LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

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\SOM-EPA-BG111920MA.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.584	39	42	45	rBV3	6156	8469	0.69%	0.063%
2	3.884	89	93	96	rBV	2678	4876	0.39%	0.037%
3	4.007	111	114	117	rVV	1968	2812	0.23%	0.021%
4	4.031	117	118	121	rVB2	3004	2117	0.17%	0.016%
5	4.207	146	148	151	rVB	2467	2286	0.18%	0.017%
6	4.319	162	167	170	rBV	1437	2370	0.19%	0.018%
7	4.372	172	176	180	rVB4	3303	4727	0.38%	0.035%
8	4.583	209	212	216	rVB4	2148	2977	0.24%	0.022%
9	4.660	220	225	227	rBV	2023	2977	0.24%	0.022%
10	5.194	313	316	319	rBV	1544	2078	0.17%	0.016%
11	5.306	333	335	338	rVB	3421	3441	0.28%	0.026%
12	6.117	470	473	475	rBV	1844	2427	0.20%	0.018%
13	6.176	480	483	485	rVB	2109	2002	0.16%	0.015%
14	7.380	678	688	698	rBV2	186517	366131	29.63%	2.743%
15	7.562	712	719	728	rBV	105825	180052	14.57%	1.349%
16	7.774	749	755	762	rBV2	184938	324923	26.29%	2.434%
17	8.250	829	836	841	rBV	139874	238543	19.30%	1.787%
18	8.285	841	842	846	rVB2	3304	3478	0.28%	0.026%
19	8.937	946	953	962	rBV2	225086	392375	31.75%	2.940%
20	9.325	1014	1019	1020	rBV	2264	2671	0.22%	0.020%
21	9.413	1028	1034	1042	rBV	177456	321022	25.98%	2.405%
22	9.701	1079	1083	1086	rBV	1698	2589	0.21%	0.019%
23	9.824	1100	1104	1108	rVB3	5379	7815	0.63%	0.059%
24	10.141	1150	1158	1166	rBV2	173132	317494	25.69%	2.379%
25	10.682	1242	1250	1258	rBV	241883	434346	35.15%	3.254%
26	10.935	1289	1293	1295	rBV	1683	2288	0.19%	0.017%
27	11.076	1309	1317	1324	rBV	166439	306519	24.80%	2.297%
28	11.193	1327	1337	1348	rBV	158686	289487	23.43%	2.169%
29	11.528	1385	1394	1399	rBV2	12177	22994	1.86%	0.172%
30	11.569	1399	1401	1405	rVB2	2005	2171	0.18%	0.016%
31	11.810	1439	1442	1444	rBV2	1824	2490	0.20%	0.019%
32	12.515	1560	1562	1568	rVB2	1926	2897	0.23%	0.022%
33	12.574	1568	1572	1574	rBV2	2010	2833	0.23%	0.021%
34	12.627	1579	1581	1583	rBV	3280	3233	0.26%	0.024%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

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\SOM-EPA-BG111920MA.M
Title : SVOA CALIBRATION

35	13.402	1709	1713	1715	rVB	2015	2028	0.16%	0.015%
36	13.537	1728	1736	1738	rBV	1947	3622	0.29%	0.027%
37	13.673	1754	1759	1761	rBV	2663	2872	0.23%	0.022%
38	13.743	1766	1771	1774	rBV2	4113	6798	0.55%	0.051%
39	14.254	1851	1858	1863	rBV	442626	652188	52.78%	4.886%
40	14.301	1863	1866	1872	rVB	104185	141093	11.42%	1.057%
41	14.560	1902	1910	1917	rVB	432693	678926	54.94%	5.087%
42	14.666	1926	1928	1931	rBV	1850	2442	0.20%	0.018%
43	14.742	1938	1941	1943	rVB2	2927	2685	0.22%	0.020%
44	14.865	1954	1962	1968	rBV	254721	413893	33.49%	3.101%
45	15.024	1982	1989	1996	rBV2	210884	351390	28.44%	2.633%
46	15.106	2001	2003	2006	rVB	2804	2545	0.21%	0.019%
47	15.612	2086	2089	2093	rVB	2521	2818	0.23%	0.021%
48	15.670	2096	2099	2104	rVV	1639	2943	0.24%	0.022%
49	15.847	2122	2129	2137	rVB	567587	854270	69.13%	6.400%
50	15.946	2141	2146	2155	rBV	203859	308884	25.00%	2.314%
51	16.087	2164	2170	2173	rVB2	7811	10328	0.84%	0.077%
52	16.211	2186	2191	2193	rBV	2187	3199	0.26%	0.024%
53	16.469	2231	2235	2237	rVB	1652	2179	0.18%	0.016%
54	16.522	2241	2244	2246	rBV	2849	3226	0.26%	0.024%
55	16.622	2259	2261	2264	rVB4	3751	3541	0.29%	0.027%
56	16.687	2270	2272	2275	rVB4	2817	2085	0.17%	0.016%
57	16.769	2282	2286	2288	rBV	1865	2377	0.19%	0.018%
58	16.822	2294	2295	2298	rVB2	2932	2183	0.18%	0.016%
59	16.875	2303	2304	2308	rVB2	2559	2599	0.21%	0.019%
60	16.916	2308	2311	2315	rBV	2400	3170	0.26%	0.024%
61	17.028	2327	2330	2332	rBV	3214	2635	0.21%	0.020%
62	17.251	2365	2368	2371	rVB	1942	1991	0.16%	0.015%
63	17.339	2379	2383	2385	rBV2	1921	2867	0.23%	0.021%
64	17.527	2412	2415	2417	rBV3	2641	2764	0.22%	0.021%
65	17.597	2419	2427	2435	rVB	376736	571595	46.25%	4.283%
66	17.691	2435	2443	2456	rBV	623814	982332	79.49%	7.360%
67	17.891	2474	2477	2480	rBV2	3432	4777	0.39%	0.036%
68	18.050	2501	2504	2505	rBV	2854	2856	0.23%	0.021%
69	18.103	2509	2513	2515	rVB2	2447	2681	0.22%	0.020%
70	18.179	2522	2526	2527	rBV	2673	2189	0.18%	0.016%
71	18.226	2531	2534	2537	rVV	2779	3118	0.25%	0.023%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

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\SOM-EPA-BG111920MA.M
Title : SVOA CALIBRATION

72	18.267	2539	2541	2543	rVB	2586	2178	0.18%	0.016%
73	18.684	2609	2612	2614	rBV2	2398	2832	0.23%	0.021%
74	18.755	2621	2624	2625	rBV2	2227	2027	0.16%	0.015%
75	18.914	2650	2651	2653	rBV2	2310	2003	0.16%	0.015%
76	19.019	2666	2669	2670	rBV	1700	2020	0.16%	0.015%
77	19.190	2694	2698	2704	rVB4	8542	13398	1.08%	0.100%
78	19.237	2704	2706	2708	rBV	2011	2222	0.18%	0.017%
79	19.260	2708	2710	2714	rBV2	2016	2212	0.18%	0.017%
80	19.525	2752	2755	2758	rBV4	4047	6576	0.53%	0.049%
81	19.595	2765	2767	2773	rVB2	10156	14228	1.15%	0.107%
82	19.742	2790	2792	2794	rBV3	4852	4109	0.33%	0.031%
83	19.777	2796	2798	2802	rVV3	2553	3523	0.29%	0.026%
84	19.854	2808	2811	2815	rVB4	6075	8514	0.69%	0.064%
85	19.912	2819	2821	2822	rBV2	3465	2352	0.19%	0.018%
86	19.959	2823	2829	2837	rVV	841078	1235748	100.00%	9.258%
87	20.253	2875	2879	2882	rBV	137842	145997	11.81%	1.094%
88	20.294	2882	2886	2890	rVB	234870	268057	21.69%	2.008%
89	20.377	2898	2900	2901	rBV2	3553	3279	0.27%	0.025%
90	21.258	3045	3050	3053	rBV2	70525	92020	7.45%	0.689%
91	21.293	3053	3056	3061	rVB	134789	160307	12.97%	1.201%
92	21.481	3084	3088	3099	rBV	108701	190695	15.43%	1.429%
93	21.875	3148	3155	3164	rBV	397007	688220	55.69%	5.156%
94	22.398	3241	3244	3248	rBV5	24824	32444	2.63%	0.243%
95	22.445	3248	3252	3260	rVB3	59997	103149	8.35%	0.773%
96	23.872	3491	3495	3500	rBV6	23248	41353	3.35%	0.310%
97	23.937	3501	3506	3514	rVB5	52091	112132	9.07%	0.840%
98	25.030	3682	3692	3704	rVB	404201	1171963	94.84%	8.781%
99	25.265	3721	3732	3748	rVB2	219723	715403	57.89%	5.360%
100	31.593	4807	4809	4811	rBV3	6013	4264	0.35%	0.032%

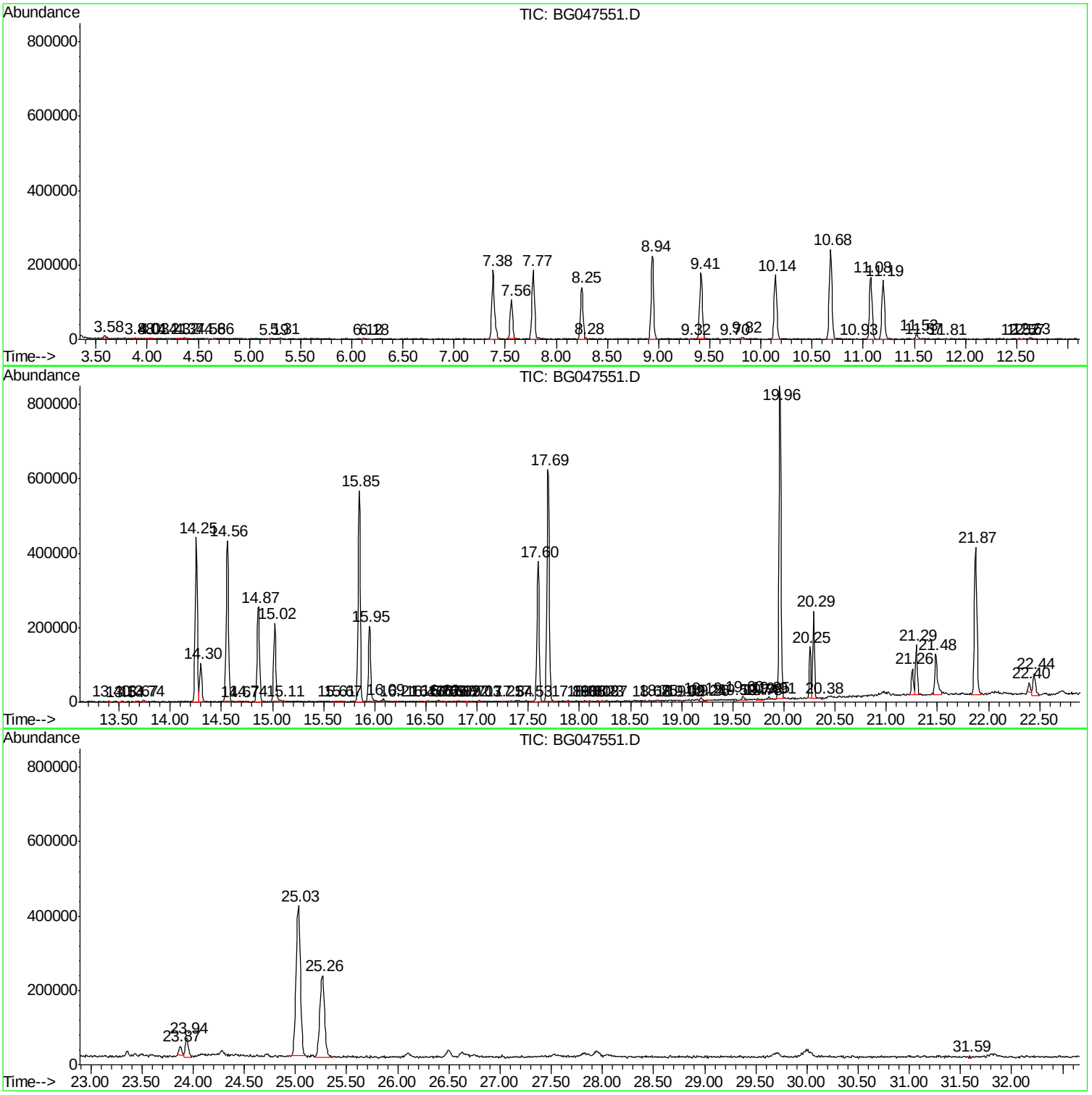
Sum of corrected areas: 13347224

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

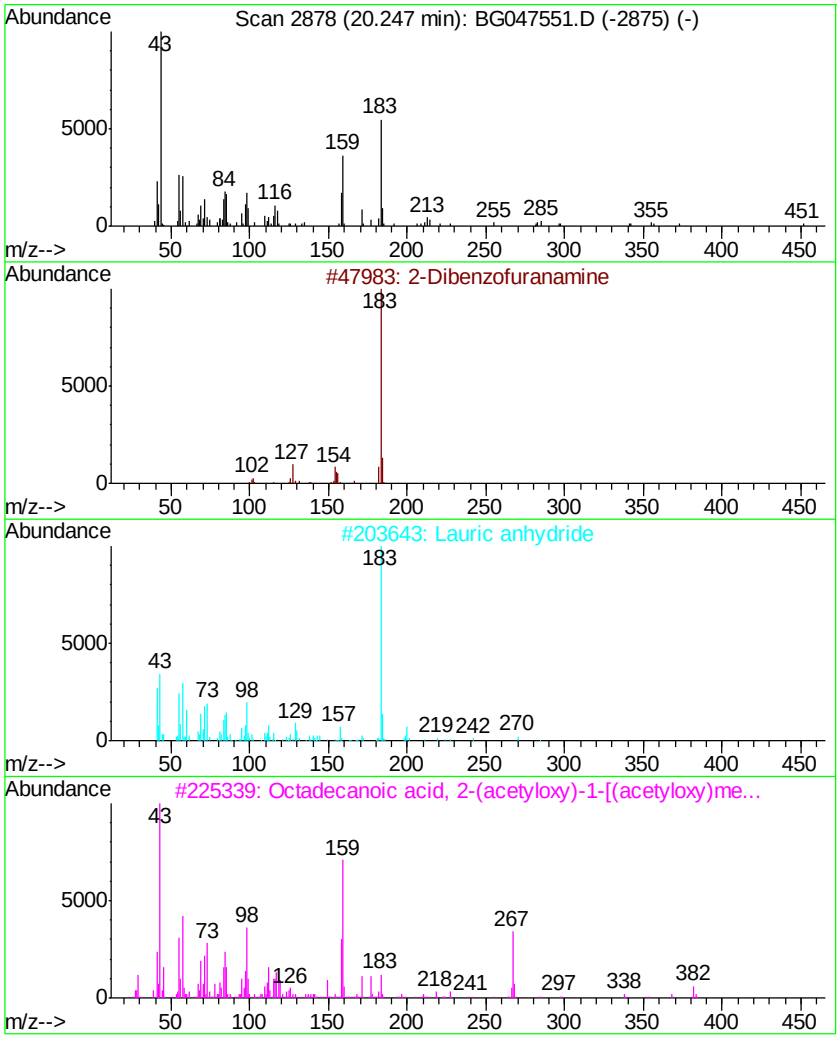
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

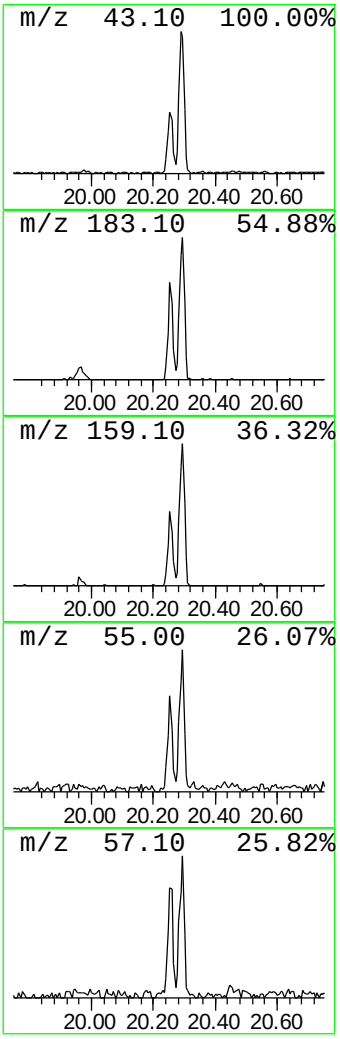
****

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.25	4.24 ng/ul	145997	Chrysene-d12	21.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dibenzofuranamine	183	C12H9NO	003693-22-9	47
2	Lauric anhydride	382	C24H46O3	000645-66-9	47
3	Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	46
4	Lauric acid, 3,4-dichlorophenyl ...	344	C18H26Cl2O2	1000357-92-7	38
5	Fumaric acid, isohexyl pentafluo...	366	C16H15F5O4	1000348-09-7	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

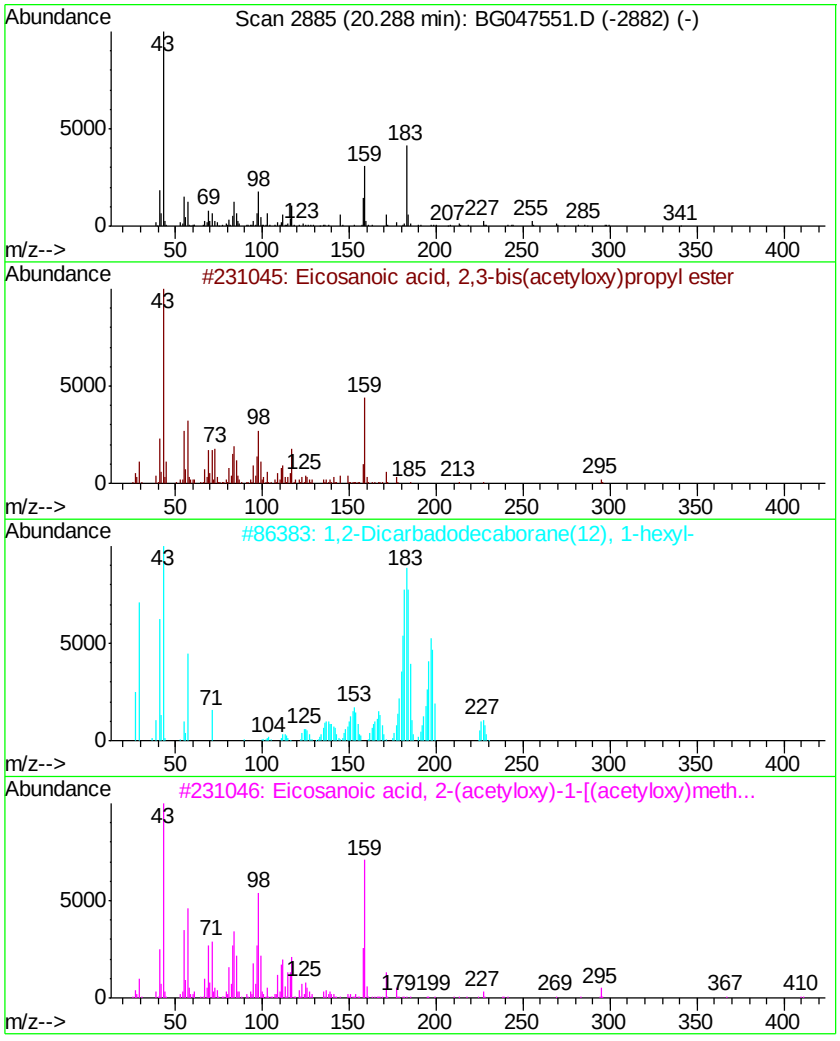
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

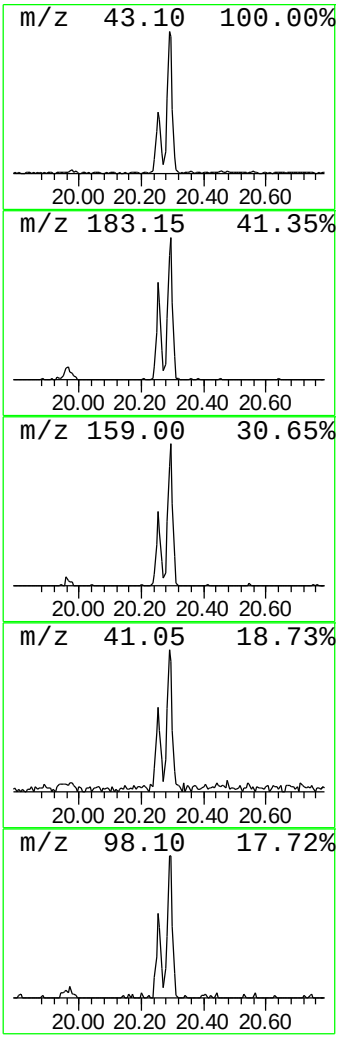
****

Peak Number 2 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.29	7.79 ng/ul	268057	Chrysene-d12	21.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	37
2	1,2-Dicarbadodecaborane(12), 1-h...	230	C8H24B10	020740-05-0	18
3	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	10
4	Dodecanoic acid, 2-hydroxy-1-(hy...	274	C15H30O4	001678-45-1	10
5	4,5,6-Trimethyltetrahydro-1,3-ox...	159	C7H13NOS	085333-98-8	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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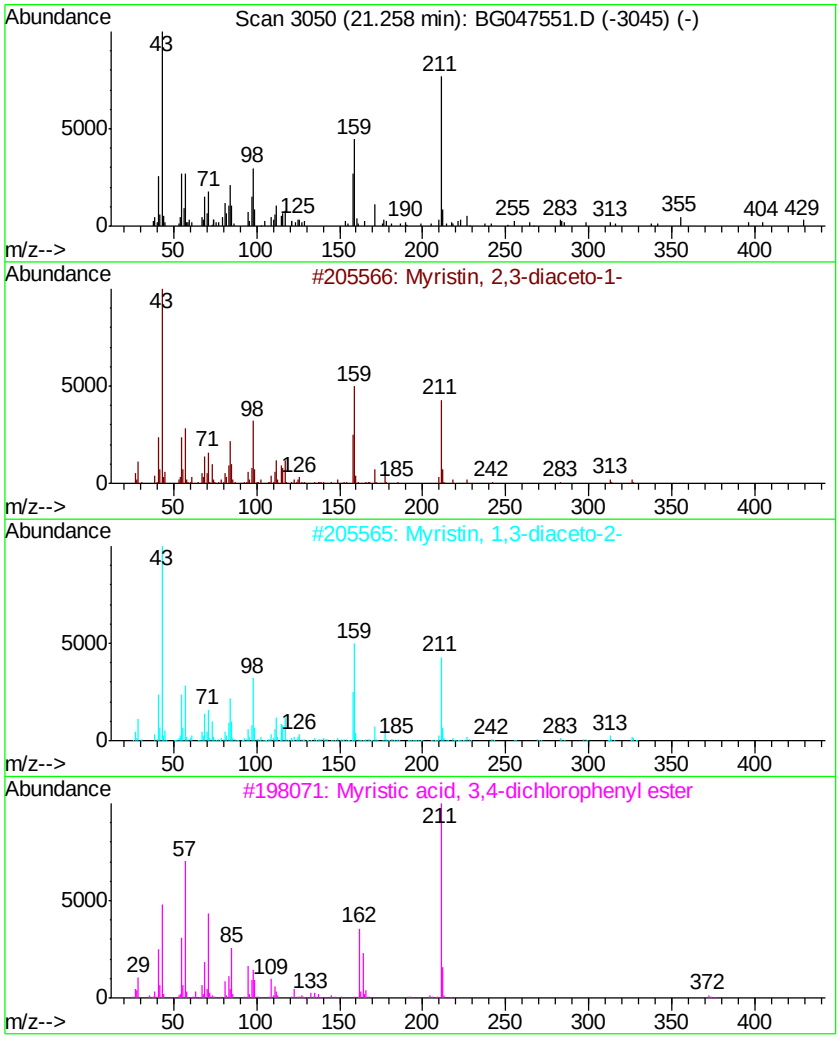
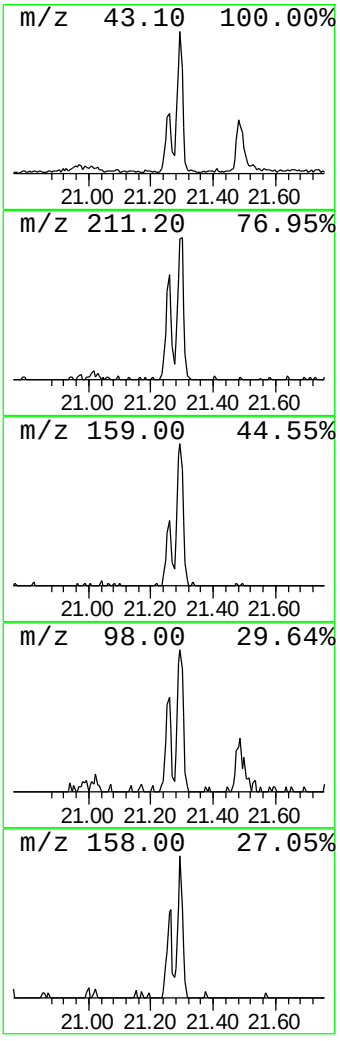
Peak Number 3 Myristin, 2,3-diaceto-1- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.26	2.67 ng/ul	92020	Chrysene-d12	21.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	64
2	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	58
3	Myristic acid, 3,4-dichlorophenyl...	372	C20H30Cl2O2	1000357-93-1	35
4	6-Thiopyrazolo[3,4-d]pyrimidin-4...	211	C6H5N5O2S	096555-42-9	27
5	[1,1'-Biphenyl]-2-ol, 5-(1,1-dim...	226	C16H18O	000577-92-4	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

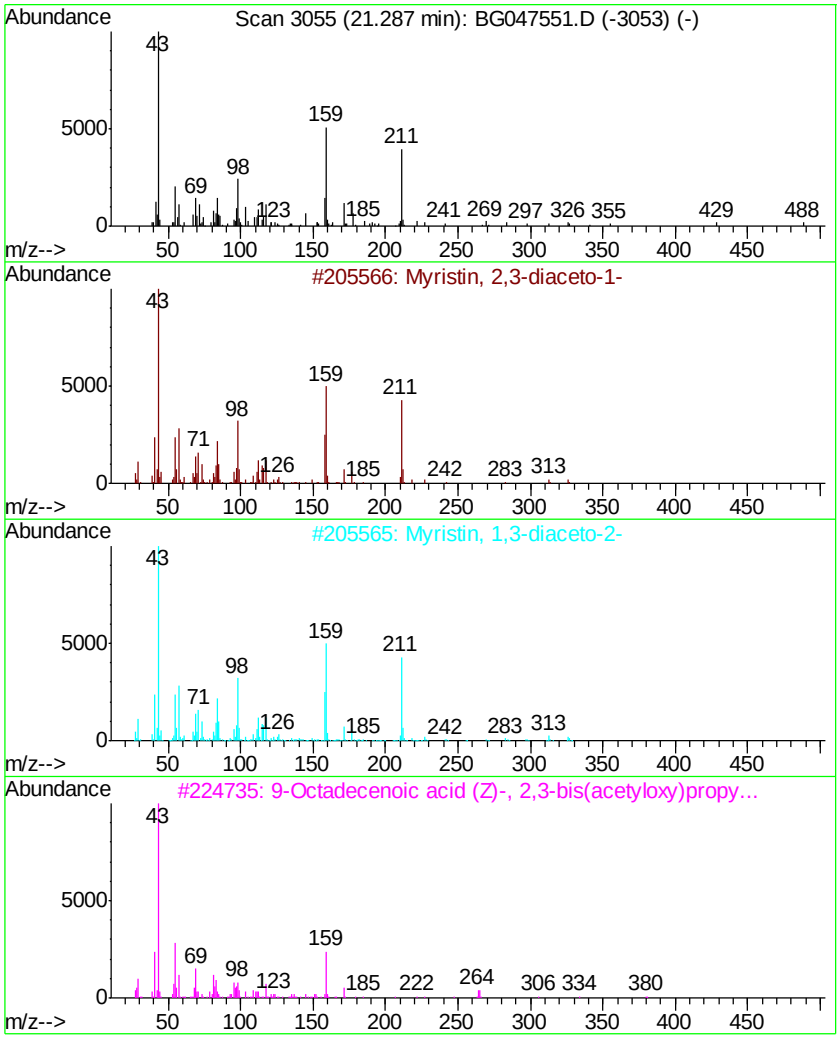
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

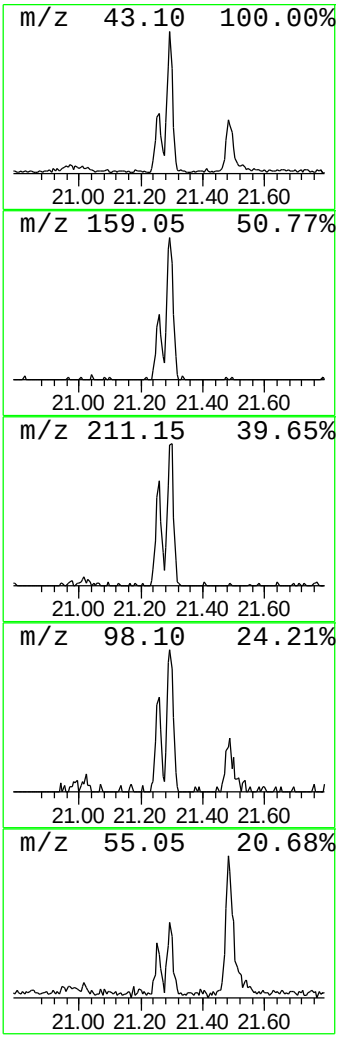
****

Peak Number 4 Myristin, 1,3-diaceto-2- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	4.66 ng/ul	160307	Chrysene-d12	21.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Myristin, 2,3-diaceto-1-	386	C21H38O6	014473-55-3	81
2	Myristin, 1,3-diaceto-2-	386	C21H38O6	014290-23-4	81
3	9-Octadecenoic acid (Z)-, 2,3-bi...	440	C25H44O6	055401-64-4	32
4	Eicosanoic acid, 2,3-bis(acetylo...	470	C27H50O6	055429-67-9	14
5	4,5,6-Trimethyltetrahydro-1,3-ox...	159	C7H13NOS	085333-98-8	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

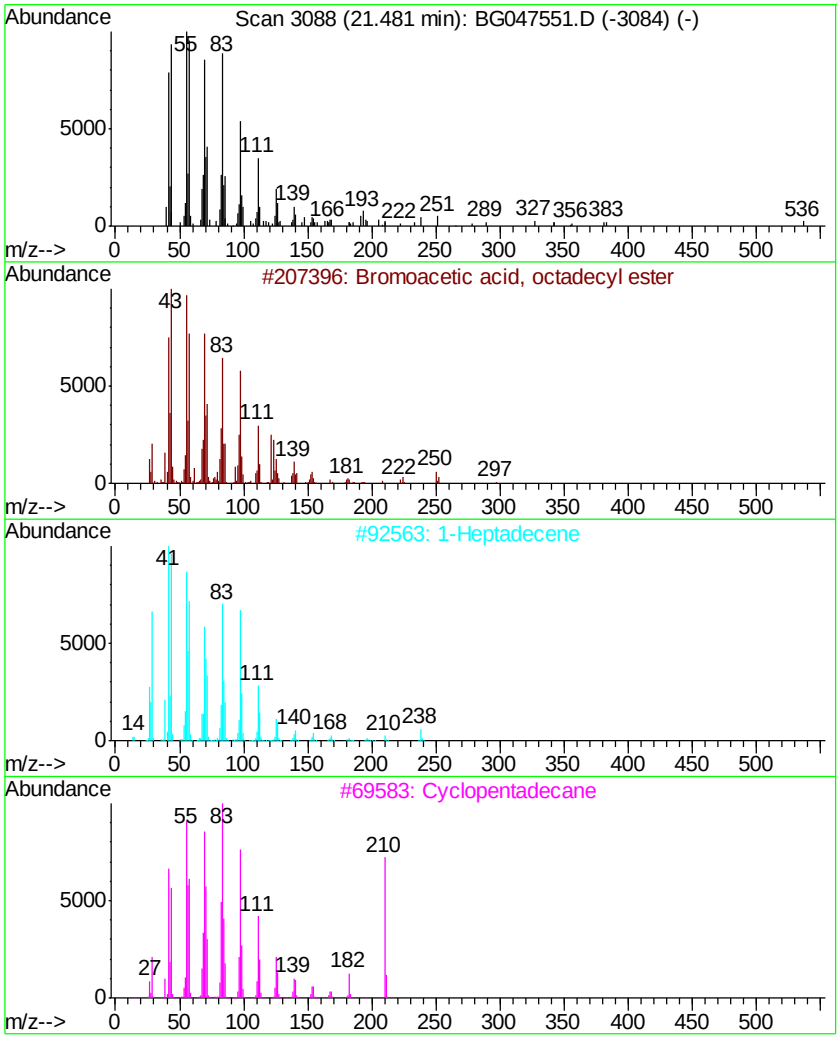
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

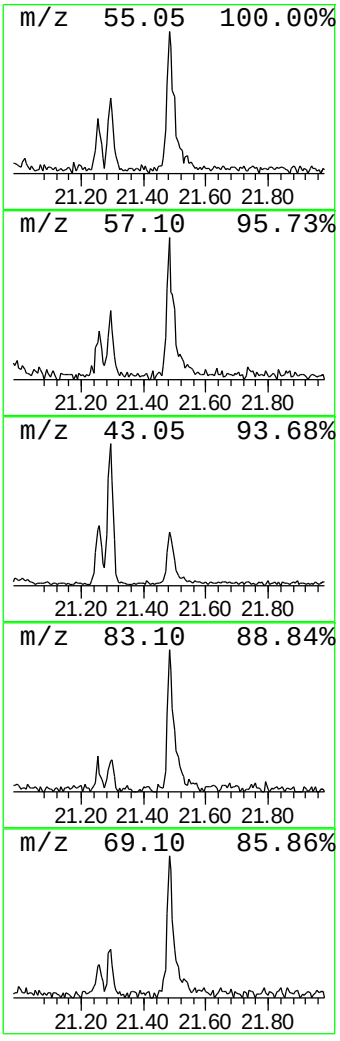
****

Peak Number 5 Bromoacetic acid, octadecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.48	5.54 ng/ul	190695	Chrysene-d12	21.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	1-Heptadecene	238	C17H34	006765-39-5	83
3	Cyclopentadecane	210	C15H30	000295-48-7	80
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	78
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	78





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

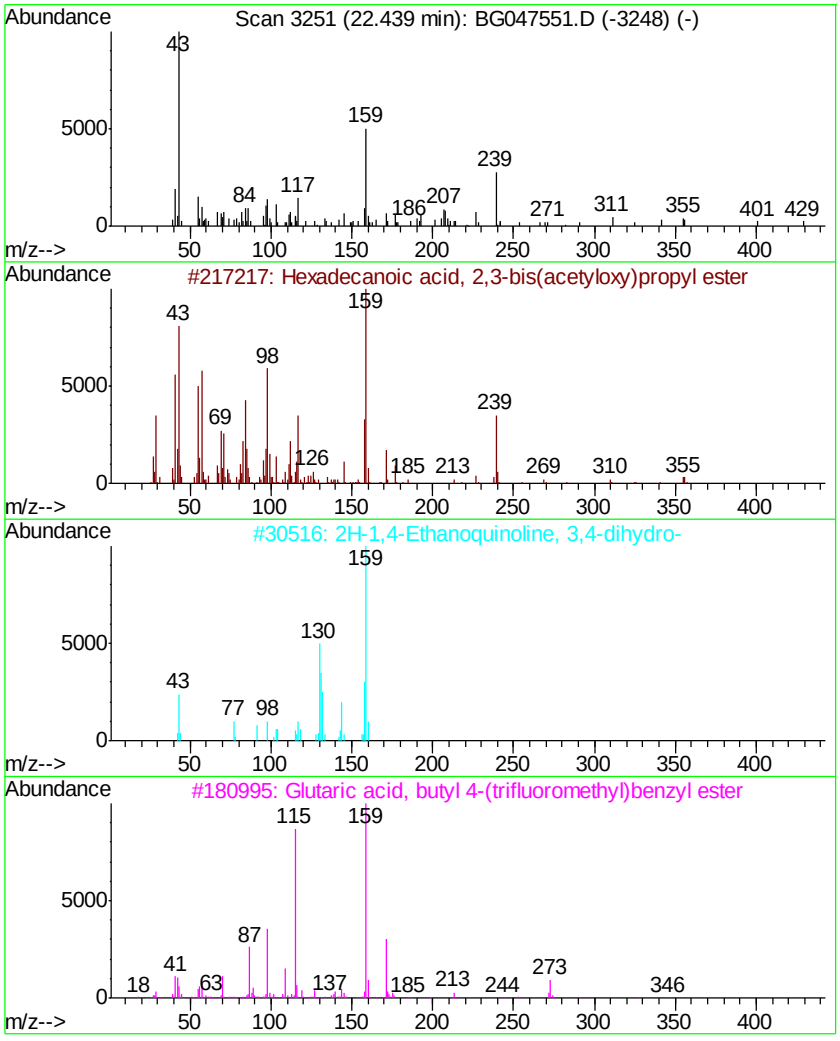
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

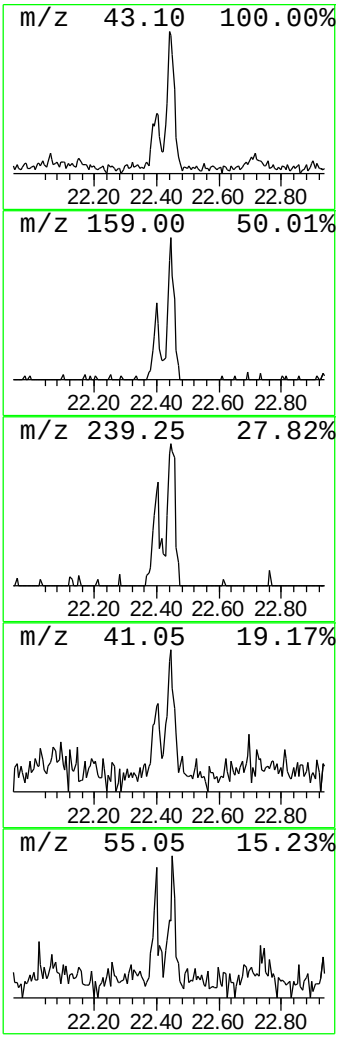
****

Peak Number 6 Hexadecanoic acid, 2,3-bis(... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.44	3.00 ng/ul	103149	Chrysene-d12	21.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2,3-bis(acetv...	414	C23H42O6	055268-70-7	86
2	2H-1,4-Ethanoquinoline, 3,4-dihv...	159	C11H13N	004363-25-1	38
3	Glutaric acid, butyl 4-(trifluor...	346	C17H21F3O4	1000377-57-9	32
4	Glutaric acid, isobutyl 4-(trifl...	346	C17H21F3O4	1000377-57-8	32
5	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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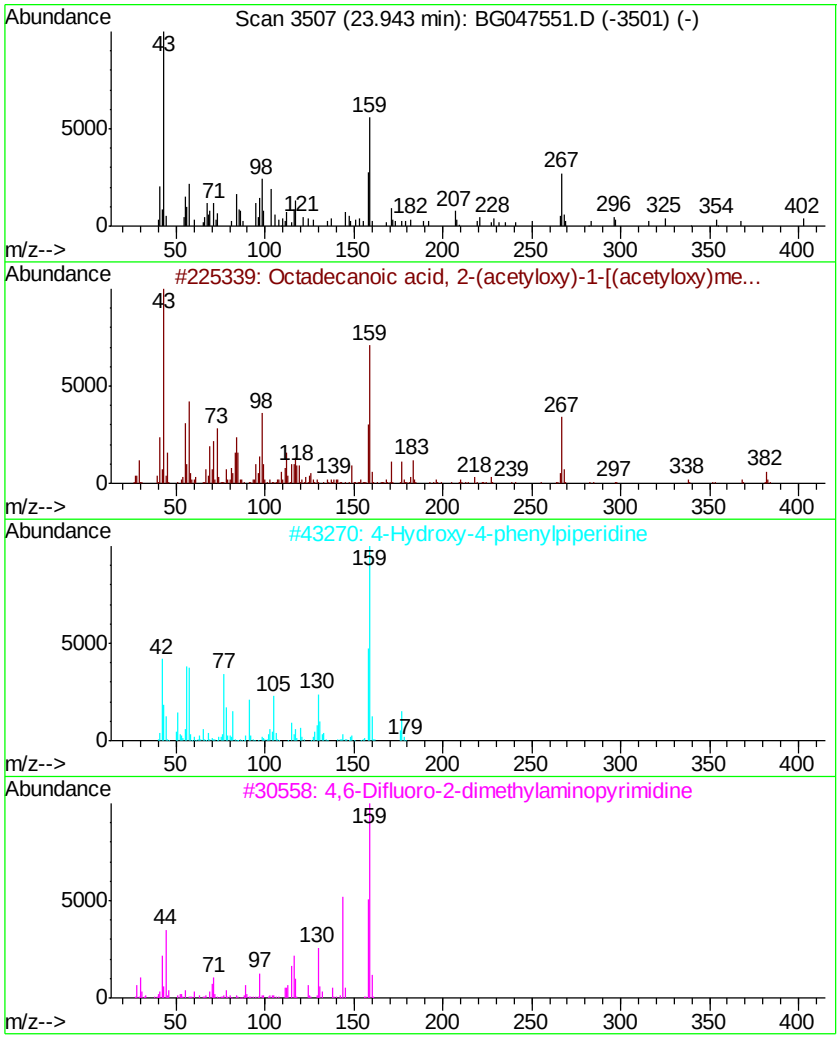
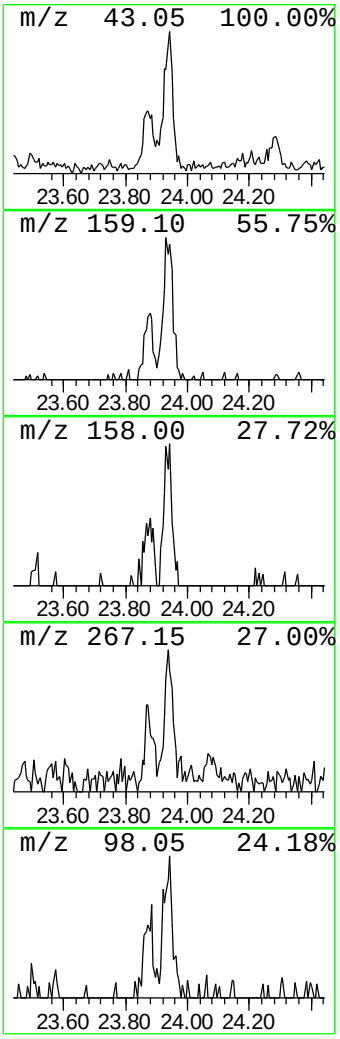
Peak Number 7 unknown-03 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.94	3.13 ng/ul	112132	Perylene-d12	25.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, 2-(acetyloxy)...	442	C25H46O6	055401-62-2	37
2	4-Hydroxy-4-phenylpiperidine	177	C11H15NO	040807-61-2	35
3	4,6-Difluoro-2-dimethylaminopyri...	159	C6H7F2N3	165258-63-9	25
4	Eicosanoic acid, 2-(acetyloxy)-1...	470	C27H50O6	055429-68-0	22
5	Nonanoic acid, tetradecyl ester	354	C23H46O2	1000340-28-1	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG120320\
Data File : BG047551.D
Acq On : 3 Dec 2020 23:29
Operator : CG/JU
Sample : L4866-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C0BC8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\SOM-EPA-BG111920MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown-01	20.25	4.2	ng/ul	145997	5	21.87	688220	20.0
unknown-02	20.29	7.8	ng/ul	268057	5	21.87	688220	20.0
Myristin, 2,3-dia...	21.26	2.7	ng/ul	92020	5	21.87	688220	20.0
Myristin, 1,3-dia...	21.29	4.7	ng/ul	160307	5	21.87	688220	20.0
Bromoacetic acid,...	21.48	5.5	ng/ul	190695	5	21.87	688220	20.0
Hexadecanoic acid...	22.44	3.0	ng/ul	103149	5	21.87	688220	20.0
unknown-03	23.94	3.1	ng/ul	112132	6	25.26	715403	20.0