

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
 Data File : BP005420.D
 Acq On : 29 Apr 2021 21:13
 Operator : CG/JU
 Sample : M2217-22
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 HTRCV2-GRAB-TS01-02

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-BP042921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005420.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.770	279	286	294	rBV	27923	42554	1.68%	0.329%
2	5.228	356	364	376	rBV	499777	704092	27.84%	5.442%
3	6.817	626	634	653	rBV	473622	731787	28.93%	5.656%
4	7.622	764	771	779	rBV	122636	192373	7.61%	1.487%
5	8.787	962	969	983	rBV	284360	471629	18.65%	3.646%
6	10.410	1238	1245	1255	rBV	137261	236850	9.36%	1.831%
7	12.904	1660	1669	1678	rBV	839586	1199736	47.43%	9.274%
8	13.757	1806	1814	1822	rBV	29455	46168	1.83%	0.357%
9	14.293	1898	1905	1912	rBV	222622	330037	13.05%	2.551%
10	15.798	2153	2161	2171	rBV	814684	1170357	46.27%	9.046%
11	17.057	2368	2375	2380	rBV	320492	447686	17.70%	3.460%
12	17.904	2515	2519	2523	rBV3	26039	36176	1.43%	0.280%
13	17.963	2524	2529	2538	rVV	127415	173924	6.88%	1.344%
14	19.086	2713	2720	2727	rBV	43554	79854	3.16%	0.617%
15	19.204	2736	2740	2749	rBV3	38494	55683	2.20%	0.430%
16	19.439	2774	2780	2783	rBV	20119	34714	1.37%	0.268%
17	19.639	2808	2814	2822	rBV	2203835	2529401	100.00%	19.551%
18	20.845	3013	3019	3021	rBV	88580	143933	5.69%	1.113%
19	20.880	3021	3025	3032	rVV2	273298	541834	21.42%	4.188%
20	20.951	3032	3037	3045	rVV	442338	586055	23.17%	4.530%
21	21.010	3045	3047	3052	rVB	23581	26746	1.06%	0.207%
22	21.163	3067	3073	3078	rBV	548774	737350	29.15%	5.699%
23	21.763	3168	3175	3184	rVB2	193799	349281	13.81%	2.700%
24	22.439	3286	3290	3294	rVB3	72601	98279	3.89%	0.760%
25	22.716	3333	3337	3341	rBV	109238	165107	6.53%	1.276%
26	22.769	3342	3346	3355	rVB2	202729	362645	14.34%	2.803%
27	23.416	3450	3456	3467	rVB	370602	668244	26.42%	5.165%
28	23.610	3485	3489	3500	rVB4	99403	184213	7.28%	1.424%
29	23.951	3542	3547	3554	rVB	127899	234725	9.28%	1.814%
30	24.045	3558	3563	3574	rVB2	150589	355808	14.07%	2.750%

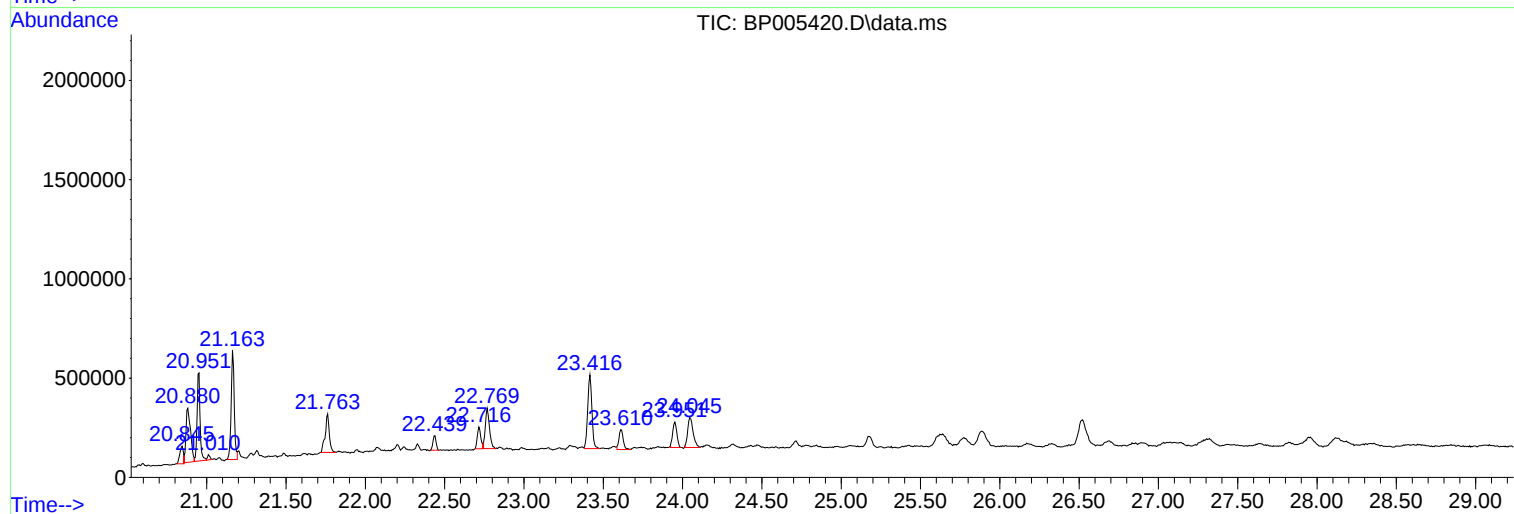
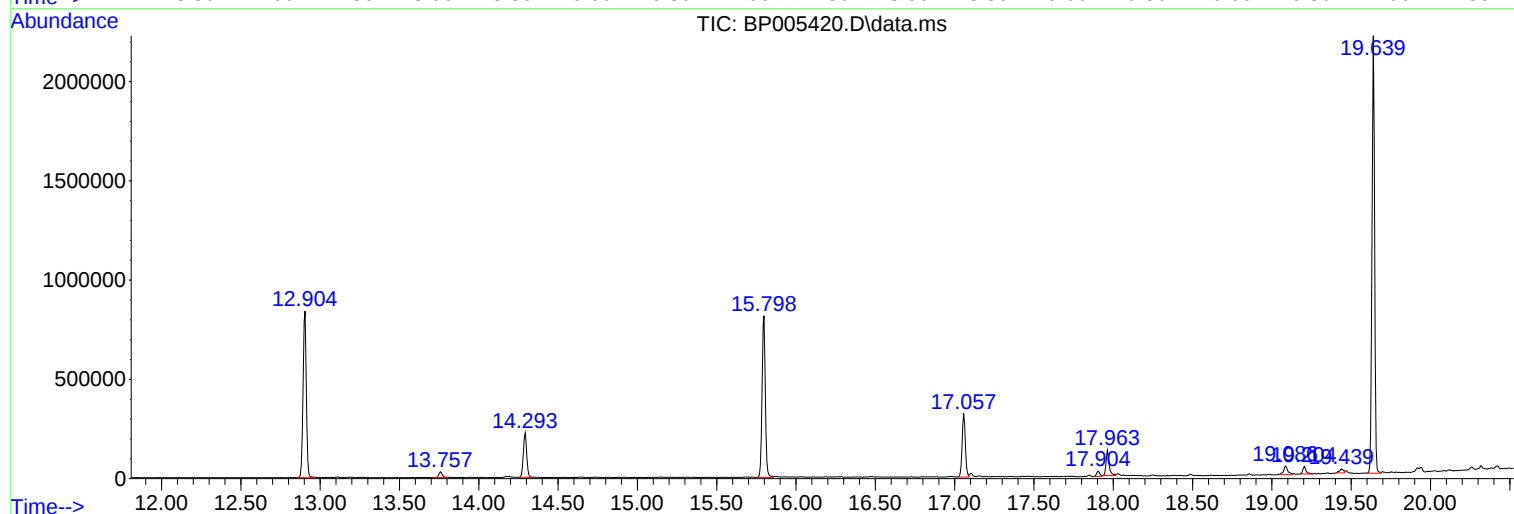
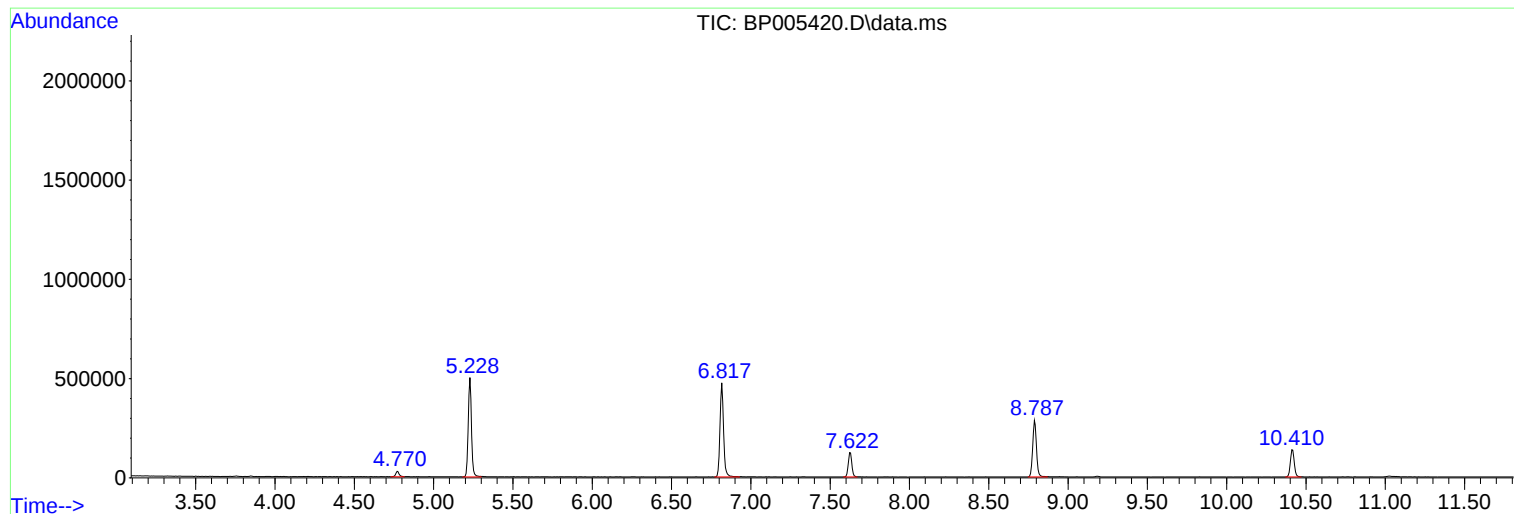
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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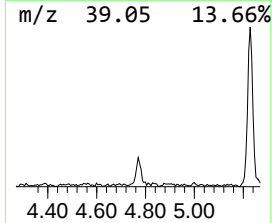
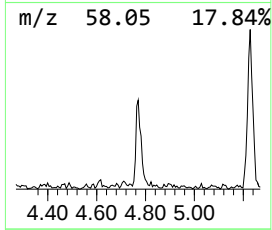
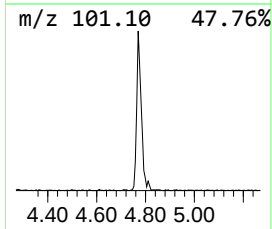
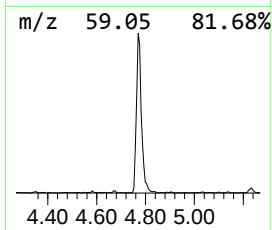
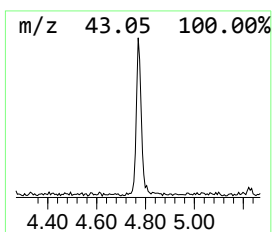
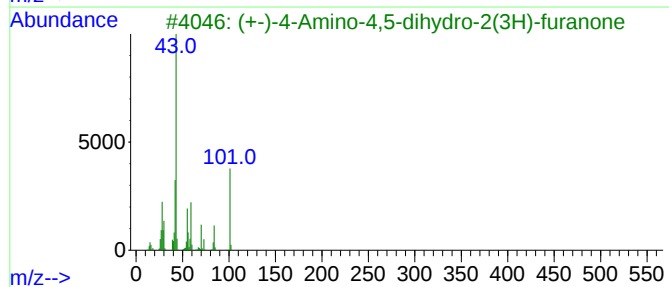
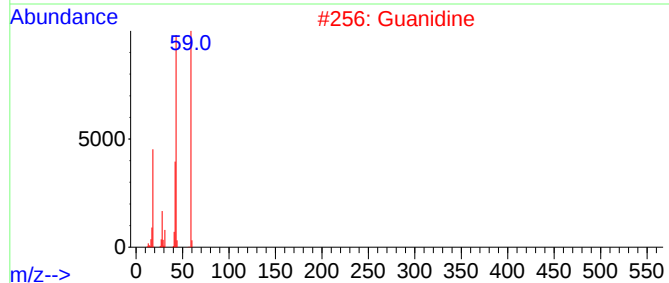
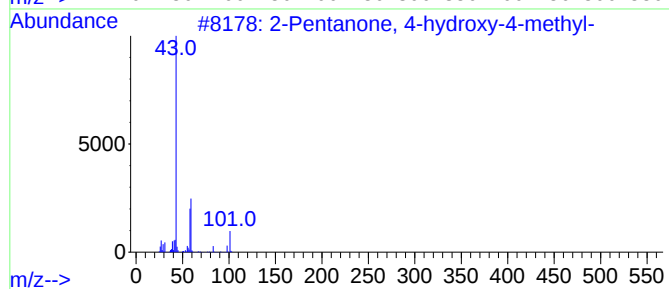
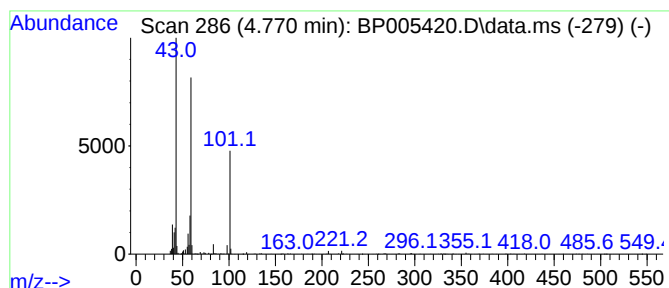
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.770	4.42 ng	42554	1,4-Dichlorobenzene-d4	7.628

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Guanidine	59	CH5N3	000113-00-8	43		
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43		
4	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	38		
5	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	36		



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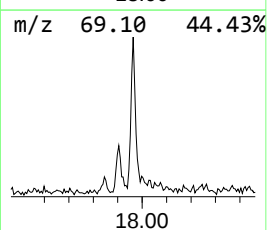
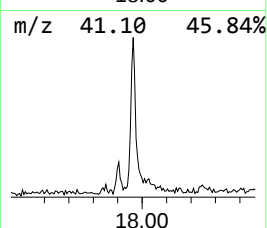
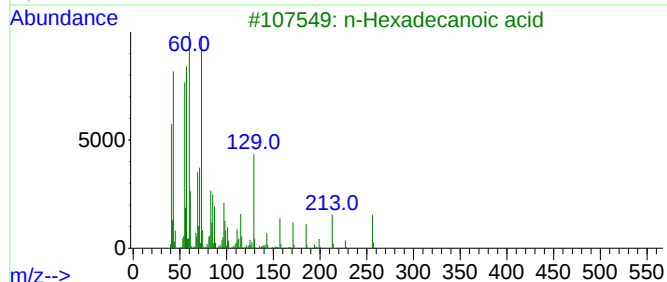
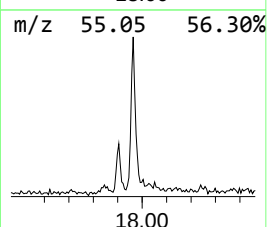
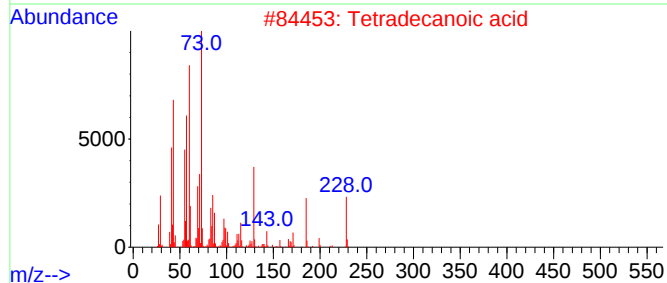
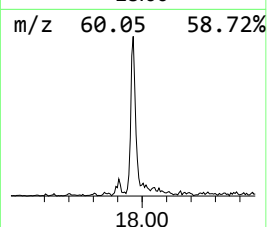
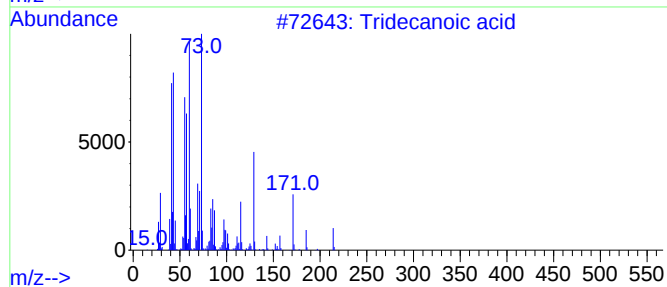
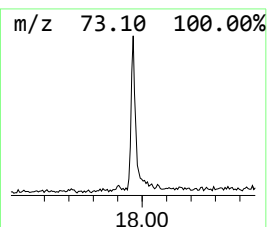
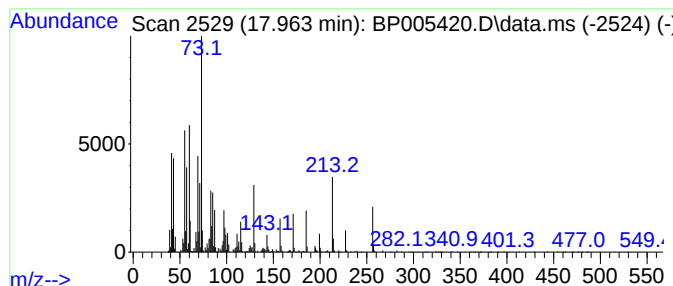
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.963	7.77 ng	173924	Phenanthrene-d10	17.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	83
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5			Octadecanoic acid	284	C18H36O2	000057-11-4	38



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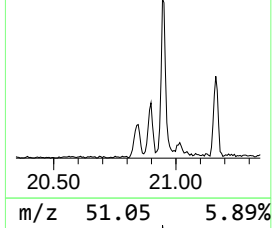
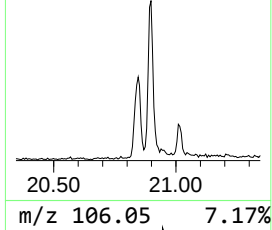
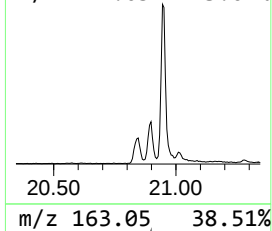
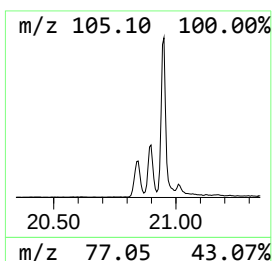
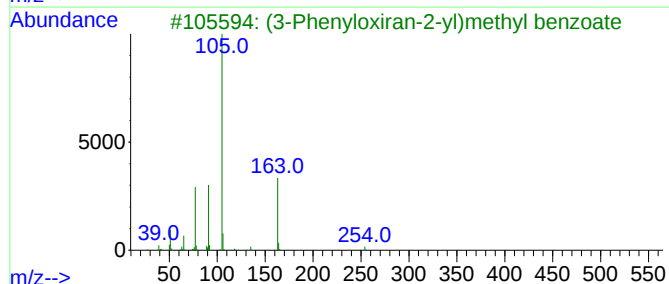
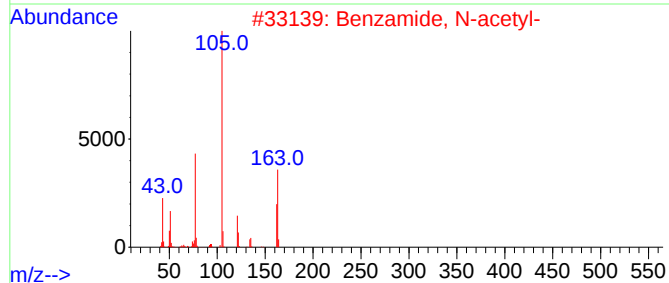
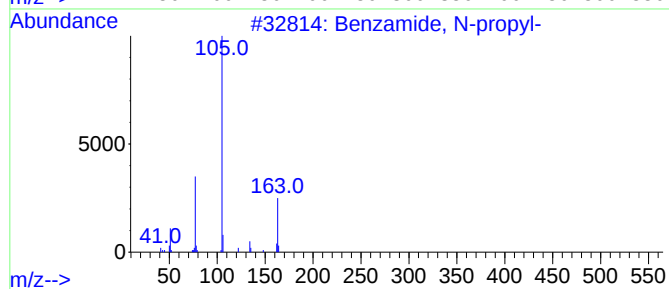
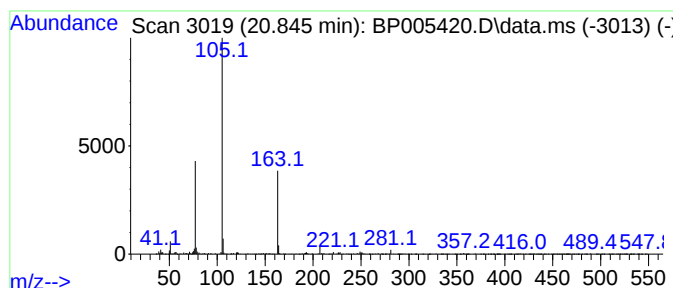
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BNA_P
ClientSampleId :
HTCRV2-GRAB-TS01-02

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzamide, N-propyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.845	3.90 ng	143933	Chrysene-d12	21.163	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
2	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	72
3	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	40
4	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	40
5	Benzamide, N-(2,3-dihydro-6-benz...	395	C24H17N3O3	186965-74-2	25



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Instrument :
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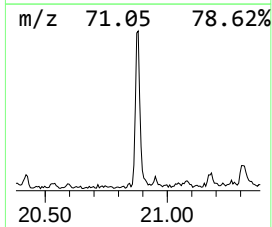
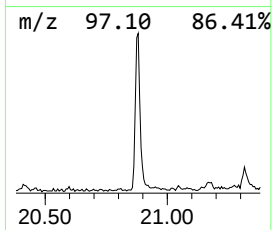
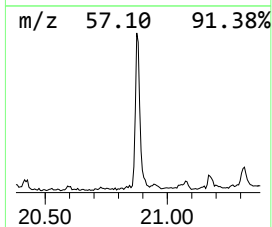
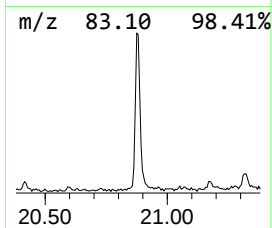
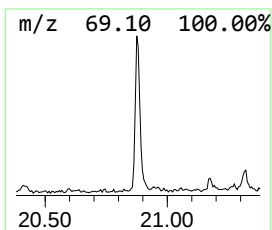
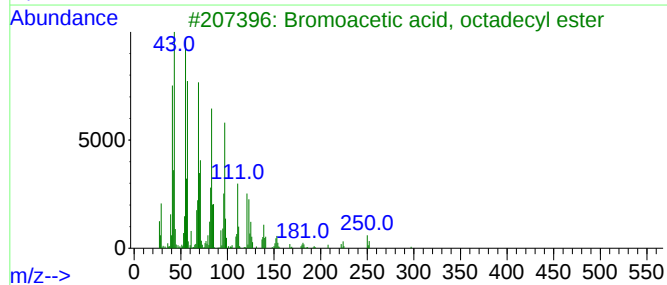
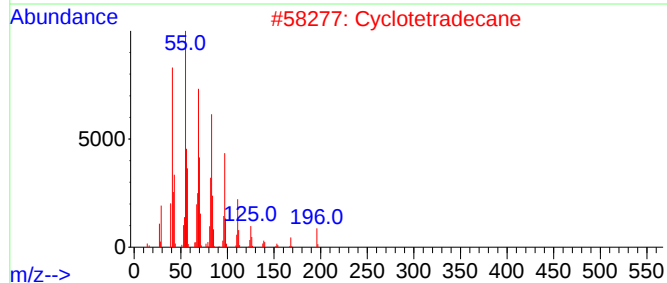
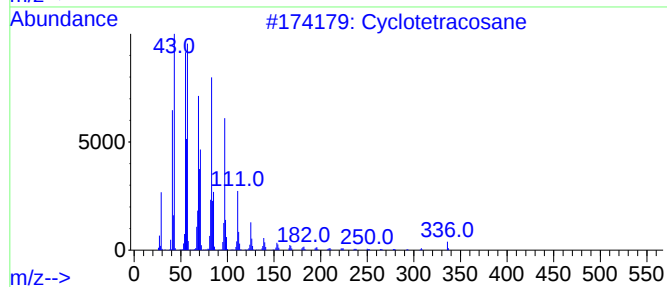
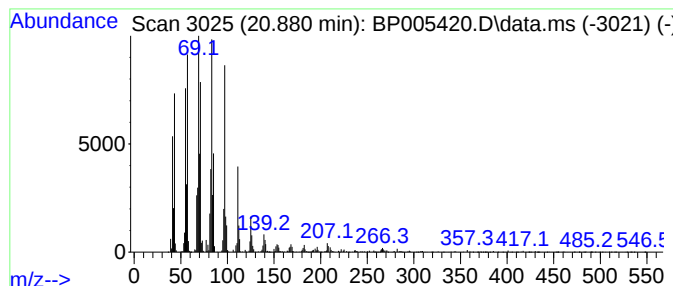
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Cyclotetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.881	14.70 ng	541834	Chrysene-d12	21.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	87
2			Cyclotetradecane	196	C14H28	000295-17-0	86
3			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	83
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	76
5			1-Hexacosanol	382	C26H54O	000506-52-5	76



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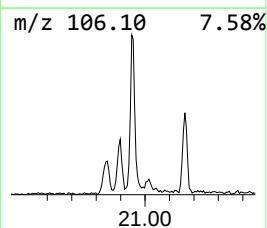
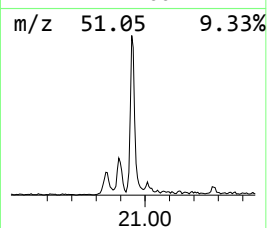
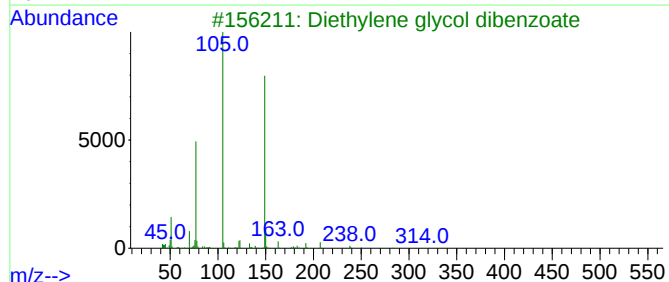
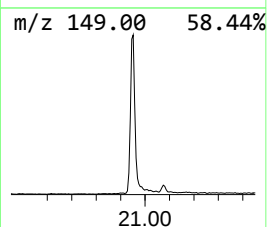
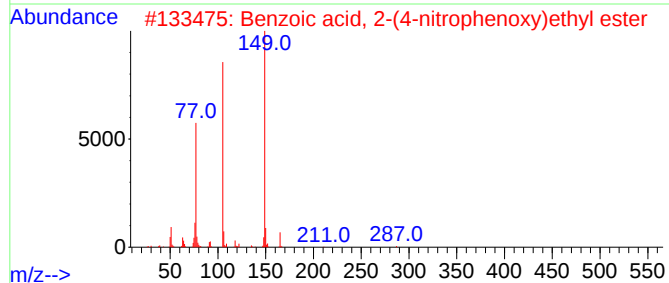
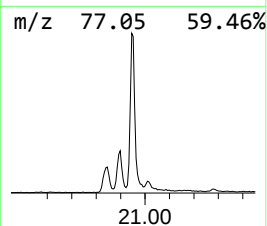
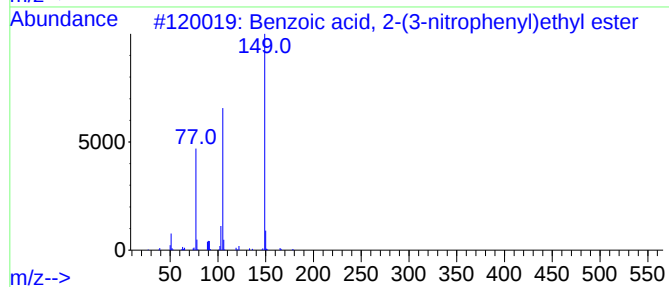
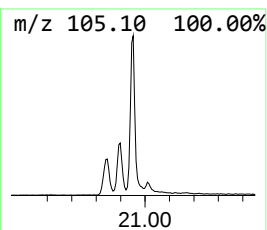
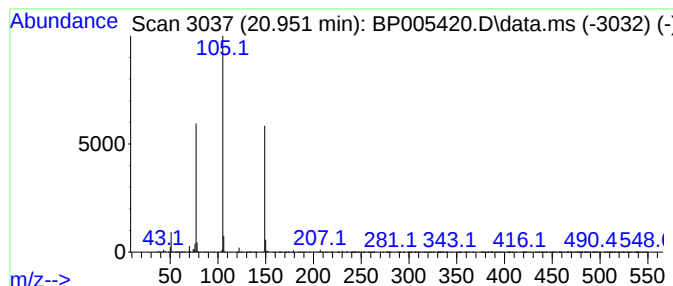
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Benzoic acid, 2-(3-nitrophe... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.951	15.90 ng	586055	Chrysene-d12	21.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78
2			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
3			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
4			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	50
5			Benzoyl bromide	184	C7H5BrO	000618-32-6	47



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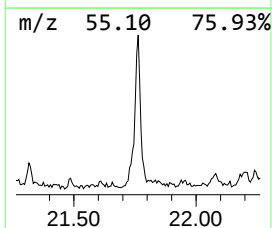
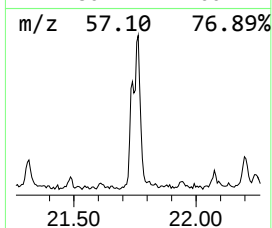
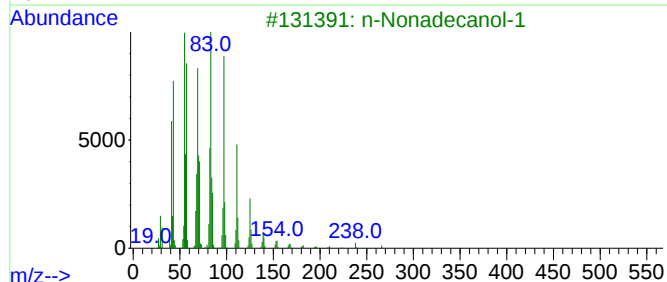
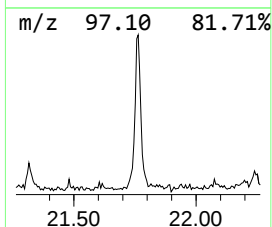
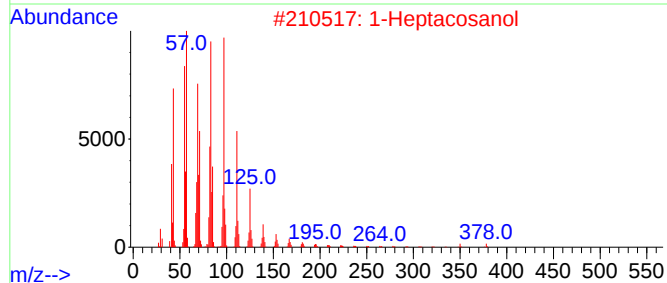
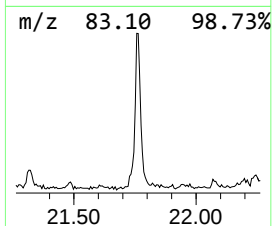
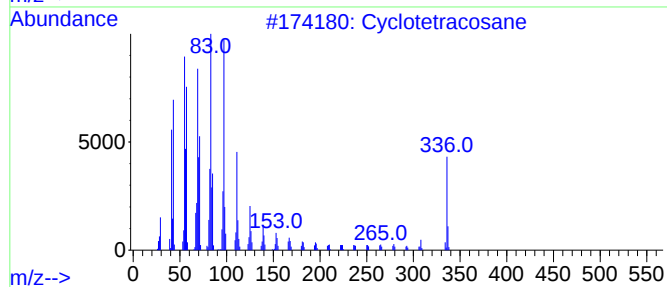
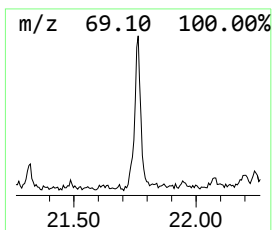
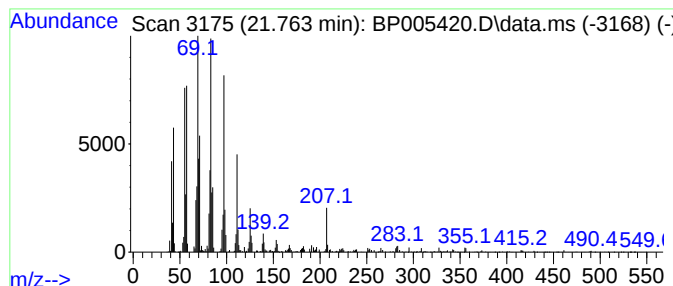
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.763	9.47 ng	349281	Chrysene-d12	21.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	94
2			1-Heptacosanol	396	C27H56O	002004-39-9	93
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	70
4			Behenic alcohol	326	C22H46O	000661-19-8	70
5			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005420.D
Acq On : 29 Apr 2021 21:13
Operator : CG/JU
Sample : M2217-22
Misc :
ALS Vial : 17 Sample Multiplier: 1

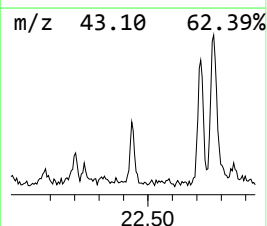
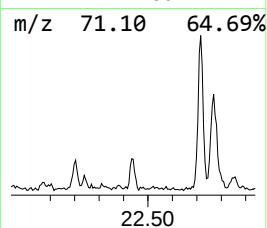
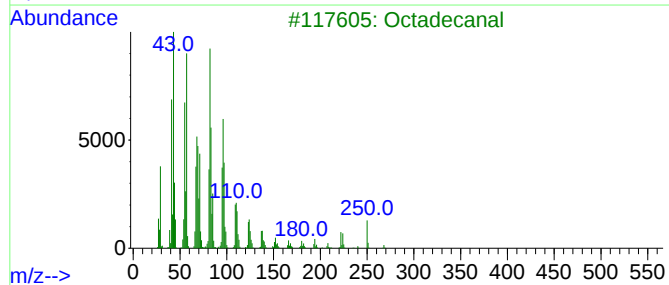
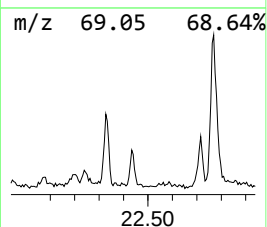
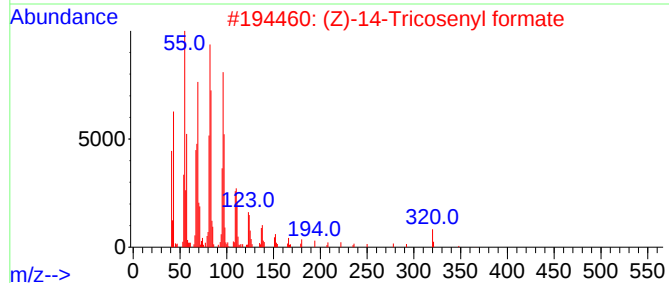
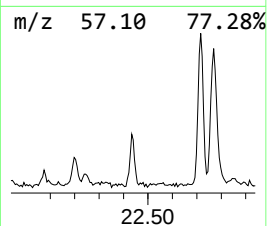
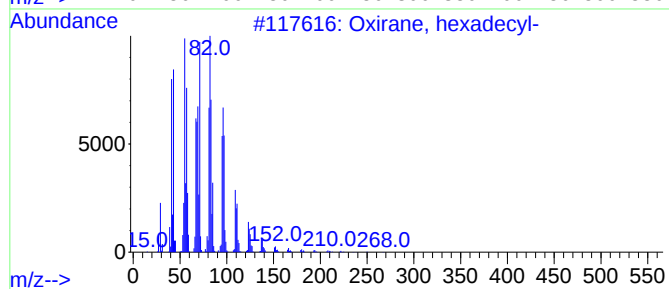
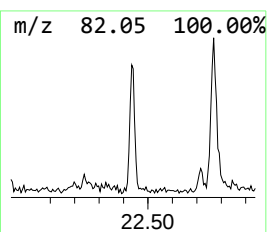
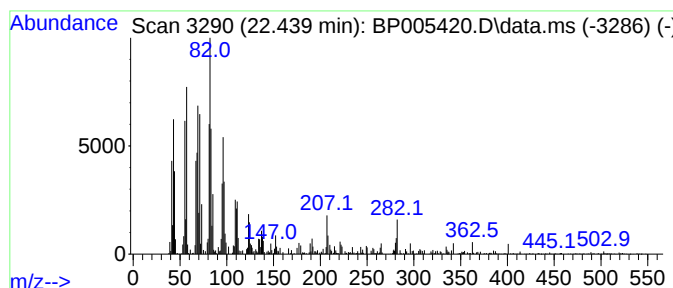
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.439	2.94 ng	98279	Perylene-d12		23.416	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	91
2	(Z)-14-Tricosenyl formate		366	C24H46O2	077899-10-6	90
3	Octadecanal		268	C18H36O	000638-66-4	80
4	9-Octadecen-1-ol, (Z)-		268	C18H36O	000143-28-2	78
5	16-Heptadecenal		252	C17H32O	1000144-57-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005420.D
Acq On : 29 Apr 2021 21:13
Operator : CG/JU
Sample : M2217-22
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HTCRV2-GRAB-TS01-02

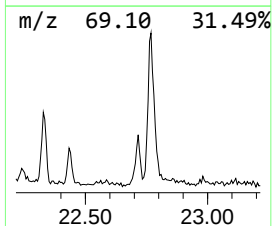
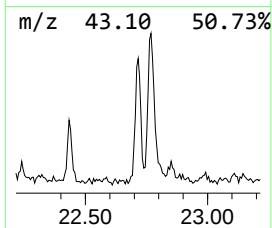
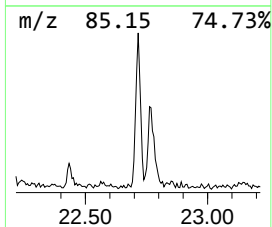
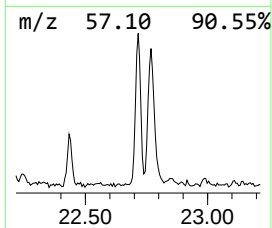
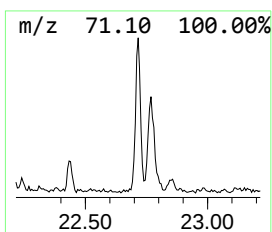
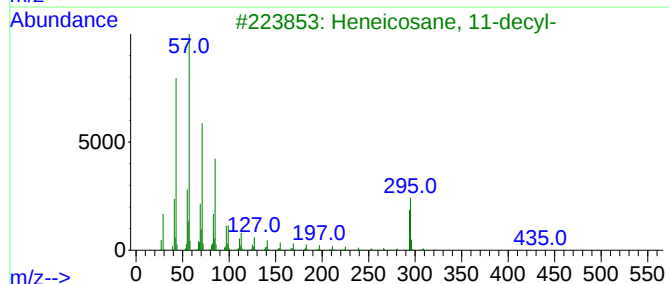
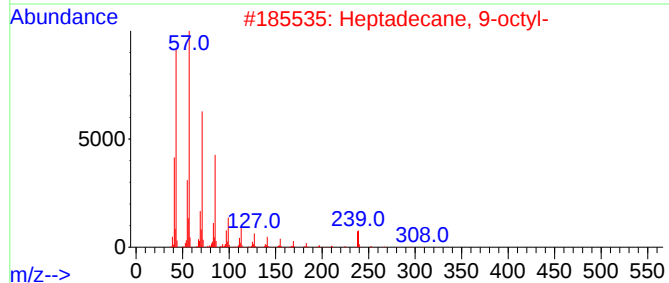
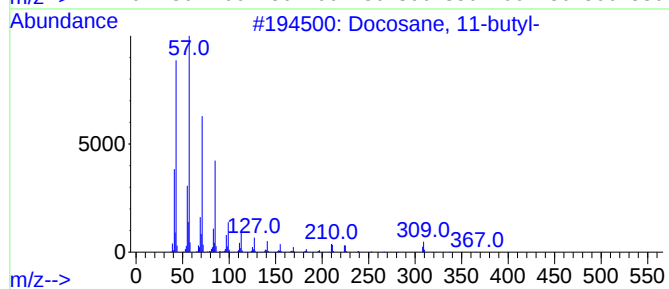
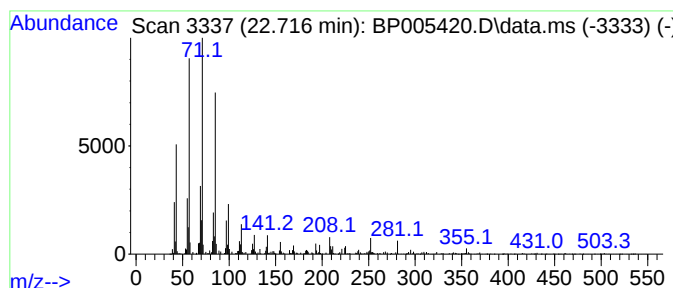
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Docosane, 11-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.716	4.94 ng	165107	Perylene-d12	23.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3			Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
4			Octacosane	394	C28H58	000630-02-4	87
5			Docosane, 5-butyl-	366	C26H54	055282-16-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005420.D
Acq On : 29 Apr 2021 21:13
Operator : CG/JU
Sample : M2217-22
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HTCRV2-GRAB-TS01-02

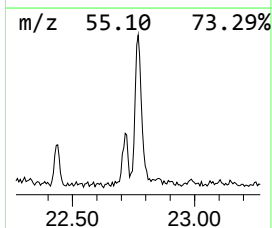
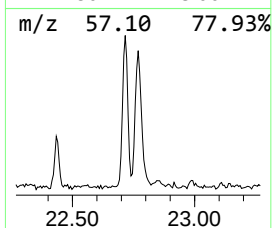
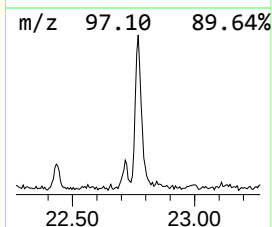
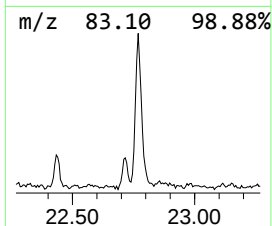
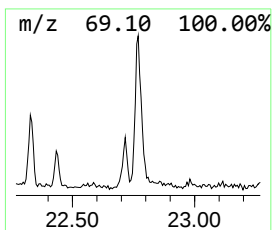
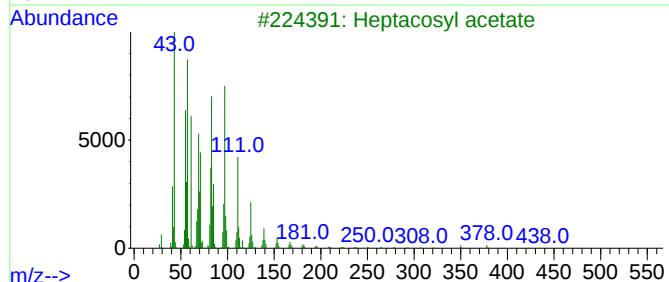
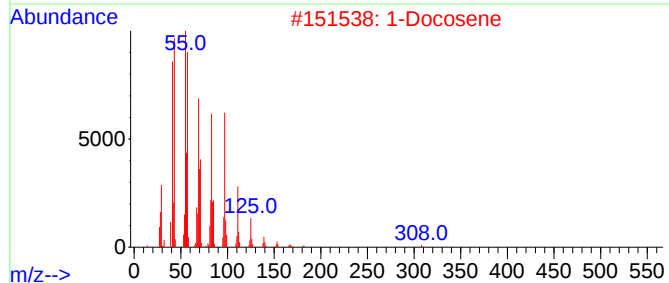
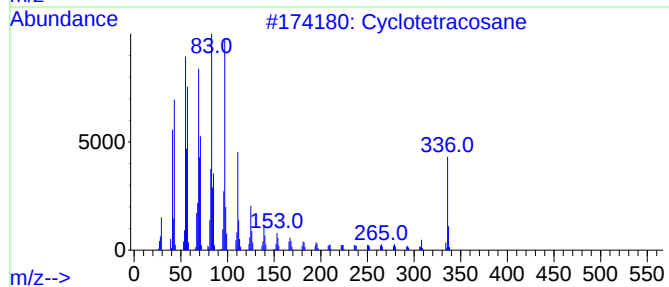
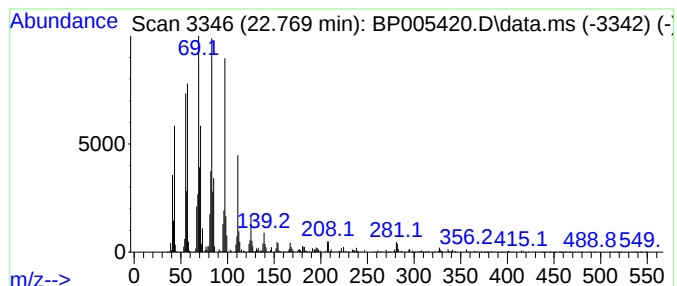
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.769	10.85 ng	362645	Perylene-d12	23.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	91
2			1-Docosene	308	C22H44	001599-67-3	80
3			Heptacosyl acetate	438	C29H58O2	1000351-78-2	78
4			Cyclotetradecane	196	C14H28	000295-17-0	70
5			1-Triacontanol	438	C30H62O	000593-50-0	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005420.D
Acq On : 29 Apr 2021 21:13
Operator : CG/JU
Sample : M2217-22
Misc :
ALS Vial : 17 Sample Multiplier: 1

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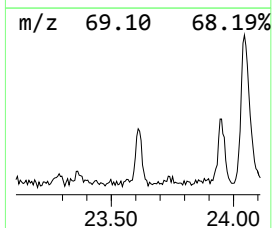
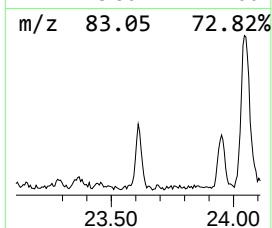
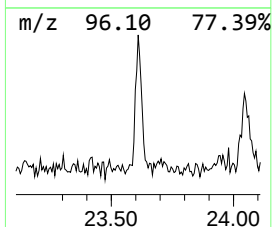
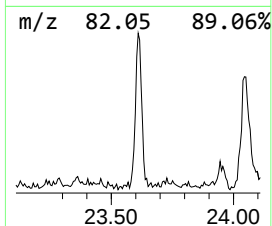
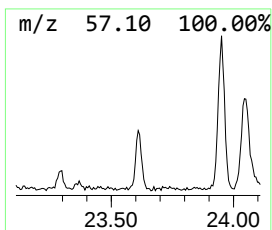
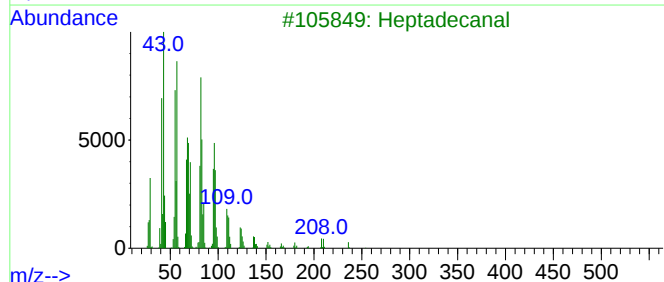
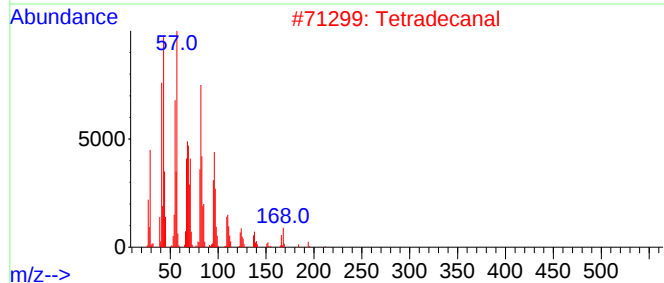
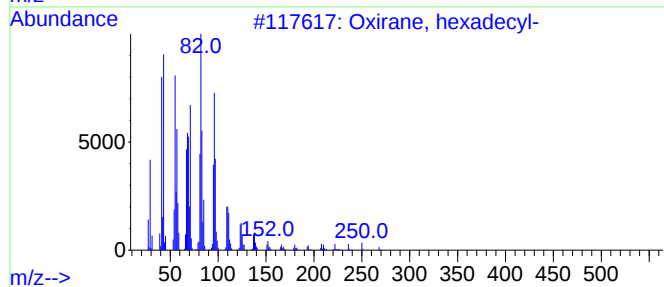
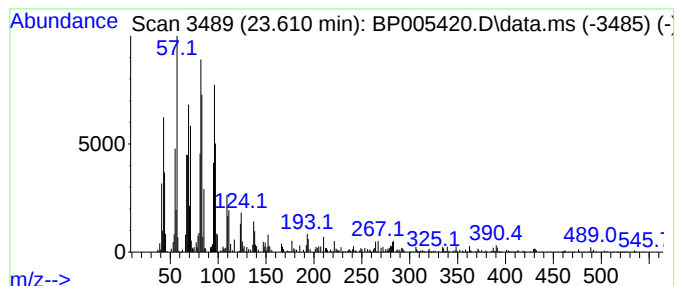
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Tetradecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.610	5.51 ng	184213	Perylene-d12	23.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2		Tetradecanal	212	C14H28O	000124-25-4	87
3		Heptadecanal	254	C17H34O	1000376-70-0	86
4		Hexadecanal	240	C16H32O	000629-80-1	86
5		Pentadecanal	226	C15H30O	002765-11-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005420.D
Acq On : 29 Apr 2021 21:13
Operator : CG/JU
Sample : M2217-22
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
HTCRV2-GRAB-TS01-02

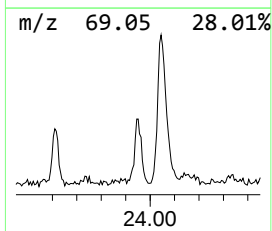
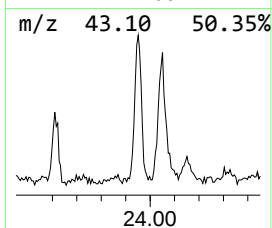
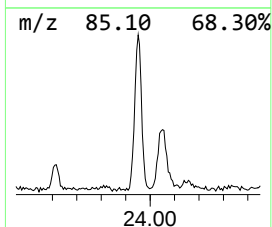
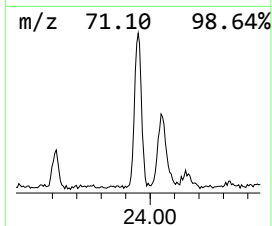
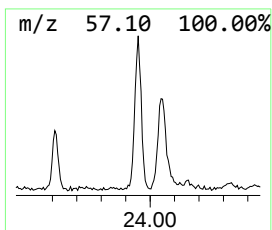
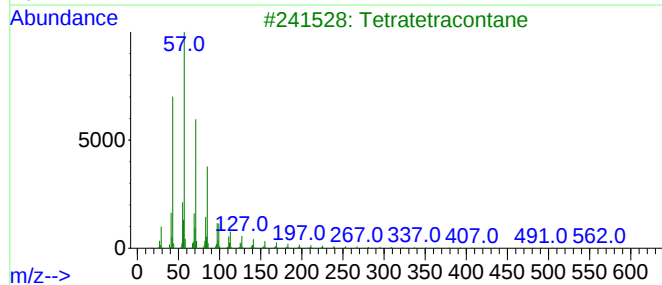
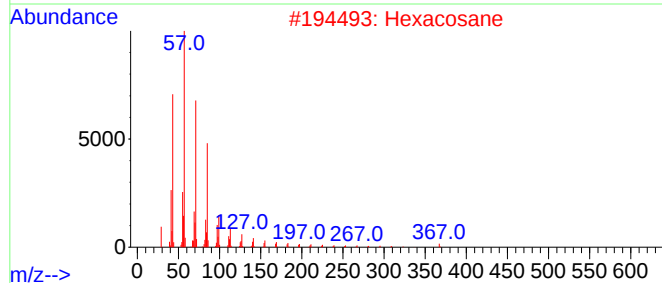
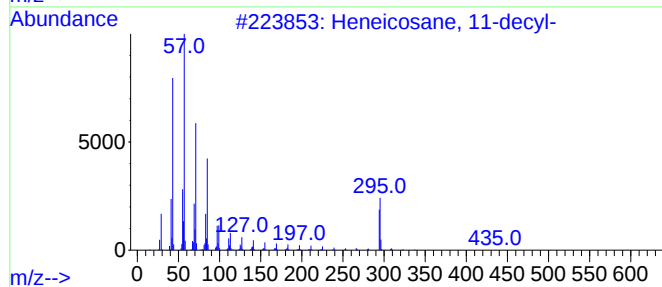
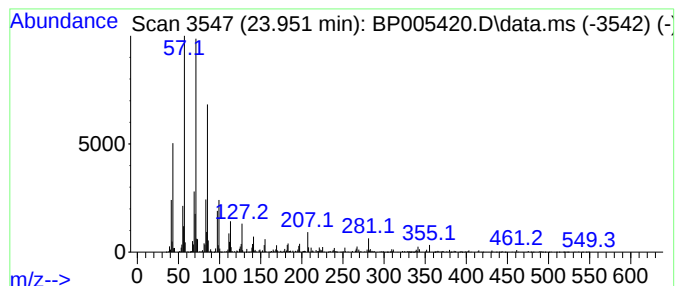
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Heneicosane, 11-decyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.951	7.03 ng	234725	Perylene-d12	23.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	93
2		Hexacosane	366	C26H54	000630-01-3	90
3		Tetratetracontane	619	C44H90	007098-22-8	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	90
5		Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005420.D
Acq On : 29 Apr 2021 21:13
Operator : CG/JU
Sample : M2217-22
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HTCRV2-GRAB-TS01-02

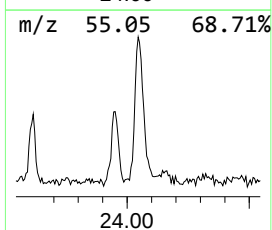
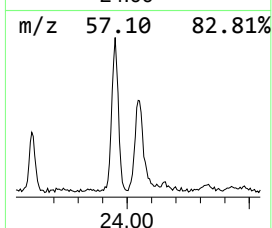
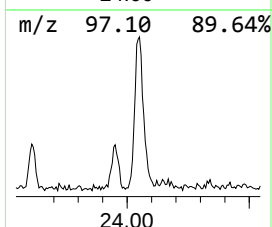
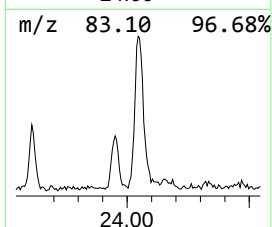
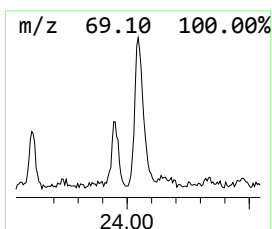
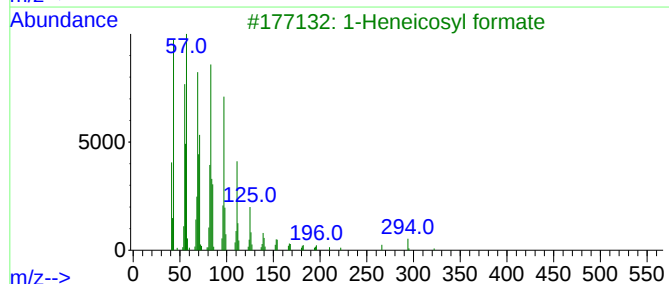
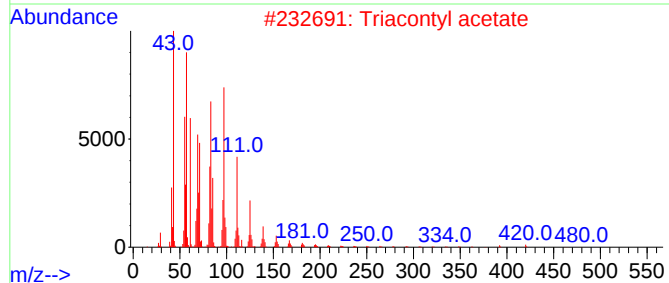
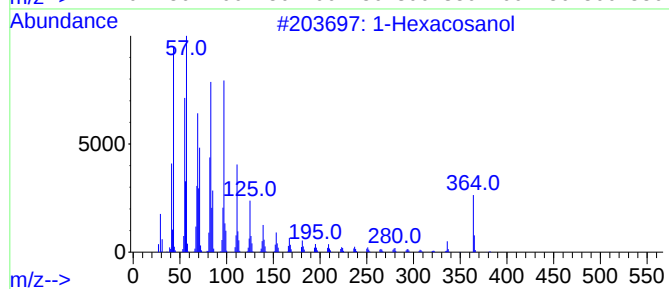
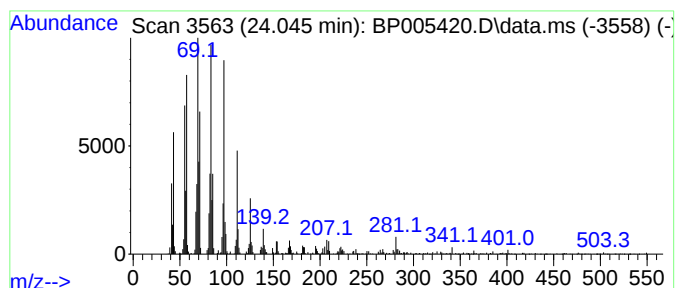
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 1-Hexacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.045	10.65 ng	355808	Perylene-d12	23.416

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol		382	C26H54O	000506-52-5	95
2	Triacontyl acetate		480	C32H64O2	041755-58-2	93
3	1-Heneicosyl formate		340	C22H44O2	077899-03-7	91
4	Trifluoroacetic acid, pentadecyl...		324	C17H31F3O2	959010-23-2	91
5	1-Heptacosanol		396	C27H56O	002004-39-9	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042921\
Data File : BP005420.D
Acq On : 29 Apr 2021 21:13
Operator : CG/JU
Sample : M2217-22
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
HTCRV2-GRAB-TS01-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.770	4.4	ng	42554	1	7.628	192373	20.0
Tridecanoic acid	17.963	7.8	ng	173924	4	17.057	447686	20.0
Benzamide, N-pr...	20.845	3.9	ng	143933	5	21.163	737350	20.0
Cyclotetracosane	20.881	14.7	ng	541834	5	21.163	737350	20.0
Benzoic acid, 2...	20.951	15.9	ng	586055	5	21.163	737350	20.0
1-Heptacosanol	21.763	9.5	ng	349281	5	21.163	737350	20.0
Oxirane, hexade...	22.439	2.9	ng	98279	6	23.416	668244	20.0
Docosane, 11-bu...	22.716	4.9	ng	165107	6	23.416	668244	20.0
1-Docosene	22.769	10.9	ng	362645	6	23.416	668244	20.0
Tetradecanal	23.610	5.5	ng	184213	6	23.416	668244	20.0
Heneicosane, 11...	23.951	7.0	ng	234725	6	23.416	668244	20.0
1-Hexacosanol	24.045	10.7	ng	355808	6	23.416	668244	20.0