

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
 Data File : BF137045.D
 Acq On : 12 Jan 2024 13:28
 Operator : CG\JU
 Sample : PB158404BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB158404BL

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: BF137045.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	516	rBV	42631	76158	2.15%	0.382%
2	5.446	566	571	574	rBV	2478539	2538191	71.74%	12.734%
3	6.446	735	741	744	rBV	2214509	2539544	71.78%	12.741%
4	6.787	795	799	802	rBV	563773	466472	13.18%	2.340%
5	7.351	889	895	898	rBV	1477374	1743243	49.27%	8.746%
6	8.063	1011	1016	1019	rBV	655781	622176	17.59%	3.121%
7	9.145	1193	1200	1203	rBV	3264964	3304293	93.40%	16.577%
8	9.816	1310	1314	1318	rBV	820809	717475	20.28%	3.599%
9	10.622	1446	1451	1454	rBV	1913392	1903691	53.81%	9.551%
10	11.310	1565	1568	1572	rBV	857277	787654	22.26%	3.952%
11	12.916	1835	1841	1844	rBV	3359024	3537970	100.00%	17.750%
12	13.969	2016	2020	2029	rVB	553311	572745	16.19%	2.873%
13	14.745	2148	2152	2156	rVB	58163	62624	1.77%	0.314%
14	15.086	2205	2210	2217	rVB	72905	87503	2.47%	0.439%
15	15.463	2268	2274	2282	rVB2	355116	542926	15.35%	2.724%
16	15.921	2347	2352	2362	rVB	74619	123492	3.49%	0.620%
17	16.439	2435	2440	2449	rVB	66703	125619	3.55%	0.630%
18	17.057	2540	2545	2553	rVB2	48744	99197	2.80%	0.498%
19	17.786	2663	2669	2676	rVB4	33530	81691	2.31%	0.410%

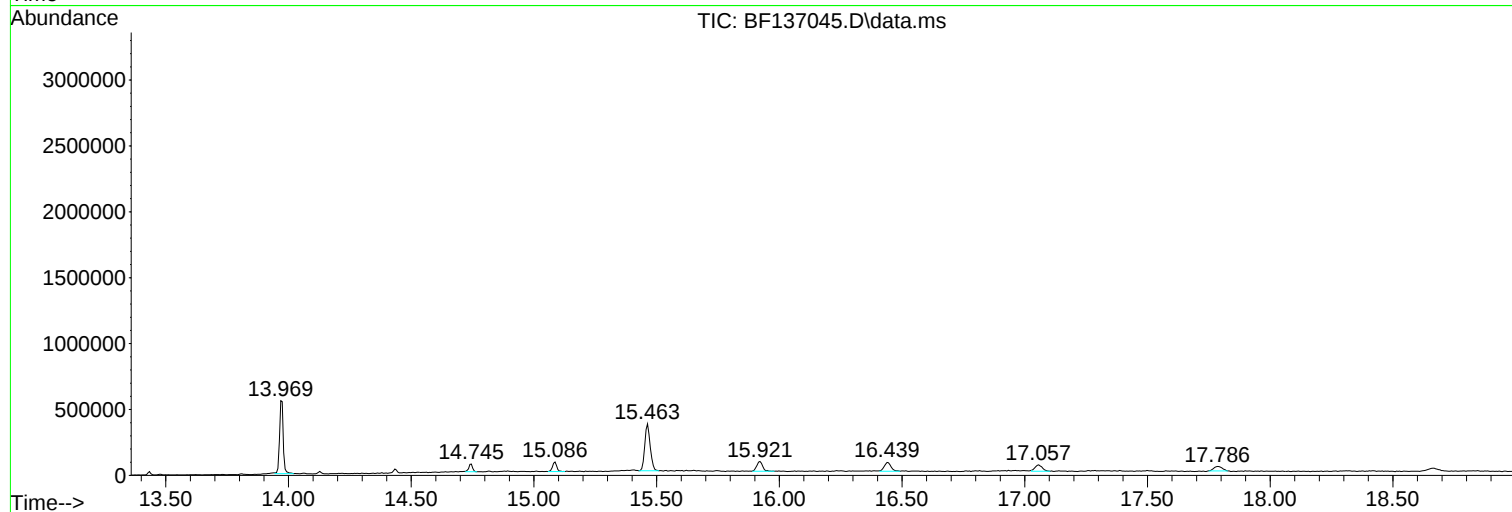
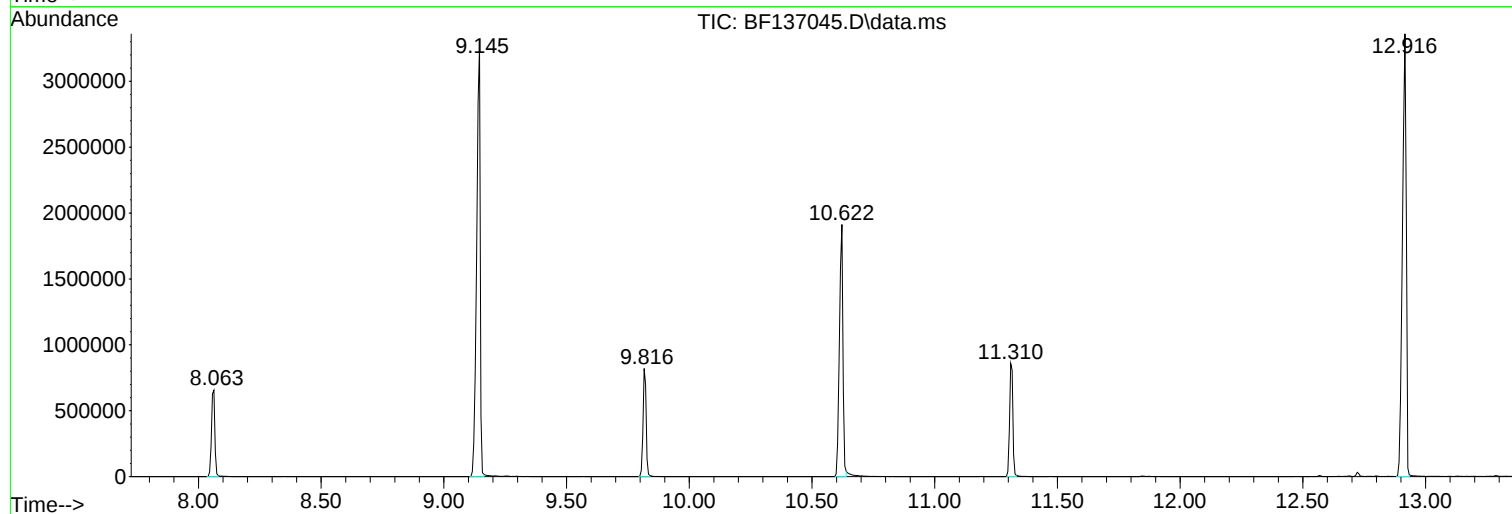
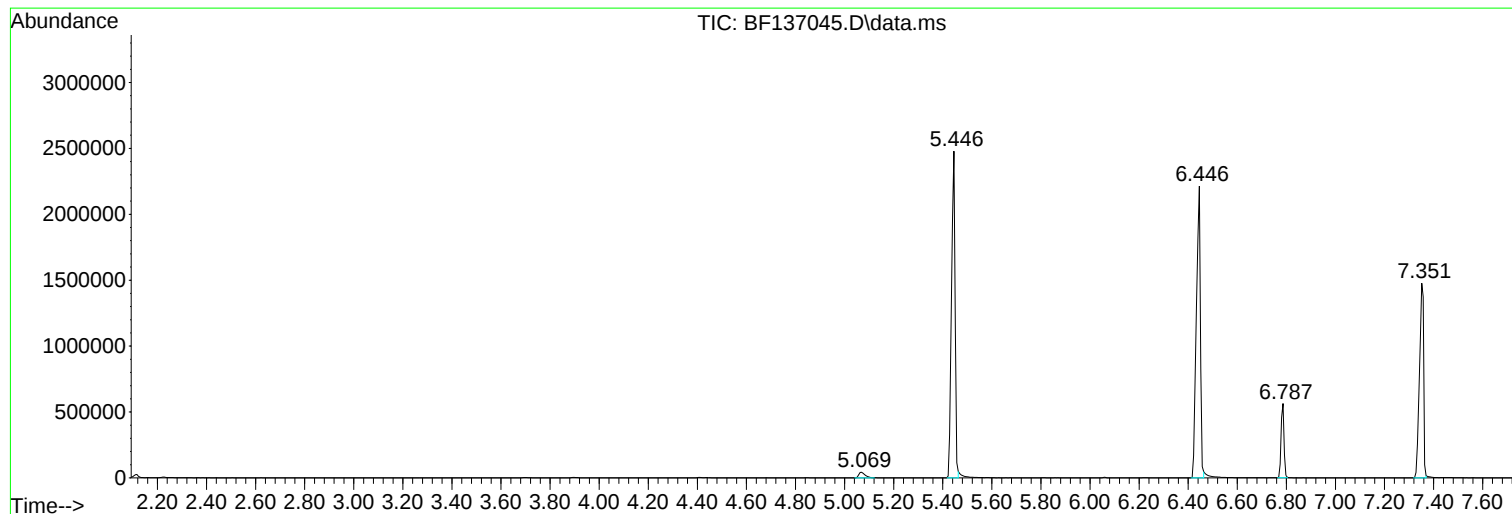
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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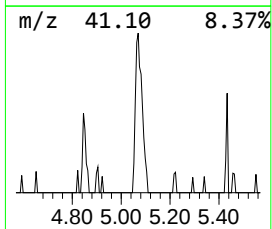
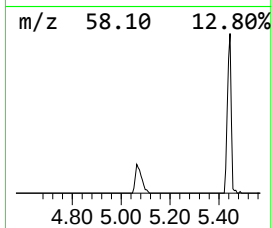
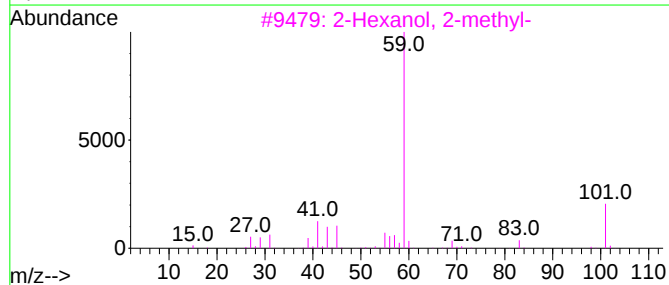
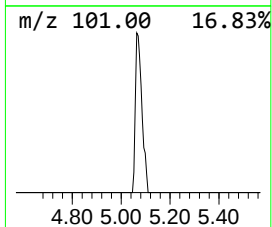
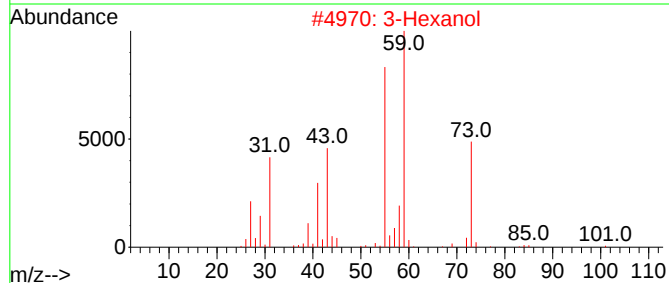
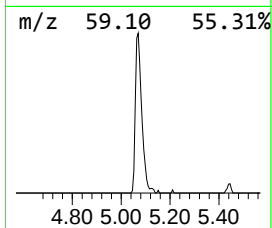
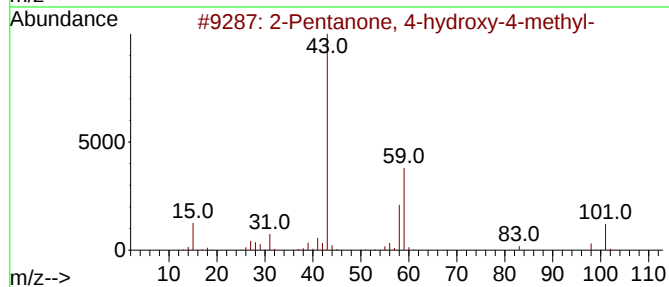
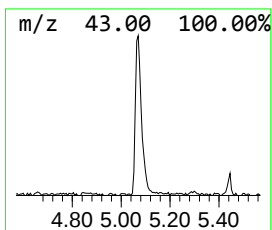
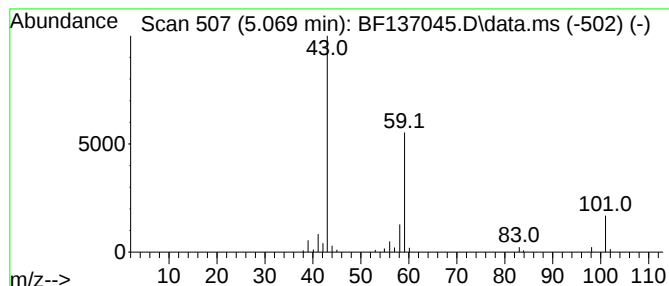
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	3.27 ng	76158	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hexanol	102	C6H14O	000623-37-0	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		



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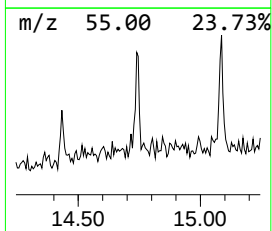
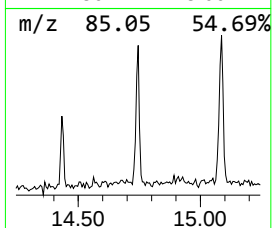
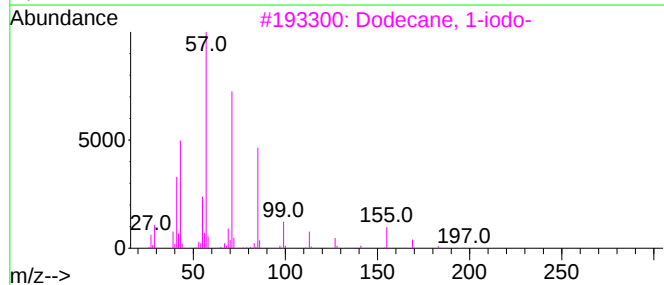
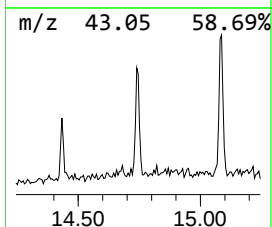
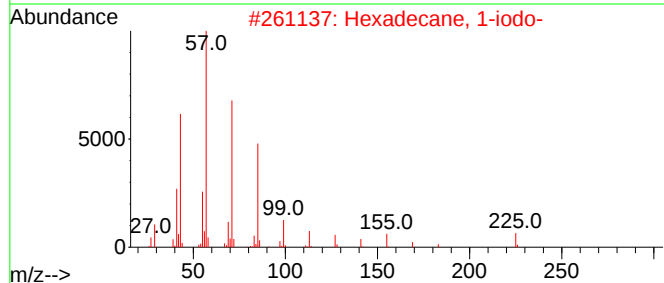
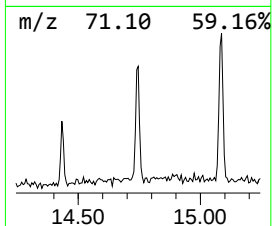
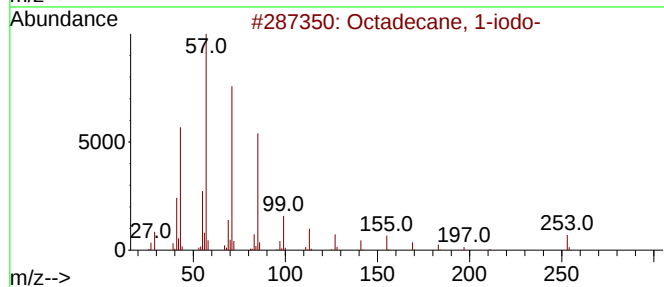
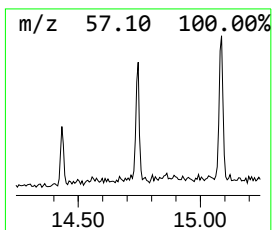
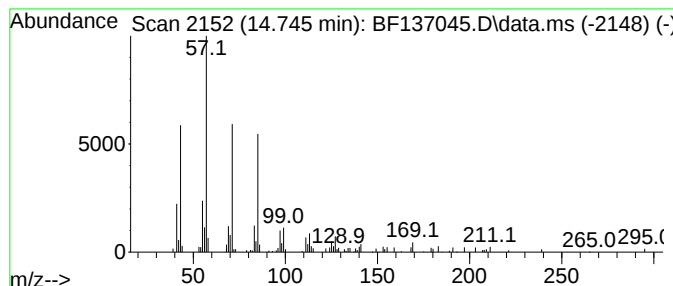
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	2.31 ng	62624	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
3		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
4		Nonadecane	268	C19H40	000629-92-5	83
5		Tetratetracontane	619	C44H90	007098-22-8	81



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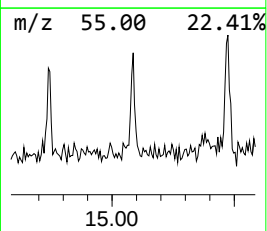
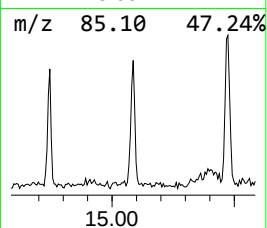
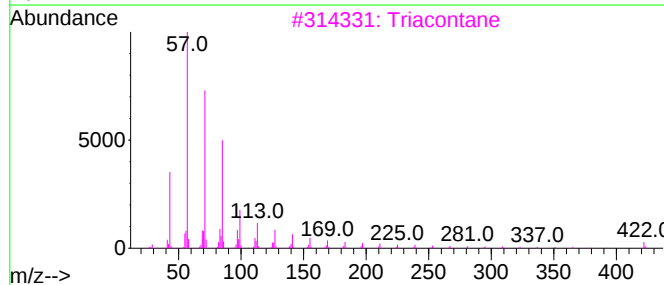
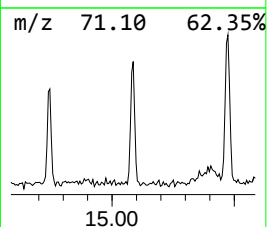
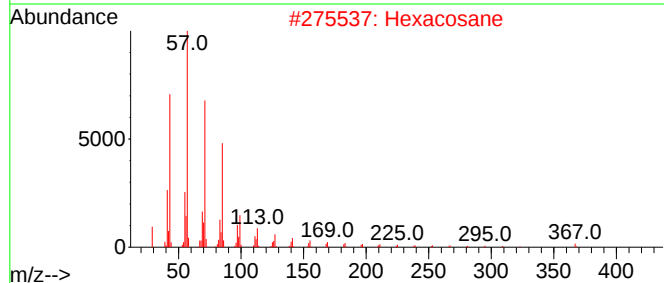
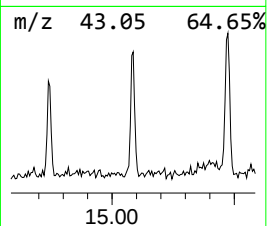
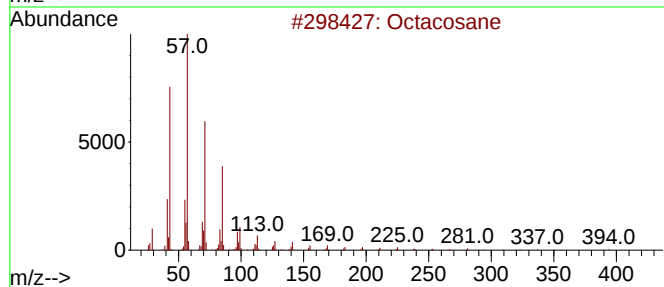
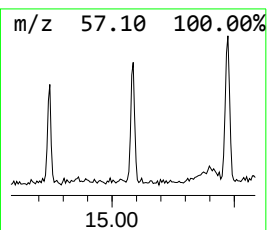
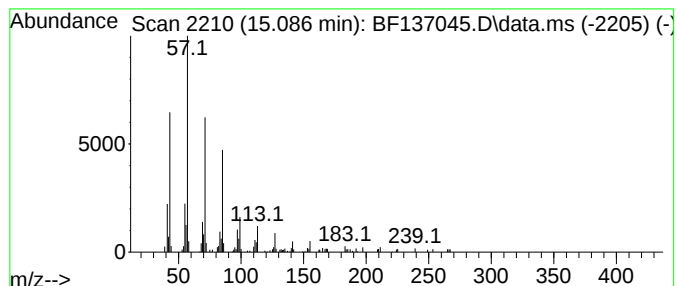
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	3.22 ng	87503	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	90
2		Hexacosane	366	C26H54	000630-01-3	90
3		Triacontane	422	C30H62	000638-68-6	90
4		Tetratetracontane	619	C44H90	007098-22-8	90
5		Heneicosane	296	C21H44	000629-94-7	90



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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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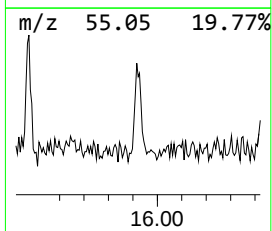
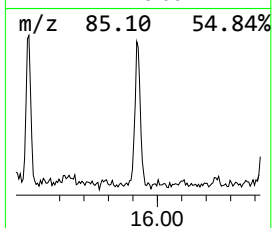
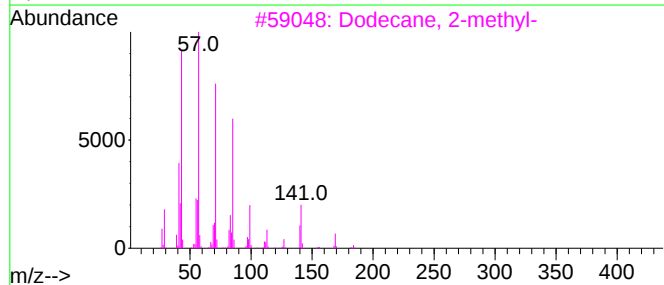
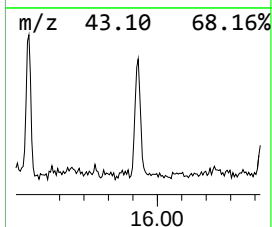
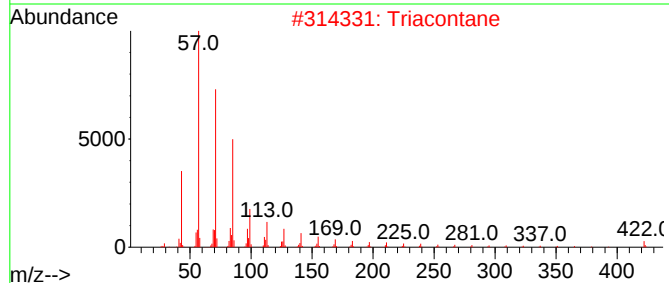
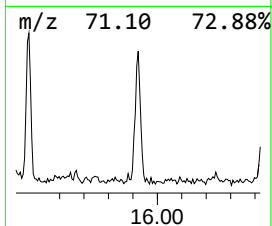
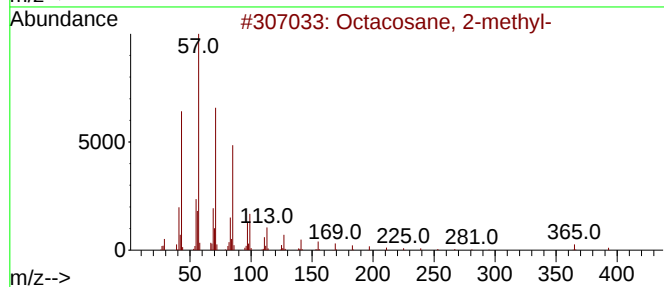
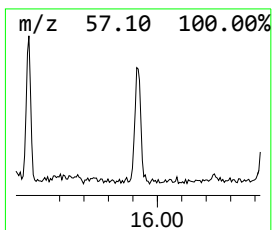
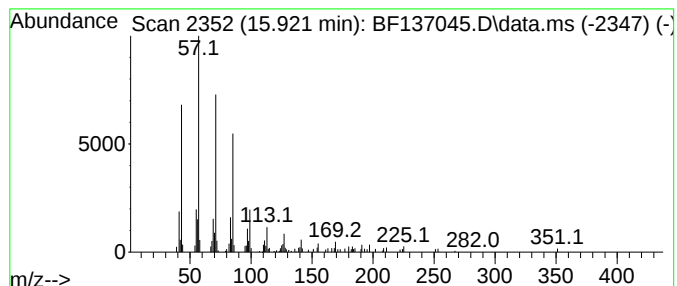
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Peak Number 4 Octacosane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	4.55 ng	123492	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2		Triacontane	422	C30H62	000638-68-6	90
3		Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
4		Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
5		Heneicosane	296	C21H44	000629-94-7	87



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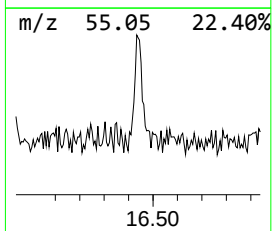
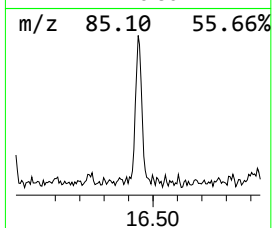
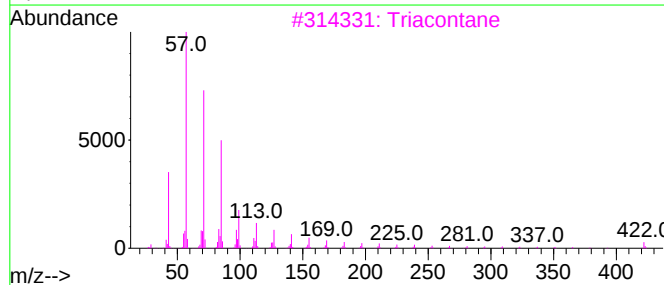
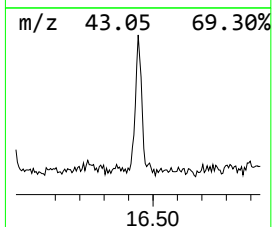
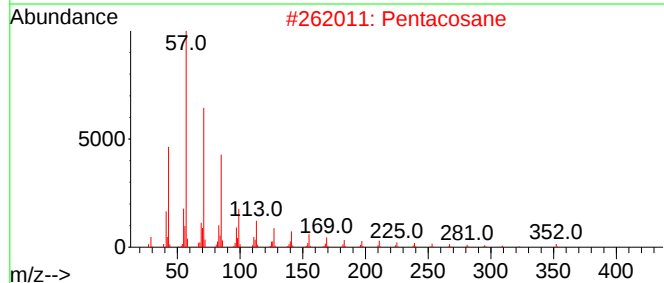
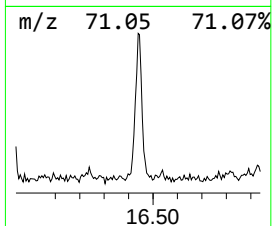
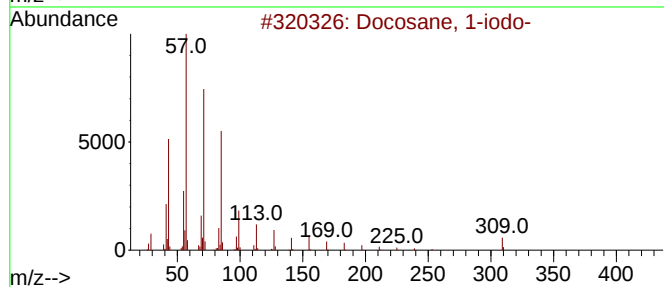
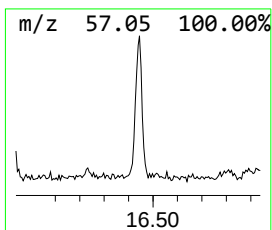
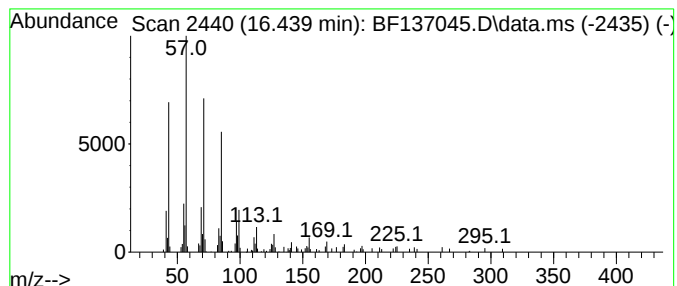
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Docosane, 1-iodo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.439	4.63 ng	125619	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
2			Pentacosane	352	C25H52	000629-99-2	90
3			Triacontane	422	C30H62	000638-68-6	90
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



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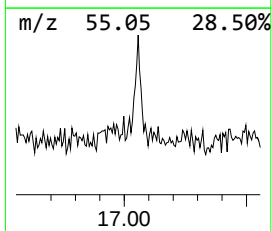
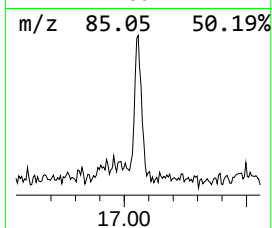
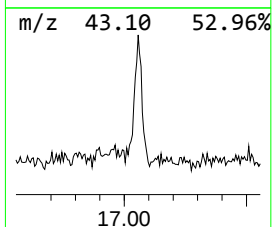
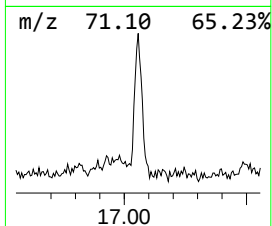
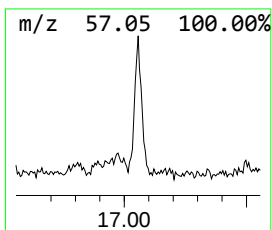
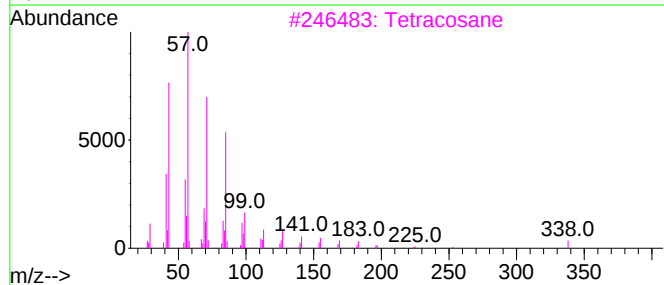
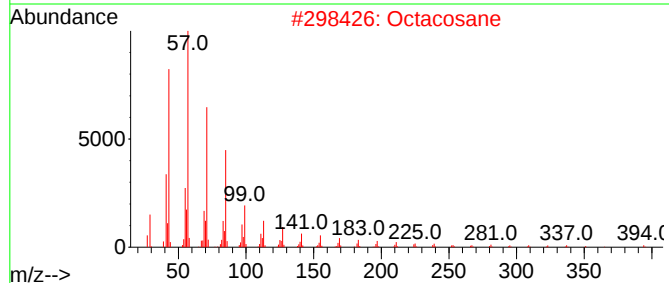
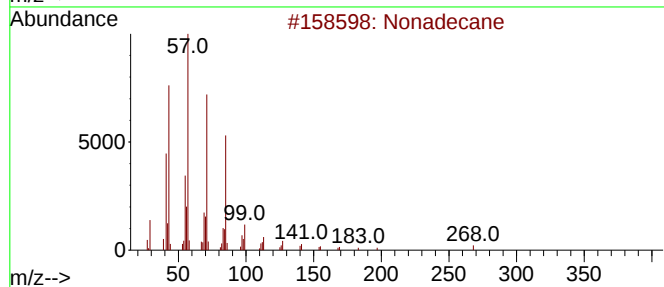
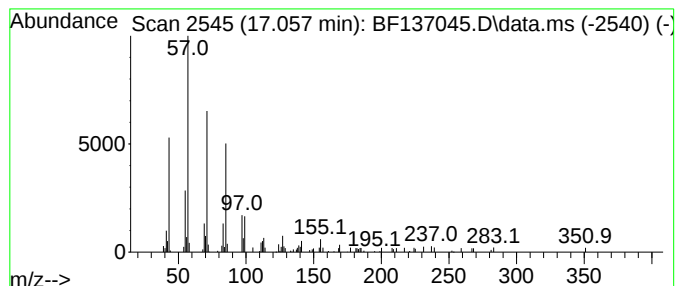
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.057	3.65 ng	99197	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Tetracosane	338	C24H50	000646-31-1	87
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137045.D
Acq On : 12 Jan 2024 13:28
Operator : CG\JU
Sample : PB158404BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158404BL

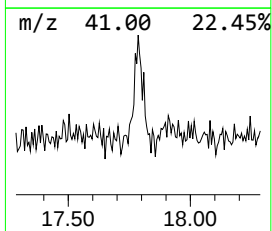
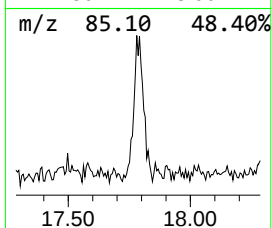
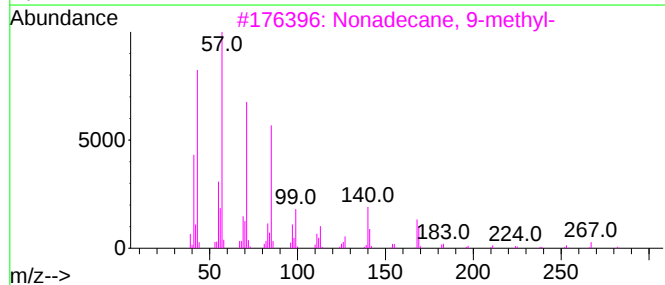
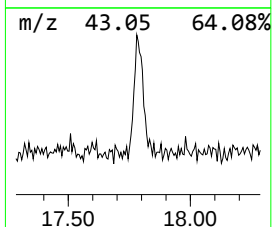
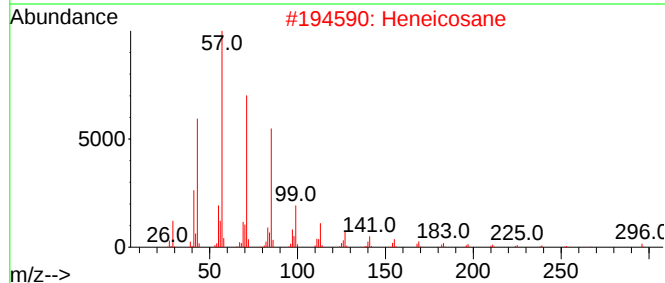
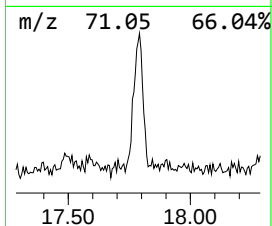
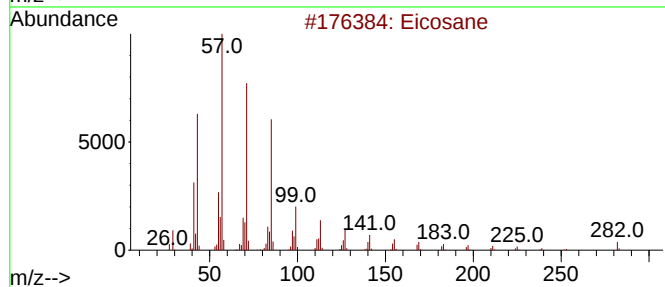
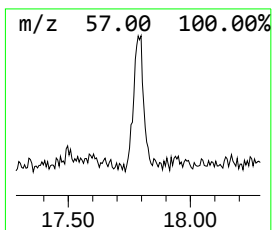
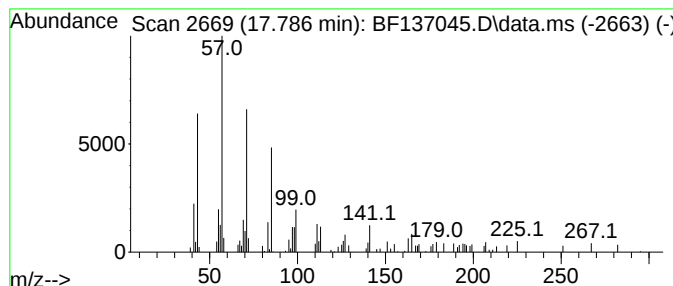
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.786	3.01 ng	81691	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	91
2	Heneicosane			296	C21H44	000629-94-7	83
3	Nonadecane, 9-methyl-			282	C20H42	013287-24-6	80
4	Hexacosane			366	C26H54	000630-01-3	80
5	Pentacosane			352	C25H52	000629-99-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
Data File : BF137045.D
Acq On : 12 Jan 2024 13:28
Operator : CG\JU
Sample : PB158404BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158404BL

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	76158	1	6.787	466472	20.0
Octadecane, 1-i...	14.745	2.3	ng	62624	6	15.463	542926	20.0
Octacosane	15.086	3.2	ng	87503	6	15.463	542926	20.0
Octacosane, 2-m...	15.921	4.5	ng	123492	6	15.463	542926	20.0
Docosane, 1-iodo-	16.439	4.6	ng	125619	6	15.463	542926	20.0
Nonadecane	17.057	3.6	ng	99197	6	15.463	542926	20.0
Eicosane	17.786	3.0	ng	81691	6	15.463	542926	20.0