

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
 Data File : BF138048.D
 Acq On : 28 May 2024 15:38
 Operator : CG\JU
 Sample : P2615-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR200035

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.381	43	50	56	rVB	809877	1074314	33.00%	4.715%
2	5.663	603	608	611	rBV	2942605	2634214	80.91%	11.561%
3	6.651	771	776	779	rBV	2468960	2588486	79.50%	11.361%
4	7.034	838	841	845	rBV	1020037	794295	24.40%	3.486%
5	7.598	932	937	940	rBV	1879153	1648821	50.64%	7.236%
6	8.210	1038	1041	1047	rBV2	74588	106230	3.26%	0.466%
7	8.316	1056	1059	1063	rBV	1176020	973377	29.90%	4.272%
8	9.275	1219	1222	1226	rBV4	82002	142355	4.37%	0.625%
9	9.316	1226	1229	1233	rVV3	151197	194006	5.96%	0.851%
10	9.398	1238	1243	1246	rBV	3403596	3255822	100.00%	14.289%
11	9.469	1252	1255	1259	rBV	314131	361714	11.11%	1.588%
12	9.786	1306	1309	1312	rBV	1149221	928949	28.53%	4.077%
13	9.845	1316	1319	1322	rVV	387625	397005	12.19%	1.742%
14	9.945	1333	1336	1338	rBV2	889609	780810	23.98%	3.427%
15	9.969	1338	1340	1341	rVV2	322243	254073	7.80%	1.115%
16	9.992	1341	1344	1347	rVB	1439899	1231964	37.84%	5.407%
17	10.033	1348	1351	1353	rBV2	404179	484877	14.89%	2.128%
18	10.069	1354	1357	1358	rVV	674934	738838	22.69%	3.243%
19	10.086	1358	1360	1362	rVB	1159175	895187	27.49%	3.929%
20	10.422	1415	1417	1421	rBV3	519372	527303	16.20%	2.314%
21	10.498	1427	1430	1433	rVB	1444482	1207263	37.08%	5.299%
22	10.886	1494	1496	1500	rBV2	1012830	982415	30.17%	4.312%
23	15.821	2333	2335	2340	rVB	493681	582639	17.90%	2.557%

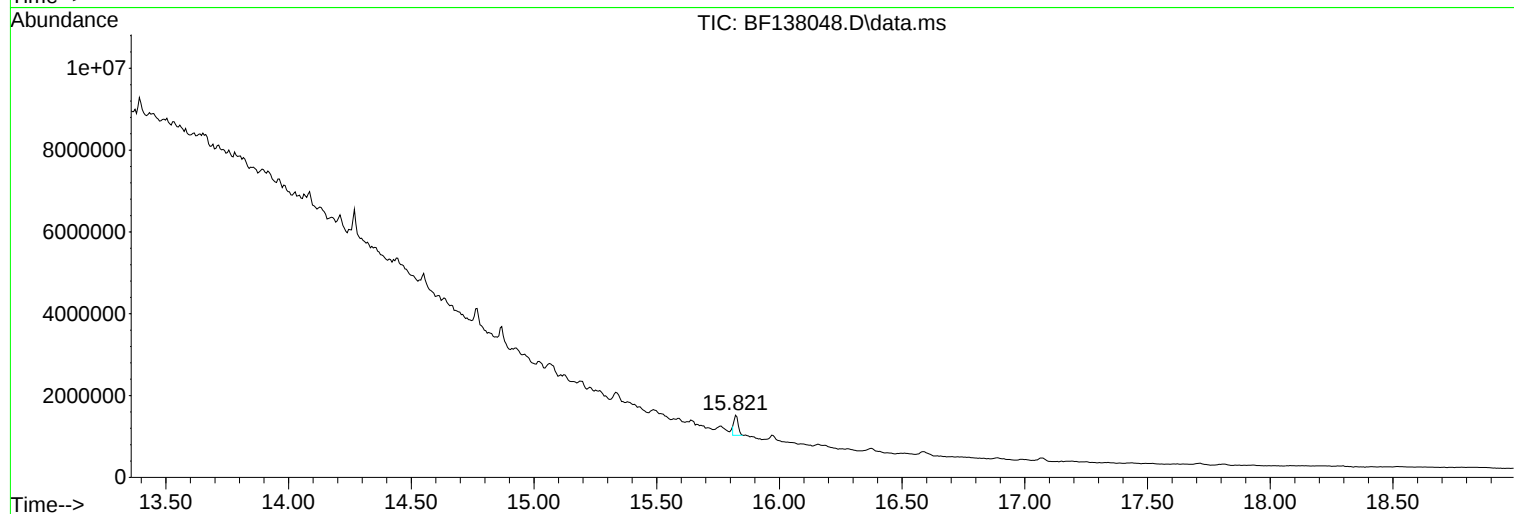
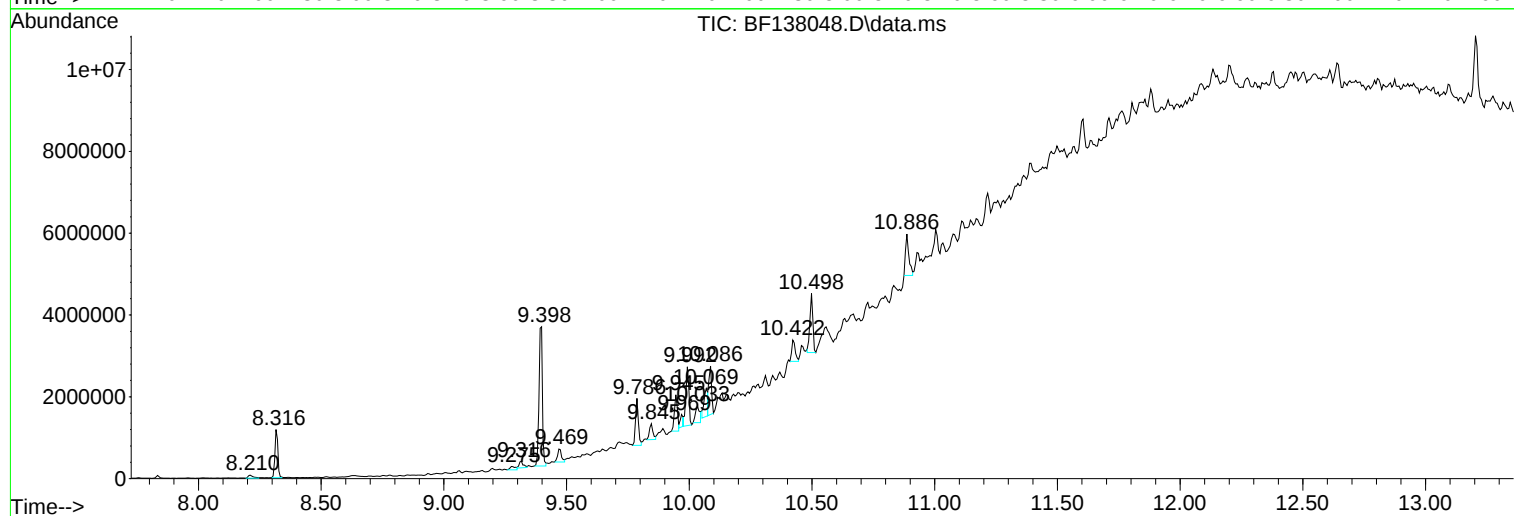
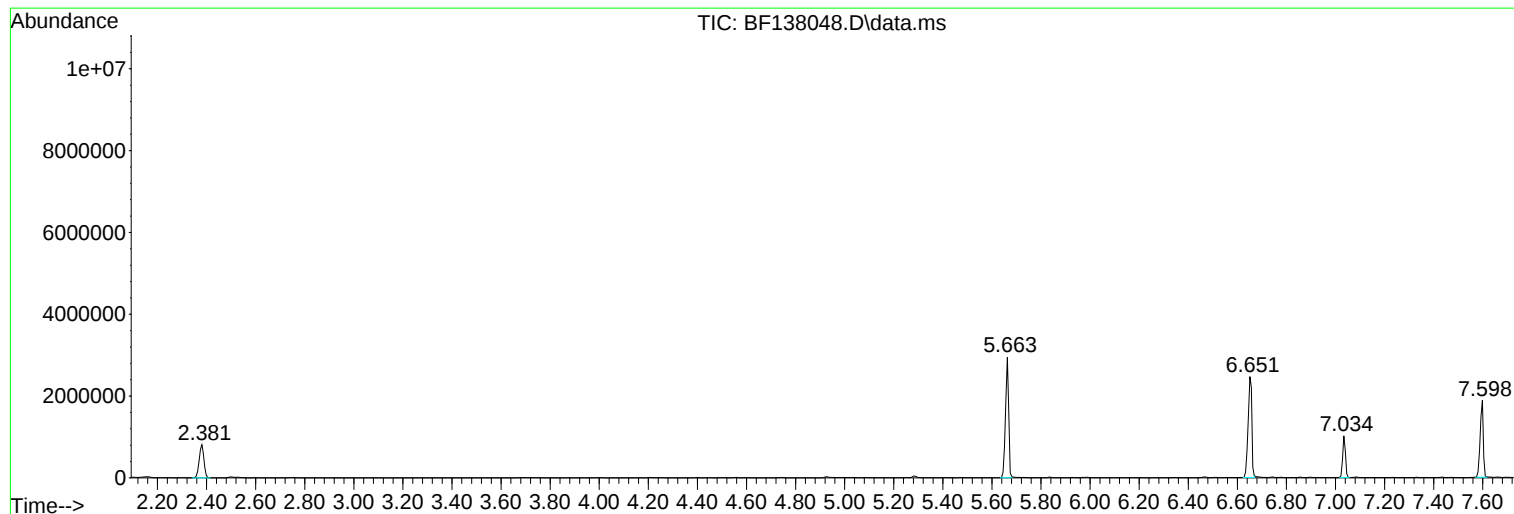
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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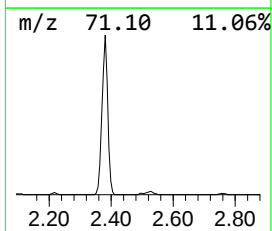
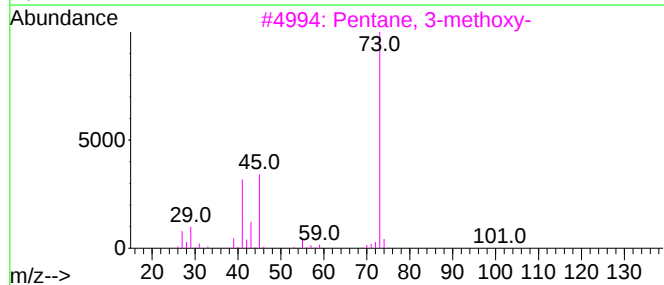
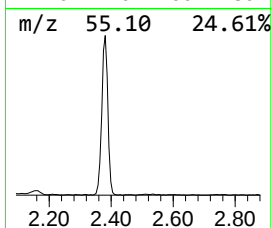
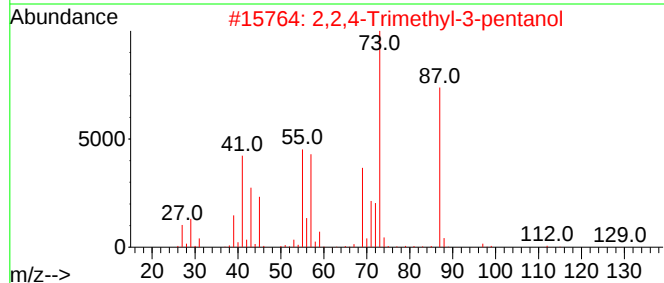
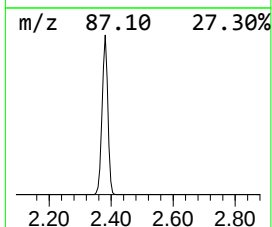
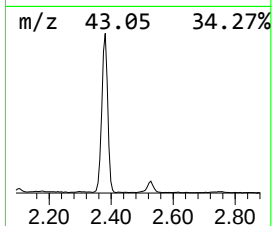
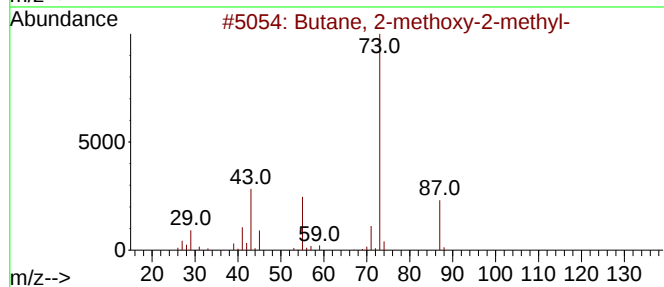
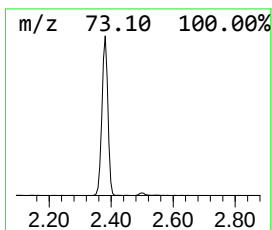
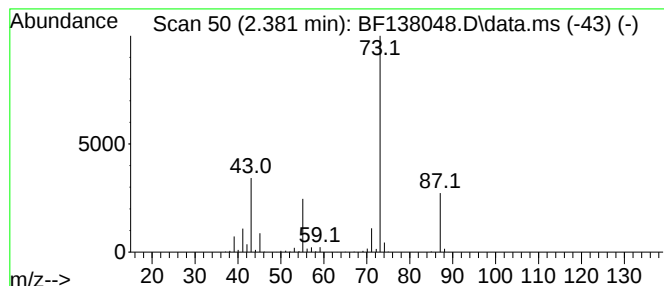
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.381	27.05 ng	1074310	1,4-Dichlorobenzene-d4	7.034

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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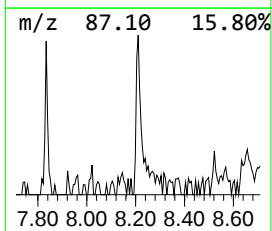
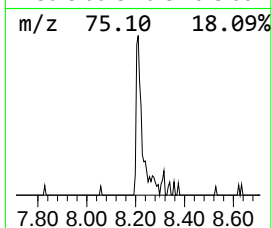
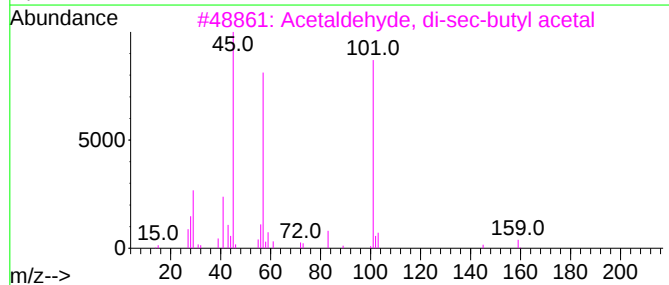
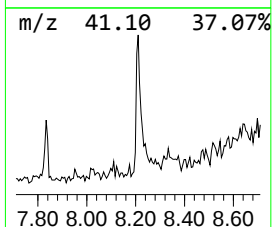
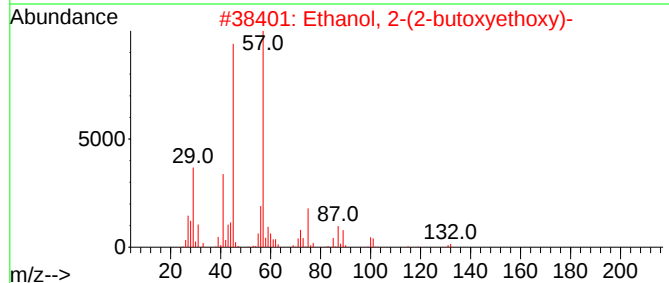
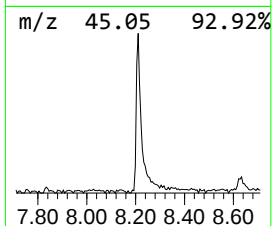
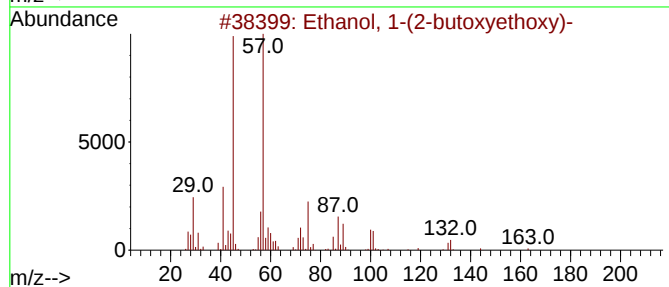
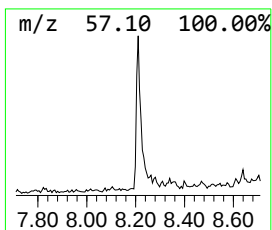
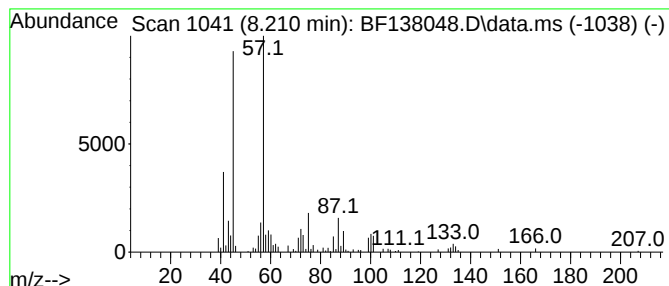
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.210	2.18 ng	106230	Naphthalene-d8	8.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	86
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
3			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	53
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Butane, 1,1'-[ethylidenebis(oxy)]...	174	C10H22O2	000871-22-7	47



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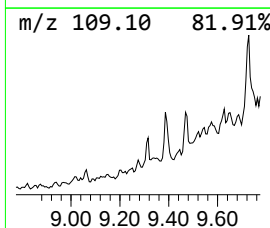
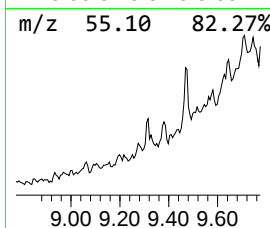
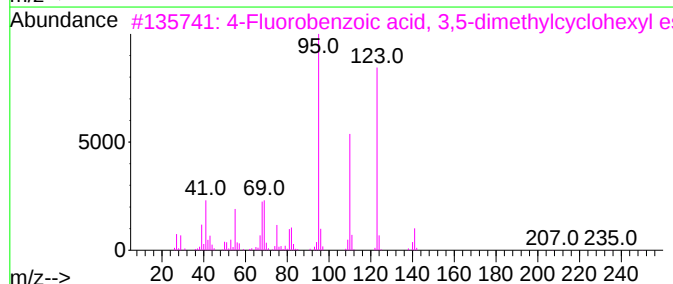
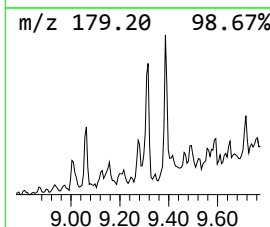
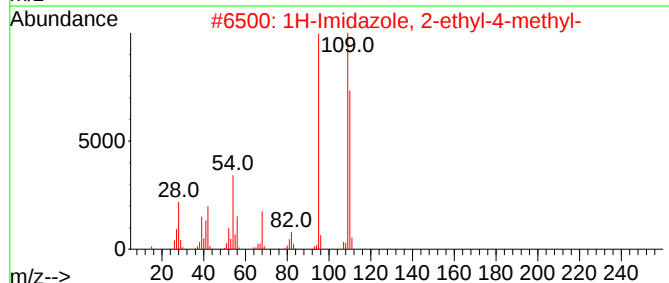
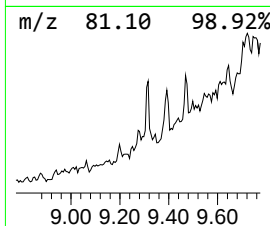
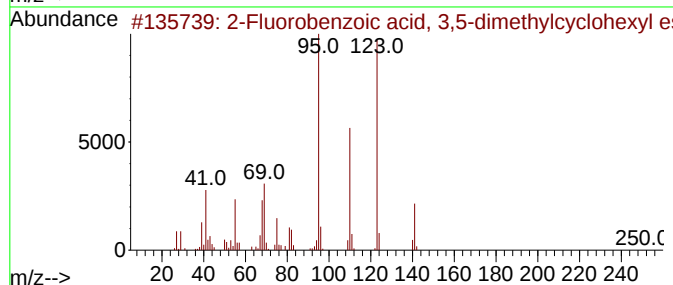
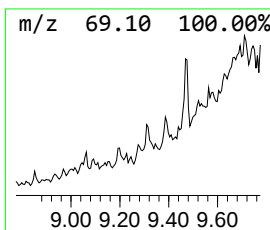
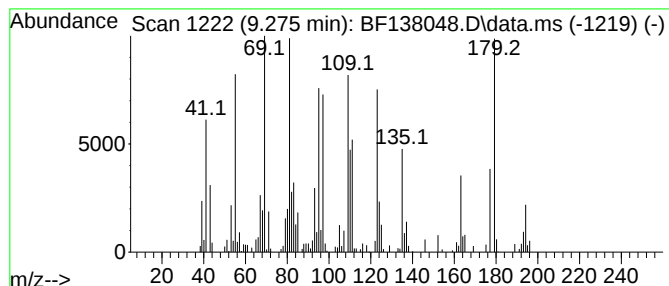
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.275 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.275	3.18 ng	142355	Acenaphthene-d10	10.086

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Fluorobenzoic acid, 3,5-dimeth...	250	C15H19F02	1000278-96-6	22
2		1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	22
3		4-Fluorobenzoic acid, 3,5-dimeth...	250	C15H19F02	1000279-07-3	22
4		Isoxazole, 3,4-dimethyl-5-(2-thi...	179	C9H9N0S	056421-65-9	18
5		Phosphine, bis(1-methylethyl)phe...	194	C12H19P	006372-43-6	18



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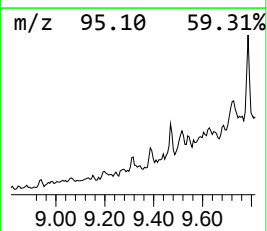
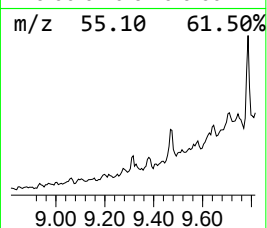
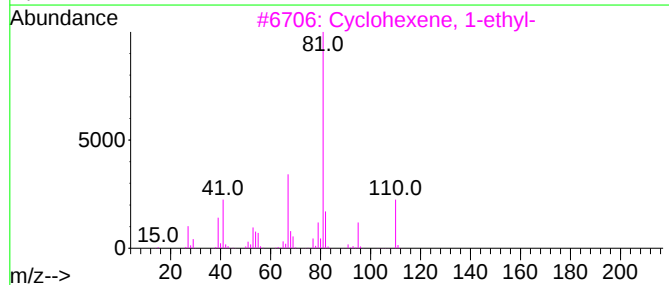
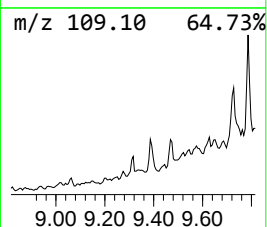
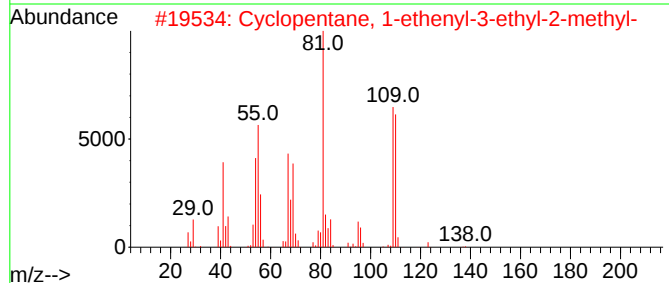
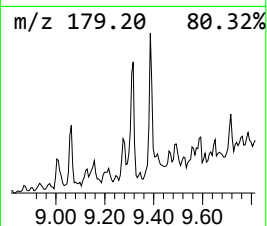
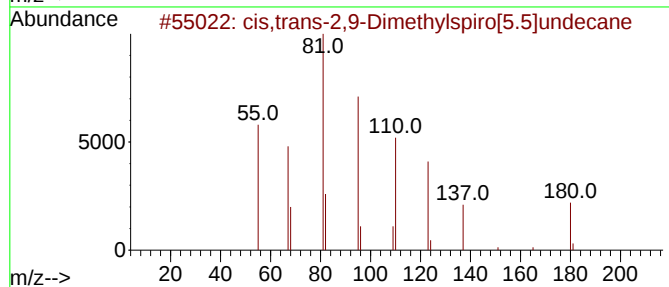
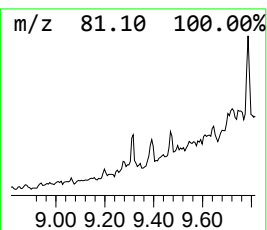
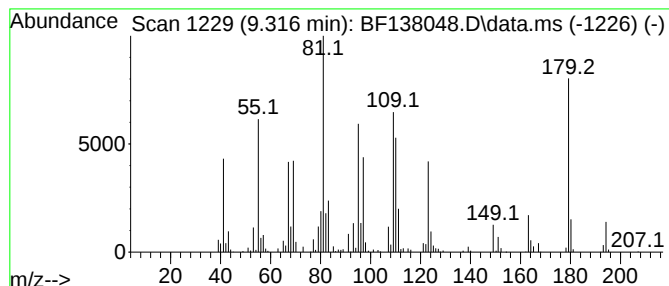
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Peak Number 4 cis,trans-2,9-Dimethylspiro... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.316	4.33 ng	194006	Acenaphthene-d10		10.086	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	cis,trans-2,9-Dimethylspiro[5.5]...		180	C13H24	095530-74-8	55
2	Cyclopentane, 1-ethenyl-3-ethyl-...		138	C10H18	055170-98-4	35
3	Cyclohexene, 1-ethyl-		110	C8H14	001453-24-3	30
4	Cyclohexane, ethylidene-		110	C8H14	001003-64-1	27
5	1-Octanone, 1-(2-furanyl)-		194	C12H18O2	005456-77-9	25



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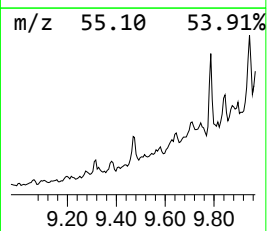
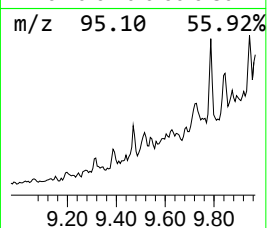
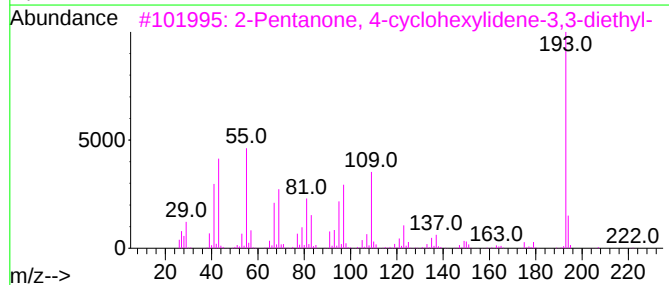
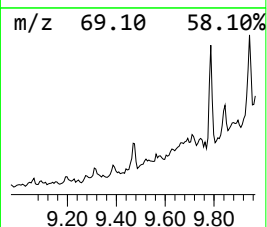
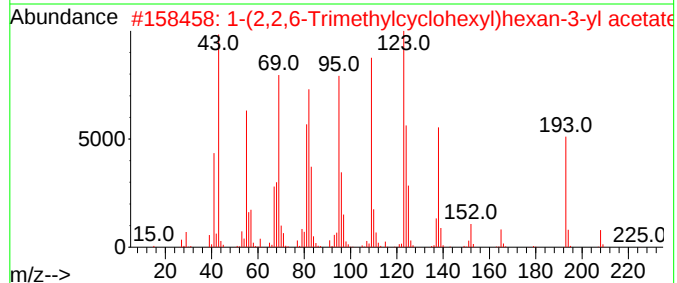
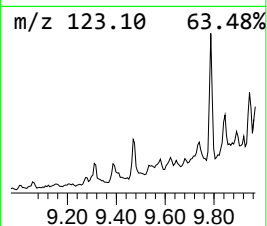
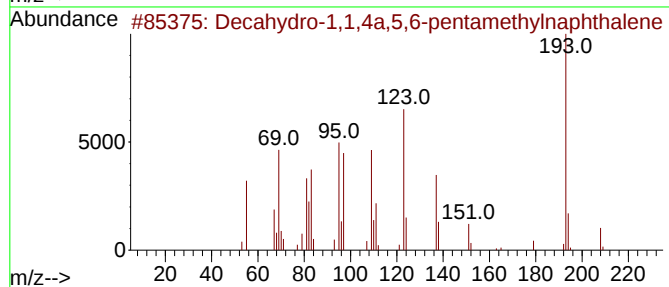
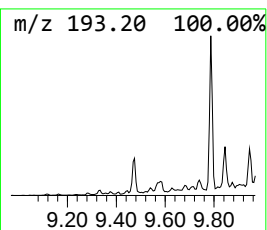
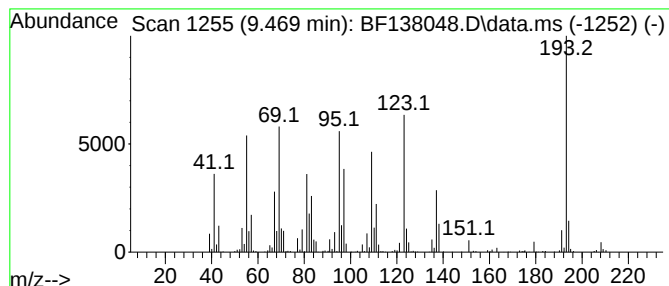
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Peak Number 5 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD			R.T.	
9.469	8.08 ng	361714	Acenaphthene-d10			10.086	
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	83
2			1-(2,2,6-Trimethylcyclohexyl)hex...	268	C17H32O2	1000498-96-1	53
3			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	52
4			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
5			1-Anthracenamine	193	C14H11N	000610-49-1	35



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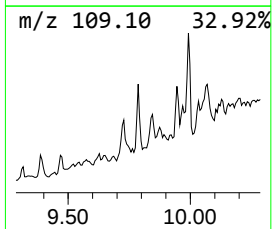
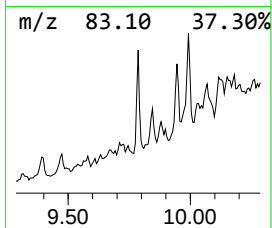
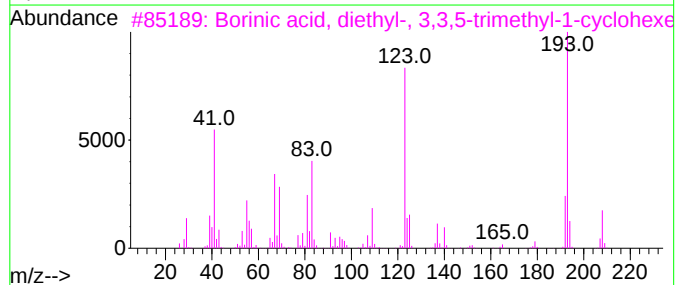
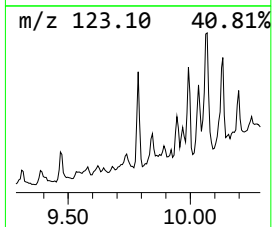
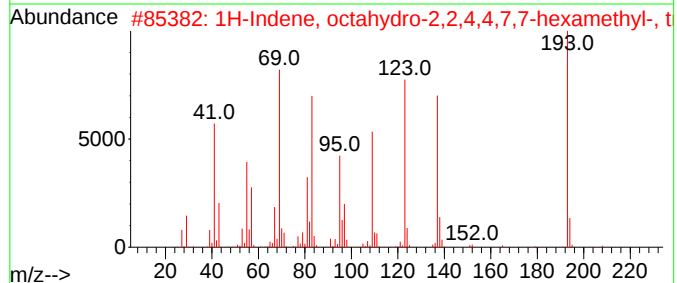
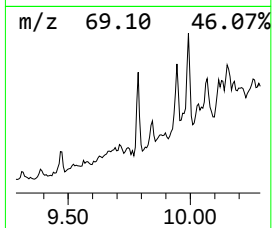
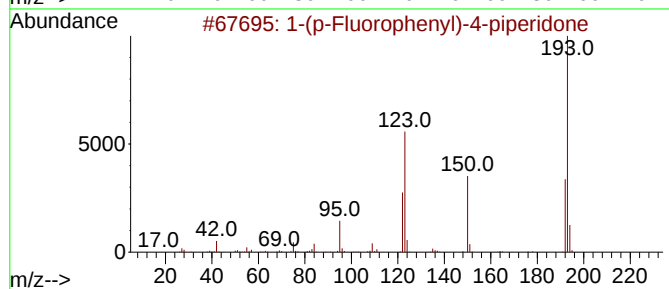
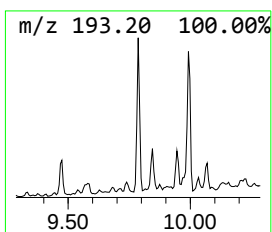
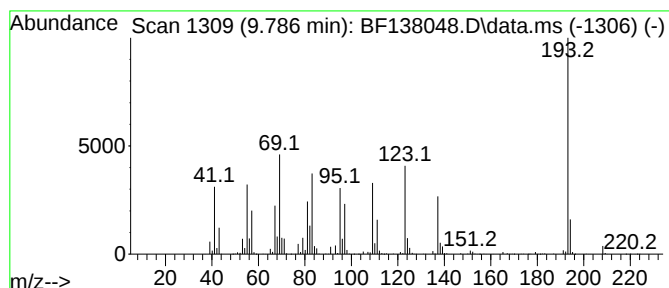
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 1-(p-Fluorophenyl)-4-piperi... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.786	20.75 ng	928949	Acenaphthene-d10	10.086	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	50
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43
3	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	40
4	9-Phenanthrenamine	193	C14H11N	000947-73-9	38
5	2-Anthracenamine	193	C14H11N	000613-13-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138048.D
Acq On : 28 May 2024 15:38
Operator : CG\JU
Sample : P2615-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

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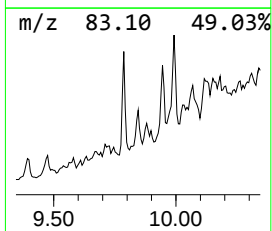
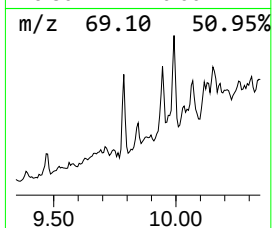
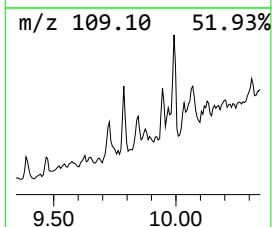
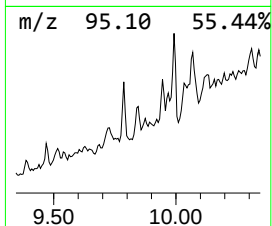
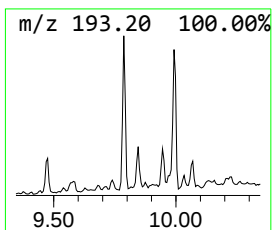
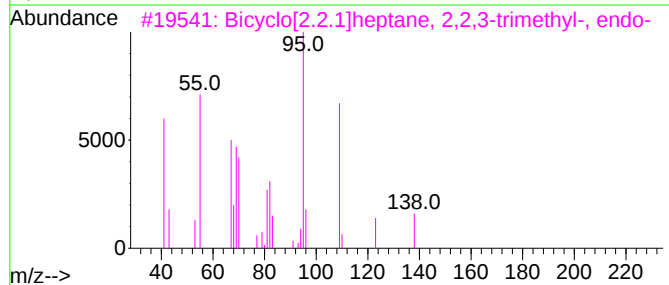
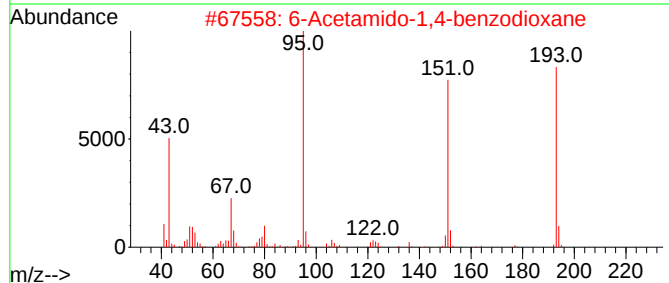
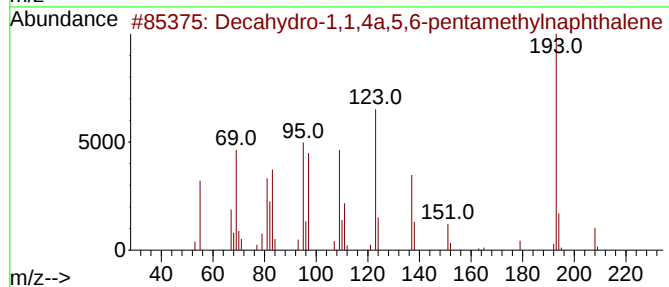
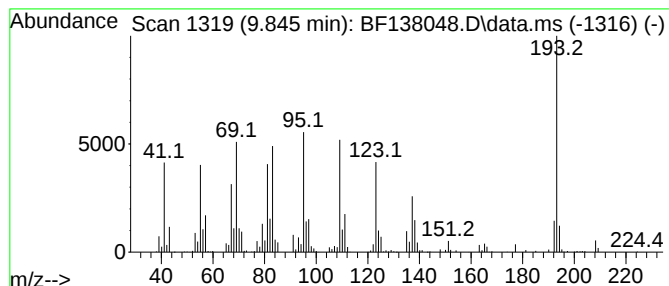
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown9.845 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.845	8.87 ng	397005	Acenaphthene-d10	10.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	49
2			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	38
3			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	30
4			[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	18
5			3-Phenylindole	193	C14H11N	001504-16-1	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138048.D
Acq On : 28 May 2024 15:38
Operator : CG\JU
Sample : P2615-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

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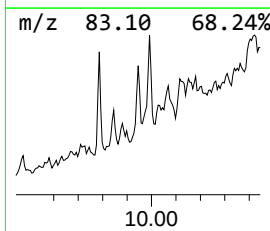
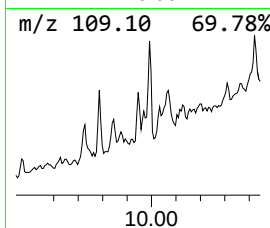
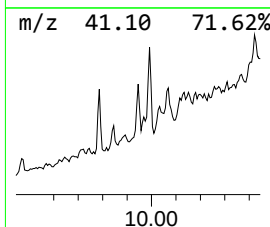
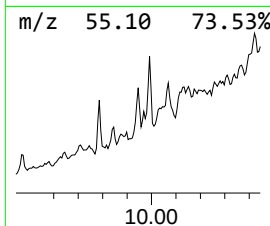
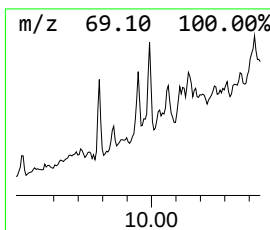
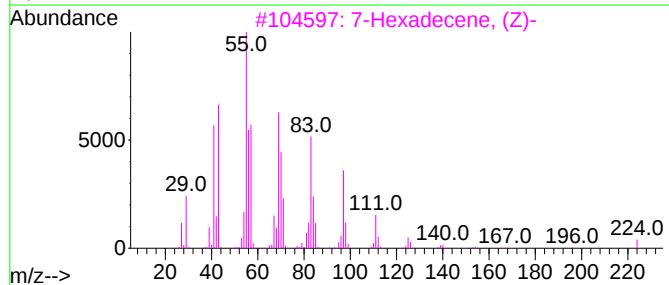
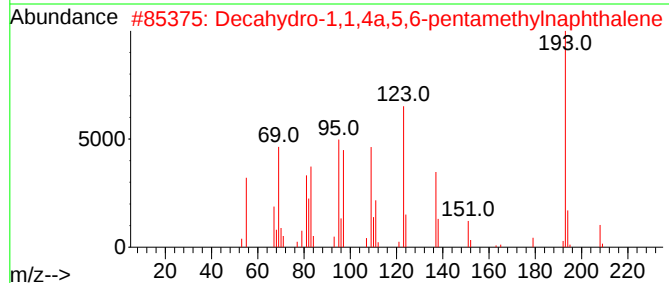
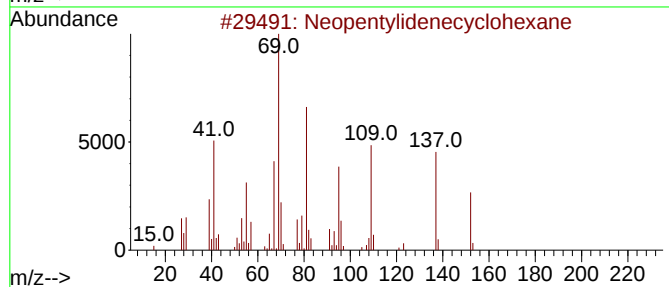
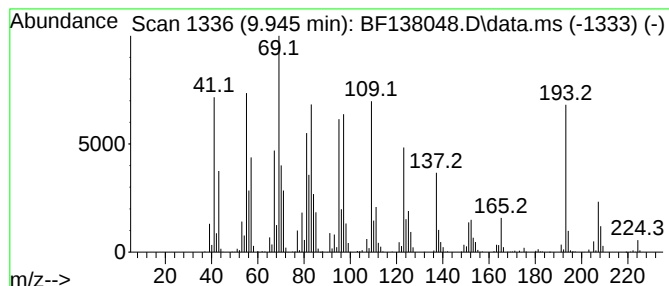
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown9.945 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.945	17.44 ng	780810	Acenaphthene-d10	10.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neopentylidenecyclohexane	152	C11H20	039546-80-0	43
2			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	43
3			7-Hexadecene, (Z)-	224	C16H32	035507-09-6	38
4			Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	30
5			Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138048.D
Acq On : 28 May 2024 15:38
Operator : CG\JU
Sample : P2615-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

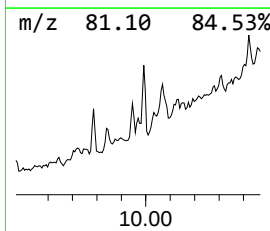
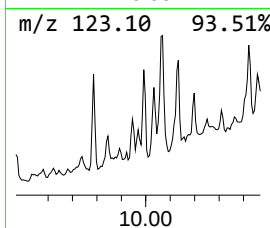
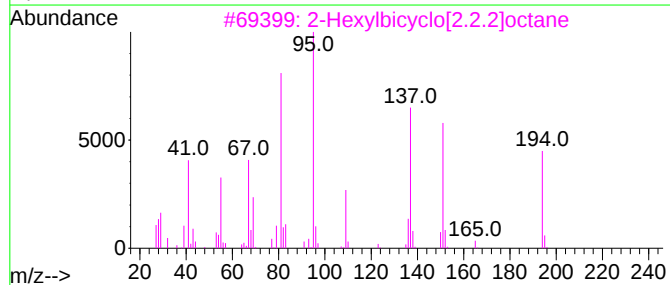
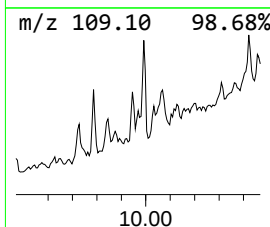
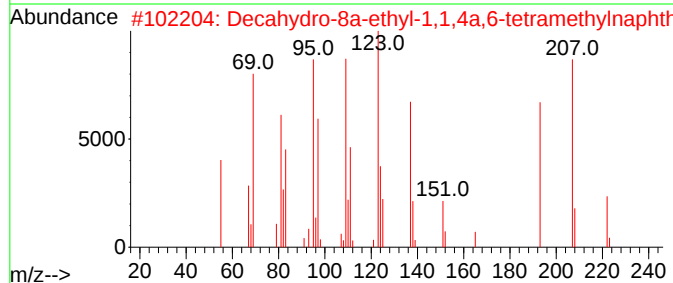
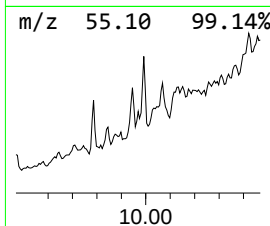
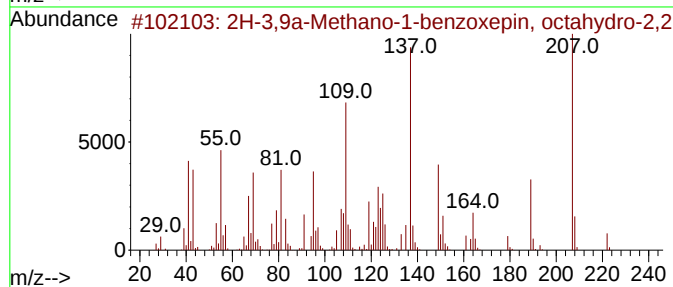
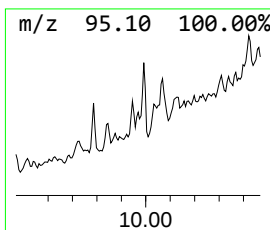
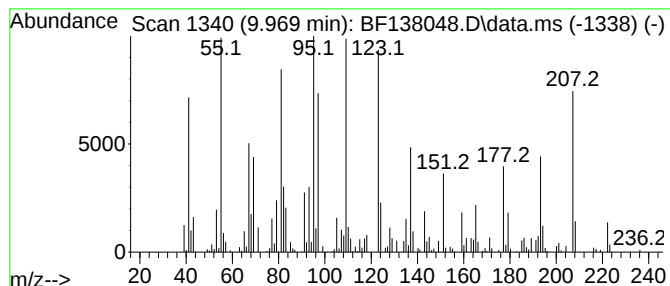
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown9.969 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.969	5.68 ng	254073	Acenaphthene-d10	10.086	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-3,9a-Methano-1-benzoxepin, oc...	222	C15H26O	005956-09-2	45
2	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	42
3	2-Hexylbicyclo[2.2.2]octane	194	C14H26	1000435-94-1	38
4	1-Hexylbicyclo[2.2.2]octane	194	C14H26	1000435-94-2	27
5	(1aR,3S,3aS,7R,7aR,7bS)-(-)-1a,2...	222	C15H26O	028329-86-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138048.D
Acq On : 28 May 2024 15:38
Operator : CG\JU
Sample : P2615-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

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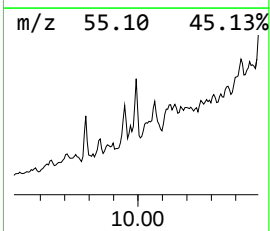
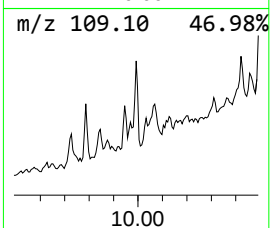
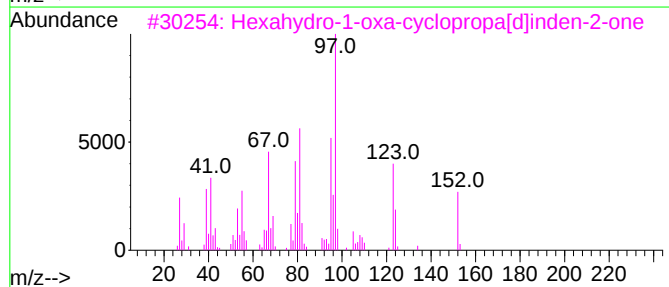
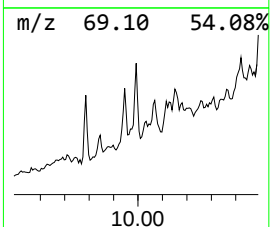
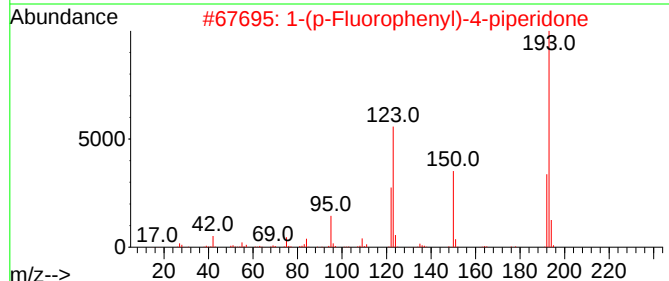
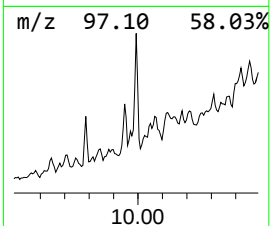
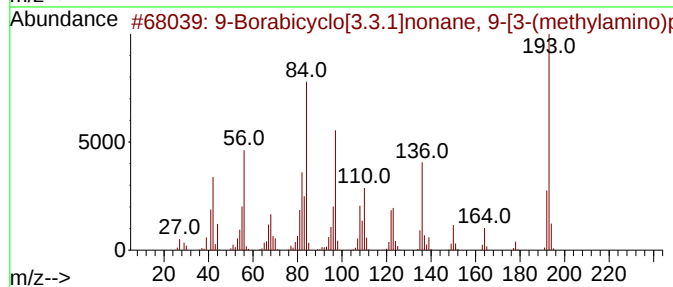
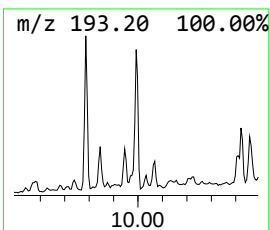
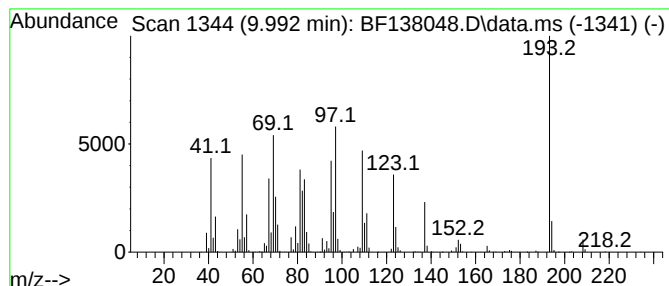
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown9.992 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.992	27.52 ng	1231960	Acenaphthene-d10	10.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1010162-56-0	43		
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38		
3	Hexahydro-1-oxa-cyclopropa[d]ind...	152	C9H12O2	037643-23-5	27		
4	Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	27		
5	s-Triazine, 2-amino-4-(morpholin...	278	C13H22N6O	021868-45-1	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138048.D
Acq On : 28 May 2024 15:38
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Sample : P2615-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

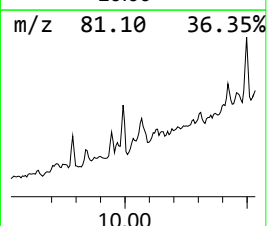
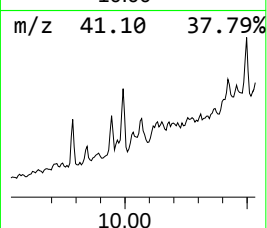
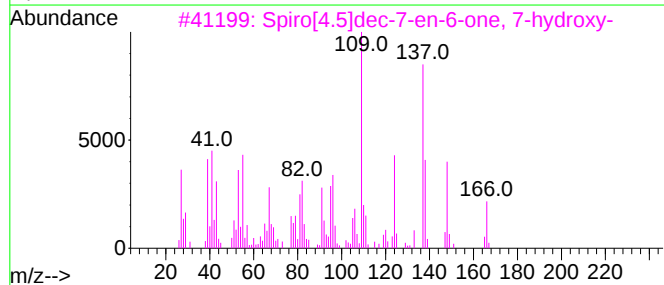
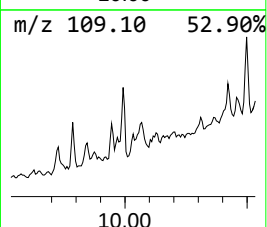
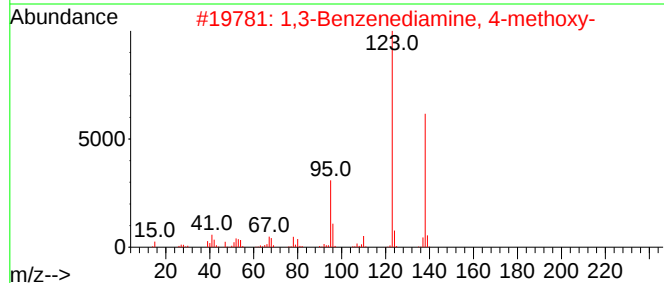
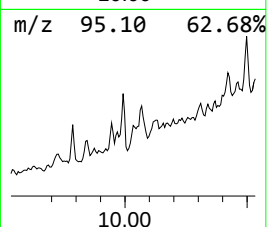
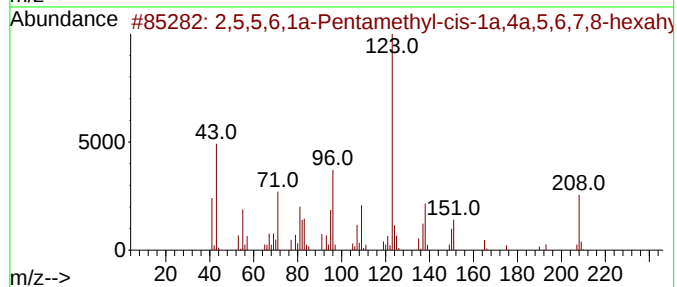
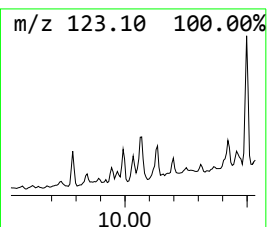
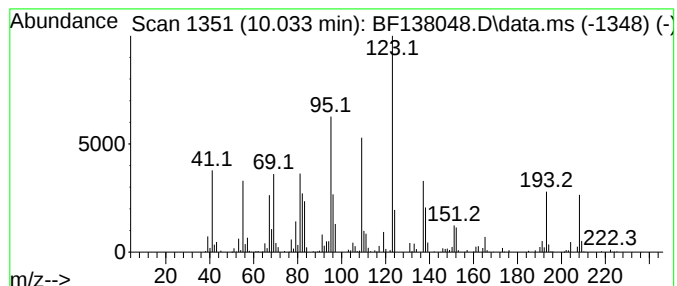
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2,5,5,6,1a-Pentamethyl-cis-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.033	10.83 ng	484877	Acenaphthene-d10	10.086	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5,5,6,1a-Pentamethyl-cis-1a,4a...	208	C14H24O	1010215-77-9	53
2	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	47
3	Spiro[4.5]dec-7-en-6-one, 7-hydr...	166	C10H14O2	108573-05-3	42
4	Ethanone, 1-(3-fluorophenyl)-	138	C8H7FO	000455-36-7	38
5	Cyclohexene, 1,4,6,6-tetramethyl-	138	C10H18	070092-37-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138048.D
Acq On : 28 May 2024 15:38
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Misc :
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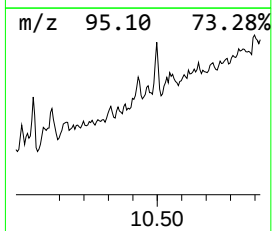
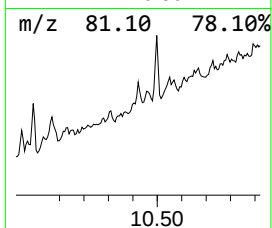
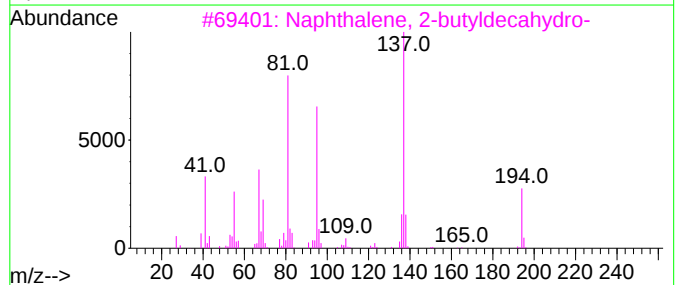
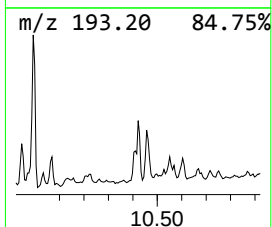
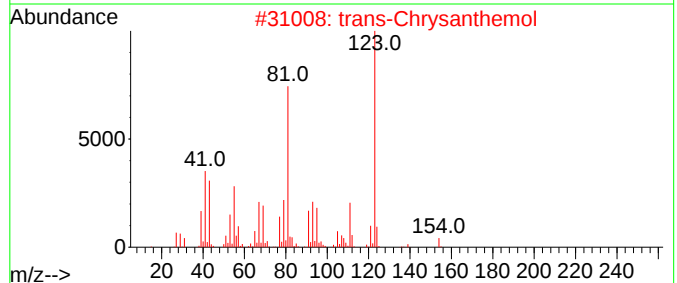
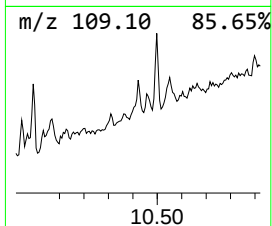
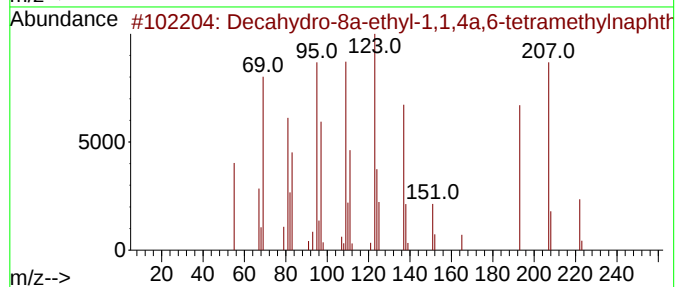
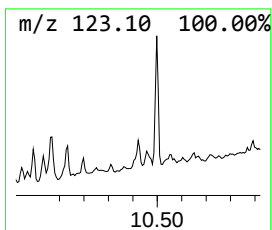
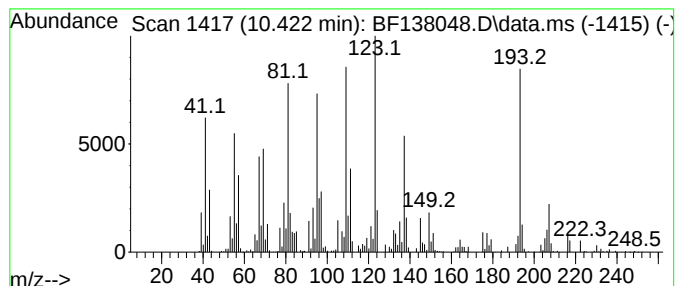
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Decahydro-8a-ethyl-1,1,4a,6... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.422	11.78 ng	527303	Acenaphthene-d10	10.086	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-8a-ethyl-1,1,4a,6-tetr...	222	C16H30	1000100-23-6	50
2	trans-Chrysanthemol	154	C10H18O	018383-58-9	38
3	Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	38
4	formamide, N-(4-butoxyphenyl)-	193	C11H15NO2	1000400-28-0	20
5	di-t-Butylacetylene	138	C10H18	017530-24-4	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138048.D
Acq On : 28 May 2024 15:38
Operator : CG\JU
Sample : P2615-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200035

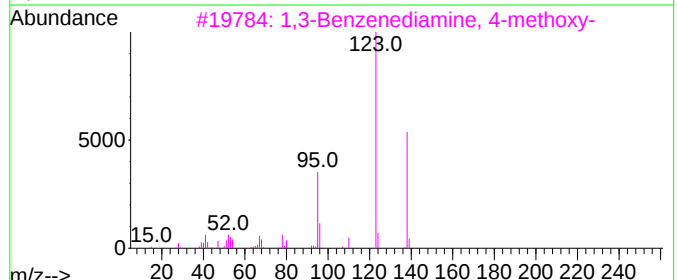
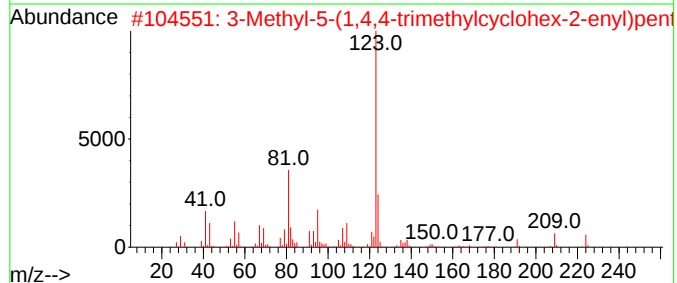
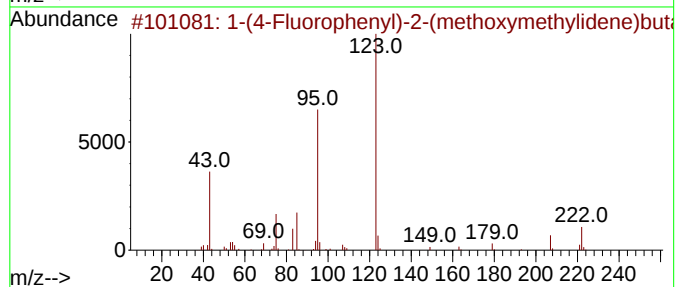
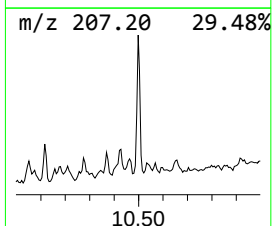
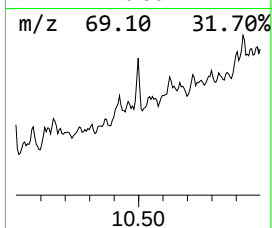
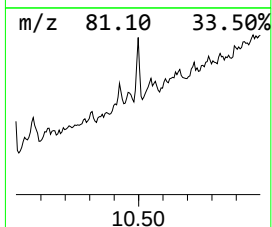
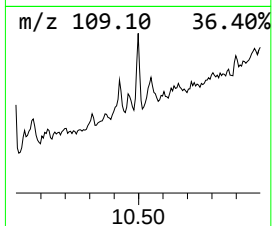
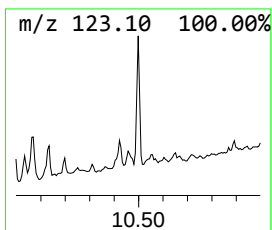
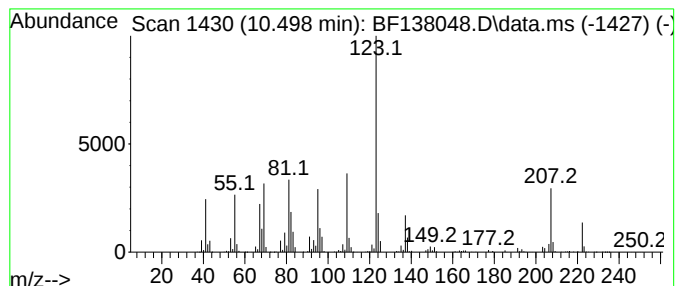
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 1-(4-Fluorophenyl)-2-(metho... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.498	26.97 ng	1207260	Acenaphthene-d10	10.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Fluorophenyl)-2-(methoxymet...	222	C12H11FO3	1000388-14-4	50		
2	3-Methyl-5-(1,4,4-trimethylcyclo...	224	C15H28O	1000187-09-1	50		
3	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	000615-05-4	47		
4	Benzamide, 3-fluoro-N-(2-phenyle...	313	C20H24FNO	1000451-30-5	47		
5	4-Nitrophenyl bicyclo[4.1.0]hept...	261	C14H15NO4	328938-65-4	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052824\
Data File : BF138048.D
Acq On : 28 May 2024 15:38
Operator : CG\JU
Sample : P2615-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200035

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF051424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.381	27.1	ng	1074310	1	7.034	794295	20.0
Ethanol, 1-(2-b...	8.210	2.2	ng	106230	2	8.316	973377	20.0
unknown9.275	9.275	3.2	ng	142355	3	10.086	895187	20.0
cis,trans-2,9-D...	9.316	4.3	ng	194006	3	10.086	895187	20.0
Decahydro-1,1,4...	9.469	8.1	ng	361714	3	10.086	895187	20.0
1-(p-Fluorophen...	9.786	20.8	ng	928949	3	10.086	895187	20.0
unknown9.845	9.845	8.9	ng	397005	3	10.086	895187	20.0
unknown9.945	9.945	17.4	ng	780810	3	10.086	895187	20.0
unknown9.969	9.969	5.7	ng	254073	3	10.086	895187	20.0
unknown9.992	9.992	27.5	ng	1231960	3	10.086	895187	20.0
2,5,5,6,1a-Pent...	10.033	10.8	ng	484877	3	10.086	895187	20.0
Decahydro-8a-et...	10.422	11.8	ng	527303	3	10.086	895187	20.0
1-(4-Fluorophen...	10.498	27.0	ng	1207260	3	10.086	895187	20.0