

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
 Data File : BP006187.D
 Acq On : 12 Jul 2021 18:30
 Operator : CG/JU
 Sample : M3001-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 N9994

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006187.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.440	392	400	417	rBV	2463904	3884921	67.31%	9.203%
2	7.051	667	674	690	rBV	2209612	3922650	67.97%	9.292%
3	7.857	801	811	821	rBV	714546	1167929	20.24%	2.767%
4	9.028	1003	1010	1018	rBV	1448158	2513546	43.55%	5.954%
5	10.451	1243	1252	1260	rBV	481705	924986	16.03%	2.191%
6	10.663	1281	1288	1294	rBV	909477	1500565	26.00%	3.555%
7	12.375	1574	1579	1588	rVB	140692	305883	5.30%	0.725%
8	12.475	1593	1596	1606	rVB4	108599	223096	3.87%	0.528%
9	12.580	1610	1614	1619	rBV3	119064	225679	3.91%	0.535%
10	13.122	1700	1706	1715	rVB	4013176	5771495	100.00%	13.672%
11	13.275	1728	1732	1736	rBV2	244146	345184	5.98%	0.818%
12	13.910	1836	1840	1845	rVB	1384494	1972915	34.18%	4.674%
13	14.027	1856	1860	1870	rBV3	1057376	2070139	35.87%	4.904%
14	14.233	1890	1895	1900	rBV4	1019247	2204025	38.19%	5.221%
15	14.322	1906	1910	1917	rVB	2407816	3638340	63.04%	8.619%
16	14.457	1930	1933	1936	rBV	986667	1593875	27.62%	3.776%
17	14.498	1937	1940	1948	rVB2	1818062	3162636	54.80%	7.492%
18	15.286	2070	2074	2078	rBV2	3054443	4427810	76.72%	10.489%
19	23.721	3504	3508	3514	rVB2	1333463	2359255	40.88%	5.589%

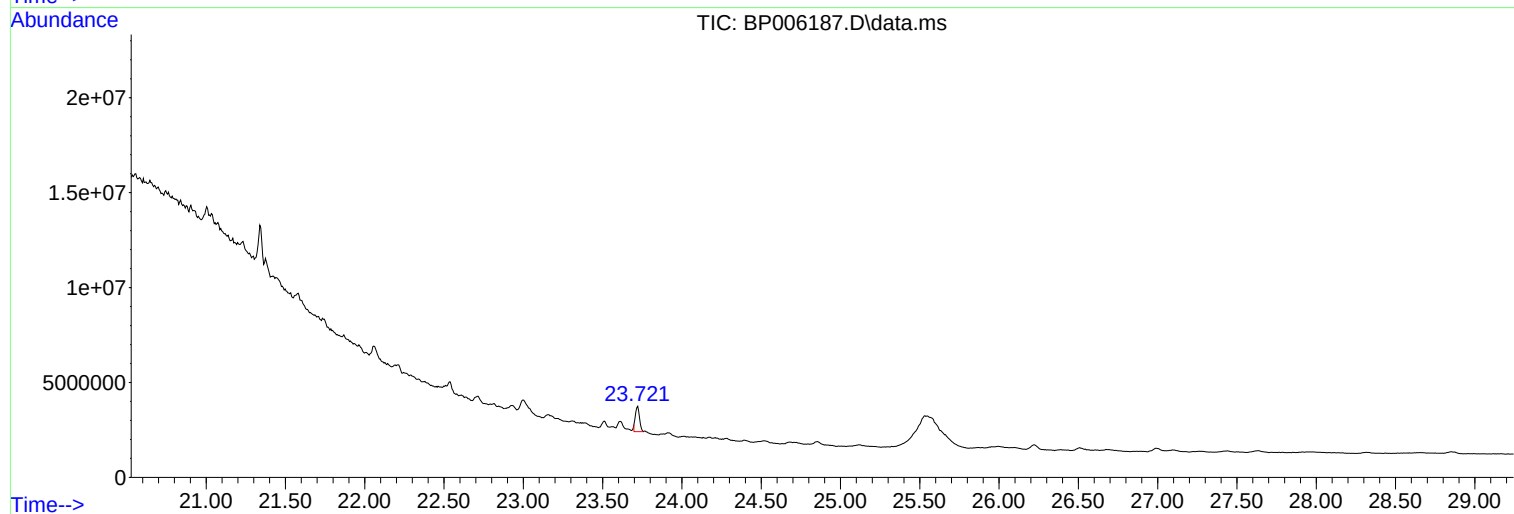
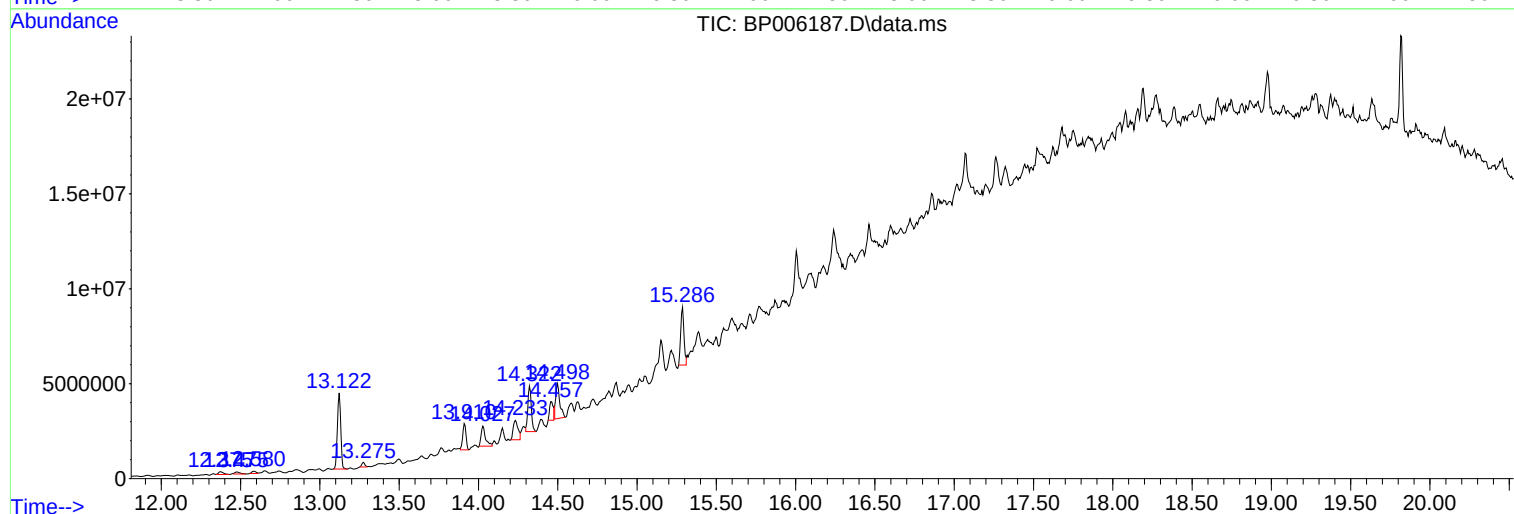
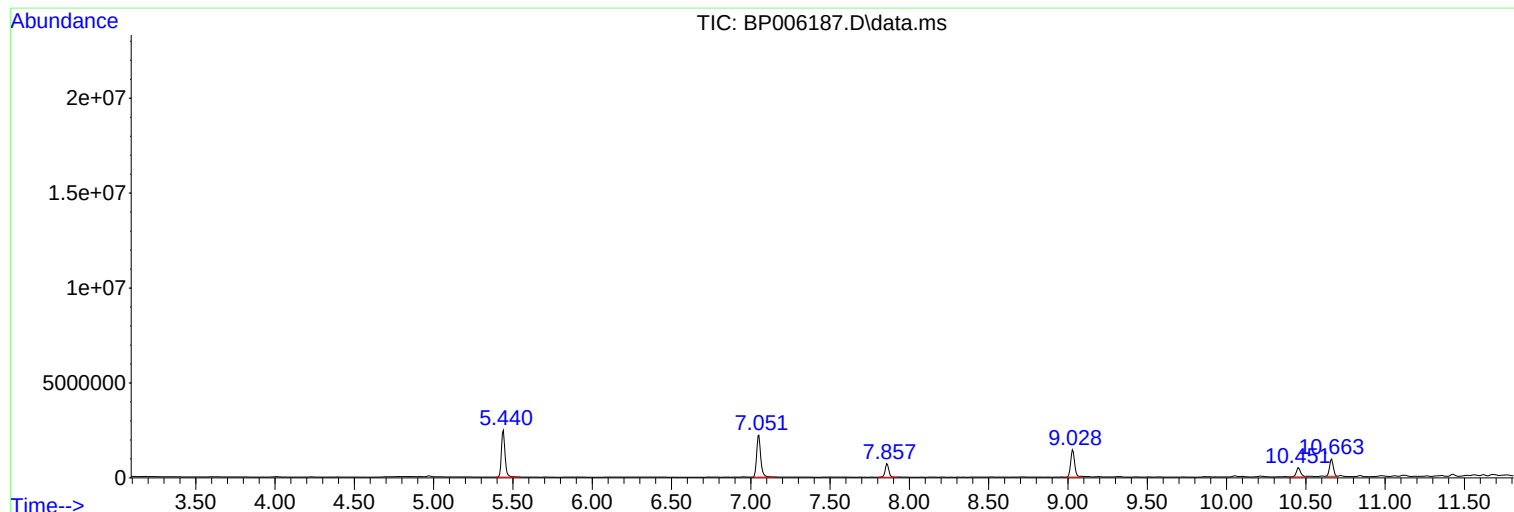
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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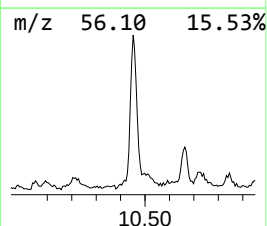
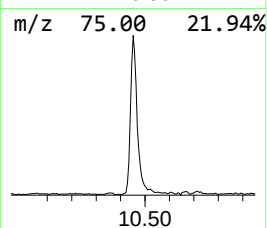
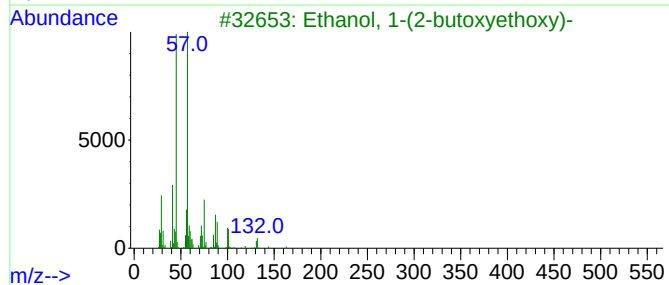
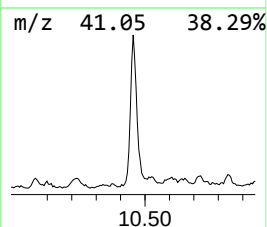
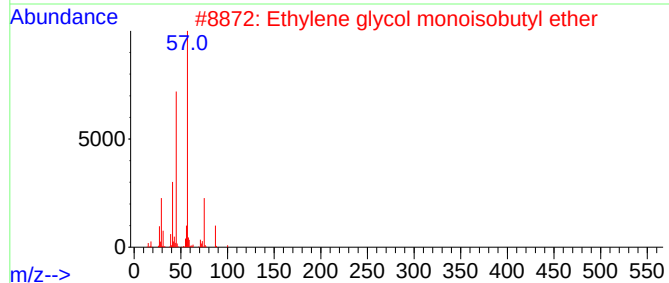
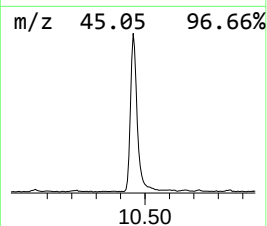
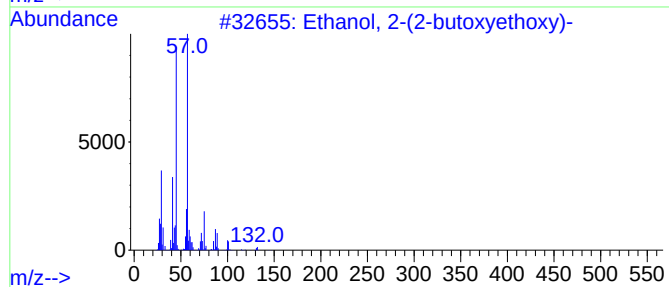
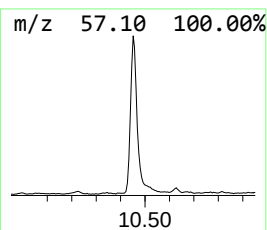
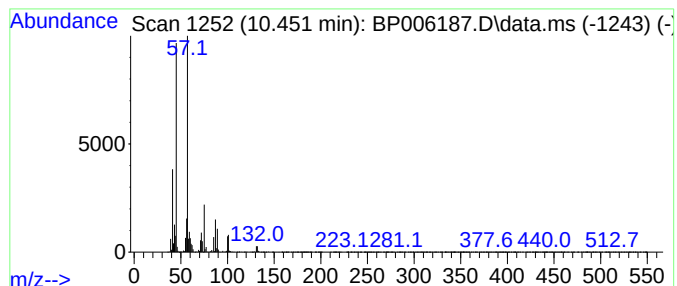
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	12.33 ng	924986	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	49
5			Tetraethylene glycol	194	C8H18O5	000112-60-7	47



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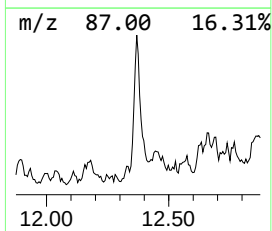
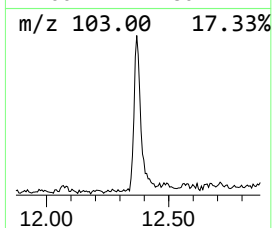
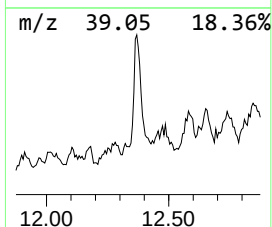
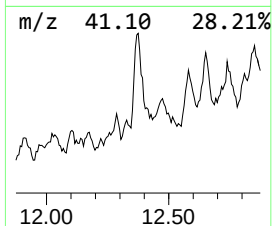
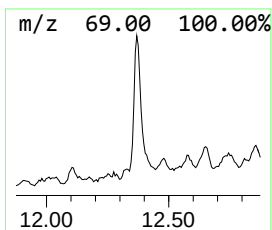
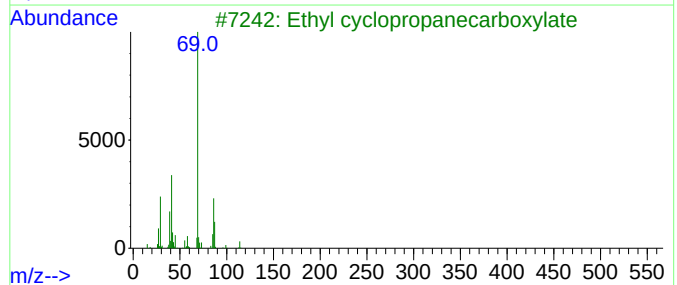
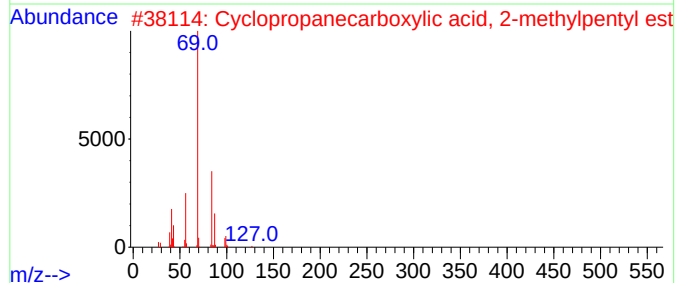
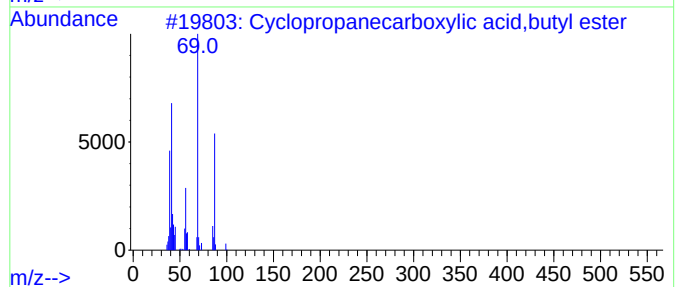
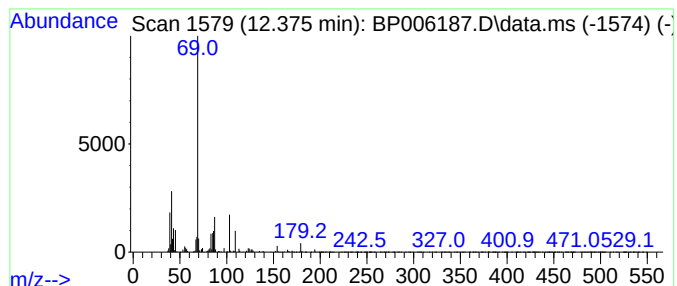
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown12.375 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.375	4.08 ng	305883	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	45
2			Cyclopropanecarboxylic acid, 2-m...	170	C10H18O2	1000354-65-8	38
3			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	36
4			6-Bromohexanoic acid, pent-2-en-...	258	C11H15BrO2	1000299-28-8	28
5			2-Propenoic acid, 2-methyl-, 1,2...	198	C10H14O4	000097-90-5	25



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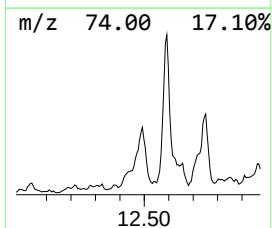
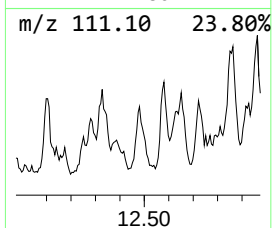
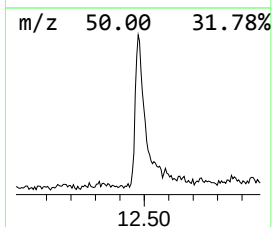
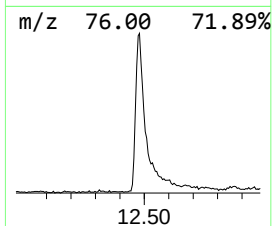
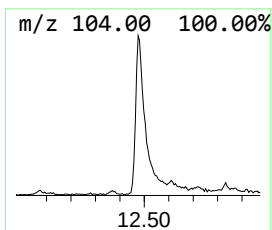
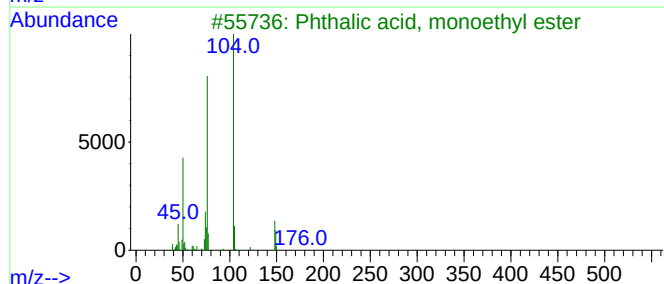
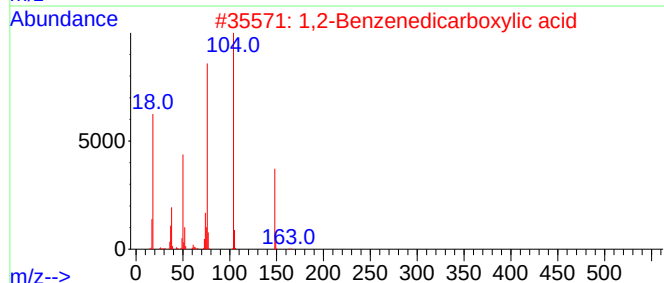
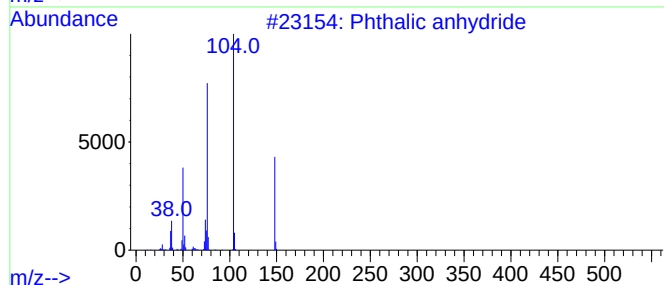
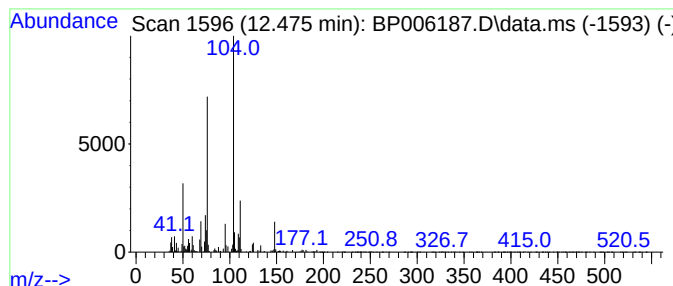
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phthalic anhydride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.475	2.97 ng	223096	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic anhydride	148	C8H4O3	000085-44-9	89
2			1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	59
3			Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	59
4			Bicyclo[4.2.0]octa-1,3,5-triene...	132	C8H4O2	006383-11-5	53
5			3-Ethylideneisobenzofuranone	160	C10H8O2	004767-63-9	53



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Misc :
ALS Vial : 6 Sample Multiplier: 1

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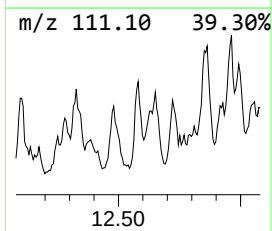
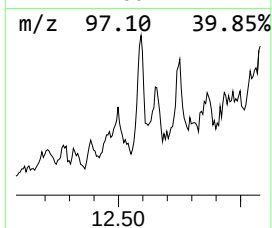
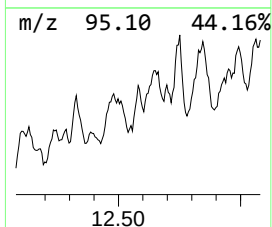
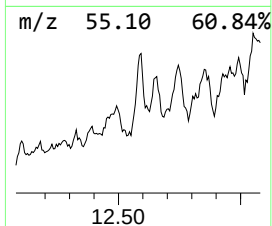
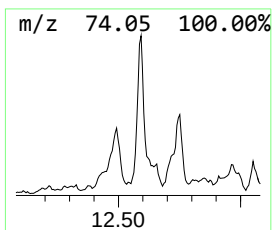
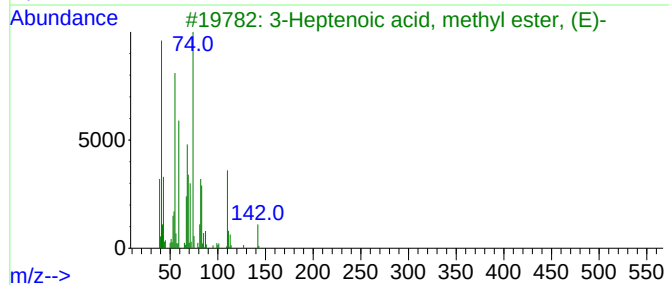
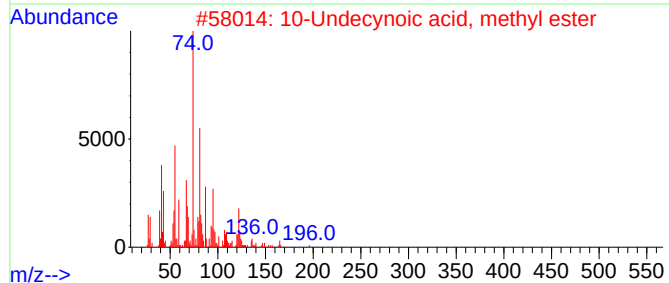
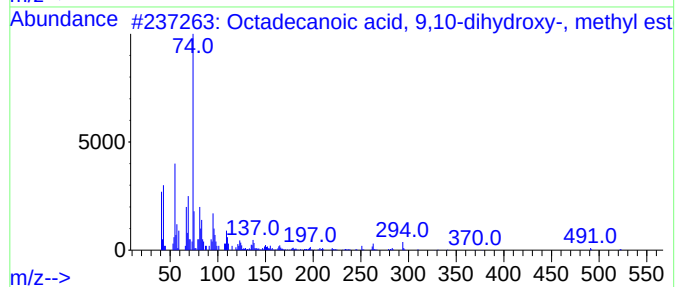
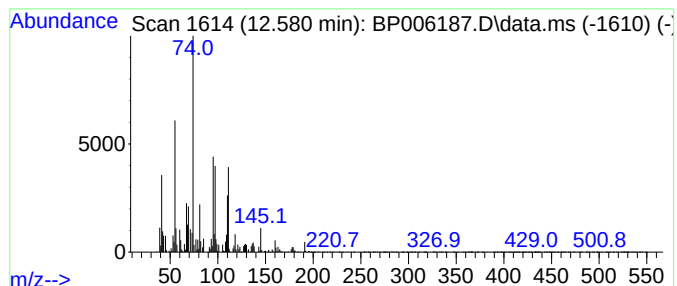
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.581 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.581	3.01 ng	225679	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, 9,10-dihydrox...	522	C23H36F6O6	021987-19-9	25
2			10-Undecynoic acid, methyl ester	196	C12H20O2	002777-66-4	25
3			3-Heptenoic acid, methyl ester, ...	142	C8H14O2	054004-30-7	17
4			Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	14
5			Cyclohexanecarboxylic acid, 1-cy...	224	C14H24O2	1000279-52-6	12



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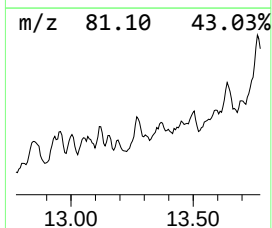
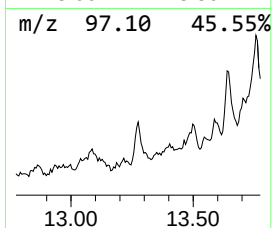
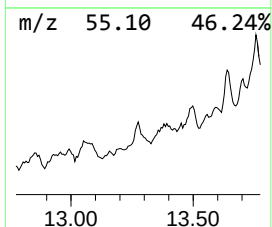
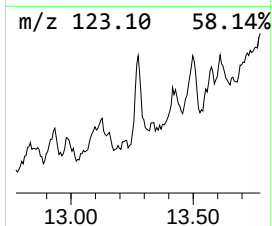
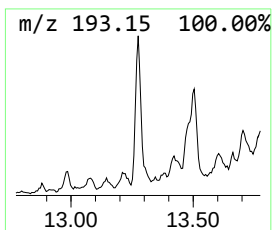
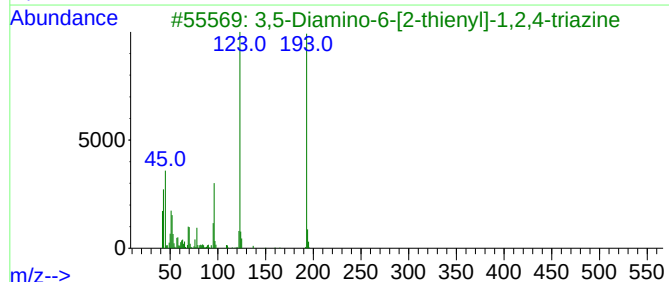
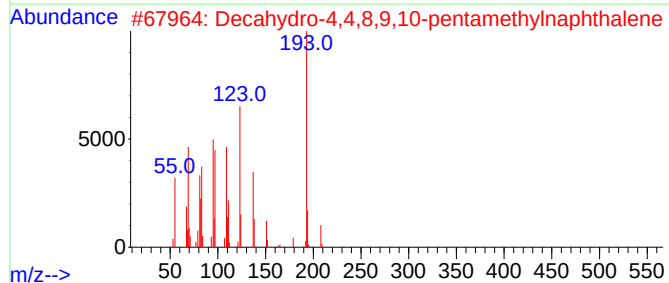
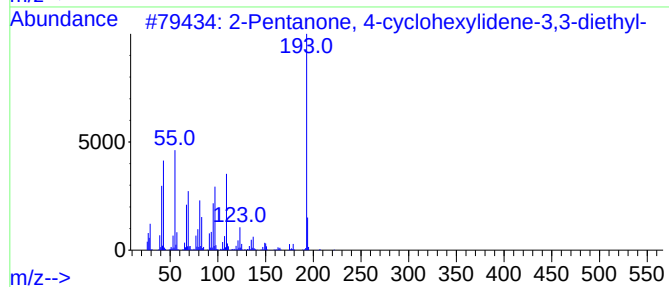
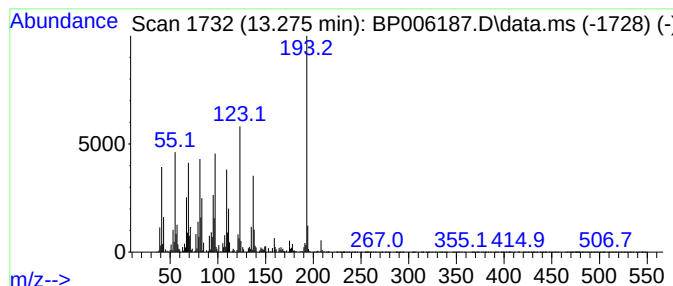
Instrument :
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ClientSampled :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-cyclohexylid... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.275	2.18 ng	345184	Acenaphthene-d10		14.498	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...		222	C15H26O	313253-65-5	53
2	Decahydro-4,4,8,9,10-pentamethyl...		208	C15H28	080655-44-3	46
3	3,5-Diamino-6-[2-thienyl]-1,2,4-...		193	C7H7N5S	058848-66-1	35
4	m-Nitrobenzaldehyde dimethylhydr...		193	C9H11N3O2	032787-76-1	14
5	[1,1'-Biphenyl]-4-acetonitrile		193	C14H11N	031603-77-7	14



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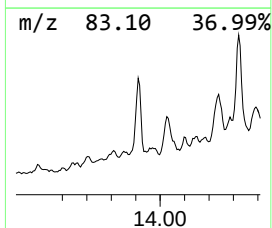
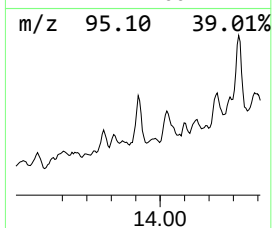
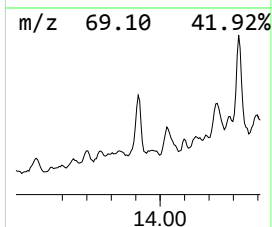
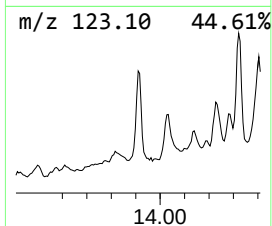
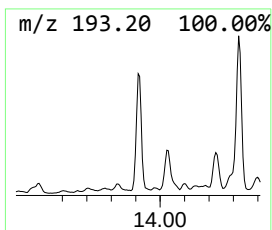
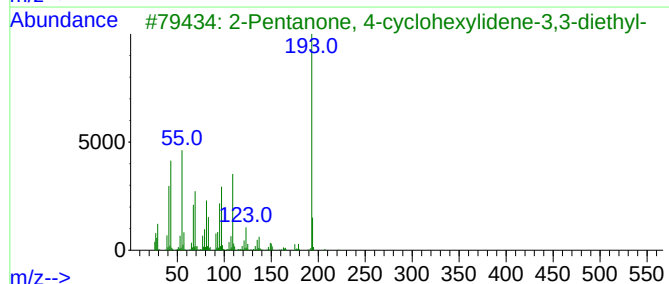
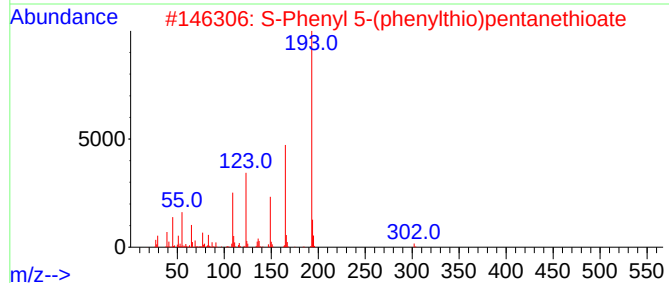
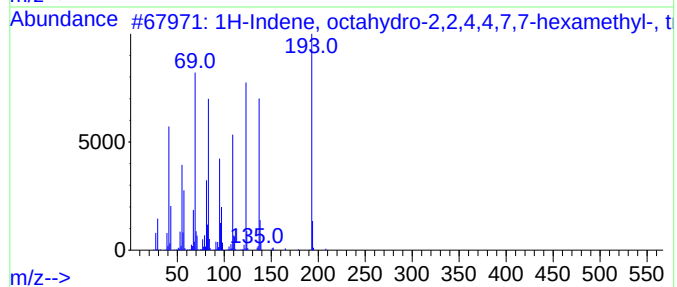
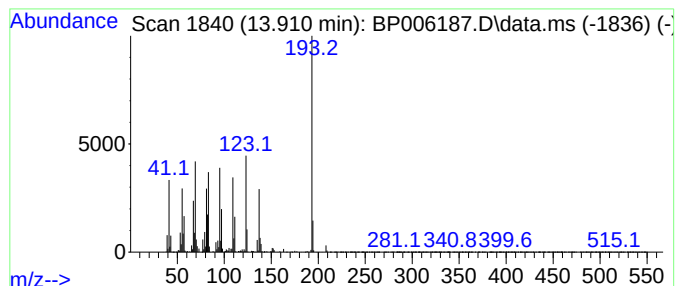
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown13.910 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	12.48 ng	1972920	Acenaphthene-d10	14.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	45		
2	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	37		
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37		
4	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21B02	074630-04-9	32		
5	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
Data File : BP006187.D
Acq On : 12 Jul 2021 18:30
Operator : CG/JU
Sample : M3001-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

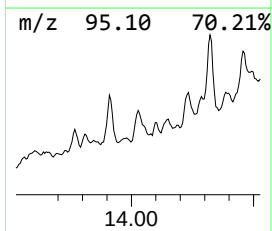
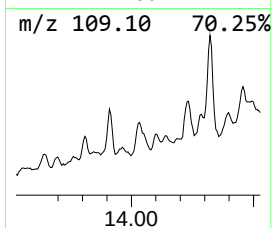
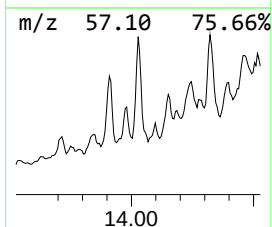
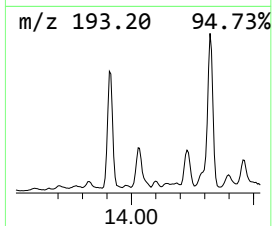
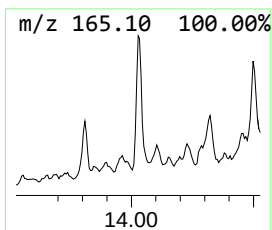
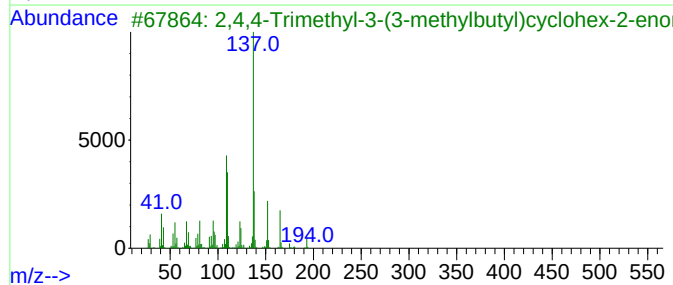
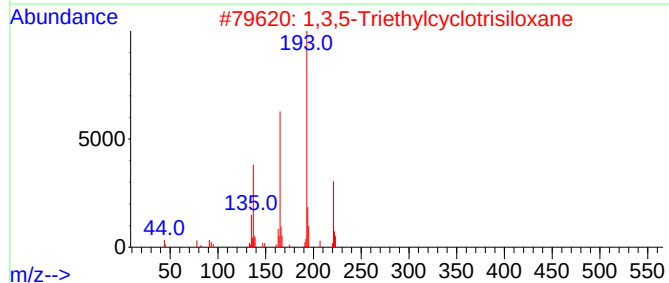
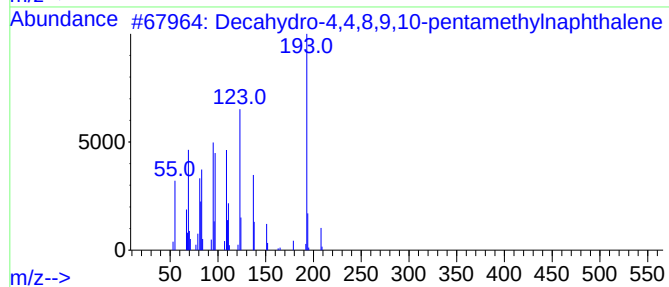
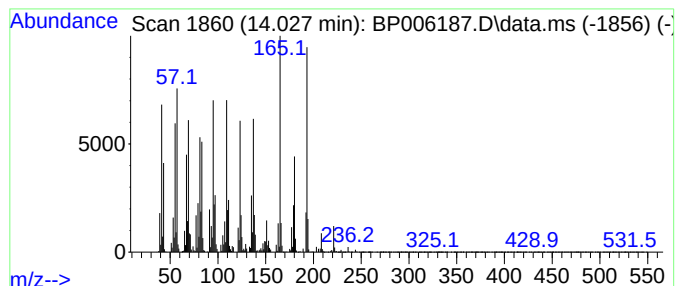
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Decahydro-4,4,8,9,10-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.028	13.09 ng	2070140	Acenaphthene-d10	14.498	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	70
2	1,3,5-Triethylcyclotrisiloxane	222	C6H18O3Si3	018442-02-9	64
3	2,4,4-Trimethyl-3-(3-methylbutyl...	208	C14H24O	088725-82-0	58
4	1,3-Pentadiene, 2,4-di-t-butyl-	180	C13H24	132850-21-6	50
5	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
Data File : BP006187.D
Acq On : 12 Jul 2021 18:30
Operator : CG/JU
Sample : M3001-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

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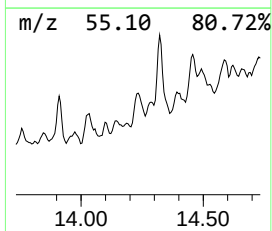
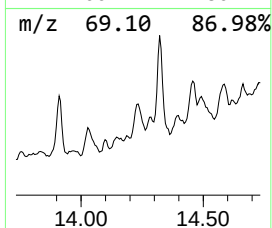
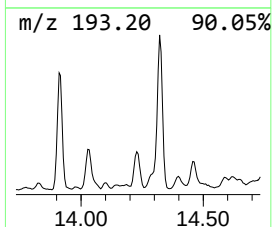
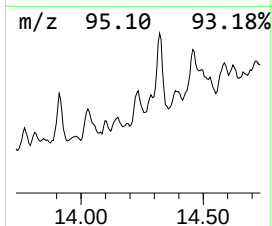
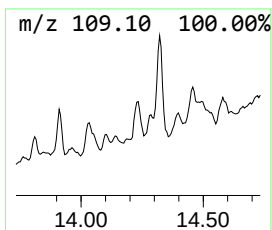
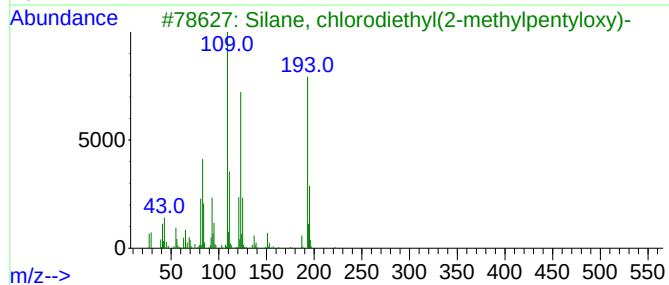
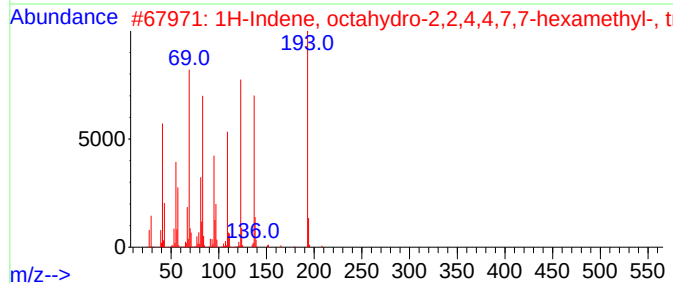
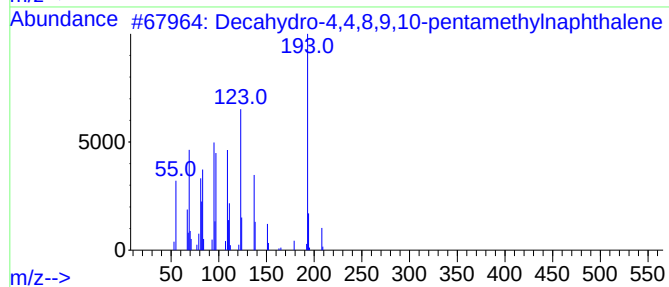
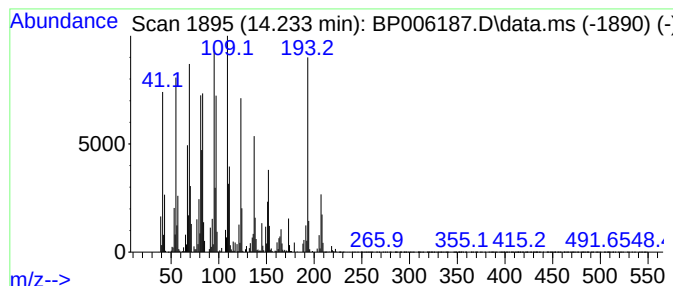
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.233 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	13.94 ng	2204030	Acenaphthene-d10	14.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	90
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	47
3			Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	46
4			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	38
5			Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
Data File : BP006187.D
Acq On : 12 Jul 2021 18:30
Operator : CG/JU
Sample : M3001-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
N9994

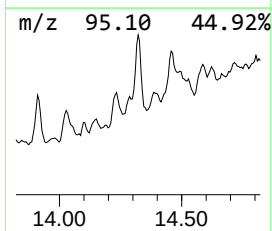
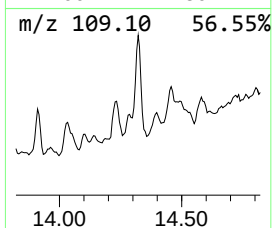
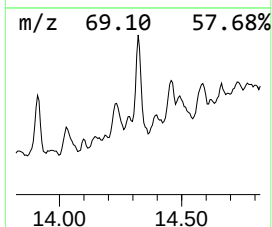
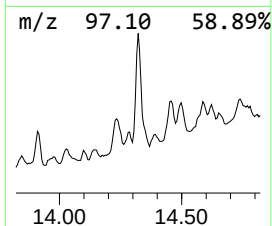
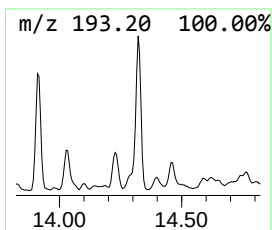
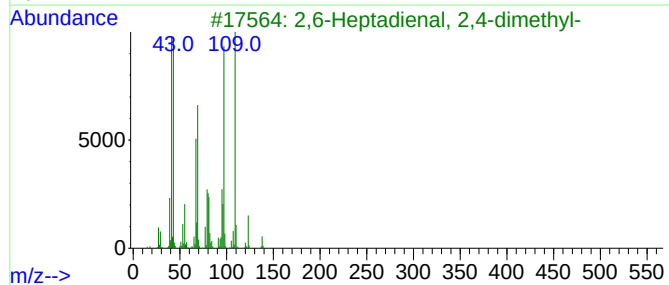
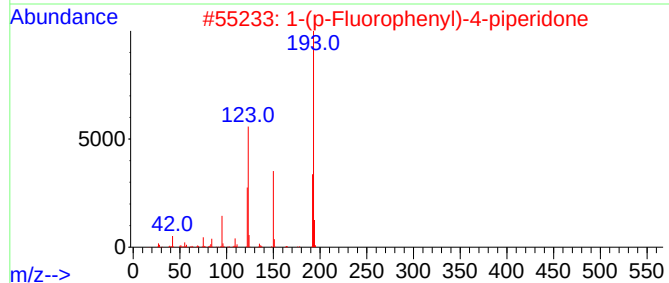
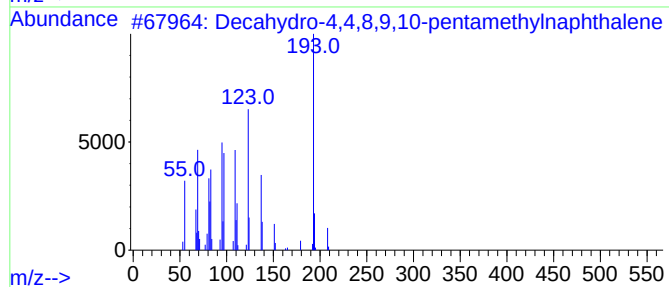
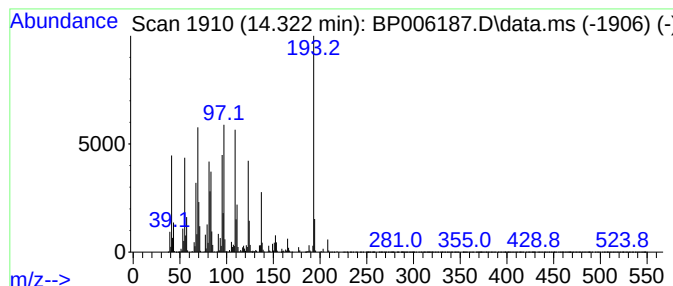
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown14.322 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.322	23.01 ng	3638340	Acenaphthene-d10	14.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	47
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
3			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	35
4			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	25
5			Pyrazole, 5-methyl-3-(5-nitro-2-...	193	C8H7N3O3	016239-90-0	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
Data File : BP006187.D
Acq On : 12 Jul 2021 18:30
Operator : CG/JU
Sample : M3001-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

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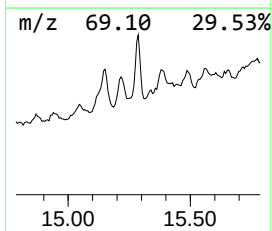
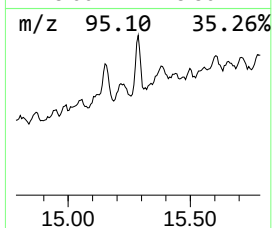
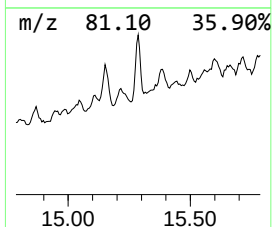
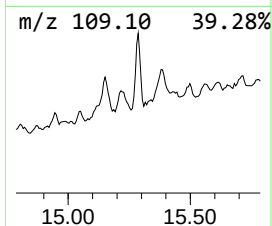
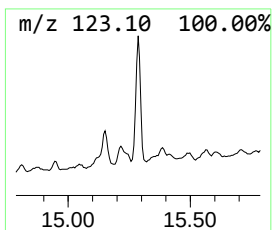
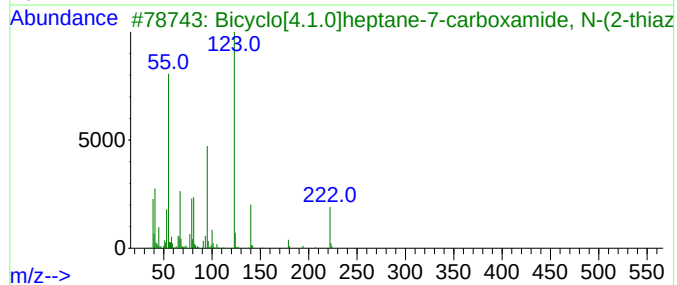
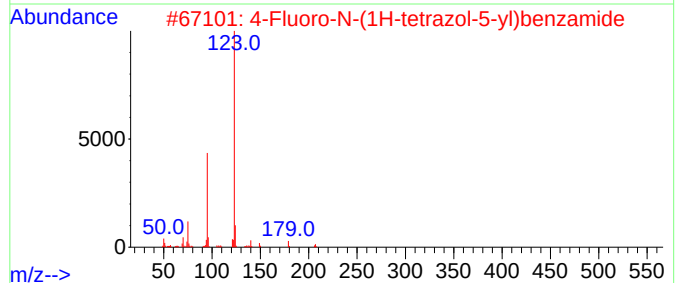
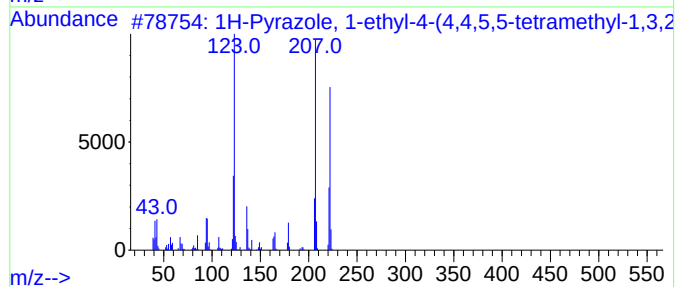
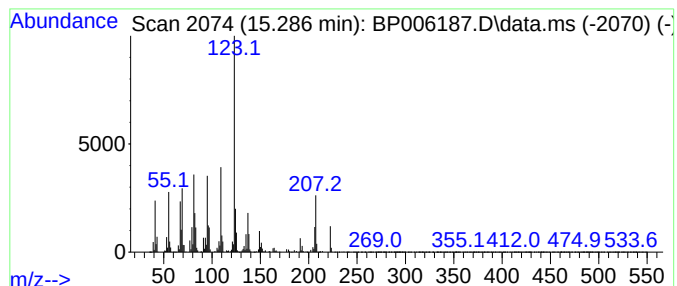
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.286 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	28.00 ng	4427810	Acenaphthene-d10	14.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrazole, 1-ethyl-4-(4,4,5,5-...	222	C11H19BN2O2	1000319-69-6	47
2			4-Fluoro-N-(1H-tetrazol-5-yl)ben...	207	C8H6FN5O	1000306-76-6	43
3			Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2O5	329912-72-3	38
4			3-Fluorobenzoic acid, 3-methylbu...	208	C12H13F02	154559-38-3	38
5			Furan, 2-methyl-5-(1,1,5-trimeth...	206	C14H22O	077143-15-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP071221\
Data File : BP006187.D
Acq On : 12 Jul 2021 18:30
Operator : CG/JU
Sample : M3001-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
N9994

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.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
Ethanol, 2-(2-b...	10.451	12.3	ng	924986	2	10.663	1500570	20.0
unknown12.375	12.375	4.1	ng	305883	2	10.663	1500570	20.0
Phthalic anhydride	12.475	3.0	ng	223096	2	10.663	1500570	20.0
unknown12.581	12.581	3.0	ng	225679	2	10.663	1500570	20.0
2-Pentanone, 4-...	13.275	2.2	ng	345184	3	14.498	3162640	20.0
unknown13.910	13.910	12.5	ng	1972920	3	14.498	3162640	20.0
Decahydro-4,4,8...	14.028	13.1	ng	2070140	3	14.498	3162640	20.0
unknown14.233	14.233	13.9	ng	2204030	3	14.498	3162640	20.0
unknown14.322	14.322	23.0	ng	3638340	3	14.498	3162640	20.0
unknown15.286	15.286	28.0	ng	4427810	3	14.498	3162640	20.0