LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBZW2

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: BG056785.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.445	320	324	329	rVB2	7070	10471	3.29%	0.276%
2	5.685	363	365	366	rBV	1447	738	0.23%	0.019%
3	6.549	510	512	514	rVB	1296	851	0.27%	0.022%
4	6.573	514	516	517	rBV	1064	770	0.24%	0.020%
5	7.542	675	681	687	rVB	39199	67008	21.08%	1.766%
6	7.718	705	711	718	rBV	25372	42325	13.31%	1.116%
7	7.830	728	730	733	rBV	757	623	0.20%	0.016%
8	7.871	735	737	742	rVV4	1805	2178	0.69%	0.057%
9	7.942	742	749	756	rVB	32781	55660	17.51%	1.467%
10	8.206	792	794	796	rBV	1247	1037	0.33%	0.027%
11	8.418	823	830	837	rVB	54411	87749	27.60%	2.313%
12	8.723	880	882	886	rVB3	1089	1271	0.40%	0.033%
13	9.105	940	947	953	rVB2	40076	65821	20.70%	1.735%
14	9.170	956	958	959	rBV	1054	648	0.20%	0.017%
15	9.246	967	971	973	rBV2	1679	2413	0.76%	0.064%
16	9.593	1022	1030	1036	rBV	38208	66563	20.94%	1.754%
17	9.969	1092	1094	1098	rBV2	1028	1212	0.38%	0.032%
18	10.321	1148	1154	1161	rBV2	33643	56399	17.74%	1.486%
19	10.862	1239	1246	1252	rVB	46875	80881	25.44%	2.132%
20	11.067	1276	1281	1286	rVB4	6623	9504	2.99%	0.250%
21	11.155	1293	1296	1300	rVB2	629	934	0.29%	0.025%
22	11.255	1305	1313	1322	rBV	76330	136001	42.78%	3.584%
23	11.373	1327	1333	1343	rVB	31531	57068	17.95%	1.504%
24	12.724	1561	1563	1572	rVB3	1137	1757	0.55%	0.046%
25	12.806	1572	1577	1580	rBV2	884	1245	0.39%	0.033%
26	13.141	1631	1634	1638	rBV	549	652	0.21%	0.017%
27	13.735	1731	1735	1741	rVB4	9128	11903	3.74%	0.314%
28	13.817	1747	1749	1754	rBV2	1160	1389	0.44%	0.037%
29	13.893	1757	1762	1765	rBV3	1806	2148	0.68%	0.057%
30	14.070	1789	1792	1795	rBV2	545	769	0.24%	0.020%
31	14.134	1800	1803	1805	rVB2	708	652	0.21%	0.017%
32	14.346	1834	1839	1844	rVV3	28091	37776	11.88%	0.996%
33	14.405	1844	1849	1856	rVB	102434	145152	45.65%	3.826%
34	14.663	1889	1893	1895	rVB	477	607	0.19%	0.016%
35	14.722	1895	1903	1909	rBV2	108296	168555	53.02%	4.442%
36	15.022	1943	1954	1960	rVB2	142421	231125	72.70%	6.092%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBZW2

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	15.174	1972	1980	1987	rBV	47693	73335	23.07%	1.933%
38	15.274	1993	1997	2001	rBV	473	705	0.22%	0.019%
39	15.327	2003	2006	2009	rVV	598	704	0.22%	0.019%
40	15.403	2016	2019	2023	rBV2	1070	1291	0.41%	0.034%
41	15.756	2075	2079	2083	rBV3	7479	8755	2.75%	0.231%
42	15.938	2106	2110	2113	rBV	547	712	0.22%	0.019%
43	16.003	2114	2121	2128	rVV2	147813	216053	67.96%	5.694%
44	16.103	2132	2138	2145	rVB	42909	63343	19.92%	1.669%
45	16.349	2174	2180	2185	rBV	17025	24446	7.69%	0.644%
46	16.655	2230	2232	2237	rVB	559	622	0.20%	0.016%
47	17.419	2359	2362	2366	rVB2	4414	4761	1.50%	0.125%
48	17.754	2413	2419	2430	rBV	191112	287038	90.28%	7.565%
49	17.854	2430	2436	2443	rVB	160642	235982	74.22%	6.220%
50	17.912	2443	2446	2449	rBV	1586	1732	0.54%	0.046%
51	18.388	2524	2527	2531	rVB	2926	2922	0.92%	0.077%
52	18.594	2557	2562	2569	rBV2	19035	26894	8.46%	0.709%
53	18.670	2573	2575	2576	rVV2	1069	1087	0.34%	0.029%
54	18.711	2579	2582	2583	rVV2	870	709	0.22%	0.019%
55	18.841	2602	2604	2609	rVB3	2844	3642	1.15%	0.096%
56	18.929	2617	2619	2621	rBV	768	679	0.21%	0.018%
57	19.011	2629	2633	2636	rVB	14016	13947	4.39%	0.368%
58	19.275	2675	2678	2679	rBV2	650	628	0.20%	0.017%
59	19.328	2684	2687	2689	rVB	842	775	0.24%	0.020%
60	19.358	2689	2692	2693	rBV2	674	648	0.20%	0.017%
61	19.399	2696	2699	2702	rVB2	962	982	0.31%	0.026%
62	19.505	2713	2717	2719	rBV2	1347	1620	0.51%	0.043%
63	19.552	2724	2725	2727	rBV	1094	773	0.24%	0.020%
64	19.604	2732	2734	2737	rBV2	903	960	0.30%	0.025%
65	19.651	2739	2742	2744	rBV2	621	801	0.25%	0.021%
66	19.681	2744	2747	2750	rVB3	2180	2660	0.84%	0.070%
67	19.745	2754	2758	2761	rVV4	1880	2698	0.85%	0.071%
68	19.839	2773	2774	2777	rBV	2633	2938	0.92%	0.077%
69	20.039	2806	2808	2812	rVB3	2634	2389	0.75%	0.063%
70	20.110	2814	2820	2828	rVB	218637	305955	96.23%	8.064%
71	20.221	2836	2839	2842	rBV3	775	1177	0.37%	0.031%
72	20.251	2842	2844	2845	rVB	1507	722	0.23%	0.019%
73	20.333	2856	2858	2860	rBV2	1179	1321	0.42%	0.035%
74	20.450	2876	2878	2880	rBV2	1145	729	0.23%	0.019%
75	20.533	2890	2892	2896	rBV	2160	2240	0.70%	0.059%
76	20.762	2929	2931	2935	rVB3	2124	1691	0.53%	0.045%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBZW2

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

77	20.850	2943	2946	2950	rBV4	3664	3915	1.23%	0.103%
78	20.897	2950	2954	2958	rBV5	8728	10726	3.37%	0.283%
79	21.291	3017	3021	3022	rVB2	1934	2352	0.74%	0.062%
80	21.461	3045	3050	3056	rBV	42768	57591	18.11%	1.518%
81	21.637	3072	3080	3087	rBV5	27855	54664	17.19%	1.441%
82	22.060	3146	3152	3159	rVB	181228	312166	98.19%	8.227%
83	22.489	3222	3225	3230	rBV7	2825	4229	1.33%	0.111%
84	23.412	3381	3382	3385	rVB3	2321	1361	0.43%	0.036%
85	23.435	3385	3386	3388	rBV2	2098	1026	0.32%	0.027%
86	23.488	3394	3395	3398	rBV2	1875	2217	0.70%	0.058%
87	24.334	3537	3539	3540	rVB	2347	1222	0.38%	0.032%
88	24.481	3562	3564	3566	rBV3	1934	1862	0.59%	0.049%
89	24.522	3568	3571	3578	rVB5	7823	16486	5.19%	0.435%
90	25.339	3701	3710	3720	rVB	95855	271221	85.31%	7.148%
91	25.456	3728	3730	3732	rBV3	1831	1684	0.53%	0.044%
92	25.586	3739	3752	3763	rBV2	103089	317934	100.00%	8.379%
93	28.124	4183	4184	4185	rBV	1780	709	0.22%	0.019%
94	28.811	4299	4301	4302	rBV2	1985	1502	0.47%	0.040%
95	29.205	4364	4368	4370	rBV5	2147	3333	1.05%	0.088%
96	30.750	4629	4631	4634	rBV4	2162	2489	0.78%	0.066%
97	31.156	4699	4700	4702	rBV	1717	1367	0.43%	0.036%
98	31.608	4776	4777	4778	rBV	2604	1404	0.44%	0.037%
99	31.690	4779	4791	4793	rBV8	23801	68712	21.61%	1.811%
100	31.943	4832	4834	4835	rBV2	1686	1118	0.35%	0.029%

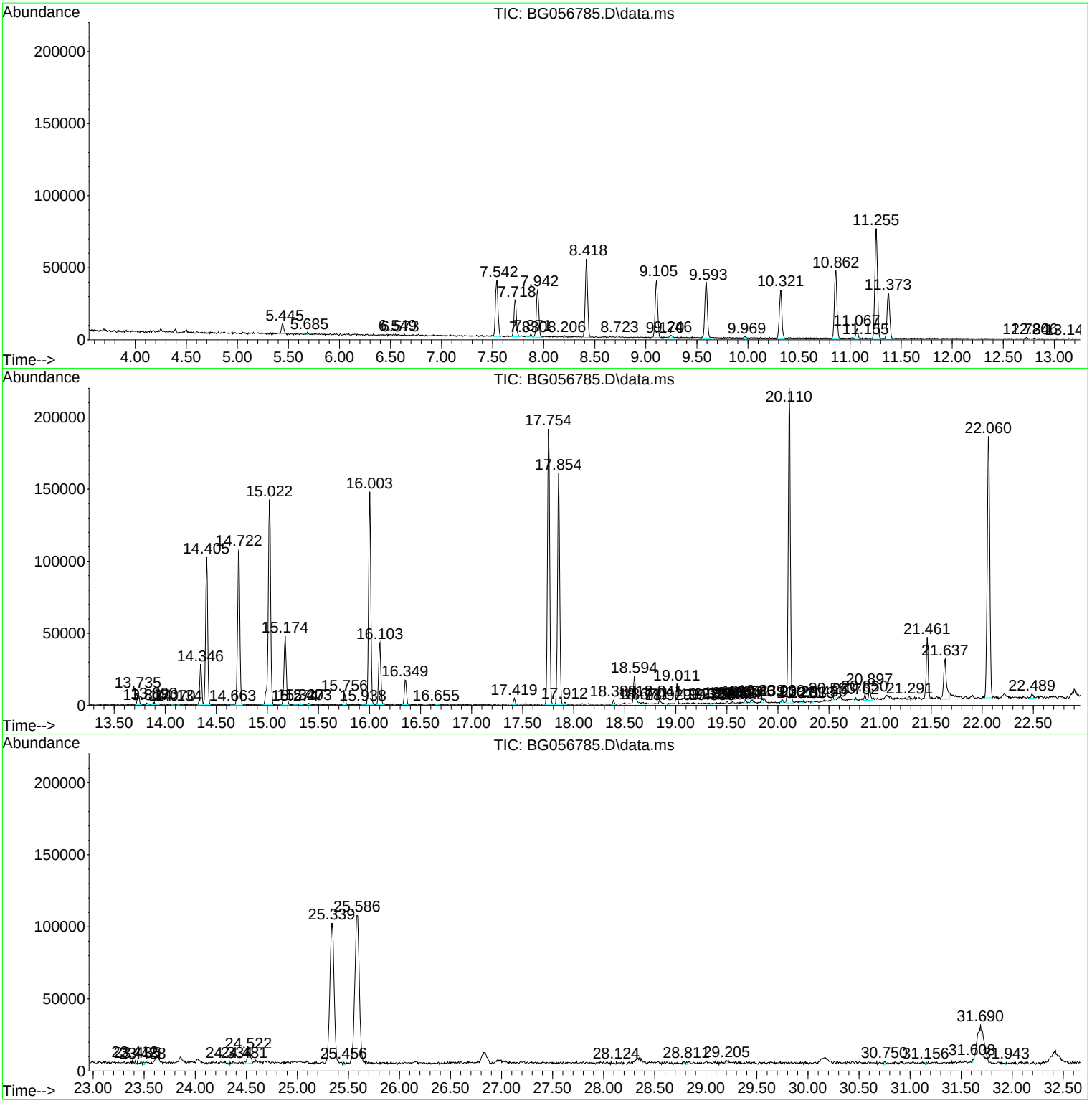
Sum of corrected areas: 3794211

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW2

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\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW2

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

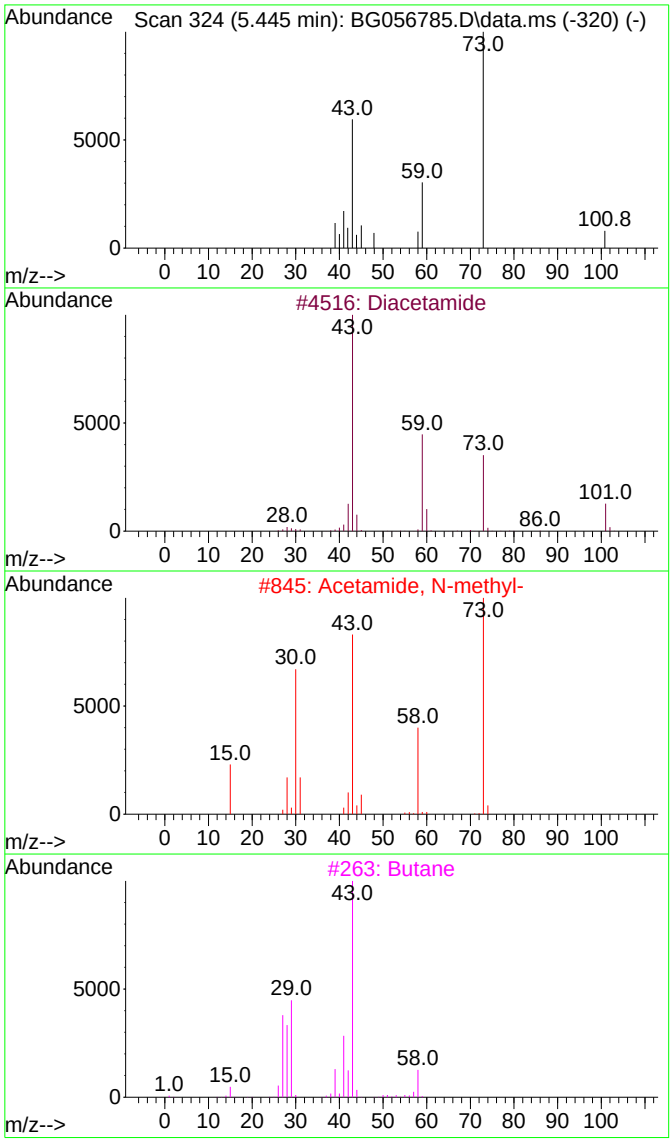
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

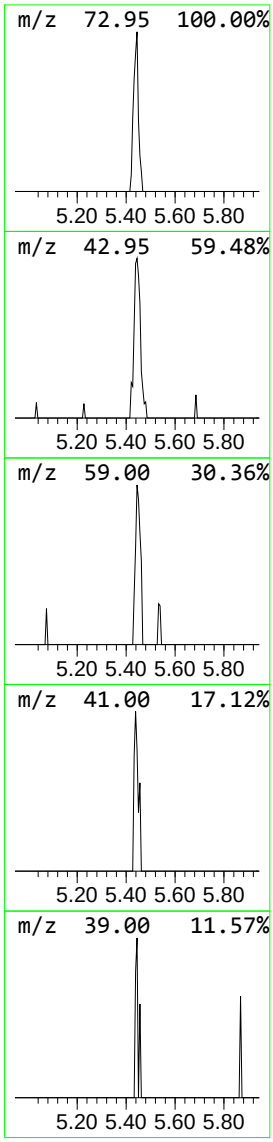
****

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.445	2.39 ng/ul	10471	1,4-Dichlorobenzene-d4	8.418

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diacetamide	101	C4H7NO2	000625-77-4	45
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3	Butane	58	C4H10	000106-97-8	9
4	Butane	58	C4H10	000106-97-8	9
5	1-Hexanamine	101	C6H15N	000111-26-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW2

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

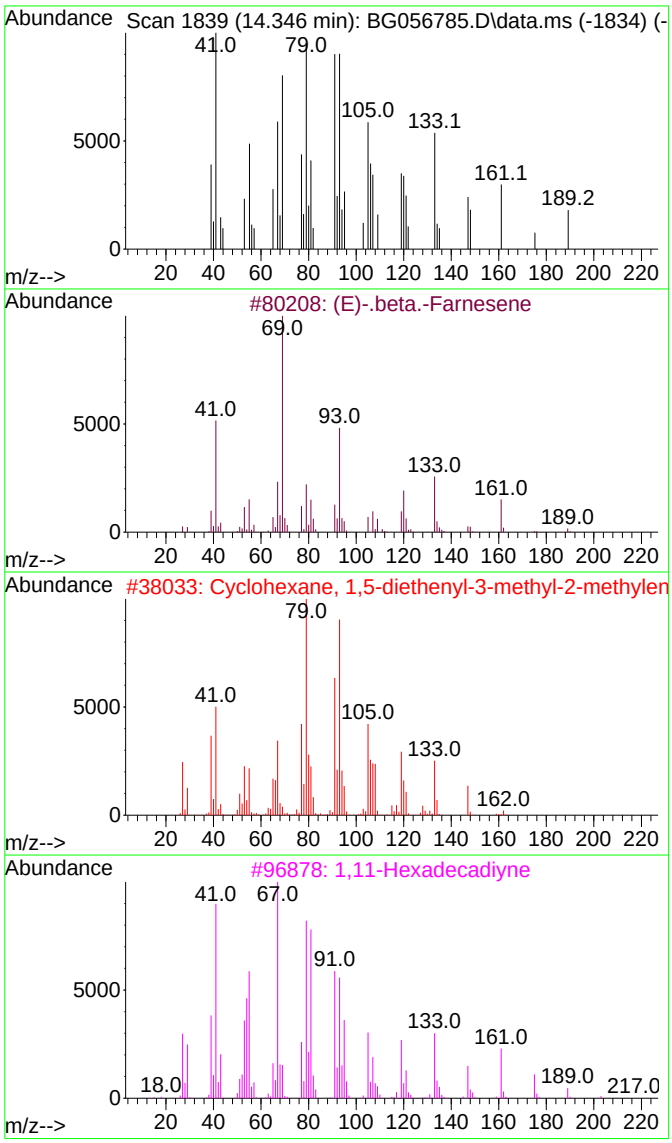
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

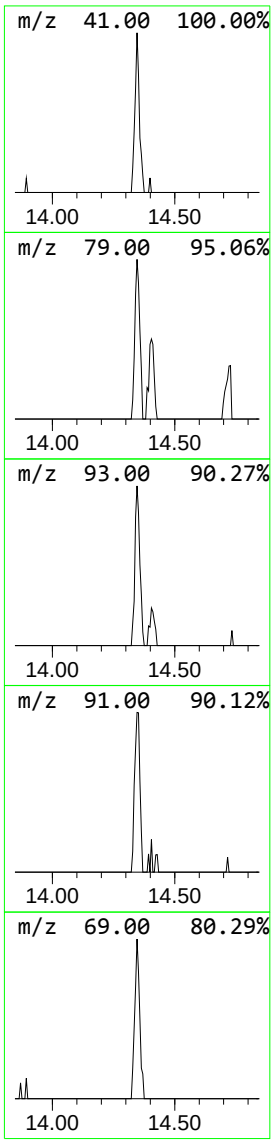
****

Peak Number 2 (E)-.beta.-Farnesene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.346	3.27 ng/ul	37776	Acenaphthene-d10	15.022

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-.beta.-Farnesene	204	C15H24	018794-84-8	50
2	Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	50
3	1,11-Hexadecadiyne	218	C16H26	071673-32-0	47
4	1,3,6,10-Dodecatetraene, 3,7,11-...	204	C15H24	026560-14-5	43
5	3-Ethylidenecycloheptene	122	C9H14	1000211-16-7	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW2

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

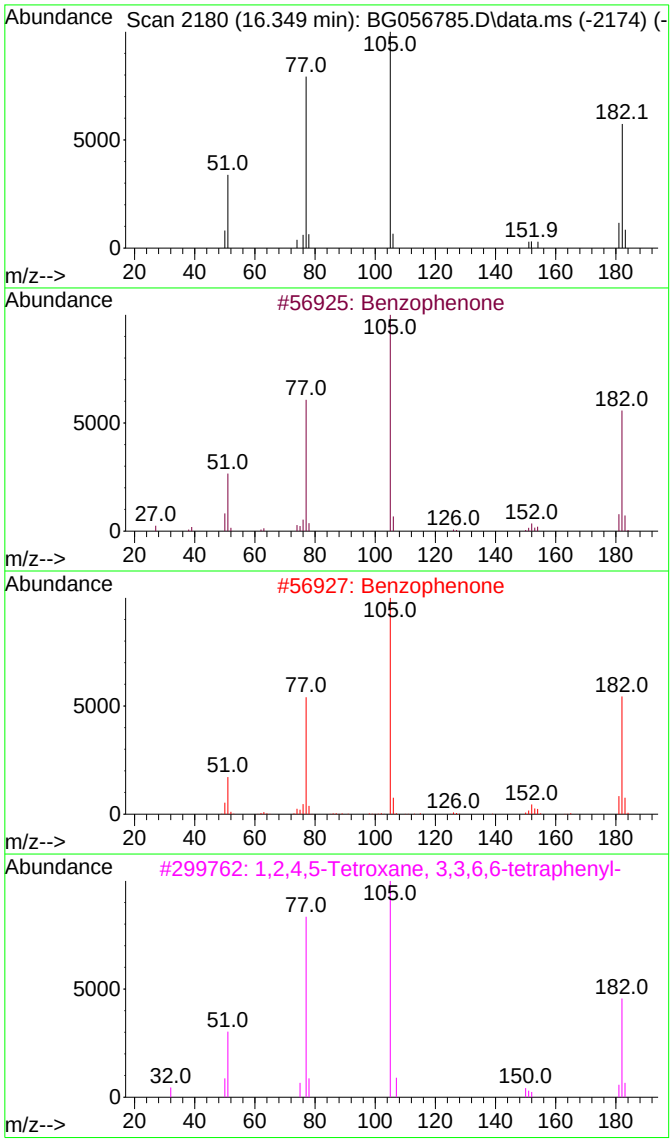
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

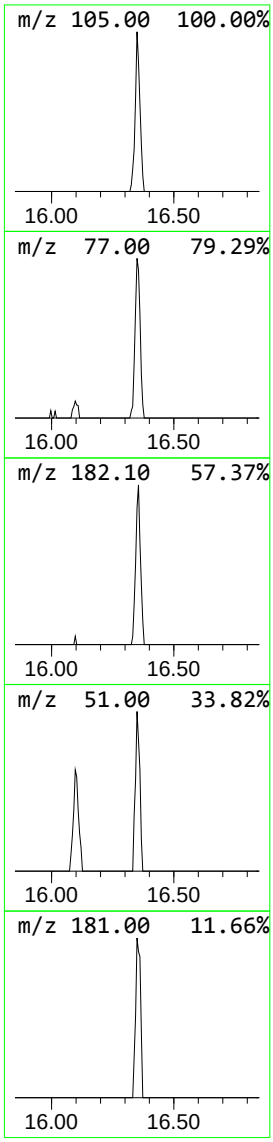
****

Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.349	2.12 ng/ul	24446	Acenaphthene-d10	15.022

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	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
4	Benzophenone	182	C13H10O	000119-61-9	72
5	Benzophenone	182	C13H10O	000119-61-9	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW2

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

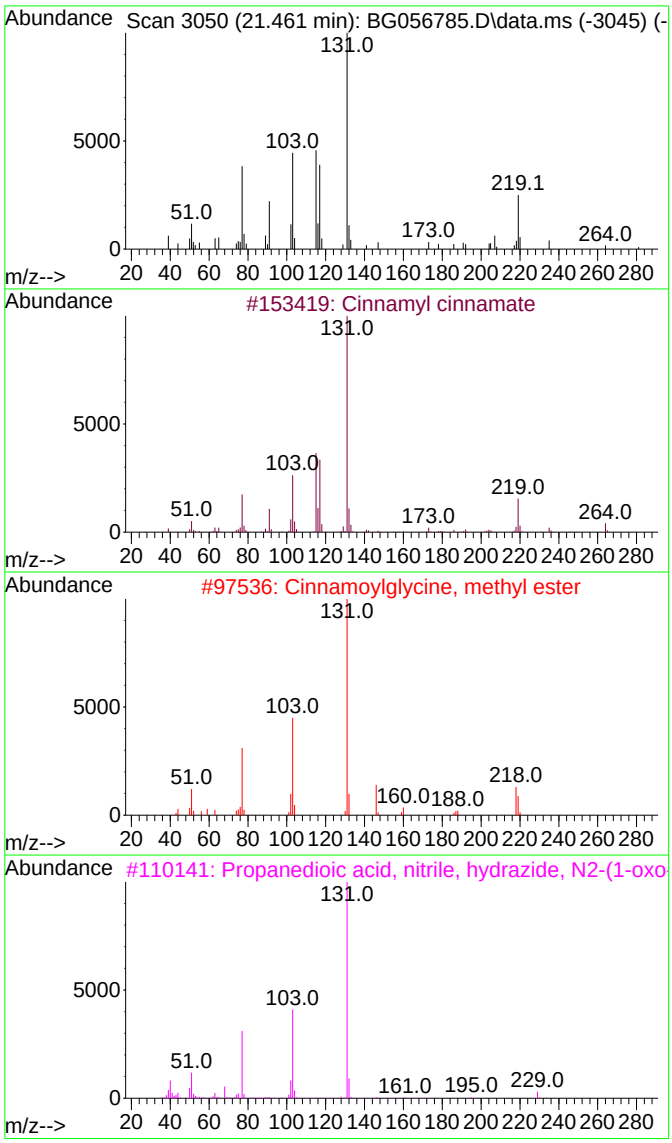
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

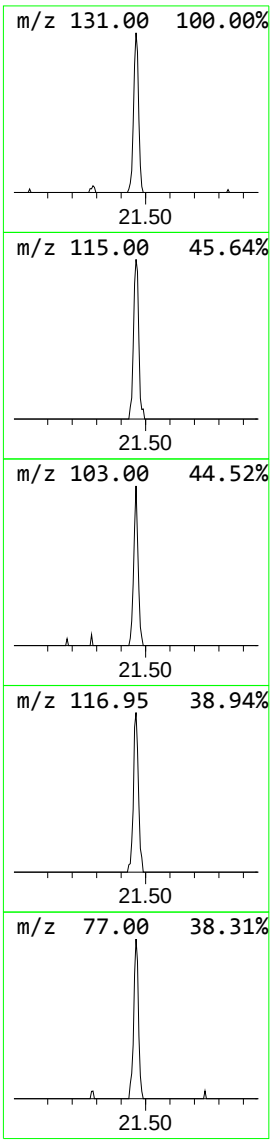
****

Peak Number 4 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.461	3.69 ng/ul	57591	Chrysene-d12	22.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	72
2	Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	47
3	Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	46
4	(2E)-N-(4-Methylphenyl)-3-phenyl...	237	C16H15NO	134430-88-9	43
5	(Z)-N-(2-Hydroxyethyl)-3-phenyla...	233	C13H15NO3	1000512-63-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW2

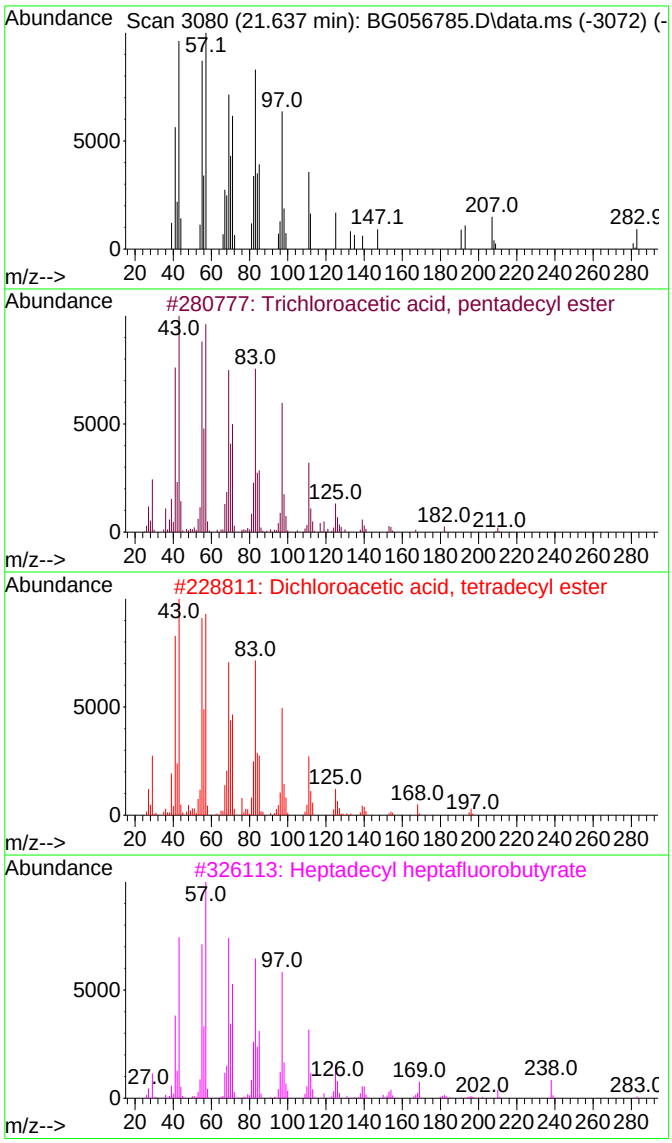
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

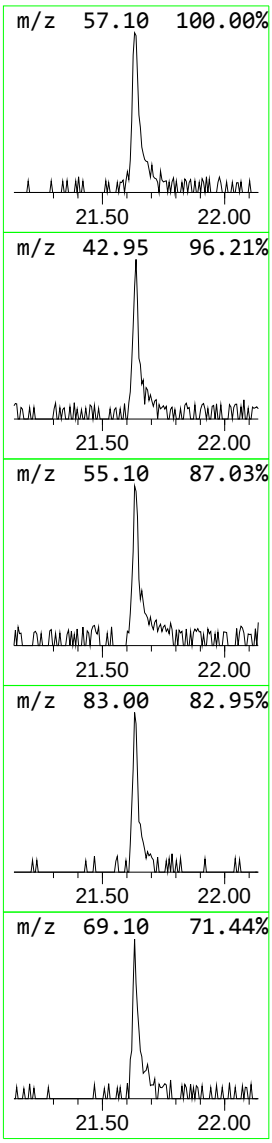
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.637	3.50 ng/ul	54664	Chrysene-d12	22.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	90
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW2

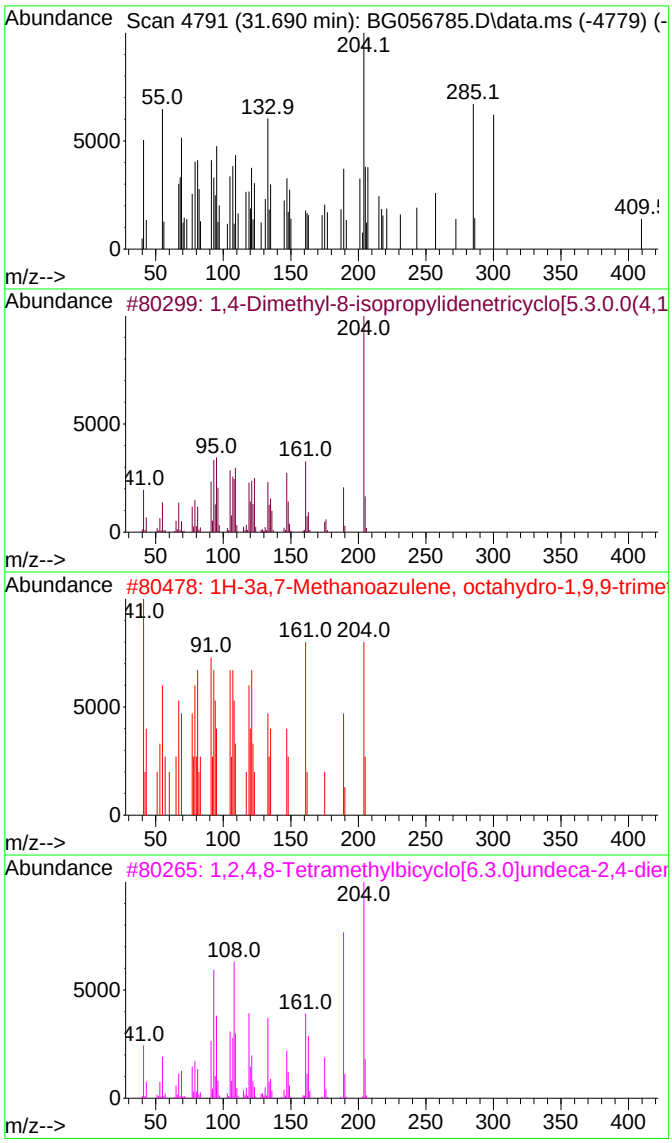
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

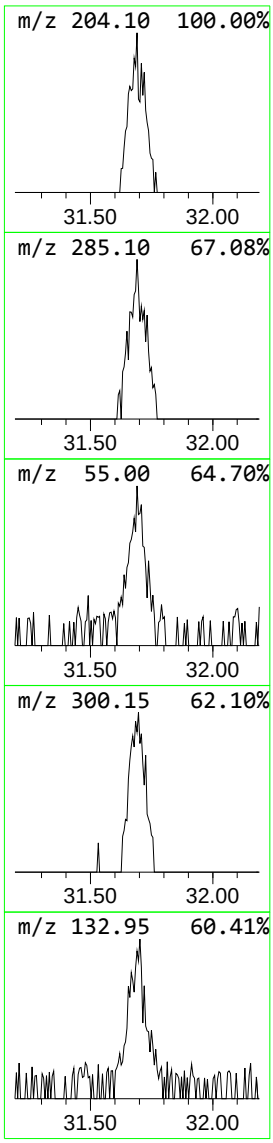
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,4-Dimethyl-8-isopropylide... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.690	4.32 ng/ul	68712	Perylene-d12	25.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	60
2	1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	50
3	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	47
4	(8R,10S,13S)-13-Methyl-3,17-diox...	300	C19H24O3	1000497-96-3	45
5	Cedrene	204	C15H24	011028-42-5	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030123\
Data File : BG056785.D
Acq On : 2 Mar 2023 6:11
Operator : CG/JU
Sample : 01649-15
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZW2

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	5.445	2.4	ng/ul	10471	1	8.418	87749	20.0
(E)-.beta.-Farn...	14.346	3.3	ng/ul	37776	3	15.022	231125	20.0
Benzophenone	16.349	2.1	ng/ul	24446	3	15.022	231125	20.0
Cinnamyl cinnamate	21.461	3.7	ng/ul	57591	5	22.060	312166	20.0
Trichloroacetic...	21.637	3.5	ng/ul	54664	5	22.060	312166	20.0
1,4-Dimethyl-8-...	31.690	4.3	ng/ul	68712	6	25.586	317934	20.0