

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
 Data File : BG051170.D
 Acq On : 22 Nov 2021 14:47
 Operator : CG/JU
 Sample : M4781-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ETGI-354

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_G\Methods\8270-BG111921.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051170.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.262	297	302	313	rBV	38667	60390	3.34%	0.641%
2	5.744	377	384	394	rBV	460990	748395	41.33%	7.944%
3	7.360	651	659	674	rBV	460227	811176	44.80%	8.610%
4	8.206	795	803	814	rVB	88060	155488	8.59%	1.650%
5	9.381	995	1003	1017	rBV	280709	512289	28.29%	5.438%
6	10.780	1235	1241	1261	rVB2	21411	42394	2.34%	0.450%
7	11.032	1277	1284	1292	rBV	126826	232029	12.81%	2.463%
8	13.459	1686	1697	1704	rBV	674817	1079328	59.61%	11.457%
9	14.834	1923	1931	1939	rBV	213223	348010	19.22%	3.694%
10	16.326	2179	2185	2201	rBV	609064	948749	52.40%	10.071%
11	17.589	2393	2400	2406	rBV	308929	496269	27.41%	5.268%
12	20.174	2834	2840	2846	rBV	1363215	1810699	100.00%	19.220%
13	21.473	3056	3061	3073	rBV2	52084	103111	5.69%	1.095%
14	21.884	3125	3131	3140	rBV2	290837	518138	28.62%	5.500%
15	22.671	3260	3265	3269	rBV	38510	67372	3.72%	0.715%
16	23.600	3417	3423	3431	rVB2	27965	56831	3.14%	0.603%
17	23.770	3447	3452	3459	rVB2	36011	73691	4.07%	0.782%
18	24.240	3526	3532	3540	rVB2	49773	108903	6.01%	1.156%
19	24.323	3541	3546	3554	rBV6	22571	60911	3.36%	0.647%
20	25.292	3700	3711	3721	rVB2	168835	499729	27.60%	5.305%
21	25.803	3790	3798	3808	rVB2	61343	170533	9.42%	1.810%
22	26.438	3898	3906	3916	rVB2	47799	138642	7.66%	1.472%
23	26.602	3923	3934	3947	rBV7	27480	129418	7.15%	1.374%
24	28.717	4285	4294	4308	rVB5	45084	177498	9.80%	1.884%
25	30.151	4530	4538	4553	rVB5	15983	70802	3.91%	0.752%

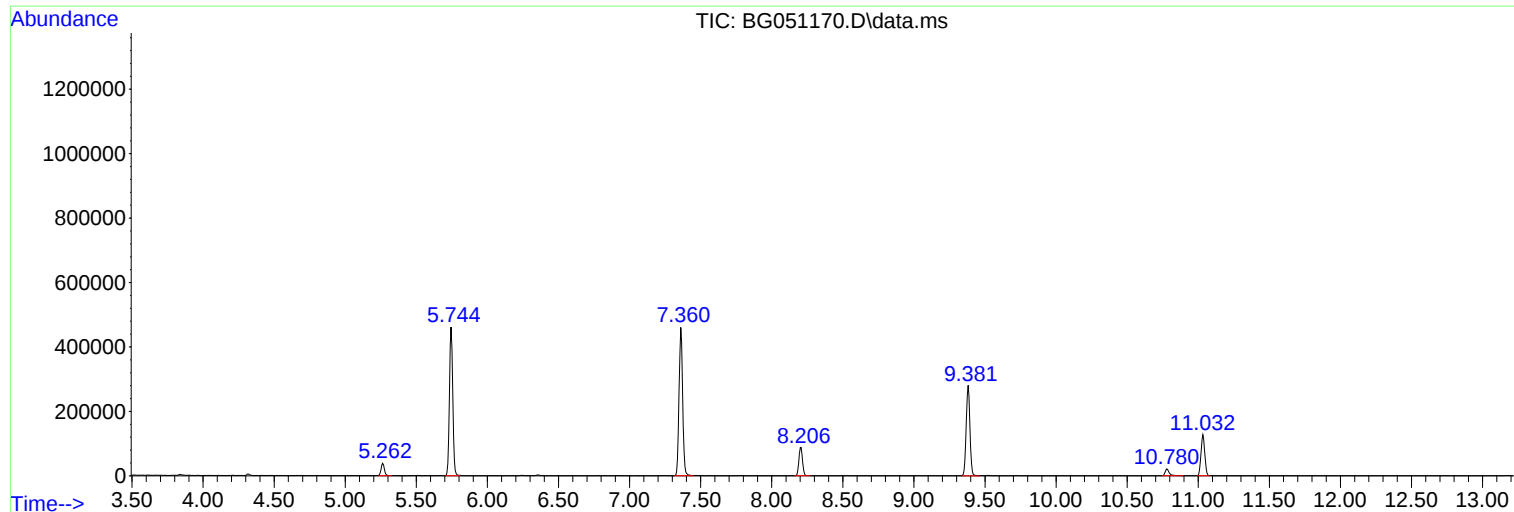
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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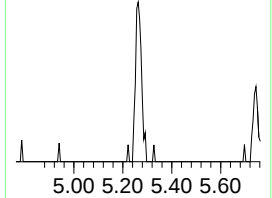
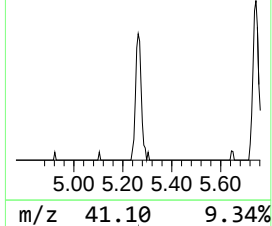
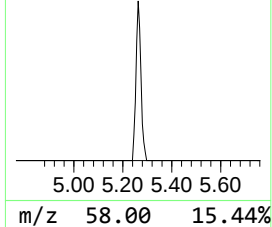
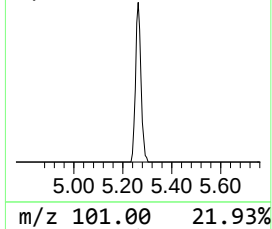
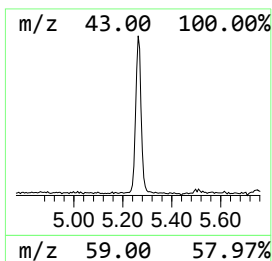
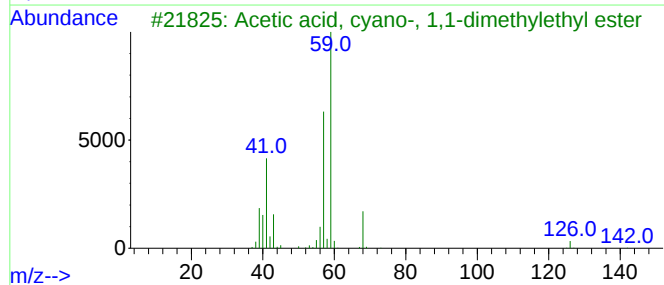
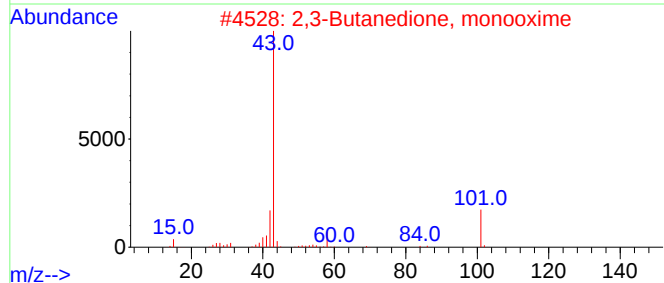
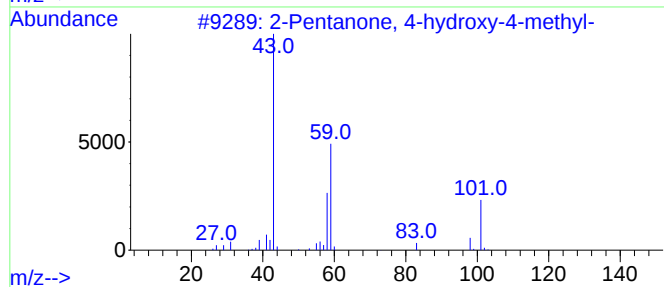
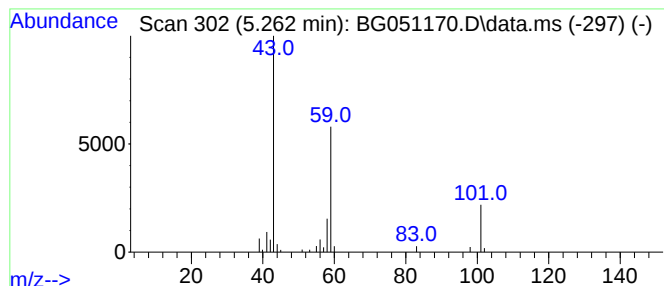
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.262	7.77 ng	60390	1,4-Dichlorobenzene-d4	8.206

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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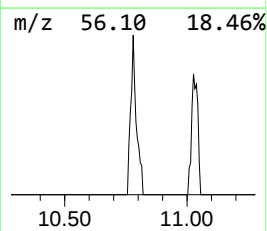
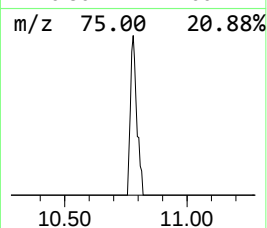
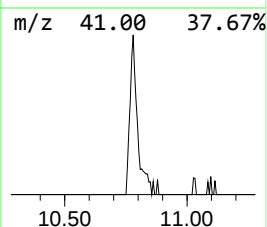
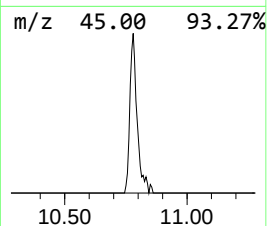
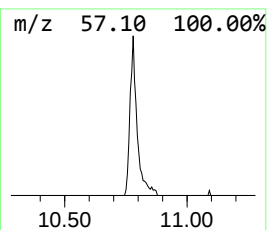
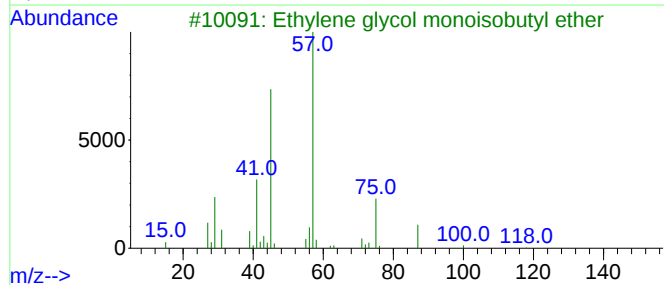
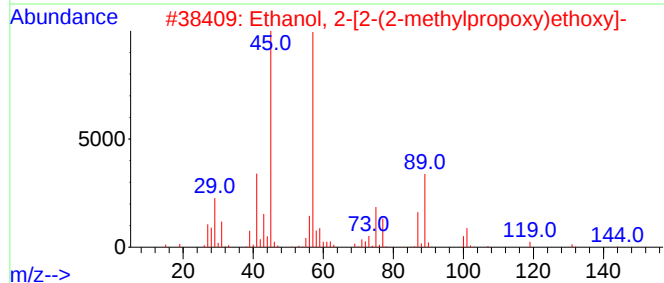
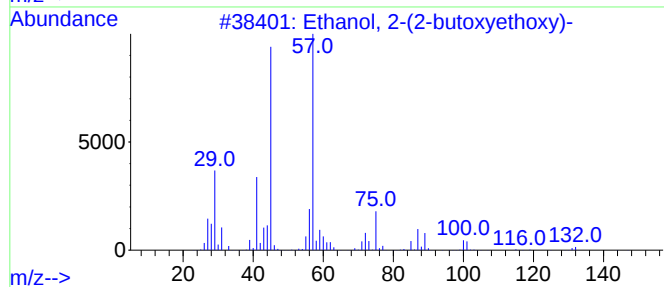
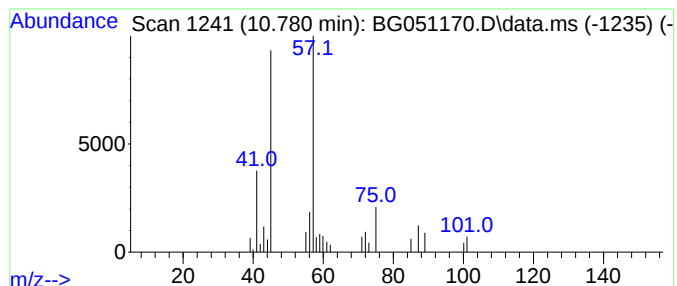
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.780	3.65 ng	42394	Naphthalene-d8	11.032

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	56
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50



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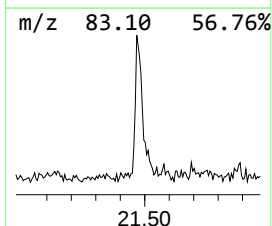
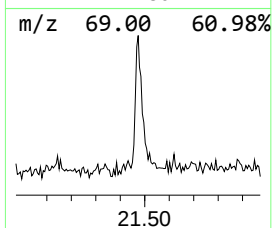
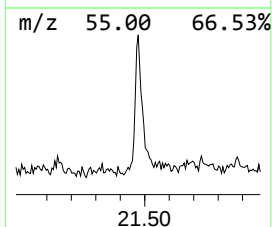
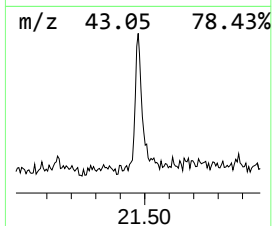
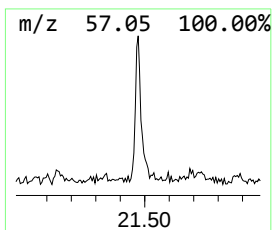
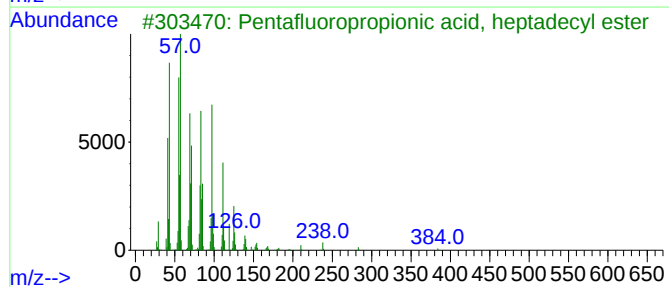
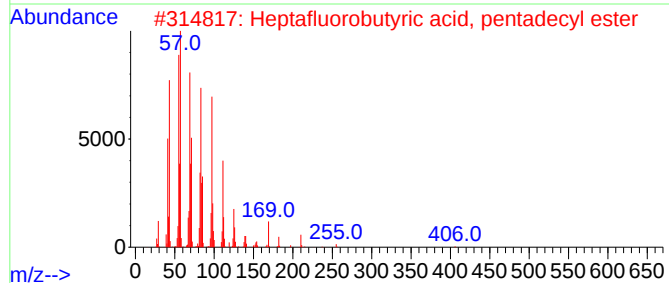
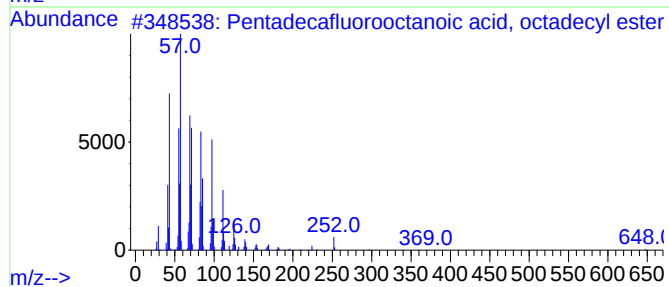
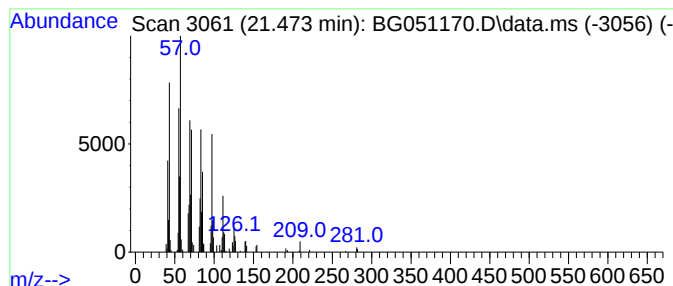
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Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.473	3.98 ng	103111	Chrysene-d12	21.884

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
3			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90



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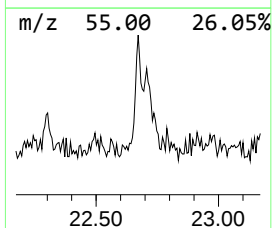
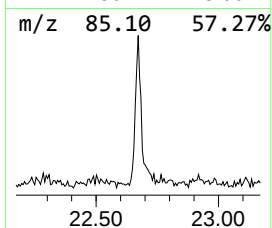
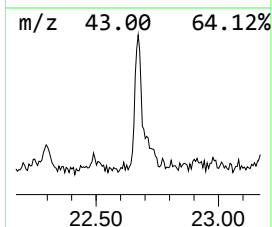
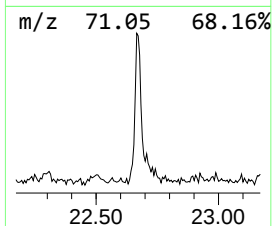
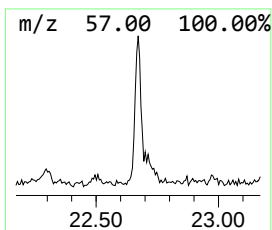
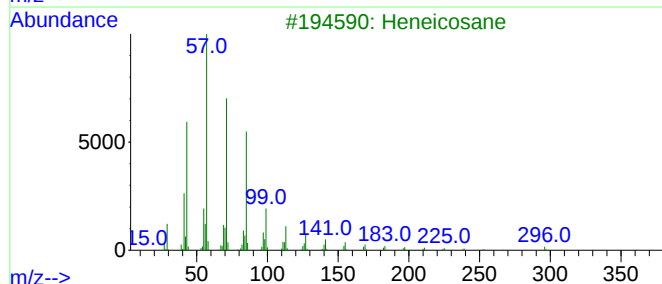
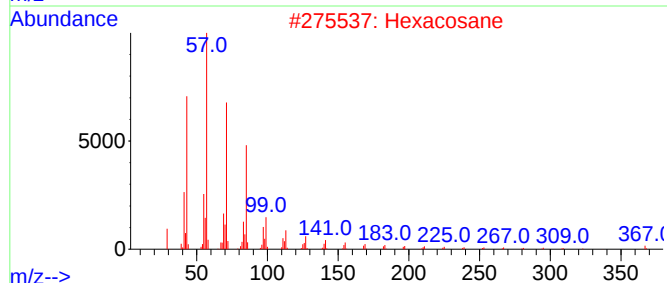
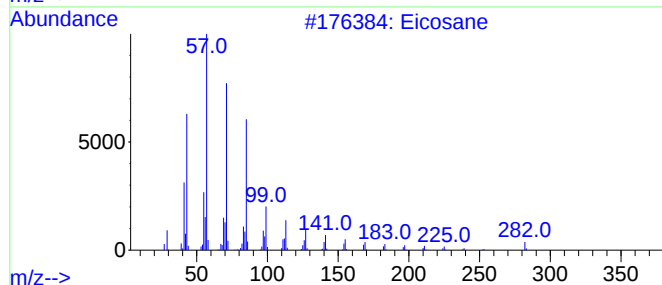
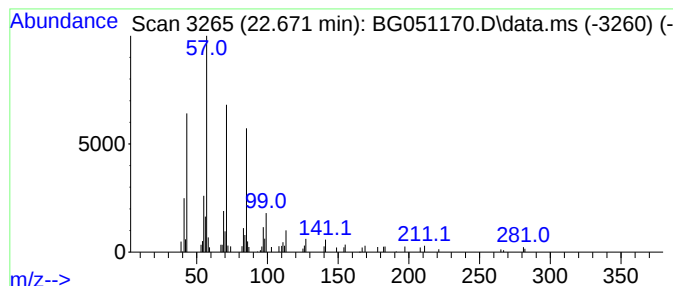
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Peak Number 4 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.672	2.60 ng	67372	Chrysene-d12	21.884

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Hexacosane	366	C26H54	000630-01-3	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Octacosane	394	C28H58	000630-02-4	87
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



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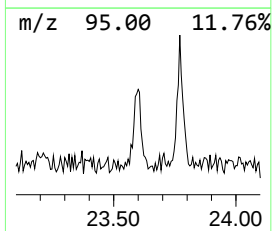
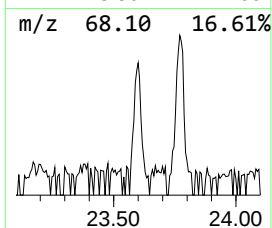
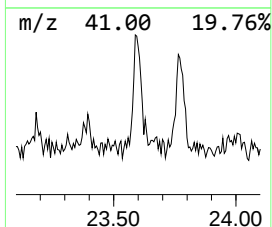
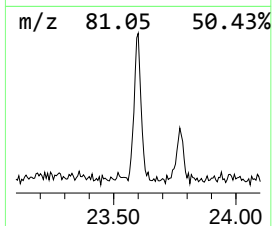
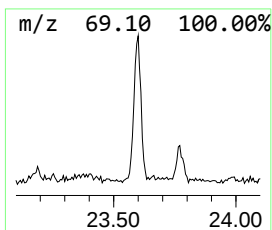
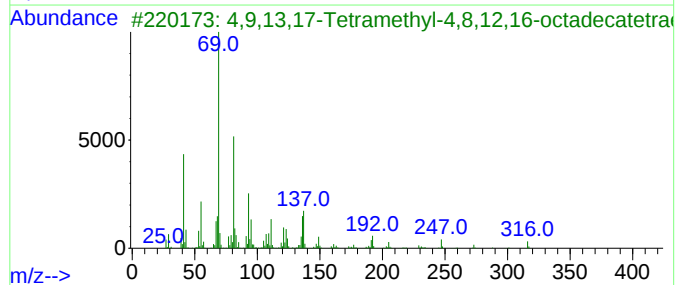
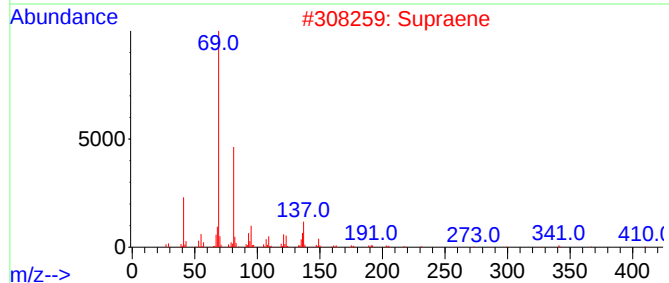
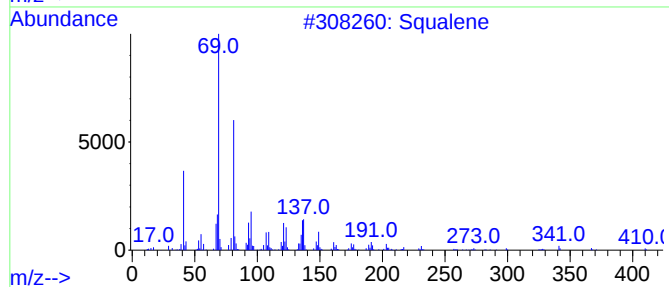
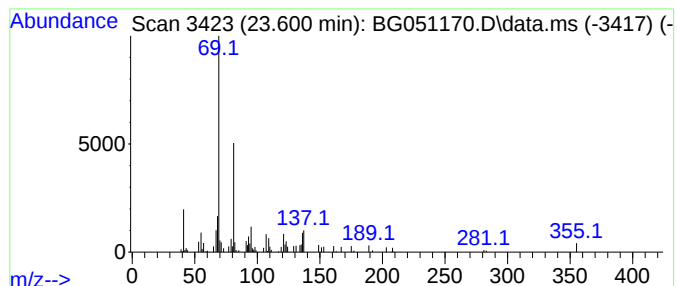
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Peak Number 5 Squalene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.600	2.27 ng	56831	Perylene-d12	25.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Supraene	410	C30H50	007683-64-9	87
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5			trans-Farnesol	222	C15H26O	000106-28-5	72



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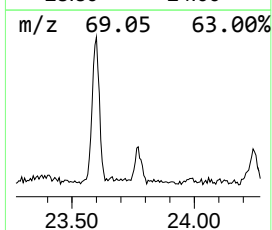
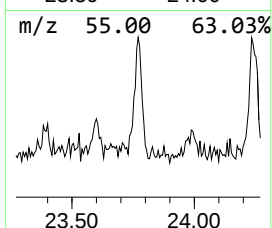
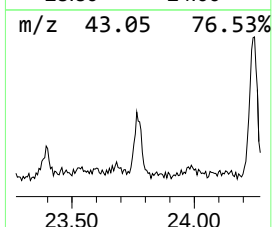
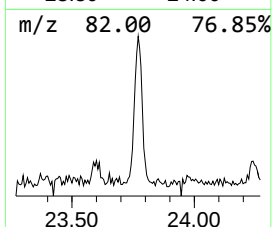
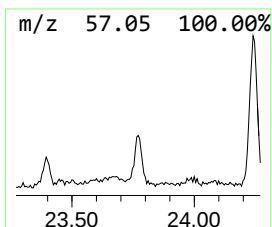
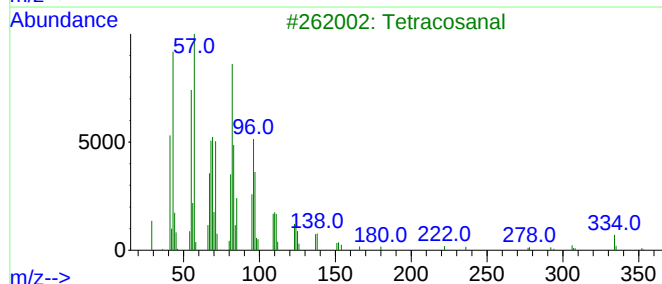
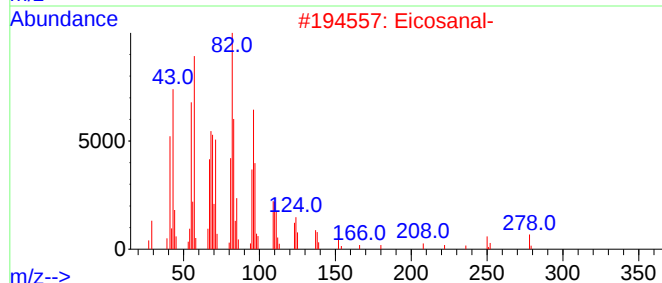
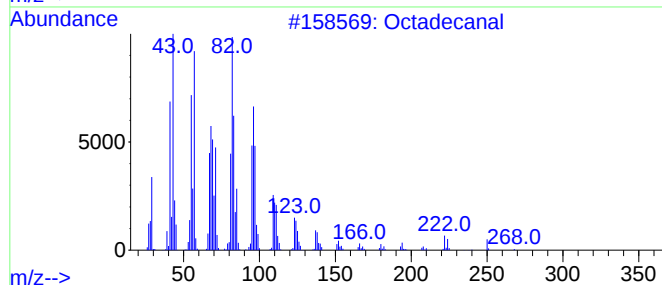
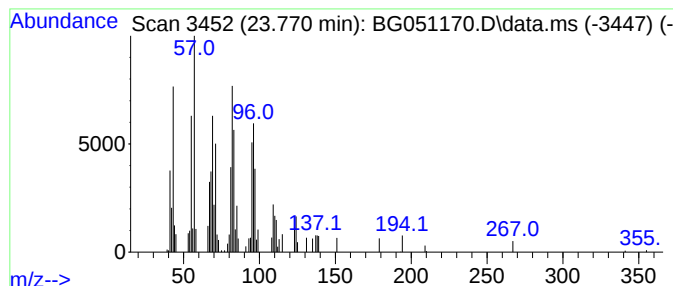
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosanal- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.770	2.95 ng	73691	Perylene-d12	25.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	87
2			Eicosanal-	296	C20H40O	002400-66-0	87
3			Tetracosanal	352	C24H48O	057866-08-7	87
4			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
5			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051170.D
Acq On : 22 Nov 2021 14:47
Operator : CG/JU
Sample : M4781-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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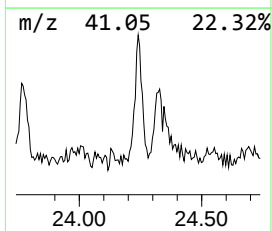
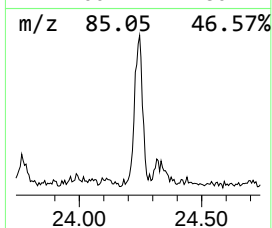
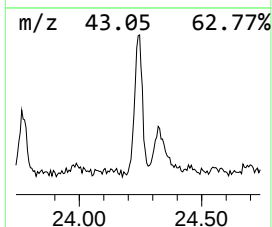
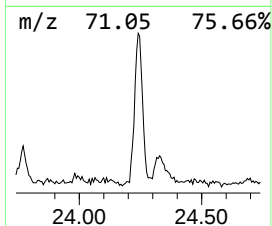
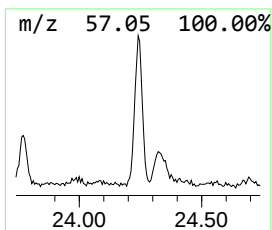
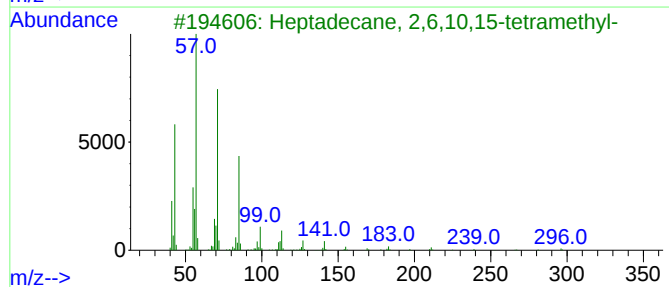
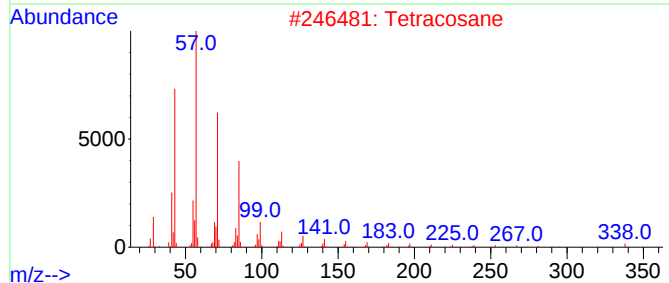
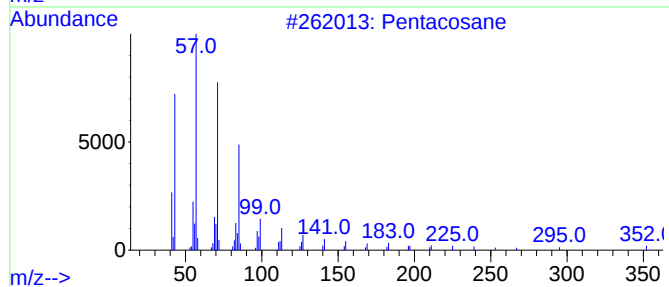
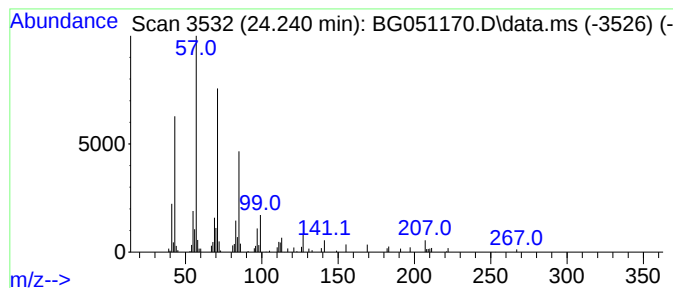
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.240	4.36 ng	108903	Perylene-d12	25.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	87
2			Tetracosane	338	C24H50	000646-31-1	87
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
4			Heptacosane	380	C27H56	000593-49-7	74
5			Octacosane	394	C28H58	000630-02-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051170.D
Acq On : 22 Nov 2021 14:47
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Sample : M4781-01
Misc :
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Instrument :
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ClientSampleId :
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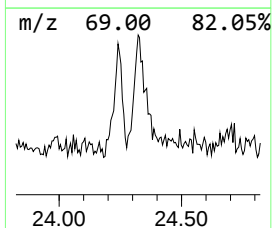
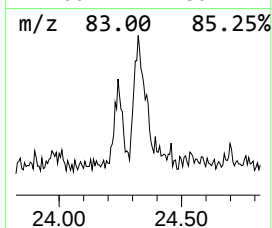
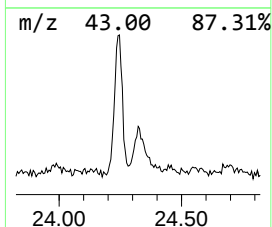
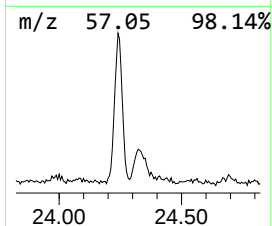
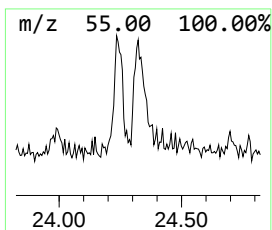
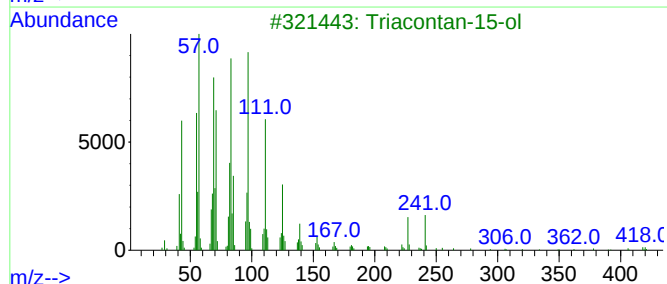
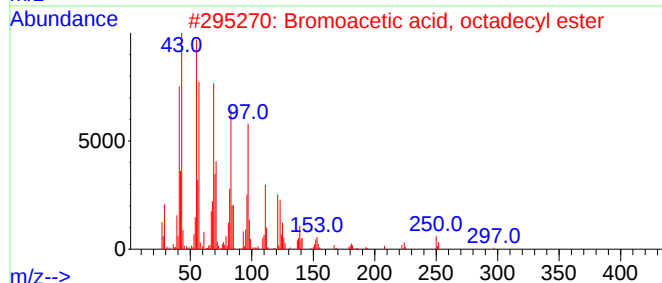
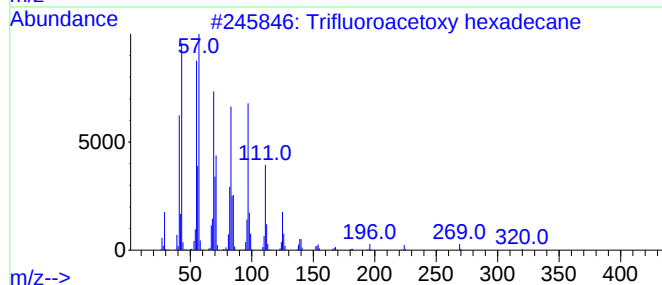
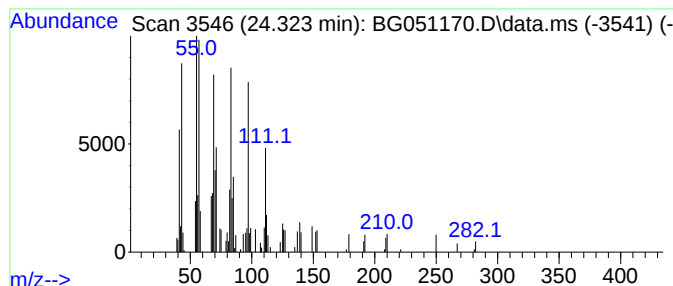
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.323	2.44 ng	60911	Perylene-d12	25.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	87
3			Triacontan-15-ol	438	C30H62O	031849-26-0	86
4			Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	83
5			Fumaric acid, hexadecyl 2-methyl...	394	C24H42O4	1000330-55-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051170.D
Acq On : 22 Nov 2021 14:47
Operator : CG/JU
Sample : M4781-01
Misc :
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Instrument :
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ClientSampleId :
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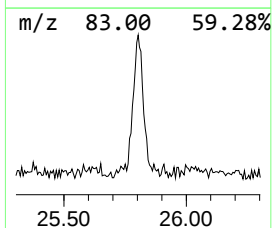
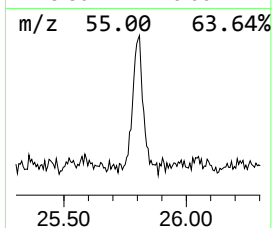
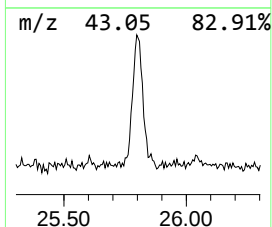
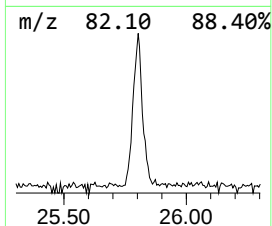
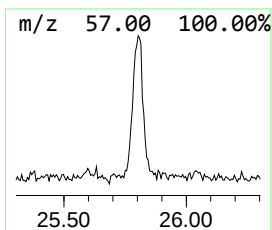
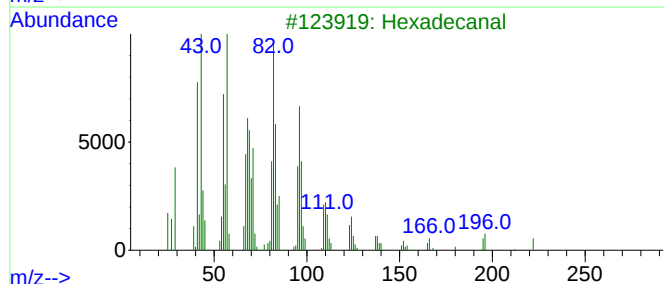
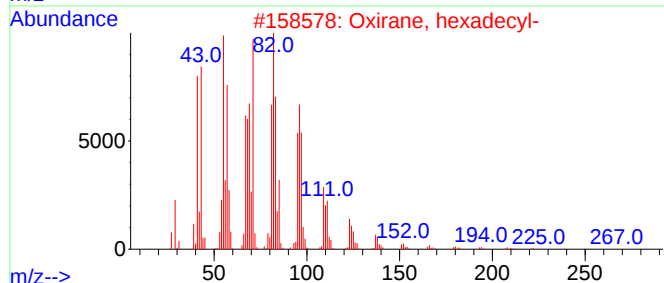
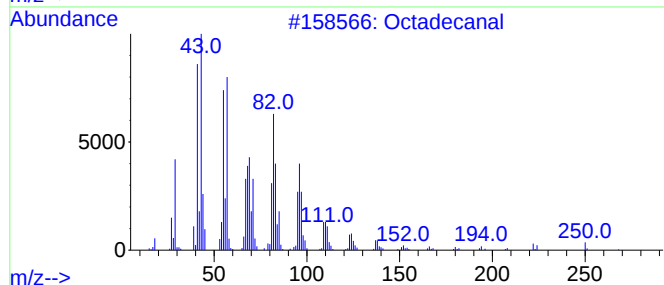
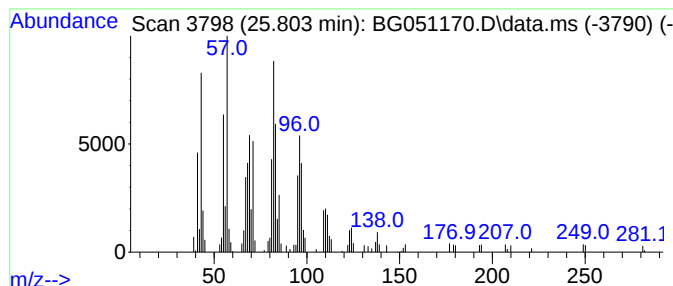
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.803	6.83 ng	170533	Perylene-d12	25.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	91
2			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3			Hexadecanal	240	C16H32O	000629-80-1	90
4			Eicosanal	296	C20H40O	002400-66-0	87
5			Tetradecanal	212	C14H28O	000124-25-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051170.D
Acq On : 22 Nov 2021 14:47
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Sample : M4781-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

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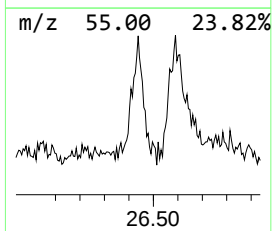
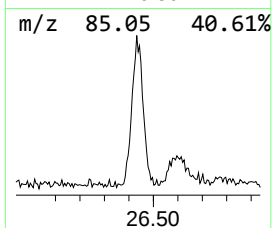
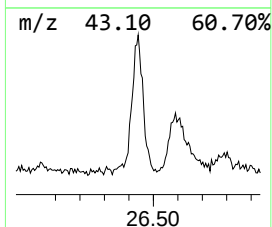
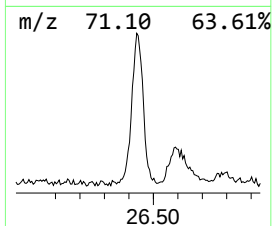
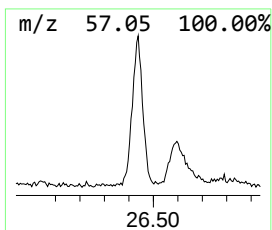
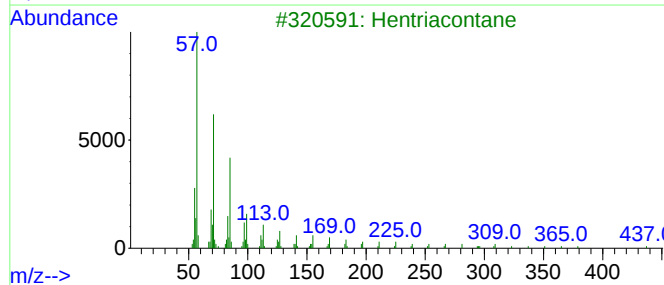
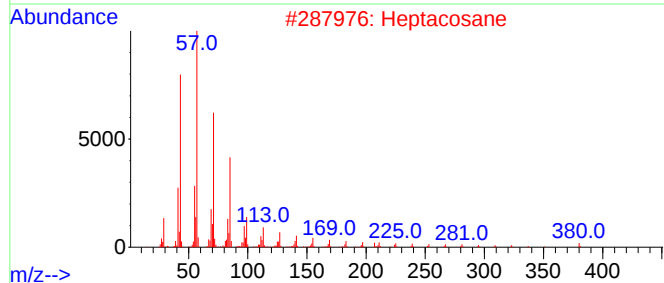
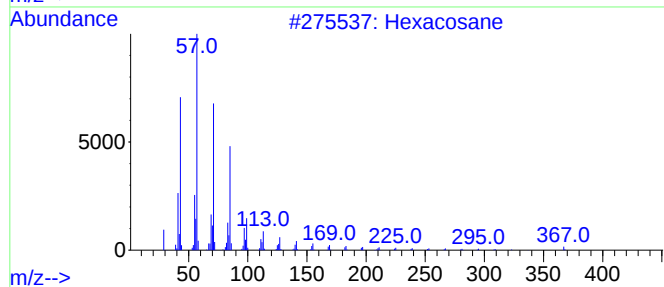
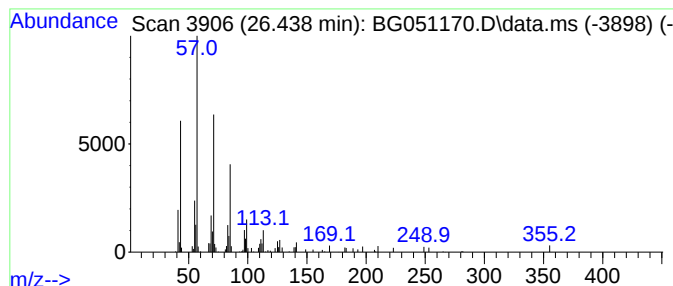
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.438	5.55 ng	138642	Perylene-d12	25.292

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexacosane	366	C26H54	000630-01-3	91
2		Heptacosane	380	C27H56	000593-49-7	91
3		Hentriacontane	437	C31H64	000630-04-6	91
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
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Operator : CG/JU
Sample : M4781-01
Misc :
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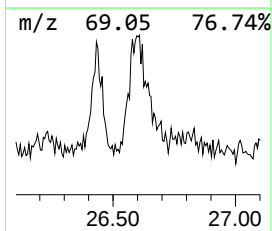
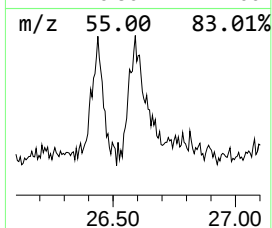
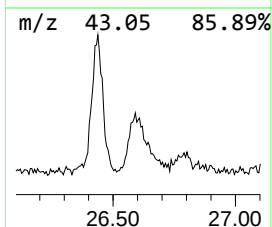
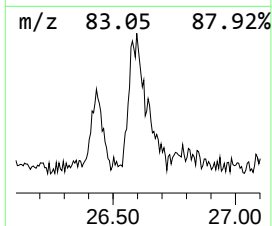
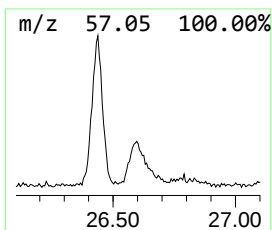
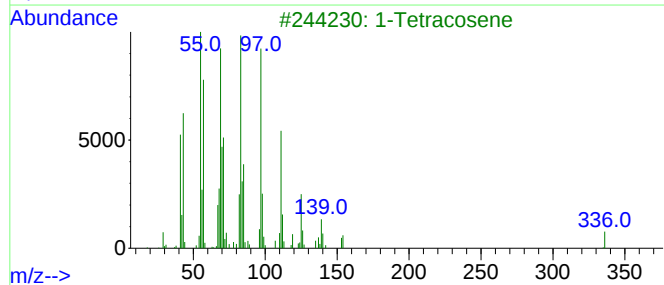
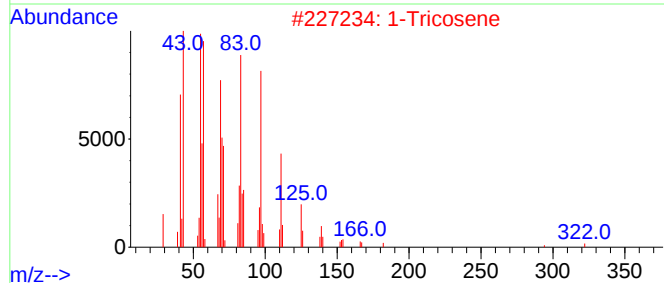
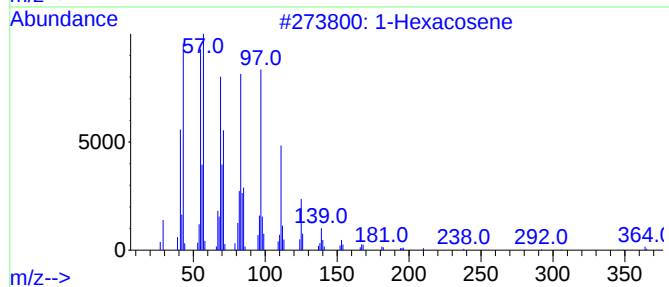
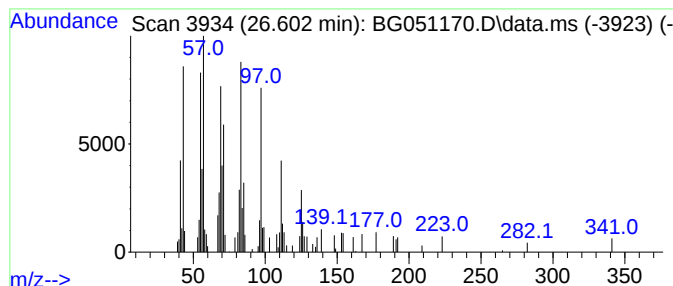
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Hexacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.602	5.18 ng	129418	Perylene-d12	25.292	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	91
2	1-Tricosene	322	C23H46	018835-32-0	90
3	1-Tetracosene	336	C24H48	010192-32-2	87
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	76
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
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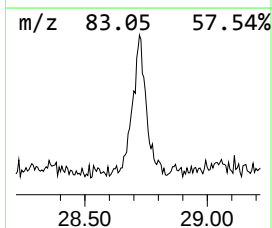
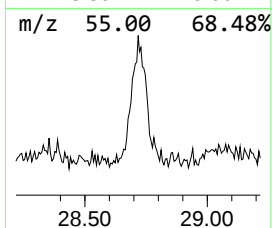
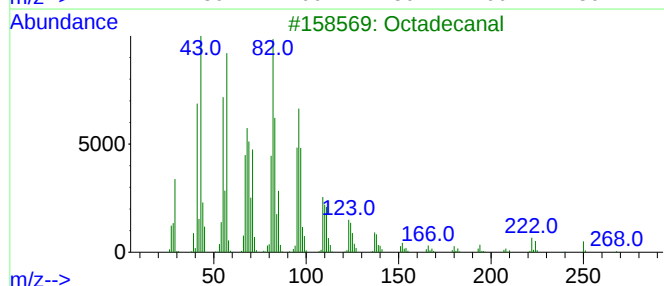
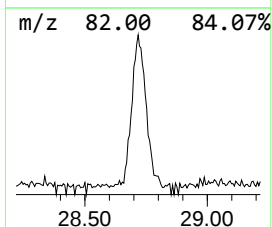
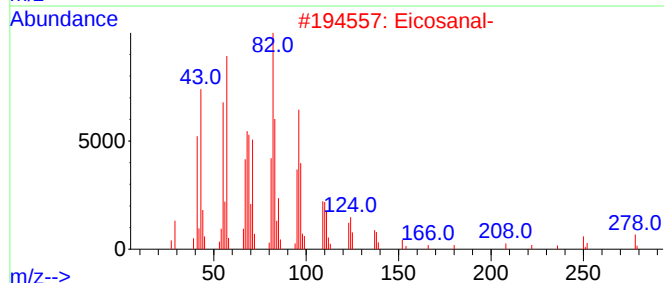
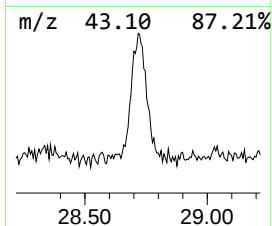
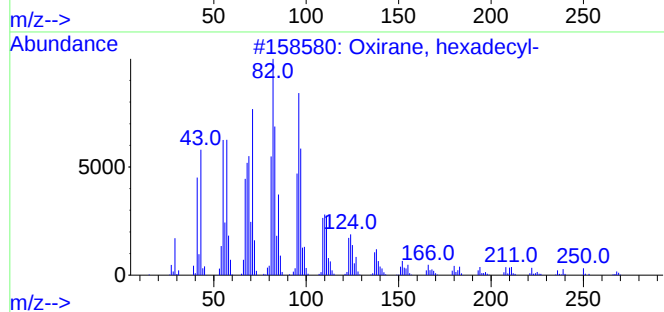
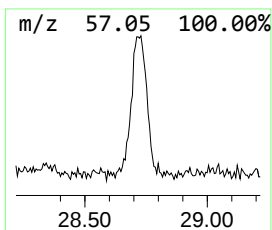
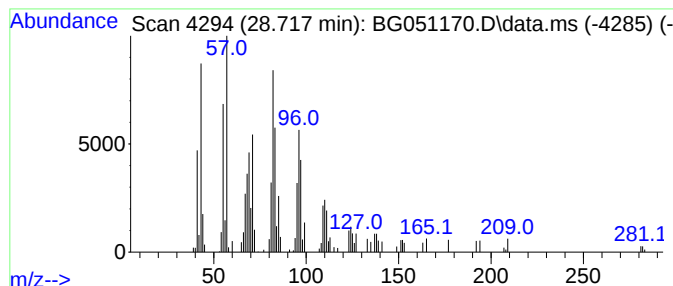
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Oxirane, hexadecyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
28.717	7.10 ng	177498	Perylene-d12		25.292	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-		268	C18H36O	007390-81-0	94
2	Eicosanal-		296	C20H40O	002400-66-0	74
3	Octadecanal		268	C18H36O	000638-66-4	72
4	Oxirane, heptadecyl-		282	C19H38O	067860-04-2	64
5	1,16-Hexadecanediol		258	C16H34O2	007735-42-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051170.D
Acq On : 22 Nov 2021 14:47
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Sample : M4781-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
ETGI-354

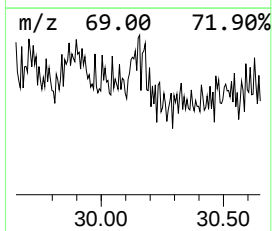
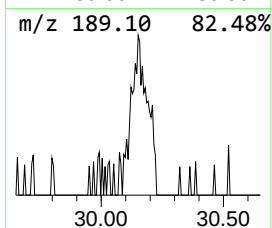
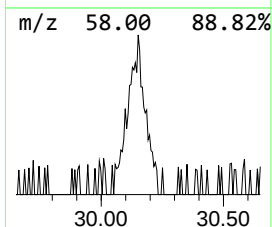
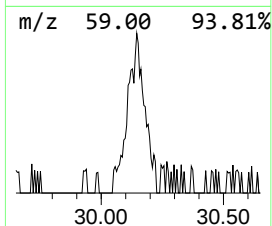
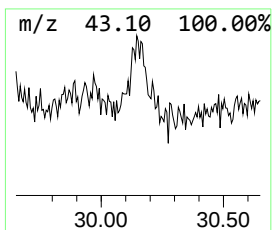
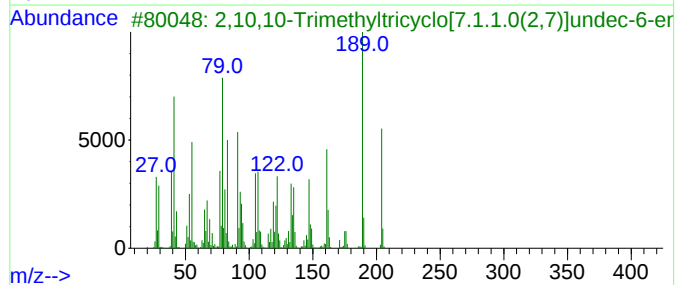
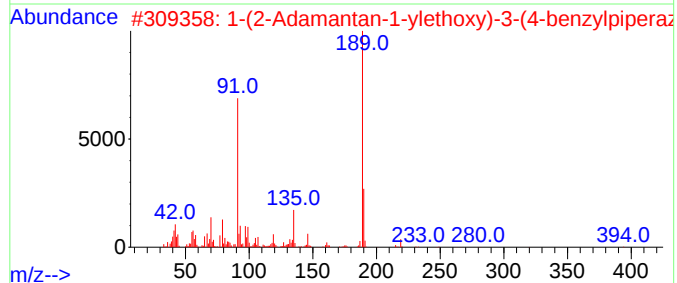
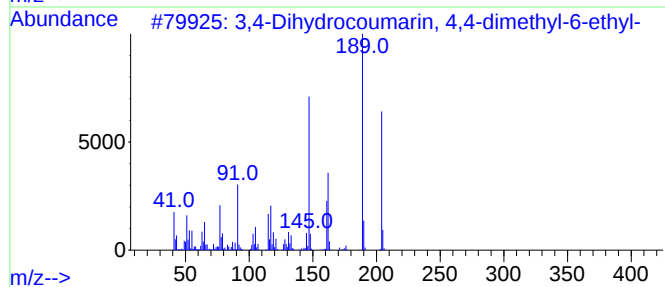
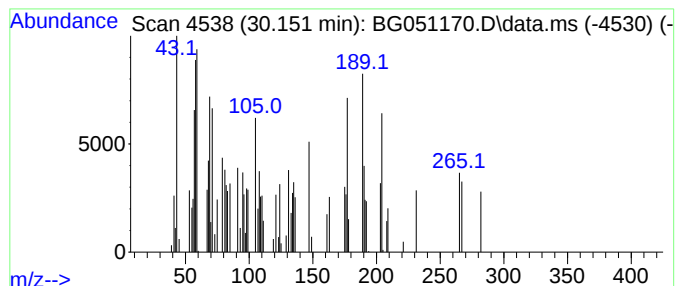
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown30.151 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.151	2.83 ng	70802	Perylene-d12	25.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dihydrocoumarin, 4,4-dimethy...	204	C13H16O2	029423-74-3	22		
2	1-(2-Adamantan-1-ylethoxy)-3-(4-...	412	C26H40N2O2	1000264-46-7	10		
3	2,10,10-Trimethyltricyclo[7.1.1...	204	C14H20O	1000210-81-9	10		
4	Spiro[5.5]undec-2-ene, 3,7,7-tri...	204	C15H24	018431-82-8	10		
5	3-Decanol	158	C10H22O	001565-81-7	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112221\
Data File : BG051170.D
Acq On : 22 Nov 2021 14:47
Operator : CG/JU
Sample : M4781-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ETGI-354

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.262	7.8	ng	60390	1	8.206	155488	20.0
Ethanol, 2-(2-b...	10.780	3.6	ng	42394	2	11.032	232029	20.0
Pentadecafluoro...	21.473	4.0	ng	103111	5	21.884	518138	20.0
Eicosane	22.672	2.6	ng	67372	5	21.884	518138	20.0
Squalene	23.600	2.3	ng	56831	6	25.292	499729	20.0
Eicosanal-	23.770	3.0	ng	73691	6	25.292	499729	20.0
Pentacosane	24.240	4.4	ng	108903	6	25.292	499729	20.0
Trifluoroacetox...	24.323	2.4	ng	60911	6	25.292	499729	20.0
Octadecanal	25.803	6.8	ng	170533	6	25.292	499729	20.0
Hexacosane	26.438	5.5	ng	138642	6	25.292	499729	20.0
1-Hexacosene	26.602	5.2	ng	129418	6	25.292	499729	20.0
Oxirane, hexade...	28.717	7.1	ng	177498	6	25.292	499729	20.0
unknown30.151	30.151	2.8	ng	70802	6	25.292	499729	20.0