LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122422\
Data File : BG056106.D
Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBYF5

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-BG122422.M
Title : SVOA CALIBRATION

Signal : TIC: BG056106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.372	9	14	27	rVB	106408	158885	11.43%	1.027%
2	3.648	57	61	68	rBV2	7553	12072	0.87%	0.078%
3	4.083	132	135	149	rBV	80106	130493	9.39%	0.844%
4	4.195	151	154	163	rVB2	6973	10761	0.77%	0.070%
5	4.653	228	232	241	rVB3	10274	16398	1.18%	0.106%
6	5.082	296	305	311	rBV2	9061	13467	0.97%	0.087%
7	5.458	362	369	376	rBV	1106	2652	0.19%	0.017%
8	7.473	706	712	725	rVB	135879	230881	16.61%	1.493%
9	7.649	735	742	751	rVB	102119	169827	12.21%	1.098%
10	7.867	772	779	788	rBV	126100	223528	16.08%	1.445%
11	8.343	854	860	870	rVB	122625	209140	15.04%	1.352%
12	9.036	969	978	988	rBV	163701	278512	20.03%	1.801%
13	9.518	1051	1060	1069	rBV	123192	216534	15.57%	1.400%
14	9.906	1120	1126	1130	rVB2	3525	5613	0.40%	0.036%
15	10.246	1174	1184	1191	rVB	105259	187474	13.48%	1.212%
16	10.781	1268	1275	1283	rBV	215413	380459	27.36%	2.460%
17	11.181	1335	1343	1352	rBB	178583	321249	23.11%	2.077%
18	11.304	1353	1364	1372	rBV	135632	253464	18.23%	1.639%
19	12.738	1603	1608	1613	rBV	5094	6678	0.48%	0.043%
20	13.155	1675	1679	1683	rVB	6199	7640	0.55%	0.049%
21	14.342	1873	1881	1889	rBV	433376	628314	45.19%	4.063%
22	14.465	1898	1902	1905	rBV2	2584	3916	0.28%	0.025%
23	14.506	1905	1909	1913	rVV	7195	10557	0.76%	0.068%
24	14.653	1927	1934	1941	rVB	507660	791933	56.96%	5.121%
25	14.953	1978	1985	1992	rBV	367080	589895	42.43%	3.814%
26	15.111	2005	2012	2021	rBV	137592	220294	15.84%	1.424%
27	15.276	2035	2040	2044	rVB4	2573	3408	0.25%	0.022%
28	15.940	2146	2153	2163	rVV	695638	1090746	78.45%	7.053%
29	16.040	2164	2170	2177	rVB	152182	225544	16.22%	1.458%
30	16.169	2190	2192	2199	rVB3	4247	5171	0.37%	0.033%
31	16.292	2206	2213	2220	rBV	394493	581647	41.84%	3.761%
32	16.374	2226	2227	2230	rVB3	4988	3825	0.28%	0.025%
33	16.404	2230	2232	2235	rBV4	3961	4945	0.36%	0.032%
34	16.562	2254	2259	2261	rBV5	4205	7081	0.51%	0.046%
35	16.598	2263	2265	2266	rVV	3903	2910	0.21%	0.019%
36	16.645	2268	2273	2275	rVV6	8136	12810	0.92%	0.083%

LSC Area Percent Report

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Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DBYF5

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-BG122422.M
Title : SVOA CALIBRATION

37	16.686	2278	2280	2283	rVV4	3189	3907	0.28%	0.025%
38	16.721	2284	2286	2288	rVV3	3329	3058	0.22%	0.020%
39	16.751	2288	2291	2294	rVV5	5319	6985	0.50%	0.045%
40	16.792	2296	2298	2301	rVV4	4219	4760	0.34%	0.031%
41	16.856	2303	2309	2316	rVV	39460	65309	4.70%	0.422%
42	16.933	2321	2322	2324	rBV2	5345	3303	0.24%	0.021%
43	17.021	2333	2337	2339	rBV5	3488	5028	0.36%	0.033%
44	17.044	2339	2341	2342	rVV2	6075	4553	0.33%	0.029%
45	17.232	2371	2373	2376	rVB4	4252	4927	0.35%	0.032%
46	17.262	2376	2378	2381	rBV4	3627	3403	0.24%	0.022%
47	17.356	2391	2394	2399	rVB5	3671	5525	0.40%	0.036%
48	17.409	2399	2403	2408	rVB5	3461	5721	0.41%	0.037%
49	17.691	2443	2451	2457	rBV	516382	780261	56.12%	5.045%
50	17.738	2457	2459	2461	rVV3	5717	5754	0.41%	0.037%
51	17.790	2461	2468	2475	rVV	721924	1085444	78.07%	7.019%
52	17.849	2475	2478	2483	rVB3	4804	5698	0.41%	0.037%
53	18.043	2501	2511	2512	rBV2	2477	4870	0.35%	0.031%
54	18.319	2554	2558	2564	rBV6	4625	9216	0.66%	0.060%
55	18.384	2564	2569	2572	rBV3	6267	10332	0.74%	0.067%
56	18.478	2580	2585	2590	rBV6	11931	18227	1.31%	0.118%
57	18.537	2590	2595	2603	rVV2	107793	147620	10.62%	0.955%
58	18.613	2606	2608	2611	rVV2	4496	5135	0.37%	0.033%
59	18.660	2613	2616	2619	rBV4	3880	5599	0.40%	0.036%
60	18.719	2623	2626	2627	rBV4	2601	2524	0.18%	0.016%
61	18.742	2627	2630	2635	rVB5	10645	15322	1.10%	0.099%
62	18.801	2637	2640	2647	rBV3	14330	21132	1.52%	0.137%
63	18.895	2655	2656	2662	rVB6	4340	7012	0.50%	0.045%
64	18.960	2662	2667	2675	rBV7	24438	36607	2.63%	0.237%
65	19.054	2679	2683	2687	rBV5	7022	10199	0.73%	0.066%
66	19.124	2692	2695	2701	rVB4	15691	20829	1.50%	0.135%
67	19.171	2701	2703	2705	rBV3	3246	2918	0.21%	0.019%
68	19.206	2708	2709	2713	rVB3	2464	2662	0.19%	0.017%
69	19.324	2727	2729	2732	rBV3	4297	5432	0.39%	0.035%
70	19.471	2747	2754	2757	rBV7	14551	28849	2.07%	0.187%
71	19.612	2771	2778	2779	rBV7	12645	21618	1.55%	0.140%
72	19.653	2782	2785	2786	rBV3	8687	8499	0.61%	0.055%
73	19.688	2786	2791	2792	rBV4	17259	27594	1.98%	0.178%
74	19.718	2794	2796	2799	rBV3	8919	14161	1.02%	0.092%
75	19.794	2805	2809	2810	rBV3	41173	55593	4.00%	0.359%
76	19.853	2811	2819	2821	rVV8	81255	189914	13.66%	1.228%

LSC Area Percent Report

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Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBYF5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Title : SVOA CALIBRATION

77	20.053	2847	2853	2862	rVB	969563	1390318	100.00%	8.990%
78	20.188	2871	2876	2881	rBV	332837	423057	30.43%	2.736%
79	20.317	2894	2898	2901	rBV6	9827	12444	0.90%	0.080%
80	20.534	2929	2935	2941	rBV2	49013	82199	5.91%	0.532%
81	20.664	2946	2957	2958	rBV9	20674	59476	4.28%	0.385%
82	20.799	2978	2980	2984	rVB4	13814	15878	1.14%	0.103%
83	20.869	2990	2992	2995	rVB4	6517	4852	0.35%	0.031%
84	21.574	3108	3112	3126	rVB4	69495	141954	10.21%	0.918%
85	21.991	3175	3183	3198	rVB2	503235	965413	69.44%	6.242%
86	22.632	3290	3292	3293	rBV2	6970	3544	0.25%	0.023%
87	24.330	3579	3581	3582	rBV2	7241	5082	0.37%	0.033%
88	24.424	3595	3597	3603	rVB5	21011	37722	2.71%	0.244%
89	25.223	3722	3733	3743	rBV2	456339	1342453	96.56%	8.680%
90	25.458	3762	3773	3788	rVB	303264	965930	69.48%	6.246%
91	25.722	3816	3818	3821	rBV4	5953	5312	0.38%	0.034%
92	25.781	3826	3828	3829	rBV2	7506	4654	0.33%	0.030%
93	26.339	3921	3923	3924	rBV2	7369	5282	0.38%	0.034%
94	26.704	3978	3985	3994	rVB5	41107	117037	8.42%	0.757%
95	27.708	4155	4156	4158	rVB2	7340	3381	0.24%	0.022%
96	27.973	4199	4201	4202	rBV2	5015	4855	0.35%	0.031%
97	29.653	4485	4487	4490	rVB4	9801	8446	0.61%	0.055%
98	29.994	4536	4545	4559	rVB5	39689	165183	11.88%	1.068%
99	30.293	4593	4596	4598	rBV4	9192	12139	0.87%	0.078%
100	31.574	4812	4814	4815	rBV2	7070	4355	0.31%	0.028%

Sum of corrected areas: 15465189

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Data File : BG056106.D
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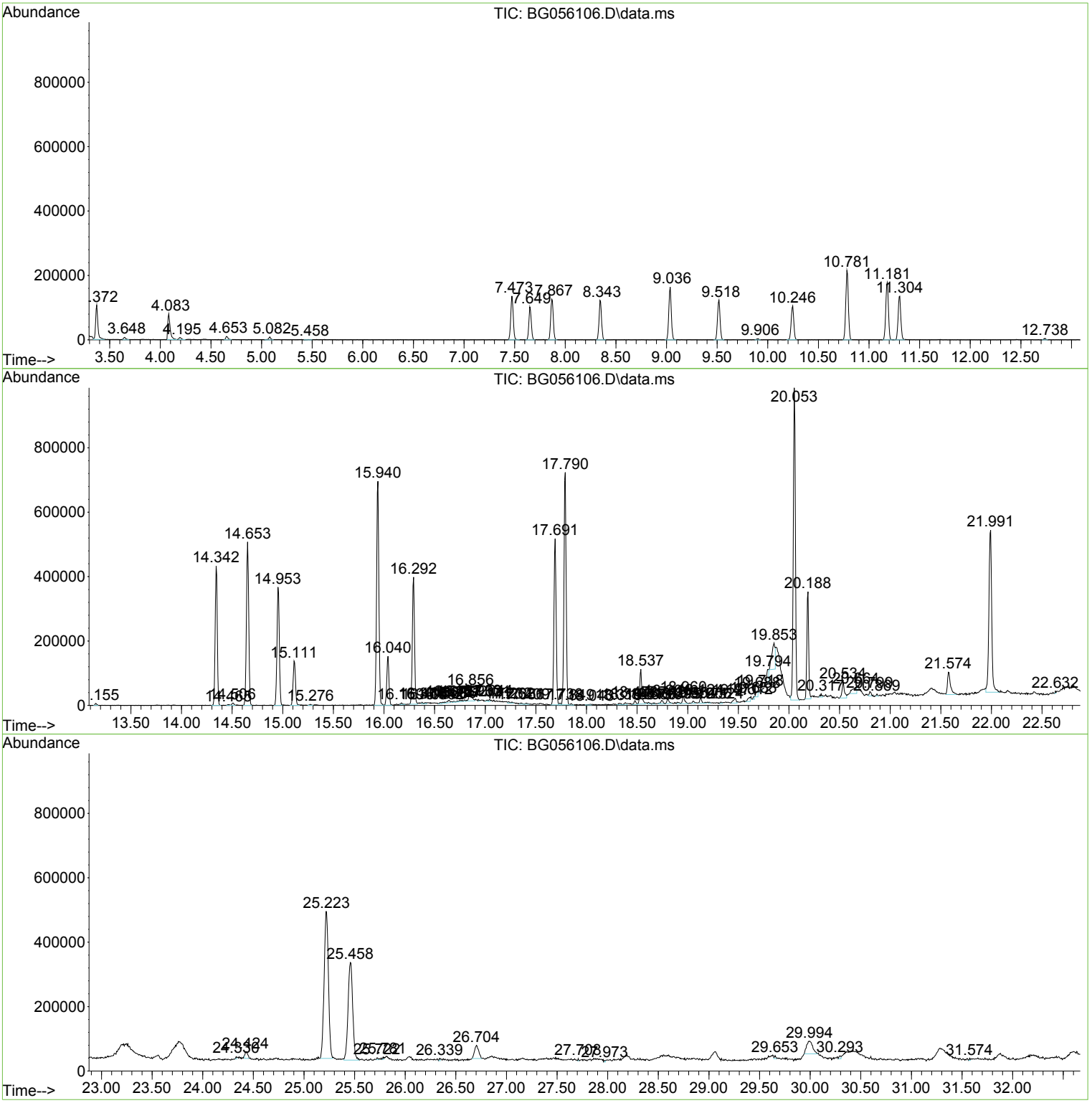
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBYF5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122422\
Data File : BG056106.D
Acq On : 25 Dec 2022 2:36
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Sample : N6017-07
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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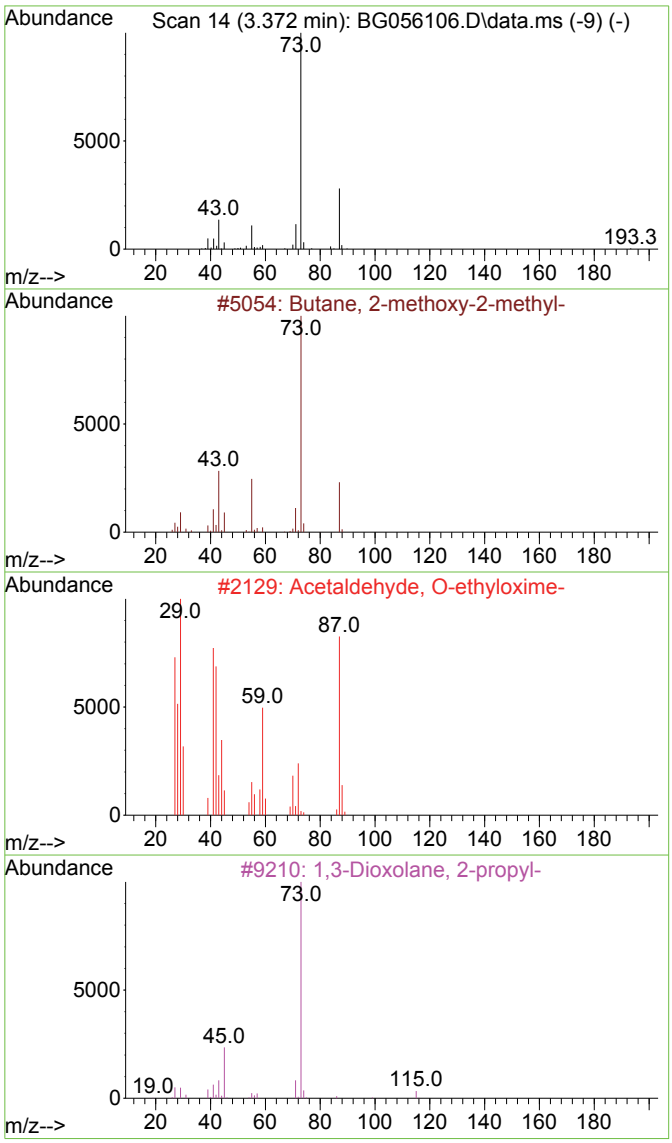
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Quant Title : SVOA CALIBRATION

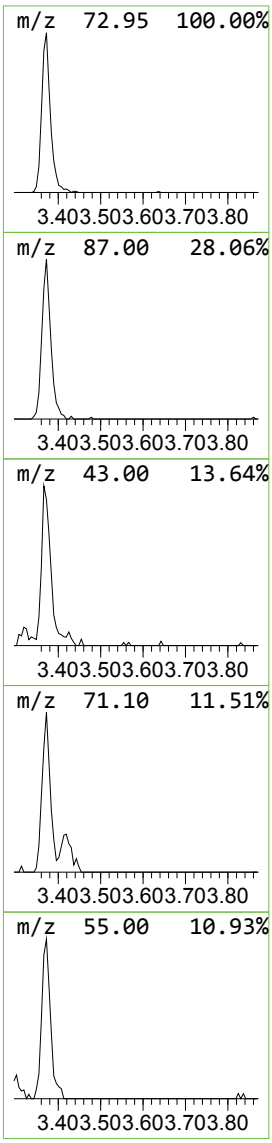
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.372	15.19 ng/ul	158885	1,4-Dichlorobenzene-d4	8.343

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	39
2	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9
3	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
4	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	7





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122422\
Data File : BG056106.D
Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBYF5

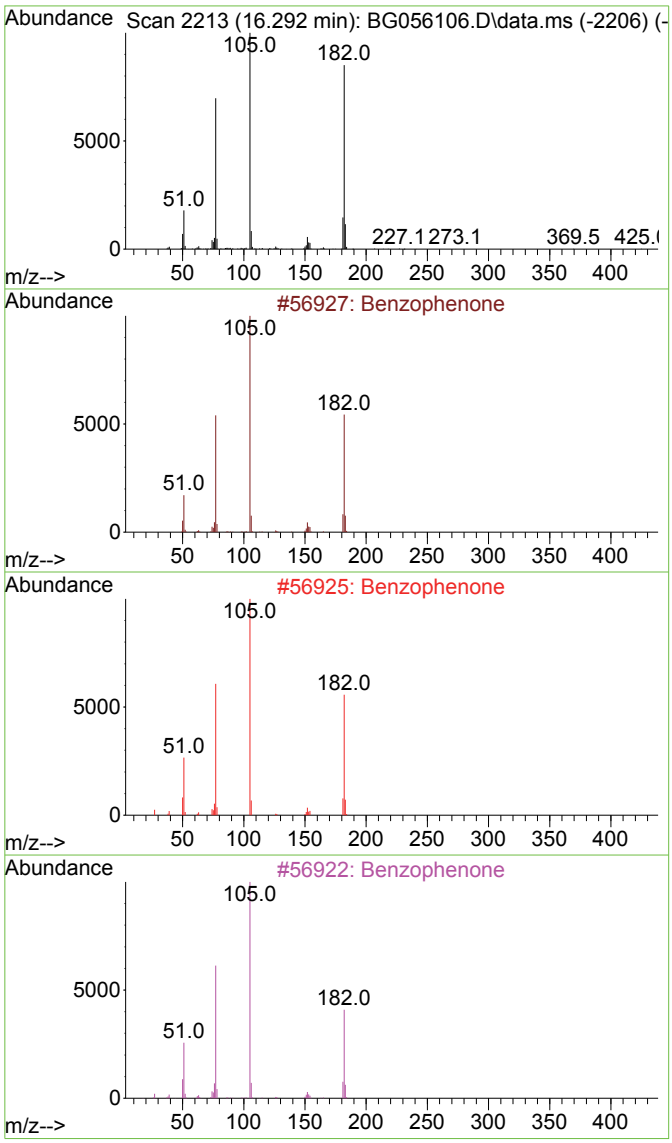
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Quant Title : SVOA CALIBRATION

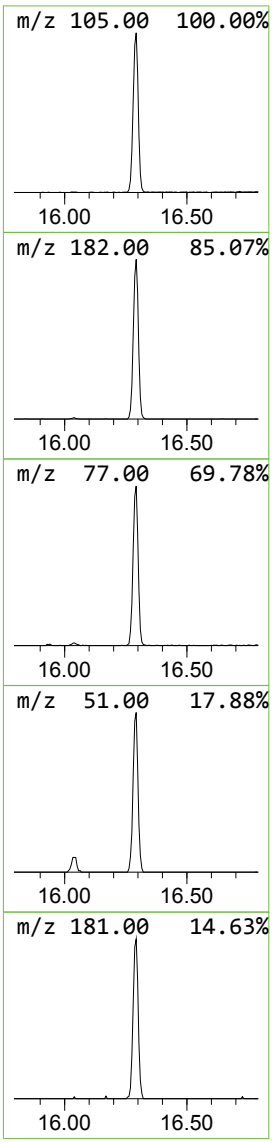
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.292	19.72 ng/ul	581647	Acenaphthene-d10	14.953

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Benzophenone	182	C13H10O	000119-61-9	94
3	Benzophenone	182	C13H10O	000119-61-9	87
4	Benzophenone	182	C13H10O	000119-61-9	81
5	1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122422\
Data File : BG056106.D
Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBYF5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Quant Title : SVOA CALIBRATION

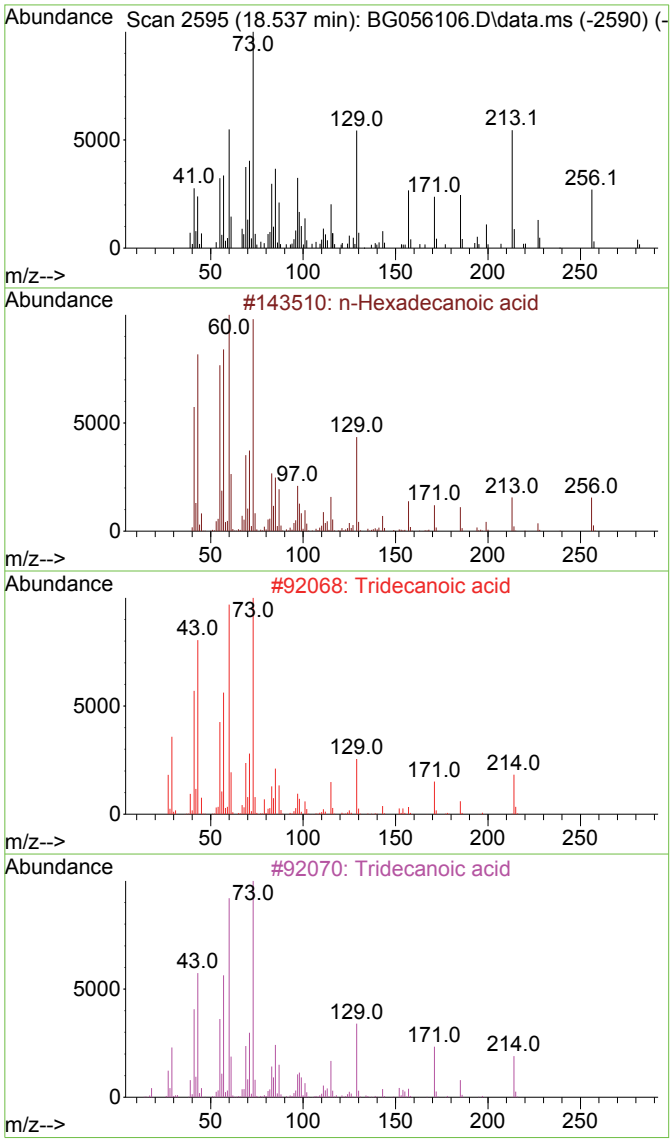
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

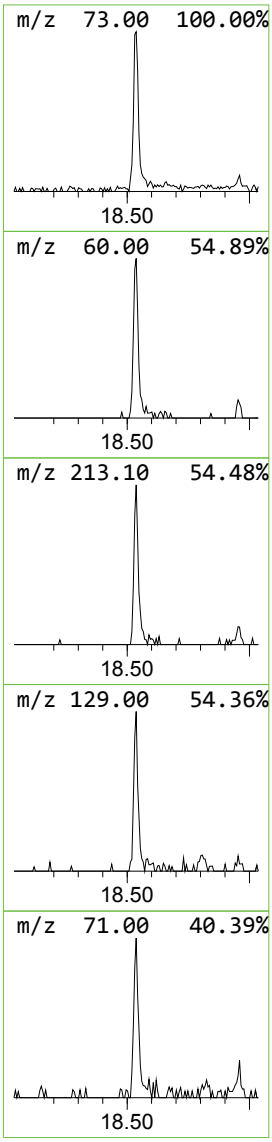
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.537	3.78 ng/ul	147620	Phenanthrene-d10	17.691

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Tridecanoic acid	214	C13H26O2	000638-53-9	78
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Quant Title : SVOA CALIBRATION

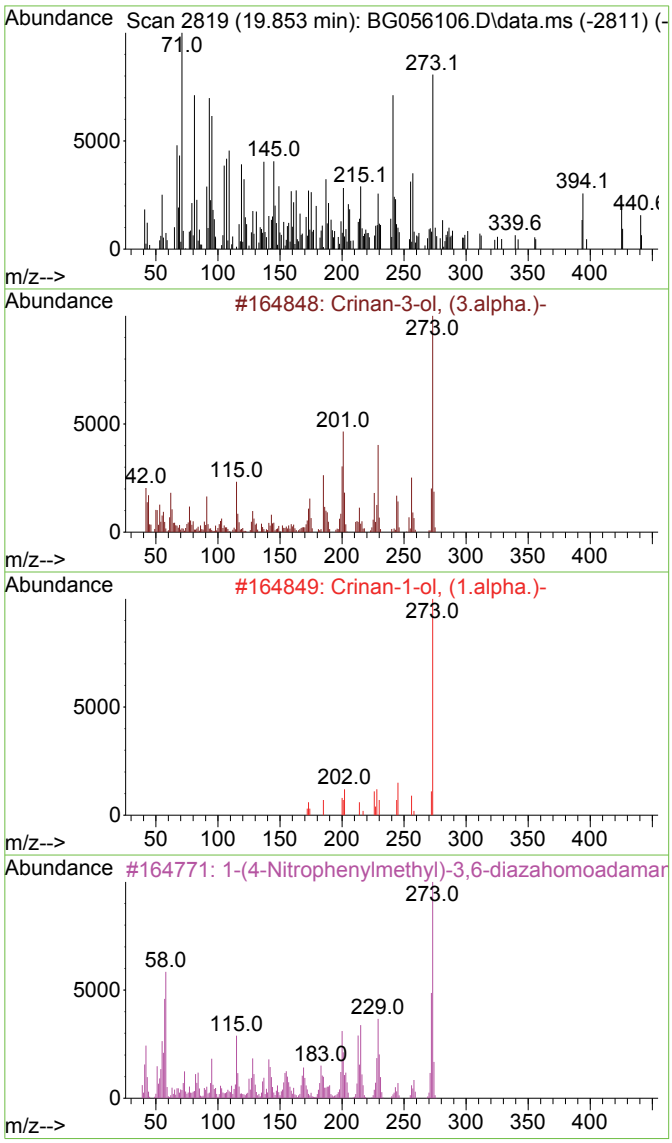
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

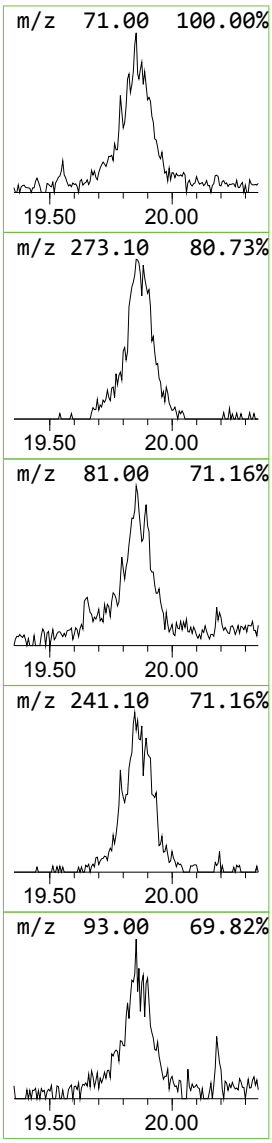
****

Peak Number 4 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.853	3.93 ng/ul	189914	Chrysene-d12	21.985

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Crinan-3-ol, (3.alpha.)-	273	C16H19NO3	010438-97-8	45
2	Crinan-1-ol, (1.alpha.)-	273	C16H19NO3	041928-89-6	35
3	1-(4-Nitrophenylmethyl)-3,6-diaz...	273	C15H19N3O2	148988-02-7	25
4	4H-[1,2,4]Triazole-3-thiol, 5-(3...	273	C10H13F2N5S	1000303-04-6	25
5	1-(4-Methyl-6-chloro-quinolin-2-...	273	C14H12ClN3O	111784-26-0	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122422\
Data File : BG056106.D
Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBYF5

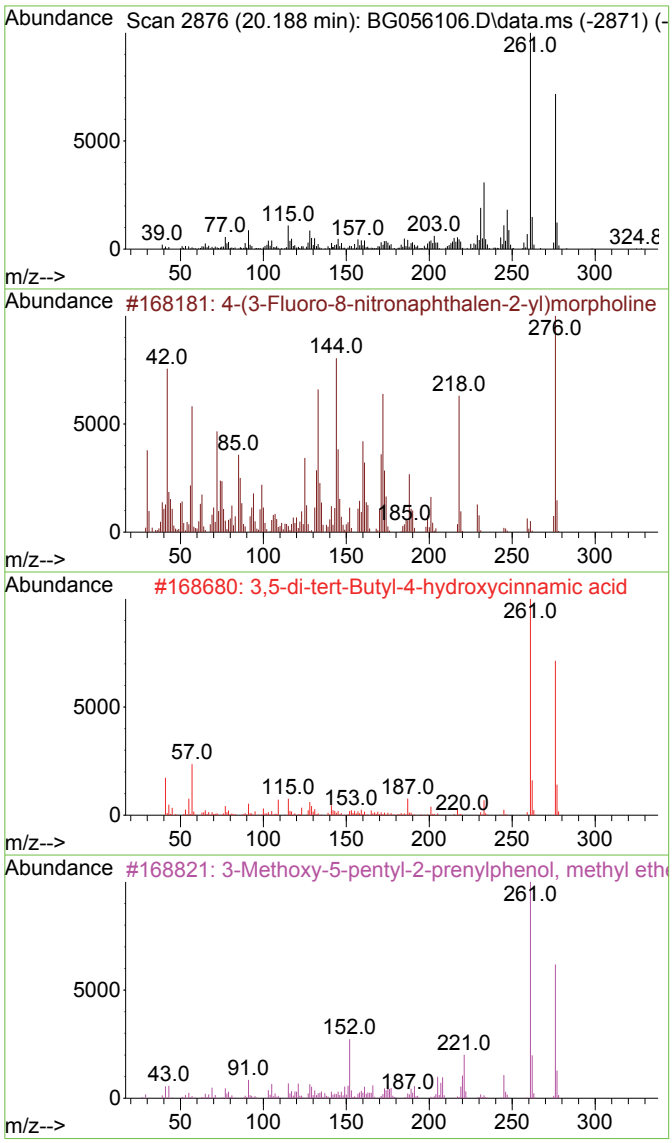
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Quant Title : SVOA CALIBRATION

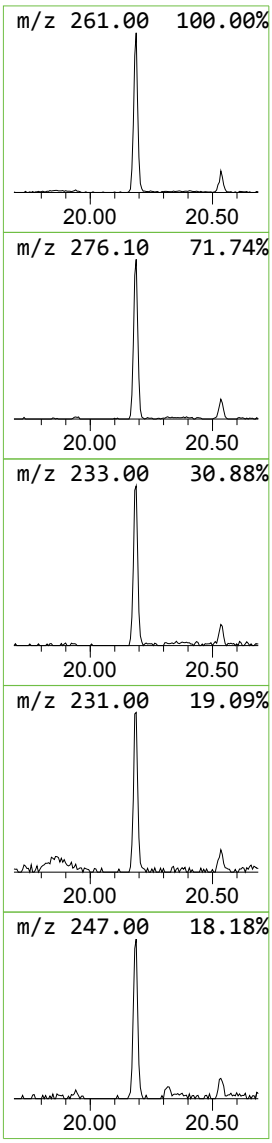
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4-(3-Fluoro-8-nitronaphthal... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.188	8.76 ng/ul	423057	Chrysene-d12	21.985

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(3-Fluoro-8-nitronaphthalen-2-...	276	C14H13FN2O3	1000409-37-1	91
2	3,5-di-tert-Butyl-4-hydroxycinna...	276	C17H24O3	022014-01-3	62
3	3-Methoxy-5-pentyl-2-prenylpheno...	276	C18H28O2	083036-53-7	62
4	5H-Furo[3,2-g][1]benzopyran-5-on...	276	C14H12O6	000668-10-0	60
5	(1H)Pyrrole, 3,4-dimethyl-5-meth...	276	C15H20N2OS	1000197-22-6	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122422\
Data File : BG056106.D
Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBYF5

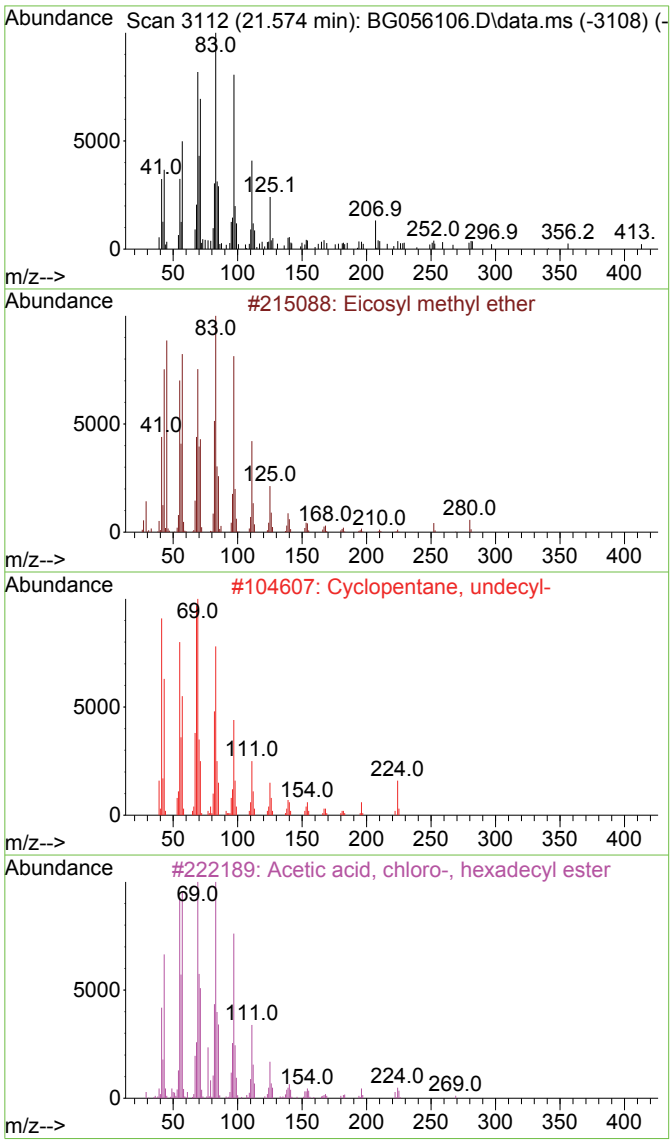
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Quant Title : SVOA CALIBRATION

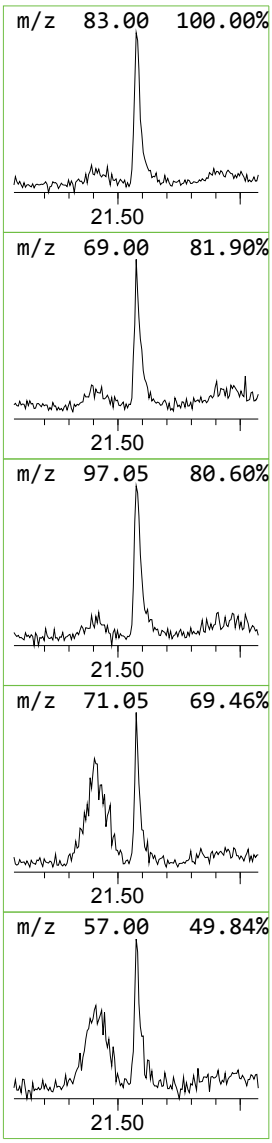
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Eicosyl methyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.574	2.94 ng/ul	141954	Chrysene-d12	21.985

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosyl methyl ether	312	C21H44O	1000406-29-4	83
2	Cyclopentane, undecyl-	224	C16H32	006785-23-5	80
3	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	64
4	Cyclopentane, nonyl-	196	C14H28	002882-98-6	62
5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122422\
Data File : BG056106.D
Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBYF5

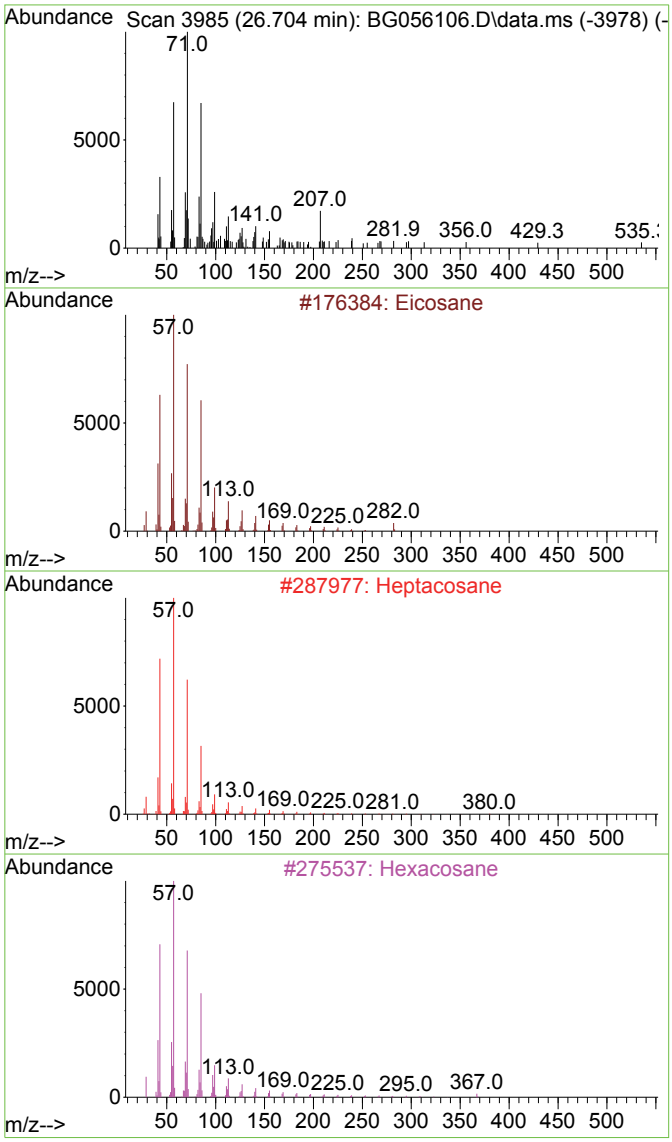
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Quant Title : SVOA CALIBRATION

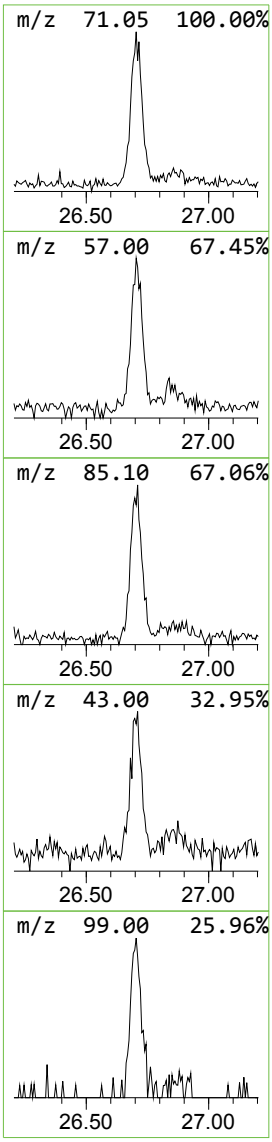
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.703	2.42 ng/ul	117037	Perylene-d12	25.458

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heptacosane	380	C27H56	000593-49-7	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Pentacosane	352	C25H52	000629-99-2	87
5	Hentriacontane	437	C31H64	000630-04-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122422\
Data File : BG056106.D
Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBYF5

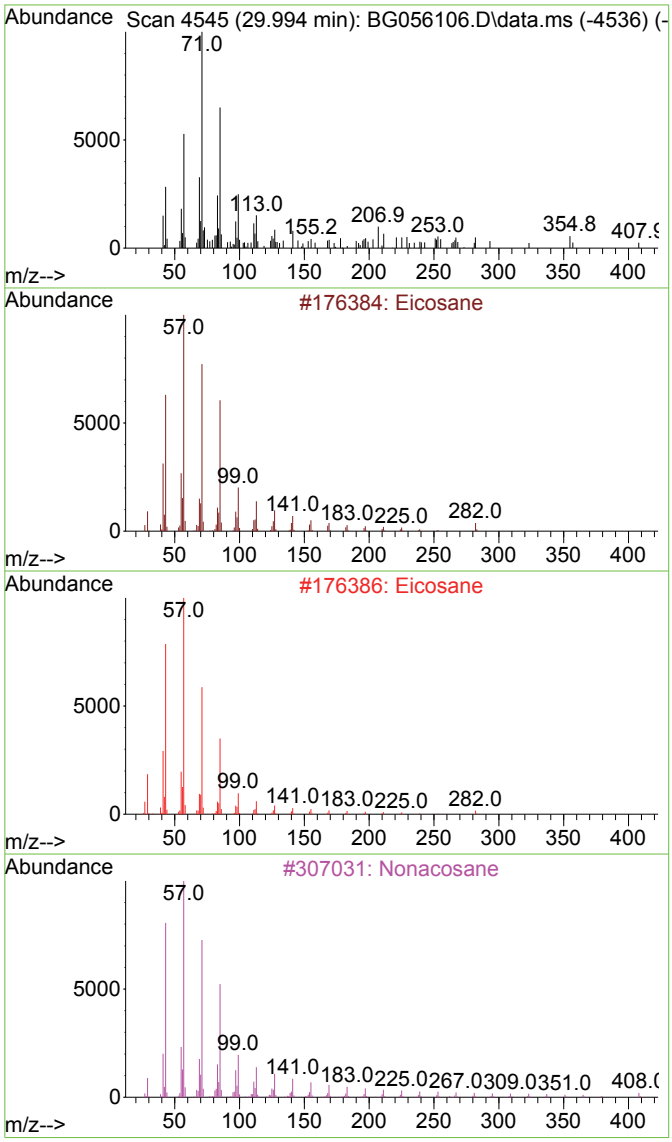
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.M
Quant Title : SVOA CALIBRATION

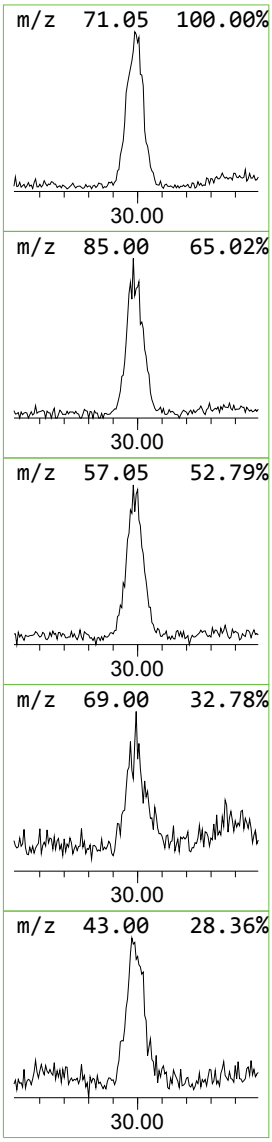
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.994	3.42 ng/ul	165183	Perylene-d12	25.458

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	78
2	Eicosane	282	C20H42	000112-95-8	76
3	Nonacosane	408	C29H60	000630-03-5	74
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	72
5	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122422\
Data File : BG056106.D
Acq On : 25 Dec 2022 2:36
Operator : CG/JU
Sample : N6017-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DBYF5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG122422.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	3.372	15.2	ng/ul	158885	1	8.343	209140	20.0
Benzophenone	16.292	19.7	ng/ul	581647	3	14.953	589895	20.0
n-Hexadecanoic ...	18.537	3.8	ng/ul	147620	4	17.691	780261	20.0
unknown-02	19.853	3.9	ng/ul	189914	5	21.985	965413	20.0
4-(3-Fluoro-8-n...	20.188	8.8	ng/ul	423057	5	21.985	965413	20.0
Eicosyl methyl ...	21.574	2.9	ng/ul	141954	5	21.985	965413	20.0
(DEL) Alkane: S...	26.703	2.4	ng/ul	117037	6	25.458	965930	20.0
(DEL) Alkane: S...	29.994	3.4	ng/ul	165183	6	25.458	965930	20.0