

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
 Data File : BM038178.D
 Acq On : 21 Dec 2022 18:51
 Operator : CG/JU
 Sample : N6014-19
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DBXS9

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: BM038178.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.393	31	35	44	rVB	37868	59157	1.43%	0.109%
2	3.746	93	95	101	rBV5	2762	4638	0.11%	0.009%
3	3.828	105	109	125	rBV	557836	928891	22.40%	1.715%
4	4.058	144	148	153	rVB7	3647	6740	0.16%	0.012%
5	4.158	162	165	171	rBV	9996	14532	0.35%	0.027%
6	4.540	227	230	235	rVB7	3475	4474	0.11%	0.008%
7	5.116	325	328	334	rVB9	4988	8612	0.21%	0.016%
8	7.204	675	683	693	rVB	801777	1275572	30.75%	2.355%
9	7.369	702	711	720	rBV	593402	905491	21.83%	1.672%
10	7.569	738	745	754	rBV	837187	1283977	30.96%	2.370%
11	8.040	818	825	833	rVV	663201	1039046	25.05%	1.918%
12	8.098	833	835	841	rVB6	3389	4169	0.10%	0.008%
13	8.757	939	947	957	rBV	986987	1598536	38.54%	2.951%
14	9.210	1017	1024	1033	rBV	778316	1283800	30.95%	2.370%
15	9.363	1048	1050	1056	rVB7	5849	7670	0.18%	0.014%
16	9.592	1084	1089	1094	rBV3	6846	10900	0.26%	0.020%
17	9.798	1120	1124	1129	rVB3	4012	7467	0.18%	0.014%
18	9.939	1140	1148	1158	rVB	664462	1103839	26.61%	2.038%
19	10.363	1215	1220	1222	rBV5	3691	6266	0.15%	0.012%
20	10.475	1232	1239	1250	rBV	1114756	1794485	43.27%	3.313%
21	10.857	1296	1304	1312	rVB	927852	1536146	37.04%	2.836%
22	10.934	1312	1317	1321	rBV6	6022	11819	0.28%	0.022%
23	10.998	1321	1328	1341	rVV	1006214	1683866	40.60%	3.108%
24	12.251	1535	1541	1545	rBV7	3313	5884	0.14%	0.011%
25	12.433	1566	1572	1577	rBV2	18610	29765	0.72%	0.055%
26	12.945	1655	1659	1665	rBV6	7454	12278	0.30%	0.023%
27	13.475	1744	1749	1757	rVB6	8080	12972	0.31%	0.024%
28	13.627	1768	1775	1777	rBV8	3689	8922	0.22%	0.016%
29	13.651	1777	1779	1782	rVB4	4789	5076	0.12%	0.009%
30	14.080	1842	1852	1860	rBV	1884467	2550625	61.50%	4.708%
31	14.186	1866	1870	1873	rVB6	4083	5225	0.13%	0.010%
32	14.310	1887	1891	1894	rBV5	3946	7812	0.19%	0.014%
33	14.363	1894	1900	1910	rVB	2090967	3130666	75.48%	5.779%
34	14.545	1924	1931	1937	rVB8	5445	10423	0.25%	0.019%
35	14.669	1945	1952	1959	rBV	1391708	1971213	47.53%	3.639%
36	14.869	1977	1986	1999	rBV	785175	1158270	27.93%	2.138%

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Max Peaks: 100

Stop Thrs : 0

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

37	15.027	2009	2013	2016	rBV6	5131	7309	0.18%	0.013%
38	15.069	2016	2020	2026	rVV6	22429	35439	0.85%	0.065%
39	15.227	2043	2047	2049	rBV5	2991	4550	0.11%	0.008%
40	15.292	2053	2058	2060	rBV6	3668	4955	0.12%	0.009%
41	15.427	2077	2081	2082	rBV4	4126	4628	0.11%	0.009%
42	15.445	2082	2084	2087	rVV4	4759	5978	0.14%	0.011%
43	15.486	2087	2091	2096	rVB6	5303	9000	0.22%	0.017%
44	15.657	2113	2120	2128	rVB	2832468	3827191	92.27%	7.065%
45	15.774	2134	2140	2148	rBV	388797	530103	12.78%	0.979%
46	15.892	2156	2160	2165	rBV5	14407	21511	0.52%	0.040%
47	15.974	2170	2174	2175	rVV4	4124	4346	0.10%	0.008%
48	16.016	2175	2181	2190	rVB	124025	174781	4.21%	0.323%
49	16.186	2207	2210	2215	rBV6	4854	8716	0.21%	0.016%
50	16.233	2215	2218	2221	rVB5	4146	4698	0.11%	0.009%
51	16.357	2234	2239	2244	rBV10	6190	10173	0.25%	0.019%
52	16.427	2247	2251	2252	rBV4	4727	5439	0.13%	0.010%
53	16.574	2272	2276	2280	rVB7	6484	8679	0.21%	0.016%
54	16.663	2286	2291	2294	rBV7	8664	13664	0.33%	0.025%
55	16.792	2308	2313	2319	rBV2	55897	79615	1.92%	0.147%
56	16.845	2319	2322	2327	rVB7	5415	8602	0.21%	0.016%
57	17.080	2358	2362	2366	rBV6	4644	7981	0.19%	0.015%
58	17.145	2370	2373	2377	rVV6	8339	13019	0.31%	0.024%
59	17.192	2379	2381	2389	rVV8	6690	14082	0.34%	0.026%
60	17.257	2389	2392	2394	rVV4	9353	10318	0.25%	0.019%
61	17.286	2394	2397	2405	rVB7	12448	23252	0.56%	0.043%
62	17.351	2405	2408	2411	rBV3	9632	12405	0.30%	0.023%
63	17.410	2411	2418	2426	rVV	1592940	2204247	53.14%	4.069%
64	17.510	2428	2435	2441	rVV	2817338	3836810	92.51%	7.083%
65	17.557	2441	2443	2447	rVV3	28562	40154	0.97%	0.074%
66	17.592	2447	2449	2455	rVB7	18906	25637	0.62%	0.047%
67	17.663	2455	2461	2470	rBV3	32126	71019	1.71%	0.131%
68	17.780	2477	2481	2486	rVB5	11543	19273	0.46%	0.036%
69	17.921	2501	2505	2508	rVB6	8941	11808	0.28%	0.022%
70	18.004	2516	2519	2525	rBV7	11379	15723	0.38%	0.029%
71	18.057	2526	2528	2533	rVB5	9839	11382	0.27%	0.021%
72	18.157	2540	2545	2552	rBV2	67843	119273	2.88%	0.220%
73	18.227	2552	2557	2562	rBV2	40739	62184	1.50%	0.115%
74	18.286	2562	2567	2577	rBV	881358	1193793	28.78%	2.204%
75	18.568	2613	2615	2617	rBV3	9650	10904	0.26%	0.020%
76	18.633	2622	2626	2633	rVV2	33873	54563	1.32%	0.101%

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 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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 Title : SVOA CALIBRATION

77	18.704	2634	2638	2642	rVB	66553	76798	1.85%	0.142%
78	18.892	2667	2670	2675	rVB3	17072	21478	0.52%	0.040%
79	18.945	2677	2679	2683	rVB5	11156	11874	0.29%	0.022%
80	19.357	2742	2749	2754	rBV3	46723	87280	2.10%	0.161%
81	19.433	2754	2762	2774	rBV5	150187	423021	10.20%	0.781%
82	19.557	2778	2783	2796	rBV	2376463	3250288	78.36%	6.000%
83	19.792	2817	2823	2835	rVB	3311951	4147640	100.00%	7.656%
84	20.756	2984	2987	2991	rBV	160154	176730	4.26%	0.326%
85	20.792	2991	2993	2997	rVB3	56640	66549	1.60%	0.123%
86	21.262	3069	3073	3080	rBV	583498	779756	18.80%	1.439%
87	21.574	3121	3126	3132	rVB	1483961	1839832	44.36%	3.396%
88	23.868	3509	3516	3526	rVB2	1791340	3512420	84.68%	6.484%
89	24.027	3537	3543	3551	rVB2	876075	1754444	42.30%	3.239%
90	28.532	4303	4309	4324	rVB5	612841	2007007	48.39%	3.705%

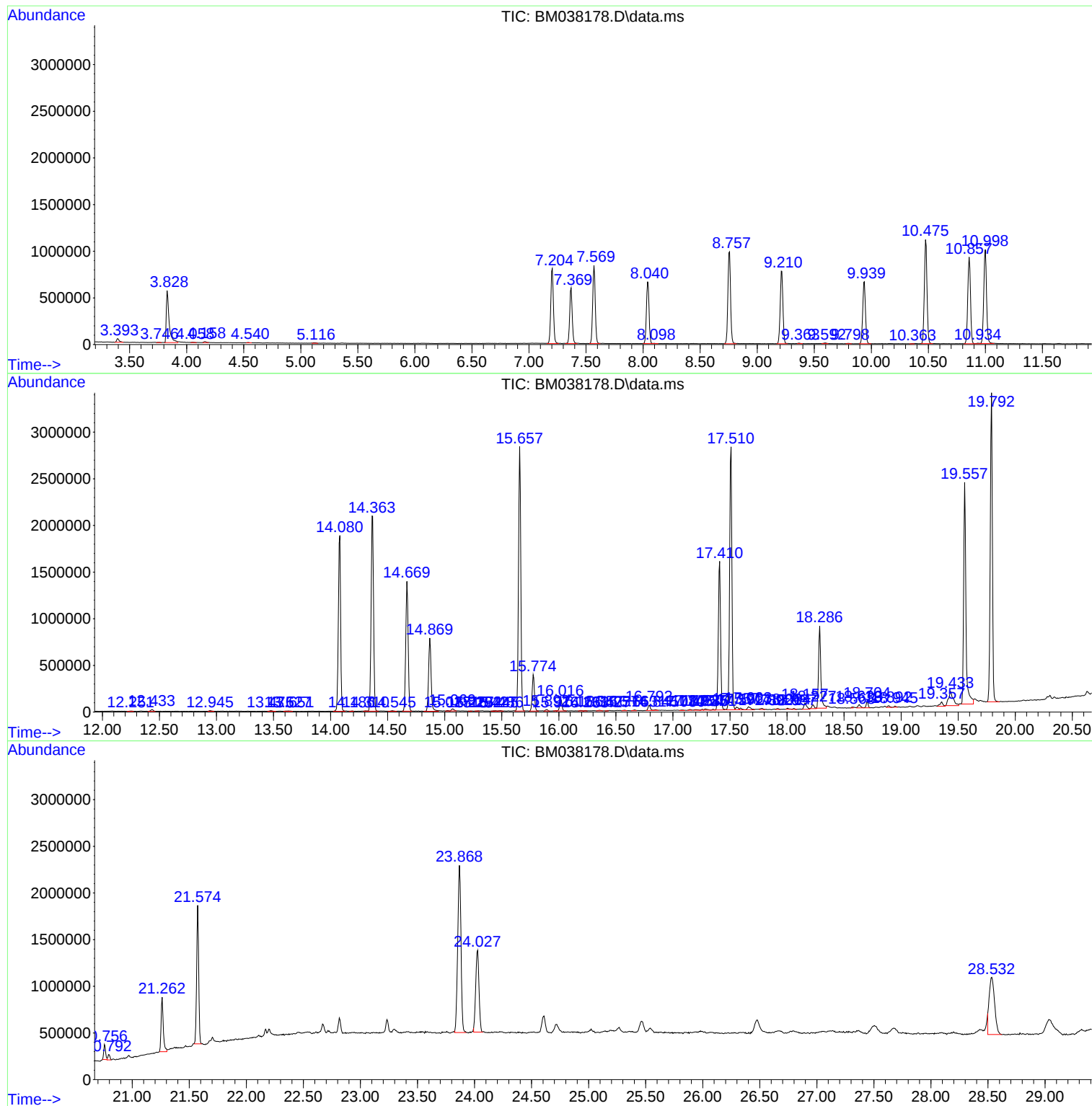
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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



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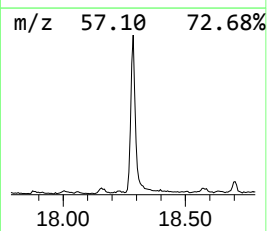
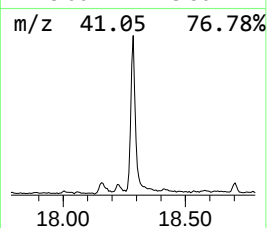
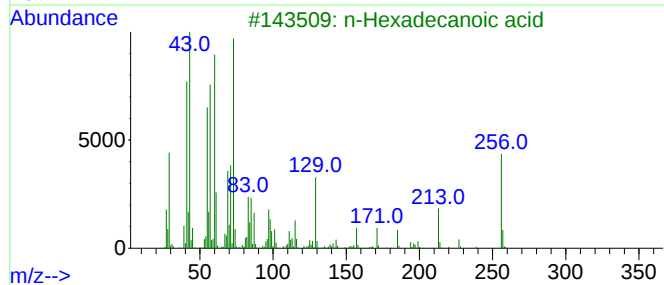
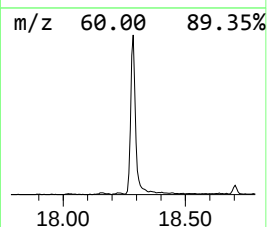
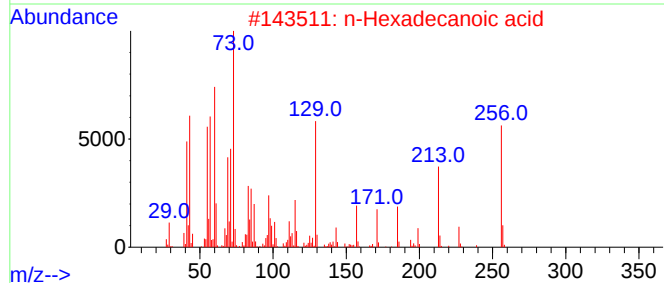
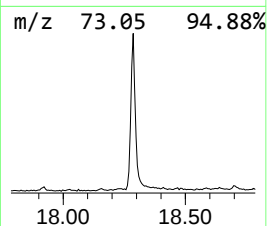
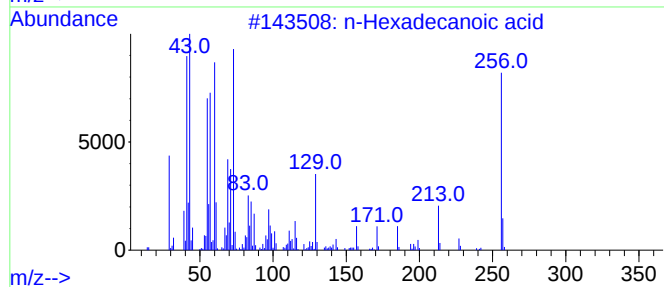
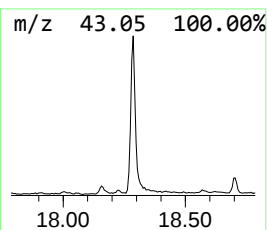
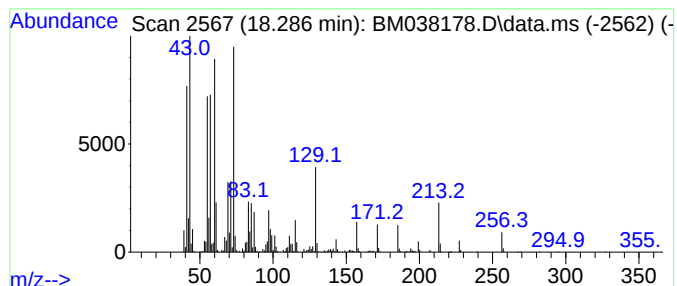
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	10.83 ng/ul	1193790	Phenanthrene-d10	17.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5			Tridecanoic acid	214	C13H26O2	000638-53-9	93



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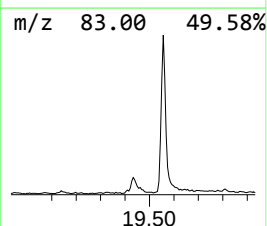
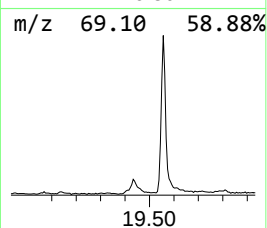
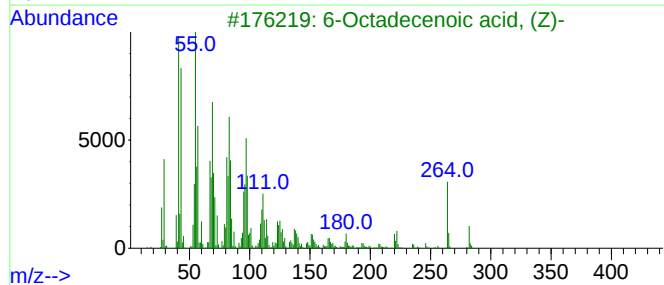
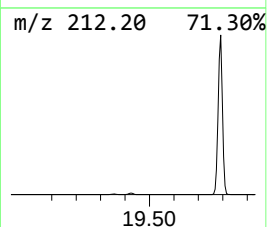
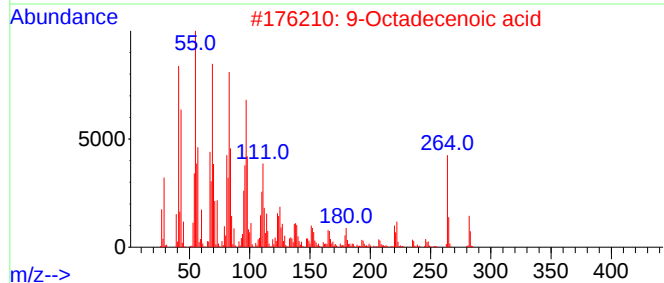
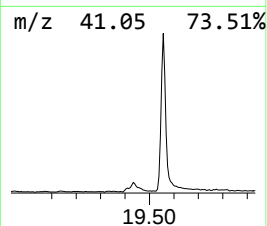
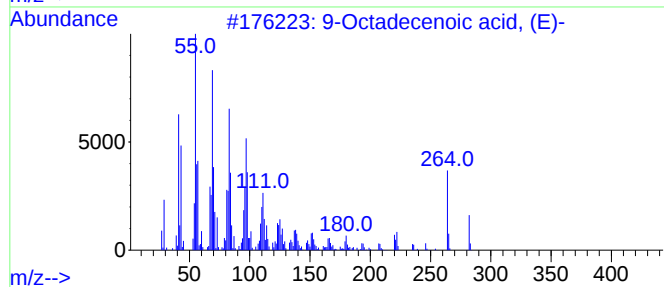
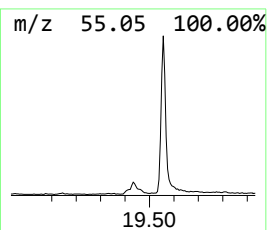
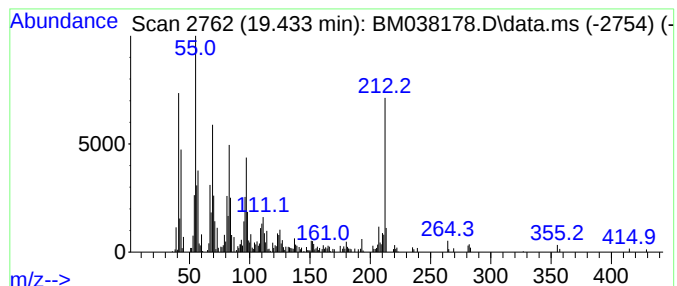
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 9-Octadecenoic acid, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.433	3.84 ng/ul	423021	Phenanthrene-d10		17.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-		282	C18H34O2	000112-79-8	95
2	9-Octadecenoic acid		282	C18H34O2	002027-47-6	91
3	6-Octadecenoic acid, (Z)-		282	C18H34O2	000593-39-5	70
4	cis-Vaccenic acid		282	C18H34O2	000506-17-2	70
5	Oleic Acid		282	C18H34O2	000112-80-1	62



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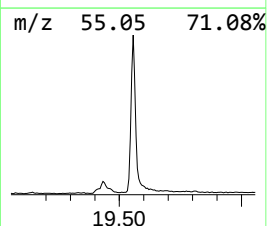
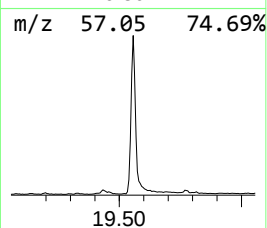
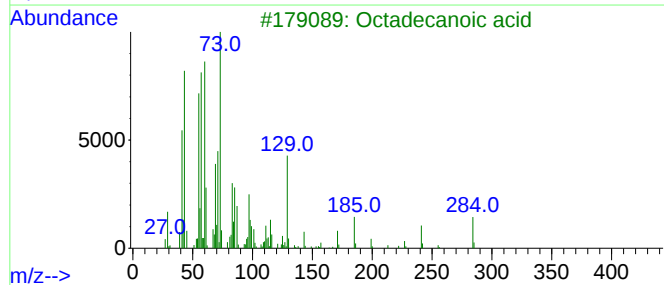
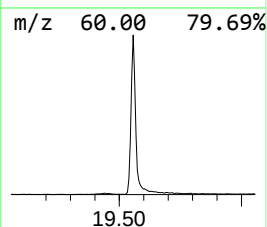
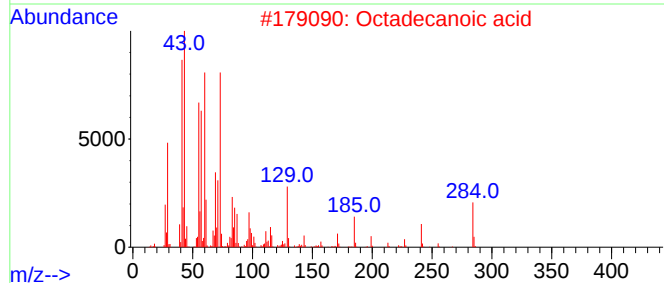
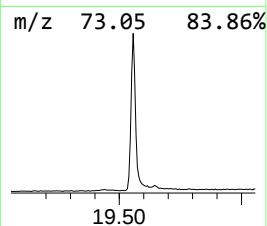
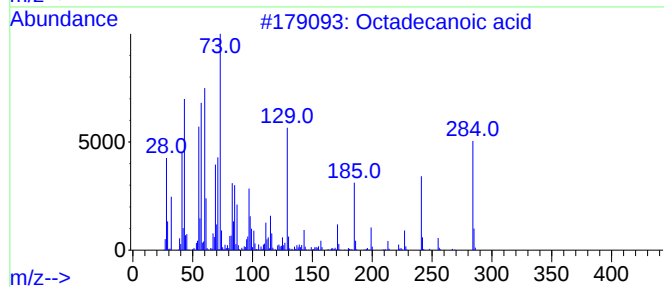
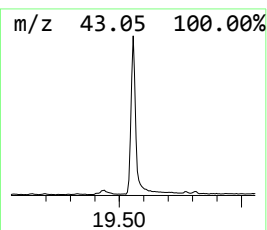
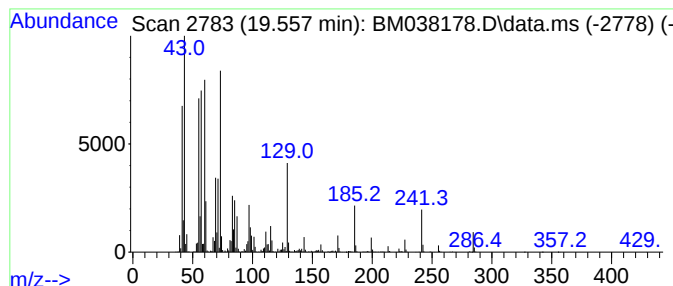
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.557	35.33 ng/ul	3250290	Chrysene-d12	21.574

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	98
4			Octadecanoic acid	284	C18H36O2	000057-11-4	93
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	81



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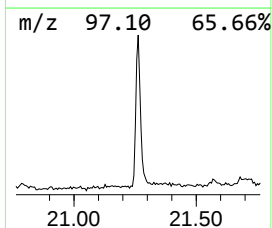
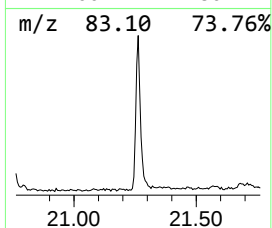
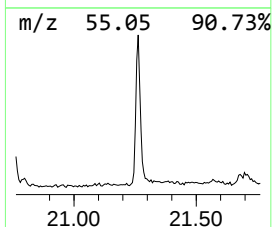
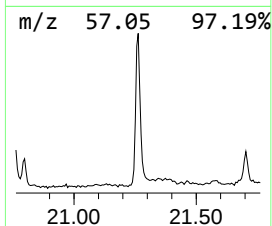
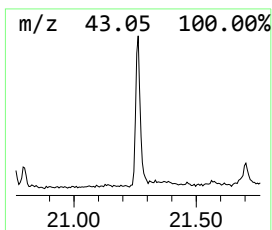
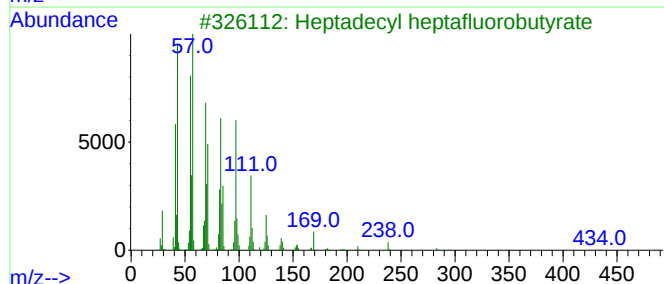
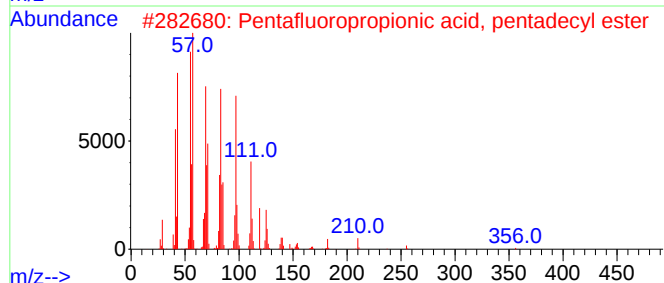
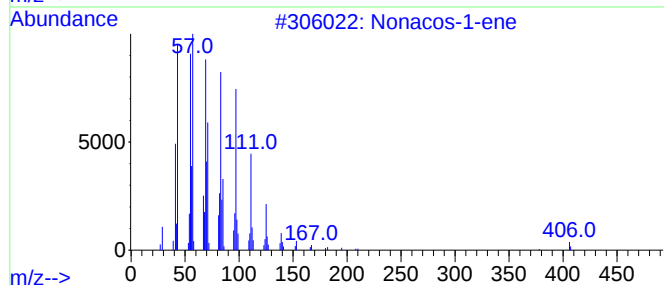
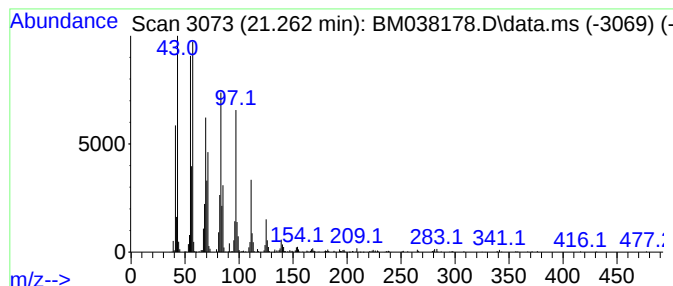
Instrument :
BNA_M
ClientSampleId :
DBXS9

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 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.262	8.48 ng/ul	779756	Chrysene-d12	21.574	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacos-1-ene	406	C29H58	018835-35-3	94
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038178.D
Acq On : 21 Dec 2022 18:51
Operator : CG/JU
Sample : N6014-19
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXS9

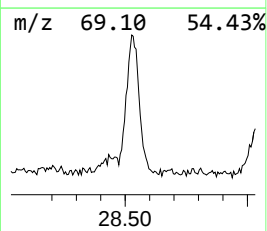
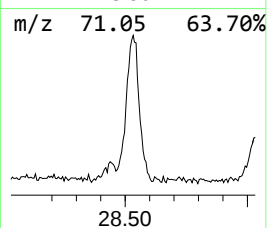
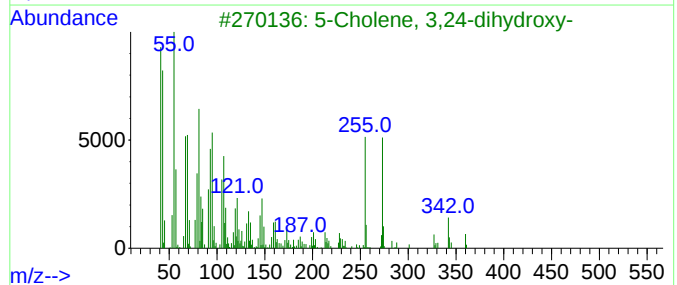
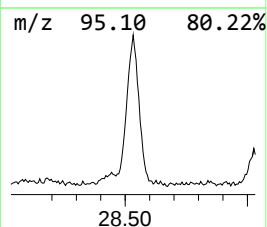
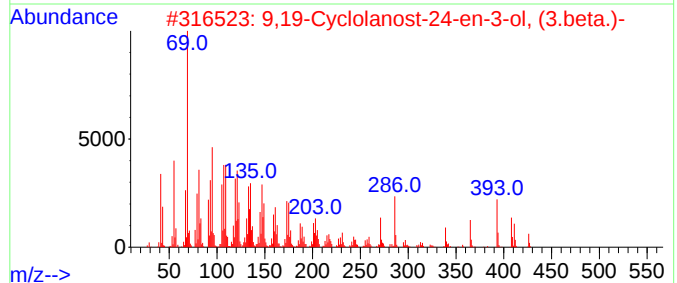
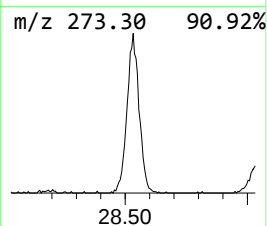
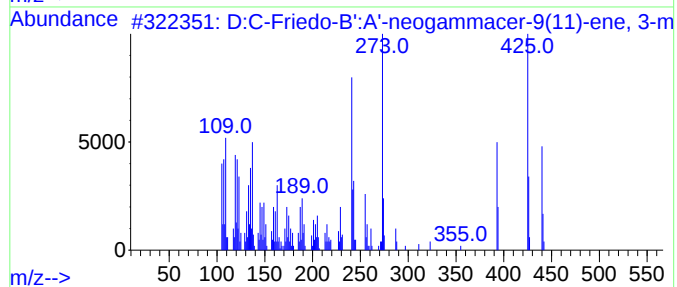
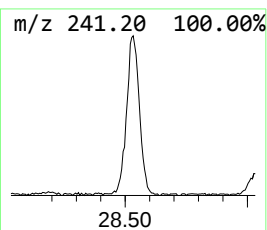
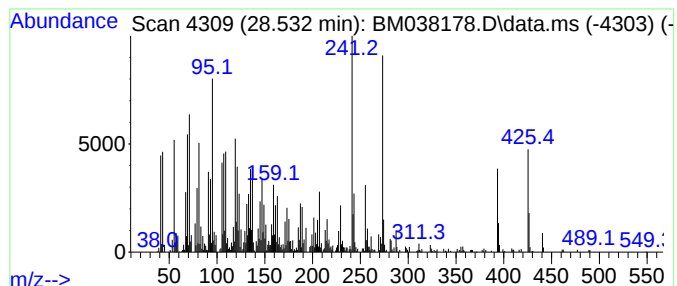
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.532	22.88 ng/ul	2007010	Perylene-d12	24.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	38
2			9,19-Cyclolanost-24-en-3-ol, (3...	426	C30H50O	000469-38-5	27
3			5-Cholene, 3,24-dihydroxy-	360	C24H40O2	1000251-69-2	22
4			1-(4-Methyl-6-chloro-quinolin-2-...	273	C14H12ClN3O	111784-26-0	14
5			9,19-Cyclo-9.beta.-lanostane-3.b...	444	C30H52O2	026525-84-8	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038178.D
Acq On : 21 Dec 2022 18:51
Operator : CG/JU
Sample : N6014-19
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXS9

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.286	10.8	ng/ul	1193790	4	17.410	2204250	20.0
9-Octadecenoic ...	19.433	3.8	ng/ul	423021	4	17.410	2204250	20.0
Octadecanoic acid	19.557	35.3	ng/ul	3250290	5	21.574	1839830	20.0
(DEL) Alkane: S...	21.262	8.5	ng/ul	779756	5	21.574	1839830	20.0
unknown-01	28.532	22.9	ng/ul	2007010	6	24.027	1754440	20.0