LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062318.D
Acq On : 8 Aug 2024 3:49
Operator : MA/JU
Sample : P3437-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

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: BG062318.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	29	rVB	13358	21810	1.08%	0.094%
2	3.681	63	67	77	rBV	38705	63760	3.15%	0.273%
3	3.828	88	92	107	rBV	85076	145427	7.18%	0.624%
4	4.169	146	150	158	rVB6	3418	7431	0.37%	0.032%
5	6.043	465	469	477	rVB2	5520	10329	0.51%	0.044%
6	7.112	643	651	660	rBV	85372	151181	7.47%	0.648%
7	7.288	674	681	691	rBV	173656	288401	14.24%	1.237%
8	7.488	708	715	721	rBV	219344	364369	17.99%	1.563%
9	7.547	721	725	730	rVV	16821	25946	1.28%	0.111%
10	7.588	730	732	738	rVB5	2938	4630	0.23%	0.020%
11	7.958	788	795	802	rBV	270393	445158	21.98%	1.909%
12	8.017	802	805	812	rVB5	4870	7590	0.37%	0.033%
13	8.305	849	854	858	rBV3	2150	3293	0.16%	0.014%
14	8.651	905	913	922	rBV	227484	389771	19.25%	1.672%
15	9.109	984	991	998	rBV	216825	371701	18.36%	1.594%
16	9.286	1015	1021	1024	rBV3	1964	2944	0.15%	0.013%
17	9.673	1075	1087	1094	rBV	27788	44298	2.19%	0.190%
18	9.826	1106	1113	1121	rBV	173139	302998	14.96%	1.300%
19	10.049	1148	1151	1156	rVB4	2430	3255	0.16%	0.014%
20	10.367	1197	1205	1213	rBV	341675	592247	29.25%	2.540%
21	10.748	1262	1270	1278	rBV	404821	721553	35.63%	3.095%
22	10.878	1283	1292	1306	rBV	303365	546744	27.00%	2.345%
23	10.995	1306	1312	1313	rBV3	2757	3261	0.16%	0.014%
24	11.095	1325	1329	1335	rBV3	2198	3945	0.19%	0.017%
25	11.289	1356	1362	1365	rBV3	8877	14613	0.72%	0.063%
26	11.389	1373	1379	1385	rBV	23554	40275	1.99%	0.173%
27	11.483	1389	1395	1404	rVV	95402	174568	8.62%	0.749%
28	11.577	1407	1411	1417	rVV6	6032	11519	0.57%	0.049%
29	11.647	1419	1423	1426	rVV3	2461	4281	0.21%	0.018%
30	11.688	1429	1430	1438	rVB3	2298	2968	0.15%	0.013%
31	12.334	1535	1540	1545	rVB3	6211	9987	0.49%	0.043%
32	12.940	1639	1643	1647	rBV4	2985	5040	0.25%	0.022%
33	13.198	1682	1687	1692	rVV3	7160	12355	0.61%	0.053%
34	13.415	1720	1724	1730	rBV4	4462	5881	0.29%	0.025%
35	13.480	1732	1735	1739	rVB4	3645	5792	0.29%	0.025%
36	13.580	1749	1752	1757	rVB4	3089	5128	0.25%	0.022%

LSC Area Percent Report

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Acq On : 8 Aug 2024 3:49
Operator : MA/JU
Sample : P3437-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

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	13.780	1780	1786	1787	rBV3	2139	3140	0.16%	0.013%
38	13.985	1814	1821	1829	rVV	668883	940406	46.44%	4.034%
39	14.114	1837	1843	1848	rVB4	23326	34057	1.68%	0.146%
40	14.267	1857	1869	1877	rVV2	678903	1110061	54.82%	4.762%
41	14.484	1904	1906	1912	rVV3	6267	10612	0.52%	0.046%
42	14.573	1913	1921	1932	rVB	765940	1190158	58.78%	5.105%
43	14.649	1932	1934	1937	rBV4	3106	3256	0.16%	0.014%
44	14.755	1944	1952	1953	rBV2	93611	138783	6.85%	0.595%
45	14.808	1959	1961	1972	rVB	911820	977451	48.27%	4.193%
46	14.913	1975	1979	1984	rVB7	5644	8555	0.42%	0.037%
47	14.990	1990	1992	1996	rBV4	4975	6379	0.32%	0.027%
48	15.119	2011	2014	2020	rVB6	6706	9312	0.46%	0.040%
49	15.184	2021	2025	2027	rBV4	3146	4237	0.21%	0.018%
50	15.231	2030	2033	2036	rBV4	8202	11844	0.58%	0.051%
51	15.313	2045	2047	2051	rBV5	3298	4809	0.24%	0.021%
52	15.377	2054	2058	2064	rBV7	7789	14970	0.74%	0.064%
53	15.442	2067	2069	2074	rVB4	4471	4972	0.25%	0.021%
54	15.565	2083	2090	2099	rBV	979510	1461624	72.18%	6.270%
55	15.671	2101	2108	2117	rBV	224626	334897	16.54%	1.437%
56	15.736	2117	2119	2124	rVV4	6630	9975	0.49%	0.043%
57	15.794	2127	2129	2134	rVB5	5696	10355	0.51%	0.044%
58	15.877	2141	2143	2146	rBV4	4392	5380	0.27%	0.023%
59	16.006	2163	2165	2168	rVB4	5815	4863	0.24%	0.021%
60	16.071	2172	2176	2182	rVV3	26788	42660	2.11%	0.183%
61	16.123	2182	2185	2191	rVB8	9311	13075	0.65%	0.056%
62	16.223	2198	2202	2210	rVB	22473	37397	1.85%	0.160%
63	16.429	2234	2237	2239	rBV4	4253	5333	0.26%	0.023%
64	16.452	2239	2241	2244	rVV4	4263	4614	0.23%	0.020%
65	16.723	2283	2287	2292	rBV9	17220	28481	1.41%	0.122%
66	16.875	2310	2313	2318	rBV7	11259	21323	1.05%	0.091%
67	17.187	2364	2366	2367	rBV2	6875	5268	0.26%	0.023%
68	17.245	2372	2376	2380	rVV3	32826	46549	2.30%	0.200%
69	17.316	2382	2388	2393	rVB	928060	1346274	66.49%	5.775%
70	17.410	2399	2404	2411	rVB	1047675	1571428	77.61%	6.741%
71	17.492	2416	2418	2424	rVB6	14364	22028	1.09%	0.094%
72	17.710	2450	2455	2459	rBV7	15663	21782	1.08%	0.093%
73	17.997	2501	2504	2508	rVB5	18243	25202	1.24%	0.108%
74	18.091	2516	2520	2524	rBV6	18689	28246	1.39%	0.121%
75	18.221	2536	2542	2552	rBV	336922	528560	26.10%	2.267%
76	19.072	2685	2687	2696	rVB10	14824	25775	1.27%	0.111%

LSC Area Percent Report

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Acq On : 8 Aug 2024 3:49
Operator : MA/JU
Sample : P3437-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

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

77	19.166	2700	2703	2707	rVB3	36899	43061	2.13%	0.185%
78	19.260	2717	2719	2722	rVB4	19270	18135	0.90%	0.078%
79	19.337	2729	2732	2735	rBV2	16360	23727	1.17%	0.102%
80	19.489	2754	2758	2772	rBV	128689	199393	9.85%	0.855%
81	19.695	2787	2793	2802	rVB	1294805	1903273	93.99%	8.164%
82	21.234	3050	3055	3065	rBV	221913	329441	16.27%	1.413%
83	21.469	3093	3095	3101	rVB	32659	40256	1.99%	0.173%
84	21.551	3103	3109	3123	rVB2	924590	1526148	75.37%	6.546%
85	22.380	3245	3250	3257	rBV4	30084	62697	3.10%	0.269%
86	23.231	3389	3395	3406	rVB	126412	245901	12.14%	1.055%
87	23.390	3420	3422	3425	rBV3	7077	6596	0.33%	0.028%
88	23.825	3490	3496	3505	rBV	41919	97630	4.82%	0.419%
89	24.430	3589	3599	3616	rVB	768773	2024901	100.00%	8.686%
90	24.641	3625	3635	3647	rVV	591686	1633427	80.67%	7.007%
91	24.747	3648	3653	3661	rVB4	23339	55646	2.75%	0.239%
92	24.888	3676	3677	3679	rBV2	5547	3604	0.18%	0.015%
93	25.840	3833	3839	3848	rVB4	26038	67615	3.34%	0.290%
94	25.940	3848	3856	3866	rBV4	20999	74624	3.69%	0.320%
95	26.110	3883	3885	3888	rBV3	5432	6349	0.31%	0.027%
96	26.785	3993	4000	4002	rBV7	16330	33143	1.64%	0.142%
97	27.150	4057	4062	4063	rBV4	12003	16522	0.82%	0.071%
98	27.972	4200	4202	4207	rVB5	3559	4772	0.24%	0.020%
99	28.583	4304	4306	4309	rBV4	3521	3795	0.19%	0.016%
100	32.155	4912	4914	4918	rBV5	2669	3699	0.18%	0.016%

Sum of corrected areas: 23312895

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062318.D
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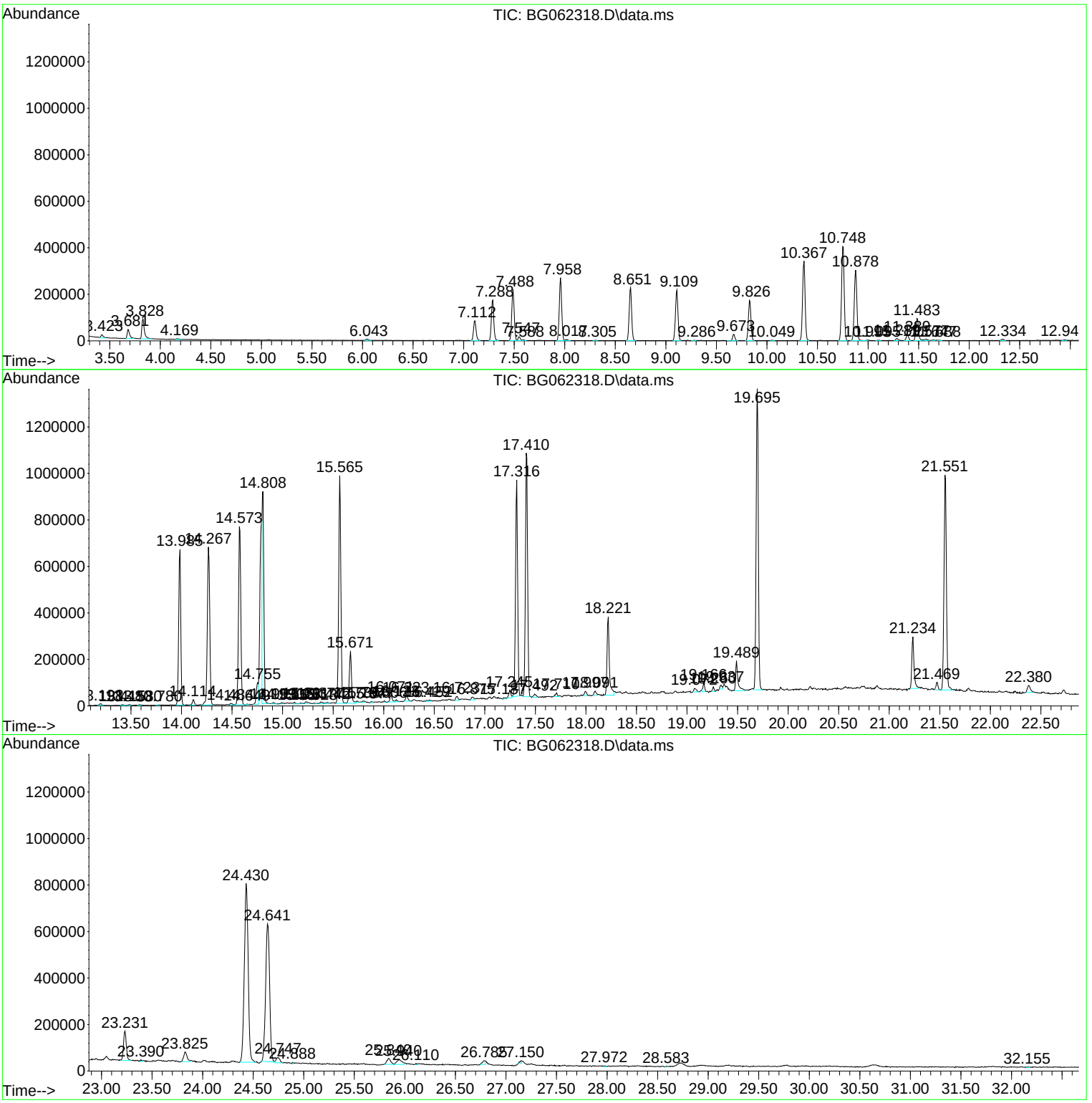
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

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\BG080824\
Data File : BG062318.D
Acq On : 8 Aug 2024 3:49
Operator : MA/JU
Sample : P3437-04
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

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

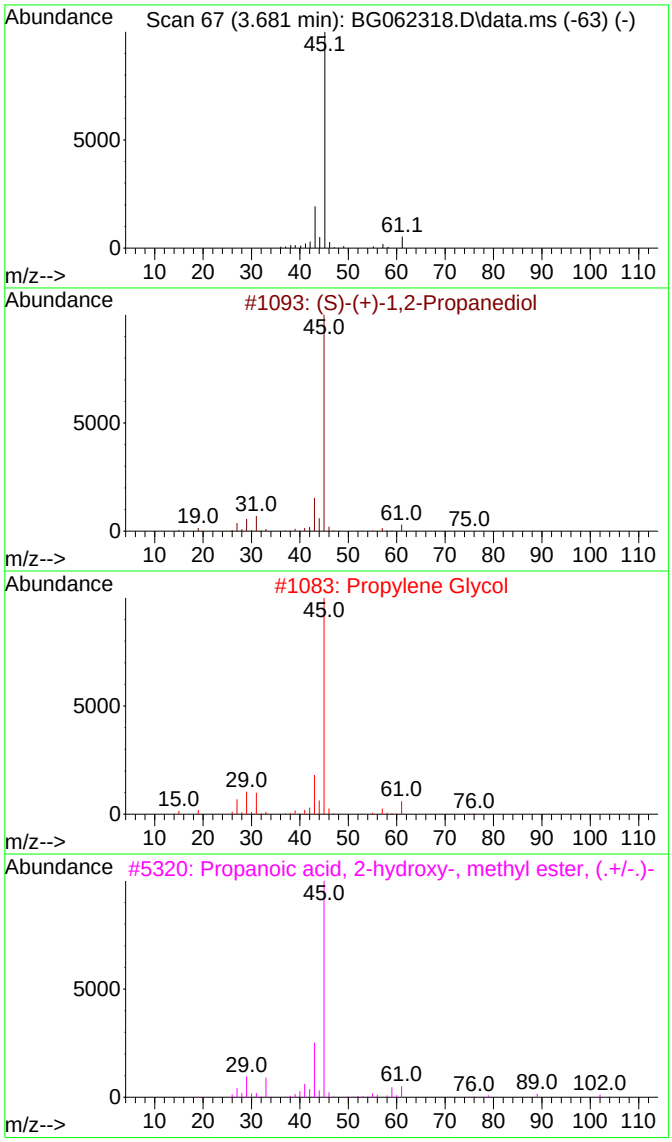
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

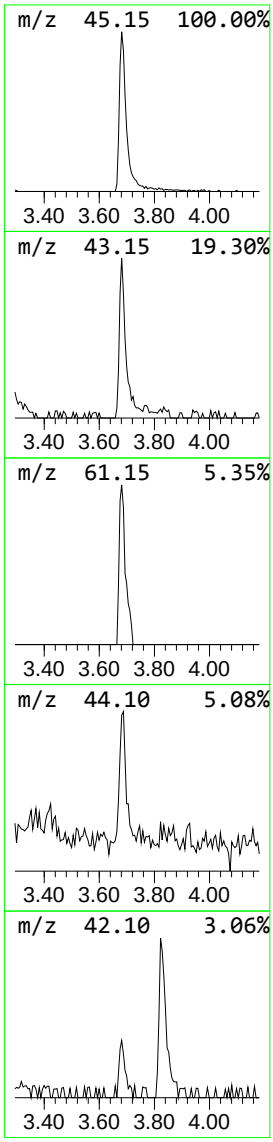
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.681	2.86 ng/ul	63760	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	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	43
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	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\BG080824\
Data File : BG062318.D
Acq On : 8 Aug 2024 3:49
Operator : MA/JU
Sample : P3437-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

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

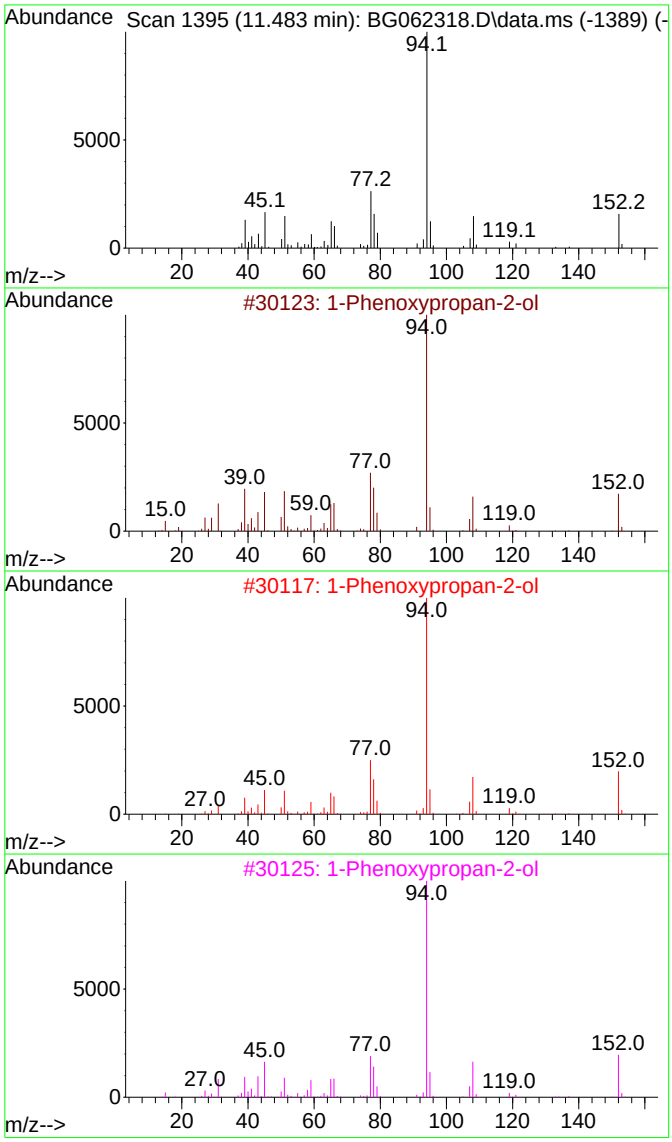
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

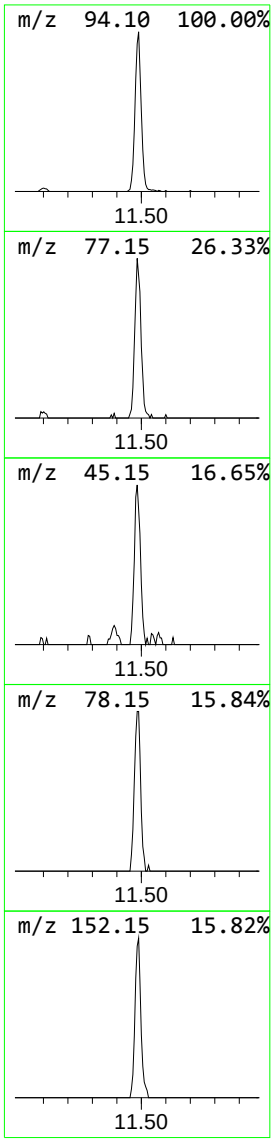
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.483	4.84 ng/ul	174568	Naphthalene-d8	10.754

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	96
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
5	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
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Operator : MA/JU
Sample : P3437-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

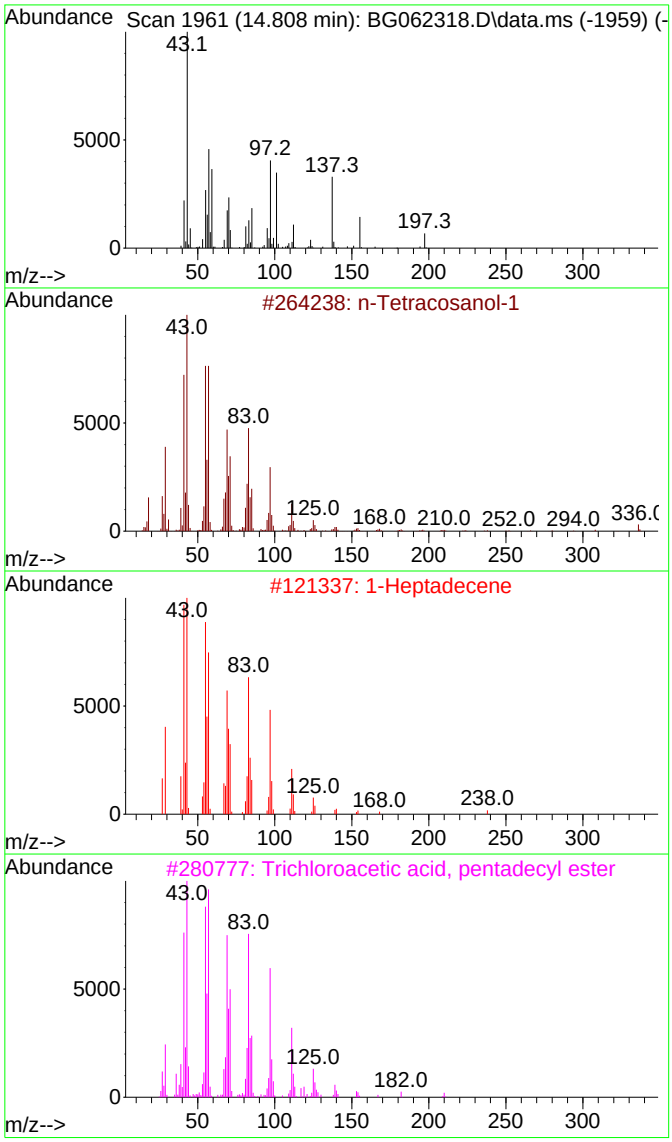
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

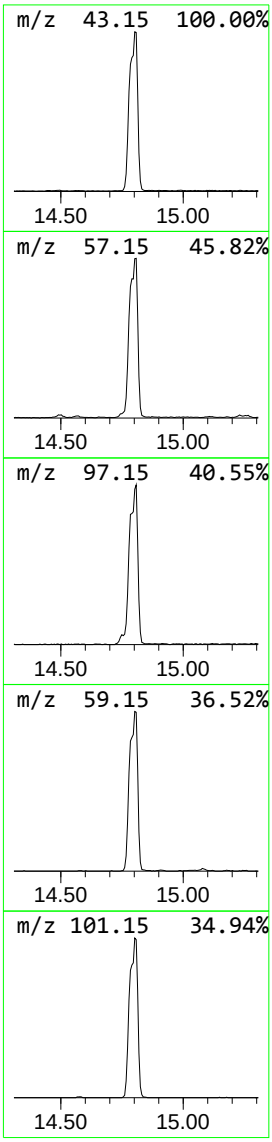
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.808	16.43 ng/ul	977451	Acenaphthene-d10	14.573

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	32
2	1-Heptadecene	238	C17H34	006765-39-5	17
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	13
4	3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	12
5	1-Hexacosanol	382	C26H54O	000506-52-5	12





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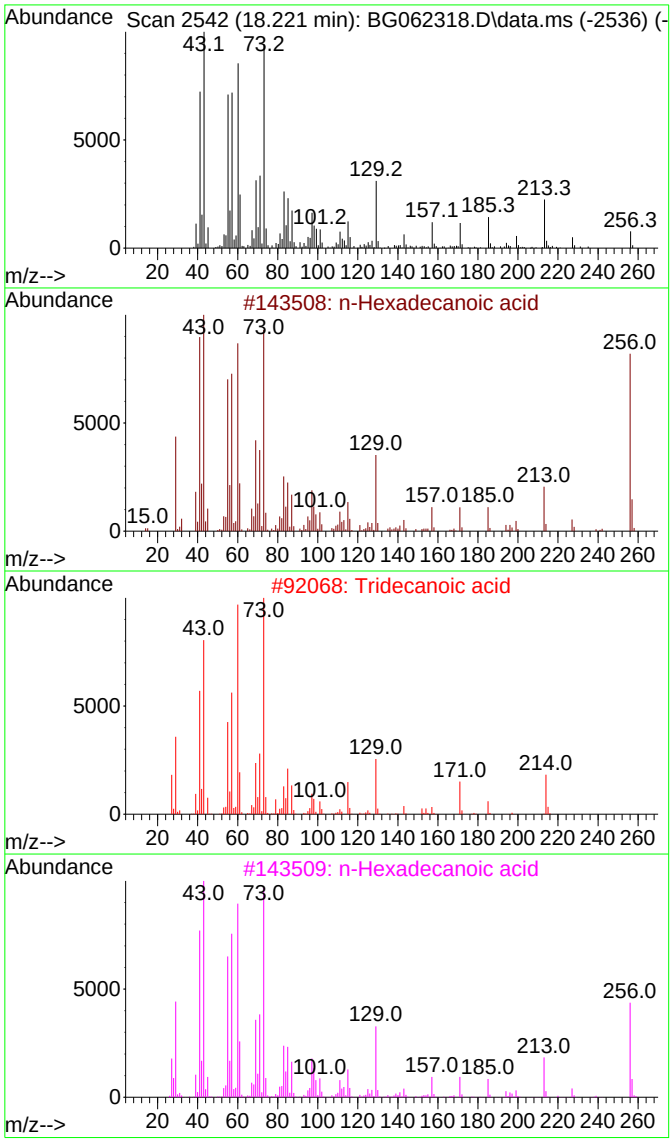
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

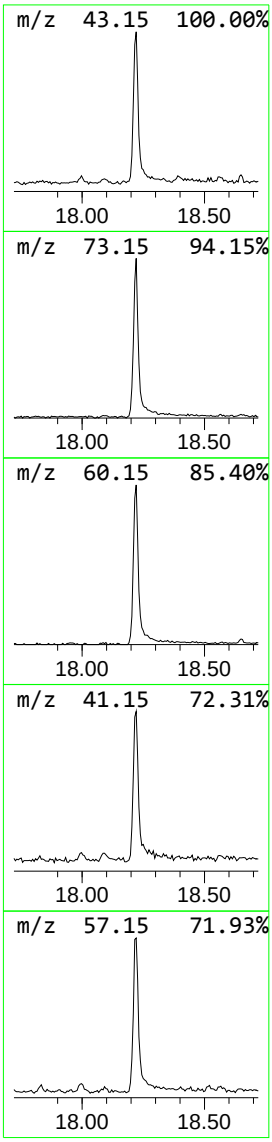
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.221	7.85 ng/ul	528560	Phenanthrene-d10	17.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062318.D
Acq On : 8 Aug 2024 3:49
Operator : MA/JU
Sample : P3437-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

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

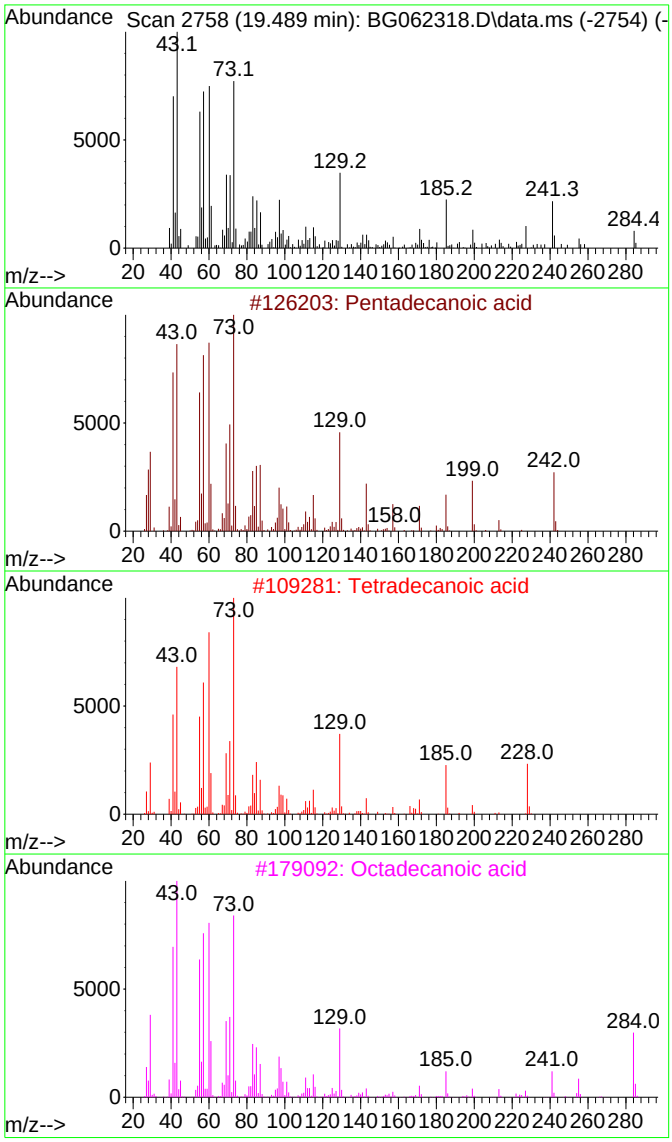
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

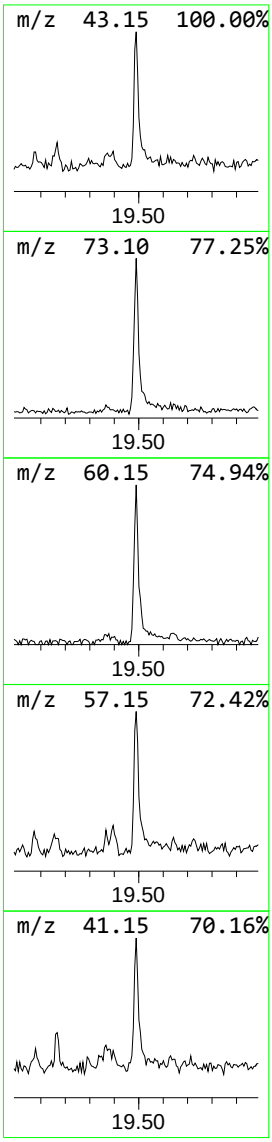
****

Peak Number 5 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.490	2.61 ng/ul	199393	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	Octadecanoic acid	284	C18H36O2	000057-11-4	74
4	Octadecanoic acid	284	C18H36O2	000057-11-4	72
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





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Data File : BG062318.D
Acq On : 8 Aug 2024 3:49
Operator : MA/JU
Sample : P3437-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

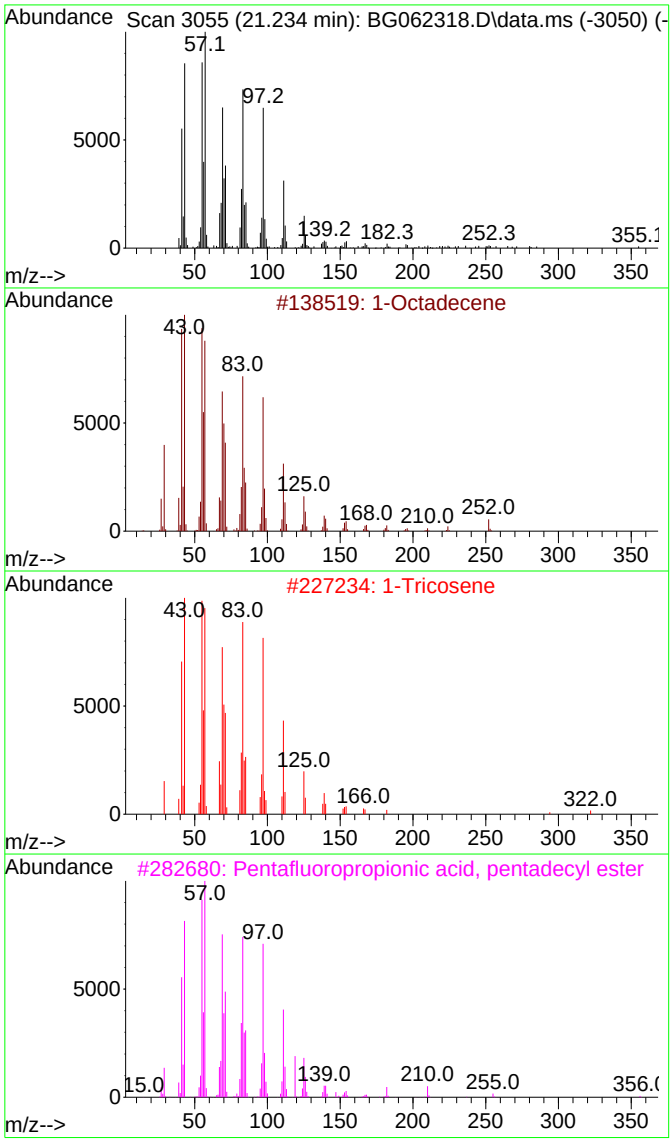
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

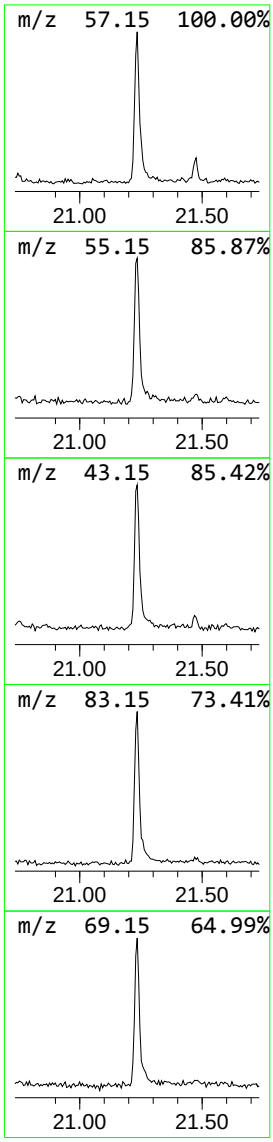
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.234	4.32 ng/ul	329441	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	95
2	1-Tricosene	322	C23H46	018835-32-0	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062318.D
Acq On : 8 Aug 2024 3:49
Operator : MA/JU
Sample : P3437-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

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

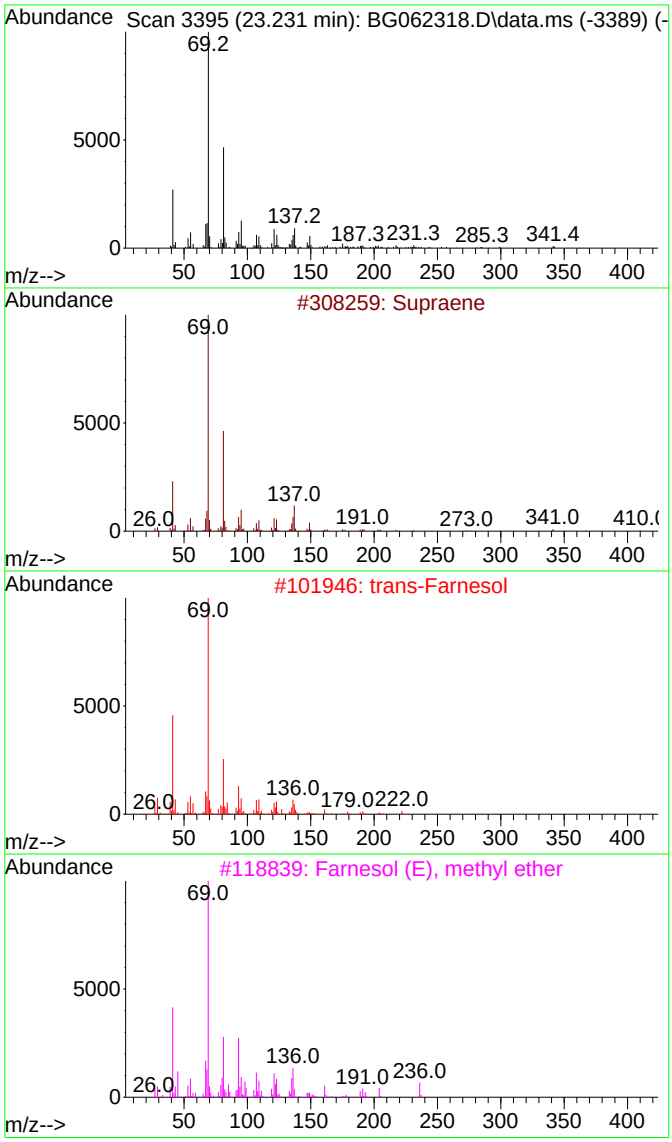
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

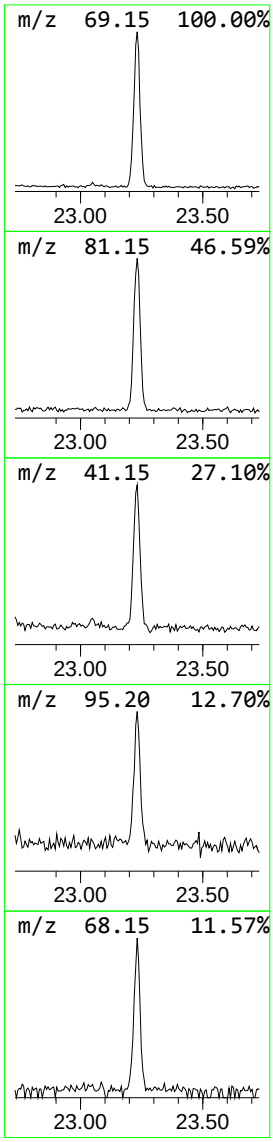
****

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.232	3.01 ng/ul	245901	Perylene-d12	24.647

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	trans-Farnesol	222	C15H26O	000106-28-5	78
3	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72
4	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72
5	4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062318.D
Acq On : 8 Aug 2024 3:49
Operator : MA/JU
Sample : P3437-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :

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...	3.681	2.9	ng/ul	63760	1	7.958	445158	20.0
1-Phenoxypropan...	11.483	4.8	ng/ul	174568	2	10.754	721553	20.0
unknown-01	14.808	16.4	ng/ul	977451	3	14.573	1190160	20.0
n-Hexadecanoic ...	18.221	7.8	ng/ul	528560	4	17.316	1346270	20.0
Pentadecanoic acid	19.490	2.6	ng/ul	199393	5	21.551	1526150	20.0
(DEL) Alkane: S...	21.234	4.3	ng/ul	329441	5	21.551	1526150	20.0
Supraene	23.232	3.0	ng/ul	245901	6	24.647	1633430	20.0