LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : E05W7

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: BG062321.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.421	19	22	31	rVB3	12590	20185	1.38%	0.107%
2	3.679	63	66	74	rBV	20367	33334	2.28%	0.177%
3	3.826	87	91	106	rBV	66481	116888	7.99%	0.619%
4	6.041	462	468	479	rVB	10450	17969	1.23%	0.095%
5	7.110	643	650	661	rVB	72658	129016	8.82%	0.684%
6	7.286	673	680	693	rVB	101568	174736	11.95%	0.926%
7	7.486	707	714	721	rBV	138266	242607	16.59%	1.285%
8	7.550	721	725	731	rVB	11195	16550	1.13%	0.088%
9	7.956	785	794	801	rBV	234969	408983	27.97%	2.167%
10	8.014	801	804	810	rVB4	7487	12269	0.84%	0.065%
11	8.649	904	912	923	rBV	166903	280070	19.15%	1.484%
12	9.107	983	990	1003	rBV	128932	221433	15.14%	1.173%
13	9.671	1080	1086	1094	rVB	45168	70747	4.84%	0.375%
14	9.830	1106	1113	1121	rBV	98884	175508	12.00%	0.930%
15	9.965	1129	1136	1146	rBV3	12736	27833	1.90%	0.147%
16	10.241	1177	1183	1188	rBV3	4724	8099	0.55%	0.043%
17	10.364	1197	1204	1218	rVB	195130	349146	23.87%	1.850%
18	10.752	1262	1270	1280	rVB	383911	665319	45.50%	3.525%
19	10.875	1282	1291	1302	rBV	256080	476347	32.57%	2.524%
20	11.286	1354	1361	1366	rBV2	15490	25016	1.71%	0.133%
21	11.486	1388	1395	1406	rBV	118372	213683	14.61%	1.132%
22	13.196	1682	1686	1691	rBV3	4724	7673	0.52%	0.041%
23	13.419	1720	1724	1729	rVV2	3375	5925	0.41%	0.031%
24	13.983	1813	1820	1830	rVV	350229	507758	34.72%	2.690%
25	14.229	1857	1862	1863	rVV2	11558	15826	1.08%	0.084%
26	14.265	1863	1868	1877	rVB	371133	589835	40.33%	3.125%
27	14.488	1900	1906	1910	rBV3	3579	5825	0.40%	0.031%
28	14.576	1913	1921	1928	rVV	685440	1059666	72.46%	5.614%
29	14.682	1933	1939	1942	rVB4	8334	11657	0.80%	0.062%
30	14.752	1942	1951	1952	rBV	72657	108156	7.40%	0.573%
31	14.788	1952	1957	1958	rVV	607382	892831	61.05%	4.730%
32	14.805	1958	1960	1968	rVV	722128	782359	53.50%	4.145%
33	14.911	1974	1978	1984	rVV5	3473	7204	0.49%	0.038%
34	14.987	1987	1991	1996	rVV5	9623	13877	0.95%	0.074%
35	15.316	2041	2047	2051	rBV5	5228	8623	0.59%	0.046%
36	15.381	2054	2058	2065	rVB6	5486	10068	0.69%	0.053%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

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	15.445	2065	2069	2071	rBV3	4930	6713	0.46%	0.036%
38	15.563	2083	2089	2096	rBV	520390	776795	53.12%	4.115%
39	15.669	2101	2107	2115	rBV2	111221	171214	11.71%	0.907%
40	15.739	2115	2119	2122	rVV	5155	6713	0.46%	0.036%
41	15.945	2148	2154	2158	rBV7	4123	8183	0.56%	0.043%
42	16.004	2158	2164	2165	rBV5	4308	6426	0.44%	0.034%
43	16.115	2178	2183	2188	rBV4	6617	11256	0.77%	0.060%
44	16.233	2201	2203	2209	rVB5	6269	9021	0.62%	0.048%
45	16.303	2209	2215	2219	rBV4	9588	17100	1.17%	0.091%
46	16.720	2282	2286	2288	rBV3	7288	9230	0.63%	0.049%
47	16.879	2309	2313	2317	rVV4	8910	12308	0.84%	0.065%
48	16.932	2318	2322	2327	rVV4	4483	7321	0.50%	0.039%
49	17.043	2337	2341	2345	rBV5	6125	10047	0.69%	0.053%
50	17.090	2346	2349	2352	rVV4	8425	10840	0.74%	0.057%
51	17.131	2354	2356	2363	rVB7	6539	7598	0.52%	0.040%
52	17.249	2371	2376	2378	rBV3	9938	12897	0.88%	0.068%
53	17.314	2380	2387	2394	rVV	806463	1227664	83.95%	6.504%
54	17.413	2397	2404	2412	rVV	586362	877748	60.02%	4.650%
55	17.496	2414	2418	2422	rVB7	4451	6685	0.46%	0.035%
56	17.701	2451	2453	2458	rVB4	5567	6730	0.46%	0.036%
57	17.825	2471	2474	2478	rBV5	7000	10758	0.74%	0.057%
58	17.995	2500	2503	2508	rVB	15955	20275	1.39%	0.107%
59	18.083	2515	2518	2526	rVB6	8951	13482	0.92%	0.071%
60	18.218	2535	2541	2550	rBV	372037	547241	37.42%	2.899%
61	18.559	2597	2599	2604	rVB5	3905	6513	0.45%	0.035%
62	18.647	2611	2614	2617	rBV5	5373	6674	0.46%	0.035%
63	18.882	2650	2654	2658	rBV7	7522	8822	0.60%	0.047%
64	19.023	2672	2678	2682	rBV6	13728	23861	1.63%	0.126%
65	19.076	2682	2687	2689	rBV5	8235	12820	0.88%	0.068%
66	19.164	2694	2702	2707	rVB6	41385	67813	4.64%	0.359%
67	19.264	2716	2719	2722	rBV3	10189	11416	0.78%	0.060%
68	19.299	2722	2725	2727	rBV3	9415	9840	0.67%	0.052%
69	19.340	2727	2732	2734	rVV3	31342	46850	3.20%	0.248%
70	19.370	2734	2737	2746	rVB9	25767	52508	3.59%	0.278%
71	19.487	2753	2757	2766	rBV	127547	186310	12.74%	0.987%
72	19.640	2781	2783	2786	rVB3	9145	8106	0.55%	0.043%
73	19.693	2786	2792	2800	rVV	760147	1077447	73.68%	5.708%
74	19.757	2800	2803	2806	rVB3	19355	19729	1.35%	0.105%
75	20.116	2859	2864	2869	rBV6	10170	18109	1.24%	0.096%
76	20.216	2877	2881	2884	rBV4	16197	20082	1.37%	0.106%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

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

77	20.257	2884	2888	2892	rVB	40924	46481	3.18%	0.246%
78	20.603	2944	2947	2948	rBV3	6895	6051	0.41%	0.032%
79	20.750	2964	2972	2975	rVV2	43214	69302	4.74%	0.367%
80	20.779	2975	2977	2981	rVB5	10649	11816	0.81%	0.063%
81	20.856	2987	2990	2993	rBV2	6251	7370	0.50%	0.039%
82	21.232	3049	3054	3064	rBV	330454	520253	35.58%	2.756%
83	21.549	3101	3108	3119	rBV2	837315	1394020	95.32%	7.386%
84	21.778	3143	3147	3153	rVB	49223	70940	4.85%	0.376%
85	22.371	3242	3248	3258	rVB2	57310	119228	8.15%	0.632%
86	22.524	3270	3274	3277	rBV5	23265	37463	2.56%	0.198%
87	22.653	3293	3296	3301	rBV7	10931	18759	1.28%	0.099%
88	23.047	3358	3363	3369	rVB2	41868	77093	5.27%	0.408%
89	23.229	3387	3394	3403	rVB2	79299	153242	10.48%	0.812%
90	23.828	3490	3496	3501	rBV2	42744	88602	6.06%	0.469%
91	24.427	3587	3598	3611	rBV	422174	1105469	75.59%	5.857%
92	24.639	3623	3634	3645	rBV	530838	1462400	100.00%	7.748%
93	24.745	3645	3652	3659	rVB2	41623	96014	6.57%	0.509%
94	25.837	3831	3838	3846	rBV3	37077	99104	6.78%	0.525%
95	25.937	3848	3855	3872	rVB6	32406	113110	7.73%	0.599%
96	26.783	3992	3999	4006	rBV6	13415	41624	2.85%	0.221%
97	27.141	4051	4060	4071	rBV4	30645	104183	7.12%	0.552%
98	28.716	4318	4328	4346	rVB8	25886	116125	7.94%	0.615%
99	29.756	4499	4505	4506	rBV5	11146	19751	1.35%	0.105%
100	30.032	4550	4552	4560	rVB9	7834	12340	0.84%	0.065%

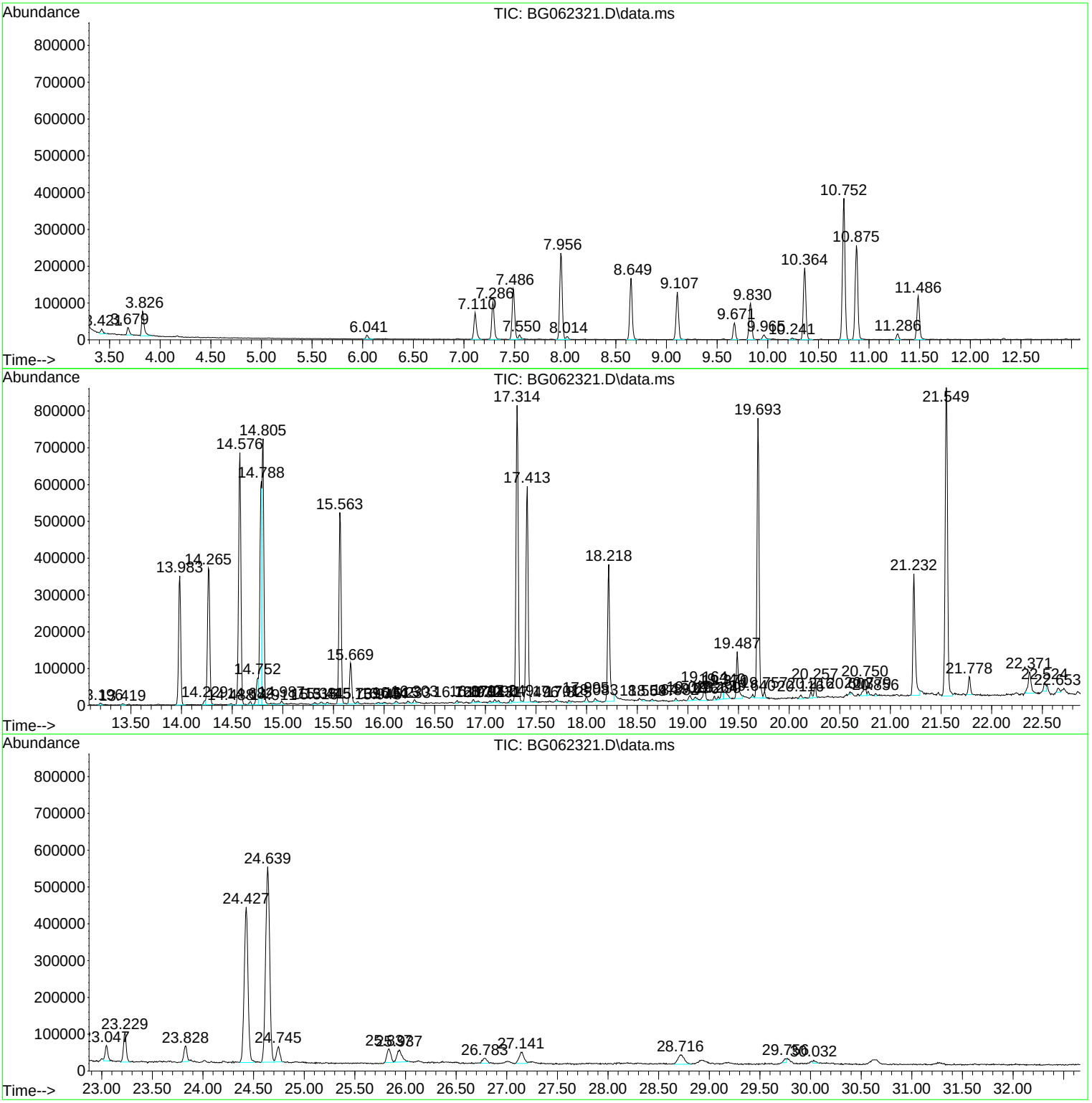
Sum of corrected areas: 18874906

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

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 : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

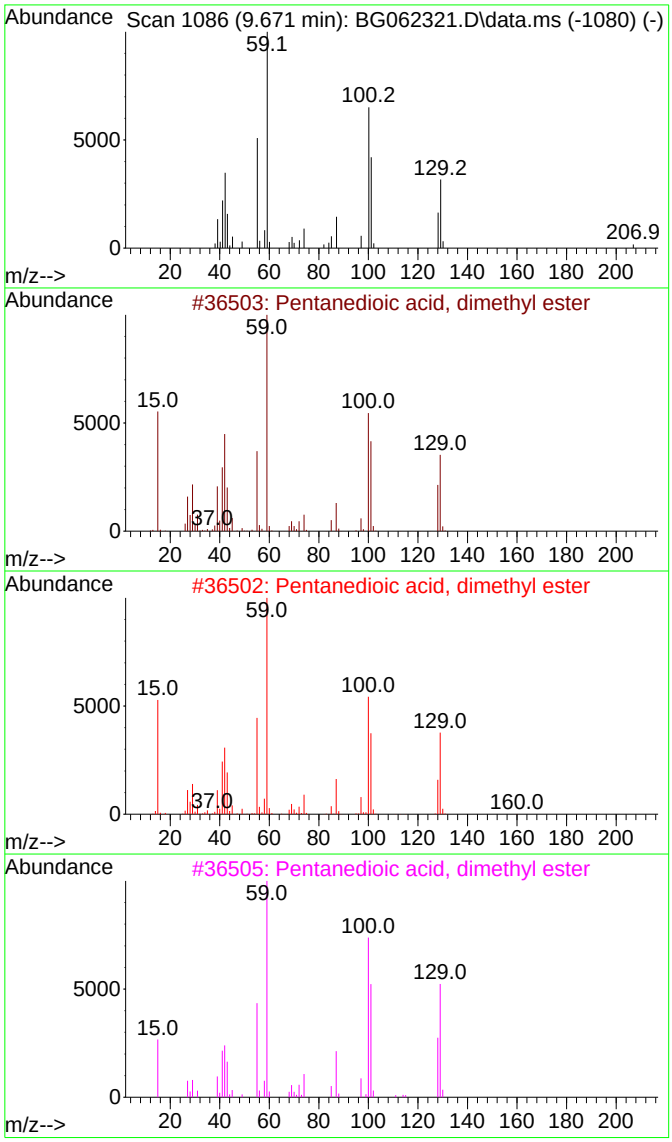
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

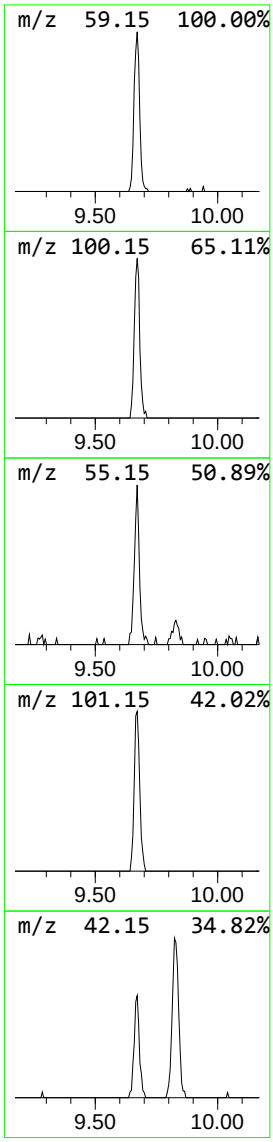
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentanedioic acid, dimethyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.671	2.13 ng/ul	70747	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	83
2	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	78
3	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	64
4	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	59
5	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

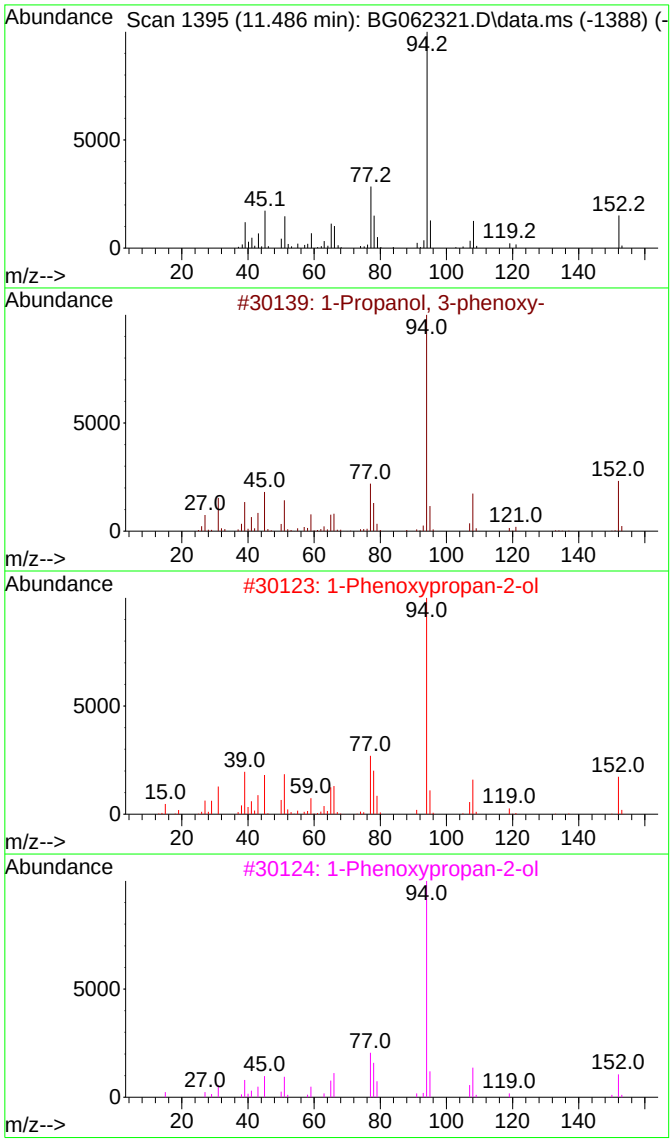
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

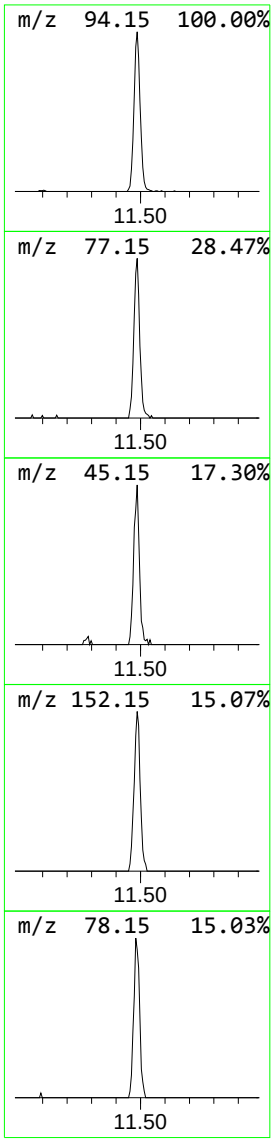
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propanol, 3-phenoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.486	6.42 ng/ul	213683	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	70
3	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	64
4	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

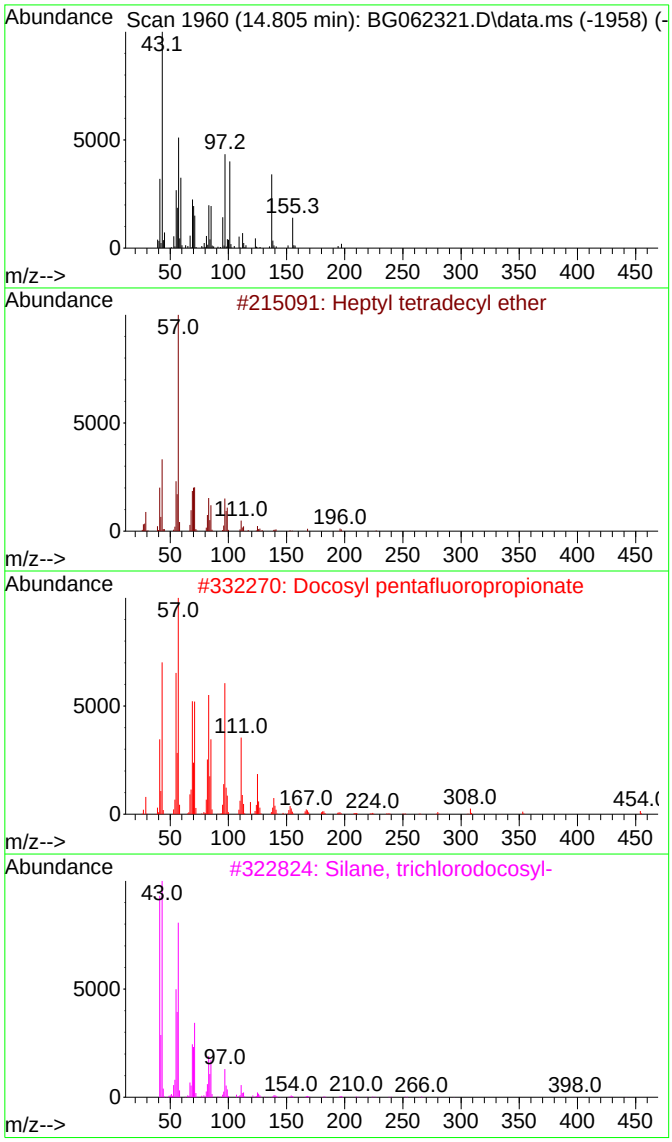
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

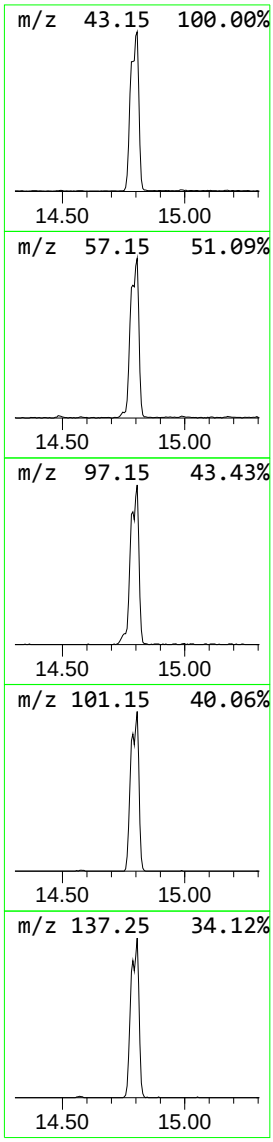
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.805	14.77 ng/ul	782359	Acenaphthene-d10	14.576

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptyl tetradecyl ether	312	C21H44O	1000406-39-3	16
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	12
3	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	12
4	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	12
5	6,10,13-Trimethyltetradecanol	256	C17H36O	1000131-71-0	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

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

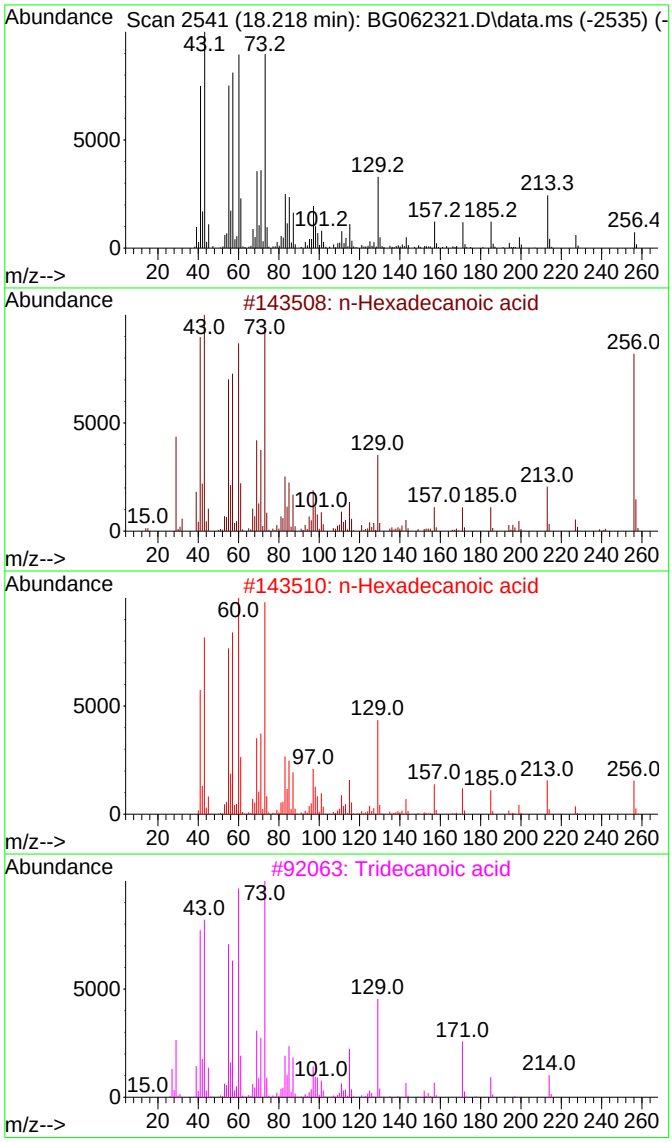
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

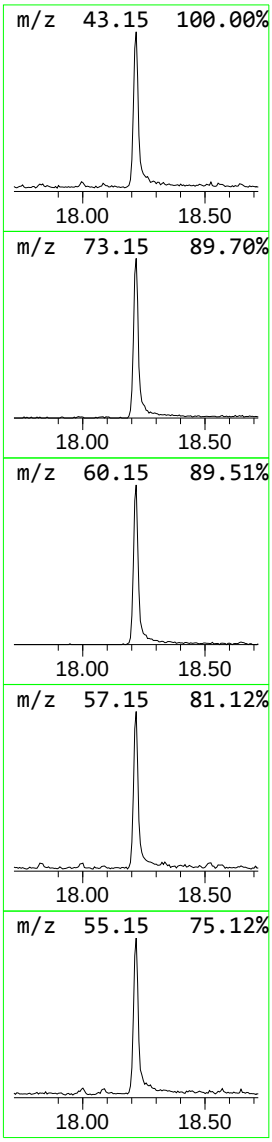
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.218	8.92 ng/ul	547241	Phenanthrene-d10	17.314

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

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

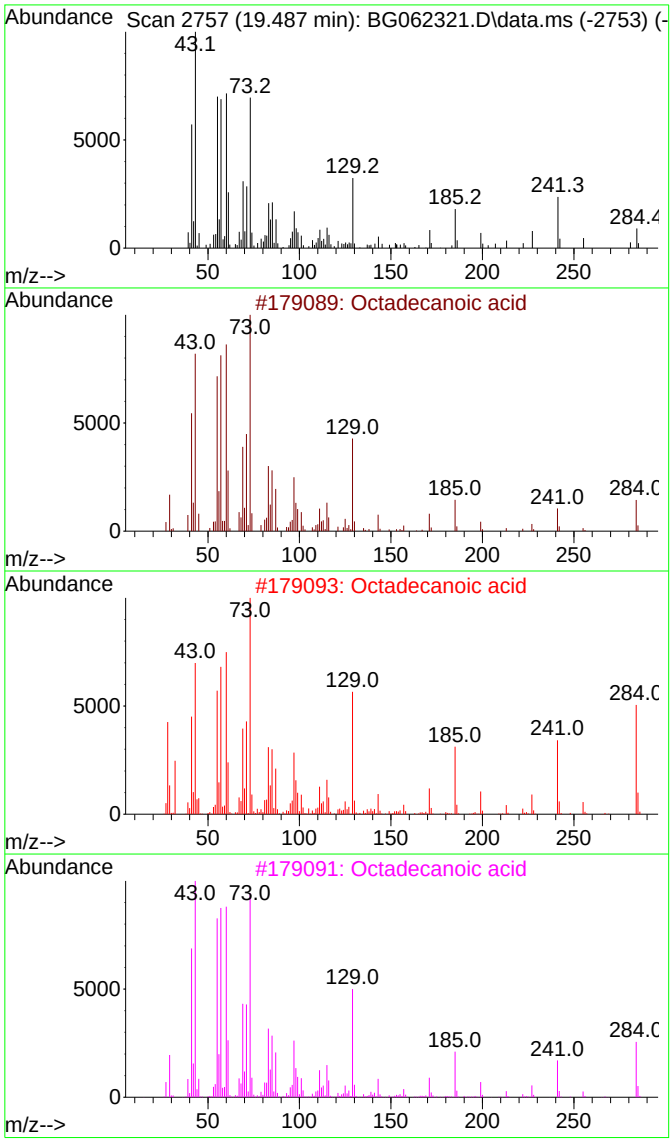
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

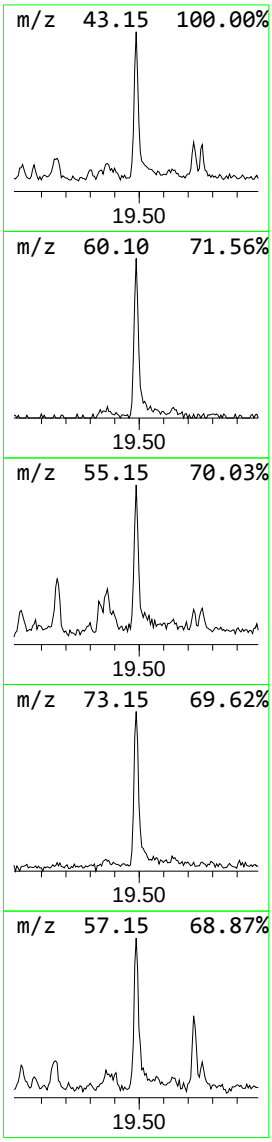
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.487	2.67 ng/ul	186310	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	83
3	Octadecanoic acid	284	C18H36O2	000057-11-4	76
4	Octadecanoic acid	284	C18H36O2	000057-11-4	74
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64





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Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

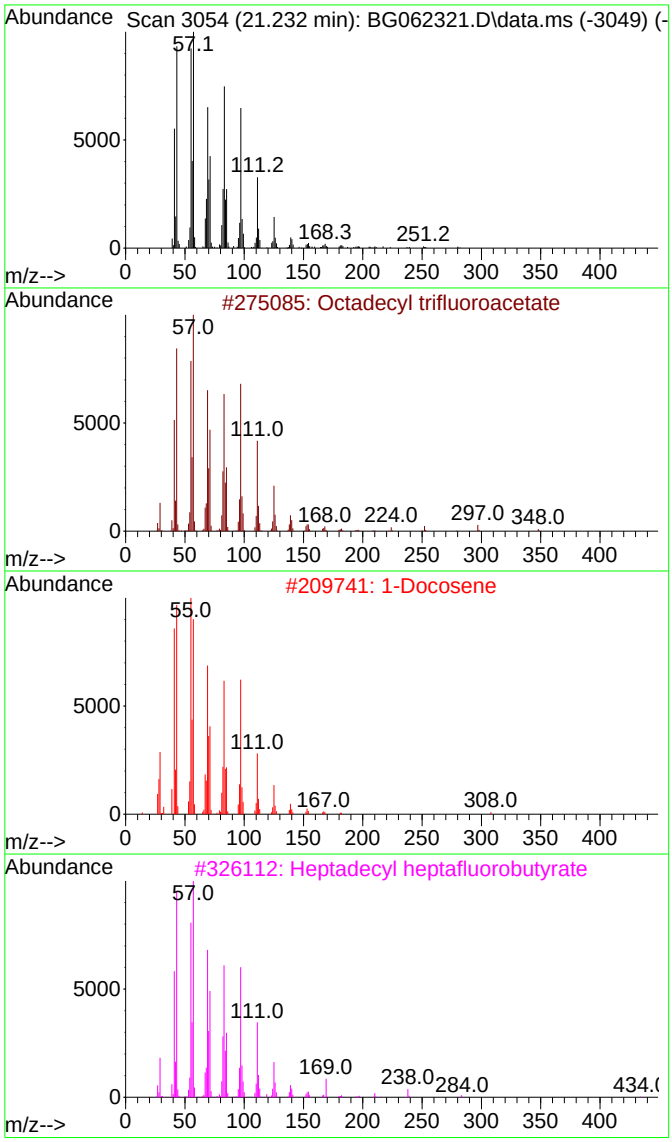
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG080524.MA.M
Quant Title : SVOA CALIBRATION

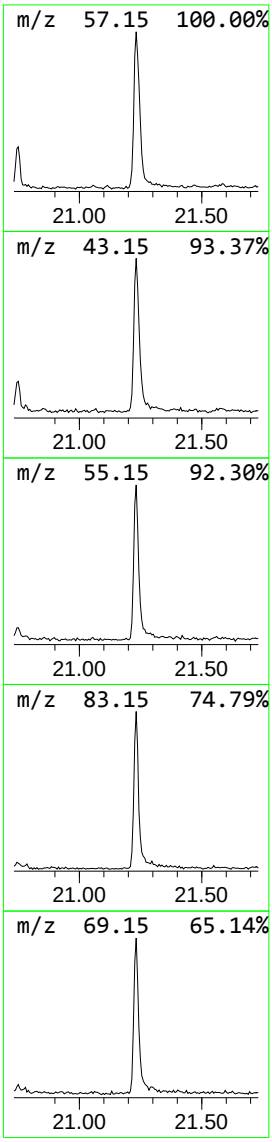
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Octadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.232	7.46 ng/ul	520253	Chrysene-d12	21.555

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

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

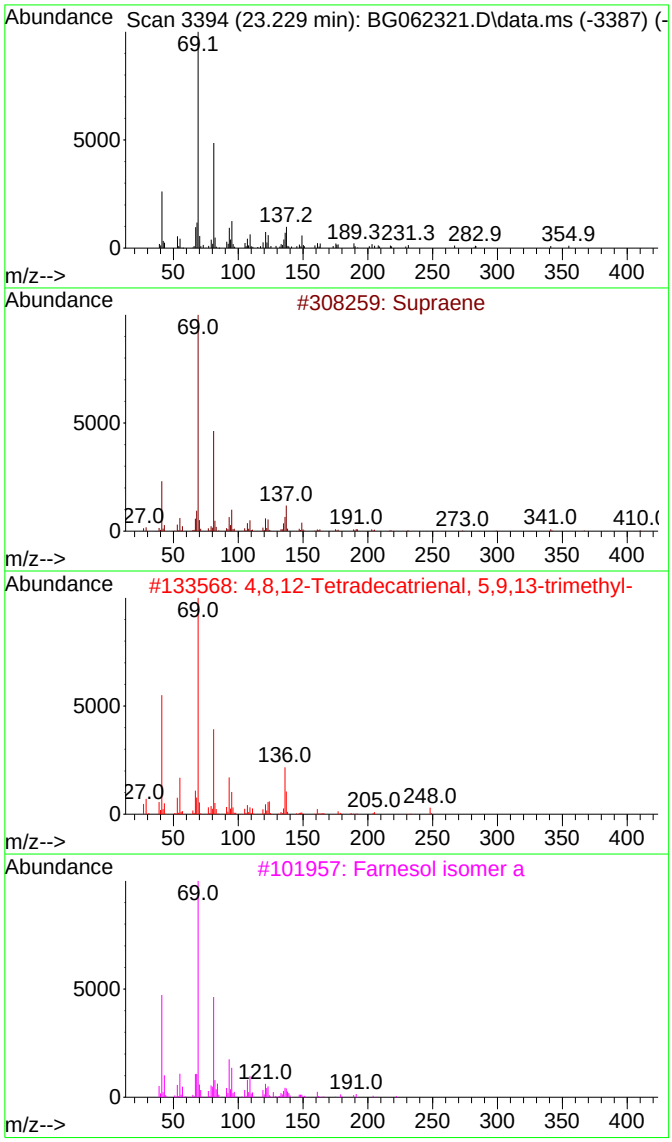
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

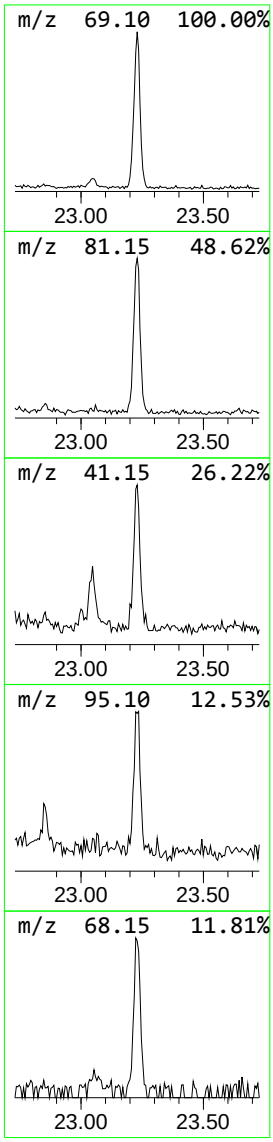
****

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.229	2.10 ng/ul	153242	Perylene-d12	24.639

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
3	Farnesol isomer a	222	C15H26O	1000108-92-4	72
4	Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	64
5	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080824\
Data File : BG062321.D
Acq On : 8 Aug 2024 5:53
Operator : MA/JU
Sample : P3437-06
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
E05W7

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
Pentanedioic ac...	9.671	2.1	ng/ul	70747	2	10.752	665319	20.0
1-Propanol, 3-p...	11.486	6.4	ng/ul	213683	2	10.752	665319	20.0
unknown-01	14.805	14.8	ng/ul	782359	3	14.576	1059670	20.0
n-Hexadecanoic ...	18.218	8.9	ng/ul	547241	4	17.314	1227660	20.0
Octadecanoic acid	19.487	2.7	ng/ul	186310	5	21.555	1394020	20.0
Octadecyl trifl...	21.232	7.5	ng/ul	520253	5	21.555	1394020	20.0
Supraene	23.229	2.1	ng/ul	153242	6	24.639	1462400	20.0