

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
 Data File : BF133207.D
 Acq On : 03 May 2023 15:09
 Operator : CG\JU
 Sample : 02583-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CF-25

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133207.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.340	548	553	580	rBV	3462670	3862753	85.40%	12.031%
2	6.369	723	728	731	rBV	3937708	3883213	85.86%	12.095%
3	6.728	786	789	793	rVB	1387906	1083802	23.96%	3.376%
4	7.292	881	885	888	rBV	3002848	2561191	56.63%	7.977%
5	8.010	1004	1007	1011	rBV	1713126	1475186	32.62%	4.595%
6	9.092	1187	1191	1194	rBV	5150240	4522984	100.00%	14.088%
7	9.763	1302	1305	1309	rBV	1960577	1626654	35.96%	5.067%
8	10.475	1423	1426	1430	rBV	416575	317466	7.02%	0.989%
9	10.551	1435	1439	1452	rBV	846941	838432	18.54%	2.611%
10	11.204	1543	1550	1554	rBV2	70105	89801	1.99%	0.280%
11	11.245	1554	1557	1561	rVB	1815069	1473151	32.57%	4.588%
12	11.557	1606	1610	1614	rVB	47703	57796	1.28%	0.180%
13	11.639	1619	1624	1630	rVB	51652	72527	1.60%	0.226%
14	11.780	1640	1648	1661	rBV2	229124	456269	10.09%	1.421%
15	12.051	1688	1694	1701	rVB	185658	266056	5.88%	0.829%
16	12.363	1742	1747	1754	rVV	112214	144338	3.19%	0.450%
17	12.433	1755	1759	1765	rVB	103981	129615	2.87%	0.404%
18	12.557	1775	1780	1792	rBV2	153778	328565	7.26%	1.023%
19	12.833	1823	1827	1831	rBV	3746780	3491614	77.20%	10.875%
20	13.792	1984	1990	1991	rBV	82411	127734	2.82%	0.398%
21	13.880	2001	2005	2009	rVB	1132699	1017810	22.50%	3.170%
22	14.063	2033	2036	2040	rBV	56500	50497	1.12%	0.157%
23	14.368	2085	2088	2090	rBV	57971	57893	1.28%	0.180%
24	14.451	2095	2102	2104	rBV2	369190	737505	16.31%	2.297%
25	14.663	2136	2138	2143	rVB	81803	85819	1.90%	0.267%
26	14.986	2190	2193	2199	rVB	90742	95437	2.11%	0.297%
27	15.304	2242	2247	2251	rBV	1010557	1129211	24.97%	3.517%
28	15.351	2251	2255	2259	rVB2	74356	97684	2.16%	0.304%
29	15.762	2321	2325	2331	rVB2	78989	123867	2.74%	0.386%
30	16.709	2480	2486	2495	rVB4	148223	407031	9.00%	1.268%
31	18.115	2717	2725	2744	rVB4	335381	1493955	33.03%	4.653%

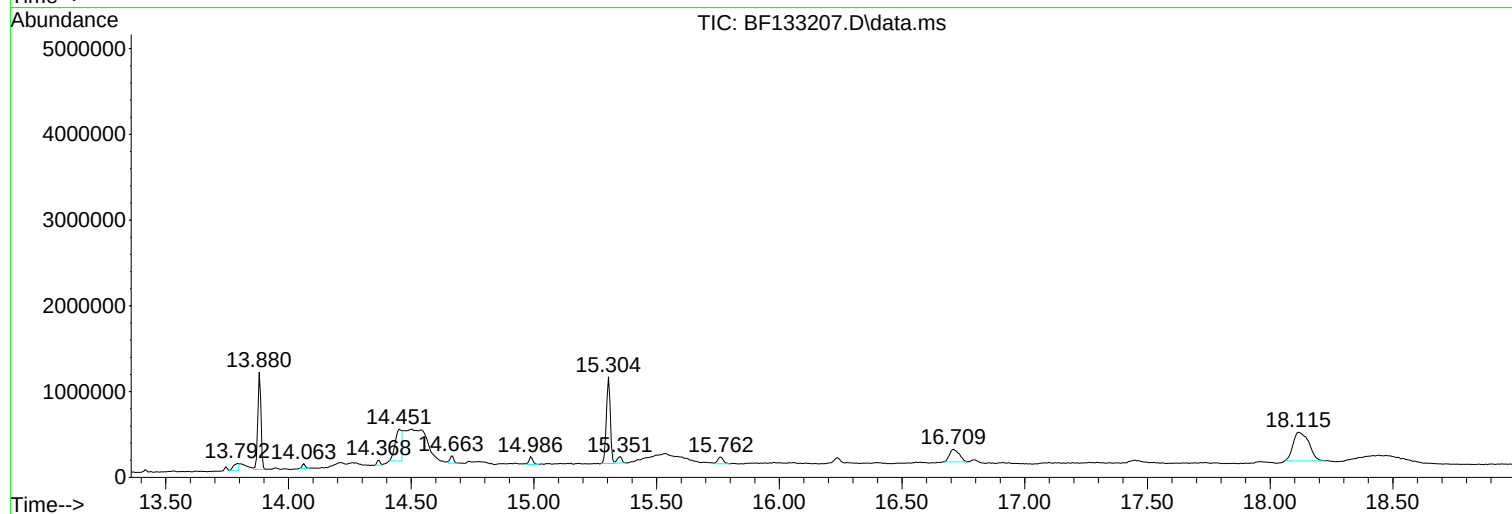
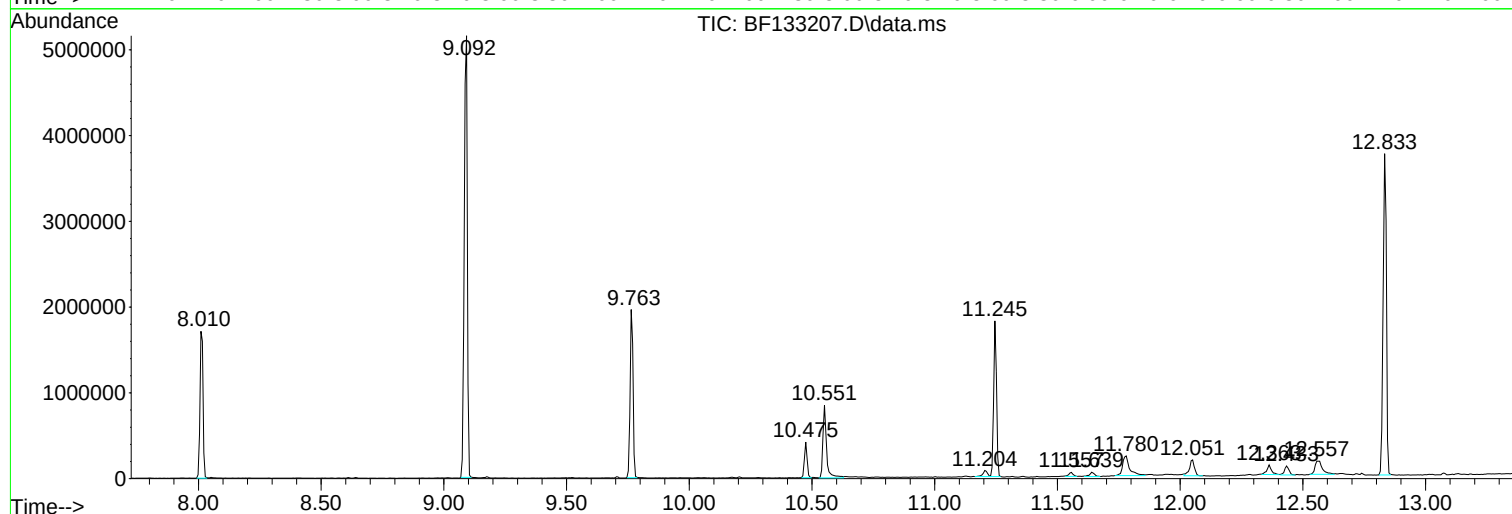
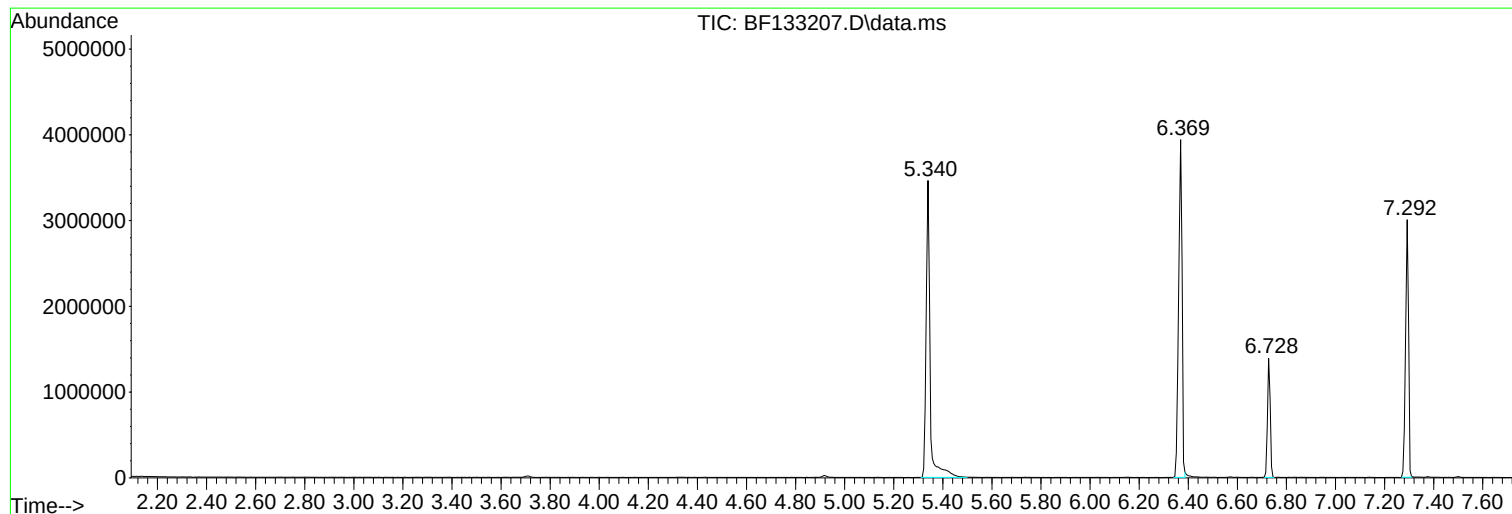
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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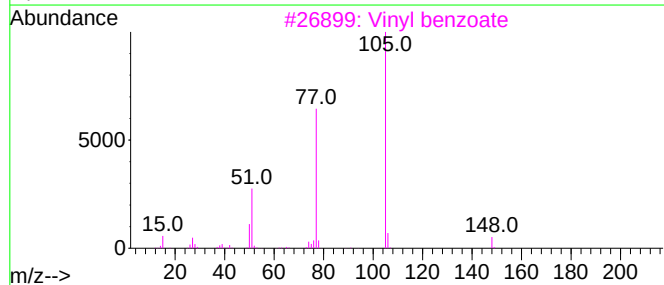
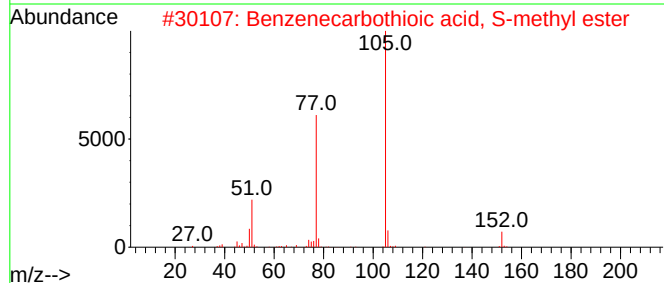
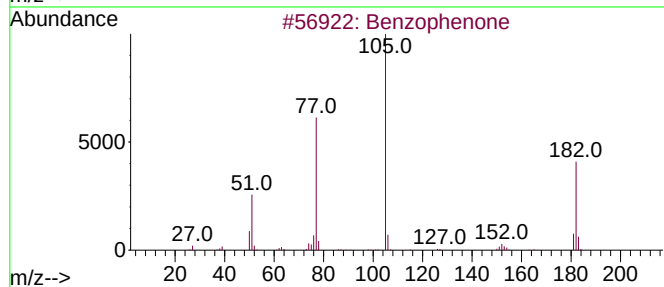
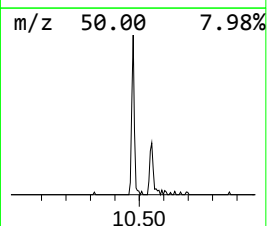
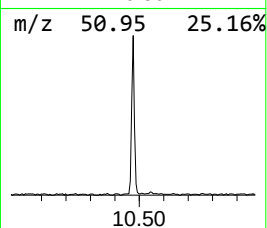
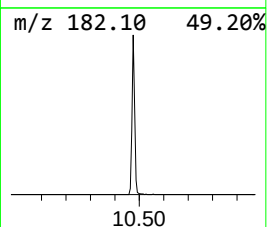
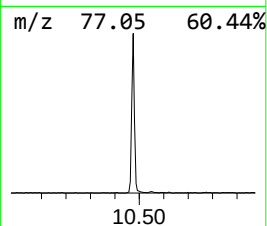
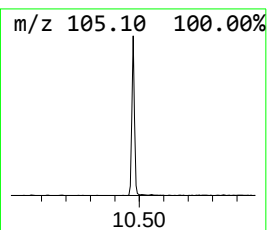
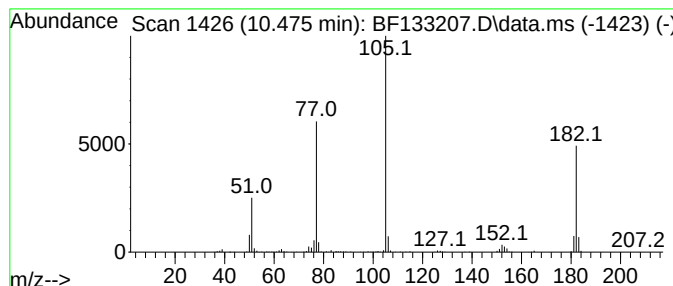
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.90 ng	317466	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			Vinyl benzoate	148	C9H8O2	000769-78-8	47
4			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47
5			N-Methylbenzamide, N-heptafluoro...	331	C12H8F7NO2	1000446-97-2	47



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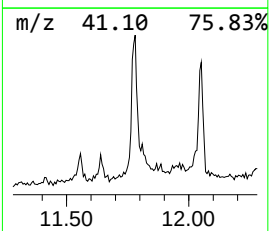
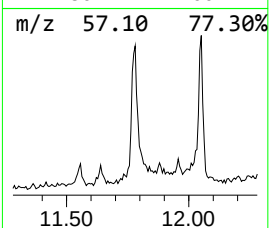
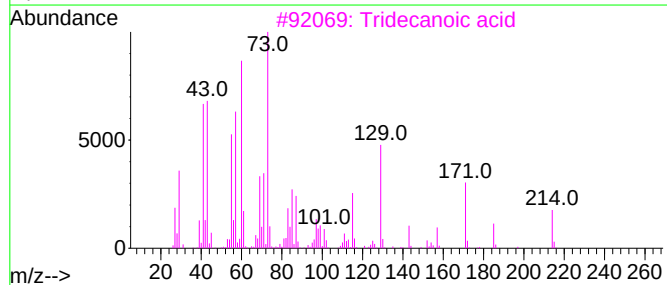
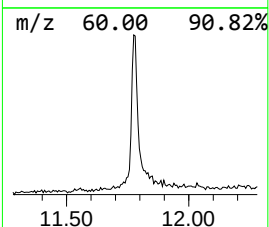
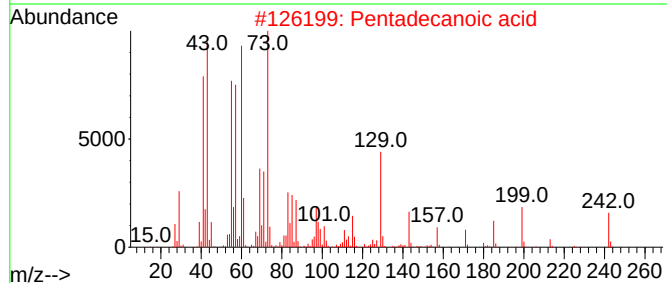
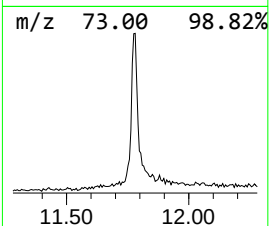
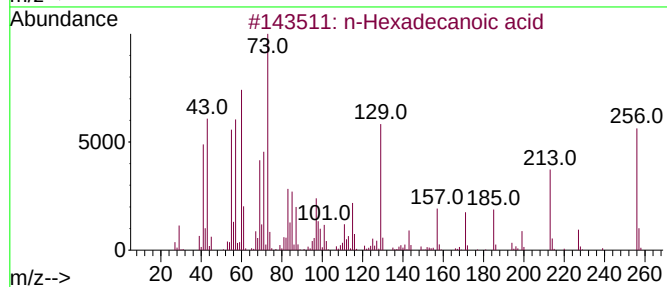
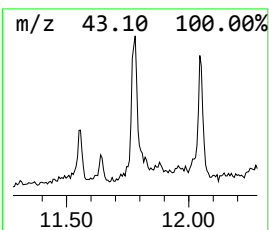
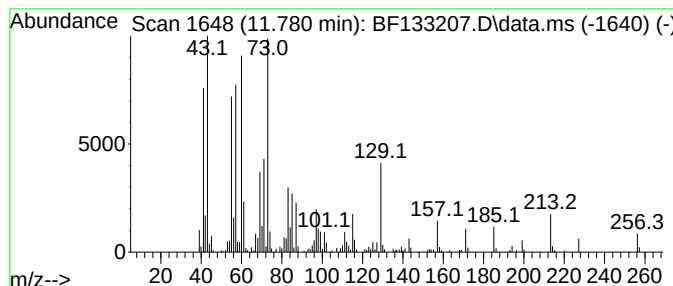
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.780	6.19 ng	456269	Phenanthrene-d10	11.245

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	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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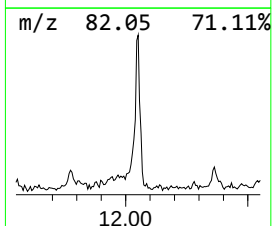
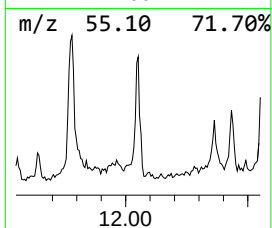
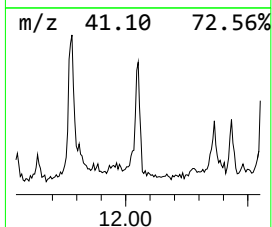
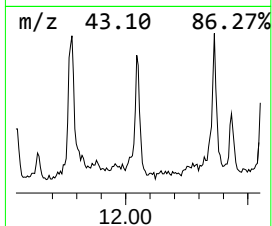
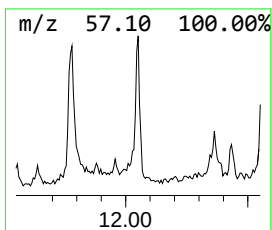
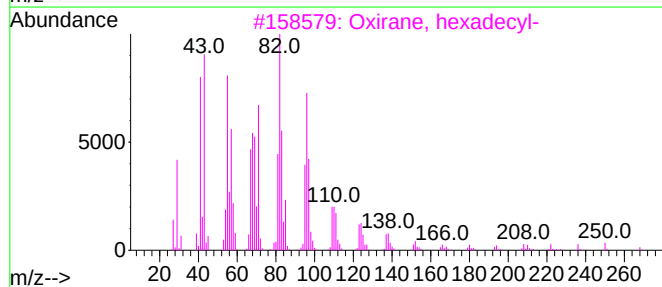
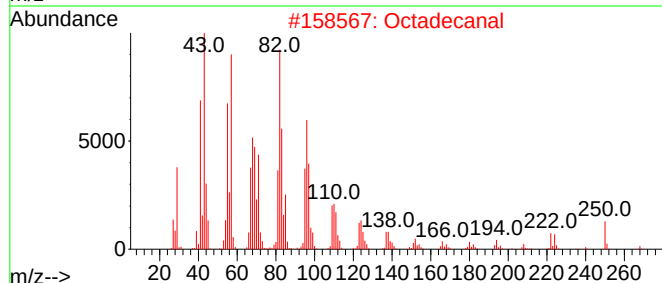
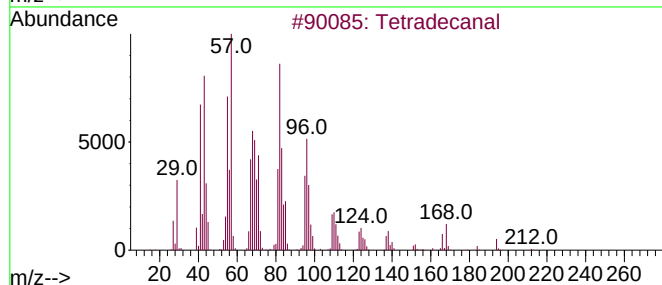
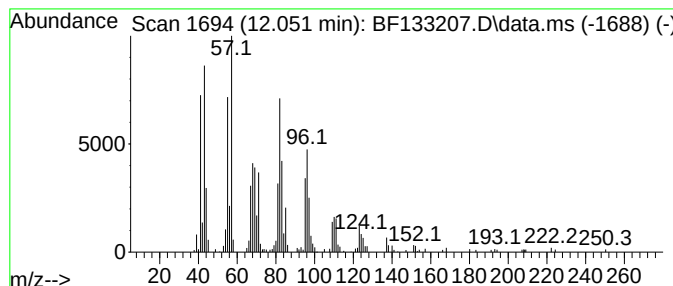
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tetradecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.051	3.61 ng	266056	Phenanthrene-d10		11.245	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Tetradecanal		212	C14H28O	000124-25-4	91
2	Octadecanal		268	C18H36O	000638-66-4	91
3	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	91
4	17-Octadecenal		266	C18H34O	056554-86-0	91
5	18-Nonadecen-1-ol		282	C19H38O	1000142-89-2	90



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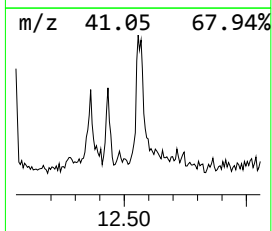
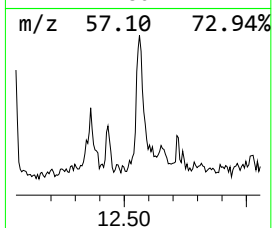
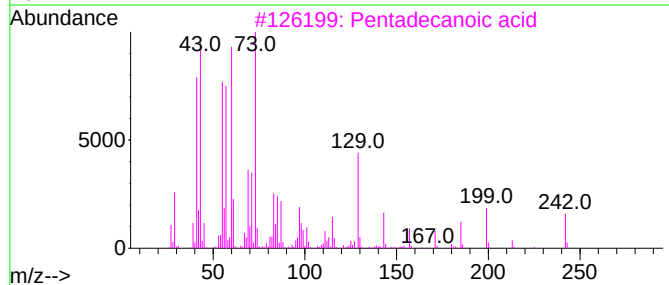
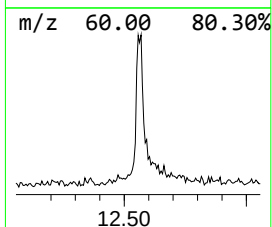
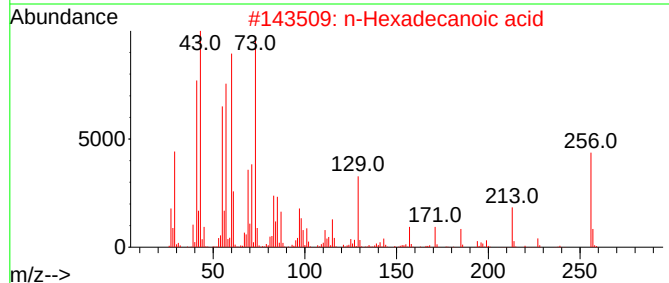
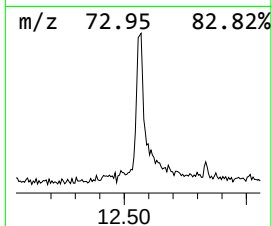
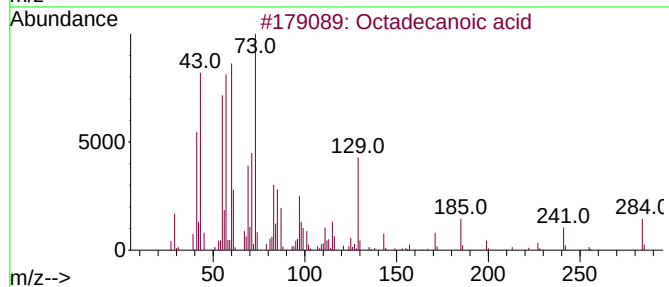
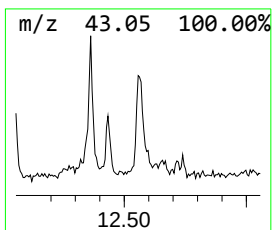
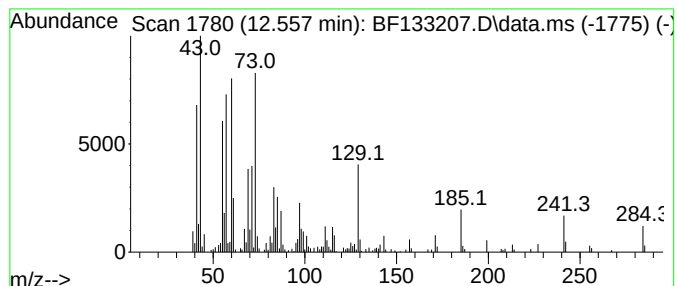
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	4.46 ng	328565	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



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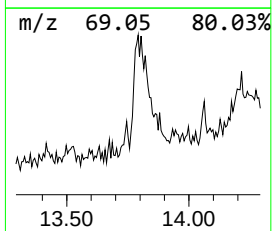
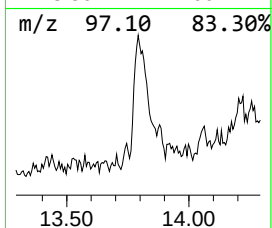
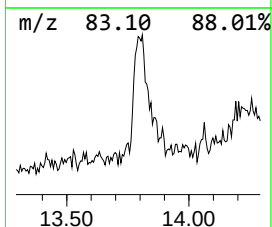
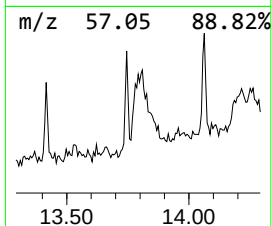
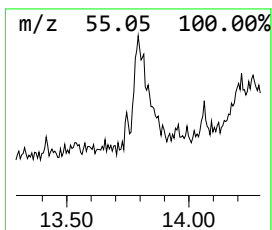
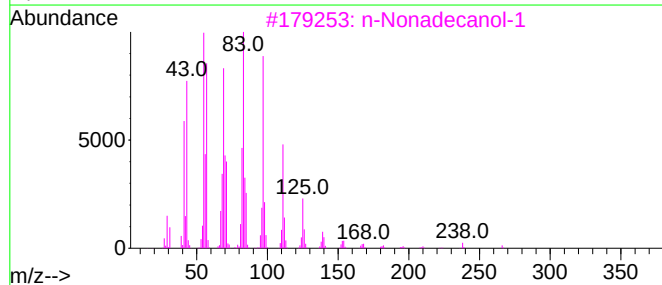
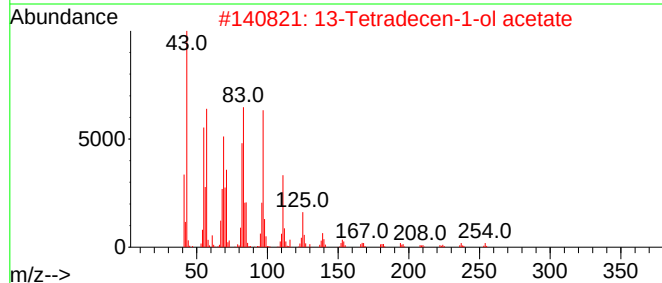
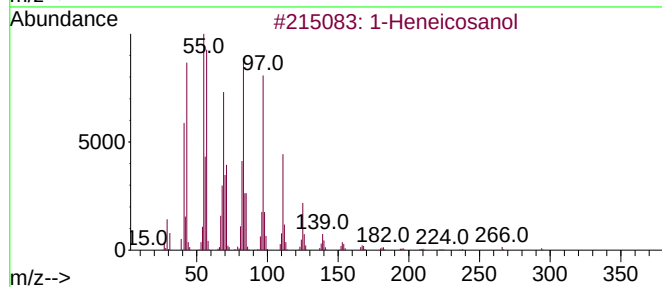
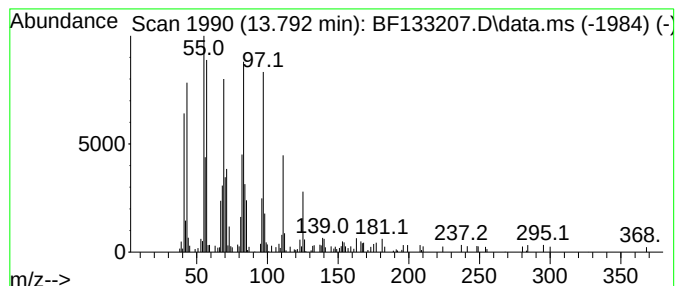
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	2.51 ng	127734	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	93
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			Eicosyl methyl ether	312	C21H44O	1000406-29-4	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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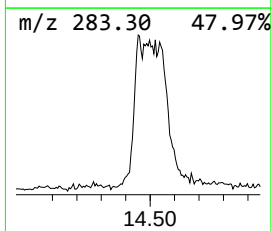
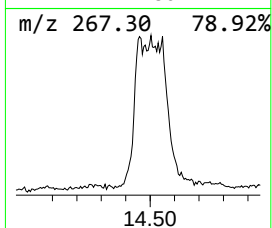
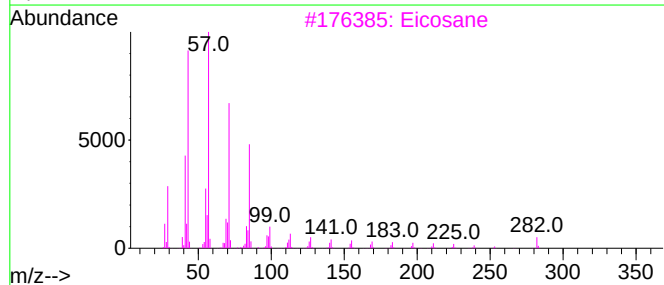
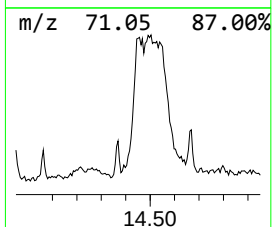
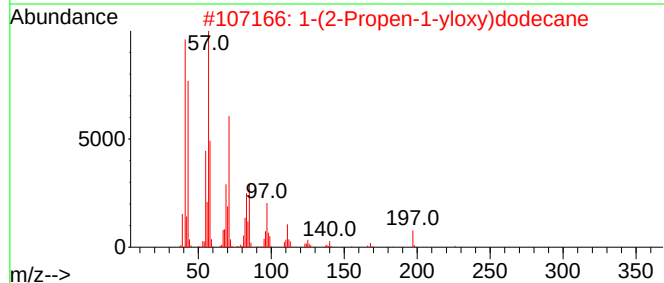
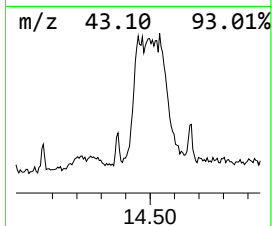
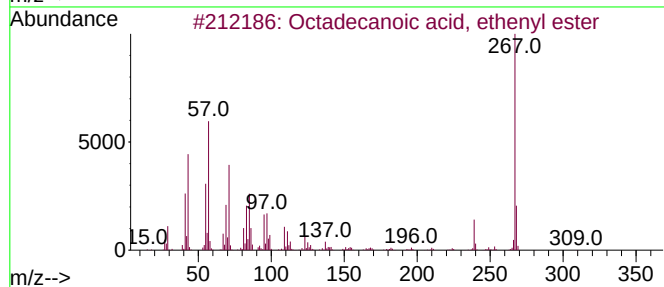
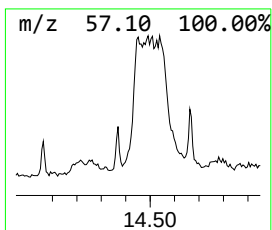
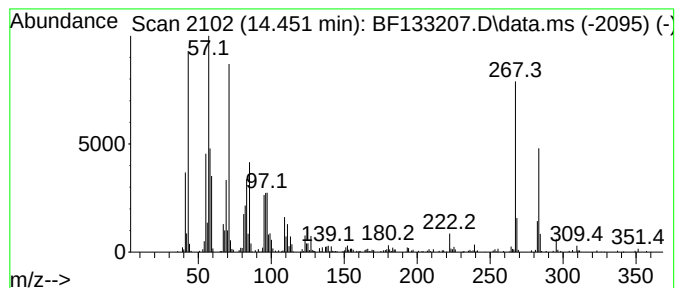
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid, ethenyl ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	14.49 ng	737505	Chrysene-d12	13.880

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	58
2		1-(2-Propen-1-yloxy)dodecane	226	C15H30O	006145-80-8	46
3		Eicosane	282	C20H42	000112-95-8	44
4		2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	30
5		Nonadecane	268	C19H40	000629-92-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133207.D
Acq On : 03 May 2023 15:09
Operator : CG\JU
Sample : 02583-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-25

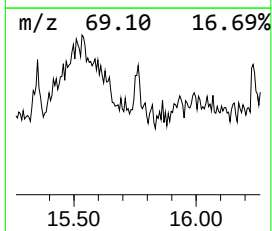
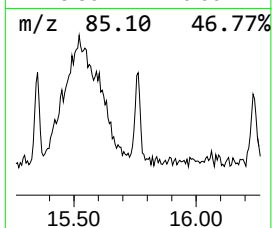
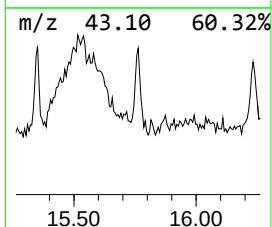
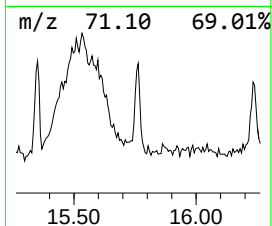
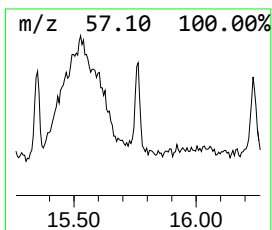
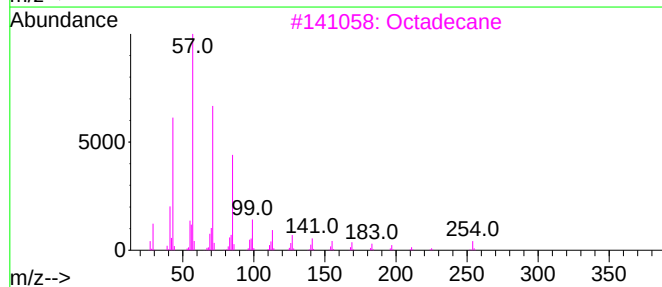
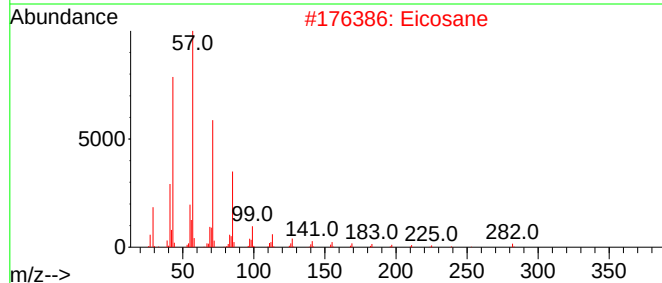
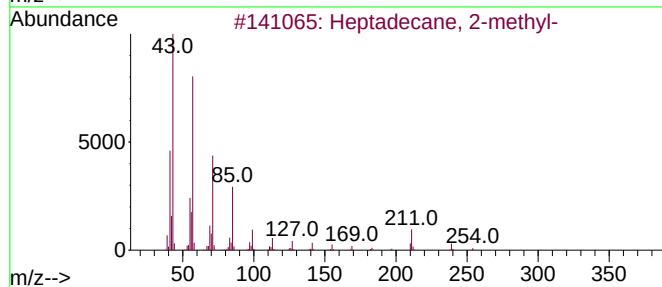
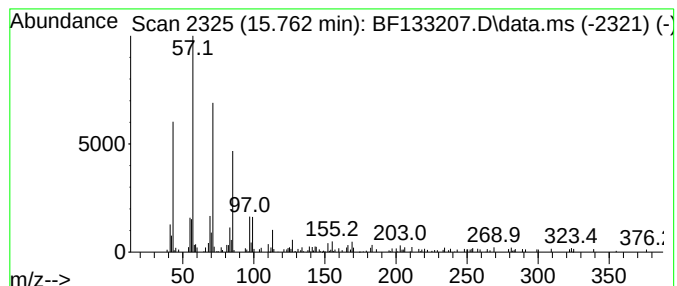
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.762	2.19 ng	123867	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 2-methyl-	254	C18H38	001560-89-0	90
2			Eicosane	282	C20H42	000112-95-8	90
3			Octadecane	254	C18H38	000593-45-3	90
4			Nonacosane	408	C29H60	000630-03-5	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133207.D
Acq On : 03 May 2023 15:09
Operator : CG\JU
Sample : 02583-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-25

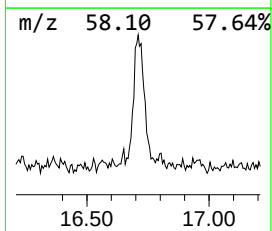
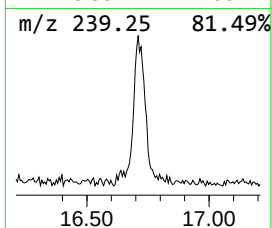
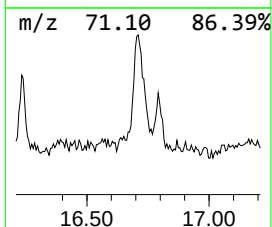
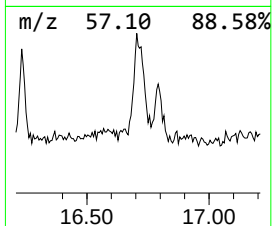
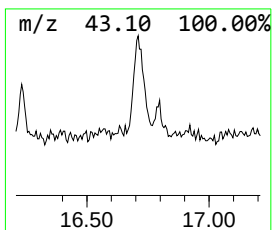
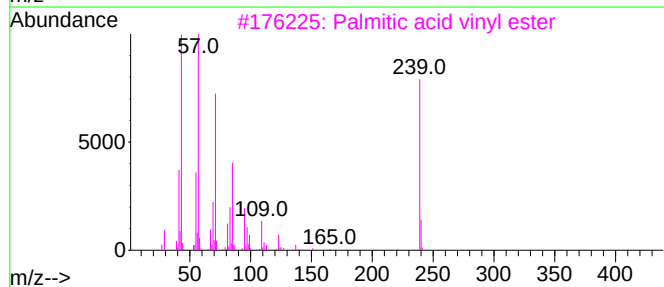
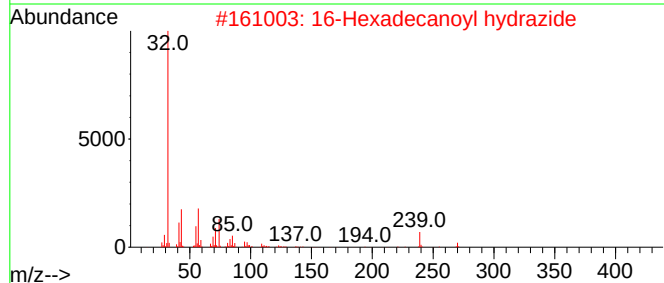
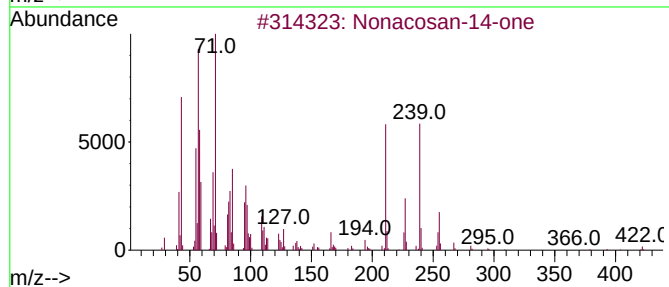
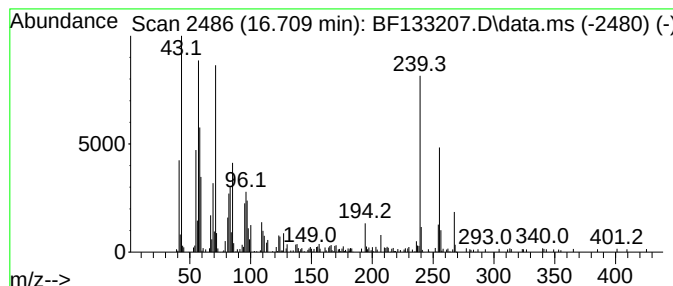
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonacosan-14-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.709	7.21 ng	407031	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacosan-14-one	422	C29H58O	034394-11-1	76
2			16-Hexadecanoyl hydrazide	270	C16H34N2O	002619-88-7	68
3			Palmitic acid vinyl ester	282	C18H34O2	000693-38-9	49
4			Hexadecanoic acid, 4-nitrophenyl...	377	C22H35NO4	001492-30-4	47
5			1-(2-Propen-1-yloxy)dodecane	226	C15H30O	006145-80-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133207.D
Acq On : 03 May 2023 15:09
Operator : CG\JU
Sample : 02583-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

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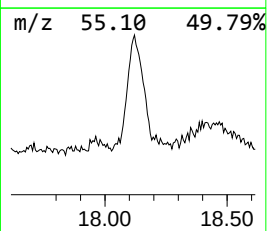
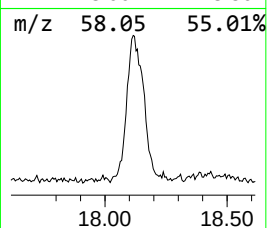
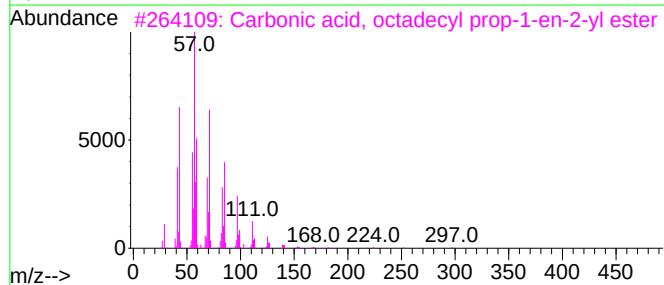
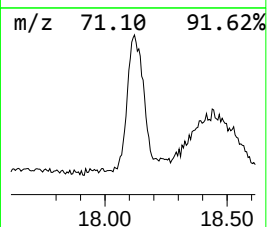
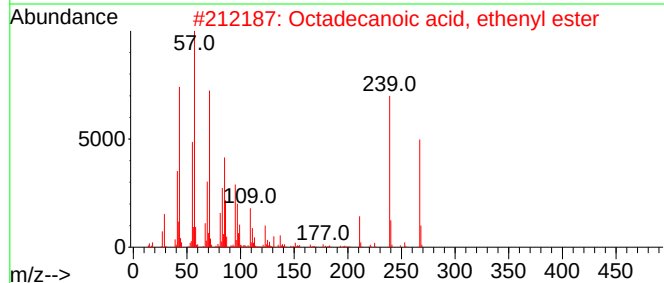
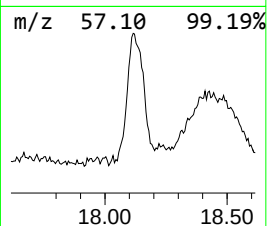
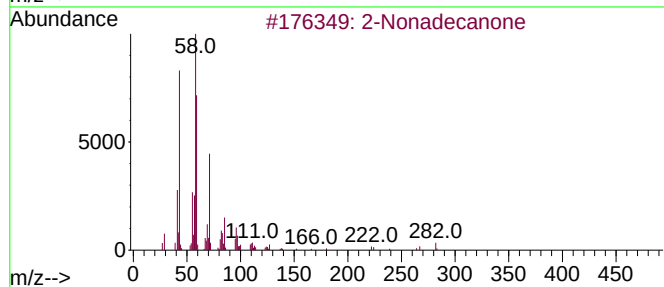
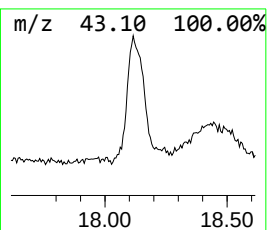
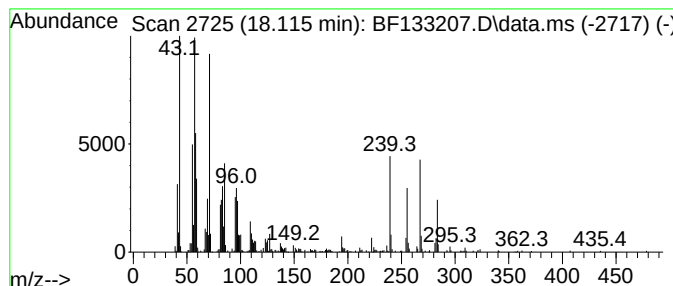
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Nonadecanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.115	26.46 ng	1493960	Perylene-d12	15.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonadecanone		282	C19H38O	000629-66-3	50
2	Octadecanoic acid, ethenyl ester		310	C20H38O2	000111-63-7	43
3	Carbonic acid, octadecyl prop-1-...		354	C22H42O3	1000383-11-5	38
4	Ether, methyl 1-tetradecenyl		226	C15H30O	026537-05-3	38
5	1-(2-Propen-1-yloxy)dodecane		226	C15H30O	006145-80-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050323\
Data File : BF133207.D
Acq On : 03 May 2023 15:09
Operator : CG\JU
Sample : 02583-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Benzophenone	10.475	3.9	ng	317466	3	9.763	1626650	20.0
n-Hexadecanoic ...	11.780	6.2	ng	456269	4	11.245	1473150	20.0
Tetradecanal	12.051	3.6	ng	266056	4	11.245	1473150	20.0
Octadecanoic acid	12.557	4.5	ng	328565	4	11.245	1473150	20.0
1-Heneicosanol	13.792	2.5	ng	127734	5	13.880	1017810	20.0
Octadecanoic ac...	14.451	14.5	ng	737505	5	13.880	1017810	20.0
Heptadecane, 2-...	15.762	2.2	ng	123867	6	15.304	1129210	20.0
Nonacosan-14-one	16.709	7.2	ng	407031	6	15.304	1129210	20.0
2-Nonadecanone	18.115	26.5	ng	1493960	6	15.304	1129210	20.0