

Data Path : T:\svoasrv\HPCHEM1\BNA_F\Data\BF032425\
 Data File : BF142055.D
 Acq On : 24 Mar 2025 15:25
 Operator : RC/JU
 Sample : Q1606-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 N48965

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 : T:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142055.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.434	555	568	574	rBV	6891559	17759515	100.00%	45.659%
2	5.504	575	580	585	rVV	1370209	1644892	9.26%	4.229%
3	5.669	596	608	613	rVB3	160618	301064	1.70%	0.774%
4	5.840	630	637	648	rVB	1686218	3005083	16.92%	7.726%
5	6.498	741	749	756	rBV	808108	1153717	6.50%	2.966%
6	6.751	788	792	797	rVB2	236912	449095	2.53%	1.155%
7	6.875	808	813	817	rBV	763634	1034273	5.82%	2.659%
8	6.934	819	823	834	rVB4	574149	1200225	6.76%	3.086%
9	7.216	862	871	876	rBV6	147127	438196	2.47%	1.127%
10	7.434	900	908	913	rVB	1817895	3038953	17.11%	7.813%
11	7.581	925	933	937	rBV6	238913	650949	3.67%	1.674%
12	7.645	940	944	946	rBV4	178654	277989	1.57%	0.715%
13	8.098	1018	1021	1025	rBV2	214624	365639	2.06%	0.940%
14	8.157	1027	1031	1034	rBV	743759	1055977	5.95%	2.715%
15	9.239	1211	1215	1223	rBV	2002349	5277408	29.72%	13.568%
16	14.810	2158	2162	2168	rVB	911476	1242894	7.00%	3.195%

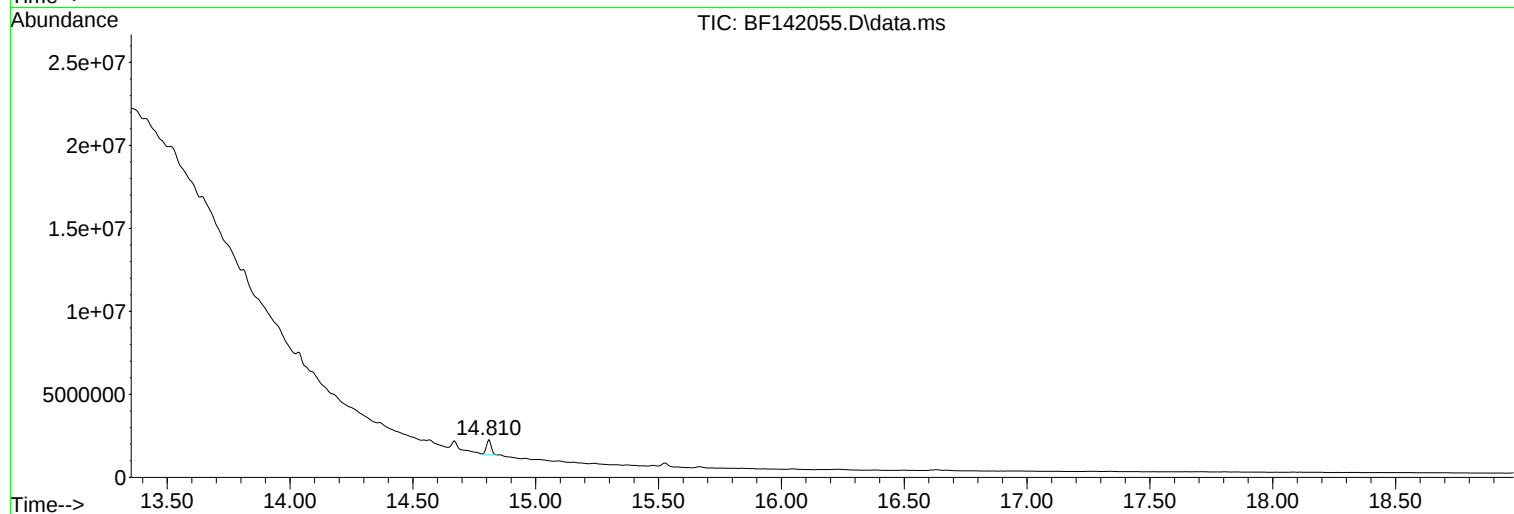
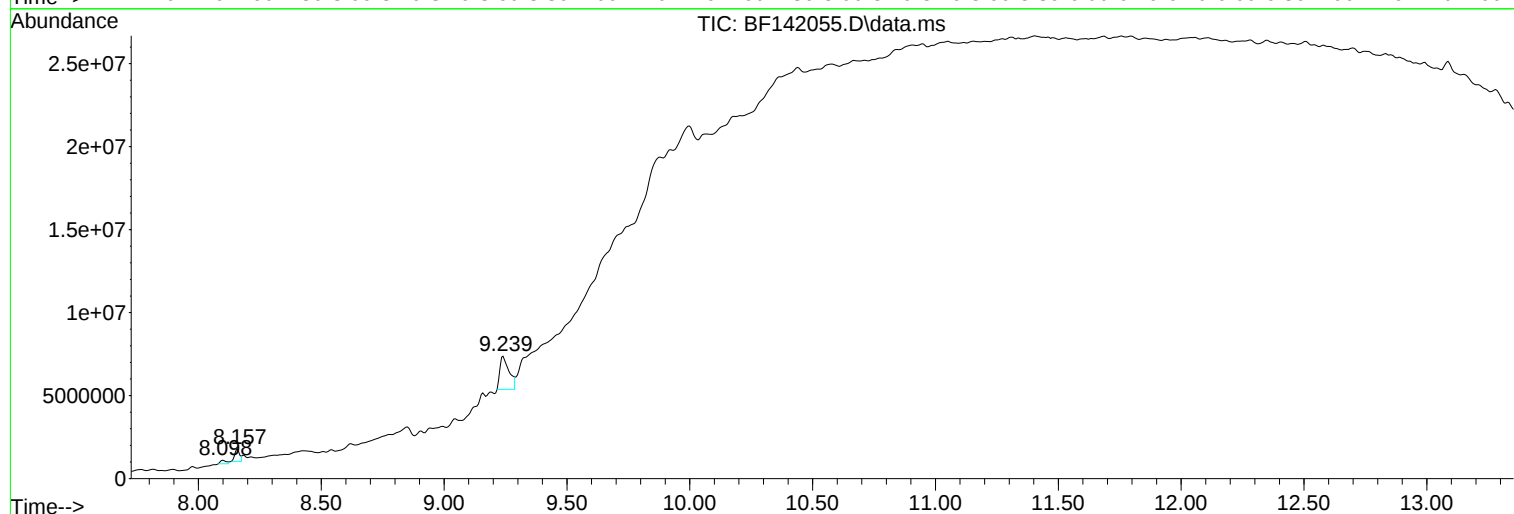
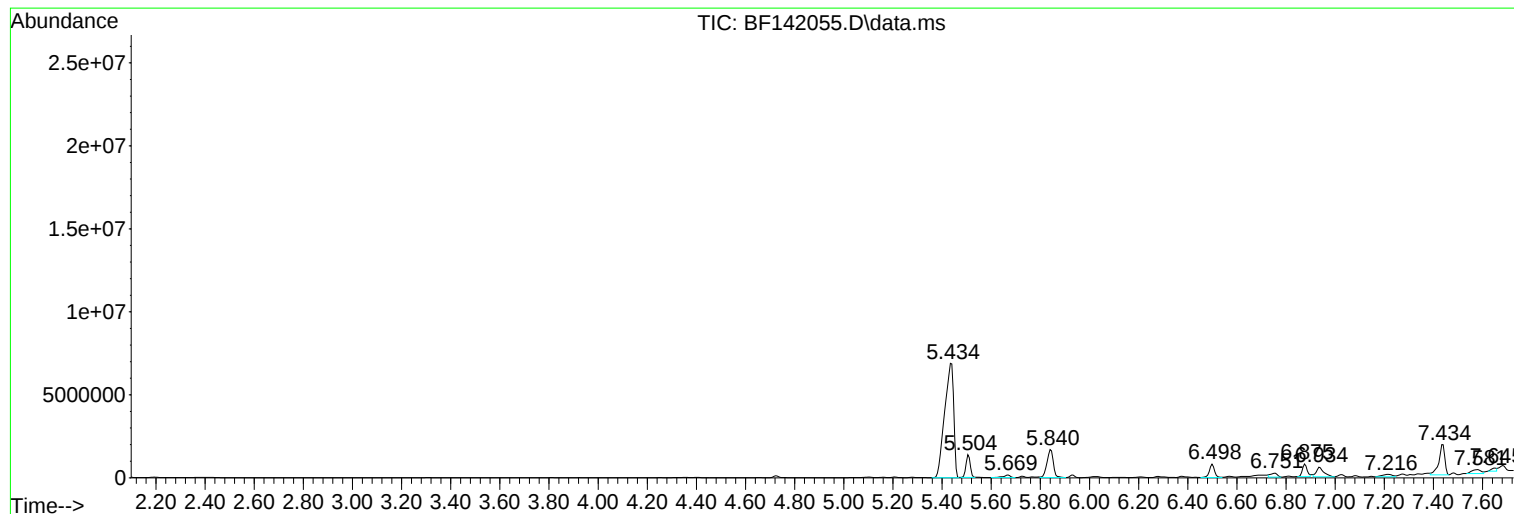
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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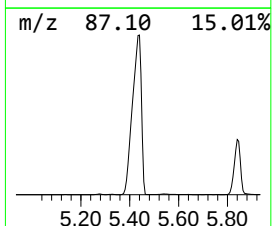
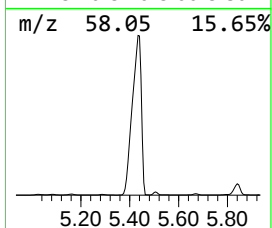
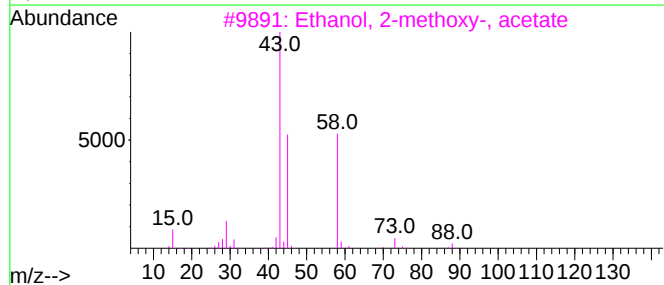
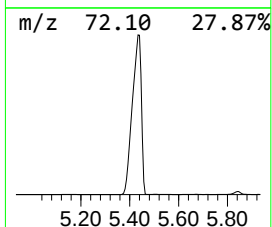
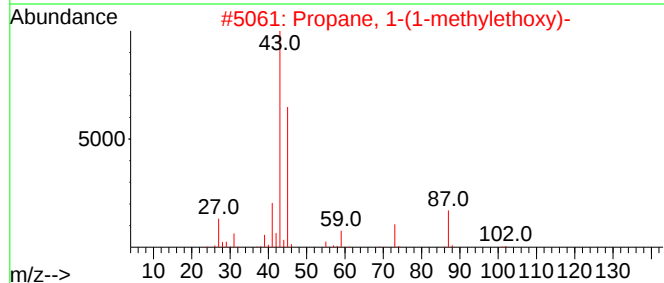
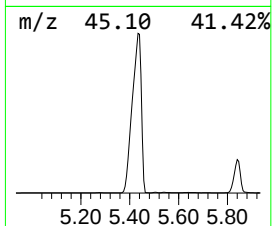
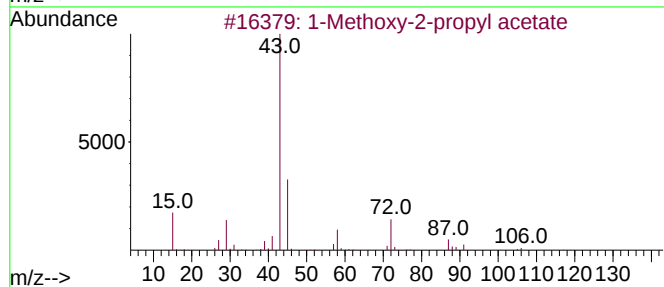
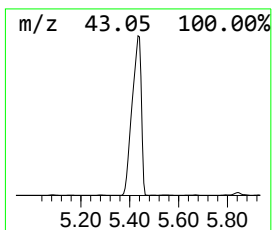
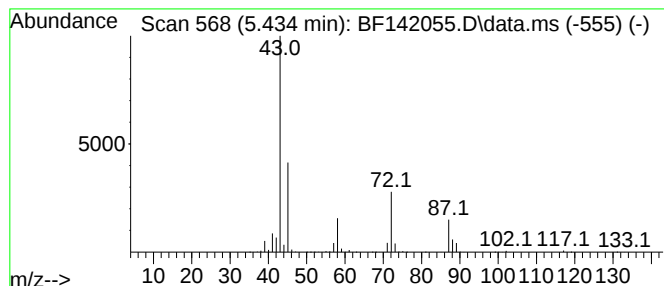
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Methoxy-2-propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.434	343.42 ng	17759500	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methoxy-2-propyl acetate	132	C6H12O3	000108-65-6	83
2			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	38
3			Ethanol, 2-methoxy-, acetate	118	C5H10O3	000110-49-6	37
4			Ethanol, 2-propoxy-	104	C5H12O2	002807-30-9	23
5			Propanal, 2-methyl-	72	C4H8O	000078-84-2	22



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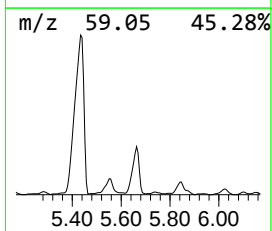
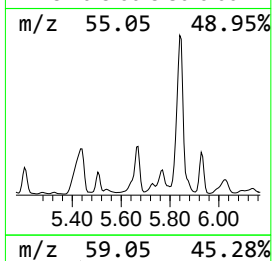
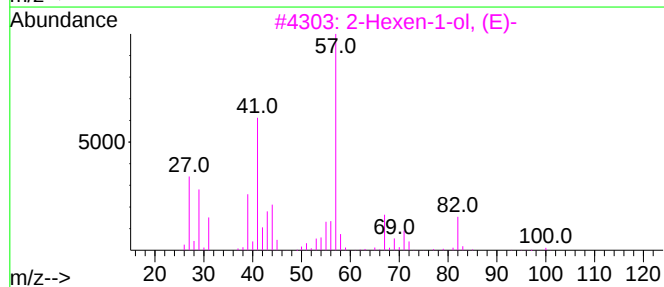
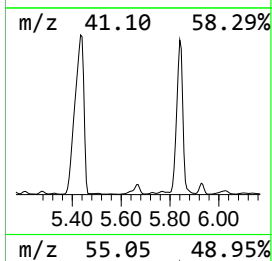
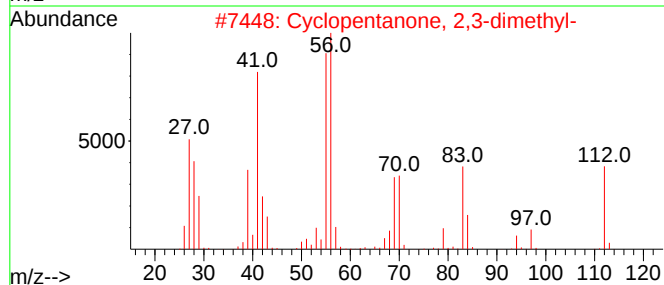
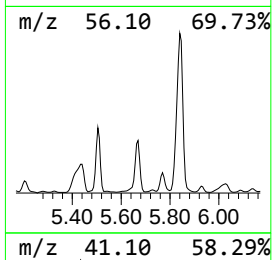
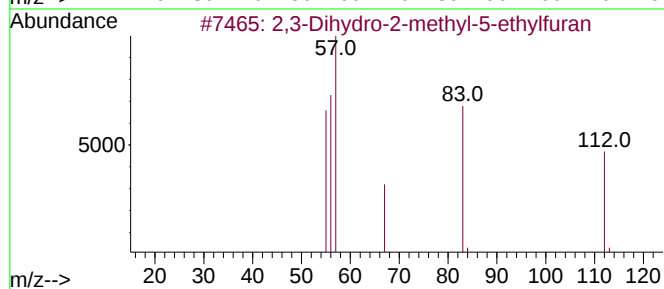
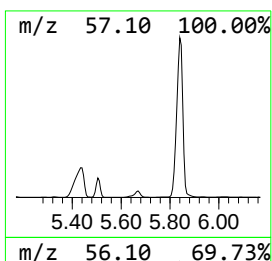
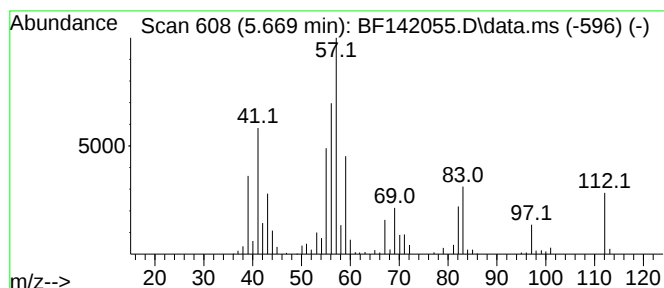
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.669 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.669	5.82 ng	301064	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,3-Dihydro-2-methyl-5-ethylfuran	112	C7H12O	1000288-51-4	38
2		Cyclopentanone, 2,3-dimethyl-	112	C7H12O	1000151-06-7	35
3		2-Hexen-1-ol, (E)-	100	C6H12O	000928-95-0	30
4		2-Heptene, 6-methyl-	112	C8H16	073548-72-8	25
5		Pentanal, 3-methyl-	100	C6H12O	015877-57-3	22



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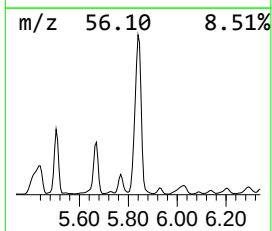
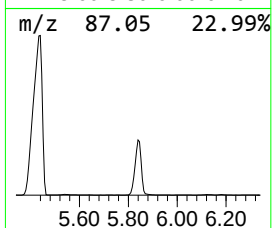
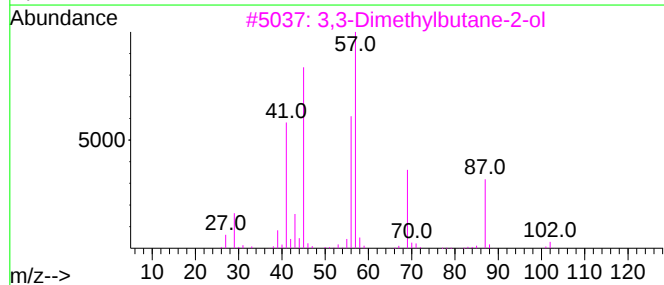
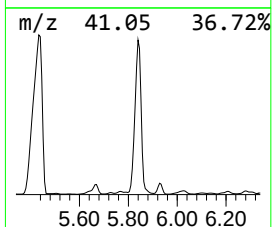
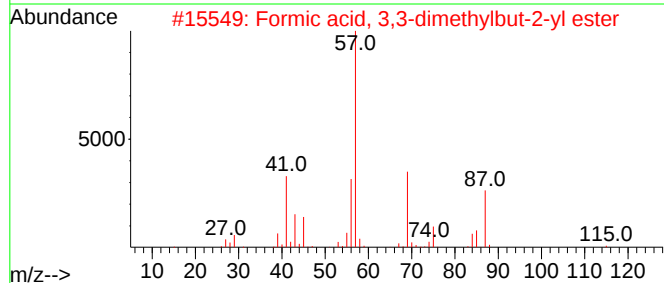
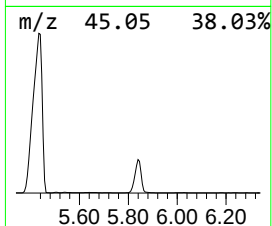
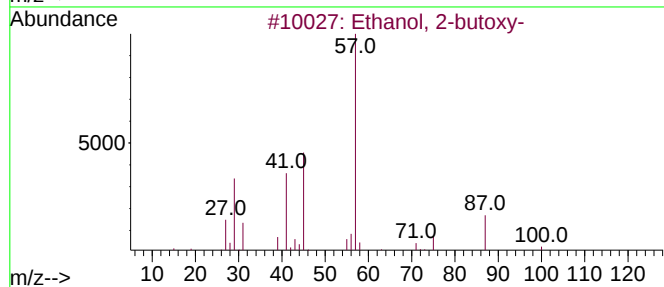
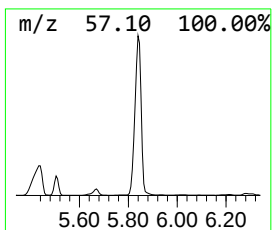
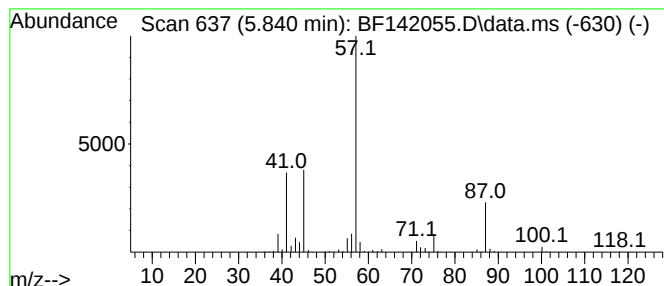
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.840	58.11 ng	3005080	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2			Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	59
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	37
4			n-Butyl ether	130	C8H18O	000142-96-1	37
5			Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	28



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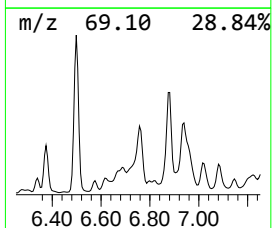
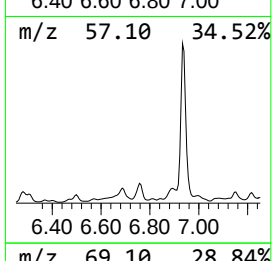
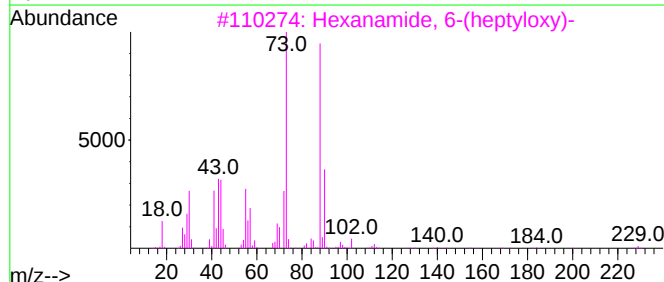
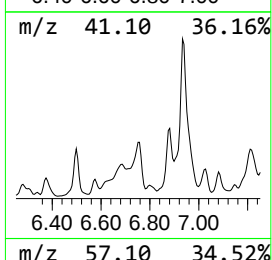
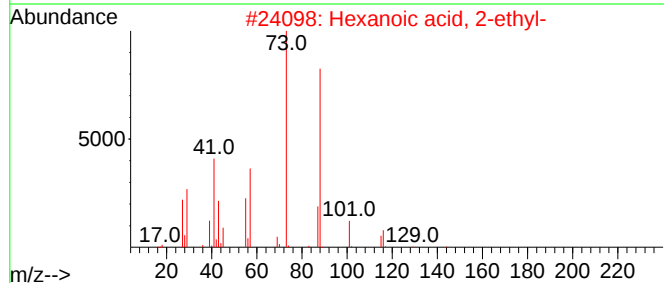
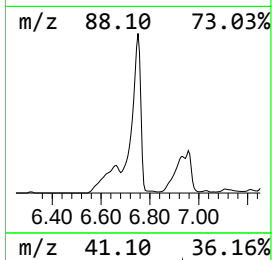
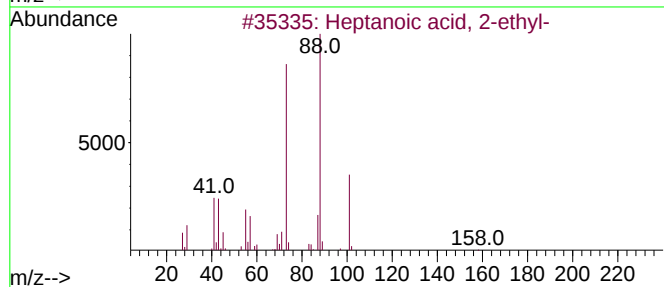
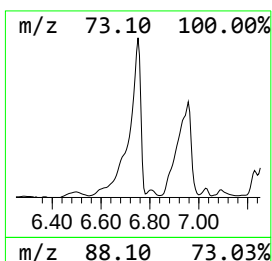
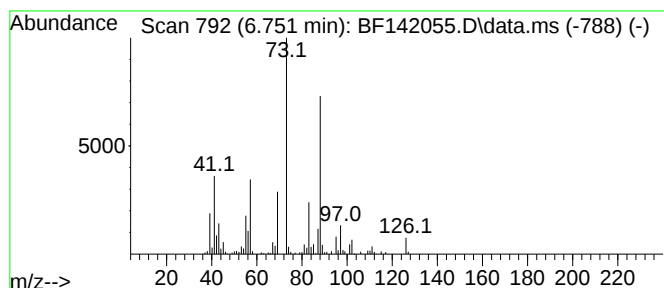
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown6.751 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.751	8.68 ng	449095	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	37
2			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	28
3			Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	27
4			Cyclohexanecarboxylic acid, .alpha.-...	170	C10H18O2	006051-00-9	23
5			3-Dodecyloxypropanoic acid, Me d...	272	C16H32O3	1000497-89-8	17



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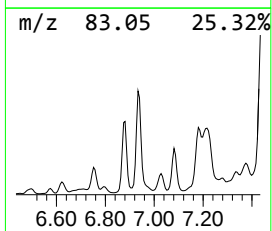
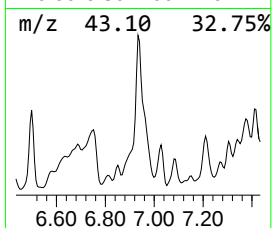
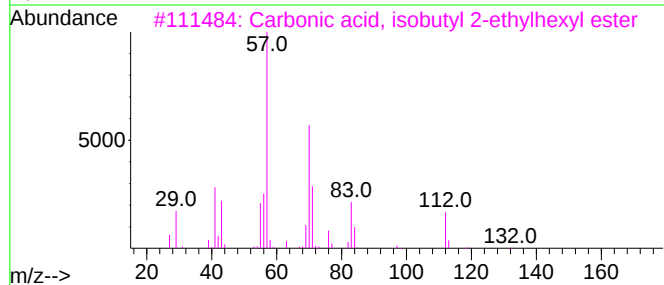
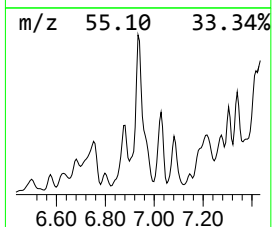
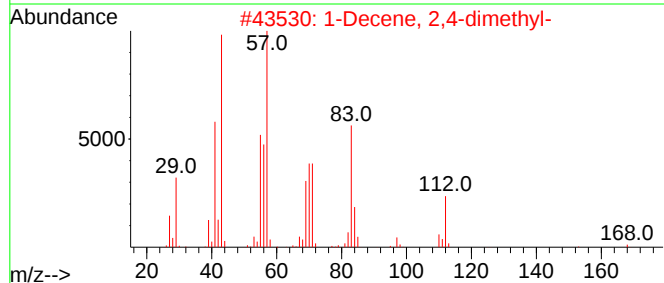
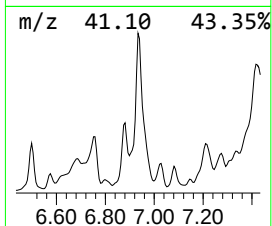
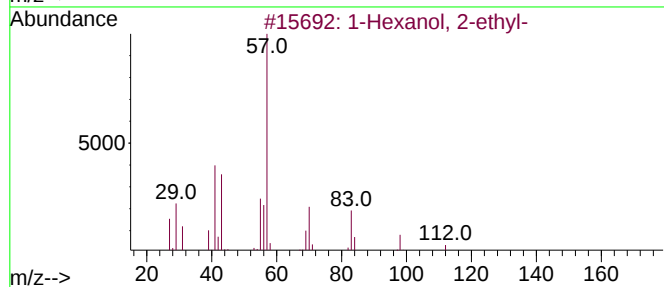
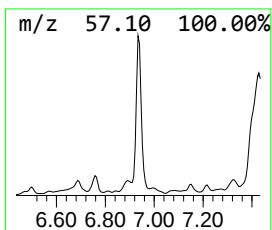
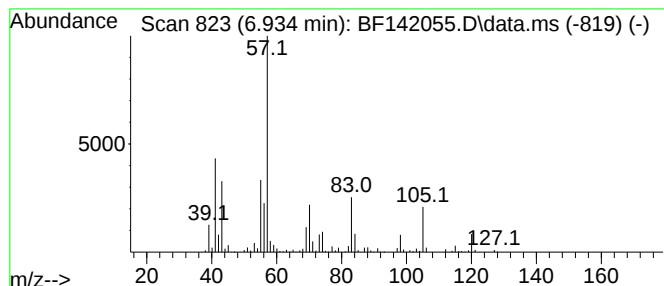
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.934	23.21 ng	1200230	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	58
2			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	43
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	38
4			2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	38
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	35



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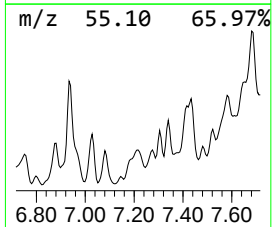
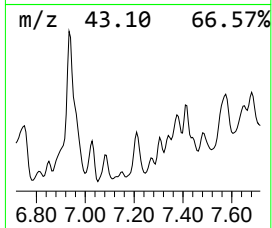
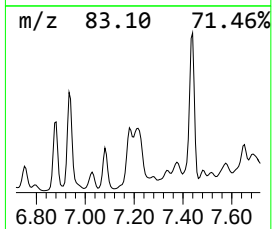
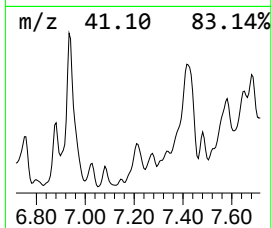
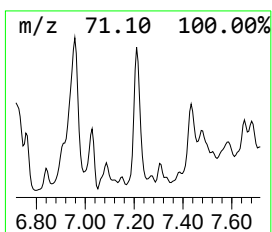
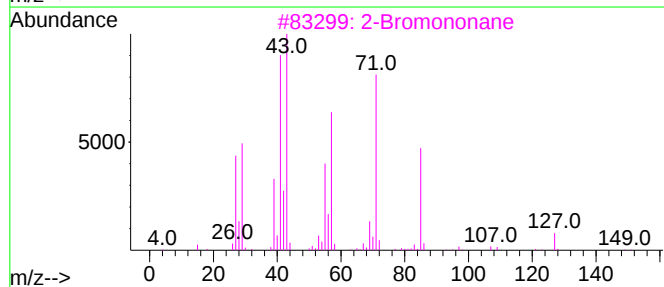
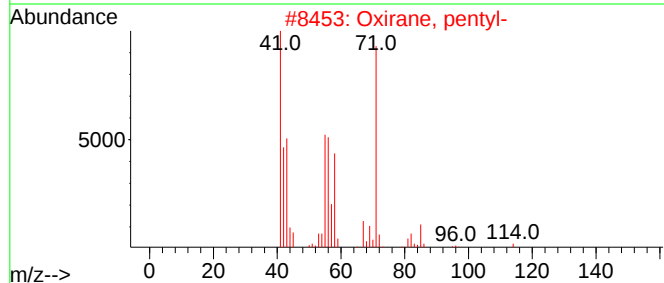
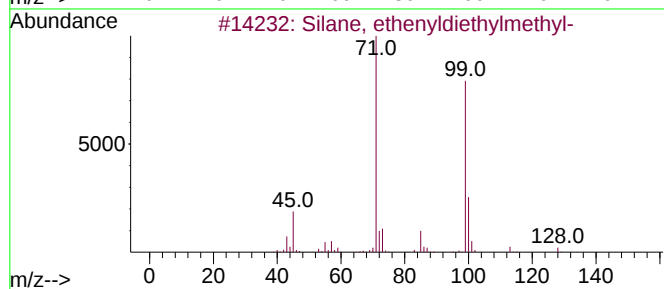
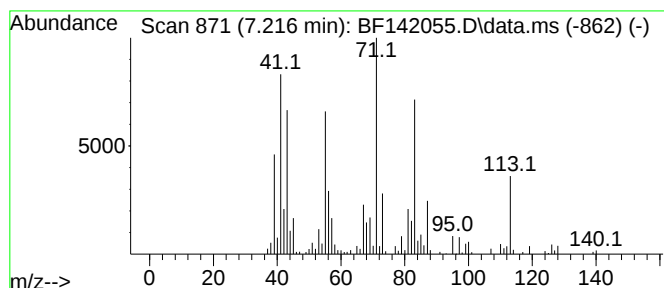
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown7.216 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.216	8.47 ng	438196	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Silane, ethenyldiethylmethyl-	128	C7H16Si	018292-29-0	27
2			Oxirane, pentyl-	114	C7H14O	005063-65-0	22
3			2-Bromononane	206	C9H19Br	002216-35-5	22
4			Butanoic acid, 2-hexenyl ester, ...	170	C10H18O2	053398-83-7	22
5			2-Furanmethanol, tetrahydro-	102	C5H10O2	000097-99-4	22



Data Path : T:\svoasrv\HPCHEM1\BNA_F\Data\BF032425\
Data File : BF142055.D
Acq On : 24 Mar 2025 15:25
Operator : RC/JU
Sample : Q1606-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N48965

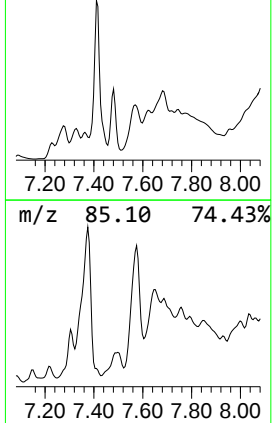
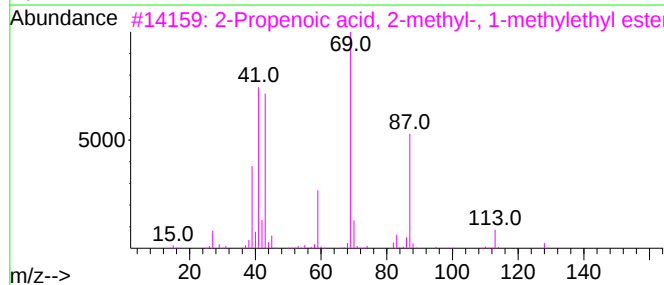
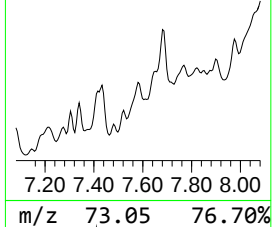
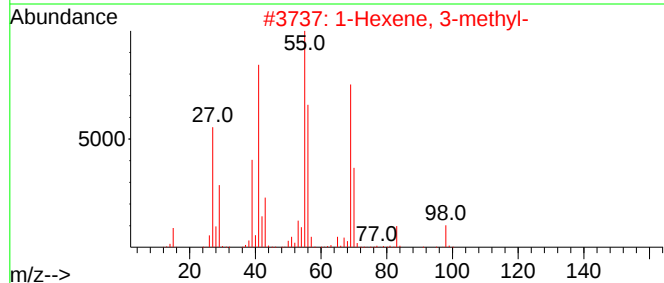
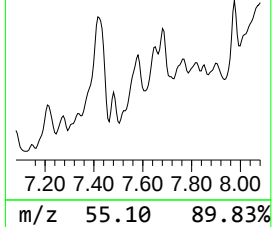
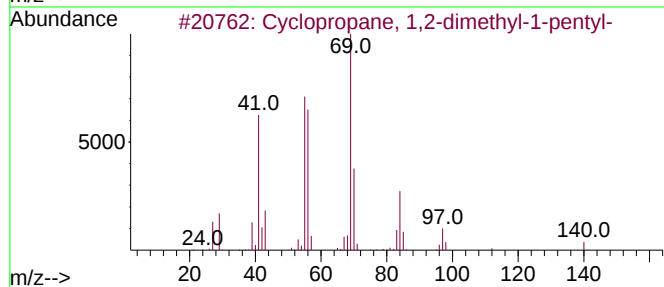
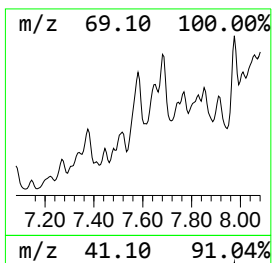
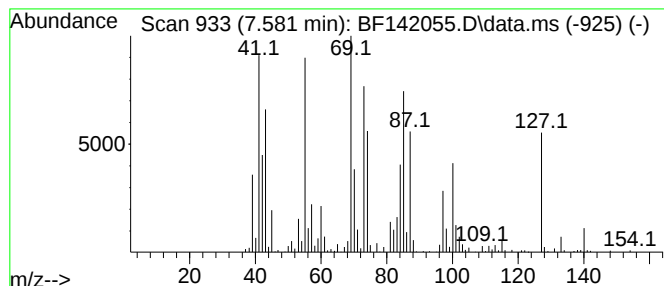
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.581 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.581	12.33 ng	650949	Naphthalene-d8	8.157

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	27
2		1-Hexene, 3-methyl-	98	C7H14	003404-61-3	15
3		2-Propenoic acid, 2-methyl-, 1-m...	128	C7H12O2	004655-34-9	14
4		4-Octanol	130	C8H18O	000589-62-8	14
5		Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	14



Data Path : T:\svoasrv\HPCHEM1\BNA_F\Data\BF032425\
Data File : BF142055.D
Acq On : 24 Mar 2025 15:25
Operator : RC/JU
Sample : Q1606-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N48965

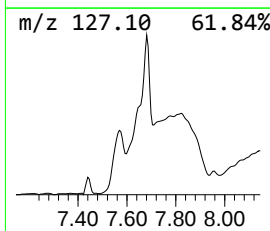
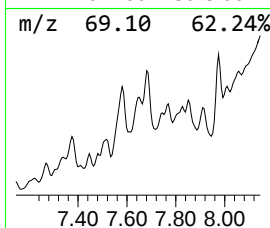
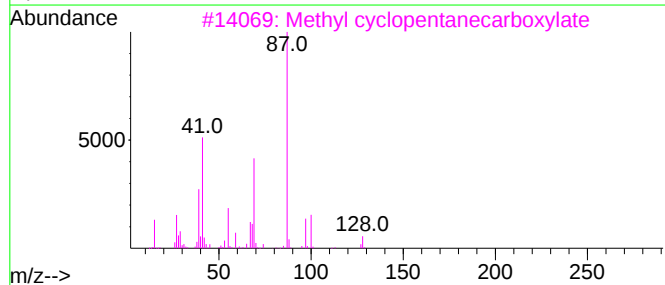
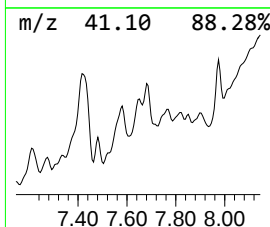
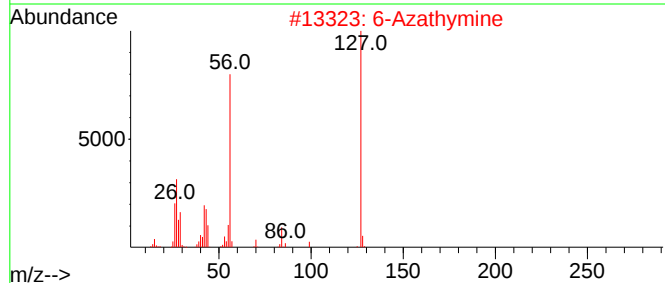
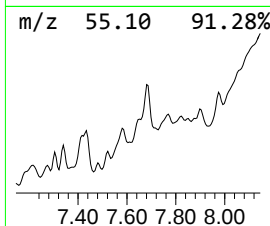
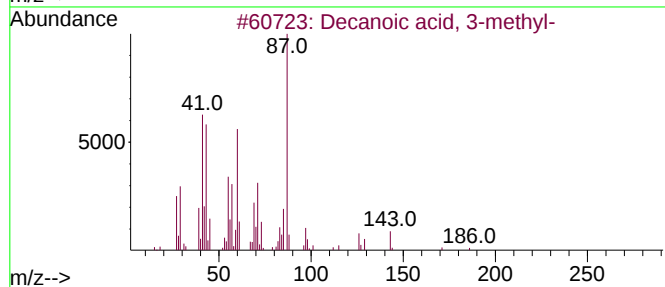
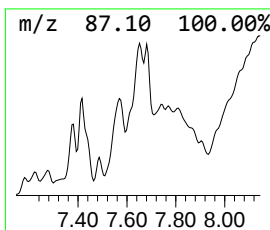
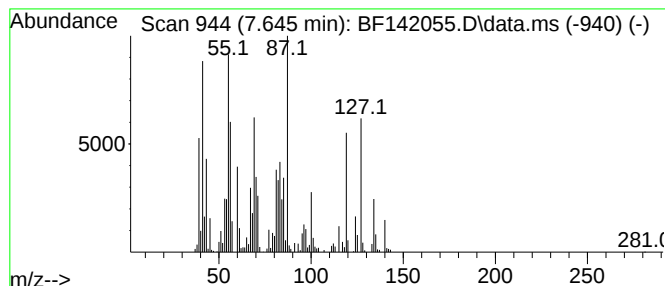
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown7.645 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.645	5.27 ng	277989	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanoic acid, 3-methyl-	186	C11H22O2	060308-82-9	12
2			6-Azathymine	127	C4H5N3O2	000932-53-6	11
3			Methyl cyclopentanecarboxylate	128	C7H12O2	004630-80-2	10
4			4-Pentenal	84	C5H8O	002100-17-6	10
5			7-Octenoic acid	142	C8H14O2	018719-24-9	10



Data Path : T:\svoasrv\HPCHEM1\BNA_F\Data\BF032425\
Data File : BF142055.D
Acq On : 24 Mar 2025 15:25
Operator : RC/JU
Sample : Q1606-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

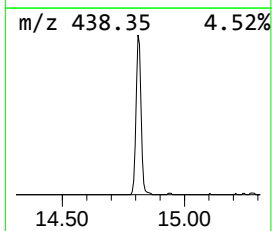
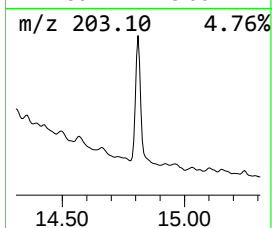
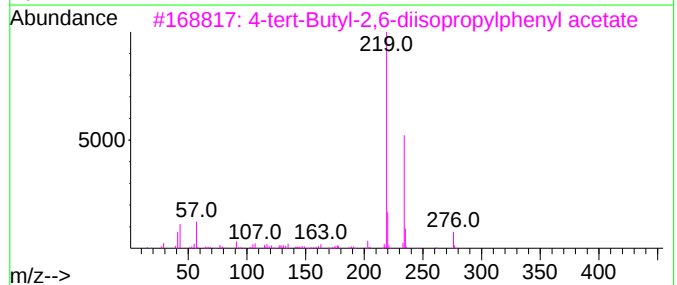
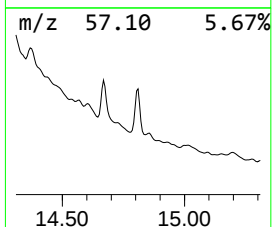
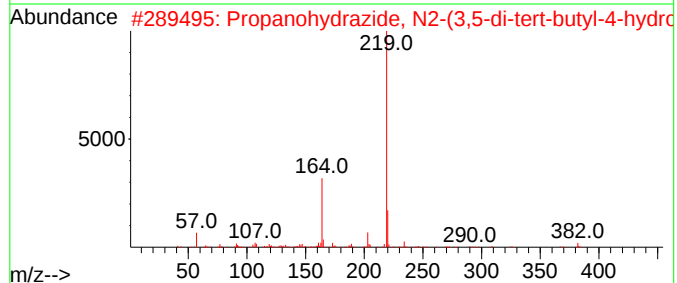
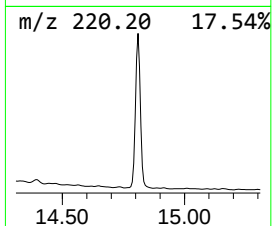
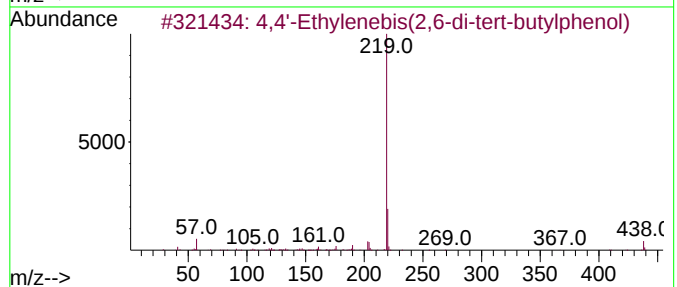
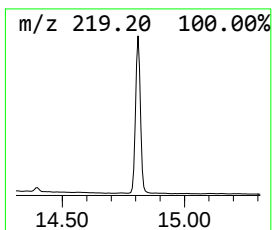
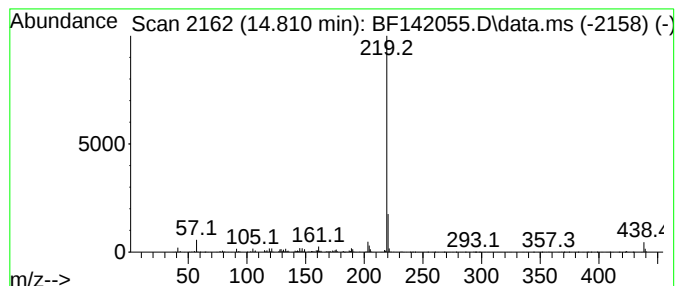
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 4,4'-Ethylenebis(2,6-di-ter... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.810	20.00 ng	1242890	Perylene-d12	15.527	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Ethylenebis(2,6-di-tert-but...	438	C30H46O2	001516-94-5	93
2	Propanohydrazide, N2-(3,5-di-ter...	382	C24H34N2O2	304870-86-8	78
3	4-tert-Butyl-2,6-diisopropylphen...	276	C18H28O2	1000236-32-0	72
4	2-Methyl-4-phenylquinoline	219	C16H13N	001721-92-2	72
5	5,8-Methano-1H-[1,2,4]triazolo[1...	395	C25H21N3O2	1000142-91-6	64



Data Path : T:\svoasrv\HPCHEM1\BNA_F\Data\BF032425\
Data File : BF142055.D
Acq On : 24 Mar 2025 15:25
Operator : RC/JU
Sample : Q1606-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N48965

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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-Methoxy-2-pro...	5.434	343.4	ng	17759500	1	6.875	1034270	20.0
unknown5.669	5.669	5.8	ng	301064	1	6.875	1034270	20.0
Ethanol, 2-butoxy-	5.840	58.1	ng	3005080	1	6.875	1034270	20.0
unknown6.751	6.751	8.7	ng	449095	1	6.875	1034270	20.0
1-Hexanol, 2-et...	6.934	23.2	ng	1200230	1	6.875	1034270	20.0
unknown7.216	7.216	8.5	ng	438196	1	6.875	1034270	20.0
unknown7.581	7.581	12.3	ng	650949	2	8.157	1055980	20.0
unknown7.645	7.645	5.3	ng	277989	2	8.157	1055980	20.0
4,4'-Ethylenebi...	14.810	20.0	ng	1242890	6	15.527	1242890	20.0