

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
 Data File : BM043409.D
 Acq On : 19 Dec 2023 00:46
 Operator : MA/JU
 Sample : 05807-09
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0AZ1

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-BM121523.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM043409.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.387	30	34	46	rVB	194568	278155	0.21%	0.063%
2	3.675	80	83	95	rVB	87175	143220	0.11%	0.032%
3	3.810	102	106	125	rBV	1965579	2970042	2.28%	0.671%
4	4.028	137	143	155	rVB	127701	241321	0.19%	0.055%
5	5.304	350	360	386	rBV4	52391757	130029519	100.00%	29.368%
6	7.151	667	674	688	rBV	2848410	4661707	3.59%	1.053%
7	7.334	698	705	717	rVB	2387372	3683361	2.83%	0.832%
8	7.522	728	737	748	rBV	2871910	4709358	3.62%	1.064%
9	7.881	790	798	807	rBV	5262173	8355296	6.43%	1.887%
10	8.051	811	827	845	rBV2	50481330	121239862	93.24%	27.383%
11	8.345	869	877	891	rVB	3267911	5249019	4.04%	1.186%
12	8.704	930	938	945	rBV	3429732	5544059	4.26%	1.252%
13	9.163	1008	1016	1027	rBV	2676450	4532804	3.49%	1.024%
14	9.733	1106	1113	1124	rBV2	113828	197981	0.15%	0.045%
15	9.886	1129	1139	1156	rBV	2228846	3799412	2.92%	0.858%
16	10.422	1221	1230	1237	rBV	3233384	5469093	4.21%	1.235%
17	10.663	1264	1271	1285	rBV2	414946	834910	0.64%	0.189%
18	10.798	1285	1294	1302	rBV	2563668	4404650	3.39%	0.995%
19	10.945	1310	1319	1336	rBV	3033705	5295064	4.07%	1.196%
20	11.180	1352	1359	1368	rVB	172729	301349	0.23%	0.068%
21	11.551	1414	1422	1433	rBV	111828	228712	0.18%	0.052%
22	13.421	1734	1740	1750	rBV2	145805	300765	0.23%	0.068%
23	14.045	1837	1846	1852	rBV	4658871	6800601	5.23%	1.536%
24	14.315	1885	1892	1905	rVB	5965446	9071544	6.98%	2.049%
25	14.621	1933	1944	1951	rBV	3475217	5162879	3.97%	1.166%
26	14.821	1971	1978	1992	rBV	2371255	3643606	2.80%	0.823%
27	15.615	2105	2113	2120	rBV	7308805	10206146	7.85%	2.305%
28	15.733	2127	2133	2147	rBV	2082629	2920399	2.25%	0.660%
29	17.362	2404	2410	2416	rBV	3609039	5240393	4.03%	1.184%
30	17.468	2421	2428	2436	rVB	7074698	10110130	7.78%	2.283%
31	18.262	2557	2563	2575	rBV	677192	1170349	0.90%	0.264%
32	19.192	2717	2721	2727	rVB	115867	138868	0.11%	0.031%
33	19.386	2750	2754	2758	rBV2	112659	172149	0.13%	0.039%
34	19.539	2776	2780	2791	rBV2	161792	277957	0.21%	0.063%
35	19.750	2809	2816	2823	rBV	7929743	10491838	8.07%	2.370%
36	20.268	2900	2904	2907	rBV2	148763	215273	0.17%	0.049%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
 Data File : BM043409.D
 Acq On : 19 Dec 2023 00:46
 Operator : MA/JU
 Sample : 05807-09
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0AZ1

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-BM121523.MA.M
 Title : SVOA CALIBRATION

37	20.303	2907	2910	2916	rVB	544200	585065	0.45%	0.132%
38	20.797	2991	2994	2998	rVB	178388	193060	0.15%	0.044%
39	20.950	3016	3020	3025	rBV	734512	954658	0.73%	0.216%
40	21.027	3030	3033	3037	rVB4	105603	141191	0.11%	0.032%
41	21.144	3048	3053	3058	rBV	3019945	3698714	2.84%	0.835%
42	21.186	3058	3060	3066	rVB2	119822	146489	0.11%	0.033%
43	21.256	3068	3072	3075	rBV	2641189	3613660	2.78%	0.816%
44	21.286	3075	3077	3082	rVB	1622080	1738393	1.34%	0.393%
45	21.539	3116	3120	3128	rVB	4017535	5334312	4.10%	1.205%
46	21.709	3146	3149	3155	rVB	262324	340085	0.26%	0.077%
47	22.197	3225	3232	3242	rBV3	1813341	3493166	2.69%	0.789%
48	23.256	3407	3412	3416	rBV	1483219	2481941	1.91%	0.561%
49	23.303	3416	3420	3432	rVB	1395807	2588198	1.99%	0.585%
50	23.809	3498	3506	3516	rBV2	5158988	10252197	7.88%	2.316%
51	23.968	3526	3533	3549	rVB	2470711	5225136	4.02%	1.180%
52	24.650	3644	3649	3657	rVB	518475	1109539	0.85%	0.251%
53	24.744	3658	3665	3676	rBV	1011014	2454034	1.89%	0.554%
54	24.879	3683	3688	3699	rVB4	448824	1599729	1.23%	0.361%
55	25.415	3774	3779	3789	rVB	456078	1086615	0.84%	0.245%
56	27.656	4152	4160	4172	rVB2	889471	2854792	2.20%	0.645%
57	28.503	4291	4304	4323	rVB3	3715511	14771142	11.36%	3.336%

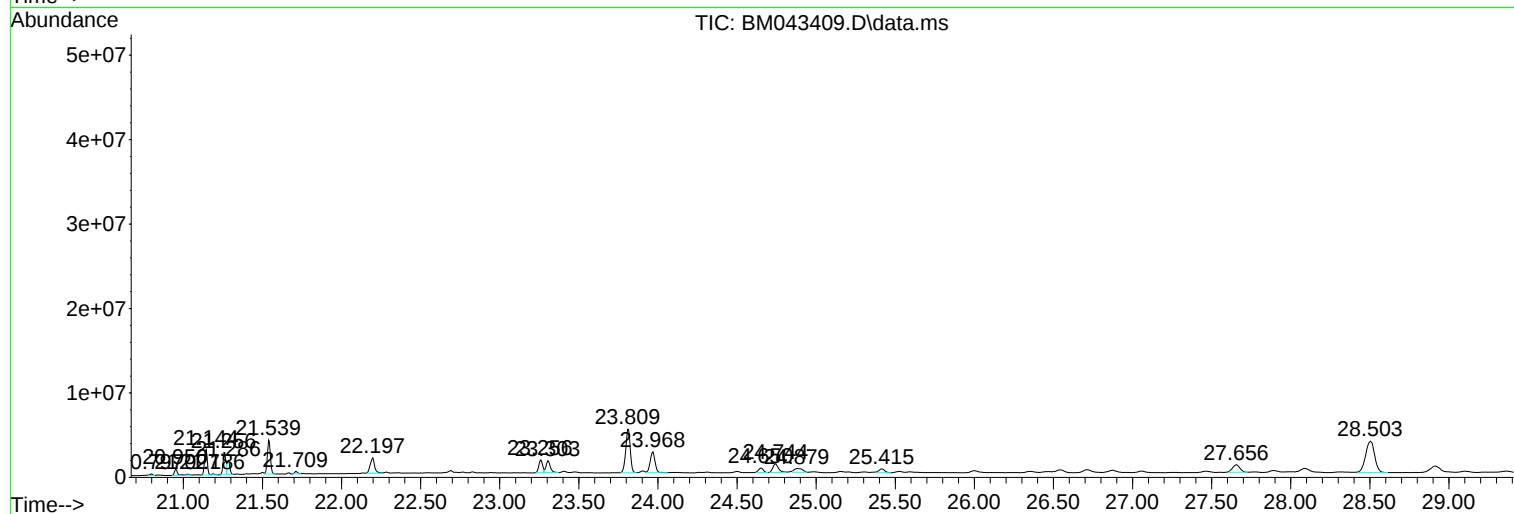
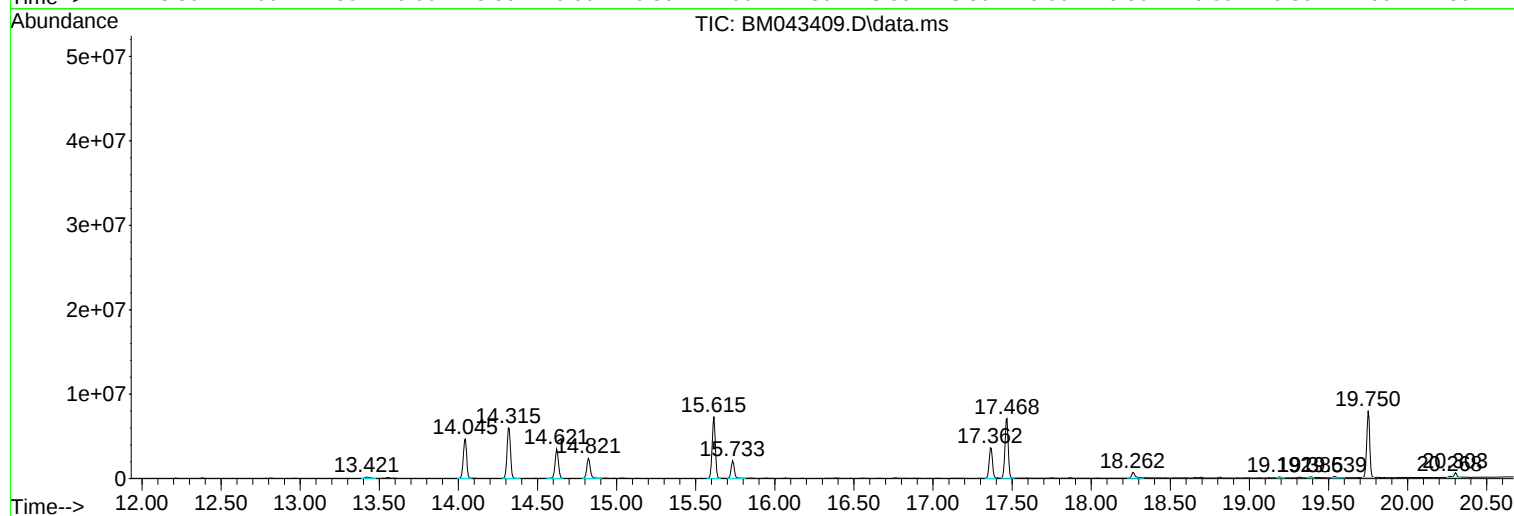
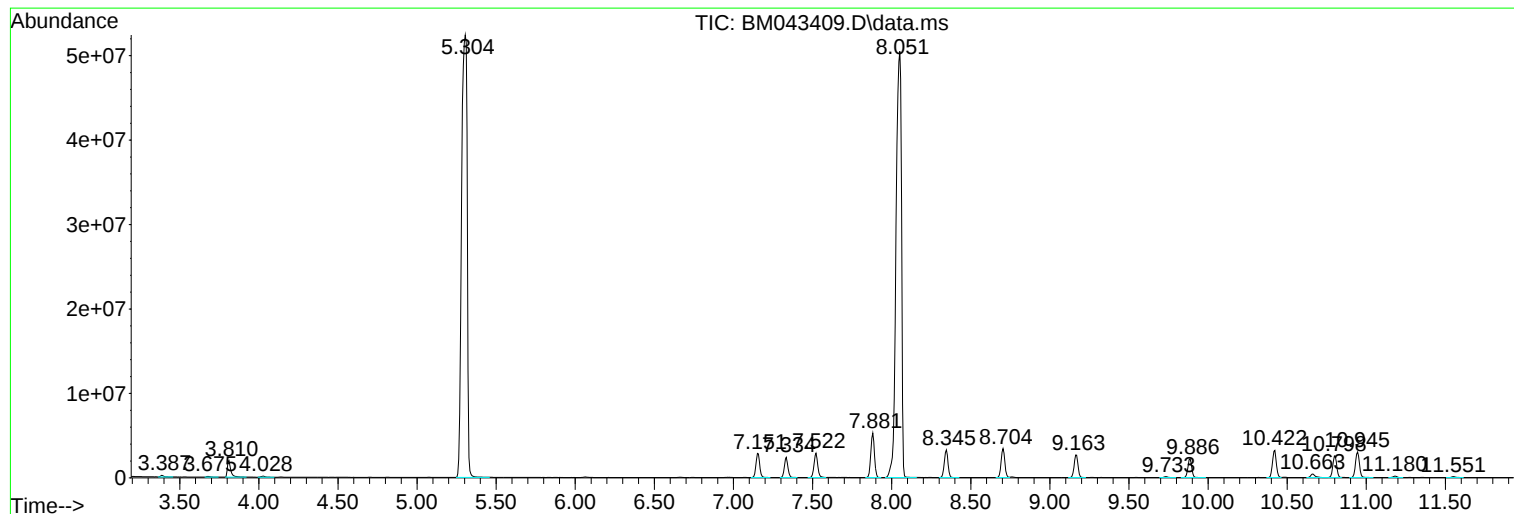
Sum of corrected areas: 442753907

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

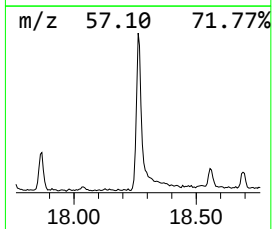
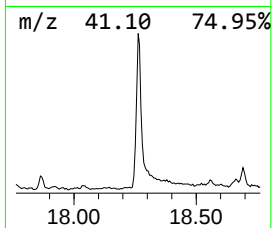
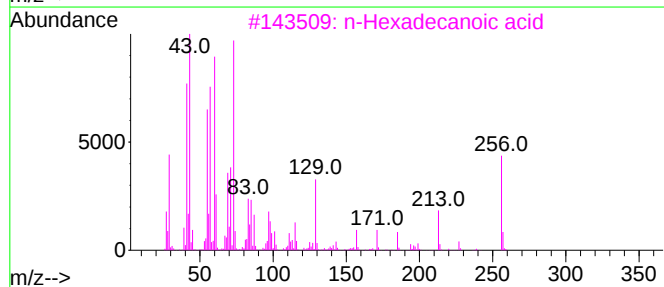
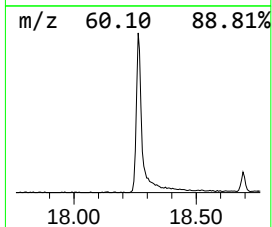
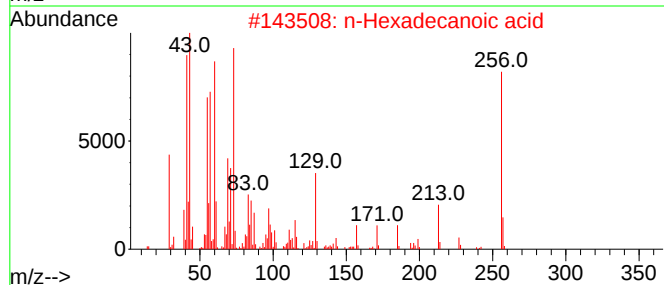
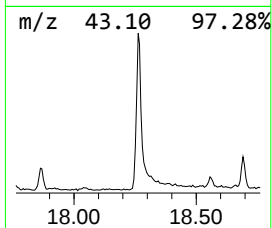
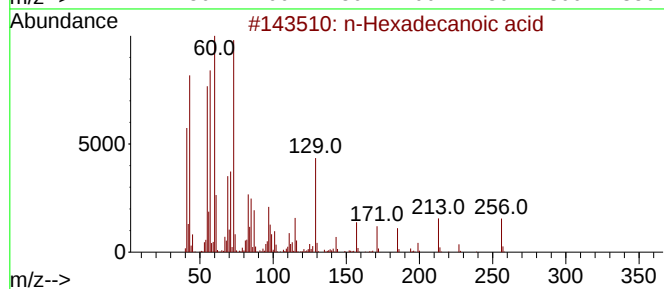
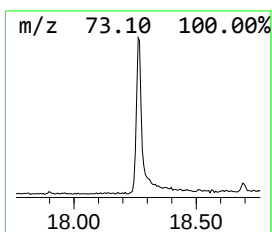
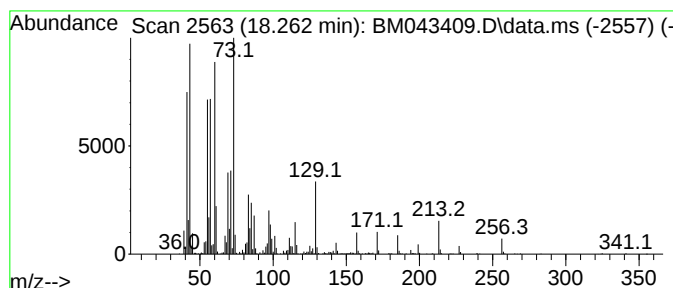
Instrument :
BNA_M
ClientSampleId :
C0AZ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.262	4.47 ng/ul	1170350	Phenanthrene-d10	17.362	
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	96
5	Tridecanoic acid	214	C13H26O2	000638-53-9	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

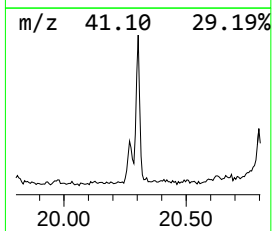
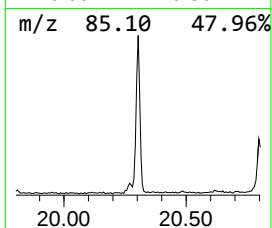
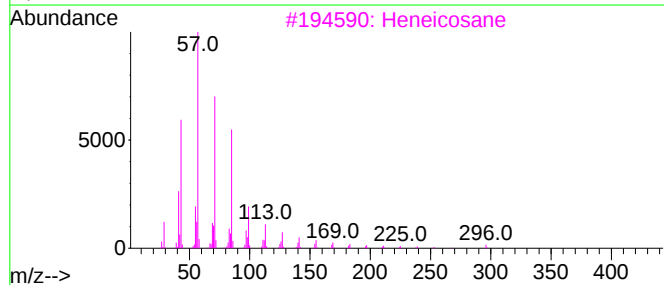
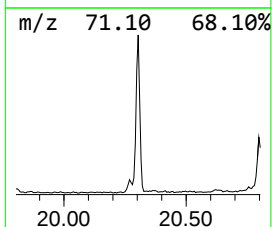
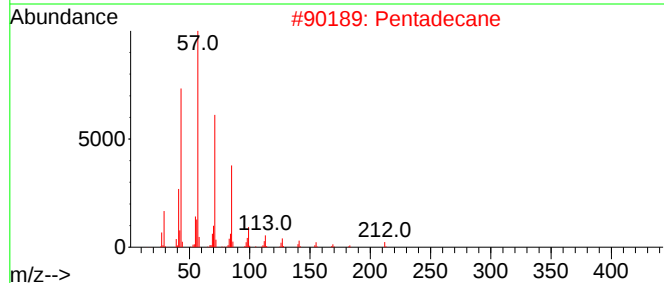
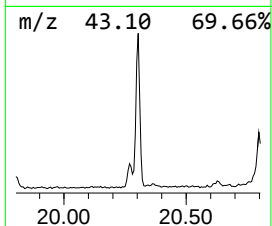
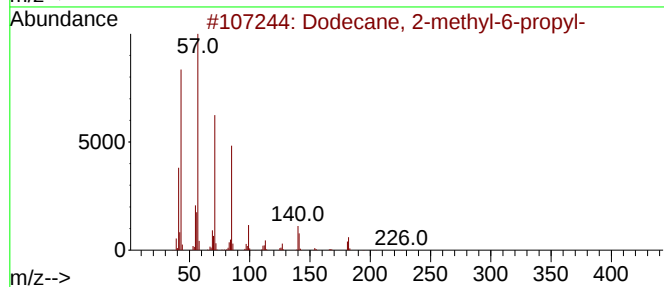
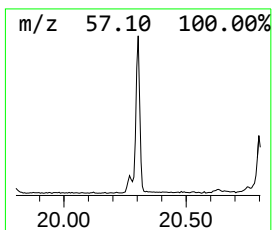
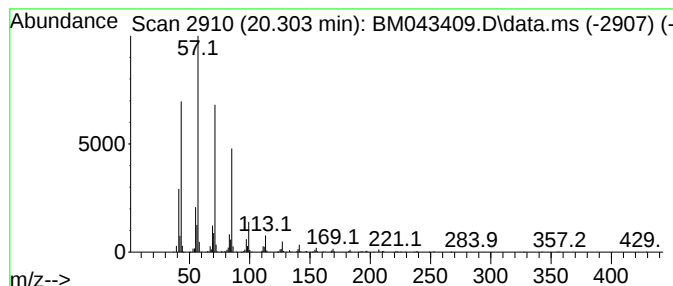
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.303	2.19 ng/ul	585065	Chrysene-d12	21.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	93
2			Pentadecane	212	C15H32	000629-62-9	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

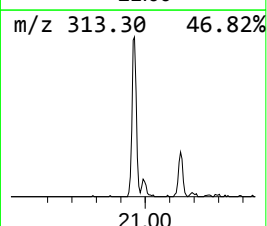
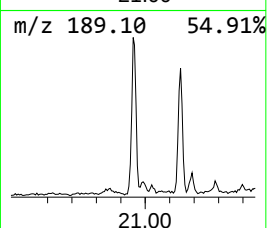
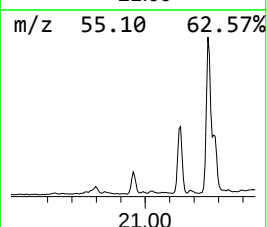
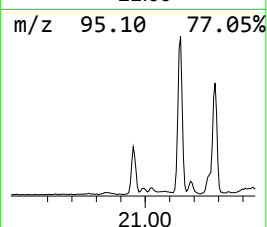
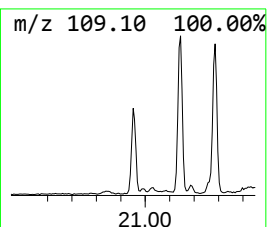
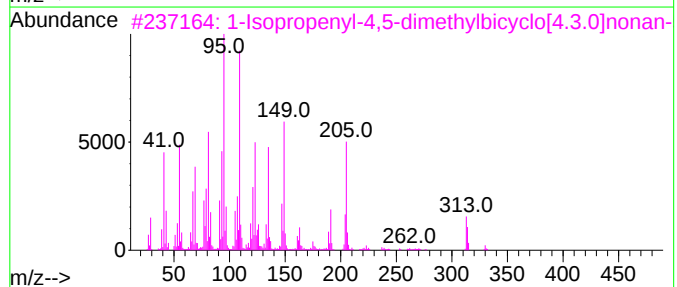
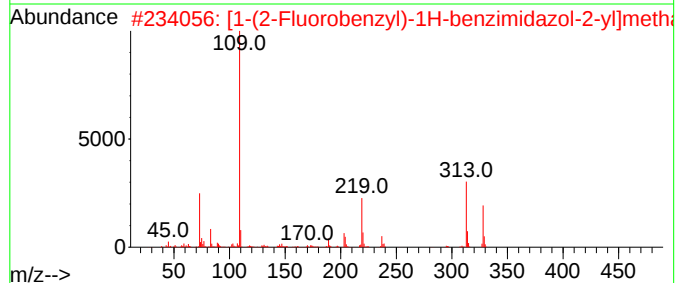
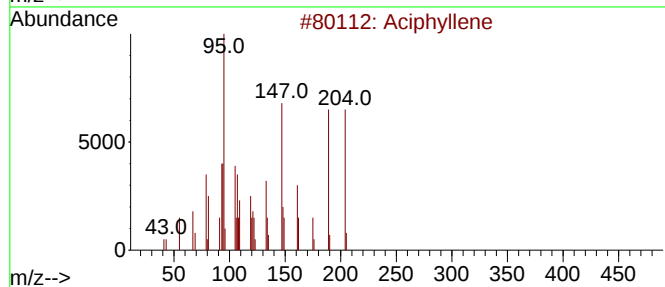
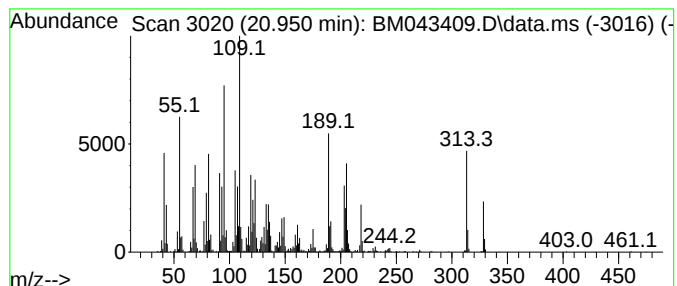
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-01 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.950	3.58 ng/ul	954658	Chrysene-d12	21.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aciphyllene	204	C15H24	087745-31-1	30
2			[1-(2-Fluorobenzyl)-1H-benzimida...	328	C18H21FN2OSi	1010474-87-2	30
3			1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30OS	1000195-85-4	25
4			4-(3,5-Dimethylpyrazol-1-yl)-1,2...	189	C8H7N5O	1000436-50-1	20
5			4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

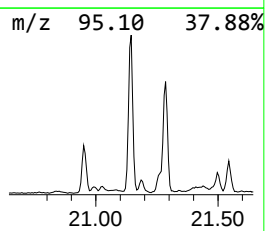
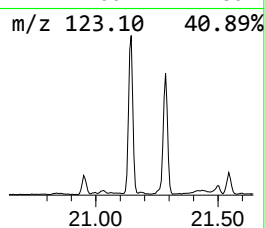
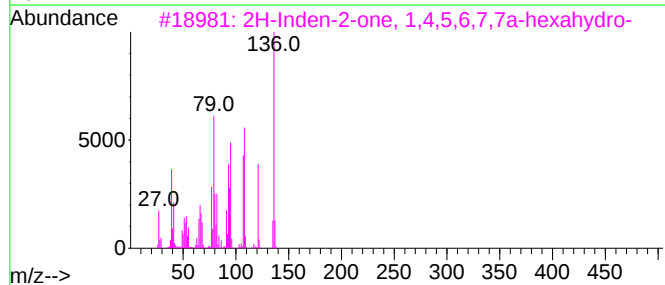
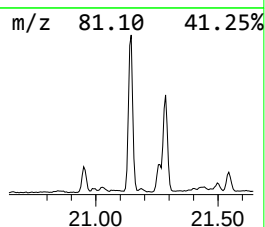
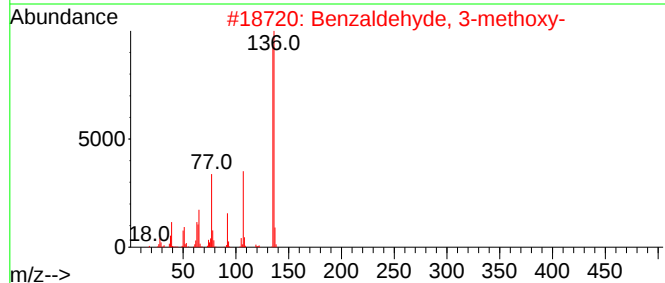
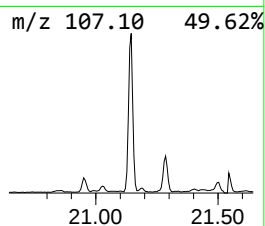
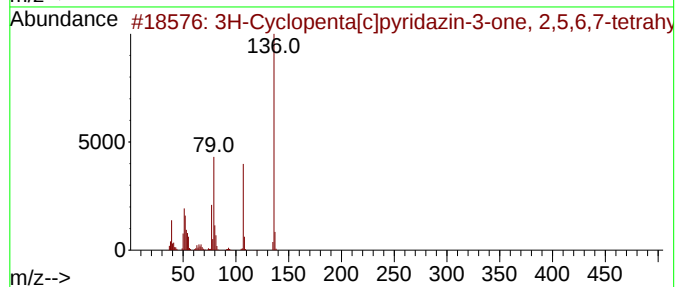
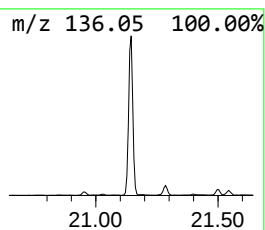
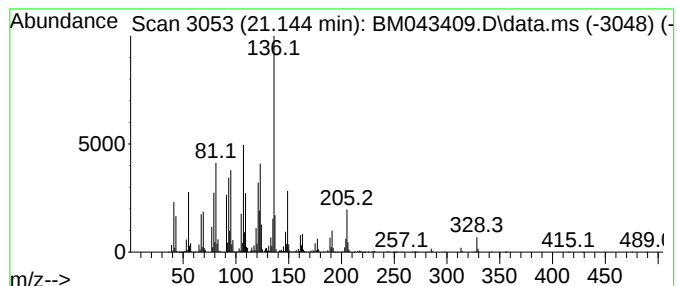
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.144	13.87 ng/ul	3698710	Chrysene-d12	21.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3H-Cyclopenta[c]pyridazin-3-one,...	136	C7H8N2O	1000338-22-1	35
2			Benzaldehyde, 3-methoxy-	136	C8H8O2	000591-31-1	35
3			2H-Inden-2-one, 1,4,5,6,7,7a-hex...	136	C9H12O	039163-29-6	35
4			Allopurinol	136	C5H4N4O	000315-30-0	22
5			2-Hydroxy-3-methylbenzaldehyde	136	C8H8O2	000824-42-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

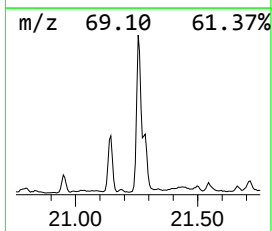
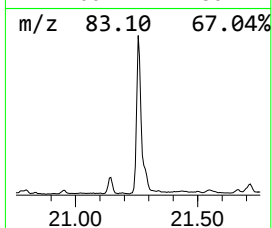
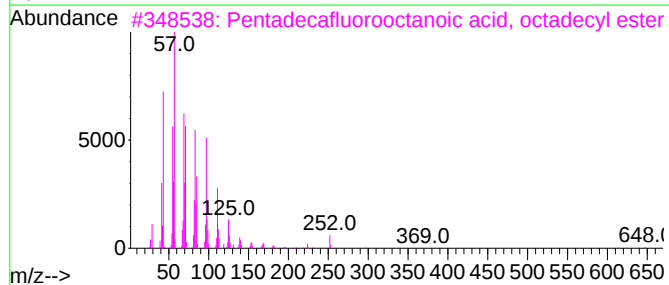
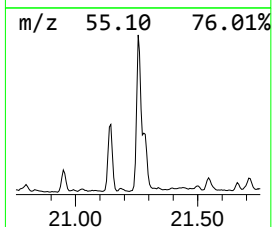
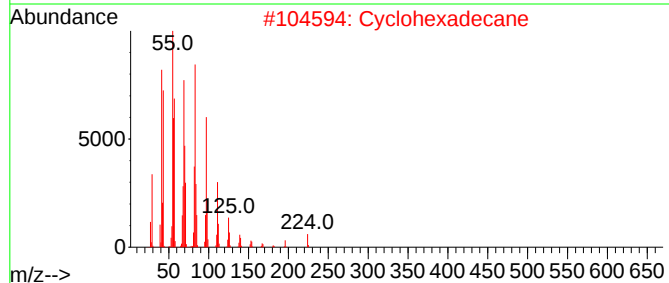
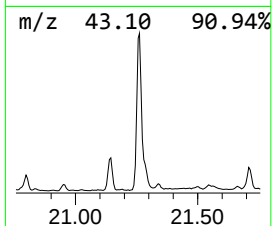
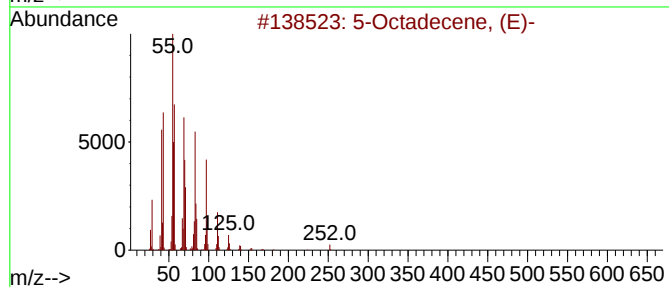
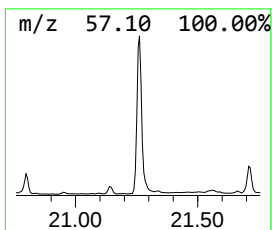
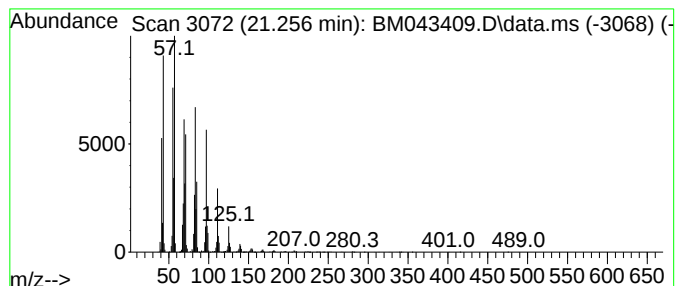
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.256	13.55 ng/ul	3613660	Chrysene-d12	21.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	94
2			Cyclohexadecane	224	C16H32	000295-65-8	94
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
4			17-Pentatriacontene	491	C35H70	006971-40-0	91
5			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

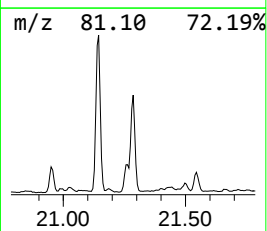
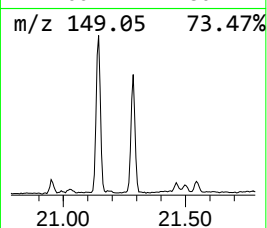
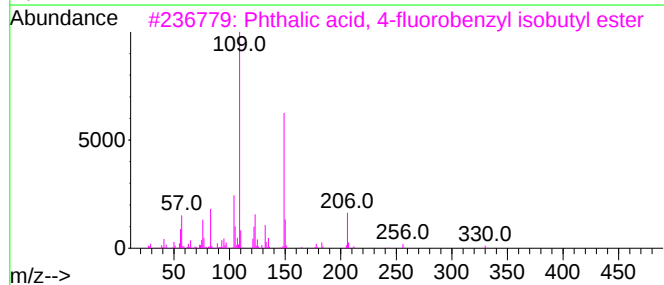
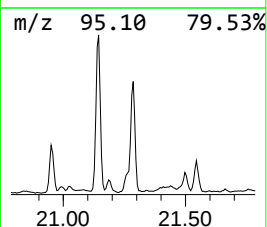
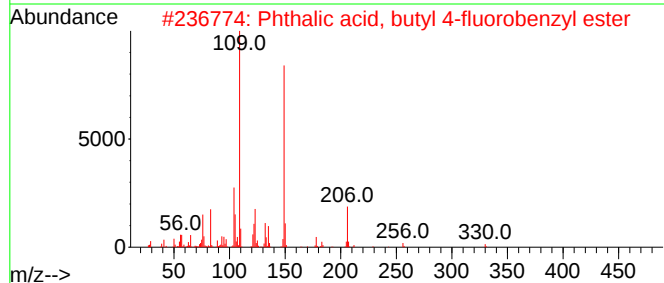
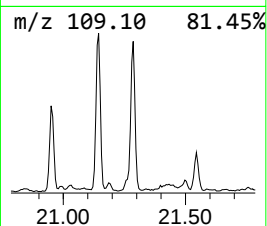
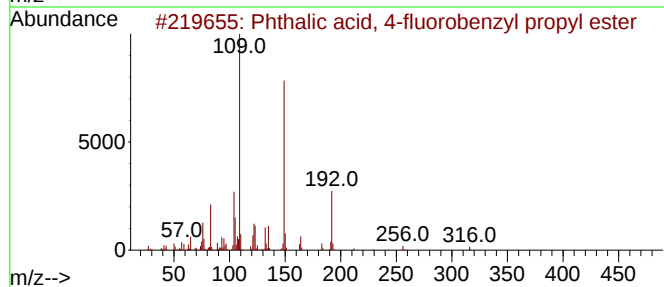
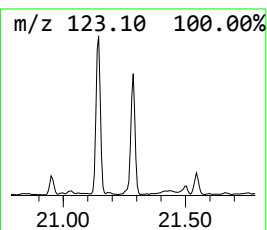
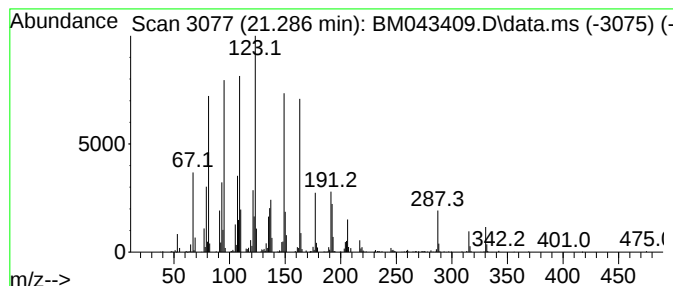
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-03 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.286	6.52 ng/ul	1738390	Chrysene-d12	21.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 4-fluorobenzyl pr...	316	C18H17F04	1010377-74-1	38
2			Phthalic acid, butyl 4-fluoroben...	330	C19H19F04	1000377-74-3	30
3			Phthalic acid, 4-fluorobenzyl is...	330	C19H19F04	1000377-74-2	27
4			Phthalic acid, 2-fluorobenzyl is...	330	C19H19F04	1010371-07-2	27
5			Ethyl 2-(4-fluorobenzamido)benzoate	287	C16H14FN03	305377-07-5	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

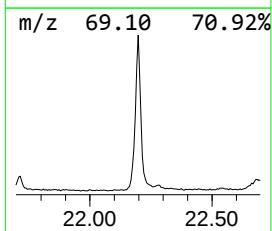
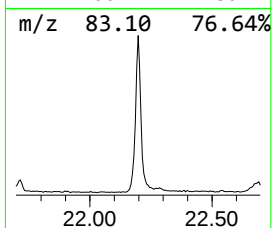
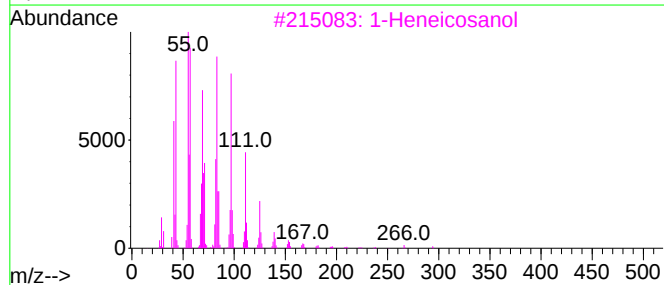
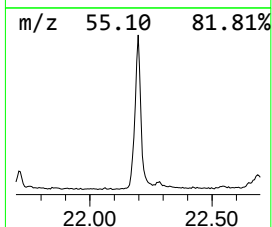
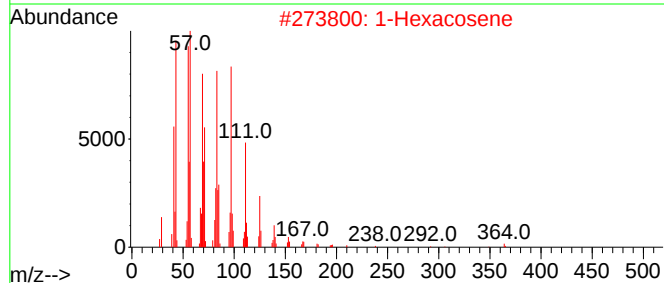
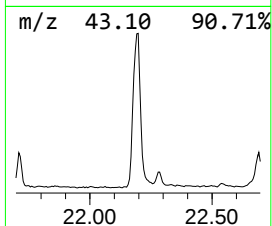
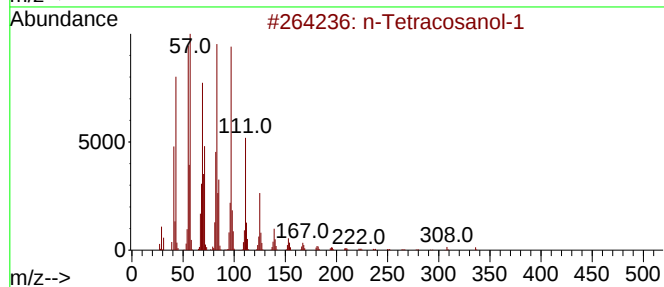
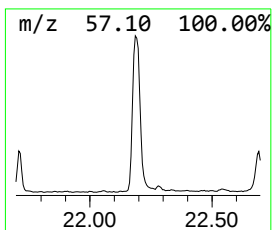
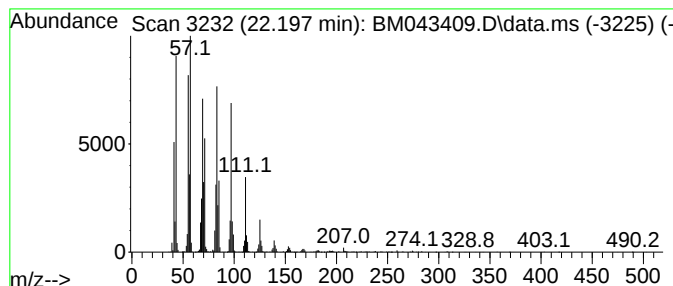
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 10 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.197	13.10 ng/ul	3493170	Chrysene-d12	21.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1			354	C24H50O	000506-51-4	94
2	1-Hexacosene			364	C26H52	018835-33-1	94
3	1-Heneicosanol			312	C21H44O	015594-90-8	93
4	1-Heptacosanol			396	C27H56O	002004-39-9	91
5	1-Hexacosanol			382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

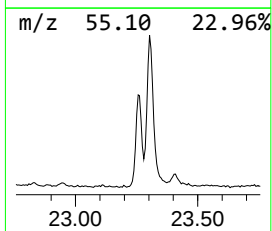
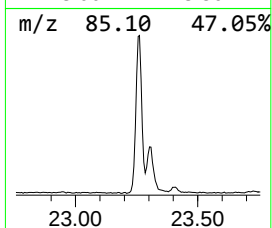
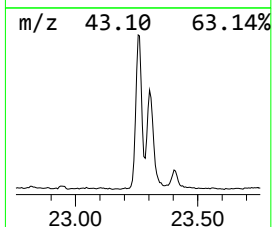
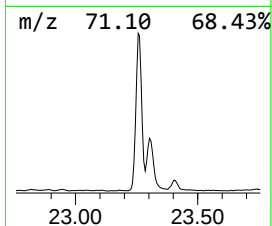
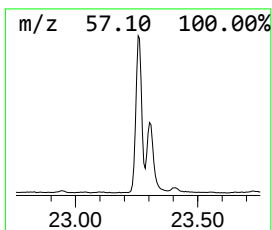
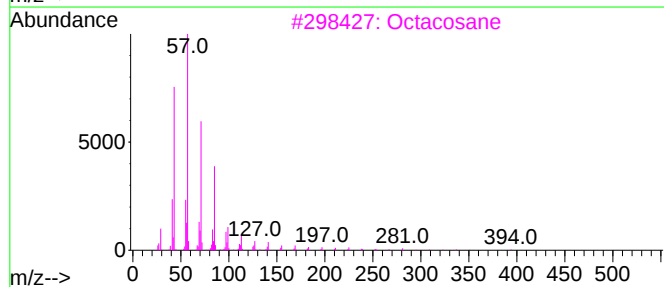
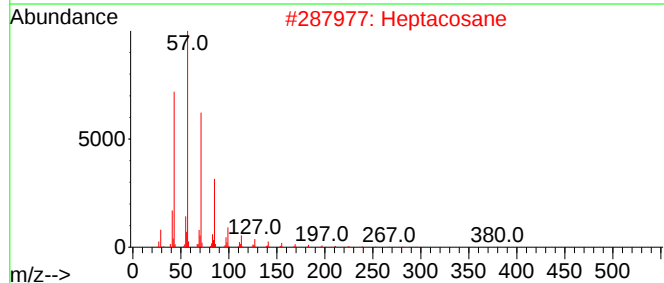
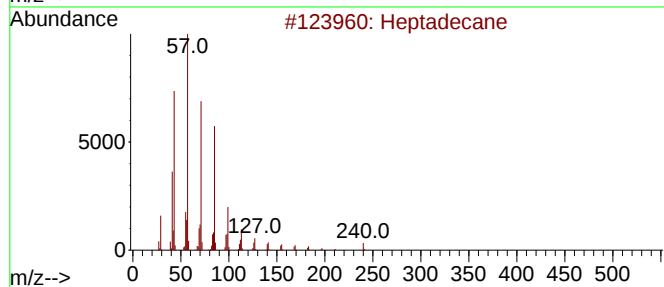
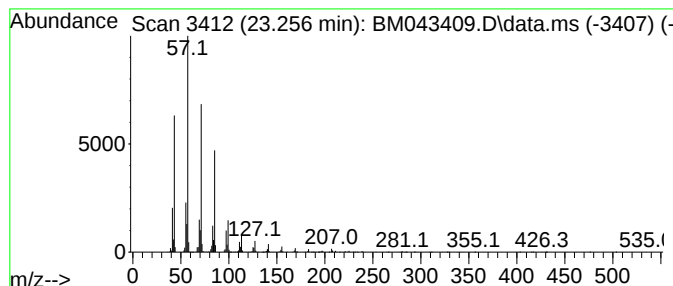
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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.
23.256	9.50 ng/ul	2481940	Perylene-d12	23.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	93
2			Heptacosane	380	C27H56	000593-49-7	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

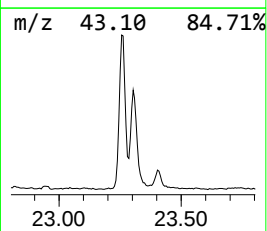
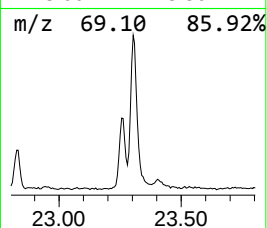
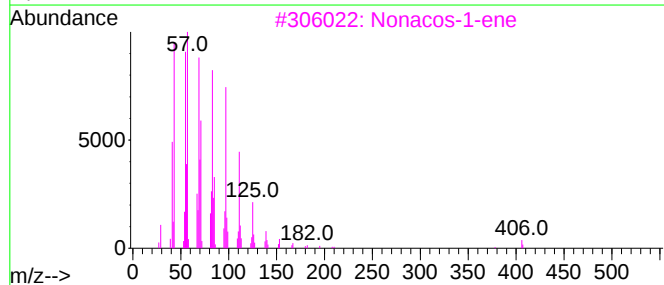
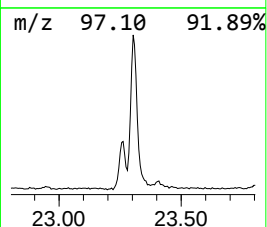
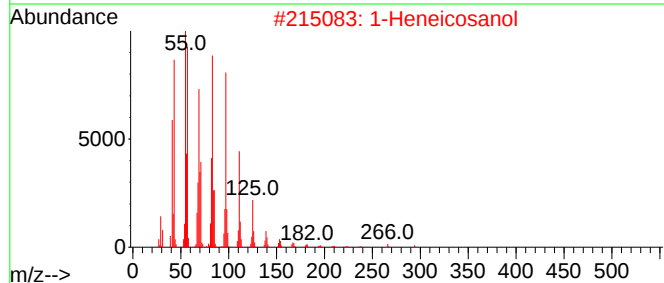
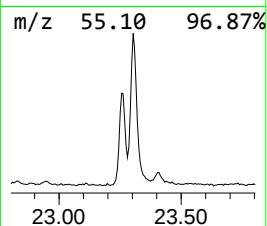
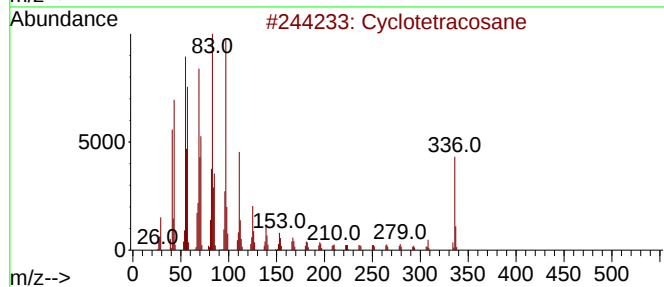
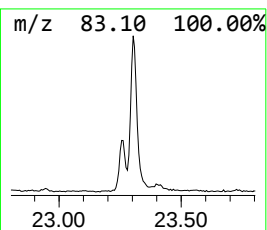
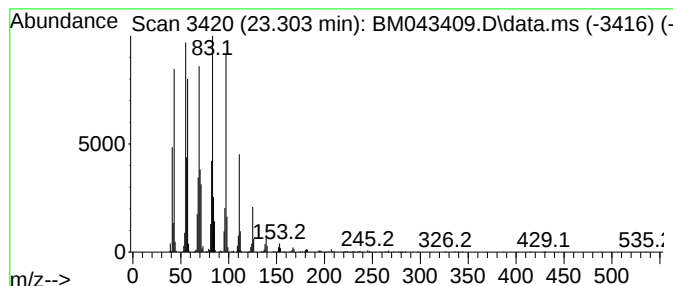
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 12 (DEL) Alkane: Cyclic23.303 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.303	9.91 ng/ul	2588200	Perylene-d12	23.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	91
3		Nonacos-1-ene	406	C29H58	018835-35-3	91
4		Octacosanol	410	C28H58O	000557-61-9	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

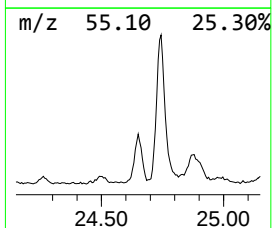
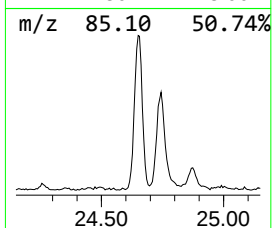
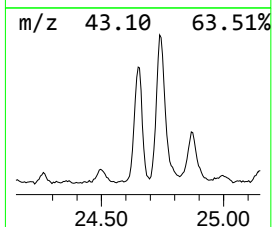
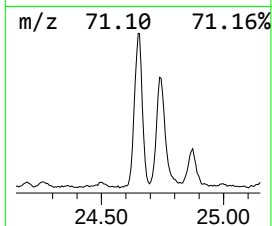
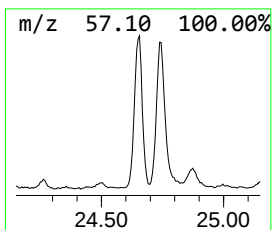
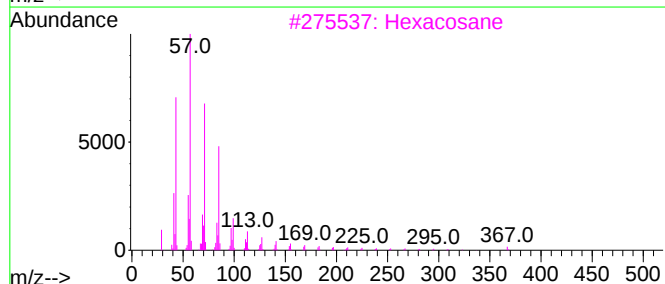
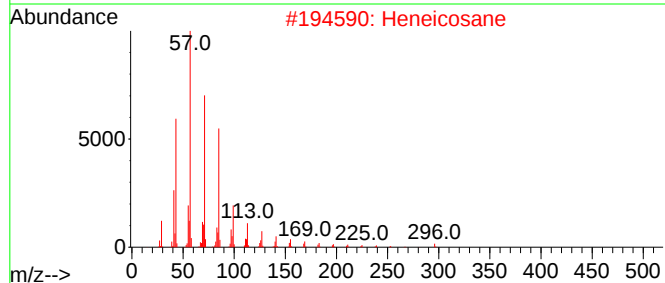
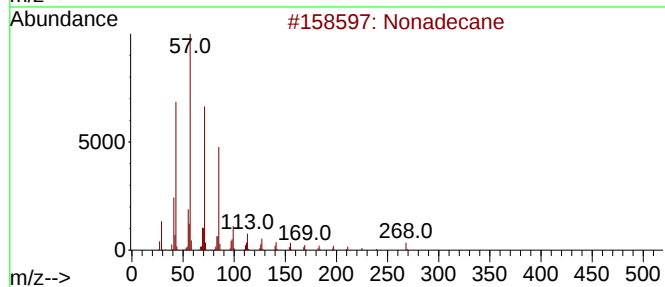
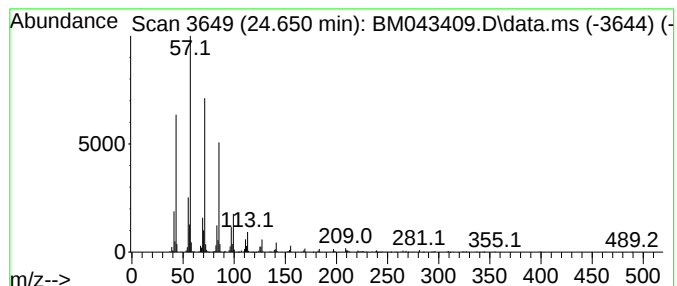
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 13 (DEL) Alkane: Straight-Chai... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.650	4.25 ng/ul	1109540	Perylene-d12	23.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Hexatriacontane	507	C36H74	000630-06-8	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

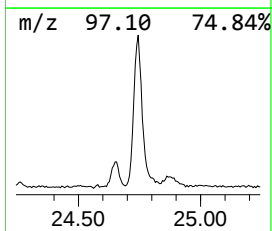
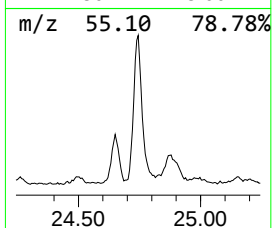
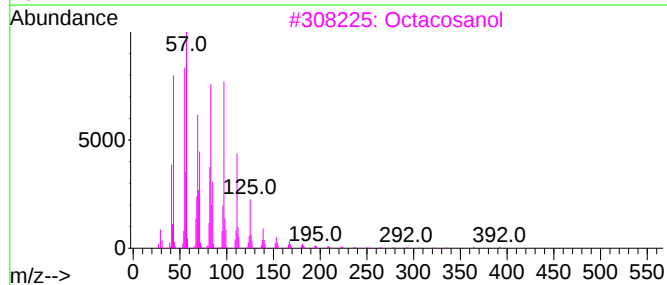
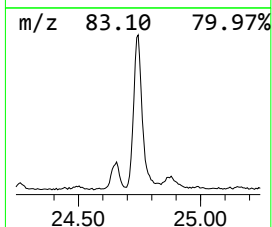
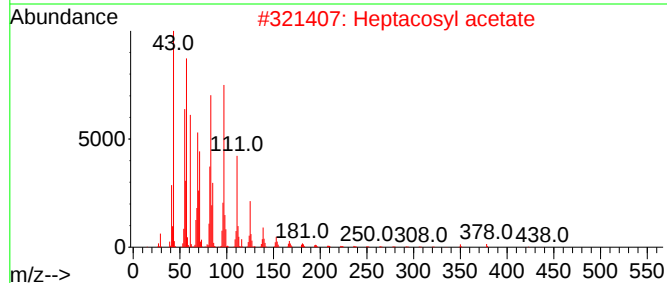
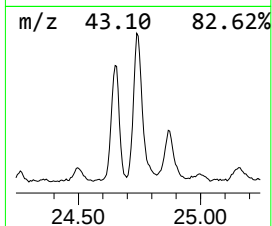
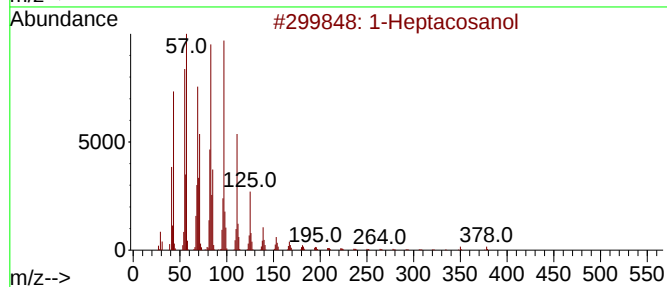
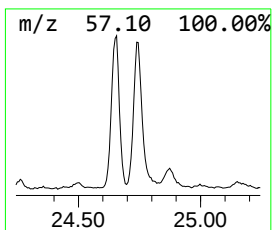
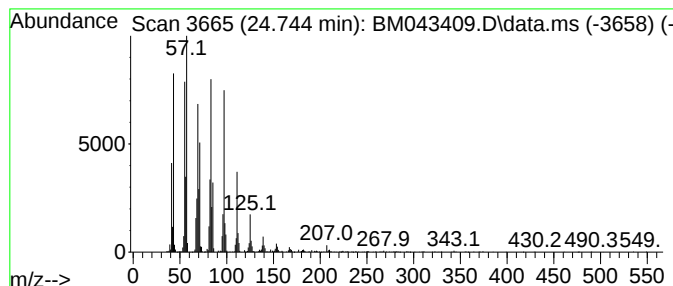
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 14 1-Heptacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.744	9.39 ng/ul	2454030	Perylene-d12	23.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol			396	C27H56O	002004-39-9	95
2	Heptacosyl acetate			438	C29H58O2	1000351-78-2	95
3	Octacosanol			410	C28H58O	000557-61-9	95
4	n-Tetracosanol-1			354	C24H50O	000506-51-4	94
5	1-Tricosene			322	C23H46	018835-32-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

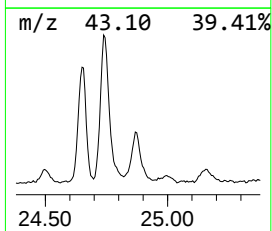
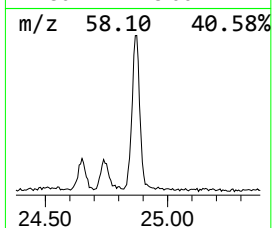
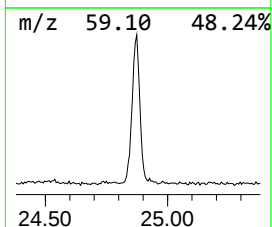
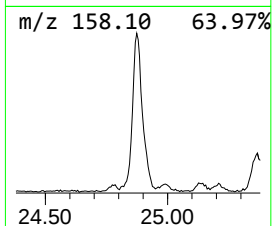
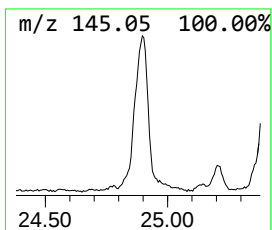
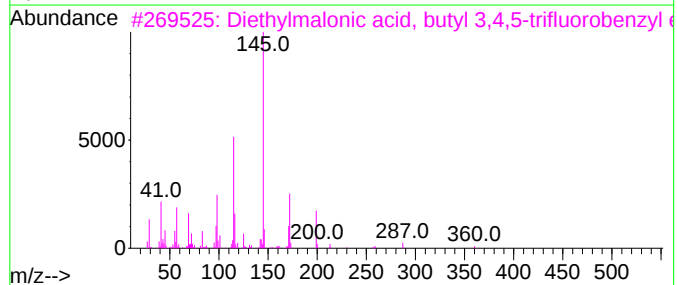
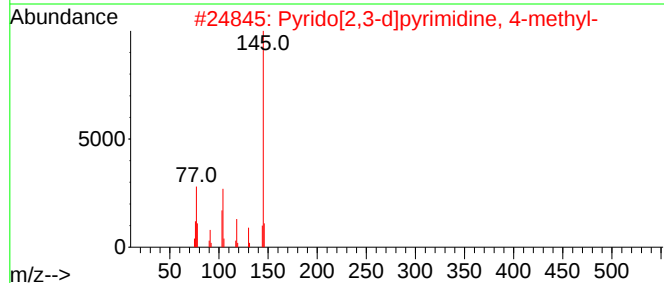
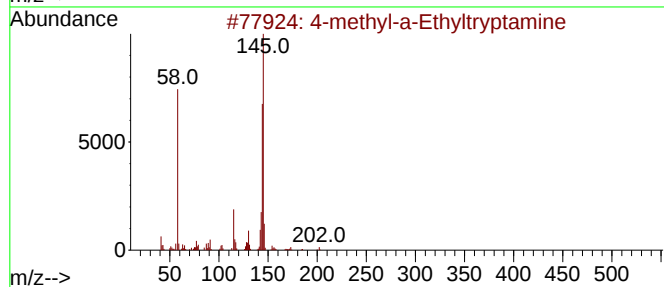
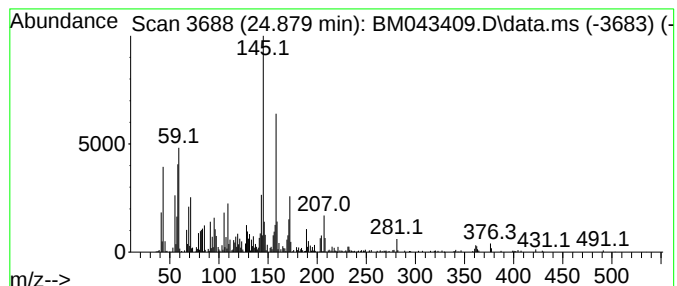
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 15 unknown-04

Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.880	6.12 ng/ul	1599730	Perylene-d12	23.968	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-methyl-a-Ethyltryptamine	202	C13H18N2	028289-30-7	35
2	Pyrido[2,3-d]pyrimidine, 4-methyl-	145	C8H7N3	028732-71-0	27
3	Diethylmalonic acid, butyl 3,4,5...	360	C18H23F3O4	1000369-27-3	25
4	Glycine, N-methyl-N-(4-cyanophen...	204	C11H12N2O2	1010452-61-8	18
5	1H-Indole, 5,7-dimethyl-	145	C10H11N	054020-53-0	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

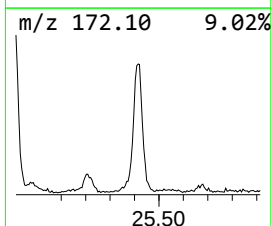
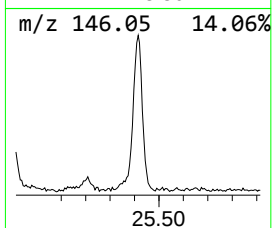
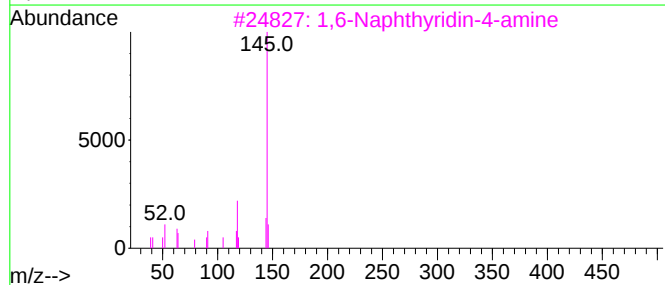
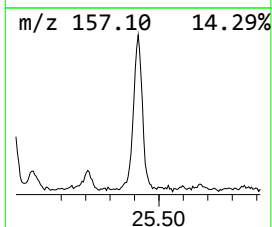
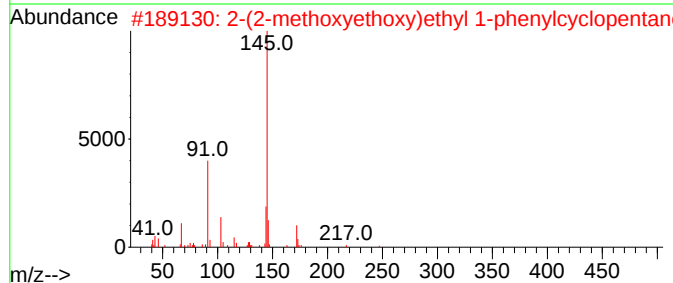
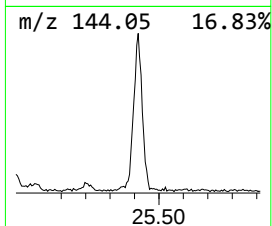
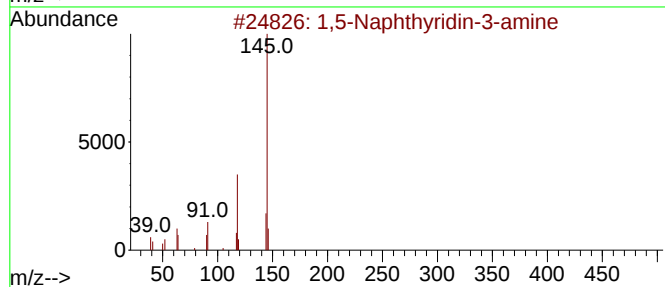
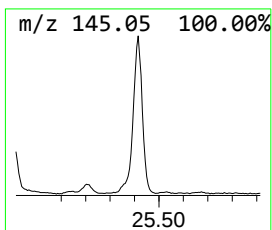
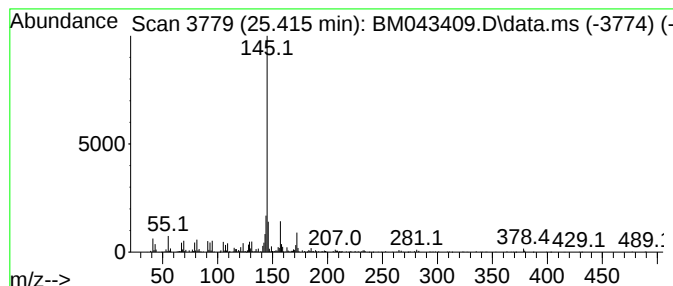
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 16 1,5-Naphthyridin-3-amine Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.415	4.16 ng/ul	1086620	Perylene-d12	23.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Naphthyridin-3-amine	145	C8H7N3	014756-77-5	64
2			2-(2-methoxyethoxy)ethyl 1-pheny...	292	C17H24O4	1000456-43-5	64
3			1,6-Naphthyridin-4-amine	145	C8H7N3	028593-08-0	59
4			.alpha.,.beta.-D-Glucopyranoside...	350	C17H34O5S	1000160-71-9	50
5			1H-Indole, 1,2-dimethyl-	145	C10H11N	000875-79-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AZ1

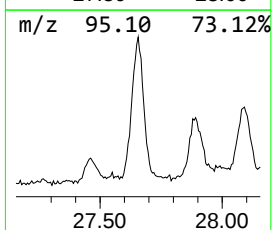
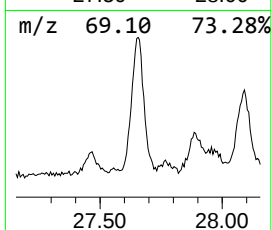
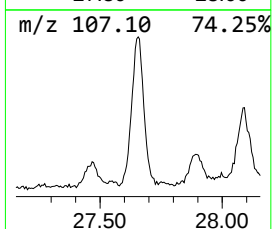
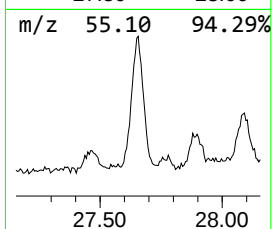
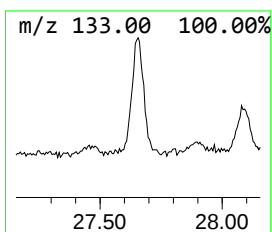
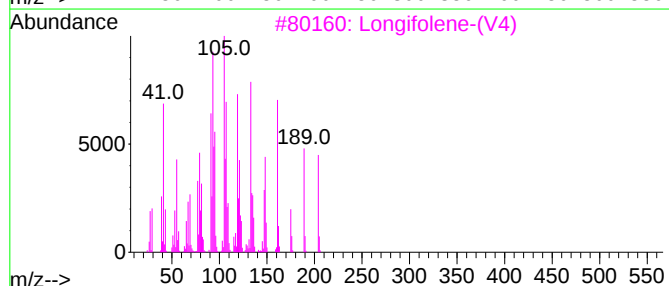
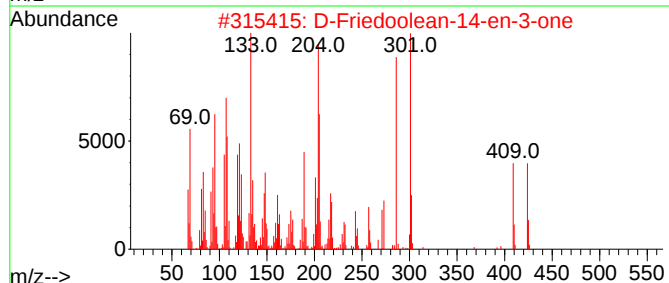
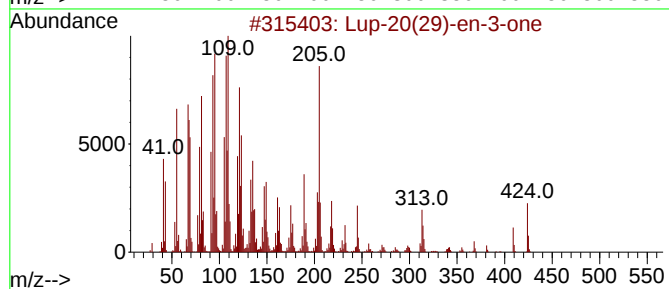
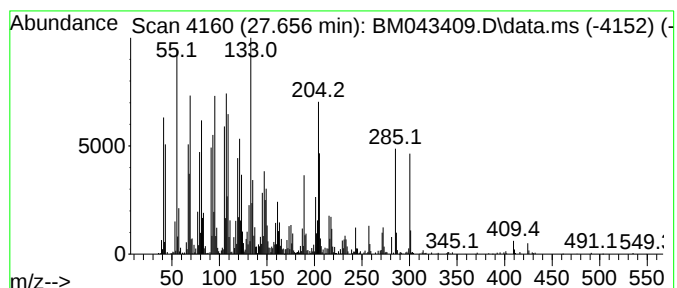
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 17 Lup-20(29)-en-3-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.656	10.93 ng/ul	2854790	Perylene-d12	23.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	64
2		D-Friedoolean-14-en-3-one	424	C30H48O	000514-07-8	58
3		Longifolene-(V4)	204	C15H24	061262-67-7	52
4		Valerena-4,7(11)-diene	204	C15H24	351222-66-7	46
5		Thunbergol	290	C20H34O	025269-17-4	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043409.D
Acq On : 19 Dec 2023 00:46
Operator : MA/JU
Sample : 05807-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

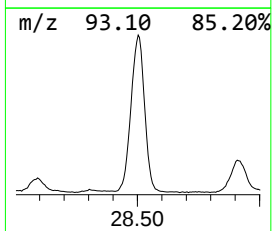
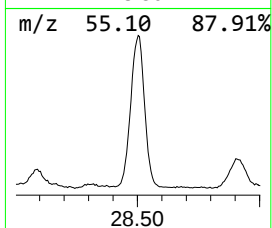
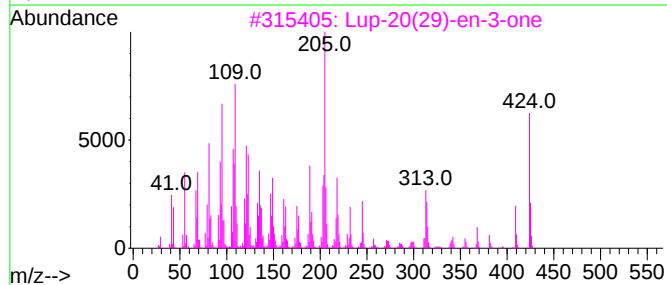
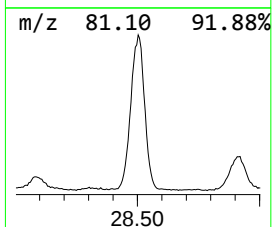
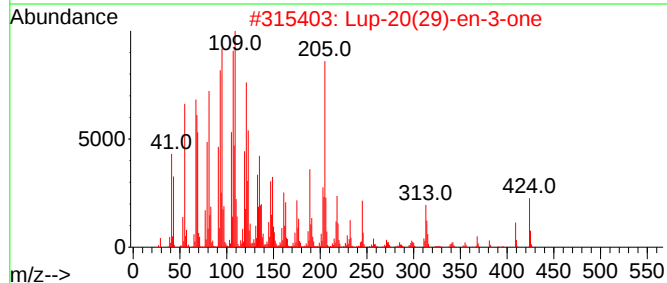
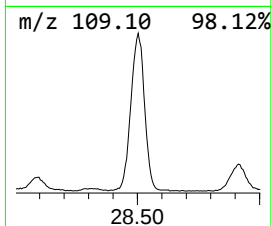
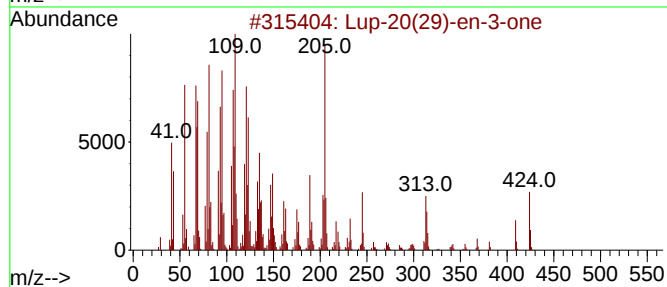
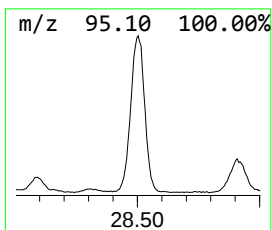
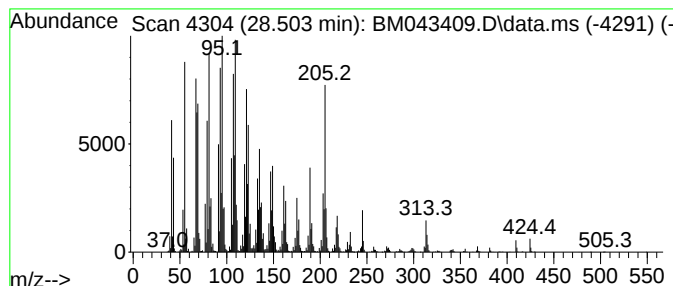
Instrument :
BNA_M
ClientSampleId :
C0AZ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 18 6,10-Dimethyl-3-(1-methylet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.503	56.54 ng/ul	14771100	Perylene-d12	23.968	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
3	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	95
4	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	64
5	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
 Data File : BM043409.D
 Acq On : 19 Dec 2023 00:46
 Operator : MA/JU
 Sample : 05807-09
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 C0AZ1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.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
n-Hexadecanoic ...	18.262	4.5	ng/ul	1170350	4	17.362	5240390	20.0
(DEL) Alkane: S...	20.303	2.2	ng/ul	585065	5	21.538	5334310	20.0
unknown-01	20.950	3.6	ng/ul	954658	5	21.538	5334310	20.0
unknown-02	21.144	13.9	ng/ul	3698710	5	21.538	5334310	20.0
(DEL) Alkane: S...	21.256	13.6	ng/ul	3613660	5	21.538	5334310	20.0
unknown-03	21.286	6.5	ng/ul	1738390	5	21.538	5334310	20.0
n-Tetracosanol-1	22.197	13.1	ng/ul	3493170	5	21.538	5334310	20.0
(DEL) Alkane: S...	23.256	9.5	ng/ul	2481940	6	23.968	5225140	20.0
(DEL) Alkane: C...	23.303	9.9	ng/ul	2588200	6	23.968	5225140	20.0
(DEL) Alkane: S...	24.650	4.3	ng/ul	1109540	6	23.968	5225140	20.0
1-Heptacosanol	24.744	9.4	ng/ul	2454030	6	23.968	5225140	20.0
unknown-04	24.880	6.1	ng/ul	1599730	6	23.968	5225140	20.0
1,5-Naphthyridi...	25.415	4.2	ng/ul	1086620	6	23.968	5225140	20.0
Lup-20(29)-en-3...	27.656	10.9	ng/ul	2854790	6	23.968	5225140	20.0
6,10-Dimethyl-3...	28.503	56.5	ng/ul	14771100	6	23.968	5225140	20.0