

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
 Data File : BP007938.D
 Acq On : 11 Nov 2021 01:36
 Operator : CG/JU
 Sample : M4577-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB-4

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: BP007938.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	378	rBV	1964941	2800808	52.14%	6.811%
2	7.028	629	636	649	rBV	1701658	2752359	51.24%	6.693%
3	7.852	768	776	784	rBV	491928	780070	14.52%	1.897%
4	9.010	965	973	989	rBV	1090102	1779654	33.13%	4.328%
5	10.440	1209	1216	1224	rBV2	70215	128864	2.40%	0.313%
6	10.651	1242	1252	1259	rBV	564878	940068	17.50%	2.286%
7	13.116	1664	1671	1679	rBV	1901080	2841124	52.90%	6.909%
8	13.263	1689	1696	1704	rVB2	89514	139350	2.59%	0.339%
9	14.263	1861	1866	1871	rBV3	58682	82332	1.53%	0.200%
10	14.339	1871	1879	1884	rVV5	74928	125877	2.34%	0.306%
11	14.492	1897	1905	1913	rBV	805838	1271980	23.68%	3.093%
12	14.563	1913	1917	1924	rVB2	63792	94902	1.77%	0.231%
13	14.745	1943	1948	1955	rVB2	53162	80210	1.49%	0.195%
14	14.816	1955	1960	1969	rVB	38892	61651	1.15%	0.150%
15	15.981	2152	2158	2170	rBV	2203282	3286770	61.19%	7.993%
16	16.216	2193	2198	2204	rVB	49970	69377	1.29%	0.169%
17	16.639	2264	2270	2280	rBV2	73541	144376	2.69%	0.351%
18	17.245	2365	2373	2381	rBV	1096578	1625350	30.26%	3.953%
19	18.139	2521	2525	2532	rBV	259279	368089	6.85%	0.895%
20	18.457	2574	2579	2585	rVB3	38033	77219	1.44%	0.188%
21	19.233	2708	2711	2713	rBV2	57679	75404	1.40%	0.183%
22	19.263	2713	2716	2722	rVV	115419	214506	3.99%	0.522%
23	19.316	2722	2725	2731	rVV	72387	112477	2.09%	0.274%
24	19.374	2731	2735	2749	rVB3	98718	183381	3.41%	0.446%
25	19.810	2803	2809	2815	rBV	3362524	4233806	78.82%	10.296%
26	20.086	2853	2856	2860	rBV4	48676	64539	1.20%	0.157%
27	20.439	2914	2916	2920	rVB3	70226	67980	1.27%	0.165%
28	21.051	3016	3020	3025	rBV	877837	1098173	20.45%	2.671%
29	21.333	3063	3068	3074	rBV	1633590	2260261	42.08%	5.497%
30	21.974	3172	3177	3188	rBV	1593181	2339500	43.56%	5.689%
31	22.233	3218	3221	3226	rVB	194371	256413	4.77%	0.624%
32	22.604	3281	3284	3290	rVB2	232294	325258	6.06%	0.791%
33	23.068	3358	3363	3371	rVB	625433	1098817	20.46%	2.672%
34	23.745	3472	3478	3490	rVB2	1158421	2387025	44.44%	5.805%
35	27.215	4062	4068	4079	rVB5	531224	1582109	29.46%	3.847%
36	28.650	4302	4312	4330	rVB3	1393392	5371240	100.00%	13.062%

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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

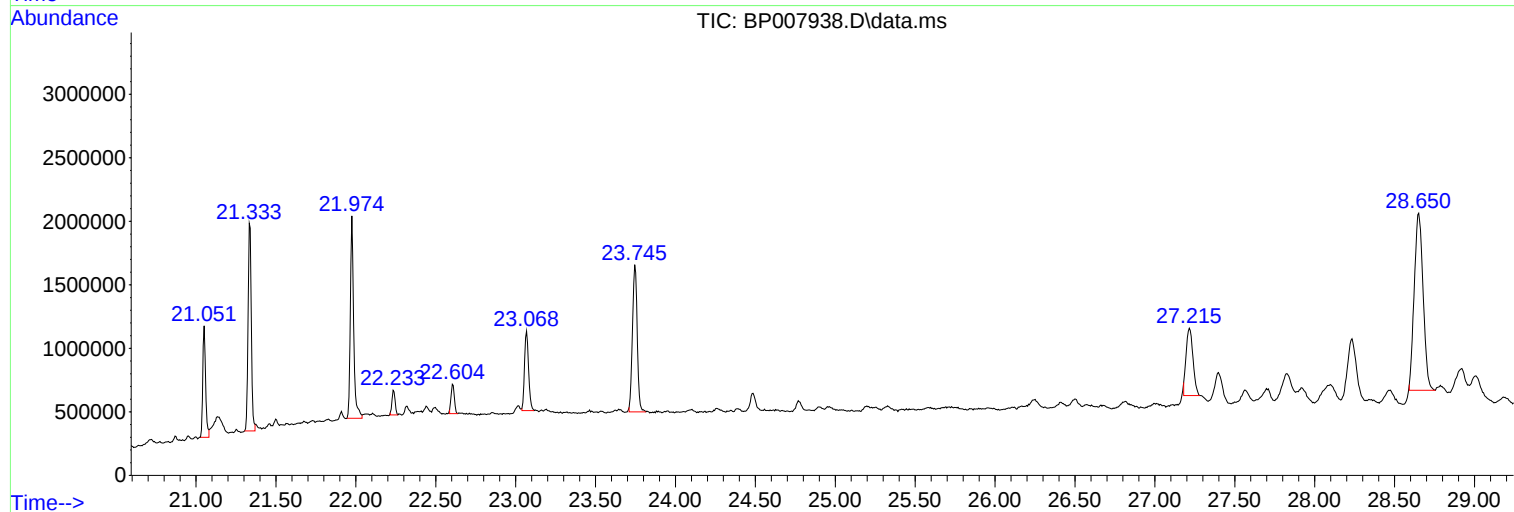
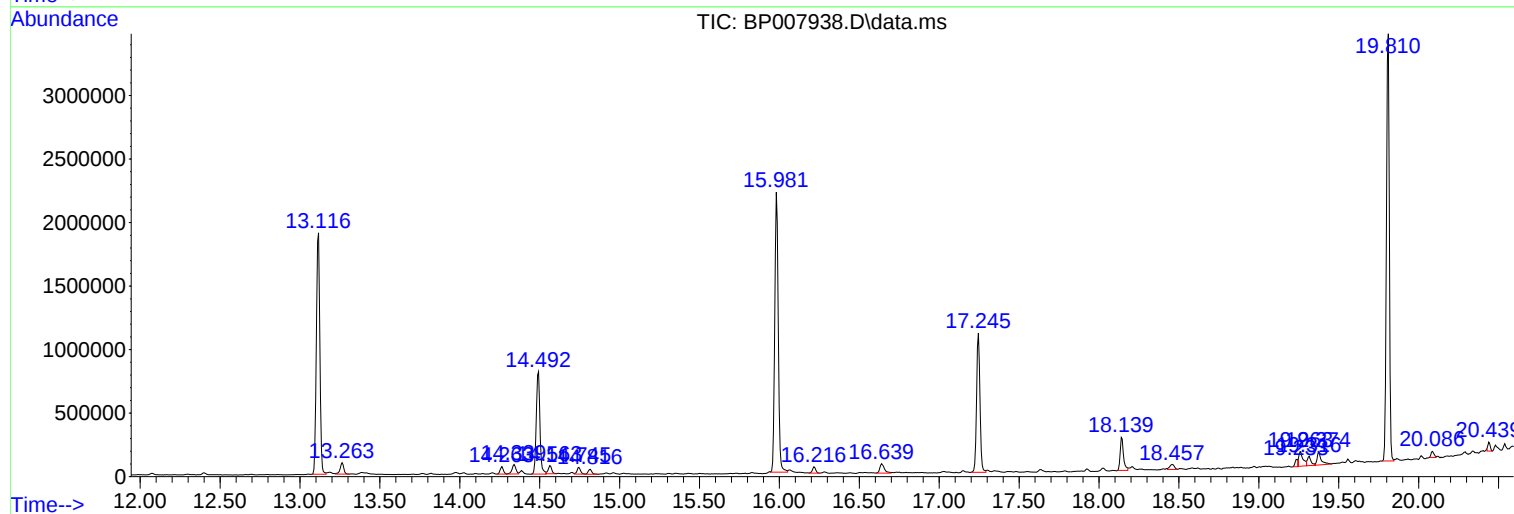
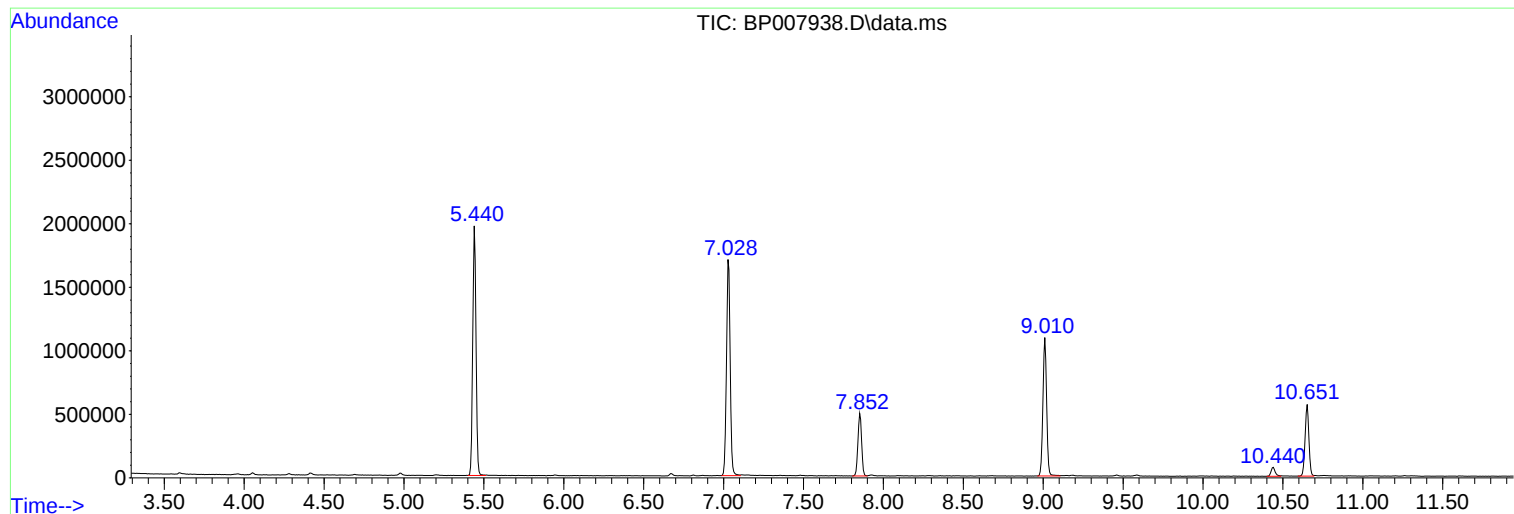
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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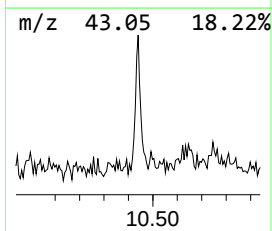
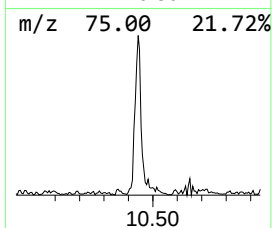
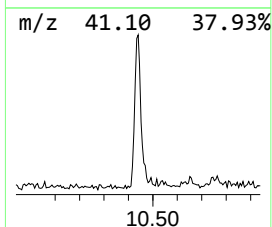
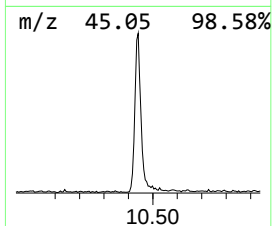
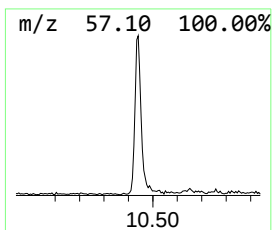
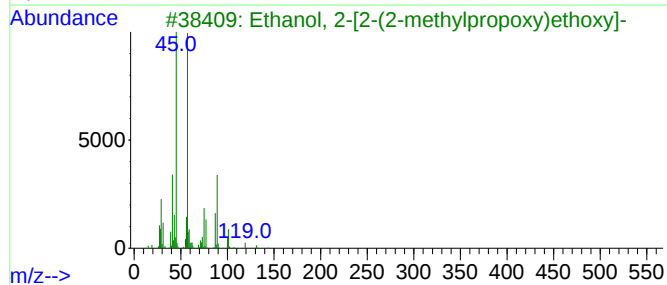
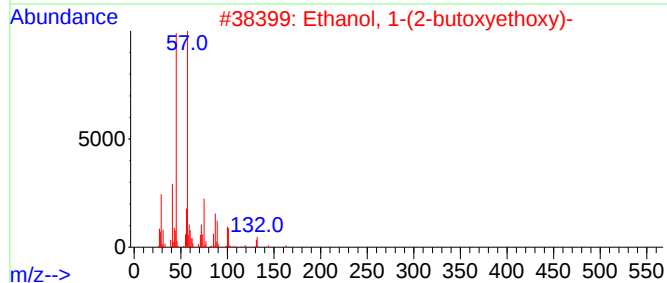
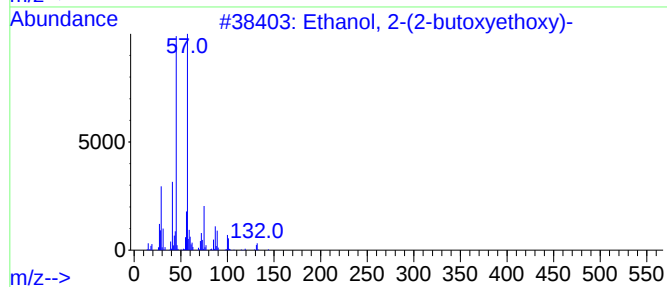
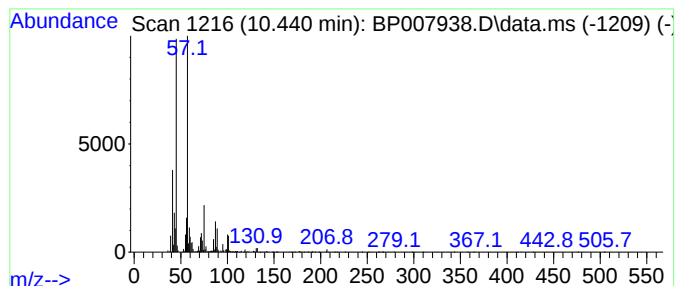
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.440	2.74 ng	128864	Naphthalene-d8	10.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50



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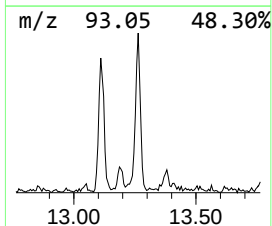
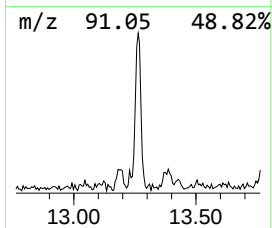
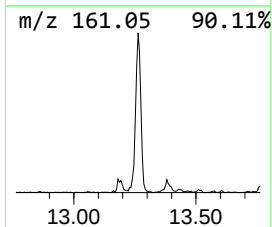
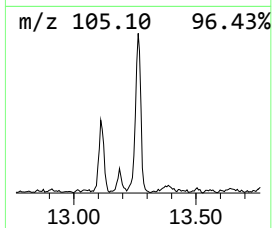
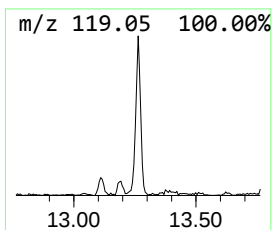
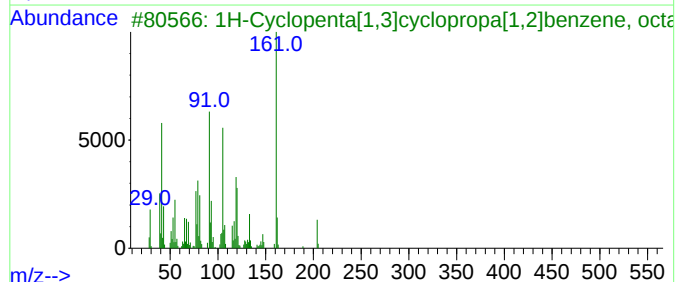
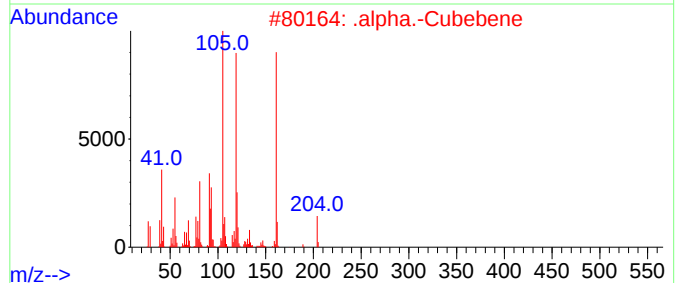
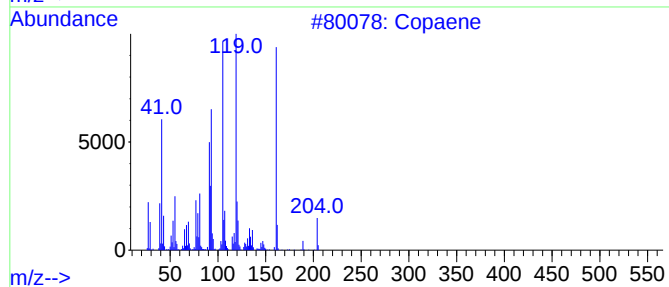
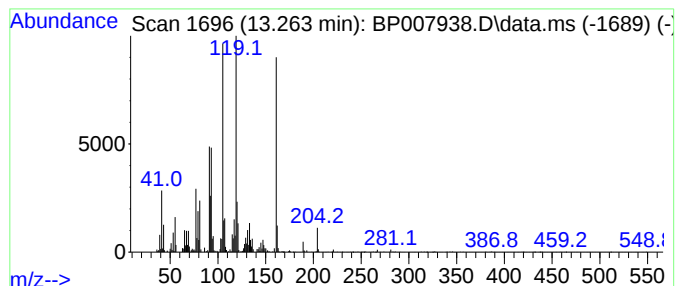
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Copaene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.263	2.19 ng	139350	Acenaphthene-d10	14.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Copaene	204	C15H24	003856-25-5	98
2			.alpha.-Cubebene	204	C15H24	017699-14-8	91
3			1H-Cyclopenta[1,3]cyclopropa[1,2...]	204	C15H24	013744-15-5	60
4			Naphthalene, 1,2,3,4,4a,7-hexahy...	204	C15H24	016728-99-7	55
5			(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	55



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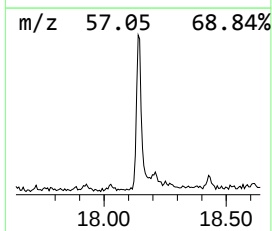
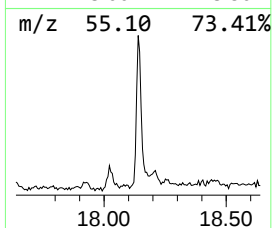
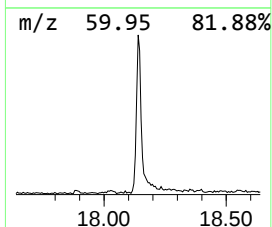
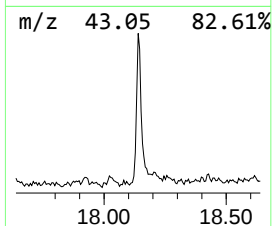
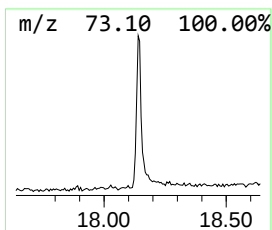
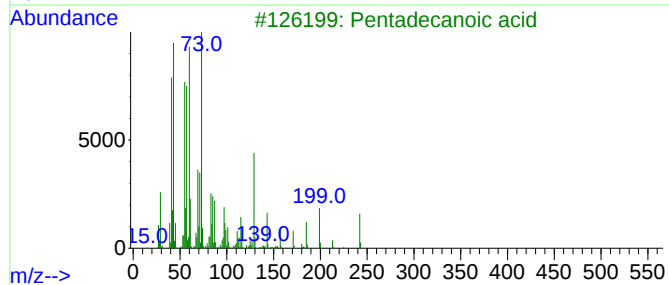
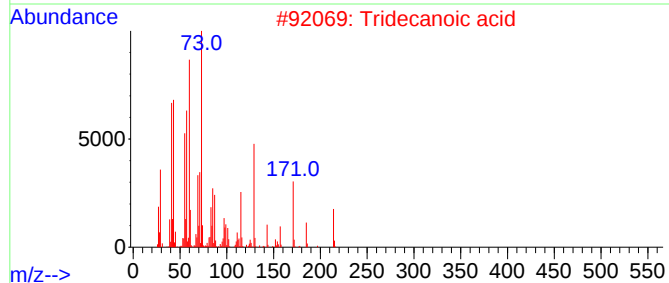
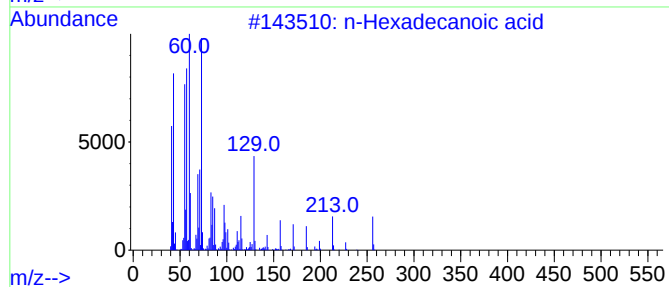
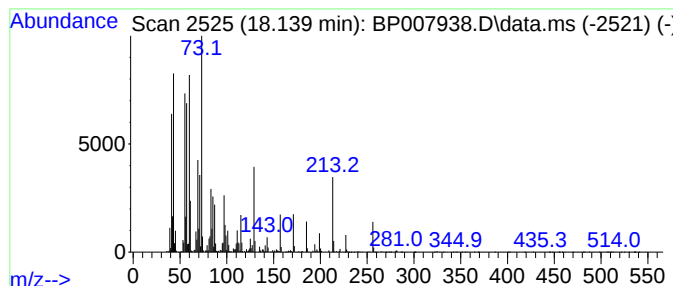
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.139	4.53 ng	368089	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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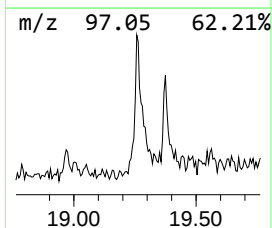
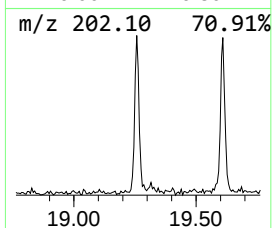
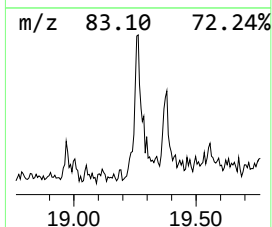
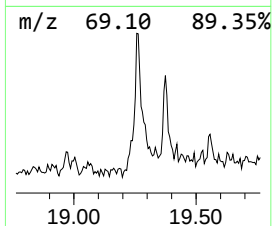
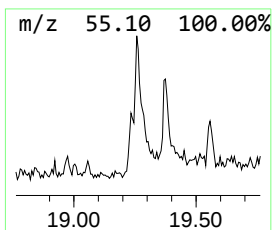
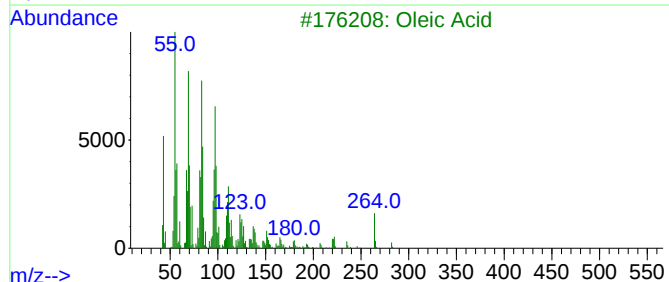
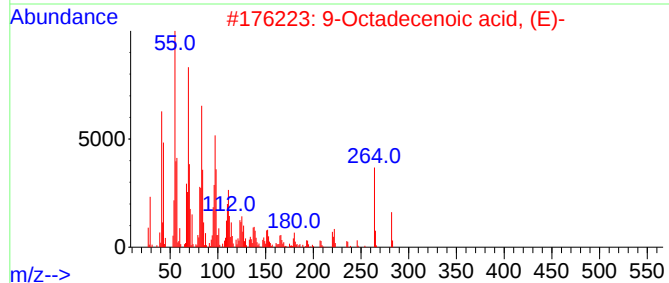
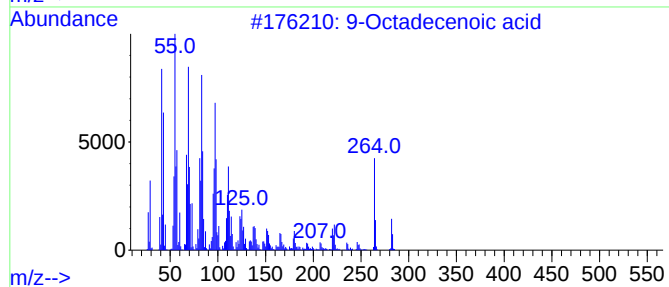
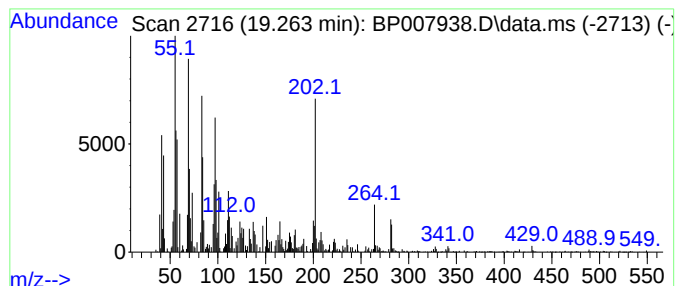
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 9-Octadecenoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.263	2.64 ng	214506	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid	282	C18H34O2	002027-47-6	89
2			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	70
3			Oleic Acid	282	C18H34O2	000112-80-1	64
4			Oleyl alcohol, trifluoroacetate	364	C20H35F3O2	1000352-68-4	55
5			Fumaric acid, 2,2-dichloroethyl ...	394	C19H32Cl2O4	1000348-58-1	49



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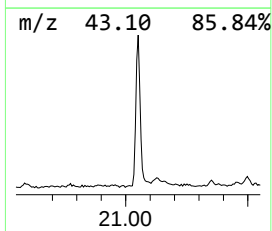
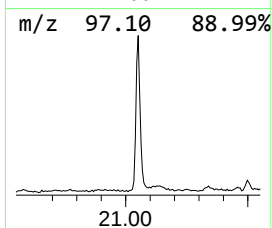
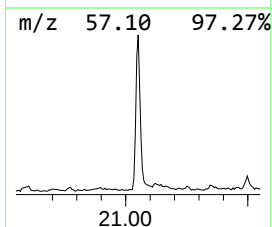
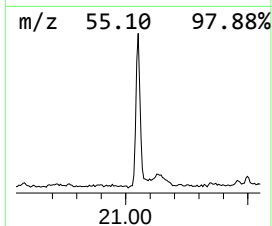
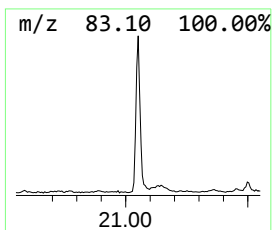
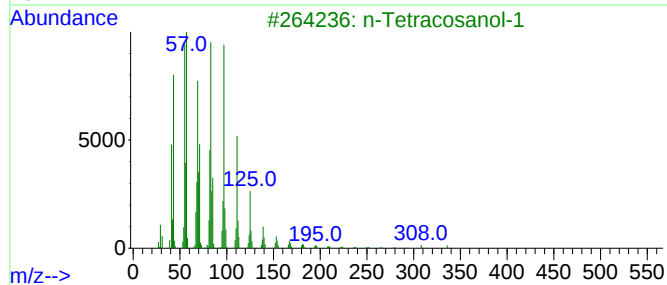
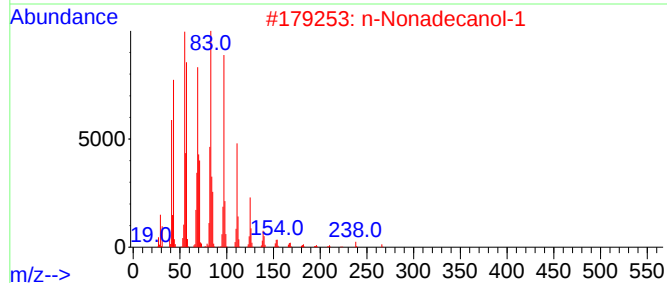
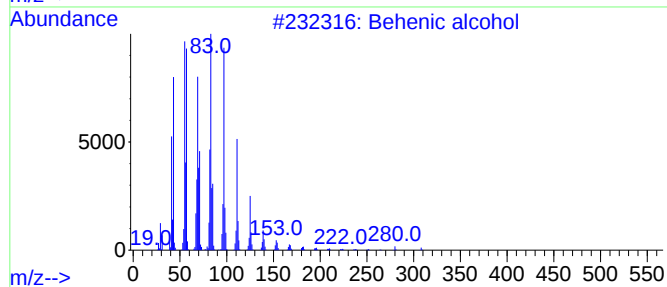
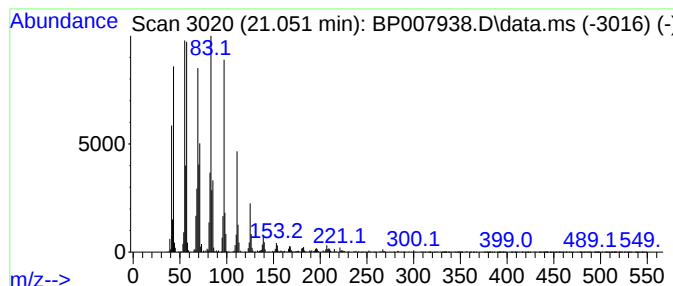
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Peak Number 5 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	9.72 ng	1098170	Chrysene-d12	21.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	94
5			Pentacos-1-ene	350	C25H50	016980-85-1	94



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Data File : BP007938.D
Acq On : 11 Nov 2021 01:36
Operator : CG/JU
Sample : M4577-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-4

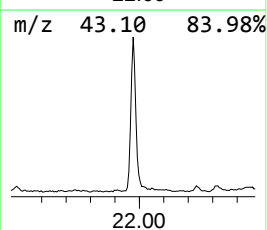
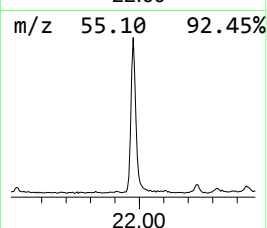
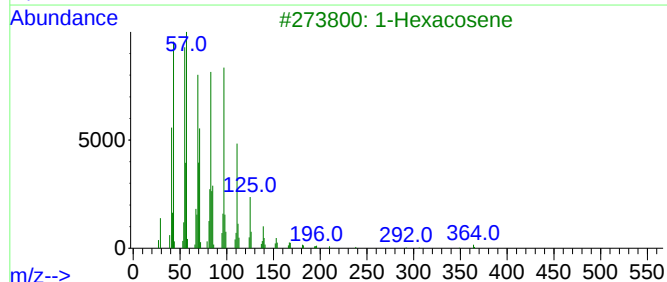
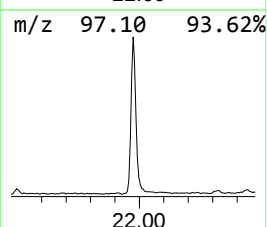
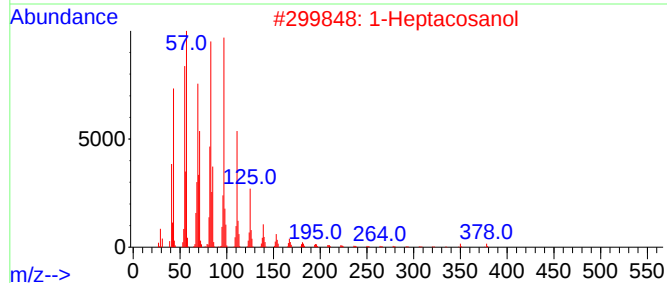
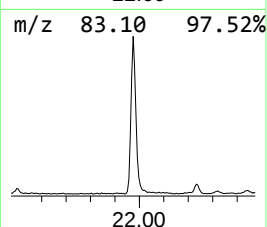
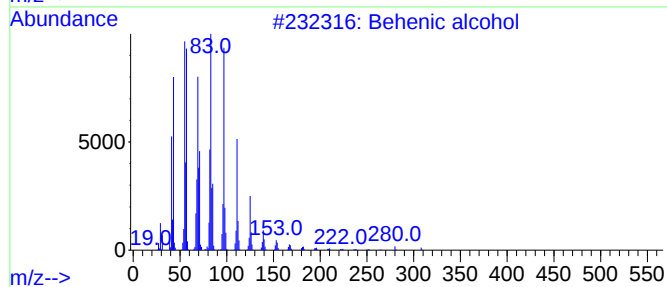
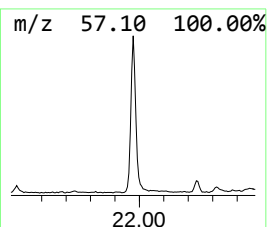
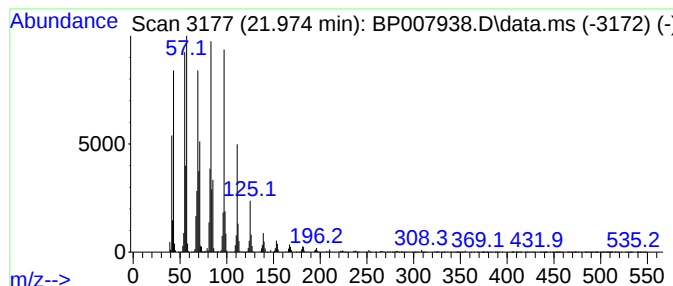
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.974	20.70 ng	2339500	Chrysene-d12	21.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			1-Heptacosanol	396	C27H56O	002004-39-9	95
3			1-Hexacosene	364	C26H52	018835-33-1	95
4			9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
Data File : BP007938.D
Acq On : 11 Nov 2021 01:36
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Misc :
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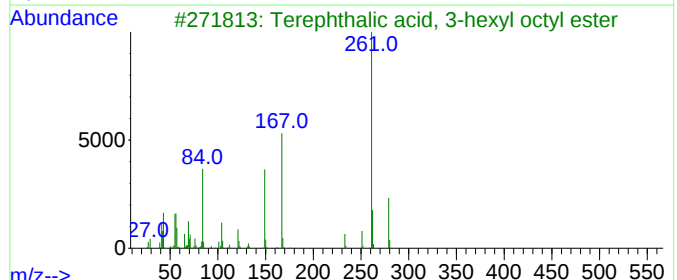
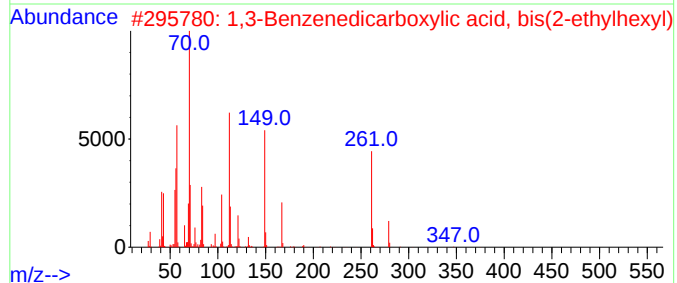
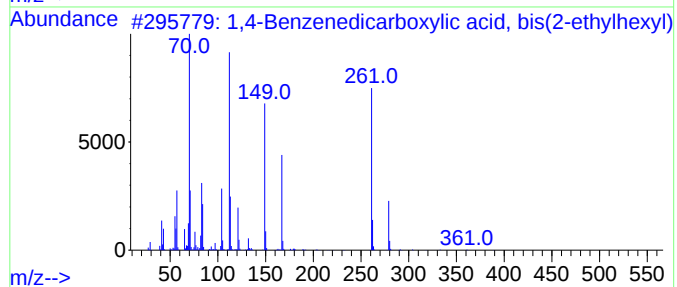
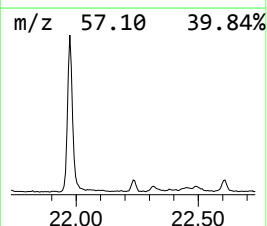
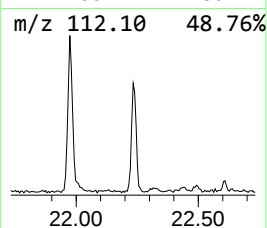
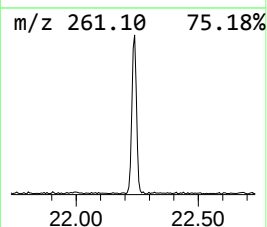
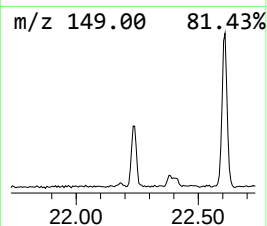
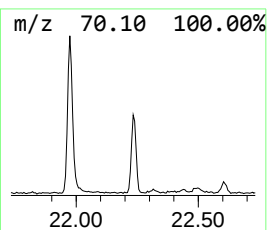
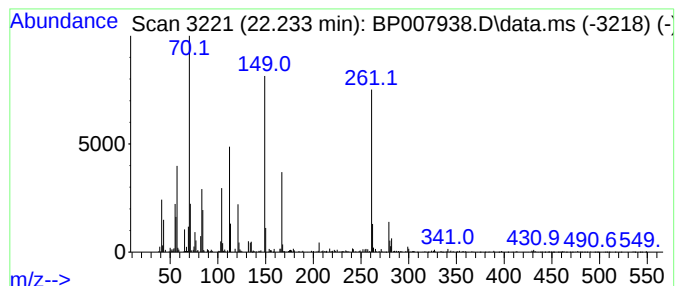
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.233	2.27 ng	256413	Chrysene-d12	21.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	83
2			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	53
3			Terephthalic acid, 3-hexyl octyl...	362	C22H34O4	1000356-23-1	38
4			Cyclohexanamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	18
5			Diethyl Phthalate	222	C12H14O4	000084-66-2	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
Data File : BP007938.D
Acq On : 11 Nov 2021 01:36
Operator : CG/JU
Sample : M4577-04
Misc :
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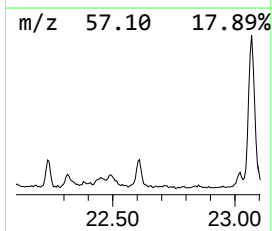
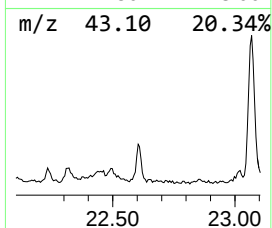
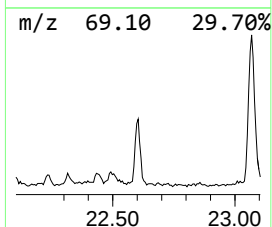
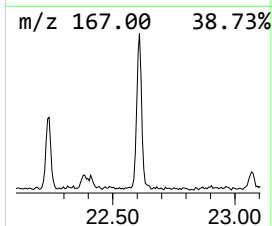
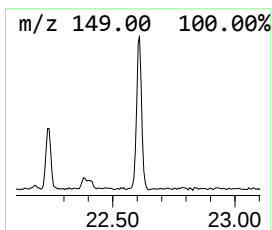
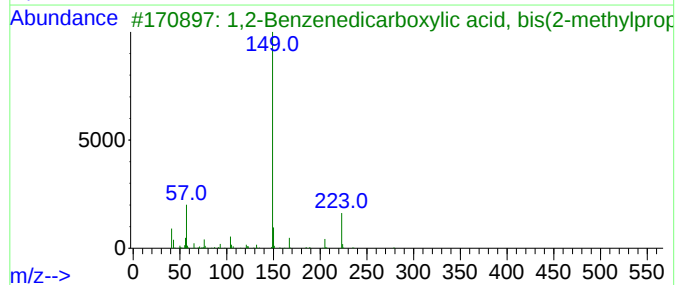
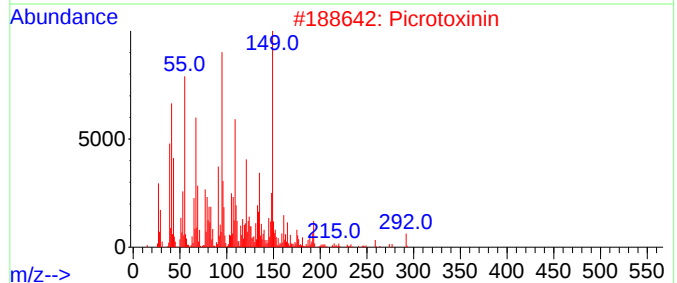
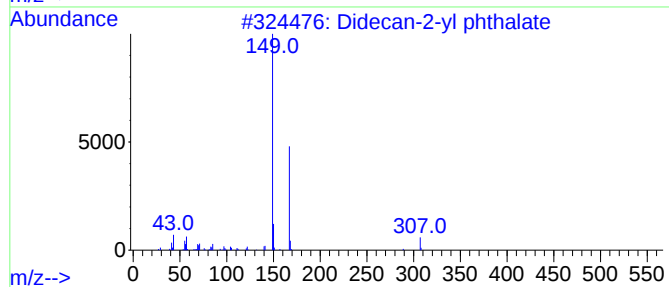
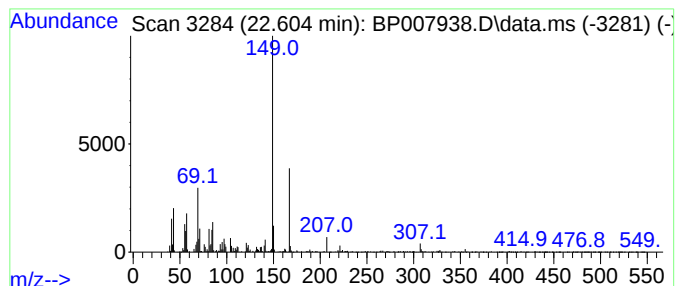
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Didecan-2-yl phthalate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.604	2.73 ng	325258	Perylene-d12	23.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Didecan-2-yl phthalate	446	C28H46O4	028029-89-2	80
2			Picrotoxinin	292	C15H16O6	017617-45-7	55
3			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	55
4			1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	007299-89-0	53
5			1,2-Benzenedicarboxylic acid, mo...	292	C17H24O4	024539-59-1	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
Data File : BP007938.D
Acq On : 11 Nov 2021 01:36
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Sample : M4577-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

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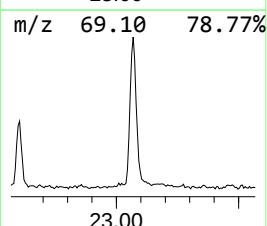
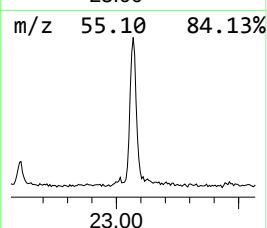
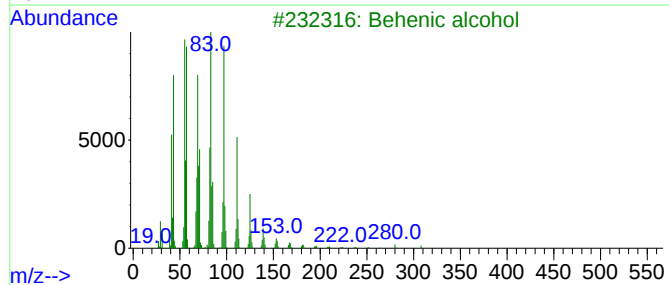
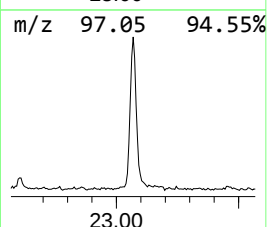
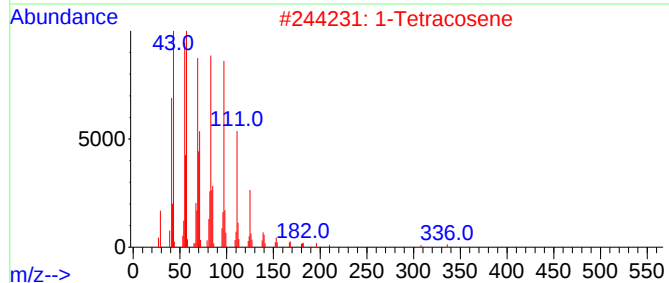
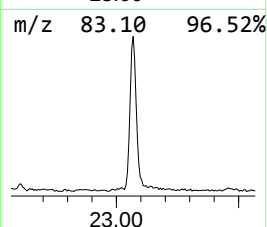
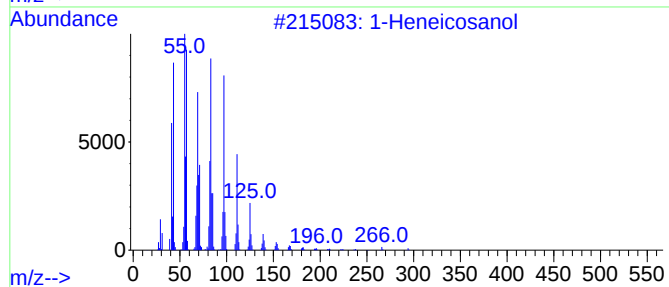
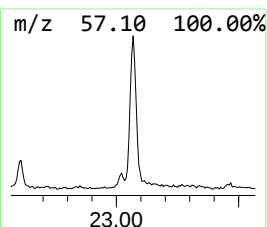
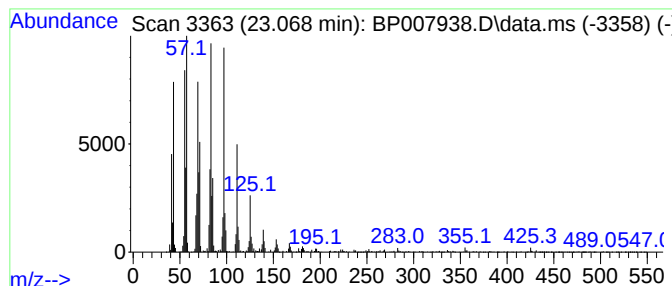
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.068	9.21 ng	1098820	Perylene-d12	23.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol			312	C21H44O	015594-90-8	95
2	1-Tetracosene			336	C24H48	010192-32-2	94
3	Behenic alcohol			326	C22H46O	000661-19-8	94
4	Nonacos-1-ene			406	C29H58	018835-35-3	94
5	n-Tetracosanol-1			354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
Data File : BP007938.D
Acq On : 11 Nov 2021 01:36
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Sample : M4577-04
Misc :
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Instrument :
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ClientSampleId :
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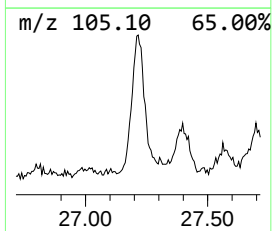
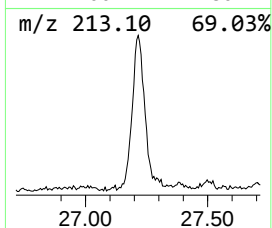
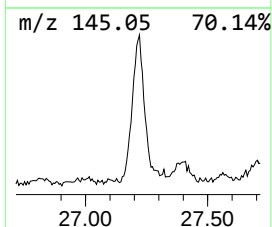
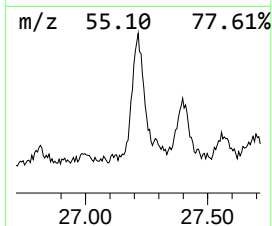
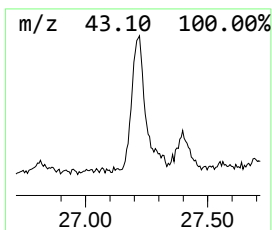
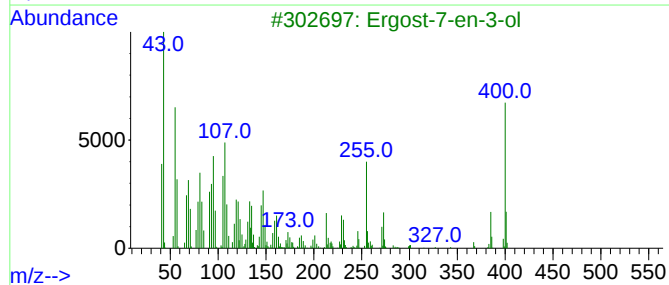
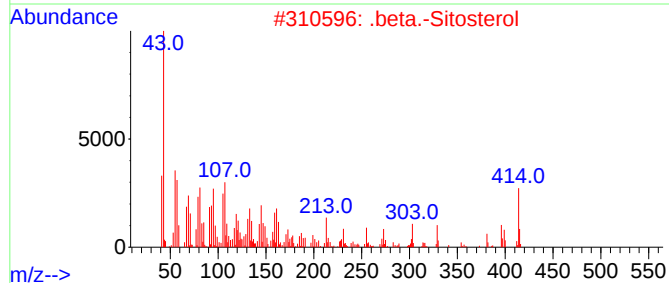
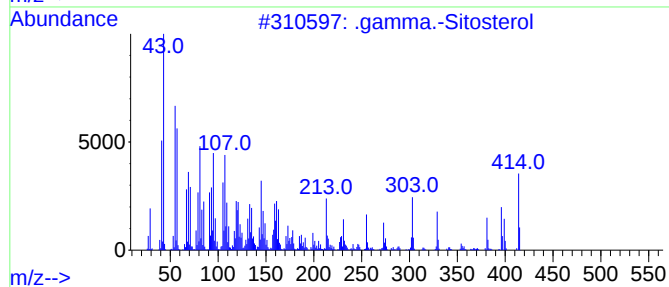
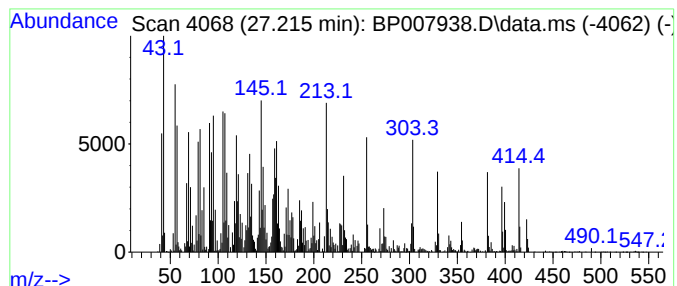
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.215	13.26 ng	1582110	Perylene-d12	23.745

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitosterol	414	C29H50O	000083-47-6	98
2			.beta.-Sitosterol	414	C29H50O	000083-46-5	87
3			Ergost-7-en-3-ol	400	C28H48O	116179-22-7	40
4			Stigmast-7-en-3-ol, (3.beta.,5.a...	414	C29H50O	000521-03-9	30
5			17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
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Sample : M4577-04
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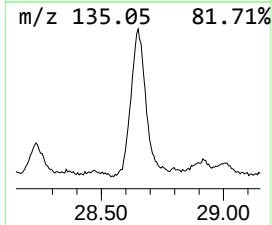
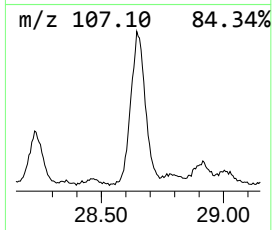
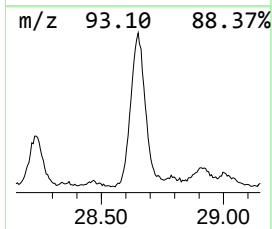
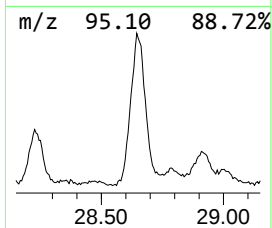
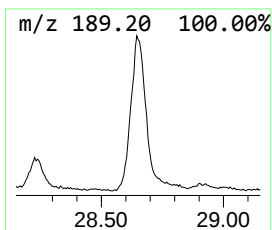
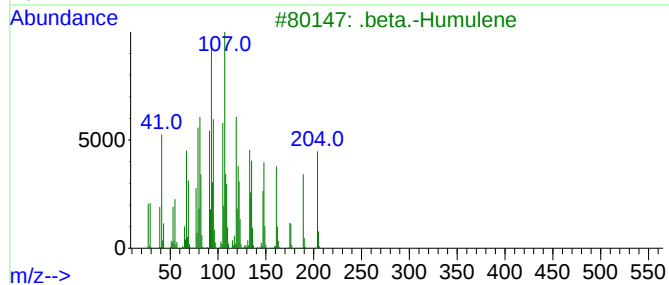
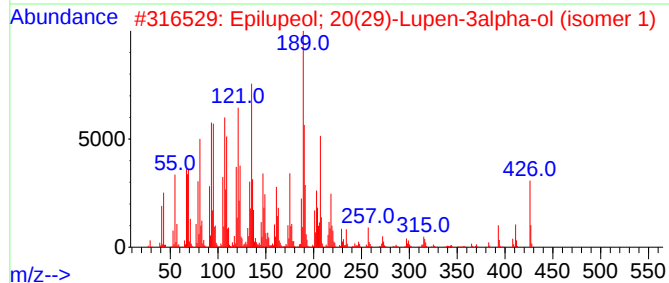
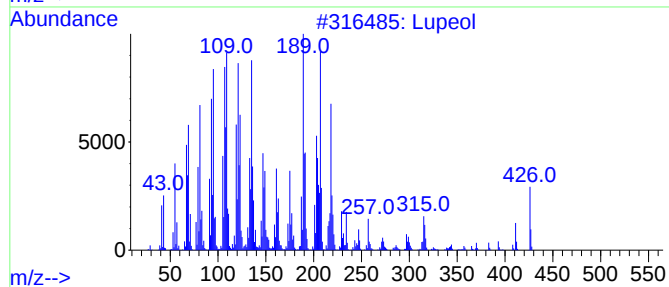
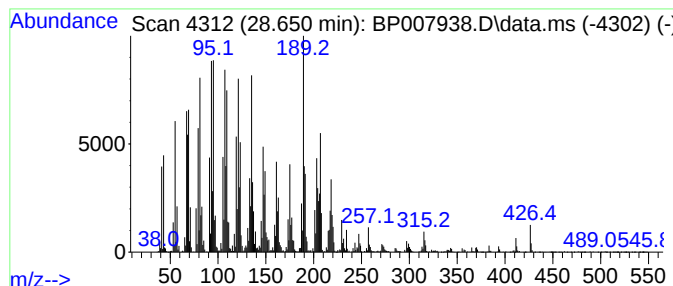
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Lupeol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.650	45.00 ng	5371240	Perylene-d12	23.745	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lupeol	426	C30H50O	000545-47-1	99
2	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-3	95
3	.beta.-Humulene	204	C15H24	000116-04-1	91
4	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	62
5	Epilupeol; 20(29)-Lupen-3alpha-o...	468	C32H52O2	1010513-01-8	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111021\
 Data File : BP007938.D
 Acq On : 11 Nov 2021 01:36
 Operator : CG/JU
 Sample : M4577-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
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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\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Copaene	13.263	2.2	ng	139350	3	14.492	1271980	20.0
n-Hexadecanoic ...	18.139	4.5	ng	368089	4	17.245	1625350	20.0
9-Octadecenoic ...	19.263	2.6	ng	214506	4	17.245	1625350	20.0
n-Nonadecanol-1	21.051	9.7	ng	1098170	5	21.333	2260260	20.0
Behenic alcohol	21.974	20.7	ng	2339500	5	21.333	2260260	20.0
1,4-Benzenedica...	22.233	2.3	ng	256413	5	21.333	2260260	20.0
Didecan-2-yl ph...	22.604	2.7	ng	325258	6	23.745	2387030	20.0
1-Heneicosanol	23.068	9.2	ng	1098820	6	23.745	2387030	20.0
.gamma.-Sitosterol	27.215	13.3	ng	1582110	6	23.745	2387030	20.0
Lupeol	28.650	45.0	ng	5371240	6	23.745	2387030	20.0