LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111023\
Data File : BP018050.D
Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A4970

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_P\Methods\SFAM-EPA-BP111023.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP018050.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.146	8	10	16	rVB5	11814	13796	0.58%	0.049%
2	3.234	21	25	30	rBV	15518	21613	0.91%	0.077%
3	3.575	78	83	86	rBV3	10948	14866	0.63%	0.053%
4	3.675	97	100	109	rBV	56003	96221	4.06%	0.344%
5	3.840	124	128	131	rBV3	6349	11392	0.48%	0.041%
6	3.875	131	134	140	rVB3	19769	26626	1.12%	0.095%
7	3.964	146	149	155	rVB2	9148	13922	0.59%	0.050%
8	4.311	205	208	213	rVV4	8137	16740	0.71%	0.060%
9	4.358	213	216	223	rVV3	24979	38216	1.61%	0.136%
10	5.146	344	350	359	rVV10	8062	20993	0.89%	0.075%
11	5.222	359	363	371	rVV	14470	26615	1.12%	0.095%
12	5.305	372	377	385	rVV	30509	55137	2.33%	0.197%
13	5.664	432	438	444	rBV	19406	27958	1.18%	0.100%
14	5.893	470	477	491	rVV	1050786	1631484	68.84%	5.826%
15	6.452	568	572	590	rVB2	70345	142146	6.00%	0.508%
16	6.858	634	641	648	rVV	47983	94563	3.99%	0.338%
17	6.922	648	652	663	rVV2	33112	66336	2.80%	0.237%
18	7.022	663	669	680	rVV2	82981	174879	7.38%	0.625%
19	7.099	680	682	687	rVB3	9607	12926	0.55%	0.046%
20	7.199	693	699	709	rVB	281936	433747	18.30%	1.549%
21	7.375	722	729	737	rBV	288140	489382	20.65%	1.748%
22	7.628	765	772	777	rVB4	8751	18284	0.77%	0.065%
23	7.846	803	809	823	rBV2	272182	543057	22.91%	1.939%
24	7.952	823	827	831	rVV3	15737	23944	1.01%	0.086%
25	8.128	848	857	867	rBV2	40852	101070	4.26%	0.361%
26	8.428	902	908	912	rBV2	22950	43012	1.81%	0.154%
27	8.481	912	917	926	rVV2	28531	66583	2.81%	0.238%
28	8.575	926	933	942	rVV	234124	458853	19.36%	1.639%
29	8.646	942	945	948	rVV3	14268	24037	1.01%	0.086%
30	8.710	951	956	963	rVV	56100	91204	3.85%	0.326%
31	8.957	990	998	1006	rBV	249866	414228	17.48%	1.479%
32	9.057	1006	1015	1021	rVV	381581	676386	28.54%	2.415%
33	9.116	1021	1025	1028	rVV2	39427	64144	2.71%	0.229%
34	9.157	1028	1032	1043	rVB	98200	175638	7.41%	0.627%
35	9.434	1072	1079	1090	rBV	27635	67817	2.86%	0.242%
36	9.604	1103	1108	1121	rVB2	51003	87521	3.69%	0.313%

LSC Area Percent Report

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Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

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_P\Methods\SFAM-EPA-BP111023.MA.M
Title : SVOA CALIBRATION

37	9.769	1126	1136	1149	rBV	308813	555292	23.43%	1.983%
38	9.875	1149	1154	1157	rBV7	9169	18507	0.78%	0.066%
39	9.922	1157	1162	1167	rVV	125650	203750	8.60%	0.728%
40	9.975	1168	1171	1178	rVB3	39829	68853	2.91%	0.246%
41	10.146	1191	1200	1212	rVB2	68853	139831	5.90%	0.499%
42	10.299	1218	1226	1236	rBV	380485	707479	29.85%	2.526%
43	10.510	1257	1262	1269	rVB8	12474	21393	0.90%	0.076%
44	10.575	1269	1273	1277	rBV5	16581	28160	1.19%	0.101%
45	10.669	1283	1289	1294	rBV	393168	667337	28.16%	2.383%
46	10.851	1313	1320	1330	rVV	268970	516774	21.80%	1.845%
47	10.946	1330	1336	1346	rVB	147606	247680	10.45%	0.884%
48	11.163	1370	1373	1379	rVB2	10698	14834	0.63%	0.053%
49	11.228	1379	1384	1391	rBV4	25353	44759	1.89%	0.160%
50	11.369	1401	1408	1415	rBV	37807	70932	2.99%	0.253%
51	11.451	1415	1422	1432	rBV2	51468	111035	4.68%	0.397%
52	11.634	1446	1453	1458	rBV3	14013	31284	1.32%	0.112%
53	11.716	1465	1467	1476	rVB7	9104	14866	0.63%	0.053%
54	11.834	1484	1487	1492	rVV2	12150	16698	0.70%	0.060%
55	12.257	1553	1559	1565	rVB4	6274	13522	0.57%	0.048%
56	12.522	1598	1604	1607	rBV2	10382	17400	0.73%	0.062%
57	12.828	1647	1656	1664	rBV2	88785	168770	7.12%	0.603%
58	13.004	1680	1686	1692	rBV	22752	40019	1.69%	0.143%
59	13.087	1694	1700	1708	rVV	127307	182860	7.72%	0.653%
60	13.363	1739	1747	1755	rBV2	61996	106265	4.48%	0.379%
61	13.487	1760	1768	1777	rBV	230518	415466	17.53%	1.484%
62	13.781	1815	1818	1822	rVV2	11429	15466	0.65%	0.055%
63	13.945	1839	1846	1851	rVV	847032	1128241	47.60%	4.029%
64	13.987	1851	1853	1864	rVB3	47913	73547	3.10%	0.263%
65	14.140	1875	1879	1885	rVV9	7190	14653	0.62%	0.052%
66	14.222	1885	1893	1904	rVV	912918	1298611	54.79%	4.637%
67	14.316	1904	1909	1912	rVV7	9091	17201	0.73%	0.061%
68	14.363	1914	1917	1923	rVV6	9377	17187	0.73%	0.061%
69	14.422	1923	1927	1936	rVV	23992	45389	1.92%	0.162%
70	14.522	1936	1944	1952	rVV	522950	768611	32.43%	2.745%
71	14.816	1989	1994	2008	rBV4	30878	93074	3.93%	0.332%
72	15.145	2046	2050	2055	rVB8	7079	11447	0.48%	0.041%
73	15.269	2067	2071	2076	rVB2	16295	23034	0.97%	0.082%
74	15.351	2079	2085	2093	rVB2	48308	75645	3.19%	0.270%
75	15.528	2108	2115	2123	rBV	1112104	1579711	66.65%	5.641%
76	15.681	2135	2141	2152	rBV	405704	601244	25.37%	2.147%

LSC Area Percent Report

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Data File : BP018050.D
Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A4970

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

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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Title : SVOA CALIBRATION

77	15.763	2152	2155	2163	rVB9	9286	17660	0.75%	0.063%
78	15.881	2170	2175	2178	rBV2	26284	41377	1.75%	0.148%
79	15.963	2186	2189	2196	rVB9	9391	17556	0.74%	0.063%
80	16.375	2254	2259	2262	rBV5	9969	19327	0.82%	0.069%
81	16.545	2282	2288	2295	rBV4	9233	18289	0.77%	0.065%
82	17.304	2410	2417	2428	rBV	682174	948202	40.01%	3.386%
83	17.404	2428	2434	2446	rBV2	1275078	1808716	76.31%	6.459%
84	17.563	2458	2461	2466	rVB	10267	14303	0.60%	0.051%
85	17.751	2486	2493	2499	rBV6	9596	19445	0.82%	0.069%
86	17.939	2519	2525	2532	rBV	1057031	1321121	55.74%	4.718%
87	18.151	2556	2561	2573	rVV2	57590	104189	4.40%	0.372%
88	18.245	2573	2577	2583	rVB	15034	22668	0.96%	0.081%
89	18.363	2593	2597	2602	rBV	38606	51392	2.17%	0.184%
90	18.410	2603	2605	2612	rVB6	10298	12387	0.52%	0.044%
91	19.227	2740	2744	2748	rBV3	17526	22213	0.94%	0.079%
92	19.298	2752	2756	2760	rVV2	19456	27385	1.16%	0.098%
93	19.392	2768	2772	2781	rBV4	53399	94106	3.97%	0.336%
94	19.533	2793	2796	2801	rVB	41755	46252	1.95%	0.165%
95	19.657	2812	2817	2825	rBV	1707709	2184991	92.19%	7.803%
96	20.645	2982	2985	2990	rBV5	47344	60766	2.56%	0.217%
97	21.210	3078	3081	3087	rVB3	50054	66169	2.79%	0.236%
98	21.433	3114	3119	3128	rBV	796543	1076822	45.43%	3.845%
99	23.768	3508	3516	3524	rBV2	1182912	2370077	100.00%	8.464%
100	23.933	3537	3544	3557	rVB	557336	1165390	49.17%	4.162%

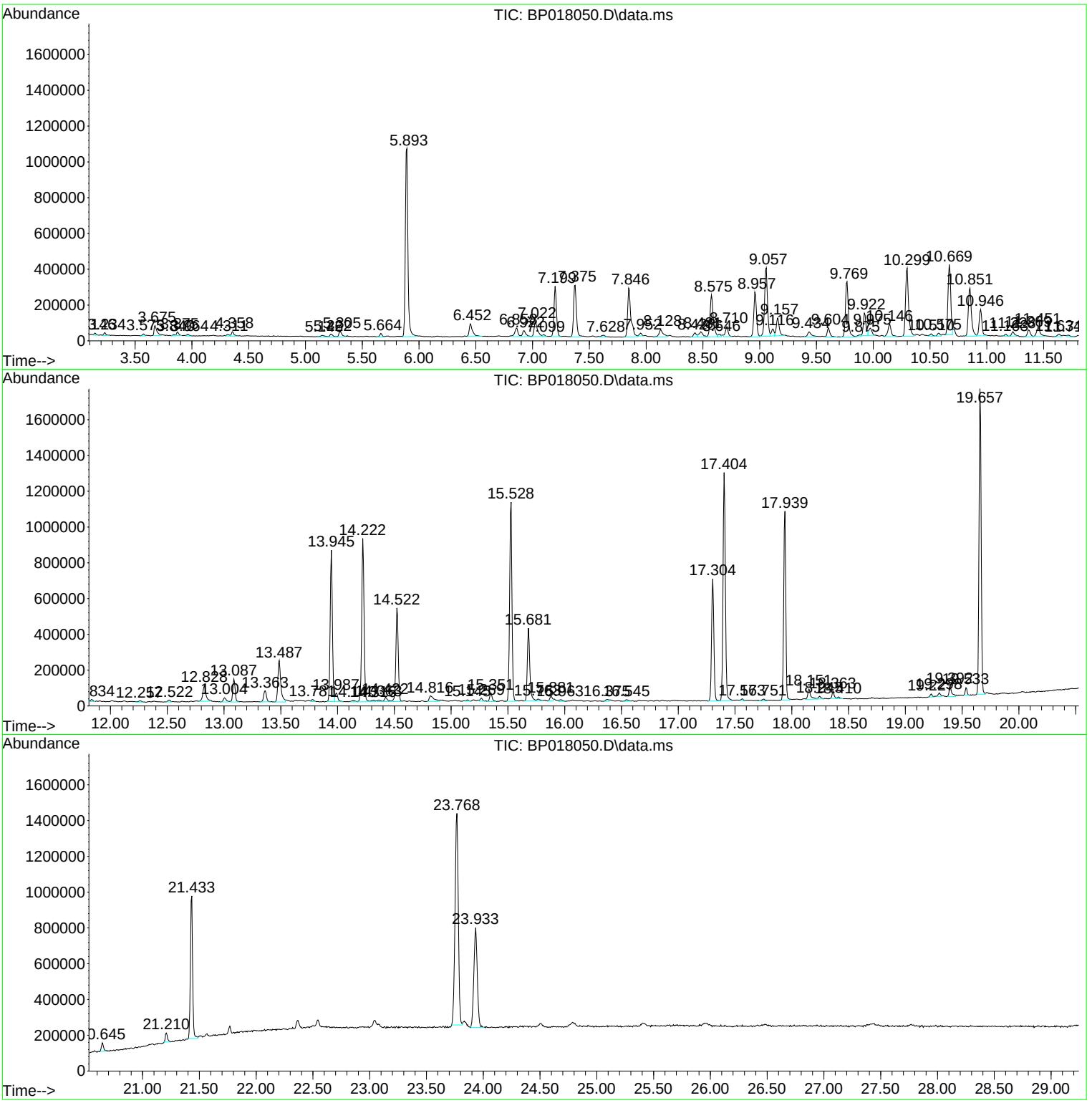
Sum of corrected areas: 28002966

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111023\
Data File : BP018050.D
Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111023\
Data File : BP018050.D
Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

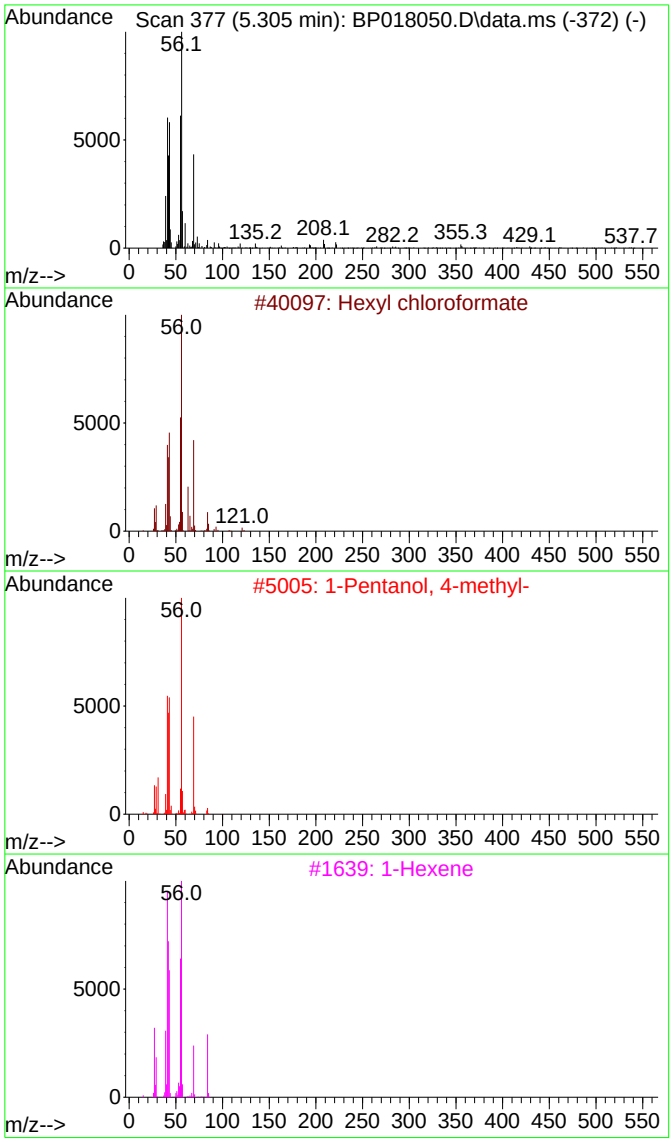
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

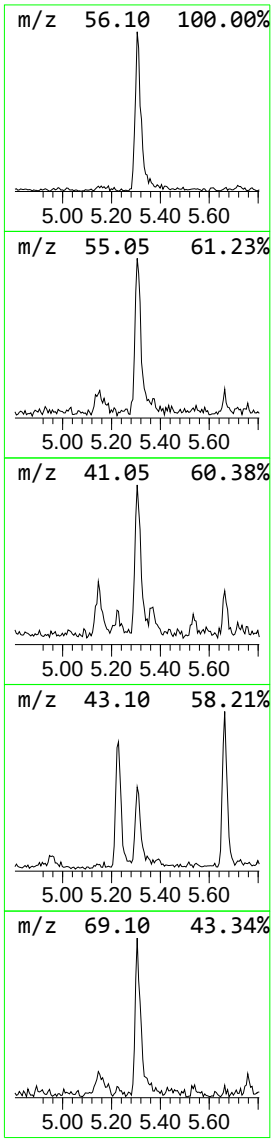
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexyl chloroformate Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.305	2.03 ng/ul	55137	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	64
2	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	64
3	1-Hexene	84	C6H12	000592-41-6	64
4	Cyclopropane, propyl-	84	C6H12	002415-72-7	50
5	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111023\
Data File : BP018050.D
Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

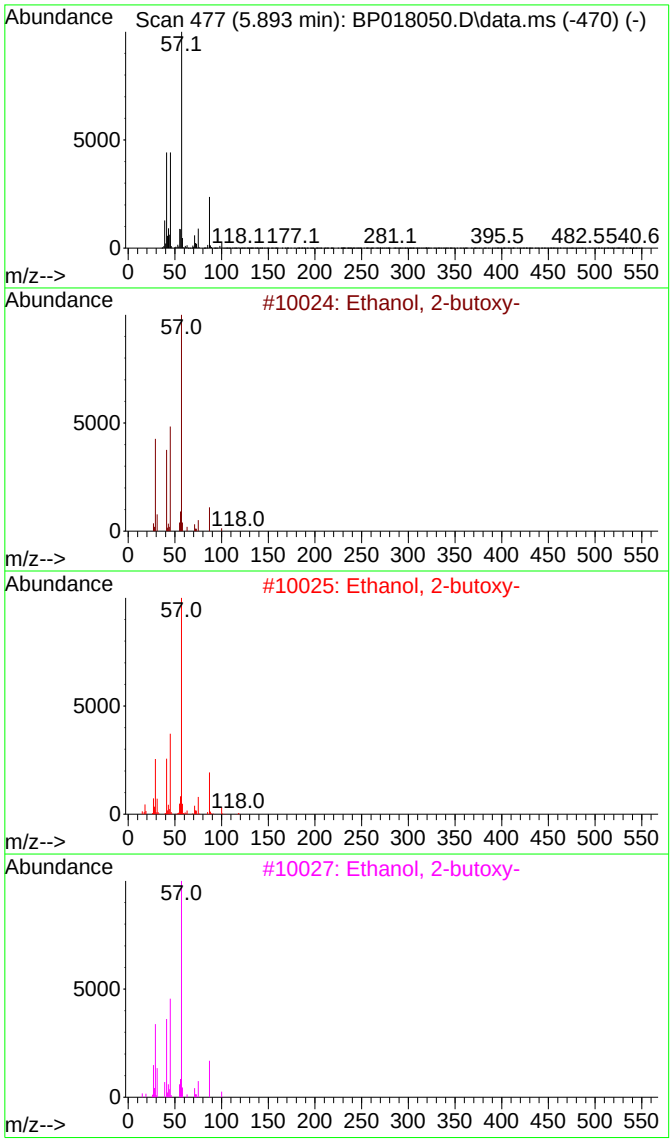
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

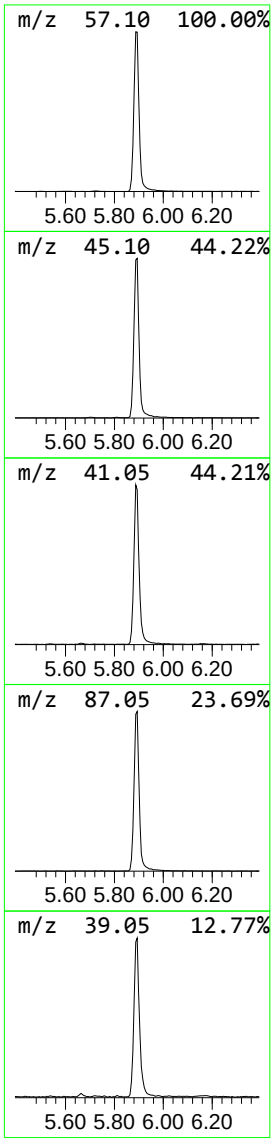
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.893	60.09 ng/ul	1631480	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
3	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
4	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	53
5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111023\
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Sample : 05013-01
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ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

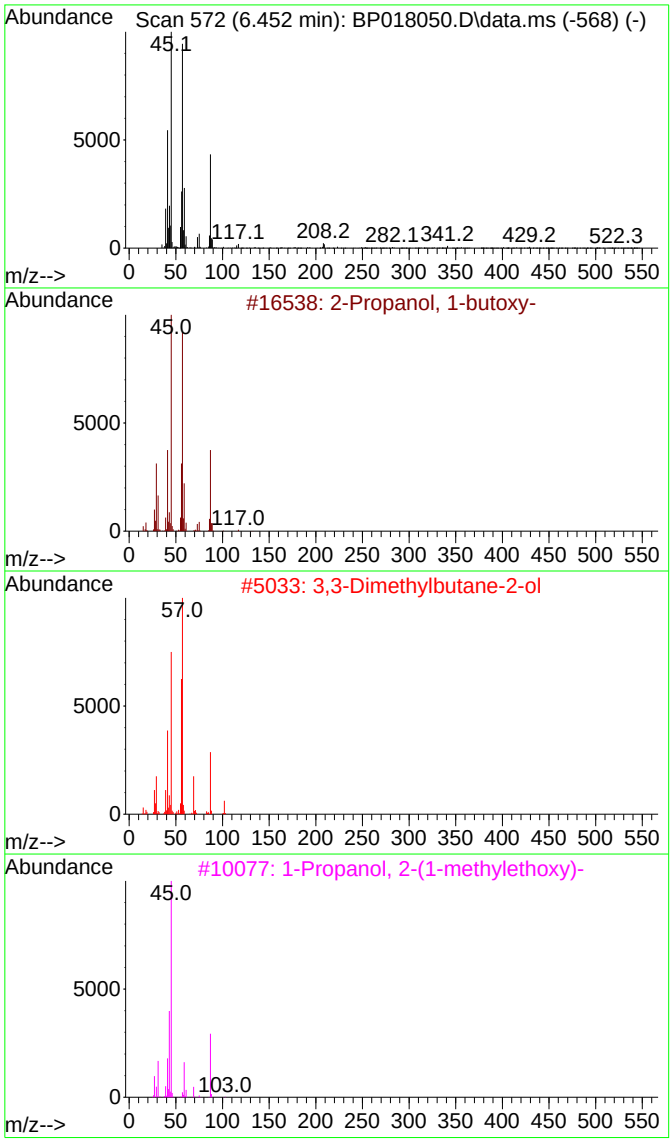
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

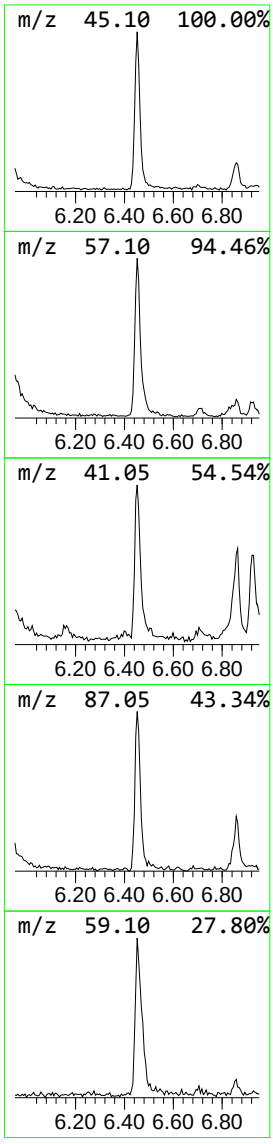
****

Peak Number 3 2-Propanol, 1-butoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.452	5.24 ng/ul	142146	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	72
2	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	59
3	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	59
4	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	59
5	Acetaldehyde isobutyl propyl acetal	160	C9H20O2	1000431-63-1	50





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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

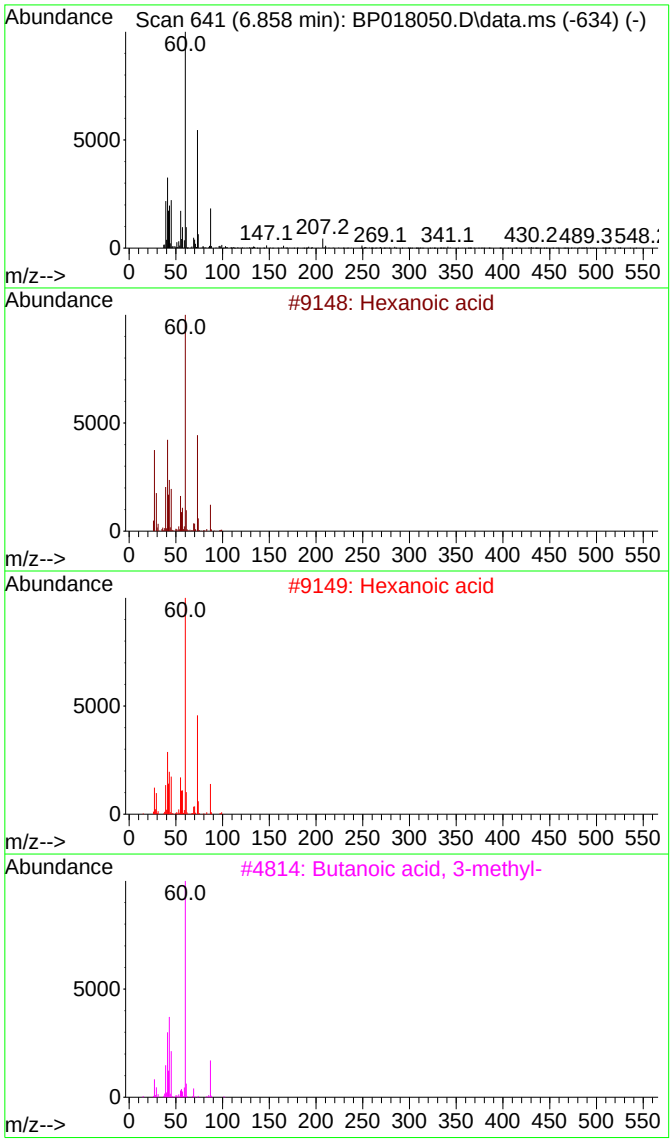
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

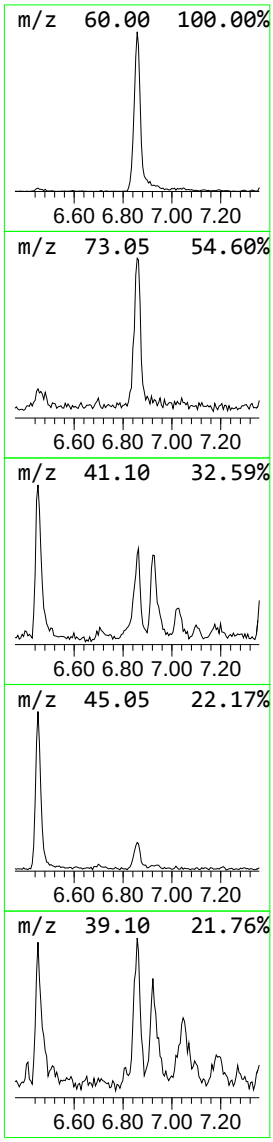
****

Peak Number 4 Hexanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.858	3.48 ng/ul	94563	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	83
2	Hexanoic acid	116	C6H12O2	000142-62-1	78
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
4	Heptanoic acid	130	C7H14O2	000111-14-8	72
5	Hexanoic acid	116	C6H12O2	000142-62-1	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111023\
Data File : BP018050.D
Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

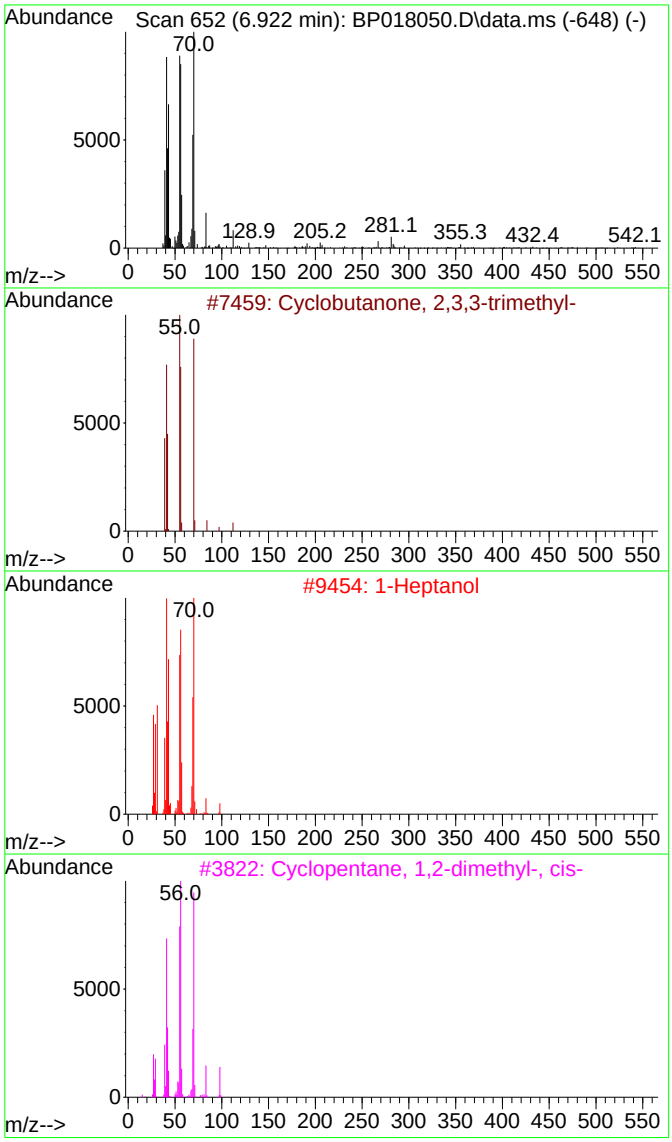
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

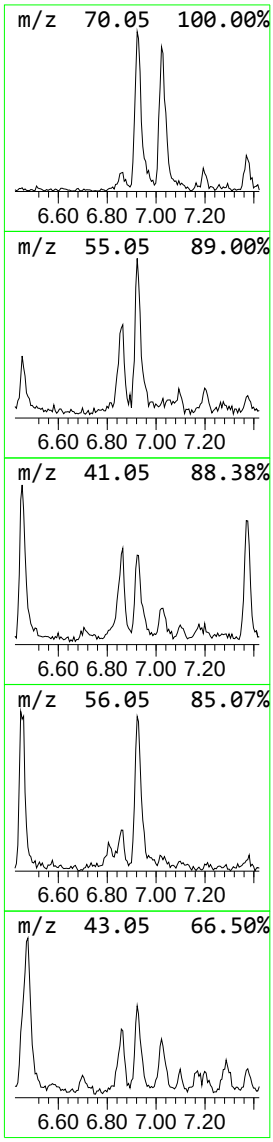
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclobutanone, 2,3,3-trimet... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.922	2.44 ng/ul	66336	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutanone, 2,3,3-trimethyl-	112	C7H12O	028290-01-9	78
2	1-Heptanol	116	C7H16O	000111-70-6	78
3	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	72
4	1-Heptanol	116	C7H16O	000111-70-6	72
5	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	64





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Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

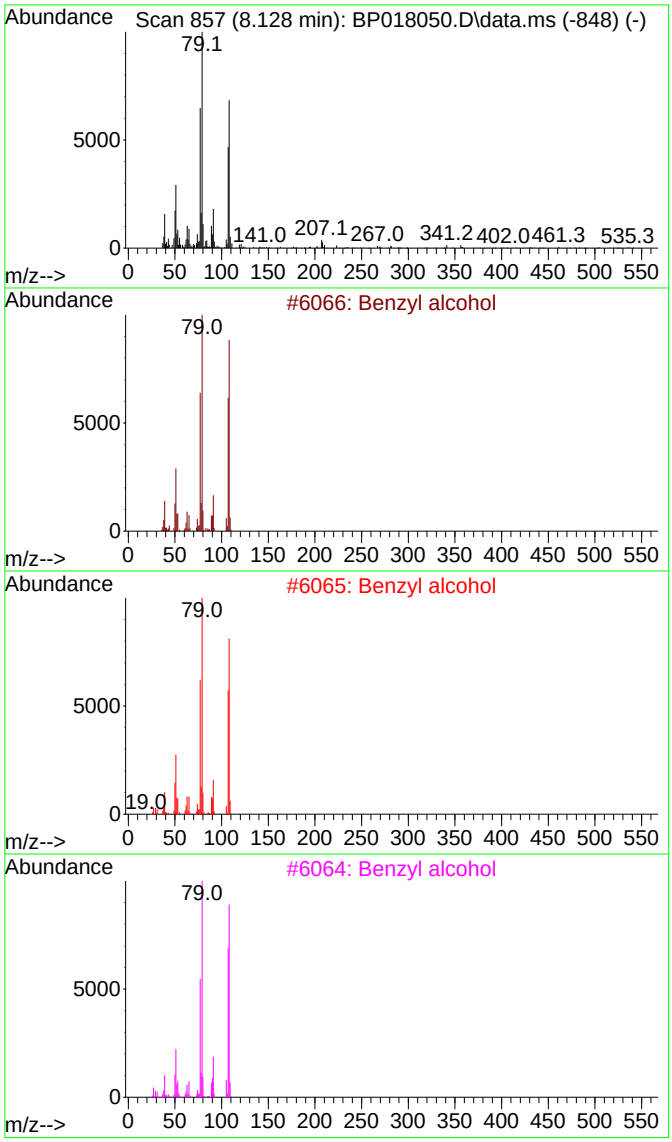
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

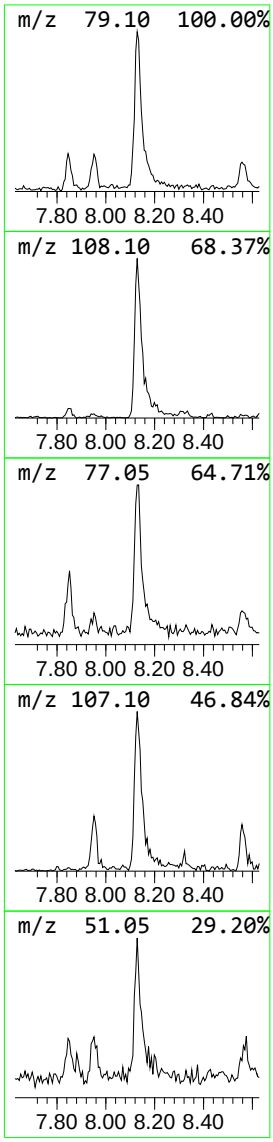
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzyl alcohol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.128	3.72 ng/ul	101070	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzyl alcohol	108	C7H8O	000100-51-6	97
2	Benzyl alcohol	108	C7H8O	000100-51-6	96
3	Benzyl alcohol	108	C7H8O	000100-51-6	94
4	Benzyl alcohol	108	C7H8O	000100-51-6	91
5	N-Cbz-glycylglycine p-nitropheny...	387	C18H17N3O7	013574-81-7	91





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Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

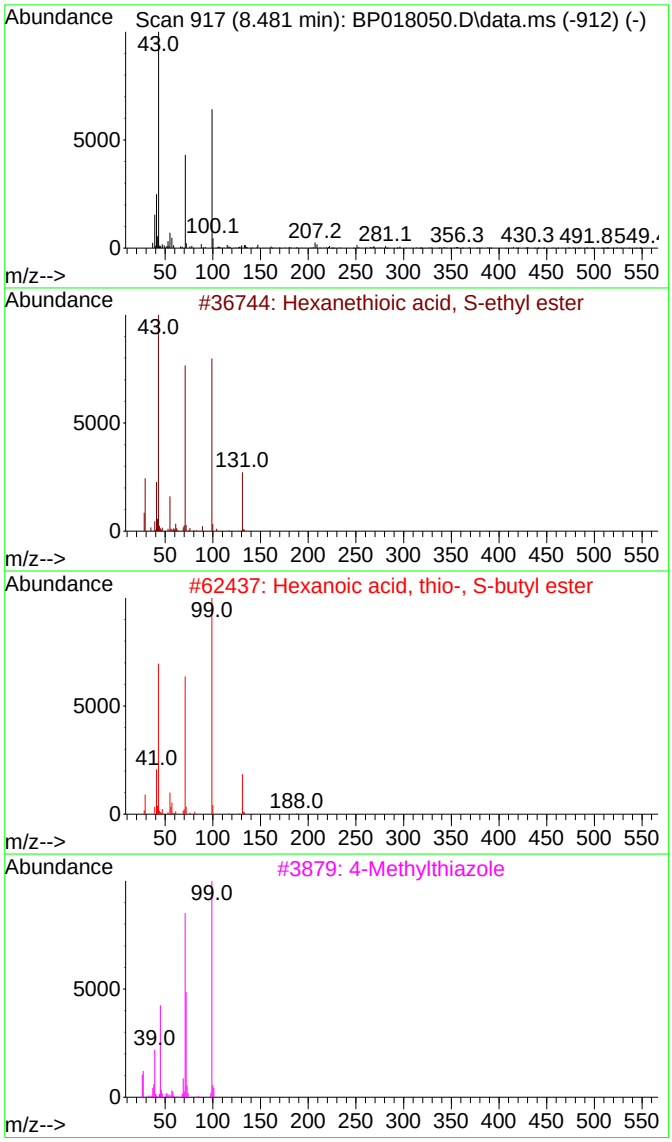
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

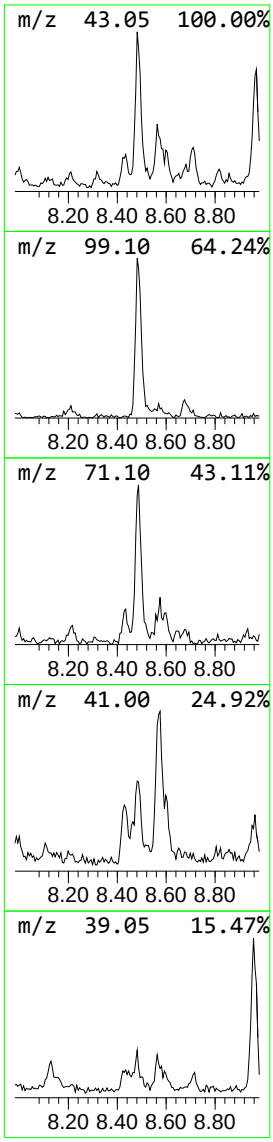
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Hexanethioic acid, S-ethyl ... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	2.45 ng/ul	66583	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanethioic acid, S-ethyl ester	160	C8H16OS	002450-12-6	72
2	Hexanoic acid, thio-, S-butyl ester	188	C10H20OS	002432-79-3	72
3	4-Methylthiazole	99	C4H5NS	000693-95-8	64
4	Pentanoic acid, 2-methyl-, anhyd...	214	C12H22O3	063169-61-9	64
5	1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	64





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Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Title : SVOA CALIBRATION

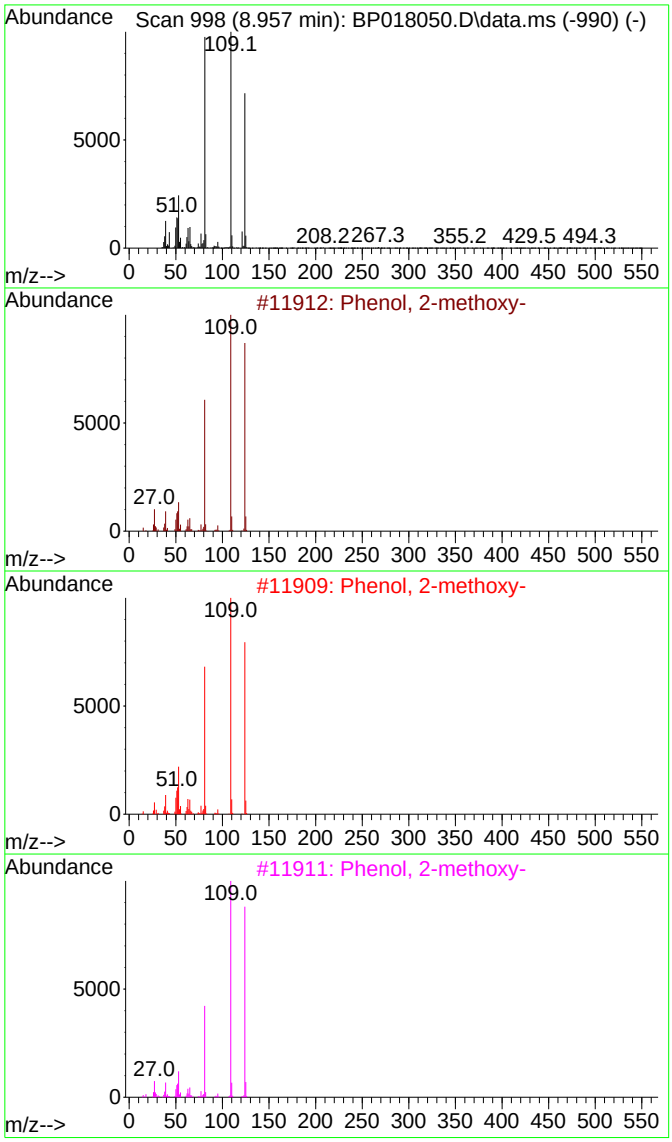
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

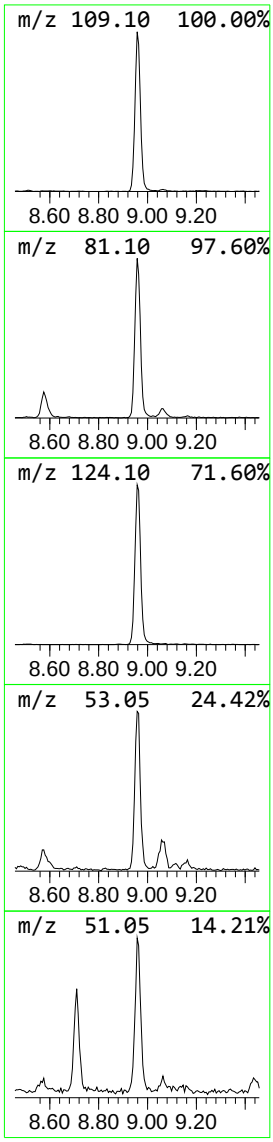
****

Peak Number 8 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.957	15.26 ng/ul	414228	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	91
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	91
3	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	86
4	Mequinol	124	C7H8O2	000150-76-5	70
5	Mequinol	124	C7H8O2	000150-76-5	70





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Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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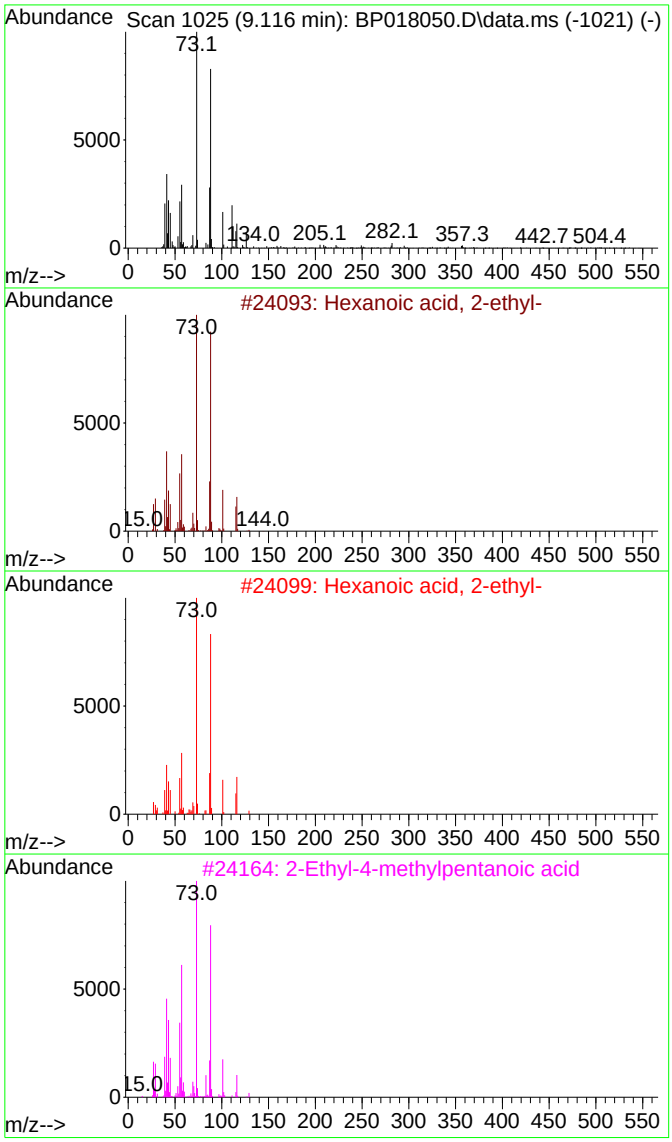
Quant Title : SVOA CALIBRATION

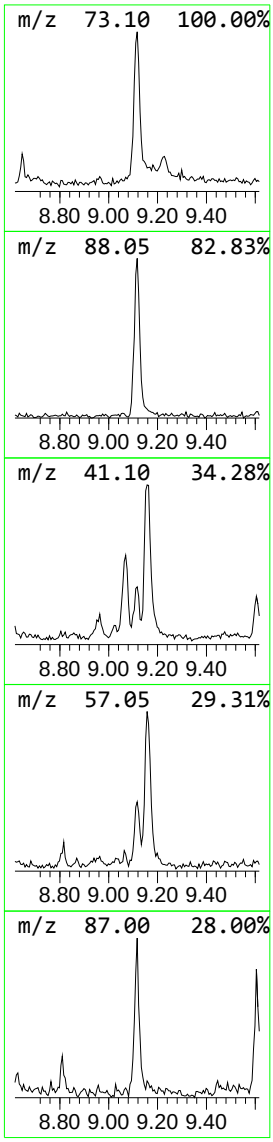
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Hexanoic acid, 2-ethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.116	2.36 ng/ul	64144	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	59
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	59
3	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	59
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	53
5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	53





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Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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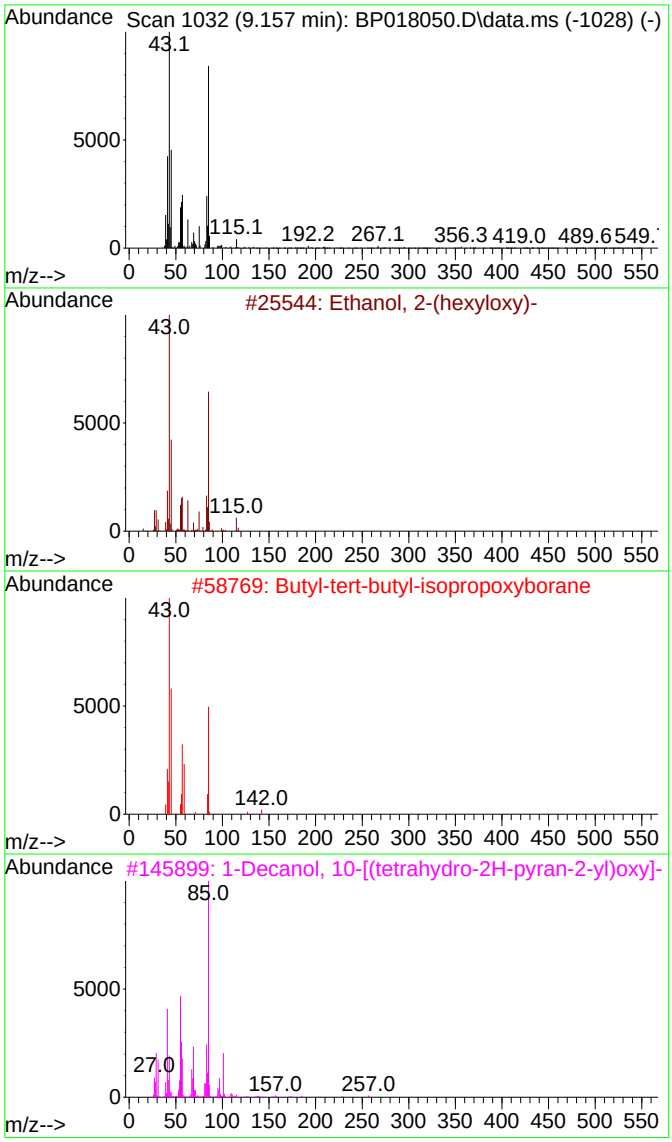
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

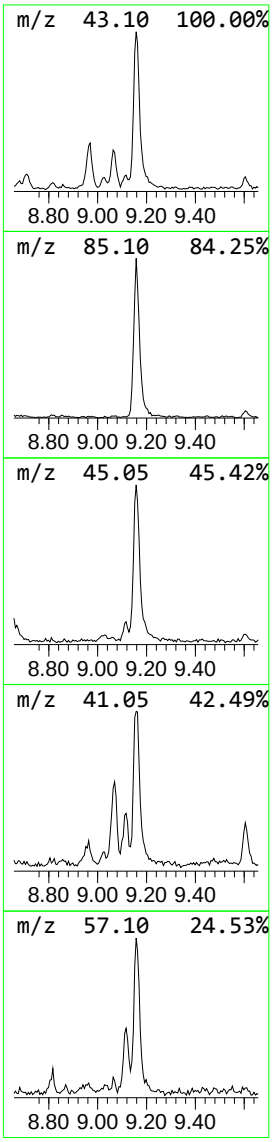
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Ethanol, 2-(hexyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.157	6.47 ng/ul	175638	1,4-Dichlorobenzene-d4	7.846

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexyloxy)-	146	C8H18O2	000112-25-4	72
2	Butyl-tert-butyl-isopropoxyborane	184	C11H25BO	097782-82-6	50
3	1-Decanol, 10-[(tetrahydro-2H-py...	258	C15H30O3	043047-93-4	50
4	Heptane, 2-(hexyloxy)-	200	C13H28O	074663-79-9	47
5	Sulfurous acid, isohexyl hexyl e...	250	C12H26O3S	1000309-12-8	43





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Sample : 05013-01
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ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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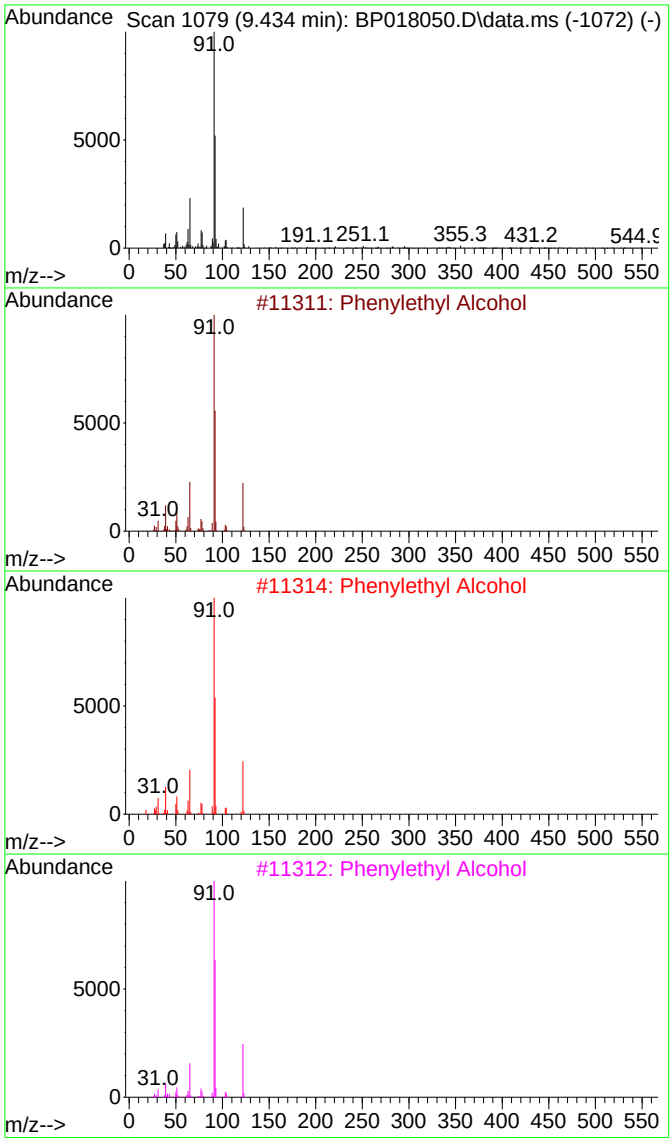
Quant Title : SVOA CALIBRATION

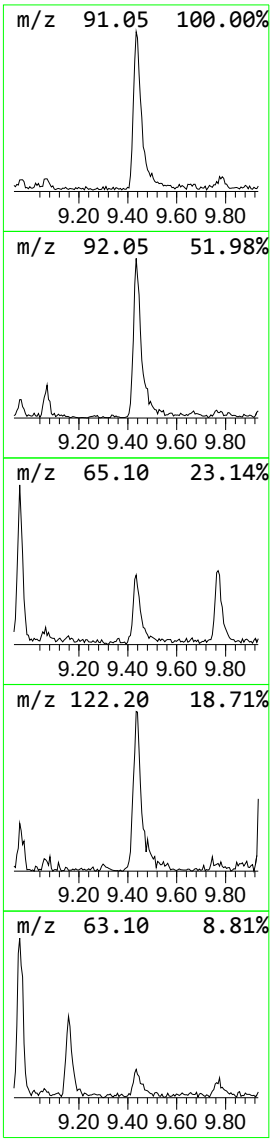
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Phenylethyl Alcohol Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.434	2.03 ng/ul	67817	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenylethyl Alcohol	122	C8H10O	000060-12-8	95
2	Phenylethyl Alcohol	122	C8H10O	000060-12-8	94
3	Phenylethyl Alcohol	122	C8H10O	000060-12-8	72
4	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	64
5	Toluene	92	C7H8	000108-88-3	58





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Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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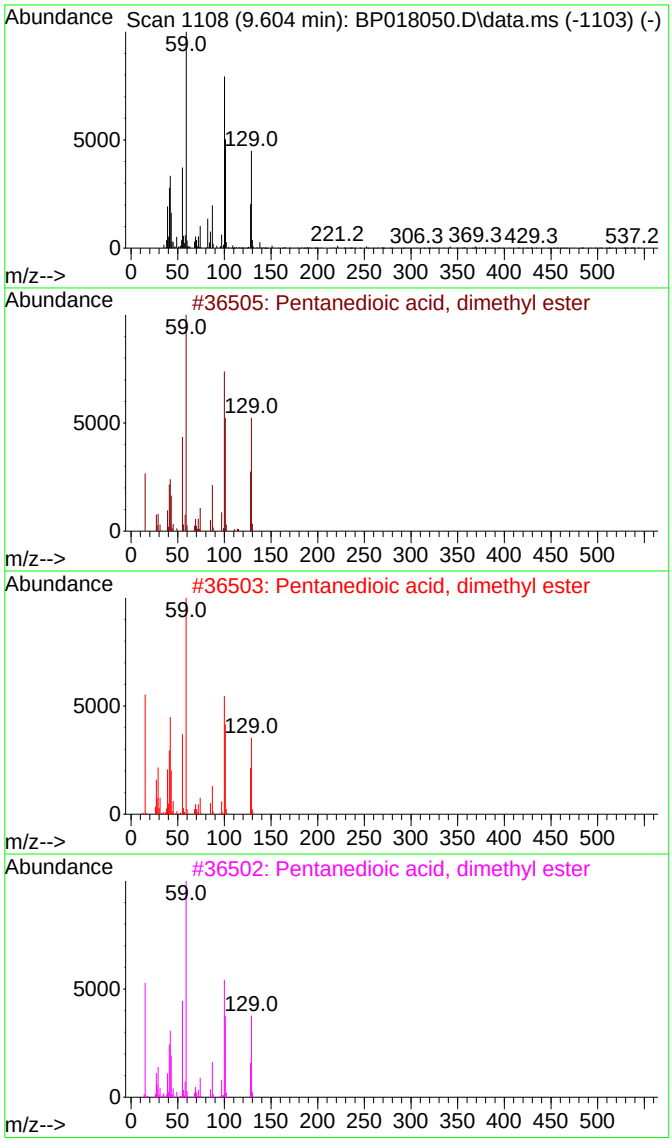
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

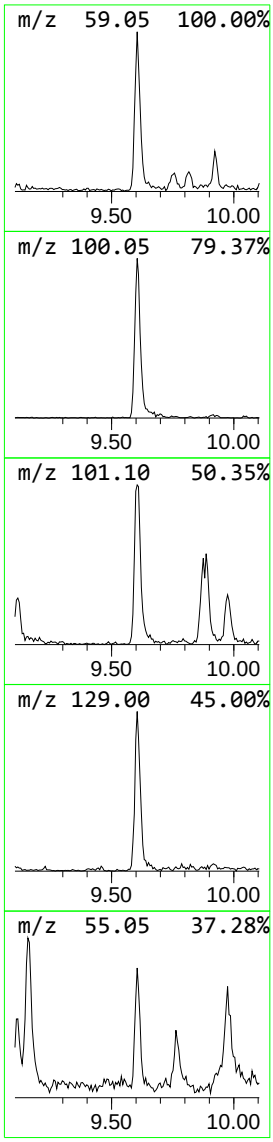
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Pentanedioic acid, dimethyl... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.604	2.62 ng/ul	87521	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	87
2	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	83
3	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	74
4	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	50
5	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	47





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Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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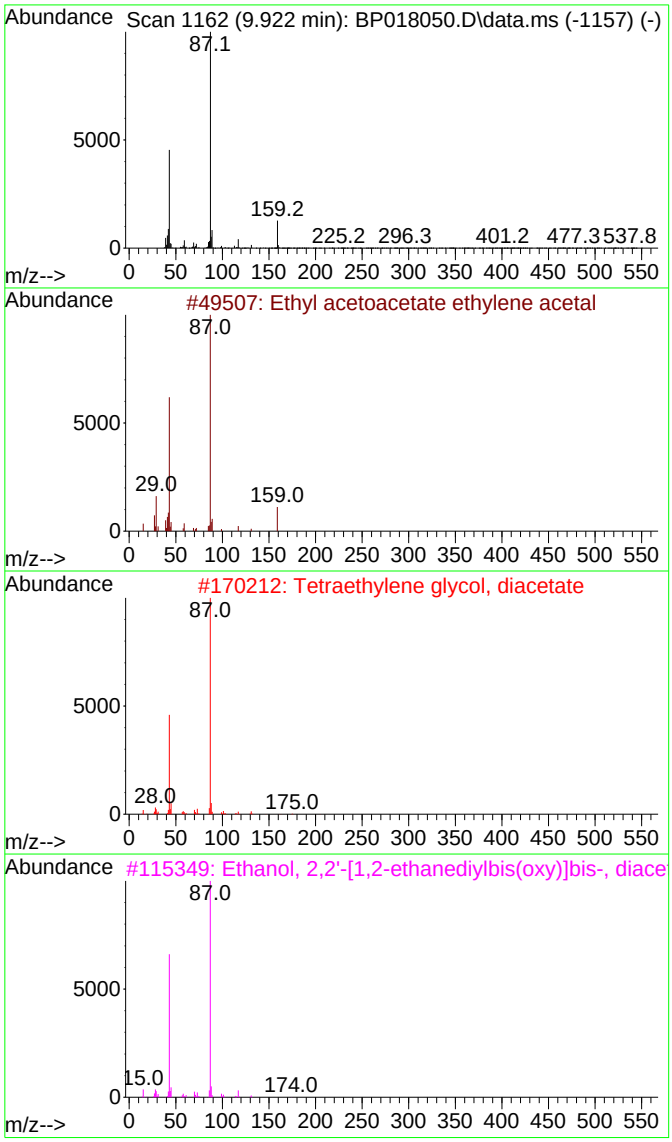
Quant Title : SVOA CALIBRATION

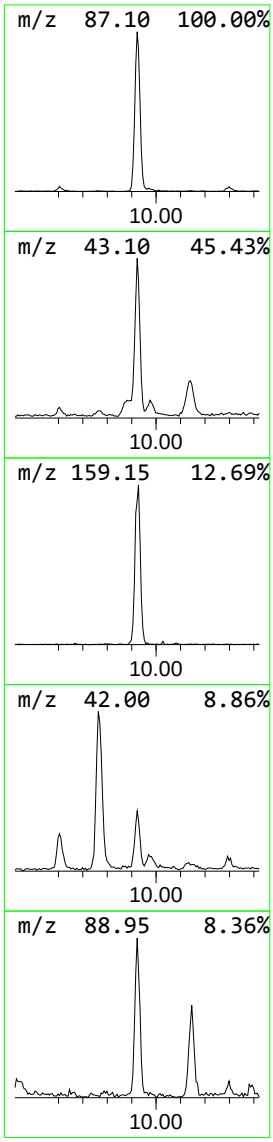
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Ethyl acetoacetate ethylene... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.922	6.11 ng/ul	203750	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl acetoacetate ethylene acetal	174	C8H14O4	006413-10-1	78
2	Tetraethylene glycol, diacetate	278	C12H22O7	022790-12-1	64
3	Ethanol, 2,2'-[1,2-ethanediylbis...	234	C10H18O6	000111-21-7	59
4	2-[2-[2-[2-[2-(2-Acetyloxyethoxy...	366	C16H30O9	024997-24-8	50
5	Ethyl acetoacetate ethylene acetal	174	C8H14O4	006413-10-1	47





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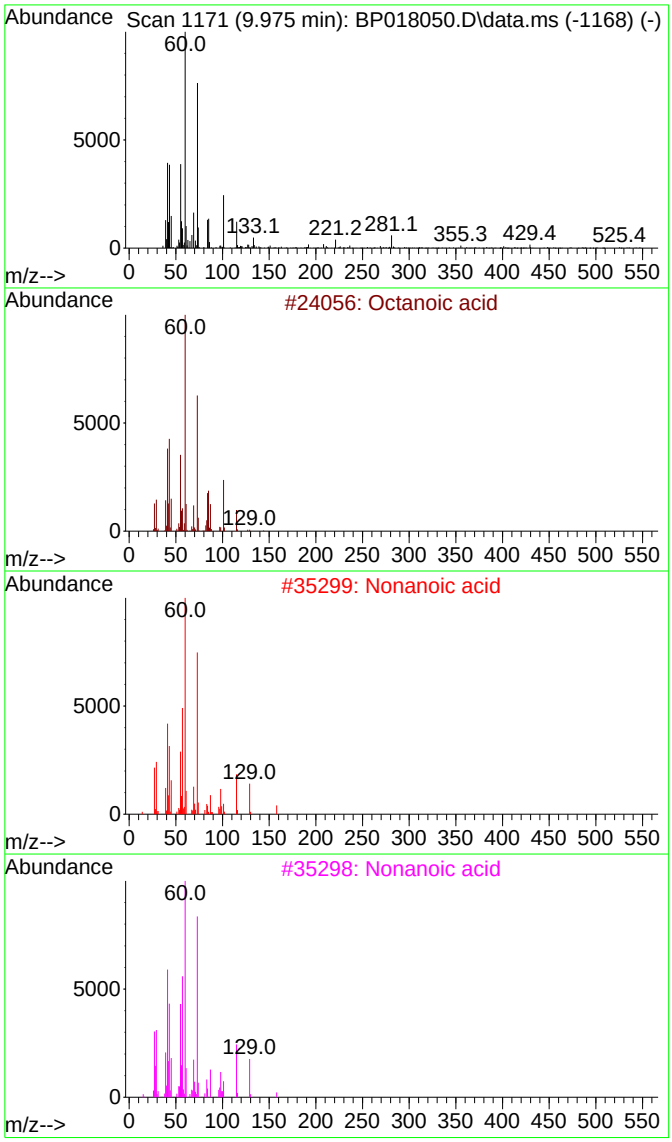
Quant Title : SVOA CALIBRATION

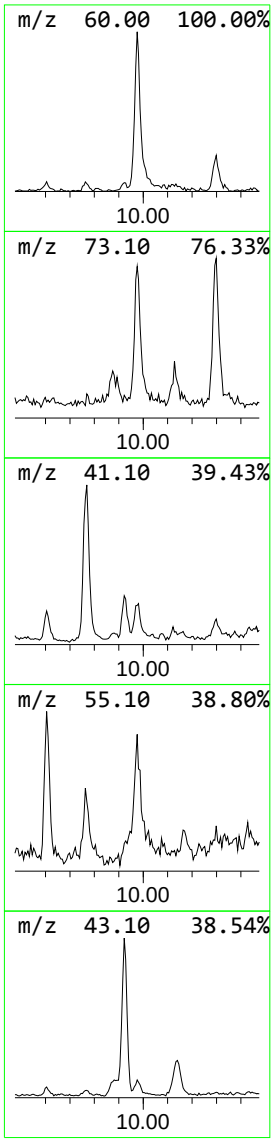
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Octanoic acid Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.975	2.06 ng/ul	68853	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	64
2	Nonanoic acid	158	C9H18O2	000112-05-0	59
3	Nonanoic acid	158	C9H18O2	000112-05-0	59
4	Pentanoic acid	102	C5H10O2	000109-52-4	53
5	Octanoic acid	144	C8H16O2	000124-07-2	53





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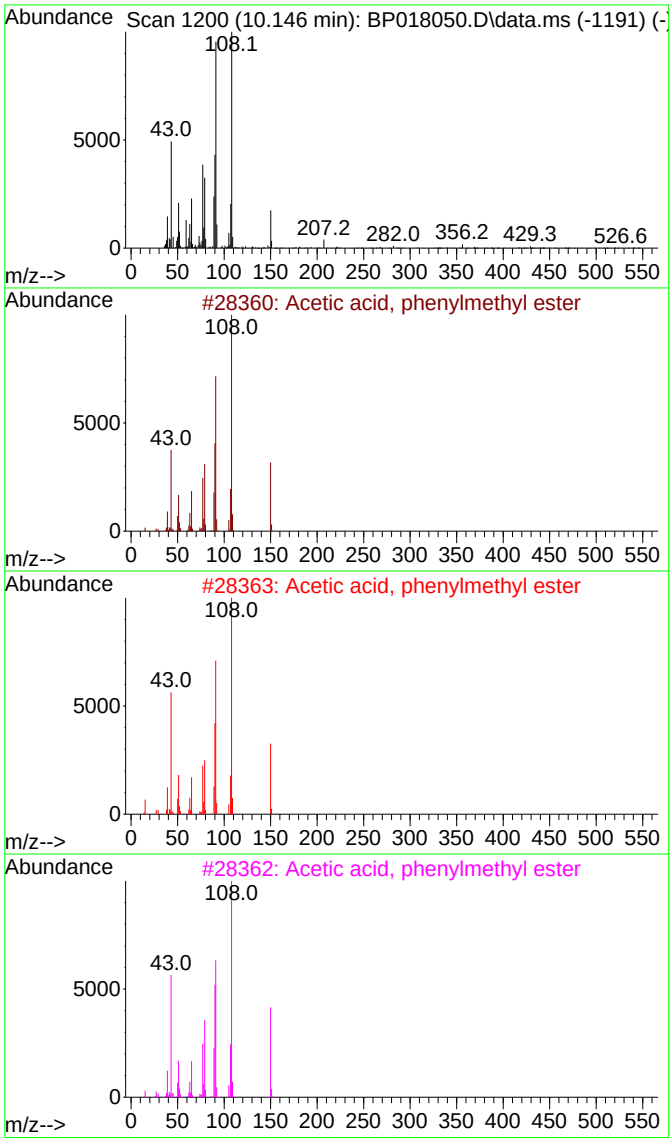
Quant Title : SVOA CALIBRATION

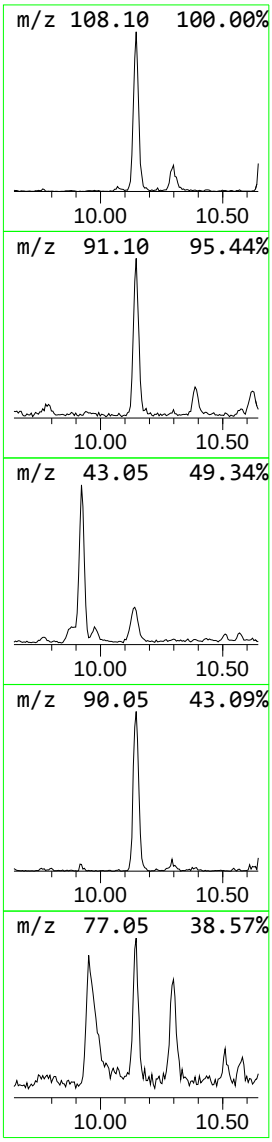
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 Acetic acid, phenylmethyl e... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.146	4.19 ng/ul	139831	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	94
2	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	90
3	Acetic acid, phenylmethyl ester	150	C9H10O2	000140-11-4	81
4	Benzylcarbamate	151	C8H9NO2	000621-84-1	64
5	Glycyl-l-glutamic acid, N-carbob...	338	C15H18N2O7	1010130-29-9	58





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Quant Title : SVOA CALIBRATION

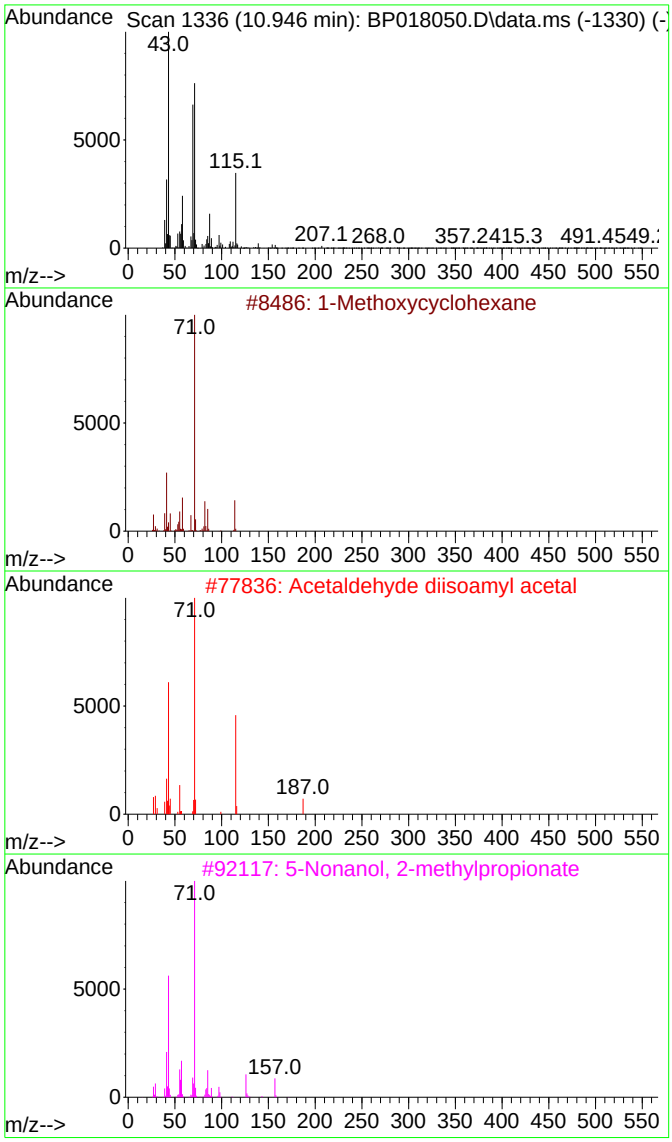
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

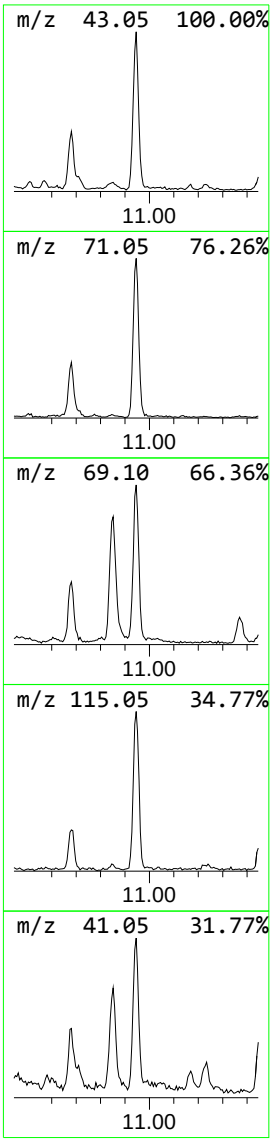
****

Peak Number 16 1-Methoxycyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.946	7.42 ng/ul	247680	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methoxycyclohexane	114	C7H14O	000931-56-6	50
2	Acetaldehyde diisoamyl acetal	202	C12H26O2	1000430-80-1	50
3	5-Nonanol, 2-methylpropionate	214	C13H26O2	1000463-47-6	47
4	2,3'-Bifuran, octahydro-	142	C8H14O2	073373-15-6	47
5	Cyclopropanemethanol, .alpha.-bu...	128	C8H16O	004379-16-2	47





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Operator : MA/JU
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Misc :
ALS Vial : 27 Sample Multiplier: 1

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

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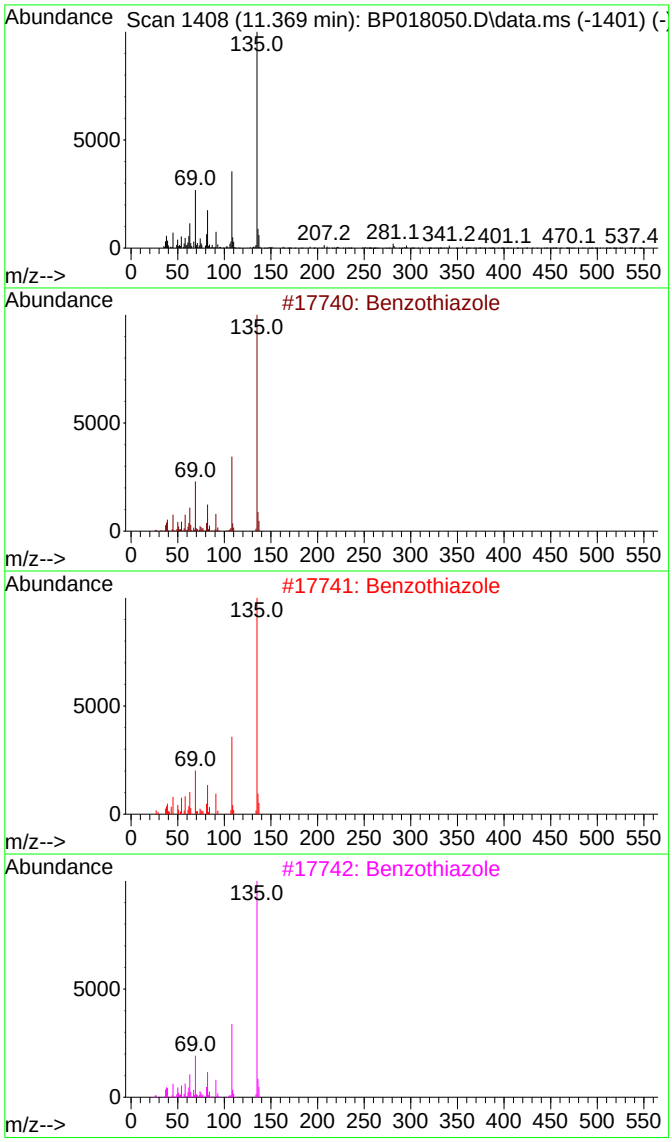
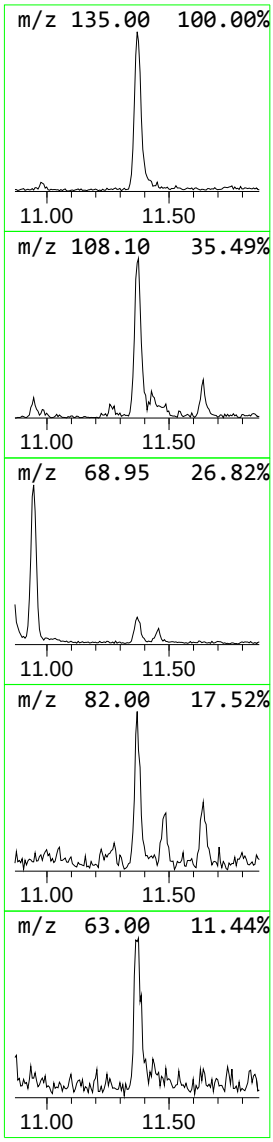
Peak Number 17 Benzothiazole Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.369	2.13 ng/ul	70932	Naphthalene-d8	10.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	94
2	Benzothiazole	135	C7H5NS	000095-16-9	91
3	Benzothiazole	135	C7H5NS	000095-16-9	91
4	Benzothiazole	135	C7H5NS	000095-16-9	90
5	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	86





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Data File : BP018050.D
Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

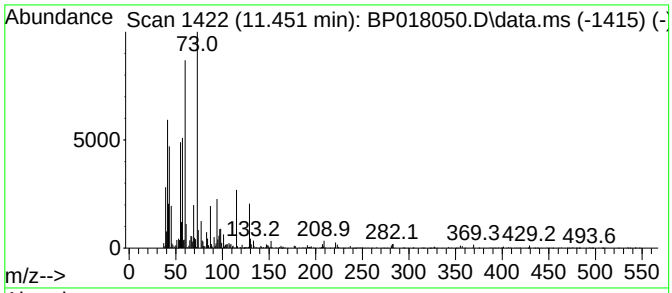
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

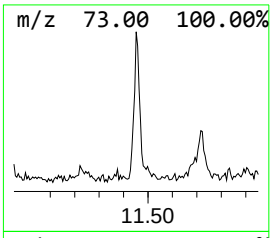
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

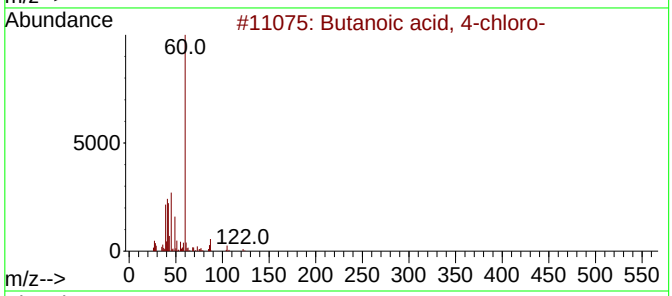
****
Peak Number 18 Butanoic acid, 4-chloro- Concentration Rank 14

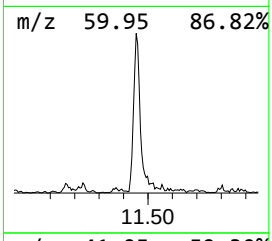
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.451	3.33 ng/ul	111035	Naphthalene-d8	10.669

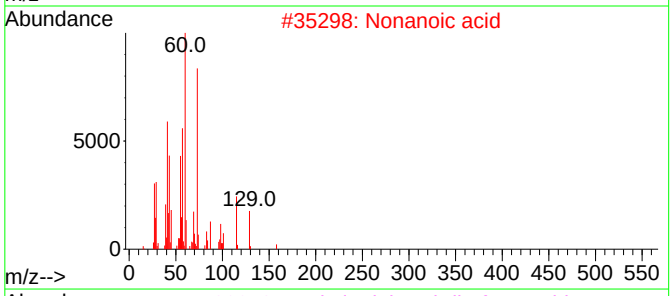
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	50
2	Nonanoic acid	158	C9H18O2	000112-05-0	47
3	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	47
4	Butanoic acid	88	C4H8O2	000107-92-6	47
5	Nonanoic acid	158	C9H18O2	000112-05-0	47

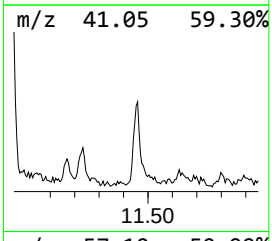


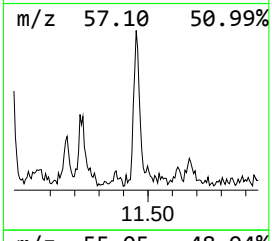


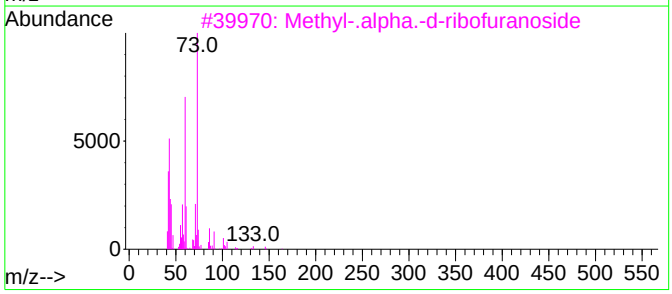


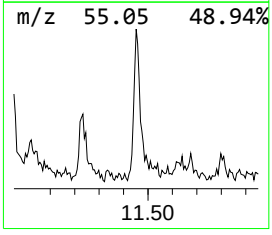












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Acq On : 11 Nov 2023 05:38
Operator : MA/JU
Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

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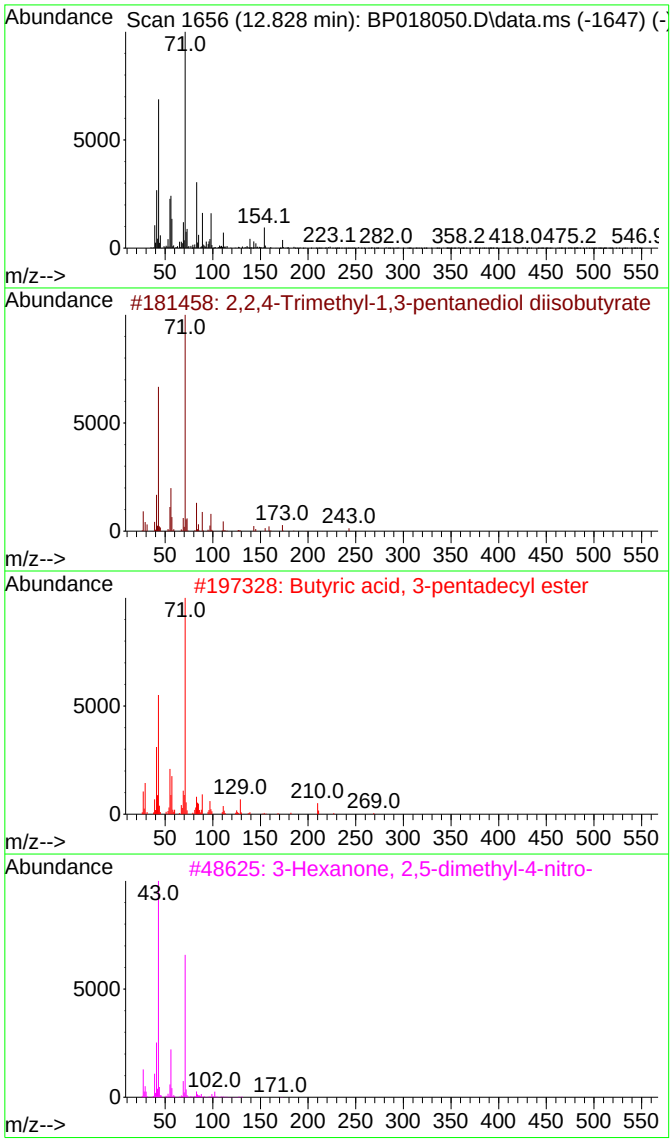
Quant Title : SVOA CALIBRATION

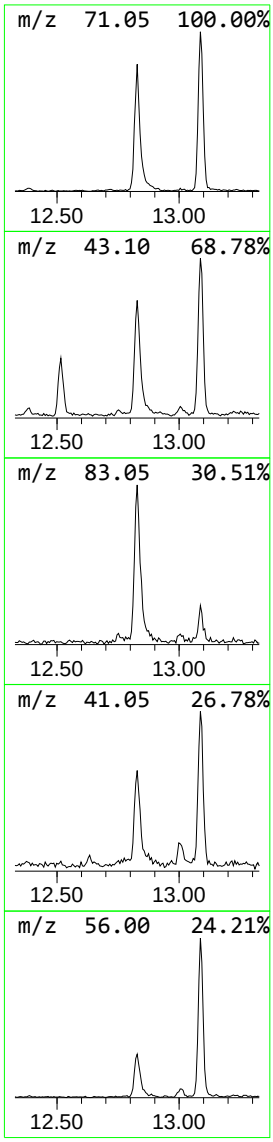
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.828	4.39 ng/ul	168770	Acenaphthene-d10	14.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
2	Butyric acid, 3-pentadecyl ester	298	C19H38O2	1000280-57-3	43
3	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
4	Butyric acid, 3-tridecyl ester	270	C17H34O2	1000280-56-8	43
5	Butanoic acid, 1-methylhexyl ester	186	C11H22O2	039026-94-3	42





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Data File : BP018050.D
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Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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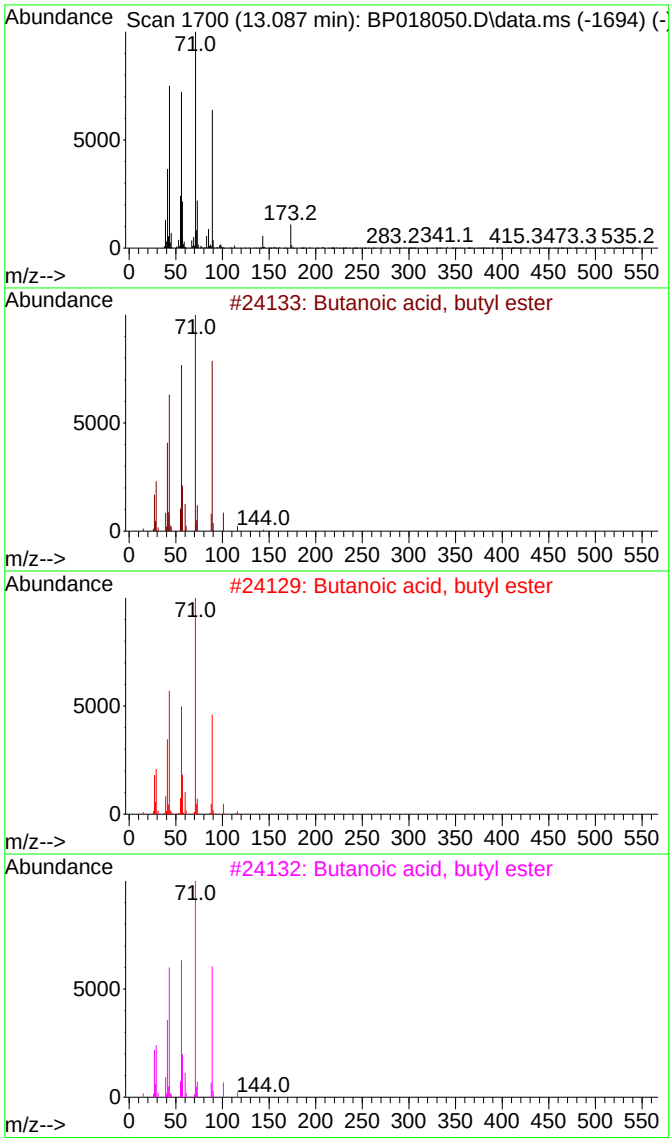
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

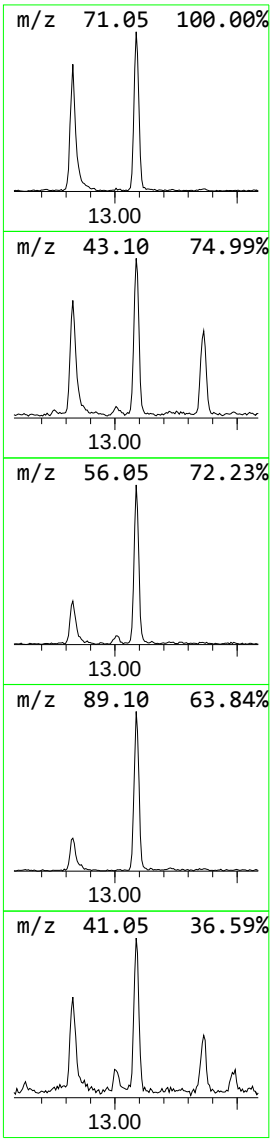
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Butanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.087	4.76 ng/ul	182860	Acenaphthene-d10	14.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	83
2	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	59
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	56
5	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	56





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Sample : 05013-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

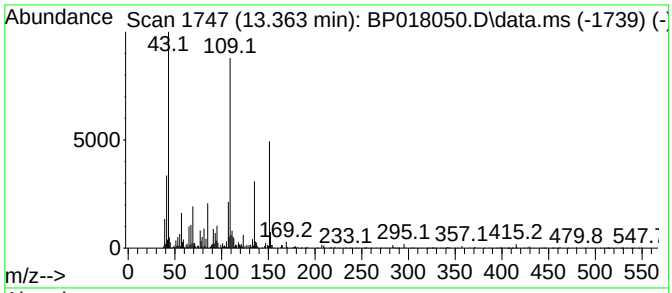
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

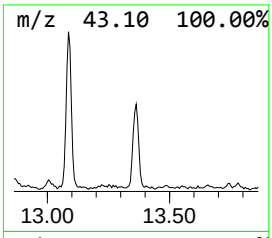
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

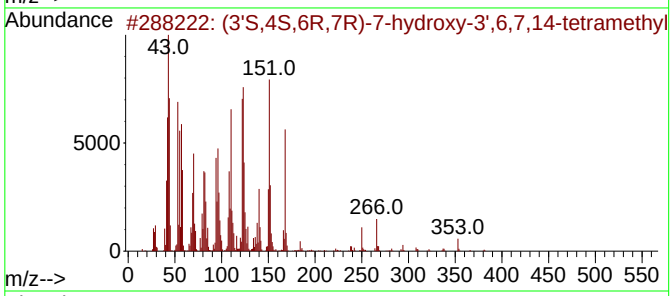
****
Peak Number 21 (3'S,4S,6R,7R)-7-hydroxy-3'... Concentration Rank 15

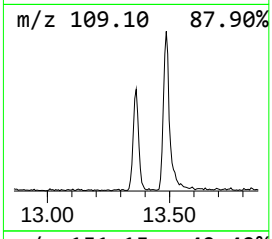
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.363	2.77 ng/ul	106265	Acenaphthene-d10	14.522

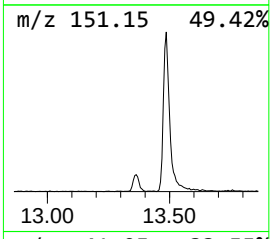
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3'S,4S,6R,7R)-7-hydroxy-3',6,7,...	381	C19H27NO7	1010497-93-7	90
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	62
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	49
4	Metacetamol	151	C8H9NO2	000621-42-1	49
5	Metacetamol	151	C8H9NO2	000621-42-1	47

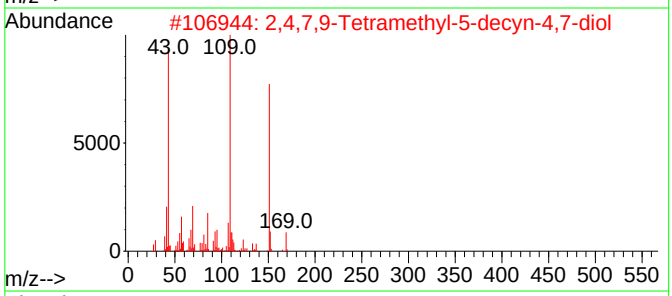


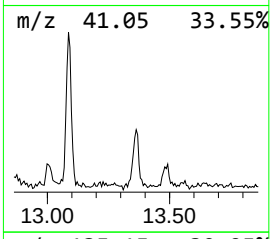


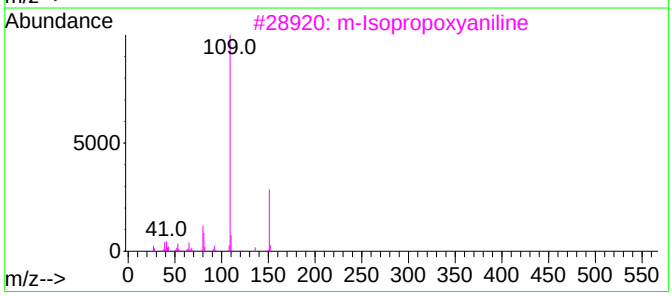


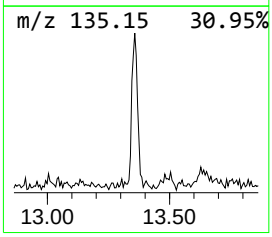












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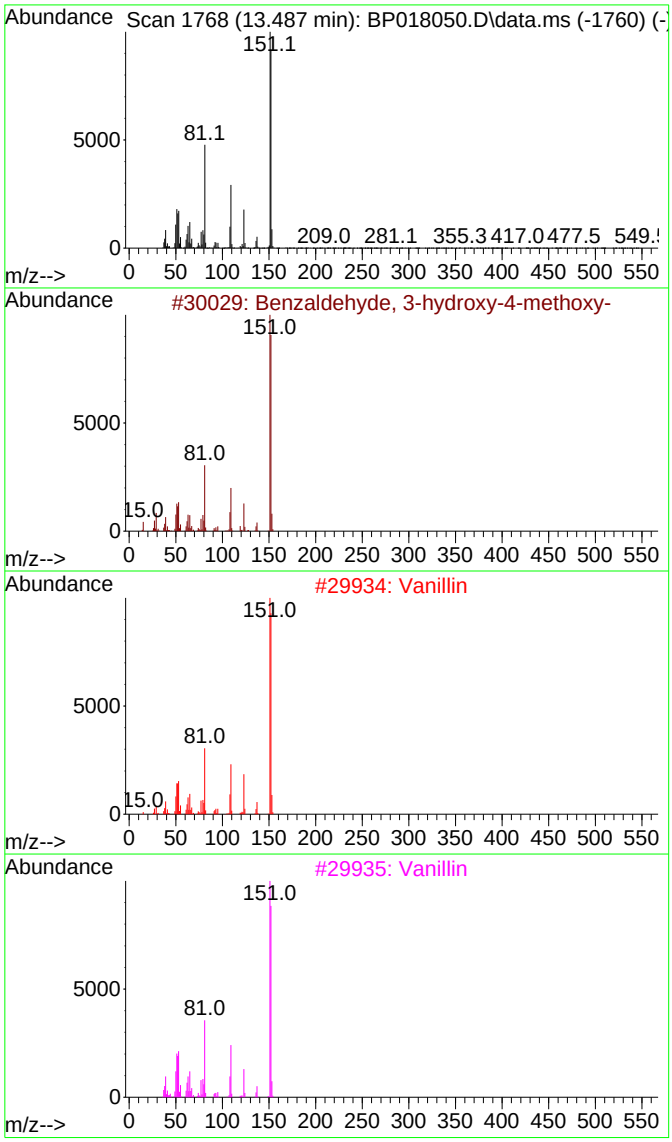
Quant Title : SVOA CALIBRATION

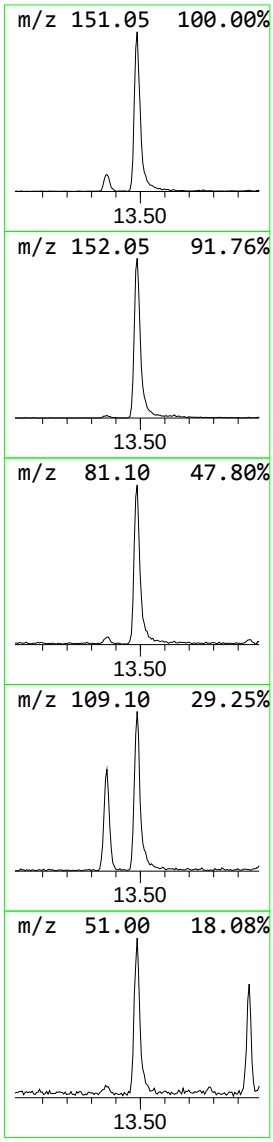
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 22 Benzaldehyde, 3-hydroxy-4-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.487	10.81 ng/ul	415466	Acenaphthene-d10	14.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
2	Vanillin	152	C8H8O3	000121-33-5	97
3	Vanillin	152	C8H8O3	000121-33-5	96
4	Vanillin	152	C8H8O3	000121-33-5	96
5	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	95





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ClientSampleId :
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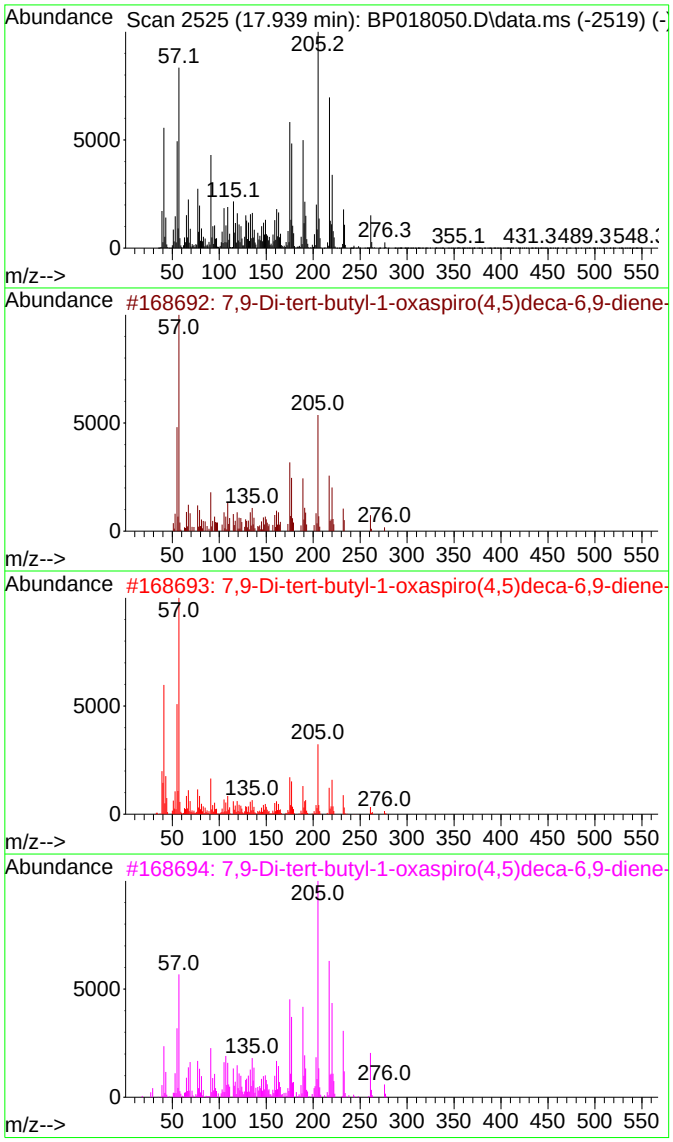
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

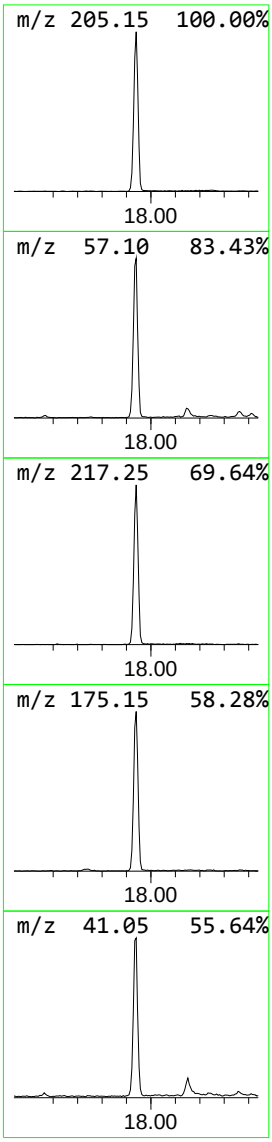
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 23 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	27.87 ng/ul	1321120	Phenanthrene-d10	17.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	98
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	97
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	87
4	2,5-Cyclohexadien-1-one, 2,6-bis...	232	C16H24O	006738-27-8	83
5	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	66





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BNA_P
ClientSampleId :
A4970

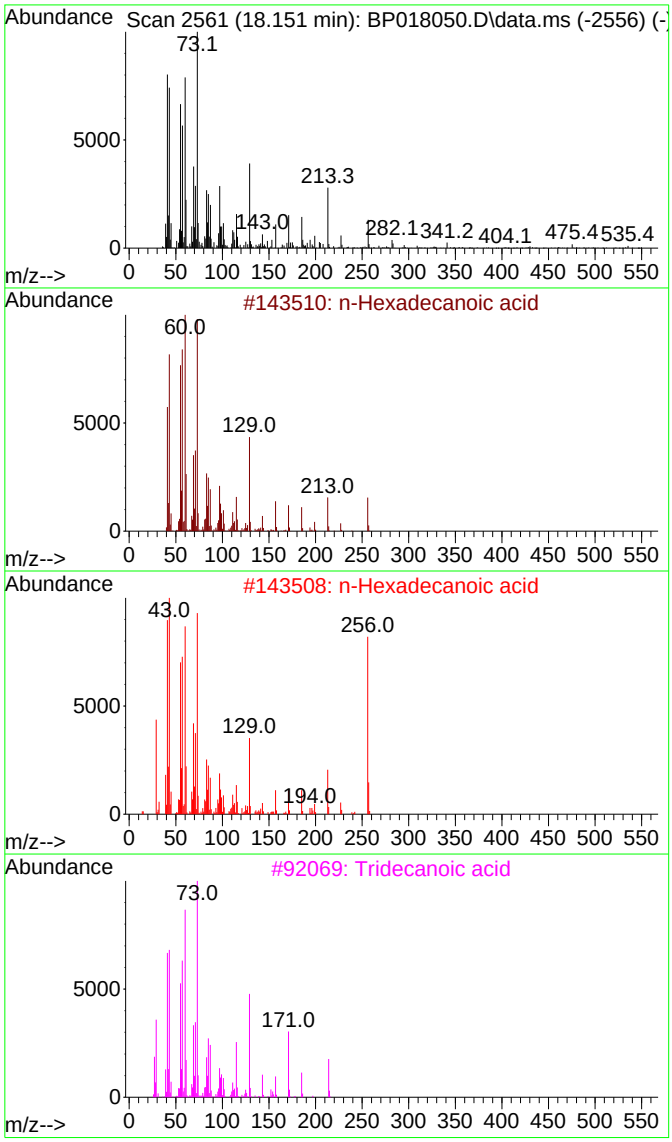
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

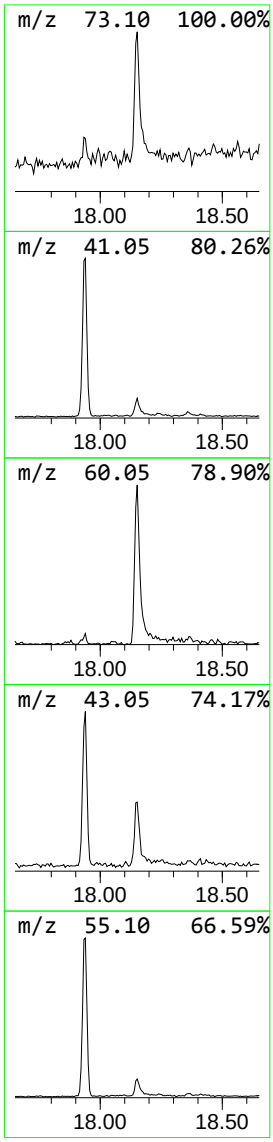
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 24 n-Hexadecanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	2.20 ng/ul	104189	Phenanthrene-d10	17.304

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	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	89





Tentatively Identified Compound (LSC) summary

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Data File : BP018050.D
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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4970

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP111023.MA.M
Quant Title : SVOA CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexyl chlorofor...	5.305	2.0	ng/ul	55137	1	7.846	543057	20.0
Ethanol, 2-butoxy-	5.893	60.1	ng/ul	1631480	1	7.846	543057	20.0
2-Propanol, 1-b...	6.452	5.2	ng/ul	142146	1	7.846	543057	20.0
Hexanoic acid	6.858	3.5	ng/ul	94563	1	7.846	543057	20.0
Cyclobutanone, ...	6.922	2.4	ng/ul	66336	1	7.846	543057	20.0
Benzyl alcohol	8.128	3.7	ng/ul	101070	1	7.846	543057	20.0
Hexanethioic ac...	8.481	2.5	ng/ul	66583	1	7.846	543057	20.0
Phenol, 2-methoxy-	8.957	15.3	ng/ul	414228	1	7.846	543057	20.0
Hexanoic acid, ...	9.116	2.4	ng/ul	64144	1	7.846	543057	20.0
Ethanol, 2-(hex...	9.157	6.5	ng/ul	175638	1	7.846	543057	20.0
Phenylethyl Alc...	9.434	2.0	ng/ul	67817	2	10.669	667337	20.0
Pentanedioic ac...	9.604	2.6	ng/ul	87521	2	10.669	667337	20.0
Ethyl acetoacet...	9.922	6.1	ng/ul	203750	2	10.669	667337	20.0
Octanoic acid	9.975	2.1	ng/ul	68853	2	10.669	667337	20.0
Acetic acid, ph...	10.146	4.2	ng/ul	139831	2	10.669	667337	20.0
1-Methoxycycloh...	10.946	7.4	ng/ul	247680	2	10.669	667337	20.0
Benzothiazole	11.369	2.1	ng/ul	70932	2	10.669	667337	20.0
Butanoic acid, ...	11.451	3.3	ng/ul	111035	2	10.669	667337	20.0
2,2,4-Trimethyl...	12.828	4.4	ng/ul	168770	3	14.522	768611	20.0
Butanoic acid, ...	13.087	4.8	ng/ul	182860	3	14.522	768611	20.0
(3'S,4S,6R,7R)-...	13.363	2.8	ng/ul	106265	3	14.522	768611	20.0
Benzaldehyde, 3...	13.487	10.8	ng/ul	415466	3	14.522	768611	20.0
7,9-Di-tert-but...	17.939	27.9	ng/ul	1321120	4	17.304	948202	20.0
n-Hexadecanoic ...	18.151	2.2	ng/ul	104189	4	17.304	948202	20.0