

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122123\
 Data File : BM043508.D
 Acq On : 21 Dec 2023 18:23
 Operator : MA/JU
 Sample : 05912-12
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 BH3N8

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_M\Methods\SFAM-EPA-BM121523.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM043508.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.287	15	17	23	rVB2	19540	26770	0.53%	0.051%
2	3.375	28	32	41	rVB	49777	67344	1.34%	0.129%
3	3.805	101	105	121	rBV	154772	277759	5.53%	0.530%
4	4.022	138	142	149	rVB2	48155	75473	1.50%	0.144%
5	4.122	155	159	166	rVB	22982	32899	0.65%	0.063%
6	4.334	191	195	201	rVB	21415	31005	0.62%	0.059%
7	4.499	219	223	231	rVB	37478	52346	1.04%	0.100%
8	4.987	304	306	310	rVB5	8382	9669	0.19%	0.018%
9	5.452	381	385	391	rVV	47349	73883	1.47%	0.141%
10	5.504	391	394	399	rVB4	8217	12135	0.24%	0.023%
11	5.810	440	446	455	rVB	73784	113934	2.27%	0.217%
12	6.022	478	482	484	rBV4	6850	9815	0.20%	0.019%
13	6.051	484	487	491	rVV5	6126	8170	0.16%	0.016%
14	6.969	634	643	650	rBV	68033	135802	2.70%	0.259%
15	7.069	655	660	665	rVV2	69332	115987	2.31%	0.221%
16	7.128	665	670	680	rVB	227198	404990	8.06%	0.773%
17	7.251	687	691	695	rBV3	12352	19986	0.40%	0.038%
18	7.310	695	701	712	rVB	825193	1328170	26.44%	2.534%
19	7.428	718	721	726	rVB2	14274	21228	0.42%	0.041%
20	7.498	726	733	743	rBV	736840	1179173	23.48%	2.250%
21	7.593	745	749	752	rVB5	5024	8500	0.17%	0.016%
22	7.975	807	814	820	rBV	761817	1249382	24.87%	2.384%
23	8.034	820	824	835	rVB	74217	123719	2.46%	0.236%
24	8.234	853	858	862	rBV8	10514	20674	0.41%	0.039%
25	8.487	897	901	905	rBV7	7004	12278	0.24%	0.023%
26	8.545	905	911	915	rVV	37287	62891	1.25%	0.120%
27	8.598	915	920	927	rVB	23437	46065	0.92%	0.088%
28	8.681	927	934	945	rBV	555484	988082	19.67%	1.885%
29	8.804	951	955	965	rVB	29273	50906	1.01%	0.097%
30	9.075	994	1001	1007	rBV	239442	395323	7.87%	0.754%
31	9.145	1007	1013	1021	rVB	981264	1607237	32.00%	3.067%
32	9.310	1036	1041	1050	rVB9	13284	24690	0.49%	0.047%
33	9.522	1072	1077	1086	rVB	27933	45135	0.90%	0.086%
34	9.863	1126	1135	1146	rBV	641857	1105331	22.01%	2.109%
35	10.098	1168	1175	1184	rBV	69871	129784	2.58%	0.248%
36	10.304	1204	1210	1216	rVB10	7434	16439	0.33%	0.031%

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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_M\Methods\SFAM-EPA-BM121523.MA.M
 Title : SVOA CALIBRATION

37	10.398	1216	1226	1240	rBV	950741	1621971	32.29%	3.095%
38	10.551	1249	1252	1257	rVB7	5377	9451	0.19%	0.018%
39	10.692	1263	1276	1283	rBV7	35857	110064	2.19%	0.210%
40	10.781	1283	1291	1297	rVV	1044980	1759862	35.04%	3.358%
41	10.839	1297	1301	1308	rVB3	25174	44882	0.89%	0.086%
42	10.922	1308	1315	1327	rBV	778353	1397179	27.82%	2.666%
43	11.445	1401	1404	1416	rVB6	11244	23739	0.47%	0.045%
44	11.575	1420	1426	1434	rBV	65594	115492	2.30%	0.220%
45	11.951	1484	1490	1494	rBV3	14456	23508	0.47%	0.045%
46	12.022	1497	1502	1504	rVV4	8846	13478	0.27%	0.026%
47	12.069	1504	1510	1515	rVV	71785	124822	2.49%	0.238%
48	12.110	1515	1517	1523	rVB7	9539	13978	0.28%	0.027%
49	12.369	1556	1561	1568	rVB2	19036	31133	0.62%	0.059%
50	12.828	1634	1639	1645	rBV8	7159	14610	0.29%	0.028%
51	12.886	1645	1649	1656	rBV6	18923	39435	0.79%	0.075%
52	12.969	1658	1663	1669	rVB7	9255	20010	0.40%	0.038%
53	13.222	1701	1706	1712	rBV5	18028	30386	0.60%	0.058%
54	13.357	1725	1729	1735	rBV9	11225	18369	0.37%	0.035%
55	13.451	1741	1745	1750	rBV4	7927	14303	0.28%	0.027%
56	13.510	1750	1755	1756	rVV	25376	34242	0.68%	0.065%
57	13.539	1756	1760	1774	rVB	156403	269651	5.37%	0.515%
58	14.027	1831	1843	1857	rBV	1879530	2667617	53.11%	5.090%
59	14.139	1857	1862	1865	rVB6	9960	15465	0.31%	0.030%
60	14.304	1876	1890	1898	rBV	2134613	3258509	64.87%	6.218%
61	14.474	1915	1919	1928	rVB7	14041	27261	0.54%	0.052%
62	14.604	1934	1941	1953	rBV	1487273	2156808	42.94%	4.116%
63	14.692	1953	1956	1968	rVB5	15323	30168	0.60%	0.058%
64	14.810	1968	1976	1984	rBV	130975	260519	5.19%	0.497%
65	15.039	2007	2015	2021	rVB6	28283	50228	1.00%	0.096%
66	15.286	2052	2057	2063	rBV	22097	39853	0.79%	0.076%
67	15.404	2072	2077	2084	rBV4	21808	47237	0.94%	0.090%
68	15.598	2101	2110	2120	rBV	2846058	3981564	79.27%	7.598%
69	15.716	2122	2130	2139	rBV	742903	1058063	21.07%	2.019%
70	15.833	2148	2150	2155	rVB6	11224	16761	0.33%	0.032%
71	15.892	2155	2160	2165	rVB9	8002	15360	0.31%	0.029%
72	15.968	2167	2173	2180	rBV2	17468	26720	0.53%	0.051%
73	16.316	2227	2232	2236	rBV5	11654	18504	0.37%	0.035%
74	16.380	2238	2243	2248	rVB6	13638	23340	0.46%	0.045%
75	16.439	2248	2253	2256	rBV6	5744	9116	0.18%	0.017%
76	17.086	2359	2363	2365	rBV5	7736	10942	0.22%	0.021%

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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

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 Title : SVOA CALIBRATION

77	17.110	2365	2367	2371	rVV3	15133	18769	0.37%	0.036%
78	17.168	2373	2377	2383	rVB5	10743	18442	0.37%	0.035%
79	17.351	2402	2408	2418	rVV	1700645	2348893	46.76%	4.482%
80	17.451	2418	2425	2436	rVV	3028780	4333501	86.28%	8.269%
81	17.645	2453	2458	2460	rBV2	17478	24227	0.48%	0.046%
82	17.851	2489	2493	2501	rBV2	26620	40607	0.81%	0.077%
83	18.021	2517	2522	2528	rBV	564032	695021	13.84%	1.326%
84	18.204	2548	2553	2557	rVB8	4361	8388	0.17%	0.016%
85	18.245	2557	2560	2566	rBV3	29267	45108	0.90%	0.086%
86	18.321	2571	2573	2583	rVB3	19580	44141	0.88%	0.084%
87	18.498	2601	2603	2607	rVB3	9494	10571	0.21%	0.020%
88	18.545	2607	2611	2616	rBV	32939	43579	0.87%	0.083%
89	18.733	2639	2643	2650	rBV2	24671	36404	0.72%	0.069%
90	19.004	2687	2689	2696	rVB3	15130	20383	0.41%	0.039%
91	19.174	2715	2718	2723	rVB2	20821	27551	0.55%	0.053%
92	19.304	2735	2740	2744	rBV4	38959	56864	1.13%	0.109%
93	19.374	2748	2752	2755	rBV2	30989	40689	0.81%	0.078%
94	19.521	2774	2777	2785	rBV5	27531	46496	0.93%	0.089%
95	19.739	2808	2814	2823	rBV	3597860	4725938	94.09%	9.018%
96	20.745	2983	2985	2989	rVB5	29137	33539	0.67%	0.064%
97	21.527	3113	3118	3127	rBV	1781240	2409954	47.98%	4.599%
98	22.333	3251	3255	3264	rBV	267057	429761	8.56%	0.820%
99	23.791	3495	3503	3514	rBV2	2549865	5022833	100.00%	9.585%
100	23.944	3523	3529	3541	rVB	1263810	2596162	51.69%	4.954%

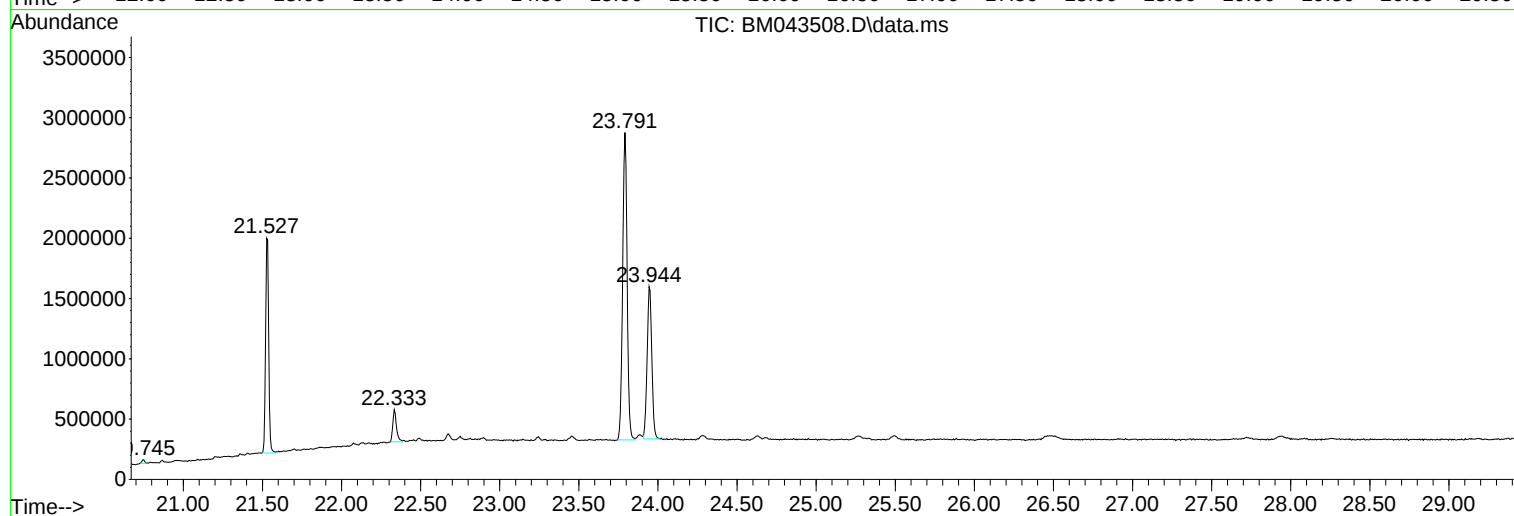
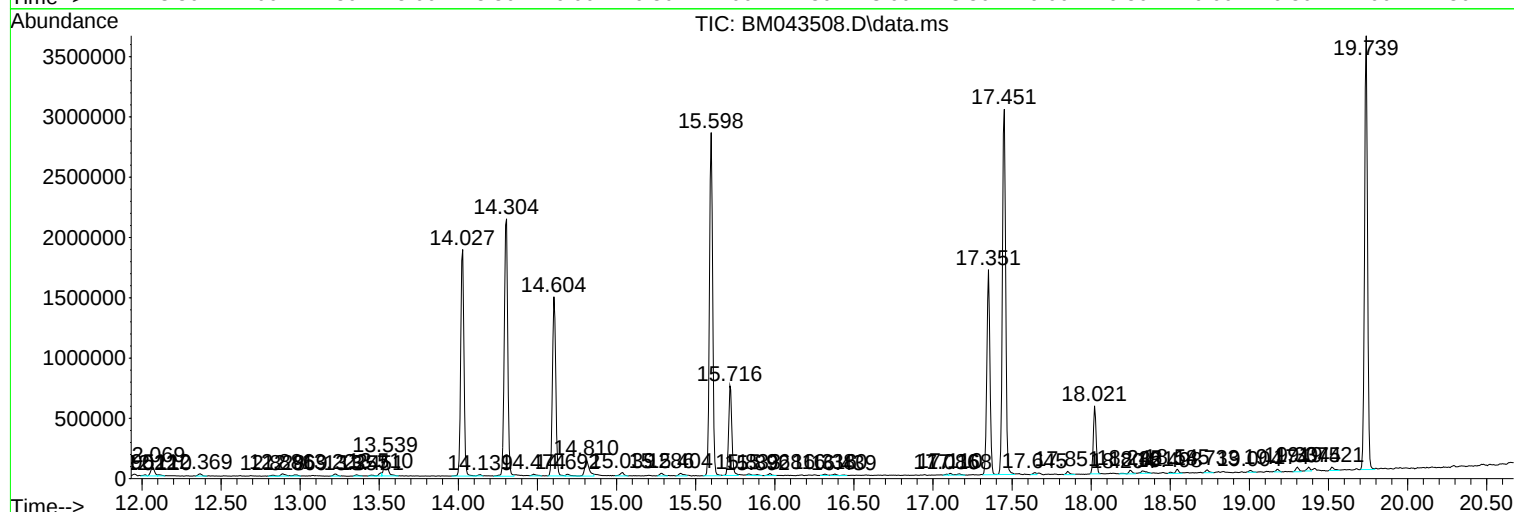
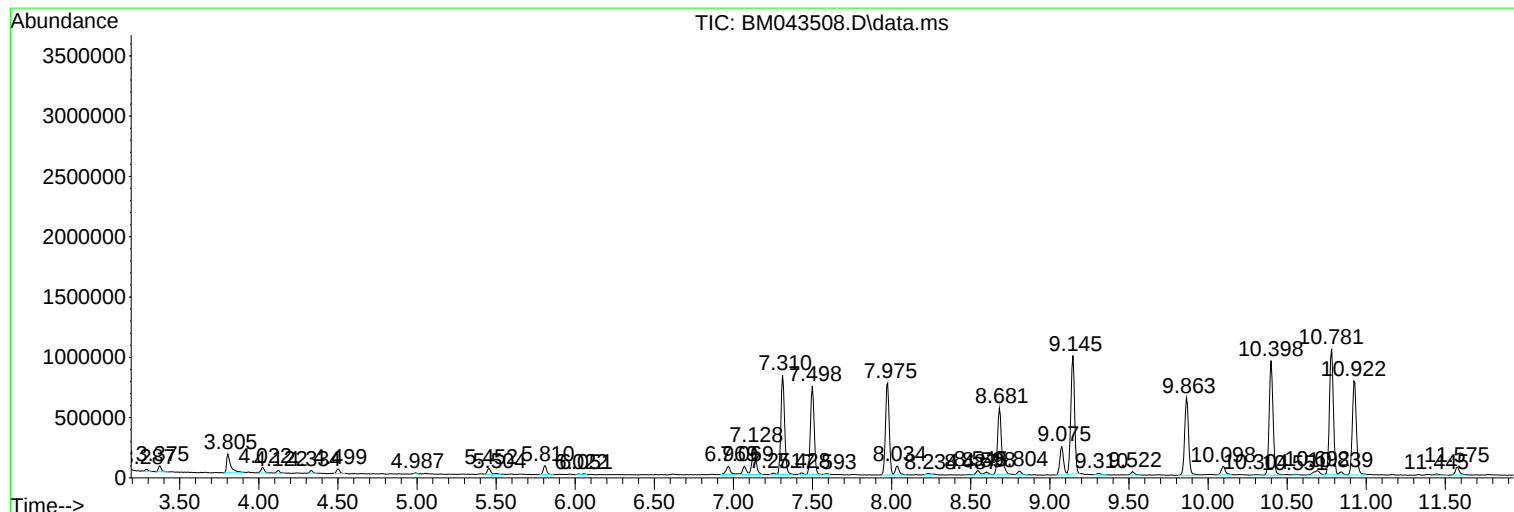
Sum of corrected areas: 52405395

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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122123\
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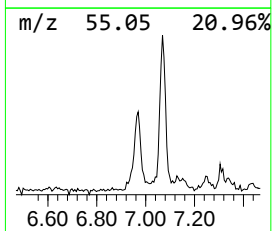
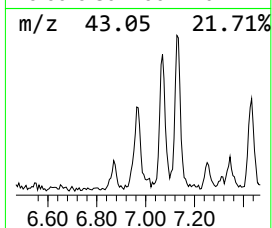
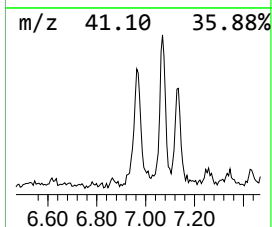
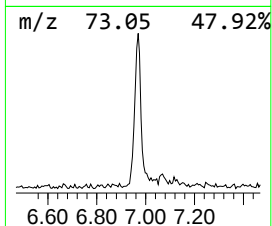
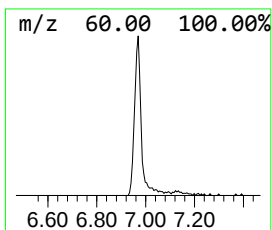
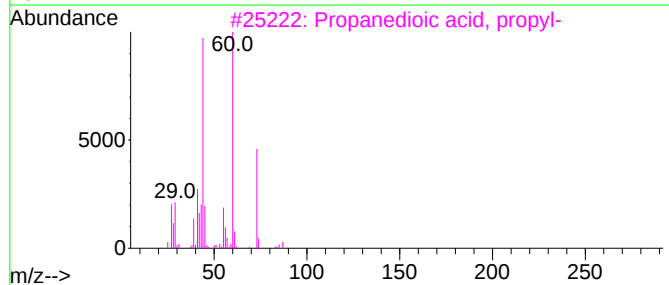
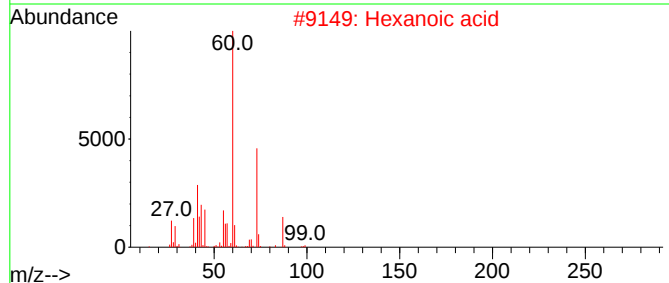
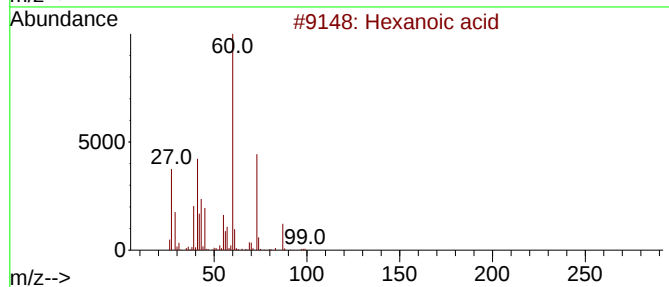
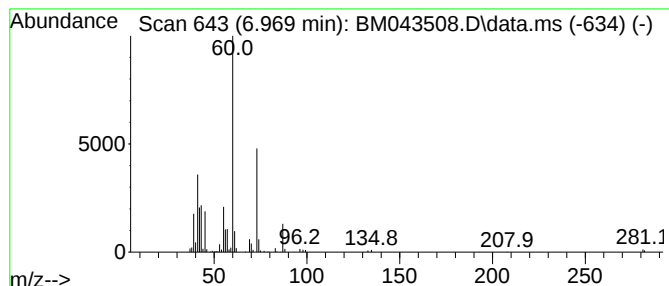
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Hexanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.969	2.17 ng/ul	135802	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	90
2			Hexanoic acid	116	C6H12O2	000142-62-1	86
3			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	78
4			Hexanoic acid	116	C6H12O2	000142-62-1	72
5			Hexanoic acid	116	C6H12O2	000142-62-1	72



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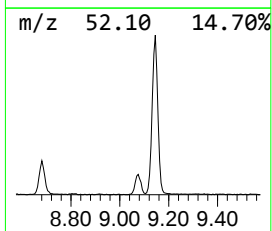
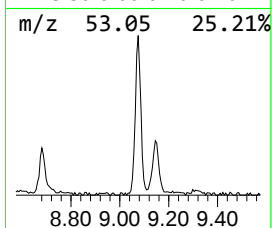
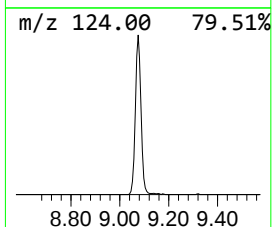
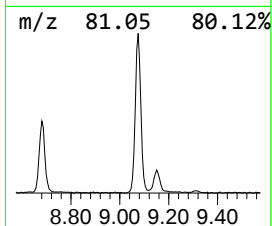
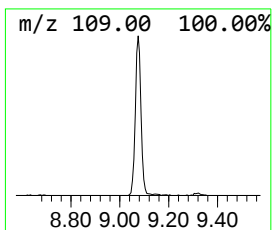
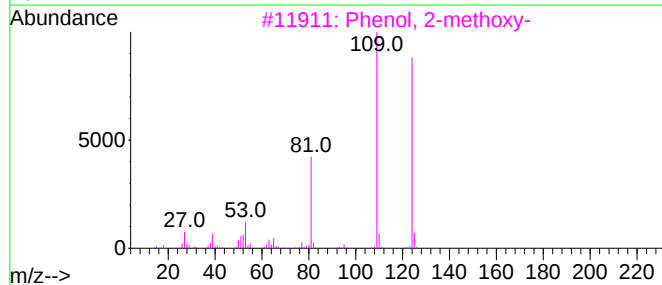
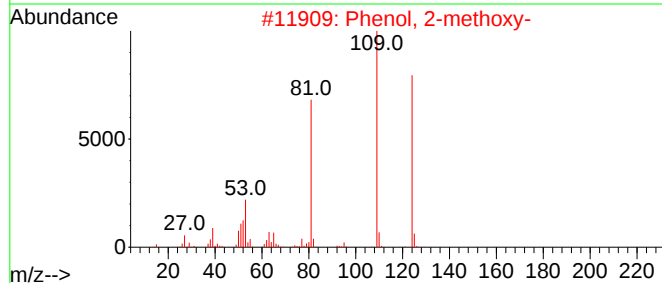
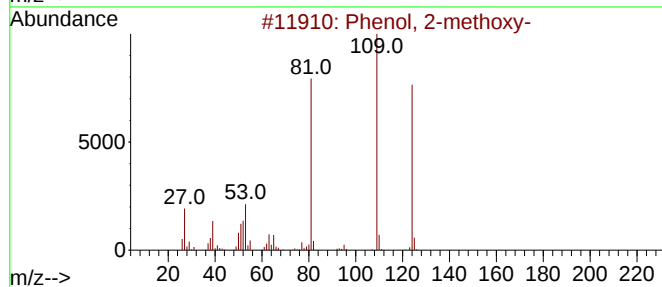
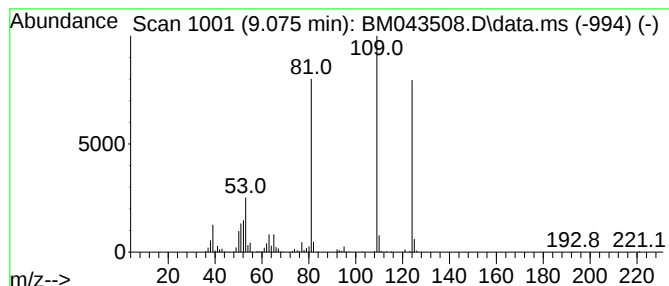
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Phenol, 2-methoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.075	6.33 ng/ul	395323	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	97
2			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
3			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	95
4			Mequinol	124	C7H8O2	000150-76-5	91
5			Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	90



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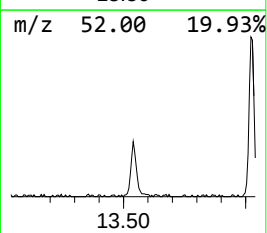
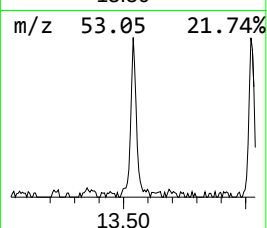
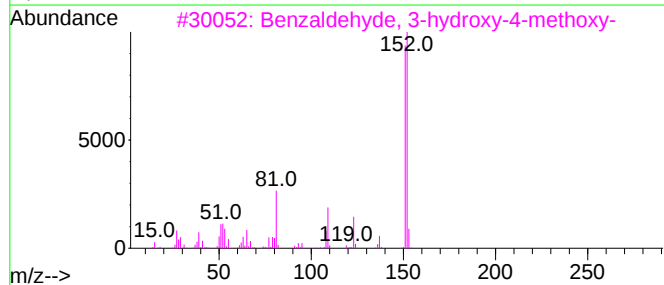
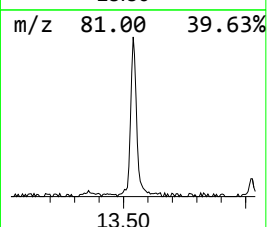
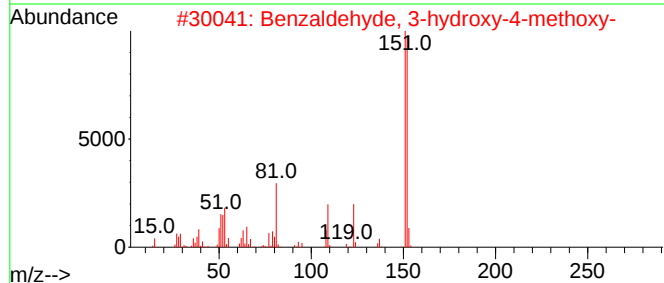
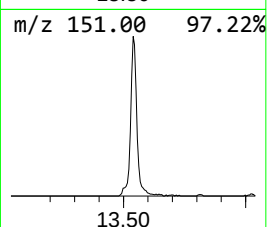
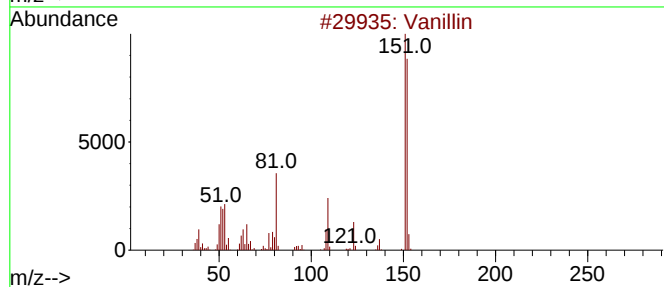
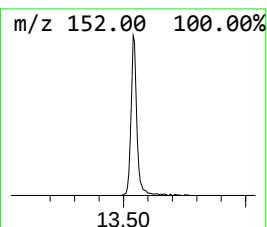
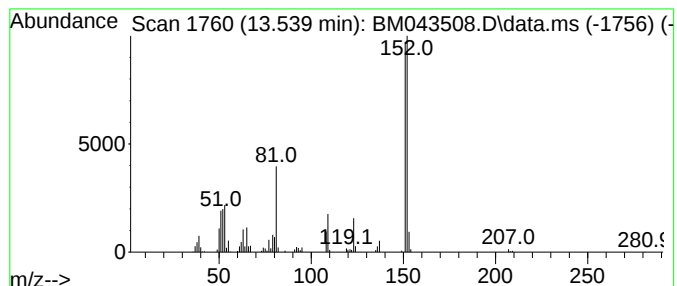
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Vanillin Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.539	2.50 ng/ul	269651	Acenaphthene-d10	14.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin	152	C8H8O3	000121-33-5	96
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	95
3			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	95
4			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94
5			Vanillin	152	C8H8O3	000121-33-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122123\
Data File : BM043508.D
Acq On : 21 Dec 2023 18:23
Operator : MA/JU
Sample : 05912-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BH3N8

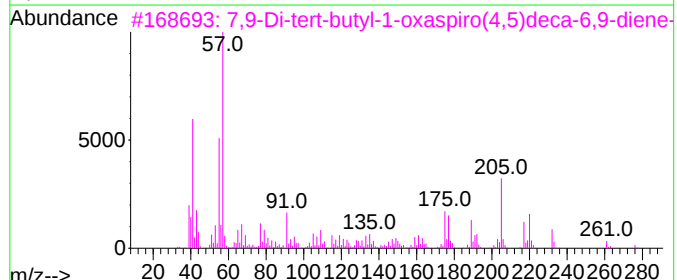
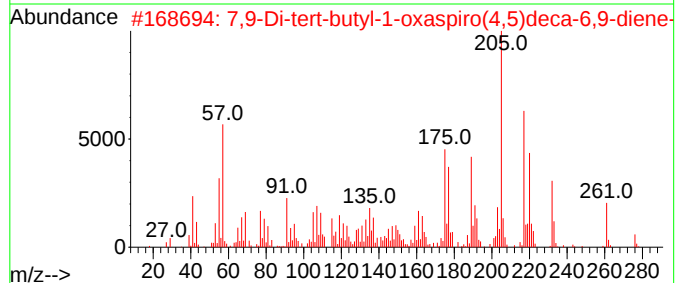
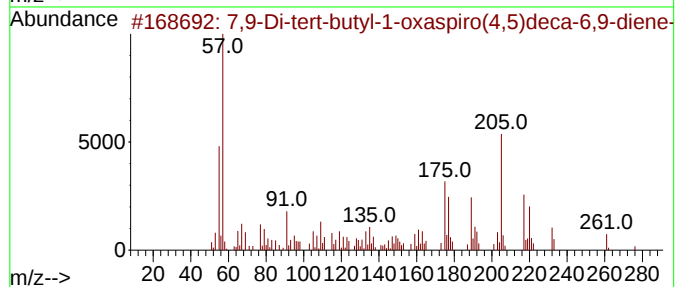
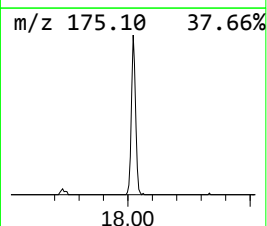
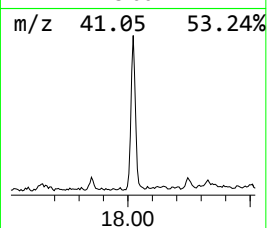
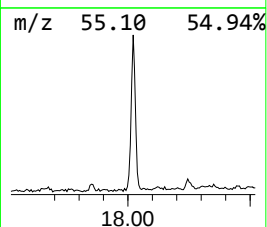
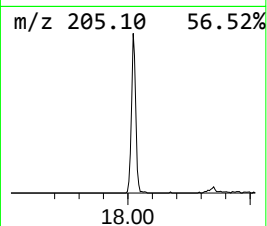
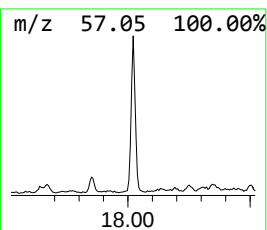
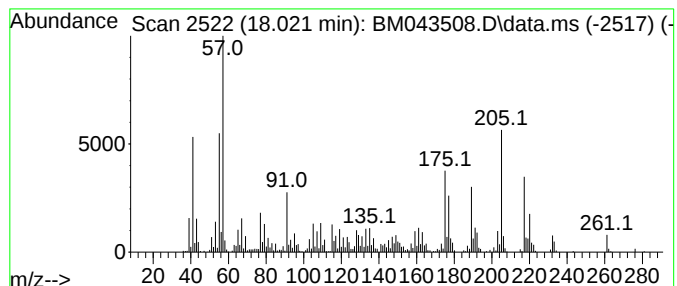
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.021	5.92 ng/ul	695021	Phenanthrene-d10	17.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99		
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	64		
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	60		
4	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	46		
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	41		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122123\
Data File : BM043508.D
Acq On : 21 Dec 2023 18:23
Operator : MA/JU
Sample : 05912-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BH3N8

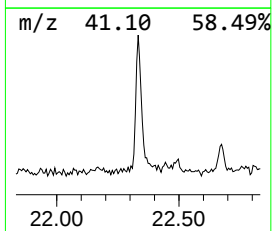
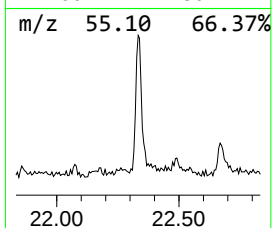
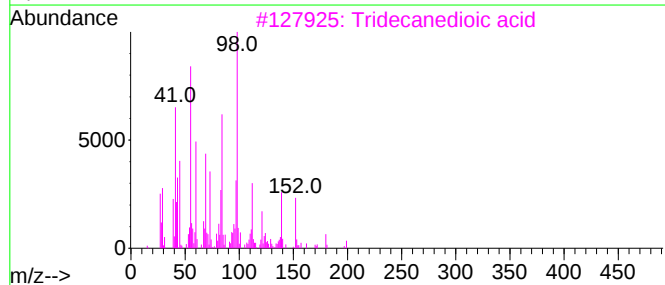
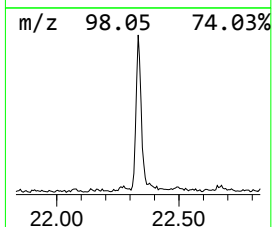
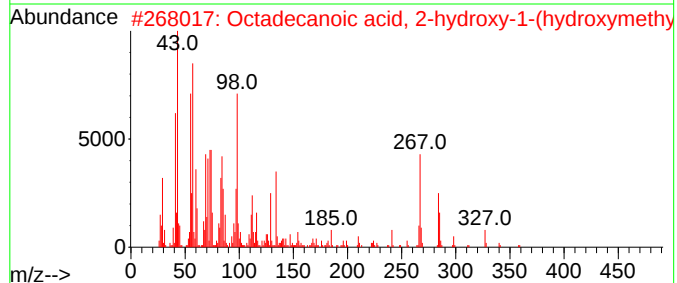
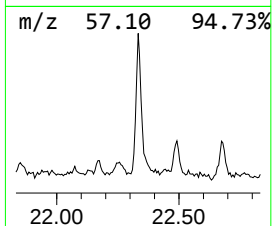
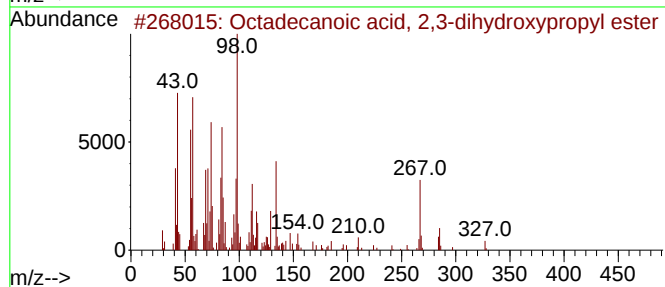
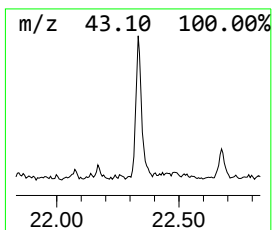
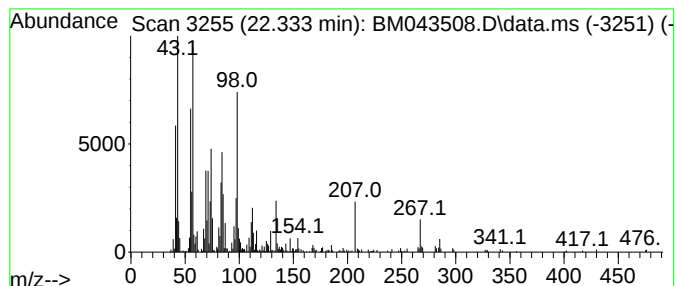
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octadecanoic acid, 2,3-dihy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.333	3.57 ng/ul	429761	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, 2,3-dihydroxy...	358	C21H42O4	000123-94-4	74
2			Octadecanoic acid, 2-hydroxy-1-(...	358	C21H42O4	000621-61-4	64
3			Tridecanedioic acid	244	C13H24O4	000505-52-2	49
4			Dodecanoyl chloride	218	C12H23ClO	000112-16-3	38
5			Acetonitrile, isothiocyanato-	98	C3H2N2S	032772-75-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122123\
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Operator : MA/JU
Sample : 05912-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BH3N8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.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
Hexanoic acid	6.969	2.2	ng/ul	135802	1	7.975	1249380	20.0
Phenol, 2-methoxy-	9.075	6.3	ng/ul	395323	1	7.975	1249380	20.0
Vanillin	13.539	2.5	ng/ul	269651	3	14.604	2156810	20.0
7,9-Di-tert-but...	18.021	5.9	ng/ul	695021	4	17.351	2348890	20.0
Octadecanoic ac...	22.333	3.6	ng/ul	429761	5	21.533	2409950	20.0