

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
 Data File : BF136105.D
 Acq On : 02 Nov 2023 20:02
 Operator : CG\JU
 Sample : 05049-04
 Misc :
 ALS Vial : 16 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: BF136105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.039	498	502	506	rVB	59341	63474	1.67%	0.348%
2	5.445	566	571	574	rBV	1422143	1376935	36.14%	7.553%
3	6.445	737	741	744	rBV	1000830	835320	21.92%	4.582%
4	6.816	801	804	808	rVB	825137	656437	17.23%	3.601%
5	7.386	895	901	903	rBV	2174949	2153924	56.53%	11.815%
6	7.457	910	913	918	rBV	67554	51267	1.35%	0.281%
7	8.098	1018	1022	1025	rBV	1164462	868733	22.80%	4.765%
8	8.439	1075	1080	1084	rBV	89926	88891	2.33%	0.488%
9	9.180	1202	1206	1209	rBV	4507584	3810406	100.00%	20.901%
10	9.298	1222	1226	1230	rBV	148006	124094	3.26%	0.681%
11	9.857	1317	1321	1324	rBV	1231282	935129	24.54%	5.129%
12	10.651	1451	1456	1459	rBV	2373139	2113760	55.47%	11.594%
13	11.351	1571	1575	1578	rBV	884421	811128	21.29%	4.449%
14	11.886	1661	1666	1671	rBV	173120	167654	4.40%	0.920%
15	12.680	1797	1801	1811	rBV2	41878	52015	1.37%	0.285%
16	12.768	1813	1816	1821	rVB	83915	71185	1.87%	0.390%
17	12.951	1843	1847	1850	rBV	3176168	2786332	73.12%	15.283%
18	13.886	1998	2006	2022	rBV6	34332	125552	3.29%	0.689%
19	14.004	2022	2026	2032	rVB	695016	597607	15.68%	3.278%
20	15.492	2274	2279	2286	rVB	449680	541148	14.20%	2.968%

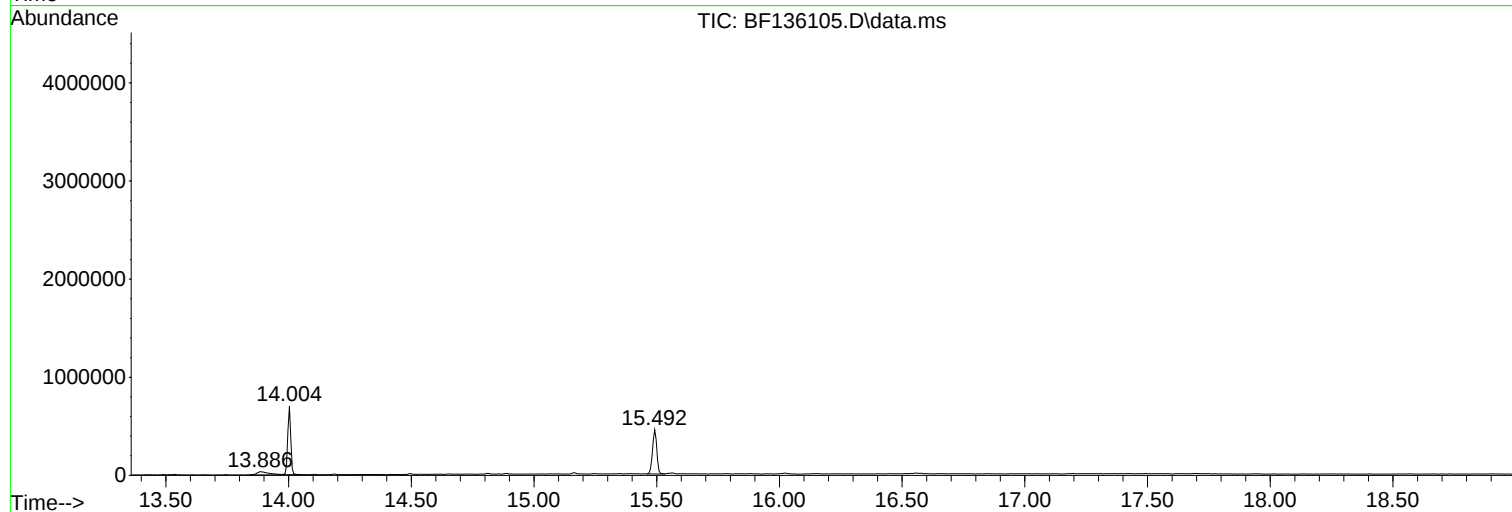
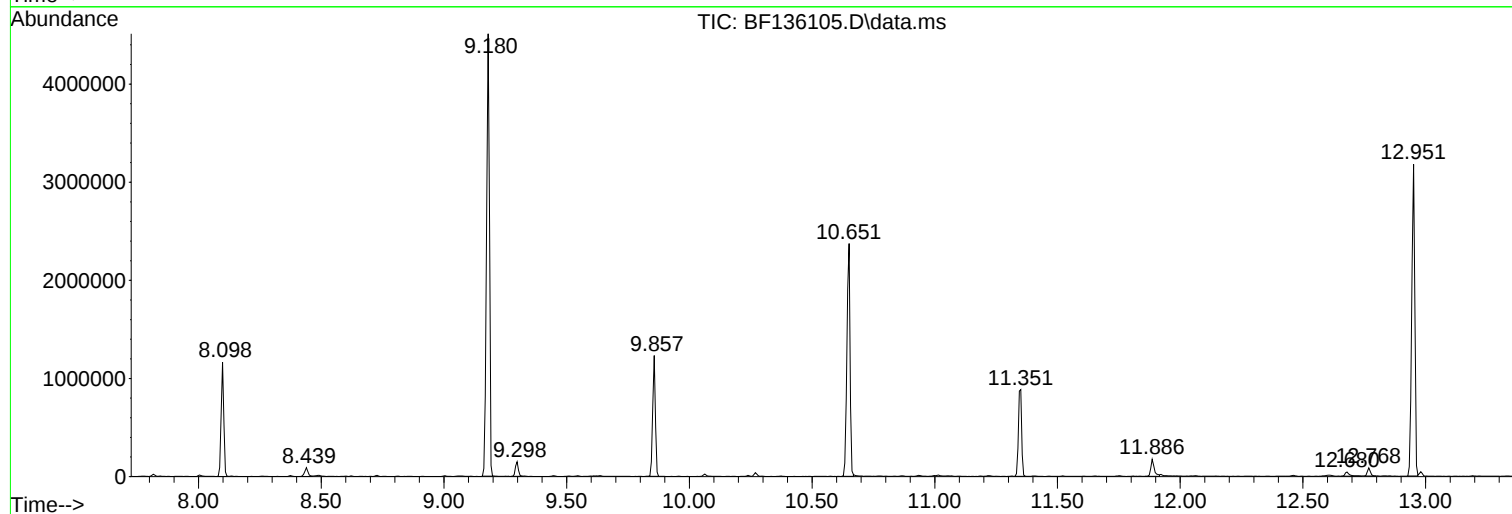
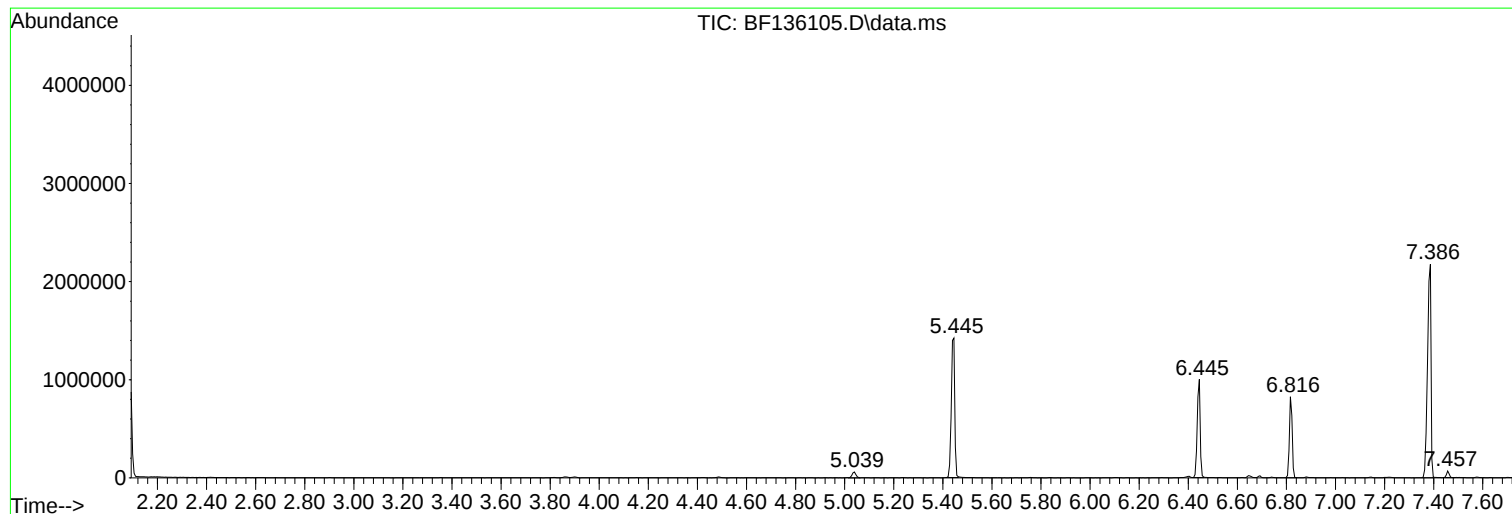
Sum of corrected areas: 18230991

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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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Data File : BF136105.D
Acq On : 02 Nov 2023 20:02
Operator : CG\JU
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Instrument :
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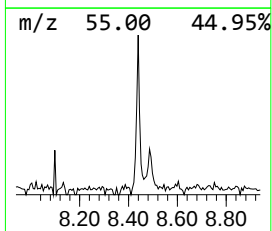
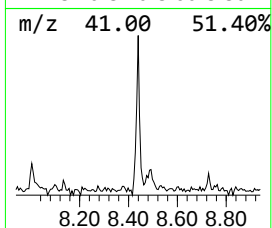
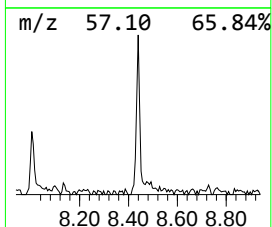
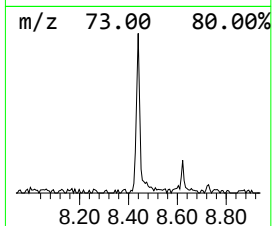
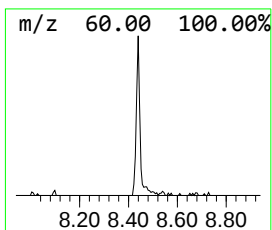
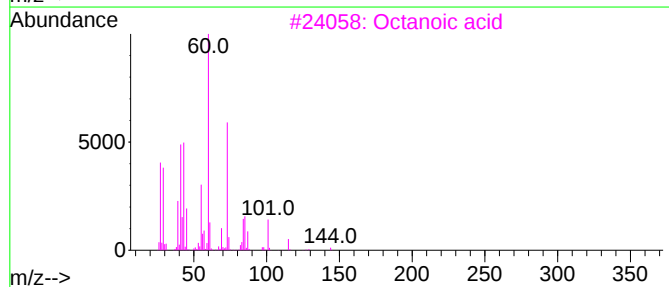
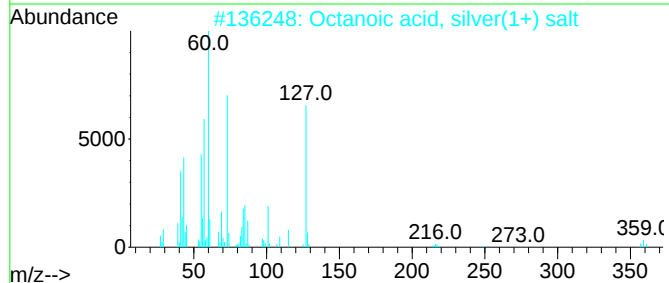
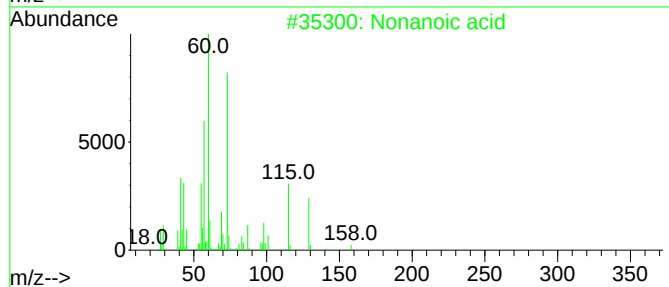
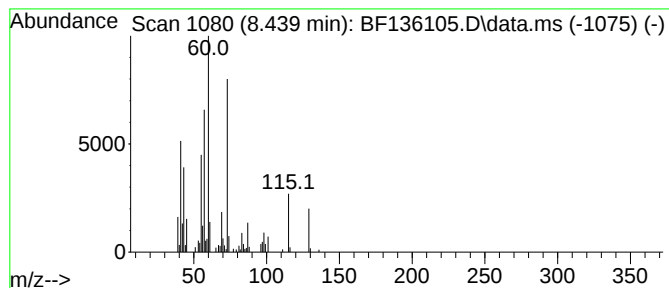
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Nonanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.439	2.05 ng	88891	Naphthalene-d8	8.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	91
2			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	52
3			Octanoic acid	144	C8H16O2	000124-07-2	50
4			Heptanoic acid	130	C7H14O2	000111-14-8	47
5			Hexanoic acid	116	C6H12O2	000142-62-1	47



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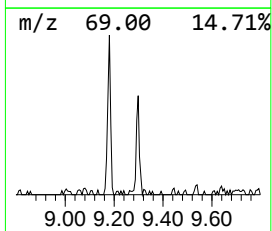
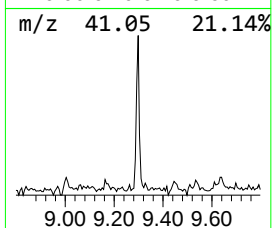
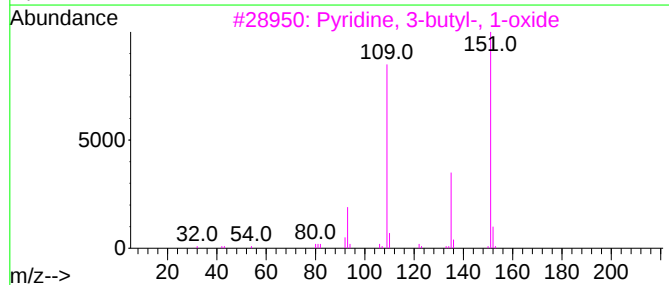
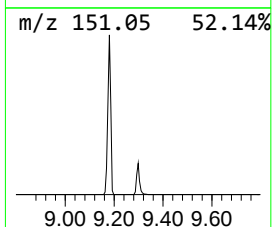
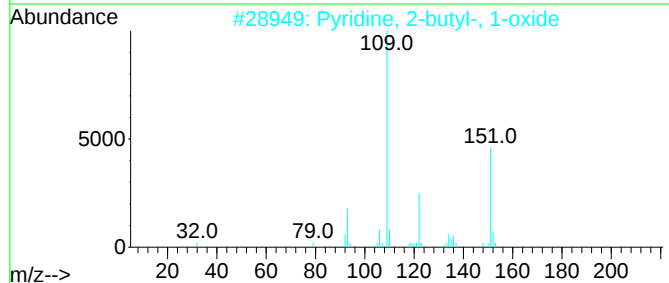
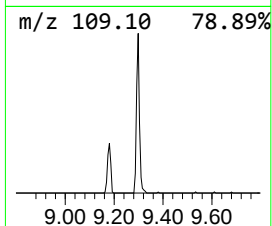
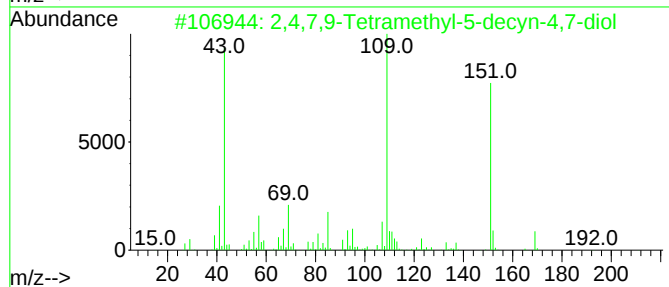
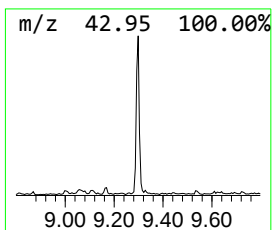
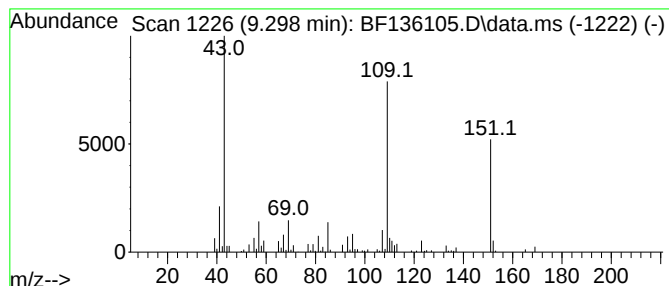
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.298	2.65 ng	124094	Acenaphthene-d10	9.857

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91	
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59	
3	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	59	
4	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	59	
5	Metacetamol	151	C8H9NO2	000621-42-1	59	



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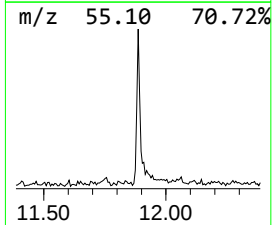
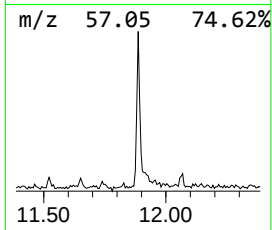
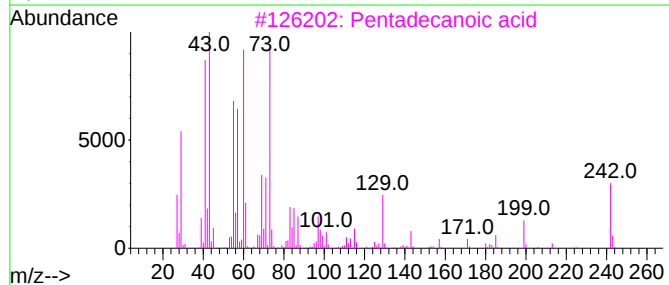
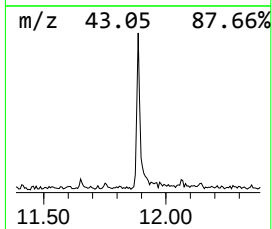
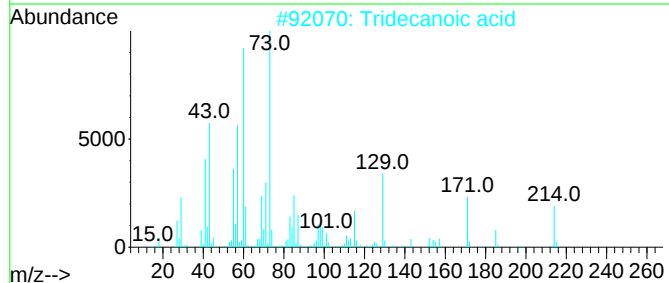
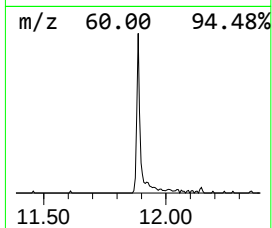
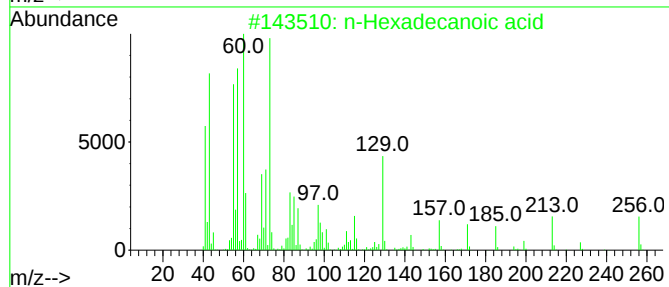
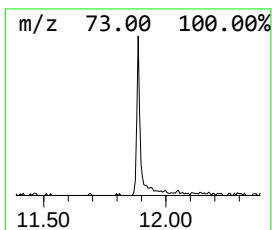
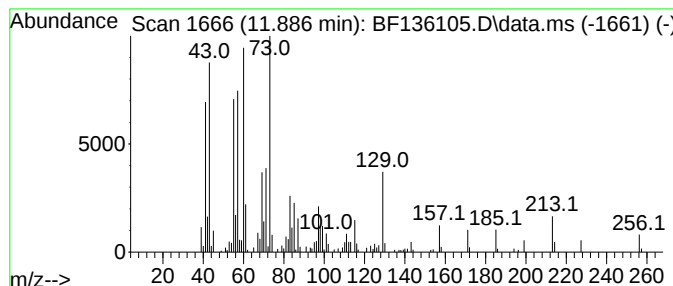
Instrument :
BNA_F
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.886	4.13 ng	167654	Phenanthrene-d10	11.351	
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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Undecanoic acid	186	C11H22O2	000112-37-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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Instrument :
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ClientSampleId :
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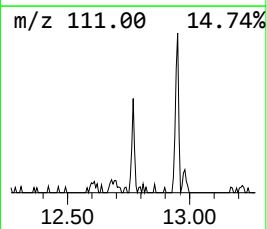
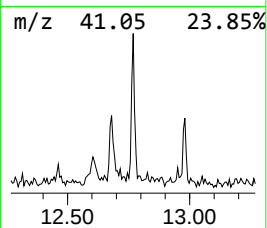
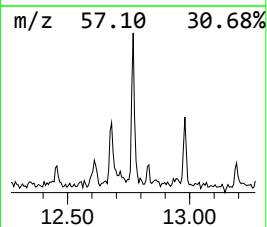
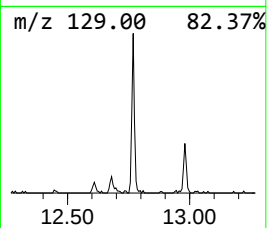
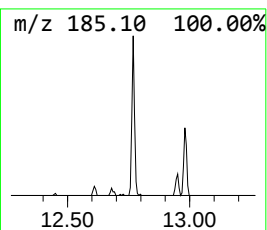
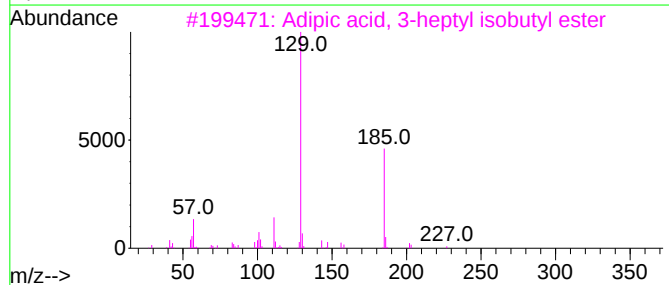
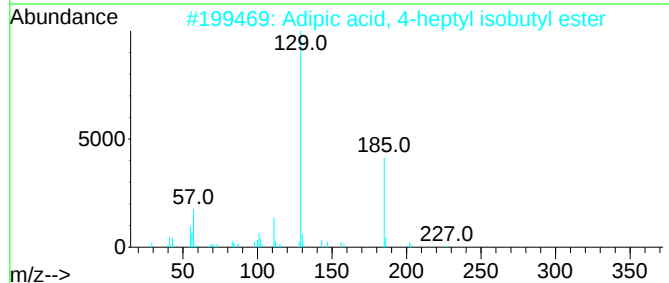
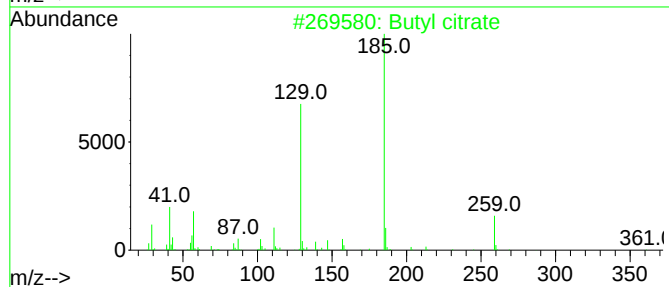
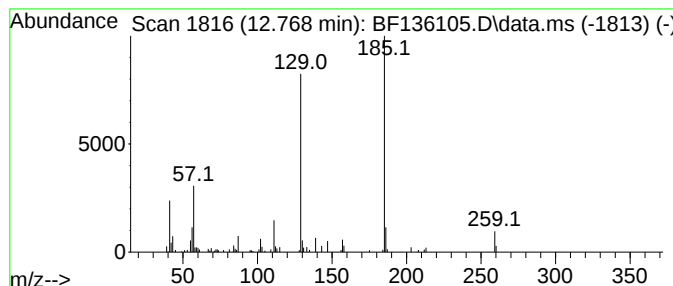
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Butyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	2.38 ng	71185	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	90
2			Adipic acid, 4-heptyl isobutyl e...	300	C17H32O4	1000349-73-6	78
3			Adipic acid, 3-heptyl isobutyl e...	300	C17H32O4	1000353-64-8	78
4			Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	72
5			Adipic acid, butyl trans-2-methy...	298	C17H30O4	1000324-74-6	72



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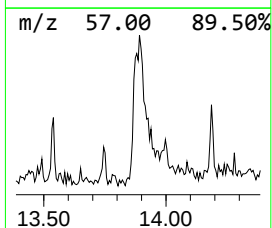
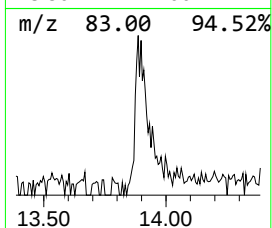
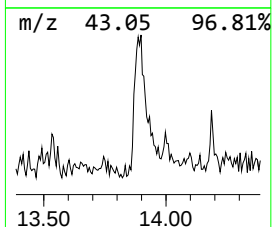
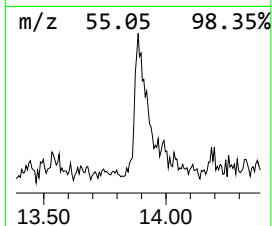
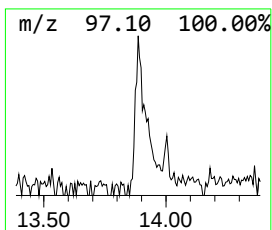
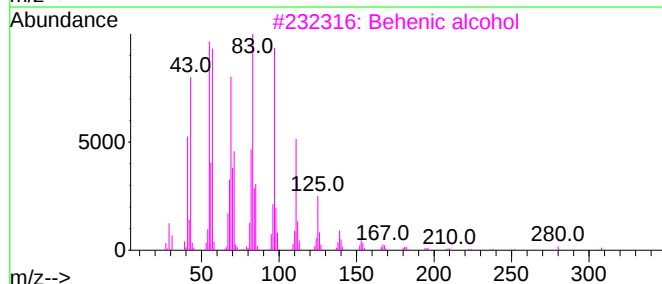
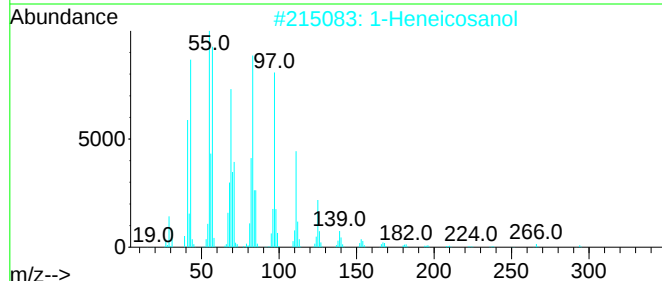
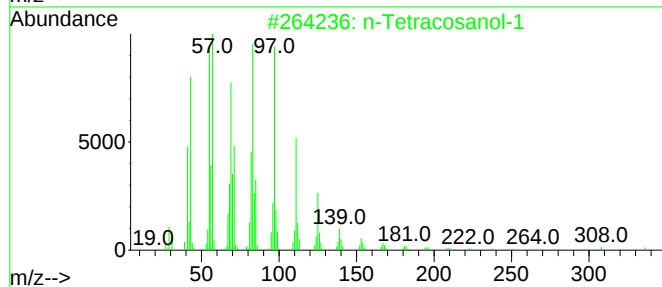
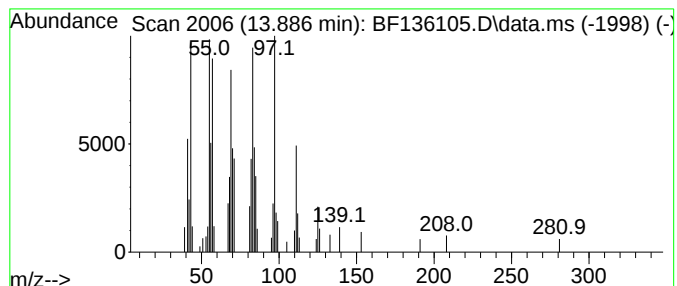
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Tetracosanol-1 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.886	4.20 ng	125552	Chrysene-d12	14.004	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	1-Nonadecene	266	C19H38	018435-45-5	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Nonanoic acid	8.439	2.0	ng	88891	2	8.098	868733	20.0
2,4,7,9-Tetrame...	9.298	2.6	ng	124094	3	9.857	935129	20.0
n-Hexadecanoic ...	11.886	4.1	ng	167654	4	11.351	811128	20.0
Butyl citrate	12.768	2.4	ng	71185	5	14.004	597607	20.0
n-Tetracosanol-1	13.886	4.2	ng	125552	5	14.004	597607	20.0