

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
 Data File : BF132023.D
 Acq On : 11 Jan 2023 14:29
 Operator : CG\JU
 Sample : PB150096BL
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB150096BL

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-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132023.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.999	491	495	514	rBV	233718	403141	7.72%	1.440%
2	5.404	560	564	568	rBV	2795966	3110703	59.53%	11.113%
3	6.428	733	738	741	rBV	2653101	3194438	61.14%	11.412%
4	6.775	794	797	801	rBV	726289	626623	11.99%	2.239%
5	7.357	889	896	899	rBV	1845213	2132635	40.82%	7.619%
6	8.069	1011	1017	1020	rBV	933945	846825	16.21%	3.025%
7	9.151	1194	1201	1204	rBV	4067196	4335067	82.97%	15.486%
8	9.828	1310	1316	1320	rBV	1190499	1075741	20.59%	3.843%
9	10.628	1446	1452	1455	rBV	2835530	2973388	56.91%	10.622%
10	11.322	1565	1570	1574	rBV	1364912	1209613	23.15%	4.321%
11	12.733	1806	1810	1813	rBV	146754	114976	2.20%	0.411%
12	12.927	1837	1843	1845	rBV	5005892	5225001	100.00%	18.666%
13	13.439	1927	1930	1934	rVB	141055	117818	2.25%	0.421%
14	13.974	2017	2021	2025	rBV	1088206	947270	18.13%	3.384%
15	14.739	2147	2151	2156	rBV	91841	92076	1.76%	0.329%
16	15.074	2205	2208	2214	rVB	114662	136047	2.60%	0.486%
17	15.445	2265	2271	2280	rVB2	558890	784570	15.02%	2.803%
18	15.880	2340	2345	2350	rBV	105454	154224	2.95%	0.551%
19	16.380	2424	2430	2437	rBV	95683	167037	3.20%	0.597%
20	16.962	2521	2529	2536	rBV2	65386	135996	2.60%	0.486%
21	17.651	2638	2646	2654	rVB3	54272	131212	2.51%	0.469%
22	18.462	2777	2784	2792	rVB5	28912	78274	1.50%	0.280%

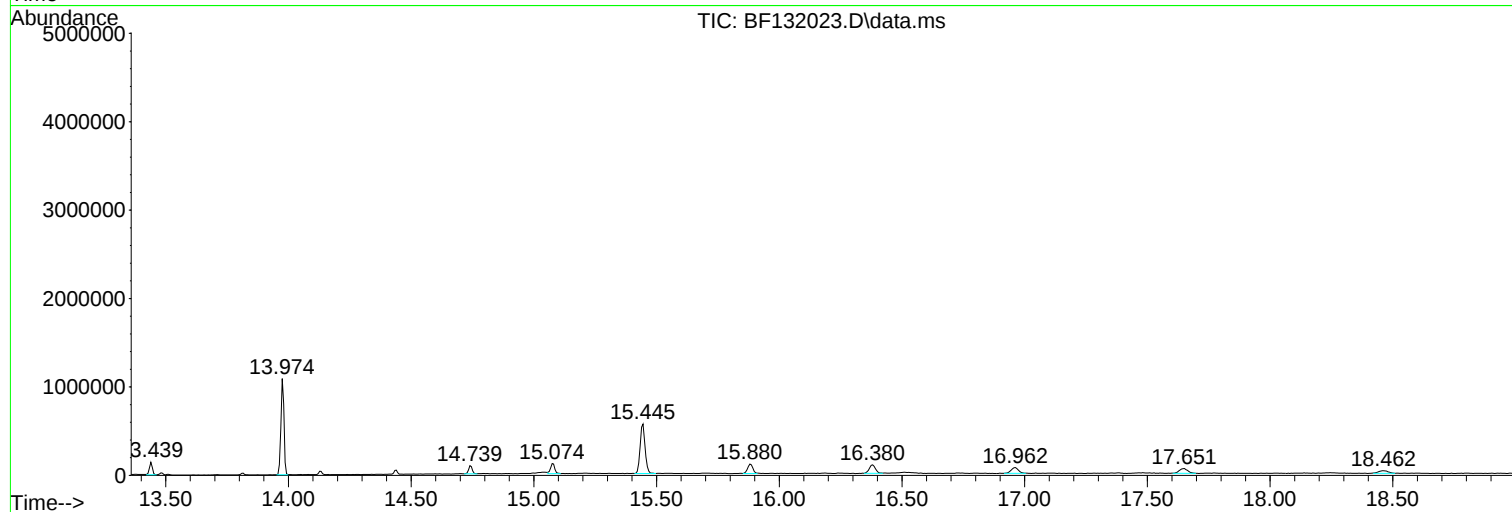
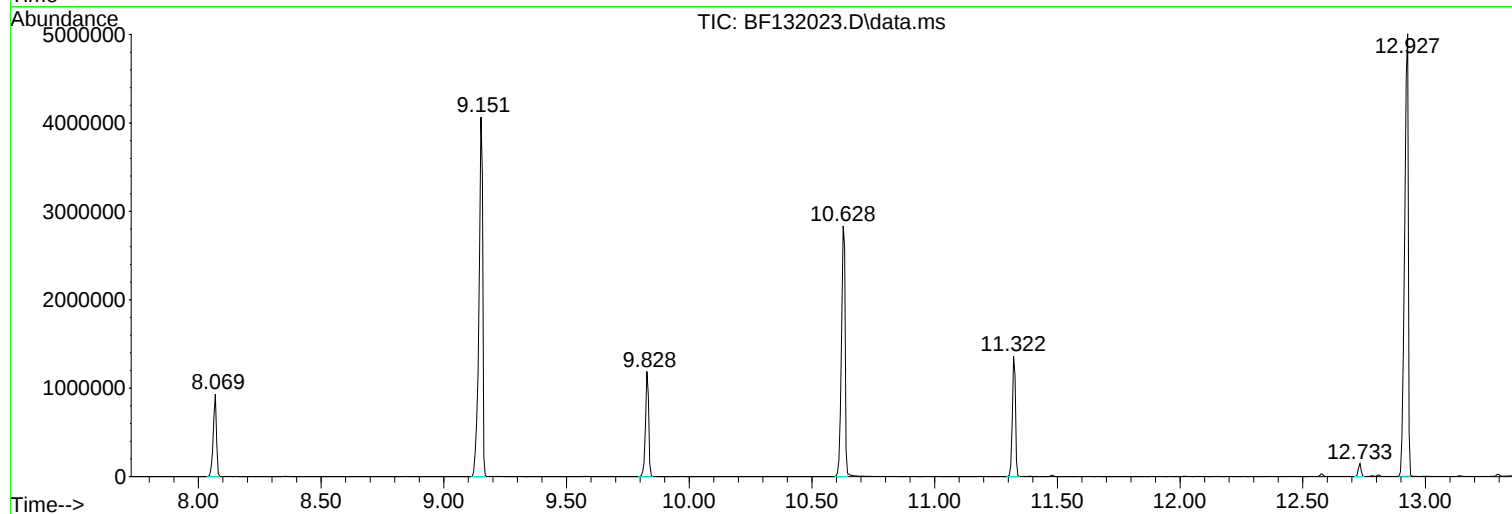
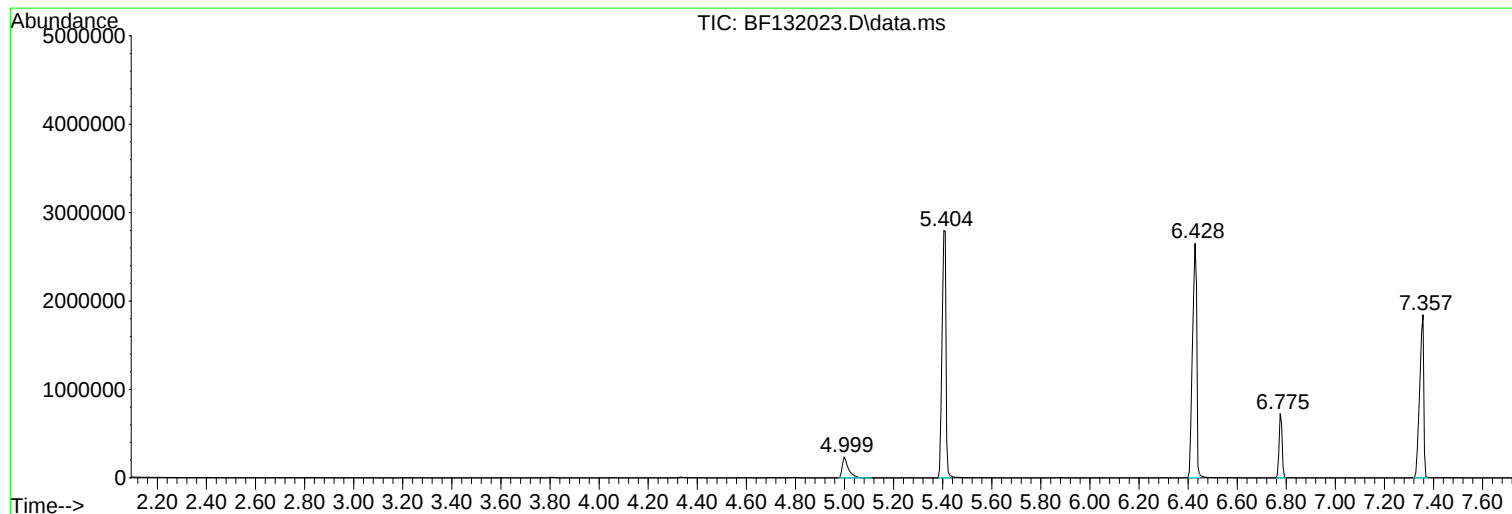
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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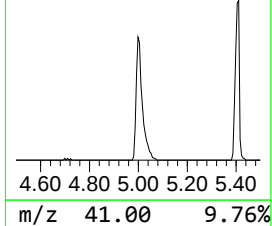
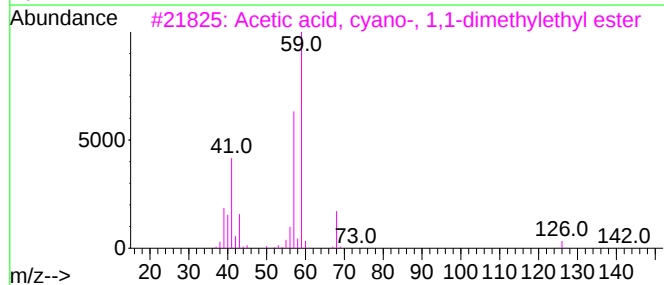
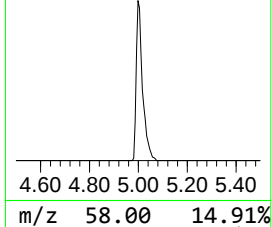
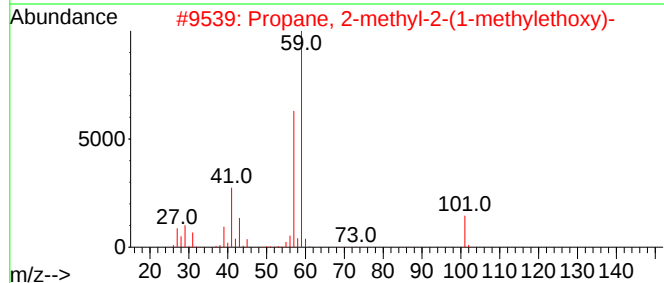
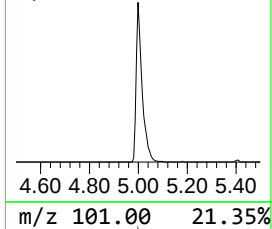
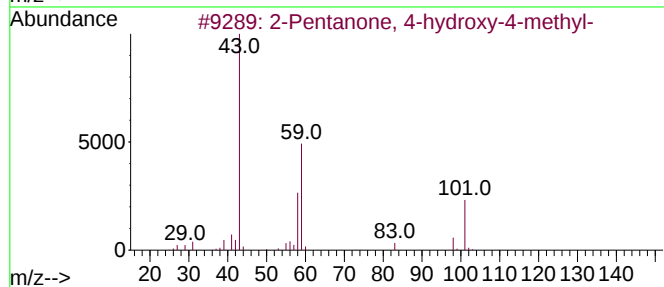
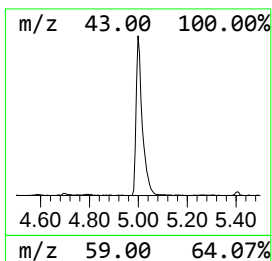
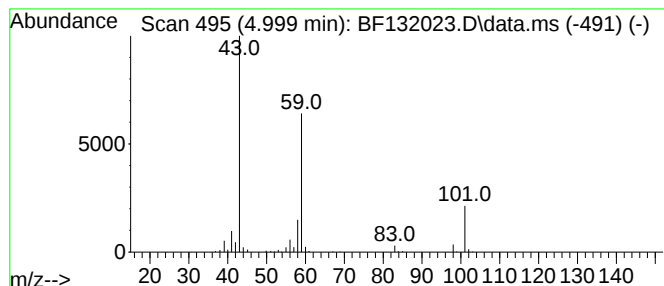
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.999	12.87 ng	403141	1,4-Dichlorobenzene-d4	6.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50	
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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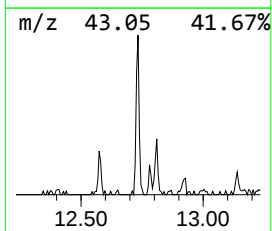
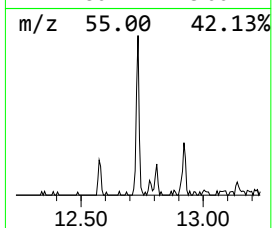
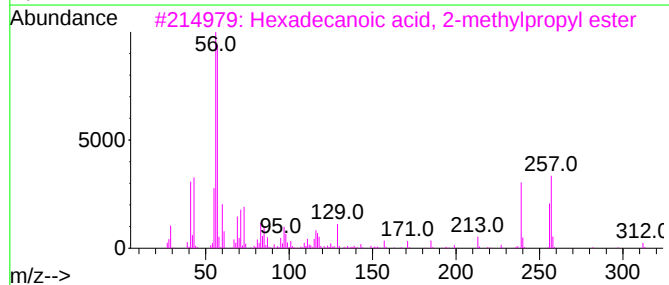
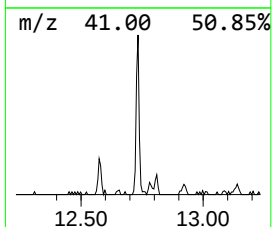
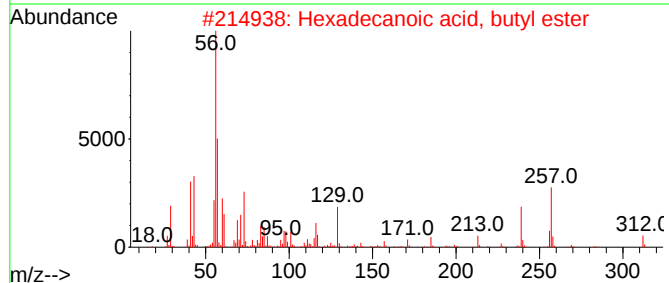
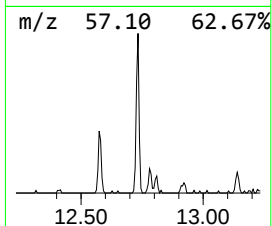
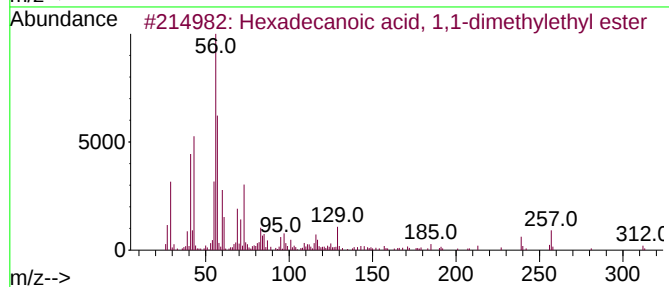
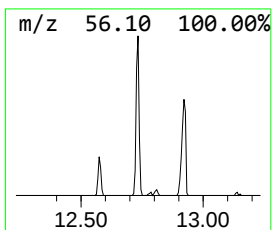
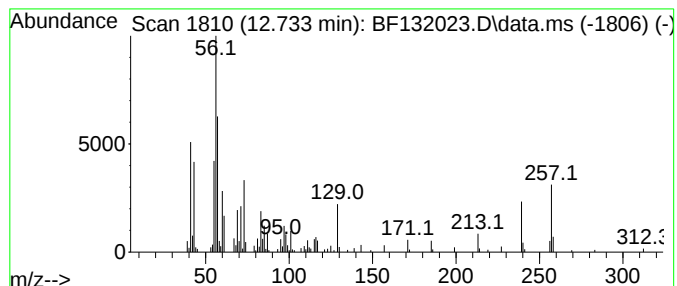
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ClientSampleId :
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Hexadecanoic acid, 1,1-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.733	2.43 ng	114976	Chrysene-d12	13.974	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	92
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	90
4	2-Isopropyl-3-vinyloxirane	112	C7H12O	070777-23-0	35
5	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30



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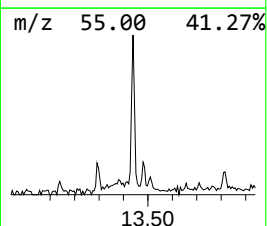
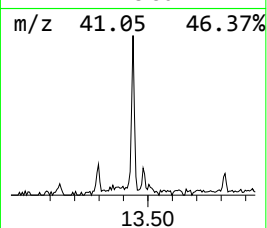
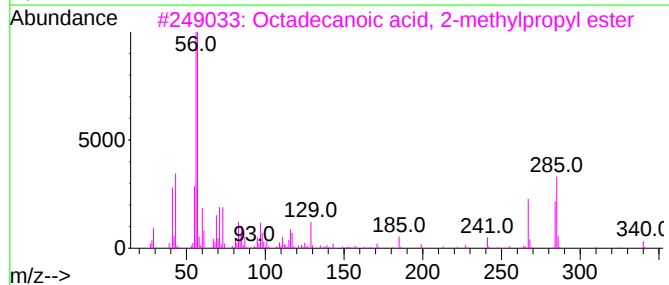
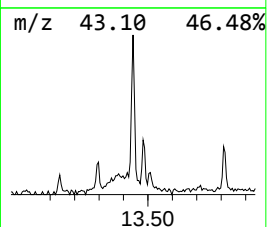
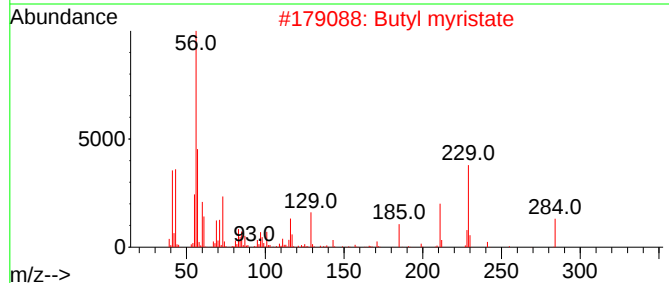
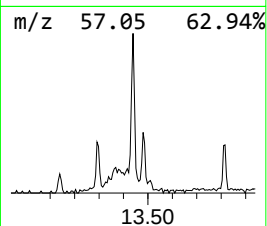
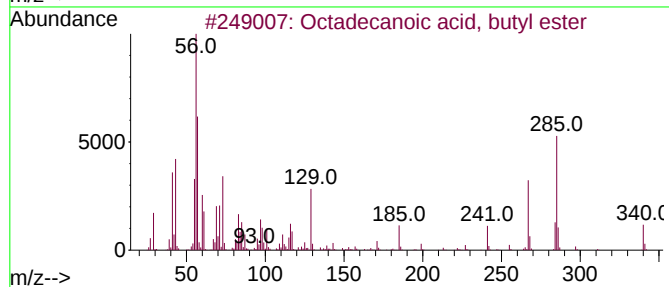
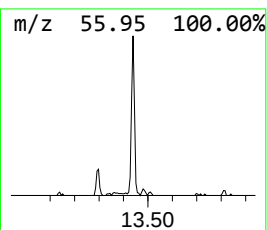
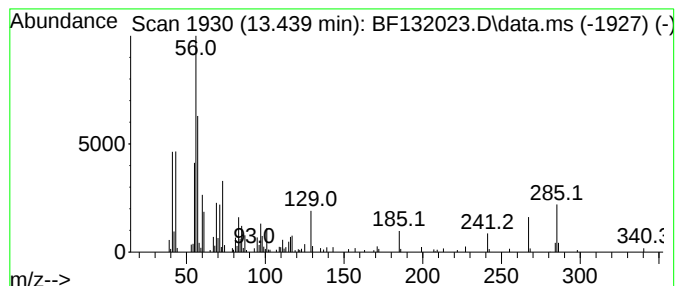
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Peak Number 3 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.439	2.49 ng	117818	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2			Butyl myristate	284	C18H36O2	000110-36-1	72
3			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	38
4			(1-Propylcyclopropyl)methanamine	113	C7H15N	1368512-93-9	27
5			2-Butyl-1-decene	196	C14H28	051655-65-3	27



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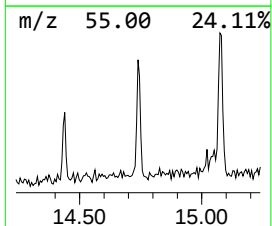
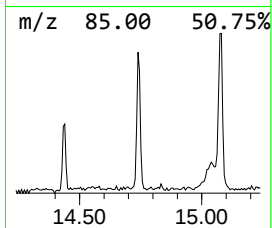
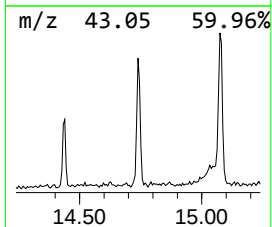
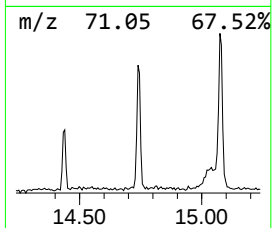
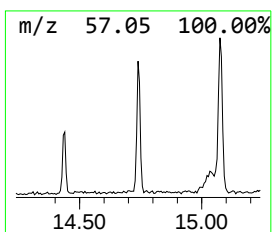
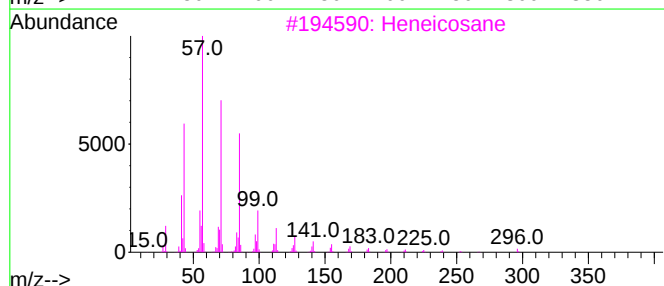
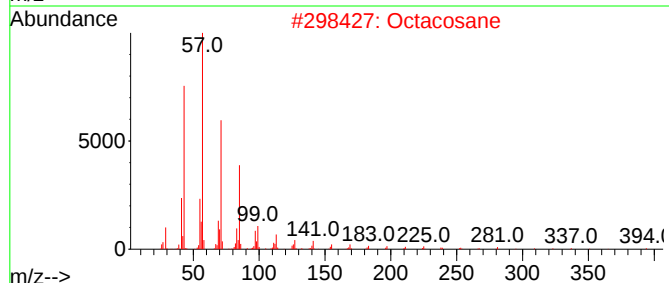
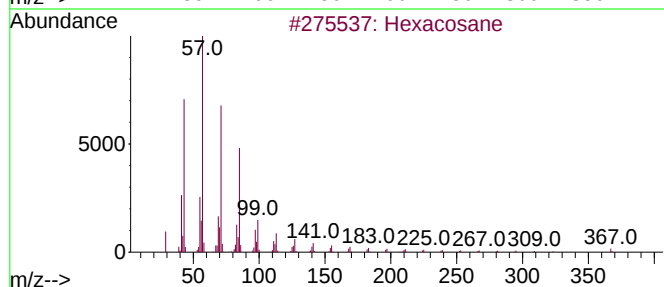
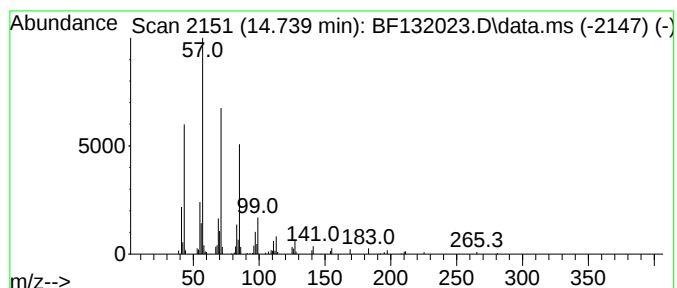
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Peak Number 4 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	2.35 ng	92076	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			2-Methyltetracosane	352	C25H52	001560-78-7	91
5			Tetratetracontane	619	C44H90	007098-22-8	87



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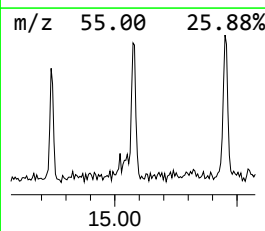
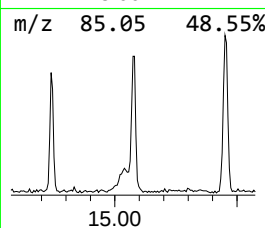
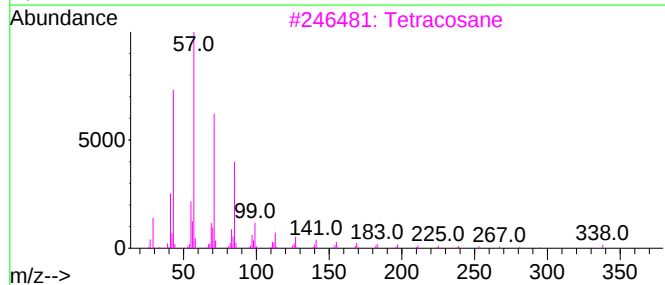
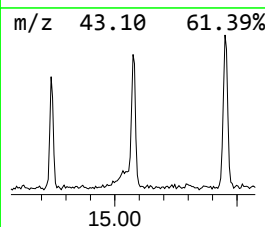
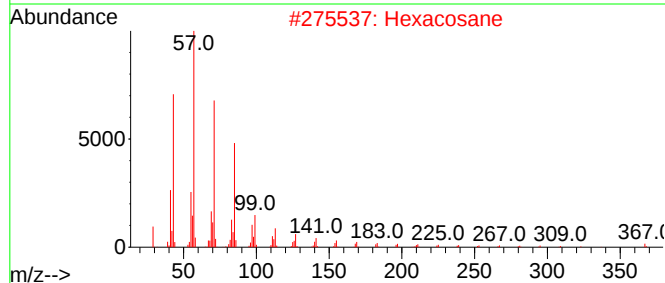
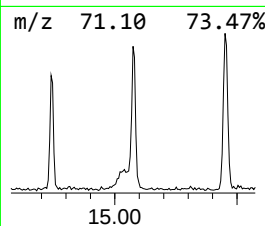
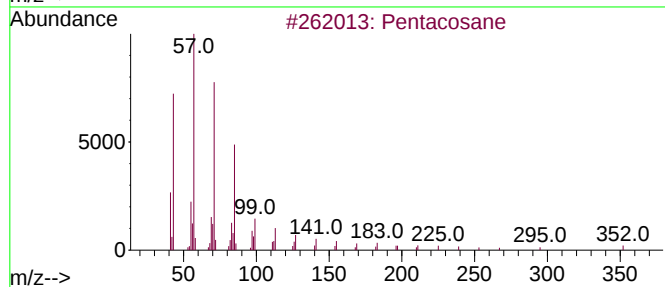
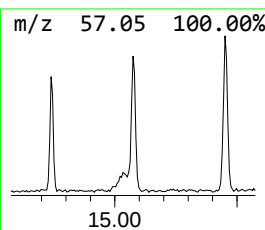
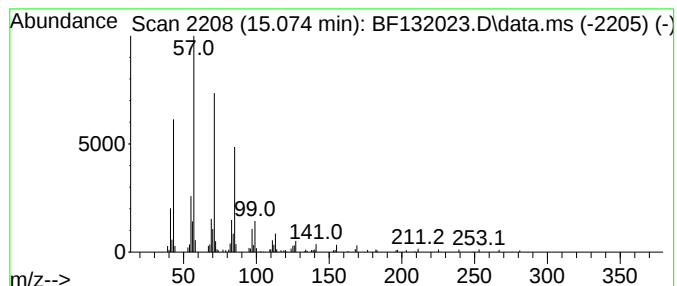
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Peak Number 5 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.074	3.47 ng	136047	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Tetratetracontane	619	C44H90	007098-22-8	91
5			Triacontane	422	C30H62	000638-68-6	87



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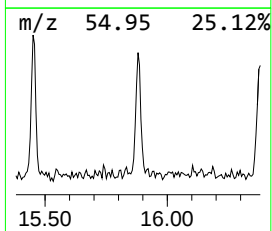
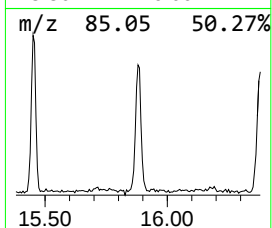
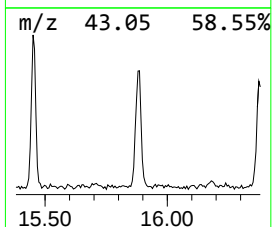
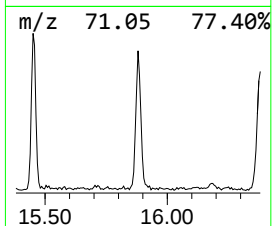
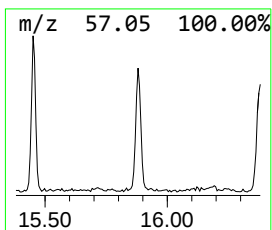
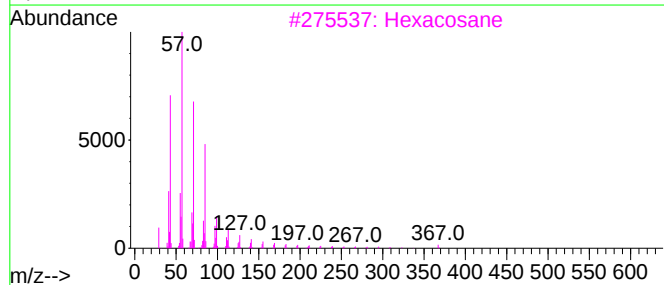
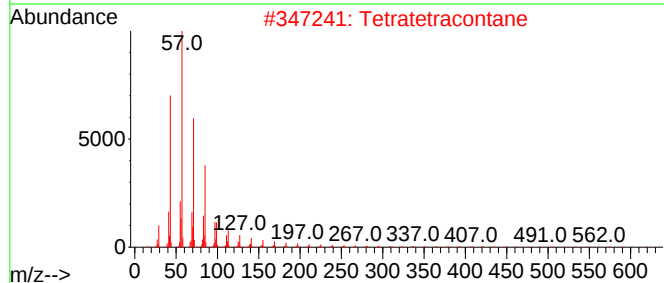
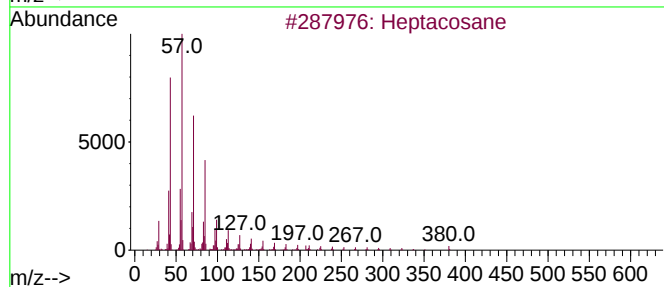
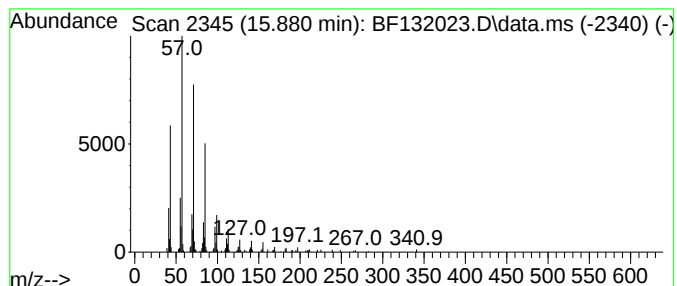
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
15.880	3.93 ng	154224	Perylene-d12	15.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132023.D
Acq On : 11 Jan 2023 14:29
Operator : CG\JU
Sample : PB150096BL
Misc :
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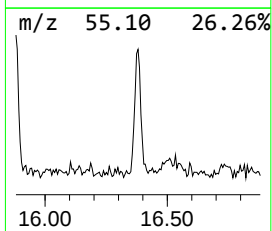
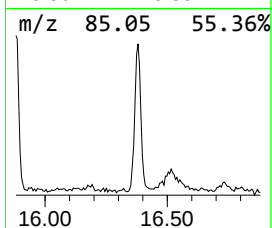
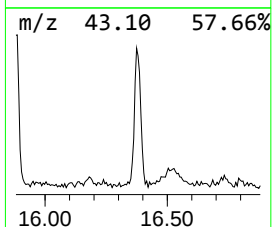
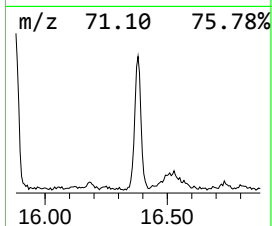
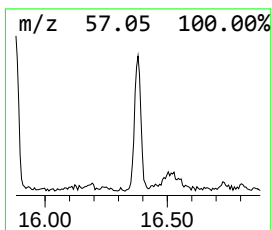
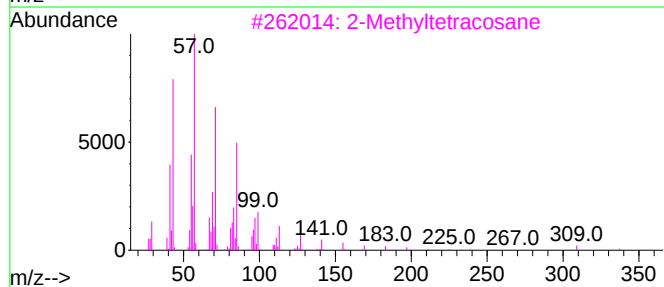
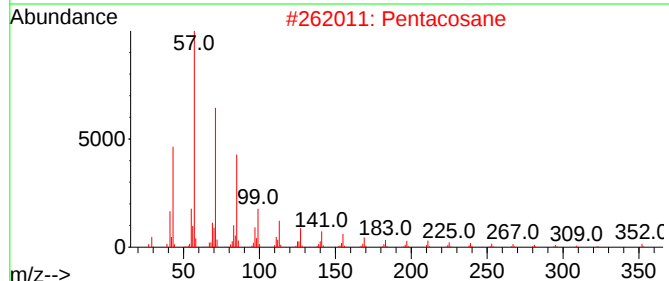
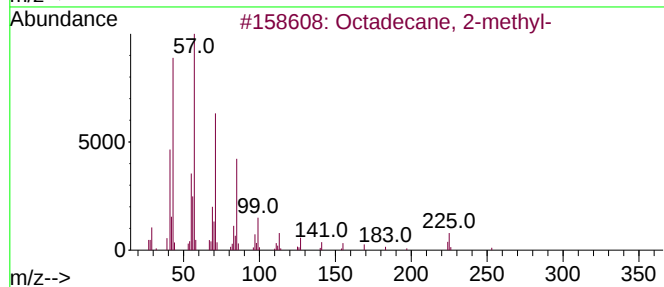
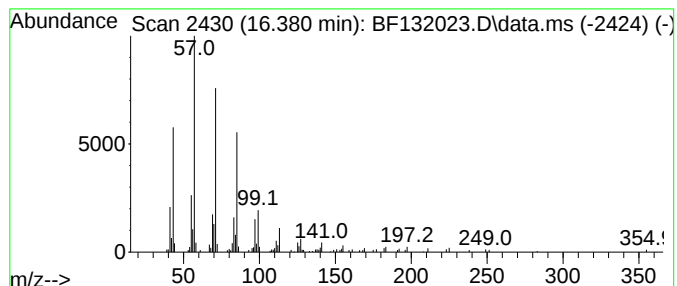
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.380	4.26 ng	167037	Perylene-d12	15.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
2	Pentacosane	352	C25H52	000629-99-2	90
3	2-Methyltetracosane	352	C25H52	001560-78-7	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132023.D
Acq On : 11 Jan 2023 14:29
Operator : CG\JU
Sample : PB150096BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150096BL

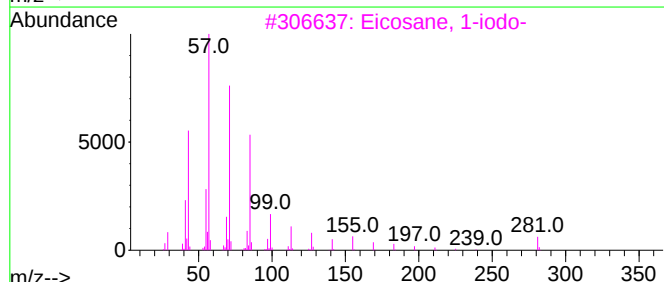
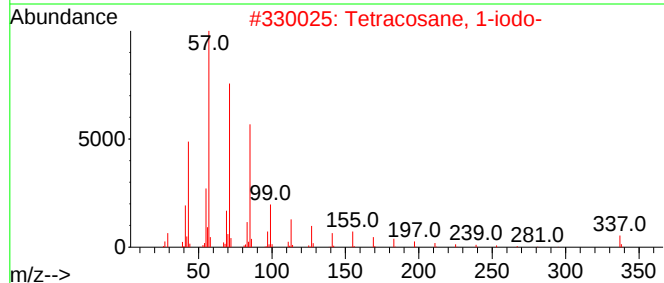
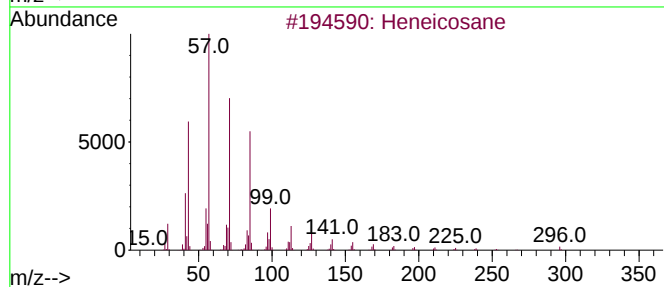
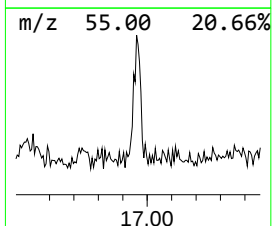
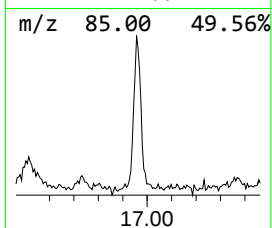
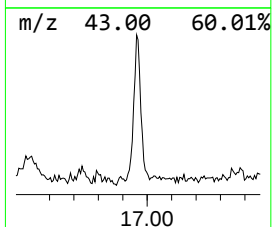
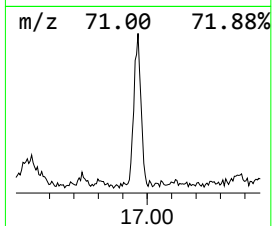
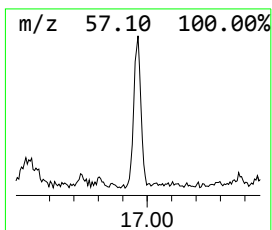
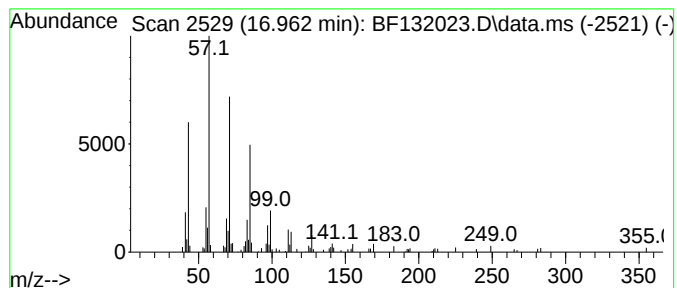
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.962	3.47 ng	135996	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	87
2			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	83
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
4			Hexacosane	366	C26H54	000630-01-3	83
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132023.D
Acq On : 11 Jan 2023 14:29
Operator : CG\JU
Sample : PB150096BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

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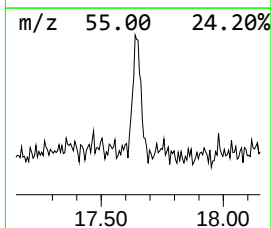
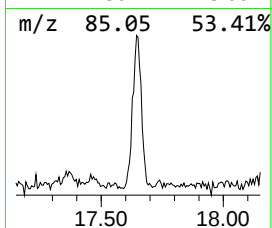
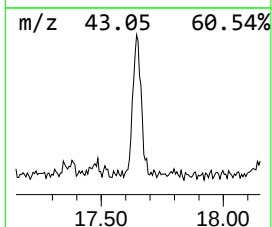
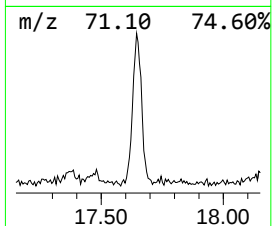
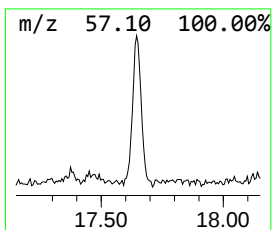
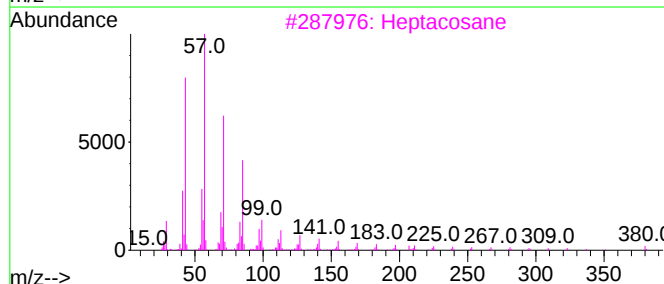
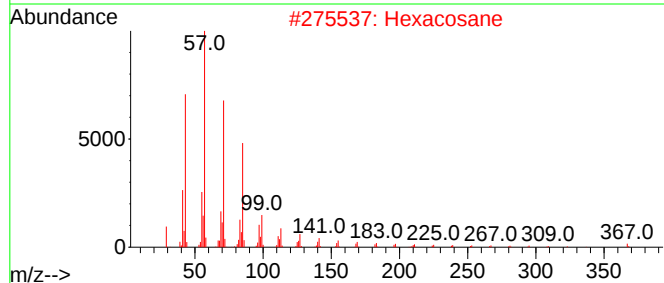
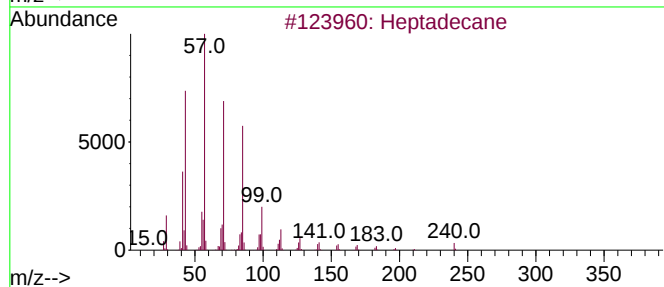
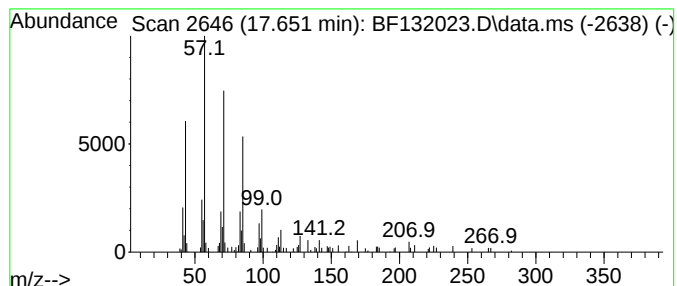
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.651	3.34 ng	131212	Perylene-d12	15.439

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Eicosane	282	C20H42	000112-95-8	91
5		10-Methylnonadecane	282	C20H42	056862-62-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011123\
Data File : BF132023.D
Acq On : 11 Jan 2023 14:29
Operator : CG\JU
Sample : PB150096BL
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB150096BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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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Hexadecanoic ac...	12.733	2.4	ng	114976	5	13.974	947270	20.0
Octadecanoic ac...	13.439	2.5	ng	117818	5	13.974	947270	20.0
Hexacosane	14.739	2.4	ng	92076	6	15.439	784570	20.0
Pentacosane	15.074	3.5	ng	136047	6	15.439	784570	20.0
Heptacosane	15.880	3.9	ng	154224	6	15.439	784570	20.0
Octadecane, 2-m...	16.380	4.3	ng	167037	6	15.439	784570	20.0
Heneicosane	16.962	3.5	ng	135996	6	15.439	784570	20.0
Heptadecane	17.651	3.3	ng	131212	6	15.439	784570	20.0