

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020725\
 Data File : BF141509.D
 Acq On : 07 Feb 2025 15:58
 Operator : RC/JU
 Sample : Q1304-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RB21140

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-BF020625.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141509.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.404	557	563	578	rBV	930083	1311637	81.41%	15.798%
2	6.422	731	736	754	rBV	1029020	1394558	86.56%	16.797%
3	6.787	793	798	805	rBV	399265	496427	30.81%	5.979%
4	6.863	805	811	827	rBV	114852	329794	20.47%	3.972%
5	7.345	884	893	898	rBV	674049	940256	58.36%	11.325%
6	8.069	1009	1016	1020	rBV	531985	772093	47.92%	9.300%
7	8.363	1062	1066	1068	rBV4	91901	134881	8.37%	1.625%
8	8.451	1078	1081	1084	rBV3	102796	146776	9.11%	1.768%
9	8.610	1105	1108	1111	rBV4	128584	192826	11.97%	2.322%
10	8.951	1164	1166	1170	rBV4	209060	240583	14.93%	2.898%
11	9.145	1195	1199	1203	rBV	1131663	1611173	100.00%	19.406%
12	9.233	1211	1214	1218	rBV3	516268	731515	45.40%	8.811%

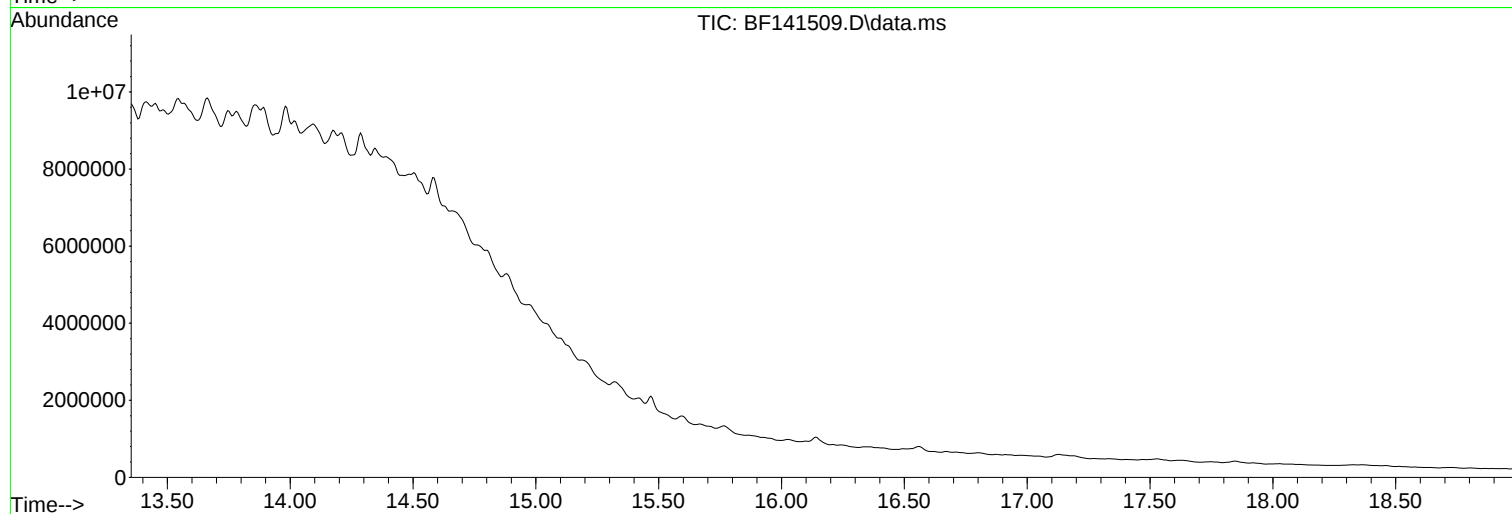
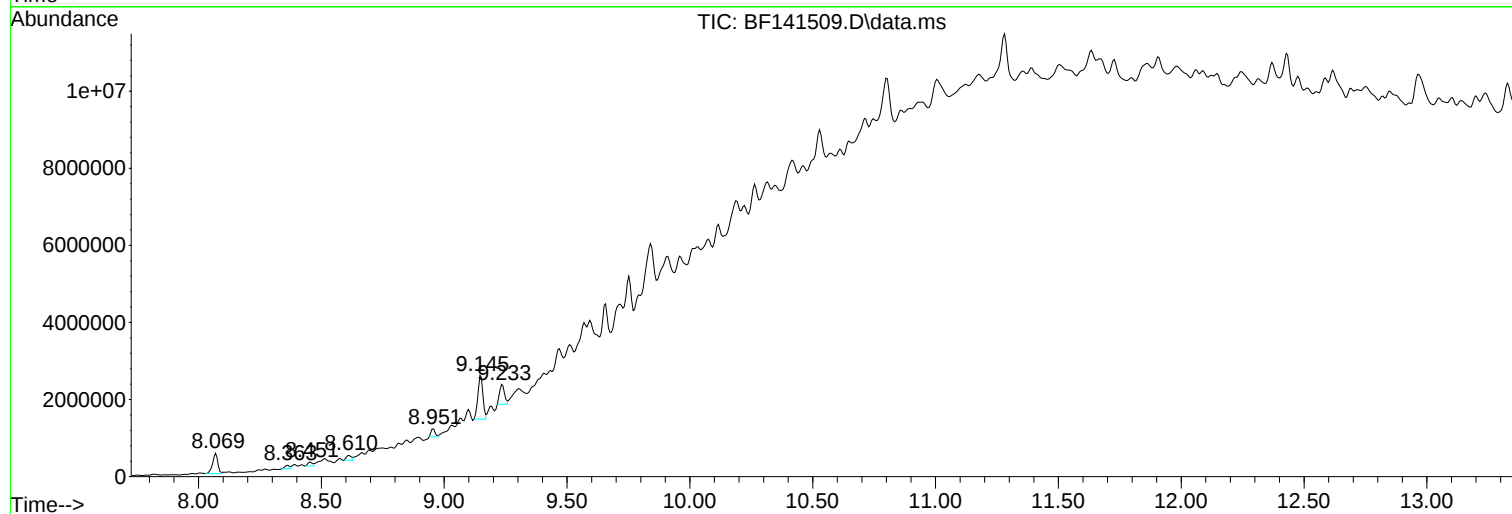
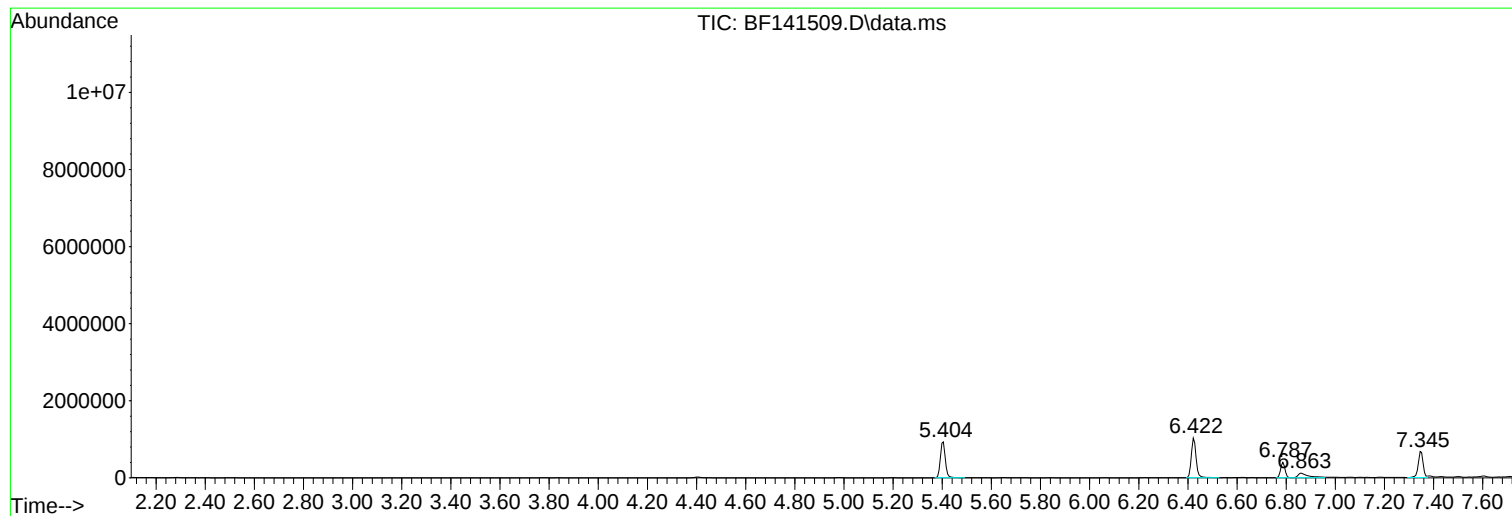
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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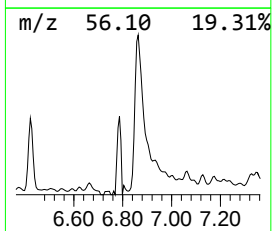
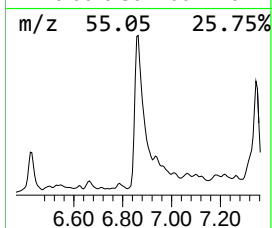
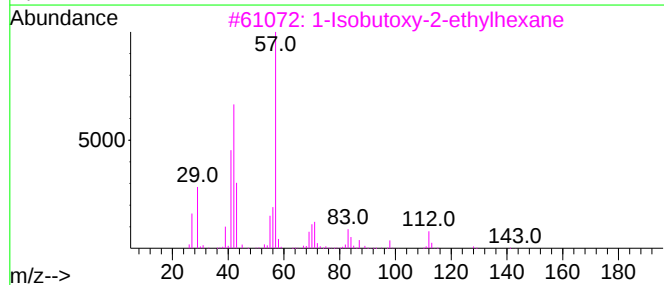
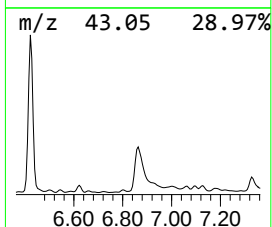
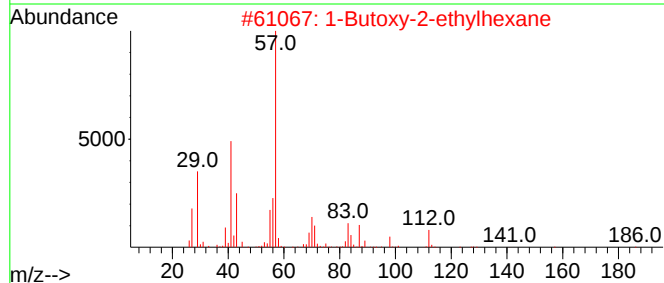
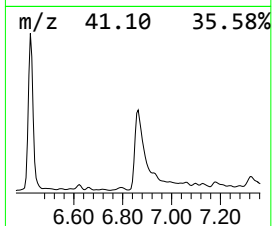
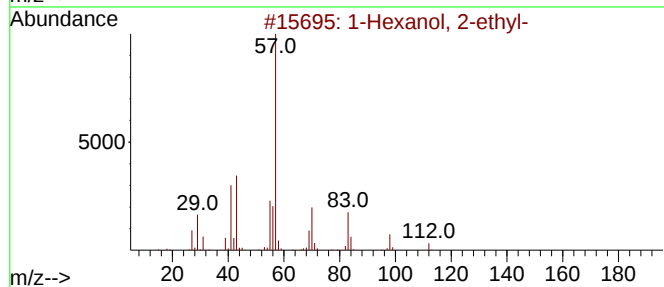
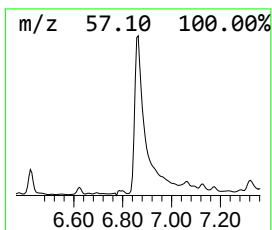
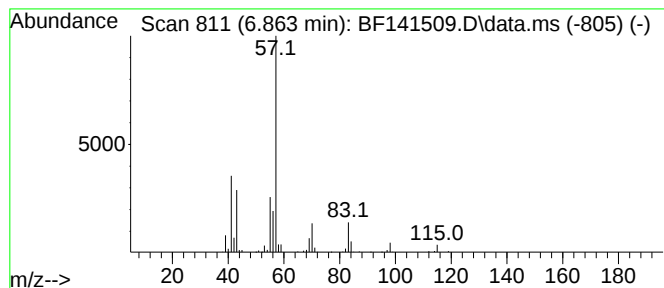
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.863	13.29 ng	329794	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	50
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50
4			1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	47
5			Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	47



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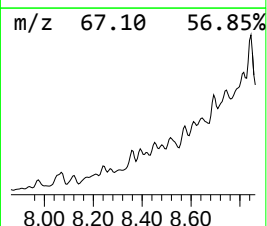
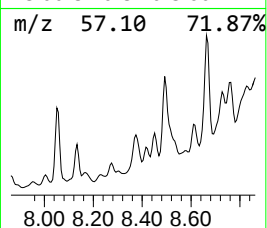
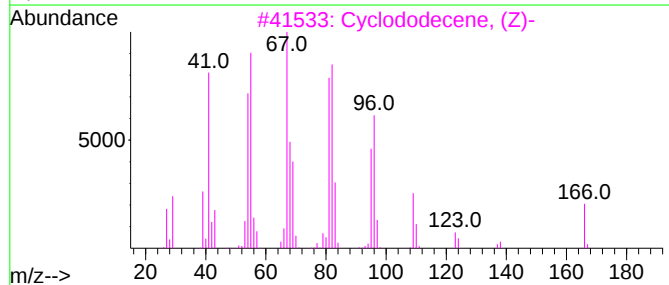
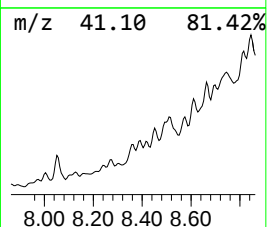
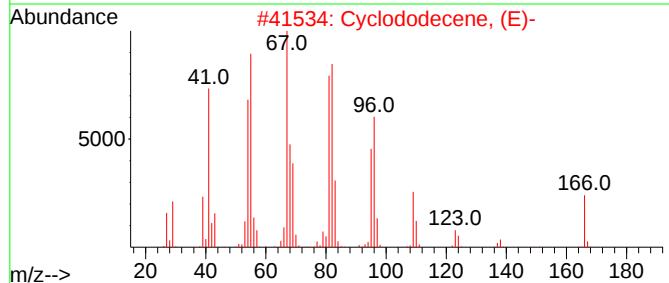
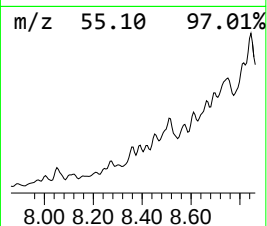
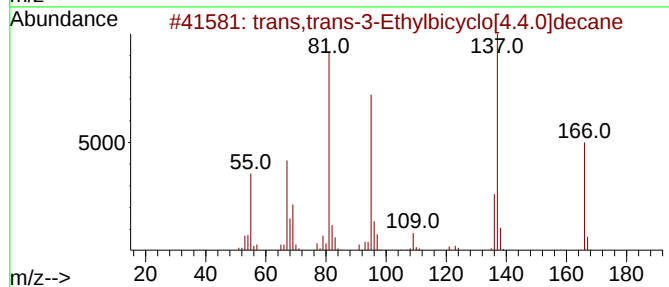
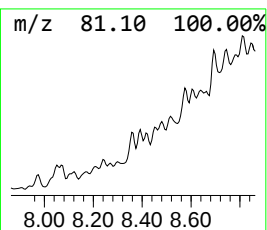
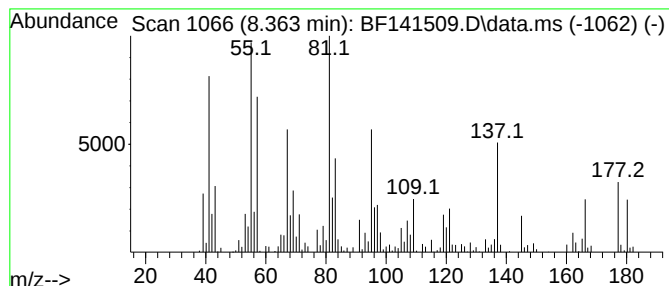
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Peak Number 2 trans,trans-3-Ethylbicyclo[... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.363	3.49 ng	134881	Naphthalene-d8	8.069

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		trans,trans-3-Ethylbicyclo[4.4.0...	166	C12H22	058462-32-1	53
2		Cyclododecene, (E)-	166	C12H22	001486-75-5	49
3		Cyclododecene, (Z)-	166	C12H22	001129-89-1	49
4		cis,cis-2,8-Dimethylspiro[5.5]un...	180	C13H24	095530-75-9	43
5		Bicyclo[4.1.0]heptane, 2-methyl-...	180	C13H24	055937-92-3	43



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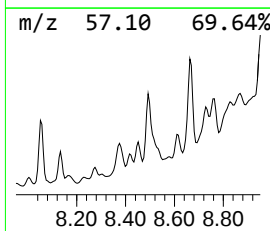
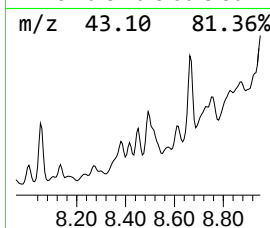
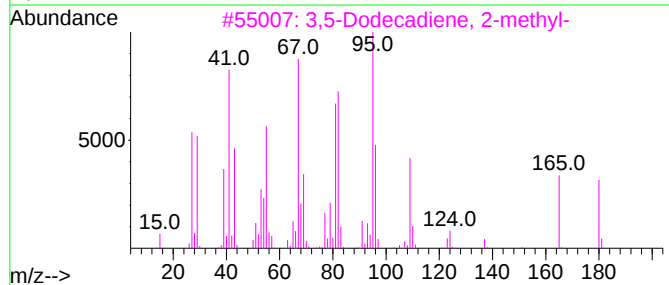
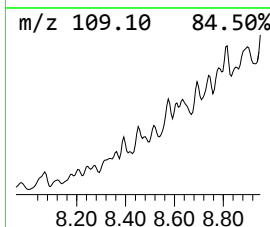
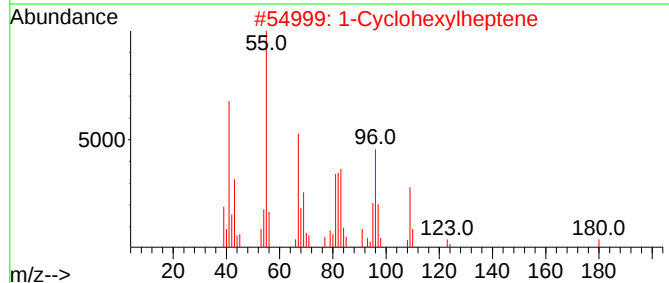
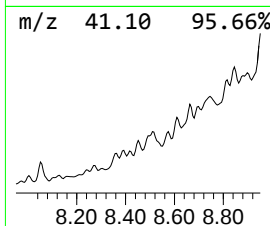
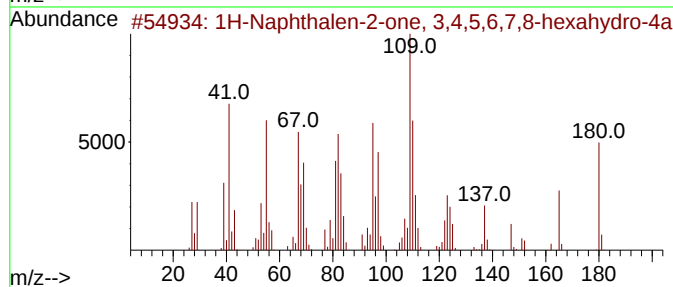
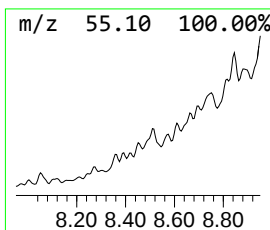
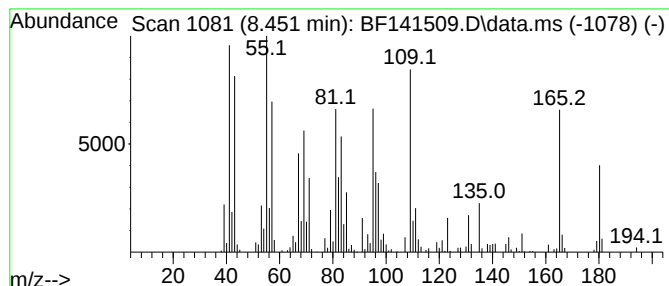
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Peak Number 3 unknown8.451 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.451	3.80 ng	146776	Naphthalene-d8	8.069	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Naphthalen-2-one, 3,4,5,6,7,8...	180	C12H20O	1010164-27-1	49
2	1-Cyclohexylheptene	180	C13H24	114614-83-4	49
3	3,5-Dodecadiene, 2-methyl-	180	C13H24	055638-51-2	41
4	2-Hexanone, 3-cyclohexylidene-4-...	208	C14H24O	1000150-19-2	38
5	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	35



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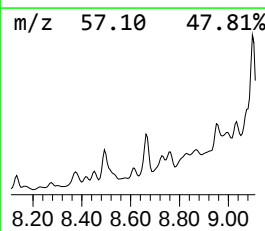
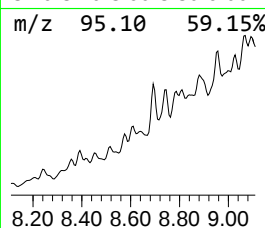
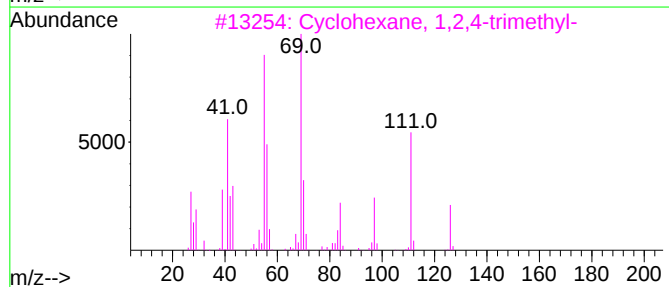
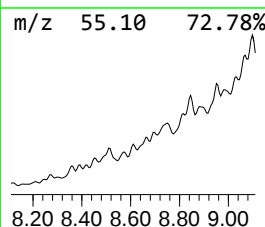
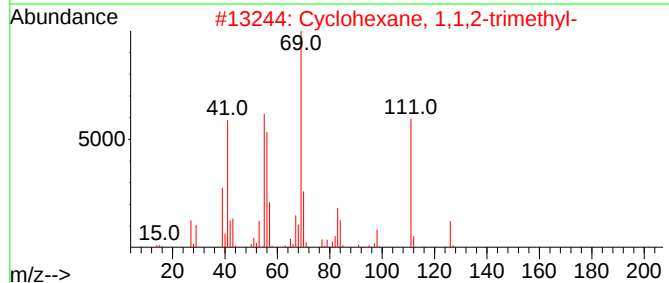
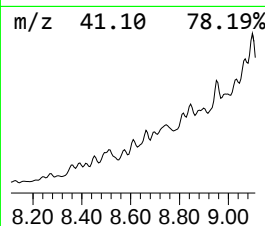
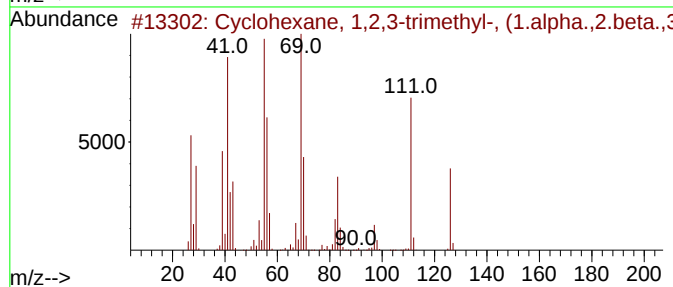
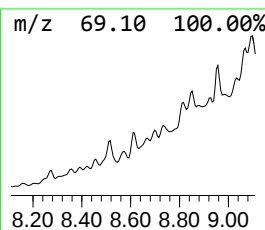
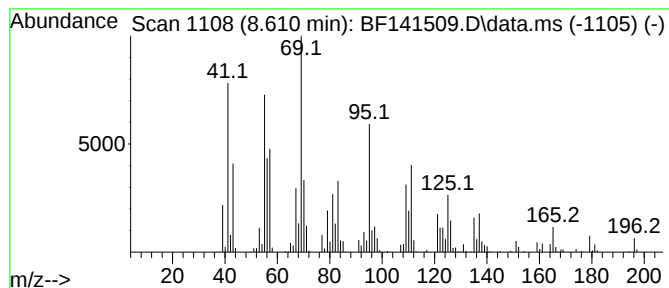
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Peak Number 4 Cyclohexane, 1,2,3-trimethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.610	4.99 ng	192826	Naphthalene-d8	8.069

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	001678-81-5	55
2		Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	46
3		Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	46
4		trans-3,5-Dimethylcyclohexanone	126	C8H14O	007214-49-5	38
5		2,3,4-Trimethyl-hex-3-enal	140	C9H16O	1000193-72-9	38



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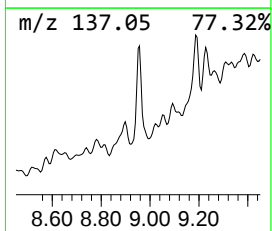
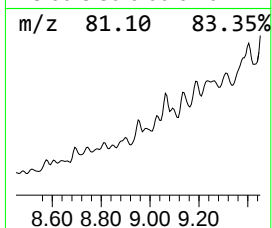
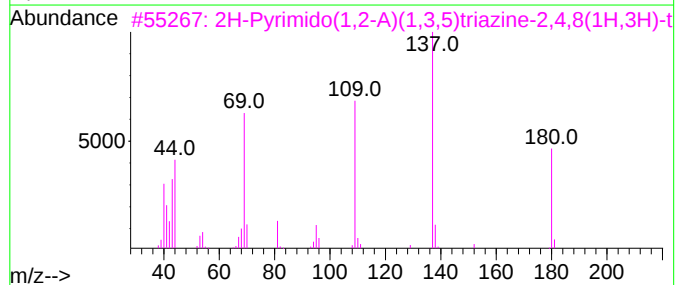
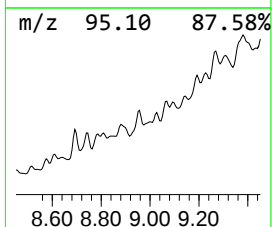
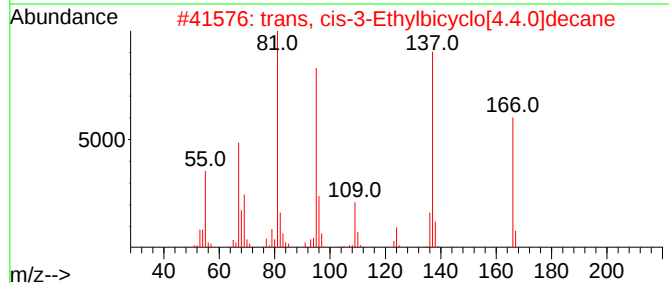
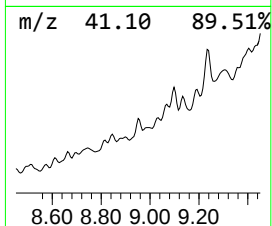
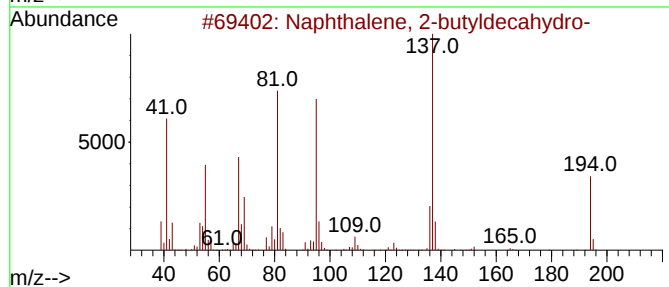
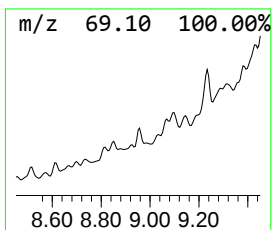
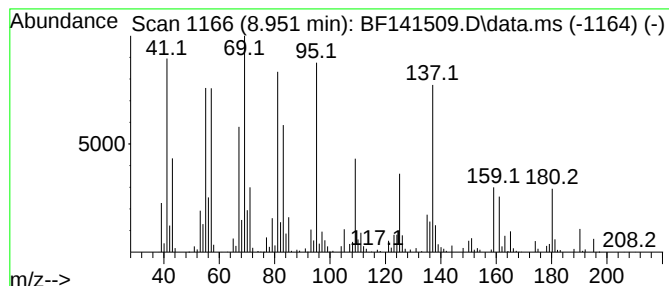
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Peak Number 5 unknown8.951 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.951	6.23 ng	240583	Naphthalene-d8	8.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	38
2			trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	38
3			2H-Pyrimido(1,2-A)(1,3,5)triazin...	180	C6H4N4O3	1000433-55-0	35
4			2-(2-Hydroxycycloheptyl)-furan	180	C11H16O2	1000145-02-9	30
5			3-Oxabicyclo[3.2.1]octane-2,4-di...	260	C10H13BrO3	013441-28-6	27



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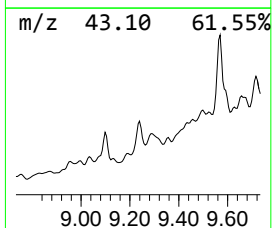
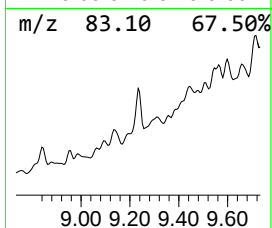
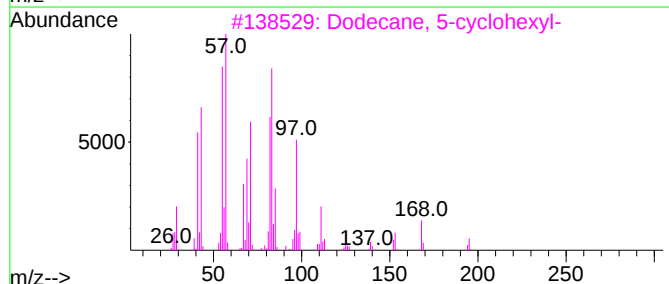
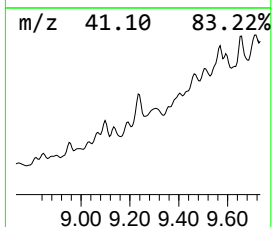
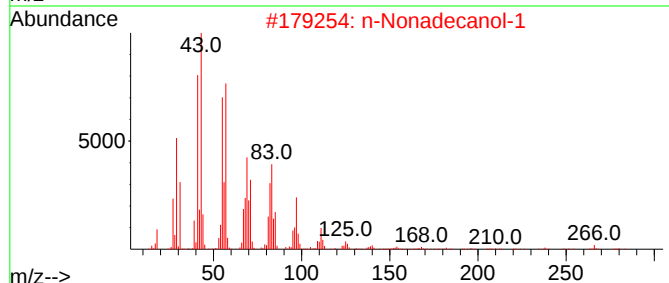
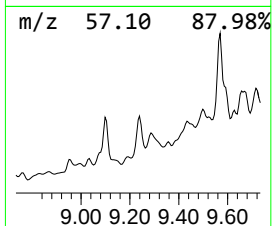
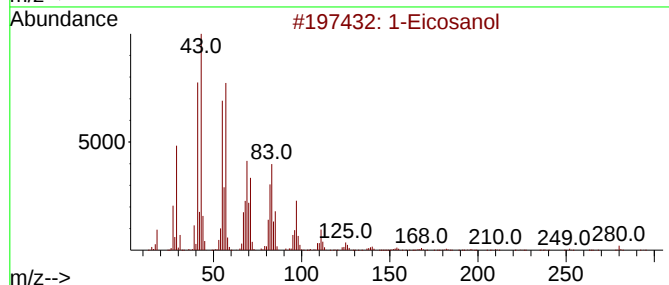
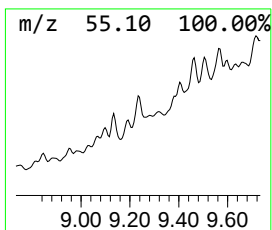
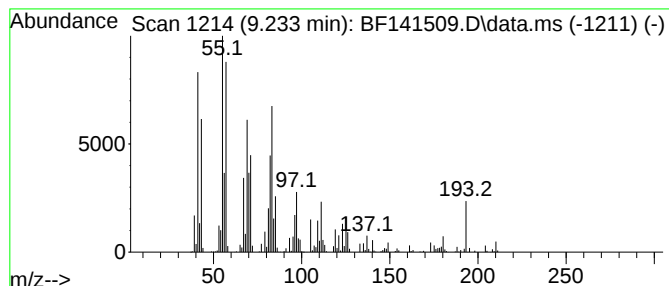
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Eicosanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.233	20.00 ng	731515	Acenaphthene-d10	9.839

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Eicosanol	298	C20H42O	000629-96-9	64
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	59
3		Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	53
4		17-Pentatriacontene	491	C35H70	006971-40-0	50
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020725\
Data File : BF141509.D
Acq On : 07 Feb 2025 15:58
Operator : RC/JU
Sample : Q1304-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB21140

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF020625.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-Hexanol, 2-et...	6.863	13.3	ng	329794	1	6.787	496427	20.0
trans,trans-3-E...	8.363	3.5	ng	134881	2	8.069	772093	20.0
unknown8.451	8.451	3.8	ng	146776	2	8.069	772093	20.0
Cyclohexane, 1,...	8.610	5.0	ng	192826	2	8.069	772093	20.0
unknown8.951	8.951	6.2	ng	240583	2	8.069	772093	20.0
1-Eicosanol	9.233	20.0	ng	731515	3	9.839	731515	20.0