

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
 Data File : BP007934.D
 Acq On : 10 Nov 2021 23:21
 Operator : CG/JU
 Sample : M4577-03
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-3

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_P\Methods\8270E-BP110221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007934.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.440	359	366	379	rBV	1587448	2258144	48.49%	8.932%
2	7.028	629	636	650	rBV	1379802	2195681	47.15%	8.685%
3	7.852	769	776	784	rVB	376252	575558	12.36%	2.277%
4	9.010	965	973	982	rBV	823847	1355442	29.11%	5.361%
5	10.440	1210	1216	1229	rBV	42855	89266	1.92%	0.353%
6	10.651	1242	1252	1262	rBV	406425	680279	14.61%	2.691%
7	13.116	1664	1671	1686	rBV	1754312	2724198	58.50%	10.775%
8	13.398	1713	1719	1726	rVB3	34820	59157	1.27%	0.234%
9	14.492	1898	1905	1914	rBV	566921	906488	19.47%	3.585%
10	15.980	2152	2158	2181	rBV	1739904	2688904	57.74%	10.635%
11	17.245	2366	2373	2386	rBV	768884	1182430	25.39%	4.677%
12	18.139	2521	2525	2534	rBV	111950	159973	3.44%	0.633%
13	19.057	2677	2681	2686	rBV	56891	58700	1.26%	0.232%
14	19.810	2803	2809	2817	rBV	3727162	4656924	100.00%	18.420%
15	20.086	2852	2856	2860	rBV2	71728	95562	2.05%	0.378%
16	20.439	2913	2916	2920	rVB2	45057	47603	1.02%	0.188%
17	21.051	3016	3020	3025	rBV	443556	550094	11.81%	2.176%
18	21.333	3064	3068	3074	rBV	1213705	1625413	34.90%	6.429%
19	21.974	3173	3177	3187	rBV	311405	470838	10.11%	1.862%
20	22.239	3218	3222	3229	rVB	357660	487718	10.47%	1.929%
21	22.604	3280	3284	3290	rVB2	415859	584227	12.55%	2.311%
22	23.745	3472	3478	3490	rVB2	877491	1829850	39.29%	7.238%

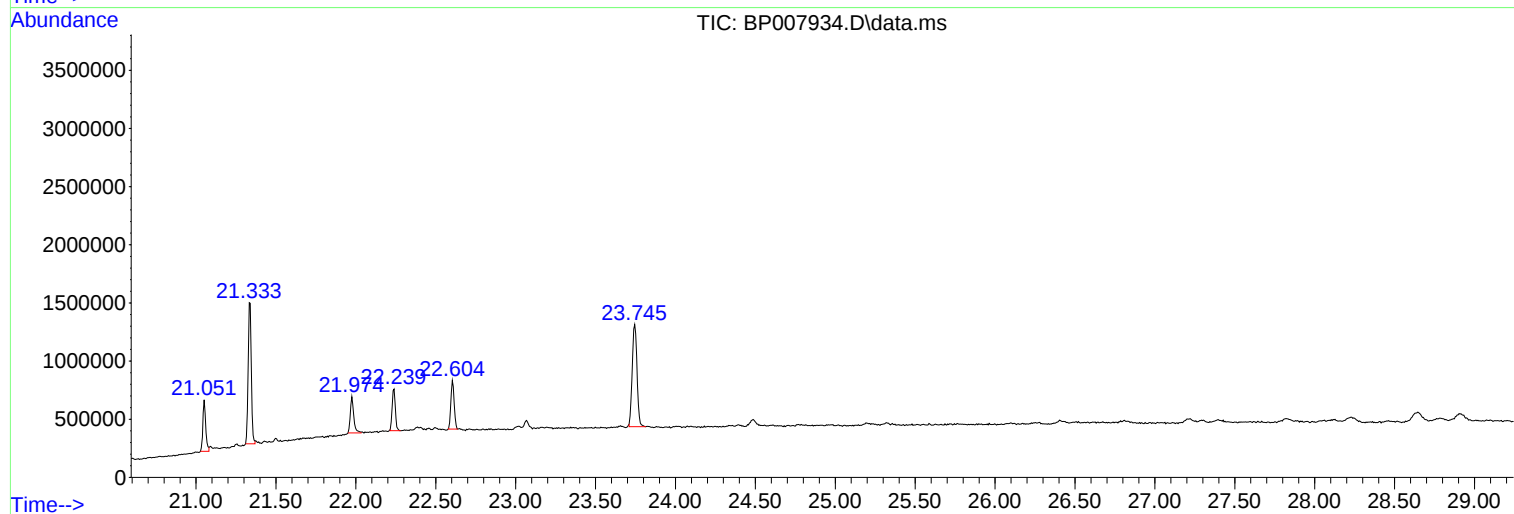
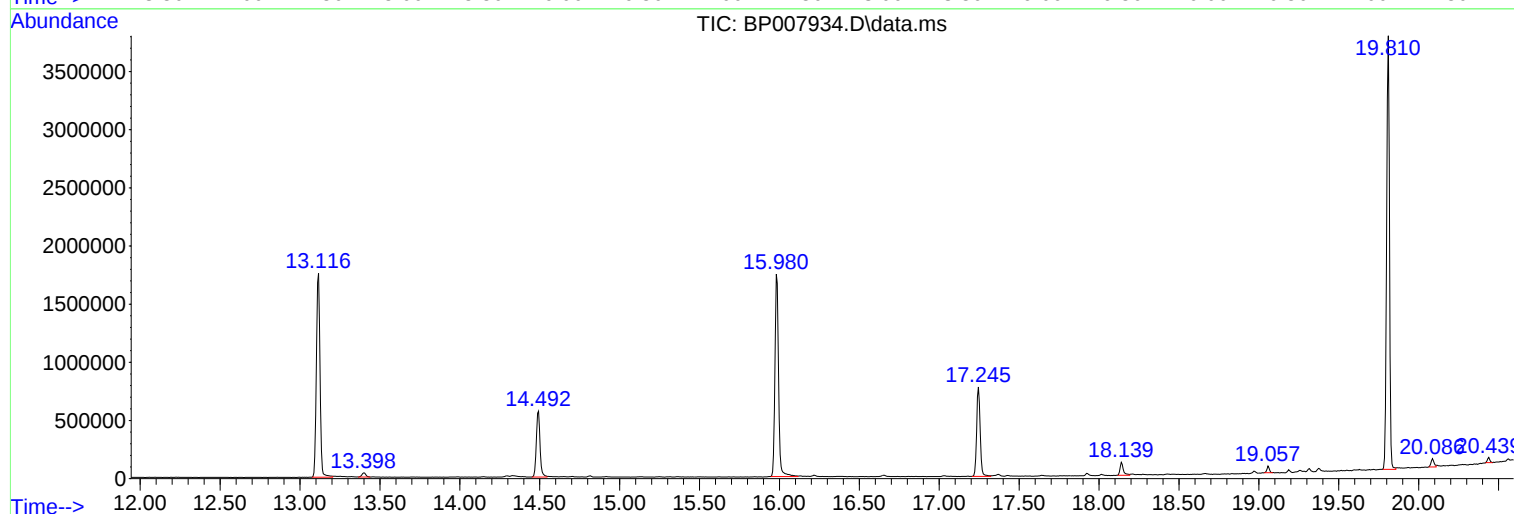
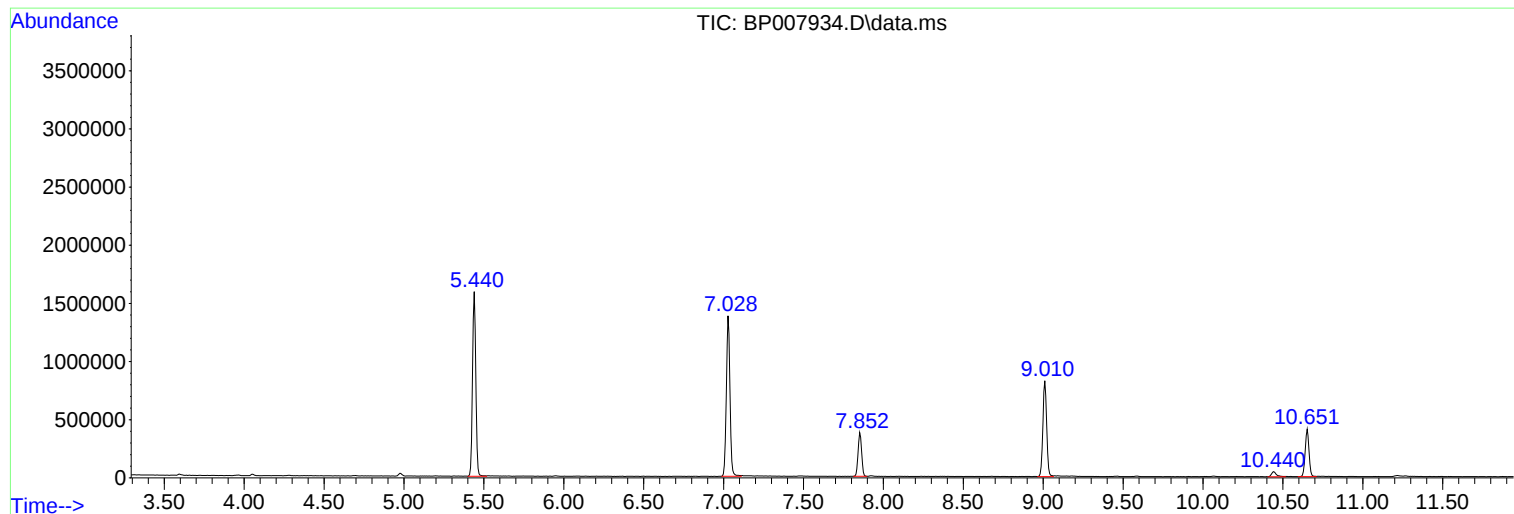
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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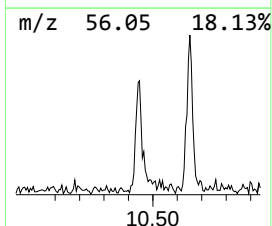
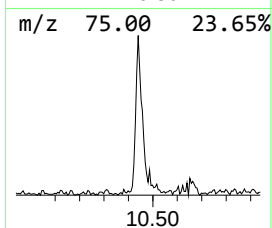
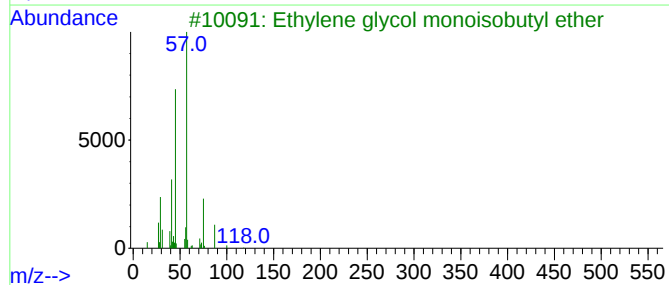
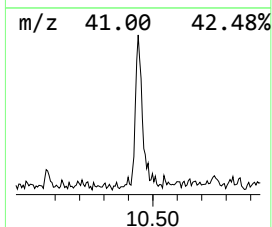
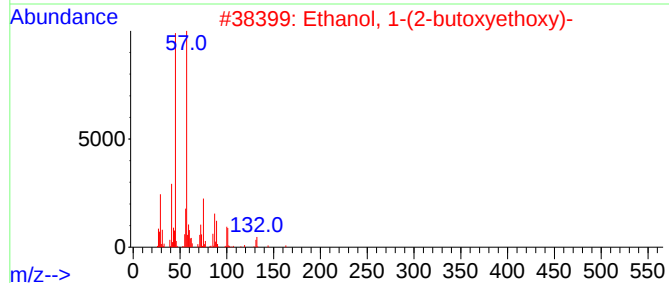
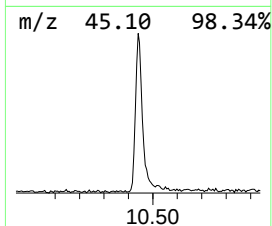
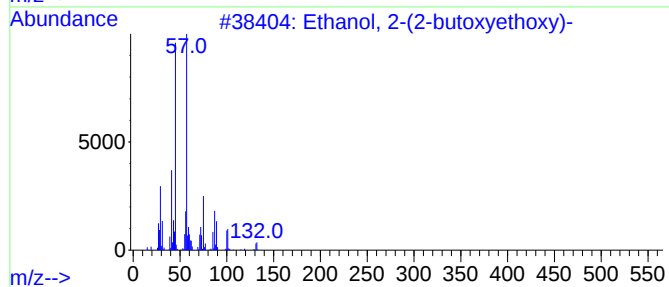
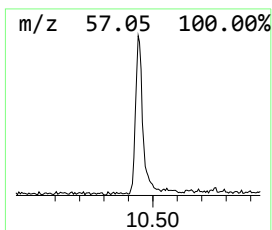
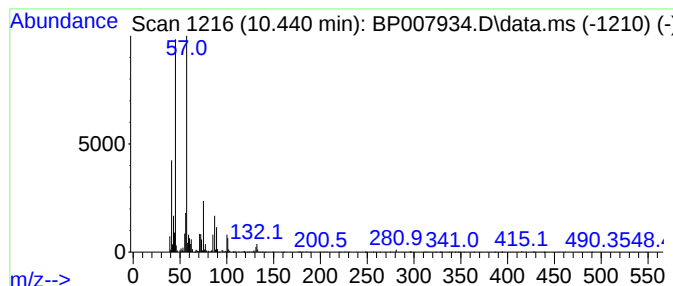
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.440	2.62 ng	89266	Naphthalene-d8	10.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	86
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	58



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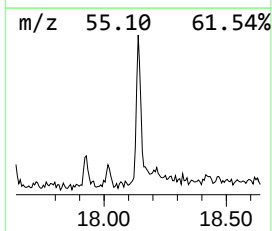
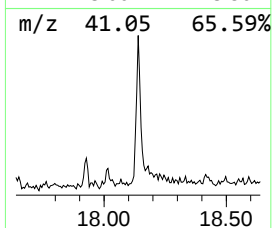
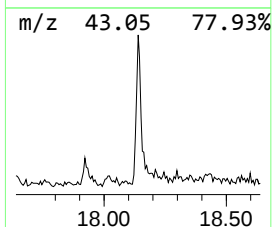
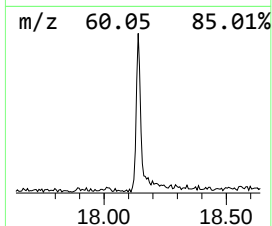
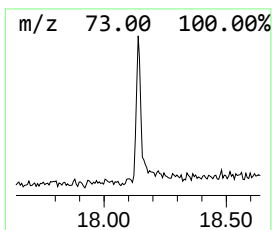
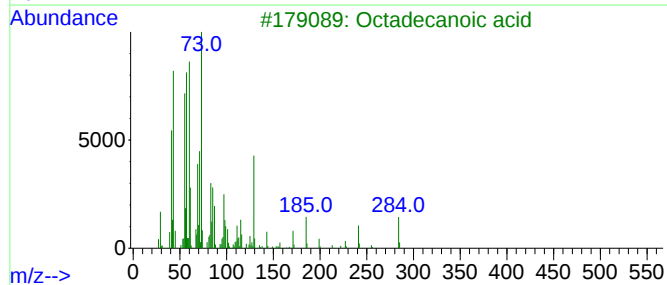
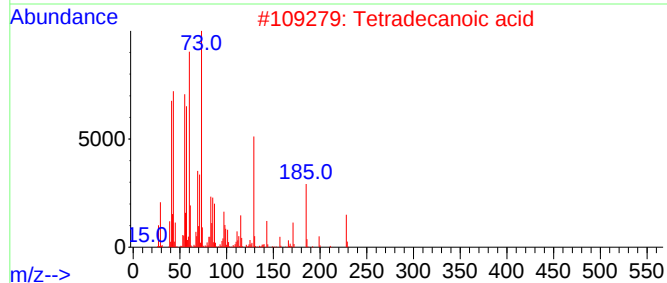
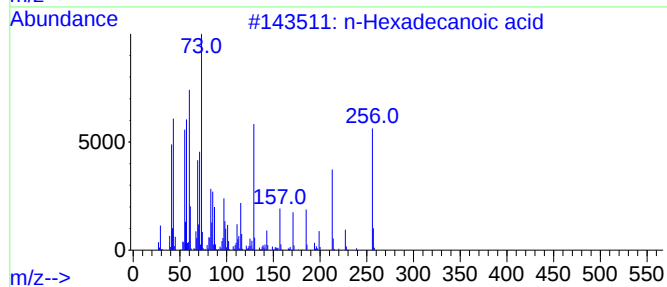
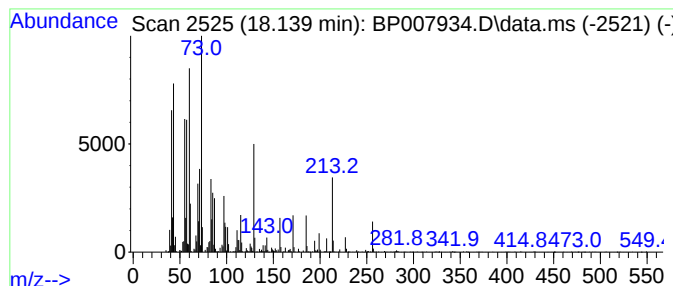
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	2.71 ng	159973	Phenanthrene-d10	17.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3		Octadecanoic acid	284	C18H36O2	000057-11-4	90
4		Tridecanoic acid	214	C13H26O2	000638-53-9	87
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	83



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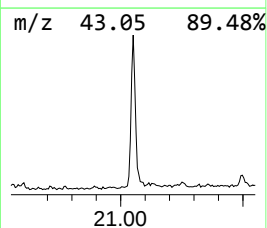
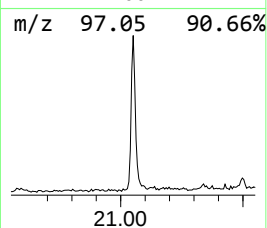
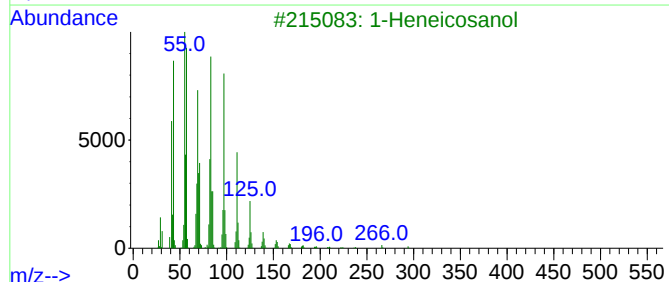
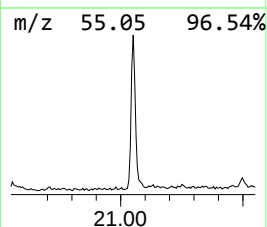
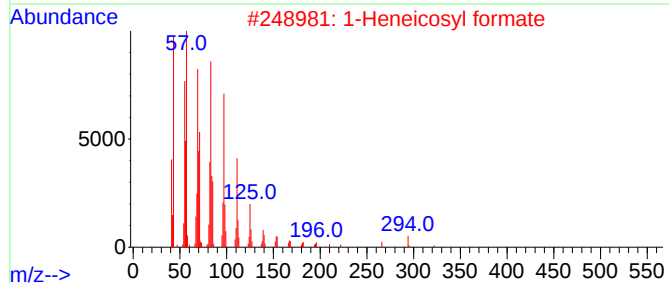
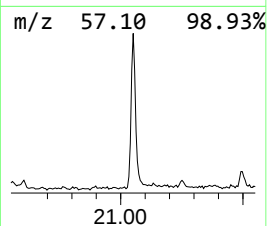
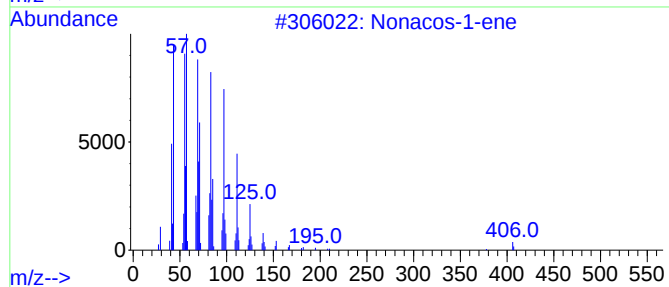
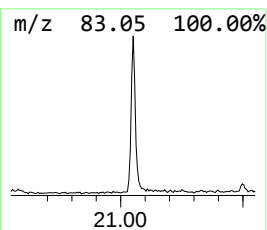
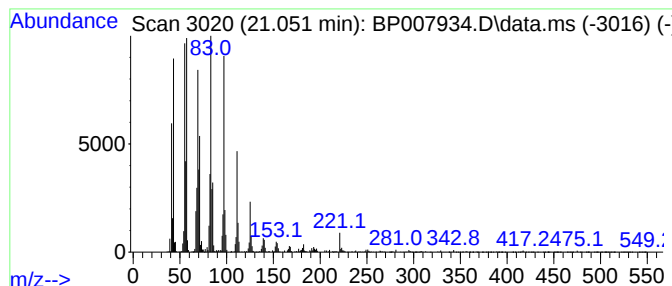
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Peak Number 3 Nonacos-1-ene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	6.77 ng	550094	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonacos-1-ene	406	C29H58	018835-35-3	98
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	98
3			1-Heneicosanol	312	C21H44O	015594-90-8	95
4			1-Tetracosene	336	C24H48	010192-32-2	94
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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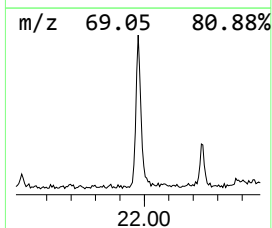
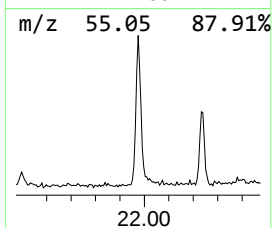
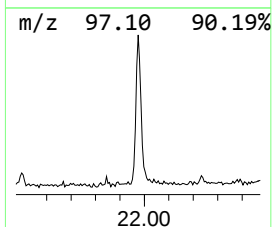
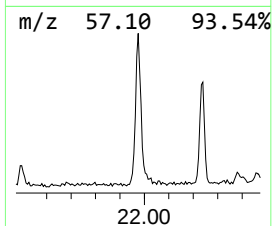
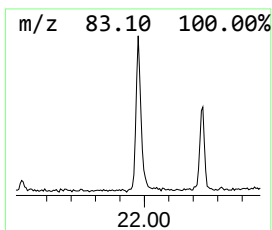
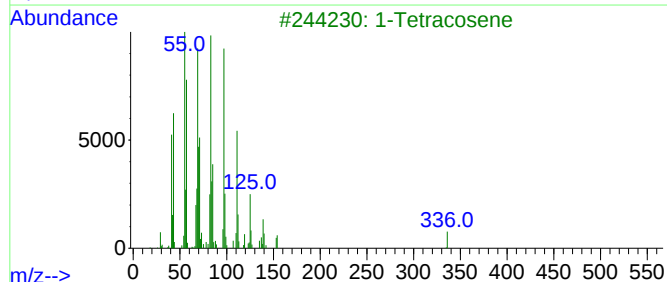
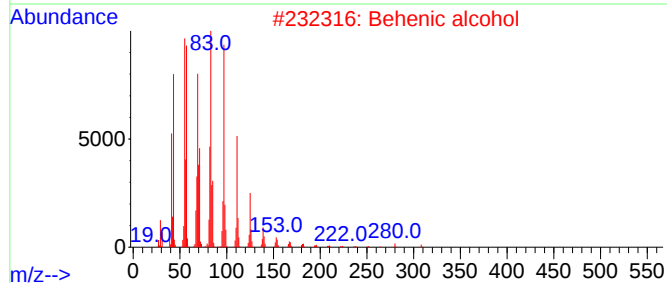
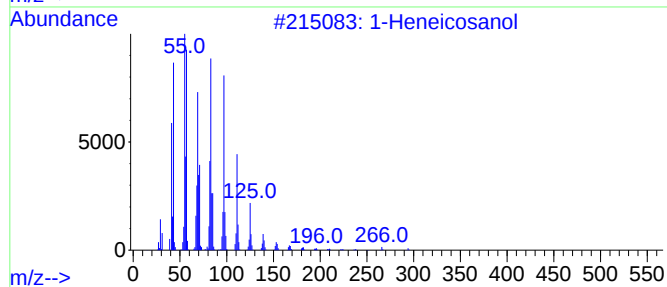
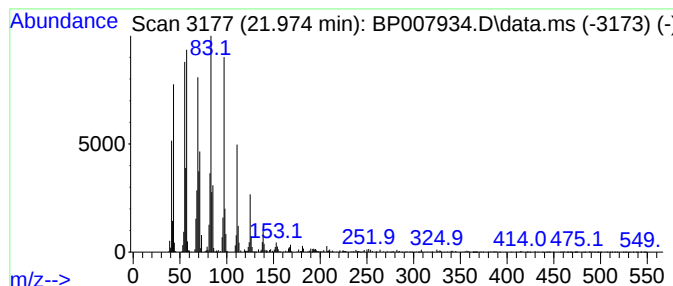
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.974	5.79 ng	470838	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Behenic alcohol	326	C22H46O	000661-19-8	95
3			1-Tetracosene	336	C24H48	010192-32-2	94
4			1-(Ethenesulfonyl)dodecane	260	C14H28O2S	030719-66-5	93
5			E-15-Heptadecenal	252	C17H32O	1000130-97-9	93



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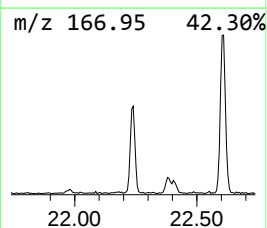
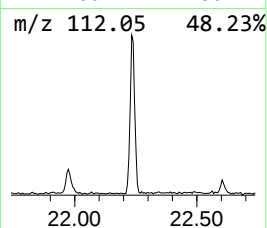
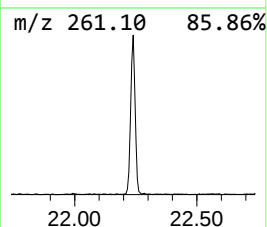
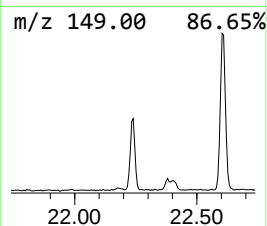
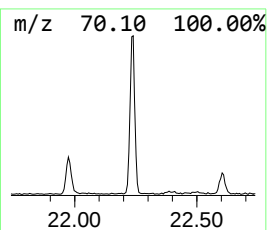
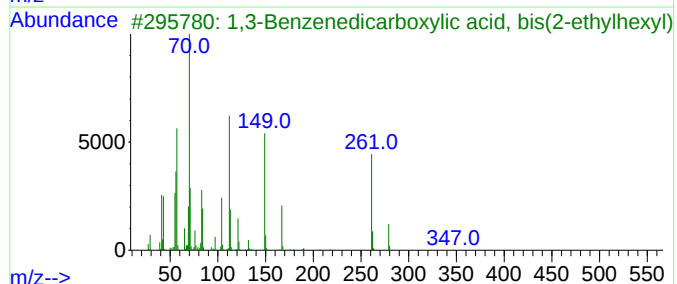
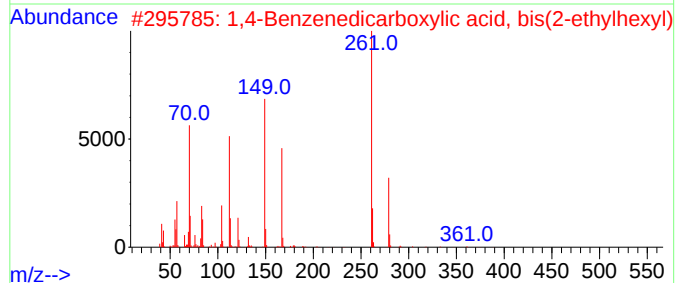
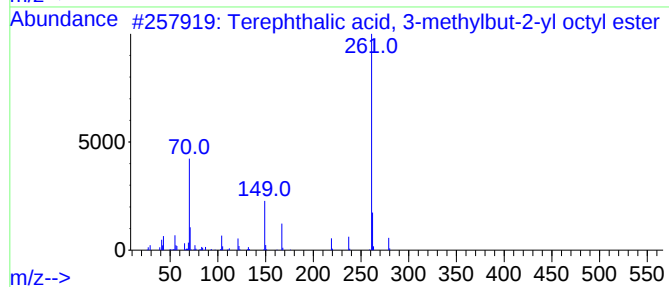
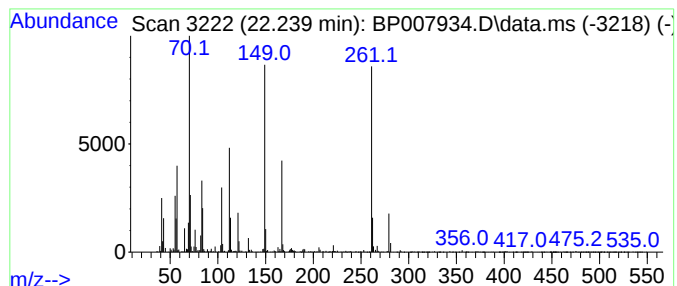
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Terephthalic acid, 3-methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.239	6.00 ng	487718	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	72
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
4			Terephthalic acid, but-3-enyl oc...	332	C20H28O4	1000356-33-8	38
5			Isophthalic acid, octyl tridec-2...	456	C29H44O4	1000343-92-0	38



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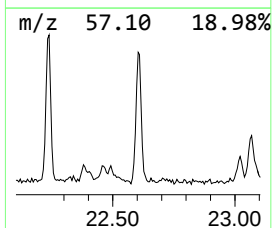
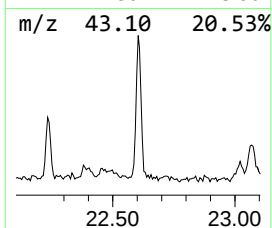
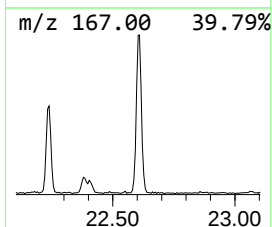
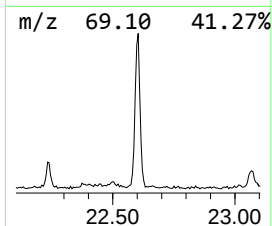
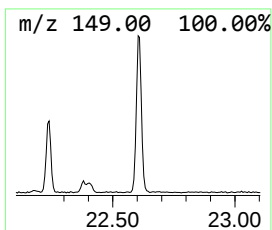
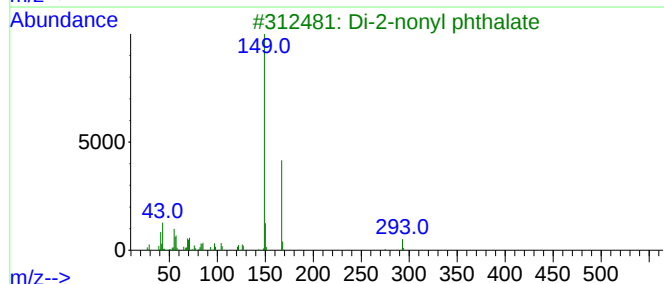
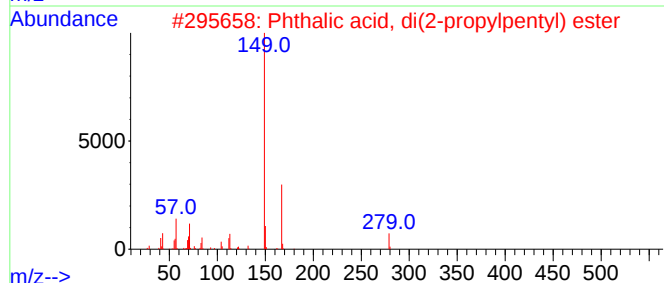
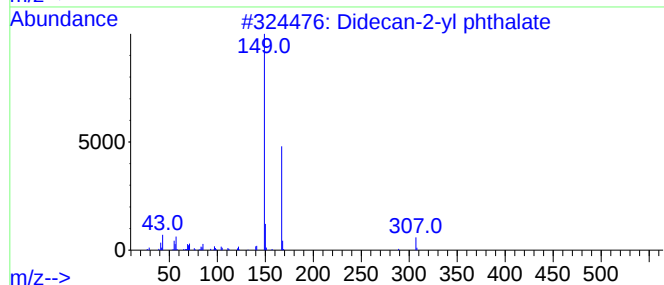
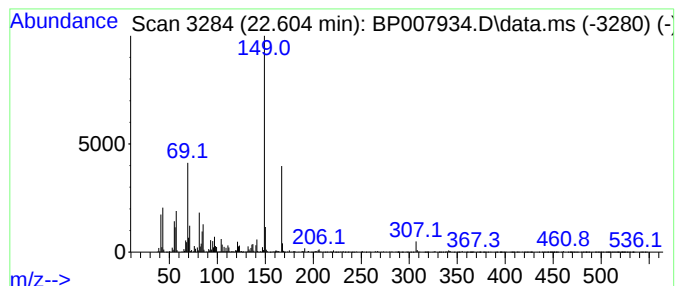
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Didecan-2-yl phthalate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.604	6.39 ng	584227	Perylene-d12	23.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Didecan-2-yl phthalate	446	C28H46O4	028029-89-2	86
2			Phthalic acid, di(2-propylpentyl)...	390	C24H38O4	1000377-93-5	72
3			Di-2-nonyl phthalate	418	C26H42O4	059431-96-8	64
4			Phthalic acid, di(6-methylhept-2...	390	C24H38O4	1000377-97-3	64
5			Phthalic acid, isohexyl pentadec...	460	C29H48O4	1000308-98-3	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
Data File : BP007934.D
Acq On : 10 Nov 2021 23:21
Operator : CG/JU
Sample : M4577-03
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.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
Ethanol, 2-(2-b...	10.440	2.6	ng	89266	2	10.651	680279	20.0
n-Hexadecanoic ...	18.139	2.7	ng	159973	4	17.245	1182430	20.0
Nonacos-1-ene	21.051	6.8	ng	550094	5	21.339	1625410	20.0
1-Heneicosanol	21.974	5.8	ng	470838	5	21.339	1625410	20.0
Terephthalic ac...	22.239	6.0	ng	487718	5	21.339	1625410	20.0
Didecan-2-yl ph...	22.604	6.4	ng	584227	6	23.745	1829850	20.0