LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051123\
Data File : BG057396.D
Acq On : 11 May 2023 12:39
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : JREA7

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-BG042823.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG057396.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.646	14	18	20	rBV2	1125	1353	0.21%	0.028%
2	3.934	65	67	71	rBV	453	672	0.10%	0.014%
3	4.199	110	112	116	rVB2	1358	1826	0.28%	0.038%
4	4.246	117	120	123	rBB2	788	733	0.11%	0.015%
5	4.439	151	153	158	rVB	788	947	0.14%	0.020%
6	5.397	311	316	318	rBB2	549	766	0.12%	0.016%
7	7.506	669	675	685	rBV2	27410	47893	7.33%	1.009%
8	7.670	697	703	710	rBB2	19515	32366	4.95%	0.682%
9	7.894	735	741	748	rBB	26640	43964	6.73%	0.926%
10	8.369	815	822	829	rBB	57241	96874	14.82%	2.040%
11	9.063	934	940	952	rBB2	31493	56916	8.71%	1.199%
12	9.198	957	963	971	rBB2	3377	6245	0.96%	0.132%
13	9.544	1016	1022	1029	rBV	26539	45898	7.02%	0.967%
14	10.273	1141	1146	1154	rVB2	22755	39126	5.98%	0.824%
15	10.819	1233	1239	1247	rBV	34195	62151	9.51%	1.309%
16	11.201	1297	1304	1311	rBV	86336	149448	22.86%	3.147%
17	11.260	1311	1314	1317	rVB	678	902	0.14%	0.019%
18	11.336	1320	1327	1334	rBV	10402	18695	2.86%	0.394%
19	12.763	1567	1570	1573	rBV2	737	668	0.10%	0.014%
20	12.946	1597	1601	1603	rVB2	609	850	0.13%	0.018%
21	13.838	1749	1753	1756	rVB2	752	945	0.14%	0.020%
22	13.909	1759	1765	1772	rVB3	1736	3182	0.49%	0.067%
23	13.974	1772	1776	1779	rBV	411	708	0.11%	0.015%
24	14.361	1837	1842	1849	rVB	79821	109164	16.70%	2.299%
25	14.679	1890	1896	1905	rBV2	85324	131792	20.16%	2.776%
26	14.978	1940	1947	1955	rBV	152637	228211	34.91%	4.806%
27	15.178	1976	1981	1990	rBV2	12876	26883	4.11%	0.566%
28	15.965	2109	2115	2122	rBV	111705	169785	25.97%	3.576%
29	16.083	2130	2135	2145	rBV2	20966	33912	5.19%	0.714%
30	16.312	2170	2174	2180	rVB	14127	19557	2.99%	0.412%
31	16.876	2268	2270	2273	rVB2	1512	1567	0.24%	0.033%
32	16.987	2282	2289	2293	rVB2	509	706	0.11%	0.015%
33	17.393	2352	2358	2362	rBV5	1824	3636	0.56%	0.077%
34	17.504	2376	2377	2381	rBV	758	746	0.11%	0.016%
35	17.580	2386	2390	2396	rVB2	1127	2100	0.32%	0.044%
36	17.639	2396	2400	2403	rBV	536	889	0.14%	0.019%

LSC Area Percent Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREA7

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-BG042823.MA.M
Title : SVOA CALIBRATION

37	17.721	2406	2414	2420	rBV	188914	285648	43.69%	6.016%
38	17.815	2425	2430	2441	rVV2	121149	182992	27.99%	3.854%
39	17.892	2441	2443	2447	rVB	780	723	0.11%	0.015%
40	18.068	2470	2473	2475	rBV	706	667	0.10%	0.014%
41	18.127	2480	2483	2485	rVV	602	865	0.13%	0.018%
42	18.156	2485	2488	2490	rVB2	1140	1177	0.18%	0.025%
43	18.456	2532	2539	2542	rBV3	1913	3119	0.48%	0.066%
44	18.562	2552	2557	2566	rBV3	25750	42687	6.53%	0.899%
45	18.702	2579	2581	2586	rVB4	2745	3080	0.47%	0.065%
46	18.767	2589	2592	2593	rBV2	1323	1203	0.18%	0.025%
47	18.838	2602	2604	2608	rVB2	1682	1819	0.28%	0.038%
48	18.879	2608	2611	2616	rBV4	1333	2460	0.38%	0.052%
49	18.979	2624	2628	2634	rVB3	29076	38890	5.95%	0.819%
50	19.020	2634	2635	2637	rBV2	1270	846	0.13%	0.018%
51	19.125	2651	2653	2654	rBV2	1186	789	0.12%	0.017%
52	19.161	2654	2659	2664	rVB3	39794	52270	8.00%	1.101%
53	19.255	2674	2675	2678	rVB	1420	714	0.11%	0.015%
54	19.296	2678	2682	2689	rBV2	9208	11360	1.74%	0.239%
55	19.378	2693	2696	2697	rBV	1356	1177	0.18%	0.025%
56	19.419	2700	2703	2707	rBV4	2736	4266	0.65%	0.090%
57	19.454	2707	2709	2712	rVB3	5691	5000	0.76%	0.105%
58	19.537	2722	2723	2725	rVB2	1910	1000	0.15%	0.021%
59	19.584	2730	2731	2733	rVB2	1711	1094	0.17%	0.023%
60	19.625	2733	2738	2739	rBV3	4295	5119	0.78%	0.108%
61	19.748	2757	2759	2762	rVB3	4201	3702	0.57%	0.078%
62	19.783	2762	2765	2768	rVB3	7018	5557	0.85%	0.117%
63	19.871	2778	2780	2785	rVB4	3235	4303	0.66%	0.091%
64	20.024	2803	2806	2809	rVB4	6140	5965	0.91%	0.126%
65	20.083	2809	2816	2824	rBV	162494	234209	35.83%	4.933%
66	20.171	2829	2831	2835	rBV5	2226	3459	0.53%	0.073%
67	20.500	2883	2887	2890	rBV	23937	31384	4.80%	0.661%
68	20.547	2892	2895	2899	rVV2	15404	20709	3.17%	0.436%
69	21.246	3012	3014	3020	rVB4	8968	11819	1.81%	0.249%
70	21.593	3068	3073	3086	rBV2	219922	589142	90.12%	12.408%
71	21.986	3136	3140	3142	rBV3	47765	67536	10.33%	1.422%
72	22.027	3143	3147	3158	rVB2	177676	322109	49.27%	6.784%
73	22.127	3160	3164	3168	rVB2	53041	73074	11.18%	1.539%
74	22.815	3277	3281	3283	rBV2	16694	23061	3.53%	0.486%
75	22.856	3283	3288	3314	rVB3	170056	653738	100.00%	13.768%
76	23.355	3369	3373	3388	rVB5	26804	65435	10.01%	1.378%

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Instrument :
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ClientSampleId :
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Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
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Title : SVOA CALIBRATION

77	23.514	3396	3400	3406	rBV2	31957	50179	7.68%	1.057%
78	24.430	3550	3556	3564	rVB2	52090	121741	18.62%	2.564%
79	25.294	3695	3703	3713	rVB	66610	183685	28.10%	3.868%
80	25.540	3736	3745	3755	rVB	100736	286418	43.81%	6.032%

Sum of corrected areas: 4748266

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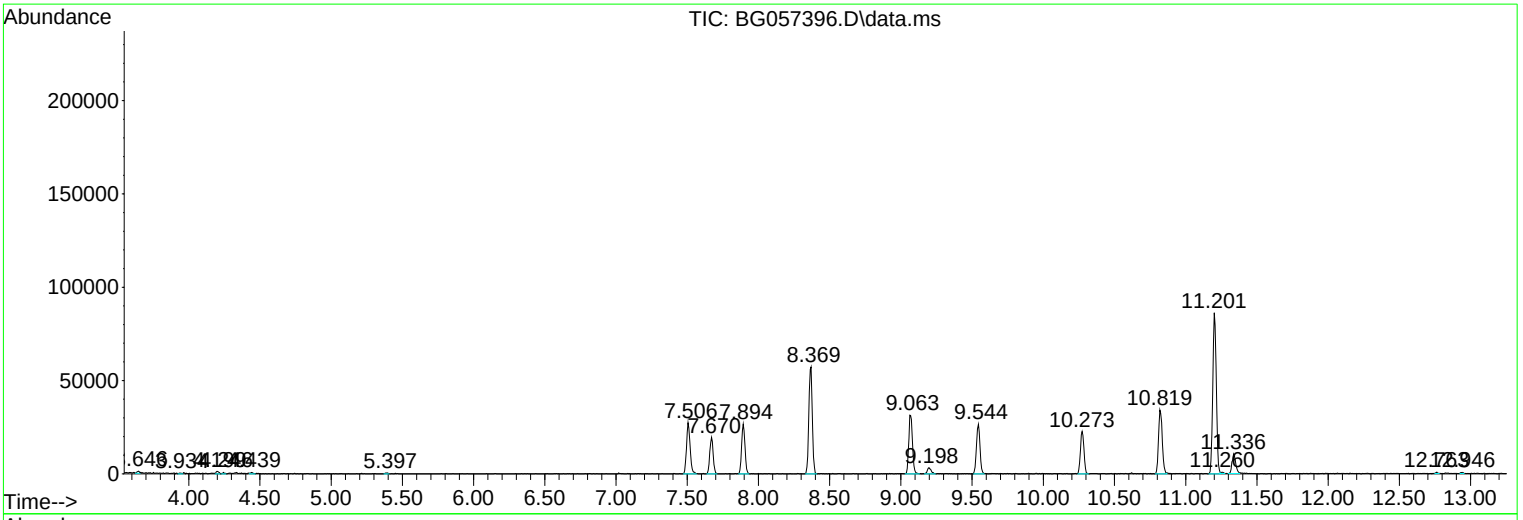
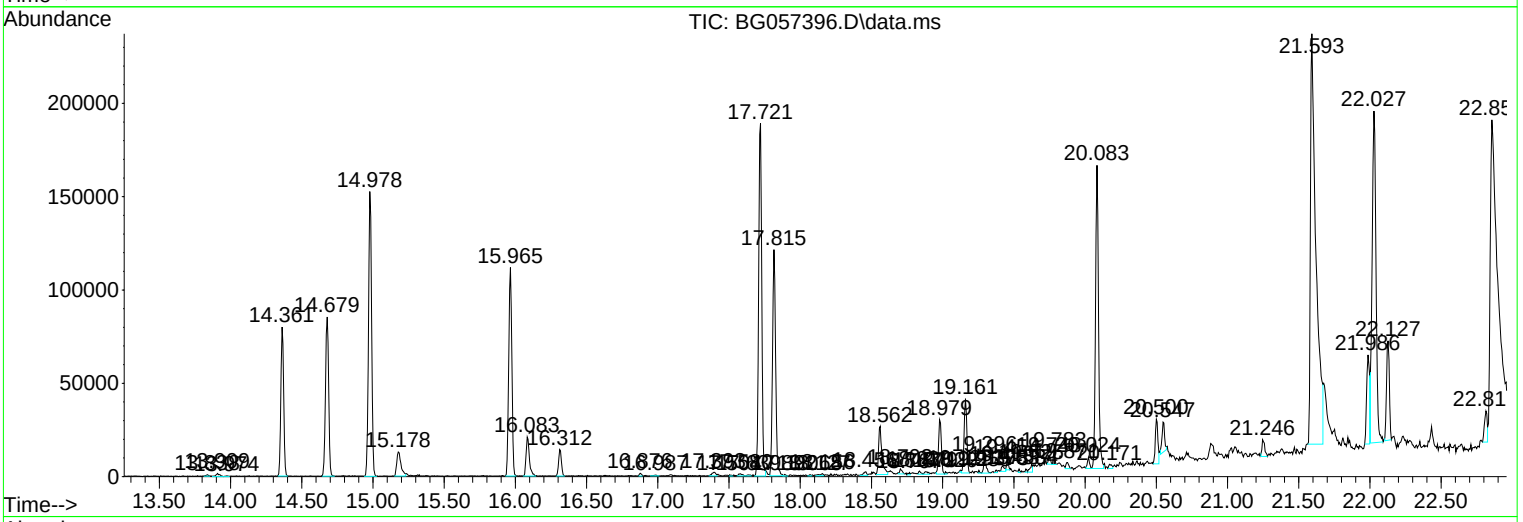
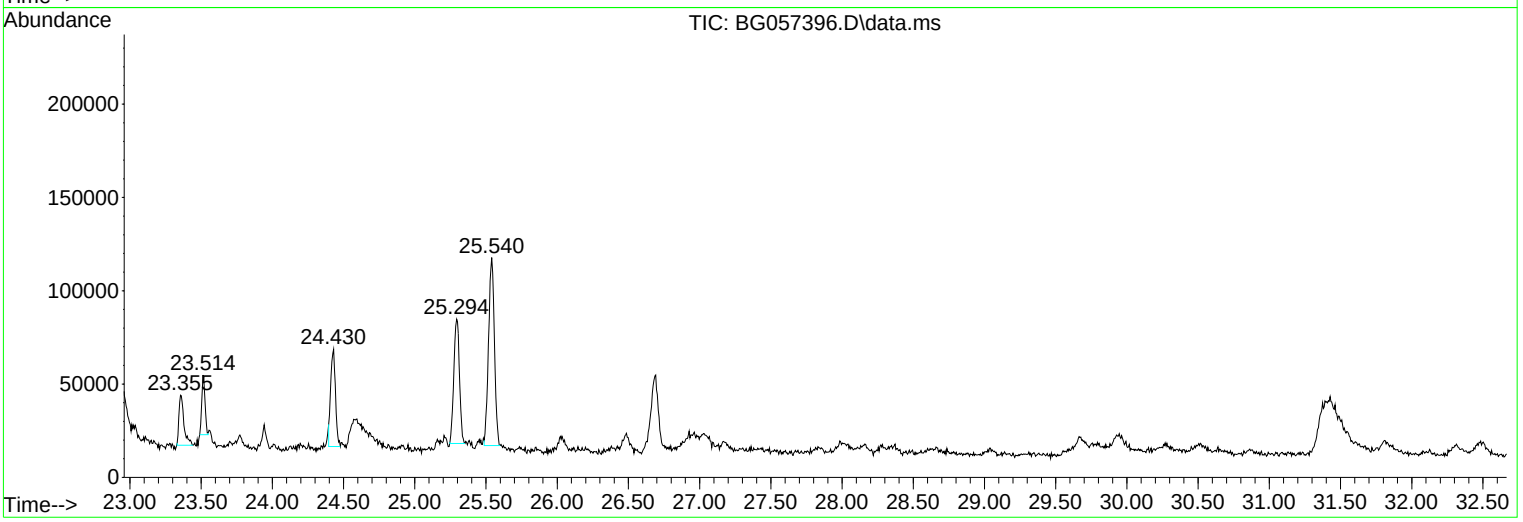
Instrument :
BNA_G
ClientSampleId :
JREA7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051123\
Data File : BG057396.D
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Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREA7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

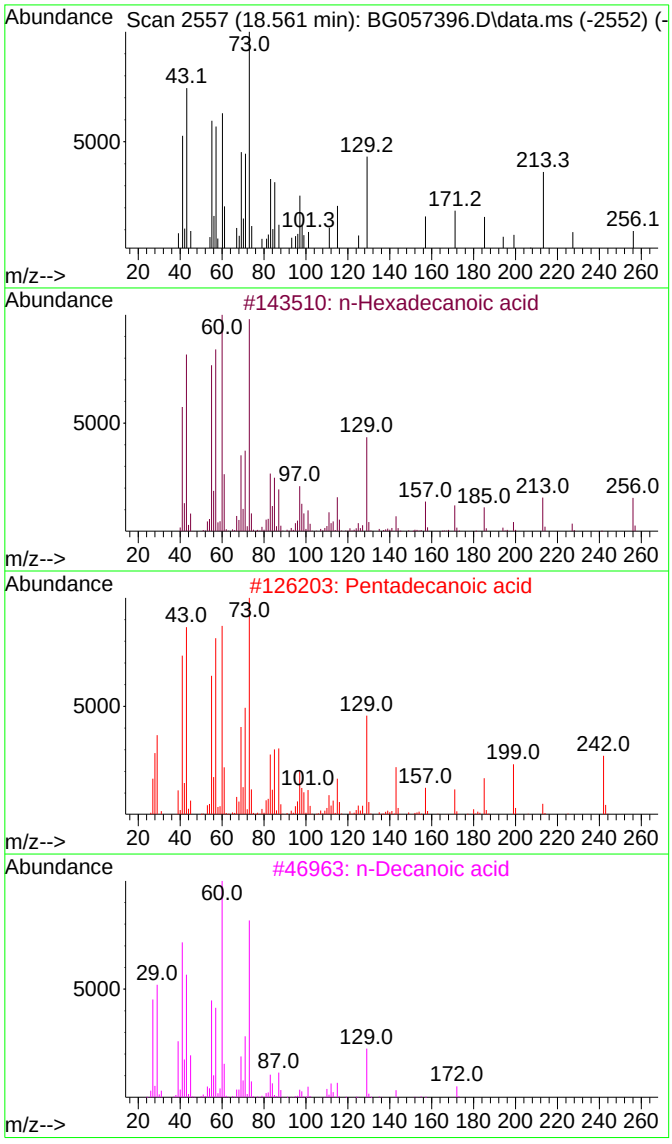
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

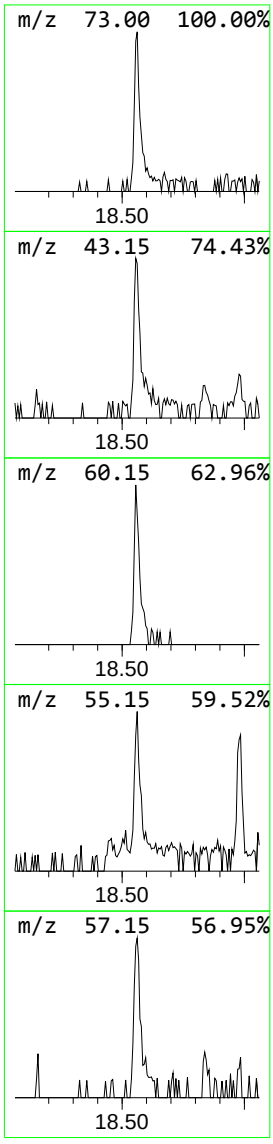
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.561	2.99 ng/ul	42687	Phenanthrene-d10	17.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	n-Decanoic acid	172	C10H20O2	000334-48-5	43
4	Tridecanoic acid	214	C13H26O2	000638-53-9	43
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051123\
Data File : BG057396.D
Acq On : 11 May 2023 12:39
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREA7

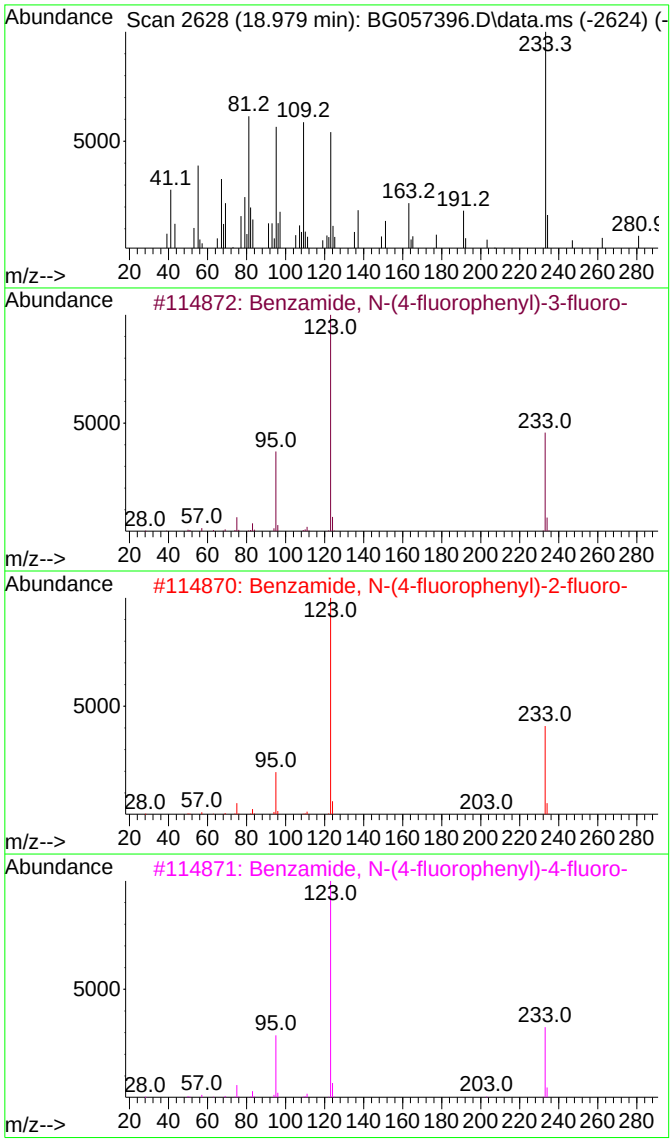
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

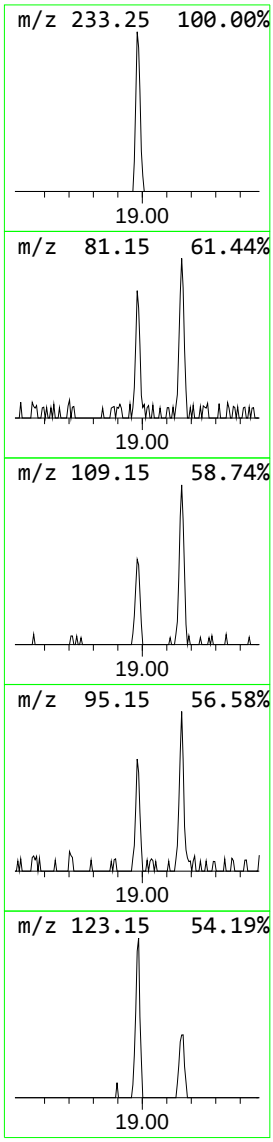
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzamide, N-(4-fluoropheny... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.979	2.72 ng/ul	38890	Phenanthrene-d10	17.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-(4-fluorophenyl)-3-...	233	C13H9F2NO	1010307-16-3	50
2	Benzamide, N-(4-fluorophenyl)-2-...	233	C13H9F2NO	1000307-07-9	50
3	Benzamide, N-(4-fluorophenyl)-4-...	233	C13H9F2NO	1000307-10-1	50
4	8-Hydroxy-5,8a-dimethyl-3-methyl...	262	C15H18O4	1379770-19-0	43
5	Silane, tetra-2-propenyl-	192	C12H20Si	001112-66-9	35





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Sample : 02591-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREA7

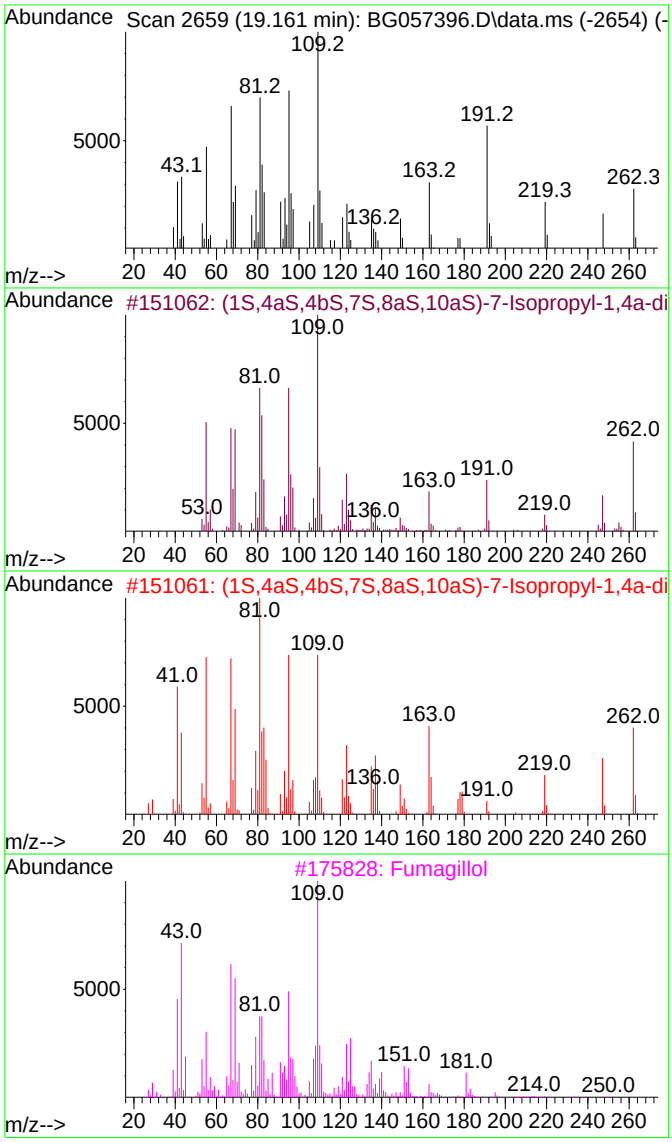
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

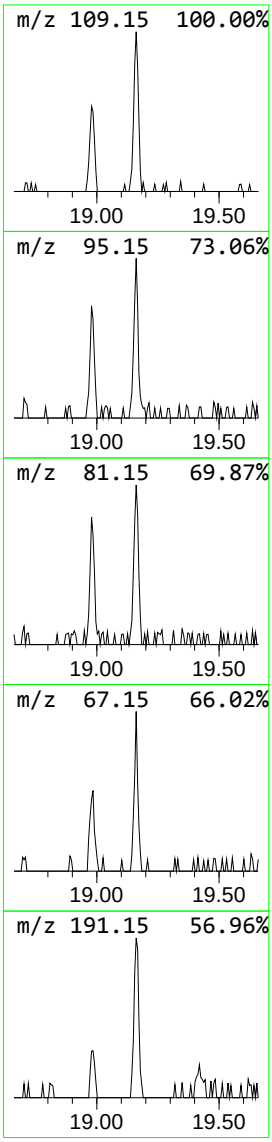
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (1S,4aS,4bS,7S,8aS,10aS)-7-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.161	3.66 ng/ul	52270	Phenanthrene-d10	17.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S,4aS,4bS,7S,8aS,10aS)-7-Isopr...	262	C19H34	002221-95-6	95
2	(1S,4aS,4bS,7S,8aS,10aS)-7-Isopr...	262	C19H34	002221-95-6	50
3	Fumagillol	282	C16H26O4	108102-51-8	43
4	3-[(4-Fluorophenyl)methyl]-1,2,3...	192	C9H9FN4	1000435-39-8	38
5	Longipinane, (E)-	206	C15H26	1000156-14-5	35





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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

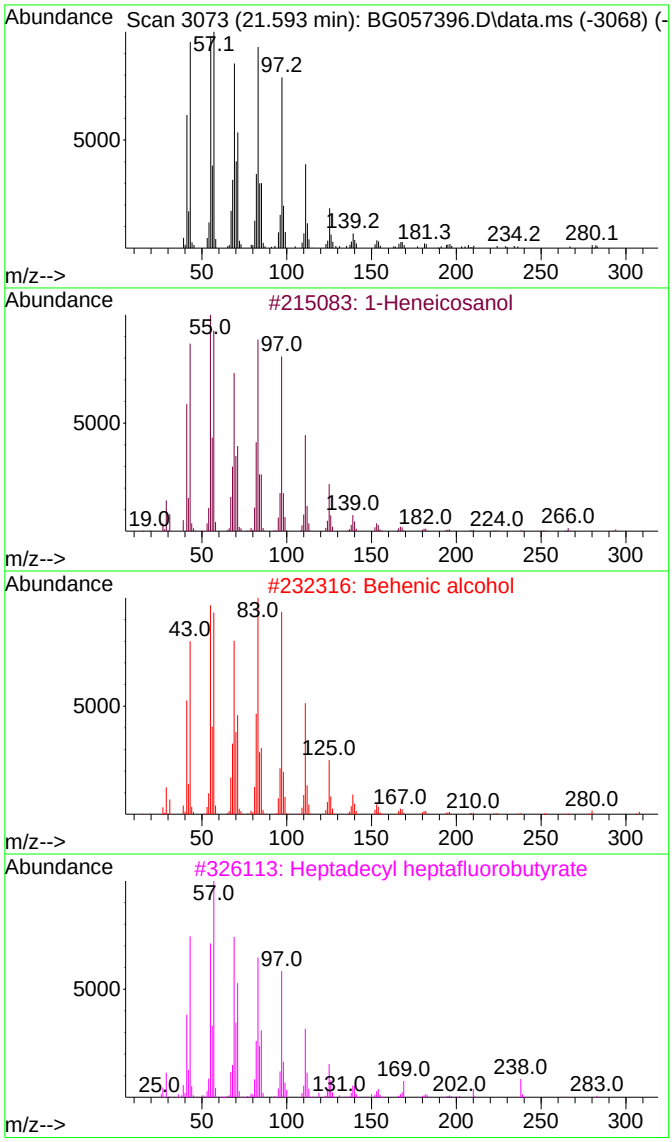
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

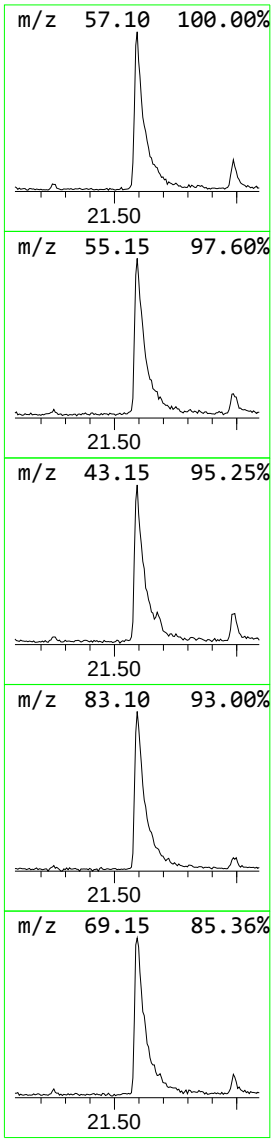
****

Peak Number 4 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.593	36.58 ng/ul	589142	Chrysene-d12	22.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94





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Sample : 02591-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREA7

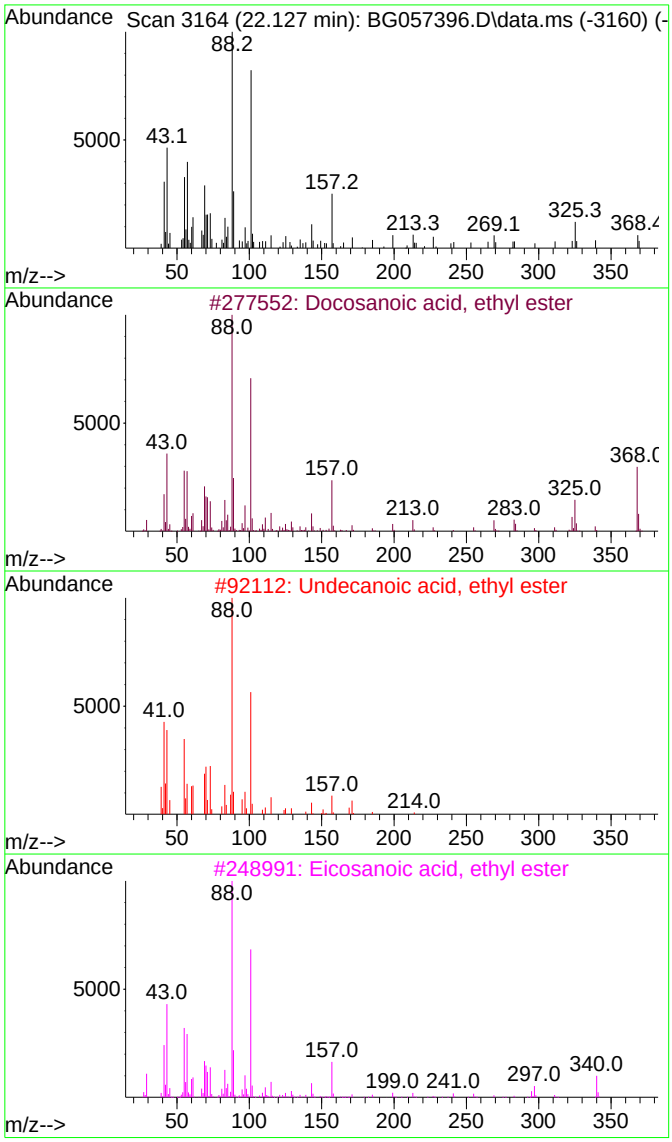
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

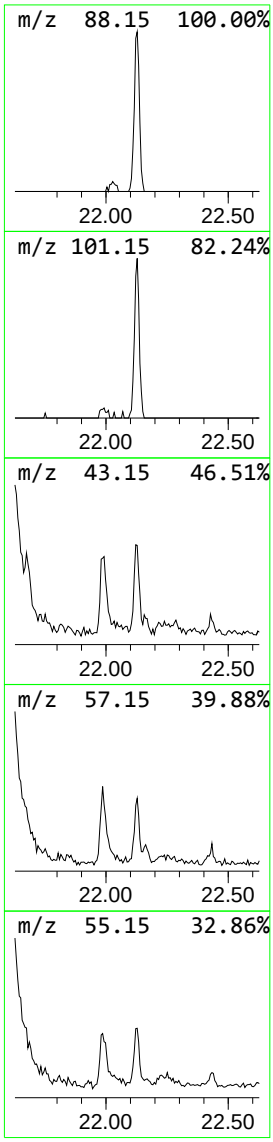
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Docosanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.127	4.54 ng/ul	73074	Chrysene-d12	22.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, ethyl ester	368	C24H48O2	005908-87-2	91
2	Undecanoic acid, ethyl ester	214	C13H26O2	000627-90-7	81
3	Eicosanoic acid, ethyl ester	340	C22H44O2	018281-05-5	80
4	Nonadecanoic acid, ethyl ester	326	C21H42O2	018281-04-4	80
5	Hexadecanoic acid, ethyl ester	284	C18H36O2	000628-97-7	72





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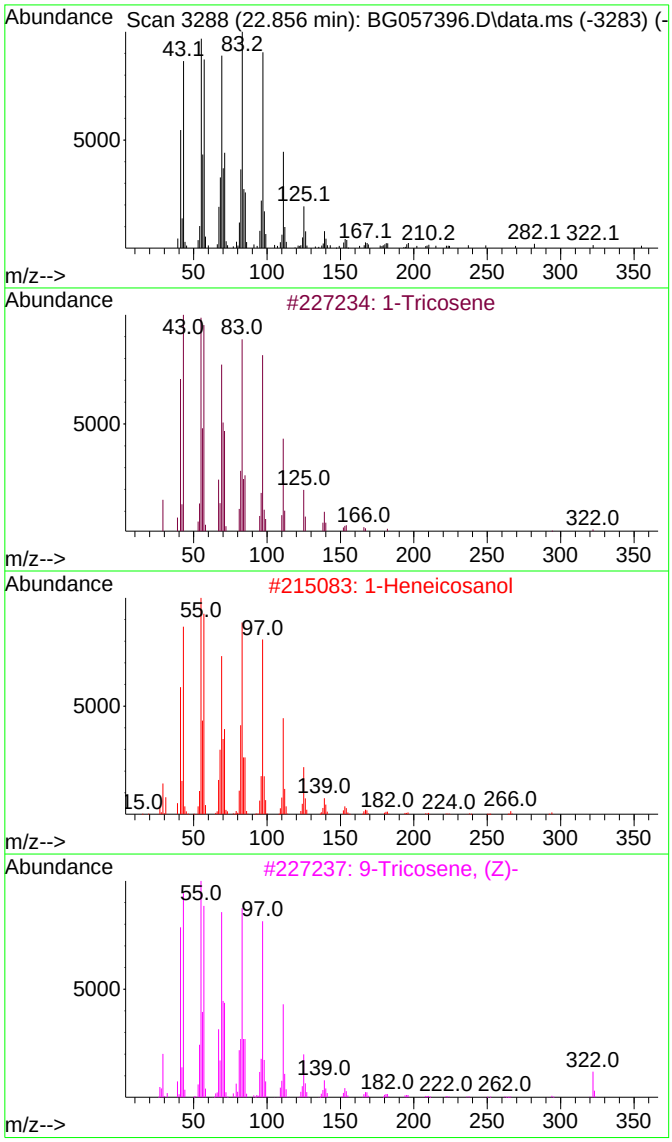
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

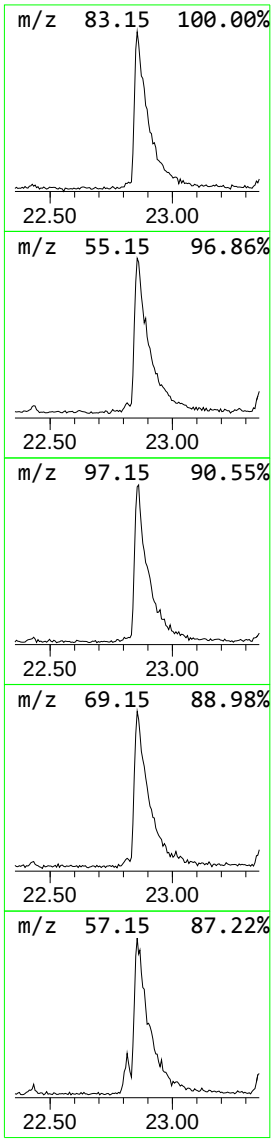
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.856	40.59 ng/ul	653738	Chrysene-d12	22.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	96
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	1-Hexacosene	364	C26H52	018835-33-1	93





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Data File : BG057396.D
Acq On : 11 May 2023 12:39
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREA7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

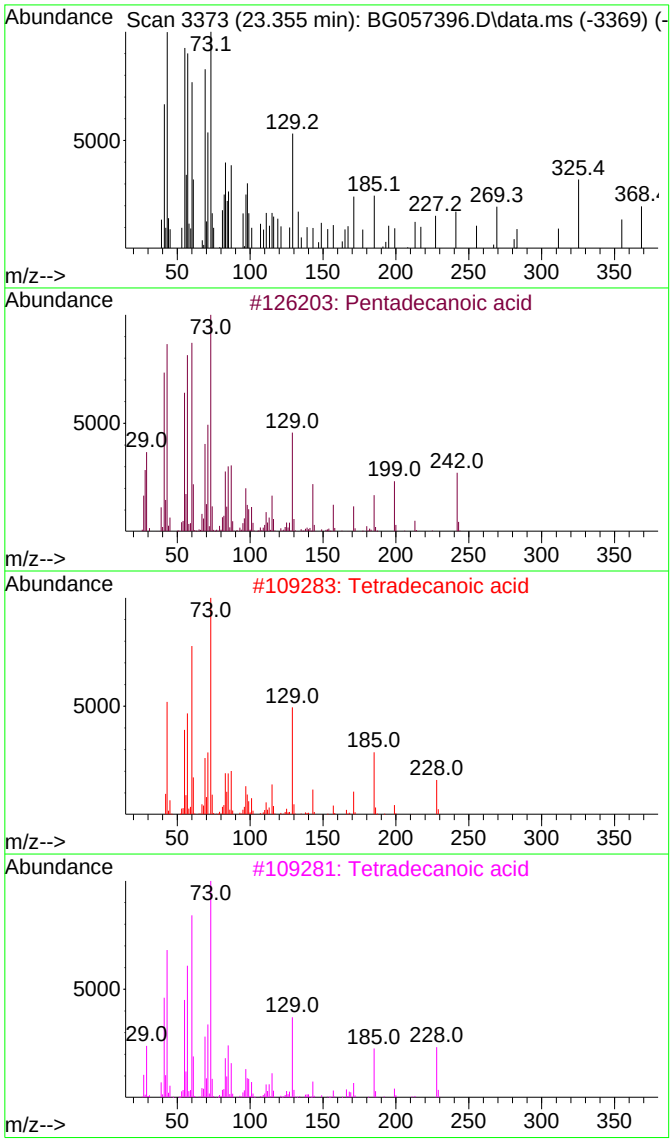
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

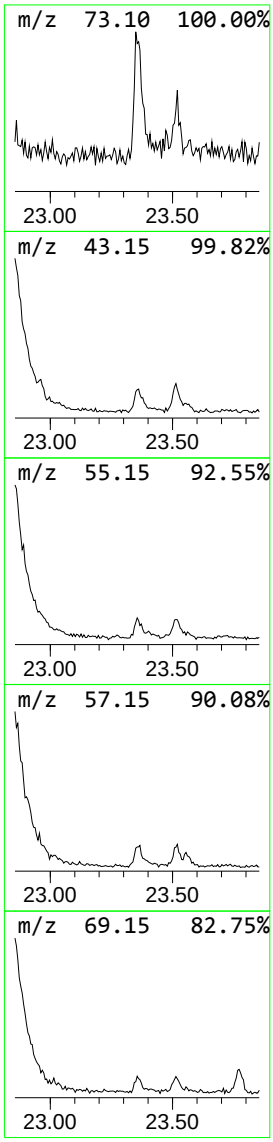
****

Peak Number 7 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.355	4.06 ng/ul	65435	Chrysene-d12	22.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	38
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	35
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	35
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	35
5	Octadecanoic acid	284	C18H36O2	000057-11-4	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051123\
Data File : BG057396.D
Acq On : 11 May 2023 12:39
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREA7

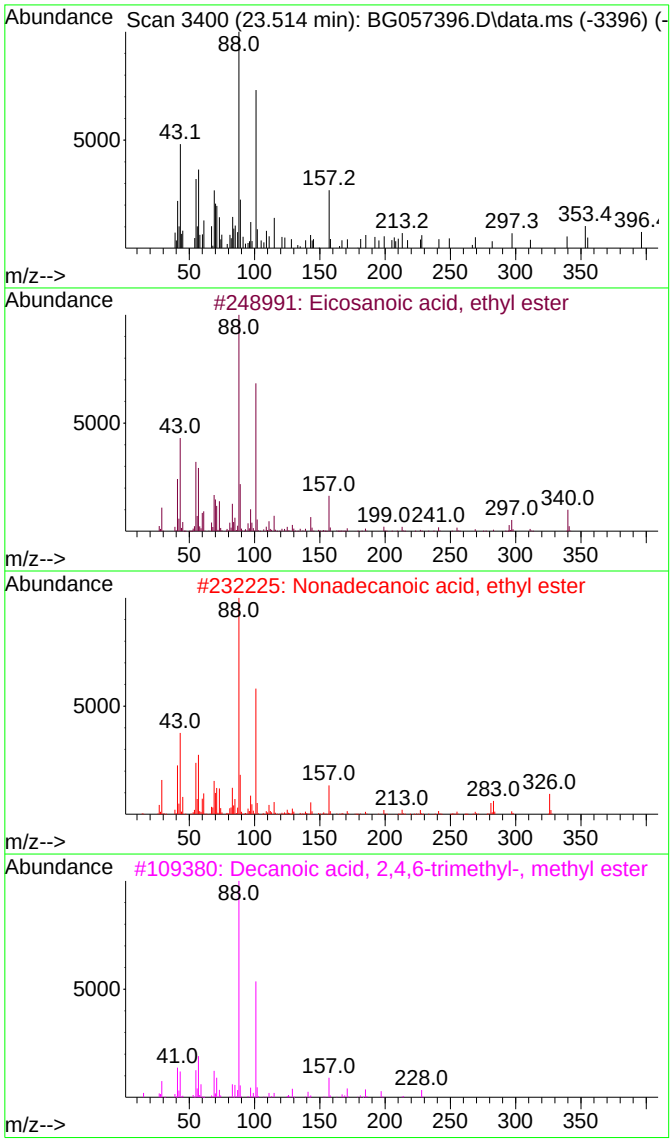
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.M
Quant Title : SVOA CALIBRATION

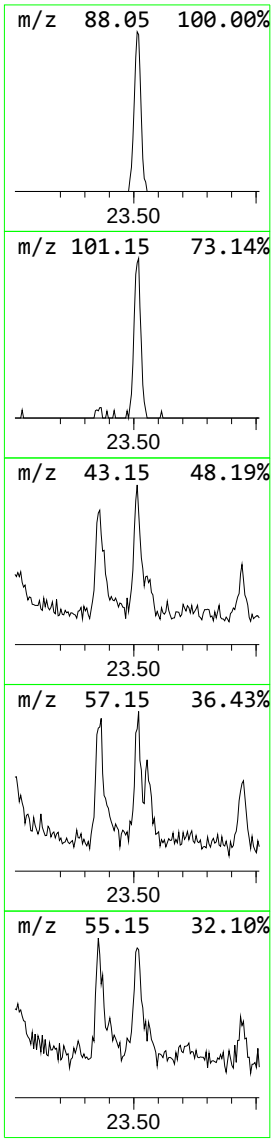
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Eicosanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.514	3.12 ng/ul	50179	Chrysene-d12	22.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, ethyl ester	340	C22H44O2	018281-05-5	74
2	Nonadecanoic acid, ethyl ester	326	C21H42O2	018281-04-4	72
3	Decanoic acid, 2,4,6-trimethyl-,...	228	C14H28O2	055955-72-1	64
4	Eicosanoic acid, ethyl ester	340	C22H44O2	018281-05-5	64
5	Hexadecanoic acid, ethyl ester	284	C18H36O2	000628-97-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051123\
Data File : BG057396.D
Acq On : 11 May 2023 12:39
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
JREA7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG042823.MA.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
n-Hexadecanoic ...	18.561	3.0	ng/ul	42687	4	17.721	285648	20.0
Benzamide, N-(4...	18.979	2.7	ng/ul	38890	4	17.721	285648	20.0
(1S,4aS,4bS,7S,...	19.161	3.7	ng/ul	52270	4	17.721	285648	20.0
1-Heneicosanol	21.593	36.6	ng/ul	589142	5	22.027	322109	20.0
Docosanoic acid...	22.127	4.5	ng/ul	73074	5	22.027	322109	20.0
(DEL) Alkane: S...	22.856	40.6	ng/ul	653738	5	22.027	322109	20.0
unknown-01	23.355	4.1	ng/ul	65435	5	22.027	322109	20.0
Eicosanoic acid...	23.514	3.1	ng/ul	50179	5	22.027	322109	20.0