

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
 Data File : BF140170.D
 Acq On : 30 Oct 2024 20:51
 Operator : RC/JU
 Sample : P4613-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ARS20-0001

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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140170.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.493	572	578	587	rBV	1255419	1649096	98.03%	17.842%
2	6.163	684	692	699	rVB	268761	358201	21.29%	3.876%
3	6.504	744	750	755	rBV	1272792	1682200	100.00%	18.200%
4	6.887	810	815	821	rVB	529707	682842	40.59%	7.388%
5	7.016	828	837	843	rBV	339110	483664	28.75%	5.233%
6	7.445	899	910	914	rBV	860898	1328180	78.95%	14.370%
7	7.528	919	924	928	rBV4	144153	217773	12.95%	2.356%
8	7.693	948	952	958	rVB2	217513	306897	18.24%	3.320%
9	7.763	959	964	968	rBV4	101624	204666	12.17%	2.214%
10	7.810	968	972	976	rVV2	231739	306550	18.22%	3.317%
11	8.069	1013	1016	1021	rVB3	193175	260022	15.46%	2.813%
12	8.169	1026	1033	1037	rVV	803398	1451884	86.31%	15.709%
13	8.222	1039	1042	1045	rVB3	249727	310673	18.47%	3.361%

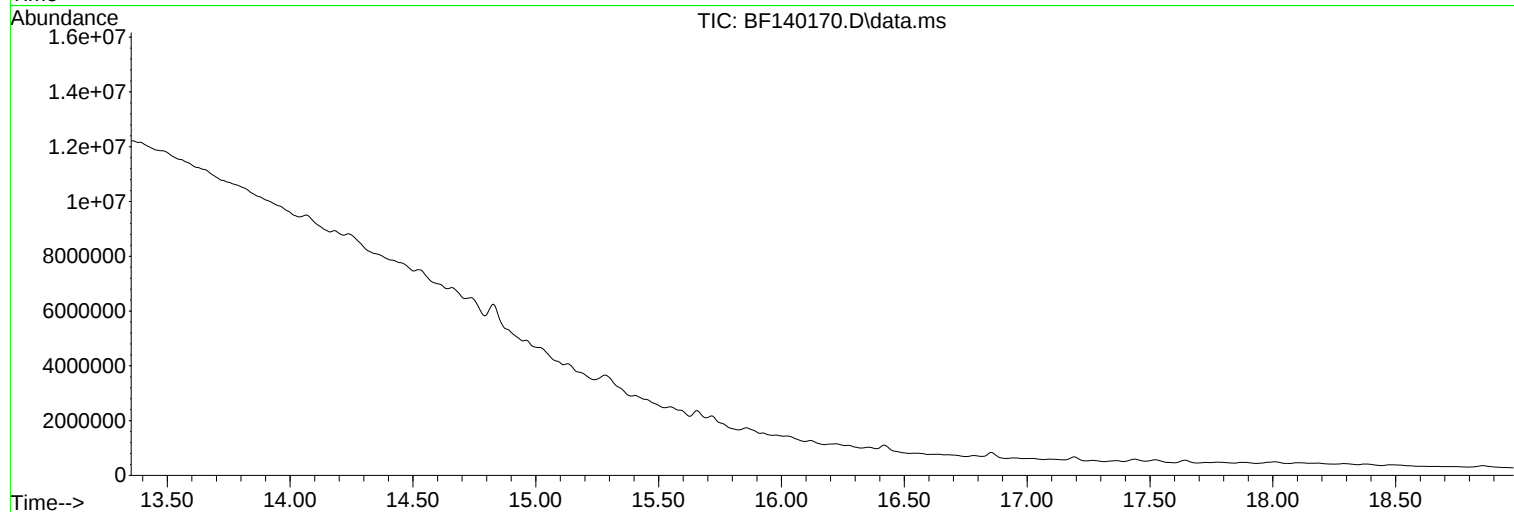
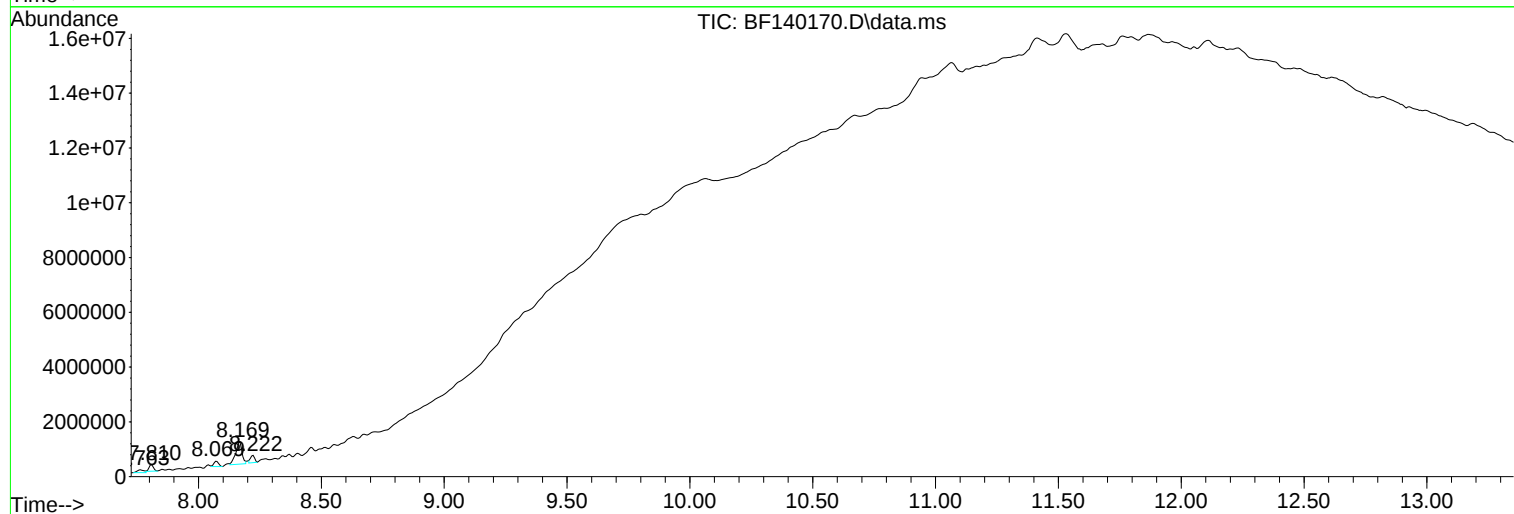
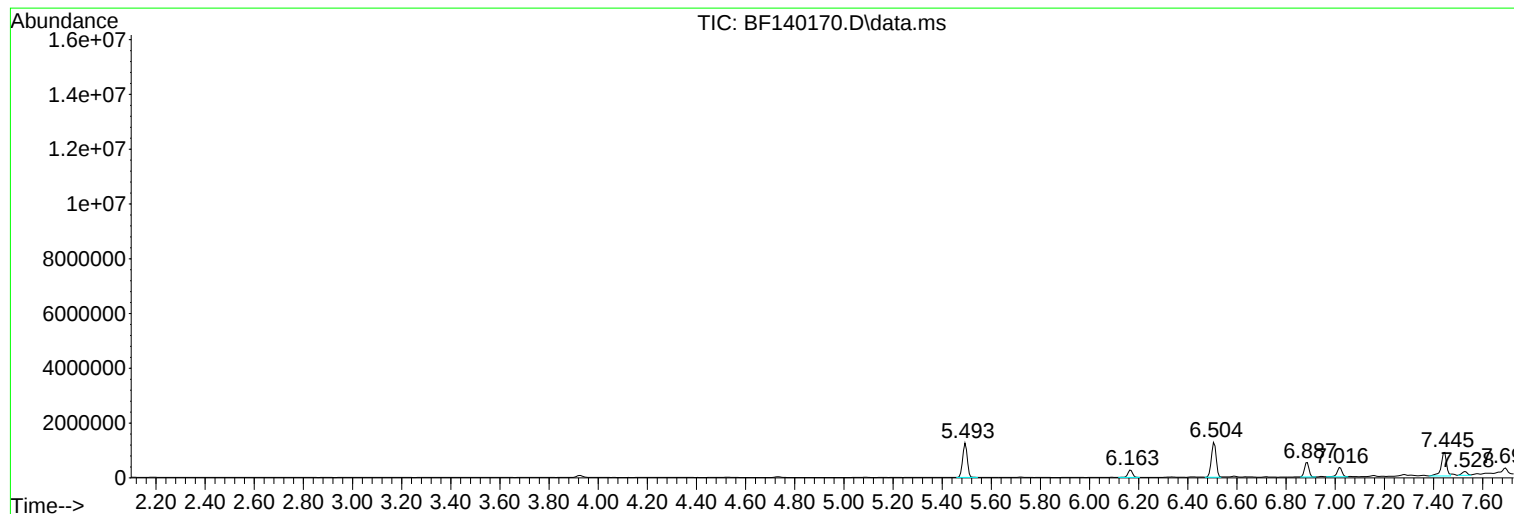
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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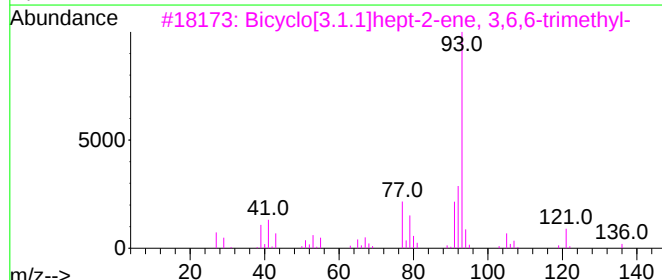
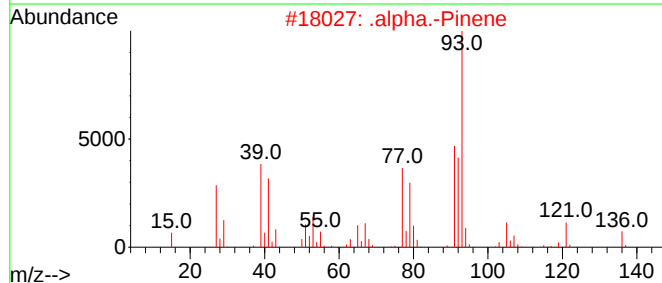
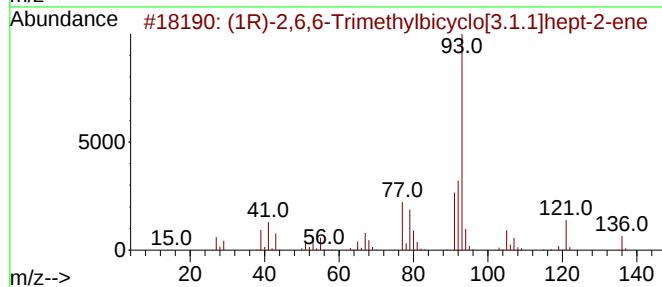
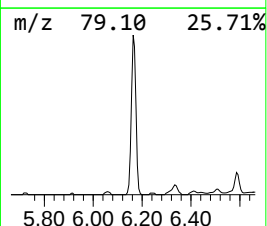
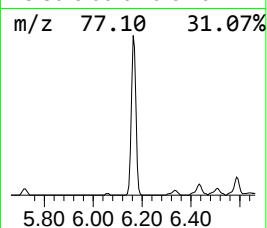
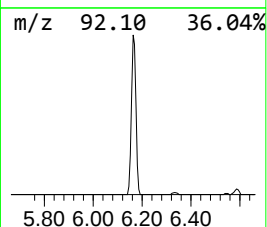
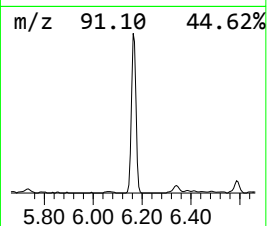
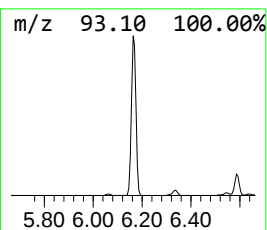
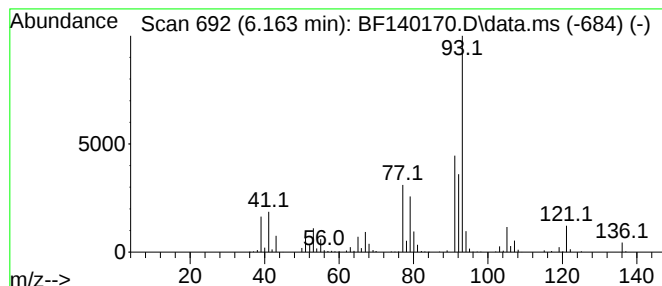
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.163	10.49 ng	358201	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	95		
2	.alpha.-Pinene	136	C10H16	000080-56-8	94		
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	94		
4	(+)-3-Carene	136	C10H16	000498-15-7	91		
5	Tricyclo[2.2.1.0(2,6)]heptane, 1,1,2-trimethyl-	136	C10H16	000508-32-7	91		



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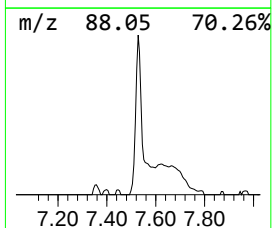
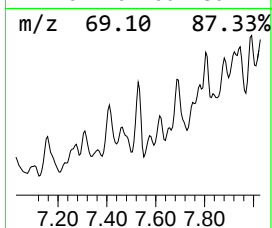
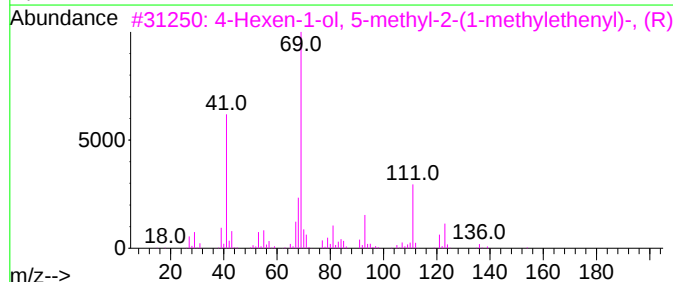
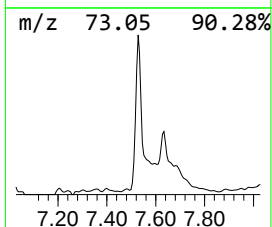
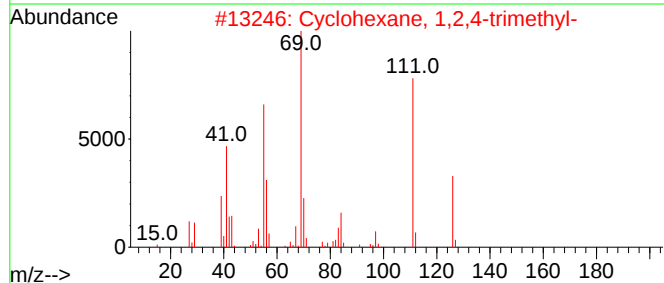
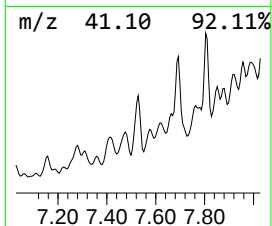
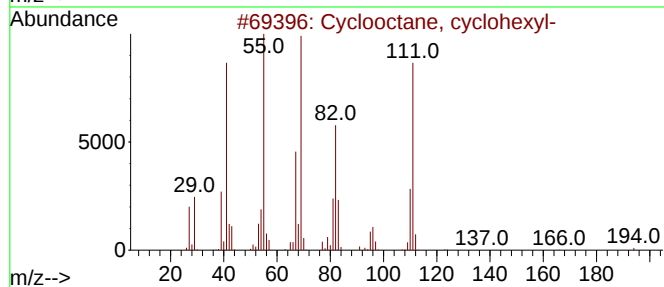
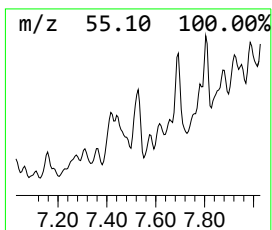
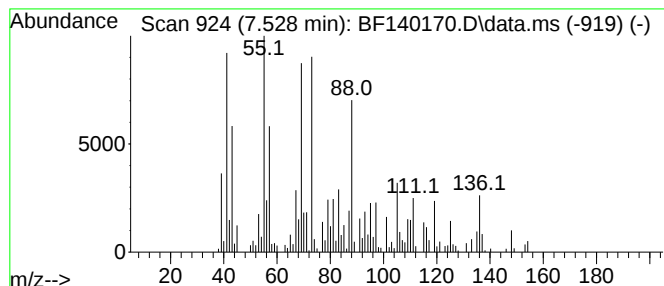
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Peak Number 2 unknown7.528 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.528	3.00 ng	217773	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane, cyclohexyl-	194	C14H26	092369-78-3	27
2			Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	25
3			4-Hexen-1-ol, 5-methyl-2-(1-meth...	154	C10H18O	000498-16-8	22
4			Oct-3-enoic acid, oct-3-en-2-yl ...	252	C16H28O2	1010406-95-0	22
5			Cyclohexane, (1,2-dimethylpropyl)-	154	C11H22	051284-29-8	22



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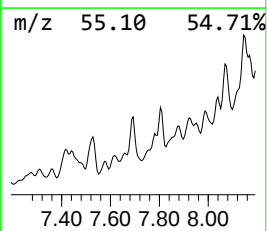
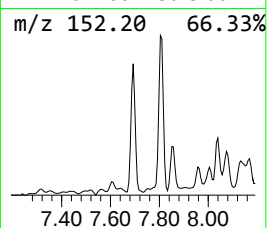
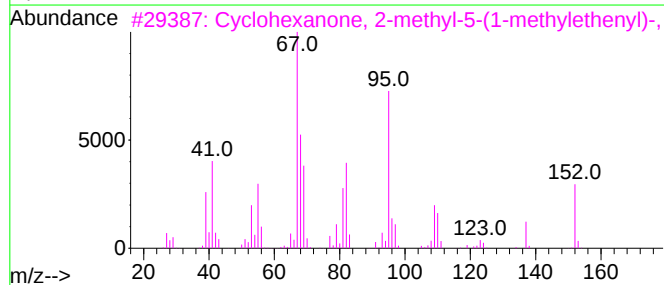
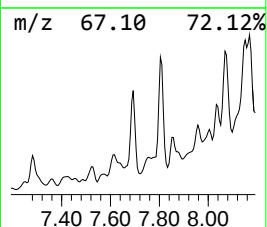
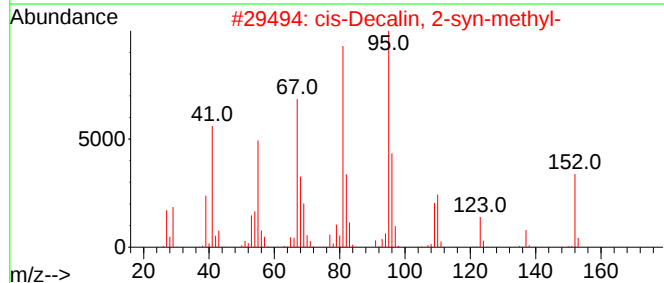
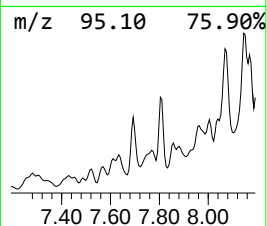
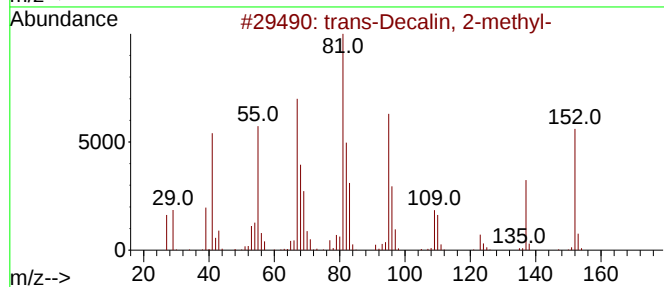
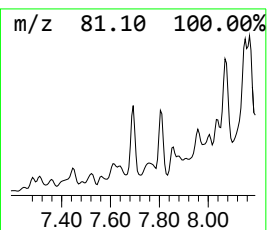
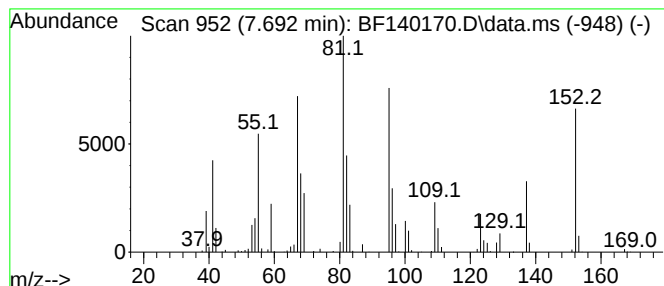
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Peak Number 3 trans-Decalin, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.692	4.23 ng	306897	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	93
2			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	81
3			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	60
4			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	53
5			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	52



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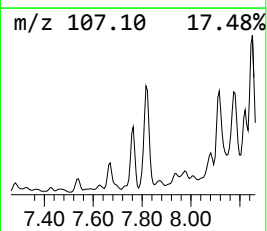
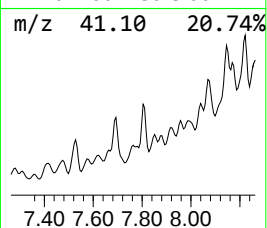
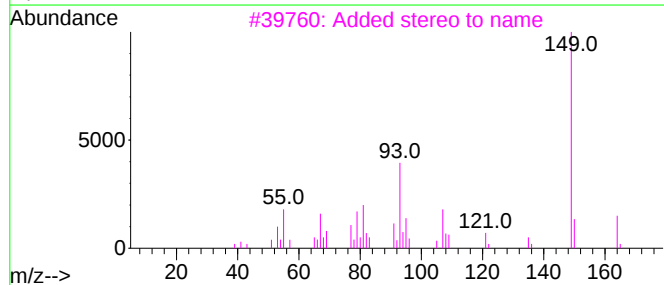
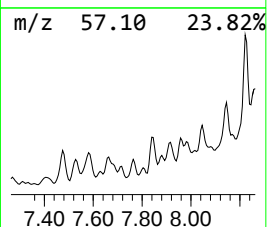
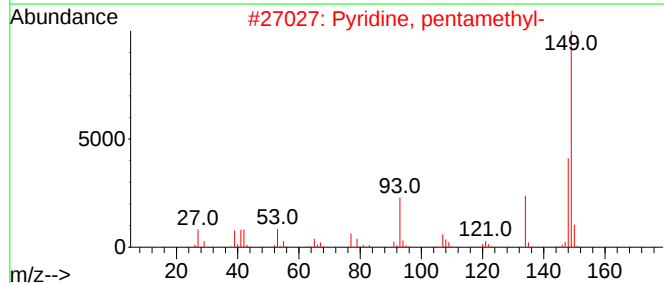
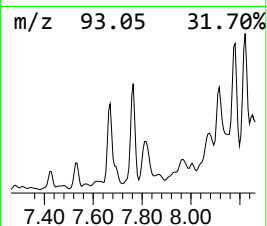
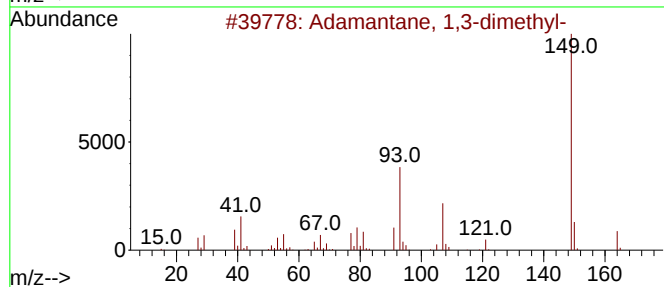
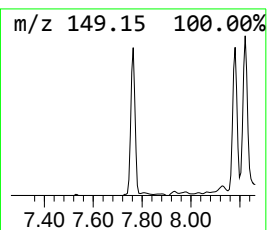
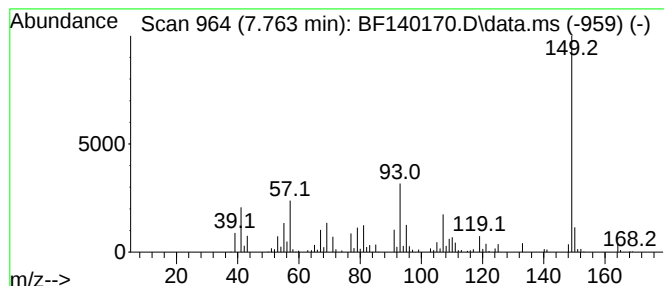
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Peak Number 4 Adamantane, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.763	2.82 ng	204666	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	72
2			Pyridine, pentamethyl-	149	C10H15N	003748-83-2	53
3			Added stereo to name	164	C12H20	024145-88-8	50
4			2-t-Butyl-5-[hydroxy-(2,4,6-trim...	306	C18H26O4	092572-63-9	50
5			2-(Heptyloxycarbonyl)benzoic acid	264	C15H20O4	024539-58-0	50



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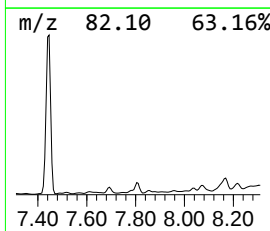
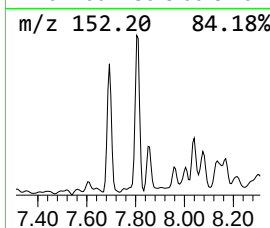
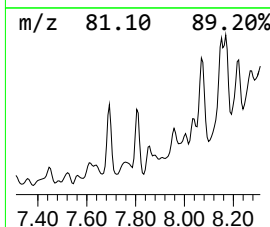
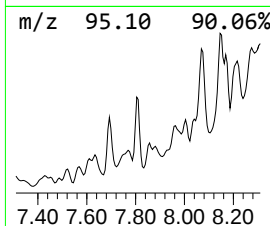
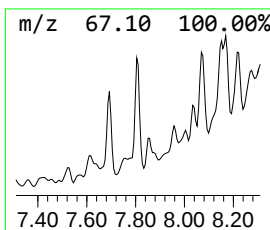
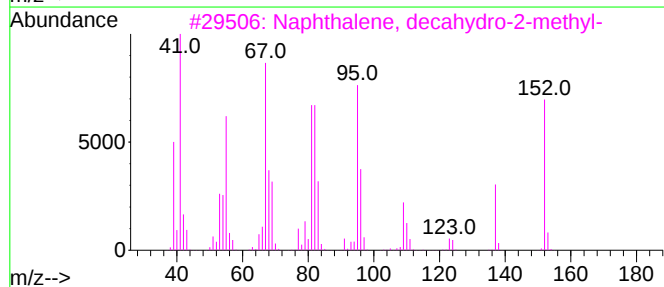
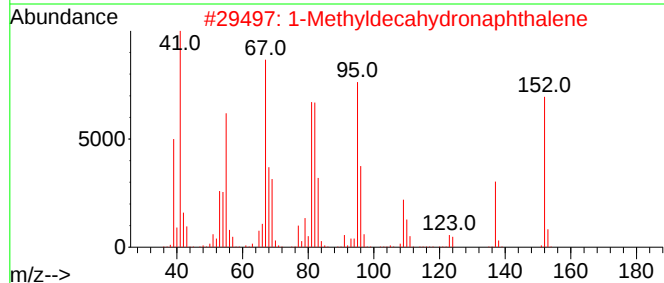
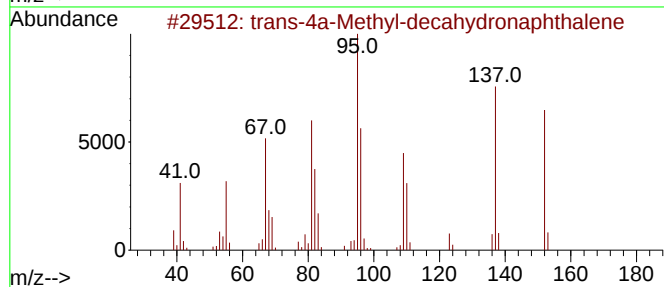
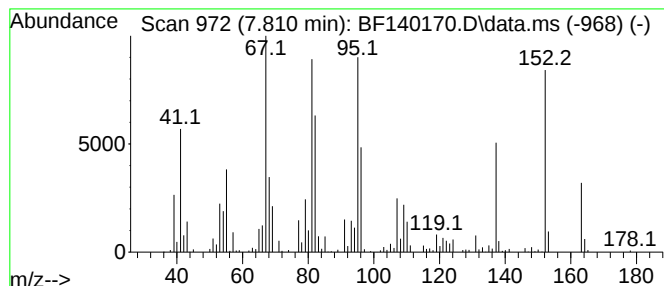
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Peak Number 5 trans-4a-Methyl-decahydrona... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.810	4.22 ng	306550	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	89
2			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	78
3			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	78
4			Spiro[5.5]undecane	152	C11H20	000180-43-8	60
5			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	58



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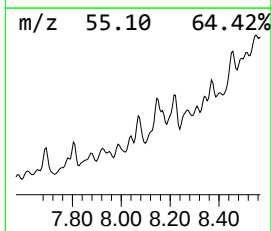
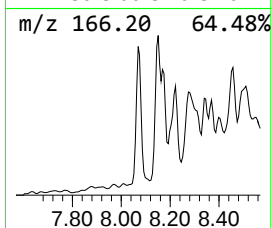
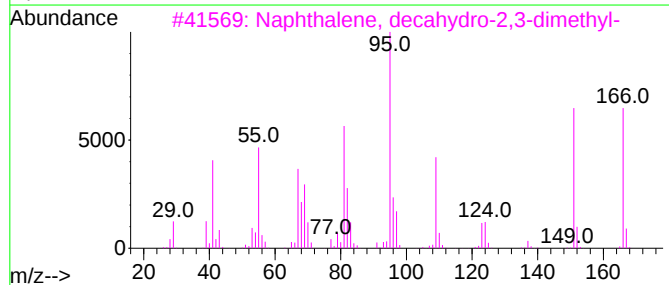
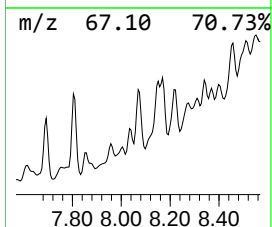
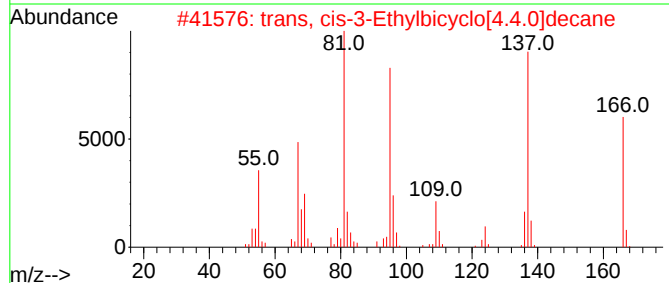
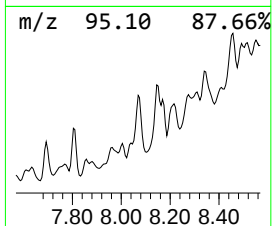
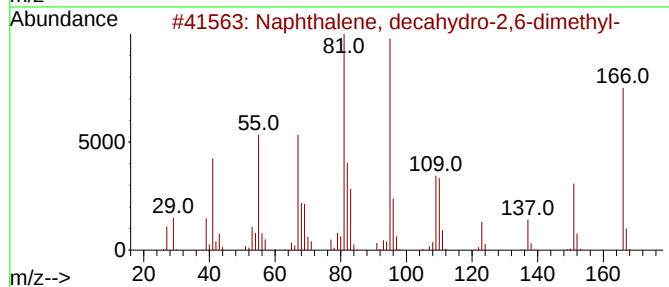
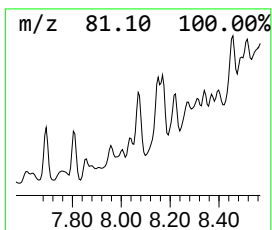
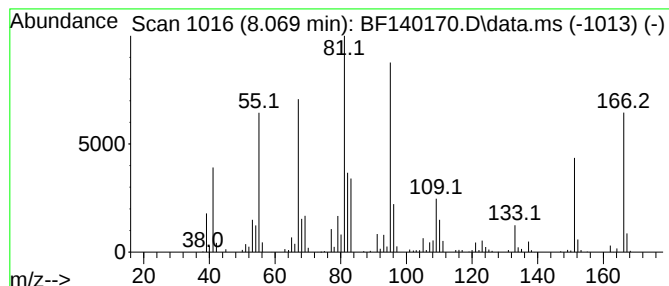
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Naphthalene, decahydro-2,6-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.069	3.58 ng	260022	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	87
2			trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	74
3			Naphthalene, decahydro-2,3-dimet...	166	C12H22	001008-80-6	70
4			1H-Indene, 1-ethyloctahydro-7a-m...	166	C12H22	056324-71-1	62
5			cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140170.D
Acq On : 30 Oct 2024 20:51
Operator : RC/JU
Sample : P4613-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-0001

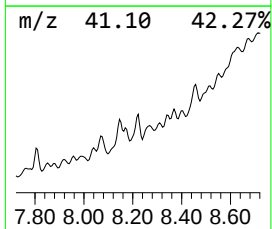
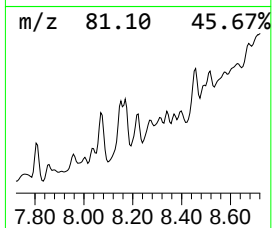
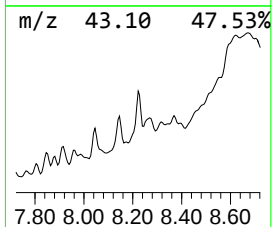
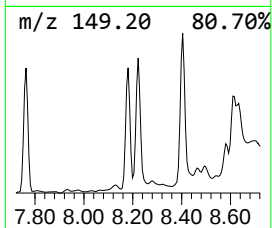
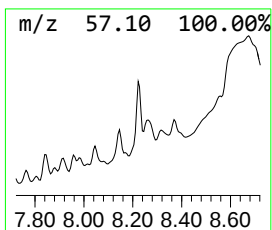
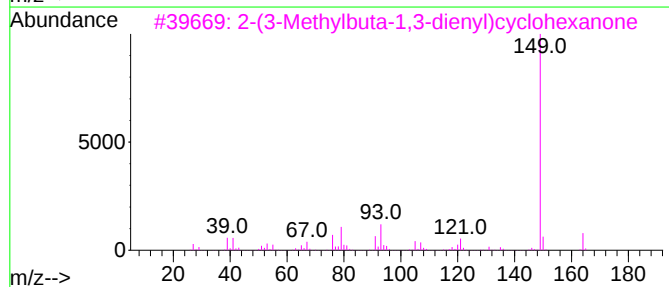
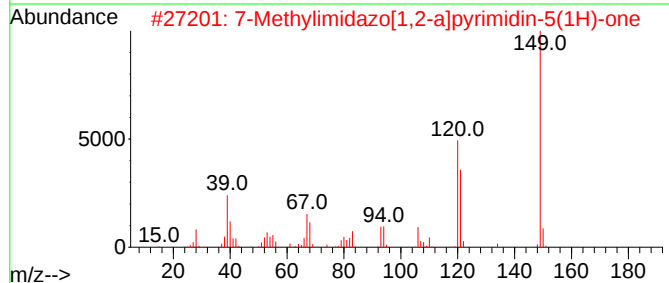
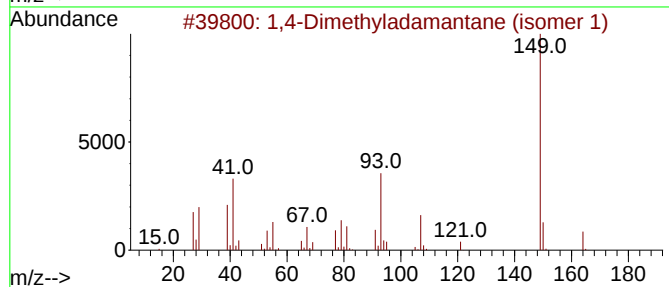
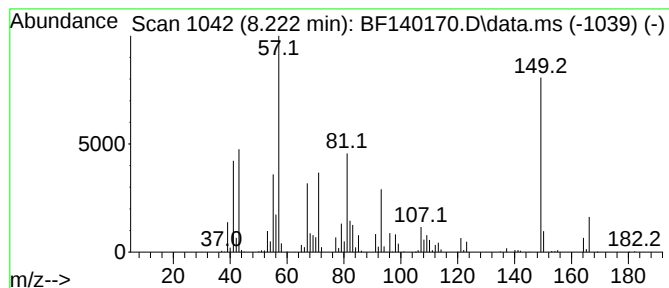
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,4-Dimethyladamantane (iso... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.222	4.28 ng	310673	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dimethyladamantane (isomer 1)	164	C12H20	1000460-67-0	58		
2	7-Methylimidazo[1,2-a]pyrimidin-...	149	C7H7N3O	039567-76-5	43		
3	2-(3-Methylbuta-1,3-dienyl)cyclo...	164	C11H16O	1000191-75-5	38		
4	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	38		
5	Benzothiazole, 2-methyl-	149	C8H7NS	000120-75-2	35		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140170.D
Acq On : 30 Oct 2024 20:51
Operator : RC/JU
Sample : P4613-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ARS20-0001

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(1R)-2,6,6-Trim...	6.163	10.5	ng	358201	1	6.887	682842	20.0
unknown7.528	7.528	3.0	ng	217773	2	8.163	1451880	20.0
trans-Decalin, ...	7.692	4.2	ng	306897	2	8.163	1451880	20.0
Adamantane, 1,3...	7.763	2.8	ng	204666	2	8.163	1451880	20.0
trans-4a-Methyl...	7.810	4.2	ng	306550	2	8.163	1451880	20.0
Naphthalene, de...	8.069	3.6	ng	260022	2	8.163	1451880	20.0
1,4-Dimethylada...	8.222	4.3	ng	310673	2	8.163	1451880	20.0