

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
 Data File : BM016588.D
 Acq On : 24 Aug 2018 15:03
 Operator : SJ/JU
 Sample : J4522-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-1R

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.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	3.616	52	56	68	rVB	499903	676485	2.29%	0.679%
2	3.922	105	108	115	rVB	255137	336629	1.14%	0.338%
3	4.440	193	196	202	rVB	292410	416905	1.41%	0.418%
4	5.163	314	319	329	rVB	214213	392170	1.33%	0.393%
5	5.551	380	385	399	rBV	972608	1622962	5.49%	1.628%
6	7.187	656	663	670	rBV	593085	1061947	3.59%	1.065%
7	7.257	670	675	682	rVB2	166244	305981	1.04%	0.307%
8	7.463	698	710	716	rBV3	120239	315135	1.07%	0.316%
9	7.534	716	722	736	rBV	2680559	4446698	15.04%	4.461%
10	8.010	796	803	814	rBV	498013	956568	3.24%	0.960%
11	8.104	814	819	828	rVB	306630	497721	1.68%	0.499%
12	8.322	840	856	860	rBV	3364190	5908965	19.99%	5.928%
13	8.363	860	863	869	rVB	1470147	2374250	8.03%	2.382%
14	8.475	877	882	886	rBV2	653423	1132044	3.83%	1.136%
15	9.104	972	989	992	rBV4	419281	1182088	4.00%	1.186%
16	9.192	996	1004	1012	rBV2	2349736	5486123	18.56%	5.504%
17	9.792	1098	1106	1108	rBV2	221253	378185	1.28%	0.379%
18	9.828	1108	1112	1117	rVB	432784	661507	2.24%	0.664%
19	10.192	1165	1174	1182	rBV	763686	1262453	4.27%	1.267%
20	10.816	1275	1280	1291	rVB	617657	1248435	4.22%	1.252%
21	13.263	1690	1696	1704	rBV	8799444	12410644	41.98%	12.451%
22	14.110	1835	1840	1847	rBV	350778	547308	1.85%	0.549%
23	14.651	1926	1932	1939	rBV2	1096936	1777489	6.01%	1.783%
24	16.145	2179	2186	2197	rBV	10819427	14560740	49.26%	14.608%
25	17.392	2392	2398	2407	rBV	1869373	2688977	9.10%	2.698%
26	18.245	2539	2543	2552	rBV2	230168	343525	1.16%	0.345%
27	19.980	2832	2838	2845	rBV	26636872	29560066	100.00%	29.656%
28	21.533	3098	3102	3109	rBV	2821826	3584962	12.13%	3.597%
29	23.815	3484	3490	3500	rBV	1779661	3540759	11.98%	3.552%

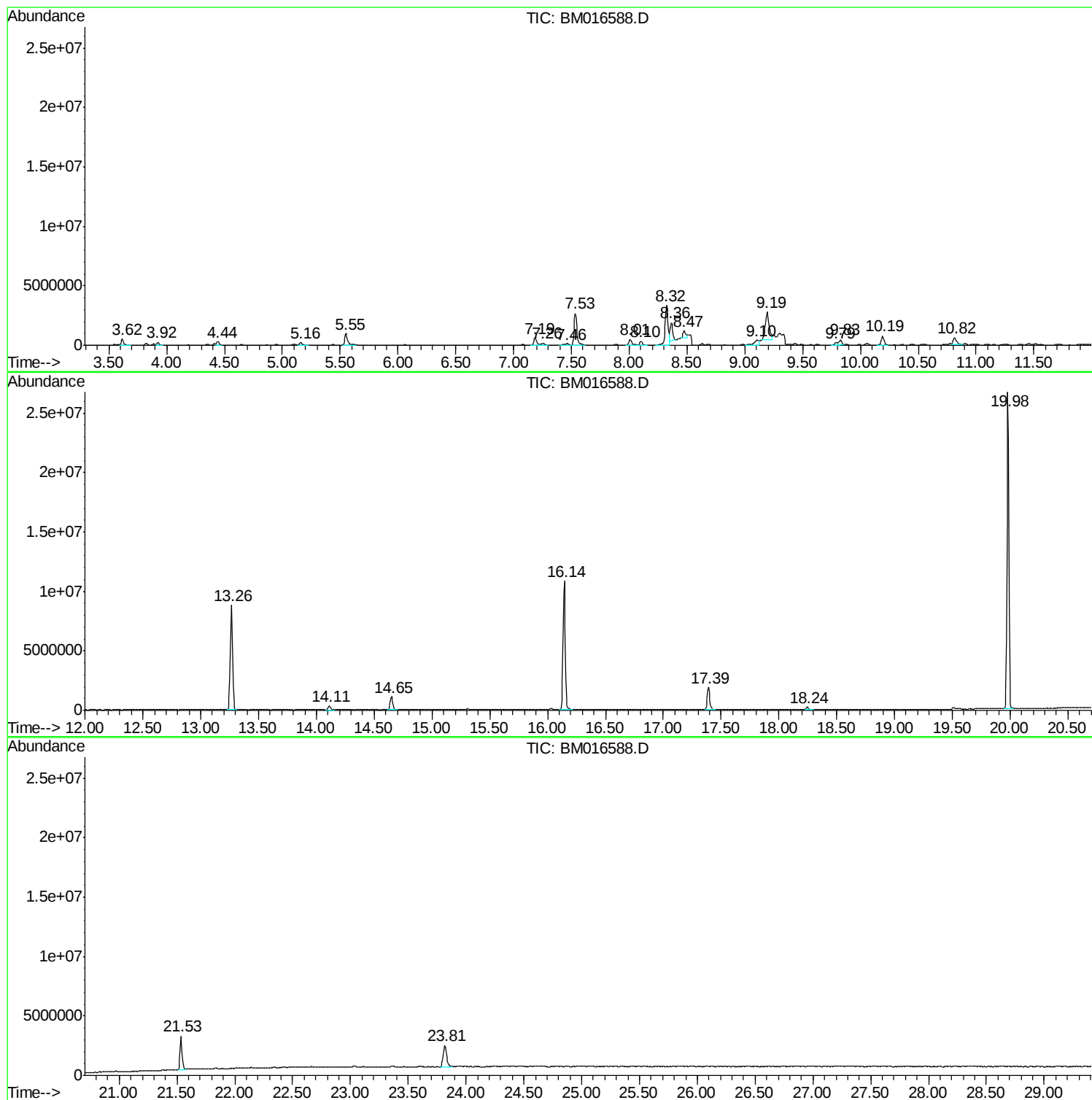
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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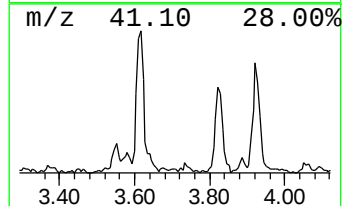
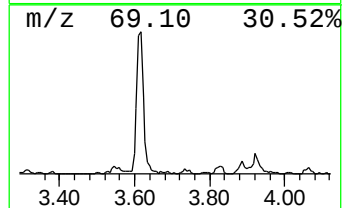
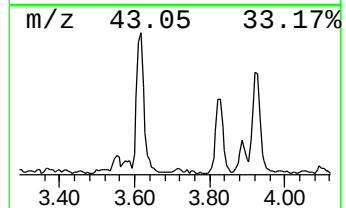
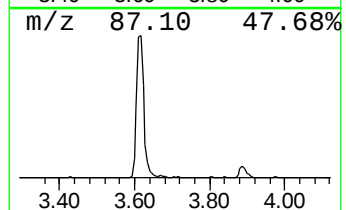
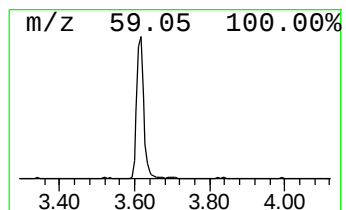
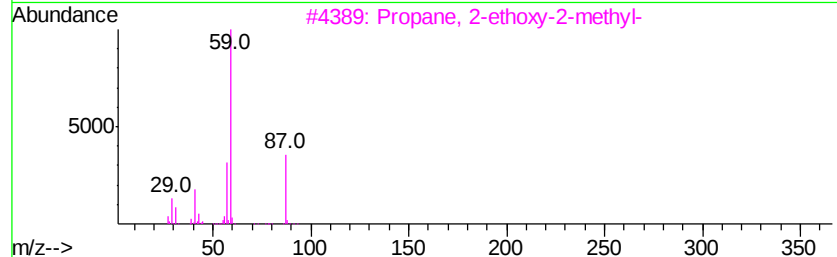
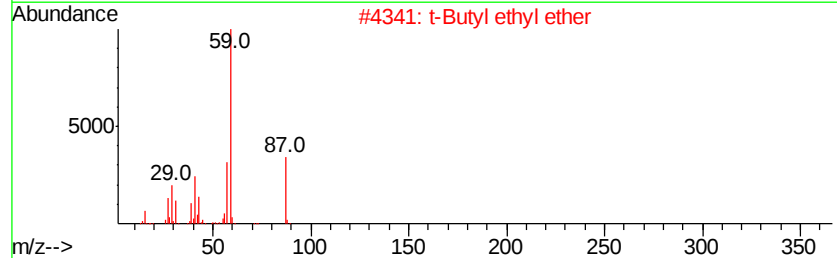
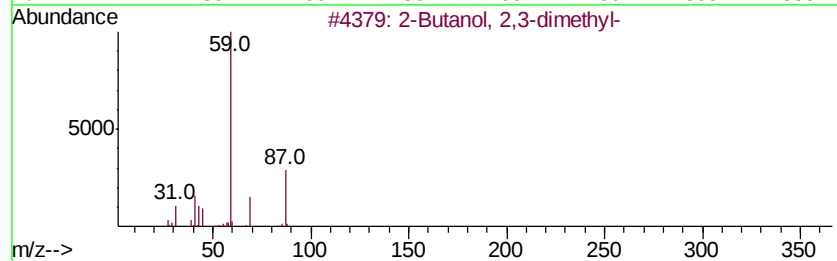
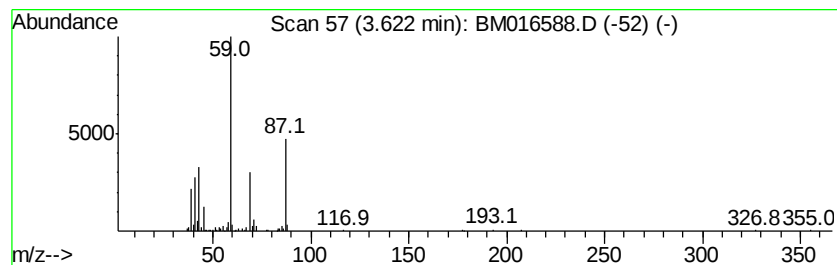
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.62	14.14 ng	676485	1,4-Dichlorobenzene-d4	8.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2			t-Butyl ethyl ether	102	C6H14O	1000118-18-4	50
3			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
4			Amylene Hydrate	88	C5H12O	000075-85-4	47
5			2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	47



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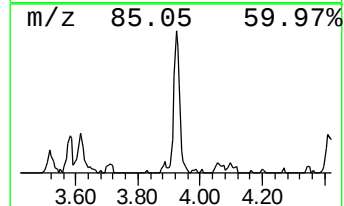
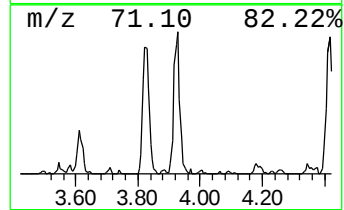
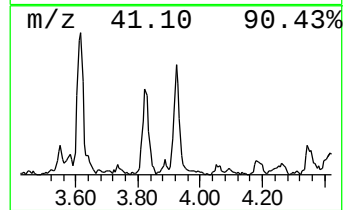
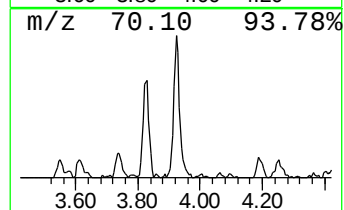
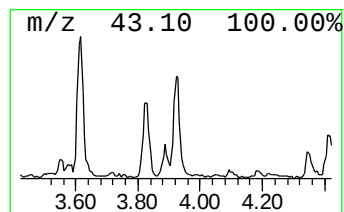
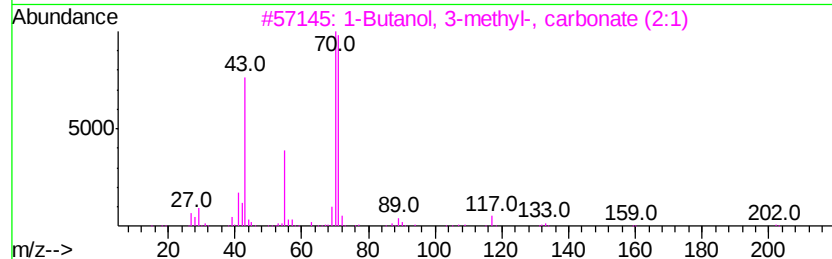
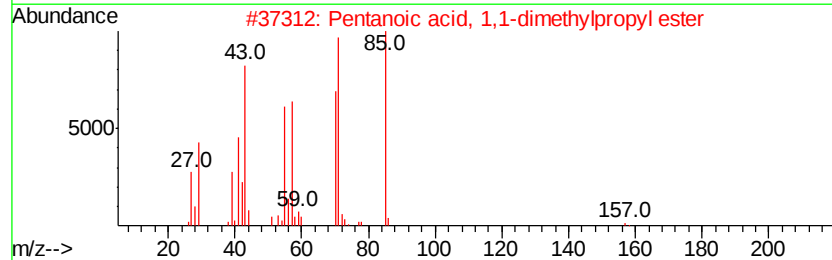
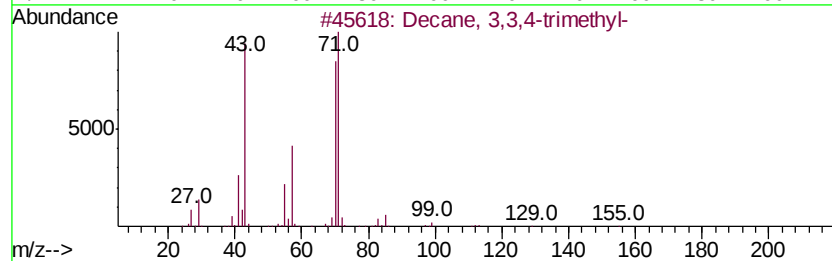
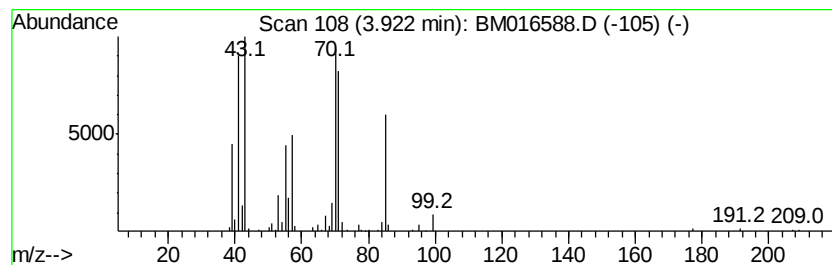
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Peak Number 2 unknown3.92 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.92	7.04 ng	336629	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	47
2		Pentanoic acid, 1,1-dimethylprop...	172	C10H20O2	117421-32-6	47
3		1-Butanol, 3-methyl-, carbonate ...	202	C11H22O3	002050-95-5	47
4		Tridecane, 7-propyl-	226	C16H34	055045-09-5	43
5		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	43



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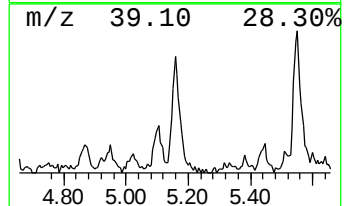
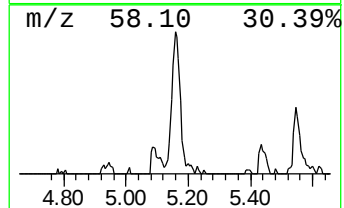
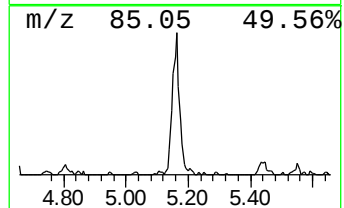
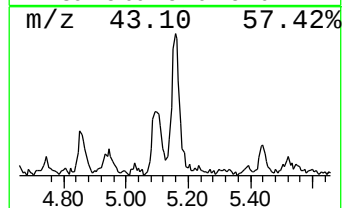
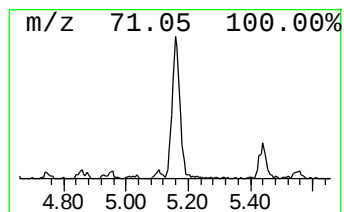
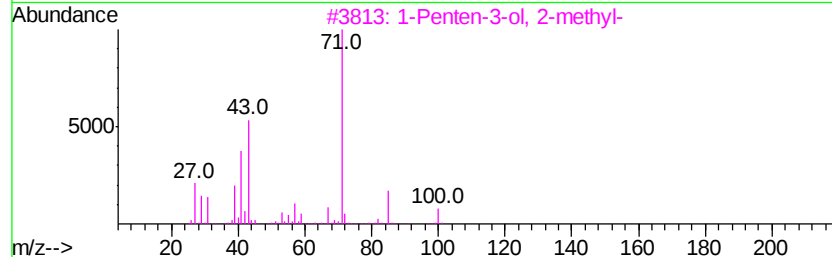
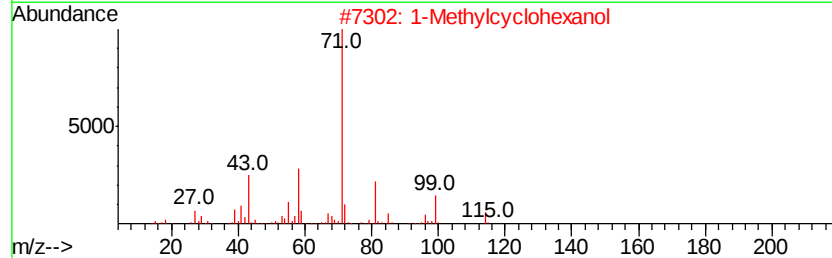
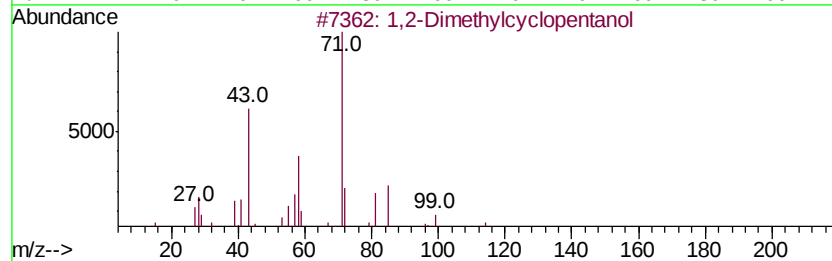
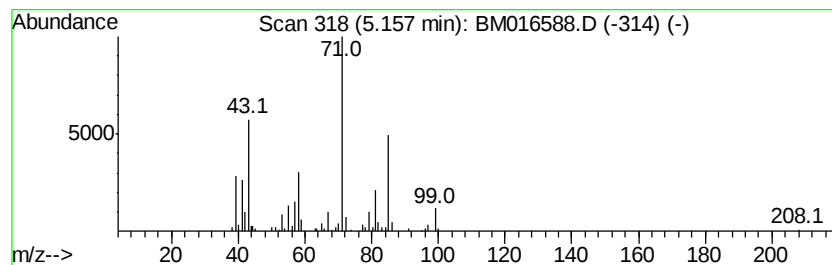
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Peak Number 4 1,2-Dimethylcyclopentanol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	8.20 ng	392170	1,4-Dichlorobenzene-d4	8.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dimethylcyclopentanol	114	C7H14O	019550-45-9	59
2			1-Methylcyclohexanol	114	C7H14O	000590-67-0	53
3			1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	50
4			Oxirane, butyl-	100	C6H12O	001436-34-6	47
5			1-Penten-3-ol, 3-methyl-	100	C6H12O	000918-85-4	47



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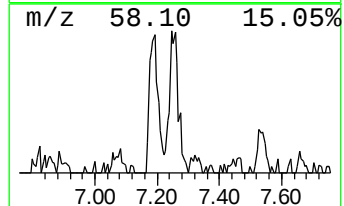
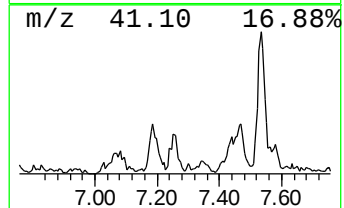
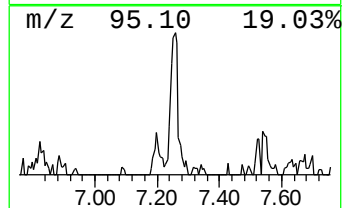
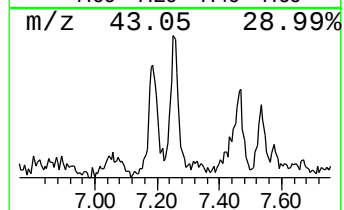
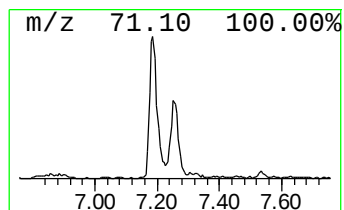
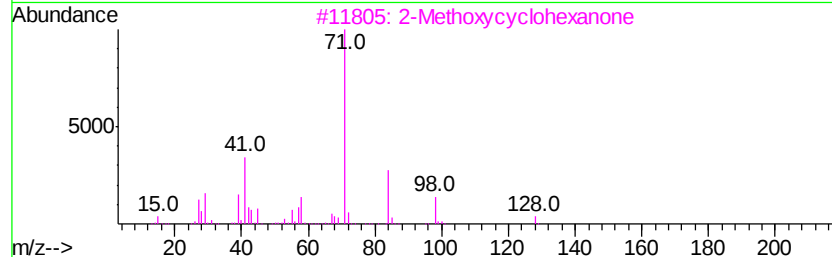
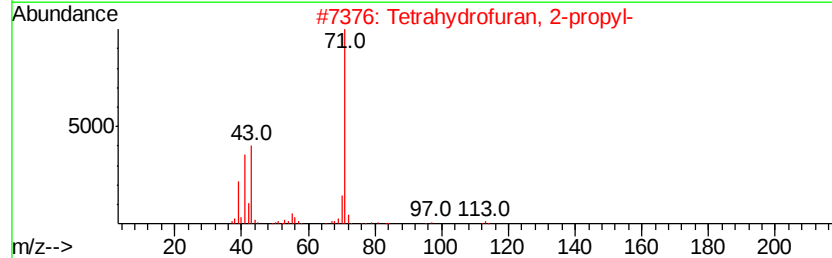
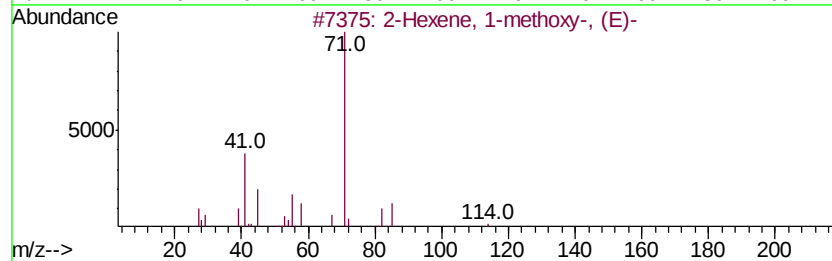
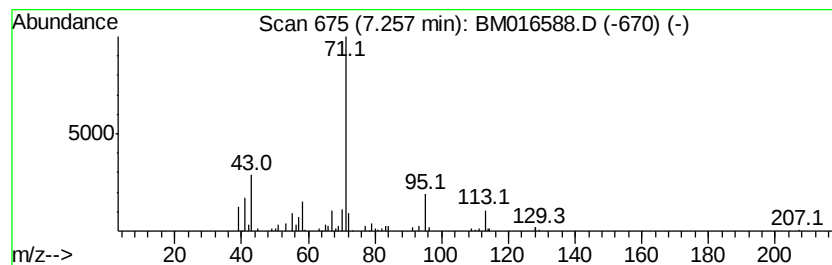
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Peak Number 5 2-Hexene, 1-methoxy-, (E)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.		
7.26	6.40 ng	305981	1,4-Dichlorobenzene-d4	8.01		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2	Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	53
2		Tetrahydrofuran, 2-propyl-	114	C7H14O	003208-22-8	50
3		2-Methoxycyclohexanone	128	C7H12O2	007429-44-9	50
4		trans-2-Methyl-4-hexen-3-ol	114	C7H14O	096346-76-8	47
5		Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	40



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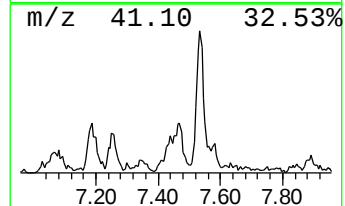
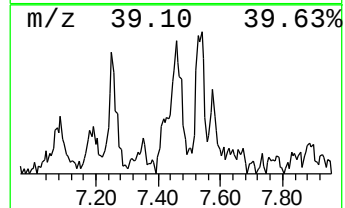
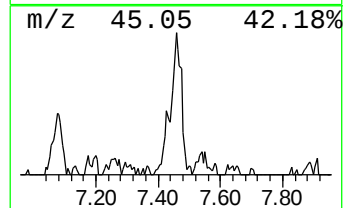
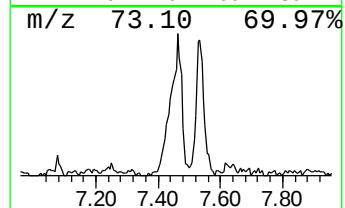
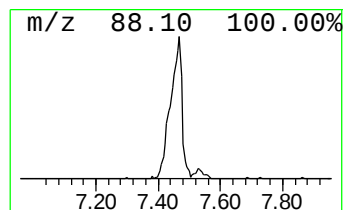
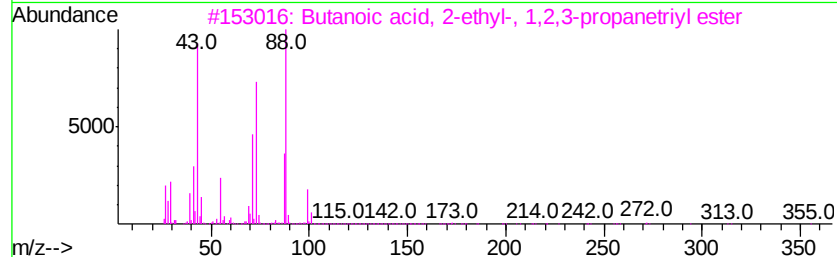
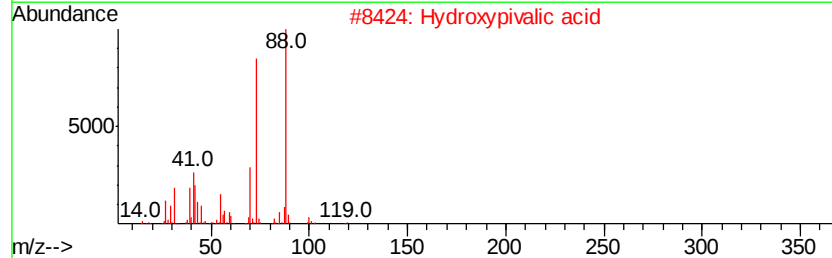
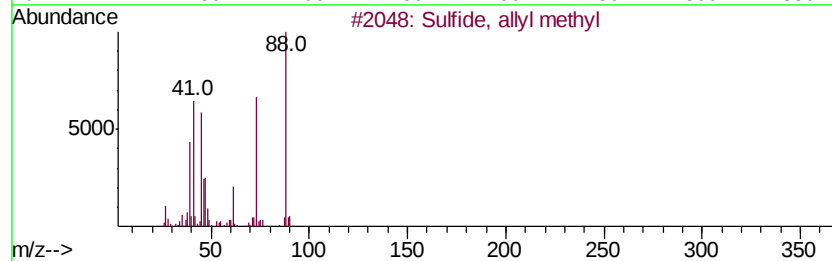
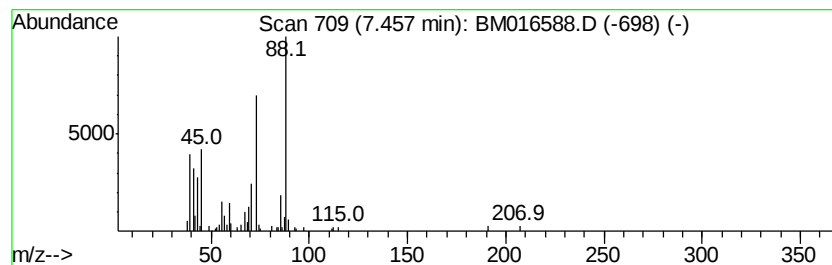
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Sulfide, allyl methyl Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	6.59 ng	315135	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfide, allyl methyl	88	C4H8S	010152-76-8	53
2		Hydroxypivalic acid	118	C5H10O3	004835-90-9	50
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	50
4		Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	40
5		1,4-Dioxane	88	C4H8O2	000123-91-1	38



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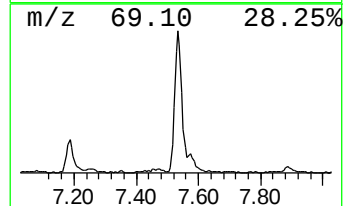
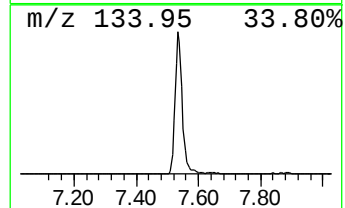
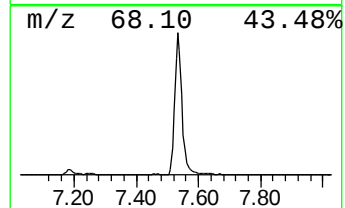
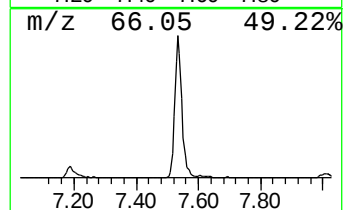
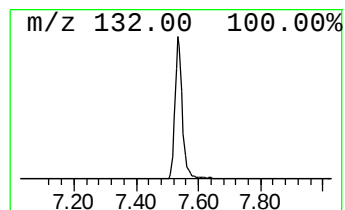
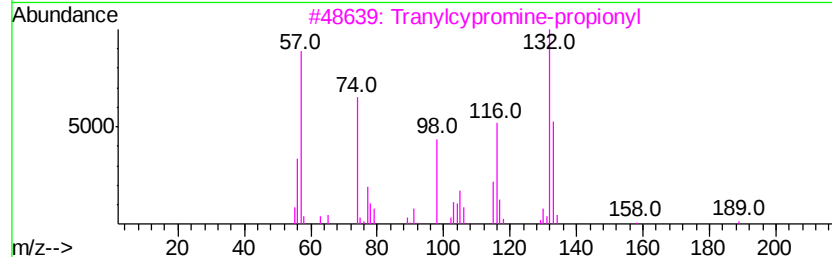
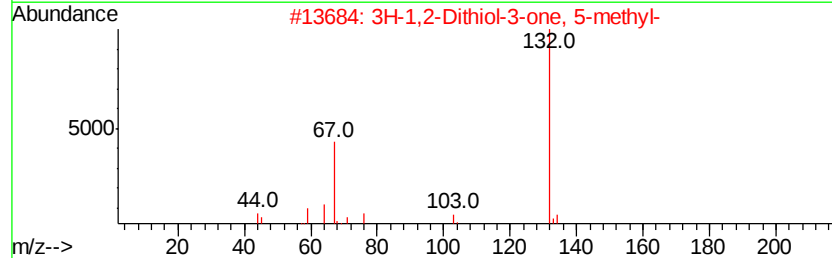
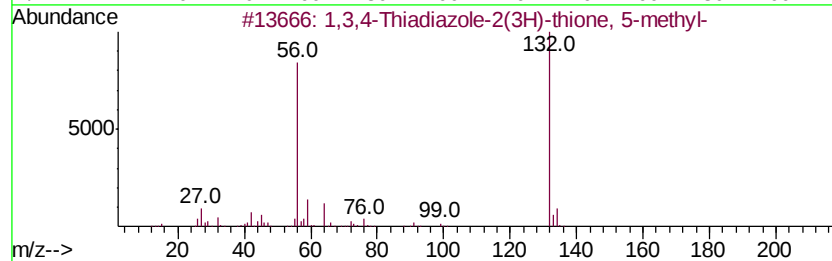
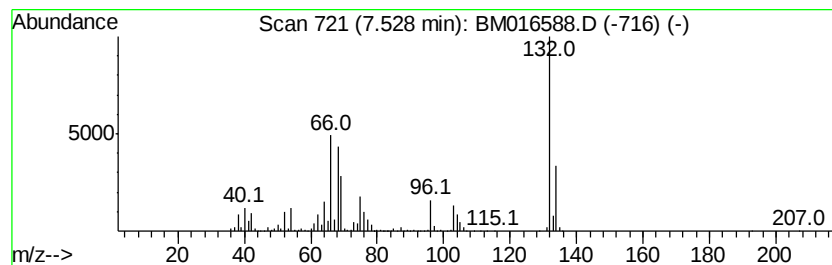
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.53 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	92.97 ng	4446700	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	10
5		5-Aminoindole	132	C8H8N2	005192-03-0	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016588.D
Acq On : 24 Aug 2018 15:03
Operator : SJ/JU
Sample : J4522-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-1R

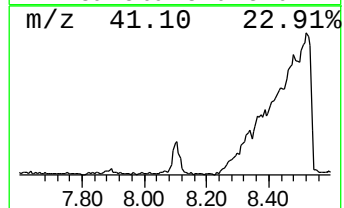
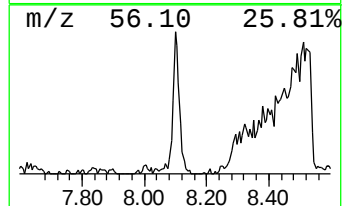
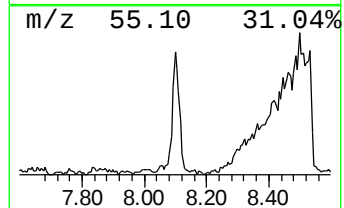
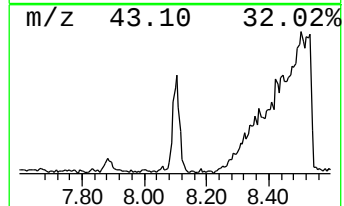
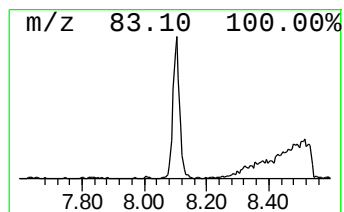
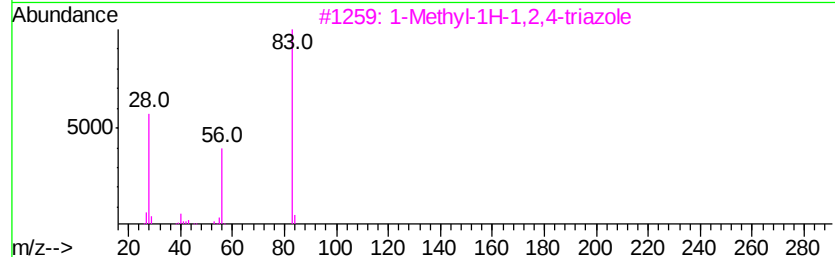
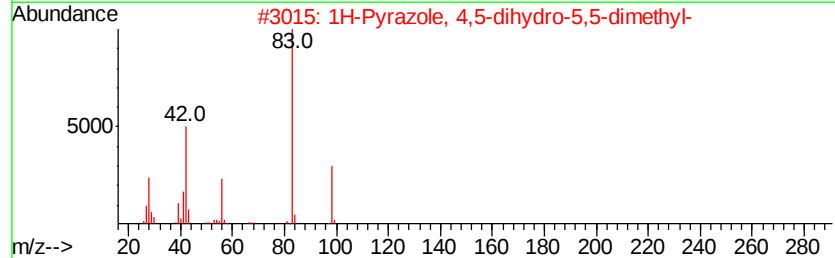
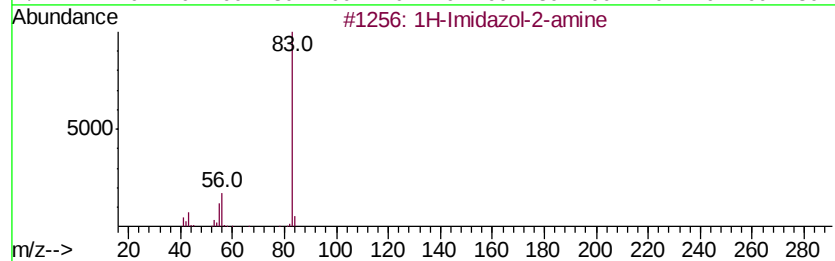
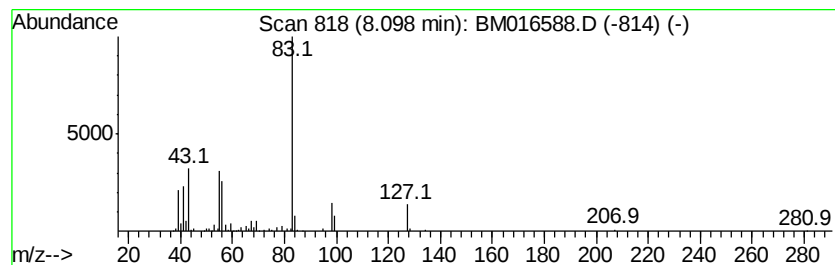
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1H-Imidazol-2-amine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.10	10.41 ng	497721	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Imidazol-2-amine	83	C3H5N3	007720-39-0	53
2		1H-Pyrazole, 4,5-dihydro-5,5-dim...	98	C5H10N2	004320-85-8	53
3		1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	43
4		1,5-Heptadien-4-one, 3,3,6-trime...	152	C10H16O	000546-49-6	38
5		Propanedinitrile, dicyclohexyl-	230	C15H22N2	074764-28-6	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016588.D
Acq On : 24 Aug 2018 15:03
Operator : SJ/JU
Sample : J4522-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1R

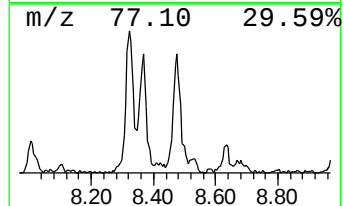
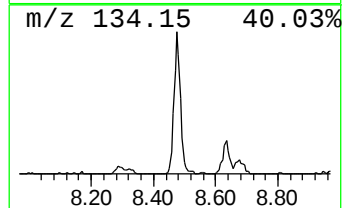
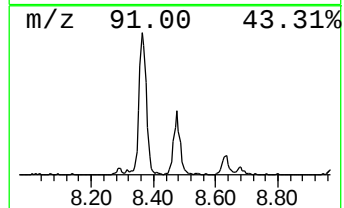
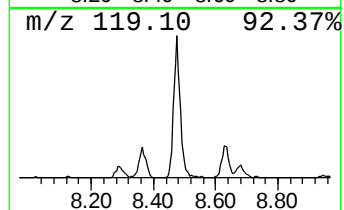
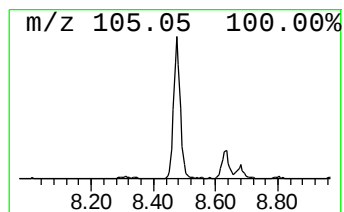
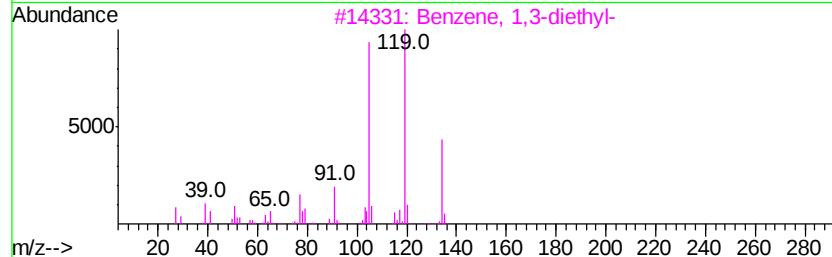
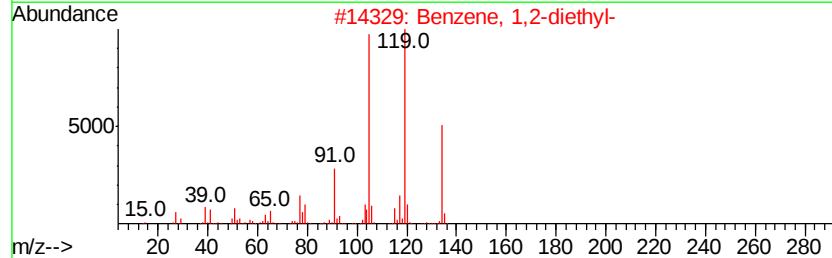
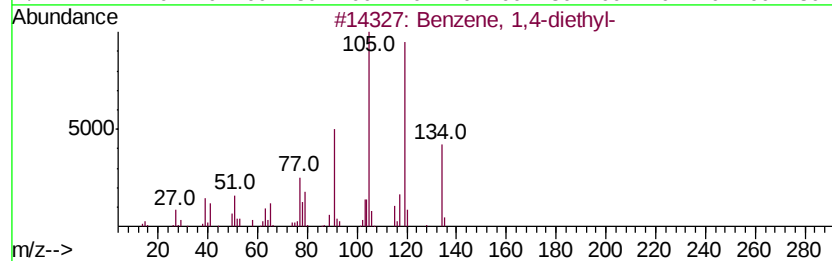
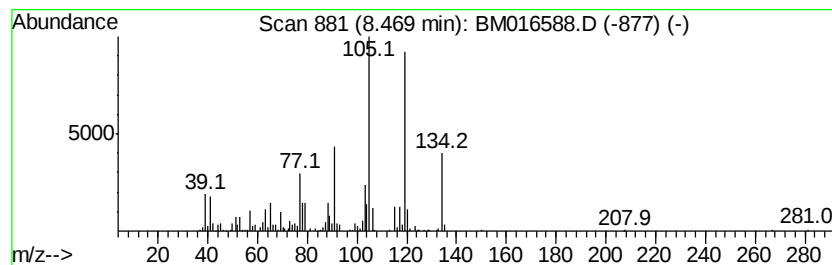
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzene, 1,4-diethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	23.67 ng	1132040	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	96
2		Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	94
3		Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	93
4		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	87
5		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016588.D
Acq On : 24 Aug 2018 15:03
Operator : SJ/JU
Sample : J4522-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

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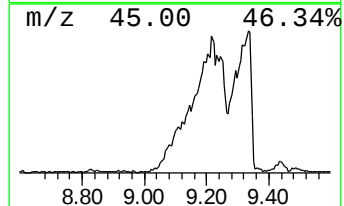
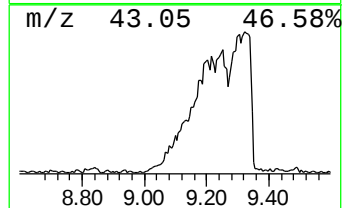
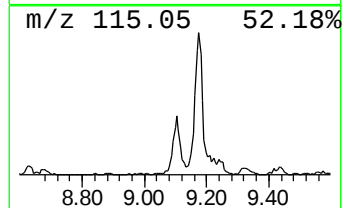
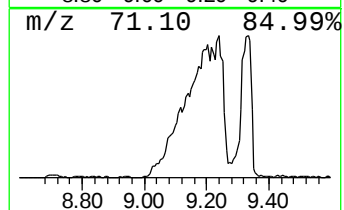
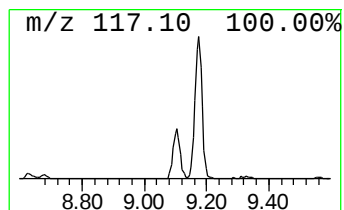
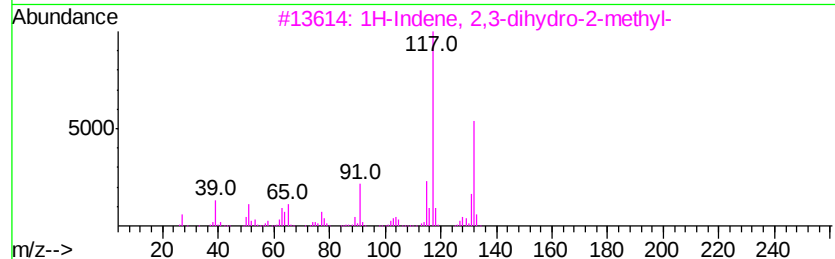
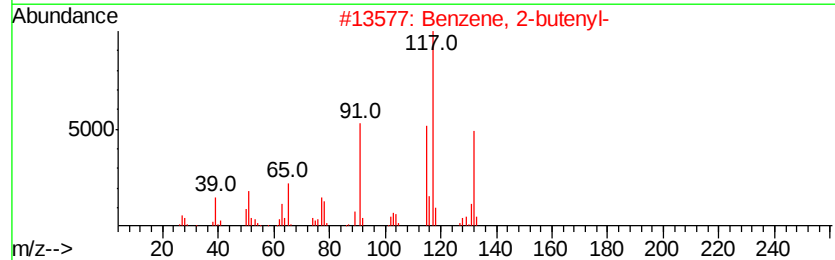
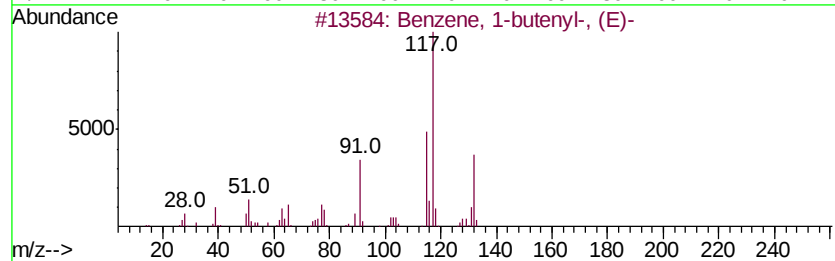
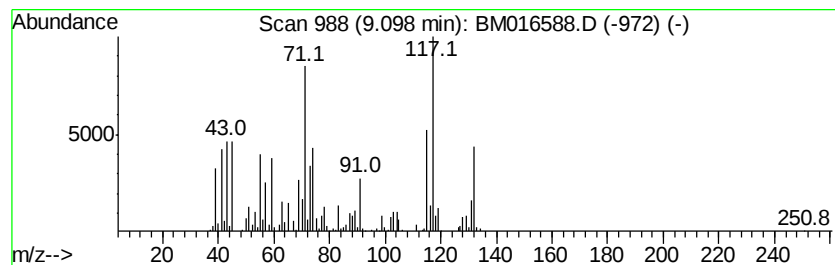
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzene, 1-butenyl-, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.10	24.72 ng	1182090	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-butenyl-, (E)-	132	C10H12	001005-64-7	60
2		Benzene, 2-butenyl-	132	C10H12	001560-06-1	46
3		1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	42
4		1-Phenyl-1-butene	132	C10H12	000824-90-8	42
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016588.D
Acq On : 24 Aug 2018 15:03
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Sample : J4522-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

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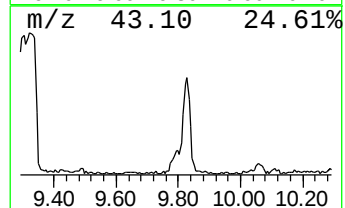
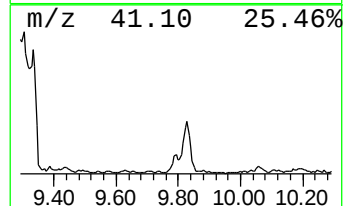
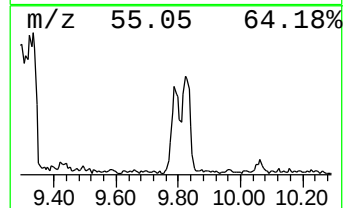
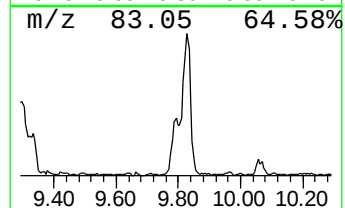
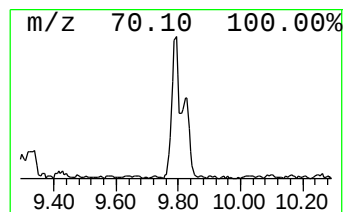
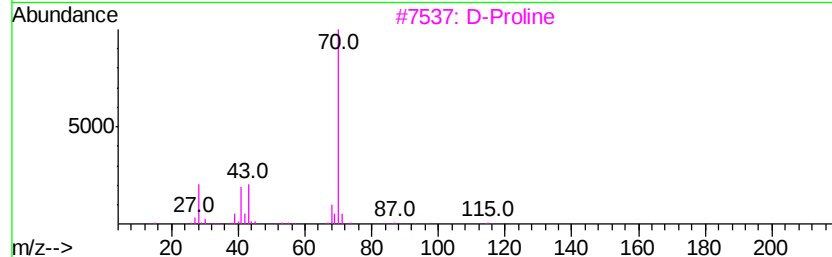
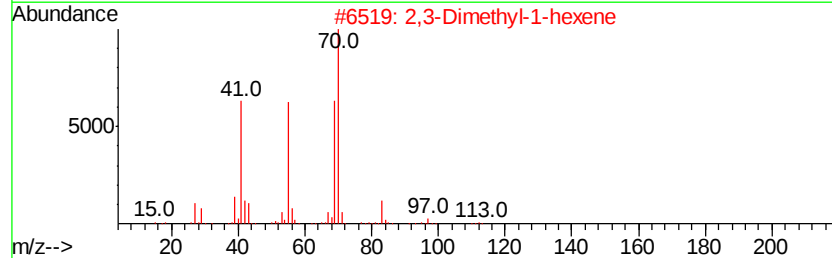
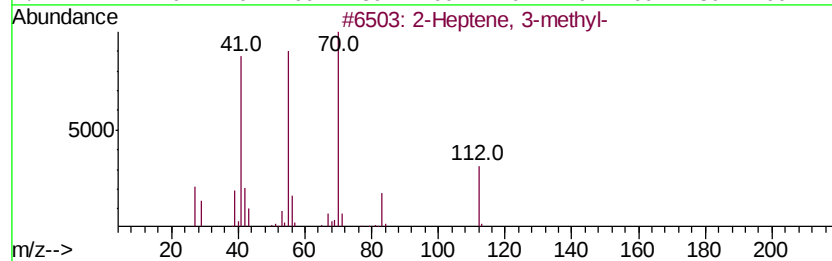
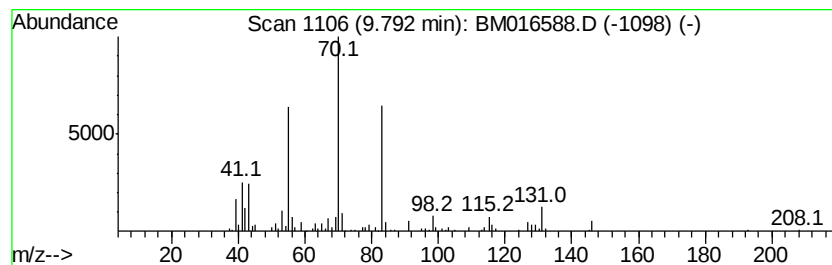
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown9.79 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.79	6.06 ng	378185	Naphthalene-d8	10.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptene, 3-methyl-	112	C8H16	003404-75-9	43
2			2,3-Dimethyl-1-hexene	112	C8H16	016746-86-4	43
3			D-Proline	115	C5H9NO2	000344-25-2	38
4			Heptane, 3-methylene-	112	C8H16	001632-16-2	38
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016588.D
Acq On : 24 Aug 2018 15:03
Operator : SJ/JU
Sample : J4522-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-1R

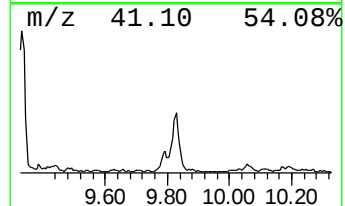
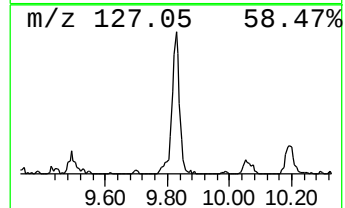
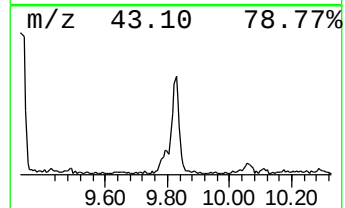
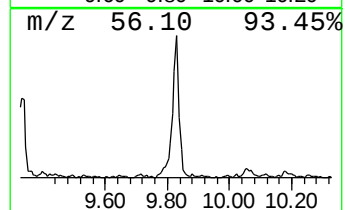
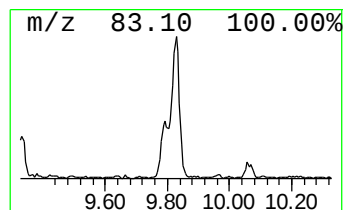
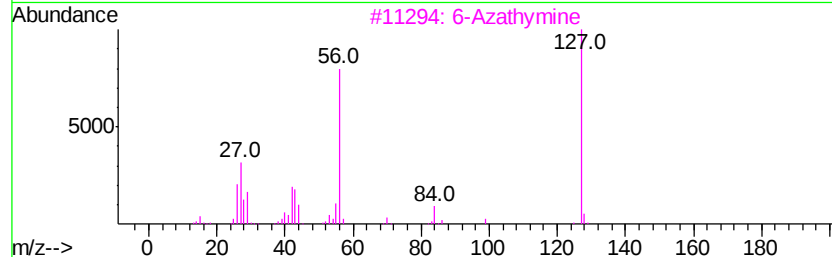
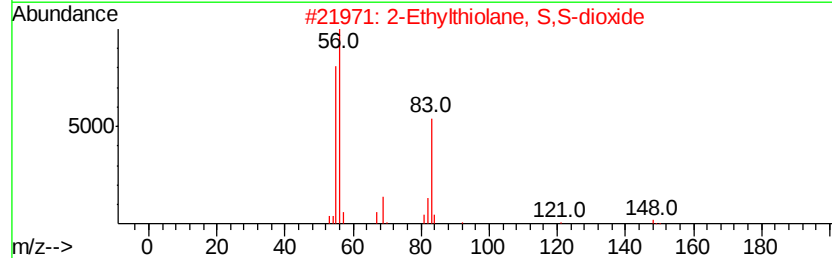
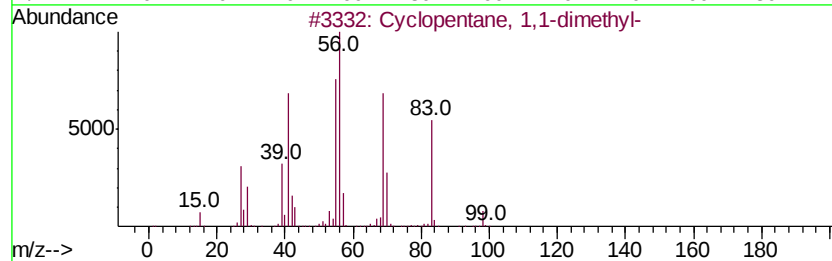
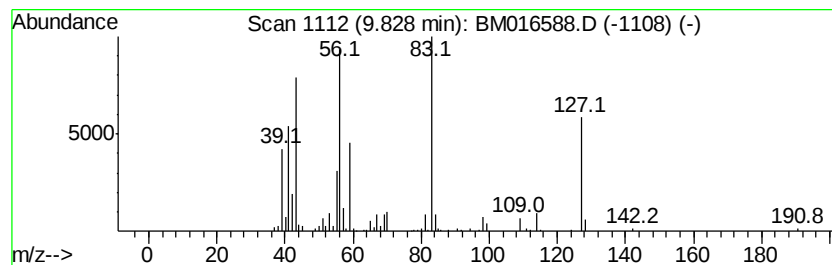
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown9.83 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	10.60 ng	661507	Napthalene-d8	10.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	38
2			2-Ethylthiolane, S,S-dioxide	148	C6H12O2S	010178-59-3	38
3			6-Azathymine	127	C4H5N3O2	000932-53-6	27
4			2,5-Pyrrolidinedione, 1-ethyl-	127	C6H9NO2	002314-78-5	27
5			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
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Misc :
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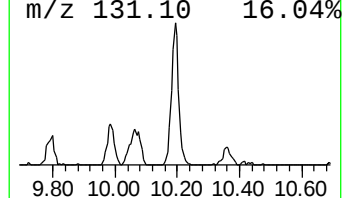
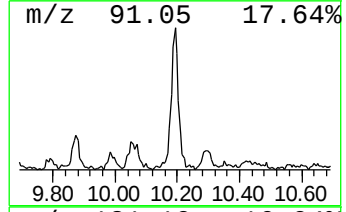
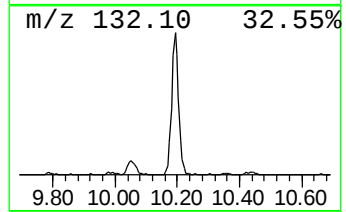
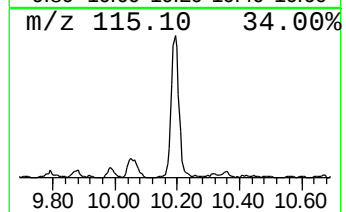
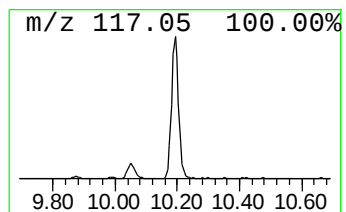
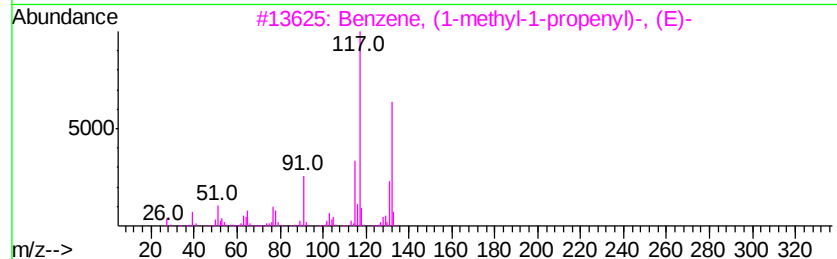
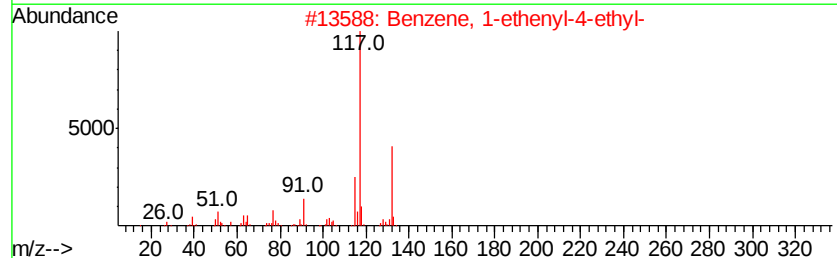
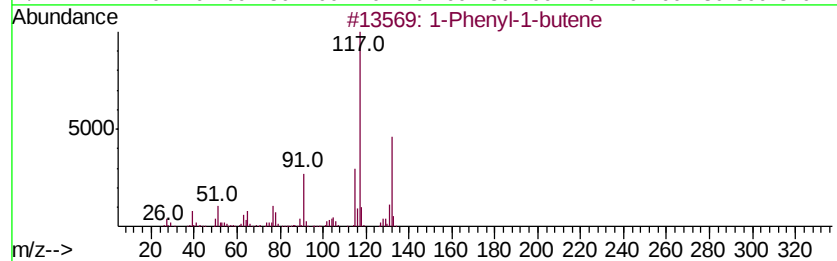
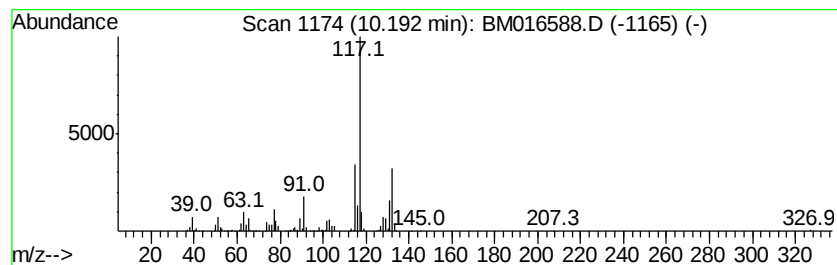
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Phenyl-1-butene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	20.22 ng	1262450	Napthalene-d8	10.82
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Phenyl-1-butene	132 C10H12	000824-90-8 94
2		Benzene, 1-ethenyl-4-ethyl-	132 C10H12	003454-07-7 93
3		Benzene, (1-methyl-1-propenyl)-,...	132 C10H12	000768-00-3 91
4		Benzene, 2-ethenyl-1,3-dimethyl-	132 C10H12	002039-90-9 91
5		Benzene, 1-methyl-2-(2-propenyl)-	132 C10H12	001587-04-8 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082418\
Data File : BM016588.D
Acq On : 24 Aug 2018 15:03
Operator : SJ/JU
Sample : J4522-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

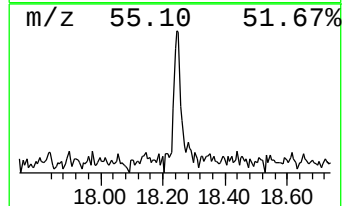
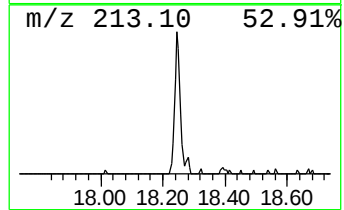
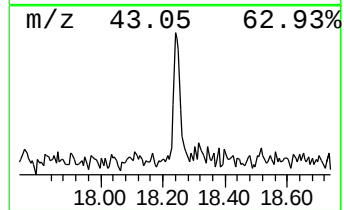
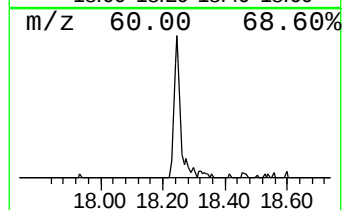
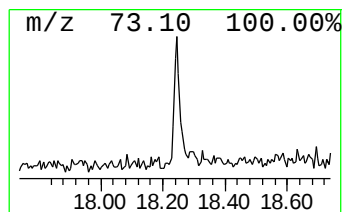
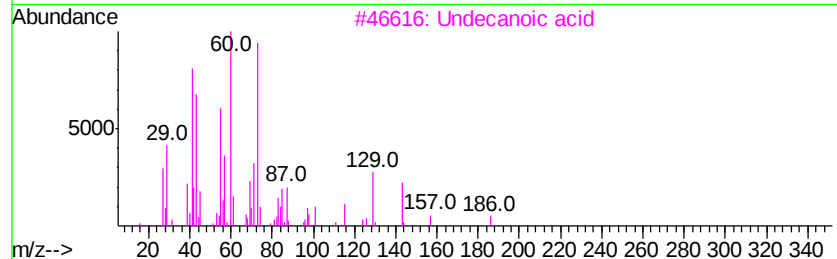
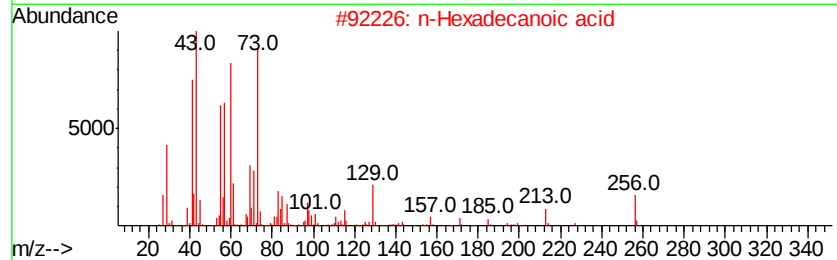
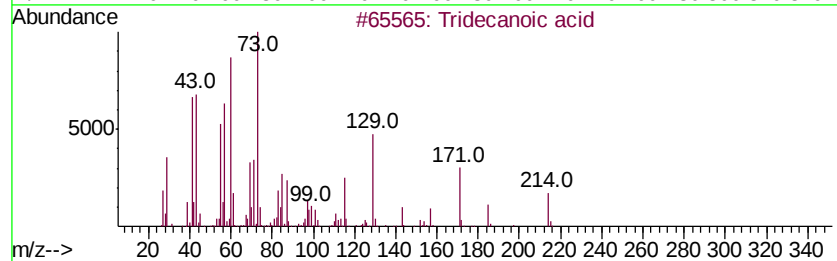
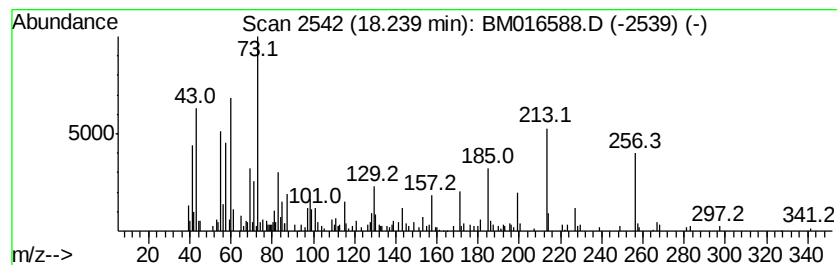
Instrument :
BNA_M
ClientSampleId :
MW-1R

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Tridecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.24	2.56 ng	343525	Phenanthrene-d10		17.39
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	83
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3	Undecanoic acid	186	C11H22O2	000112-37-8	35
4	Nonanoic acid	158	C9H18O2	000112-05-0	30
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM082418\
Data File : BM016588.D
Acq On : 24 Aug 2018 15:03
Operator : SJ/JU
Sample : J4522-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-1R

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butanol, 2,3-di...	3.62	14.1	ng	676485	1	8.01	956568	20.0
unknown3.92	3.92	7.0	ng	336629	1	8.01	956568	20.0
1,2-Dimethylcyclo...	5.16	8.2	ng	392170	1	8.01	956568	20.0
2-Hexene, 1-metho...	7.26	6.4	ng	305981	1	8.01	956568	20.0
Sulfide, allyl me...	7.46	6.6	ng	315135	1	8.01	956568	20.0
unknown7.53	7.53	93.0	ng	4446700	1	8.01	956568	20.0
1H-Imidazol-2-amine	8.10	10.4	ng	497721	1	8.01	956568	20.0
Benzene, 1,4-diet...	8.47	23.7	ng	1132040	1	8.01	956568	20.0
Benzene, 1-buteny...	9.10	24.7	ng	1182090	1	8.01	956568	20.0
unknown9.79	9.79	6.1	ng	378185	2	10.82	1248440	20.0
unknown9.83	9.83	10.6	ng	661507	2	10.82	1248440	20.0
1-Phenyl-1-butene	10.19	20.2	ng	1262450	2	10.82	1248440	20.0
Tridecanoic acid	18.24	2.6	ng	343525	4	17.39	2688980	20.0