

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
 Data File : BF137037.D
 Acq On : 11 Jan 2024 14:15
 Operator : CG\JU
 Sample : PB158373BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB158373BL

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-BF122023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137037.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	502	507	519	rBV	42502	77272	2.32%	0.395%
2	5.445	566	571	574	rBV	2460872	2545859	76.42%	13.018%
3	6.445	735	741	744	rBV	2257409	2530792	75.97%	12.941%
4	6.786	795	799	802	rBV	577293	470708	14.13%	2.407%
5	7.357	889	896	898	rBV	1449687	1735213	52.09%	8.873%
6	8.063	1011	1016	1019	rBV	707564	615551	18.48%	3.148%
7	9.145	1193	1200	1203	rBV	3410419	3257812	97.79%	16.659%
8	9.822	1310	1315	1318	rBV	816986	707797	21.25%	3.619%
9	10.622	1446	1451	1454	rBV	1878577	1807767	54.26%	9.244%
10	11.316	1565	1569	1572	rBV	930123	766978	23.02%	3.922%
11	12.915	1835	1841	1844	rBV	2942296	3331449	100.00%	17.036%
12	13.945	2004	2016	2017	rBV7	19016	36892	1.11%	0.189%
13	13.974	2017	2021	2034	rVB	572816	565094	16.96%	2.890%
14	14.745	2148	2152	2157	rVB	54366	58829	1.77%	0.301%
15	15.092	2207	2211	2216	rVB	65231	74082	2.22%	0.379%
16	15.468	2269	2275	2289	rVB2	327232	546381	16.40%	2.794%
17	15.927	2348	2353	2358	rVB	71721	113920	3.42%	0.583%
18	16.445	2436	2441	2449	rVB2	70073	122347	3.67%	0.626%
19	17.068	2541	2547	2555	rVB	50040	107346	3.22%	0.549%
20	17.798	2666	2671	2680	rVB2	35083	83665	2.51%	0.428%

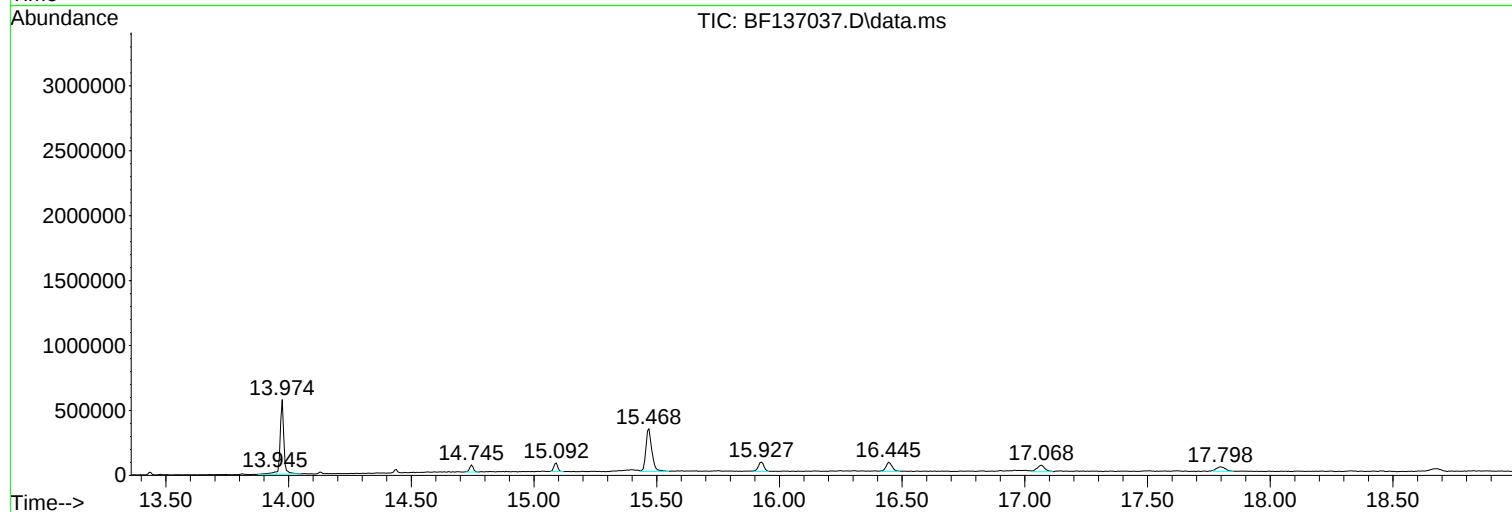
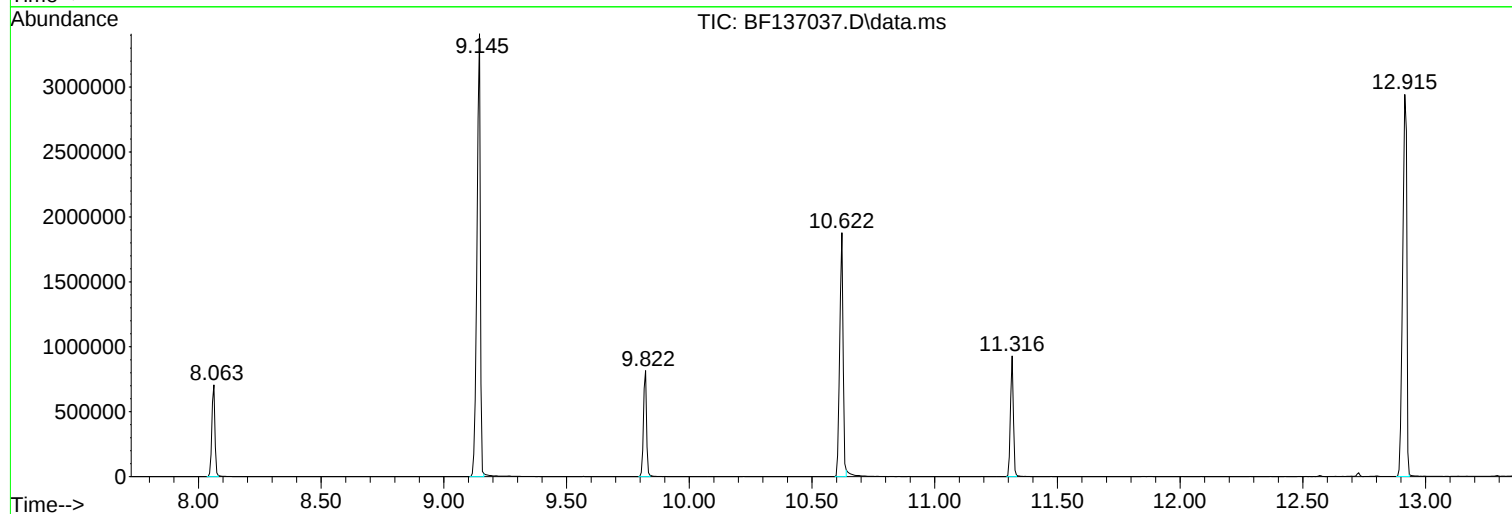
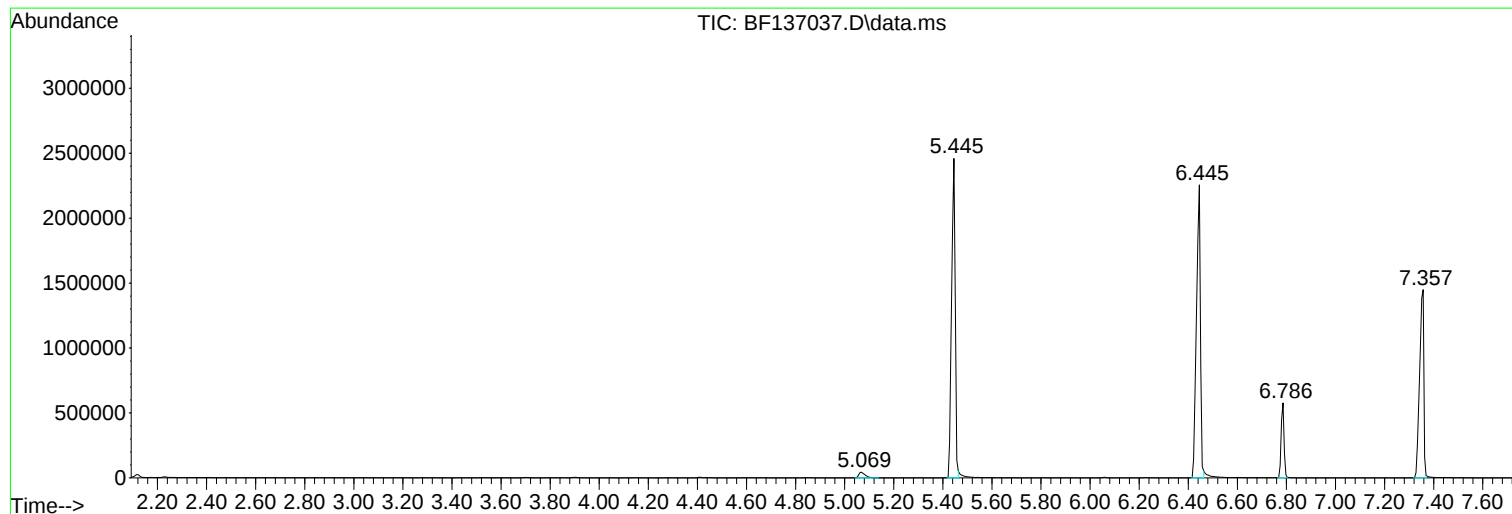
Sum of corrected areas: 19555754

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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Data File : BF137037.D
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Operator : CG\JU
Sample : PB158373BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158373BL

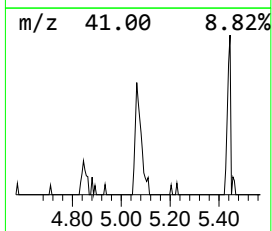
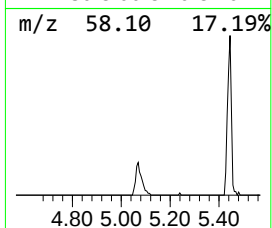
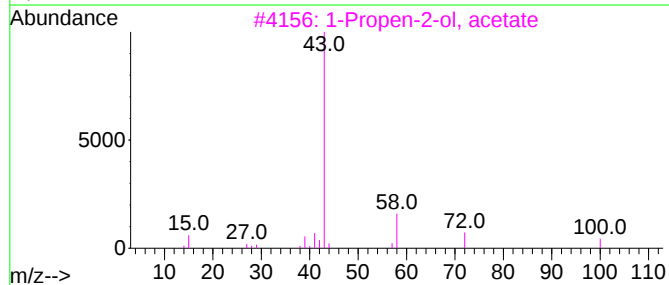
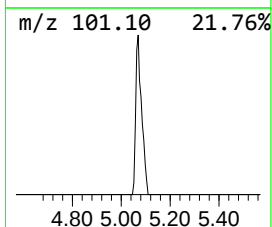
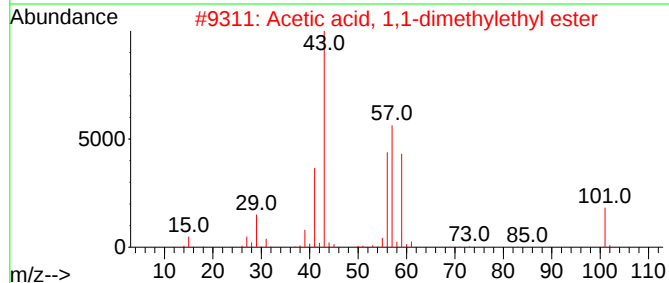
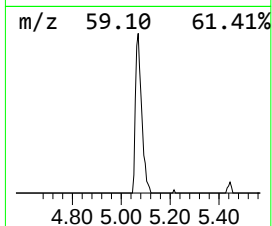
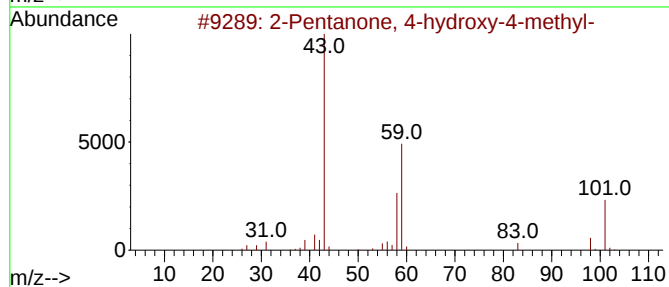
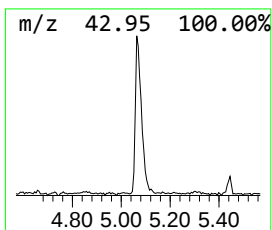
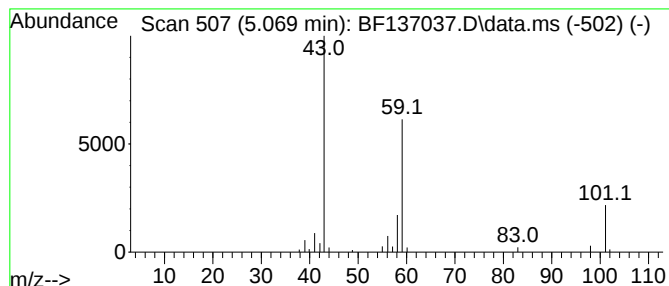
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	3.28 ng	77272	1,4-Dichlorobenzene-d4	6.786

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Acetone	58	C3H6O	000067-64-1	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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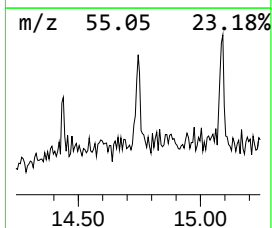
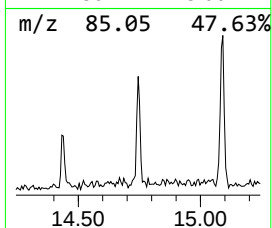
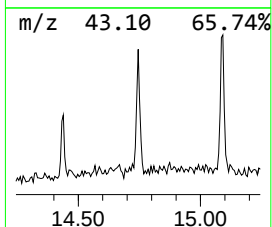
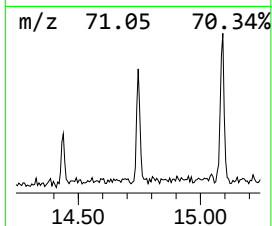
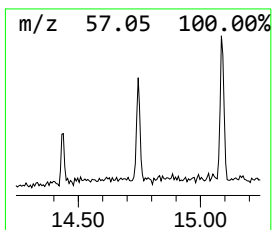
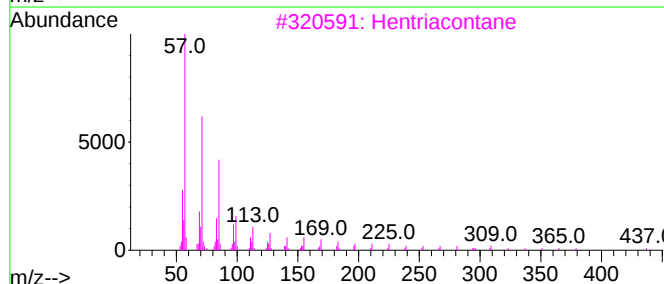
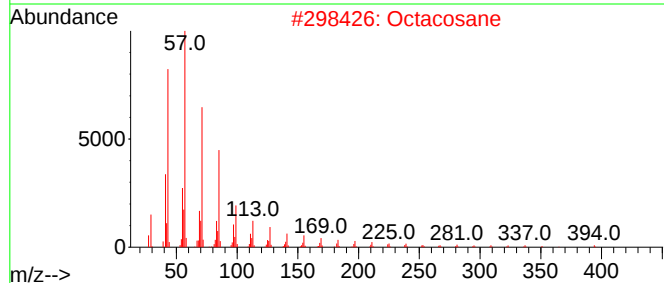
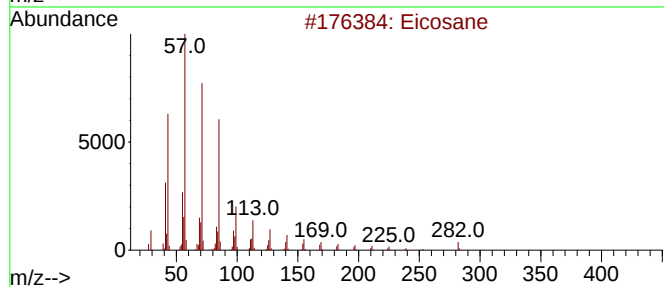
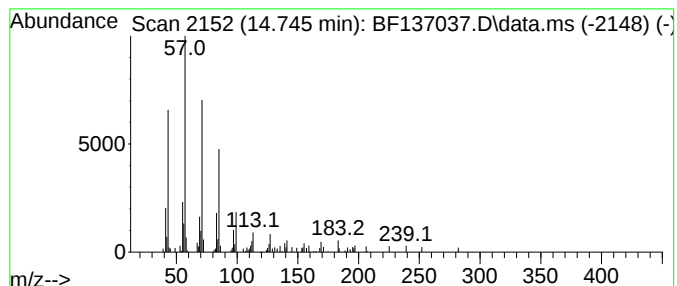
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	2.15 ng	58829	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	95
2	Octacosane			394	C28H58	000630-02-4	91
3	Hentriacontane			437	C31H64	000630-04-6	91
4	Heneicosane			296	C21H44	000629-94-7	90
5	Tetratetracontane			619	C44H90	007098-22-8	90



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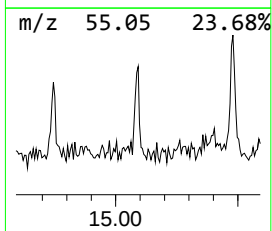
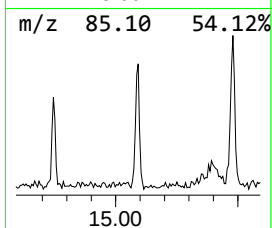
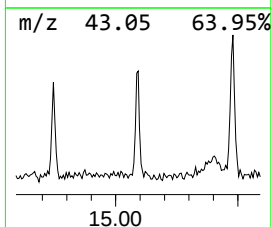
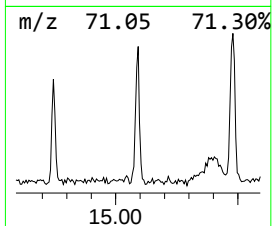
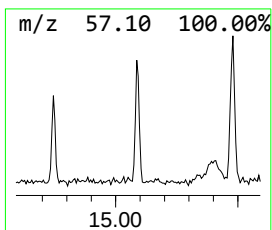
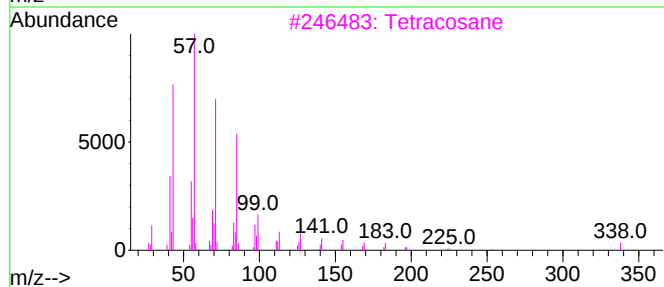
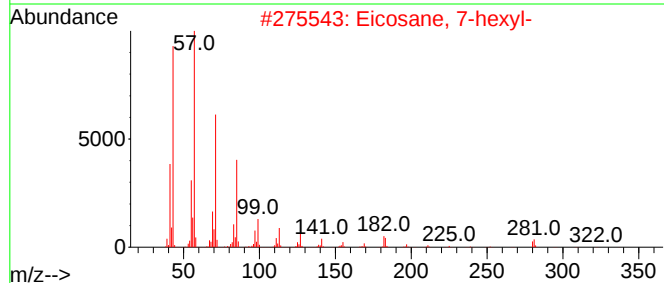
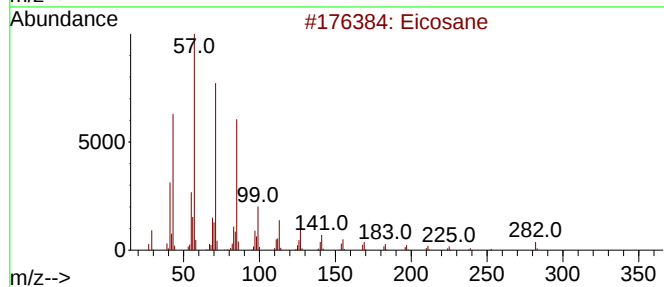
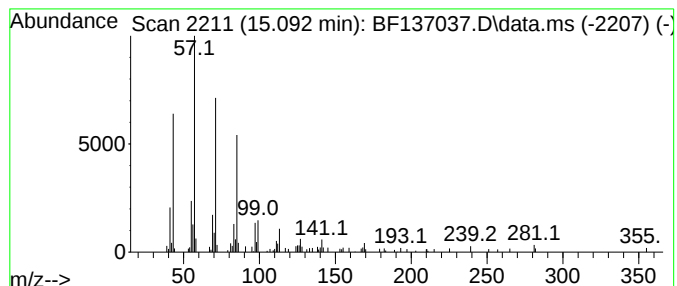
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Eicosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.092	2.71 ng	74082	Perylene-d12		15.462	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	94
2	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	91
3	Tetracosane		338	C24H50	000646-31-1	90
4	Hexacosane		366	C26H54	000630-01-3	90
5	Heneicosane		296	C21H44	000629-94-7	90



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Data File : BF137037.D
Acq On : 11 Jan 2024 14:15
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Sample : PB158373BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

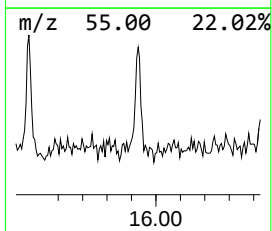
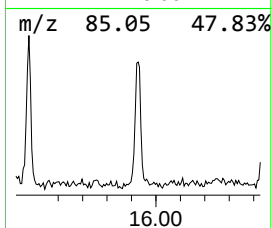
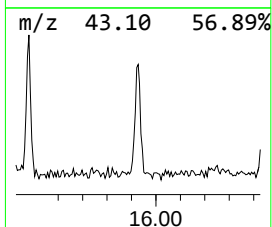
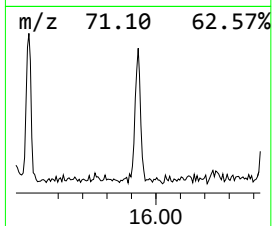
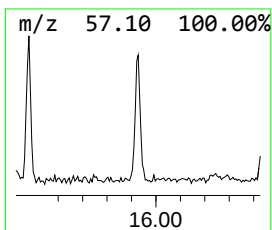
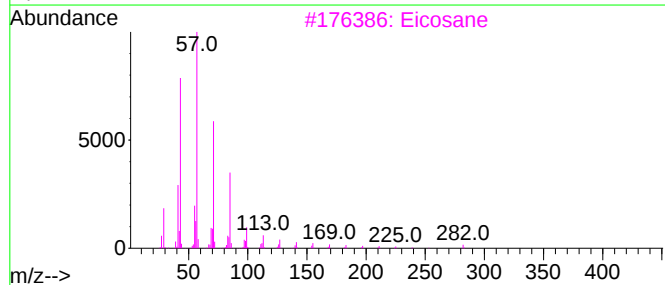
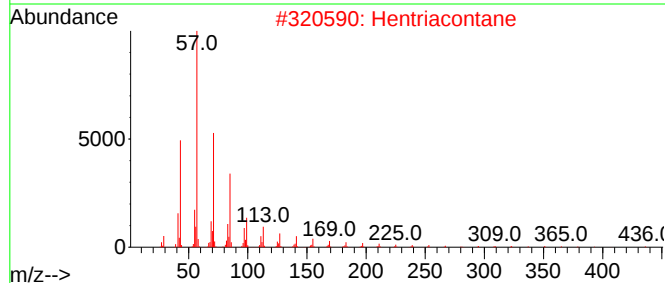
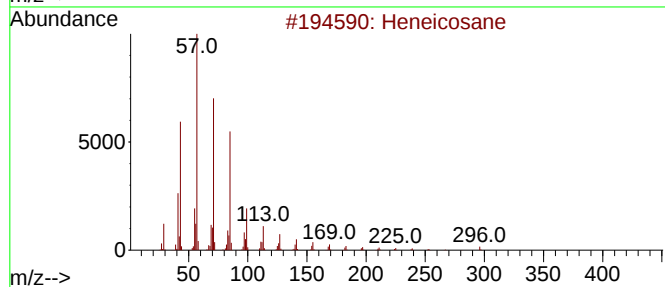
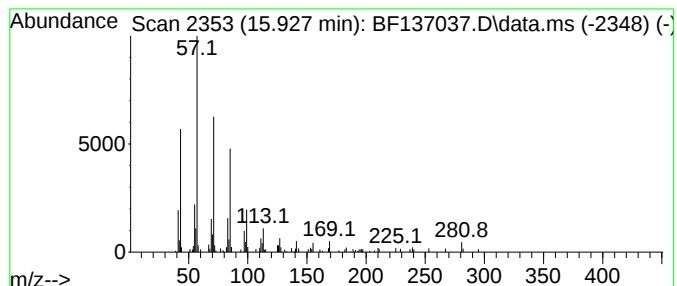
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heneicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.927	4.17 ng	113920	Perylene-d12	15.462	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Eicosane	282	C20H42	000112-95-8	90
4	Pentacosane	352	C25H52	000629-99-2	87
5	Hexacosane	366	C26H54	000630-01-3	87



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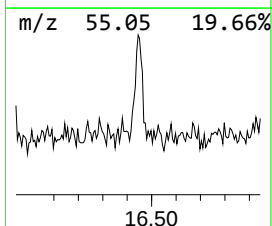
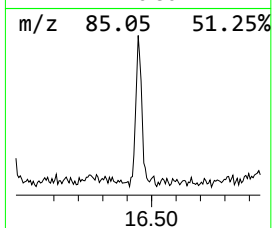
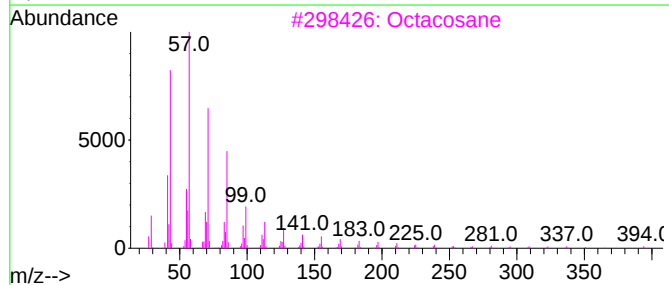
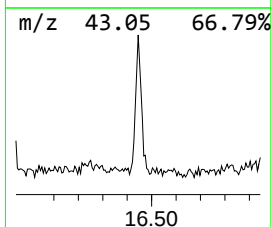
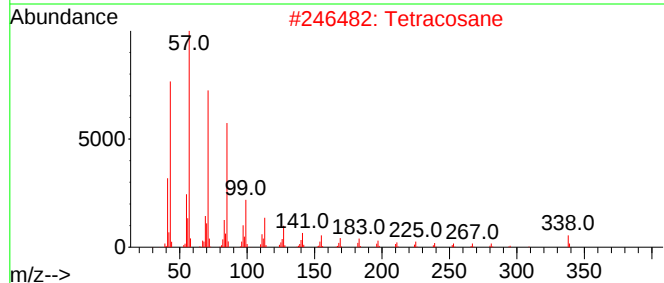
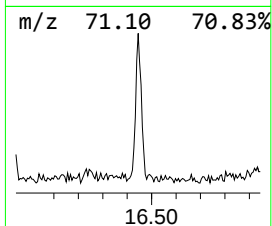
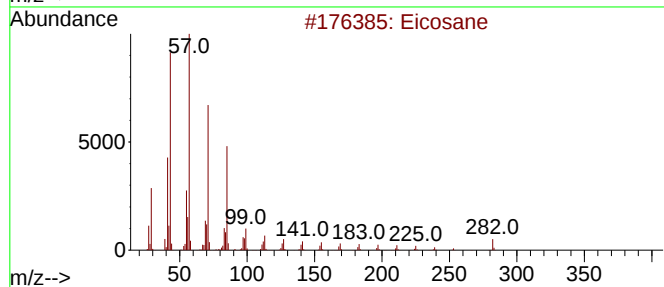
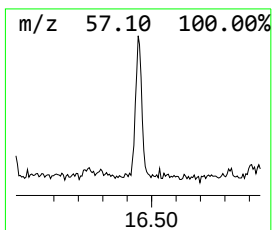
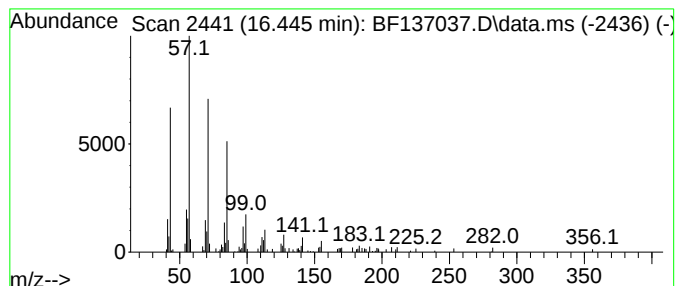
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Tetracosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	4.48 ng	122347	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Tetracosane	338	C24H50	000646-31-1	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
5			Tetratetracontane	619	C44H90	007098-22-8	90



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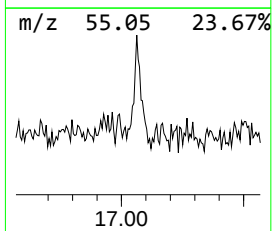
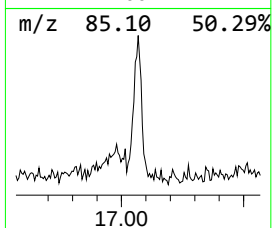
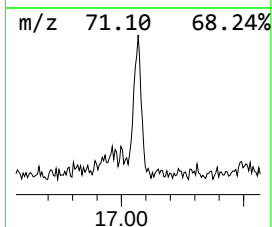
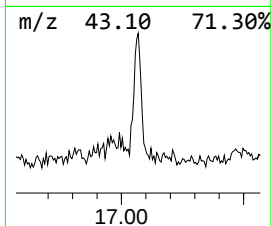
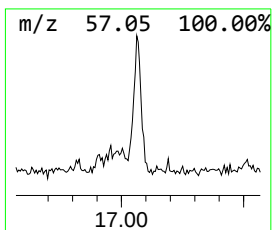
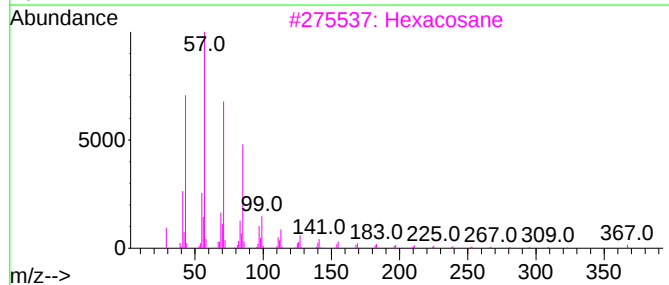
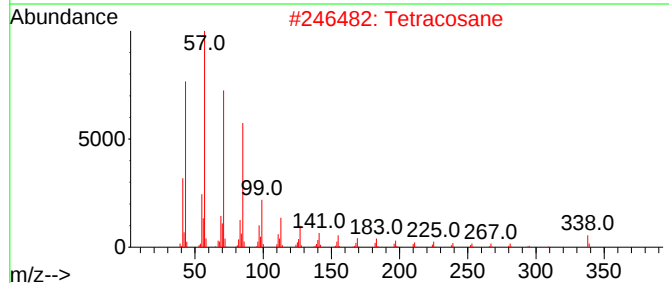
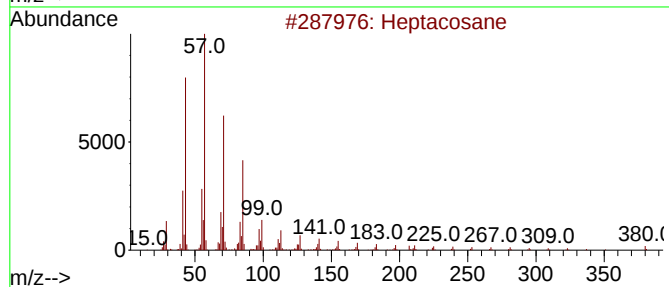
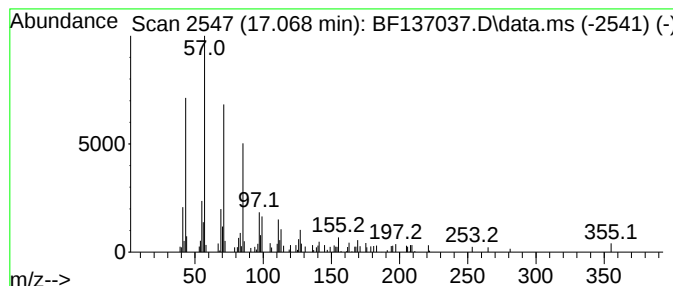
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.068	3.93 ng	107346	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Tetracosane	338	C24H50	000646-31-1	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Tetratetracontane	619	C44H90	007098-22-8	86
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137037.D
Acq On : 11 Jan 2024 14:15
Operator : CG\JU
Sample : PB158373BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158373BL

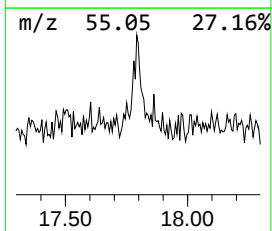
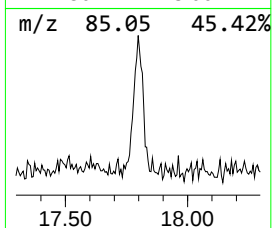
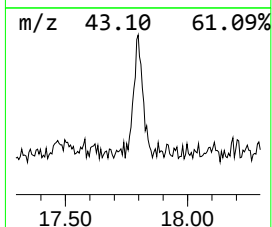
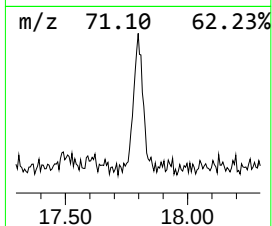
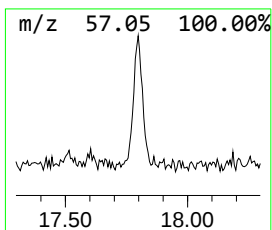
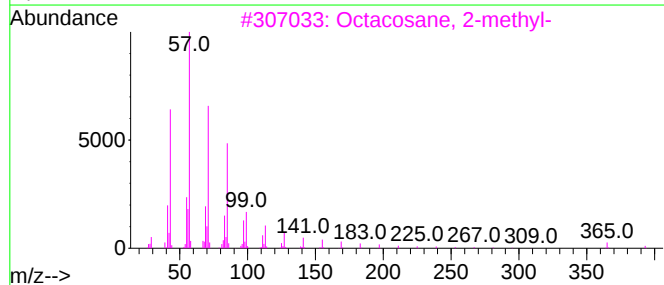
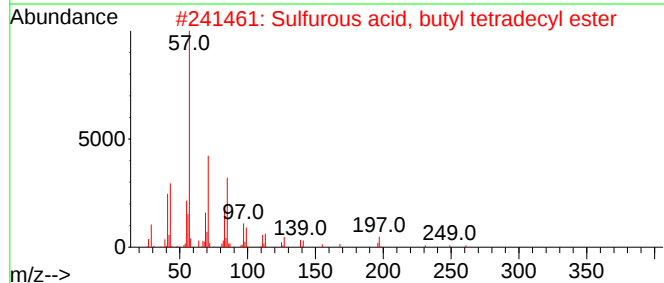
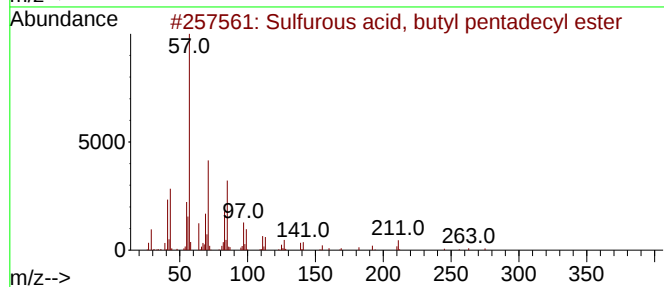
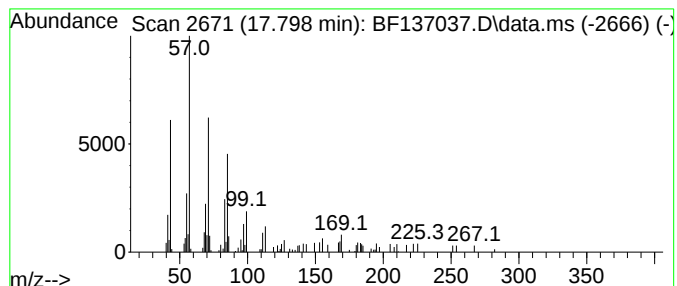
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, butyl penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.797	3.06 ng	83665	Perylene-d12	15.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	86
2			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	86
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	83
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	68
5			Octacosane	394	C28H58	000630-02-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011124\
Data File : BF137037.D
Acq On : 11 Jan 2024 14:15
Operator : CG\JU
Sample : PB158373BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158373BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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-...	5.069	3.3	ng	77272	1	6.786	470708	20.0
Eicosane	14.745	2.1	ng	58829	6	15.462	546381	20.0
Eicosane, 7-hexyl-	15.092	2.7	ng	74082	6	15.462	546381	20.0
Heneicosane	15.927	4.2	ng	113920	6	15.462	546381	20.0
Tetracosane	16.445	4.5	ng	122347	6	15.462	546381	20.0
Heptacosane	17.068	3.9	ng	107346	6	15.462	546381	20.0
Sulfurous acid,...	17.797	3.1	ng	83665	6	15.462	546381	20.0