

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
 Data File : BF135873.D
 Acq On : 19 Oct 2023 04:30
 Operator : CG\JU
 Sample : 04858-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-2

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135873.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	486	489	501	rBV	101109	140041	9.98%	1.327%
2	5.381	556	560	581	rBV	1204170	1377534	98.14%	13.055%
3	6.398	729	733	751	rBV	1326522	1403648	100.00%	13.302%
4	6.740	787	791	798	rBV	462712	392466	27.96%	3.719%
5	7.304	884	887	899	rBV	882639	838145	59.71%	7.943%
6	8.016	1005	1008	1017	rBV	546822	473522	33.74%	4.487%
7	9.098	1188	1192	1195	rBV	1398710	1268642	90.38%	12.023%
8	9.216	1208	1212	1216	rVB	21190	20308	1.45%	0.192%
9	9.775	1304	1307	1319	rVB	520724	431350	30.73%	4.088%
10	10.575	1439	1443	1459	rBV	772818	705311	50.25%	6.684%
11	11.275	1558	1562	1565	rBV	471677	419003	29.85%	3.971%
12	11.804	1649	1652	1665	rBV	217412	239790	17.08%	2.272%
13	12.498	1767	1770	1772	rBV	51633	58171	4.14%	0.551%
14	12.521	1772	1774	1784	rVV4	59007	117489	8.37%	1.113%
15	12.598	1784	1787	1799	rVV2	93616	135989	9.69%	1.289%
16	12.692	1801	1803	1805	rVV	21901	20714	1.48%	0.196%
17	12.727	1807	1809	1814	rVB	34964	33866	2.41%	0.321%
18	12.869	1829	1833	1836	rBV	1435566	1216381	86.66%	11.527%
19	13.357	1910	1916	1922	rBV	333950	352164	25.09%	3.337%
20	13.433	1926	1929	1933	rBV6	12998	21639	1.54%	0.205%
21	13.810	1989	1993	2002	rBV7	40924	114405	8.15%	1.084%
22	13.939	2011	2015	2019	rBV	491985	462949	32.98%	4.387%
23	15.421	2263	2267	2273	rVB	242917	308507	21.98%	2.924%

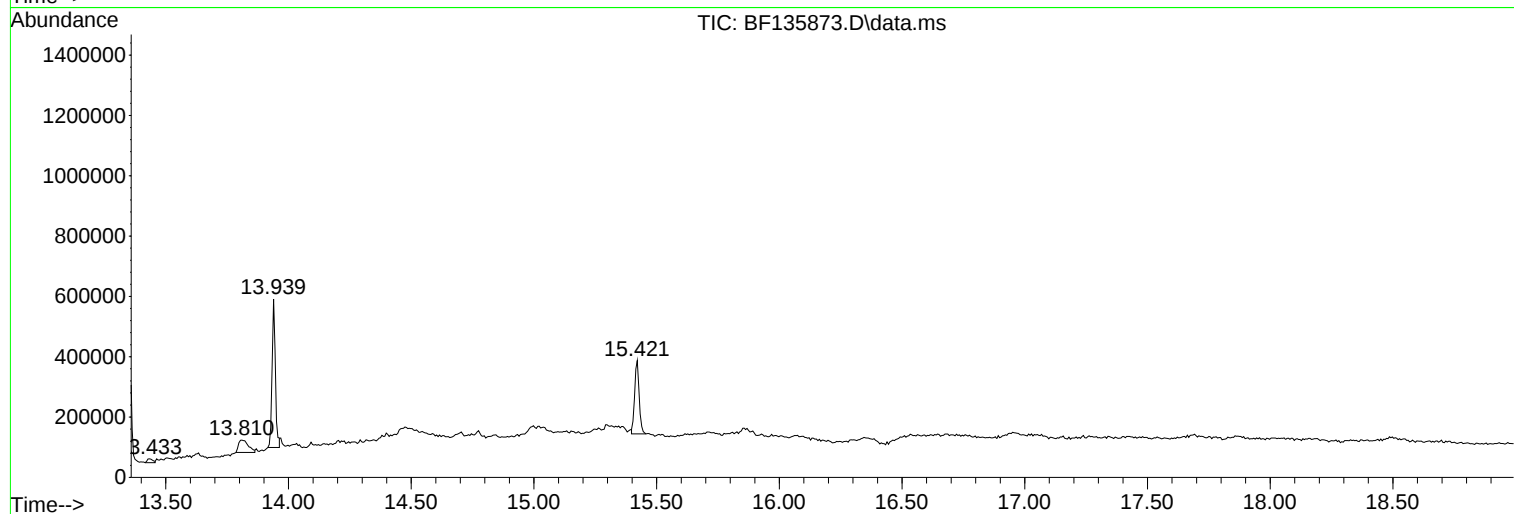
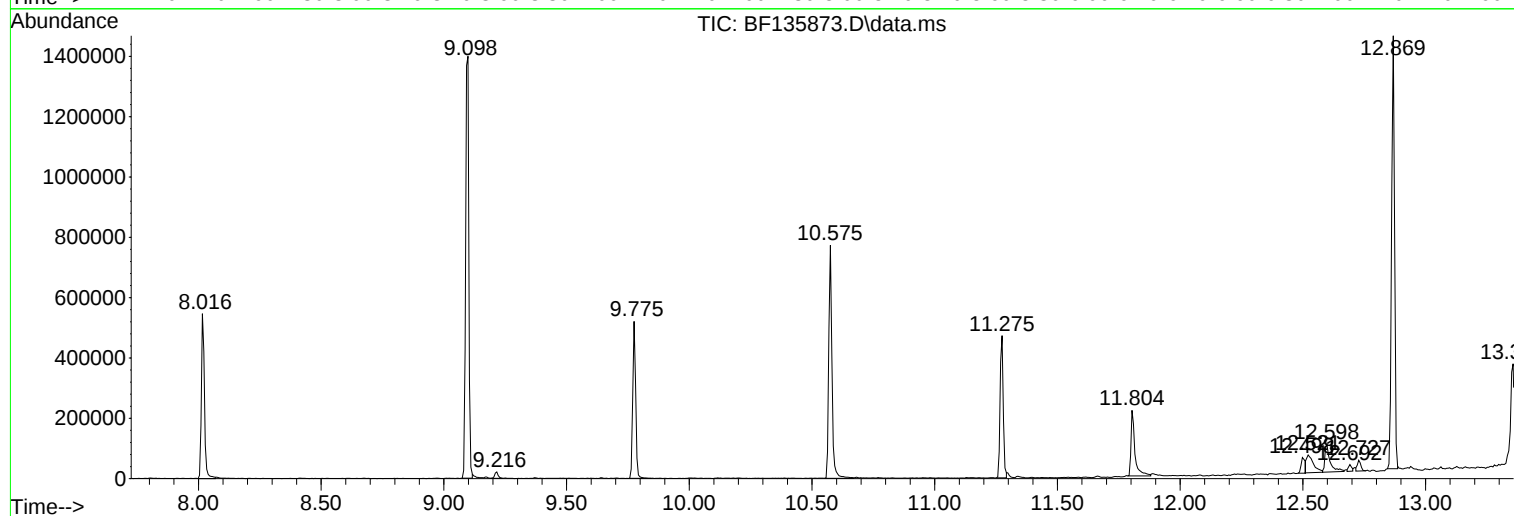
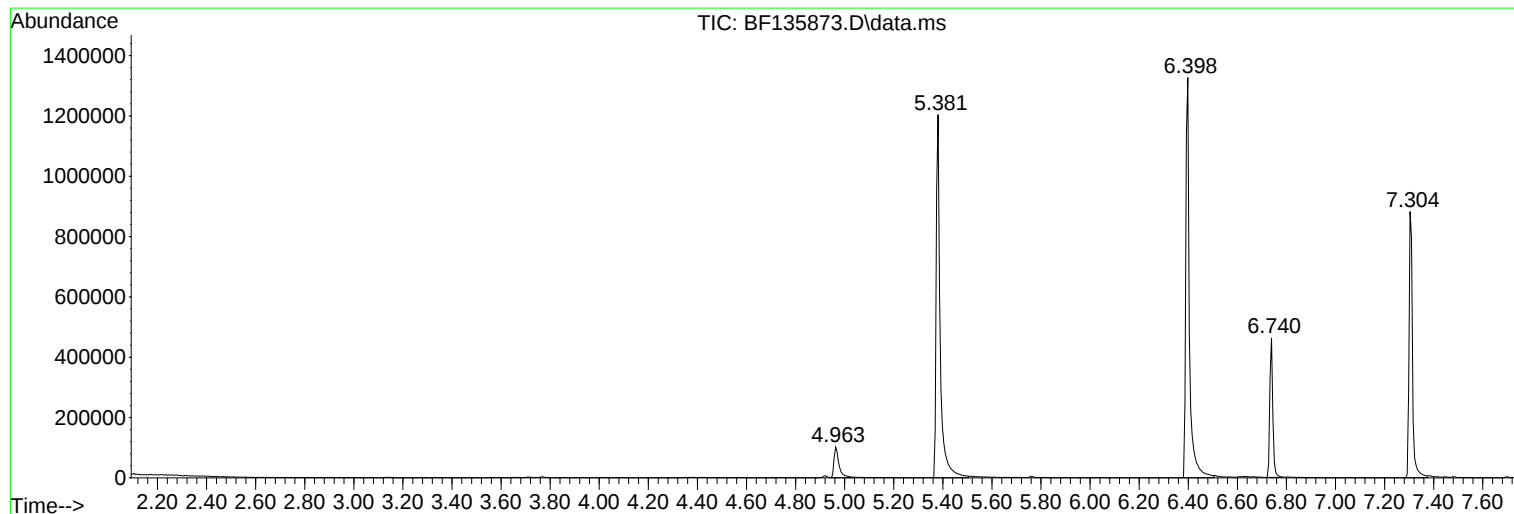
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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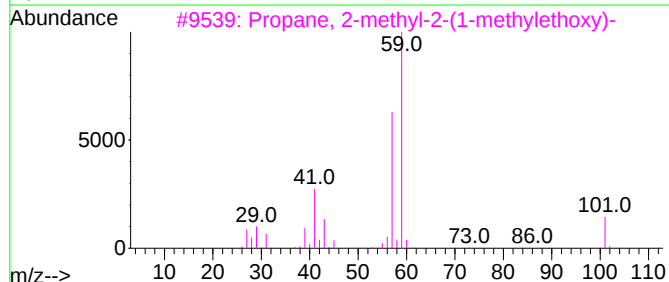
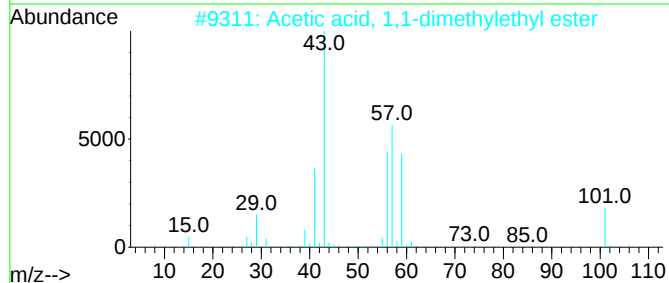
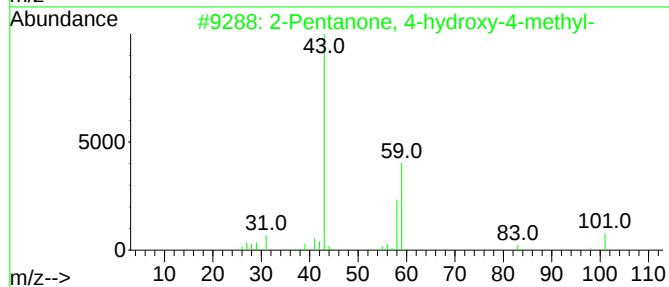
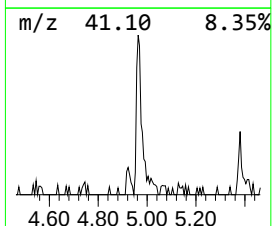
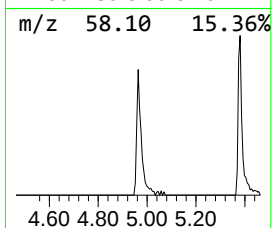
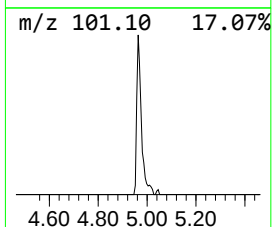
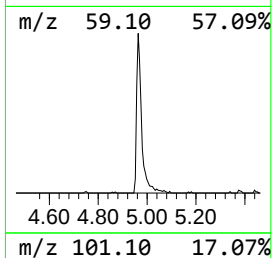
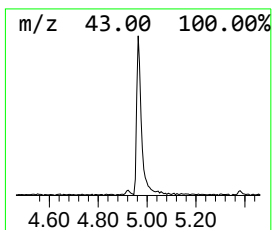
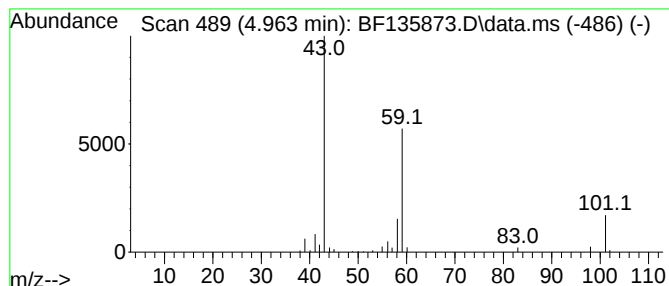
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	7.14 ng	140041	1,4-Dichlorobenzene-d4	6.740

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



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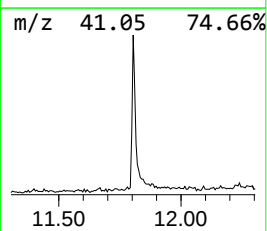
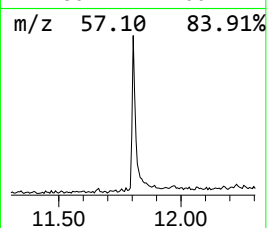
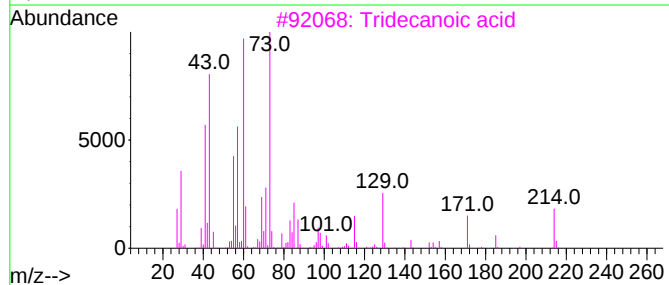
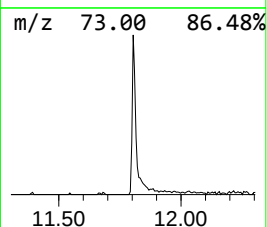
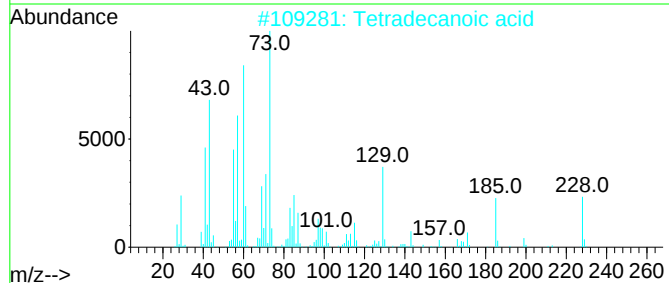
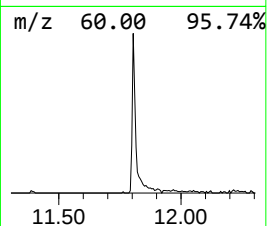
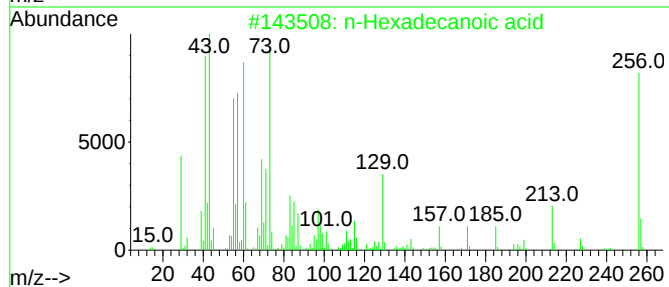
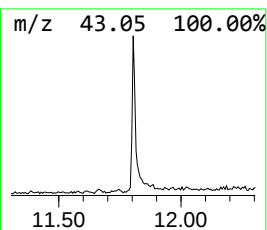
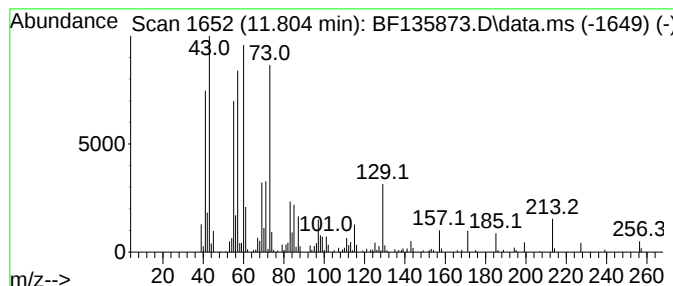
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	11.45 ng	239790	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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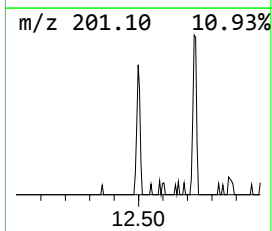
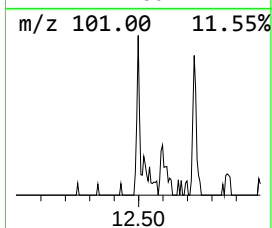
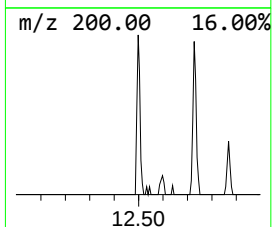
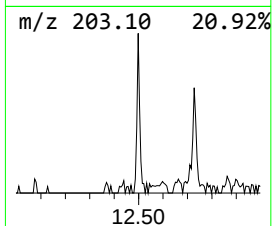
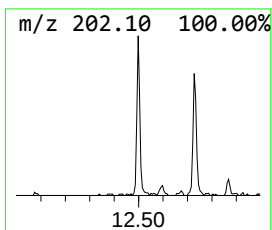
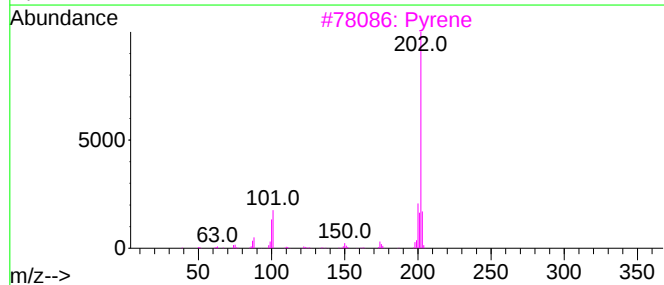
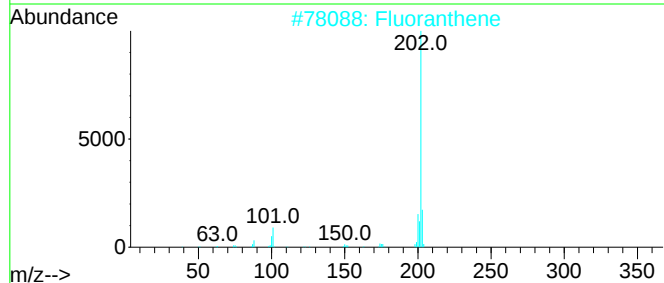
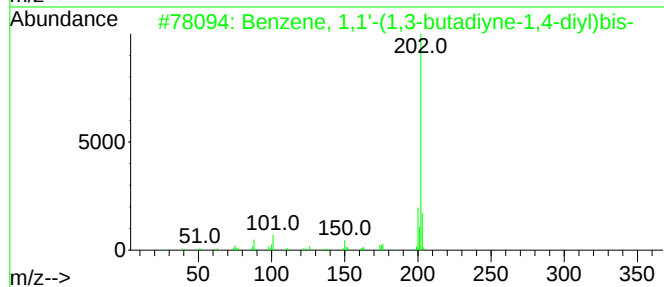
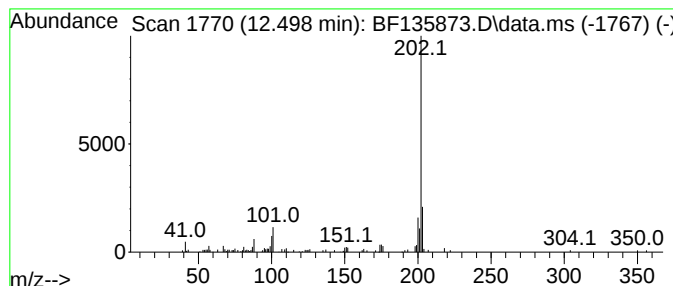
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	2.78 ng	58171	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	93
2			Fluoranthene	202	C16H10	000206-44-0	90
3			Pyrene	202	C16H10	000129-00-0	87
4			1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	50
5			4-Benzyl-1-(1-methyl-2-[(trimeth...	469	C27H43NO2Si2	1000408-11-0	40



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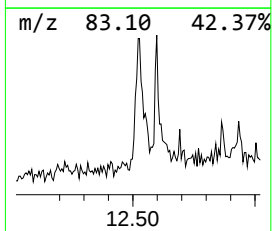
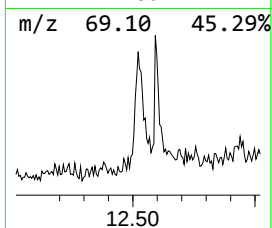
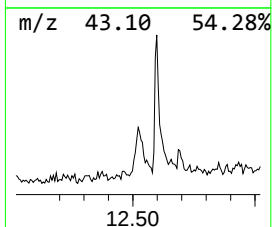
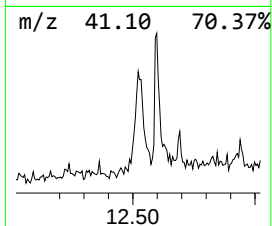
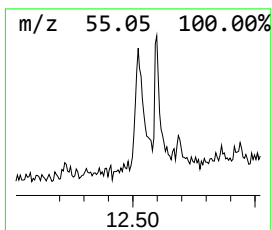
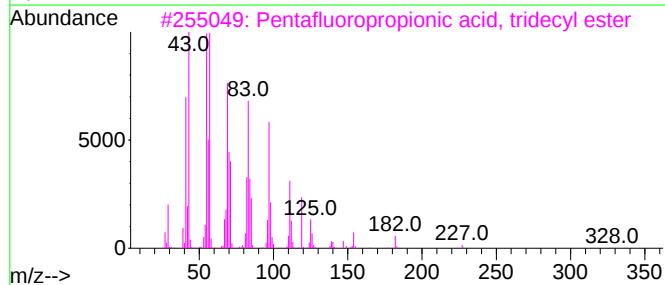
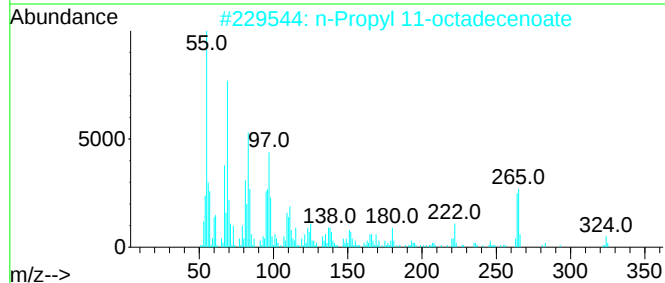
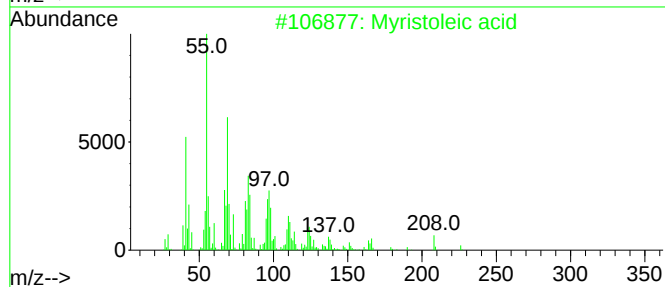
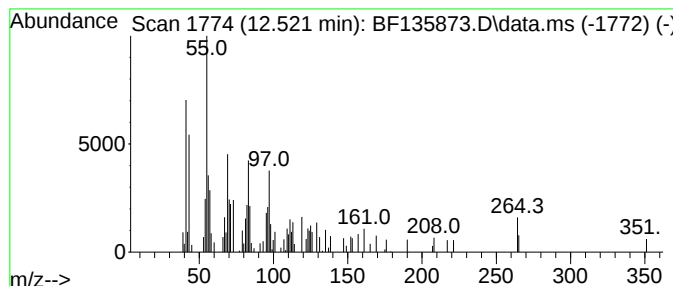
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Myristoleic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.522	5.61 ng	117489	Phenanthrene-d10	11.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Myristoleic acid	226	C14H26O2	000544-64-9	64
2			n-Propyl 11-octadecenoate	324	C21H40O2	1000336-71-7	64
3			Pentafluoropropionic acid, tridecyl ester	346	C16H27F5O2	959261-22-4	55
4			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	49
5			5-Bromovaleric acid, tetradecyl ester	376	C19H37BrO2	1000292-29-1	49



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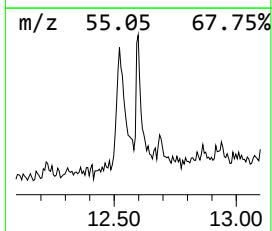
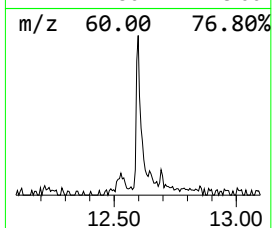
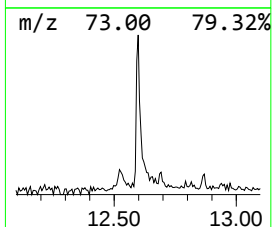
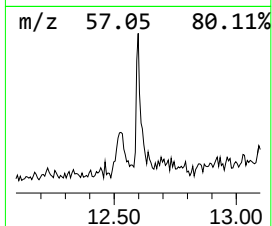
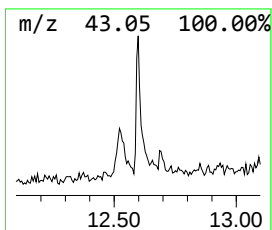
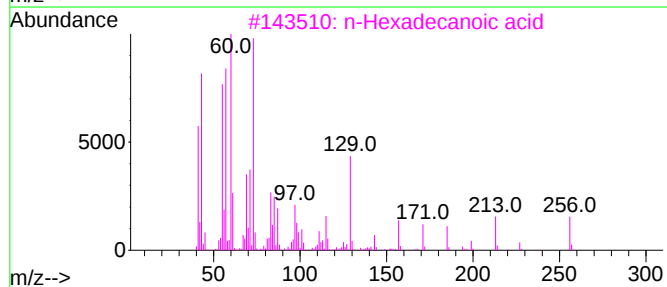
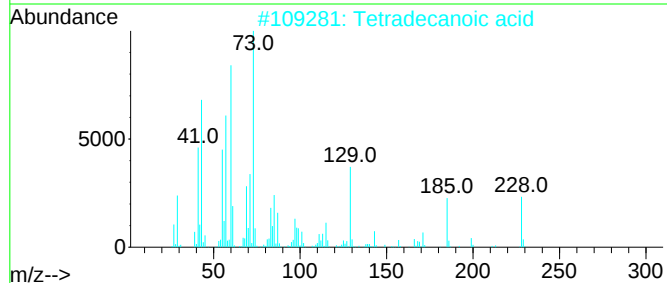
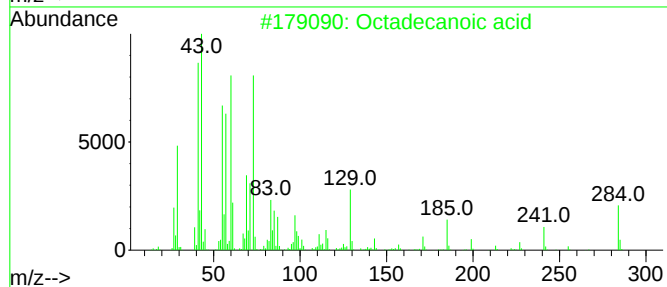
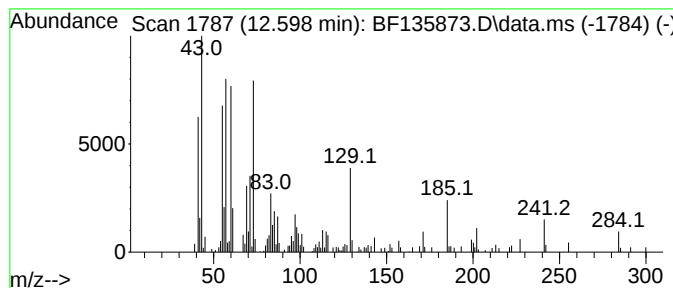
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.598	6.49 ng	135989	Phenanthrene-d10	11.275

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	81
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5			Tridecanoic acid	214	C13H26O2	000638-53-9	62



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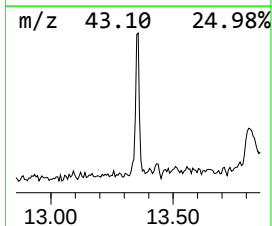
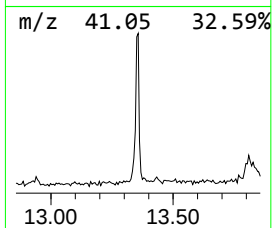
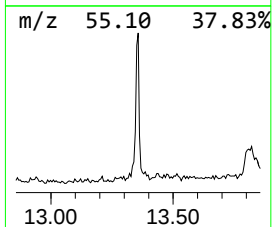
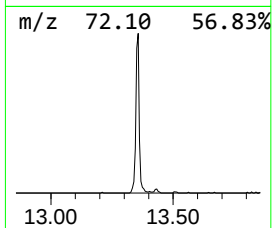
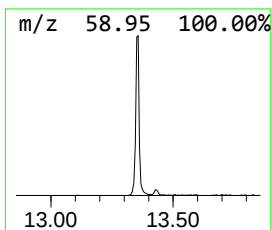
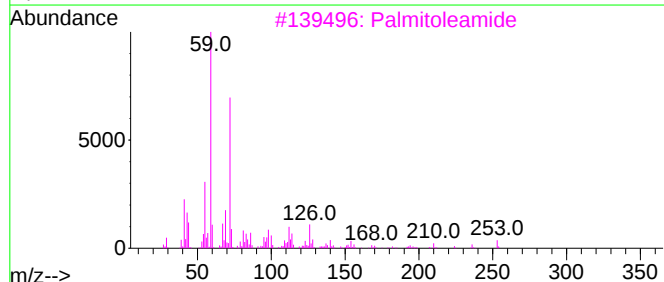
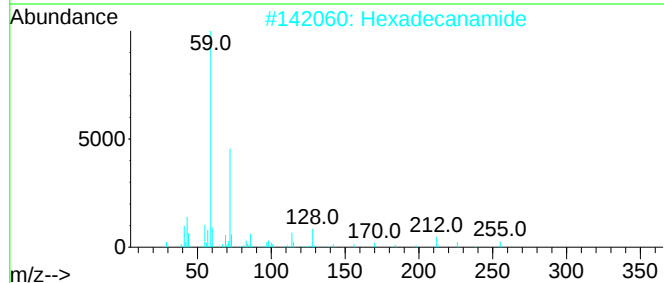
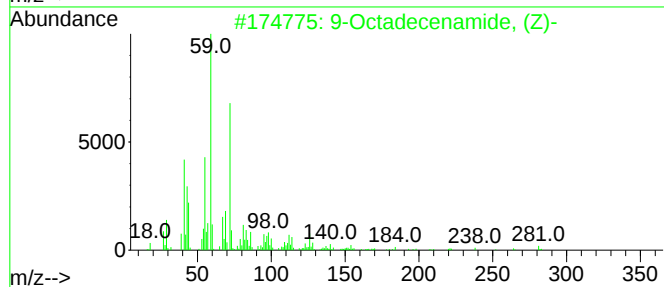
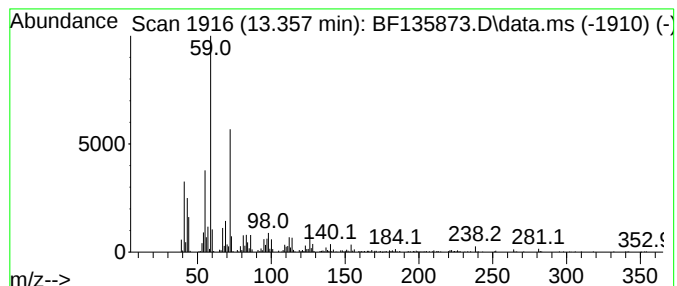
Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.357	15.21 ng	352164	Chrysene-d12	13.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Hexadecanamide	255	C16H33NO	000629-54-9	78
3	Palmitoleamide	253	C16H31NO	106010-22-4	72
4	Dodecanamide	199	C12H25NO	001120-16-7	59
5	Octanamide	143	C8H17NO	000629-01-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135873.D
Acq On : 19 Oct 2023 04:30
Operator : CG\JU
Sample : 04858-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

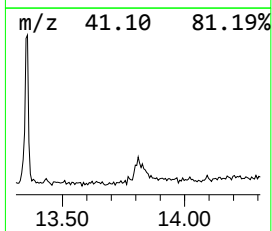
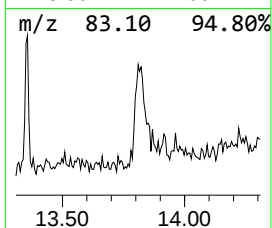
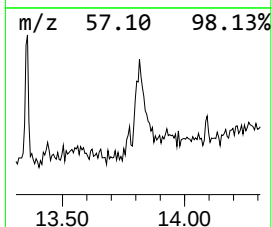
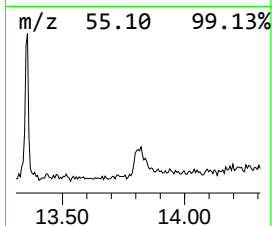
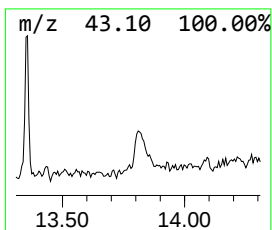
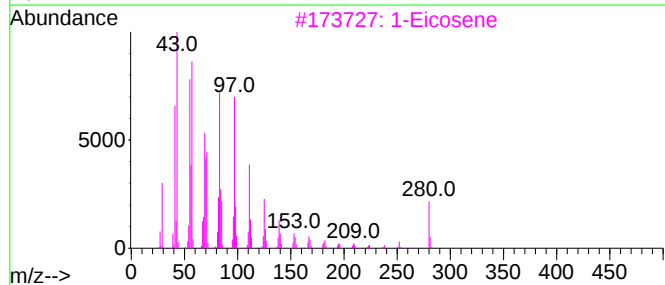
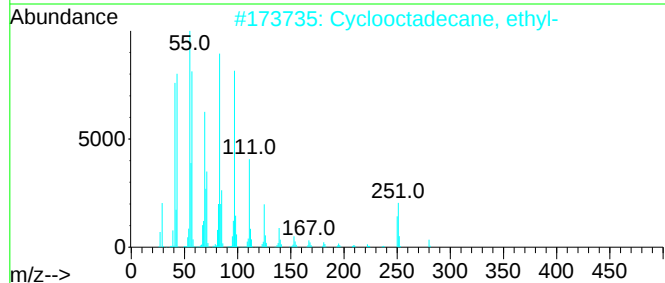
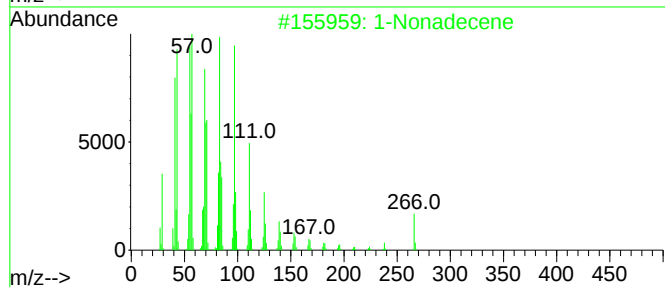
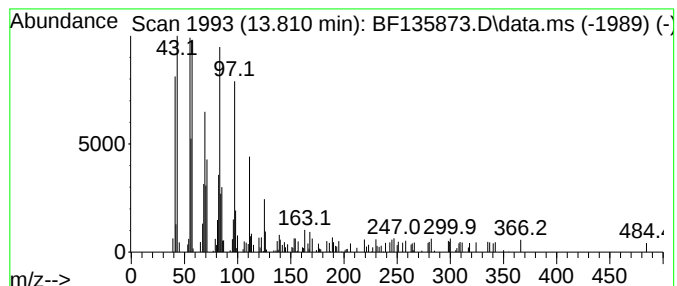
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	4.94 ng	114405	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	94
2	Cyclooctadecane, ethyl-			280	C20H40	1000151-22-5	94
3	1-Eicosene			280	C20H40	003452-07-1	94
4	Cycloeicosane			280	C20H40	000296-56-0	93
5	9-Nonadecene			266	C19H38	031035-07-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
Data File : BF135873.D
Acq On : 19 Oct 2023 04:30
Operator : CG\JU
Sample : 04858-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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-...	4.963	7.1	ng	140041	1	6.740	392466	20.0
n-Hexadecanoic ...	11.804	11.4	ng	239790	4	11.275	419003	20.0
Benzene, 1,1'-(...	12.498	2.8	ng	58171	4	11.275	419003	20.0
Myristoleic acid	12.522	5.6	ng	117489	4	11.275	419003	20.0
Octadecanoic acid	12.598	6.5	ng	135989	4	11.275	419003	20.0
9-Octadecenamid...	13.357	15.2	ng	352164	5	13.939	462949	20.0
1-Nonadecene	13.810	4.9	ng	114405	5	13.939	462949	20.0