

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062822\
 Data File : BG054117.D
 Acq On : 28 Jun 2022 14:03
 Operator : CG/JU
 Sample : N3472-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20071

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_G\Methods\8270-BG061322.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054117.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.643	375	384	392	rBV	190988	364477	62.23%	10.588%
2	6.137	460	468	477	rVB	115078	217578	37.15%	6.321%
3	7.230	645	654	662	rBV2	209783	425458	72.64%	12.360%
4	8.070	789	797	803	rBV	106348	207214	35.38%	6.020%
5	8.129	803	807	816	rVB	76547	148264	25.31%	4.307%
6	9.227	988	994	1001	rVB	128319	233410	39.85%	6.781%
7	10.878	1265	1275	1284	rBV2	143895	436853	74.58%	12.691%
8	11.583	1391	1395	1401	rVB5	89479	174094	29.72%	5.058%
9	11.654	1402	1407	1413	rVV6	78700	158534	27.07%	4.605%
10	11.795	1426	1431	1437	rBV4	104162	223689	38.19%	6.498%
11	12.682	1578	1582	1589	rVB	160015	266980	45.58%	7.756%
12	13.258	1677	1680	1684	rVB	407539	585725	100.00%	17.016%

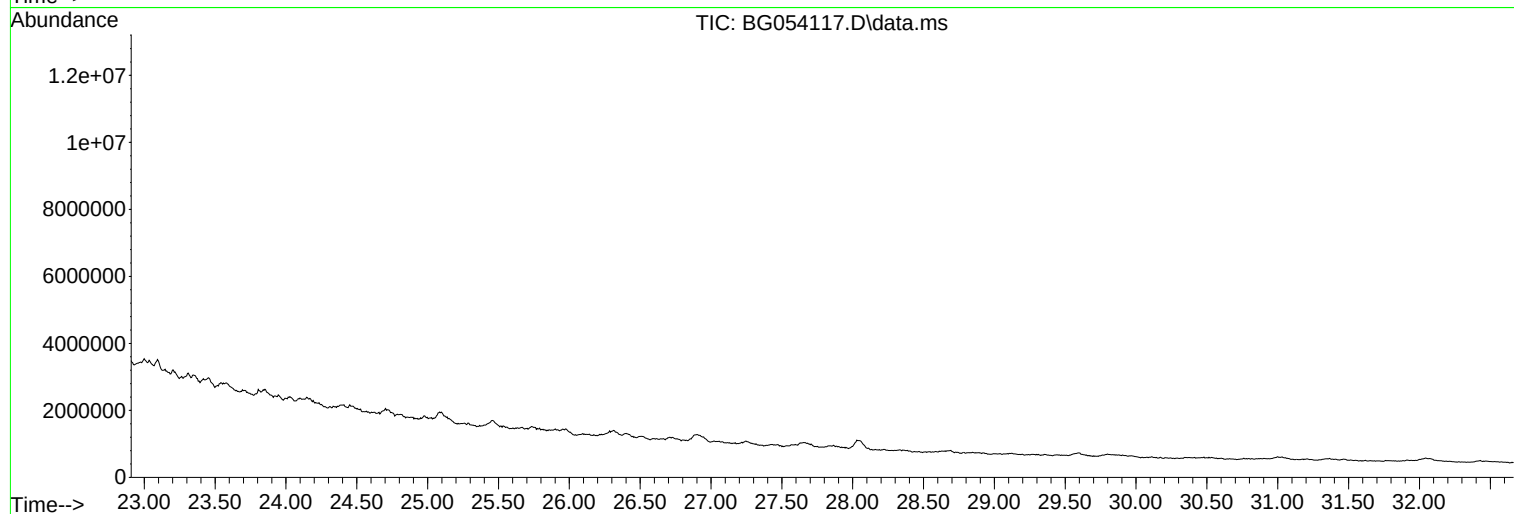
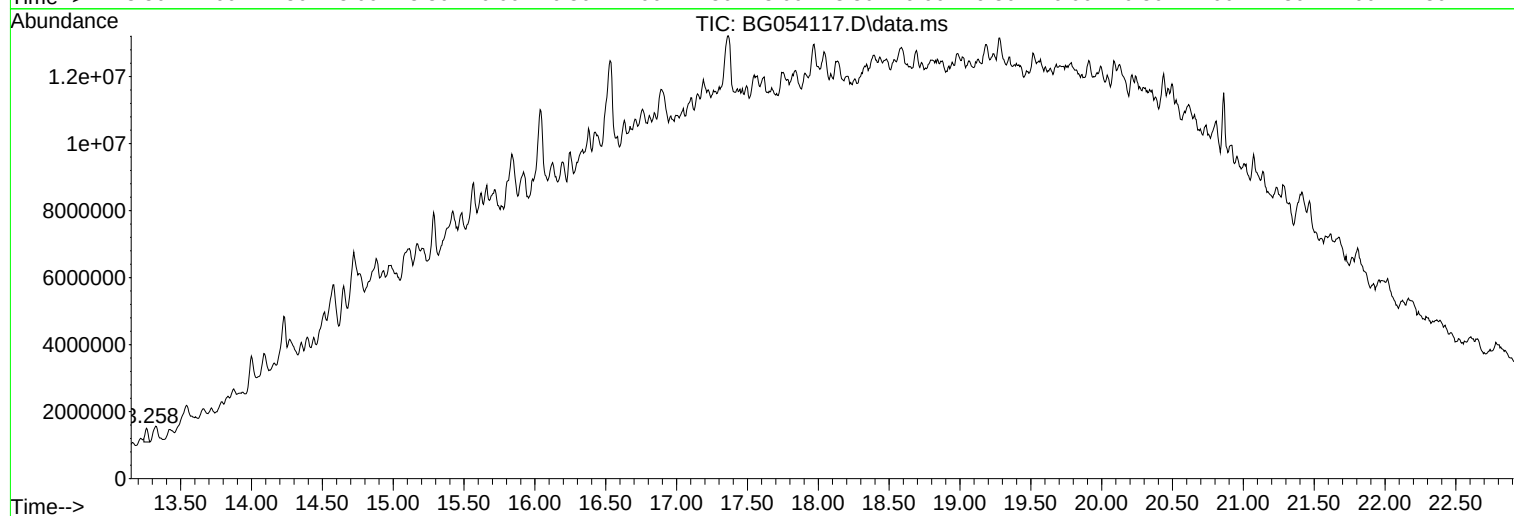
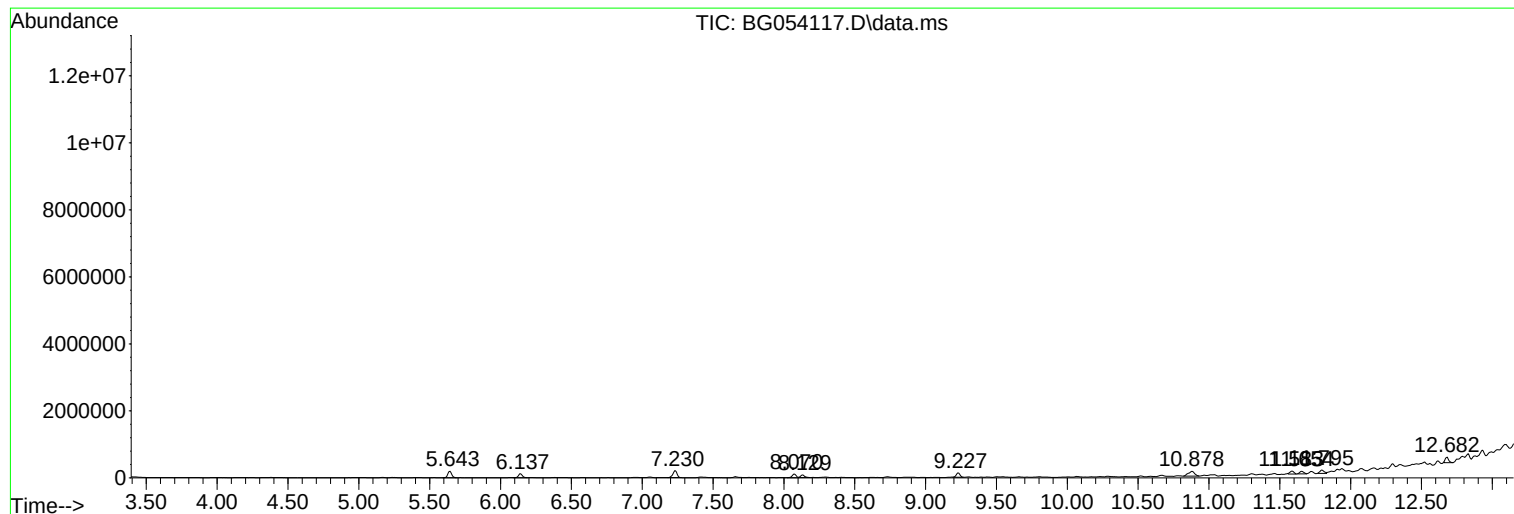
Sum of corrected areas: 3442276

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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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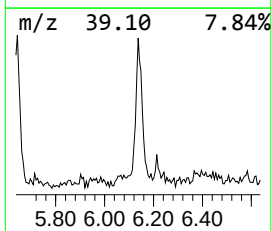
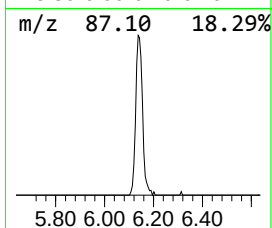
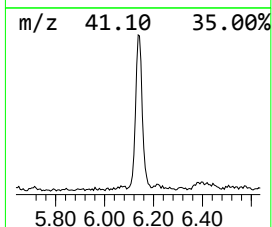
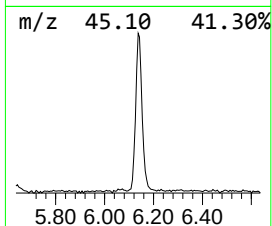
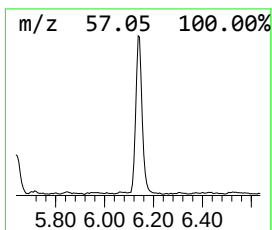
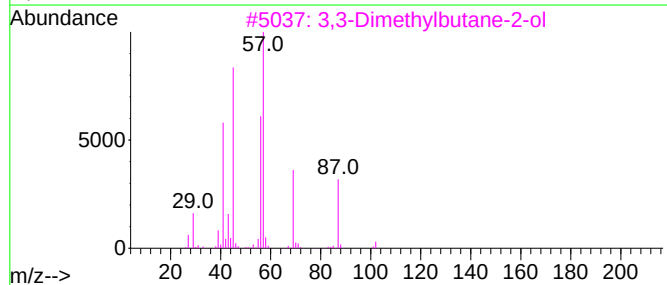
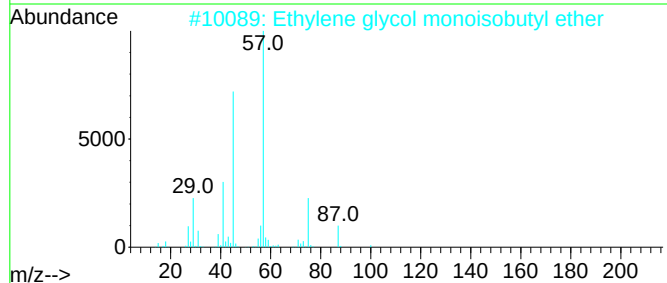
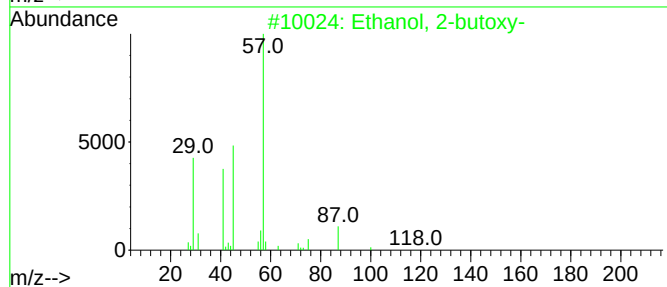
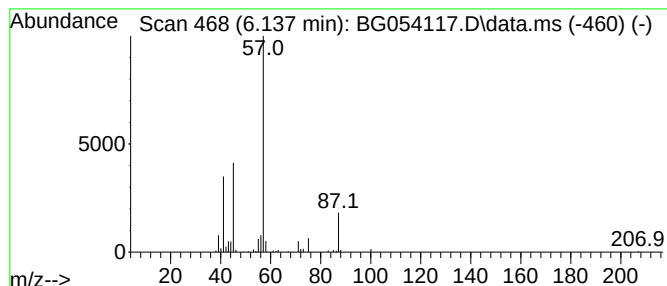
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.137	21.00 ng	217578	1,4-Dichlorobenzene-d4	8.070

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	56
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	36
4			Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	17
5			1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	17



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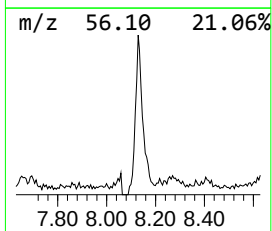
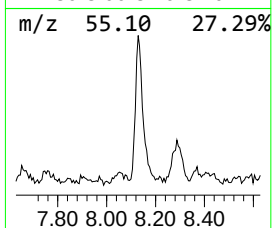
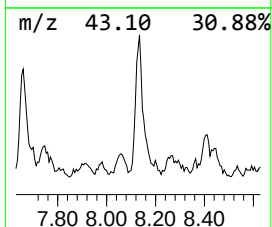
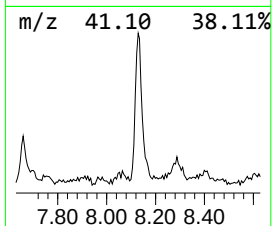
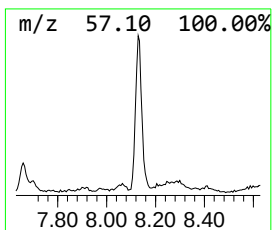
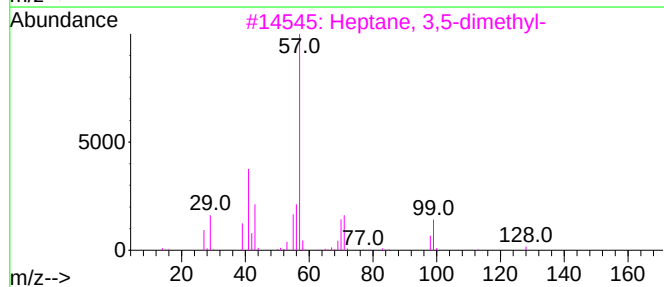
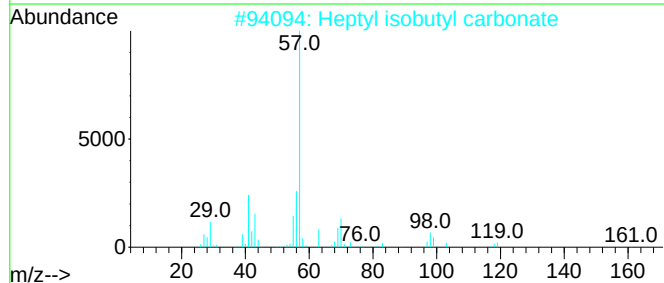
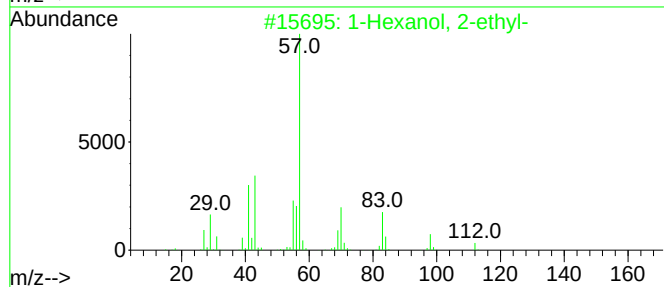
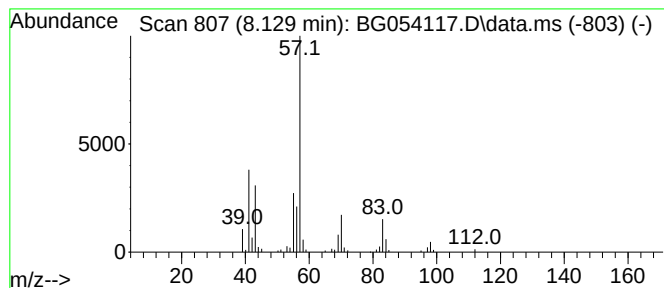
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.129	14.31 ng	148264	1,4-Dichlorobenzene-d4	8.070

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	59
3		Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	53
4		1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	53
5		Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	50



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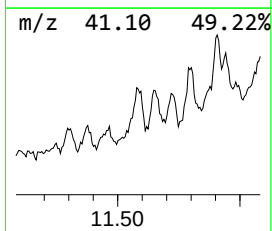
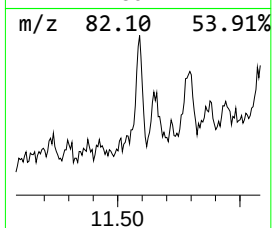
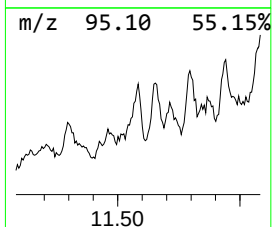
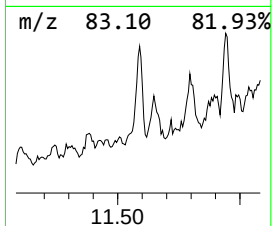
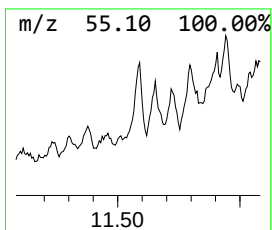
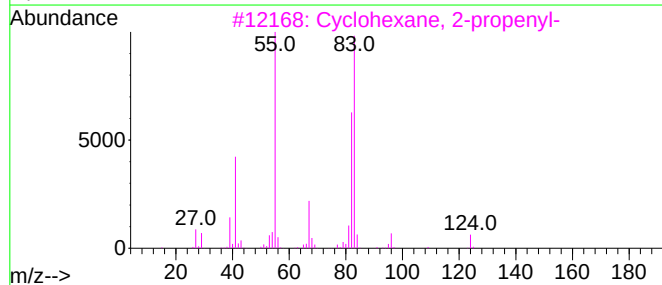
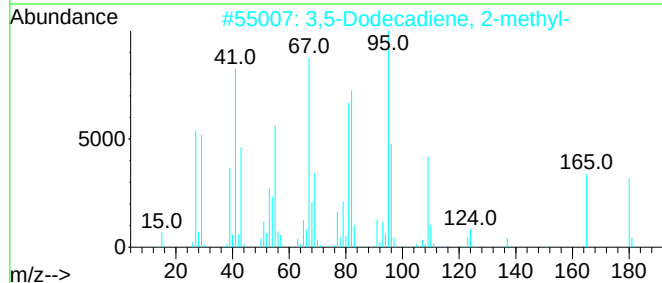
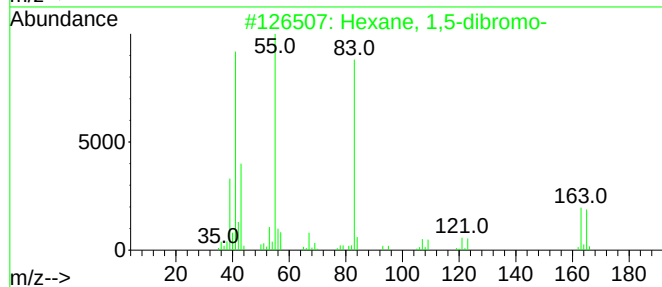
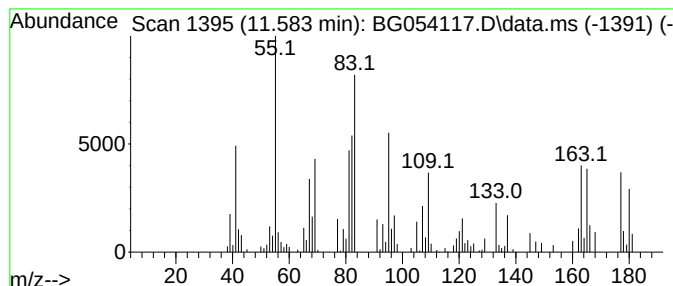
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Peak Number 3 unknown11.584 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.584	7.97 ng	174094	Naphthalene-d8	10.878

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 1,5-dibromo-	242	C6H12Br2	000627-96-3	38
2			3,5-Dodecadiene, 2-methyl-	180	C13H24	055638-51-2	30
3			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	22
4			3-Cyclohexyl-1-propyne	122	C9H14	1010342-45-9	22
5			Cyclohexane, hexyl-	168	C12H24	004292-75-5	22



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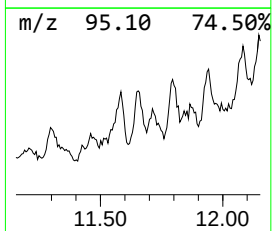
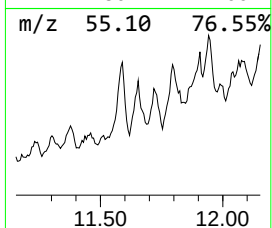
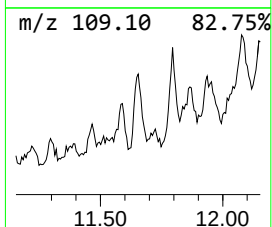
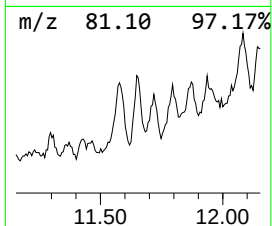
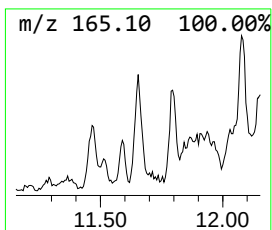
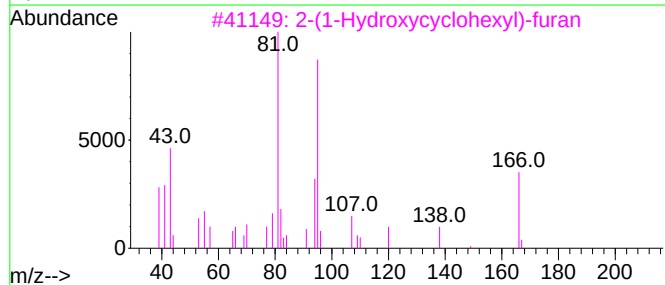
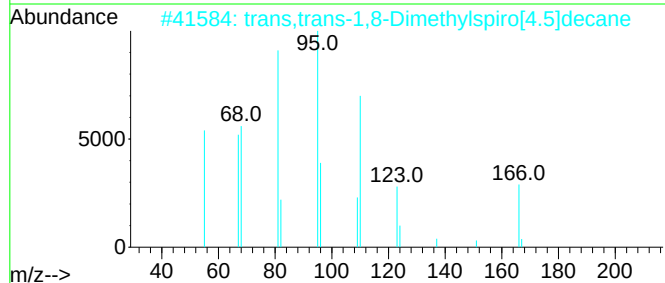
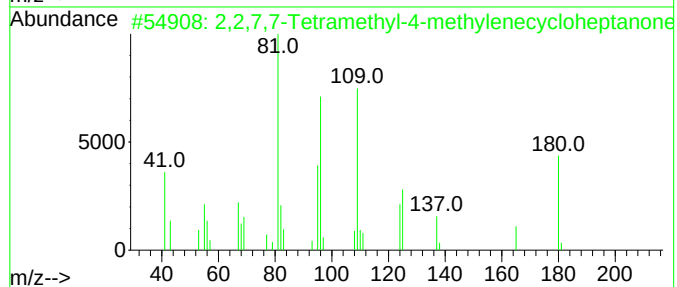
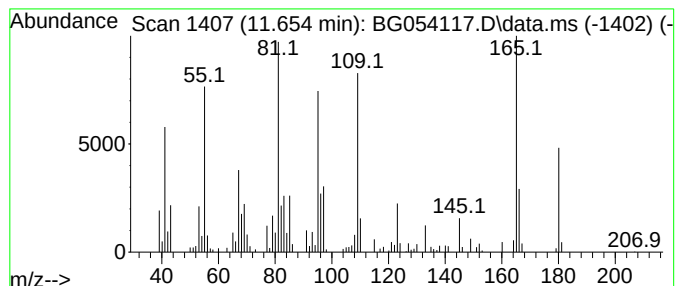
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown11.654 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.654	7.26 ng	158534	Naphthalene-d8	10.878

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,7,7-Tetramethyl-4-methylenec...	180	C12H20O	1000424-29-1	43		
2	trans,trans-1,8-Dimethylspiro[4...	166	C12H22	1000111-72-8	38		
3	2-(1-Hydroxycyclohexyl)-furan	166	C10H14O2	036169-67-2	30		
4	1-Heptylcyclohexene	180	C13H24	015232-86-7	25		
5	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	25		



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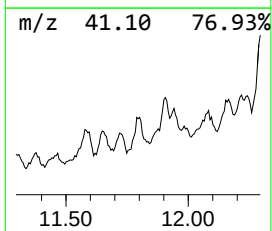
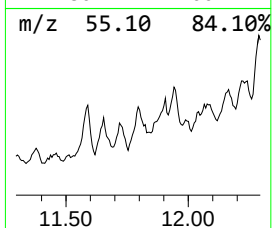
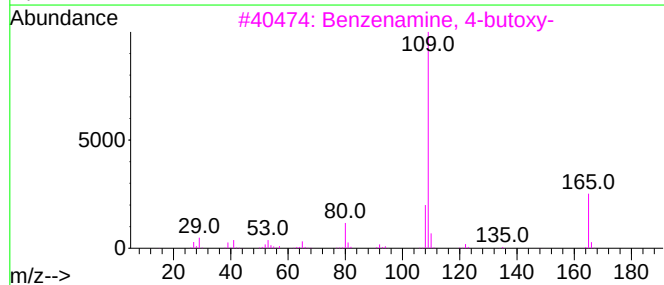
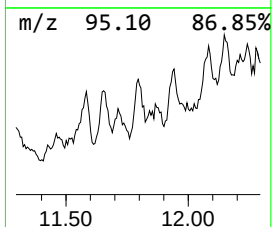
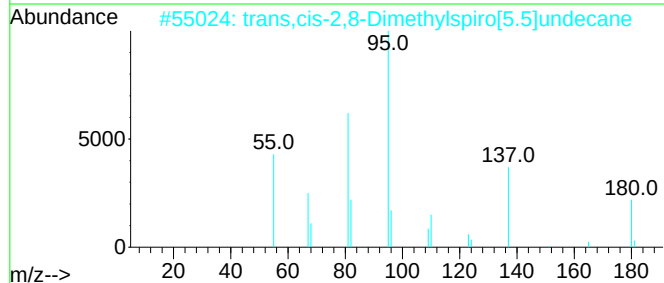
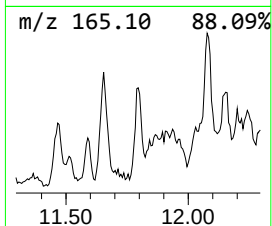
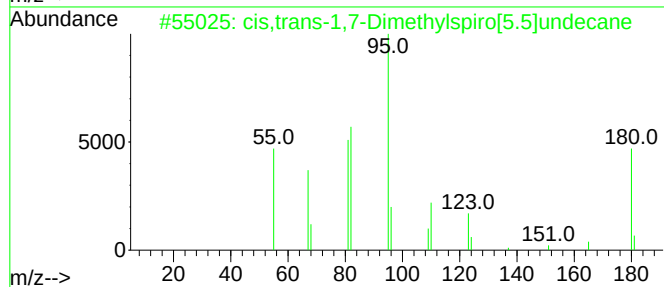
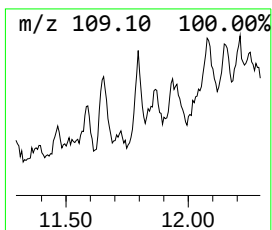
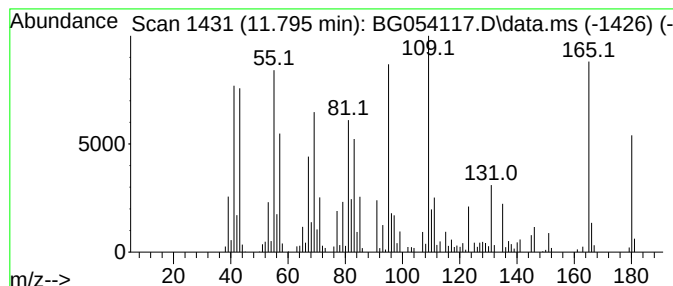
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Peak Number 5 unknown11.795 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.795	10.24 ng	223689	Naphthalene-d8	10.878

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis,trans-1,7-Dimethylspiro[5.5]...	180	C13H24	1000111-73-1	42
2			trans,cis-2,8-Dimethylspiro[5.5]...	180	C13H24	095472-52-9	38
3			Benzenamine, 4-butoxy-	165	C10H15NO	004344-55-2	30
4			Naphthalene, decahydro-1,2-dimet...	166	C12H22	003604-14-6	25
5			2,4,4,7-Tetramethyl-octa-5,7-die...	180	C12H20O	1000190-70-6	22



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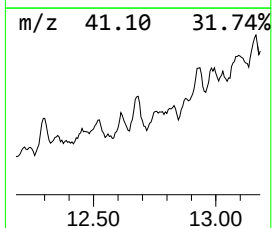
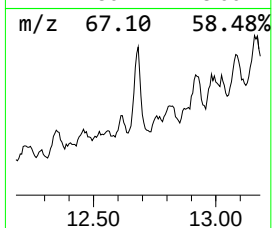
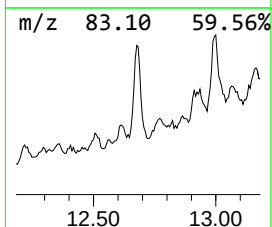
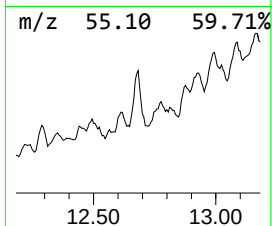
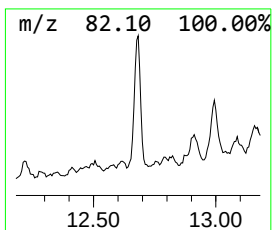
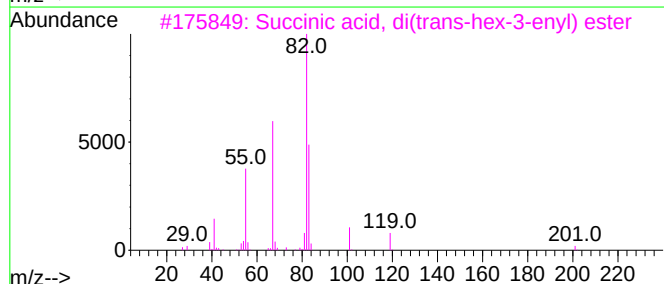
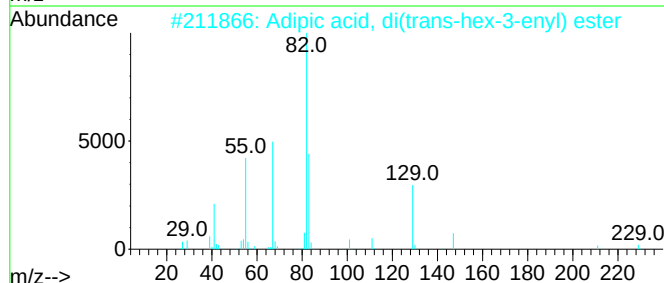
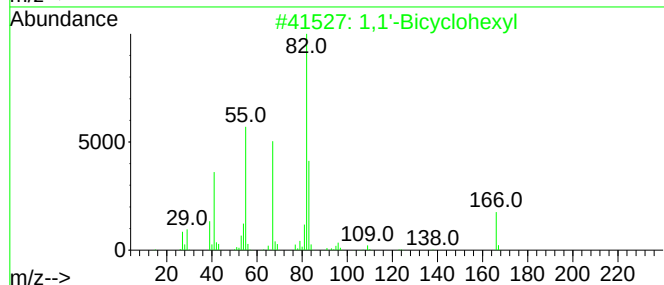
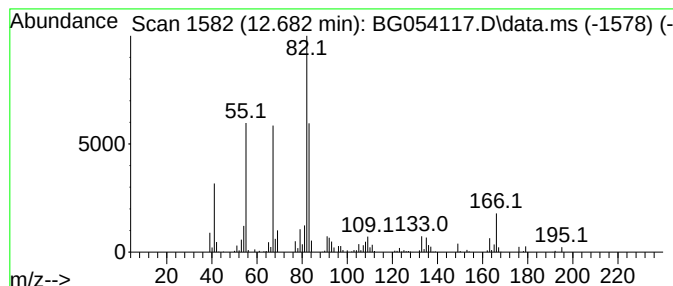
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,1'-Bicyclohexyl Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.682	12.22 ng	266980	Naphthalene-d8	10.878

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1'-Bicyclohexyl	166	C12H22	000092-51-3	87
2			Adipic acid, di(trans-hex-3-enyl...)	310	C18H30O4	1000354-02-3	64
3			Succinic acid, di(trans-hex-3-en...)	282	C16H26O4	1000353-43-7	64
4			Fumaric acid, di(trans-hex-3-eny...)	280	C16H24O4	1000348-90-0	50
5			4-Methyl-1,3-pentadiene	82	C6H10	000926-56-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062822\
Data File : BG054117.D
Acq On : 28 Jun 2022 14:03
Operator : CG/JU
Sample : N3472-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20071

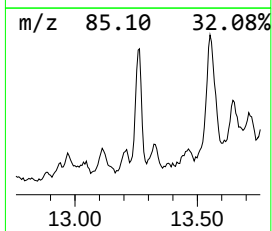
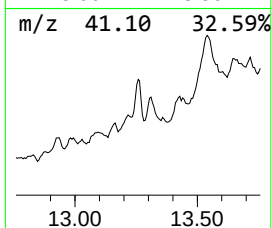
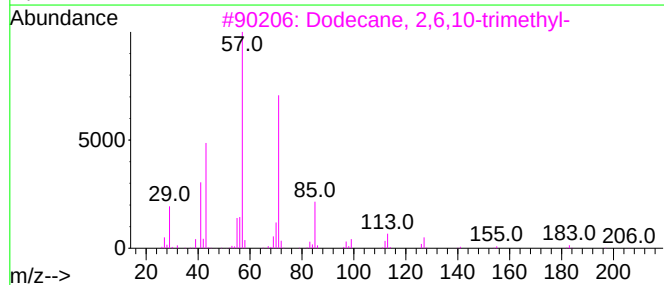
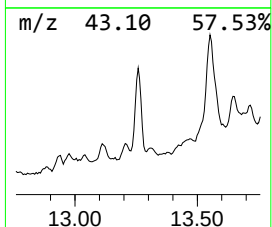
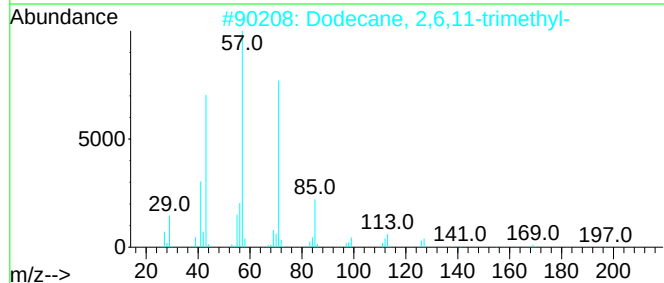
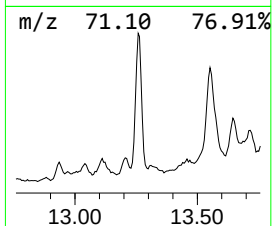
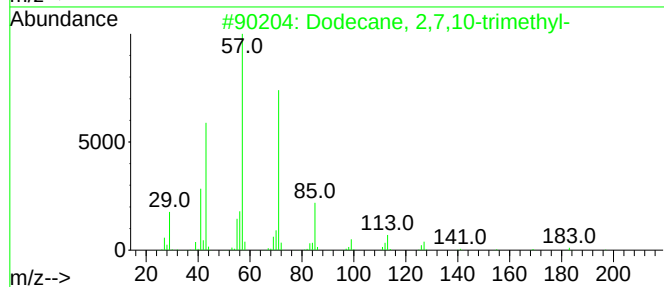
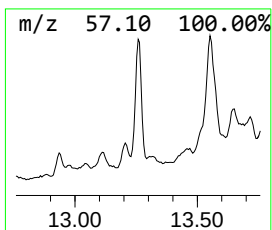
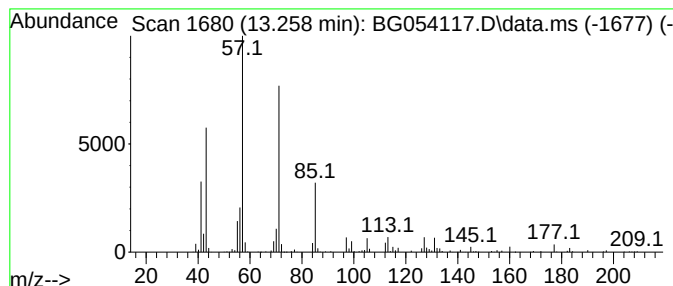
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecane, 2,7,10-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.258	20.00 ng	585725	Acenaphthene-d10	14.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	90
2			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	83
3			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	80
4			Decane, 5-propyl-	184	C13H28	017312-62-8	72
5			Undecane, 2-methyl-	170	C12H26	007045-71-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062822\
Data File : BG054117.D
Acq On : 28 Jun 2022 14:03
Operator : CG/JU
Sample : N3472-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20071

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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
Ethanol, 2-butoxy-	6.137	21.0	ng	217578	1	8.070	207214	20.0
1-Hexanol, 2-et...	8.129	14.3	ng	148264	1	8.070	207214	20.0
unknown11.584	11.584	8.0	ng	174094	2	10.878	436853	20.0
unknown11.654	11.654	7.3	ng	158534	2	10.878	436853	20.0
unknown11.795	11.795	10.2	ng	223689	2	10.878	436853	20.0
1,1'-Bicyclohexyl	12.682	12.2	ng	266980	2	10.878	436853	20.0
Dodecane, 2,7,1...	13.258	20.0	ng	585725	3	14.733	585725	20.0