

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
 Data File : BF132703.D
 Acq On : 08 Mar 2023 22:07
 Operator : CG\JU
 Sample : 01829-10
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-10-20230306

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132703.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.204	441	445	452	rVB	1166061	1334324	48.25%	8.062%
2	5.610	510	514	522	rBV	2876758	2765661	100.00%	16.709%
3	6.616	682	685	694	rVB	2546601	2567673	92.84%	15.513%
4	6.986	745	748	751	rBV	909488	710599	25.69%	4.293%
5	7.551	840	844	847	rBV	2094579	1768432	63.94%	10.684%
6	8.269	963	966	969	rBV	899614	798748	28.88%	4.826%
7	8.345	976	979	986	rBV	664915	663164	23.98%	4.007%
8	8.804	1050	1057	1060	rBV4	185004	296647	10.73%	1.792%
9	9.045	1096	1098	1102	rBV	135709	144563	5.23%	0.873%
10	9.345	1146	1149	1152	rBV	3066777	2761223	99.84%	16.682%
11	9.375	1152	1154	1156	rVV	326977	225763	8.16%	1.364%
12	9.410	1158	1160	1161	rBV	285020	219841	7.95%	1.328%
13	9.427	1161	1163	1166	rVB2	288477	292911	10.59%	1.770%
14	9.616	1192	1195	1199	rVB	1779216	1484366	53.67%	8.968%
15	9.898	1241	1243	1246	rBV	571519	517703	18.72%	3.128%

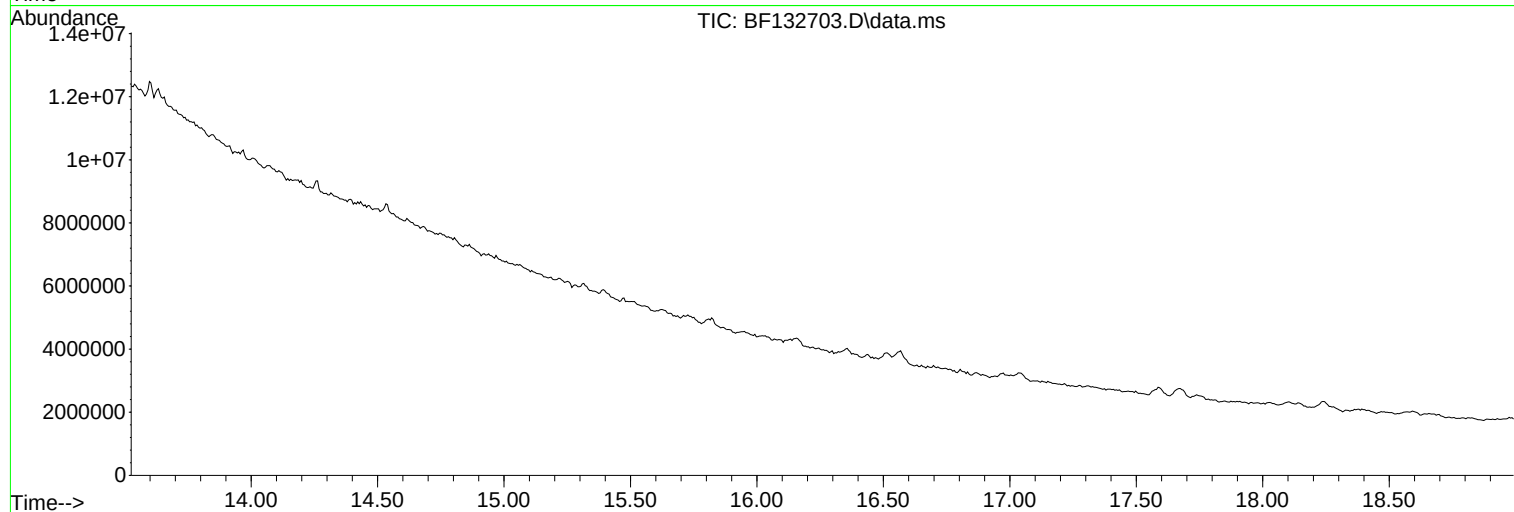
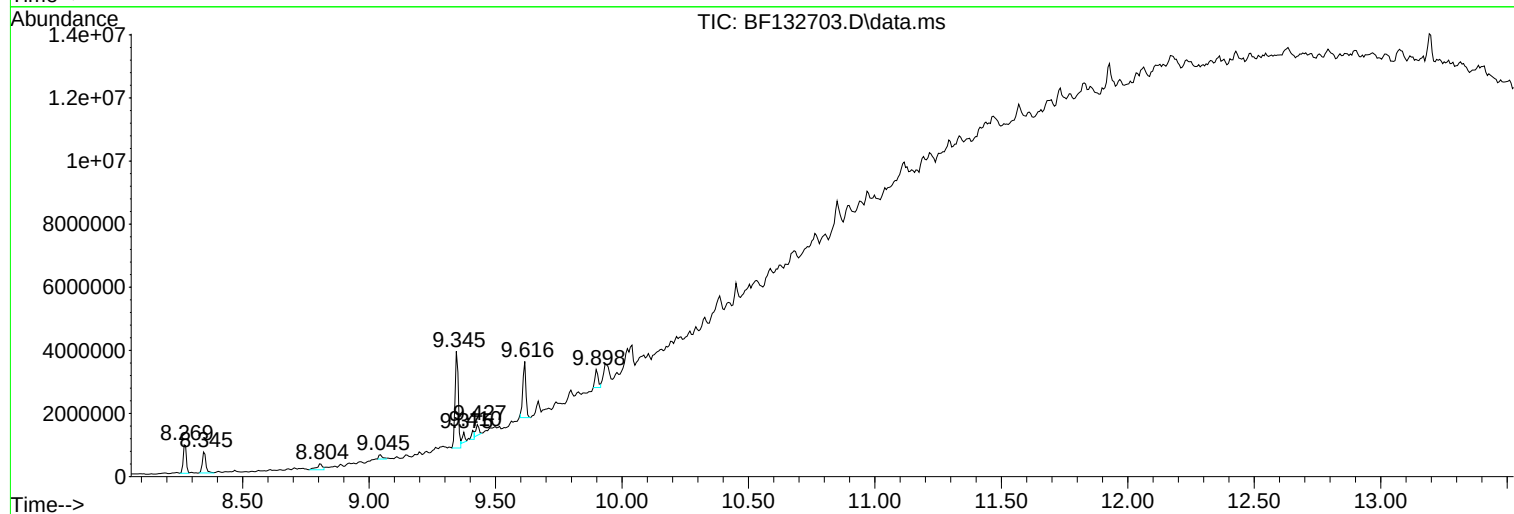
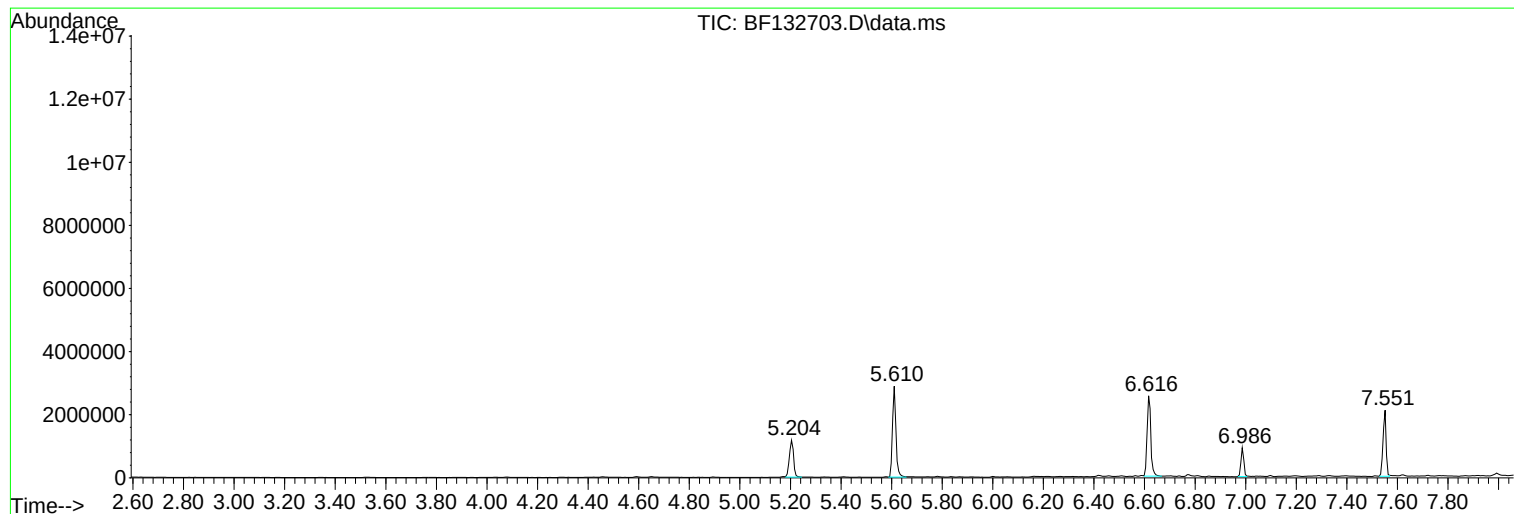
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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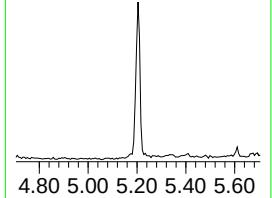
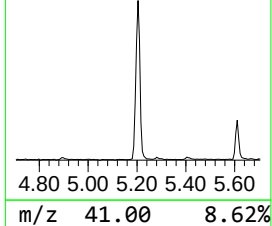
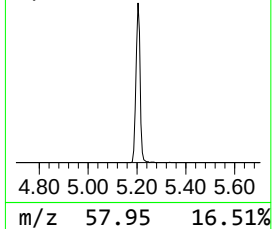
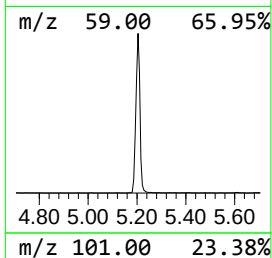
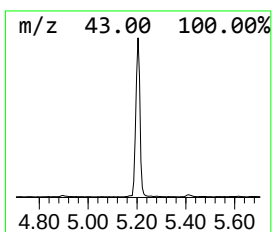
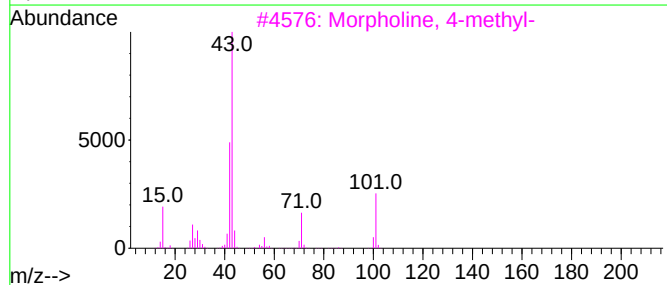
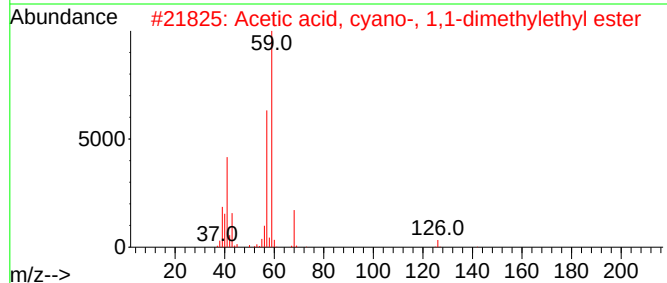
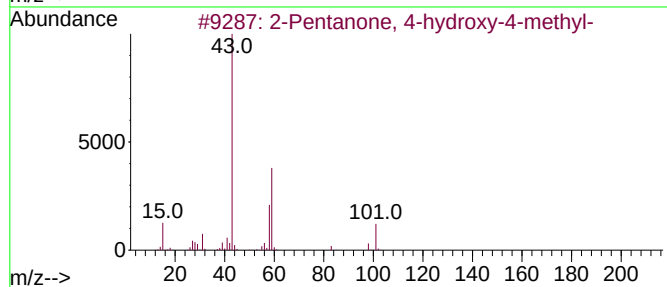
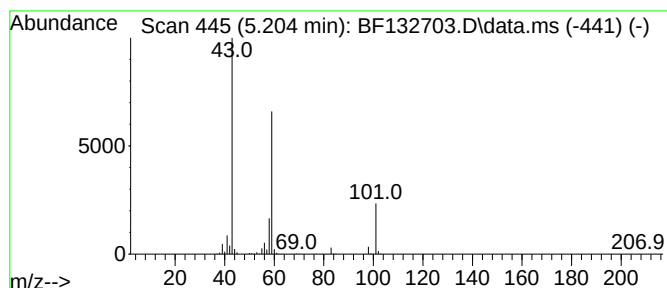
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.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.
5.204	37.55 ng	1334320	1,4-Dichlorobenzene-d4	6.986

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Guanidine	59	CH5N3	000113-00-8	9



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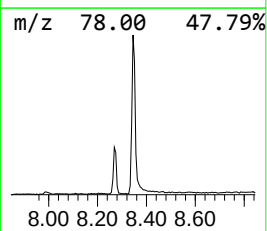
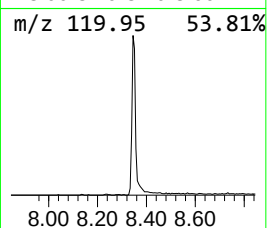
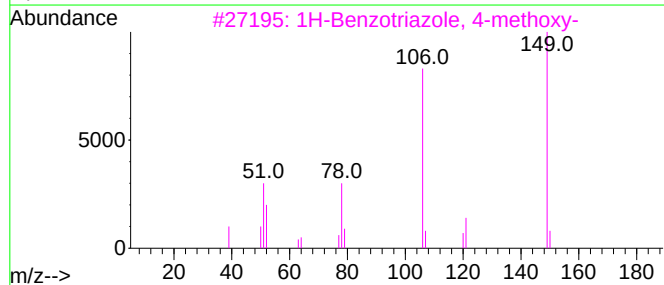
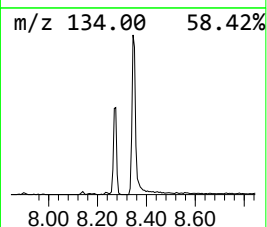
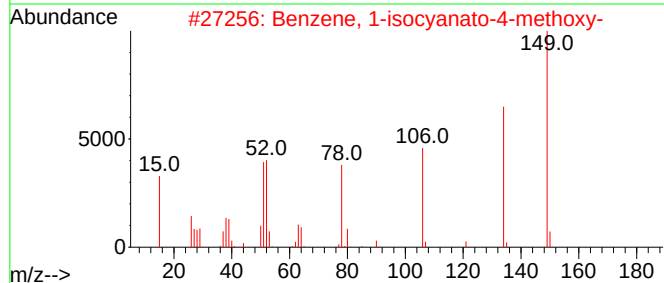
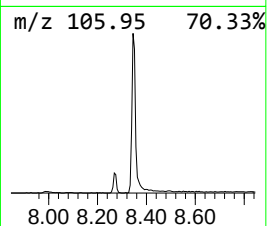
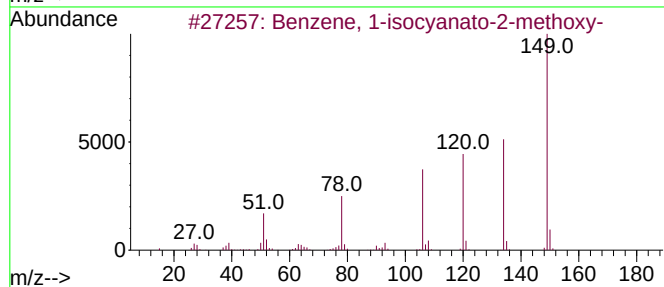
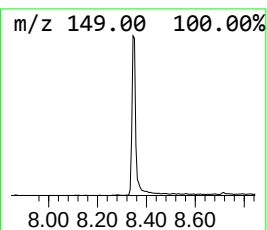
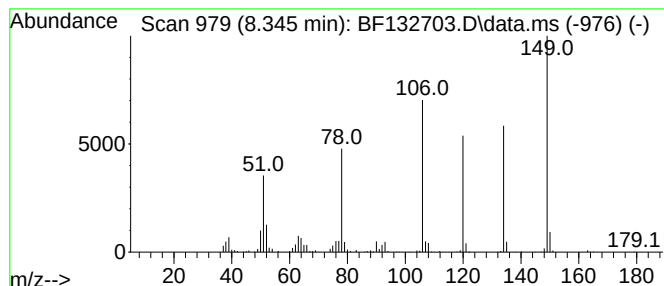
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-isocyanato-2-met... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.345	16.61 ng	663164	Naphthalene-d8	8.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-isocyanato-2-methoxy-	149	C8H7NO2	000700-87-8	81
2			Benzene, 1-isocyanato-4-methoxy-	149	C8H7NO2	005416-93-3	72
3			1H-Benzotriazole, 4-methoxy-	149	C7H7N3O	027799-90-2	47
4			N,N-Dimethylnicotinamide	150	C8H10N2O	006972-69-6	47
5			1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	46



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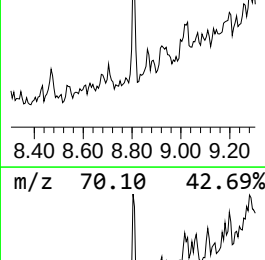
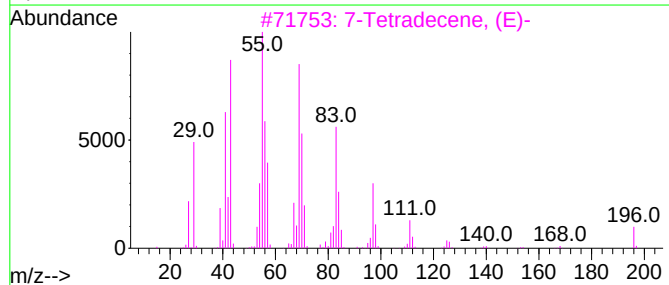
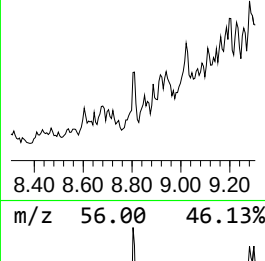
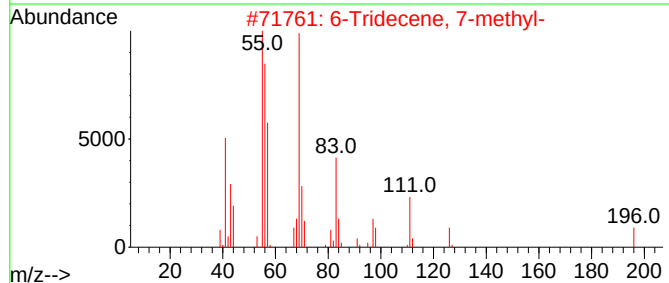
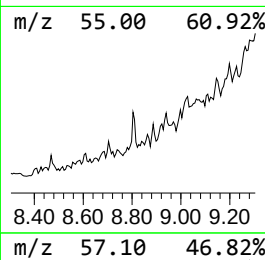
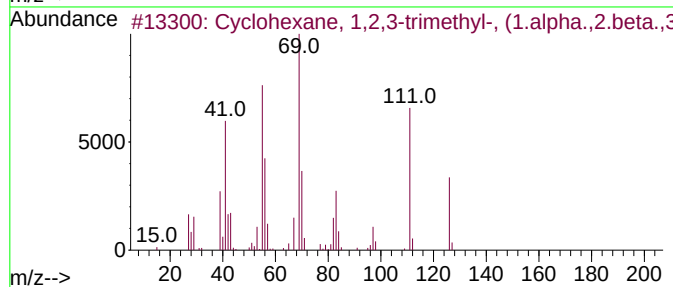
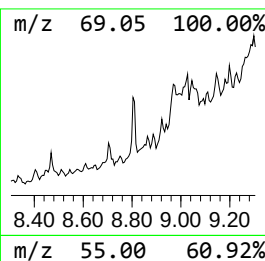
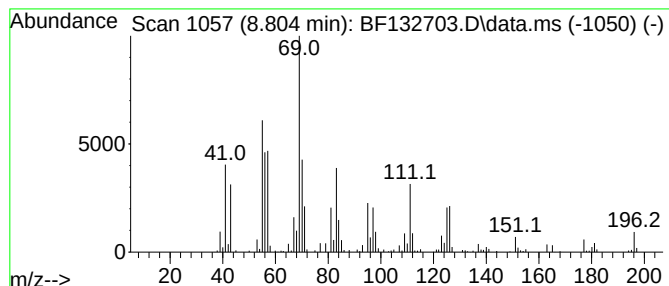
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexane, 1,2,3-trimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.804	7.43 ng	296647	Naphthalene-d8	8.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	001678-81-5	68
2			6-Tridecene, 7-methyl-	196	C14H28	024949-42-6	68
3			7-Tetradecene, (E)-	196	C14H28	041446-63-3	55
4			Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	007667-55-2	52
5			7-Tetradecene, (Z)-	196	C14H28	041446-60-0	50



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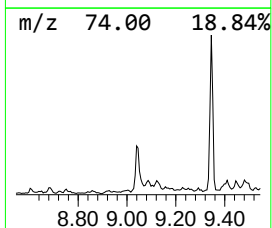
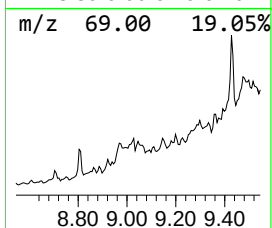
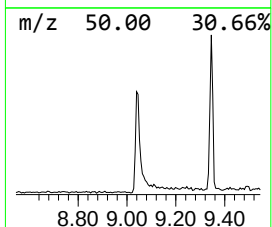
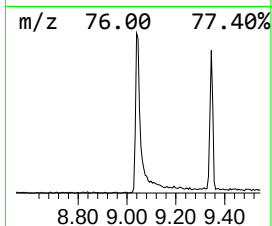
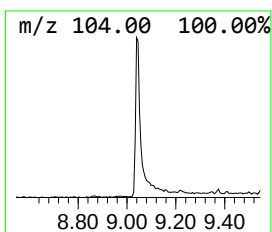
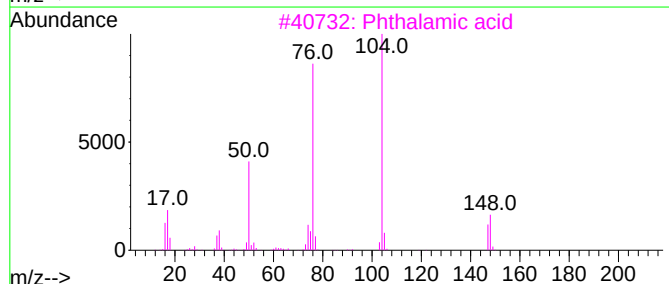
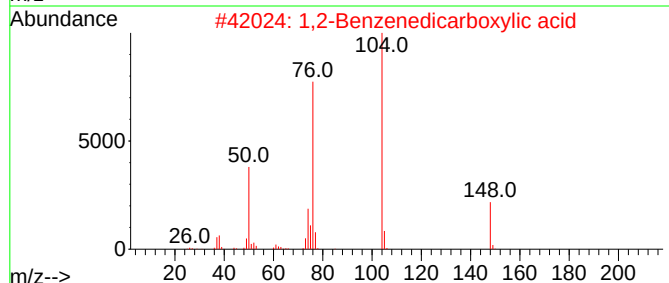
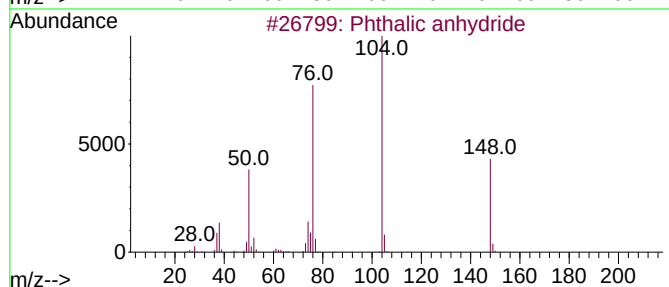
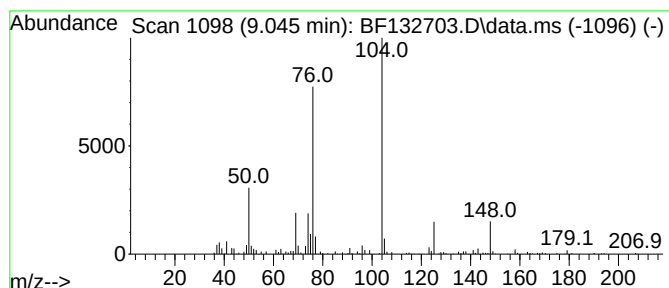
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phthalic anhydride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.045	3.62 ng	144563	Naphthalene-d8	8.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic anhydride	148	C8H4O3	000085-44-9	94
2			1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	90
3			Phthalamic acid	165	C8H7NO3	000088-97-1	83
4			Bicyclo[4.2.0]octa-1,3,5-triene-...	132	C8H4O2	006383-11-5	83
5			Indan-1,2,3-trione	160	C9H4O3	000938-24-9	83



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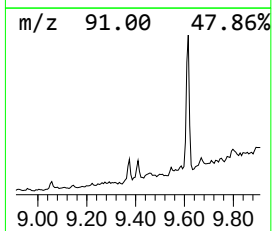
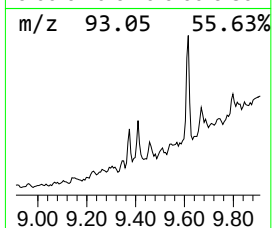
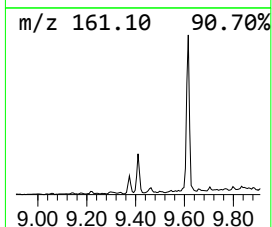
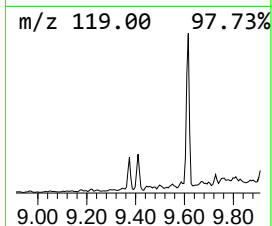
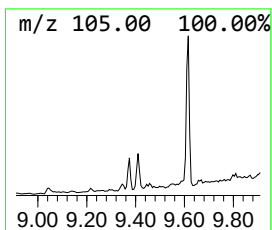
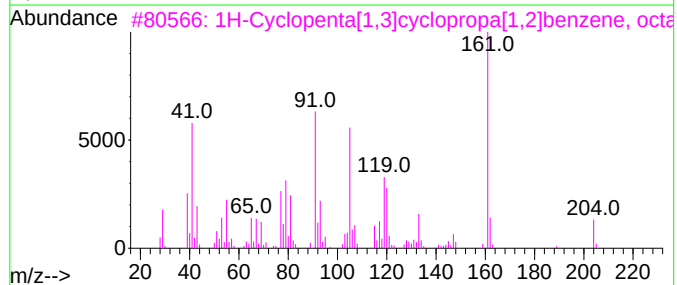
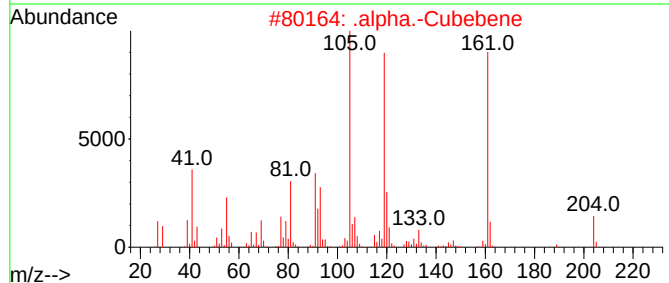
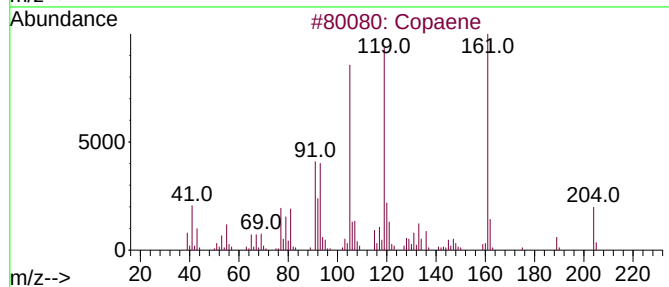
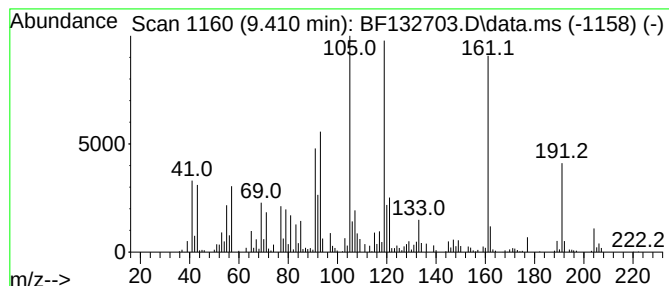
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Copaene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.410	8.49 ng	219841	Acenaphthene-d10	10.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Copaene	204	C15H24	003856-25-5	98
2			.alpha.-Cubebene	204	C15H24	017699-14-8	92
3			1H-Cyclopenta[1,3]cyclopropa[1,2...]	204	C15H24	013744-15-5	86
4			1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	001461-03-6	55
5			Tricyclo[5.4.0.0(2,8)]undec-9-en...	204	C15H24	005989-08-2	49



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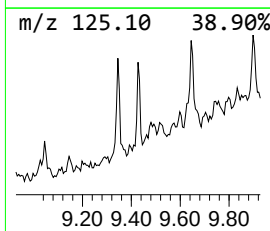
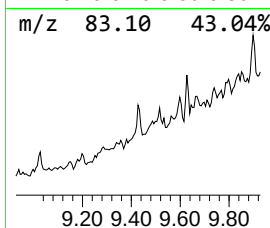
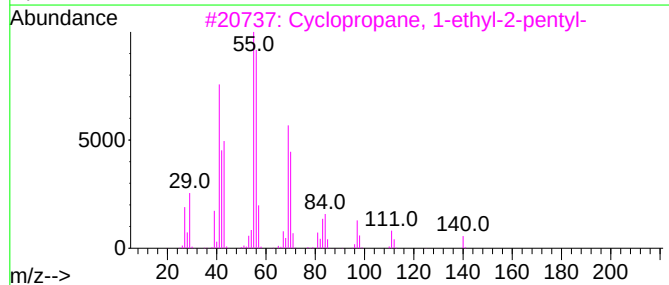
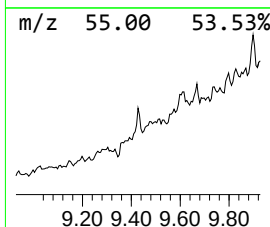
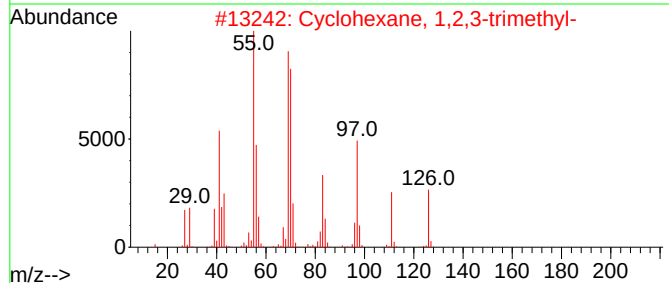
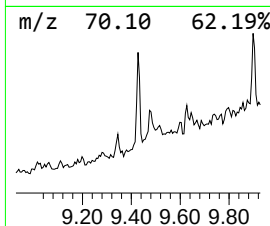
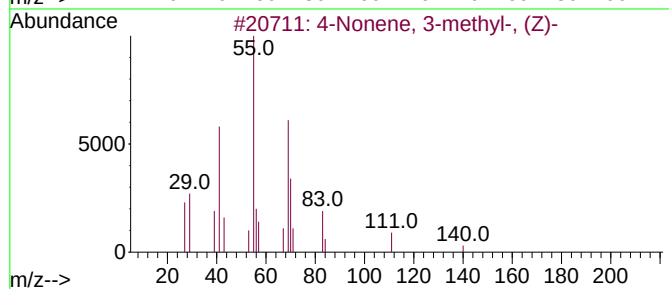
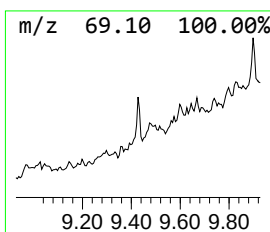
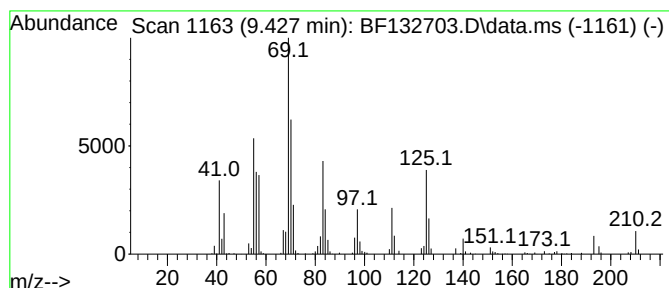
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4-Nonene, 3-methyl-, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.427	11.32 ng	292911	Acenaphthene-d10	10.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Nonene, 3-methyl-, (Z)-	140	C10H20	063830-69-3	53
2			Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	47
3			Cyclopropane, 1-ethyl-2-pentyl-	140	C10H20	062238-08-8	47
4			6-Dodecene, (E)-	168	C12H24	007206-17-9	43
5			3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132703.D
Acq On : 08 Mar 2023 22:07
Operator : CG\JU
Sample : 01829-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

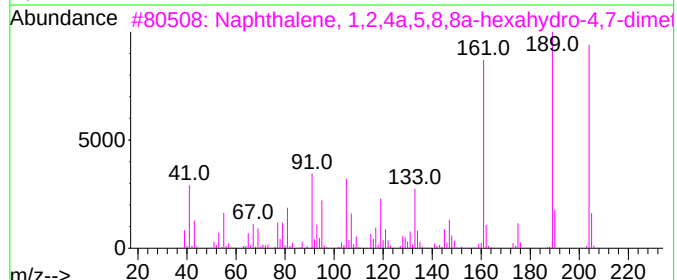
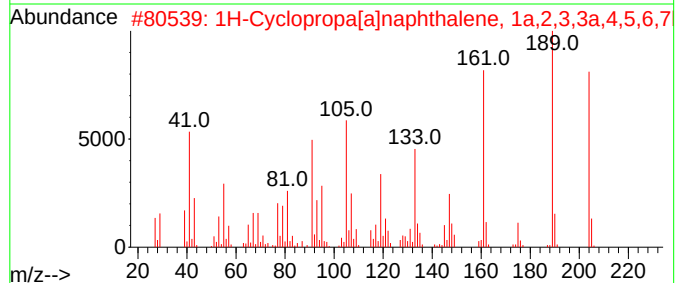
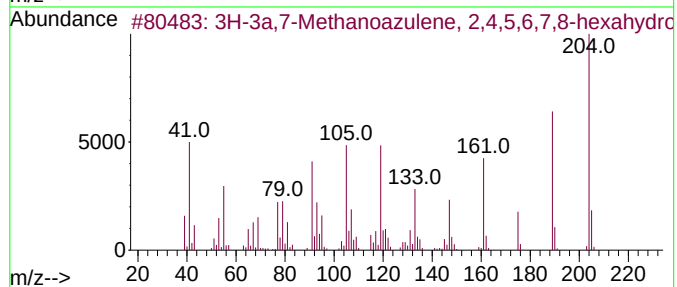
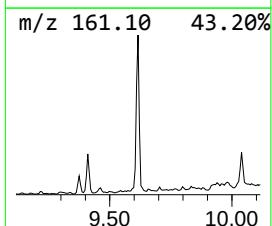
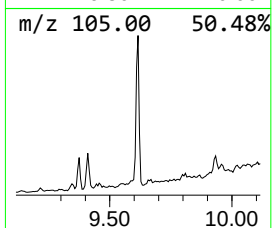
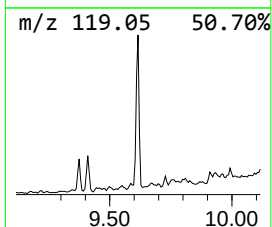
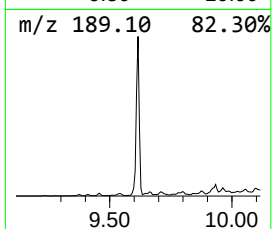
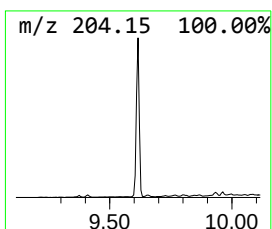
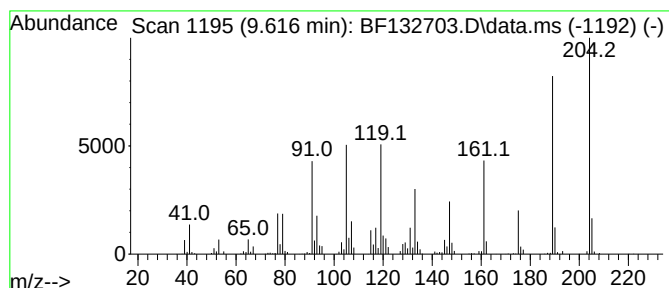
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ClientSampleId :
SS-10-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3H-3a,7-Methanoazulene, 2,4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.616	57.34 ng	1484370	Acenaphthene-d10		10.039	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3H-3a,7-Methanoazulene, 2,4,5,6,...		204	C15H24	002387-78-2	94
2	1H-Cyclopropa[a]naphthalene, 1a,...		204	C15H24	000489-29-2	93
3	Naphthalene, 1,2,4a,5,8,8a-hexah...		204	C15H24	005951-61-1	89
4	2H-1,3-Oxazine, 2-[(2,6-dimethyl...		204	C12H16N2O	054708-09-7	76
5	1H-Cycloprop[e]azulene, 1a,2,3,4...		204	C15H24	000489-40-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132703.D
Acq On : 08 Mar 2023 22:07
Operator : CG\JU
Sample : 01829-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-10-20230306

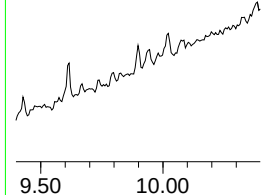
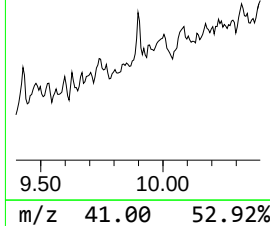
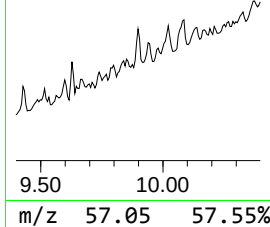
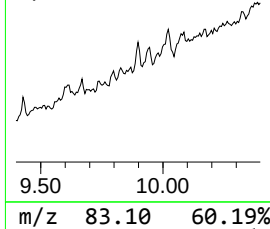
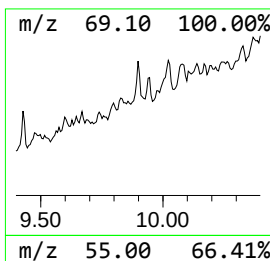
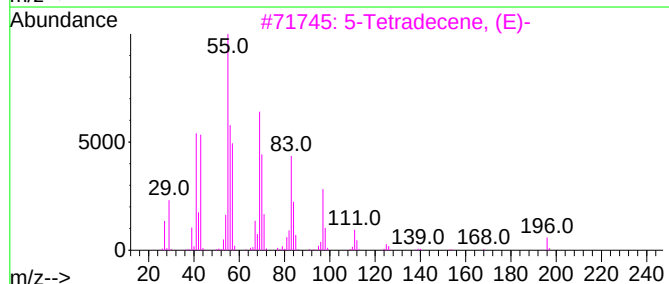
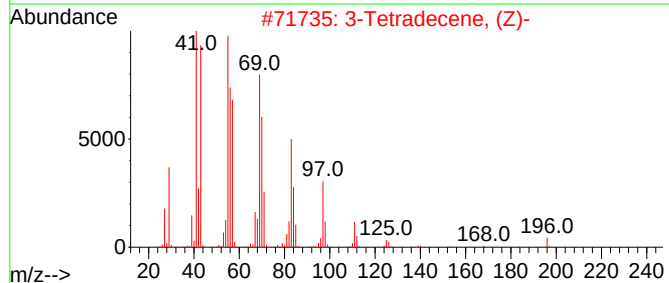
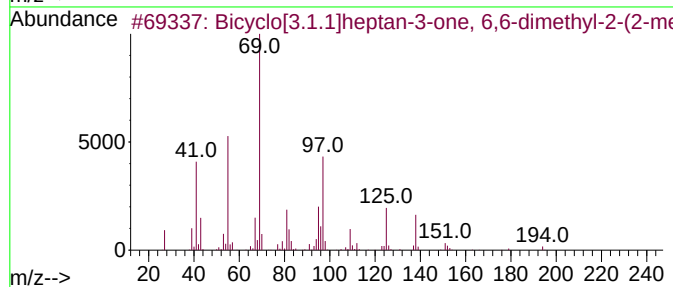
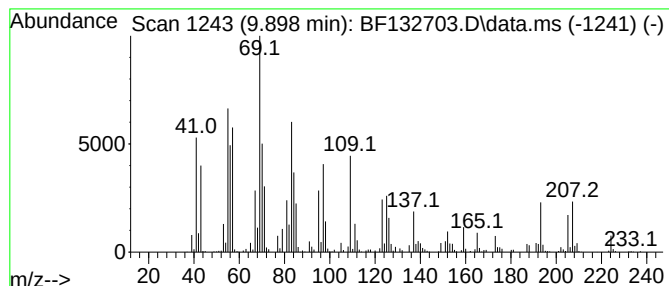
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown9.898 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.898	20.00 ng	517703	Acenaphthene-d10	10.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptan-3-one, 6,6-...	194	C13H22O	1000163-97-9	45
2			3-Tetradecene, (Z)-	196	C14H28	041446-67-7	43
3			5-Tetradecene, (E)-	196	C14H28	041446-66-6	38
4			7-Tetradecene	196	C14H28	010374-74-0	38
5			2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030823\
Data File : BF132703.D
Acq On : 08 Mar 2023 22:07
Operator : CG\JU
Sample : 01829-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-10-20230306

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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-...	5.204	37.5	ng	1334320	1	6.986	710599	20.0
Benzene, 1-isoc...	8.345	16.6	ng	663164	2	8.275	798748	20.0
Cyclohexane, 1,...	8.804	7.4	ng	296647	2	8.275	798748	20.0
Phthalic anhydride	9.045	3.6	ng	144563	2	8.275	798748	20.0
Copaene	9.410	8.5	ng	219841	3	10.039	517703	20.0
4-Nonene, 3-met...	9.427	11.3	ng	292911	3	10.039	517703	20.0
3H-3a,7-Methano...	9.616	57.3	ng	1484370	3	10.039	517703	20.0
unknown9.898	9.898	20.0	ng	517703	3	10.039	517703	20.0