

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
 Data File : BF136112.D
 Acq On : 02 Nov 2023 23:38
 Operator : CG\JU
 Sample : 05050-10
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B5

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-BF103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136112.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	502	506	513	rVB	87373	113282	3.07%	0.520%
2	5.451	566	572	575	rBV	3041226	3310137	89.79%	15.194%
3	6.457	736	743	746	rBV	2744367	3103036	84.17%	14.243%
4	6.645	772	775	786	rBV	57313	61349	1.66%	0.282%
5	6.816	801	804	808	rVB	739758	584374	15.85%	2.682%
6	7.381	895	900	903	rBV	1971329	2067829	56.09%	9.492%
7	8.098	1018	1022	1025	rBV	1040780	780178	21.16%	3.581%
8	9.181	1202	1206	1209	rBV	4327145	3686474	100.00%	16.922%
9	9.298	1223	1226	1230	rVB	47819	41698	1.13%	0.191%
10	9.857	1317	1321	1324	rBV	1089629	848201	23.01%	3.893%
11	10.651	1451	1456	1459	rBV	2301546	2091703	56.74%	9.601%
12	11.345	1571	1574	1578	rBV	892786	762047	20.67%	3.498%
13	11.886	1662	1666	1682	rBV2	244544	275290	7.47%	1.264%
14	12.680	1798	1801	1810	rBV	48205	63200	1.71%	0.290%
15	12.951	1842	1847	1850	rBV	3184163	2798107	75.90%	12.844%
16	13.869	2000	2003	2005	rBV	47268	52387	1.42%	0.240%
17	13.898	2005	2008	2022	rVV3	43157	120891	3.28%	0.555%
18	14.004	2022	2026	2029	rVV	593543	516397	14.01%	2.370%
19	15.492	2273	2279	2284	rBV	422286	509143	13.81%	2.337%

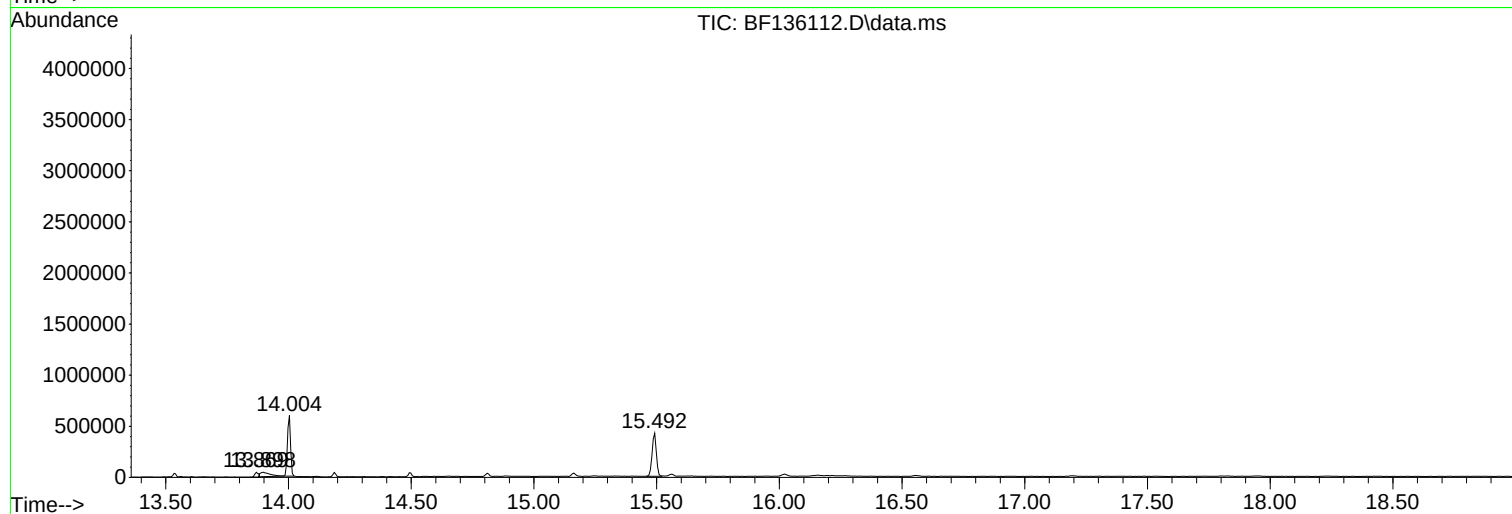
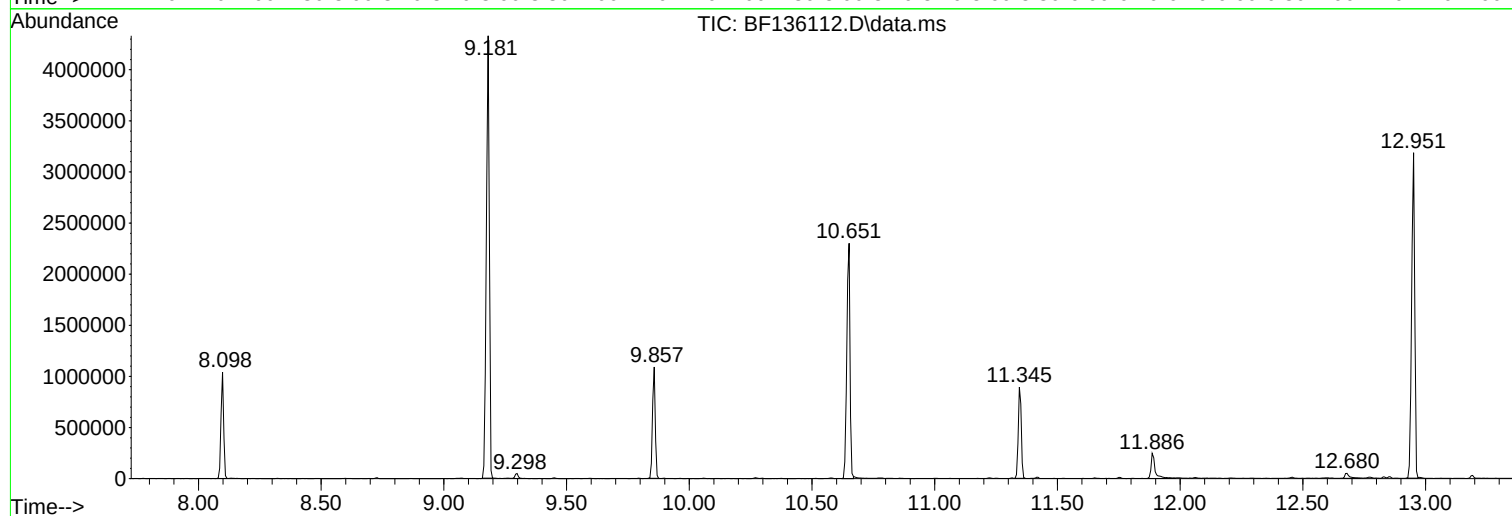
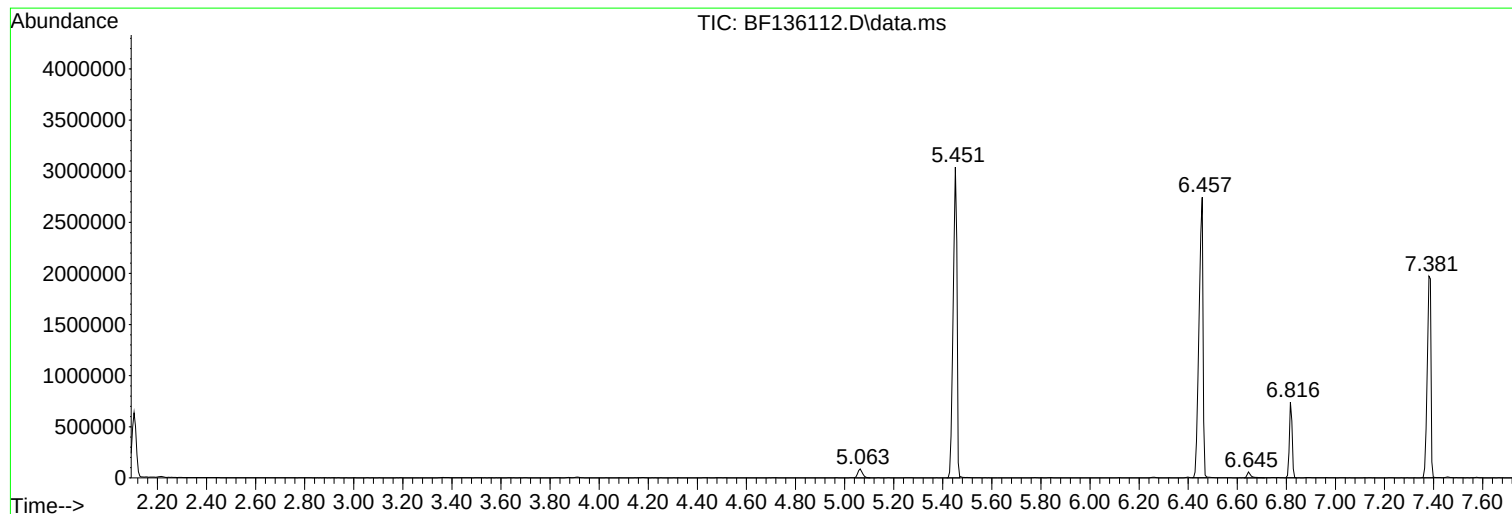
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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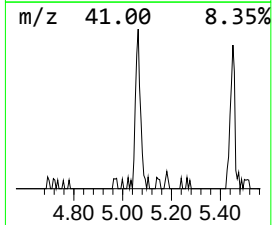
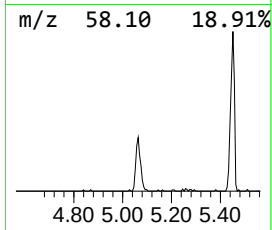
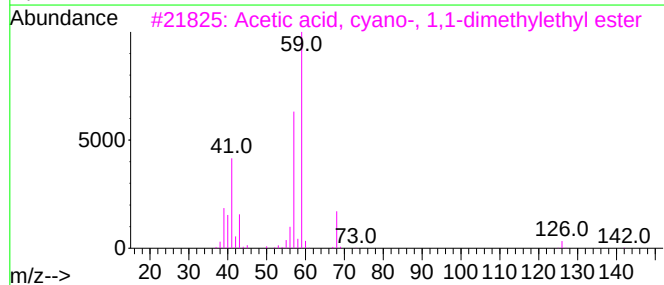
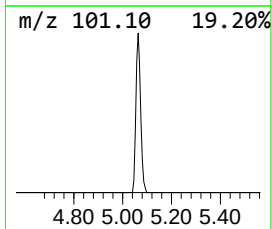
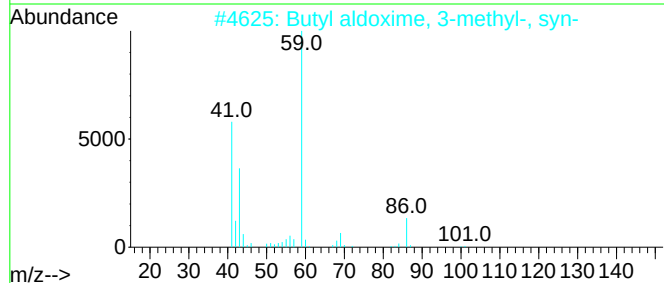
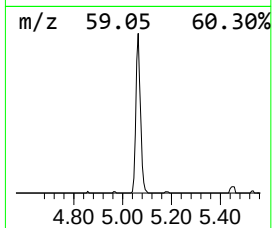
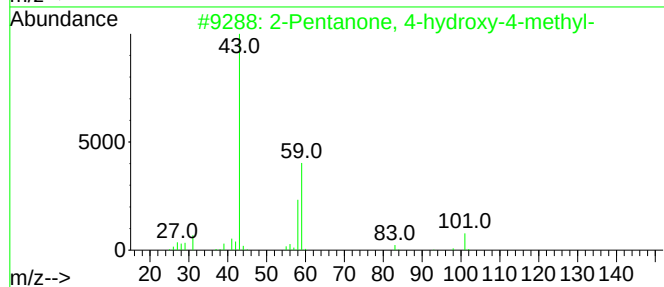
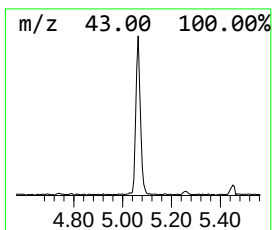
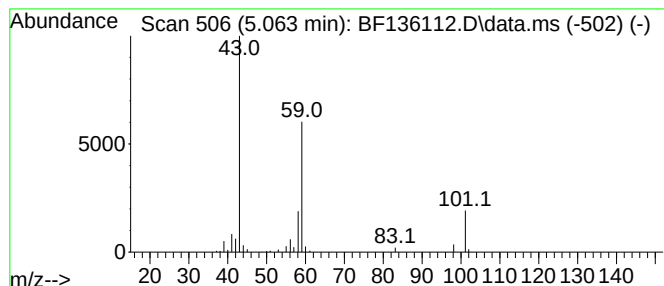
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	3.88 ng	113282	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Acetone	58	C3H6O	000067-64-1	14		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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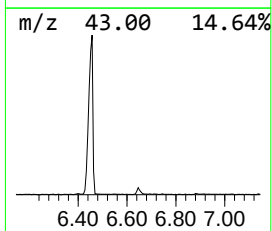
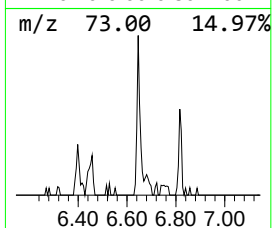
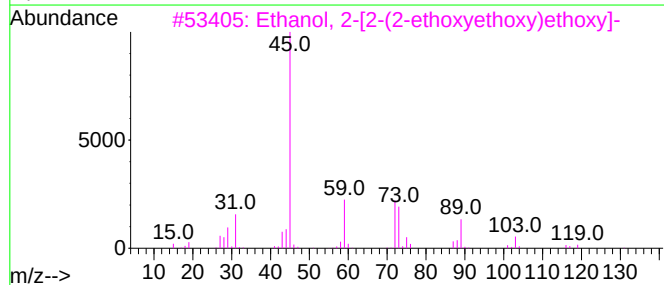
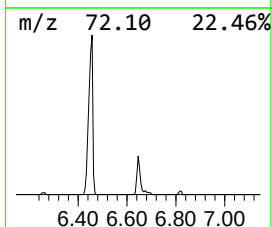
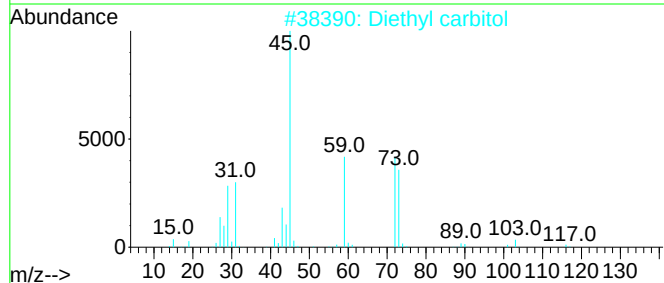
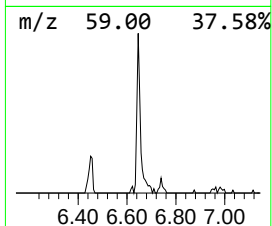
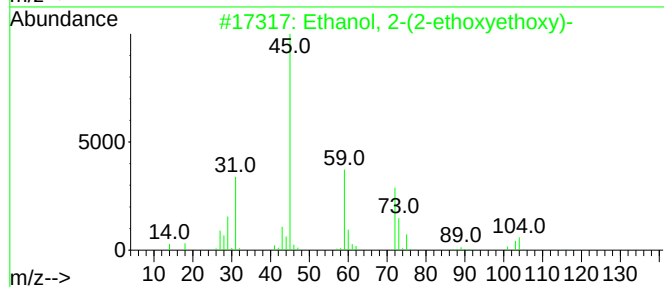
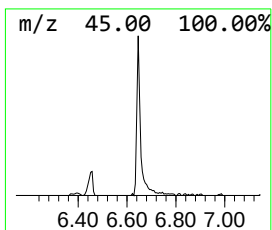
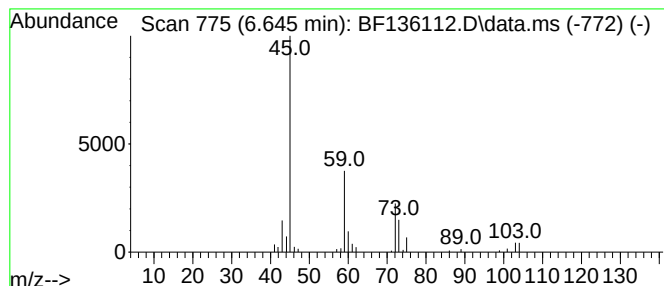
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.645	2.10 ng	61349	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
4			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	36



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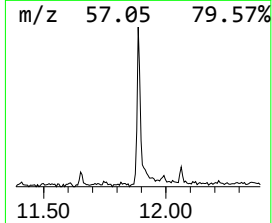
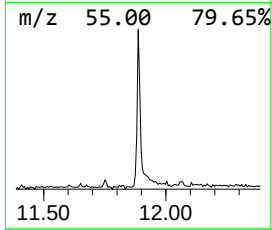
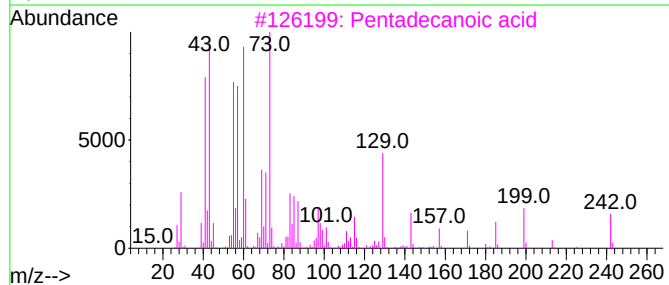
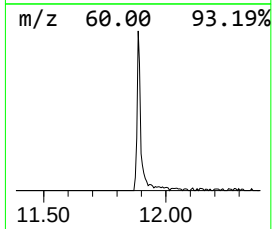
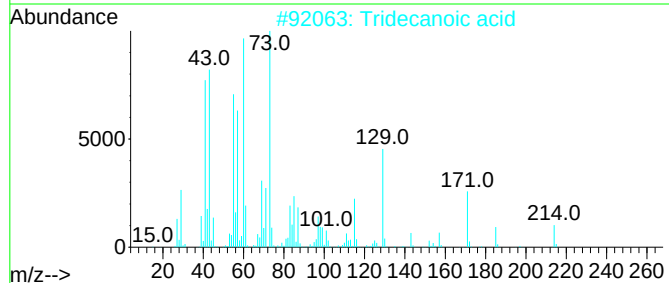
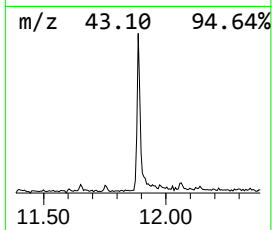
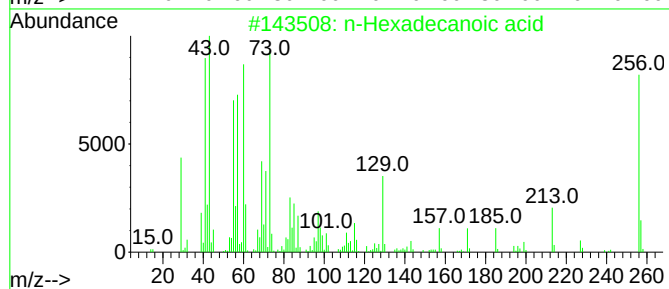
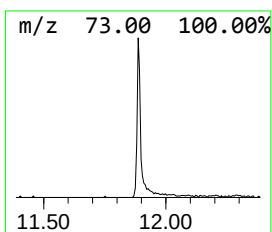
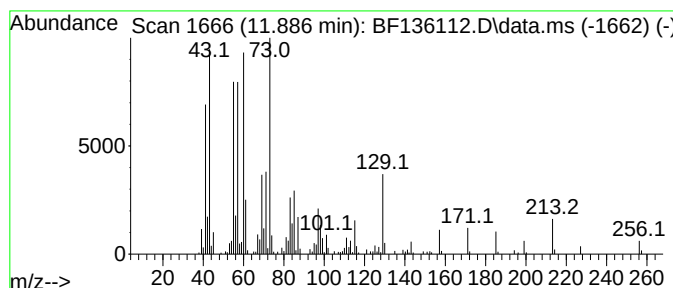
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.886	7.23 ng	275290	Phenanthrene-d10	11.345	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Dodecanoic acid	200	C12H24O2	000143-07-7	80



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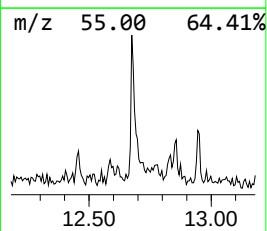
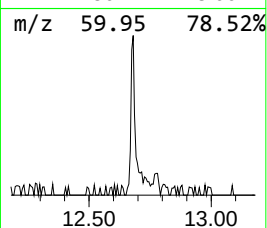
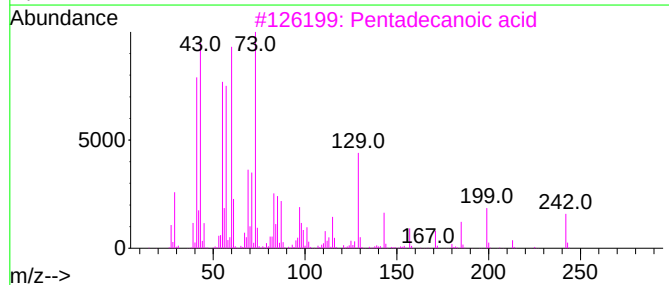
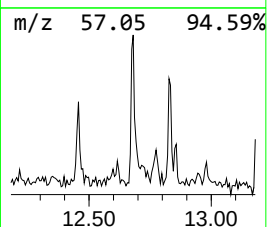
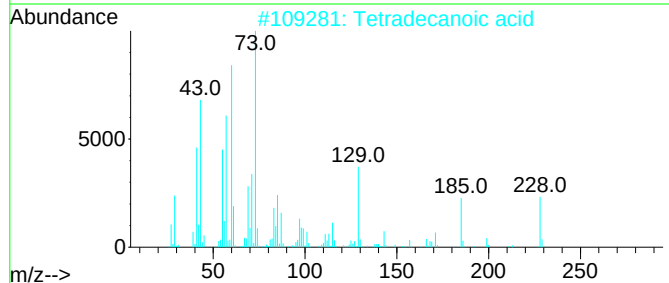
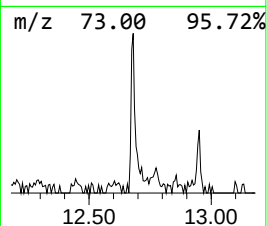
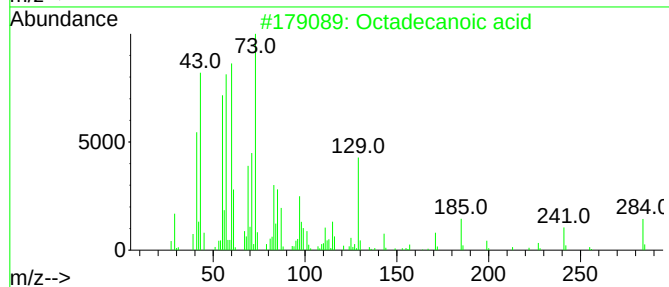
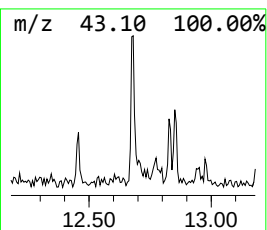
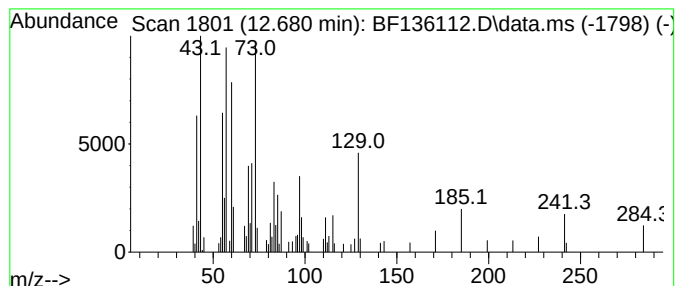
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.45 ng	63200	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	59



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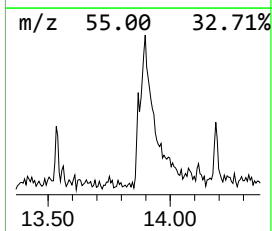
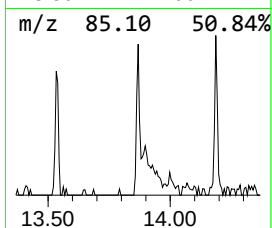
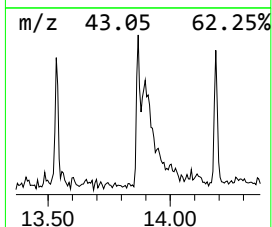
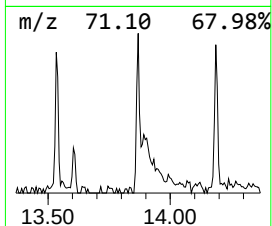
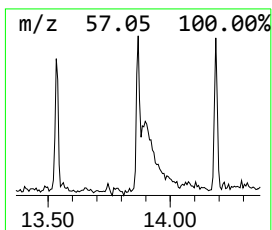
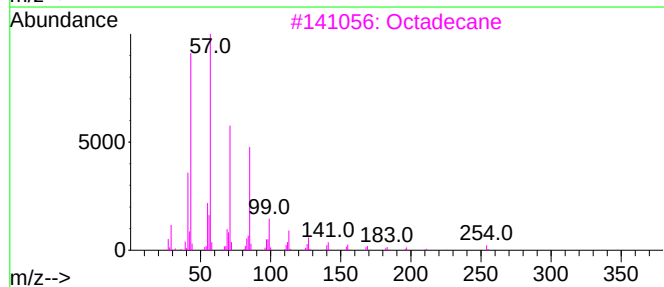
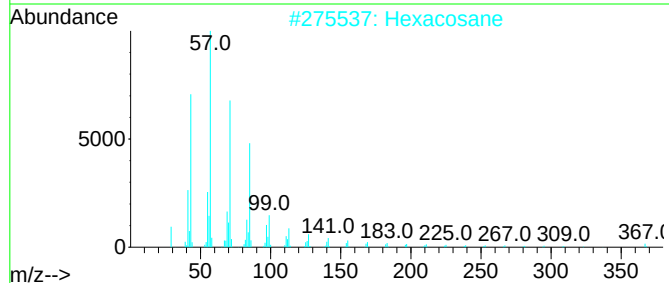
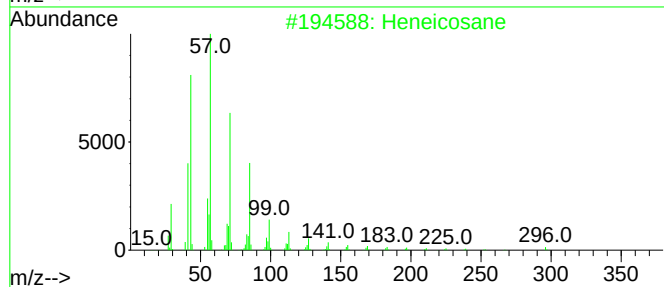
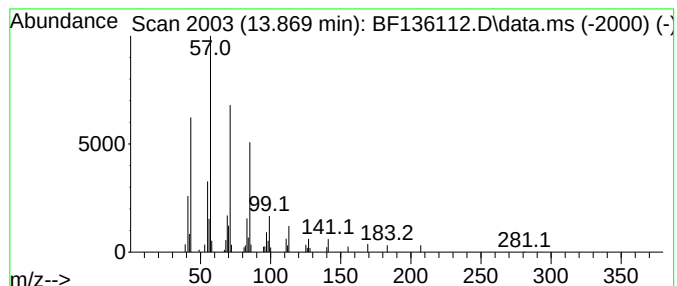
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Peak Number 5 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	2.03 ng	52387	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	90
3			Octadecane	254	C18H38	000593-45-3	90
4			Docosane	310	C22H46	000629-97-0	90
5			Heptadecane	240	C17H36	000629-78-7	87



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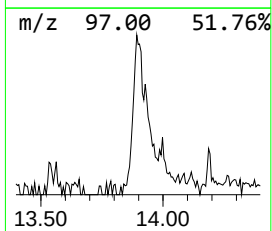
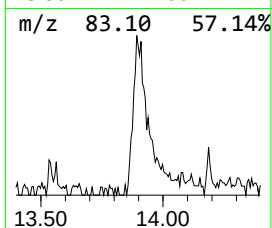
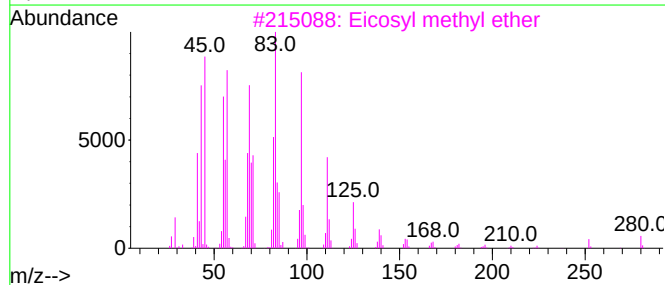
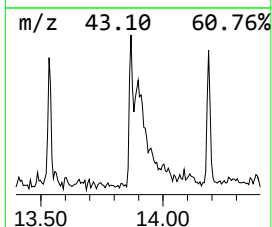
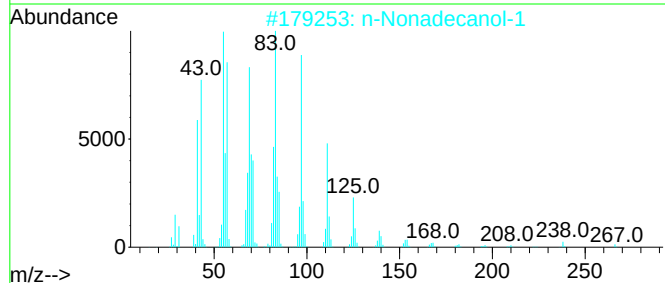
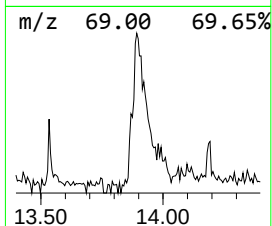
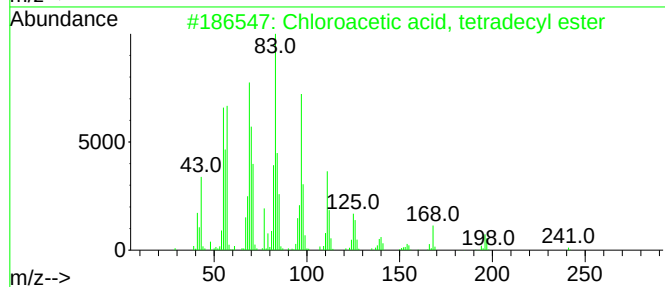
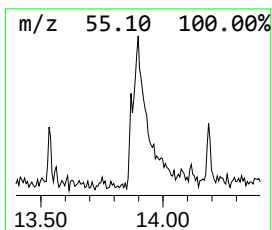
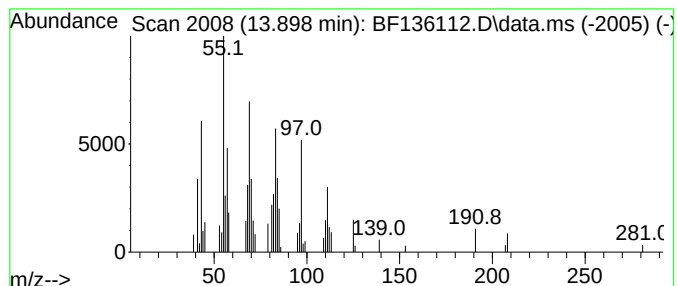
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ClientSampleId :
B5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Chloroacetic acid, tetradec... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	4.68 ng	120891	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	83
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	74
3	Eicosyl methyl ether	312	C21H44O	1000406-29-4	74
4	Behenic alcohol	326	C22H46O	000661-19-8	74
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136112.D
Acq On : 02 Nov 2023 23:38
Operator : CG\JU
Sample : 05050-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.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-...	5.063	3.9	ng	113282	1	6.816	584374	20.0
Ethanol, 2-(2-e...	6.645	2.1	ng	61349	1	6.816	584374	20.0
n-Hexadecanoic ...	11.886	7.2	ng	275290	4	11.345	762047	20.0
Octadecanoic acid	12.680	2.5	ng	63200	5	14.004	516397	20.0
Heneicosane	13.868	2.0	ng	52387	5	14.004	516397	20.0
Chloroacetic ac...	13.898	4.7	ng	120891	5	14.004	516397	20.0