LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBZU2

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: BG056740.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.143	101	103	109	rBV	12757	17649	5.46%	0.449%
2	4.384	142	144	147	rVB3	2490	2915	0.90%	0.074%
3	4.572	174	176	178	rVB2	1332	1123	0.35%	0.029%
4	4.601	178	181	183	rBV3	1679	1995	0.62%	0.051%
5	5.447	320	325	330	rVB3	9405	14598	4.51%	0.371%
6	5.635	355	357	361	rVV3	875	1118	0.35%	0.028%
7	6.734	542	544	546	rBV	972	917	0.28%	0.023%
8	6.840	559	562	564	rBV	761	966	0.30%	0.025%
9	7.092	603	605	608	rVB	1353	952	0.29%	0.024%
10	7.539	676	681	691	rVB	40250	70044	21.66%	1.782%
11	7.721	706	712	718	rVB	26559	45100	13.95%	1.147%
12	7.944	743	750	756	rVB	34618	59125	18.28%	1.504%
13	8.420	824	831	839	rVB	50273	83701	25.88%	2.130%
14	8.726	881	883	887	rVB2	1229	1331	0.41%	0.034%
15	9.107	941	948	954	rVV2	47092	79830	24.69%	2.031%
16	9.160	956	957	962	rVB3	1343	1471	0.45%	0.037%
17	9.248	966	972	977	rVV3	6486	11220	3.47%	0.285%
18	9.589	1024	1030	1038	rVB	38484	66180	20.47%	1.684%
19	9.977	1092	1096	1100	rVB2	858	1411	0.44%	0.036%
20	10.318	1148	1154	1160	rBV3	30505	52999	16.39%	1.348%
21	10.858	1239	1246	1253	rVB2	47251	83852	25.93%	2.133%
22	11.017	1270	1273	1276	rVB2	842	970	0.30%	0.025%
23	11.070	1279	1282	1286	rBV3	1191	1796	0.56%	0.046%
24	11.258	1307	1314	1320	rVV	70011	125415	38.78%	3.191%
25	11.375	1327	1334	1341	rBV	34252	61468	19.01%	1.564%
26	12.033	1444	1446	1450	rVB2	900	1145	0.35%	0.029%
27	12.727	1560	1564	1567	rBV2	1271	1654	0.51%	0.042%
28	12.803	1575	1577	1581	rBV3	899	1015	0.31%	0.026%
29	13.021	1609	1614	1619	rBV2	485	950	0.29%	0.024%
30	13.538	1697	1702	1707	rVB2	3014	3821	1.18%	0.097%
31	13.737	1733	1736	1740	rBV3	2563	2721	0.84%	0.069%
32	13.825	1747	1751	1757	rVB2	2196	3180	0.98%	0.081%
33	13.890	1757	1762	1766	rBV3	3594	4201	1.30%	0.107%
34	14.407	1844	1850	1856	rVV	106050	150847	46.65%	3.838%
35	14.724	1897	1904	1913	rVB	103655	170677	52.78%	4.342%
36	14.801	1913	1917	1920	rBV	571	936	0.29%	0.024%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBZU2

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	14.883	1928	1931	1934	rVB2	1529	1513	0.47%	0.038%
38	14.989	1945	1949	1950	rBV	11117	12581	3.89%	0.320%
39	15.024	1950	1955	1961	rVV	134847	208607	64.51%	5.307%
40	15.077	1961	1964	1968	rVB4	1631	1968	0.61%	0.050%
41	15.171	1974	1980	1991	rBV	49407	80113	24.77%	2.038%
42	15.259	1991	1995	1998	rVV3	1822	2460	0.76%	0.063%
43	15.318	2001	2005	2009	rBV	1098	1362	0.42%	0.035%
44	15.759	2077	2080	2085	rVB3	2189	2533	0.78%	0.064%
45	15.911	2104	2106	2109	rBV3	1437	1190	0.37%	0.030%
46	16.005	2115	2122	2130	rVB	152063	224407	69.40%	5.709%
47	16.099	2133	2138	2146	rVB	43527	64692	20.01%	1.646%
48	16.352	2175	2181	2187	rBV	24836	36734	11.36%	0.935%
49	16.405	2187	2190	2193	rVV3	2118	2582	0.80%	0.066%
50	16.428	2193	2194	2198	rVV2	1541	1559	0.48%	0.040%
51	16.464	2198	2200	2205	rVB2	1982	2179	0.67%	0.055%
52	16.563	2213	2217	2220	rVB	748	1007	0.31%	0.026%
53	17.427	2361	2364	2365	rVV3	2154	2463	0.76%	0.063%
54	17.451	2365	2368	2375	rVB3	14387	17877	5.53%	0.455%
55	17.756	2414	2420	2427	rVB	201012	300934	93.06%	7.656%
56	17.856	2430	2437	2444	rBV	177321	260795	80.65%	6.635%
57	17.921	2444	2448	2451	rBV3	5800	6065	1.88%	0.154%
58	18.068	2470	2473	2475	rBV2	3188	3211	0.99%	0.082%
59	18.191	2493	2494	2500	rVB2	809	1193	0.37%	0.030%
60	18.397	2523	2529	2536	rBV2	1544	2459	0.76%	0.063%
61	18.496	2542	2546	2552	rVB3	3011	4020	1.24%	0.102%
62	18.596	2558	2563	2571	rBV4	16685	29945	9.26%	0.762%
63	18.720	2581	2584	2588	rVV3	4251	4795	1.48%	0.122%
64	18.761	2588	2591	2593	rVV	1260	1436	0.44%	0.037%
65	18.814	2596	2600	2604	rVV4	9458	12740	3.94%	0.324%
66	18.849	2604	2606	2610	rVV4	1489	2043	0.63%	0.052%
67	18.920	2615	2618	2619	rBV2	843	1054	0.33%	0.027%
68	18.972	2622	2627	2630	rBV4	8639	11089	3.43%	0.282%
69	19.014	2630	2634	2641	rVV2	17006	18765	5.80%	0.477%
70	19.078	2641	2645	2652	rVB3	9292	12141	3.75%	0.309%
71	19.155	2655	2658	2659	rBV2	1120	1103	0.34%	0.028%
72	19.202	2659	2666	2671	rVB5	2190	4222	1.31%	0.107%
73	19.401	2697	2700	2704	rBV2	2241	3205	0.99%	0.082%
74	19.442	2704	2707	2712	rVB4	2263	3117	0.96%	0.079%
75	19.648	2740	2742	2743	rBV	1683	1062	0.33%	0.027%
76	19.848	2771	2776	2781	rBV5	3325	4798	1.48%	0.122%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZU2

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	19.959	2793	2795	2799	rVB3	1283	1272	0.39%	0.032%
78	20.012	2802	2804	2805	rBV	1399	997	0.31%	0.025%
79	20.053	2808	2811	2812	rBV2	1038	1048	0.32%	0.027%
80	20.112	2815	2821	2827	rVV	229431	323364	100.00%	8.227%
81	20.159	2827	2829	2834	rVB4	7773	7723	2.39%	0.196%
82	20.224	2836	2840	2843	rBV6	2872	3680	1.14%	0.094%
83	20.341	2856	2860	2867	rVB4	16564	22099	6.83%	0.562%
84	20.435	2872	2876	2880	rBV2	30284	34297	10.61%	0.873%
85	20.529	2889	2892	2897	rBV4	11215	15564	4.81%	0.396%
86	20.618	2901	2907	2911	rVV2	28792	35002	10.82%	0.891%
87	20.647	2911	2912	2914	rVB2	2342	1267	0.39%	0.032%
88	20.811	2936	2940	2945	rVB	15782	18557	5.74%	0.472%
89	20.911	2955	2957	2959	rBV2	1916	1932	0.60%	0.049%
90	20.941	2959	2962	2965	rVV2	6727	8348	2.58%	0.212%
91	21.105	2987	2990	2995	rVB5	3203	3813	1.18%	0.097%
92	21.276	3017	3019	3020	rVB2	2254	1200	0.37%	0.031%
93	21.640	3077	3081	3088	rBV4	20457	30538	9.44%	0.777%
94	22.069	3147	3154	3163	rVB	177420	305725	94.55%	7.778%
95	23.309	3363	3365	3368	rBV4	2564	2179	0.67%	0.055%
96	23.867	3456	3460	3468	rVB3	15062	32013	9.90%	0.814%
97	25.347	3703	3712	3723	rVB3	99967	290201	89.74%	7.383%
98	25.594	3744	3754	3765	rVB	101832	301205	93.15%	7.663%
99	28.314	4215	4217	4218	rBV2	2229	1692	0.52%	0.043%
100	31.170	4701	4703	4705	rBV3	2442	1512	0.47%	0.038%

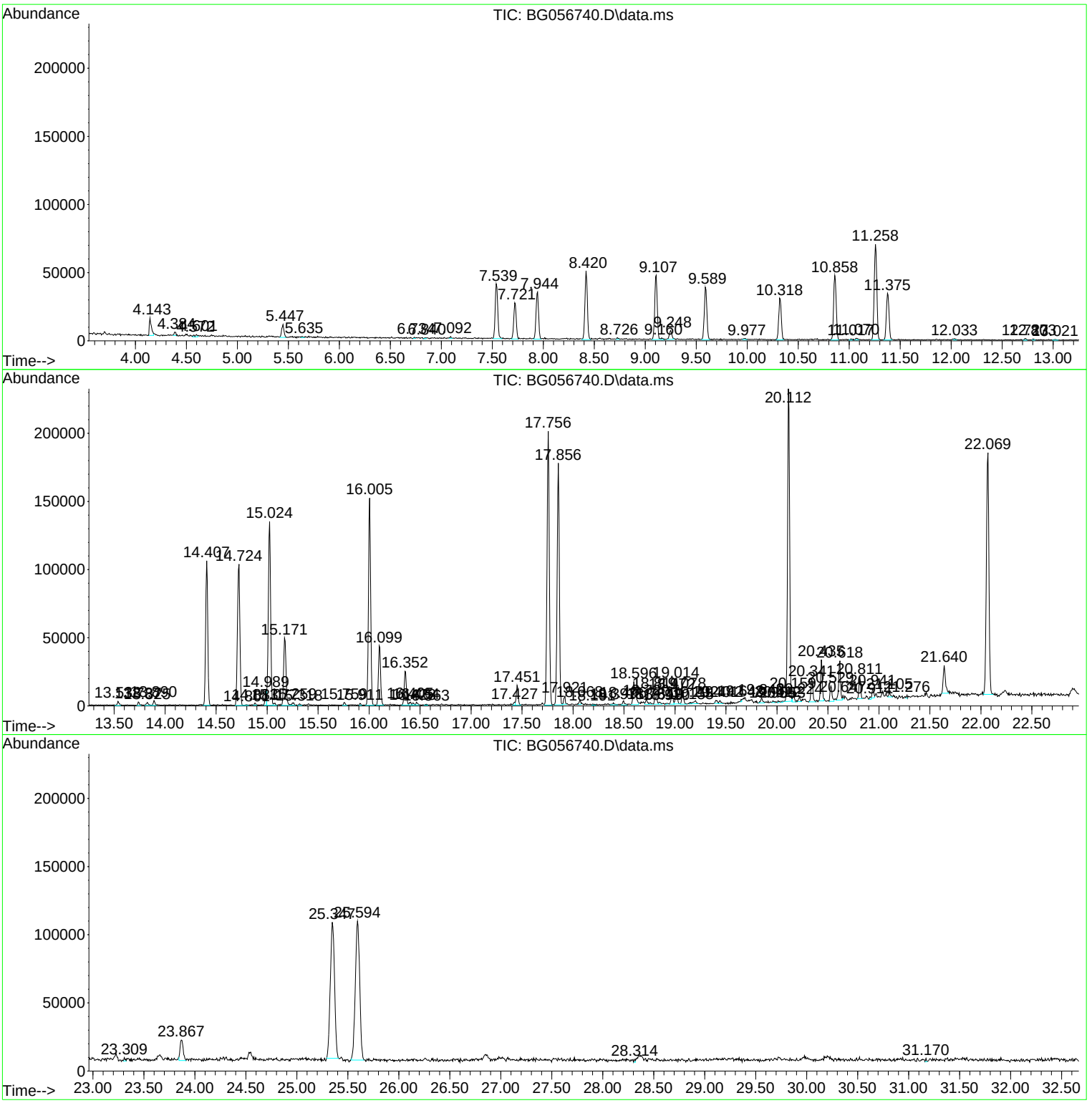
Sum of corrected areas: 3930540

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZU2

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\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZU2

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

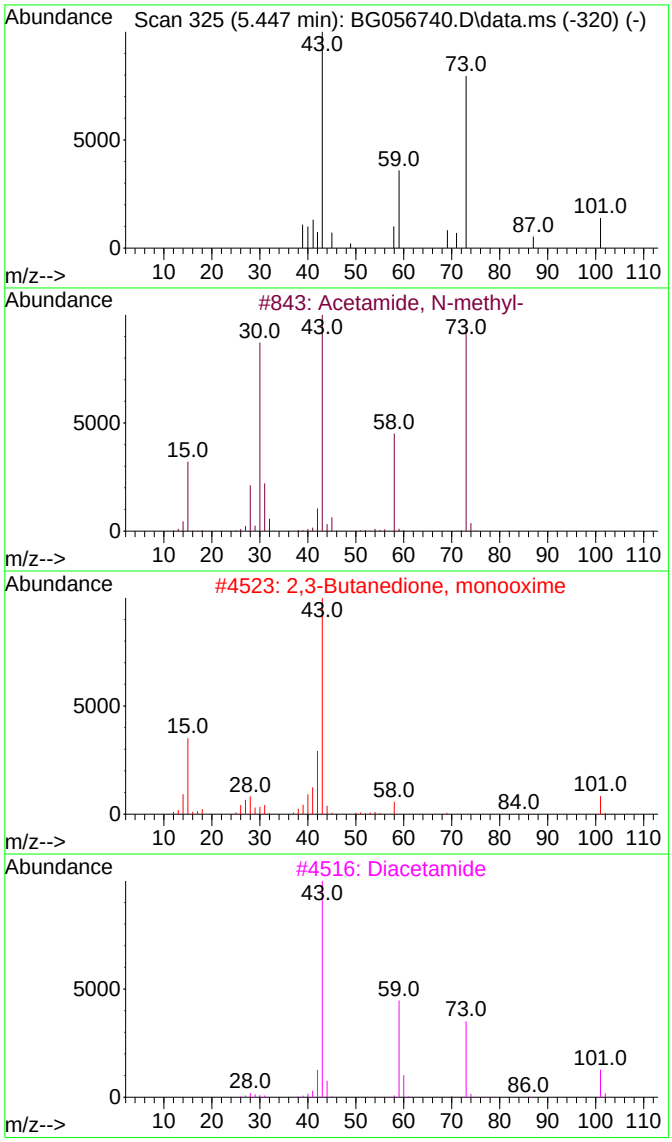
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

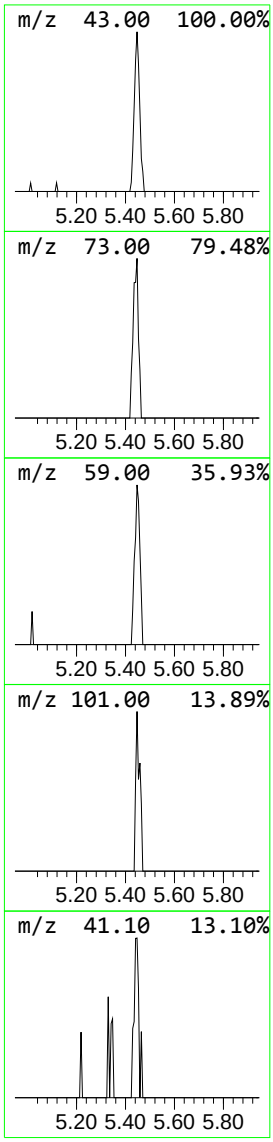
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.447	3.49 ng/ul	14598	1,4-Dichlorobenzene-d4	8.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
3	Diacetamide	101	C4H7NO2	000625-77-4	7
4	Diacetamide	101	C4H7NO2	000625-77-4	7
5	Guanidine, methyl-	73	C2H7N3	000471-29-4	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZU2

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

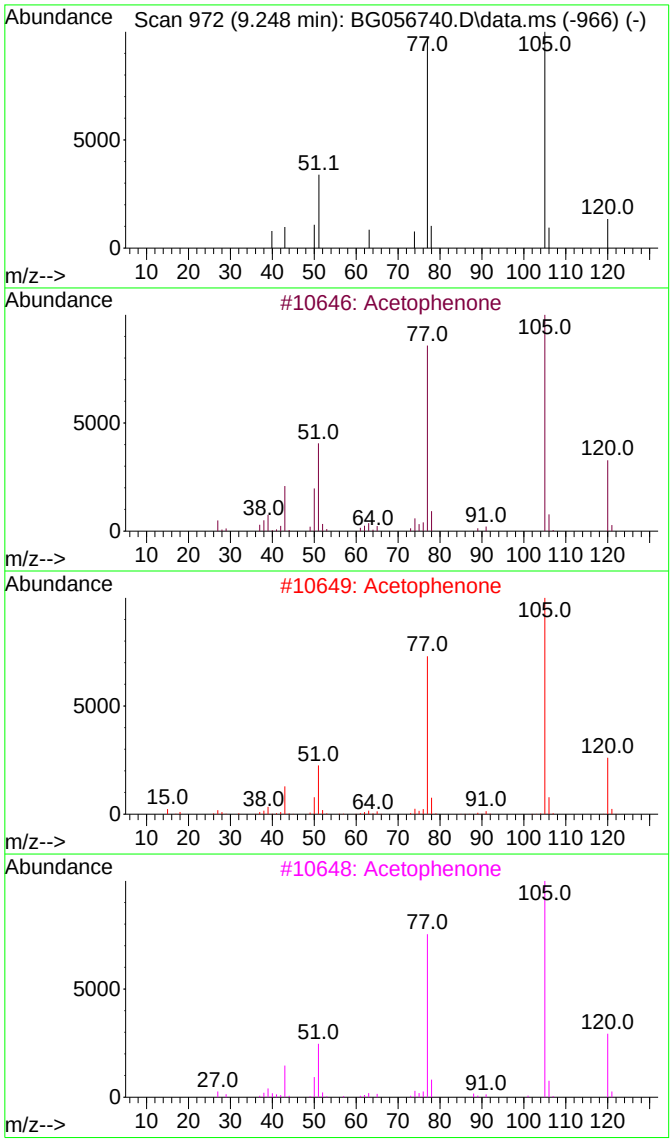
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

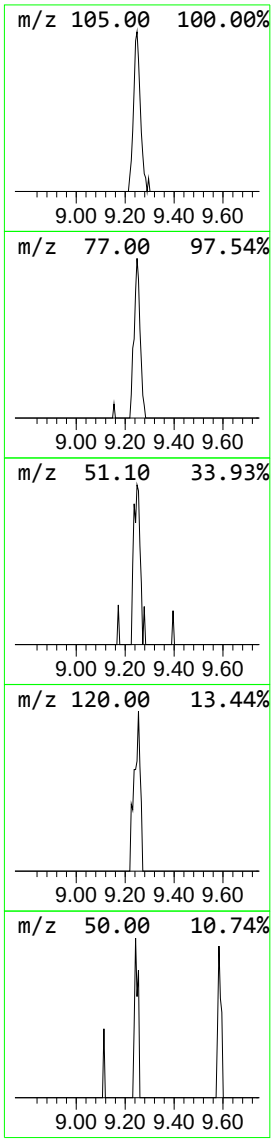
****

Peak Number 2 Acetophe none Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.248	2.68 ng/ul	11220	1,4-Dichlorobenzene-d4	8.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone	120	C8H8O	000098-86-2	83
2	Acetophenone	120	C8H8O	000098-86-2	83
3	Acetophenone	120	C8H8O	000098-86-2	83
4	Acetophenone	120	C8H8O	000098-86-2	83
5	Acetophenone	120	C8H8O	000098-86-2	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZU2

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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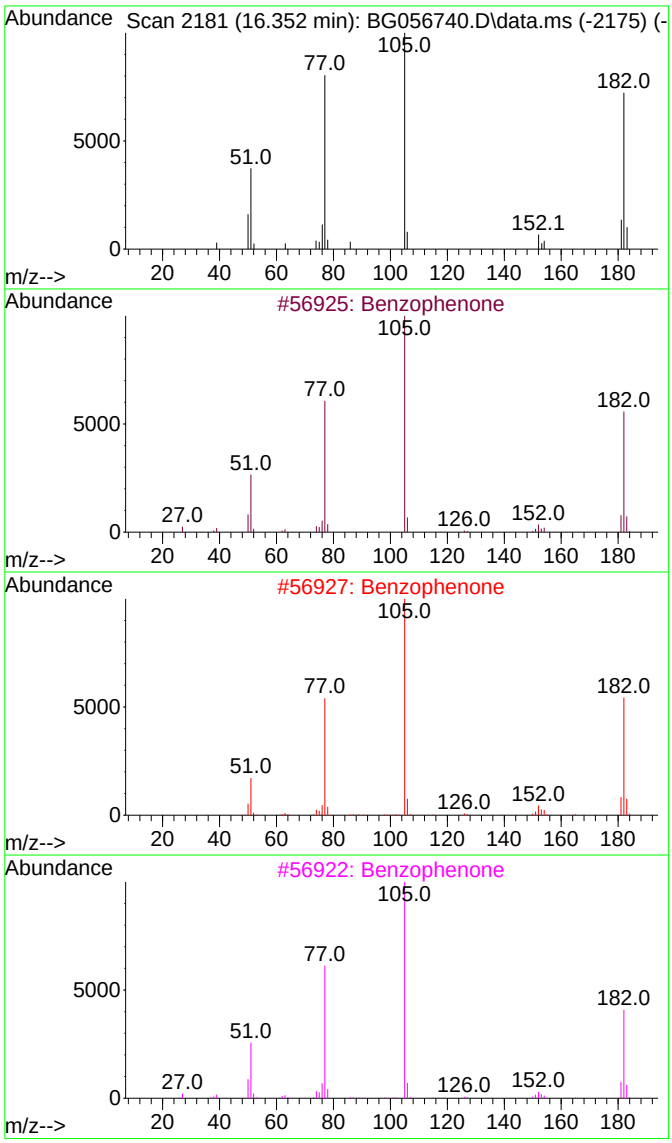
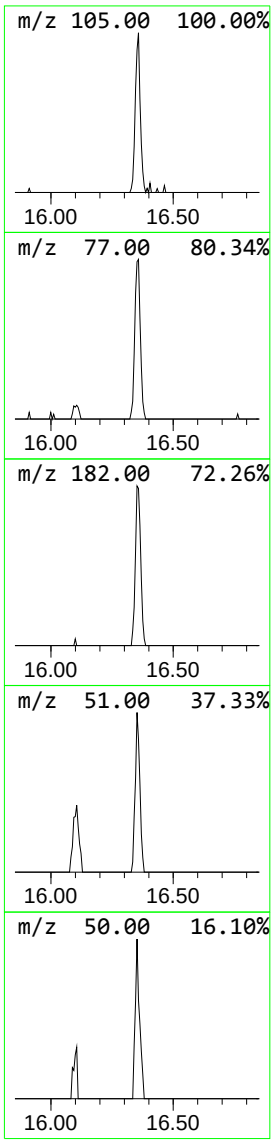
Peak Number 3 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.352	3.52 ng/ul	36734	Acenaphthene-d10	15.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	91
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZU2

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

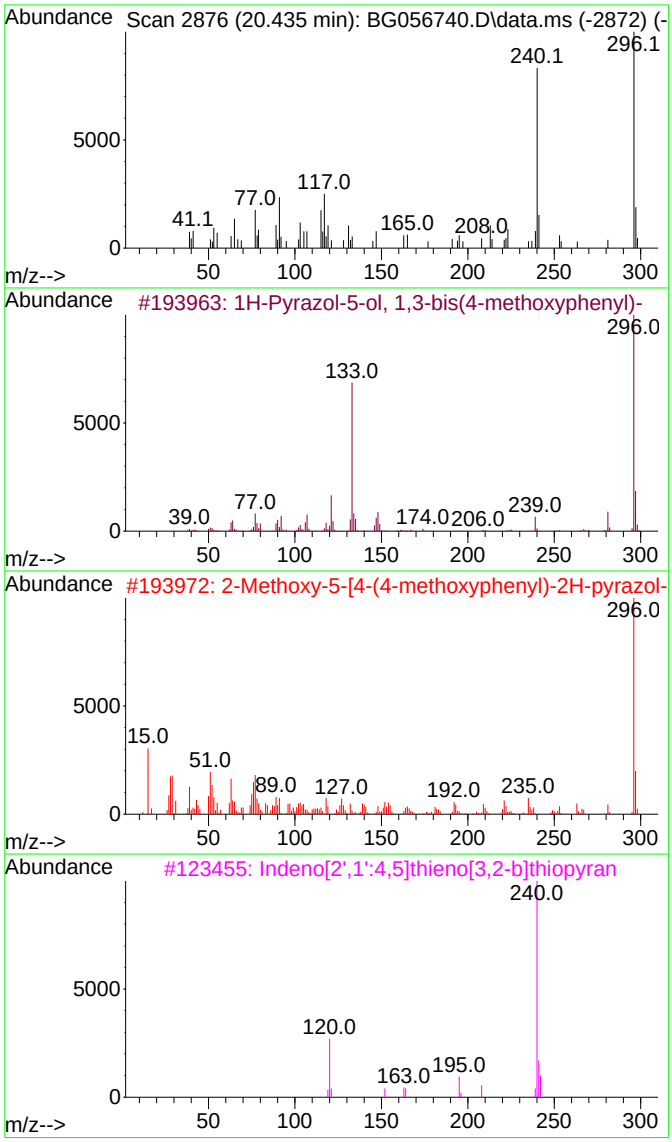
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

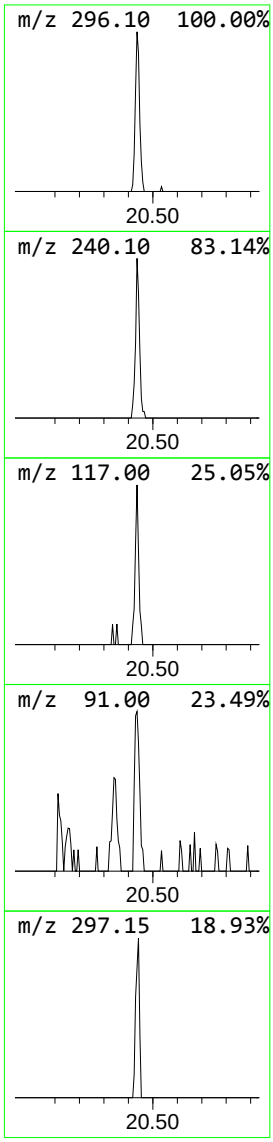
****

Peak Number 4 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.435	2.24 ng/ul	34297	Chrysene-d12	22.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazol-5-ol, 1,3-bis(4-metho...	296	C17H16N2O3	1000337-80-1	38
2	2-Methoxy-5-[4-(4-methoxyphenyl)...	296	C17H16N2O3	1000489-30-8	38
3	Indeno[2',1':4,5]thieno[3,2-b]th...	240	C14H8S2	056830-85-4	30
4	Thiazolidine-2,4-dione, 3-phenyl...	296	C15H12N4OS	309283-86-1	30
5	[1,1'-Biphenyl]-4,4'-diamine, 3,...	240	C16H20N2	054827-17-7	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZU2

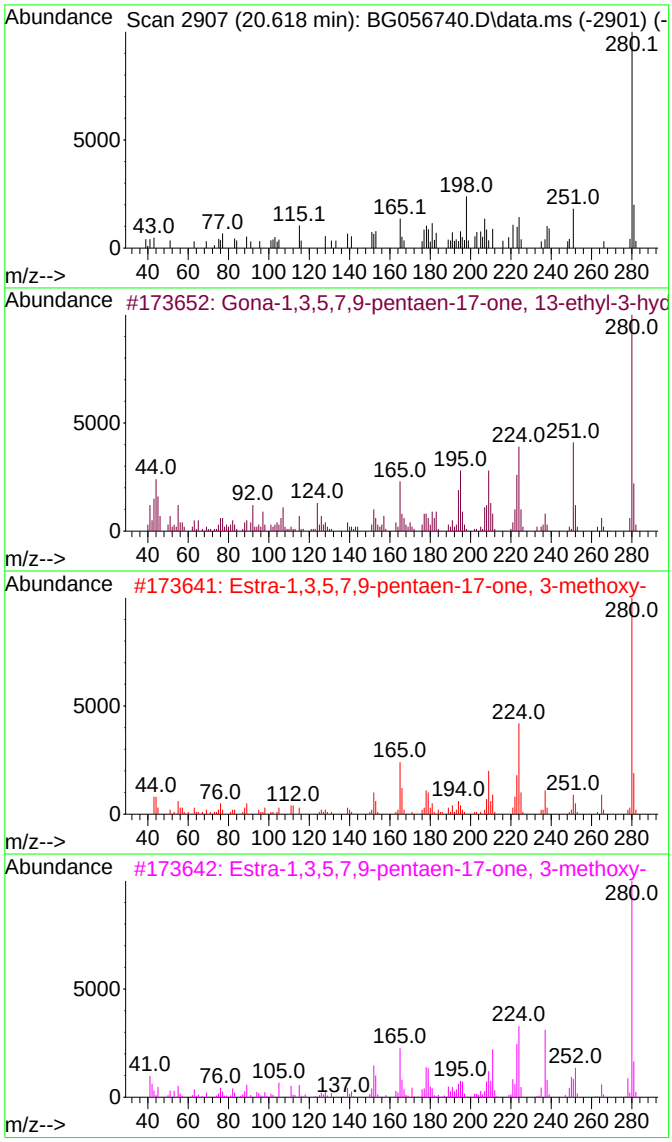
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

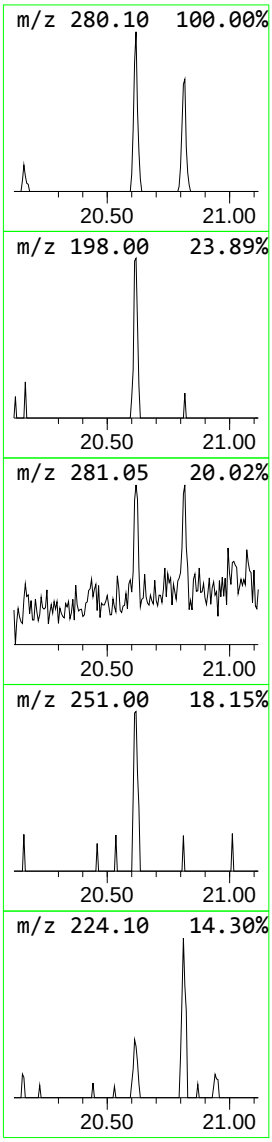
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Gona-1,3,5,7,9-pentaen-17-o... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.618	2.29 ng/ul	35002	Chrysene-d12	22.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Gona-1,3,5,7,9-pentaen-17-one, 1...	280	C19H20O2	030788-51-3	76
2	Estra-1,3,5,7,9-pentaen-17-one, ...	280	C19H20O2	003907-67-3	70
3	Estra-1,3,5,7,9-pentaen-17-one, ...	280	C19H20O2	003907-67-3	62
4	3,5-Bis(3-methoxyphenyl)-1H-pyra...	280	C17H16N2O2	1159988-49-4	58
5	4H-Pirazino[3,2,1-j,k]carbazole-...	280	C18H20N2O	313647-35-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZU2

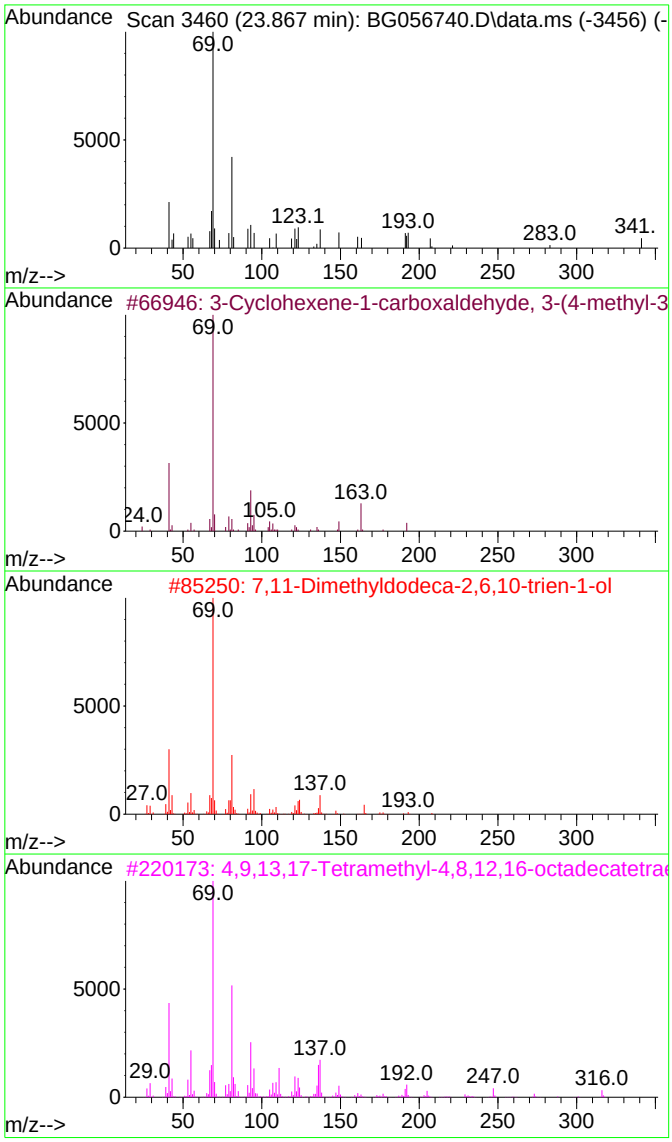
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

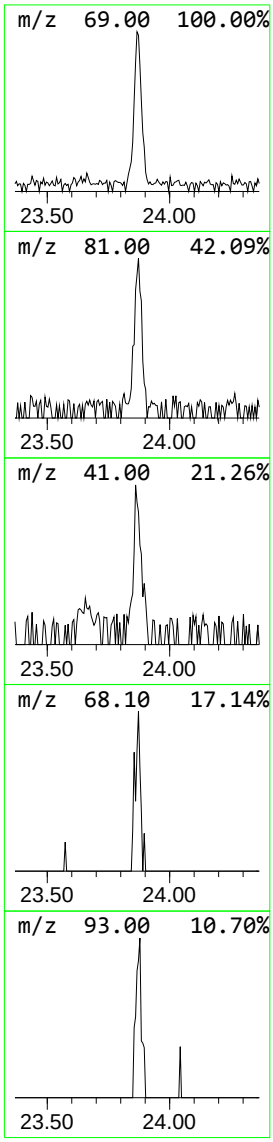
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Cyclohexene-1-carboxaldeh... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.867	2.13 ng/ul	32013	Perylene-d12	25.600

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	53
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	53
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	50
4	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	47
5	Squalene	410	C30H50	000111-02-4	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056740.D
Acq On : 27 Feb 2023 21:35
Operator : CG/JU
Sample : 01648-14
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZU2

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	5.447	3.5	ng/ul	14598	1	8.420	83701	20.0
Acetophe none	9.248	2.7	ng/ul	11220	1	8.420	83701	20.0
Benzophenone	16.352	3.5	ng/ul	36734	3	15.024	208607	20.0
unknown-02	20.435	2.2	ng/ul	34297	5	22.069	305725	20.0
Gona-1,3,5,7,9-...	20.618	2.3	ng/ul	35002	5	22.069	305725	20.0
3-Cyclohexene-1...	23.867	2.1	ng/ul	32013	6	25.600	301205	20.0