

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080625\
 Data File : BF143337.D
 Acq On : 06 Aug 2025 18:40
 Operator : RC/JU
 Sample : Q2774-09 2X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 248

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-BF071725.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF143337.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	6	12	28	rVB	231903	378789	40.06%	4.402%
2	5.181	503	508	516	rBV	67628	93003	9.84%	1.081%
3	5.593	572	578	589	rBV	624190	804258	85.05%	9.345%
4	6.587	742	747	758	rVB	613813	777653	82.24%	9.036%
5	6.963	806	811	820	rVB	488174	613743	64.90%	7.132%
6	7.363	873	879	891	rVB3	17085	39717	4.20%	0.462%
7	7.516	897	905	910	rBV	429098	552647	58.44%	6.422%
8	7.663	924	930	937	rVB4	35304	95316	10.08%	1.108%
9	7.992	982	986	993	rVB3	26490	42304	4.47%	0.492%
10	8.063	993	998	1006	rBV	81634	146033	15.44%	1.697%
11	8.145	1007	1012	1015	rBV5	20724	39003	4.12%	0.453%
12	8.240	1022	1028	1033	rBV	608946	846449	89.51%	9.836%
13	8.328	1040	1043	1048	rVB2	40419	58655	6.20%	0.682%
14	8.387	1048	1053	1057	rBV3	45739	78208	8.27%	0.909%
15	8.569	1076	1084	1088	rBV	99199	203884	21.56%	2.369%
16	8.657	1095	1099	1102	rBV	48951	67202	7.11%	0.781%
17	8.739	1110	1113	1116	rVB2	50008	56248	5.95%	0.654%
18	8.787	1116	1121	1125	rBV2	76351	137689	14.56%	1.600%
19	8.934	1142	1146	1148	rBV3	33734	55236	5.84%	0.642%
20	8.957	1148	1150	1153	rVB	44041	43462	4.60%	0.505%
21	9.022	1157	1161	1165	rBV2	61345	81708	8.64%	0.949%
22	9.069	1165	1169	1171	rBV2	61710	91337	9.66%	1.061%
23	9.187	1185	1189	1194	rBV3	83604	146504	15.49%	1.702%
24	9.245	1195	1199	1200	rBV2	72531	97614	10.32%	1.134%
25	9.316	1206	1211	1216	rVB	765563	945632	100.00%	10.988%
26	9.716	1276	1279	1282	rBV2	190392	241161	25.50%	2.802%
27	9.916	1310	1313	1317	rVB	307837	371626	39.30%	4.318%
28	9.998	1324	1327	1331	rVB	650096	842874	89.13%	9.794%
29	15.651	2284	2288	2299	rVB	270232	467764	49.47%	5.435%
30	16.968	2508	2512	2518	rVB2	107472	190124	20.11%	2.209%

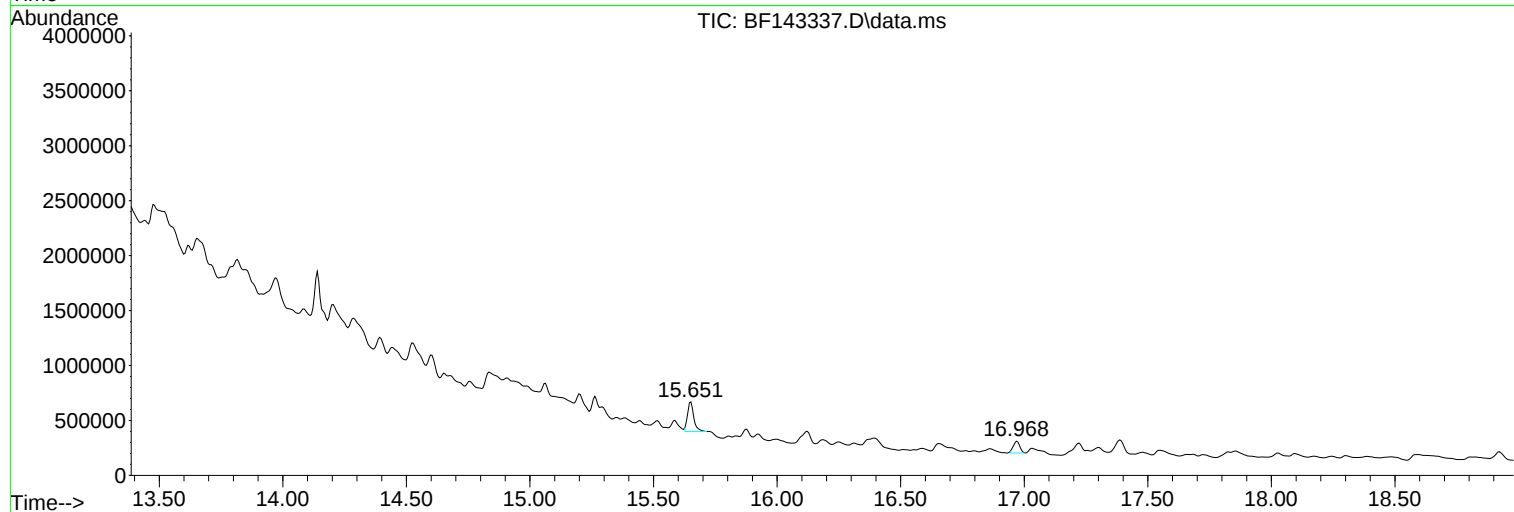
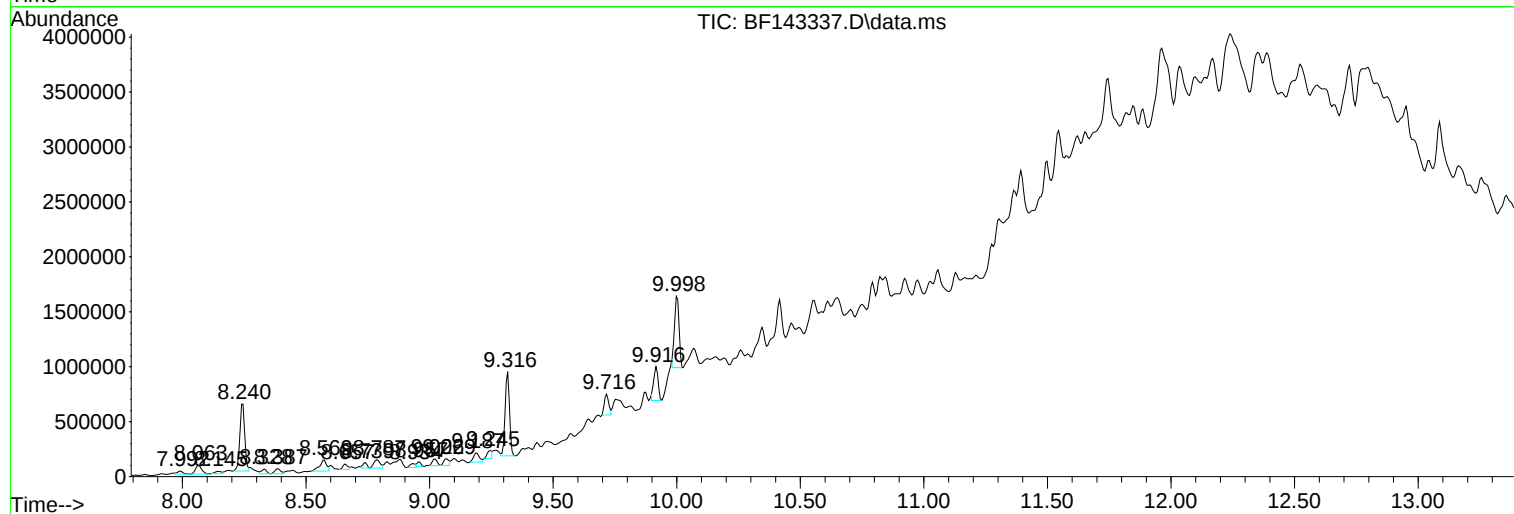
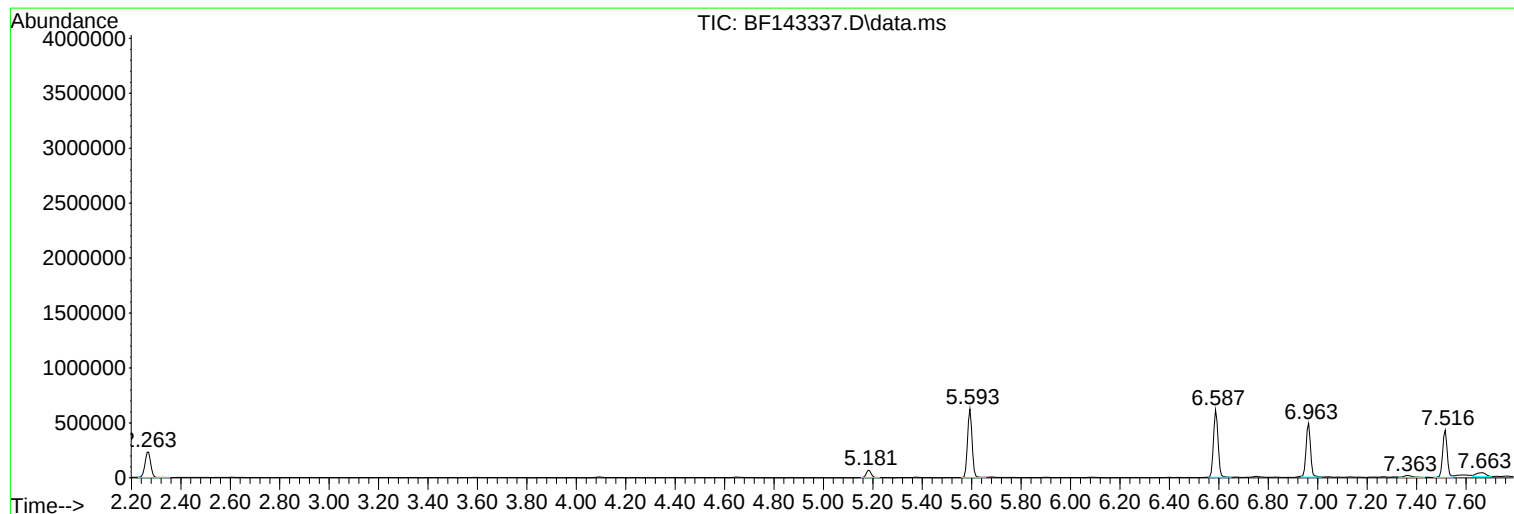
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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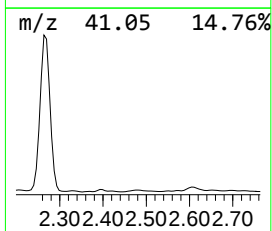
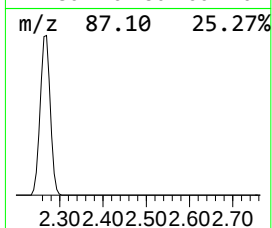
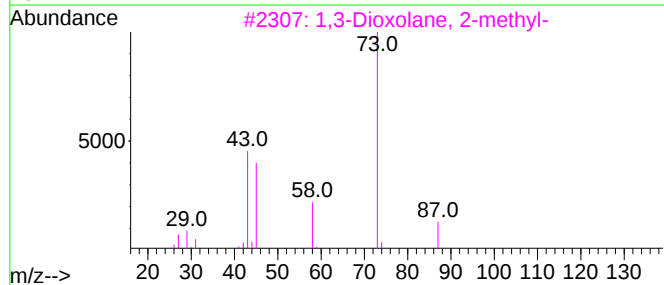
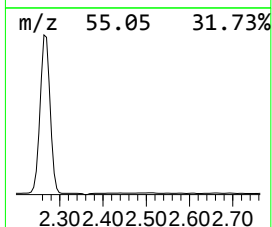
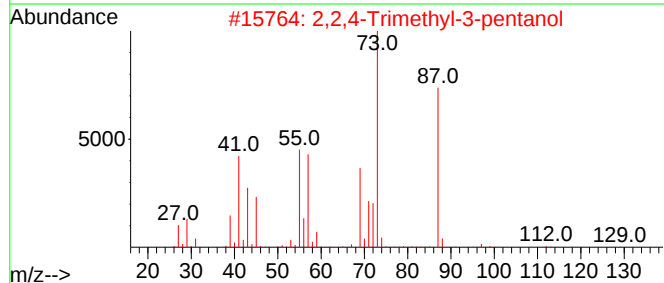
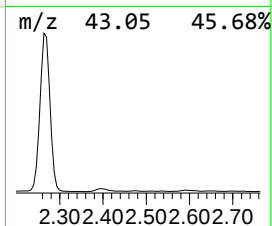
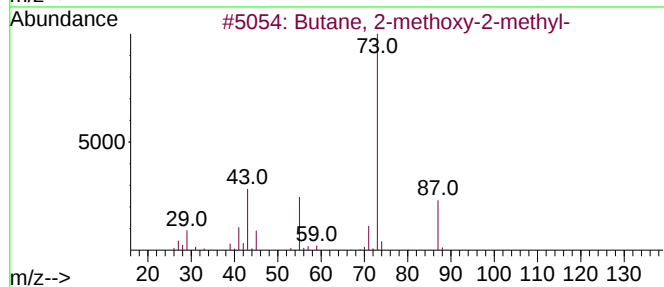
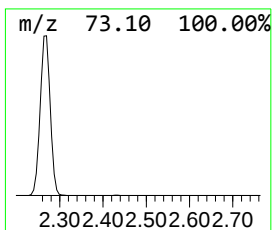
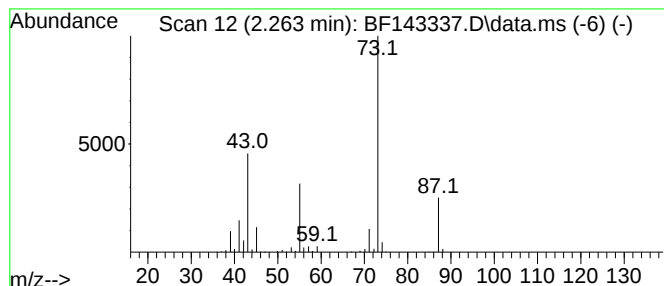
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	12.34 ng	378789	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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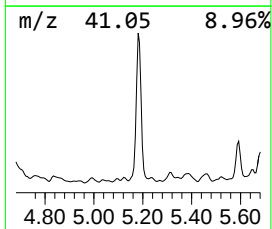
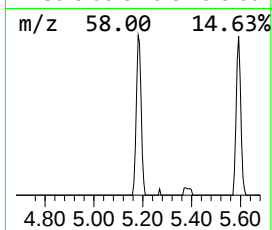
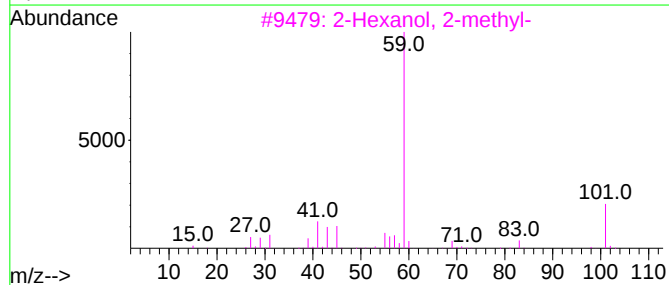
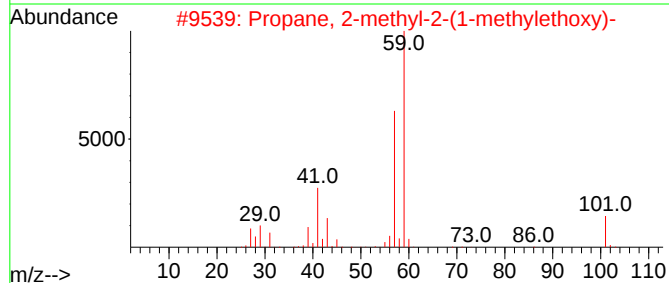
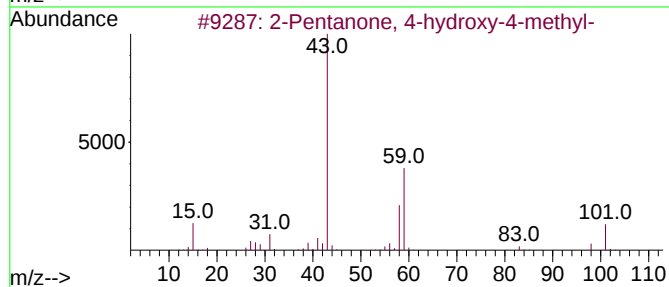
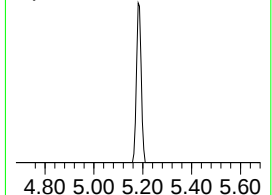
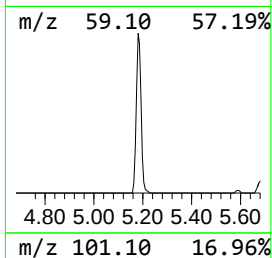
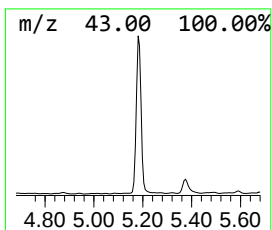
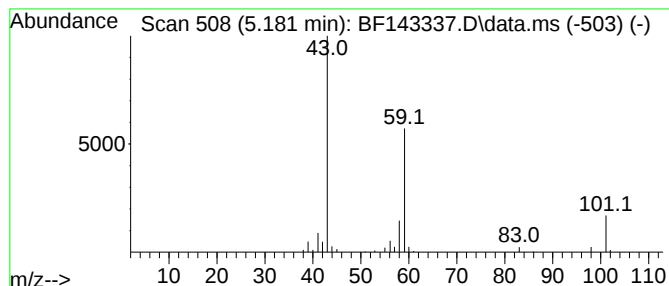
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	3.03 ng	93003	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27



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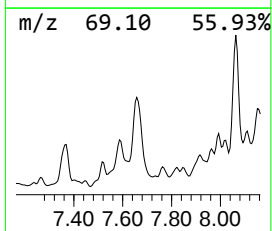
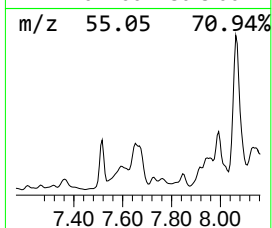
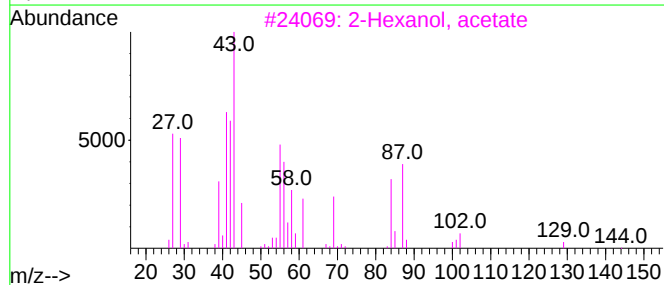
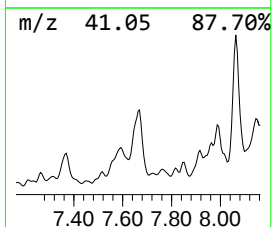
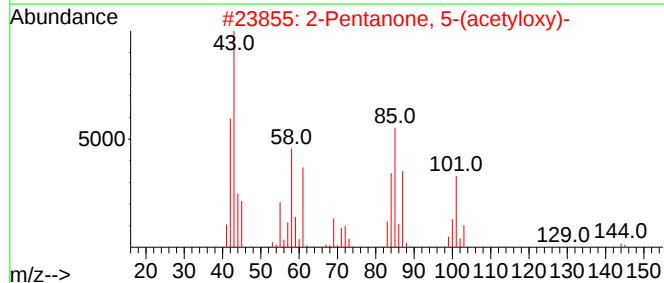
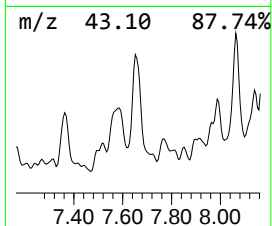
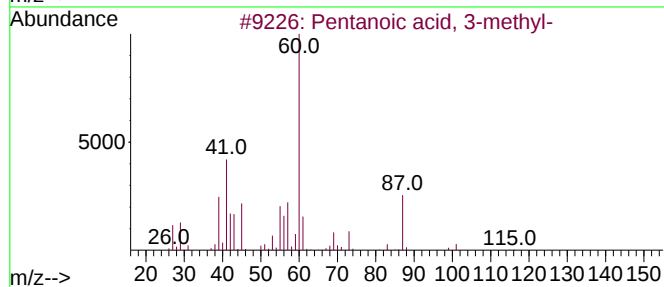
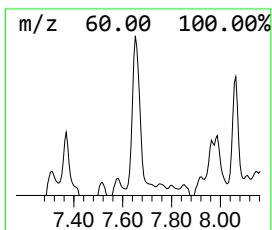
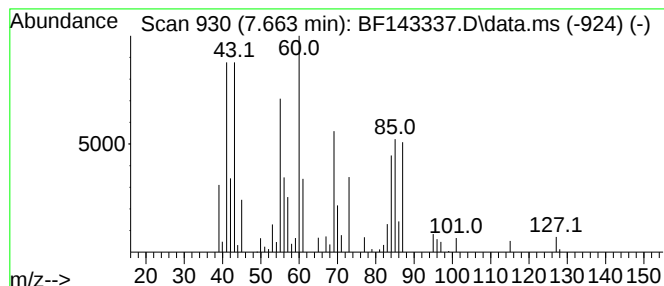
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.663 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.663	2.25 ng	95316	Naphthalene-d8	8.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	37
2			2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	25
3			2-Hexanol, acetate	144	C8H16O2	005953-49-1	16
4			Acetic acid, 2-ethylbutyl ester	144	C8H16O2	010031-87-5	14
5			Piperidine, 1-acetyl-	127	C7H13NO	000618-42-8	14



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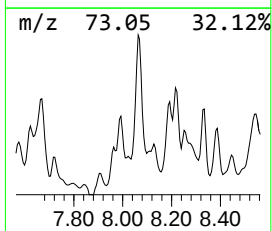
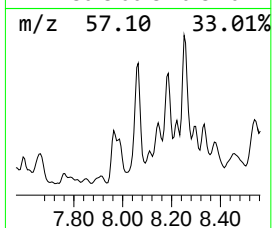
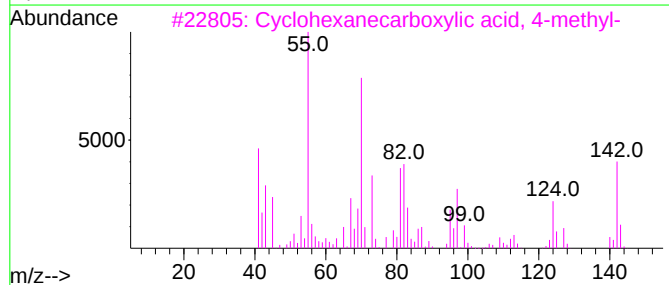
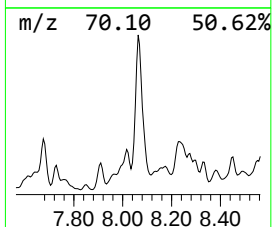
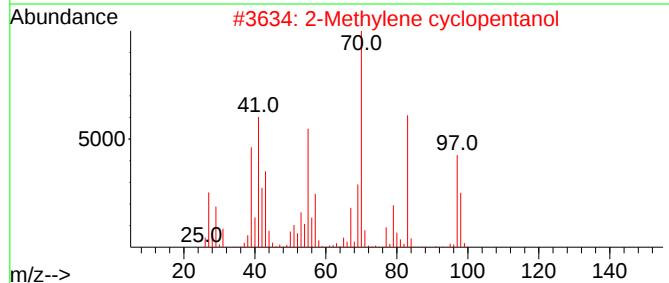
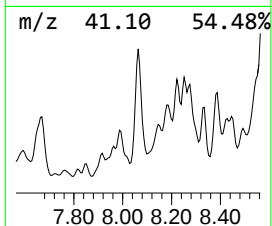
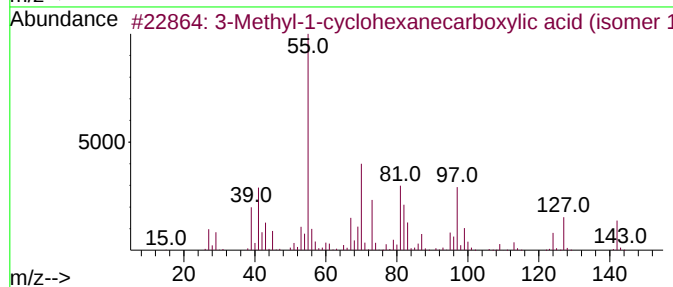
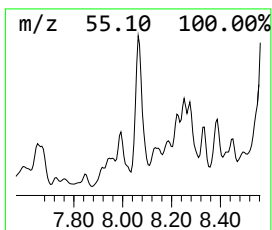
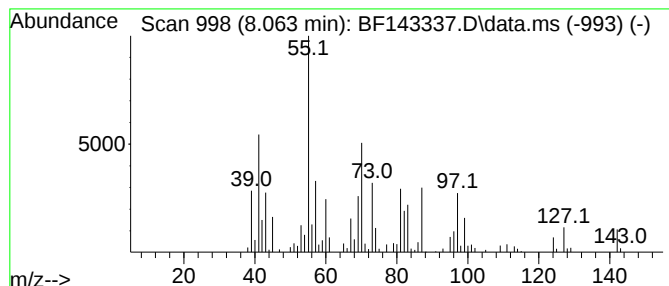
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Peak Number 4 3-Methyl-1-cyclohexanecarbo... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.063	3.45 ng	146033	Naphthalene-d8	8.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-1-cyclohexanecarboxylic...	142	C8H14O2	1000453-57-0	55
2			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	30
3			Cyclohexanecarboxylic acid, 4-me...	142	C8H14O2	004331-54-8	22
4			3-Hexenoic acid, (Z)-	114	C6H10O2	001775-43-5	14
5			3-Pyrrolidin-2-yl-propionic acid	143	C7H13NO2	1000193-88-0	14



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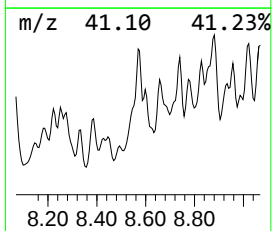
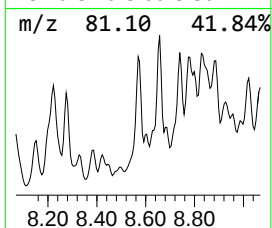
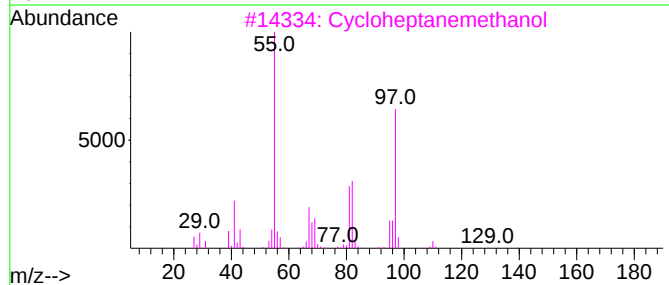
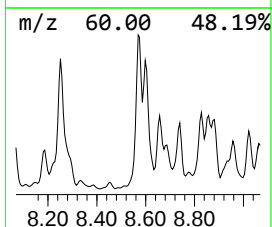
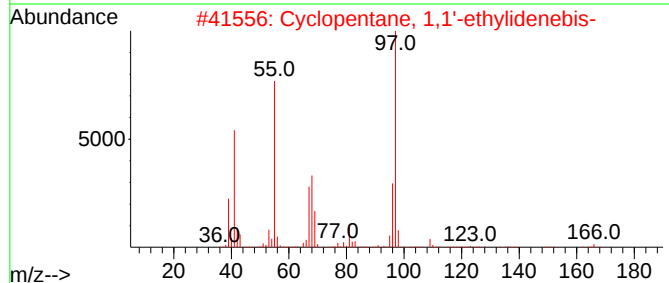
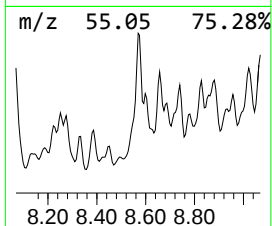
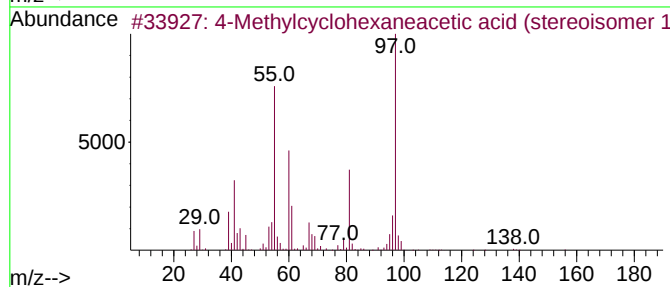
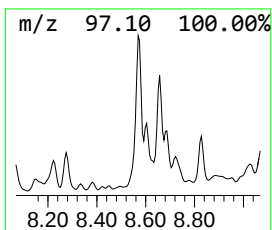
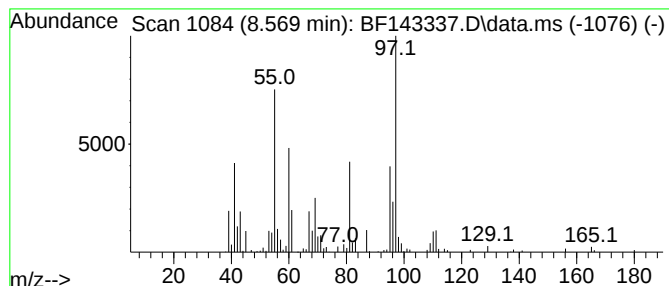
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Peak Number 5 4-Methylcyclohexaneacetic a... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.569	4.82 ng	203884	Naphthalene-d8	8.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methylcyclohexaneacetic acid (...)	156	C9H16O2	1000453-59-3	53
2			Cyclopentane, 1,1'-ethylidenebis-	166	C12H22	004413-21-2	43
3			Cycloheptanemethanol	128	C8H16O	004448-75-3	43
4			1,2-Octanediol	146	C8H18O2	001117-86-8	38
5			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	38



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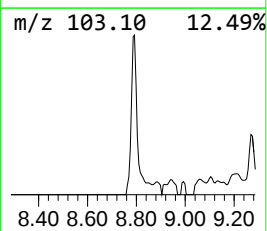
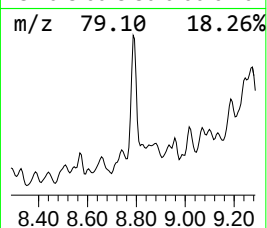
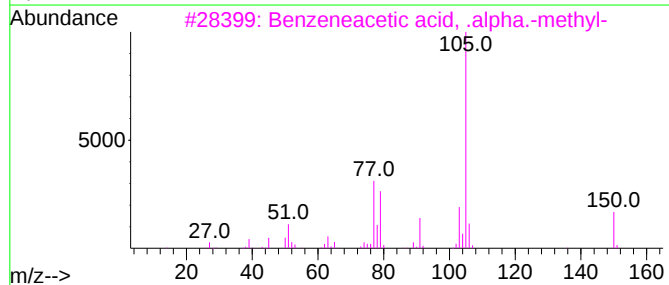
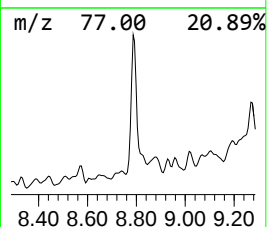
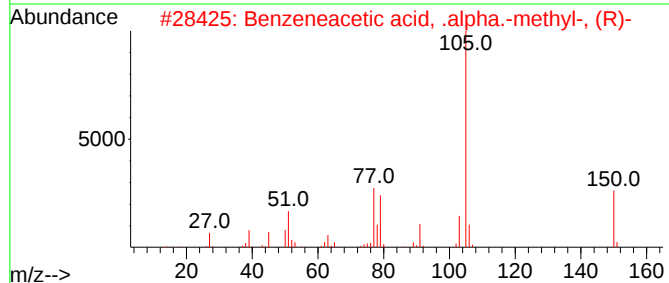
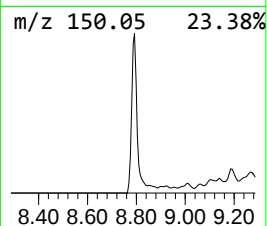
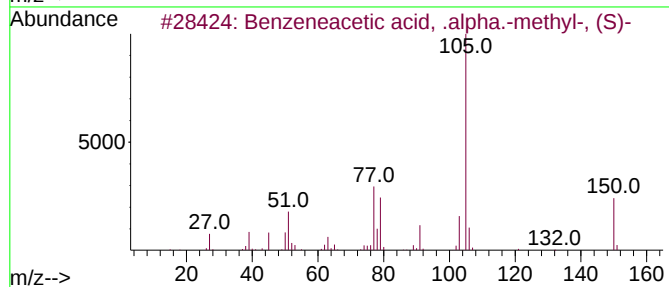
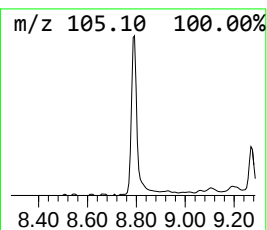
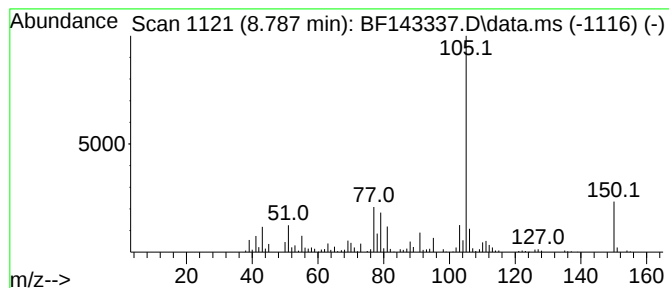
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzeneacetic acid, .alpha.... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	3.25 ng	137689	Naphthalene-d8	8.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-24-3	95
2			Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-26-5	93
3			Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	92
4			m-Tolylacetic acid	150	C9H10O2	000621-36-3	81
5			p-Tolylacetic acid	150	C9H10O2	000622-47-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080625\
Data File : BF143337.D
Acq On : 06 Aug 2025 18:40
Operator : RC/JU
Sample : Q2774-09 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

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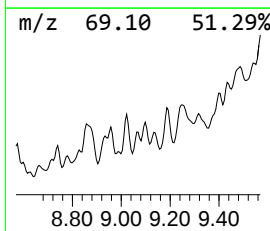
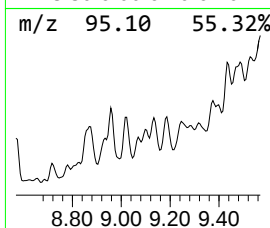
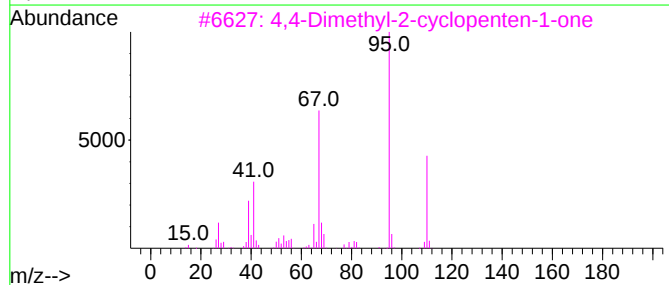
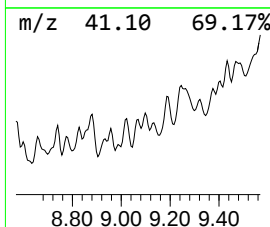
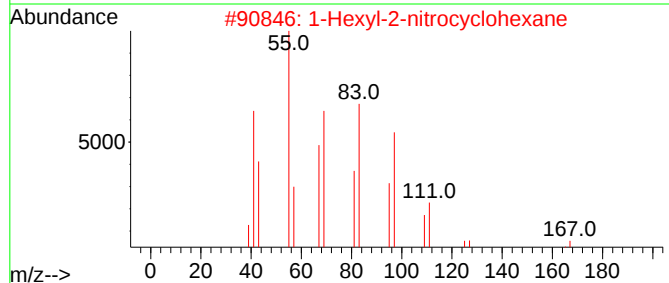
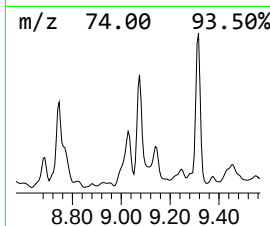
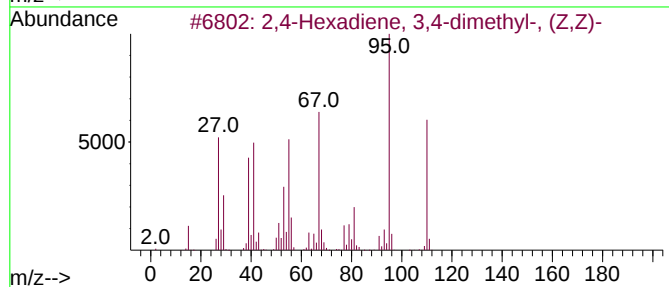
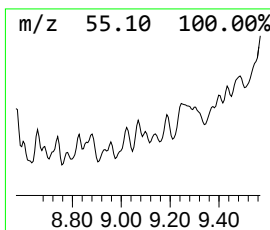
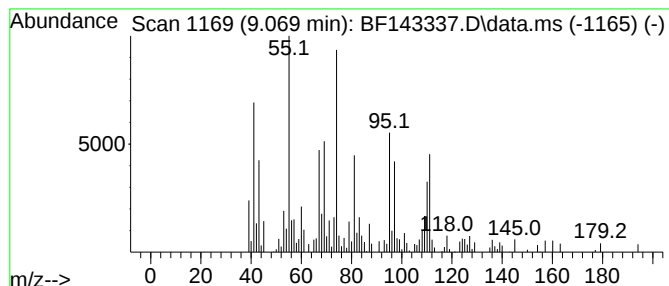
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.069 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.069	2.16 ng	91337	Naphthalene-d8	8.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	35		
2	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	30		
3	4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	22		
4	1,2,3,4-Hexadecanetetrol, [2R-(2...	290	C16H34O4	136953-06-5	22		
5	2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	18		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080625\
Data File : BF143337.D
Acq On : 06 Aug 2025 18:40
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Sample : Q2774-09 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

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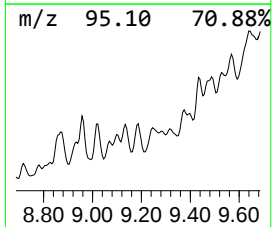
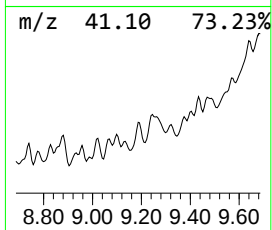
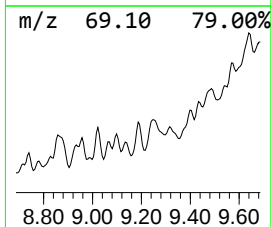
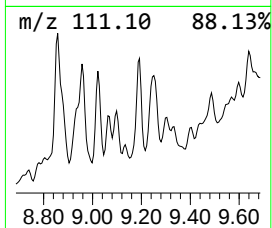
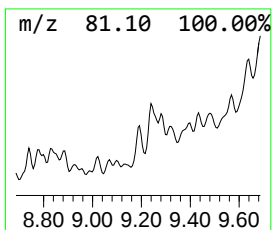
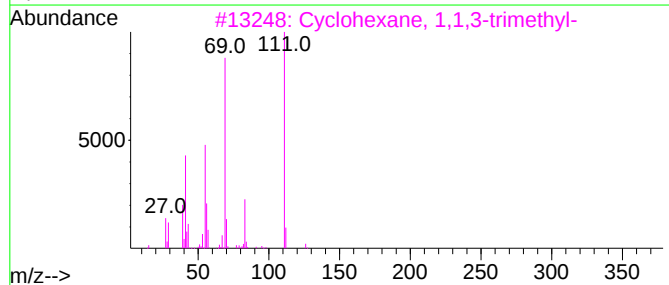
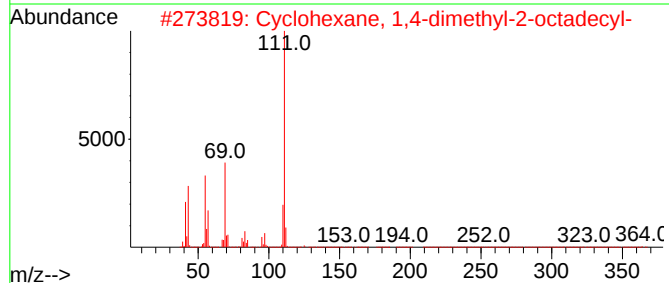
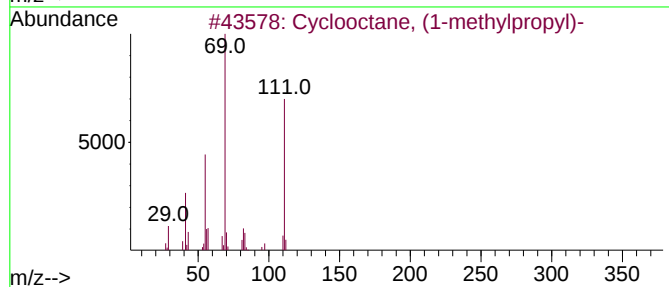
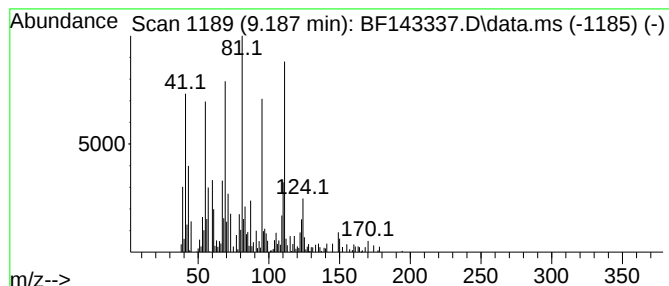
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.187 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.187	3.48 ng	146504	Acenaphthene-d10	10.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	35
2		Cyclohexane, 1,4-dimethyl-2-octa...	364	C26H52	055282-02-5	35
3		Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	30
4		Cyclooctane, cyclohexyl-	194	C14H26	092369-78-3	30
5		Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080625\
Data File : BF143337.D
Acq On : 06 Aug 2025 18:40
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Sample : Q2774-09 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

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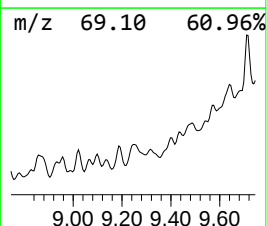
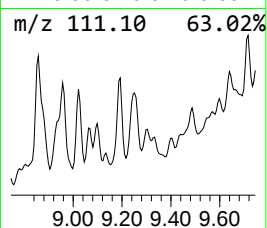
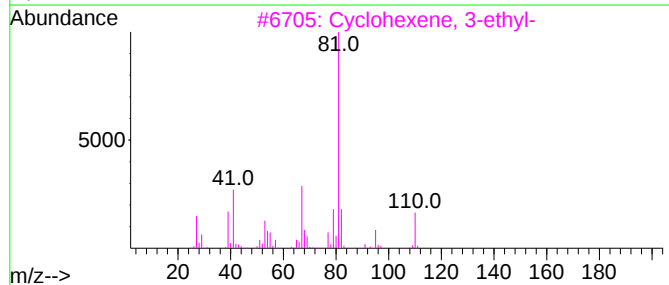
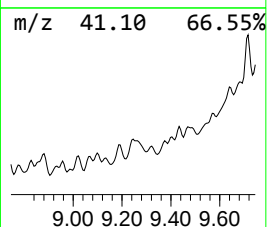
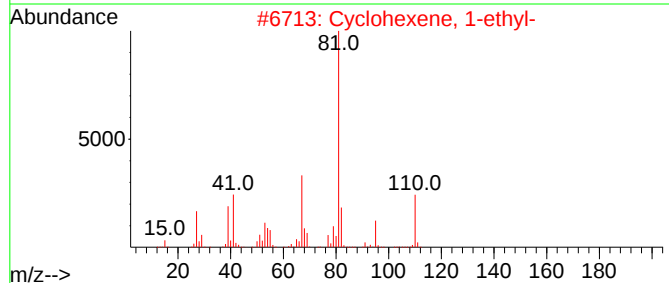
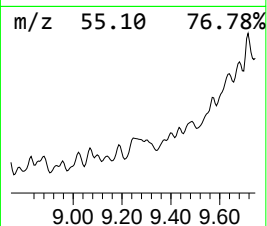
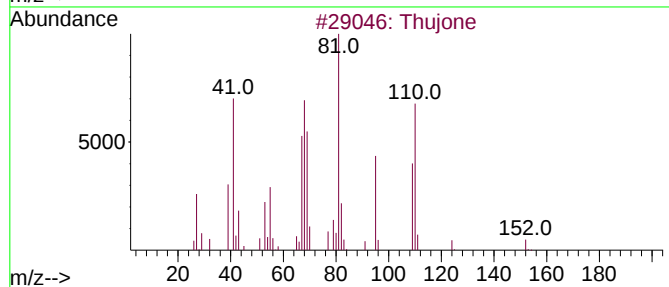
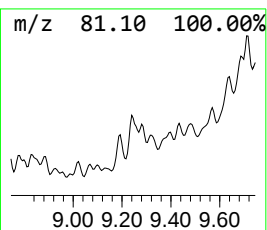
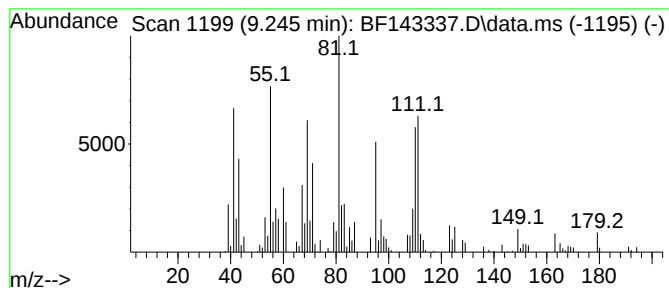
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown9.245 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.245	2.32 ng	97614	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thujone	152	C10H16O	000546-80-5	45
2			Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	38
3			Cyclohexene, 3-ethyl-	110	C8H14	002808-71-1	38
4			2,4-Heptadienal, (E,E)-	110	C7H10O	004313-03-5	30
5			Cyclohexane, ethylidene-	110	C8H14	001003-64-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080625\
Data File : BF143337.D
Acq On : 06 Aug 2025 18:40
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Sample : Q2774-09 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

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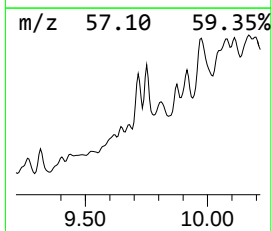
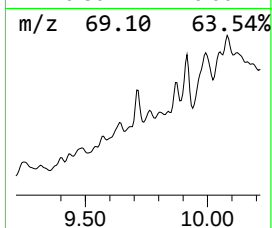
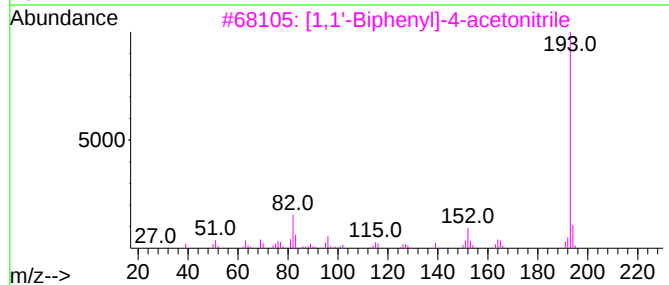
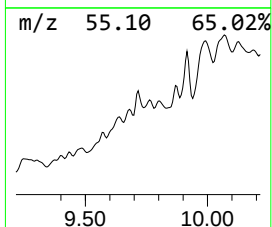
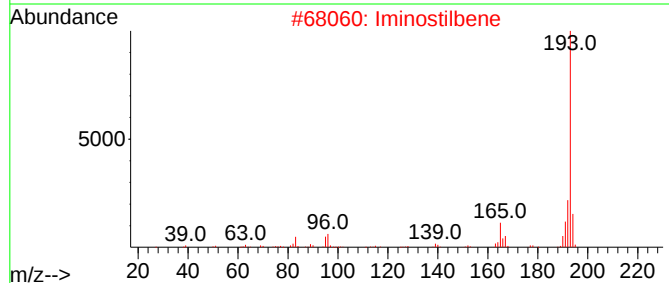
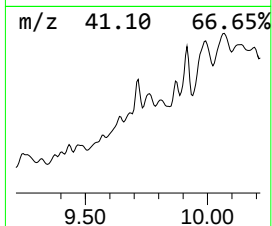
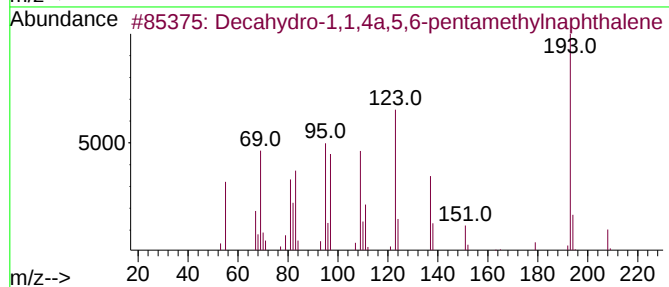
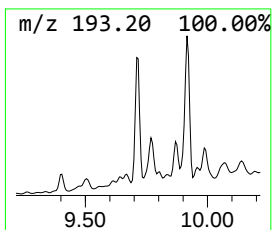
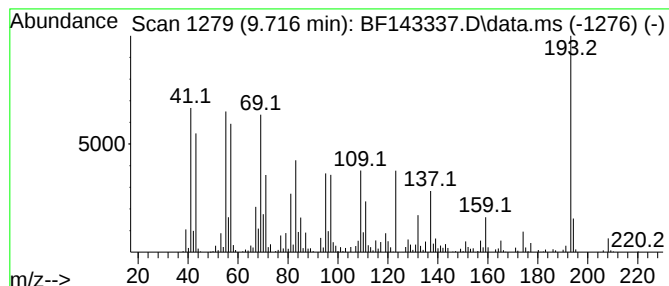
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.716	5.72 ng	241161	Acenaphthene-d10	10.004

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	70
2		Iminostilbene	193	C14H11N	000256-96-2	30
3		[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	30
4		5-Amino-2-fluorobenzonitrile, TM...	208	C10H13FN2Si	1000478-92-3	25
5		1H-Indole, 2-phenyl-	193	C14H11N	000948-65-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080625\
Data File : BF143337.D
Acq On : 06 Aug 2025 18:40
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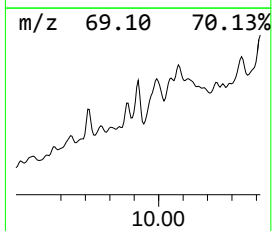
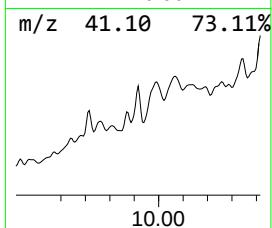
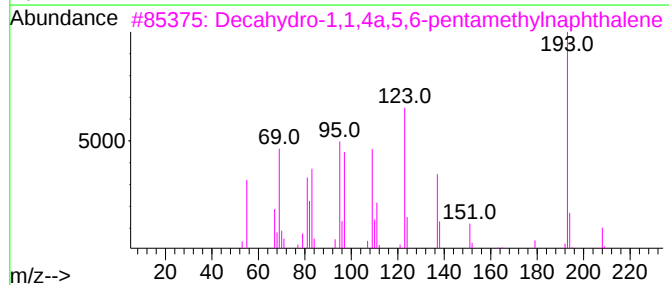
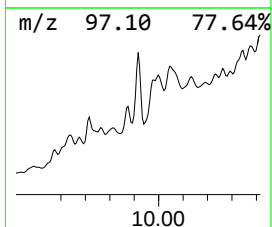
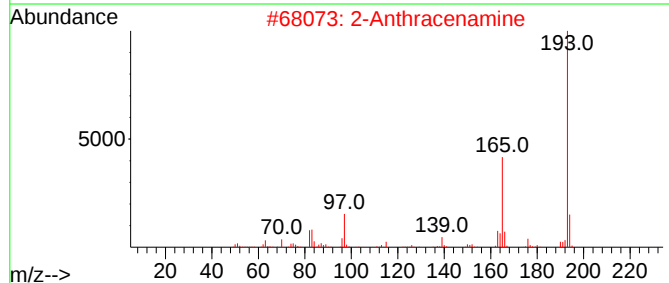
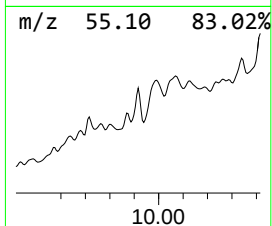
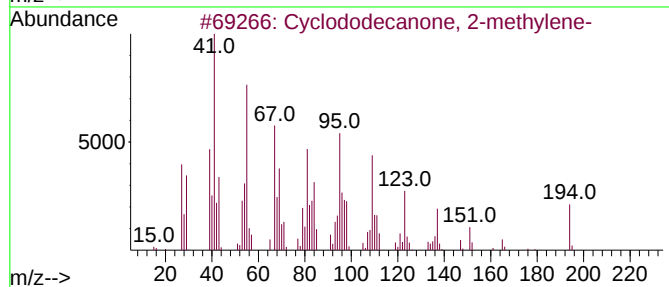
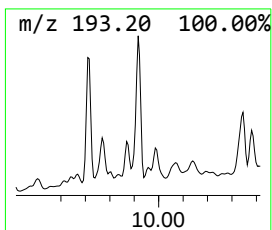
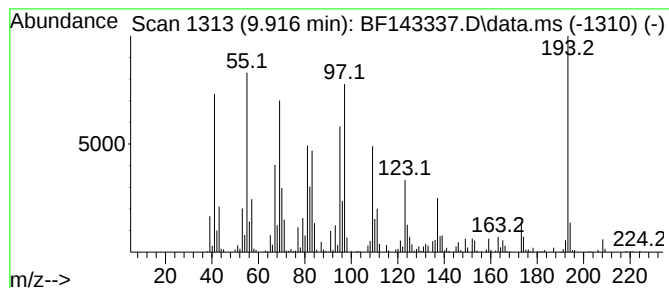
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclododecanone, 2-methylene- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.916	8.82 ng	371626	Acenaphthene-d10		10.004	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclododecanone, 2-methylene-		194	C13H22O	003045-76-9	52
2	2-Anthracenamine		193	C14H11N	000613-13-8	50
3	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	38
4	Cyclohexane, 2,4-diisopropyl-1,1...		196	C14H28	1000149-60-5	30
5	4-Amino-N-hydroxypyrazolo[3,2-c]...		193	C6H7N7O	1000443-50-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080625\
Data File : BF143337.D
Acq On : 06 Aug 2025 18:40
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Sample : Q2774-09 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

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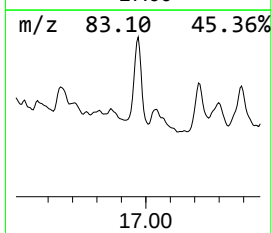
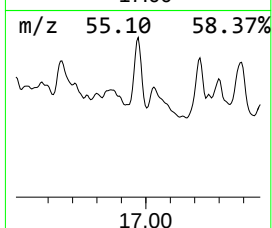
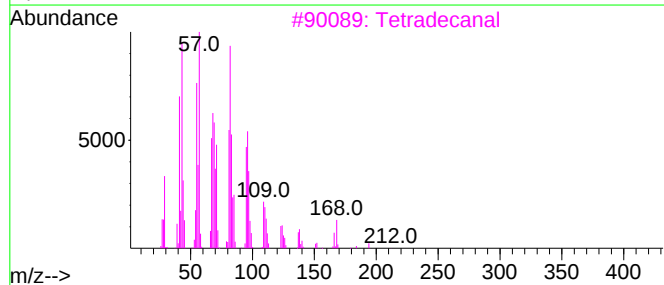
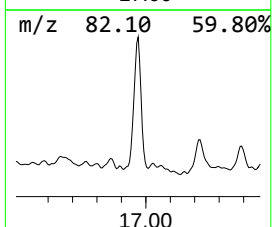
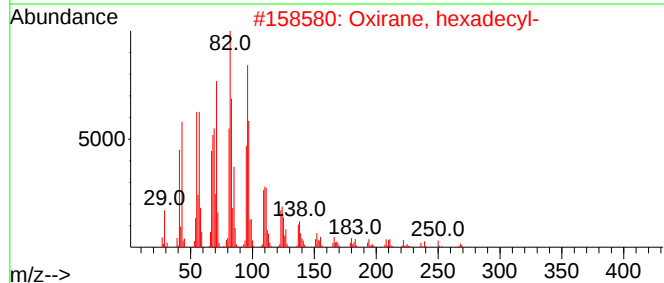
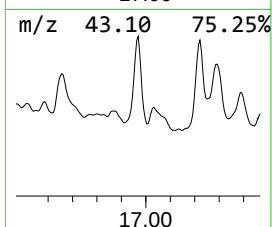
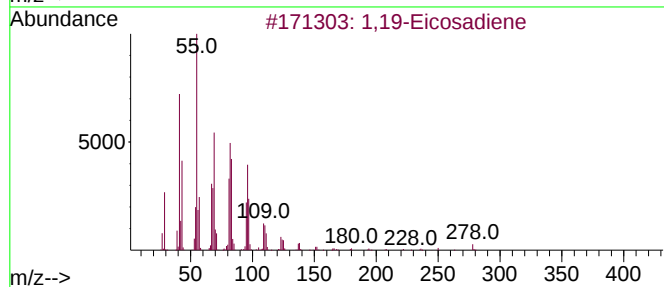
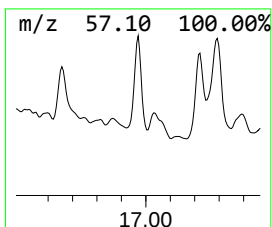
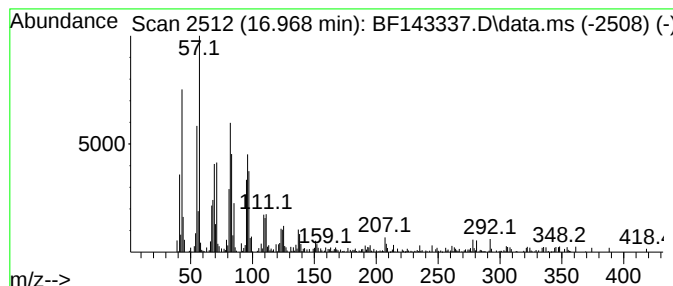
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,19-Eicosadiene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.968	8.13 ng	190124	Perylene-d12	15.651

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,19-Eicosadiene	278	C20H38	014811-95-1	92
2		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3		Tetradecanal	212	C14H28O	000124-25-4	91
4		Tetracosanal	352	C24H48O	057866-08-7	76
5		Cyclododecanol	184	C12H24O	001724-39-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080625\
Data File : BF143337.D
Acq On : 06 Aug 2025 18:40
Operator : RC/JU
Sample : Q2774-09 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
248

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071725.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...	2.263	12.3	ng	378789	1	6.963	613743	20.0
2-Pentanone, 4-...	5.181	3.0	ng	93003	1	6.963	613743	20.0
unknown7.663	7.663	2.3	ng	95316	2	8.245	846449	20.0
3-Methyl-1-cycl...	8.063	3.5	ng	146033	2	8.245	846449	20.0
4-Methylcyclohe...	8.569	4.8	ng	203884	2	8.245	846449	20.0
Benzeneacetic a...	8.787	3.3	ng	137689	2	8.245	846449	20.0
unknown9.069	9.069	2.2	ng	91337	2	8.245	846449	20.0
unknown9.187	9.187	3.5	ng	146504	3	10.004	842874	20.0
unknown9.245	9.245	2.3	ng	97614	3	10.004	842874	20.0
Decahydro-1,1,4...	9.716	5.7	ng	241161	3	10.004	842874	20.0
Cyclododecanone...	9.916	8.8	ng	371626	3	10.004	842874	20.0
1,19-Eicosadiene	16.968	8.1	ng	190124	6	15.651	467764	20.0