LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030323\
Data File : BG056814.D
Acq On : 3 Mar 2023 21:56
Operator : CG/JU
Sample : 01711-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAC1

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: BG056814.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.438	320	323	329	rVB3	4447	6369	1.61%	0.135%
2	7.077	597	602	610	rVB	36841	60672	15.35%	1.289%
3	7.536	674	680	687	rBV	43894	74972	18.97%	1.593%
4	7.718	706	711	719	rVB	29475	50741	12.84%	1.078%
5	7.853	731	734	740	rVB4	3405	4563	1.15%	0.097%
6	7.935	743	748	757	rVB	37975	65487	16.57%	1.392%
7	8.417	824	830	838	rBV2	49958	84926	21.49%	1.805%
8	9.104	940	947	954	rBV2	50235	82636	20.91%	1.756%
9	9.239	967	970	976	rVB2	2532	3687	0.93%	0.078%
10	9.586	1023	1029	1036	rBV	44399	77626	19.64%	1.650%
11	9.968	1091	1094	1095	rBV2	1113	933	0.24%	0.020%
12	10.315	1148	1153	1160	rVV2	36954	64405	16.30%	1.369%
13	10.855	1239	1245	1252	rBV	56148	97799	24.75%	2.078%
14	11.255	1306	1313	1320	rVB	77672	135643	34.33%	2.883%
15	11.378	1328	1334	1341	rVB	40415	72632	18.38%	1.544%
16	11.701	1386	1389	1392	rVB2	1431	1547	0.39%	0.033%
17	12.806	1574	1577	1580	rVB2	813	1054	0.27%	0.022%
18	13.388	1674	1676	1680	rBV	806	748	0.19%	0.016%
19	13.816	1746	1749	1753	rVB	846	781	0.20%	0.017%
20	13.899	1756	1763	1767	rBV4	4863	6741	1.71%	0.143%
21	14.345	1833	1839	1844	rBV2	68024	98310	24.88%	2.089%
22	14.404	1844	1849	1858	rVB	114422	168423	42.62%	3.579%
23	14.721	1895	1903	1912	rBV	122751	195985	49.60%	4.165%
24	14.845	1922	1924	1928	rBV2	1593	2247	0.57%	0.048%
25	14.968	1937	1945	1949	rBV2	44355	62529	15.82%	1.329%
26	15.021	1949	1954	1960	rVV	140607	216975	54.91%	4.611%
27	15.068	1961	1962	1970	rVB2	1702	3387	0.86%	0.072%
28	15.174	1974	1980	1986	rBV2	51110	79415	20.10%	1.688%
29	15.250	1990	1993	1997	rBV3	3302	3781	0.96%	0.080%
30	15.403	2016	2019	2023	rBV4	1805	2029	0.51%	0.043%
31	16.002	2114	2121	2128	rBV	172887	256420	64.89%	5.449%
32	16.102	2133	2138	2144	rBV	48492	72235	18.28%	1.535%
33	16.349	2173	2180	2186	rBV	25914	38243	9.68%	0.813%
34	16.466	2195	2200	2205	rBV4	5593	8800	2.23%	0.187%
35	17.171	2317	2320	2323	rBV	569	818	0.21%	0.017%
36	17.453	2364	2368	2372	rVB3	2801	2866	0.73%	0.061%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030323\
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Acq On : 3 Mar 2023 21:56
Operator : CG/JU
Sample : 01711-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBAC1

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	17.753	2413	2419	2425	rBV	198913	293901	74.37%	6.246%
38	17.853	2429	2436	2443	rVV	191825	284328	71.95%	6.043%
39	17.912	2443	2446	2449	rVB2	1921	1346	0.34%	0.029%
40	18.499	2543	2546	2548	rVB2	1136	1266	0.32%	0.027%
41	18.558	2553	2556	2558	rBV	669	801	0.20%	0.017%
42	18.593	2558	2562	2570	rBV2	16462	24313	6.15%	0.517%
43	18.670	2574	2575	2577	rBV	1658	870	0.22%	0.018%
44	18.822	2600	2601	2605	rVV	887	1029	0.26%	0.022%
45	18.852	2605	2606	2611	rVB	1627	1245	0.32%	0.026%
46	19.010	2629	2633	2639	rVB4	5077	9139	2.31%	0.194%
47	19.128	2650	2653	2657	rBV2	700	923	0.23%	0.020%
48	19.198	2661	2665	2673	rVB2	20006	30385	7.69%	0.646%
49	19.334	2684	2688	2692	rBV	5035	5914	1.50%	0.126%
50	19.404	2696	2700	2702	rBV2	1416	1722	0.44%	0.037%
51	19.498	2715	2716	2721	rVB2	1006	746	0.19%	0.016%
52	19.586	2729	2731	2732	rBV	1002	801	0.20%	0.017%
53	19.680	2743	2747	2751	rVB6	2372	3332	0.84%	0.071%
54	19.745	2755	2758	2763	rBV2	2628	3417	0.86%	0.073%
55	19.815	2766	2770	2773	rBV4	5818	6778	1.72%	0.144%
56	19.845	2773	2775	2778	rVV3	3006	2736	0.69%	0.058%
57	19.903	2781	2785	2787	rBV2	773	798	0.20%	0.017%
58	19.950	2792	2793	2797	rBV3	642	728	0.18%	0.015%
59	20.109	2814	2820	2827	rVB	263830	359332	90.93%	7.637%
60	20.344	2859	2860	2862	rBV	1400	812	0.21%	0.017%
61	20.438	2873	2876	2877	rBV2	3854	3383	0.86%	0.072%
62	20.468	2878	2881	2887	rVB	15036	18574	4.70%	0.395%
63	20.538	2887	2893	2895	rBV3	3404	4605	1.17%	0.098%
64	20.562	2895	2897	2898	rBV	1637	847	0.21%	0.018%
65	20.614	2902	2906	2909	rBV4	10869	13303	3.37%	0.283%
66	20.697	2917	2920	2923	rBV3	1986	2503	0.63%	0.053%
67	20.973	2965	2967	2969	rVB3	1736	1101	0.28%	0.023%
68	21.026	2974	2976	2979	rVB4	2360	2449	0.62%	0.052%
69	21.202	3004	3006	3007	rBV2	1969	1732	0.44%	0.037%
70	21.220	3007	3009	3013	rVV5	4374	4718	1.19%	0.100%
71	21.278	3015	3019	3025	rVV2	12983	18615	4.71%	0.396%
72	21.460	3044	3050	3056	rVB	289279	395164	100.00%	8.398%
73	21.631	3075	3079	3091	rVB6	20843	38532	9.75%	0.819%
74	21.842	3114	3115	3116	rBV	1868	805	0.20%	0.017%
75	22.060	3146	3152	3162	rVB2	188594	325295	82.32%	6.913%
76	22.189	3172	3174	3175	rBV	1889	999	0.25%	0.021%

LSC Area Percent Report

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Sample : 01711-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAC1

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-BG022323.M
Title : SVOA CALIBRATION

77	22.553	3234	3236	3238	rBV2	2076	1619	0.41%	0.034%
78	23.053	3319	3321	3322	rVB2	2151	919	0.23%	0.020%
79	23.106	3328	3330	3331	rBV2	1655	1218	0.31%	0.026%
80	24.522	3564	3571	3579	rVB3	10643	24789	6.27%	0.527%
81	24.592	3581	3583	3584	rBV2	1737	953	0.24%	0.020%
82	25.039	3657	3659	3660	rBV2	1713	759	0.19%	0.016%
83	25.338	3700	3710	3721	rVB2	116592	334464	84.64%	7.108%
84	25.579	3741	3751	3762	rBV2	108254	328250	83.07%	6.976%
85	25.732	3776	3777	3779	rBV	1628	1008	0.26%	0.021%
86	26.378	3886	3887	3888	rBV	2368	1026	0.26%	0.022%
87	26.396	3888	3890	3891	rVV2	1441	934	0.24%	0.020%
88	26.560	3917	3918	3921	rBV3	1622	1216	0.31%	0.026%
89	26.825	3955	3963	3967	rBV7	6709	16265	4.12%	0.346%
90	28.311	4214	4216	4218	rBV3	2119	1888	0.48%	0.040%
91	28.946	4322	4324	4325	rBV	1921	956	0.24%	0.020%
92	29.028	4336	4338	4341	rBV4	1960	2116	0.54%	0.045%
93	29.410	4401	4403	4407	rVB2	1758	1485	0.38%	0.032%
94	30.350	4561	4563	4566	rBV3	1992	1606	0.41%	0.034%
95	30.456	4579	4581	4584	rBV3	1979	1565	0.40%	0.033%
96	31.061	4682	4684	4685	rBV2	1578	1256	0.32%	0.027%
97	31.214	4708	4710	4711	rVB2	1892	886	0.22%	0.019%
98	31.560	4767	4769	4770	rVB2	1878	1100	0.28%	0.023%
99	31.731	4796	4798	4799	rVB	1667	788	0.20%	0.017%
100	31.790	4806	4808	4811	rBV3	2033	2610	0.66%	0.055%

Sum of corrected areas: 4705388

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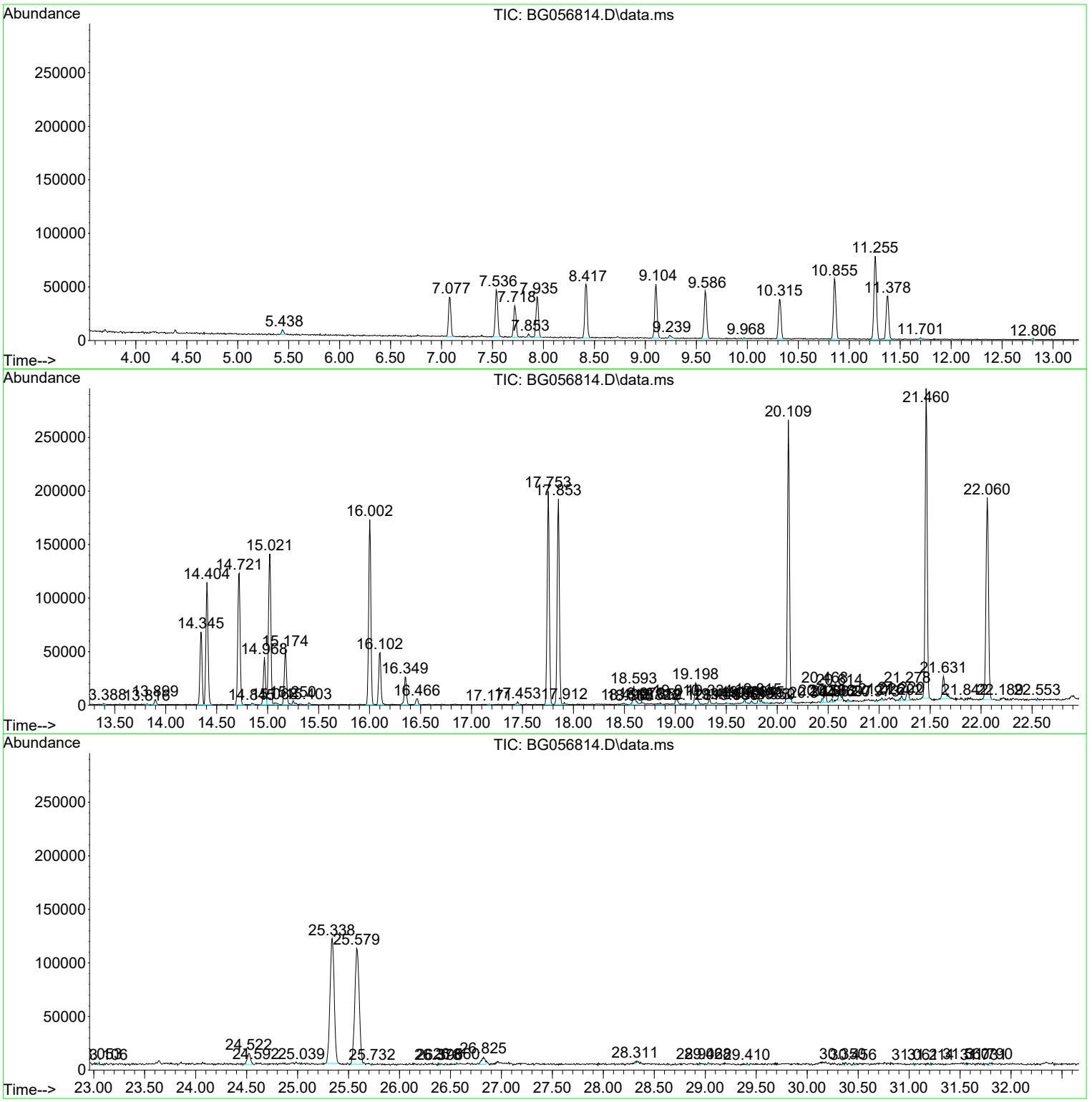
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAC1

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\BG030323\
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Instrument :
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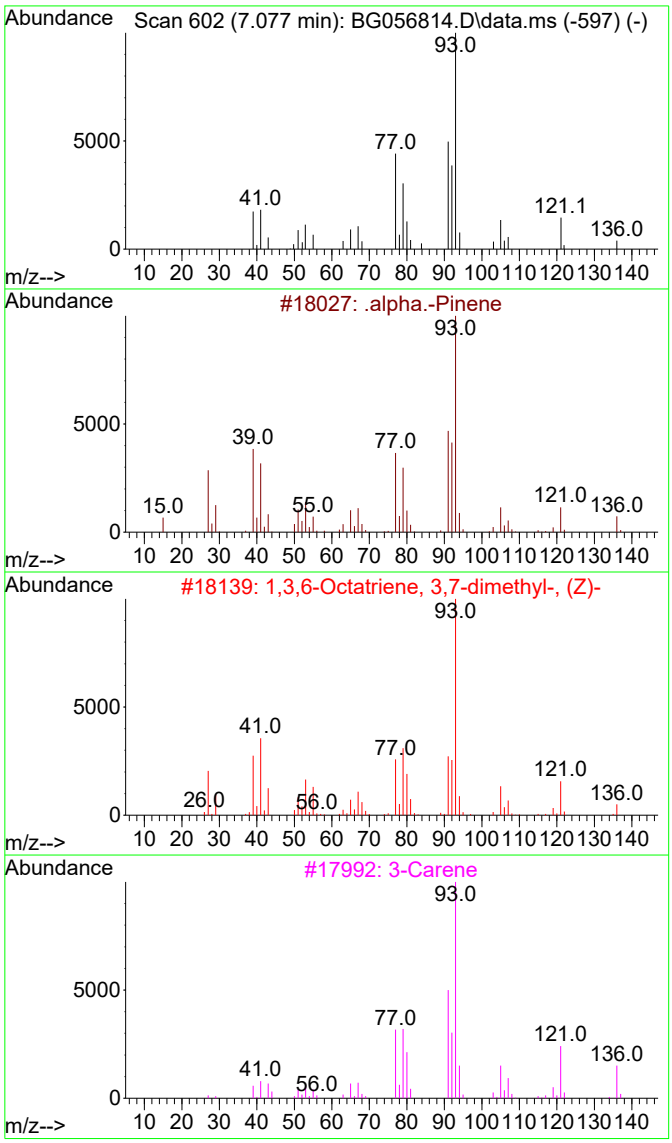
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

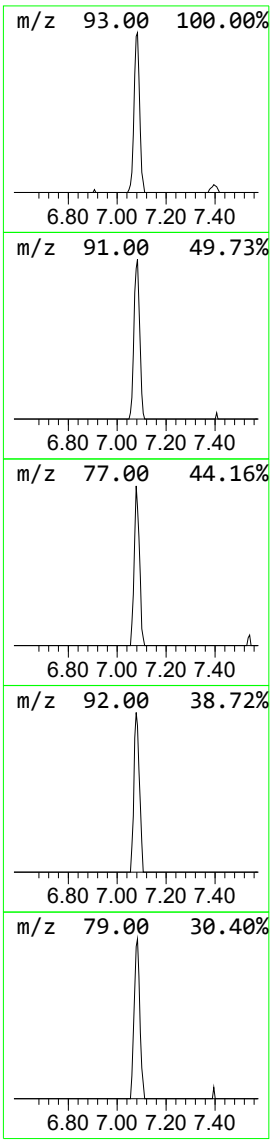
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 .alpha.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.077	14.29 ng/ul	60672	1,4-Dichlorobenzene-d4	8.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	94
2	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	92
3	3-Carene	136	C10H16	013466-78-9	78
4	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	70
5	trans-.beta.-Ocimene	136	C10H16	003779-61-1	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030323\
Data File : BG056814.D
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAC1

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

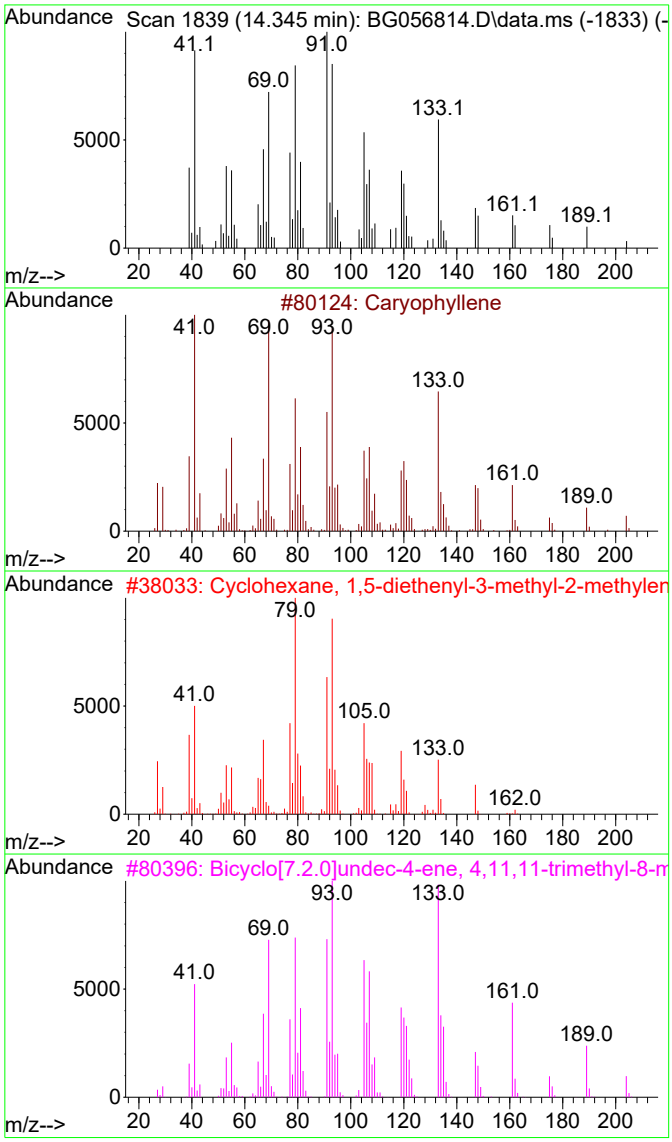
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

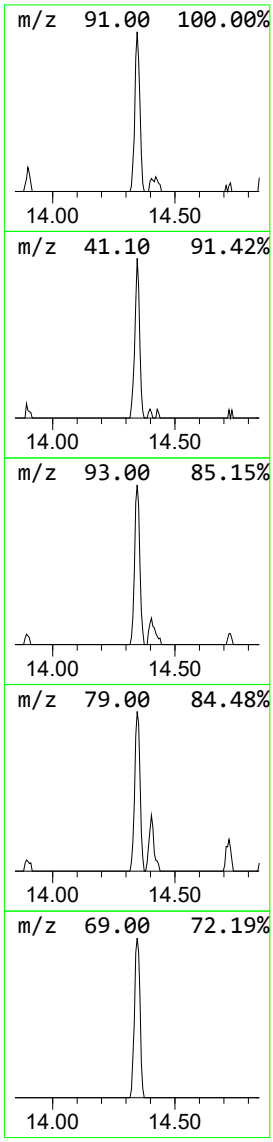
****

Peak Number 2 Caryophyllene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.345	9.06 ng/ul	98310	Acenaphthene-d10	15.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	91
2	Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	90
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	89
4	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	83
5	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	64





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAC1

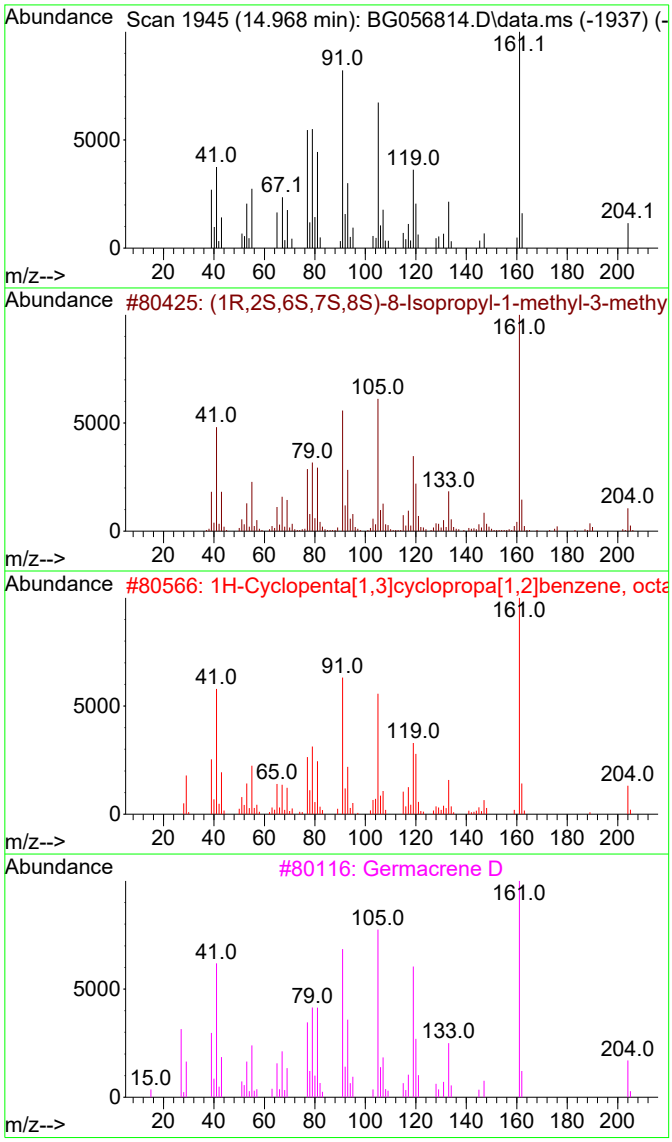
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

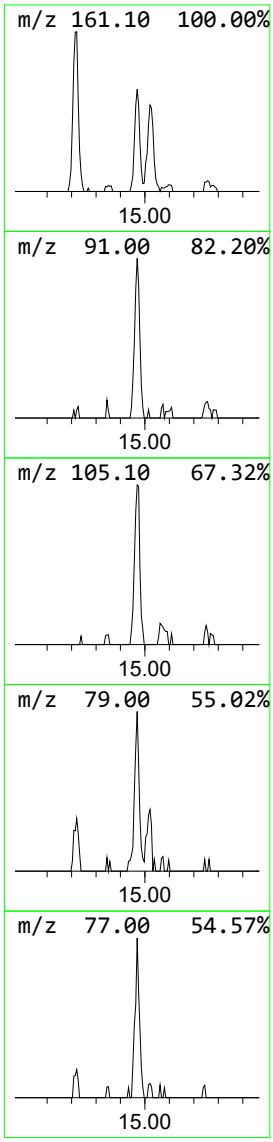
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (1R,2S,6S,7S,8S)-8-Isopropy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	5.76 ng/ul	62529	Acenaphthene-d10	15.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	93
2	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	93
3	Germacrene D	204	C15H24	023986-74-5	92
4	1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	70
5	Germacrene D	204	C15H24	023986-74-5	70





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

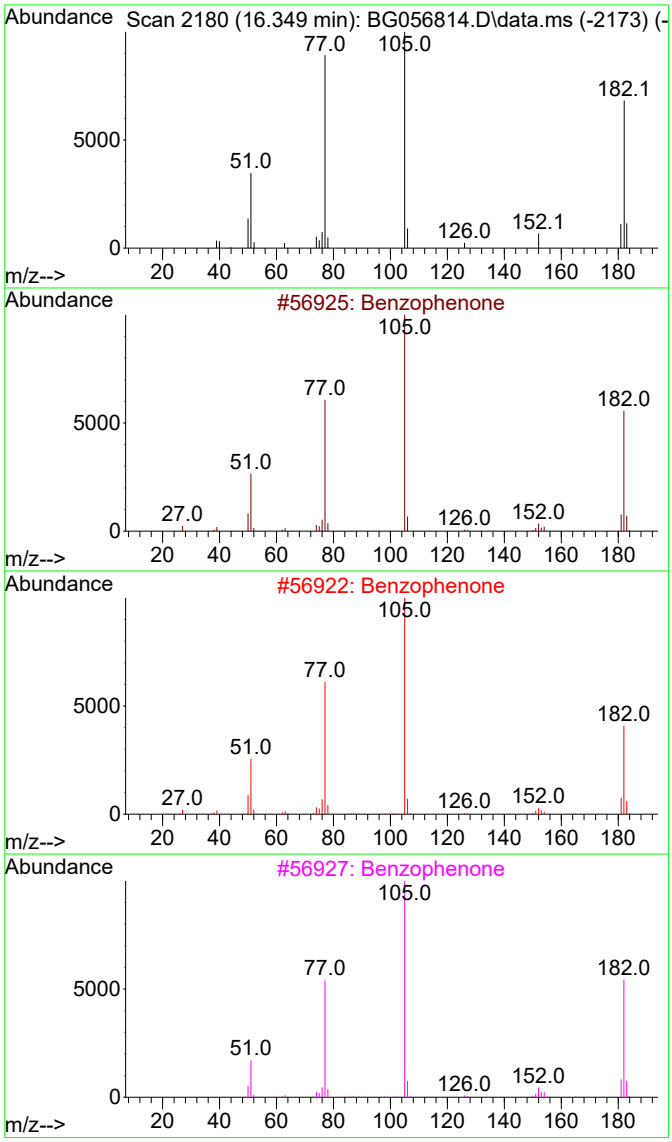
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

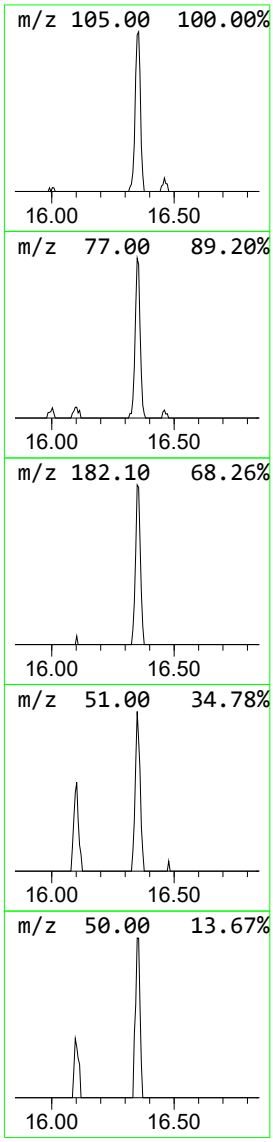
****

Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.349	3.53 ng/ul	38243	Acenaphthene-d10	15.021

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	91
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	76





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Data File : BG056814.D
Acq On : 3 Mar 2023 21:56
Operator : CG/JU
Sample : 01711-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAC1

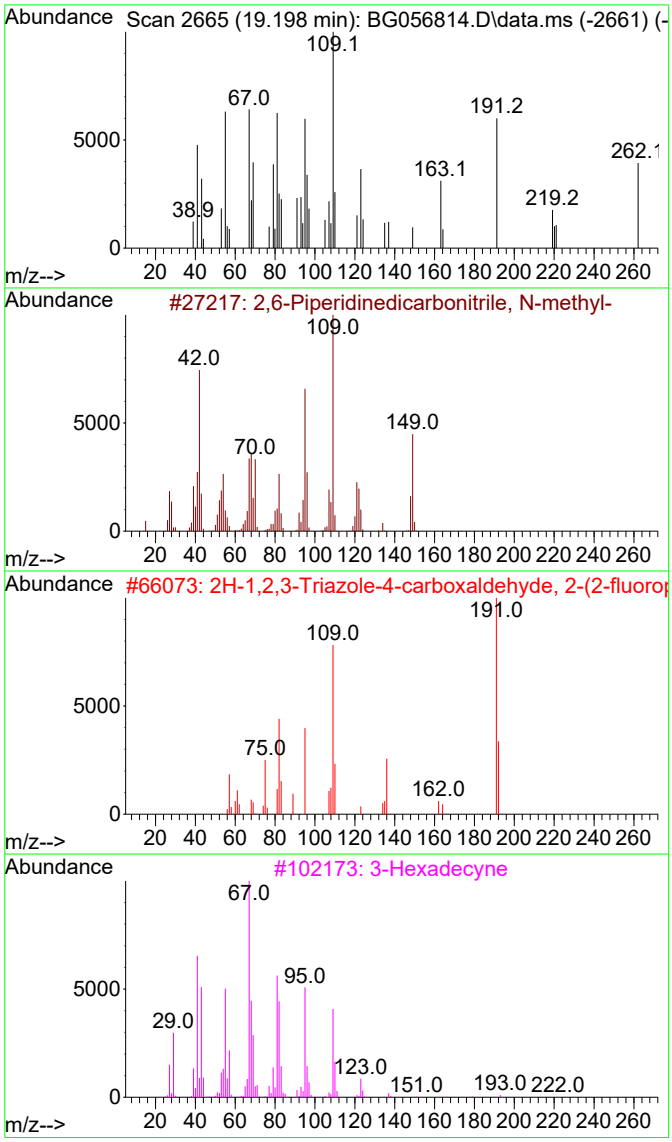
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

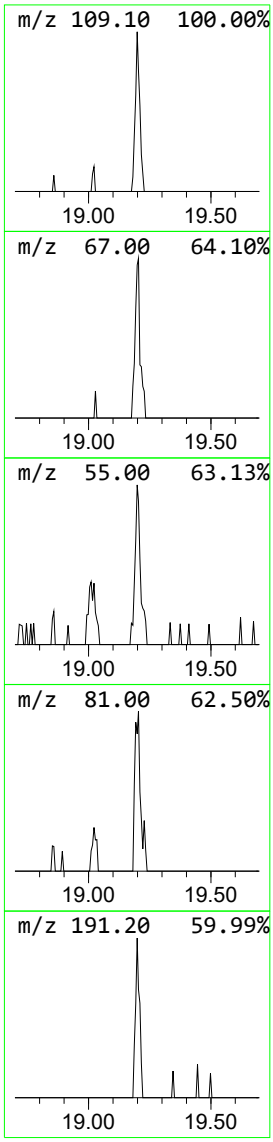
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,6-Piperidinedicarbonitril... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.198	2.07 ng/ul	30385	Phenanthrene-d10	17.753

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Piperidinedicarbonitrile, N-...	149	C8H11N3	090090-68-9	50
2	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	43
3	3-Hexadecyne	222	C16H30	061886-62-2	27
4	1,3-Di(cyclohexyl)but-1-ene	220	C16H28	1000214-97-4	25
5	7-Tetradecyne	194	C14H26	035216-11-6	22





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Data File : BG056814.D
Acq On : 3 Mar 2023 21:56
Operator : CG/JU
Sample : 01711-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAC1

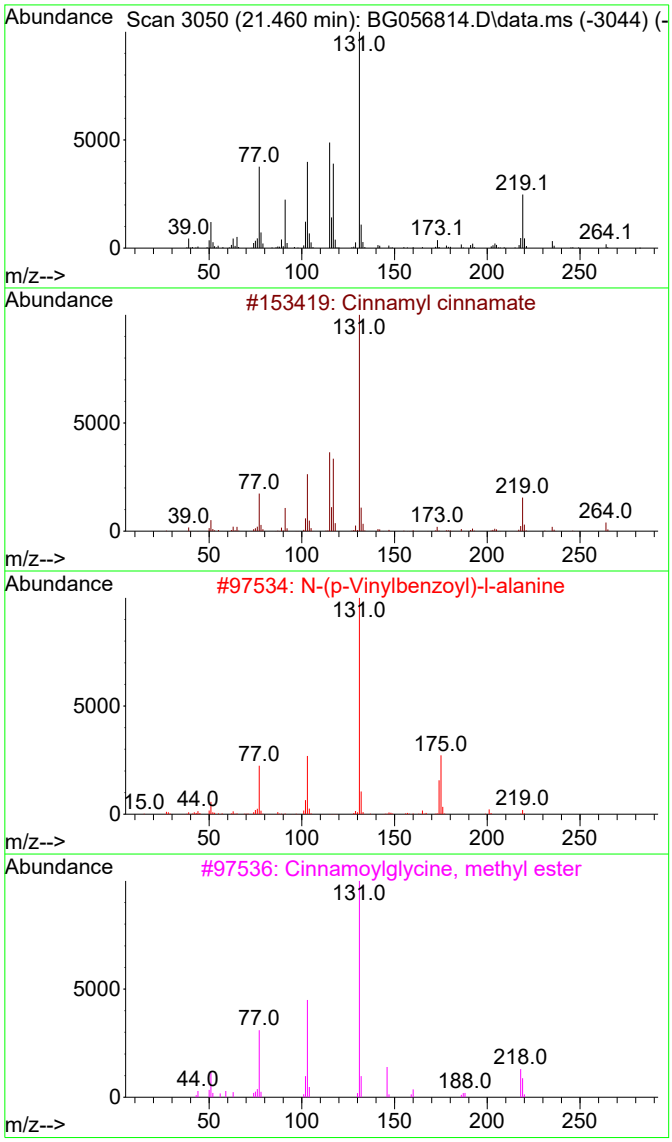
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

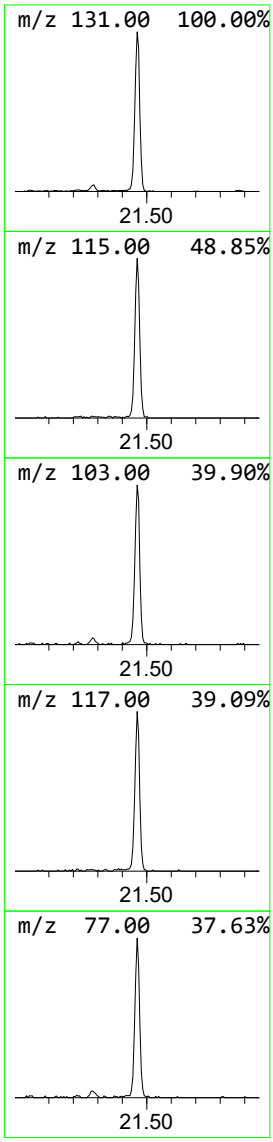
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.461	24.30 ng/ul	395164	Chrysene-d12	22.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	47
3	Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	47
4	2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	001754-62-7	47
5	1-(2-Vinylphenyl)propan-1-one	160	C11H12O	052095-41-7	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030323\
Data File : BG056814.D
Acq On : 3 Mar 2023 21:56
Operator : CG/JU
Sample : 01711-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAC1

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

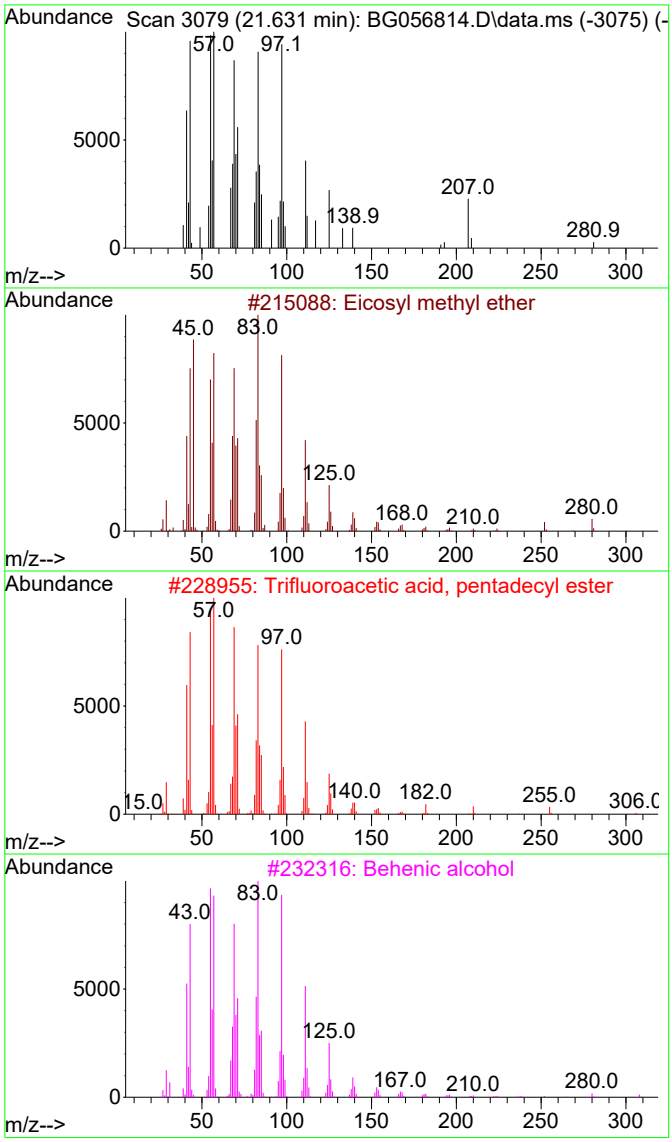
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

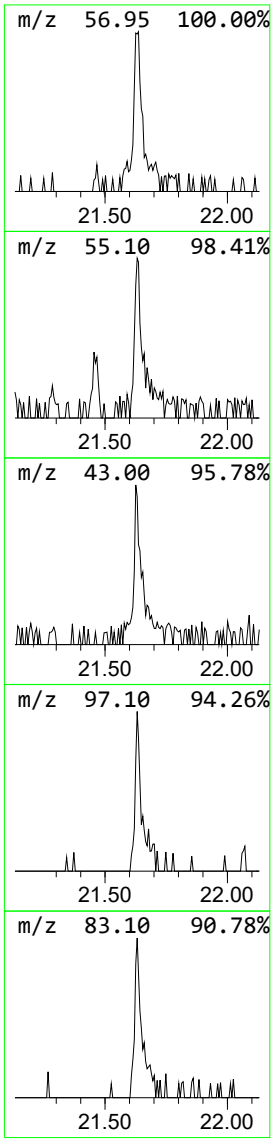
****

Peak Number 7 Eicosyl methyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.631	2.37 ng/ul	38532	Chrysene-d12	22.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl methyl ether	312	C21H44O	1000406-29-4	91
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5	1-Hexadecanol	242	C16H34O	036653-82-4	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030323\
Data File : BG056814.D
Acq On : 3 Mar 2023 21:56
Operator : CG/JU
Sample : 01711-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBAC1

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
.alpha.-Pinene	7.077	14.3	ng/ul	60672	1	8.417	84926	20.0
Caryophyllene	14.345	9.1	ng/ul	98310	3	15.021	216975	20.0
(1R,2S,6S,7S,8S...	14.968	5.8	ng/ul	62529	3	15.021	216975	20.0
Benzophenone	16.349	3.5	ng/ul	38243	3	15.021	216975	20.0
2,6-Piperidined...	19.198	2.1	ng/ul	30385	4	17.753	293901	20.0
Cinnamyl cinnamate	21.461	24.3	ng/ul	395164	5	22.060	325295	20.0
Eicosyl methyl ...	21.631	2.4	ng/ul	38532	5	22.060	325295	20.0