

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
 Data File : BP019022.D
 Acq On : 22 Dec 2023 04:41
 Operator : MA/JU
 Sample : 05808-07
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0AZ9

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_P\Methods\SFAM-EPA-BP120123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP019022.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.252	24	28	35	rVB	25305	33156	0.15%	0.058%
2	3.899	134	138	143	rVB	15630	25978	0.12%	0.045%
3	4.228	189	194	198	rBV	52057	70416	0.32%	0.122%
4	4.640	260	264	272	rVB	30542	41185	0.19%	0.072%
5	4.916	307	311	320	rVB	25389	36990	0.17%	0.064%
6	6.993	651	664	680	rBV2	363086	725712	3.32%	1.260%
7	7.157	686	692	703	rVB	298418	459480	2.10%	0.798%
8	7.351	717	725	734	rBV	373417	589328	2.70%	1.023%
9	7.440	734	740	747	rVV	11789	22233	0.10%	0.039%
10	7.816	797	804	814	rBV	482868	763374	3.49%	1.325%
11	8.534	916	926	938	rBV	371029	610473	2.79%	1.060%
12	8.645	938	945	958	rVV	457276	723055	3.31%	1.255%
13	8.787	962	969	980	rVB2	10662	29904	0.14%	0.052%
14	8.981	995	1002	1010	rBV	345799	552431	2.53%	0.959%
15	9.698	1115	1124	1135	rBV	274386	472470	2.16%	0.820%
16	9.887	1146	1156	1164	rBV	110113	234844	1.07%	0.408%
17	10.063	1179	1186	1193	rBV	41622	70289	0.32%	0.122%
18	10.240	1208	1216	1231	rVB	460973	768940	3.52%	1.335%
19	10.610	1271	1279	1287	rBV	619895	1039444	4.76%	1.805%
20	10.757	1295	1304	1315	rBV	277292	510756	2.34%	0.887%
21	11.163	1364	1373	1383	rBV3	34867	87363	0.40%	0.152%
22	11.410	1409	1415	1426	rVB	37944	80254	0.37%	0.139%
23	13.257	1720	1729	1738	rBV5	14586	33699	0.15%	0.059%
24	13.357	1741	1746	1750	rBV2	19374	29628	0.14%	0.051%
25	13.869	1825	1833	1842	rBV	886645	1216745	5.57%	2.113%
26	14.145	1869	1880	1894	rBV	976209	1450262	6.64%	2.518%
27	14.451	1924	1932	1941	rBV	999251	1526060	6.98%	2.650%
28	14.669	1962	1969	1981	rBV	292262	559385	2.56%	0.971%
29	14.769	1981	1986	1991	rVV	41598	70315	0.32%	0.122%
30	14.822	1991	1995	2000	rVV4	17143	29918	0.14%	0.052%
31	14.880	2000	2005	2013	rVB4	19381	34587	0.16%	0.060%
32	15.445	2095	2101	2110	rBV	1332616	1902787	8.71%	3.304%
33	15.575	2117	2123	2131	rBV	343809	487715	2.23%	0.847%
34	16.222	2229	2233	2241	rVB5	19910	34581	0.16%	0.060%
35	16.504	2274	2281	2286	rBV	35084	51838	0.24%	0.090%
36	16.669	2305	2309	2315	rVV	17916	26891	0.12%	0.047%

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37	17.016	2363	2368	2374	rVB	43033	62053	0.28%	0.108%
38	17.204	2392	2400	2407	rBV	1390413	1984550	9.08%	3.446%
39	17.304	2411	2417	2428	rVV	1457235	2056403	9.41%	3.570%
40	17.704	2482	2485	2490	rBV	23581	31845	0.15%	0.055%
41	17.974	2527	2531	2538	rVB	44958	61532	0.28%	0.107%
42	18.098	2547	2552	2561	rBV	379548	532516	2.44%	0.925%
43	18.416	2603	2606	2610	rVB4	19906	26410	0.12%	0.046%
44	18.616	2637	2640	2642	rBV	21865	26089	0.12%	0.045%
45	18.651	2642	2646	2653	rVB2	120453	163354	0.75%	0.284%
46	18.874	2680	2684	2688	rBV	114274	145833	0.67%	0.253%
47	18.916	2688	2691	2698	rVV2	47089	76652	0.35%	0.133%
48	19.333	2758	2762	2768	rBV	186239	240070	1.10%	0.417%
49	19.545	2792	2798	2804	rBV	2159008	2813748	12.87%	4.885%
50	20.357	2934	2936	2938	rBV2	54750	60526	0.28%	0.105%
51	20.892	2998	3027	3043	rBV2	4263465	21856481	100.00%	37.948%
52	21.015	3044	3048	3056	rVB2	514725	809283	3.70%	1.405%
53	21.298	3091	3096	3102	rVB	1987259	2469607	11.30%	4.288%
54	21.898	3195	3198	3200	rBV	205274	257704	1.18%	0.447%
55	21.927	3200	3203	3209	rVB3	290427	466174	2.13%	0.809%
56	22.633	3320	3323	3333	rVB2	321268	491776	2.25%	0.854%
57	22.933	3370	3374	3379	rVB	324911	473332	2.17%	0.822%
58	22.992	3380	3384	3394	rVB2	419259	835498	3.82%	1.451%
59	23.504	3465	3471	3484	rVB2	1456094	2908489	13.31%	5.050%
60	23.656	3491	3497	3516	rVB	1327496	2778209	12.71%	4.824%
61	23.892	3533	3537	3543	rBV	311513	564817	2.58%	0.981%

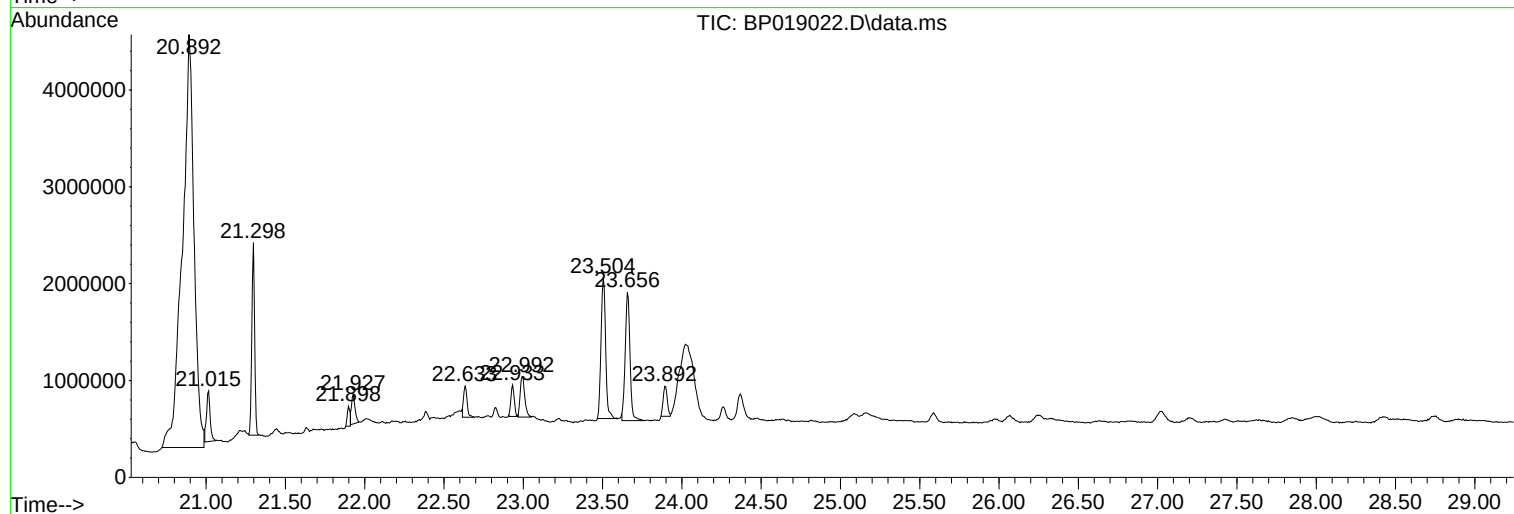
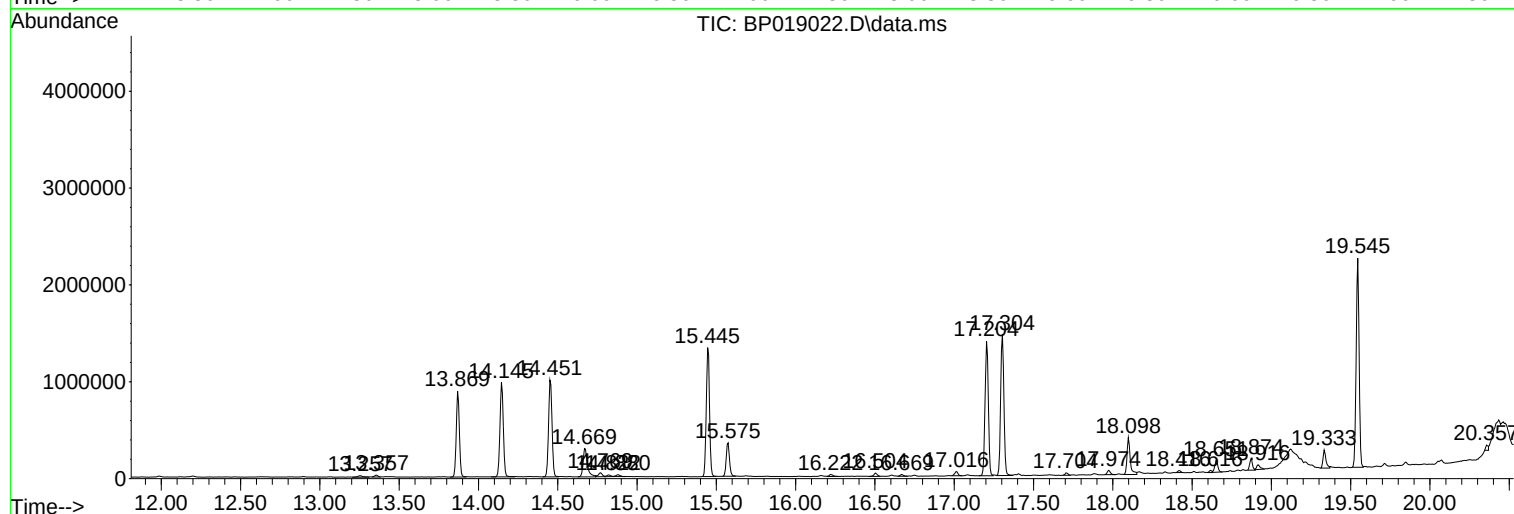
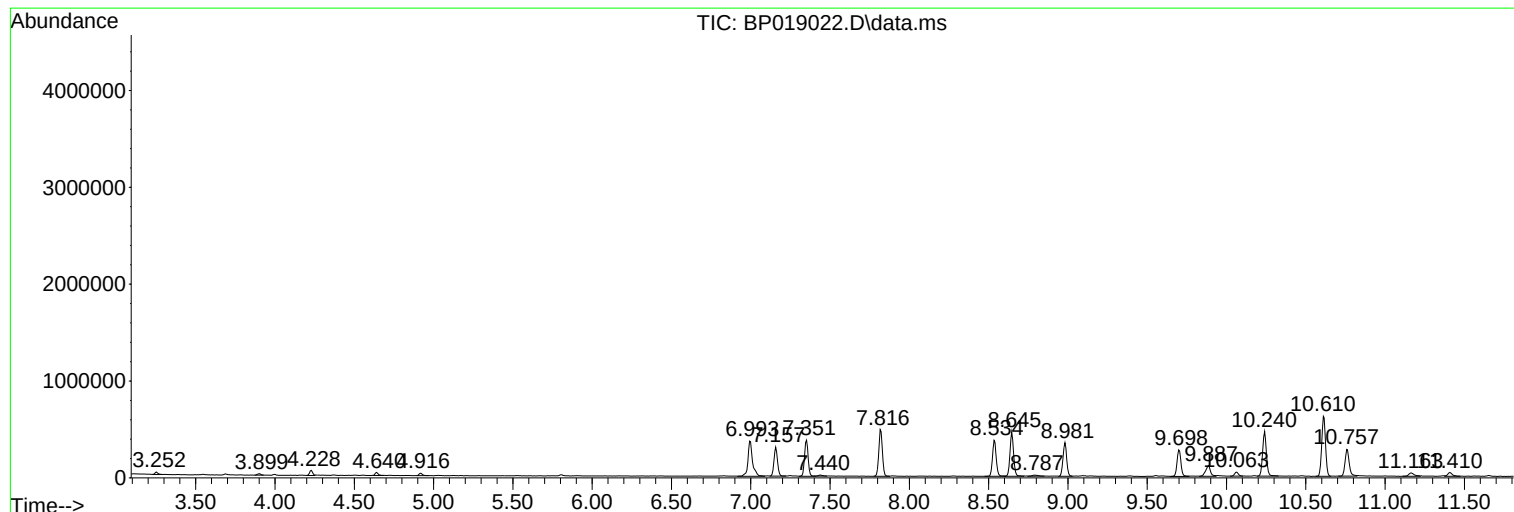
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Quant Title : SVOA CALIBRATION

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



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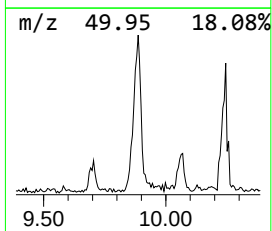
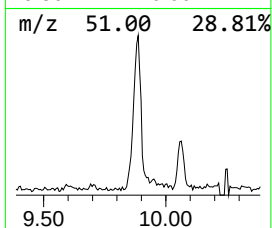
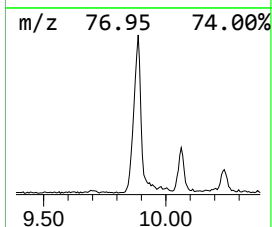
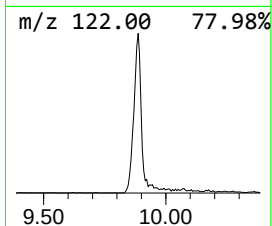
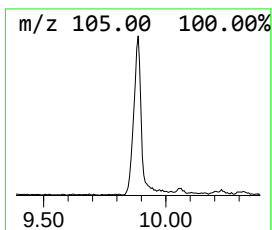
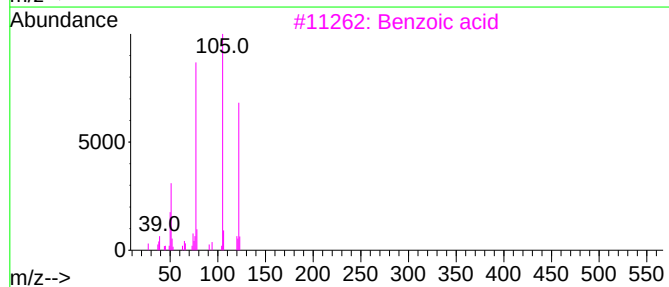
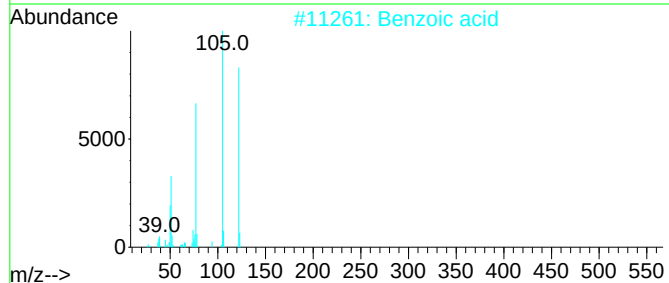
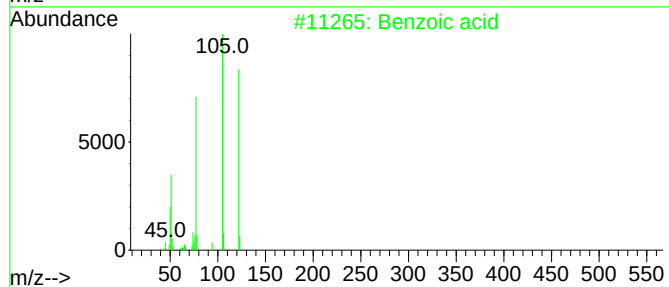
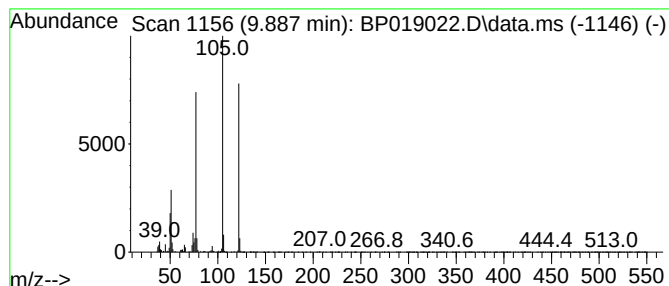
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.887	4.52 ng/ul	234844	Naphthalene-d8	10.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid	122	C7H6O2	000065-85-0	96
2			Benzoic acid	122	C7H6O2	000065-85-0	94
3			Benzoic acid	122	C7H6O2	000065-85-0	94
4			Benzoic acid	122	C7H6O2	000065-85-0	91
5			Methanol, oxo-, benzoate	150	C8H6O3	1000305-65-2	90



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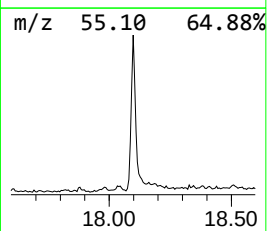
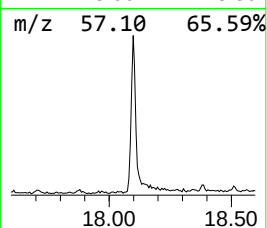
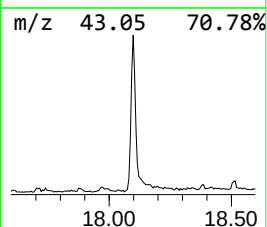
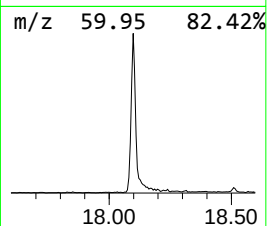
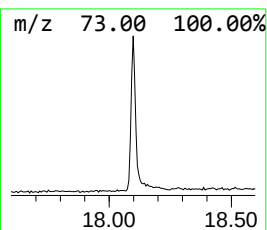
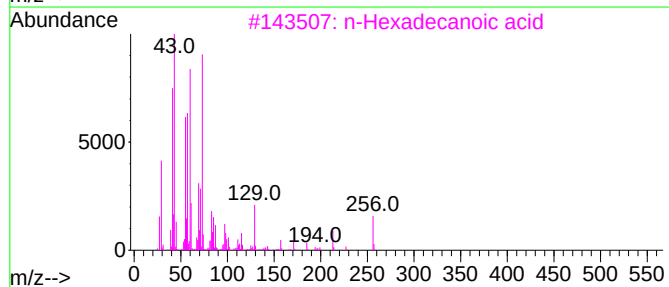
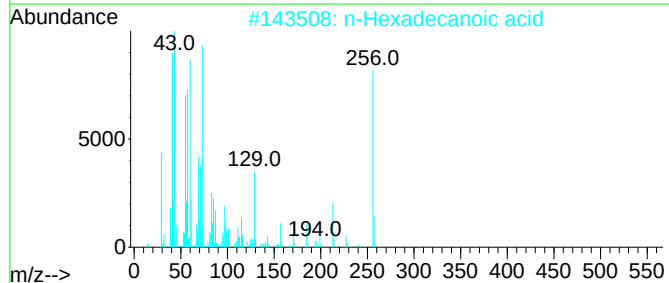
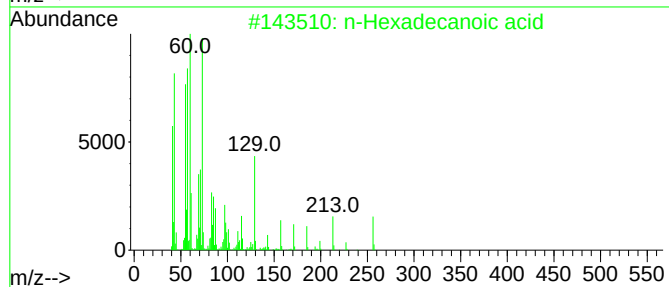
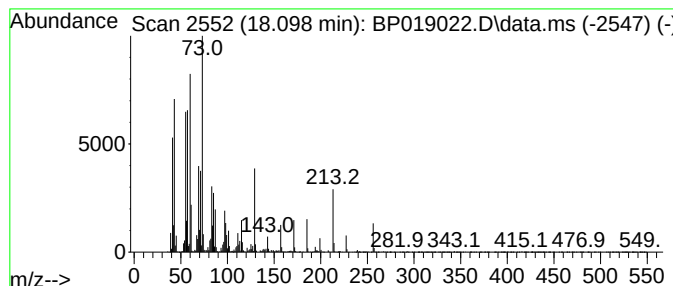
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.098	5.37 ng/ul	532516	Phenanthrene-d10	17.204

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	95
4			Octadecanoic acid	284	C18H36O2	000057-11-4	93
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	91



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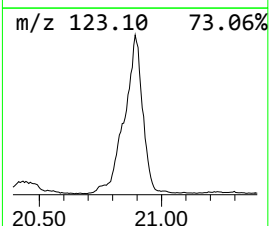
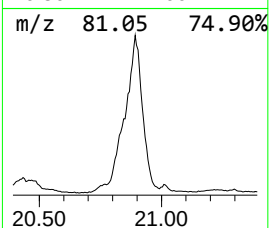
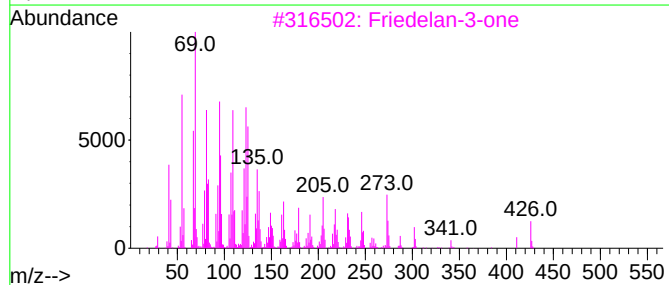
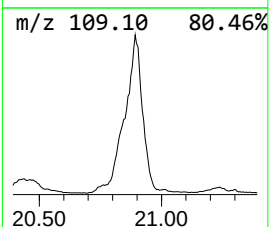
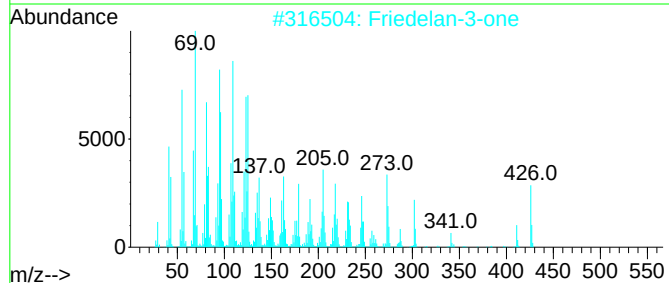
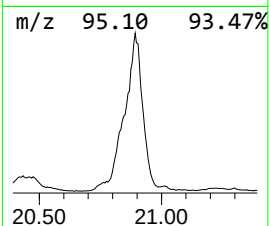
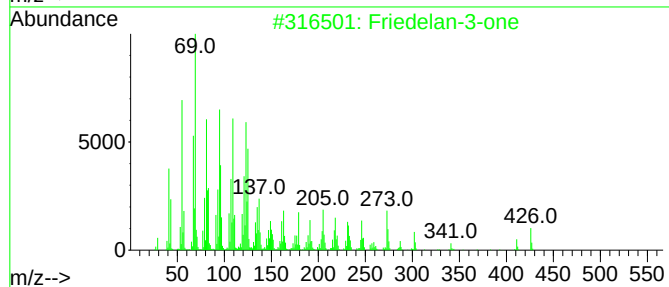
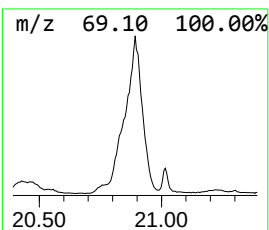
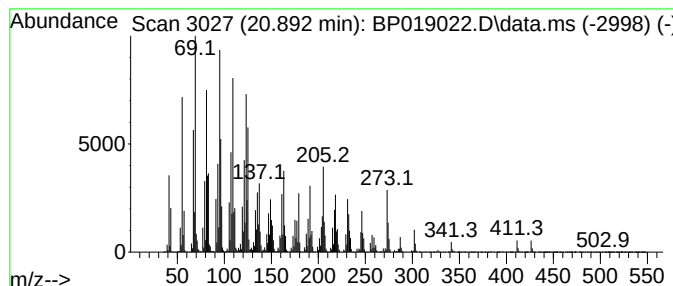
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	177.00 ng/ul	21856500	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Friedelan-3-one	426	C30H50O	000559-74-0	99
2			Friedelan-3-one	426	C30H50O	000559-74-0	99
3			Friedelan-3-one	426	C30H50O	000559-74-0	95
4			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
5			5-Cyclohexyl-1-pentene	152	C11H20	005729-54-4	56



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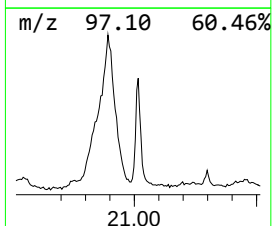
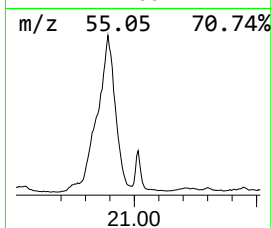
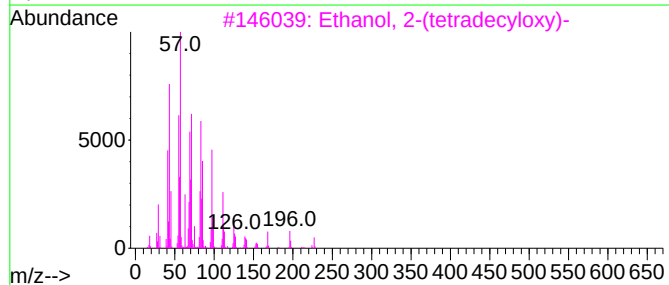
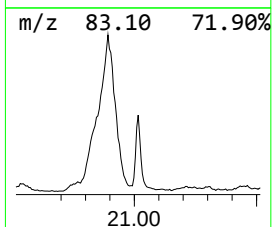
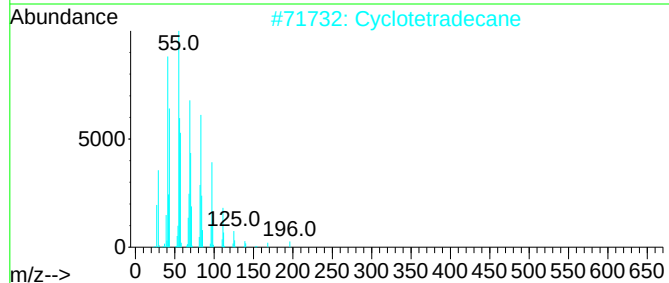
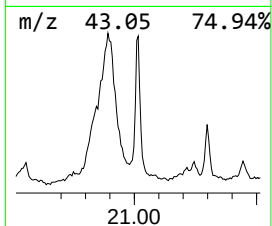
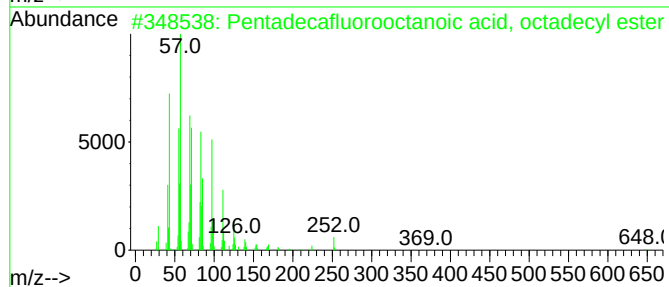
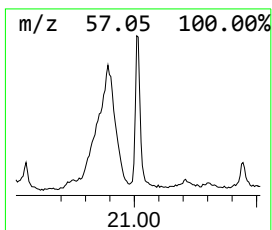
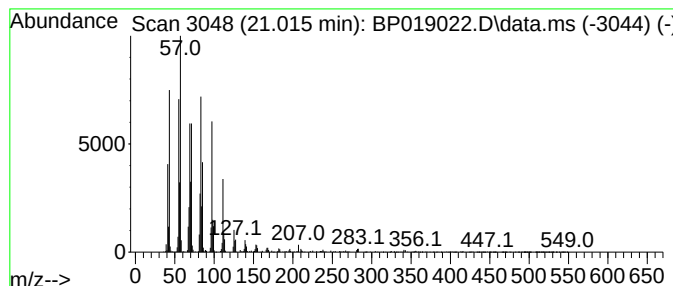
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.015	6.55 ng/ul	809283	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Cyclotetradecane	196	C14H28	000295-17-0	90
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	81
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81



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C0AZ9

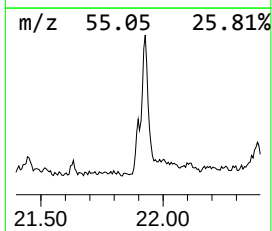
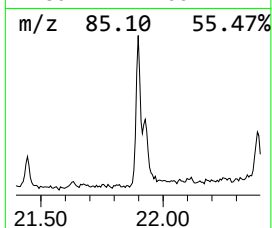
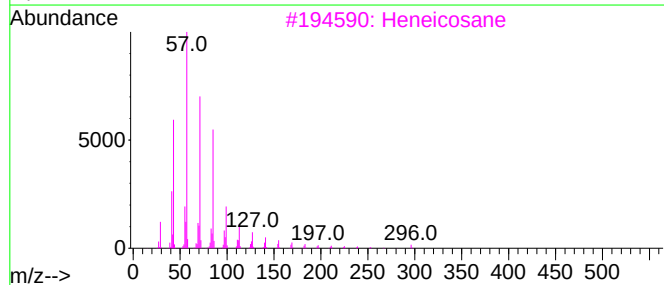
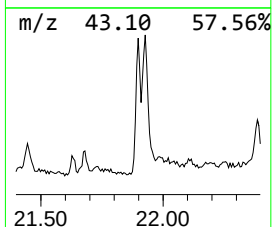
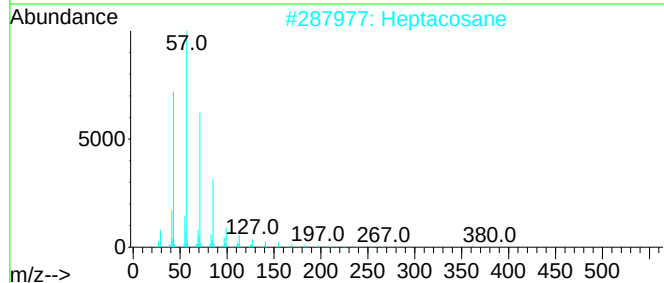
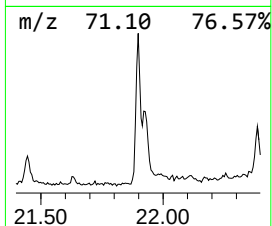
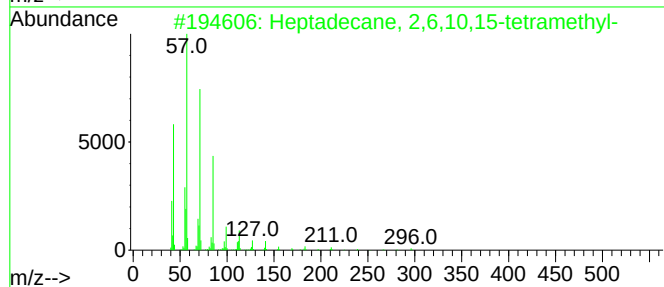
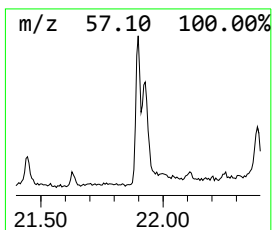
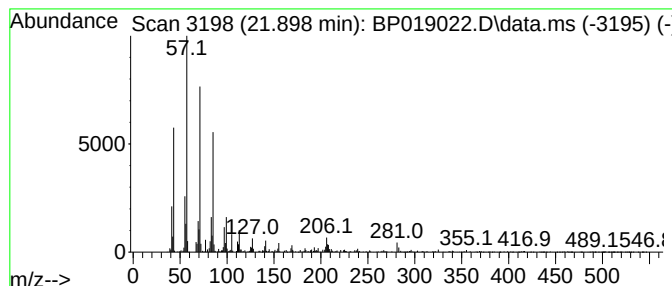
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.898	2.09 ng/ul	257704	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	96
2			Heptacosane	380	C27H56	000593-49-7	94
3			Heneicosane	296	C21H44	000629-94-7	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019022.D
Acq On : 22 Dec 2023 04:41
Operator : MA/JU
Sample : 05808-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AZ9

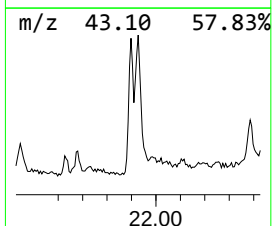
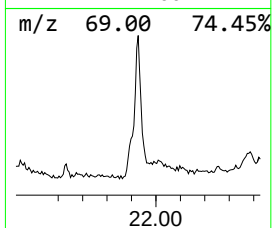
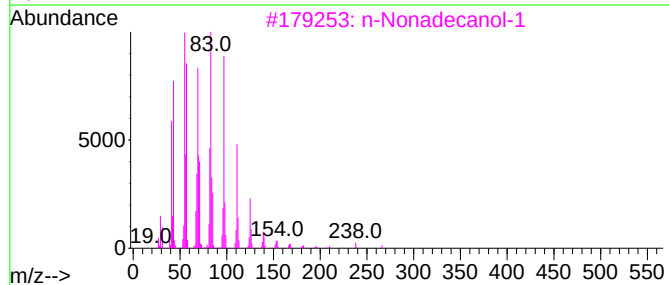
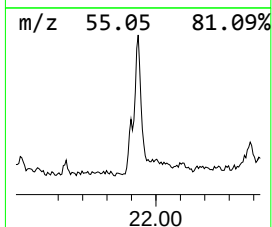
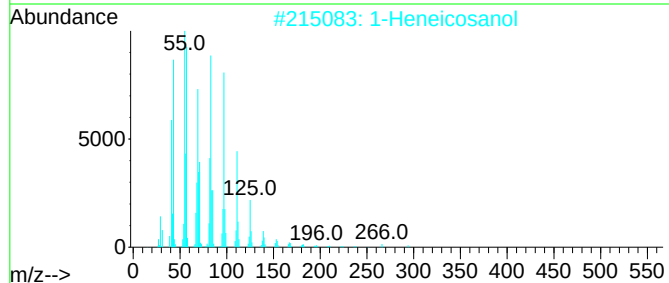
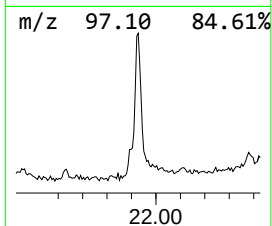
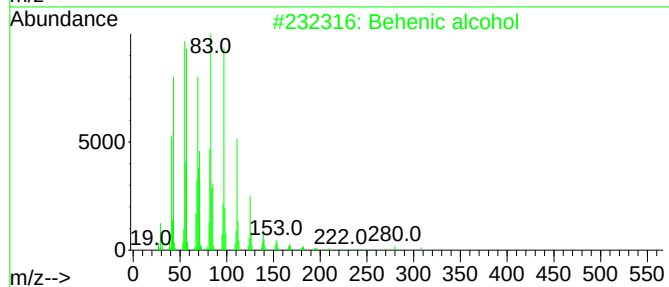
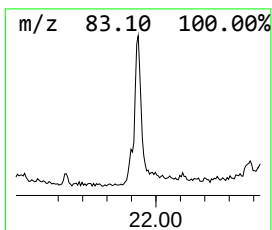
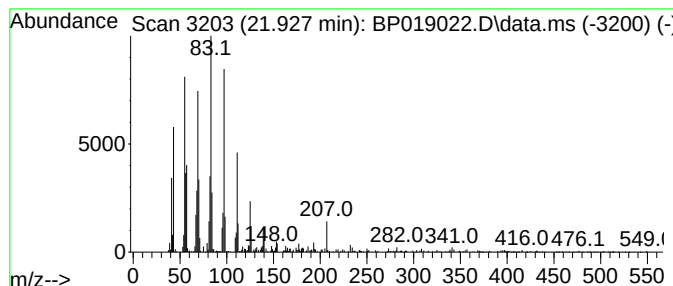
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.927	3.78 ng/ul	466174	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			Heptacosyl acetate	438	C29H58O2	1000351-78-2	87
5			1-Docosene	308	C22H44	001599-67-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019022.D
Acq On : 22 Dec 2023 04:41
Operator : MA/JU
Sample : 05808-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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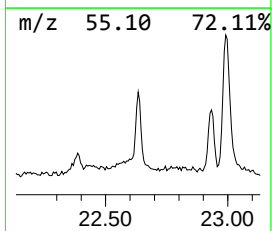
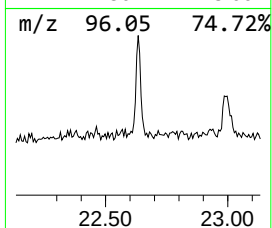
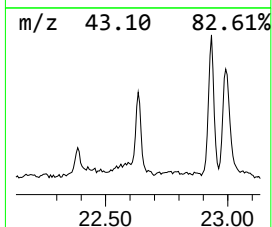
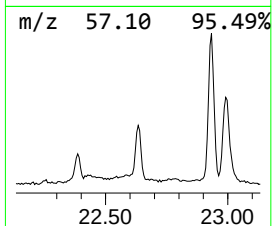
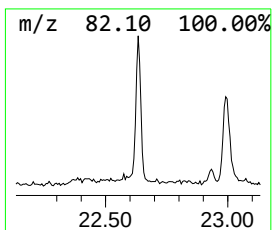
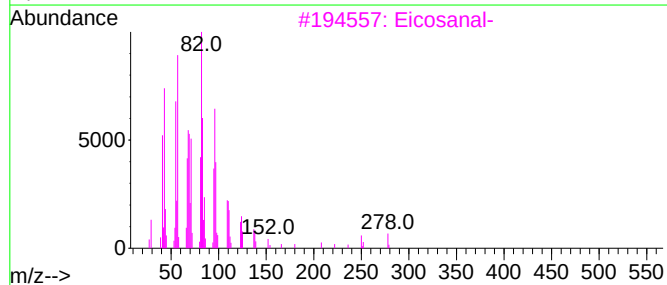
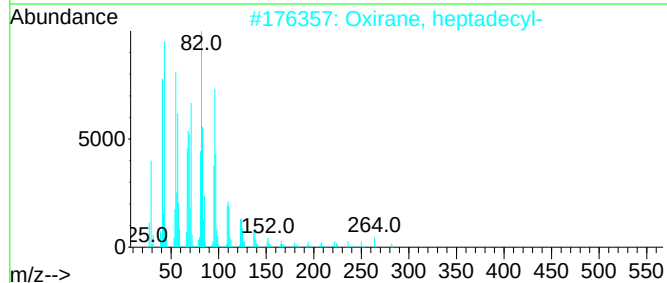
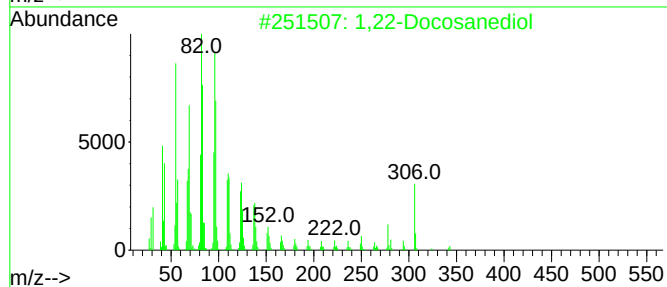
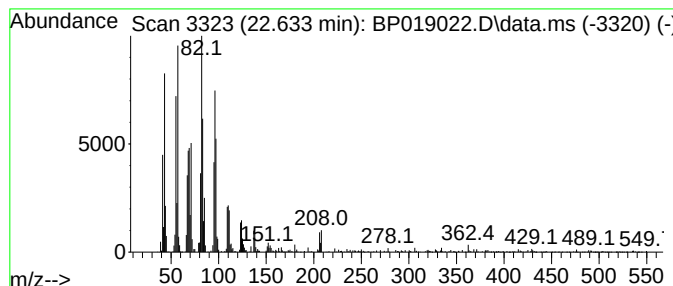
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 1,22-Docosanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.633	3.54 ng/ul	491776	Perylene-d12	23.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,22-Docosanediol	342	C22H46O2	022513-81-1	95
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3			Eicosanal-	296	C20H40O	002400-66-0	91
4			Tricosanal	338	C23H46O	072934-02-2	90
5			Octadecanal	268	C18H36O	000638-66-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019022.D
Acq On : 22 Dec 2023 04:41
Operator : MA/JU
Sample : 05808-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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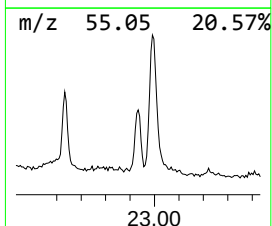
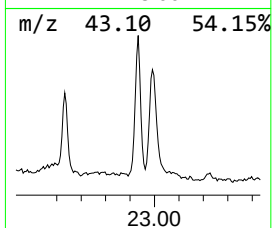
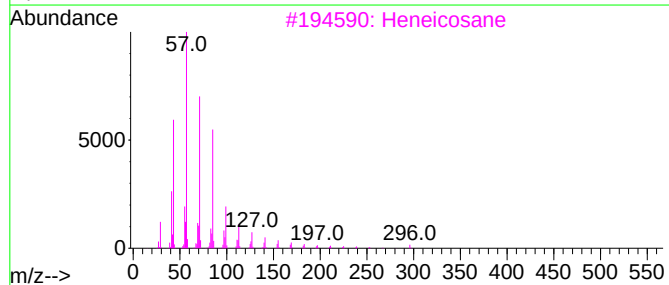
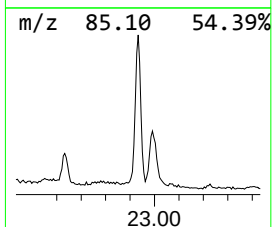
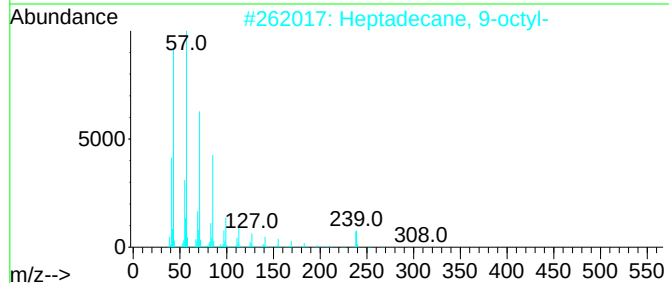
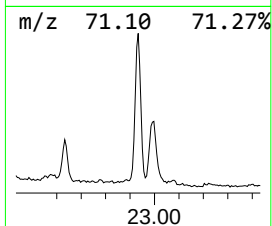
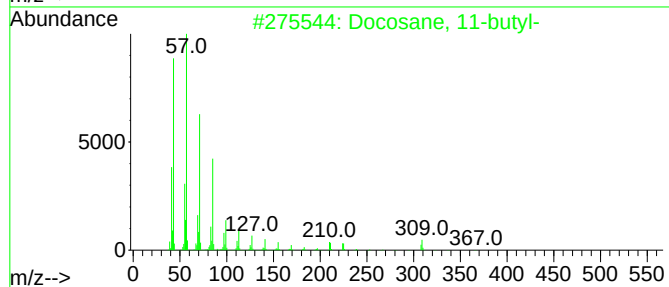
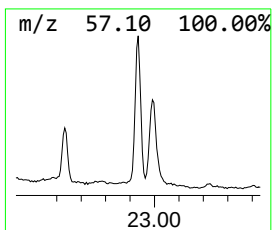
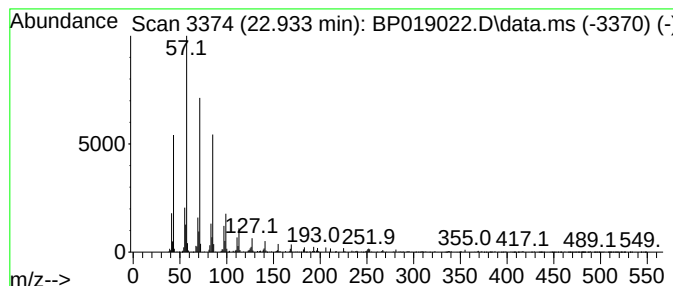
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.933	3.41 ng/ul	473332	Perylene-d12	23.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Heptacosane	380	C27H56	000593-49-7	90
5			Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019022.D
Acq On : 22 Dec 2023 04:41
Operator : MA/JU
Sample : 05808-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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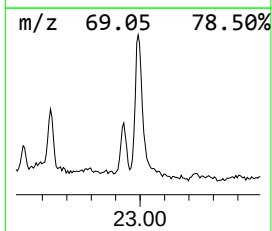
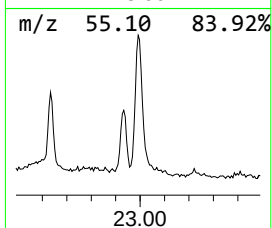
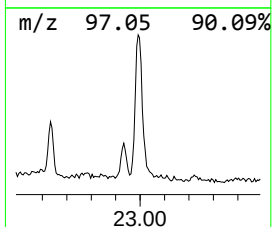
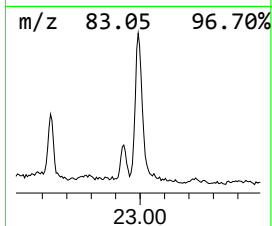
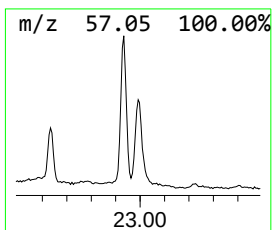
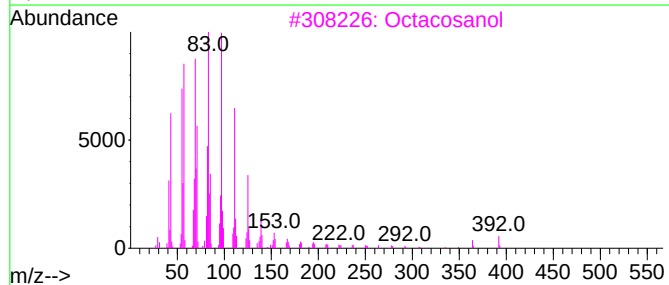
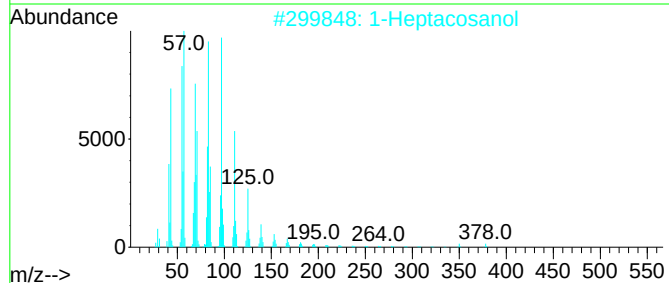
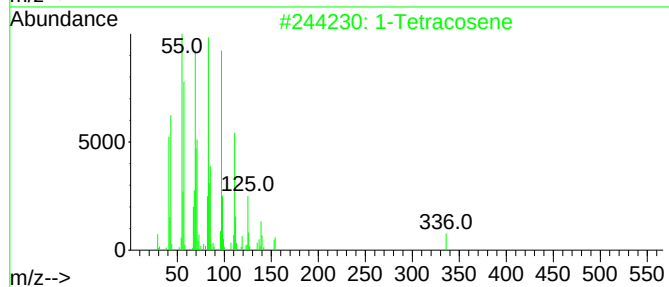
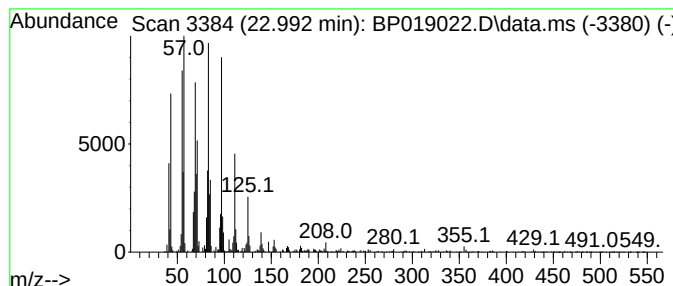
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.992	6.01 ng/ul	835498	Perylene-d12	23.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene			336	C24H48	010192-32-2	96
2	1-Heptacosanol			396	C27H56O	002004-39-9	95
3	Octacosanol			410	C28H58O	000557-61-9	95
4	Cyclotetracosane			336	C24H48	000297-03-0	95
5	1-Hexacosene			364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019022.D
Acq On : 22 Dec 2023 04:41
Operator : MA/JU
Sample : 05808-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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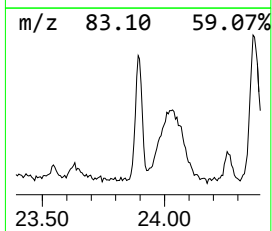
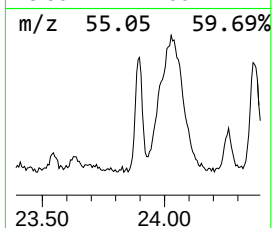
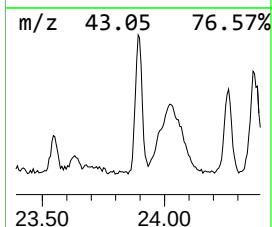
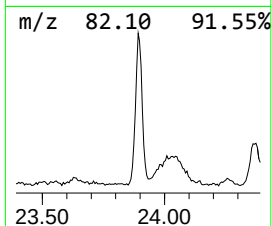
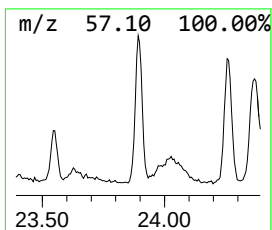
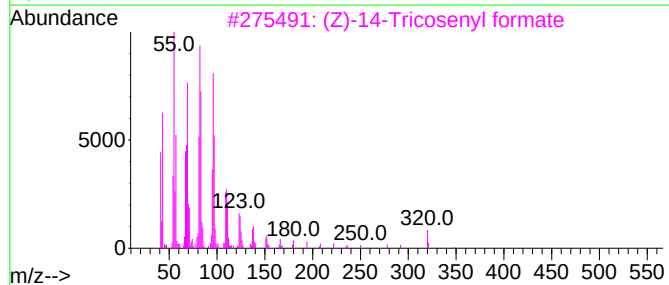
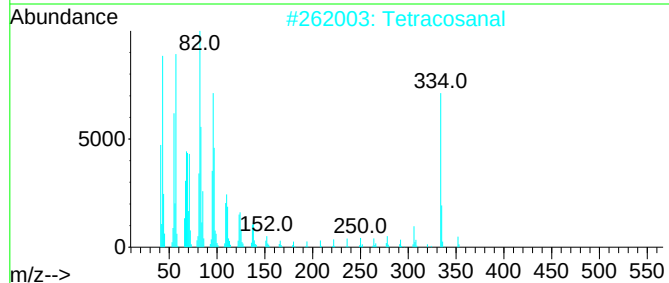
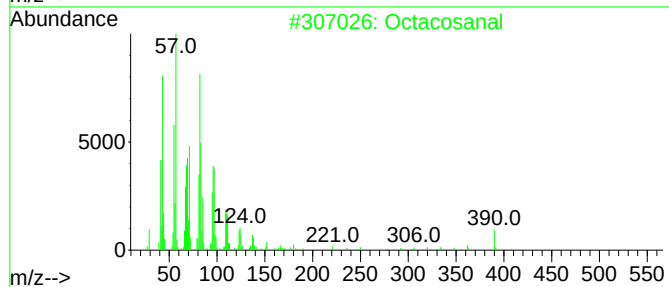
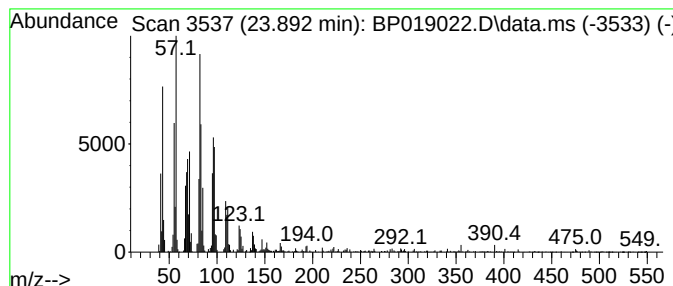
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 Octacosanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.892	4.07 ng/ul	564817	Perylene-d12	23.657

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanal	408	C28H56O	022725-64-0	91
2			Tetracosanal	352	C24H48O	057866-08-7	90
3			(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	90
4			1,19-Eicosadiene	278	C20H38	014811-95-1	89
5			Hexadecanal	240	C16H32O	000629-80-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019022.D
Acq On : 22 Dec 2023 04:41
Operator : MA/JU
Sample : 05808-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.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
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n-Hexadecanoic ...	18.098	5.4	ng/ul	532516	4	17.204	1984550	20.0
5-Bromo-4-oxo-4...	20.892	177.0	ng/ul	21856500	5	21.298	2469610	20.0
Pentadecafluoro...	21.015	6.5	ng/ul	809283	5	21.298	2469610	20.0
(DEL) Alkane: S...	21.898	2.1	ng/ul	257704	5	21.298	2469610	20.0
Behenic alcohol	21.927	3.8	ng/ul	466174	5	21.298	2469610	20.0
1,22-Docosanediol	22.633	3.5	ng/ul	491776	6	23.657	2778210	20.0
(DEL) Alkane: S...	22.933	3.4	ng/ul	473332	6	23.657	2778210	20.0
(DEL) Alkane: S...	22.992	6.0	ng/ul	835498	6	23.657	2778210	20.0
Octacosanal	23.892	4.1	ng/ul	564817	6	23.657	2778210	20.0