

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090119\
 Data File : BM022492.D
 Acq On : 02 Sep 2019 00:22
 Operator : HP/JU
 Sample : K4562-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-02-20-22

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.128	359	364	370	rBV	145003	224319	35.55%	5.662%
2	5.175	370	372	383	rVB3	19440	34373	5.45%	0.868%
3	6.704	627	632	647	rBV	130788	260695	41.32%	6.580%
4	7.045	684	690	703	rBB	163871	274822	43.56%	6.937%
5	7.504	763	768	776	rBB	44456	65315	10.35%	1.649%
6	7.816	815	821	830	rBB	125612	207505	32.89%	5.238%
7	8.686	963	969	986	rBV	62115	144683	22.93%	3.652%
8	10.286	1235	1241	1259	rBV	32297	72858	11.55%	1.839%
9	12.774	1659	1664	1677	rBV	157254	276512	43.83%	6.979%
10	13.663	1810	1815	1828	rBB2	17073	30652	4.86%	0.774%
11	14.174	1897	1902	1912	rBB	66086	101064	16.02%	2.551%
12	15.686	2154	2159	2173	rBV	198207	323065	51.20%	8.154%
13	16.951	2368	2374	2379	rBV2	94691	165223	26.19%	4.170%
14	16.992	2379	2381	2390	rVB2	12288	13747	2.18%	0.347%
15	17.274	2427	2429	2433	rVB	7734	8689	1.38%	0.219%
16	17.833	2519	2524	2531	rBV2	19091	29272	4.64%	0.739%
17	19.121	2740	2743	2749	rBV3	9679	14795	2.34%	0.373%
18	19.580	2816	2821	2831	rBV	518590	630929	100.00%	15.925%
19	19.874	2867	2871	2874	rBV	9201	9889	1.57%	0.250%
20	20.374	2951	2956	2959	rBV4	9928	13056	2.07%	0.330%
21	20.556	2984	2987	2990	rBV3	8345	8503	1.35%	0.215%
22	20.756	3018	3021	3026	rBV7	9996	12362	1.96%	0.312%
23	20.844	3031	3036	3046	rBV5	39280	73169	11.60%	1.847%
24	20.944	3049	3053	3056	rBV	10198	13298	2.11%	0.336%
25	21.068	3071	3074	3079	rVB5	6512	8006	1.27%	0.202%
26	21.156	3084	3089	3099	rBV	166197	258413	40.96%	6.523%
27	21.274	3106	3109	3115	rBV3	20260	23211	3.68%	0.586%
28	21.462	3138	3141	3148	rBV7	13480	19996	3.17%	0.505%
29	21.697	3177	3181	3184	rBV2	43235	46636	7.39%	1.177%
30	22.138	3253	3256	3264	rVB2	26803	33290	5.28%	0.840%
31	22.621	3334	3338	3343	rBV	85014	103632	16.43%	2.616%
32	23.338	3454	3460	3473	rBV2	134403	278267	44.10%	7.024%
33	23.762	3528	3532	3540	rVB2	40876	73052	11.58%	1.844%
34	26.309	3961	3965	3973	rVB10	48431	108518	17.20%	2.739%

LSC Area Percent Report

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BM082919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

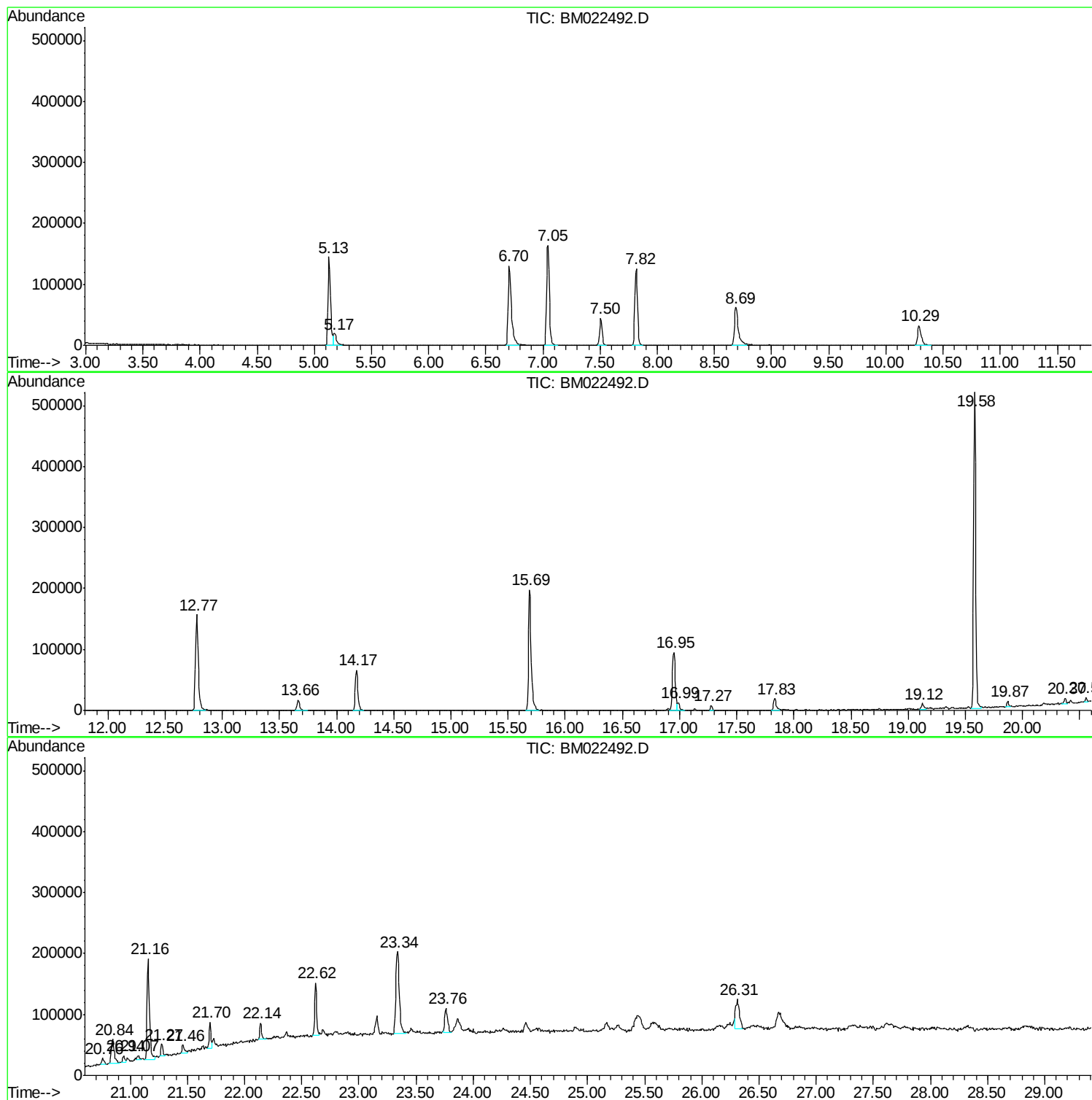
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082919.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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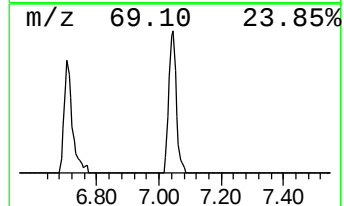
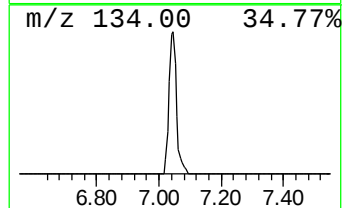
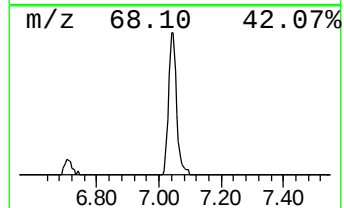
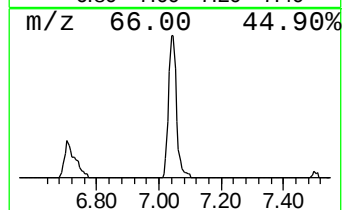
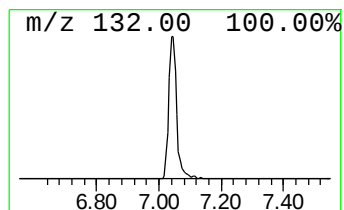
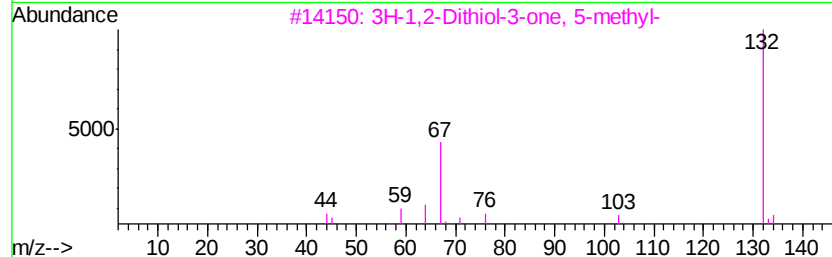
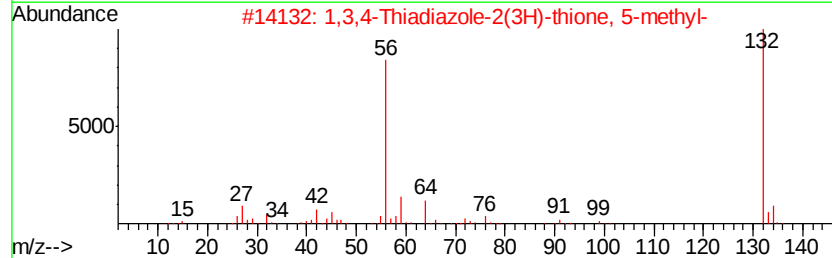
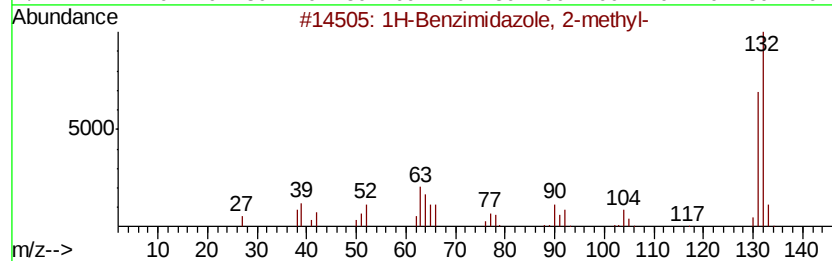
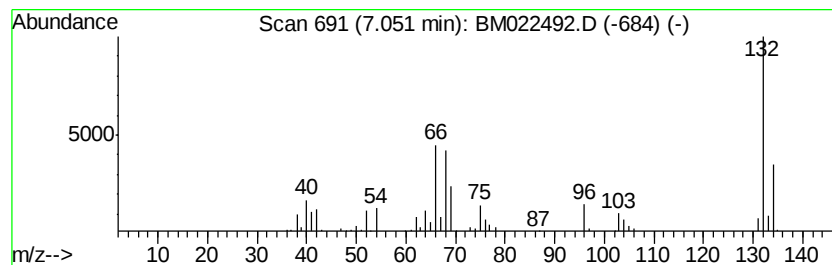
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	84.15 ng	274822	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	18
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10



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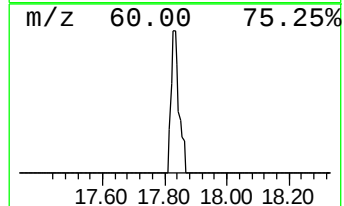
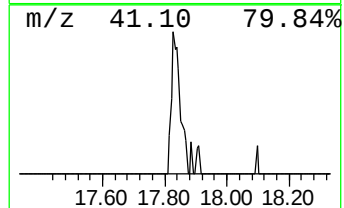
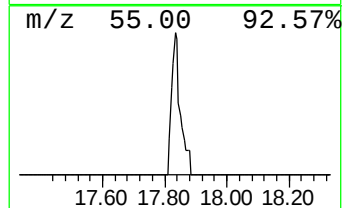
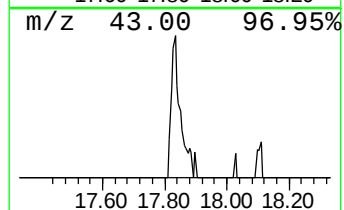
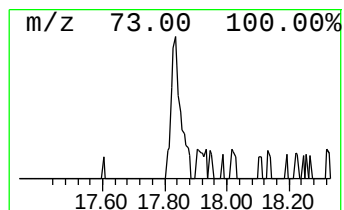
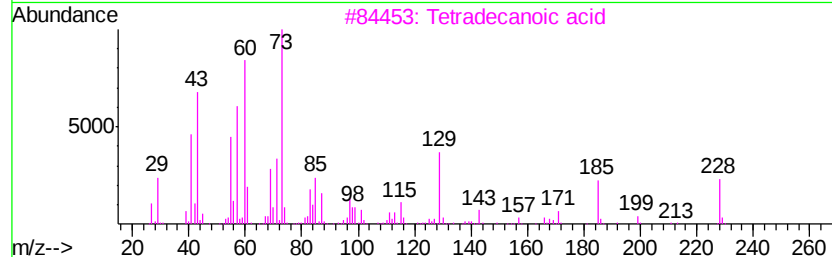
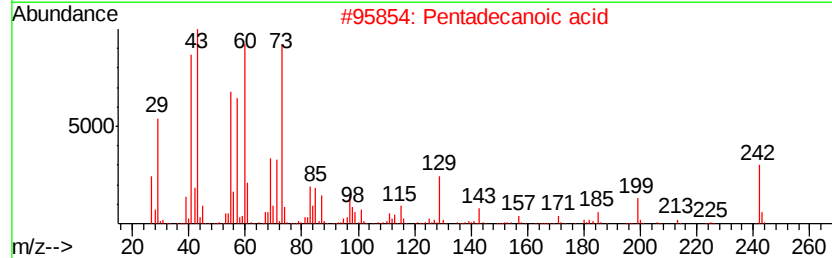
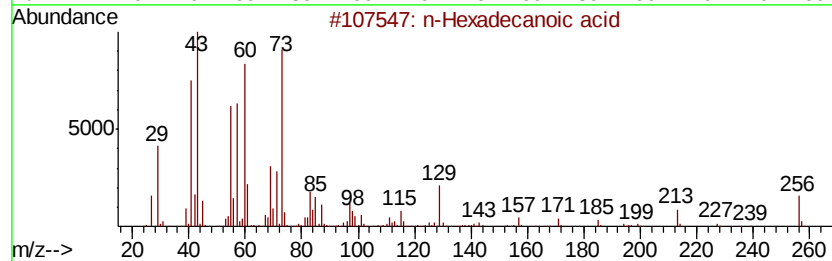
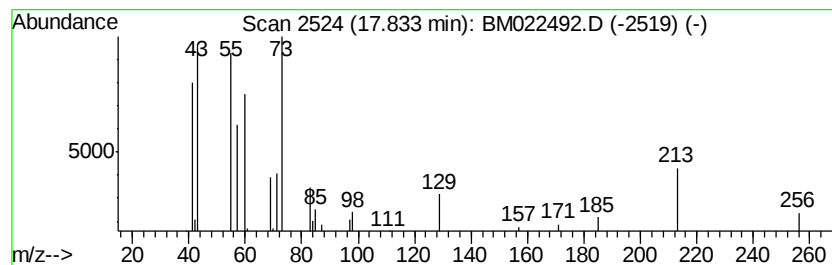
Instrument :
BNA_M
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.83	3.54 ng	29272	Phenanthrene-d10		16.94
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	43
5	Tridecanoic acid	214	C13H26O2	000638-53-9	43



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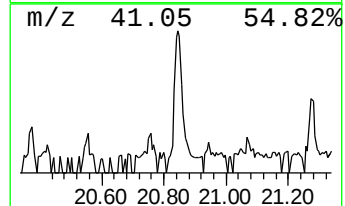
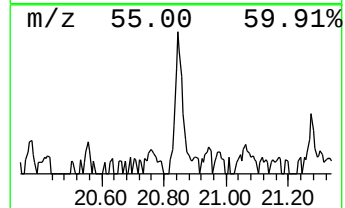
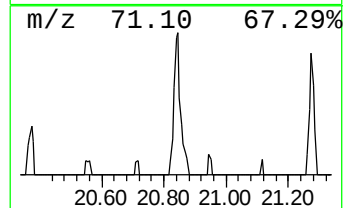
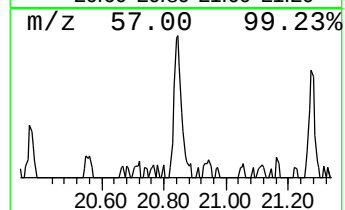
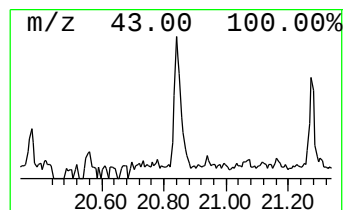
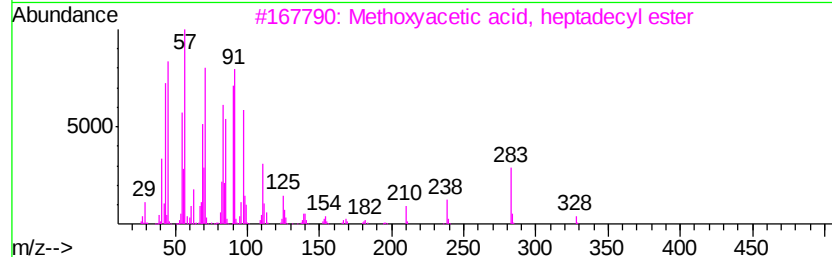
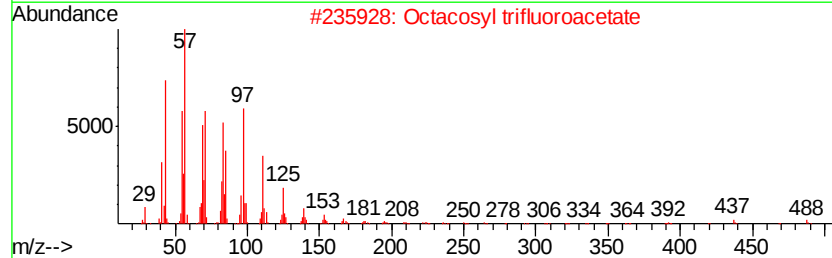
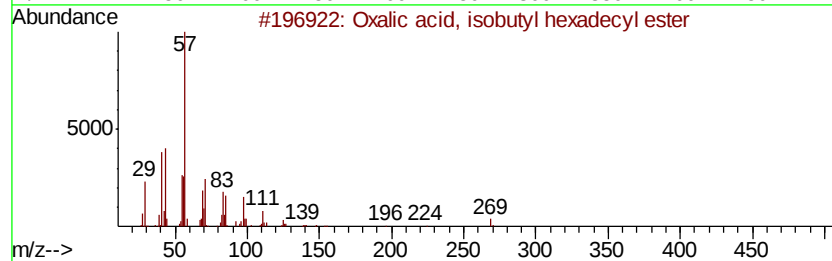
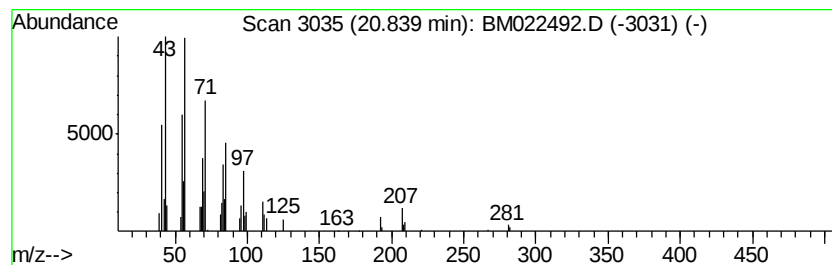
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Oxalic acid, isobutyl hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.84	5.66 ng	73169	Chrysene-d12	21.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
3		Methoxyacetic acid, heptadecyl e...	328	C20H40O3	1000282-99-1	83
4		Oxalic acid, cyclobutyl octadecyl...	396	C24H44O4	1000309-70-8	83
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	83



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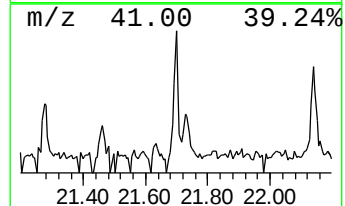
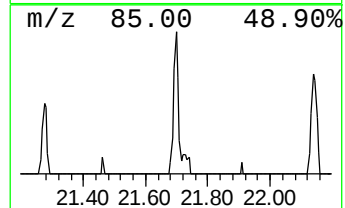
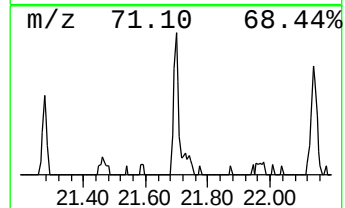
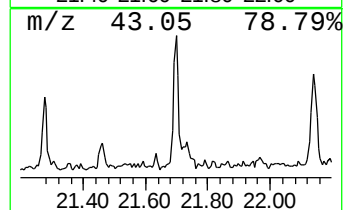
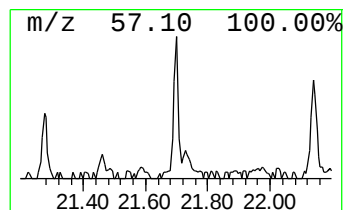
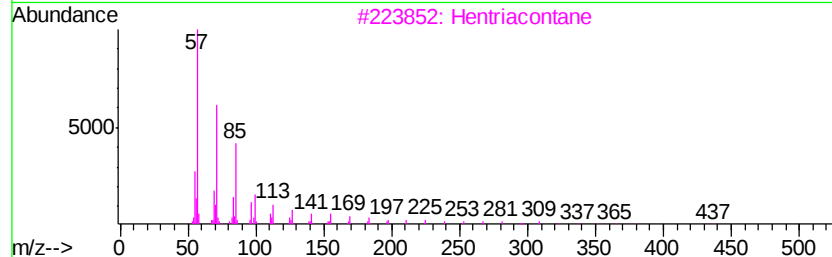
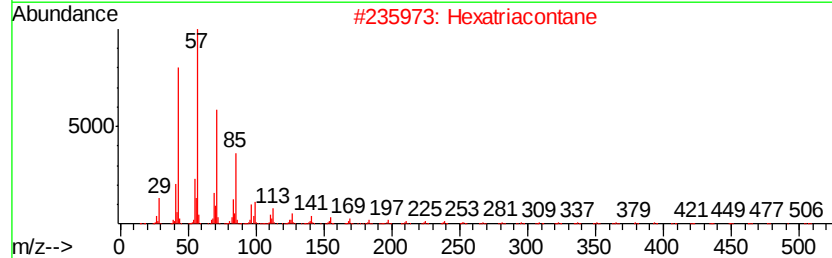
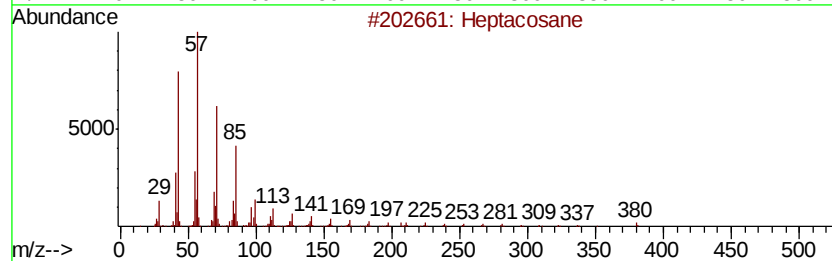
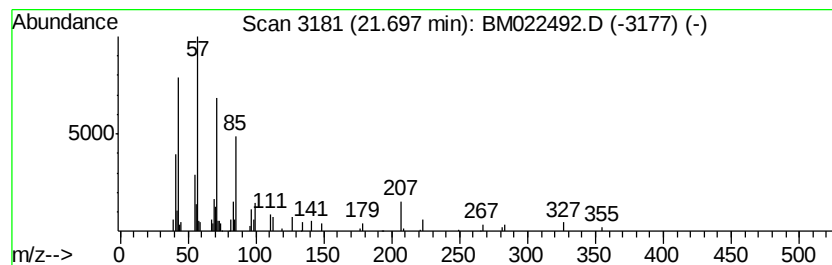
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.70	3.61 ng	46636	Chrysene-d12	21.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	87
2	Hexatriacontane		507	C36H74	000630-06-8	87
3	Hentriacontane		437	C31H64	000630-04-6	87
4	Hexacosane		366	C26H54	000630-01-3	87
5	10-Methylnonadecane		282	C20H42	056862-62-5	83



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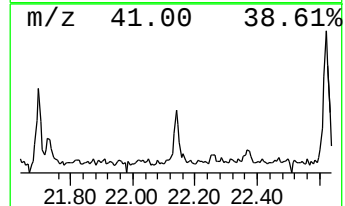
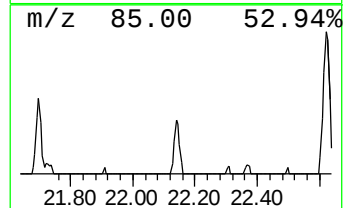
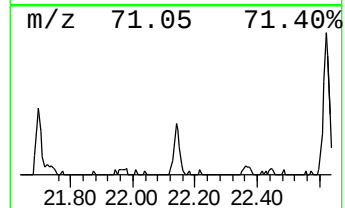
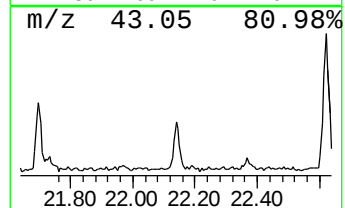
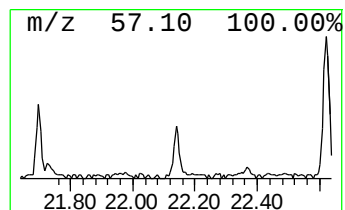
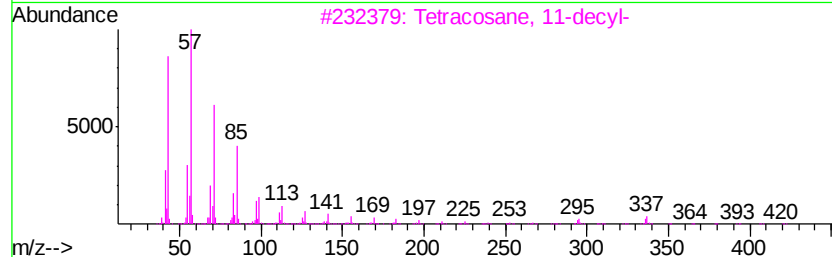
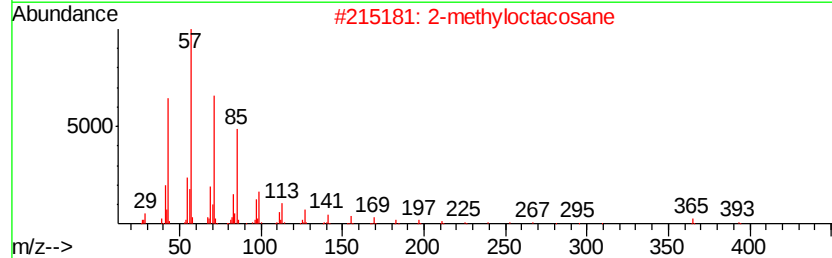
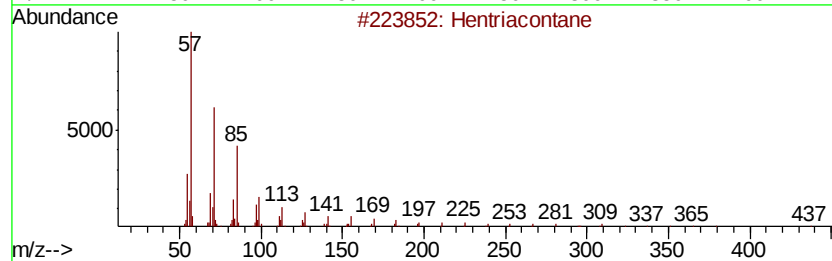
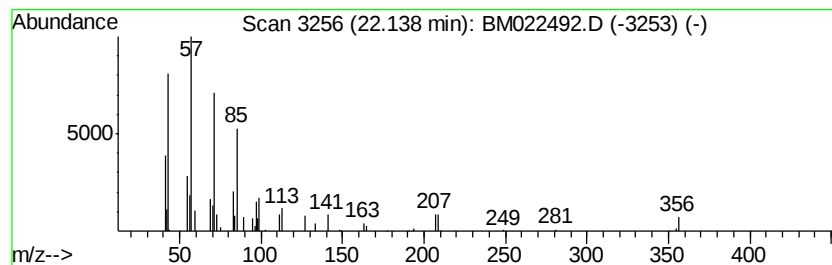
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 Peak Number 6 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
22.14	2.58 ng	33290	Chrysene-d12		21.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	87
2			2-methyloctacosane	408	C29H60	1000376-72-8	87
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
4			Tetratetracontane	619	C44H90	007098-22-8	87
5			2-methylhexacosane	380	C27H56	1000376-72-7	87



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Sample : K4562-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-02-20-22

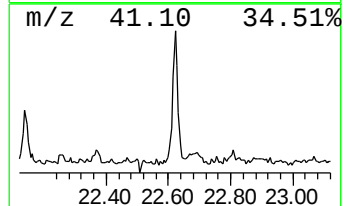
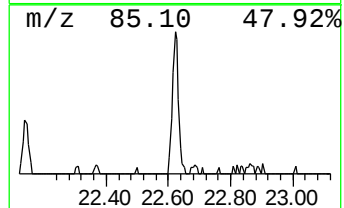
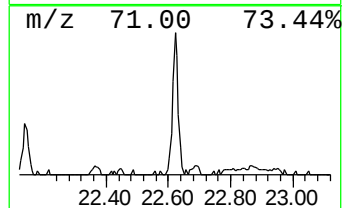
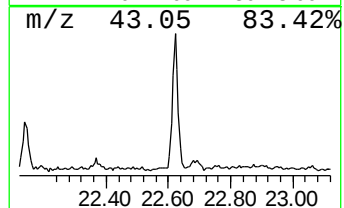
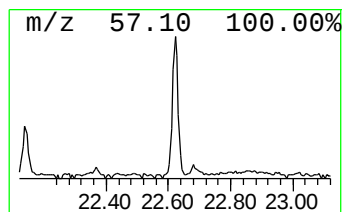
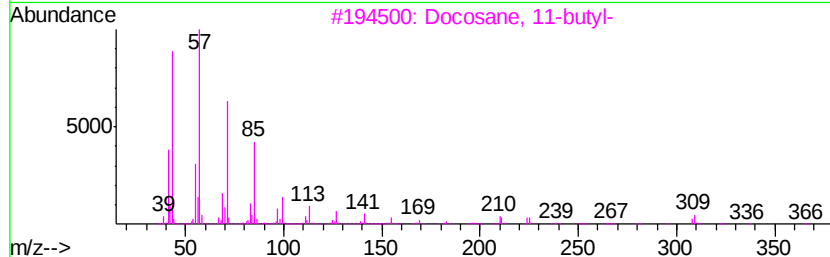
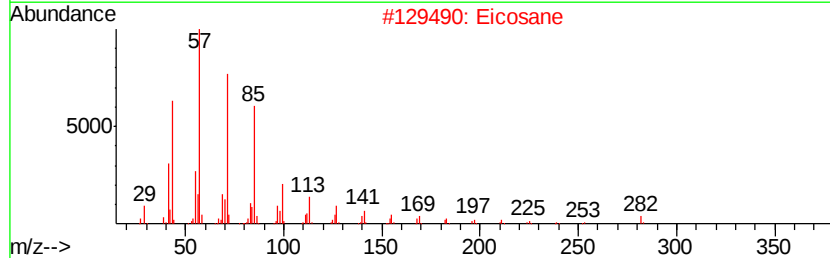
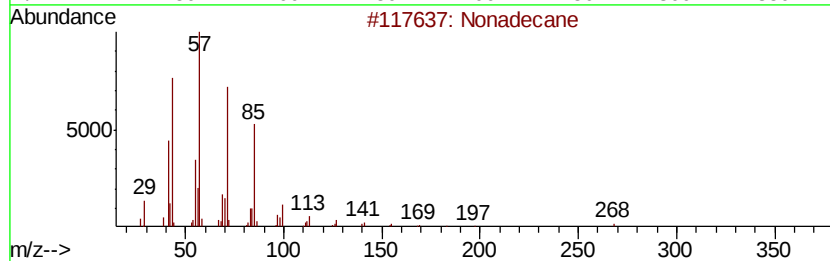
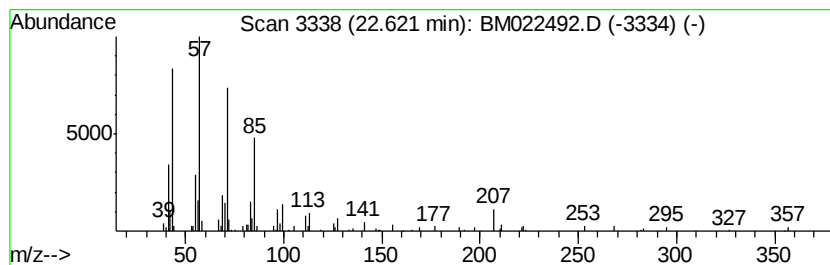
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.62	7.45 ng	103632	Perylene-d12	23.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	95
2		Eicosane	282	C20H42	000112-95-8	93
3		Docosane, 11-butyl-	366	C26H54	013475-76-8	90
4		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090119\
Data File : BM022492.D
Acq On : 02 Sep 2019 00:22
Operator : HP/JU
Sample : K4562-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-02-20-22

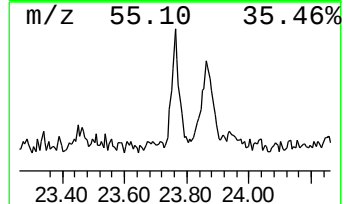
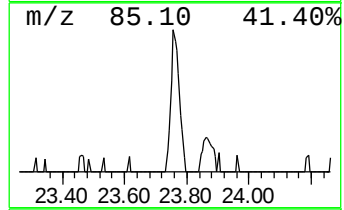
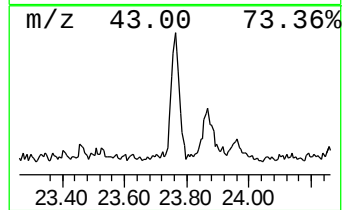
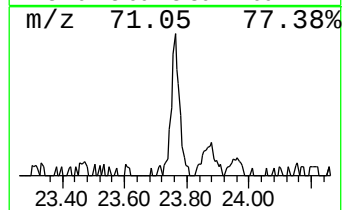
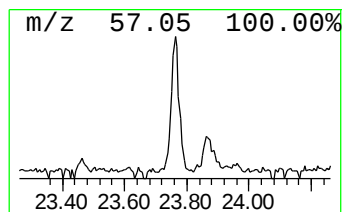
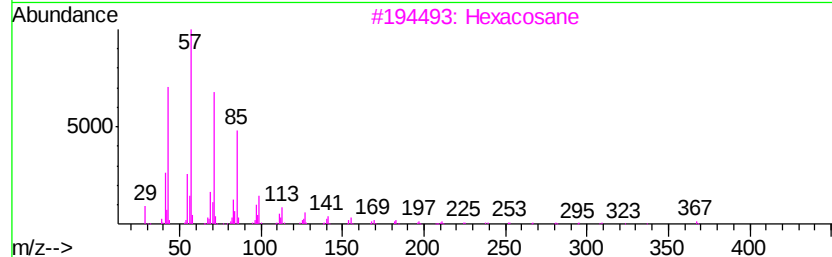
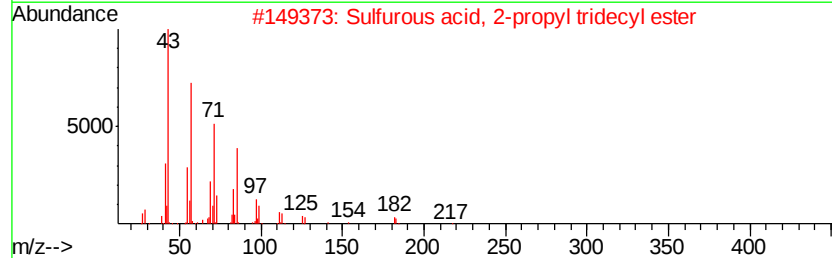
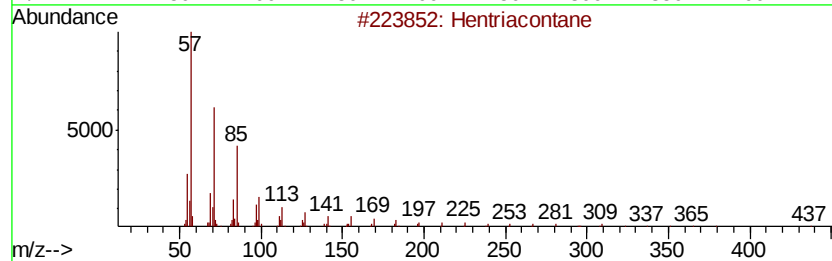
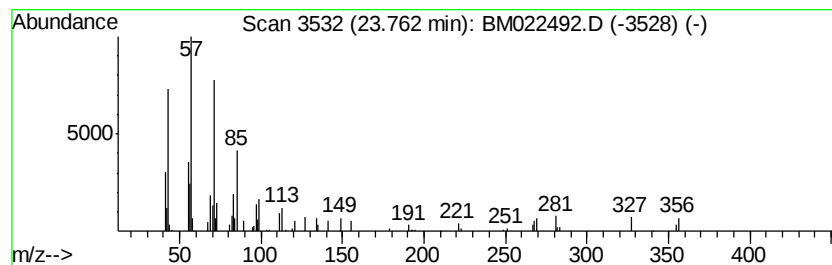
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Sulfurous acid, 2-propyl tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.76	5.25 ng	73052	Perylene-d12	23.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	87
2		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	83
3		Hexacosane	366	C26H54	000630-01-3	83
4		Tetratetracontane	619	C44H90	007098-22-8	83
5		Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090119\
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Sample : K4562-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-02-20-22

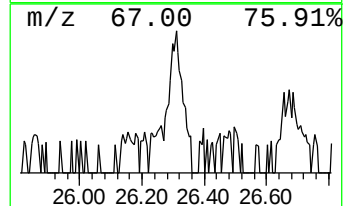
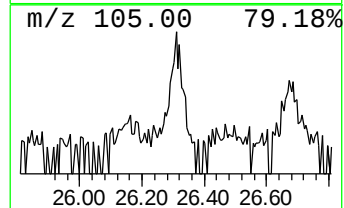
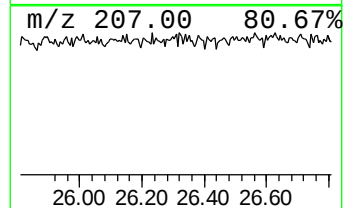
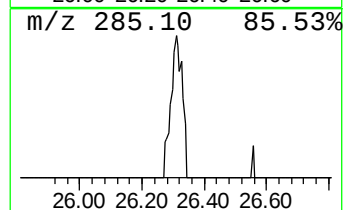
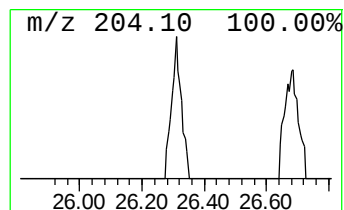
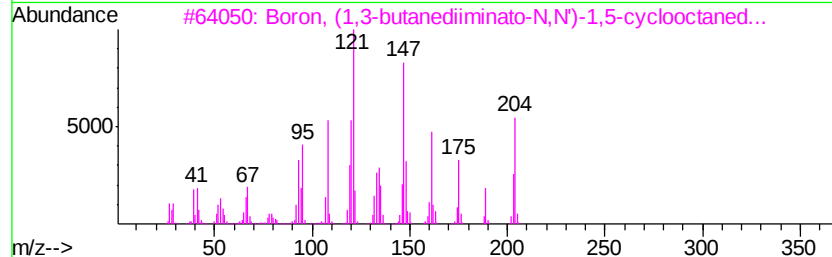
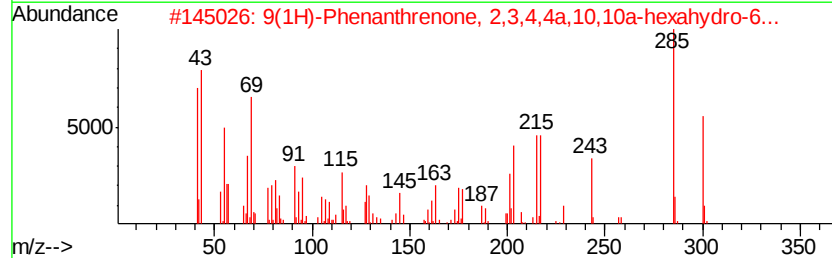
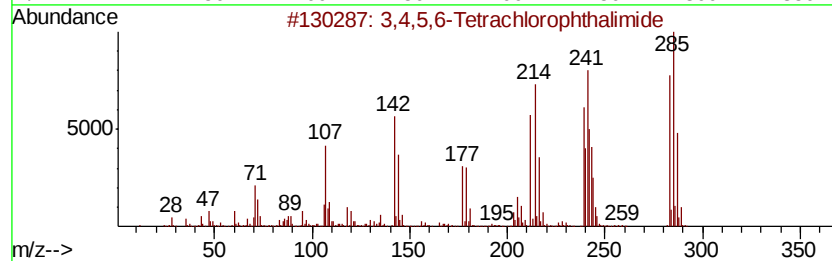
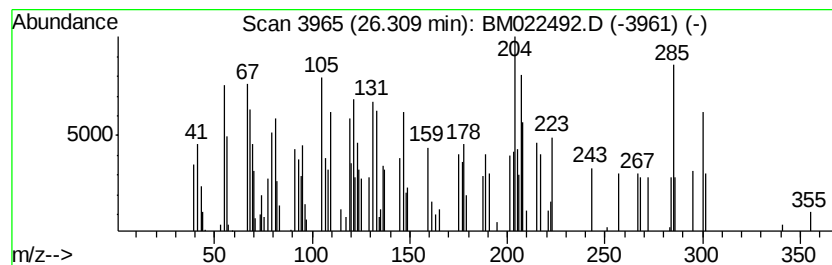
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 3,4,5,6-Tetrachlorophthalimide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.31	7.80 ng	108518	Perylene-d12	23.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,4,5,6-Tetrachlorophthalimide	283	C8HCl4N02	001571-13-7	56
2		9(1H)-Phenanthrenone, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	35
3		Boron, (1,3-butanediiminato-N,N'...	204	C12H21BN2	136704-98-8	25
4		4H-1-Benzopyran-4-one, 3,7-dihyd...	300	C16H12O6	057396-72-2	18
5		1,4-Methanoazulen-9-ol, decahydr...	222	C15H26O	000465-24-7	15



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM090119\
Data File : BM022492.D
Acq On : 02 Sep 2019 00:22
Operator : HP/JU
Sample : K4562-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-02-20-22

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.05	7.05	84.2	ng	274822	1	7.50	65315	20.0
n-Hexadecanoic acid	17.83	3.5	ng	29272	4	16.94	165223	20.0
Oxalic acid, isob...	20.84	5.7	ng	73169	5	21.16	258413	20.0
Heptacosane	21.70	3.6	ng	46636	5	21.16	258413	20.0
Hentriacontane	22.14	2.6	ng	33290	5	21.16	258413	20.0
Nonadecane	22.62	7.5	ng	103632	6	23.34	278267	20.0
Sulfurous acid, 2...	23.76	5.3	ng	73052	6	23.34	278267	20.0
3,4,5,6-Tetrachlo...	26.31	7.8	ng	108518	6	23.34	278267	20.0