LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

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: BG061618.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.466	26	30	37	rVB3	18329	25333	1.37%	0.138%
2	3.736	72	76	81	rBV	27336	39887	2.16%	0.217%
3	3.901	100	104	108	rBV4	18957	28373	1.54%	0.154%
4	4.001	118	121	124	rBV3	12451	13390	0.73%	0.073%
5	4.077	128	134	138	rBV6	2444	5110	0.28%	0.028%
6	4.224	157	159	165	rVB4	7303	7784	0.42%	0.042%
7	4.600	220	223	228	rVB5	4000	5654	0.31%	0.031%
8	4.741	242	247	251	rBV	8730	10582	0.57%	0.057%
9	4.794	251	256	260	rVB2	15995	24539	1.33%	0.133%
10	5.041	296	298	301	rVV4	3739	4557	0.25%	0.025%
11	5.147	312	316	323	rVB3	28584	43529	2.36%	0.236%
12	5.505	374	377	381	rBV4	3019	3953	0.21%	0.021%
13	6.128	481	483	491	rVB3	6972	10591	0.57%	0.058%
14	6.997	629	631	638	rVV5	4095	8373	0.45%	0.045%
15	7.209	660	667	675	rVV3	236361	423299	22.96%	2.298%
16	7.397	691	699	706	rBV	178984	284083	15.41%	1.542%
17	7.597	726	733	740	rVV	221495	376316	20.41%	2.043%
18	7.661	740	744	751	rVV5	9815	20384	1.11%	0.111%
19	8.073	808	814	820	rVV	185578	305312	16.56%	1.658%
20	8.131	822	824	827	rVB3	6197	5406	0.29%	0.029%
21	8.413	870	872	876	rVB3	3825	3959	0.21%	0.021%
22	8.466	876	881	883	rBV	4044	6089	0.33%	0.033%
23	8.760	923	931	938	rBV	256122	434001	23.54%	2.356%
24	8.901	950	955	961	rVB3	25465	43080	2.34%	0.234%
25	9.066	979	983	987	rVB4	2982	4036	0.22%	0.022%
26	9.165	996	1000	1002	rBV3	3779	4378	0.24%	0.024%
27	9.236	1005	1012	1020	rVV	213174	372329	20.20%	2.021%
28	9.324	1023	1027	1031	rVB4	4027	5991	0.32%	0.033%
29	9.794	1101	1107	1113	rVB4	20668	35341	1.92%	0.192%
30	9.959	1128	1135	1143	rVB2	162607	289333	15.69%	1.571%
31	10.053	1148	1151	1152	rBV2	5725	6483	0.35%	0.035%
32	10.064	1152	1153	1156	rVB2	7068	5247	0.28%	0.028%
33	10.311	1191	1195	1201	rBV3	4480	9348	0.51%	0.051%
34	10.370	1201	1205	1208	rBV2	3222	4888	0.27%	0.027%
35	10.493	1216	1226	1235	rBV	280806	504108	27.34%	2.737%
36	10.581	1239	1241	1244	rVB2	4522	4760	0.26%	0.026%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : A4BP4

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	10.658	1251	1254	1256	rBV2	4104	3989	0.22%	0.022%
38	10.887	1285	1293	1304	rBV	269176	483847	26.24%	2.627%
39	11.010	1309	1314	1322	rVB	144438	273119	14.81%	1.483%
40	11.310	1362	1365	1368	rVB3	3915	5067	0.27%	0.028%
41	11.345	1368	1371	1375	rBV2	2567	4474	0.24%	0.024%
42	11.410	1378	1382	1388	rVV6	13548	23572	1.28%	0.128%
43	11.539	1401	1404	1406	rVB2	3364	3841	0.21%	0.021%
44	11.621	1410	1418	1429	rBV2	43836	93231	5.06%	0.506%
45	11.933	1468	1471	1475	rBV4	3553	4037	0.22%	0.022%
46	12.403	1544	1551	1555	rVV3	7931	17199	0.93%	0.093%
47	12.462	1558	1561	1566	rVV4	9387	12753	0.69%	0.069%
48	12.532	1570	1573	1577	rBV3	4651	6131	0.33%	0.033%
49	12.826	1621	1623	1626	rBV2	3999	4142	0.22%	0.022%
50	13.290	1701	1702	1705	rBV2	5036	4334	0.24%	0.024%
51	13.525	1738	1742	1746	rBV3	2889	4045	0.22%	0.022%
52	13.637	1760	1761	1763	rBV2	4463	4111	0.22%	0.022%
53	13.666	1763	1766	1773	rVV5	9459	16880	0.92%	0.092%
54	13.819	1785	1792	1793	rBV	3562	5876	0.32%	0.032%
55	13.878	1799	1802	1805	rVB3	5792	8720	0.47%	0.047%
56	14.107	1835	1841	1847	rBV	550500	777161	42.15%	4.219%
57	14.336	1877	1880	1884	rVV3	7844	11996	0.65%	0.065%
58	14.395	1884	1890	1898	rVB	591999	933181	50.62%	5.066%
59	14.700	1935	1942	1950	rBV2	451738	706511	38.32%	3.836%
60	14.865	1962	1970	1975	rBV	282472	441742	23.96%	2.398%
61	14.970	1985	1988	1991	rVB4	5470	6902	0.37%	0.037%
62	15.023	1991	1997	2001	rBV5	13784	26560	1.44%	0.144%
63	15.105	2006	2011	2014	rBV6	13469	23696	1.29%	0.129%
64	15.305	2044	2045	2049	rVV2	3222	4032	0.22%	0.022%
65	15.552	2083	2087	2089	rBV5	4393	5679	0.31%	0.031%
66	15.593	2093	2094	2098	rVB4	4688	4526	0.25%	0.025%
67	15.687	2102	2110	2116	rBV	798703	1214018	65.85%	6.591%
68	15.746	2116	2120	2122	rVV4	16137	20050	1.09%	0.109%
69	15.787	2122	2127	2134	rVB	209984	313457	17.00%	1.702%
70	15.922	2148	2150	2151	rBV2	5830	5735	0.31%	0.031%
71	16.016	2163	2166	2168	rBV2	3935	5650	0.31%	0.031%
72	16.051	2170	2172	2174	rVV2	5797	4989	0.27%	0.027%
73	16.322	2217	2218	2221	rBV2	4048	4385	0.24%	0.024%
74	16.345	2221	2222	2225	rVV	6530	4136	0.22%	0.022%
75	16.410	2229	2233	2240	rVB7	9766	18350	1.00%	0.100%
76	16.662	2273	2276	2279	rBV5	5945	10238	0.56%	0.056%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

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	16.715	2283	2285	2288	rBV3	6569	8241	0.45%	0.045%
78	17.080	2346	2347	2349	rBV2	6787	4688	0.25%	0.025%
79	17.197	2365	2367	2370	rVB3	7917	9346	0.51%	0.051%
80	17.256	2375	2377	2379	rBV2	6734	5157	0.28%	0.028%
81	17.444	2403	2409	2413	rBV	604415	926054	50.23%	5.028%
82	17.485	2413	2416	2420	rVV	126625	176122	9.55%	0.956%
83	17.538	2420	2425	2437	rVB2	858997	1352423	73.36%	7.343%
84	17.802	2468	2470	2471	rBV2	5453	4580	0.25%	0.025%
85	18.026	2504	2508	2509	rBV4	8349	8757	0.47%	0.048%
86	18.196	2535	2537	2538	rBV2	9954	8355	0.45%	0.045%
87	18.331	2555	2560	2570	rBV4	234962	402716	21.84%	2.186%
88	18.513	2586	2591	2594	rBV4	27658	50141	2.72%	0.272%
89	18.748	2627	2631	2636	rBV7	16783	30910	1.68%	0.168%
90	18.813	2639	2642	2644	rVV2	19514	21957	1.19%	0.119%
91	19.218	2708	2711	2716	rVB5	36587	52847	2.87%	0.287%
92	19.489	2752	2757	2765	rVB	371404	539224	29.25%	2.928%
93	19.606	2773	2777	2784	rVB3	99045	138035	7.49%	0.749%
94	19.823	2808	2814	2827	rBV2	999780	1843659	100.00%	10.010%
95	21.369	3073	3077	3083	rBV3	210903	298413	16.19%	1.620%
96	21.616	3116	3119	3124	rVB	95717	132872	7.21%	0.721%
97	21.704	3127	3134	3139	rBV3	614032	1208203	65.53%	6.560%
98	23.907	3502	3509	3518	rBV2	137960	472661	25.64%	2.566%
99	24.706	3638	3645	3654	rBV2	351524	895379	48.57%	4.861%
100	24.935	3677	3684	3693	rVB3	347128	925774	50.21%	5.026%

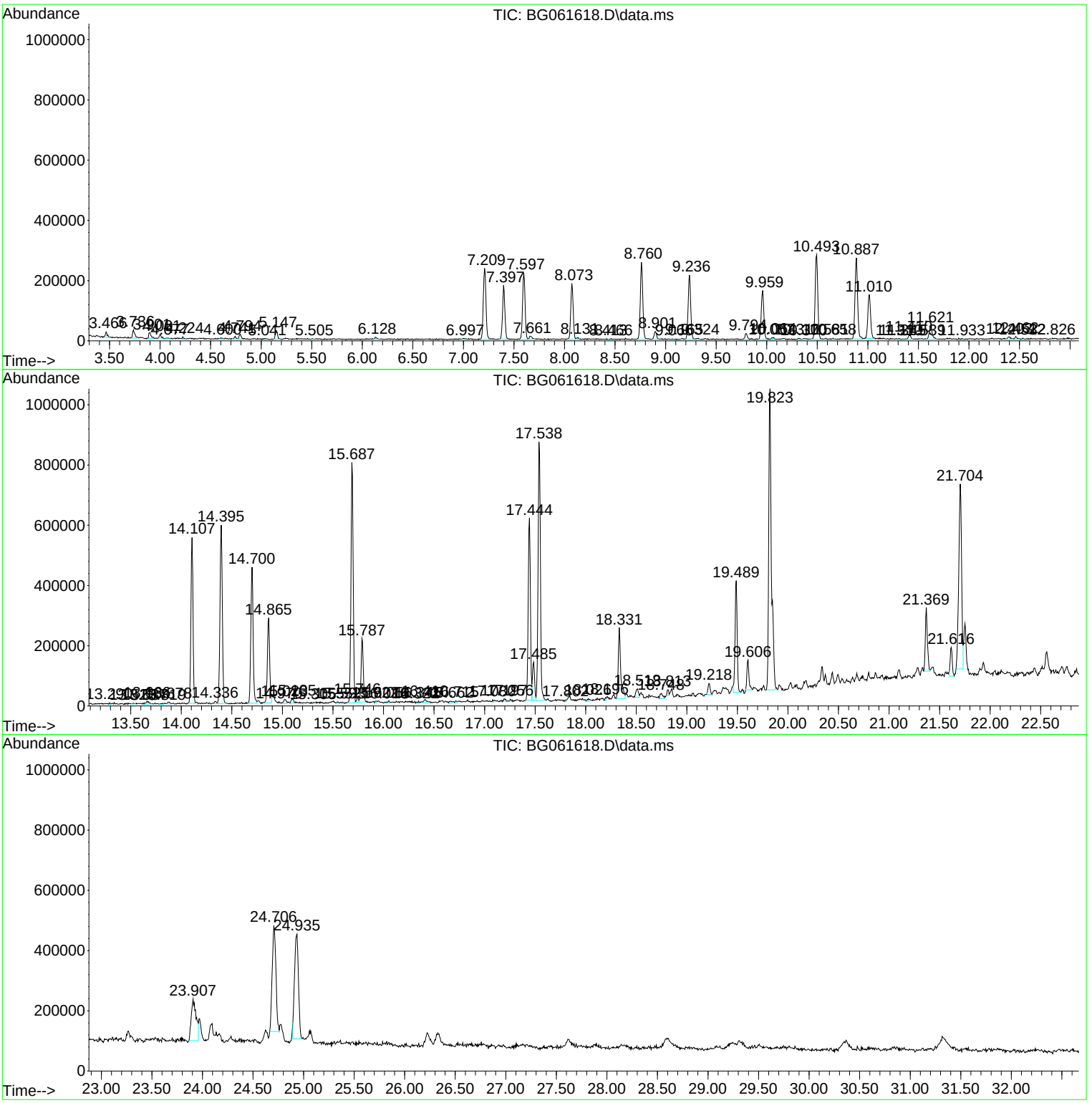
Sum of corrected areas: 18418702

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

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 : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

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

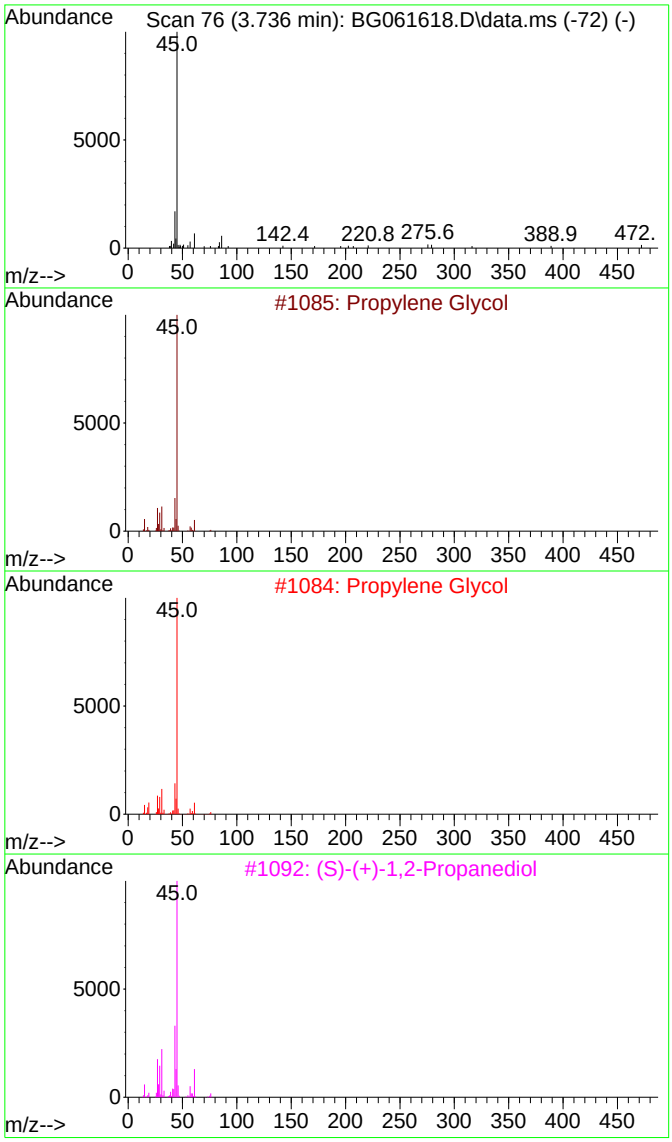
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

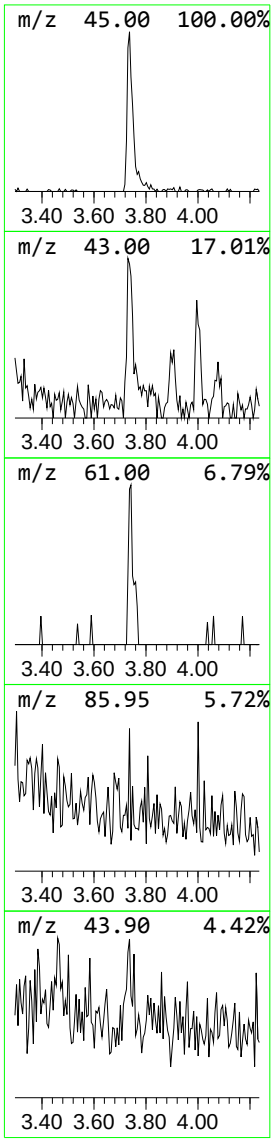
****

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.736	2.61 ng/ul	39887	1,4-Dichlorobenzene-d4	8.073

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

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

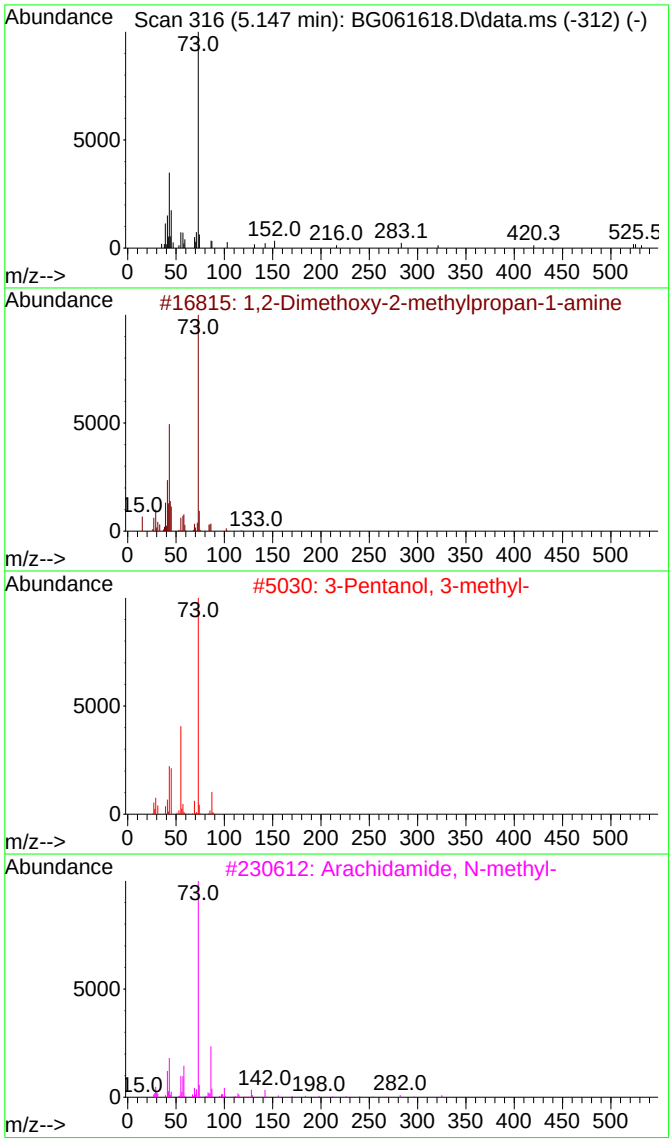
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

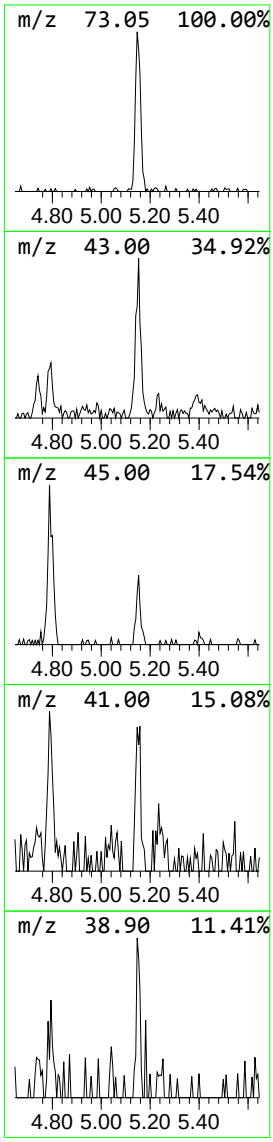
****

Peak Number 2 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.147	2.85 ng/ul	43529	1,4-Dichlorobenzene-d4	8.073

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dimethoxy-2-methylpropan-1-a...	133	C6H15NO2	1000445-17-2	23
2	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	12
3	Arachidamide, N-methyl-	325	C21H43NO	1000420-44-0	12
4	2-Methylbutane-1,4-diol, 3-(1-et...	192	C9H20O4	088481-54-3	12
5	Tripropylene glycol monomethyl e...	320	C16H36O4Si	1000367-06-9	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

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

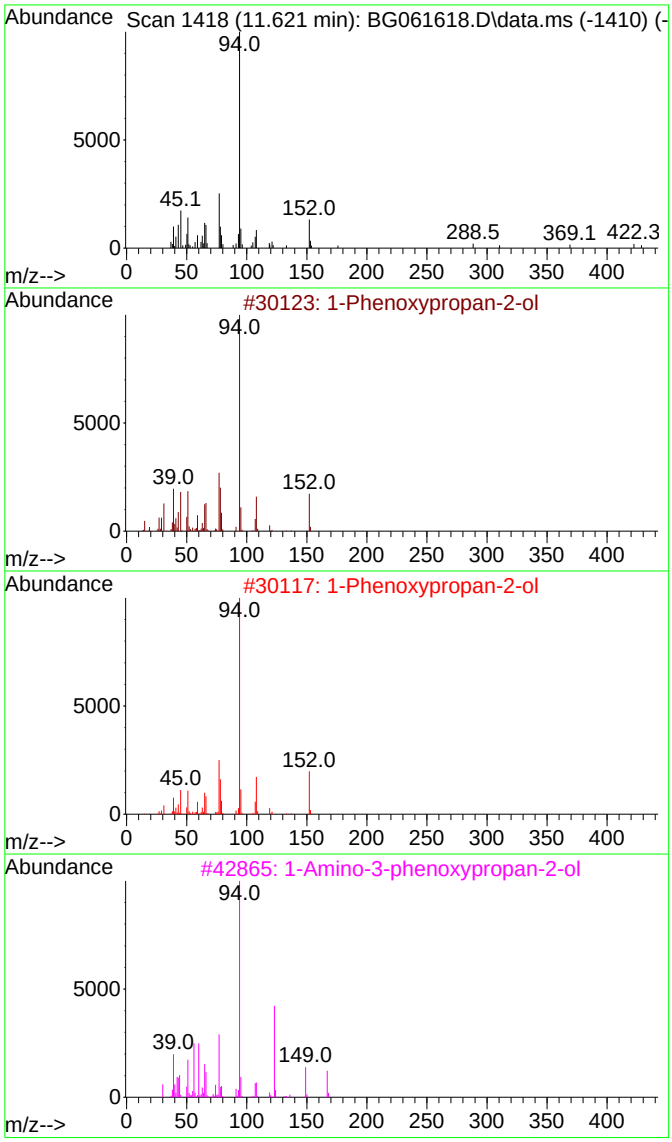
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

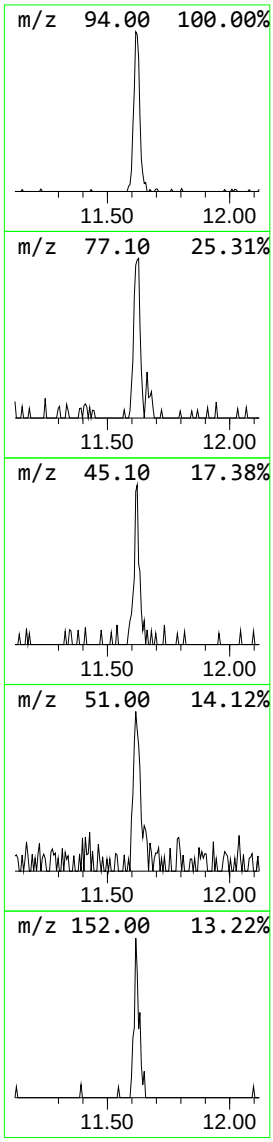
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.621	3.85 ng/ul	93231	Naphthalene-d8	10.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	90
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
3	1-Amino-3-phenoxypropan-2-ol	167	C9H13NO2	004287-19-8	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5	Pentanenitrile, 5-phenoxy-	175	C11H13NO	016728-56-6	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

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

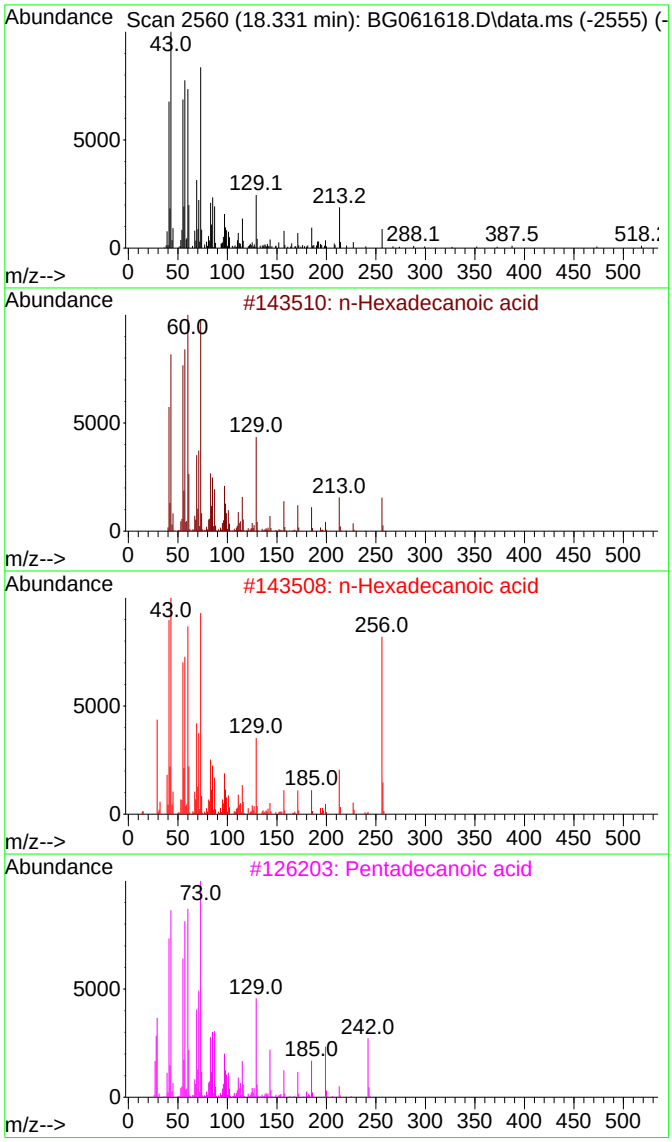
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

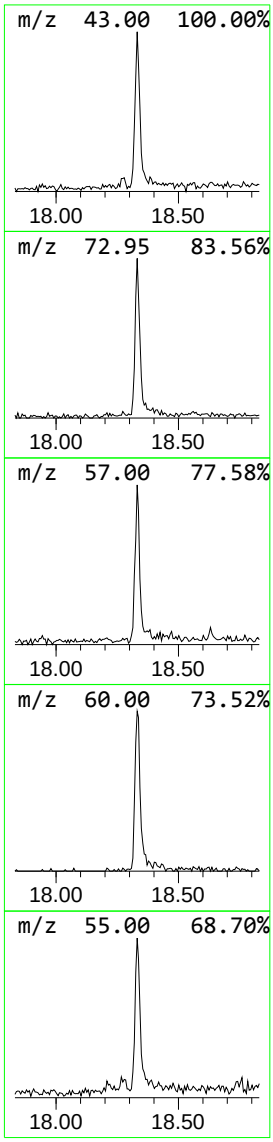
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.331	8.70 ng/ul	402716	Phenanthrene-d10	17.444

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

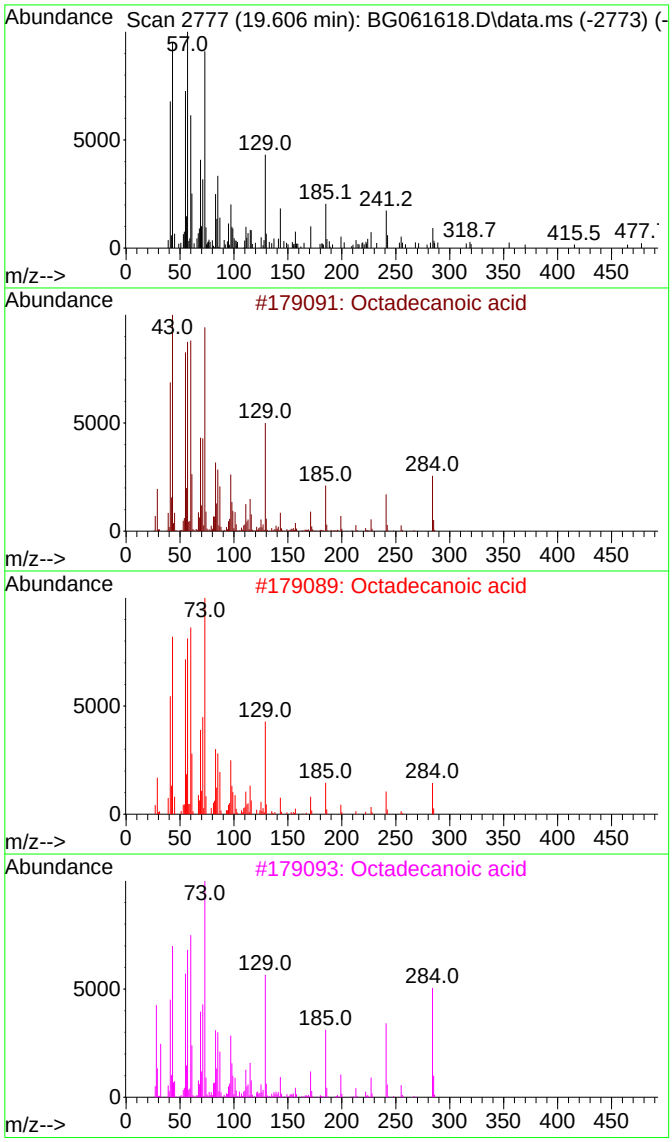
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

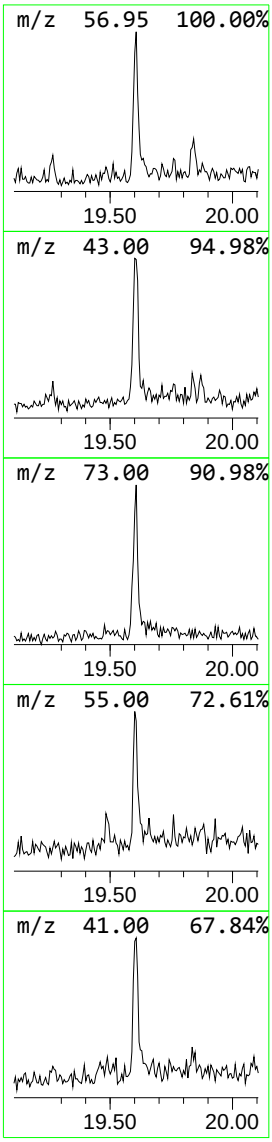
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.606	2.28 ng/ul	138035	Chrysene-d12	21.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	97
3	Octadecanoic acid	284	C18H36O2	000057-11-4	97
4	Octadecanoic acid	284	C18H36O2	000057-11-4	94
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

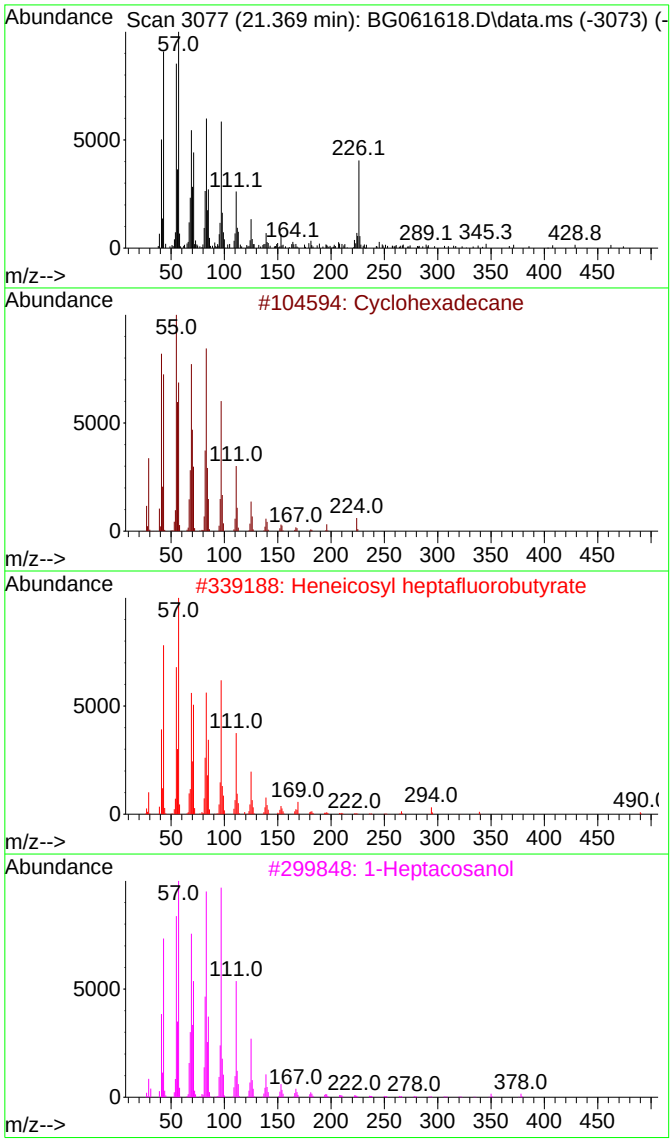
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG062024.MA.M
Quant Title : SVOA CALIBRATION

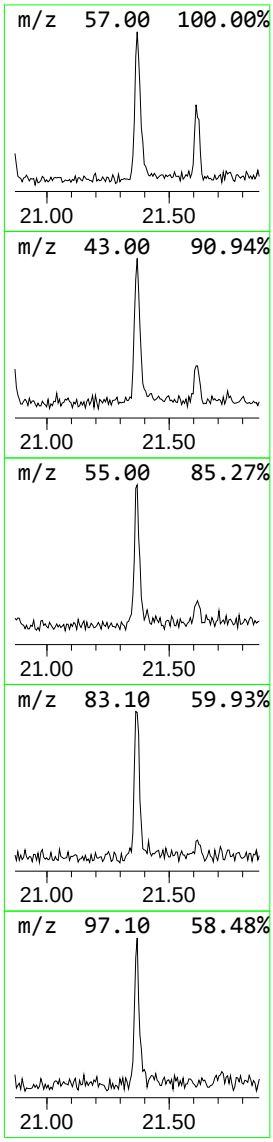
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Cyclic21.369 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.369	4.94 ng/ul	298413	Chrysene-d12	21.704

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	76
3	1-Heptacosanol	396	C27H56O	002004-39-9	76
4	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	76
5	Cyclotetracosane	336	C24H48	000297-03-0	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062124\
Data File : BG061618.D
Acq On : 21 Jun 2024 13:26
Operator : MA/JU
Sample : P2754-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
A4BP4

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
unknown-01	3.736	2.6	ng/ul	39887	1	8.073	305312	20.0
unknown-02	5.147	2.9	ng/ul	43529	1	8.073	305312	20.0
1-Phenoxypropan...	11.621	3.9	ng/ul	93231	2	10.887	483847	20.0
n-Hexadecanoic ...	18.331	8.7	ng/ul	402716	4	17.444	926054	20.0
Octadecanoic acid	19.606	2.3	ng/ul	138035	5	21.704	1208200	20.0
(DEL) Alkane: C...	21.369	4.9	ng/ul	298413	5	21.704	1208200	20.0