

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
 Data File : BG061709.D
 Acq On : 25 Jun 2024 19:18
 Operator : MA/JU
 Sample : P2873-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C0SH8

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: BG061709.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.467	24	30	36	rBV2	23860	36603	1.23%	0.126%
2	3.731	71	75	83	rBV	118447	184614	6.20%	0.636%
3	3.884	98	101	113	rBV	326603	509037	17.10%	1.754%
4	4.166	146	149	153	rVB5	2984	4783	0.16%	0.016%
5	4.231	156	160	163	rBV5	6907	10427	0.35%	0.036%
6	4.589	217	221	225	rVB4	3701	6731	0.23%	0.023%
7	5.147	311	316	321	rVB3	12723	20603	0.69%	0.071%
8	5.300	338	342	344	rBV3	3131	4767	0.16%	0.016%
9	5.330	344	347	353	rVB3	3270	6252	0.21%	0.022%
10	5.388	353	357	359	rBV4	3836	5574	0.19%	0.019%
11	5.717	409	413	419	rVB4	3208	6149	0.21%	0.021%
12	5.929	445	449	450	rVB4	4785	5551	0.19%	0.019%
13	6.129	480	483	488	rVB3	11614	17351	0.58%	0.060%
14	7.028	631	636	639	rBV5	8954	14817	0.50%	0.051%
15	7.086	644	646	648	rBV3	3597	4184	0.14%	0.014%
16	7.216	660	668	676	rBV	393790	661340	22.22%	2.279%
17	7.398	691	699	707	rVB	258424	423988	14.25%	1.461%
18	7.598	724	733	739	rBV	348741	579671	19.48%	1.997%
19	7.656	739	743	751	rVB2	50851	83843	2.82%	0.289%
20	7.903	781	785	788	rVB3	3608	6309	0.21%	0.022%
21	8.073	805	814	820	rBV	192259	332984	11.19%	1.147%
22	8.214	835	838	843	rBV5	3212	5328	0.18%	0.018%
23	8.579	897	900	902	rVB3	5681	4404	0.15%	0.015%
24	8.767	925	932	939	rBV	479500	799648	26.87%	2.756%
25	9.237	1004	1012	1022	rVB	350060	636398	21.38%	2.193%
26	9.319	1022	1026	1029	rBV4	7045	10595	0.36%	0.037%
27	9.413	1041	1042	1048	rVB3	4666	6199	0.21%	0.021%
28	9.789	1098	1106	1114	rVB5	25028	47681	1.60%	0.164%
29	9.959	1126	1135	1142	rBV	316929	558464	18.77%	1.924%
30	10.159	1165	1169	1173	rVB3	4898	8164	0.27%	0.028%
31	10.359	1199	1203	1207	rBV5	3947	6763	0.23%	0.023%
32	10.494	1218	1226	1235	rBV	491740	850468	28.58%	2.931%
33	10.882	1284	1292	1298	rBV	297213	548731	18.44%	1.891%
34	10.935	1298	1301	1307	rVV	43624	68092	2.29%	0.235%
35	11.017	1307	1315	1322	rVB	469184	860545	28.92%	2.965%
36	11.411	1376	1382	1386	rBV5	16500	22785	0.77%	0.079%

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37	11.616	1411	1417	1424	rBV	104693	197995	6.65%	0.682%
38	11.834	1452	1454	1457	rBV2	4117	5408	0.18%	0.019%
39	12.010	1480	1484	1487	rVB3	2951	4804	0.16%	0.017%
40	12.033	1487	1488	1491	rBV2	5811	6215	0.21%	0.021%
41	12.075	1494	1495	1498	rVB2	5042	4409	0.15%	0.015%
42	12.345	1537	1541	1542	rBV4	3754	4887	0.16%	0.017%
43	12.462	1557	1561	1565	rVB4	6943	10141	0.34%	0.035%
44	12.533	1570	1573	1578	rVB3	11479	14409	0.48%	0.050%
45	12.645	1590	1592	1596	rBV3	3445	5061	0.17%	0.017%
46	12.750	1607	1610	1614	rBV5	11166	15492	0.52%	0.053%
47	12.780	1614	1615	1619	rVB3	5167	4777	0.16%	0.016%
48	12.821	1619	1622	1624	rBV2	2851	3929	0.13%	0.014%
49	13.050	1658	1661	1664	rBV3	6535	9472	0.32%	0.033%
50	13.303	1700	1704	1709	rBV3	6025	12532	0.42%	0.043%
51	13.743	1776	1779	1782	rBV3	3970	4001	0.13%	0.014%
52	13.867	1798	1800	1802	rBV2	5127	4908	0.16%	0.017%
53	14.108	1834	1841	1846	rBV	896122	1332262	44.77%	4.591%
54	14.149	1846	1848	1853	rVB4	5086	7018	0.24%	0.024%
55	14.184	1853	1854	1857	rBV3	4729	4851	0.16%	0.017%
56	14.343	1875	1881	1883	rBV4	19507	31489	1.06%	0.109%
57	14.395	1883	1890	1897	rVB	1025542	1661695	55.84%	5.726%
58	14.589	1920	1923	1925	rBV3	4393	4125	0.14%	0.014%
59	14.701	1935	1942	1949	rVV	547531	838280	28.17%	2.889%
60	14.766	1949	1953	1957	rVB6	11543	17842	0.60%	0.061%
61	14.877	1965	1972	1984	rBV	597040	1038320	34.89%	3.578%
62	15.100	2007	2010	2015	rVB6	15722	21786	0.73%	0.075%
63	15.294	2033	2043	2046	rBV3	65670	192619	6.47%	0.664%
64	15.688	2104	2110	2117	rBV	1405499	2178635	73.21%	7.507%
65	15.741	2117	2119	2122	rVV3	9303	8291	0.28%	0.029%
66	15.794	2122	2128	2138	rVB	502388	734546	24.68%	2.531%
67	15.929	2149	2151	2154	rVB4	9209	7711	0.26%	0.027%
68	16.046	2167	2171	2172	rBV3	5045	5027	0.17%	0.017%
69	16.223	2200	2201	2202	rBV	9395	5933	0.20%	0.020%
70	16.305	2212	2215	2216	rBV3	5398	5076	0.17%	0.017%
71	16.405	2229	2232	2234	rVB3	9377	10222	0.34%	0.035%
72	16.628	2267	2270	2273	rVB3	5543	4701	0.16%	0.016%
73	16.828	2300	2304	2310	rBV8	10048	17350	0.58%	0.060%
74	16.975	2327	2329	2332	rBV4	5233	6349	0.21%	0.022%
75	17.257	2375	2377	2380	rVB4	7912	5697	0.19%	0.020%
76	17.445	2402	2409	2414	rBV	802204	1225933	41.19%	4.224%

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Title : SVOA CALIBRATION

77	17.539	2419	2425	2434	rVV2	1652463	2612994	87.80%	9.004%
78	17.615	2436	2438	2443	rVB6	22104	26302	0.88%	0.091%
79	18.109	2519	2522	2527	rVB6	23251	29016	0.97%	0.100%
80	18.332	2554	2560	2566	rBV	353355	511829	17.20%	1.764%
81	19.595	2771	2775	2780	rBV4	103577	140004	4.70%	0.482%
82	19.824	2808	2814	2823	rBV	2005955	2813304	94.53%	9.694%
83	21.358	3071	3075	3088	rVB2	258531	413372	13.89%	1.424%
84	21.704	3129	3134	3141	rVB	720322	1195812	40.18%	4.121%
85	24.713	3636	3646	3660	rBV2	1086179	2976008	100.00%	10.255%
86	24.930	3675	3683	3694	rBV3	449091	1267307	42.58%	4.367%

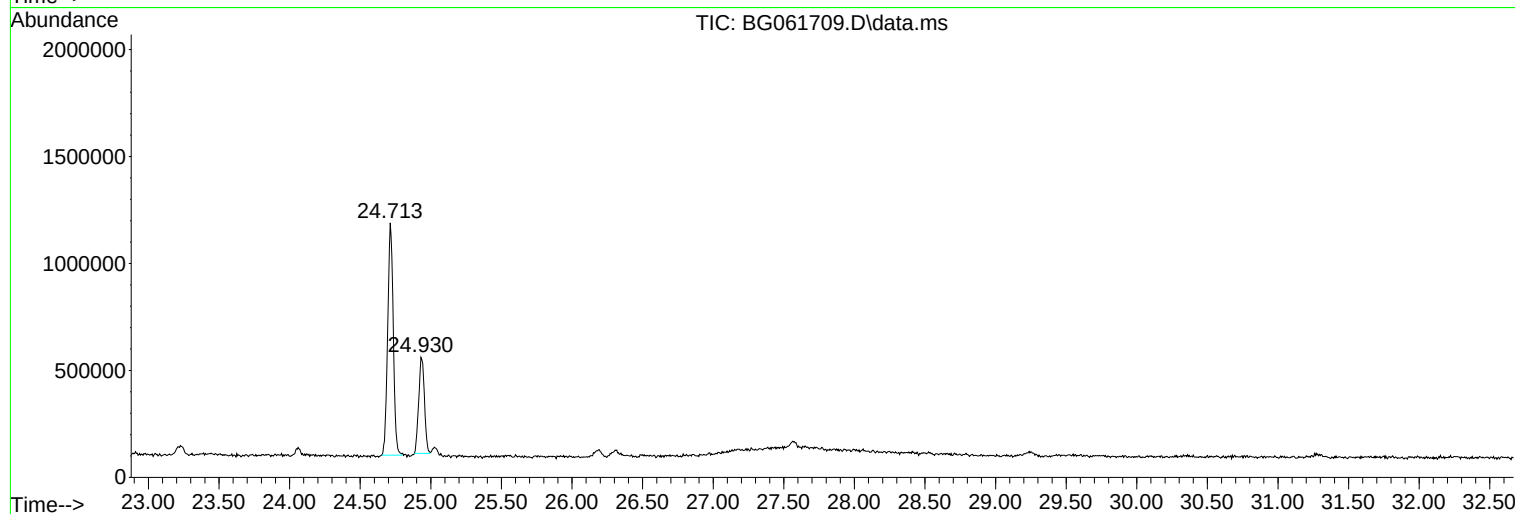
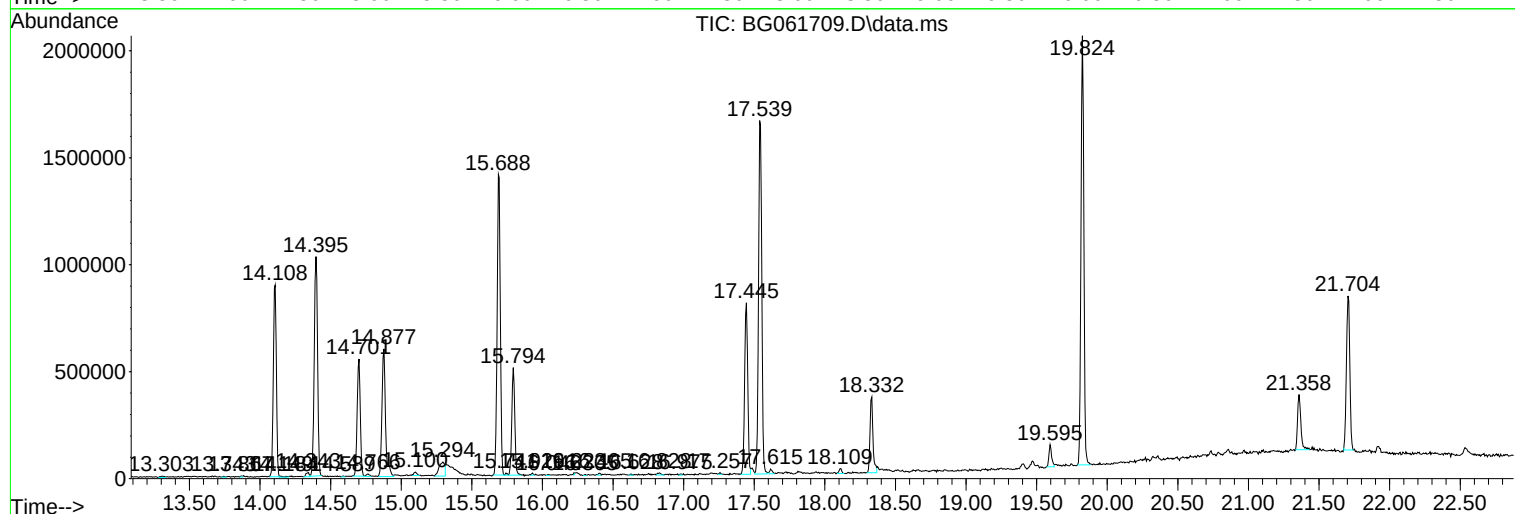
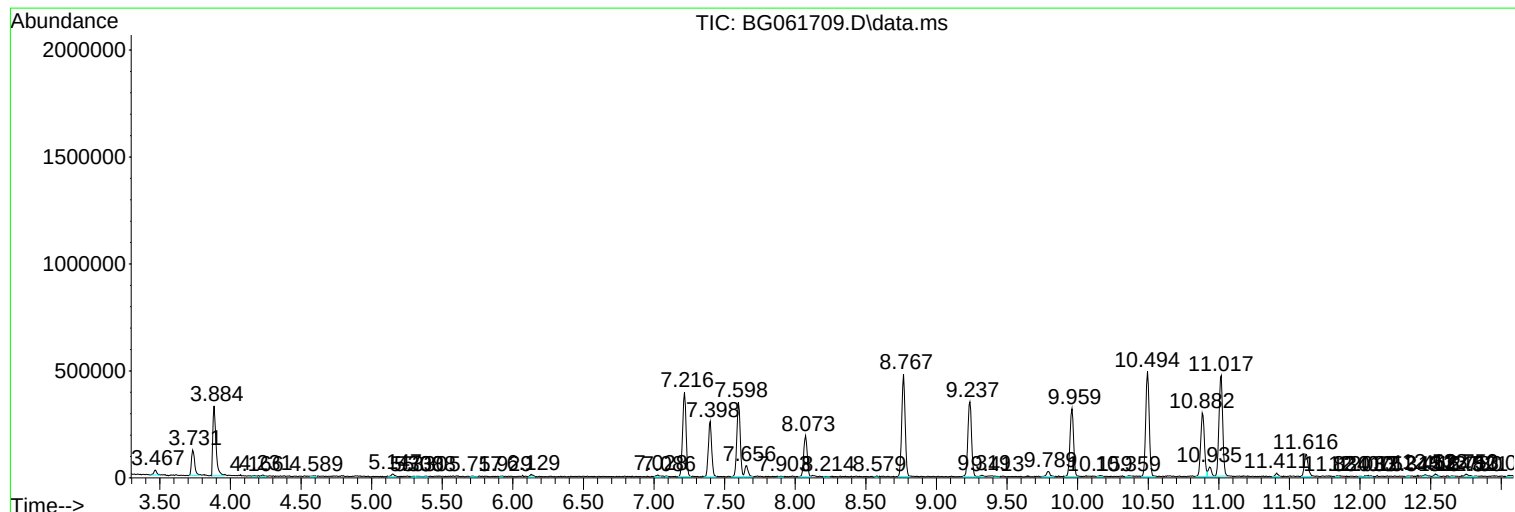
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

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



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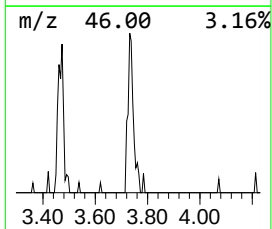
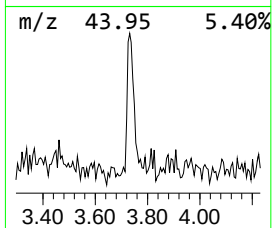
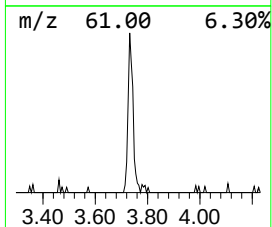
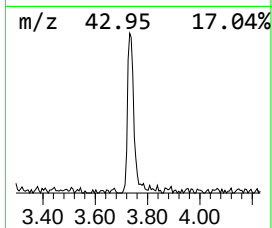
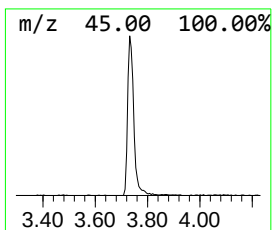
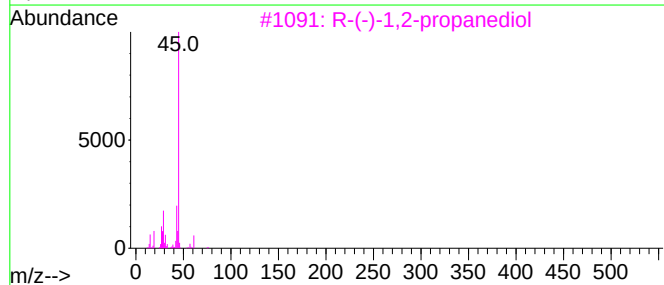
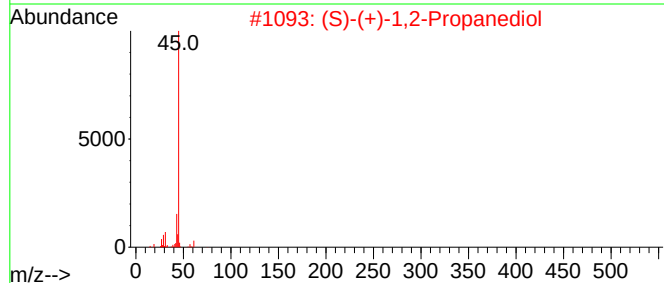
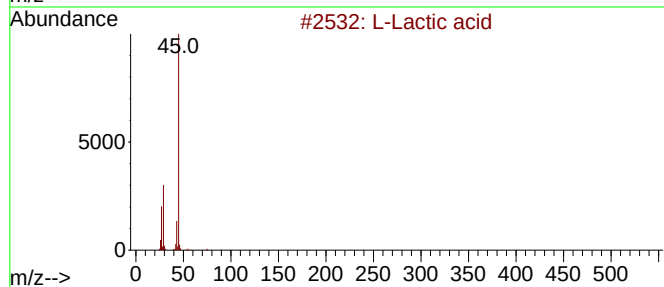
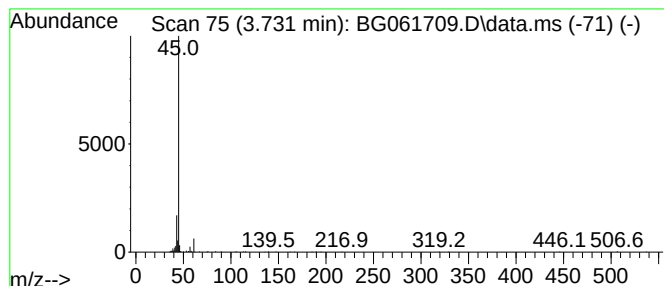
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 L-Lactic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.731	11.09 ng/ul	184614	1,4-Dichlorobenzene-d4	8.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Lactic acid	90	C3H6O3	000079-33-4	50
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
4			Propylene Glycol	76	C3H8O2	000057-55-6	38
5			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9



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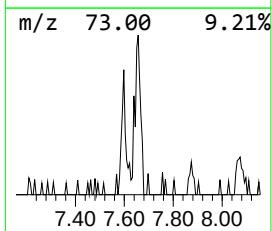
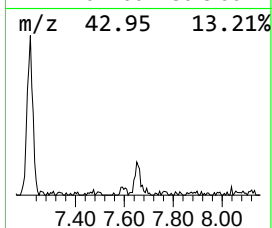
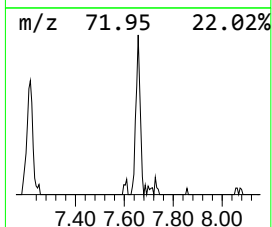
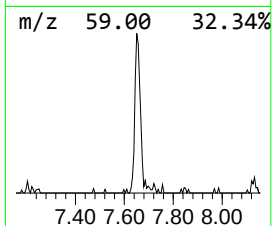
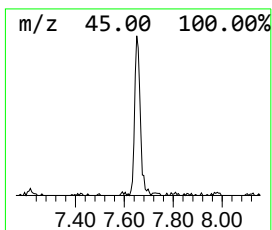
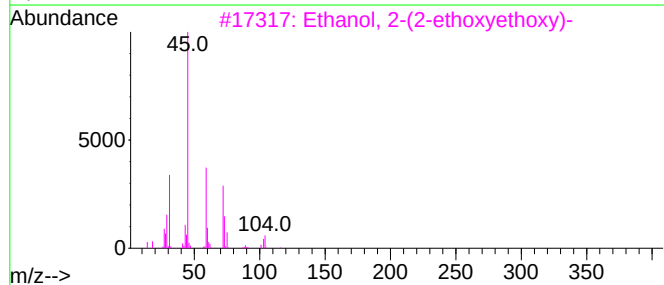
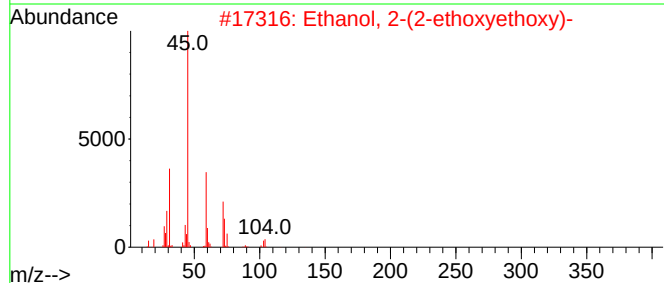
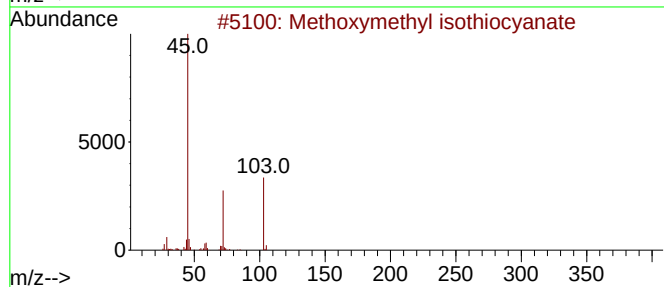
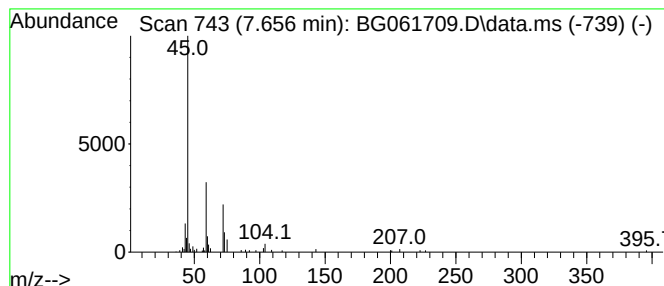
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Methoxymethyl isothiocyanate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.656	5.04 ng/ul	83843	1,4-Dichlorobenzene-d4	8.073

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methoxymethyl isothiocyanate	103	C3H5NOS	019900-84-6	53
2			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	50
3			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	50
4			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	50
5			Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	42



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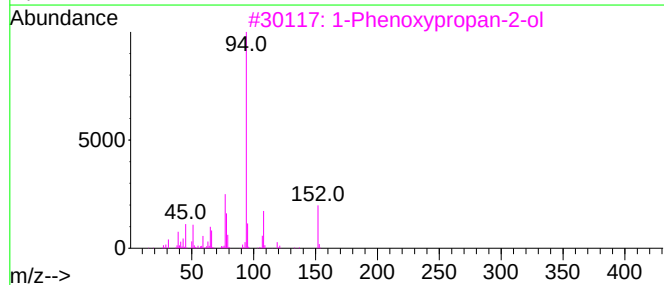
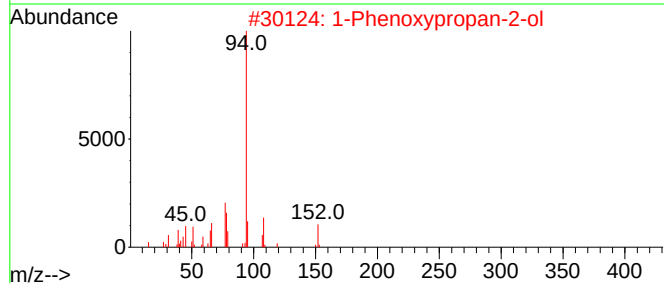
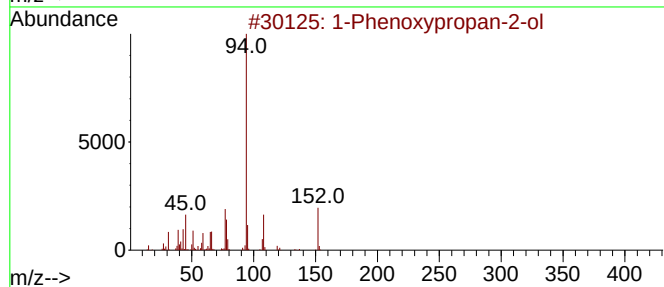
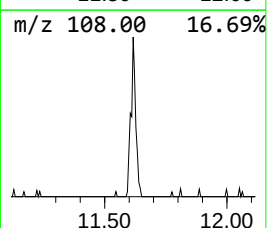
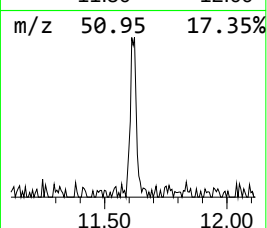
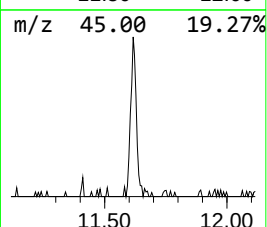
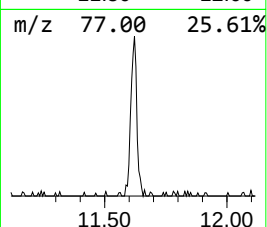
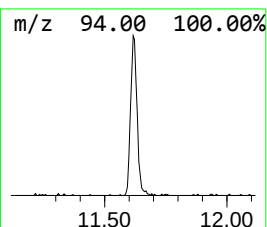
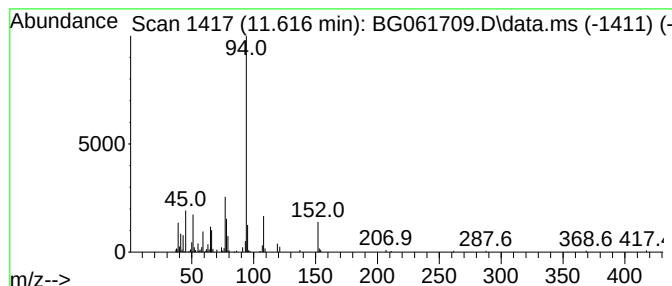
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	7.22 ng/ul	197995	Naphthalene-d8	10.882

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
4			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	90
5			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87



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C0SH8

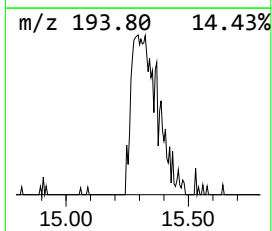
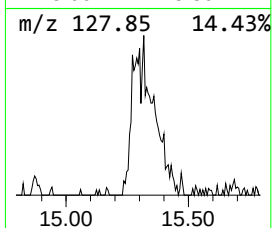
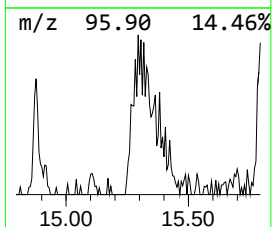
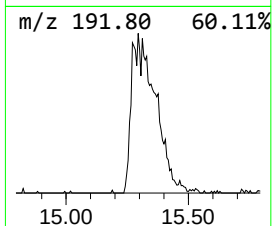
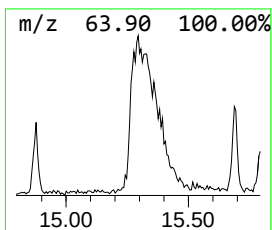
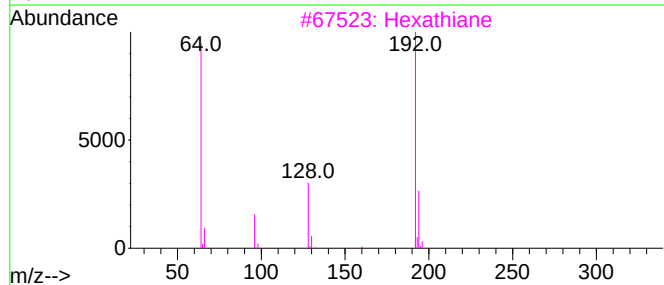
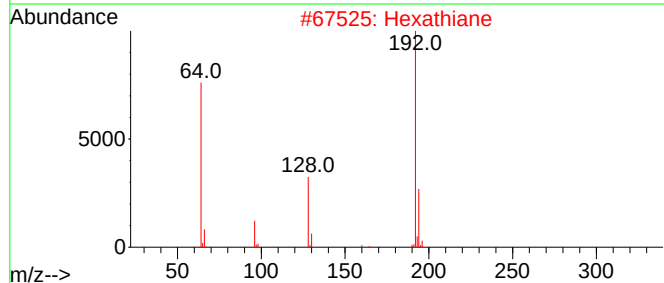
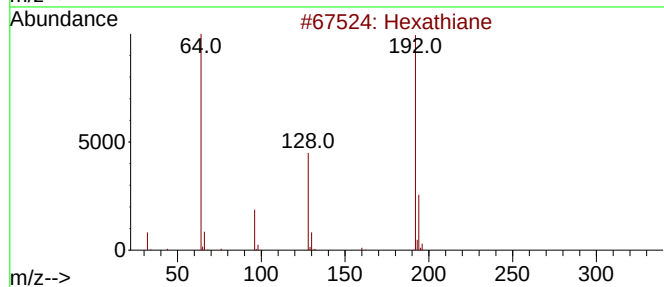
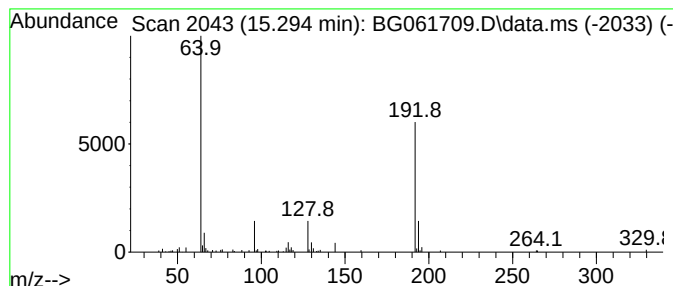
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Hexathiane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.294	4.60 ng/ul	192619	Acenaphthene-d10	14.701

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiane	192	S6	013798-23-7	91
2			Hexathiane	192	S6	013798-23-7	91
3			Hexathiane	192	S6	013798-23-7	91
4			Cyclic octaatomic sulfur	256	S8	010544-50-0	40
5			Cyclic octaatomic sulfur	256	S8	010544-50-0	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061709.D
Acq On : 25 Jun 2024 19:18
Operator : MA/JU
Sample : P2873-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0SH8

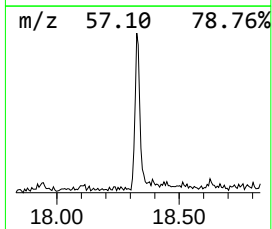
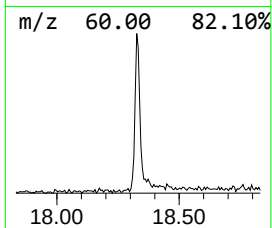
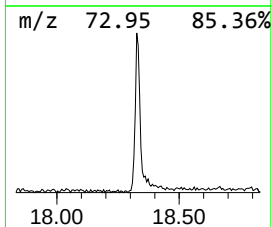
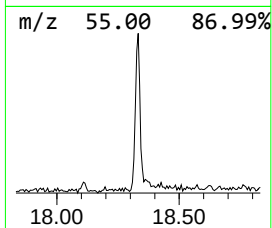
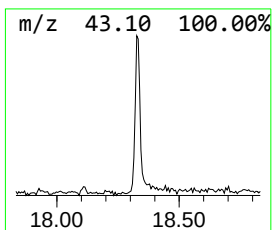
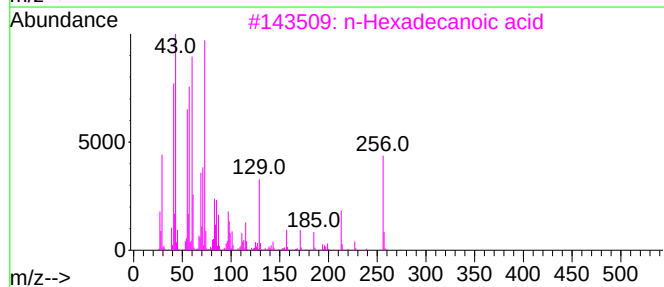
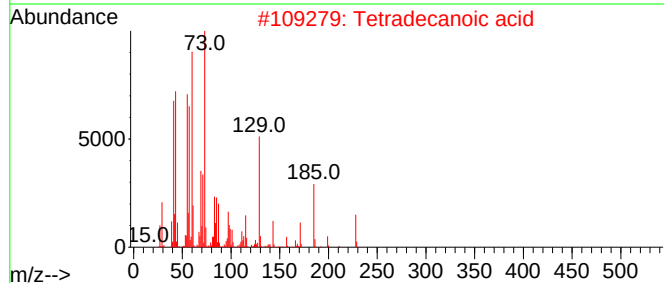
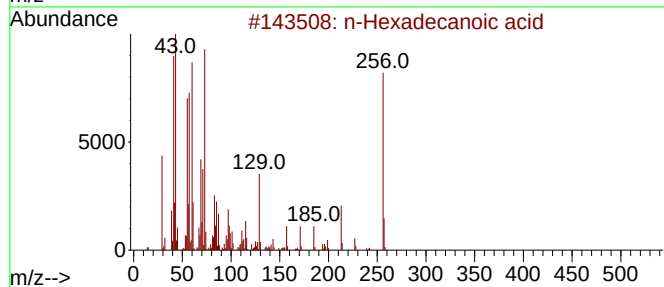
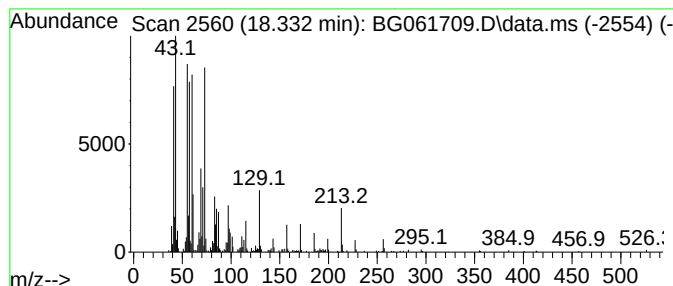
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.332	8.35 ng/ul	511829	Phenanthrene-d10	17.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5			Tridecanoic acid	214	C13H26O2	000638-53-9	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061709.D
Acq On : 25 Jun 2024 19:18
Operator : MA/JU
Sample : P2873-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0SH8

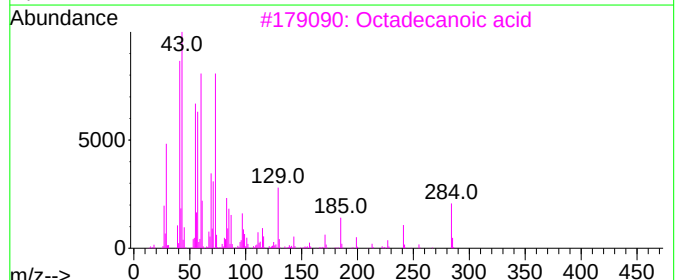
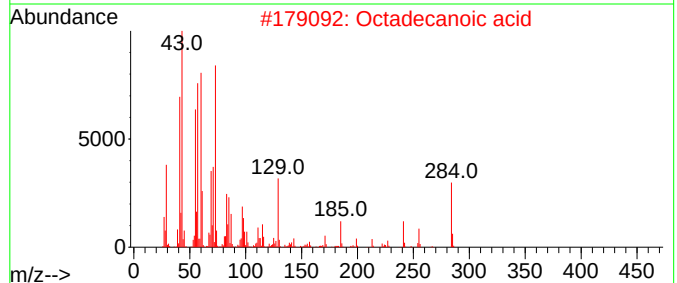
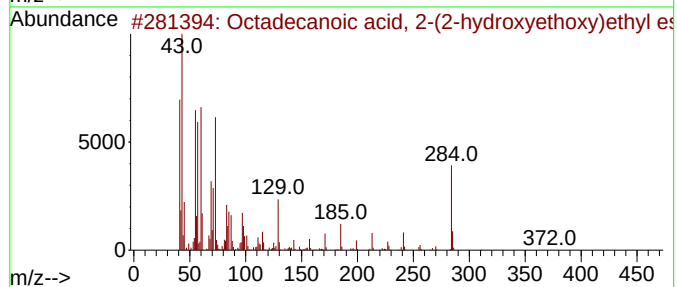
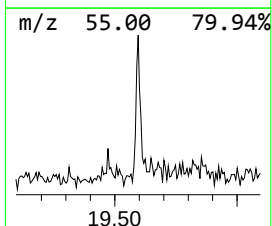
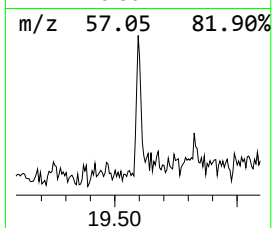
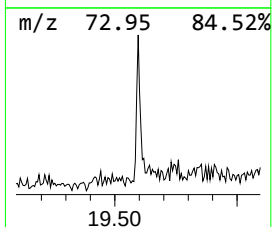
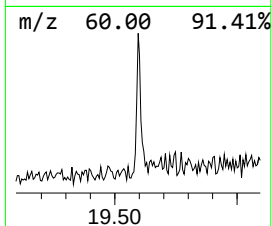
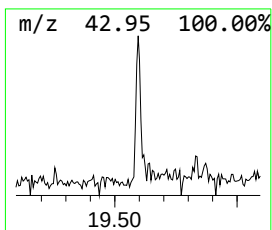
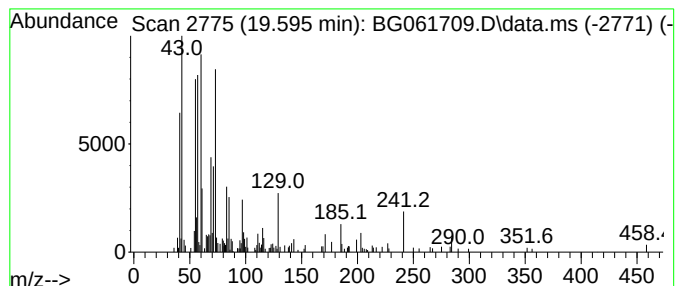
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Octadecanoic acid, 2-(2-hyd... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.595	2.34 ng/ul	140004	Chrysene-d12	21.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
2			Octadecanoic acid	284	C18H36O2	000057-11-4	86
3			Octadecanoic acid	284	C18H36O2	000057-11-4	80
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061709.D
Acq On : 25 Jun 2024 19:18
Operator : MA/JU
Sample : P2873-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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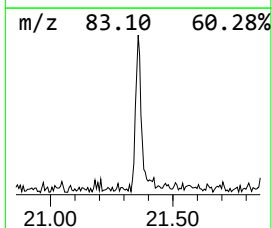
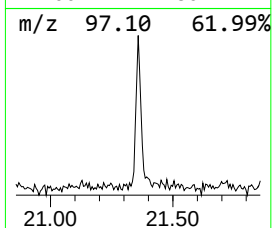
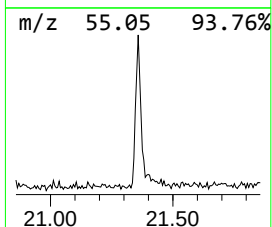
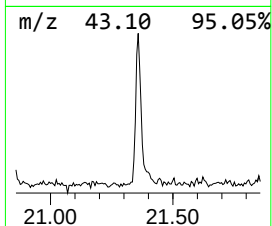
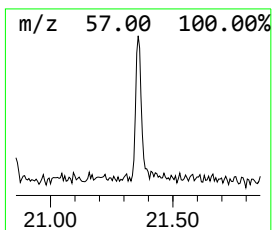
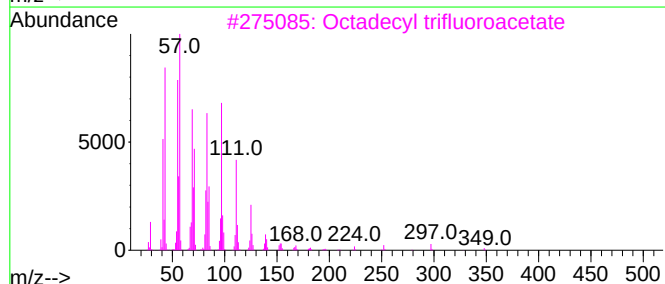
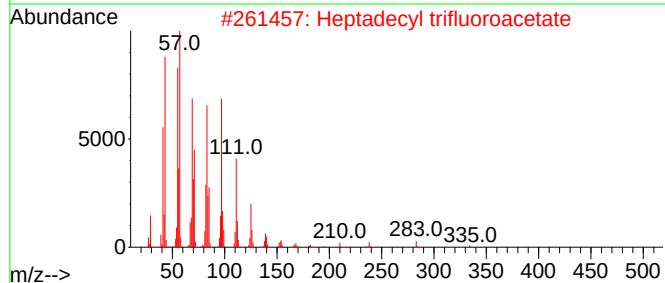
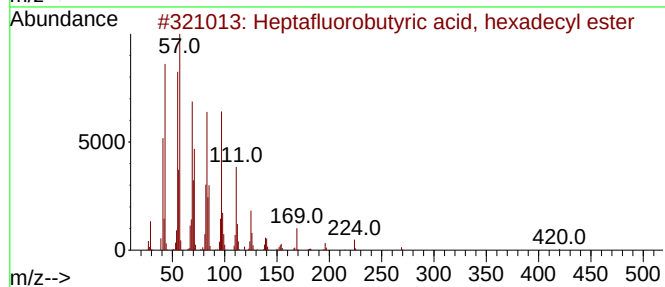
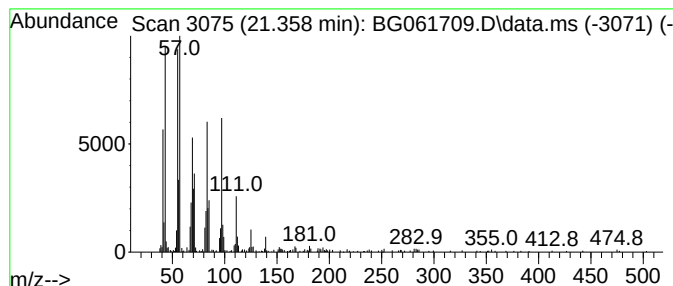
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.358	6.91 ng/ul	413372	Chrysene-d12	21.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062424\
Data File : BG061709.D
Acq On : 25 Jun 2024 19:18
Operator : MA/JU
Sample : P2873-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0SH8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.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
L-Lactic acid	3.731	11.1	ng/ul	184614	1	8.073	332984	20.0
Methoxymethyl i...	7.656	5.0	ng/ul	83843	1	8.073	332984	20.0
1-Phenoxypropan...	11.616	7.2	ng/ul	197995	2	10.882	548731	20.0
Hexathiane	15.294	4.6	ng/ul	192619	3	14.701	838280	20.0
n-Hexadecanoic ...	18.332	8.3	ng/ul	511829	4	17.445	1225930	20.0
Octadecanoic ac...	19.595	2.3	ng/ul	140004	5	21.710	1195810	20.0
Heptafluorobuty...	21.358	6.9	ng/ul	413372	5	21.710	1195810	20.0