LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056737.D
Acq On : 27 Feb 2023 19:31
Operator : CG/JU
Sample : 01648-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBZT9

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: BG056737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.114	96	98	100	rBV	1593	1240	0.35%	0.029%
2	4.143	100	103	114	rVV2	9486	18743	5.36%	0.432%
3	5.447	320	325	332	rVB2	18120	28220	8.07%	0.650%
4	5.729	371	373	375	rBV	1155	999	0.29%	0.023%
5	5.829	388	390	392	rBV3	1321	1199	0.34%	0.028%
6	6.182	448	450	452	rBV2	828	815	0.23%	0.019%
7	6.493	501	503	505	rBV2	738	844	0.24%	0.019%
8	7.081	598	603	608	rBV4	4384	6510	1.86%	0.150%
9	7.504	672	675	676	rBV	835	767	0.22%	0.018%
10	7.539	676	681	692	rVB2	43308	76197	21.79%	1.755%
11	7.721	706	712	718	rVB	31791	49550	14.17%	1.141%
12	7.862	731	736	738	rBV2	1031	1064	0.30%	0.025%
13	7.939	743	749	756	rBV	37308	63225	18.08%	1.456%
14	8.420	824	831	840	rBV	59342	97858	27.98%	2.254%
15	9.108	941	948	954	rBV	47912	80404	22.99%	1.852%
16	9.243	964	971	980	rBV4	7075	13708	3.92%	0.316%
17	9.590	1023	1030	1036	rBV	39007	72343	20.68%	1.667%
18	9.971	1091	1095	1099	rVB2	1335	2209	0.63%	0.051%
19	10.318	1148	1154	1161	rVB2	33336	59084	16.89%	1.361%
20	10.659	1208	1212	1216	rVB3	4179	5932	1.70%	0.137%
21	10.794	1230	1235	1240	rVV5	2568	4413	1.26%	0.102%
22	10.859	1240	1246	1254	rVB2	52714	92054	26.32%	2.121%
23	11.258	1305	1314	1325	rBV	85488	151929	43.44%	3.500%
24	11.382	1328	1335	1344	rVB2	33683	60802	17.38%	1.401%
25	12.621	1540	1546	1550	rBV2	394	749	0.21%	0.017%
26	12.668	1550	1554	1559	rVB4	3035	3656	1.05%	0.084%
27	12.803	1573	1577	1580	rBV3	988	1008	0.29%	0.023%
28	13.708	1727	1731	1735	rBV	538	863	0.25%	0.020%
29	13.744	1735	1737	1743	rVB2	400	746	0.21%	0.017%
30	13.826	1747	1751	1755	rVB4	2649	3801	1.09%	0.088%
31	14.225	1814	1819	1823	rVB3	2591	3030	0.87%	0.070%
32	14.349	1836	1840	1844	rBV2	20030	27570	7.88%	0.635%
33	14.407	1844	1850	1856	rVV	117792	168877	48.28%	3.890%
34	14.472	1856	1861	1863	rVV2	3357	4336	1.24%	0.100%
35	14.507	1863	1867	1873	rVB2	26054	35293	10.09%	0.813%
36	14.660	1890	1893	1896	rBV	906	1147	0.33%	0.026%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
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Acq On : 27 Feb 2023 19:31
Operator : CG/JU
Sample : 01648-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZT9

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	14.719	1896	1903	1910	rBV2	123372	190373	54.43%	4.386%
38	14.877	1927	1930	1934	rBV	2811	2868	0.82%	0.066%
39	14.971	1942	1946	1949	rBV3	10189	14015	4.01%	0.323%
40	15.024	1949	1955	1961	rVV	159446	241444	69.03%	5.562%
41	15.071	1961	1963	1968	rVB	893	892	0.26%	0.021%
42	15.171	1974	1980	1988	rBV	49965	78176	22.35%	1.801%
43	15.254	1992	1994	1998	rVB2	1482	1418	0.41%	0.033%
44	15.324	2003	2006	2011	rBV2	844	1684	0.48%	0.039%
45	15.406	2017	2020	2022	rBV	787	751	0.21%	0.017%
46	15.829	2089	2092	2097	rBV3	2903	3858	1.10%	0.089%
47	16.006	2115	2122	2129	rBV	168509	250832	71.72%	5.778%
48	16.100	2133	2138	2146	rVB	48069	69918	19.99%	1.611%
49	16.288	2169	2170	2174	rVB	795	744	0.21%	0.017%
50	16.352	2174	2181	2188	rBV	48084	72634	20.77%	1.673%
51	16.869	2267	2269	2274	rVB	741	805	0.23%	0.019%
52	16.916	2274	2277	2280	rBV	1042	1292	0.37%	0.030%
53	17.427	2359	2364	2368	rBV	1256	1696	0.48%	0.039%
54	17.551	2380	2385	2386	rBV	866	1262	0.36%	0.029%
55	17.756	2414	2420	2430	rVB	227011	333939	95.48%	7.693%
56	17.856	2430	2437	2443	rVV	186795	284781	81.42%	6.560%
57	17.915	2444	2447	2452	rVB2	5415	5500	1.57%	0.127%
58	18.097	2474	2478	2480	rBV	623	850	0.24%	0.020%
59	18.256	2502	2505	2508	rBV2	692	817	0.23%	0.019%
60	18.350	2520	2521	2524	rBV	1090	766	0.22%	0.018%
61	18.450	2532	2538	2540	rBV2	835	848	0.24%	0.020%
62	18.497	2542	2546	2548	rBV3	1133	1364	0.39%	0.031%
63	18.597	2559	2563	2572	rBV2	15155	21508	6.15%	0.495%
64	18.661	2572	2574	2576	rVV2	1277	1345	0.38%	0.031%
65	18.714	2579	2583	2585	rBV	1148	1350	0.39%	0.031%
66	18.843	2603	2605	2609	rVB2	1528	1492	0.43%	0.034%
67	18.896	2609	2614	2615	rBV2	1251	1486	0.42%	0.034%
68	18.932	2618	2620	2623	rBV2	757	858	0.25%	0.020%
69	19.014	2630	2634	2637	rBV	11215	11442	3.27%	0.264%
70	19.120	2649	2652	2653	rBV2	1642	1765	0.50%	0.041%
71	19.137	2653	2655	2657	rVV	2011	1589	0.45%	0.037%
72	19.184	2661	2663	2666	rVV2	1778	1436	0.41%	0.033%
73	19.243	2670	2673	2675	rBV2	909	833	0.24%	0.019%
74	19.343	2687	2690	2691	rBV	1004	914	0.26%	0.021%
75	19.402	2697	2700	2703	rBV2	1842	1975	0.56%	0.045%
76	19.443	2704	2707	2711	rVV3	1717	1680	0.48%	0.039%

LSC Area Percent Report

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Operator : CG/JU
Sample : 01648-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZT9

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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Peak separation: 5

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

77	19.513	2716	2719	2724	rVB3	1151	1691	0.48%	0.039%
78	19.613	2732	2736	2737	rBV2	1913	1908	0.55%	0.044%
79	19.684	2745	2748	2754	rVB6	4695	8268	2.36%	0.190%
80	19.742	2756	2758	2762	rVB2	1755	1845	0.53%	0.043%
81	19.854	2774	2777	2781	rVB4	1892	2357	0.67%	0.054%
82	19.954	2791	2794	2796	rBV2	1946	1970	0.56%	0.045%
83	20.113	2816	2821	2828	rVB	242492	349756	100.00%	8.057%
84	20.195	2833	2835	2836	rBV	1462	1069	0.31%	0.025%
85	20.236	2840	2842	2843	rVB2	1390	768	0.22%	0.018%
86	20.395	2867	2869	2870	rBV2	1521	1125	0.32%	0.026%
87	20.536	2890	2893	2897	rBV	8303	10756	3.08%	0.248%
88	20.600	2902	2904	2909	rVB4	3817	4503	1.29%	0.104%
89	20.729	2925	2926	2927	rBV	1937	968	0.28%	0.022%
90	20.818	2940	2941	2943	rBV2	1958	1821	0.52%	0.042%
91	21.070	2980	2984	2987	rVB	9719	10588	3.03%	0.244%
92	21.170	2999	3001	3004	rBV3	1900	1459	0.42%	0.034%
93	21.282	3018	3020	3026	rBV4	2431	4167	1.19%	0.096%
94	21.464	3046	3051	3056	rBV	46585	64421	18.42%	1.484%
95	21.640	3077	3081	3089	rBV3	42482	71990	20.58%	1.658%
96	22.063	3147	3153	3164	rVB2	201984	348500	99.64%	8.028%
97	23.873	3457	3461	3469	rVB4	14131	28646	8.19%	0.660%
98	23.943	3469	3473	3474	rBV2	3557	4178	1.19%	0.096%
99	25.348	3702	3712	3728	rVB2	110996	316613	90.52%	7.294%
100	25.594	3744	3754	3765	rVB2	118044	347180	99.26%	7.998%

Sum of corrected areas: 4340932

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
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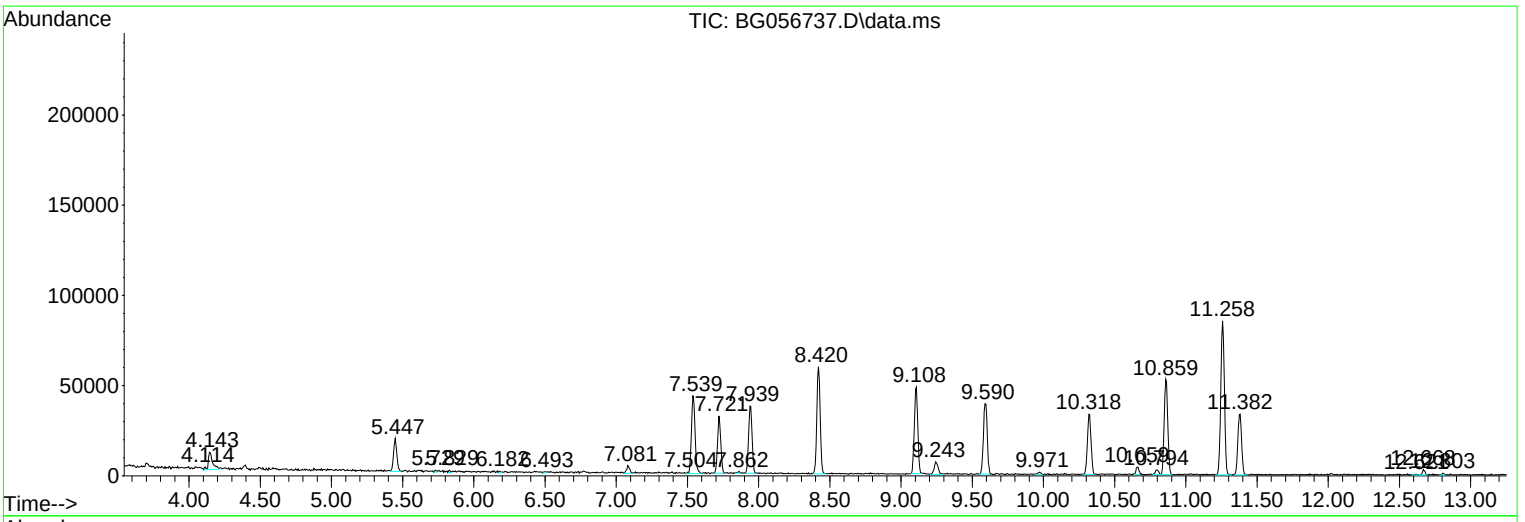
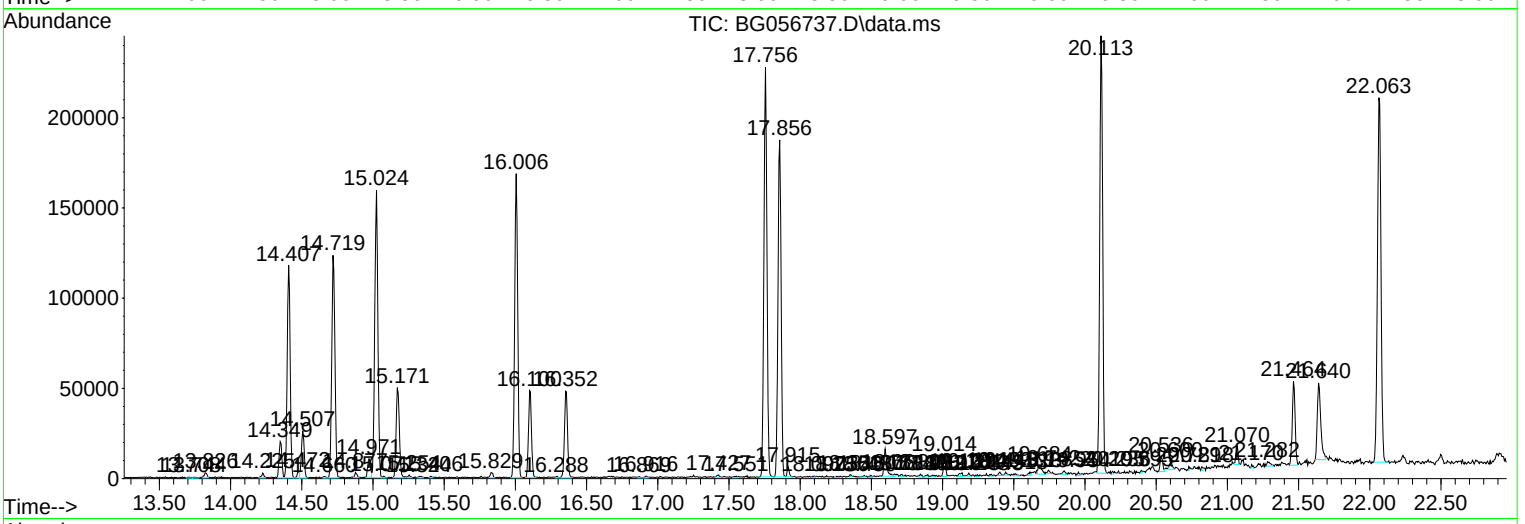
Sample : 01648-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

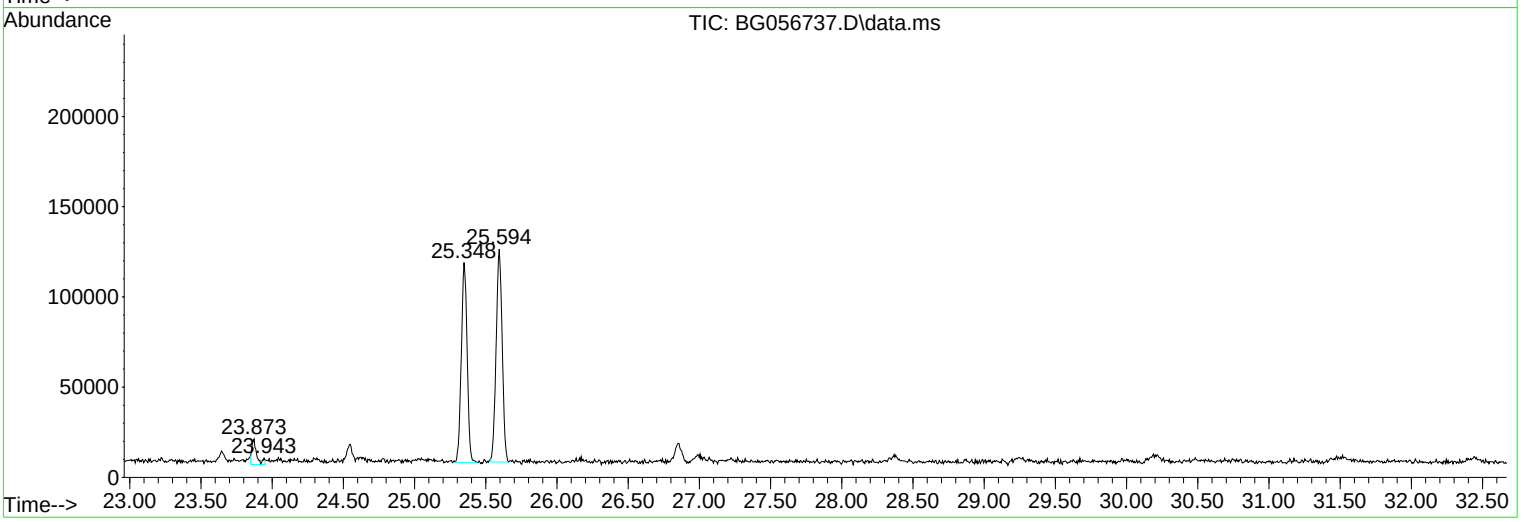
Instrument :
BNA_G
ClientSampleId :
DBZT9

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 : BG056737.D
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Operator : CG/JU
Sample : 01648-11
Misc :
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Instrument :
BNA_G
ClientSampleId :
DBZT9

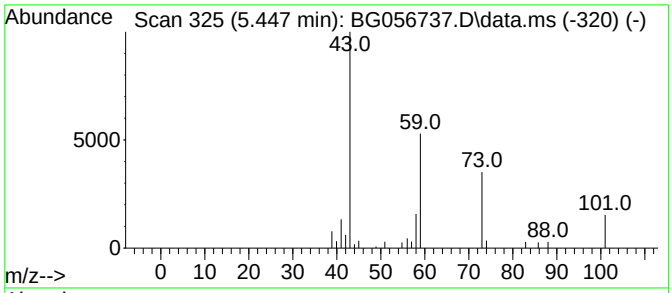
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

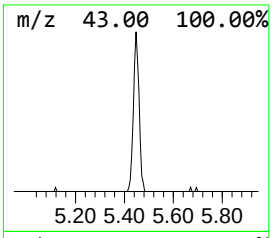
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

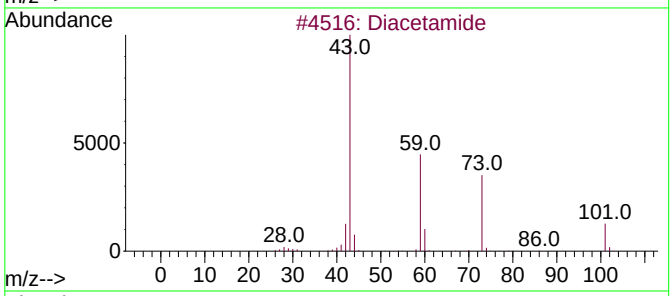
****
Peak Number 1 Diacetamide Concentration Rank 2

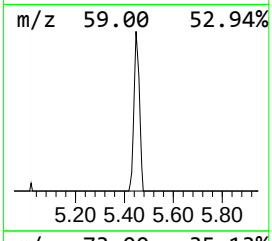
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.447	5.77 ng/ul	28220	1,4-Dichlorobenzene-d4	8.420

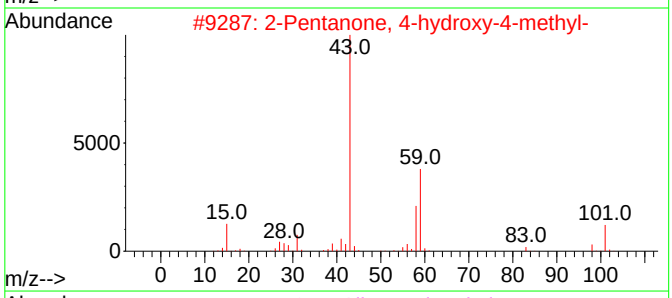
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diacetamide	101	C4H7NO2	000625-77-4	59
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
3	Silane, trimethyl-	74	C3H10Si	000993-07-7	38
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	37
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	28

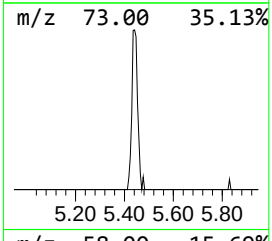


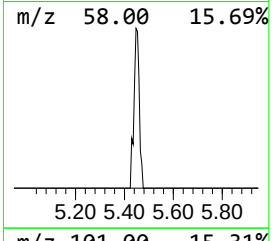


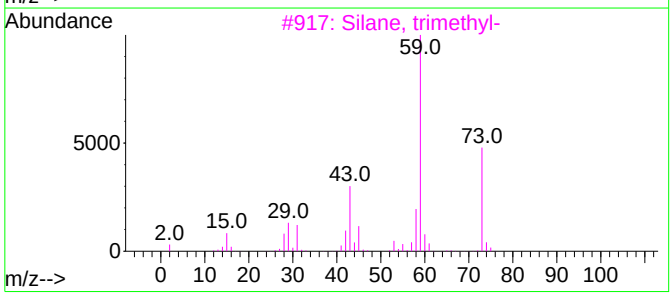


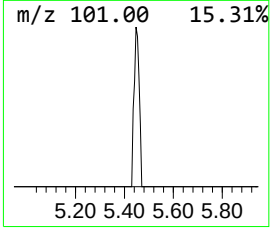












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056737.D
Acq On : 27 Feb 2023 19:31
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZT9

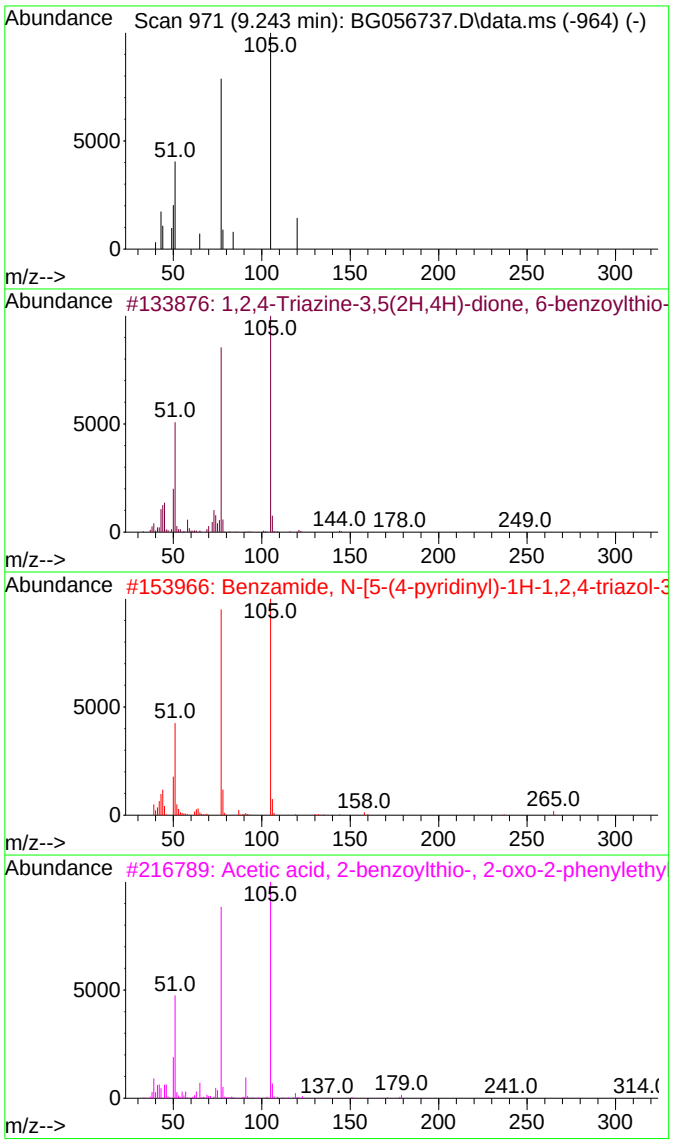
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG022323.M
Quant Title : SVOA CALIBRATION

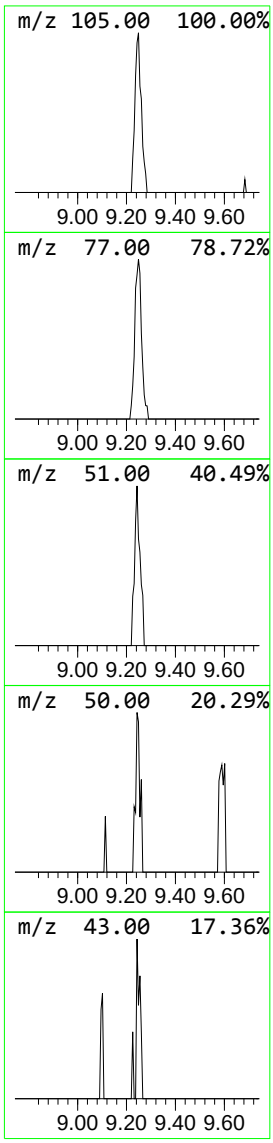
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,2,4-Triazine-3,5(2H,4H)-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.243	2.80 ng/ul	13708	1,4-Dichlorobenzene-d4	8.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	72
2	Benzamide, N-[5-(4-pyridinyl)-1H...	265	C14H11N5O	1000319-96-5	72
3	Acetic acid, 2-benzoylthio-, 2-o...	314	C17H14O4S	1000260-20-1	56
4	Benzoylformic acid	150	C8H6O3	000611-73-4	40
5	Acetophenone	120	C8H8O	000098-86-2	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056737.D
Acq On : 27 Feb 2023 19:31
Operator : CG/JU
Sample : 01648-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZT9

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

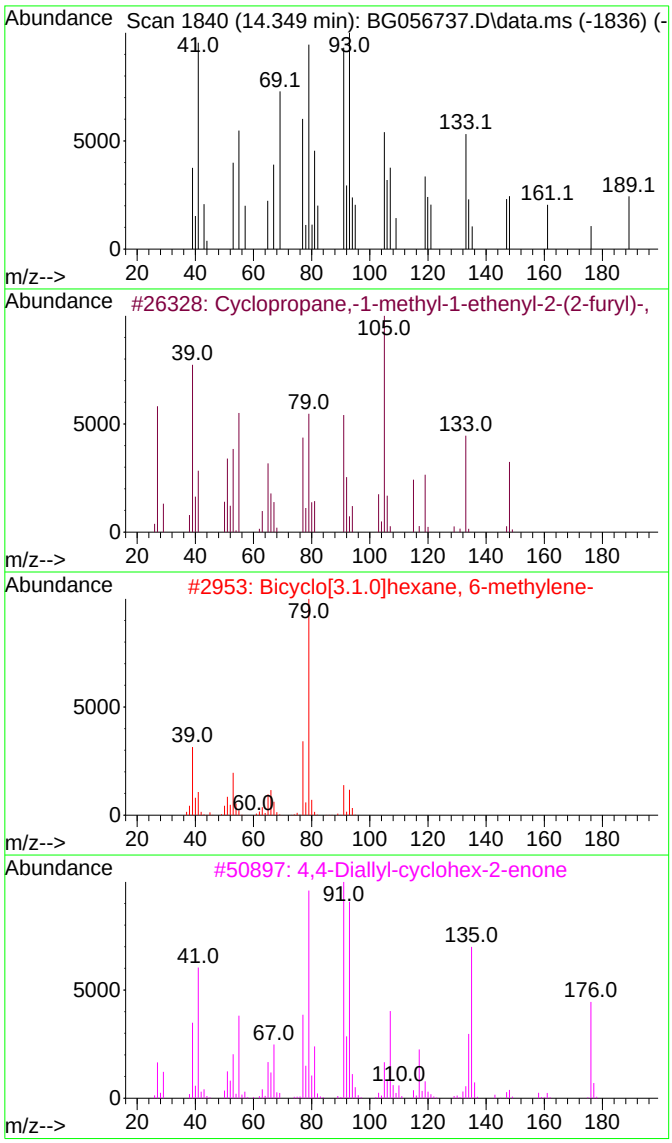
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

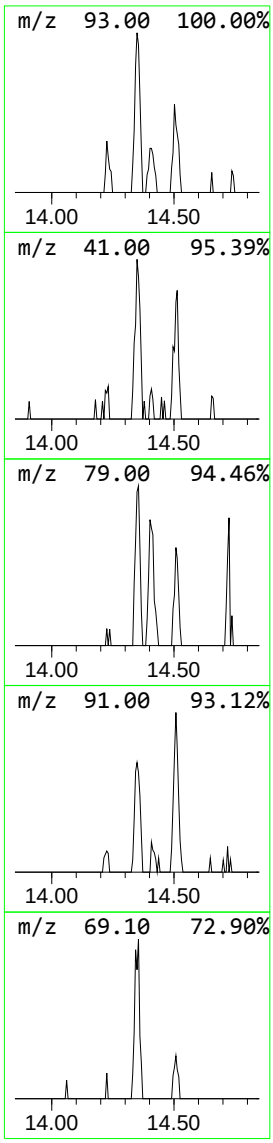
****

Peak Number 3 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.349	2.28 ng/ul	27570	Acenaphthene-d10	15.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane,-1-methyl-1-ethenyl...	148	C10H12O	1000221-96-9	49
2	Bicyclo[3.1.0]hexane, 6-methylene-	94	C7H10	054211-16-4	38
3	4,4-Diallyl-cyclohex-2-enone	176	C12H16O	1000186-50-1	38
4	trans-.alpha.-Bergamotene	204	C15H24	013474-59-4	35
5	Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	35





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Data File : BG056737.D
Acq On : 27 Feb 2023 19:31
Operator : CG/JU
Sample : 01648-11
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZT9

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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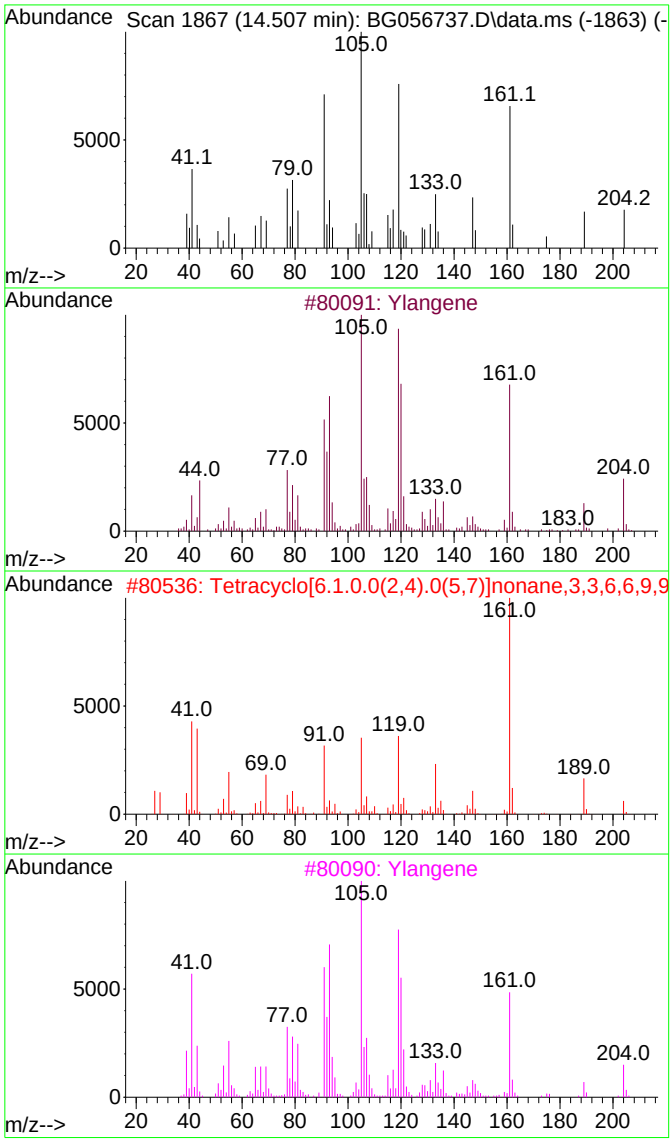
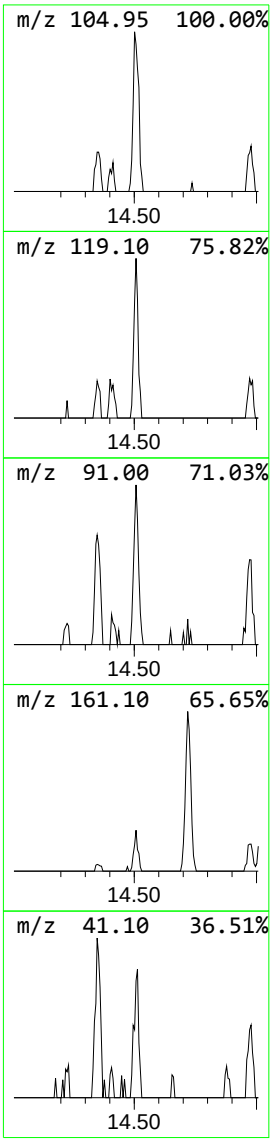
Peak Number 4 Ylangene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.507	2.92 ng/ul	35293	Acenaphthene-d10	15.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ylangene	204	C15H24	014912-44-8	87
2	Tetracyclo[6.1.0.0(2,4).0(5,7)]n...	204	C15H24	051898-92-1	87
3	Ylangene	204	C15H24	014912-44-8	81
4	cis-muurola-3,5-diene	204	C15H24	1000365-95-4	60
5	Ylangene	204	C15H24	014912-44-8	58





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Acq On : 27 Feb 2023 19:31
Operator : CG/JU
Sample : 01648-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZT9

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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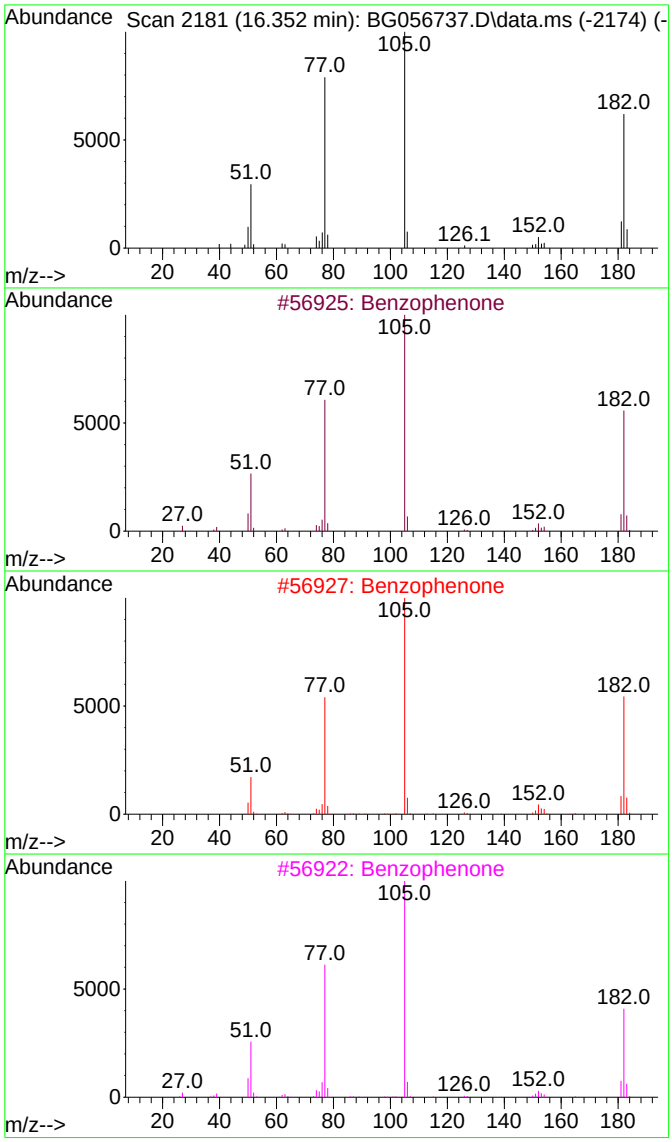
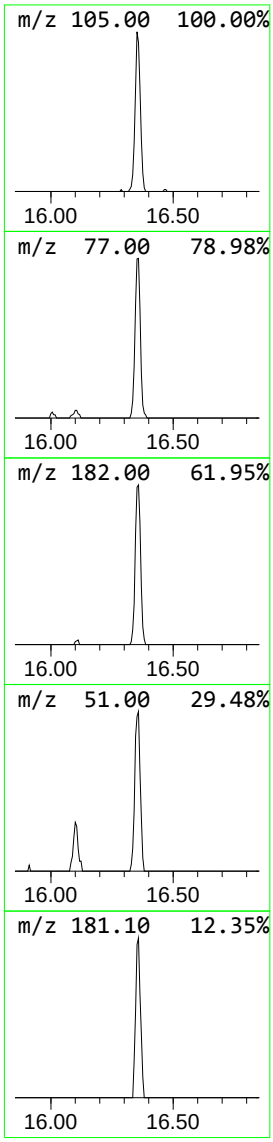
Peak Number 5 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.352	6.02 ng/ul	72634	Acenaphthene-d10	15.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	94
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	90





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Operator : CG/JU
Sample : 01648-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZT9

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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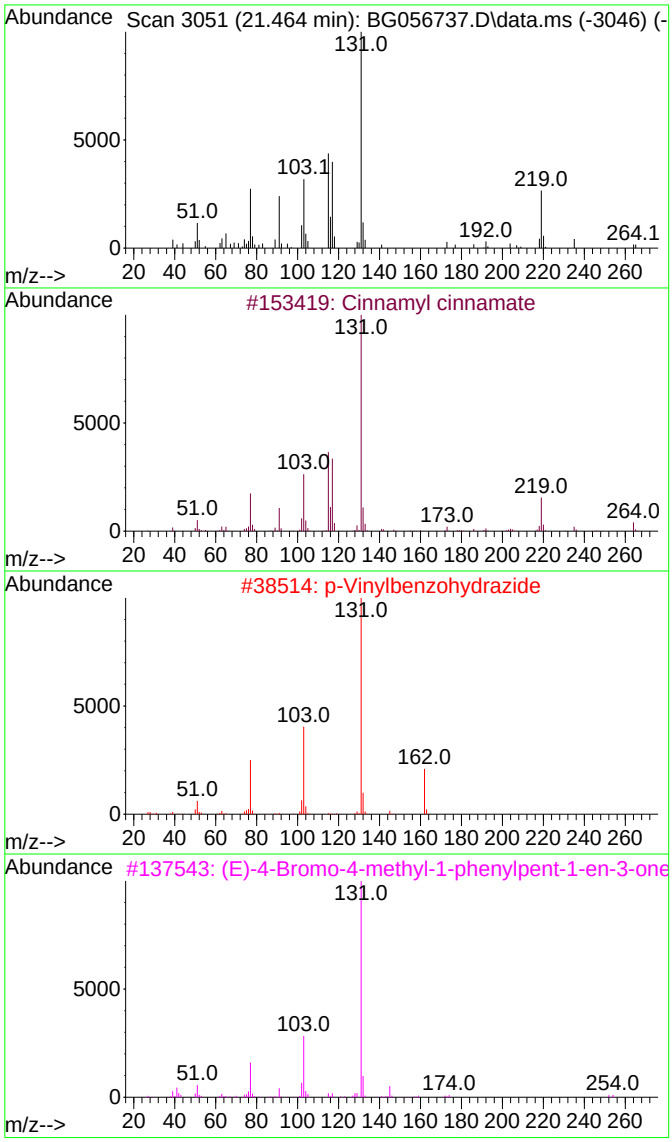
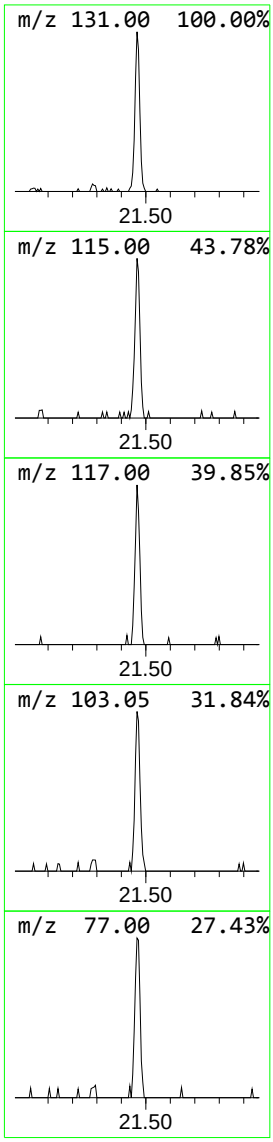
Peak Number 6 Cinnamyl cinnamate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.464	3.70 ng/ul	64421	Chrysene-d12	22.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	38
3	(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	38
4	Imidazo[1,2-a]pyridine-3-methana...	219	C11H17N3Si	1000497-61-2	38
5	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	38





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Data File : BG056737.D
Acq On : 27 Feb 2023 19:31
Operator : CG/JU
Sample : 01648-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZT9

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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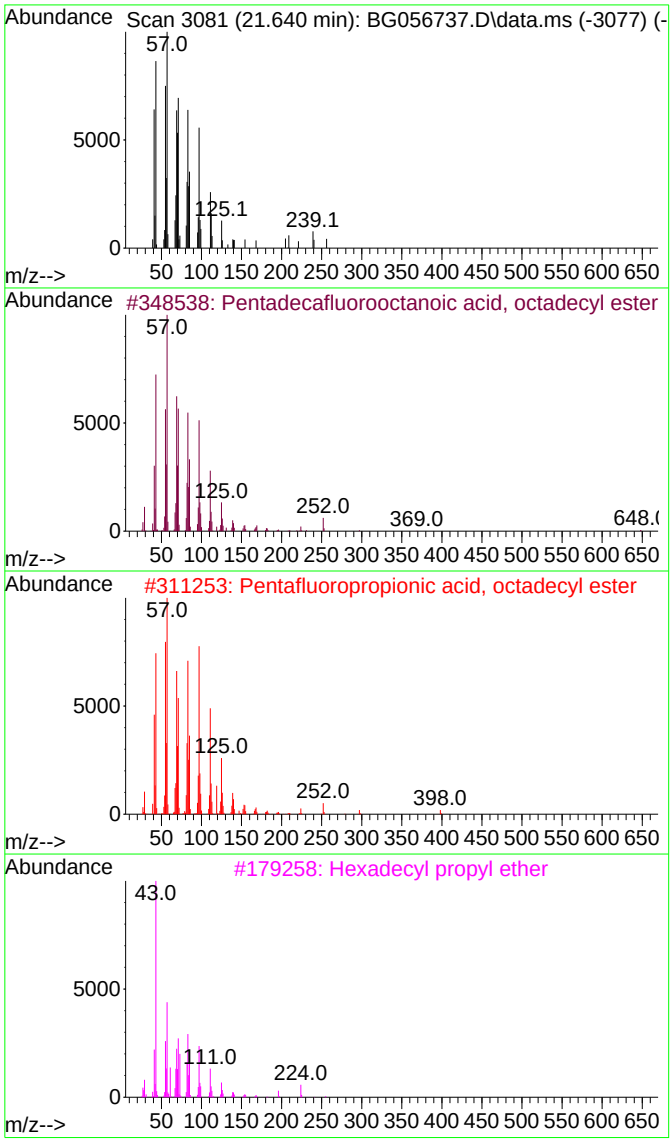
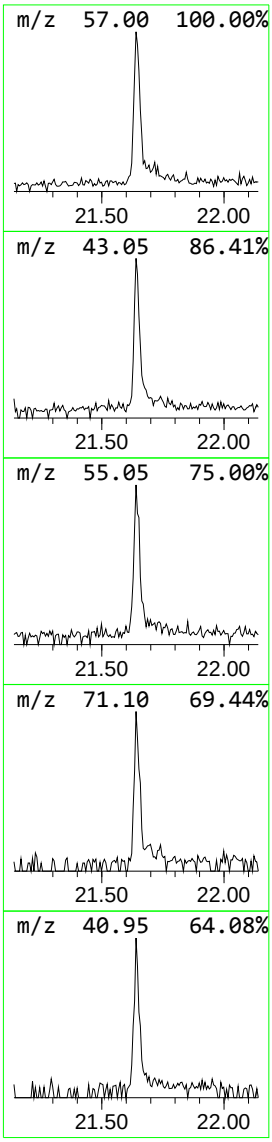
Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.640	4.13 ng/ul	71990	Chrysene-d12	22.063

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	83
3	Hexadecyl propyl ether	284	C19H40O	1000406-27-9	83
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	76
5	1-Octadecanol	270	C18H38O	000112-92-5	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG022723\
Data File : BG056737.D
Acq On : 27 Feb 2023 19:31
Operator : CG/JU
Sample : 01648-11
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBZT9

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
Diacetamide	5.447	5.8	ng/ul	28220	1	8.420	97858	20.0
1,2,4-Triazine-...	9.243	2.8	ng/ul	13708	1	8.420	97858	20.0
unknown-01	14.349	2.3	ng/ul	27570	3	15.024	241444	20.0
Ylangene	14.507	2.9	ng/ul	35293	3	15.024	241444	20.0
Benzophenone	16.352	6.0	ng/ul	72634	3	15.024	241444	20.0
Cinnamyl cinnamate	21.464	3.7	ng/ul	64421	5	22.063	348500	20.0
Pentadecafluoro...	21.640	4.1	ng/ul	71990	5	22.063	348500	20.0