LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
Data File : BG056801.D
Acq On : 2 Mar 2023 22:16
Operator : CG/JU
Sample : 01710-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBAB3

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-BG022323.M
Title : SVOA CALIBRATION

Signal : TIC: BG056801.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.254	118	122	126	rVB3	5480	7640	2.25%	0.181%
2	5.441	320	324	331	rVB3	6838	10670	3.14%	0.252%
3	7.538	675	681	689	rVB2	49658	85975	25.31%	2.033%
4	7.721	705	712	719	rBV	30530	50219	14.78%	1.187%
5	7.938	743	749	757	rVB	40142	65977	19.42%	1.560%
6	8.414	824	830	839	rBV2	53561	89103	26.23%	2.107%
7	8.725	879	883	890	rBV4	4764	7048	2.07%	0.167%
8	8.913	910	915	917	rBV2	728	1266	0.37%	0.030%
9	9.101	941	947	955	rVB2	49505	83196	24.49%	1.967%
10	9.248	967	972	980	rVB4	4764	9095	2.68%	0.215%
11	9.589	1023	1030	1039	rVB2	43347	76912	22.64%	1.818%
12	9.971	1092	1095	1098	rVB3	959	1222	0.36%	0.029%
13	10.318	1148	1154	1161	rVB2	36515	65533	19.29%	1.549%
14	10.453	1175	1177	1183	rVB4	1470	1878	0.55%	0.044%
15	10.746	1223	1227	1232	rBV3	1042	2140	0.63%	0.051%
16	10.858	1240	1246	1254	rVV2	58017	100740	29.65%	2.382%
17	11.011	1269	1272	1279	rVB4	3719	5788	1.70%	0.137%
18	11.064	1279	1281	1286	rBV2	1137	1525	0.45%	0.036%
19	11.258	1307	1314	1321	rVB	78847	139114	40.95%	3.289%
20	11.375	1328	1334	1342	rBV2	27398	50308	14.81%	1.189%
21	12.021	1441	1444	1447	rVB2	1139	1020	0.30%	0.024%
22	12.803	1575	1577	1584	rVV4	1131	1549	0.46%	0.037%
23	12.873	1584	1589	1594	rVB	16436	23569	6.94%	0.557%
24	13.743	1732	1737	1738	rBV3	1315	1518	0.45%	0.036%
25	13.819	1747	1750	1754	rVB	1718	1688	0.50%	0.040%
26	13.884	1759	1761	1765	rBV2	1029	1141	0.34%	0.027%
27	13.931	1765	1769	1772	rVV3	1236	1358	0.40%	0.032%
28	14.348	1835	1840	1844	rBV3	9081	11324	3.33%	0.268%
29	14.407	1844	1850	1857	rVB	119886	166235	48.93%	3.930%
30	14.718	1897	1903	1910	rVB2	126299	198371	58.39%	4.690%
31	15.018	1944	1954	1961	rBV	144981	230623	67.88%	5.452%
32	15.177	1974	1981	1988	rBV	51577	80403	23.67%	1.901%
33	15.341	2002	2009	2011	rBV2	1287	2126	0.63%	0.050%
34	15.400	2018	2019	2024	rVB	933	1054	0.31%	0.025%
35	15.464	2024	2030	2031	rBV	811	837	0.25%	0.020%
36	15.758	2076	2080	2083	rVB	1475	1571	0.46%	0.037%

LSC Area Percent Report

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Operator : CG/JU
Sample : 01710-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAB3

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-BG022323.M
Title : SVOA CALIBRATION

37	16.005	2115	2122	2131	rBV	168328	256617	75.53%	6.067%
38	16.099	2133	2138	2144	rBV	55946	78616	23.14%	1.859%
39	16.352	2173	2181	2187	rBV	38444	54335	15.99%	1.285%
40	16.534	2210	2212	2219	rVV2	441	863	0.25%	0.020%
41	16.657	2230	2233	2235	rBV	827	847	0.25%	0.020%
42	16.710	2239	2242	2245	rVB	844	1107	0.33%	0.026%
43	17.421	2358	2363	2365	rVB2	1230	1221	0.36%	0.029%
44	17.597	2389	2393	2396	rBV	1322	1969	0.58%	0.047%
45	17.756	2412	2420	2426	rBV	196413	298740	87.93%	7.063%
46	17.856	2430	2437	2443	rVB	168995	255345	75.16%	6.037%
47	17.909	2443	2446	2449	rBV2	2720	2824	0.83%	0.067%
48	17.938	2449	2451	2454	rVB3	1702	1396	0.41%	0.033%
49	18.009	2458	2463	2464	rBV2	992	1498	0.44%	0.035%
50	18.249	2501	2504	2507	rBV	1193	987	0.29%	0.023%
51	18.379	2523	2526	2527	rBV	993	1106	0.33%	0.026%
52	18.490	2542	2545	2552	rVB4	3006	4938	1.45%	0.117%
53	18.549	2552	2555	2557	rBV2	1554	1527	0.45%	0.036%
54	18.590	2557	2562	2572	rBV2	29644	46501	13.69%	1.099%
55	18.714	2582	2583	2586	rBV	1054	988	0.29%	0.023%
56	18.831	2600	2603	2604	rBV	1183	1172	0.34%	0.028%
57	18.872	2608	2610	2614	rVB	962	1103	0.32%	0.026%
58	18.949	2621	2623	2626	rVB	908	1036	0.30%	0.024%
59	19.007	2629	2633	2637	rBV3	5468	6499	1.91%	0.154%
60	19.113	2647	2651	2656	rVB5	1370	2611	0.77%	0.062%
61	19.184	2660	2663	2664	rBV3	1318	908	0.27%	0.021%
62	19.378	2693	2696	2697	rBV3	875	1128	0.33%	0.027%
63	19.401	2697	2700	2703	rVV3	2115	2280	0.67%	0.054%
64	19.454	2707	2709	2712	rVV2	1181	944	0.28%	0.022%
65	19.507	2714	2718	2720	rVV2	2218	2526	0.74%	0.060%
66	19.607	2731	2735	2736	rBV3	1734	2176	0.64%	0.051%
67	19.730	2753	2756	2758	rBV4	3376	3855	1.13%	0.091%
68	19.812	2769	2770	2772	rBV2	1441	1149	0.34%	0.027%
69	19.842	2772	2775	2778	rBV3	5574	7220	2.13%	0.171%
70	20.112	2815	2821	2829	rVB	238282	339745	100.00%	8.032%
71	20.188	2832	2834	2835	rVB2	1800	834	0.25%	0.020%
72	20.271	2846	2848	2851	rBV3	1760	2120	0.62%	0.050%
73	20.365	2862	2864	2865	rBV2	1523	912	0.27%	0.022%
74	20.459	2876	2880	2884	rBV4	4696	7098	2.09%	0.168%
75	20.494	2884	2886	2887	rBV2	1739	885	0.26%	0.021%
76	20.535	2889	2893	2897	rBV	12166	18411	5.42%	0.435%

LSC Area Percent Report

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Sample : 01710-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAB3

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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Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Title : SVOA CALIBRATION

77	20.664	2913	2915	2917	rBV3	1743	1055	0.31%	0.025%
78	20.835	2941	2944	2946	rBV4	2241	2825	0.83%	0.067%
79	20.876	2949	2951	2952	rBV2	3608	2202	0.65%	0.052%
80	21.064	2979	2983	2986	rBV	13047	18262	5.38%	0.432%
81	21.093	2986	2988	2991	rVB4	4479	3662	1.08%	0.087%
82	21.463	3046	3051	3056	rVB	47912	66301	19.51%	1.567%
83	21.540	3061	3064	3067	rBV5	3171	4758	1.40%	0.112%
84	21.634	3075	3080	3093	rBV2	42971	80292	23.63%	1.898%
85	21.904	3122	3126	3129	rVB4	3489	4788	1.41%	0.113%
86	22.063	3146	3153	3159	rBV2	179901	308424	90.78%	7.292%
87	22.492	3223	3226	3233	rVB9	8492	13139	3.87%	0.311%
88	22.909	3290	3297	3303	rBV7	18297	39693	11.68%	0.938%
89	24.530	3567	3573	3578	rVB5	13555	26113	7.69%	0.617%
90	25.341	3701	3711	3723	rVB2	100817	292833	86.19%	6.923%
91	25.588	3743	3753	3765	rVB3	101893	311505	91.69%	7.365%
92	25.935	3810	3812	3813	rVB	2727	1096	0.32%	0.026%
93	26.828	3958	3964	3975	rVB6	14558	44479	13.09%	1.052%
94	29.566	4428	4430	4432	rBV3	2367	2194	0.65%	0.052%
95	29.853	4477	4479	4480	rBV2	2372	1079	0.32%	0.026%
96	31.076	4685	4687	4689	rBV2	1975	2487	0.73%	0.059%
97	31.904	4825	4828	4829	rBV3	2608	2241	0.66%	0.053%
98	32.022	4846	4848	4849	rBV2	2437	1348	0.40%	0.032%
99	32.333	4899	4901	4902	rBV2	2214	1232	0.36%	0.029%
100	32.556	4937	4939	4940	rBV2	2431	2008	0.59%	0.047%

Sum of corrected areas: 4229789

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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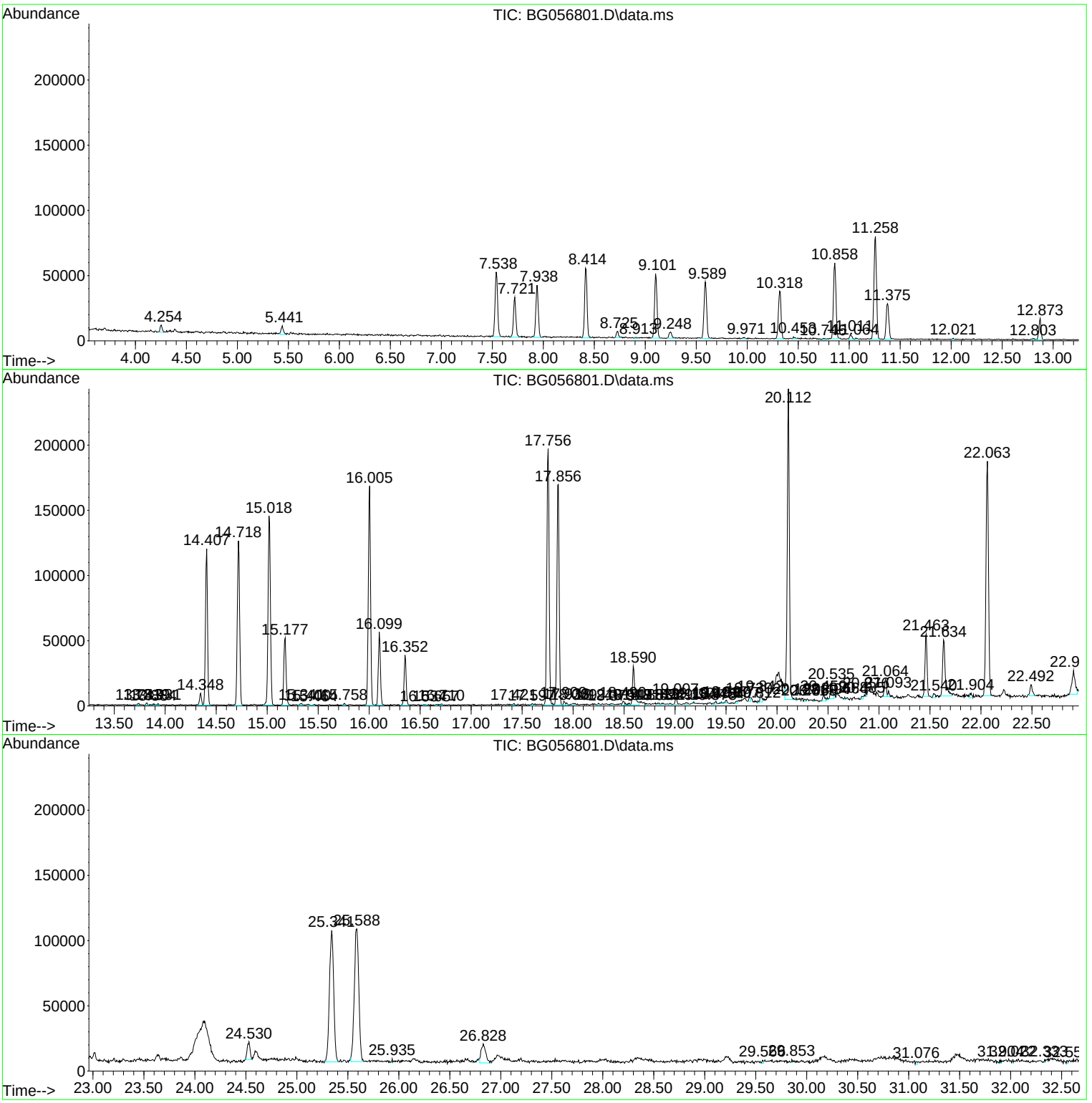
ClientSampleId :
DBAB3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
Data File : BG056801.D
Acq On : 2 Mar 2023 22:16
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Misc :
ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
DBAB3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

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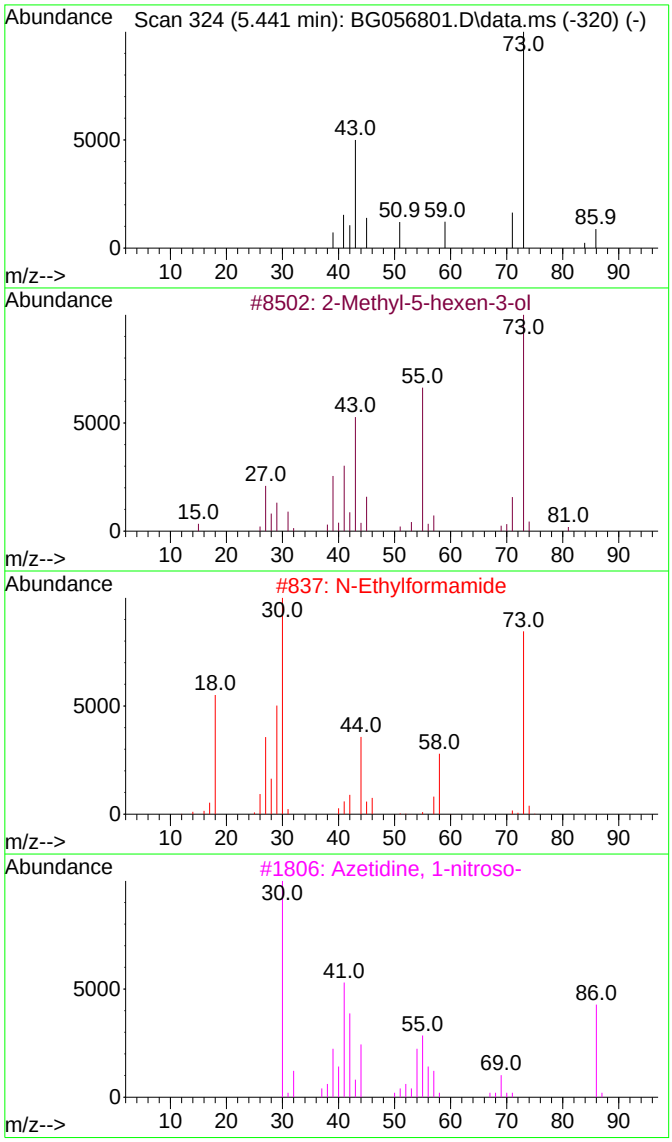
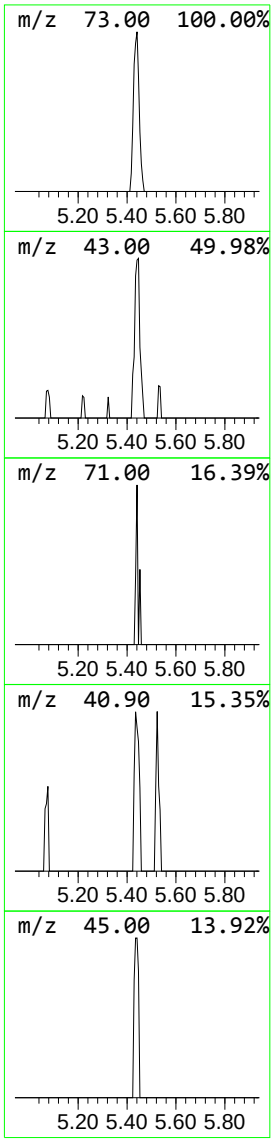
Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.441	2.39 ng/ul	10670	1,4-Dichlorobenzene-d4	8.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
2	N-Ethylformamide	73	C3H7NO	000627-45-2	5
3	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	4
4	1,4-Butanediamine	88	C4H12N2	000110-60-1	4
5	N-Ethylformamide	73	C3H7NO	000627-45-2	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
Data File : BG056801.D
Acq On : 2 Mar 2023 22:16
Operator : CG/JU
Sample : 01710-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

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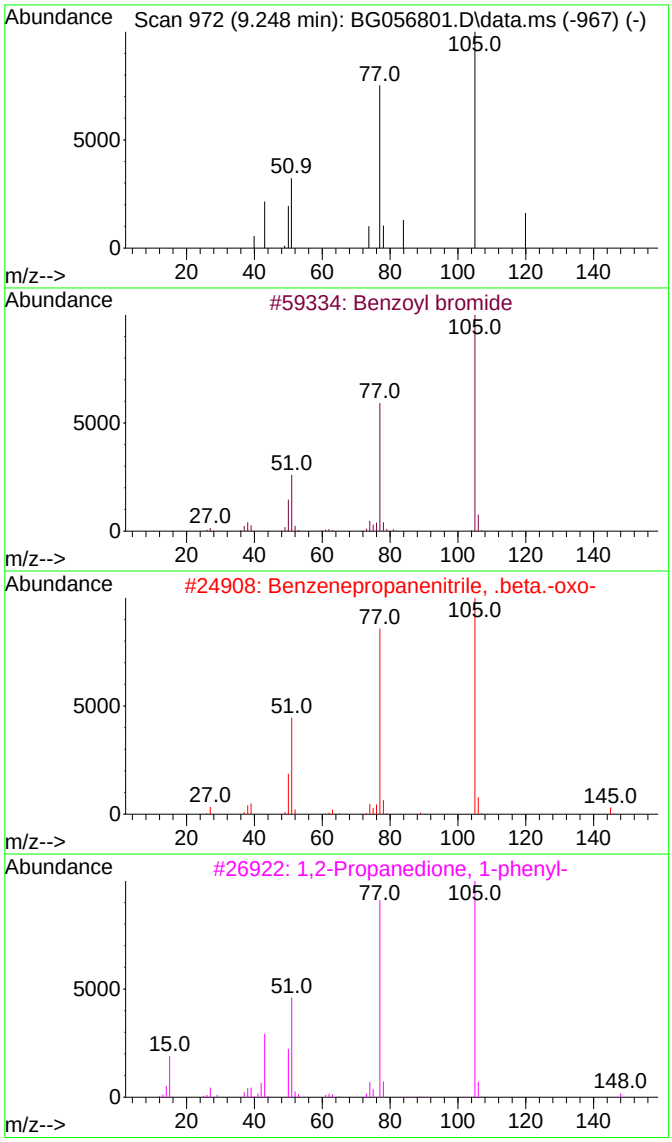
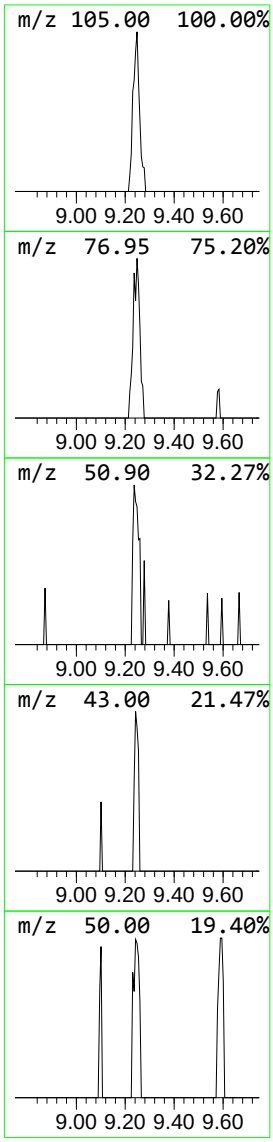
Peak Number 2 Benzoyl bromide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.248	2.04 ng/ul	9095	1,4-Dichlorobenzene-d4	8.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoyl bromide	184	C7H5BrO	000618-32-6	56
2	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	56
3	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	56
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	56
5	Acetophenone	120	C8H8O	000098-86-2	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

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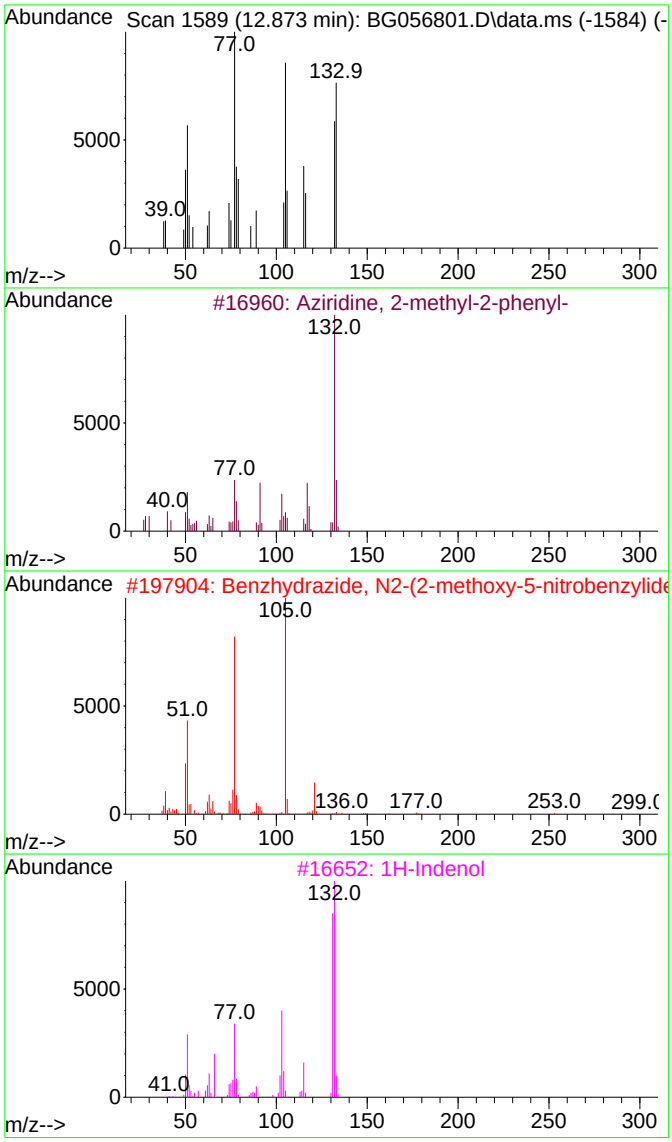
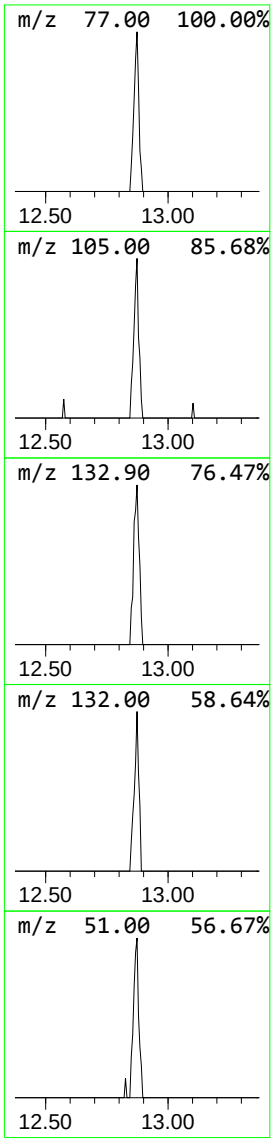
Peak Number 3 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.873	3.39 ng/ul	23569	Naphthalene-d8	11.258

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 2-methyl-2-phenyl-	133	C9H11N	022596-57-2	38
2	Benzhydrazide, N2-(2-methoxy-5-n...	299	C15H13N3O4	349572-84-5	35
3	1H-Indenol	132	C9H8O	056631-57-3	17
4	ethanone, 2-chloro-2,2-difluoro-...	190	C8H5ClF2O	1000400-22-4	16
5	Benzamide	121	C7H7NO	000055-21-0	12





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

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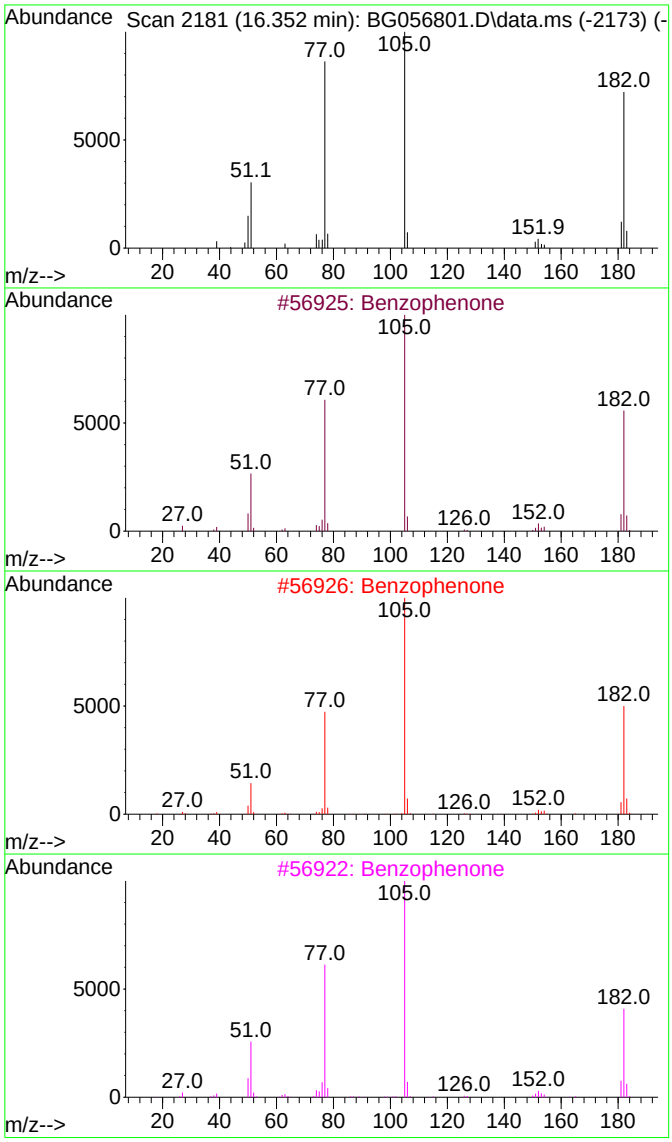
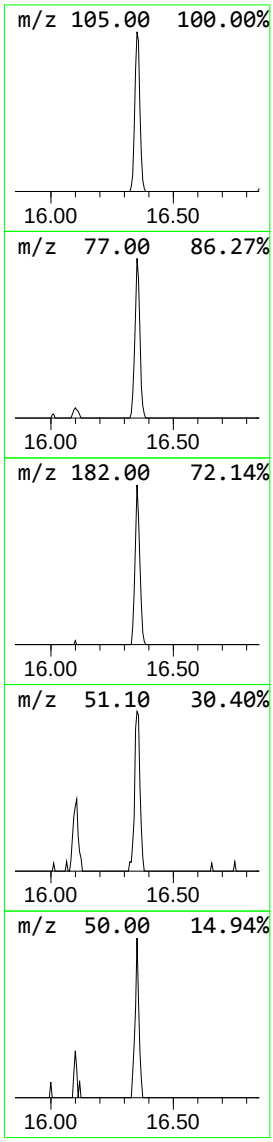
Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.352	4.71 ng/ul	54335	Acenaphthene-d10	15.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	94
2	Benzophenone	182	C13H10O	000119-61-9	91
3	Benzophenone	182	C13H10O	000119-61-9	76
4	Benzophenone	182	C13H10O	000119-61-9	72
5	Benzophenone	182	C13H10O	000119-61-9	68





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Data File : BG056801.D
Acq On : 2 Mar 2023 22:16
Operator : CG/JU
Sample : 01710-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAB3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

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

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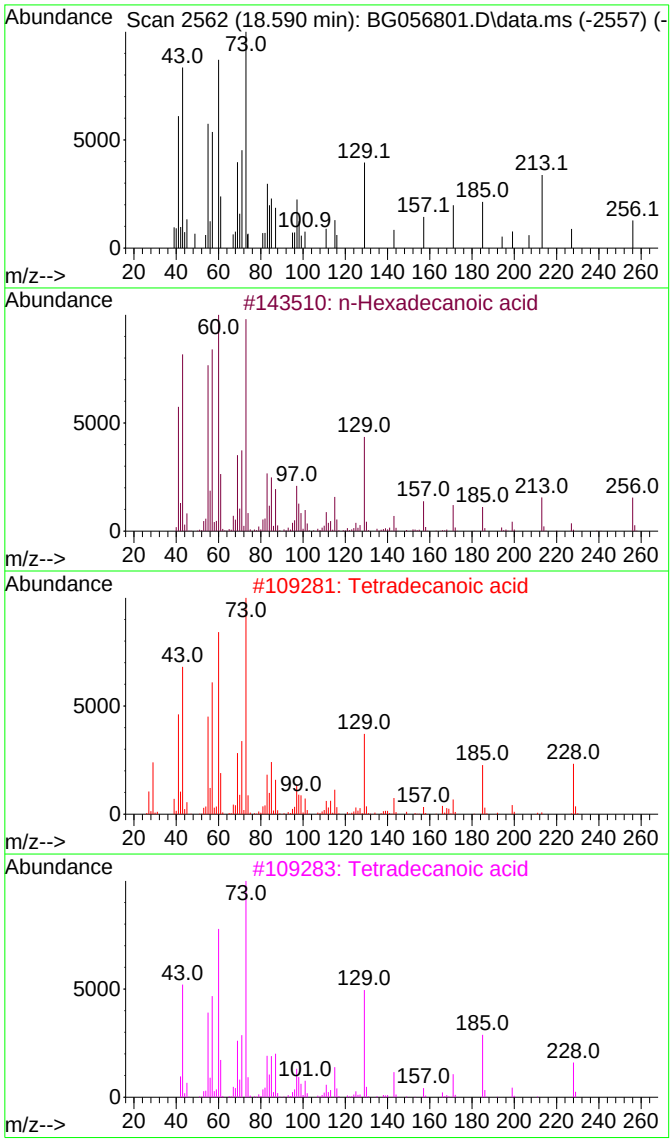
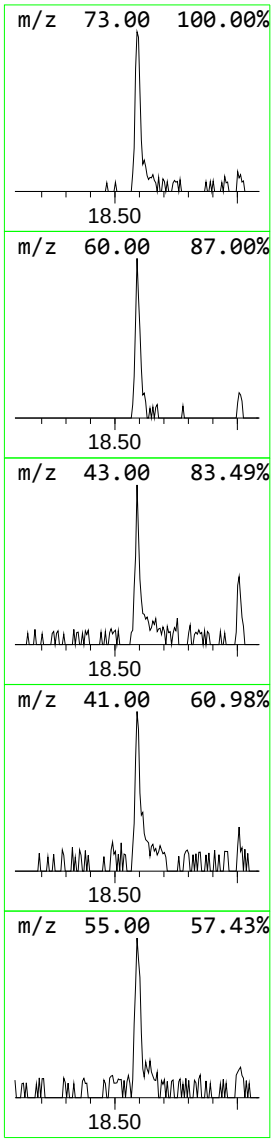
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.590	3.11 ng/ul	46501	Phenanthrene-d10	17.756

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030223\
Data File : BG056801.D
Acq On : 2 Mar 2023 22:16
Operator : CG/JU
Sample : 01710-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAB3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

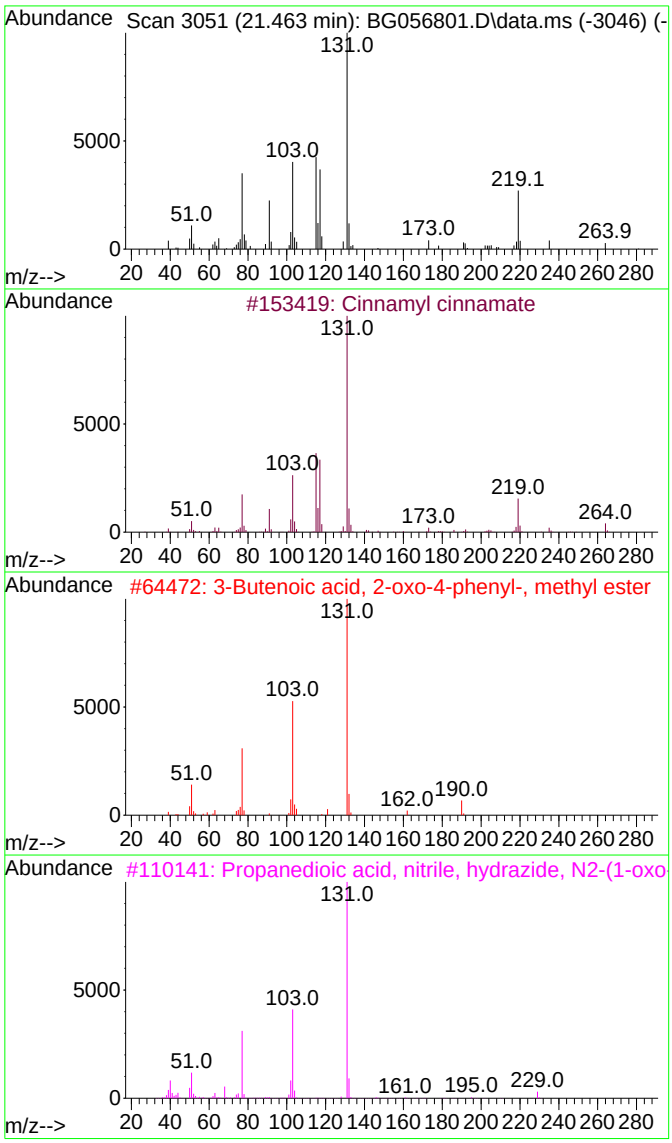
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

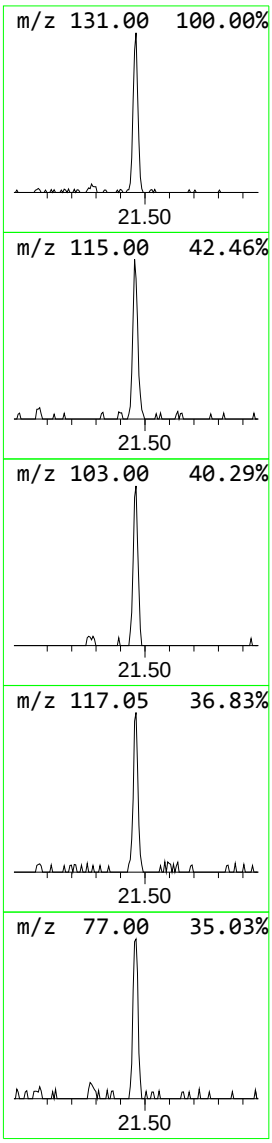
****

Peak Number 6 Cinnamyl cinnamate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.463	4.30 ng/ul	66301	Chrysene-d12	22.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	58
2	3-Butenoic acid, 2-oxo-4-phenyl-...	190	C11H10O3	1000142-22-4	49
3	Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	49
4	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47
5	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47





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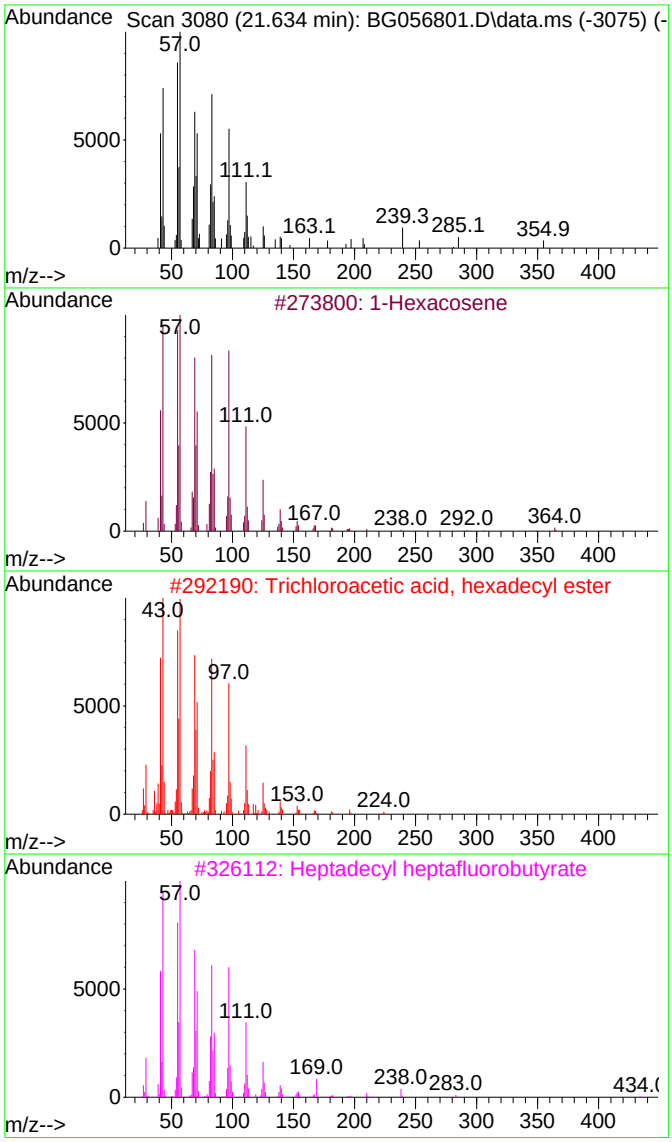
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

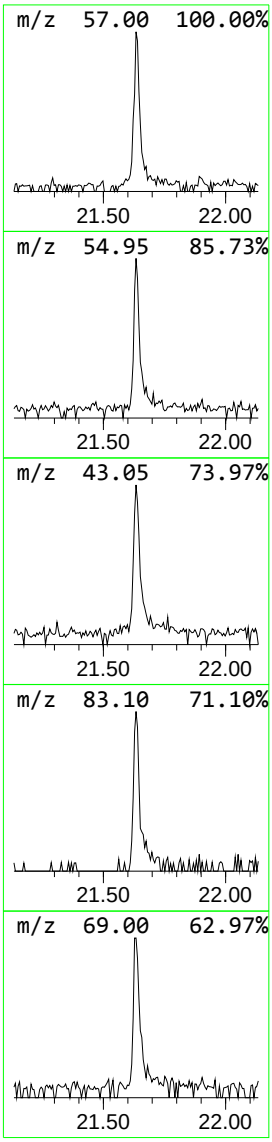
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.634	5.21 ng/ul	80292	Chrysene-d12	22.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	90
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
5	1-Hexacosanol	382	C26H54O	000506-52-5	90





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Data File : BG056801.D
Acq On : 2 Mar 2023 22:16
Operator : CG/JU
Sample : 01710-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAB3

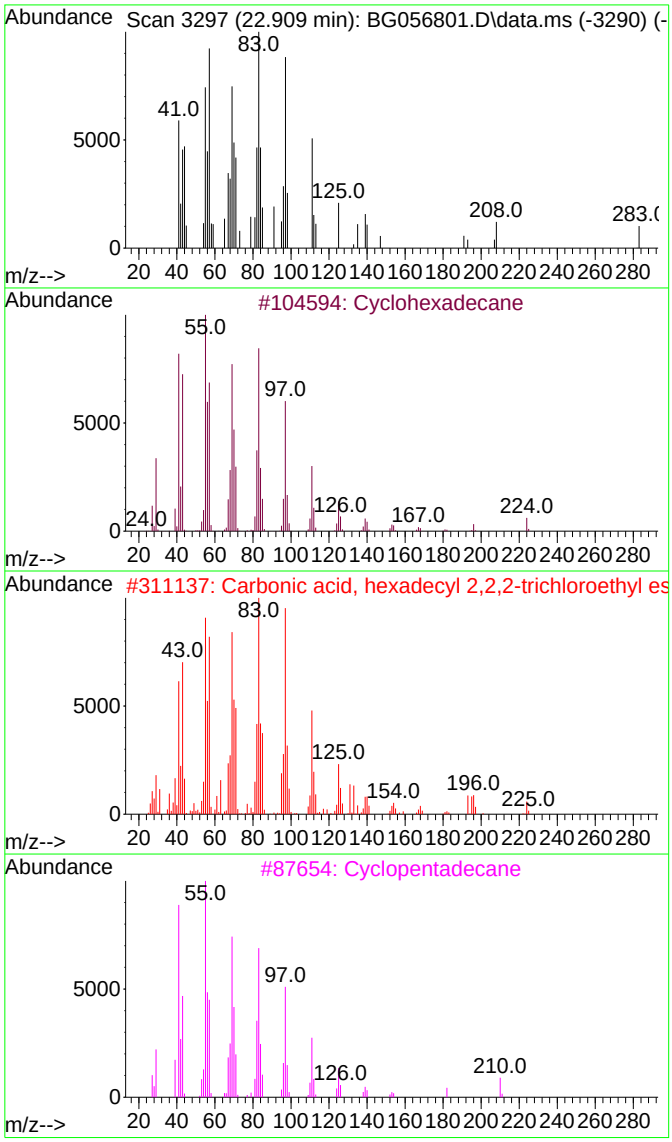
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

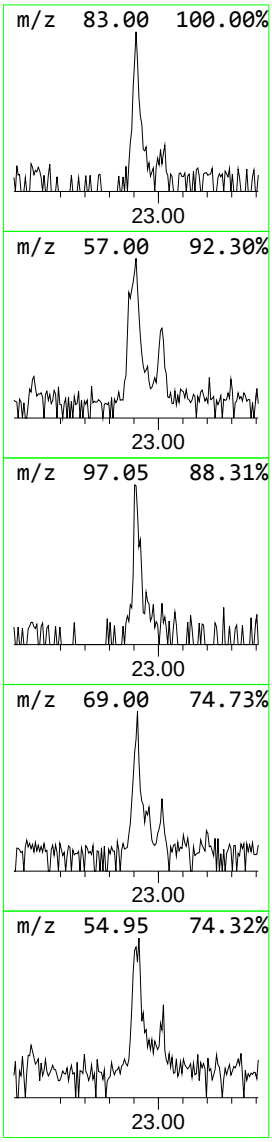
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Cyclic22.909 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.909	2.57 ng/ul	39693	Chrysene-d12	22.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	91
2	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	91
3	Cyclopentadecane	210	C15H30	000295-48-7	91
4	Cyclotetradecane	196	C14H28	000295-17-0	91
5	n-Pentadecanol	228	C15H32O	000629-76-5	90





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Sample : 01710-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAB3

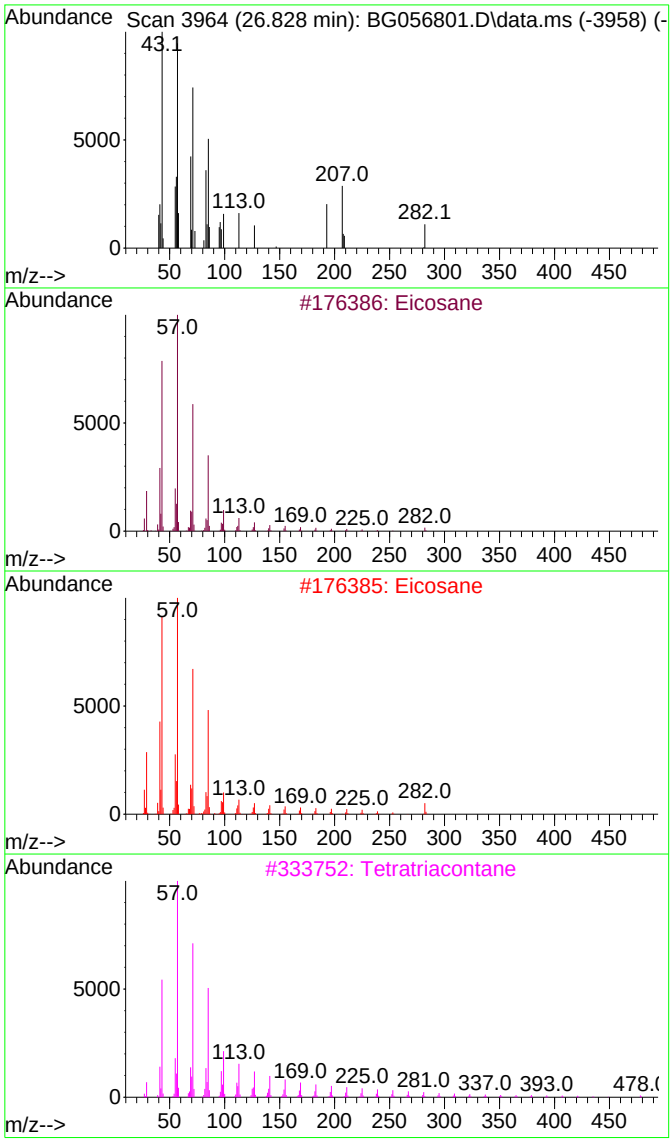
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

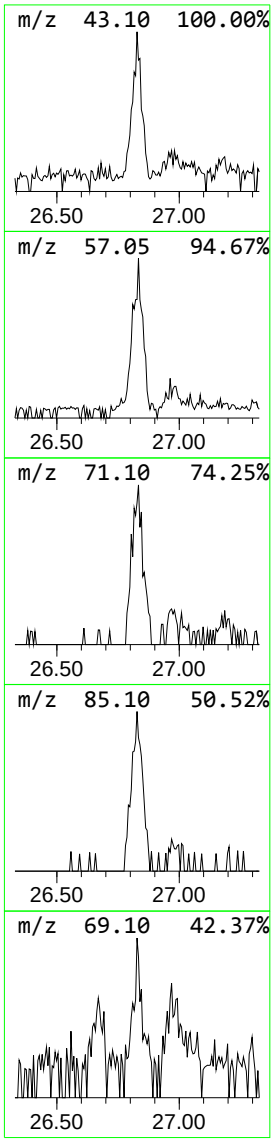
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.828	2.86 ng/ul	44479	Perylene-d12	25.588

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	68
2	Eicosane	282	C20H42	000112-95-8	58
3	Tetratriacontane	479	C34H70	014167-59-0	53
4	Eicosane, 3-methyl-	296	C21H44	006418-46-8	53
5	Hexadecane	226	C16H34	000544-76-3	53





Tentatively Identified Compound (LSC) summary

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Data File : BG056801.D
Acq On : 2 Mar 2023 22:16
Operator : CG/JU
Sample : 01710-16
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAB3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.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	5.441	2.4	ng/ul	10670	1	8.420	89103	20.0
Benzoyl bromide	9.248	2.0	ng/ul	9095	1	8.420	89103	20.0
unknown-02	12.873	3.4	ng/ul	23569	2	11.258	139114	20.0
Benzophenone	16.352	4.7	ng/ul	54335	3	15.018	230623	20.0
n-Hexadecanoic ...	18.590	3.1	ng/ul	46501	4	17.756	298740	20.0
Cinnamyl cinnamate	21.463	4.3	ng/ul	66301	5	22.063	308424	20.0
(DEL) Alkane: S...	21.634	5.2	ng/ul	80292	5	22.063	308424	20.0
(DEL) Alkane: C...	22.909	2.6	ng/ul	39693	5	22.063	308424	20.0
(DEL) Alkane: S...	26.828	2.9	ng/ul	44479	6	25.588	311505	20.0