

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
 Data File : BF130389.D
 Acq On : 23 Sep 2022 14:13
 Operator : CG\JU
 Sample : N4780-11
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-2

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130389.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.840	463	468	483	rBV	425933	666492	21.43%	2.741%
2	5.263	535	540	551	rBV	2687039	2727588	87.70%	11.217%
3	6.298	711	716	731	rBV	2516863	2786790	89.61%	11.460%
4	6.651	772	776	779	rBV	759729	586842	18.87%	2.413%
5	7.216	867	872	875	rBV	1720902	1838967	59.13%	7.562%
6	7.934	989	994	997	rBV	933905	815448	26.22%	3.353%
7	9.016	1172	1178	1181	rBV	3099535	3110033	100.00%	12.789%
8	9.686	1287	1292	1295	rBV	1046383	873132	28.07%	3.591%
9	10.475	1422	1426	1443	rBV	1898746	1919474	61.72%	7.893%
10	11.169	1540	1544	1547	rVB	968762	775804	24.95%	3.190%
11	11.698	1626	1634	1654	rVB	425108	716158	23.03%	2.945%
12	11.857	1658	1661	1669	rVB7	27420	43952	1.41%	0.181%
13	12.357	1743	1746	1749	rBV2	47015	55439	1.78%	0.228%
14	12.404	1749	1754	1758	rVV7	50822	125928	4.05%	0.518%
15	12.492	1761	1769	1782	rVB	1580807	2207971	71.00%	9.080%
16	12.757	1810	1814	1817	rBV	3018201	2574305	82.77%	10.586%
17	13.245	1888	1897	1906	rBV4	87141	318263	10.23%	1.309%
18	13.798	1987	1991	1995	rBV	631366	559614	17.99%	2.301%
19	13.904	2005	2009	2015	rVB	81044	108098	3.48%	0.445%
20	14.121	2040	2046	2052	rBV	109957	205478	6.61%	0.845%
21	14.286	2071	2074	2077	rVB2	31760	32907	1.06%	0.135%
22	14.763	2148	2155	2162	rBV2	80065	169202	5.44%	0.696%
23	15.192	2223	2228	2232	rBV	506292	585917	18.84%	2.409%
24	15.433	2263	2269	2279	rVB3	63714	171657	5.52%	0.706%
25	15.598	2288	2297	2300	rBV8	76198	222006	7.14%	0.913%
26	16.221	2398	2403	2412	rVB3	47066	119829	3.85%	0.493%

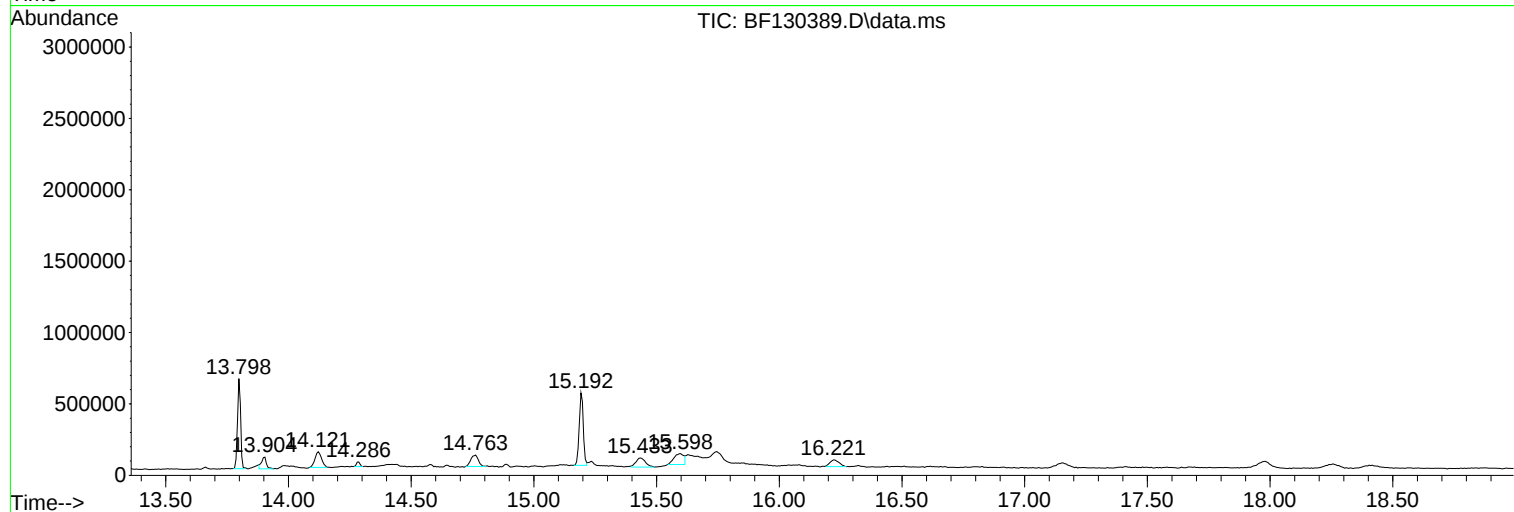
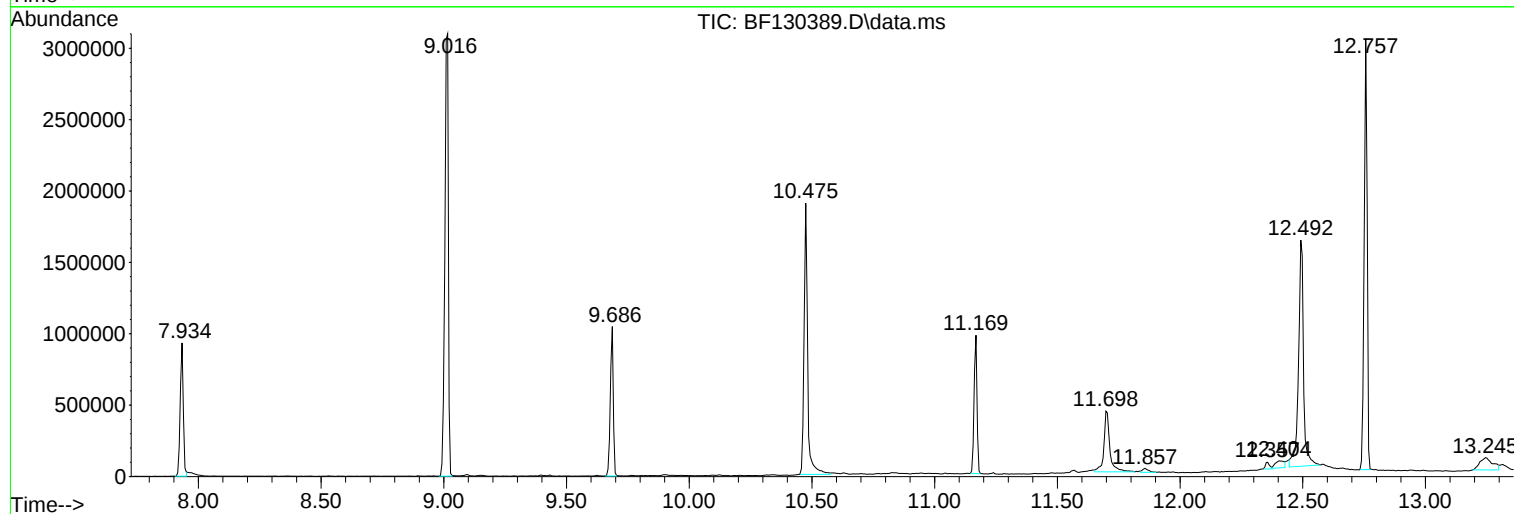
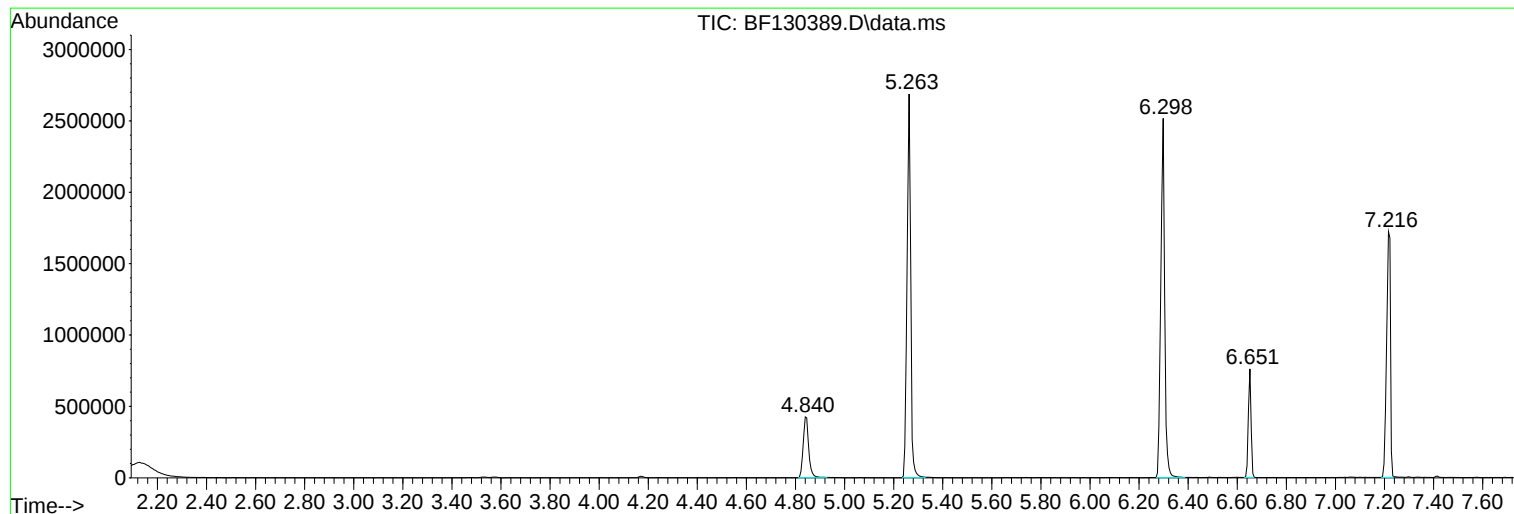
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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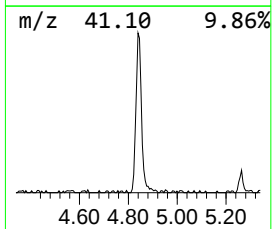
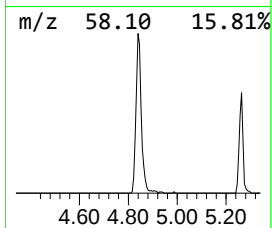
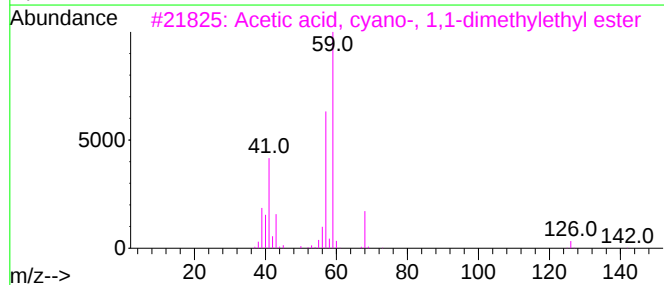
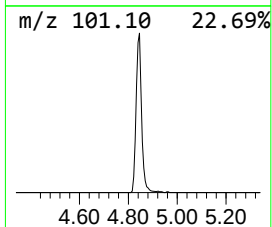
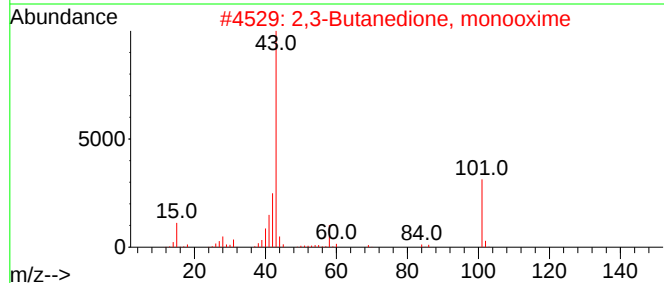
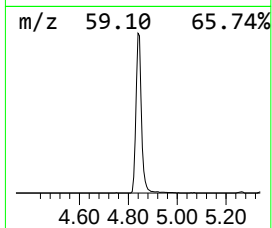
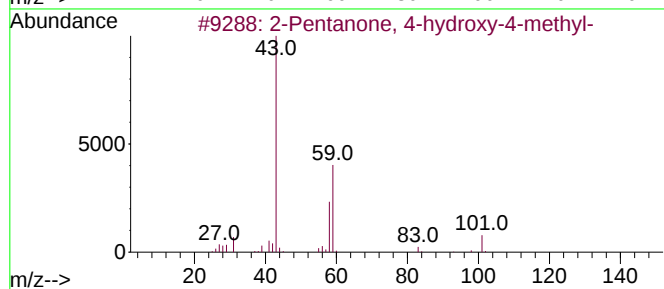
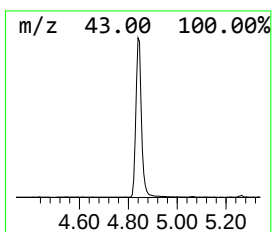
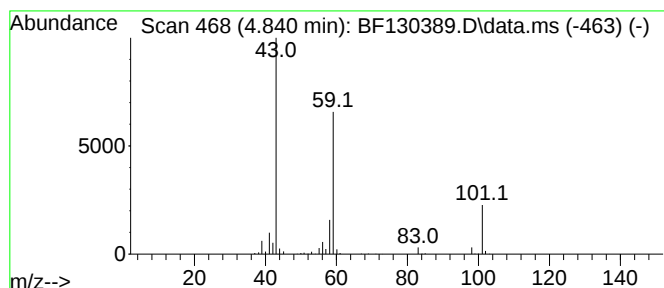
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.840	22.71 ng	666492	1,4-Dichlorobenzene-d4	6.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Acetone	58	C3H6O	000067-64-1	10		



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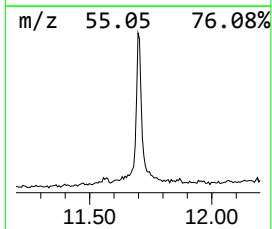
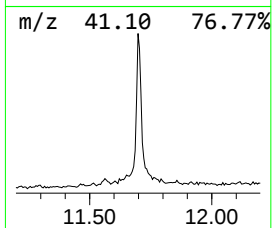
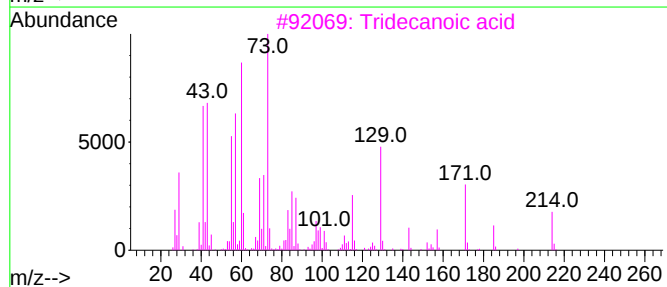
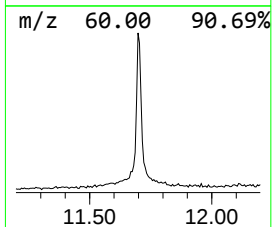
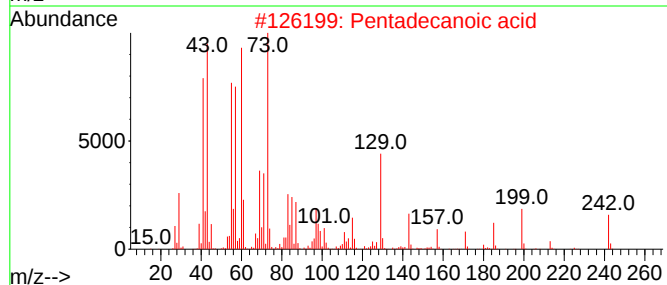
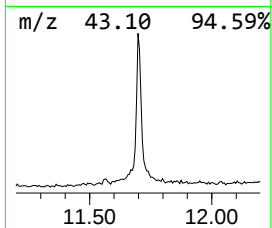
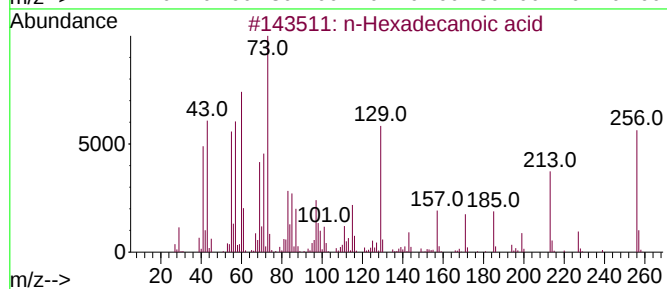
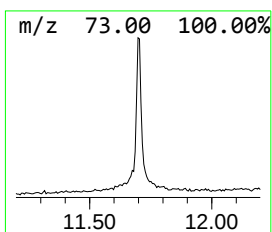
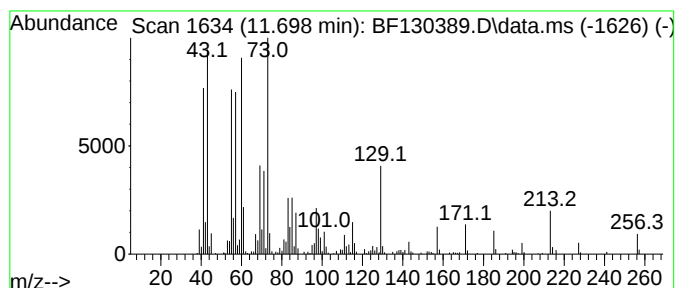
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.698	18.46 ng	716158	Phenanthrene-d10		11.169	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
3	Tridecanoic acid		214	C13H26O2	000638-53-9	92
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
5	n-Decanoic acid		172	C10H20O2	000334-48-5	68



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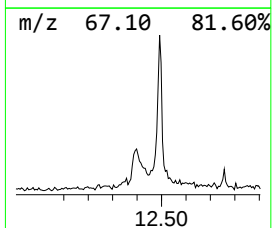
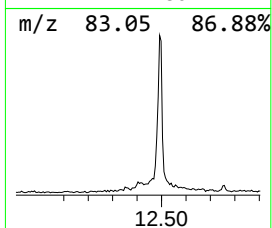
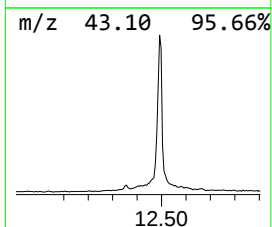
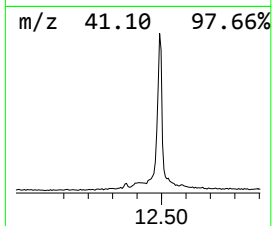
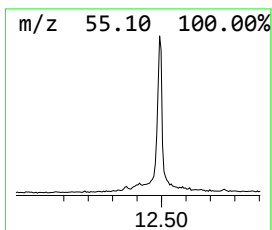
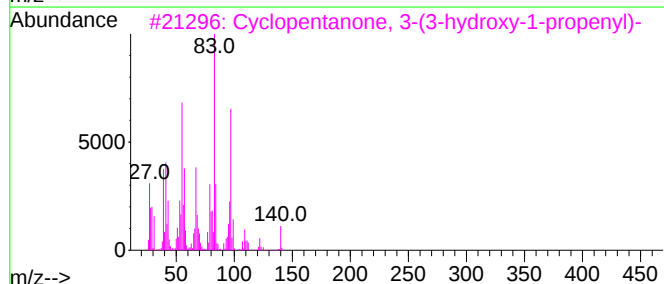
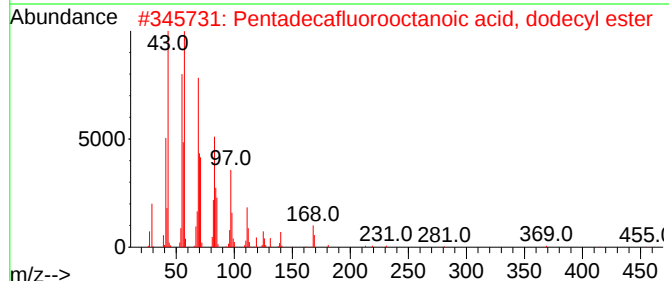
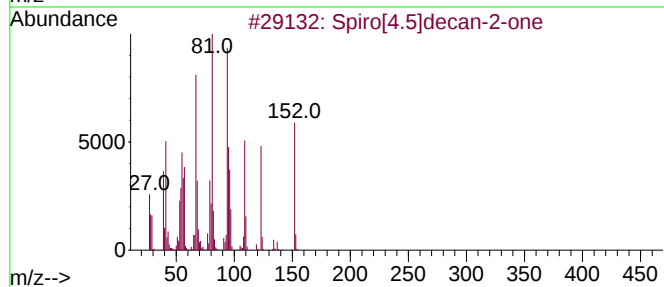
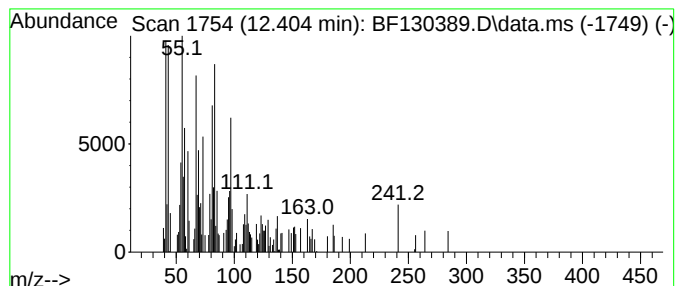
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown12.404 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.404	3.25 ng	125928	Phenanthrene-d10	11.169	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[4.5]decan-2-one	152	C10H16O	003643-16-1	44
2	Pentadecafluorooctanoic acid, do...	582	C20H25F15O2	1000406-04-2	43
3	Cyclopentanone, 3-(3-hydroxy-1-p...	140	C8H12O2	074473-08-8	38
4	Z-1,8-Dodecadiene	166	C12H22	1010245-71-5	35
5	9,12-Octadecadienoyl chloride, (...	298	C18H31ClO	007459-33-8	30



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Instrument :
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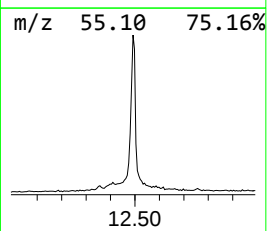
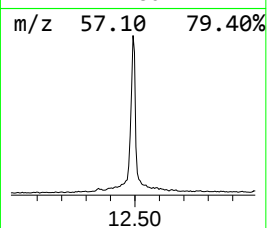
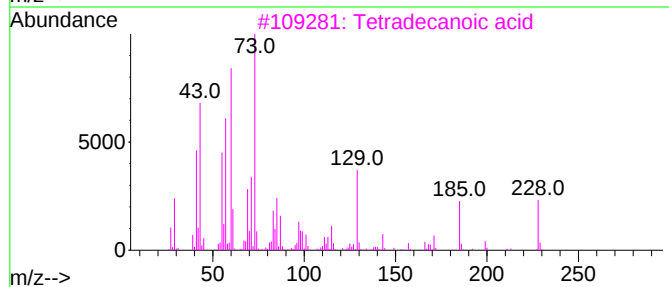
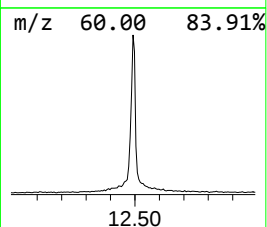
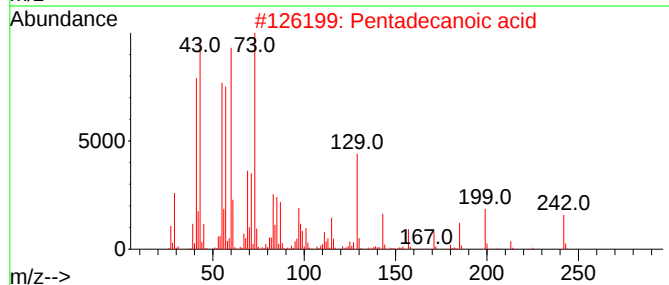
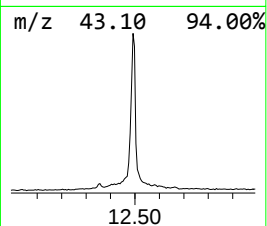
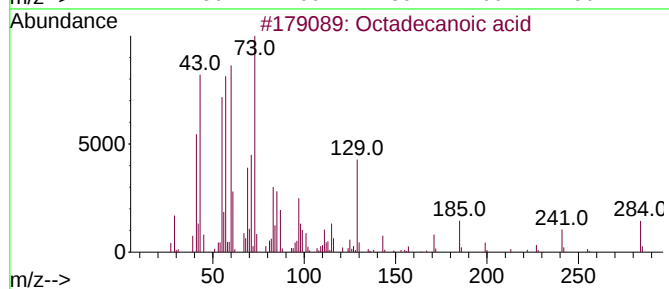
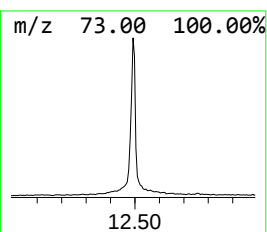
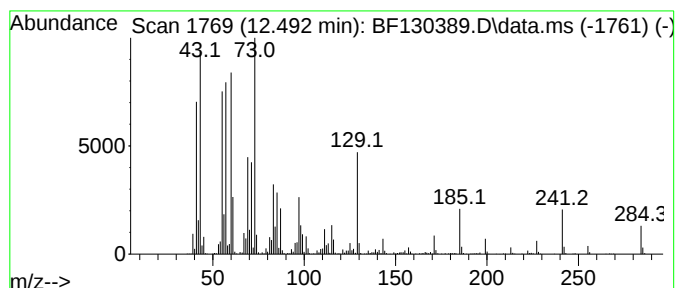
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	78.91 ng	2207970	Chrysene-d12	13.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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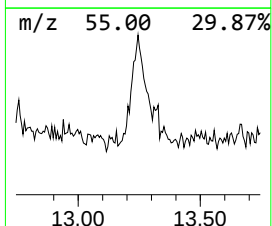
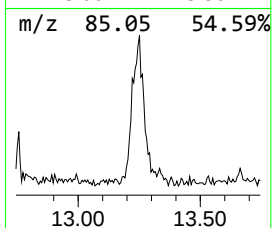
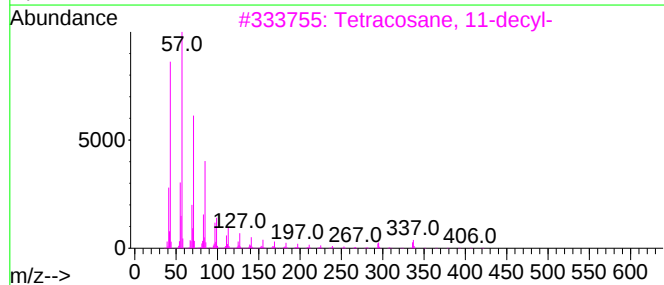
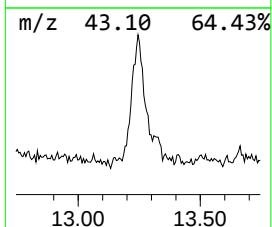
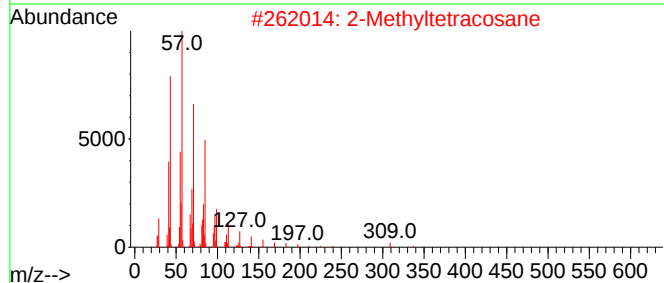
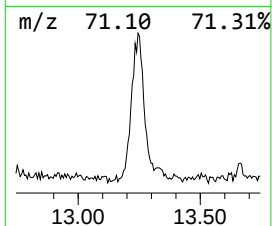
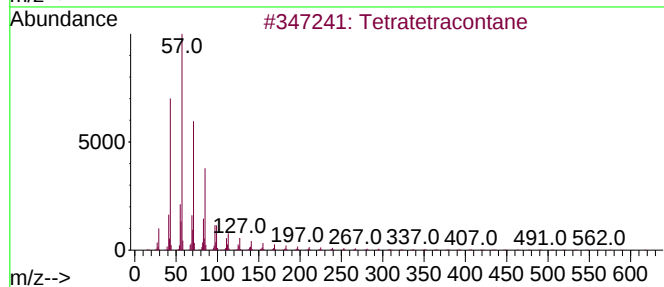
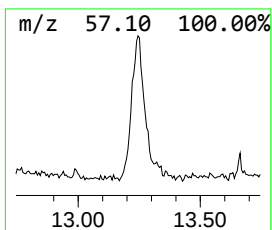
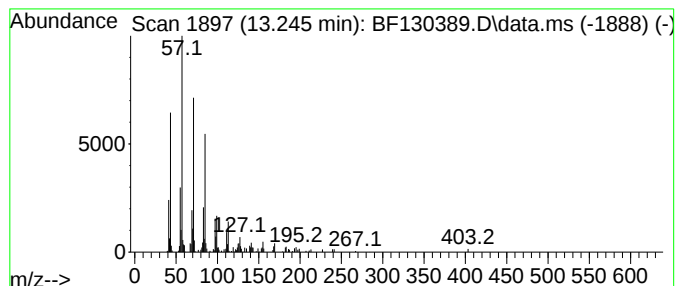
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.245	11.37 ng	318263	Chrysene-d12	13.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			2-Methyltetracosane	352	C25H52	001560-78-7	91
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
4			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90
5			Hexacosane	366	C26H54	000630-01-3	87



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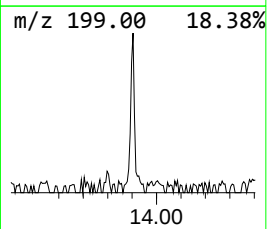
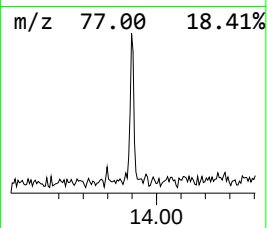
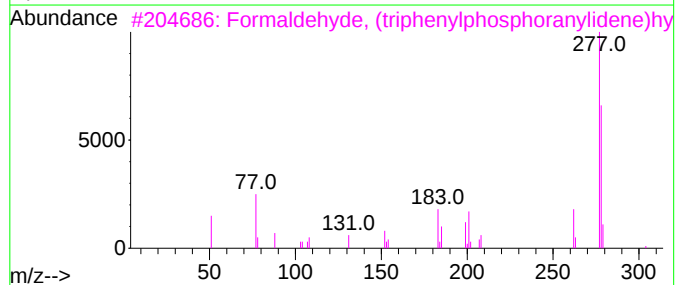
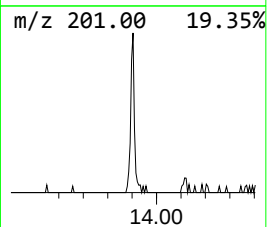
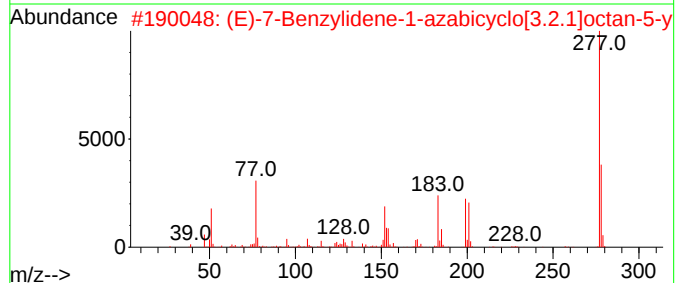
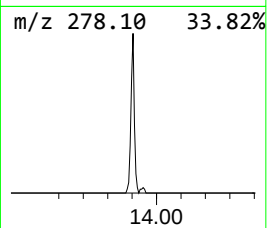
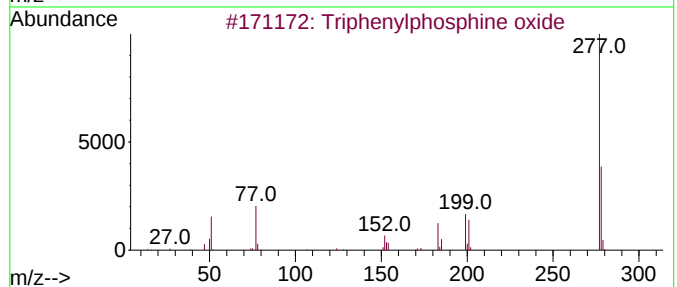
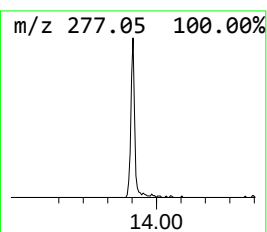
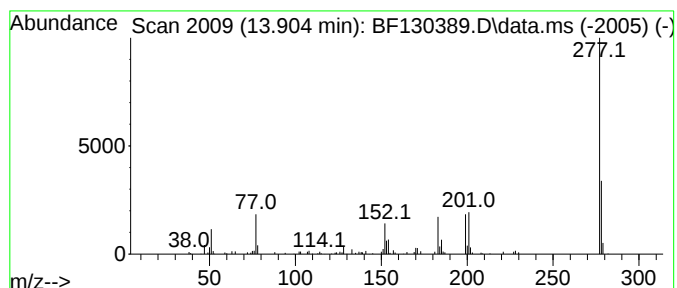
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.86 ng	108098	Chrysene-d12	13.798

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	C15H19N03S	1000483-83-4	58
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	40
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	33
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130389.D
Acq On : 23 Sep 2022 14:13
Operator : CG\JU
Sample : N4780-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

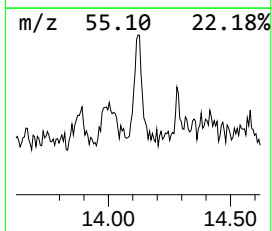
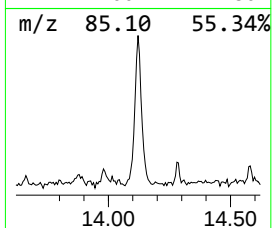
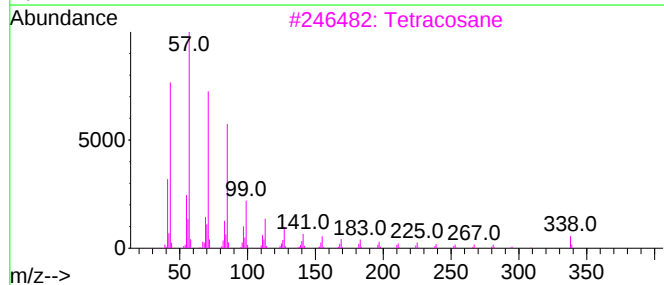
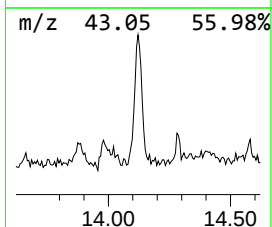
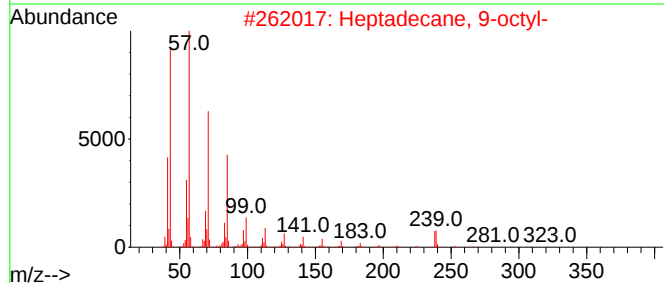
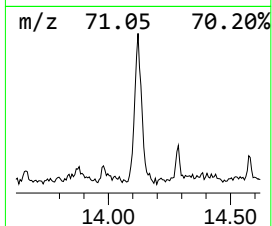
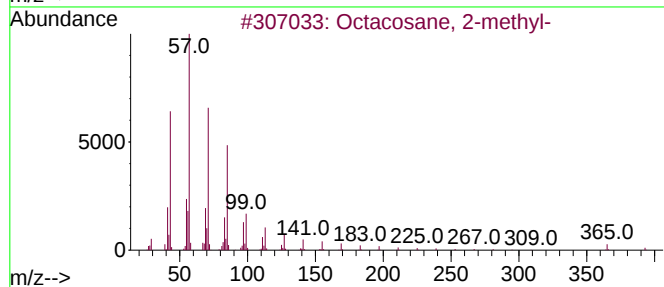
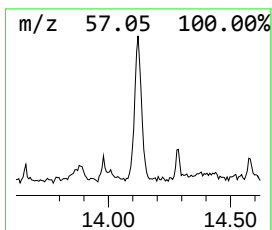
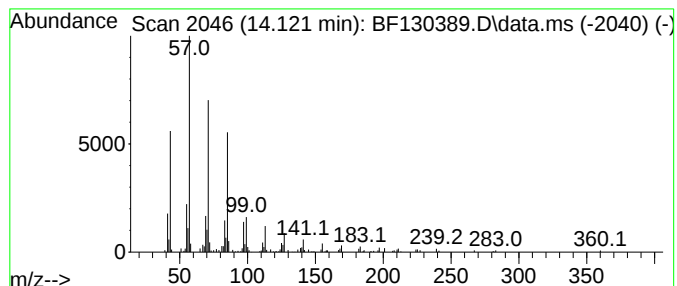
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	7.34 ng	205478	Chrysene-d12	13.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Tetracosane	338	C24H50	000646-31-1	90
4			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
5			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130389.D
Acq On : 23 Sep 2022 14:13
Operator : CG\JU
Sample : N4780-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

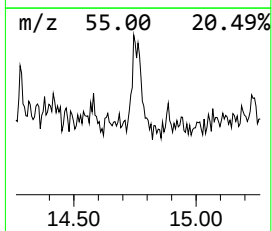
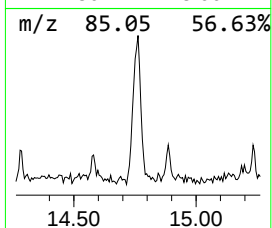
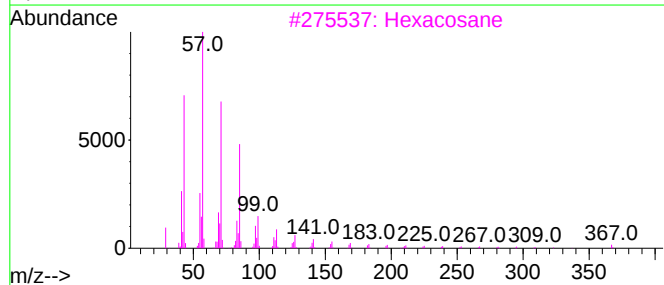
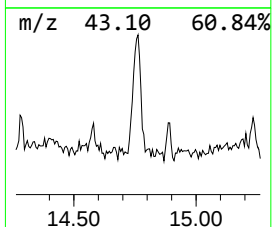
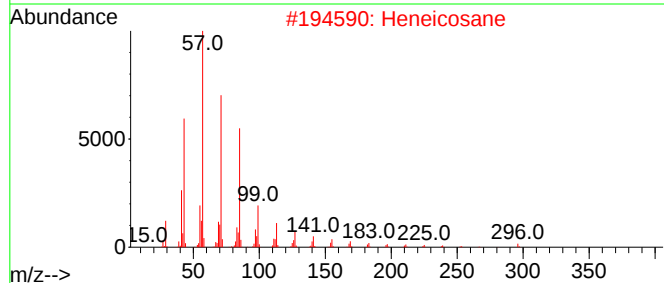
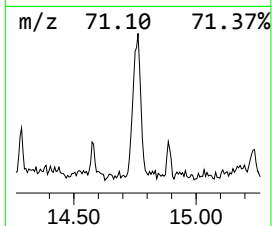
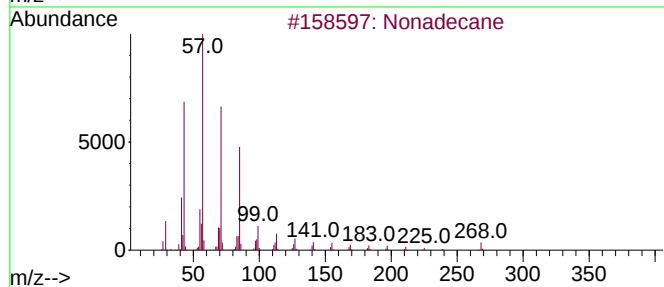
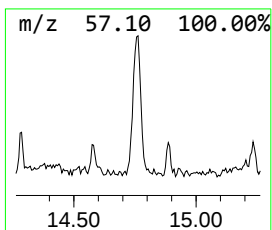
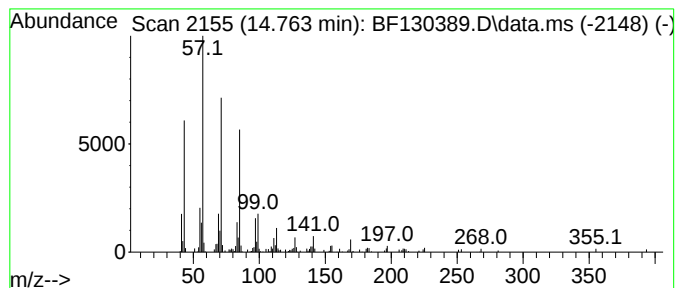
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.762	5.78 ng	169202	Perylene-d12	15.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Heneicosane	296	C21H44	000629-94-7	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87
5			Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130389.D
Acq On : 23 Sep 2022 14:13
Operator : CG\JU
Sample : N4780-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

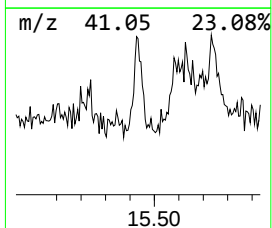
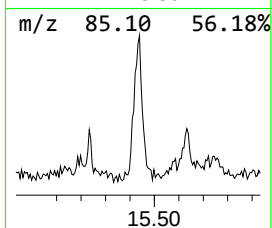
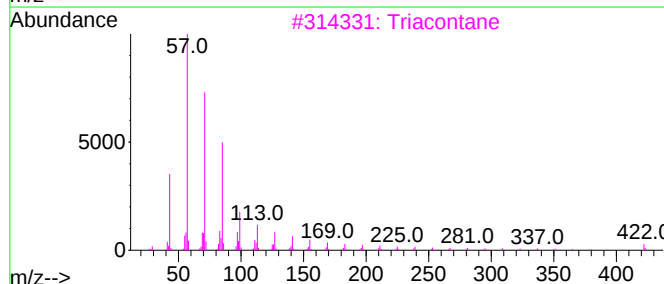
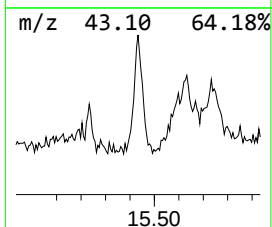
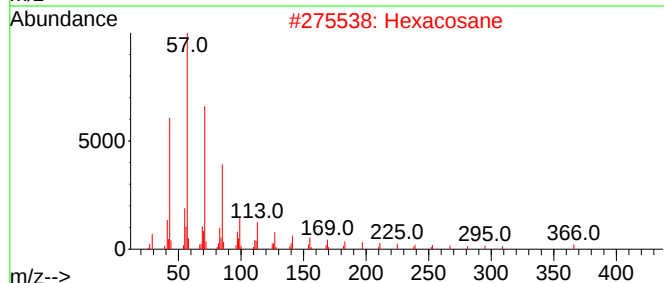
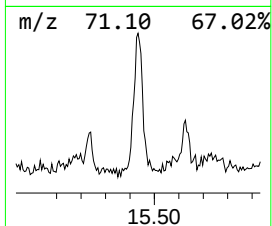
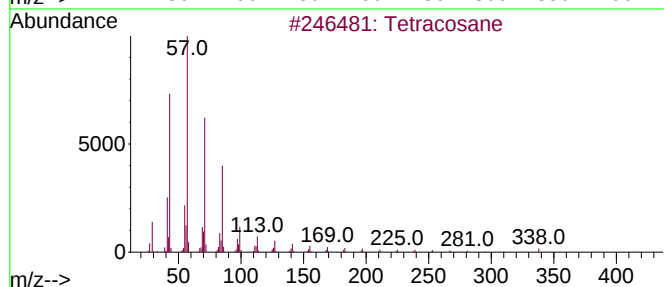
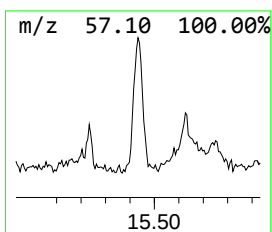
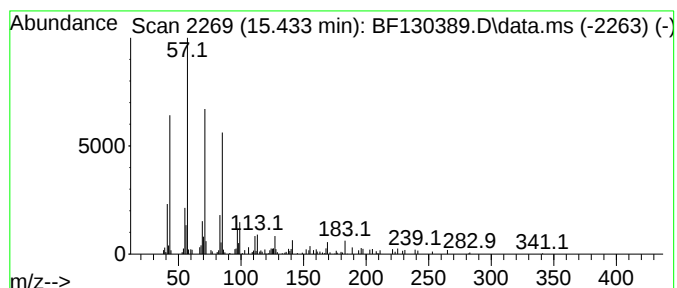
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.433	5.86 ng	171657	Perylene-d12	15.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Triacontane	422	C30H62	000638-68-6	87
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5	Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130389.D
Acq On : 23 Sep 2022 14:13
Operator : CG\JU
Sample : N4780-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

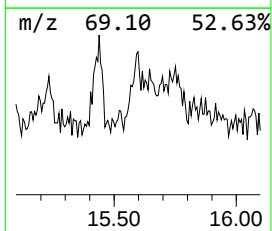
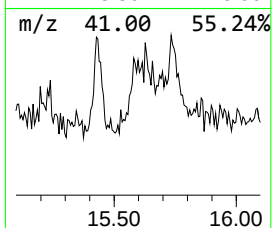
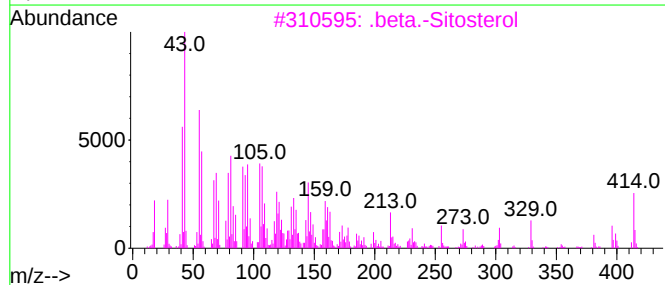
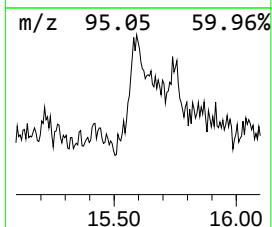
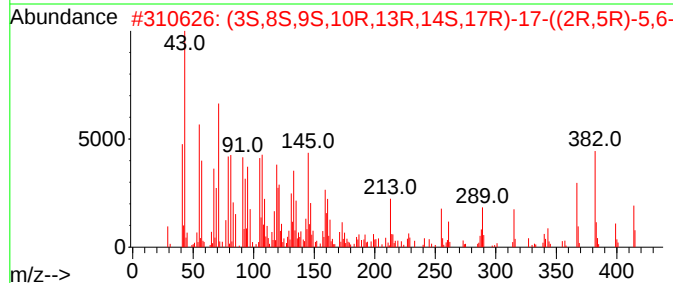
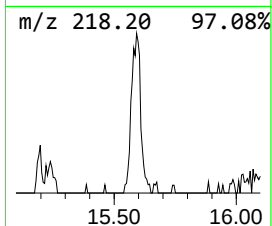
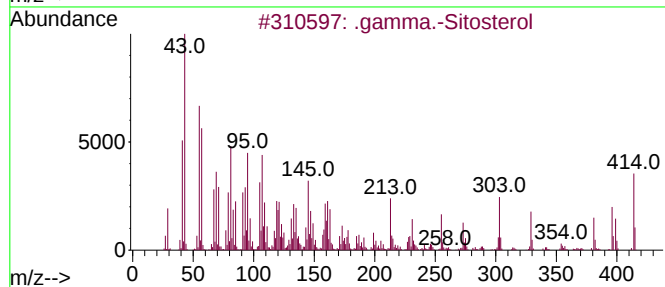
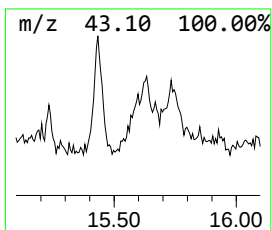
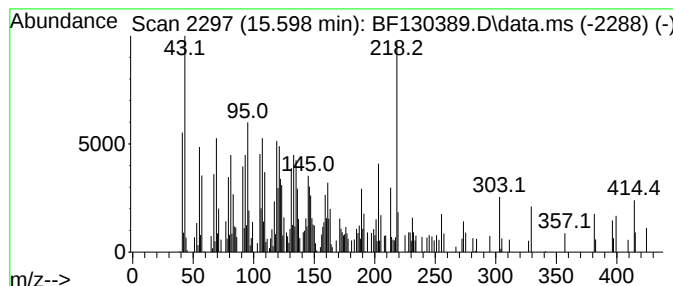
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.598	7.58 ng	222006	Perylene-d12	15.192	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	76
2	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	70
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	62
4	4,6,6-Trimethyl-2-(3-methylbuta-...	218	C15H22O	1000190-22-2	60
5	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130389.D
Acq On : 23 Sep 2022 14:13
Operator : CG\JU
Sample : N4780-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

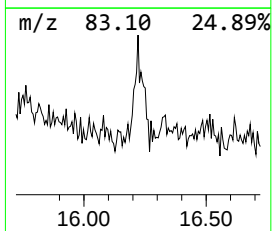
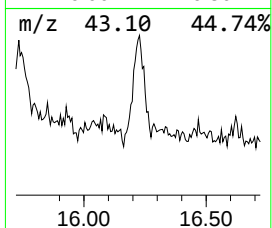
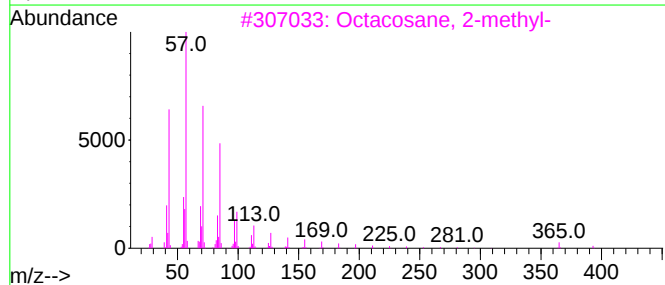
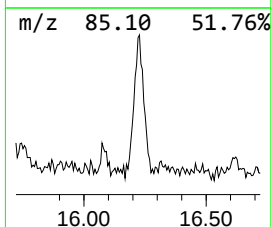
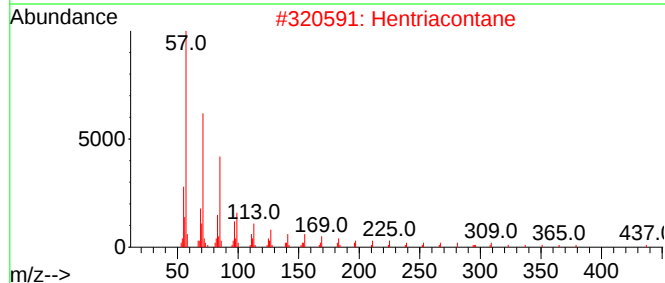
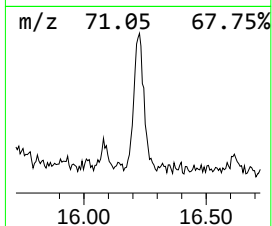
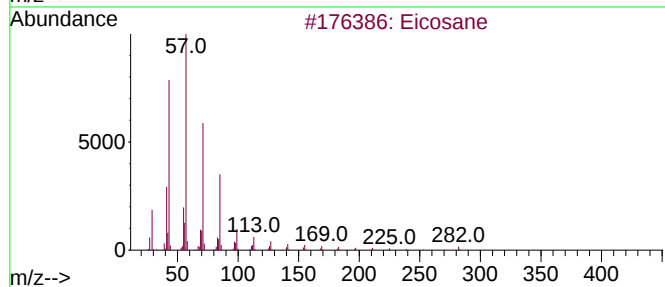
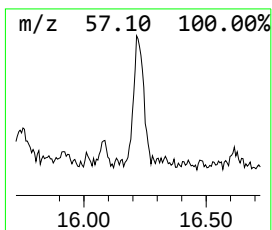
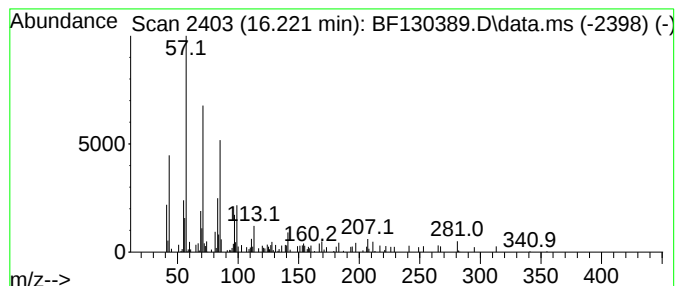
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.221	4.09 ng	119829	Perylene-d12	15.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	90
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	86
4			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	86
5			Tetratetracontane	619	C44H90	007098-22-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092322\
Data File : BF130389.D
Acq On : 23 Sep 2022 14:13
Operator : CG\JU
Sample : N4780-11
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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n-Hexadecanoic ...	11.698	18.5	ng	716158	4	11.169	775804	20.0
unknown12.404	12.404	3.3	ng	125928	4	11.169	775804	20.0
Octadecanoic acid	12.492	78.9	ng	2207970	5	13.798	559614	20.0
Tetratetracontane	13.245	11.4	ng	318263	5	13.798	559614	20.0
Triphenylphosph...	13.904	3.9	ng	108098	5	13.798	559614	20.0
Octacosane, 2-m...	14.121	7.3	ng	205478	5	13.798	559614	20.0
Nonadecane	14.762	5.8	ng	169202	6	15.192	585917	20.0
Tetracosane	15.433	5.9	ng	171657	6	15.192	585917	20.0
.gamma.-Sitosterol	15.598	7.6	ng	222006	6	15.192	585917	20.0
Eicosane	16.221	4.1	ng	119829	6	15.192	585917	20.0