LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062455.D
Acq On : 16 Aug 2024 23:09
Operator : MA/JU
Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : E0CL1

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-BG081424.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG062455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.423	19	23	28	rVB2	12882	18839	0.75%	0.082%
2	3.682	63	67	77	rVB	23715	40501	1.60%	0.177%
3	3.829	87	92	102	rBV	72683	112468	4.45%	0.491%
4	4.163	146	149	153	rVB4	3775	4705	0.19%	0.021%
5	4.622	222	227	234	rVB5	3214	6292	0.25%	0.027%
6	4.692	234	239	245	rVB5	13135	22306	0.88%	0.097%
7	4.957	281	284	289	rBV6	3491	4752	0.19%	0.021%
8	5.068	297	303	310	rBV3	4039	6595	0.26%	0.029%
9	6.002	458	462	465	rBV2	2388	3157	0.12%	0.014%
10	6.037	465	468	475	rVB2	5933	9962	0.39%	0.044%
11	6.220	494	499	506	rVB4	7969	14321	0.57%	0.063%
12	7.112	645	651	660	rBV	87209	149433	5.92%	0.653%
13	7.283	672	680	690	rBV	200422	329813	13.06%	1.441%
14	7.488	708	715	722	rBV	244854	409650	16.22%	1.790%
15	7.547	722	725	731	rVB	13492	20966	0.83%	0.092%
16	7.958	788	795	802	rBV	235435	402806	15.95%	1.760%
17	8.017	802	805	810	rVB4	4551	6974	0.28%	0.030%
18	8.328	853	858	860	rBV4	2356	3463	0.14%	0.015%
19	8.652	905	913	922	rBV	238490	406036	16.08%	1.774%
20	8.728	922	926	930	rVB4	2003	3250	0.13%	0.014%
21	9.110	983	991	999	rBV	261839	460621	18.24%	2.012%
22	9.280	1015	1020	1023	rVB3	1843	2572	0.10%	0.011%
23	9.556	1063	1067	1072	rVB3	2831	3989	0.16%	0.017%
24	9.668	1080	1086	1091	rBV	22619	32031	1.27%	0.140%
25	9.832	1106	1114	1122	rBV	221422	394772	15.63%	1.725%
26	10.367	1197	1205	1214	rBV	367785	636986	25.22%	2.783%
27	10.749	1260	1270	1280	rVB	378785	660201	26.14%	2.884%
28	10.878	1285	1292	1303	rVB	205011	385367	15.26%	1.684%
29	11.277	1355	1360	1367	rVB6	8117	13766	0.55%	0.060%
30	11.354	1370	1373	1375	rVV3	2719	3279	0.13%	0.014%
31	11.395	1375	1380	1386	rVB	17444	29743	1.18%	0.130%
32	11.483	1388	1395	1406	rBV	73617	135990	5.38%	0.594%
33	12.223	1520	1521	1527	rVB2	2424	3189	0.13%	0.014%
34	12.329	1534	1539	1544	rVB2	7732	11355	0.45%	0.050%
35	12.940	1639	1643	1649	rBV4	3347	5326	0.21%	0.023%
36	13.004	1649	1654	1661	rVV2	11271	19815	0.78%	0.087%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062455.D
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Operator : MA/JU
Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

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-BG081424.MA.M
Title : SVOA CALIBRATION

37	13.187	1681	1685	1689	rBV4	2736	5265	0.21%	0.023%
38	13.416	1719	1724	1730	rBV6	6162	10271	0.41%	0.045%
39	13.545	1742	1746	1749	rBV4	1838	3105	0.12%	0.014%
40	13.592	1749	1754	1759	rVV7	4461	7397	0.29%	0.032%
41	13.762	1779	1783	1787	rBV5	2652	3699	0.15%	0.016%
42	13.980	1814	1820	1826	rBV	724686	1011382	40.04%	4.418%
43	14.056	1828	1833	1838	rVV3	2654	5403	0.21%	0.024%
44	14.109	1839	1842	1847	rVB4	4605	7313	0.29%	0.032%
45	14.220	1856	1861	1863	rBV3	15172	22118	0.88%	0.097%
46	14.267	1863	1869	1877	rVB2	790155	1259213	49.86%	5.501%
47	14.485	1902	1906	1910	rVB5	2417	3202	0.13%	0.014%
48	14.573	1913	1921	1929	rVB	647200	1038728	41.13%	4.538%
49	14.755	1946	1952	1958	rBV	103977	177101	7.01%	0.774%
50	14.896	1971	1976	1977	rBV3	2197	2594	0.10%	0.011%
51	14.984	1987	1991	1996	rBV6	6065	9971	0.39%	0.044%
52	15.149	2015	2019	2020	rBV4	2233	2895	0.11%	0.013%
53	15.313	2041	2047	2051	rBV6	5510	10758	0.43%	0.047%
54	15.366	2051	2056	2061	rVV7	7741	16900	0.67%	0.074%
55	15.425	2064	2066	2071	rVV6	4804	7371	0.29%	0.032%
56	15.472	2071	2074	2077	rVB4	3150	4222	0.17%	0.018%
57	15.566	2083	2090	2099	rVB	1129080	1632165	64.62%	7.130%
58	15.671	2102	2108	2115	rBV	334836	480564	19.03%	2.099%
59	15.801	2128	2130	2133	rBV4	4739	4987	0.20%	0.022%
60	15.930	2151	2152	2159	rVB7	4192	6548	0.26%	0.029%
61	16.112	2179	2183	2185	rBV3	4412	6637	0.26%	0.029%
62	16.224	2200	2202	2203	rVV2	4336	3415	0.14%	0.015%
63	16.241	2203	2205	2209	rVB5	4970	7294	0.29%	0.032%
64	16.288	2209	2213	2216	rBV5	7403	10425	0.41%	0.046%
65	16.318	2216	2218	2221	rVB3	6696	6030	0.24%	0.026%
66	16.535	2252	2255	2257	rBV3	3465	3479	0.14%	0.015%
67	16.576	2259	2262	2264	rBV4	2225	2543	0.10%	0.011%
68	16.717	2283	2286	2291	rVB6	7544	8090	0.32%	0.035%
69	16.758	2291	2293	2296	rBV4	4026	3475	0.14%	0.015%
70	16.799	2298	2300	2308	rVB9	10486	19128	0.76%	0.084%
71	16.870	2308	2312	2316	rBV6	10290	18787	0.74%	0.082%
72	17.034	2338	2340	2342	rBV3	3833	2893	0.11%	0.013%
73	17.075	2345	2347	2351	rVV4	4255	5040	0.20%	0.022%
74	17.316	2381	2388	2396	rVB	823131	1219810	48.30%	5.329%
75	17.410	2398	2404	2411	rBV	1174893	1776804	70.35%	7.762%
76	17.487	2414	2417	2419	rBV4	4493	4509	0.18%	0.020%

LSC Area Percent Report

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Operator : MA/JU
Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

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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Title : SVOA CALIBRATION

77	17.827	2469	2475	2477	rBV7	7689	16693	0.66%	0.073%
78	17.986	2499	2502	2506	rVB4	17670	21046	0.83%	0.092%
79	18.209	2535	2540	2550	rBV	341159	496638	19.66%	2.170%
80	18.867	2650	2652	2656	rBV5	8499	10514	0.42%	0.046%
81	19.267	2716	2720	2723	rBV5	17024	22711	0.90%	0.099%
82	19.331	2727	2731	2734	rBV	31385	49732	1.97%	0.217%
83	19.478	2752	2756	2763	rBV	206210	302946	11.99%	1.323%
84	19.695	2787	2793	2798	rBV	1588079	2525674	100.00%	11.034%
85	20.553	2935	2939	2946	rBV	194975	326573	12.93%	1.427%
86	21.223	3048	3053	3064	rBV2	241793	371726	14.72%	1.624%
87	21.558	3103	3110	3119	rBV	822666	1373783	54.39%	6.002%
88	24.436	3590	3600	3612	rVB	812394	2196106	86.95%	9.594%
89	24.648	3627	3636	3654	rVB	542920	1569565	62.14%	6.857%

Sum of corrected areas: 22890529

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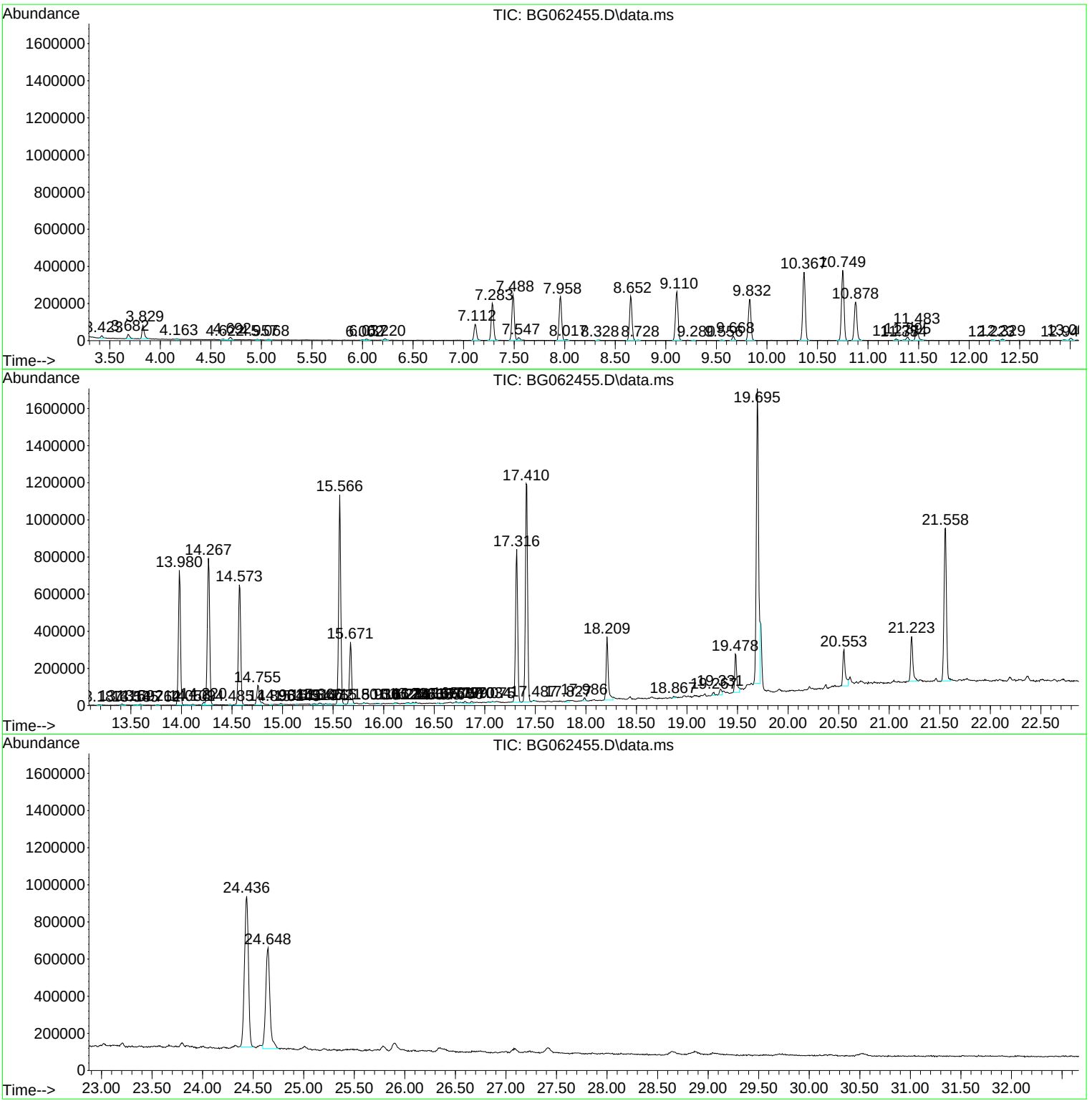
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.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\BG081524\
Data File : BG062455.D
Acq On : 16 Aug 2024 23:09
Operator : MA/JU
Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

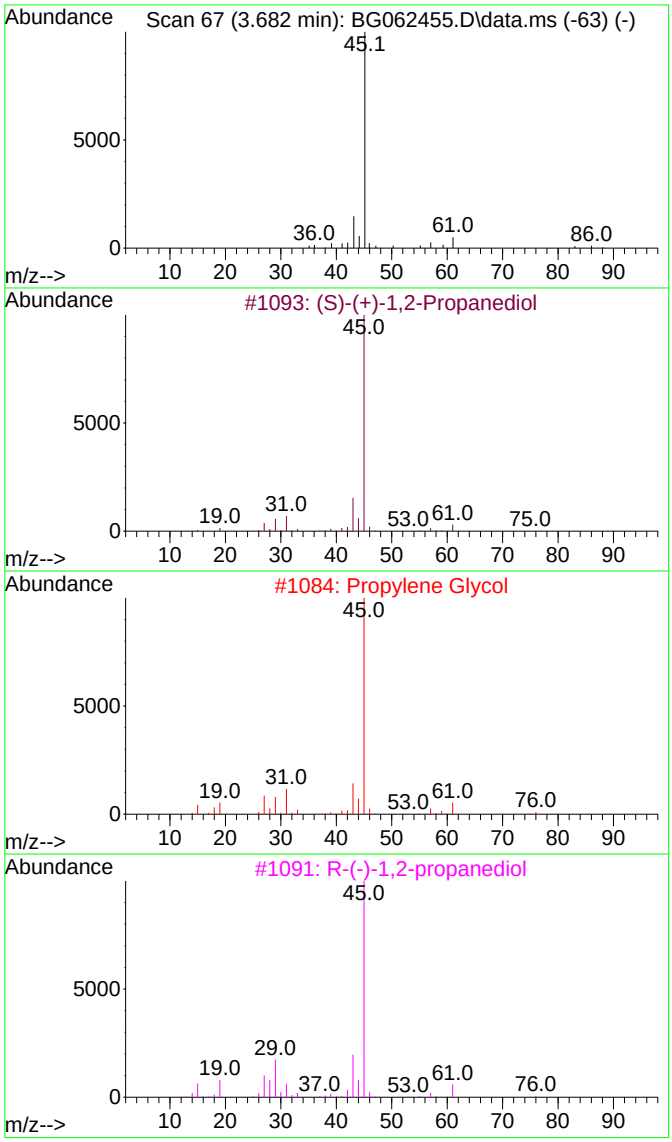
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

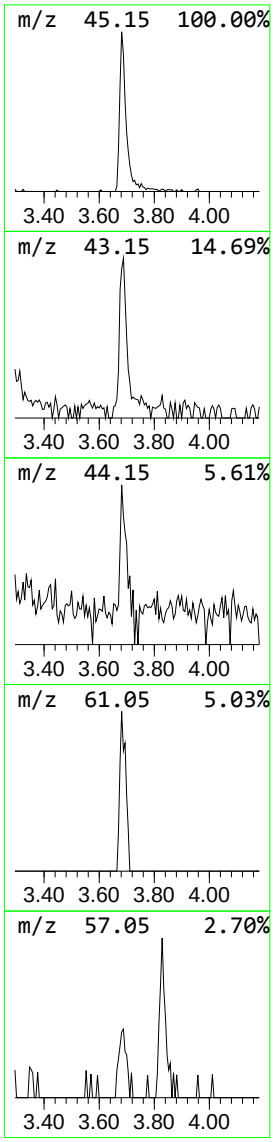
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.682	2.01 ng/ul	40501	1,4-Dichlorobenzene-d4	7.958

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
2	Propylene Glycol	76	C3H8O2	000057-55-6	43
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
4	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
5	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062455.D
Acq On : 16 Aug 2024 23:09
Operator : MA/JU
Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

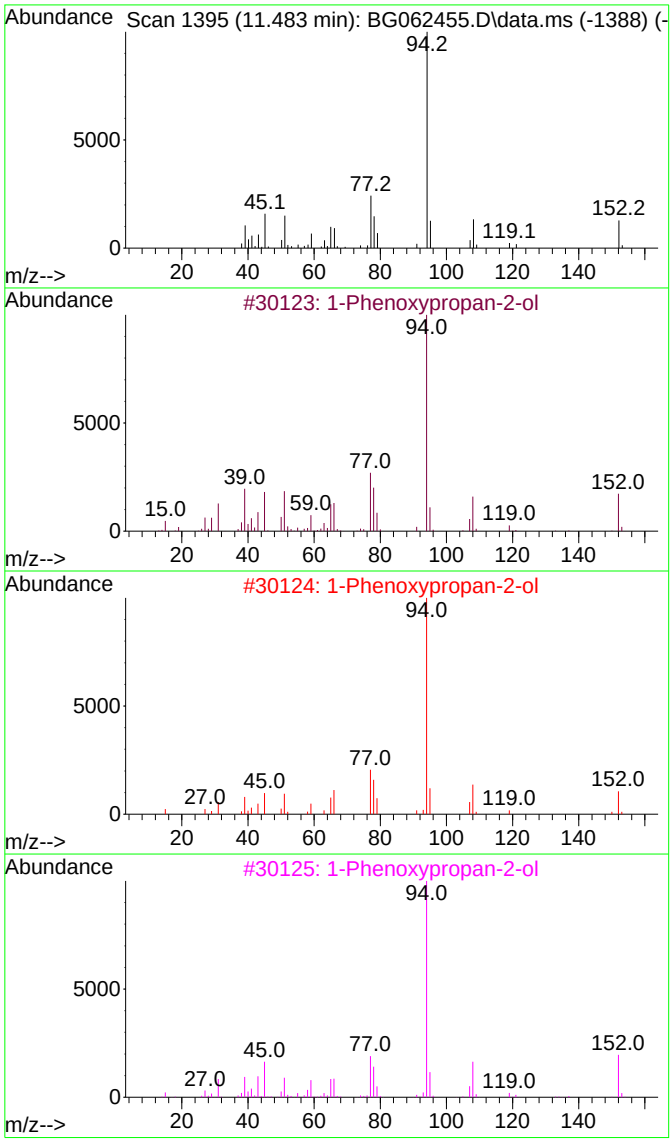
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

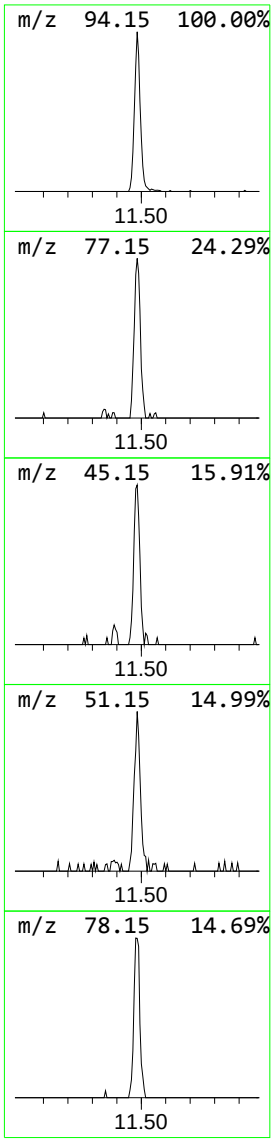
****

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.483	4.12 ng/ul	135990	Naphthalene-d8	10.749

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
4	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062455.D
Acq On : 16 Aug 2024 23:09
Operator : MA/JU
Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

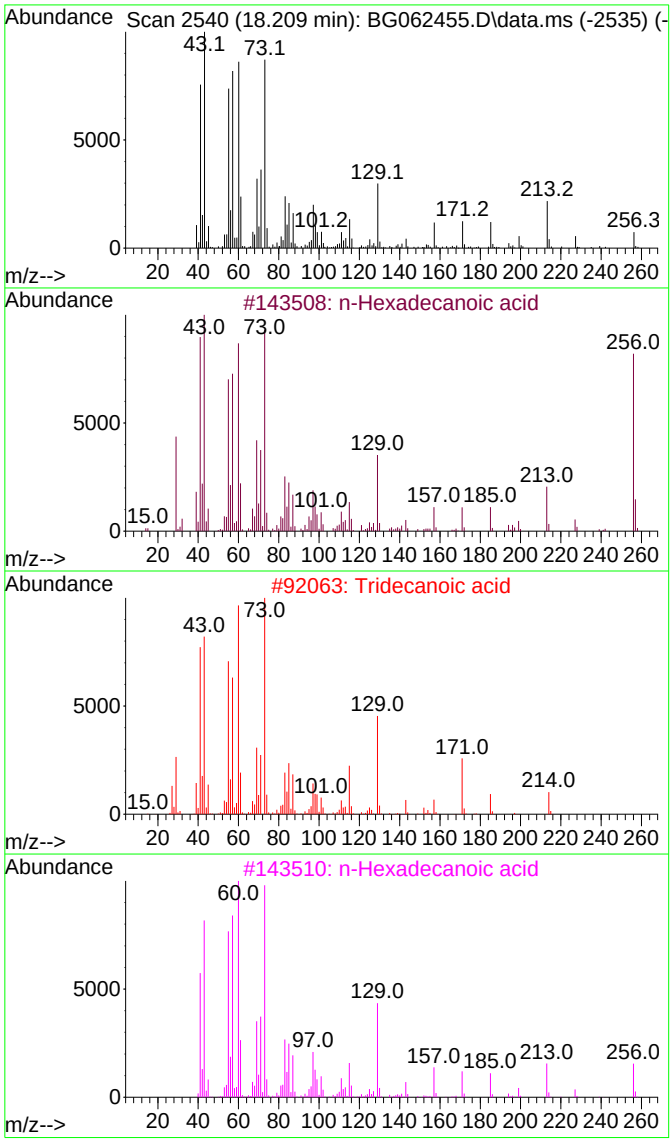
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

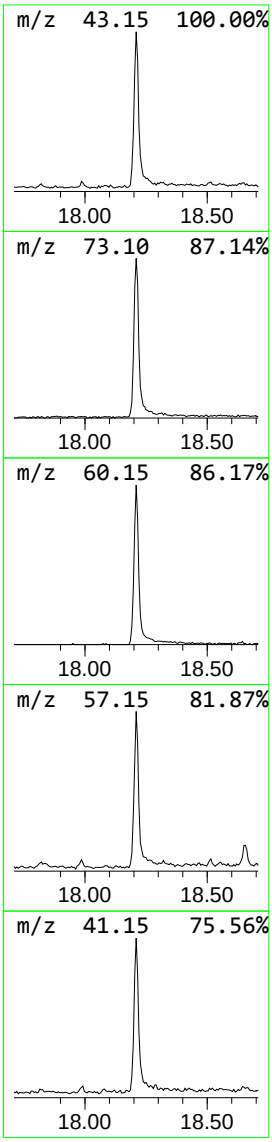
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	8.14 ng/ul	496638	Phenanthrene-d10	17.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87





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Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

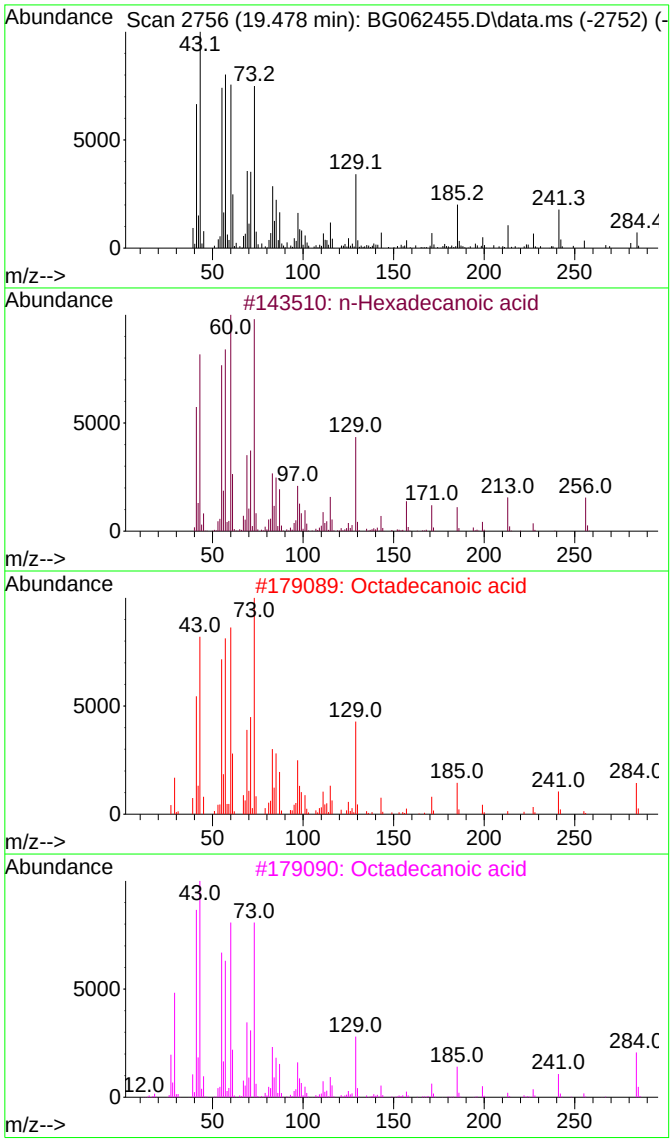
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

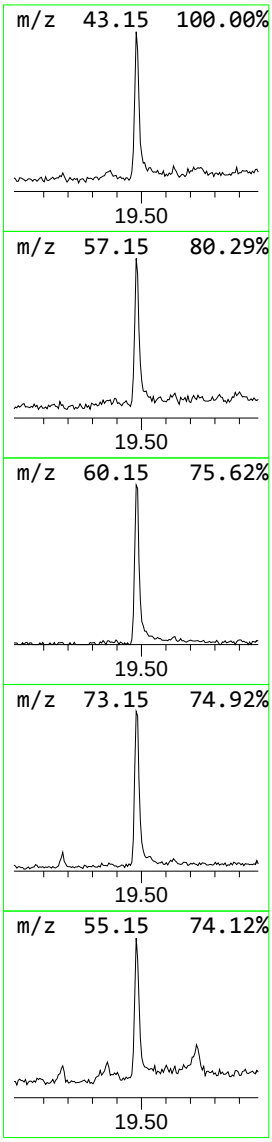
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.478	4.41 ng/ul	302946	Chrysene-d12	21.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	Octadecanoic acid	284	C18H36O2	000057-11-4	83
3	Octadecanoic acid	284	C18H36O2	000057-11-4	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062455.D
Acq On : 16 Aug 2024 23:09
Operator : MA/JU
Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

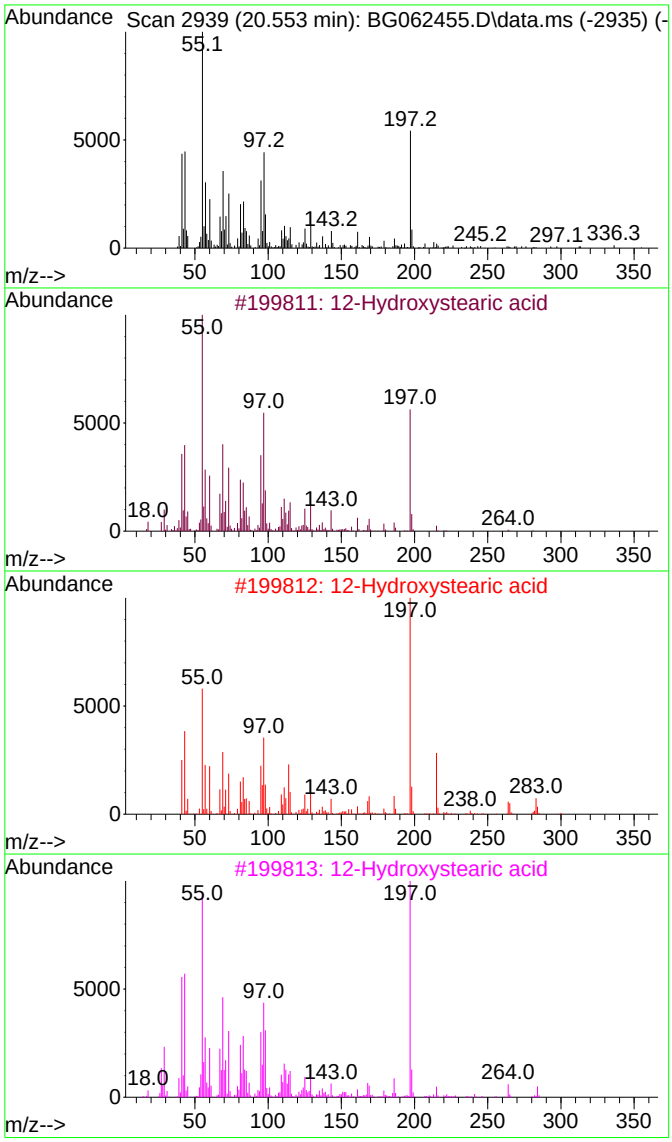
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

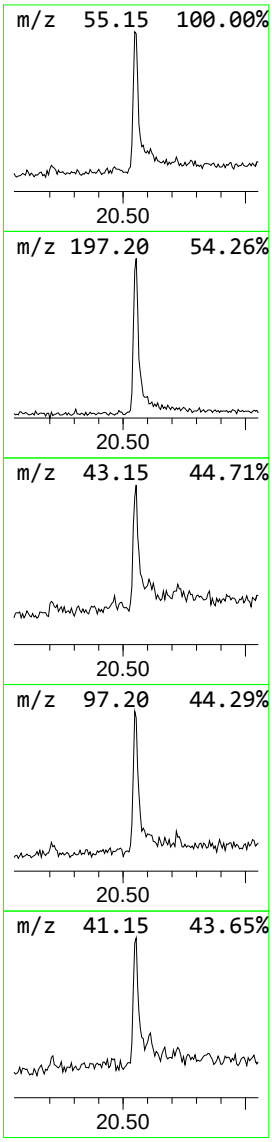
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 12-Hydroxystearic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.553	4.75 ng/ul	326573	Chrysene-d12	21.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	90
2	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	83
3	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	35
4	5-Methoxy-1,3-benzothiazol-2-yl ...	197	C8H7NOS2	1000476-84-0	22
5	Oleic Acid	282	C18H34O2	000112-80-1	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062455.D
Acq On : 16 Aug 2024 23:09
Operator : MA/JU
Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

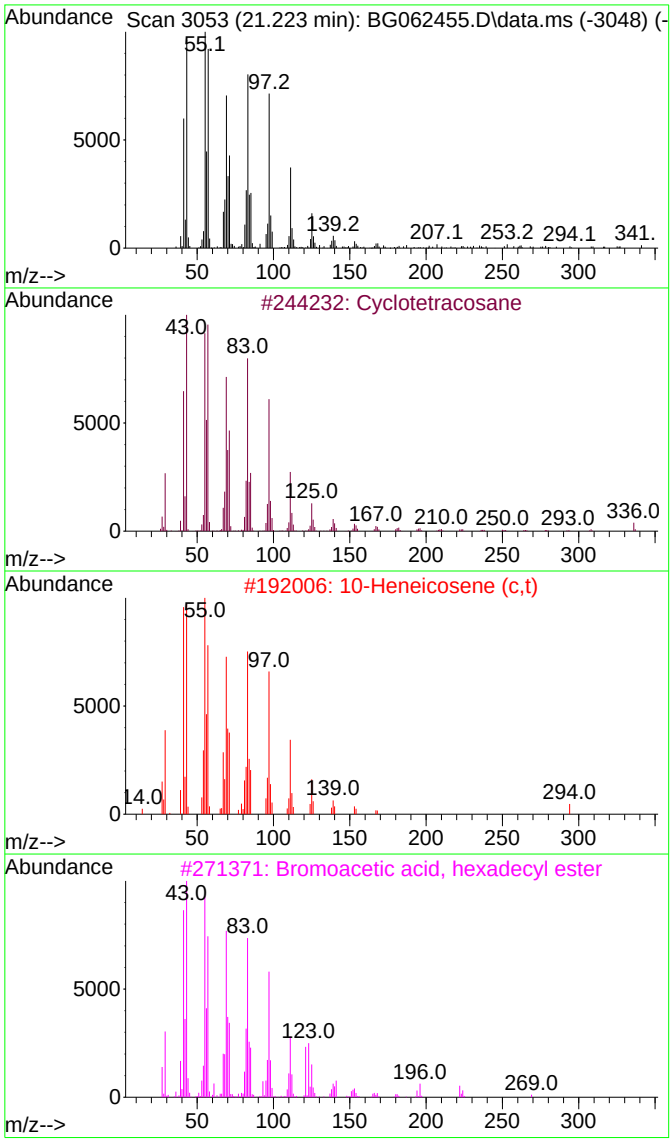
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.MA.M
Quant Title : SVOA CALIBRATION

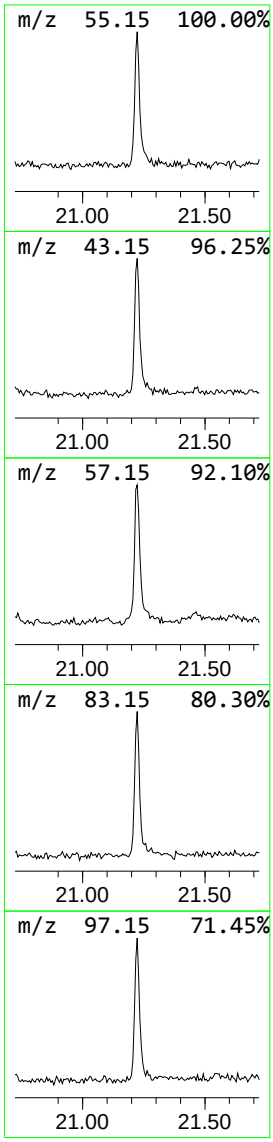
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Cyclic21.223 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.223	5.41 ng/ul	371726	Chrysene-d12	21.558

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	94
2	10-Heneicosene (c,t)	294	C21H42	095008-11-0	94
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
4	1-Docosene	308	C22H44	001599-67-3	91
5	Octacosanol	410	C28H58O	000557-61-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081524\
Data File : BG062455.D
Acq On : 16 Aug 2024 23:09
Operator : MA/JU
Sample : P3603-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E0CL1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG081424.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
(S)-(+)-1,2-Pro...	3.682	2.0	ng/ul	40501	1	7.958	402806	20.0
1-Phenoxypropan...	11.483	4.1	ng/ul	135990	2	10.749	660201	20.0
n-Hexadecanoic ...	18.209	8.1	ng/ul	496638	4	17.316	1219810	20.0
Octadecanoic acid	19.478	4.4	ng/ul	302946	5	21.558	1373780	20.0
12-Hydroxystear...	20.553	4.8	ng/ul	326573	5	21.558	1373780	20.0
(DEL) Alkane: C...	21.223	5.4	ng/ul	371726	5	21.558	1373780	20.0