LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033024\
Data File : BM044832.D
Acq On : 30 Mar 2024 15:03
Operator : MA/JU
Sample : P1887-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0798

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_M\Methods\SFAM-EPA-BM030524.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM044832.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.234	22	25	29	rBV3	9276	12606	1.17%	0.096%
2	3.522	70	74	83	rVB2	7678	15626	1.45%	0.119%
3	3.640	91	94	96	rBV2	7444	10021	0.93%	0.076%
4	3.734	106	110	117	rVB	55427	73122	6.78%	0.557%
5	3.805	119	122	125	rVB4	6444	7508	0.70%	0.057%
6	3.928	142	143	149	rVB4	7592	8930	0.83%	0.068%
7	4.146	175	180	184	rBV2	12069	18333	1.70%	0.140%
8	4.216	189	192	195	rBV5	2714	3503	0.32%	0.027%
9	4.287	202	204	212	rVB8	11247	17502	1.62%	0.133%
10	4.346	212	214	215	rBV2	3853	2669	0.25%	0.020%
11	4.475	232	236	243	rVB7	7846	12134	1.12%	0.093%
12	4.728	274	279	284	rBV7	3407	7159	0.66%	0.055%
13	4.816	290	294	299	rBV4	6010	11150	1.03%	0.085%
14	4.928	309	313	320	rBV5	8405	15264	1.41%	0.116%
15	6.093	506	511	513	rBV6	2685	3990	0.37%	0.030%
16	6.704	609	615	618	rBV7	3854	6825	0.63%	0.052%
17	6.846	632	639	651	rVV	134296	235870	21.86%	1.798%
18	7.016	662	668	677	rBV	108398	176330	16.34%	1.344%
19	7.199	693	699	708	rVB	139675	226948	21.03%	1.730%
20	7.275	708	712	715	rVV5	5252	6469	0.60%	0.049%
21	7.299	715	716	722	rVB6	3170	4535	0.42%	0.035%
22	7.363	722	727	734	rBV9	4955	11648	1.08%	0.089%
23	7.663	772	778	786	rBV	343174	554837	51.41%	4.230%
24	8.375	892	899	912	rVV	114358	206478	19.13%	1.574%
25	8.498	915	920	928	rVB2	19523	33783	3.13%	0.258%
26	8.828	969	976	989	rVV	134838	233228	21.61%	1.778%
27	8.945	993	996	997	rVV3	3752	3600	0.33%	0.027%
28	8.987	997	1003	1009	rVB4	16275	29585	2.74%	0.226%
29	9.193	1034	1038	1040	rBV4	2776	2683	0.25%	0.020%
30	9.540	1090	1097	1106	rBV	105821	187955	17.42%	1.433%
31	9.734	1125	1130	1132	rBV5	2800	4669	0.43%	0.036%
32	9.910	1156	1160	1166	rVB8	3123	6120	0.57%	0.047%
33	10.075	1181	1188	1202	rBV	118517	251918	23.34%	1.921%
34	10.445	1239	1251	1258	rVV	430675	755034	69.96%	5.756%
35	10.545	1262	1268	1269	rBV5	1985	3500	0.32%	0.027%
36	10.616	1275	1280	1288	rVB8	4084	7712	0.71%	0.059%

LSC Area Percent Report

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Sample : P1887-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0798

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_M\Methods\SFAM-EPA-BM030524.MA.M
Title : SVOA CALIBRATION

37	10.975	1338	1341	1346	rBV5	4166	7202	0.67%	0.055%
38	11.216	1378	1382	1384	rVV4	1900	2930	0.27%	0.022%
39	11.263	1384	1390	1394	rVV6	7702	16174	1.50%	0.123%
40	11.410	1409	1415	1420	rBV6	4756	10737	0.99%	0.082%
41	11.869	1489	1493	1499	rVB7	4935	8798	0.82%	0.067%
42	11.963	1506	1509	1514	rBV6	3229	5385	0.50%	0.041%
43	12.604	1614	1618	1621	rBV4	1981	2977	0.28%	0.023%
44	12.786	1643	1649	1652	rBV8	3113	5823	0.54%	0.044%
45	12.833	1652	1657	1659	rVB5	3223	3605	0.33%	0.027%
46	13.128	1703	1707	1712	rVB3	6316	10026	0.93%	0.076%
47	13.210	1715	1721	1725	rVV5	12340	18431	1.71%	0.141%
48	13.657	1791	1797	1799	rBV7	2279	3593	0.33%	0.027%
49	13.733	1802	1810	1819	rBV	242560	363094	33.64%	2.768%
50	13.828	1824	1826	1833	rVB7	3271	5835	0.54%	0.044%
51	13.922	1838	1842	1843	rBV4	2700	2912	0.27%	0.022%
52	14.004	1849	1856	1864	rBV	303392	447358	41.45%	3.411%
53	14.210	1884	1891	1898	rBV6	9051	22184	2.06%	0.169%
54	14.310	1902	1908	1917	rVV	586431	893783	82.82%	6.814%
55	14.469	1930	1935	1938	rVB5	1998	2839	0.26%	0.022%
56	14.551	1942	1949	1965	rBV2	58598	168520	15.62%	1.285%
57	14.745	1977	1982	1988	rBV8	6998	12927	1.20%	0.099%
58	14.839	1995	1998	2001	rVB5	2261	2644	0.24%	0.020%
59	15.116	2039	2045	2049	rBV6	5434	10361	0.96%	0.079%
60	15.169	2049	2054	2059	rVV3	8127	14024	1.30%	0.107%
61	15.310	2071	2078	2088	rBV	361253	565441	52.39%	4.311%
62	15.451	2097	2102	2113	rBV	83614	135932	12.60%	1.036%
63	15.551	2118	2119	2121	rVV2	3470	3109	0.29%	0.024%
64	15.569	2121	2122	2127	rVV5	4360	5500	0.51%	0.042%
65	15.733	2148	2150	2154	rVB5	2650	2757	0.26%	0.021%
66	16.039	2198	2202	2205	rBV4	10784	16250	1.51%	0.124%
67	16.104	2210	2213	2215	rBV3	3472	3989	0.37%	0.030%
68	16.121	2215	2216	2219	rVB3	3683	2657	0.25%	0.020%
69	16.210	2227	2231	2236	rVB7	3880	6153	0.57%	0.047%
70	16.486	2275	2278	2279	rBV3	3354	4192	0.39%	0.032%
71	16.621	2293	2301	2304	rBV7	7097	12366	1.15%	0.094%
72	16.786	2325	2329	2330	rBV3	3306	3853	0.36%	0.029%
73	16.839	2333	2338	2340	rBV	10364	12908	1.20%	0.098%
74	16.886	2342	2346	2348	rBV5	3557	5350	0.50%	0.041%
75	16.968	2356	2360	2362	rBV5	1905	2761	0.26%	0.021%
76	17.004	2364	2366	2368	rVV3	3003	3093	0.29%	0.024%

LSC Area Percent Report

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Acq On : 30 Mar 2024 15:03
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Sample : P1887-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0798

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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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM030524.MA.M
Title : SVOA CALIBRATION

77	17.068	2370	2377	2388	rVV	698945	991691	91.89%	7.560%
78	17.168	2388	2394	2402	rVV	441349	619787	57.43%	4.725%
79	17.468	2441	2445	2453	rVB8	14014	23928	2.22%	0.182%
80	17.574	2460	2463	2466	rVV3	8367	8880	0.82%	0.068%
81	17.751	2490	2493	2498	rVB6	7432	8092	0.75%	0.062%
82	17.857	2506	2511	2520	rBV6	6022	15507	1.44%	0.118%
83	17.974	2526	2531	2541	rBV	173306	293139	27.16%	2.235%
84	18.274	2579	2582	2586	rVB5	11203	13689	1.27%	0.104%
85	18.410	2602	2605	2610	rVB3	22275	26135	2.42%	0.199%
86	18.521	2621	2624	2626	rBV4	5834	7962	0.74%	0.061%
87	18.786	2667	2669	2672	rBV4	5961	6079	0.56%	0.046%
88	18.910	2687	2690	2693	rBV4	12885	16174	1.50%	0.123%
89	18.968	2697	2700	2702	rVB	12532	13951	1.29%	0.106%
90	19.121	2722	2726	2727	rBV2	48450	55149	5.11%	0.420%
91	19.145	2727	2730	2743	rVB	192952	338492	31.37%	2.581%
92	19.268	2747	2751	2759	rBV	271753	396146	36.71%	3.020%
93	19.468	2780	2785	2793	rBV	567148	782722	72.53%	5.967%
94	20.033	2878	2881	2884	rBV	34289	35134	3.26%	0.268%
95	20.357	2932	2936	2945	rBV	269198	380226	35.23%	2.899%
96	20.533	2963	2966	2969	rVB2	52618	54476	5.05%	0.415%
97	20.998	3041	3045	3049	rBV	156184	192323	17.82%	1.466%
98	21.268	3086	3091	3095	rBV	830397	1072935	99.42%	8.180%
99	23.362	3442	3447	3452	rVB2	394818	687350	63.69%	5.240%
100	23.503	3466	3471	3480	rVB	587717	1079202	100.00%	8.228%

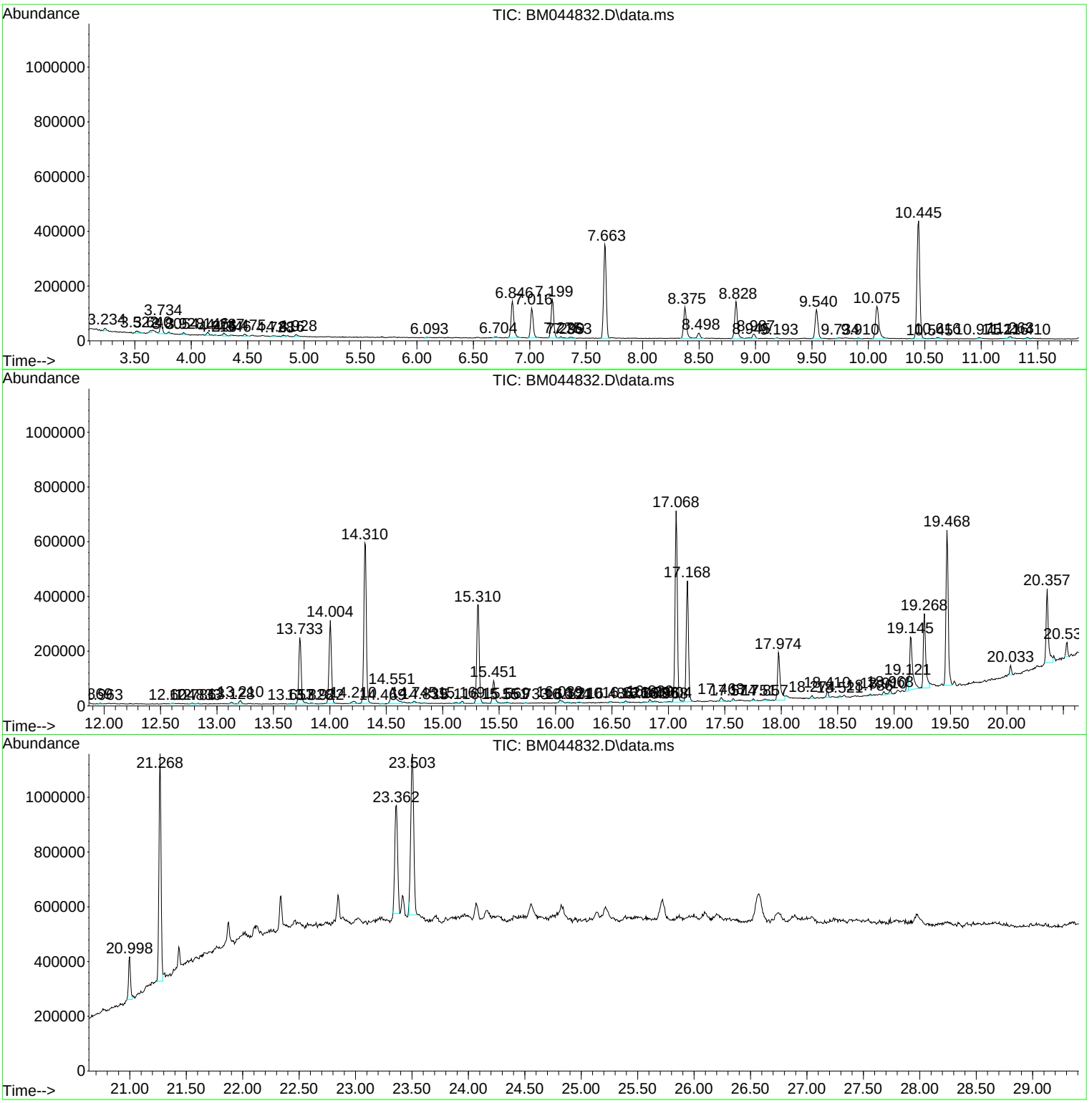
Sum of corrected areas: 13116886

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033024\
Data File : BM044832.D
Acq On : 30 Mar 2024 15:03
Operator : MA/JU
Sample : P1887-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0798

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM030524.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033024\
Data File : BM044832.D
Acq On : 30 Mar 2024 15:03
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Sample : P1887-05
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM030524.MA.M
Quant Title : SVOA CALIBRATION

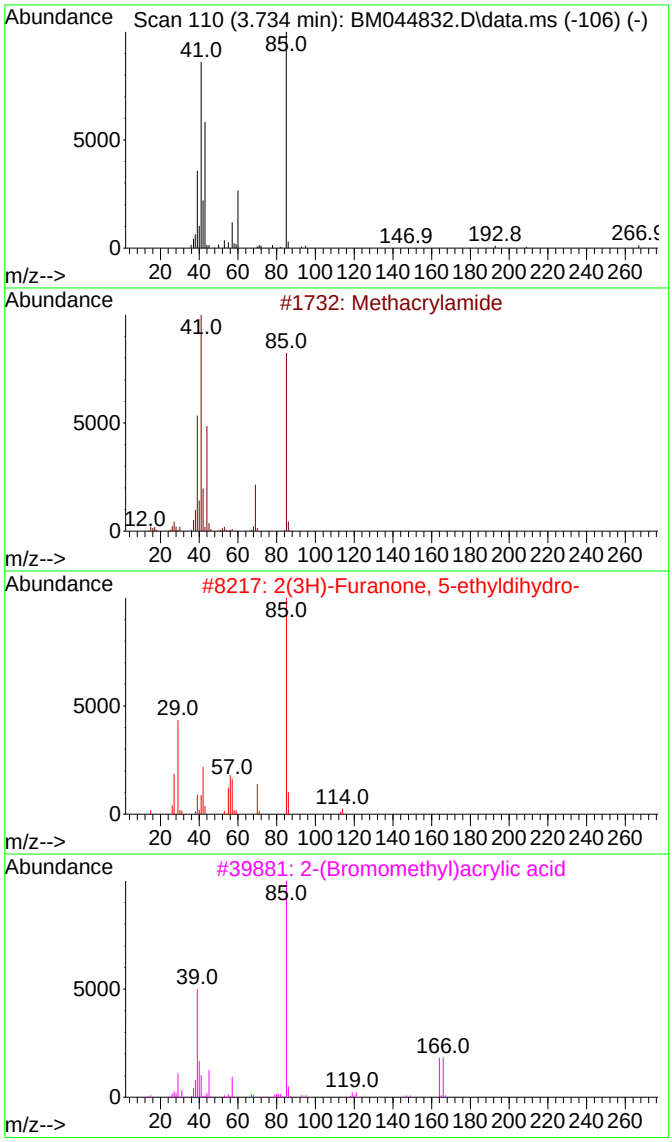
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

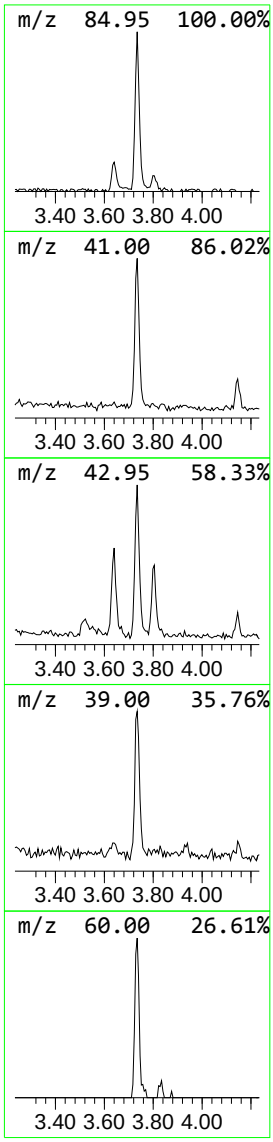
****

Peak Number 1 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.734	2.64 ng/ul	73122	1,4-Dichlorobenzene-d4	7.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methacrylamide	85	C4H7NO	000079-39-0	38
2	2(3H)-Furanone, 5-ethyldihydro-	114	C6H10O2	000695-06-7	33
3	2-(Bromomethyl)acrylic acid	164	C4H5BrO2	072707-66-5	9
4	n-Butyl nitrite	103	C4H9NO2	000544-16-1	9
5	Pentane, 2-bromo-4-methyl-	164	C6H13Br	030310-22-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033024\
Data File : BM044832.D
Acq On : 30 Mar 2024 15:03
Operator : MA/JU
Sample : P1887-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0798

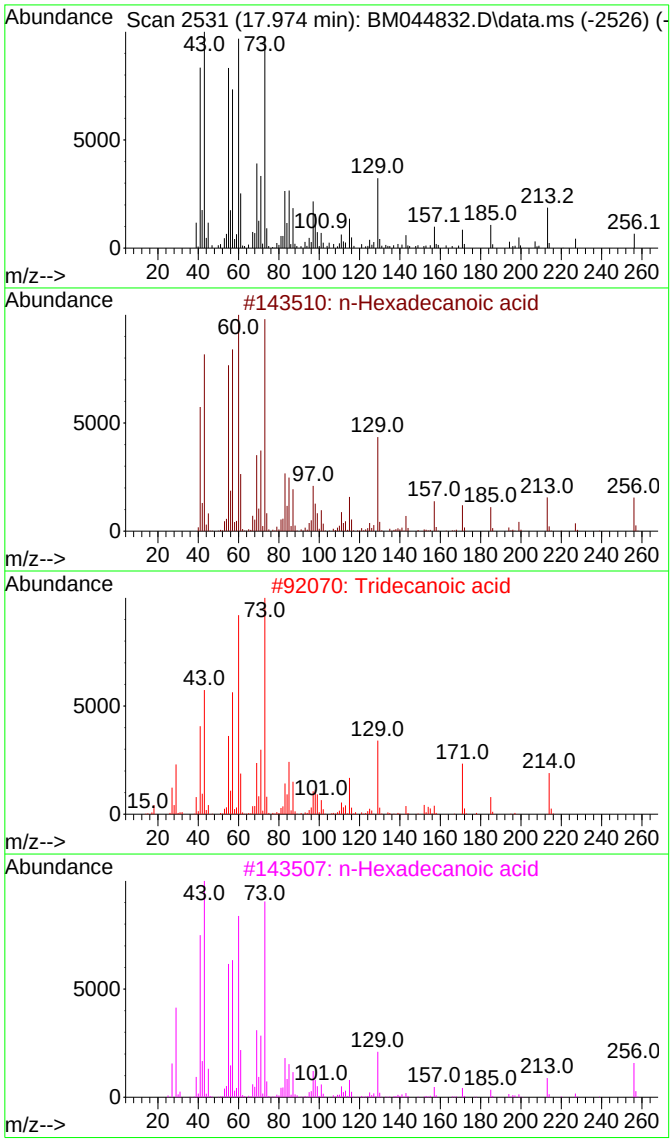
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM030524.MA.M
Quant Title : SVOA CALIBRATION

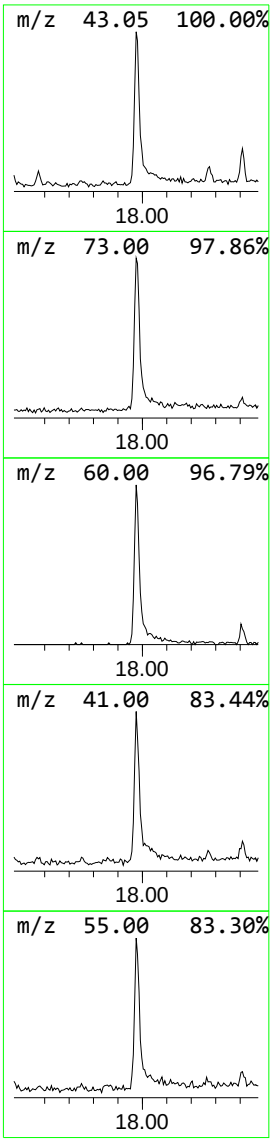
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	5.91 ng/ul	293139	Phenanthrene-d10	17.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	74





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Instrument :
BNA_M
ClientSampleId :
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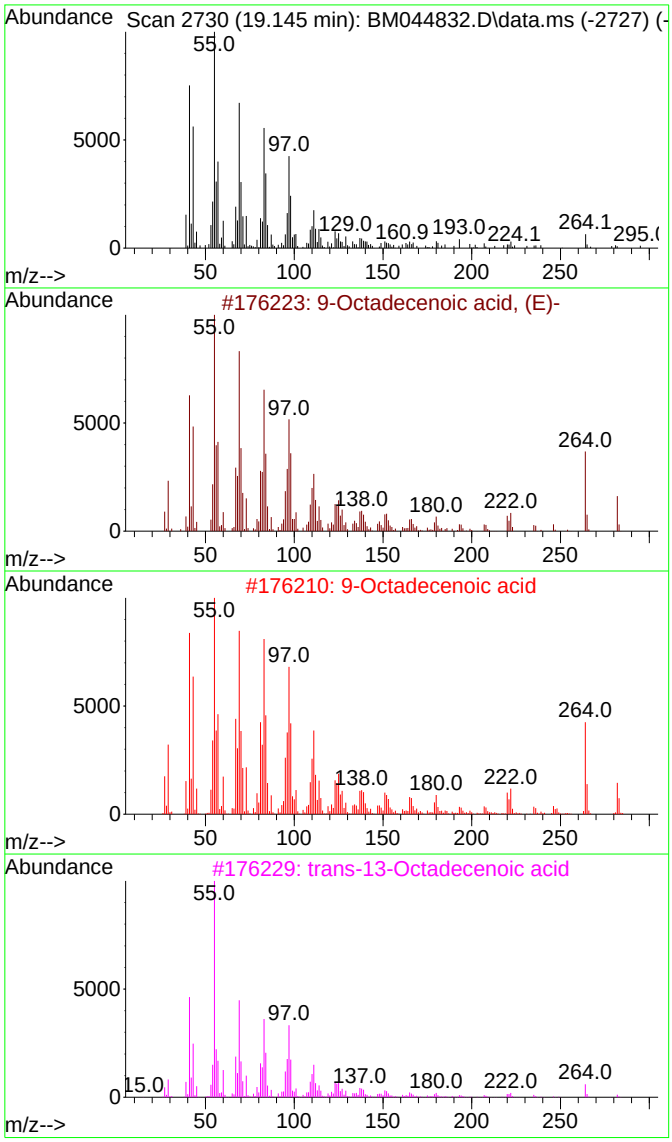
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM030524.MA.M
Quant Title : SVOA CALIBRATION

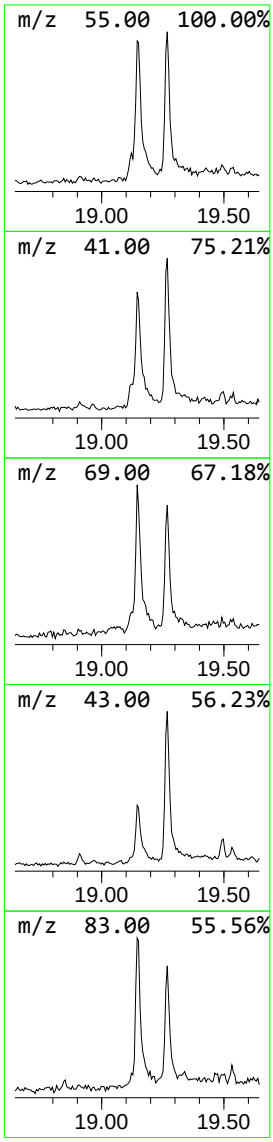
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9-Octadecenoic acid, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.145	6.83 ng/ul	338492	Phenanthrene-d10	17.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	94
2	9-Octadecenoic acid	282	C18H34O2	002027-47-6	93
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	92
4	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	87
5	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	86





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM030524.MA.M
Quant Title : SVOA CALIBRATION

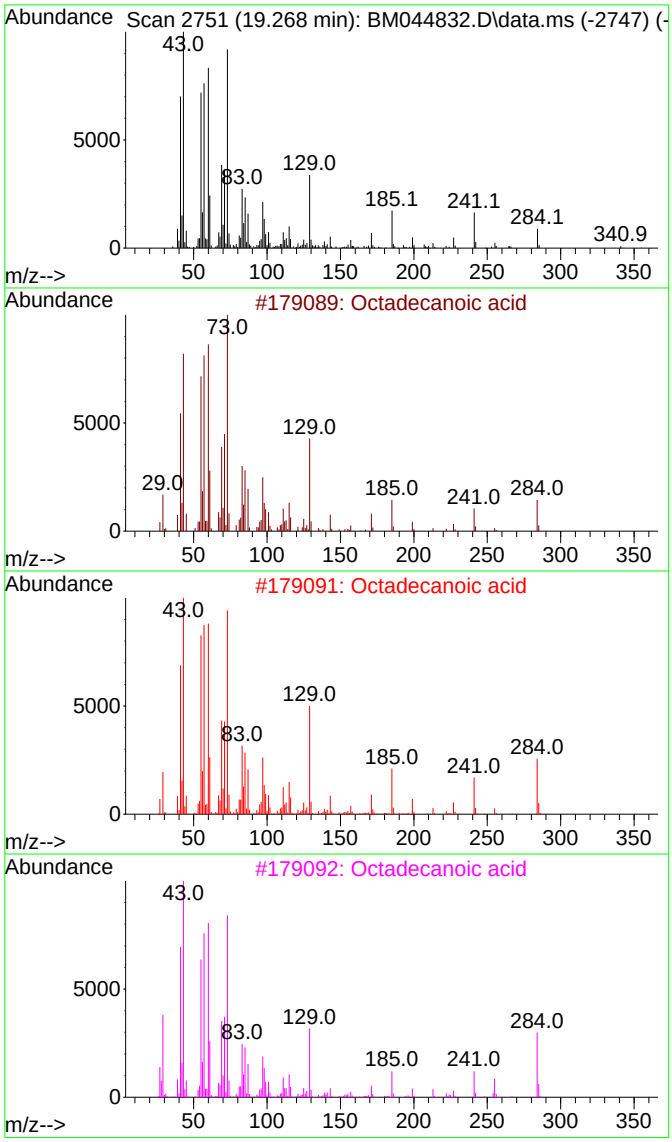
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

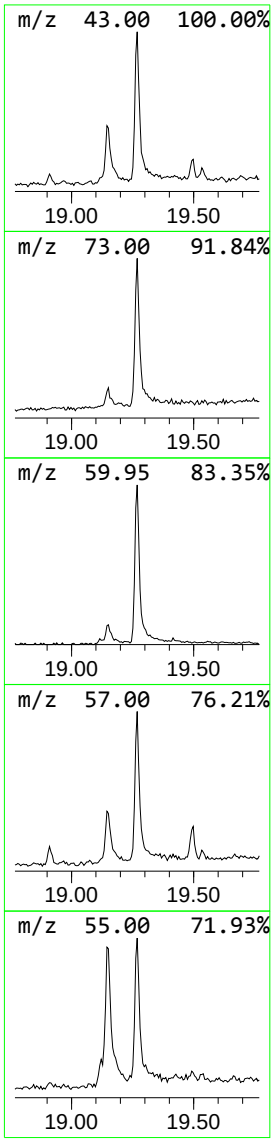
****

Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.268	7.38 ng/ul	396146	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	98
3	Octadecanoic acid	284	C18H36O2	000057-11-4	95
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033024\
Data File : BM044832.D
Acq On : 30 Mar 2024 15:03
Operator : MA/JU
Sample : P1887-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0798

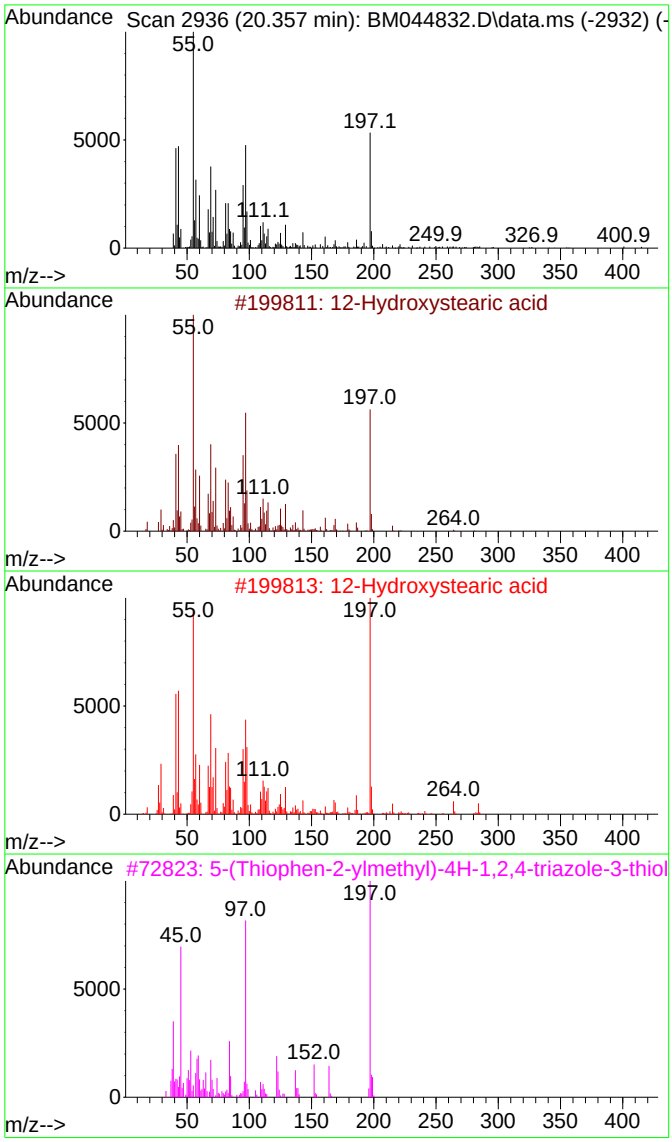
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM030524.MA.M
Quant Title : SVOA CALIBRATION

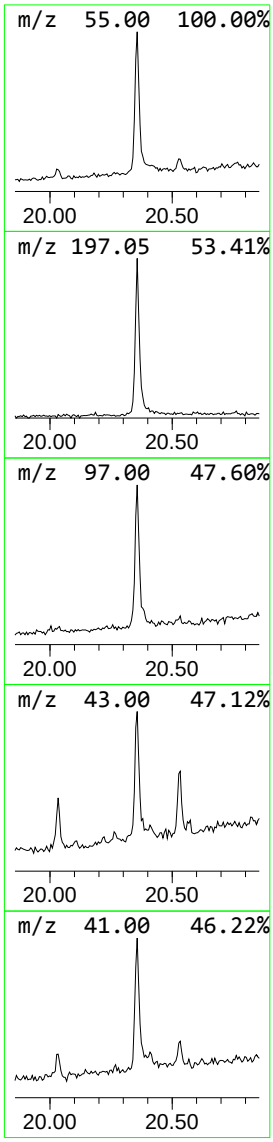
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 12-Hydroxystearic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.357	7.09 ng/ul	380226	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	91
2	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	58
3	5-(Thiophen-2-ylmethyl)-4H-1,2,4...	197	C7H7N3S2	1000409-63-8	35
4	5-Methoxy-2-nitrobenzoic acid	197	C8H7NO5	001882-69-5	27
5	Tetradecanoic acid, 2-oxo-, ethy...	270	C16H30O3	160941-13-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033024\
Data File : BM044832.D
Acq On : 30 Mar 2024 15:03
Operator : MA/JU
Sample : P1887-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0798

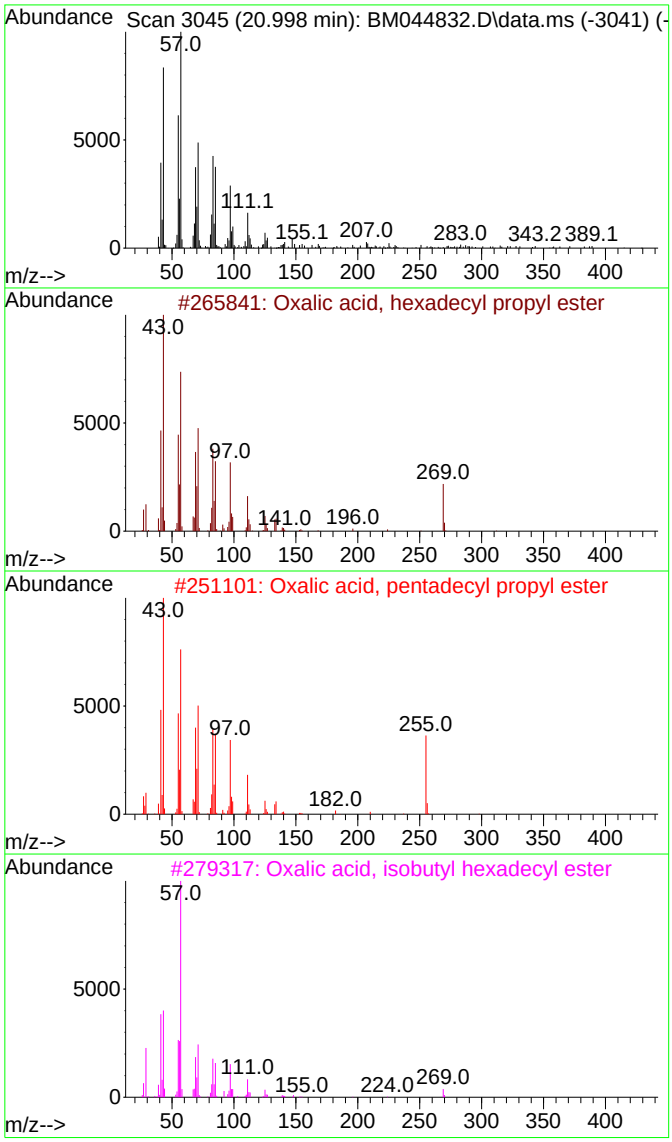
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM030524.MA.M
Quant Title : SVOA CALIBRATION

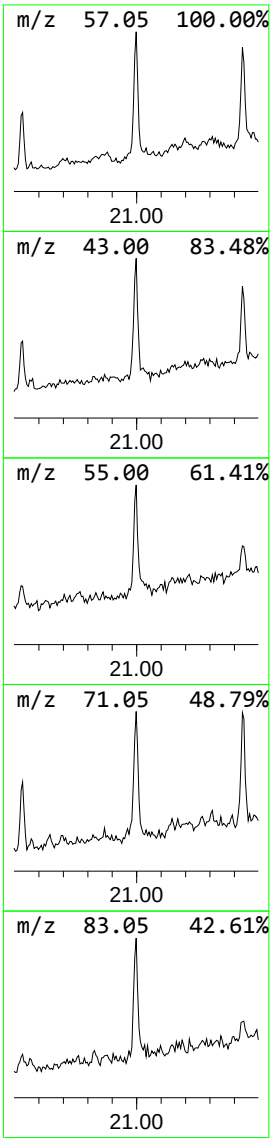
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Oxalic acid, hexadecyl prop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.998	3.58 ng/ul	192323	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
2	Oxalic acid, pentadecyl propyl e...	342	C20H38O4	1000309-26-8	91
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
4	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87
5	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM033024\
Data File : BM044832.D
Acq On : 30 Mar 2024 15:03
Operator : MA/JU
Sample : P1887-05
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
E0798

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM030524.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
unknown-01	3.734	2.6	ng/ul	73122	1	7.669	554837	20.0
n-Hexadecanoic ...	17.974	5.9	ng/ul	293139	4	17.069	991691	20.0
9-Octadecenoic ...	19.145	6.8	ng/ul	338492	4	17.069	991691	20.0
Octadecanoic acid	19.268	7.4	ng/ul	396146	5	21.268	1072940	20.0
12-Hydroxystear...	20.357	7.1	ng/ul	380226	5	21.268	1072940	20.0
Oxalic acid, he...	20.998	3.6	ng/ul	192323	5	21.268	1072940	20.0