

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
 Data File : BG058220.D
 Acq On : 14 Jul 2023 6:40
 Operator : CG/JU
 Sample : 03418-14
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A46J3

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-BG070123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG058220.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.349	40	44	51	rVB	17068	24726	1.02%	0.096%
2	3.755	108	113	128	rBV	235882	403288	16.65%	1.572%
3	3.866	128	132	142	rVV	13742	25453	1.05%	0.099%
4	3.931	142	143	150	rVB5	2396	3255	0.13%	0.013%
5	3.996	150	154	157	rVB3	4032	5150	0.21%	0.020%
6	4.090	166	170	175	rVB6	4961	8248	0.34%	0.032%
7	4.313	203	208	213	rVB2	15439	21483	0.89%	0.084%
8	4.718	273	277	282	rVB3	3301	4568	0.19%	0.018%
9	5.000	319	325	332	rBV4	2597	5946	0.25%	0.023%
10	5.088	332	340	346	rBV4	4572	8796	0.36%	0.034%
11	6.910	646	650	651	rBV2	2014	2583	0.11%	0.010%
12	7.068	667	677	692	rBV	301860	546088	22.54%	2.129%
13	7.227	697	704	719	rVB	233613	402247	16.60%	1.568%
14	7.433	732	739	750	rBV	279875	490448	20.24%	1.912%
15	7.903	812	819	835	rVB	214806	372205	15.36%	1.451%
16	8.608	931	939	955	rBV	361968	661862	27.32%	2.580%
17	9.060	1009	1016	1029	rBV	292414	540620	22.32%	2.108%
18	9.219	1038	1043	1048	rVB6	2409	4060	0.17%	0.016%
19	9.783	1131	1139	1149	rBV	247425	450070	18.58%	1.755%
20	10.323	1224	1231	1241	rBV	384573	692422	28.58%	2.699%
21	10.705	1287	1296	1306	rBV	329372	610801	25.21%	2.381%
22	10.841	1312	1319	1334	rBV	346943	666906	27.53%	2.600%
23	12.115	1532	1536	1542	rVB2	2170	4094	0.17%	0.016%
24	12.180	1542	1547	1552	rBV3	2596	4658	0.19%	0.018%
25	12.286	1562	1565	1575	rVB3	5750	10642	0.44%	0.041%
26	12.885	1663	1667	1673	rBV4	3259	6064	0.25%	0.024%
27	13.073	1696	1699	1703	rVB3	2227	3281	0.14%	0.013%
28	13.138	1703	1710	1715	rVB2	5217	7447	0.31%	0.029%
29	13.361	1742	1748	1752	rVB4	3385	5830	0.24%	0.023%
30	13.420	1754	1758	1763	rBV4	6216	10420	0.43%	0.041%
31	13.943	1840	1847	1855	rBV	727143	1078162	44.50%	4.203%
32	14.007	1856	1858	1862	rVB3	4840	6431	0.27%	0.025%
33	14.054	1864	1866	1873	rVB4	2666	4913	0.20%	0.019%
34	14.172	1882	1886	1887	rBV2	3363	2811	0.12%	0.011%
35	14.237	1890	1897	1906	rBV	842817	1361933	56.22%	5.310%
36	14.372	1915	1920	1925	rVB6	4165	7051	0.29%	0.027%

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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-BG070123.MA.M
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37	14.425	1925	1929	1934	rBV4	5328	7958	0.33%	0.031%
38	14.495	1939	1941	1942	rBV2	3140	3018	0.12%	0.012%
39	14.536	1942	1948	1957	rVB	551539	897495	37.05%	3.499%
40	14.660	1962	1969	1973	rBV	16925	29393	1.21%	0.115%
41	14.742	1976	1983	2000	rBV	278348	539709	22.28%	2.104%
42	14.889	2006	2008	2011	rBV4	3575	3706	0.15%	0.014%
43	14.947	2014	2018	2027	rVB10	13140	25645	1.06%	0.100%
44	15.047	2032	2035	2039	rBV6	3930	6046	0.25%	0.024%
45	15.188	2057	2059	2064	rVB5	2931	4041	0.17%	0.016%
46	15.247	2067	2069	2076	rVB7	3803	7699	0.32%	0.030%
47	15.323	2078	2082	2084	rBV5	11779	16025	0.66%	0.062%
48	15.470	2104	2107	2111	rBV5	6862	10536	0.43%	0.041%
49	15.529	2111	2117	2125	rBV	1096011	1746130	72.08%	6.807%
50	15.653	2132	2138	2149	rVB	325730	517808	21.37%	2.019%
51	15.788	2156	2161	2167	rVB	56301	87659	3.62%	0.342%
52	15.893	2174	2179	2184	rBV	158941	226626	9.35%	0.884%
53	16.452	2271	2274	2279	rBV	20700	28052	1.16%	0.109%
54	16.510	2280	2284	2289	rVV	44910	67535	2.79%	0.263%
55	16.810	2332	2335	2340	rBV7	27098	40474	1.67%	0.158%
56	17.192	2397	2400	2404	rVB3	35967	46416	1.92%	0.181%
57	17.286	2410	2416	2421	rBV	745687	1154993	47.67%	4.503%
58	17.386	2427	2433	2441	rVB	1128587	1712922	70.70%	6.678%
59	17.462	2442	2446	2451	rVB4	58988	85516	3.53%	0.333%
60	17.868	2512	2515	2522	rVB4	29516	50636	2.09%	0.197%
61	18.173	2562	2567	2577	rBV	266221	455356	18.80%	1.775%
62	19.336	2762	2765	2769	rVB	65621	90201	3.72%	0.352%
63	19.442	2780	2783	2788	rBV2	58083	75238	3.11%	0.293%
64	19.677	2817	2823	2837	rVB	1411757	2250023	92.87%	8.772%
65	20.694	2992	2996	2999	rVB	53791	63690	2.63%	0.248%
66	21.187	3075	3080	3090	rBV	167795	344350	14.21%	1.342%
67	21.422	3117	3120	3126	rVB2	38809	55874	2.31%	0.218%
68	21.540	3132	3140	3146	rBV	707766	1308455	54.01%	5.101%
69	21.716	3167	3170	3176	rVB2	42184	60748	2.51%	0.237%
70	22.245	3257	3260	3266	rBV3	27593	44984	1.86%	0.175%
71	22.304	3266	3270	3277	rBV	55450	95478	3.94%	0.372%
72	22.973	3379	3384	3394	rVB2	55954	118048	4.87%	0.460%
73	23.684	3497	3505	3508	rBV3	26628	70014	2.89%	0.273%
74	23.755	3511	3517	3527	rVB2	121418	272093	11.23%	1.061%
75	24.472	3628	3639	3661	rVB2	805554	2422654	100.00%	9.445%
76	24.683	3664	3675	3689	rVV	536831	1518293	62.67%	5.919%

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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

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Peak separation: 5

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77	25.770	3851	3860	3870	rBV2	76598	228432	9.43%	0.891%
78	27.080	4075	4083	4099	rVB3	65617	231610	9.56%	0.903%
79	28.661	4344	4352	4366	rVB5	42930	163898	6.77%	0.639%

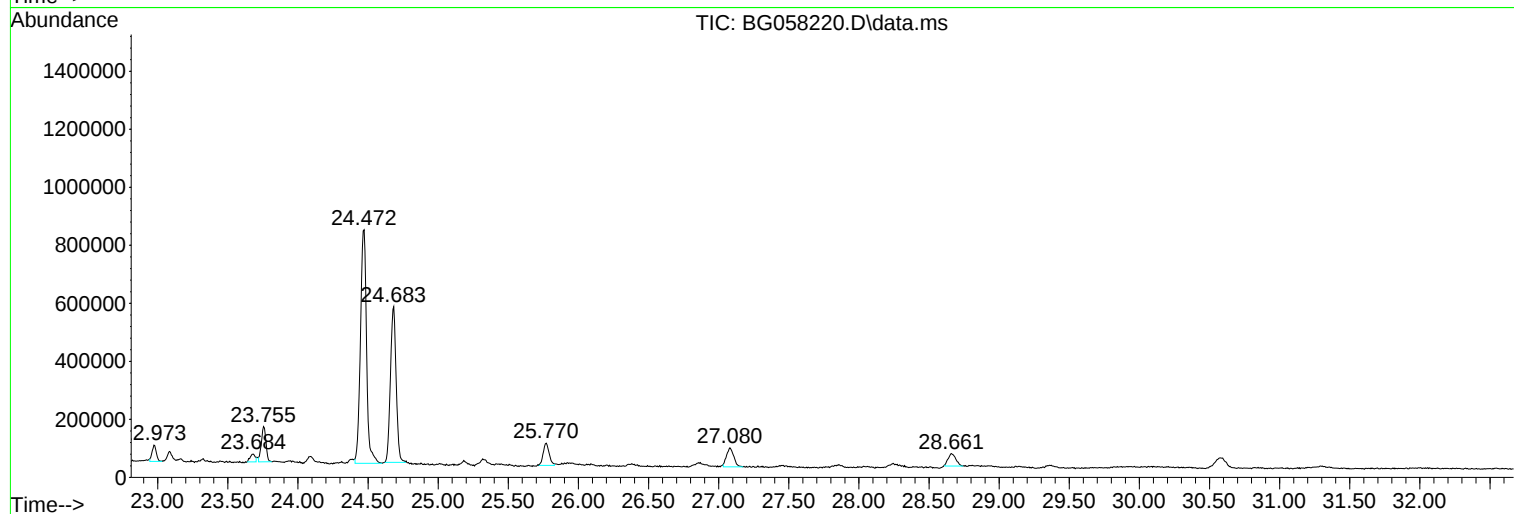
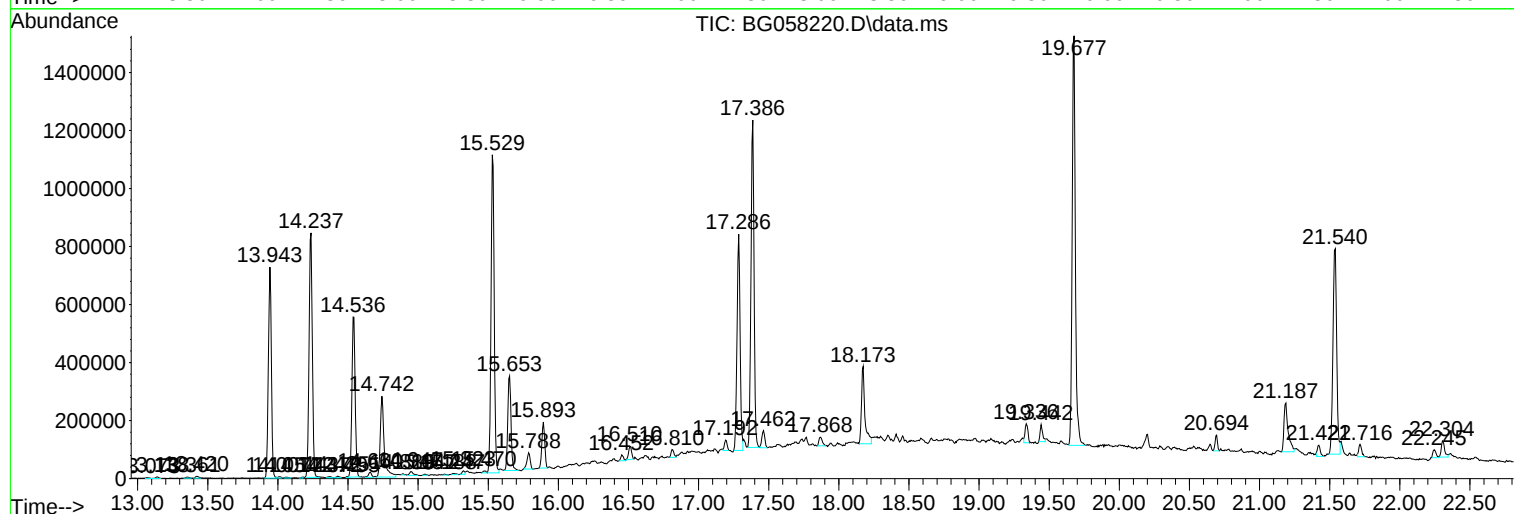
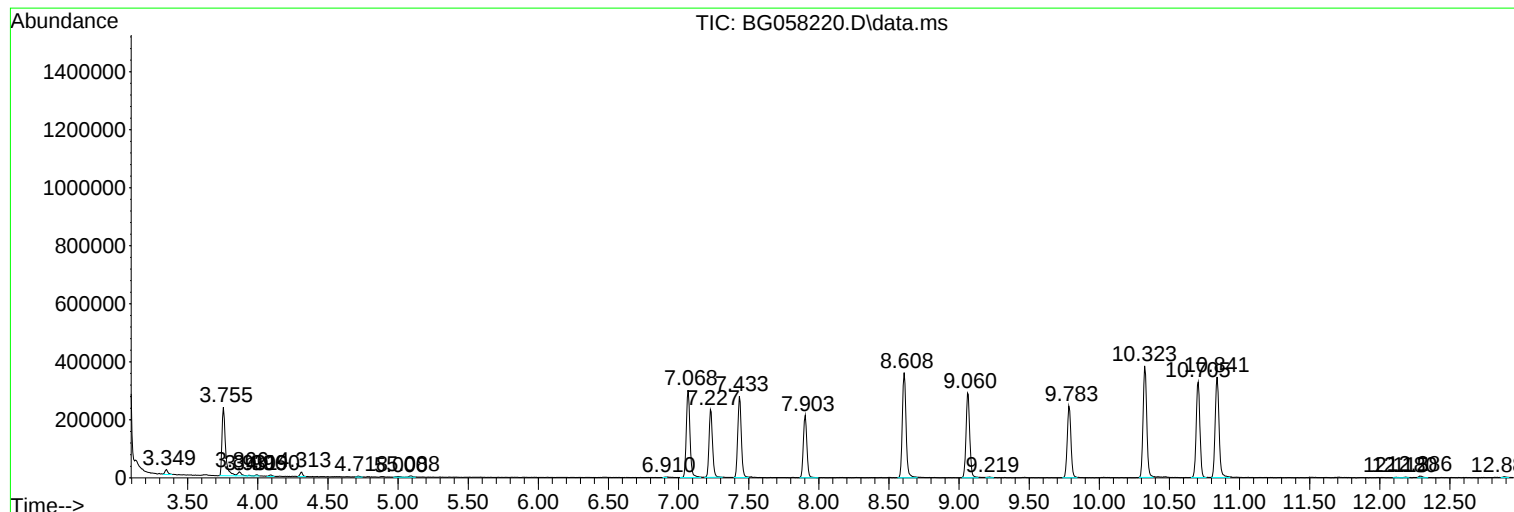
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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



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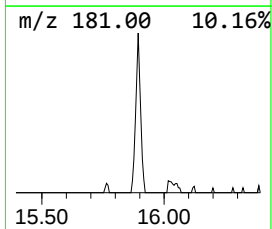
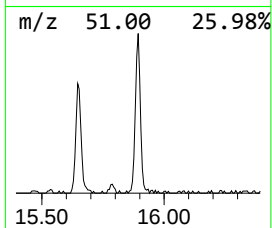
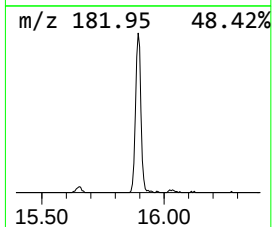
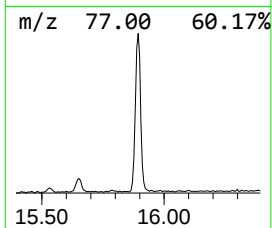
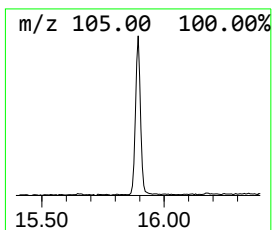
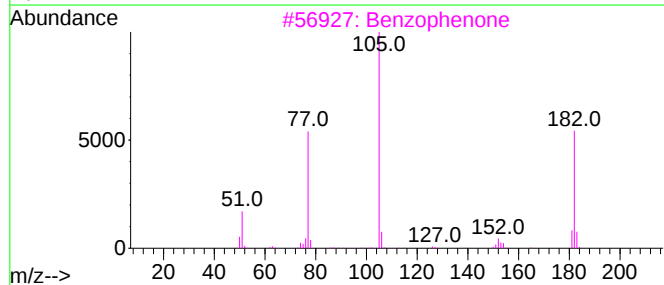
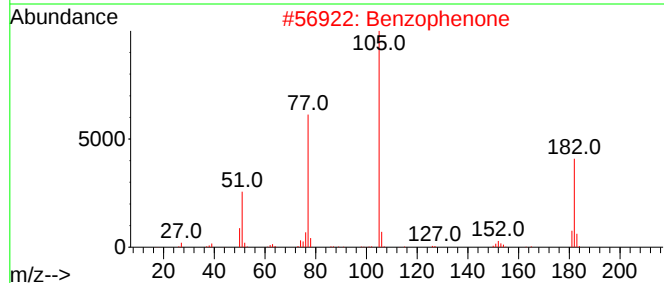
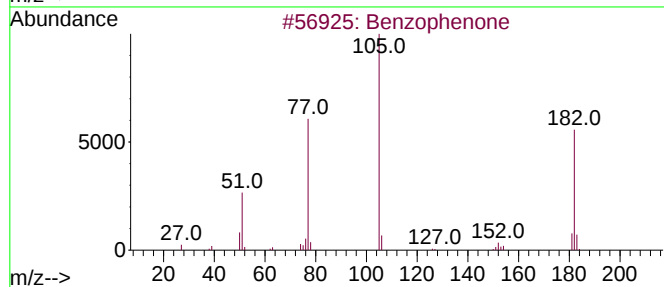
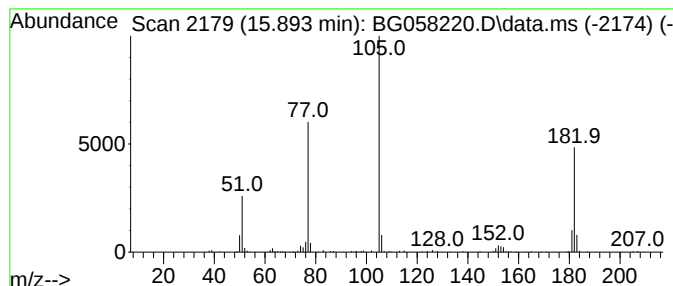
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.893	5.05 ng/ul	226626	Acenaphthene-d10	14.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzophenone	182	C13H10O	000119-61-9	96
3			Benzophenone	182	C13H10O	000119-61-9	95
4			Benzophenone	182	C13H10O	000119-61-9	94
5			Benzophenone	182	C13H10O	000119-61-9	86



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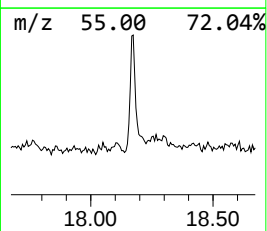
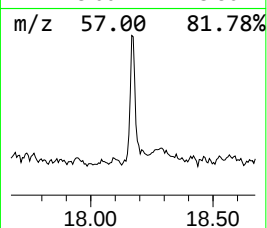
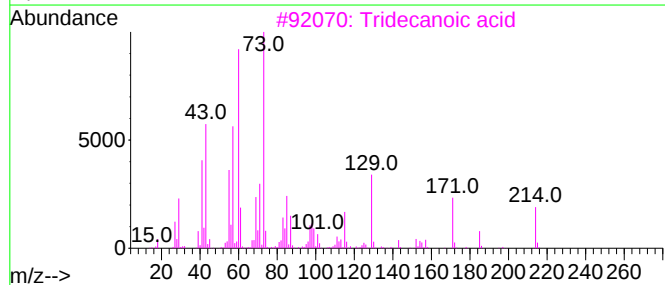
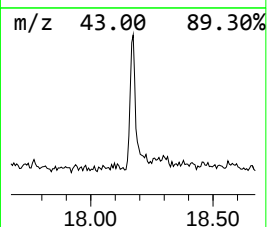
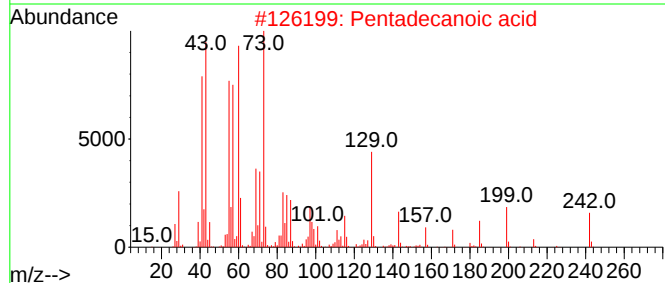
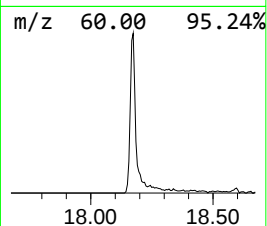
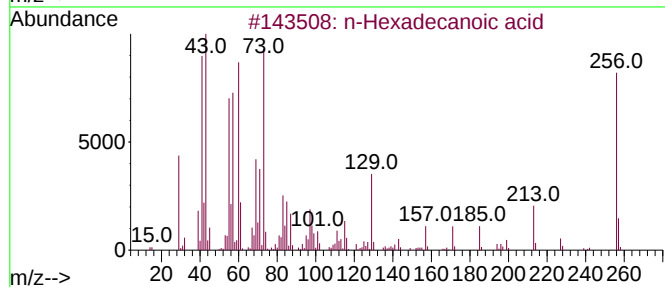
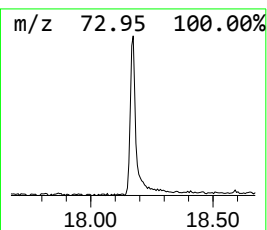
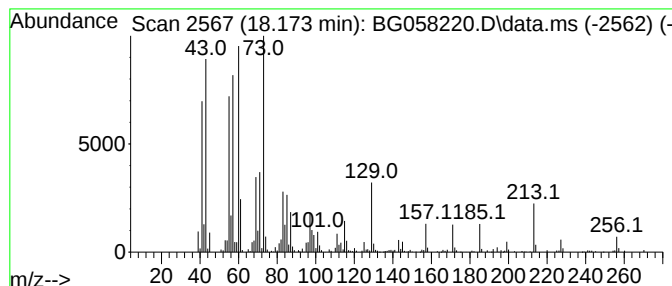
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.173	7.88 ng/ul	455356	Phenanthrene-d10	17.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	94
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87



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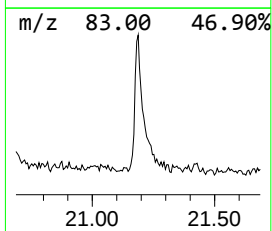
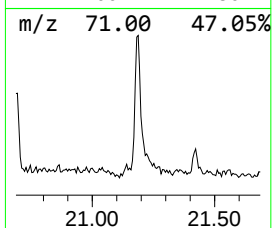
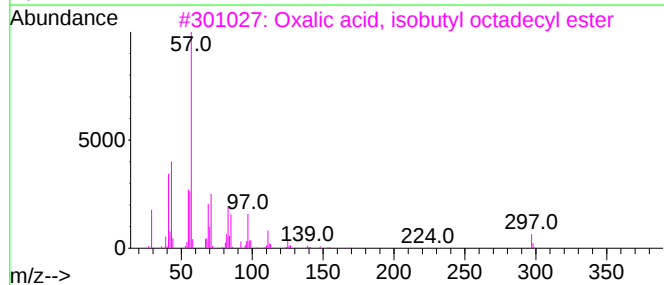
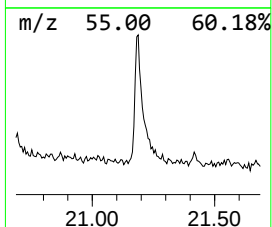
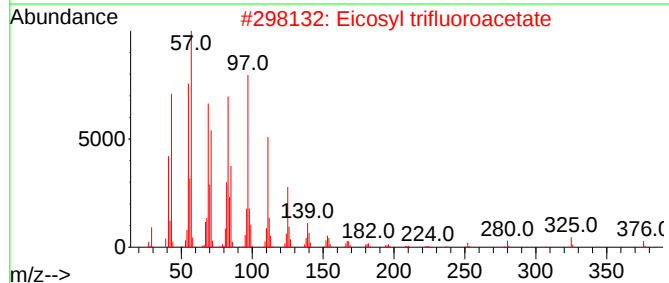
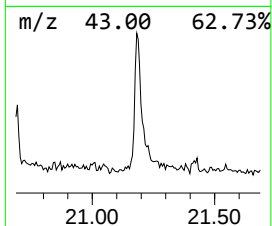
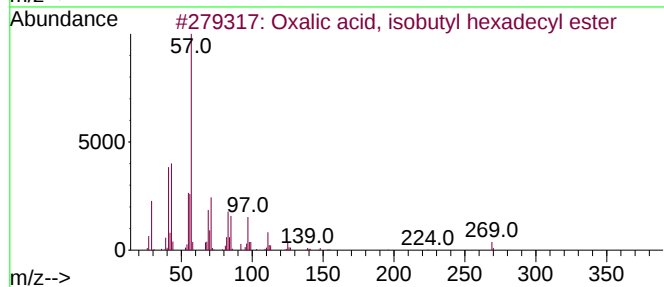
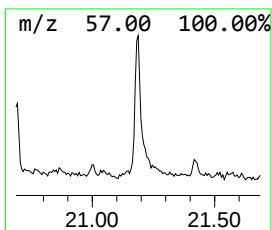
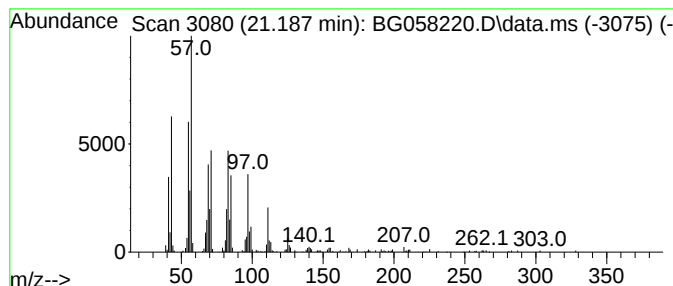
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Oxalic acid, isobutyl hexadecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.187	5.26 ng/ul	344350	Chrysene-d12	21.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	87
3			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87
4			Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83



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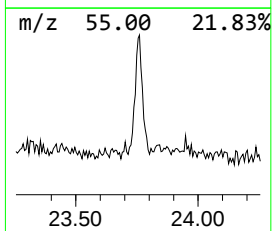
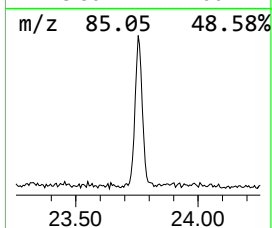
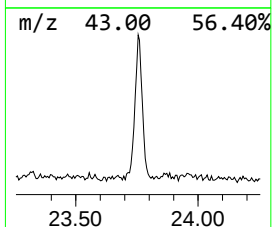
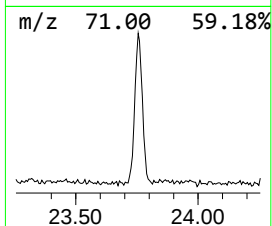
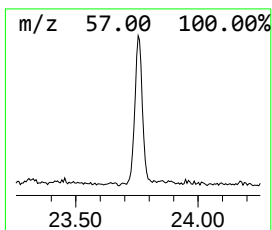
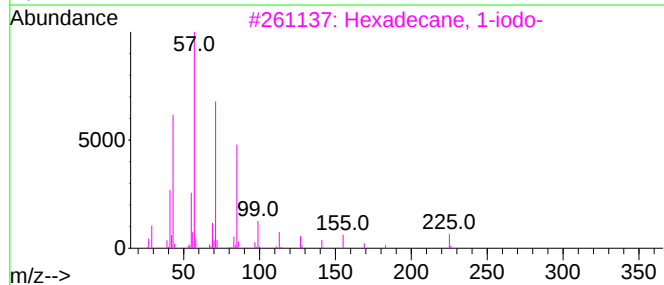
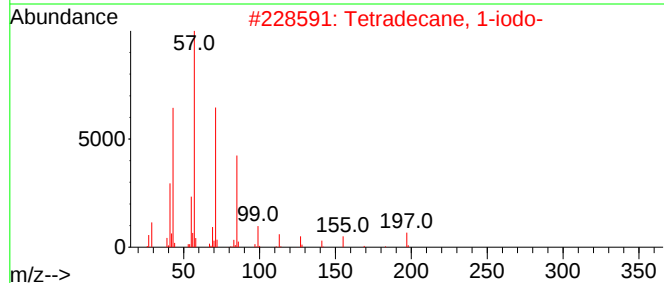
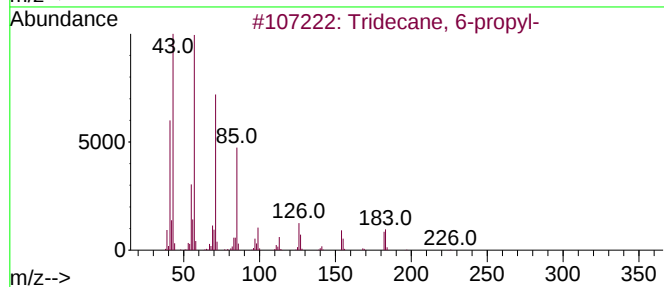
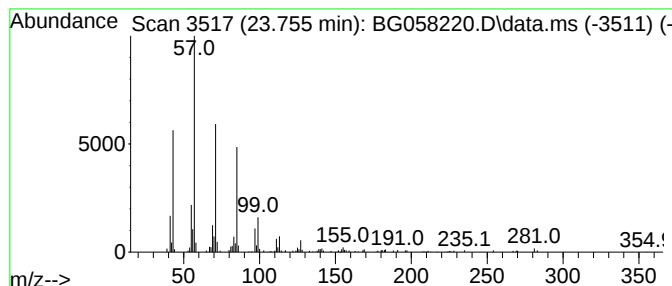
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.755	3.58 ng/ul	272093	Perylene-d12	24.683

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 6-propyl-	226	C16H34	055045-10-8	83
2		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
3		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
4		Heneicosane	296	C21H44	000629-94-7	72
5		Hexatriacontane	507	C36H74	000630-06-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
Data File : BG058220.D
Acq On : 14 Jul 2023 6:40
Operator : CG/JU
Sample : 03418-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A46J3

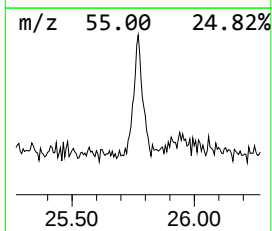
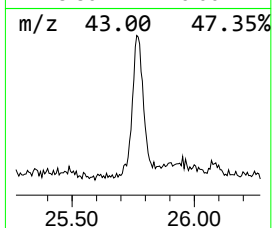
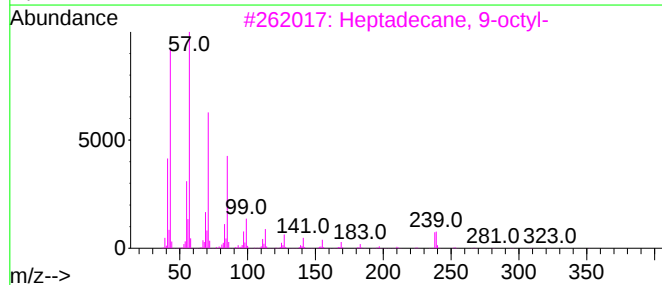
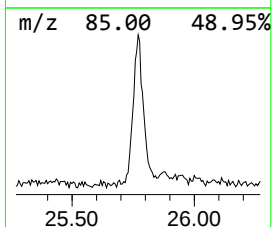
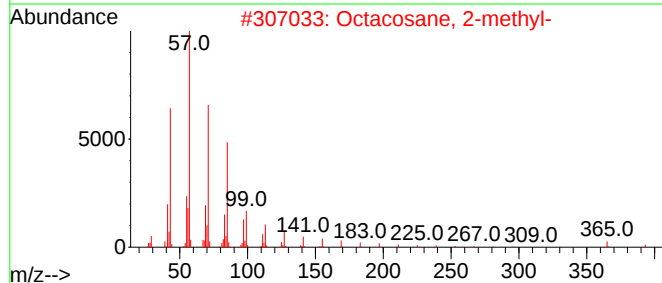
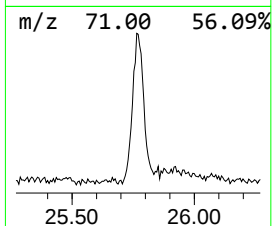
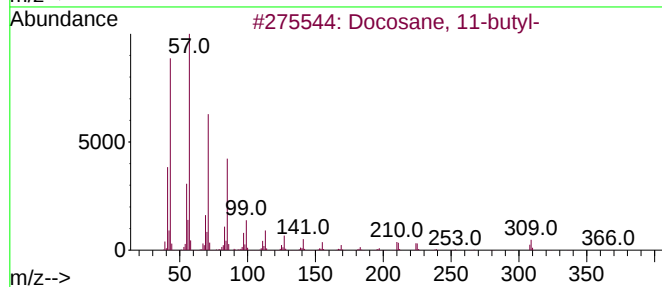
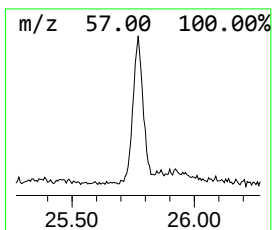
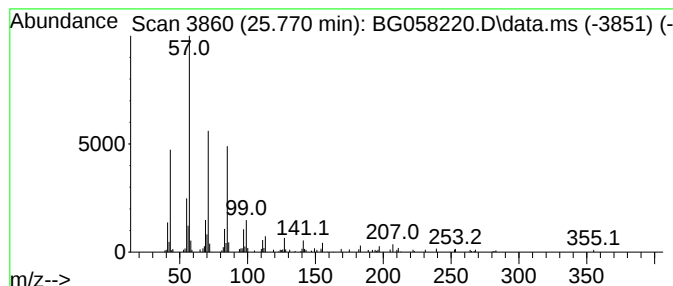
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.770	3.01 ng/ul	228432	Perylene-d12	24.683

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosane, 11-butyl-	366	C26H54	013475-76-8	87
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4		Nonadecane	268	C19H40	000629-92-5	87
5		Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
Data File : BG058220.D
Acq On : 14 Jul 2023 6:40
Operator : CG/JU
Sample : 03418-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

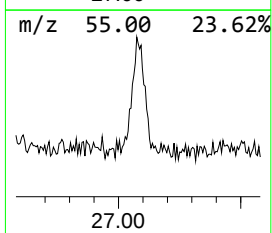
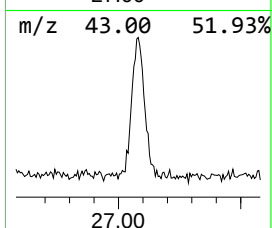
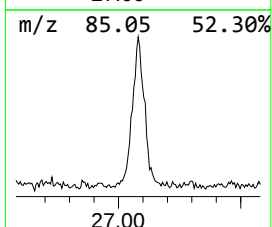
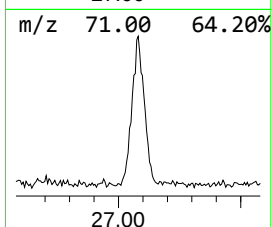
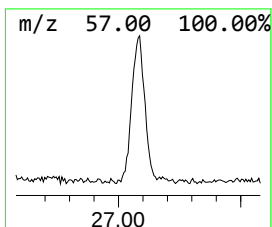
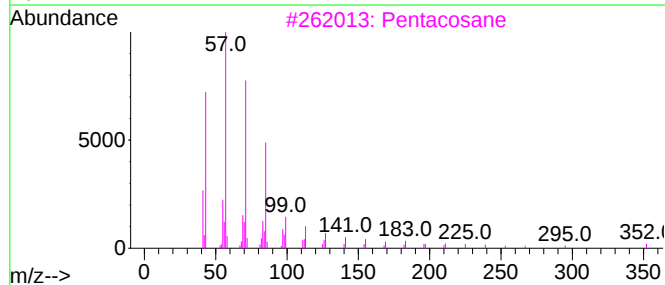
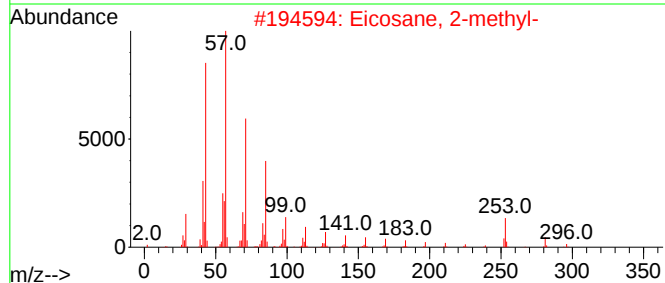
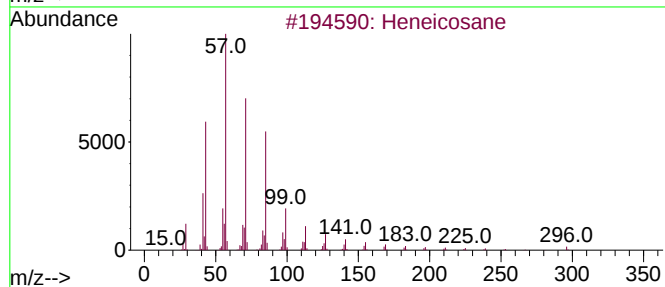
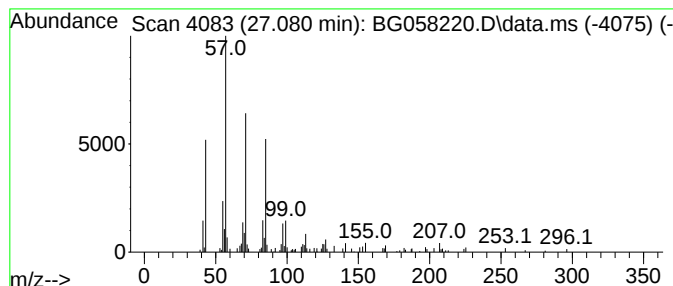
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
27.080	3.05 ng/ul	231610	Perylene-d12	24.683	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Eicosane, 2-methyl-	296	C21H44	001560-84-5	93
3	Pentacosane	352	C25H52	000629-99-2	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
Data File : BG058220.D
Acq On : 14 Jul 2023 6:40
Operator : CG/JU
Sample : 03418-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

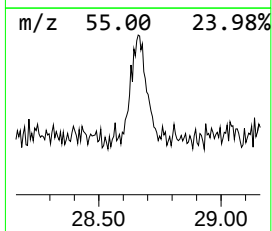
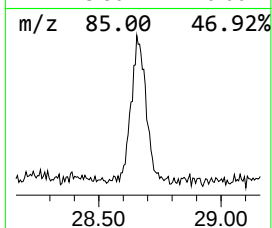
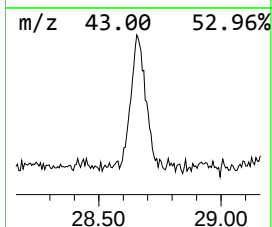
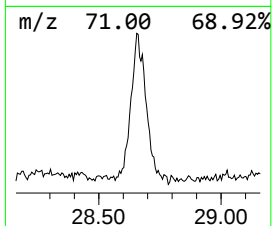
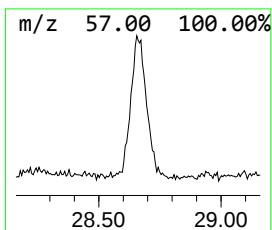
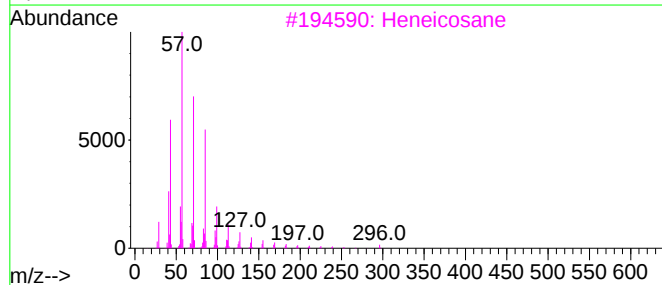
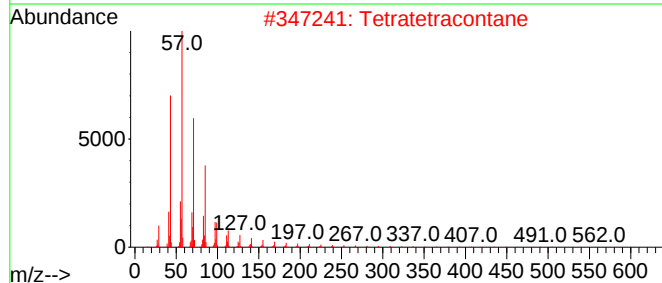
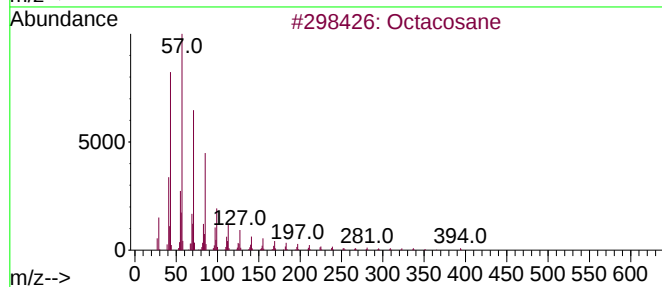
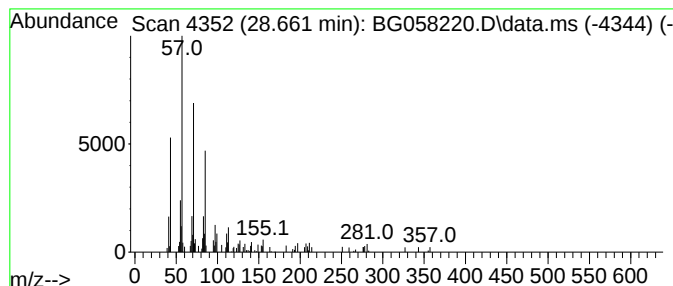
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.661	2.16 ng/ul	163898	Perylene-d12	24.683	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	86
2	Tetratetracontane	619	C44H90	007098-22-8	83
3	Heneicosane	296	C21H44	000629-94-7	83
4	Hexatriacontane	507	C36H74	000630-06-8	80
5	Hexacosane	366	C26H54	000630-01-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG071323\
Data File : BG058220.D
Acq On : 14 Jul 2023 6:40
Operator : CG/JU
Sample : 03418-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A46J3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.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
Benzophenone	15.893	5.0	ng/ul	226626	3	14.542	897495	20.0
n-Hexadecanoic ...	18.173	7.9	ng/ul	455356	4	17.286	1154990	20.0
Oxalic acid, is...	21.187	5.3	ng/ul	344350	5	21.540	1308460	20.0
(DEL) Alkane: S...	23.755	3.6	ng/ul	272093	6	24.683	1518290	20.0
(DEL) Alkane: S...	25.770	3.0	ng/ul	228432	6	24.683	1518290	20.0
(DEL) Alkane: S...	27.080	3.0	ng/ul	231610	6	24.683	1518290	20.0
(DEL) Alkane: S...	28.661	2.2	ng/ul	163898	6	24.683	1518290	20.0