

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121421\
 Data File : BG051546.D
 Acq On : 15 Dec 2021 21:05
 Operator : CG/JU
 Sample : M4995-09
 Misc :
 ALS Vial : 44 Sample Multiplier: 1

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-BG121421.M

Title : SVOA CALIBRATION

Signal : TIC: BG051546.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.582	11	16	17	rBV3	8685	12597	0.87%	0.104%
2	3.600	17	19	23	rVV	10659	16316	1.12%	0.135%
3	3.641	23	26	34	rVB2	14445	23241	1.60%	0.192%
4	4.040	90	94	102	rBV2	17616	34443	2.37%	0.285%
5	4.387	148	153	156	rBV3	2165	2688	0.18%	0.022%
6	4.933	241	246	252	rVV3	11411	19595	1.35%	0.162%
7	7.406	659	667	678	rBV	46536	85160	5.85%	0.704%
8	7.583	690	697	705	rBV	126984	211218	14.51%	1.745%
9	7.800	727	734	742	rBV	132539	230785	15.85%	1.907%
10	7.900	744	751	753	rBV2	944	1609	0.11%	0.013%
11	8.282	808	816	822	rBV	112592	192227	13.20%	1.589%
12	8.470	844	848	850	rBV	1013	1552	0.11%	0.013%
13	8.969	926	933	940	rBV2	117703	202321	13.90%	1.672%
14	9.357	996	999	1003	rBV	1319	1882	0.13%	0.016%
15	9.445	1007	1014	1024	rVV	171876	305017	20.95%	2.521%
16	9.527	1024	1028	1030	rVB	1471	1691	0.12%	0.014%
17	9.885	1082	1089	1093	rVV2	5142	8118	0.56%	0.067%
18	10.179	1131	1139	1148	rVB	137544	246277	16.92%	2.035%
19	10.720	1222	1231	1238	rBV	212774	366591	25.18%	3.029%
20	10.872	1250	1257	1261	rVB3	1941	3845	0.26%	0.032%
21	11.119	1290	1299	1307	rBV	148576	272730	18.73%	2.254%
22	11.237	1311	1319	1326	rVV	161950	288792	19.84%	2.387%
23	12.141	1468	1473	1476	rVB	1151	1994	0.14%	0.016%
24	12.511	1531	1536	1541	rBV3	2925	4027	0.28%	0.033%
25	12.687	1563	1566	1569	rVB3	3082	4273	0.29%	0.035%
26	12.881	1596	1599	1606	rVB	1255	1963	0.13%	0.016%
27	13.046	1623	1627	1631	rVB	1302	2150	0.15%	0.018%
28	13.281	1664	1667	1669	rBV2	1765	1703	0.12%	0.014%
29	13.298	1669	1670	1675	rVB	1183	1551	0.11%	0.013%
30	13.463	1693	1698	1703	rVB2	1471	2323	0.16%	0.019%
31	13.522	1705	1708	1711	rBV3	1286	1524	0.10%	0.013%
32	13.739	1738	1745	1753	rBV3	6858	12824	0.88%	0.106%
33	14.303	1832	1841	1847	rBV	475665	673275	46.25%	5.564%
34	14.532	1877	1880	1885	rVV3	5981	8934	0.61%	0.074%
35	14.608	1885	1893	1900	rVV	470855	743363	51.06%	6.143%
36	14.685	1903	1906	1909	rVB2	1249	1510	0.10%	0.012%

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 Title : SVOA CALIBRATION

37	14.796	1921	1925	1933	rBV3	3841	6708	0.46%	0.055%
38	14.914	1937	1945	1952	rVB	264150	417751	28.69%	3.452%
39	15.067	1965	1971	1977	rBV	55994	93022	6.39%	0.769%
40	15.178	1986	1990	1993	rVB2	1252	1638	0.11%	0.014%
41	15.243	1998	2001	2005	rVB2	1436	2258	0.16%	0.019%
42	15.296	2005	2010	2016	rBV4	2746	4895	0.34%	0.040%
43	15.478	2035	2041	2042	rBV3	1424	1511	0.10%	0.012%
44	15.537	2048	2051	2054	rBV2	2235	2470	0.17%	0.020%
45	15.631	2065	2067	2072	rVB2	3120	3349	0.23%	0.028%
46	15.701	2074	2079	2083	rBV4	11911	18358	1.26%	0.152%
47	15.736	2083	2085	2088	rVB3	1859	2482	0.17%	0.021%
48	15.901	2106	2113	2121	rBV	663243	986313	67.75%	8.151%
49	15.995	2123	2129	2139	rBV	232999	346457	23.80%	2.863%
50	16.136	2150	2153	2158	rVB3	3374	3821	0.26%	0.032%
51	16.253	2170	2173	2175	rVB3	2337	2629	0.18%	0.022%
52	16.300	2178	2181	2184	rVV3	2811	3033	0.21%	0.025%
53	16.394	2192	2197	2204	rBV2	13349	20152	1.38%	0.167%
54	16.529	2219	2220	2221	rBV	3012	1792	0.12%	0.015%
55	16.576	2224	2228	2231	rVV4	2876	4002	0.27%	0.033%
56	16.600	2231	2232	2235	rVB2	3036	2378	0.16%	0.020%
57	16.670	2241	2244	2245	rBV3	2071	2182	0.15%	0.018%
58	16.782	2258	2263	2268	rBV6	2873	4886	0.34%	0.040%
59	16.899	2277	2283	2287	rBV5	7099	12354	0.85%	0.102%
60	16.946	2289	2291	2293	rBV2	3595	3713	0.26%	0.031%
61	17.017	2299	2303	2304	rBV3	1368	1701	0.12%	0.014%
62	17.117	2316	2320	2324	rBV3	2528	3483	0.24%	0.029%
63	17.187	2327	2332	2333	rBV3	1768	2341	0.16%	0.019%
64	17.358	2358	2361	2363	rBV3	2803	3469	0.24%	0.029%
65	17.393	2364	2367	2371	rBV4	6022	6060	0.42%	0.050%
66	17.557	2391	2395	2396	rBV3	3369	3861	0.27%	0.032%
67	17.657	2405	2412	2418	rVV	366984	554222	38.07%	4.580%
68	17.757	2422	2429	2437	rVB	798560	1234134	84.77%	10.199%
69	17.880	2448	2450	2451	rBV2	1739	1495	0.10%	0.012%
70	18.021	2471	2474	2476	rBV4	2850	3278	0.23%	0.027%
71	18.115	2487	2490	2492	rBV3	2048	1924	0.13%	0.016%
72	18.139	2492	2494	2499	rVB5	4617	5758	0.40%	0.048%
73	18.180	2499	2501	2502	rBV2	2889	2549	0.18%	0.021%
74	18.215	2505	2507	2510	rBV	1238	1568	0.11%	0.013%
75	18.303	2521	2522	2530	rVB6	2952	5042	0.35%	0.042%
76	18.415	2540	2541	2543	rBV2	1957	1488	0.10%	0.012%

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 Title : SVOA CALIBRATION

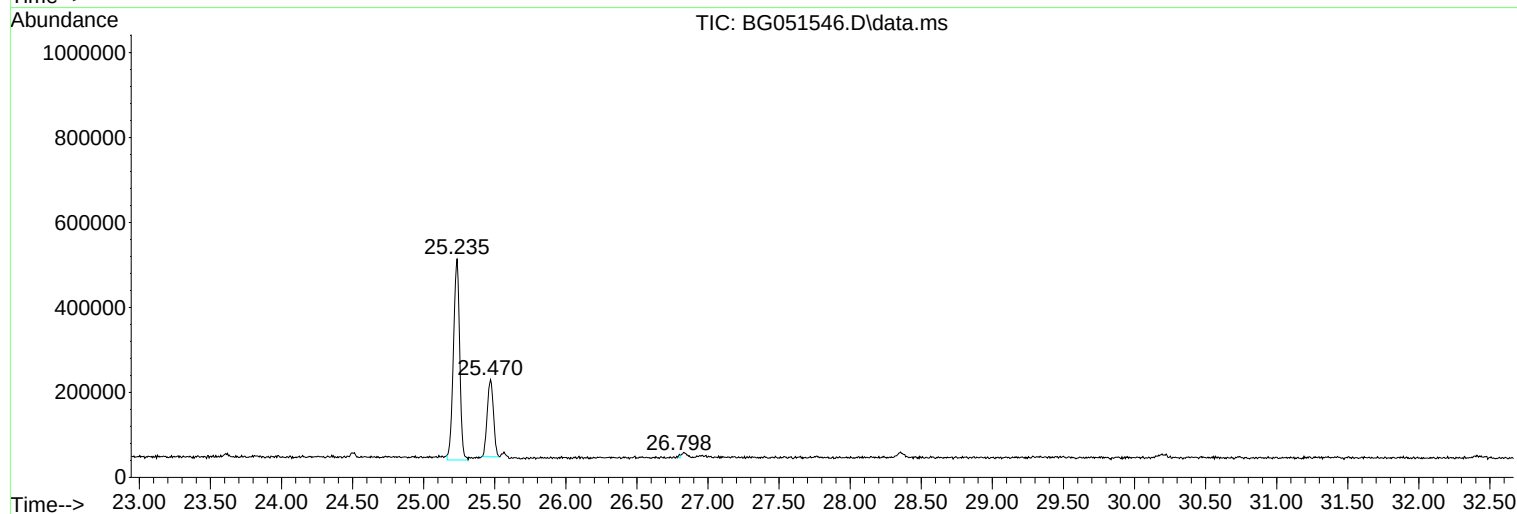
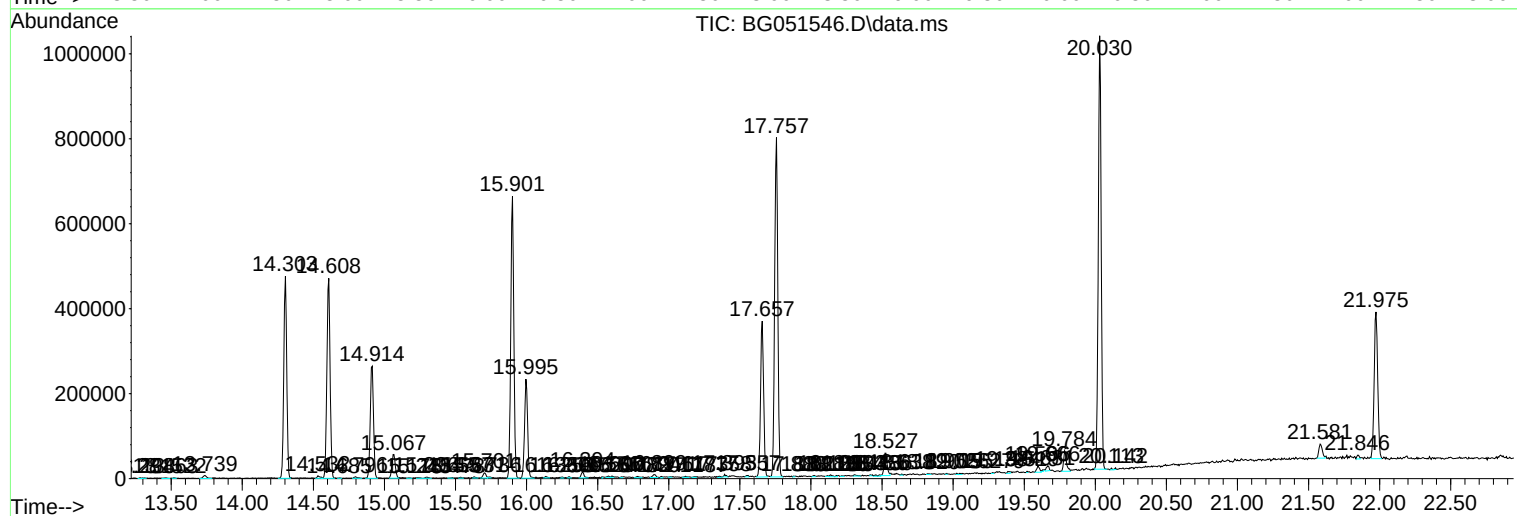
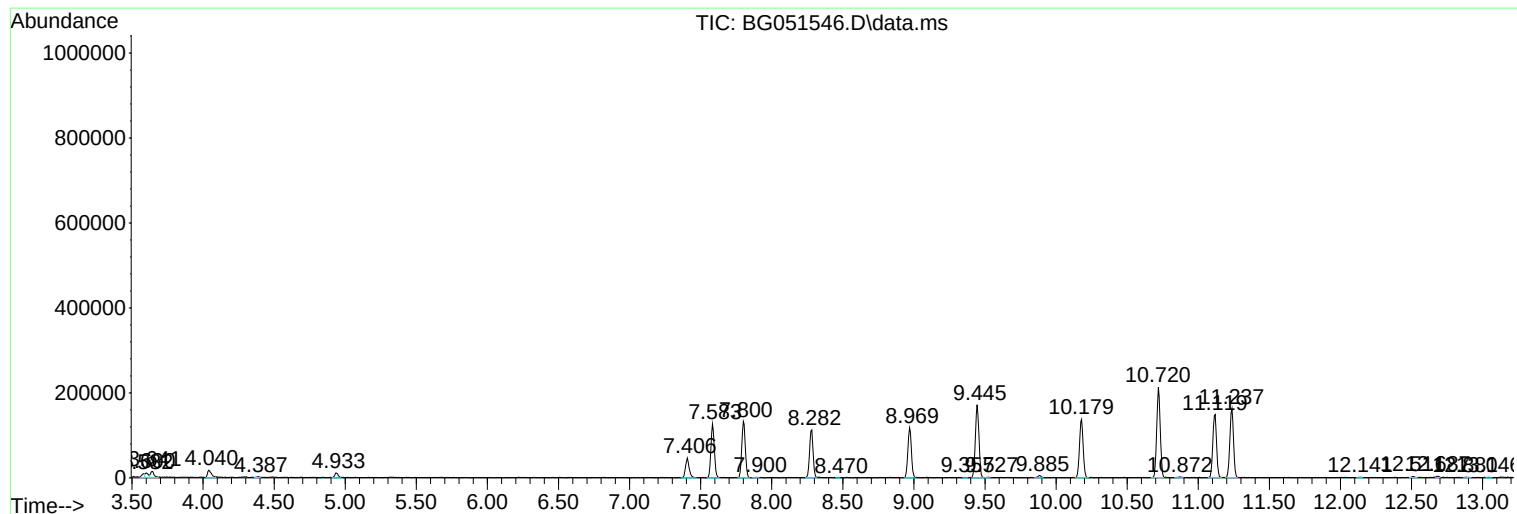
77	18.456	2545	2548	2550	rVB3	3068	3136	0.22%	0.026%
78	18.486	2550	2553	2554	rBV2	3331	3291	0.23%	0.027%
79	18.527	2554	2560	2565	rBV2	52800	81184	5.58%	0.671%
80	18.638	2577	2579	2581	rVB3	2778	1931	0.13%	0.016%
81	18.820	2608	2610	2614	rBV5	2224	3101	0.21%	0.026%
82	18.955	2631	2633	2634	rBV2	2254	1474	0.10%	0.012%
83	19.026	2644	2645	2647	rVB2	3034	1504	0.10%	0.012%
84	19.055	2647	2650	2651	rBV3	2663	2784	0.19%	0.023%
85	19.279	2686	2688	2689	rBV2	2361	1625	0.11%	0.013%
86	19.384	2704	2706	2709	rBV3	4784	6170	0.42%	0.051%
87	19.519	2728	2729	2730	rBV	3198	1459	0.10%	0.012%
88	19.596	2738	2742	2746	rBV3	15042	21028	1.44%	0.174%
89	19.631	2746	2748	2749	rVV2	4268	3271	0.22%	0.027%
90	19.666	2751	2754	2757	rVB2	11596	14748	1.01%	0.122%
91	19.784	2770	2774	2781	rBV2	48349	67222	4.62%	0.556%
92	20.030	2810	2816	2825	rVB	1020171	1455881	100.00%	12.031%
93	20.113	2828	2830	2833	rBV3	4037	3150	0.22%	0.026%
94	20.142	2833	2835	2836	rBV2	4013	2183	0.15%	0.018%
95	21.581	3076	3080	3086	rBV5	33237	55768	3.83%	0.461%
96	21.846	3123	3125	3128	rBV3	9167	10830	0.74%	0.089%
97	21.975	3141	3147	3154	rVB	345212	589283	40.48%	4.870%
98	25.235	3690	3702	3715	rVB2	473854	1443457	99.15%	11.929%
99	25.470	3733	3742	3752	rVB2	181567	549185	37.72%	4.538%
100	26.798	3966	3968	3969	rBV2	8044	6552	0.45%	0.054%

Sum of corrected areas: 12100853

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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



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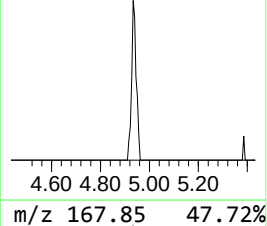
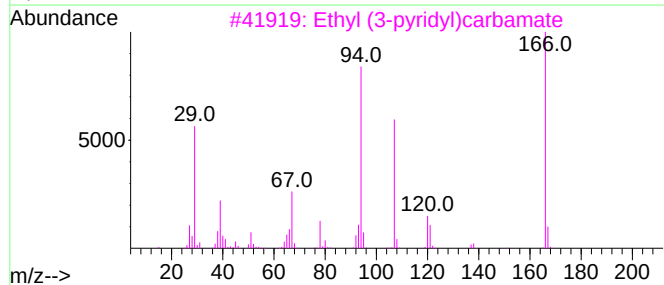
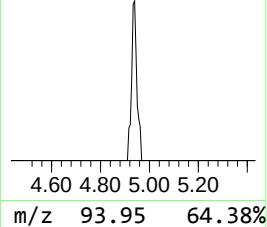
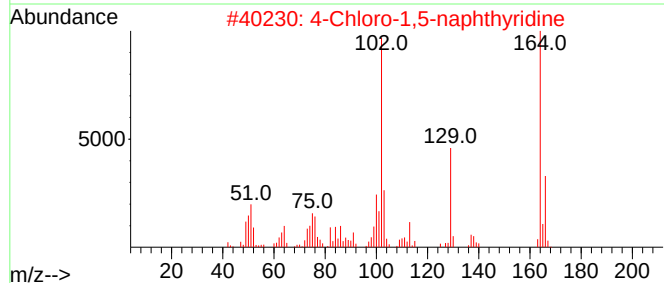
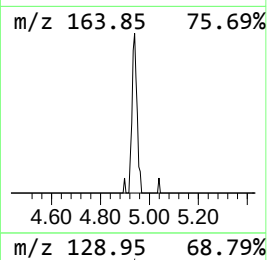
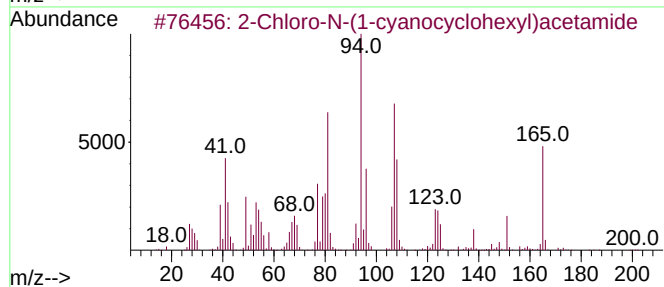
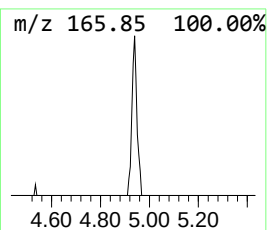
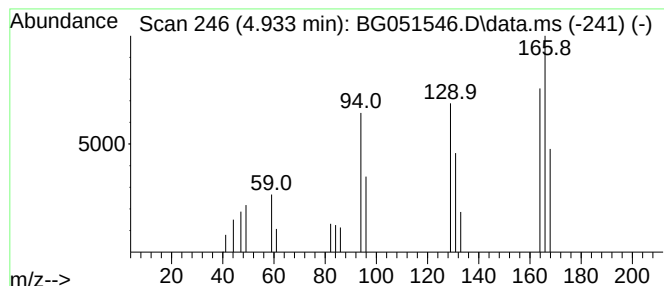
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.933	2.04 ng/ul	19595	1,4-Dichlorobenzene-d4	8.276

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloro-N-(1-cyanocyclohexyl)ac...	200	C9H13ClN2O	078734-78-8	9		
2	4-Chloro-1,5-naphthyridine	164	C8H5ClN2	007689-63-6	7		
3	Ethyl (3-pyridyl)carbamate	166	C8H10N2O2	006276-11-5	5		
4	Phosphorodichloridothioic acid, ...	164	CH3Cl2OPS	002523-94-6	5		
5	4-Chloro-2-aminopyrimidine	129	C4H4ClN3	003993-78-0	5		



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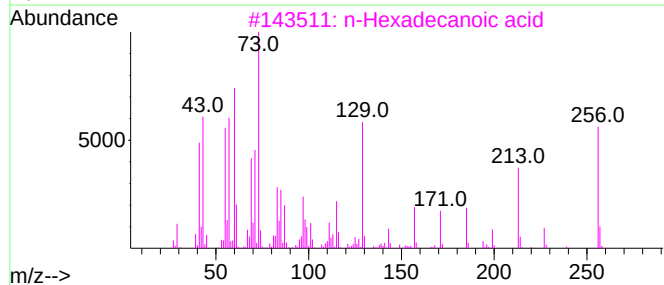
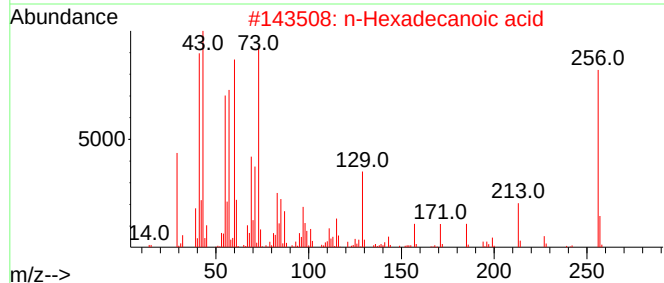
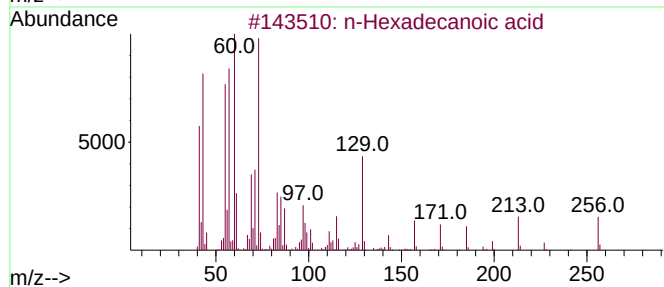
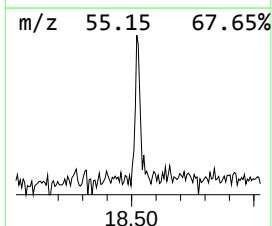
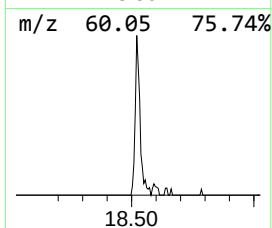
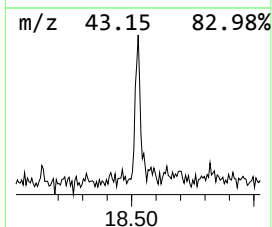
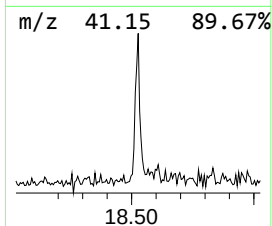
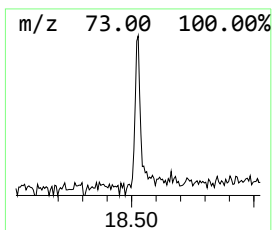
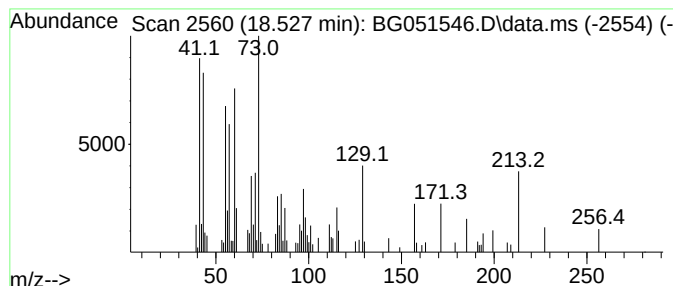
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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.
18.527	2.93 ng/ul	81184	Phenanthrene-d10	17.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	68



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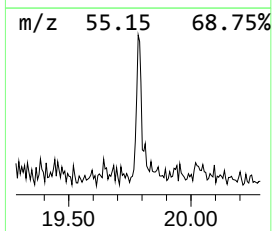
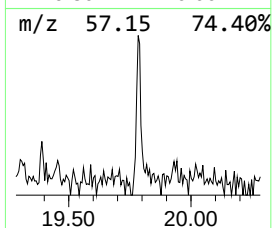
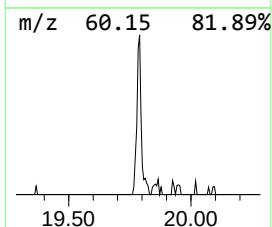
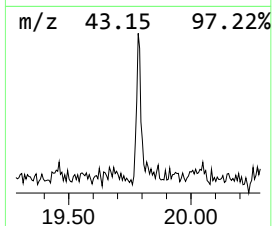
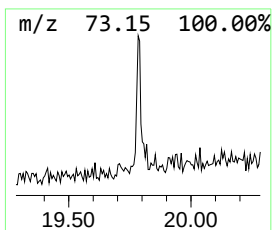
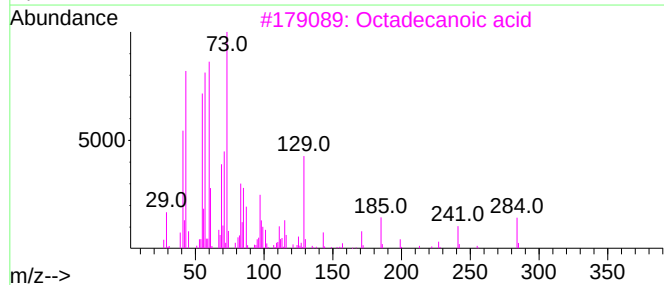
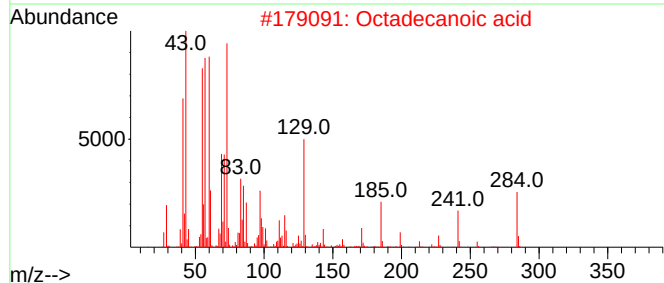
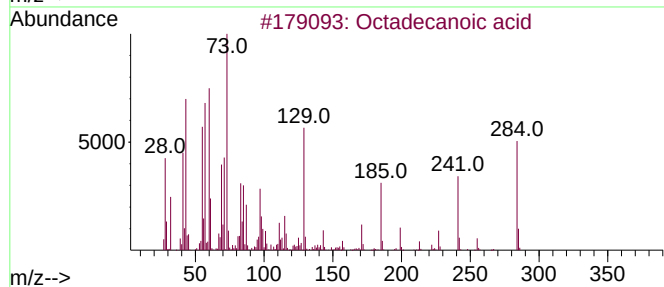
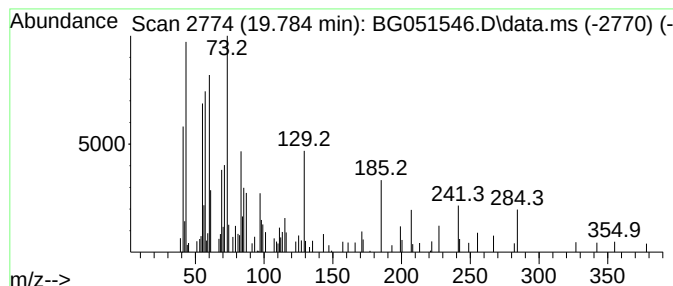
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.784	2.43 ng/ul	67222	Phenanthrene-d10	17.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid			284	C18H36O2	000057-11-4	99
2	Octadecanoic acid			284	C18H36O2	000057-11-4	99
3	Octadecanoic acid			284	C18H36O2	000057-11-4	98
4	Octadecanoic acid			284	C18H36O2	000057-11-4	97
5	Octadecanoic acid			284	C18H36O2	000057-11-4	96



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Acq On : 15 Dec 2021 21:05
Operator : CG/JU
Sample : M4995-09
Misc :
ALS Vial : 44 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG121421.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	4.933	2.0	ng/ul	19595	1	8.276	192227	20.0
n-Hexadecanoic ...	18.527	2.9	ng/ul	81184	4	17.657	554222	20.0
Octadecanoic acid	19.784	2.4	ng/ul	67222	4	17.657	554222	20.0