

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
 Data File : BF136103.D
 Acq On : 02 Nov 2023 19:01
 Operator : CG\JU
 Sample : 05049-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B2

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: BF136103.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	498	502	509	rVB	64699	71666	1.76%	0.351%
2	5.446	566	571	574	rBV	1799583	1604988	39.39%	7.866%
3	6.446	737	741	744	rBV	1226818	980299	24.06%	4.805%
4	6.816	801	804	808	rBV	844983	698312	17.14%	3.422%
5	7.387	895	901	904	rBV	2370699	2331420	57.22%	11.426%
6	7.463	910	914	918	rBV2	52387	58474	1.44%	0.287%
7	8.004	1003	1006	1011	rBV	46438	49693	1.22%	0.244%
8	8.098	1018	1022	1025	rBV	1272958	932946	22.90%	4.572%
9	8.451	1075	1082	1085	rBV	199635	221397	5.43%	1.085%
10	9.181	1202	1206	1209	rBV	4625334	4074365	100.00%	19.969%
11	9.857	1317	1321	1324	rBV	1348405	1053873	25.87%	5.165%
12	10.269	1388	1391	1398	rVB	137649	110634	2.72%	0.542%
13	10.651	1451	1456	1459	rBV	2661732	2364248	58.03%	11.587%
14	11.351	1571	1575	1578	rVB	911292	802482	19.70%	3.933%
15	11.886	1662	1666	1670	rBV	201689	198948	4.88%	0.975%
16	12.610	1782	1789	1795	rBV	42738	58498	1.44%	0.287%
17	12.680	1798	1801	1812	rVV	61420	79293	1.95%	0.389%
18	12.769	1812	1816	1824	rVB	527418	427168	10.48%	2.094%
19	12.951	1843	1847	1850	rBV	3079091	2721769	66.80%	13.340%
20	12.980	1850	1852	1856	rVB	315056	245962	6.04%	1.205%
21	13.898	2001	2008	2022	rBV5	30688	83131	2.04%	0.407%
22	14.004	2022	2026	2030	rBV	711493	588349	14.44%	2.884%
23	14.886	2173	2176	2181	rVB	49419	50629	1.24%	0.248%
24	15.492	2274	2279	2286	rVB	498759	595129	14.61%	2.917%

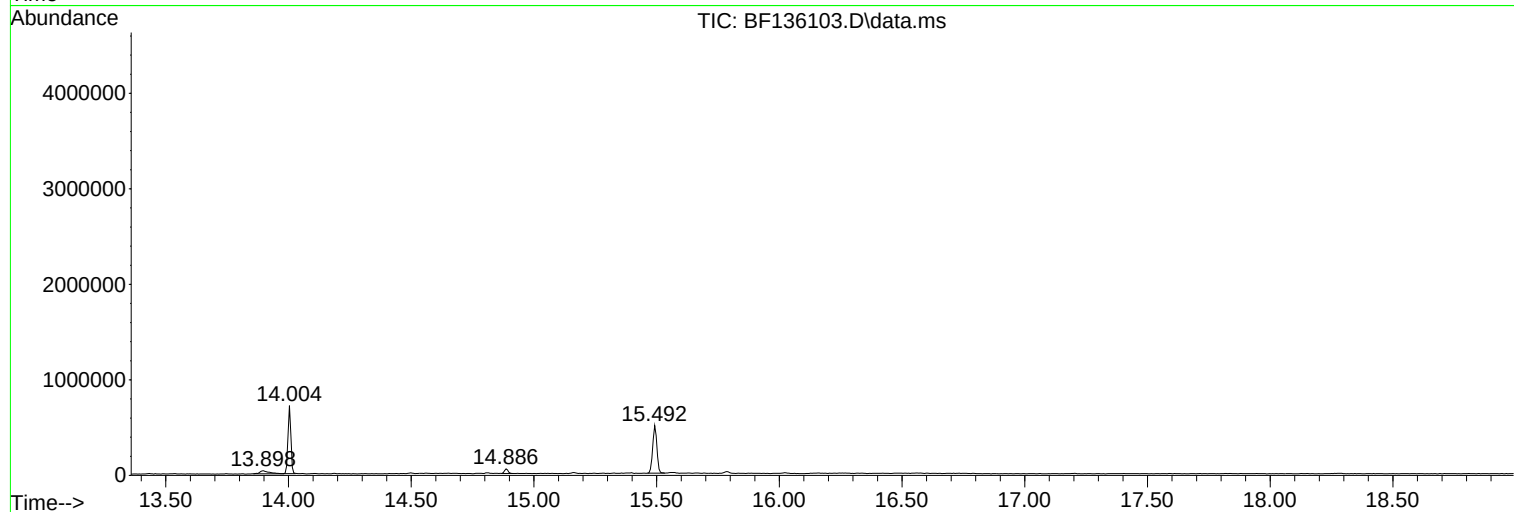
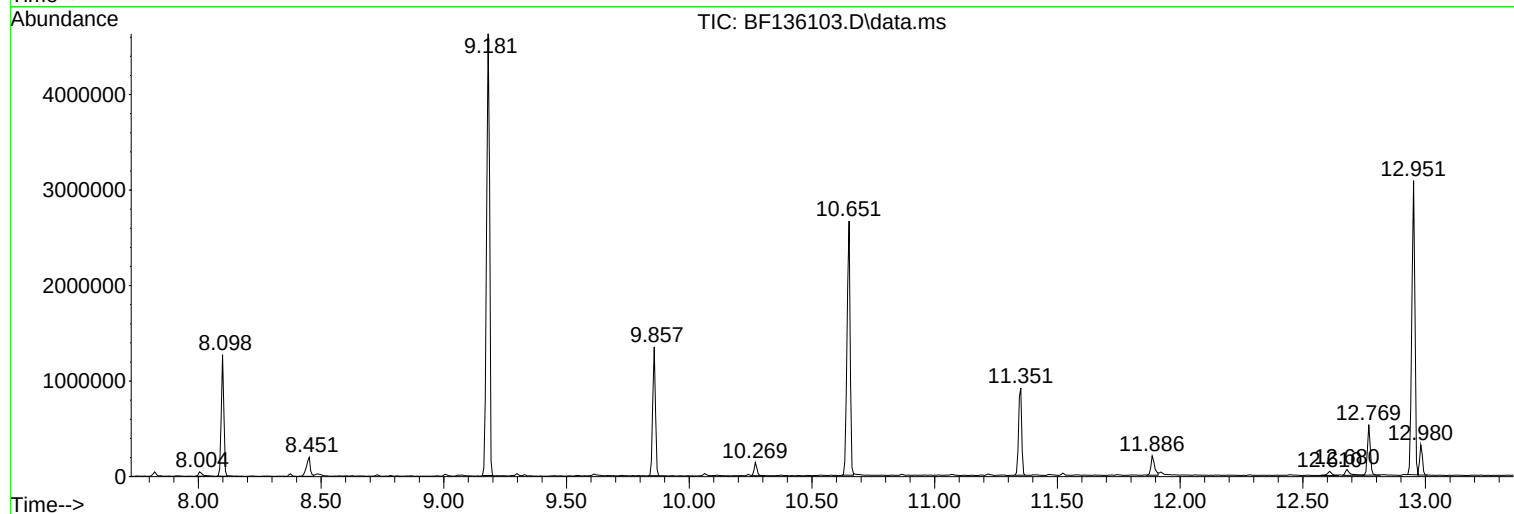
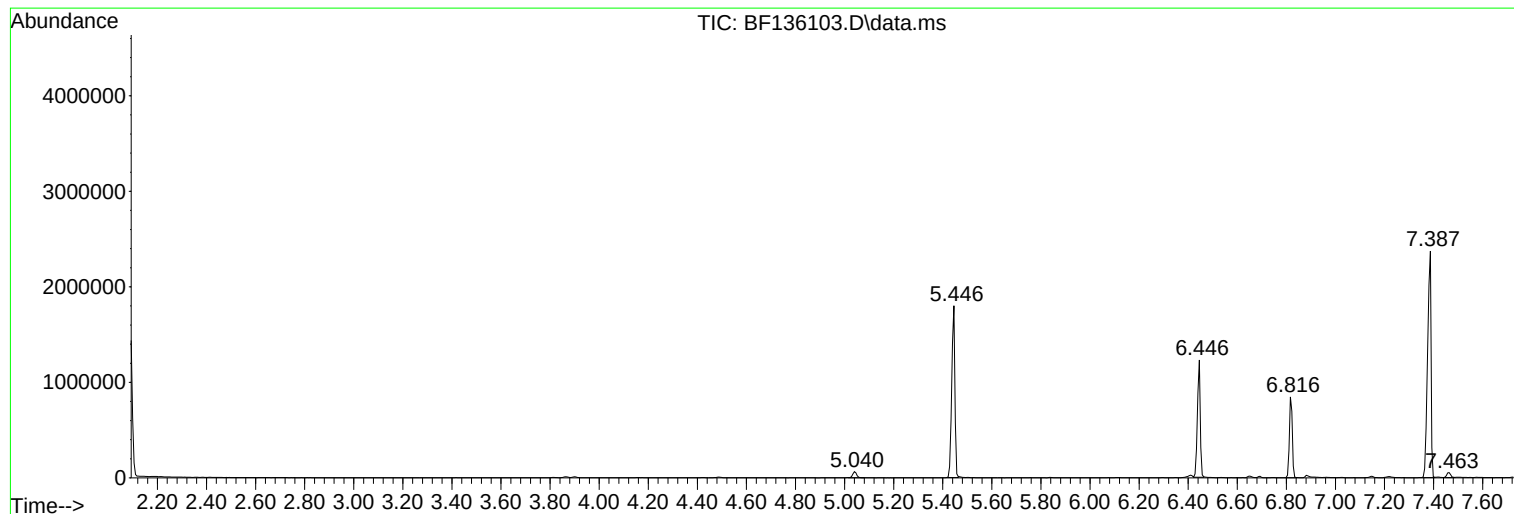
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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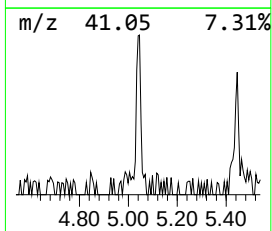
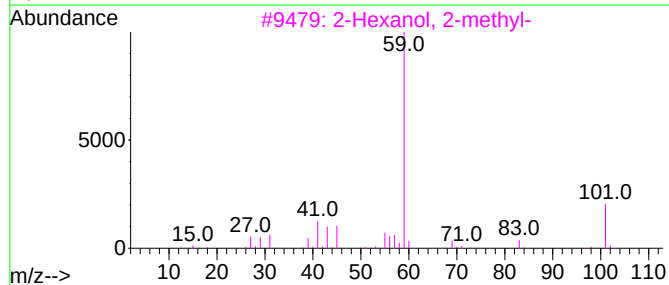
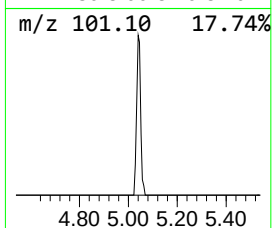
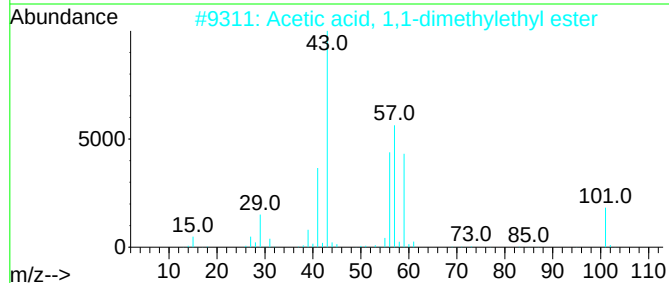
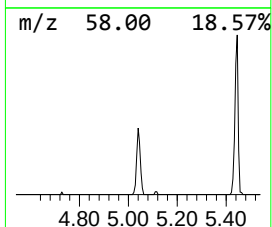
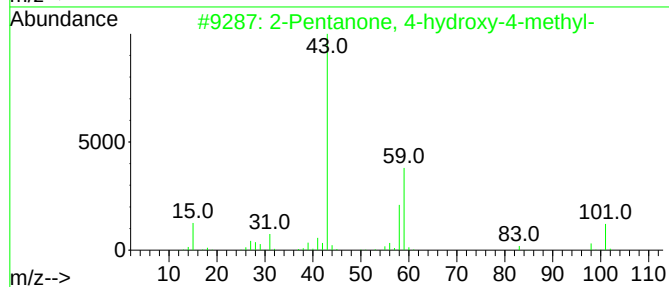
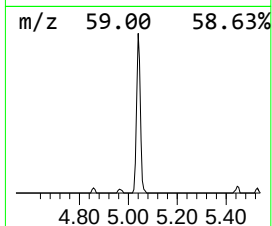
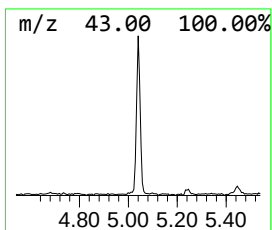
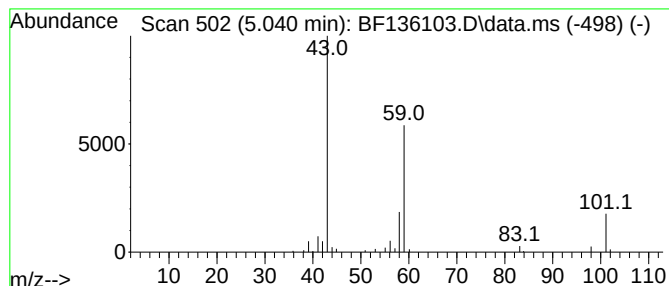
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.05 ng	71666	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	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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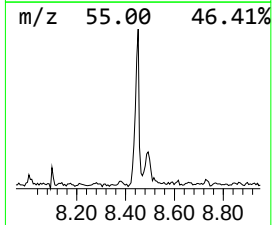
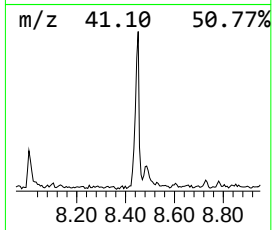
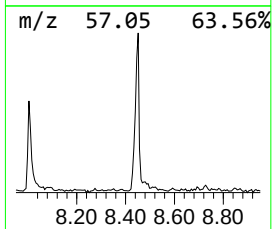
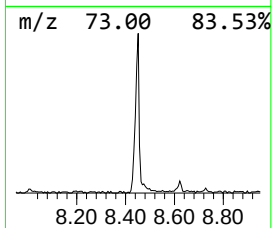
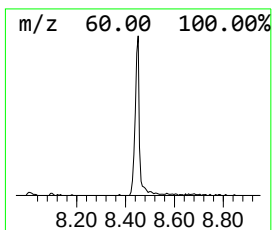
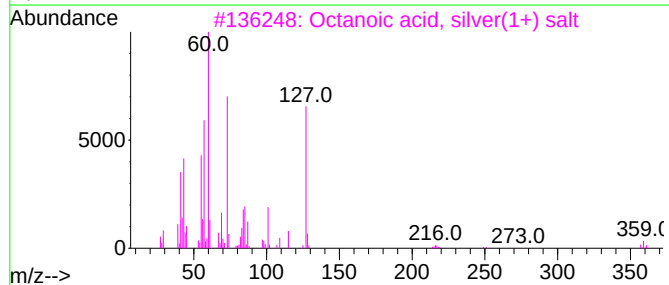
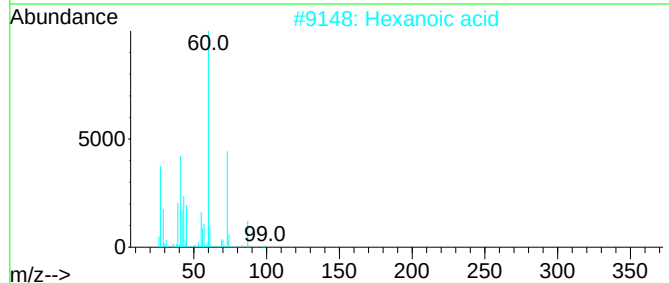
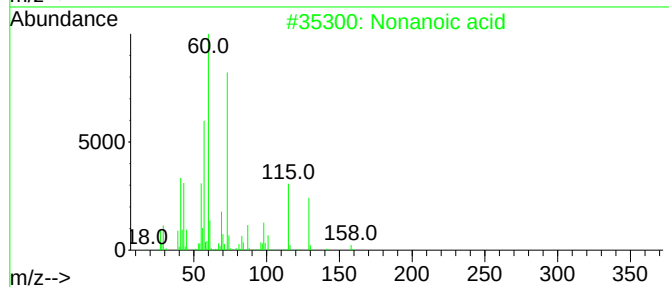
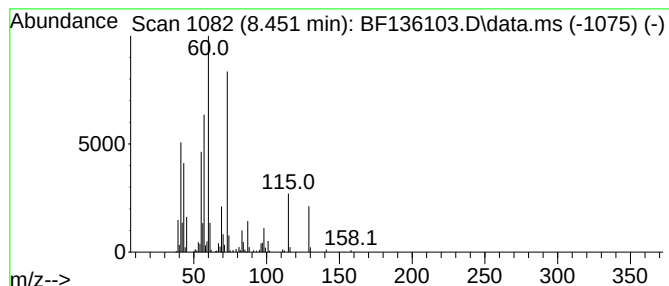
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Nonanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.451	4.75 ng	221397	Naphthalene-d8	8.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	91
2			Hexanoic acid	116	C6H12O2	000142-62-1	50
3			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	50
4			Pentanoic acid	102	C5H10O2	000109-52-4	47
5			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43



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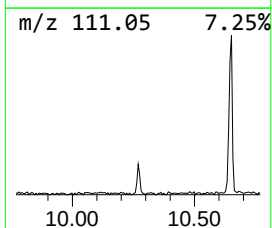
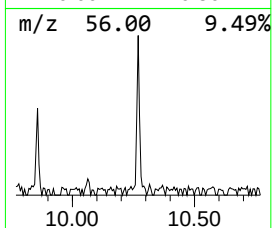
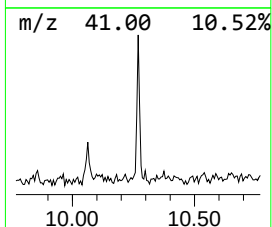
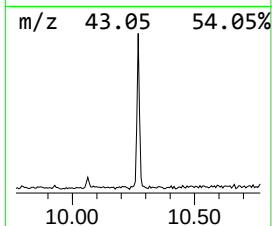
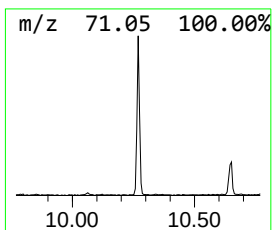
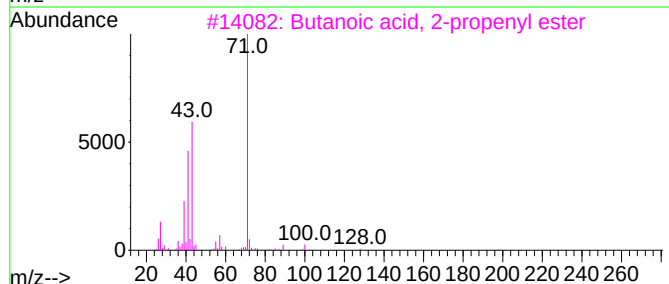
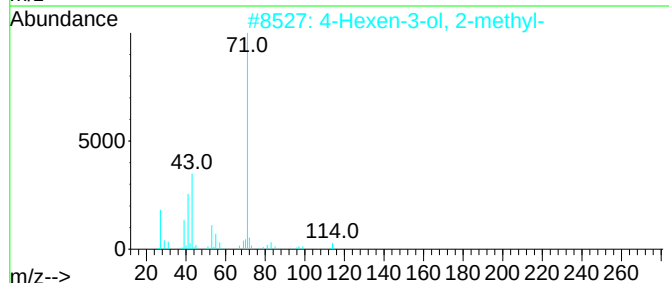
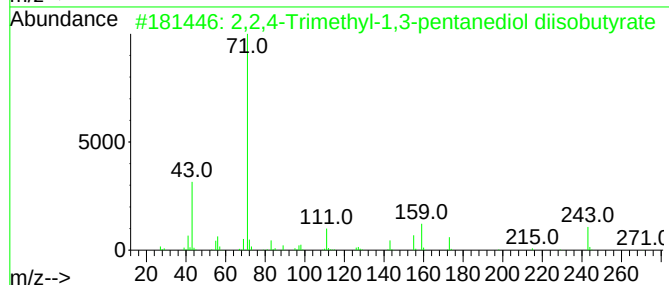
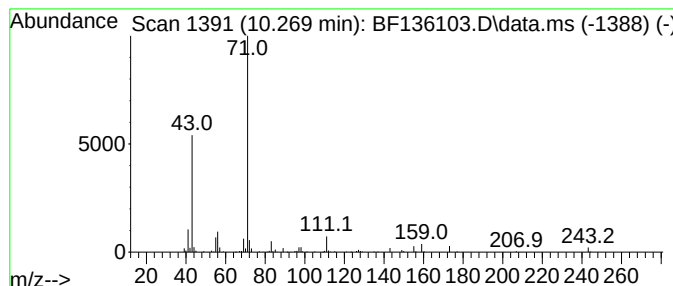
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.269	2.10 ng	110634	Acenaphthene-d10	9.857	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	83
2	4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	53
3	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	53
4	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	50
5	2,2'-Bifuran, octahydro-	142	C8H14O2	001592-33-2	45



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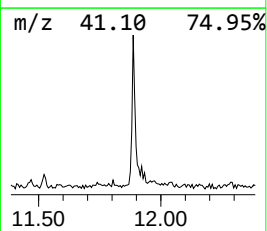
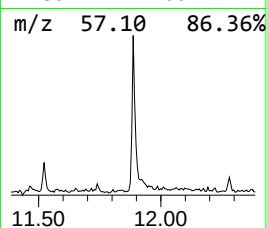
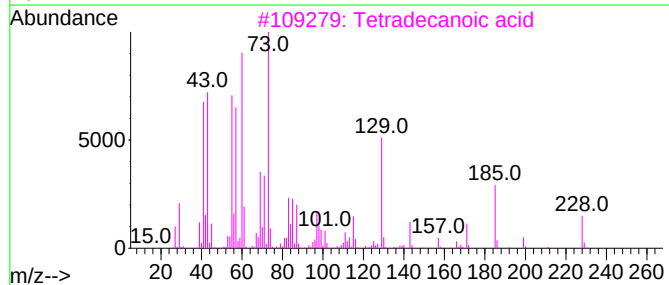
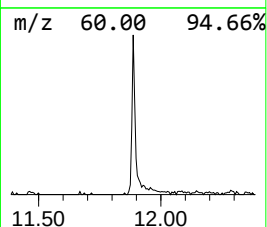
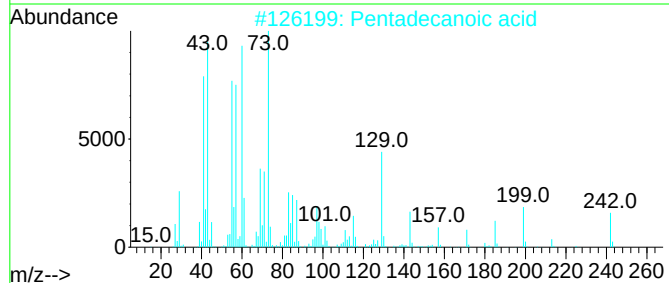
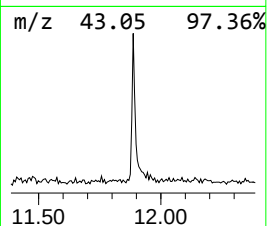
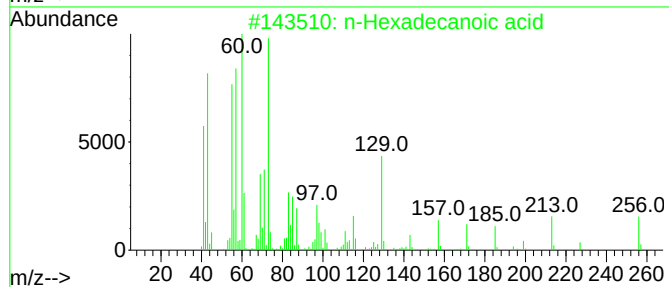
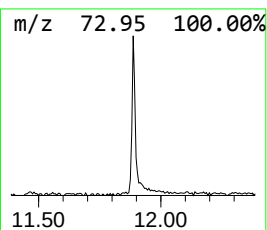
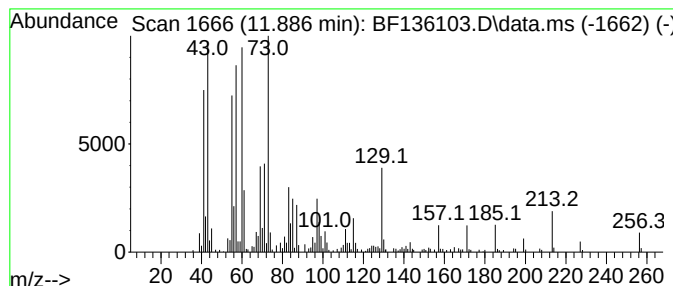
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	4.96 ng	198948	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Tridecanoic acid	214	C13H26O2	000638-53-9	86
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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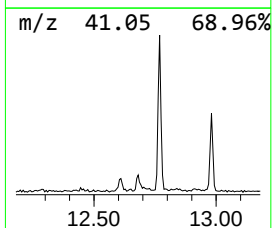
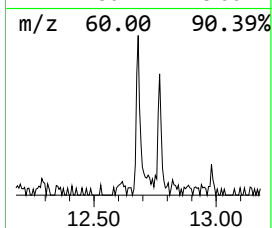
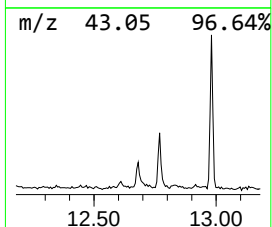
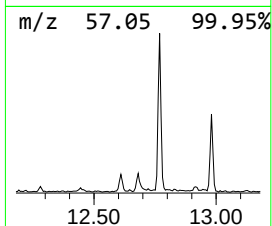
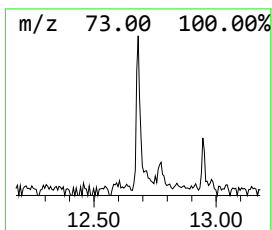
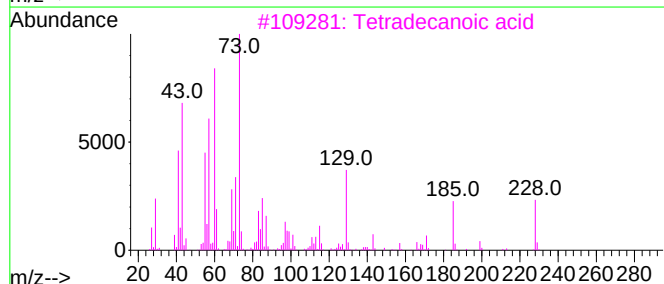
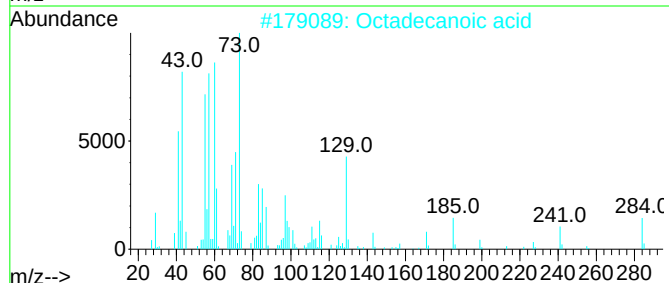
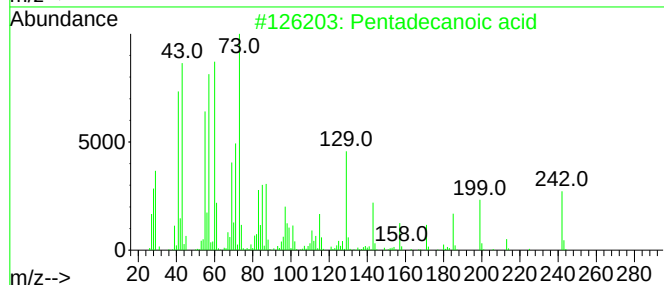
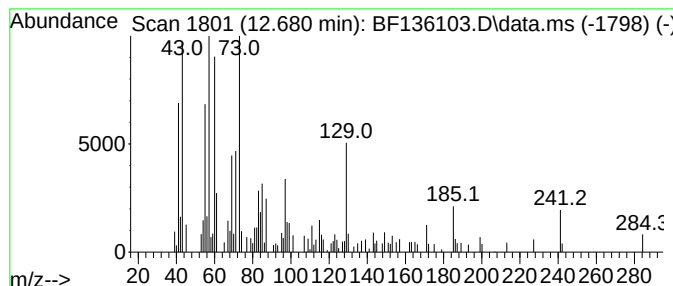
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.681	2.70 ng	79293	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2			Octadecanoic acid	284	C18H36O2	000057-11-4	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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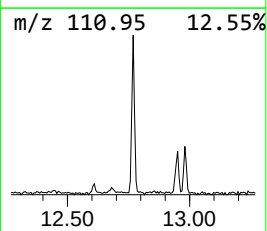
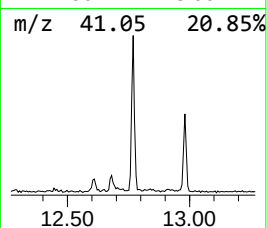
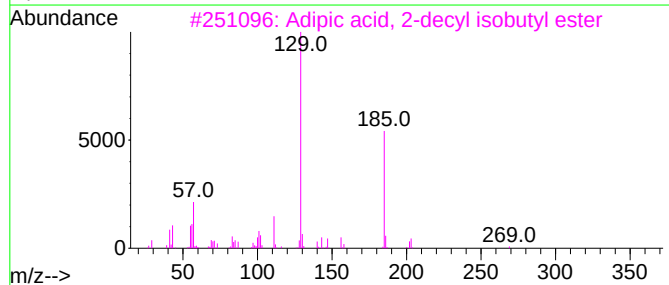
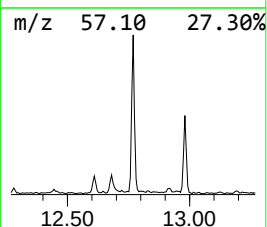
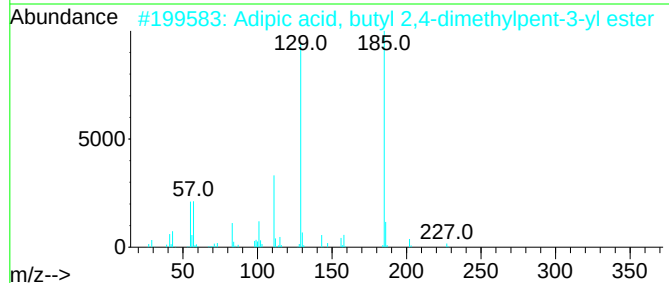
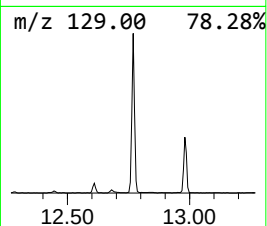
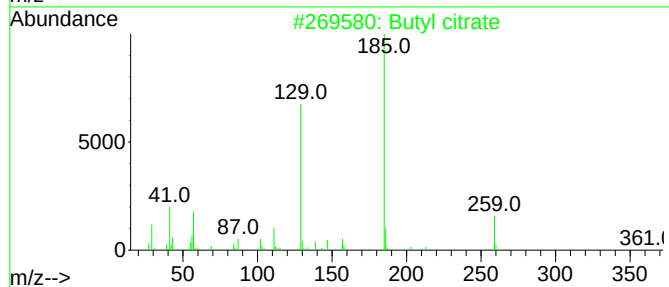
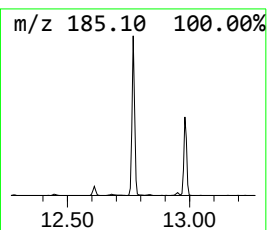
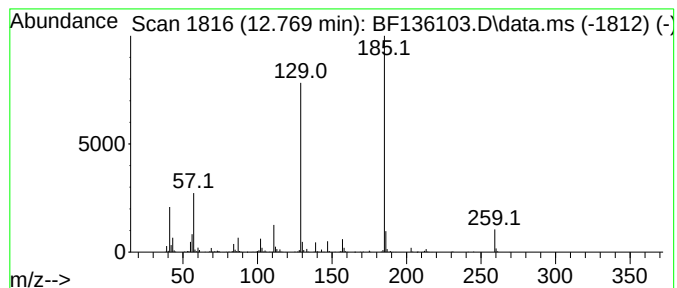
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Butyl citrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.769	14.52 ng	427168	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Adipic acid, butyl 2,4-dimethylp...	300	C17H32O4	1000349-77-7	72
3			Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	64
4			Adipic acid, 2-hexyl isobutyl ester	286	C16H30O4	1000353-70-9	64
5			Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136103.D
Acq On : 02 Nov 2023 19:01
Operator : CG\JU
Sample : 05049-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

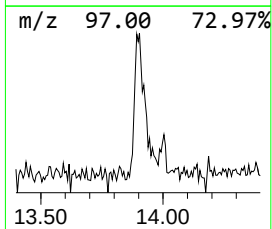
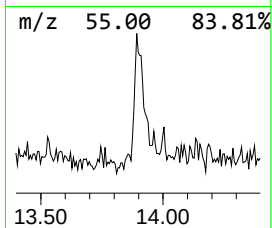
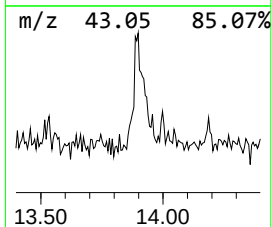
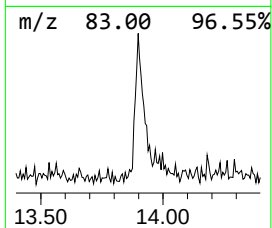
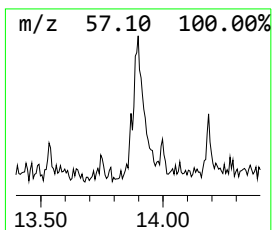
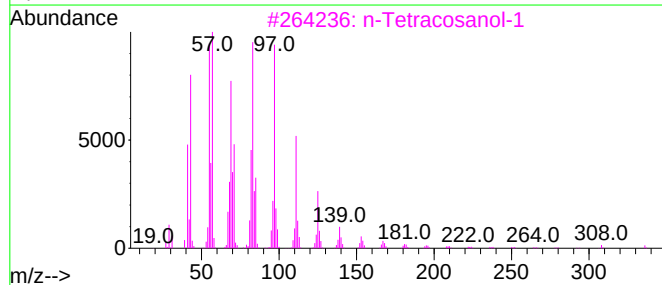
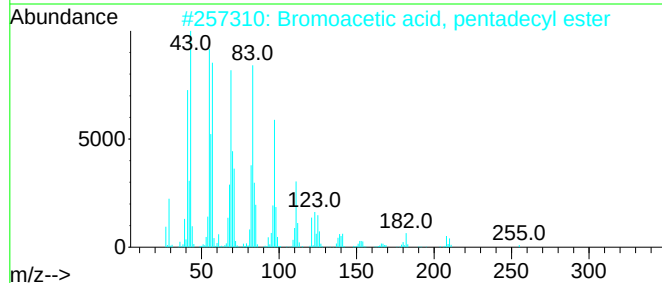
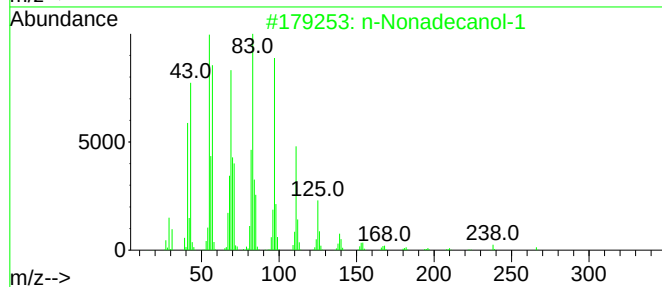
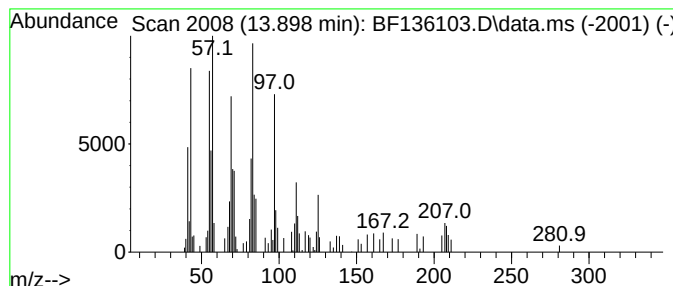
Instrument :
BNA_F
ClientSampleId :
B2

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 7 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.898	2.83 ng	83131	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
2	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	90
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
Data File : BF136103.D
Acq On : 02 Nov 2023 19:01
Operator : CG\JU
Sample : 05049-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B2

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-...	5.040	2.0	ng	71666	1	6.816	698312	20.0
Nonanoic acid	8.451	4.8	ng	221397	2	8.098	932946	20.0
2,2,4-Trimethyl...	10.269	2.1	ng	110634	3	9.857	1053870	20.0
n-Hexadecanoic ...	11.886	5.0	ng	198948	4	11.351	802482	20.0
Pentadecanoic acid	12.681	2.7	ng	79293	5	14.004	588349	20.0
Butyl citrate	12.769	14.5	ng	427168	5	14.004	588349	20.0
n-Nonadecanol-1	13.898	2.8	ng	83131	5	14.004	588349	20.0