

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
 Data File : BM015886.D
 Acq On : 11 Jul 2018 13:24
 Operator : SJ/JU
 Sample : J3925-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-1

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	5.316	338	345	354	rBV	77215	130661	2.45%	0.404%
2	5.799	421	427	443	rBV	754100	1225523	23.00%	3.793%
3	7.440	700	706	720	rBV	441672	794712	14.91%	2.460%
4	7.816	763	770	784	rBV	1673317	2717644	50.99%	8.411%
5	8.293	845	851	857	rBV	387891	629385	11.81%	1.948%
6	8.616	899	906	917	rBV	1602405	2630123	49.35%	8.140%
7	9.481	1046	1053	1066	rBV	1218351	2047694	38.42%	6.338%
8	11.122	1325	1332	1341	rBV	442347	778884	14.62%	2.411%
9	12.069	1487	1493	1503	rBV3	25541	53476	1.00%	0.166%
10	13.539	1736	1743	1758	rBV	3076164	4291981	80.53%	13.283%
11	13.751	1774	1779	1788	rBV	97654	147516	2.77%	0.457%
12	14.363	1877	1883	1889	rBV	108109	153715	2.88%	0.476%
13	14.916	1966	1977	1987	rBV2	612844	962148	18.05%	2.978%
14	15.522	2074	2080	2084	rBV	56224	71970	1.35%	0.223%
15	16.392	2222	2228	2240	rBV	2434191	3361320	63.07%	10.403%
16	16.992	2322	2330	2338	rBV3	33467	77062	1.45%	0.239%
17	17.639	2435	2440	2451	rBV	744735	1060564	19.90%	3.282%
18	18.215	2533	2538	2543	rBV	55790	83515	1.57%	0.258%
19	18.357	2557	2562	2572	rBV4	63357	127357	2.39%	0.394%
20	18.480	2578	2583	2592	rBV	550094	748321	14.04%	2.316%
21	18.562	2593	2597	2607	rVB	69522	105900	1.99%	0.328%
22	19.609	2768	2775	2783	rBV4	67190	166222	3.12%	0.514%
23	19.727	2790	2795	2804	rBV	322584	439415	8.25%	1.360%
24	19.980	2834	2838	2841	rBV2	45274	58104	1.09%	0.180%
25	20.204	2868	2876	2883	rBV	4415429	5329341	100.00%	16.494%
26	21.421	3074	3083	3091	rBV3	135232	435764	8.18%	1.349%
27	21.503	3093	3097	3103	rVV	275967	361471	6.78%	1.119%
28	21.751	3134	3139	3145	rBV	819172	1087422	20.40%	3.366%
29	21.845	3152	3155	3157	rVB	54508	54213	1.02%	0.168%
30	22.298	3229	3232	3235	rBV	73804	78394	1.47%	0.243%
31	22.786	3312	3315	3320	rVB	93664	115292	2.16%	0.357%
32	22.927	3334	3339	3347	rVB	457799	606119	11.37%	1.876%
33	23.321	3403	3406	3412	rVB2	114707	162636	3.05%	0.503%
34	23.927	3505	3509	3514	rVB3	102023	166849	3.13%	0.516%

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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

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35	24.144	3540	3546	3557	rVB	529788	1050035	19.70%	3.250%
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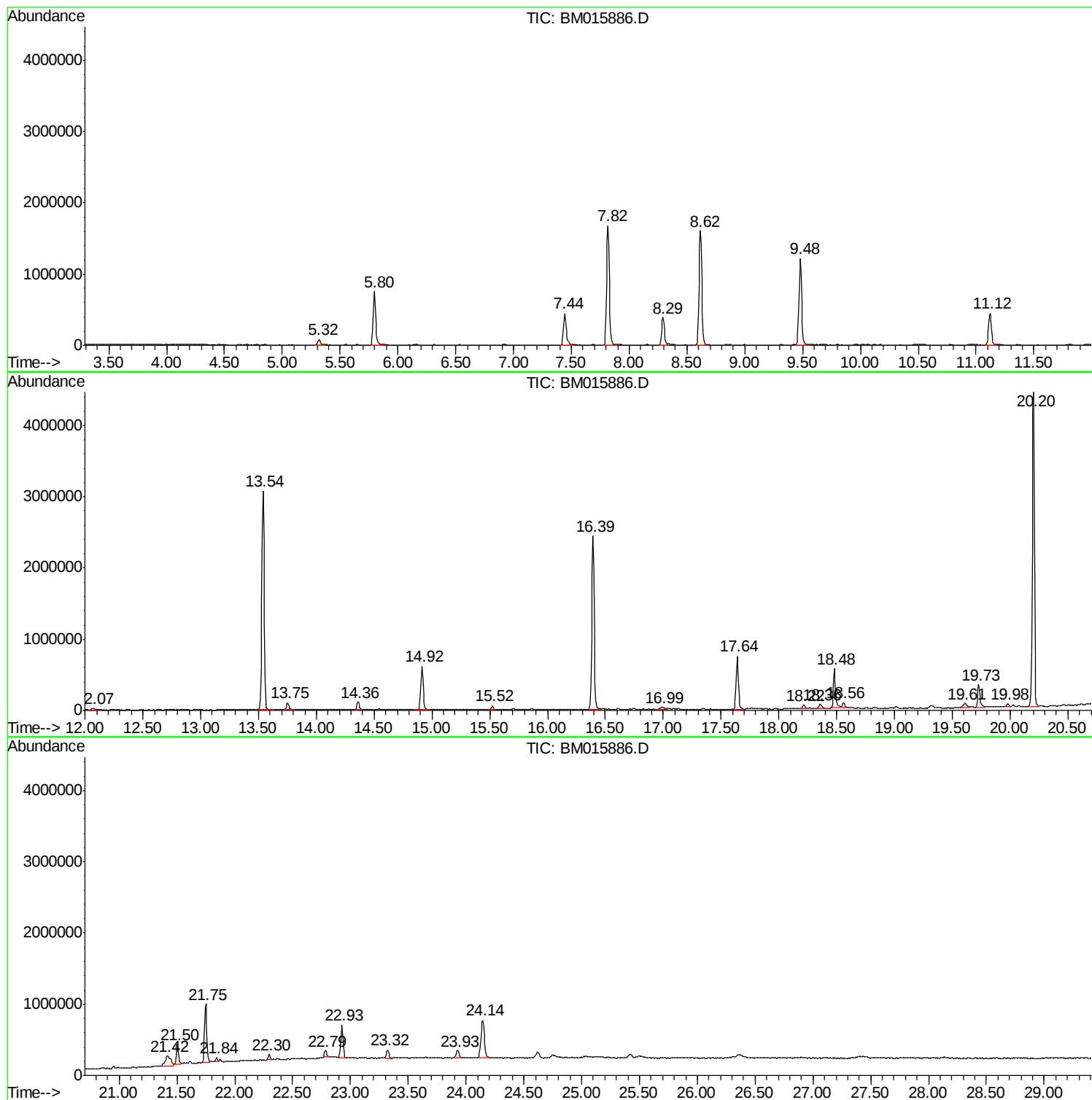
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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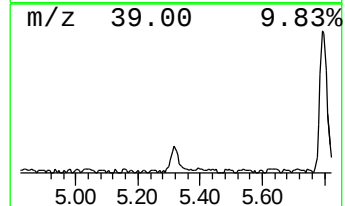
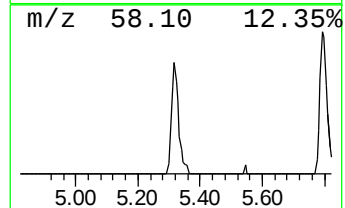
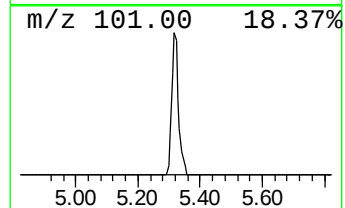
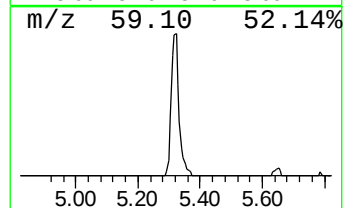
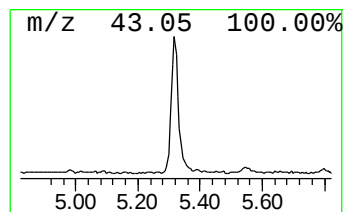
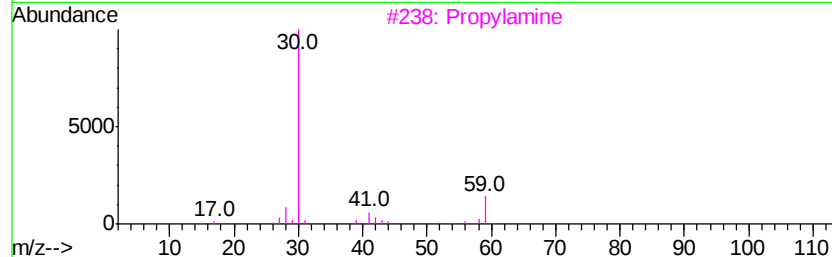
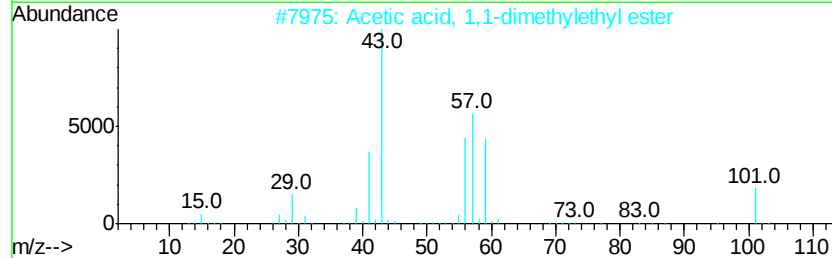
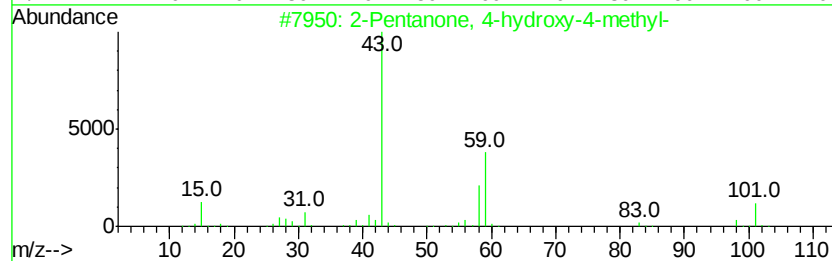
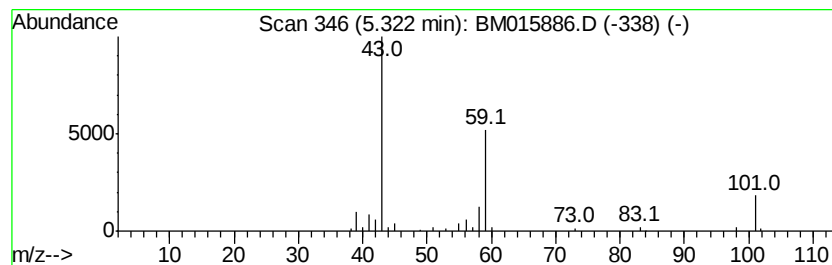
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	4.15 ng	130661	1,4-Dichlorobenzene-d4	8.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Propylamine	59	C3H9N	000107-10-8	38
4			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12



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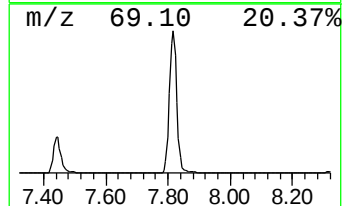
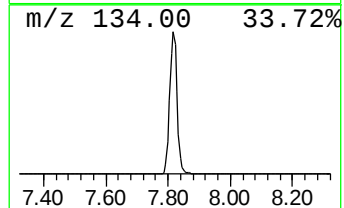
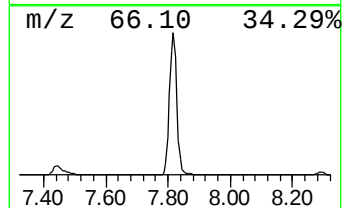
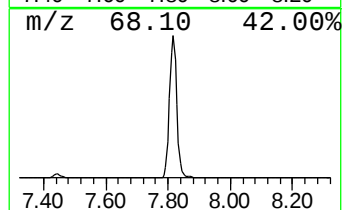
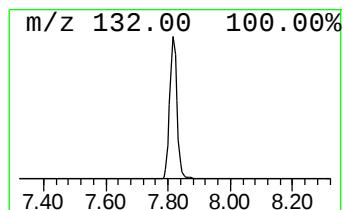
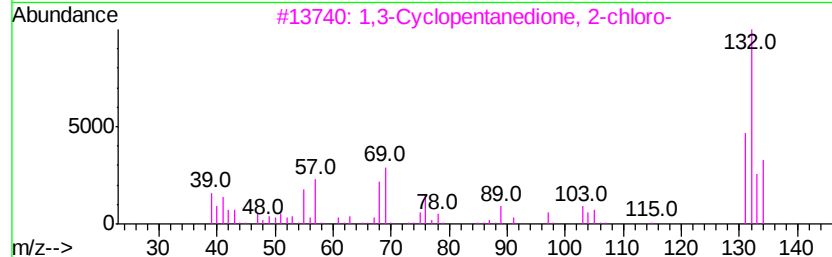
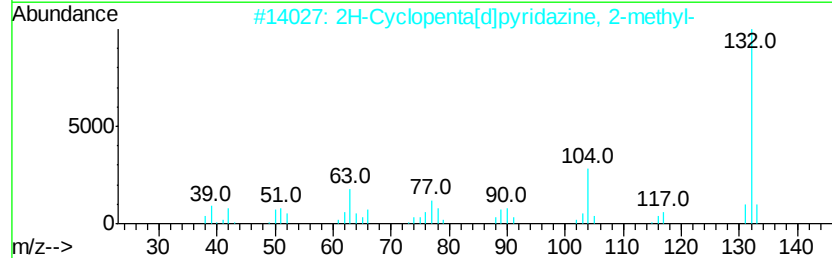
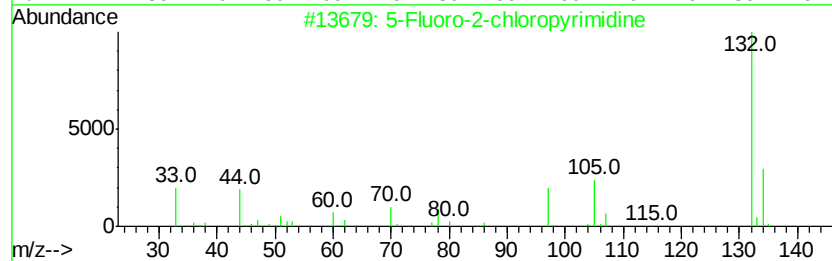
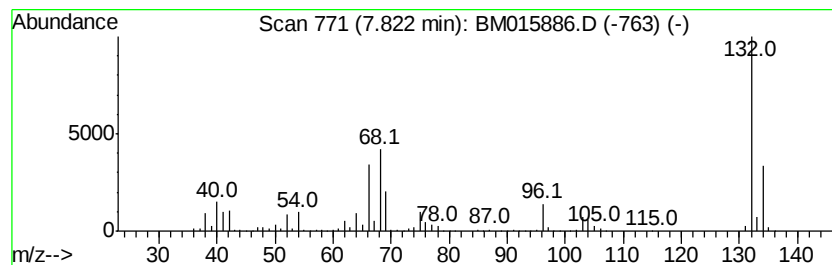
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	86.36 ng	2717640	1,4-Dichlorobenzene-d4	8.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	22
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22



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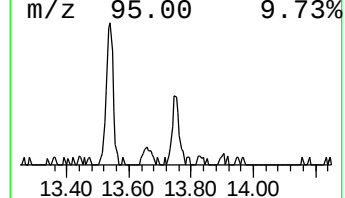
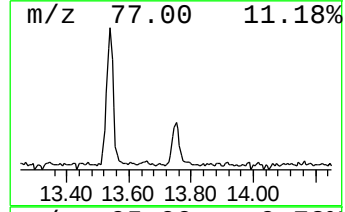
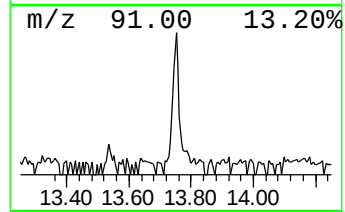
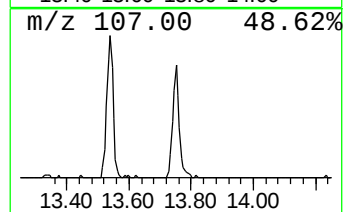
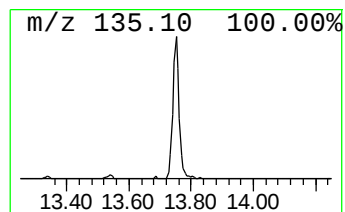
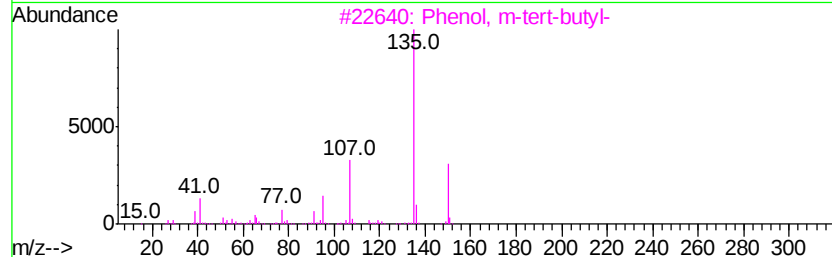
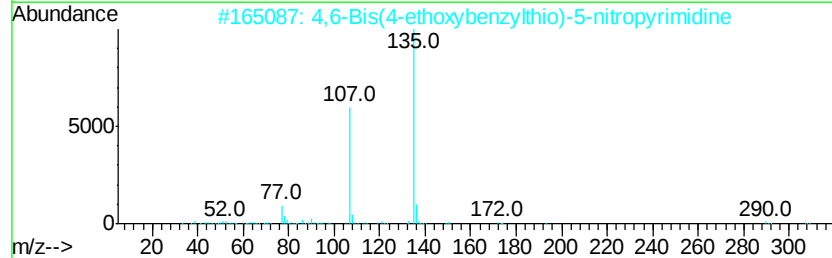
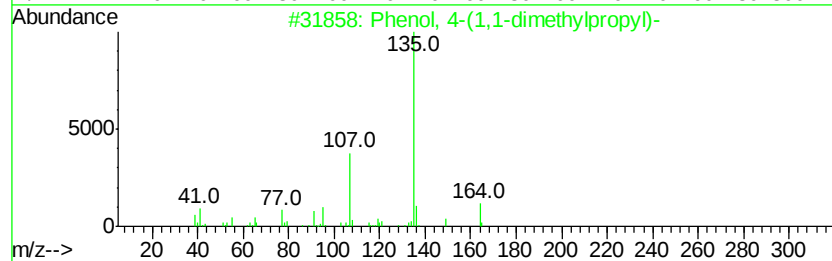
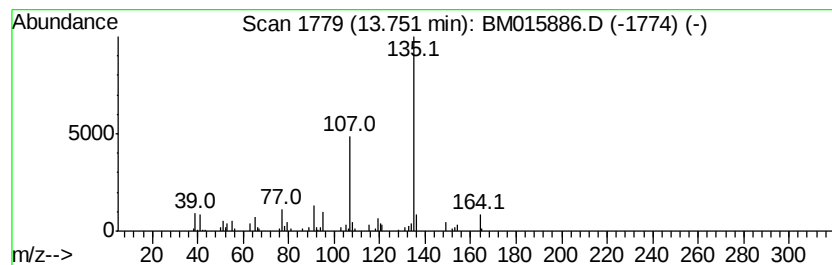
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Phenol, 4-(1,1-dimethylprop... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	3.07 ng	147516	Acenaphthene-d10	14.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2		4,6-Bis(4-ethoxybenzylthio)-5-ni...	457	C22H23N3O4S2	325957-76-4	59
3		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	59
4		2-Aziridinone, 1-(1-adamantyl)-3...	273	C18H27NO	026905-18-0	50
5		Benzene, 1-methoxy-4-(1-methylpr...	164	C11H16O	004917-90-2	47



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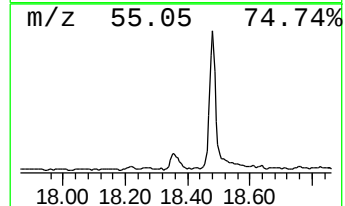
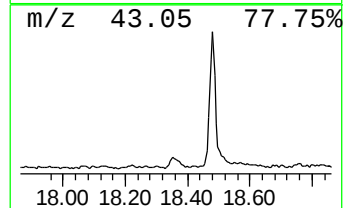
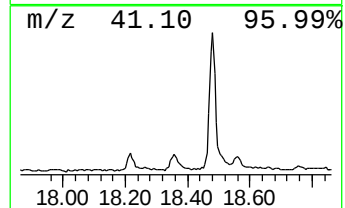
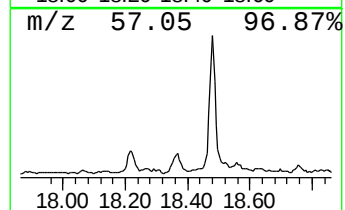
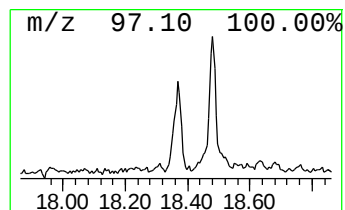
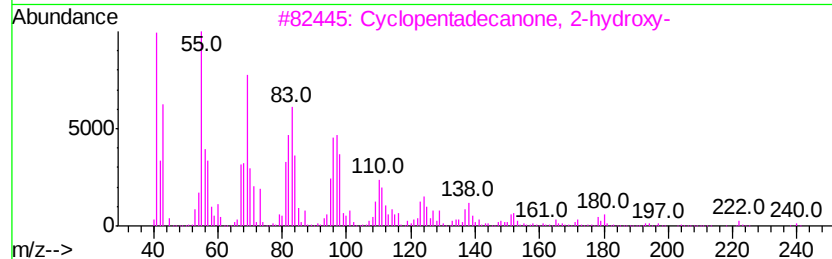
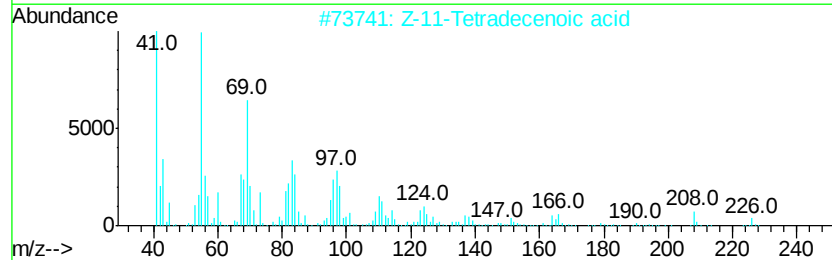
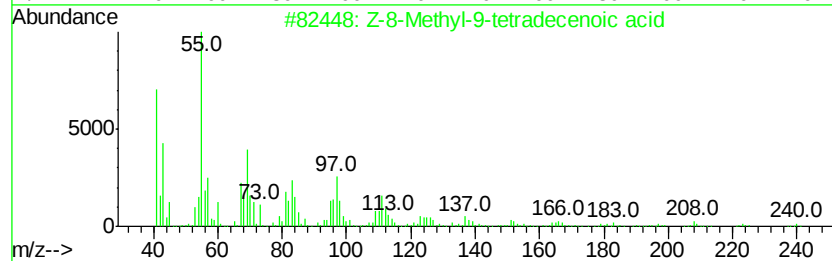
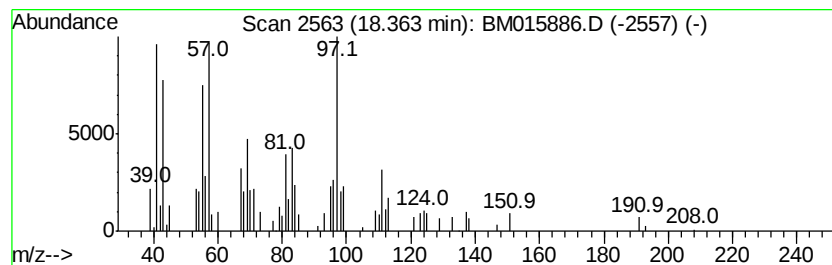
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Peak Number 5 unknown18.36 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	2.40 ng	127357	Phenanthrene-d10	17.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Z-8-Methyl-9-tetradecenoic acid	240	C15H28O2	1000130-84-5	47
2		Z-11-Tetradecenoic acid	226	C14H26O2	1000130-83-3	43
3		Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	43
4		(1S,15S)-Bicyclo[13.1.0]hexadeca...	236	C16H28O	102572-89-4	43
5		E-9-Tetradecenoic acid	226	C14H26O2	1000131-35-8	43



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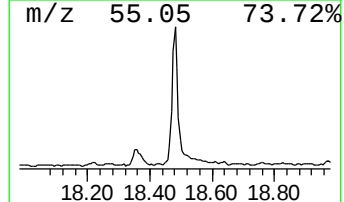
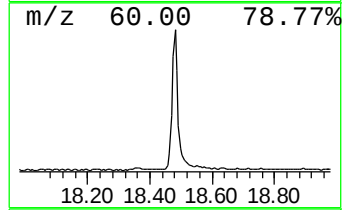
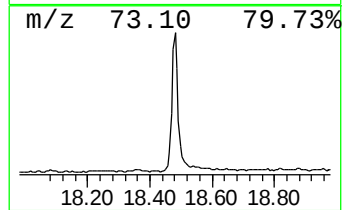
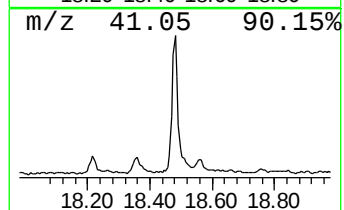
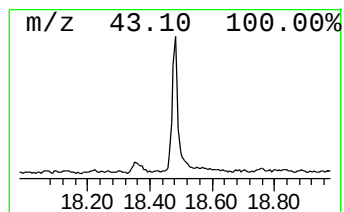
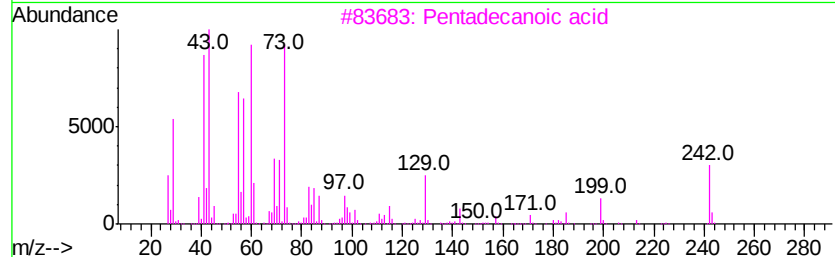
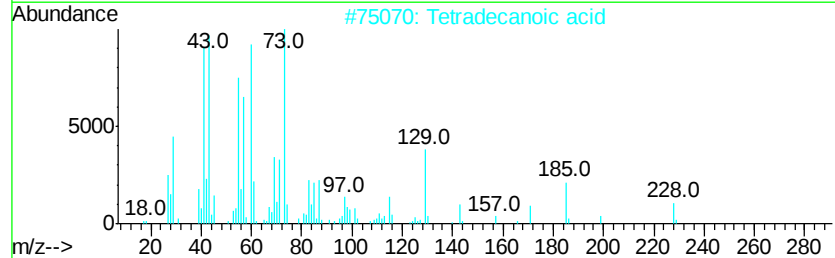
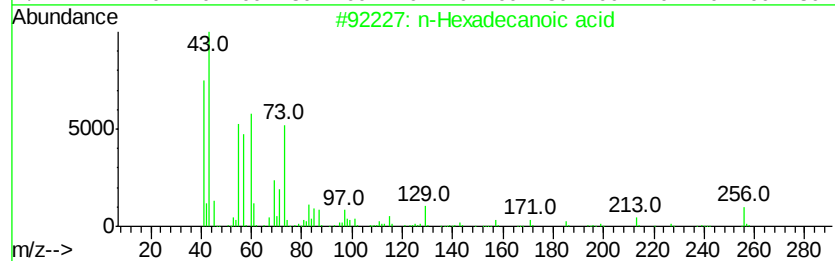
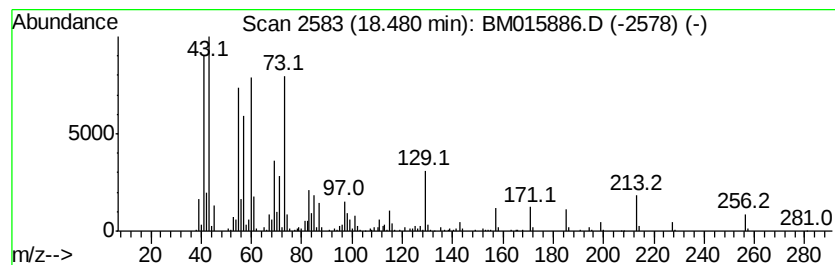
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.48	14.11 ng	748321	Phenanthrene-d10	17.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015886.D
Acq On : 11 Jul 2018 13:24
Operator : SJ/JU
Sample : J3925-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

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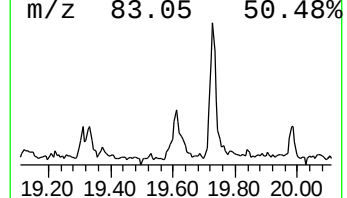
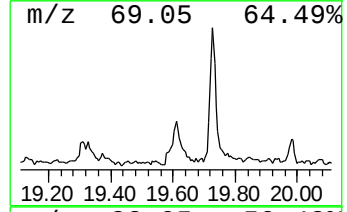
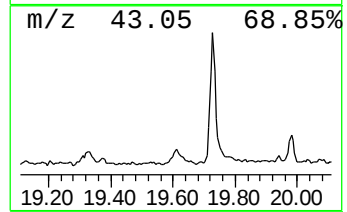
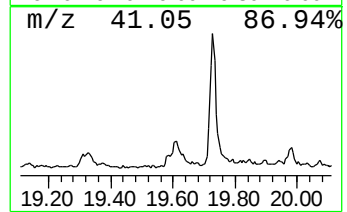
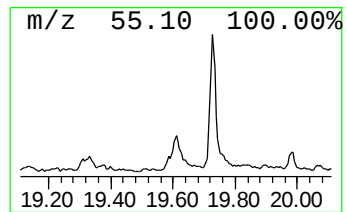
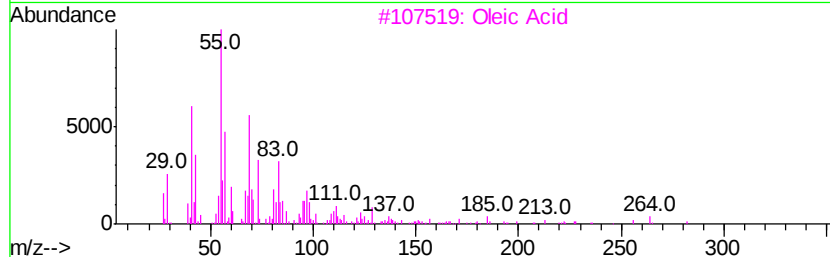
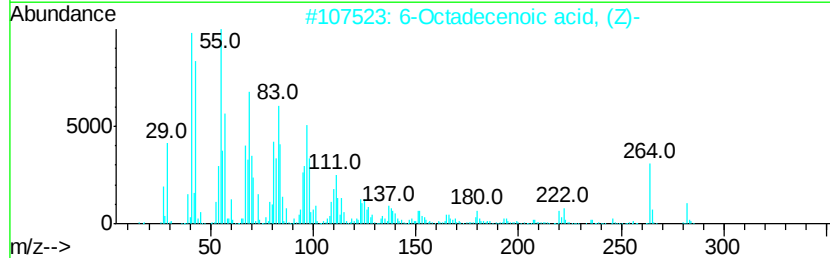
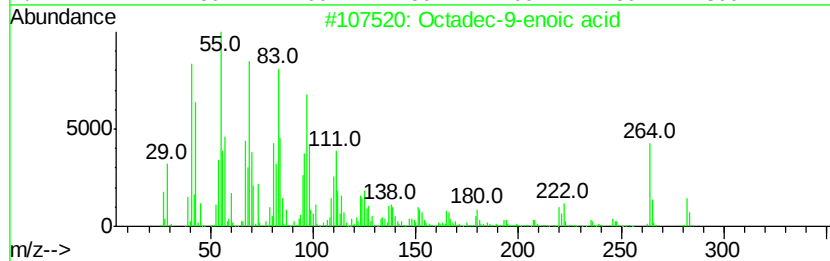
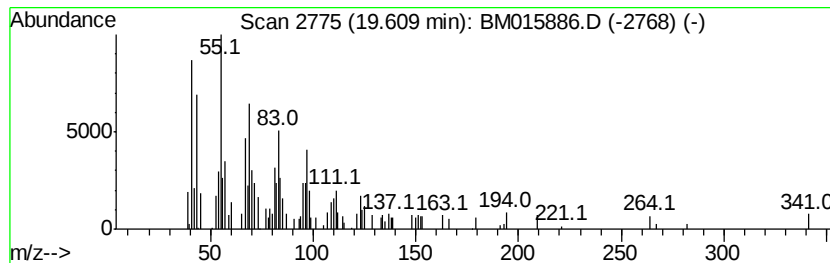
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadec-9-enoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	3.13 ng	166222	Phenanthrene-d10	17.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	96
2	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	90
3	Oleic Acid	282	C18H34O2	000112-80-1	90
4	Aspidospermidin-17-ol, 1-acetyl-...	414	C23H30N2O5	002122-26-1	87
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015886.D
Acq On : 11 Jul 2018 13:24
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Sample : J3925-01
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ALS Vial : 3 Sample Multiplier: 1

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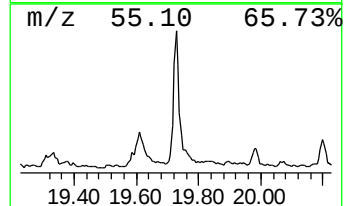
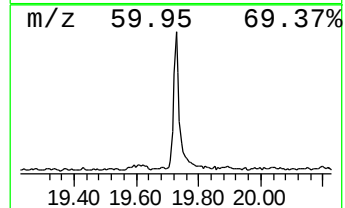
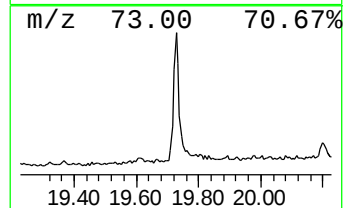
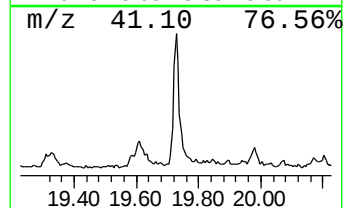
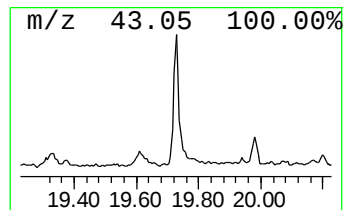
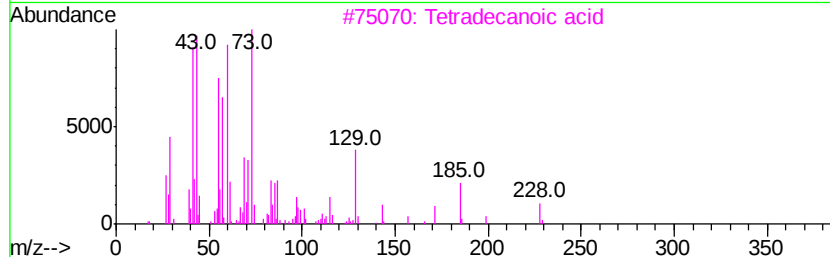
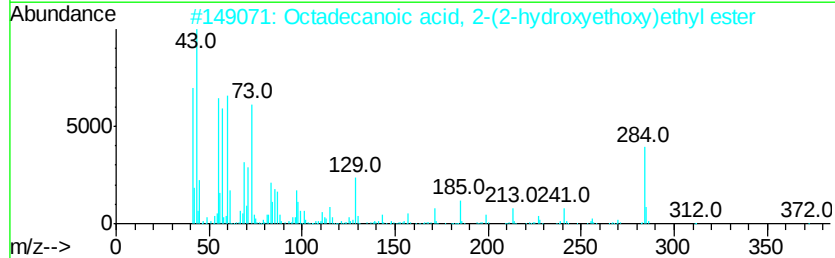
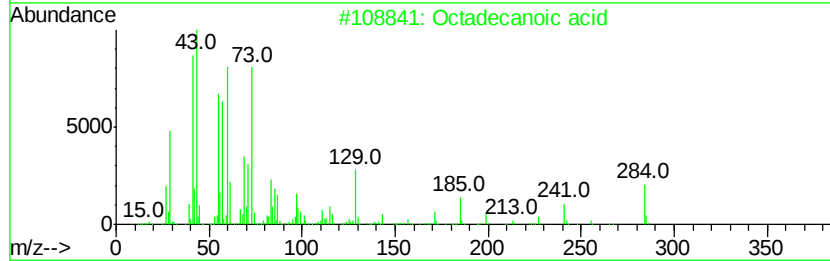
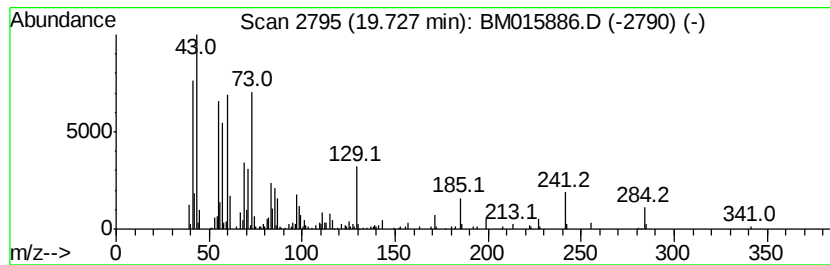
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	8.08 ng	439415	Chrysene-d12	21.75

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	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		Dodecanoic acid	200	C12H24O2	000143-07-7	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015886.D
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Sample : J3925-01
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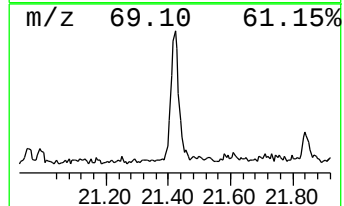
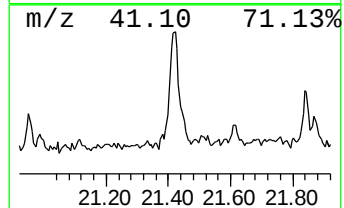
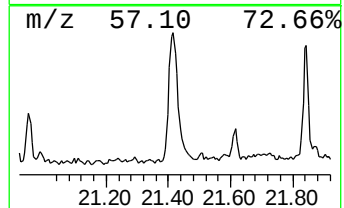
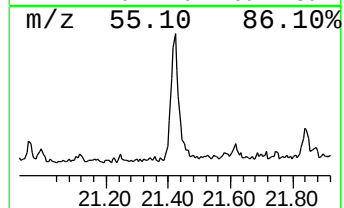
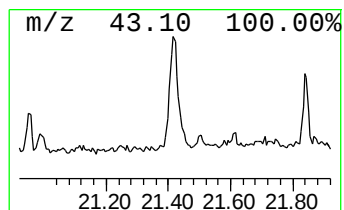
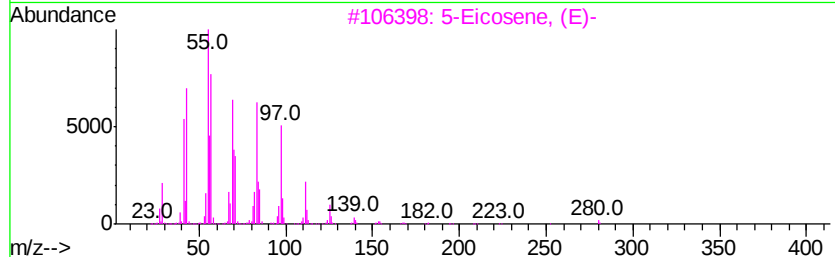
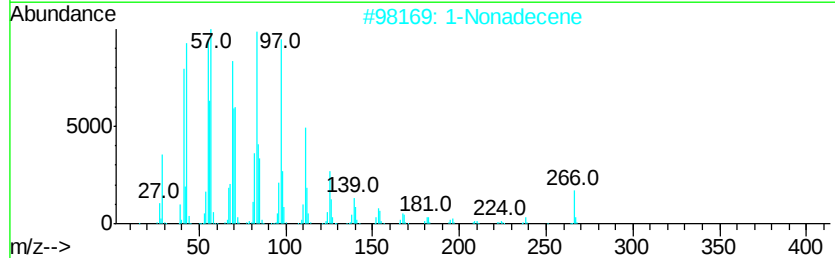
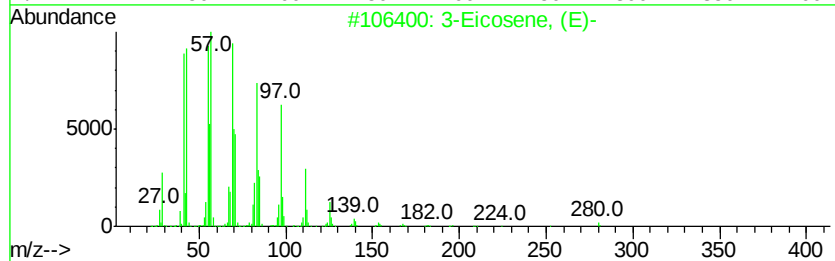
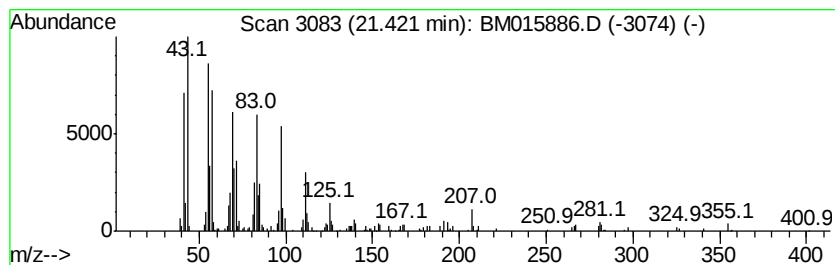
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	8.01 ng	435764	Chrysene-d12	21.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Eicosene, (E)-	280	C20H40	074685-33-9	99
2		1-Nonadecene	266	C19H38	018435-45-5	98
3		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
4		1-Eicosene	280	C20H40	003452-07-1	96
5		Cycloeicosane	280	C20H40	000296-56-0	95



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
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Sample : J3925-01
Misc :
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Instrument :
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ClientSampleId :
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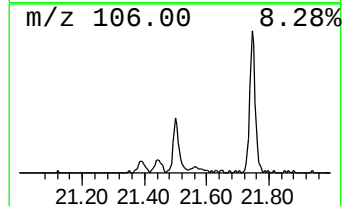
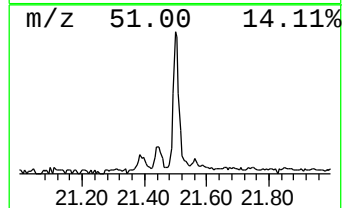
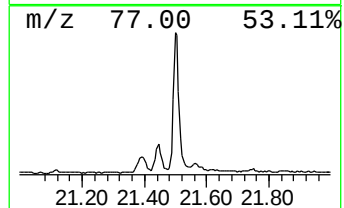
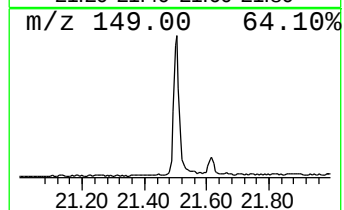
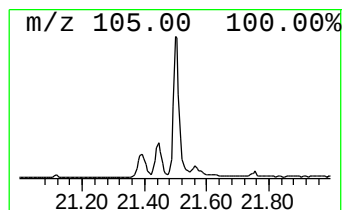
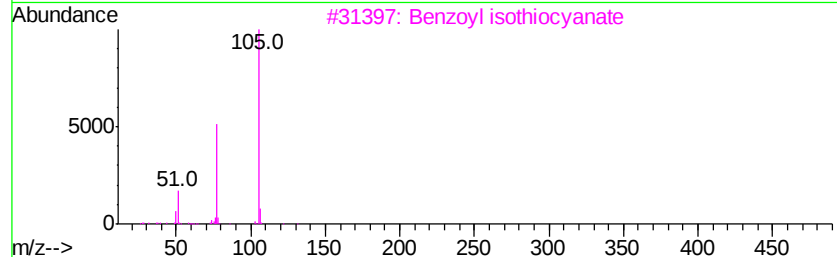
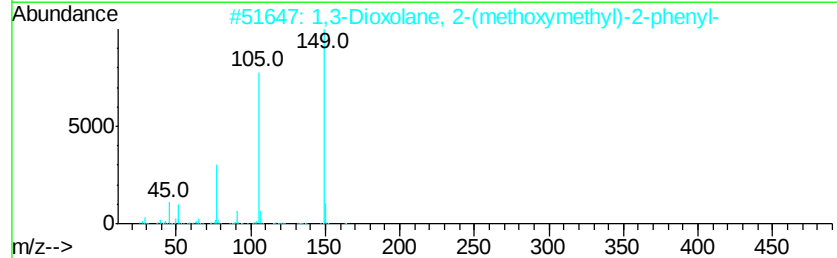
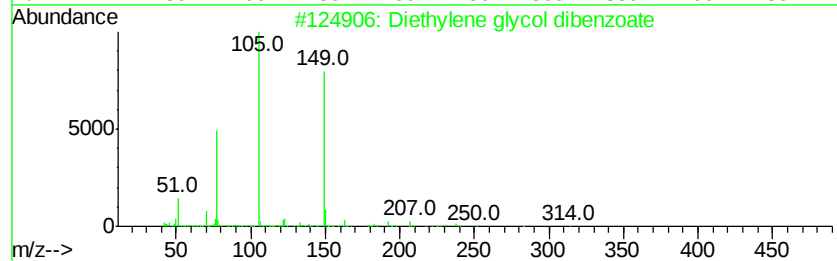
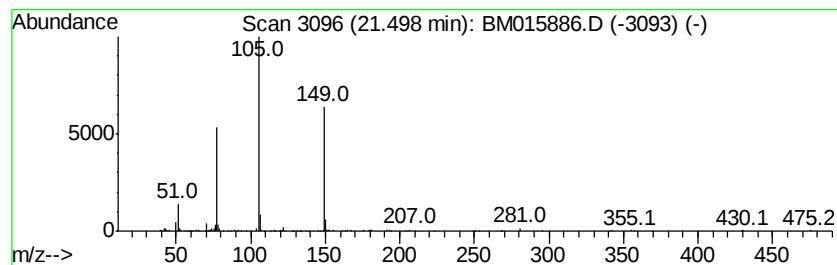
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Diethylene glycol dibenzoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	6.65 ng	361471	Chrysene-d12	21.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	78
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	53
3			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
4			Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	47
5			Benzaldehyde, 4-cyano-, benzoylh...	249	C15H11N3O	195066-12-7	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015886.D
Acq On : 11 Jul 2018 13:24
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ClientSampleId :
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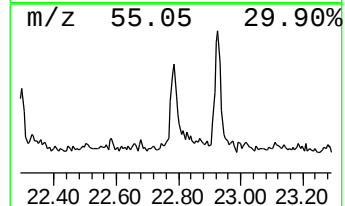
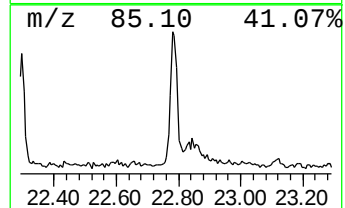
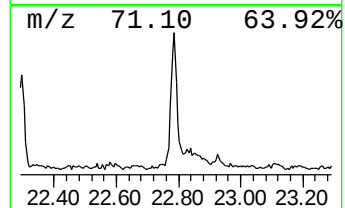
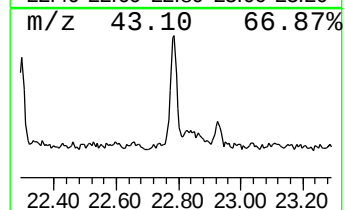
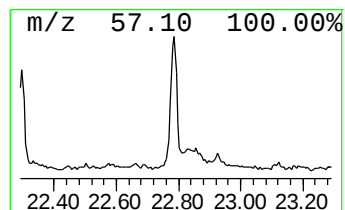
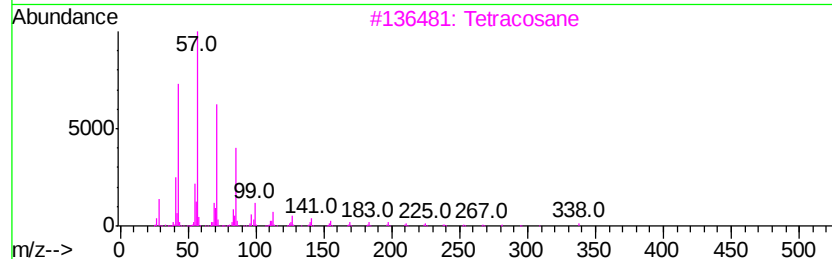
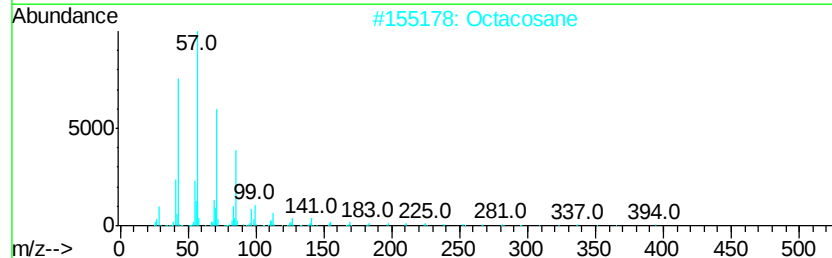
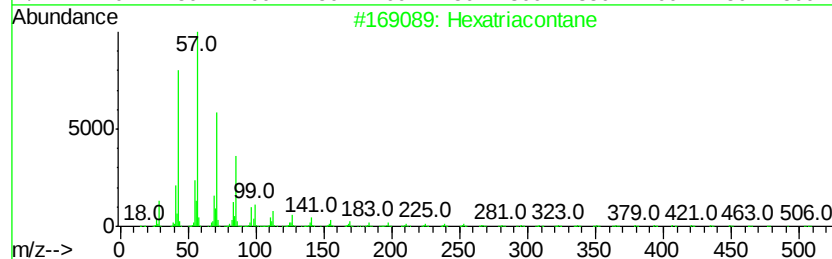
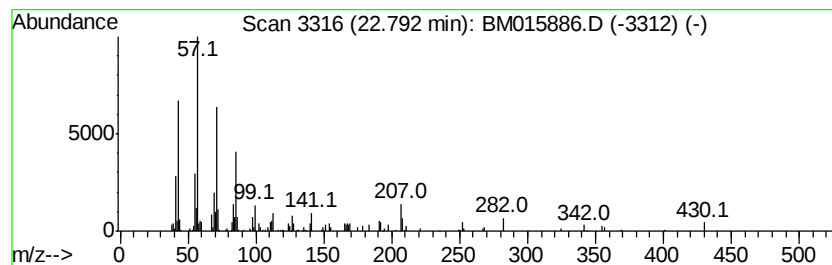
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexatriacontane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.79	2.12 ng	115292	Chrysene-d12	21.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexatriacontane	507	C36H74	000630-06-8	81
2		Octacosane	394	C28H58	000630-02-4	81
3		Tetracosane	338	C24H50	000646-31-1	81
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	81
5		Heptacosane	380	C27H56	000593-49-7	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
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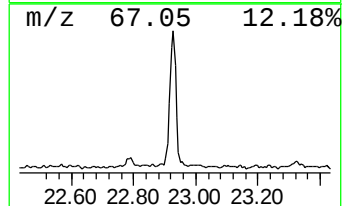
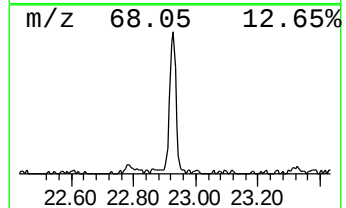
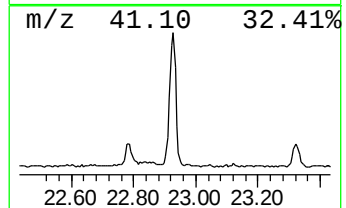
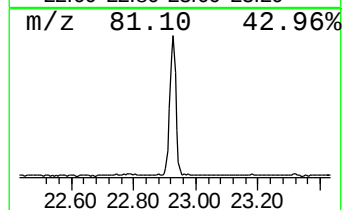
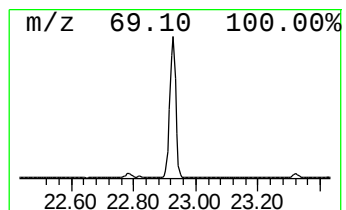
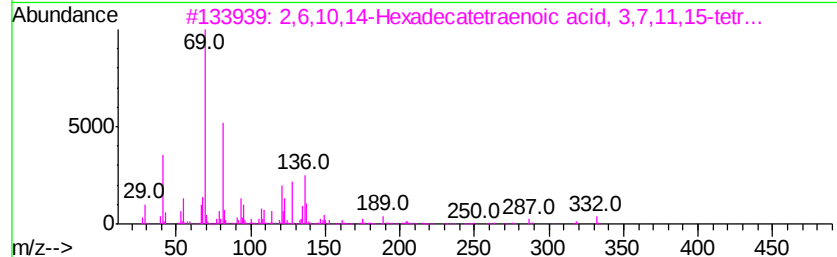
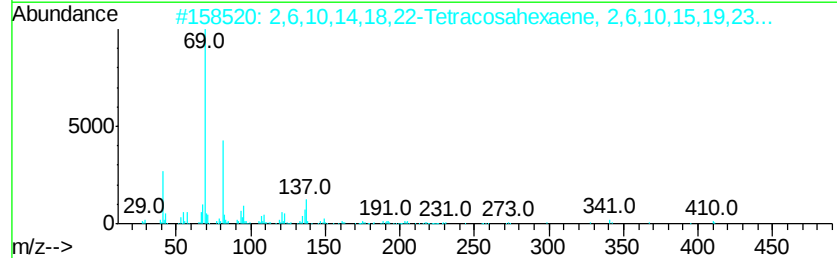
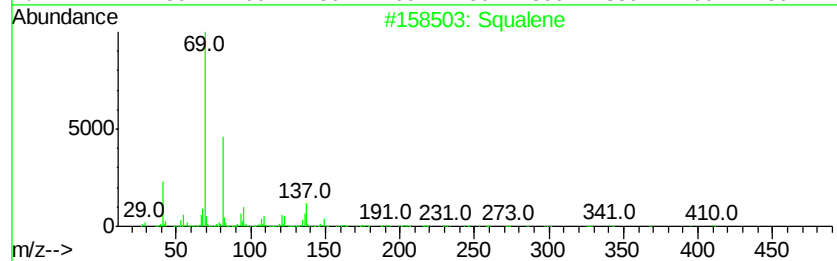
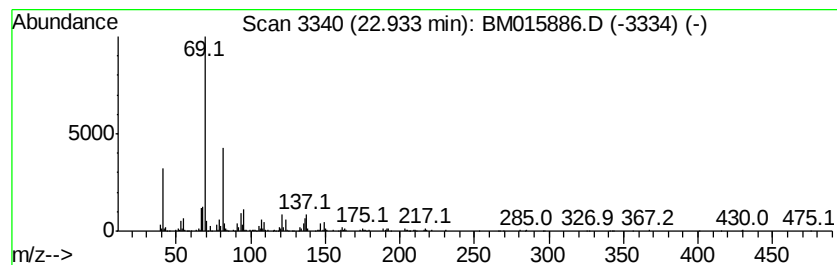
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.93	11.15 ng	606119	Chrysene-d12	21.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 91
2	2,6,10,14,18,22-Tetracosahexaene...		410 C30H50	000111-02-4 80
3	2,6,10,14-Hexadecatetraenoic aci...		332 C22H36O2	024035-35-6 78
4	4,9,13,17-Tetramethyl-4,8,12,16-...		316 C22H36O	056882-09-8 78
5	7,11-Dimethyldodeca-2,6,10-trien...		208 C14H24O	125529-10-4 74



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
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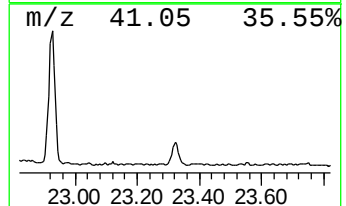
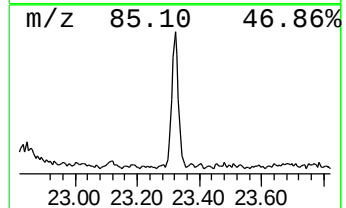
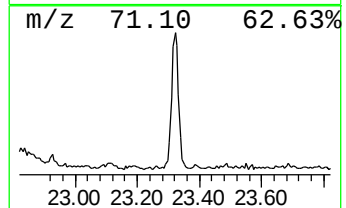
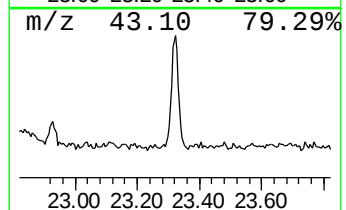
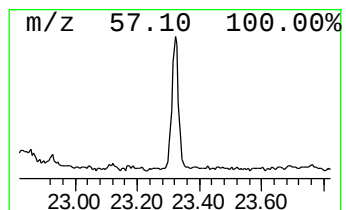
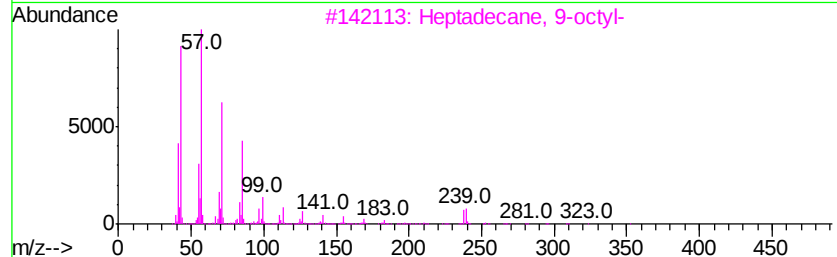
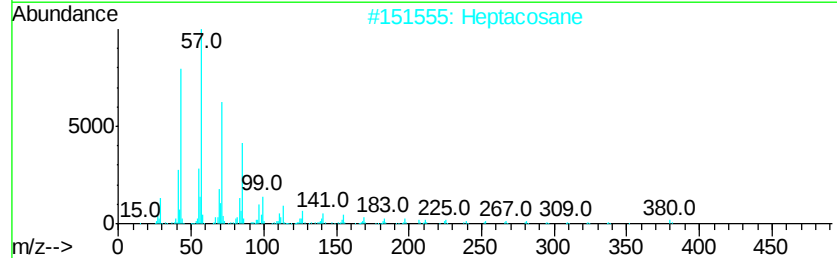
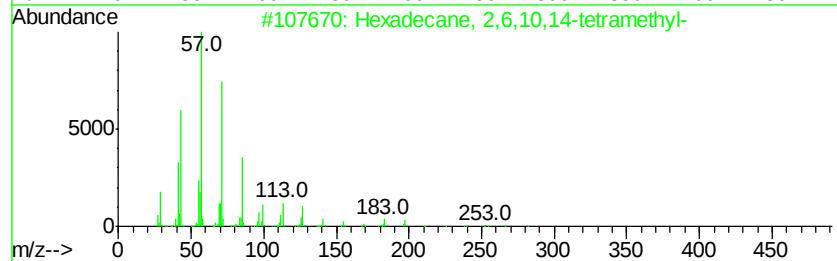
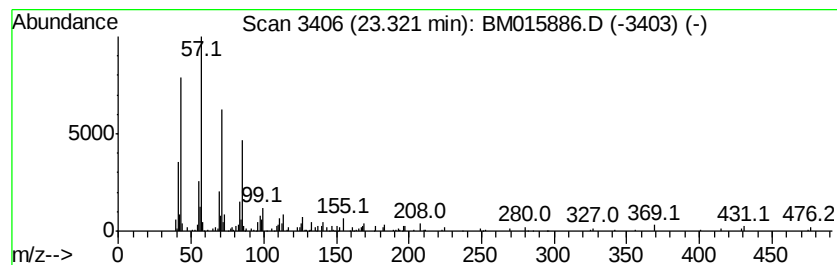
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexadecane, 2,6,10,14-tetra... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.32	3.10 ng	162636	Perylene-d12	24.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	95
2		Heptacosane	380	C27H56	000593-49-7	87
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	87
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
 Data File : BM015886.D
 Acq On : 11 Jul 2018 13:24
 Operator : SJ/JU
 Sample : J3925-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

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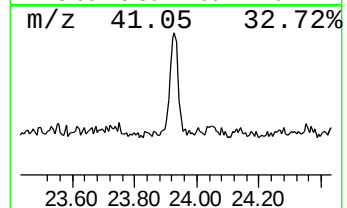
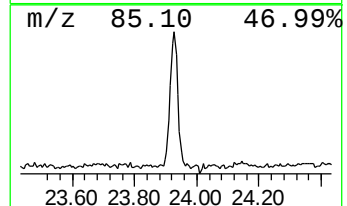
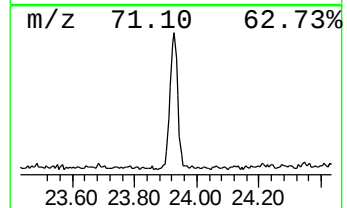
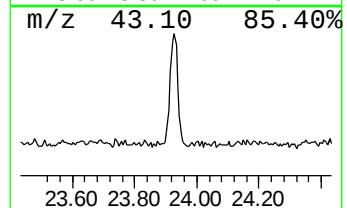
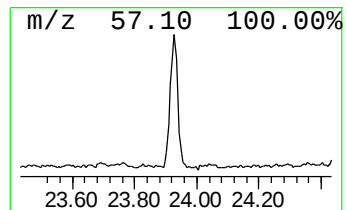
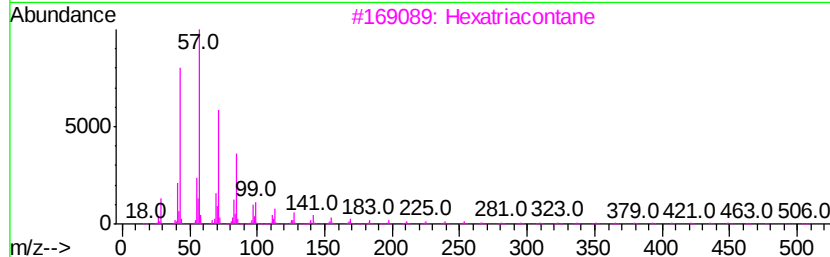
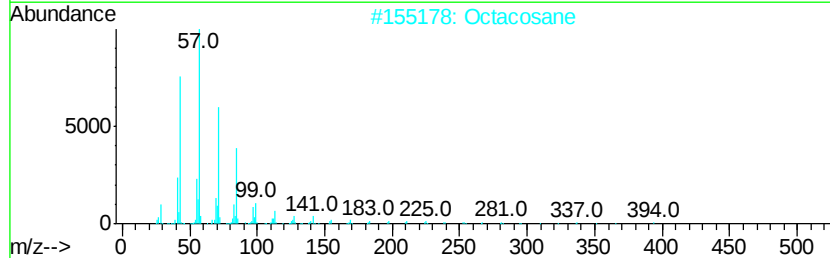
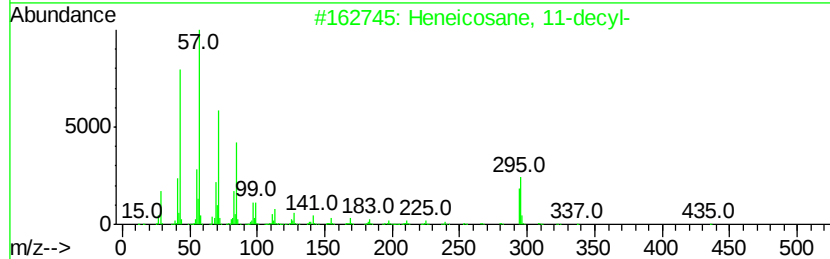
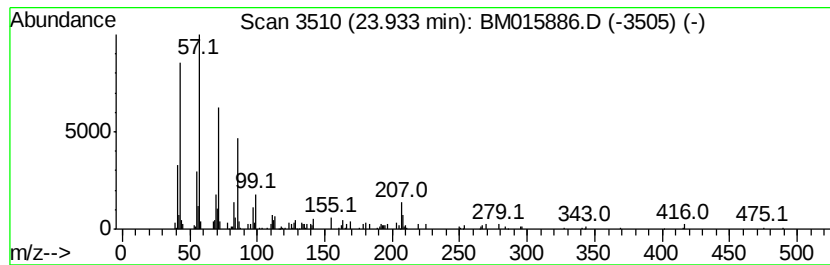
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 14 Heneicosane, 11-decyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	3.18 ng	166849	Perylene-d12	24.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Hexatriacontane	507	C36H74	000630-06-8	90
4		Heptacosane	380	C27H56	000593-49-7	90
5		Tetratetracontane	619	C44H90	007098-22-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM071118\
Data File : BM015886.D
Acq On : 11 Jul 2018 13:24
Operator : SJ/JU
Sample : J3925-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-1

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
2-Pentanone, 4-hy...	5.32	4.2 ng		130661	1	8.29	629385	20.0
unknown7.82	7.82	86.4 ng		2717640	1	8.29	629385	20.0
Phenol, 4-(1,1-di...	13.75	3.1 ng		147516	3	14.91	962148	20.0
unknown18.36	18.36	2.4 ng		127357	4	17.64	1060560	20.0
n-Hexadecanoic acid	18.48	14.1 ng		748321	4	17.64	1060560	20.0
Octadec-9-enoic acid	19.61	3.1 ng		166222	4	17.64	1060560	20.0
Octadecanoic acid	19.73	8.1 ng		439415	5	21.75	1087420	20.0
3-Eicosene, (E)-	21.42	8.0 ng		435764	5	21.75	1087420	20.0
Diethylene glycol...	21.50	6.7 ng		361471	5	21.75	1087420	20.0
Hexatriacontane	22.79	2.1 ng		115292	5	21.75	1087420	20.0
Squalene	22.93	11.2 ng		606119	5	21.75	1087420	20.0
Hexadecane, 2,6,1...	23.32	3.1 ng		162636	6	24.14	1050040	20.0
Heneicosane, 11-d...	23.93	3.2 ng		166849	6	24.14	1050040	20.0