

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
 Data File : BF130927.D
 Acq On : 02 Nov 2022 13:06
 Operator : CG\JU
 Sample : N5381-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 265393-7

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130927.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	21	28	33	rVB	1328309	1680065	51.51%	9.135%
2	4.510	406	412	416	rBV	30160	33918	1.04%	0.184%
3	5.151	516	521	528	rBV	166826	197558	6.06%	1.074%
4	5.540	582	587	590	rBV	1466991	1275577	39.11%	6.935%
5	6.540	752	757	764	rVB	935898	837171	25.67%	4.552%
6	6.922	818	822	826	rBV	627992	514735	15.78%	2.799%
7	7.492	912	919	921	rBV	1589205	1823451	55.91%	9.914%
8	8.210	1036	1041	1044	rBV	771146	675275	20.71%	3.672%
9	9.286	1218	1224	1227	rBV	3125906	3261380	100.00%	17.732%
10	9.681	1286	1291	1293	rBV	78576	66494	2.04%	0.362%
11	9.969	1335	1340	1344	rBV	942056	783074	24.01%	4.258%
12	10.763	1469	1475	1478	rBV	2104258	1969924	60.40%	10.711%
13	11.463	1590	1594	1597	rBV	979432	811057	24.87%	4.410%
14	11.980	1674	1682	1686	rBV	79289	131572	4.03%	0.715%
15	12.769	1810	1816	1827	rBV2	54305	105964	3.25%	0.576%
16	13.057	1860	1865	1868	rBV	3364791	3127668	95.90%	17.005%
17	13.451	1924	1932	1938	rBV2	24328	58937	1.81%	0.320%
18	14.045	2028	2033	2040	rBV4	28608	66095	2.03%	0.359%
19	14.110	2040	2044	2048	rVB	624332	541174	16.59%	2.942%
20	14.857	2168	2171	2175	rVB2	23641	34573	1.06%	0.188%
21	15.621	2296	2301	2310	rBV	295376	396610	12.16%	2.156%

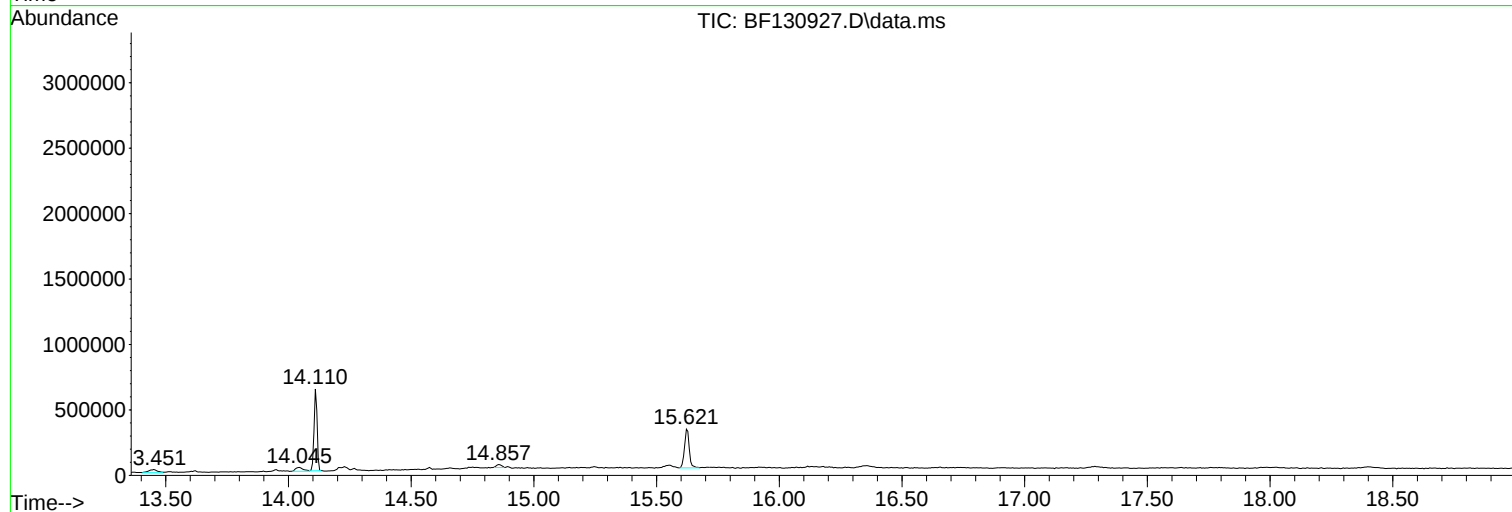
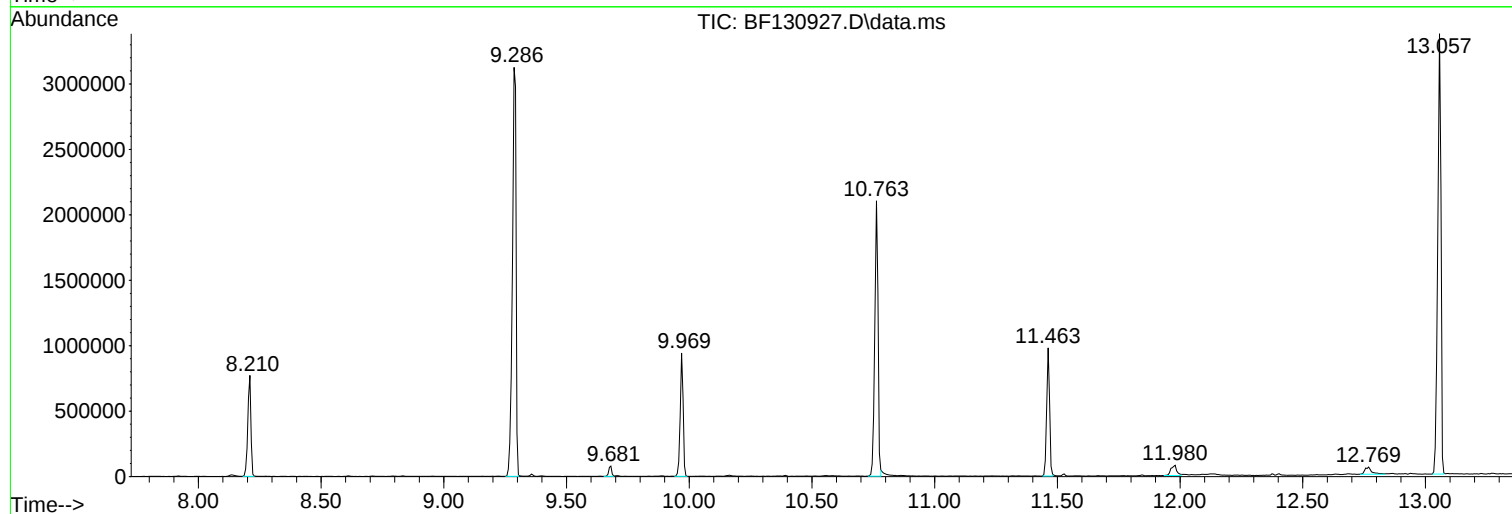
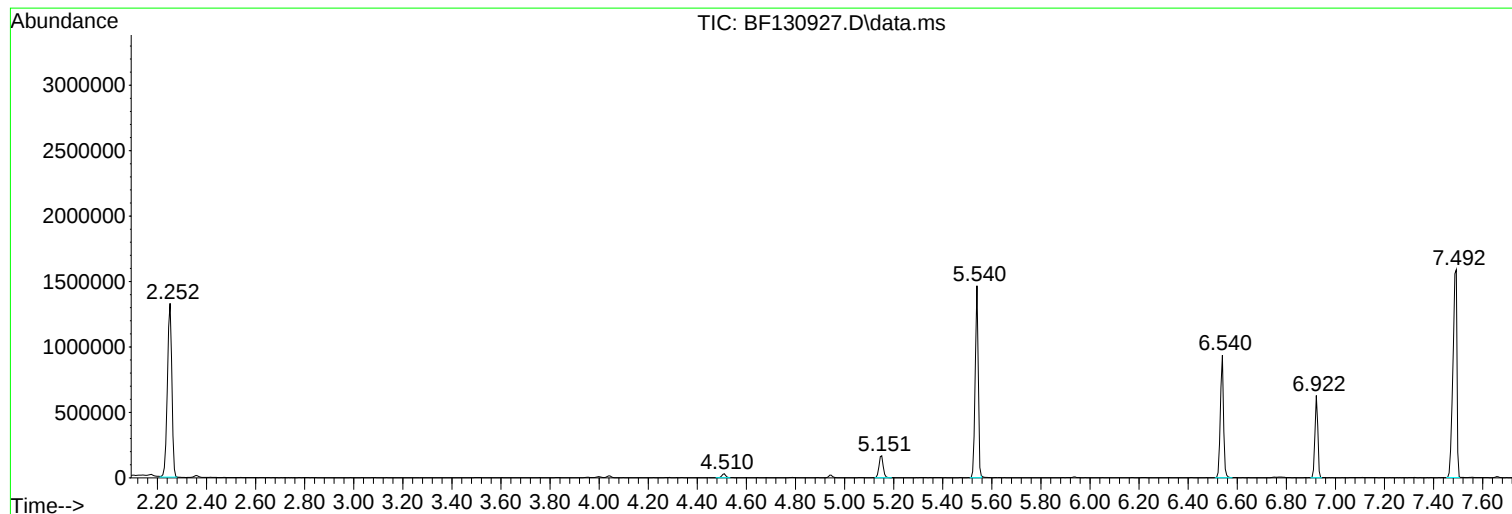
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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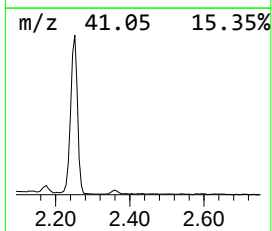
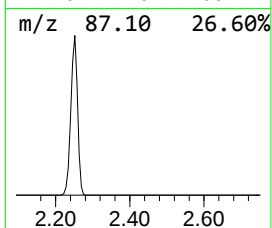
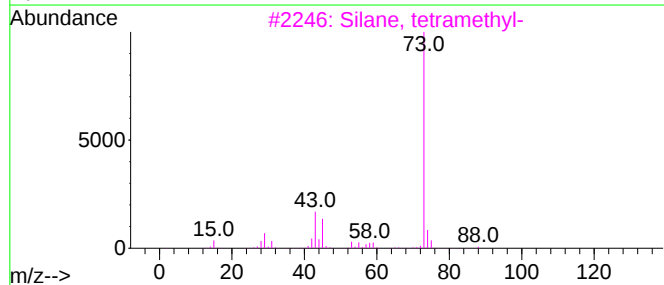
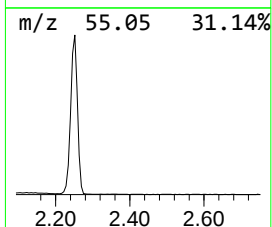
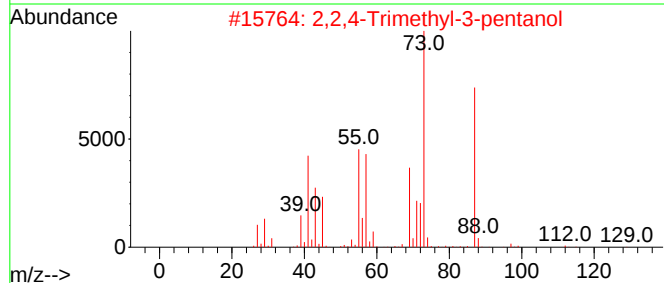
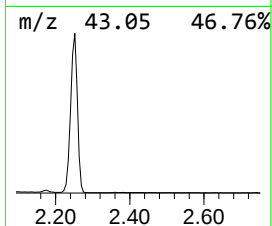
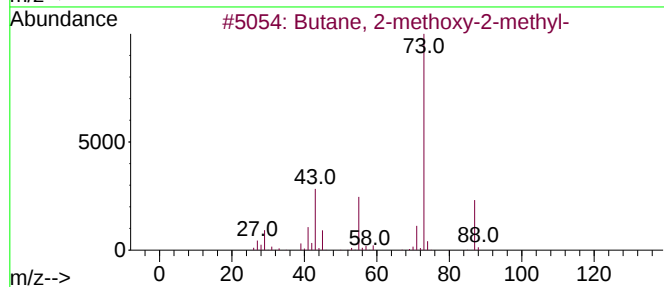
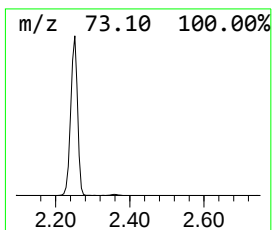
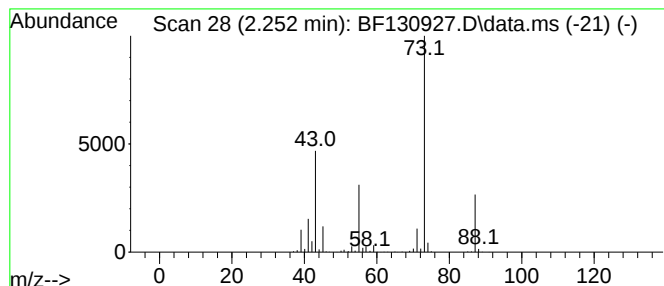
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	65.28 ng	1680070	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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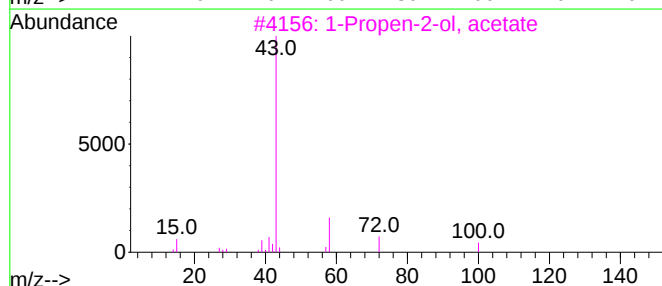
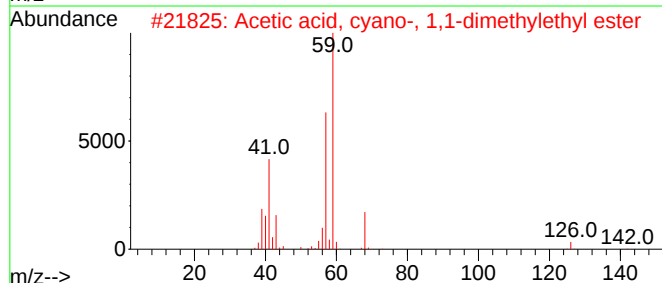
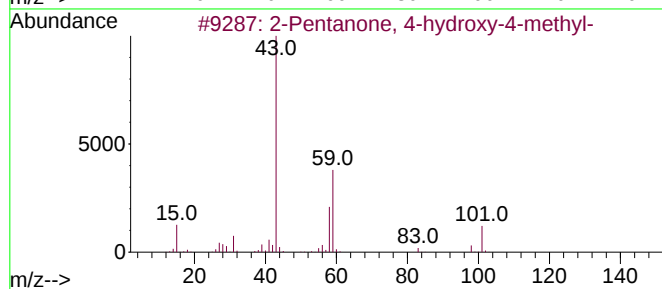
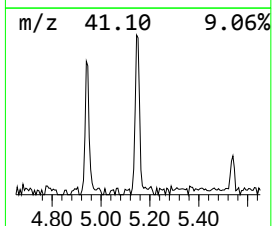
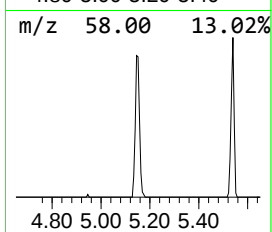
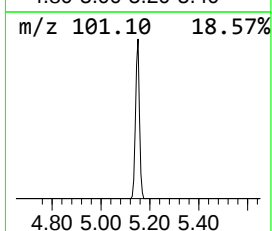
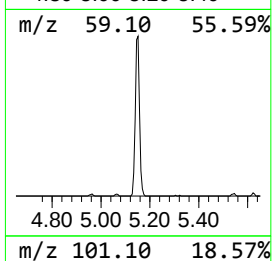
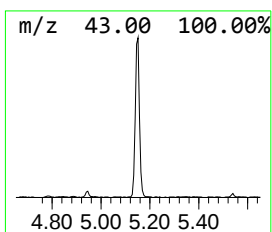
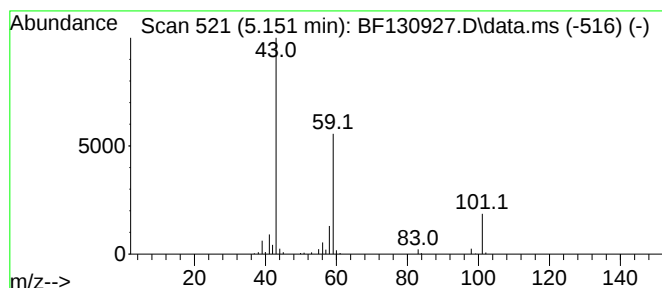
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	7.68 ng	197558	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			3-Pentanol	88	C5H12O	000584-02-1	9



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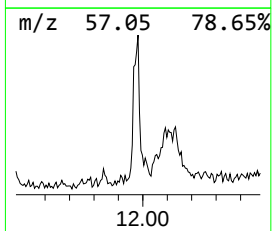
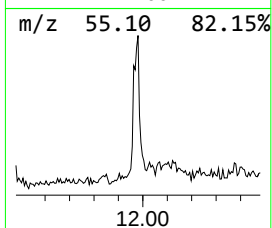
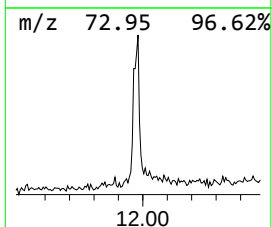
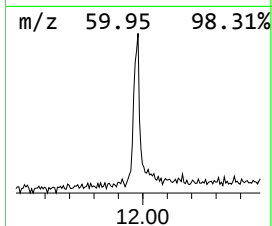
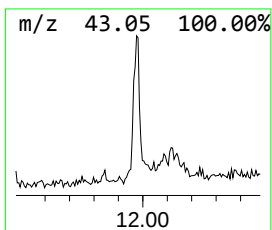
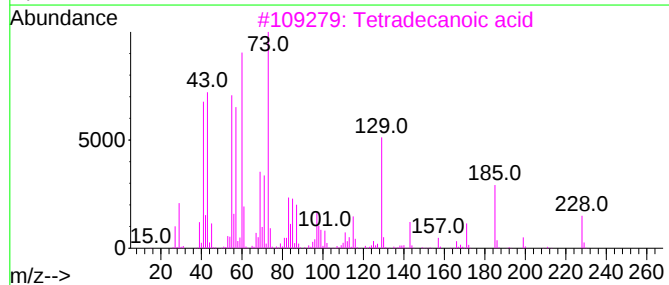
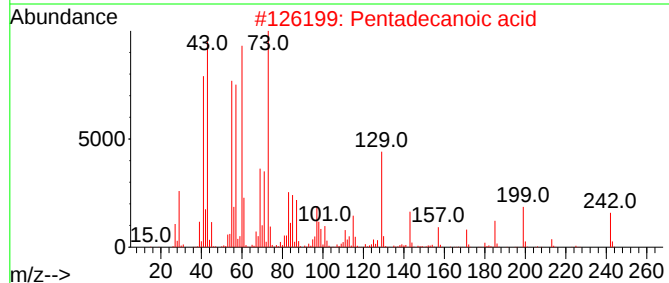
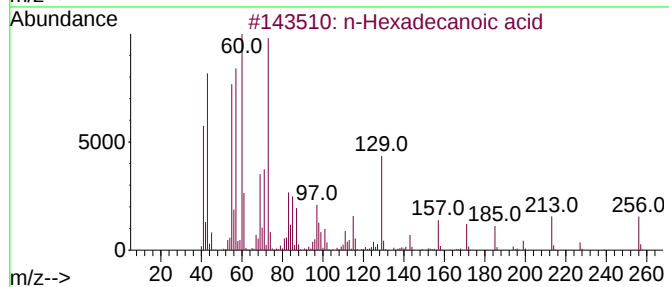
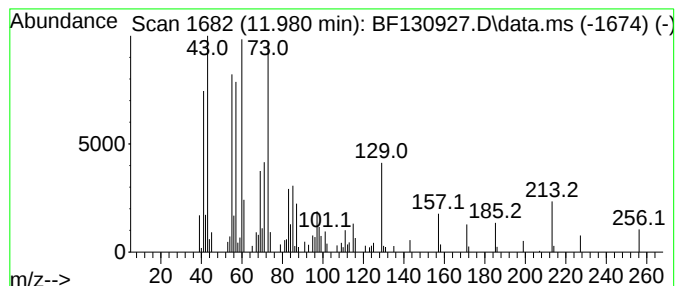
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.980	3.24 ng	131572	Phenanthrene-d10		11.463	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	87
4	n-Decanoic acid		172	C10H20O2	000334-48-5	76
5	Tridecanoic acid		214	C13H26O2	000638-53-9	74



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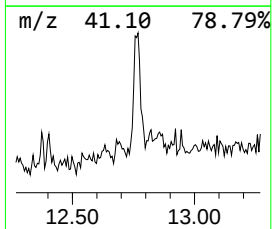
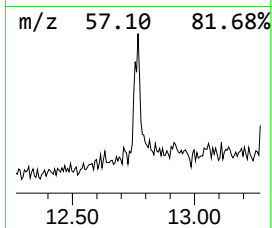
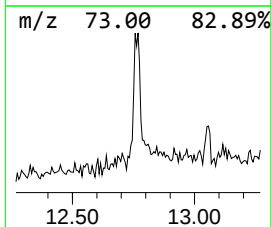
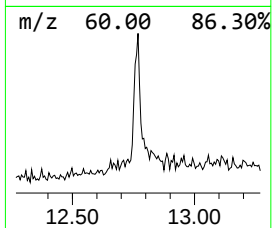
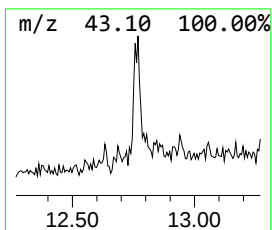
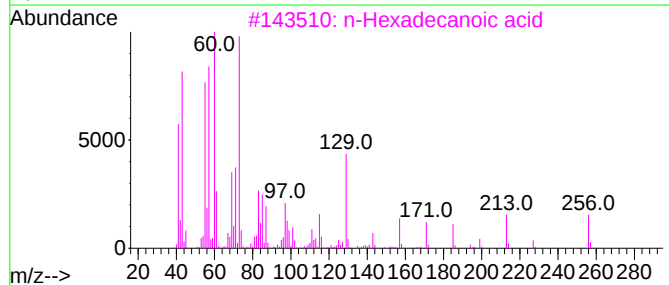
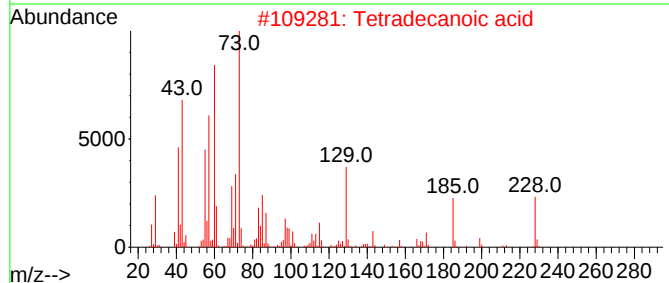
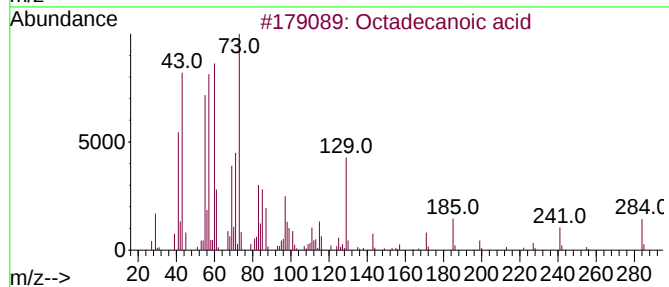
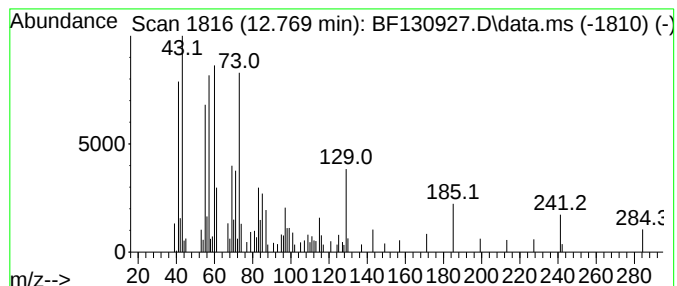
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.769	2.61 ng	105964	Phenanthrene-d10	11.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Dodecanoic acid	200	C12H24O2	000143-07-7	59
5			Tridecanoic acid	214	C13H26O2	000638-53-9	59



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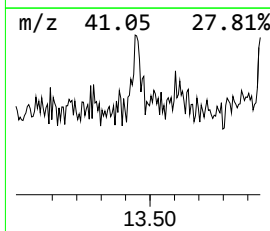
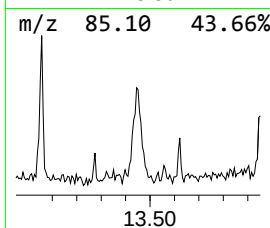
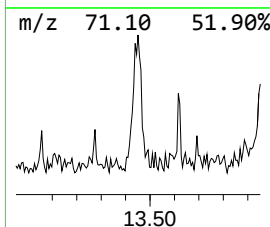
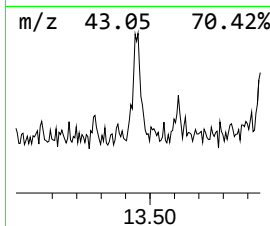
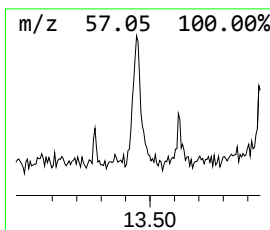
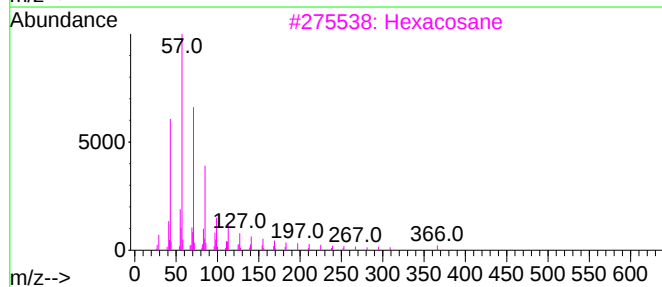
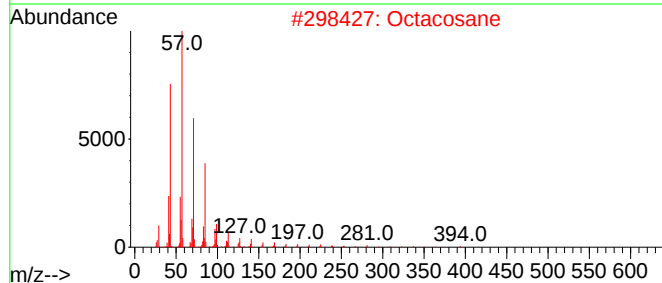
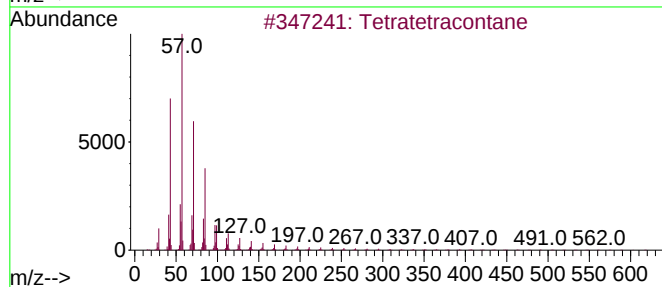
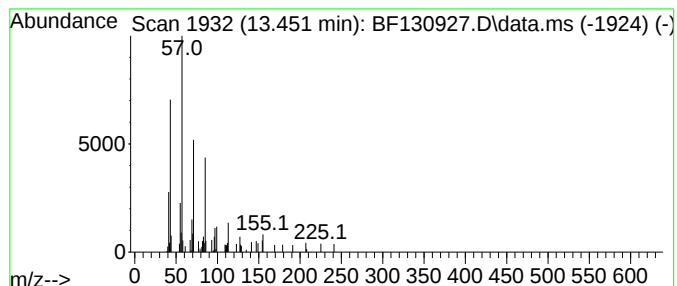
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.451	2.18 ng	58937	Chrysene-d12	14.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	78
2			Octacosane	394	C28H58	000630-02-4	72
3			Hexacosane	366	C26H54	000630-01-3	68
4			Dodecane, 3-methyl-	184	C13H28	017312-57-1	64
5			Heneicosane	296	C21H44	000629-94-7	64



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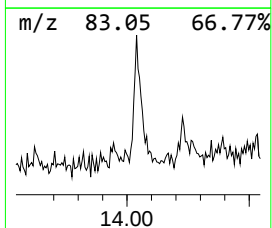
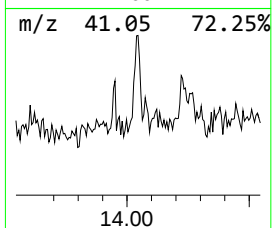
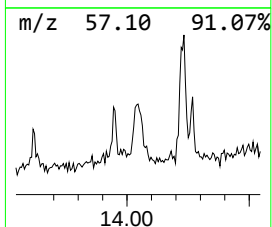
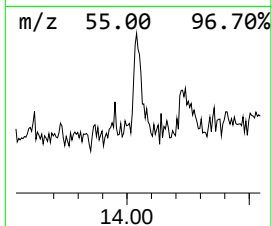
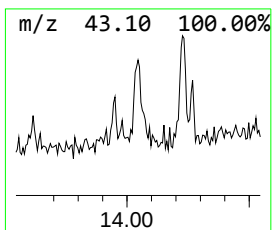
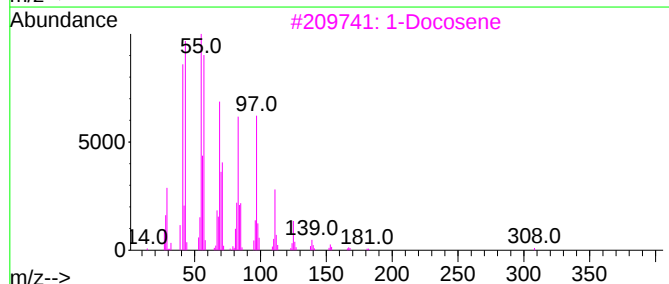
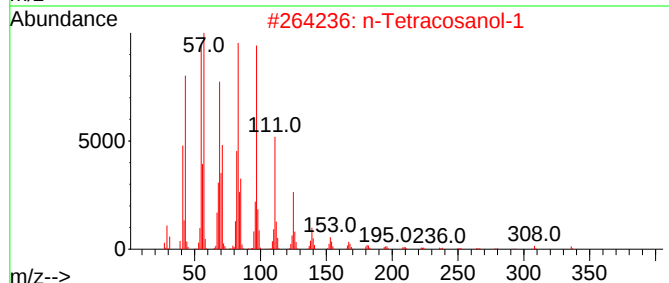
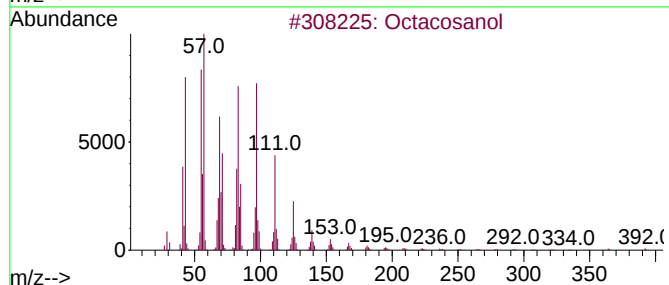
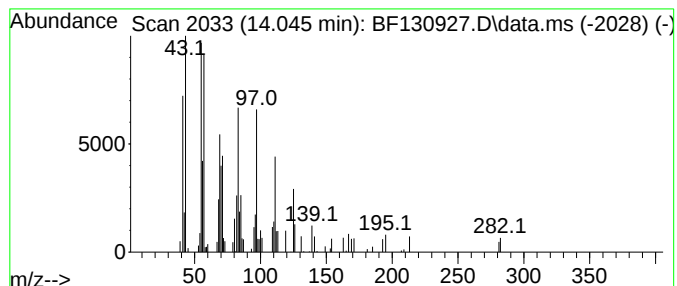
Instrument :
BNA_F
ClientSampleId :
265393-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.045	2.44 ng	66095	Chrysene-d12		14.110	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octacosanol		410	C28H58O	000557-61-9	90
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	87
3	1-Docosene		308	C22H44	001599-67-3	87
4	1-Tricosene		322	C23H46	018835-32-0	87
5	Octadecyl trifluoroacetate		366	C20H37F3O2	079392-43-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
Data File : BF130927.D
Acq On : 02 Nov 2022 13:06
Operator : CG\JU
Sample : N5381-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
265393-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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
Butane, 2-metho...	2.252	65.3	ng	1680070	1	6.922	514735	20.0
2-Pentanone, 4-...	5.151	7.7	ng	197558	1	6.922	514735	20.0
n-Hexadecanoic ...	11.980	3.2	ng	131572	4	11.463	811057	20.0
Octadecanoic acid	12.769	2.6	ng	105964	4	11.463	811057	20.0
Tetratetracontane	13.451	2.2	ng	58937	5	14.110	541174	20.0
Octacosanol	14.045	2.4	ng	66095	5	14.110	541174	20.0