LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : F7E33

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-BG080524.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG062289.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.425	19	23	29	rVB2	13885	20844	0.89%	0.091%
2	3.683	62	67	78	rBV	58909	97675	4.19%	0.424%
3	3.824	87	91	113	rVB	202067	341073	14.62%	1.482%
4	4.159	146	148	153	rVB4	2181	3084	0.13%	0.013%
5	5.075	300	304	311	rBV5	4893	8274	0.35%	0.036%
6	6.045	464	469	478	rVB2	8120	14080	0.60%	0.061%
7	7.114	643	651	661	rBV	319838	547055	23.45%	2.377%
8	7.290	674	681	689	rBV	223183	360745	15.46%	1.568%
9	7.490	708	715	722	rBV	283104	474390	20.33%	2.061%
10	7.549	722	725	732	rVV	16993	27329	1.17%	0.119%
11	7.960	788	795	802	rBV	171385	284234	12.18%	1.235%
12	8.024	802	806	812	rVB	6772	10737	0.46%	0.047%
13	8.653	906	913	925	rBV	408626	683980	29.31%	2.972%
14	9.111	983	991	1000	rBV	296550	505788	21.68%	2.198%
15	9.276	1016	1019	1024	rBV2	2106	2585	0.11%	0.011%
16	9.569	1065	1069	1075	rVB3	2194	3377	0.14%	0.015%
17	9.675	1081	1087	1093	rVB2	39188	60154	2.58%	0.261%
18	9.834	1105	1114	1121	rBV	234709	409104	17.53%	1.778%
19	10.368	1196	1205	1219	rBV	423378	728846	31.24%	3.167%
20	10.533	1226	1233	1240	rVB3	2696	4904	0.21%	0.021%
21	10.756	1263	1271	1278	rVB	271447	485174	20.79%	2.108%
22	10.879	1282	1292	1302	rBV	430300	745092	31.93%	3.238%
23	11.285	1357	1361	1366	rBV	16948	25280	1.08%	0.110%
24	11.490	1388	1396	1404	rBV	92544	160005	6.86%	0.695%
25	12.336	1531	1540	1547	rBV3	6245	11680	0.50%	0.051%
26	13.423	1720	1725	1730	rVB3	4101	5876	0.25%	0.026%
27	13.987	1814	1821	1828	rBV	772441	1136648	48.72%	4.939%
28	14.275	1859	1870	1878	rBV	890710	1451729	62.22%	6.308%
29	14.492	1904	1907	1913	rVB3	2841	3709	0.16%	0.016%
30	14.580	1915	1922	1932	rVB	504854	773491	33.15%	3.361%
31	14.751	1943	1951	1956	rBV	358854	565985	24.26%	2.459%
32	14.809	1956	1961	1966	rVB3	55796	114437	4.90%	0.497%
33	14.986	1987	1991	1995	rBV3	7258	9335	0.40%	0.041%
34	15.385	2054	2059	2065	rVB5	4616	7670	0.33%	0.033%
35	15.444	2065	2069	2072	rBV2	3512	4394	0.19%	0.019%
36	15.573	2084	2091	2097	rBV	1237452	1824287	78.19%	7.927%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

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-BG080524.MA.M
Title : SVOA CALIBRATION

37	15.673	2102	2108	2116	rBV	247380	359687	15.42%	1.563%
38	15.737	2116	2119	2124	rVB5	2793	4445	0.19%	0.019%
39	15.808	2128	2131	2136	rVB2	3669	5264	0.23%	0.023%
40	16.125	2180	2185	2190	rVB5	4753	6506	0.28%	0.028%
41	16.307	2210	2216	2219	rBV4	4563	6290	0.27%	0.027%
42	16.343	2219	2222	2227	rVB4	2434	3997	0.17%	0.017%
43	16.730	2283	2288	2292	rBV4	2113	4101	0.18%	0.018%
44	16.889	2310	2315	2319	rBV4	4470	7302	0.31%	0.032%
45	17.000	2330	2334	2337	rVV4	2219	3113	0.13%	0.014%
46	17.047	2339	2342	2347	rVV4	3360	3996	0.17%	0.017%
47	17.100	2347	2351	2354	rVV3	4803	6886	0.30%	0.030%
48	17.141	2354	2358	2364	rVB5	2286	4207	0.18%	0.018%
49	17.318	2381	2388	2396	rBV	611748	905333	38.80%	3.934%
50	17.418	2398	2405	2413	rVV	1302624	1919607	82.27%	8.341%
51	17.500	2415	2419	2424	rVB5	8459	10892	0.47%	0.047%
52	17.841	2473	2477	2479	rBV3	3123	4573	0.20%	0.020%
53	18.005	2500	2505	2510	rVB2	12250	15553	0.67%	0.068%
54	18.222	2536	2542	2552	rBV	168742	261758	11.22%	1.137%
55	18.528	2591	2594	2595	rBV	3251	2778	0.12%	0.012%
56	18.563	2599	2600	2607	rVB5	2436	3247	0.14%	0.014%
57	18.686	2618	2621	2626	rVB5	3880	4749	0.20%	0.021%
58	18.892	2652	2656	2659	rBV4	2427	3583	0.15%	0.016%
59	19.021	2675	2678	2683	rBV3	2880	4039	0.17%	0.018%
60	19.080	2685	2688	2693	rVV5	3892	6384	0.27%	0.028%
61	19.168	2701	2703	2710	rVB3	3692	4364	0.19%	0.019%
62	19.268	2715	2720	2724	rBV2	18689	26032	1.12%	0.113%
63	19.339	2727	2732	2736	rBV	17516	30734	1.32%	0.134%
64	19.374	2736	2738	2744	rVV5	7894	12084	0.52%	0.053%
65	19.491	2754	2758	2767	rBV	51606	85347	3.66%	0.371%
66	19.644	2782	2784	2787	rBV3	5363	5919	0.25%	0.026%
67	19.697	2787	2793	2801	rVV2	1523804	2289609	98.13%	9.949%
68	19.761	2801	2804	2809	rVB2	16391	19060	0.82%	0.083%
69	20.161	2870	2872	2874	rBV3	2066	2592	0.11%	0.011%
70	20.226	2878	2883	2887	rBV6	7597	12068	0.52%	0.052%
71	20.261	2887	2889	2892	rVV4	2728	2563	0.11%	0.011%
72	20.355	2903	2905	2908	rBV3	2122	2400	0.10%	0.010%
73	20.601	2945	2947	2951	rVB4	2715	2421	0.10%	0.011%
74	20.684	2959	2961	2965	rBV5	4520	6589	0.28%	0.029%
75	20.731	2967	2969	2971	rVV3	2852	2500	0.11%	0.011%
76	20.789	2976	2979	2985	rVB4	9281	11966	0.51%	0.052%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

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-BG080524.MA.M
Title : SVOA CALIBRATION

77	21.242	3051	3056	3067	rBV	128874	207604	8.90%	0.902%
78	21.559	3104	3110	3119	rBV2	657533	1023970	43.89%	4.449%
79	21.794	3146	3150	3155	rVB6	9066	14485	0.62%	0.063%
80	22.005	3184	3186	3189	rVB4	3723	2391	0.10%	0.010%
81	22.387	3248	3251	3257	rBV5	12644	22479	0.96%	0.098%
82	22.734	3308	3310	3313	rVB4	4149	3999	0.17%	0.017%
83	23.063	3363	3366	3373	rVB4	12548	20367	0.87%	0.089%
84	23.245	3391	3397	3404	rVB2	22390	38972	1.67%	0.169%
85	23.850	3495	3500	3508	rVB3	20227	37875	1.62%	0.165%
86	24.443	3590	3601	3613	rBV	889233	2333247	100.00%	10.139%
87	24.649	3627	3636	3650	rVV	400685	1077310	46.17%	4.681%
88	24.772	3650	3657	3664	rVB5	23876	61038	2.62%	0.265%
89	25.865	3837	3843	3853	rVB5	22078	63899	2.74%	0.278%
90	25.977	3853	3862	3868	rBV9	11207	40702	1.74%	0.177%
91	27.181	4061	4067	4074	rVB8	18377	47259	2.03%	0.205%
92	28.291	4254	4256	4258	rBV3	3734	2912	0.12%	0.013%
93	28.767	4330	4337	4338	rBV5	12652	21845	0.94%	0.095%
94	30.594	4647	4648	4650	rBV2	4030	2663	0.11%	0.012%
95	31.410	4785	4787	4790	rBV4	2374	2728	0.12%	0.012%

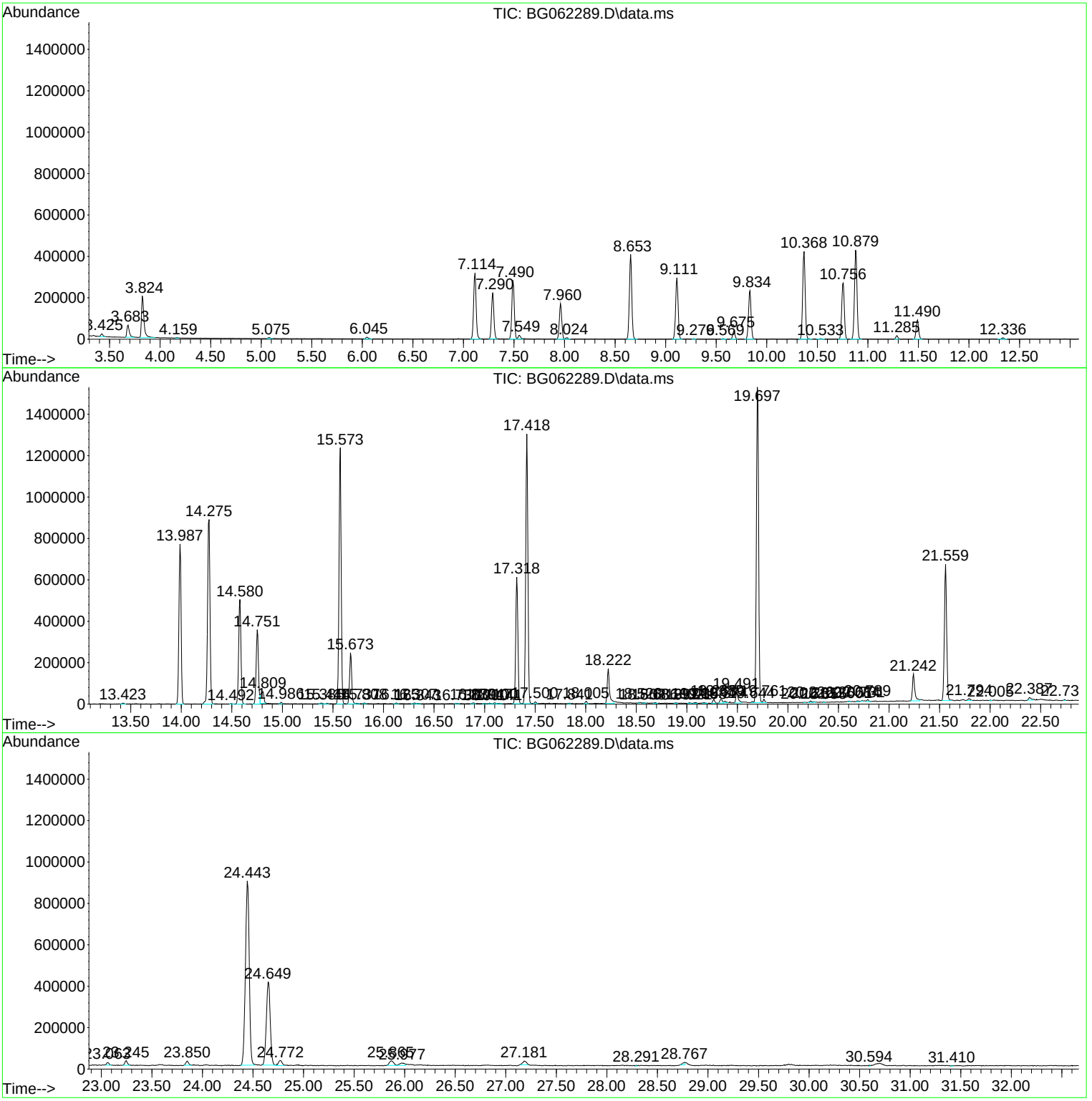
Sum of corrected areas: 23013333

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.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\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

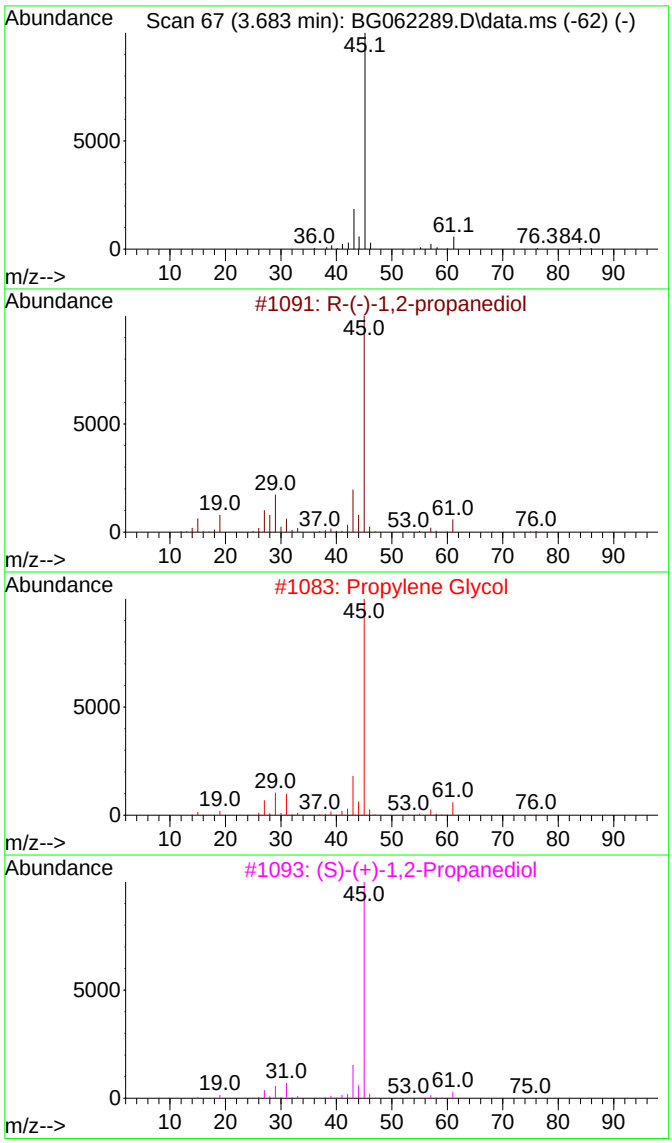
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

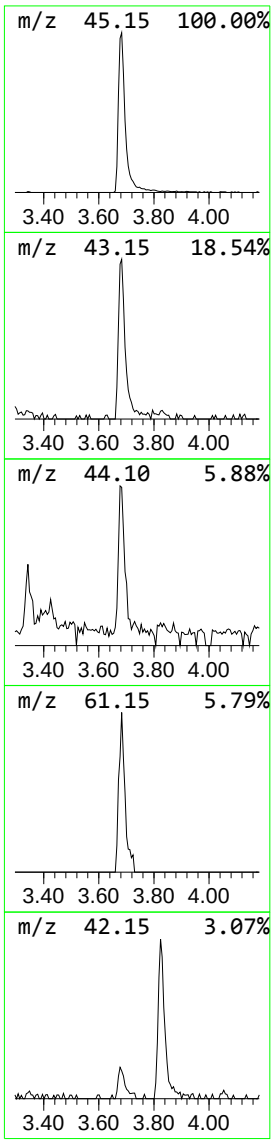
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.683	6.87 ng/ul	97675	1,4-Dichlorobenzene-d4	7.960

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
2	Propylene Glycol	76	C3H8O2	000057-55-6	78
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

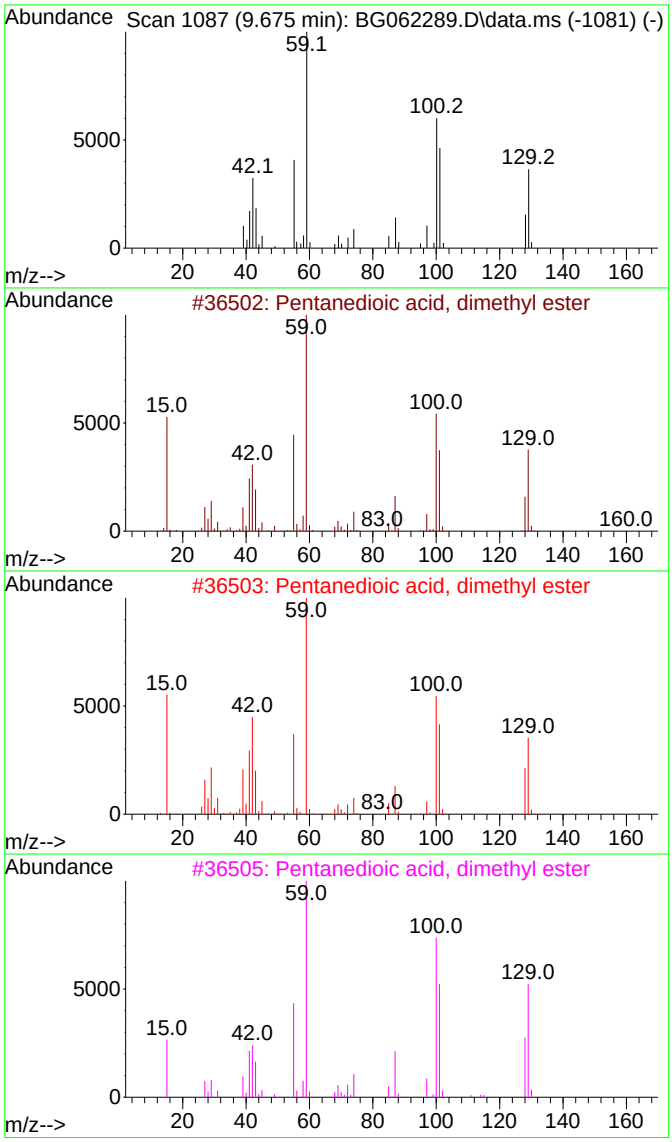
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

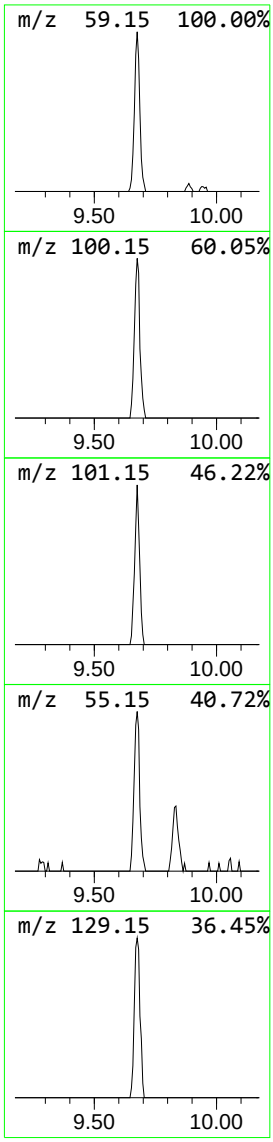
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentanedioic acid, dimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.675	2.48 ng/ul	60154	Naphthalene-d8	10.756

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	90
2	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	83
3	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	64
4	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	64
5	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

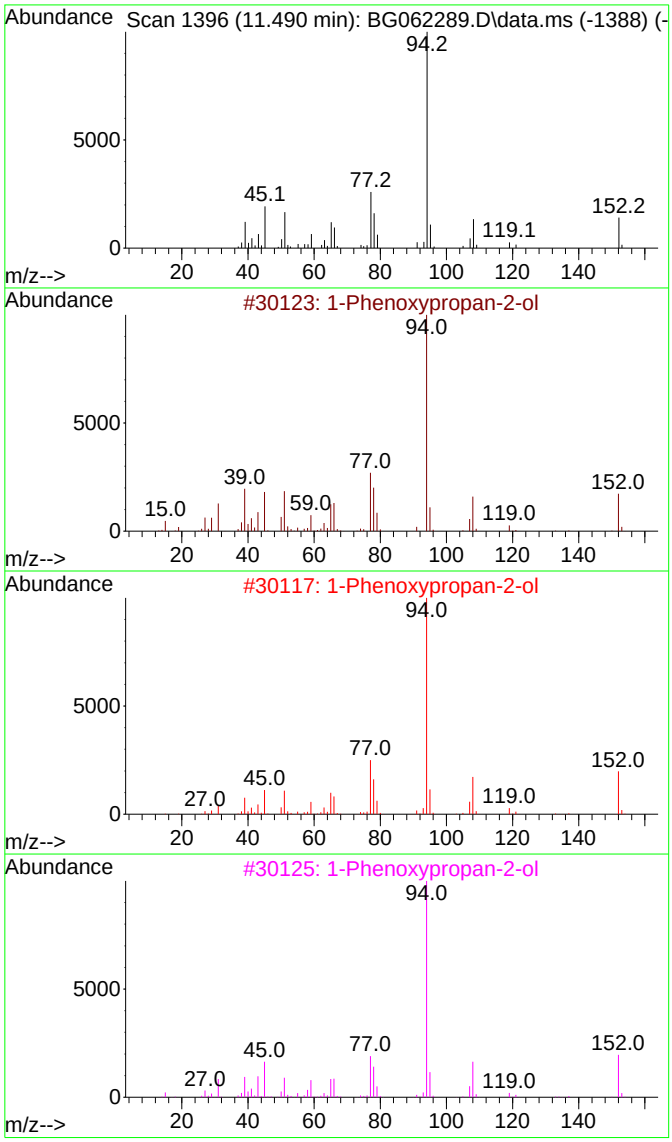
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

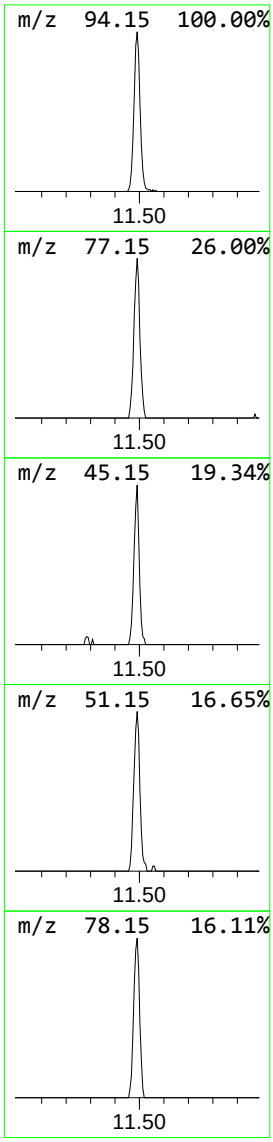
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.490	6.60 ng/ul	160005	Naphthalene-d8	10.756

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

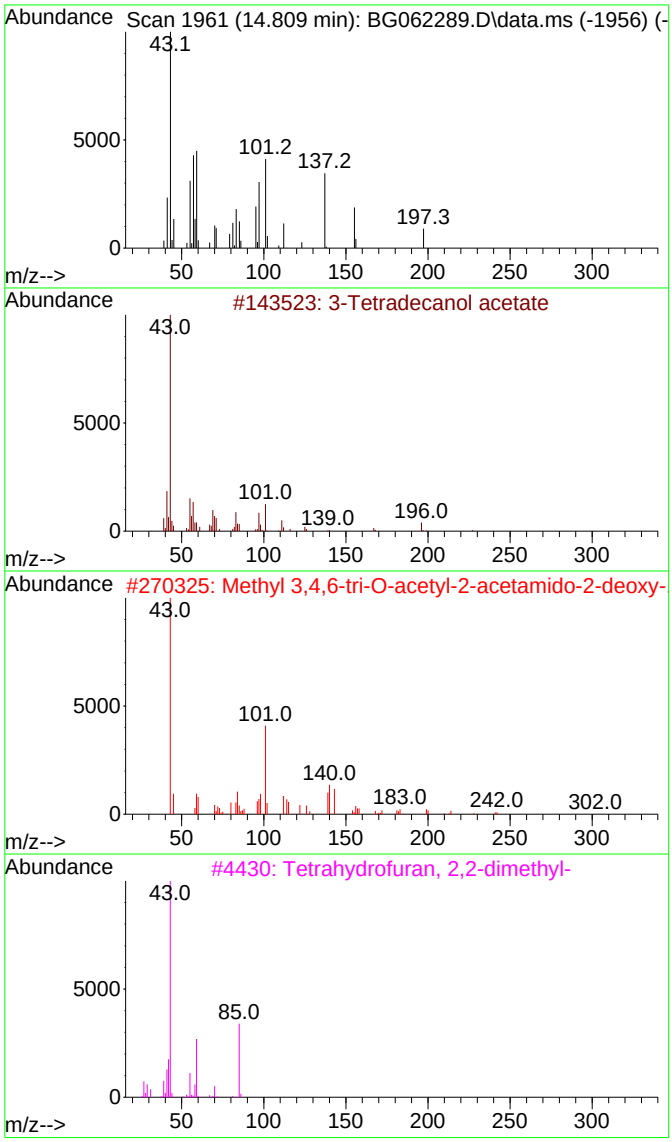
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

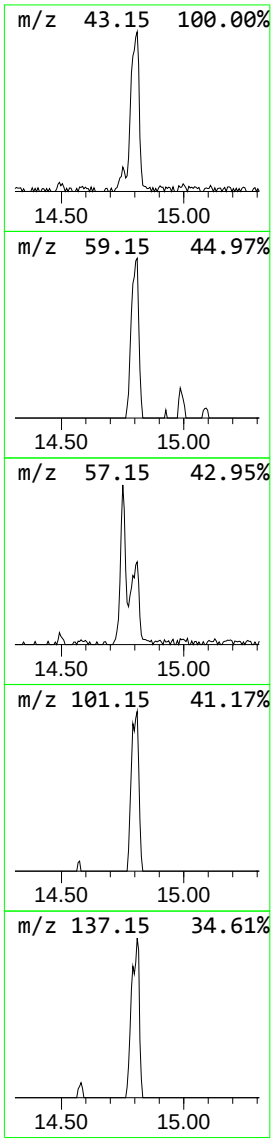
****

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.809	2.96 ng/ul	114437	Acenaphthene-d10	14.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	23
2	Methyl 3,4,6-tri-O-acetyl-2-acet...	361	C15H23NO9	002595-39-3	12
3	Tetrahydrofuran, 2,2-dimethyl-	100	C6H12O	001003-17-4	10
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

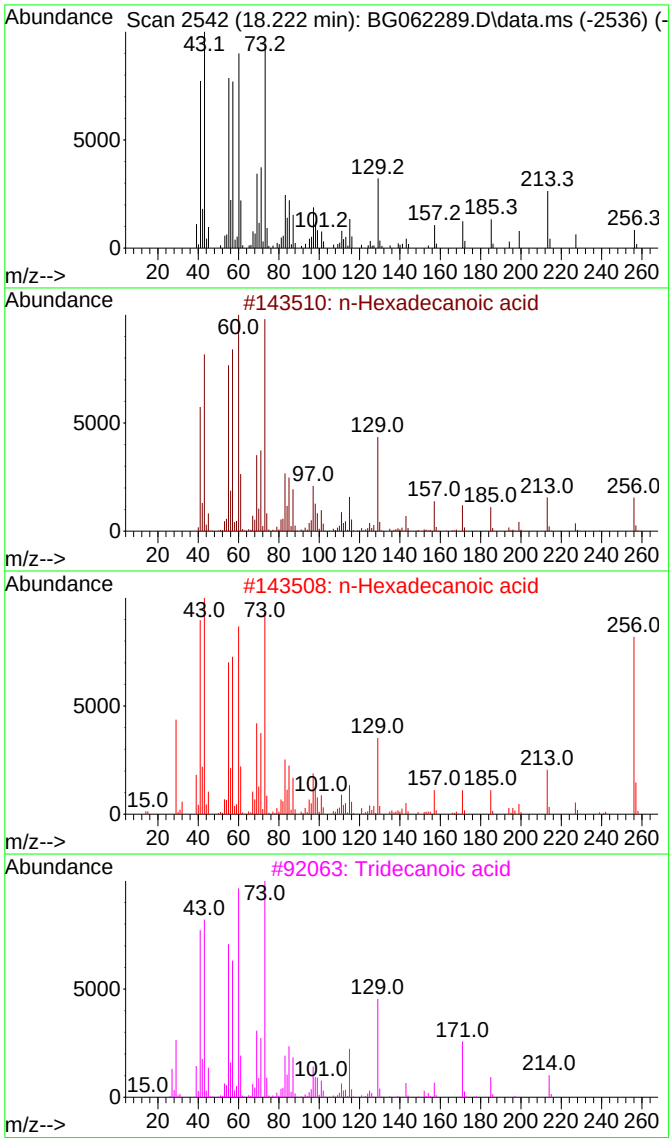
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

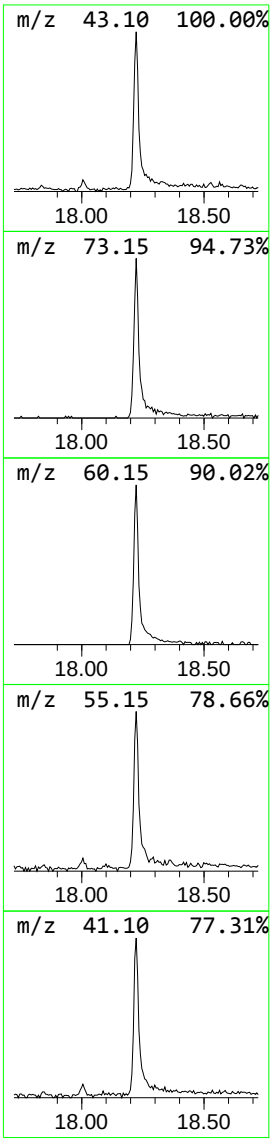
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	5.78 ng/ul	261758	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

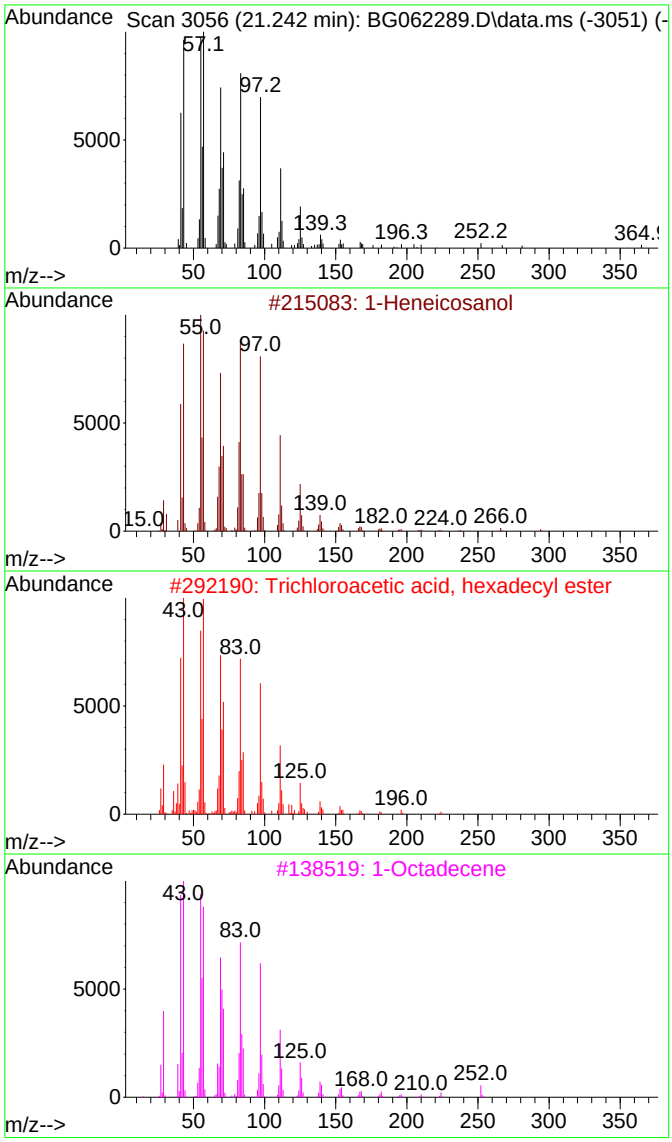
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

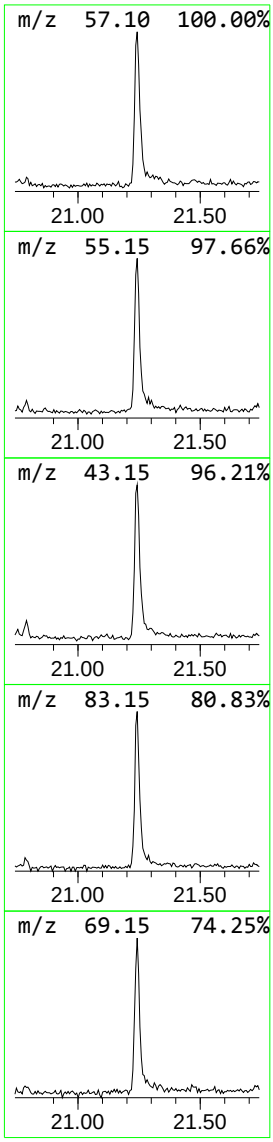
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.242	4.05 ng/ul	207604	Chrysene-d12	21.559

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
3	1-Octadecene	252	C18H36	000112-88-9	94
4	1-Tetracosene	336	C24H48	010192-32-2	94
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062289.D
Acq On : 7 Aug 2024 4:35
Operator : MA/JU
Sample : P3336-08
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F7E33

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.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...	3.683	6.9	ng/ul	97675	1	7.960	284234	20.0
Pentanedioic ac...	9.675	2.5	ng/ul	60154	2	10.756	485174	20.0
1-Phenoxypropan...	11.490	6.6	ng/ul	160005	2	10.756	485174	20.0
unknown-01	14.809	3.0	ng/ul	114437	3	14.580	773491	20.0
n-Hexadecanoic ...	18.222	5.8	ng/ul	261758	4	17.318	905333	20.0
1-Heneicosanol	21.242	4.0	ng/ul	207604	5	21.559	1023970	20.0