

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
 Data File : BF135820.D
 Acq On : 17 Oct 2023 19:28
 Operator : CG\JU
 Sample : 04895-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A-1

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: BF135820.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	485	489	508	rBV	689111	1025785	33.04%	4.721%
2	5.375	556	559	583	rBV	2545730	3034442	97.75%	13.964%
3	5.763	621	625	631	rBV	30304	37179	1.20%	0.171%
4	6.393	728	732	759	rBV	2717564	3104324	100.00%	14.286%
5	6.598	763	767	777	rBV	25210	64344	2.07%	0.296%
6	6.740	787	791	800	rVB	457911	444840	14.33%	2.047%
7	7.310	884	888	901	rBV	1945682	1954608	62.96%	8.995%
8	8.016	1005	1008	1015	rBV	613156	527700	17.00%	2.428%
9	9.092	1187	1191	1195	rBV	3104274	2905430	93.59%	13.371%
10	9.210	1208	1211	1224	rVB	262981	259712	8.37%	1.195%
11	9.775	1303	1307	1317	rBV	697683	621009	20.00%	2.858%
12	10.575	1439	1443	1455	rBV	1983807	1994577	64.25%	9.179%
13	10.681	1458	1461	1469	rVB3	20616	34796	1.12%	0.160%
14	11.269	1558	1561	1570	rBV	759750	670868	21.61%	3.087%
15	11.663	1623	1628	1633	rVB	39534	36354	1.17%	0.167%
16	11.804	1646	1652	1666	rBV2	347237	419274	13.51%	1.929%
17	12.369	1740	1748	1751	rBV3	49245	73932	2.38%	0.340%
18	12.498	1768	1770	1777	rBV2	21974	36604	1.18%	0.168%
19	12.592	1783	1786	1796	rBV	72351	103982	3.35%	0.479%
20	12.869	1828	1833	1836	rBV	3096965	2928393	94.33%	13.476%
21	13.433	1926	1929	1933	rBV2	33330	34907	1.12%	0.161%
22	13.769	1983	1986	1989	rBV	40548	38389	1.24%	0.177%
23	13.827	1989	1996	2006	rVV6	55880	191246	6.16%	0.880%
24	13.933	2011	2014	2023	rVB	482787	512135	16.50%	2.357%
25	14.086	2037	2040	2043	rBV	37769	34102	1.10%	0.157%
26	14.398	2089	2093	2099	rBV	39840	39814	1.28%	0.183%
27	14.698	2139	2144	2148	rBV2	38881	41750	1.34%	0.192%
28	14.768	2152	2156	2161	rVV	37857	40922	1.32%	0.188%
29	15.033	2198	2201	2205	rVB2	35577	39899	1.29%	0.184%
30	15.410	2261	2265	2276	rBV	304450	441741	14.23%	2.033%
31	15.845	2334	2339	2343	rVB2	25244	36769	1.18%	0.169%

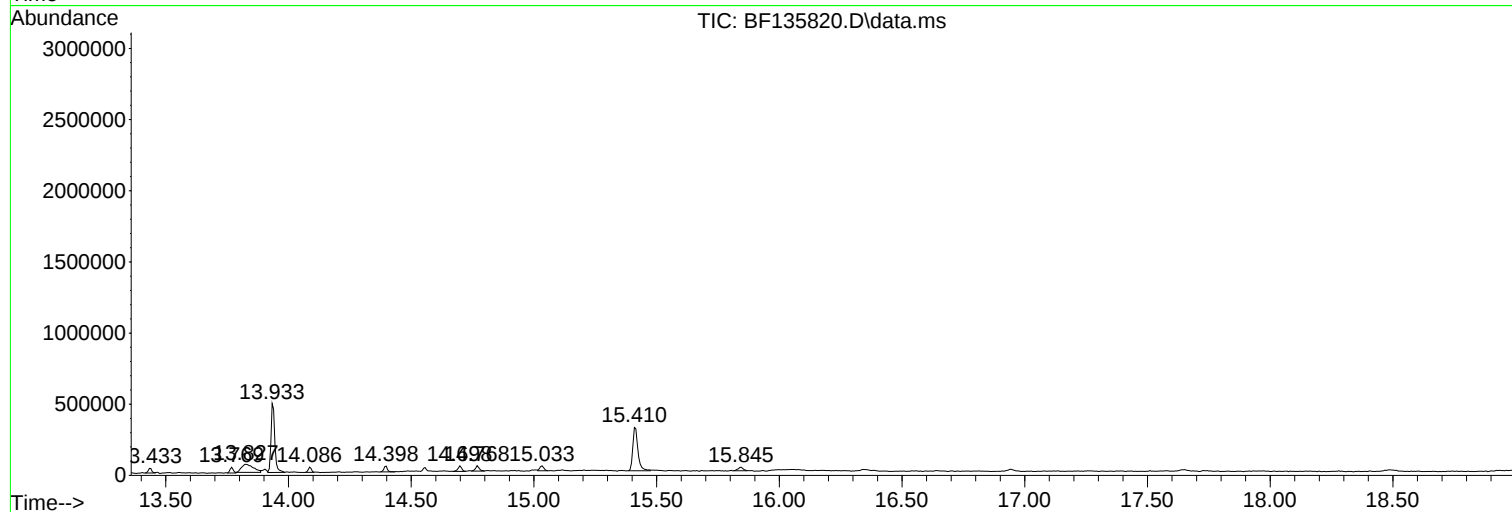
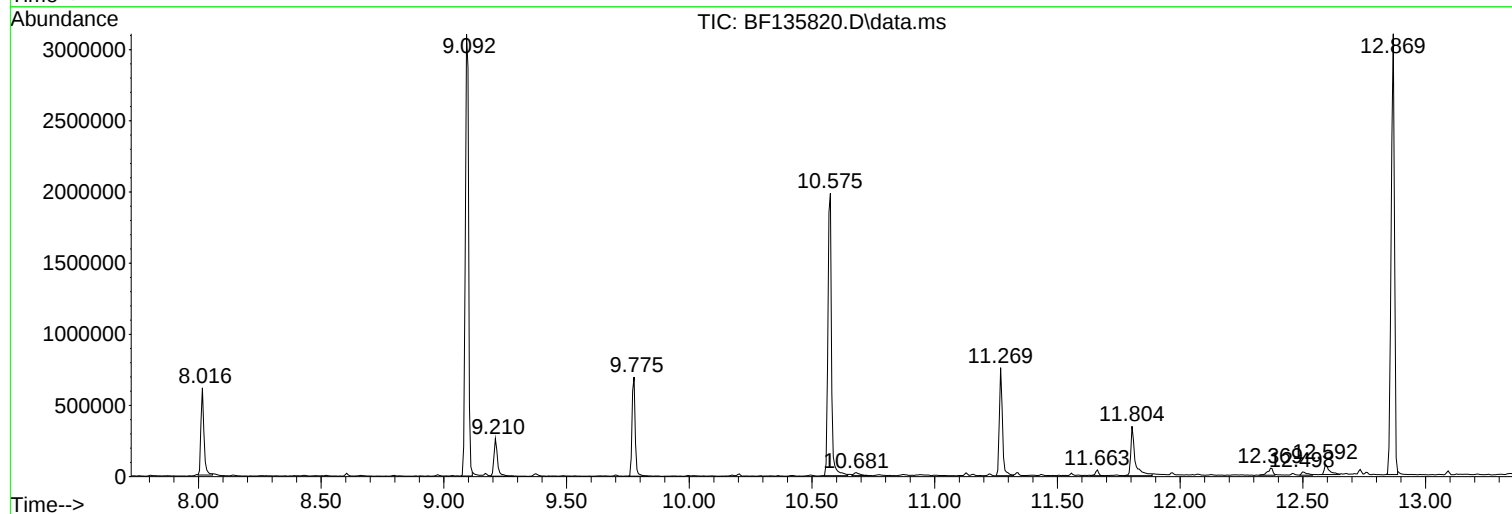
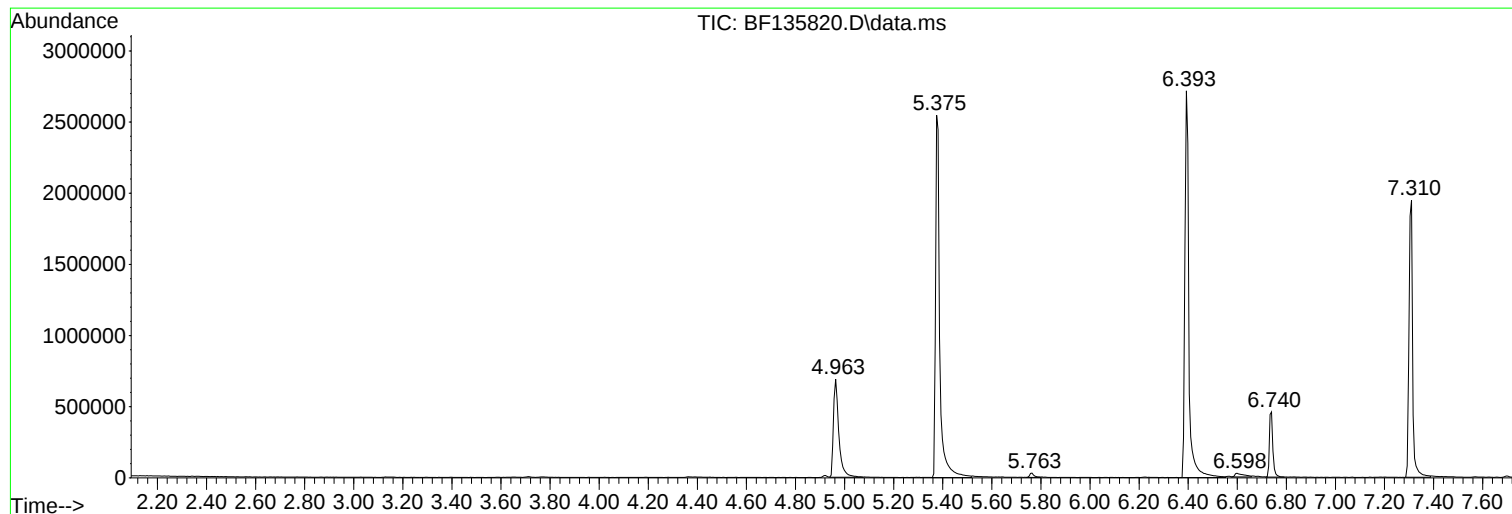
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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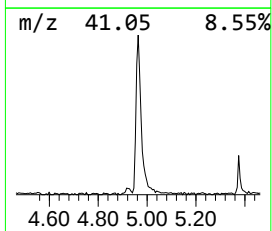
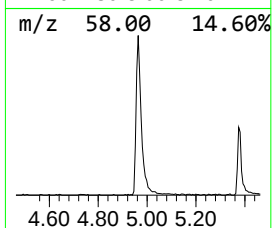
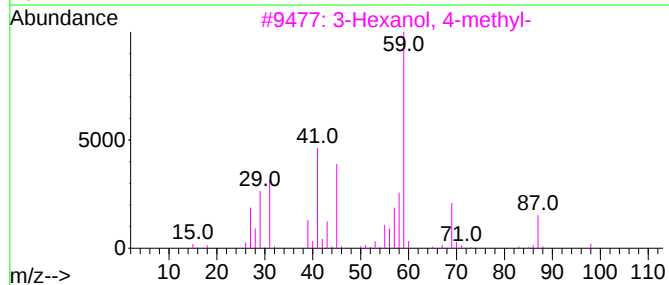
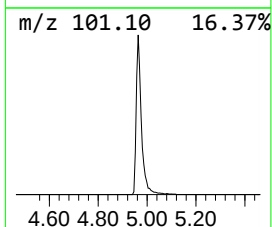
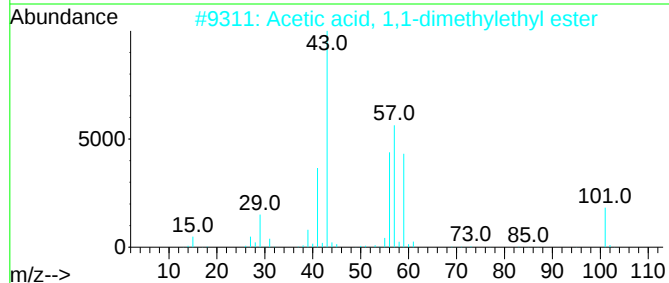
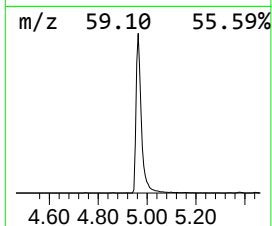
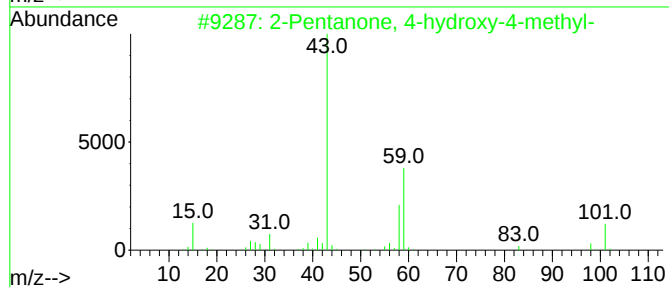
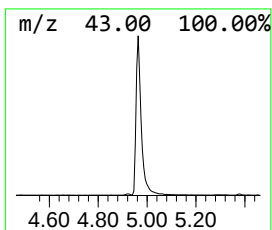
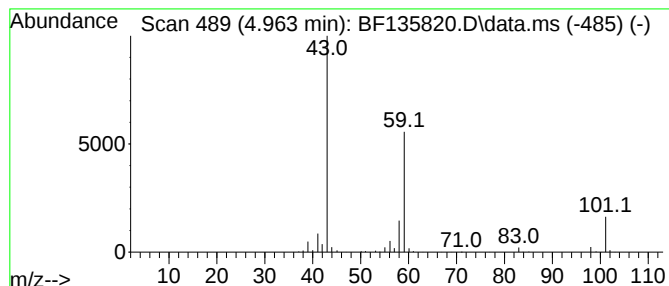
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown4.963 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	46.12 ng	1025790	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	42		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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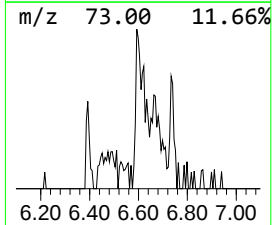
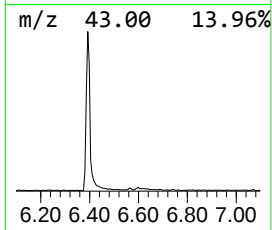
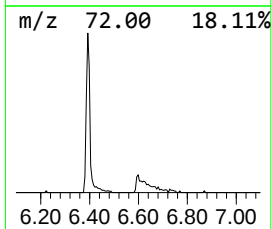
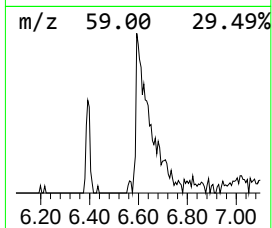
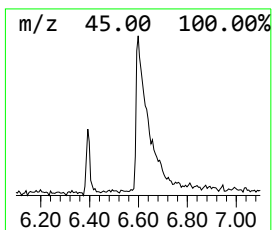
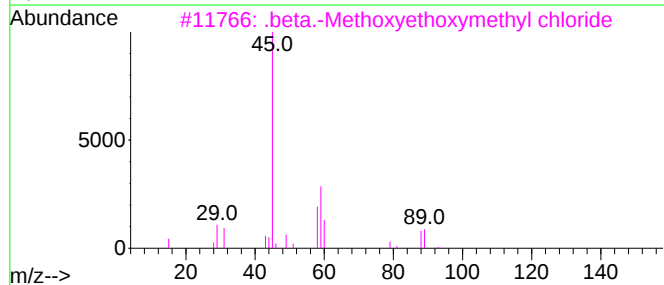
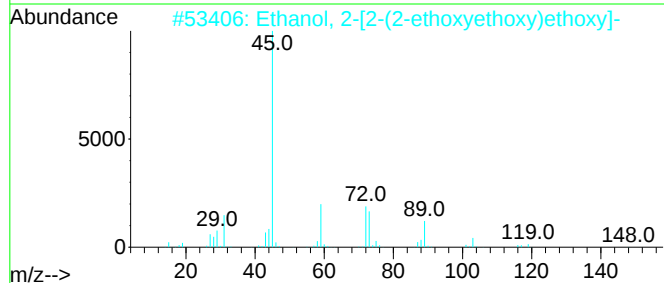
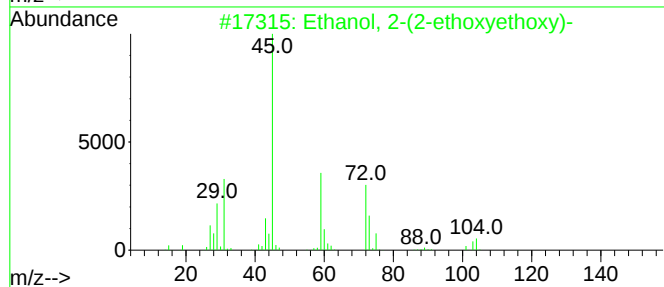
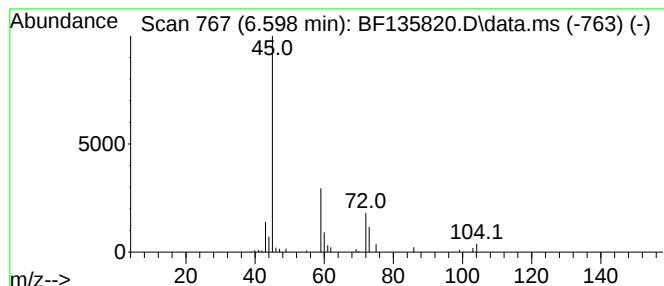
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.598	2.89 ng	64344	1,4-Dichlorobenzene-d4	6.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	50
2			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	39
3			.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	38
4			Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	33
5			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	33



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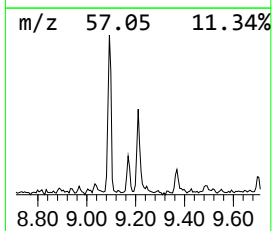
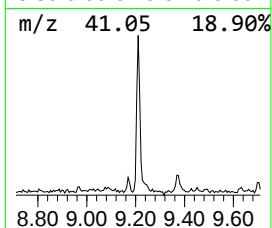
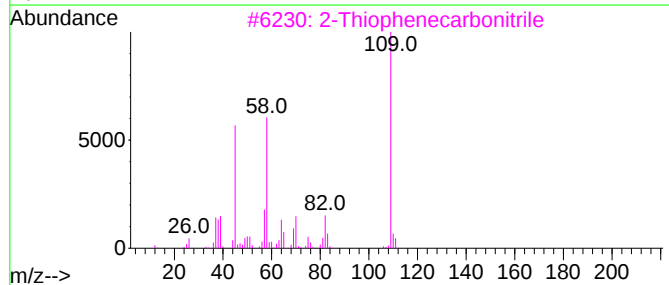
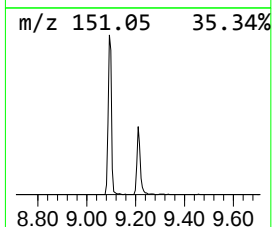
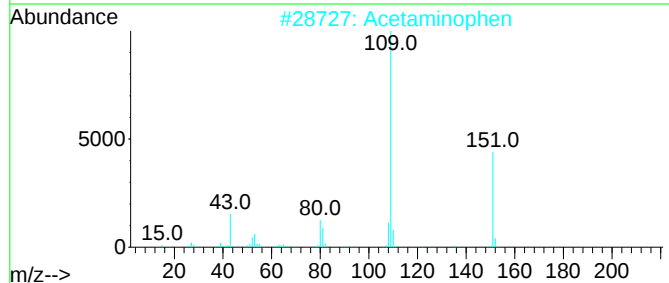
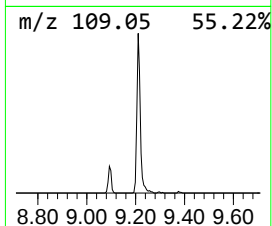
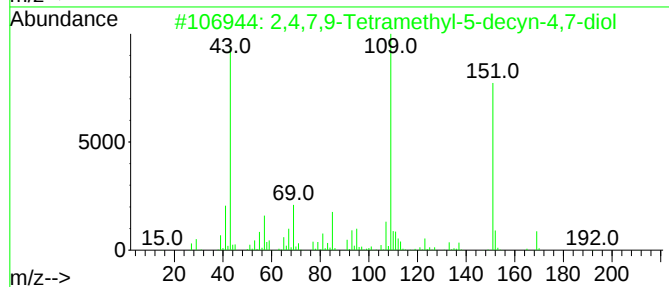
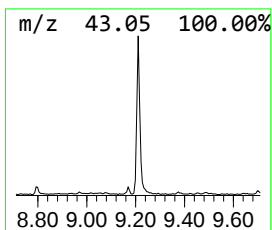
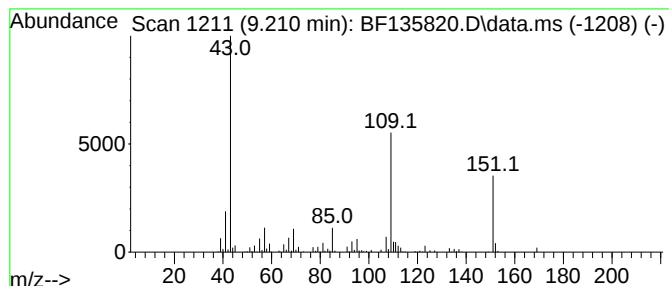
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.210	8.36 ng	259712	Acenaphthene-d10	9.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	80	
2	Acetaminophen	151	C8H9NO2	000103-90-2	47	
3	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	43	
4	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	37	
5	2,3-Dehydro-1,8-cineole	152	C10H16O	092760-25-3	37	



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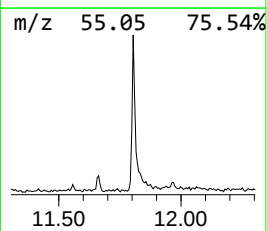
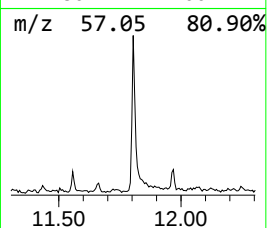
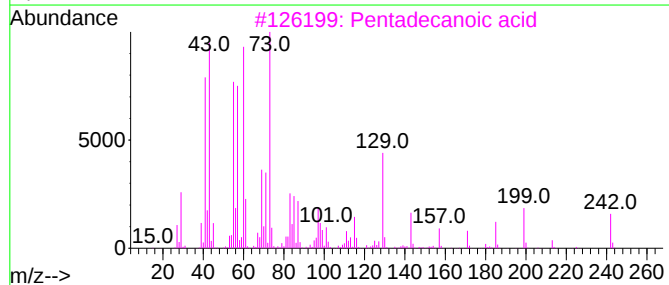
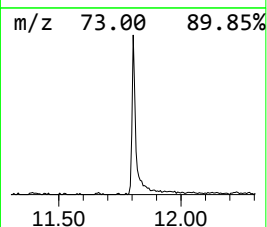
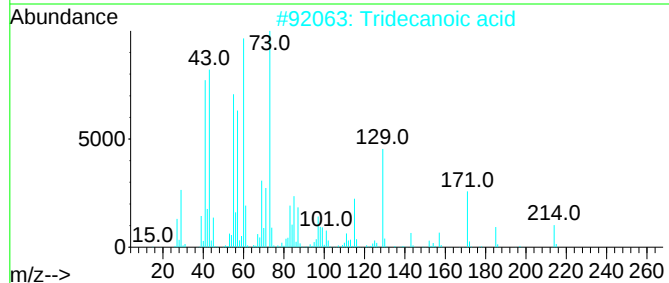
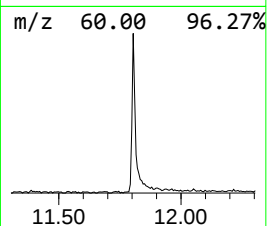
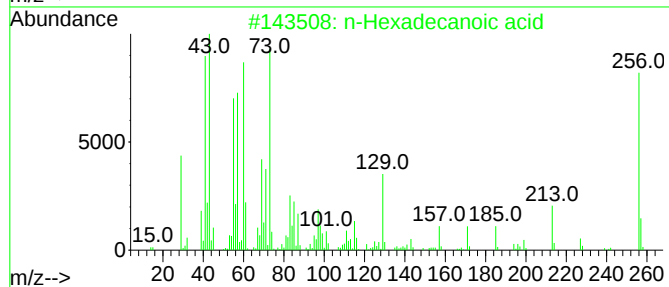
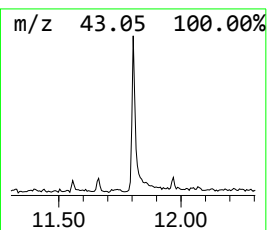
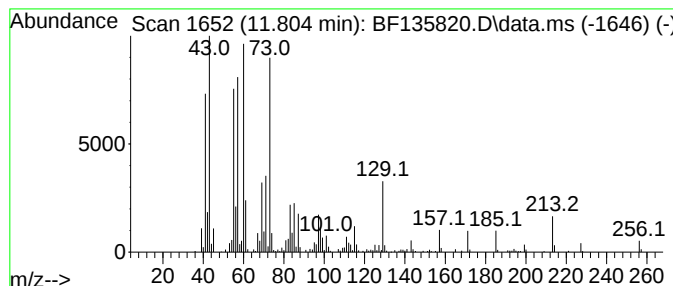
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	12.50 ng	419274	Phenanthrene-d10	11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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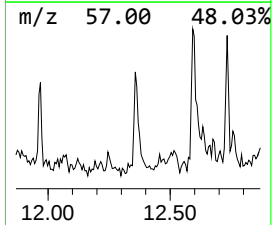
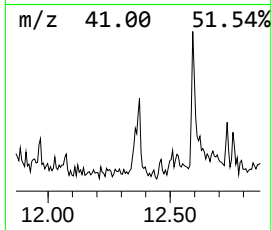
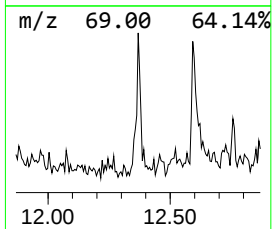
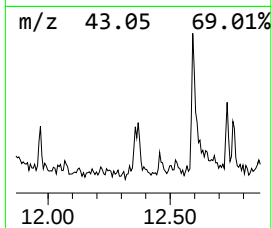
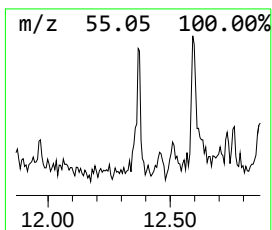
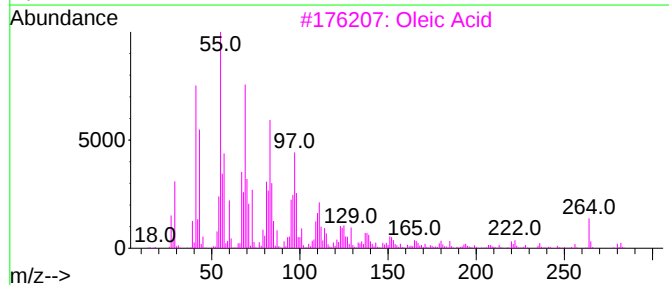
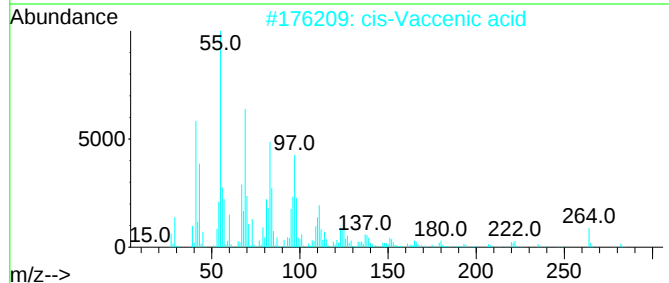
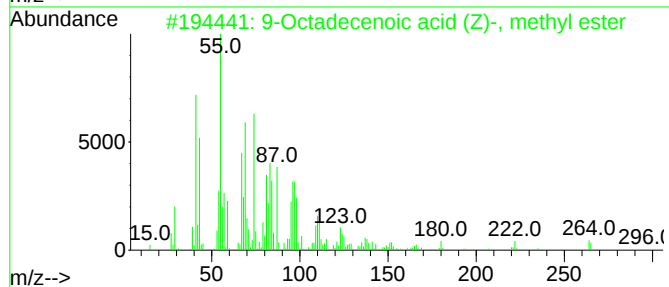
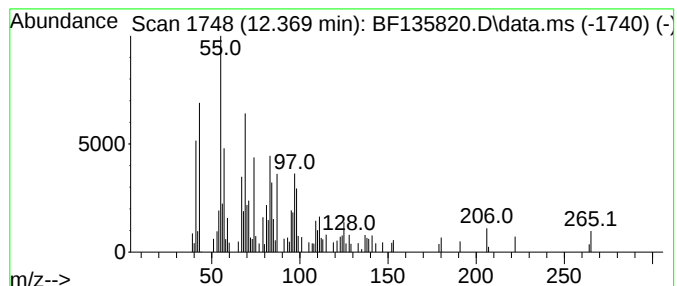
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Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.369	2.20 ng	73932	Phenanthrene-d10	11.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	52
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	49
3	Oleic Acid	282	C18H34O2	000112-80-1	38
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	30
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	30



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ALS Vial : 7 Sample Multiplier: 1

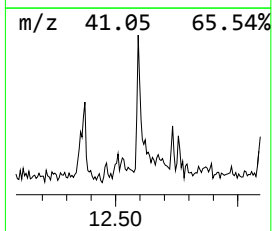
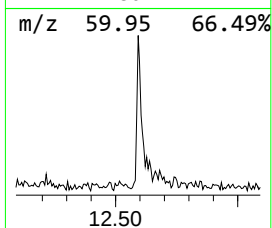
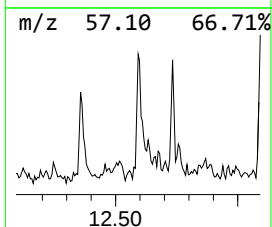
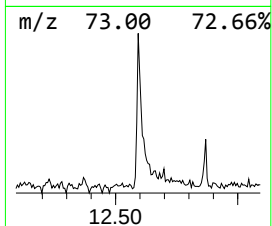
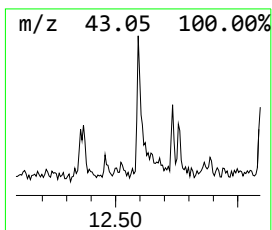
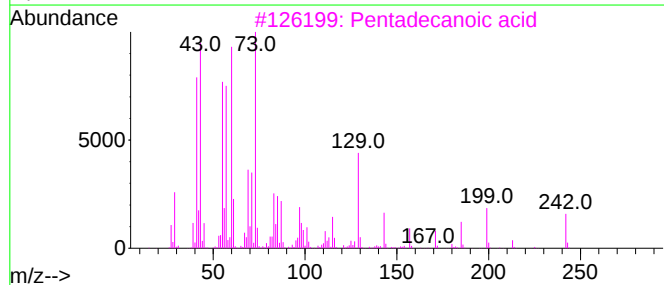
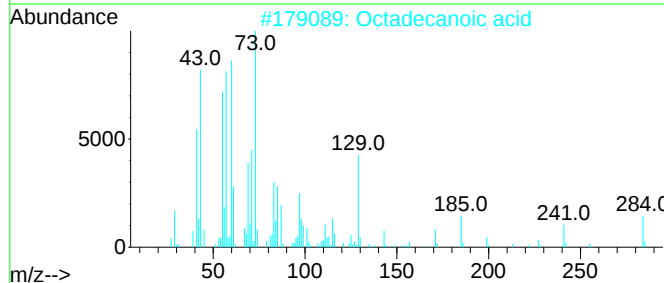
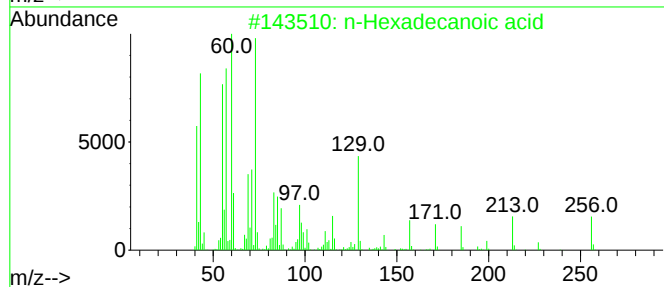
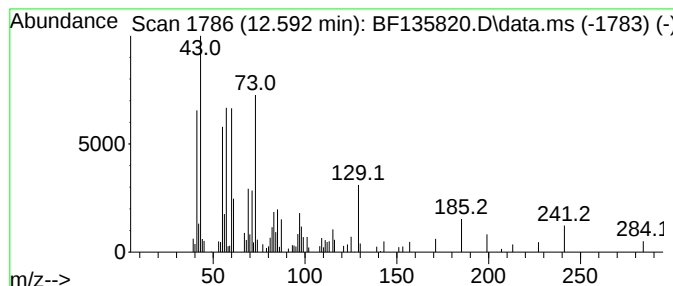
Instrument :
BNA_F
ClientSampleId :
A-1

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 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.592	3.10 ng	103982	Phenanthrene-d10		11.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	90
2	Octadecanoic acid		284	C18H36O2	000057-11-4	83
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	68
5	Tridecanoic acid		214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
Data File : BF135820.D
Acq On : 17 Oct 2023 19:28
Operator : CG\JU
Sample : 04895-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-1

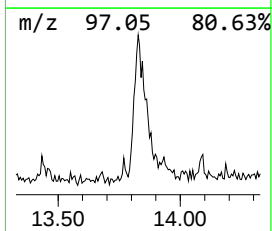
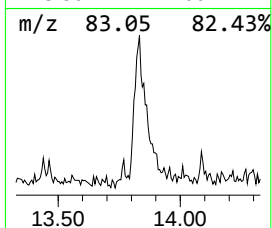
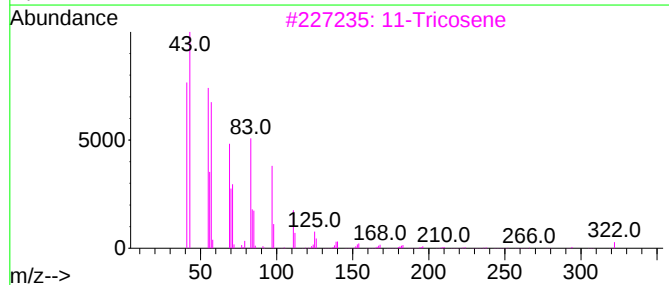
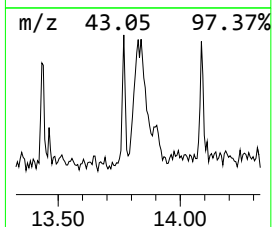
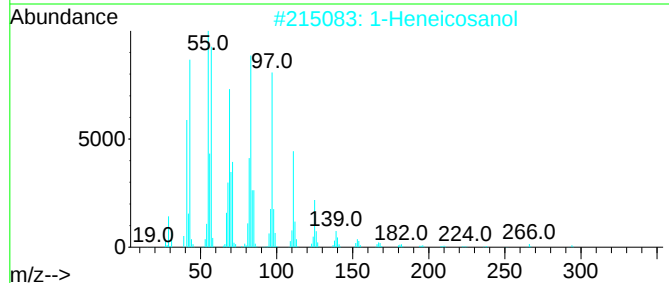
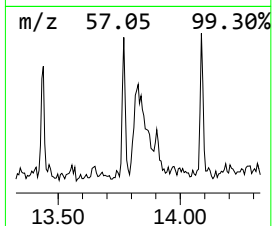
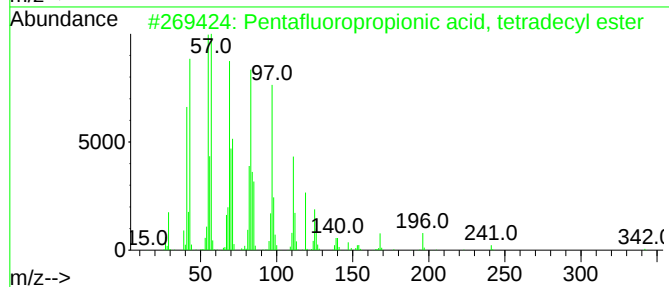
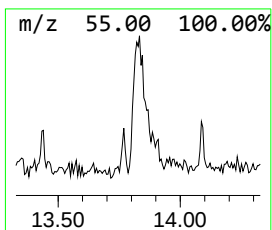
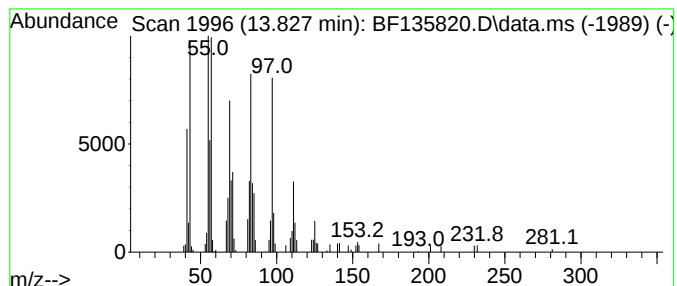
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	7.47 ng	191246	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93
2			1-Heneicosanol	312	C21H44O	015594-90-8	91
3			11-Tricosene	322	C23H46	052078-56-5	91
4			1-Docosene	308	C22H44	001599-67-3	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101723\
Data File : BF135820.D
Acq On : 17 Oct 2023 19:28
Operator : CG\JU
Sample : 04895-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A-1

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
unknown4.963	4.963	46.1	ng	1025790	1	6.740	444840	20.0
Ethanol, 2-(2-e...	6.598	2.9	ng	64344	1	6.740	444840	20.0
2,4,7,9-Tetrame...	9.210	8.4	ng	259712	3	9.775	621009	20.0
n-Hexadecanoic ...	11.804	12.5	ng	419274	4	11.269	670868	20.0
9-Octadecenoic ...	12.369	2.2	ng	73932	4	11.269	670868	20.0
Octadecanoic acid	12.592	3.1	ng	103982	4	11.269	670868	20.0
Pentafluoroprop...	13.827	7.5	ng	191246	5	13.933	512135	20.0