

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120420\
 Data File : BG047598.D
 Acq On : 5 Dec 2020 9:48
 Operator : CG/JU
 Sample : L4864-08
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0BD4

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_G\METHODS\SOM-EPA-BG111920MA.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	3.519	29	31	35	rBV3	2039	3137	0.20%	0.021%
2	3.583	38	42	47	rVV2	9765	13296	0.85%	0.087%
3	3.842	83	86	87	rBV	2335	2033	0.13%	0.013%
4	4.071	123	125	129	rVB3	3241	2841	0.18%	0.019%
5	4.218	147	150	151	rVB2	2614	2019	0.13%	0.013%
6	4.241	151	154	156	rBV2	2199	2643	0.17%	0.017%
7	4.365	172	175	180	rVB4	2753	4295	0.27%	0.028%
8	4.482	192	195	198	rBV2	2381	2440	0.16%	0.016%
9	4.747	239	240	243	rVB2	2445	2030	0.13%	0.013%
10	5.199	315	317	320	rVB	2139	2319	0.15%	0.015%
11	7.220	656	661	662	rBV	2583	2832	0.18%	0.019%
12	7.385	681	689	698	rBV	201927	382396	24.47%	2.506%
13	7.561	712	719	727	rBV	119865	207341	13.27%	1.359%
14	7.702	740	743	747	rBV	1118	2167	0.14%	0.014%
15	7.779	747	756	764	rVV	206951	363067	23.23%	2.380%
16	8.249	827	836	843	rBV2	135195	230741	14.77%	1.512%
17	8.325	848	849	853	rBV	2139	2178	0.14%	0.014%
18	8.942	945	954	961	rBV2	251108	446935	28.60%	2.930%
19	9.418	1026	1035	1044	rBV	206757	375089	24.00%	2.459%
20	9.829	1102	1105	1108	rVB2	3382	3098	0.20%	0.020%
21	10.146	1152	1159	1166	rBV2	203909	379585	24.29%	2.488%
22	10.240	1172	1175	1179	rBV2	1948	2388	0.15%	0.016%
23	10.487	1213	1217	1220	rBV2	1642	2495	0.16%	0.016%
24	10.687	1243	1251	1260	rBV	282603	511200	32.71%	3.351%
25	11.075	1310	1317	1326	rBV	169366	303647	19.43%	1.990%
26	11.198	1331	1338	1346	rBV2	241974	447149	28.62%	2.931%
27	11.521	1387	1393	1399	rBV	8173	15097	0.97%	0.099%
28	12.632	1579	1582	1588	rBV2	4415	6116	0.39%	0.040%
29	13.078	1654	1658	1661	rBV2	1399	2117	0.14%	0.014%
30	13.119	1663	1665	1670	rBV2	1300	2032	0.13%	0.013%
31	13.419	1714	1716	1721	rBV2	1712	2165	0.14%	0.014%
32	13.677	1755	1760	1762	rBV2	2518	3199	0.20%	0.021%
33	13.736	1766	1770	1771	rBV	3826	3840	0.25%	0.025%
34	14.153	1837	1841	1842	rBV	1626	2058	0.13%	0.013%

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Integration Parameters: LSCINT.P

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35	14.253	1851	1858	1863	rBV	554641	823814	52.72%	5.400%
36	14.300	1863	1866	1872	rVB2	59900	85129	5.45%	0.558%
37	14.565	1902	1911	1918	rVB	535195	858484	54.94%	5.627%
38	14.747	1936	1942	1945	rVB	2569	3328	0.21%	0.022%
39	14.864	1955	1962	1968	rBV	292535	454987	29.12%	2.982%
40	15.029	1983	1990	2002	rBV2	296388	494375	31.64%	3.240%
41	15.187	2013	2017	2020	rVB	2935	2831	0.18%	0.019%
42	15.252	2023	2028	2032	rVV3	4220	6815	0.44%	0.045%
43	15.851	2123	2130	2136	rBV	739477	1103947	70.65%	7.236%
44	15.951	2141	2147	2157	rVV	297475	447866	28.66%	2.936%
45	16.086	2167	2170	2176	rVB2	8502	13205	0.85%	0.087%
46	16.133	2176	2178	2181	rVB2	3392	2203	0.14%	0.014%
47	16.251	2193	2198	2199	rBV2	2605	2782	0.18%	0.018%
48	16.392	2219	2222	2223	rBV	2944	2157	0.14%	0.014%
49	16.521	2242	2244	2247	rBV2	2296	2802	0.18%	0.018%
50	16.615	2257	2260	2261	rBV	3325	3241	0.21%	0.021%
51	16.821	2293	2295	2296	rBV	3207	2072	0.13%	0.014%
52	16.950	2313	2317	2320	rBV	1555	2106	0.13%	0.014%
53	17.379	2389	2390	2394	rVB	2157	2468	0.16%	0.016%
54	17.538	2412	2417	2418	rBV	2404	3635	0.23%	0.024%
55	17.596	2421	2427	2435	rVV	406289	636542	40.74%	4.172%
56	17.696	2437	2444	2452	rVV	816308	1263499	80.86%	8.282%
57	17.761	2452	2455	2460	rVB3	3222	5616	0.36%	0.037%
58	17.837	2466	2468	2473	rVB	2210	3692	0.24%	0.024%
59	17.961	2487	2489	2492	rBV2	2121	2536	0.16%	0.017%
60	17.996	2493	2495	2498	rVB2	2778	2041	0.13%	0.013%
61	18.360	2556	2557	2563	rVB	1999	2404	0.15%	0.016%
62	18.460	2570	2574	2579	rVB5	3666	5451	0.35%	0.036%
63	18.536	2585	2587	2590	rVB2	3324	2064	0.13%	0.014%
64	18.736	2619	2621	2624	rBV	2255	2744	0.18%	0.018%
65	19.130	2686	2688	2689	rBV	4095	2471	0.16%	0.016%
66	19.142	2689	2690	2693	rVV2	3467	3556	0.23%	0.023%
67	19.195	2696	2699	2700	rVB3	4338	4439	0.28%	0.029%
68	19.377	2729	2730	2732	rBV2	2674	2332	0.15%	0.015%
69	19.494	2748	2750	2752	rBV2	2056	2160	0.14%	0.014%
70	19.524	2754	2755	2759	rBV3	3584	4156	0.27%	0.027%
71	19.606	2763	2769	2772	rBV2	12397	18292	1.17%	0.120%

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72	19.858	2807	2812	2816	rVB3	9234	16553	1.06%	0.108%
73	19.964	2824	2830	2838	rVB	1053697	1562630	100.00%	10.243%
74	20.093	2850	2852	2853	rBV2	3017	2513	0.16%	0.016%
75	20.170	2863	2865	2866	rBV2	3530	2631	0.17%	0.017%
76	20.252	2875	2879	2882	rBV	78356	89058	5.70%	0.584%
77	20.293	2882	2886	2890	rVB	141953	155865	9.97%	1.022%
78	20.446	2909	2912	2914	rBV4	8040	9183	0.59%	0.060%
79	20.740	2961	2962	2964	rBV2	5366	3794	0.24%	0.025%
80	21.257	3046	3050	3053	rBV2	53638	66112	4.23%	0.433%
81	21.292	3053	3056	3061	rVB	85702	104344	6.68%	0.684%
82	21.486	3083	3089	3097	rBV3	134692	235509	15.07%	1.544%
83	21.880	3149	3156	3166	rVB	393150	682318	43.66%	4.472%
84	22.403	3241	3245	3247	rBV5	19162	26021	1.67%	0.171%
85	22.444	3248	3252	3258	rVB3	45722	71081	4.55%	0.466%
86	23.930	3501	3505	3516	rVB6	38917	89642	5.74%	0.588%
87	25.041	3682	3694	3706	rVB2	480780	1418894	90.80%	9.300%
88	25.264	3724	3732	3744	rVB	228754	698047	44.67%	4.575%
89	28.384	4261	4263	4264	rBV2	6302	3843	0.25%	0.025%

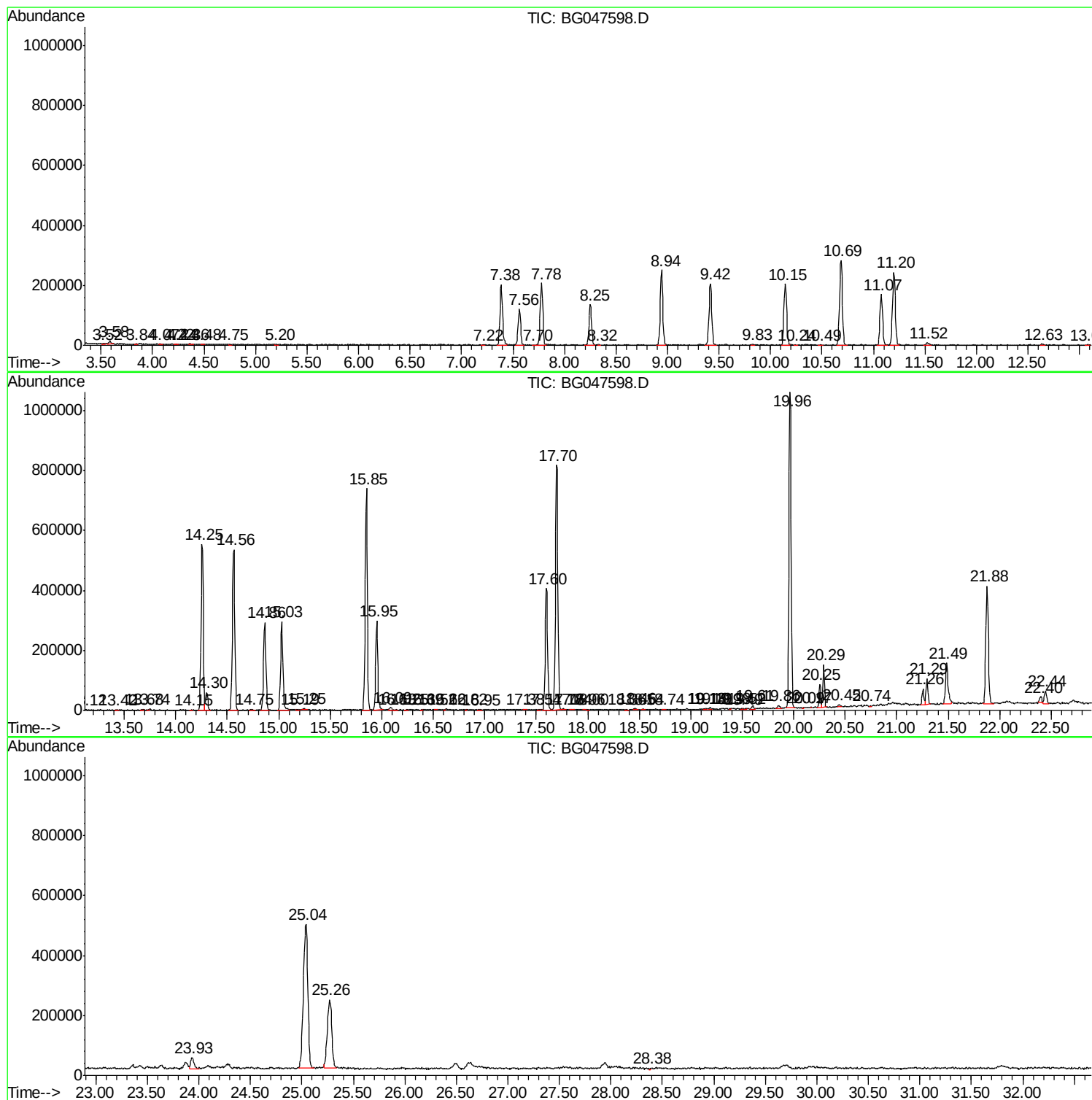
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

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



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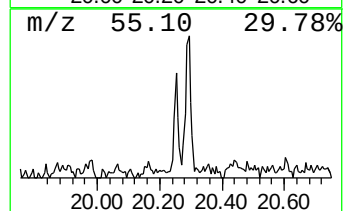
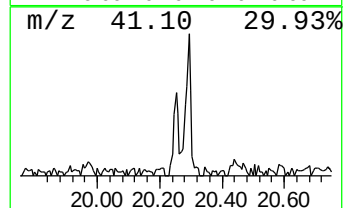
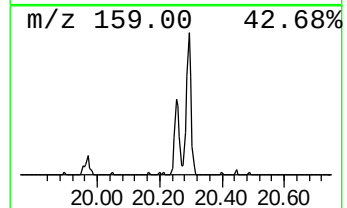
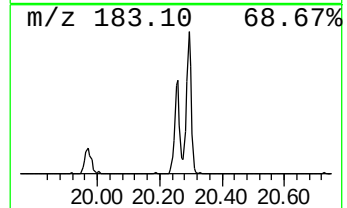
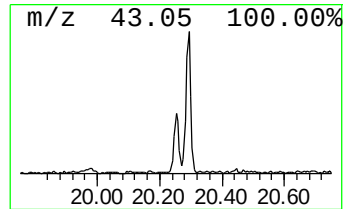
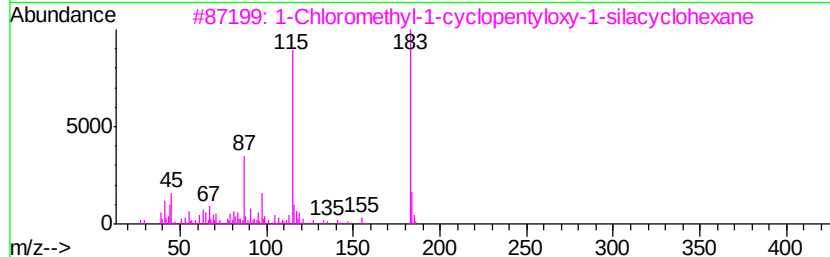
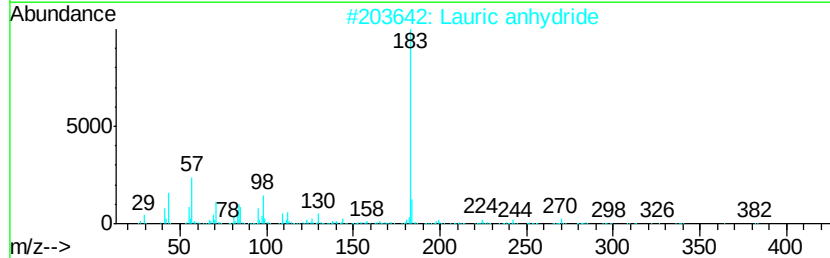
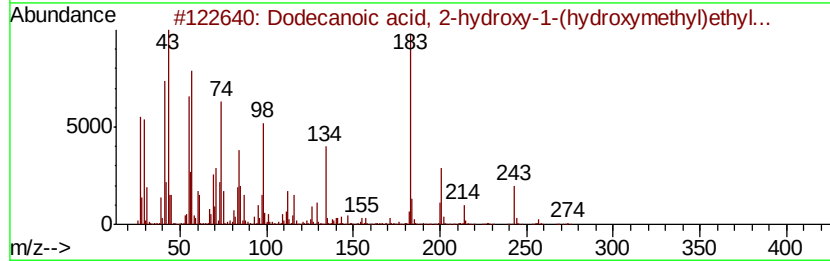
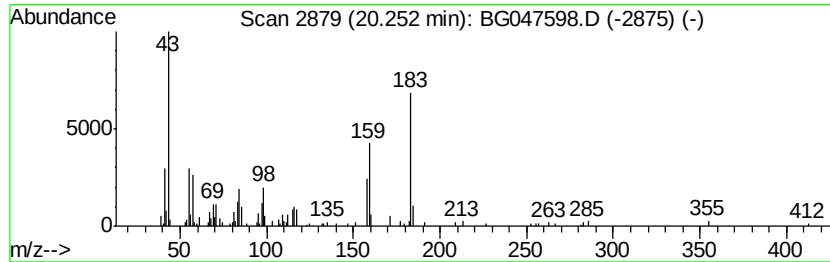
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.25	2.61 ng/ul	89058	Chrysene-d12	21.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	47
2		Lauric anhydride	382	C24H46O3	000645-66-9	35
3		1-Chloromethyl-1-cyclopentyl-oxo-...	232	C11H21ClO5	1000279-43-1	27
4		Fumaric acid, di(2-hexyl) ester	284	C16H28O4	1000348-75-8	27
5		Dodecanoic acid, ethenyl ester	226	C14H26O2	002146-71-6	22



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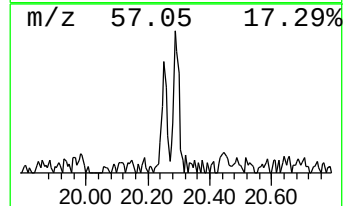
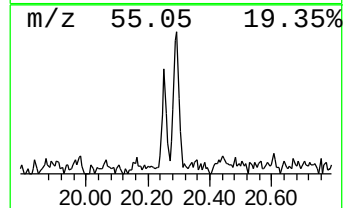
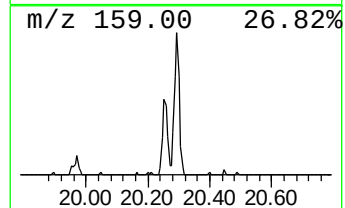
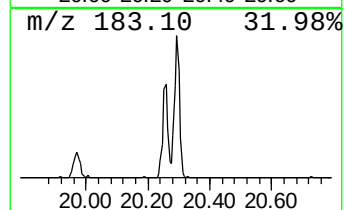
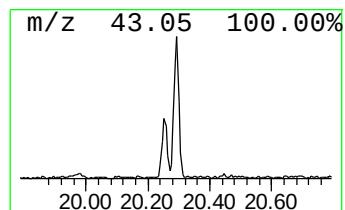
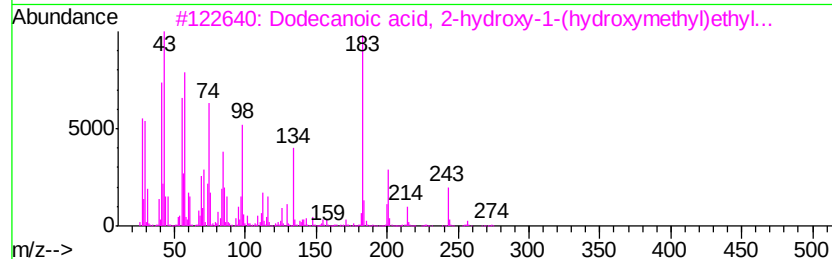
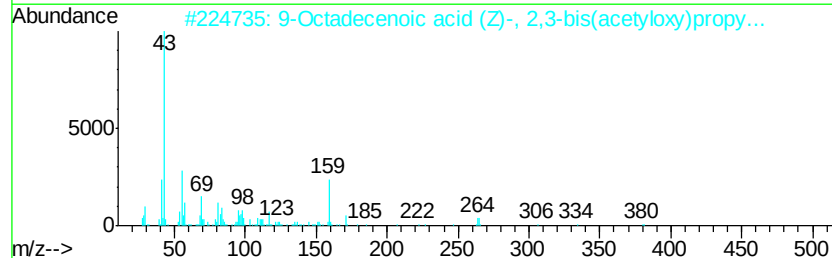
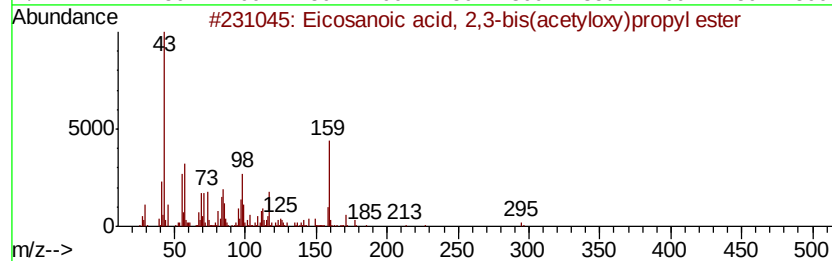
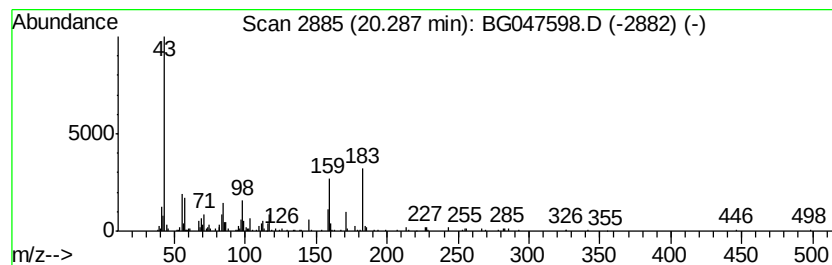
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.29	4.57 ng/ul	155865	Chrysene-d12	21.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	37
2		9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	16
3		Dodecanoic acid, 2-hydroxy-1-(hv...	274	C15H30O4	001678-45-1	12
4		Dodecanoic acid, ethenyl ester	226	C14H26O2	002146-71-6	10
5		Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	10



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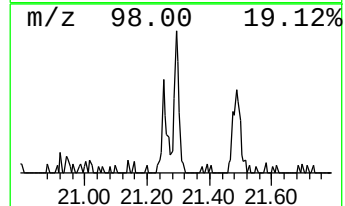
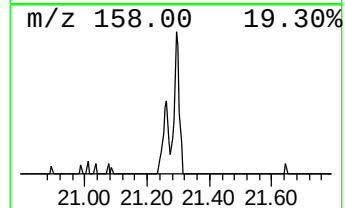
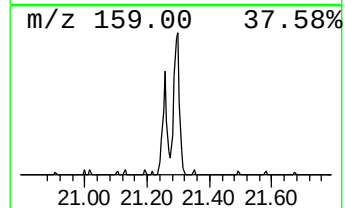
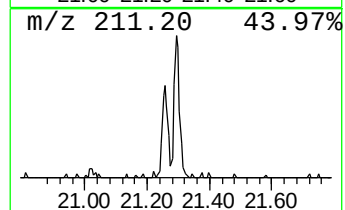
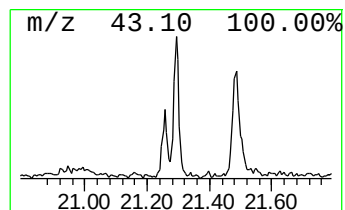
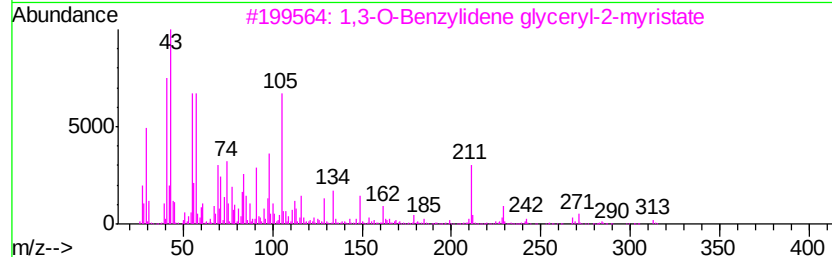
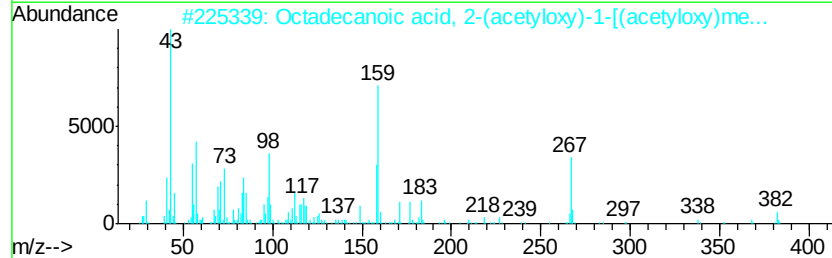
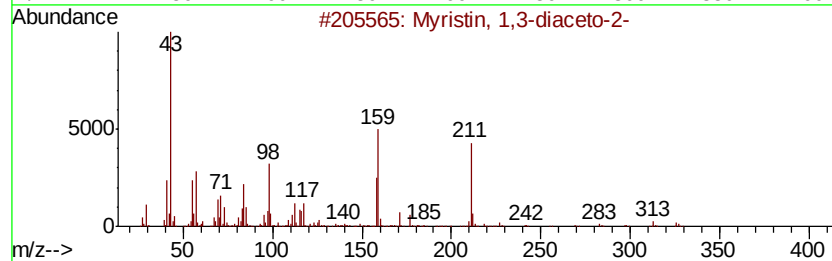
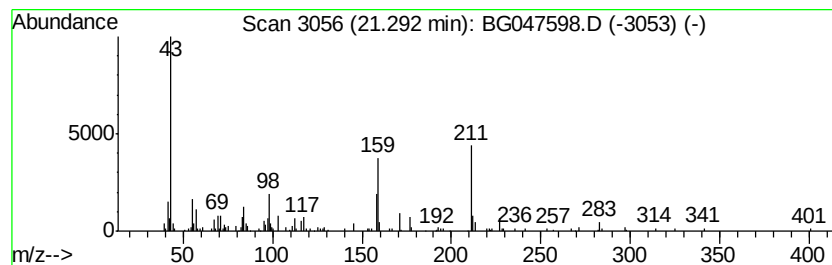
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Myristin, 1,3-diaceto-2- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.29	3.06 ng/ul	104344	Chrysene-d12	21.88		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	78	
2	Octadecanoic acid, 2-(acetyloxy)-1-	442	C25H46O6	055401-62-2	25	
3	1,3-O-Benzylidene glyceryl-2-myr...	374	C24H38O3	1000036-49-3	17	
4	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	12	
5	Eicosanoic acid, 2-(acetyloxy)-1-	470	C27H50O6	055429-68-0	10	



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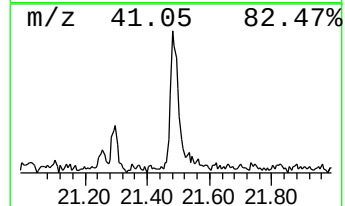
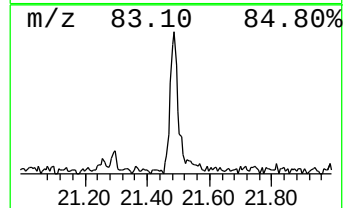
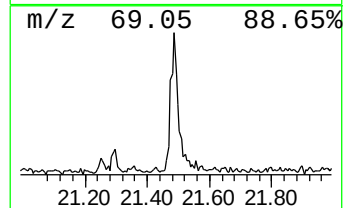
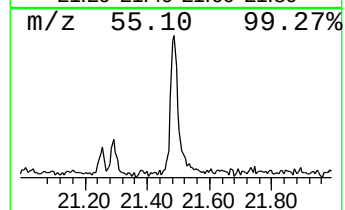
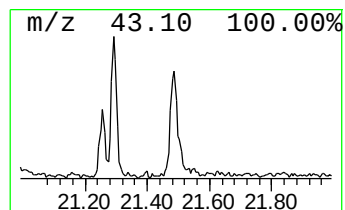
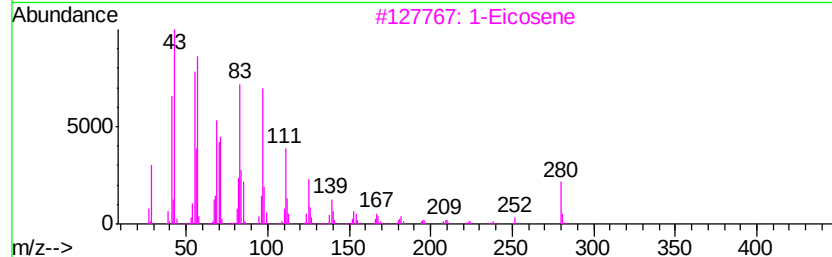
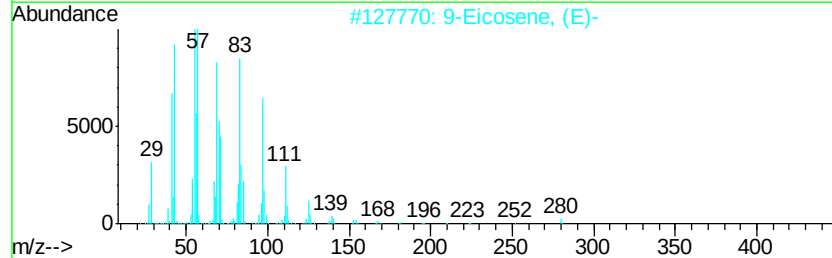
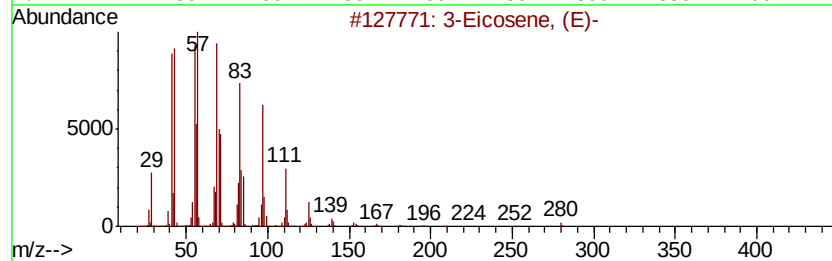
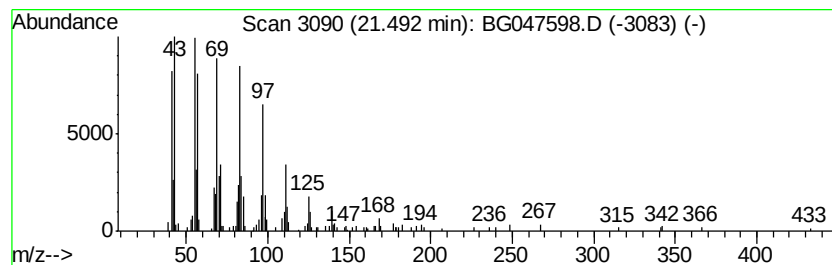
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.49	6.90 ng/ul	235509	Chrysene-d12	21.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-		280	C20H40	074685-33-9	94
2	9-Eicosene, (E)-		280	C20H40	074685-29-3	94
3	1-Eicosene		280	C20H40	003452-07-1	90
4	Cycloeicosane		280	C20H40	000296-56-0	86
5	5-Eicosene, (E)-		280	C20H40	074685-30-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120420\
Data File : BG047598.D
Acq On : 5 Dec 2020 9:48
Operator : CG/JU
Sample : L4864-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0BD4

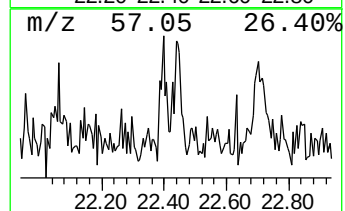
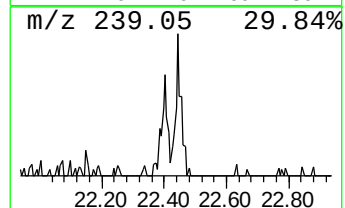
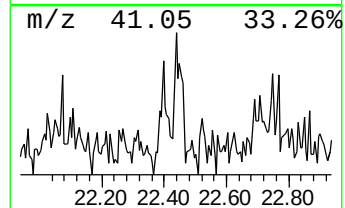
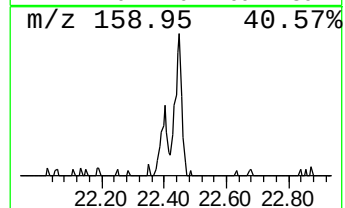
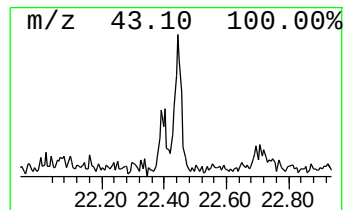
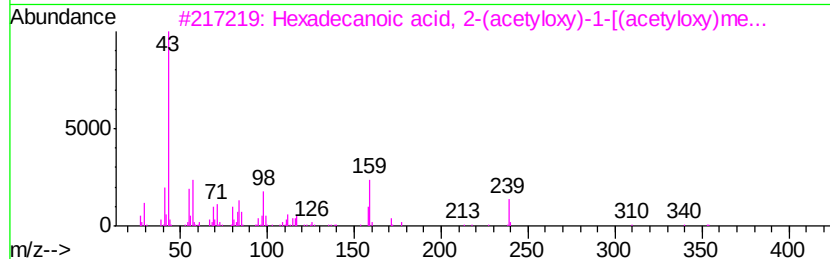
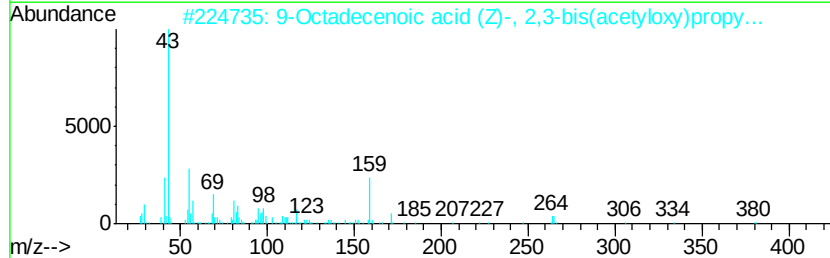
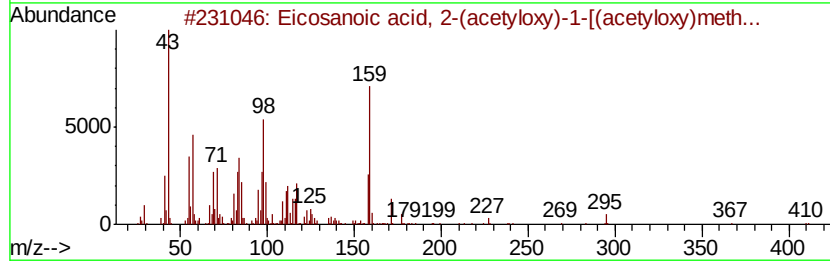
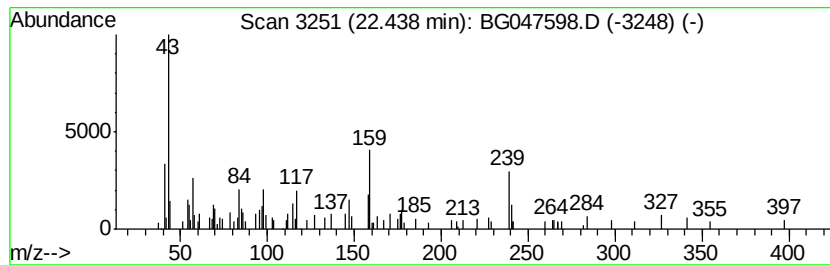
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-03 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.44	2.08 ng/ul	71081	Chrysene-d12	21.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	37	
2	9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	12	
3	Hexadecanoic acid, 2-(acetyloxy)...	414	C23H42O6	055268-69-4	10	
4	Hexadecanoic acid, 2-hydroxy-1-(...	330	C19H38O4	023470-00-0	9	
5	1,3-Dioxolane-4-methanol, 2,2-di...	174	C8H14O4	014739-11-8	9	



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120420\
Data File : BG047598.D
Acq On : 5 Dec 2020 9:48
Operator : CG/JU
Sample : L4864-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
C0BD4

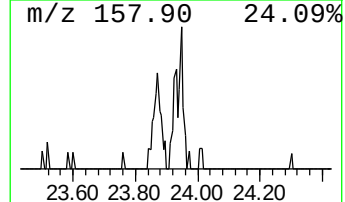
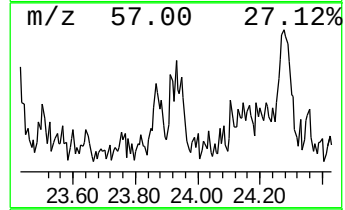
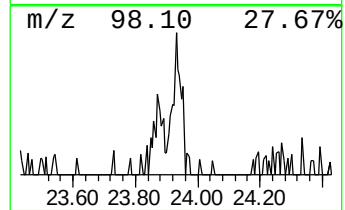
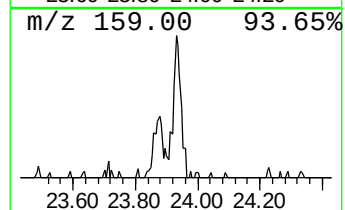
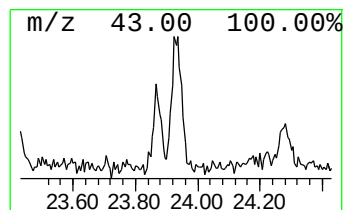
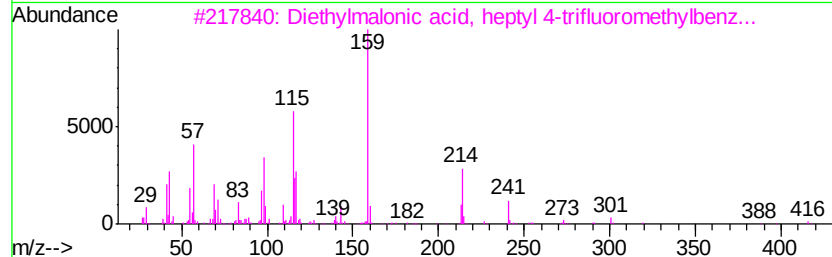
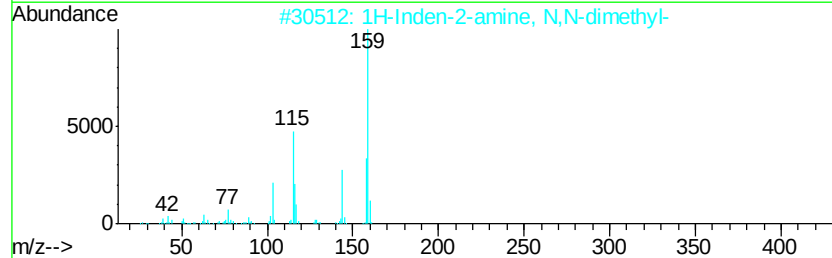
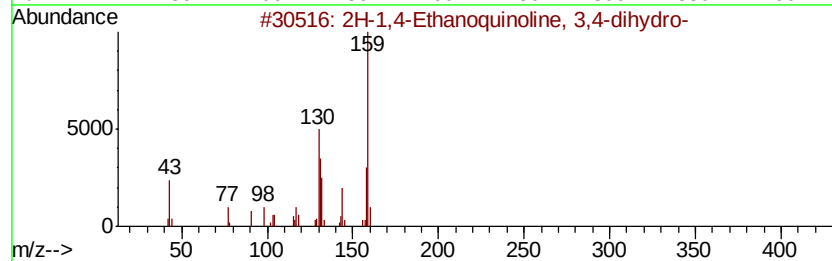
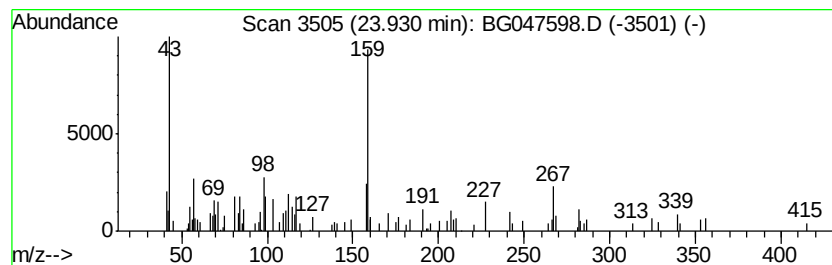
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-04 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	2.57 ng/ul	89642	Perylene-d12	25.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-1,4-Ethanoquinoline, 3,4-dihy...	159	C11H13N	004363-25-1	47
2		1H-Inden-2-amine, N,N-dimethyl-	159	C11H13N	035336-08-4	43
3		Diethylmalonic acid, heptyl 4-tr...	416	C22H31F3O4	1000368-40-5	38
4		2-Naphthalenecarboxylic acid, 1,...	250	C14H18O4	1000196-78-9	38
5		2,3,4-Trifluorobenzoic acid, 2-o...	288	C15H19F3O2	1000282-58-1	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG120420\
Data File : BG047598.D
Acq On : 5 Dec 2020 9:48
Operator : CG/JU
Sample : L4864-08
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0BD4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.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
unknown-01	20.25	2.6	ng/ul	89058	5	21.88	682318	20.0
unknown-02	20.29	4.6	ng/ul	155865	5	21.88	682318	20.0
Myristin, 1,3-dia...	21.29	3.1	ng/ul	104344	5	21.88	682318	20.0
(DEL) Alkane: Str...	21.49	6.9	ng/ul	235509	5	21.88	682318	20.0
unknown-03	22.44	2.1	ng/ul	71081	5	21.88	682318	20.0
unknown-04	23.93	2.6	ng/ul	89642	6	25.26	698047	20.0