LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062254.D
Acq On : 6 Aug 2024 2:17
Operator : MA/JU
Sample : P3361-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : E20P9

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: BG062254.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	30	rVB2	11864	18065	1.04%	0.087%
2	3.681	63	67	77	rBV	48634	79856	4.59%	0.386%
3	3.828	87	92	109	rVB	161142	267445	15.37%	1.291%
4	4.163	147	149	156	rVB6	3768	6282	0.36%	0.030%
5	6.055	466	471	475	rBV4	3478	5253	0.30%	0.025%
6	7.112	644	651	660	rBV	225469	378668	21.76%	1.828%
7	7.294	674	682	691	rBV	162157	262420	15.08%	1.267%
8	7.494	708	716	722	rBV	204068	343575	19.75%	1.659%
9	7.553	722	726	739	rVB	23441	41186	2.37%	0.199%
10	7.964	789	796	803	rBV	250292	413504	23.76%	1.997%
11	8.028	803	807	812	rVB2	3444	5249	0.30%	0.025%
12	8.657	905	914	925	rVB	288451	482155	27.71%	2.328%
13	9.115	984	992	1003	rBV	193197	337134	19.37%	1.628%
14	9.679	1082	1088	1094	rBV2	15567	23963	1.38%	0.116%
15	9.838	1107	1115	1122	rBV	148034	259847	14.93%	1.255%
16	10.372	1198	1206	1215	rBV	285523	495297	28.46%	2.392%
17	10.760	1264	1272	1279	rBV	375507	666558	38.31%	3.218%
18	10.883	1283	1293	1302	rBV	302911	535705	30.79%	2.587%
19	11.289	1358	1362	1369	rBV	6271	9402	0.54%	0.045%
20	11.494	1389	1397	1405	rBV	75466	129407	7.44%	0.625%
21	12.340	1536	1541	1547	rBV	3498	5903	0.34%	0.029%
22	12.951	1640	1645	1651	rBV2	2555	3166	0.18%	0.015%
23	13.204	1683	1688	1690	rBV2	3448	3525	0.20%	0.017%
24	13.427	1722	1726	1732	rBV3	2023	3468	0.20%	0.017%
25	13.991	1816	1822	1831	rBV	573693	827589	47.56%	3.996%
26	14.273	1859	1870	1880	rBV	659411	1039212	59.72%	5.018%
27	14.584	1916	1923	1930	rBV	686977	1075156	61.79%	5.191%
28	14.755	1945	1952	1955	rBV	234683	362497	20.83%	1.750%
29	14.796	1955	1959	1960	rBV	297368	321945	18.50%	1.554%
30	14.995	1989	1993	1996	rBV4	3521	5478	0.31%	0.026%
31	15.095	2005	2010	2014	rVB2	3087	4002	0.23%	0.019%
32	15.395	2057	2061	2065	rBV4	4217	6471	0.37%	0.031%
33	15.454	2067	2071	2074	rVV3	2633	3512	0.20%	0.017%
34	15.571	2084	2091	2099	rVV	852086	1321517	75.95%	6.381%
35	15.677	2103	2109	2118	rBV	134162	200088	11.50%	0.966%
36	15.736	2118	2119	2126	rVV4	2709	5611	0.32%	0.027%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062254.D
Acq On : 6 Aug 2024 2:17
Operator : MA/JU
Sample : P3361-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P9

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	15.812	2128	2132	2137	rVV4	4097	5919	0.34%	0.029%
38	16.129	2182	2186	2192	rVB3	11430	15884	0.91%	0.077%
39	16.311	2214	2217	2220	rBV4	3965	4593	0.26%	0.022%
40	16.487	2242	2247	2250	rVB4	2435	4283	0.25%	0.021%
41	16.587	2260	2264	2268	rBV3	1532	2714	0.16%	0.013%
42	16.893	2312	2316	2320	rBV3	3754	4667	0.27%	0.023%
43	17.051	2342	2343	2348	rVB5	2206	2555	0.15%	0.012%
44	17.104	2348	2352	2357	rBV3	5623	8067	0.46%	0.039%
45	17.322	2382	2389	2397	rBV	878263	1317962	75.74%	6.364%
46	17.422	2399	2406	2415	rVV	957077	1437848	82.63%	6.943%
47	17.504	2417	2420	2425	rVV3	3137	4755	0.27%	0.023%
48	17.651	2442	2445	2448	rVB3	3103	3040	0.17%	0.015%
49	17.715	2453	2456	2463	rVB5	5025	7994	0.46%	0.039%
50	17.850	2475	2479	2483	rBV4	2484	4719	0.27%	0.023%
51	18.015	2501	2507	2513	rVB2	24397	31076	1.79%	0.150%
52	18.226	2538	2543	2561	rBV2	80716	157593	9.06%	0.761%
53	18.532	2592	2595	2599	rBV3	3176	4796	0.28%	0.023%
54	18.884	2652	2655	2658	rBV4	2098	2976	0.17%	0.014%
55	19.031	2677	2680	2684	rVB3	3167	3797	0.22%	0.018%
56	19.090	2686	2690	2695	rVB3	10170	15390	0.88%	0.074%
57	19.149	2695	2700	2702	rBV4	7358	9997	0.57%	0.048%
58	19.178	2702	2705	2710	rVB2	50960	63206	3.63%	0.305%
59	19.272	2716	2721	2725	rBV2	11101	15505	0.89%	0.075%
60	19.319	2725	2729	2730	rBV3	6654	8372	0.48%	0.040%
61	19.337	2730	2732	2737	rVB	8673	12959	0.74%	0.063%
62	19.501	2755	2760	2769	rBV3	27207	47628	2.74%	0.230%
63	19.654	2782	2786	2788	rBV4	6726	8033	0.46%	0.039%
64	19.701	2788	2794	2803	rVV	1201280	1702418	97.84%	8.220%
65	19.771	2803	2806	2810	rVB2	12828	14159	0.81%	0.068%
66	20.229	2880	2884	2888	rBV5	9557	13282	0.76%	0.064%
67	20.271	2888	2891	2898	rVB7	3090	5565	0.32%	0.027%
68	20.500	2927	2930	2933	rBV5	2034	2831	0.16%	0.014%
69	20.635	2947	2953	2957	rVB2	16433	23649	1.36%	0.114%
70	20.699	2961	2964	2966	rVV4	4410	4697	0.27%	0.023%
71	20.741	2968	2971	2974	rVV4	5395	7074	0.41%	0.034%
72	20.764	2974	2975	2978	rVV3	7149	5636	0.32%	0.027%
73	20.799	2978	2981	2987	rVB7	5508	6091	0.35%	0.029%
74	21.252	3052	3058	3068	rBV	161107	246673	14.18%	1.191%
75	21.487	3097	3098	3101	rBV3	2971	2953	0.17%	0.014%
76	21.563	3104	3111	3119	rBV2	922882	1453864	83.55%	7.020%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062254.D
Acq On : 6 Aug 2024 2:17
Operator : MA/JU
Sample : P3361-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P9

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	21.804	3148	3152	3156	rBV4	9961	16760	0.96%	0.081%
78	22.403	3250	3254	3263	rVB5	18679	33436	1.92%	0.161%
79	22.996	3353	3355	3356	rBV2	3388	2551	0.15%	0.012%
80	23.032	3356	3361	3365	rVV7	17666	35885	2.06%	0.173%
81	23.079	3365	3369	3380	rVB2	21410	44837	2.58%	0.216%
82	23.267	3394	3401	3410	rBV2	21364	42229	2.43%	0.204%
83	23.866	3497	3503	3511	rBV2	28796	63505	3.65%	0.307%
84	24.447	3591	3602	3615	rVV	665222	1740057	100.00%	8.402%
85	24.659	3627	3638	3651	rBV2	592426	1588163	91.27%	7.668%
86	24.794	3655	3661	3672	rVB3	37160	95128	5.47%	0.459%
87	24.958	3687	3689	3694	rVB5	4285	5715	0.33%	0.028%
88	25.628	3800	3803	3804	rBV2	3886	3105	0.18%	0.015%
89	25.898	3841	3849	3859	rBV4	33605	99858	5.74%	0.482%
90	26.004	3859	3867	3875	rBV4	16361	56408	3.24%	0.272%
91	26.668	3979	3980	3983	rBV3	3295	3628	0.21%	0.018%
92	27.226	4066	4075	4085	rBV4	31994	107089	6.15%	0.517%
93	27.314	4088	4090	4093	rVB5	3446	2810	0.16%	0.014%
94	27.831	4176	4178	4182	rBV5	2577	4026	0.23%	0.019%
95	28.830	4339	4348	4360	rVB7	21060	87991	5.06%	0.425%
96	29.153	4401	4403	4405	rBV2	2477	2712	0.16%	0.013%
97	29.828	4511	4518	4519	rBV7	8561	16381	0.94%	0.079%
98	30.674	4660	4662	4664	rBV3	2752	3621	0.21%	0.017%
99	30.721	4667	4670	4671	rBV2	6174	6240	0.36%	0.030%
100	30.974	4711	4713	4717	rVB4	3469	3141	0.18%	0.015%

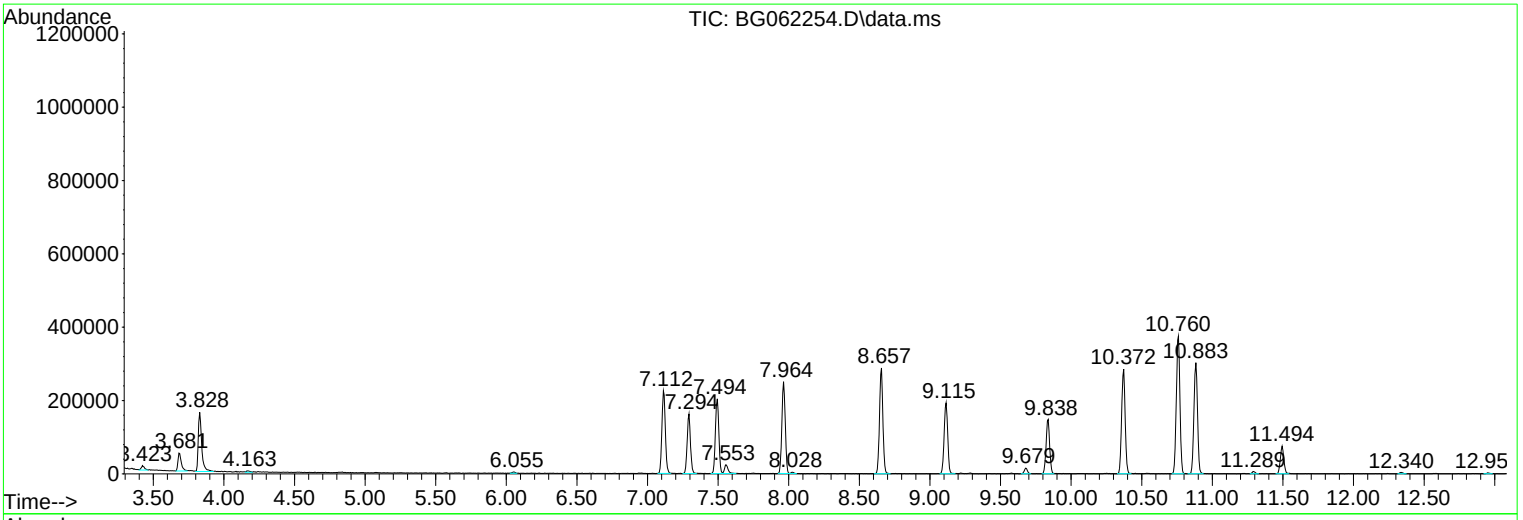
Sum of corrected areas: 20710607

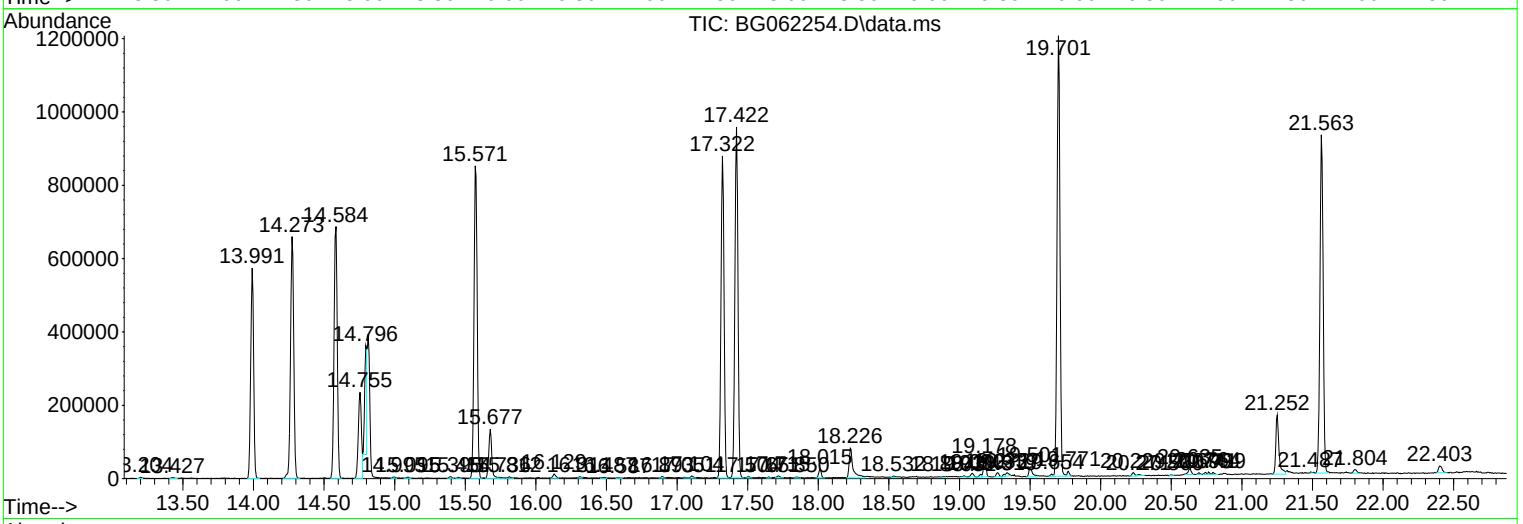
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062254.D
Acq On : 6 Aug 2024 2:17
Operator : MA/JU
Sample : P3361-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

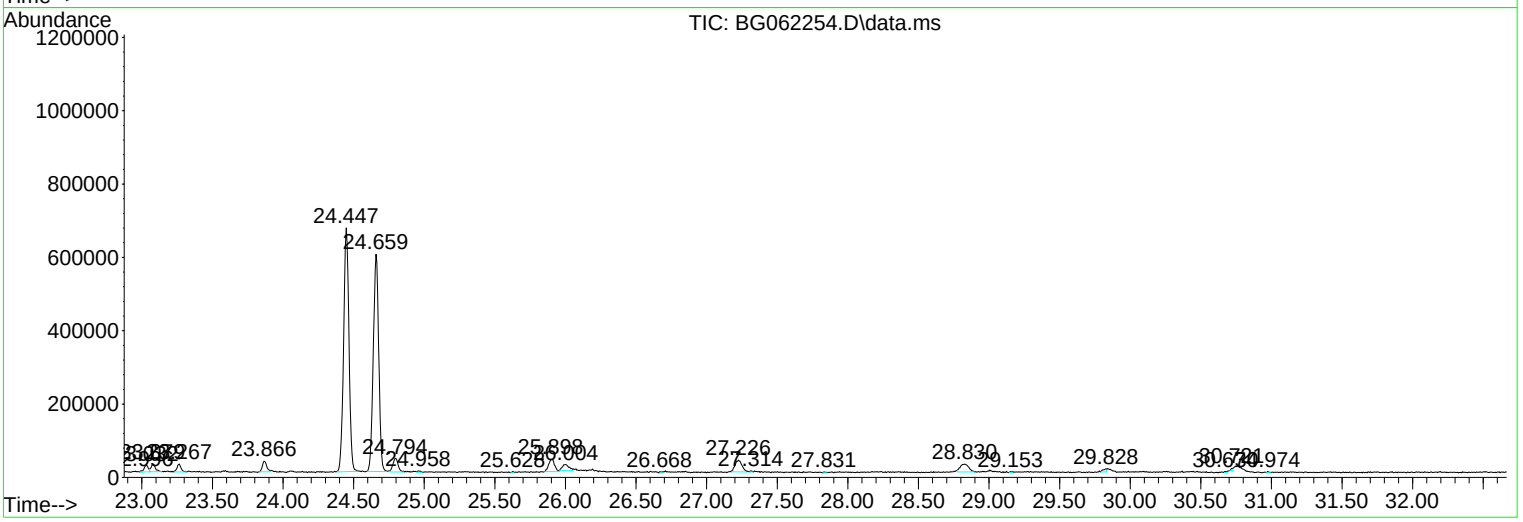
Instrument :
BNA_G
ClientSampleId :
E20P9

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 : BG062254.D
Acq On : 6 Aug 2024 2:17
Operator : MA/JU
Sample : P3361-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P9

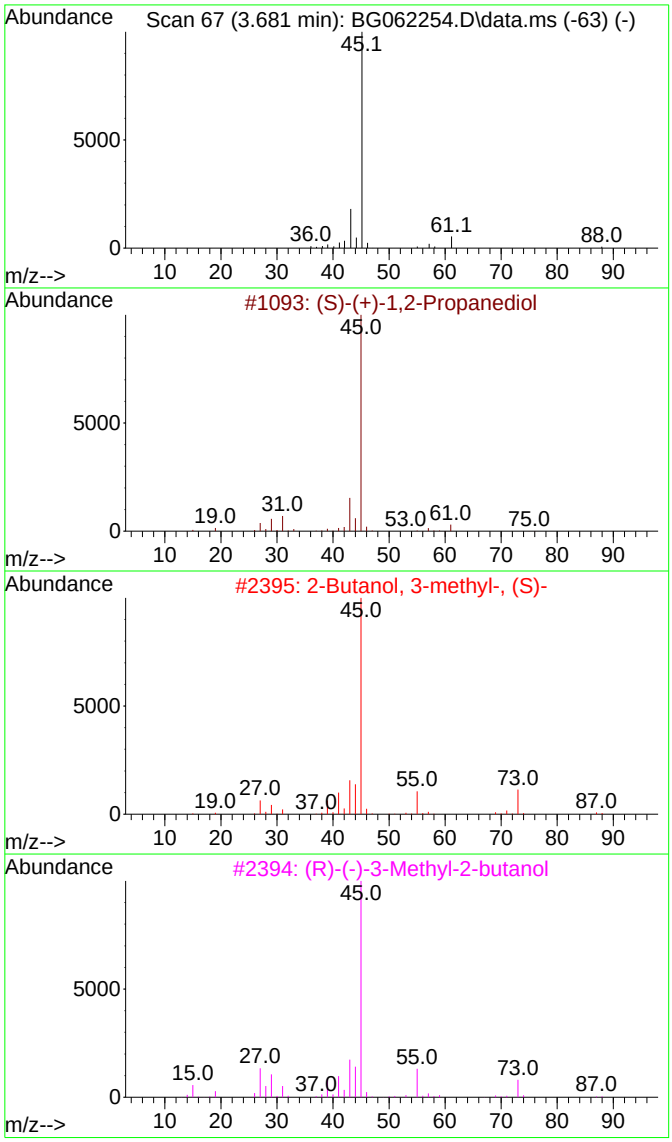
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

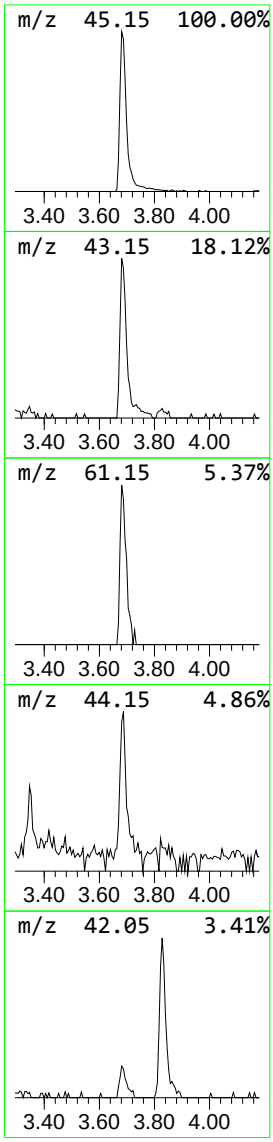
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	3.86 ng/ul	79856	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	40
2	2-Butanol, 3-methyl-, (S)-	88	C5H12O	001517-66-4	9
3	(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Propylene Glycol	76	C3H8O2	000057-55-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062254.D
Acq On : 6 Aug 2024 2:17
Operator : MA/JU
Sample : P3361-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P9

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

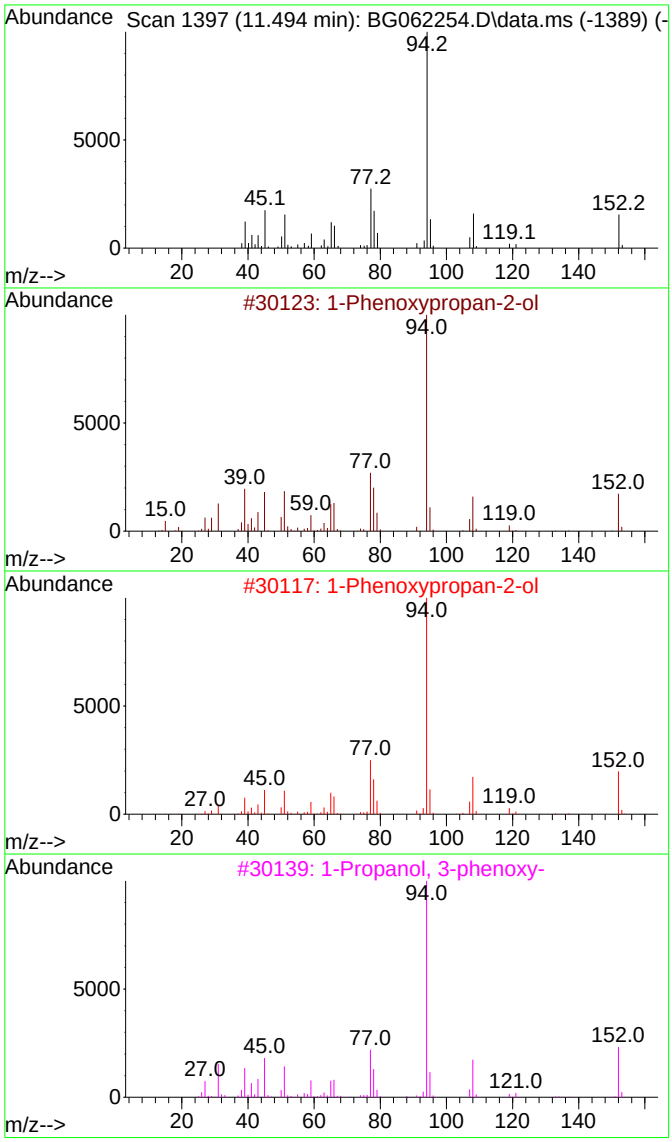
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

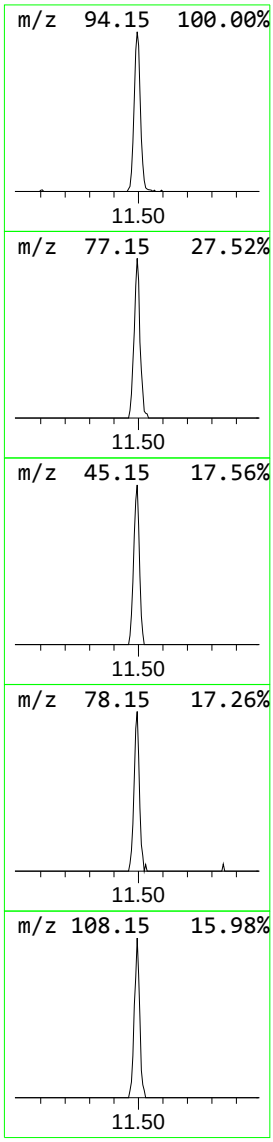
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.494	3.88 ng/ul	129407	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	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062254.D
Acq On : 6 Aug 2024 2:17
Operator : MA/JU
Sample : P3361-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P9

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

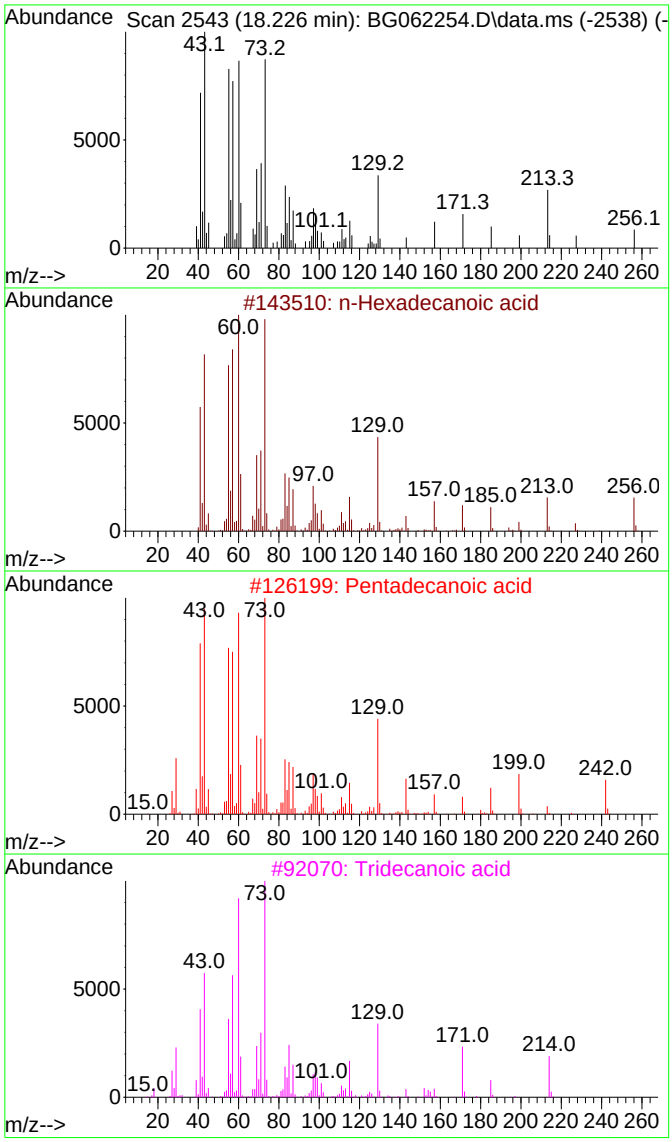
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

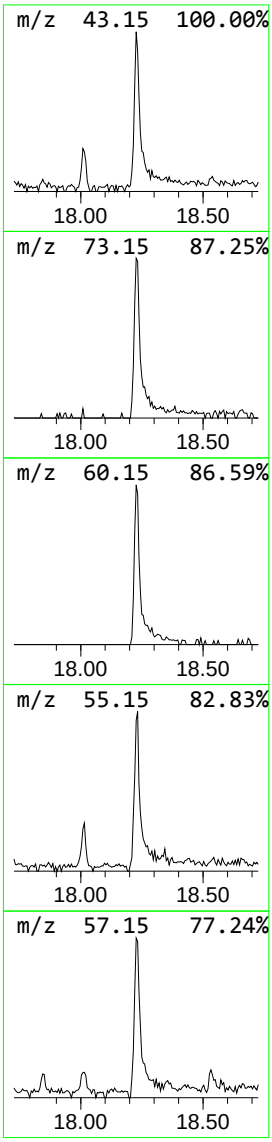
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.226	2.39 ng/ul	157593	Phenanthrene-d10	17.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062254.D
Acq On : 6 Aug 2024 2:17
Operator : MA/JU
Sample : P3361-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P9

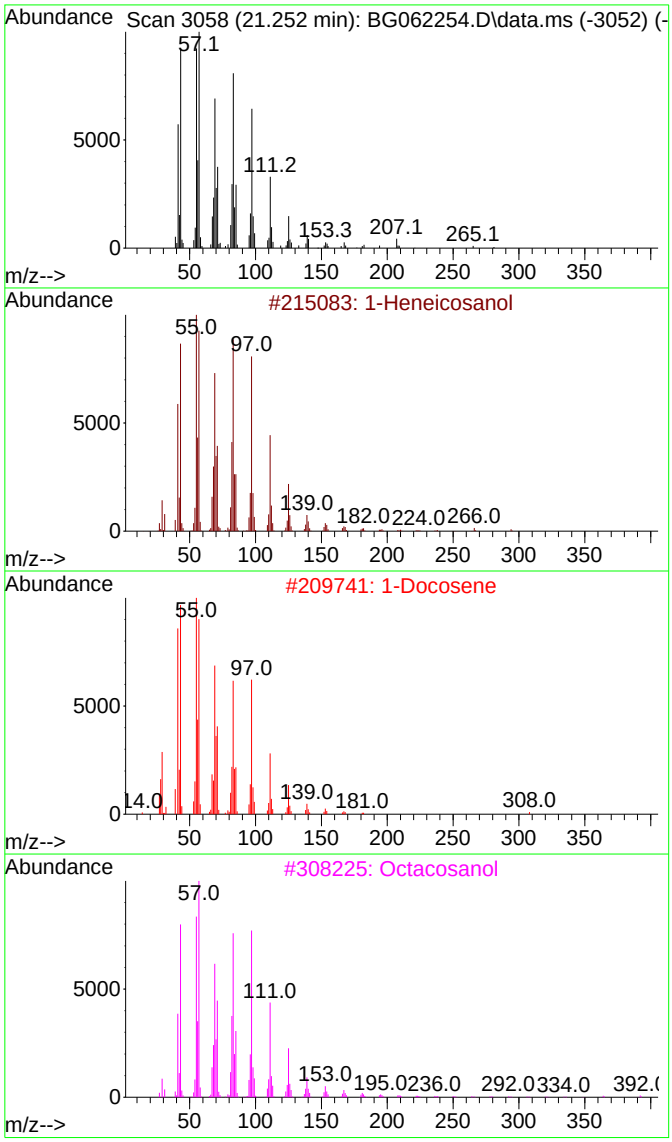
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

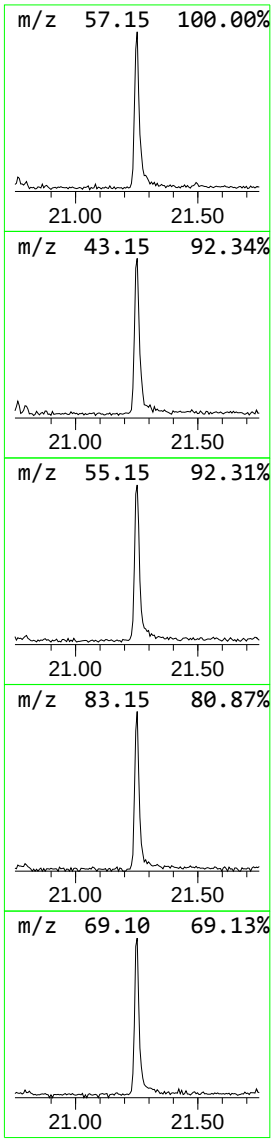
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.252	3.39 ng/ul	246673	Chrysene-d12	21.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Docosene	308	C22H44	001599-67-3	94
3	Octacosanol	410	C28H58O	000557-61-9	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080524\
Data File : BG062254.D
Acq On : 6 Aug 2024 2:17
Operator : MA/JU
Sample : P3361-19
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E20P9

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
unknown-01	3.681	3.9	ng/ul	79856	1	7.964	413504	20.0
1-Phenoxypropan...	11.494	3.9	ng/ul	129407	2	10.760	666558	20.0
n-Hexadecanoic ...	18.226	2.4	ng/ul	157593	4	17.322	1317960	20.0
1-Heneicosanol	21.252	3.4	ng/ul	246673	5	21.563	1453860	20.0