

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
 Data File : BM038148.D
 Acq On : 20 Dec 2022 23:29
 Operator : CG/JU
 Sample : N6008-22
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DBXY8

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: BM038148.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	45	rVB	39065	59111	1.00%	0.099%
2	3.834	107	110	124	rBV	269729	476994	8.04%	0.799%
3	5.128	326	330	333	rVB2	8052	11564	0.19%	0.019%
4	7.204	676	683	694	rBV	804859	1279962	21.58%	2.144%
5	7.316	698	702	705	rVV3	5989	7471	0.13%	0.013%
6	7.369	705	711	727	rVB	637630	968861	16.33%	1.623%
7	7.569	738	745	756	rBV	803039	1264603	21.32%	2.118%
8	8.045	819	826	832	rBV	687823	1100598	18.55%	1.844%
9	8.757	940	947	956	rBV	1075156	1691128	28.51%	2.833%
10	9.216	1018	1025	1038	rBV	862531	1372877	23.14%	2.300%
11	9.375	1047	1052	1055	rVB7	5050	6441	0.11%	0.011%
12	9.598	1085	1090	1095	rVB5	8362	10805	0.18%	0.018%
13	9.939	1140	1148	1156	rBV	726797	1170253	19.73%	1.960%
14	10.481	1231	1240	1250	rBV	1191573	1982927	33.43%	3.322%
15	10.857	1297	1304	1311	rBV	998336	1673425	28.21%	2.803%
16	10.910	1311	1313	1317	rVB2	10422	12611	0.21%	0.021%
17	10.998	1321	1328	1343	rBV	839489	1441548	24.30%	2.415%
18	11.322	1379	1383	1389	rBV6	4051	7988	0.13%	0.013%
19	11.633	1433	1436	1442	rBV7	7084	13044	0.22%	0.022%
20	11.863	1471	1475	1485	rVB9	3256	7012	0.12%	0.012%
21	12.092	1506	1514	1518	rBV10	4459	9368	0.16%	0.016%
22	12.251	1537	1541	1547	rBV5	8583	13005	0.22%	0.022%
23	12.433	1567	1572	1578	rBV2	21252	32763	0.55%	0.055%
24	12.510	1581	1585	1588	rVB5	5079	8101	0.14%	0.014%
25	13.057	1673	1678	1681	rBV7	3716	6181	0.10%	0.010%
26	13.480	1744	1750	1754	rBV4	14680	23784	0.40%	0.040%
27	13.522	1754	1757	1759	rVV3	8901	10627	0.18%	0.018%
28	13.557	1759	1763	1767	rVB4	6790	10497	0.18%	0.018%
29	13.657	1773	1780	1784	rVB8	6686	14533	0.24%	0.024%
30	13.992	1833	1837	1843	rBV8	4899	11607	0.20%	0.019%
31	14.080	1843	1852	1860	rBV	2289061	2990418	50.41%	5.009%
32	14.186	1867	1870	1876	rVB7	4784	7659	0.13%	0.013%
33	14.369	1894	1901	1913	rBV	2730050	3885807	65.50%	6.509%
34	14.545	1925	1931	1939	rBV6	12156	18696	0.32%	0.031%
35	14.669	1945	1952	1959	rBV	1539760	2236446	37.70%	3.746%
36	14.869	1980	1986	1997	rBV	824030	1176839	19.84%	1.971%

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

37	14.957	1997	2001	2006	rVV7	7990	15575	0.26%	0.026%
38	15.027	2008	2013	2016	rVV6	9808	17500	0.30%	0.029%
39	15.069	2016	2020	2029	rVB7	22233	39733	0.67%	0.067%
40	15.327	2059	2064	2069	rBV8	4652	7964	0.13%	0.013%

41	15.445	2078	2084	2086	rBV6	5760	8609	0.15%	0.014%
42	15.492	2089	2092	2097	rVB7	9985	12359	0.21%	0.021%
43	15.539	2097	2100	2103	rBV5	4038	6077	0.10%	0.010%
44	15.657	2114	2120	2127	rVB	3409664	4745120	79.99%	7.949%
45	15.774	2134	2140	2149	rBV	838883	1160650	19.57%	1.944%

46	15.892	2153	2160	2165	rBV3	22159	38465	0.65%	0.064%
47	15.980	2171	2175	2177	rBV4	8915	15013	0.25%	0.025%
48	16.021	2177	2182	2192	rVB	127953	183085	3.09%	0.307%
49	16.151	2202	2204	2209	rBV5	3866	6347	0.11%	0.011%
50	16.351	2233	2238	2240	rBV5	17689	25112	0.42%	0.042%

51	16.374	2240	2242	2245	rVB4	16701	18625	0.31%	0.031%
52	16.510	2261	2265	2271	rVB8	8888	17088	0.29%	0.029%
53	16.574	2273	2276	2280	rBV6	6241	9068	0.15%	0.015%
54	16.668	2289	2292	2295	rBV5	4573	6969	0.12%	0.012%
55	16.792	2309	2313	2320	rBV8	20471	34208	0.58%	0.057%

56	16.857	2320	2324	2329	rVB8	8823	12345	0.21%	0.021%
57	17.057	2352	2358	2360	rBV7	9377	17912	0.30%	0.030%
58	17.145	2369	2373	2377	rBV6	9197	16693	0.28%	0.028%
59	17.192	2378	2381	2390	rVB8	16832	31436	0.53%	0.053%
60	17.286	2393	2397	2405	rBV3	28698	54299	0.92%	0.091%

61	17.357	2405	2409	2411	rBV5	14114	19688	0.33%	0.033%
62	17.410	2412	2418	2423	rBV	1870248	2594386	43.73%	4.346%
63	17.451	2423	2425	2428	rVB	40840	42065	0.71%	0.070%
64	17.510	2429	2435	2442	rVV	3574746	4867987	82.06%	8.155%
65	17.686	2461	2465	2469	rBV6	6279	11943	0.20%	0.020%

66	17.745	2473	2475	2479	rVV5	11222	13150	0.22%	0.022%
67	18.162	2542	2546	2553	rBV4	41630	80422	1.36%	0.135%
68	18.227	2553	2557	2562	rBV	56506	87294	1.47%	0.146%
69	18.286	2562	2567	2585	rVV	862235	1293017	21.80%	2.166%
70	18.704	2635	2638	2642	rVB3	31348	37916	0.64%	0.064%

71	19.198	2719	2722	2727	rVB6	25598	33305	0.56%	0.056%
72	19.351	2746	2748	2754	rVB2	47686	59696	1.01%	0.100%
73	19.457	2763	2766	2775	rVB	232629	323133	5.45%	0.541%
74	19.551	2778	2782	2791	rBV	272447	406307	6.85%	0.681%
75	19.792	2817	2823	2834	rBV	4360247	5932159	100.00%	9.937%

76	20.280	2903	2906	2908	rBV3	41030	54489	0.92%	0.091%
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 Title : SVOA CALIBRATION

77	20.304	2908	2910	2914	rVB	73367	79672	1.34%	0.133%
78	20.756	2984	2987	2991	rBV	160442	179748	3.03%	0.301%
79	21.262	3068	3073	3083	rVB	959035	1270574	21.42%	2.128%
80	21.574	3121	3126	3131	rVB	1866872	2385277	40.21%	3.996%
81	21.921	3181	3185	3190	rVB	252838	330098	5.56%	0.553%
82	23.233	3405	3408	3412	rBV	242616	343972	5.80%	0.576%
83	23.868	3509	3516	3523	rBV2	2226745	4224596	71.22%	7.077%
84	24.021	3536	3542	3550	rVB2	997537	1977017	33.33%	3.312%
85	24.515	3620	3626	3635	rVB2	756728	1533119	25.84%	2.568%

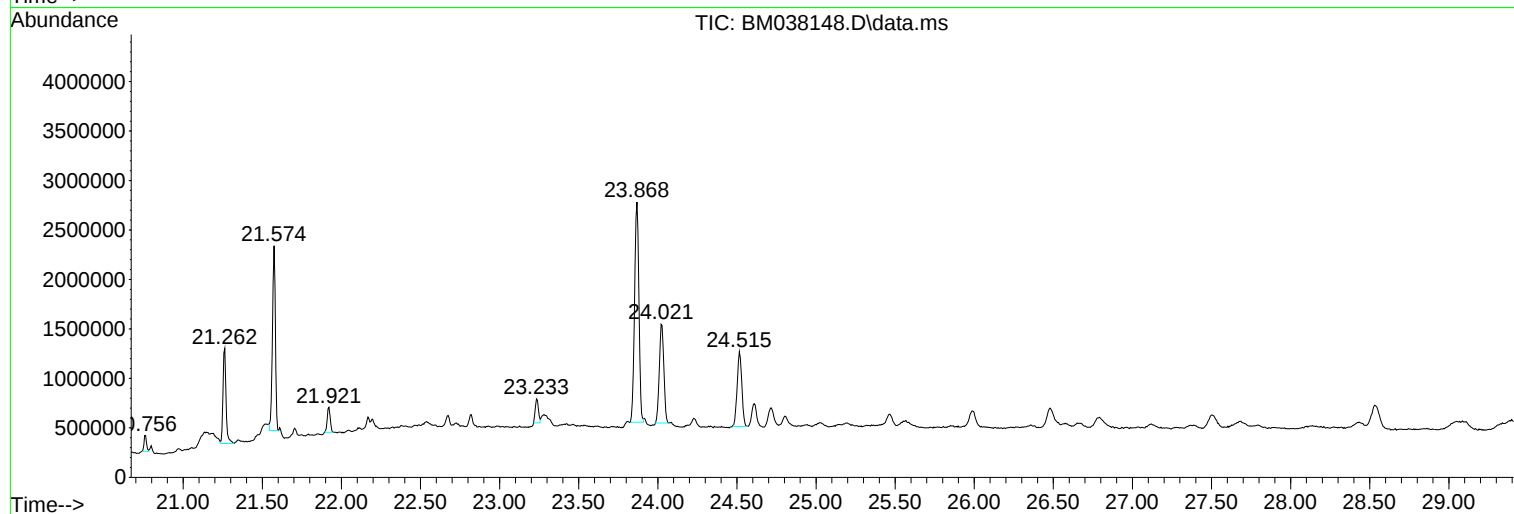
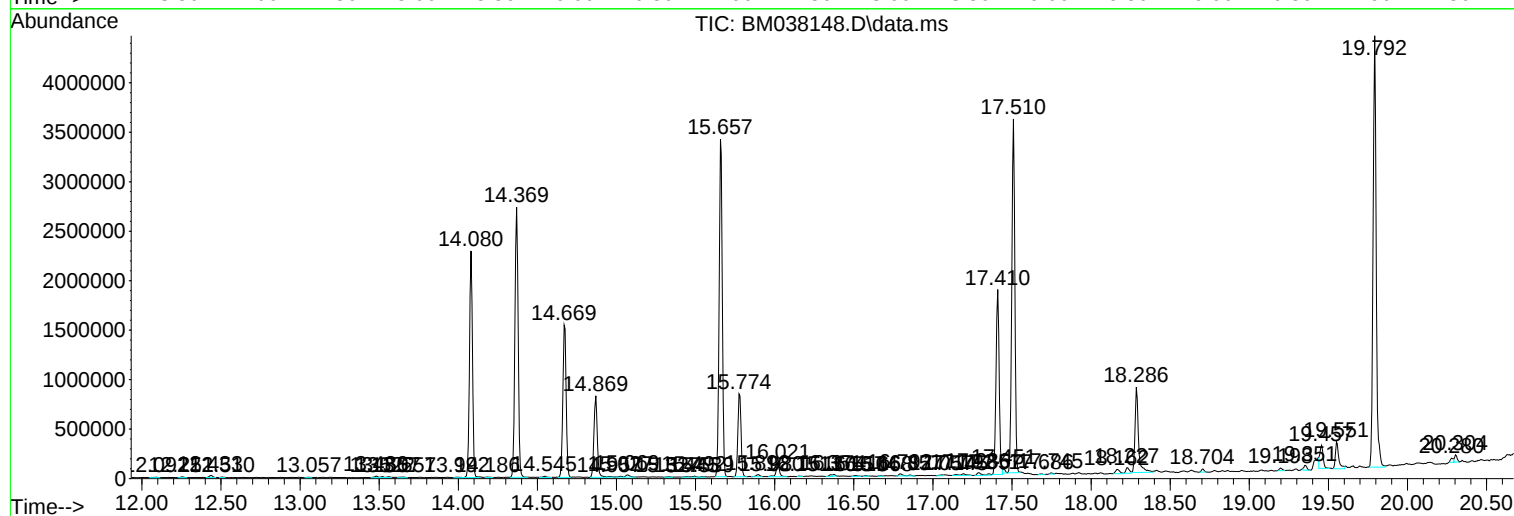
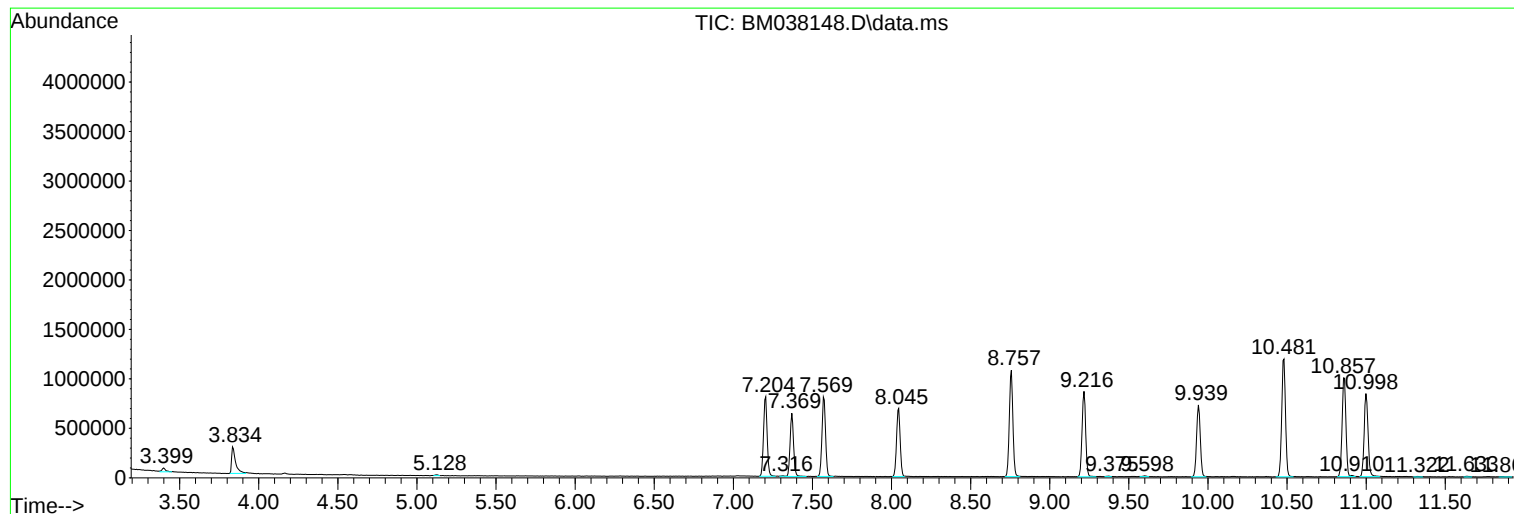
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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



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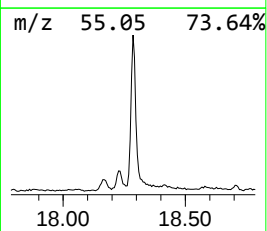
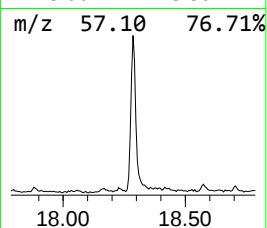
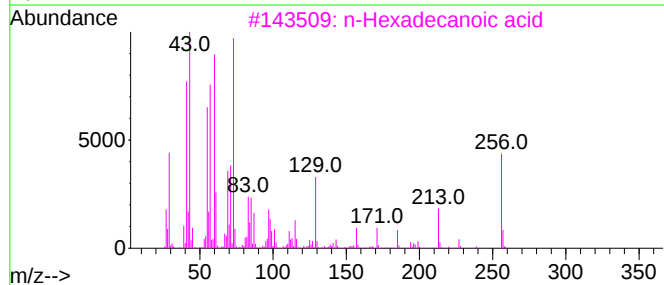
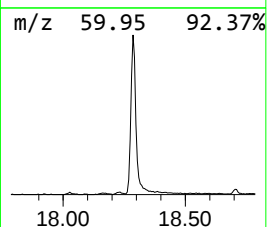
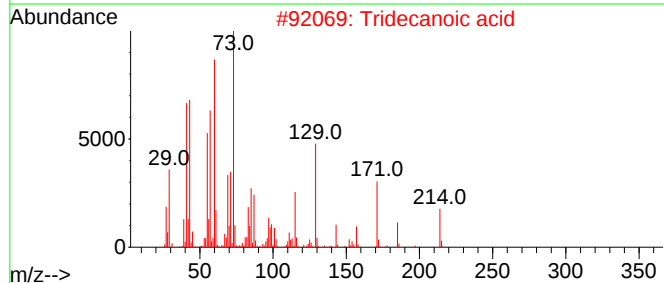
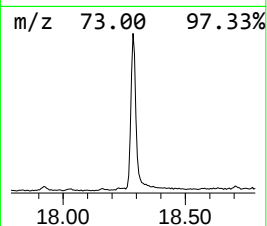
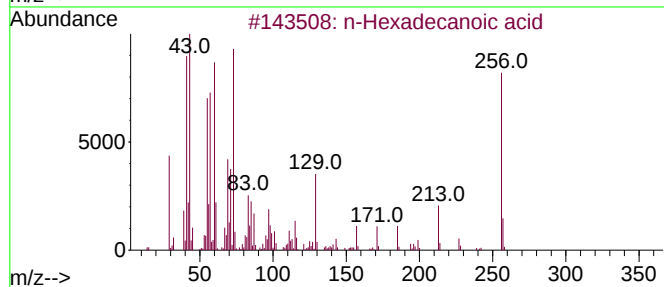
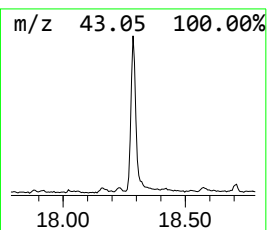
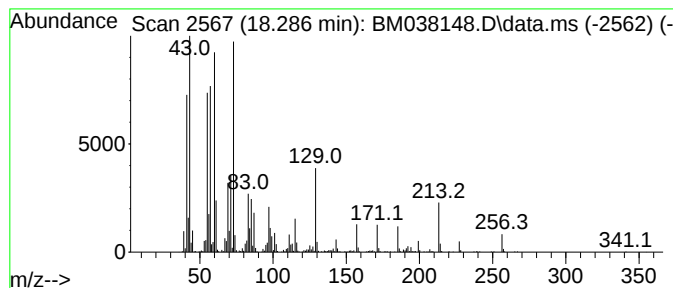
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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	9.97 ng/ul	1293020	Phenanthrene-d10	17.410

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	95
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	91



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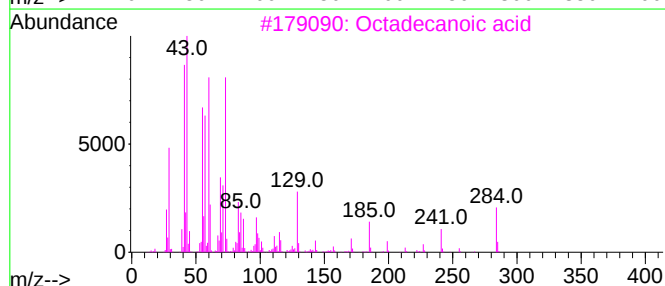
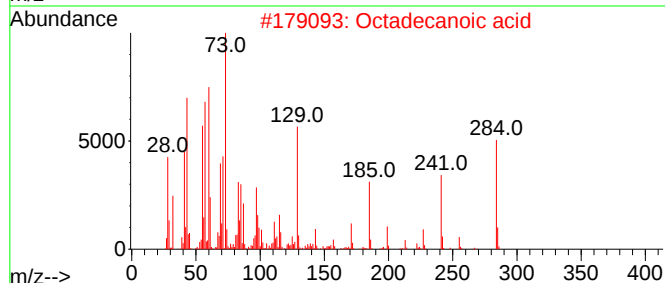
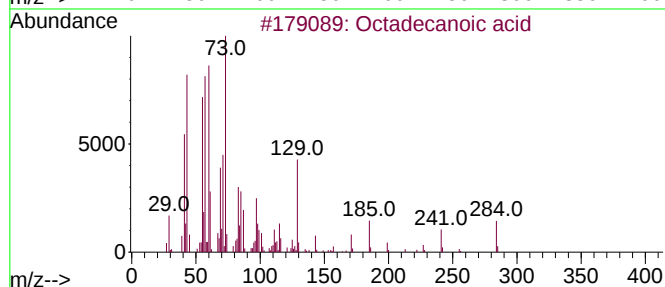
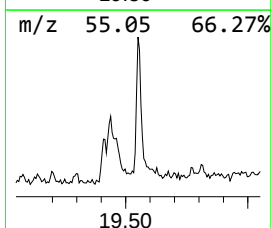
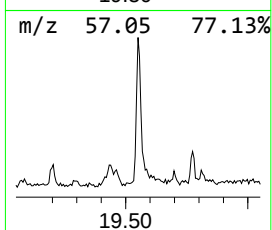
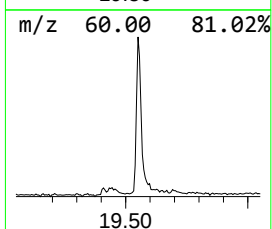
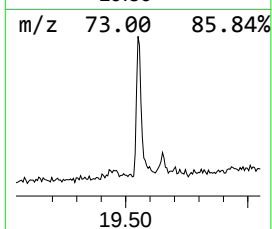
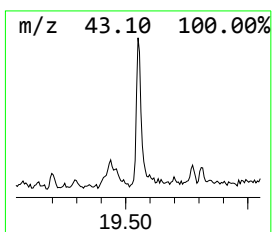
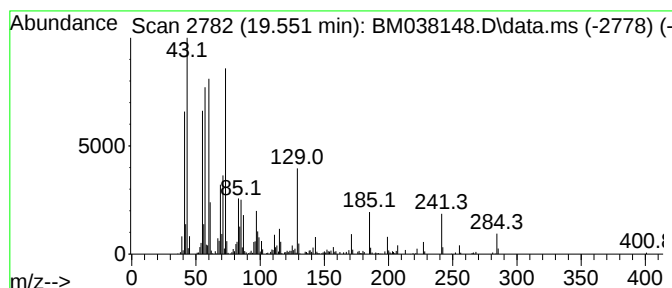
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.551	3.41 ng/ul	406307	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	99
3			Octadecanoic acid	284	C18H36O2	000057-11-4	99
4			Octadecanoic acid	284	C18H36O2	000057-11-4	96
5			Octadecanoic acid	284	C18H36O2	000057-11-4	91



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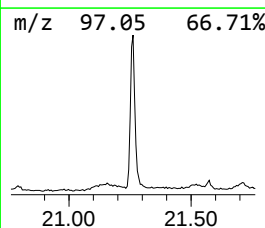
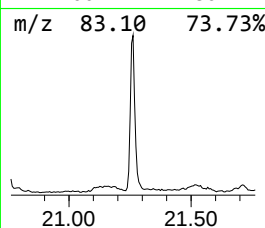
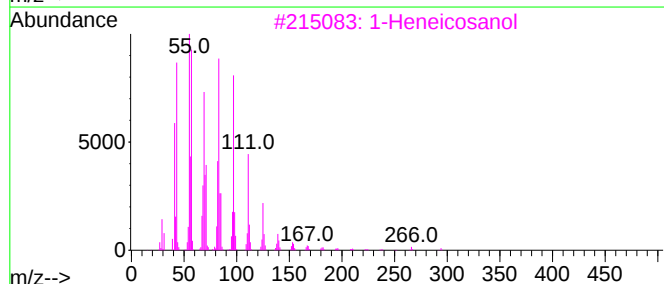
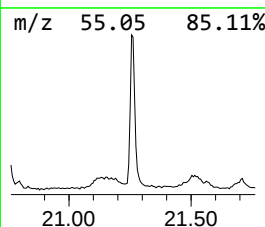
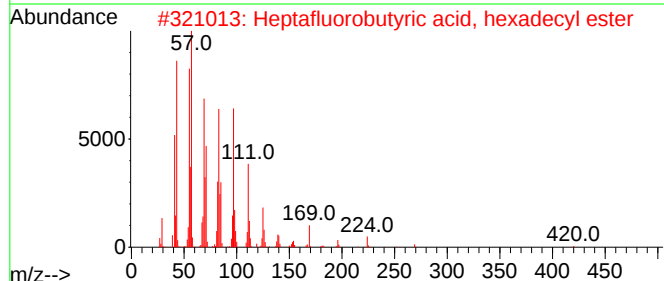
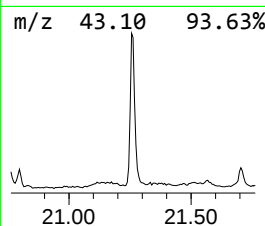
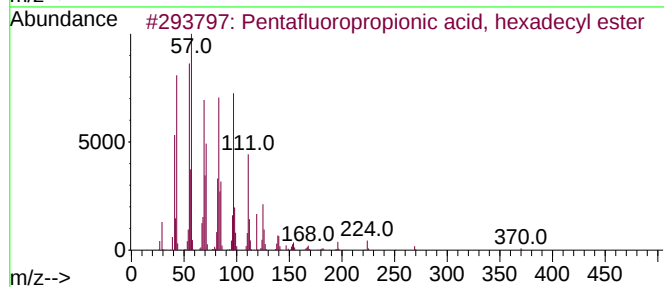
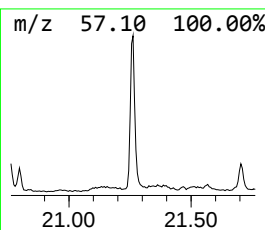
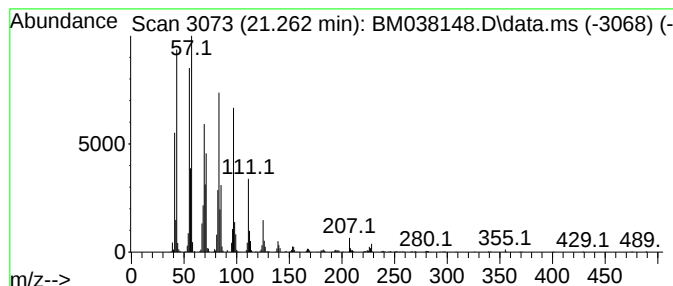
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.262	10.65 ng/ul	1270570	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
2			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



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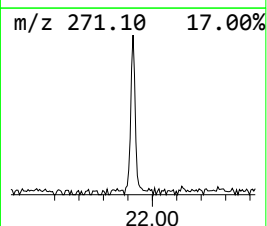
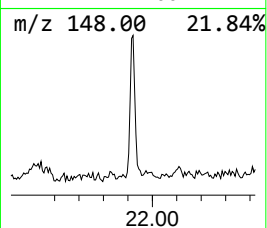
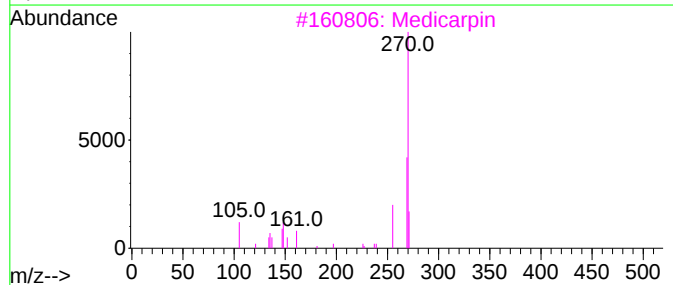
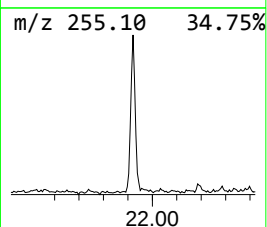
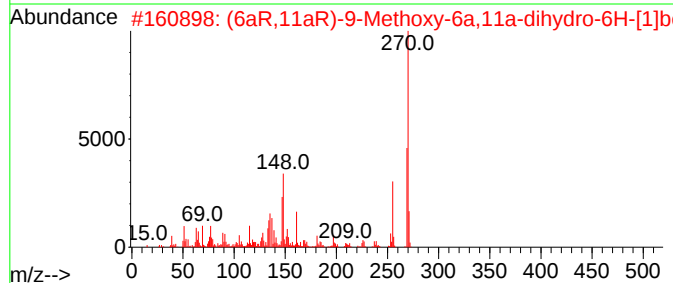
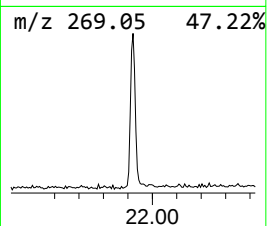
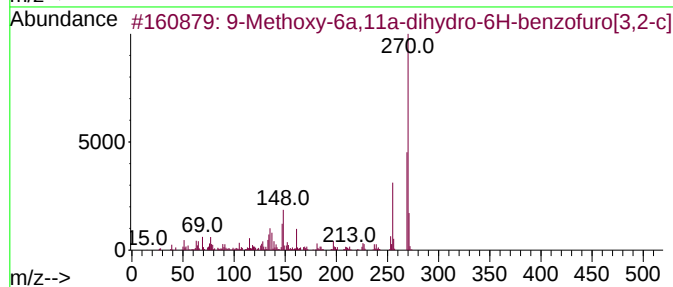
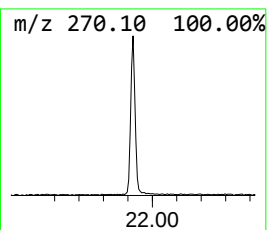
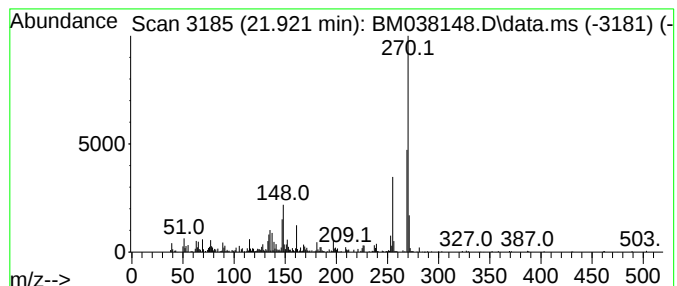
Instrument :
BNA_M
ClientSampleId :
DBXY8

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 9-Methoxy-6a,11a-dihydro-6H... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.921	2.77 ng/ul	330098	Chrysene-d12	21.574	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Methoxy-6a,11a-dihydro-6H-benz...	270	C16H14O4	607363-34-8	99
2	(6aR,11aR)-9-Methoxy-6a,11a-dihy...	270	C16H14O4	033983-40-3	98
3	Medicarpin	270	C16H14O4	032383-76-9	90
4	3-Acetoxy-9-methoxypterocarpan	312	C18H16O5	001891-12-9	68
5	9-Benzylidenexanthene	270	C20H14O	027980-52-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038148.D
Acq On : 20 Dec 2022 23:29
Operator : CG/JU
Sample : N6008-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXY8

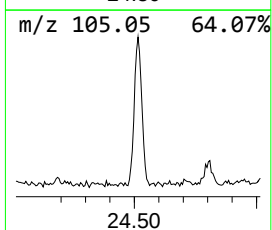
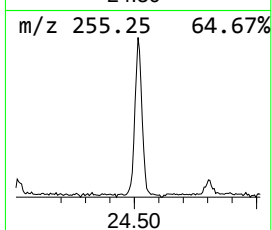
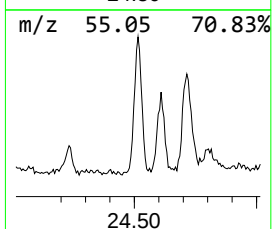
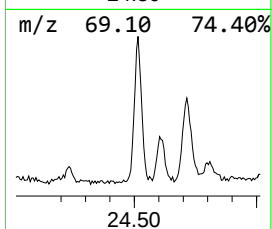
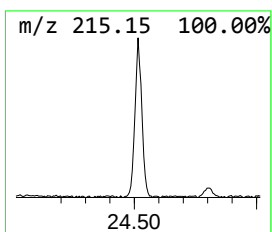
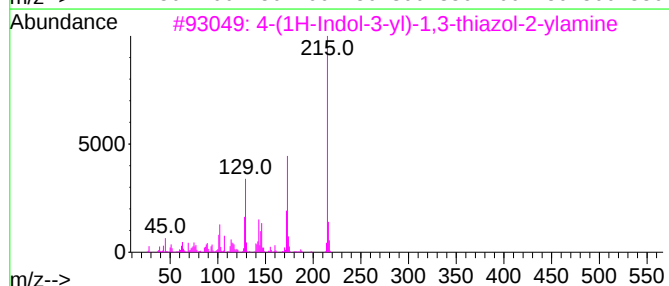
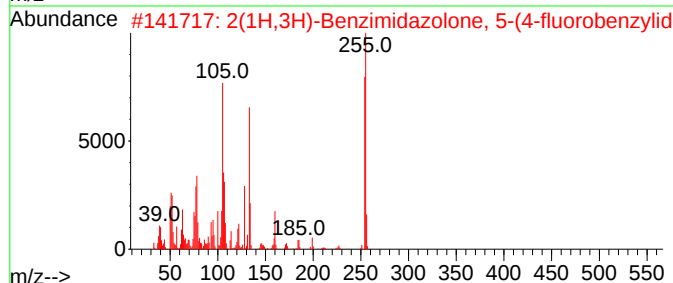
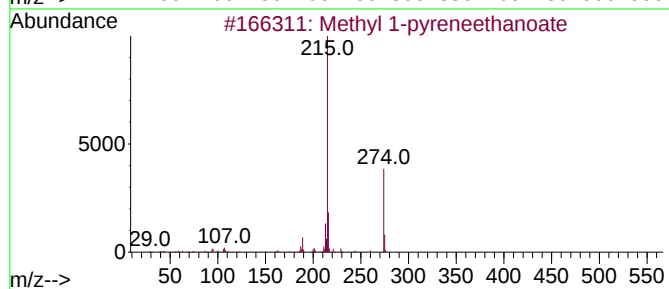
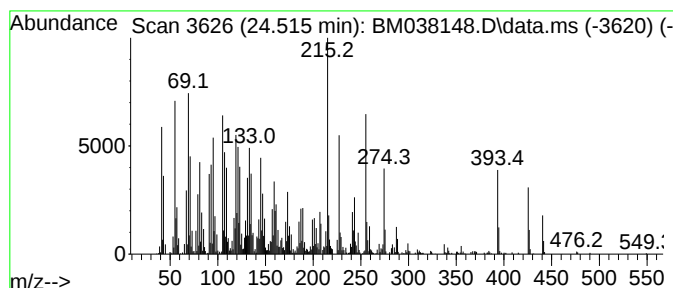
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.515	15.51 ng/ul	1533120	Perylene-d12	24.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 1-pyreneethanoate	274	C19H14O2	073654-19-0	35
2			2(1H,3H)-Benzimidazolone, 5-(4-f...	255	C14H10FN3O	332352-27-9	25
3			4-(1H-Indol-3-yl)-1,3-thiazol-2-...	215	C11H9N3S	022258-56-6	15
4			Indanidine	215	C11H13N5	085392-79-6	15
5			3-Imidazo[2,1-b][1,3]thiazol-6-y...	215	C11H9N3S	861206-26-0	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
Data File : BM038148.D
Acq On : 20 Dec 2022 23:29
Operator : CG/JU
Sample : N6008-22
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DBXY8

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.286	10.0	ng/ul	1293020	4	17.410	2594390	20.0
Octadecanoic acid	19.551	3.4	ng/ul	406307	5	21.574	2385280	20.0
Pentafluoroprop...	21.262	10.7	ng/ul	1270570	5	21.574	2385280	20.0
9-Methoxy-6a,11...	21.921	2.8	ng/ul	330098	5	21.574	2385280	20.0
unknown-01	24.515	15.5	ng/ul	1533120	6	24.027	1977020	20.0