

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062224\
 Data File : BG061647.D
 Acq On : 22 Jun 2024 13:41
 Operator : MA/JU
 Sample : P2775-16
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 A4CA1

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-BG062024.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG061647.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.470	27	31	38	rVB4	14077	22726	1.50%	0.095%
2	3.588	50	51	54	rBV2	3684	4021	0.26%	0.017%
3	3.741	73	77	83	rBV	23262	33734	2.22%	0.142%
4	3.888	99	102	113	rBV	159531	244596	16.10%	1.027%
5	4.058	129	131	134	rBV3	3485	3466	0.23%	0.015%
6	4.228	159	160	163	rVV3	4479	3550	0.23%	0.015%
7	4.593	220	222	228	rVB5	3886	5490	0.36%	0.023%
8	4.945	281	282	286	rVB3	3846	4065	0.27%	0.017%
9	5.004	290	292	294	rBV2	2605	3588	0.24%	0.015%
10	5.151	310	317	322	rBV5	7501	13730	0.90%	0.058%
11	5.392	354	358	359	rBV2	3702	4677	0.31%	0.020%
12	5.462	365	370	372	rBV3	2849	4206	0.28%	0.018%
13	5.844	430	435	436	rBV2	2444	3543	0.23%	0.015%
14	5.909	442	446	449	rBV3	3146	4988	0.33%	0.021%
15	5.985	456	459	460	rBV2	4070	3579	0.24%	0.015%
16	6.026	463	466	468	rBV3	3427	4252	0.28%	0.018%
17	6.132	480	484	490	rVB4	11157	18724	1.23%	0.079%
18	7.019	632	635	639	rBV4	5603	10062	0.66%	0.042%
19	7.213	660	668	677	rBV	284606	488861	32.17%	2.053%
20	7.272	677	678	682	rVB3	3292	3442	0.23%	0.014%
21	7.401	693	700	707	rBV	176572	290391	19.11%	1.220%
22	7.466	709	711	715	rVB2	4141	4773	0.31%	0.020%
23	7.601	727	734	741	rBV2	243341	403651	26.57%	1.695%
24	7.660	741	744	747	rBV3	8802	11010	0.72%	0.046%
25	8.077	809	815	821	rBV2	227316	382579	25.18%	1.607%
26	8.124	821	823	831	rVB4	7030	13150	0.87%	0.055%
27	8.188	831	834	836	rBV2	3888	3594	0.24%	0.015%
28	8.230	836	841	843	rBV4	2026	3450	0.23%	0.014%
29	8.606	902	905	907	rBV3	3636	4138	0.27%	0.017%
30	8.770	926	933	945	rVB2	318563	552134	36.34%	2.319%
31	8.935	958	961	964	rBV3	3510	5326	0.35%	0.022%
32	9.240	1005	1013	1021	rBV	251065	441494	29.06%	1.854%
33	9.322	1021	1027	1030	rBV5	4485	9333	0.61%	0.039%
34	9.399	1035	1040	1043	rBV4	8466	12290	0.81%	0.052%
35	9.657	1079	1084	1087	rVB5	7308	11462	0.75%	0.048%
36	9.710	1089	1093	1094	rVV2	3075	4138	0.27%	0.017%

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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
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37	9.751	1096	1100	1102	rVV2	4097	5687	0.37%	0.024%
38	9.798	1102	1108	1114	rVB4	23954	43194	2.84%	0.181%
39	9.898	1124	1125	1128	rBV	4788	4519	0.30%	0.019%
40	9.963	1128	1136	1144	rVB2	198718	360971	23.76%	1.516%

41	10.157	1167	1169	1170	rVV2	4181	4066	0.27%	0.017%
42	10.169	1170	1171	1174	rVV3	5804	3607	0.24%	0.015%
43	10.498	1217	1227	1233	rBV	327435	582035	38.31%	2.444%
44	10.885	1286	1293	1302	rBV	349239	628271	41.35%	2.639%
45	11.015	1304	1315	1322	rBV	172918	336374	22.14%	1.413%

46	11.144	1334	1337	1339	rBV2	3879	5211	0.34%	0.022%
47	11.226	1348	1351	1354	rBV3	3298	4403	0.29%	0.018%
48	11.414	1379	1383	1388	rVB5	8326	14954	0.98%	0.063%
49	11.626	1413	1419	1426	rVV2	40974	75906	5.00%	0.319%
50	11.731	1434	1437	1439	rBV2	3005	4037	0.27%	0.017%

51	11.796	1446	1448	1451	rBV	3319	3830	0.25%	0.016%
52	12.360	1539	1544	1548	rBV5	4772	9149	0.60%	0.038%
53	12.460	1558	1561	1567	rVB6	7966	13665	0.90%	0.057%
54	13.124	1671	1674	1676	rVB	5444	5580	0.37%	0.023%
55	13.159	1676	1680	1681	rBV4	4513	5345	0.35%	0.022%

56	13.523	1741	1742	1746	rBV4	4172	3900	0.26%	0.016%
57	13.600	1751	1755	1761	rVB6	9436	22186	1.46%	0.093%
58	13.664	1764	1766	1768	rVB3	6604	4720	0.31%	0.020%
59	13.870	1799	1801	1805	rBV4	5348	7333	0.48%	0.031%
60	14.017	1821	1826	1827	rBV5	3902	5306	0.35%	0.022%

61	14.105	1835	1841	1848	rBV	563750	828784	54.54%	3.481%
62	14.340	1878	1881	1884	rVV3	13822	15168	1.00%	0.064%
63	14.399	1884	1891	1900	rVB2	617361	1012011	66.60%	4.250%
64	14.475	1900	1904	1907	rBV4	3820	7029	0.46%	0.030%
65	14.646	1930	1933	1936	rBV4	5194	5884	0.39%	0.025%

66	14.704	1936	1943	1950	rVV	570208	892621	58.75%	3.749%
67	14.869	1964	1971	1977	rBV	297678	529176	34.83%	2.222%
68	14.957	1984	1986	1987	rBV	6481	4749	0.31%	0.020%
69	15.033	1995	1999	2005	rVB4	15159	26809	1.76%	0.113%
70	15.104	2005	2011	2013	rBV5	11242	21423	1.41%	0.090%

71	15.392	2059	2060	2063	rBV3	5515	4922	0.32%	0.021%
72	15.433	2063	2067	2070	rVV4	6254	9300	0.61%	0.039%
73	15.486	2074	2076	2081	rVV4	5504	8613	0.57%	0.036%
74	15.545	2083	2086	2091	rVB3	5703	8903	0.59%	0.037%
75	15.691	2105	2111	2118	rBV	818679	1240410	81.63%	5.209%

76	15.791	2123	2128	2134	rVB	193812	280836	18.48%	1.179%
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77	15.844	2134	2137	2140	rBV4	8800	10848	0.71%	0.046%
78	16.032	2167	2169	2170	rBV2	7182	4856	0.32%	0.020%
79	16.538	2253	2255	2257	rBV3	5704	5309	0.35%	0.022%
80	16.831	2301	2305	2308	rBV6	23309	31992	2.11%	0.134%
81	17.325	2386	2389	2394	rVV3	23142	33493	2.20%	0.141%
82	17.442	2403	2409	2415	rBV	724107	1073262	70.63%	4.507%
83	17.542	2420	2426	2434	rVV2	814192	1227706	80.80%	5.156%
84	17.813	2470	2472	2475	rBV4	10589	13760	0.91%	0.058%
85	18.065	2512	2515	2516	rBV3	13962	14084	0.93%	0.059%
86	18.112	2521	2523	2528	rVB5	19589	22069	1.45%	0.093%
87	18.330	2555	2560	2570	rBV	339382	509569	33.54%	2.140%
88	19.458	2749	2752	2753	rBV3	53263	55005	3.62%	0.231%
89	19.487	2754	2757	2764	rVB2	113322	198240	13.05%	0.833%
90	19.599	2772	2776	2782	rBV2	113402	163935	10.79%	0.688%
91	19.751	2800	2802	2808	rVB5	27024	28820	1.90%	0.121%
92	19.822	2808	2814	2825	rBV	1007527	1519466	100.00%	6.381%
93	21.361	3072	3076	3084	rBV	677262	936517	61.63%	3.933%
94	21.708	3129	3135	3148	rVB2	634706	1176346	77.42%	4.940%
95	22.560	3274	3280	3292	rVB2	623965	1179614	77.63%	4.954%
96	24.082	3532	3539	3543	rBV2	415738	967124	63.65%	4.062%
97	24.710	3640	3646	3655	rVB2	532138	1270823	83.64%	5.337%
98	24.934	3676	3684	3693	rVB2	418765	1149923	75.68%	4.829%
99	25.574	3787	3793	3803	rVB2	367324	904704	59.54%	3.800%
100	26.320	3913	3920	3937	rVB4	392960	1224262	80.57%	5.142%

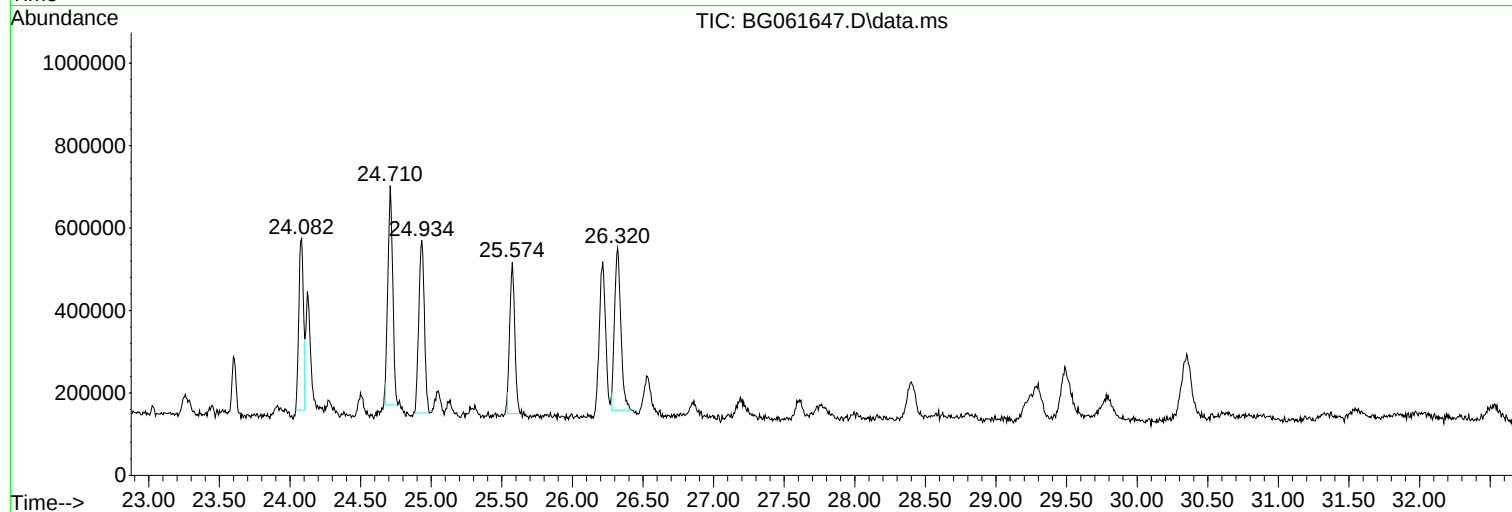
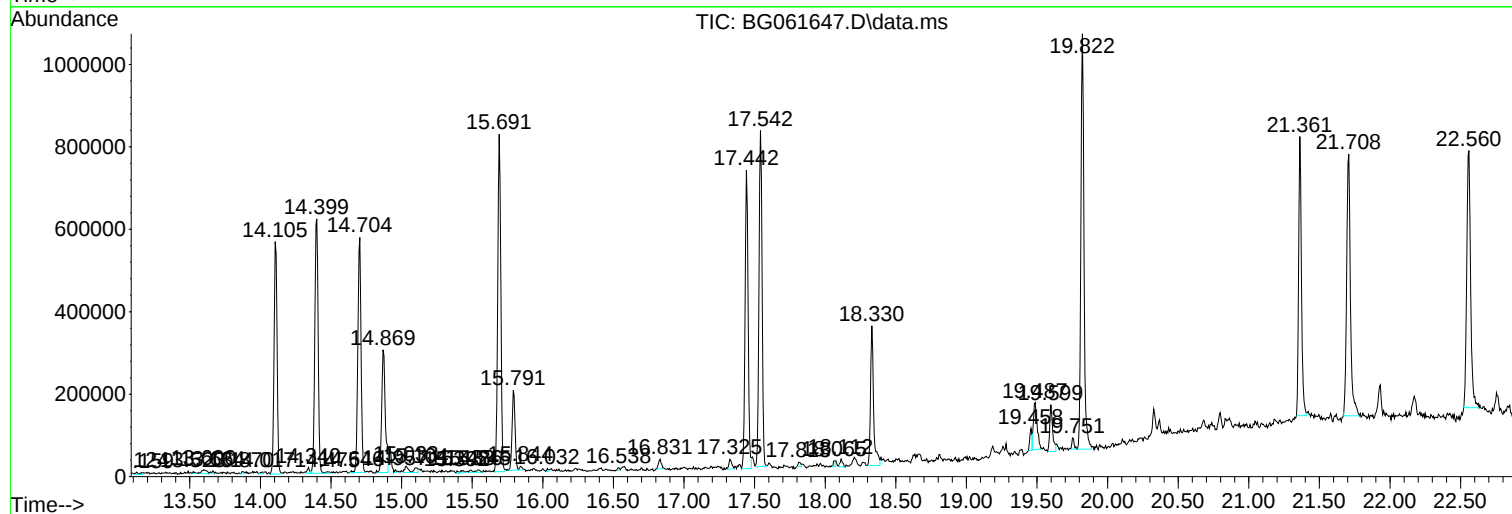
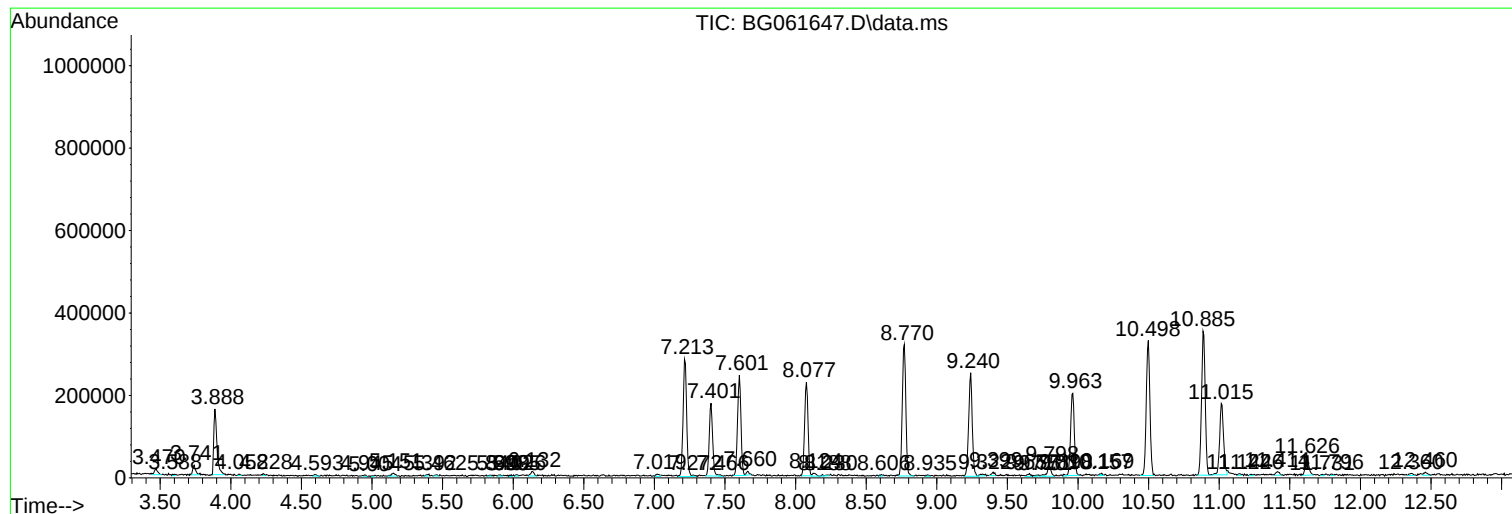
Sum of corrected areas: 23810827

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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

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



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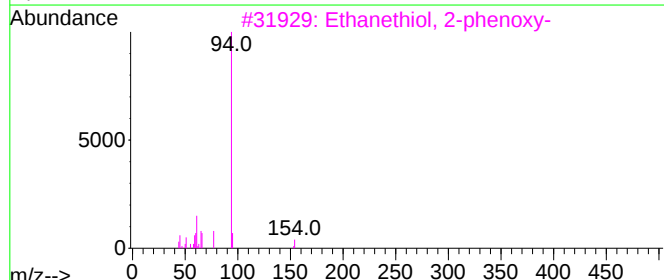
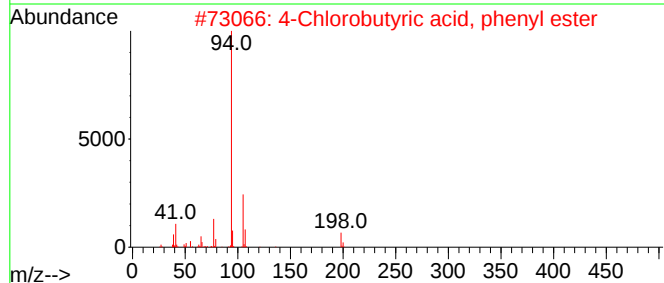
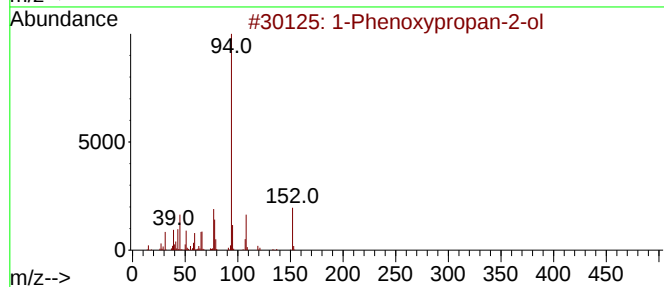
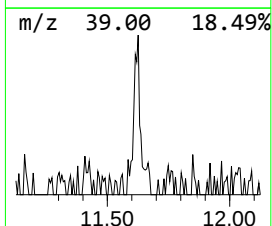
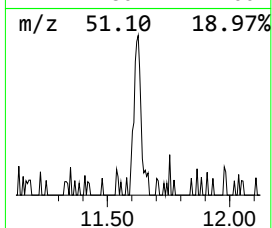
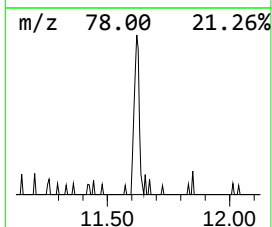
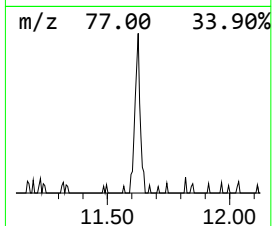
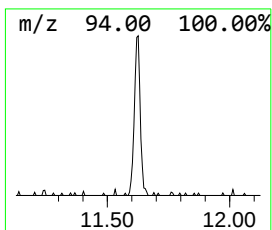
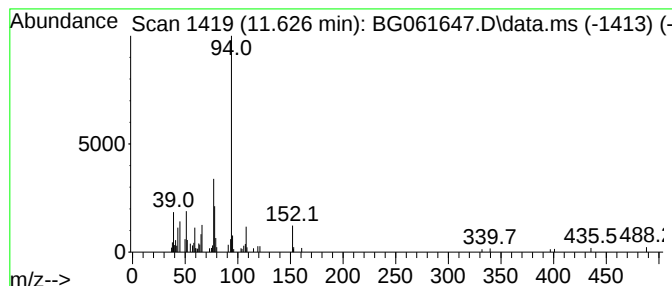
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.626	2.42 ng/ul	75906	Naphthalene-d8	10.885

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	74
2			4-Chlorobutyric acid, phenyl ester	198	C10H11ClO2	1000357-76-9	50
3			Ethanethiol, 2-phenoxy-	154	C8H10OS	006338-63-2	47
4			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	46
5			Pyrimidine, 5-methyl-	94	C5H6N2	002036-41-1	46



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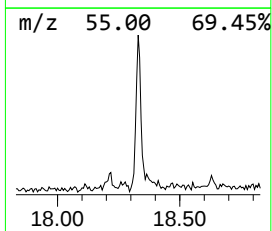
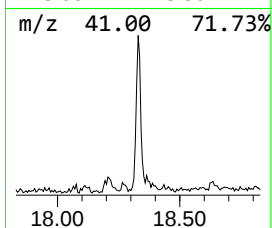
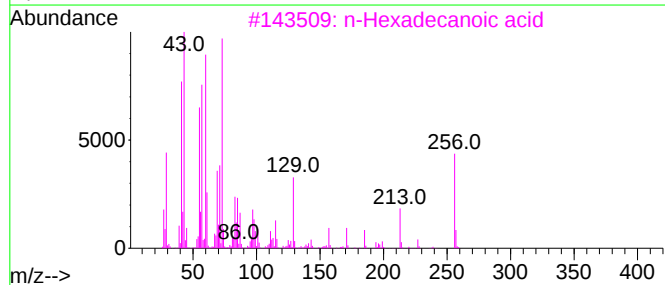
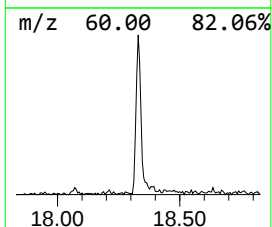
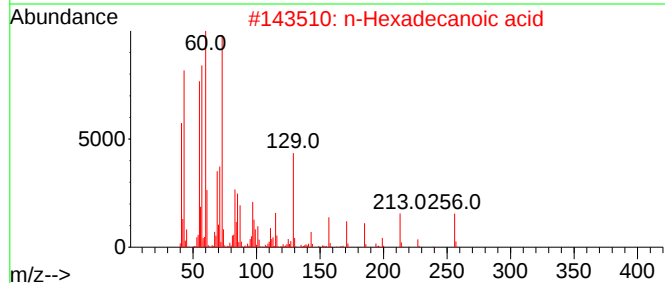
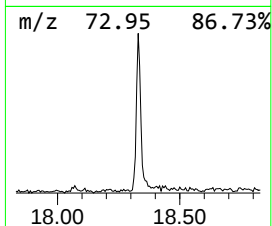
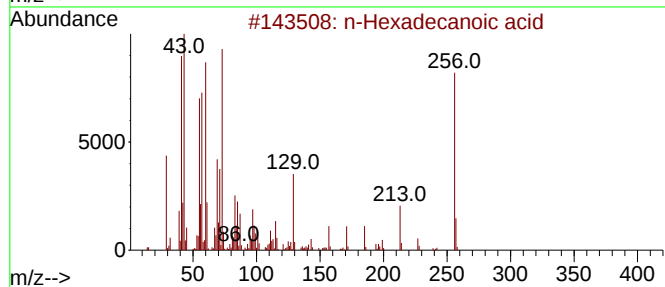
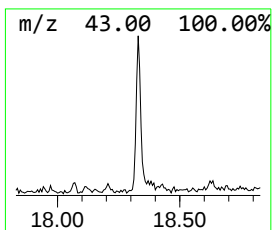
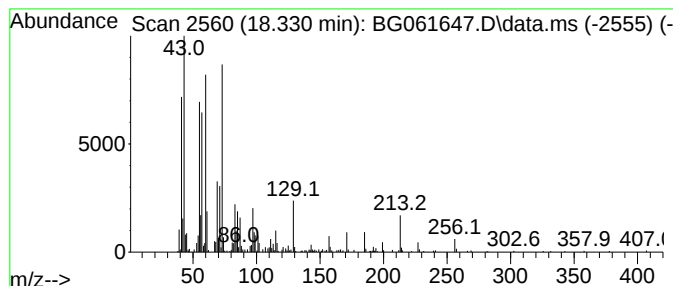
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.329	9.50 ng/ul	509569	Phenanthrene-d10	17.442

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4			Tridecanoic acid	214	C13H26O2	000638-53-9	94
5			Octadecanoic acid	284	C18H36O2	000057-11-4	90



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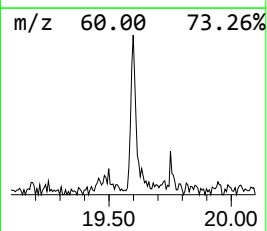
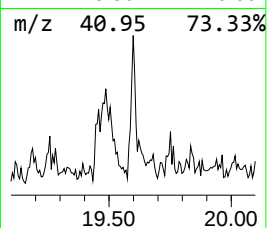
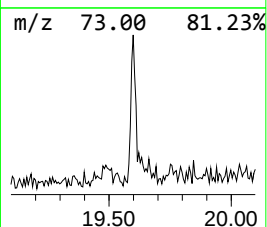
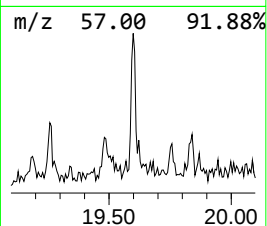
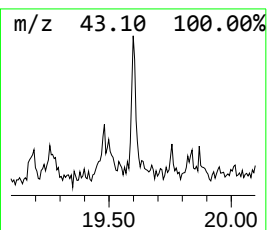
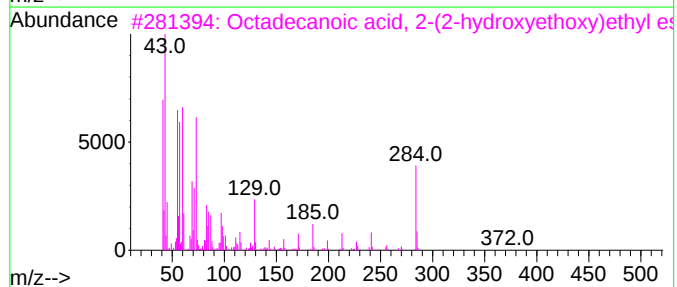
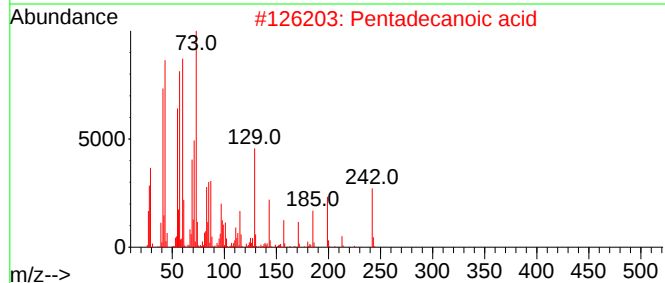
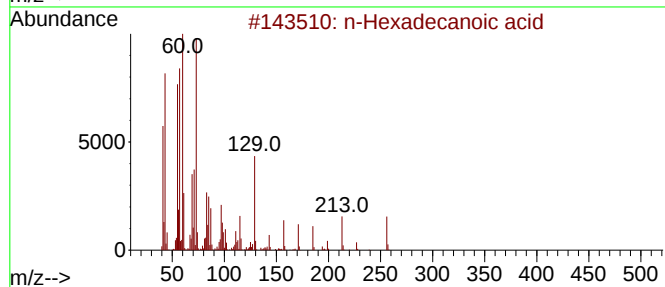
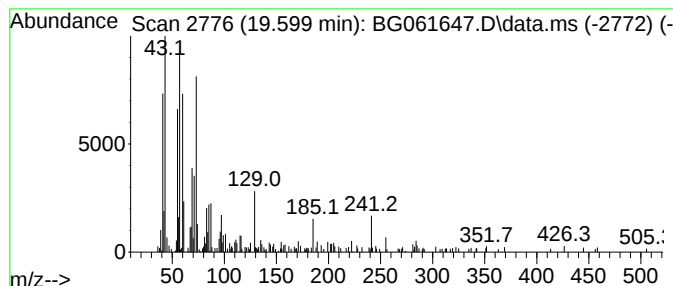
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.599	2.79 ng/ul	163935	Chrysene-d12	21.708

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	86
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062224\
Data File : BG061647.D
Acq On : 22 Jun 2024 13:41
Operator : MA/JU
Sample : P2775-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

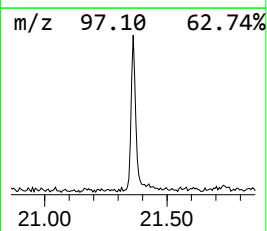
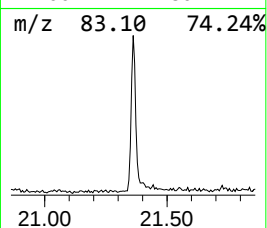
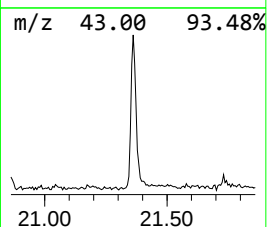
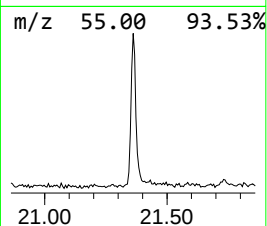
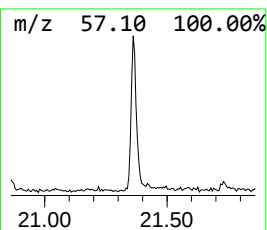
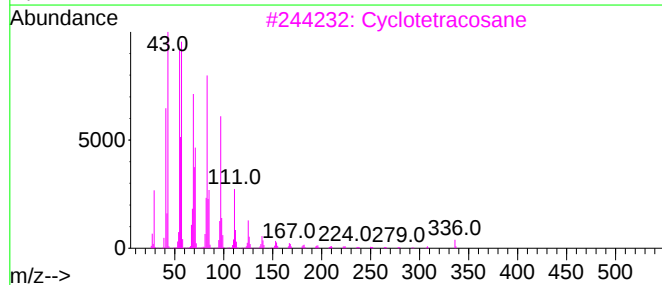
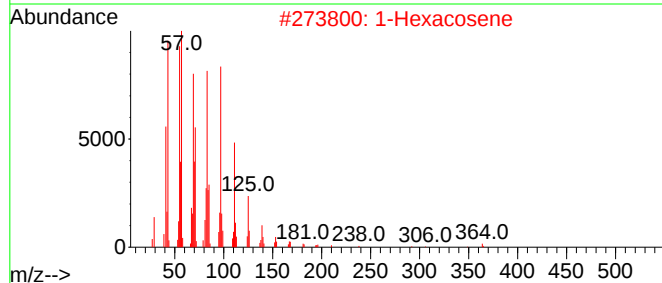
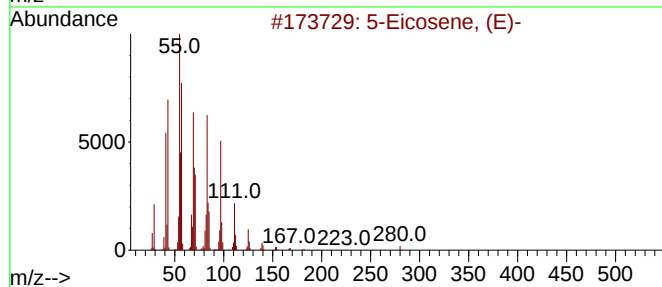
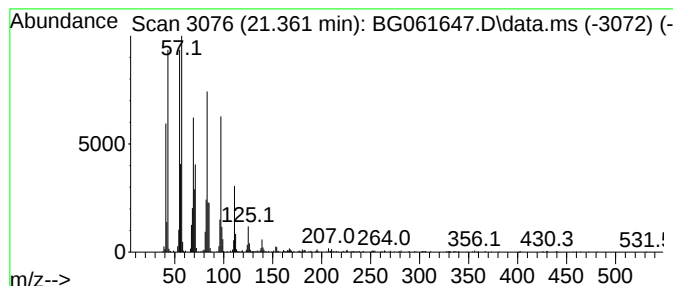
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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.	
21.361	15.92 ng/ul	936517	Chrysene-d12		21.708	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	91
2	1-Hexacosene		364	C26H52	018835-33-1	91
3	Cyclotetracosane		336	C24H48	000297-03-0	91
4	1-Heneicosyl formate		340	C22H44O2	077899-03-7	91
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062224\
Data File : BG061647.D
Acq On : 22 Jun 2024 13:41
Operator : MA/JU
Sample : P2775-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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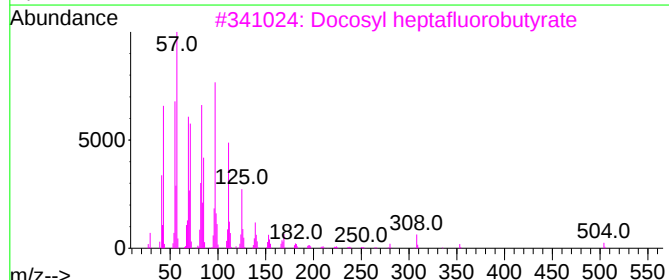
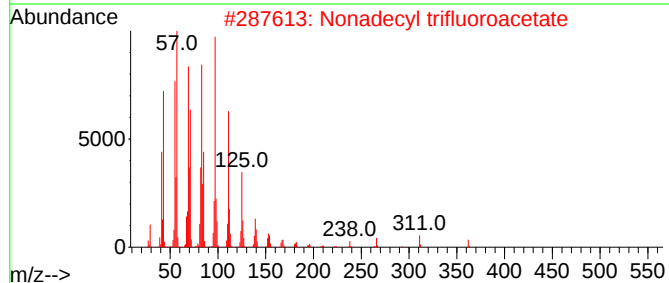
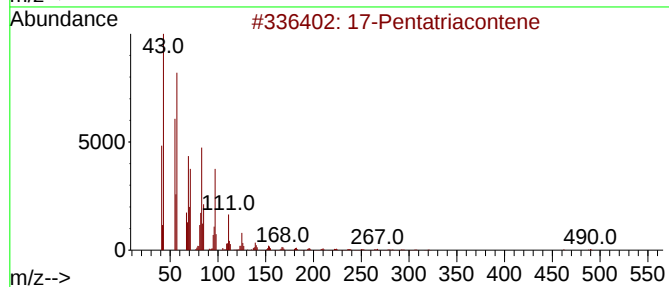
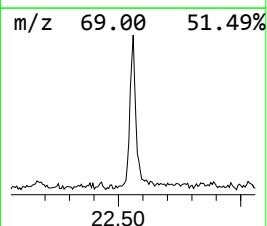
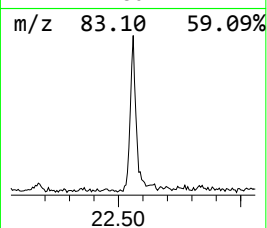
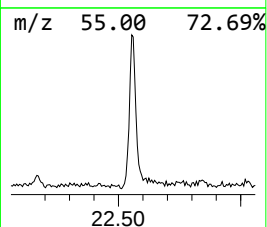
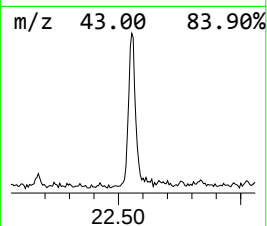
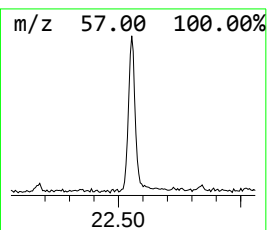
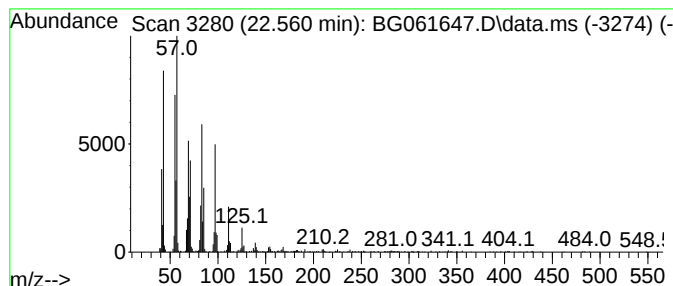
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.560	20.06 ng/ul	1179610	Chrysene-d12	21.708

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3			Docosyl heptafluorobutyrate	522	C26H45F7O2	1000351-83-1	91
4			Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	91
5			Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062224\
Data File : BG061647.D
Acq On : 22 Jun 2024 13:41
Operator : MA/JU
Sample : P2775-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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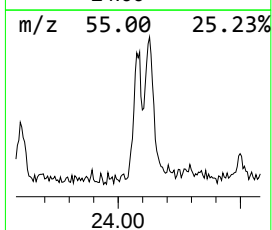
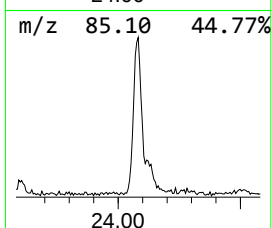
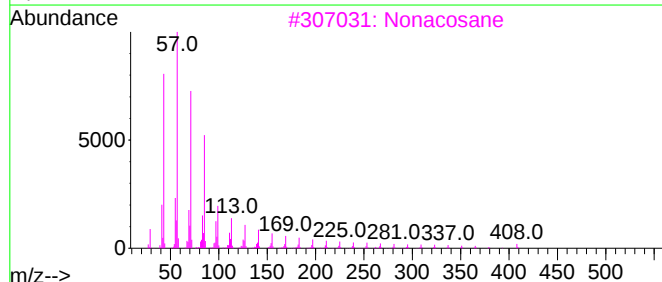
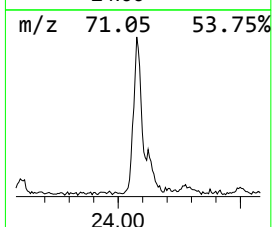
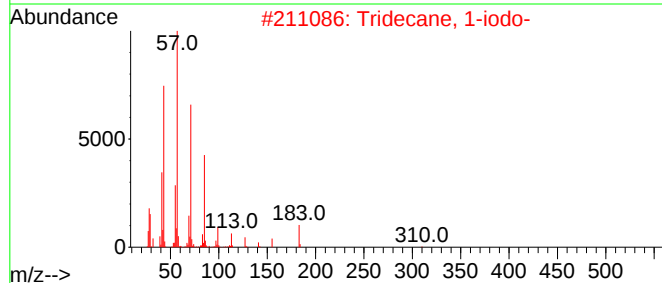
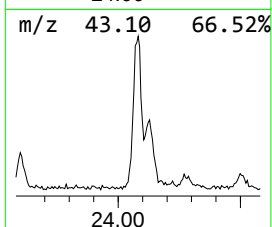
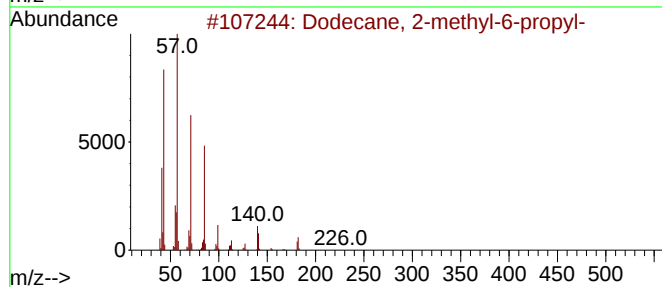
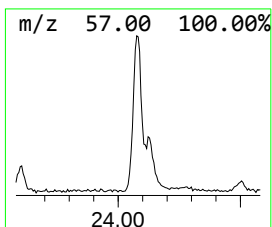
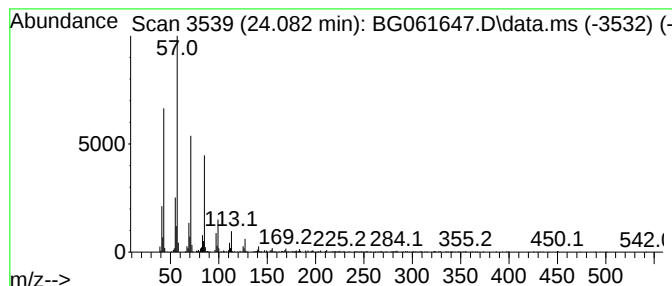
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.082	16.82 ng/ul	967124	Perylene-d12	24.934

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	87
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
3		Nonacosane	408	C29H60	000630-03-5	86
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	86
5		Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062224\
Data File : BG061647.D
Acq On : 22 Jun 2024 13:41
Operator : MA/JU
Sample : P2775-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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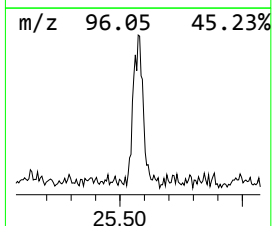
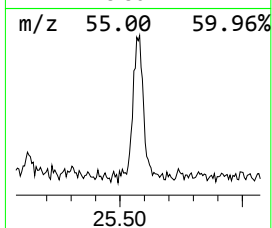
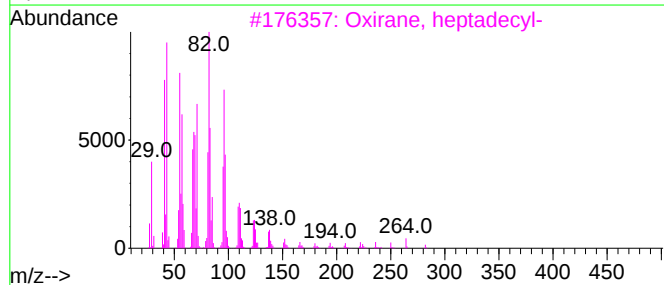
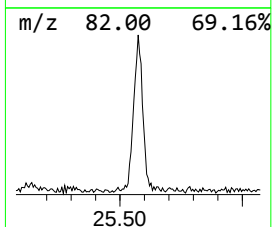
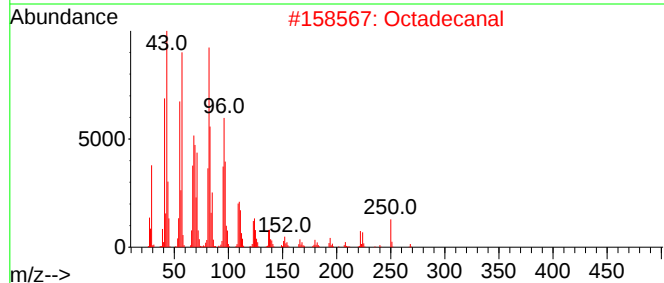
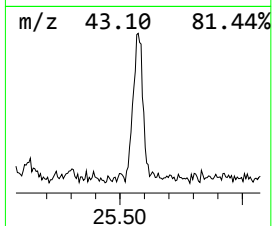
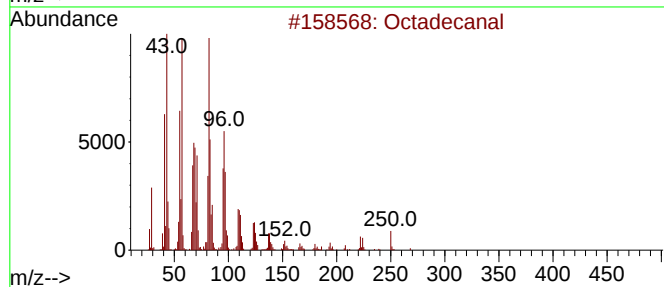
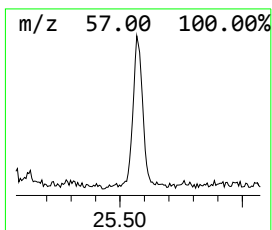
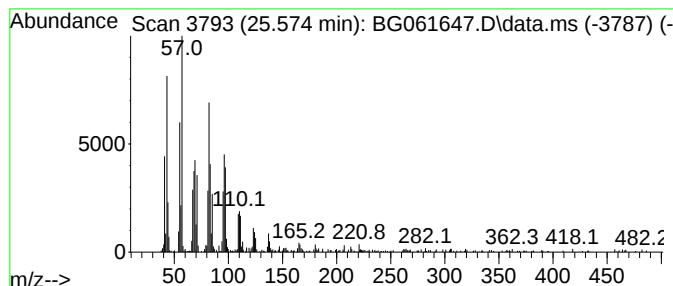
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.574	15.73 ng/ul	904704	Perylene-d12	24.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal			268	C18H36O	000638-66-4	94
2	Octadecanal			268	C18H36O	000638-66-4	93
3	Oxirane, heptadecyl-			282	C19H38O	067860-04-2	93
4	Oxirane, hexadecyl-			268	C18H36O	007390-81-0	93
5	Tricosanal			338	C23H46O	072934-02-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062224\
Data File : BG061647.D
Acq On : 22 Jun 2024 13:41
Operator : MA/JU
Sample : P2775-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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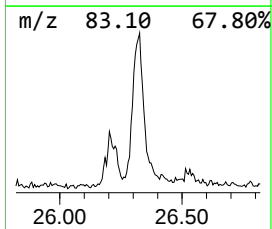
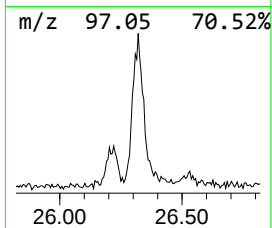
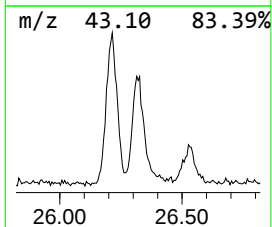
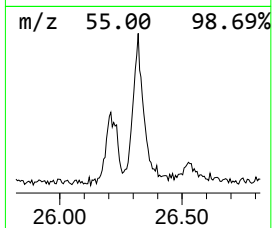
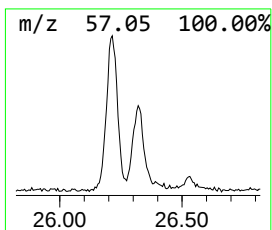
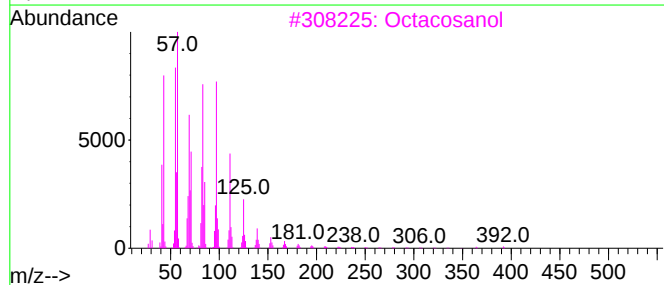
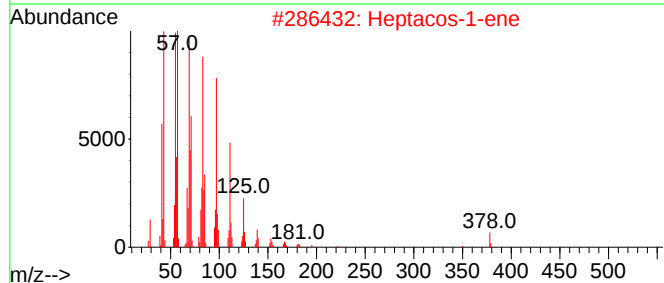
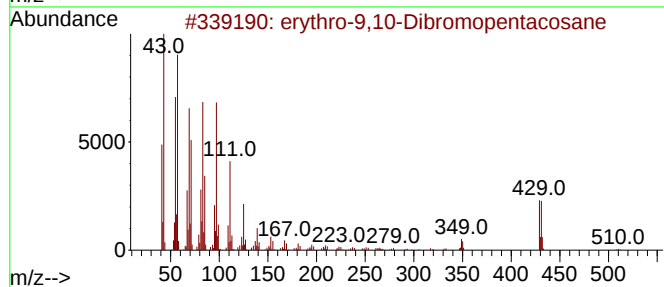
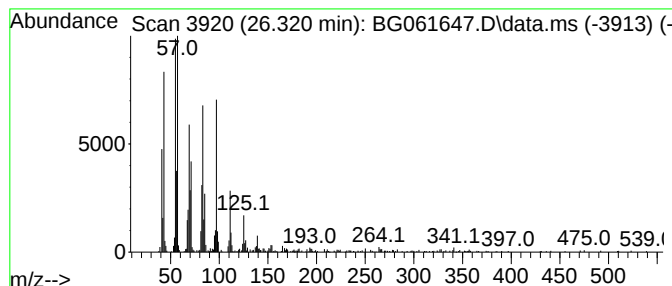
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 erythro-9,10-Dibromopentaco... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.320	21.29 ng/ul	1224260	Perylene-d12	24.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			erythro-9,10-Dibromopentacosane	508	C25H50Br2	059907-02-7	91
2			Heptacos-1-ene	378	C27H54	015306-27-1	91
3			Octacosanol	410	C28H58O	000557-61-9	91
4			Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
5			1-Hexacosene	364	C26H52	018835-33-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062224\
Data File : BG061647.D
Acq On : 22 Jun 2024 13:41
Operator : MA/JU
Sample : P2775-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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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
1-Phenoxypropan...	11.626	2.4	ng/ul	75906	2	10.885	628271	20.0
n-Hexadecanoic ...	18.329	9.5	ng/ul	509569	4	17.442	1073260	20.0
Pentadecanoic acid	19.599	2.8	ng/ul	163935	5	21.708	1176350	20.0
(DEL) Alkane: S...	21.361	15.9	ng/ul	936517	5	21.708	1176350	20.0
(DEL) Alkane: S...	22.560	20.1	ng/ul	1179610	5	21.708	1176350	20.0
(DEL) Alkane: S...	24.082	16.8	ng/ul	967124	6	24.934	1149920	20.0
Octadecanal	25.574	15.7	ng/ul	904704	6	24.934	1149920	20.0
erythro-9,10-Di...	26.320	21.3	ng/ul	1224260	6	24.934	1149920	20.0