

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101818\
 Data File : BF109960.D
 Acq On : 18 Oct 2018 14:44
 Operator : JU/SJ
 Sample : J5575-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1015-S-DH-27

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_F\METHODS\8270-BF101518.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	2.140	6	9	30	rVB	370187	740904	12.30%	1.300%
2	2.357	39	46	55	rVB	846486	1159352	19.24%	2.034%
3	5.228	524	534	544	rBV	237598	329659	5.47%	0.578%
4	5.604	592	598	601	rBV	5131103	5314403	88.22%	9.322%
5	6.598	760	767	771	rBV2	4922680	6024242	100.00%	10.567%
6	6.745	787	792	795	rBV	5424863	5556304	92.23%	9.746%
7	6.975	827	831	835	rBV	1979013	1558957	25.88%	2.734%
8	7.134	853	858	861	rBV	4754335	4266055	70.81%	7.483%
9	7.540	921	927	930	rBV	3645849	3580938	59.44%	6.281%
10	8.257	1044	1049	1053	rBV	2361884	2042138	33.90%	3.582%
11	9.334	1226	1232	1235	rBV	6315806	5979737	99.26%	10.489%
12	9.722	1294	1298	1302	rBV	720330	567812	9.43%	0.996%
13	10.022	1344	1349	1352	rBV	2307175	2230406	37.02%	3.912%
14	10.810	1478	1483	1486	rBV	3827678	3519242	58.42%	6.173%
15	11.510	1598	1602	1605	rBV	2474445	2072683	34.41%	3.636%
16	12.016	1683	1688	1699	rBV2	198599	264056	4.38%	0.463%
17	12.951	1844	1847	1850	rBV	86615	81144	1.35%	0.142%
18	13.098	1867	1872	1875	rBV	4788588	4250825	70.56%	7.456%
19	13.310	1905	1908	1911	rVB	144908	112044	1.86%	0.197%
20	13.563	1947	1951	1956	rBV	243322	354155	5.88%	0.621%
21	13.598	1956	1957	1962	rVV	101927	82506	1.37%	0.145%
22	13.651	1962	1966	1969	rVV2	221631	211821	3.52%	0.372%
23	13.980	2018	2022	2034	rBV	570820	655776	10.89%	1.150%
24	14.157	2048	2052	2055	rBV	1409002	1341692	22.27%	2.353%
25	14.251	2064	2068	2073	rBV	46582	66373	1.10%	0.116%
26	14.298	2073	2076	2081	rVB	314345	258404	4.29%	0.453%
27	14.604	2124	2128	2134	rBV	355303	325656	5.41%	0.571%
28	14.927	2178	2183	2188	rBV	371646	392638	6.52%	0.689%
29	15.010	2193	2197	2200	rBV	134498	141004	2.34%	0.247%
30	15.280	2239	2243	2250	rBV	434788	560716	9.31%	0.984%
31	15.686	2306	2312	2319	rVB2	1454639	2006048	33.30%	3.519%
32	16.151	2387	2391	2396	rBV	372513	638017	10.59%	1.119%
33	16.692	2480	2483	2492	rVB2	184828	326275	5.42%	0.572%

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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_F\METHODS\8270-BF101518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

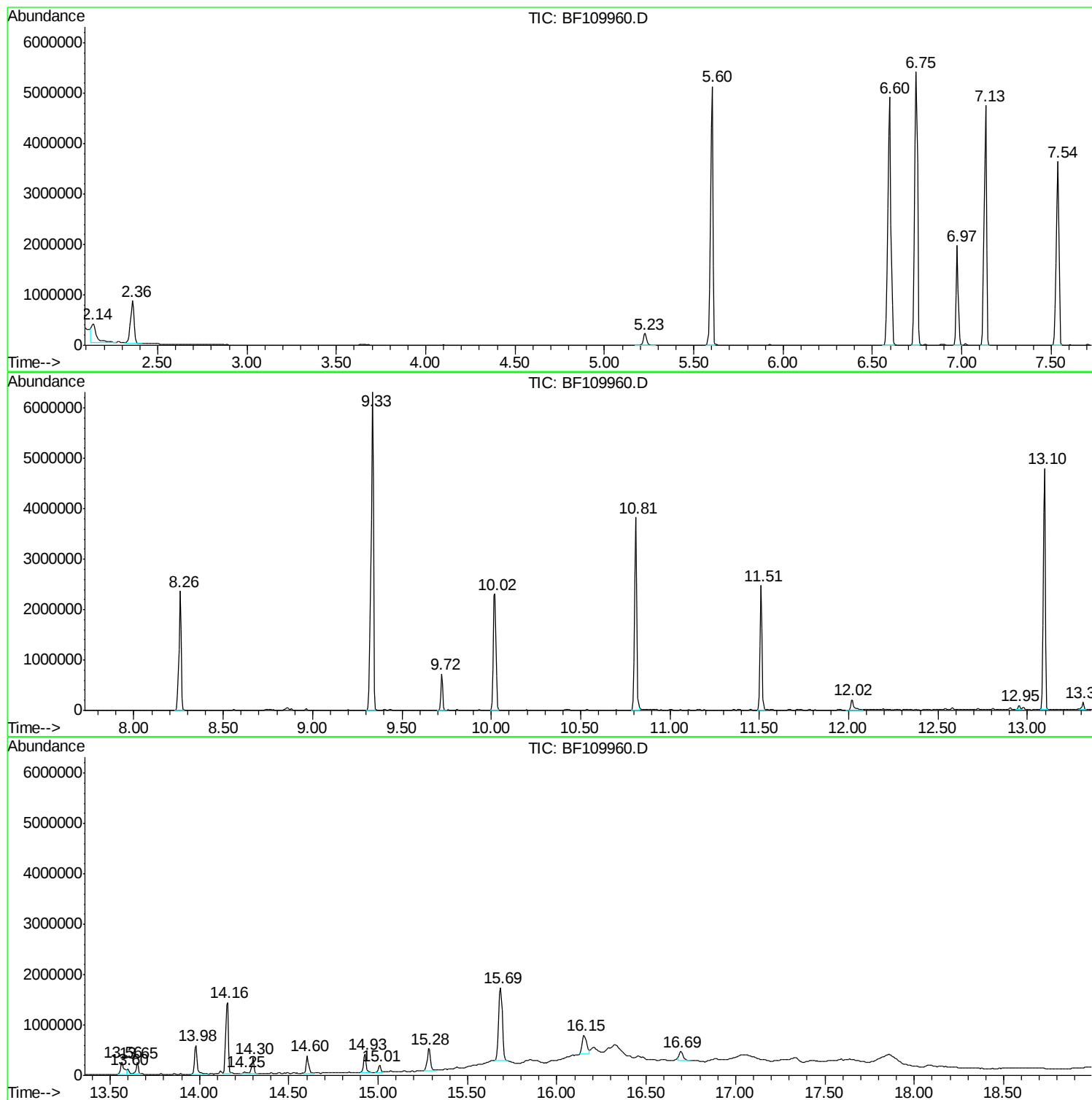
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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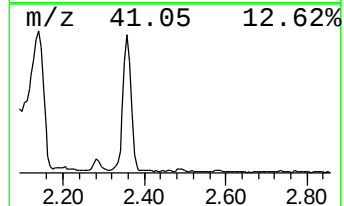
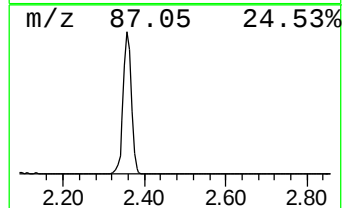
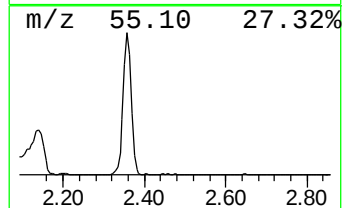
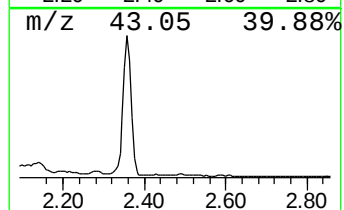
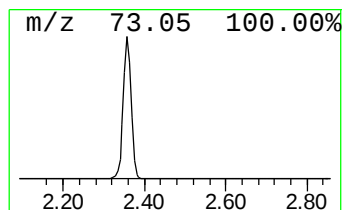
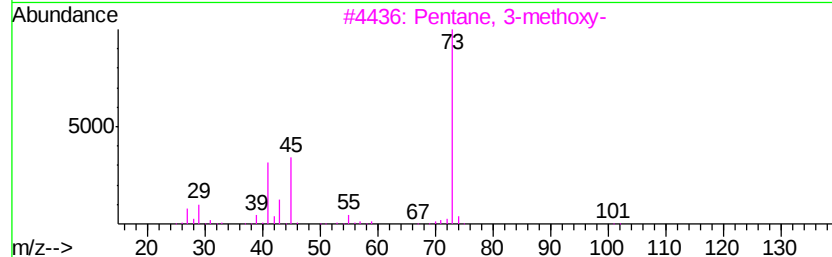
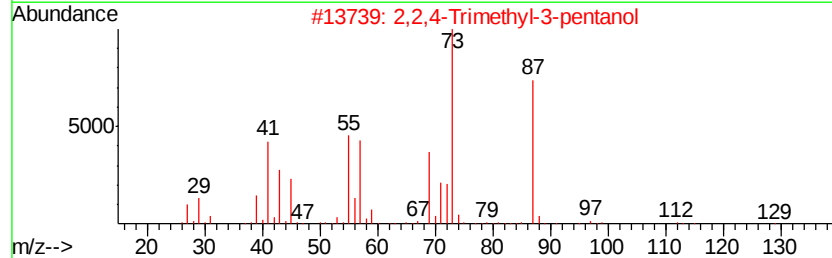
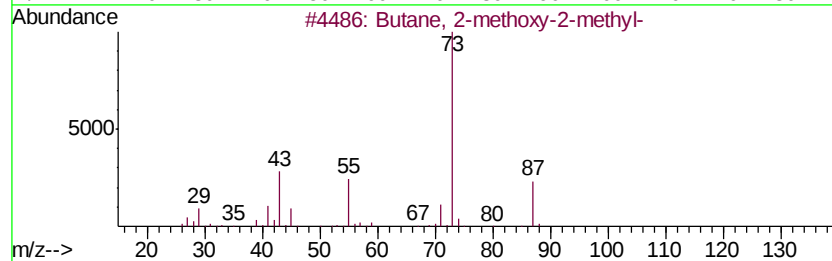
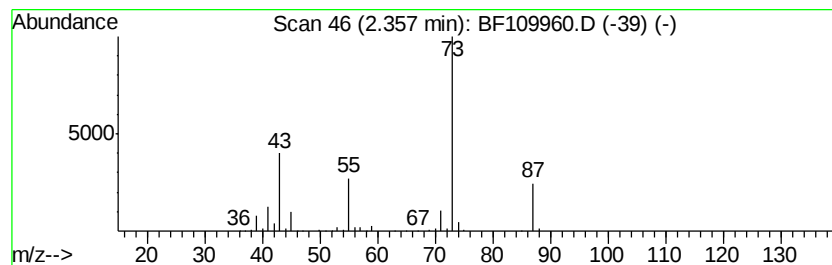
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.36	14.87 ng	1159350	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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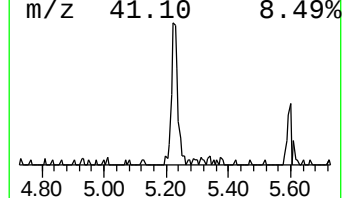
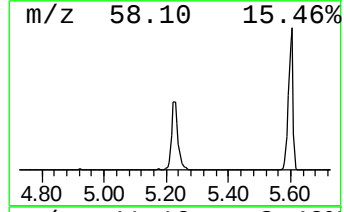
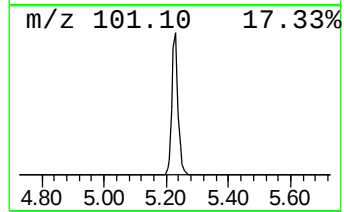
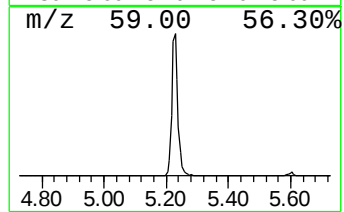
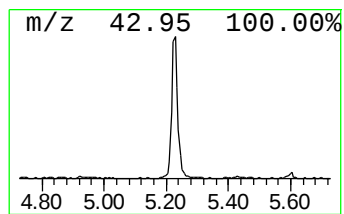
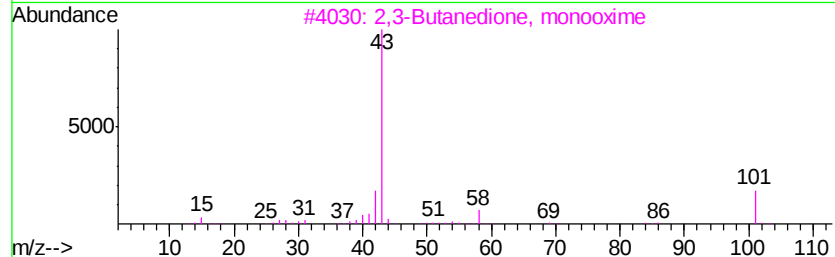
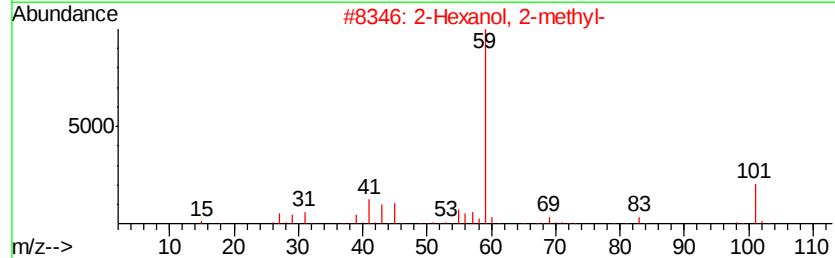
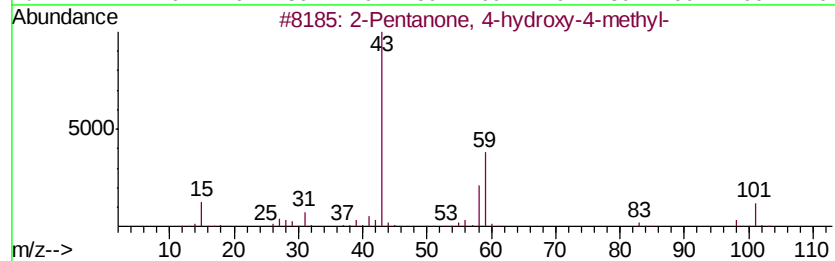
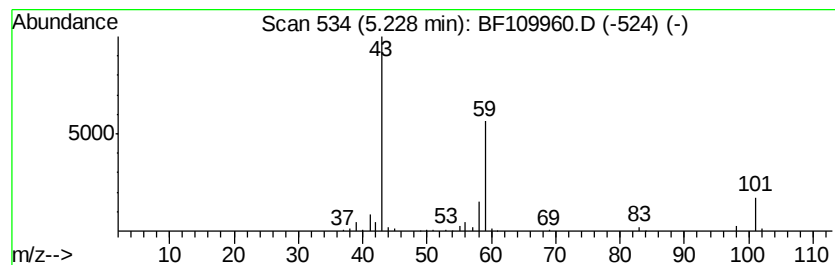
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	4.23 ng	329659	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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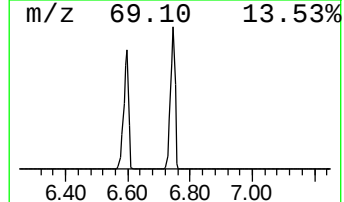
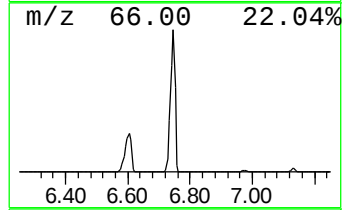
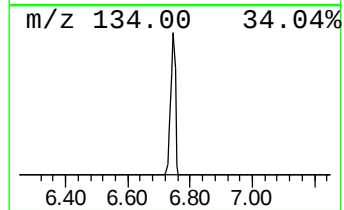
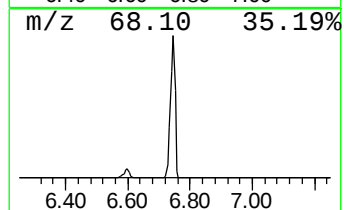
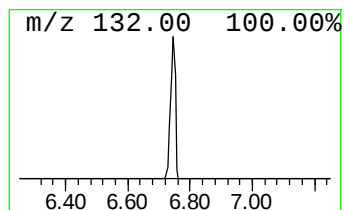
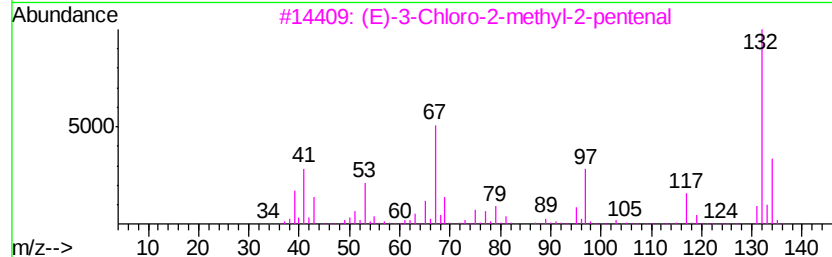
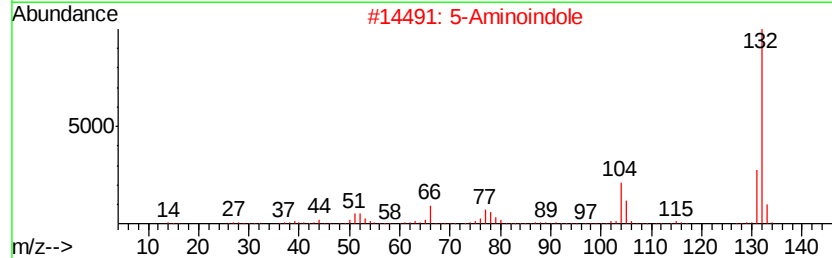
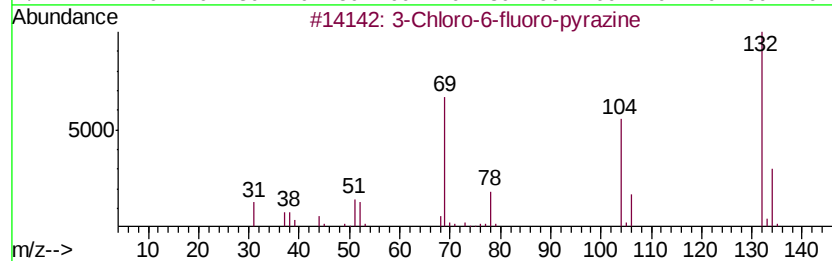
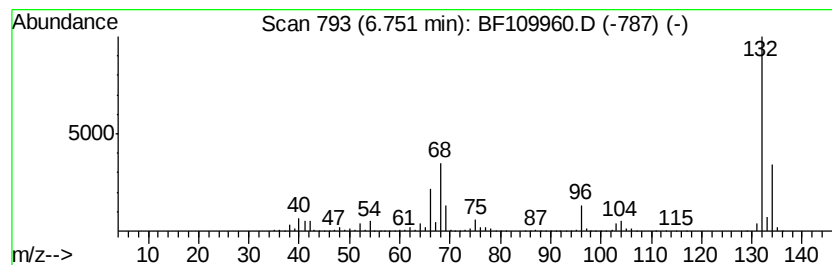
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	71.28 ng	5556300	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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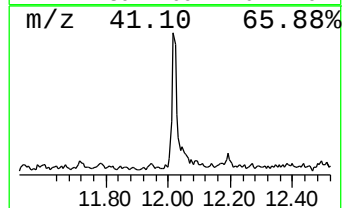
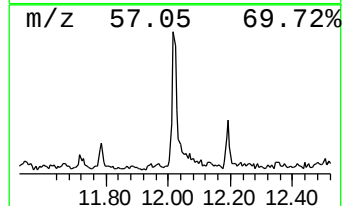
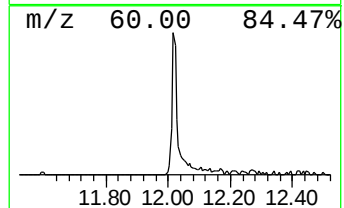
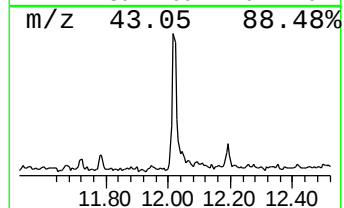
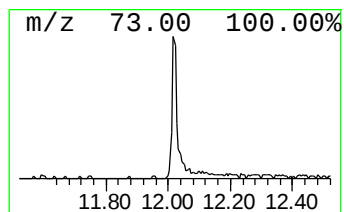
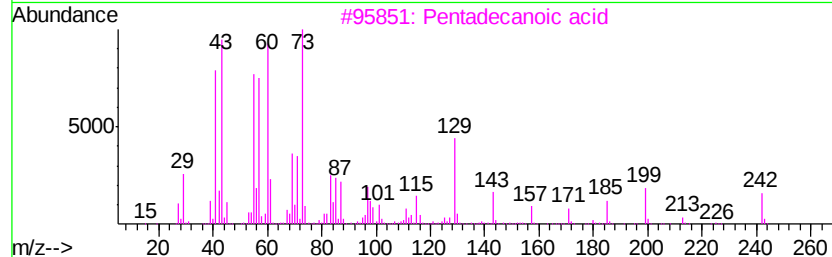
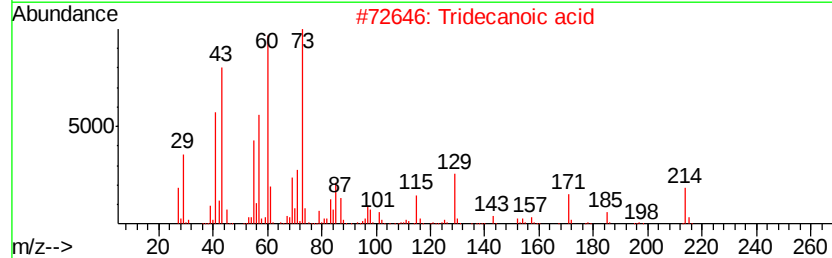
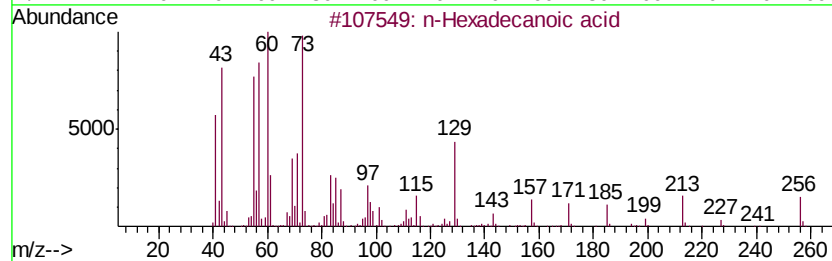
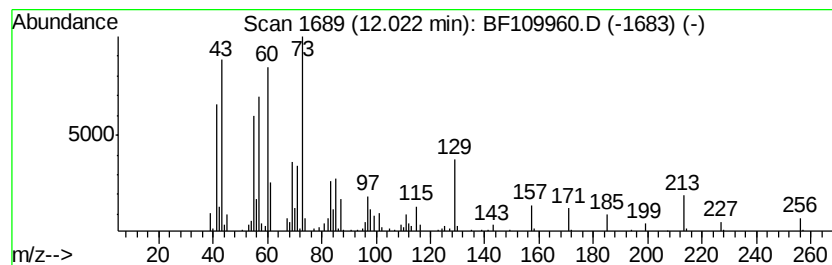
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	2.55 ng	264056	Phenanthrene-d10	11.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	74
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		Nonanoic acid	158	C9H18O2	000112-05-0	43



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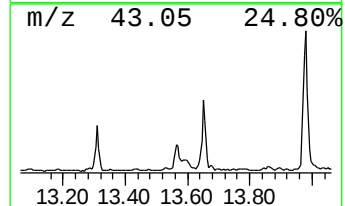
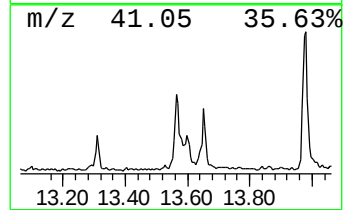
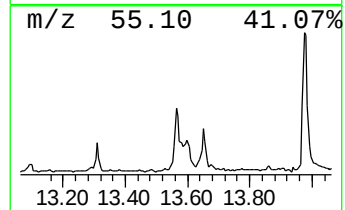
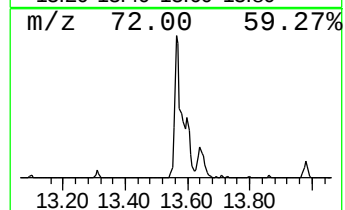
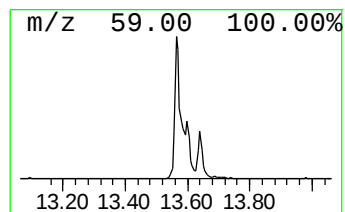
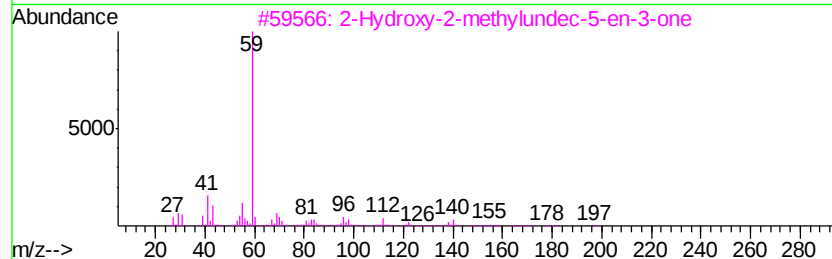
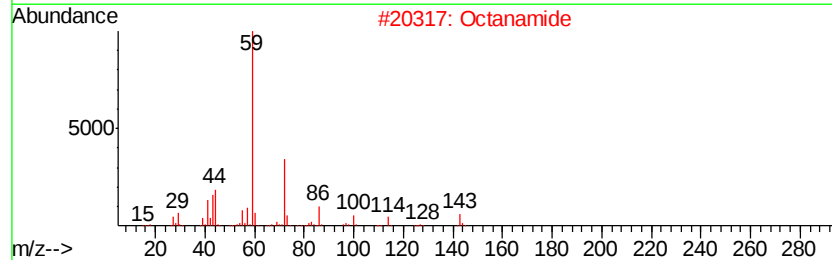
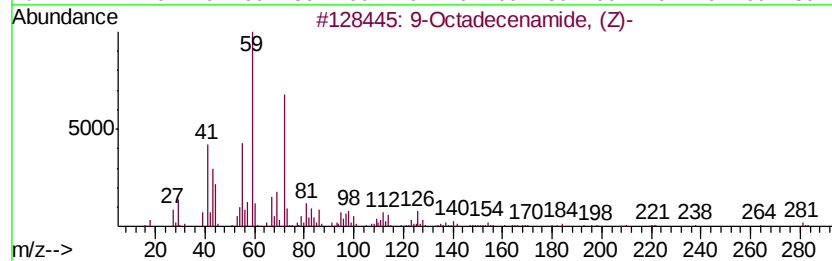
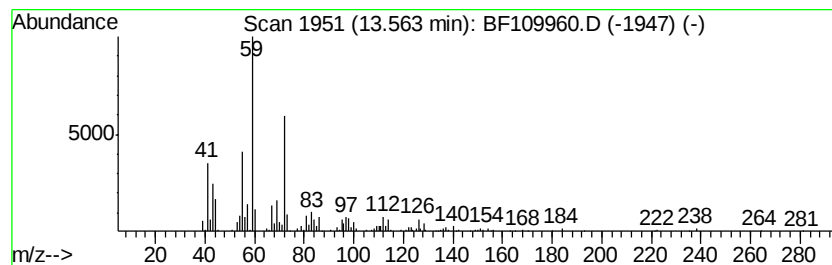
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.56	5.28 ng	354155	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		Octanamide	143	C8H17NO	000629-01-6	53
3		2-Hydroxy-2-methylundec-5-en-3-one	198	C12H22O2	1000191-46-2	43
4		2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	43
5		Oxirane, tetramethyl-	100	C6H12O	005076-20-0	43



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Acq On : 18 Oct 2018 14:44
Operator : JU/SJ
Sample : J5575-04
Misc :
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ClientSampleId :
SSSI-1015-S-DH-27

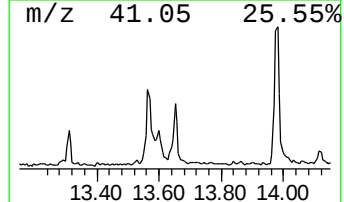
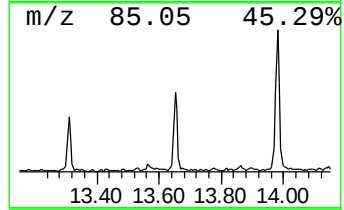
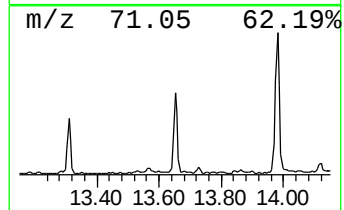
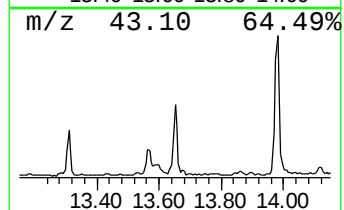
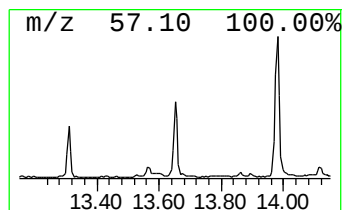
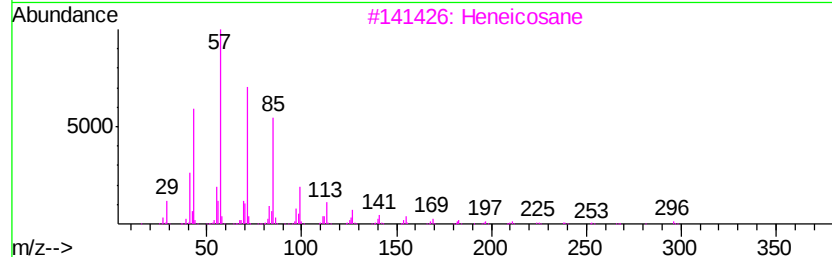
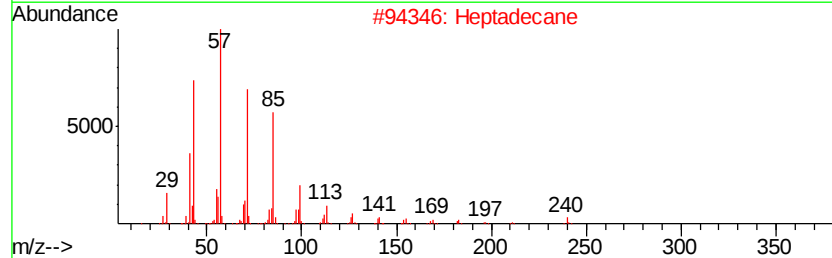
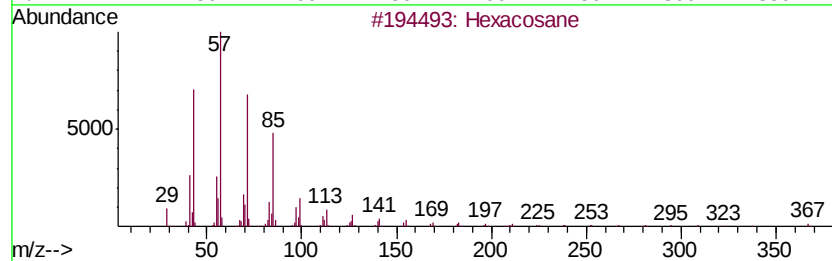
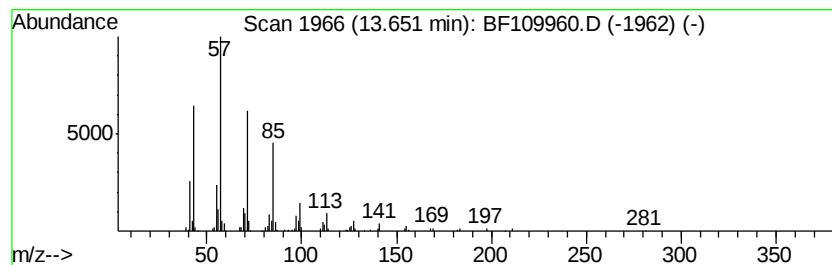
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	3.16 ng	211821	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101818\
Data File : BF109960.D
Acq On : 18 Oct 2018 14:44
Operator : JU/SJ
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Instrument :
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ClientSampleId :
SSSI-1015-S-DH-27

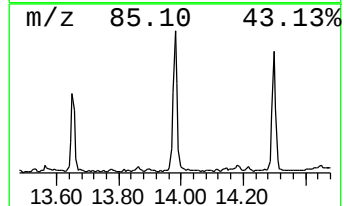
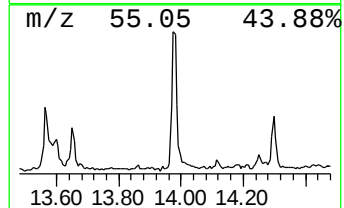
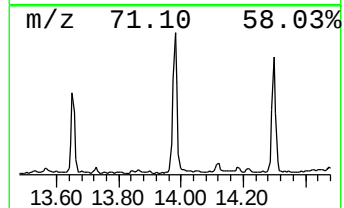
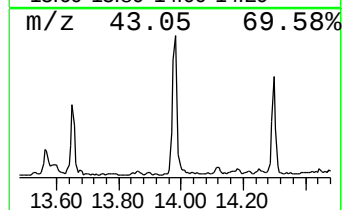
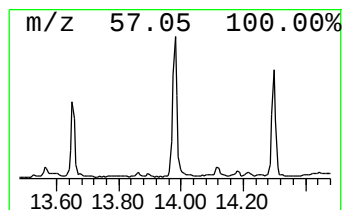
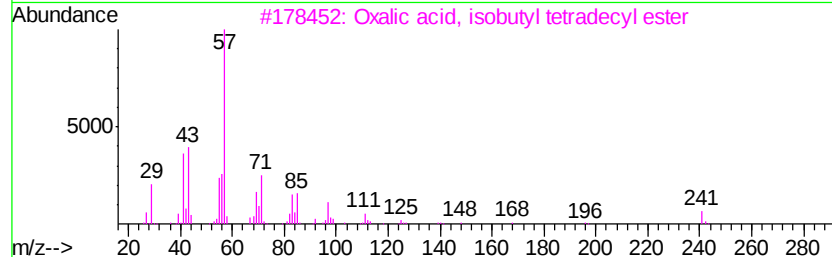
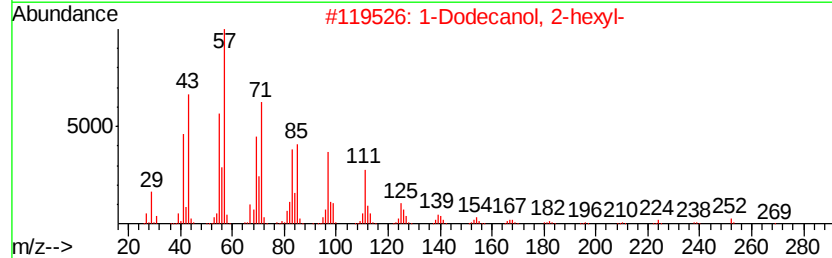
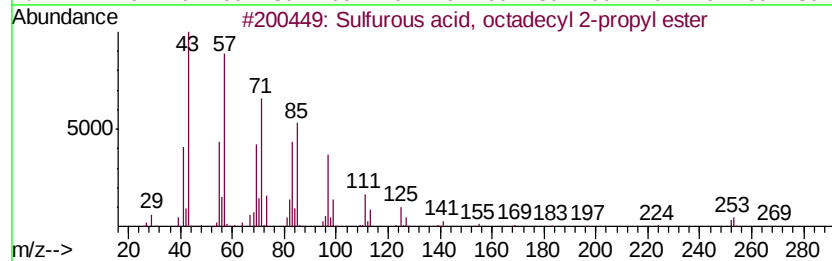
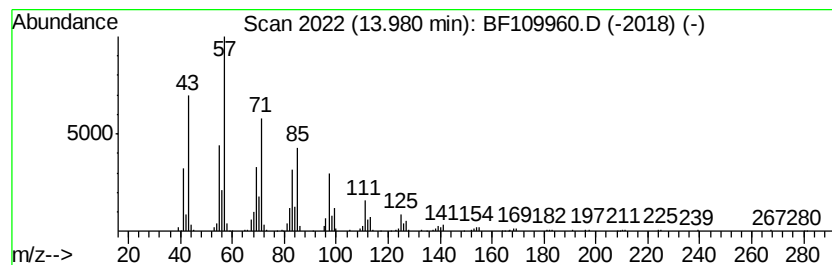
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Sulfurous acid, octadecyl 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	9.78 ng	655776	Chrysene-d12	14.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	90
2			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	83
3			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	83
4			Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	68
5			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101818\
Data File : BF109960.D
Acq On : 18 Oct 2018 14:44
Operator : JU/SJ
Sample : J5575-04
Misc :
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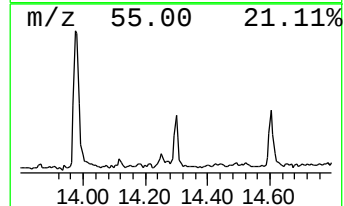
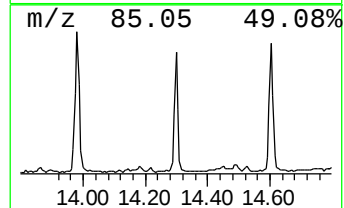
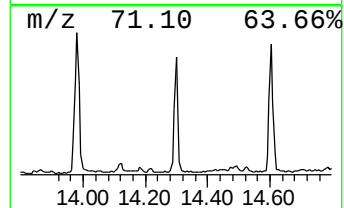
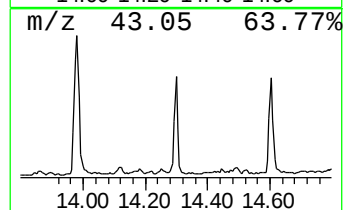
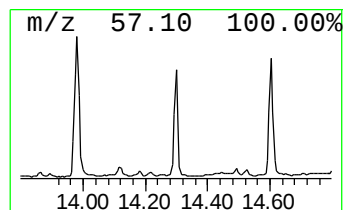
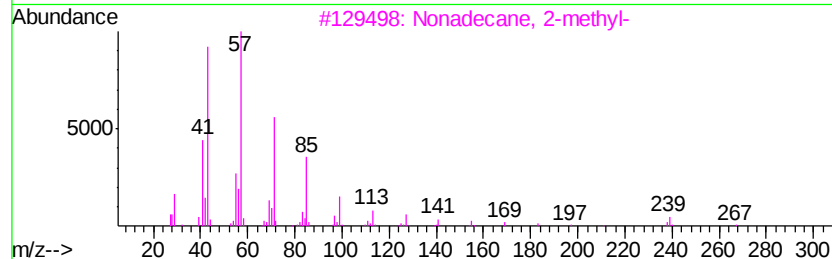
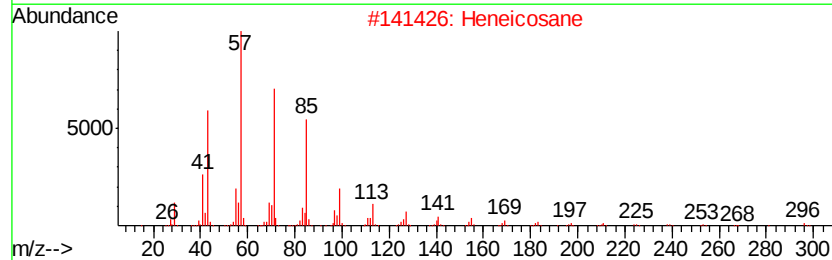
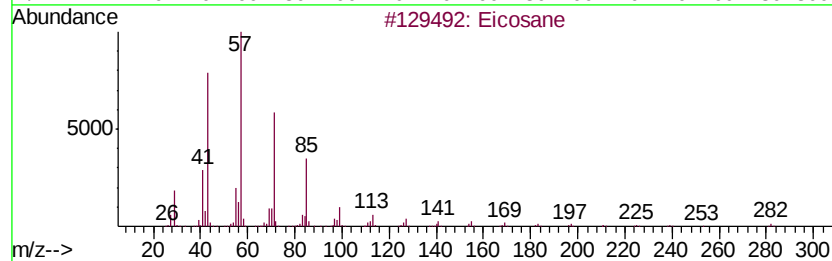
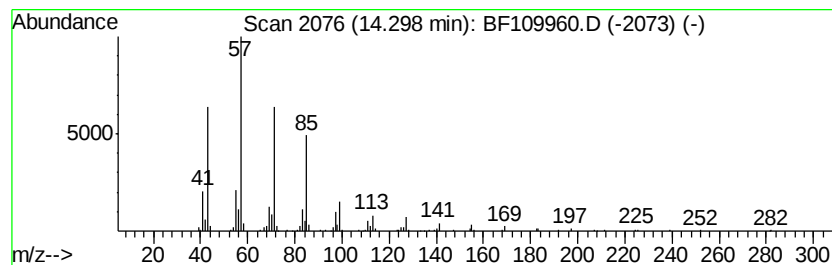
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	3.85 ng	258404	Chrysene-d12	14.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Heneicosane	296	C21H44	000629-94-7	91
3			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	91
4			Octacosane	394	C28H58	000630-02-4	83
5			Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101818\
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Acq On : 18 Oct 2018 14:44
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Sample : J5575-04
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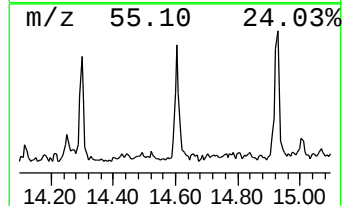
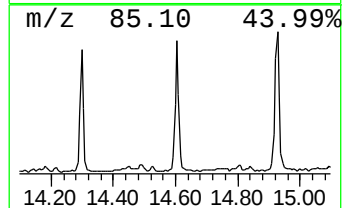
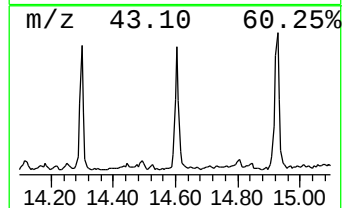
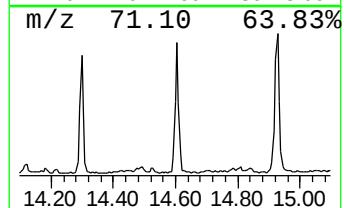
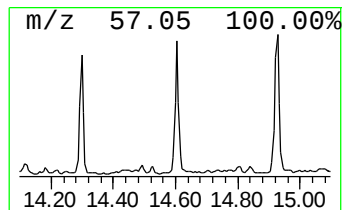
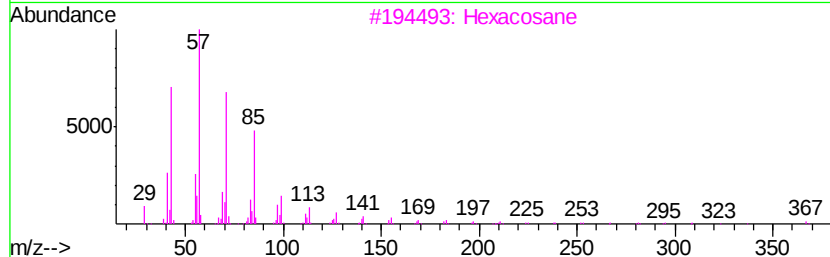
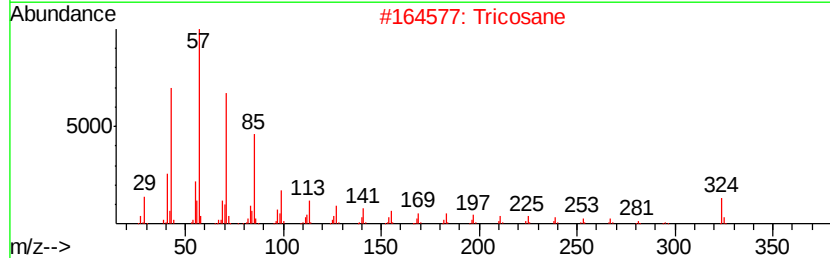
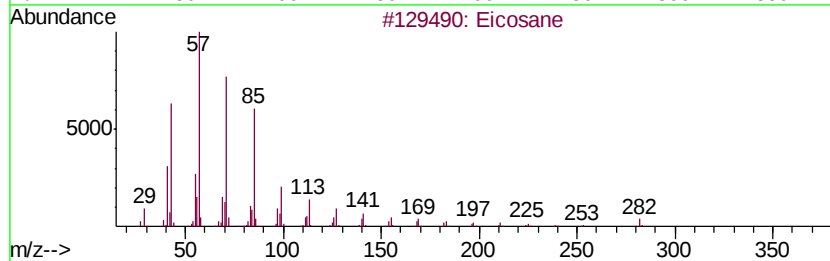
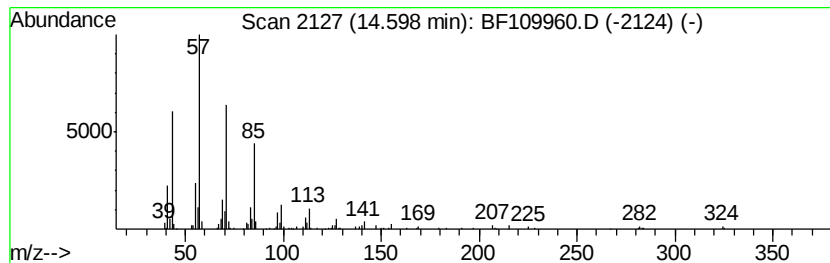
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	4.85 ng	325656	Chrysene-d12	14.16
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	97
2	Tricosane	324 C23H48	000638-67-5	93
3	Hexacosane	366 C26H54	000630-01-3	91
4	Docosane	310 C22H46	000629-97-0	91
5	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101818\
Data File : BF109960.D
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Operator : JU/SJ
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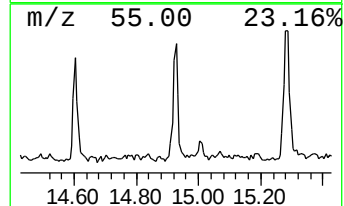
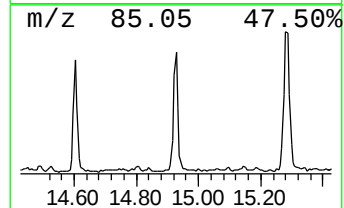
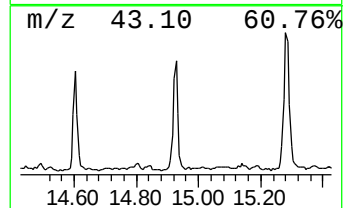
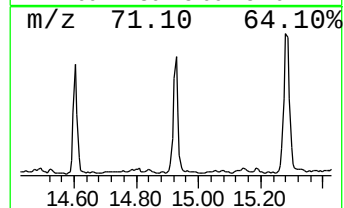
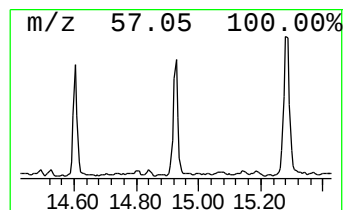
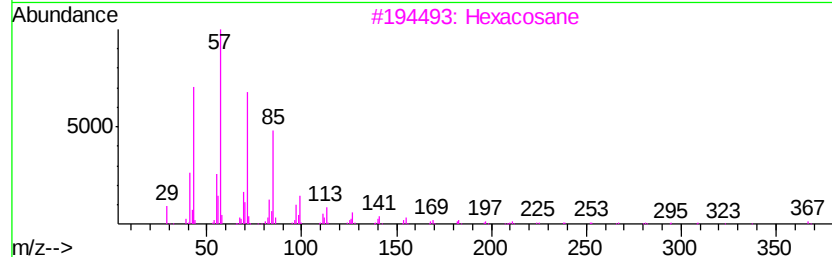
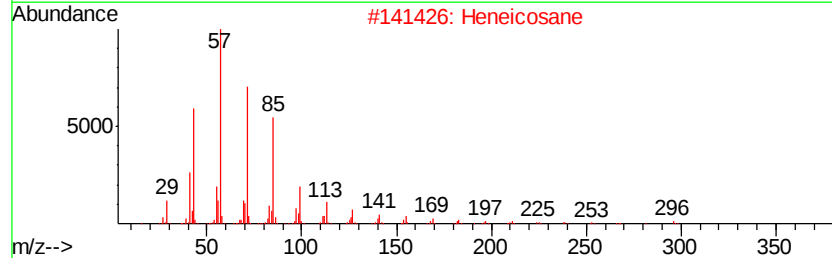
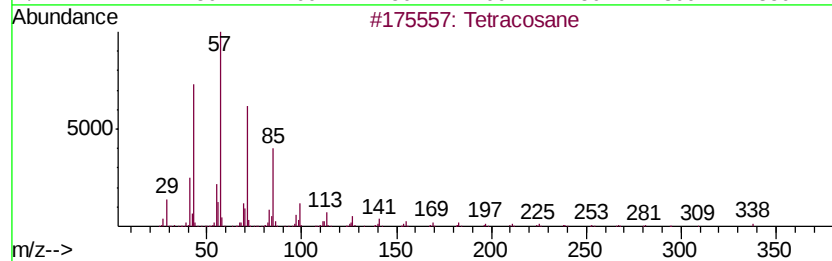
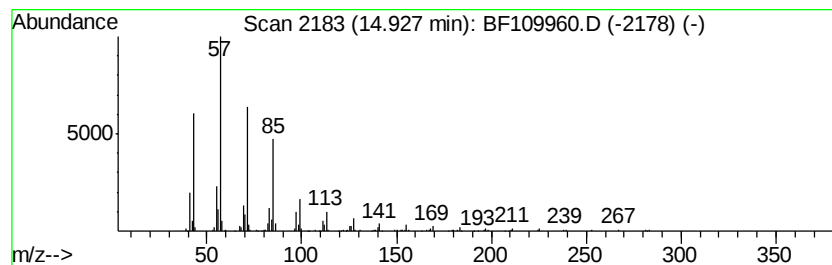
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	3.91 ng	392638	Perylene-d12	15.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5			triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101818\
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Acq On : 18 Oct 2018 14:44
Operator : JU/SJ
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ClientSampleId :
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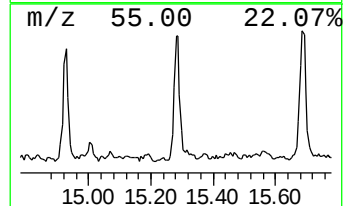
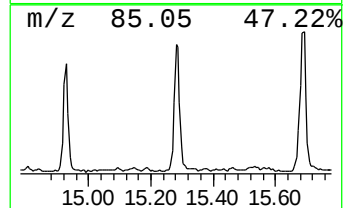
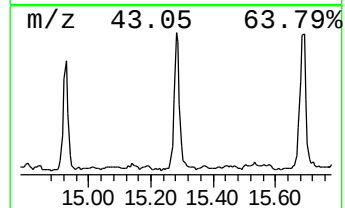
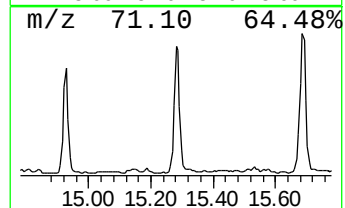
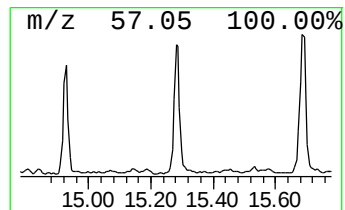
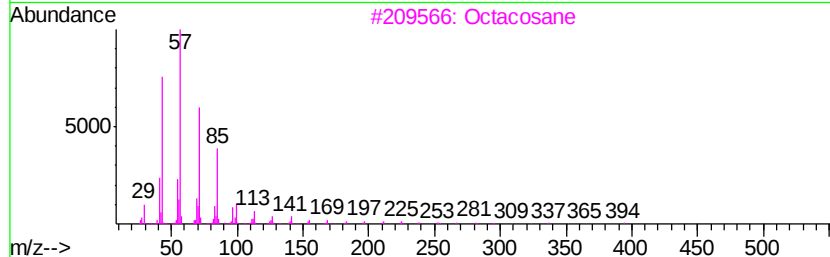
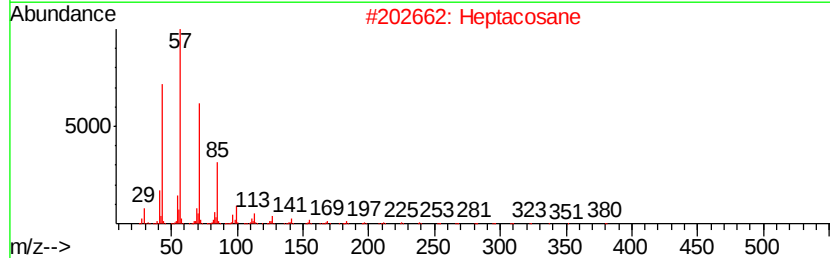
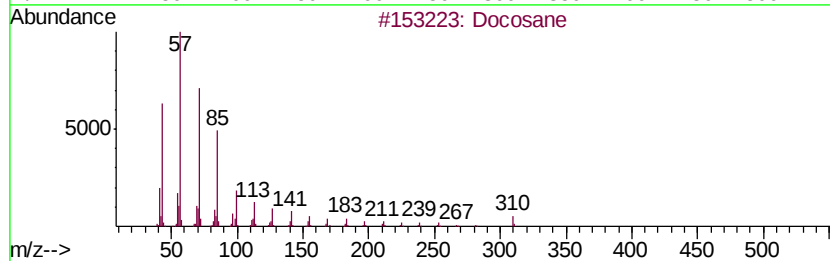
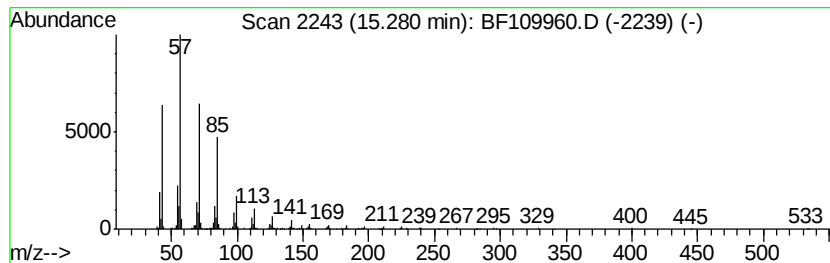
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Docosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.28	5.59 ng	560716	Perylene-d12	15.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101818\
Data File : BF109960.D
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Misc :
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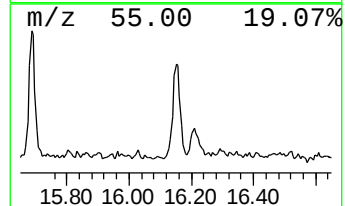
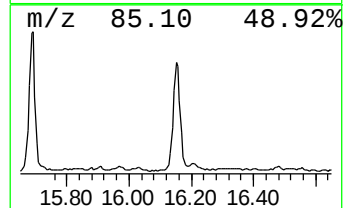
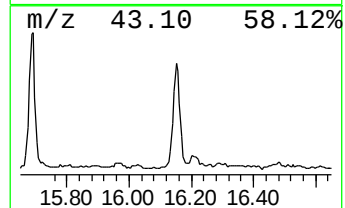
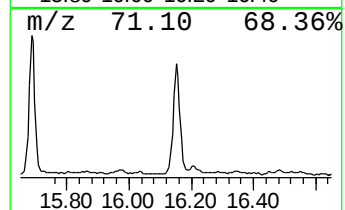
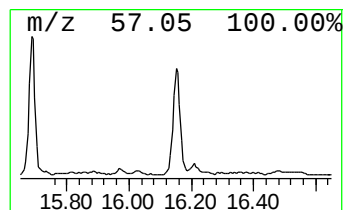
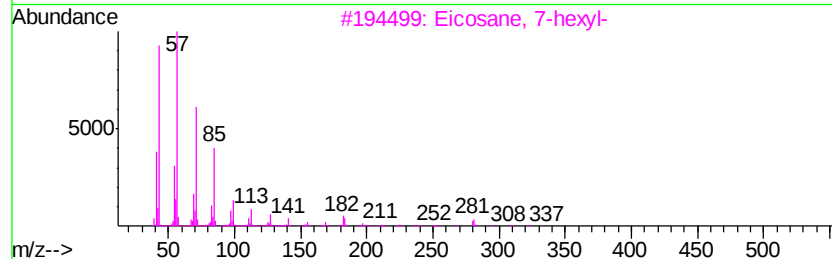
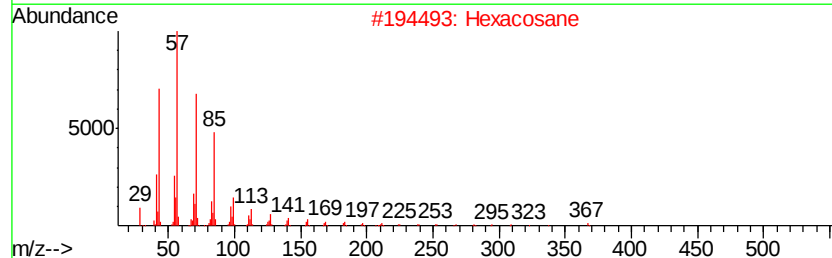
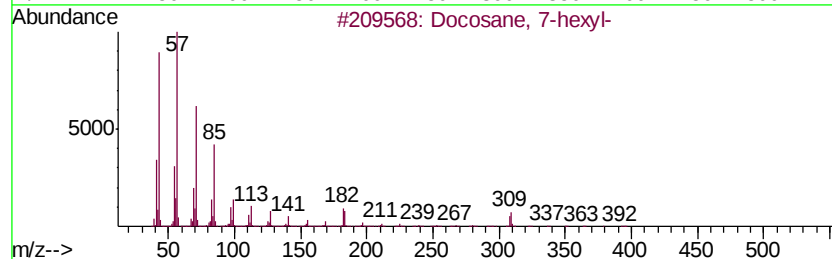
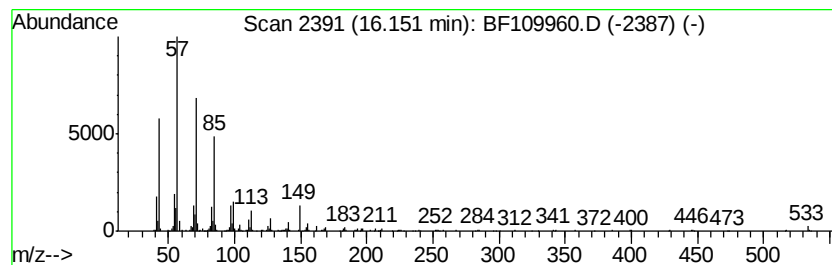
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Docosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	6.36 ng	638017	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	83
2		Hexacosane	366	C26H54	000630-01-3	83
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80
4		Octacosane	394	C28H58	000630-02-4	76
5		Tetratetracontane	619	C44H90	007098-22-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101818\
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 Acq On : 18 Oct 2018 14:44
 Operator : JU/SJ
 Sample : J5575-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1015-S-DH-27

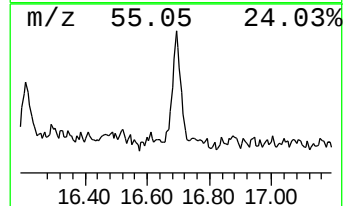
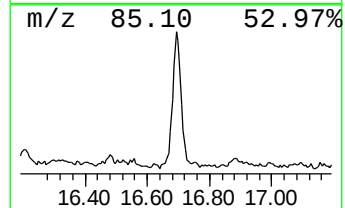
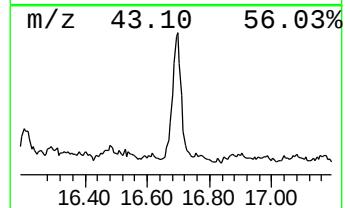
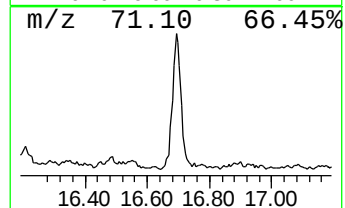
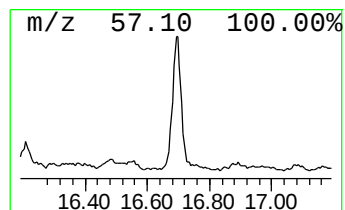
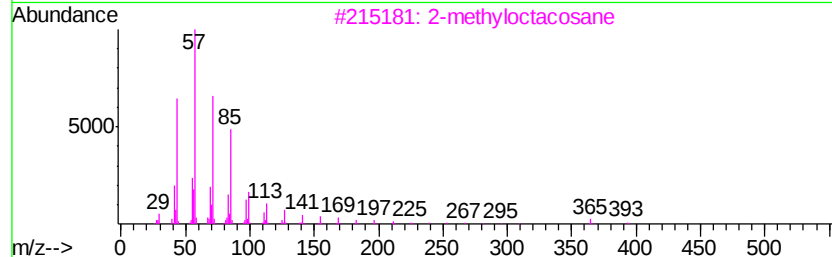
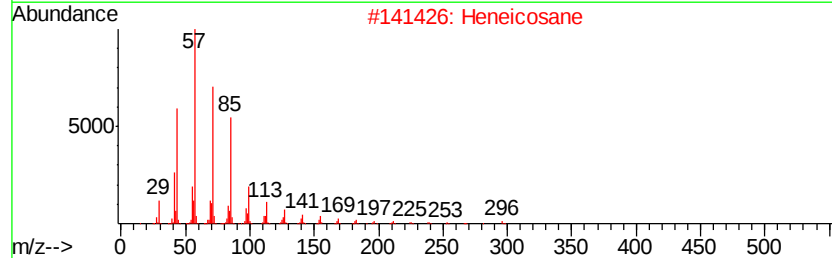
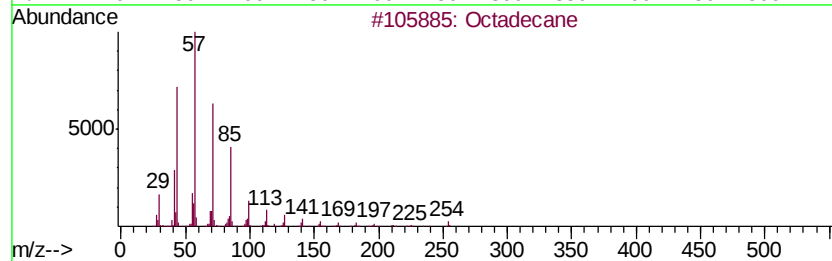
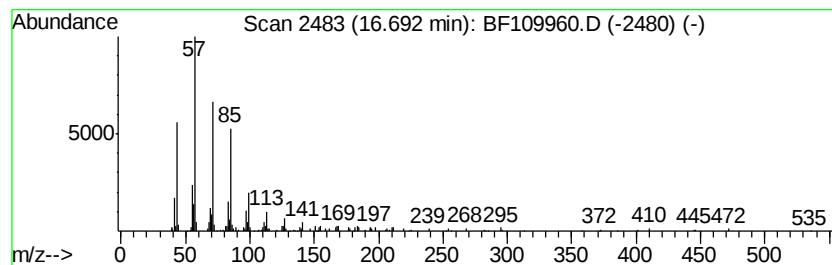
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 15 Octadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	3.25 ng	326275	Perylene-d12	15.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	94
2			Heneicosane	296	C21H44	000629-94-7	90
3			2-methyloctacosane	408	C29H60	1000376-72-8	87
4			Tetracosane	338	C24H50	000646-31-1	86
5			Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101818\
 Data File : BF109960.D
 Acq On : 18 Oct 2018 14:44
 Operator : JU/SJ
 Sample : J5575-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SSSI-1015-S-DH-27

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.36	14.9	ng	1159350	1	6.97	1558960	20.0
2-Pentanone, 4-hy...	5.23	4.2	ng	329659	1	6.97	1558960	20.0
unknown6.75	6.75	71.3	ng	5556300	1	6.97	1558960	20.0
n-Hexadecanoic acid	12.02	2.5	ng	264056	4	11.51	2072680	20.0
9-Octadecenamide,...	13.56	5.3	ng	354155	5	14.16	1341690	20.0
Hexacosane	13.65	3.2	ng	211821	5	14.16	1341690	20.0
Sulfurous acid, o...	13.98	9.8	ng	655776	5	14.16	1341690	20.0
Nonadecane, 2-met...	14.30	3.9	ng	258404	5	14.16	1341690	20.0
Eicosane	14.60	4.8	ng	325656	5	14.16	1341690	20.0
Tetracosane	14.93	3.9	ng	392638	6	15.68	2006050	20.0
Docosane	15.28	5.6	ng	560716	6	15.68	2006050	20.0
Docosane, 7-hexyl-	16.15	6.4	ng	638017	6	15.68	2006050	20.0
Octadecane	16.69	3.3	ng	326275	6	15.68	2006050	20.0