LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

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-BG062024.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG061622.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.464	28	30	37	rVB4	16153	28795	1.73%	0.152%
2	3.682	65	67	70	rBV3	3622	3606	0.22%	0.019%
3	3.734	73	76	85	rVB	33220	52419	3.15%	0.278%
4	3.899	101	104	109	rVB4	19143	25101	1.51%	0.133%
5	3.940	109	111	114	rVV4	4170	4865	0.29%	0.026%
6	3.999	118	121	126	rBV3	9041	11341	0.68%	0.060%
7	4.116	139	141	146	rVB4	3495	4087	0.25%	0.022%
8	4.539	209	213	214	rBV3	3089	3790	0.23%	0.020%
9	4.739	243	247	251	rVV6	7104	9812	0.59%	0.052%
10	4.798	252	257	261	rVB3	14909	24273	1.46%	0.128%
11	5.045	293	299	304	rBV8	3909	9455	0.57%	0.050%
12	5.150	310	317	323	rBV2	33115	53945	3.24%	0.286%
13	5.233	328	331	332	rBV3	3276	3897	0.23%	0.021%
14	5.244	332	333	342	rVB5	5980	7434	0.45%	0.039%
15	6.020	461	465	468	rVB4	4049	4712	0.28%	0.025%
16	6.143	481	486	490	rVB5	10228	17641	1.06%	0.093%
17	6.478	540	543	546	rBV4	2421	3520	0.21%	0.019%
18	6.772	590	593	595	rBV3	2310	3419	0.21%	0.018%
19	6.866	607	609	614	rBV2	3134	4234	0.25%	0.022%
20	7.007	632	633	635	rBV2	4164	3942	0.24%	0.021%
21	7.213	659	668	676	rBV	288102	490108	29.43%	2.595%
22	7.401	693	700	707	rVB	194783	316230	18.99%	1.674%
23	7.595	727	733	740	rVV	242710	437357	26.26%	2.315%
24	7.659	740	744	752	rVV2	12470	28949	1.74%	0.153%
25	7.877	777	781	784	rBV3	3054	4508	0.27%	0.024%
26	8.076	807	815	821	rBV	225683	385537	23.15%	2.041%
27	8.194	830	835	837	rBV4	3989	6125	0.37%	0.032%
28	8.429	873	875	878	rVB3	2868	3762	0.23%	0.020%
29	8.599	901	904	905	rBV3	3952	3466	0.21%	0.018%
30	8.764	926	932	941	rVV	325734	551366	33.11%	2.919%
31	8.899	949	955	959	rBV4	15950	30618	1.84%	0.162%
32	9.163	995	1000	1002	rVB2	2896	4977	0.30%	0.026%
33	9.234	1002	1012	1019	rBV	250647	453781	27.25%	2.402%
34	9.310	1023	1025	1029	rBV4	3277	4978	0.30%	0.026%
35	9.469	1048	1052	1053	rBV2	4157	4613	0.28%	0.024%
36	9.798	1101	1108	1113	rBV	24385	39891	2.40%	0.211%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
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Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

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-BG062024.MA.M
Title : SVOA CALIBRATION

37	9.957	1128	1135	1145	rBV	195559	356728	21.42%	1.888%
38	10.051	1149	1151	1152	rBV	4696	4537	0.27%	0.024%
39	10.156	1164	1169	1174	rVB6	5723	9922	0.60%	0.053%
40	10.338	1199	1200	1205	rBV4	2919	4000	0.24%	0.021%
41	10.491	1217	1226	1235	rBV	319403	576078	34.59%	3.050%
42	10.744	1264	1269	1272	rVB3	3182	4095	0.25%	0.022%
43	10.885	1286	1293	1301	rBV	331784	582022	34.95%	3.081%
44	10.938	1301	1302	1307	rVB2	5668	5435	0.33%	0.029%
45	11.014	1307	1315	1327	rBV	234853	450641	27.06%	2.386%
46	11.179	1338	1343	1346	rBV2	2359	3876	0.23%	0.021%
47	11.343	1370	1371	1376	rVB3	4884	4585	0.28%	0.024%
48	11.408	1376	1382	1388	rBV7	16139	29574	1.78%	0.157%
49	11.619	1410	1418	1430	rBV2	50706	107244	6.44%	0.568%
50	12.342	1537	1541	1542	rBV3	4710	4867	0.29%	0.026%
51	12.401	1546	1551	1556	rBV4	7894	15051	0.90%	0.080%
52	12.460	1558	1561	1562	rBV	4725	4732	0.28%	0.025%
53	12.542	1574	1575	1580	rVB3	4139	4920	0.30%	0.026%
54	12.753	1609	1611	1614	rVB3	5602	5161	0.31%	0.027%
55	12.959	1642	1646	1647	rBV3	5661	7029	0.42%	0.037%
56	13.071	1663	1665	1668	rVB4	3411	4239	0.25%	0.022%
57	13.217	1688	1690	1692	rBV2	3247	3376	0.20%	0.018%
58	13.241	1692	1694	1698	rVB3	4292	5083	0.31%	0.027%
59	13.282	1698	1701	1703	rVB3	3761	3449	0.21%	0.018%
60	13.317	1703	1707	1712	rBV5	5704	9425	0.57%	0.050%
61	13.611	1755	1757	1762	rVB3	4877	5350	0.32%	0.028%
62	13.658	1762	1765	1768	rBV4	3550	4429	0.27%	0.023%
63	13.864	1798	1800	1801	rBV	3606	3407	0.20%	0.018%
64	13.876	1801	1802	1808	rVB4	6745	7154	0.43%	0.038%
65	13.964	1813	1817	1819	rVB2	5221	4103	0.25%	0.022%
66	14.017	1823	1826	1827	rBV3	4704	5098	0.31%	0.027%
67	14.105	1832	1841	1849	rBV	583294	857132	51.47%	4.538%
68	14.199	1854	1857	1858	rVB2	4043	3753	0.23%	0.020%
69	14.246	1863	1865	1867	rBV3	4779	5274	0.32%	0.028%
70	14.346	1876	1882	1884	rBV5	11950	22314	1.34%	0.118%
71	14.398	1884	1891	1897	rVB	662305	1047885	62.92%	5.547%
72	14.534	1912	1914	1917	rVV4	5314	4276	0.26%	0.023%
73	14.698	1935	1942	1949	rVB	523181	846412	50.82%	4.481%
74	14.757	1949	1952	1959	rBV5	15289	24806	1.49%	0.131%
75	14.863	1964	1970	1976	rBV	307769	496372	29.81%	2.628%
76	15.027	1993	1998	2004	rBV8	16514	33932	2.04%	0.180%

LSC Area Percent Report

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Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

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-BG062024.MA.M
Title : SVOA CALIBRATION

77	15.098	2006	2010	2017	rVB9	18438	33425	2.01%	0.177%
78	15.286	2040	2042	2045	rVB3	4018	3736	0.22%	0.020%
79	15.350	2051	2053	2056	rVB4	5547	4506	0.27%	0.024%
80	15.415	2062	2064	2065	rBV2	5634	3541	0.21%	0.019%
81	15.497	2074	2078	2079	rBV3	6029	6176	0.37%	0.033%
82	15.691	2104	2111	2117	rBV	860730	1328096	79.75%	7.031%
83	15.744	2117	2120	2123	rVV3	18918	22126	1.33%	0.117%
84	15.791	2123	2128	2134	rVB2	227800	326993	19.63%	1.731%
85	16.408	2231	2233	2234	rBV2	7821	5423	0.33%	0.029%
86	16.749	2288	2291	2294	rBV5	7463	9599	0.58%	0.051%
87	17.319	2385	2388	2391	rVB3	24297	29832	1.79%	0.158%
88	17.442	2403	2409	2413	rBV	745831	1087351	65.29%	5.756%
89	17.483	2413	2416	2420	rVV	119620	159645	9.59%	0.845%
90	17.542	2420	2426	2435	rVB2	956117	1453684	87.29%	7.696%
91	17.812	2470	2472	2473	rBV2	12250	9468	0.57%	0.050%
92	18.029	2505	2509	2510	rBV3	50454	61552	3.70%	0.326%
93	18.329	2556	2560	2570	rBV4	200455	328355	19.72%	1.738%
94	19.487	2754	2757	2763	rVB	192494	266769	16.02%	1.412%
95	19.598	2774	2776	2785	rVB4	89173	123231	7.40%	0.652%
96	19.821	2809	2814	2824	rBV2	1043415	1665390	100.00%	8.816%
97	21.367	3074	3077	3082	rVB2	187716	267774	16.08%	1.418%
98	21.708	3130	3135	3140	rVB2	598218	999666	60.03%	5.292%
99	24.704	3640	3645	3654	rVB2	359186	912053	54.77%	4.828%
100	24.933	3676	3684	3693	rVB	431500	1156848	69.46%	6.124%

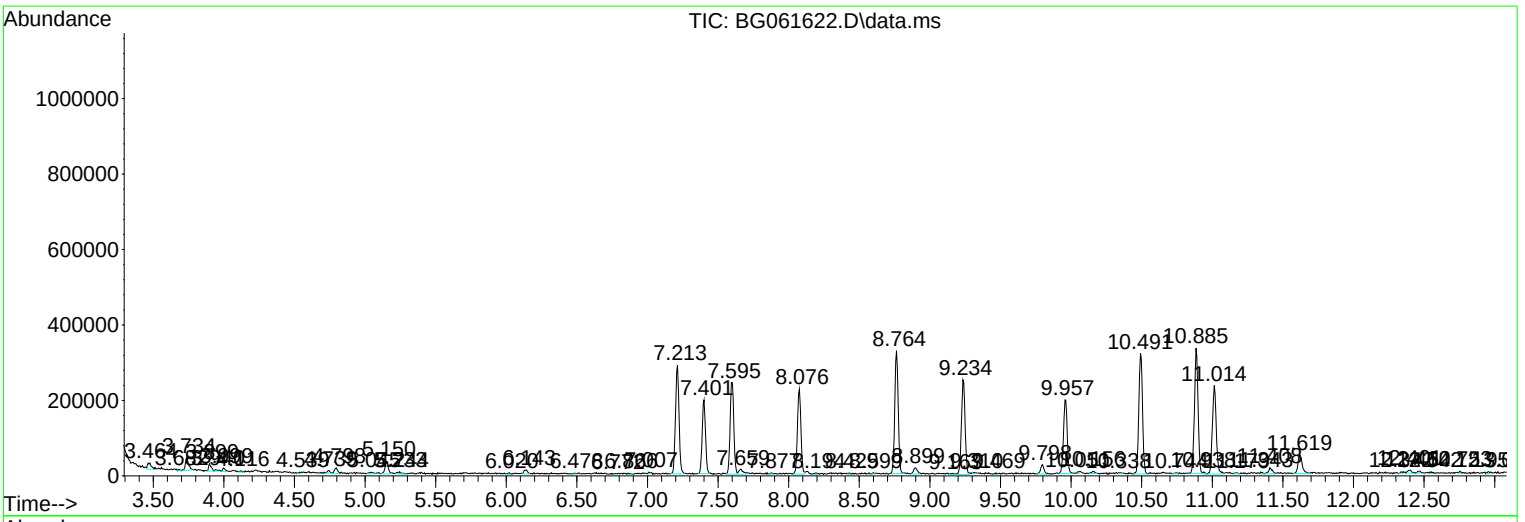
Sum of corrected areas: 18889559

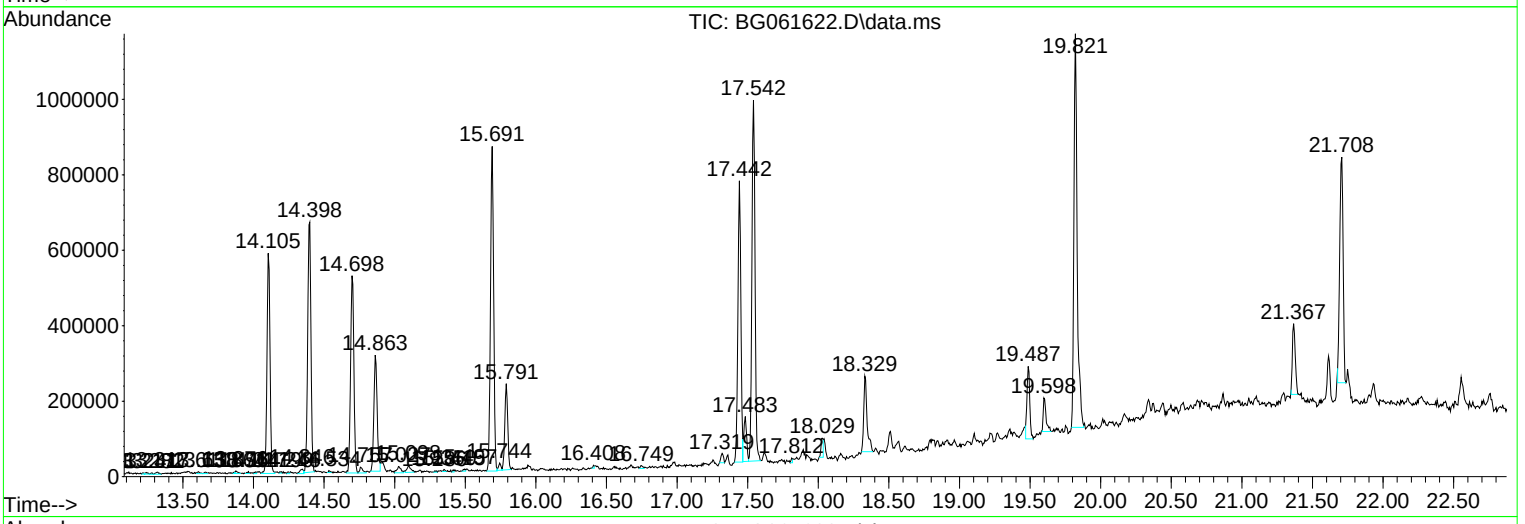
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

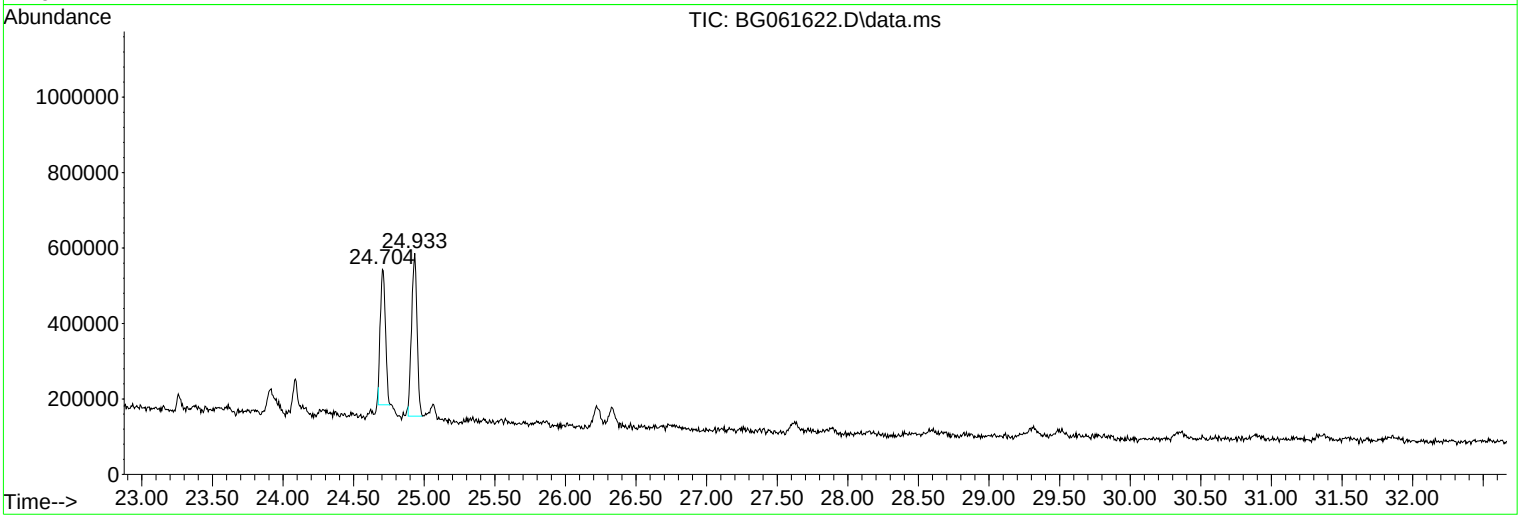
Instrument :
BNA_G
ClientSampleId :
A4BP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.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\BG062124\
Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

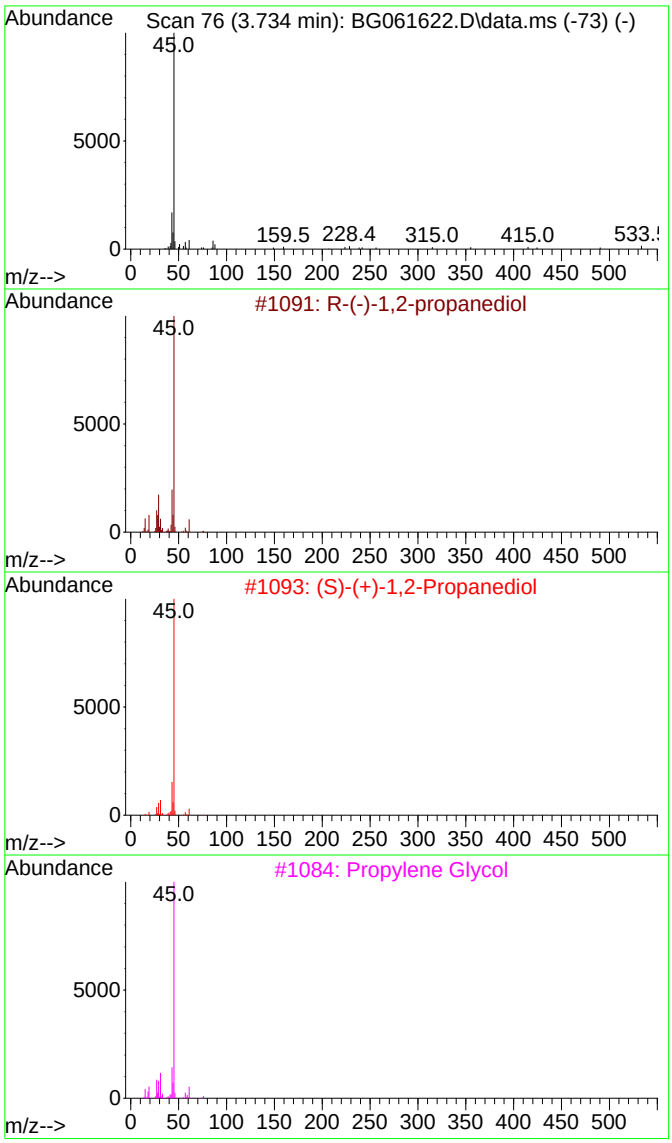
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

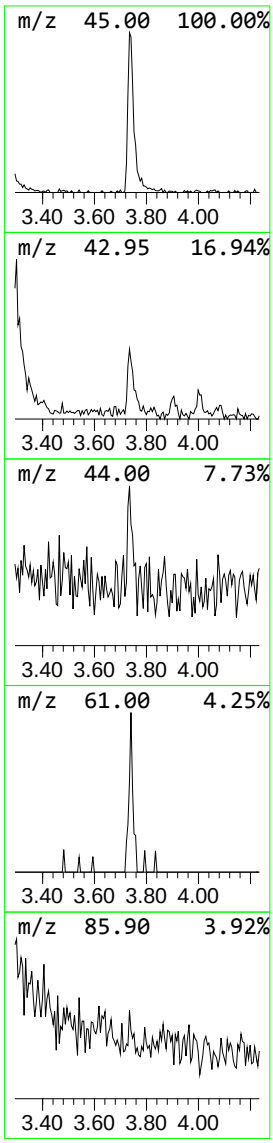
****

Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.734	2.72 ng/ul	52419	1,4-Dichlorobenzene-d4	8.071

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	50
3	Propylene Glycol	76	C3H8O2	000057-55-6	50
4	Propylene Glycol	76	C3H8O2	000057-55-6	50
5	Butane, 1-methoxy-	88	C5H12O	000628-28-4	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

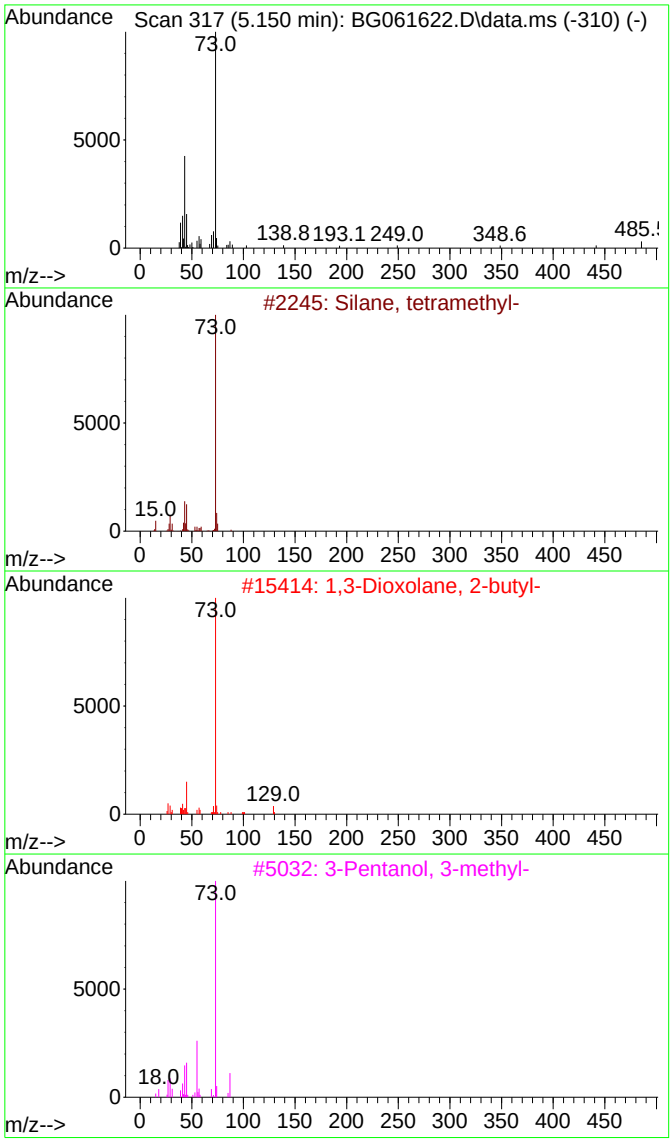
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

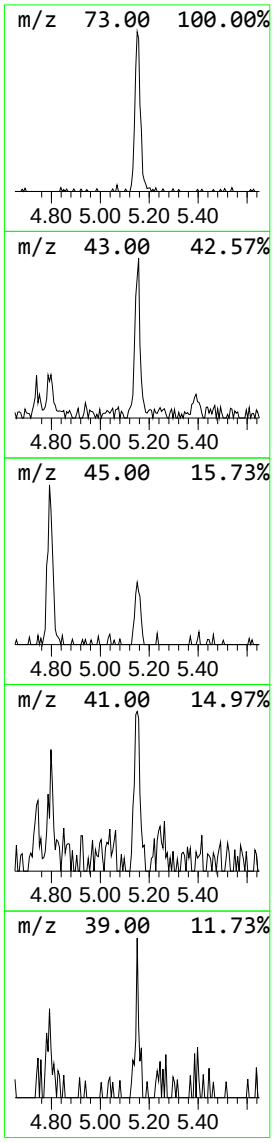
****

Peak Number 2 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.150	2.80 ng/ul	53945	1,4-Dichlorobenzene-d4	8.071

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, tetramethyl-	88	C4H12Si	000075-76-3	42
2	1,3-Dioxolane, 2-butyl-	130	C7H14O2	004360-76-3	38
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	36
5	1,3-Dioxolane, 2-(1-methylpropyl)-	130	C7H14O2	014447-25-7	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

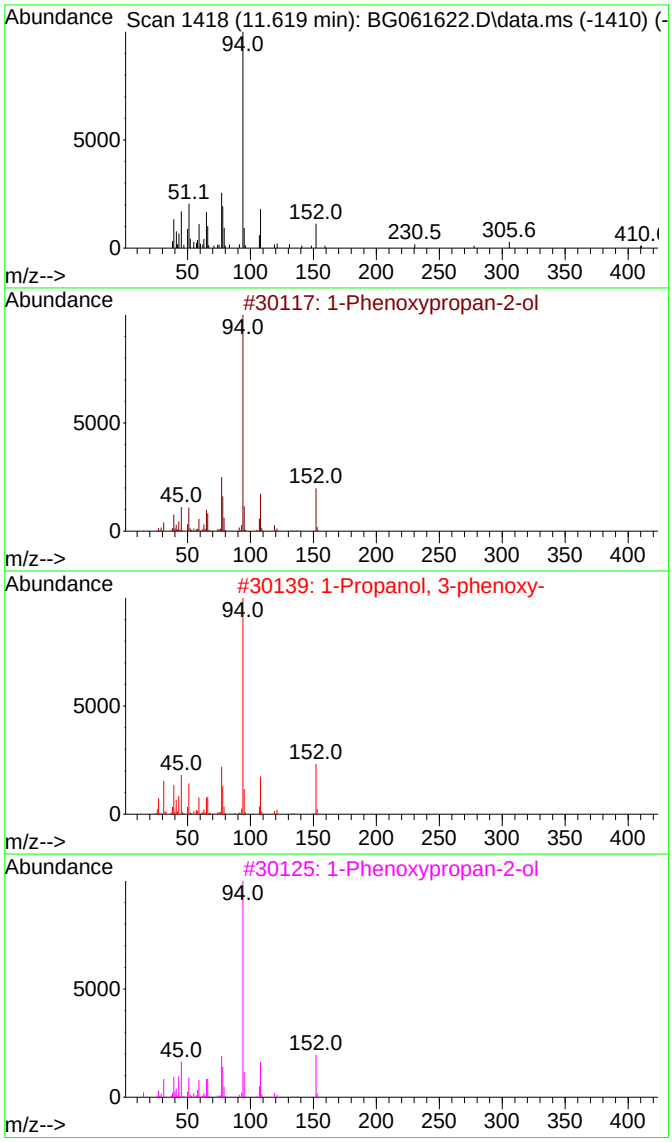
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

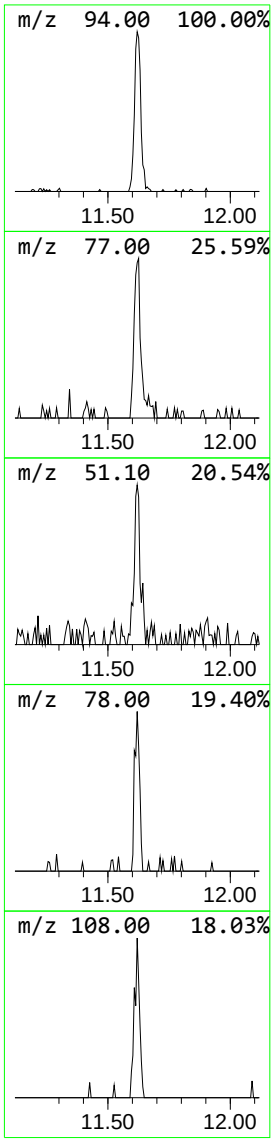
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.619	3.69 ng/ul	107244	Naphthalene-d8	10.885

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	76
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	72
5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

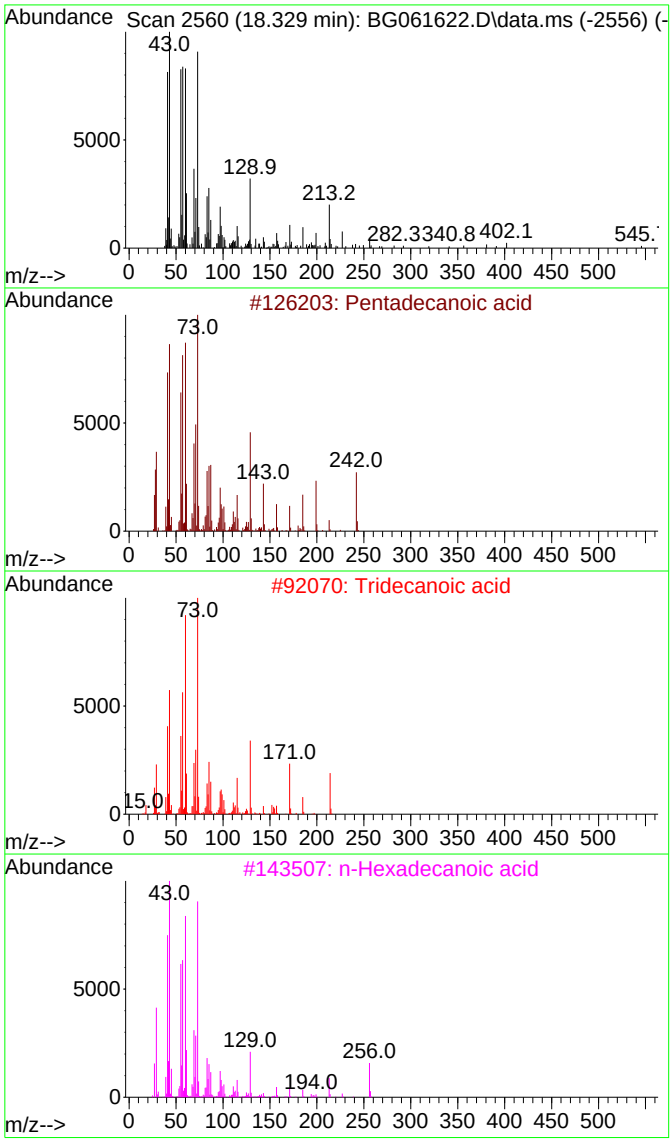
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

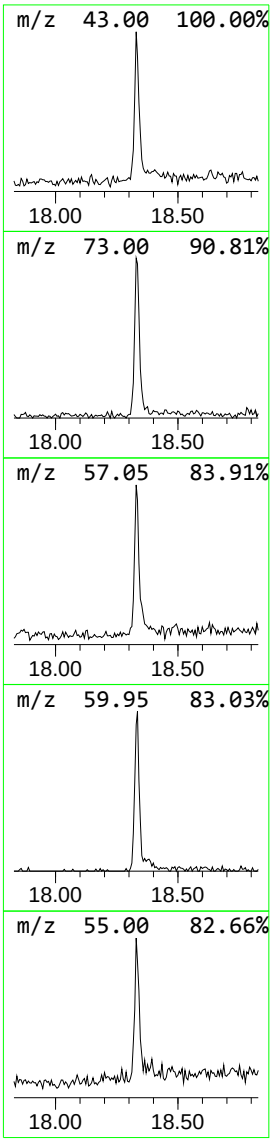
****

Peak Number 4 Pentadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.329	6.04 ng/ul	328355	Phenanthrene-d10	17.442

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
2	Tridecanoic acid	214	C13H26O2	000638-53-9	62
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
4	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	59
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

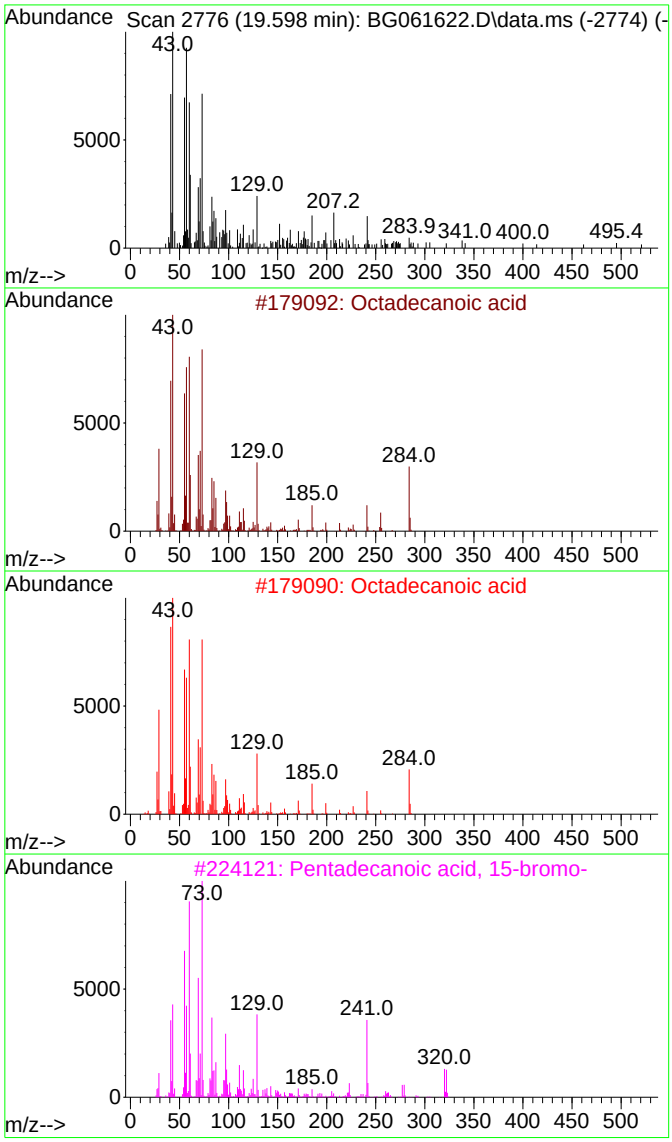
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

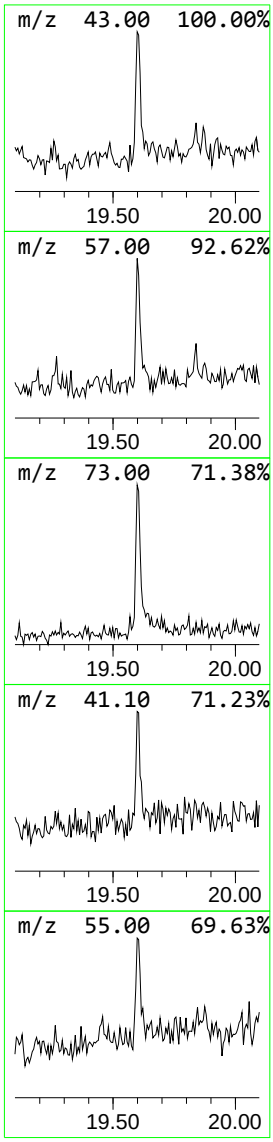
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.598	2.47 ng/ul	123231	Chrysene-d12	21.708

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	72
2	Octadecanoic acid	284	C18H36O2	000057-11-4	62
3	Pentadecanoic acid, 15-bromo-	320	C15H29BrO2	056523-59-2	53
4	Octadecanoic acid	284	C18H36O2	000057-11-4	52
5	Heptadecanoic acid	270	C17H34O2	000506-12-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

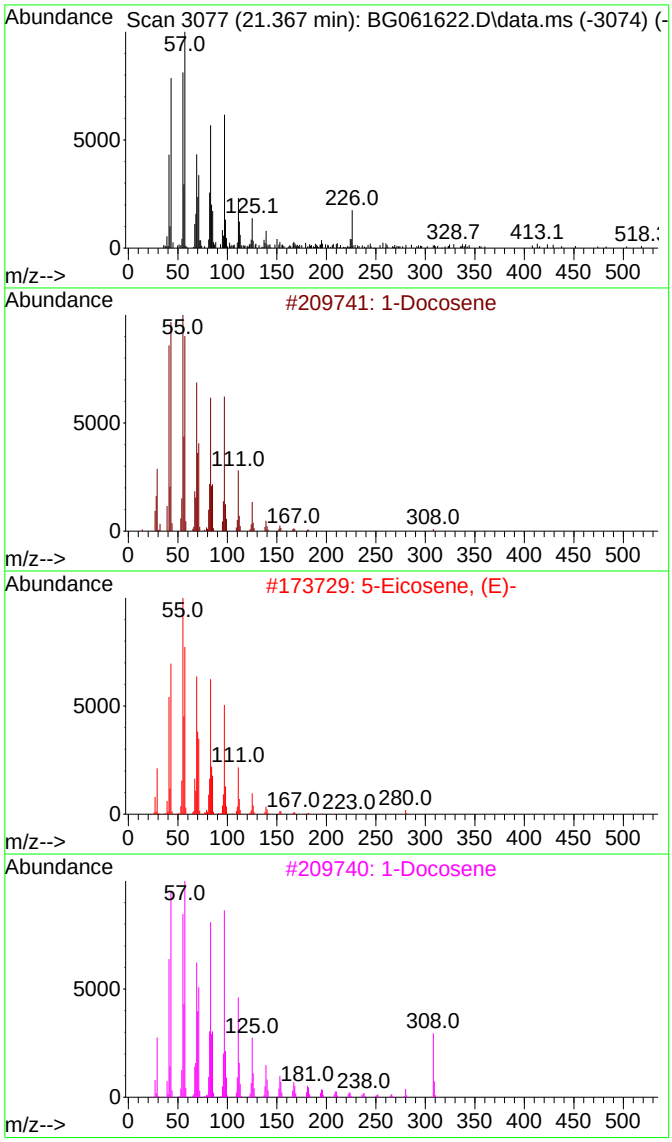
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

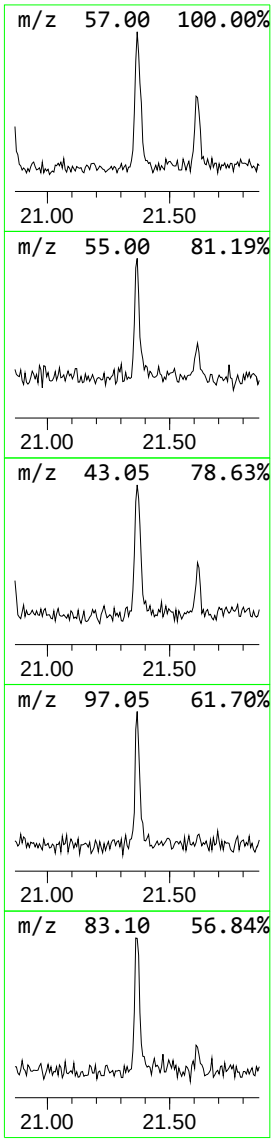
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.367	5.36 ng/ul	267774	Chrysene-d12	21.708

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	1-Docosene	308	C22H44	001599-67-3	89
4	Cyclotetracosane	336	C24H48	000297-03-0	87
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061622.D
Acq On : 21 Jun 2024 16:10
Operator : MA/JU
Sample : P2754-09
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.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
R-(-)-1,2-propa...	3.734	2.7	ng/ul	52419	1	8.071	385537	20.0
unknown-01	5.150	2.8	ng/ul	53945	1	8.071	385537	20.0
1-Phenoxypropan...	11.619	3.7	ng/ul	107244	2	10.885	582022	20.0
Pentadecanoic acid	18.329	6.0	ng/ul	328355	4	17.442	1087350	20.0
Octadecanoic acid	19.598	2.5	ng/ul	123231	5	21.708	999666	20.0
(DEL) Alkane: S...	21.367	5.4	ng/ul	267774	5	21.708	999666	20.0