

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030119\
 Data File : BM018991.D
 Acq On : 01 Mar 2019 17:44
 Operator : JU/SJ
 Sample : K1655-10
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 A0C12-2-1.5-2.0

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-BM021119.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	5.281	366	373	396	rBV	5299534	7706289	47.26%	7.532%
2	6.863	634	642	656	rBV	5557210	8802511	53.98%	8.603%
3	7.216	695	702	716	rBV	5591770	8781729	53.86%	8.583%
4	7.681	773	781	788	rBV	893826	1397631	8.57%	1.366%
5	7.998	827	835	845	rBV	3796632	5914368	36.27%	5.780%
6	8.851	972	980	999	rBV	3013087	5093742	31.24%	4.978%
7	10.469	1248	1255	1272	rBV	1114318	1939871	11.90%	1.896%
8	12.951	1669	1677	1691	rBV	7552208	11026196	67.62%	10.776%
9	13.798	1815	1821	1835	rBV	432419	649577	3.98%	0.635%
10	14.333	1905	1912	1921	rBV2	1789107	2654670	16.28%	2.594%
11	15.833	2160	2167	2182	rBV	7323997	10037564	61.56%	9.810%
12	17.086	2374	2380	2385	rBV2	2224629	3234762	19.84%	3.161%
13	17.127	2385	2387	2393	rVB	178722	237441	1.46%	0.232%
14	17.751	2488	2493	2497	rBV	180016	214099	1.31%	0.209%
15	17.980	2526	2532	2543	rBV	1140557	1713307	10.51%	1.674%
16	19.062	2712	2716	2721	rVB	147281	163361	1.00%	0.160%
17	19.151	2727	2731	2740	rVB	211019	329556	2.02%	0.322%
18	19.262	2746	2750	2761	rBV	360115	547757	3.36%	0.535%
19	19.409	2771	2775	2784	rVB	229915	271974	1.67%	0.266%
20	19.521	2790	2794	2802	rVB	168596	246376	1.51%	0.241%
21	19.727	2822	2829	2835	rBV	13277170	16305523	100.00%	15.936%
22	20.456	2950	2953	2958	rBV	353368	387722	2.38%	0.379%
23	20.521	2960	2964	2968	rVB	134861	163328	1.00%	0.160%
24	20.986	3038	3043	3053	rBV	1676215	2265850	13.90%	2.214%
25	21.286	3088	3094	3099	rBV	2951054	3892014	23.87%	3.804%
26	21.421	3113	3117	3124	rBV	425511	497471	3.05%	0.486%
27	21.850	3187	3190	3205	rVB	491242	823473	5.05%	0.805%
28	22.315	3265	3269	3276	rVB	683207	866423	5.31%	0.847%
29	22.821	3350	3355	3359	rBV	661469	953575	5.85%	0.932%
30	23.386	3447	3451	3457	rVB	528863	780876	4.79%	0.763%
31	23.533	3470	3476	3488	rVB2	1598390	3119152	19.13%	3.048%
32	24.033	3556	3561	3567	rVB	408753	728340	4.47%	0.712%
33	24.127	3573	3577	3590	rVB2	271067	573921	3.52%	0.561%

LSC Area Percent Report

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ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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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-BM021119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

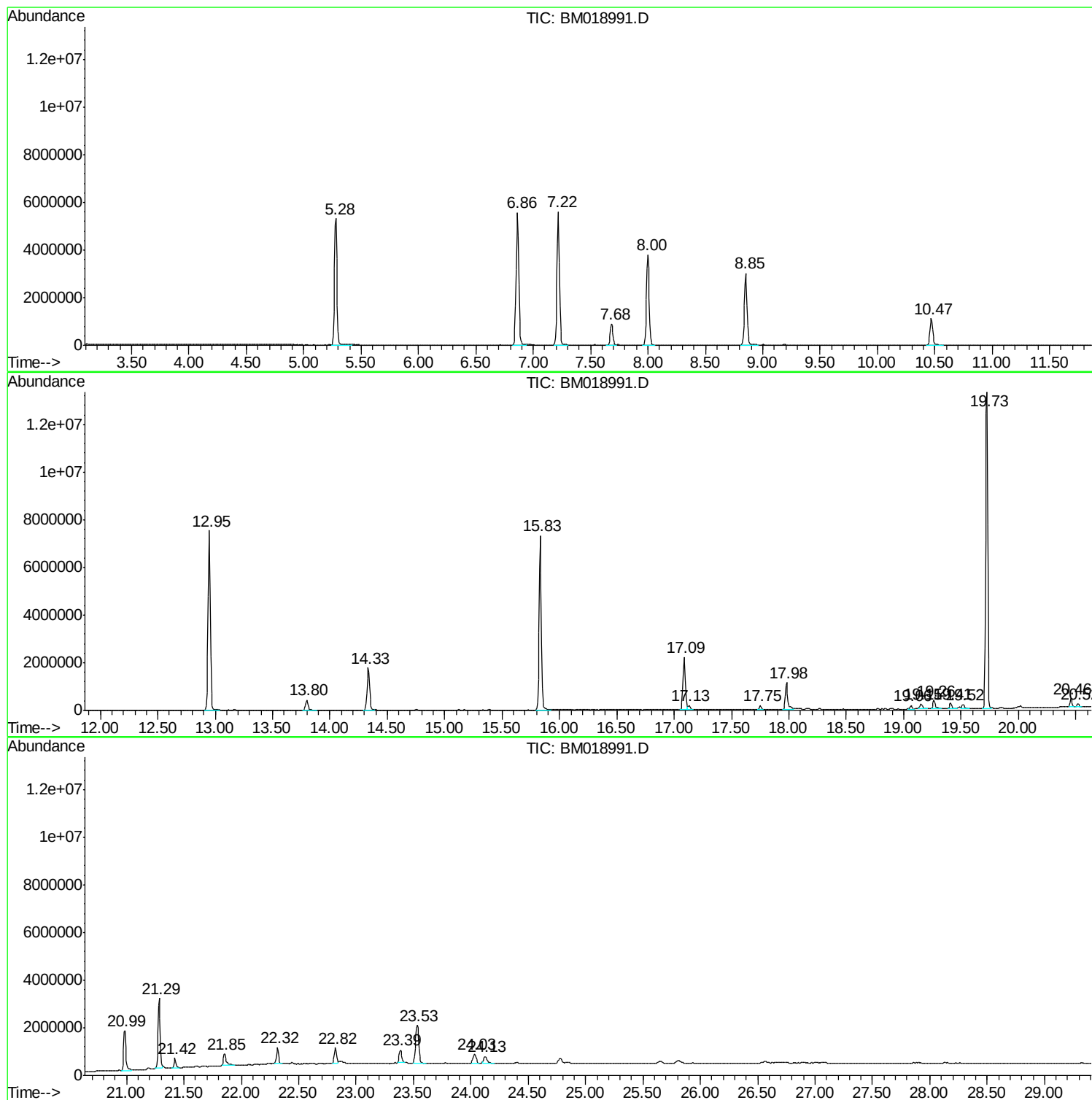
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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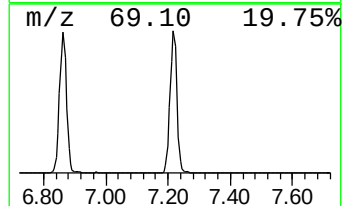
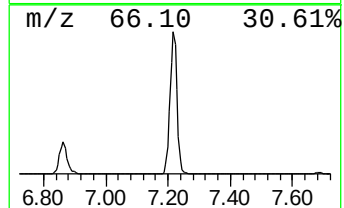
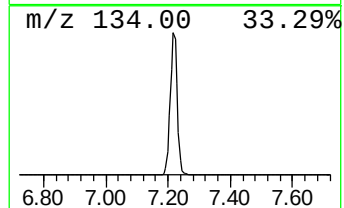
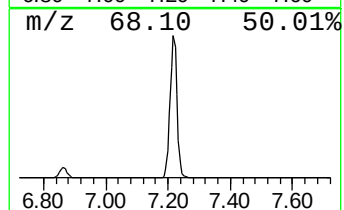
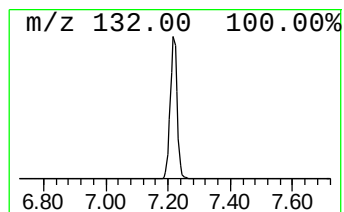
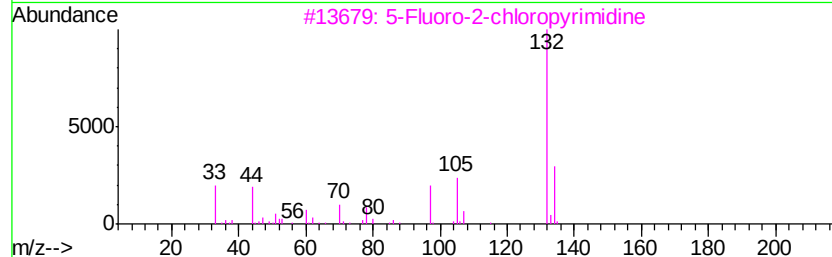
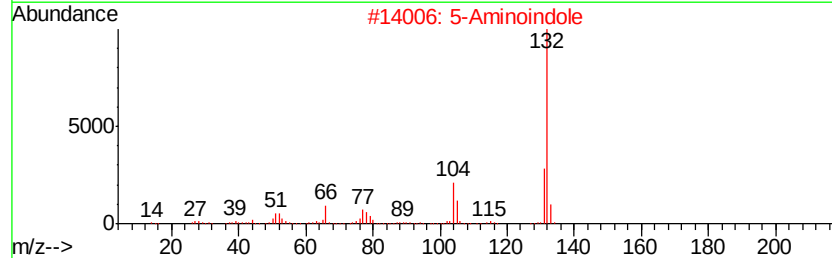
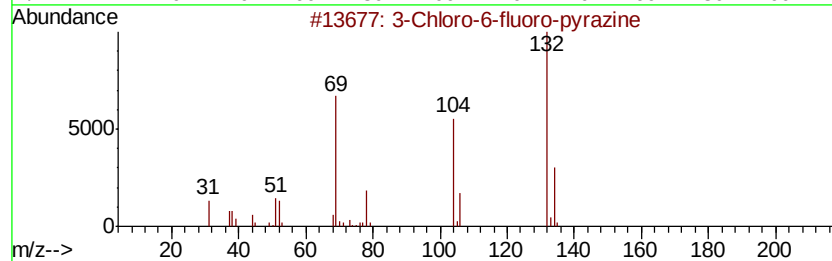
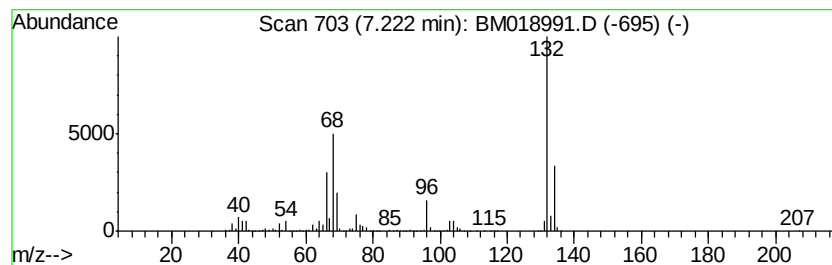
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	125.67 ng	8781730	1,4-Dichlorobenzene-d4	7.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5			(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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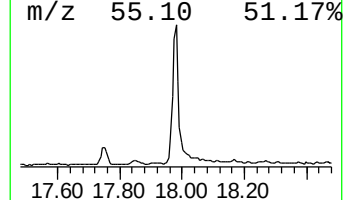
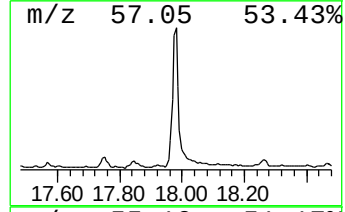
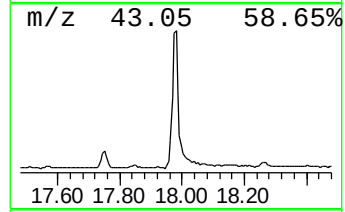
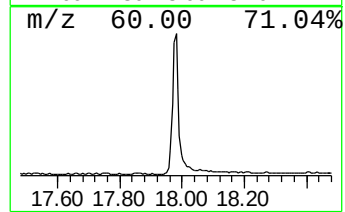
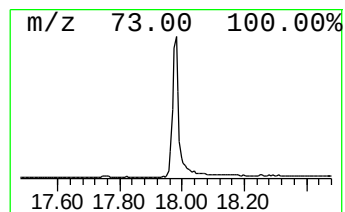
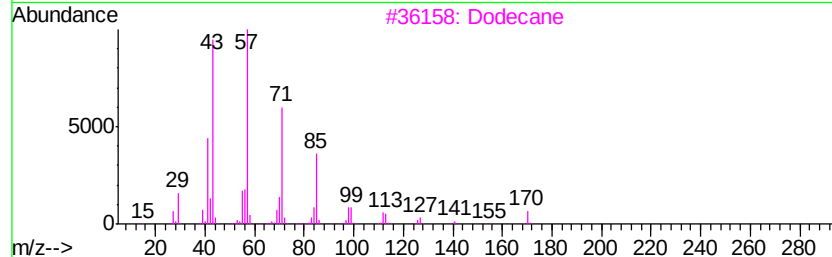
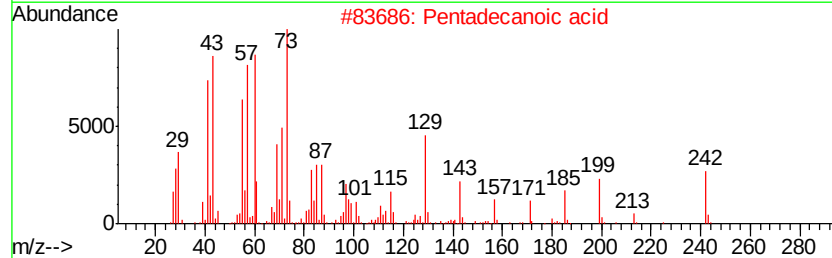
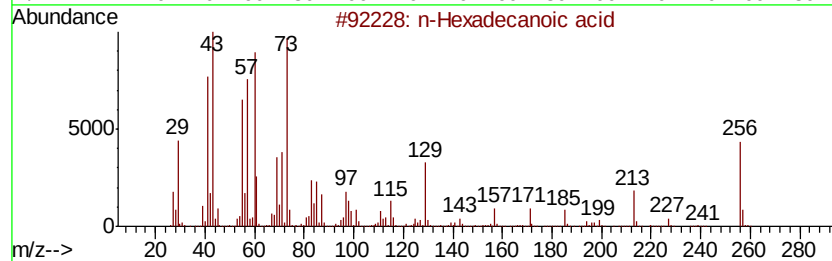
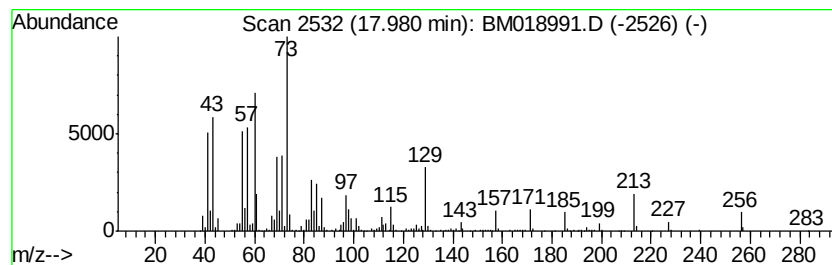
Instrument :
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.98	10.59 ng	1713310	Phenanthrene-d10		17.09
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Dodecane	170	C12H26	000112-40-3	18
4	Hexadecane	226	C16H34	000544-76-3	18
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	18



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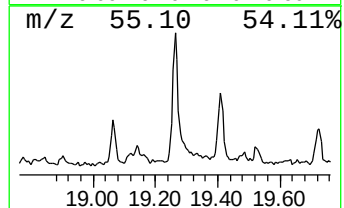
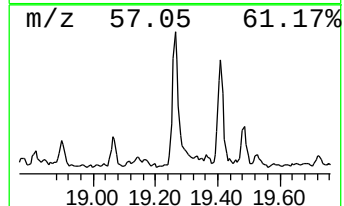
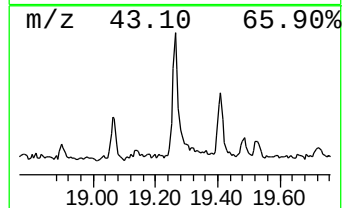
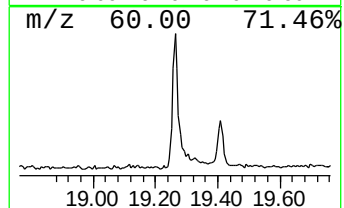
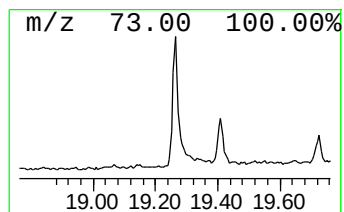
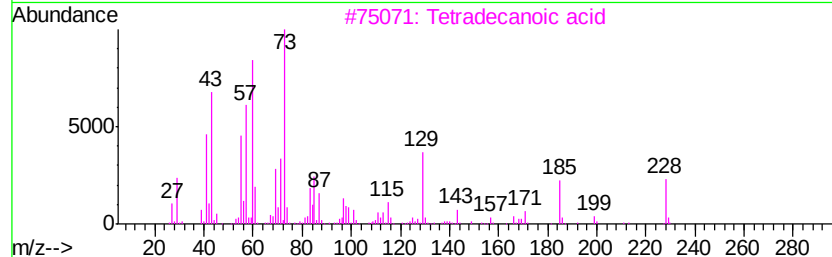
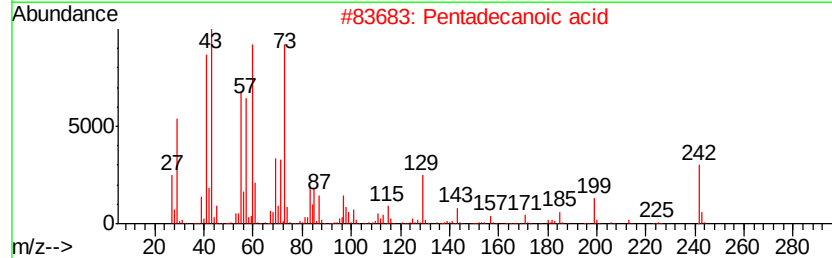
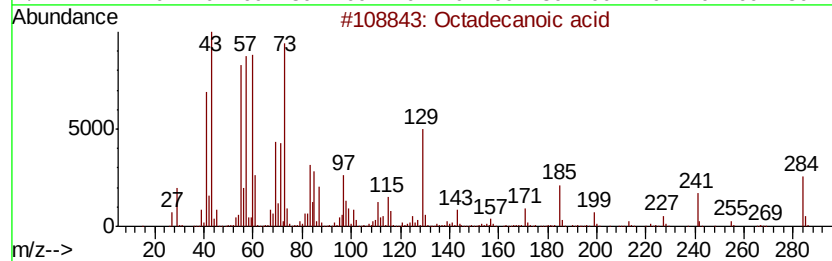
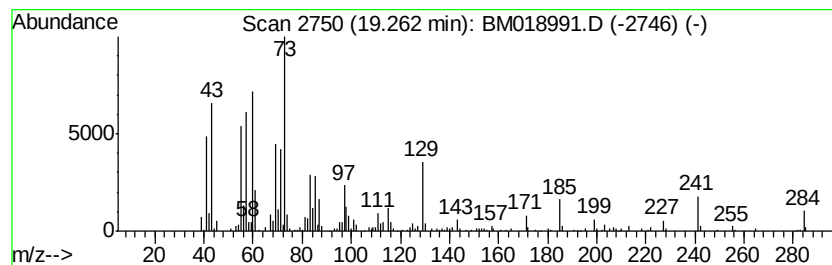
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.26	2.81 ng	547757	Chrysene-d12		21.29
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	80
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76



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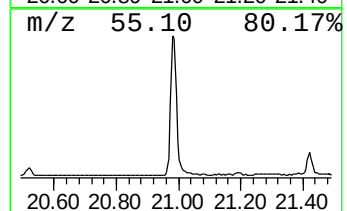
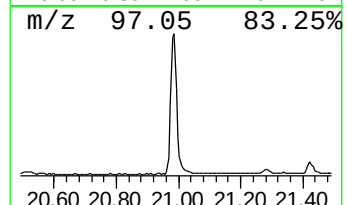
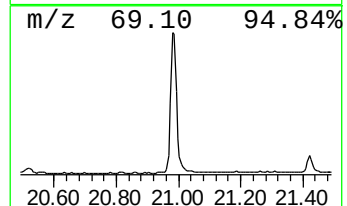
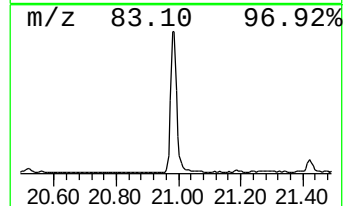
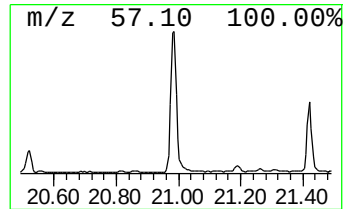
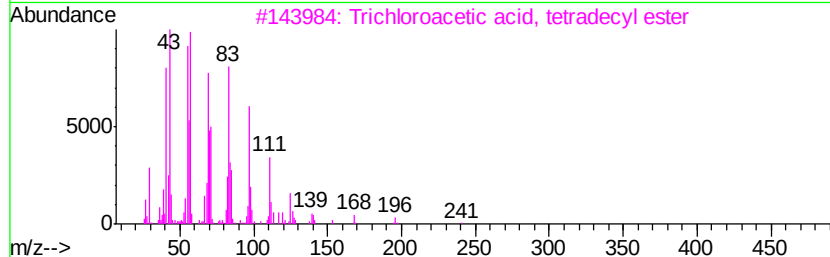
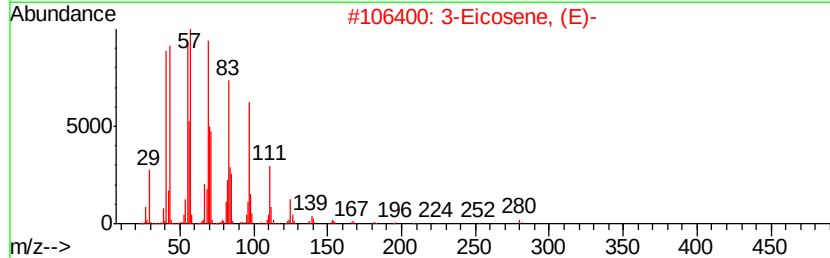
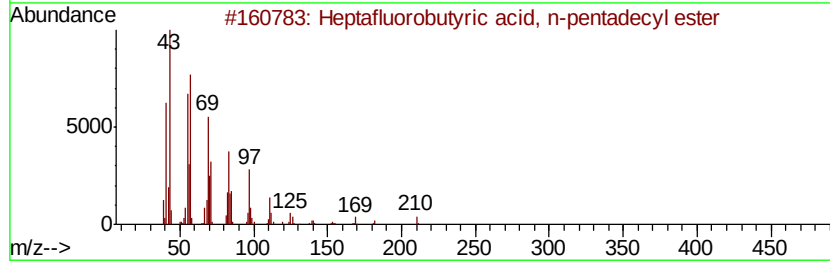
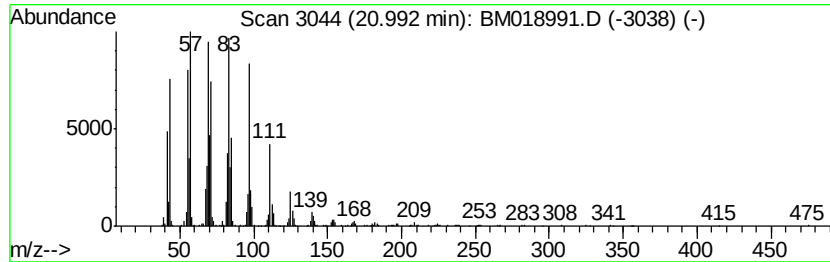
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.99	11.64 ng	2265850	Chrysene-d12		21.29	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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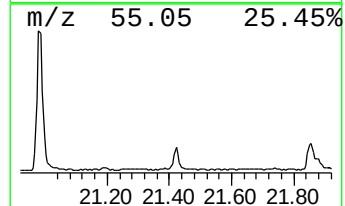
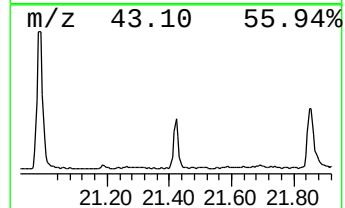
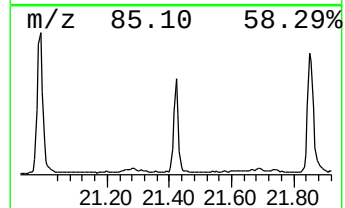
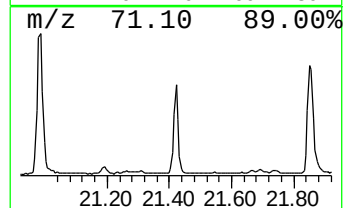
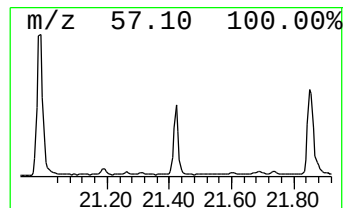
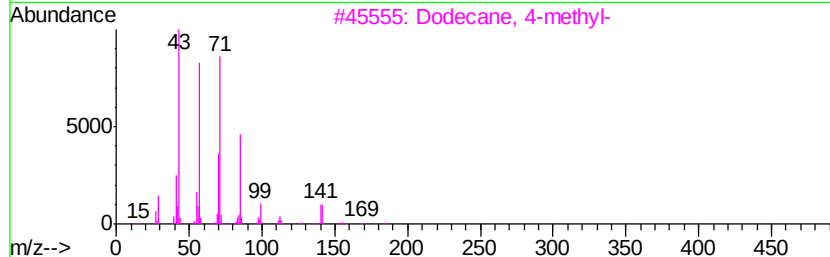
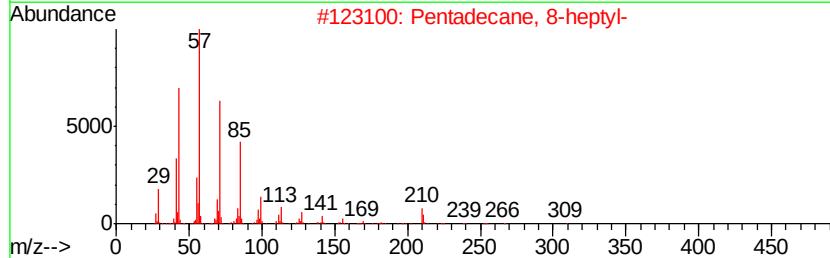
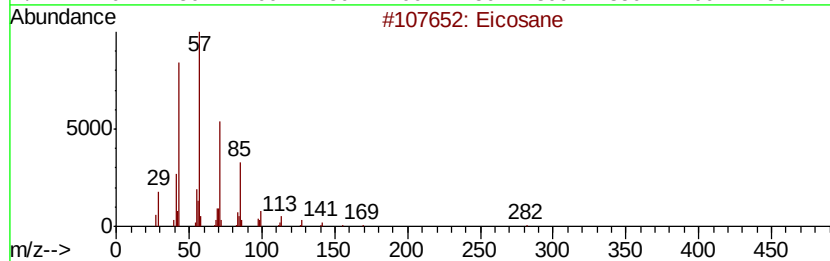
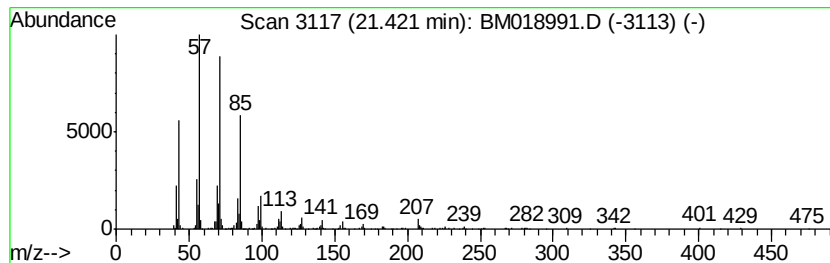
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.42	2.56 ng	497471	Chrysene-d12	21.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	86
3	Dodecane, 4-methyl-	184	C13H28	006117-97-1	83
4	Dodecane	170	C12H26	000112-40-3	83
5	Octadecane	254	C18H38	000593-45-3	83



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 Misc :
 ALS Vial : 8 Sample Multiplier: 1

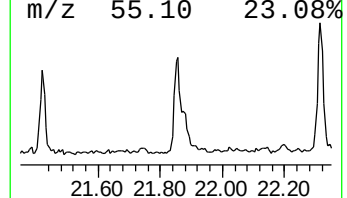
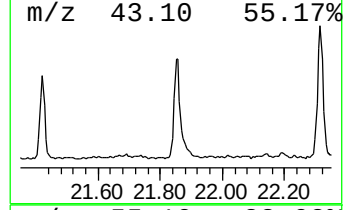
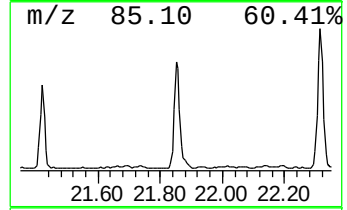
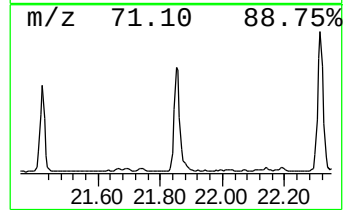
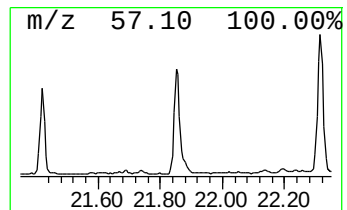
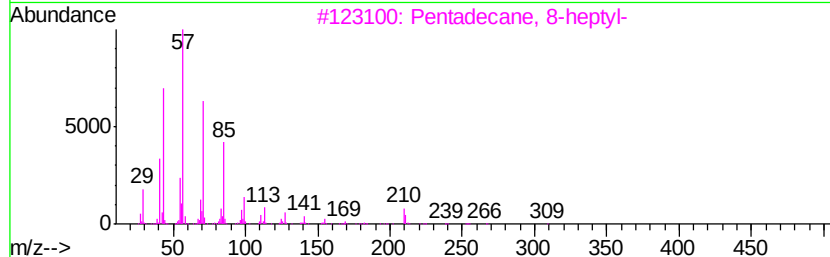
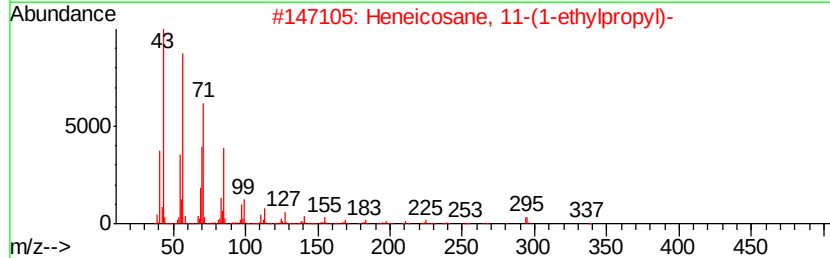
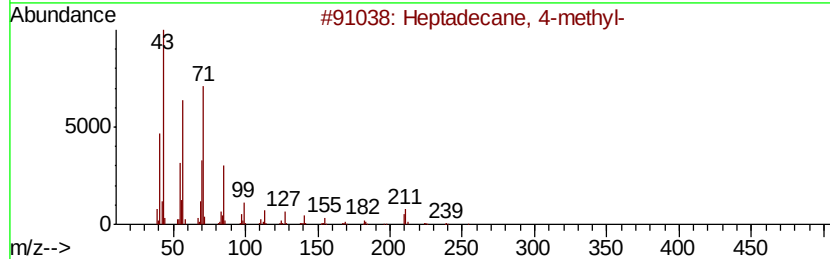
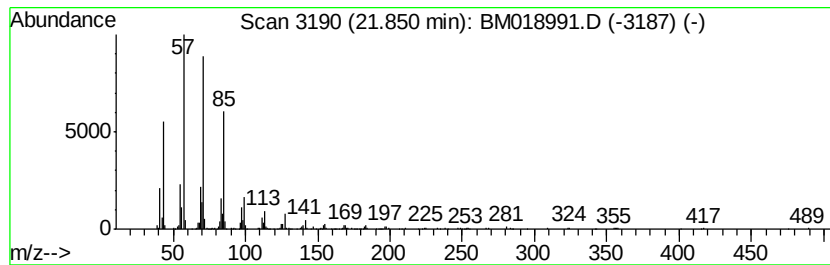
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 8 Heptadecane, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.85	4.23 ng	823473	Chrysene-d12		21.29	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 4-methyl-	254	C18H38	026429-11-8	91
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030119\
Data File : BM018991.D
Acq On : 01 Mar 2019 17:44
Operator : JU/SJ
Sample : K1655-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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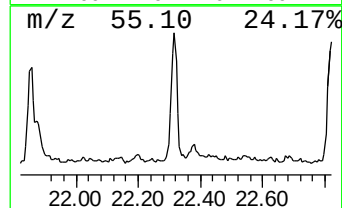
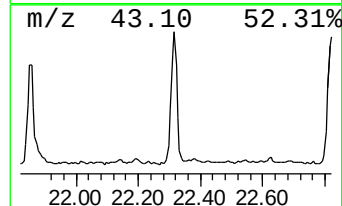
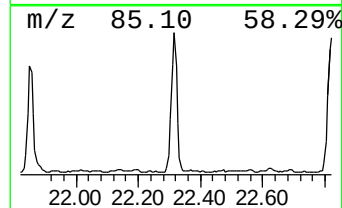
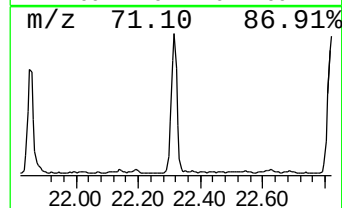
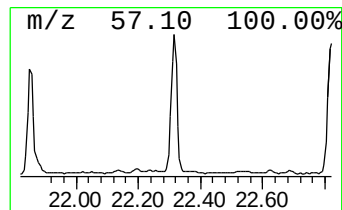
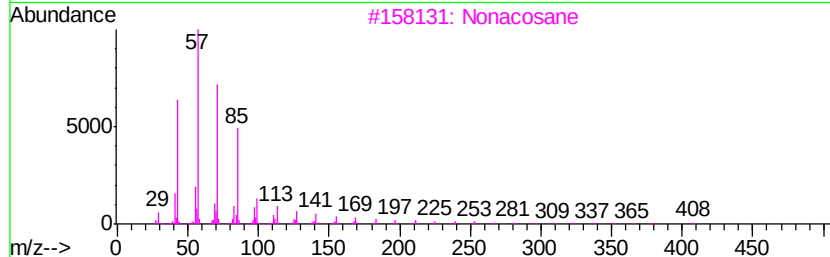
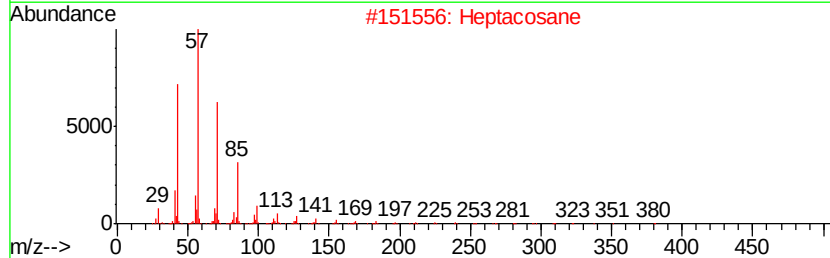
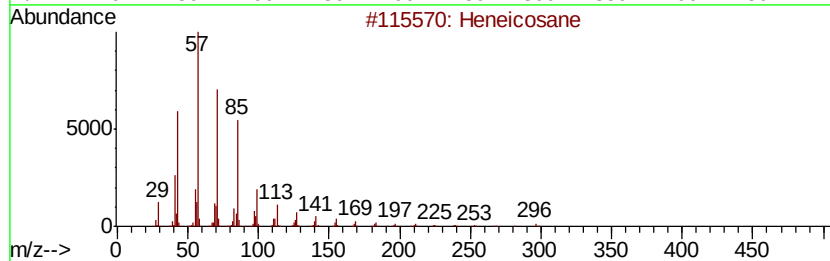
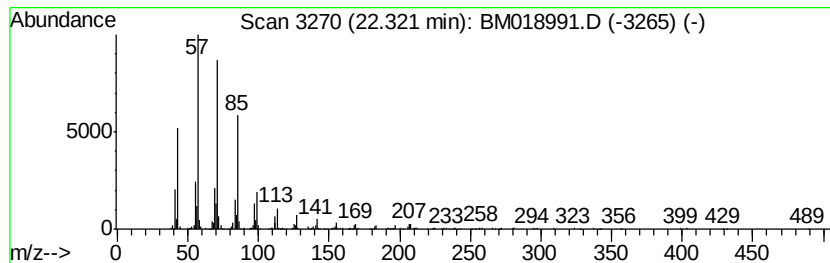
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.32	4.45 ng	866423	Chrysene-d12	21.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Nonacosane	408	C29H60	000630-03-5	90
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030119\
Data File : BM018991.D
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Sample : K1655-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

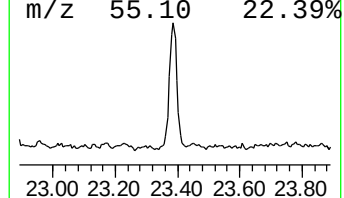
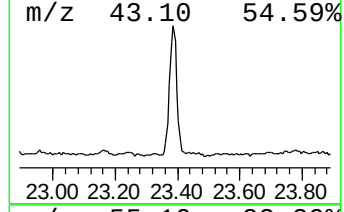
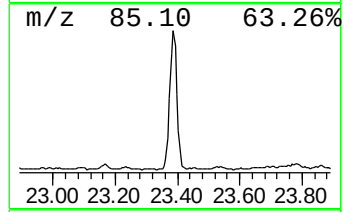
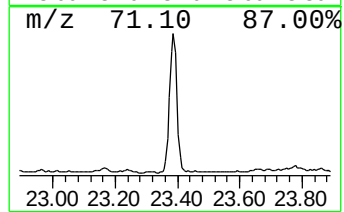
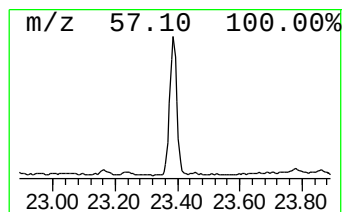
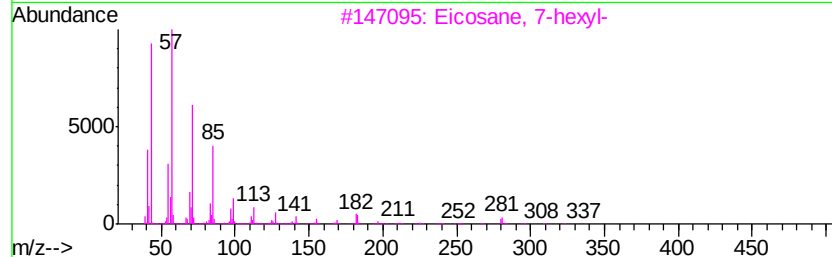
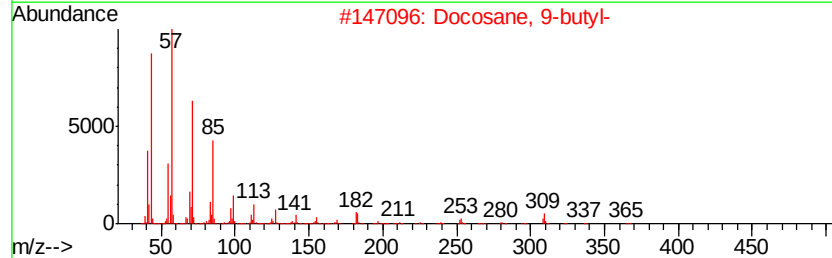
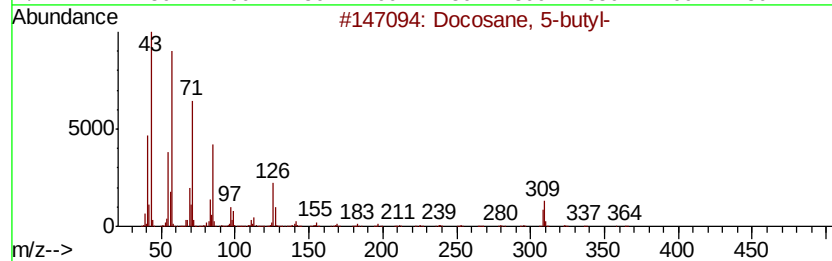
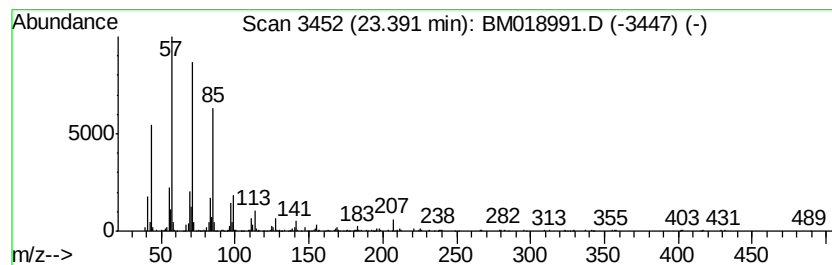
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Docosane, 5-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.39	5.01 ng	780876	Perylene-d12	23.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 5-butyl-	366	C26H54	055282-16-1	90
2	Docosane, 9-butyl-	366	C26H54	055282-14-9	90
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Tridecane, 6-propyl-	226	C16H34	055045-10-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030119\
Data File : BM018991.D
Acq On : 01 Mar 2019 17:44
Operator : JU/SJ
Sample : K1655-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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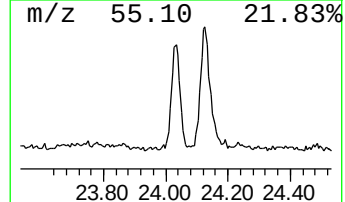
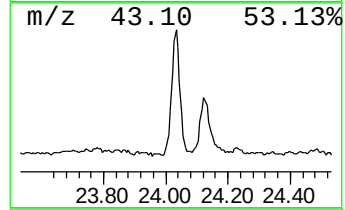
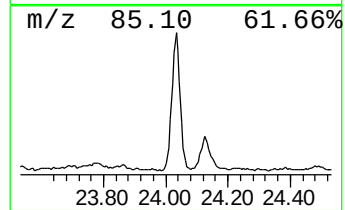
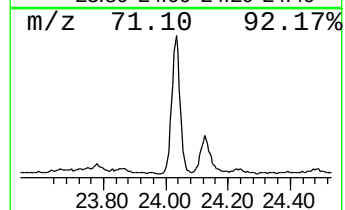
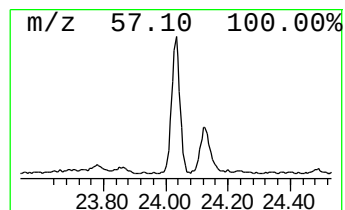
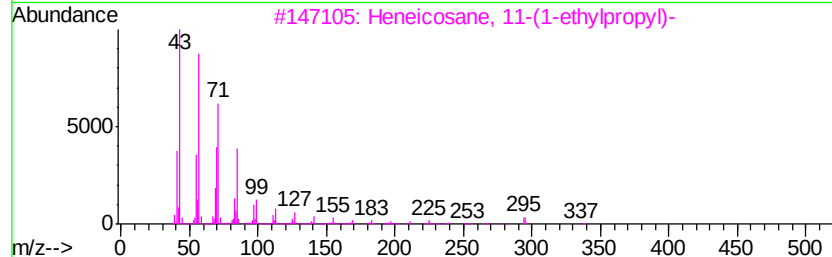
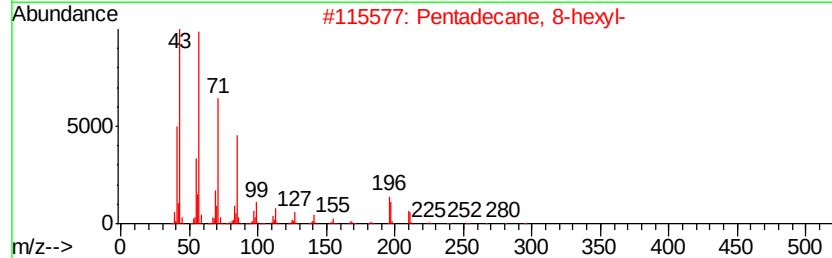
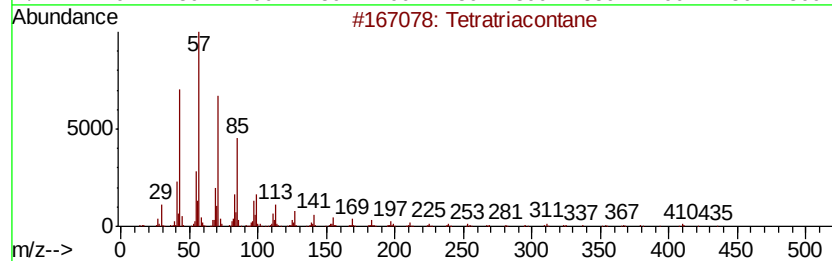
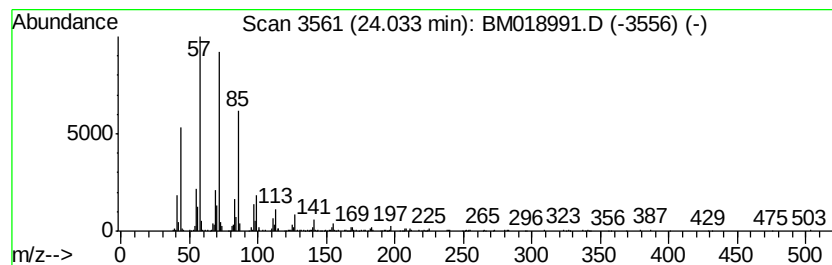
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Tetratriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.03	4.67 ng	728340	Perylene-d12	23.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratriacontane	479	C34H70	014167-59-0	91
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM030119\
Data File : BM018991.D
Acq On : 01 Mar 2019 17:44
Operator : JU/SJ
Sample : K1655-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

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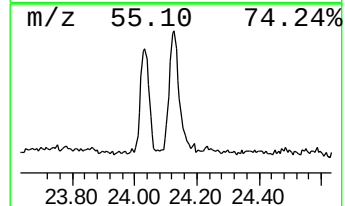
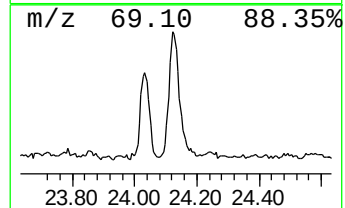
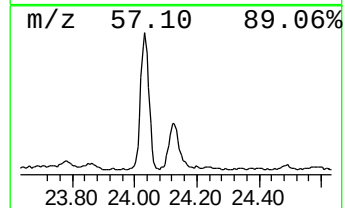
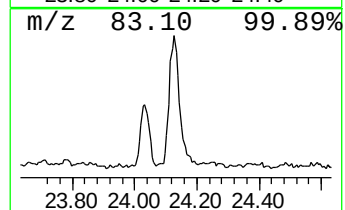
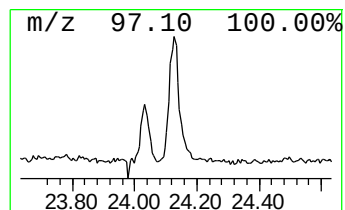
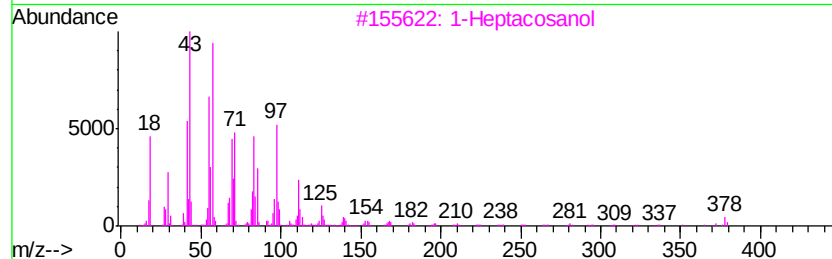
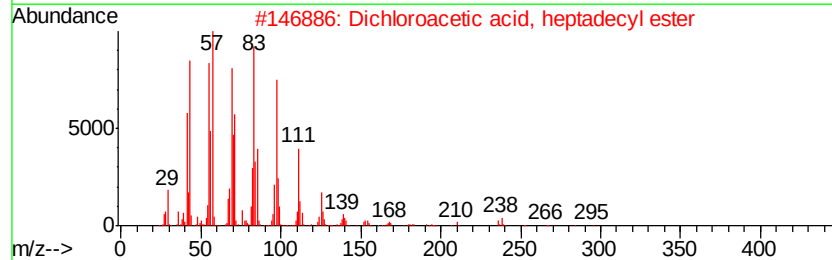
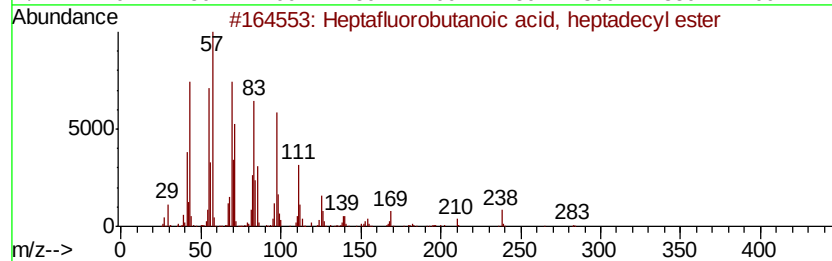
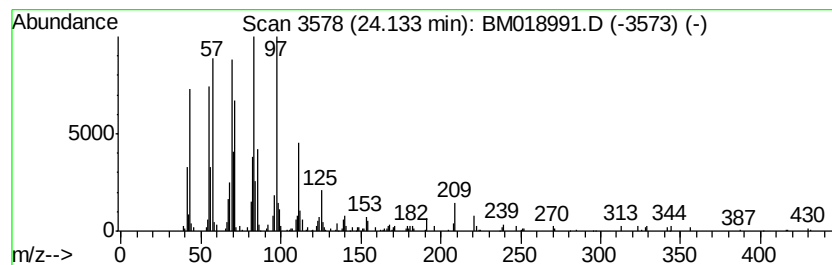
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptafluorobutanoic acid, h... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.13	3.68 ng	573921	Perylene-d12	23.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	80
3		1-Heptacosanol	396	C27H56O	002004-39-9	72
4		1-Docosene	308	C22H44	001599-67-3	62
5		1-Eicosanol	298	C20H42O	000629-96-9	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030119\
Data File : BM018991.D
Acq On : 01 Mar 2019 17:44
Operator : JU/SJ
Sample : K1655-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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 acid	17.98	10.6	ng	1713310	4	17.09	3234760	20.0
Octadecanoic acid	19.26	2.8	ng	547757	5	21.29	3892010	20.0
Heptafluorobutyri...	20.99	11.6	ng	2265850	5	21.29	3892010	20.0
Eicosane	21.42	2.6	ng	497471	5	21.29	3892010	20.0
Heptadecane, 4-me...	21.85	4.2	ng	823473	5	21.29	3892010	20.0
Heneicosane	22.32	4.5	ng	866423	5	21.29	3892010	20.0
Docosane, 5-butyl-	23.39	5.0	ng	780876	6	23.53	3119150	20.0
Tetratriacontane	24.03	4.7	ng	728340	6	23.53	3119150	20.0
Heptafluorobutano...	24.13	3.7	ng	573921	6	23.53	3119150	20.0