

Data Path : Z:\HPCHEM1\BNA M\DATA\BM020818\
 Data File : BM014198.D
 Acq On : 08 Feb 2018 18:10
 Operator : SJ/JU
 Sample : J1490-06
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 265578-SEGMENT-2C

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:\HPCHEM1\BNA_M\METHODS\8270-BM020718.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	3.434	72	76	82	rBV	216302	250361	2.87%	0.589%
2	5.087	352	357	364	rBV2	55180	91283	1.05%	0.215%
3	5.163	364	370	375	rVV	991808	1440365	16.54%	3.390%
4	5.216	375	379	389	rVB	189132	387080	4.44%	0.911%
5	5.581	434	441	446	rBV2	71090	115337	1.32%	0.271%
6	6.734	630	637	649	rBV	578628	1017648	11.68%	2.395%
7	7.081	689	696	713	rBV	2183113	3405114	39.09%	8.013%
8	7.540	768	774	784	rBV	420133	646898	7.43%	1.522%
9	7.857	820	828	842	rVB	2165106	3431976	39.40%	8.076%
10	8.334	904	909	921	rBV3	57299	147719	1.70%	0.348%
11	8.698	964	971	982	rBV	1652703	2788505	32.01%	6.562%
12	10.316	1237	1246	1251	rBV	488081	849575	9.75%	1.999%
13	10.369	1251	1255	1266	rVB5	122546	274770	3.15%	0.647%
14	11.992	1526	1531	1536	rBV3	52232	119660	1.37%	0.282%
15	12.216	1560	1569	1575	rBV6	49155	128647	1.48%	0.303%
16	12.810	1662	1670	1679	rBV	4211191	6154809	70.66%	14.484%
17	13.669	1809	1816	1822	rBV2	67767	118766	1.36%	0.279%
18	14.198	1898	1906	1912	rBV2	715509	1102732	12.66%	2.595%
19	14.263	1912	1917	1923	rVB	118386	178789	2.05%	0.421%
20	14.745	1991	1999	2006	rBV	418550	679902	7.81%	1.600%
21	15.257	2081	2086	2090	rBV2	59052	90139	1.03%	0.212%
22	15.698	2154	2161	2173	rBV	3379348	4924629	56.53%	11.589%
23	16.480	2290	2294	2300	rBV2	61473	111654	1.28%	0.263%
24	16.957	2367	2375	2381	rBV	884841	1320695	15.16%	3.108%
25	17.862	2523	2529	2534	rBV3	140104	230588	2.65%	0.543%
26	17.980	2545	2549	2555	rBV2	251844	365308	4.19%	0.860%
27	18.204	2582	2587	2594	rBV7	58239	115710	1.33%	0.272%
28	18.586	2648	2652	2662	rBV5	146169	299029	3.43%	0.704%
29	19.151	2745	2748	2754	rBV5	111636	157524	1.81%	0.371%
30	19.598	2819	2824	2832	rBV	6859938	8710821	100.00%	20.499%
31	21.162	3085	3090	3097	rVB	1104134	1466277	16.83%	3.451%
32	23.339	3454	3460	3468	rBV2	703685	1372177	15.75%	3.229%

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ALS Vial : 14 Sample Multiplier: 1

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

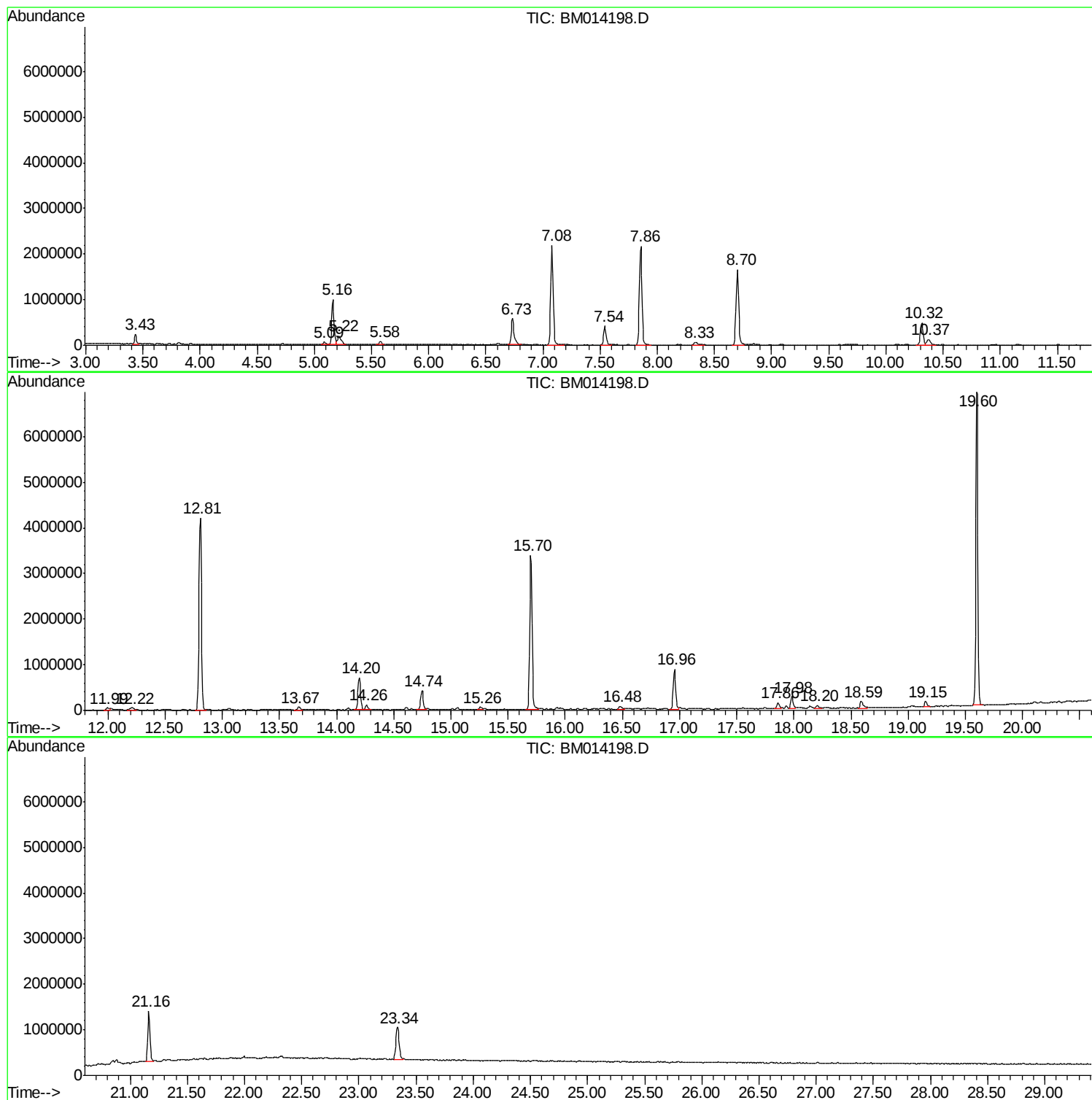
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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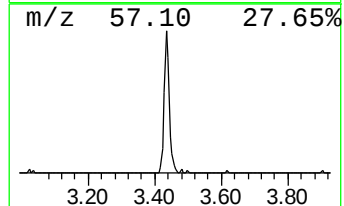
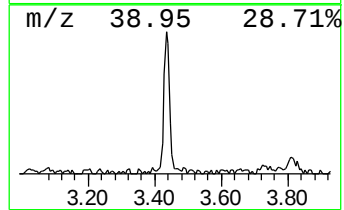
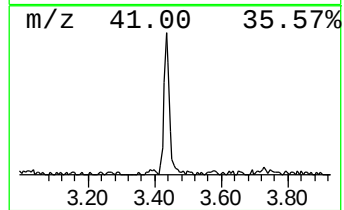
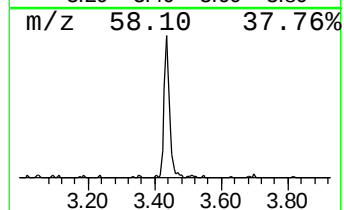
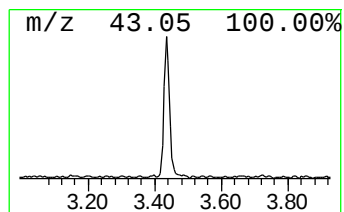
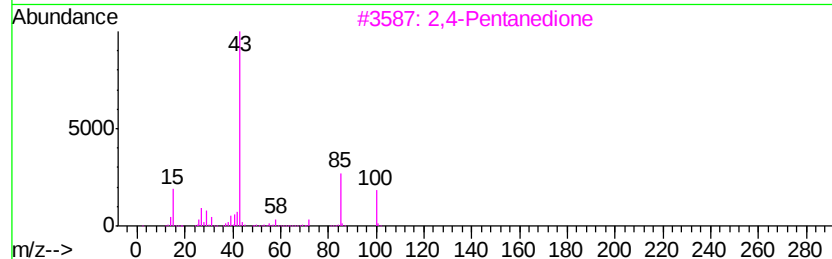
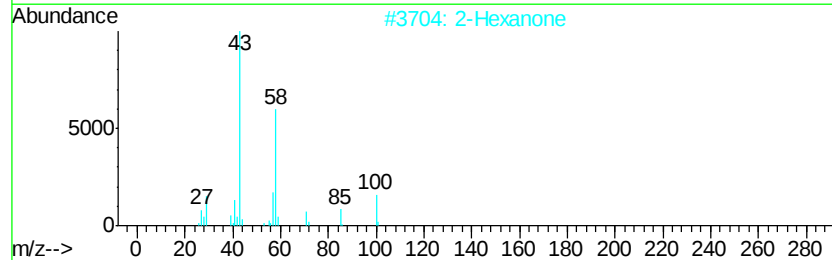
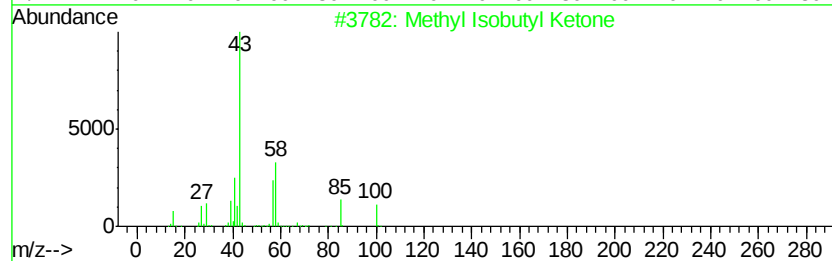
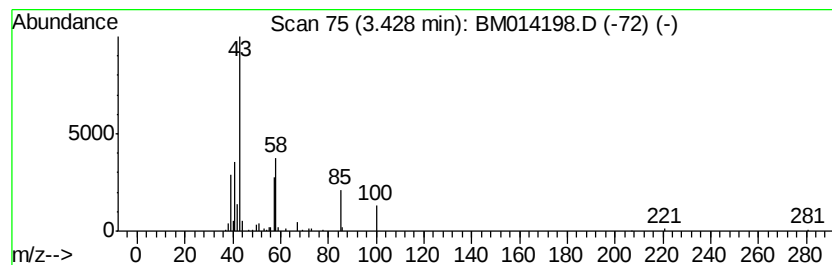
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Methyl Isobutyl Ketone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.43	7.74 ng	250361	1,4-Dichlorobenzene-d4	7.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	83
2			2-Hexanone	100	C6H12O	000591-78-6	64
3			2,4-Pentanedione	100	C5H8O2	000123-54-6	38
4			Octane	114	C8H18	000111-65-9	32
5			2,3-Pentanedione	100	C5H8O2	000600-14-6	27



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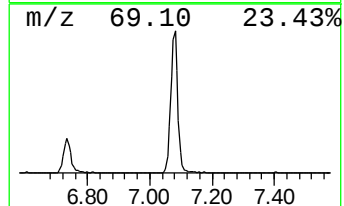
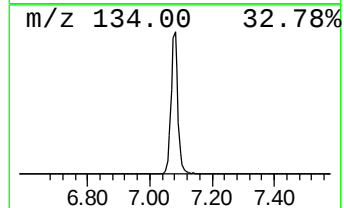
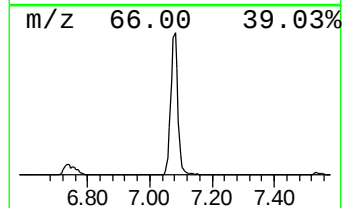
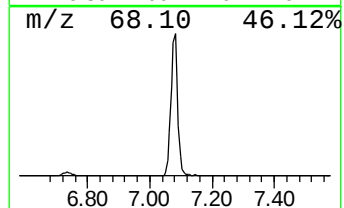
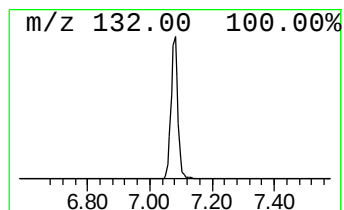
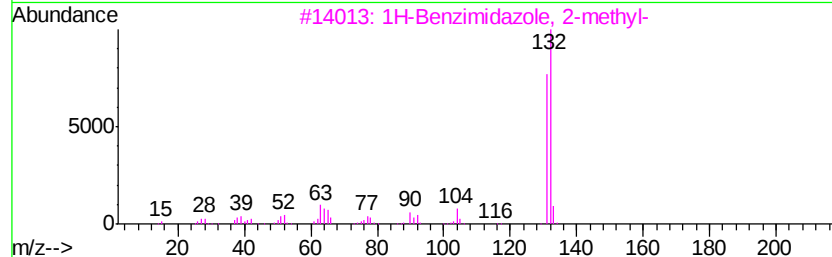
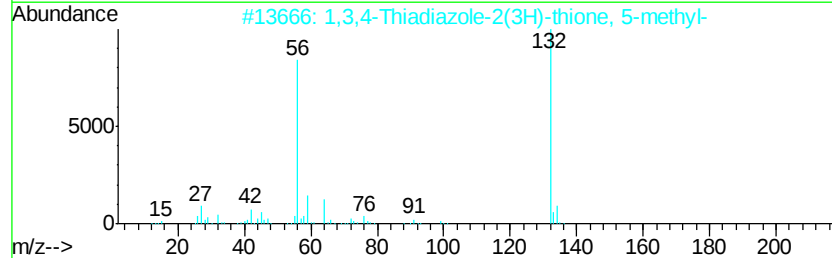
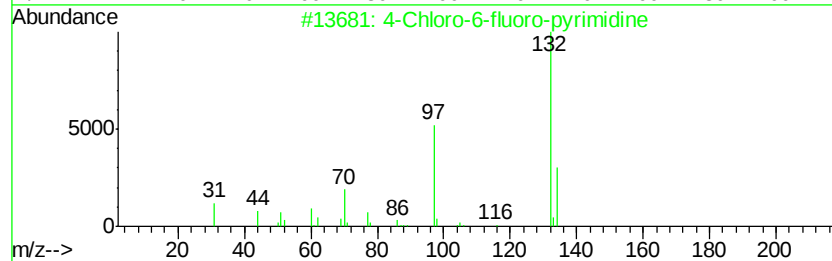
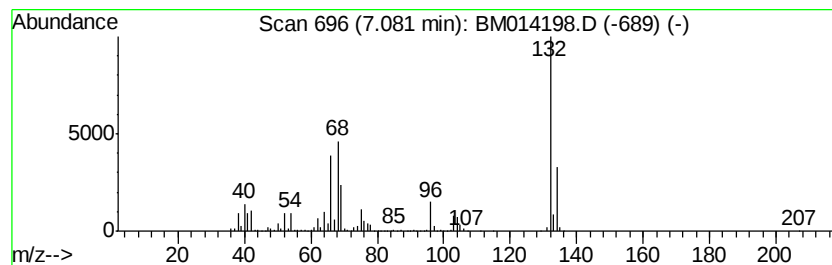
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.08 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	105.28 ng	3405110	1,4-Dichlorobenzene-d4	7.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12



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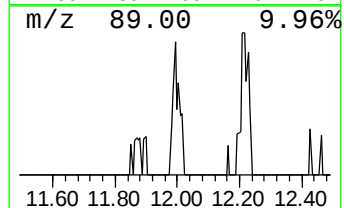
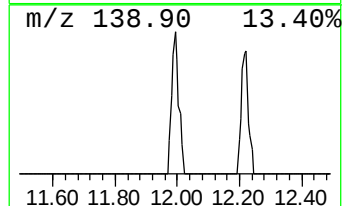
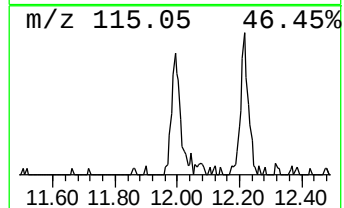
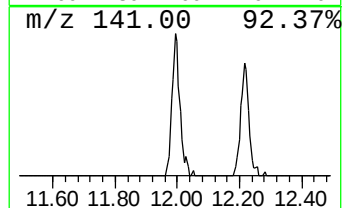
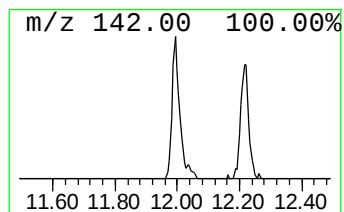
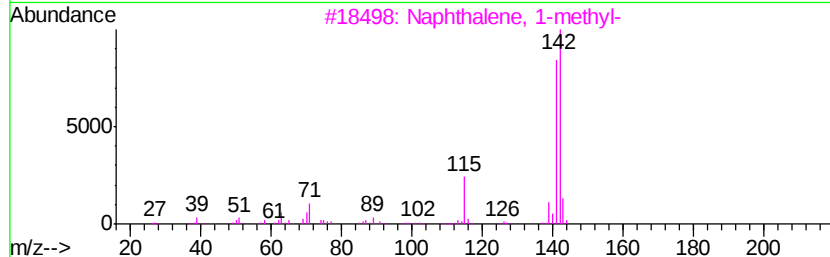
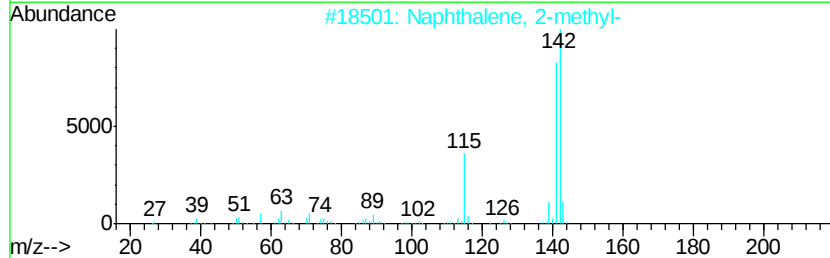
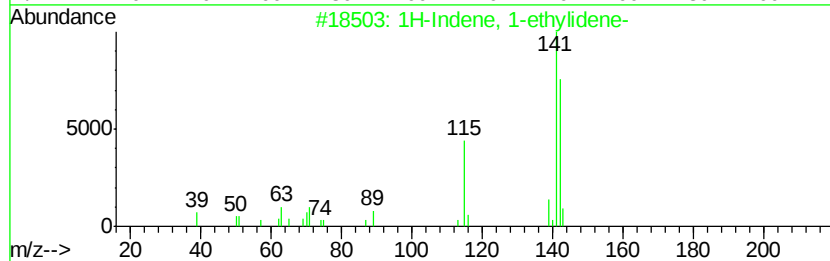
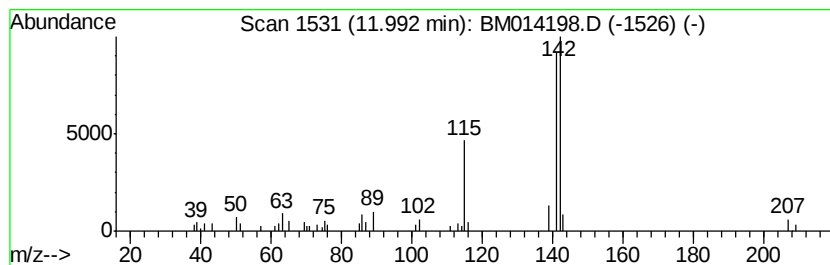
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1H-Indene, 1-ethylidene- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.82 ng	119660	Naphthalene-d8	10.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	91
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	91
3		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5		Benzocycloheptatriene	142	C11H10	000264-09-5	91



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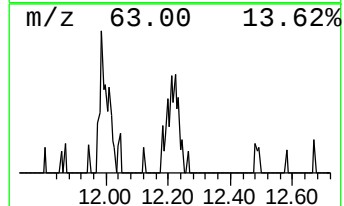
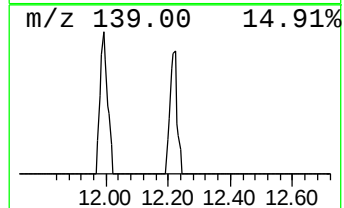
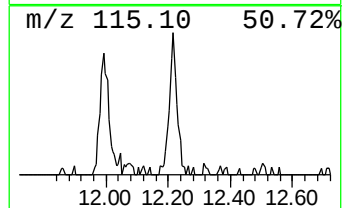
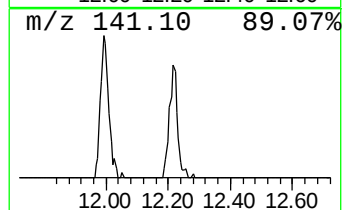
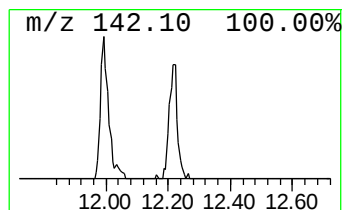
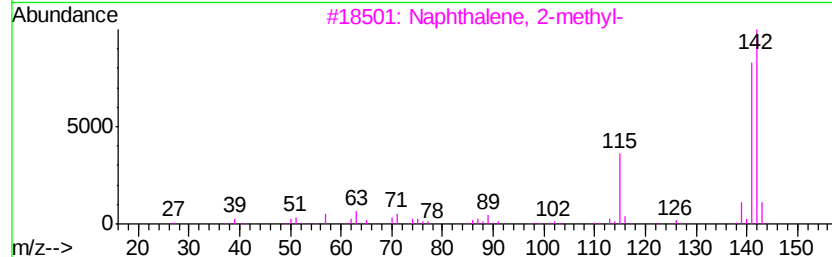
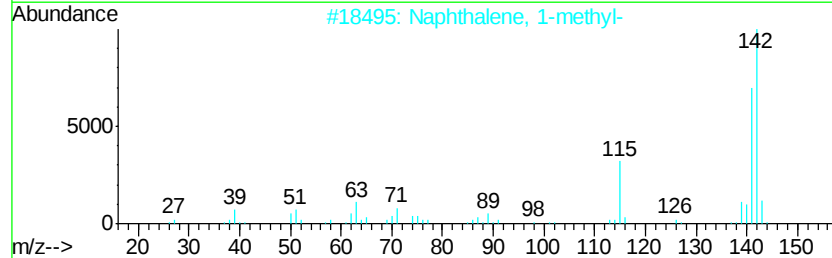
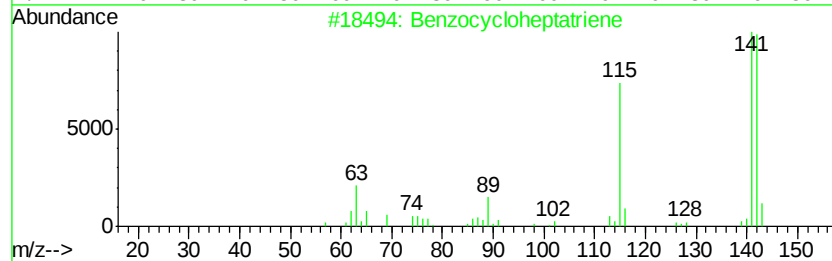
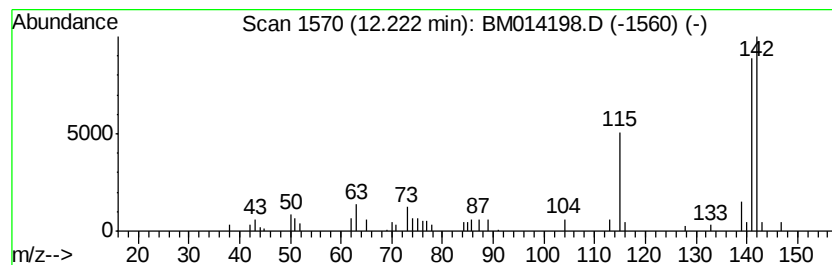
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzocycloheptatriene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.22	3.03 ng	128647	Naphthalene-d8	10.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzocycloheptatriene	142	C11H10	000264-09-5	87
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	87
3		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	83
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	83
5		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	74



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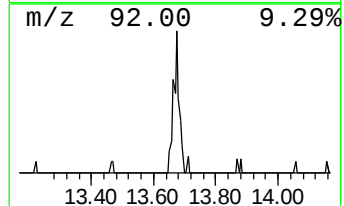
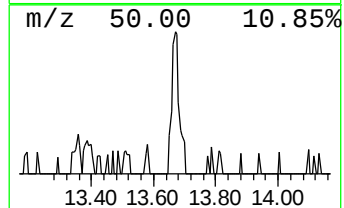
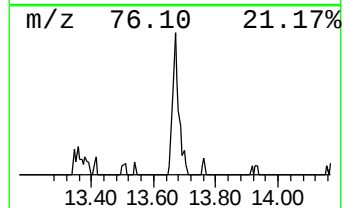
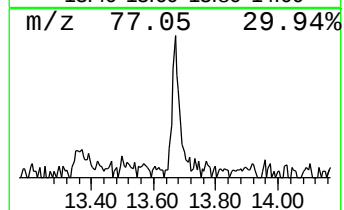
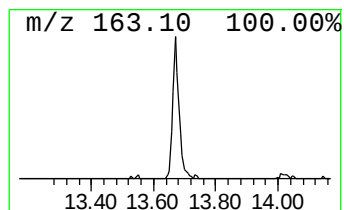
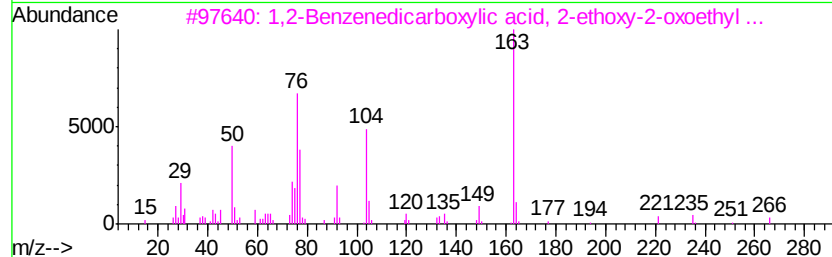
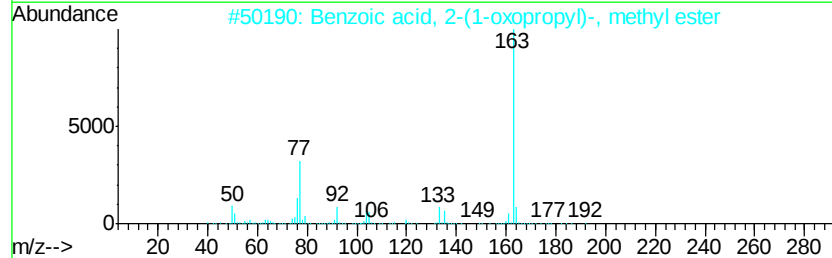
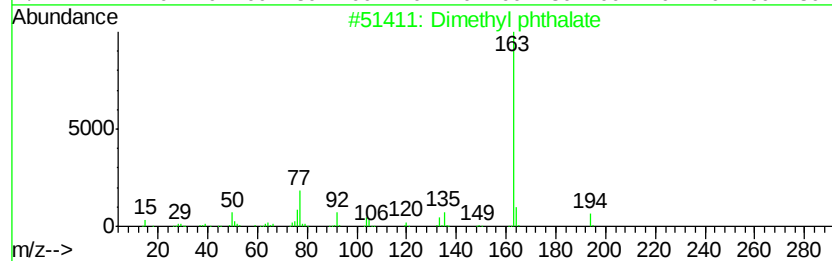
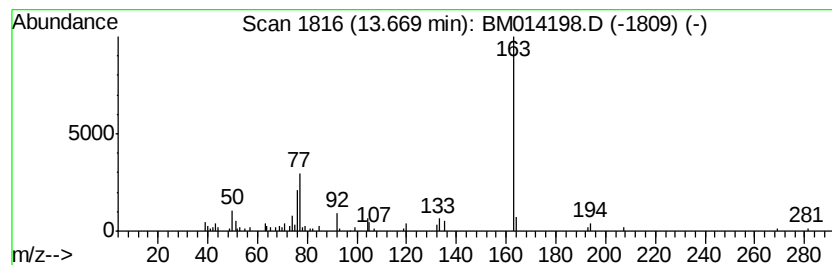
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Peak Number 9 Dimethyl phthalate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	2.15 ng	118766	Acenaphthene-d10	14.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dimethyl phthalate	194	C10H10O4	000131-11-3	87
2		Benzoic acid, 2-(1-oxopropyl)-, ...	192	C11H12O3	032025-37-9	72
3		1,2-Benzenedicarboxylic acid, 2-...	266	C13H14O6	000085-71-2	56
4		Methyl 2-ethylhexyl phthalate	292	C17H24O4	056166-83-7	50
5		1-Amino-4,6-dimethyl-2-oxo-1,2-d...	163	C8H9N3O	001562-12-5	47



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Misc :
ALS Vial : 14 Sample Multiplier: 1

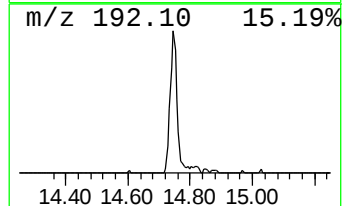
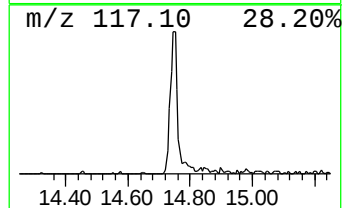
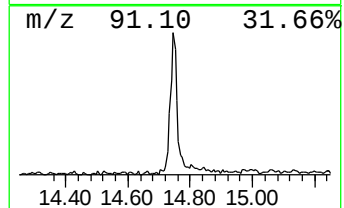
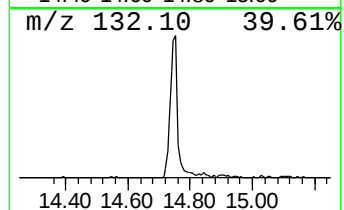
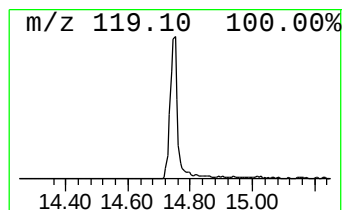
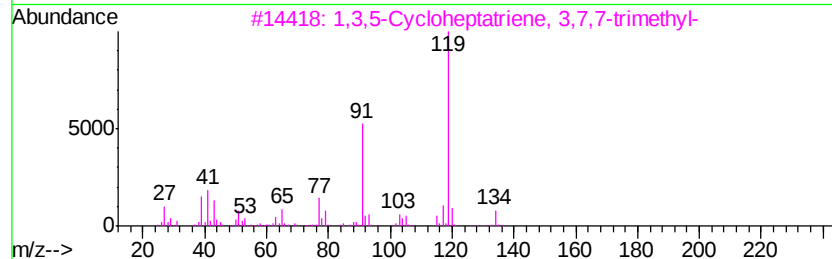
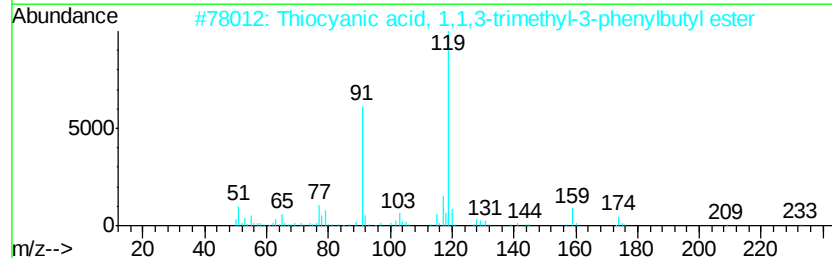
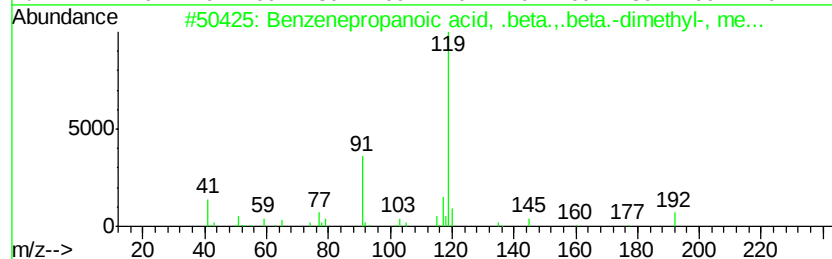
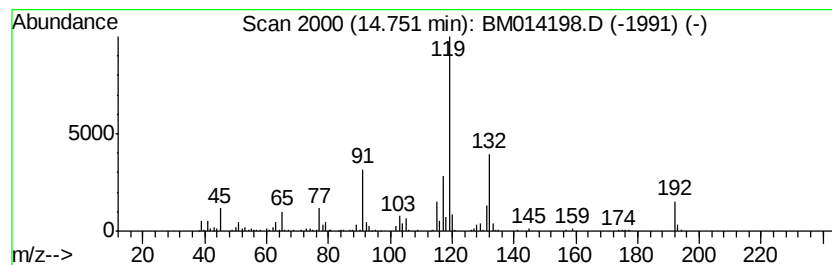
Instrument :
BNA_M
ClientSampleId :
265578-SEGMENT-2C

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM020718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown14.75 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	12.33 ng	679902	Acenaphthene-d10	14.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzenepropanoic acid, .beta.,.b...	192 C12H16O2	025080-84-6 47
2		Thiocyanic acid, 1,1,3-trimethyl...	233 C14H19NS	1000293-27-7 43
3		1,3,5-Cycloheptatriene, 3,7,7-tr...	134 C10H14	003479-89-8 43
4		Benzenebutanoic acid, 2,5-dimethyl-	192 C12H16O2	001453-06-1 43
5		Benzenepropanoic acid, .beta.,.b...	178 C11H14O2	001010-48-6 43



Data Path : Z:\HPCHEM1\BNA M\DATA\BM020818\
Data File : BM014198.D
Acq On : 08 Feb 2018 18:10
Operator : SJ/JU
Sample : J1490-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
265578-SEGMENT-2C

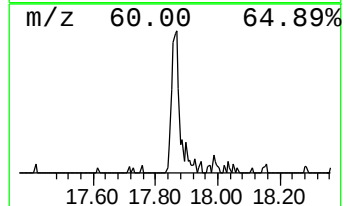
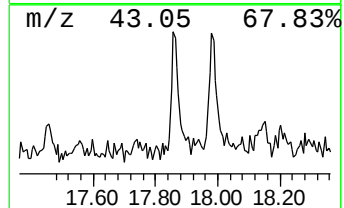
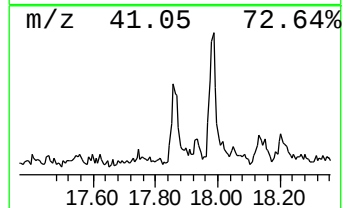
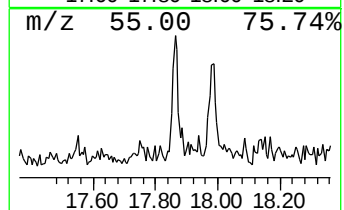
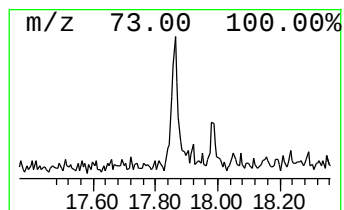
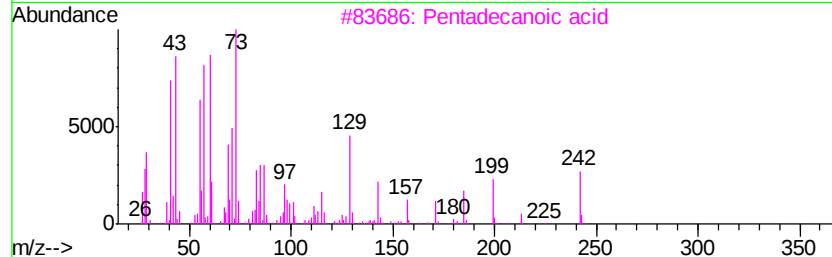
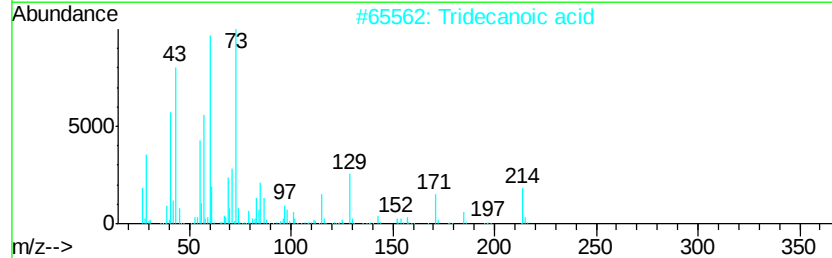
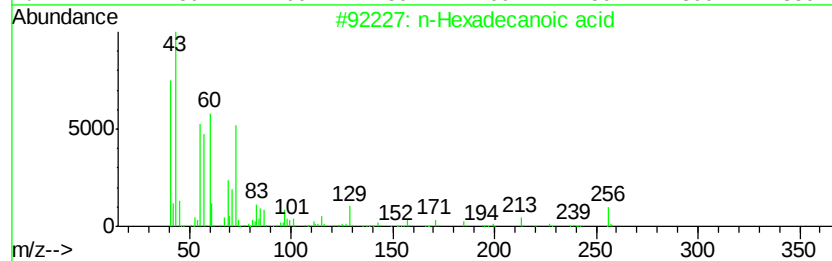
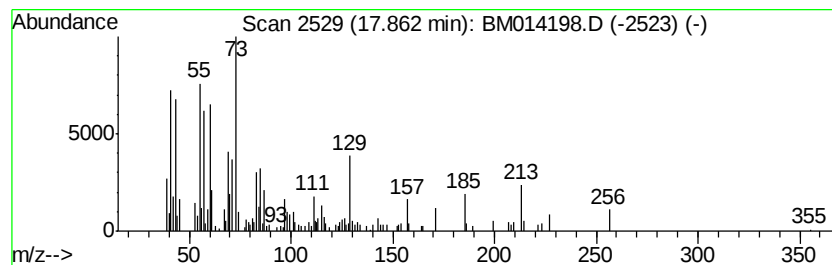
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.86	3.49 ng	230588	Phenanthrene-d10	16.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



Data Path : Z:\HPCHEM1\BNA M\DATA\BM020818\
Data File : BM014198.D
Acq On : 08 Feb 2018 18:10
Operator : SJ/JU
Sample : J1490-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
265578-SEGMENT-2C

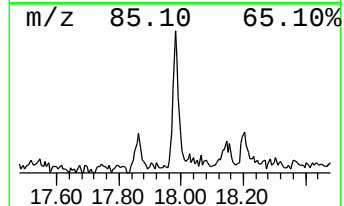
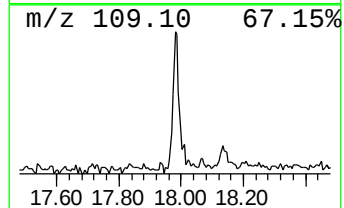
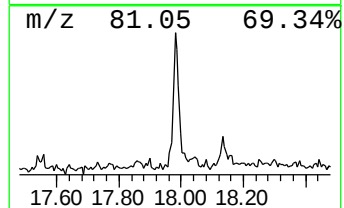
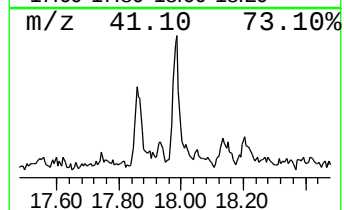
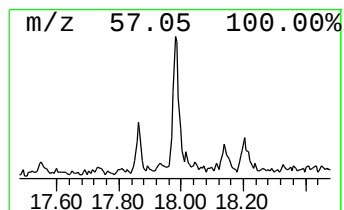
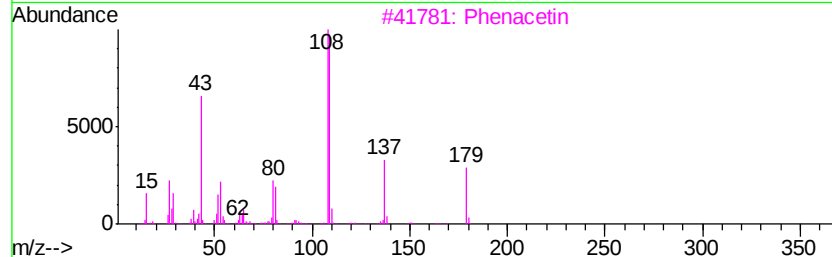
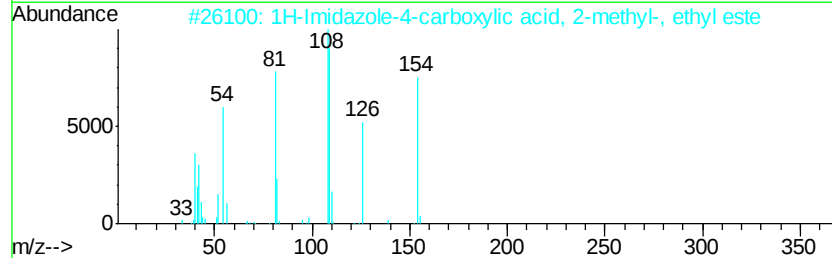
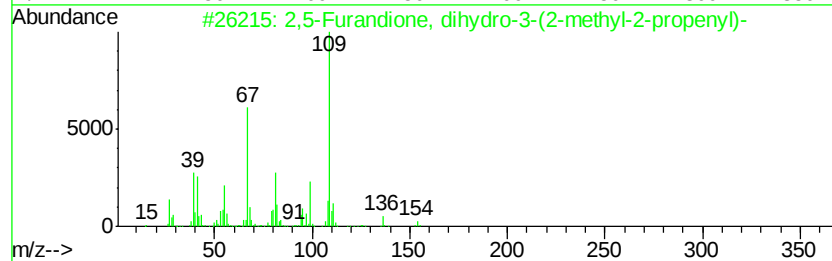
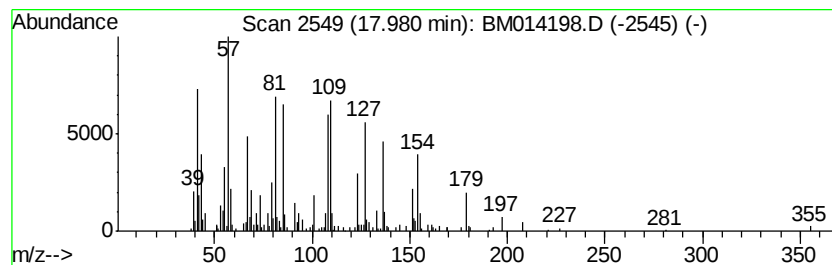
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.98 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	5.53 ng	365308	Phenanthrene-d10	16.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Furandione, dihydro-3-(2-met...	154	C8H10O3	018908-20-8	27
2			1H-Imidazole-4-carboxylic acid, ...	154	C7H10N2O2	087326-25-8	25
3			Phenacetin	179	C10H13NO2	000062-44-2	18
4			5-Fluoro-2-methylbenzoic acid	154	C8H7FO2	033184-16-6	16
5			3-Methyl-4-nitro-hex-4-enoic acid	173	C7H11NO4	1000186-07-0	14



Data Path : Z:\HPCHEM1\BNA M\DATA\BM020818\
Data File : BM014198.D
Acq On : 08 Feb 2018 18:10
Operator : SJ/JU
Sample : J1490-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
265578-SEGMENT-2C

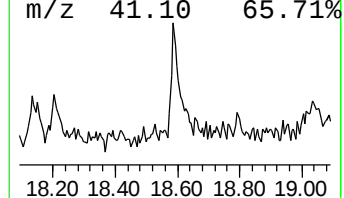
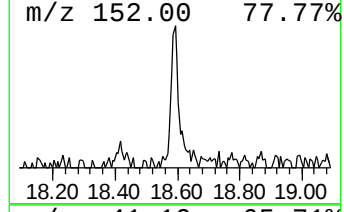
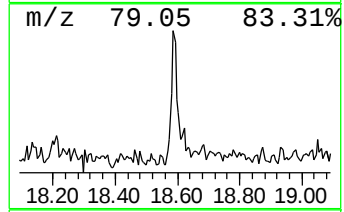
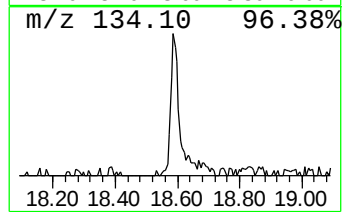
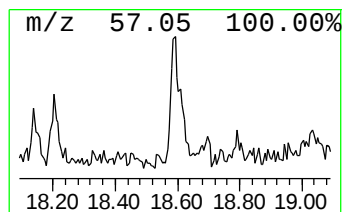
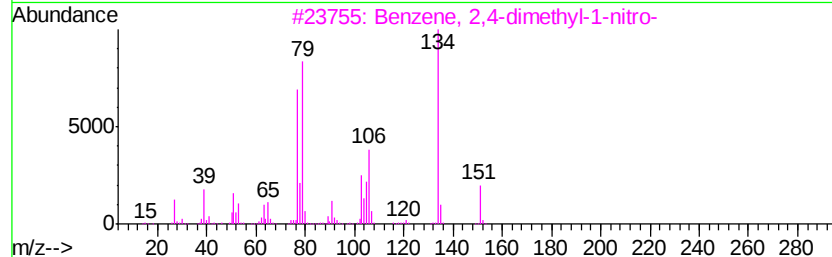
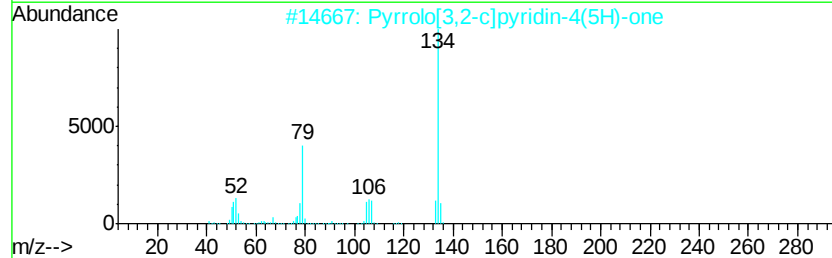
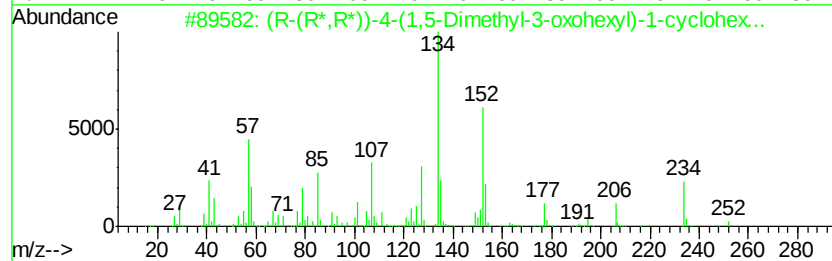
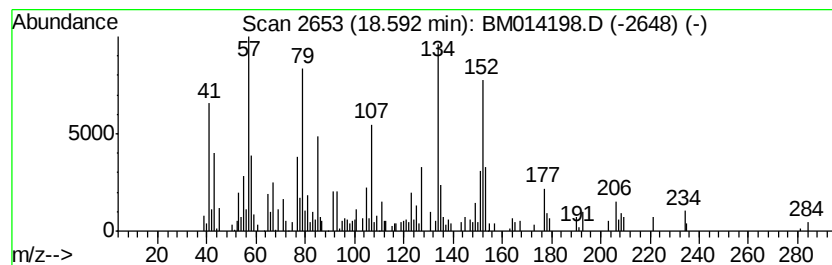
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown18.59 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.59	4.53 ng	299029	Phenanthrene-d10	16.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R-(R*,R*))	-4-(1,5-Dimethyl-3-ox...	252	C15H24O3	006753-22-6	47	
2	Pyrrolo[3,2-c]pyridin-4(5H)-one	134	C7H6N2O	054415-77-9	38		
3	Benzene, 2,4-dimethyl-1-nitro-	151	C8H9NO2	000089-87-2	35		
4	Azetidine, 1-(methylsulfonyl)-	135	C4H9NO2S	013595-45-4	25		
5	Benzenemethanol, .alpha.-methyl-	122	C8H10O	013323-81-4	25		



Data Path : Z:\HPCHEM1\BNA M\DATA\BM020818\
Data File : BM014198.D
Acq On : 08 Feb 2018 18:10
Operator : SJ/JU
Sample : J1490-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

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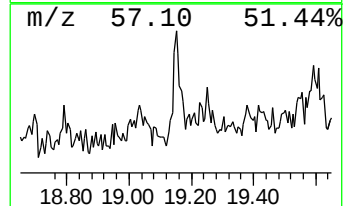
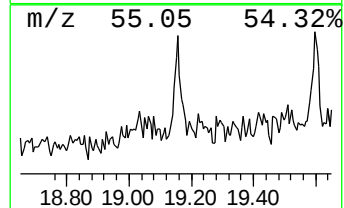
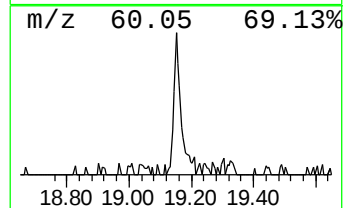
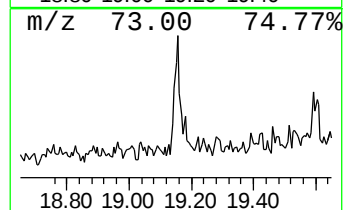
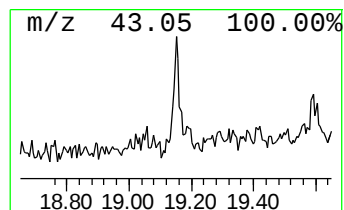
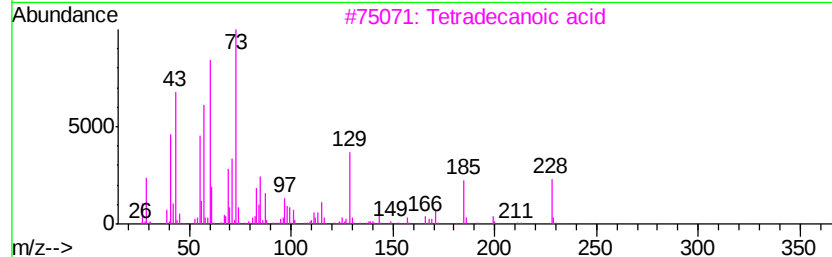
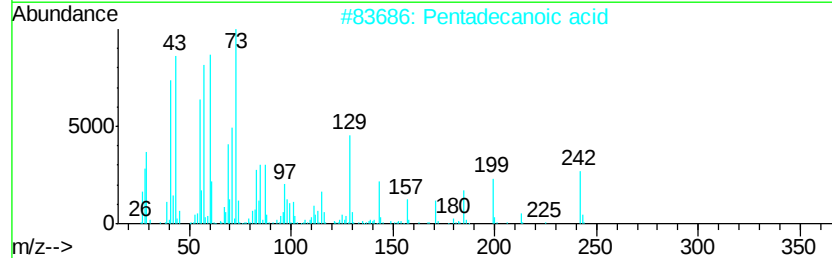
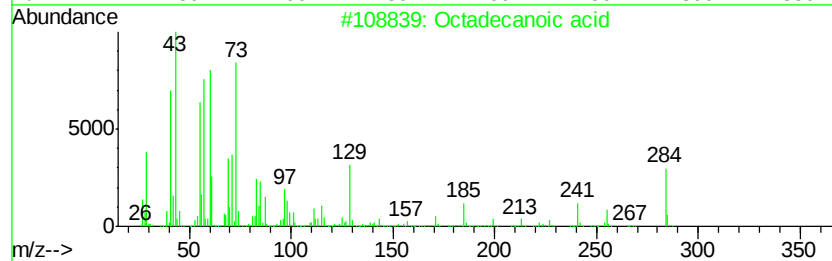
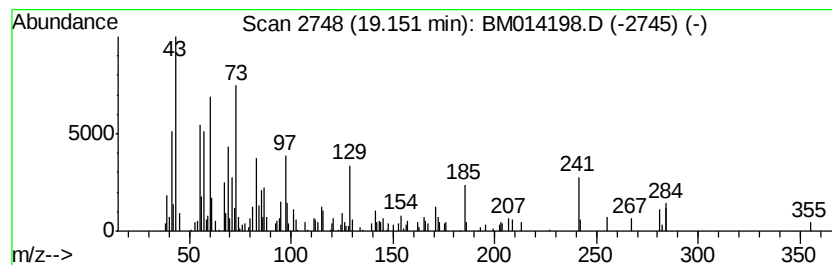
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.15	2.15 ng	157524	Chrysene-d12	21.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	55
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4			Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	47
5			Undecanoic acid	186	C11H22O2	000112-37-8	46



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM020818\
Data File : BM014198.D
Acq On : 08 Feb 2018 18:10
Operator : SJ/JU
Sample : J1490-06
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM020718.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
Methyl Isobutyl K...	3.43	7.7	ng	250361	1	7.54	646898	20.0
unknown7.08	7.08	105.3	ng	3405110	1	7.54	646898	20.0
1H-Indene, 1-ethy...	11.99	2.8	ng	119660	2	10.32	849575	20.0
Benzocycloheptatr...	12.22	3.0	ng	128647	2	10.32	849575	20.0
Dimethyl phthalate	13.67	2.1	ng	118766	3	14.20	1102730	20.0
unknown14.75	14.75	12.3	ng	679902	3	14.20	1102730	20.0
n-Hexadecanoic acid	17.86	3.5	ng	230588	4	16.96	1320700	20.0
unknown17.98	17.98	5.5	ng	365308	4	16.96	1320700	20.0
unknown18.59	18.59	4.5	ng	299029	4	16.96	1320700	20.0
Octadecanoic acid	19.15	2.1	ng	157524	5	21.16	1466280	20.0