

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042223\
 Data File : BM039577.D
 Acq On : 22 Apr 2023 15:40
 Operator : CG/JU
 Sample : 02440-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP7

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-BM041823.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM039577.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.213	26	30	38	rVB	49060	73104	0.88%	0.118%
2	3.866	138	141	146	rVB	18462	27007	0.32%	0.043%
3	3.966	154	158	165	rVB	15784	27217	0.33%	0.044%
4	5.107	346	352	363	rBV	344538	533951	6.42%	0.859%
5	5.501	416	419	423	rVB	10110	12389	0.15%	0.020%
6	7.013	670	676	688	rBV	114392	267183	3.21%	0.430%
7	7.154	694	700	721	rVB	575820	968449	11.64%	1.558%
8	7.354	728	734	754	rBV	578679	1056687	12.70%	1.699%
9	7.707	788	794	804	rBV	161733	270256	3.25%	0.435%
10	7.819	806	813	816	rBV	675366	1087016	13.06%	1.748%
11	7.854	816	819	837	rVB	620169	1029208	12.37%	1.655%
12	8.172	866	873	881	rBV	116282	198810	2.39%	0.320%
13	8.554	931	938	963	rBV	367744	813464	9.77%	1.308%
14	8.995	1005	1013	1031	rBV	616648	1188122	14.28%	1.911%
15	9.378	1074	1078	1083	rVB3	9213	12469	0.15%	0.020%
16	9.713	1127	1135	1150	rBV	505098	1003384	12.06%	1.614%
17	10.272	1222	1230	1255	rBV	555724	1388475	16.68%	2.233%
18	10.495	1262	1268	1282	rVB	115948	219870	2.64%	0.354%
19	10.630	1282	1291	1304	rBV	876898	1588269	19.08%	2.554%
20	10.789	1311	1318	1333	rBV	106341	281392	3.38%	0.453%
21	11.013	1352	1356	1362	rVB2	16195	25814	0.31%	0.042%
22	12.236	1557	1564	1570	rBV2	9479	19716	0.24%	0.032%
23	13.283	1737	1742	1746	rBV7	6311	11082	0.13%	0.018%
24	13.583	1787	1793	1798	rBV9	4497	11724	0.14%	0.019%
25	13.895	1838	1846	1863	rBV	1576165	2319190	27.87%	3.730%
26	14.171	1886	1893	1909	rBV	1792142	2706699	32.52%	4.353%
27	14.477	1939	1945	1957	rBV	1213583	1891453	22.73%	3.042%
28	14.789	1992	1998	2006	rBV7	26930	93992	1.13%	0.151%
29	15.312	2083	2087	2093	rVB9	6403	11691	0.14%	0.019%
30	15.477	2108	2115	2133	rBV	2291747	3411833	40.99%	5.487%
31	15.618	2133	2139	2149	rBV	586359	1018028	12.23%	1.637%
32	15.848	2172	2178	2189	rVB	201476	324235	3.90%	0.521%
33	16.642	2308	2313	2330	rBV	113437	267808	3.22%	0.431%
34	17.148	2395	2399	2403	rVB6	6050	9254	0.11%	0.015%
35	17.230	2407	2413	2424	rBV	1429638	2150967	25.84%	3.459%
36	17.330	2424	2430	2441	rVV	2732181	4046275	48.62%	6.507%

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37	17.418	2442	2445	2458	rVB9	30514	73724	0.89%	0.119%
38	18.142	2562	2568	2597	rBV	5390662	8322574	100.00%	13.385%
39	18.812	2678	2682	2691	rBV7	35279	86935	1.04%	0.140%
40	19.195	2744	2747	2753	rVB2	38431	54808	0.66%	0.088%
41	19.271	2757	2760	2761	rBV	47473	51308	0.62%	0.083%
42	19.300	2761	2765	2766	rVV	154857	203316	2.44%	0.327%
43	19.336	2766	2771	2781	rVV	1791909	3169519	38.08%	5.097%
44	19.418	2781	2785	2805	rVB	1775972	2899035	34.83%	4.662%
45	19.630	2816	2821	2832	rBV	3293293	4697540	56.44%	7.555%
46	20.518	2969	2972	2984	rVB2	148100	295486	3.55%	0.475%
47	21.142	3074	3078	3085	rBV3	182761	341853	4.11%	0.550%
48	21.430	3122	3127	3136	rBV	1574444	2176742	26.15%	3.501%
49	23.647	3497	3504	3516	rVB2	2280552	4559654	54.79%	7.333%
50	23.794	3524	3529	3541	rVB2	1067123	2175849	26.14%	3.499%
51	25.224	3766	3772	3785	rVB2	1078471	2704125	32.49%	4.349%

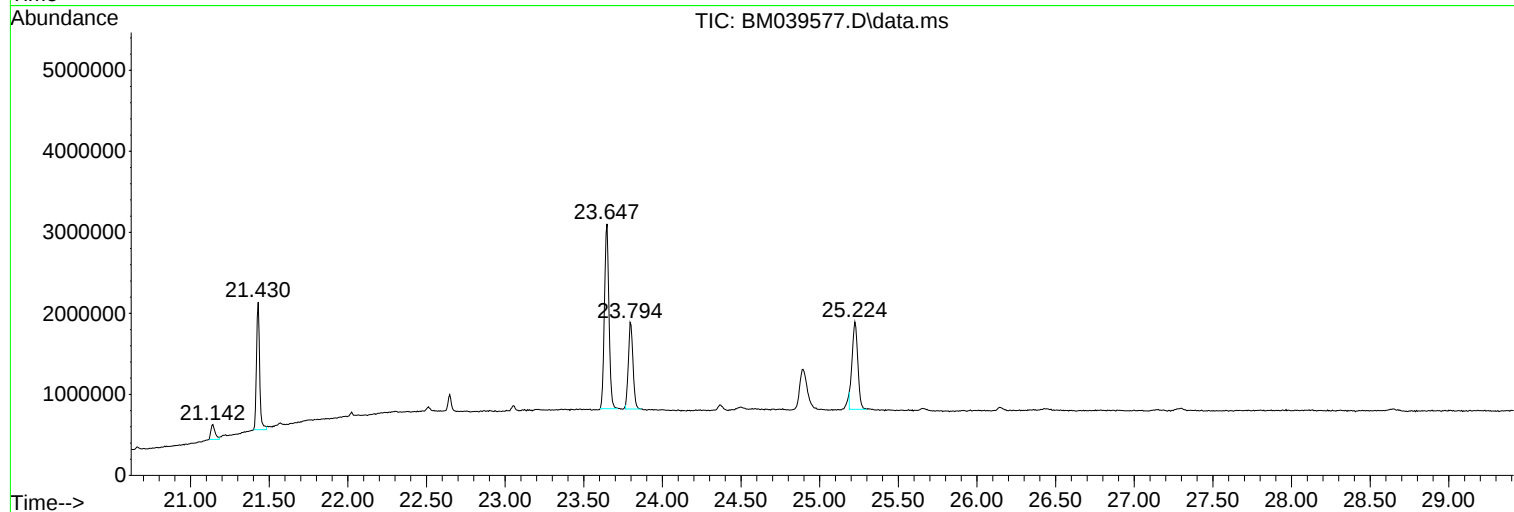
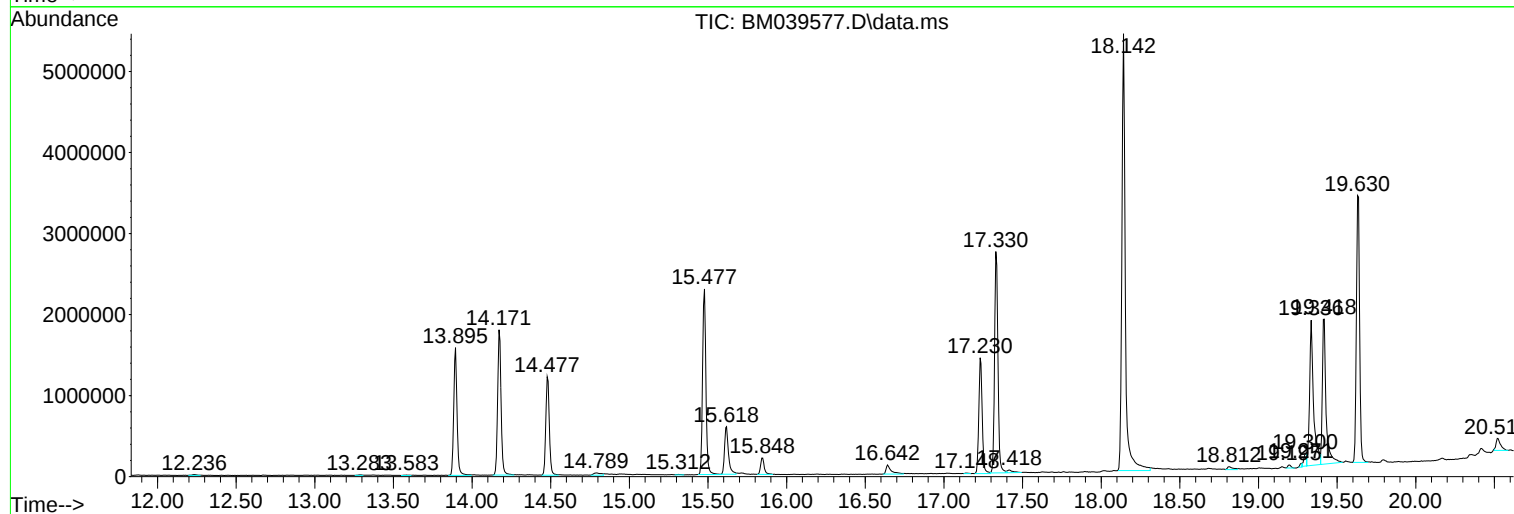
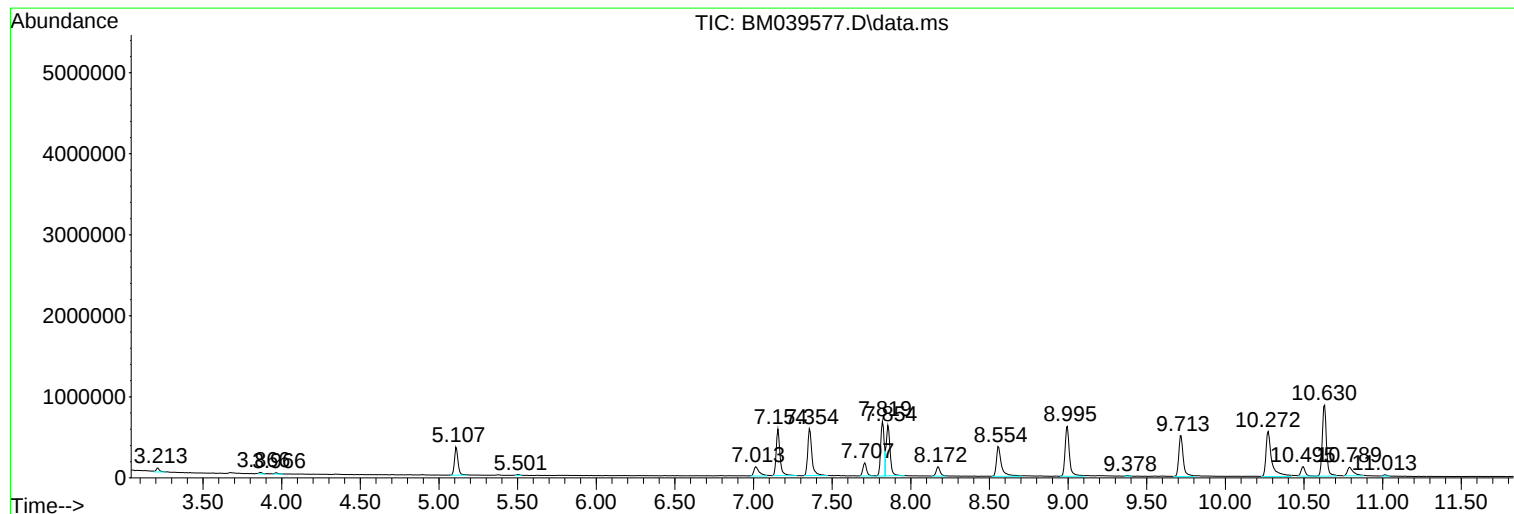
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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



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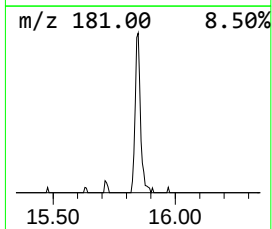
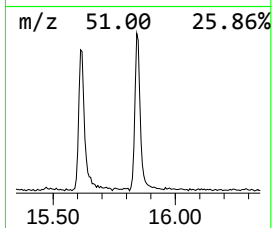
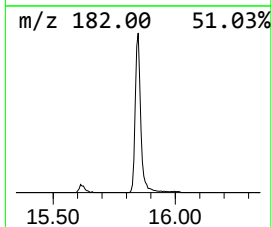
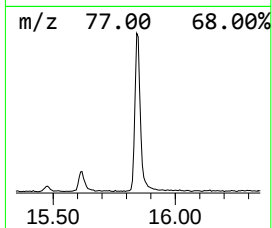
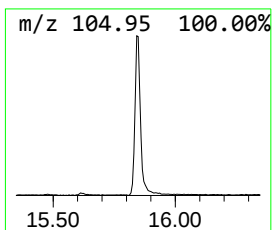
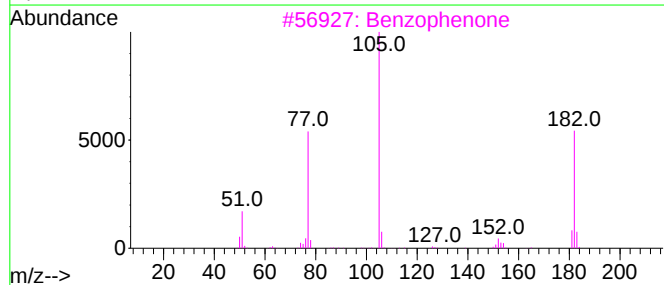
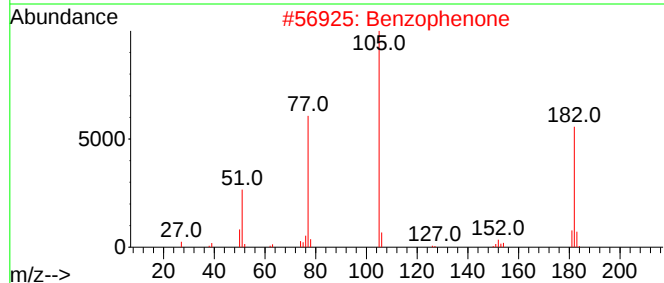
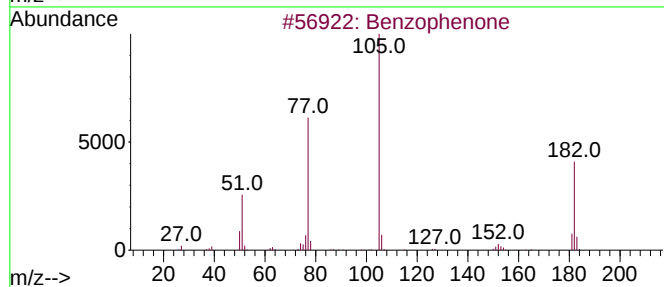
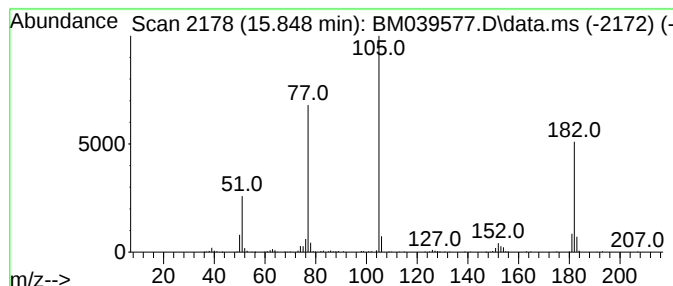
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.848	3.43 ng/ul	324235	Acenaphthene-d10	14.477

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzophenone	182	C13H10O	000119-61-9	96
3			Benzophenone	182	C13H10O	000119-61-9	95
4			Benzophenone	182	C13H10O	000119-61-9	90
5			Benzophenone	182	C13H10O	000119-61-9	90



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Instrument :
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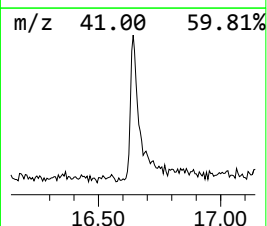
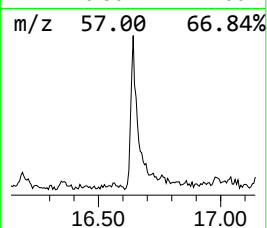
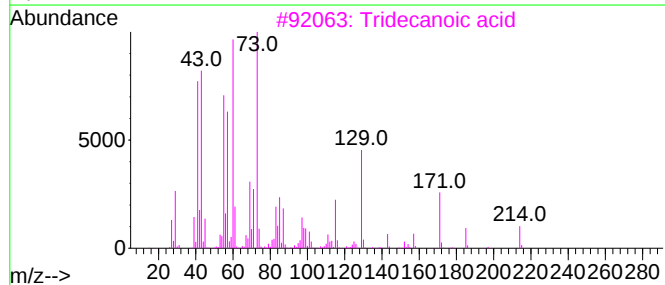
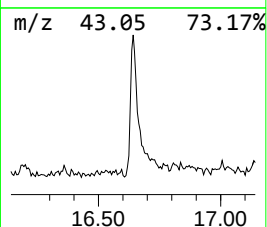
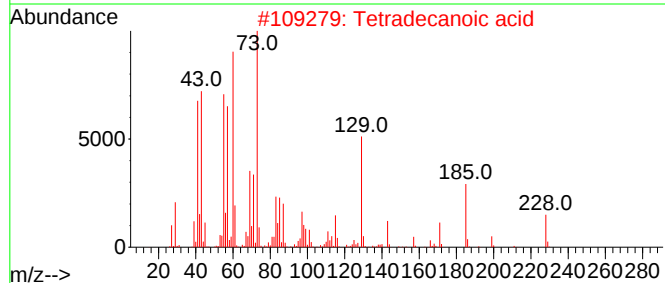
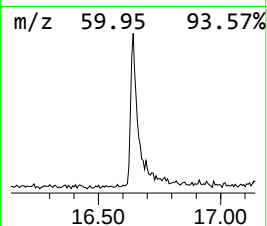
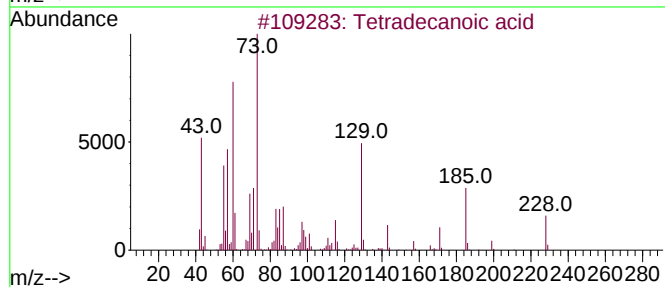
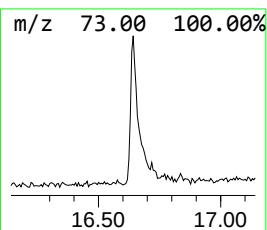
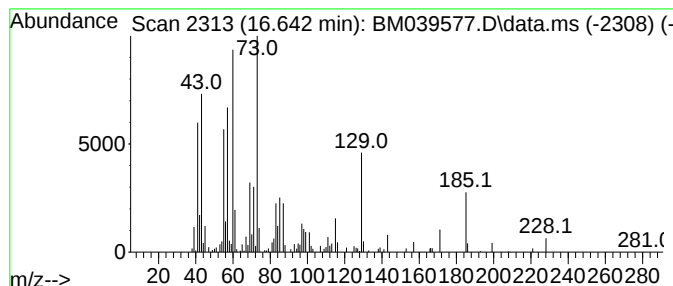
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 Tetradecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.642	2.49 ng/ul	267808	Phenanthrene-d10	17.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Undecanoic acid	186	C11H22O2	000112-37-8	76
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



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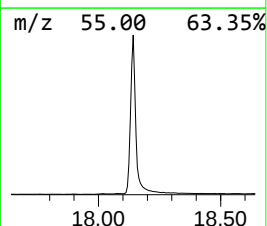
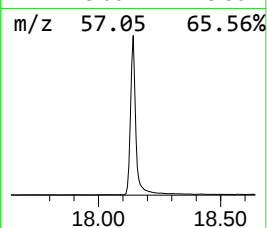
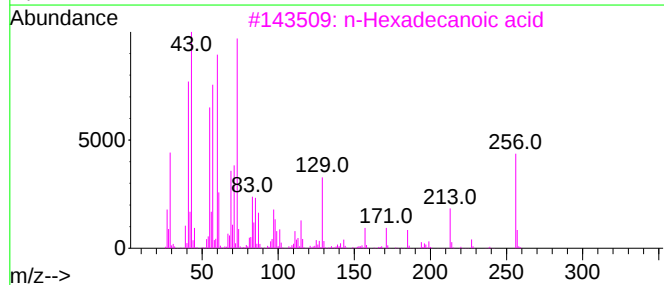
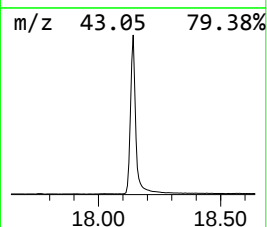
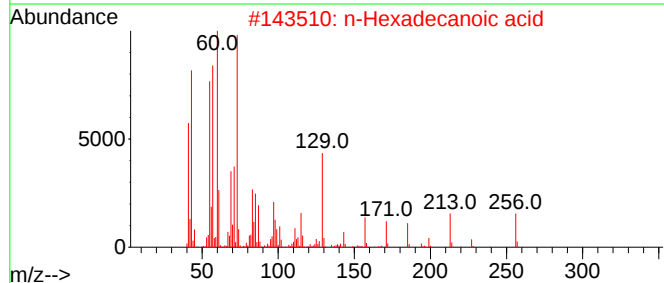
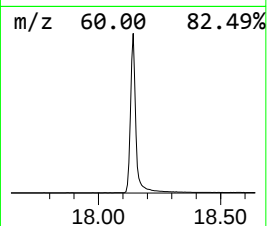
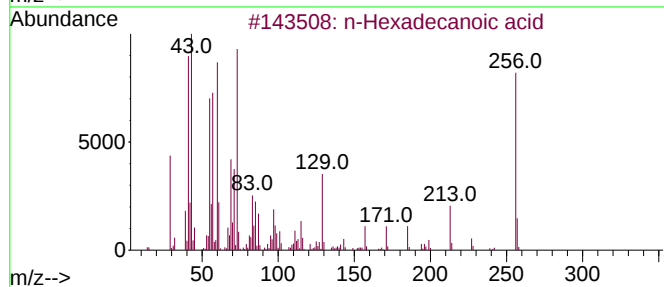
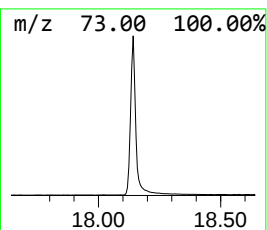
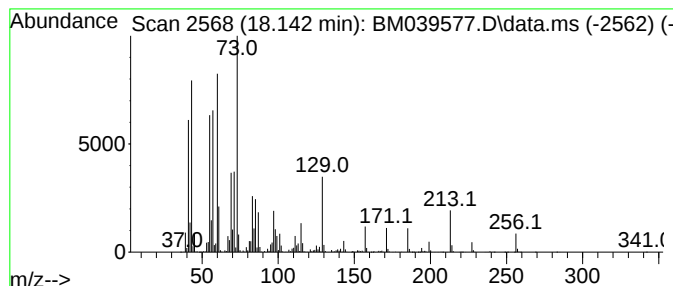
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.142	77.38 ng/ul	8322570	Phenanthrene-d10	17.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99		
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99		
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98		
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98		
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97		



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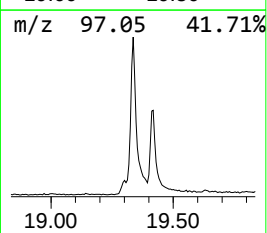
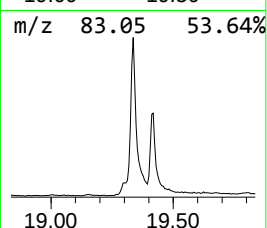
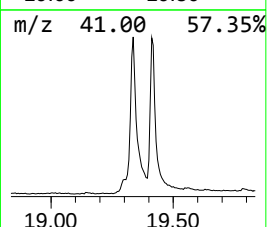
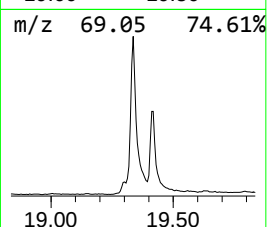
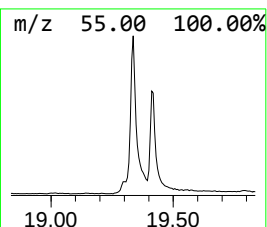
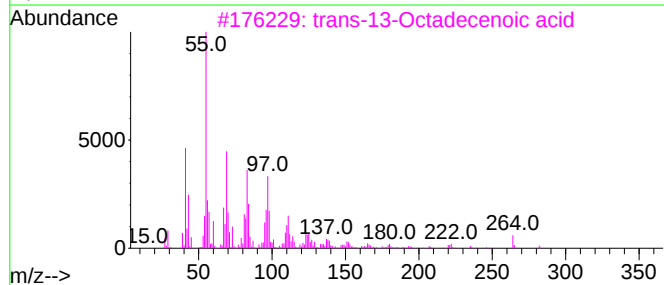
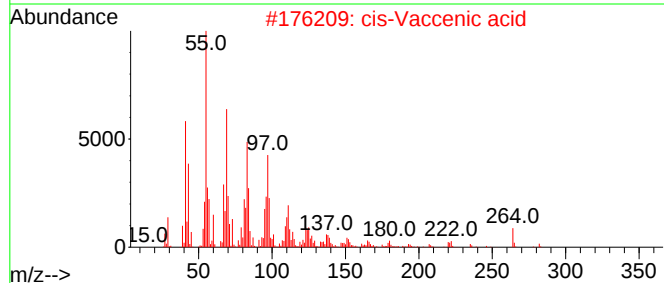
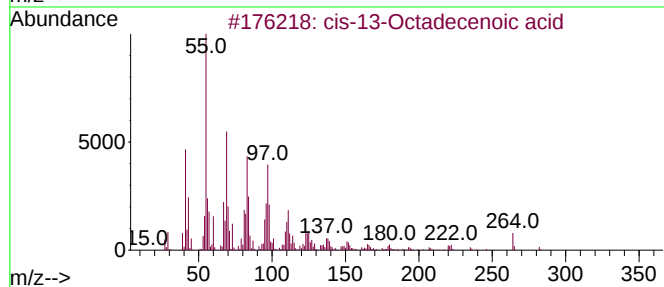
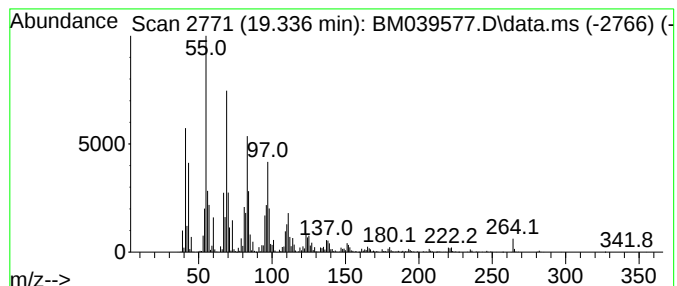
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 cis-13-Octadecenoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.336	29.12 ng/ul	3169520	Chrysene-d12	21.430	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	99
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	99
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	99
4	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	96
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	94



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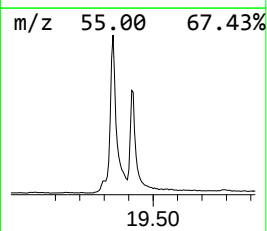
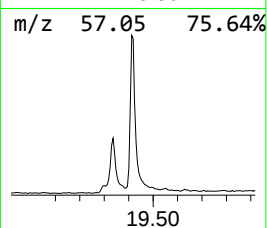
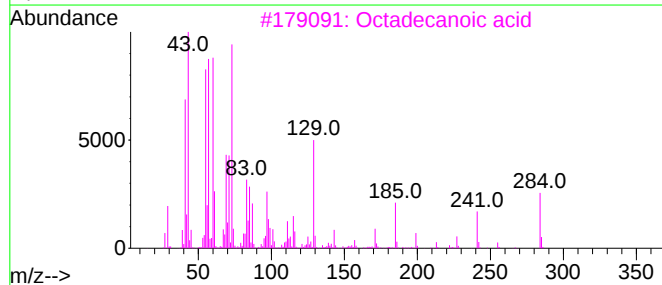
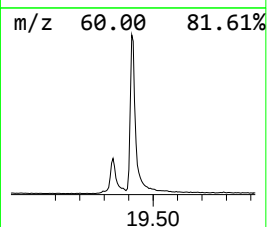
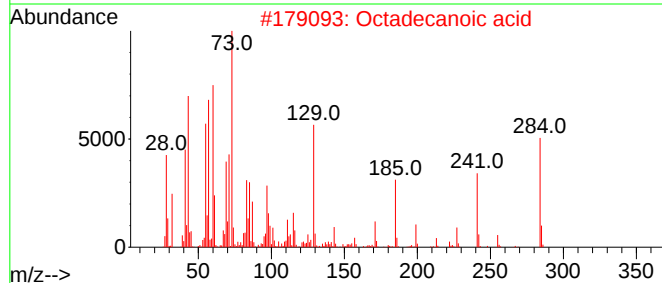
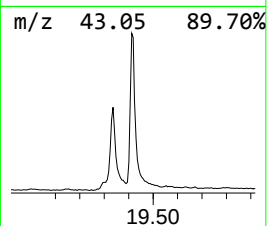
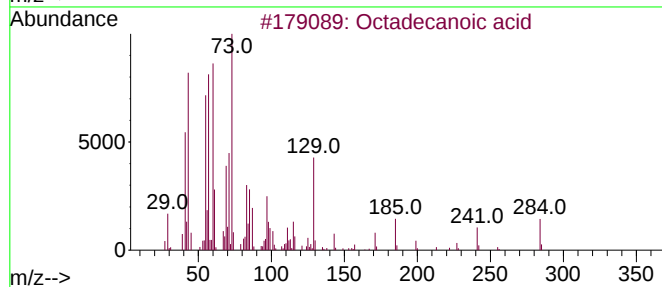
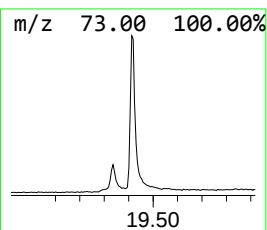
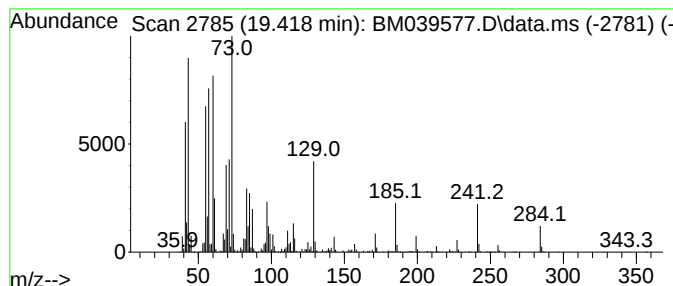
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.418	26.64 ng/ul	2899040	Chrysene-d12	21.430

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	98
5			Octadecanoic acid	284	C18H36O2	000057-11-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042223\
Data File : BM039577.D
Acq On : 22 Apr 2023 15:40
Operator : CG/JU
Sample : 02440-02
Misc :
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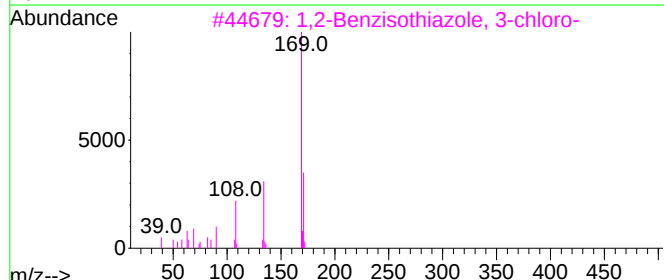
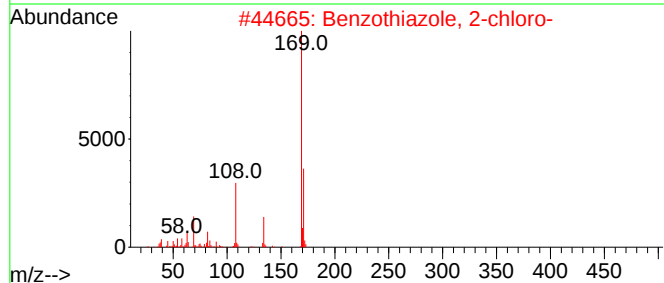
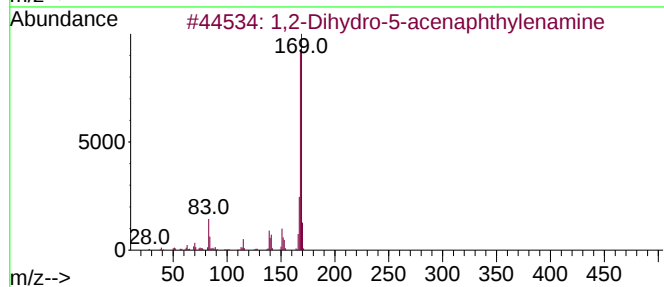
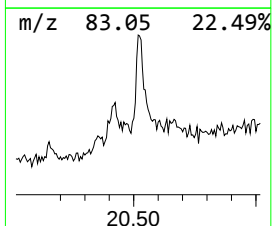
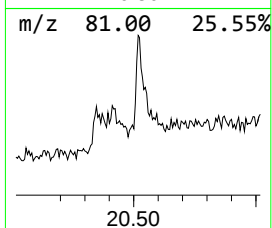
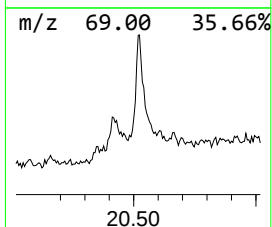
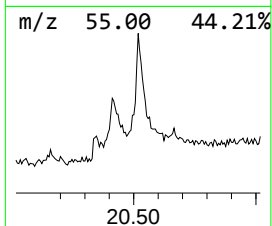
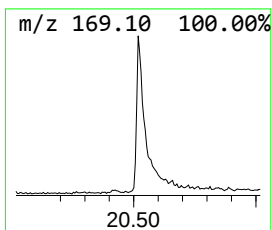
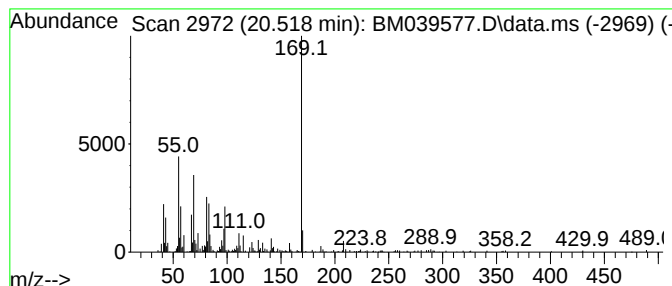
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 10 1,2-Dihydro-5-acenaphthylen... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.518	2.71 ng/ul	295486	Chrysene-d12		21.430	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,2-Dihydro-5-acenaphthylenamine		169	C12H11N	004657-93-6	50
2	Benzothiazole, 2-chloro-		169	C7H4ClNS	000615-20-3	43
3	1,2-Benzisothiazole, 3-chloro-		169	C7H4ClNS	007716-66-7	43
4	Diphenylamine		169	C12H11N	000122-39-4	43
5	Diphenylamine		169	C12H11N	000122-39-4	40



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042223\
Data File : BM039577.D
Acq On : 22 Apr 2023 15:40
Operator : CG/JU
Sample : 02440-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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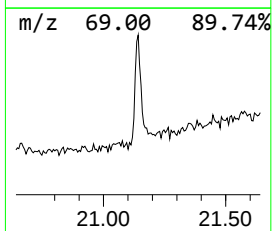
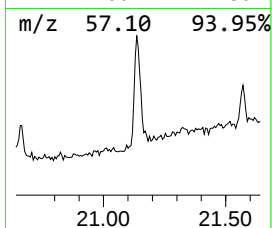
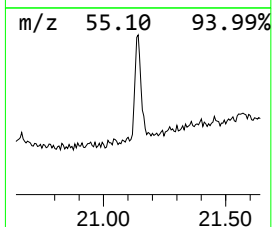
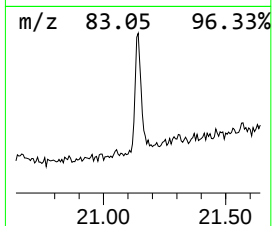
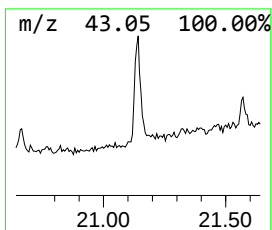
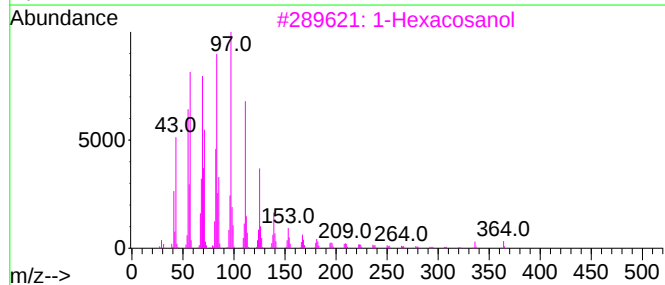
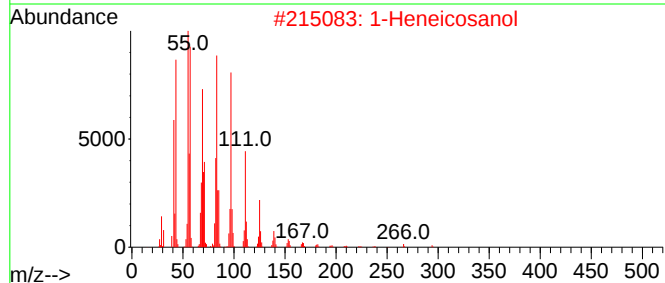
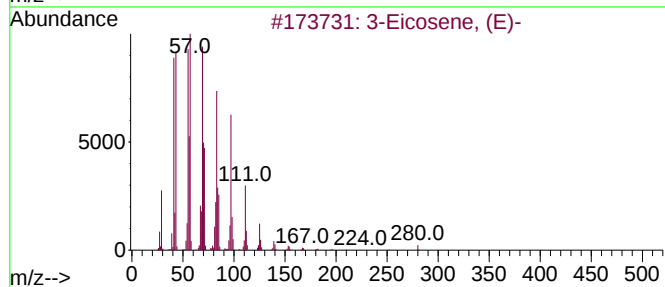
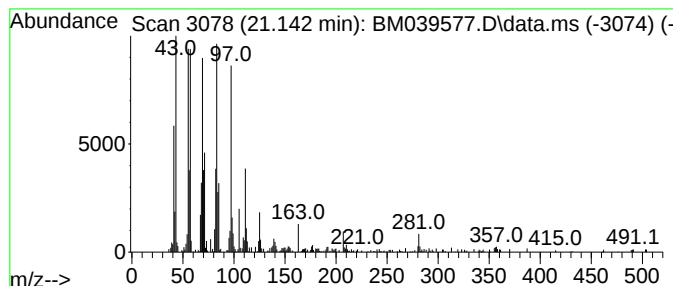
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.142	3.14 ng/ul	341853	Chrysene-d12	21.430

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-		280	C20H40	074685-33-9	98
2	1-Heneicosanol		312	C21H44O	015594-90-8	94
3	1-Hexacosanol		382	C26H54O	000506-52-5	91
4	1-Heptacosanol		396	C27H56O	002004-39-9	91
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042223\
Data File : BM039577.D
Acq On : 22 Apr 2023 15:40
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Sample : 02440-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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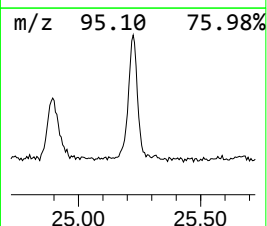
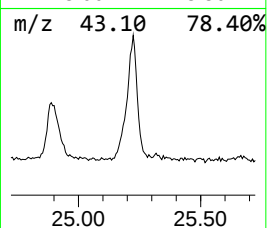
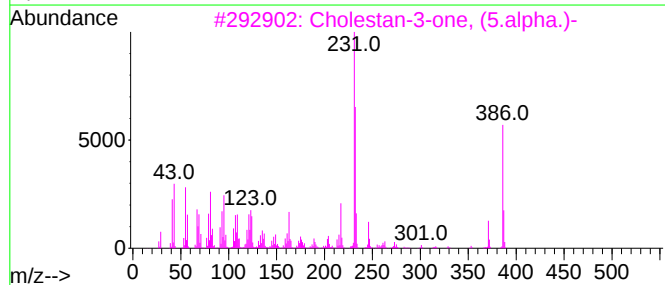
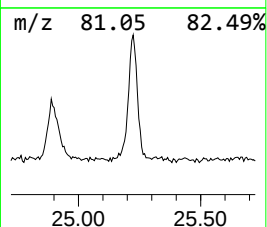
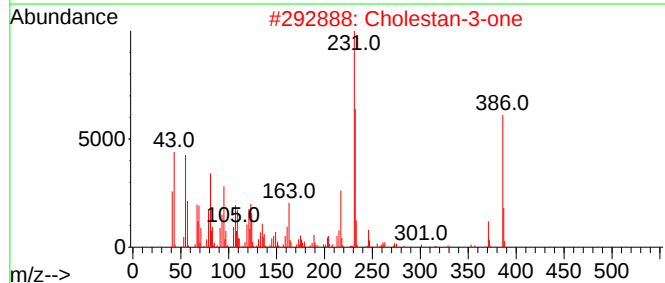
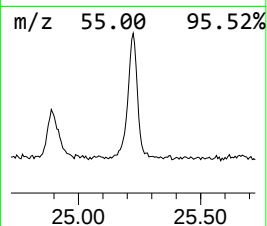
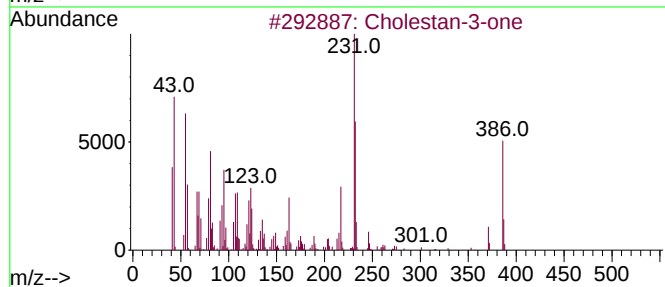
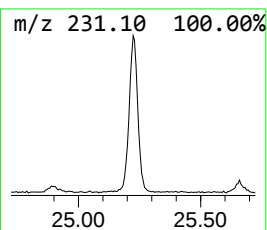
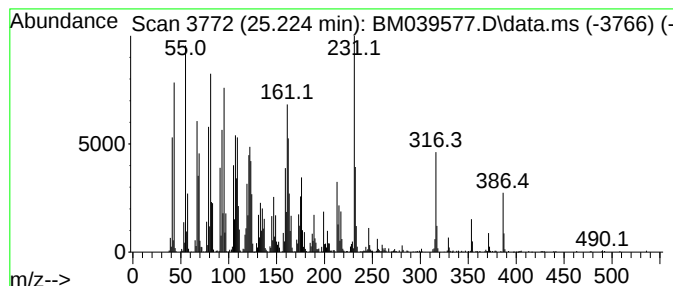
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Quant Title : SVOA CALIBRATION

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

Peak Number 12 Cholestan-3-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.224	24.86 ng/ul	2704130	Perylene-d12	23.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholestan-3-one	386	C27H46O	015600-08-5	95
2			Cholestan-3-one	386	C27H46O	015600-08-5	90
3			Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	83
4			Cholestan-2-one	386	C27H46O	1010210-43-4	80
5			Cholestan-3-one, (5.beta.)-	386	C27H46O	000601-53-6	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042223\
Data File : BM039577.D
Acq On : 22 Apr 2023 15:40
Operator : CG/JU
Sample : 02440-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM041823.MA.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
Benzophenone	15.848	3.4	ng/ul	324235	3	14.477	1891450	20.0
Tetradecanoic acid	16.642	2.5	ng/ul	267808	4	17.230	2150970	20.0
n-Hexadecanoic ...	18.142	77.4	ng/ul	8322570	4	17.230	2150970	20.0
cis-13-Octadece...	19.336	29.1	ng/ul	3169520	5	21.430	2176740	20.0
Octadecanoic acid	19.418	26.6	ng/ul	2899040	5	21.430	2176740	20.0
1,2-Dihydro-5-a...	20.518	2.7	ng/ul	295486	5	21.430	2176740	20.0
(DEL) Alkane: S...	21.142	3.1	ng/ul	341853	5	21.430	2176740	20.0
Cholestan-3-one	25.224	24.9	ng/ul	2704130	6	23.794	2175850	20.0