

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
 Data File : BG062476.D
 Acq On : 20 Aug 2024 13:49
 Operator : MA/JU
 Sample : P3504-15
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCYE7

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-BG081424.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG062476.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.406	17	20	28	rVB5	12405	19526	1.27%	0.110%
2	3.670	61	65	72	rBV	32299	49572	3.23%	0.278%
3	3.817	87	90	99	rVV3	13626	24270	1.58%	0.136%
4	4.146	143	146	151	rVB5	5174	7258	0.47%	0.041%
5	4.363	180	183	187	rVV3	2599	3219	0.21%	0.018%
6	4.781	251	254	256	rVB3	2399	2738	0.18%	0.015%
7	5.057	298	301	308	rVB4	2828	3535	0.23%	0.020%
8	6.026	462	466	470	rBV	4951	6997	0.46%	0.039%
9	6.502	544	547	555	rVB4	1767	4376	0.29%	0.025%
10	6.643	565	571	574	rBV3	3405	4481	0.29%	0.025%
11	6.931	614	620	626	rVB5	2254	4335	0.28%	0.024%
12	7.101	642	649	662	rVV	208284	367714	23.98%	2.063%
13	7.271	670	678	686	rBV	138147	224767	14.66%	1.261%
14	7.477	706	713	719	rBV	183522	307293	20.04%	1.724%
15	7.536	719	723	728	rVB	4675	6726	0.44%	0.038%
16	7.941	784	792	799	rBV	277501	464037	30.26%	2.603%
17	8.006	799	803	807	rVB3	4351	6077	0.40%	0.034%
18	8.640	903	911	922	rBV	259641	433759	28.28%	2.434%
19	9.092	982	988	996	rVB	184170	310503	20.25%	1.742%
20	9.533	1059	1063	1069	rVB4	3384	5320	0.35%	0.030%
21	9.656	1077	1084	1091	rBV3	16989	28989	1.89%	0.163%
22	9.815	1103	1111	1118	rBV	149252	259880	16.95%	1.458%
23	10.038	1145	1149	1154	rBV5	2261	3724	0.24%	0.021%
24	10.355	1194	1203	1211	rBV	254186	451422	29.44%	2.533%
25	10.508	1225	1229	1232	rBV4	2577	3513	0.23%	0.020%
26	10.737	1259	1268	1278	rBV	427638	760544	49.59%	4.267%
27	10.861	1283	1289	1298	rVB	70311	129167	8.42%	0.725%
28	11.260	1353	1357	1364	rVB3	7159	11973	0.78%	0.067%
29	11.471	1387	1393	1398	rBV3	41083	73130	4.77%	0.410%
30	11.513	1398	1400	1405	rVB5	3775	5790	0.38%	0.032%
31	12.323	1533	1538	1541	rVB3	4142	6566	0.43%	0.037%
32	12.552	1574	1577	1583	rVB2	1998	2819	0.18%	0.016%
33	13.175	1678	1683	1685	rBV	1743	2431	0.16%	0.014%
34	13.398	1717	1721	1725	rVB3	3887	4277	0.28%	0.024%
35	13.757	1779	1782	1786	rBV2	1646	2265	0.15%	0.013%
36	13.968	1812	1818	1824	rVV	465470	639648	41.71%	3.589%

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37	14.209	1853	1859	1861	rBV2	6161	7608	0.50%	0.043%
38	14.256	1861	1867	1876	rVB	529916	813792	53.07%	4.566%
39	14.467	1899	1903	1908	rVB2	6220	8254	0.54%	0.046%
40	14.561	1911	1919	1929	rBV	736989	1142436	74.50%	6.410%
41	14.749	1942	1951	1962	rBV2	198685	384666	25.08%	2.158%
42	14.967	1983	1988	1989	rBV3	4637	4120	0.27%	0.023%
43	15.125	2011	2015	2017	rBV4	1895	2273	0.15%	0.013%
44	15.360	2051	2055	2059	rBV4	3427	5721	0.37%	0.032%
45	15.413	2062	2064	2071	rBV4	3187	4483	0.29%	0.025%
46	15.478	2071	2075	2078	rVB4	2136	2547	0.17%	0.014%
47	15.554	2081	2088	2096	rBV	690933	1038591	67.72%	5.827%
48	15.660	2100	2106	2113	rBV	174365	263028	17.15%	1.476%
49	15.795	2125	2129	2130	rBV2	2479	2416	0.16%	0.014%
50	15.895	2143	2146	2149	rBV3	1934	2091	0.14%	0.012%
51	15.983	2158	2161	2165	rVB5	1906	3149	0.21%	0.018%
52	16.124	2179	2185	2189	rBV7	3280	5777	0.38%	0.032%
53	16.242	2203	2205	2208	rBV4	2113	2576	0.17%	0.014%
54	16.277	2208	2211	2215	rVV4	11787	14129	0.92%	0.079%
55	16.377	2226	2228	2231	rVB4	1898	1880	0.12%	0.011%
56	16.435	2231	2238	2244	rBV6	9435	18261	1.19%	0.102%
57	16.482	2244	2246	2249	rVV4	1456	2044	0.13%	0.011%
58	16.553	2255	2258	2260	rVB3	1941	2221	0.14%	0.012%
59	16.706	2280	2284	2287	rVV4	3874	5272	0.34%	0.030%
60	16.800	2295	2300	2301	rBV4	2233	3721	0.24%	0.021%
61	16.858	2305	2310	2313	rBV4	4773	6226	0.41%	0.035%
62	17.017	2334	2337	2341	rBV4	4026	4756	0.31%	0.027%
63	17.070	2343	2346	2347	rBV3	4227	3911	0.26%	0.022%
64	17.176	2360	2364	2369	rBV6	3070	4706	0.31%	0.026%
65	17.305	2379	2386	2393	rVB	873577	1373427	89.56%	7.706%
66	17.399	2396	2402	2412	rVB	654937	964796	62.91%	5.413%
67	17.481	2412	2416	2418	rBV5	3630	3915	0.26%	0.022%
68	17.587	2432	2434	2436	rVB3	2578	2079	0.14%	0.012%
69	17.687	2447	2451	2456	rBV7	3830	7223	0.47%	0.041%
70	17.792	2468	2469	2470	rBV	2933	1905	0.12%	0.011%
71	17.933	2489	2493	2494	rBV4	3305	4042	0.26%	0.023%
72	17.980	2496	2501	2507	rVB7	6657	11097	0.72%	0.062%
73	18.068	2513	2516	2520	rBV5	6357	7886	0.51%	0.044%
74	18.198	2533	2538	2548	rBV	160220	252226	16.45%	1.415%
75	18.386	2568	2570	2573	rBV4	4506	5417	0.35%	0.030%
76	18.450	2578	2581	2583	rBV3	2423	3060	0.20%	0.017%

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77	18.503	2586	2590	2591	rBV3	6758	8972	0.59%	0.050%
78	18.521	2591	2593	2594	rBV2	4953	4071	0.27%	0.023%
79	18.627	2607	2611	2613	rBV5	4666	6392	0.42%	0.036%
80	18.674	2615	2619	2622	rVV6	8965	13370	0.87%	0.075%
81	18.861	2648	2651	2653	rBV4	4876	6819	0.44%	0.038%
82	19.085	2681	2689	2693	rBV5	43417	75713	4.94%	0.425%
83	19.249	2714	2717	2722	rVB5	10604	13326	0.87%	0.075%
84	19.320	2724	2729	2732	rBV2	24401	42526	2.77%	0.239%
85	19.349	2732	2734	2738	rVB4	14829	16851	1.10%	0.095%
86	19.467	2750	2754	2761	rBV3	54748	87699	5.72%	0.492%
87	19.625	2778	2781	2782	rBV3	9935	10154	0.66%	0.057%
88	19.684	2785	2791	2796	rBV	882437	1323889	86.33%	7.428%
89	20.201	2875	2879	2882	rBV6	14470	23851	1.56%	0.134%
90	20.236	2882	2885	2887	rVV	15572	17600	1.15%	0.099%
91	20.724	2966	2968	2970	rBV2	14218	12262	0.80%	0.069%
92	21.176	3042	3045	3046	rBV2	20063	19914	1.30%	0.112%
93	21.211	3047	3051	3057	rVV2	134796	214034	13.96%	1.201%
94	21.540	3101	3107	3115	rBV2	892215	1444259	94.18%	8.103%
95	22.339	3238	3243	3255	rBV5	53422	137808	8.99%	0.773%
96	23.772	3482	3487	3493	rBV	49510	99851	6.51%	0.560%
97	24.413	3587	3596	3611	rVB	457254	1217469	79.39%	6.831%
98	24.624	3622	3632	3651	rVB	540332	1533559	100.00%	8.604%
99	25.441	3761	3771	3772	rBV6	63770	155458	10.14%	0.872%
100	25.870	3836	3844	3862	rVB4	88002	297427	19.39%	1.669%

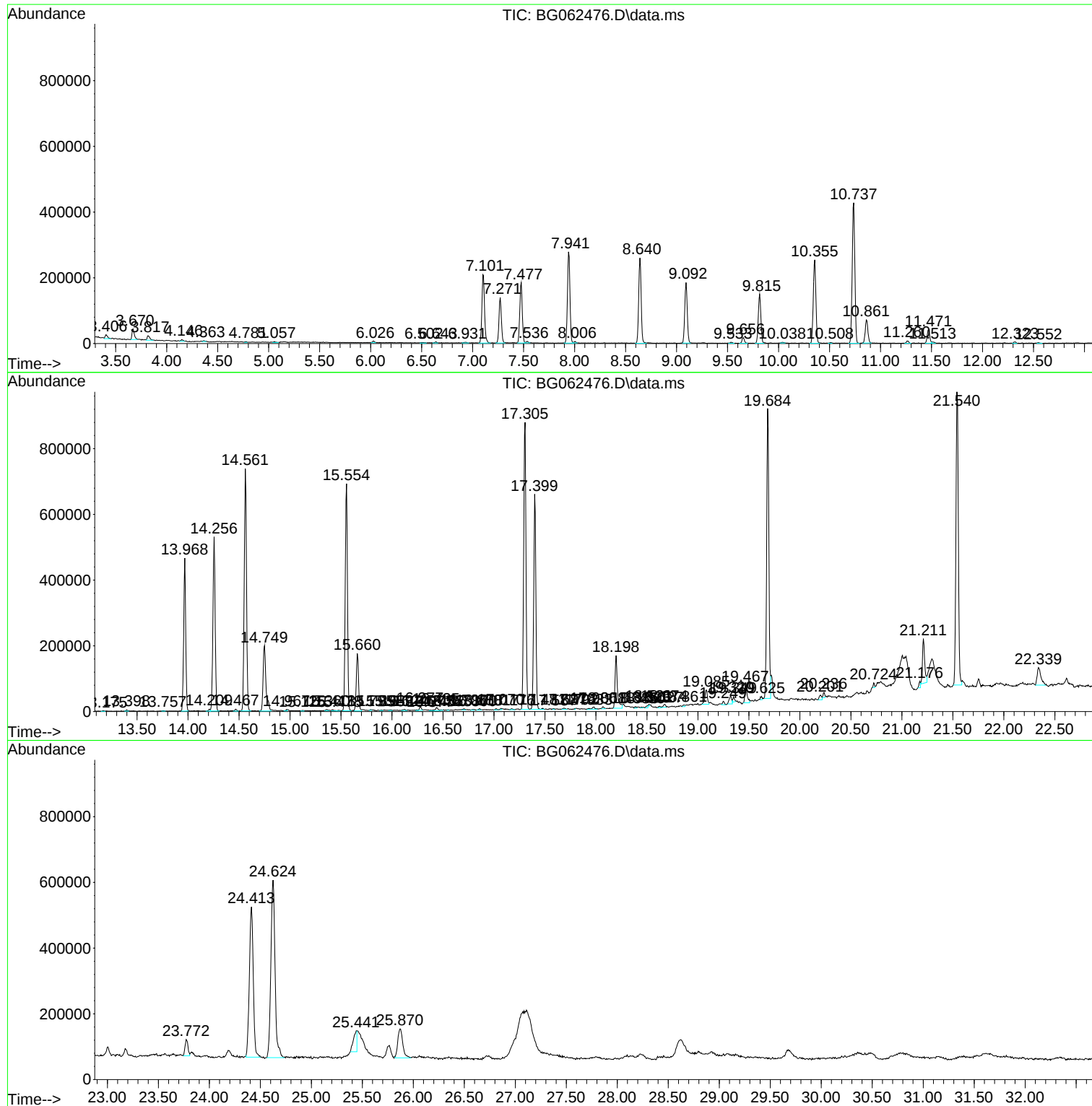
Sum of corrected areas: 17823643

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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



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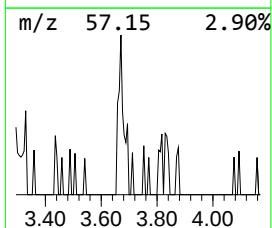
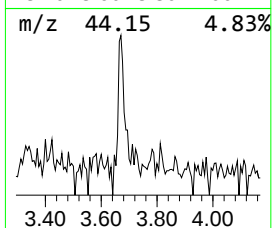
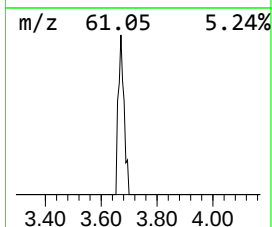
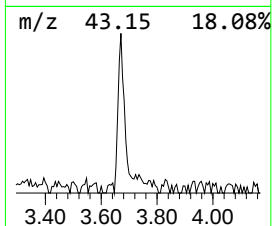
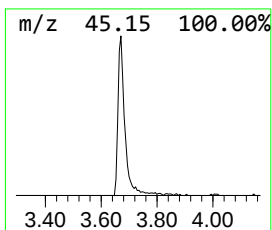
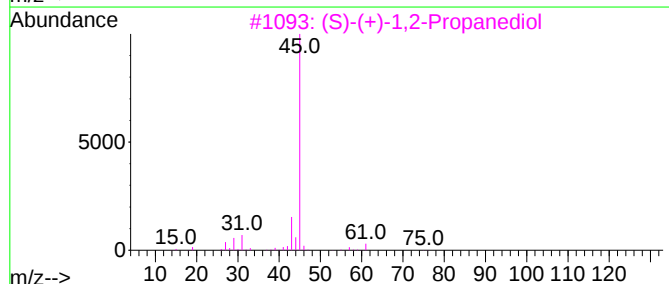
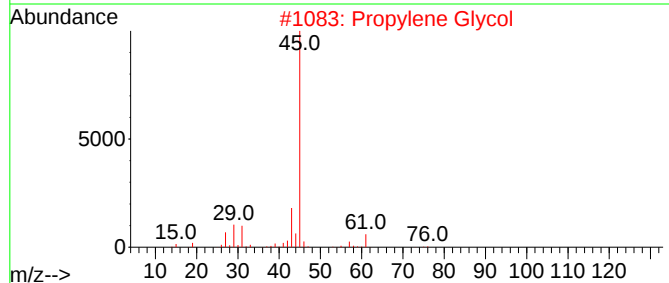
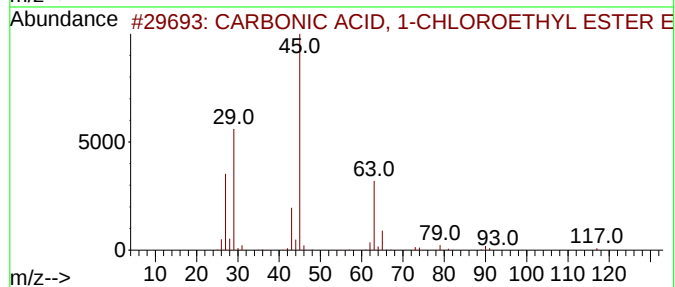
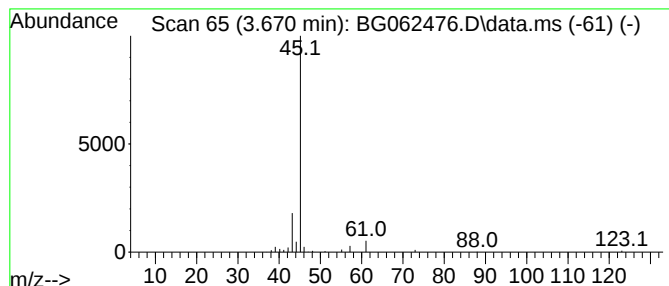
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.670	2.14 ng/ul	49572	1,4-Dichlorobenzene-d4	7.941

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			CARBONIC ACID, 1-CHLOROETHYL EST...	152	C5H9ClO3	050893-36-2	9
2			Propylene Glycol	76	C3H8O2	000057-55-6	9
3			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4			Propylene Glycol	76	C3H8O2	000057-55-6	9
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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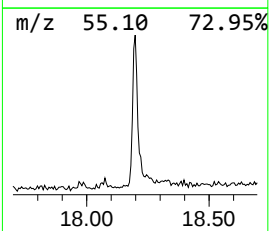
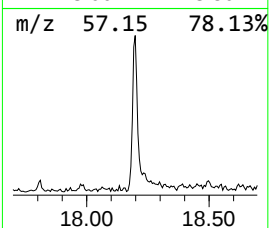
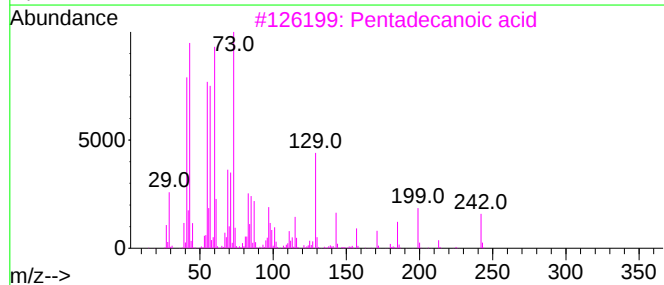
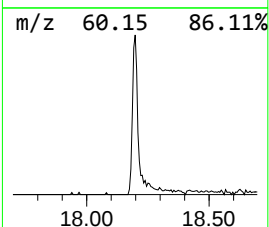
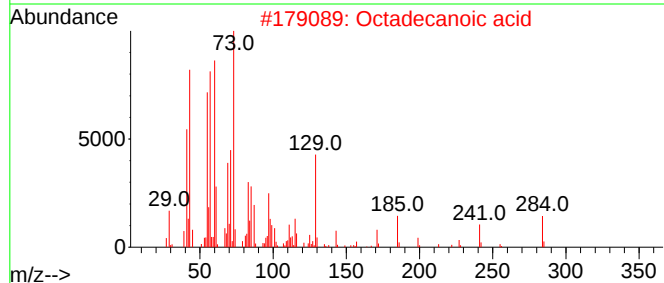
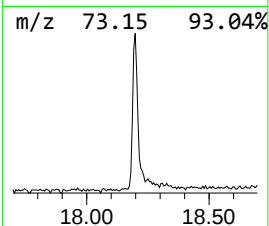
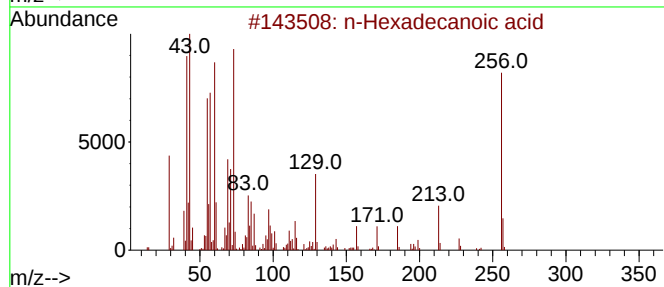
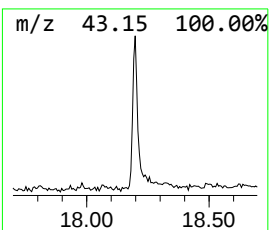
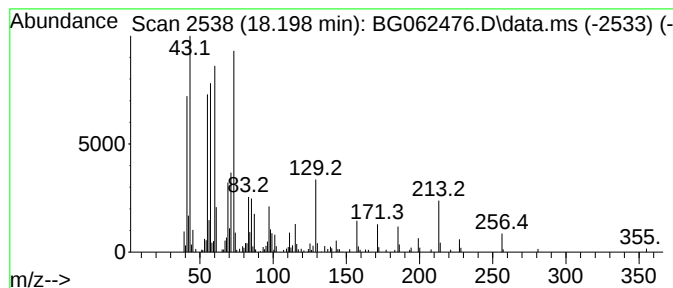
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	3.67 ng/ul	252226	Phenanthrene-d10	17.305

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	86
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83



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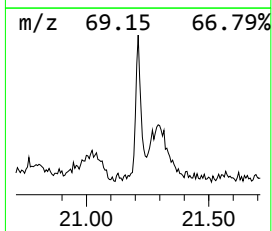
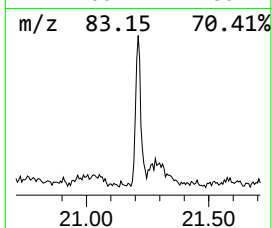
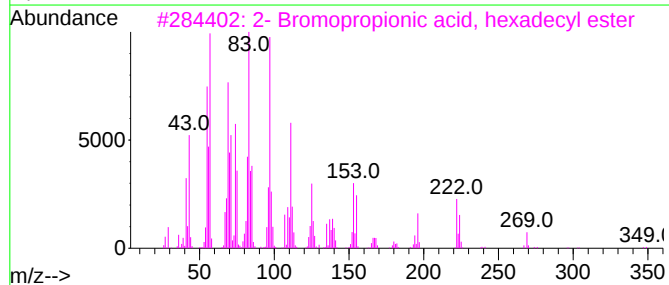
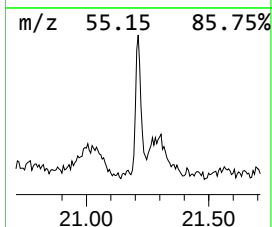
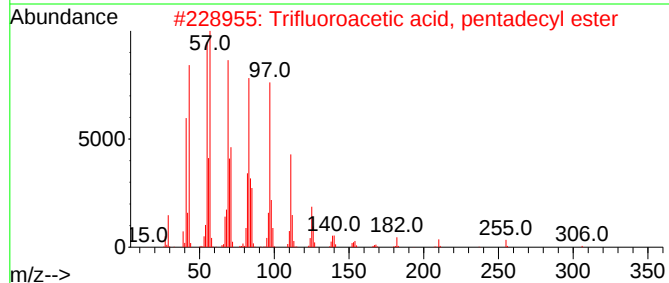
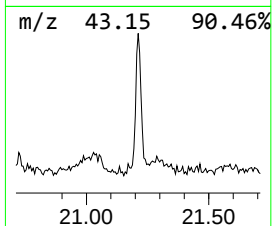
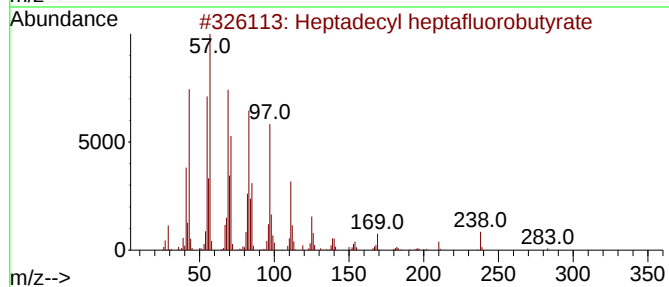
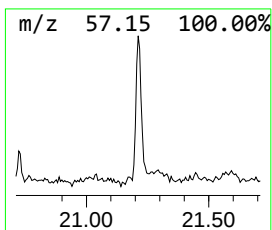
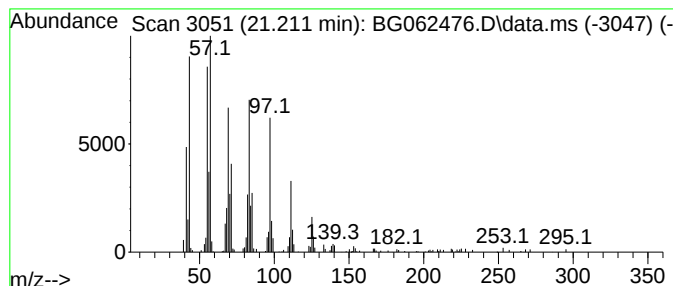
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.211	2.96 ng/ul	214034	Chrysene-d12	21.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3			2- Bromopropionic acid, hexadecy...	376	C19H37BrO2	063966-83-6	91
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
Data File : BG062476.D
Acq On : 20 Aug 2024 13:49
Operator : MA/JU
Sample : P3504-15
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE7

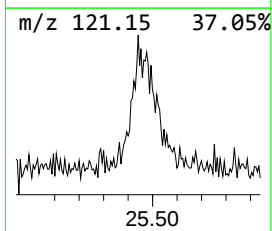
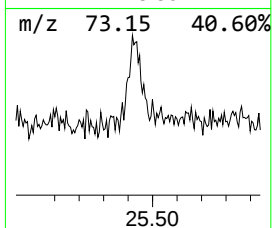
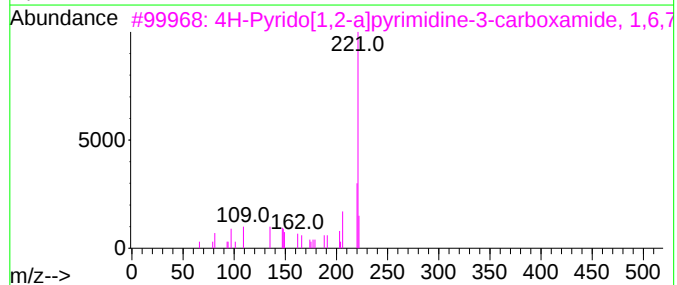
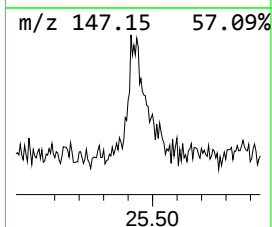
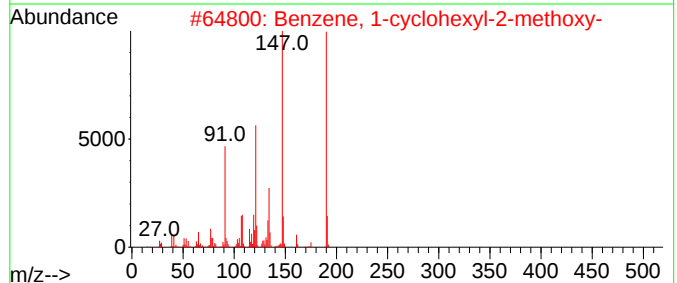
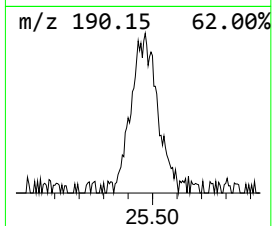
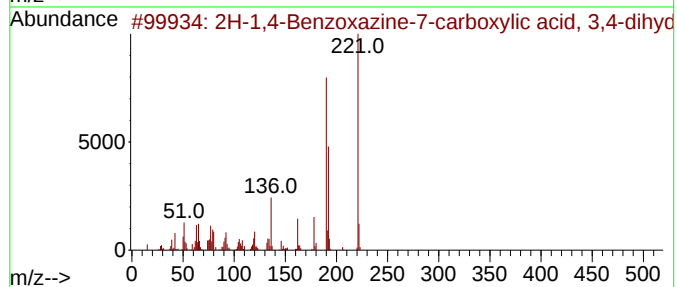
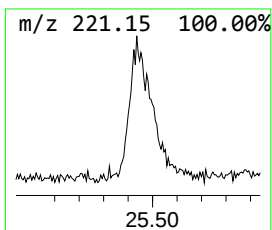
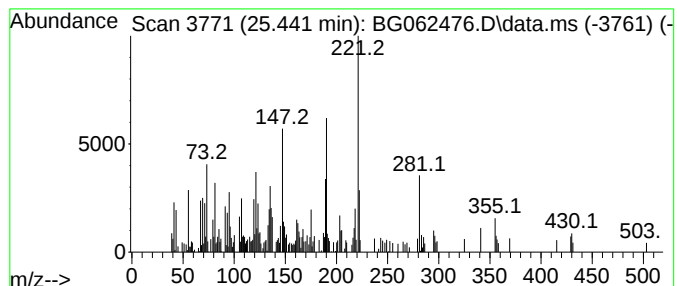
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.441	2.03 ng/ul	155458	Perylene-d12	24.624

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,4-Benzoxazine-7-carboxylic ...	221	C11H11N04	201294-27-1	49		
2	Benzene, 1-cyclohexyl-2-methoxy-	190	C13H18O	002206-48-6	38		
3	4H-Pyrido[1,2-a]pyrimidine-3-car...	221	C11H15N3O2	064399-29-7	38		
4	1,3,4-Oxadiazol-2-amine, 5-(3,4-...	221	C10H11N3O3	1000362-71-7	38		
5	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	35		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
Data File : BG062476.D
Acq On : 20 Aug 2024 13:49
Operator : MA/JU
Sample : P3504-15
Misc :
ALS Vial : 8 Sample Multiplier: 1

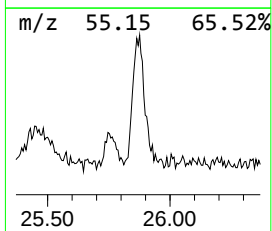
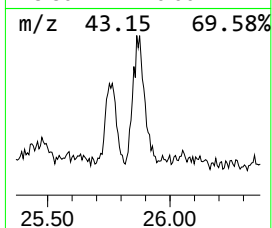
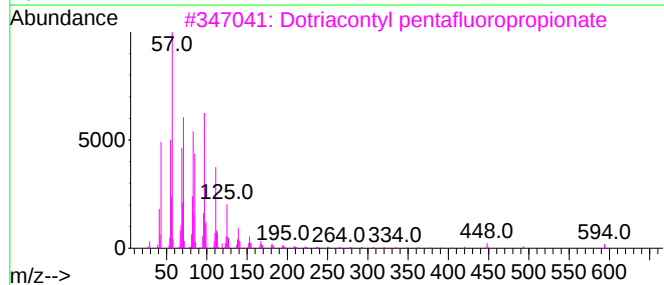
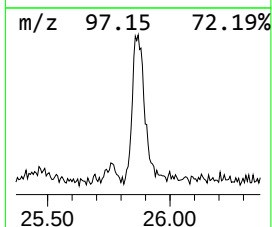
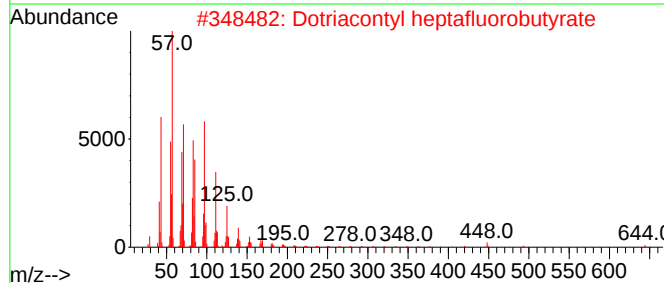
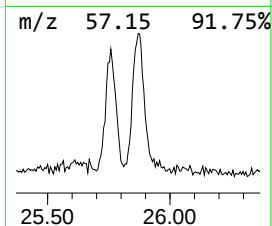
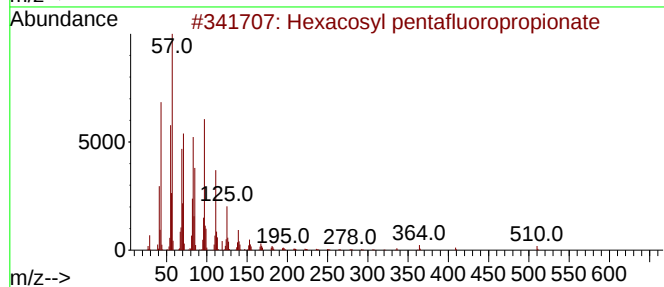
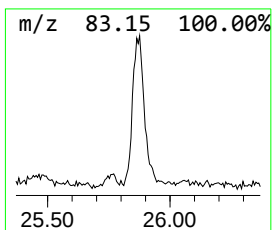
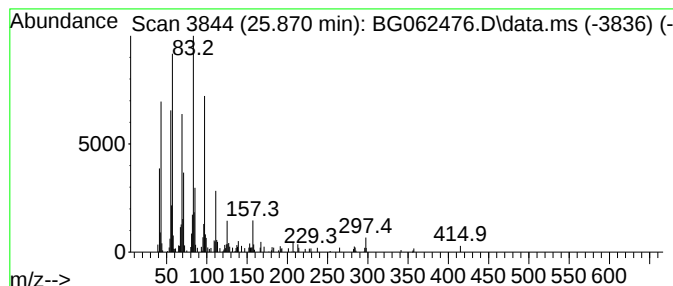
Instrument :
BNA_G
ClientSampleId :
DCYE7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 Hexacosyl pentafluoropropio... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
25.870	3.88 ng/ul	297427	Perylene-d12			24.624
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosyl pentafluoropropionate		528	C29H53F5O2	1000351-81-2	50
2	Dotriacontyl heptafluorobutyrate		662	C36H65F7O2	1000351-84-2	50
3	Dotriacontyl pentafluoropropionate		612	C35H65F5O2	1010351-81-4	50
4	Heptacosyl pentafluoropropionate		542	C30H55F5O2	1000351-81-6	50
5	Octacosyl heptafluorobutyrate		606	C32H57F7O2	1010351-83-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082024\
Data File : BG062476.D
Acq On : 20 Aug 2024 13:49
Operator : MA/JU
Sample : P3504-15
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCYE7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	3.670	2.1	ng/ul	49572	1	7.941	464037	20.0
n-Hexadecanoic ...	18.198	3.7	ng/ul	252226	4	17.305	1373430	20.0
Heptadecyl hept...	21.211	3.0	ng/ul	214034	5	21.540	1444260	20.0
unknown-02	25.441	2.0	ng/ul	155458	6	24.624	1533560	20.0
Hexacosyl penta...	25.870	3.9	ng/ul	297427	6	24.624	1533560	20.0