

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120221\
 Data File : BG051331.D
 Acq On : 3 Dec 2021 16:00
 Operator : CG/JU
 Sample : M4833-18
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ESQN4

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
 Title : SVOA CALIBRATION

Signal : TIC: BG051331.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.530	3	7	14	rVB	5990	9327	1.30%	0.112%
2	3.824	53	57	68	rBV	10808	19896	2.77%	0.238%
3	3.965	77	81	95	rBV	41662	79642	11.11%	0.954%
4	4.076	95	100	107	rVB2	8304	14516	2.02%	0.174%
5	4.200	116	121	125	rVB2	5716	8451	1.18%	0.101%
6	4.311	135	140	143	rBV4	2218	4237	0.59%	0.051%
7	5.234	292	297	303	rVB5	2570	5503	0.77%	0.066%
8	6.849	567	572	577	rVV4	2180	4042	0.56%	0.048%
9	7.355	651	658	673	rVB	99102	187989	26.22%	2.252%
10	7.508	673	684	692	rBV	81962	141412	19.72%	1.694%
11	7.725	714	721	727	rVV	95257	170495	23.78%	2.043%
12	8.189	794	800	807	rBV	96046	163179	22.76%	1.955%
13	8.906	916	922	934	rBV	93341	172340	24.03%	2.065%
14	9.029	938	943	948	rVB2	2167	4339	0.61%	0.052%
15	9.370	994	1001	1009	rBV	104035	188840	26.34%	2.263%
16	10.093	1118	1124	1132	rBV	85115	156457	21.82%	1.875%
17	10.645	1211	1218	1230	rBV	111849	218905	30.53%	2.623%
18	10.757	1231	1237	1252	rBV	105269	202203	28.20%	2.423%
19	11.015	1274	1281	1289	rVB	134594	246322	34.35%	2.951%
20	11.156	1295	1305	1324	rVB	63590	137193	19.13%	1.644%
21	12.384	1505	1514	1519	rBV4	2448	4125	0.58%	0.049%
22	12.596	1544	1550	1554	rVB2	2273	3636	0.51%	0.044%
23	13.606	1719	1722	1728	rVB3	3624	5681	0.79%	0.068%
24	13.689	1728	1736	1745	rBV	42456	68052	9.49%	0.815%
25	14.217	1820	1826	1833	rBV	220128	339453	47.34%	4.067%
26	14.523	1870	1878	1886	rVB	268734	439514	61.29%	5.266%
27	14.676	1900	1904	1909	rVB	4204	5607	0.78%	0.067%
28	14.823	1922	1929	1937	rBV	224895	353830	49.34%	4.240%
29	15.052	1960	1968	1984	rBV2	55558	128082	17.86%	1.535%
30	15.193	1989	1992	1995	rVV3	2207	3889	0.54%	0.047%
31	15.246	1995	2001	2003	rVV6	4548	6969	0.97%	0.084%
32	15.627	2062	2066	2070	rVB3	4923	6307	0.88%	0.076%
33	15.815	2090	2098	2109	rVB	354382	550766	76.81%	6.599%
34	15.945	2115	2120	2129	rBV	69971	112446	15.68%	1.347%
35	16.027	2129	2134	2142	rVB4	3387	7526	1.05%	0.090%
36	16.256	2167	2173	2178	rVB3	3209	4652	0.65%	0.056%

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37	16.485	2207	2212	2213	rVV2	6343	7175	1.00%	0.086%
38	16.503	2213	2215	2221	rVV3	9037	13615	1.90%	0.163%
39	16.803	2261	2266	2269	rBV2	2786	4129	0.58%	0.049%
40	17.096	2312	2316	2321	rVB4	2510	3226	0.45%	0.039%
41	17.278	2343	2347	2351	rVB2	6976	8936	1.25%	0.107%
42	17.331	2351	2356	2360	rBV3	4264	7066	0.99%	0.085%
43	17.572	2391	2397	2403	rVV	287290	444591	62.00%	5.327%
44	17.613	2403	2404	2408	rVV2	3987	4056	0.57%	0.049%
45	17.672	2408	2414	2422	rVV	380686	581674	81.12%	6.970%
46	17.754	2424	2428	2432	rVB5	3822	5138	0.72%	0.062%
47	17.819	2434	2439	2442	rBV5	1930	2769	0.39%	0.033%
48	17.937	2453	2459	2461	rBV5	2065	3304	0.46%	0.040%
49	18.019	2467	2473	2479	rBV2	5154	8480	1.18%	0.102%
50	18.166	2492	2498	2499	rVV5	3861	5991	0.84%	0.072%
51	18.195	2499	2503	2509	rVV	26529	35499	4.95%	0.425%
52	18.512	2552	2557	2558	rBV2	2164	3084	0.43%	0.037%
53	18.624	2572	2576	2582	rBV3	10943	13764	1.92%	0.165%
54	18.683	2582	2586	2588	rVV3	6548	8027	1.12%	0.096%
55	18.706	2588	2590	2598	rVB4	5943	9293	1.30%	0.111%
56	18.835	2610	2612	2617	rVV5	1687	2767	0.39%	0.033%
57	18.906	2619	2624	2628	rVV4	7964	10614	1.48%	0.127%
58	18.953	2630	2632	2638	rVV5	3134	4680	0.65%	0.056%
59	19.012	2638	2642	2645	rVB3	1924	3218	0.45%	0.039%
60	19.047	2645	2648	2651	rBV3	2560	3744	0.52%	0.045%
61	19.082	2651	2654	2657	rVB2	6614	7687	1.07%	0.092%
62	19.288	2684	2689	2690	rBV2	2515	2634	0.37%	0.032%
63	19.329	2692	2696	2698	rBV3	10334	13980	1.95%	0.168%
64	19.358	2698	2701	2704	rVV	77481	85952	11.99%	1.030%
65	19.388	2704	2706	2710	rVB4	11379	11915	1.66%	0.143%
66	19.435	2710	2714	2717	rBV3	15294	16828	2.35%	0.202%
67	19.482	2717	2722	2726	rBV2	29138	47983	6.69%	0.575%
68	19.588	2737	2740	2743	rVV2	6806	8548	1.19%	0.102%
69	19.623	2743	2746	2750	rVB	6505	8472	1.18%	0.102%
70	19.687	2750	2757	2759	rBV7	8784	13999	1.95%	0.168%
71	19.734	2763	2765	2771	rVB7	8374	10545	1.47%	0.126%
72	19.799	2773	2776	2782	rBV6	4956	7553	1.05%	0.090%
73	19.899	2789	2793	2796	rBV4	5871	8442	1.18%	0.101%
74	19.952	2796	2802	2815	rVB	488287	717066	100.00%	8.592%
75	20.075	2819	2823	2826	rBV6	4393	6101	0.85%	0.073%
76	20.128	2830	2832	2835	rVB4	3106	2668	0.37%	0.032%

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77	20.181	2838	2841	2848	rVB7	9030	12986	1.81%	0.156%
78	20.234	2848	2850	2853	rBV4	3103	3920	0.55%	0.047%
79	20.434	2880	2884	2887	rBV5	9005	11766	1.64%	0.141%
80	20.498	2892	2895	2899	rVB4	8634	11732	1.64%	0.141%
81	20.551	2901	2904	2909	rBV7	5337	7943	1.11%	0.095%
82	20.627	2911	2917	2920	rBV7	6744	11243	1.57%	0.135%
83	20.716	2928	2932	2933	rBV4	8547	9332	1.30%	0.112%
84	20.774	2940	2942	2946	rBV4	5591	5582	0.78%	0.067%
85	20.933	2966	2969	2973	rVB6	6275	6912	0.96%	0.083%
86	21.462	3055	3059	3060	rBV3	12513	14400	2.01%	0.173%
87	21.709	3099	3101	3106	rVB4	7314	9178	1.28%	0.110%
88	21.873	3122	3129	3138	rBV	263054	460180	64.18%	5.514%
89	22.649	3256	3261	3267	rBV4	11508	18342	2.56%	0.220%
90	23.371	3379	3384	3390	rVB3	13531	24398	3.40%	0.292%
91	23.571	3411	3418	3426	rVB2	37567	82908	11.56%	0.993%
92	23.747	3443	3448	3453	rVB6	13336	25058	3.49%	0.300%
93	24.211	3521	3527	3536	rVB3	24294	56994	7.95%	0.683%
94	25.034	3656	3667	3678	rBV	209081	620131	86.48%	7.430%
95	25.269	3689	3707	3718	rBV3	149718	481854	67.20%	5.774%
96	26.391	3890	3898	3909	rVB4	24377	72276	10.08%	0.866%
97	27.255	4043	4045	4049	rBV5	2565	4347	0.61%	0.052%
98	27.813	4134	4140	4150	rVB4	15047	46698	6.51%	0.560%
99	29.517	4428	4430	4431	rBV2	4610	3707	0.52%	0.044%
100	31.215	4716	4719	4720	rBV3	2655	2971	0.41%	0.036%

Sum of corrected areas: 8345894

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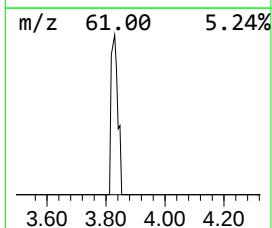
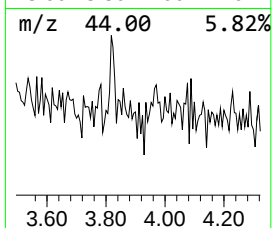
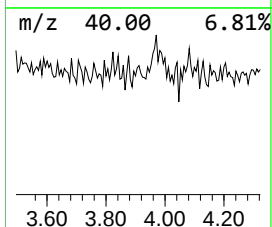
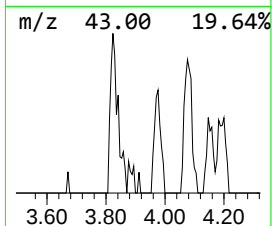
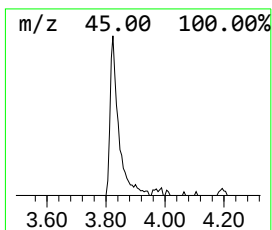
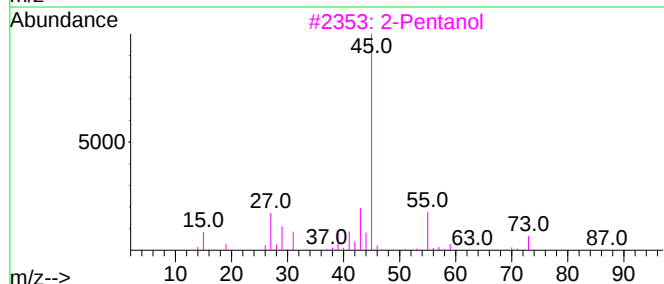
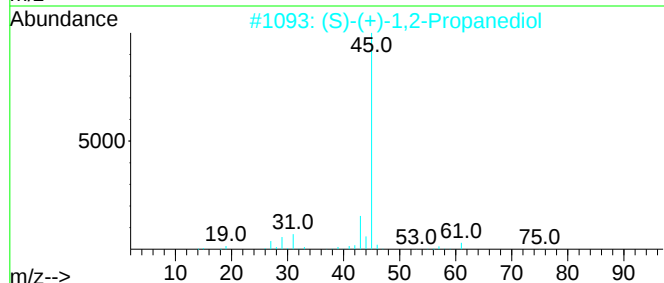
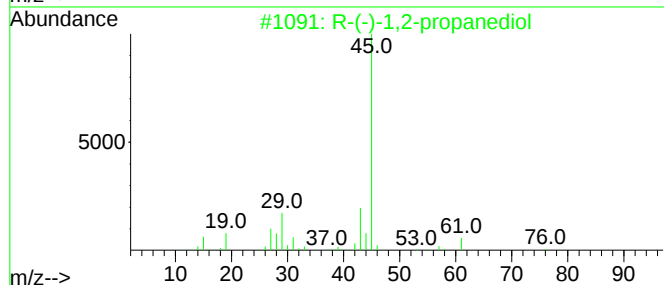
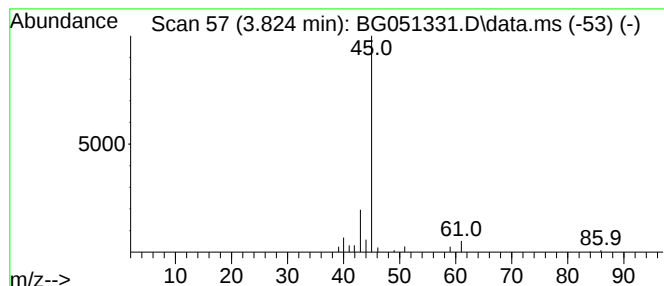
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.824	2.44 ng/ul	19896	1,4-Dichlorobenzene-d4	8.189

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	43
3	2-Pentanol			88	C5H12O	006032-29-7	40
4	Butanenitrile, 2-(methoxymethoxy)			129	C6H11NO2	1000196-86-5	9
5	Propylene Glycol			76	C3H8O2	000057-55-6	9



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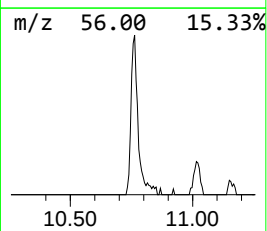
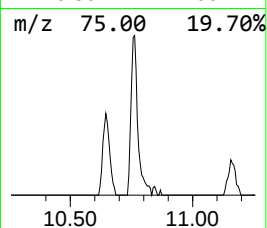
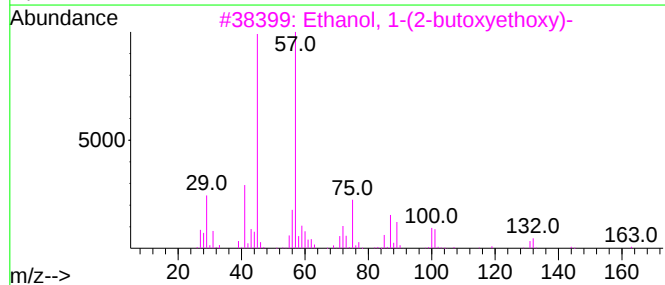
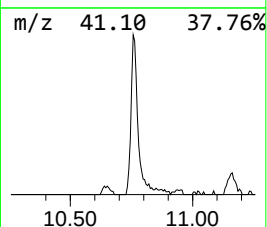
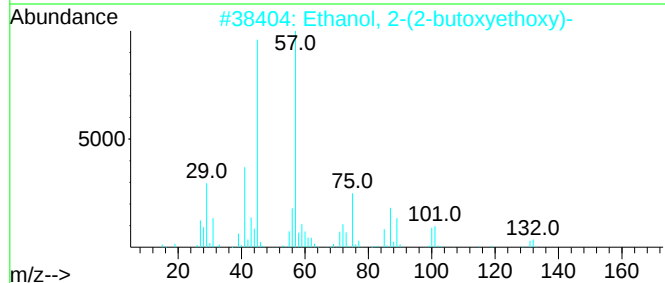
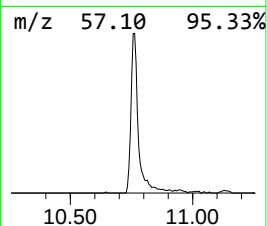
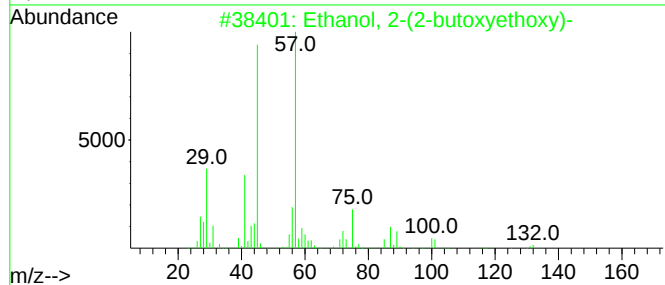
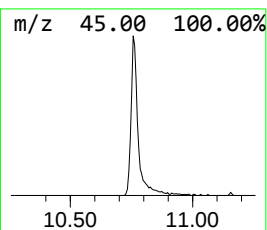
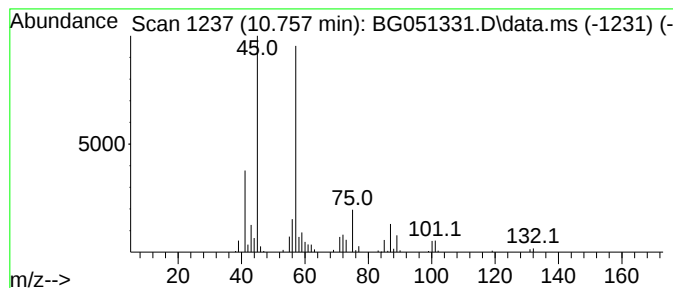
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	16.42 ng/ul	202203	Naphthalene-d8	11.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
4			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
5			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83



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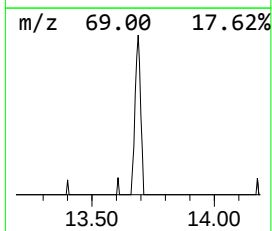
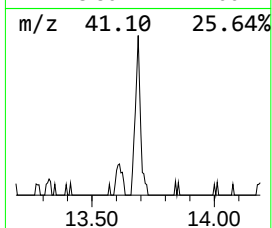
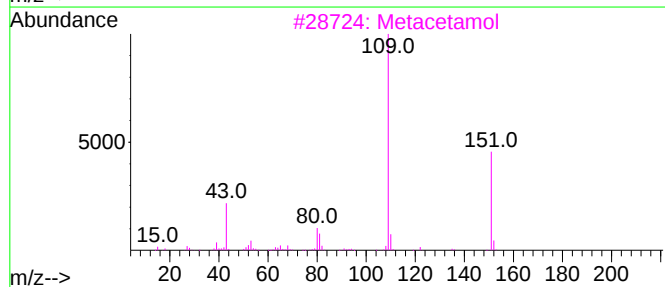
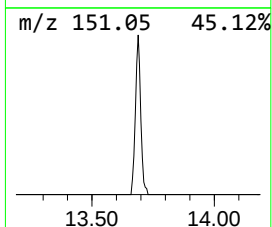
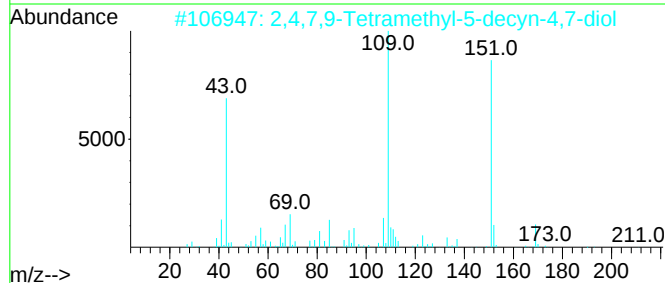
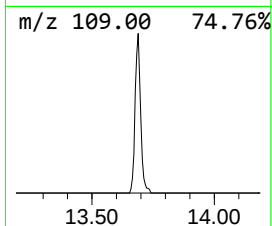
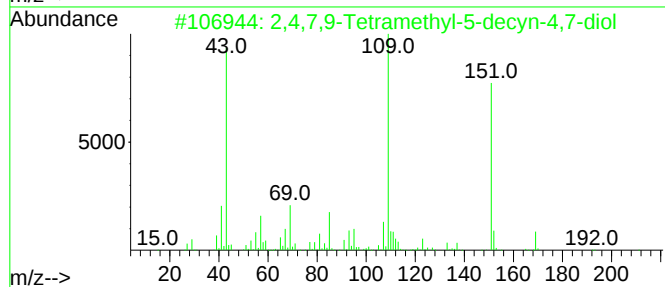
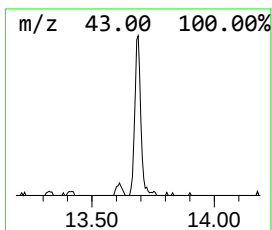
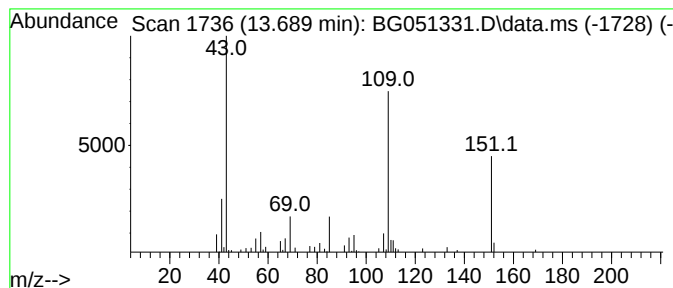
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	3.85 ng/ul	68052	Acenaphthene-d10	14.823

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91		
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90		
3	Metacetamol	151	C8H9NO2	000621-42-1	58		
4	Metacetamol	151	C8H9NO2	000621-42-1	53		
5	Metacetamol	151	C8H9NO2	000621-42-1	53		



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ClientSampleId :
ESQN4

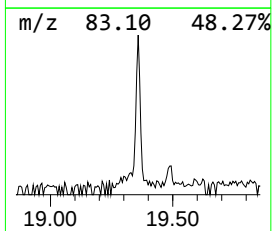
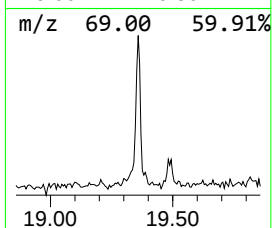
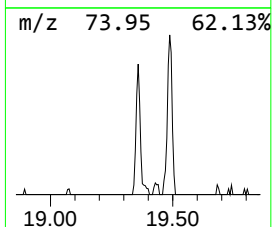
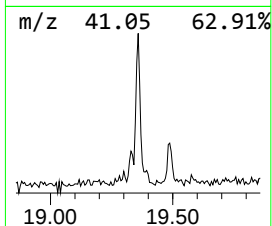
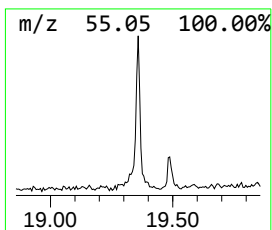
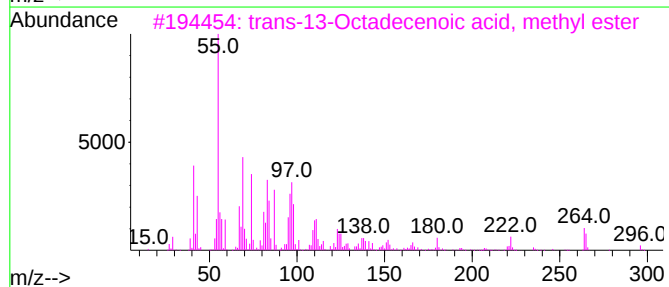
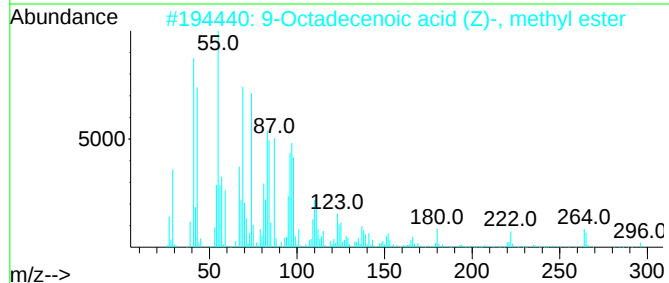
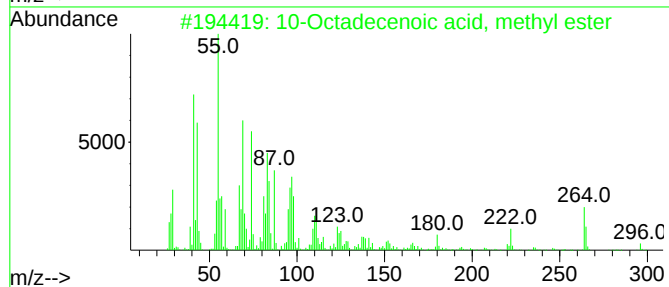
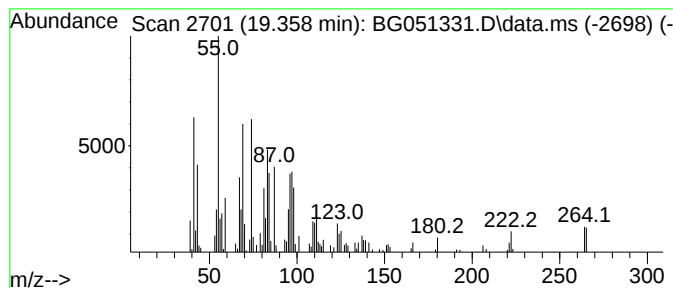
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 10-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.358	3.87 ng/ul	85952	Phenanthrene-d10	17.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
4			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5			6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120221\
Data File : BG051331.D
Acq On : 3 Dec 2021 16:00
Operator : CG/JU
Sample : M4833-18
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ESQN4

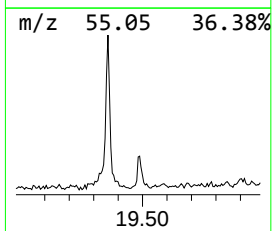
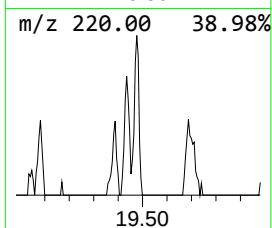
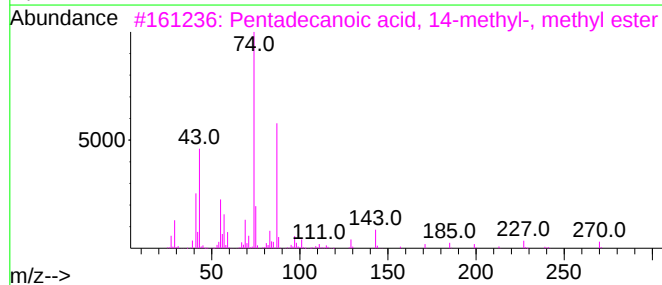
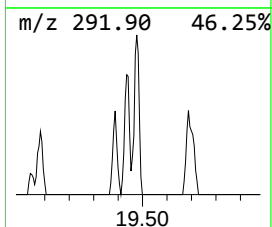
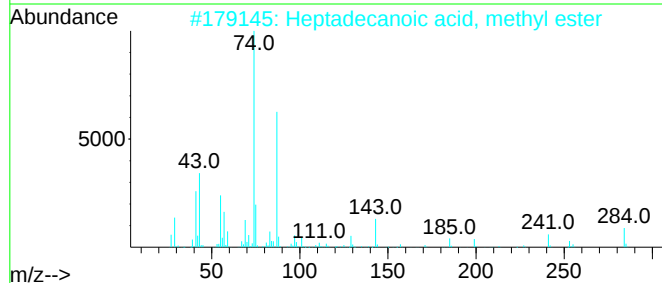
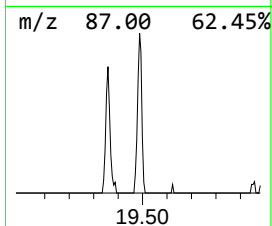
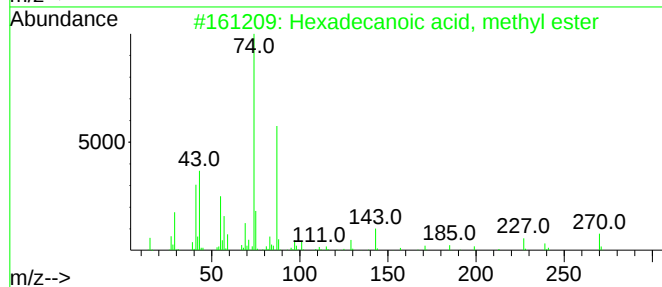
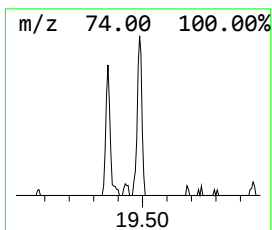
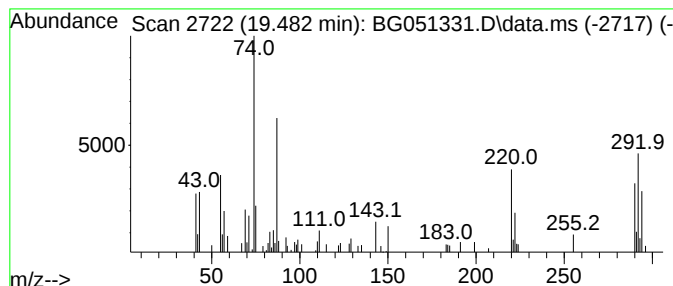
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.482	2.16 ng/ul	47983	Phenanthrene-d10	17.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	30
2			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	30
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	30
4			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	30
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120221\
Data File : BG051331.D
Acq On : 3 Dec 2021 16:00
Operator : CG/JU
Sample : M4833-18
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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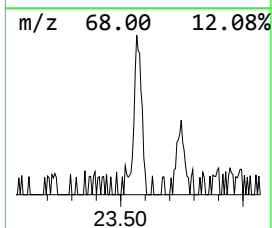
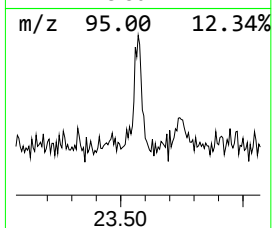
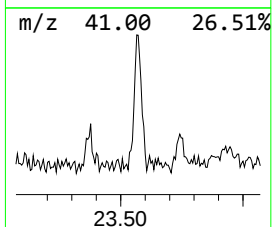
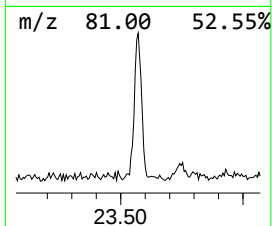
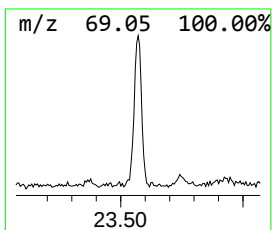
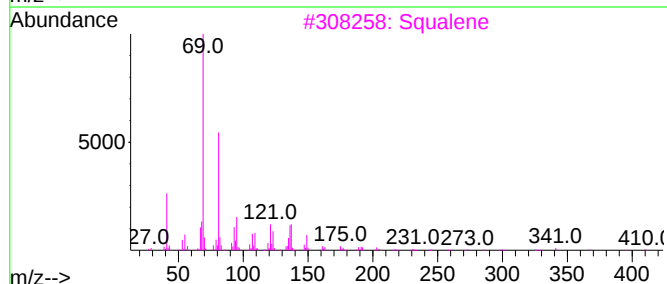
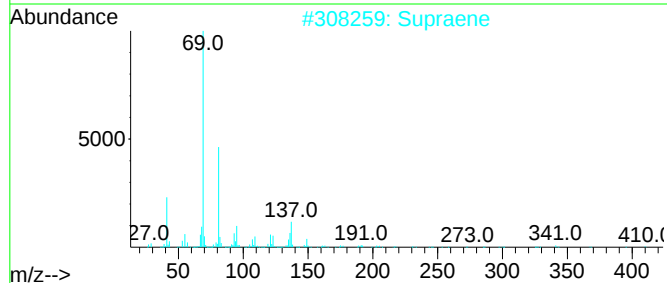
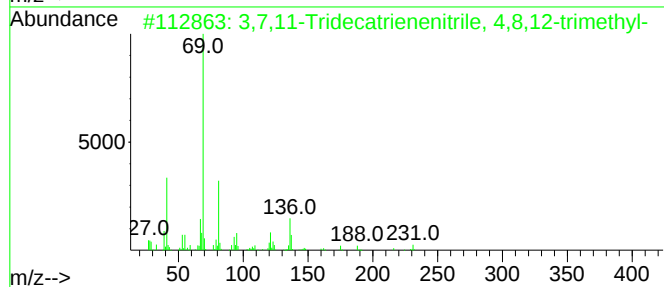
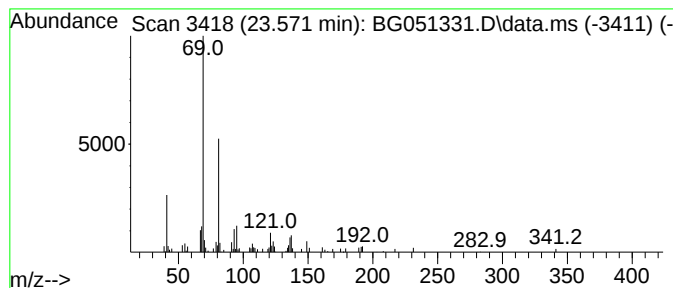
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3,7,11-Tridecatrienitrile... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.571	3.60 ng/ul	82908	Chrysene-d12	21.873

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	87		
2	Supraene	410	C30H50	007683-64-9	86		
3	Squalene	410	C30H50	000111-02-4	83		
4	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64		
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120221\
Data File : BG051331.D
Acq On : 3 Dec 2021 16:00
Operator : CG/JU
Sample : M4833-18
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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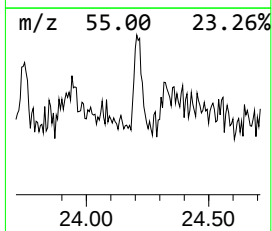
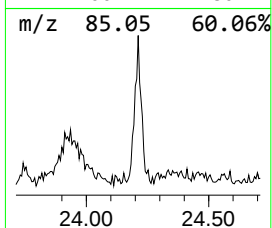
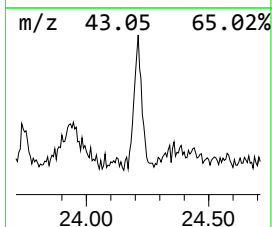
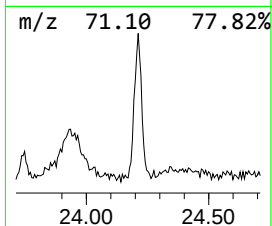
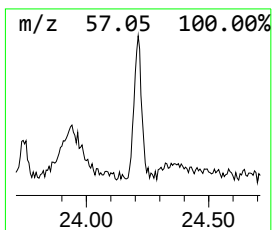
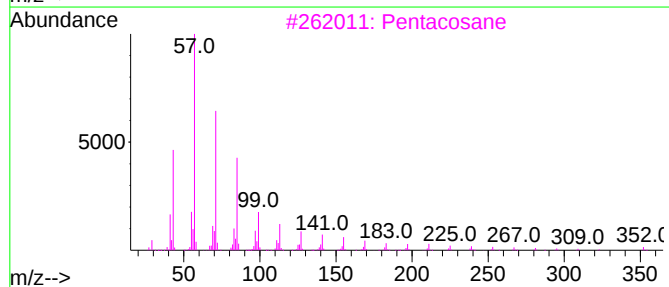
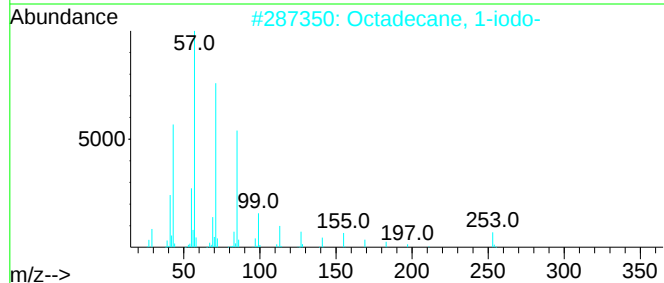
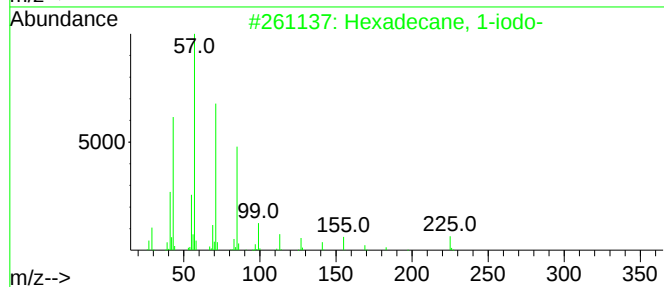
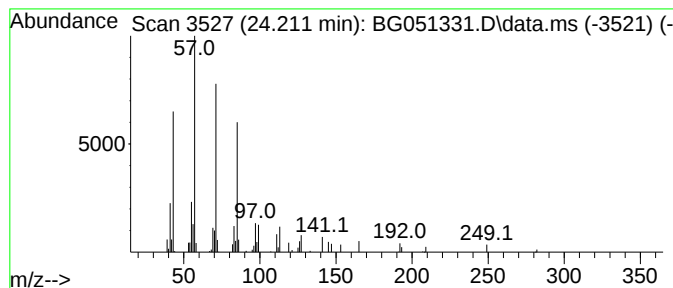
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.212	2.37 ng/ul	56994	Perylene-d12	25.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
3			Pentacosane	352	C25H52	000629-99-2	80
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5			Eicosane	282	C20H42	000112-95-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120221\
Data File : BG051331.D
Acq On : 3 Dec 2021 16:00
Operator : CG/JU
Sample : M4833-18
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ESQN4

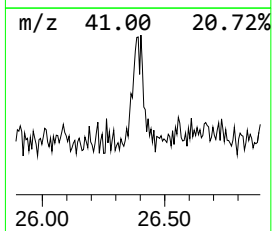
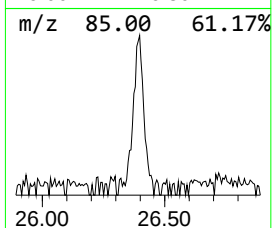
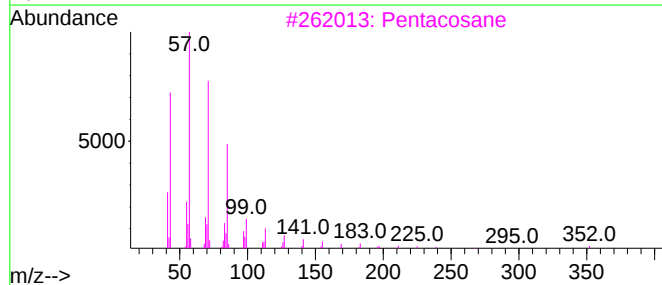
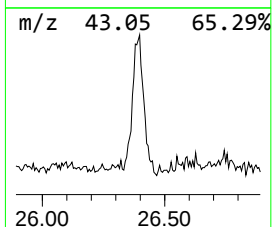
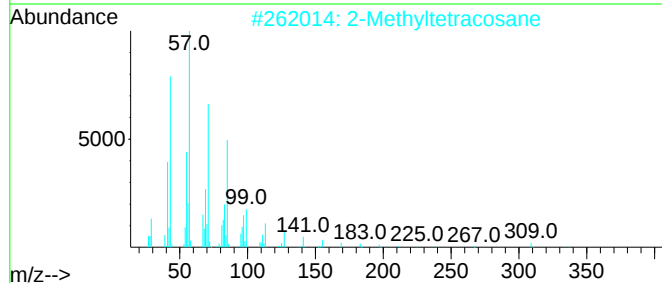
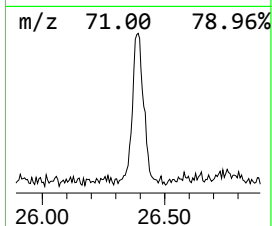
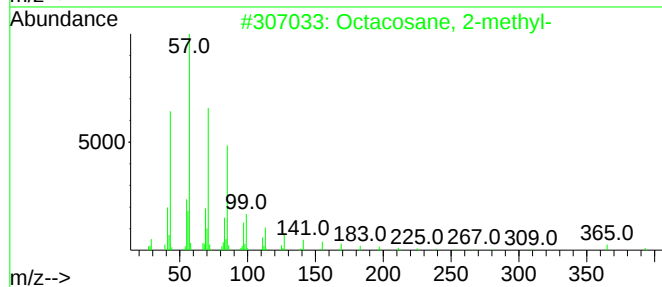
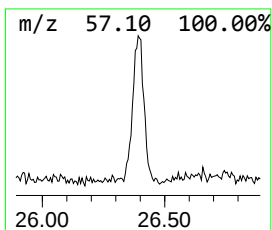
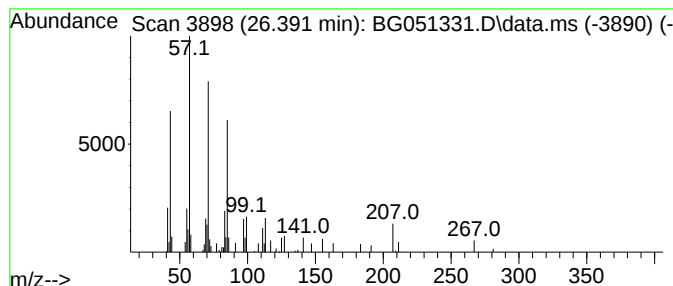
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.391	3.00 ng/ul	72276	Perylene-d12	25.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2			2-Methyltetracosane	352	C25H52	001560-78-7	90
3			Pentacosane	352	C25H52	000629-99-2	87
4			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	86
5			Tetratetracontane	619	C44H90	007098-22-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG120221\
Data File : BG051331.D
Acq On : 3 Dec 2021 16:00
Operator : CG/JU
Sample : M4833-18
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ESQN4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG112321.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Ethanol, 2-(2-b...	10.757	16.4	ng/ul	202203	2	11.021	246322	20.0
2,4,7,9-Tetrame...	13.688	3.9	ng/ul	68052	3	14.823	353830	20.0
10-Octadecenoic...	19.358	3.9	ng/ul	85952	4	17.572	444591	20.0
unknown-02	19.482	2.2	ng/ul	47983	4	17.572	444591	20.0
3,7,11-Tridecat...	23.571	3.6	ng/ul	82908	5	21.873	460180	20.0
Hexadecane, 1-i...	24.212	2.4	ng/ul	56994	6	25.269	481854	20.0
(DEL) Alkane: S...	26.391	3.0	ng/ul	72276	6	25.269	481854	20.0