

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
 Data File : BN029549.D
 Acq On : 07 Feb 2024 16:53
 Operator : MA/JU
 Sample : P1303-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 C0FH2

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_N\Methods\SFAM-EPA-BN020724.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BN029549.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.328	37	41	50	rVB	60082	80720	2.50%	0.188%
2	3.740	107	111	130	rBV	626987	1018611	31.56%	2.370%
3	4.063	163	166	172	rVB	16639	23080	0.72%	0.054%
4	5.011	325	327	332	rVB3	6877	8301	0.26%	0.019%
5	5.987	489	493	496	rBV7	3225	4560	0.14%	0.011%
6	6.687	610	612	614	rBV3	3200	3636	0.11%	0.008%
7	6.869	639	643	646	rVB5	2907	4308	0.13%	0.010%
8	7.052	667	674	685	rBV	803478	1308717	40.55%	3.045%
9	7.228	698	704	720	rVB	700691	1091121	33.81%	2.539%
10	7.410	728	735	747	rVB	833290	1303975	40.41%	3.034%
11	7.516	750	753	758	rBV4	4489	6646	0.21%	0.015%
12	7.887	809	816	822	rBV	748669	1204791	37.33%	2.803%
13	7.952	822	827	835	rVB	33786	54705	1.70%	0.127%
14	8.593	929	936	949	rBV	964703	1520476	47.12%	3.538%
15	9.051	1005	1014	1025	rBV	767413	1250294	38.74%	2.909%
16	9.216	1039	1042	1047	rVB6	4381	6933	0.21%	0.016%
17	9.451	1076	1082	1084	rBV4	5481	9554	0.30%	0.022%
18	9.634	1111	1113	1117	rVB4	3143	3626	0.11%	0.008%
19	9.769	1128	1136	1148	rBV	526900	891544	27.63%	2.074%
20	10.210	1208	1211	1213	rBV4	3897	3666	0.11%	0.009%
21	10.304	1219	1227	1238	rBV	877073	1452473	45.01%	3.380%
22	10.687	1284	1292	1302	rVB	937074	1624728	50.35%	3.780%
23	10.828	1308	1316	1330	rBV	865632	1545583	47.89%	3.596%
24	12.116	1530	1535	1541	rBV7	10258	15302	0.47%	0.036%
25	12.275	1556	1562	1567	rBV2	15126	26323	0.82%	0.061%
26	12.328	1570	1571	1578	rVB6	2238	3380	0.10%	0.008%
27	12.751	1638	1643	1646	rBV7	2314	3498	0.11%	0.008%
28	12.857	1656	1661	1663	rBV6	3046	3556	0.11%	0.008%
29	12.939	1668	1675	1678	rBV6	4224	7209	0.22%	0.017%
30	13.069	1691	1697	1703	rVB8	2884	5778	0.18%	0.013%
31	13.357	1742	1746	1753	rVB2	18185	26609	0.82%	0.062%
32	13.428	1753	1758	1766	rBV2	33217	54228	1.68%	0.126%
33	13.498	1766	1770	1774	rVB6	2538	4520	0.14%	0.011%
34	13.757	1807	1814	1828	rBV2	90554	191818	5.94%	0.446%
35	13.951	1840	1847	1853	rBV	1380947	1940941	60.15%	4.516%
36	14.063	1861	1866	1868	rVV6	4375	4890	0.15%	0.011%

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37	14.222	1882	1893	1907	rBV	1672804	2411596	74.73%	5.611%
38	14.439	1926	1930	1933	rBV5	3335	5516	0.17%	0.013%
39	14.528	1938	1945	1953	rBV	1275854	1839735	57.01%	4.281%
40	14.681	1967	1971	1973	rBV3	12406	16162	0.50%	0.038%
41	14.728	1973	1979	1983	rVV	538510	770353	23.87%	1.792%
42	14.781	1983	1988	1999	rVB	499080	784031	24.30%	1.824%
43	14.957	2011	2018	2025	rVB10	13303	32911	1.02%	0.077%
44	15.069	2036	2037	2042	rVB4	3443	3401	0.11%	0.008%
45	15.198	2056	2059	2062	rVB4	2174	3390	0.11%	0.008%
46	15.386	2087	2091	2096	rBV6	7348	12042	0.37%	0.028%
47	15.522	2107	2114	2123	rBV	1983216	2872047	89.00%	6.683%
48	15.645	2128	2135	2146	rBV	448857	651819	20.20%	1.517%
49	15.763	2150	2155	2160	rBV8	7991	12873	0.40%	0.030%
50	16.175	2222	2225	2229	rBV6	4083	7078	0.22%	0.016%
51	16.310	2244	2248	2251	rVB6	5120	7024	0.22%	0.016%
52	16.692	2308	2313	2316	rBV4	8254	10969	0.34%	0.026%
53	16.763	2321	2325	2327	rVB5	2940	3469	0.11%	0.008%
54	16.880	2342	2345	2347	rBV4	2969	3294	0.10%	0.008%
55	17.104	2379	2383	2386	rVB6	5195	7020	0.22%	0.016%
56	17.186	2393	2397	2399	rBV5	3870	4451	0.14%	0.010%
57	17.280	2406	2413	2419	rBV	1387187	2001786	62.03%	4.658%
58	17.380	2423	2430	2440	rVV	1900710	2819331	87.36%	6.560%
59	17.480	2440	2447	2452	rVB8	22933	45091	1.40%	0.105%
60	17.680	2475	2481	2486	rVB9	6116	13380	0.41%	0.031%
61	17.792	2497	2500	2505	rBV5	4139	8642	0.27%	0.020%
62	17.927	2520	2523	2526	rBV5	4016	5602	0.17%	0.013%
63	17.969	2527	2530	2534	rVB5	4898	6570	0.20%	0.015%
64	18.057	2541	2545	2554	rBV5	11312	24039	0.74%	0.056%
65	18.133	2554	2558	2560	rBV5	4755	5776	0.18%	0.013%
66	18.192	2562	2568	2578	rBV	271821	412501	12.78%	0.960%
67	18.492	2615	2619	2622	rBV6	5152	8108	0.25%	0.019%
68	18.627	2639	2642	2645	rVB4	12334	13440	0.42%	0.031%
69	18.857	2679	2681	2683	rBV3	4072	3239	0.10%	0.008%
70	18.992	2699	2704	2707	rBV7	6056	10239	0.32%	0.024%
71	19.351	2754	2765	2775	rBV4	54442	167699	5.20%	0.390%
72	19.474	2782	2786	2792	rBV	91498	118480	3.67%	0.276%
73	19.674	2814	2820	2830	rBV	2298978	3227074	100.00%	7.509%
74	19.898	2856	2858	2859	rBV2	4866	3602	0.11%	0.008%
75	20.216	2908	2912	2914	rBV5	14055	20523	0.64%	0.048%
76	20.245	2914	2917	2923	rVB4	15476	24429	0.76%	0.057%

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Title : SVOA CALIBRATION

77	21.204	3076	3080	3087	rBV	269241	381559	11.82%	0.888%
78	21.474	3121	3126	3139	rBV2	1503704	2072519	64.22%	4.822%
79	21.657	3155	3157	3161	rVB	34031	40756	1.26%	0.095%
80	22.127	3234	3237	3242	rVB4	46423	72427	2.24%	0.169%
81	22.757	3341	3344	3353	rVB2	83145	129915	4.03%	0.302%
82	23.698	3497	3504	3517	rBV2	1521715	3059070	94.79%	7.118%
83	23.851	3524	3530	3540	rVB	1021963	2111911	65.44%	4.914%

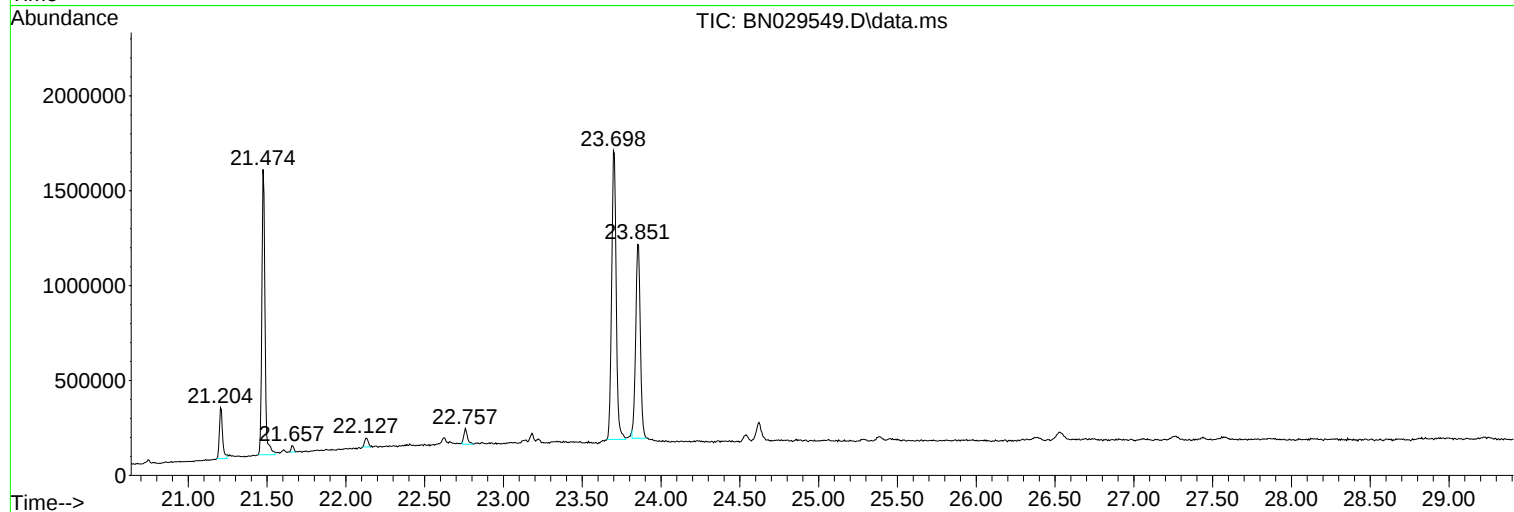
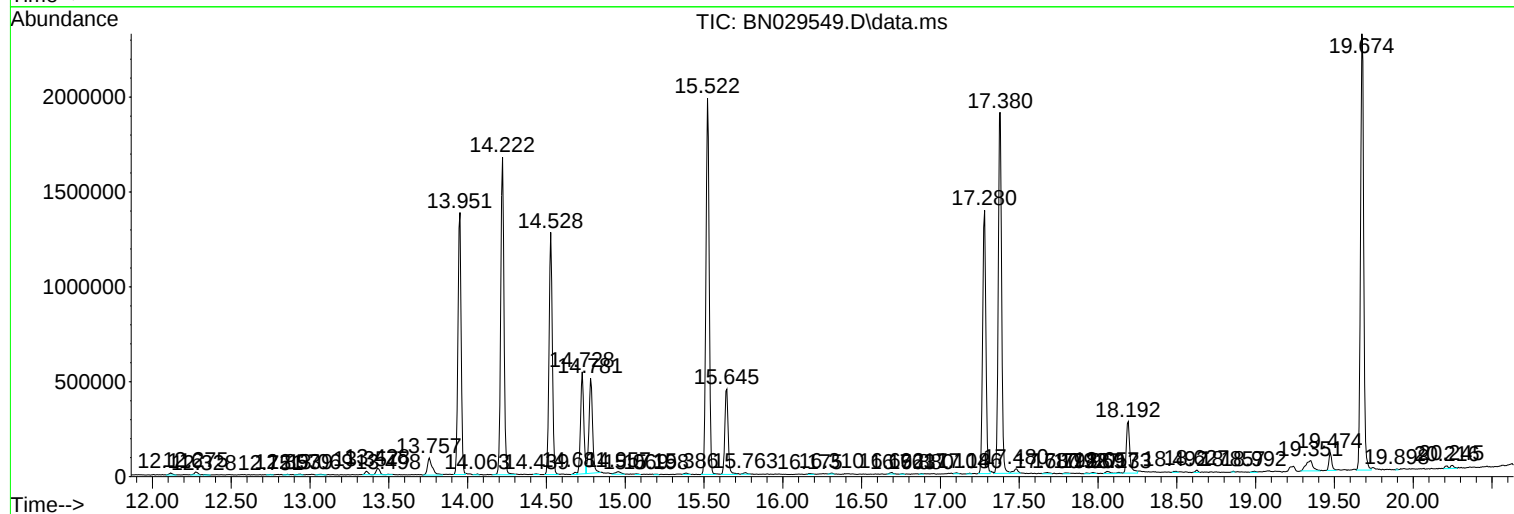
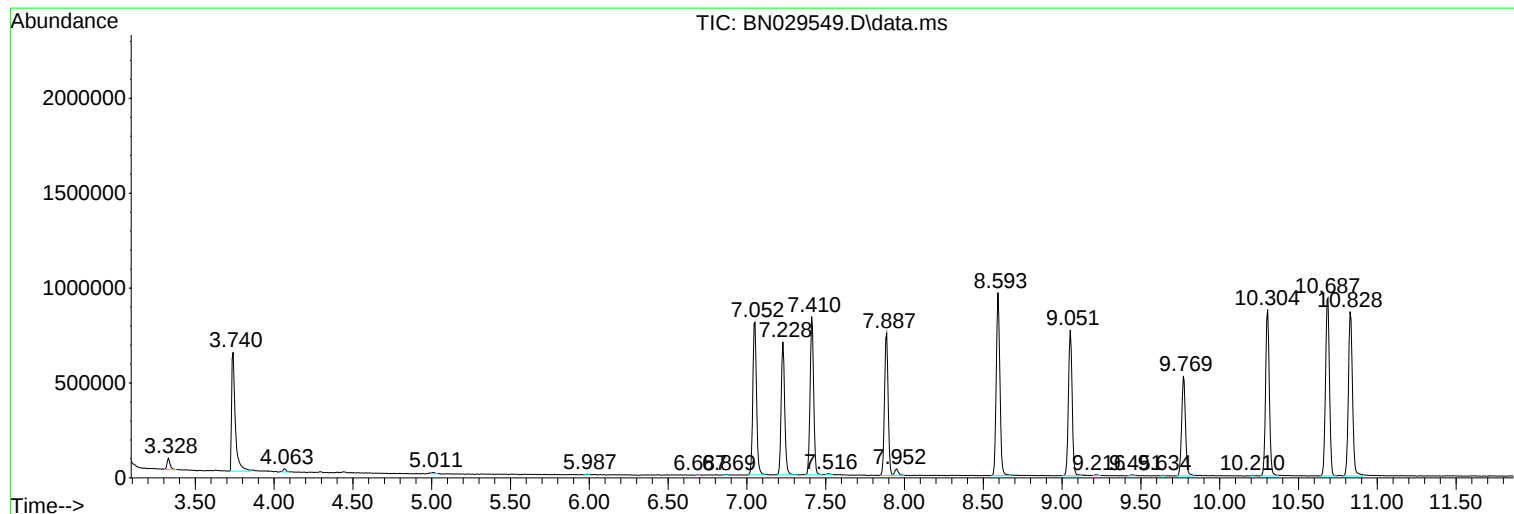
Sum of corrected areas: 42976989

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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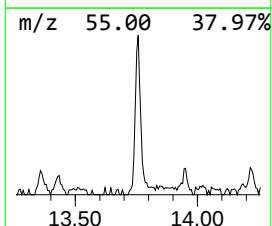
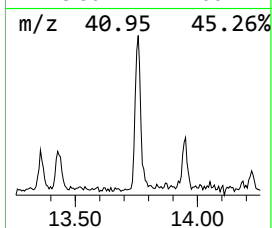
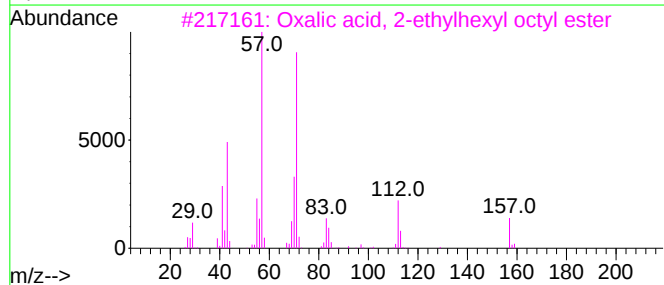
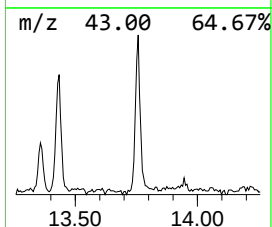
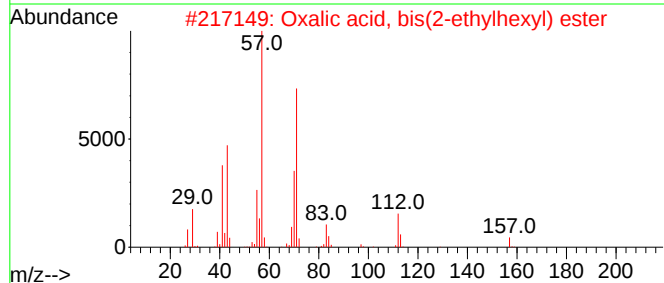
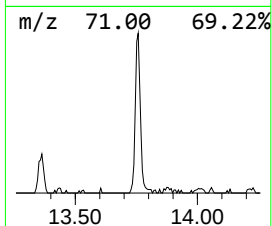
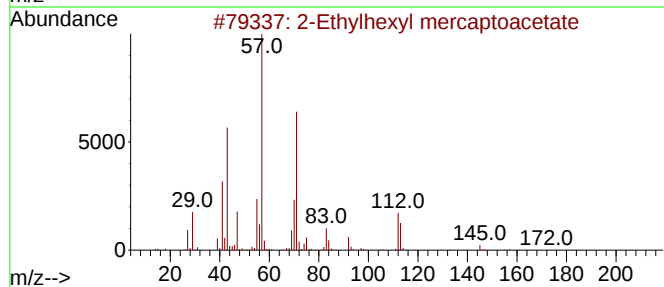
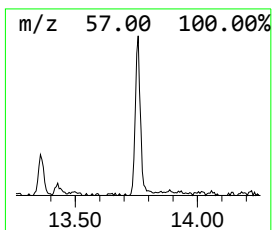
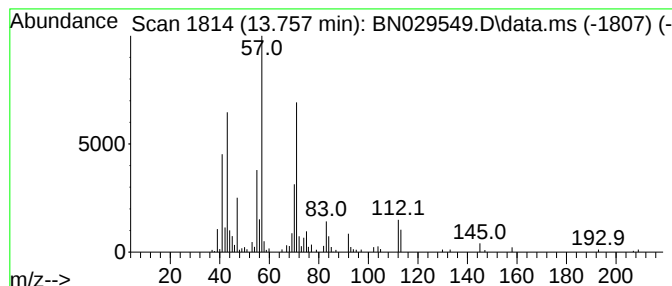
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 2-Ethylhexyl mercaptoacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	2.09 ng/ul	191818	Acenaphthene-d10	14.528

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	86
2			Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	64
3			Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	58
4			Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1010309-38-5	58
5			Oxalic acid, butyl 2-ethylhexyl ...	258	C14H26O4	1000309-38-6	53



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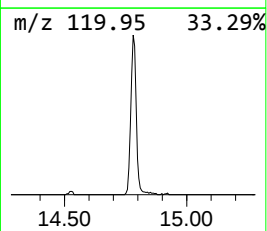
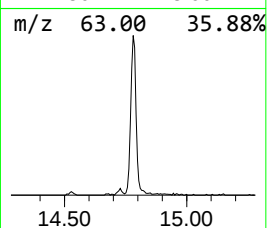
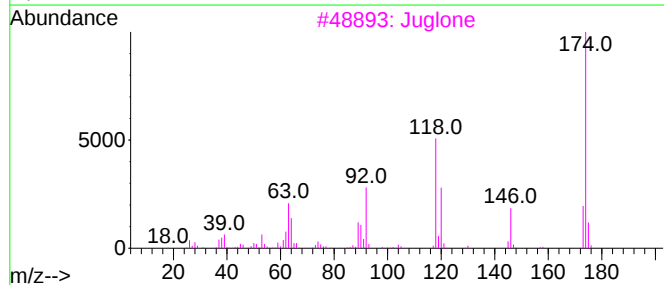
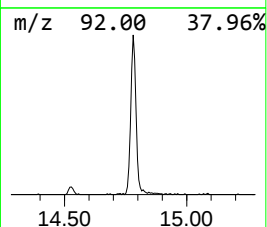
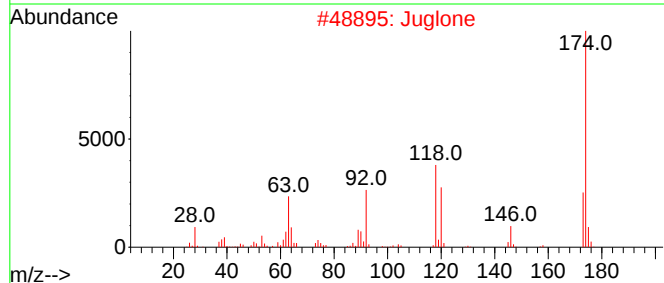
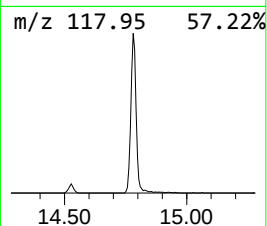
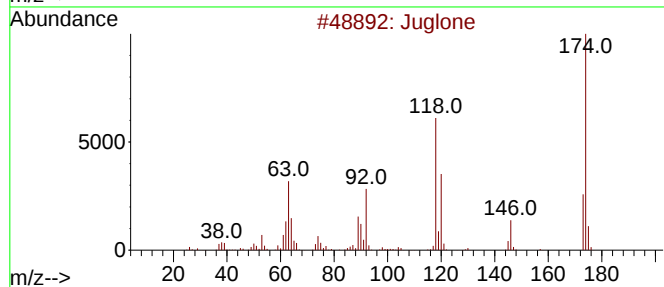
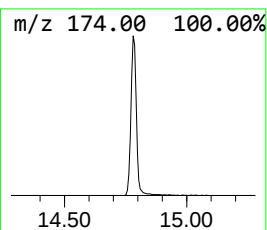
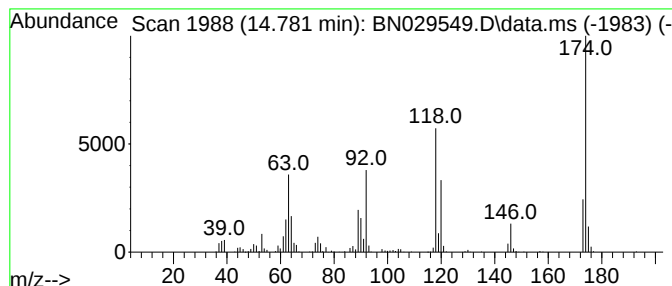
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Juglone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.781	8.52 ng/ul	784031	Acenaphthene-d10	14.528

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone			174	C10H6O3	000481-39-0	99
2	Juglone			174	C10H6O3	000481-39-0	95
3	Juglone			174	C10H6O3	000481-39-0	94
4	Juglone			174	C10H6O3	000481-39-0	64
5	1-Methyl-5-(4-methylphenyl)tetra...			174	C9H10N4	068826-33-5	52



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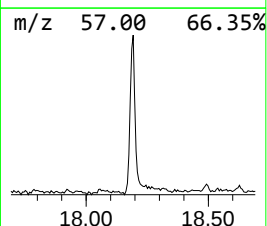
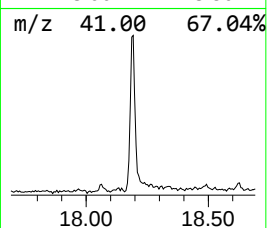
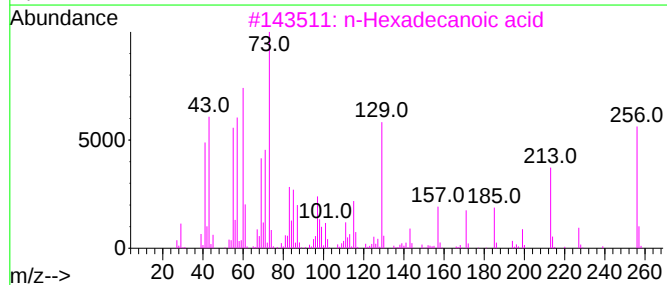
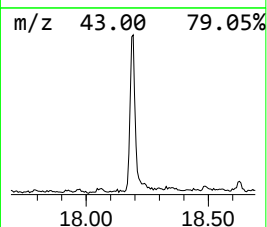
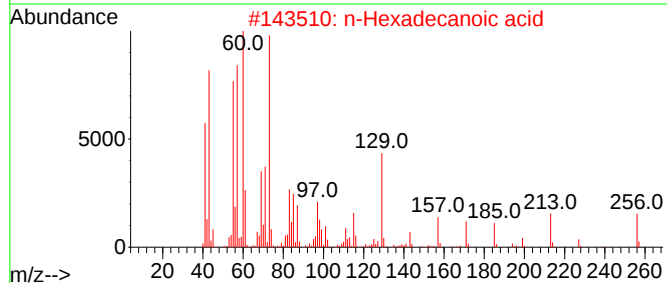
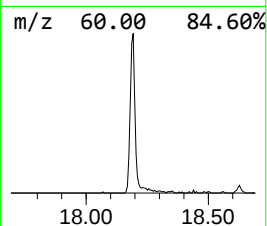
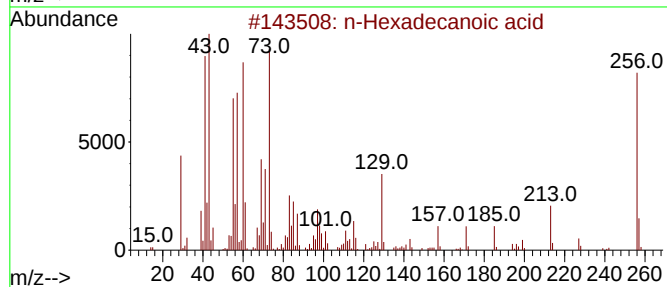
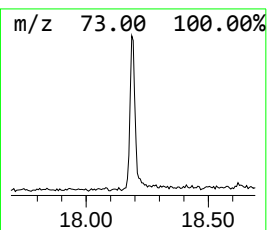
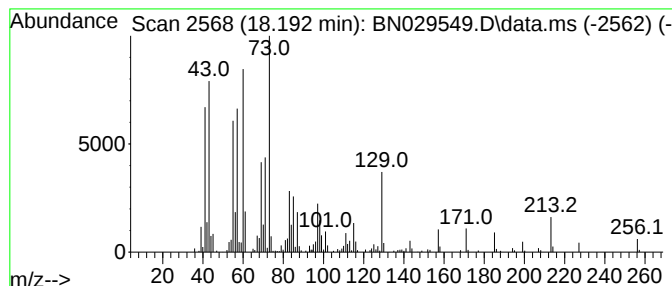
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	4.12 ng/ul	412501	Phenanthrene-d10	17.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	81



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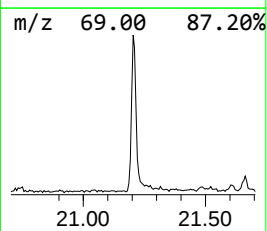
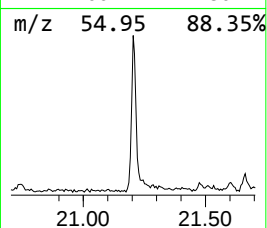
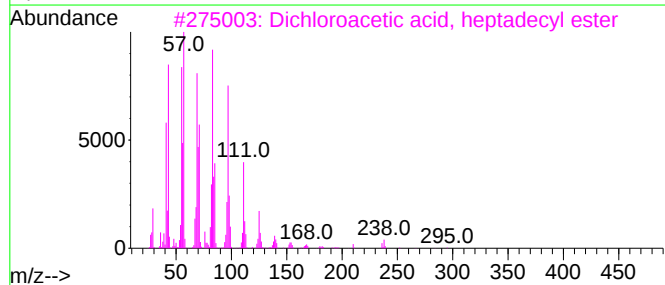
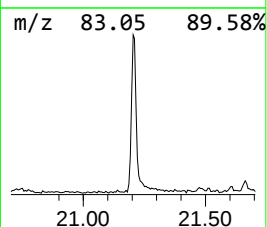
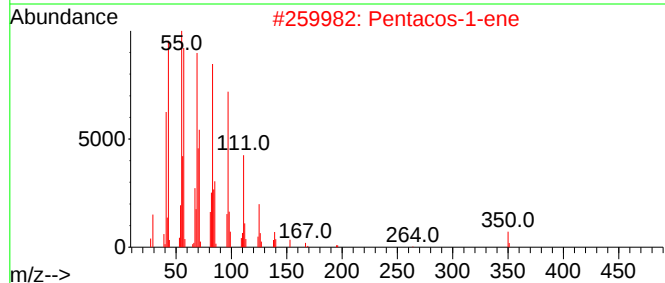
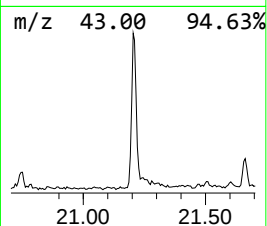
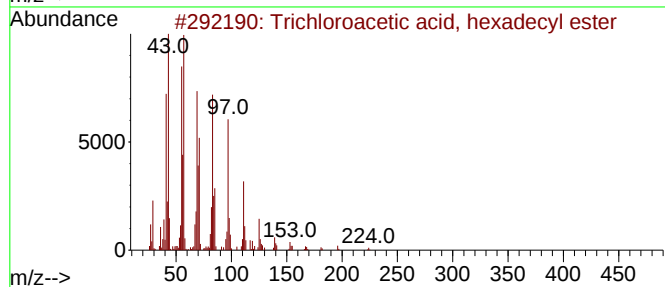
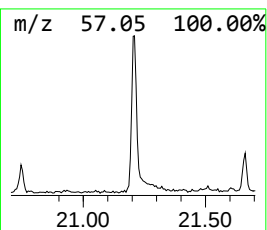
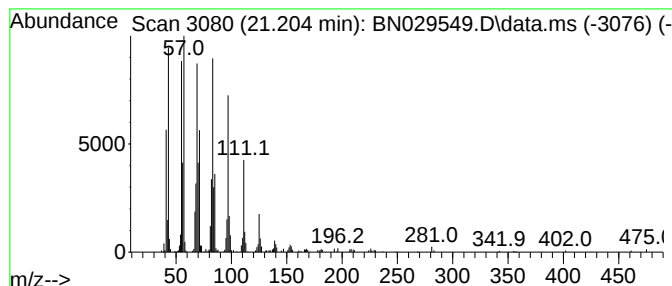
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.204	3.68 ng/ul	381559	Chrysene-d12	21.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			Pentacos-1-ene	350	C25H50	016980-85-1	94
3			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4			Heptacos-1-ene	378	C27H54	015306-27-1	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
Data File : BN029549.D
Acq On : 07 Feb 2024 16:53
Operator : MA/JU
Sample : P1303-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0FH2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.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
2-Ethylhexyl me...	13.757	2.1	ng/ul	191818	3	14.528	1839740	20.0
Juglone	14.781	8.5	ng/ul	784031	3	14.528	1839740	20.0
n-Hexadecanoic ...	18.192	4.1	ng/ul	412501	4	17.280	2001790	20.0
Trichloroacetic...	21.204	3.7	ng/ul	381559	5	21.474	2072520	20.0