

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
 Data File : BF130034.D
 Acq On : 29 Aug 2022 14:47
 Operator : CG\JU
 Sample : N4355-13
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-14

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-BF081422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130034.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.904	441	445	458	rBV	285553	347602	7.03%	1.424%
2	5.340	516	519	539	rBV	1429991	1702051	34.43%	6.975%
3	5.710	579	582	589	rVB	81962	72362	1.46%	0.297%
4	6.363	690	693	708	rBV	1036459	1275859	25.81%	5.228%
5	6.698	747	750	758	rBV	872095	741338	15.00%	3.038%
6	7.275	843	848	851	rBV	2718221	2599524	52.58%	10.652%
7	7.981	964	968	972	rBV	1165059	1014289	20.52%	4.156%
8	9.057	1146	1151	1154	rBV	4968383	4943761	100.00%	20.259%
9	9.734	1262	1266	1270	rBV	1408806	1150189	23.27%	4.713%
10	10.533	1398	1402	1405	rBV	3379222	2840915	57.46%	11.641%
11	11.222	1516	1519	1523	rBV	1326223	1115577	22.57%	4.571%
12	11.504	1563	1567	1575	rVB5	29019	66174	1.34%	0.271%
13	11.604	1581	1584	1589	rVB	173931	148714	3.01%	0.609%
14	11.751	1604	1609	1627	rBV2	217232	283645	5.74%	1.162%
15	11.992	1647	1650	1659	rVB10	34657	68848	1.39%	0.282%
16	12.310	1701	1704	1715	rVV	105659	113085	2.29%	0.463%
17	12.398	1716	1719	1722	rVB	124975	104501	2.11%	0.428%
18	12.533	1737	1742	1747	rBV	99117	136336	2.76%	0.559%
19	12.810	1784	1789	1792	rBV	4844511	4233310	85.63%	17.347%
20	13.757	1945	1950	1959	rBV5	48318	149157	3.02%	0.611%
21	13.869	1966	1969	1975	rBV	683829	622683	12.60%	2.552%
22	15.298	2208	2212	2220	rVB	529911	673463	13.62%	2.760%

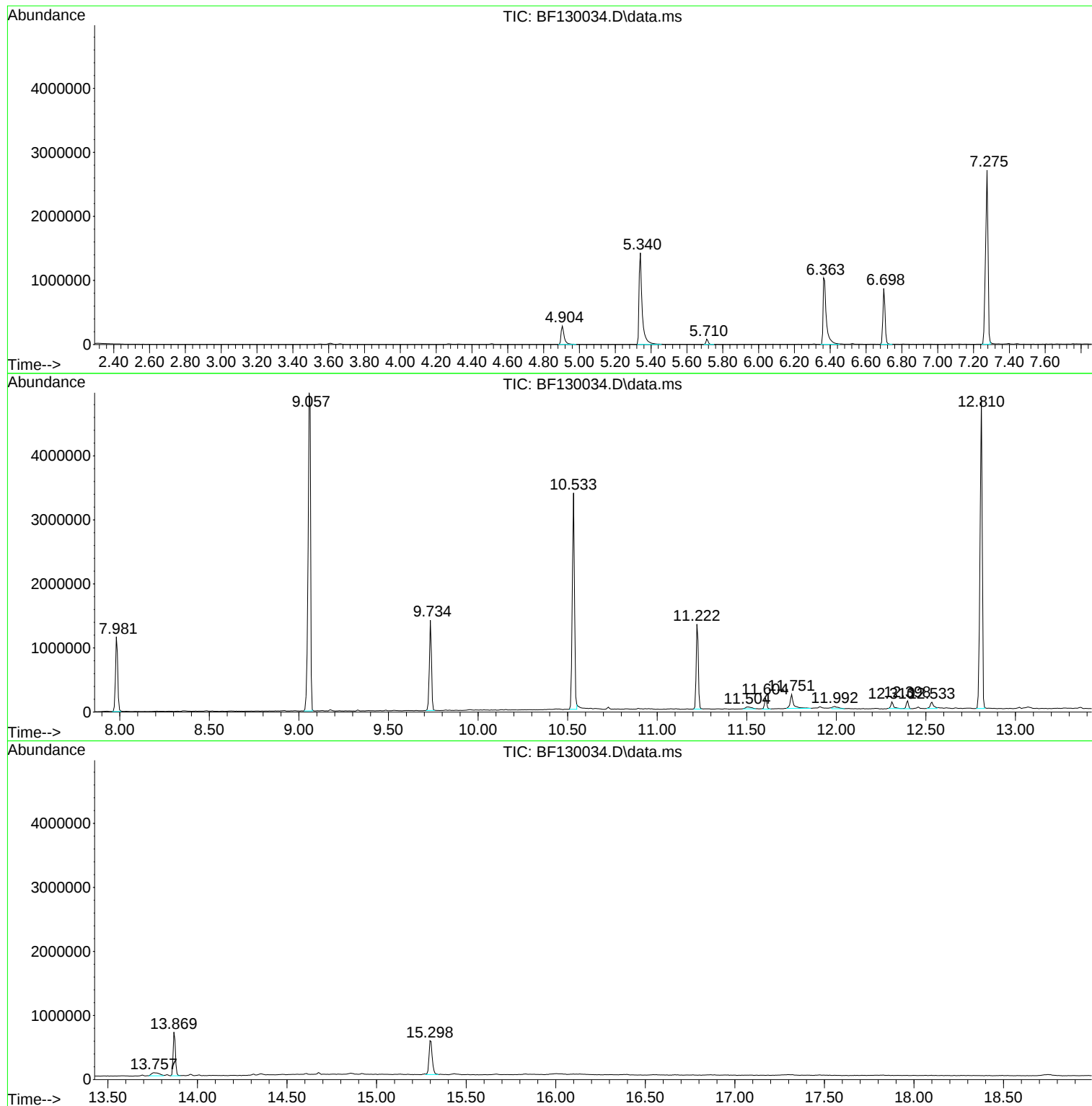
Sum of corrected areas: 24403383

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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Instrument :
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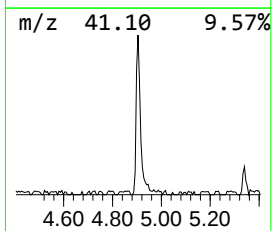
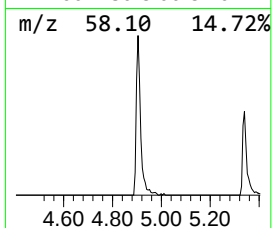
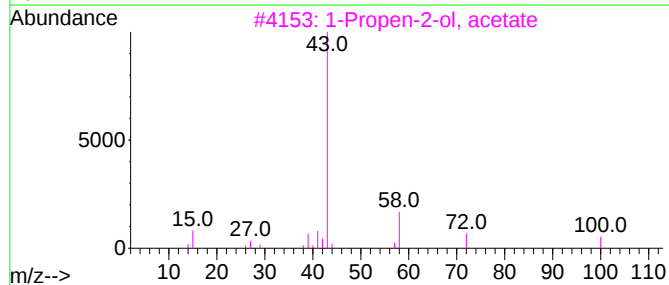
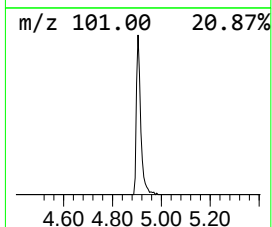
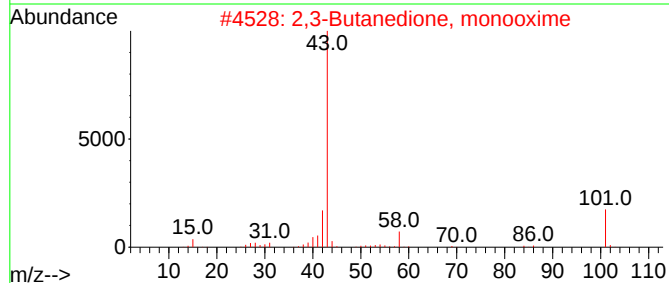
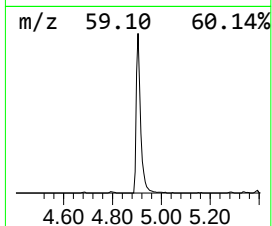
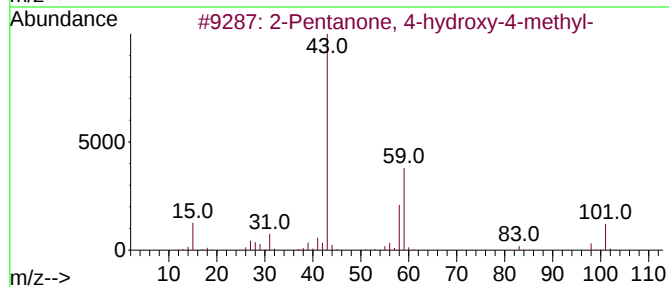
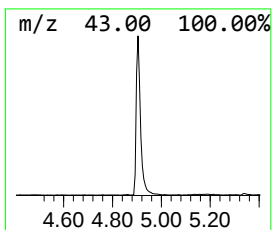
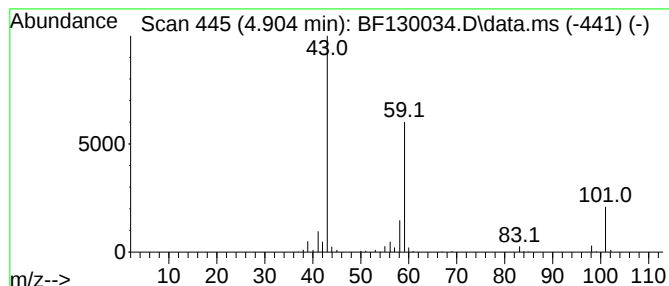
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.904	9.38 ng	347602	1,4-Dichlorobenzene-d4	6.698

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	12
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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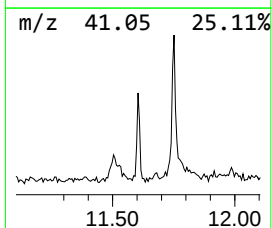
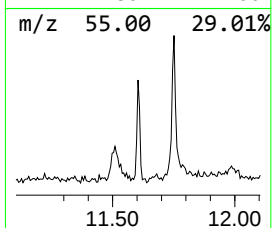
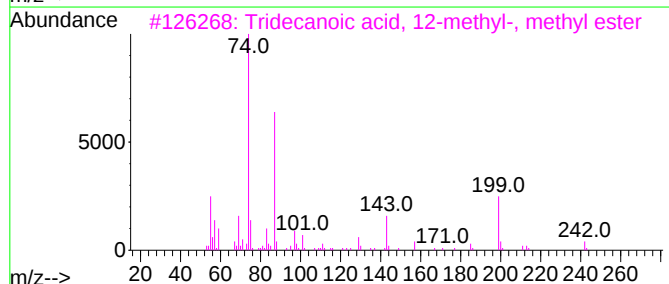
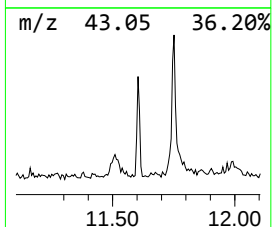
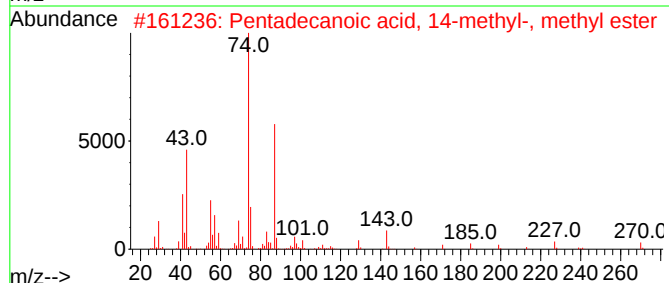
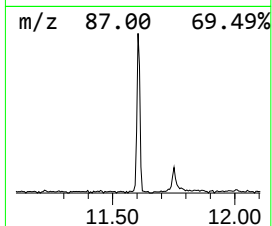
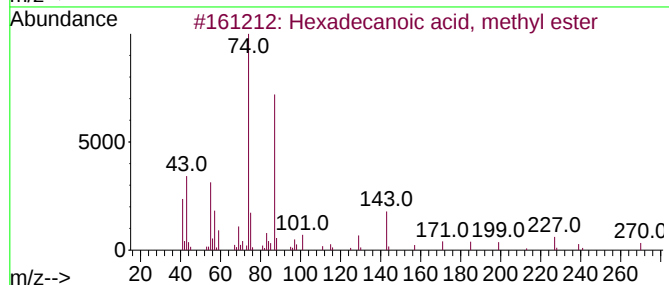
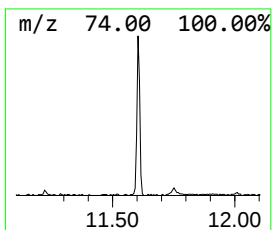
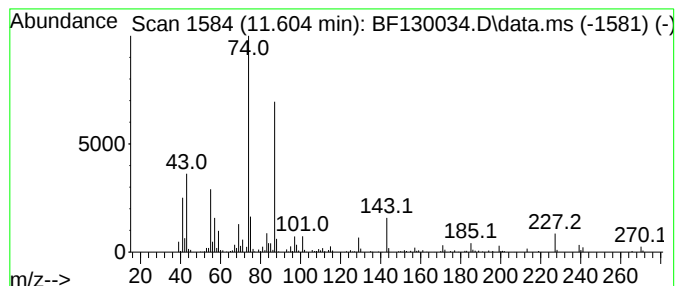
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.604	2.67 ng	148714	Phenanthrene-d10	11.222	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	87
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	86



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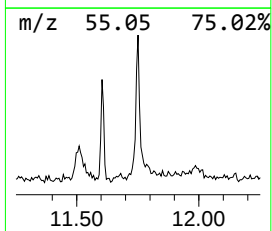
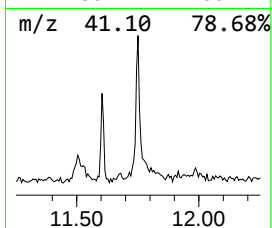
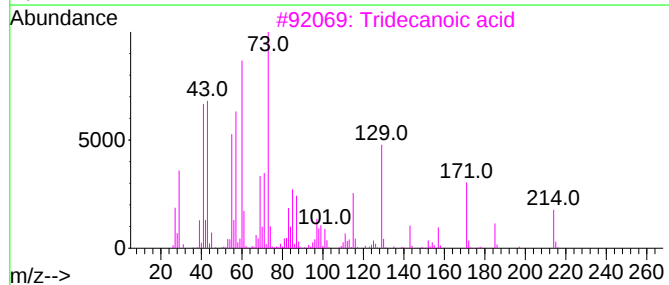
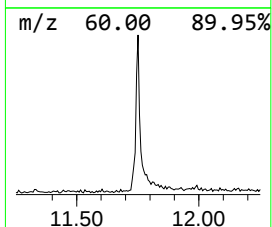
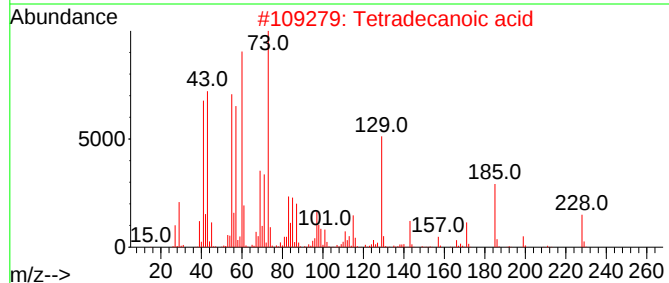
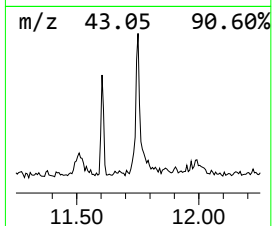
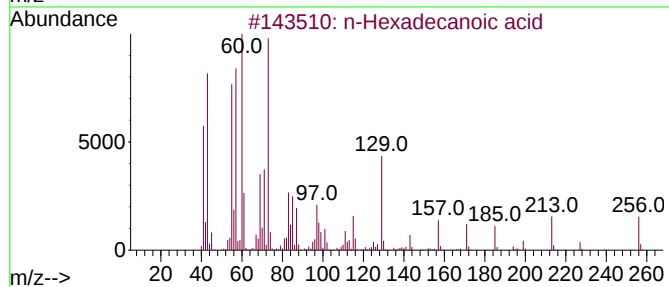
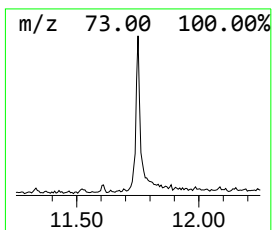
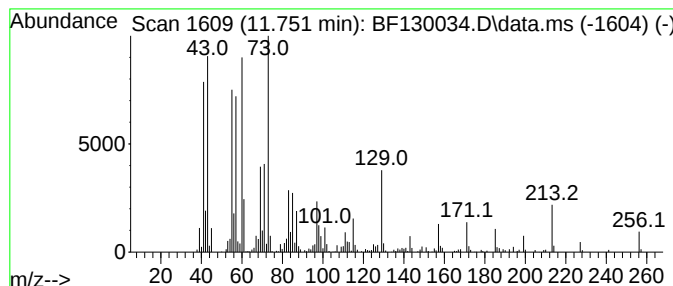
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.751	5.09 ng	283645	Phenanthrene-d10	11.222

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	97
3			Tridecanoic acid	214	C13H26O2	000638-53-9	95
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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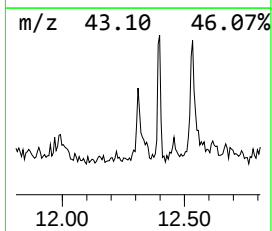
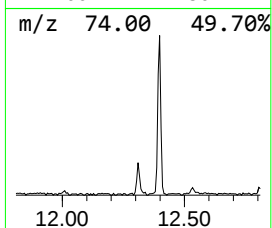
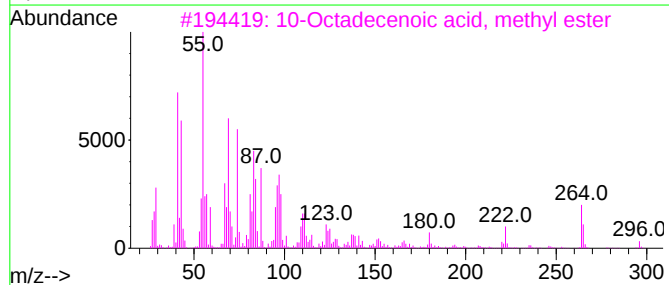
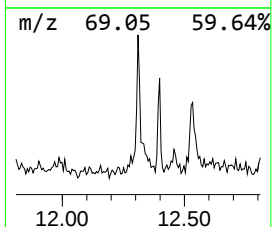
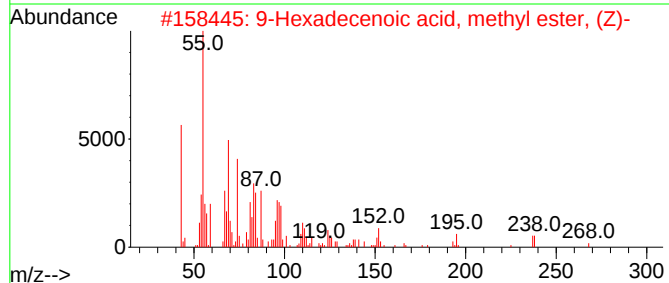
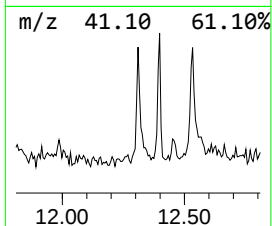
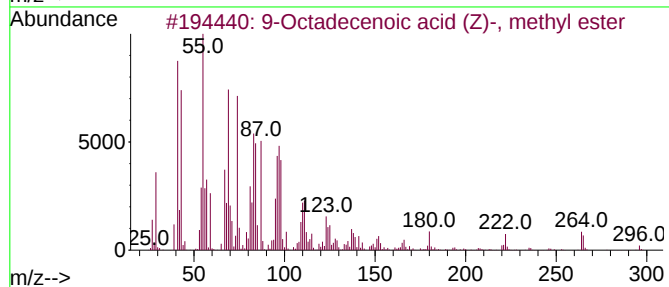
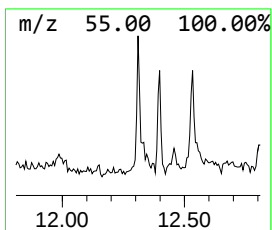
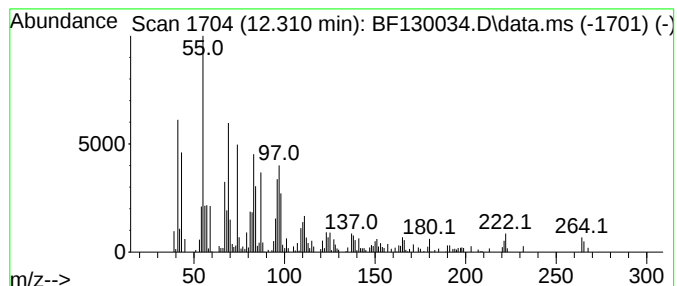
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.310	2.03 ng	113085	Phenanthrene-d10	11.222	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	93
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91



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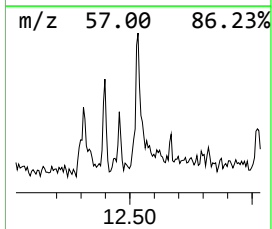
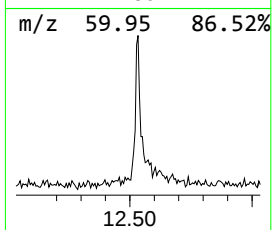
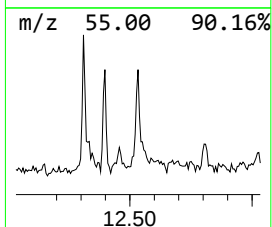
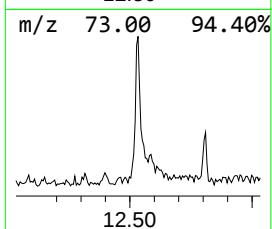
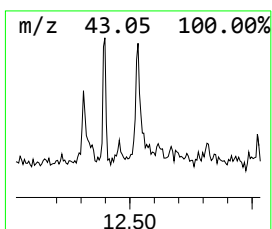
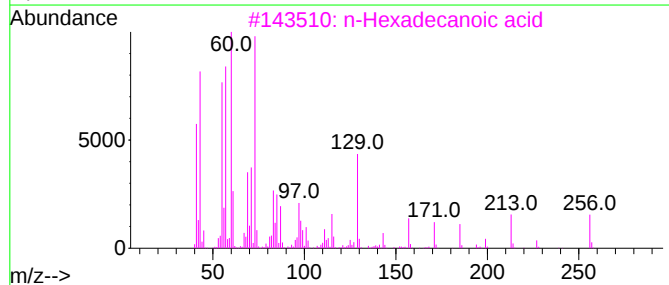
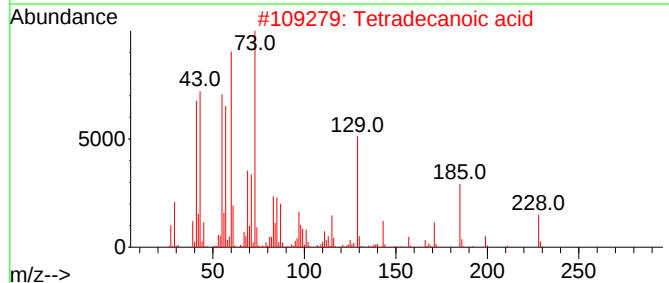
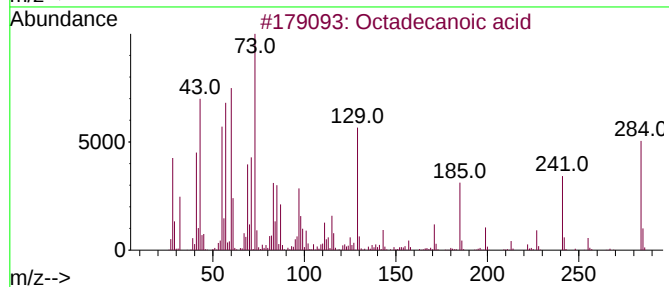
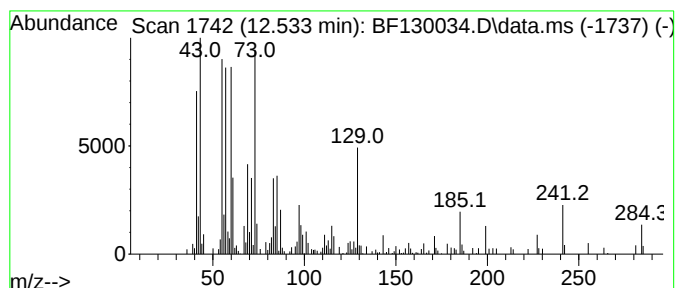
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.533	2.44 ng	136336	Phenanthrene-d10	11.222	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	64



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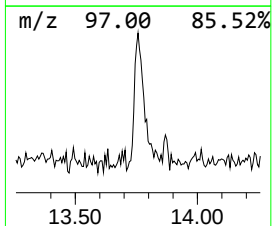
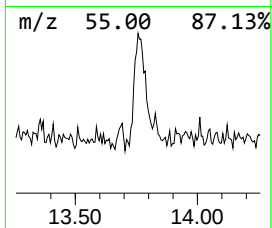
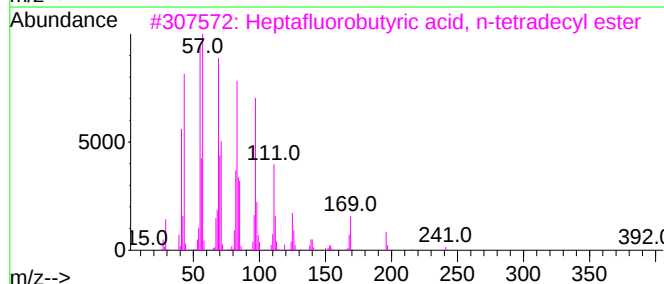
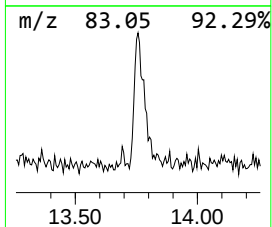
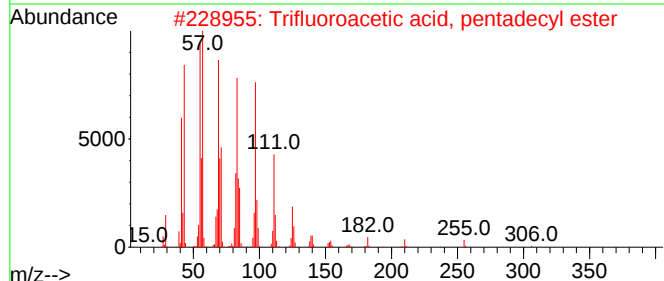
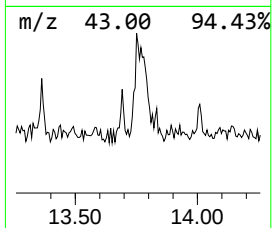
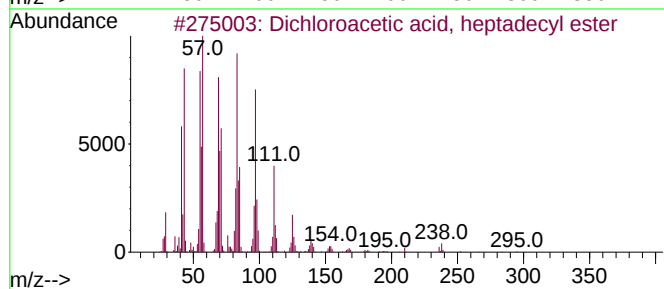
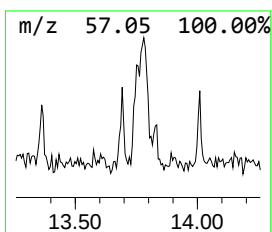
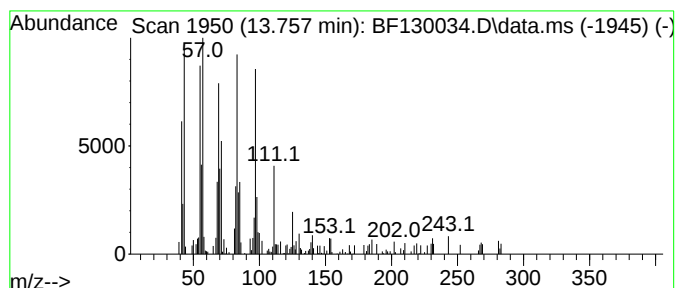
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	4.79 ng	149157	Chrysene-d12	13.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082922\
Data File : BF130034.D
Acq On : 29 Aug 2022 14:47
Operator : CG\JU
Sample : N4355-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-14

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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-...	4.904	9.4	ng	347602	1	6.698	741338	20.0
Hexadecanoic ac...	11.604	2.7	ng	148714	4	11.222	1115580	20.0
n-Hexadecanoic ...	11.751	5.1	ng	283645	4	11.222	1115580	20.0
9-Octadecenoic ...	12.310	2.0	ng	113085	4	11.222	1115580	20.0
Octadecanoic acid	12.533	2.4	ng	136336	4	11.222	1115580	20.0
Dichloroacetic ...	13.757	4.8	ng	149157	5	13.869	622683	20.0