LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038166.D
Acq On : 21 Dec 2022 11:33
Operator : CG/JU
Sample : N6014-11
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXS2

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-BM120722.M
Title : SVOA CALIBRATION

Signal : TIC: BM038166.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	32	36	41	rVB	33020	43702	1.52%	0.104%
2	3.834	107	110	130	rBV	325713	540018	18.75%	1.288%
3	4.163	163	166	170	rVB	14985	17200	0.60%	0.041%
4	4.816	275	277	282	rBV5	2945	3469	0.12%	0.008%
5	5.122	325	329	337	rVB4	11061	20013	0.69%	0.048%
6	6.804	611	615	617	rBV5	2008	3670	0.13%	0.009%
7	7.028	648	653	656	rBV7	5337	8248	0.29%	0.020%
8	7.198	676	682	694	rBV	644169	1014761	35.23%	2.420%
9	7.369	703	711	719	rBV	483548	738565	25.64%	1.761%
10	7.569	737	745	754	rBV	670170	1031795	35.82%	2.461%
11	8.040	818	825	832	rBV	695246	1066426	37.02%	2.543%
12	8.098	832	835	840	rVB7	4294	6202	0.22%	0.015%
13	8.316	870	872	877	rVB5	2635	3738	0.13%	0.009%
14	8.751	939	946	957	rBV	780782	1243971	43.19%	2.967%
15	9.216	1017	1025	1033	rBV	616300	1011877	35.13%	2.413%
16	9.369	1043	1051	1056	rVB9	7867	15132	0.53%	0.036%
17	9.598	1083	1090	1096	rVB3	12992	19710	0.68%	0.047%
18	9.804	1123	1125	1130	rVB6	2307	3745	0.13%	0.009%
19	9.939	1137	1148	1159	rBV	520220	861626	29.91%	2.055%
20	10.157	1181	1185	1188	rBV4	3224	4535	0.16%	0.011%
21	10.363	1216	1220	1225	rBV6	4353	8598	0.30%	0.021%
22	10.475	1232	1239	1250	rBV	863466	1386274	48.13%	3.306%
23	10.857	1297	1304	1311	rBV	958386	1574508	54.66%	3.755%
24	10.998	1321	1328	1342	rVV	682266	1161421	40.32%	2.770%
25	11.198	1359	1362	1366	rVB5	3250	4906	0.17%	0.012%
26	11.528	1412	1418	1421	rBV8	3431	5937	0.21%	0.014%
27	11.639	1433	1437	1441	rBV5	4314	7160	0.25%	0.017%
28	12.080	1509	1512	1514	rBV4	3187	3950	0.14%	0.009%
29	12.163	1524	1526	1530	rBV5	2399	3991	0.14%	0.010%
30	12.251	1536	1541	1546	rVB6	6613	10602	0.37%	0.025%
31	12.345	1551	1557	1562	rVB7	3052	7098	0.25%	0.017%
32	12.392	1562	1565	1567	rBV4	4322	4811	0.17%	0.011%
33	12.433	1567	1572	1577	rVV	12945	20837	0.72%	0.050%
34	13.198	1699	1702	1705	rVB4	3177	4437	0.15%	0.011%
35	13.480	1745	1750	1754	rBV	16202	21807	0.76%	0.052%
36	13.604	1767	1771	1772	rVV2	3932	5000	0.17%	0.012%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038166.D
Acq On : 21 Dec 2022 11:33
Operator : CG/JU
Sample : N6014-11
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXS2

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-BM120722.M
Title : SVOA CALIBRATION

37	13.621	1772	1774	1781	rVB7	5417	8983	0.31%	0.021%
38	14.074	1844	1851	1859	rBV	1324694	1833925	63.67%	4.374%
39	14.133	1859	1861	1866	rVB6	4824	5245	0.18%	0.013%
40	14.245	1877	1880	1884	rBV6	2798	3610	0.13%	0.009%
41	14.298	1887	1889	1891	rVV3	4944	4190	0.15%	0.010%
42	14.369	1894	1901	1911	rVB	1585945	2328621	80.84%	5.553%
43	14.545	1925	1931	1936	rVB5	9686	16363	0.57%	0.039%
44	14.668	1946	1952	1961	rVB	1460102	2024952	70.30%	4.829%
45	14.868	1979	1986	1998	rBV	492279	750238	26.05%	1.789%
46	14.980	2002	2005	2009	rVB6	3810	5352	0.19%	0.013%
47	15.027	2009	2013	2016	rBV5	3966	5870	0.20%	0.014%
48	15.068	2016	2020	2027	rVB8	18279	30824	1.07%	0.074%
49	15.327	2061	2064	2067	rVB4	3787	4199	0.15%	0.010%
50	15.421	2077	2080	2082	rBV4	4550	4543	0.16%	0.011%
51	15.439	2082	2083	2088	rVV5	4095	5281	0.18%	0.013%
52	15.492	2088	2092	2096	rVB6	6909	9140	0.32%	0.022%
53	15.615	2107	2113	2114	rBV6	4340	7201	0.25%	0.017%
54	15.657	2114	2120	2129	rVB	2109352	2778135	96.45%	6.625%
55	15.774	2134	2140	2149	rVV	376515	504715	17.52%	1.204%
56	15.892	2157	2160	2166	rVB5	10345	17134	0.59%	0.041%
57	15.980	2173	2175	2176	rBV2	4550	3788	0.13%	0.009%
58	16.015	2176	2181	2188	rVB	248218	335503	11.65%	0.800%
59	16.292	2224	2228	2232	rBV6	2982	4701	0.16%	0.011%
60	16.357	2235	2239	2240	rBV3	7916	9655	0.34%	0.023%
61	16.433	2248	2252	2253	rBV4	5636	6521	0.23%	0.016%
62	16.498	2259	2263	2270	rBV8	12937	24038	0.83%	0.057%
63	16.574	2273	2276	2281	rVB7	15551	21618	0.75%	0.052%
64	16.751	2304	2306	2309	rBV4	3223	3638	0.13%	0.009%
65	16.792	2309	2313	2317	rBV3	20942	29564	1.03%	0.071%
66	16.898	2329	2331	2334	rBV4	4291	5109	0.18%	0.012%
67	17.145	2369	2373	2377	rBV6	8978	15468	0.54%	0.037%
68	17.286	2393	2397	2404	rBV2	42843	66582	2.31%	0.159%
69	17.351	2404	2408	2411	rVV5	22535	30683	1.07%	0.073%
70	17.409	2412	2418	2427	rVV	1626067	2275030	78.98%	5.426%
71	17.504	2427	2434	2441	rVV	1975996	2813409	97.67%	6.710%
72	17.562	2441	2444	2447	rVV5	16393	21778	0.76%	0.052%
73	17.604	2447	2451	2456	rVB8	12876	19915	0.69%	0.047%
74	17.745	2471	2475	2478	rBV6	14124	20998	0.73%	0.050%
75	17.774	2478	2480	2485	rVB5	10263	15981	0.55%	0.038%
76	17.921	2502	2505	2510	rVB6	12940	17636	0.61%	0.042%

LSC Area Percent Report

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Acq On : 21 Dec 2022 11:33
Operator : CG/JU
Sample : N6014-11
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXS2

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
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Title : SVOA CALIBRATION

77	18.021	2518	2522	2526	rBV7	8306	15922	0.55%	0.038%
78	18.062	2526	2529	2532	rVB5	13565	16764	0.58%	0.040%
79	18.168	2540	2547	2553	rBV3	35093	74290	2.58%	0.177%
80	18.227	2553	2557	2562	rBV3	49899	78472	2.72%	0.187%
81	18.286	2562	2567	2577	rBV	797508	1116372	38.76%	2.662%
82	18.586	2612	2618	2623	rBV9	25620	52359	1.82%	0.125%
83	18.704	2634	2638	2642	rBV	56661	66684	2.32%	0.159%
84	18.951	2677	2680	2682	rBV4	11810	11308	0.39%	0.027%
85	19.198	2719	2722	2725	rBV3	15212	18510	0.64%	0.044%
86	19.356	2745	2749	2754	rVB3	34779	45389	1.58%	0.108%
87	19.409	2754	2758	2760	rBV	94734	124233	4.31%	0.296%
88	19.433	2760	2762	2765	rVV2	32381	39641	1.38%	0.095%
89	19.551	2778	2782	2793	rBV	280335	416326	14.45%	0.993%
90	19.792	2817	2823	2834	rVB	2210719	2880415	100.00%	6.869%
91	20.303	2908	2910	2915	rVB2	47403	45242	1.57%	0.108%
92	20.762	2984	2988	2991	rBV	151591	176040	6.11%	0.420%
93	20.797	2991	2994	2997	rVB	63508	69830	2.42%	0.167%
94	21.262	3069	3073	3082	rBV	636278	891580	30.95%	2.126%
95	21.468	3105	3108	3111	rBV	88668	90712	3.15%	0.216%
96	21.574	3121	3126	3131	rBV	1495481	1885479	65.46%	4.497%
97	23.233	3405	3408	3413	rVB	200344	292206	10.14%	0.697%
98	23.868	3509	3516	3532	rVB2	1348651	2702637	93.83%	6.445%
99	24.027	3537	3543	3557	rVB2	954346	1908393	66.25%	4.551%
100	24.609	3637	3642	3652	rVB	454997	932926	32.39%	2.225%

Sum of corrected areas: 41931606

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
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ALS Vial : 34 Sample Multiplier: 1

Instrument :
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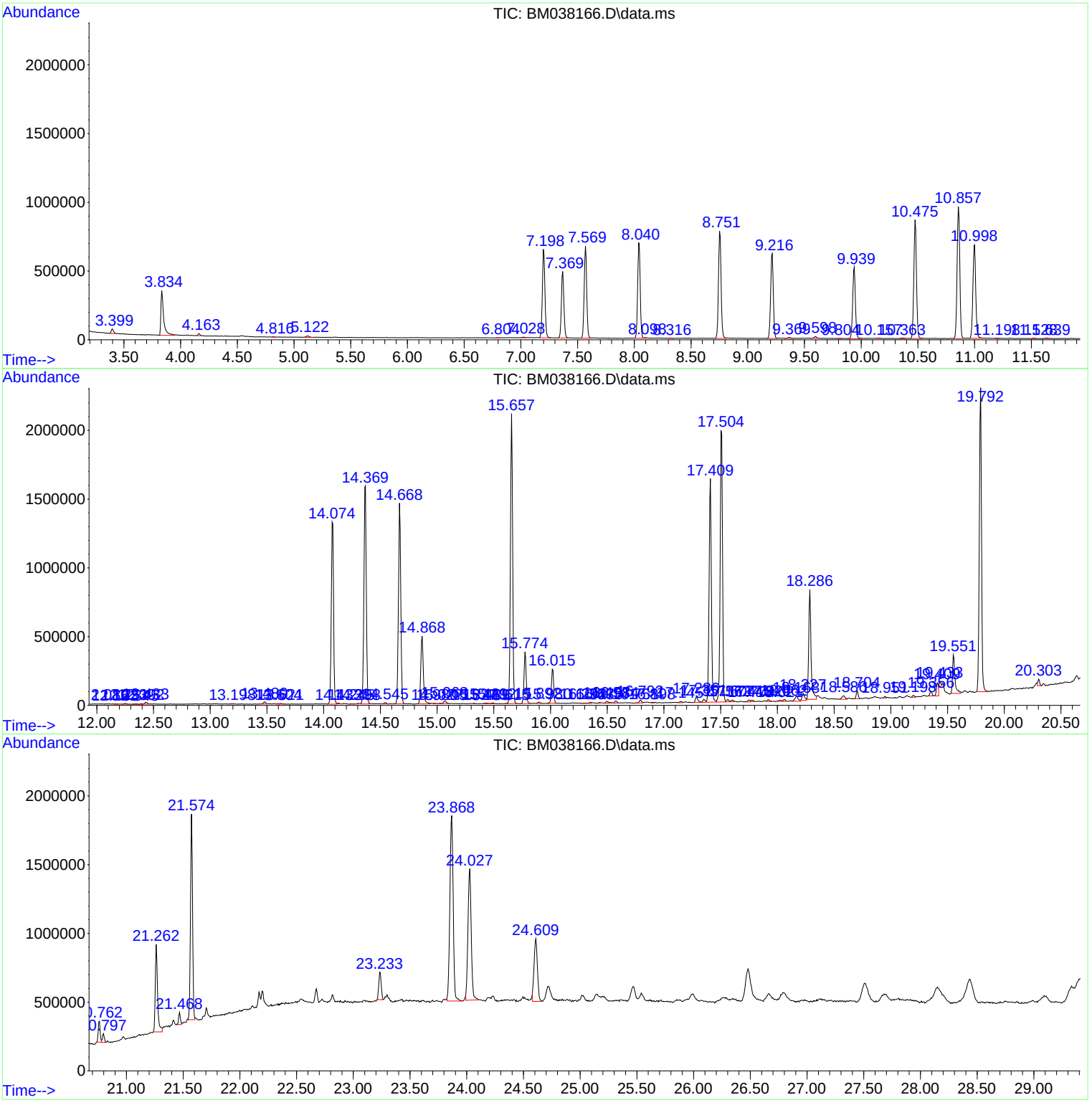
ClientSampleId :
DBXS2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038166.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

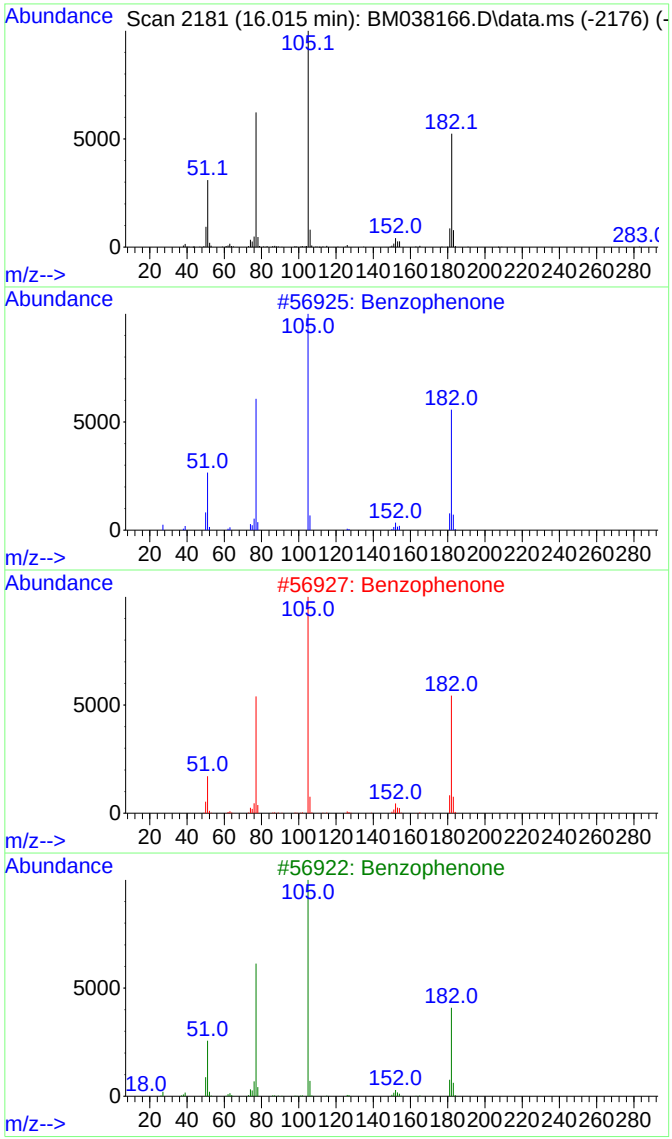
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

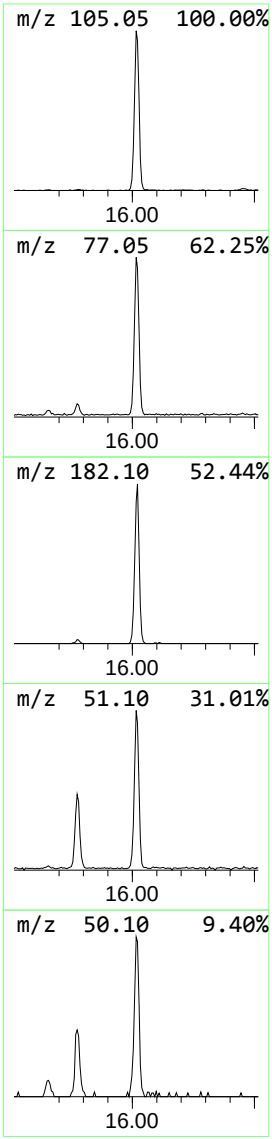
****

Peak Number 1 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	3.31 ng/ul	335503	Acenaphthene-d10	14.669

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
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	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038166.D
Acq On : 21 Dec 2022 11:33
Operator : CG/JU
Sample : N6014-11
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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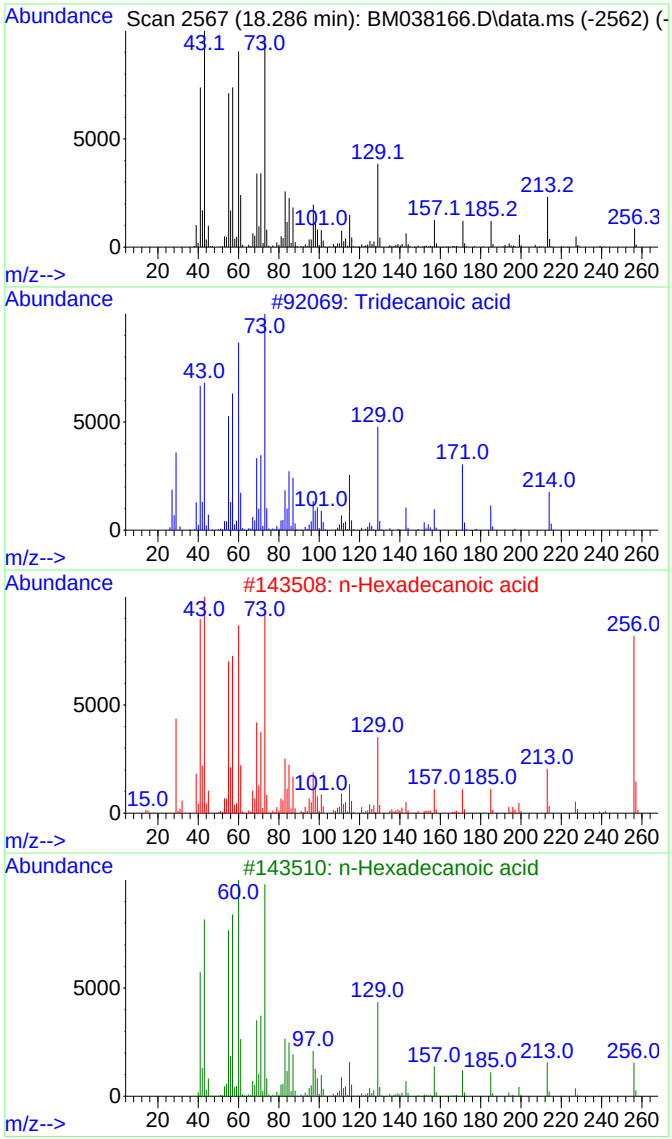
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

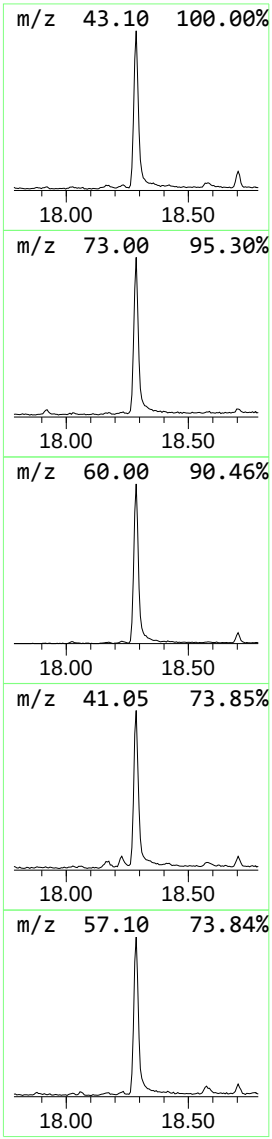
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Tridecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	9.81 ng/ul	1116370	Phenanthrene-d10	17.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Tridecanoic acid	214	C13H26O2	000638-53-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
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ALS Vial : 34 Sample Multiplier: 1

Instrument :
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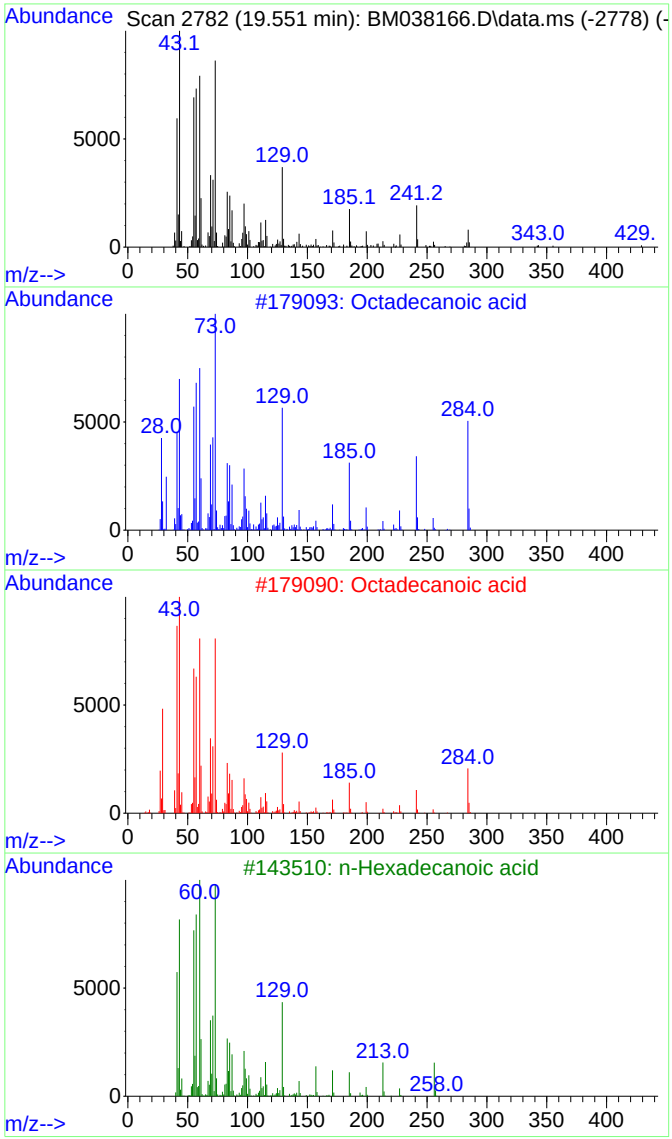
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

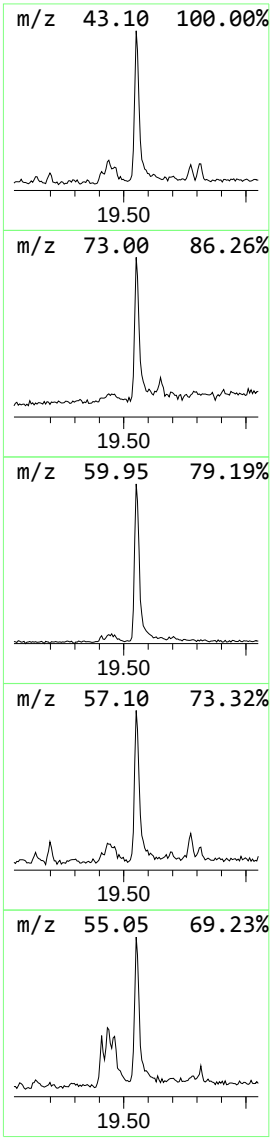
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	4.42 ng/ul	416326	Chrysene-d12	21.574

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	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Octadecanoic acid	284	C18H36O2	000057-11-4	93





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ALS Vial : 34 Sample Multiplier: 1

Instrument :
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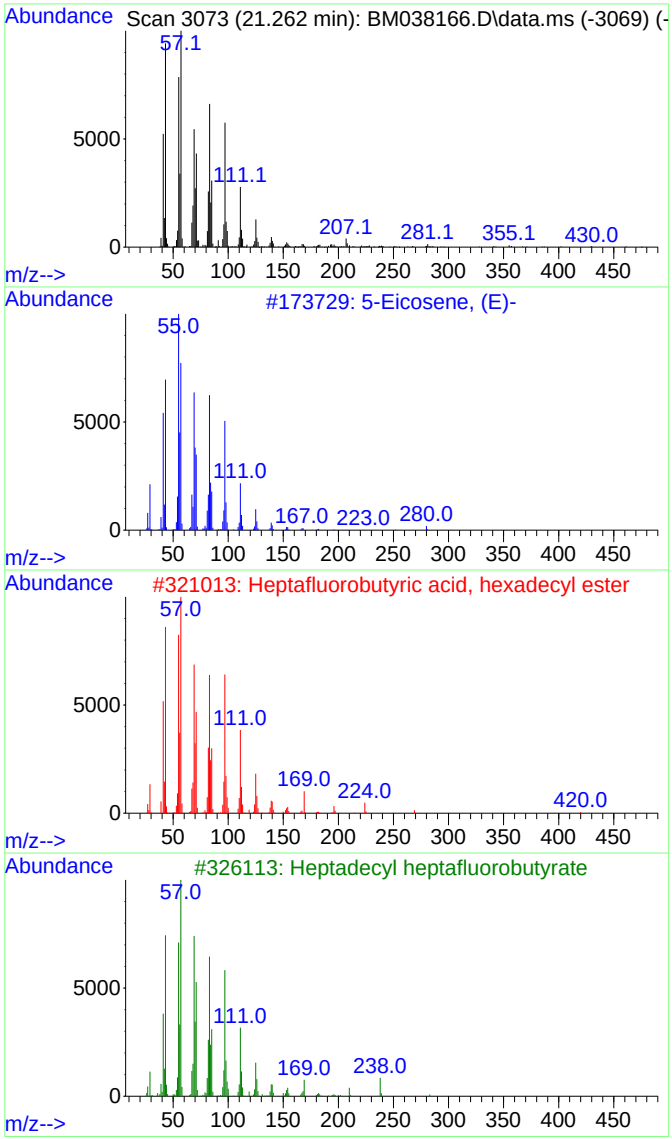
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

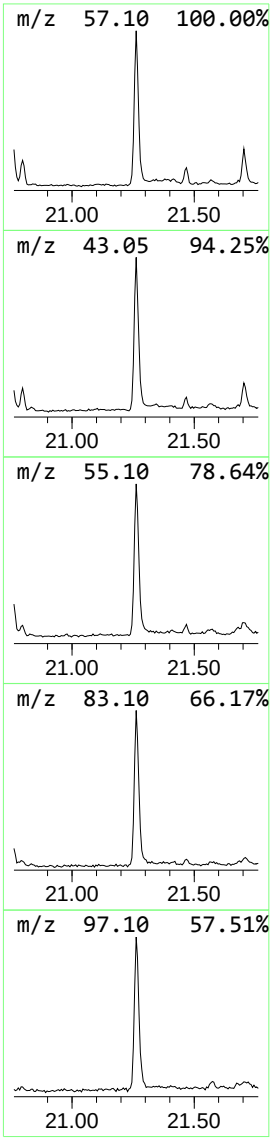
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.262	9.46 ng/ul	891580	Chrysene-d12	21.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	1-Hexacosene	364	C26H52	018835-33-1	94





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Data File : BM038166.D
Acq On : 21 Dec 2022 11:33
Operator : CG/JU
Sample : N6014-11
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXS2

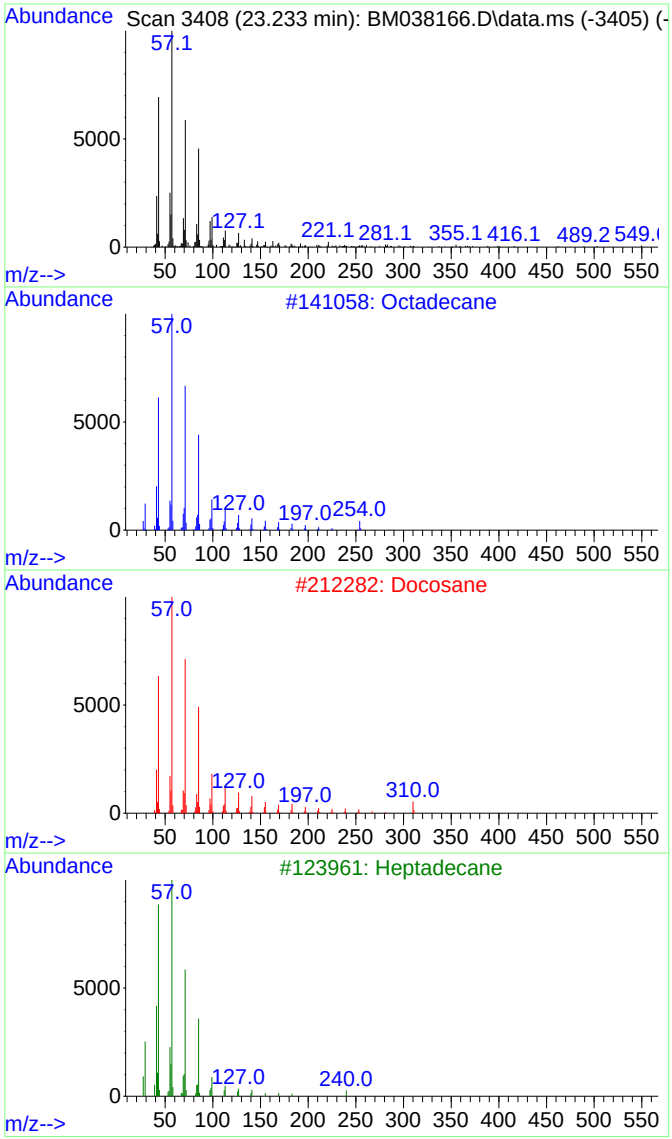
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

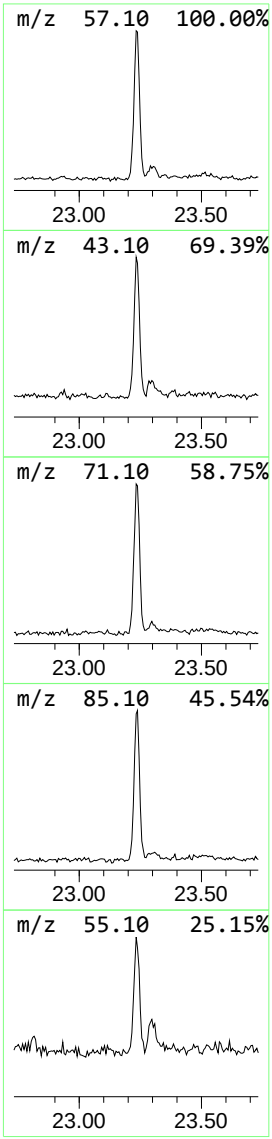
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.233	3.06 ng/ul	292206	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	96
2	Docosane	310	C22H46	000629-97-0	95
3	Heptadecane	240	C17H36	000629-78-7	94
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5	Hexatriacontane	507	C36H74	000630-06-8	90





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Data File : BM038166.D
Acq On : 21 Dec 2022 11:33
Operator : CG/JU
Sample : N6014-11
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXS2

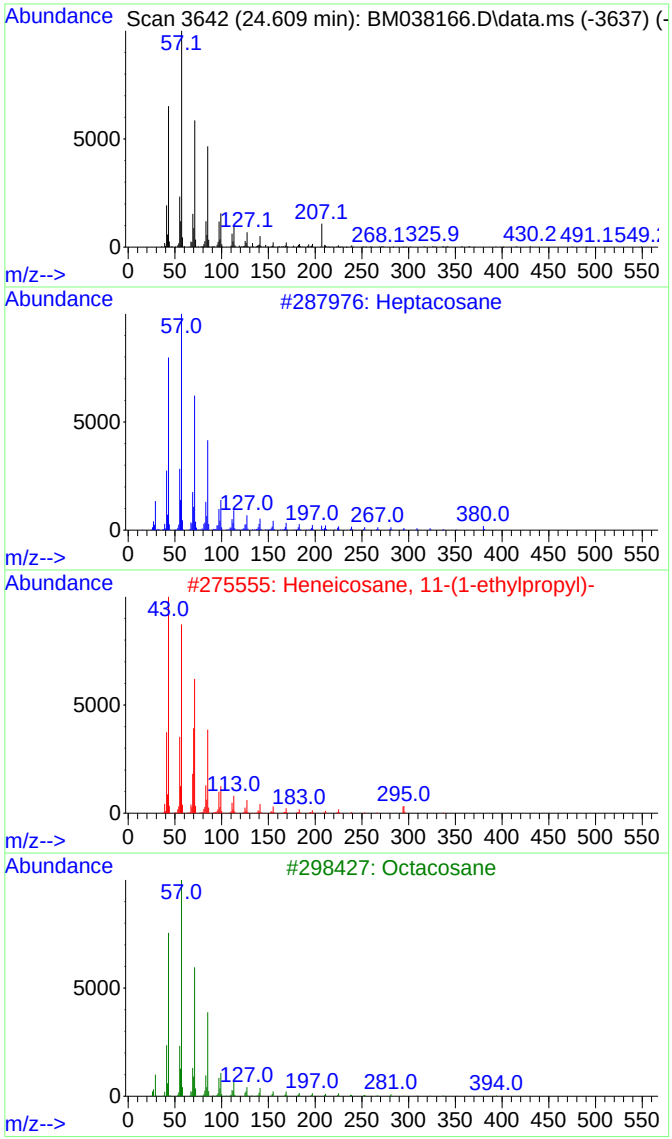
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

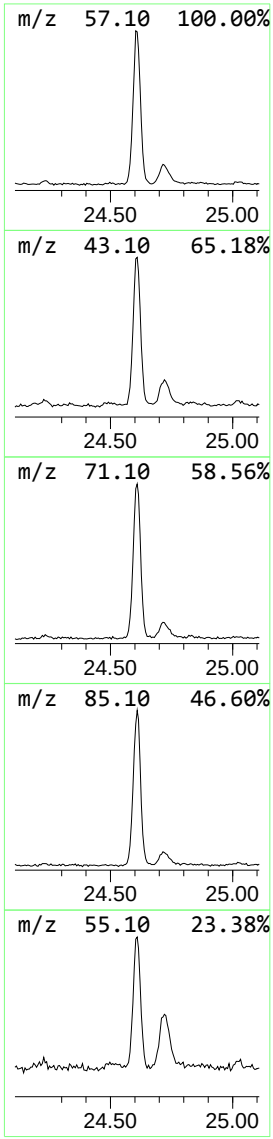
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.609	9.78 ng/ul	932926	Perylene-d12	24.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	83
3	Octacosane	394	C28H58	000630-02-4	83
4	Eicosane	282	C20H42	000112-95-8	83
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038166.D
Acq On : 21 Dec 2022 11:33
Operator : CG/JU
Sample : N6014-11
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXS2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.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
Benzophenone	16.015	3.3	ng/ul	335503	3	14.669	2024950	20.0
Tridecanoic acid	18.286	9.8	ng/ul	1116370	4	17.410	2275030	20.0
Octadecanoic acid	19.551	4.4	ng/ul	416326	5	21.574	1885480	20.0
(DEL) Alkane: S...	21.262	9.5	ng/ul	891580	5	21.574	1885480	20.0
(DEL) Alkane: S...	23.233	3.1	ng/ul	292206	6	24.027	1908390	20.0
(DEL) Alkane: S...	24.609	9.8	ng/ul	932926	6	24.027	1908390	20.0