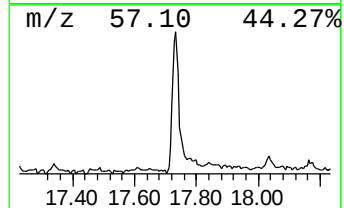
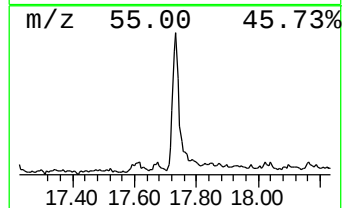
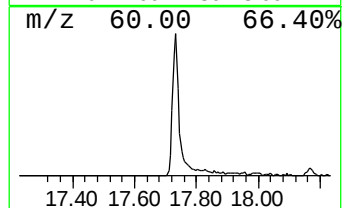
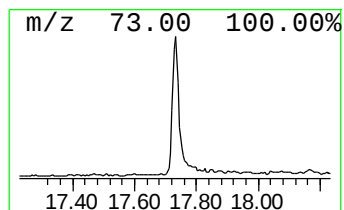
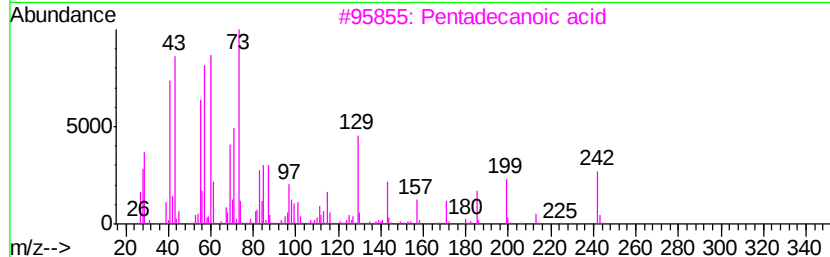
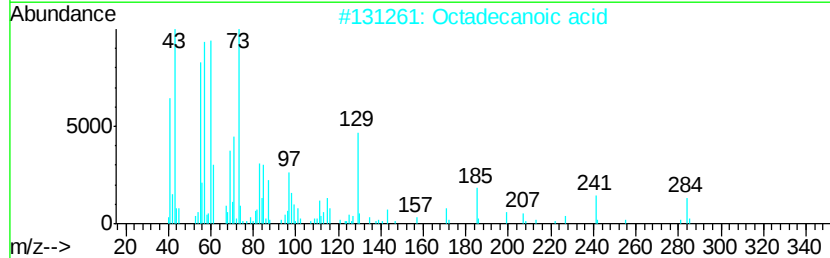
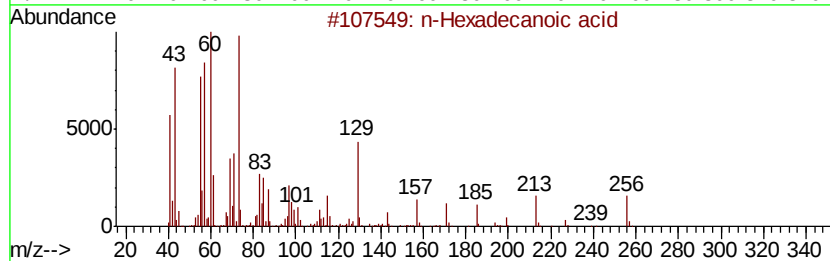
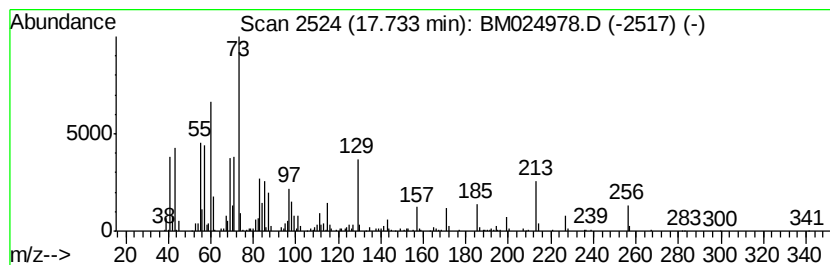
Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM020620MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD			R.T.	
17.73	3.39 ng/ul	655129	Phenanthrene-d10			16.79	
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2			Octadecanoic acid	284	C18H36O2	000057-11-4	74
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Tridecanoic acid	214	C13H26O2	000638-53-9	58



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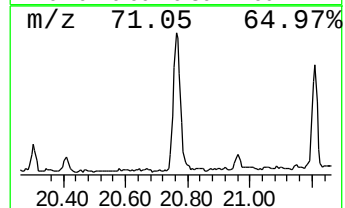
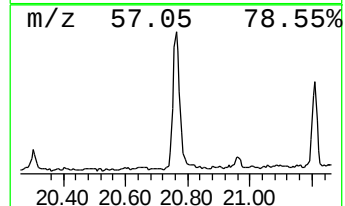
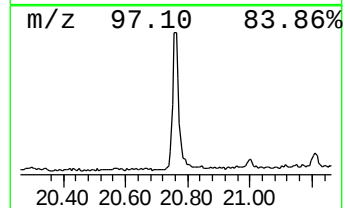
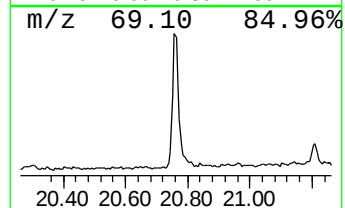
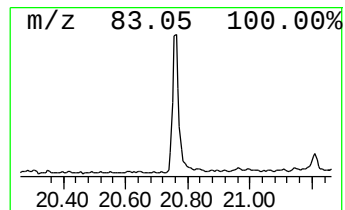
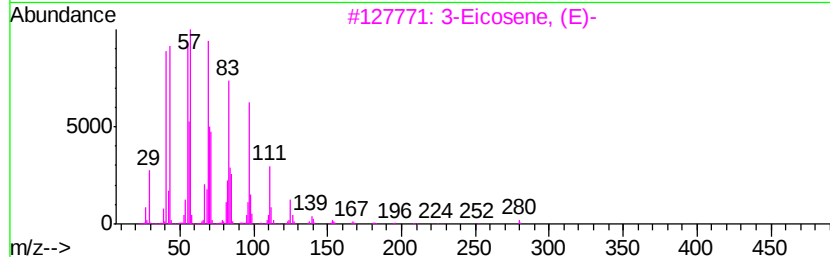
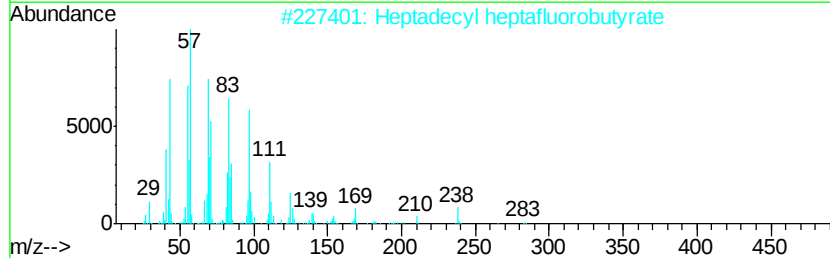
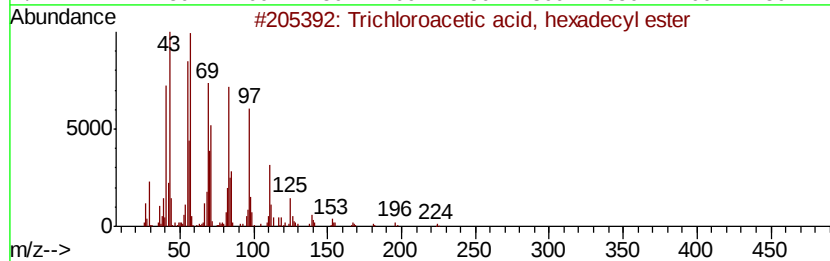
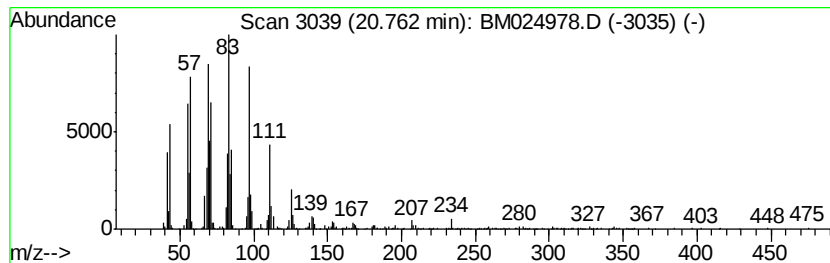
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.76	4.82 ng/ul	1019140	Chrysene-d12	21.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	87
4		1-Hexadecanol	242	C16H34O	036653-82-4	83
5		Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	83



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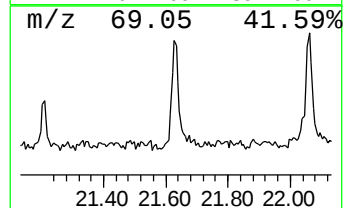
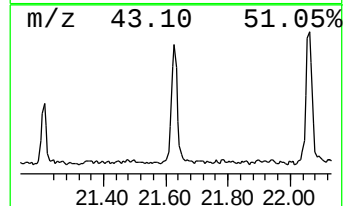
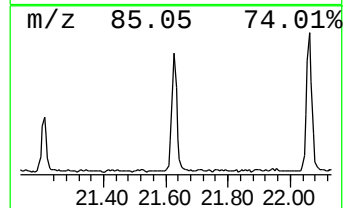
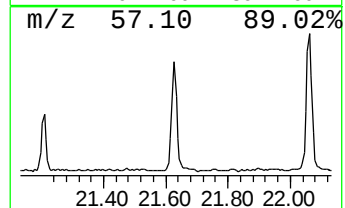
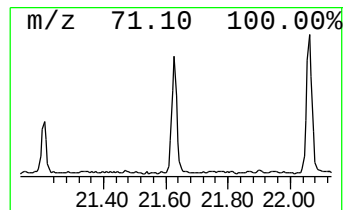
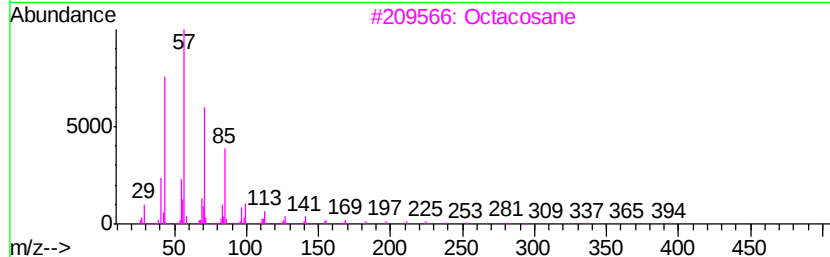
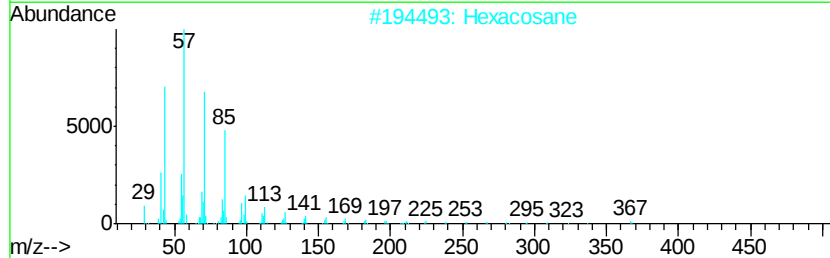
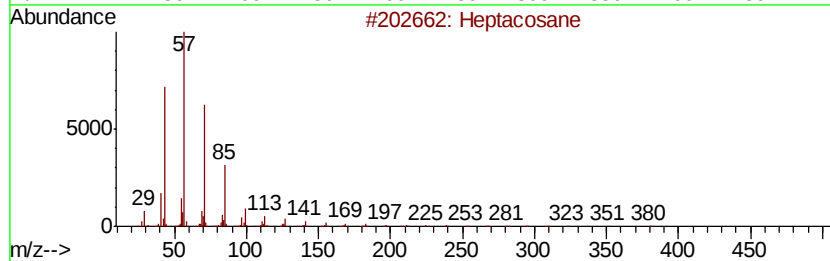
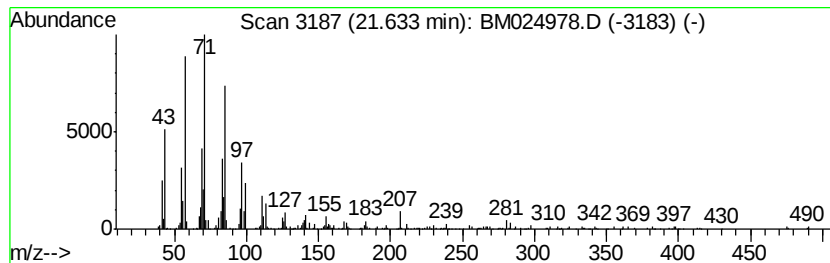
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Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.63	2.66 ng/ul	562799	Chrysene-d12	21.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	93
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane	296	C21H44	000629-94-7	87
5		Tetratetracontane	619	C44H90	007098-22-8	87



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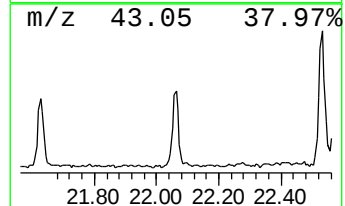
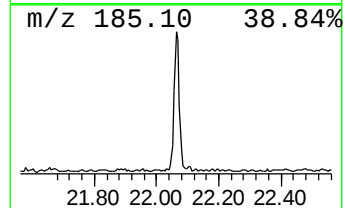
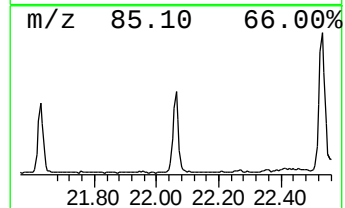
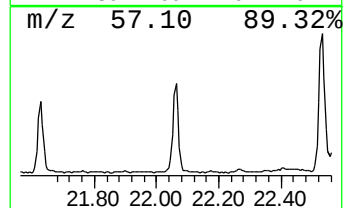
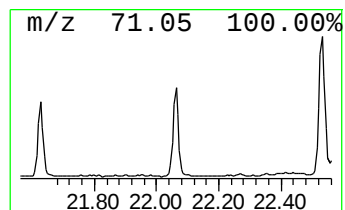
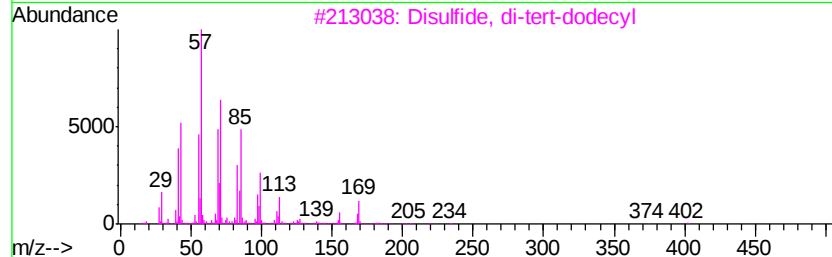
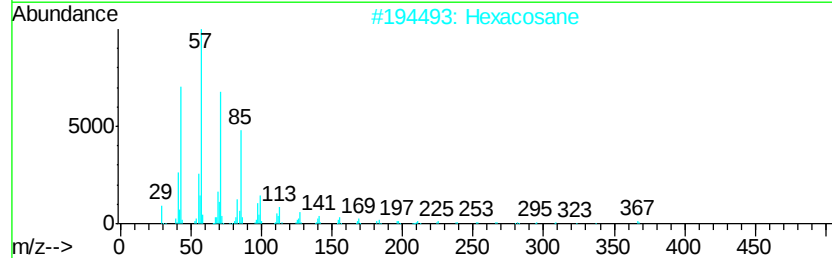
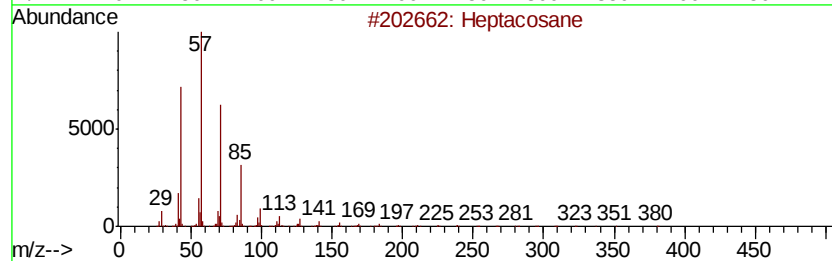
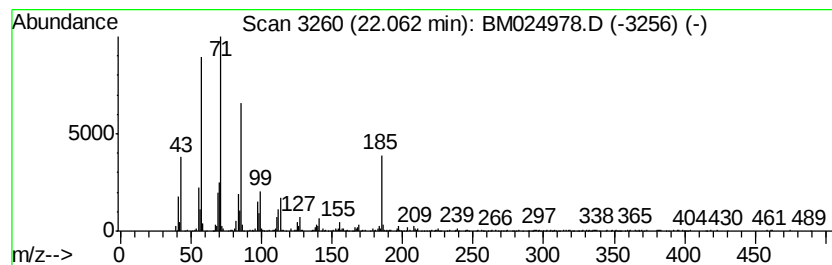
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.06	3.14 ng/ul	626092	Perylene-d12	23.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	93
2		Hexacosane	366	C26H54	000630-01-3	64
3		Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	64
4		Octacosane	394	C28H58	000630-02-4	62
5		Tetratetracontane	619	C44H90	007098-22-8	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021920\
Data File : BM024978.D
Acq On : 20 Feb 2020 12:14
Operator : CG/JU
Sample : L1423-22
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C5B02

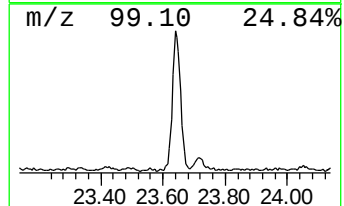
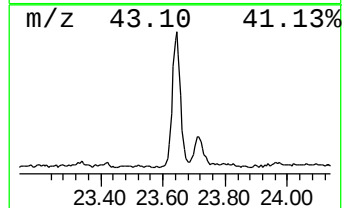
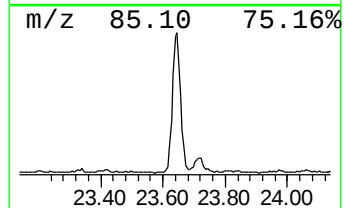
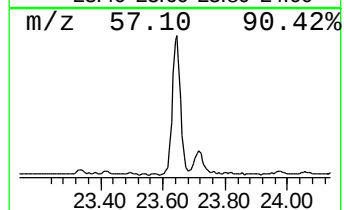
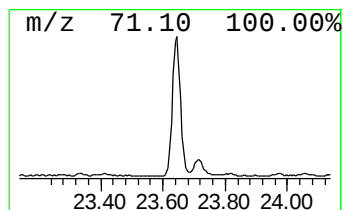
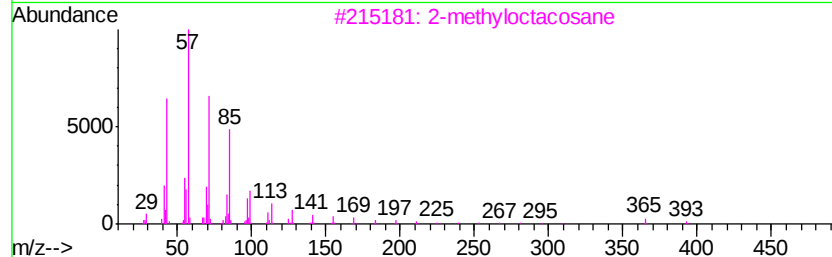
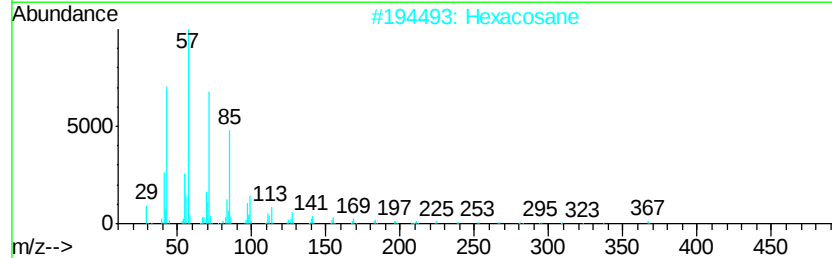
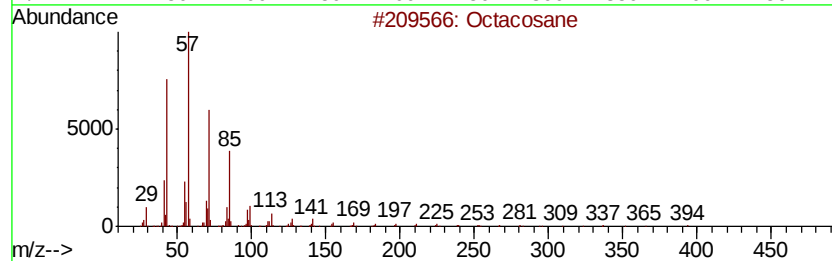
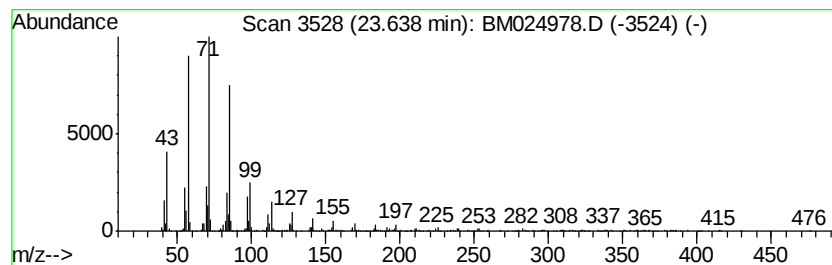
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.64	6.22 ng/ul	1241320	Perylene-d12	23.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	90
2		Hexacosane	366	C26H54	000630-01-3	90
3		2-methyloctacosane	408	C29H60	1000376-72-8	90
4		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
5		Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021920\
Data File : BM024978.D
Acq On : 20 Feb 2020 12:14
Operator : CG/JU
Sample : L1423-22
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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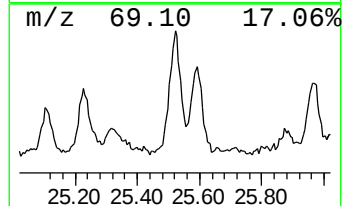
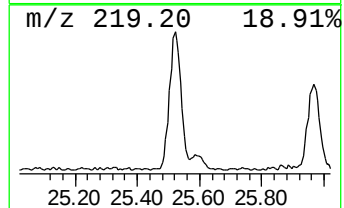
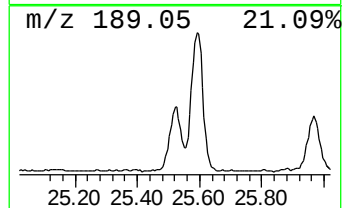
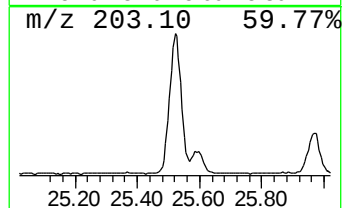
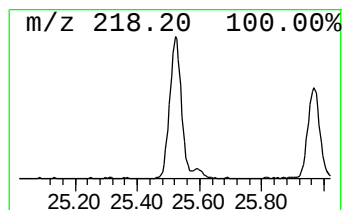
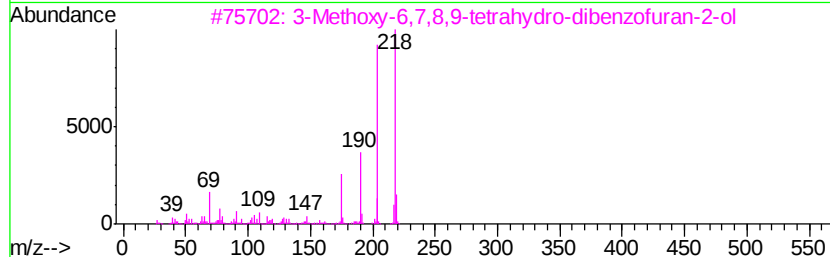
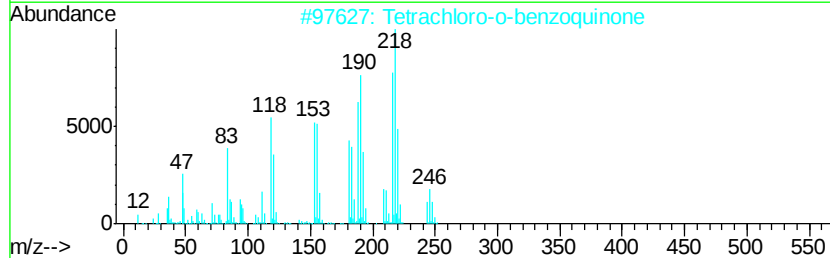
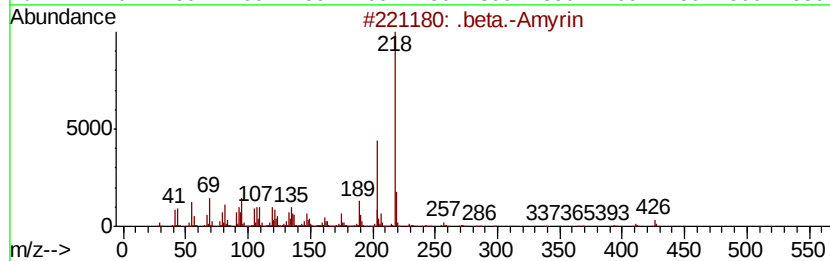
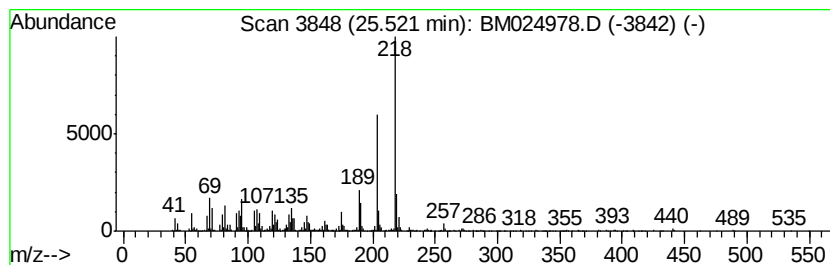
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 .beta.-Amyrin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.52	10.89 ng/ul	2172090	Perylene-d12	23.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Amyrin	426	C30H50O	000559-70-6	87
2		Tetrachloro-o-benzoquinone	244	C6Cl4O2	002435-53-2	83
3		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	81
4		.beta.-Amyrin trimethylsilyl ether	498	C33H58OSi	001721-67-1	72
5		.beta.-Amyrin	426	C30H50O	000559-70-6	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021920\
Data File : BM024978.D
Acq On : 20 Feb 2020 12:14
Operator : CG/JU
Sample : L1423-22
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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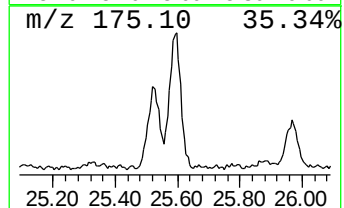
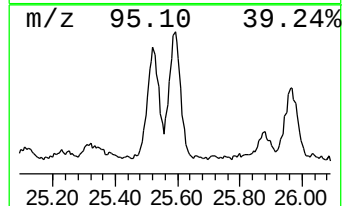
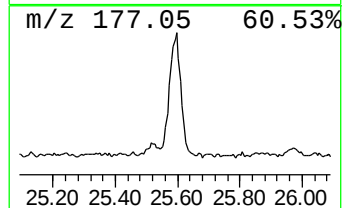
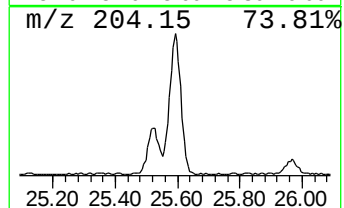
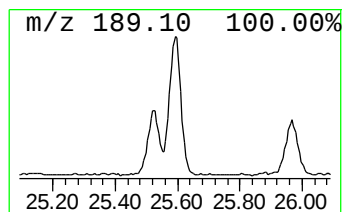
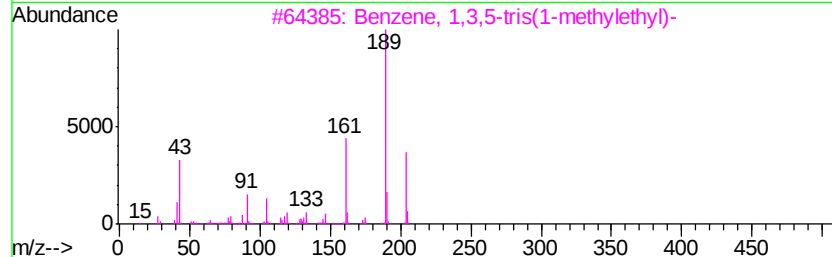
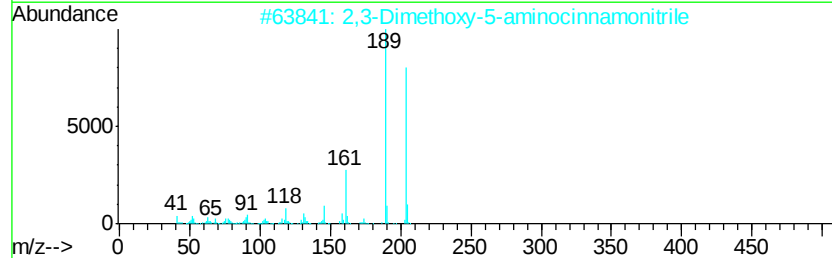
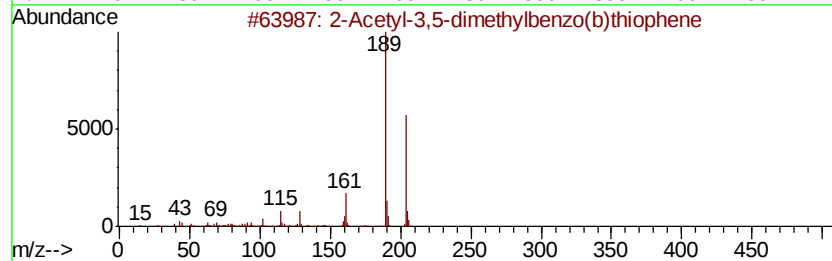
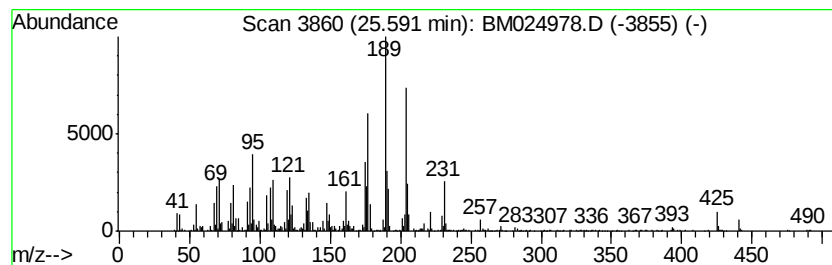
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.59	11.14 ng/ul	2222310	Perylene-d12	23.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Acetyl-3,5-dimethylbenzo(b)thi...	204	C12H12OS	006179-05-1	43
2		2,3-Dimethoxy-5-aminocinnamitrile	204	C11H12N2O2	1000214-46-5	38
3		Benzene, 1,3,5-tris(1-methylethyl)-	204	C15H24	000717-74-8	38
4		2-Acetyl-3,7-dimethylbenzo(b)thi...	204	C12H12OS	006179-06-2	38
5		1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021920\
Data File : BM024978.D
Acq On : 20 Feb 2020 12:14
Operator : CG/JU
Sample : L1423-22
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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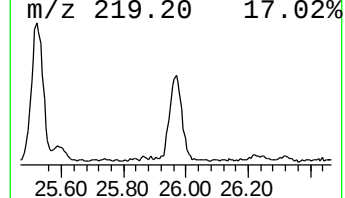
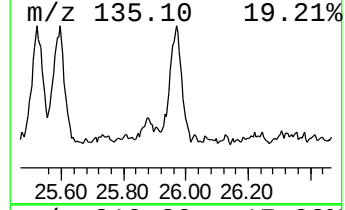
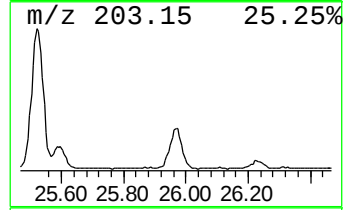
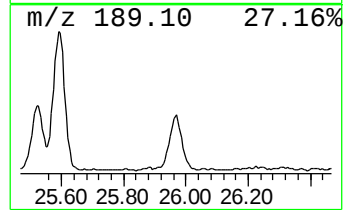
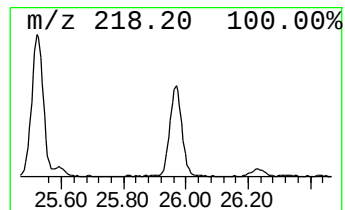
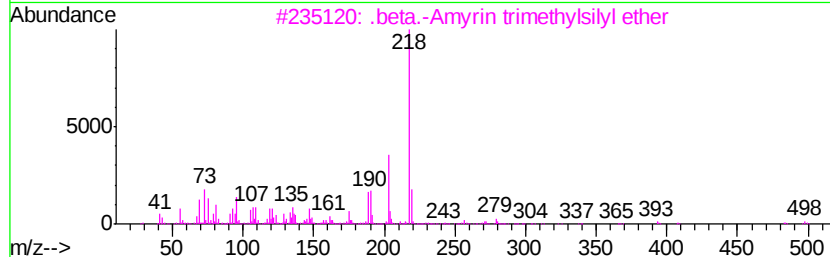
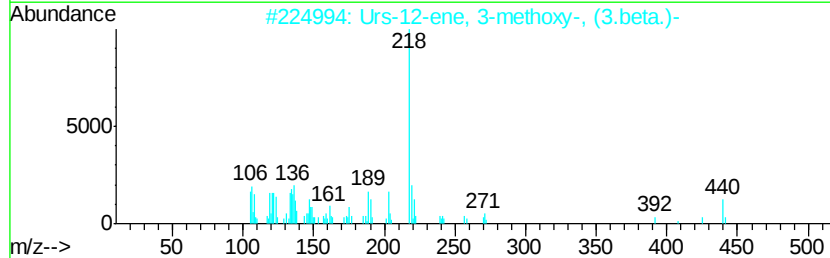
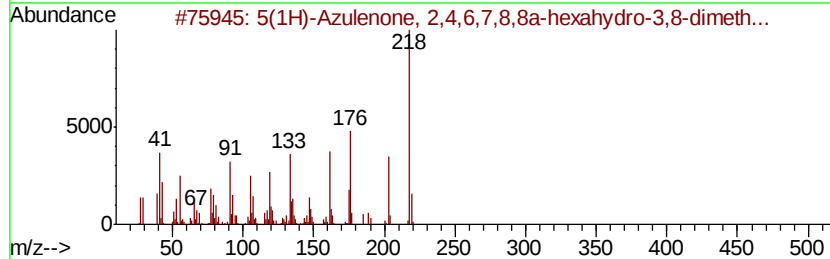
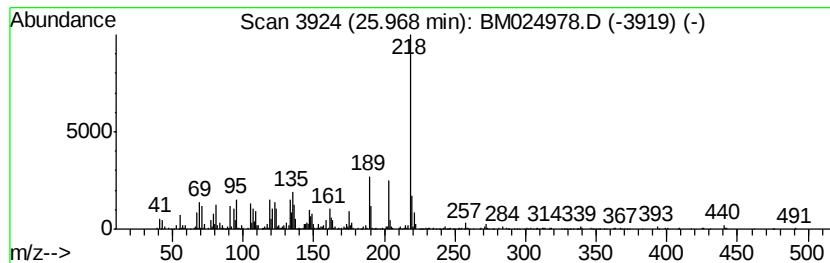
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 5(1H)-Azulenone, 2,4,6,7,8,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.97	7.28 ng/ul	1452390	Perylene-d12	23.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	76
2		Urs-12-ene, 3-methoxy-, (3.beta.)-	440	C31H52O	014021-28-4	64
3		.beta.-Amyrin trimethylsilyl ether	498	C33H58OSi	001721-67-1	64
4		.alpha.-Amyrin	426	C30H50O	000638-95-9	64
5		Urs-12-en-24-oic acid, 3-oxo-, m...	468	C31H48O3	020475-86-9	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM021920\
Data File : BM024978.D
Acq On : 20 Feb 2020 12:14
Operator : CG/JU
Sample : L1423-22
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C5B02

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic acid	17.73	3.4	ng/ul	655129	4	16.79	3865250	20.0
Trichloroacetic a...	20.76	4.8	ng/ul	1019140	5	21.00	4226970	20.0
(DEL) Alkane: Str...	21.63	2.7	ng/ul	562799	5	21.00	4226970	20.0
(DEL) Alkane: Str...	22.06	3.1	ng/ul	626092	6	23.10	3989130	20.0
(DEL) Alkane: Str...	23.64	6.2	ng/ul	1241320	6	23.10	3989130	20.0
.beta.-Amyrin	25.52	10.9	ng/ul	2172090	6	23.10	3989130	20.0
unknown-01	25.59	11.1	ng/ul	2222310	6	23.10	3989130	20.0
5(1H)-Azulenone, ...	25.97	7.3	ng/ul	1452390	6	23.10	3989130	20.0