LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057977.D
Acq On : 4 Jul 2023 7:02
Operator : CG/JU
Sample : 03247-17
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : DCGM3

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-BG070123.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BG057977.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	3	5	22	rVB	1600403	1901435	100.00%	11.821%
2	3.376	45	49	55	rVB	10909	15287	0.80%	0.095%
3	3.799	116	121	130	rBV3	13715	22808	1.20%	0.142%
4	3.899	133	138	145	rVV	41384	58212	3.06%	0.362%
5	3.975	147	151	155	rVV3	5760	10103	0.53%	0.063%
6	4.022	155	159	165	rVB	14047	21457	1.13%	0.133%
7	4.122	173	176	183	rVB4	3373	5637	0.30%	0.035%
8	4.674	266	270	276	rVB5	5218	8087	0.43%	0.050%
9	4.921	308	312	319	rVB4	3072	4072	0.21%	0.025%
10	5.033	327	331	336	rVB3	3458	5440	0.29%	0.034%
11	5.127	342	347	354	rVB	6973	11664	0.61%	0.073%
12	6.619	596	601	606	rVB6	3564	6678	0.35%	0.042%
13	6.931	649	654	659	rBV7	3734	6819	0.36%	0.042%
14	7.101	675	683	692	rBV	159297	278285	14.64%	1.730%
15	7.265	704	711	722	rBV	135379	223718	11.77%	1.391%
16	7.471	737	746	756	rBV	168605	279420	14.70%	1.737%
17	7.935	816	825	834	rVB	136653	235241	12.37%	1.463%
18	8.646	939	946	954	rBV	110241	197282	10.38%	1.227%
19	8.770	960	967	974	rVB3	6548	13264	0.70%	0.082%
20	9.099	1016	1023	1032	rBV	169246	295352	15.53%	1.836%
21	9.821	1139	1146	1158	rVB	132411	233456	12.28%	1.451%
22	10.362	1228	1238	1247	rBV	204576	357879	18.82%	2.225%
23	10.744	1294	1303	1311	rBV	215667	383159	20.15%	2.382%
24	10.873	1318	1325	1333	rBV	75959	153895	8.09%	0.957%
25	11.267	1388	1392	1396	rVB3	3589	4611	0.24%	0.029%
26	11.525	1432	1436	1441	rBV4	2799	4839	0.25%	0.030%
27	11.760	1469	1476	1483	rBV3	3837	6918	0.36%	0.043%
28	12.148	1538	1542	1548	rVB3	2523	4302	0.23%	0.027%
29	12.324	1568	1572	1577	rVB2	3398	4323	0.23%	0.027%
30	12.395	1577	1584	1589	rVB5	3082	6038	0.32%	0.038%
31	13.100	1699	1704	1709	rVB3	3697	6186	0.33%	0.038%
32	13.176	1712	1717	1720	rBV4	2451	4105	0.22%	0.026%
33	13.388	1749	1753	1760	rVB	4952	7699	0.40%	0.048%
34	13.458	1760	1765	1768	rBV3	6146	8945	0.47%	0.056%
35	13.564	1779	1783	1787	rVB4	5866	7718	0.41%	0.048%
36	13.893	1833	1839	1843	rBV4	2383	4696	0.25%	0.029%

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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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Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Title : SVOA CALIBRATION

37	13.975	1844	1853	1861	rVV	370600	533971	28.08%	3.320%
38	14.046	1861	1865	1870	rVB2	6078	7101	0.37%	0.044%
39	14.263	1895	1902	1912	rVV2	429259	687645	36.16%	4.275%
40	14.463	1931	1936	1944	rVB3	7161	13806	0.73%	0.086%
41	14.575	1944	1955	1962	rBV	329596	531997	27.98%	3.307%
42	14.768	1982	1988	1997	rBV	120398	202198	10.63%	1.257%
43	14.915	2008	2013	2019	rVB3	10717	16227	0.85%	0.101%
44	14.974	2019	2023	2029	rVB6	6785	12033	0.63%	0.075%
45	15.356	2083	2088	2092	rBV5	4034	8232	0.43%	0.051%
46	15.409	2092	2097	2102	rVB3	7148	10180	0.54%	0.063%
47	15.562	2116	2123	2135	rBV	558423	858421	45.15%	5.337%
48	15.679	2137	2143	2154	rVB	131480	201109	10.58%	1.250%
49	15.814	2158	2166	2173	rVB6	3726	9653	0.51%	0.060%
50	15.926	2179	2185	2190	rVV	67793	102516	5.39%	0.637%
51	16.190	2226	2230	2235	rBV5	3002	5517	0.29%	0.034%
52	16.290	2239	2247	2252	rBV4	14544	28885	1.52%	0.180%
53	16.408	2260	2267	2273	rBV3	8541	17508	0.92%	0.109%
54	16.701	2314	2317	2321	rBV3	7510	10101	0.53%	0.063%
55	16.848	2336	2342	2346	rBV2	11382	15816	0.83%	0.098%
56	16.966	2358	2362	2367	rBV5	6725	10664	0.56%	0.066%
57	17.060	2374	2378	2382	rVB4	16843	21198	1.11%	0.132%
58	17.201	2397	2402	2409	rBV	48848	75708	3.98%	0.471%
59	17.265	2409	2413	2416	rVV2	29219	43122	2.27%	0.268%
60	17.313	2416	2421	2426	rVV	413889	631706	33.22%	3.927%
61	17.354	2426	2428	2432	rVV	44603	58528	3.08%	0.364%
62	17.412	2432	2438	2446	rVV	545992	828612	43.58%	5.152%
63	17.495	2448	2452	2460	rVB5	9678	17895	0.94%	0.111%
64	17.595	2465	2469	2471	rBV5	4846	5897	0.31%	0.037%
65	17.694	2481	2486	2487	rBV4	5853	8748	0.46%	0.054%
66	17.718	2487	2490	2496	rVB2	8523	14335	0.75%	0.089%
67	17.800	2500	2504	2509	rBV3	9110	14594	0.77%	0.091%
68	17.900	2517	2521	2522	rBV4	2987	4158	0.22%	0.026%
69	17.971	2530	2533	2538	rVB6	5876	8518	0.45%	0.053%
70	18.082	2545	2552	2558	rBV5	26846	48311	2.54%	0.300%
71	18.141	2558	2562	2567	rBV	31898	47778	2.51%	0.297%
72	18.200	2567	2572	2587	rVV2	300688	461705	24.28%	2.870%
73	18.376	2598	2602	2607	rBV3	16828	31449	1.65%	0.196%
74	18.417	2607	2609	2614	rVB2	9726	13176	0.69%	0.082%
75	18.493	2618	2622	2626	rBV3	31880	48925	2.57%	0.304%
76	18.629	2641	2645	2648	rBV6	5544	9881	0.52%	0.061%

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77	18.687	2651	2655	2659	rVV2	20238	25363	1.33%	0.158%
78	18.723	2659	2661	2665	rVB5	6473	9574	0.50%	0.060%
79	18.799	2671	2674	2680	rVB8	6303	10340	0.54%	0.064%
80	19.105	2722	2726	2727	rBV	18383	20478	1.08%	0.127%
81	19.199	2740	2742	2744	rBV3	5943	4681	0.25%	0.029%
82	19.246	2747	2750	2751	rBV2	10362	10397	0.55%	0.065%
83	19.334	2760	2765	2766	rBV3	26444	36255	1.91%	0.225%
84	19.369	2766	2771	2778	rVB	221578	358481	18.85%	2.229%
85	19.469	2784	2788	2800	rVB3	67337	98974	5.21%	0.615%
86	19.616	2811	2813	2816	rVB4	10549	8483	0.45%	0.053%
87	19.698	2822	2827	2831	rBV	716085	1105861	58.16%	6.875%
88	20.050	2882	2887	2893	rBV4	16344	39572	2.08%	0.246%
89	20.227	2913	2917	2922	rVB3	57737	86681	4.56%	0.539%
90	20.720	2998	3001	3005	rVB2	44547	49799	2.62%	0.310%
91	20.973	3040	3044	3049	rVB	35407	54547	2.87%	0.339%
92	21.214	3081	3085	3095	rVB3	163660	284613	14.97%	1.769%
93	21.455	3123	3126	3132	rVB	58605	75899	3.99%	0.472%
94	21.566	3137	3145	3150	rVV2	424056	845953	44.49%	5.259%
95	21.613	3150	3153	3161	rVB	104598	160806	8.46%	1.000%
96	22.354	3274	3279	3292	rBV4	68513	193324	10.17%	1.202%
97	23.729	3507	3513	3520	rBV2	78319	226357	11.90%	1.407%
98	24.516	3639	3647	3655	rBV2	327675	839964	44.18%	5.222%
99	24.733	3676	3684	3696	rBV	250387	710151	37.35%	4.415%
100	25.855	3869	3875	3887	rVB2	123729	351205	18.47%	2.183%

Sum of corrected areas: 16084612

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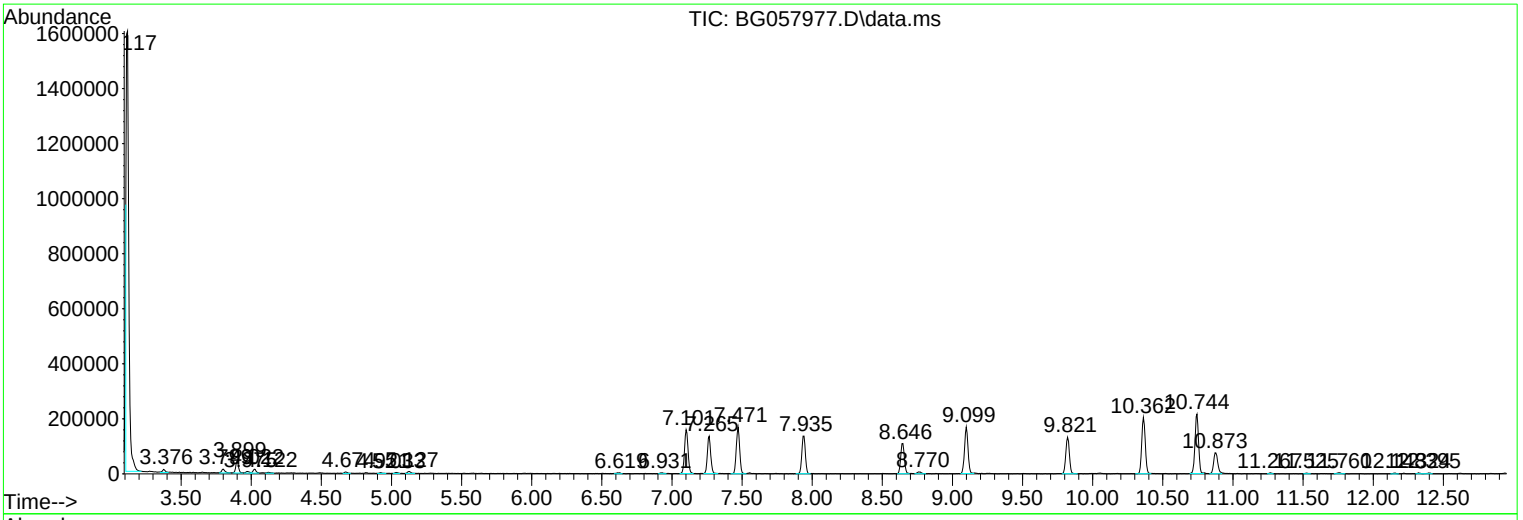
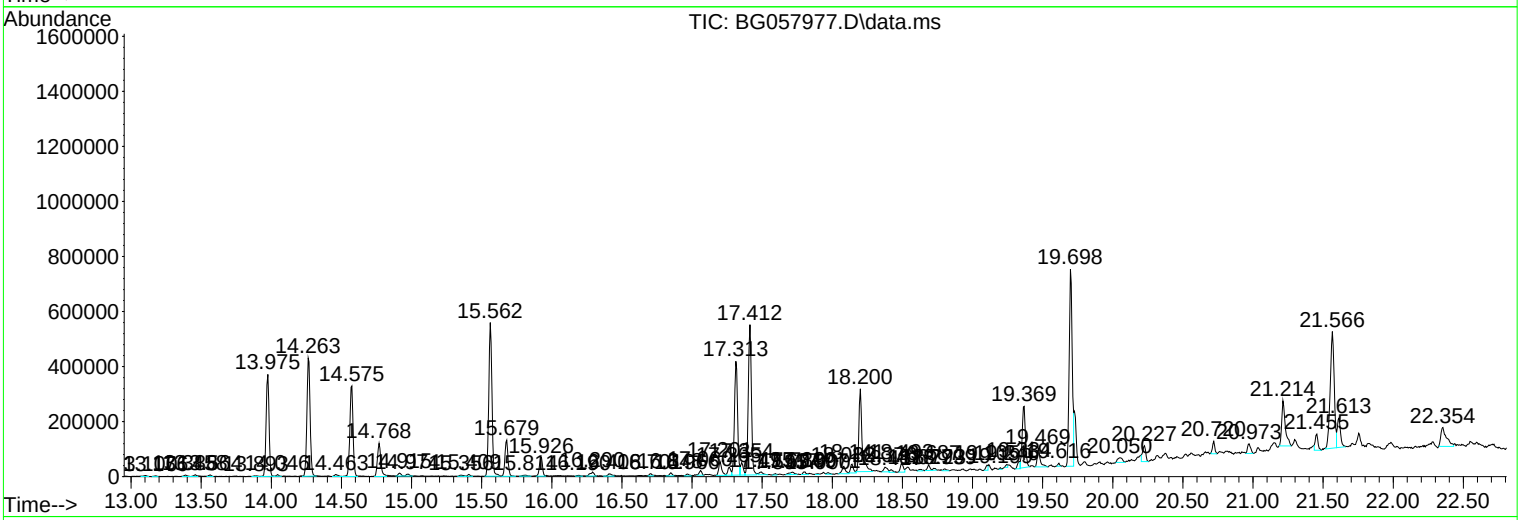
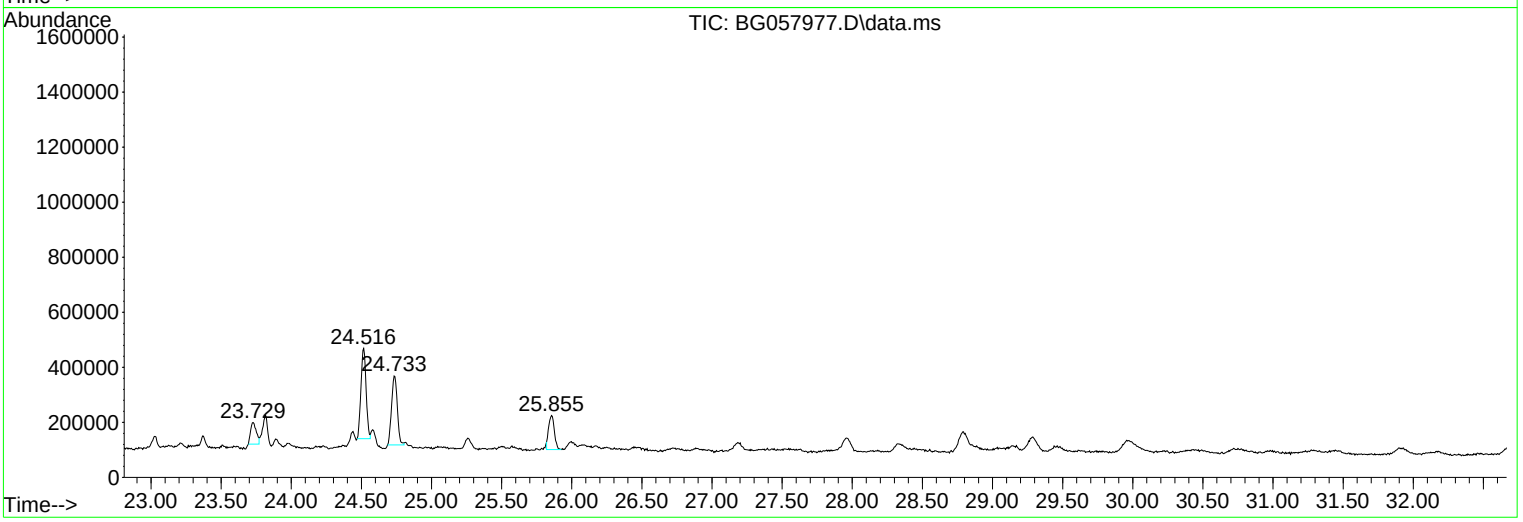
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

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







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ClientSampleId :
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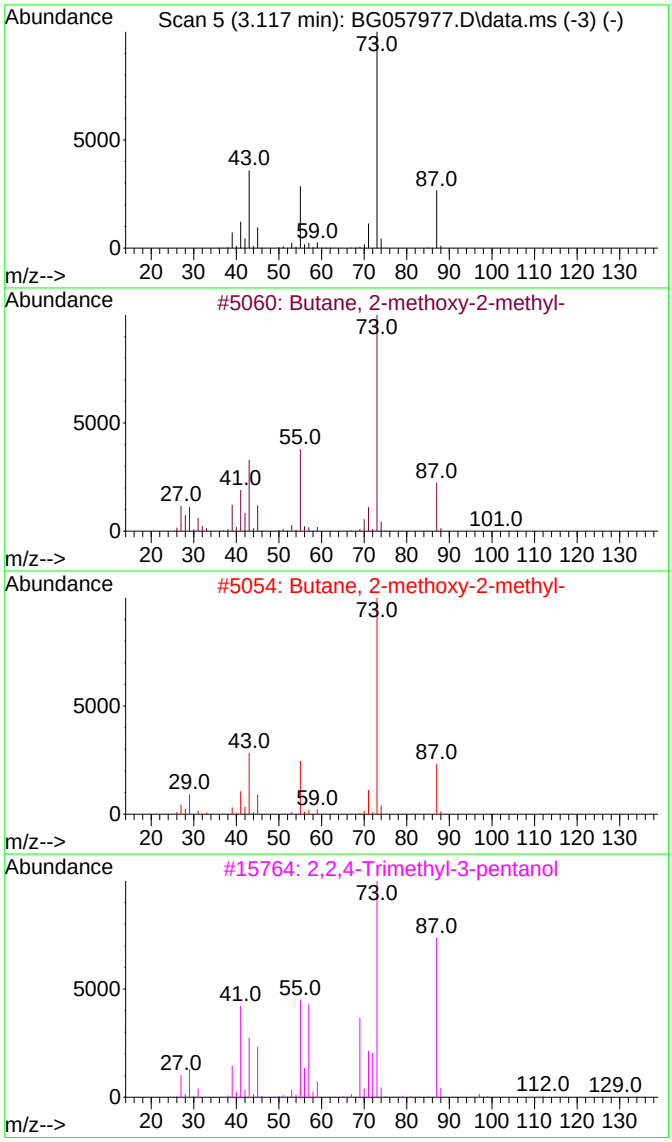
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

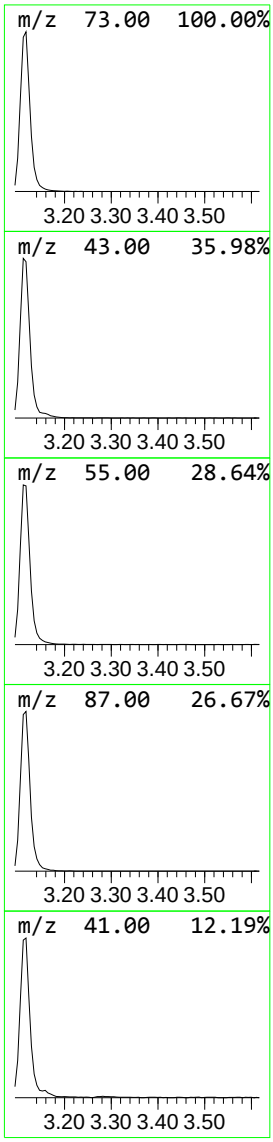
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.117	161.66 ng/ul	1901440	1,4-Dichlorobenzene-d4	7.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17





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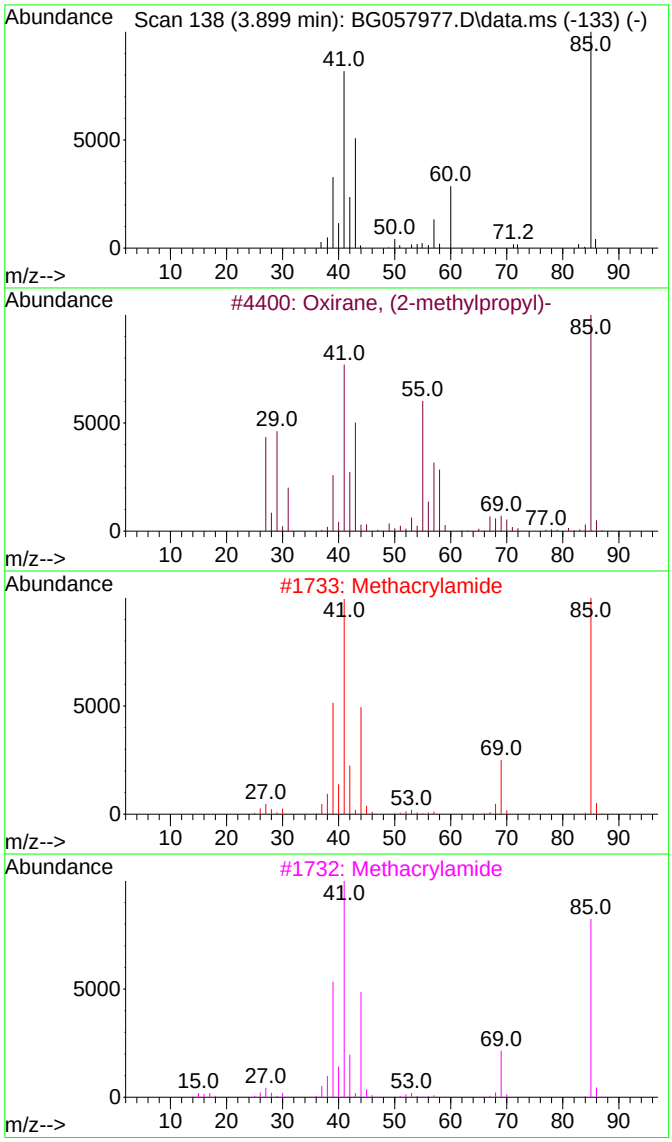
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

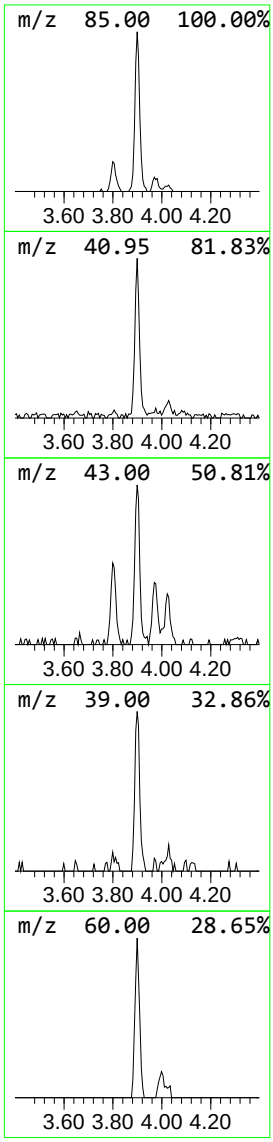
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.899	4.95 ng/ul	58212	1,4-Dichlorobenzene-d4	7.941

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, (2-methylpropyl)-	100	C6H12O	023850-78-4	36
2	Methacrylamide	85	C4H7NO	000079-39-0	36
3	Methacrylamide	85	C4H7NO	000079-39-0	36
4	2-Pyrrolidinone	85	C4H7NO	000616-45-5	28
5	5-Hydroxypentanal	102	C5H10O2	004221-03-8	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

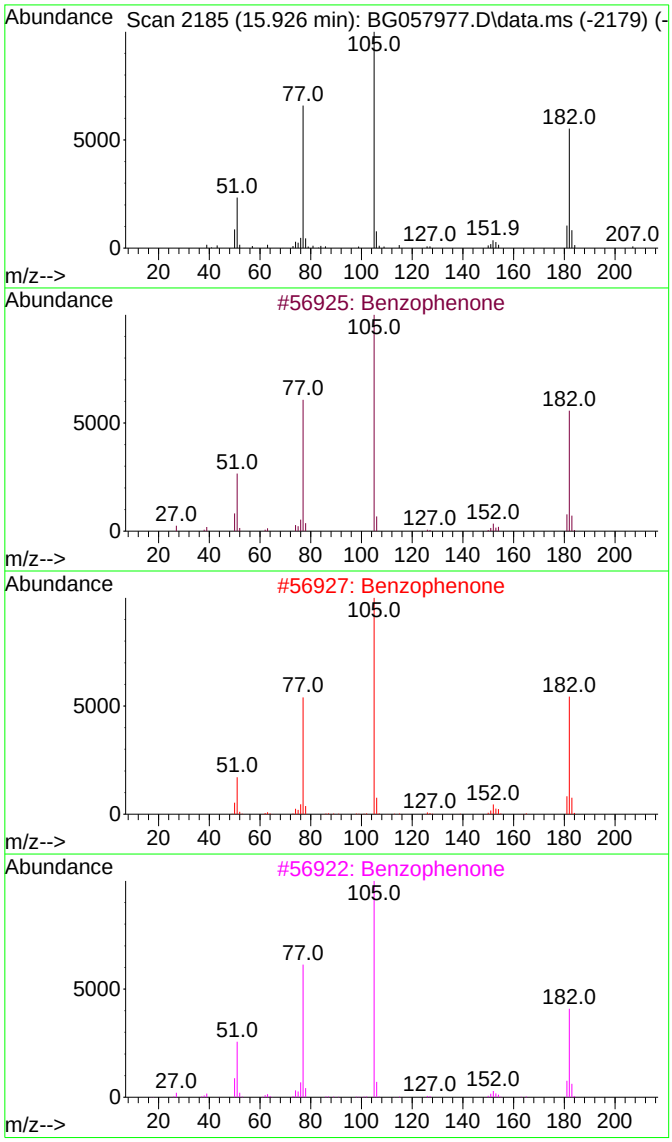
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

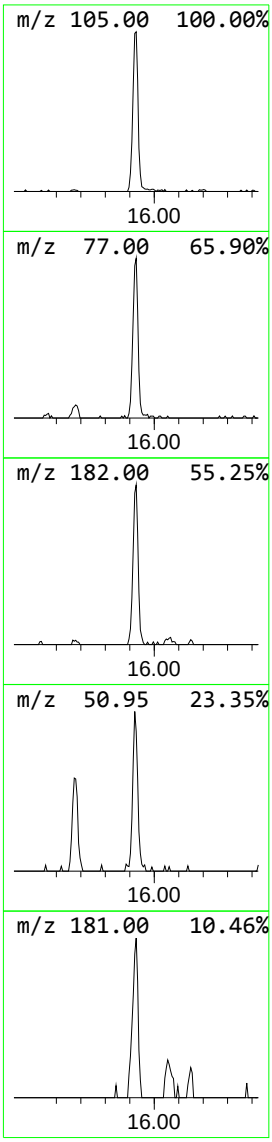
****

Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.926	3.85 ng/ul	102516	Acenaphthene-d10	14.569

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	94
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	91





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

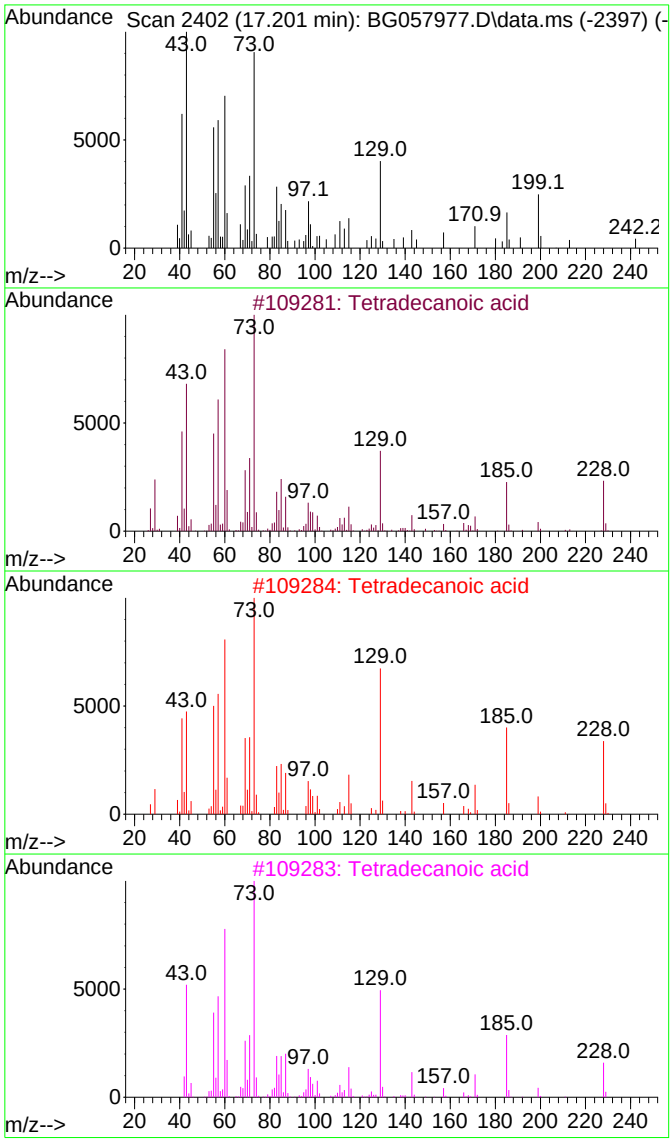
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

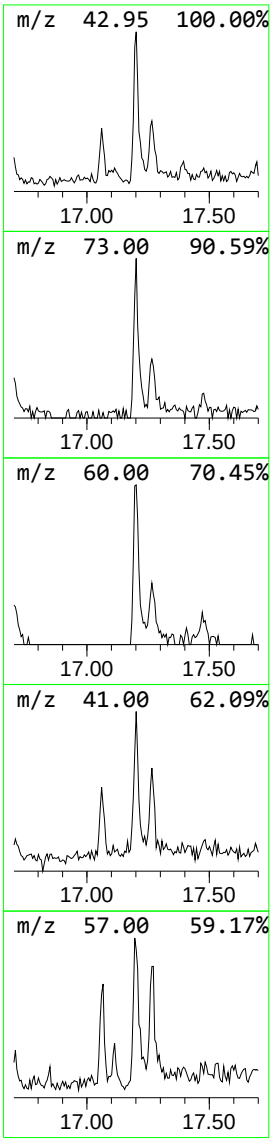
****

Peak Number 4 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.201	2.40 ng/ul	75708	Phenanthrene-d10	17.313

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	55
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





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Sample : 03247-17
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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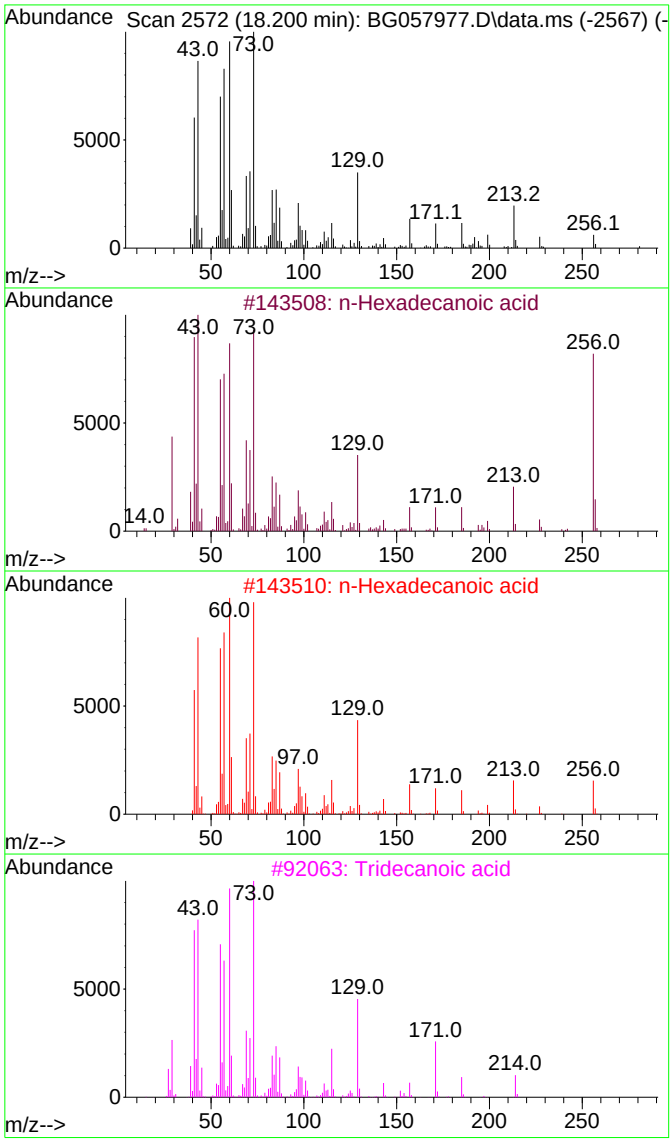
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

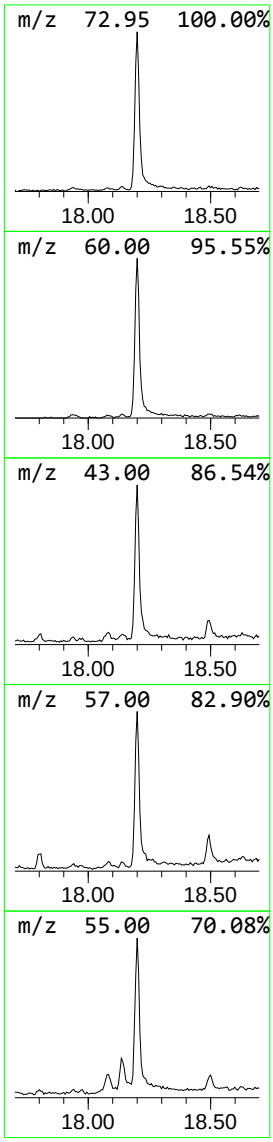
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.200	14.62 ng/ul	461705	Phenanthrene-d10	17.313

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87





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Data File : BG057977.D
Acq On : 4 Jul 2023 7:02
Operator : CG/JU
Sample : 03247-17
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

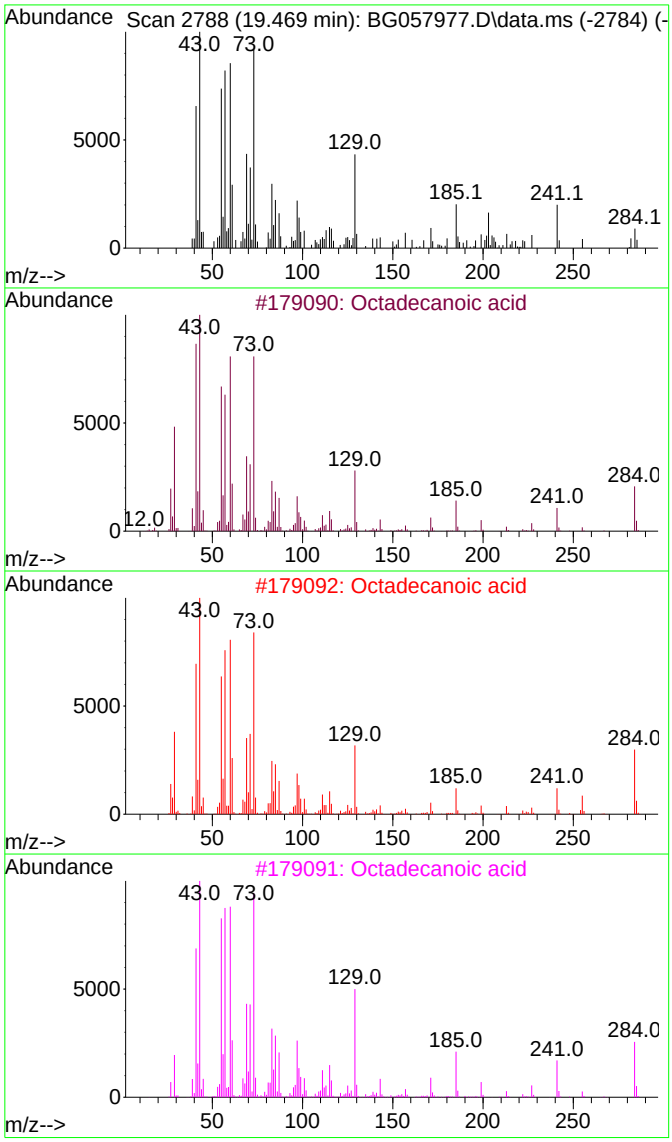
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

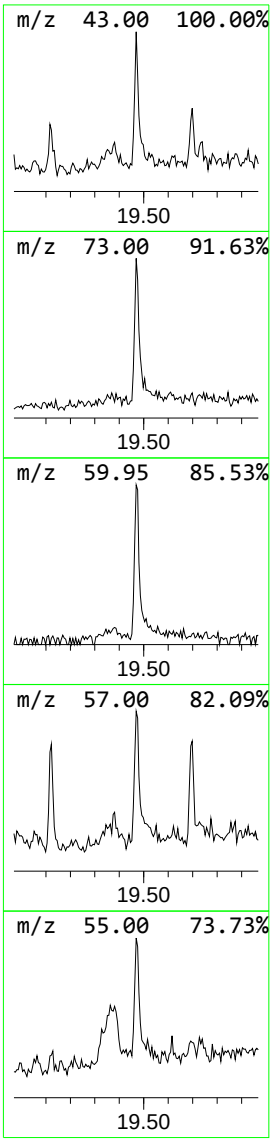
****

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.469	2.34 ng/ul	98974	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	80





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Acq On : 4 Jul 2023 7:02
Operator : CG/JU
Sample : 03247-17
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM3

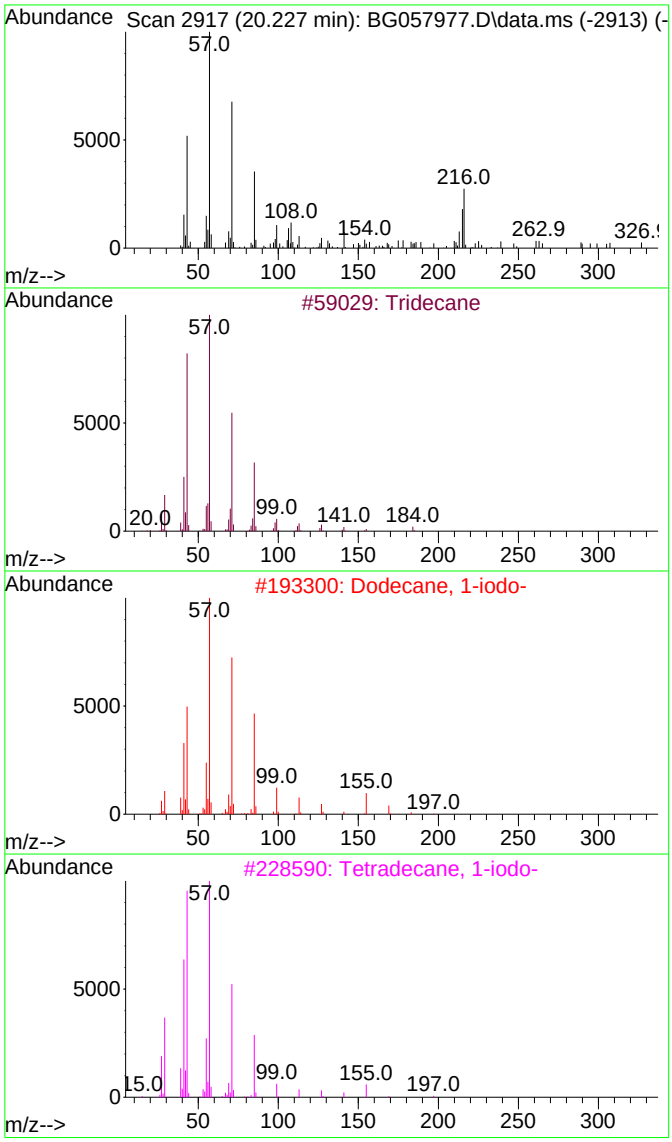
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

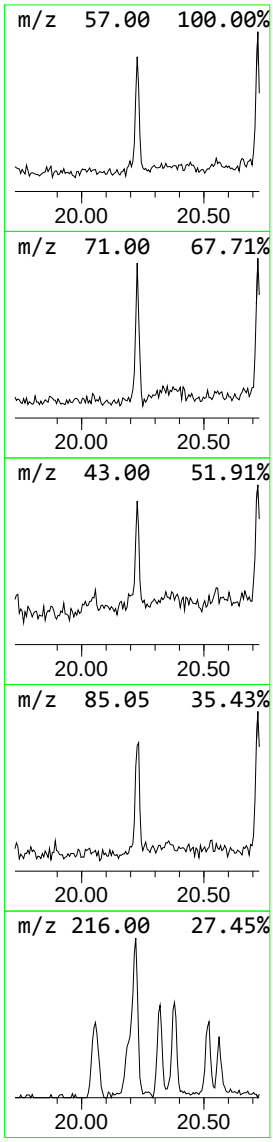
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.227	2.05 ng/ul	86681	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	49
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	47
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	47
4	Dodecyl 4-nitrophenyl ether	307	C18H29NO3	065039-18-1	47
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	43





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Acq On : 4 Jul 2023 7:02
Operator : CG/JU
Sample : 03247-17
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM3

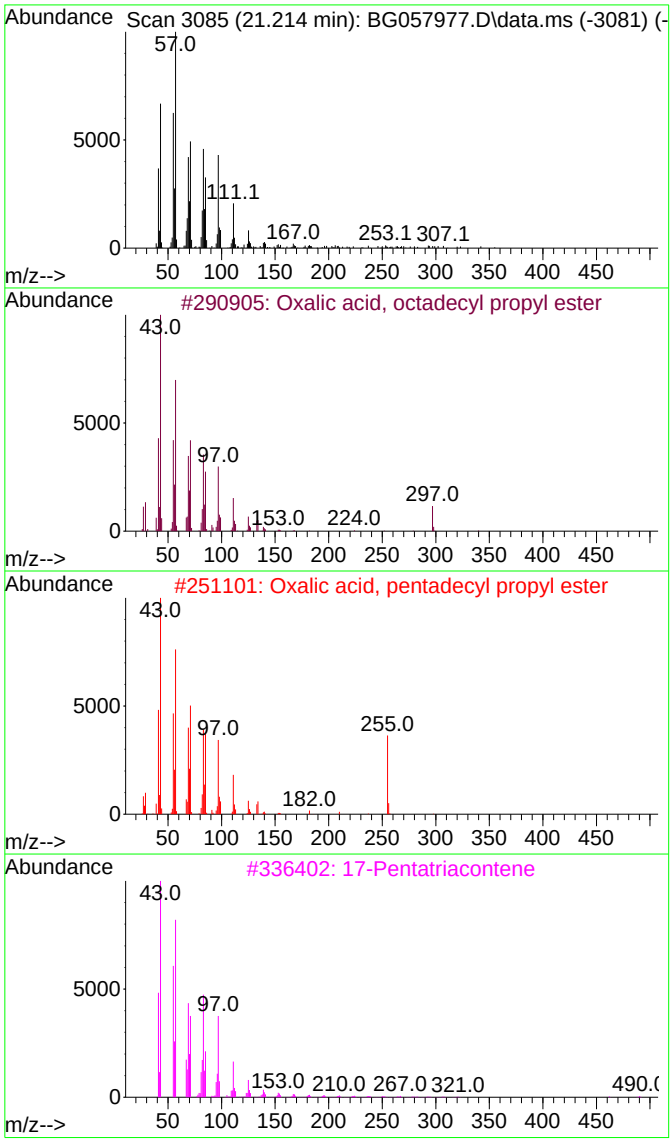
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

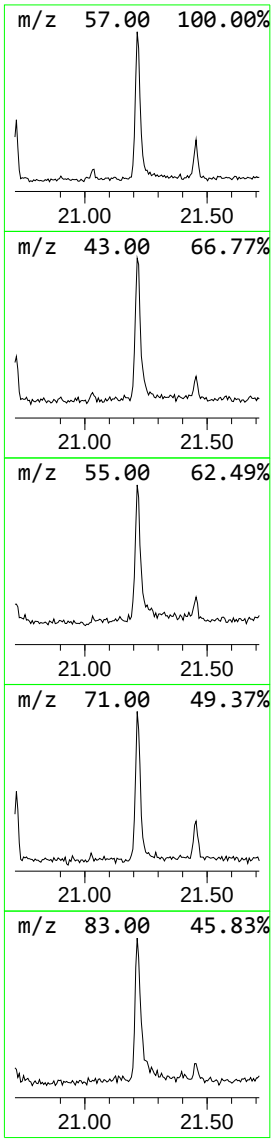
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Oxalic acid, octadecyl prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.214	6.73 ng/ul	284613	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	91
2	Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	90
5	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	90





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Data File : BG057977.D
Acq On : 4 Jul 2023 7:02
Operator : CG/JU
Sample : 03247-17
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

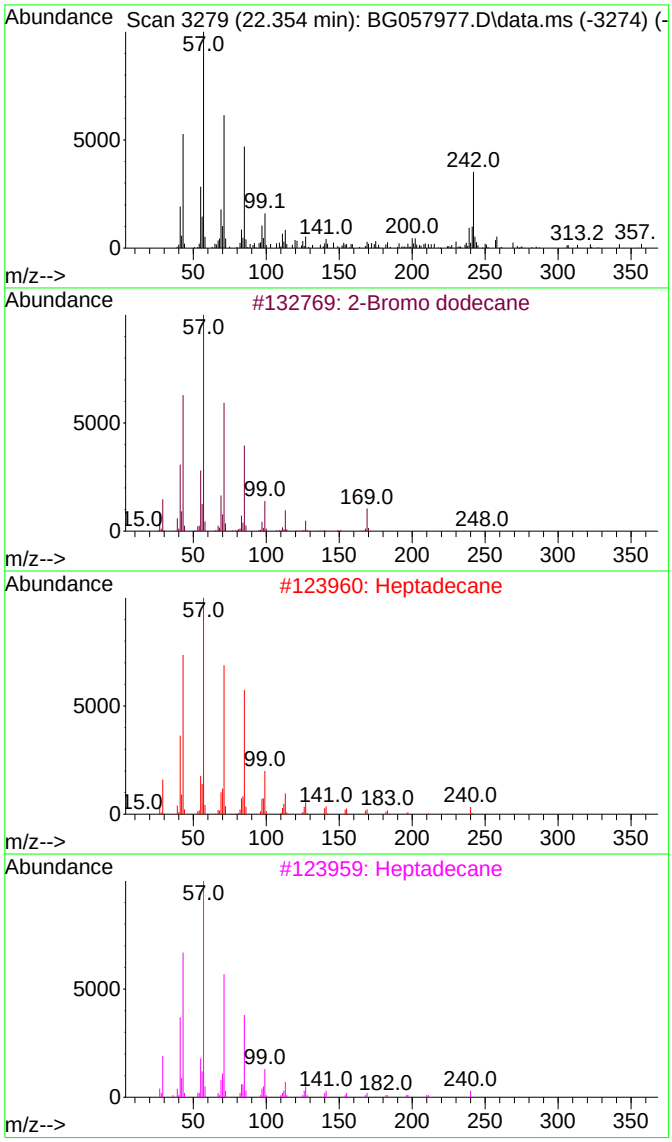
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

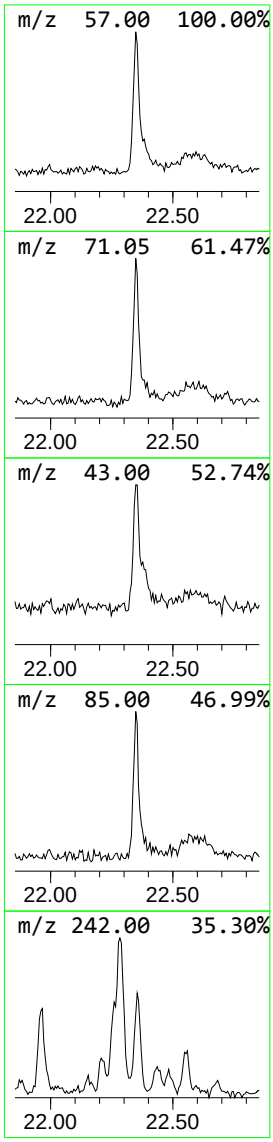
****

Peak Number 9 2-Bromo dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.354	4.57 ng/ul	193324	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
2	Heptadecane	240	C17H36	000629-78-7	78
3	Heptadecane	240	C17H36	000629-78-7	70
4	Hexacosane	366	C26H54	000630-01-3	70
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057977.D
Acq On : 4 Jul 2023 7:02
Operator : CG/JU
Sample : 03247-17
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM3

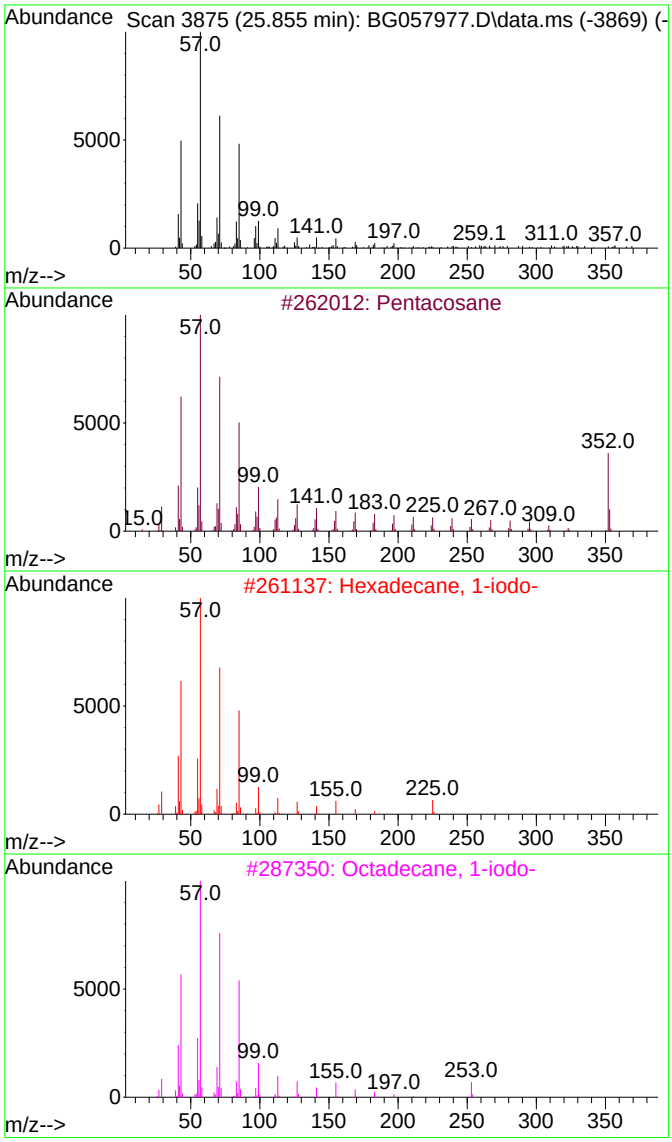
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.MA.M
Quant Title : SVOA CALIBRATION

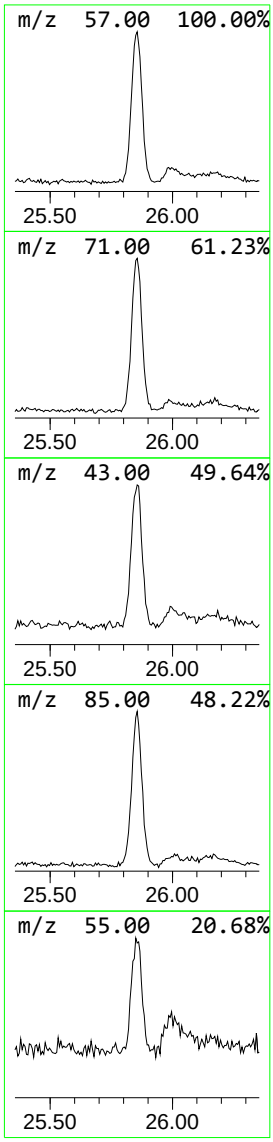
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.855	9.89 ng/ul	351205	Perylene-d12	24.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
4	Heptacosane	380	C27H56	000593-49-7	68
5	Hentriacontane	437	C31H64	000630-04-6	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070323\
Data File : BG057977.D
Acq On : 4 Jul 2023 7:02
Operator : CG/JU
Sample : 03247-17
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DCGM3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG070123.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
Butane, 2-metho...	3.117	161.7	ng/ul	1901440	1	7.941	235241	20.0
unknown-01	3.899	5.0	ng/ul	58212	1	7.941	235241	20.0
Benzophenone	15.926	3.9	ng/ul	102516	3	14.569	531997	20.0
Tetradecanoic acid	17.201	2.4	ng/ul	75708	4	17.313	631706	20.0
n-Hexadecanoic ...	18.200	14.6	ng/ul	461705	4	17.313	631706	20.0
Octadecanoic acid	19.469	2.3	ng/ul	98974	5	21.566	845953	20.0
(DEL) Alkane: S...	20.227	2.0	ng/ul	86681	5	21.566	845953	20.0
Oxalic acid, oc...	21.214	6.7	ng/ul	284613	5	21.566	845953	20.0
2-Bromo dodecane	22.354	4.6	ng/ul	193324	5	21.566	845953	20.0
(DEL) Alkane: S...	25.855	9.9	ng/ul	351205	6	24.733	710151	20.0