

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
 Data File : BM047130.D
 Acq On : 09 Aug 2024 21:05
 Operator : RC/JU
 Sample : P3498-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 E08L9

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-BM080224.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM047130.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.011	18	21	28	rVB	59141	73702	1.59%	0.141%
2	3.281	64	67	73	rBV	25586	32615	0.71%	0.063%
3	3.417	86	90	102	rBV	52418	93482	2.02%	0.179%
4	3.699	135	138	143	rVB	16770	23708	0.51%	0.045%
5	4.052	194	198	202	rBV3	15491	18358	0.40%	0.035%
6	4.958	348	352	360	rVB8	6414	12185	0.26%	0.023%
7	5.528	445	449	455	rVB	28344	42006	0.91%	0.081%
8	5.687	470	476	480	rBV9	7444	12530	0.27%	0.024%
9	6.452	599	606	616	rBV2	62076	109780	2.37%	0.211%
10	6.587	623	629	641	rVB	269919	441054	9.54%	0.846%
11	6.740	648	655	667	rBV	701370	1064365	23.02%	2.042%
12	6.928	679	687	697	rBV	791006	1225292	26.50%	2.350%
13	7.022	700	703	712	rVV3	21597	40822	0.88%	0.078%
14	7.099	712	716	723	rVB7	10317	21035	0.45%	0.040%
15	7.381	757	764	774	rBV	851927	1330581	28.78%	2.552%
16	7.463	774	778	787	rVB4	35249	69238	1.50%	0.133%
17	7.993	862	868	875	rBV	33718	60286	1.30%	0.116%
18	8.105	879	887	897	rBV	690377	1089132	23.55%	2.089%
19	8.528	952	959	968	rBV	815061	1290345	27.91%	2.475%
20	8.705	980	989	998	rBV7	20501	47628	1.03%	0.091%
21	8.975	1030	1035	1040	rVB6	7772	14201	0.31%	0.027%
22	9.116	1051	1059	1065	rVV2	70169	110993	2.40%	0.213%
23	9.240	1073	1080	1089	rBV	674383	1040331	22.50%	1.996%
24	9.440	1108	1114	1117	rBV8	8721	12997	0.28%	0.025%
25	9.528	1122	1129	1137	rBV	144779	251768	5.45%	0.483%
26	9.775	1164	1171	1184	rBV	971208	1604298	34.70%	3.077%
27	9.957	1196	1202	1210	rBV6	12927	24734	0.53%	0.047%
28	10.140	1226	1233	1241	rVB	1094891	1814073	39.23%	3.480%
29	10.293	1248	1259	1274	rBV	520939	944803	20.43%	1.812%
30	10.716	1326	1331	1337	rVB3	20024	30420	0.66%	0.058%
31	10.793	1339	1344	1349	rVB3	12729	20365	0.44%	0.039%
32	10.898	1355	1362	1371	rBV	165077	303524	6.56%	0.582%
33	10.998	1371	1379	1389	rVV	283908	506541	10.96%	0.972%
34	11.116	1394	1399	1408	rVB9	18132	43742	0.95%	0.084%
35	11.740	1498	1505	1510	rVV2	21794	37209	0.80%	0.071%
36	12.228	1584	1588	1592	rBV7	5448	9635	0.21%	0.018%

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Integrator: RTE

Smoothing : OFF

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Min Area: 0.1 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
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37	12.328	1600	1605	1612	rVV5	14120	24207	0.52%	0.046%
38	12.575	1643	1647	1653	rVB9	4563	9452	0.20%	0.018%
39	12.645	1656	1659	1663	rVV4	5498	8737	0.19%	0.017%
40	12.804	1683	1686	1689	rBV5	5571	9197	0.20%	0.018%
41	12.887	1694	1700	1709	rBV	878415	1260286	27.26%	2.418%
42	13.057	1723	1729	1735	rBV4	20125	36142	0.78%	0.069%
43	13.263	1761	1764	1773	rVV9	17688	39753	0.86%	0.076%
44	13.469	1793	1799	1807	rVV	1552630	2170038	46.93%	4.163%
45	13.728	1836	1843	1854	rBV	1816845	2678501	57.93%	5.138%
46	13.822	1854	1859	1862	rVB5	6103	8518	0.18%	0.016%
47	13.975	1881	1885	1888	rVB4	10922	15570	0.34%	0.030%
48	14.039	1888	1896	1905	rBV	1601134	2306811	49.89%	4.425%
49	14.286	1930	1938	1954	rBV2	226762	442302	9.57%	0.848%
50	14.510	1970	1976	1983	rBV	125042	190139	4.11%	0.365%
51	14.575	1985	1987	1995	rVB8	10890	21520	0.47%	0.041%
52	14.775	2018	2021	2024	rBV4	5432	8493	0.18%	0.016%
53	14.816	2024	2028	2034	rVV	48671	67343	1.46%	0.129%
54	14.875	2035	2038	2039	rVV3	13589	11813	0.26%	0.023%
55	14.898	2039	2042	2045	rVV	16510	19844	0.43%	0.038%
56	14.934	2045	2048	2051	rVB3	12407	12683	0.27%	0.024%
57	15.045	2060	2067	2075	rBV	2373356	3277551	70.88%	6.287%
58	15.181	2084	2090	2100	rBV	685154	960749	20.78%	1.843%
59	15.286	2104	2108	2112	rVV3	12902	21198	0.46%	0.041%
60	15.345	2114	2118	2123	rVB8	8140	13818	0.30%	0.027%
61	15.398	2123	2127	2130	rBV4	7476	11086	0.24%	0.021%
62	15.445	2132	2135	2140	rVB7	13168	15814	0.34%	0.030%
63	15.498	2140	2144	2149	rBV8	6298	12285	0.27%	0.024%
64	15.639	2160	2168	2172	rBV10	8093	18726	0.40%	0.036%
65	15.692	2174	2177	2184	rBV2	14391	20521	0.44%	0.039%
66	15.804	2192	2196	2198	rBV2	21571	26831	0.58%	0.051%
67	15.828	2198	2200	2203	rVV4	10962	11639	0.25%	0.022%
68	15.863	2203	2206	2211	rVV3	20471	28025	0.61%	0.054%
69	16.245	2266	2271	2279	rVB5	26603	40780	0.88%	0.078%
70	16.386	2290	2295	2297	rVV6	12457	16958	0.37%	0.033%
71	16.422	2299	2301	2305	rVV4	6948	10055	0.22%	0.019%
72	16.475	2308	2310	2317	rVB6	6443	10028	0.22%	0.019%
73	16.598	2325	2331	2334	rBV5	23541	38252	0.83%	0.073%
74	16.651	2338	2340	2346	rVB6	7034	8533	0.18%	0.016%
75	16.798	2359	2365	2375	rVV	1915419	2631532	56.91%	5.048%
76	16.898	2375	2382	2391	rBV	2669465	3727196	80.61%	7.150%

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Integration Parameters: LSCINT.P

Integrator: RTE
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 Sampling : 1 Min Area: 0.1 % of largest Peak
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 Stop Thrs : 0 Peak Location: TOP

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77	17.033	2399	2405	2408	rBV5	17255	29263	0.63%	0.056%
78	17.186	2427	2431	2434	rBV6	7468	11325	0.24%	0.022%
79	17.339	2453	2457	2463	rBV5	11594	19757	0.43%	0.038%
80	17.492	2479	2483	2485	rBV5	18503	22221	0.48%	0.043%
81	17.610	2498	2503	2509	rBV9	9576	21155	0.46%	0.041%
82	17.739	2519	2525	2532	rBV	475891	688456	14.89%	1.321%
83	17.798	2532	2535	2540	rVB	31014	57177	1.24%	0.110%
84	17.945	2557	2560	2566	rVB7	12370	19640	0.42%	0.038%
85	18.027	2573	2574	2578	rVB4	13484	14714	0.32%	0.028%
86	18.416	2636	2640	2643	rBV6	11628	17762	0.38%	0.034%
87	18.769	2697	2700	2704	rVB3	32900	37299	0.81%	0.072%
88	18.845	2709	2713	2716	rBV2	37826	50933	1.10%	0.098%
89	18.886	2716	2720	2722	rBV3	24887	31963	0.69%	0.061%
90	18.916	2722	2725	2729	rVB4	26767	35193	0.76%	0.068%
91	19.039	2741	2746	2754	rBV	264782	413943	8.95%	0.794%
92	19.210	2769	2775	2782	rBV	3314631	4257517	92.08%	8.167%
93	19.269	2782	2785	2788	rVB2	21767	22289	0.48%	0.043%
94	19.810	2875	2877	2881	rVB	41593	39724	0.86%	0.076%
95	20.127	2927	2931	2944	rBV2	238713	444996	9.62%	0.854%
96	20.774	3037	3041	3047	rBV	456608	639771	13.84%	1.227%
97	21.033	3080	3085	3093	rBV	2122229	2772619	59.96%	5.319%
98	22.515	3332	3337	3344	rVB	409896	672306	14.54%	1.290%
99	23.551	3506	3513	3522	rVB	2170001	4623807	100.00%	8.870%
100	23.733	3537	3544	3552	rBV	1379307	3076579	66.54%	5.902%

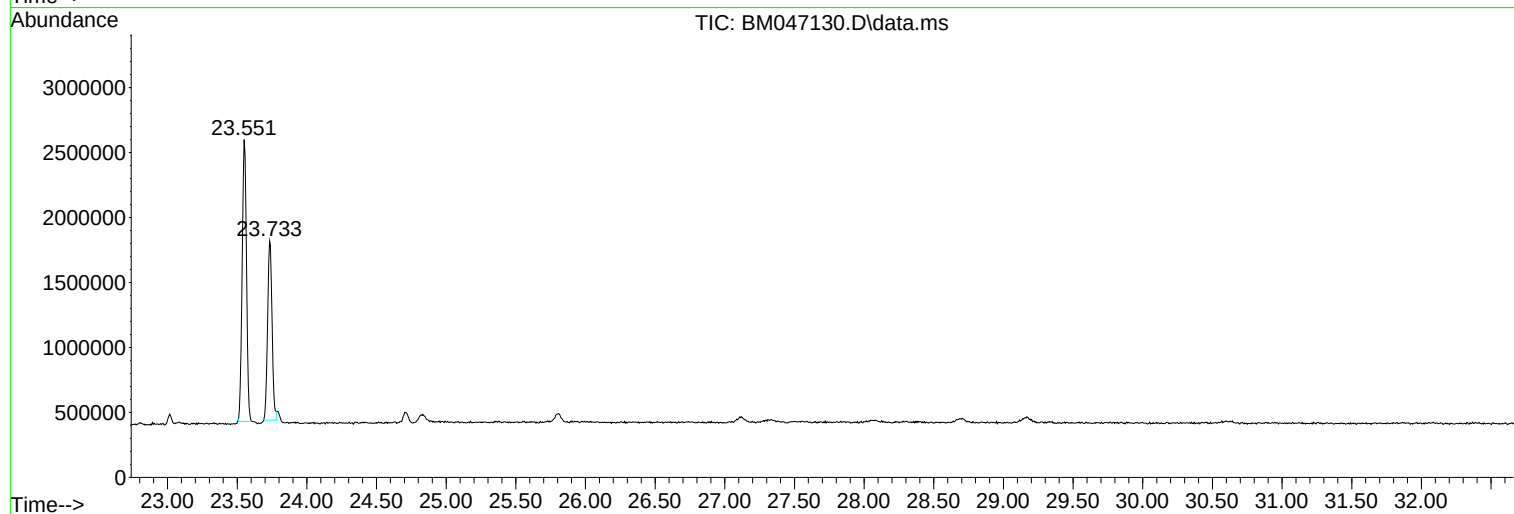
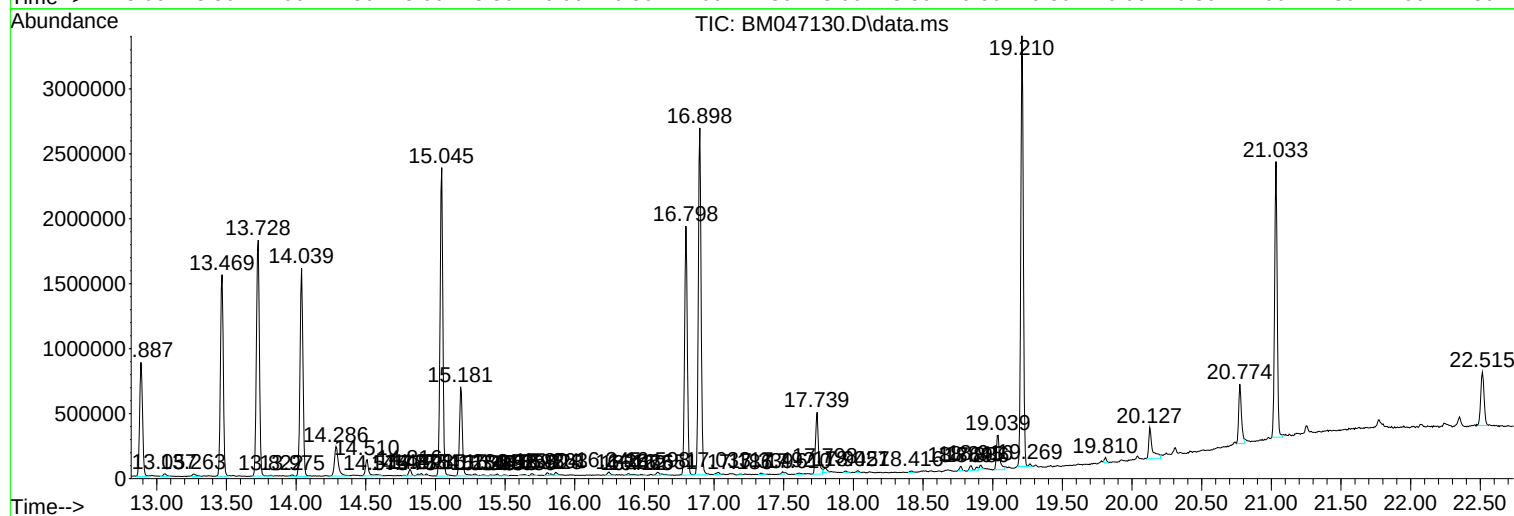
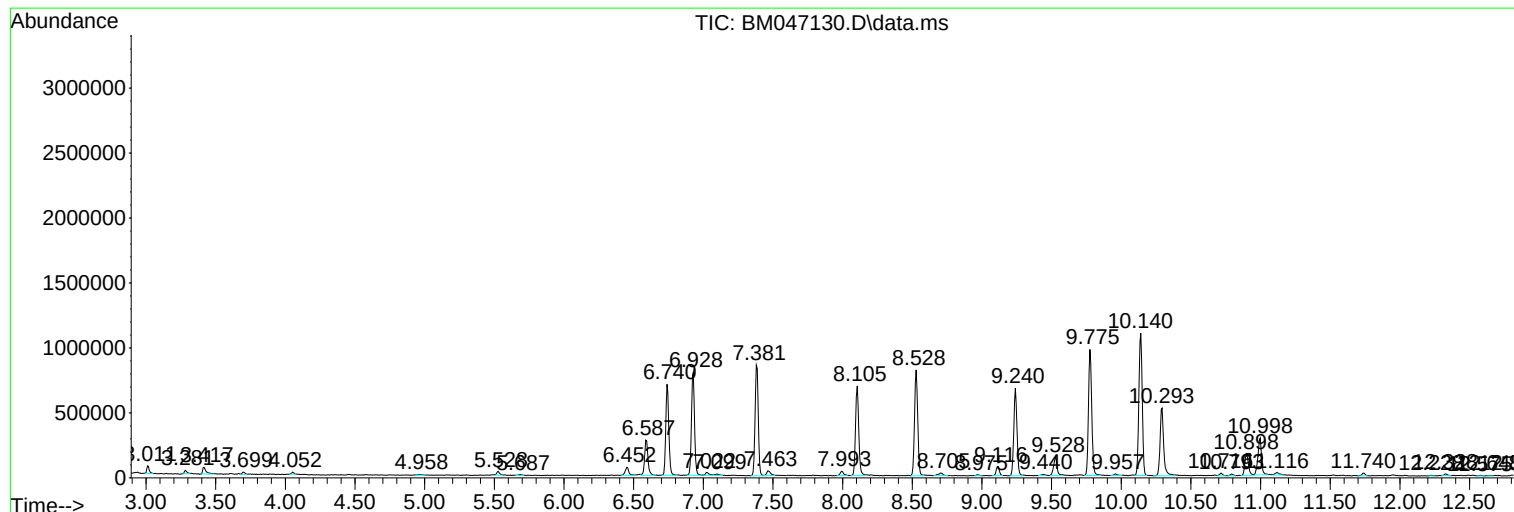
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
Quant Title : SVOA CALIBRATION

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



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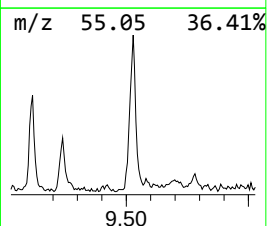
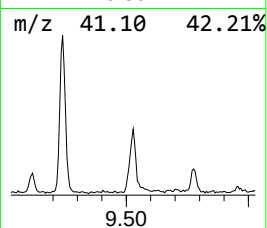
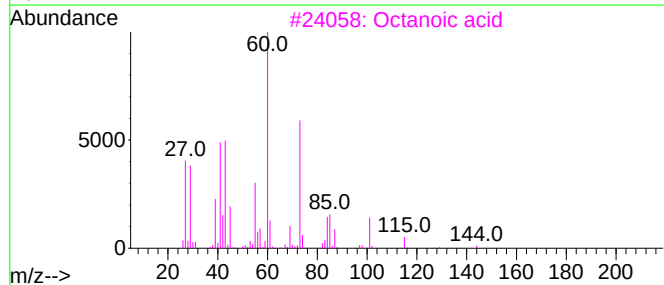
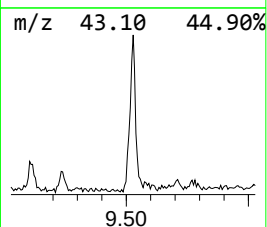
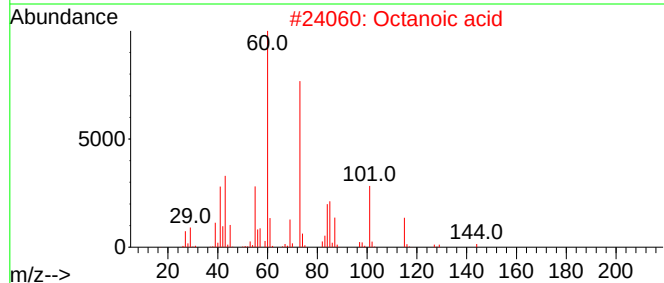
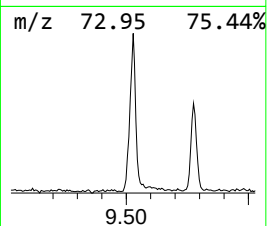
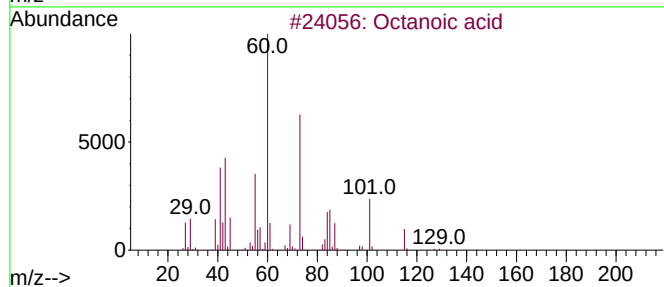
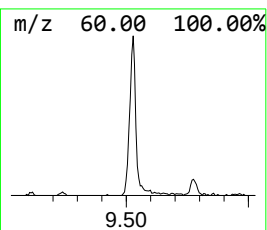
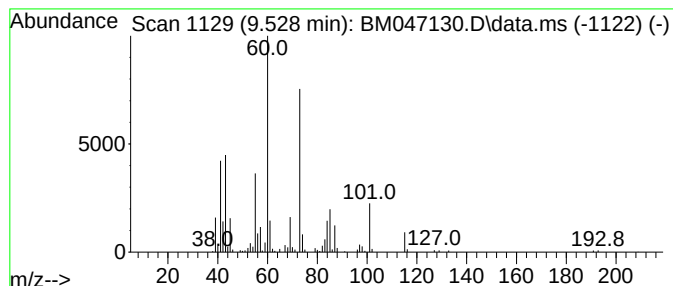
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Octanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.528	2.78 ng/ul	251768	Naphthalene-d8	10.140

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	91
2			Octanoic acid	144	C8H16O2	000124-07-2	90
3			Octanoic acid	144	C8H16O2	000124-07-2	78
4			Octanoic acid	144	C8H16O2	000124-07-2	78
5			Nonanoic acid	158	C9H18O2	000112-05-0	59



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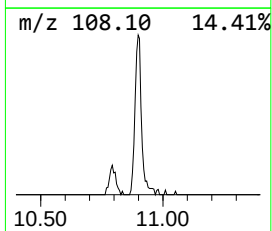
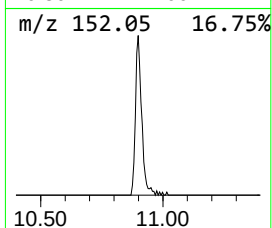
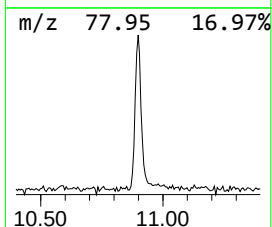
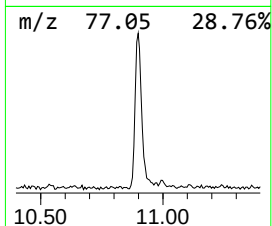
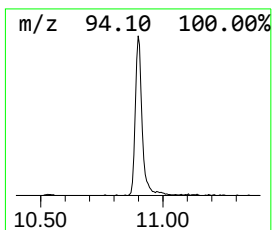
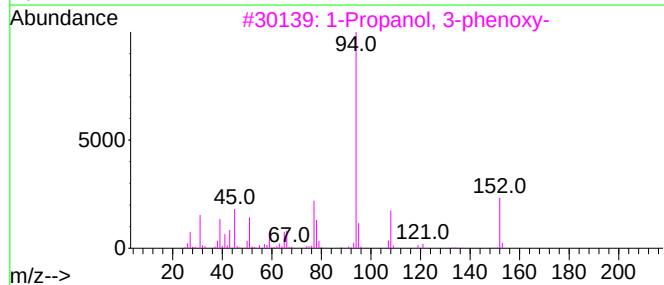
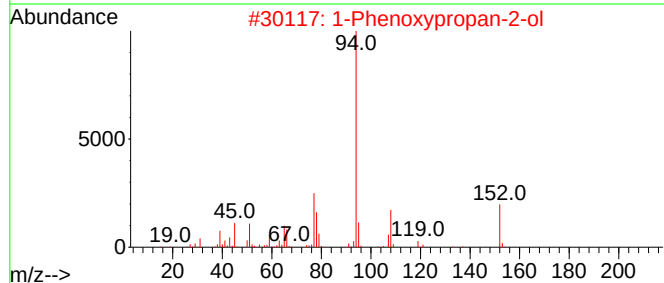
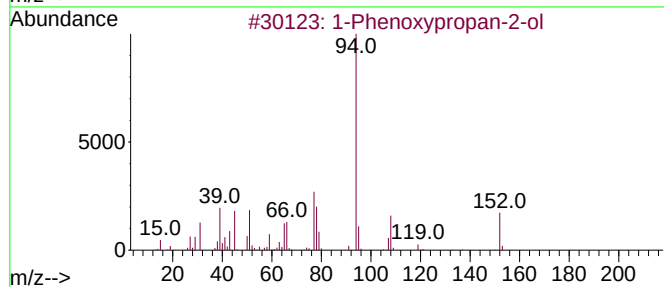
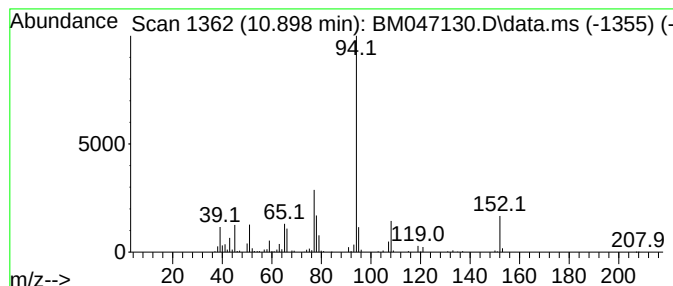
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.899	3.35 ng/ul	303524	Naphthalene-d8	10.140

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
3			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	93
4			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
5			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	83



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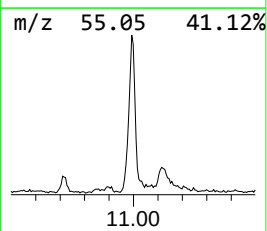
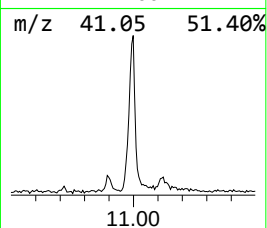
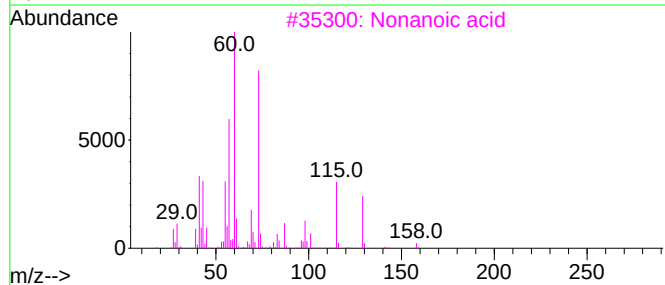
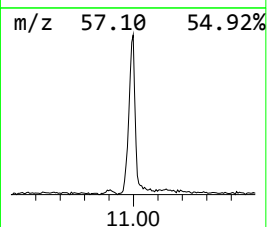
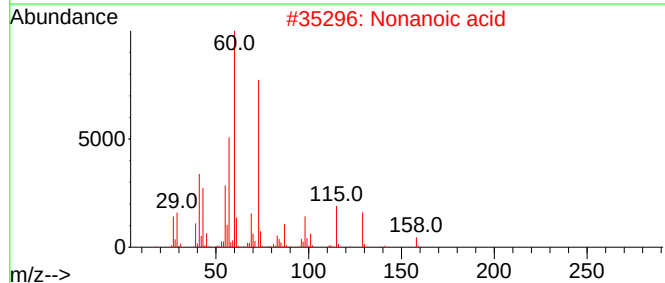
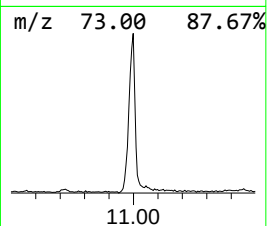
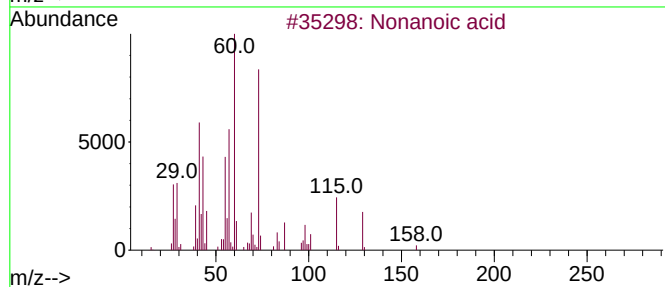
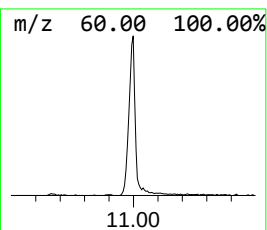
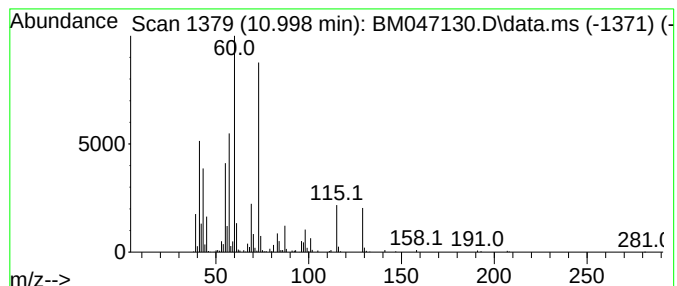
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Nonanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.999	5.58 ng/ul	506541	Naphthalene-d8	10.140

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	90
2			Nonanoic acid	158	C9H18O2	000112-05-0	86
3			Nonanoic acid	158	C9H18O2	000112-05-0	86
4			Nonanoic acid	158	C9H18O2	000112-05-0	78
5			n-Decanoic acid	172	C10H20O2	000334-48-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047130.D
Acq On : 09 Aug 2024 21:05
Operator : RC/JU
Sample : P3498-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E08L9

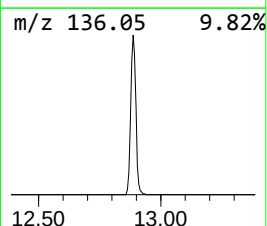
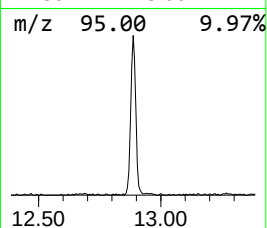
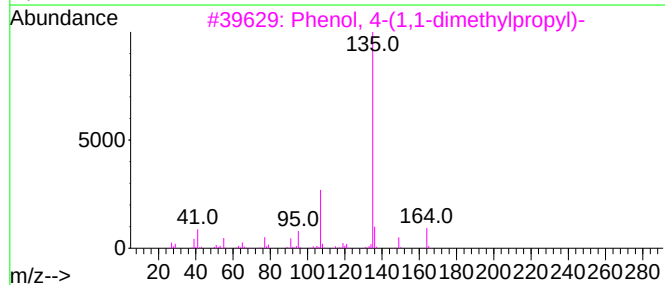
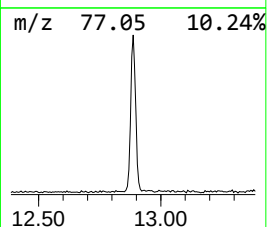
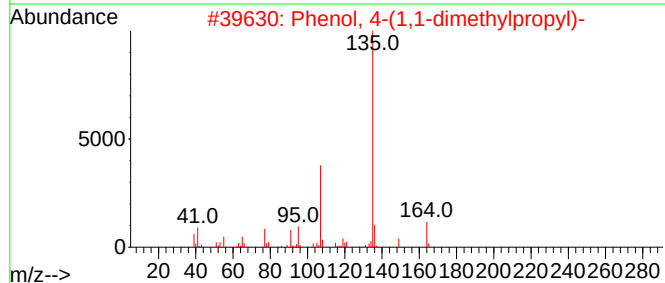
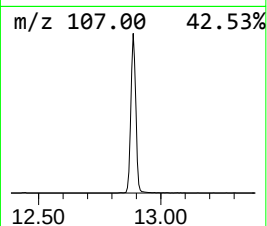
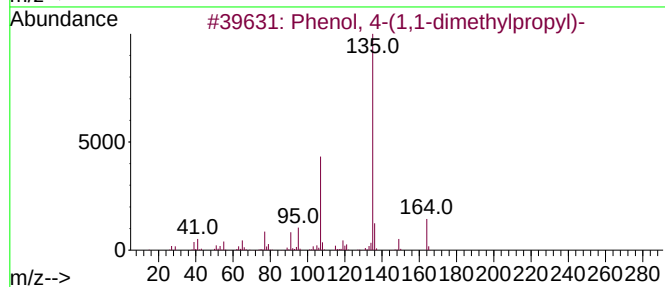
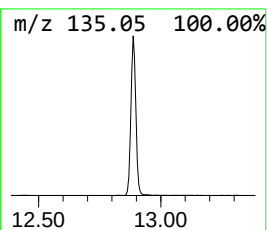
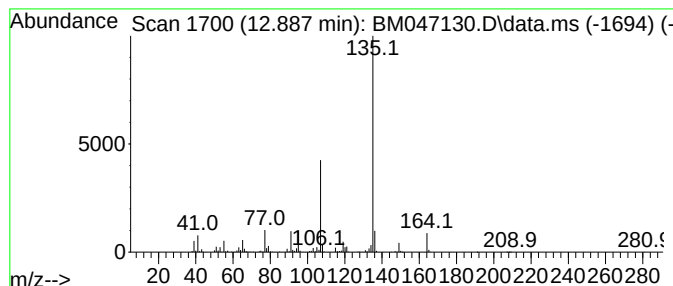
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.887	10.93 ng/ul	1260290	Acenaphthene-d10	14.040

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	93
2			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	91
3			Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	91
4			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	90
5			Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047130.D
Acq On : 09 Aug 2024 21:05
Operator : RC/JU
Sample : P3498-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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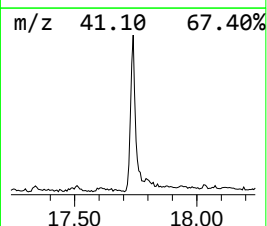
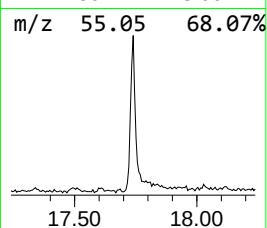
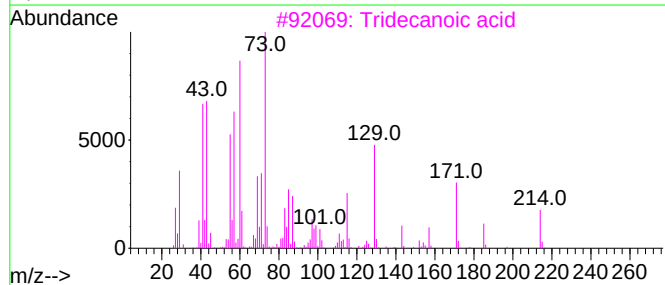
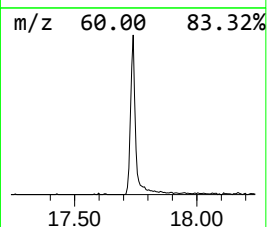
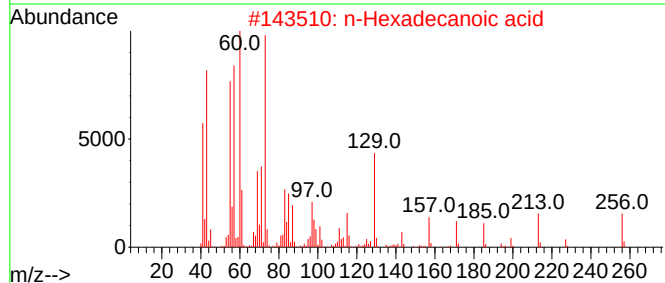
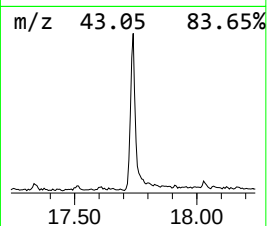
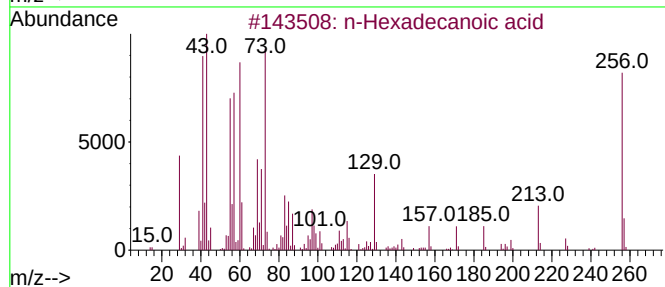
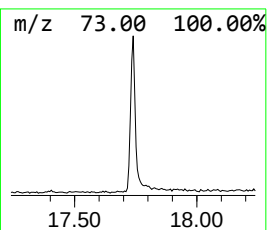
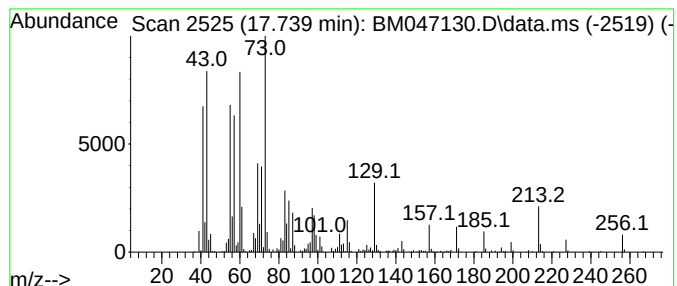
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.739	5.23 ng/ul	688456	Phenanthrene-d10	16.798

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	96
3			Tridecanoic acid	214	C13H26O2	000638-53-9	94
4			Tridecanoic acid	214	C13H26O2	000638-53-9	91
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047130.D
Acq On : 09 Aug 2024 21:05
Operator : RC/JU
Sample : P3498-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E08L9

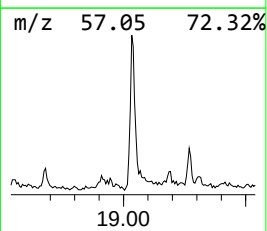
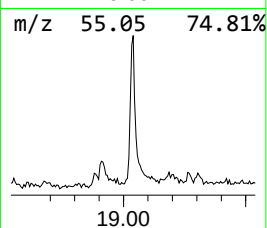
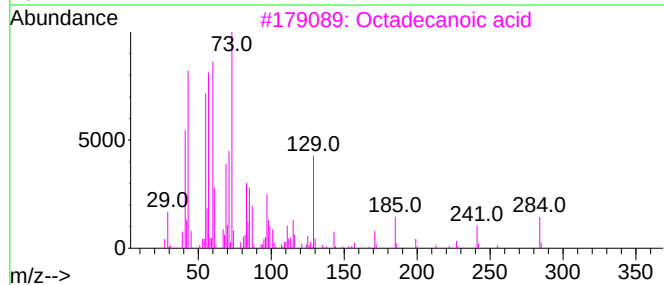
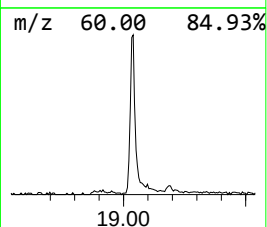
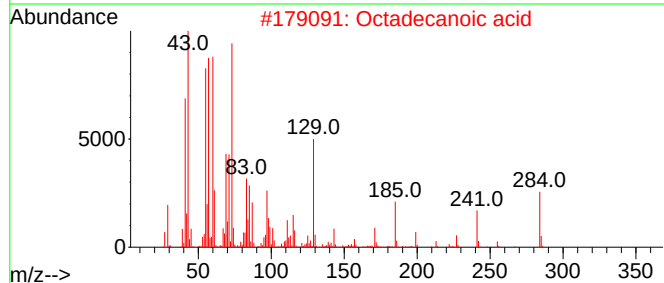
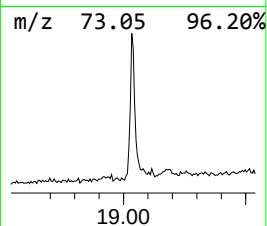
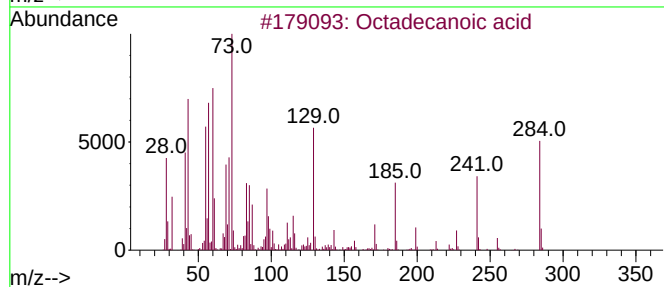
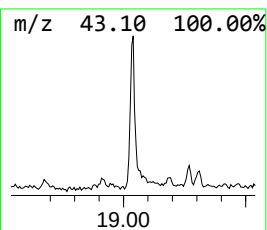
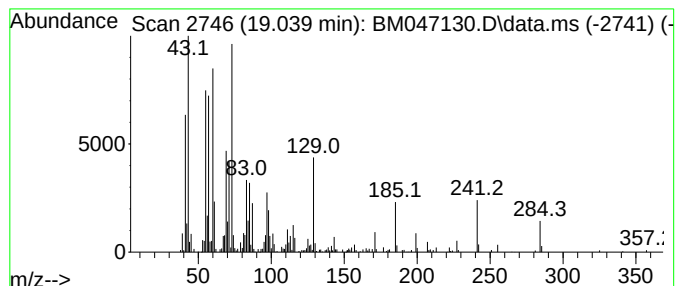
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.039	2.99 ng/ul	413943	Chrysene-d12	21.033

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	95
4			Octadecanoic acid	284	C18H36O2	000057-11-4	94
5			Octadecanoic acid	284	C18H36O2	000057-11-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047130.D
Acq On : 09 Aug 2024 21:05
Operator : RC/JU
Sample : P3498-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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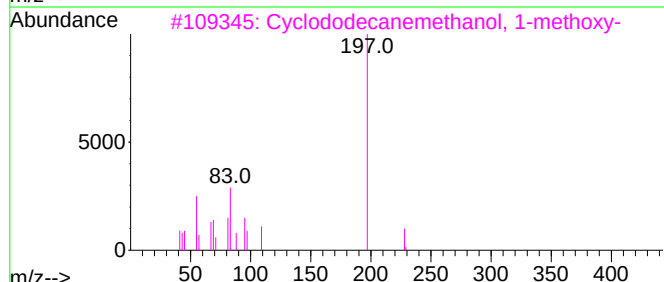
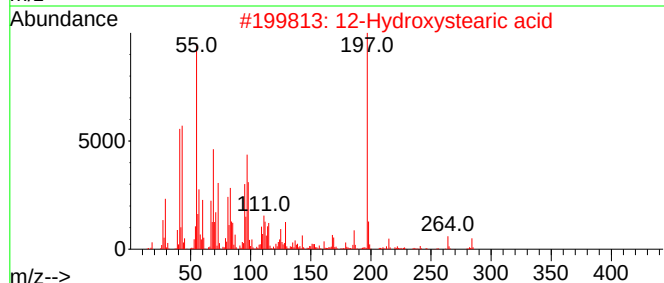
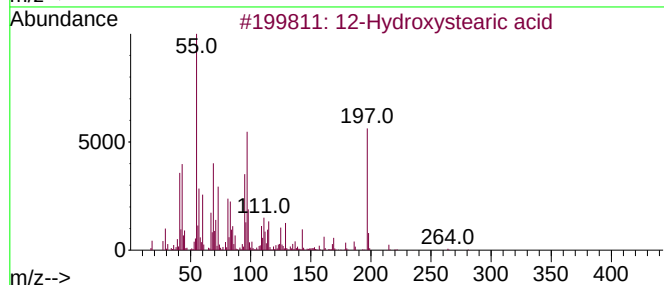
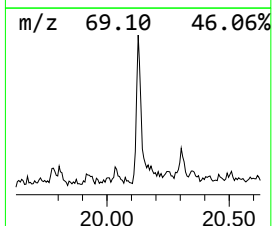
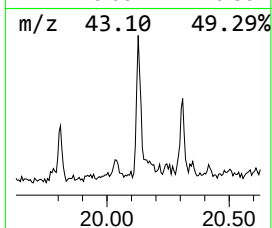
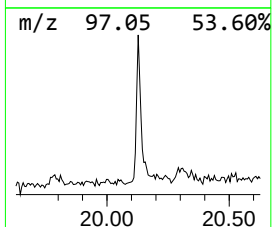
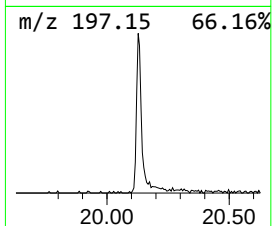
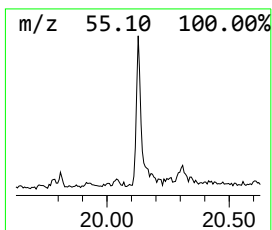
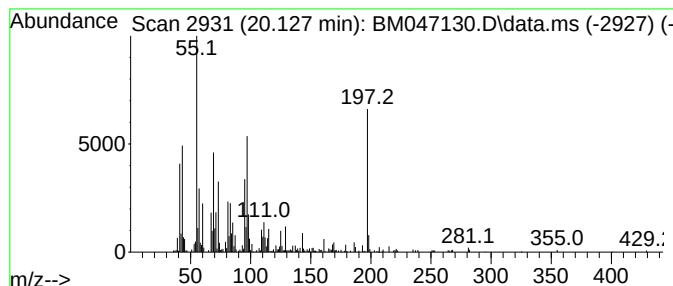
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 12-Hydroxystearic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.127	3.21 ng/ul	444996	Chrysene-d12	21.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			12-Hydroxystearic acid	300	C18H36O3	000106-14-9	94
2			12-Hydroxystearic acid	300	C18H36O3	000106-14-9	62
3			Cyclododecanemethanol, 1-methoxy-	228	C14H28O2	108682-09-3	27
4			4-Methyl-5-(2-thienyl)-2,4-dihyd...	197	C7H7N3S2	068744-66-1	27
5			4-Hydrazono-5-hydroxyimino-4,5,6...	197	C6H7N5O3	303194-86-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047130.D
Acq On : 09 Aug 2024 21:05
Operator : RC/JU
Sample : P3498-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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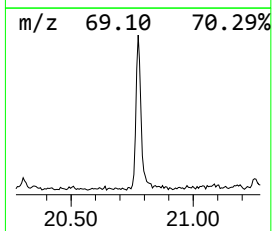
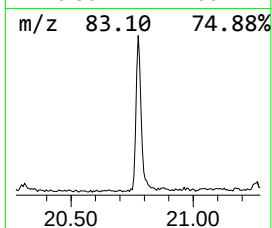
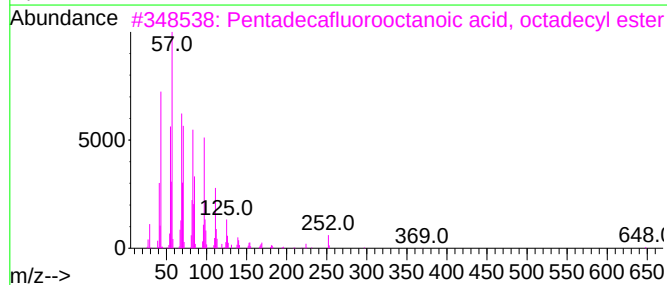
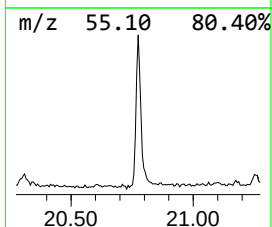
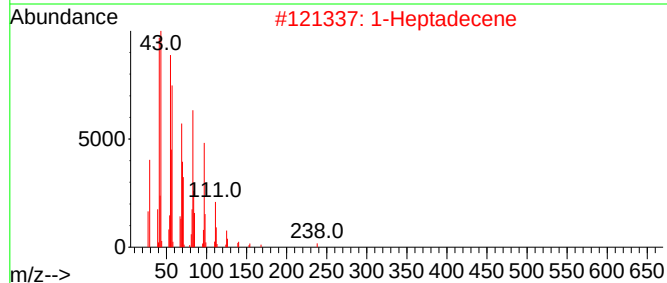
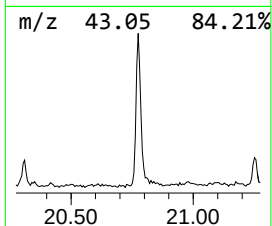
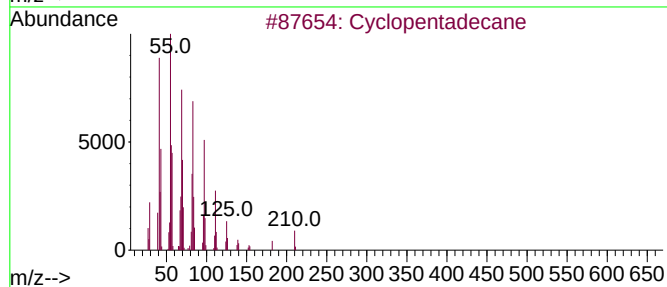
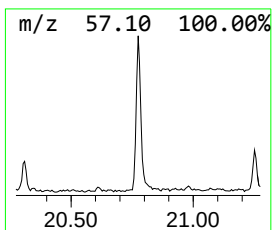
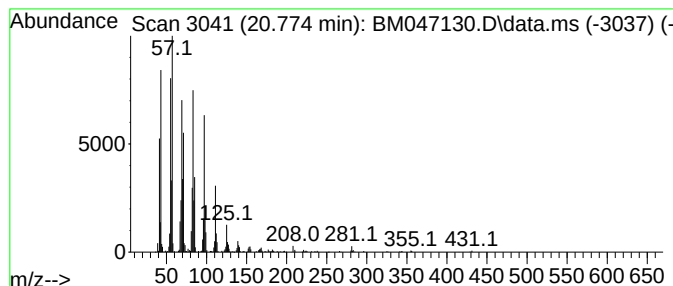
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Cyclic20.774 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.774	4.61 ng/ul	639771	Chrysene-d12	21.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			1-Heptadecene	238	C17H34	006765-39-5	94
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047130.D
Acq On : 09 Aug 2024 21:05
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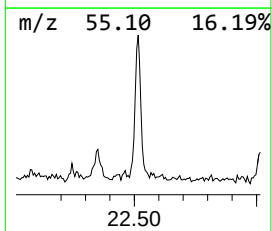
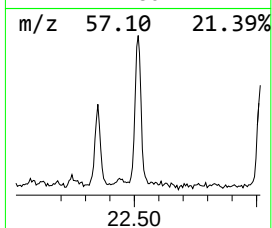
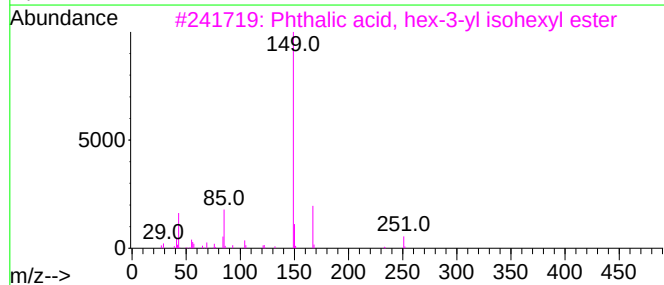
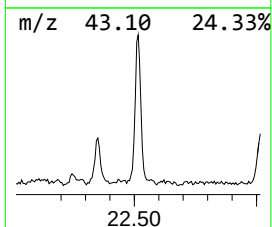
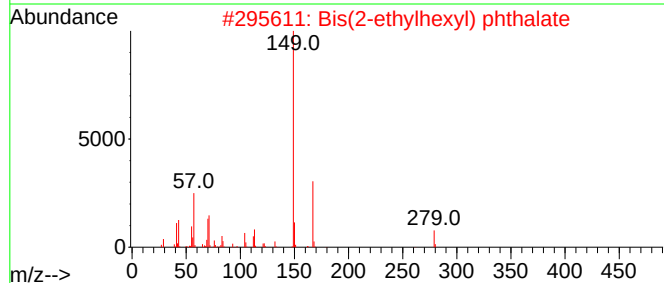
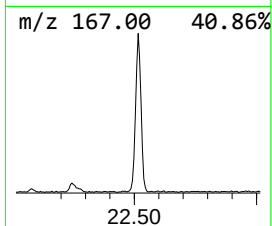
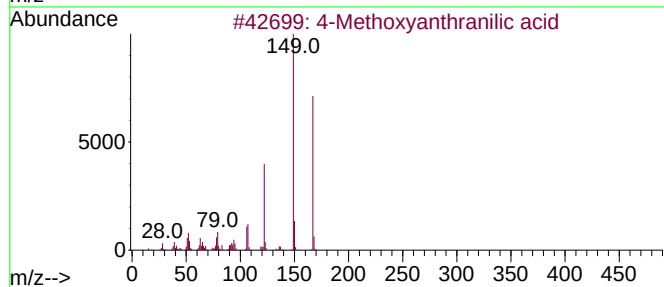
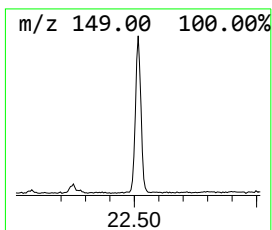
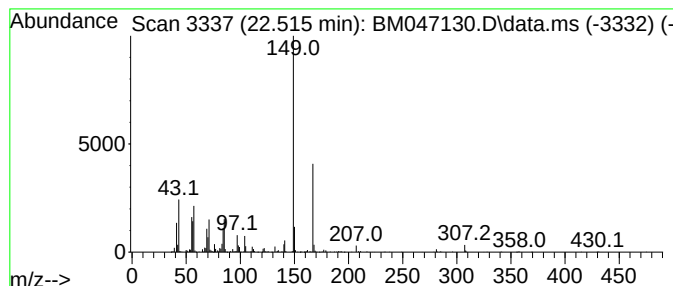
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 4-Methoxyanthranilic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.515	4.37 ng/ul	672306	Perylene-d12	23.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methoxyanthranilic acid	167	C8H9NO3	004294-95-5	64
2			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	53
3			Phthalic acid, hex-3-yl isohexyl...	334	C20H30O4	1000356-95-6	53
4			Phthalic acid, isohexyl 2-methyl...	334	C20H30O4	1000356-91-0	53
5			Phthalic acid, 2-ethylbutyl isob...	306	C18H26O4	1000356-88-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080924\
Data File : BM047130.D
Acq On : 09 Aug 2024 21:05
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Sample : P3498-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM080224.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
Octanoic acid	9.528	2.8	ng/ul	251768	2	10.140	1814070	20.0
1-Phenoxypropan...	10.899	3.4	ng/ul	303524	2	10.140	1814070	20.0
Nonanoic acid	10.999	5.6	ng/ul	506541	2	10.140	1814070	20.0
Phenol, 4-(1,1-...	12.887	10.9	ng/ul	1260290	3	14.040	2306810	20.0
n-Hexadecanoic ...	17.739	5.2	ng/ul	688456	4	16.798	2631530	20.0
Octadecanoic acid	19.039	3.0	ng/ul	413943	5	21.033	2772620	20.0
12-Hydroxystear...	20.127	3.2	ng/ul	444996	5	21.033	2772620	20.0
(DEL) Alkane: C...	20.774	4.6	ng/ul	639771	5	21.033	2772620	20.0
4-Methoxyanthra...	22.515	4.4	ng/ul	672306	6	23.733	3076580	20.0