LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062251.D
Acq On : 6 Aug 2024 00:13
Operator : MA/JU
Sample : P3361-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : E20P3

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: BG062251.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	20	23	31	rVB2	8939	13168	0.88%	0.073%
2	3.687	63	68	78	rBV	51299	86880	5.80%	0.483%
3	3.828	87	92	104	rBV	125282	203644	13.60%	1.132%
4	4.169	147	150	154	rBV3	2677	3457	0.23%	0.019%
5	5.074	301	304	308	rBV4	1533	2657	0.18%	0.015%
6	6.049	465	470	477	rBV4	3183	6248	0.42%	0.035%
7	7.112	644	651	662	rBV	177616	304417	20.33%	1.692%
8	7.294	671	682	693	rBV	128228	216899	14.48%	1.205%
9	7.494	709	716	723	rBV	169578	279613	18.67%	1.554%
10	7.559	723	727	733	rVB	18701	29965	2.00%	0.167%
11	7.964	789	796	803	rBV	234155	380736	25.42%	2.116%
12	8.029	803	807	812	rVB2	3760	4498	0.30%	0.025%
13	8.657	907	914	922	rBV	224872	387079	25.85%	2.151%
14	9.115	984	992	1001	rVB	164692	282885	18.89%	1.572%
15	9.579	1066	1071	1075	rVB2	1517	2758	0.18%	0.015%
16	9.679	1084	1088	1094	rVB2	13522	20627	1.38%	0.115%
17	9.838	1107	1115	1122	rBV	124456	212367	14.18%	1.180%
18	10.372	1196	1206	1213	rBV	228959	401990	26.84%	2.234%
19	10.537	1228	1234	1239	rBV4	1374	2629	0.18%	0.015%
20	10.760	1264	1272	1280	rVB	367347	632818	42.25%	3.516%
21	10.883	1286	1293	1303	rBV	248761	436225	29.13%	2.424%
22	11.295	1355	1363	1367	rBV4	5867	9374	0.63%	0.052%
23	11.494	1389	1397	1404	rBV	64095	108593	7.25%	0.603%
24	12.340	1537	1541	1545	rBV	3371	4931	0.33%	0.027%
25	13.204	1685	1688	1692	rBV2	1957	2736	0.18%	0.015%
26	13.433	1722	1727	1733	rVB3	2506	4368	0.29%	0.024%
27	13.991	1815	1822	1830	rVB	489641	689857	46.06%	3.833%
28	14.273	1855	1870	1879	rBV	526380	868660	58.00%	4.827%
29	14.584	1915	1923	1930	rBV	659002	1014222	67.72%	5.636%
30	14.755	1944	1952	1956	rBV	208726	325291	21.72%	1.808%
31	14.796	1956	1959	1960	rBV	39891	41338	2.76%	0.230%
32	14.996	1988	1993	1998	rBV5	2824	6002	0.40%	0.033%
33	15.095	2006	2010	2013	rVB2	2249	2659	0.18%	0.015%
34	15.395	2056	2061	2065	rBV2	3979	7080	0.47%	0.039%
35	15.454	2067	2071	2075	rVV	2295	3266	0.22%	0.018%
36	15.571	2085	2091	2103	rVB	713098	1099401	73.41%	6.109%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062251.D
Acq On : 6 Aug 2024 00:13
Operator : MA/JU
Sample : P3361-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P3

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	15.677	2103	2109	2119	rBV	113849	168988	11.28%	0.939%
38	15.818	2129	2133	2135	rBV2	2783	2801	0.19%	0.016%
39	16.129	2181	2186	2192	rBV3	9367	13005	0.87%	0.072%
40	16.311	2213	2217	2222	rBV3	3674	6143	0.41%	0.034%
41	16.893	2313	2316	2321	rBV4	3780	5035	0.34%	0.028%
42	17.110	2347	2353	2355	rBV2	5355	6475	0.43%	0.036%
43	17.322	2382	2389	2399	rVV	832001	1248167	83.34%	6.936%
44	17.422	2399	2406	2417	rVV	816257	1190190	79.47%	6.614%
45	17.510	2417	2421	2423	rVV	3493	3297	0.22%	0.018%
46	17.715	2453	2456	2460	rVB3	3275	5210	0.35%	0.029%
47	17.845	2476	2478	2483	rVV4	3033	3406	0.23%	0.019%
48	18.015	2502	2507	2511	rVB	21129	25447	1.70%	0.141%
49	18.227	2538	2543	2552	rBV	82107	137143	9.16%	0.762%
50	18.532	2590	2595	2599	rVV6	4165	6828	0.46%	0.038%
51	19.031	2677	2680	2686	rVB5	3217	5199	0.35%	0.029%
52	19.090	2686	2690	2697	rVB4	9135	14146	0.94%	0.079%
53	19.184	2697	2706	2710	rBV6	25590	36789	2.46%	0.204%
54	19.272	2717	2721	2726	rBV2	11373	15981	1.07%	0.089%
55	19.349	2726	2734	2737	rBV2	10672	21972	1.47%	0.122%
56	19.501	2755	2760	2766	rVV4	29848	45545	3.04%	0.253%
57	19.660	2783	2787	2788	rVV3	6304	8257	0.55%	0.046%
58	19.701	2788	2794	2800	rVV	1009036	1422333	94.97%	7.904%
59	19.771	2803	2806	2810	rVB3	15082	17012	1.14%	0.095%
60	20.065	2849	2856	2857	rBV7	2134	3707	0.25%	0.021%
61	20.236	2881	2885	2888	rVB3	6409	8479	0.57%	0.047%
62	20.271	2888	2891	2895	rBV4	4042	5454	0.36%	0.030%
63	20.500	2926	2930	2931	rBV4	3362	4061	0.27%	0.023%
64	20.588	2943	2945	2946	rVV2	4319	3482	0.23%	0.019%
65	20.635	2946	2953	2960	rVV5	16939	34214	2.28%	0.190%
66	20.700	2960	2964	2967	rVV4	8096	10165	0.68%	0.056%
67	20.735	2968	2970	2973	rVV2	5728	7425	0.50%	0.041%
68	20.770	2973	2976	2978	rVV4	6893	7964	0.53%	0.044%
69	20.799	2978	2981	2984	rVB5	6801	8566	0.57%	0.048%
70	20.876	2993	2994	2999	rBV4	2813	3010	0.20%	0.017%
71	21.252	3053	3058	3065	rBV	119053	174595	11.66%	0.970%
72	21.475	3087	3096	3097	rBV7	7626	17156	1.15%	0.095%
73	21.493	3097	3099	3101	rBV3	6255	6304	0.42%	0.035%
74	21.563	3104	3111	3118	rBV2	889201	1439323	96.10%	7.998%
75	22.403	3250	3254	3260	rBV4	15901	29132	1.95%	0.162%
76	22.844	3325	3329	3330	rBV3	3000	4497	0.30%	0.025%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062251.D
Acq On : 6 Aug 2024 00:13
Operator : MA/JU
Sample : P3361-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P3

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	23.032	3356	3361	3365	rBV5	16232	31241	2.09%	0.174%
78	23.079	3366	3369	3378	rVB2	21350	41194	2.75%	0.229%
79	23.267	3396	3401	3406	rVV3	15213	26603	1.78%	0.148%
80	23.325	3409	3411	3417	rBV7	4916	7125	0.48%	0.040%
81	23.737	3478	3481	3485	rVB5	4552	5547	0.37%	0.031%
82	23.872	3498	3504	3510	rBV2	32766	70697	4.72%	0.393%
83	24.447	3588	3602	3618	rBV	553797	1487593	99.33%	8.266%
84	24.659	3627	3638	3652	rBV	552384	1497682	100.00%	8.322%
85	24.800	3654	3662	3668	rBV	36261	88666	5.92%	0.493%
86	25.135	3717	3719	3722	rVB4	2813	2767	0.18%	0.015%
87	25.540	3786	3788	3791	rBV4	2720	3293	0.22%	0.018%
88	25.687	3809	3813	3814	rBV4	4844	4915	0.33%	0.027%
89	25.705	3814	3816	3821	rVB6	5468	6193	0.41%	0.034%
90	25.910	3841	3851	3859	rBV4	35998	110283	7.36%	0.613%
91	25.998	3859	3866	3875	rBV4	10345	37347	2.49%	0.208%
92	26.574	3961	3964	3966	rBV4	2586	2992	0.20%	0.017%
93	27.226	4066	4075	4085	rBV4	30425	110735	7.39%	0.615%
94	28.037	4211	4213	4217	rBV5	2332	3058	0.20%	0.017%
95	28.824	4338	4347	4348	rBV5	19319	38841	2.59%	0.216%
96	29.781	4507	4510	4511	rBV3	2979	3643	0.24%	0.020%
97	29.799	4511	4513	4514	rVV2	3644	2641	0.18%	0.015%
98	29.823	4515	4517	4522	rVV6	4796	8385	0.56%	0.047%
99	29.987	4543	4545	4547	rBV3	2621	2734	0.18%	0.015%
100	30.357	4588	4608	4609	rBV3	33951	125404	8.37%	0.697%

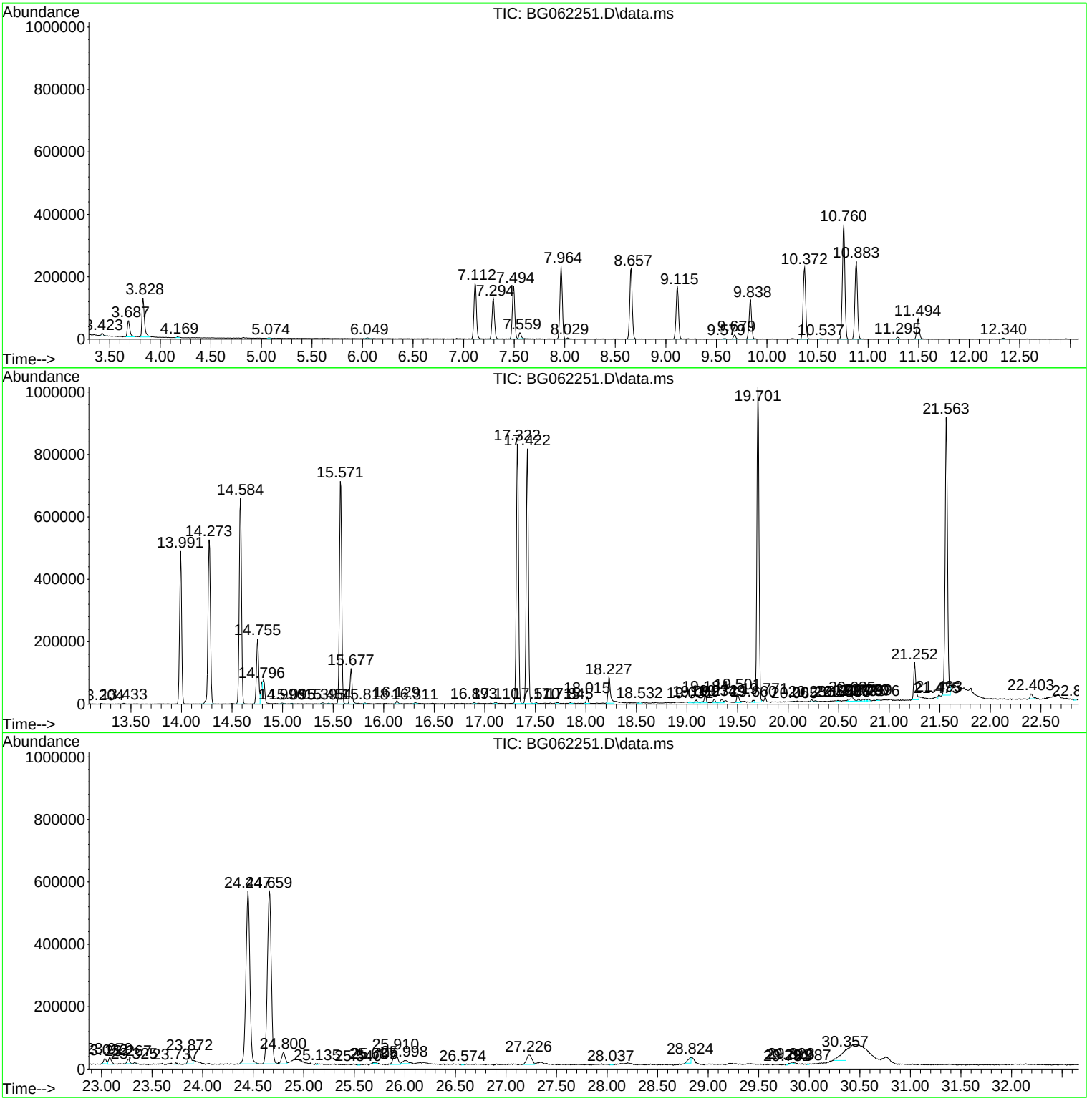
Sum of corrected areas: 17995820

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062251.D
Acq On : 6 Aug 2024 00:13
Operator : MA/JU
Sample : P3361-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P3

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 : BG062251.D
Acq On : 6 Aug 2024 00:13
Operator : MA/JU
Sample : P3361-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P3

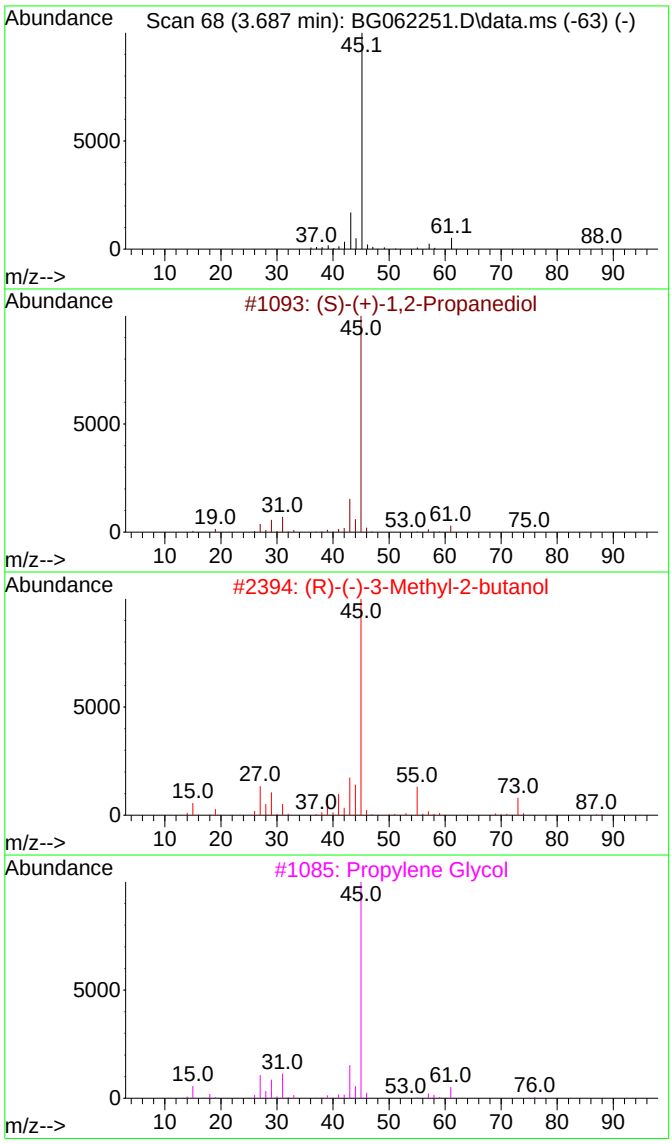
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

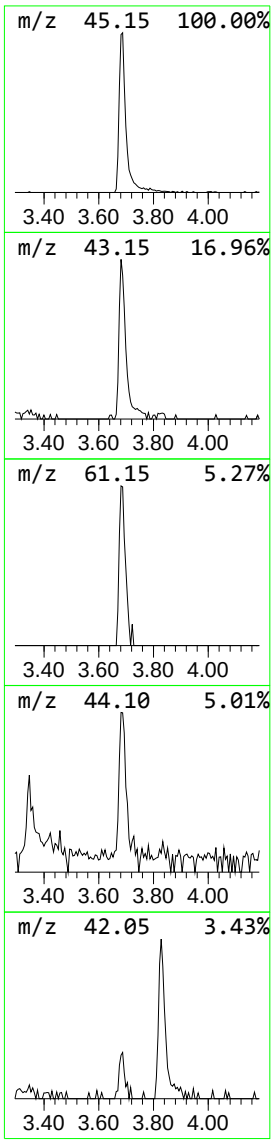
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.687	4.56 ng/ul	86880	1,4-Dichlorobenzene-d4	7.964

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	40
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	L-Lactic acid	90	C3H6O3	000079-33-4	9
5	Isopropyl Alcohol	60	C3H8O	000067-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062251.D
Acq On : 6 Aug 2024 00:13
Operator : MA/JU
Sample : P3361-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P3

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

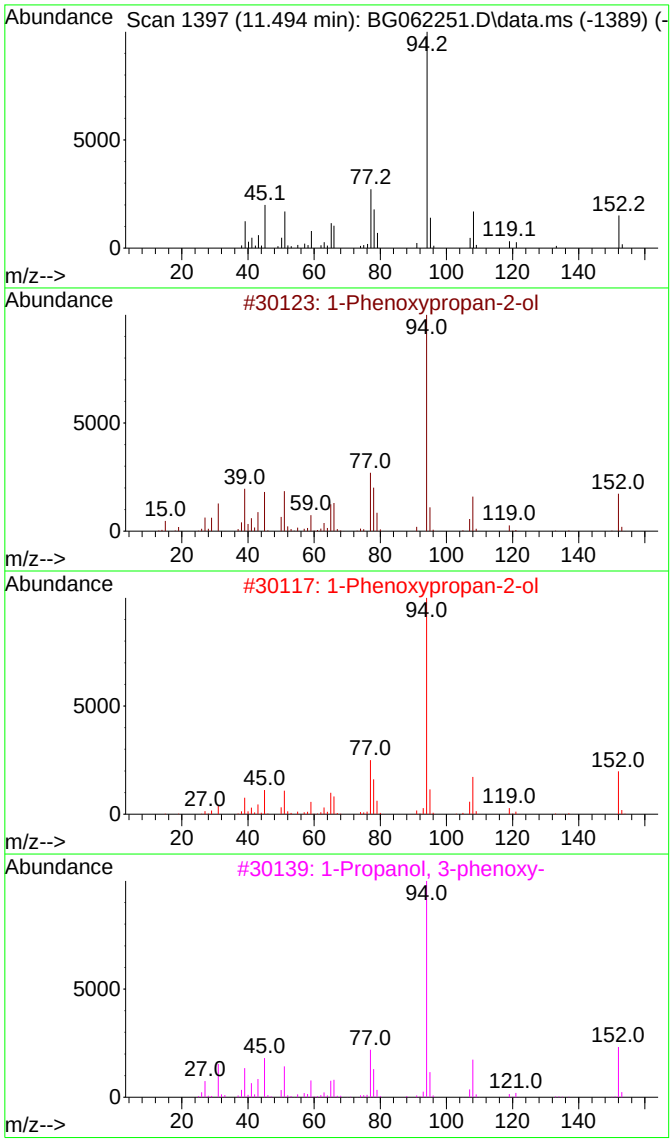
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

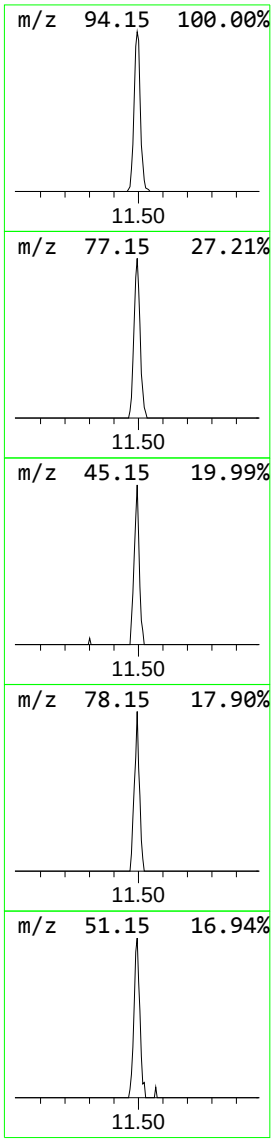
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.494	3.43 ng/ul	108593	Naphthalene-d8	10.760

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-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	94
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	93
5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062251.D
Acq On : 6 Aug 2024 00:13
Operator : MA/JU
Sample : P3361-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P3

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

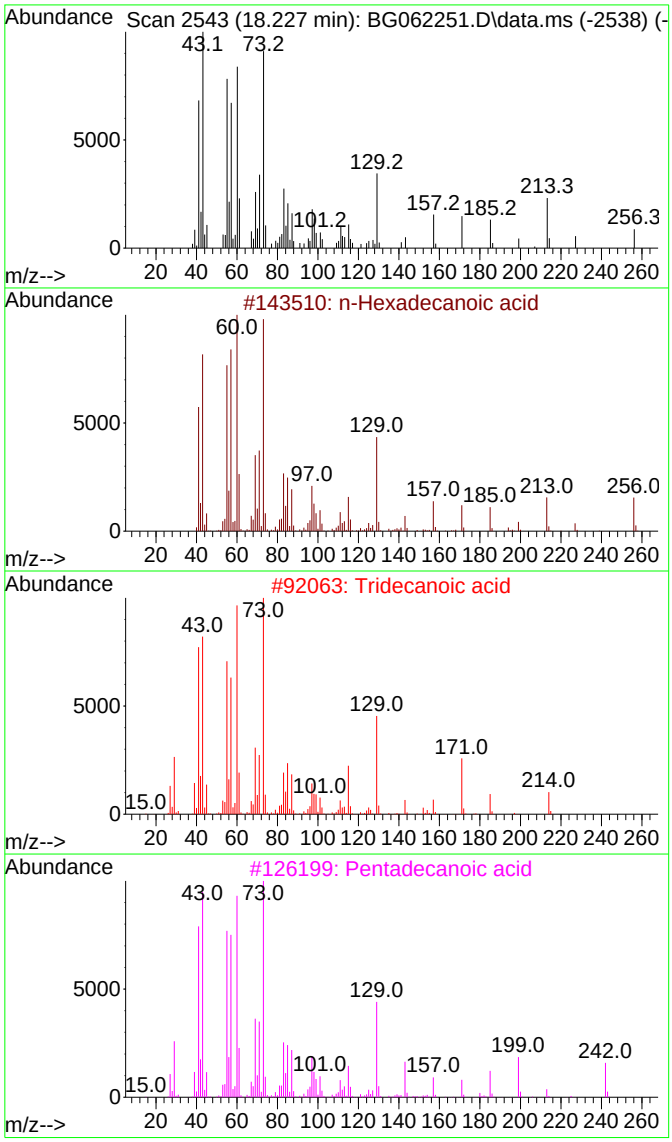
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

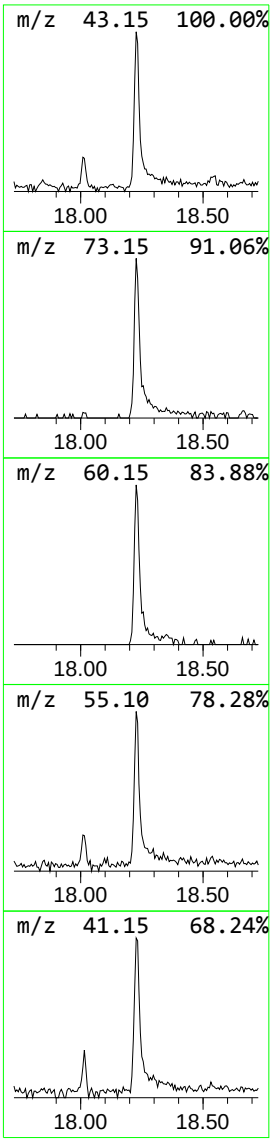
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.227	2.20 ng/ul	137143	Phenanthrene-d10	17.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062251.D
Acq On : 6 Aug 2024 00:13
Operator : MA/JU
Sample : P3361-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P3

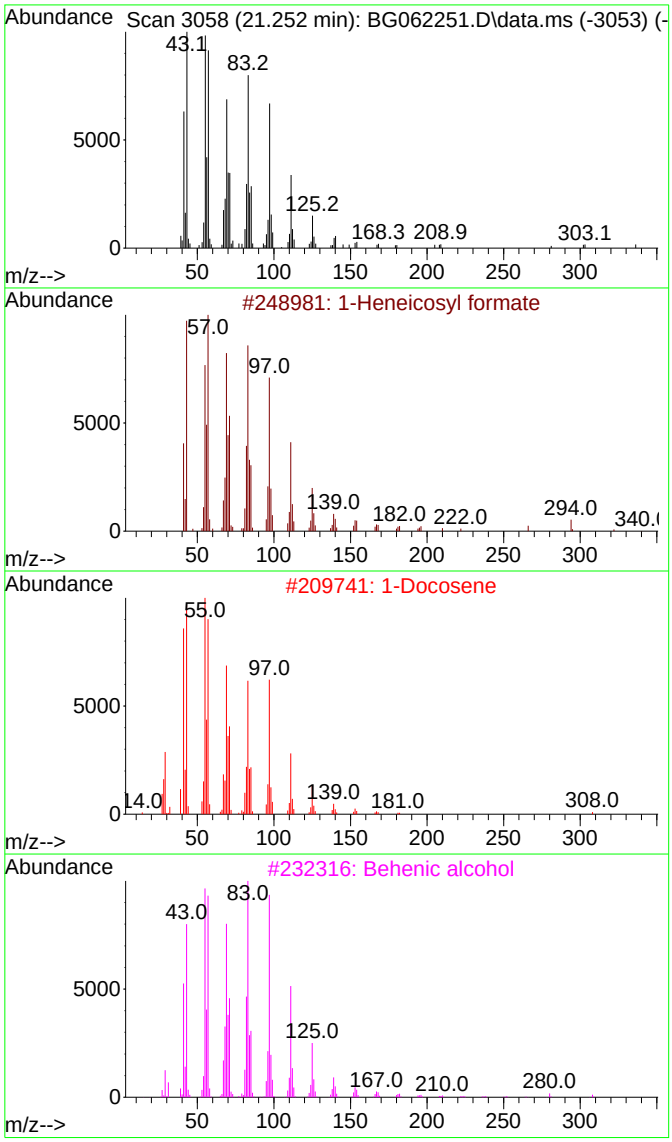
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

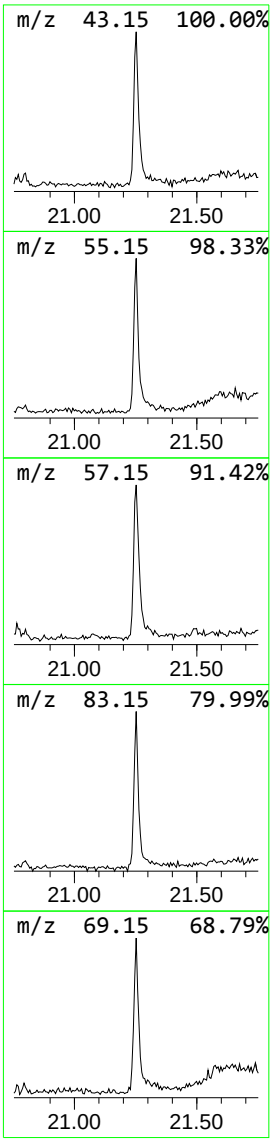
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.252	2.43 ng/ul	174595	Chrysene-d12	21.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062251.D
Acq On : 6 Aug 2024 00:13
Operator : MA/JU
Sample : P3361-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P3

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
(S)-(+)-1,2-Pro...	3.687	4.6	ng/ul	86880	1	7.964	380736	20.0
1-Phenoxypropan...	11.494	3.4	ng/ul	108593	2	10.760	632818	20.0
n-Hexadecanoic ...	18.227	2.2	ng/ul	137143	4	17.322	1248170	20.0
1-Heneicosyl fo...	21.252	2.4	ng/ul	174595	5	21.563	1439320	20.0