LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061845.D
Acq On : 2 Jul 2024 13:43
Operator : MA/JU
Sample : P2963-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A4CS8

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: BG061845.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.458	25	29	34	rVB4	17436	25940	1.36%	0.117%
2	3.605	50	54	56	rBV4	4260	5629	0.30%	0.025%
3	3.728	71	75	81	rBV	39982	72811	3.83%	0.327%
4	3.887	99	102	107	rBV4	16882	28162	1.48%	0.127%
5	3.987	115	119	127	rVB3	26137	45309	2.38%	0.204%
6	4.063	129	132	134	rBV3	4212	4251	0.22%	0.019%
7	4.169	148	150	151	rBV2	4876	4064	0.21%	0.018%
8	4.216	154	158	165	rVB3	13590	23762	1.25%	0.107%
9	4.292	167	171	172	rBV3	3459	4687	0.25%	0.021%
10	4.533	210	212	213	rBV2	4116	3569	0.19%	0.016%
11	4.580	216	220	228	rVB9	5637	13821	0.73%	0.062%
12	4.721	243	244	246	rVV2	5933	5721	0.30%	0.026%
13	4.780	250	254	258	rVV3	19711	30554	1.61%	0.137%
14	4.815	258	260	267	rVB5	7107	12557	0.66%	0.056%
15	5.015	293	294	297	rBV2	3792	3733	0.20%	0.017%
16	5.138	308	315	323	rBV2	75816	124504	6.54%	0.560%
17	5.232	325	331	336	rBV4	8065	16109	0.85%	0.072%
18	6.049	464	470	475	rBV7	6131	12087	0.64%	0.054%
19	6.120	478	482	488	rVB4	17348	23214	1.22%	0.104%
20	6.684	574	578	581	rVB5	2687	4044	0.21%	0.018%
21	6.848	603	606	607	rBV	4074	3947	0.21%	0.018%
22	6.919	617	618	621	rBV2	4634	3748	0.20%	0.017%
23	6.983	625	629	630	rBV3	3515	4277	0.22%	0.019%
24	7.001	630	632	634	rBV2	4198	4000	0.21%	0.018%
25	7.083	644	646	649	rBV3	4343	3878	0.20%	0.017%
26	7.218	661	669	678	rBV	516188	873314	45.88%	3.928%
27	7.383	691	697	707	rVB	330678	524507	27.56%	2.359%
28	7.588	726	732	739	rBV	440496	772543	40.59%	3.474%
29	7.641	739	741	742	rBV	8962	6695	0.35%	0.030%
30	8.058	805	812	818	rBV2	284303	484445	25.45%	2.179%
31	8.111	818	821	827	rVB3	14057	21834	1.15%	0.098%
32	8.299	850	853	856	rBV4	3367	3586	0.19%	0.016%
33	8.617	904	907	909	rBV4	2435	3632	0.19%	0.016%
34	8.763	925	932	943	rVB	561447	956456	50.25%	4.302%
35	8.887	948	953	958	rVB2	23106	41577	2.18%	0.187%
36	9.228	1003	1011	1017	rBV	449225	795544	41.80%	3.578%

LSC Area Percent Report

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Operator : MA/JU
Sample : P2963-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CS8

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	9.375	1032	1036	1040	rVB5	5597	8640	0.45%	0.039%
38	9.610	1072	1076	1080	rBV3	7814	12348	0.65%	0.056%
39	9.692	1088	1090	1093	rVB4	3606	3616	0.19%	0.016%
40	9.774	1097	1104	1111	rBV2	54096	85879	4.51%	0.386%
41	9.944	1126	1133	1141	rVV	395172	713543	37.49%	3.209%
42	10.085	1152	1157	1158	rBV4	5147	7156	0.38%	0.032%
43	10.162	1166	1170	1178	rVB8	7574	17734	0.93%	0.080%
44	10.297	1192	1193	1197	rVB3	5606	4015	0.21%	0.018%
45	10.491	1218	1226	1233	rVB2	583991	1021151	53.65%	4.593%
46	10.708	1260	1263	1266	rBV5	5077	5051	0.27%	0.023%
47	10.873	1284	1291	1297	rBV	413976	710768	37.34%	3.197%
48	11.002	1307	1313	1322	rBV2	132893	257866	13.55%	1.160%
49	11.131	1333	1335	1338	rVB4	2945	3602	0.19%	0.016%
50	11.184	1343	1344	1348	rVB3	3903	3444	0.18%	0.015%
51	11.225	1348	1351	1353	rBV3	4895	4591	0.24%	0.021%
52	11.290	1356	1362	1364	rBV4	7055	12413	0.65%	0.056%
53	11.343	1369	1371	1374	rVV	3203	3495	0.18%	0.016%
54	11.390	1374	1379	1385	rVB5	23829	36384	1.91%	0.164%
55	11.601	1408	1415	1422	rBV	66816	125788	6.61%	0.566%
56	11.760	1440	1442	1445	rBV4	5461	6392	0.34%	0.029%
57	11.877	1458	1462	1467	rVB5	5967	9952	0.52%	0.045%
58	12.171	1510	1512	1514	rBV	5217	4027	0.21%	0.018%
59	12.271	1525	1529	1533	rBV3	12744	19471	1.02%	0.088%
60	12.447	1555	1559	1563	rBV4	10164	17027	0.89%	0.077%
61	12.518	1567	1571	1576	rVB3	10512	17785	0.93%	0.080%
62	12.735	1600	1608	1614	rBV8	8873	16443	0.86%	0.074%
63	12.894	1633	1635	1639	rVB5	5276	6648	0.35%	0.030%
64	12.929	1639	1641	1643	rBV2	6276	6389	0.34%	0.029%
65	13.011	1652	1655	1657	rBV2	4417	4616	0.24%	0.021%
66	13.211	1688	1689	1694	rVB4	6188	7676	0.40%	0.035%
67	13.288	1699	1702	1703	rBV3	5919	6513	0.34%	0.029%
68	13.499	1736	1738	1742	rBV3	16785	20182	1.06%	0.091%
69	13.581	1750	1752	1753	rBV2	6166	4462	0.23%	0.020%
70	13.658	1764	1765	1770	rVB4	5731	6421	0.34%	0.029%
71	13.869	1796	1801	1806	rVB7	10446	21268	1.12%	0.096%
72	13.987	1820	1821	1822	rBV	7296	4486	0.24%	0.020%
73	14.010	1822	1825	1830	rVB5	11740	18660	0.98%	0.084%
74	14.093	1831	1839	1845	rBV	919592	1345618	70.69%	6.052%
75	14.204	1854	1858	1859	rBV4	6176	6123	0.32%	0.028%
76	14.322	1873	1878	1882	rBV6	15401	26944	1.42%	0.121%

LSC Area Percent Report

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Acq On : 2 Jul 2024 13:43
Operator : MA/JU
Sample : P2963-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CS8

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_G\Methods\SFAM-EPA-BG062024.MA.M
Title : SVOA CALIBRATION

77	14.386	1882	1889	1900	rVV	1011122	1590254	83.55%	7.152%
78	14.568	1917	1920	1926	rVB5	15184	23893	1.26%	0.107%
79	14.686	1934	1940	1947	rVB	580132	938012	49.28%	4.219%
80	14.756	1949	1952	1959	rVB8	11536	23575	1.24%	0.106%
81	14.815	1959	1962	1963	rVB3	7019	5726	0.30%	0.026%
82	14.827	1963	1964	1967	rBV3	3754	4769	0.25%	0.021%
83	14.886	1967	1974	1983	rBV	499985	841717	44.22%	3.786%
84	15.038	1996	2000	2003	rBV4	25785	38179	2.01%	0.172%
85	15.085	2005	2008	2013	rVB4	25637	42476	2.23%	0.191%
86	15.520	2080	2082	2086	rVB3	17793	18743	0.98%	0.084%
87	15.679	2103	2109	2115	rBV	1221980	1857203	97.57%	8.353%
88	15.791	2123	2128	2138	rVB	238596	327254	17.19%	1.472%
89	16.143	2186	2188	2190	rBV3	7892	5941	0.31%	0.027%
90	16.384	2226	2229	2231	rBV3	23498	31939	1.68%	0.144%
91	17.171	2361	2363	2367	rBV2	20633	22161	1.16%	0.100%
92	17.436	2402	2408	2412	rBV	702385	1070541	56.24%	4.815%
93	17.477	2412	2415	2419	rVV	189163	257575	13.53%	1.158%
94	17.536	2419	2425	2433	rVB2	1203012	1903438	100.00%	8.561%
95	17.912	2487	2489	2494	rBV3	25124	32518	1.71%	0.146%
96	18.311	2553	2557	2561	rBV2	154539	224793	11.81%	1.011%
97	18.493	2586	2588	2593	rVB4	46165	63335	3.33%	0.285%
98	19.480	2752	2756	2761	rVB	411393	545796	28.67%	2.455%
99	19.815	2808	2813	2817	rBV	1211780	1869353	98.21%	8.407%
100	21.337	3069	3072	3083	rVB2	608003	912644	47.95%	4.105%

Sum of corrected areas: 22234933

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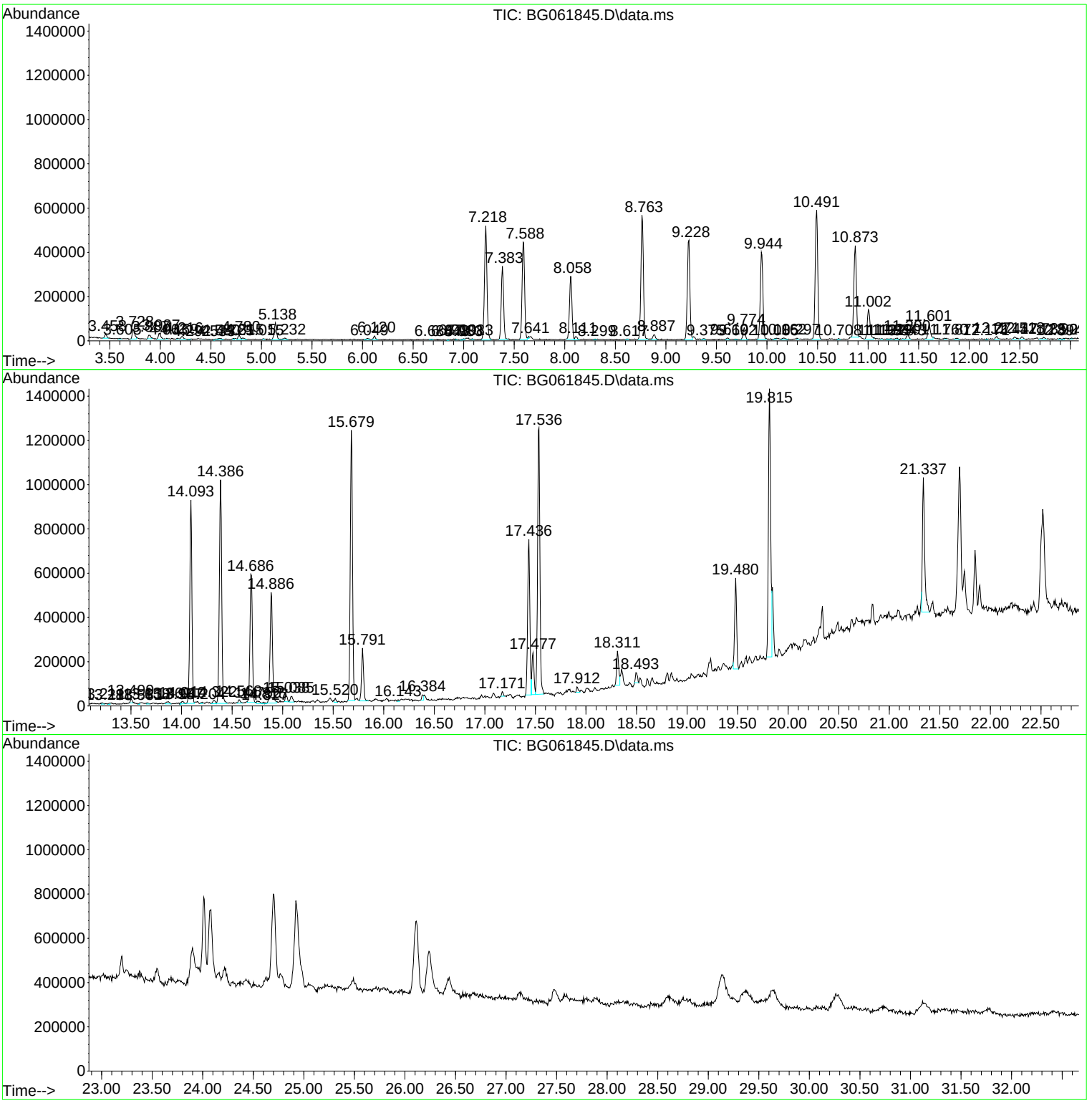
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CS8

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\BG070124\
Data File : BG061845.D
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Sample : P2963-17
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Instrument :
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ClientSampleId :
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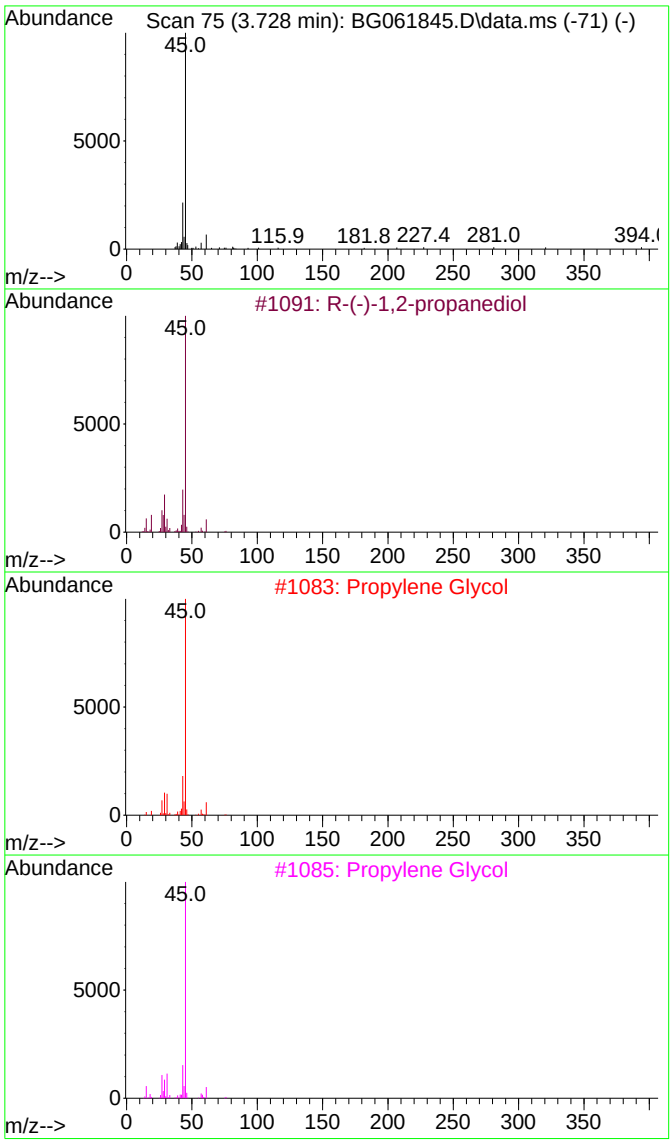
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

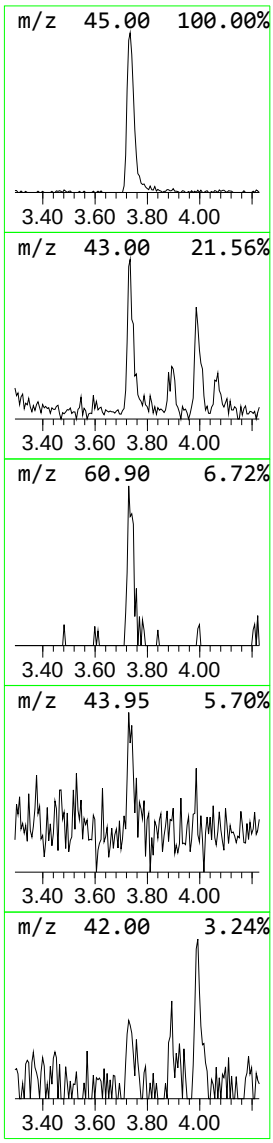
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.728	3.01 ng/ul	72811	1,4-Dichlorobenzene-d4	8.058

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	80
2	Propylene Glycol	76	C3H8O2	000057-55-6	80
3	Propylene Glycol	76	C3H8O2	000057-55-6	72
4	Propylene Glycol	76	C3H8O2	000057-55-6	56
5	2,4-Pentanediol	104	C5H12O2	000625-69-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061845.D
Acq On : 2 Jul 2024 13:43
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Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CS8

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

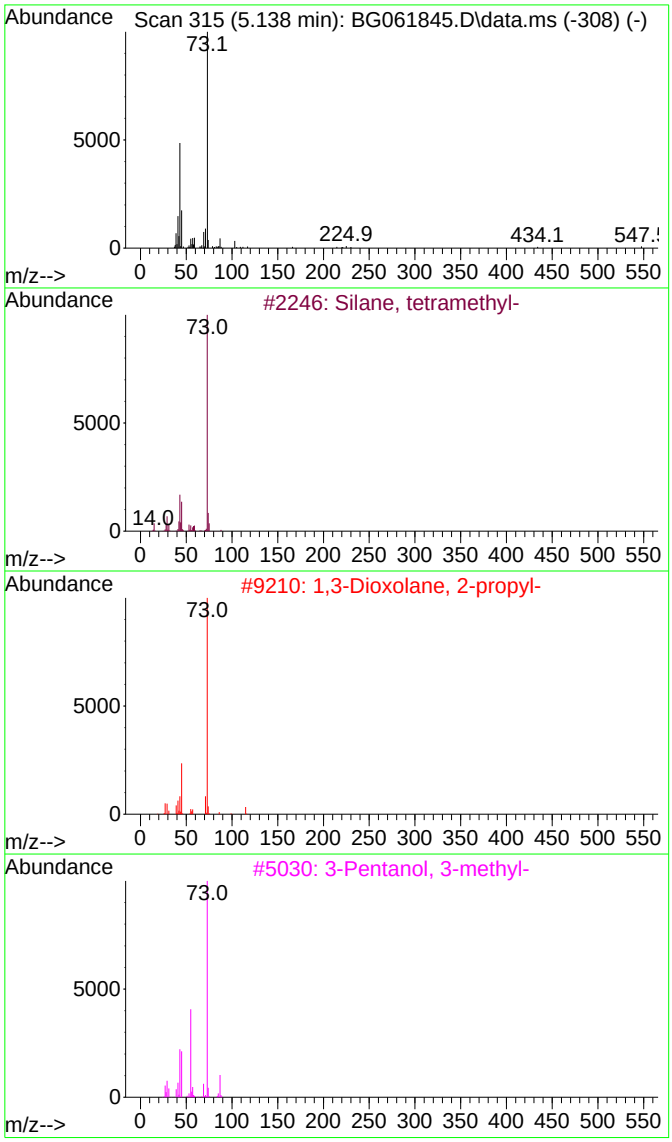
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

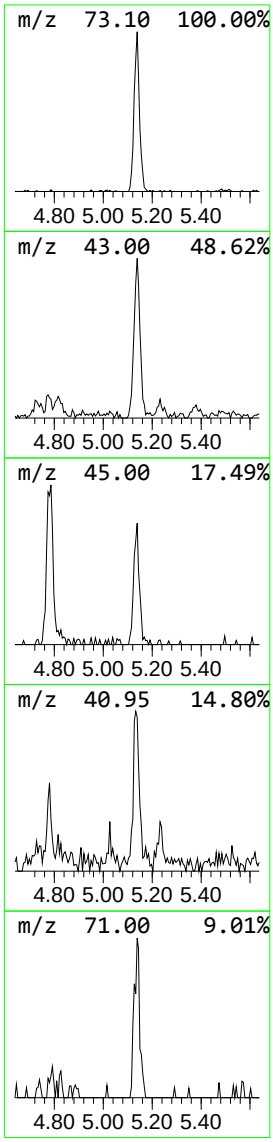
****

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.138	5.14 ng/ul	124504	1,4-Dichlorobenzene-d4	8.058

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
2	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	28
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061845.D
Acq On : 2 Jul 2024 13:43
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ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CS8

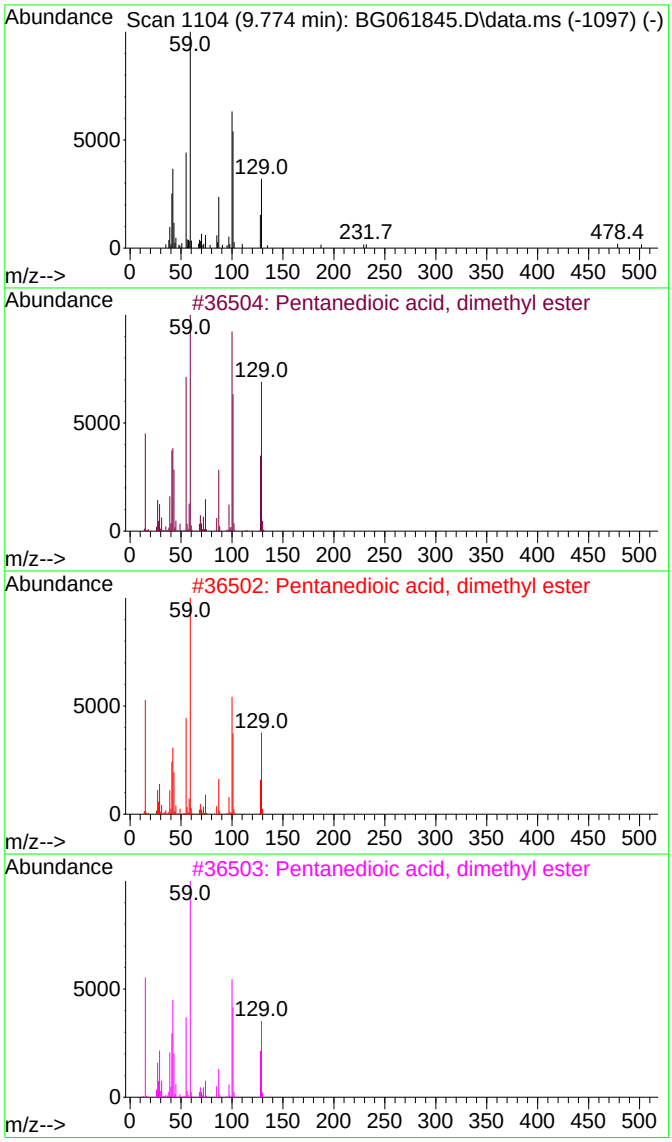
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

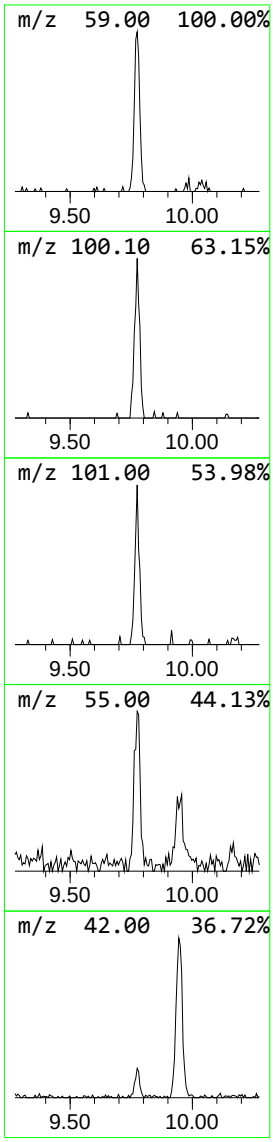
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentanedioic acid, dimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.774	2.42 ng/ul	85879	Naphthalene-d8	10.873

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	74
2	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	74
3	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	56
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	37
5	Hydrazine, (1-methylethyl)-	74	C3H10N2	002257-52-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061845.D
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Operator : MA/JU
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Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
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ClientSampleId :
A4CS8

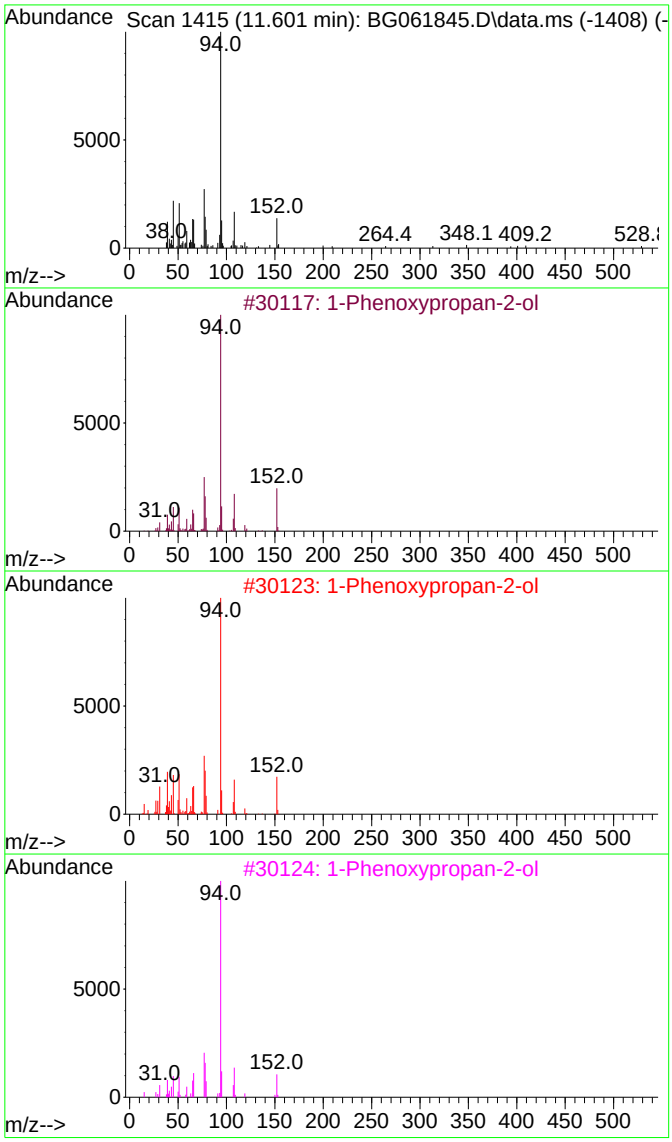
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

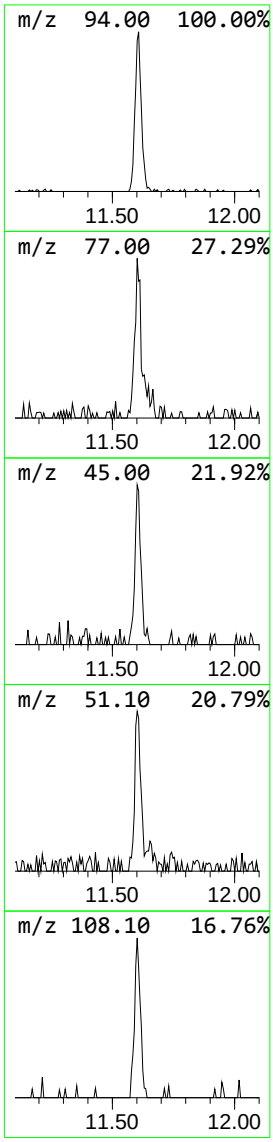
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.601	3.54 ng/ul	125788	Naphthalene-d8	10.873

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	90
4	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061845.D
Acq On : 2 Jul 2024 13:43
Operator : MA/JU
Sample : P2963-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CS8

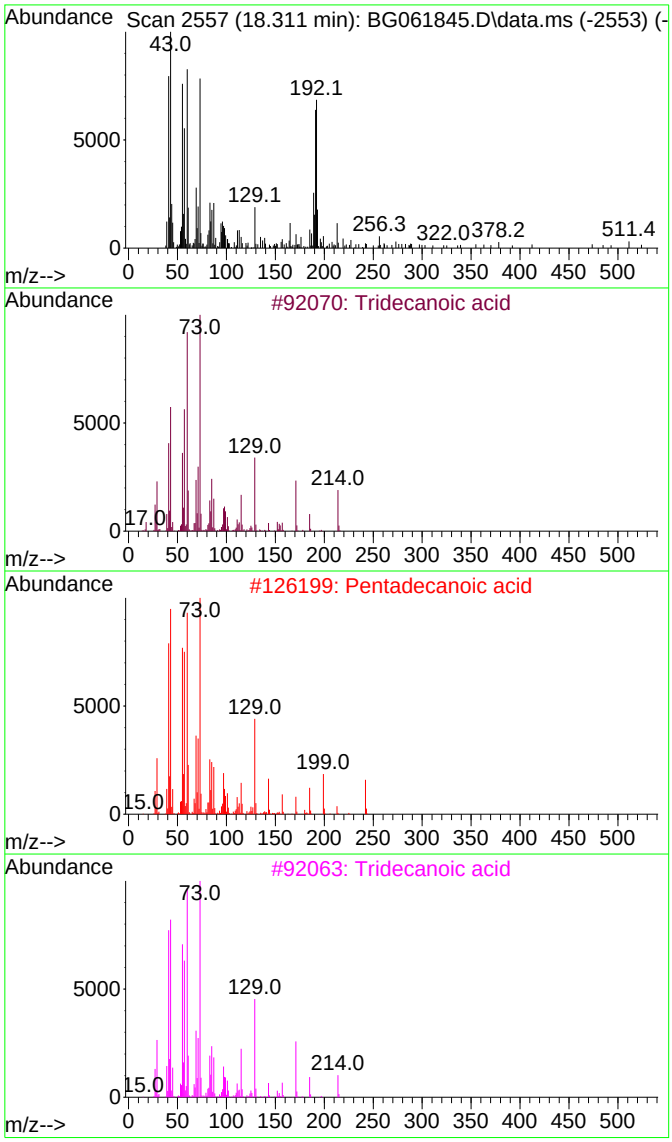
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

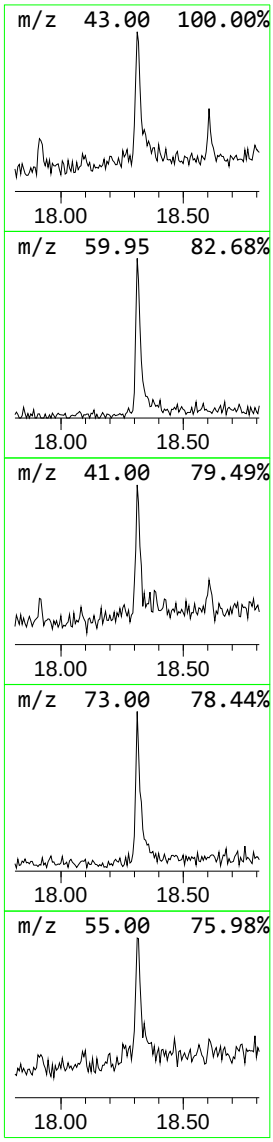
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.311	4.20 ng/ul	224793	Phenanthrene-d10	17.436

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	52
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3	Tridecanoic acid	214	C13H26O2	000638-53-9	52
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	50
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061845.D
Acq On : 2 Jul 2024 13:43
Operator : MA/JU
Sample : P2963-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CS8

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

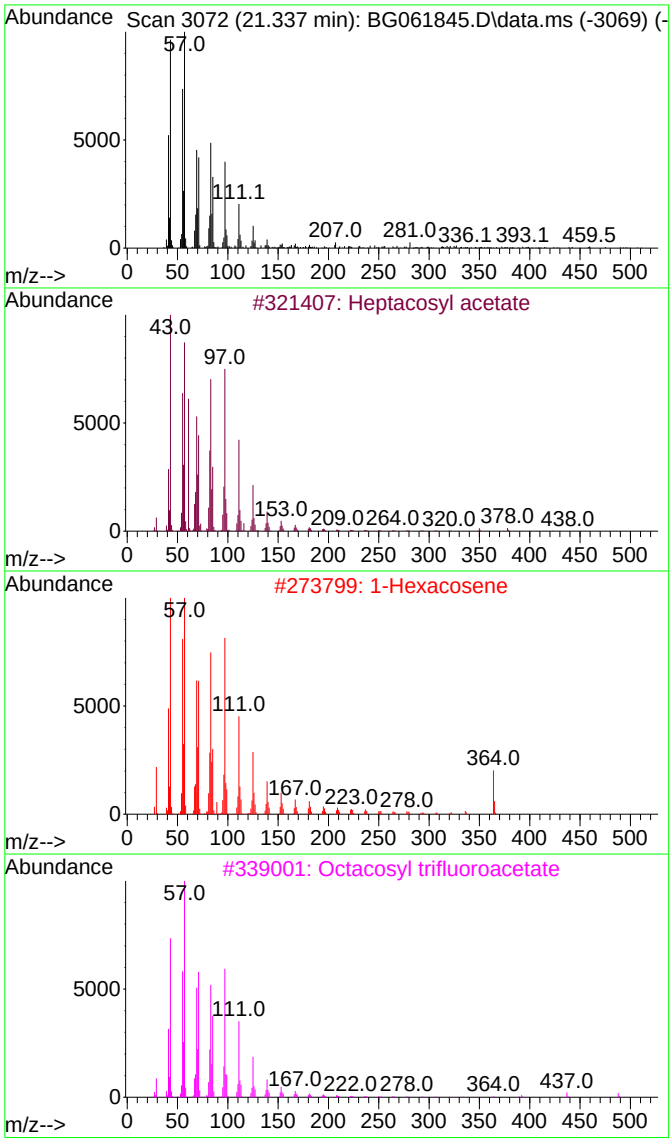
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

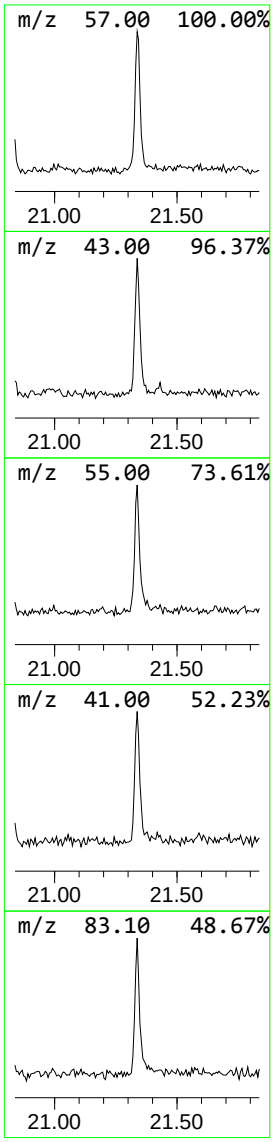
****

Peak Number 6 Heptacosyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.337	20.00 ng/ul	912644	Chrysene-d12	21.695

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl acetate	438	C29H58O2	1000351-78-2	95
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070124\
Data File : BG061845.D
Acq On : 2 Jul 2024 13:43
Operator : MA/JU
Sample : P2963-17
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4CS8

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...	3.728	3.0	ng/ul	72811	1	8.058	484445	20.0
unknown-01	5.138	5.1	ng/ul	124504	1	8.058	484445	20.0
Pentanedioic ac...	9.774	2.4	ng/ul	85879	2	10.873	710768	20.0
1-Phenoxypropan...	11.601	3.5	ng/ul	125788	2	10.873	710768	20.0
Tridecanoic acid	18.311	4.2	ng/ul	224793	4	17.436	1070540	20.0
Heptacosyl acetate	21.337	20.0	ng/ul	912644	5	21.695	912644	20.0