

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
 Data File : BM015928.D
 Acq On : 12 Jul 2018 23:10
 Operator : SJ/JU
 Sample : J3951-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 071018-TIPC-E-U-M

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-BM070518.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	5.793	421	426	439	rBV	590390	935905	14.62%	3.263%
2	7.440	700	706	721	rBV	388388	679472	10.61%	2.369%
3	7.810	762	769	783	rBV	1177238	1921475	30.01%	6.699%
4	8.287	844	850	856	rBV	343621	563670	8.80%	1.965%
5	8.610	898	905	915	rBV	1609832	2581251	40.32%	8.999%
6	9.475	1044	1052	1064	rBV	1301974	2200794	34.38%	7.672%
7	11.110	1324	1330	1341	rBV	407733	718438	11.22%	2.505%
8	13.533	1735	1742	1751	rBV	3123521	4374366	68.33%	15.250%
9	14.357	1876	1882	1891	rBV	94073	132395	2.07%	0.462%
10	14.904	1964	1975	1983	rBV3	564424	922727	14.41%	3.217%
11	16.163	2184	2189	2194	rBV	181408	216190	3.38%	0.754%
12	16.386	2221	2227	2242	rBV	1574857	2261966	35.33%	7.886%
13	17.633	2433	2439	2450	rBV	705894	1015892	15.87%	3.542%
14	18.468	2574	2581	2593	rBV	134430	200621	3.13%	0.699%
15	19.651	2779	2782	2790	rVB4	45054	69582	1.09%	0.243%
16	19.721	2790	2794	2800	rBV	99636	127602	1.99%	0.445%
17	20.198	2869	2875	2880	rBV	5490220	6402243	100.00%	22.319%
18	20.945	2998	3002	3006	rBV2	94048	111696	1.74%	0.389%
19	21.403	3076	3080	3091	rBV2	123351	208480	3.26%	0.727%
20	21.745	3133	3138	3145	rVB	822106	1071812	16.74%	3.737%
21	21.839	3150	3154	3158	rVB	142255	166103	2.59%	0.579%
22	22.292	3227	3231	3234	rVB	132191	159430	2.49%	0.556%
23	22.774	3310	3313	3319	rVB	143016	187981	2.94%	0.655%
24	23.315	3401	3405	3411	rVB	131292	193783	3.03%	0.676%
25	23.915	3504	3507	3512	rVB	114018	179629	2.81%	0.626%
26	24.133	3538	3544	3556	rBV2	529650	1081060	16.89%	3.769%

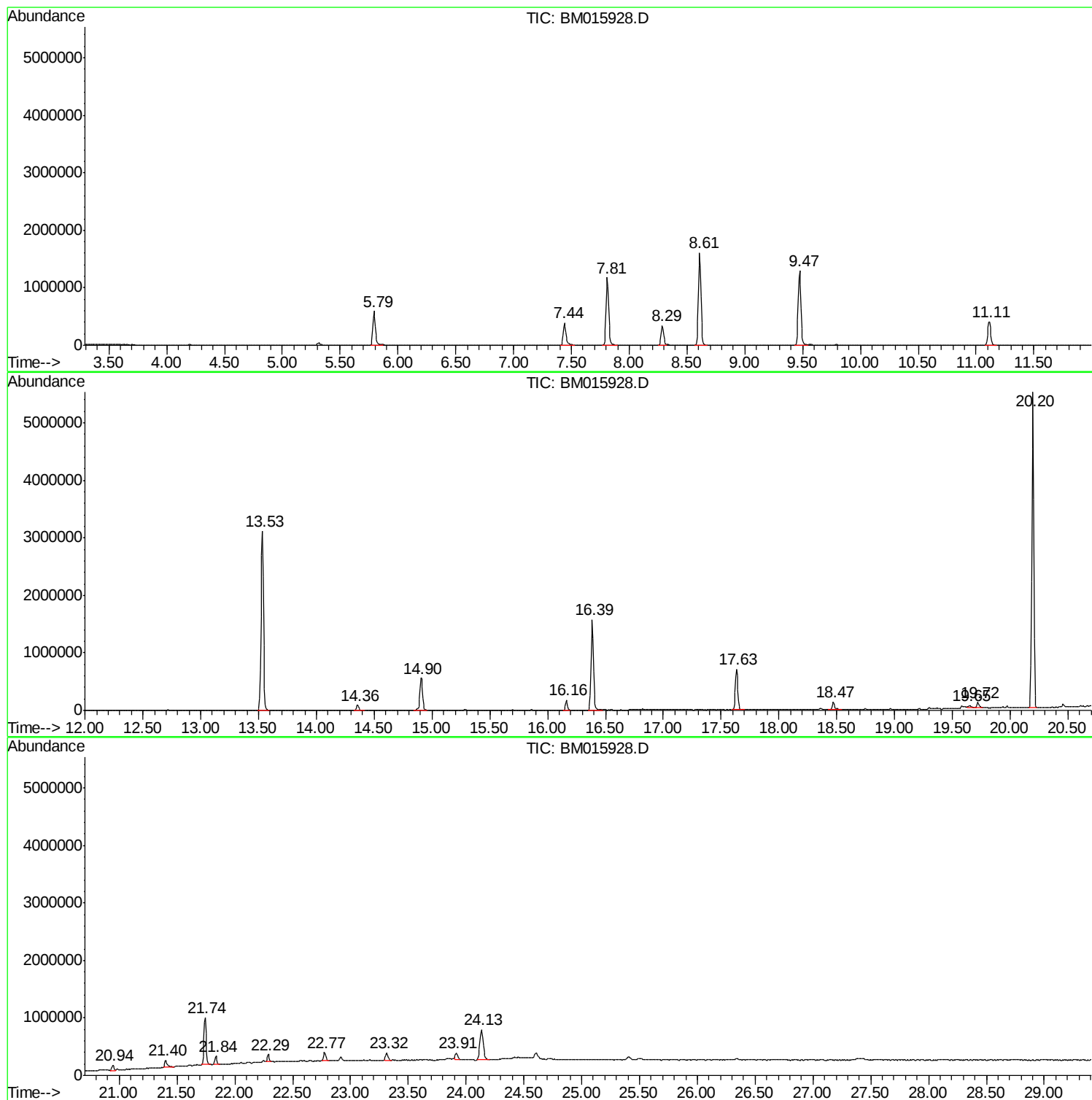
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM070518.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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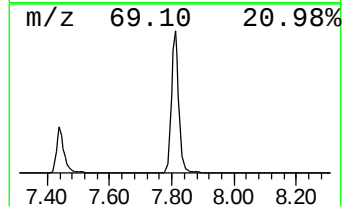
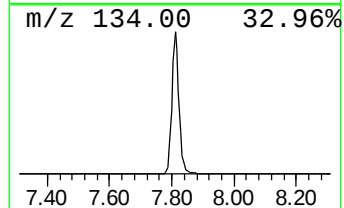
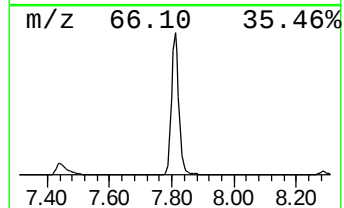
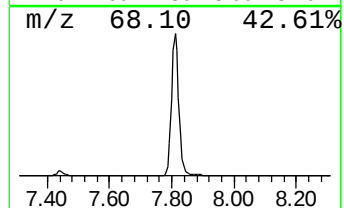
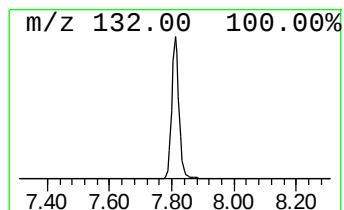
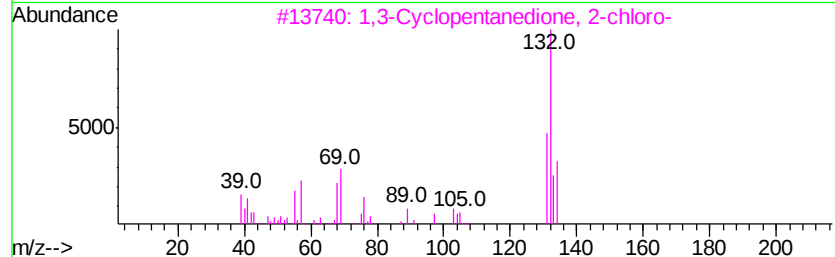
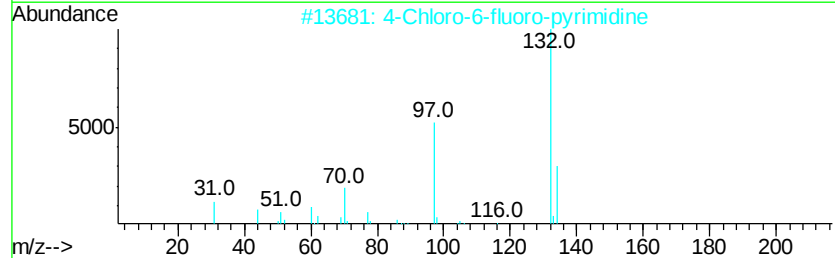
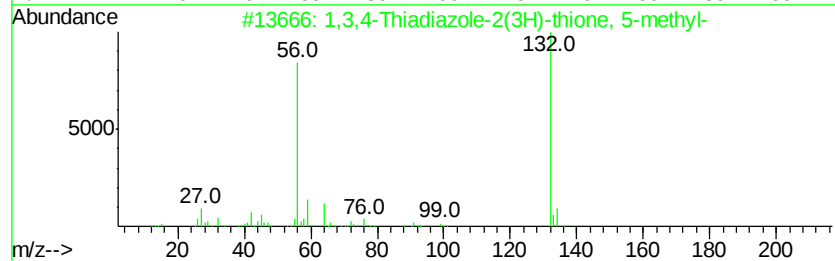
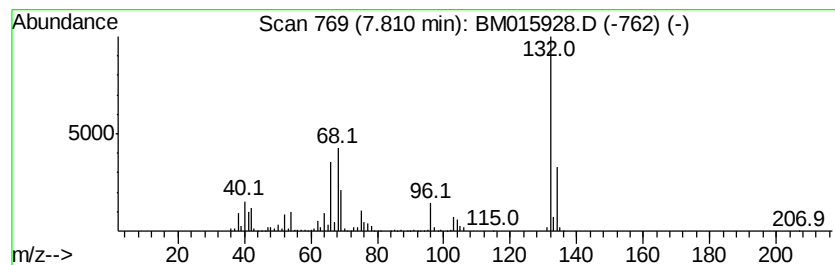
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.81 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	68.18 ng	1921480	1,4-Dichlorobenzene-d4	8.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
2			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3			1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22



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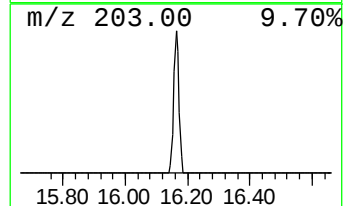
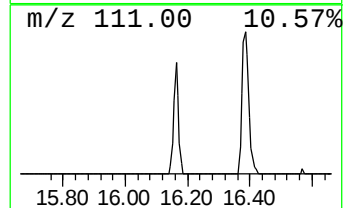
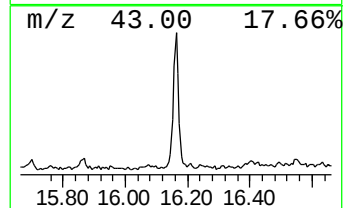
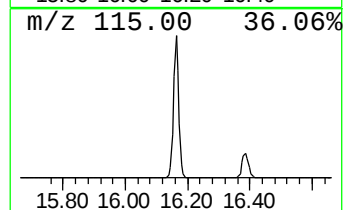
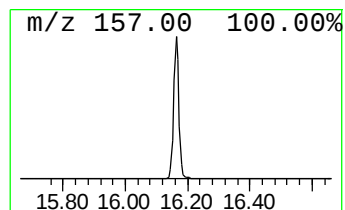
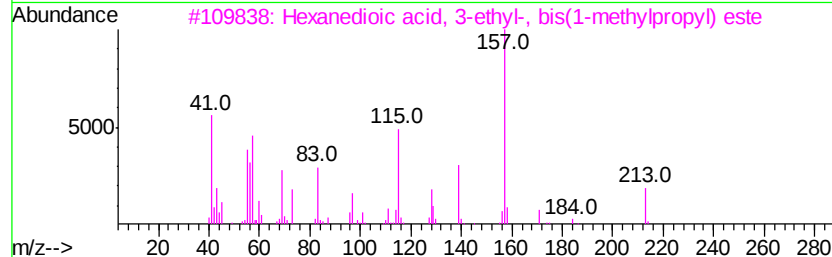
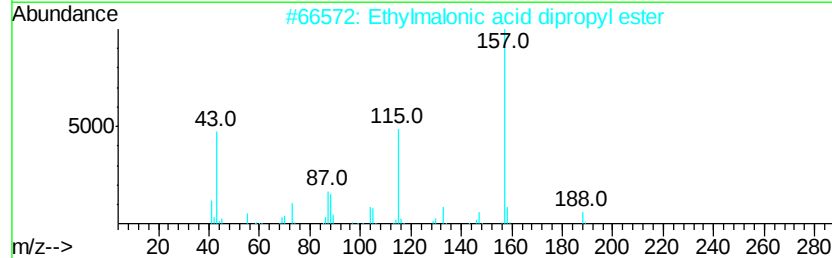
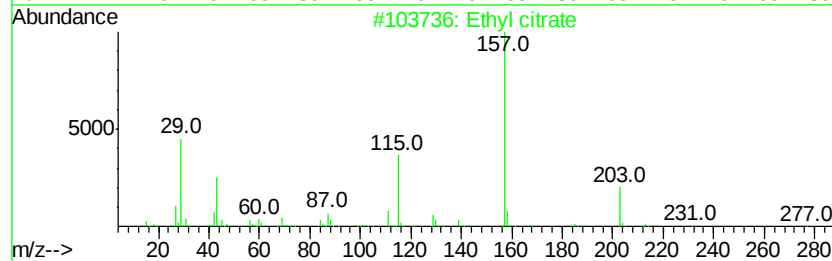
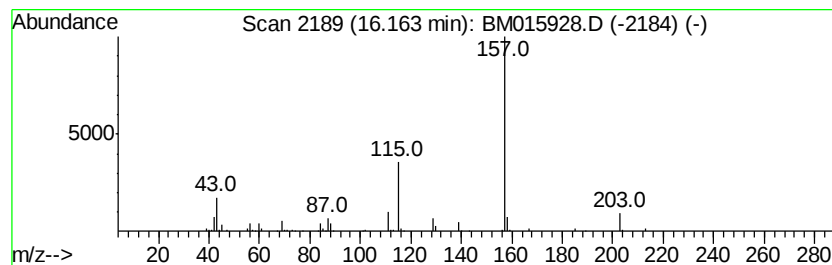
Instrument :
BNA_M
ClientSampleId :
071018-TIPC-E-U-M

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Peak Number 3 Ethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	4.69 ng	216190	Acenaphthene-d10	14.90
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Ethyl citrate	276 C12H20O7	000077-93-0 78
2		Ethylmalonic acid dipropyl ester	216 C11H20O4	001113-91-3 64
3		Hexanedioic acid, 3-ethyl-, bis(...	286 C16H30O4	057983-54-7 39
4		1-Amino-2-methylnaphthalene	157 C11H11N	002246-44-8 38
5		Pyrimidine, 2-methylthio-4-hydro...	157 C5H7N3OS	001074-41-5 33



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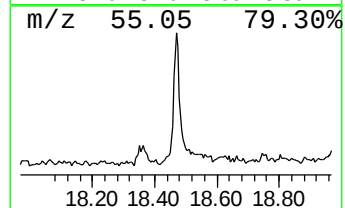
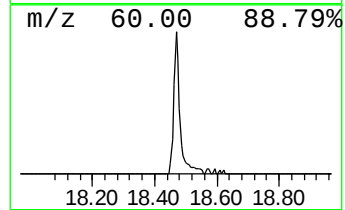
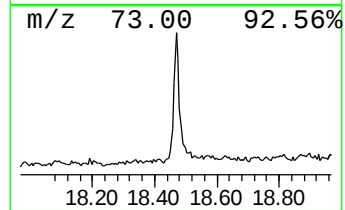
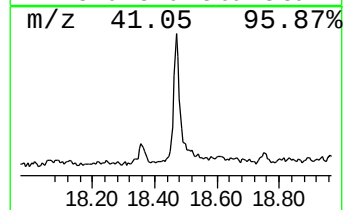
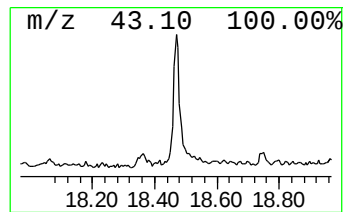
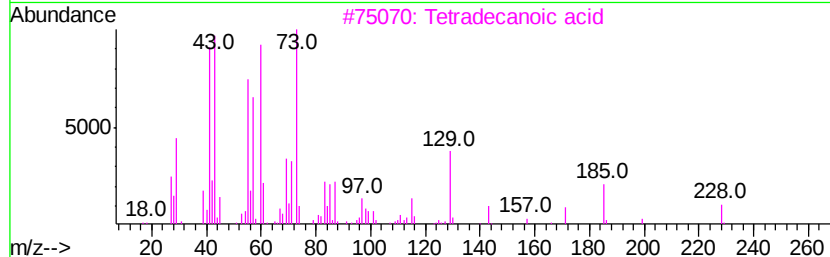
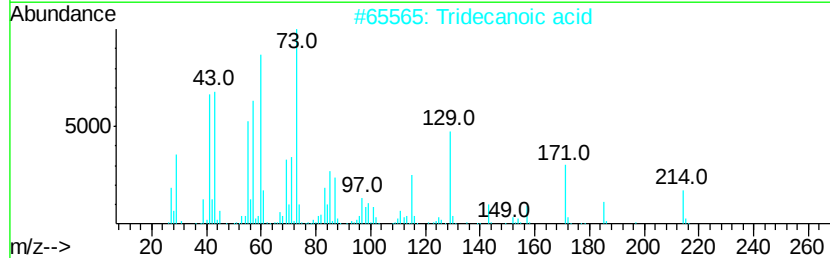
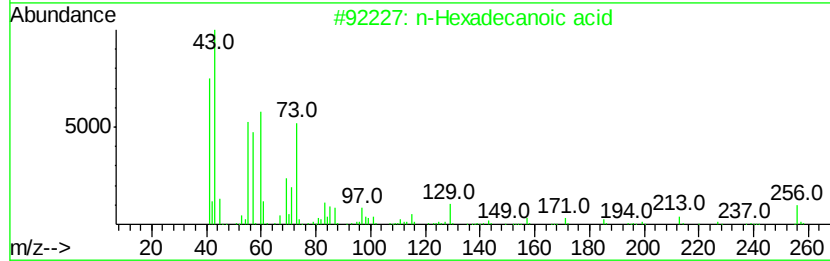
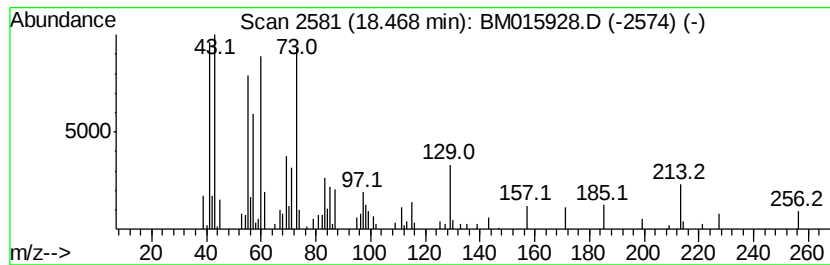
Instrument :
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TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.47	3.95 ng	200621	Phenanthrene-d10		17.63
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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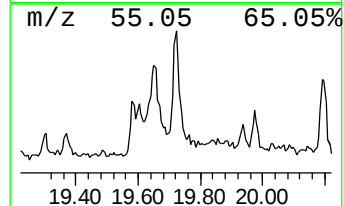
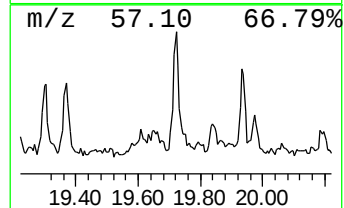
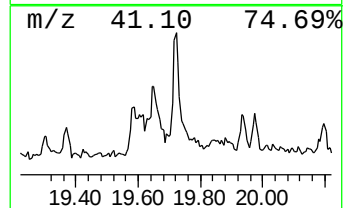
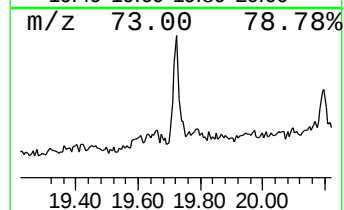
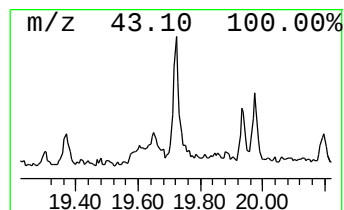
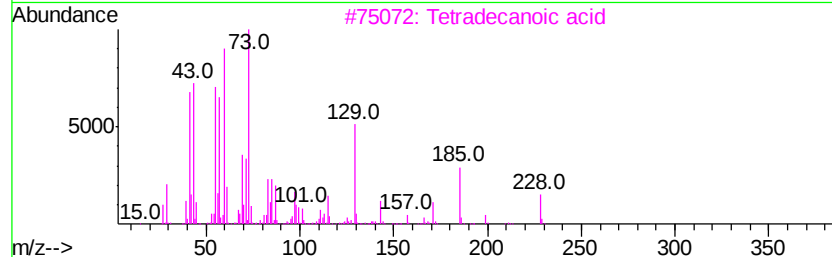
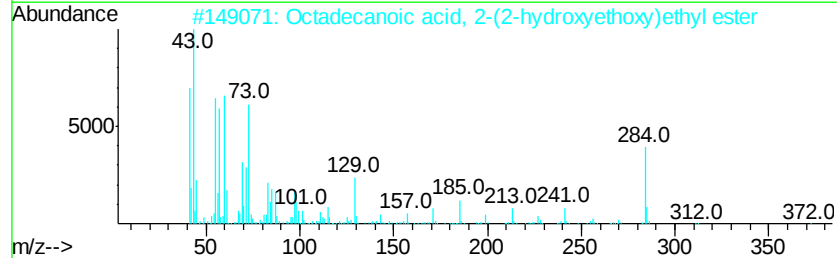
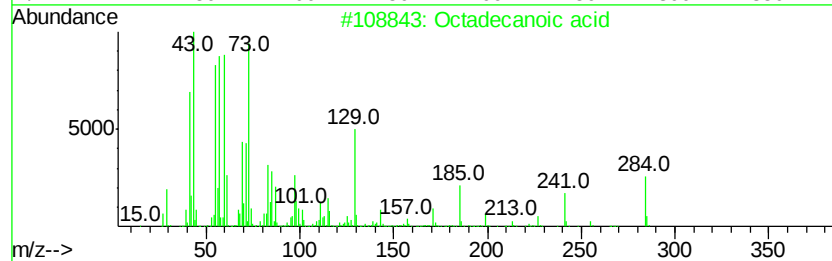
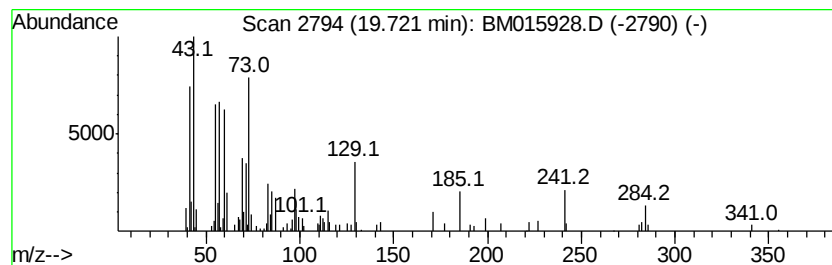
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Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.72	2.38 ng	127602	Chrysene-d12	21.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5		12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	43



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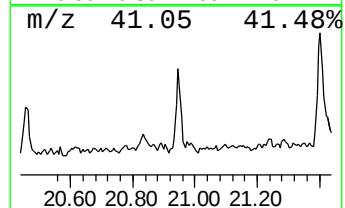
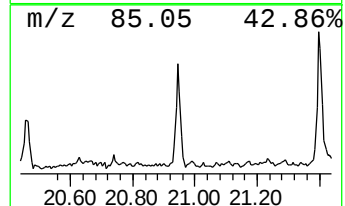
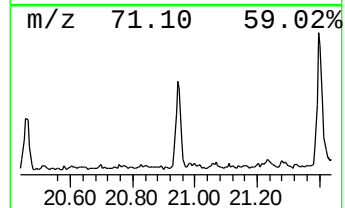
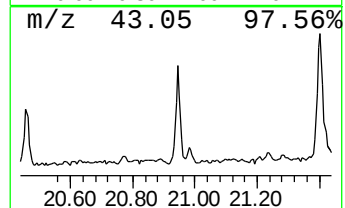
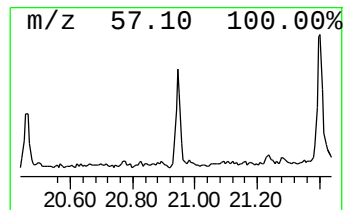
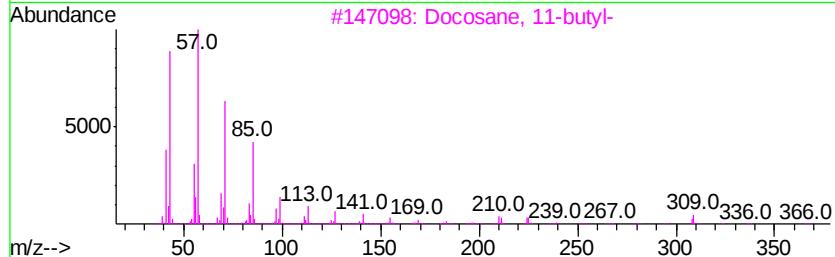
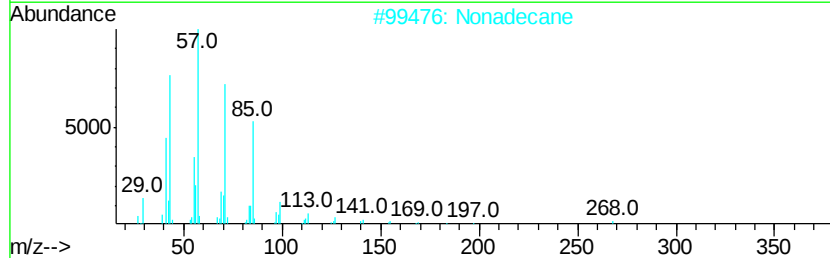
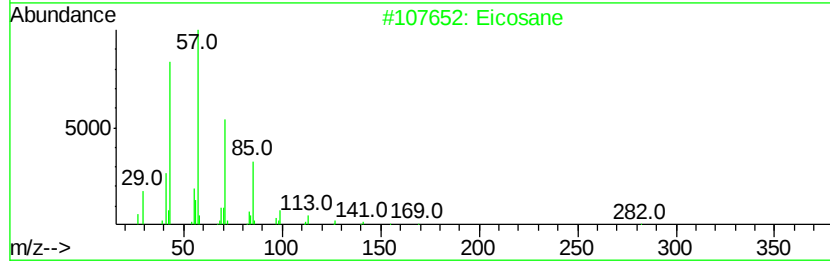
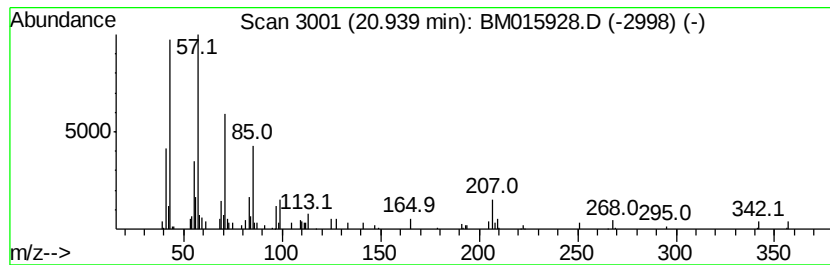
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Peak Number 6 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
20.94	2.08 ng	111696	Chrysene-d12		21.74
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Nonadecane	268	C19H40	000629-92-5	83
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	83
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	83
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	83



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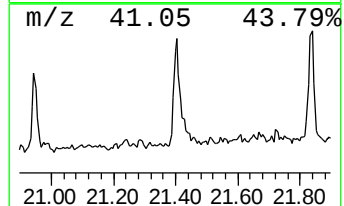
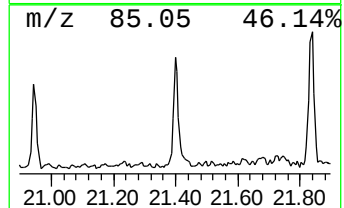
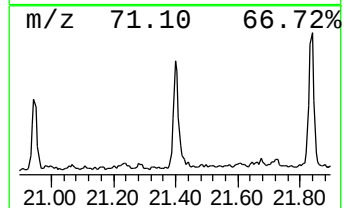
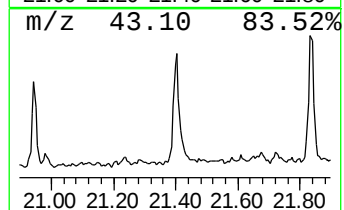
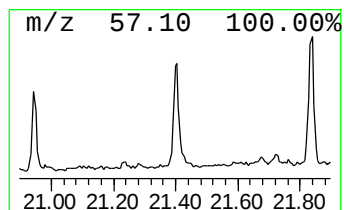
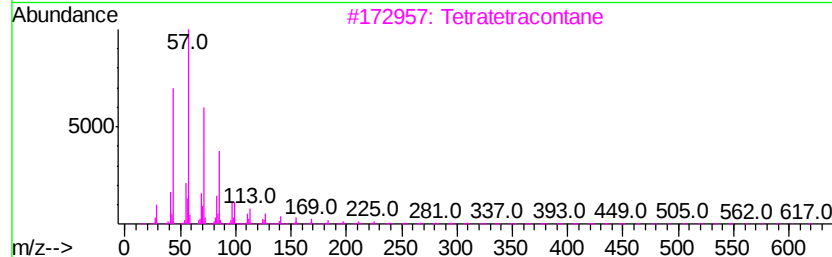
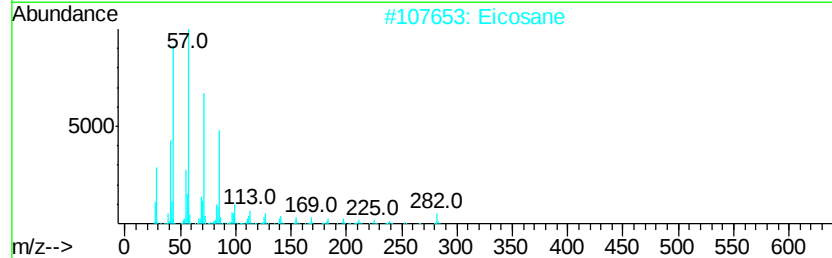
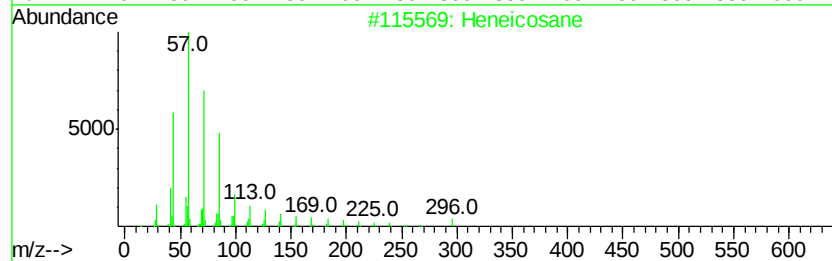
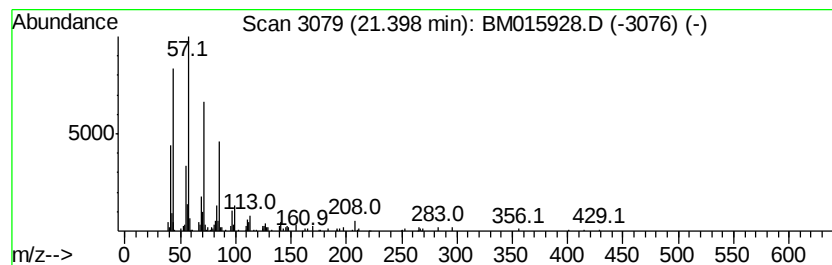
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	3.89 ng	208480	Chrysene-d12	21.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Eicosane	282	C20H42	000112-95-8	95
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Tritetracontane	605	C43H88	007098-21-7	91
5	Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015928.D
Acq On : 12 Jul 2018 23:10
Operator : SJ/JU
Sample : J3951-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
071018-TIPC-E-U-M

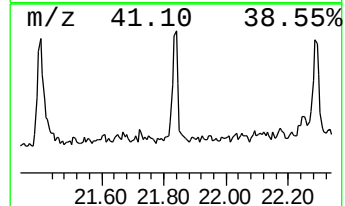
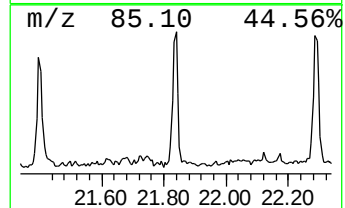
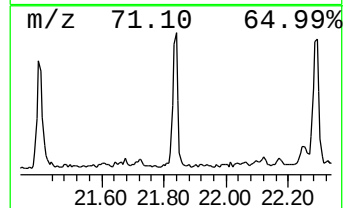
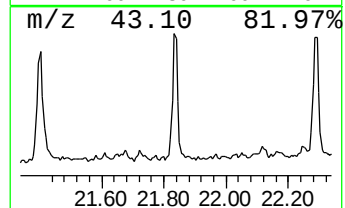
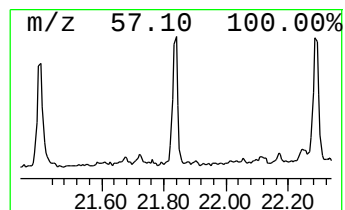
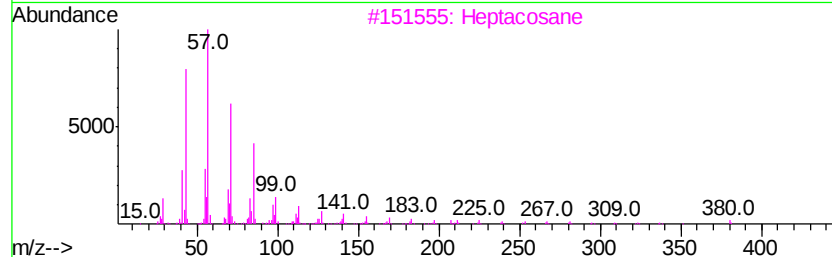
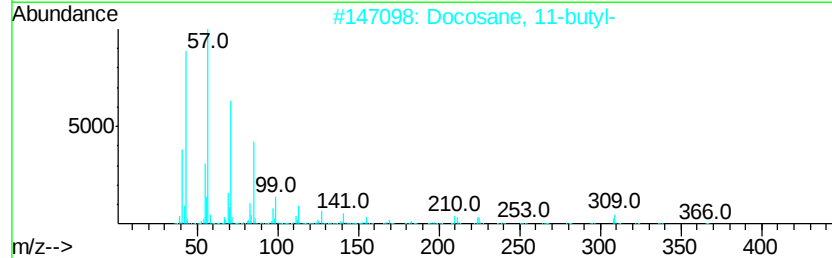
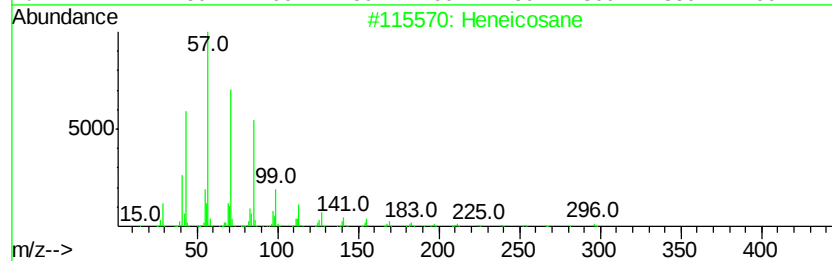
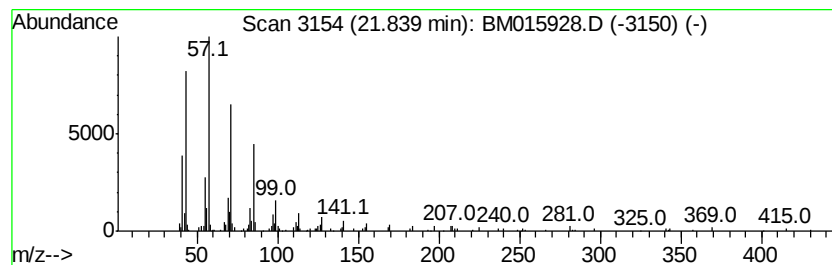
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Docosane, 11-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.84	3.10 ng	166103	Chrysene-d12	21.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	99
2		Docosane, 11-butyl-	366	C26H54	013475-76-8	87
3		Heptacosane	380	C27H56	000593-49-7	87
4		Heptadecane	240	C17H36	000629-78-7	87
5		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015928.D
Acq On : 12 Jul 2018 23:10
Operator : SJ/JU
Sample : J3951-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

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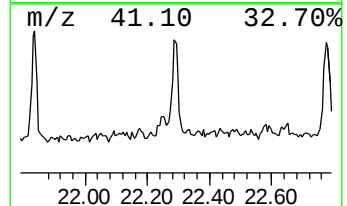
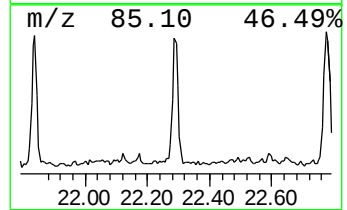
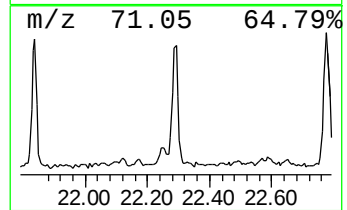
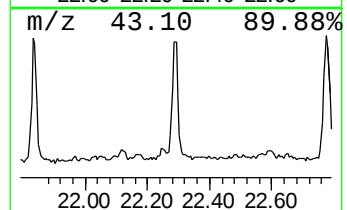
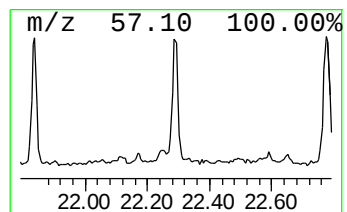
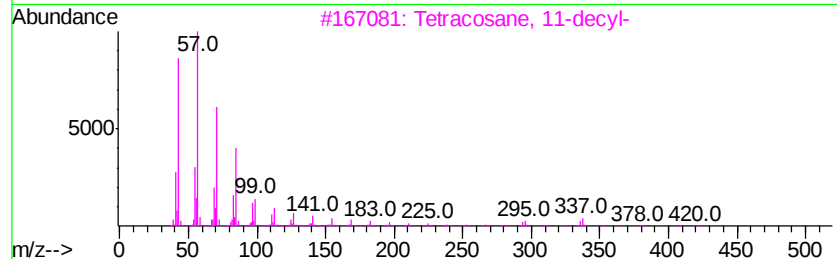
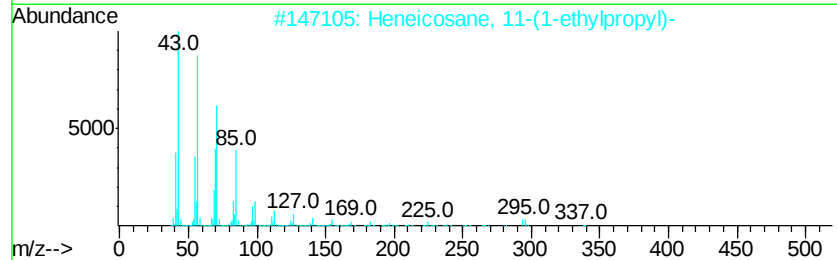
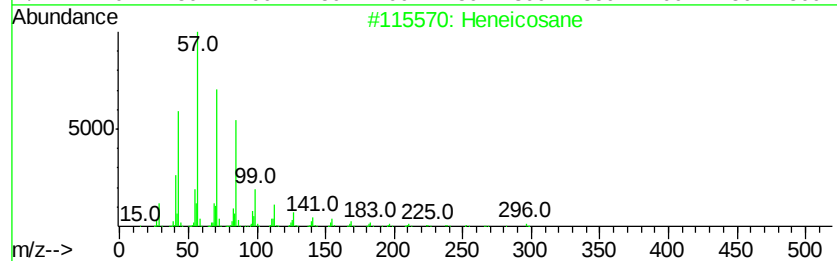
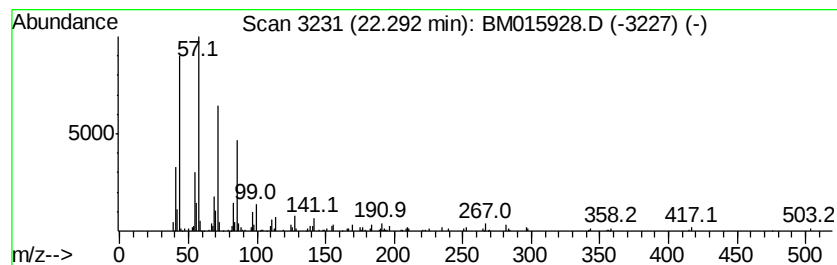
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane, 11-(1-ethylpro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.29	2.97 ng	159430	Chrysene-d12	21.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	93
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015928.D
Acq On : 12 Jul 2018 23:10
Operator : SJ/JU
Sample : J3951-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

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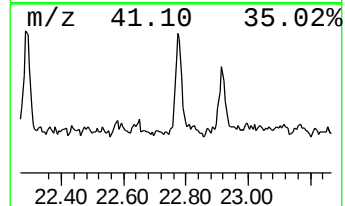
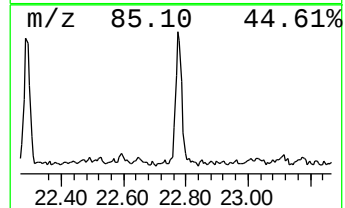
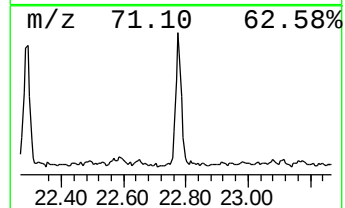
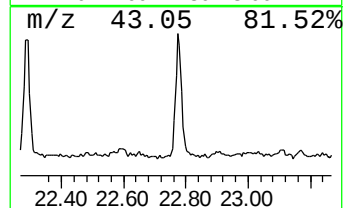
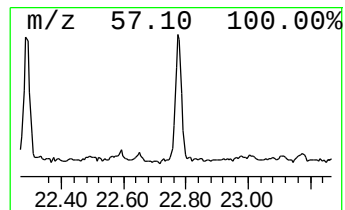
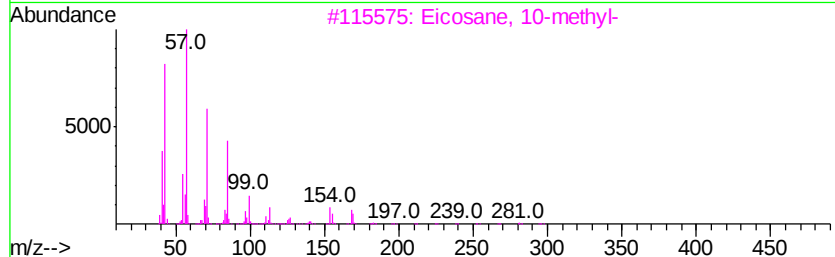
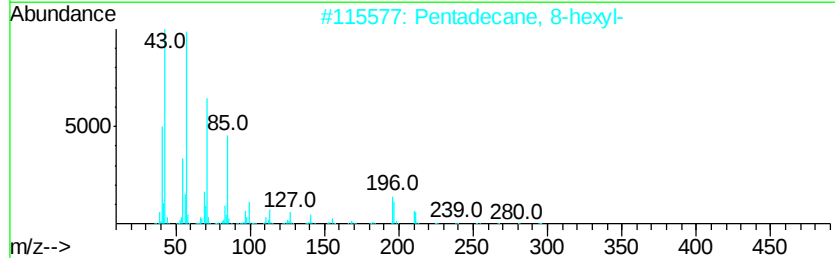
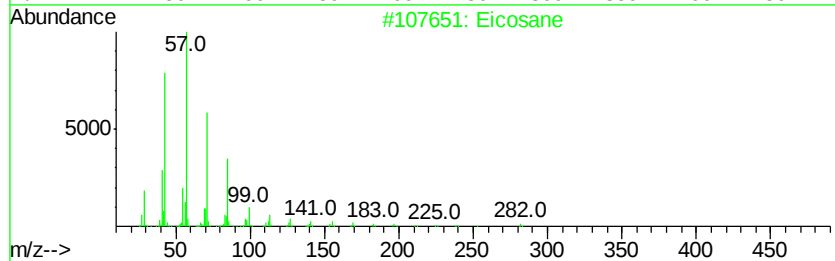
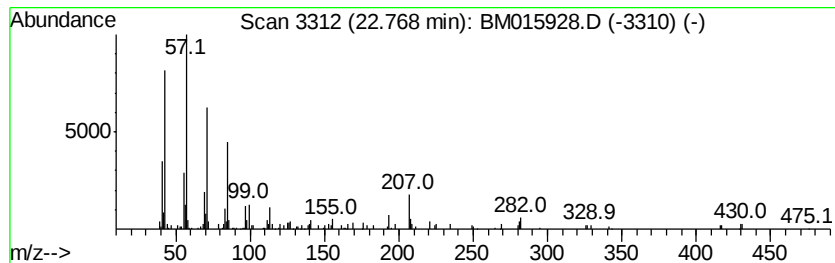
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentadecane, 8-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	3.51 ng	187981	Chrysene-d12	21.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	97
2			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	89
4			Octacosane	394	C28H58	000630-02-4	87
5			Docosane, 11-butyl-	366	C26H54	013475-76-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015928.D
Acq On : 12 Jul 2018 23:10
Operator : SJ/JU
Sample : J3951-02
Misc :
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Instrument :
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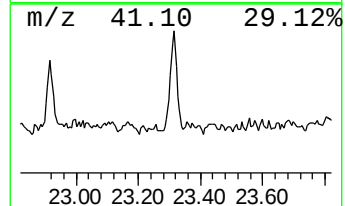
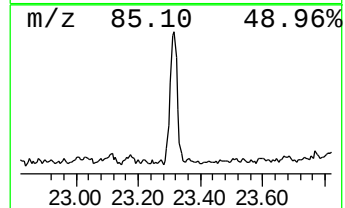
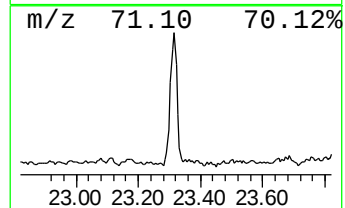
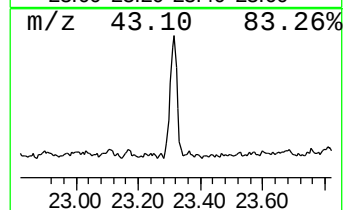
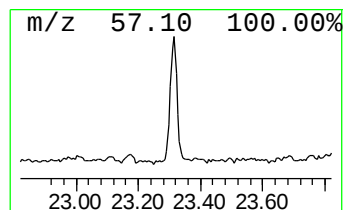
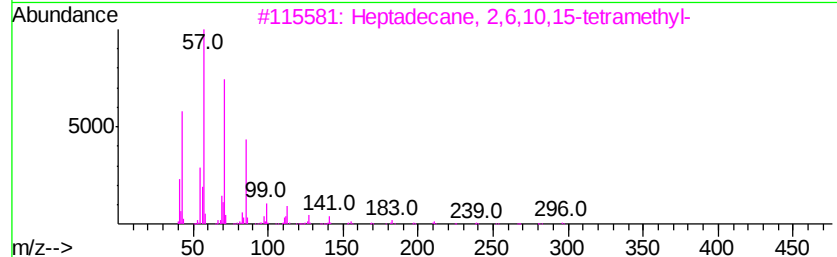
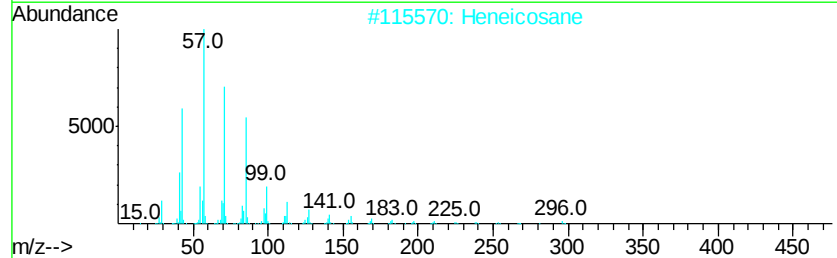
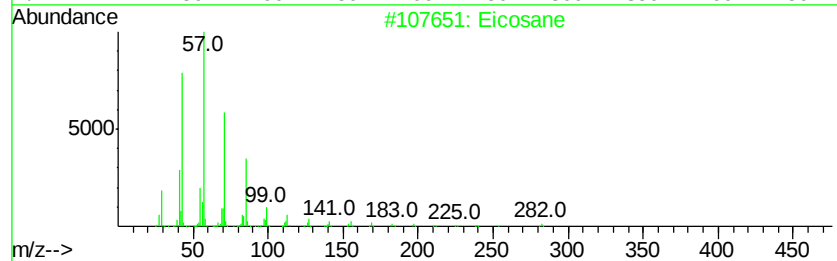
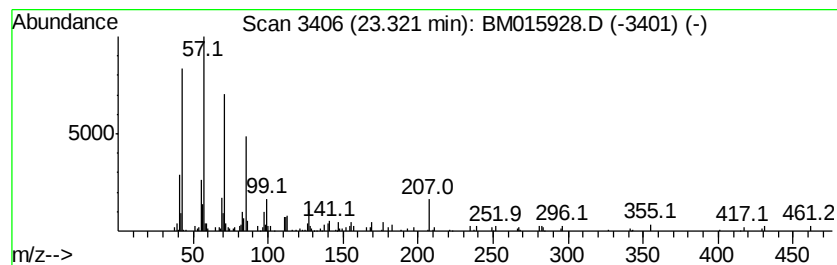
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.32	3.59 ng	193783	Perylene-d12	24.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	97
2			Heneicosane	296	C21H44	000629-94-7	94
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
4			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	83
5			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071218\
Data File : BM015928.D
Acq On : 12 Jul 2018 23:10
Operator : SJ/JU
Sample : J3951-02
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
071018-TIPC-E-U-M

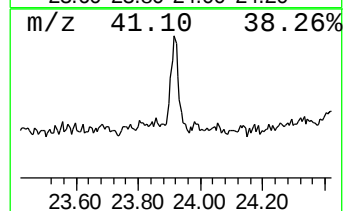
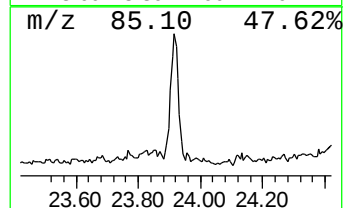
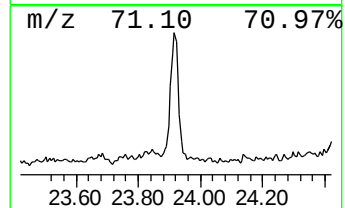
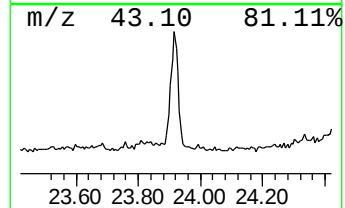
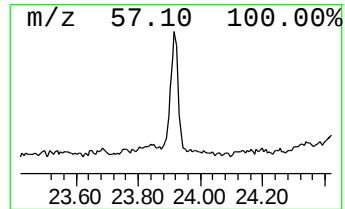
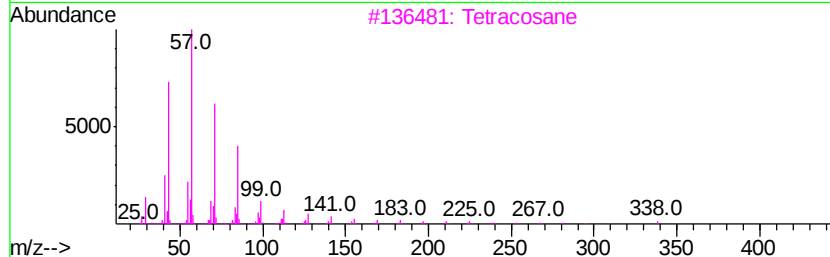
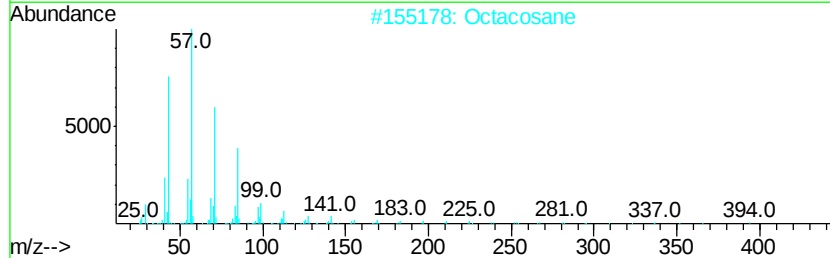
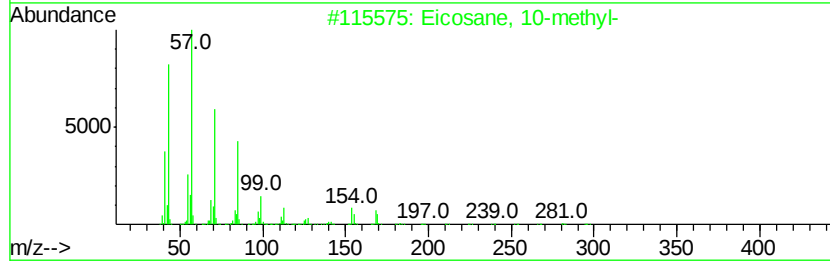
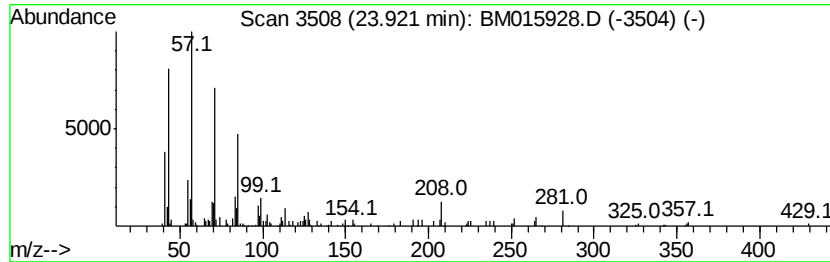
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane, 10-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	3.32 ng	179629	Perylene-d12	24.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2		Octacosane	394	C28H58	000630-02-4	90
3		Tetracosane	338	C24H50	000646-31-1	87
4		Heneicosane	296	C21H44	000629-94-7	87
5		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM071218\
Data File : BM015928.D
Acq On : 12 Jul 2018 23:10
Operator : SJ/JU
Sample : J3951-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
071018-TIPC-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.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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Ethyl citrate	16.16	4.7	ng	216190	3	14.90	922727	20.0
n-Hexadecanoic acid	18.47	4.0	ng	200621	4	17.63	1015890	20.0
Octadecanoic acid	19.72	2.4	ng	127602	5	21.74	1071810	20.0
Eicosane	20.94	2.1	ng	111696	5	21.74	1071810	20.0
Heneicosane	21.40	3.9	ng	208480	5	21.74	1071810	20.0
Docosane, 11-butyl-	21.84	3.1	ng	166103	5	21.74	1071810	20.0
Heneicosane, 11-(...	22.29	3.0	ng	159430	5	21.74	1071810	20.0
Pentadecane, 8-he...	22.77	3.5	ng	187981	5	21.74	1071810	20.0
Heptadecane, 2,6,...	23.32	3.6	ng	193783	6	24.13	1081060	20.0
Eicosane, 10-methyl-	23.92	3.3	ng	179629	6	24.13	1081060	20.0