

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
 Data File : BF142368.D
 Acq On : 14 May 2025 16:17
 Operator : RC/JU
 Sample : Q2014-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MOO-25-0145

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-BF050525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142368.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.498	556	562	572	rVB	791632	1015703	38.14%	5.101%
2	6.510	728	734	740	rBV	897092	1114472	41.85%	5.597%
3	6.898	795	800	807	rBV	817893	1001051	37.59%	5.027%
4	7.298	863	868	873	rBV	608279	785425	29.49%	3.944%
5	7.457	885	895	899	rBV	679880	976436	36.67%	4.904%
6	7.545	905	910	914	rBV5	83389	128750	4.83%	0.647%
7	7.687	930	934	942	rVB	117408	189767	7.13%	0.953%
8	7.781	946	950	954	rBV	159747	204727	7.69%	1.028%
9	7.834	954	959	965	rBV5	145423	241094	9.05%	1.211%
10	7.998	981	987	990	rBV6	50944	124508	4.68%	0.625%
11	8.134	1006	1010	1012	rBV2	139122	180275	6.77%	0.905%
12	8.181	1012	1018	1024	rVV	1085491	1776888	66.73%	8.923%
13	8.239	1025	1028	1031	rVV2	227920	291405	10.94%	1.463%
14	8.269	1031	1033	1040	rVB	143814	205049	7.70%	1.030%
15	8.422	1055	1059	1061	rBV	239065	318002	11.94%	1.597%
16	8.481	1066	1069	1073	rVB3	375536	528214	19.84%	2.653%
17	8.569	1081	1084	1087	rBV3	187891	282695	10.62%	1.420%
18	8.604	1087	1090	1091	rVV	248692	291270	10.94%	1.463%
19	8.651	1092	1098	1102	rVB3	511092	1113635	41.82%	5.593%
20	8.775	1116	1119	1122	rBV2	305271	348359	13.08%	1.749%
21	8.875	1133	1136	1142	rBV5	319052	583928	21.93%	2.932%
22	9.181	1186	1188	1190	rBV3	415784	420426	15.79%	2.111%
23	9.257	1198	1201	1206	rBV	1450495	1917475	72.01%	9.629%
24	9.345	1212	1216	1220	rBV3	1059501	1673589	62.85%	8.405%
25	9.657	1266	1269	1275	rBV3	1472474	2662931	100.00%	13.373%
26	15.563	2268	2273	2295	rVB	822666	1536564	57.70%	7.717%

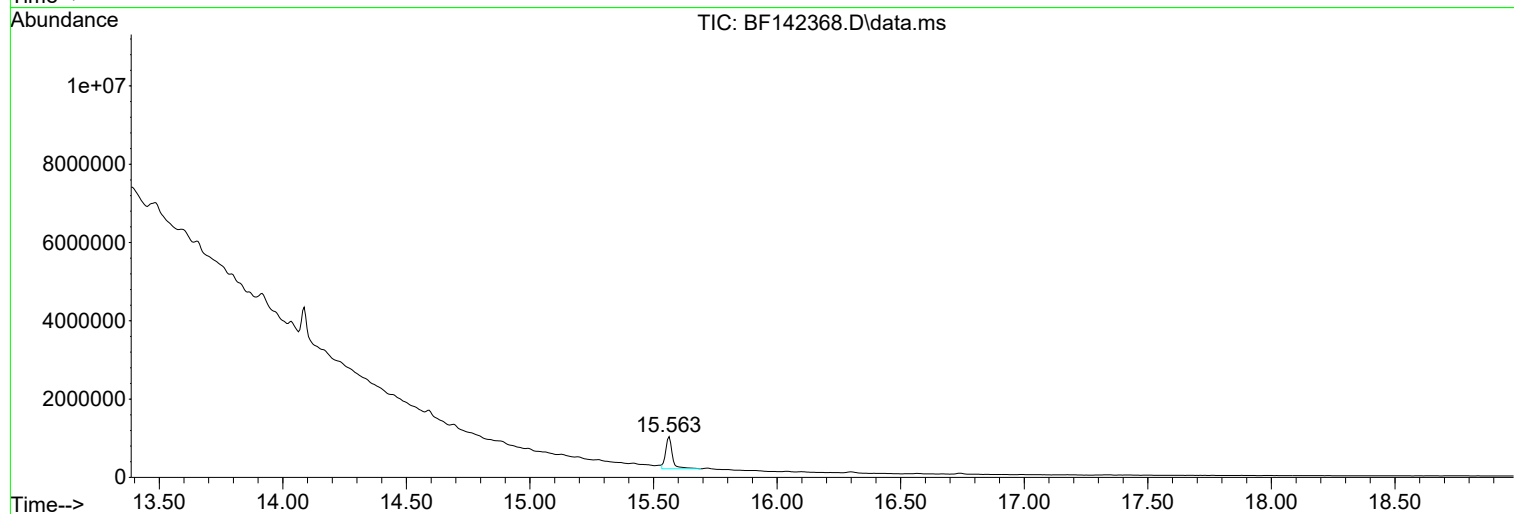
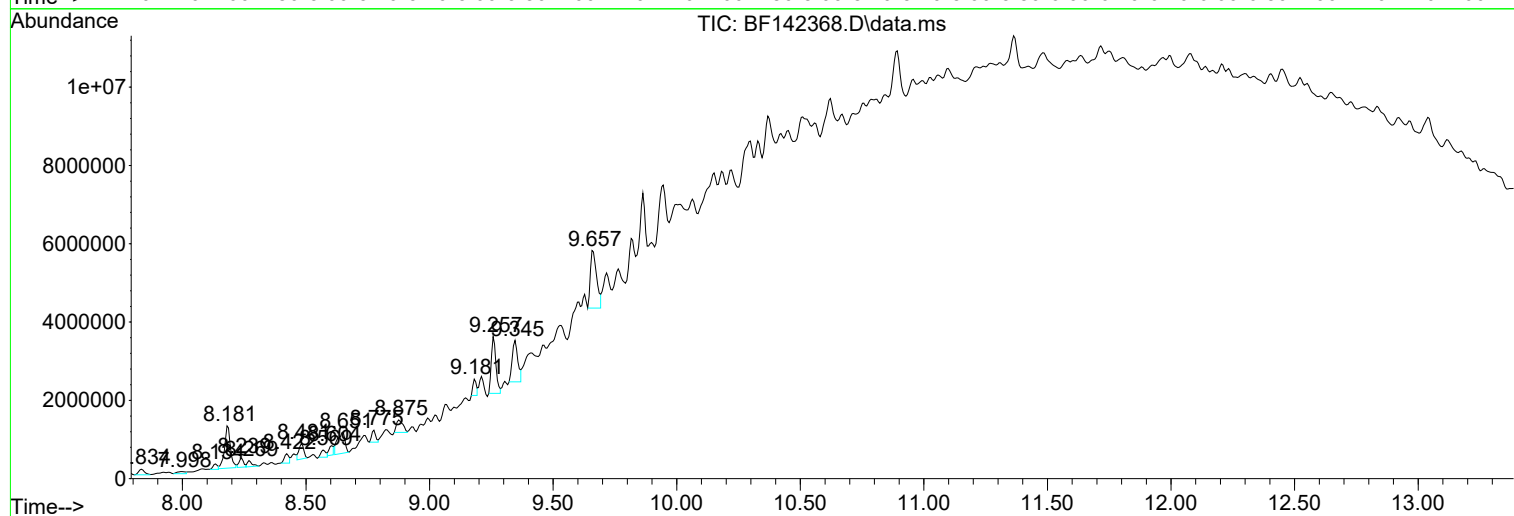
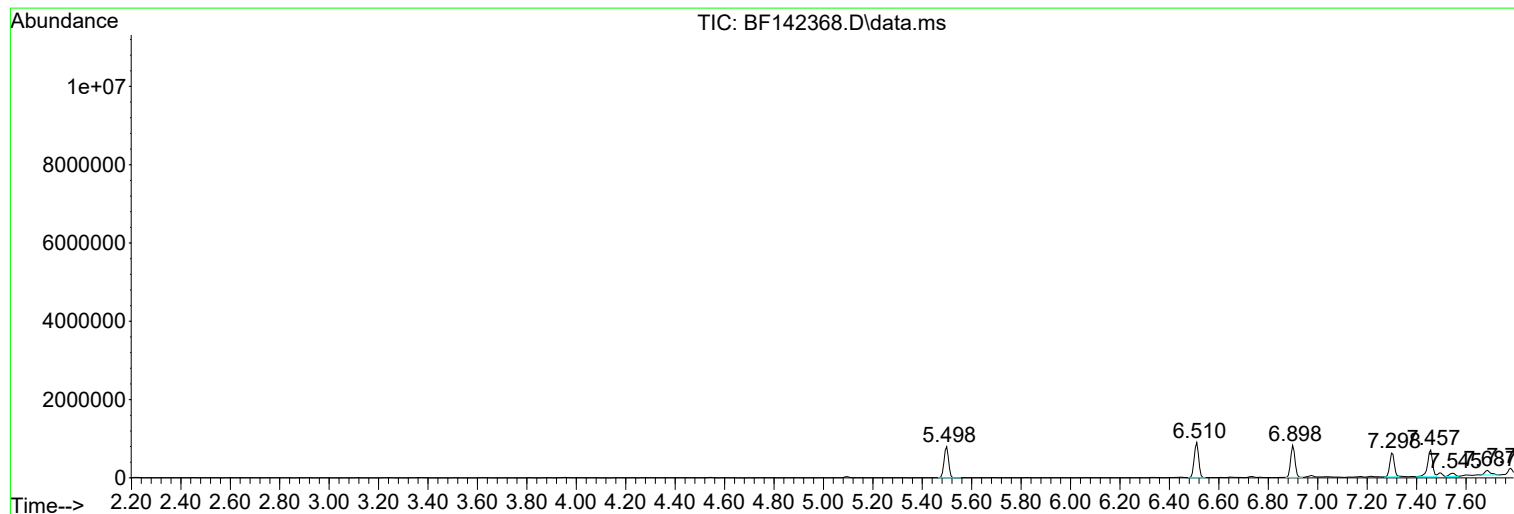
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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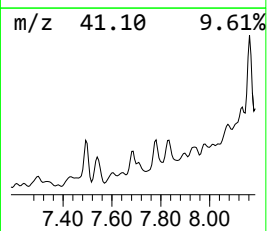
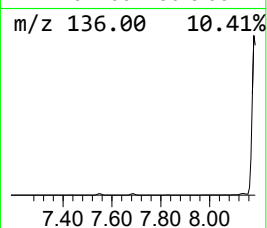
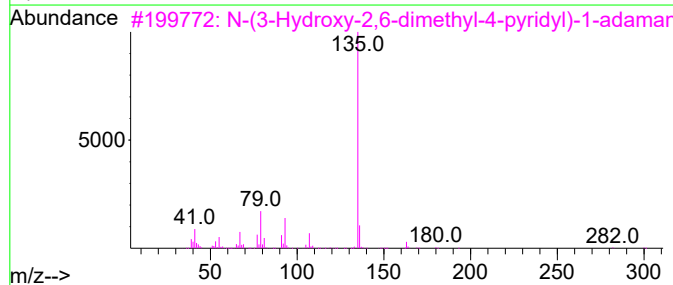
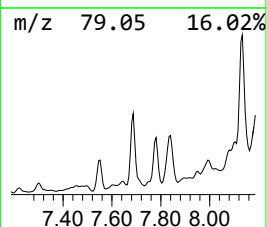
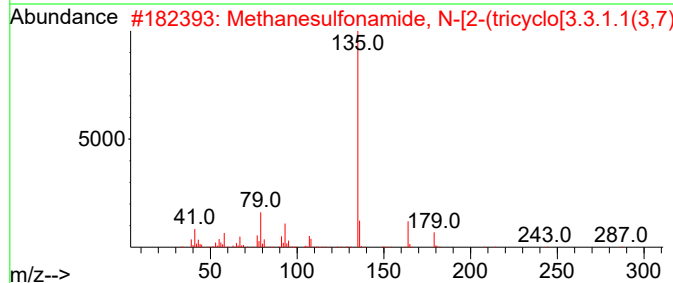
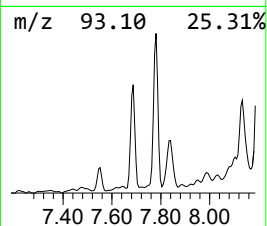
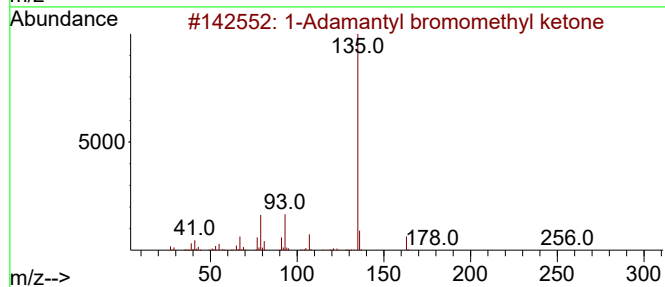
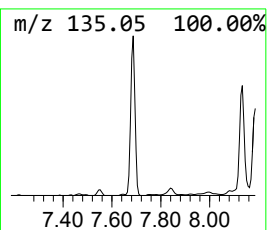
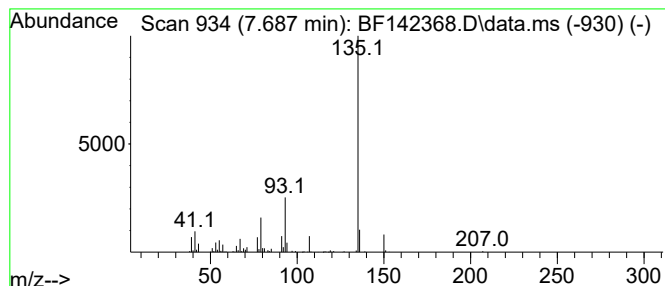
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Adamantyl bromomethyl ketone Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.687	2.14 ng	189767	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Adamantyl bromomethyl ketone	256	C12H17BrO	005122-82-7	80
2			Methanesulfonamide, N-[2-(tricyc...	287	C14H25NO3S	1000337-64-7	72
3			N-(3-Hydroxy-2,6-dimethyl-4-pyri...	300	C18H24N2O2	1000260-99-3	72
4			Adamantane-1-carbohydrazide	194	C11H18N2O	017846-15-0	72
5			Adamantane-1-carboxylic acid, (2...	332	C23H24O2	294876-57-6	72



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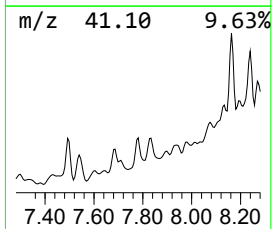
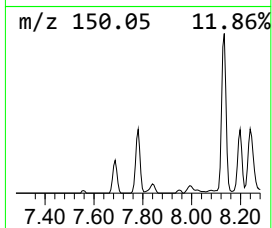
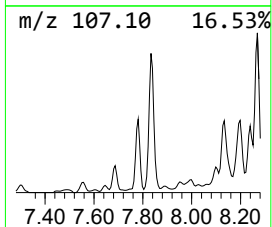
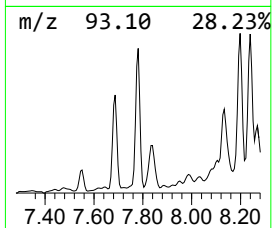
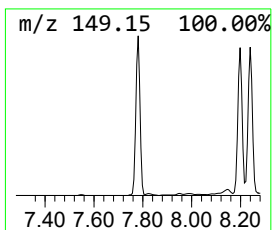
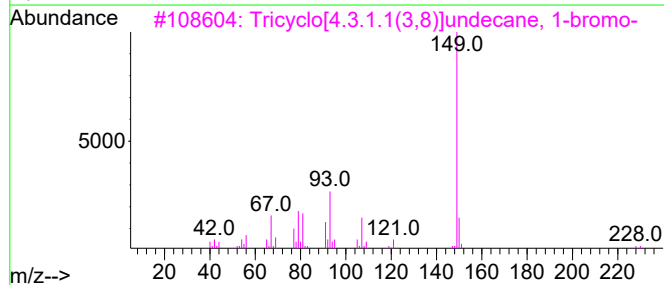
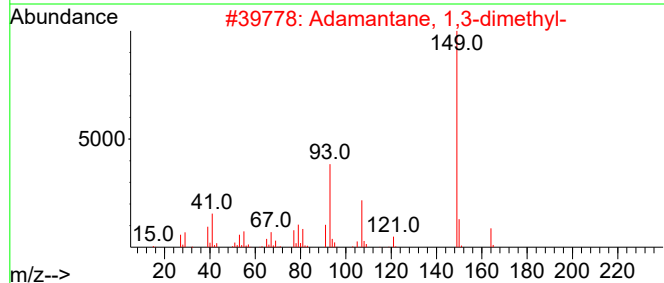
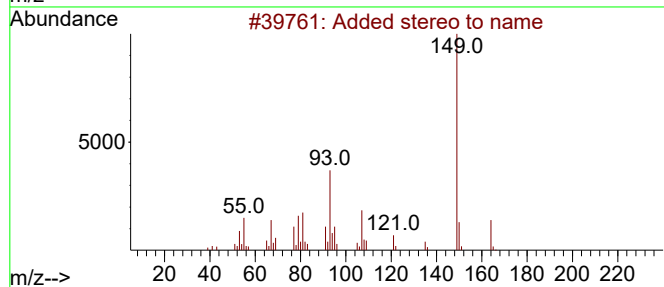
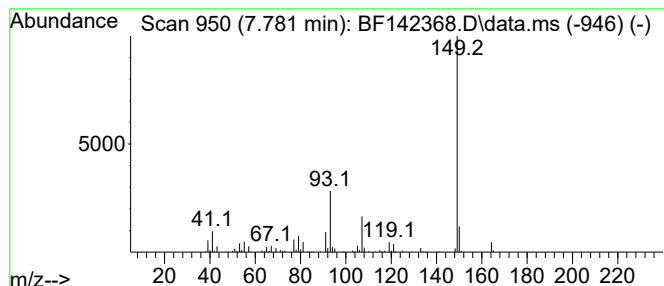
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Adamantane, 1,3-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.781	2.30 ng	204727	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Added stereo to name			164	C12H20	024145-89-9	72
2	Adamantane, 1,3-dimethyl-			164	C12H20	000702-79-4	64
3	Tricyclo[4.3.1.1(3,8)]undecane, ...			228	C11H17Br	021898-96-4	56
4	o-Toluic acid, 1-adamantylmethyl...			284	C19H24O2	1000292-22-6	53
5	2'-Hydroxy-4',5'-dimethylacetoph...			164	C10H12O2	036436-65-4	53



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ALS Vial : 10 Sample Multiplier: 1

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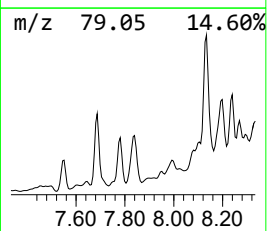
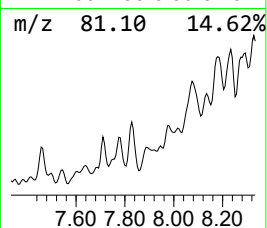
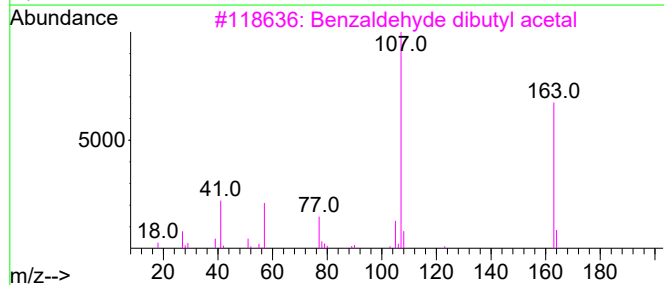
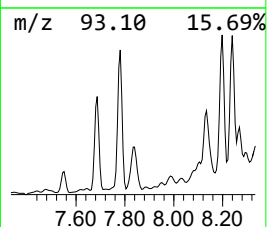
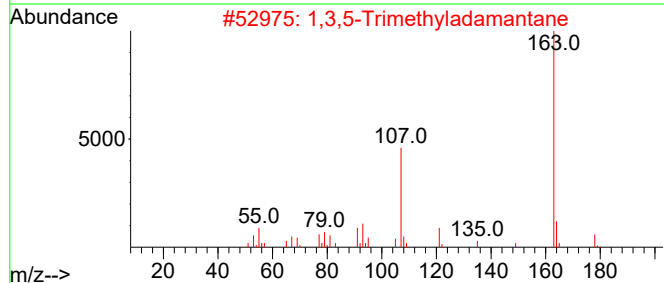
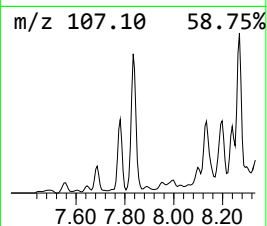
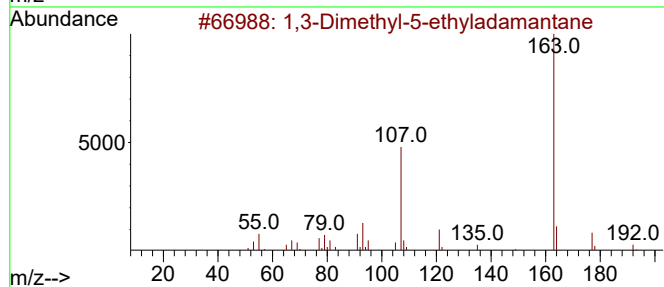
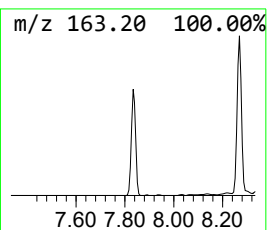
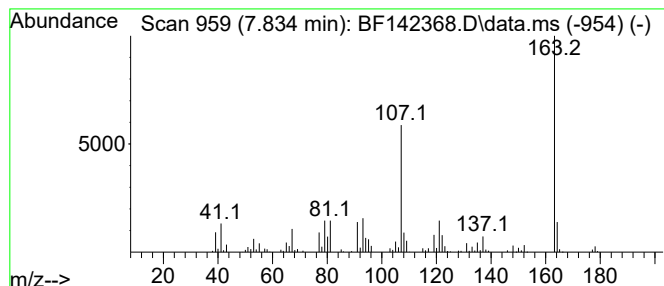
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1,3-Dimethyl-5-ethyladamantane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.834	2.71 ng	241094	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dimethyl-5-ethyladamantane	192	C14H24	001687-35-0	86
2			1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	72
3			Benzaldehyde dibutyl acetal	236	C15H24O2	1000431-61-9	64
4			l-Tyrophanamide	180	C9H12N2O2	1000131-25-3	59
5			1,4-Methanophthalazine, 1,4,4a,5...	206	C13H22N2	109746-14-7	53



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ALS Vial : 10 Sample Multiplier: 1

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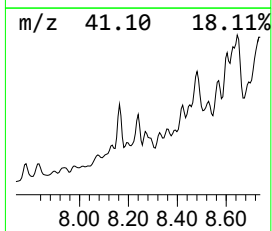
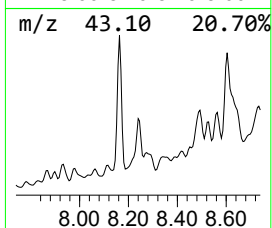
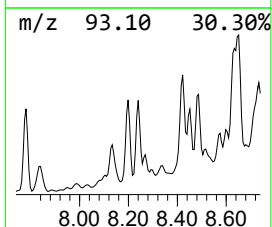
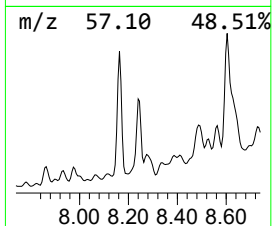
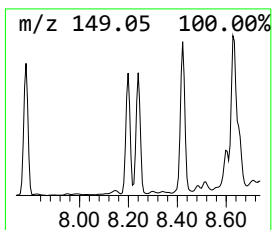
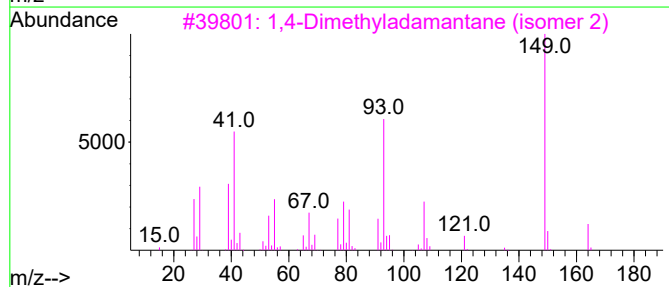
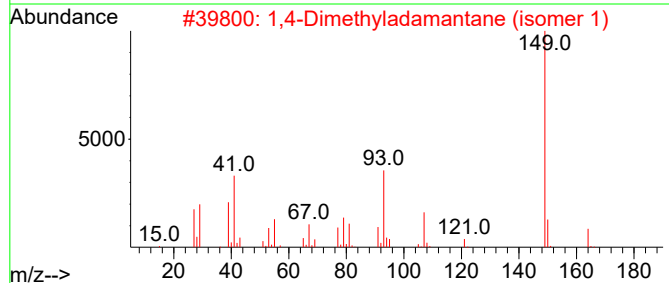
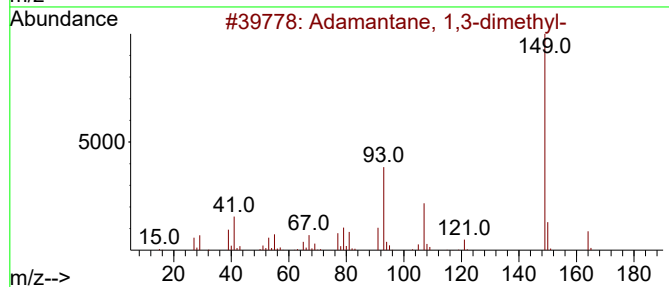
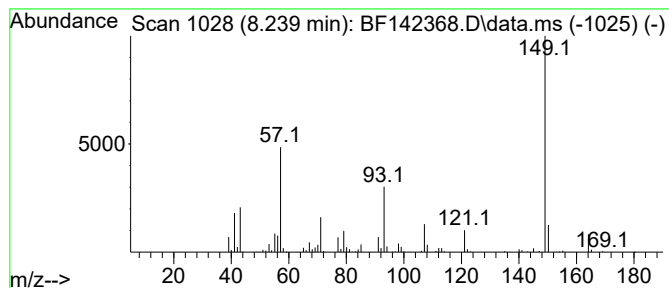
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Peak Number 4 1,4-Dimethyladamantane (iso... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.239	3.28 ng	291405	Naphthalene-d8	8.181

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	87
2		1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	80
3		1,4-Dimethyladamantane (isomer 2)	164	C12H20	1000460-67-1	49
4		1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	47
5		Added stereo to name	164	C12H20	024145-89-9	47



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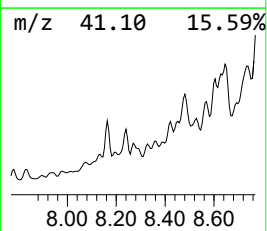
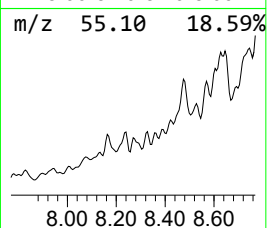
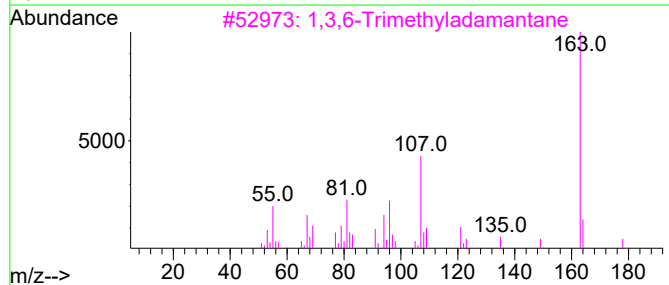
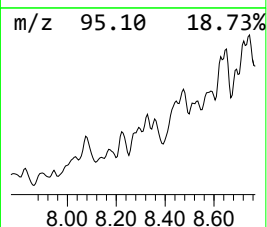
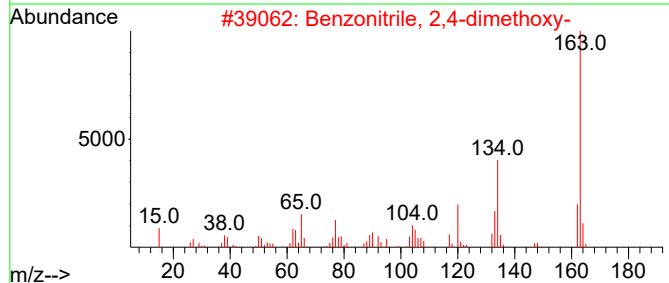
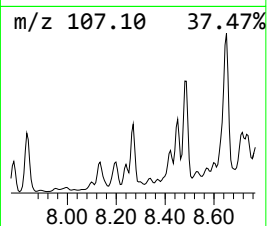
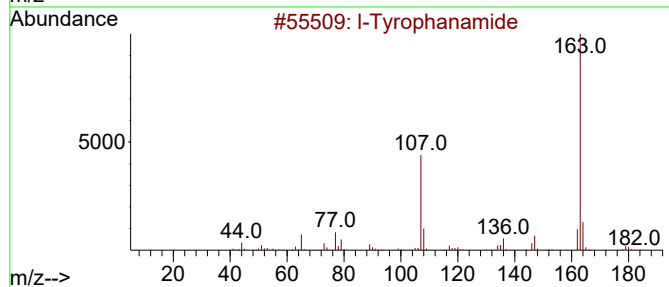
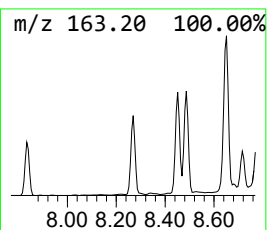
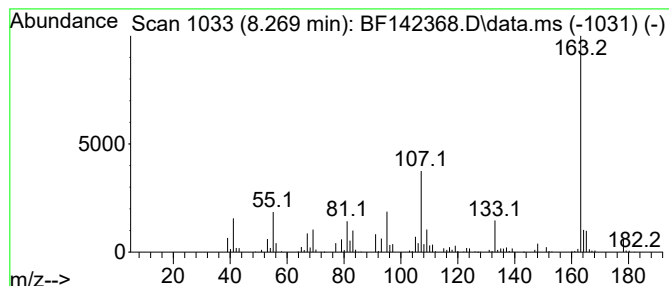
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Peak Number 5 1-Tyrophanamide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.269	2.31 ng	205049	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tyrophanamide	180	C9H12N2O2	1000131-25-3	50
2			Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	47
3			1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	45
4			6-Ethyl-1,3-benzothiazol-2-amine	178	C9H10N2S	021224-16-8	43
5			9H-Purin-6-amine,N,9-dimethyl-	163	C7H9N5	002009-52-1	42



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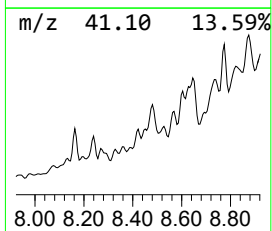
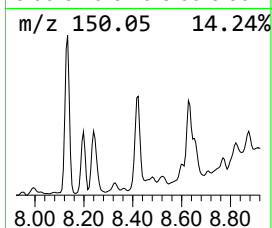
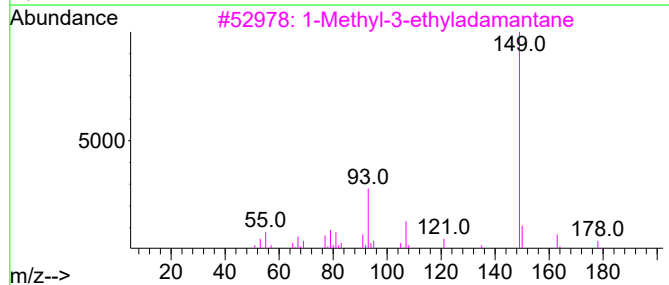
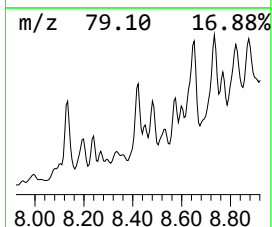
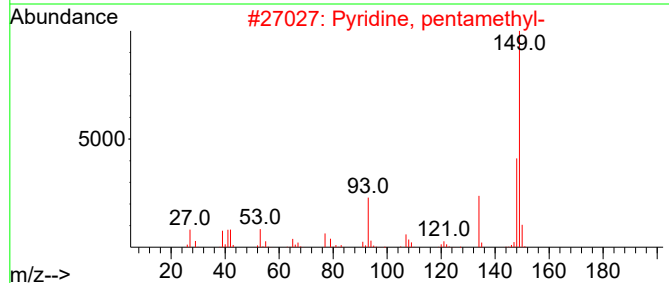
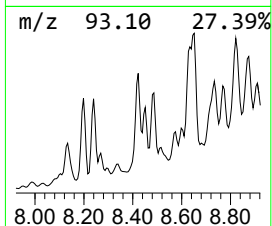
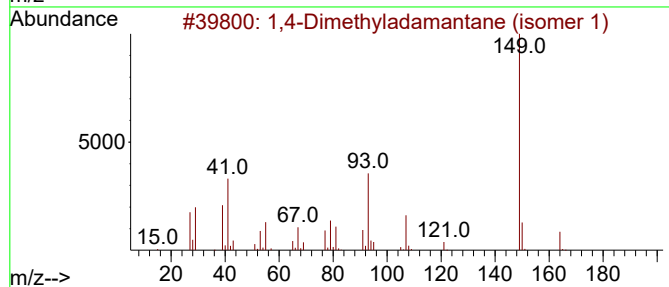
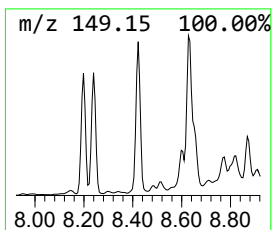
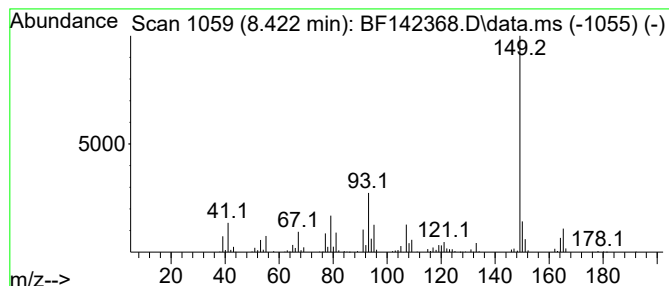
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pyridine, pentamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.422	3.58 ng	318002	Naphthalene-d8	8.181

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	81
2		Pyridine, pentamethyl-	149	C10H15N	003748-83-2	64
3		1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	64
4		1H-S-Triazolo[1,5-a]pyridin-4-yl...	149	C7H7N3O	013980-64-8	50
5		3-Methyl-1-adamantanecarboxylic ...	194	C12H18O2	1000504-38-9	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142368.D
Acq On : 14 May 2025 16:17
Operator : RC/JU
Sample : Q2014-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-25-0145

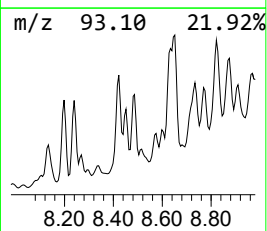
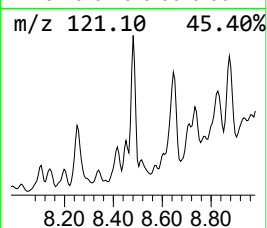
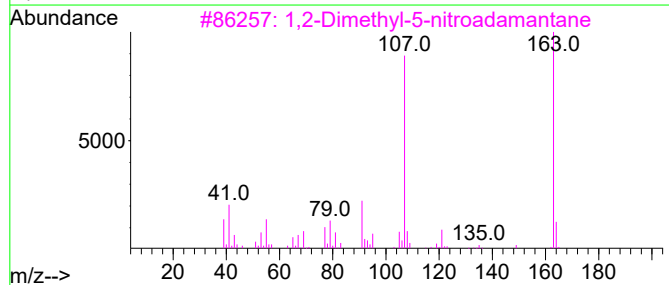
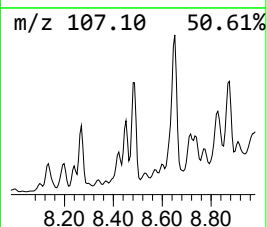
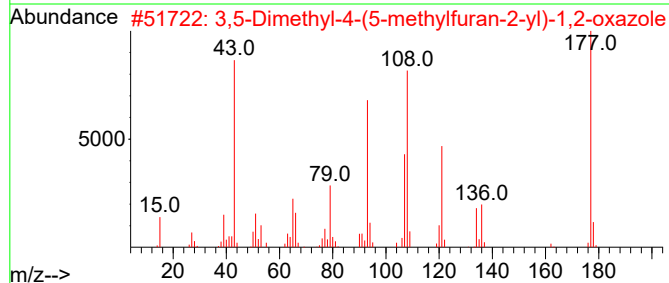
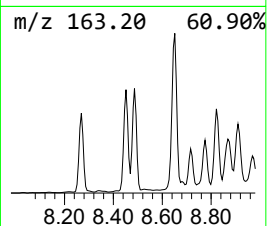
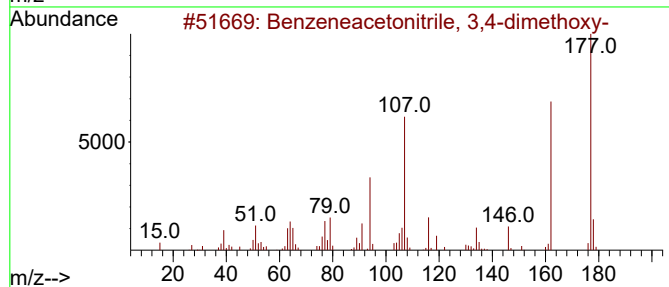
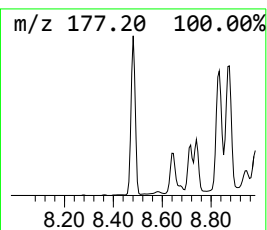
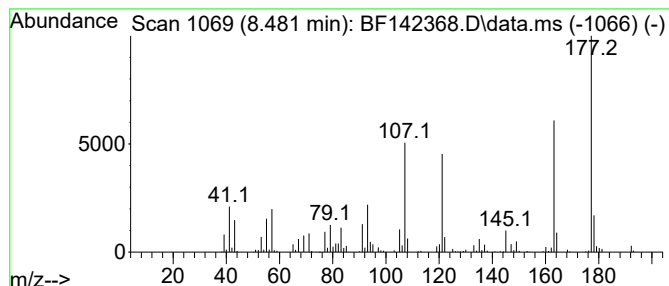
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.481 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.481	5.95 ng	528214	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetonitrile, 3,4-dimethoxy-	177	C10H11NO2	000093-17-4	43
2			3,5-Dimethyl-4-(5-methylfuran-2-...	177	C10H11NO2	1000411-58-9	43
3			1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	27
4			1,3,5,6-Tetramethyladamantane	192	C14H24	034694-70-7	27
5			1,3,5,7-Tetramethyl-adamantane	192	C14H24	001687-36-1	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142368.D
Acq On : 14 May 2025 16:17
Operator : RC/JU
Sample : Q2014-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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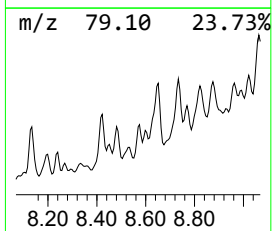
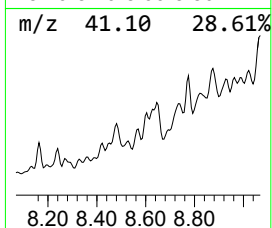
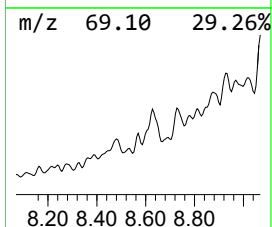
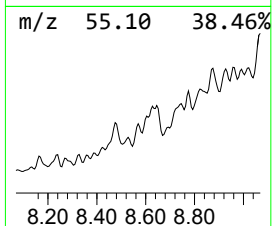
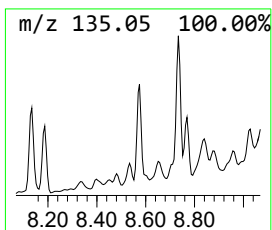
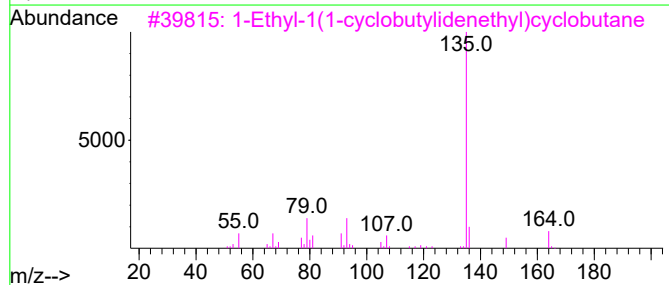
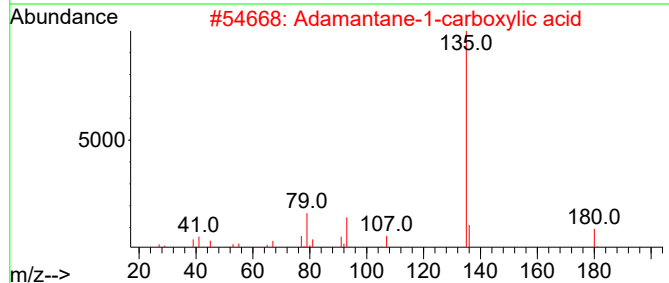
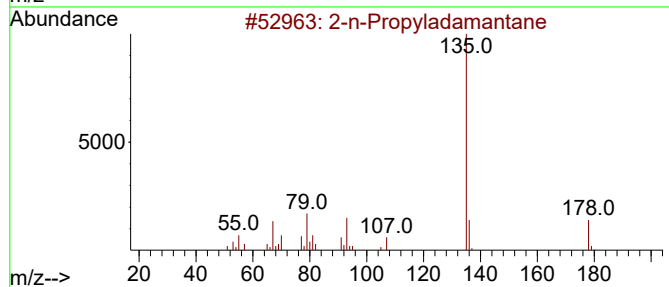
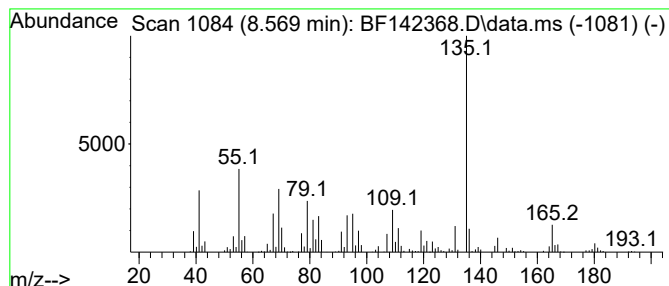
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-n-Propyladamantane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.569	3.18 ng	282695	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-n-Propyladamantane	178	C13H22	014451-88-8	53
2			Adamantane-1-carboxylic acid	180	C11H16O2	000828-51-3	49
3			1-Ethyl-1(1-cyclobutylidenethyl)...	164	C12H20	1000215-13-7	49
4			4-Amino-2,6-dimethyl-3-pyridyl 1...	300	C18H24N2O2	1000260-99-2	47
5			N-(3-Hydroxy-2,6-dimethyl-4-pyri...	300	C18H24N2O2	1000260-99-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142368.D
Acq On : 14 May 2025 16:17
Operator : RC/JU
Sample : Q2014-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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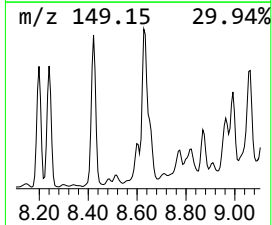
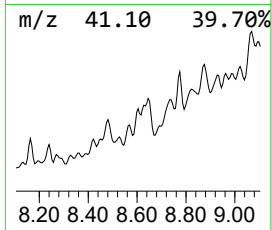
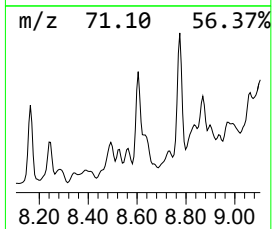
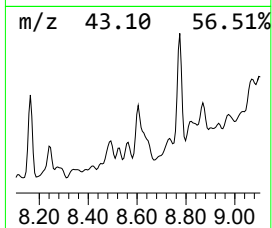
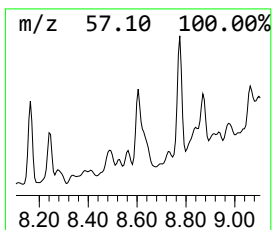
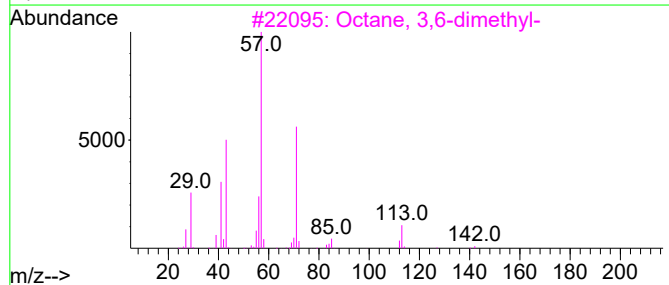
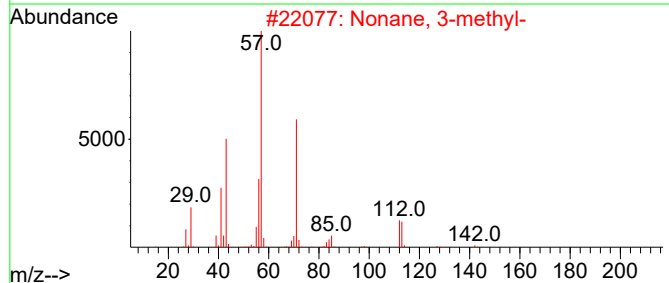
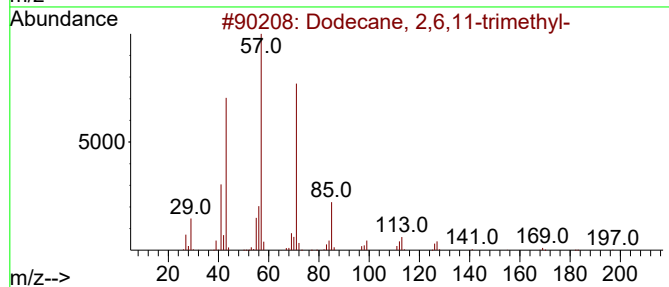
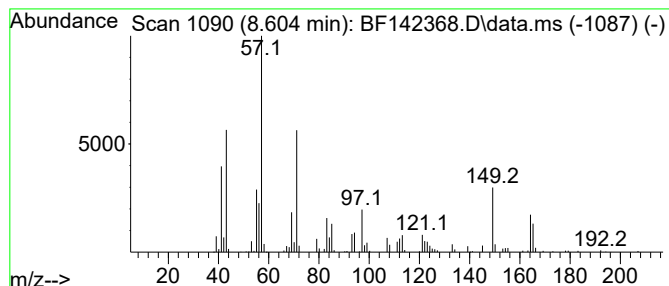
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.604 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.604	3.28 ng	291270	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	43
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	38
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	38
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	35
5			Phthalic acid, ethyl furfuryl ester	278	C15H18O5	1000314-91-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142368.D
Acq On : 14 May 2025 16:17
Operator : RC/JU
Sample : Q2014-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

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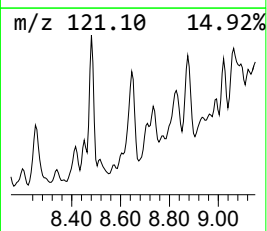
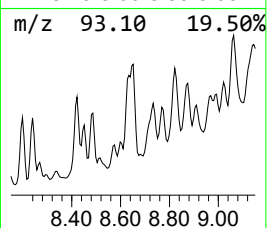
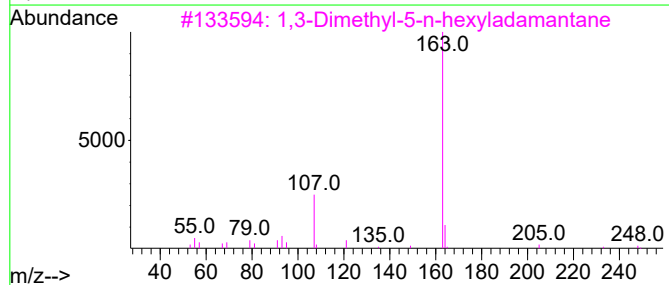
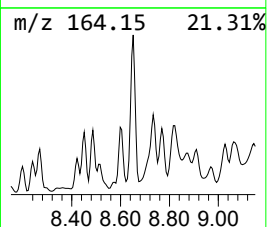
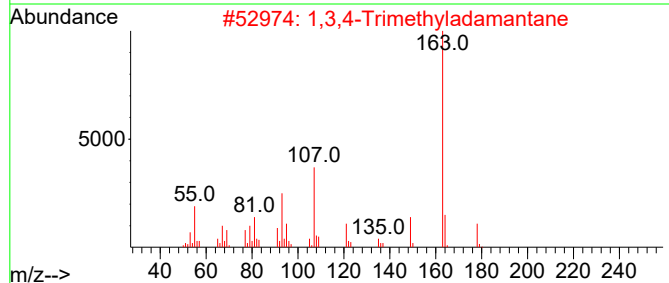
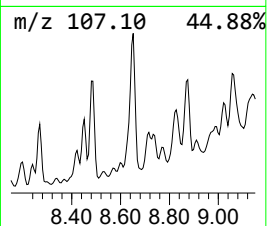
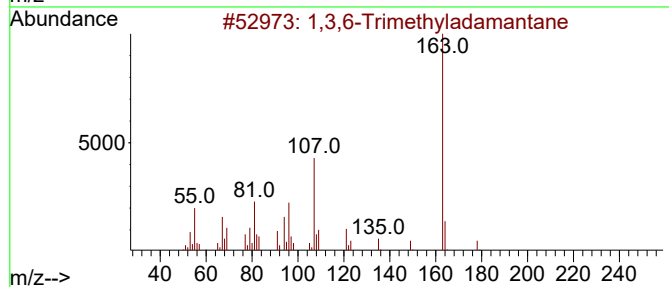
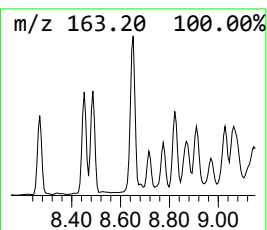
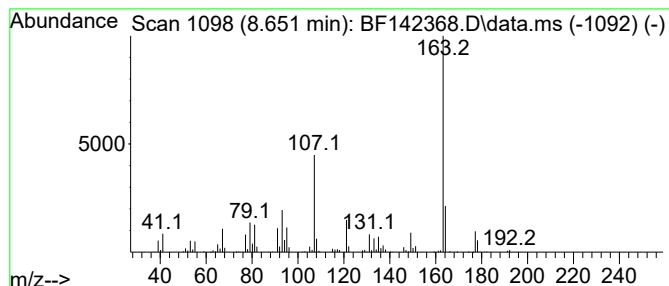
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,3,6-Trimethyladamantane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.651	12.53 ng	1113640	Naphthalene-d8	8.181

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3,6-Trimethyladamantane	178	C13H22	024139-37-5	64
2		1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	64
3		1,3-Dimethyl-5-n-hexyladamantane	248	C18H32	052873-50-4	59
4		1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	53
5		1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142368.D
Acq On : 14 May 2025 16:17
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ALS Vial : 10 Sample Multiplier: 1

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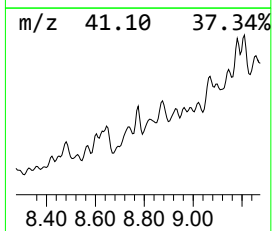
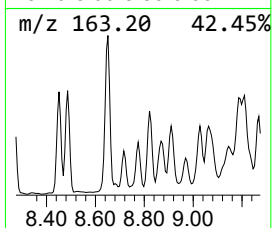
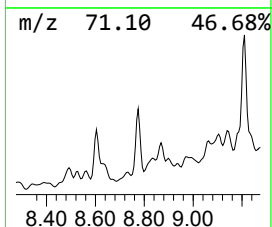
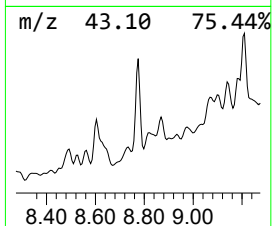
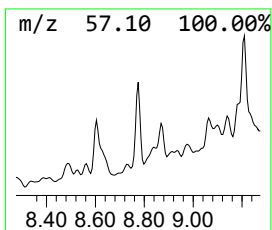
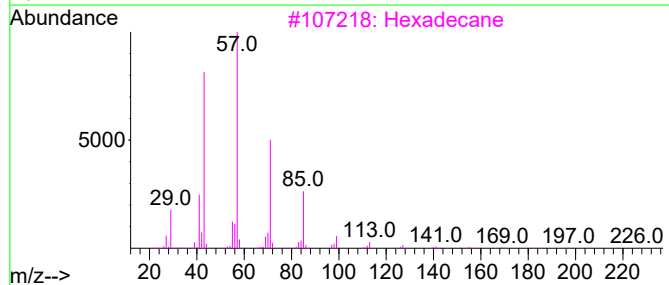
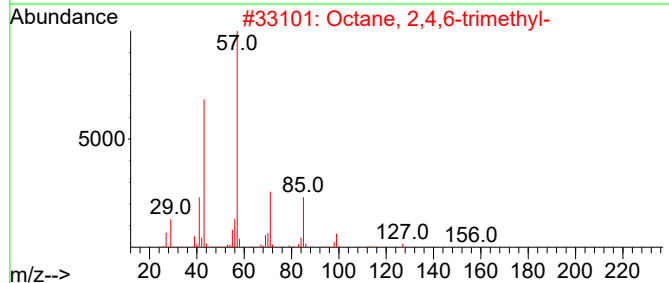
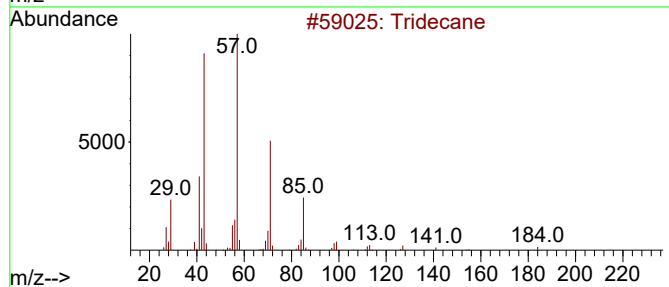
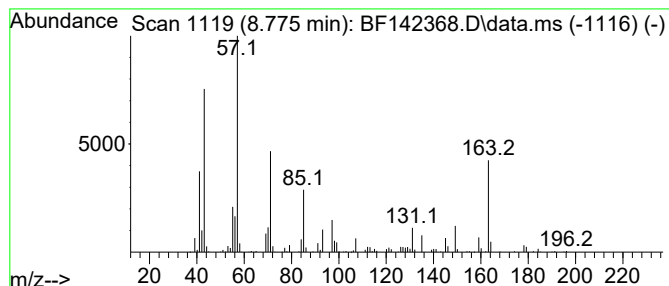
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.775	3.92 ng	348359	Naphthalene-d8	8.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	90
2			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	43
3			Hexadecane	226	C16H34	000544-76-3	43
4			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	38
5			Dodecane	170	C12H26	000112-40-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
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Acq On : 14 May 2025 16:17
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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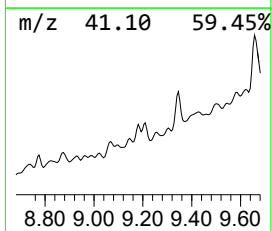
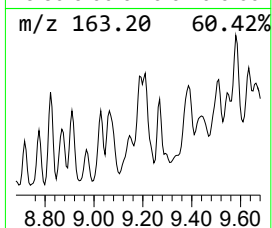
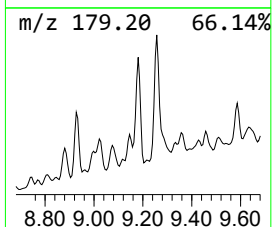
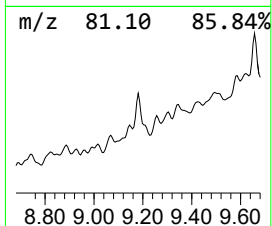
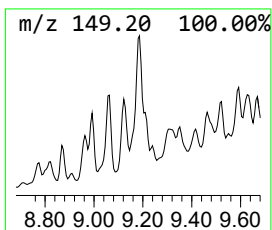
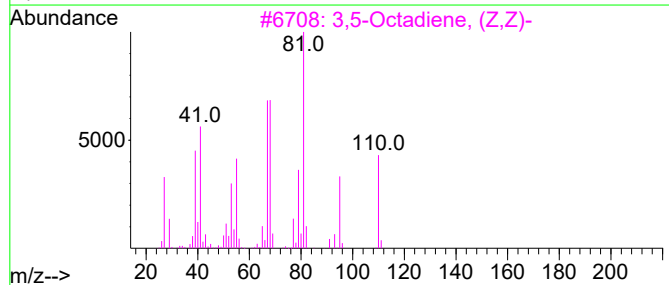
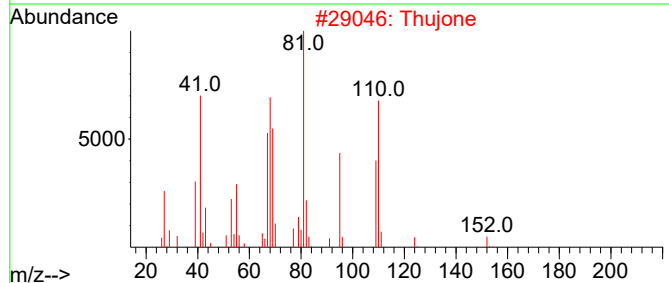
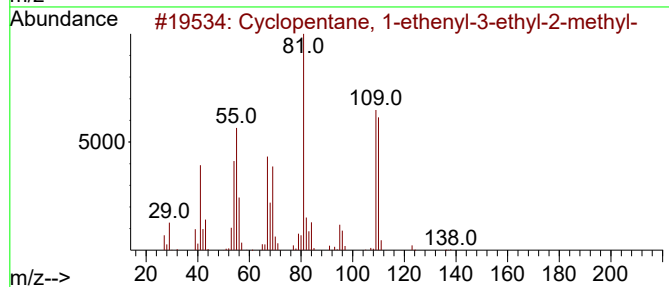
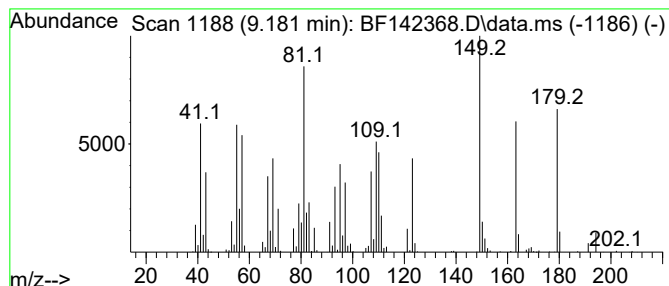
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown9.181 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.181	3.16 ng	420426	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-ethenyl-3-ethyl-...	138	C10H18	055170-98-4	30
2			Thujone	152	C10H16O	000546-80-5	27
3			3,5-Octadiene, (Z,Z)-	110	C8H14	007348-80-3	22
4			3-Heptyne, 5-methyl-	110	C8H14	061228-09-9	22
5			2-Propenyl-3-vinylloxirane	110	C7H10O	070597-49-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142368.D
Acq On : 14 May 2025 16:17
Operator : RC/JU
Sample : Q2014-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-25-0145

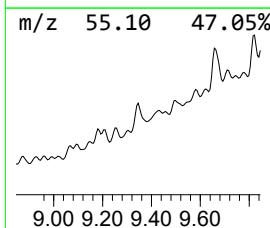
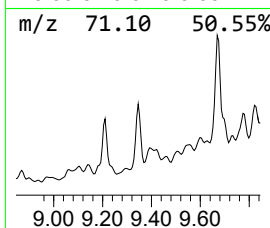
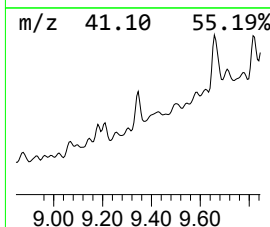
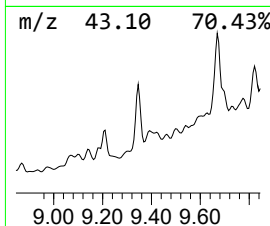
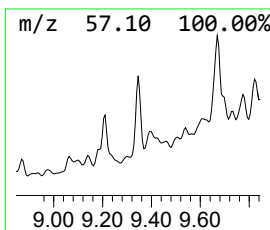
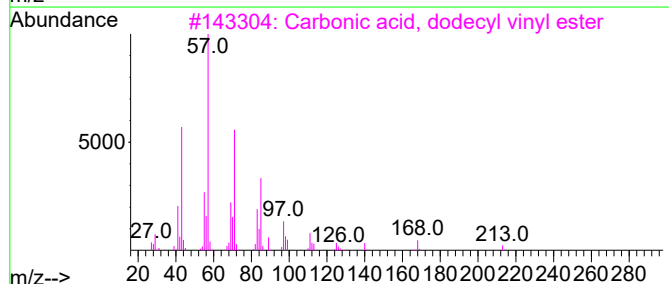
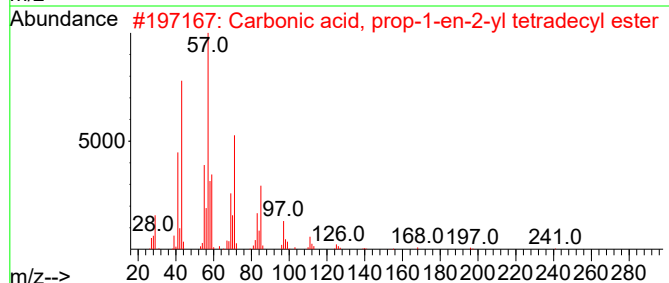
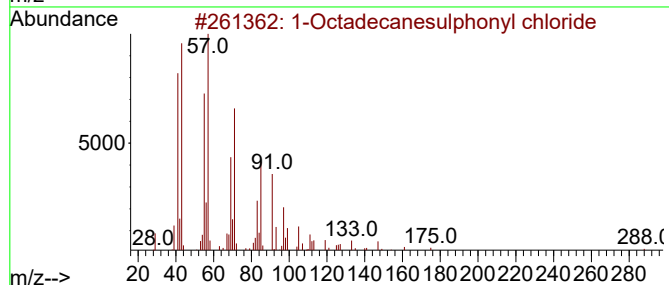
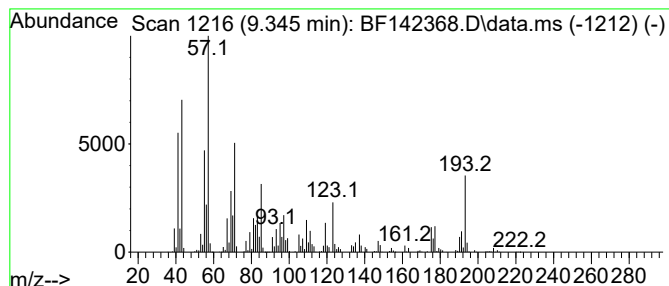
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown9.345 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	12.57 ng	1673590	Acenaphthene-d10	9.951

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	41
2		Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	41
3		Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	38
4		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	38
5		Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142368.D
Acq On : 14 May 2025 16:17
Operator : RC/JU
Sample : Q2014-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-25-0145

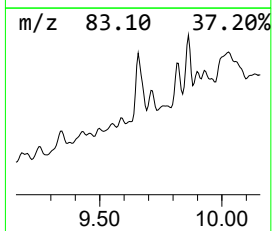
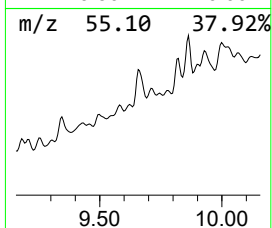
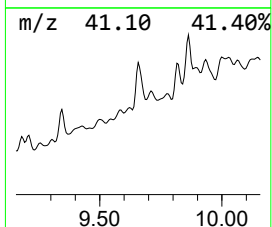
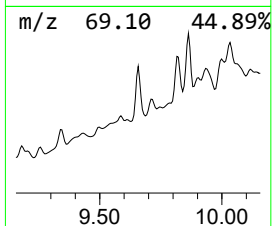
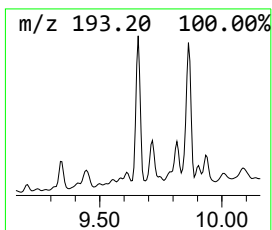
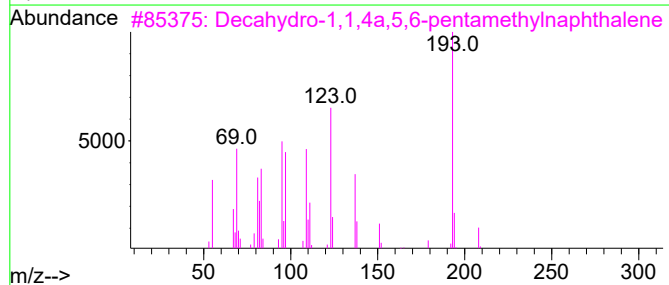
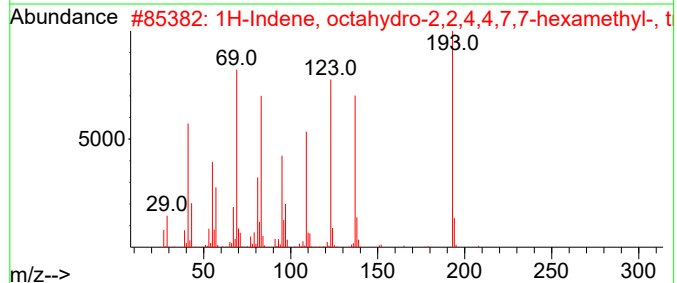
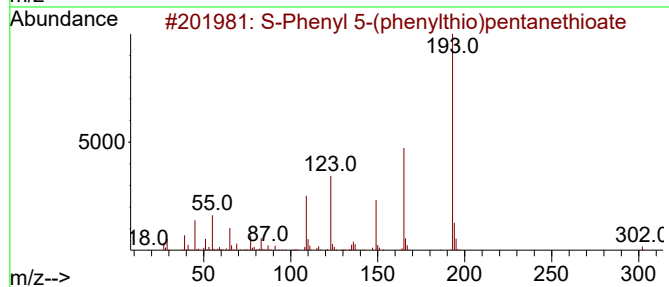
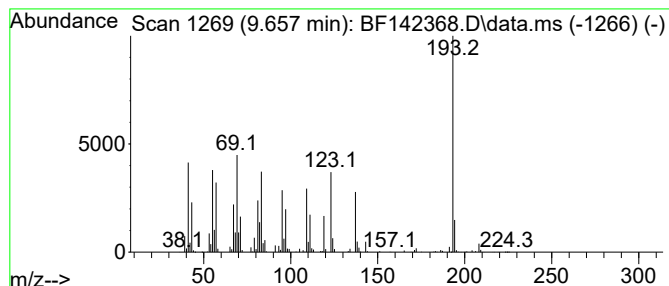
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown9.657 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.657	20.00 ng	2662930	Acenaphthene-d10	9.951

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	47		
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	43		
3	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	38		
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38		
5	2-Anthracenamine	193	C14H11N	000613-13-8	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142368.D
Acq On : 14 May 2025 16:17
Operator : RC/JU
Sample : Q2014-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-25-0145

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.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
1-Adamantyl bro...	7.687	2.1	ng	189767	2	8.181	1776890	20.0
Adamantane, 1,3...	7.781	2.3	ng	204727	2	8.181	1776890	20.0
1,3-Dimethyl-5-...	7.834	2.7	ng	241094	2	8.181	1776890	20.0
1,4-Dimethylada...	8.239	3.3	ng	291405	2	8.181	1776890	20.0
1-Tyrophanamide	8.269	2.3	ng	205049	2	8.181	1776890	20.0
Pyridine, penta...	8.422	3.6	ng	318002	2	8.181	1776890	20.0
unknown8.481	8.481	6.0	ng	528214	2	8.181	1776890	20.0
2-n-Propyladama...	8.569	3.2	ng	282695	2	8.181	1776890	20.0
unknown8.604	8.604	3.3	ng	291270	2	8.181	1776890	20.0
1,3,6-Trimethyl...	8.651	12.5	ng	1113640	2	8.181	1776890	20.0
Tridecane	8.775	3.9	ng	348359	2	8.181	1776890	20.0
unknown9.181	9.181	3.2	ng	420426	3	9.951	2662930	20.0
unknown9.345	9.345	12.6	ng	1673590	3	9.951	2662930	20.0
unknown9.657	9.657	20.0	ng	2662930	3	9.951	2662930	20.0