

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
 Data File : BP019047.D
 Acq On : 22 Dec 2023 19:27
 Operator : MA/JU
 Sample : 05835-10
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0AQ7

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: BP019047.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	37	rVB	34079	44424	0.42%	0.065%
2	3.540	74	77	82	rBV	13563	20402	0.19%	0.030%
3	3.670	95	99	117	rBV	395624	583474	5.50%	0.860%
4	3.993	151	154	159	rVB2	9889	13346	0.13%	0.020%
5	5.128	340	347	361	rVB	5930117	8913317	84.06%	13.141%
6	6.993	656	664	676	rBV	509274	788772	7.44%	1.163%
7	7.158	685	692	705	rVB	401499	625486	5.90%	0.922%
8	7.346	717	724	735	rBV	498914	800697	7.55%	1.180%
9	7.705	777	785	790	rBV2	11472	20143	0.19%	0.030%
10	7.816	797	804	808	rBV	529885	861683	8.13%	1.270%
11	7.852	808	810	825	rVB	183711	255065	2.41%	0.376%
12	8.534	918	926	933	rBV	630219	1014906	9.57%	1.496%
13	8.593	933	936	941	rVB	18433	29487	0.28%	0.043%
14	8.981	994	1002	1010	rBV	448906	742496	7.00%	1.095%
15	9.105	1018	1023	1028	rBV3	11206	20452	0.19%	0.030%
16	9.552	1094	1099	1107	rVB3	19028	29644	0.28%	0.044%
17	9.646	1107	1115	1118	rBV	15083	27442	0.26%	0.040%
18	9.699	1118	1124	1138	rVB	379959	609232	5.75%	0.898%
19	10.240	1208	1216	1231	rBV	608174	1071049	10.10%	1.579%
20	10.534	1259	1266	1272	rBV	18754	38558	0.36%	0.057%
21	10.610	1272	1279	1287	rVB	669124	1093670	10.31%	1.612%
22	10.757	1293	1304	1316	rBV	579646	1087066	10.25%	1.603%
23	11.369	1402	1408	1414	rBV3	19563	41213	0.39%	0.061%
24	12.199	1543	1549	1557	rBV2	12088	21418	0.20%	0.032%
25	13.351	1736	1745	1749	rBV2	14750	24601	0.23%	0.036%
26	13.869	1826	1833	1840	rBV	1154810	1603416	15.12%	2.364%
27	13.940	1840	1845	1850	rVB6	6915	14440	0.14%	0.021%
28	14.146	1872	1880	1891	rBV	1347662	1978391	18.66%	2.917%
29	14.451	1925	1932	1942	rBV	1035447	1524559	14.38%	2.248%
30	14.669	1962	1969	1983	rBV	381218	738693	6.97%	1.089%
31	14.875	2000	2004	2010	rVB9	7619	13044	0.12%	0.019%
32	15.445	2094	2101	2116	rBV	1869296	2633547	24.84%	3.883%
33	15.569	2116	2122	2131	rBV	482200	669800	6.32%	0.987%
34	15.681	2138	2141	2151	rVB4	9550	19129	0.18%	0.028%
35	16.234	2231	2235	2241	rVB5	7714	12575	0.12%	0.019%
36	16.610	2295	2299	2308	rBV8	16232	36480	0.34%	0.054%

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37	17.204	2393	2400	2406	rBV	1424457	1974478	18.62%	2.911%
38	17.298	2410	2416	2427	rVV	2001763	2922266	27.56%	4.308%
39	17.598	2459	2467	2473	rBV10	11167	27810	0.26%	0.041%
40	17.975	2527	2531	2538	rVB10	8376	15376	0.14%	0.023%
41	18.092	2546	2551	2561	rBV	179609	271151	2.56%	0.400%
42	18.510	2618	2622	2625	rVB3	21901	24443	0.23%	0.036%
43	18.986	2701	2703	2708	rVB3	13365	15582	0.15%	0.023%
44	19.116	2722	2725	2731	rBV2	33569	44064	0.42%	0.065%
45	19.186	2733	2737	2740	rBV	37399	53734	0.51%	0.079%
46	19.328	2757	2761	2766	rBV	73301	103845	0.98%	0.153%
47	19.539	2791	2797	2804	rBV	2865651	3786357	35.71%	5.582%
48	20.598	2974	2977	2980	rBV4	39527	56318	0.53%	0.083%
49	20.716	2993	2997	3001	rBV2	202213	250118	2.36%	0.369%
50	20.786	3006	3009	3014	rVB5	95725	119446	1.13%	0.176%
51	20.898	3024	3028	3033	rBV	2486165	3037805	28.65%	4.479%
52	21.016	3043	3048	3049	rBV	498364	645778	6.09%	0.952%
53	21.039	3049	3052	3057	rVB2	959489	1192340	11.24%	1.758%
54	21.251	3085	3088	3091	rVB2	181853	190541	1.80%	0.281%
55	21.292	3091	3095	3101	rVB	2075954	2597700	24.50%	3.830%
56	21.898	3195	3198	3199	rBV	95922	113384	1.07%	0.167%
57	21.927	3199	3203	3213	rVB	442244	784959	7.40%	1.157%
58	22.927	3369	3373	3379	rBV	238961	356144	3.36%	0.525%
59	23.498	3464	3470	3483	rVB2	2131824	4326521	40.80%	6.379%
60	23.651	3490	3496	3514	rVB	1376108	2851118	26.89%	4.203%
61	25.039	3727	3732	3745	rVB	412337	988736	9.32%	1.458%
62	27.186	4090	4097	4113	rVB3	790551	2452591	23.13%	3.616%
63	28.004	4224	4236	4251	rVB2	2875797	10604139	100.00%	15.634%

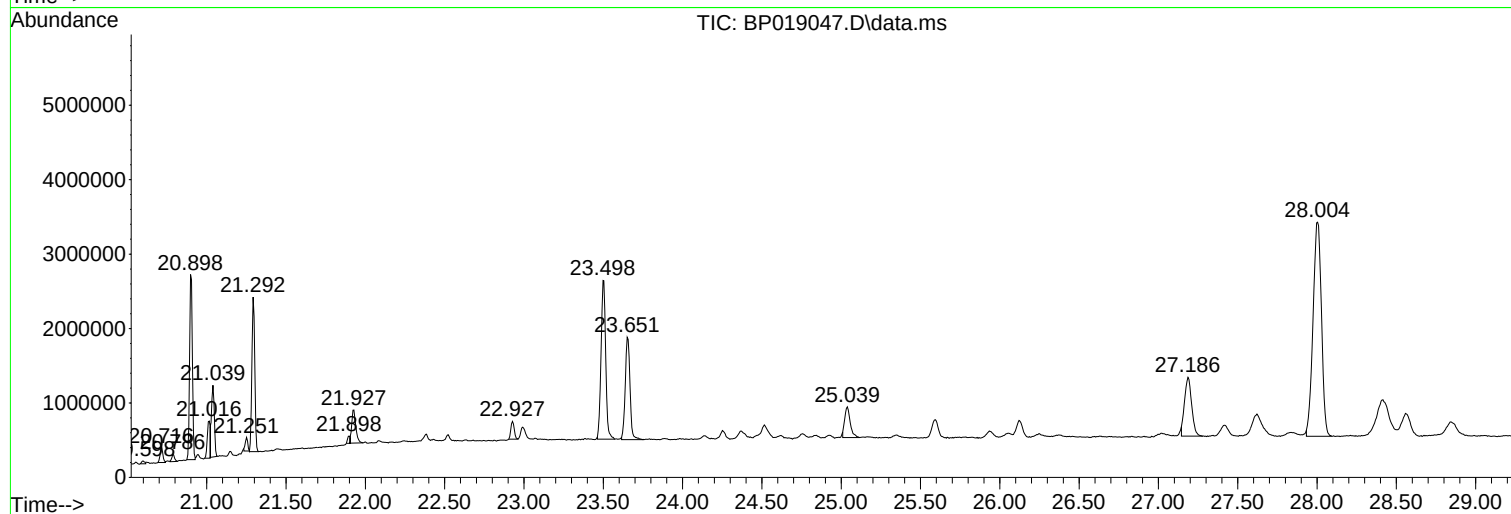
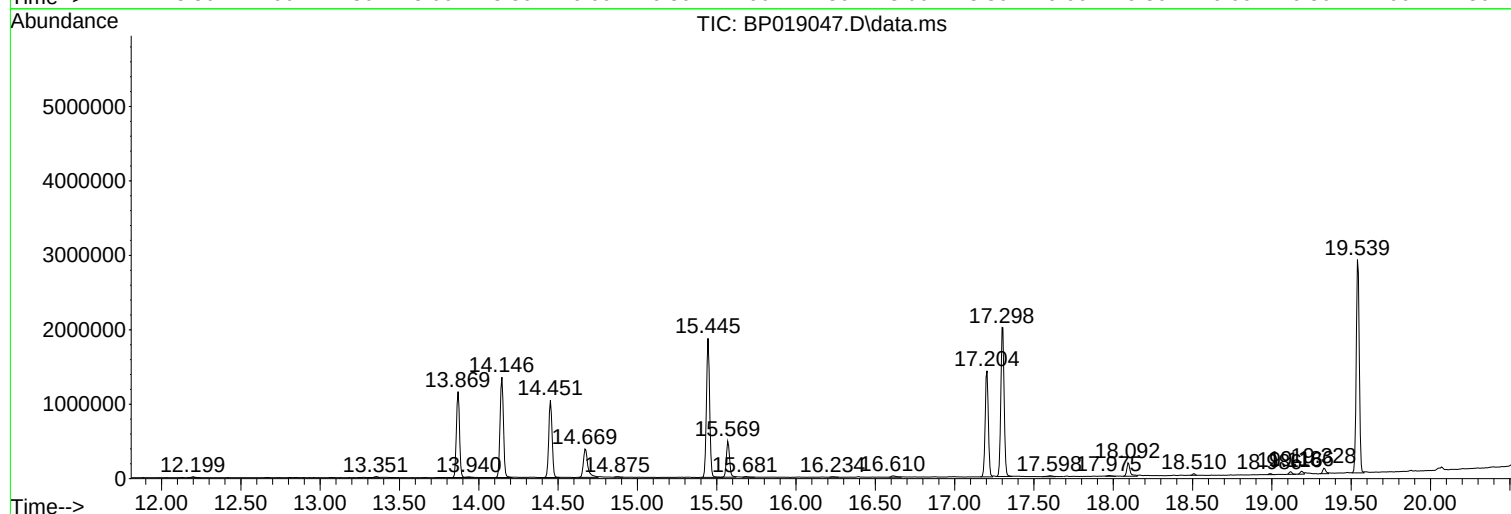
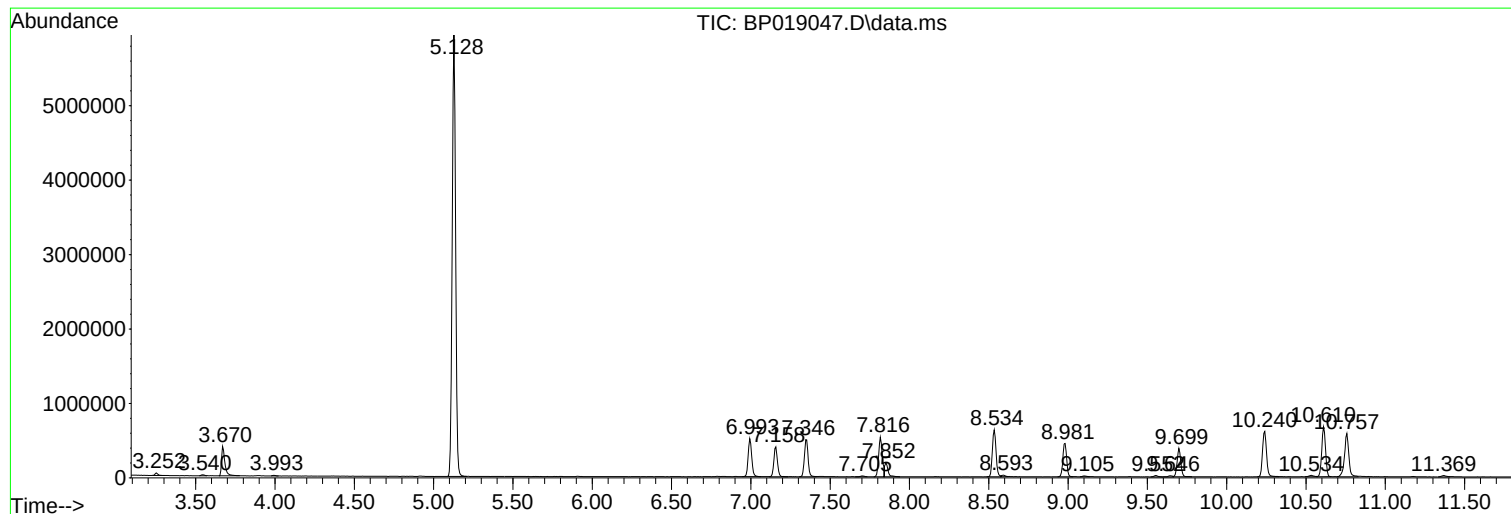
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Quant Title : SVOA CALIBRATION

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



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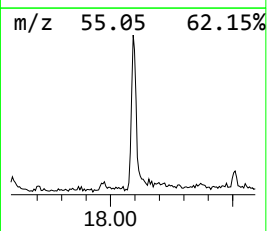
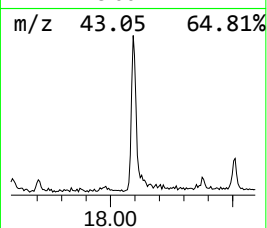
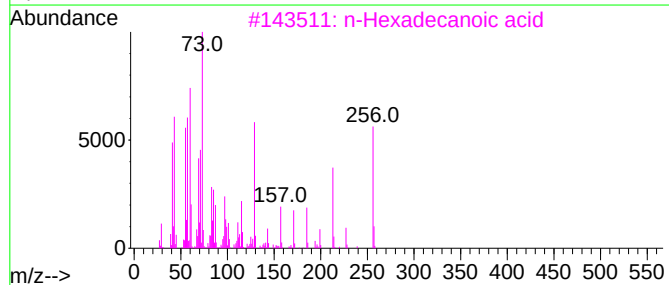
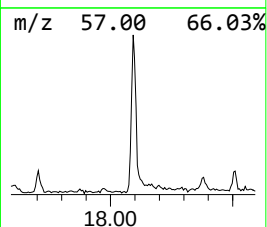
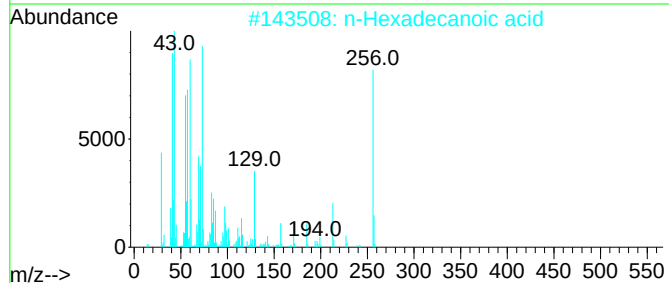
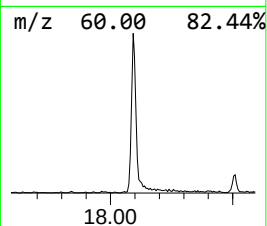
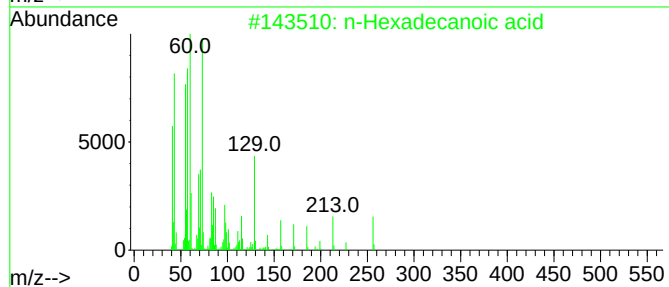
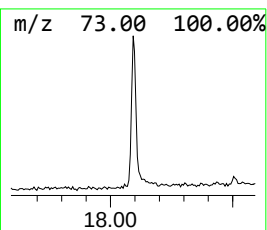
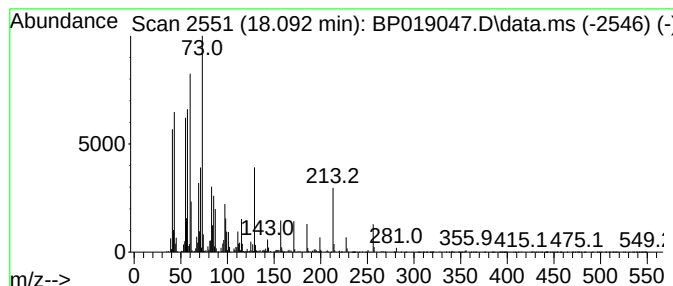
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	2.75 ng/ul	271151	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	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5			Octadecanoic acid	284	C18H36O2	000057-11-4	93



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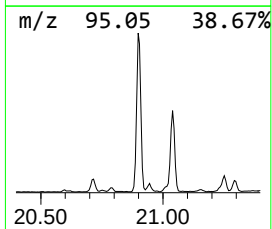
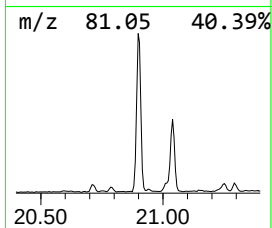
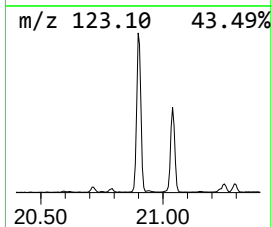
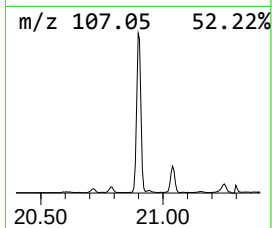
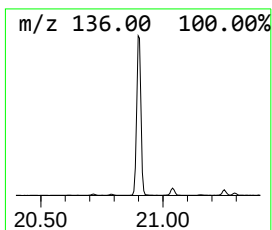
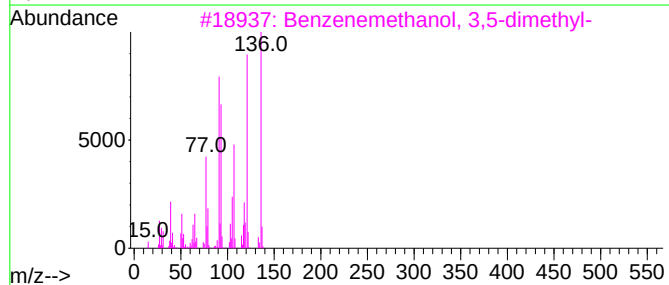
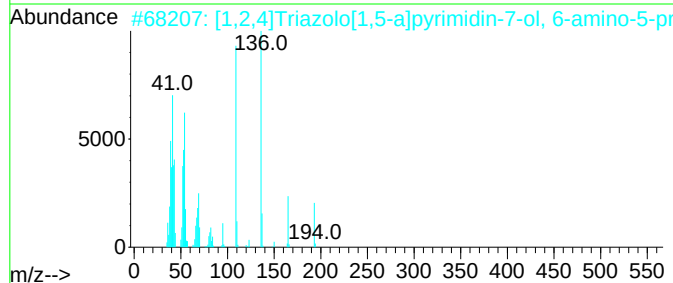
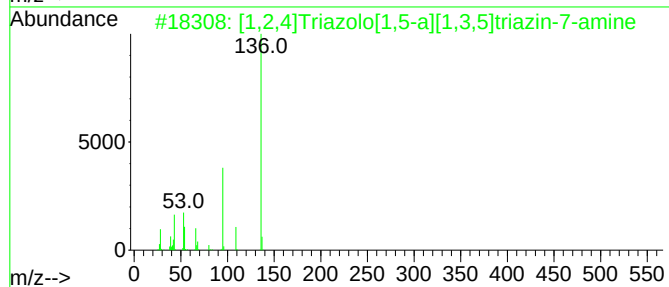
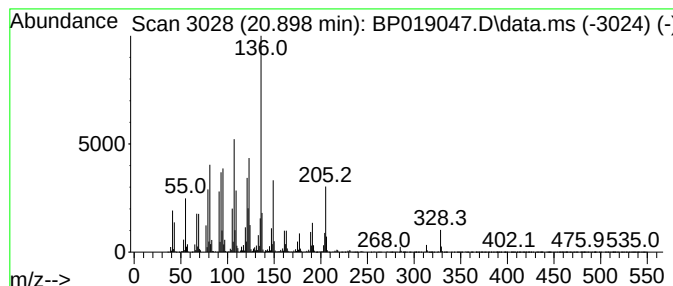
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.898	23.39 ng/ul	3037810	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,2,4]Triazolo[1,5-a][1,3,5]tri...	136	C4H4N6	001489-04-9	38		
2	[1,2,4]Triazolo[1,5-a]pyrimidin-...	193	C8H11N5O	1000362-66-7	35		
3	Benzenemethanol, 3,5-dimethyl-	136	C9H12O	027129-87-9	27		
4	3,3-Dimethyl-6-methylenecyclohexene	122	C9H14	020185-16-4	25		
5	Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	074806-55-6	22		



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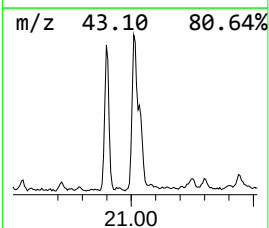
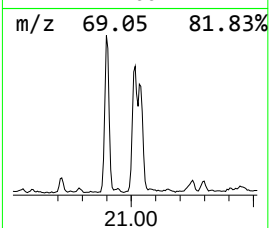
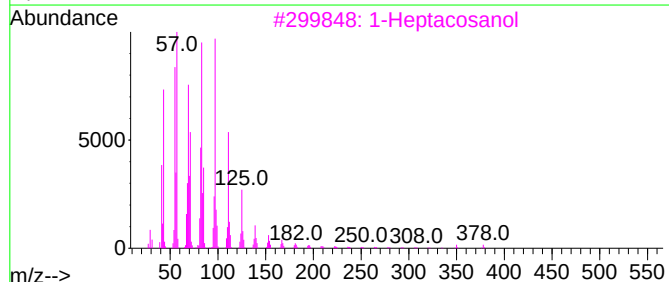
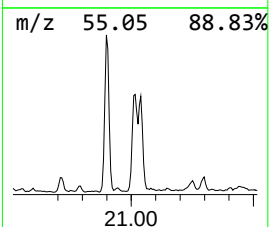
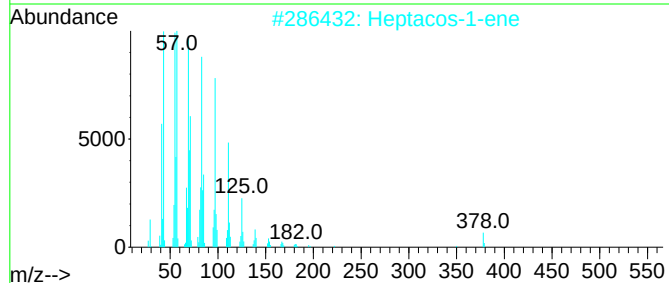
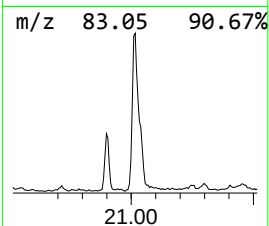
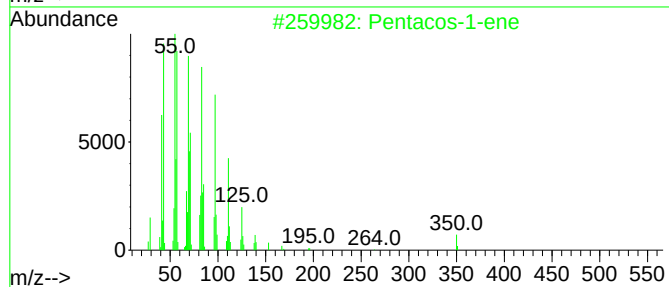
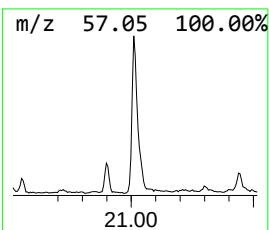
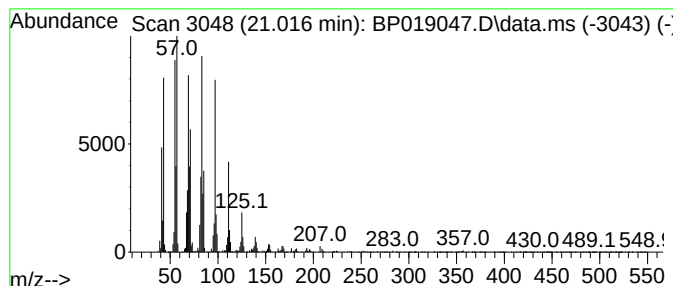
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 Pentacos-1-ene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.016	4.97 ng/ul	645778	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacos-1-ene	350	C25H50	016980-85-1	94
2			Heptacos-1-ene	378	C27H54	015306-27-1	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			1-Hexacosene	364	C26H52	018835-33-1	93



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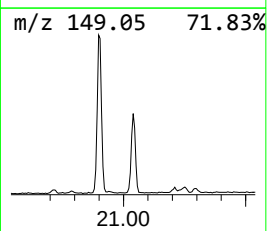
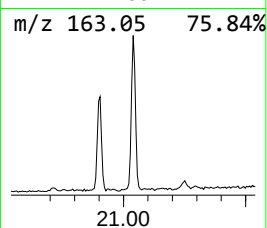
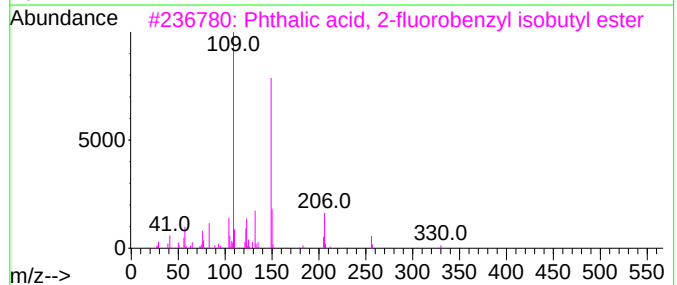
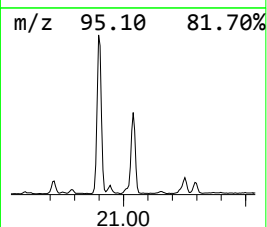
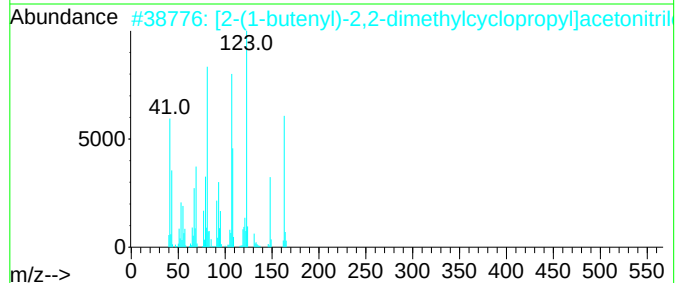
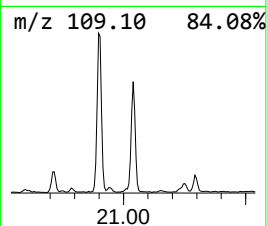
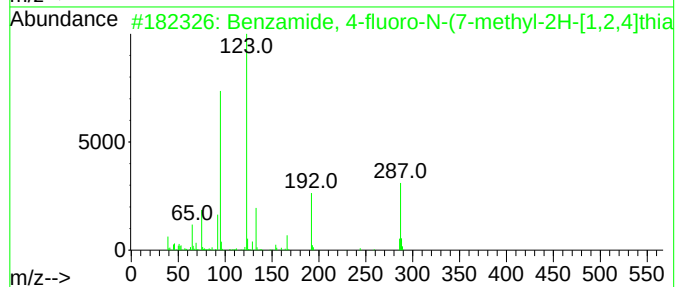
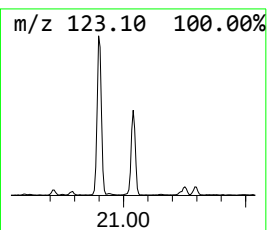
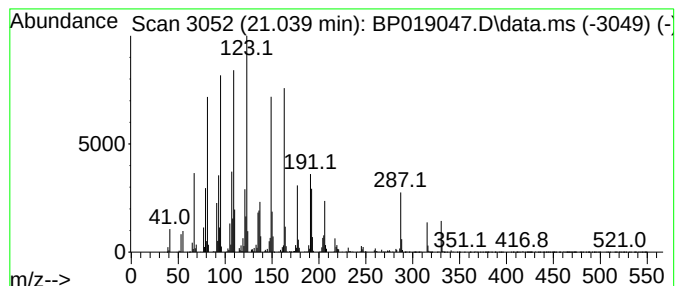
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.039	9.18 ng/ul	1192340	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, 4-fluoro-N-(7-methyl-...	287	C14H10FN3OS	1000350-88-7	38
2			[2-(1-butenyl)-2,2-dimethylcyclo...	163	C11H17N	1000111-15-4	25
3			Phthalic acid, 2-fluorobenzyl is...	330	C19H19F04	1010371-07-2	22
4			Phthalic acid, butyl 4-fluoroben...	330	C19H19F04	1000377-74-3	14
5			Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	14



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ClientSampleId :
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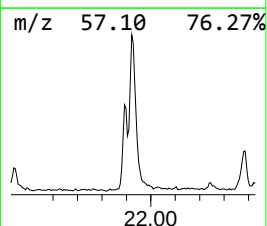
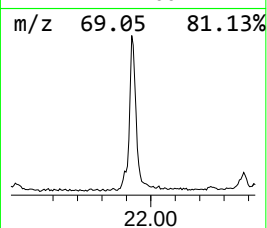
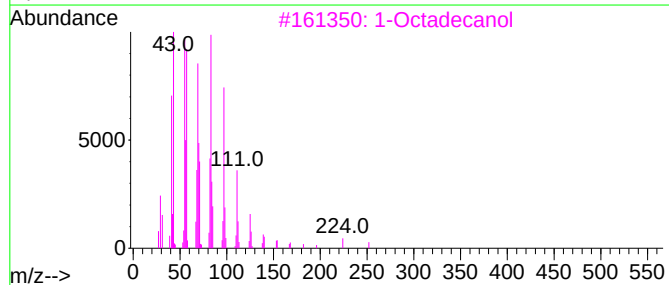
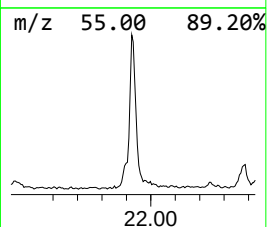
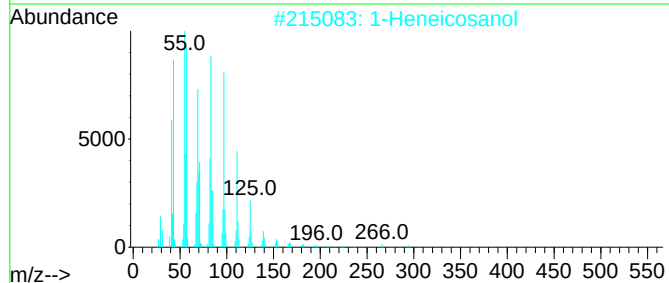
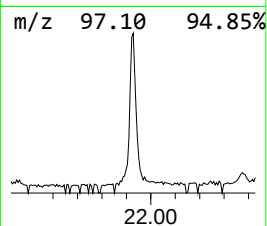
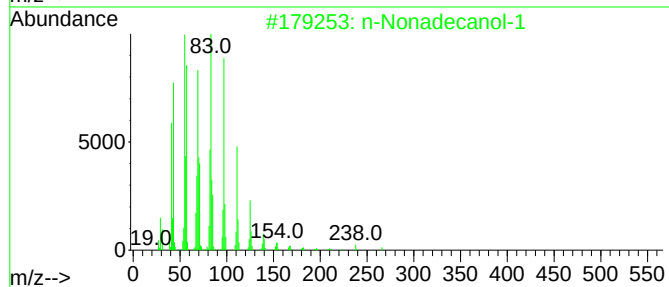
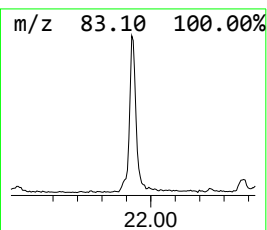
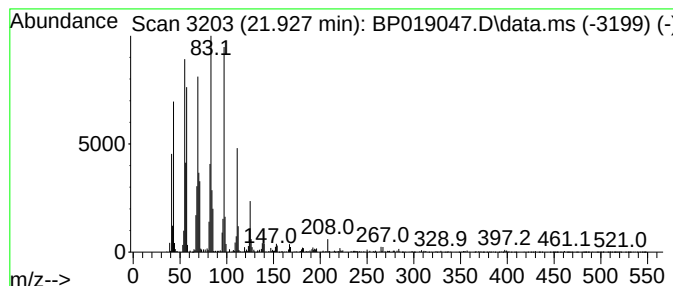
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 n-Nonadecanol-1 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.927	6.04 ng/ul	784959	Chrysene-d12	21.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1			284	C19H40O	001454-84-8	94
2	1-Heneicosanol			312	C21H44O	015594-90-8	93
3	1-Octadecanol			270	C18H38O	000112-92-5	81
4	n-Heptadecanol-1			256	C17H36O	001454-85-9	81
5	1-Hexadecanol			242	C16H34O	036653-82-4	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019047.D
Acq On : 22 Dec 2023 19:27
Operator : MA/JU
Sample : 05835-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AQ7

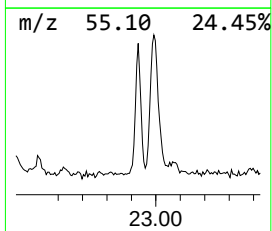
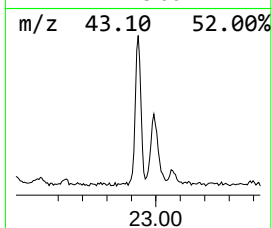
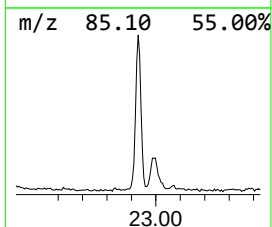
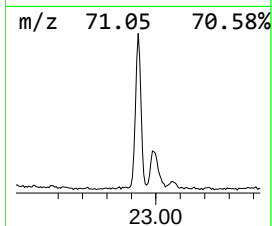
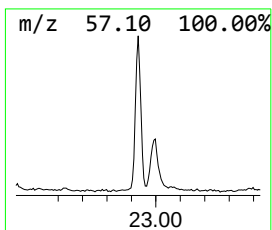
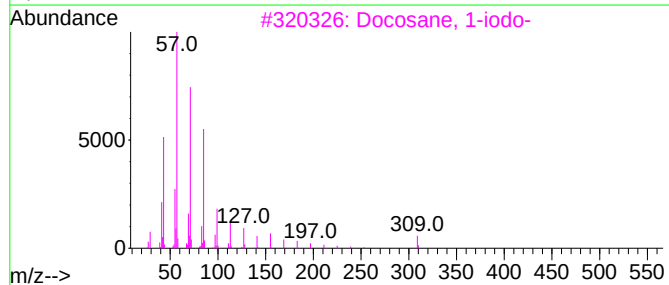
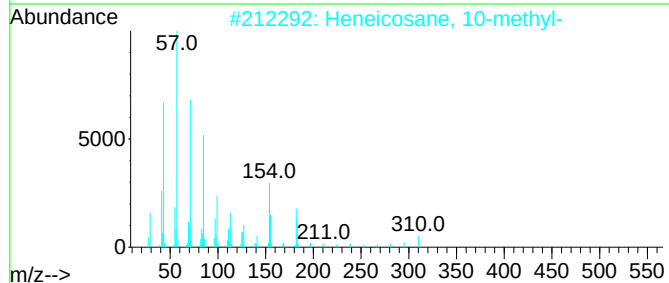
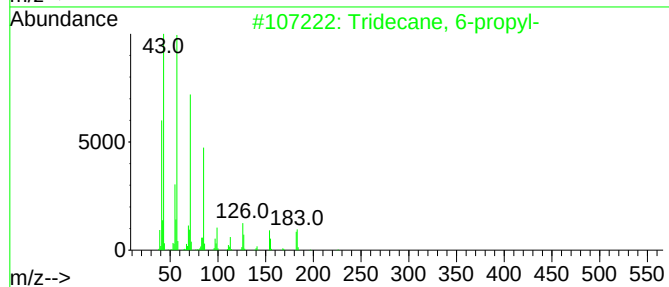
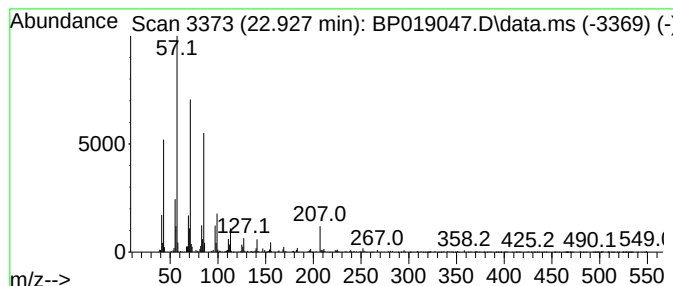
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.927	2.50 ng/ul	356144	Perylene-d12	23.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
2			Heneicosane, 10-methyl-	310	C22H46	013287-25-7	87
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
4			9-Methylheneicosane	310	C22H46	070475-51-3	87
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019047.D
Acq On : 22 Dec 2023 19:27
Operator : MA/JU
Sample : 05835-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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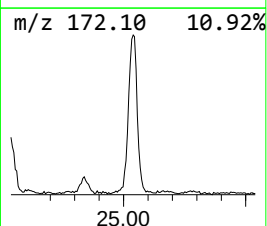
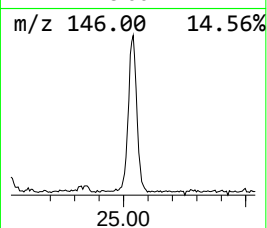
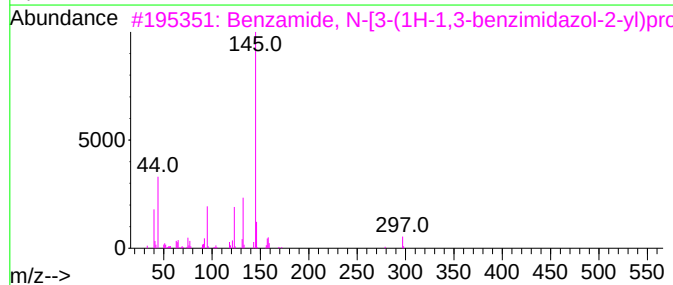
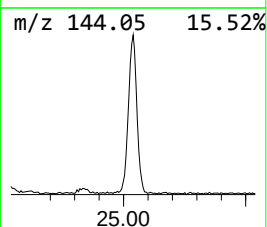
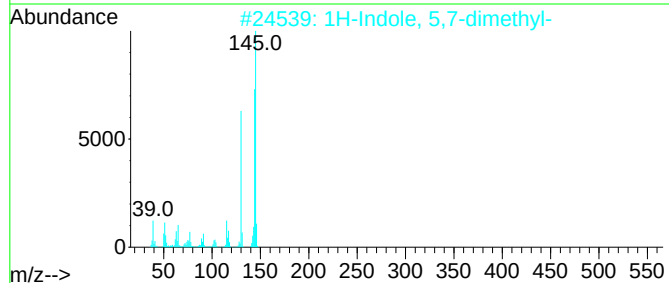
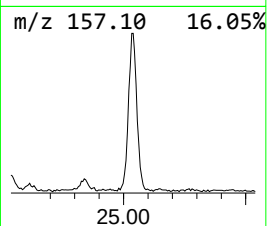
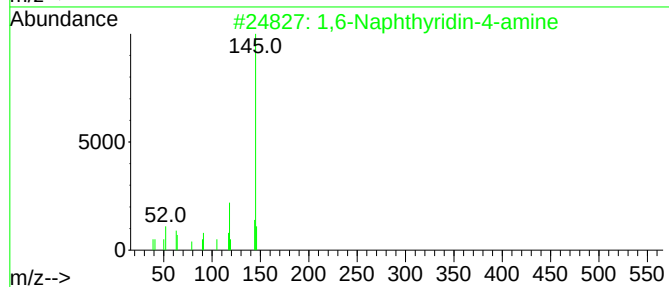
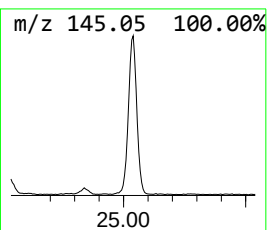
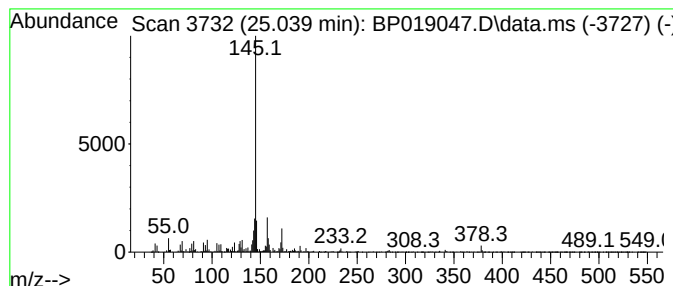
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 1,6-Naphthyridin-4-amine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.039	6.94 ng/ul	988736	Perylene-d12	23.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,6-Naphthyridin-4-amine	145	C8H7N3	028593-08-0	58
2			1H-Indole, 5,7-dimethyl-	145	C10H11N	054020-53-0	53
3			Benzamide, N-[3-(1H-1,3-benzimid...	297	C17H16FN3O	1000319-56-9	53
4			Indolizine, 2,6-dimethyl-	145	C10H11N	000769-88-0	53
5			1H-Indole, 1,2-dimethyl-	145	C10H11N	000875-79-6	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019047.D
Acq On : 22 Dec 2023 19:27
Operator : MA/JU
Sample : 05835-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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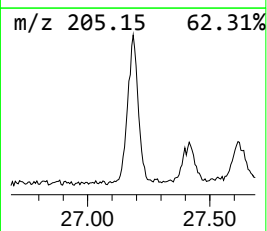
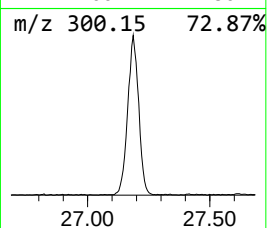
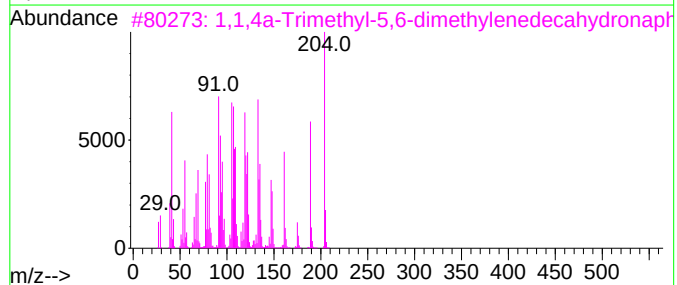
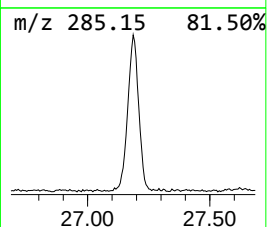
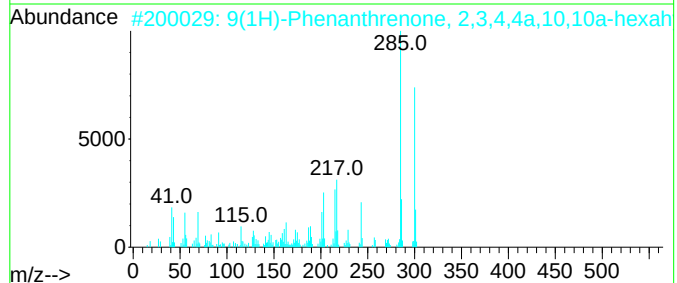
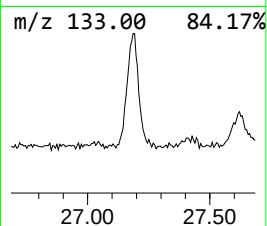
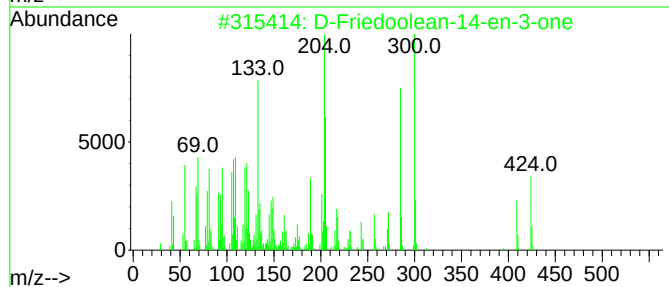
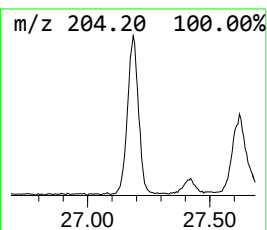
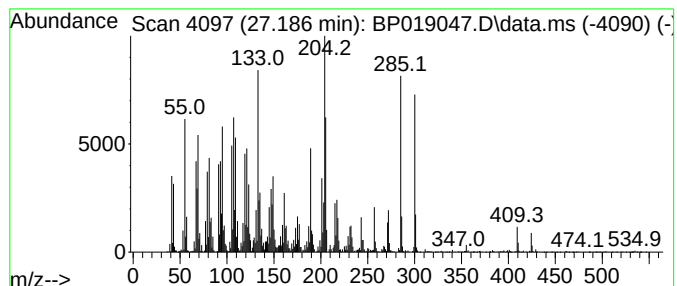
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 D-Friedoolean-14-en-3-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.186	17.20 ng/ul	2452590	Perylene-d12	23.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Friedoolean-14-en-3-one	424	C30H48O	000514-07-8	99
2			9(1H)-Phenanthrene, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	56
3			1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	46
4			1R,4S,7S,11R-2,2,4,8-Tetramethyl...	204	C15H24	1208118-28-8	41
5			2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019047.D
Acq On : 22 Dec 2023 19:27
Operator : MA/JU
Sample : 05835-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AQ7

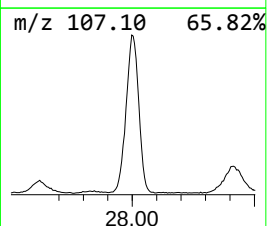
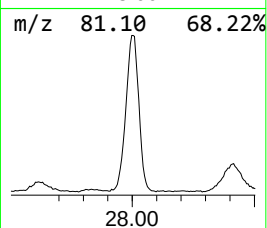
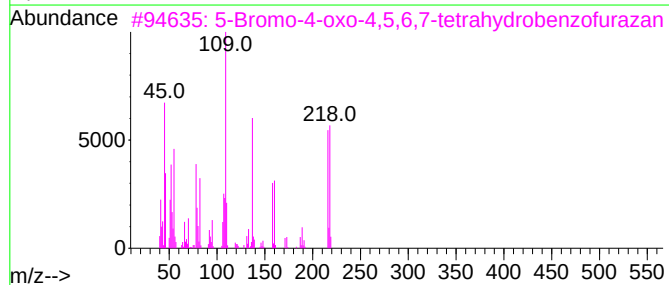
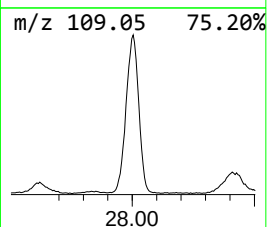
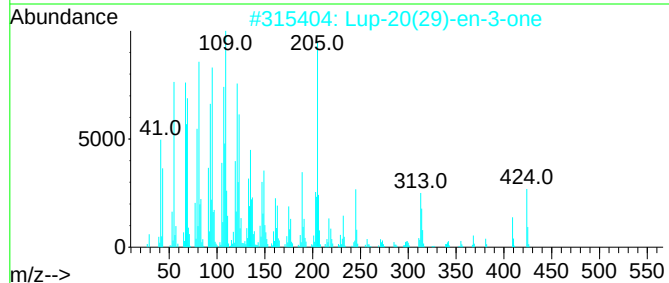
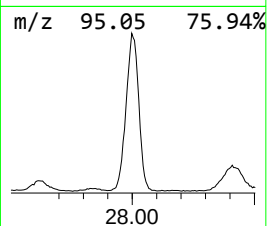
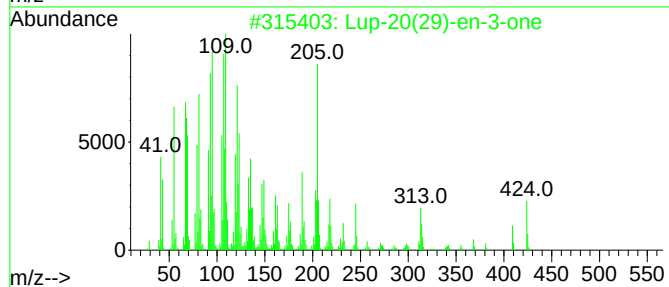
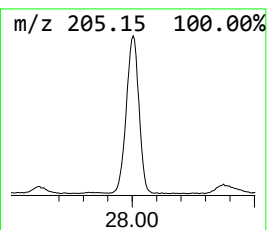
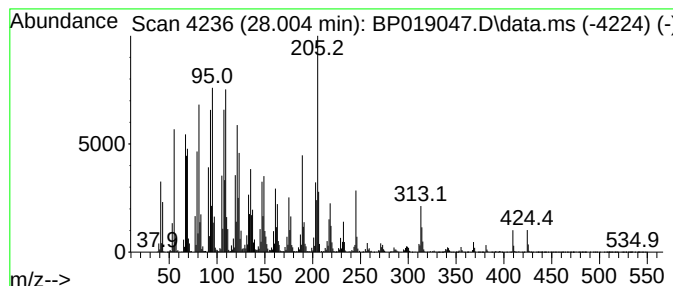
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 Lup-20(29)-en-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.004	74.39 ng/ul	10604100	Perylene-d12	23.651

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			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	91
4			D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	90
5			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122123\
Data File : BP019047.D
Acq On : 22 Dec 2023 19:27
Operator : MA/JU
Sample : 05835-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AQ7

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
n-Hexadecanoic ...	18.092	2.8	ng/ul	271151	4	17.204	1974480	20.0
unknown-01	20.898	23.4	ng/ul	3037810	5	21.292	2597700	20.0
Pentacos-1-ene	21.016	5.0	ng/ul	645778	5	21.292	2597700	20.0
unknown-02	21.039	9.2	ng/ul	1192340	5	21.292	2597700	20.0
n-Nonadecanol-1	21.927	6.0	ng/ul	784959	5	21.292	2597700	20.0
(DEL) Alkane: S...	22.927	2.5	ng/ul	356144	6	23.651	2851120	20.0
1,6-Naphthyridi...	25.039	6.9	ng/ul	988736	6	23.651	2851120	20.0
D-Friedoolean-1...	27.186	17.2	ng/ul	2452590	6	23.651	2851120	20.0
Lup-20(29)-en-3...	28.004	74.4	ng/ul	10604100	6	23.651	2851120	20.0