

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
 Data File : BF127206.D
 Acq On : 04 Mar 2022 17:45
 Operator : CG\JU
 Sample : N1793-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127206.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.498	542	546	558	rBV	1221423	1112593	31.43%	5.255%
2	6.504	713	717	719	rBV	302754	302098	8.53%	1.427%
3	6.528	719	721	728	rVB2	98157	184928	5.22%	0.874%
4	6.792	763	766	774	rVB	67069	58013	1.64%	0.274%
5	6.875	776	780	784	rVV	727751	577569	16.31%	2.728%
6	7.034	802	807	810	rBV	884743	1004478	28.37%	4.745%
7	7.445	868	877	880	rBV	2043358	2048939	57.87%	9.678%
8	7.545	884	894	902	rBV	137277	234206	6.62%	1.106%
9	7.887	948	952	961	rVB3	39461	49414	1.40%	0.233%
10	8.157	994	998	1002	rBV	845404	759120	21.44%	3.586%
11	9.239	1176	1182	1185	rBV	3902969	3482399	98.36%	16.449%
12	9.692	1251	1259	1263	rBV4	45119	111646	3.15%	0.527%
13	9.728	1263	1265	1275	rVB2	42440	55112	1.56%	0.260%
14	9.916	1288	1297	1300	rBV	920824	890483	25.15%	4.206%
15	10.716	1427	1433	1436	rBV	2782037	2502524	70.69%	11.821%
16	11.063	1486	1492	1507	rBV3	30983	114349	3.23%	0.540%
17	11.410	1547	1551	1555	rBV	1126657	893127	25.23%	4.219%
18	11.792	1612	1616	1619	rBV	1154492	1032891	29.17%	4.879%
19	11.827	1619	1622	1625	rVB	48362	48096	1.36%	0.227%
20	13.004	1816	1822	1825	rBV	3824713	3540373	100.00%	16.723%
21	13.921	1974	1978	1981	rVB	49584	51293	1.45%	0.242%
22	14.057	1997	2001	2005	rVB	828825	717427	20.26%	3.389%
23	14.151	2011	2017	2024	rBV	317383	342681	9.68%	1.619%
24	14.810	2125	2129	2135	rBV3	76915	135886	3.84%	0.642%
25	15.010	2159	2163	2167	rBV	34938	39938	1.13%	0.189%
26	15.163	2185	2189	2193	rVB2	42190	52485	1.48%	0.248%
27	15.545	2249	2254	2264	rVB2	510728	656283	18.54%	3.100%
28	15.992	2325	2330	2337	rVB	45111	67740	1.91%	0.320%
29	16.509	2412	2418	2425	rVB2	36721	66720	1.88%	0.315%
30	17.121	2517	2522	2528	rVB5	19676	37741	1.07%	0.178%

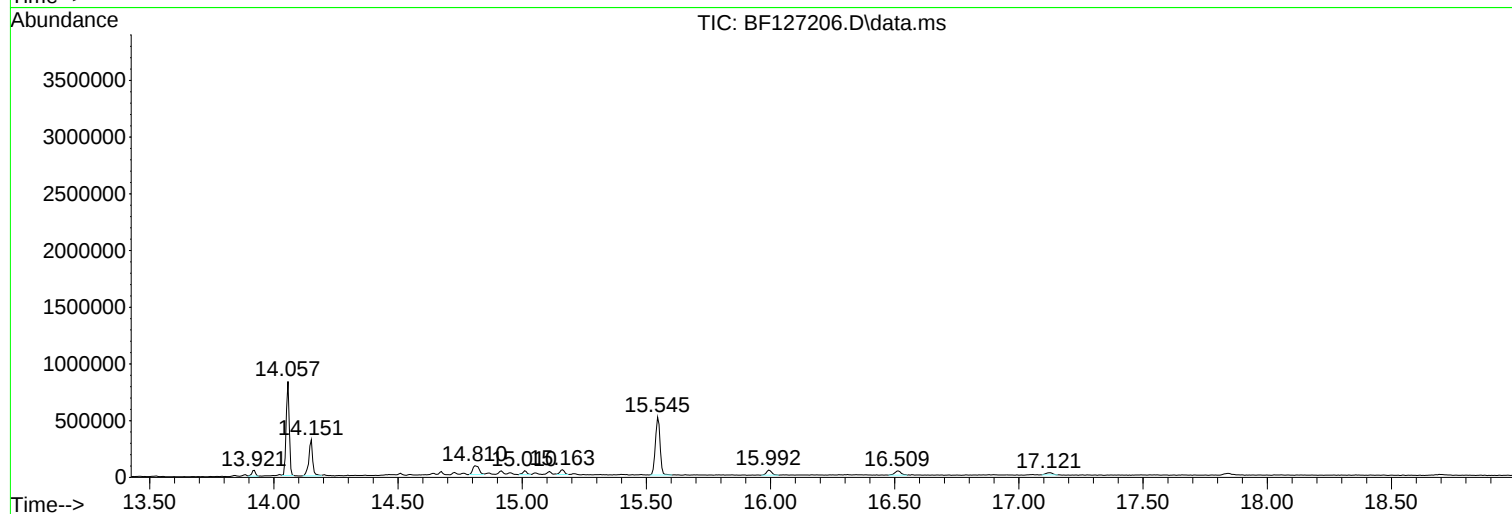
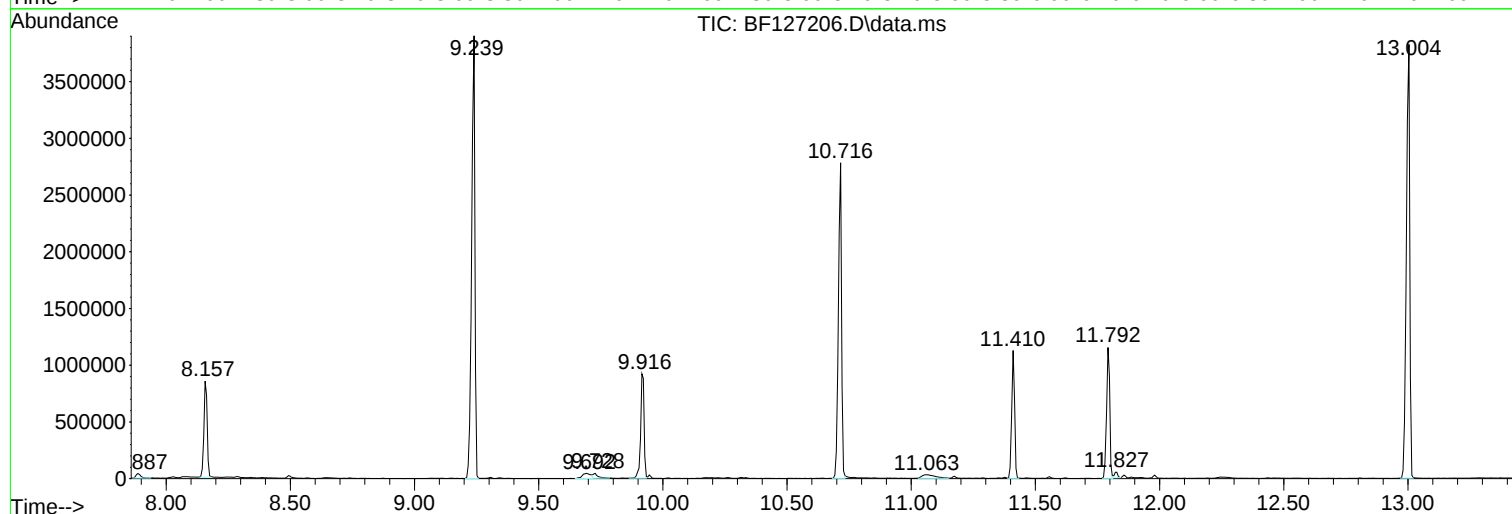
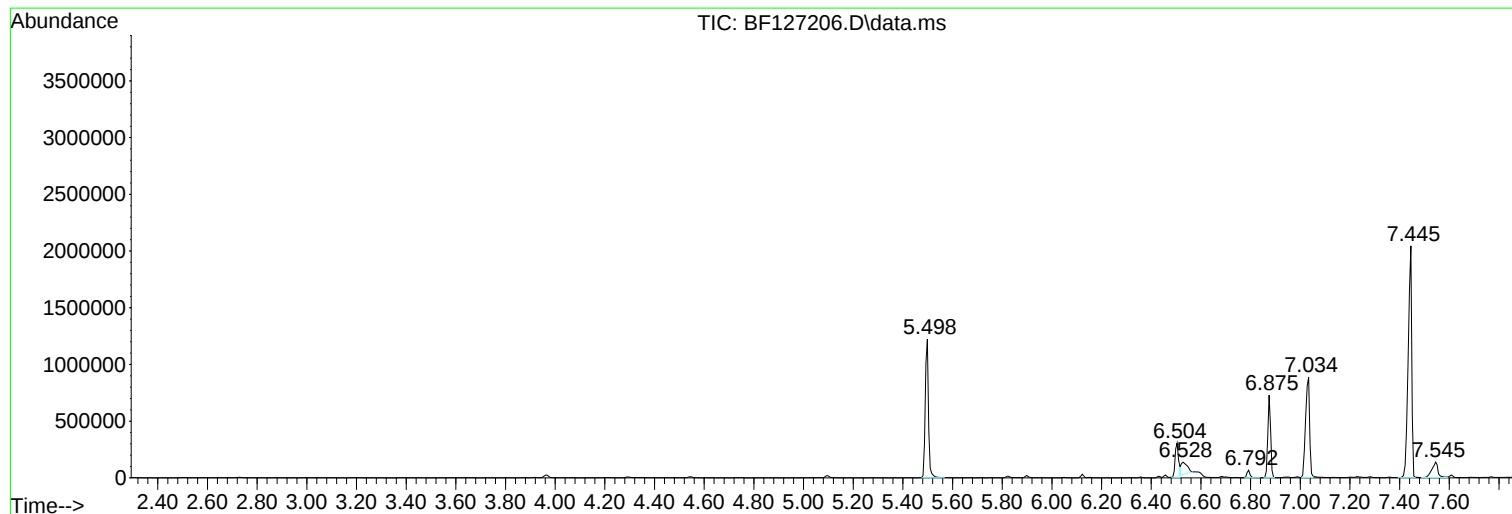
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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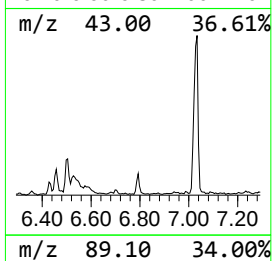
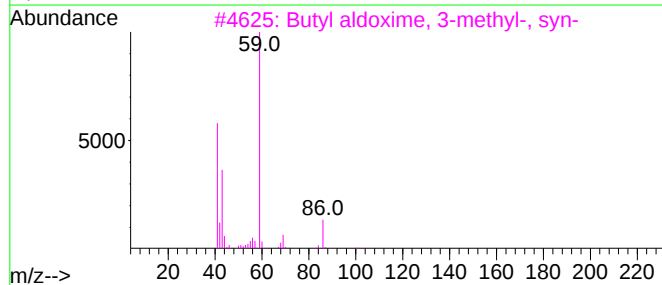
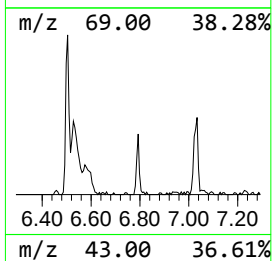
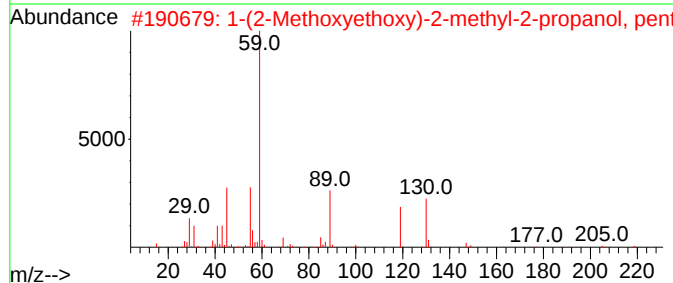
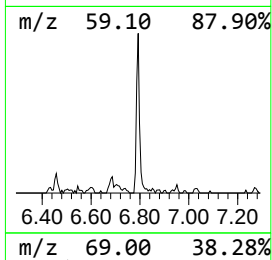
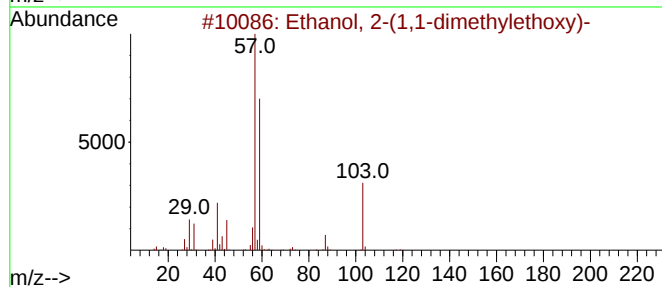
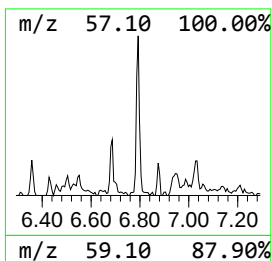
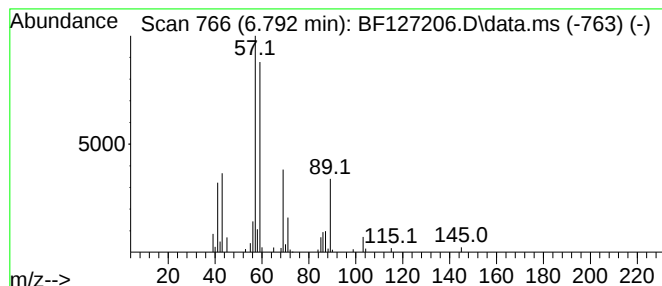
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(1,1-dimethyleth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.792	2.01 ng	58013	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(1,1-dimethylethoxy)-	118	C6H14O2	007580-85-0	53
2			1-(2-Methoxyethoxy)-2-methyl-2-p...	294	C10H15F5O4	1000364-25-8	47
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	43
4			1-Butanol, 3-methoxy-, acetate	146	C7H14O3	004435-53-4	43
5			2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	43



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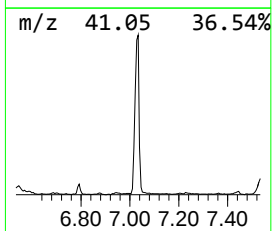
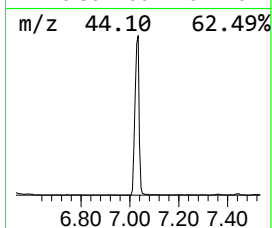
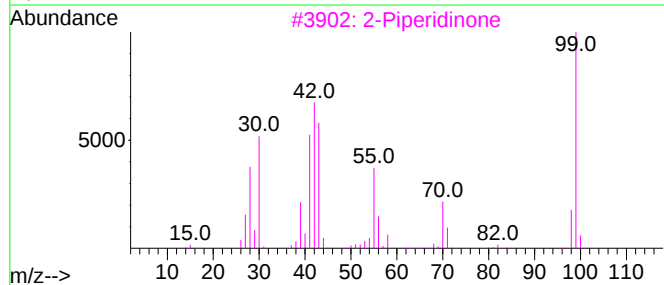
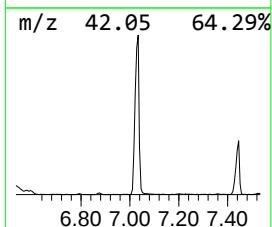
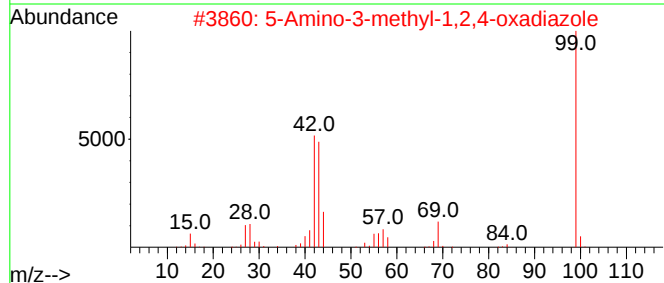
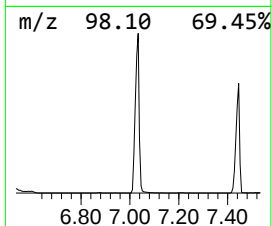
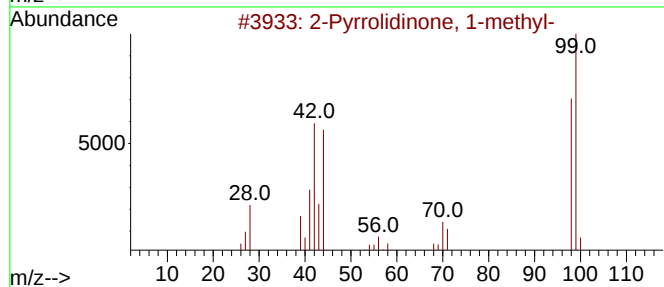
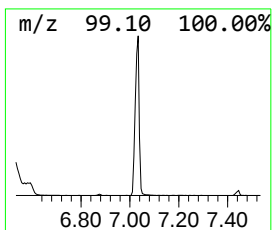
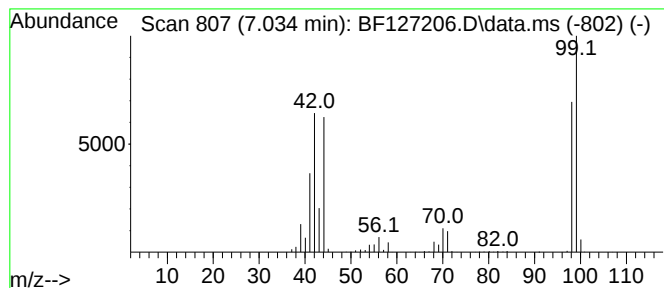
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pyrrolidinone, 1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.034	34.78 ng	1004480	1,4-Dichlorobenzene-d4	6.875

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	95
2		5-Amino-3-methyl-1,2,4-oxadiazole	99	C3H5N3O	003663-39-6	43
3		2-Piperidinone	99	C5H9NO	000675-20-7	37
4		5-Aminopentanamide	116	C5H12N2O	013023-70-6	33
5		5-.alpha.-Aminoethyltetrazole	113	C3H7N5	1000227-36-7	25



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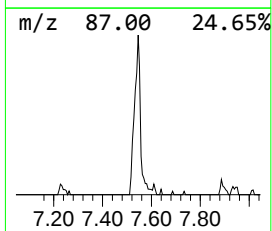
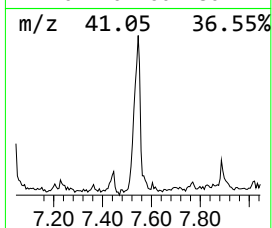
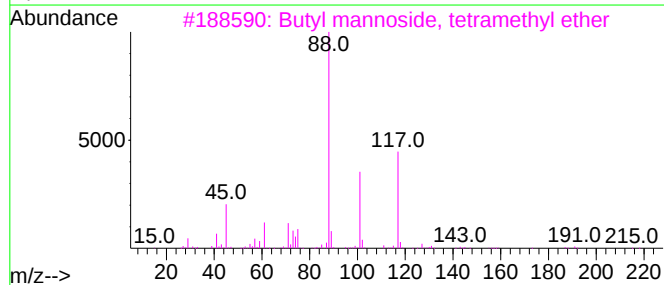
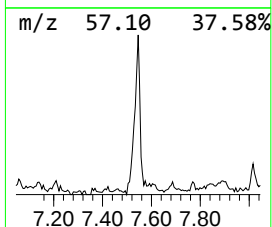
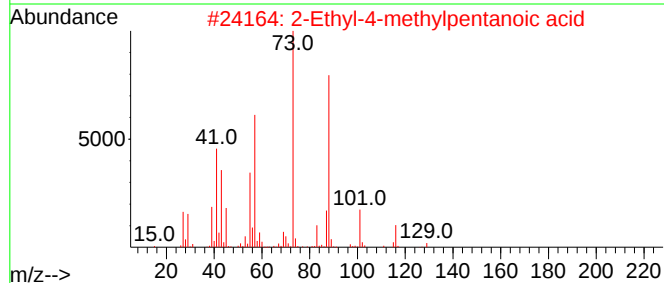
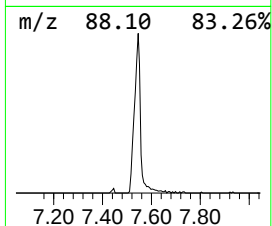
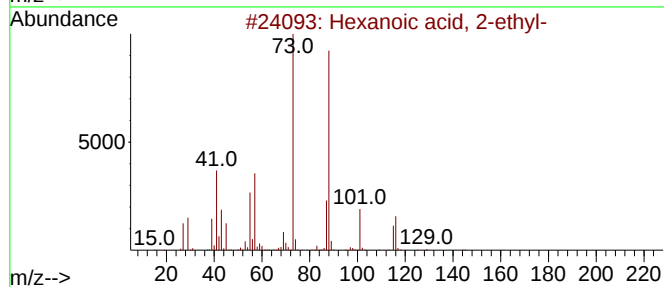
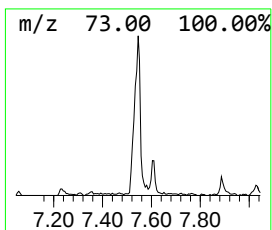
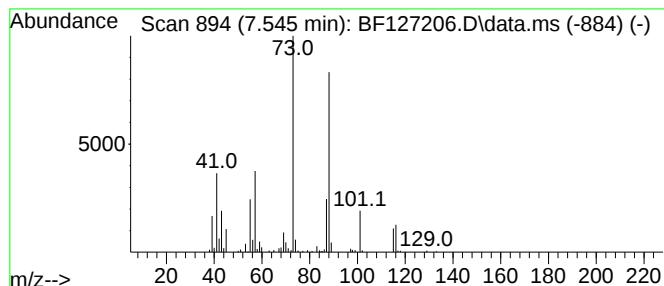
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.545	6.17 ng	234206	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	72
3			Butyl mannoside, tetramethyl ether	292	C14H28O6	1000501-84-1	50
4			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
5			Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	40



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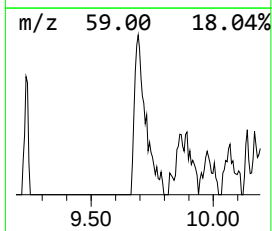
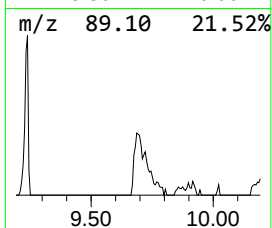
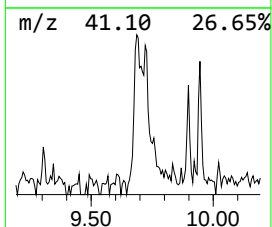
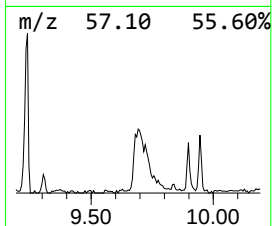
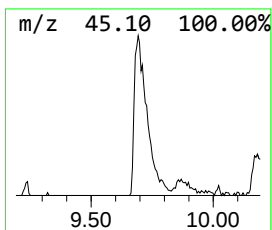
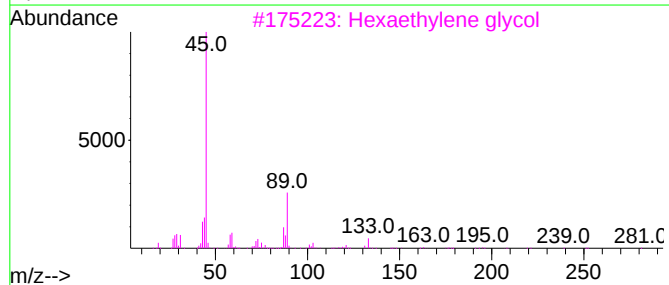
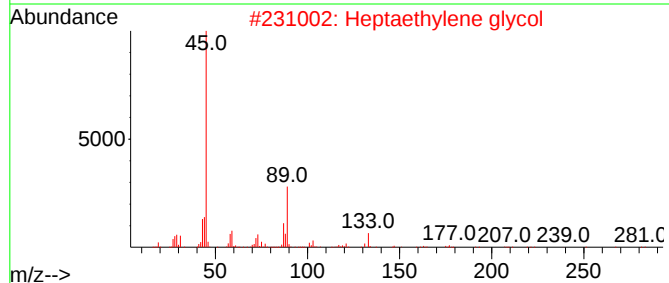
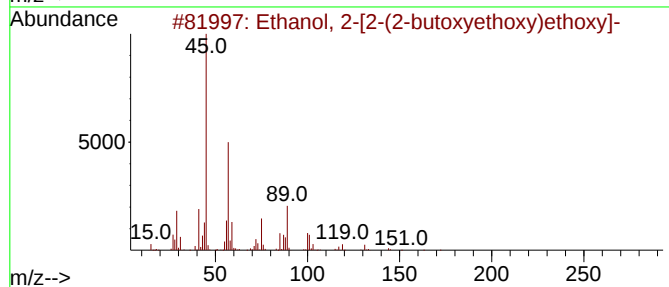
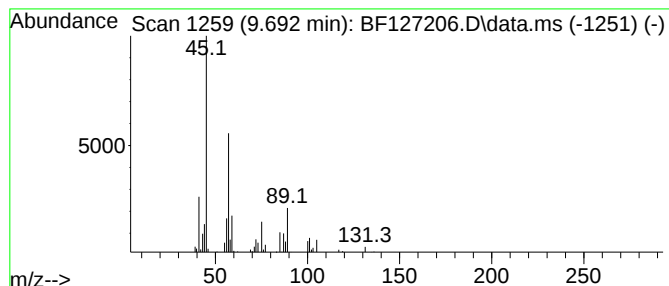
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.692	2.51 ng	111646	Acenaphthene-d10		9.916	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Ethanol, 2-[2-(2-butoxyethoxy)et...		206	C10H22O4	000143-22-6	91
2	Heptaethylene glycol		326	C14H30O8	005617-32-3	59
3	Hexaethylene glycol		282	C12H26O7	002615-15-8	59
4	2-[2-[2-[2-[2-[2-(2-Hydroxyet...		370	C16H34O9	005117-19-1	59
5	Ethanol, 2-(2-butoxyethoxy)-		162	C8H18O3	000112-34-5	59



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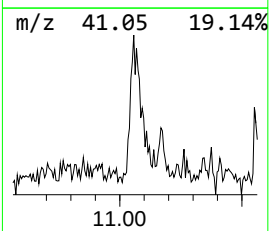
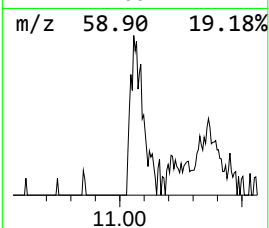
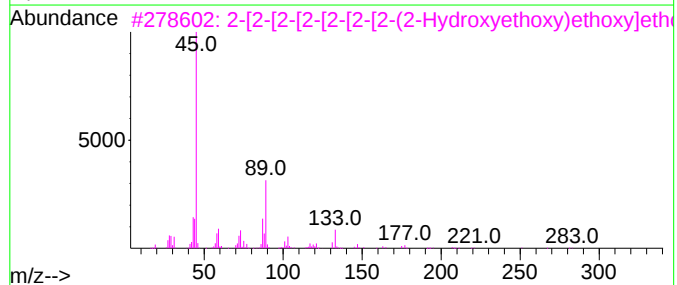
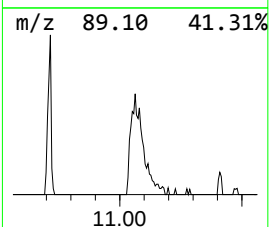
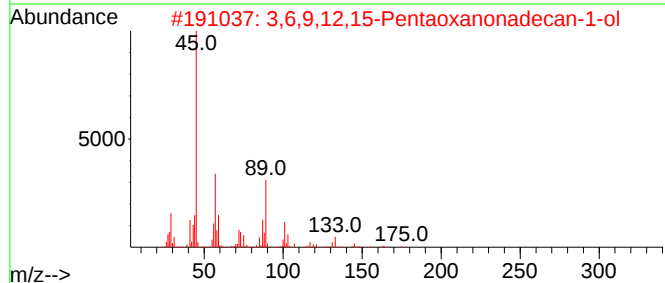
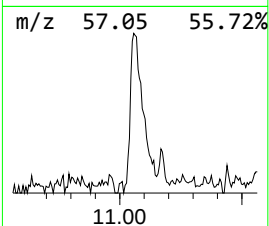
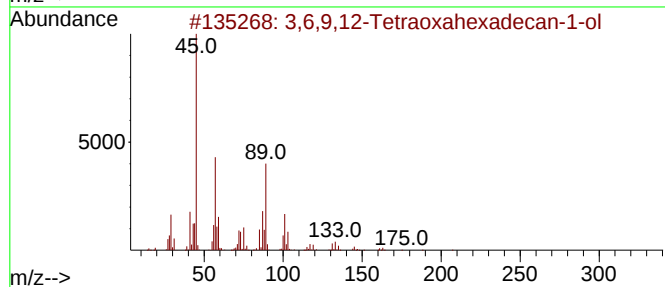
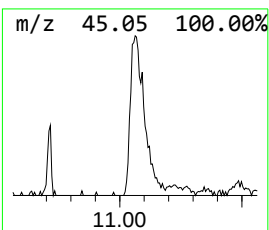
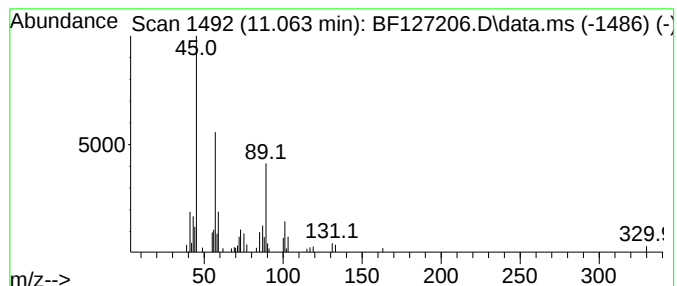
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 3,6,9,12-Tetraoxahexadecan-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.063	2.56 ng	114349	Phenanthrene-d10		11.410	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3,6,9,12-Tetraoxahexadecan-1-ol		250	C12H26O5	001559-34-8	87
2	3,6,9,12,15-Pentaoxanonadecan-1-ol		294	C14H30O6	001786-94-3	83
3	2-[2-[2-[2-[2-[2-(2-Hydroxyet...		370	C16H34O9	005117-19-1	64
4	Pentaethylene glycol		238	C10H22O6	004792-15-8	59
5	Hexaethylene glycol		282	C12H26O7	002615-15-8	59



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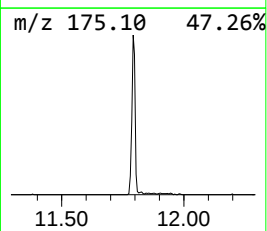
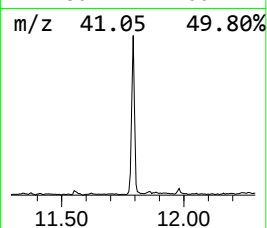
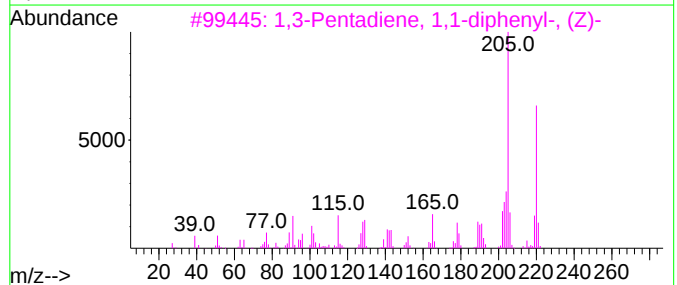
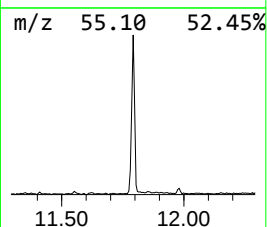
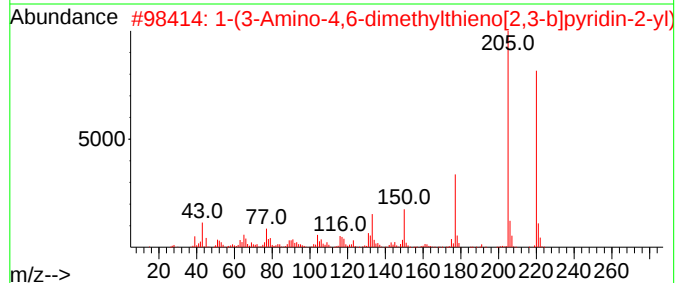
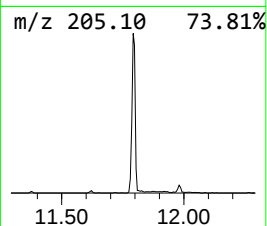
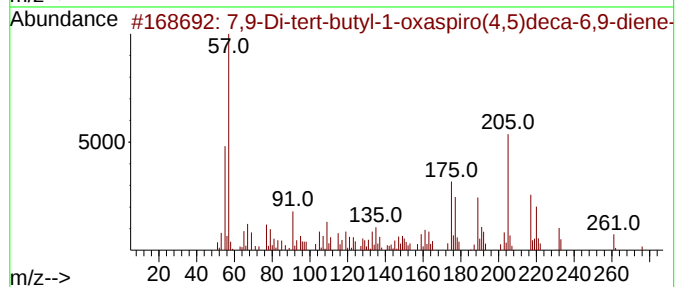
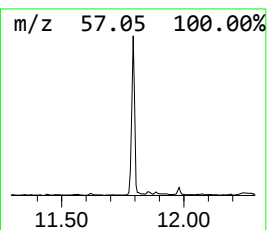
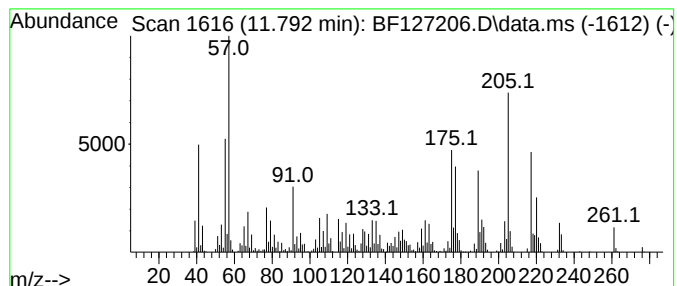
Instrument :
BNA_F
ClientSampleId :
SB-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.792	23.13 ng	1032890	Phenanthrene-d10	11.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	55
3	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	50
4	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	50
5	2-Phenazinecarbonitrile	205	C13H7N3	006479-93-2	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127206.D
Acq On : 04 Mar 2022 17:45
Operator : CG\JU
Sample : N1793-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3

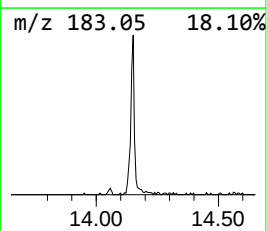
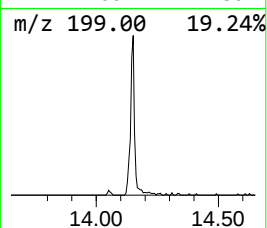
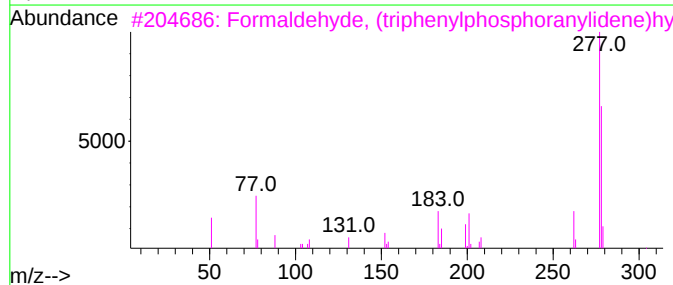
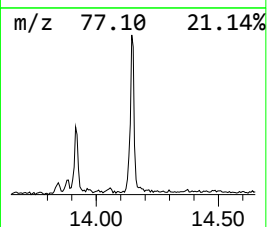
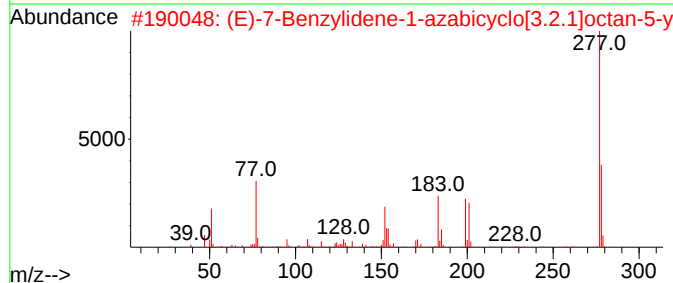
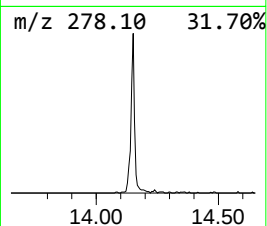
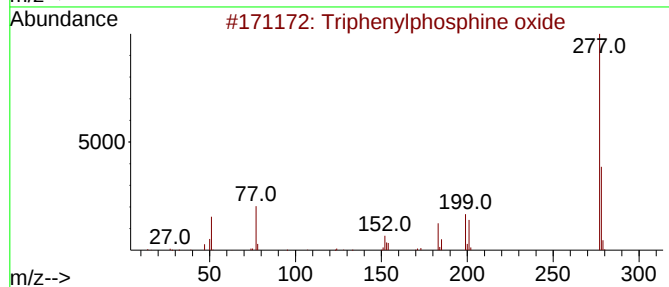
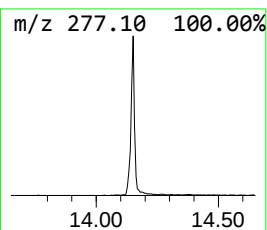
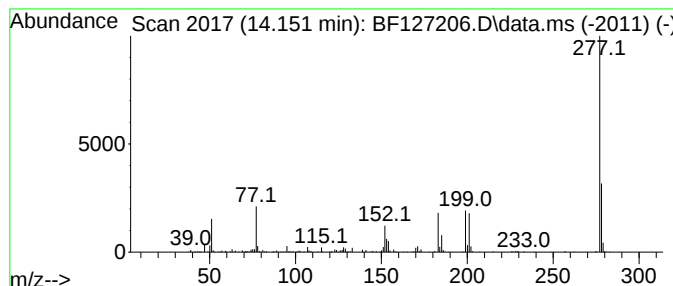
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	9.55 ng	342681	Chrysene-d12	14.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127206.D
Acq On : 04 Mar 2022 17:45
Operator : CG\JU
Sample : N1793-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

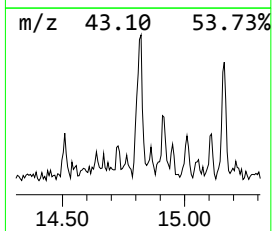
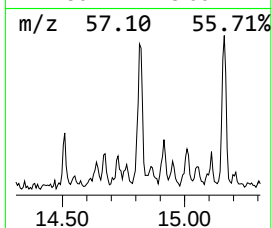
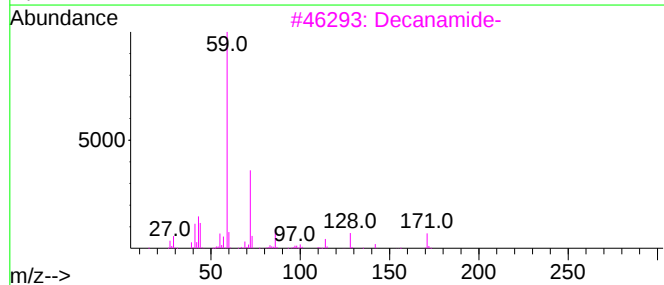
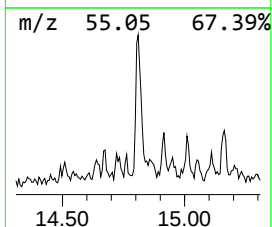
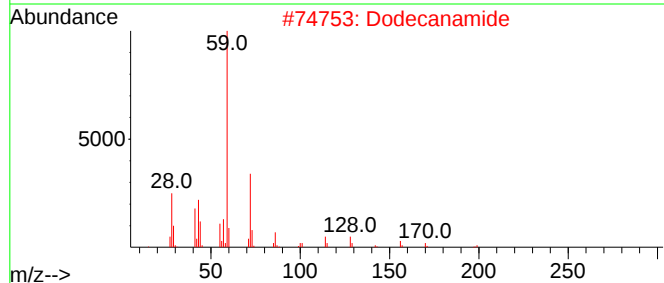
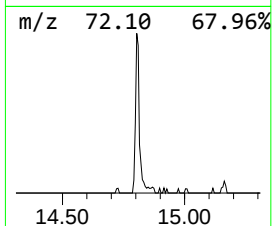
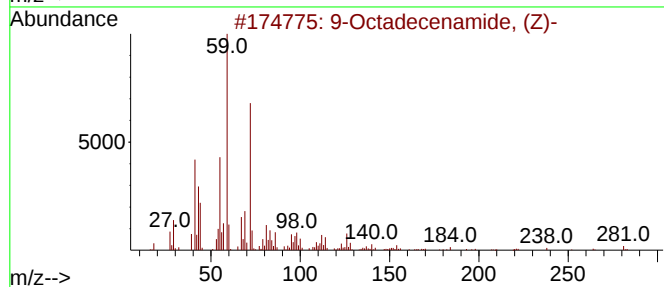
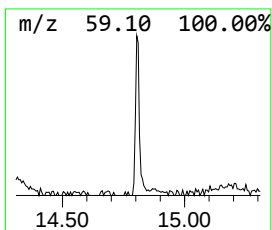
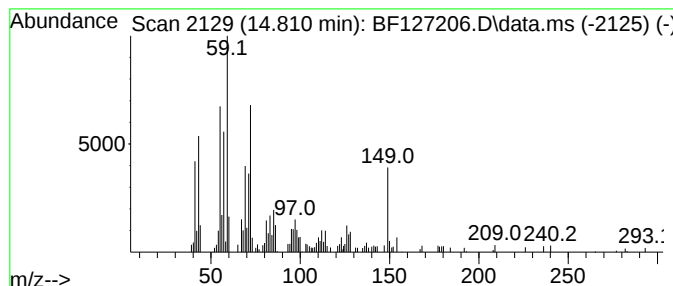
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.810	4.14 ng	135886	Perylene-d12	15.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	58
2	Dodecanamide	199	C12H25NO	001120-16-7	47
3	Decanamide-	171	C10H21NO	002319-29-1	38
4	Octadecanamide	283	C18H37NO	000124-26-5	35
5	3-Tetradecanol	214	C14H30O	001653-32-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127206.D
Acq On : 04 Mar 2022 17:45
Operator : CG\JU
Sample : N1793-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3

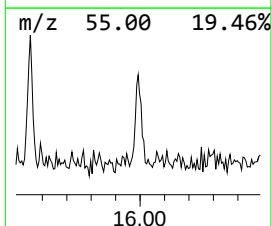
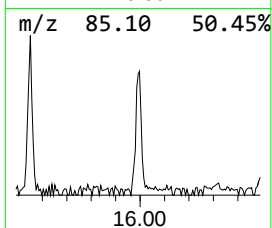
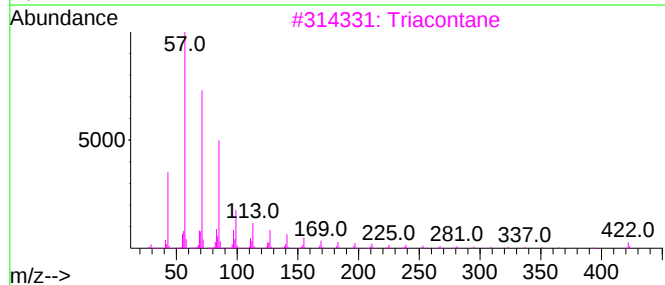
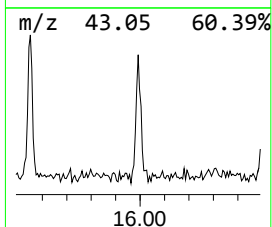
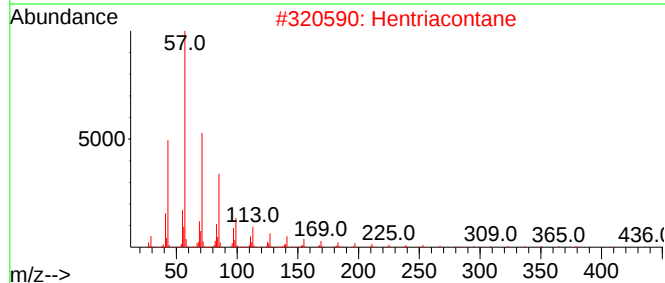
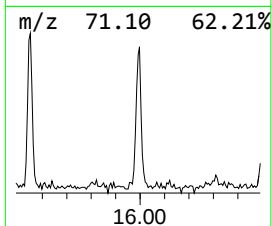
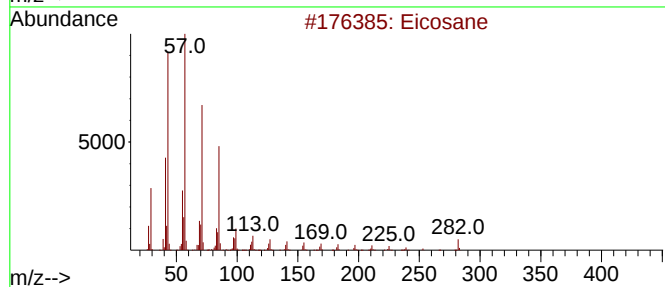
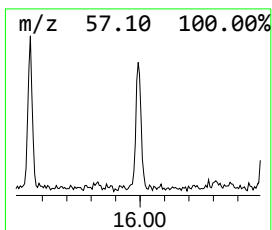
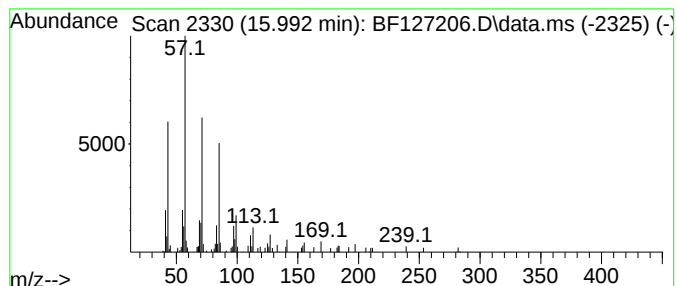
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	2.06 ng	67740	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Hentriacontane	437	C31H64	000630-04-6	91
3			Triacontane	422	C30H62	000638-68-6	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127206.D
Acq On : 04 Mar 2022 17:45
Operator : CG\JU
Sample : N1793-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

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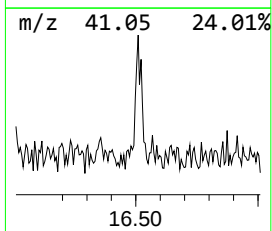
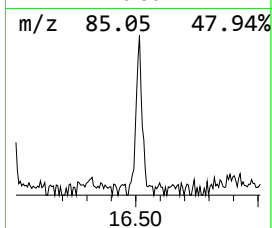
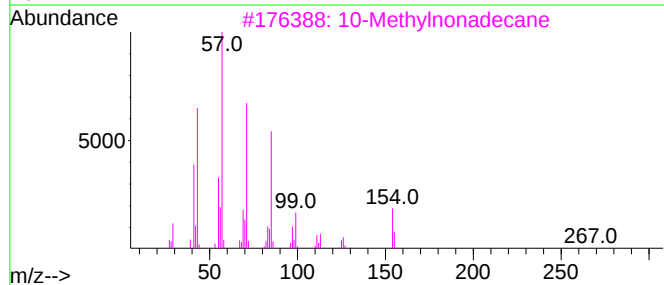
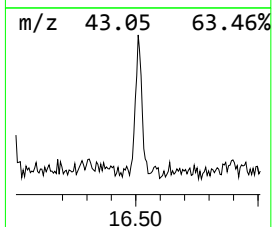
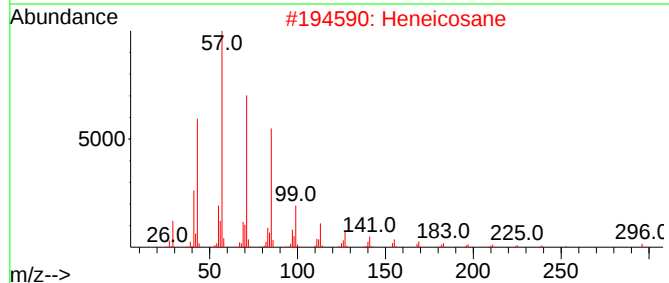
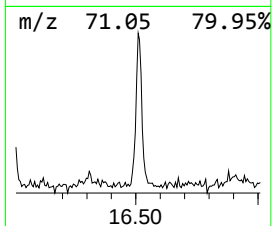
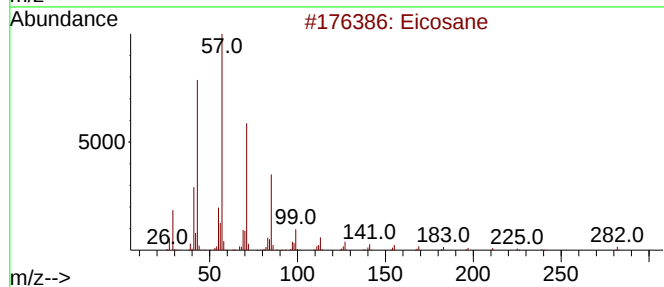
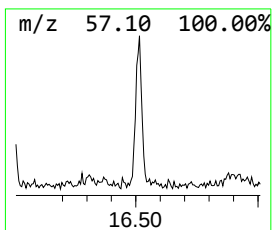
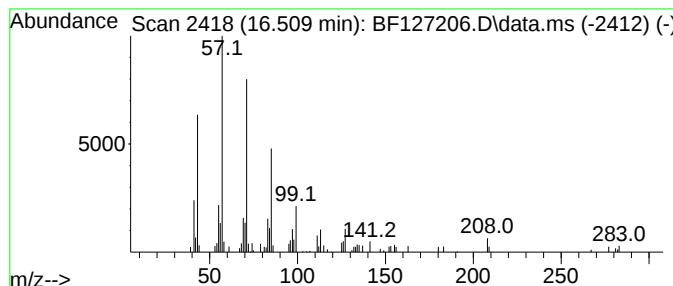
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.509	2.03 ng	66720	Perylene-d12	15.545

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		10-Methylnonadecane	282	C20H42	056862-62-5	90
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
5		Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030422\
Data File : BF127206.D
Acq On : 04 Mar 2022 17:45
Operator : CG\JU
Sample : N1793-09
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021622.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
Ethanol, 2-(1,1...	6.792	2.0	ng	58013	1	6.875	577569	20.0
2-Pyrrolidinone...	7.034	34.8	ng	1004480	1	6.875	577569	20.0
Hexanoic acid, ...	7.545	6.2	ng	234206	2	8.157	759120	20.0
Ethanol, 2-[2-(...	9.692	2.5	ng	111646	3	9.916	890483	20.0
3,6,9,12-Tetrao...	11.063	2.6	ng	114349	4	11.410	893127	20.0
7,9-Di-tert-but...	11.792	23.1	ng	1032890	4	11.410	893127	20.0
Triphenylphosph...	14.151	9.6	ng	342681	5	14.057	717427	20.0
9-Octadecenamid...	14.810	4.1	ng	135886	6	15.545	656283	20.0
Eicosane	15.992	2.1	ng	67740	6	15.545	656283	20.0
Heneicosane	16.509	2.0	ng	66720	6	15.545	656283	20.0