

Data Path : U:\HPCHEM1\BNA F\DATA\BF011118\
 Data File : BF102026.D
 Acq On : 11 Jan 2018 18:46
 Operator : SJ/JU
 Sample : J1067-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHRT-27007

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:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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	4.904	473	479	487	rVB	239243	397679	3.18%	0.739%
2	5.322	544	550	553	rBV	4253611	4583207	36.61%	8.513%
3	6.363	721	727	731	rBV	4118025	4737997	37.85%	8.800%
4	6.492	744	749	752	rBV	4378457	4467988	35.69%	8.299%
5	6.551	754	759	764	rVB2	257834	354794	2.83%	0.659%
6	6.634	769	773	776	rBV	193281	159854	1.28%	0.297%
7	6.728	785	789	792	rBV	1252965	1050496	8.39%	1.951%
8	6.834	802	807	811	rBV	276766	255945	2.04%	0.475%
9	6.881	811	815	818	rBV	3775851	3405517	27.20%	6.325%
10	7.045	839	843	849	rBV	615983	587697	4.69%	1.092%
11	7.292	880	885	888	rVB	3066425	2852789	22.79%	5.299%
12	7.328	888	891	894	rVB	372930	280212	2.24%	0.520%
13	8.010	1001	1007	1012	rBV	1533960	1609239	12.86%	2.989%
14	8.898	1144	1158	1163	rBV3	120143	530165	4.24%	0.985%
15	8.963	1163	1169	1171	rBV4	181016	392118	3.13%	0.728%
16	9.092	1186	1191	1192	rBV2	867423	1230727	9.83%	2.286%
17	9.763	1301	1305	1306	rBV2	233136	291039	2.32%	0.541%
18	10.245	1383	1387	1388	rBV3	132677	184110	1.47%	0.342%
19	10.374	1406	1409	1410	rBV2	265698	299688	2.39%	0.557%
20	10.545	1433	1438	1444	rBV2	551788	1626929	13.00%	3.022%
21	10.727	1465	1469	1470	rBV	1075078	1492575	11.92%	2.772%
22	10.833	1479	1487	1494	rBV6	3215390	12518302	100.00%	23.251%
23	11.010	1513	1517	1518	rBV	1858286	2389398	19.09%	4.438%
24	11.198	1543	1549	1550	rBV2	4321604	8141600	65.04%	15.122%

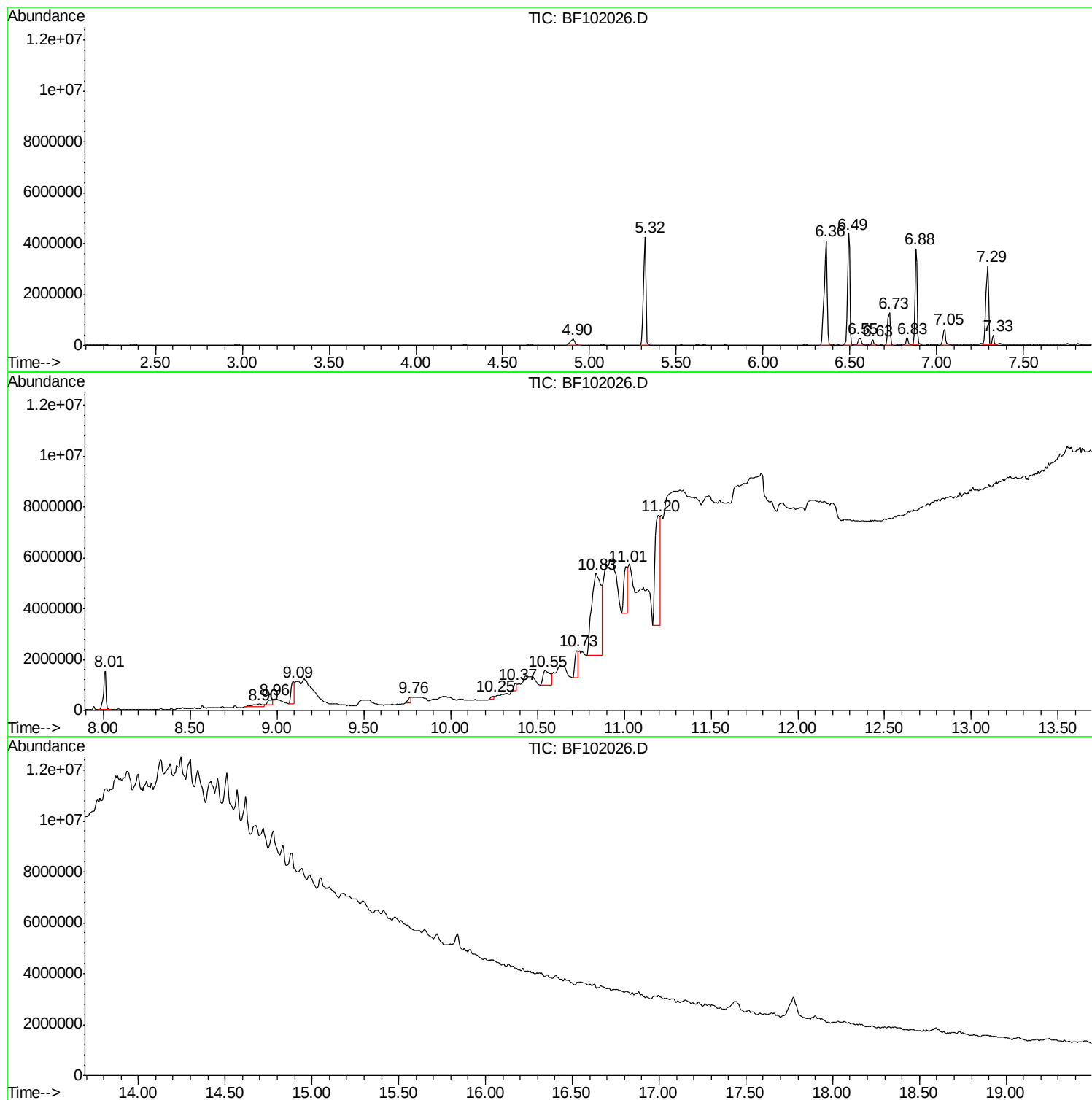
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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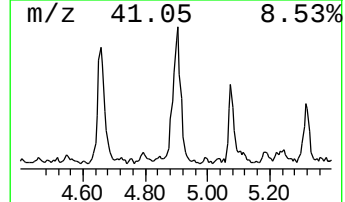
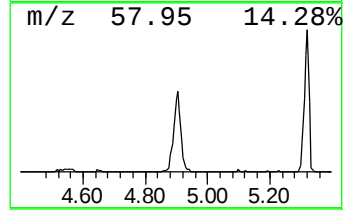
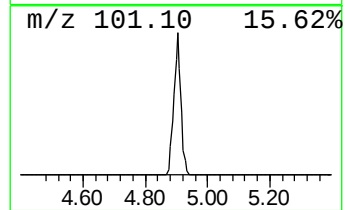
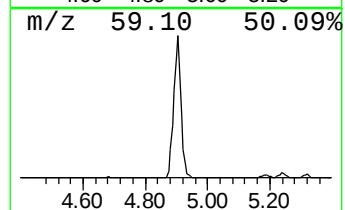
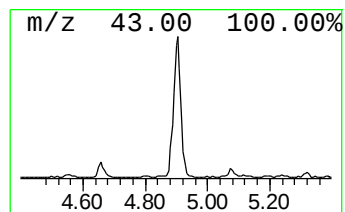
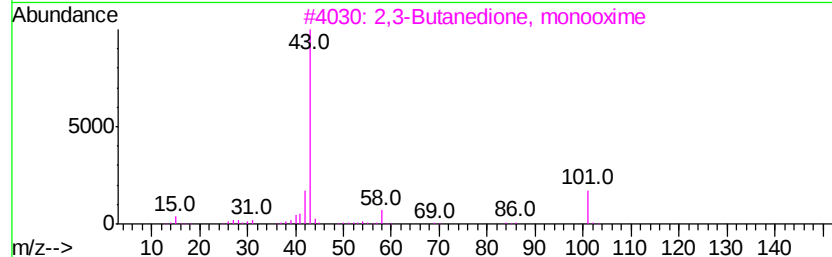
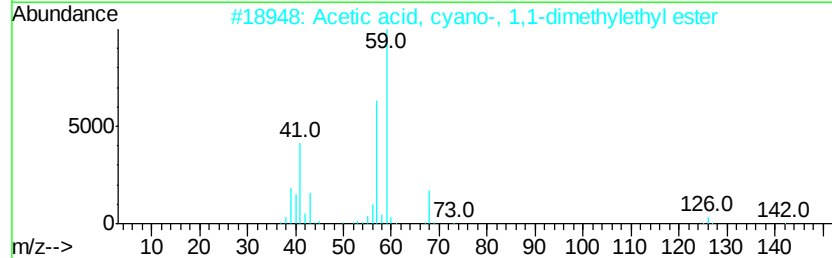
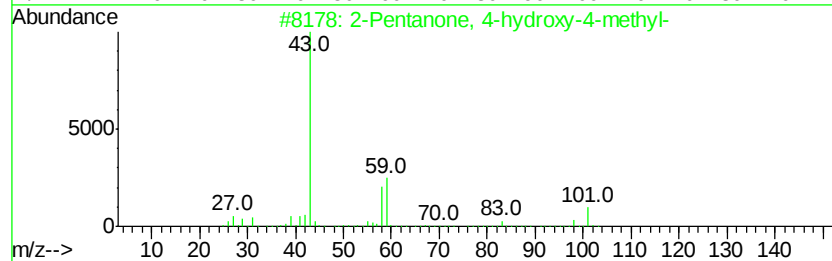
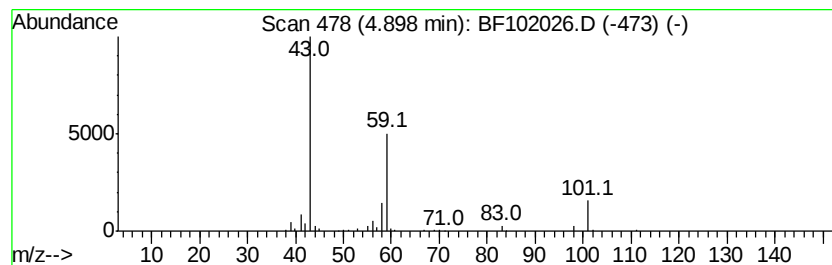
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
4.90	7.57 ng	397679	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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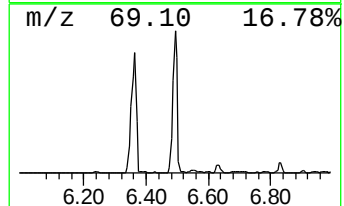
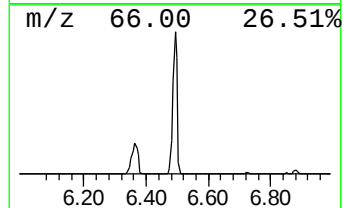
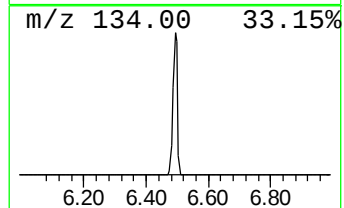
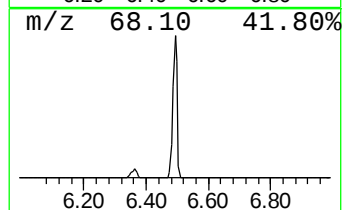
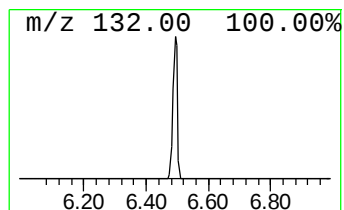
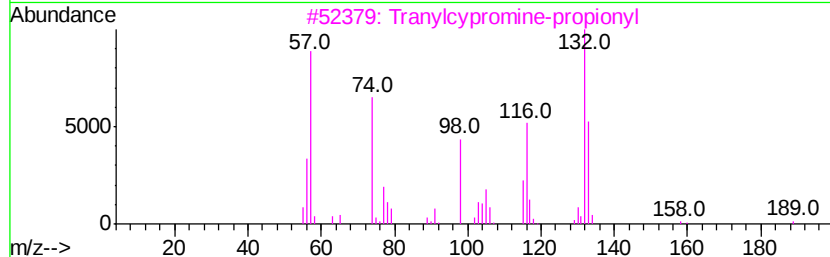
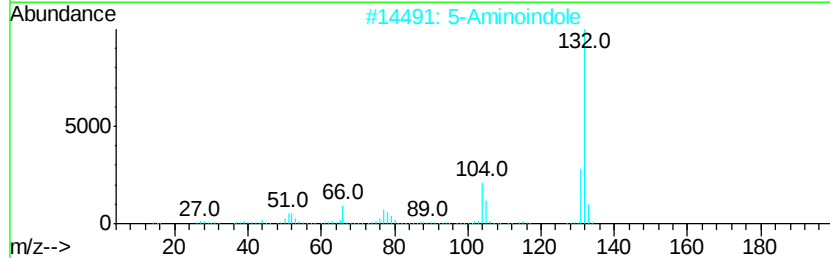
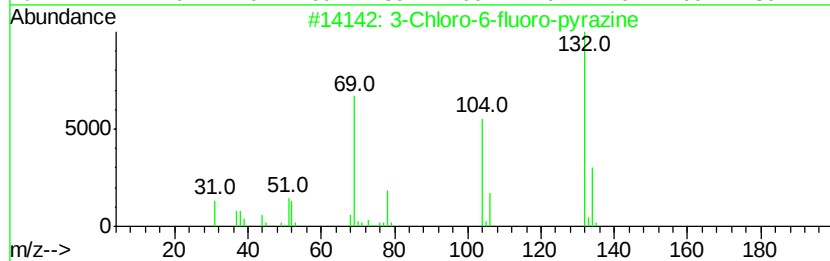
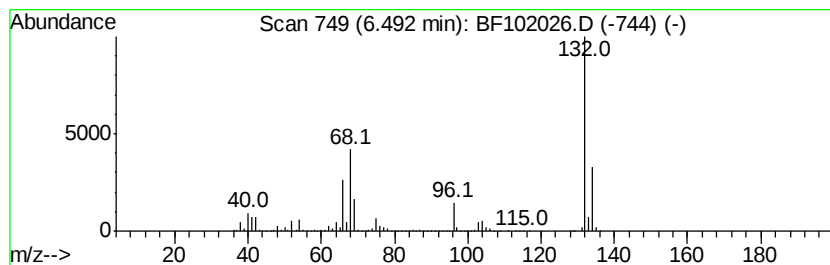
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	85.06 ng	4467990	1,4-Dichlorobenzene-d4	6.73

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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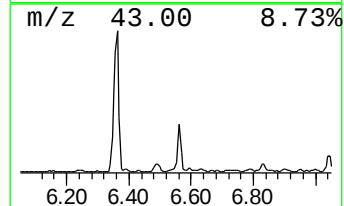
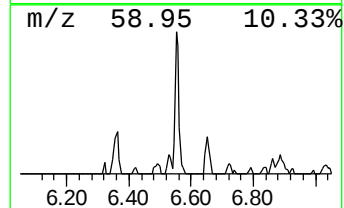
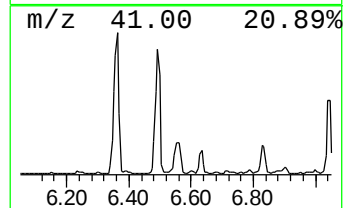
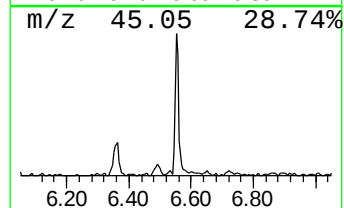
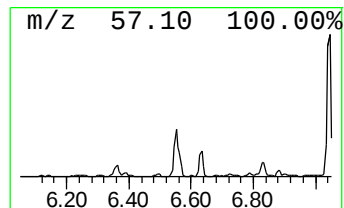
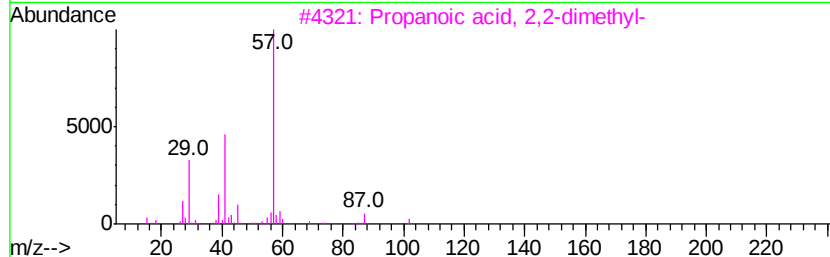
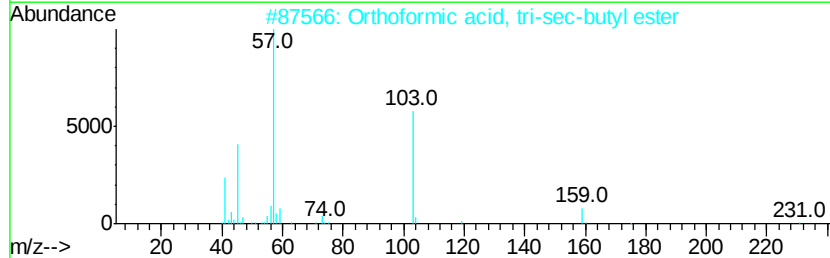
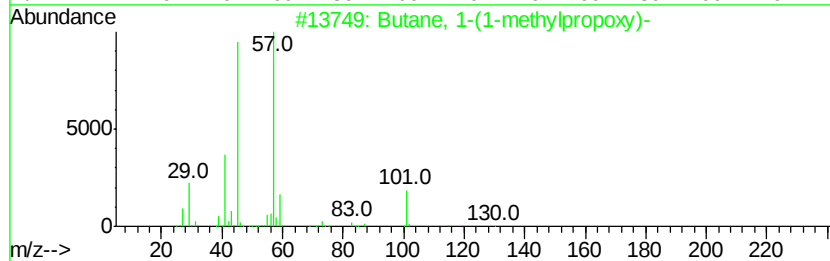
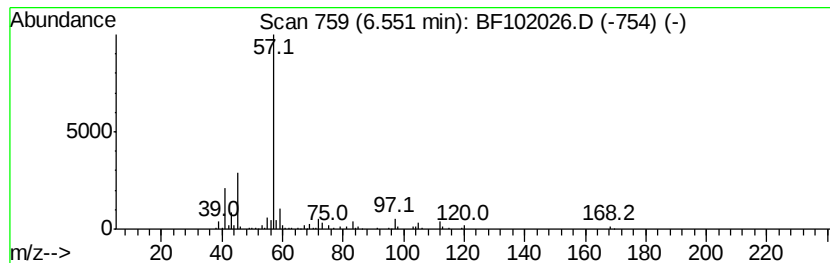
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Peak Number 3 unknown6.55 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	6.75 ng	354794	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	43
2		Orthoformic acid, tri-sec-butyl ...	232	C13H28O3	016754-48-6	42
3		Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	37
4		Nonanal	142	C9H18O	000124-19-6	32
5		Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	32



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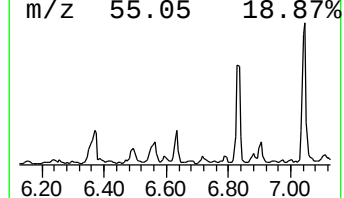
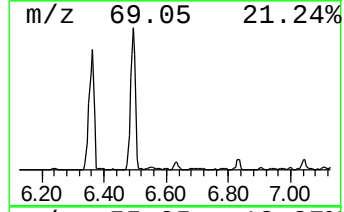
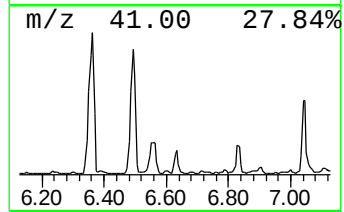
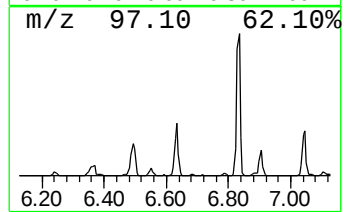
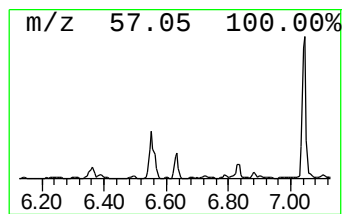
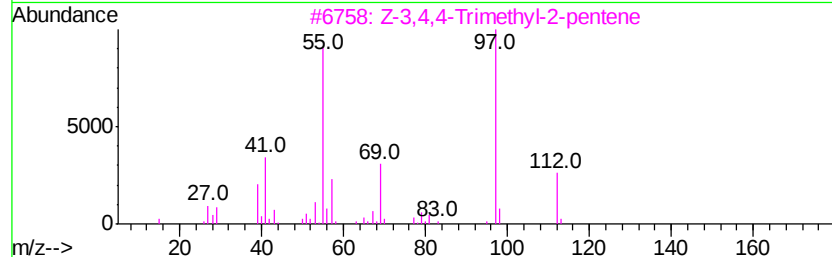
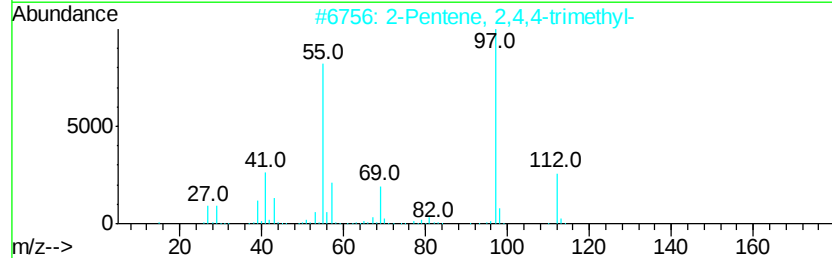
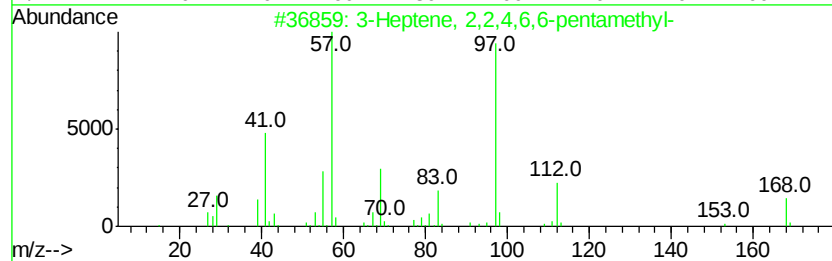
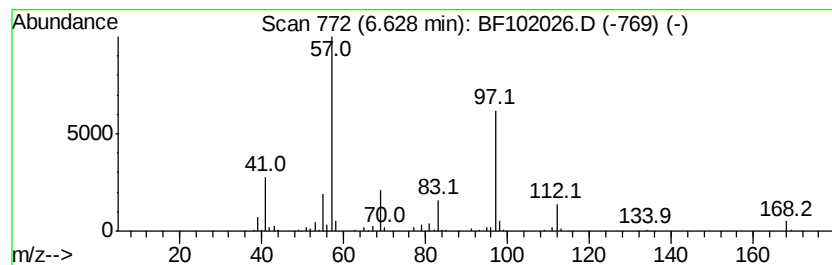
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 3-Heptene, 2,2,4,6,6-pentam... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	3.04 ng	159854	1,4-Dichlorobenzene-d4	6.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Heptene, 2,2,4,6,6-pentamethyl-	168	C12H24	000123-48-8	91
2		2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	68
3		Z-3,4,4-Trimethyl-2-pentene	112	C8H16	039761-64-3	64
4		1H-Pyrazole, 4,5-dihydro-3,5,5-t...	112	C6H12N2	003975-85-7	59
5		Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	59



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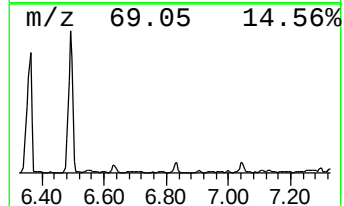
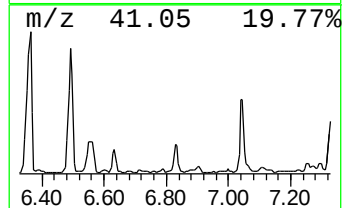
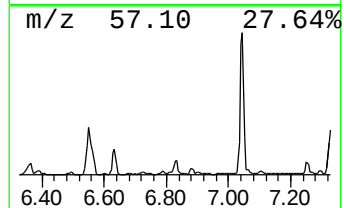
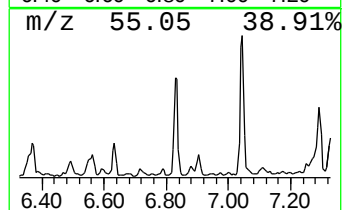
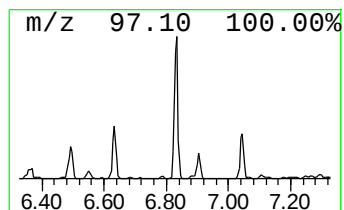
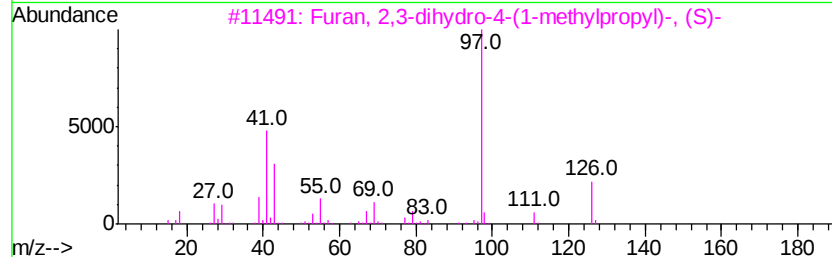
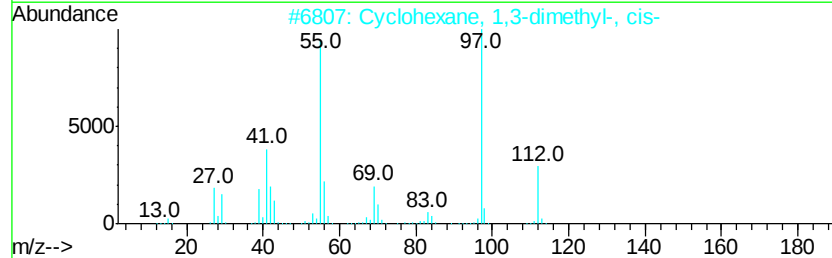
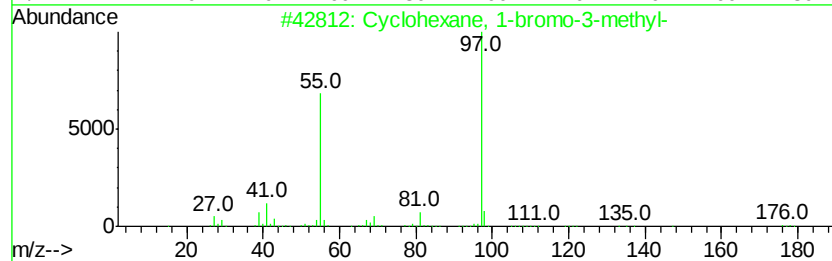
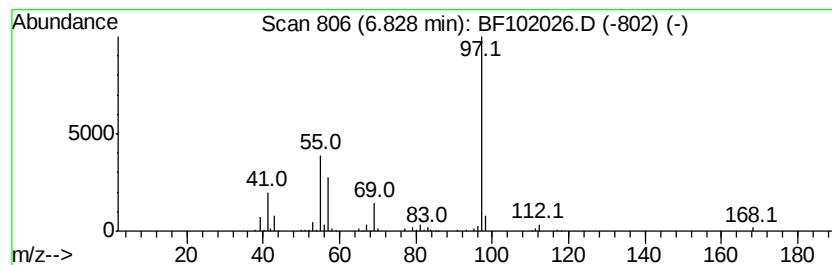
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexane, 1-bromo-3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	4.87 ng	255945	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-bromo-3-methyl-	176	C7H13Br	013905-48-1	64
2		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	56
3		Furan, 2,3-dihydro-4-(1-methylpr...	126	C8H14O	034379-54-9	50
4		3-Pentenoic acid, 2,2,4-trimethyl-	142	C8H14O2	004177-03-1	50
5		Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	50



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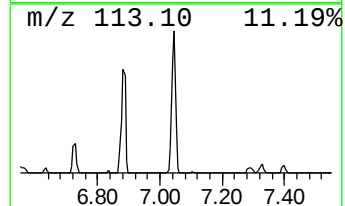
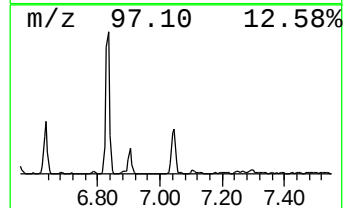
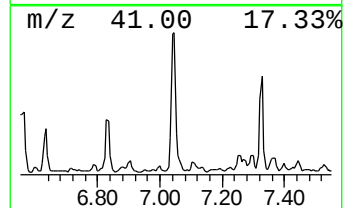
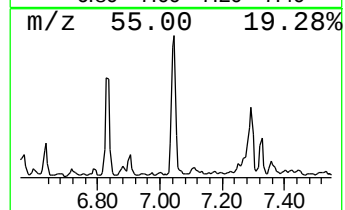
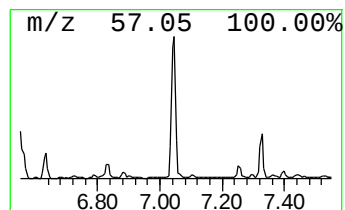
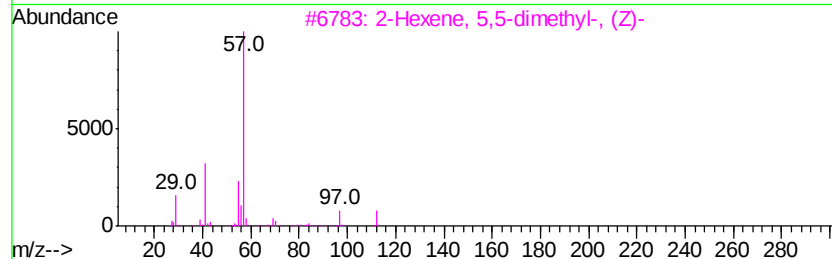
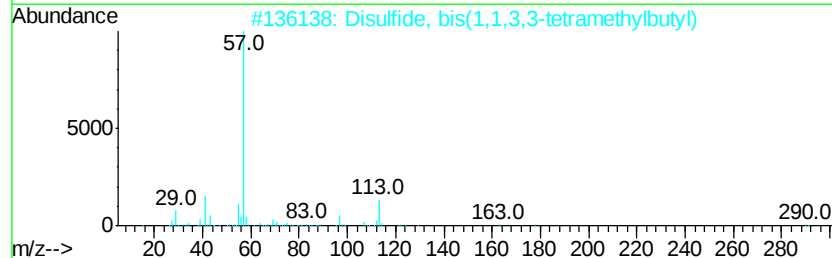
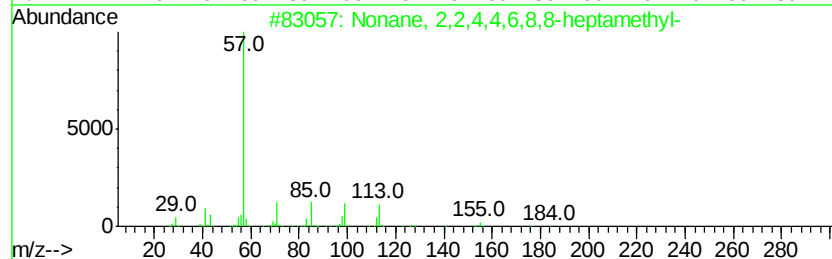
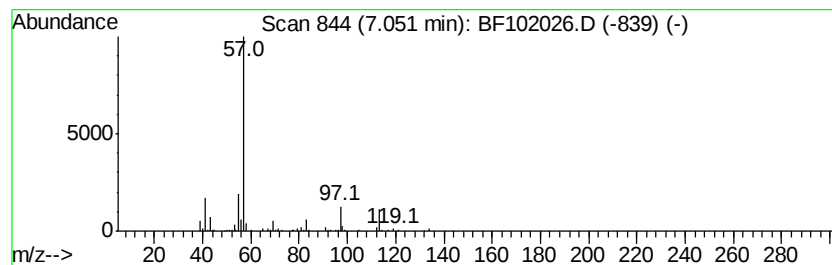
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.05 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	11.19 ng	587697	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	39
2		Disulfide, bis(1,1,3,3-tetrameth...	290	C16H34S2	029956-99-8	28
3		2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	039761-61-0	28
4		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	25
5		2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	25



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011118\
Data File : BF102026.D
Acq On : 11 Jan 2018 18:46
Operator : SJ/JU
Sample : J1067-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27007

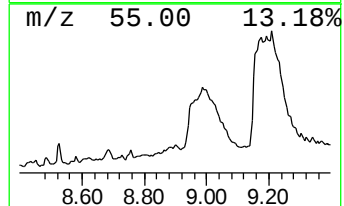
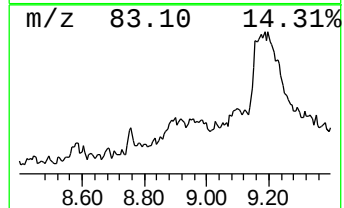
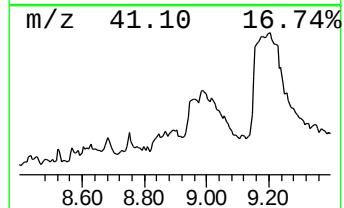
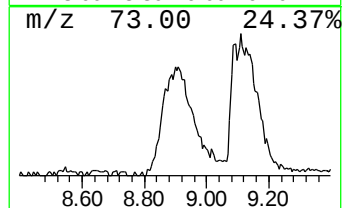
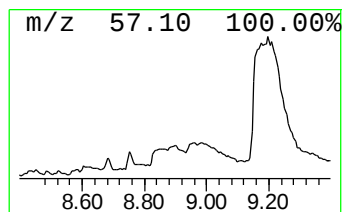
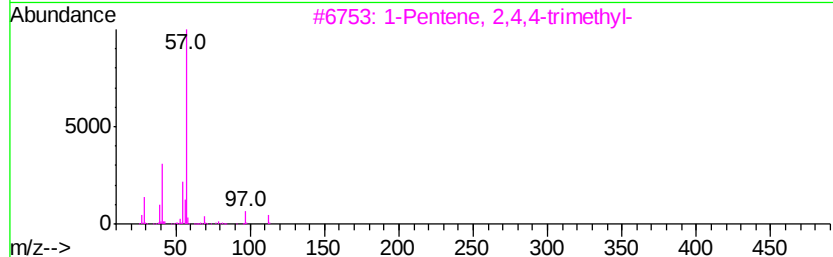
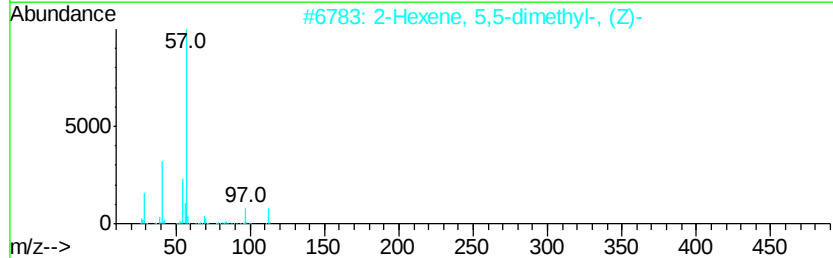
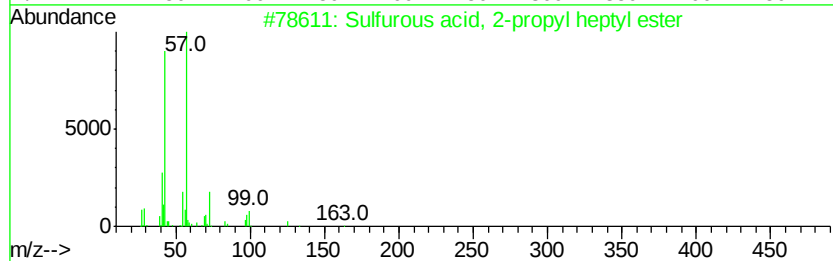
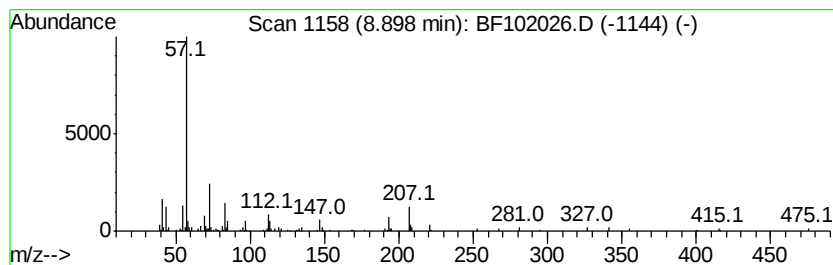
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown8.90 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	6.59 ng	530165	Naphthalene-d8	8.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-propyl heptyl ...	222	C10H22O3S	1000309-11-8	47
2			2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	039761-61-0	14
3			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	14
4			4-Decene, 2,2-dimethyl-, (Z)-	168	C12H24	055499-03-1	14
5			4-Decene, 2,2-dimethyl-, (E)-	168	C12H24	055534-69-5	10



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011118\
Data File : BF102026.D
Acq On : 11 Jan 2018 18:46
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Instrument :
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ClientSampleId :
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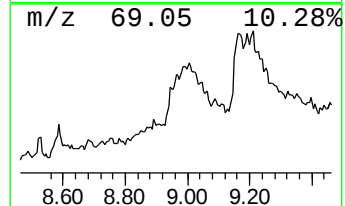
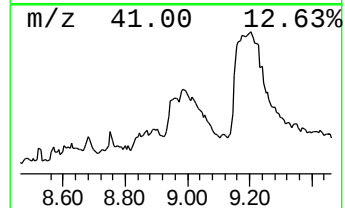
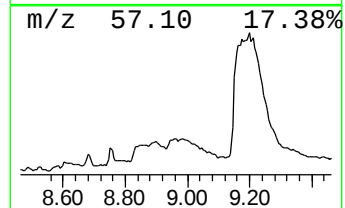
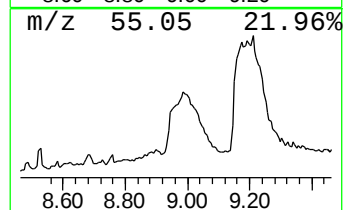
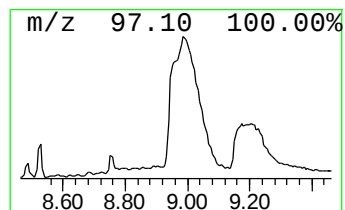
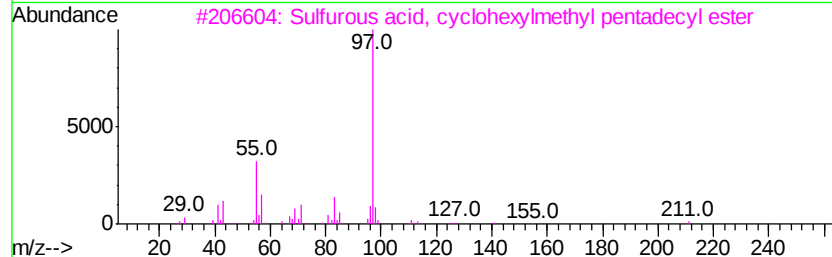
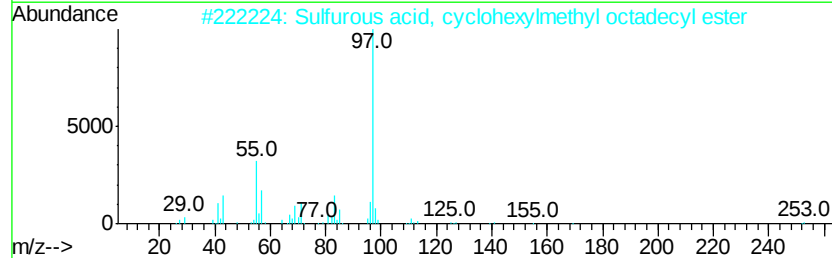
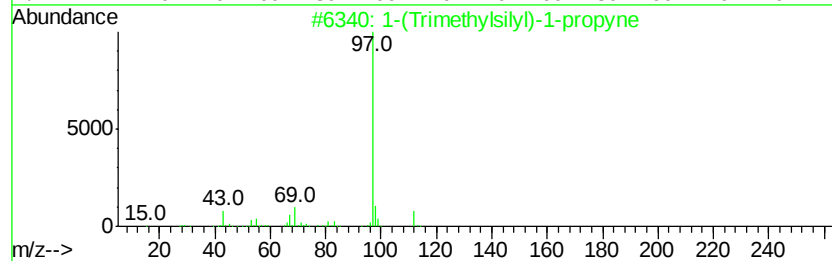
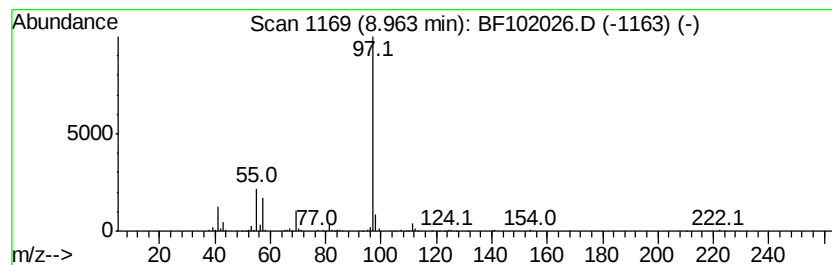
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.96 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.96	26.95 ng	392118	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	39
2		Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	28
3		Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	25
4		Hept-2-ene, 2,4,4,6-tetramethyl-	154	C11H22	103982-58-7	17
5		4H-1,2,4-Triazole, 4-ethyl-	97	C4H7N3	043183-55-7	9



Data Path : U:\HPCHEM1\BNA F\DATA\BF011118\
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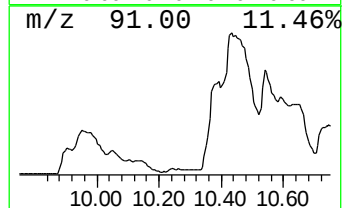
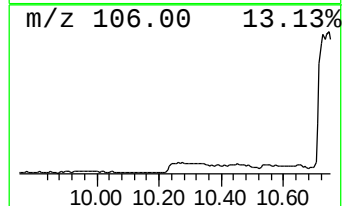
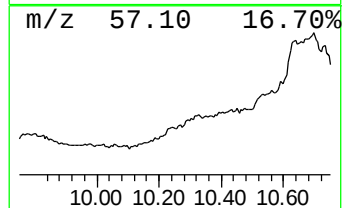
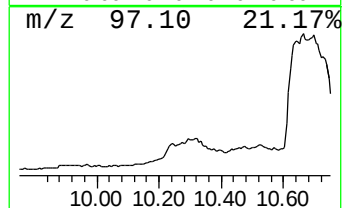
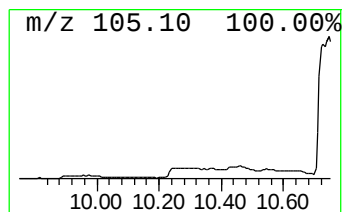
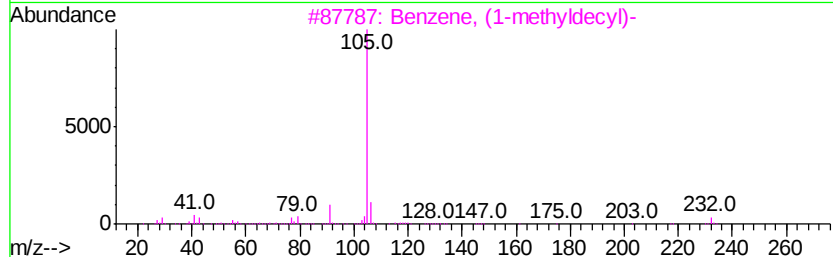
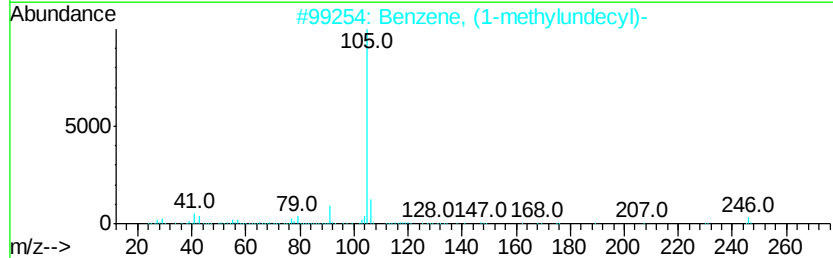
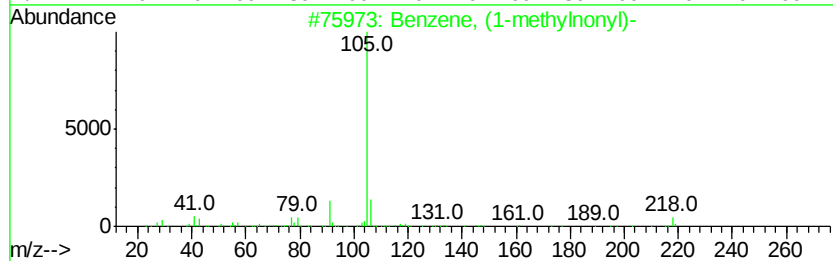
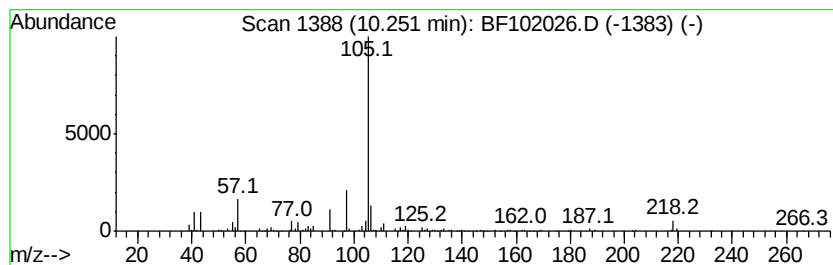
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzene, (1-methylnonyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.25	12.65 ng	184110	Acenaphthene-d10	9.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	64
2	Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	47
3	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	47
4	2-Methylbenzylamine, N,N-dihexyl-	289	C20H35N	1000310-39-7	43
5	Benzene, (1-methylpentyl)-	162	C12H18	006031-02-3	38



Data Path : U:\HPCHEM1\BNA F\DATA\BF011118\
Data File : BF102026.D
Acq On : 11 Jan 2018 18:46
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Sample : J1067-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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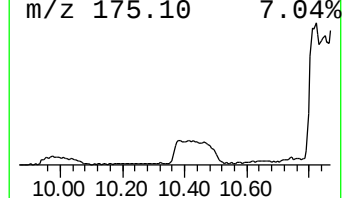
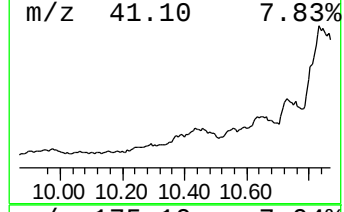
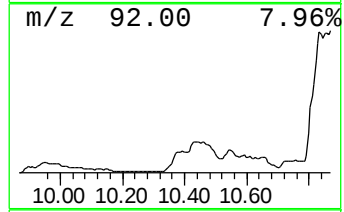
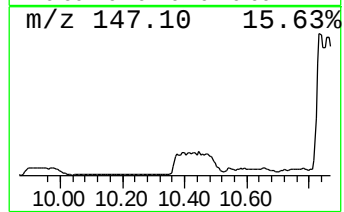
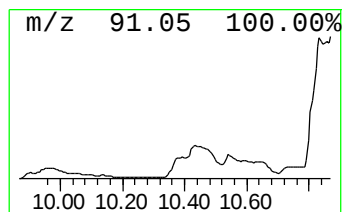
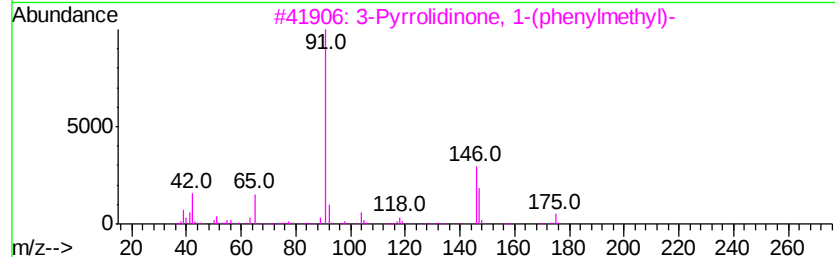
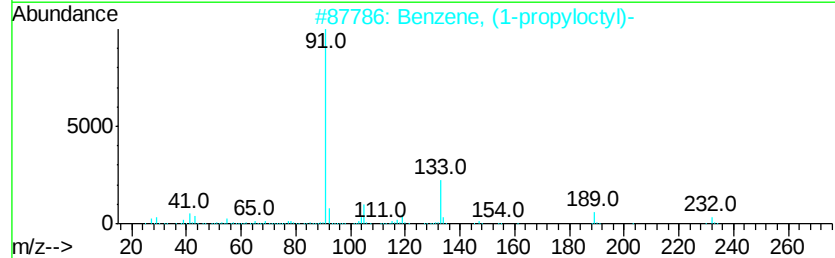
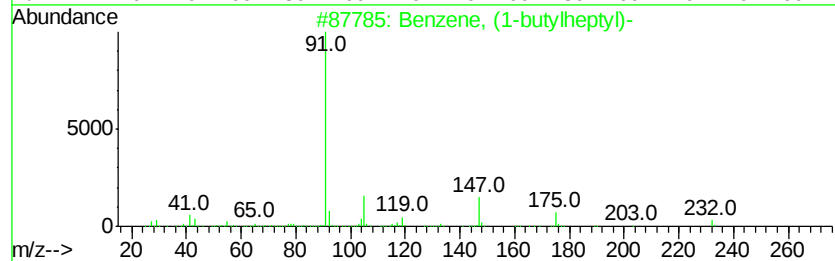
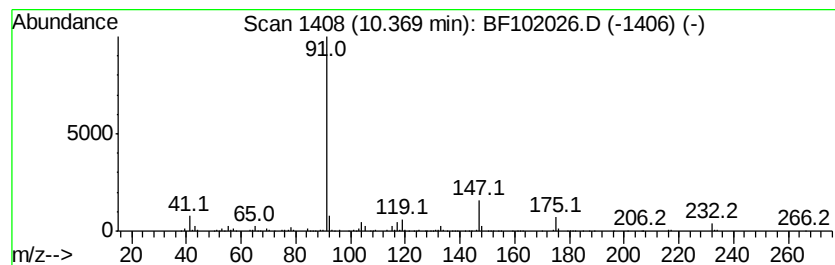
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzene, (1-butylheptyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.37	20.59 ng	299688	Acenaphthene-d10	9.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-butylheptyl)-	232	C17H28	004537-15-9	91
2		Benzene, (1-propyloctyl)-	232	C17H28	004536-86-1	64
3		3-Pyrrolidinone, 1-(phenylmethyl)-	175	C11H13NO	000775-16-6	59
4		Benzene, (1-butylloctyl)-	246	C18H30	002719-63-3	59
5		Benzene, (1-pentylhexyl)-	232	C17H28	004537-14-8	58



Data Path : U:\HPCHEM1\BNA F\DATA\BF011118\
Data File : BF102026.D
Acq On : 11 Jan 2018 18:46
Operator : SJ/JU
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Misc :
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Instrument :
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ClientSampleId :
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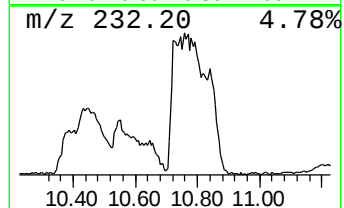
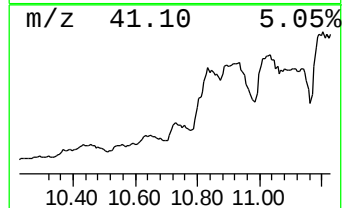
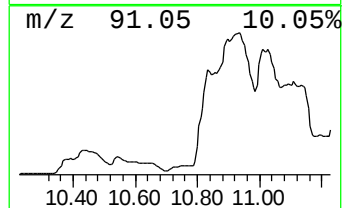
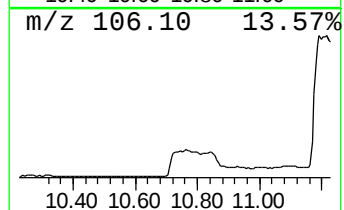
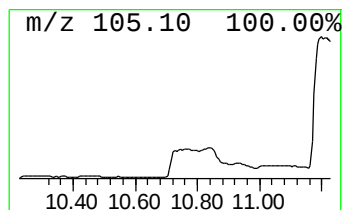
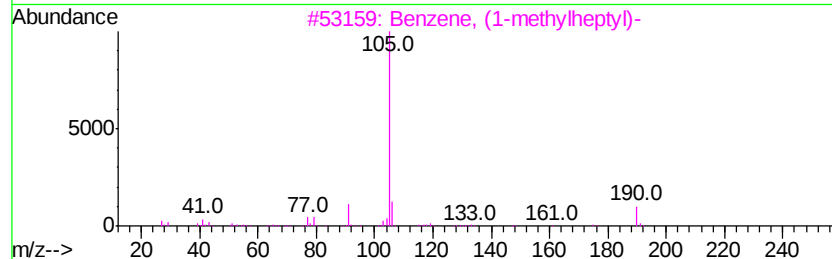
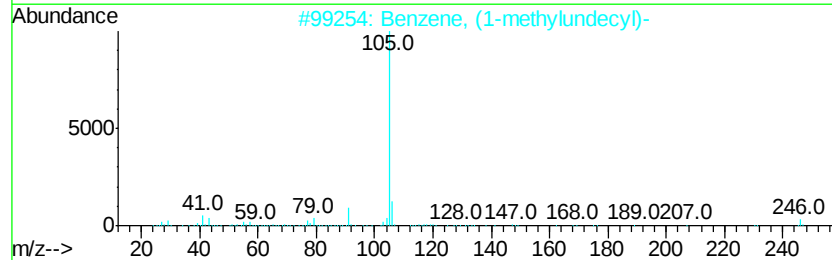
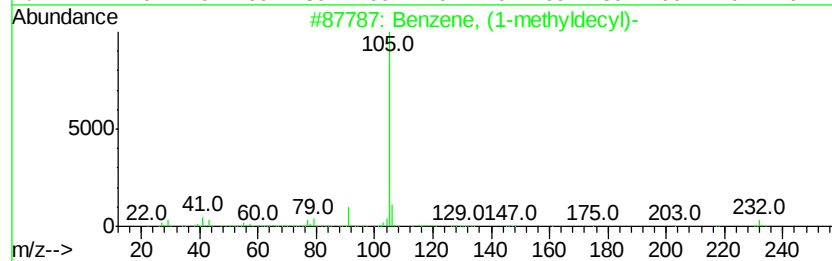
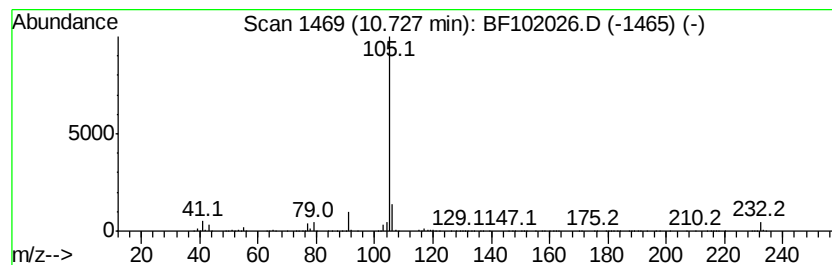
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzene, (1-methyldecyl)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	3.67 ng	1492580	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-methyldecyl)-	232	C17H28	004536-88-3	91
2		Benzene, (1-methylundecyl)-	246	C18H30	002719-61-1	72
3		Benzene, (1-methylheptyl)-	190	C14H22	000777-22-0	72
4		Benzene, (1-methylnonyl)-	218	C16H26	004537-13-7	72
5		1-Hexene, 3-methyl-6-phenyl-4-(1...	294	C21H26O	1000194-52-4	72



Data Path : U:\HPCHEM1\BNA F\DATA\BF011118\
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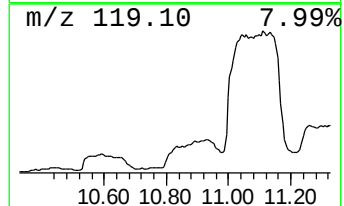
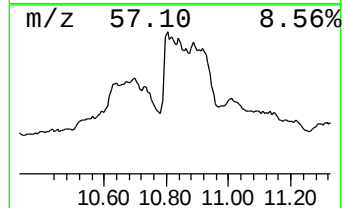
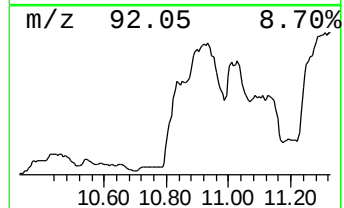
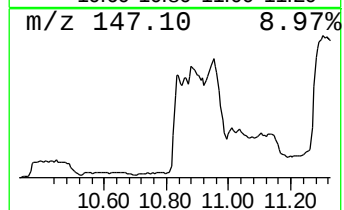
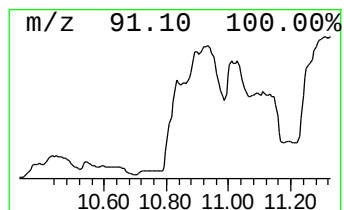
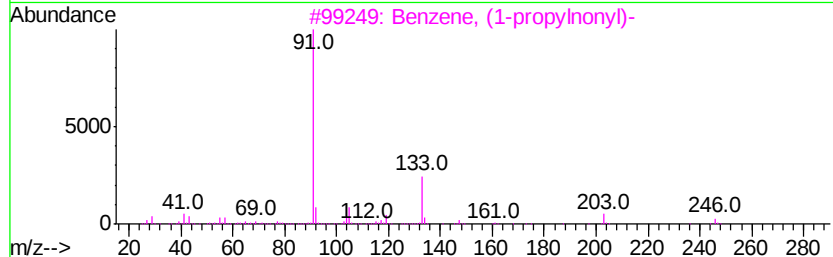
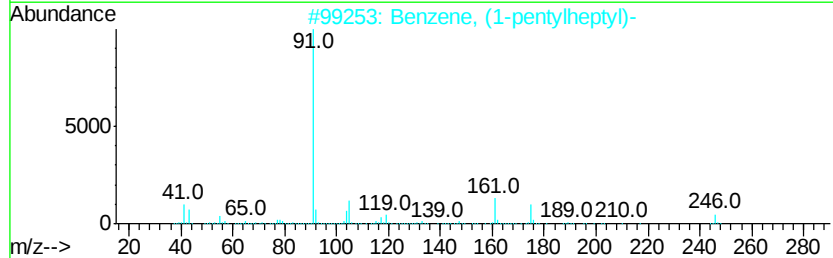
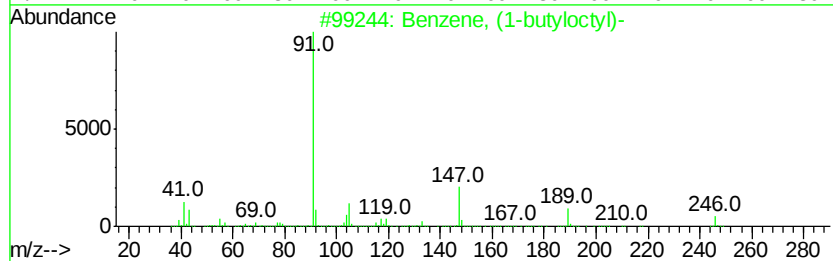
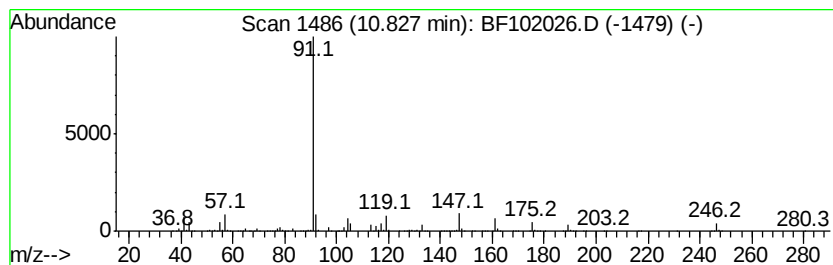
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzene, (1-butyloctyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	30.75 ng	12518300	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (1-butyloctyl)-	246	C18H30	002719-63-3	81
2		Benzene, (1-pentylheptyl)-	246	C18H30	002719-62-2	68
3		Benzene, (1-propylnonyl)-	246	C18H30	002719-64-4	64
4		Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	52
5		Benzene, (1-propyldecyl)-	260	C19H32	004534-51-4	47



Data Path : U:\HPCHEM1\BNA F\DATA\BF011118\
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Operator : SJ/JU
Sample : J1067-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

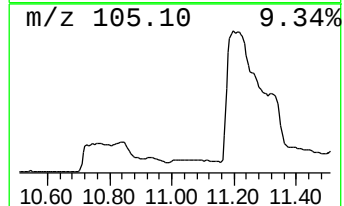
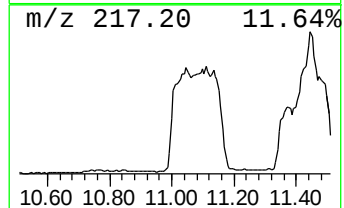
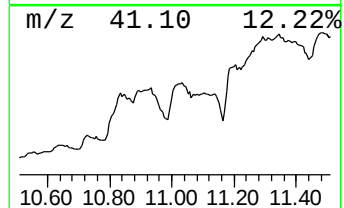
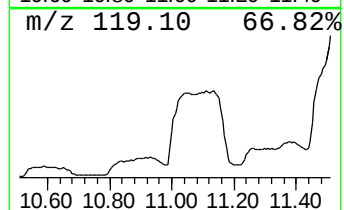
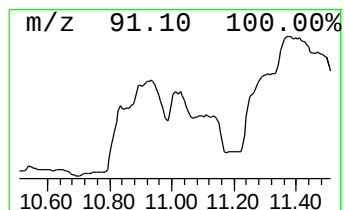
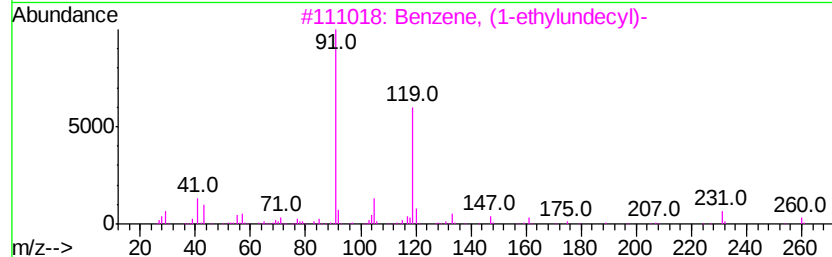
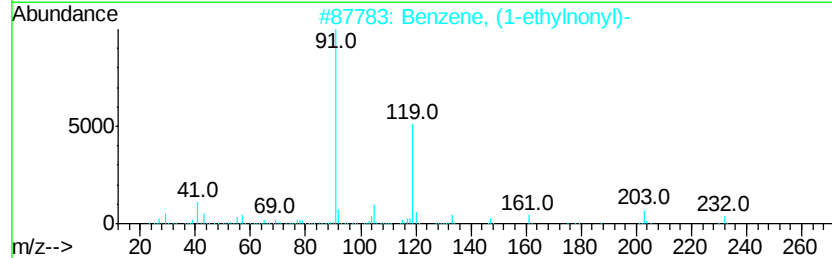
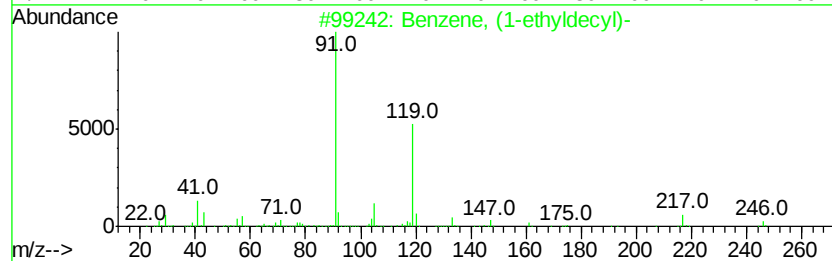
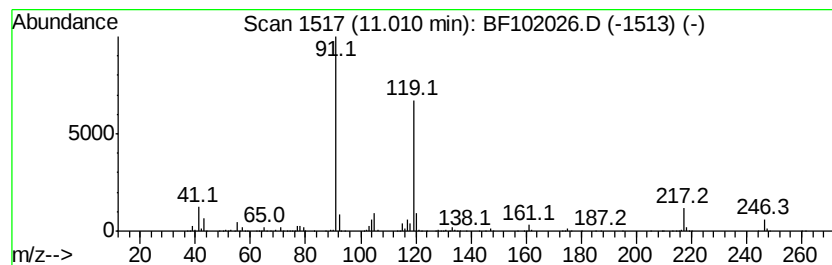
Instrument :
BNA_F
ClientSampleId :
CHRT-27007

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzene, (1-ethyldecyl)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.01	5.87 ng	2389400	Phenanthrene-d10		11.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-ethyldecyl)-	246	C18H30	002400-00-2	93
2	Benzene, (1-ethylnonyl)-	232	C17H28	004536-87-2	72
3	Benzene, (1-ethylundecyl)-	260	C19H32	004534-52-5	64
4	Benzene, (1-ethyloctyl)-	218	C16H26	004621-36-7	59
5	Benzene, (1,1-dimethyldecyl)-	246	C18H30	027854-40-6	53



Data Path : U:\HPCHEM1\BNA_F\DATA\BF011118\
Data File : BF102026.D
Acq On : 11 Jan 2018 18:46
Operator : SJ/JU
Sample : J1067-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHRT-27007

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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
2-Pentanone, 4-hy...	4.90	7.6 ng		397679	1	6.73	1050500	20.0
unknown6.49	6.49	85.1 ng		4467990	1	6.73	1050500	20.0
unknown6.55	6.55	6.8 ng		354794	1	6.73	1050500	20.0
3-Heptene, 2,2,4,...	6.63	3.0 ng		159854	1	6.73	1050500	20.0
Cyclohexane, 1-br...	6.83	4.9 ng		255945	1	6.73	1050500	20.0
unknown7.05	7.05	11.2 ng		587697	1	6.73	1050500	20.0
unknown8.90	8.90	6.6 ng		530165	2	8.01	1609240	20.0
unknown8.96	8.96	26.9 ng		392118	3	9.81	291039	20.0
Benzene, (1-methy...	10.25	12.7 ng		184110	3	9.81	291039	20.0
Benzene, (1-butyl...	10.37	20.6 ng		299688	3	9.81	291039	20.0
Benzene, (1-methy...	10.73	3.7 ng		1492580	4	11.23	8141600	20.0
Benzene, (1-butyl...	10.83	30.8 ng		12518300	4	11.23	8141600	20.0
Benzene, (1-ethyl...	11.01	5.9 ng		2389400	4	11.23	8141600	20.0