

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122022\
 Data File : BM038149.D
 Acq On : 21 Dec 2022 00:06
 Operator : CG/JU
 Sample : N6008-11
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DBXW9

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: BM038149.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	43	rBV	41699	58423	0.41%	0.091%
2	3.834	106	110	125	rBV	502507	895702	6.27%	1.390%
3	5.122	324	329	336	rVB2	16941	28293	0.20%	0.044%
4	7.204	676	683	692	rVB	806231	1257822	8.81%	1.952%
5	7.369	705	711	725	rVB	607250	920553	6.45%	1.428%
6	7.569	739	745	753	rBV	808980	1251610	8.77%	1.942%
7	8.045	819	826	832	rBV	628128	998587	6.99%	1.550%
8	8.757	940	947	956	rBV	982238	1556483	10.90%	2.415%
9	9.216	1018	1025	1037	rBV	786576	1247587	8.74%	1.936%
10	9.363	1046	1050	1057	rVB5	10441	17744	0.12%	0.028%
11	9.939	1140	1148	1158	rBV	669059	1073011	7.51%	1.665%
12	10.480	1231	1240	1247	rBV	1059762	1759136	12.32%	2.730%
13	10.857	1297	1304	1316	rBV	924538	1530701	10.72%	2.375%
14	10.998	1320	1328	1340	rBV	890144	1510227	10.58%	2.343%
15	11.639	1431	1437	1443	rBV7	10619	21073	0.15%	0.033%
16	12.433	1568	1572	1577	rBV2	17163	27109	0.19%	0.042%
17	14.080	1843	1852	1860	rBV	1823046	2421670	16.96%	3.758%
18	14.368	1894	1901	1909	rVB	2250225	3070404	21.50%	4.764%
19	14.545	1924	1931	1935	rBV8	8375	14671	0.10%	0.023%
20	14.668	1946	1952	1961	rBV	1410559	2054011	14.39%	3.187%
21	14.868	1979	1986	2000	rBV	799043	1160847	8.13%	1.801%
22	15.068	2016	2020	2028	rVV4	25224	38220	0.27%	0.059%
23	15.657	2114	2120	2127	rVB	2740690	3698070	25.90%	5.738%
24	15.780	2135	2141	2149	rBV	703547	977440	6.85%	1.517%
25	15.892	2156	2160	2166	rVB4	15044	23501	0.16%	0.036%
26	15.986	2168	2176	2178	rBV6	11666	20475	0.14%	0.032%
27	16.021	2178	2182	2186	rVB	33574	43825	0.31%	0.068%
28	16.798	2308	2314	2319	rBV5	34341	57136	0.40%	0.089%
29	17.286	2393	2397	2406	rBV5	26165	43298	0.30%	0.067%
30	17.409	2412	2418	2428	rBV	1730689	2442624	17.11%	3.790%
31	17.509	2428	2435	2441	rVV	2783844	3805551	26.65%	5.905%
32	17.562	2441	2444	2447	rVV4	17558	19261	0.13%	0.030%
33	17.774	2478	2480	2485	rVB5	18142	23524	0.16%	0.037%
34	17.921	2501	2505	2511	rVB5	14743	23508	0.16%	0.036%
35	18.168	2542	2547	2552	rBV3	35056	63946	0.45%	0.099%
36	18.227	2553	2557	2562	rVV2	49027	79094	0.55%	0.123%

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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
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37	18.286	2562	2567	2586	rVV	976562	1411889	9.89%	2.191%
38	18.415	2587	2589	2594	rVB6	18364	26589	0.19%	0.041%
39	18.633	2623	2626	2634	rVB6	19438	32388	0.23%	0.050%
40	18.703	2634	2638	2644	rVB	75877	90551	0.63%	0.141%
41	19.139	2709	2712	2716	rBV5	18408	26179	0.18%	0.041%
42	19.197	2720	2722	2728	rVB7	16756	25914	0.18%	0.040%
43	19.356	2745	2749	2754	rVB2	37348	53404	0.37%	0.083%
44	19.415	2754	2759	2760	rBV	135571	172144	1.21%	0.267%
45	19.556	2778	2783	2792	rBV	332590	472614	3.31%	0.733%
46	19.792	2817	2823	2834	rBV	3493196	4521998	31.67%	7.017%
47	20.762	2984	2988	2991	rBV	211413	225391	1.58%	0.350%
48	20.968	3021	3023	3028	rVB4	53044	63147	0.44%	0.098%
49	21.262	3068	3073	3082	rBV	685626	940834	6.59%	1.460%
50	21.574	3121	3126	3131	rVB	1803622	2287977	16.02%	3.550%
51	23.868	3509	3516	3524	rVB	1886211	3517357	24.63%	5.458%
52	24.027	3536	3543	3557	rVB2	1023795	2063105	14.45%	3.201%
53	28.556	4300	4313	4326	rVB3	3749074	14278824	100.00%	22.156%

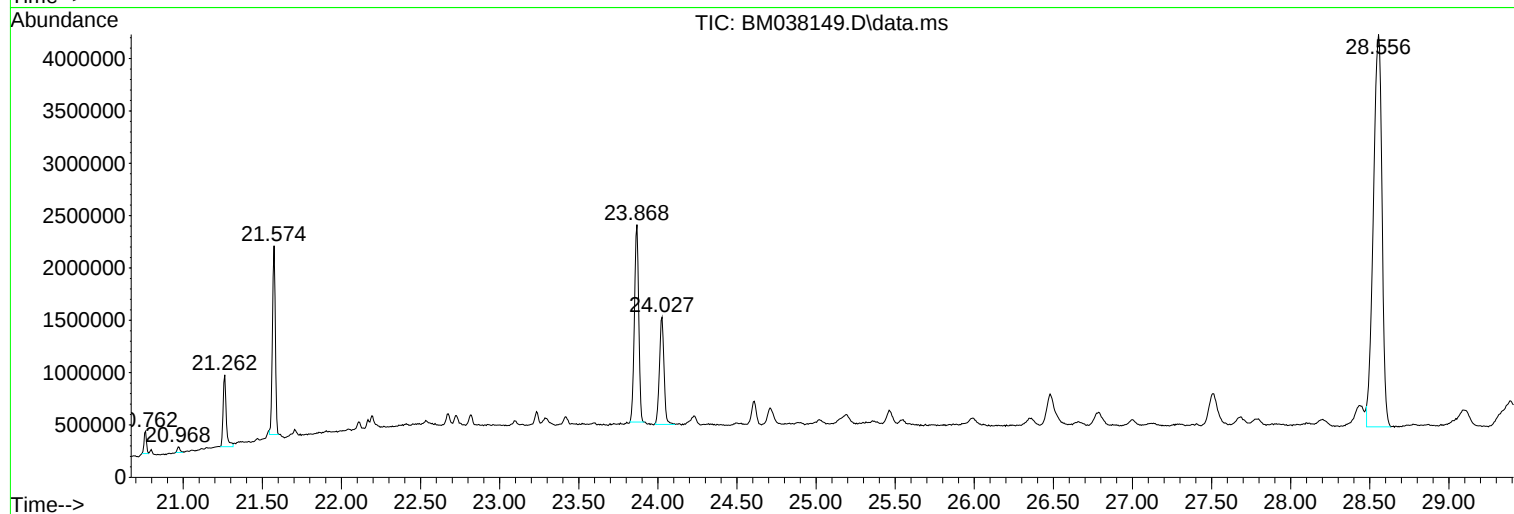
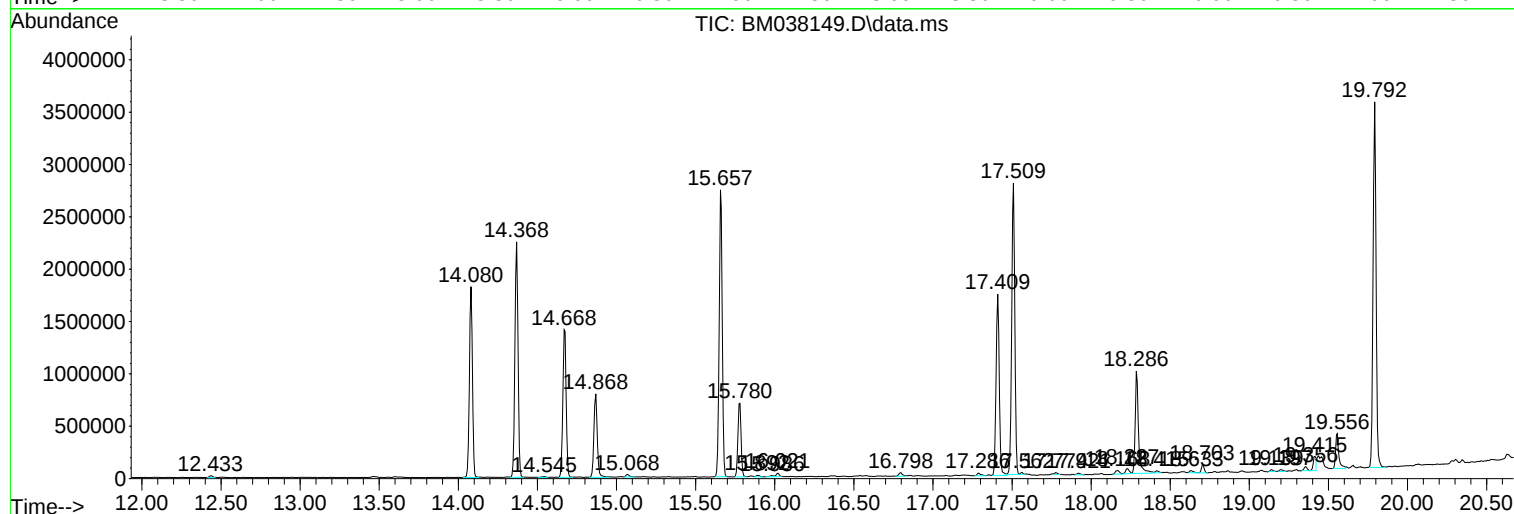
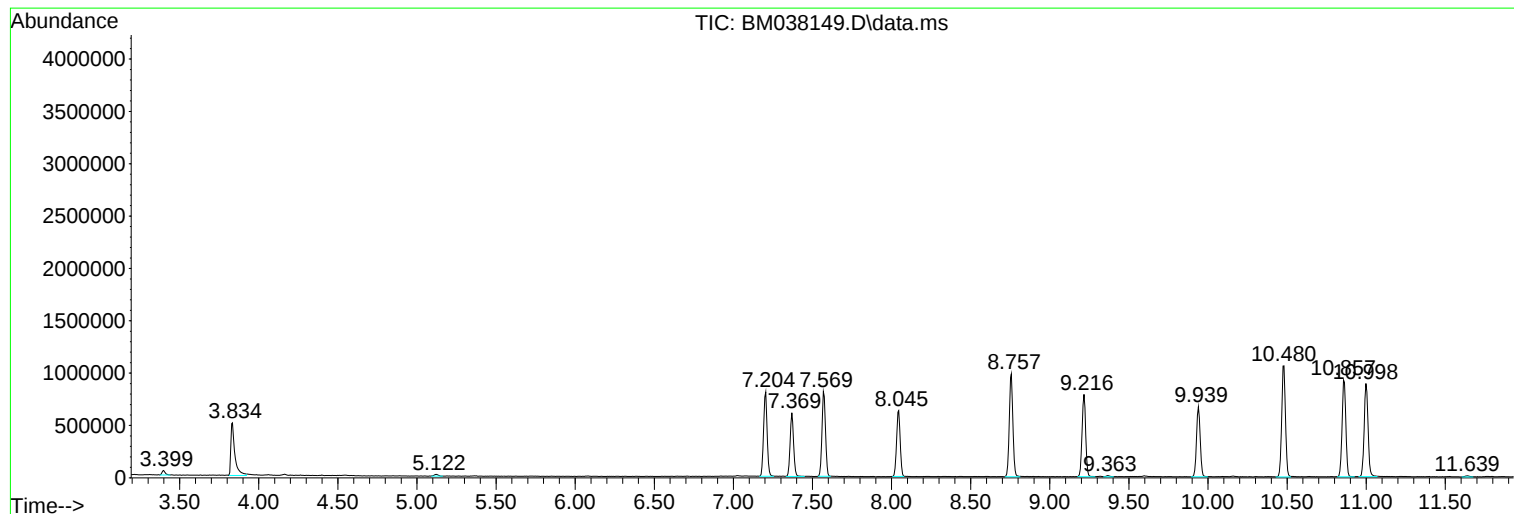
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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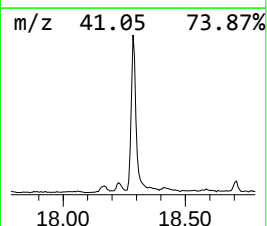
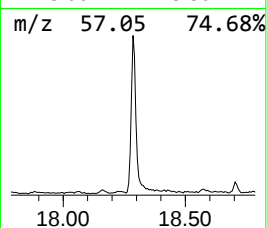
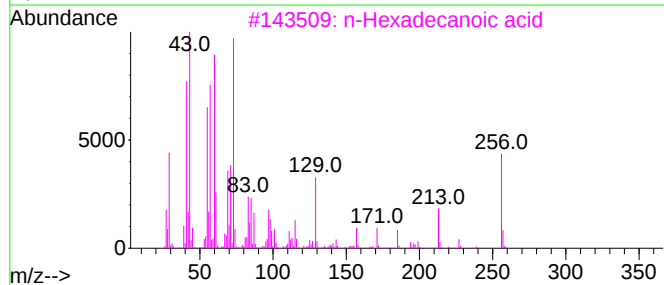
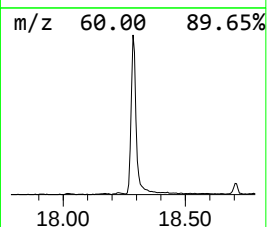
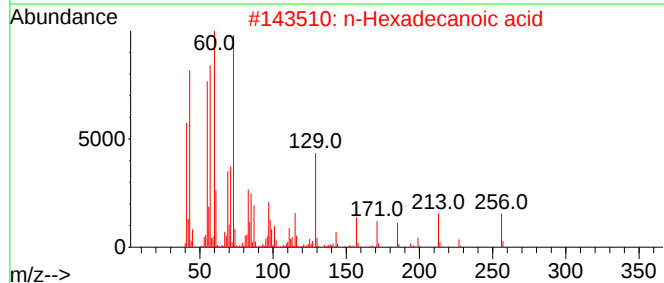
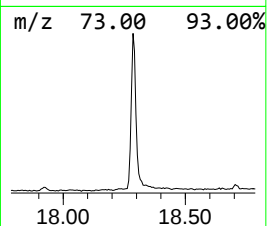
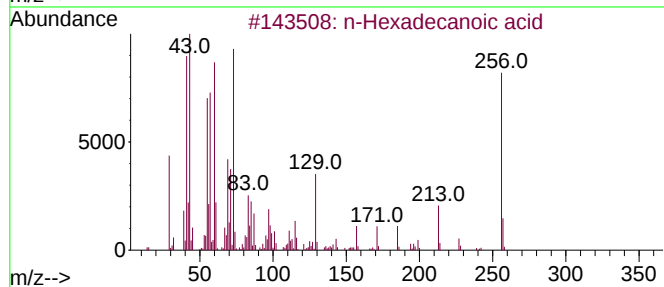
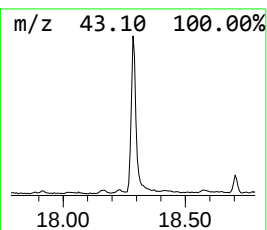
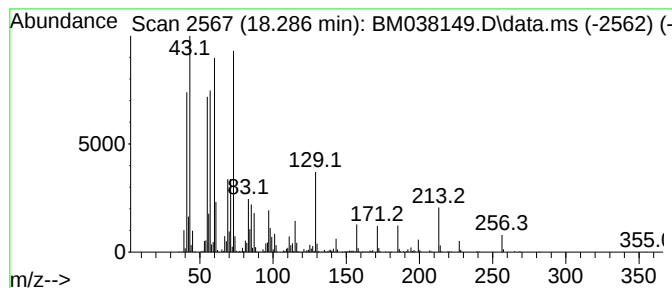
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.286	11.56 ng/ul	1411890	Phenanthrene-d10	17.409

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	94
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	89



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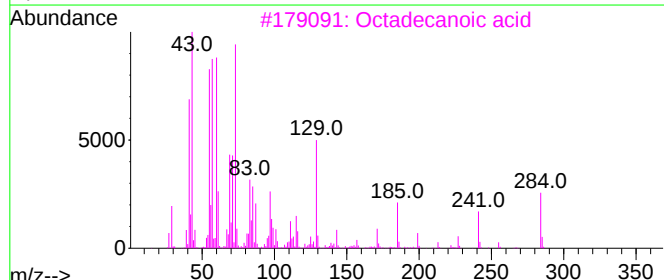
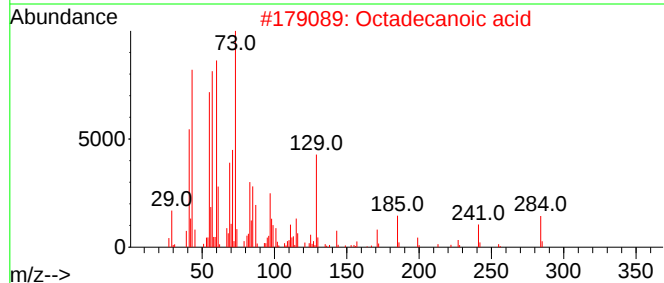
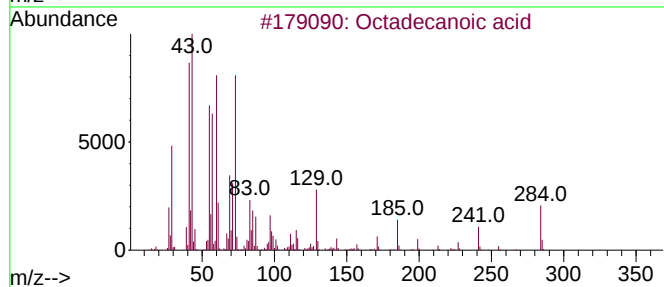
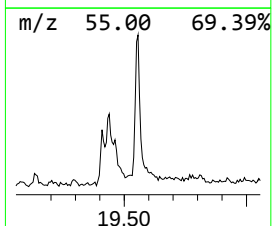
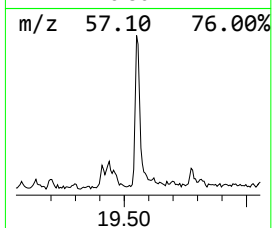
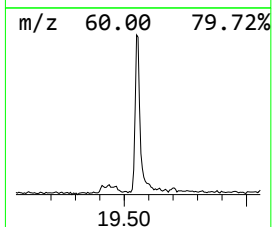
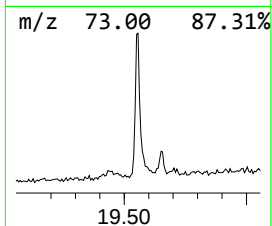
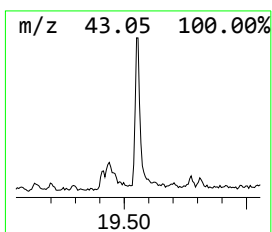
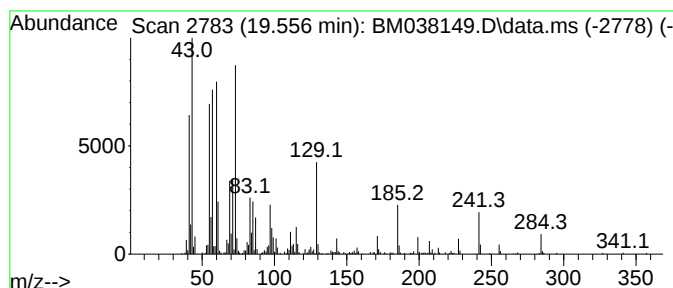
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.556	4.13 ng/ul	472614	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	94
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
5			Octadecanoic acid	284	C18H36O2	000057-11-4	90



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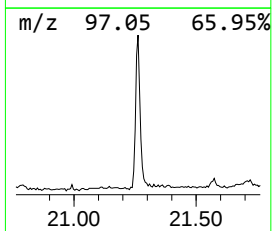
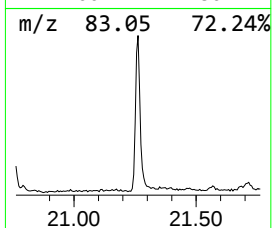
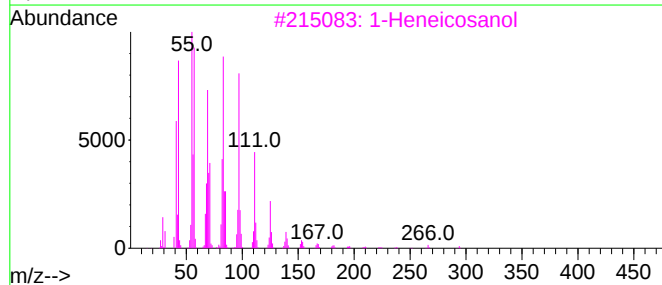
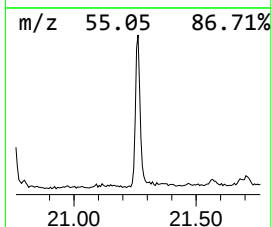
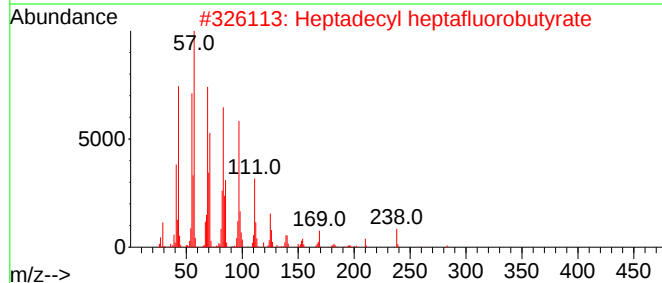
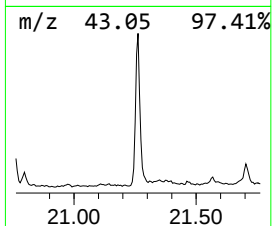
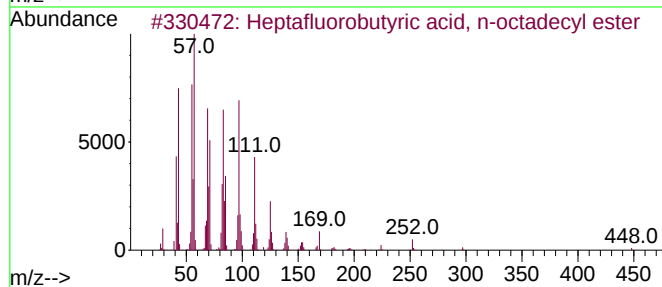
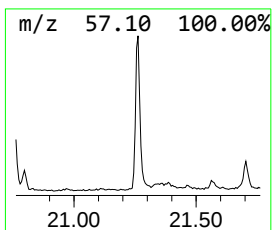
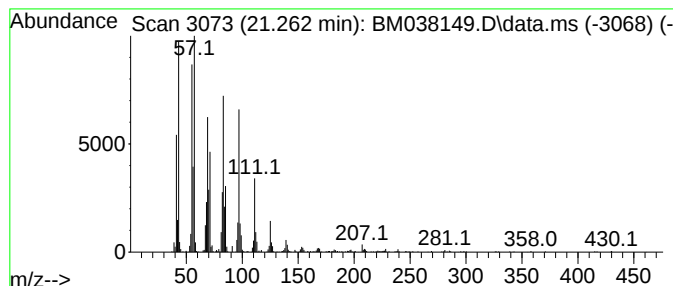
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.262	8.22 ng/ul	940834	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
5			1-Hexacosene	364	C26H52	018835-33-1	91



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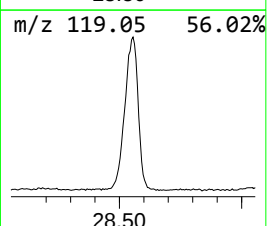
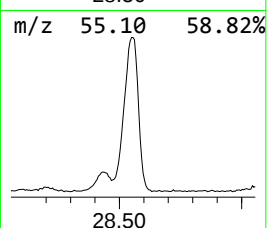
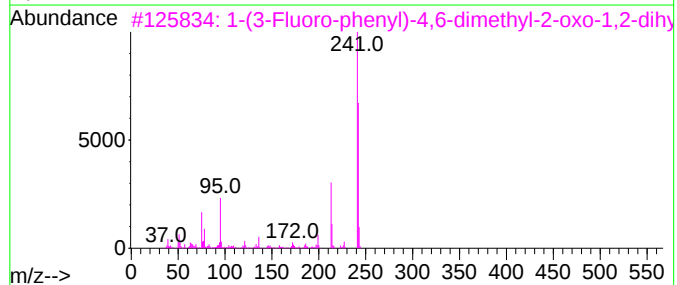
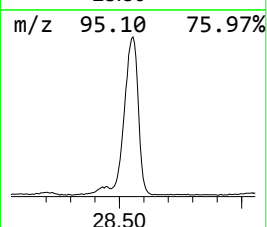
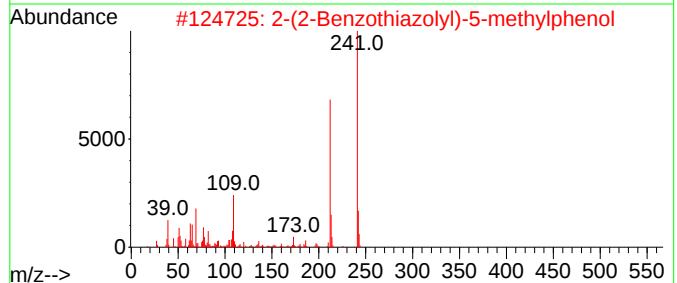
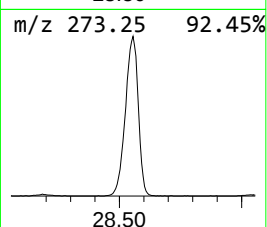
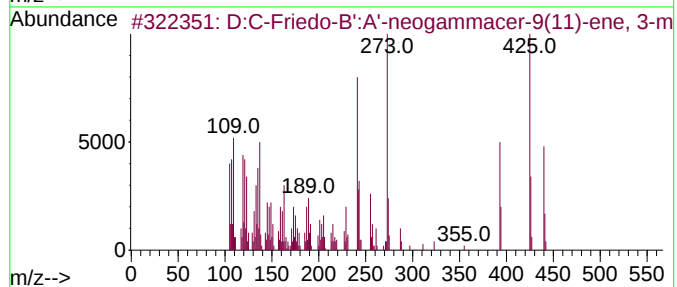
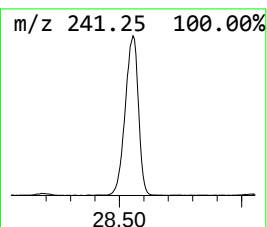
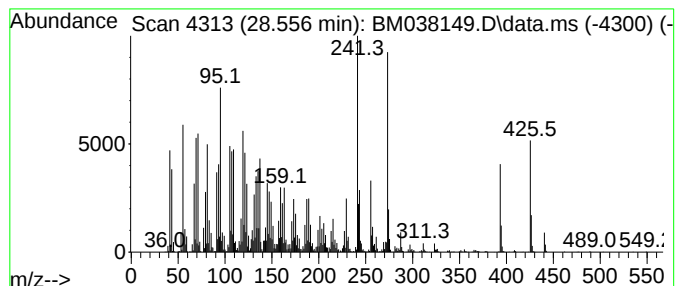
Instrument :
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.556	138.42 ng/ul	14278800	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	59
2	2-(2-Benzothiazolyl)-5-methylphenol	241	C14H11NOS	056048-54-5	25
3	1-(3-Fluoro-phenyl)-4,6-dimethyl...	242	C14H11FN2O	1000300-21-8	22
4	[1,2,4]Triazolo[1,5-a]pyrimidin...	241	C12H11N5O	1000351-09-2	22
5	Tolcapone	273	C14H11NO5	134308-13-7	15



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.286	11.6	ng/ul	1411890	4	17.409	2442620	20.0
Octadecanoic acid	19.556	4.1	ng/ul	472614	5	21.574	2287980	20.0
Heptafluorobuty...	21.262	8.2	ng/ul	940834	5	21.574	2287980	20.0
D:C-Friedo-B':A...	28.556	138.4	ng/ul	14278800	6	24.027	2063110	20.0