

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
 Data File : BF133284.D
 Acq On : 06 May 2023 02:03
 Operator : CG\JU
 Sample : 02622-03
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR-251675

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133284.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.904	474	479	486	rVB	463258	578769	18.50%	2.874%
2	5.334	548	552	555	rBV	3243238	2950758	94.32%	14.651%
3	6.369	723	728	731	rBV	3247674	2974016	95.06%	14.767%
4	6.722	785	788	792	rBV	1175335	996084	31.84%	4.946%
5	6.792	797	800	806	rVV	138501	108939	3.48%	0.541%
6	7.286	880	884	887	rBV	2197003	1915349	61.22%	9.510%
7	7.534	922	926	932	rBV3	80003	138908	4.44%	0.690%
8	7.757	959	964	968	rBV	99122	111418	3.56%	0.553%
9	8.010	1003	1007	1010	rBV	1500305	1270777	40.62%	6.310%
10	8.333	1059	1062	1065	rBV2	134528	151842	4.85%	0.754%
11	8.363	1065	1067	1070	rVV2	155876	161650	5.17%	0.803%
12	8.639	1110	1114	1118	rBV4	247503	462140	14.77%	2.295%
13	8.680	1118	1121	1123	rBV3	194389	271069	8.66%	1.346%
14	8.751	1131	1133	1135	rBV	335068	316868	10.13%	1.573%
15	8.780	1135	1138	1141	rVV2	315090	335855	10.74%	1.668%
16	8.816	1142	1144	1146	rBV2	270840	276046	8.82%	1.371%
17	8.898	1155	1158	1160	rBV4	379903	402655	12.87%	1.999%
18	9.004	1173	1176	1178	rBV2	669531	797666	25.50%	3.961%
19	9.086	1186	1190	1193	rBV	2961909	3128485	100.00%	15.533%
20	9.175	1202	1205	1208	rBV2	976908	1387568	44.35%	6.890%
21	15.327	2248	2251	2259	rVB	820226	1403411	44.86%	6.968%

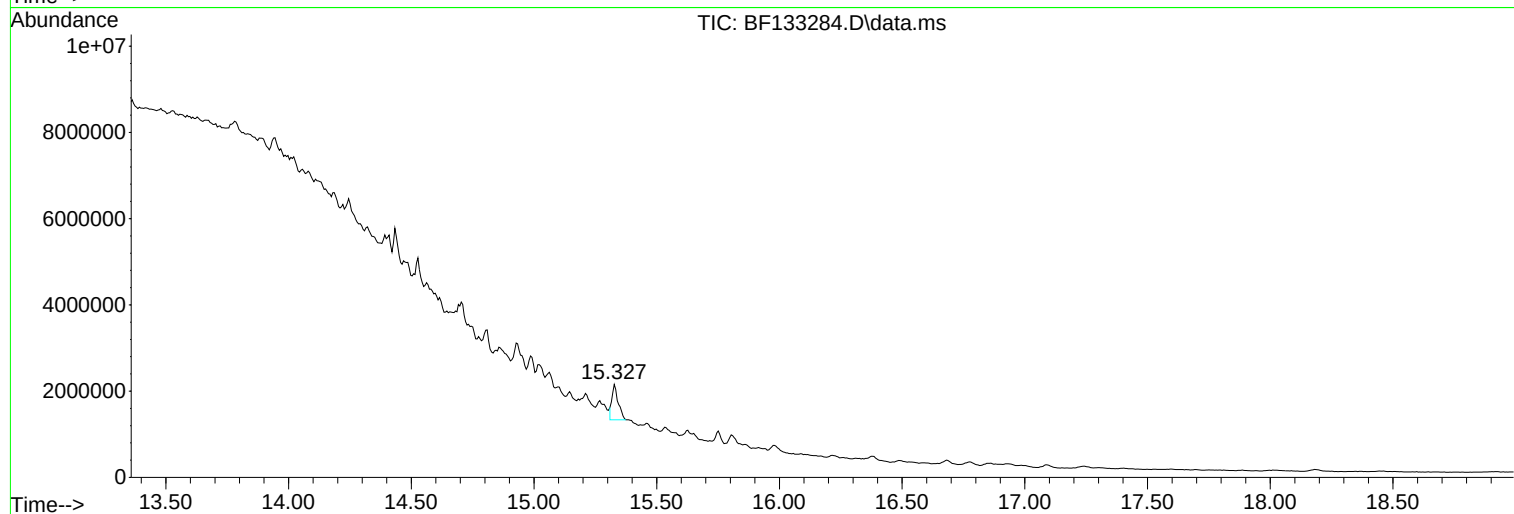
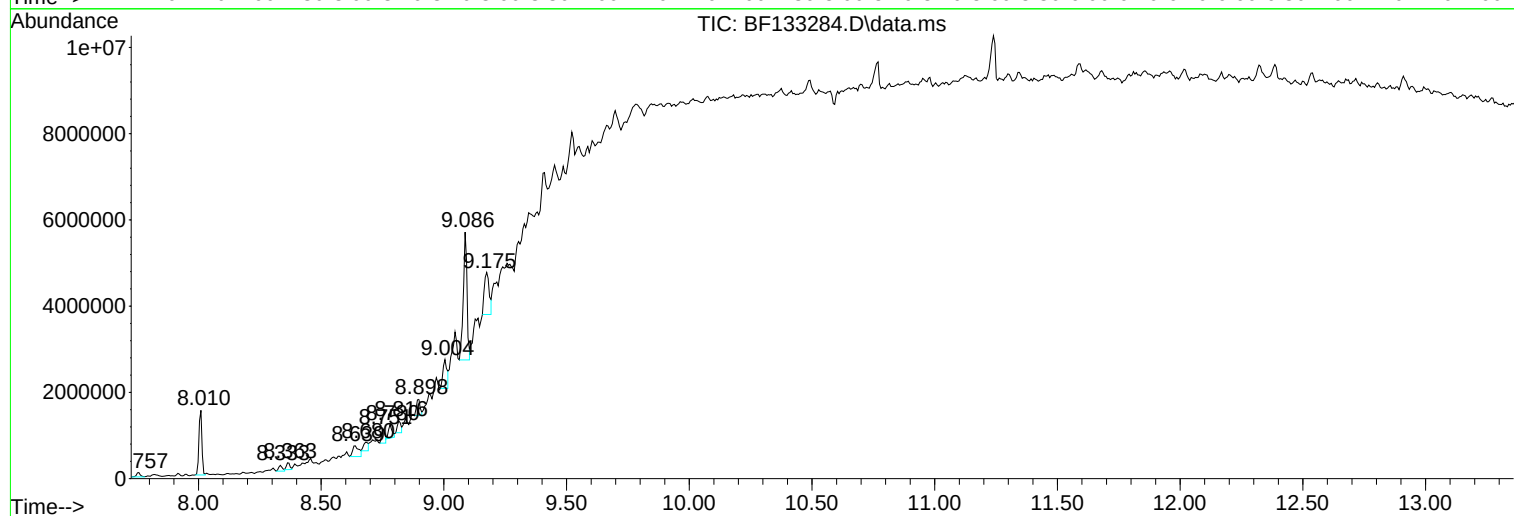
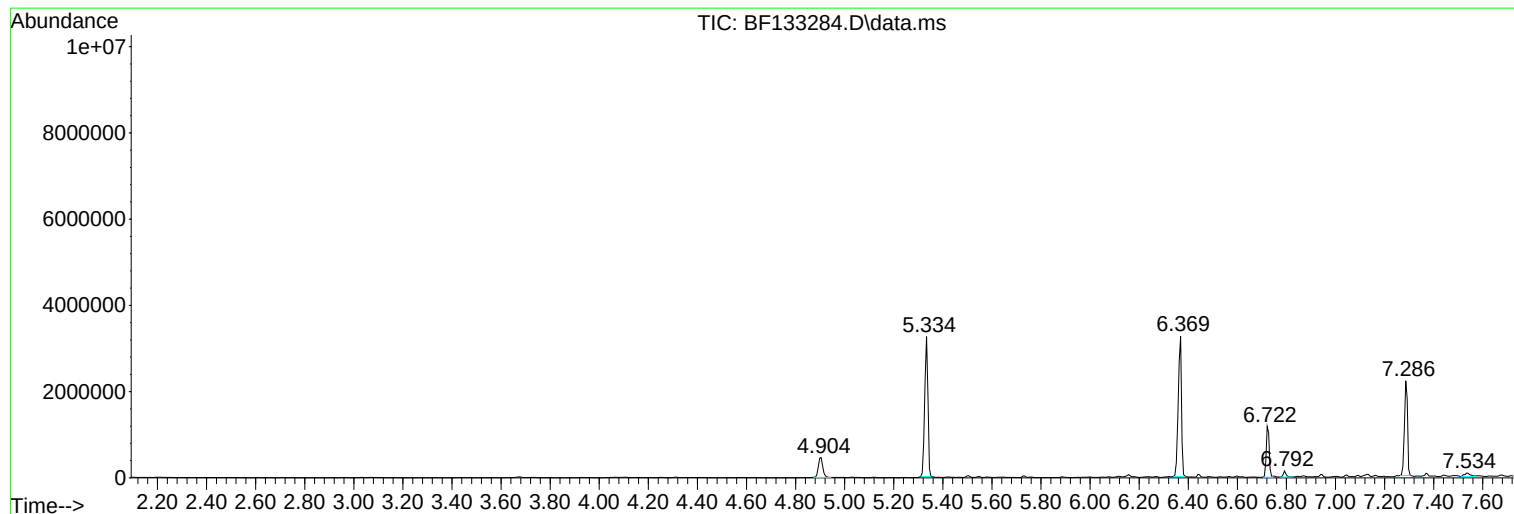
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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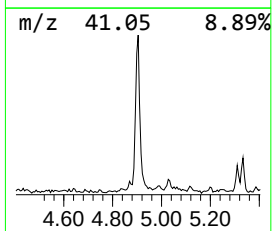
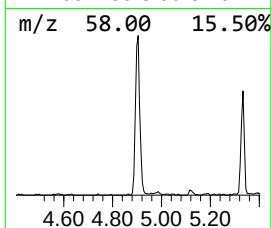
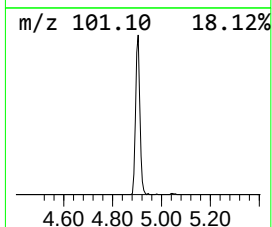
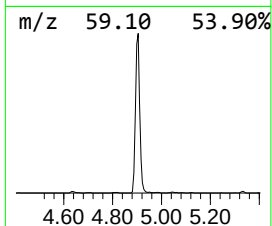
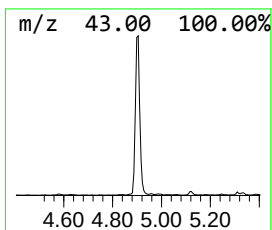
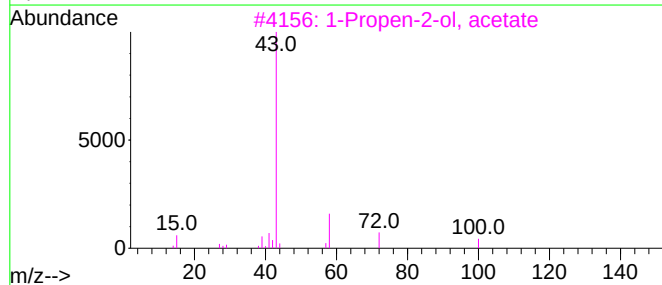
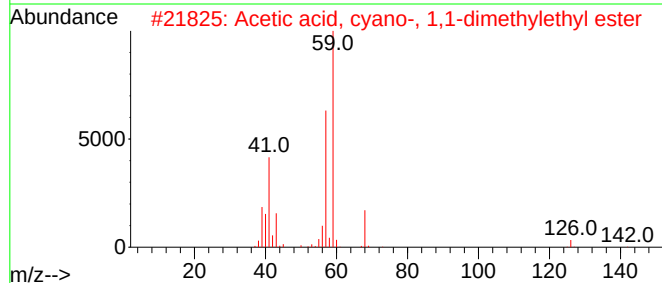
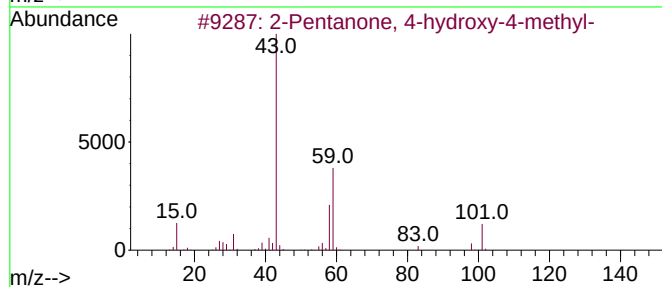
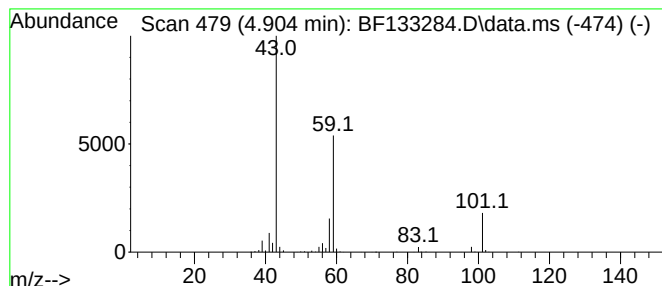
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	11.62 ng	578769	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9		



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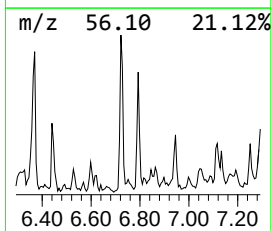
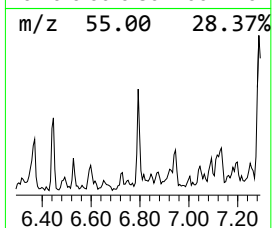
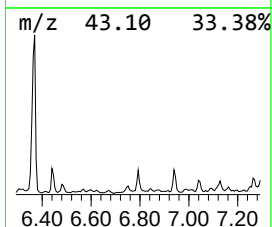
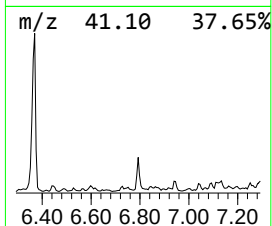
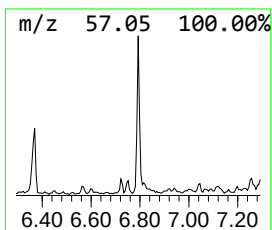
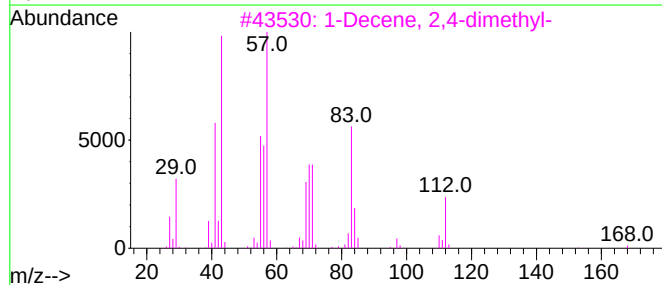
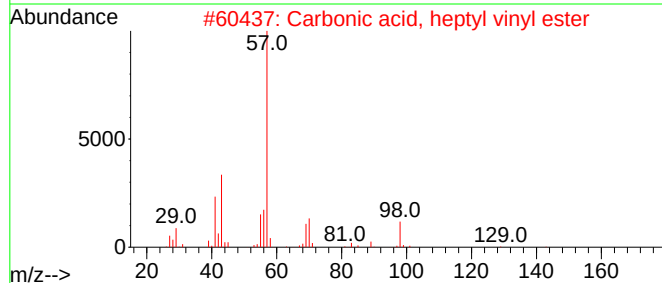
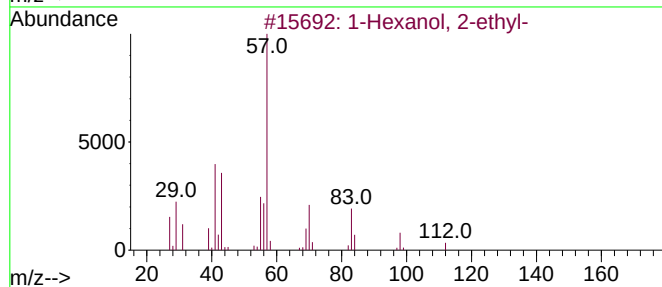
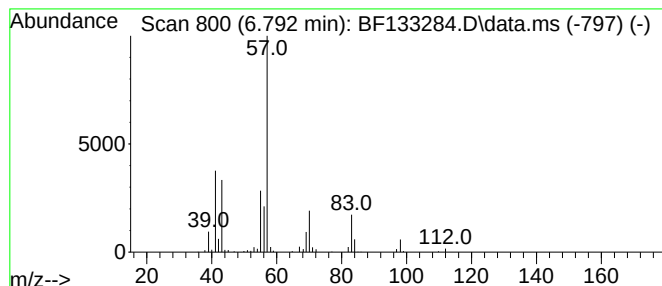
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.792	2.19 ng	108939	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
2	Carbonic acid, heptyl vinyl ester			186	C10H18O3	1010383-25-4	53
3	1-Decene, 2,4-dimethyl-			168	C12H24	055170-80-4	50
4	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	50
5	Heptyl tetradecyl ether			312	C21H44O	1000406-39-3	39



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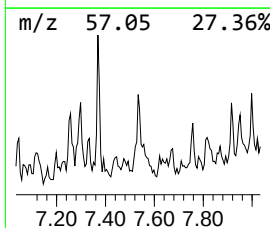
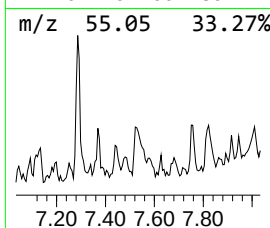
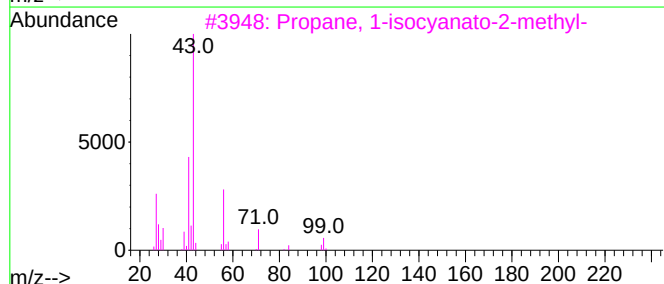
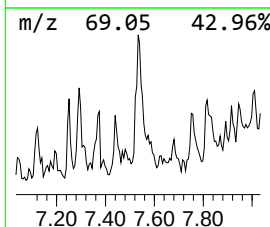
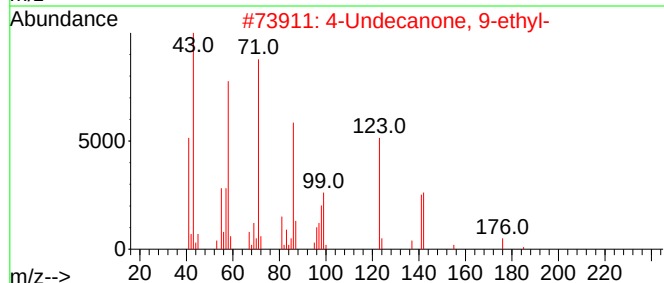
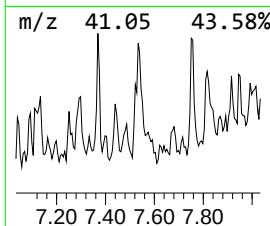
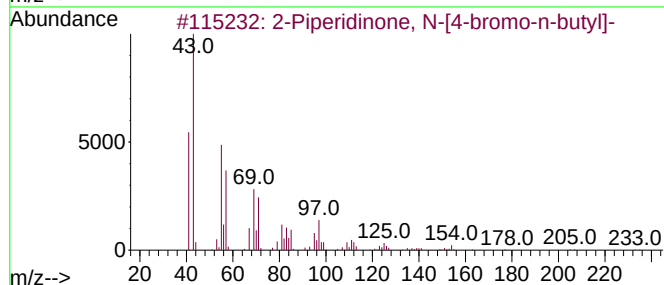
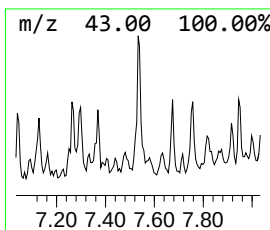
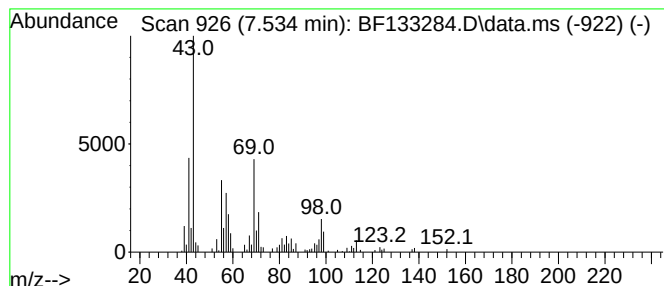
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown7.534 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.534	2.19 ng	138908	Naphthalene-d8	8.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperidinone, N-[4-bromo-n-but...	233	C9H16BrNO	195194-80-0	47		
2	4-Undecanone, 9-ethyl-	198	C13H26O	054549-96-1	47		
3	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	35		
4	Hexanoic acid, 9-decen-1-yl ester	254	C16H30O2	180252-09-9	35		
5	Oxalic acid, monoamide, n-propyl...	327	C19H37NO3	1000309-65-3	27		



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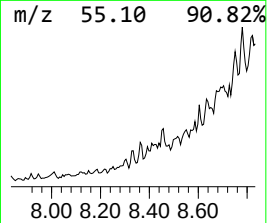
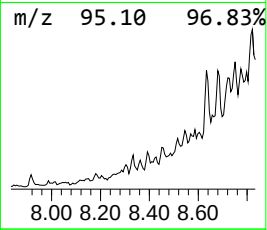
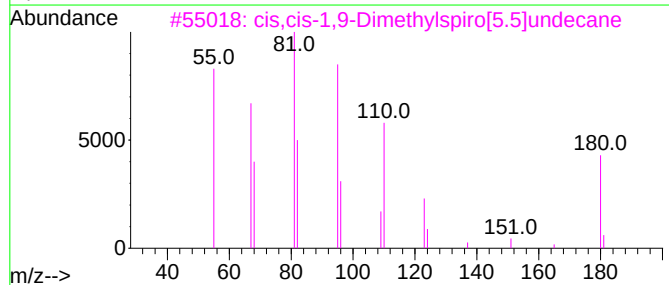
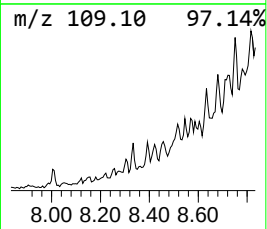
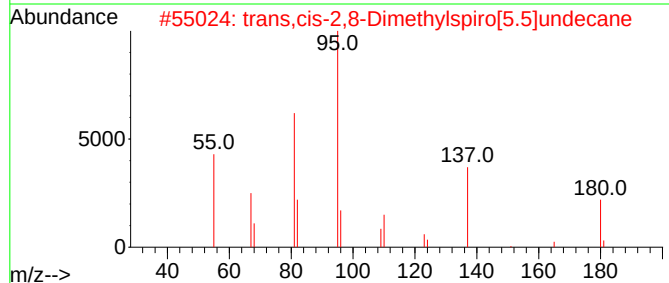
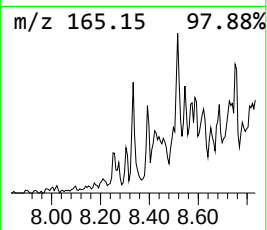
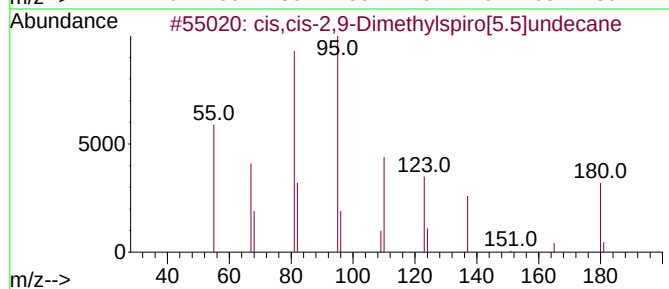
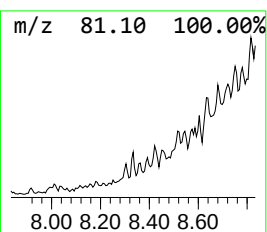
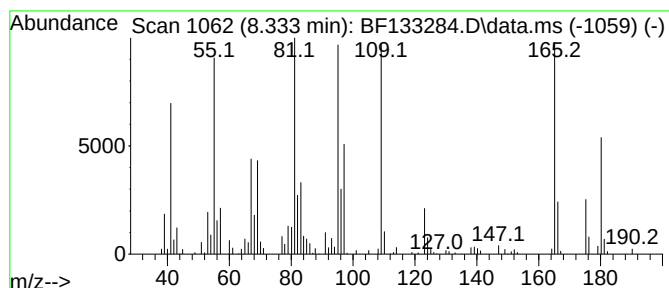
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 cis,cis-2,9-Dimethylspiro[5... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.333	2.39 ng	151842	Naphthalene-d8	8.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,cis-2,9-Dimethylspiro[5.5]un...	180	C13H24	095472-51-8	50
2	trans,cis-2,8-Dimethylspiro[5.5]...	180	C13H24	095472-52-9	46
3	cis,cis-1,9-Dimethylspiro[5.5]un...	180	C13H24	1000111-73-4	43
4	cis,trans-1,9-Dimethylspiro[5.5]...	180	C13H24	1000111-73-3	38
5	trans,cis-1,8-Dimethylspiro[4.5]...	166	C12H22	1000111-72-9	38



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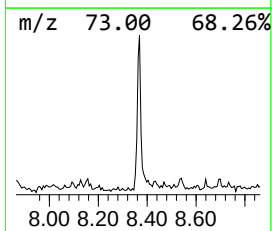
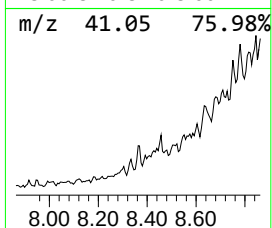
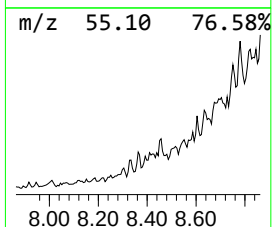
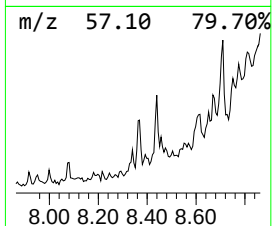
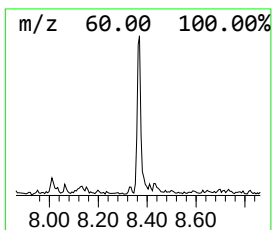
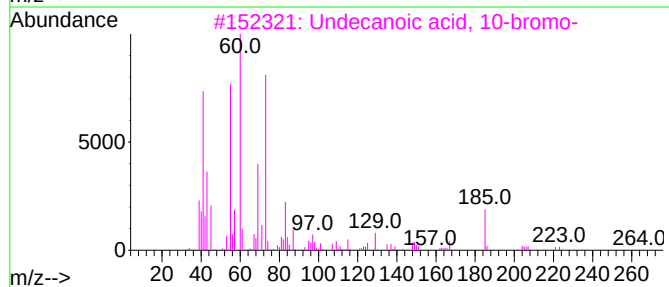
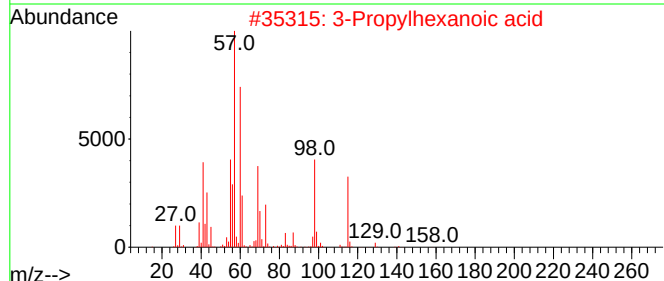
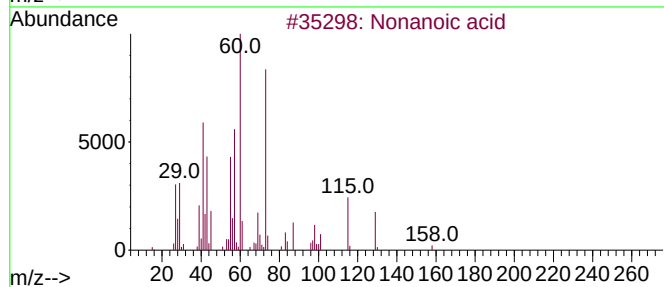
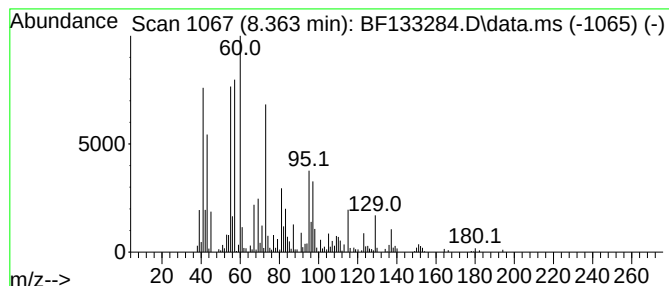
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Peak Number 5 Nonanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.363	2.54 ng	161650	Naphthalene-d8	8.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	50
2			3-Propylhexanoic acid	158	C9H18O2	025110-61-6	43
3			Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	43
4			n-Decanoic acid	172	C10H20O2	000334-48-5	38
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	27



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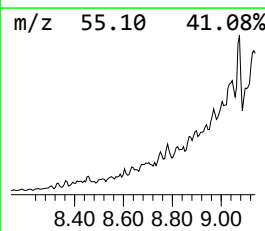
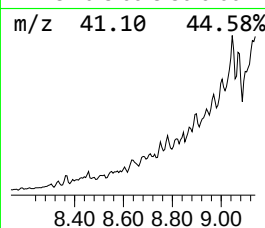
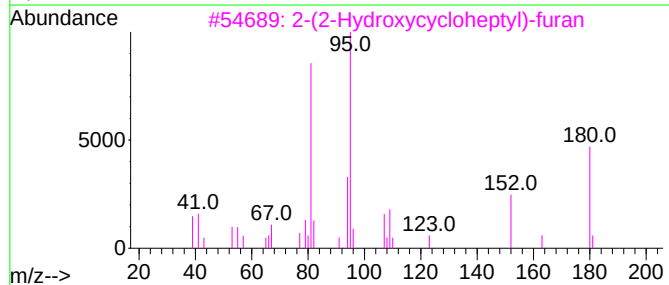
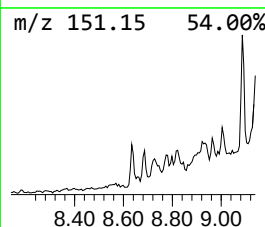
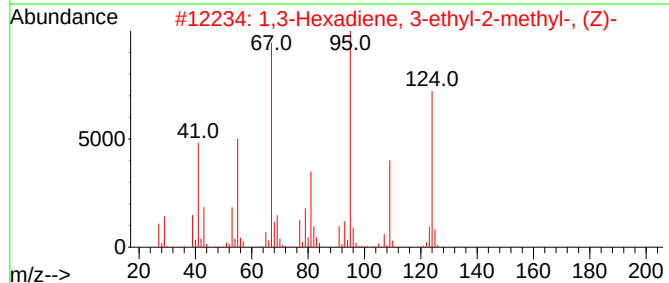
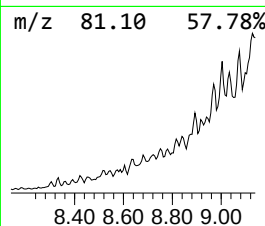
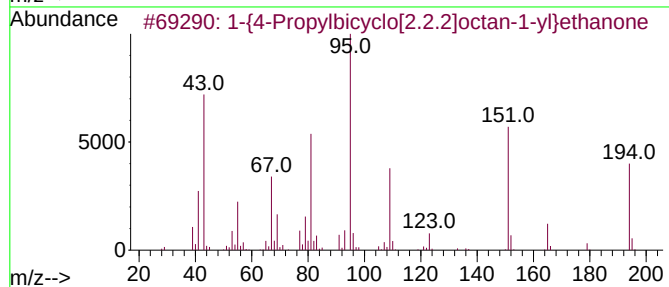
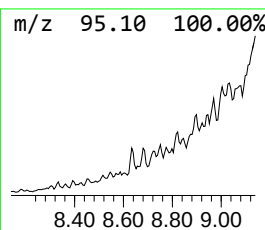
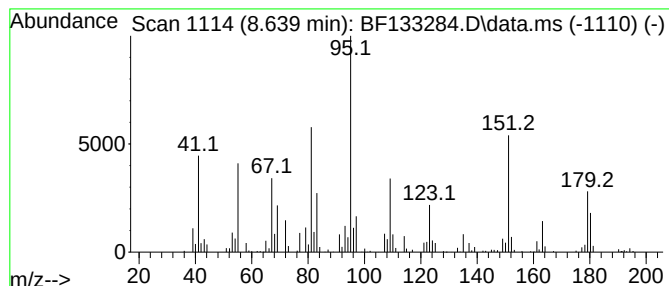
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-{4-Propylbicyclo[2.2.2]oc... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.639	7.27 ng	462140	Naphthalene-d8	8.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-{4-Propylbicyclo[2.2.2]octan-1-yl}ethanone	194	C13H22O	1000435-24-0	52
2	1,3-Hexadiene, 3-ethyl-2-methyl-, (Z)-	124	C9H16	074752-97-9	50
3	2-(2-Hydroxycycloheptyl)-furan	180	C11H16O2	1000145-02-9	43
4	2-Hexylbicyclo[2.2.2]octane	194	C14H26	1000435-94-1	43
5	6-(5-Methyl-furan-2-yl)-hexan-2-one	180	C11H16O2	1000185-87-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133284.D
Acq On : 06 May 2023 02:03
Operator : CG\JU
Sample : 02622-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

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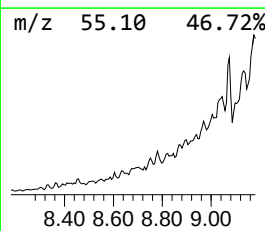
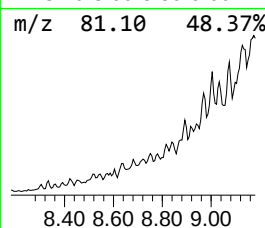
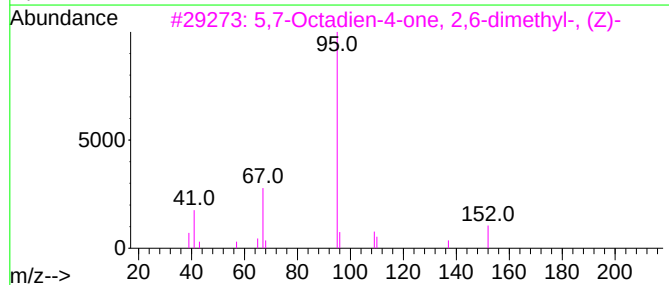
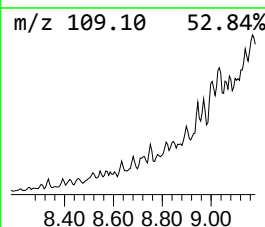
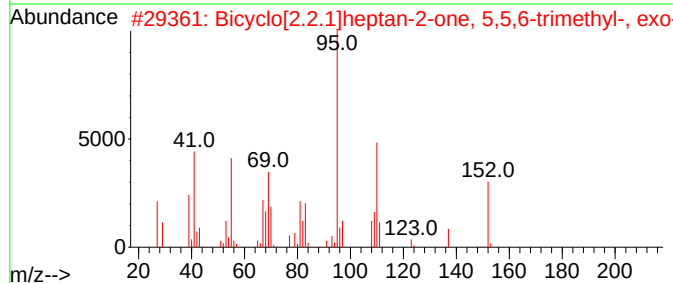
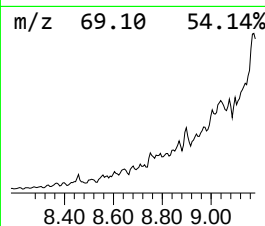
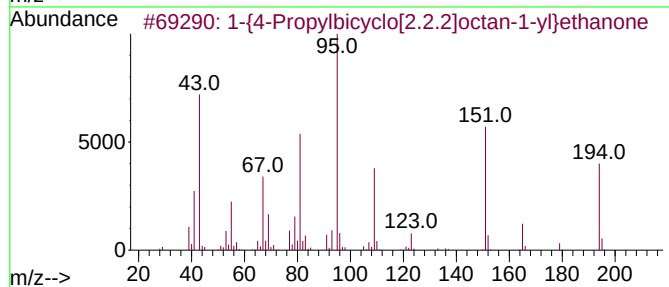
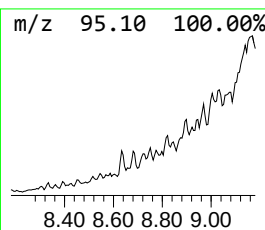
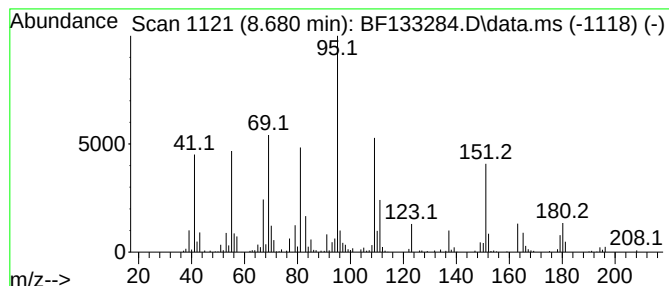
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.680 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.680	4.27 ng	271069	Naphthalene-d8	8.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1		{4-Propylbicyclo[2.2.2]octan-1...	194	C13H22O	1000435-24-0	52
2			Bicyclo[2.2.1]heptan-2-one, 5,5,...	152	C10H16O	003649-86-3	35
3			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	003588-18-9	30
4			6-Hepten-1-ol, 2-methyl-	128	C8H16O	1000132-12-0	27
5			Cyclopentene, 1-isopropyl-4,5-di...	138	C10H18	007712-74-5	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133284.D
Acq On : 06 May 2023 02:03
Operator : CG\JU
Sample : 02622-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

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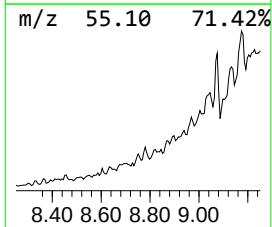
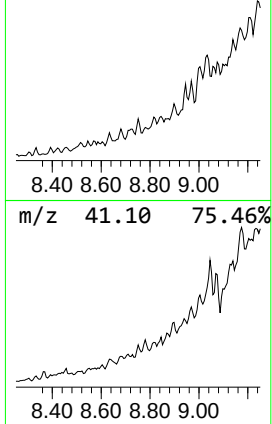
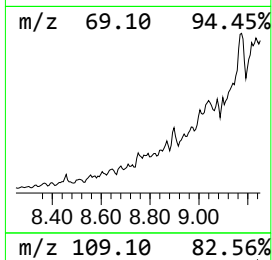
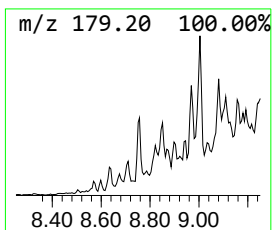
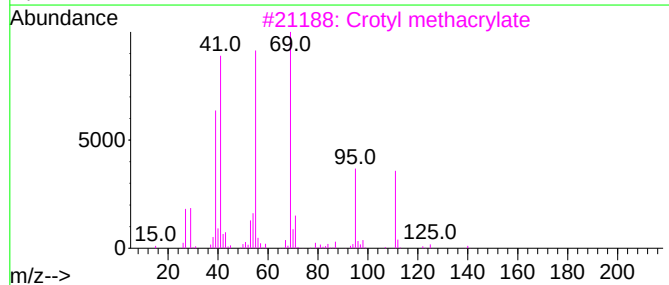
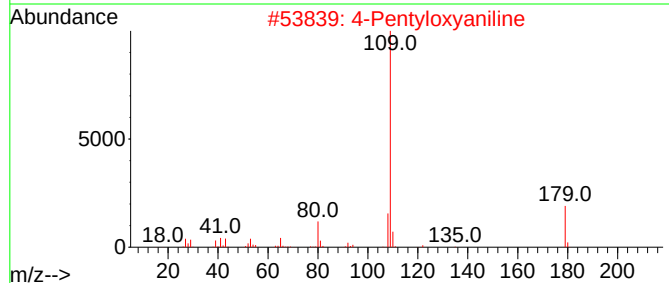
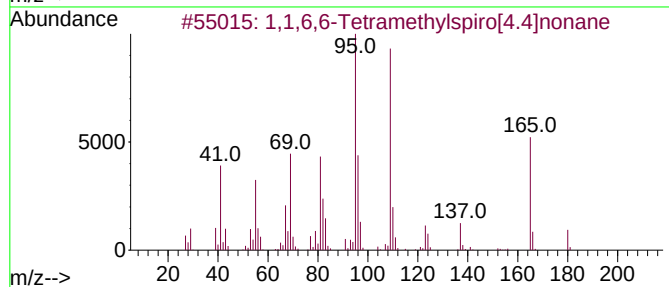
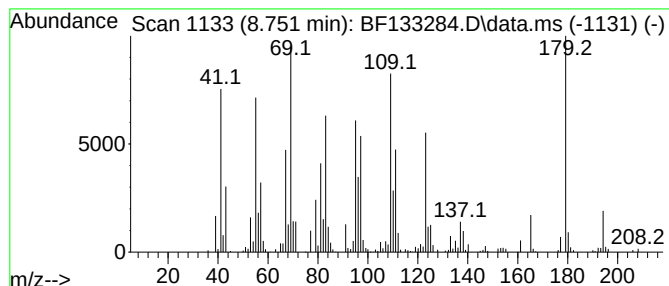
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown8.751 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.751	4.99 ng	316868	Naphthalene-d8	8.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,6,6-Tetramethylspiro[4.4]nonane	180	C13H24	074054-92-5	25		
2	4-Pentyloxyaniline	179	C11H17NO	039905-50-5	25		
3	Crotyl methacrylate	140	C8H12O2	007376-45-6	25		
4	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	22		
5	Cyclohexane, 2-ethyl-1,3-dimethyl-	140	C10H20	007045-67-2	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
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Acq On : 06 May 2023 02:03
Operator : CG\JU
Sample : 02622-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

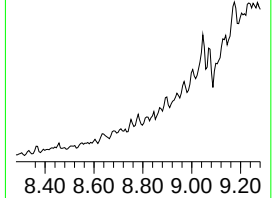
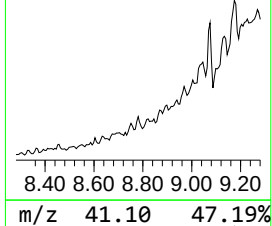
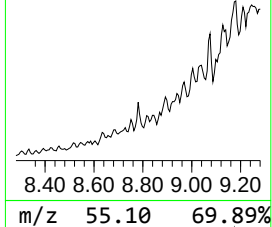
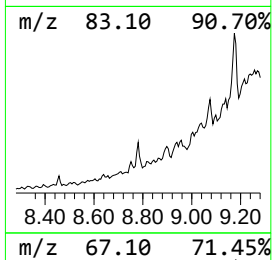
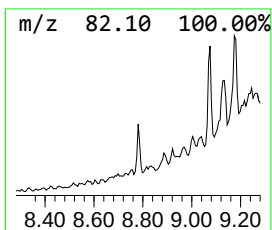
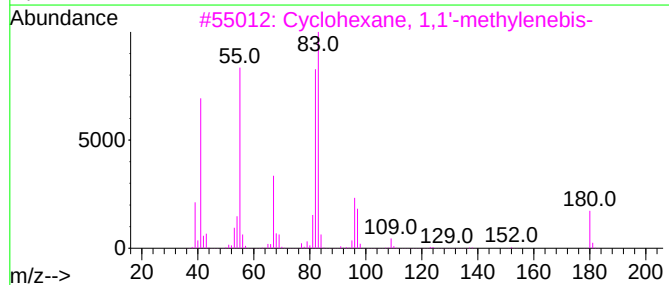
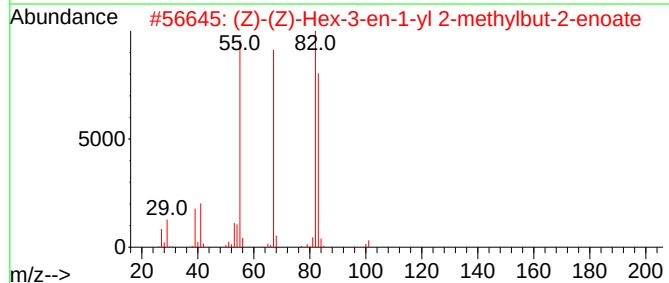
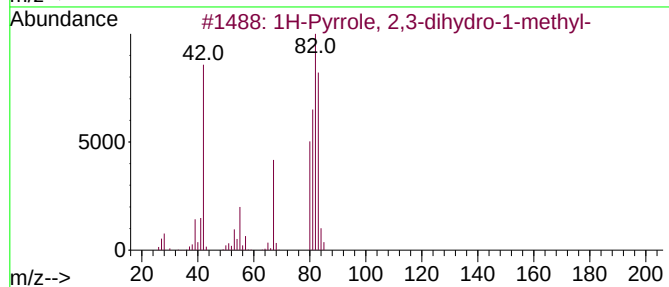
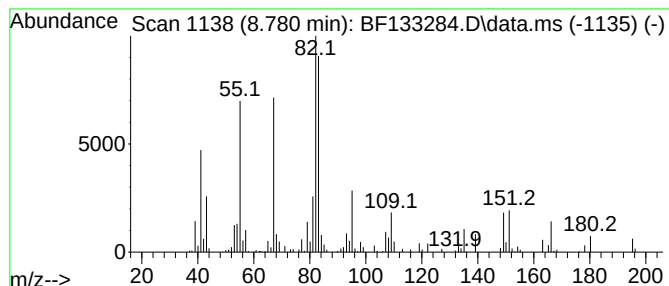
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1H-Pyrrole, 2,3-dihydro-1-m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.780	5.29 ng	335855	Naphthalene-d8	8.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	64
2	(Z)-(Z)-Hex-3-en-1-yl 2-methylbu...	182	C11H18O2	084060-80-0	50
3	Cyclohexane, 1,1'-methylenebis-	180	C13H24	003178-23-2	50
4	Hexenyl angelate, 4z-	182	C11H18O2	1000383-63-7	43
5	2(3H)-Furanone, 4,5-dihydro-4-(2...	166	C10H14O2	1000153-91-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133284.D
Acq On : 06 May 2023 02:03
Operator : CG\JU
Sample : 02622-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

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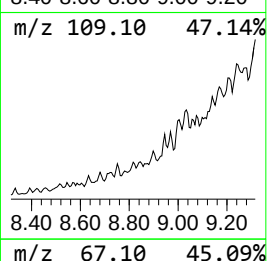
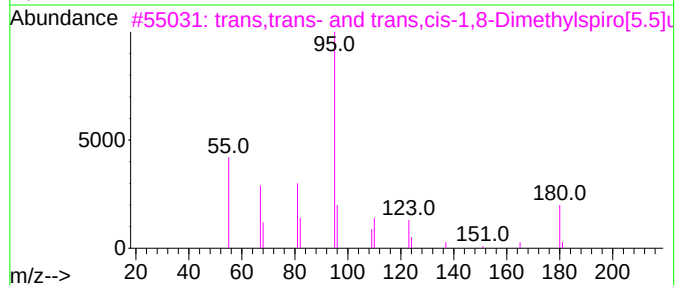
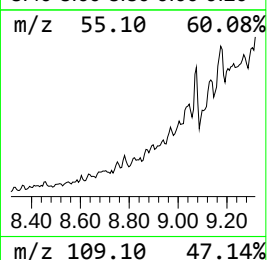
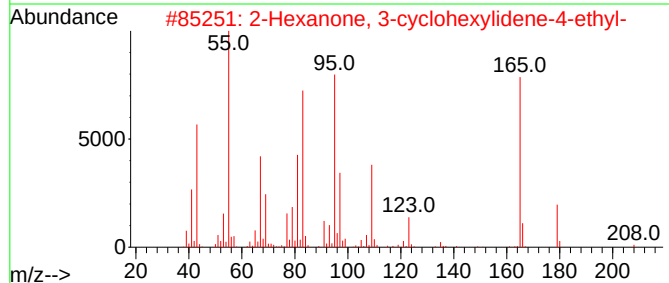
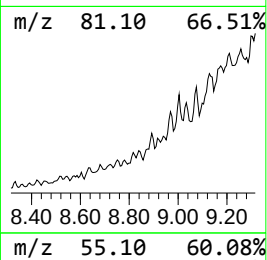
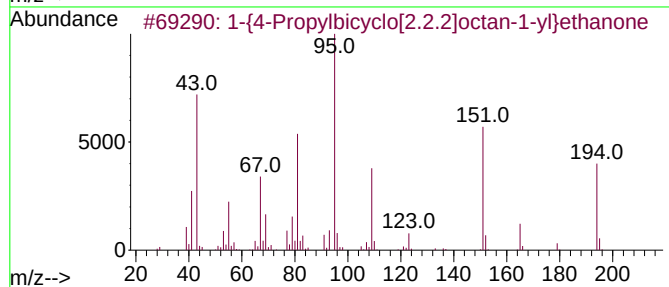
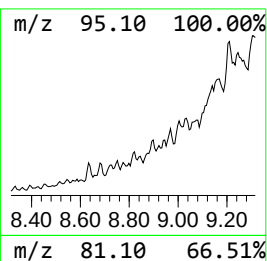
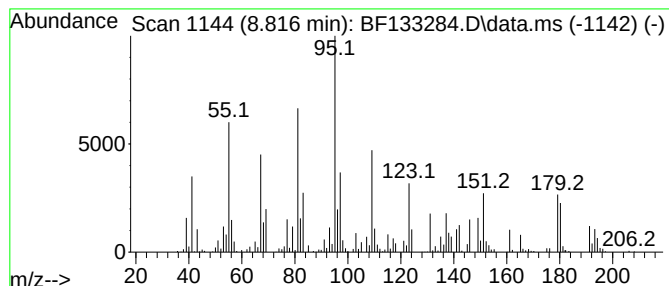
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Hexanone, 3-cyclohexylide... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.816	4.34 ng	276046	Naphthalene-d8	8.010

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1	{4-Propylbicyclo[2.2.2]octan-1...	194	C13H22O	1000435-24-0	53
2	2	Hexanone, 3-cyclohexylidene-4...	208	C14H24O	1000150-19-2	50
3	trans,trans- and trans,cis-1,8-D...	180	C13H24		1000111-73-2	46
4	2-Hexylbicyclo[2.2.2]octane	194	C14H26		1000435-94-1	46
5	cis,cis-2,8-Dimethylspiro[5.5]un...	180	C13H24		095530-75-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133284.D
Acq On : 06 May 2023 02:03
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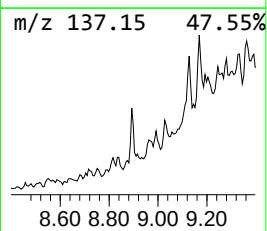
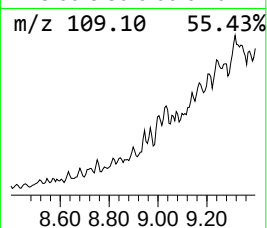
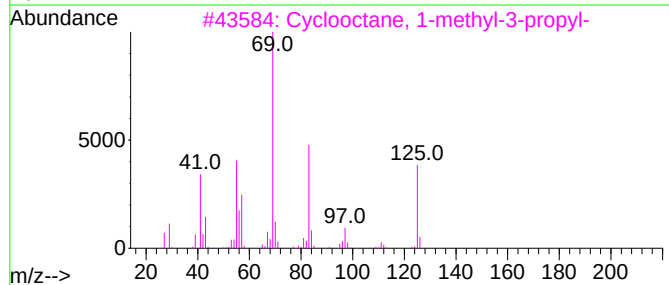
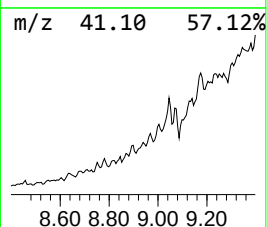
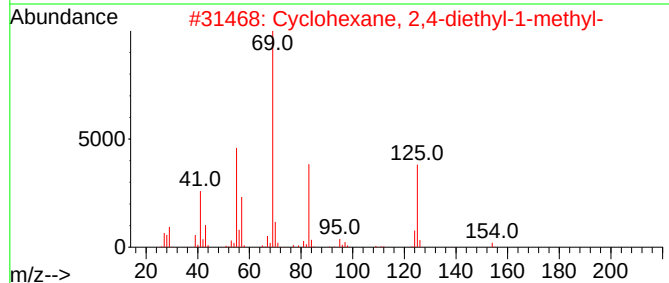
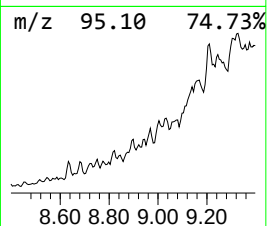
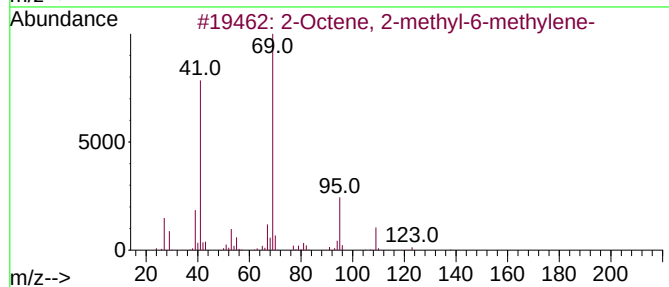
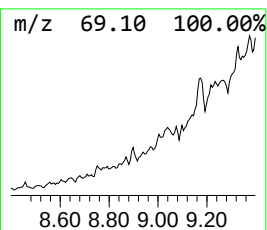
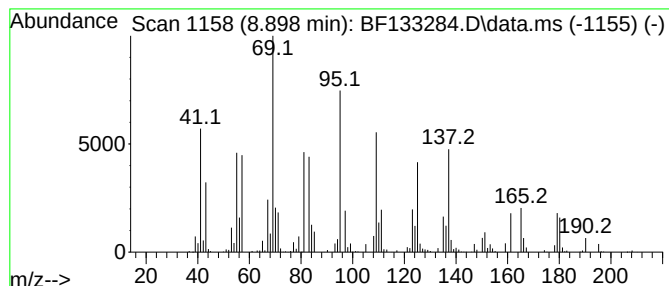
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown8.898 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.898	5.80 ng	402655	Acenaphthene-d10	9.780

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	38
2		Cyclohexane, 2,4-diethyl-1-methyl-	154	C11H22	061142-70-9	30
3		Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	27
4		Cyclohexane, 1,2-diethyl-3-methyl-	154	C11H22	061141-80-8	27
5		Bicyclo[2.2.1]heptane-2,3-dione,...	166	C10H14O2	010334-26-6	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133284.D
Acq On : 06 May 2023 02:03
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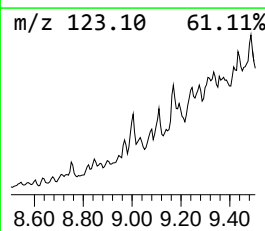
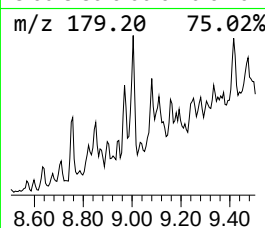
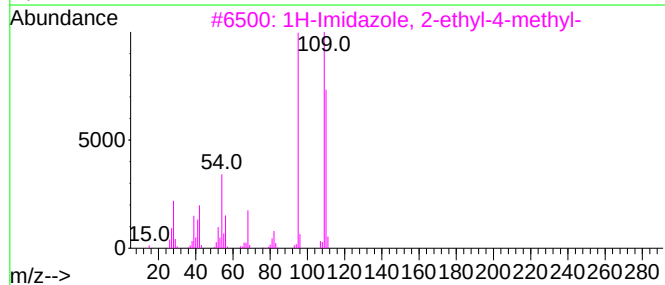
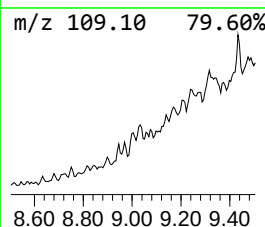
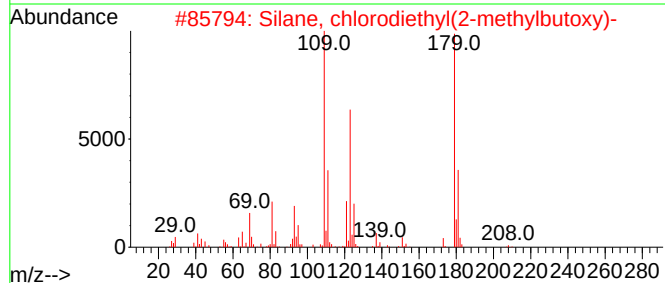
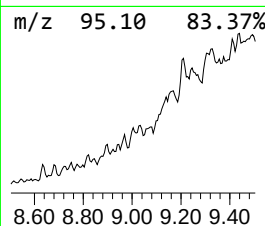
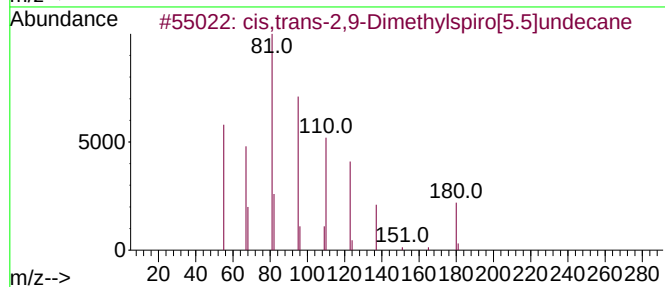
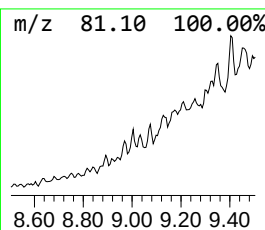
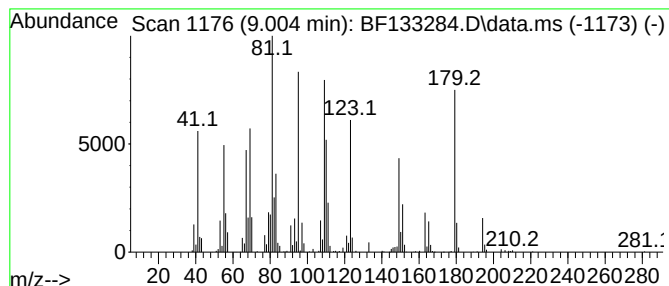
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 cis,trans-2,9-Dimethylspiro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.004	11.50 ng	797666	Acenaphthene-d10	9.780

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	50
2		Silane, chlorodiethyl(2-methylbu...	208	C9H21ClOSi	1000363-11-1	46
3		1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	30
4		2-(2-Hydroxycyclooctyl)-furan	194	C12H18O2	115754-90-0	25
5		Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133284.D
Acq On : 06 May 2023 02:03
Operator : CG\JU
Sample : 02622-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

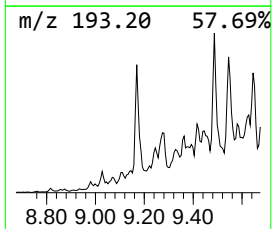
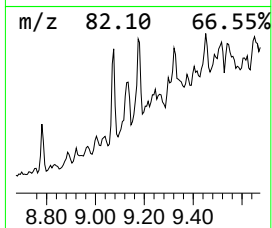
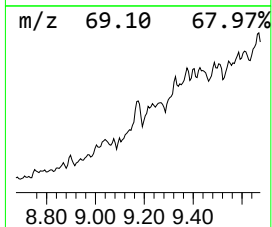
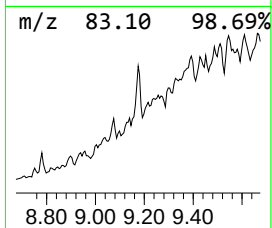
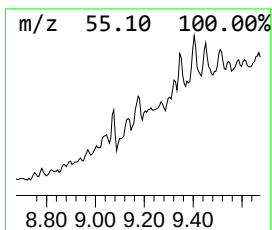
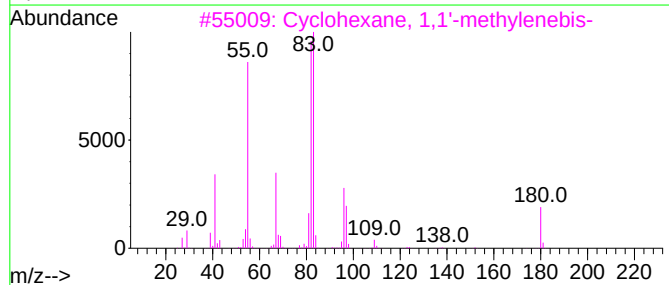
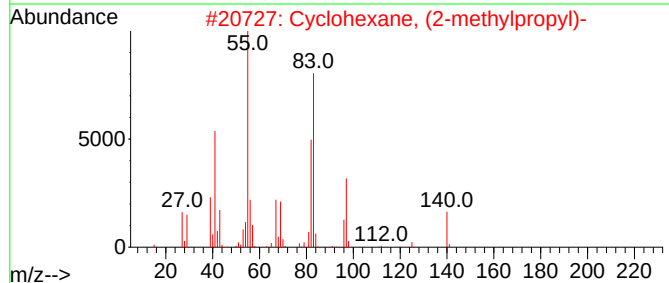
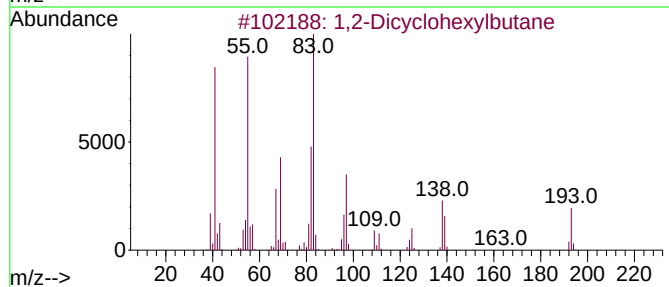
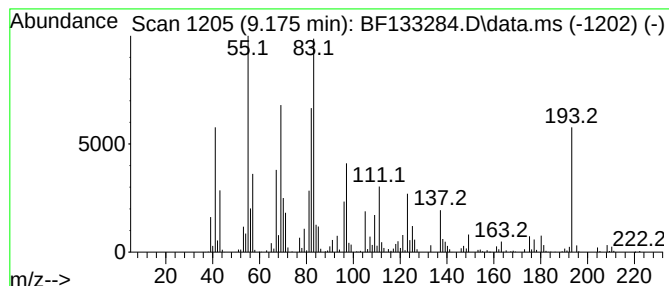
Instrument :
BNA_F
ClientSampleId :
RBR-251675

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1,2-Dicyclohexylbutane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.175	20.00 ng	1387570	Acenaphthene-d10	9.780	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dicyclohexylbutane	222	C16H30	054890-01-6	59
2	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	46
3	Cyclohexane, 1,1'-methylenebis-	180	C13H24	003178-23-2	38
4	Cyclopentane, 1-methyl-3-(1-meth...	126	C9H18	053771-88-3	38
5	Cyclohexane, octadecyl-	336	C24H48	004445-06-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133284.D
Acq On : 06 May 2023 02:03
Operator : CG\JU
Sample : 02622-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-251675

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
2-Pentanone, 4-...	4.904	11.6	ng	578769	1	6.722	996084	20.0
1-Hexanol, 2-et...	6.792	2.2	ng	108939	1	6.722	996084	20.0
unknown7.534	7.534	2.2	ng	138908	2	8.010	1270780	20.0
cis,cis-2,9-Dim...	8.333	2.4	ng	151842	2	8.010	1270780	20.0
Nonanoic acid	8.363	2.5	ng	161650	2	8.010	1270780	20.0
1-{4-Propylbicy...	8.639	7.3	ng	462140	2	8.010	1270780	20.0
unknown8.680	8.680	4.3	ng	271069	2	8.010	1270780	20.0
unknown8.751	8.751	5.0	ng	316868	2	8.010	1270780	20.0
1H-Pyrrole, 2,3...	8.780	5.3	ng	335855	2	8.010	1270780	20.0
2-Hexanone, 3-c...	8.816	4.3	ng	276046	2	8.010	1270780	20.0
unknown8.898	8.898	5.8	ng	402655	3	9.780	1387570	20.0
cis,trans-2,9-D...	9.004	11.5	ng	797666	3	9.780	1387570	20.0
1,2-Dicyclohexy...	9.175	20.0	ng	1387570	3	9.780	1387570	20.0