

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
 Data File : BF131158.D
 Acq On : 11 Nov 2022 17:34
 Operator : CG\JU
 Sample : PB148951BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB148951BL

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-BF110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131158.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	10	20	29	rVB	99480	152175	5.69%	0.835%
2	2.316	32	39	45	rBV	44984	58275	2.18%	0.320%
3	5.110	509	514	524	rVB	243818	342559	12.81%	1.881%
4	5.498	575	580	583	rBV	2526805	2499575	93.45%	13.723%
5	6.504	745	751	754	rBV	2377444	2495886	93.31%	13.702%
6	6.869	809	813	817	rBV	684259	542987	20.30%	2.981%
7	7.440	904	910	913	rBV	1409701	1458722	54.54%	8.008%
8	8.157	1027	1032	1035	rBV	587165	556440	20.80%	3.055%
9	9.234	1209	1215	1218	rBV	2909052	2674709	100.00%	14.684%
10	9.916	1325	1331	1334	rBV	762522	624983	23.37%	3.431%
11	10.710	1460	1466	1469	rBV	1788795	1568012	58.62%	8.608%
12	11.404	1580	1584	1588	rBV	790078	661818	24.74%	3.633%
13	12.998	1850	1855	1858	rBV	2916557	2657310	99.35%	14.588%
14	14.051	2030	2034	2038	rBV	736014	711742	26.61%	3.907%
15	14.145	2045	2050	2056	rBV	77355	83513	3.12%	0.458%
16	14.821	2159	2165	2169	rBV	55622	56911	2.13%	0.312%
17	15.163	2219	2223	2228	rVB	62764	69948	2.62%	0.384%
18	15.545	2283	2288	2294	rVB2	429772	543196	20.31%	2.982%
19	15.998	2360	2365	2372	rVB	66274	104260	3.90%	0.572%
20	16.515	2446	2453	2462	rBV	66540	117920	4.41%	0.647%
21	17.121	2550	2556	2562	rBV2	44117	88218	3.30%	0.484%
22	17.845	2671	2679	2687	rBV2	35557	84411	3.16%	0.463%
23	18.704	2818	2825	2834	rVB4	20521	61550	2.30%	0.338%

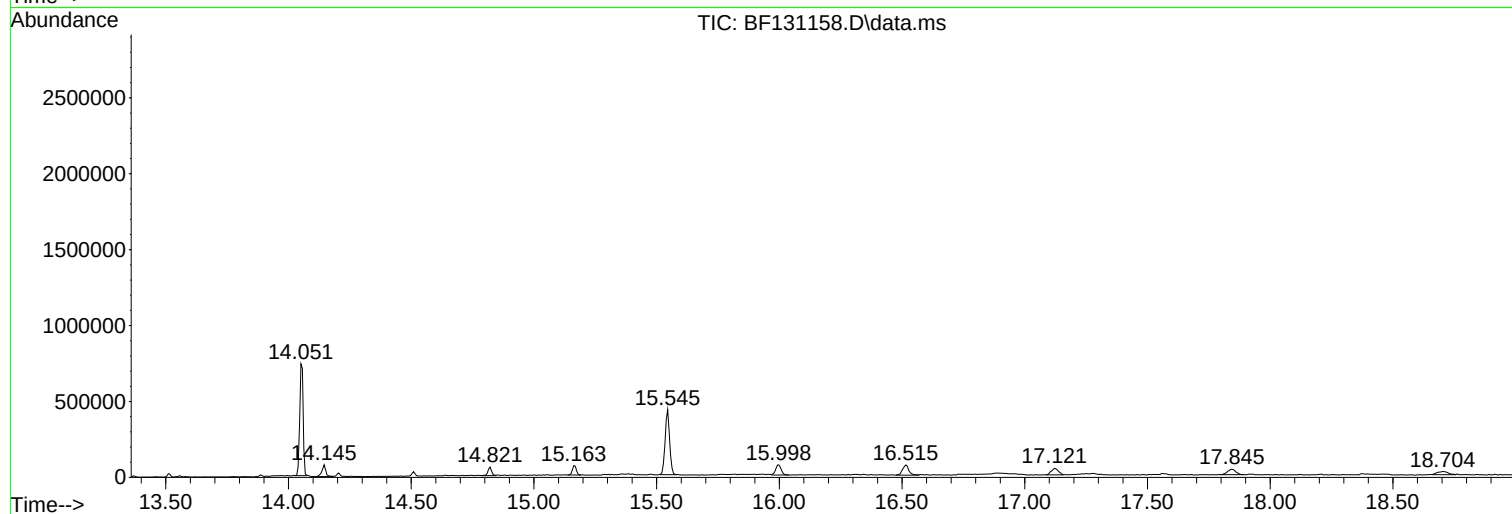
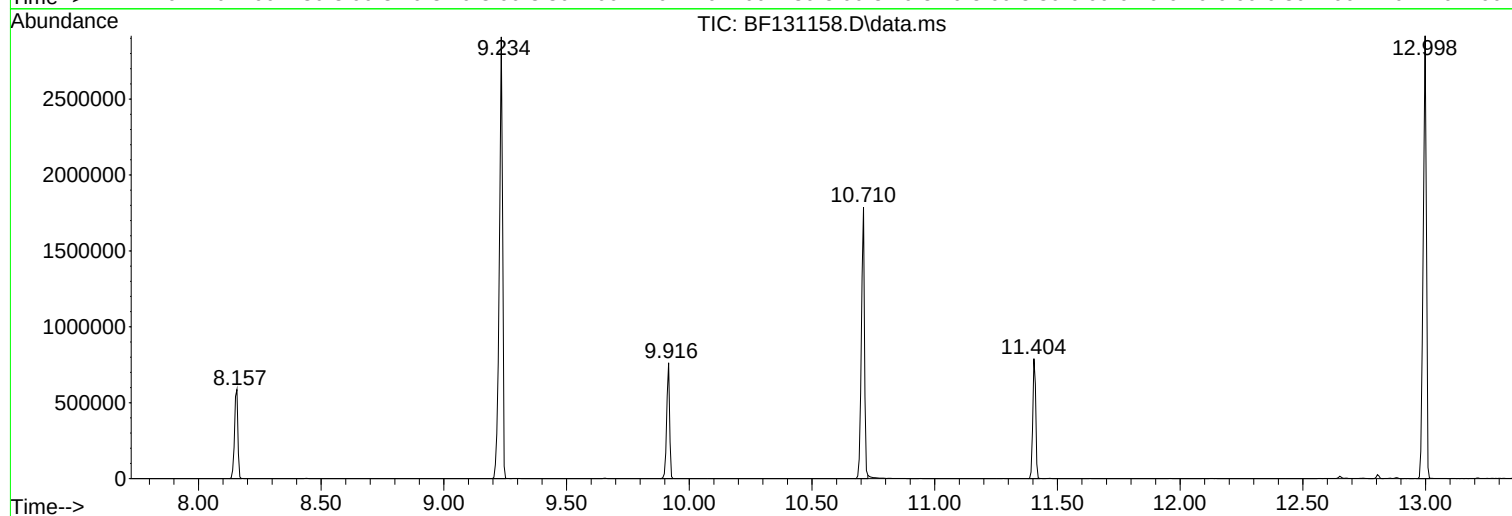
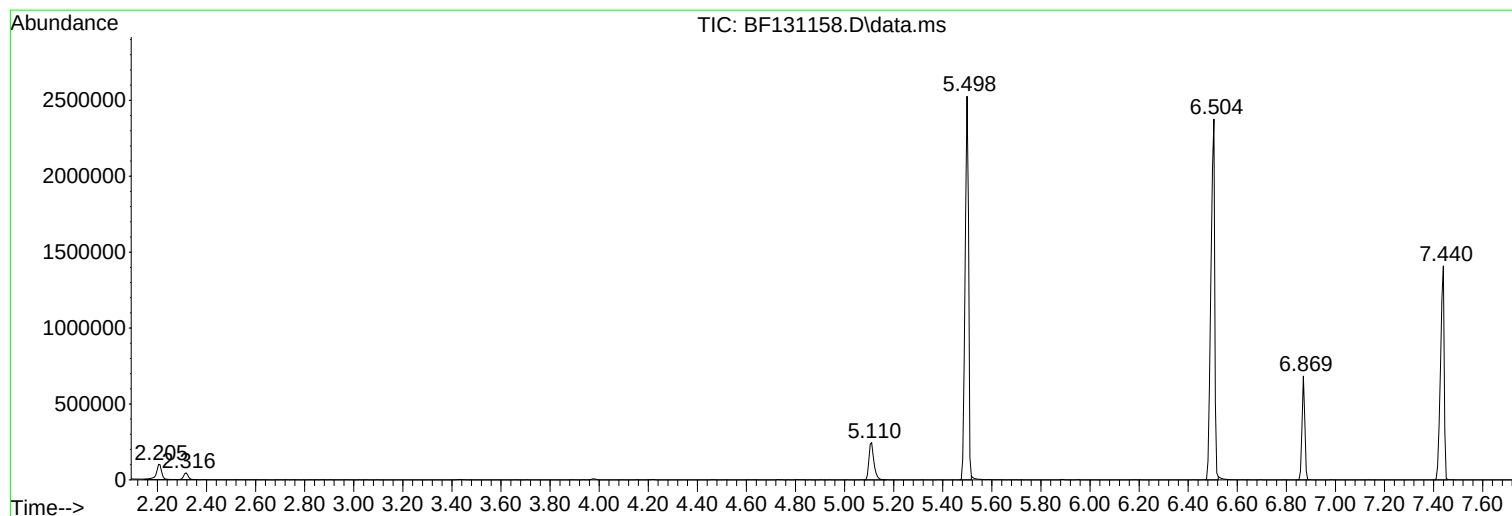
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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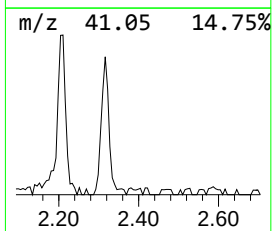
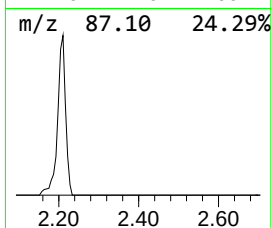
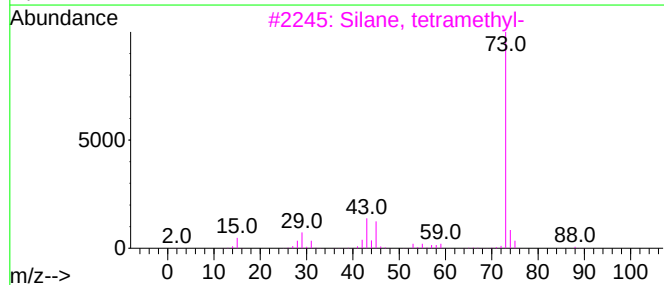
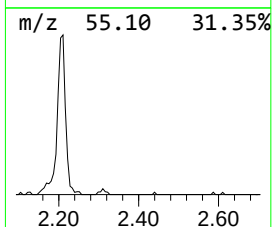
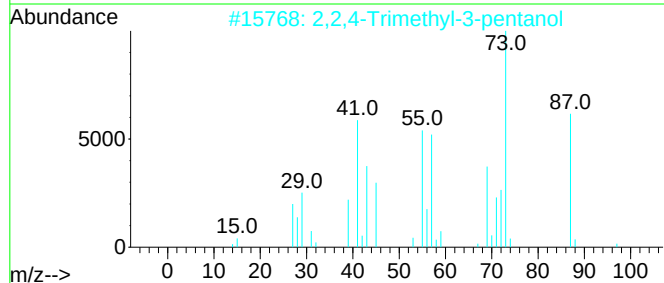
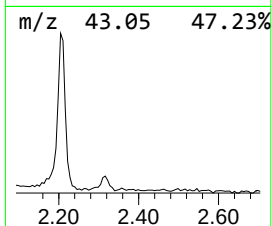
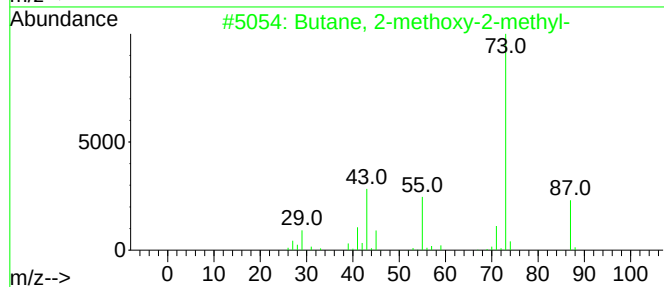
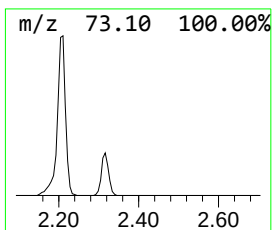
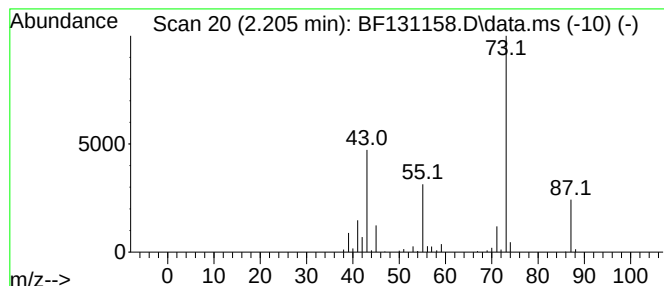
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	5.61 ng	152175	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
5			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9



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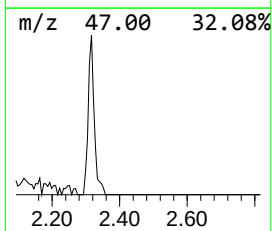
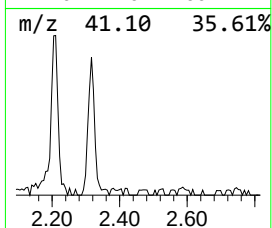
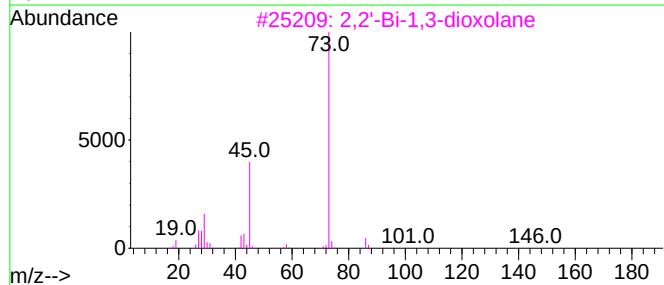
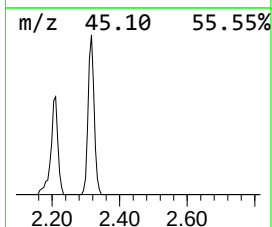
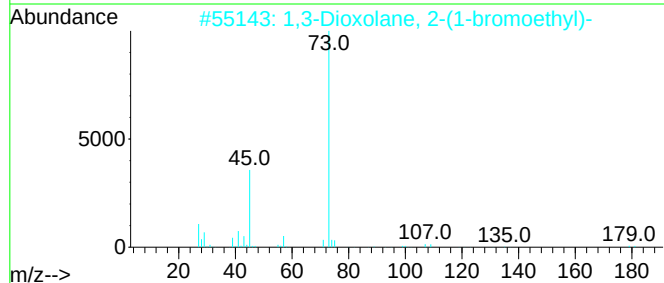
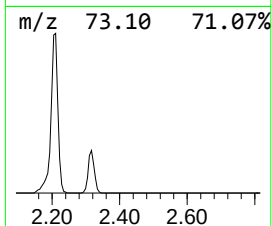
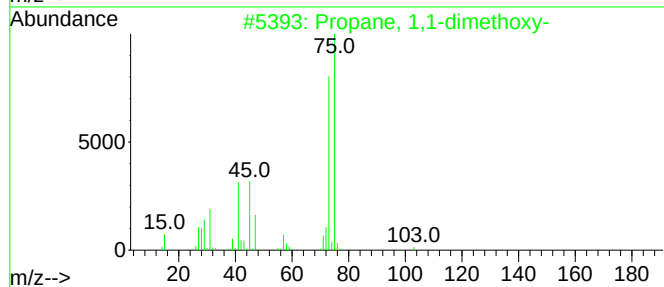
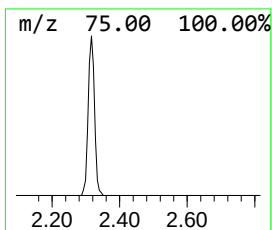
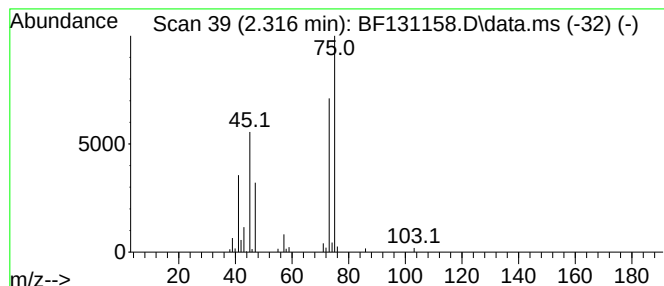
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.316	2.15 ng	58275	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	22
3			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	12
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	10
5			3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	10



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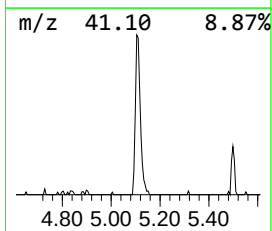
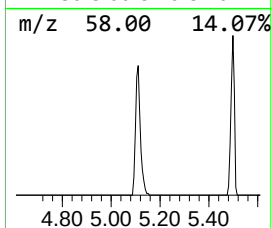
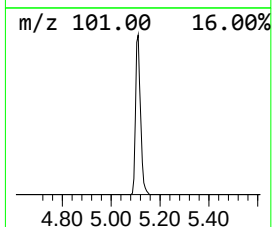
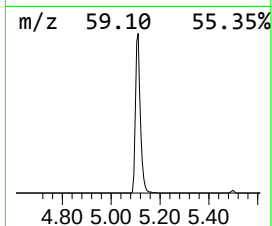
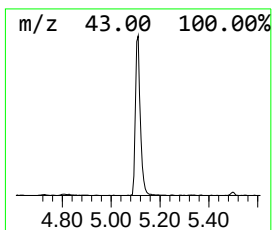
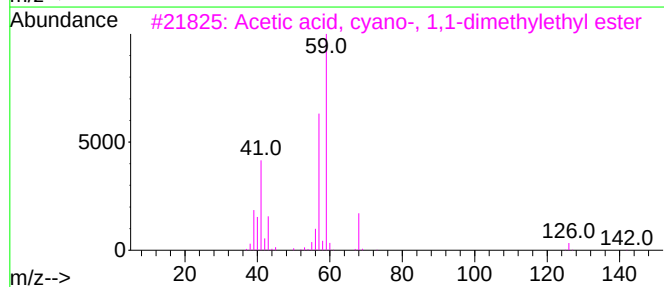
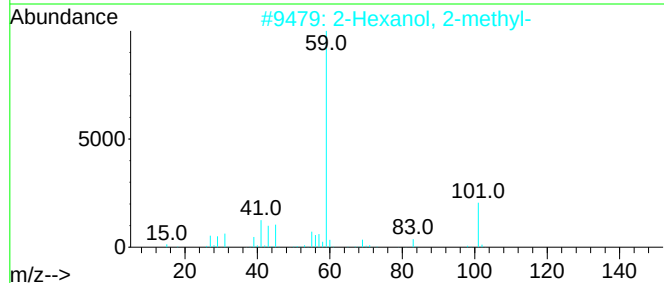
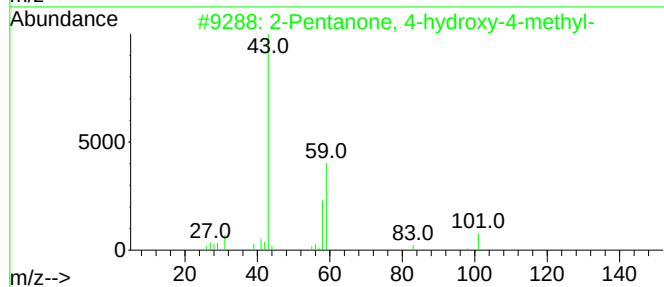
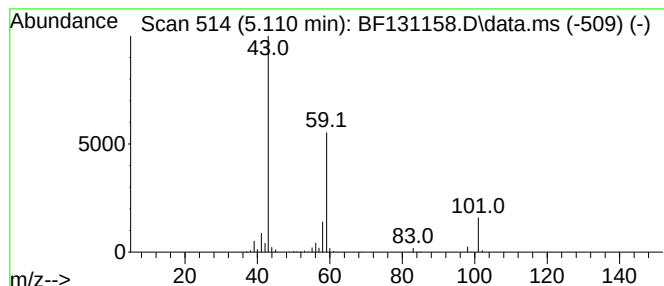
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.110	12.62 ng	342559	1,4-Dichlorobenzene-d4	6.869	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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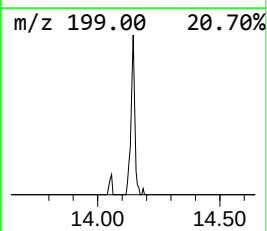
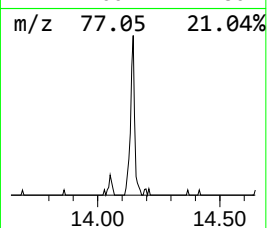
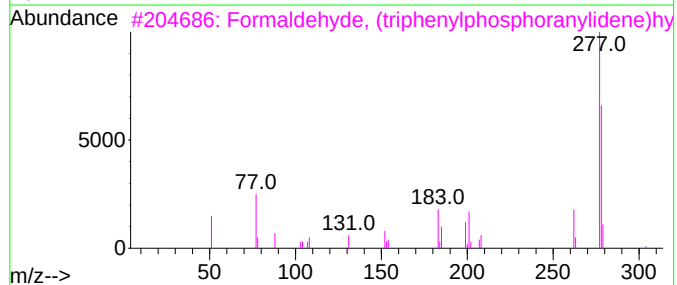
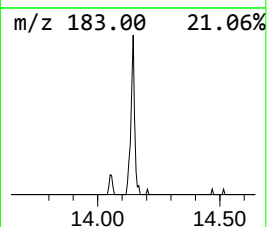
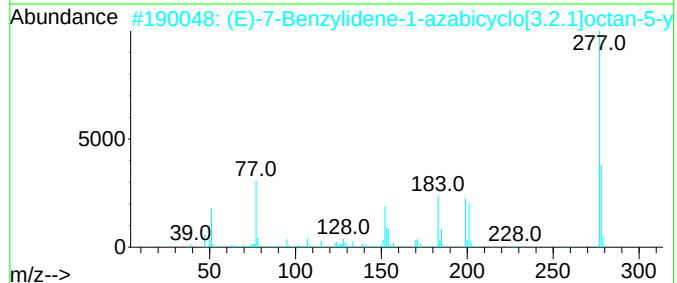
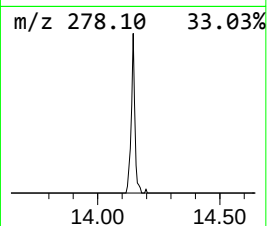
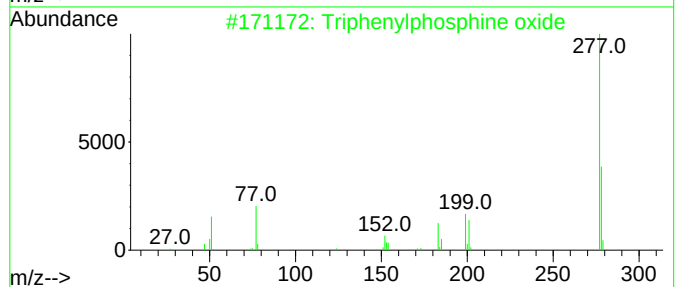
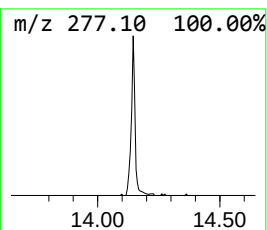
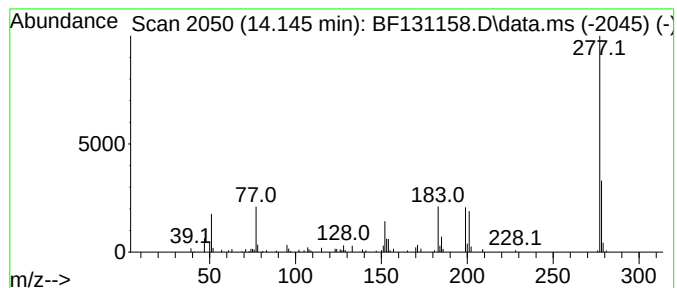
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.145	2.35 ng	83513	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	25



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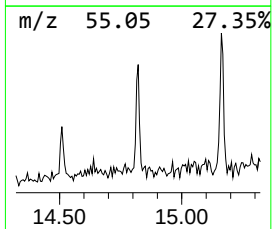
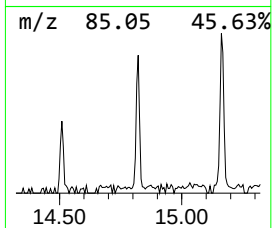
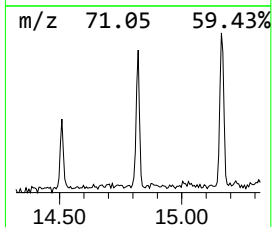
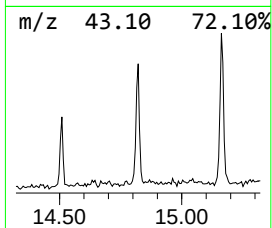
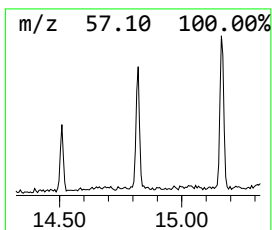
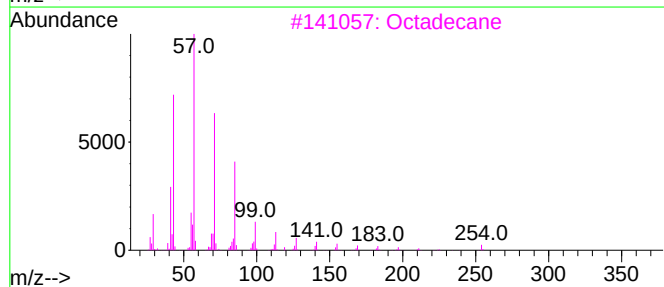
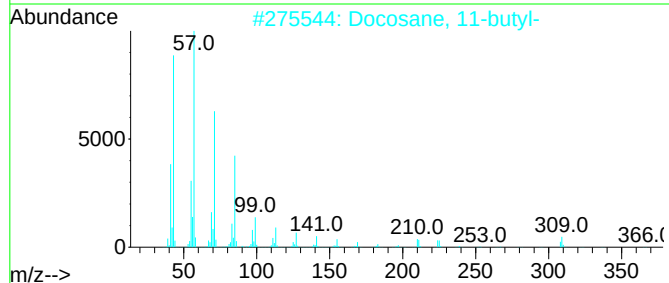
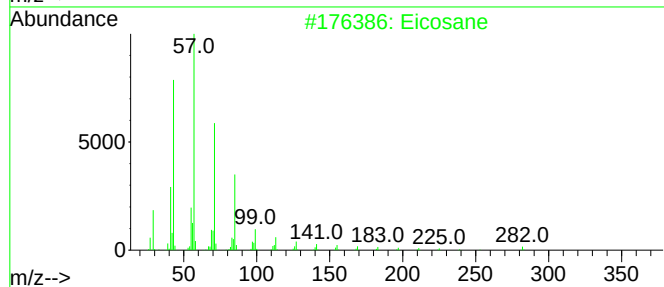
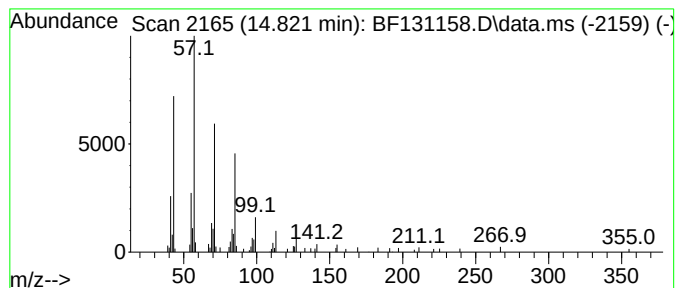
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.10 ng	56911	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Docosane, 11-butyl-	366	C26H54	013475-76-8	91
3			Octadecane	254	C18H38	000593-45-3	91
4			Heptadecane	240	C17H36	000629-78-7	91
5			Docosane	310	C22H46	000629-97-0	91



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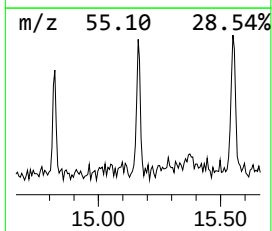
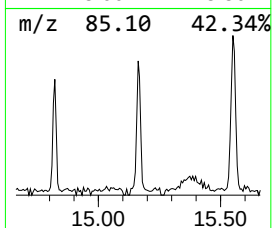
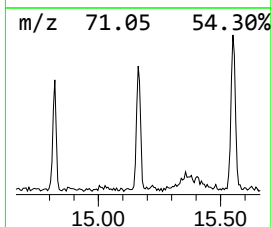
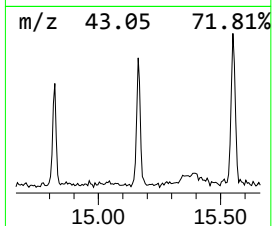
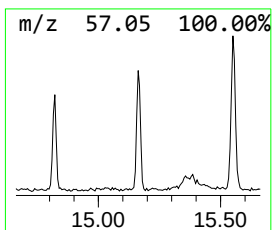
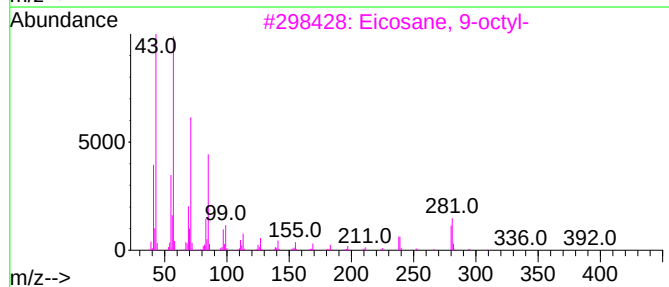
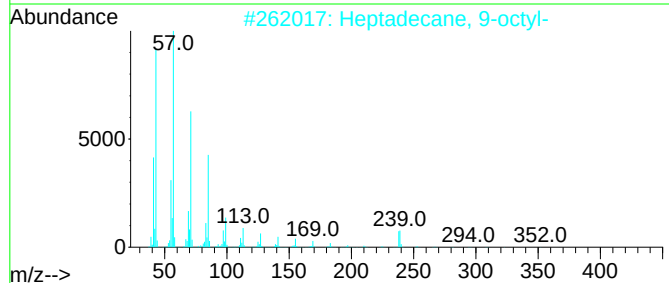
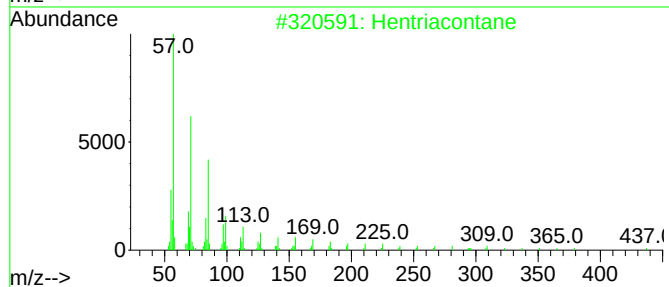
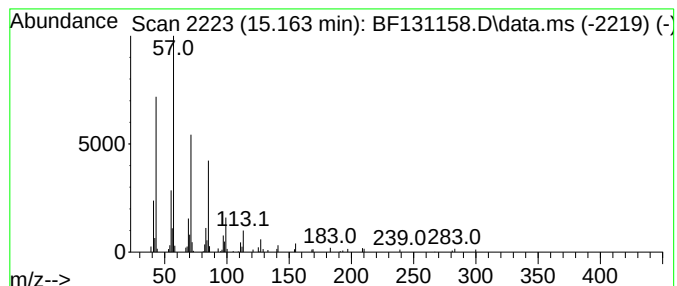
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hentriacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	2.58 ng	69948	Perylene-d12	15.545

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hentriacontane	437	C31H64	000630-04-6	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Eicosane, 9-octyl-	394	C28H58	013475-77-9	91
4		Pentacosane	352	C25H52	000629-99-2	90
5		Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131158.D
Acq On : 11 Nov 2022 17:34
Operator : CG\JU
Sample : PB148951BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148951BL

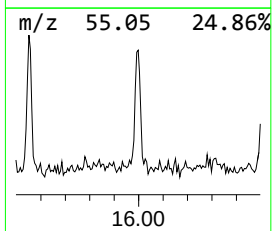
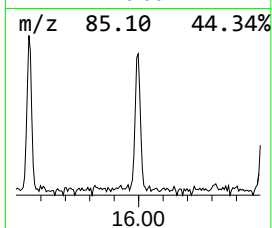
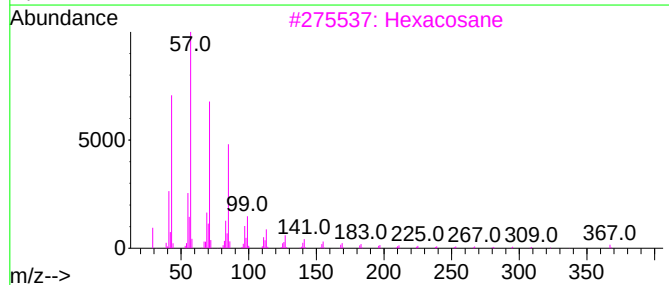
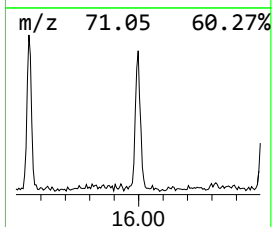
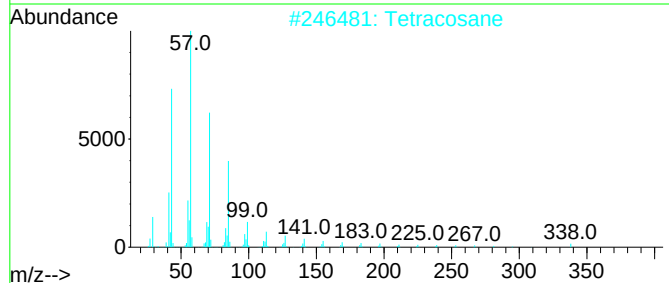
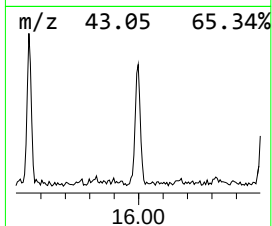
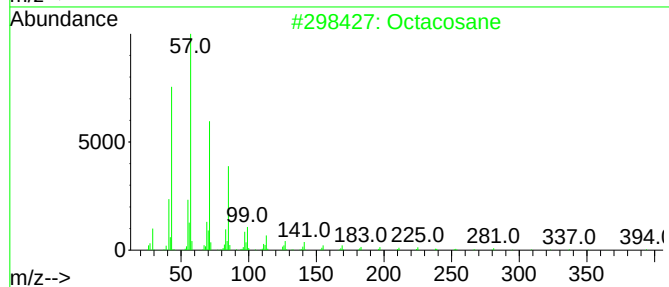
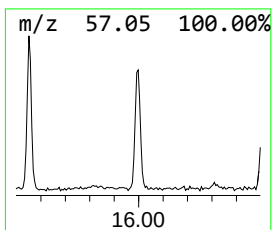
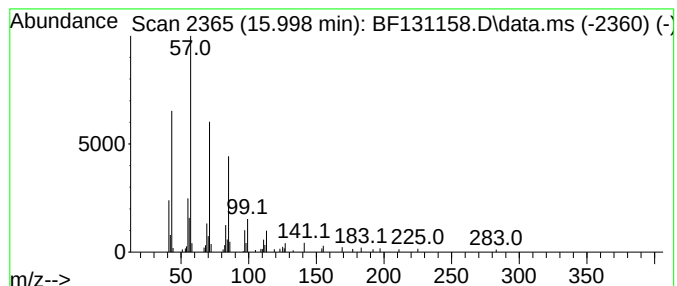
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.998	3.84 ng	104260	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Hexacosane	366	C26H54	000630-01-3	90
4			Octadecane	254	C18H38	000593-45-3	90
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131158.D
Acq On : 11 Nov 2022 17:34
Operator : CG\JU
Sample : PB148951BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

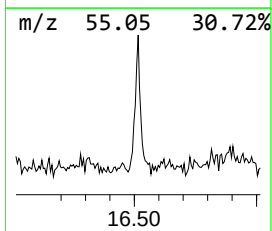
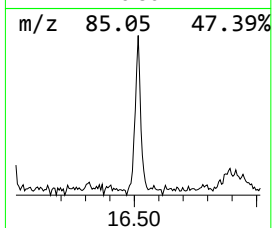
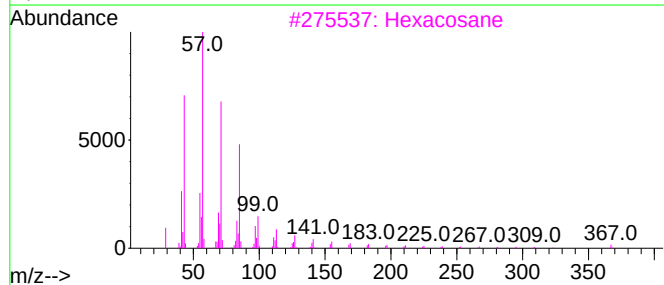
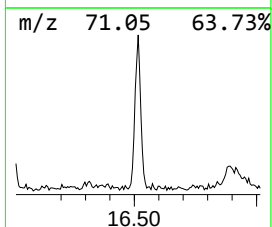
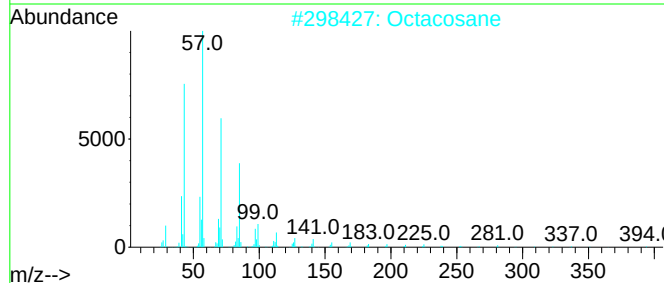
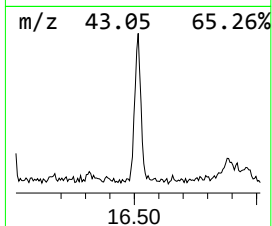
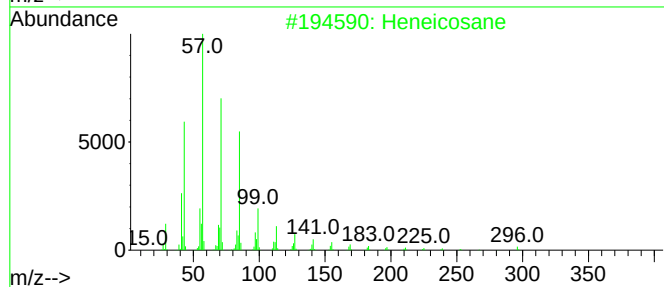
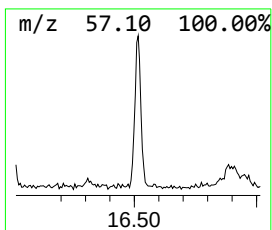
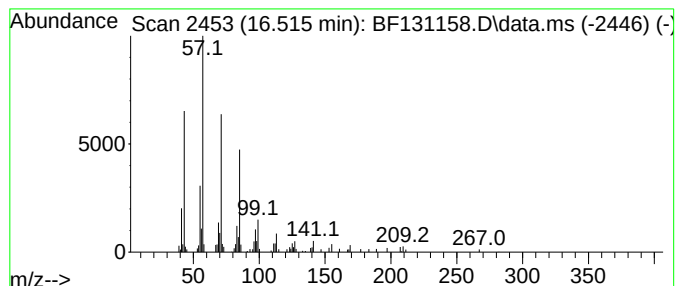
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.515	4.34 ng	117920	Perylene-d12	15.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Octadecane	254	C18H38	000593-45-3	87
5	Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131158.D
Acq On : 11 Nov 2022 17:34
Operator : CG\JU
Sample : PB148951BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148951BL

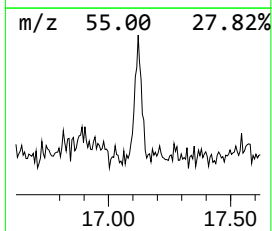
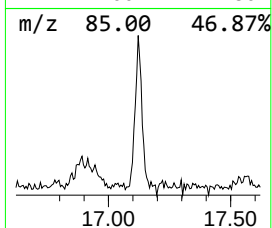
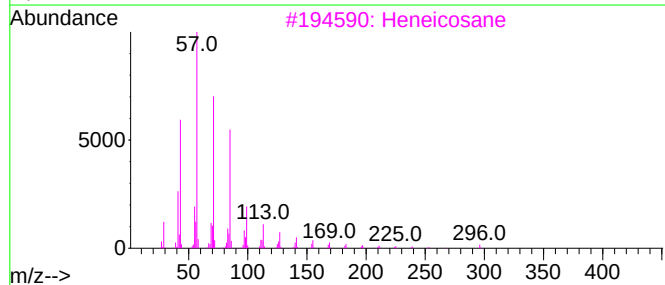
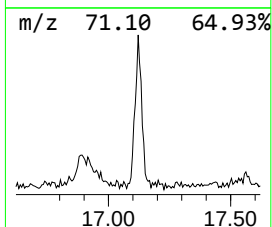
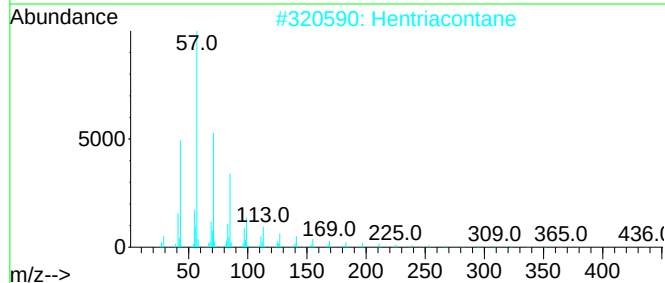
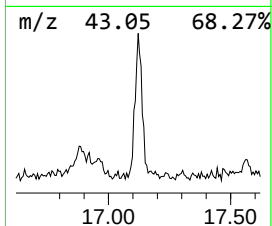
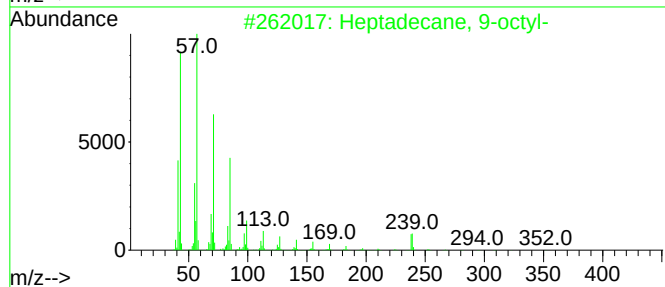
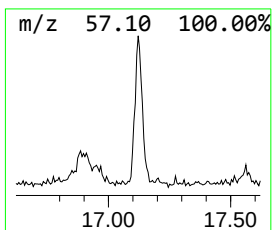
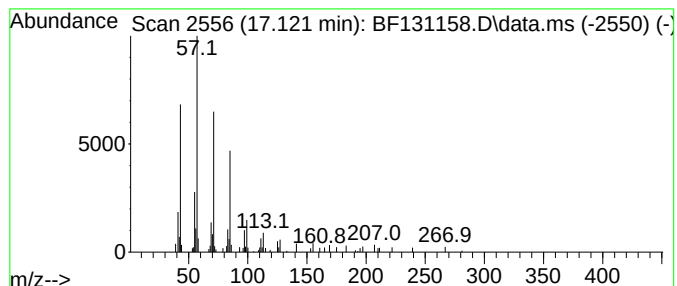
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.121	3.25 ng	88218	Perylene-d12	15.545

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2		Hentriacontane	437	C31H64	000630-04-6	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		Octacosane	394	C28H58	000630-02-4	87
5		Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131158.D
Acq On : 11 Nov 2022 17:34
Operator : CG\JU
Sample : PB148951BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

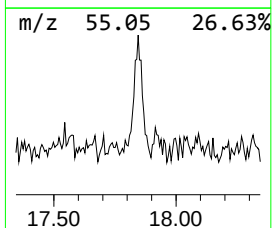
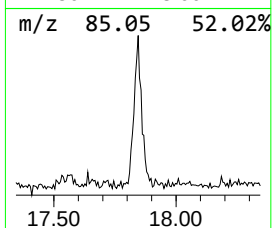
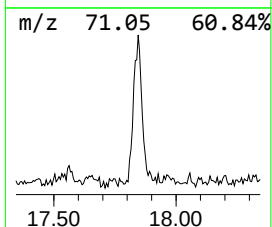
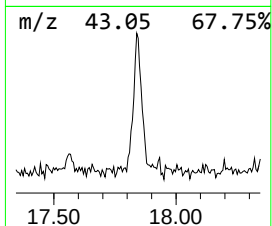
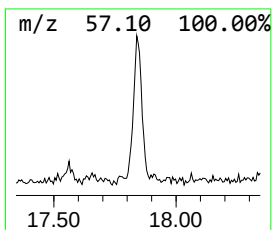
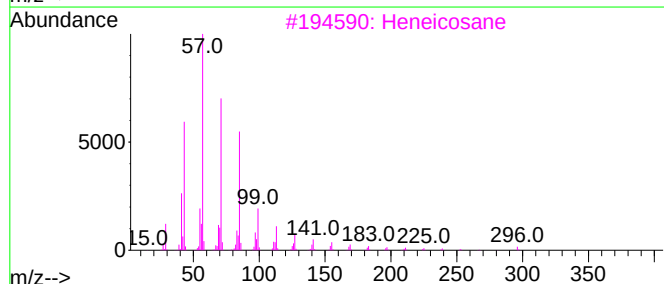
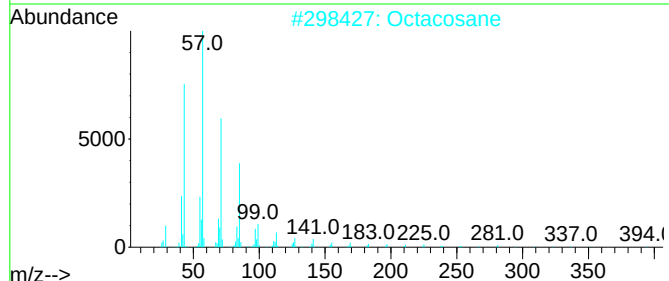
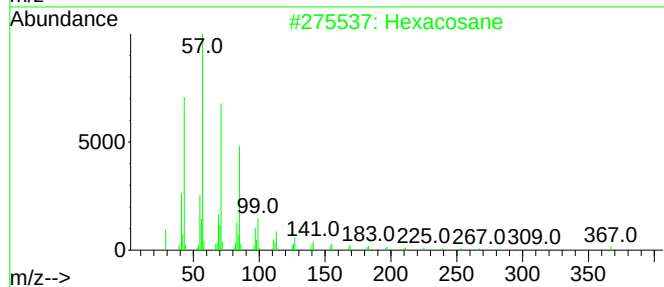
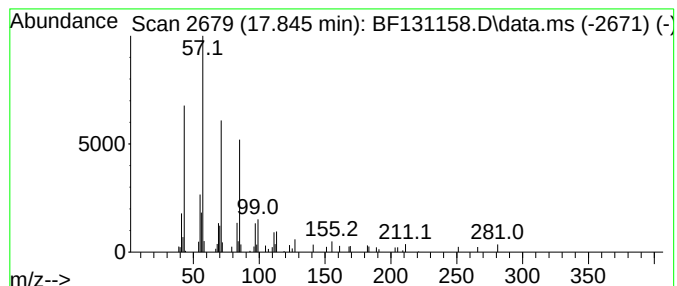
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.845	3.11 ng	84411	Perylene-d12		15.545	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	87
2	Octacosane		394	C28H58	000630-02-4	83
3	Heneicosane		296	C21H44	000629-94-7	83
4	Sulfurous acid, pentadecyl 2-pro...		334	C18H38O3S	1000309-12-6	80
5	Tetratetracontane		619	C44H90	007098-22-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131158.D
Acq On : 11 Nov 2022 17:34
Operator : CG\JU
Sample : PB148951BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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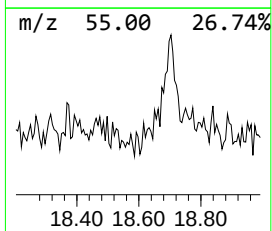
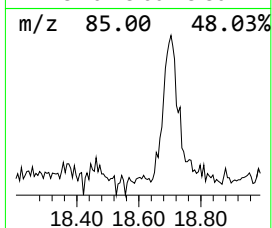
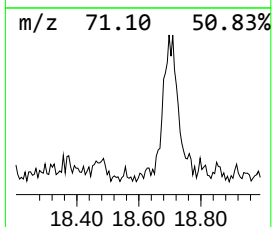
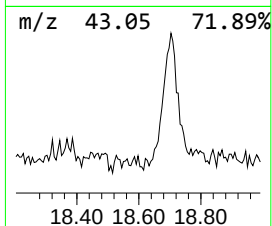
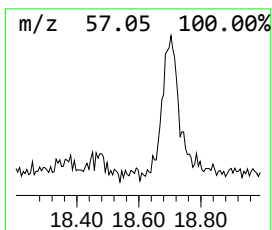
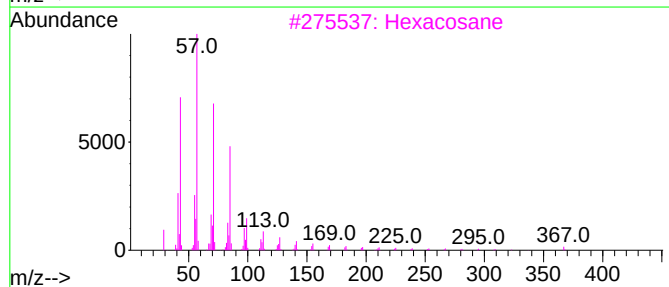
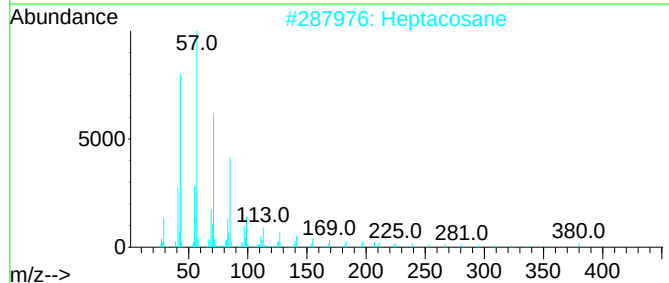
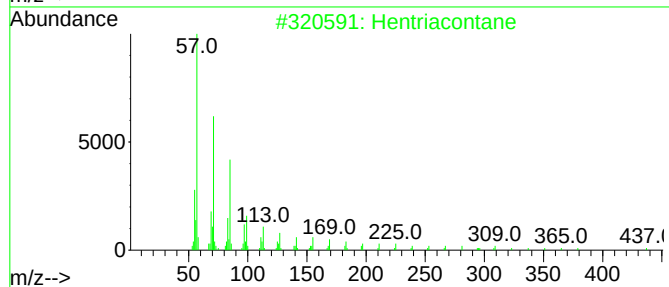
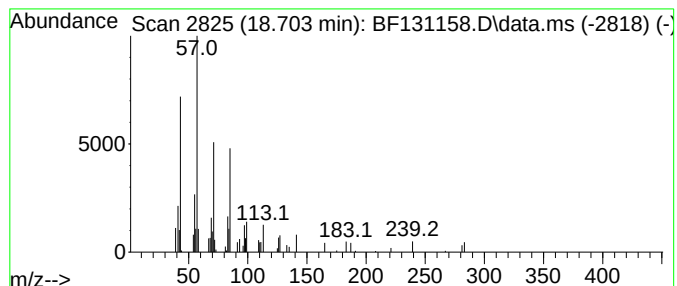
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.703	2.27 ng	61550	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	90
2			Heptacosane	380	C27H56	000593-49-7	90
3			Hexacosane	366	C26H54	000630-01-3	87
4			Isopropyl tetradecyl ether	256	C17H36O	1000406-34-0	86
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111122\
Data File : BF131158.D
Acq On : 11 Nov 2022 17:34
Operator : CG\JU
Sample : PB148951BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148951BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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
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Propane, 1,1-di...	2.316	2.1	ng	58275	1	6.869	542987	20.0
2-Pentanone, 4-...	5.110	12.6	ng	342559	1	6.869	542987	20.0
Triphenylphosph...	14.145	2.4	ng	83513	5	14.051	711742	20.0
Eicosane	14.821	2.1	ng	56911	6	15.545	543196	20.0
Hentriacontane	15.163	2.6	ng	69948	6	15.545	543196	20.0
Octacosane	15.998	3.8	ng	104260	6	15.545	543196	20.0
Heneicosane	16.515	4.3	ng	117920	6	15.545	543196	20.0
Heptadecane, 9-...	17.121	3.3	ng	88218	6	15.545	543196	20.0
Hexacosane	17.845	3.1	ng	84411	6	15.545	543196	20.0
Heptacosane	18.703	2.3	ng	61550	6	15.545	543196	20.0