LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072324\
Data File : BG062192.D
Acq On : 23 Jul 2024 19:17
Operator : MA/JU
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

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-BG071924.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG062192.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.459	25	29	32	rBV4	6850	8855	0.62%	0.054%
2	3.741	72	77	85	rBV	28737	44259	3.09%	0.270%
3	3.888	99	102	107	rBV7	6363	12561	0.88%	0.077%
4	3.988	116	119	126	rVB3	16681	23553	1.65%	0.144%
5	4.211	156	157	163	rVB4	7375	9915	0.69%	0.061%
6	4.781	250	254	257	rBV5	3813	6775	0.47%	0.041%
7	5.133	308	314	320	rBV	14828	26466	1.85%	0.162%
8	5.239	329	332	337	rVB3	5157	6497	0.45%	0.040%
9	6.919	612	618	620	rBV	1831	2700	0.19%	0.016%
10	7.148	652	657	660	rBV3	3114	3651	0.26%	0.022%
11	7.242	662	673	684	rVB	197214	342950	23.98%	2.094%
12	7.389	692	698	708	rVB	121704	195558	13.67%	1.194%
13	7.600	727	734	740	rBV	163933	295823	20.69%	1.807%
14	8.064	805	813	824	rVB	160337	279617	19.55%	1.708%
15	8.434	873	876	880	rBV2	2361	3172	0.22%	0.019%
16	8.681	913	918	921	rBV2	2449	3450	0.24%	0.021%
17	8.787	929	936	943	rBV	233776	402136	28.12%	2.456%
18	8.857	946	948	952	rVV4	2761	3496	0.24%	0.021%
19	8.904	952	956	957	rVB3	3158	3677	0.26%	0.022%
20	9.233	1005	1012	1024	rVB	180004	333533	23.32%	2.037%
21	9.339	1024	1030	1033	rBV	2176	3802	0.27%	0.023%
22	9.380	1033	1037	1040	rVB3	4805	5516	0.39%	0.034%
23	9.515	1056	1060	1063	rBV	1950	2592	0.18%	0.016%
24	9.603	1071	1075	1078	rBV3	1925	3232	0.23%	0.020%
25	9.774	1100	1104	1110	rBV3	7890	13020	0.91%	0.080%
26	9.956	1128	1135	1143	rBV	177704	313609	21.93%	1.915%
27	10.179	1170	1173	1174	rBV3	2609	3041	0.21%	0.019%
28	10.508	1220	1229	1238	rBV	267102	478560	33.46%	2.923%
29	10.708	1259	1263	1267	rVB3	2344	3187	0.22%	0.019%
30	10.819	1279	1282	1285	rVB2	3790	4132	0.29%	0.025%
31	10.878	1285	1292	1299	rBV	243055	429984	30.07%	2.626%
32	10.931	1299	1301	1310	rVB2	12280	17957	1.26%	0.110%
33	11.019	1310	1316	1323	rBV4	32325	69007	4.83%	0.421%
34	11.331	1366	1369	1371	rBV4	2503	2912	0.20%	0.018%
35	11.360	1371	1374	1377	rVV	2683	4298	0.30%	0.026%
36	11.389	1377	1379	1384	rVB4	9232	13431	0.94%	0.082%

LSC Area Percent Report

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Operator : MA/JU
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

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-BG071924.MA.M
Title : SVOA CALIBRATION

37	11.613	1411	1417	1425	rBV3	59164	114331	7.99%	0.698%
38	11.983	1477	1480	1484	rBV2	2480	3027	0.21%	0.018%
39	12.265	1526	1528	1531	rVB4	3238	3702	0.26%	0.023%
40	12.335	1536	1540	1544	rVV2	3961	4948	0.35%	0.030%
41	12.400	1546	1551	1554	rBV2	2147	3216	0.22%	0.020%
42	12.458	1557	1561	1567	rBV3	6604	12987	0.91%	0.079%
43	12.535	1570	1574	1579	rVB3	7214	11131	0.78%	0.068%
44	12.746	1606	1610	1613	rBV4	7764	9407	0.66%	0.057%
45	12.817	1616	1622	1628	rBV5	5335	14263	1.00%	0.087%
46	13.058	1659	1663	1664	rBV2	2143	2628	0.18%	0.016%
47	13.093	1667	1669	1673	rVB	2761	2580	0.18%	0.016%
48	13.128	1673	1675	1676	rBV2	3751	2641	0.18%	0.016%
49	13.210	1685	1689	1690	rBV	3268	4008	0.28%	0.024%
50	13.240	1693	1694	1698	rVV2	2699	2486	0.17%	0.015%
51	13.287	1700	1702	1703	rBV	4562	2702	0.19%	0.017%
52	13.481	1731	1735	1736	rBV	5719	6386	0.45%	0.039%
53	13.533	1742	1744	1747	rVB4	3962	3672	0.26%	0.022%
54	13.575	1747	1751	1755	rVB3	2900	4879	0.34%	0.030%
55	13.633	1755	1761	1763	rBV6	4870	10534	0.74%	0.064%
56	13.851	1795	1798	1799	rBV2	3934	4498	0.31%	0.027%
57	13.880	1800	1803	1807	rVB6	8359	11531	0.81%	0.070%
58	13.915	1807	1809	1812	rVB	2955	3129	0.22%	0.019%
59	13.939	1812	1813	1816	rBV3	3985	3659	0.26%	0.022%
60	14.009	1821	1825	1831	rVB4	8836	14695	1.03%	0.090%
61	14.092	1831	1839	1846	rBV	481001	692123	48.40%	4.227%
62	14.256	1862	1867	1870	rBV3	5066	11190	0.78%	0.068%
63	14.326	1874	1879	1884	rVV5	6164	9862	0.69%	0.060%
64	14.391	1884	1890	1898	rBV	493687	790333	55.26%	4.827%
65	14.444	1898	1899	1901	rVB2	4505	3027	0.21%	0.018%
66	14.556	1916	1918	1923	rBV3	4888	7021	0.49%	0.043%
67	14.614	1927	1928	1932	rVB3	4001	3817	0.27%	0.023%
68	14.697	1932	1942	1948	rBV	404982	657255	45.96%	4.014%
69	14.761	1948	1953	1957	rVV3	22705	35030	2.45%	0.214%
70	14.896	1967	1976	1990	rBV2	452199	1306944	91.39%	7.982%
71	15.055	1999	2003	2005	rBV4	13918	18979	1.33%	0.116%
72	15.090	2006	2009	2017	rVB2	20523	33622	2.35%	0.205%
73	15.161	2018	2021	2022	rBV2	4670	4410	0.31%	0.027%
74	15.308	2042	2046	2051	rBV4	5128	8099	0.57%	0.049%
75	15.355	2052	2054	2058	rVB5	7677	7800	0.55%	0.048%
76	15.466	2071	2073	2075	rBV3	5950	6382	0.45%	0.039%

LSC Area Percent Report

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Operator : MA/JU
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

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-BG071924.MA.M
Title : SVOA CALIBRATION

77	15.501	2078	2079	2084	rVB4	9252	11811	0.83%	0.072%
78	15.560	2087	2089	2093	rVB5	4796	4924	0.34%	0.030%
79	15.683	2104	2110	2116	rBV	640914	966426	67.58%	5.902%
80	15.736	2116	2119	2126	rVB3	27760	39441	2.76%	0.241%
81	15.807	2126	2131	2138	rBV	184517	274503	19.19%	1.676%
82	15.866	2138	2141	2143	rBV4	7059	6256	0.44%	0.038%
83	16.177	2191	2194	2198	rBV5	14531	25319	1.77%	0.155%
84	16.377	2221	2228	2231	rBV6	19615	38661	2.70%	0.236%
85	16.717	2282	2286	2287	rBV5	9123	11126	0.78%	0.068%
86	17.258	2374	2378	2384	rVB	26298	40474	2.83%	0.247%
87	17.440	2403	2409	2413	rBV	564454	858683	60.04%	5.244%
88	17.481	2413	2416	2421	rVB	362977	473047	33.08%	2.889%
89	17.540	2421	2426	2431	rBV2	670849	1006535	70.38%	6.147%
90	18.309	2554	2557	2562	rBV	58120	84028	5.88%	0.513%
91	18.362	2562	2566	2572	rVB2	89538	145727	10.19%	0.890%
92	18.503	2585	2590	2594	rBV5	94825	189430	13.25%	1.157%
93	18.538	2594	2596	2602	rVB	58840	82003	5.73%	0.501%
94	18.803	2638	2641	2645	rVB	45796	60210	4.21%	0.368%
95	19.220	2709	2712	2715	rBV3	69039	94434	6.60%	0.577%
96	19.484	2752	2757	2763	rBV	688367	979894	68.52%	5.984%
97	19.819	2809	2814	2817	rBV	818537	1249632	87.38%	7.632%
98	21.323	3066	3070	3076	rVB	275329	370215	25.89%	2.261%
99	21.699	3127	3134	3139	rBV2	625954	1430083	100.00%	8.734%
100	23.514	3438	3443	3453	rVB3	340483	701180	49.03%	4.282%

Sum of corrected areas: 16373900

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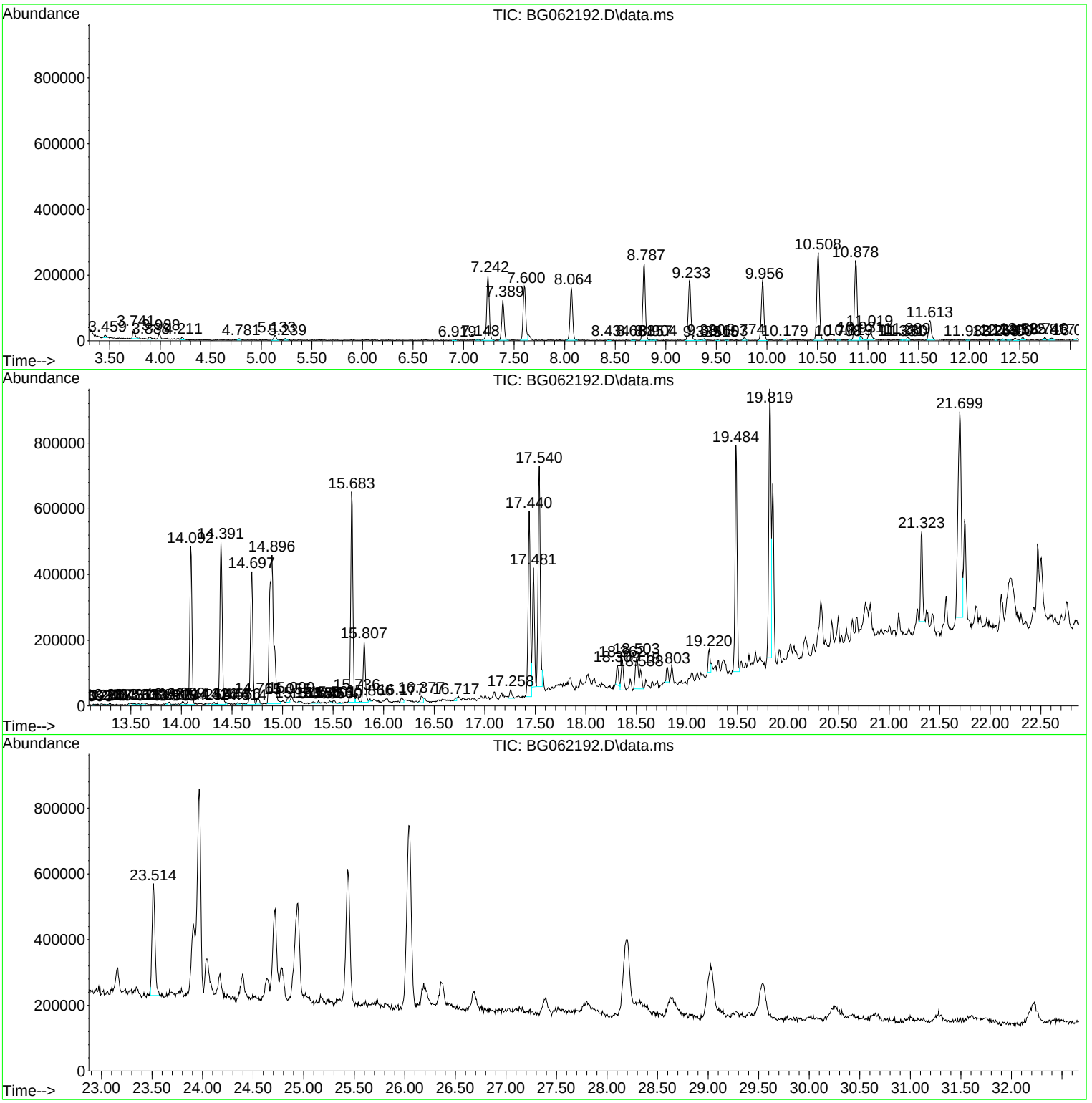
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG071924.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072324\
Data File : BG062192.D
Acq On : 23 Jul 2024 19:17
Operator : MA/JU
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

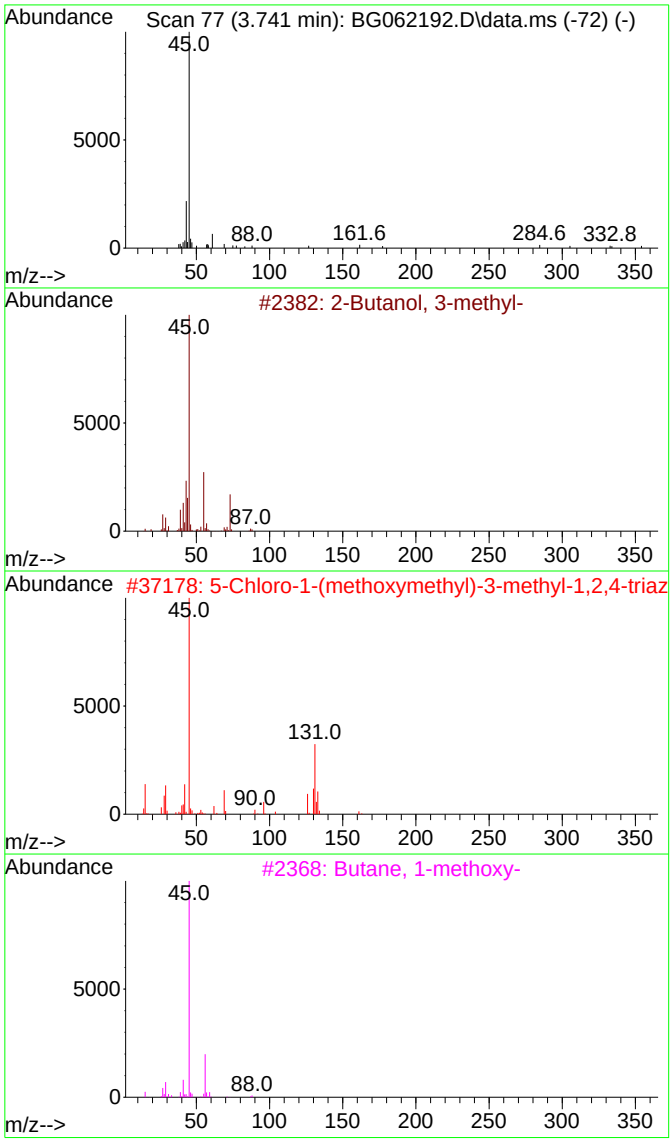
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG071924.MA.M
Quant Title : SVOA CALIBRATION

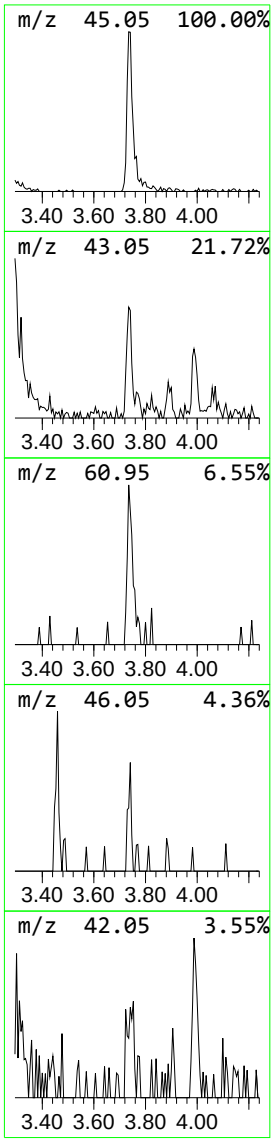
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.741	3.17 ng/ul	44259	1,4-Dichlorobenzene-d4	8.064

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
2	5-Chloro-1-(methoxymethyl)-3-met...	161	C5H8ClN3O	1000436-89-3	9
3	Butane, 1-methoxy-	88	C5H12O	000628-28-4	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072324\
Data File : BG062192.D
Acq On : 23 Jul 2024 19:17
Operator : MA/JU
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

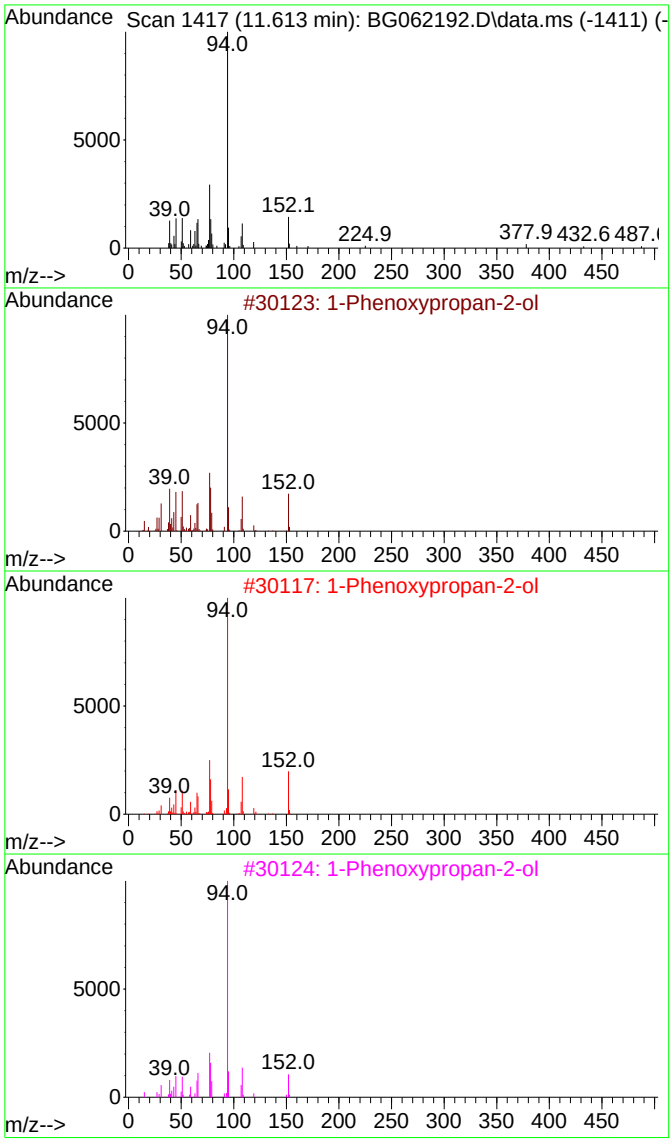
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG071924.MA.M
Quant Title : SVOA CALIBRATION

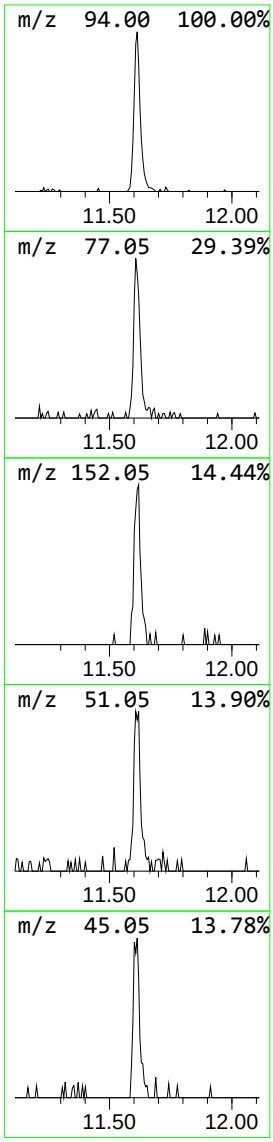
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.613	5.32 ng/ul	114331	Naphthalene-d8	10.878

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	74





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Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

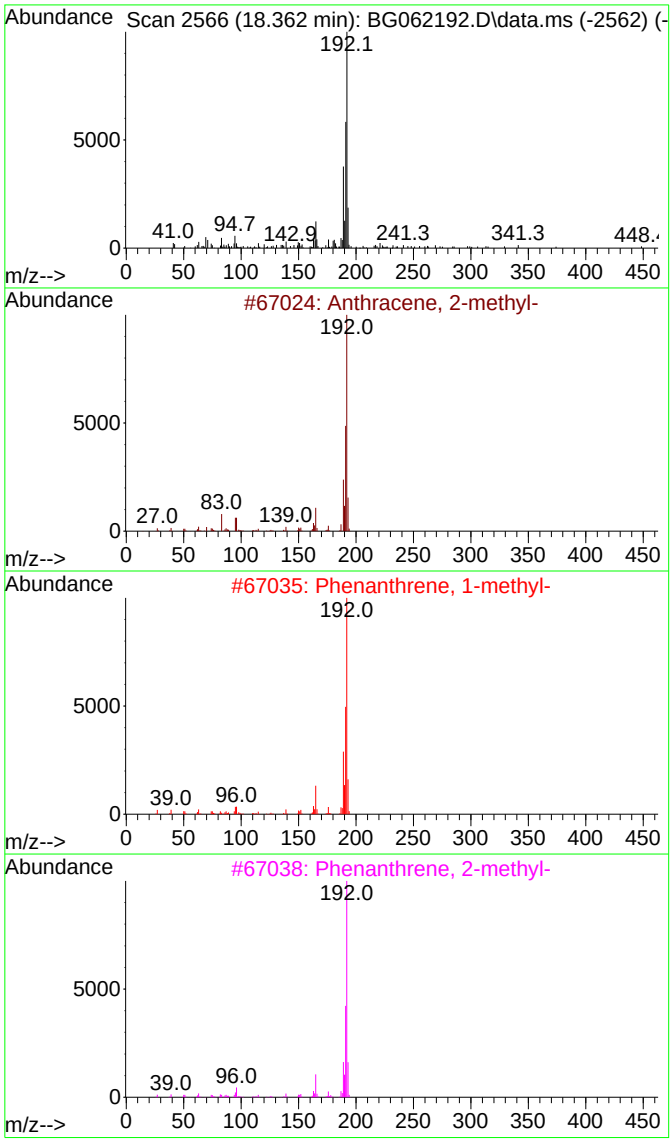
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG071924.MA.M
Quant Title : SVOA CALIBRATION

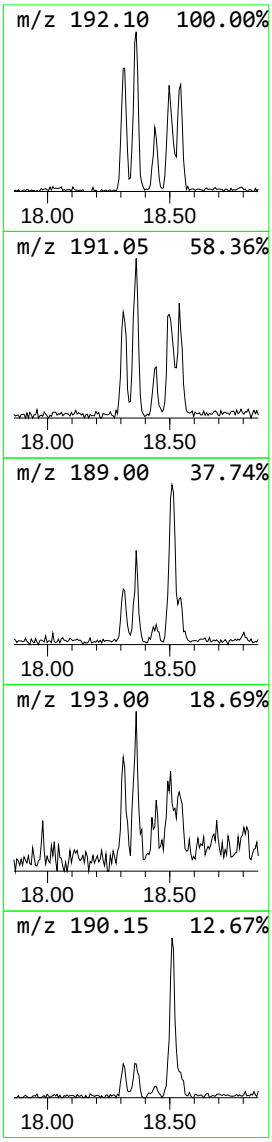
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Anthracene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.362	3.39 ng/ul	145727	Phenanthrene-d10	17.440

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072324\
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Misc :
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Instrument :
BNA_G
ClientSampleId :
A4CL0

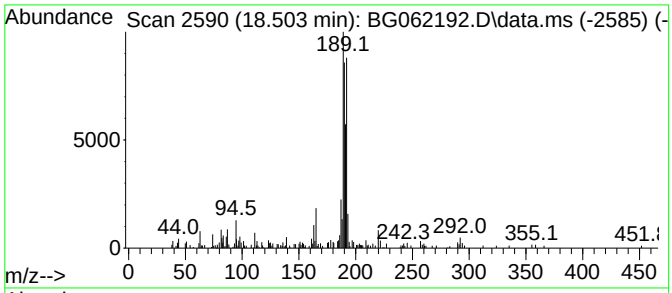
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG071924.MA.M
Quant Title : SVOA CALIBRATION

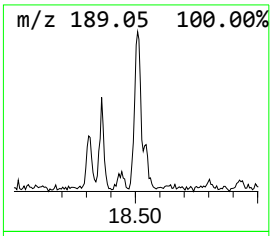
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

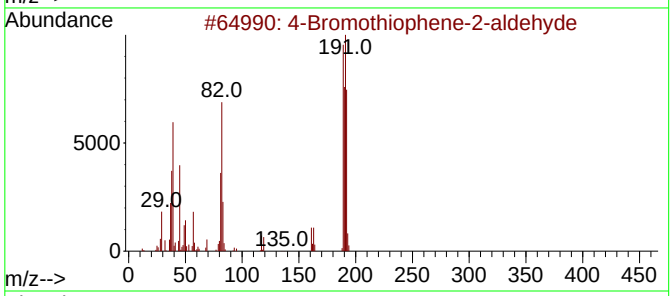
****
Peak Number 4 4-Bromothiophene-2-aldehyde Concentration Rank 4

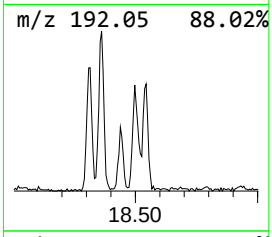
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.503	4.41 ng/ul	189430	Phenanthrene-d10	17.440

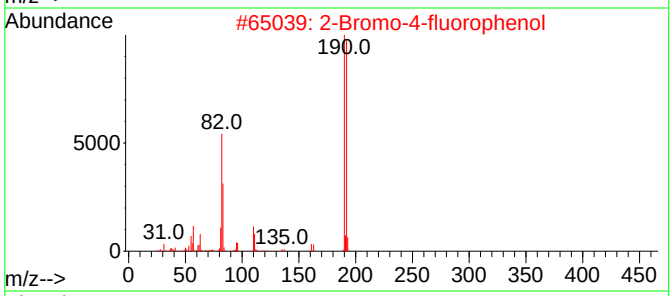
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	64
2	2-Bromo-4-fluorophenol	190	C6H4BrFO	000496-69-5	43
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38
5	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	38

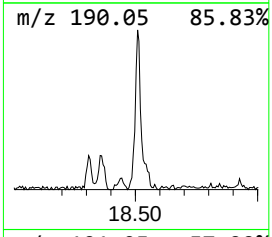


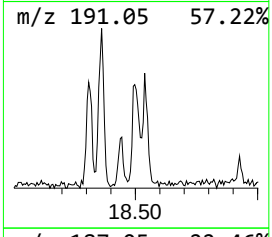


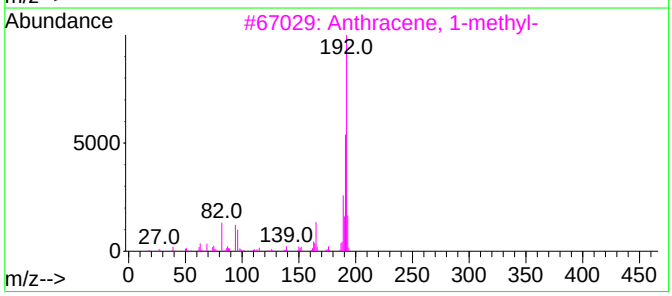


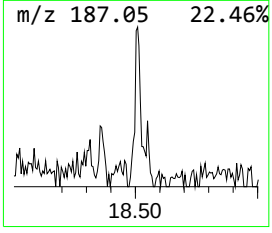












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072324\
Data File : BG062192.D
Acq On : 23 Jul 2024 19:17
Operator : MA/JU
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

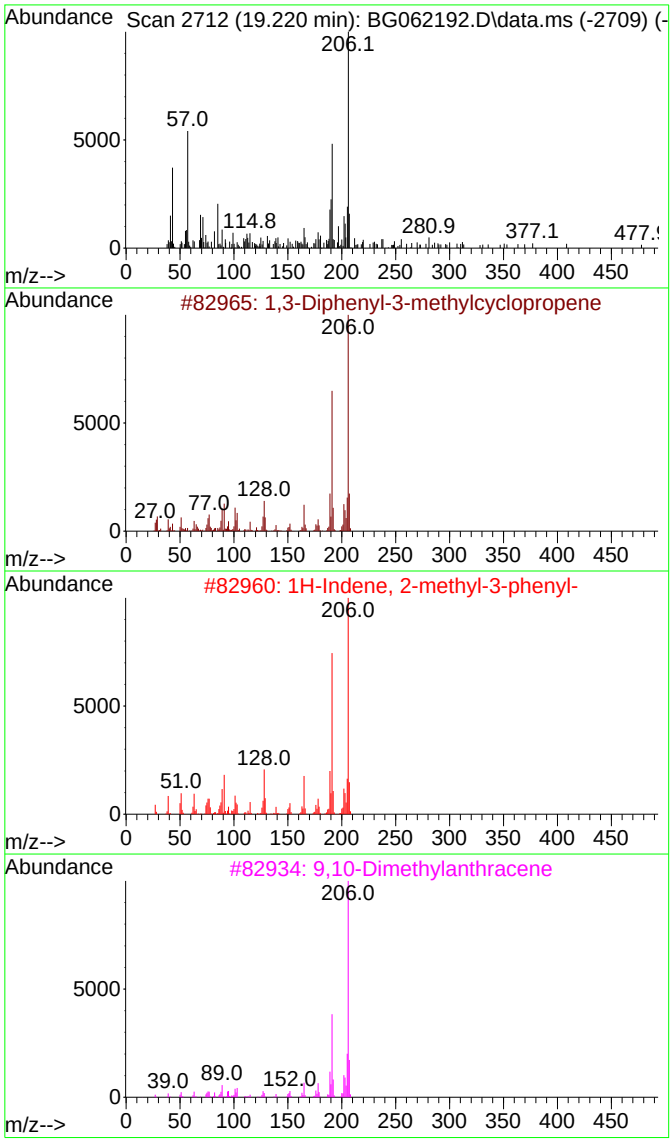
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG071924.MA.M
Quant Title : SVOA CALIBRATION

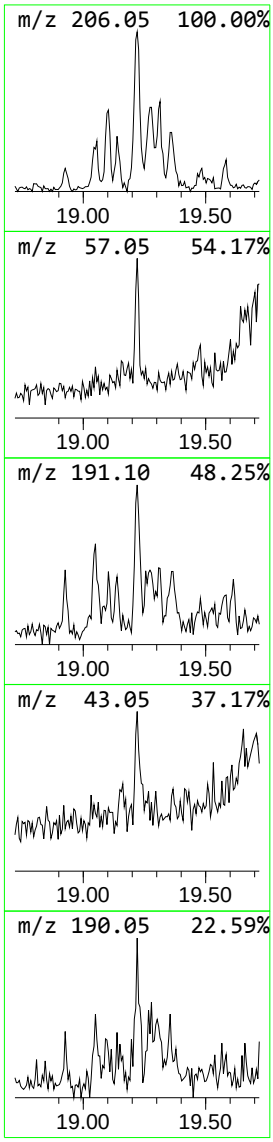
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Diphenyl-3-methylcyclop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.220	2.20 ng/ul	94434	Phenanthrene-d10	17.440

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	64
2	1H-Indene, 2-methyl-3-phenyl-	206	C16H14	035099-60-6	62
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	58
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	58
5	1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072324\
Data File : BG062192.D
Acq On : 23 Jul 2024 19:17
Operator : MA/JU
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG071924.MA.M
Quant Title : SVOA CALIBRATION

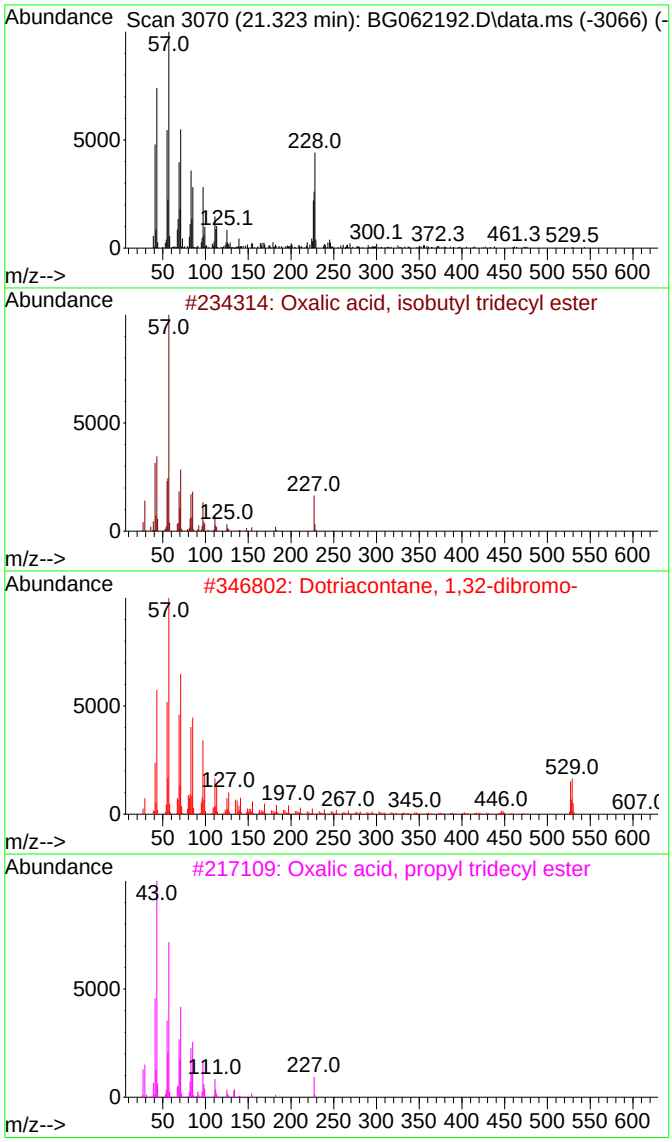
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

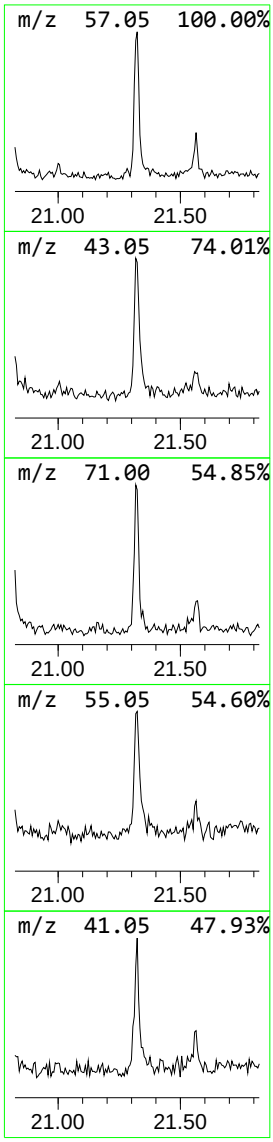
****

Peak Number 6 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.323	5.18 ng/ul	370215	Chrysene-d12	21.705

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl tridecyl e...	328	C19H36O4	1000309-37-8	49
2	Dotriacontane, 1,32-dibromo-	606	C32H64Br2	121955-26-8	25
3	Oxalic acid, propyl tridecyl ester	314	C18H34O4	1000309-26-6	22
4	Muscimol	114	C4H6N2O2	002763-96-4	22
5	Stearic acid, 3-(octadecyloxy)pr...	595	C39H78O3	017367-40-7	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072324\
Data File : BG062192.D
Acq On : 23 Jul 2024 19:17
Operator : MA/JU
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG071924.MA.M
Quant Title : SVOA CALIBRATION

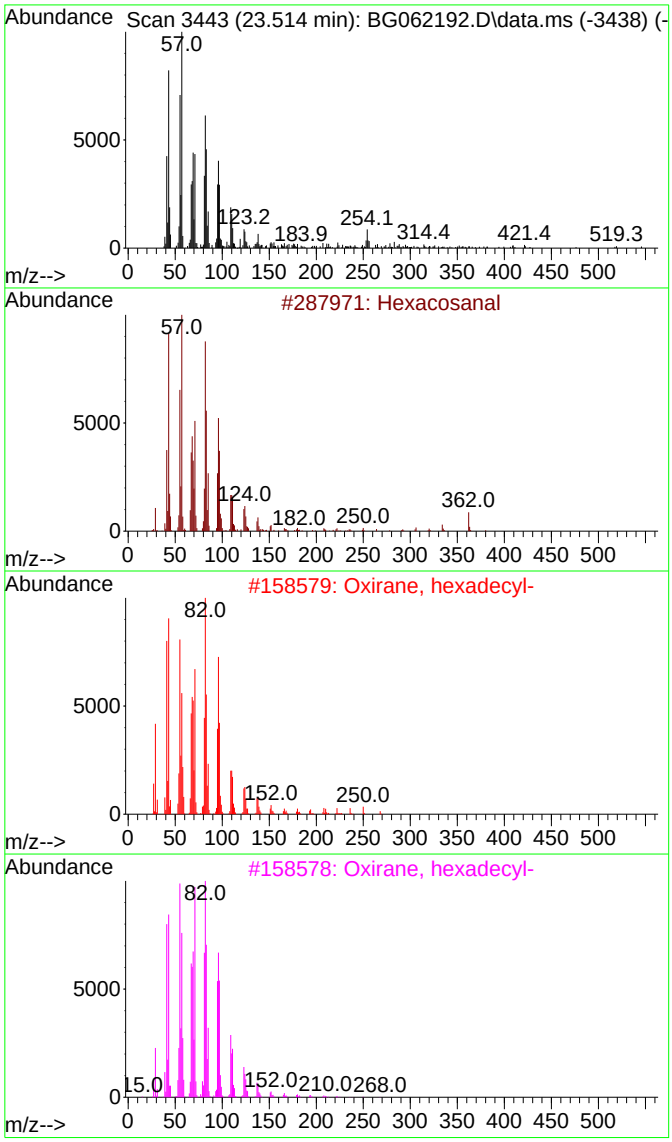
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

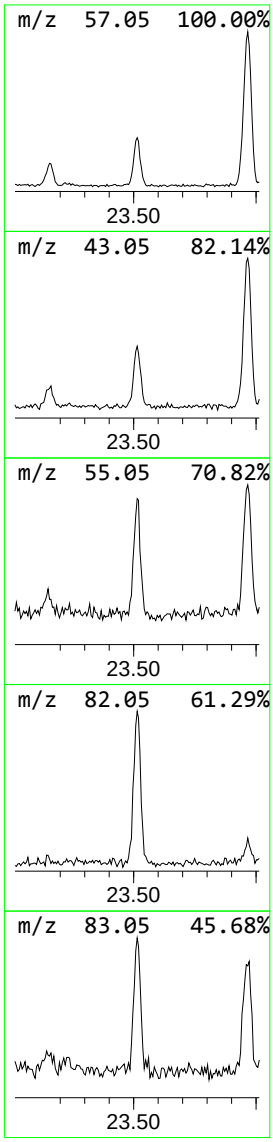
****

Peak Number 7 Hexacosanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.514	20.00 ng/ul	701180	Perylene-d12	24.942

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosanal	380	C26H52O	026627-85-0	87
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
3	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4	Tetracosanal	352	C24H48O	057866-08-7	86
5	Tetradecanal	212	C14H28O	000124-25-4	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072324\
Data File : BG062192.D
Acq On : 23 Jul 2024 19:17
Operator : MA/JU
Sample : P3263-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CL0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG071924.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
unknown-01	3.741	3.2	ng/ul	44259	1	8.064	279617	20.0
1-Phenoxypropan...	11.613	5.3	ng/ul	114331	2	10.878	429984	20.0
Anthracene, 2-m...	18.362	3.4	ng/ul	145727	4	17.440	858683	20.0
4-Bromothiophen...	18.503	4.4	ng/ul	189430	4	17.440	858683	20.0
1,3-Diphenyl-3-...	19.220	2.2	ng/ul	94434	4	17.440	858683	20.0
unknown-02	21.323	5.2	ng/ul	370215	5	21.705	1430080	20.0
Hexacosanal	23.514	20.0	ng/ul	701180	6	24.942	701180	20.0