LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080724\
Data File : BG062299.D
Acq On : 7 Aug 2024 12:39
Operator : MA/JU
Sample : P3347-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0B04

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG062299.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.422	19	23	29	rVB4	11641	18032	0.77%	0.082%
2	4.168	146	150	155	rVB	5943	7955	0.34%	0.036%
3	4.309	171	174	179	rVB4	1612	2805	0.12%	0.013%
4	4.521	206	210	220	rVB5	10254	16833	0.71%	0.077%
5	5.079	300	305	308	rBV4	1858	2703	0.11%	0.012%
6	5.467	367	371	373	rBV3	2051	3185	0.14%	0.015%
7	5.813	425	430	434	rBV3	2881	4062	0.17%	0.019%
8	6.007	458	463	468	rVB3	13081	21233	0.90%	0.097%
9	6.947	615	623	632	rBV	16588	36684	1.56%	0.168%
10	7.059	638	642	643	rBV3	2504	3854	0.16%	0.018%
11	7.112	644	651	661	rVB	119400	211628	8.99%	0.967%
12	7.288	675	681	693	rVB	207438	333834	14.17%	1.526%
13	7.488	708	715	723	rVB	260097	424891	18.04%	1.942%
14	7.957	788	795	801	rBV	217055	366725	15.57%	1.676%
15	8.022	801	806	813	rVB	24552	37599	1.60%	0.172%
16	8.516	886	890	893	rBV5	4276	6452	0.27%	0.029%
17	8.557	893	897	905	rVV4	4917	10327	0.44%	0.047%
18	8.651	906	913	925	rVV	289389	494594	21.00%	2.261%
19	8.774	927	934	939	rVB	4801	8409	0.36%	0.038%
20	9.050	975	981	984	rBV	20347	33089	1.40%	0.151%
21	9.109	984	991	1004	rVV	273059	473724	20.11%	2.165%
22	9.220	1007	1010	1015	rVV4	4449	7382	0.31%	0.034%
23	9.279	1017	1020	1025	rVB3	8242	12270	0.52%	0.056%
24	9.679	1083	1088	1092	rBV2	1821	3024	0.13%	0.014%
25	9.831	1106	1114	1123	rBV	209118	361893	15.36%	1.654%
26	9.961	1133	1136	1139	rBV3	3494	4807	0.20%	0.022%
27	10.061	1148	1153	1162	rVB3	8958	15404	0.65%	0.070%
28	10.166	1165	1171	1176	rVB4	1884	3092	0.13%	0.014%
29	10.366	1196	1205	1215	rBV	361699	633741	26.91%	2.896%
30	10.536	1227	1234	1242	rBV3	5587	9649	0.41%	0.044%
31	10.624	1245	1249	1251	rVV3	5172	7516	0.32%	0.034%
32	10.654	1251	1254	1259	rVV4	6937	12361	0.52%	0.056%
33	10.754	1263	1271	1277	rVV	348591	611028	25.94%	2.793%
34	10.812	1277	1281	1286	rVV3	11513	18441	0.78%	0.084%
35	10.877	1286	1292	1298	rVB2	65593	116343	4.94%	0.532%
36	11.388	1375	1379	1386	rBV4	1823	3209	0.14%	0.015%

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Misc :
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Instrument : BNA_G
ClientSampleId : C0B04

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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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Title : SVOA CALIBRATION

37	11.535	1398	1404	1410	rBV3	21120	37086	1.57%	0.170%
38	11.917	1467	1469	1473	rVB2	2503	2783	0.12%	0.013%
39	12.017	1480	1486	1491	rBV2	40723	69077	2.93%	0.316%
40	12.334	1535	1540	1545	rVB2	6076	10046	0.43%	0.046%
41	12.628	1585	1590	1597	rBV2	1326	2703	0.11%	0.012%
42	12.857	1626	1629	1631	rBV	2531	2758	0.12%	0.013%
43	12.945	1638	1644	1652	rVB3	5670	9552	0.41%	0.044%
44	13.033	1656	1659	1662	rVB	1812	2608	0.11%	0.012%
45	13.197	1682	1687	1691	rBV	8630	11878	0.50%	0.054%
46	13.421	1720	1725	1731	rBV	16208	22456	0.95%	0.103%
47	13.485	1731	1736	1744	rBV2	75660	116128	4.93%	0.531%
48	13.985	1815	1821	1828	rBV	742916	1070441	45.45%	4.892%
49	14.272	1860	1870	1877	rBV	816672	1300017	55.19%	5.942%
50	14.578	1915	1922	1930	rBV	676386	1018516	43.24%	4.655%
51	14.660	1930	1936	1942	rVB	14278	20851	0.89%	0.095%
52	14.748	1945	1951	1960	rBV	131103	208754	8.86%	0.954%
53	14.989	1990	1992	1998	rBV5	5092	5787	0.25%	0.026%
54	15.253	2029	2037	2042	rBV	26570	39508	1.68%	0.181%
55	15.289	2042	2043	2049	rVB3	2104	3049	0.13%	0.014%
56	15.389	2053	2060	2065	rBV5	5728	10702	0.45%	0.049%
57	15.571	2083	2091	2102	rVB	1078143	1669034	70.86%	7.628%
58	15.671	2102	2108	2122	rBV	267847	393581	16.71%	1.799%
59	15.812	2127	2132	2137	rVV4	4169	7783	0.33%	0.036%
60	15.859	2137	2140	2145	rVV2	1453	2839	0.12%	0.013%
61	15.929	2148	2152	2158	rVB	13198	19964	0.85%	0.091%
62	16.170	2191	2193	2198	rVB3	2542	3018	0.13%	0.014%
63	16.575	2257	2262	2265	rBV3	1727	3134	0.13%	0.014%
64	16.922	2317	2321	2325	rVB2	3672	4898	0.21%	0.022%
65	17.315	2375	2388	2398	rBV	780472	1153959	48.99%	5.274%
66	17.415	2398	2405	2413	rVV2	1255134	1896787	80.53%	8.669%
67	17.603	2435	2437	2441	rBV2	3401	3839	0.16%	0.018%
68	17.991	2498	2503	2508	rBV	280244	359284	15.25%	1.642%
69	18.161	2529	2532	2535	rVB3	2510	3168	0.13%	0.014%
70	18.220	2535	2542	2549	rBV	62823	101803	4.32%	0.465%
71	18.285	2551	2553	2556	rVB	4485	5498	0.23%	0.025%
72	18.426	2574	2577	2580	rBV4	1587	2622	0.11%	0.012%
73	18.467	2581	2584	2591	rVB3	5029	6018	0.26%	0.028%
74	19.260	2715	2719	2724	rBV2	17687	25592	1.09%	0.117%
75	19.330	2727	2731	2735	rBV2	14558	20658	0.88%	0.094%
76	19.407	2742	2744	2748	rVB3	2577	3388	0.14%	0.015%

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Misc :
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Instrument : BNA_G
ClientSampleId : C0B04

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
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Title : SVOA CALIBRATION

77	19.489	2753	2758	2768	rBV	43990	75045	3.19%	0.343%
78	19.648	2781	2785	2787	rBV4	6465	7965	0.34%	0.036%
79	19.700	2787	2794	2803	rVV	1534833	2257144	95.83%	10.316%
80	20.311	2895	2898	2900	rBV3	2483	3433	0.15%	0.016%
81	20.623	2947	2951	2955	rVV5	5497	8239	0.35%	0.038%
82	20.687	2960	2962	2963	rVV2	5075	4729	0.20%	0.022%
83	20.705	2963	2965	2967	rVB3	5327	4479	0.19%	0.020%
84	20.881	2992	2995	3000	rBV4	2654	5833	0.25%	0.027%
85	21.251	3051	3058	3063	rBV8	5821	11610	0.49%	0.053%
86	21.480	3095	3097	3102	rVB4	5006	5045	0.21%	0.023%
87	21.557	3104	3110	3122	rVV	805485	1251320	53.13%	5.719%
88	22.379	3248	3250	3256	rVB5	5408	6478	0.28%	0.030%
89	23.014	3351	3358	3363	rBV5	20350	42457	1.80%	0.194%
90	23.055	3363	3365	3370	rVV3	13330	19525	0.83%	0.089%
91	23.137	3372	3379	3389	rVB	150954	285323	12.11%	1.304%
92	23.842	3494	3499	3507	rVB4	14648	28720	1.22%	0.131%
93	24.441	3588	3601	3615	rBV	878649	2355322	100.00%	10.765%
94	24.647	3625	3636	3648	rBV2	492397	1380363	58.61%	6.309%
95	24.764	3648	3656	3666	rVB5	18715	55437	2.35%	0.253%
96	25.845	3835	3840	3841	rBV3	14770	19319	0.82%	0.088%
97	25.927	3852	3854	3860	rBV7	2664	5106	0.22%	0.023%
98	27.167	4058	4065	4077	rVB7	16197	49991	2.12%	0.228%
99	27.719	4157	4159	4162	rBV4	2458	3063	0.13%	0.014%
100	30.609	4649	4651	4653	rBV3	2960	3328	0.14%	0.015%

Sum of corrected areas: 21879619

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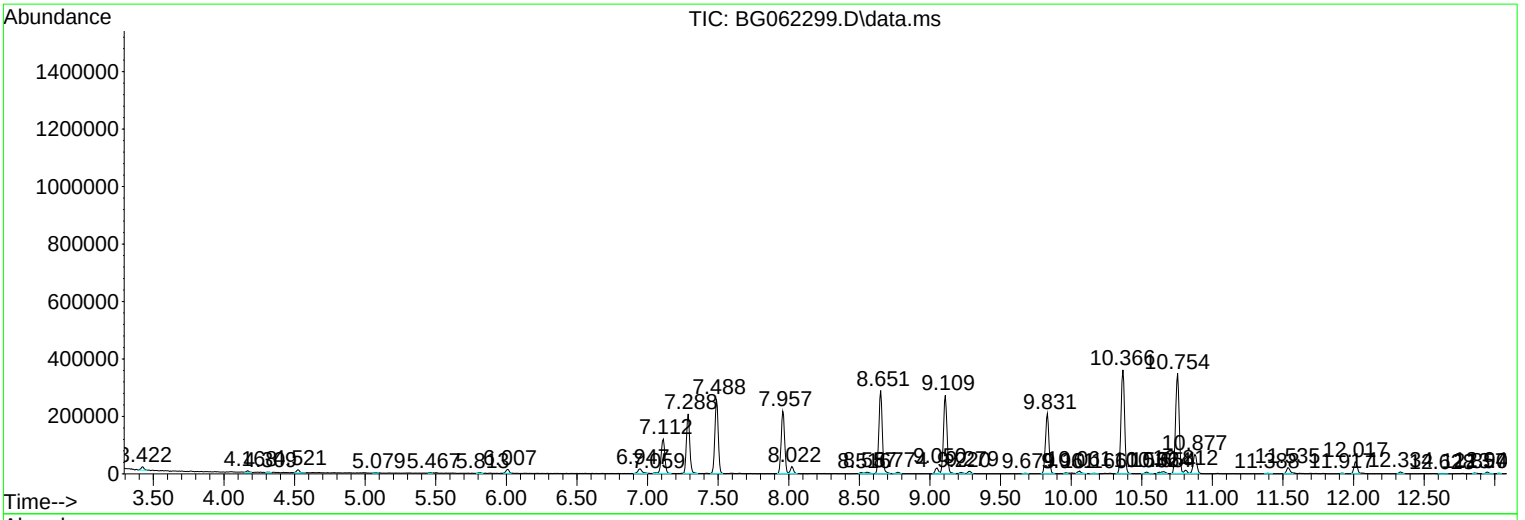
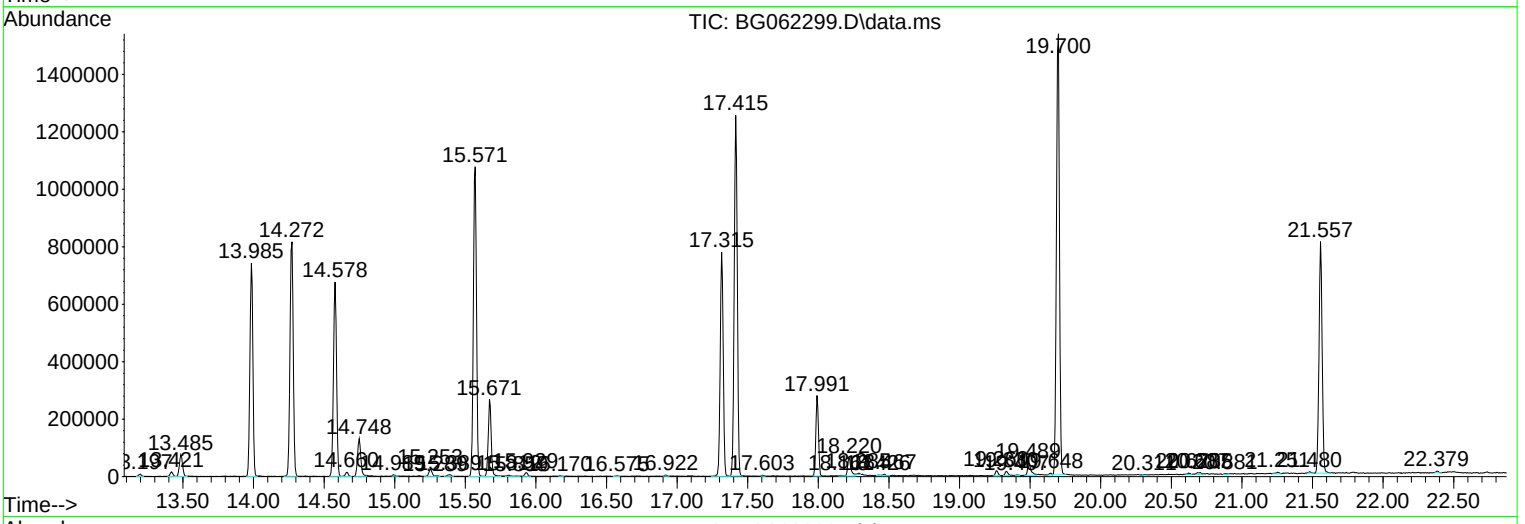
ALS Vial : 5 Sample Multiplier: 1

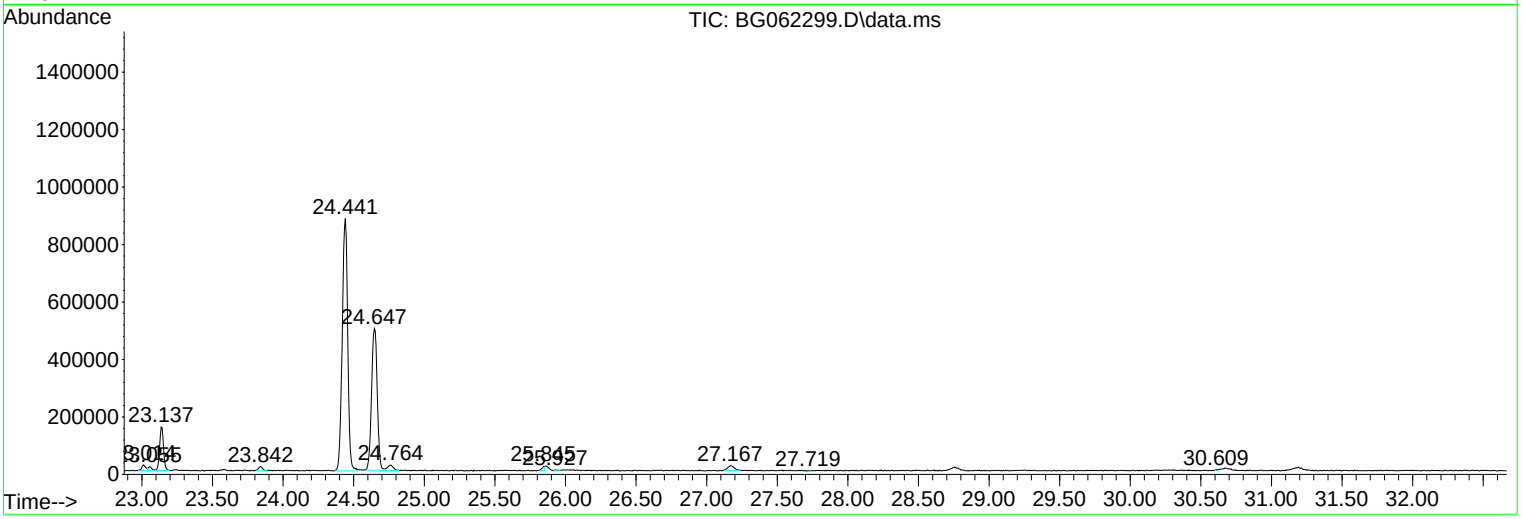
Instrument :
BNA_G
ClientSampleId :
C0B04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

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







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Data File : BG062299.D
Acq On : 7 Aug 2024 12:39
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Instrument :
BNA_G
ClientSampleId :
C0B04

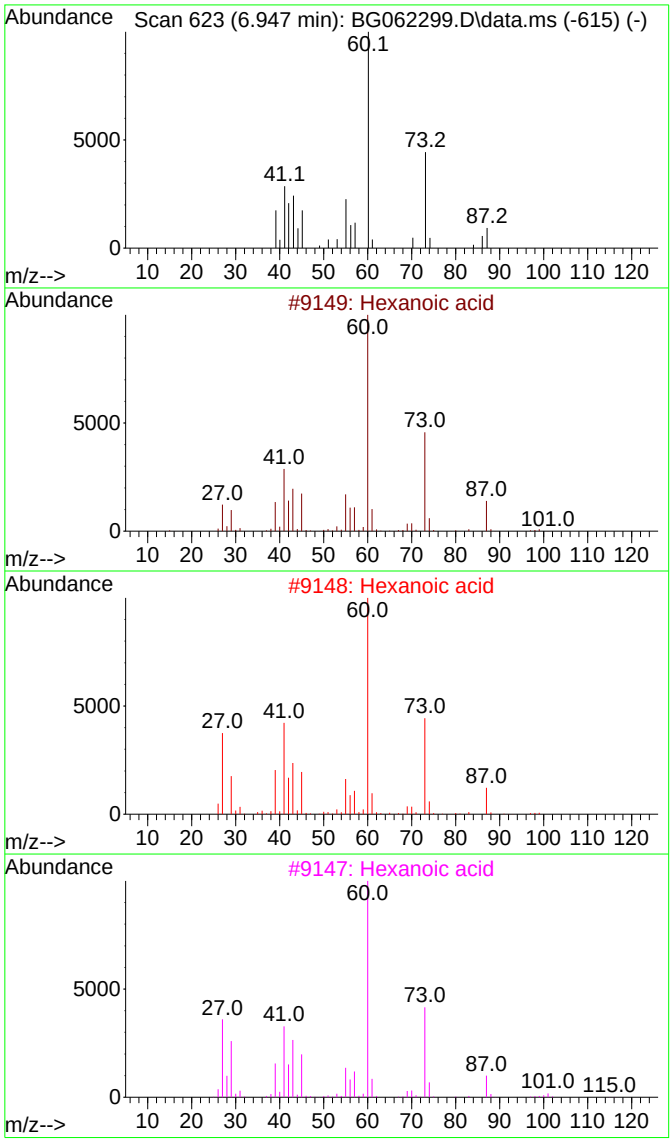
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

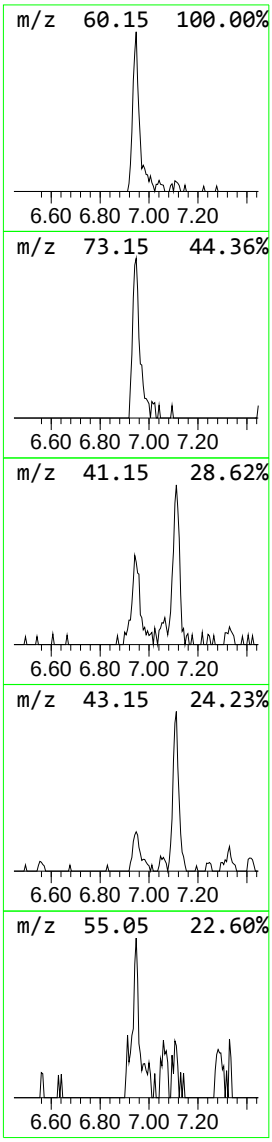
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.947	2.00 ng/ul	36684	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	72
2	Hexanoic acid	116	C6H12O2	000142-62-1	72
3	Hexanoic acid	116	C6H12O2	000142-62-1	56
4	Hexanoic acid	116	C6H12O2	000142-62-1	50
5	Pentanoic acid	102	C5H10O2	000109-52-4	50





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0B04

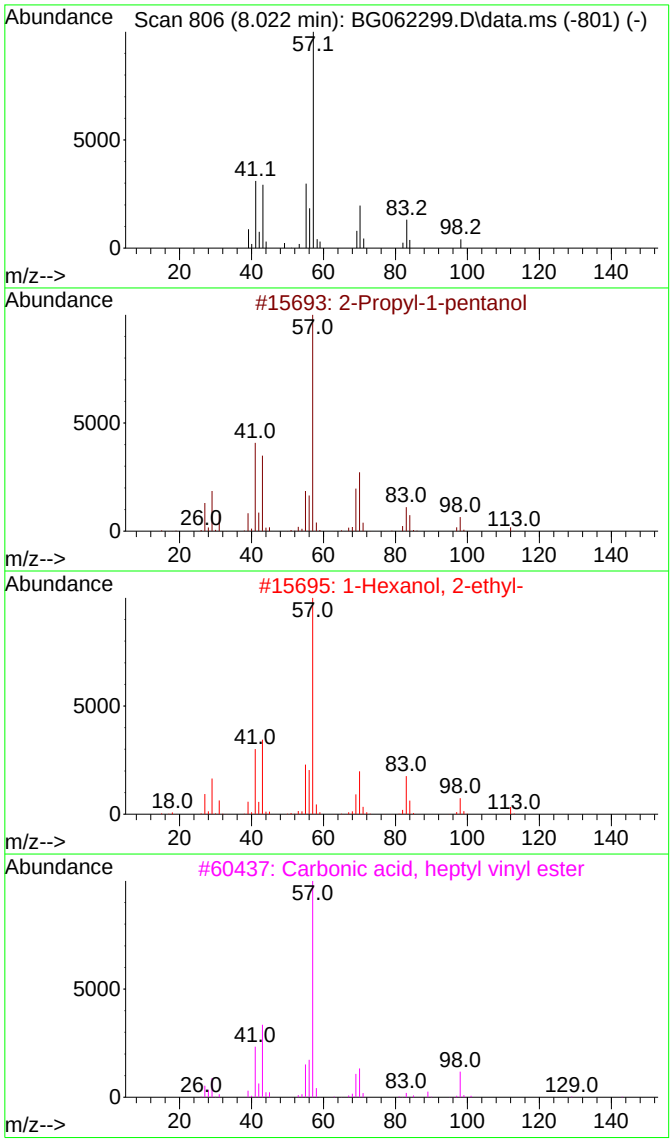
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

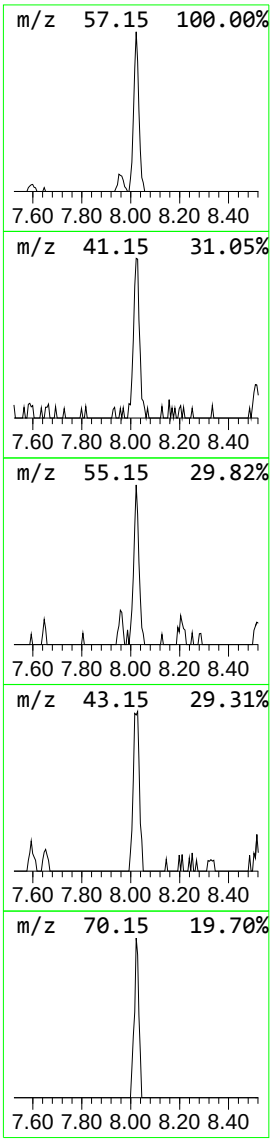
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propyl-1-pentanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	2.05 ng/ul	37599	1,4-Dichlorobenzene-d4	7.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
3	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

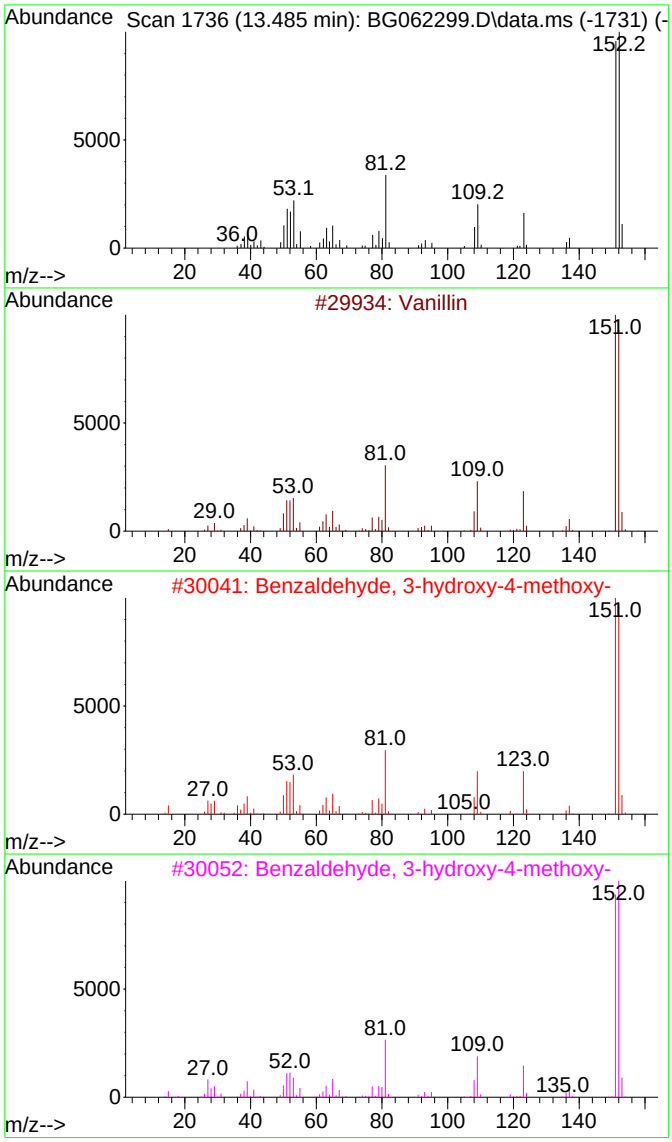
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

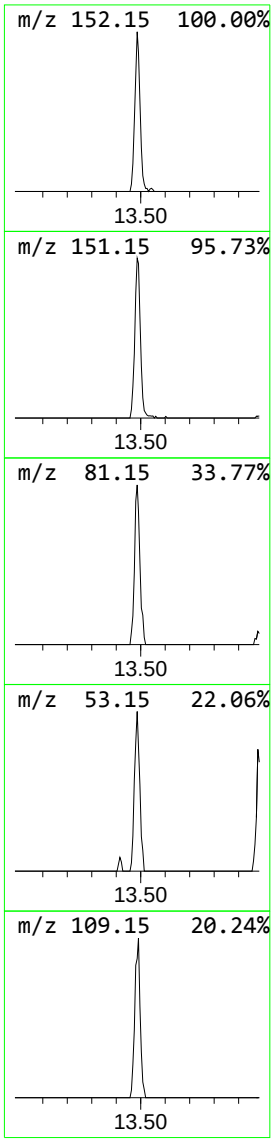
****

Peak Number 3 Vanillin Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.485	2.28 ng/ul	116128	Acenaphthene-d10	14.578

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	97
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	96
3	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	95
4	Vanillin	152	C8H8O3	000121-33-5	95
5	Vanillin	152	C8H8O3	000121-33-5	94





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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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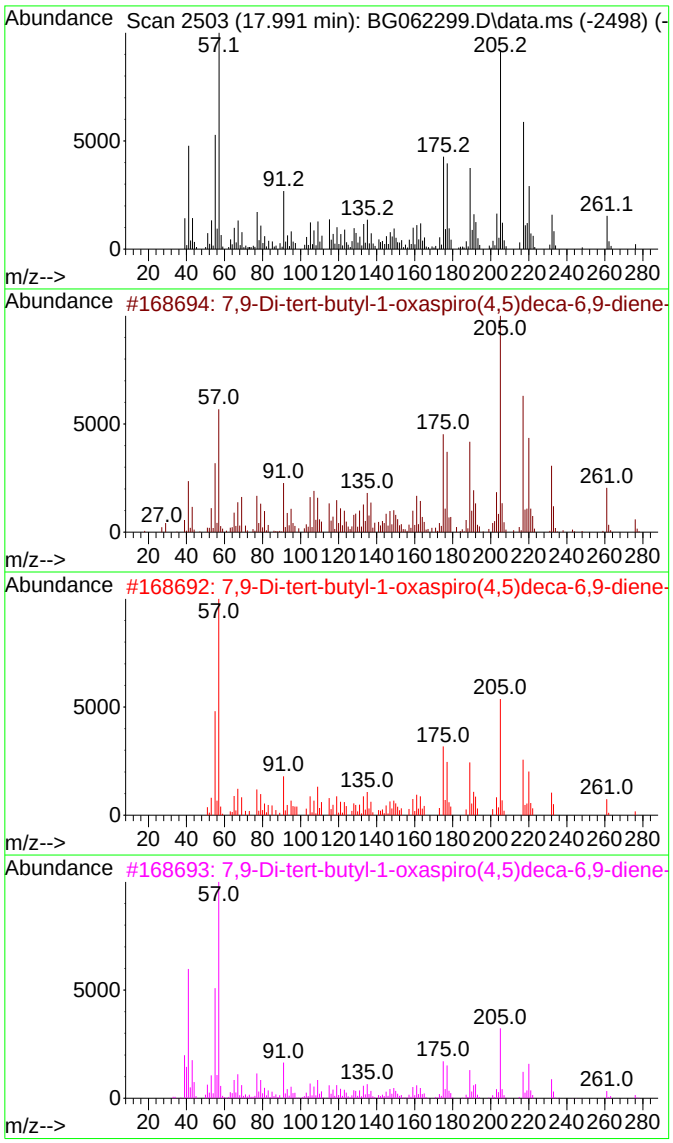
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

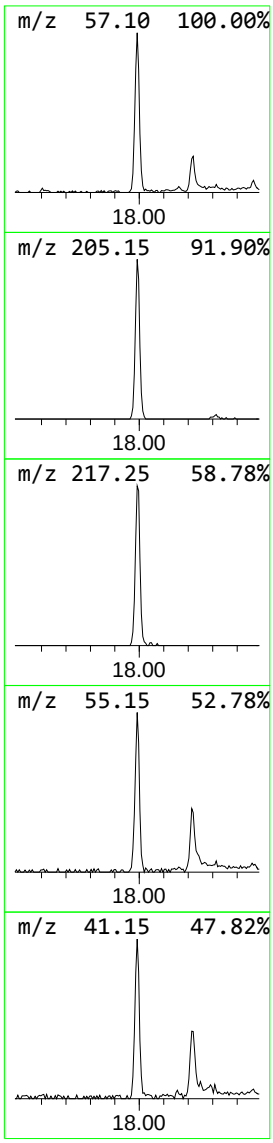
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.991	6.23 ng/ul	359284	Phenanthrene-d10	17.315

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	96
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	60
4	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	55
5	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	46





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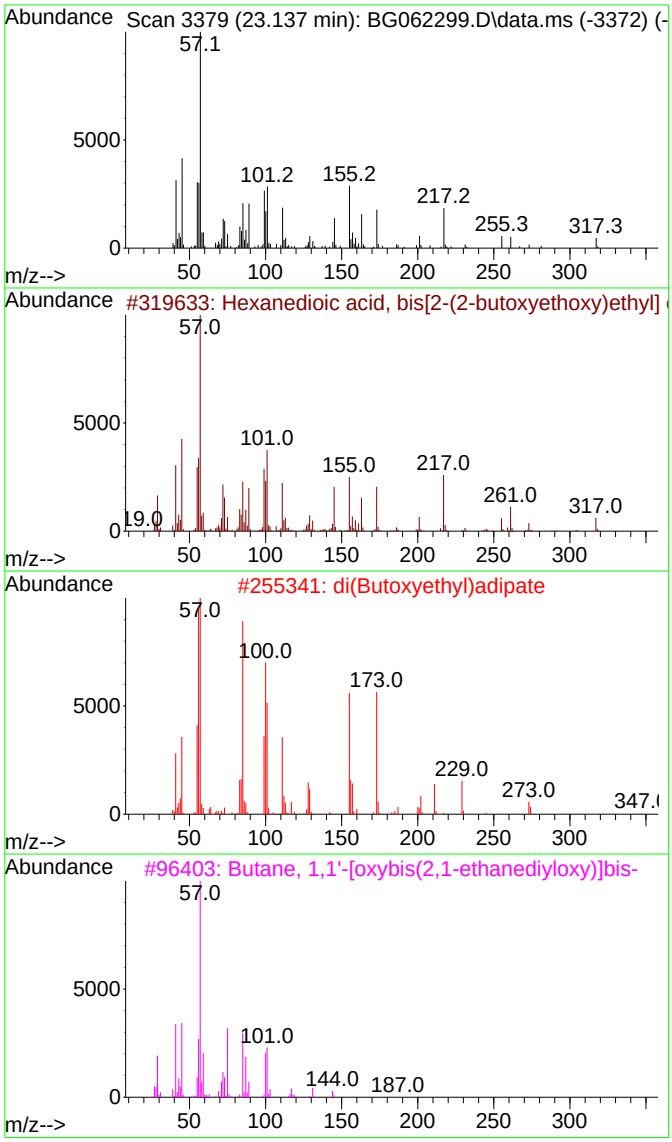
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

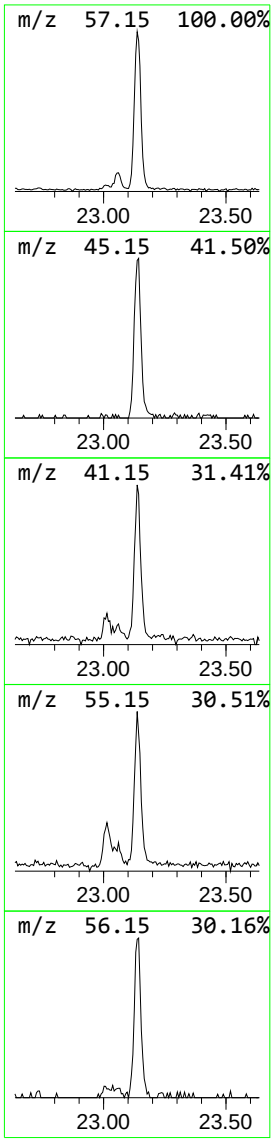
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexanedioic acid, bis[2-(2-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.137	4.13 ng/ul	285323	Perylene-d12	24.647

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	80
2	di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	37
3	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	25
4	1-Decanamine	157	C10H23N	002016-57-1	22
5	2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080724\
Data File : BG062299.D
Acq On : 7 Aug 2024 12:39
Operator : MA/JU
Sample : P3347-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C0B04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.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
Hexanoic acid	6.947	2.0	ng/ul	36684	1	7.957	366725	20.0
2-Propyl-1-pent...	8.022	2.0	ng/ul	37599	1	7.957	366725	20.0
Vanillin	13.485	2.3	ng/ul	116128	3	14.578	1018520	20.0
7,9-Di-tert-but...	17.991	6.2	ng/ul	359284	4	17.315	1153960	20.0
Hexanedioic aci...	23.137	4.1	ng/ul	285323	6	24.647	1380360	20.0