

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
 Data File : BM020322.D
 Acq On : 13 May 2019 18:45
 Operator : JU/SJ
 Sample : K2769-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P026-SS017-0002-01

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.345	395	401	409	rBV	819958	1256768	33.77%	5.866%
2	6.928	664	670	691	rVB	796972	1285122	34.54%	5.998%
3	7.292	725	732	746	rBV	852262	1396091	37.52%	6.516%
4	7.757	805	811	817	rBV	162350	257386	6.92%	1.201%
5	8.075	858	865	874	rBV	633471	1010311	27.15%	4.715%
6	8.922	1003	1009	1025	rBV	445331	804095	21.61%	3.753%
7	10.551	1277	1286	1296	rBV	170220	302627	8.13%	1.412%
8	13.021	1699	1706	1724	rBV	924097	1429374	38.41%	6.671%
9	13.863	1844	1849	1858	rBV	111507	161728	4.35%	0.755%
10	14.404	1935	1941	1955	rBV2	273971	431605	11.60%	2.014%
11	15.898	2189	2195	2211	rBV	930722	1338282	35.96%	6.246%
12	17.156	2402	2409	2418	rBV	351429	588987	15.83%	2.749%
13	18.039	2553	2559	2570	rBV	78593	136445	3.67%	0.637%
14	19.780	2850	2855	2864	rBV	1608883	2029793	54.55%	9.474%
15	21.044	3065	3070	3079	rBV	416435	560632	15.07%	2.617%
16	21.344	3116	3121	3134	rBV	508670	717657	19.29%	3.350%
17	21.939	3215	3222	3232	rBV2	280447	534247	14.36%	2.494%
18	22.627	3336	3339	3344	rVB3	78775	106722	2.87%	0.498%
19	22.903	3381	3386	3390	rBV	308075	434669	11.68%	2.029%
20	22.956	3391	3395	3406	rVB2	188215	322219	8.66%	1.504%
21	23.633	3504	3510	3521	rVB	325209	633653	17.03%	2.957%
22	23.809	3536	3540	3546	rVB2	167998	280930	7.55%	1.311%
23	24.238	3609	3613	3623	rVB6	92439	188415	5.06%	0.879%
24	25.374	3801	3806	3816	rVB3	185290	423134	11.37%	1.975%
25	27.679	4190	4198	4213	rVB7	310690	1073297	28.84%	5.009%
26	28.068	4252	4264	4285	rVB2	993656	3721145	100.00%	17.368%

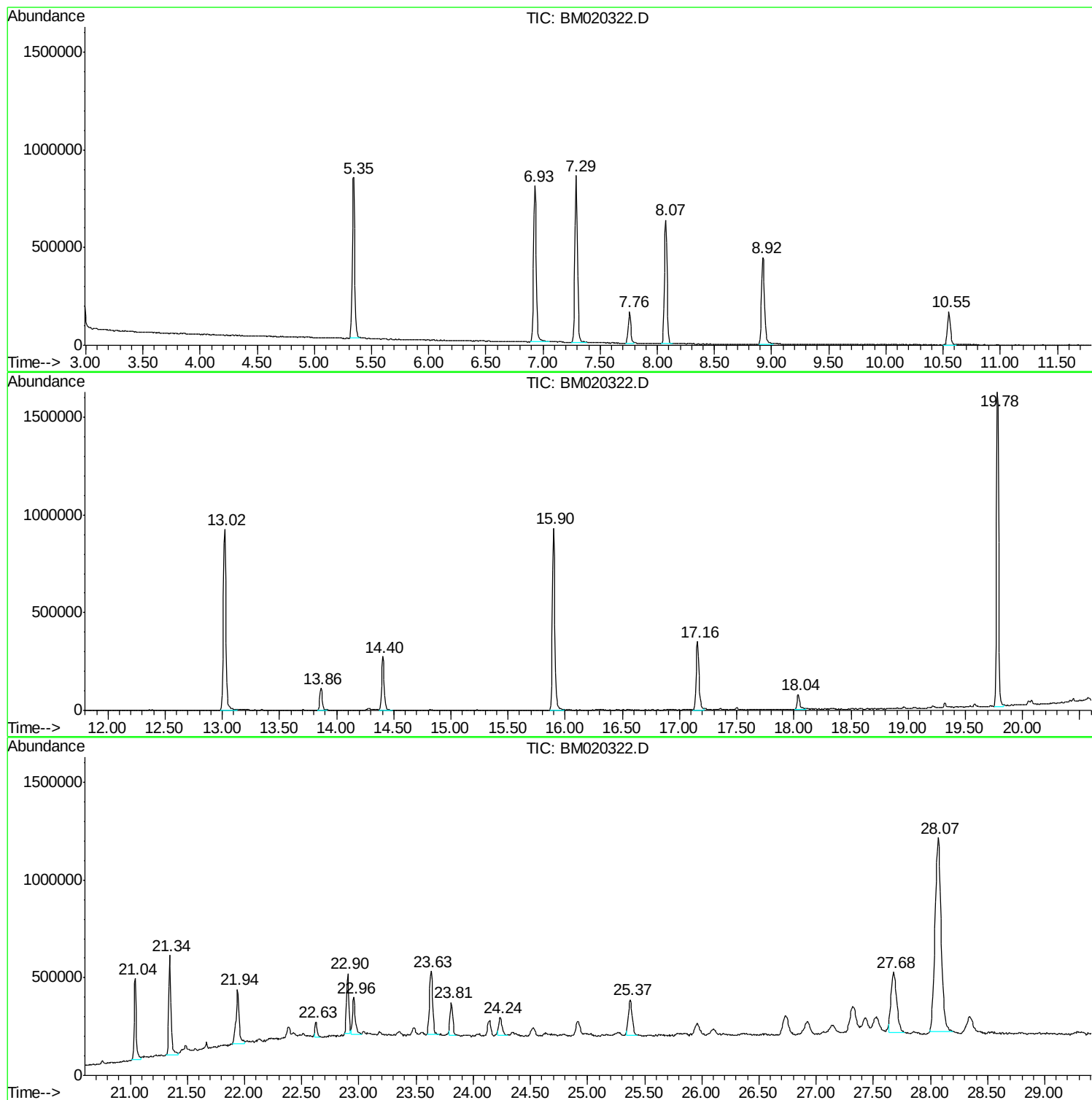
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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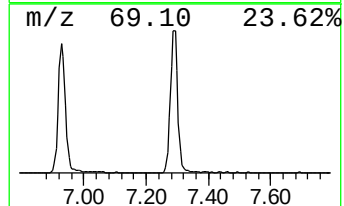
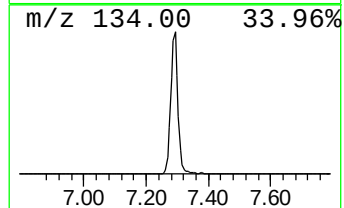
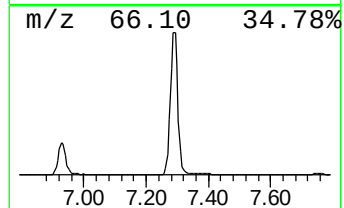
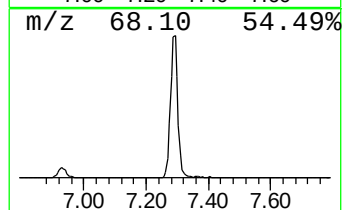
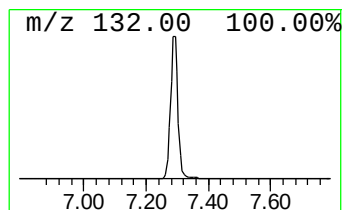
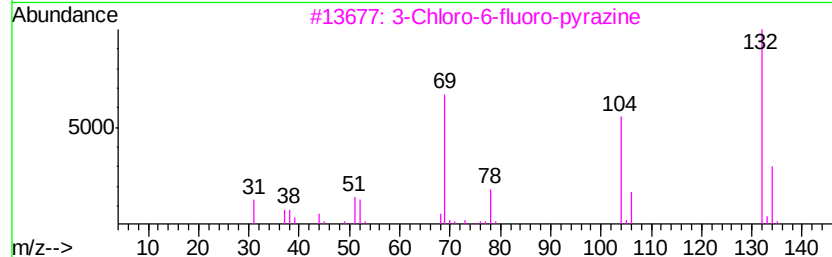
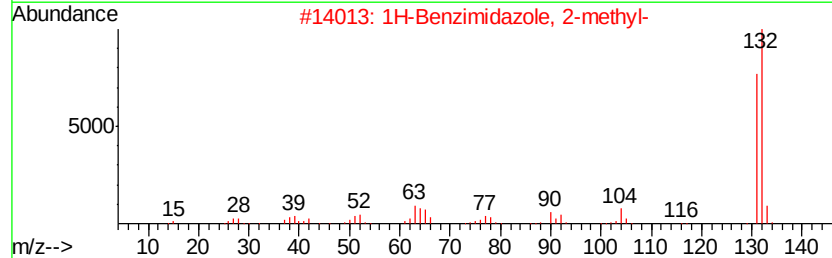
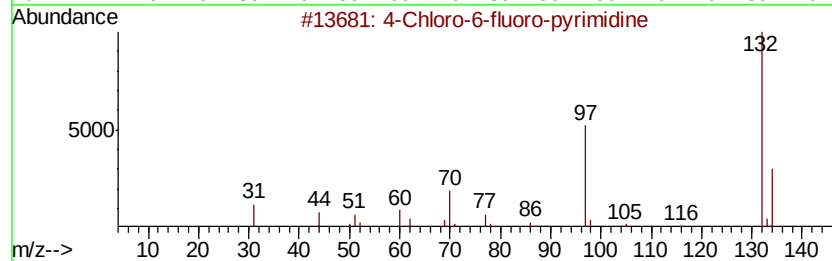
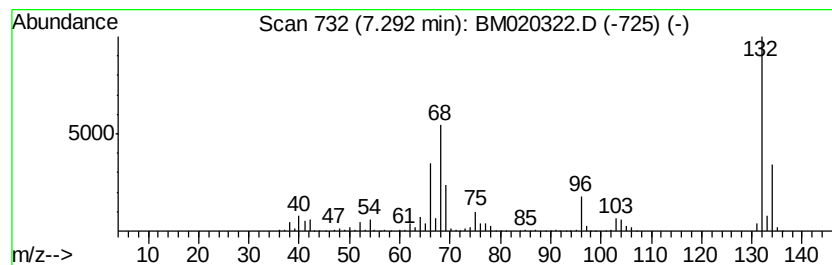
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.29 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	108.48 ng	1396090	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12



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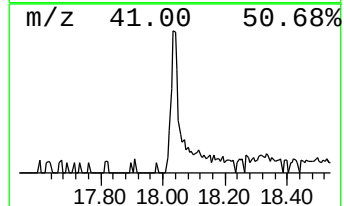
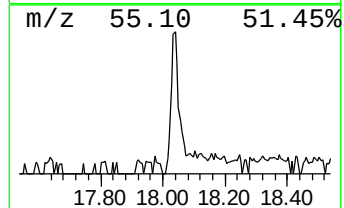
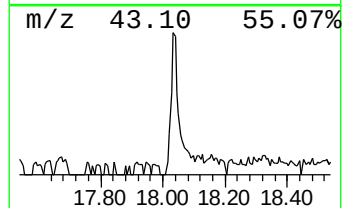
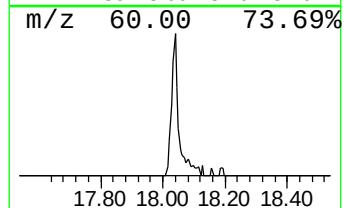
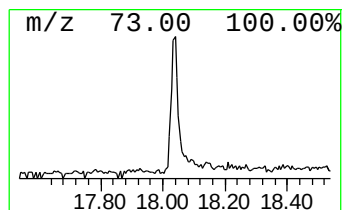
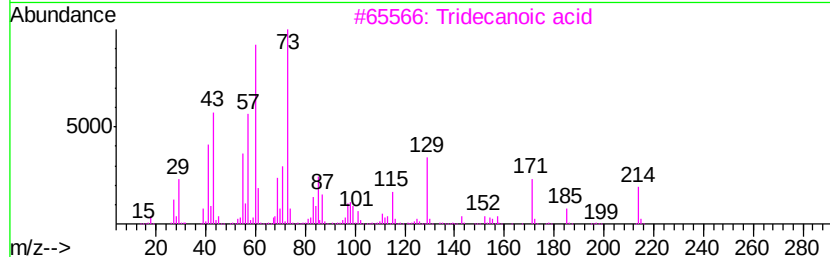
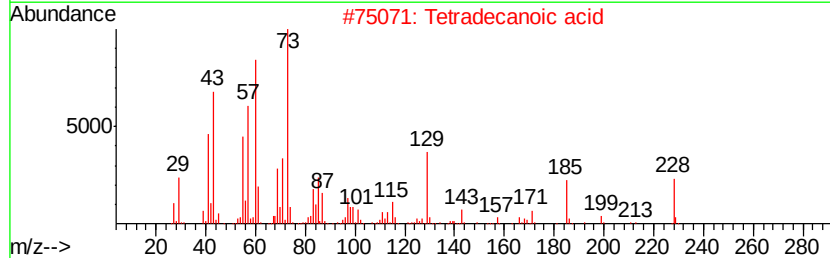
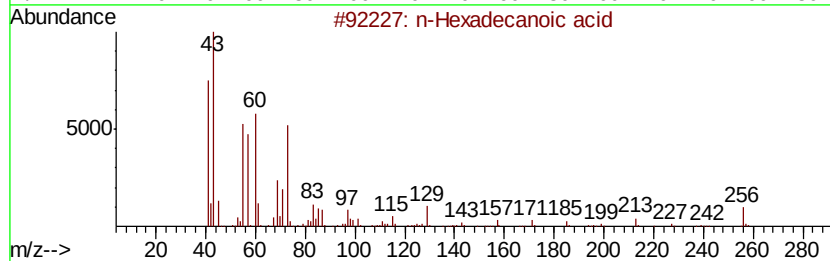
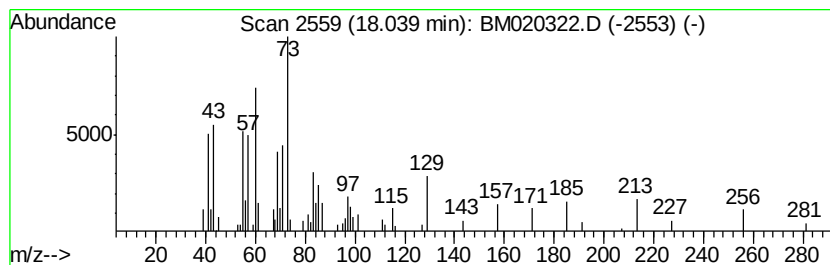
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.04	4.63 ng	136445	Phenanthrene-d10	17.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	43



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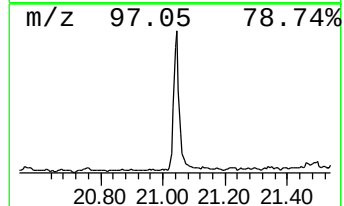
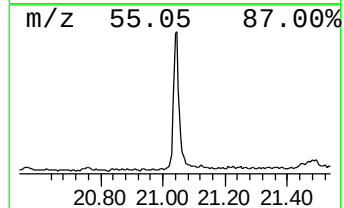
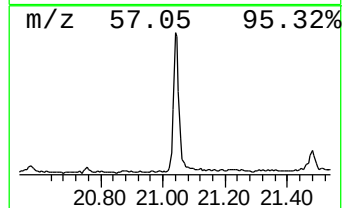
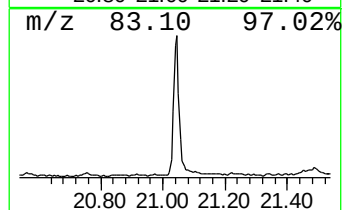
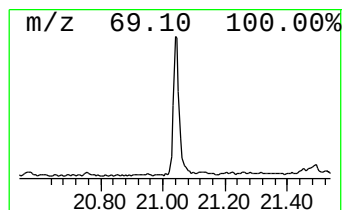
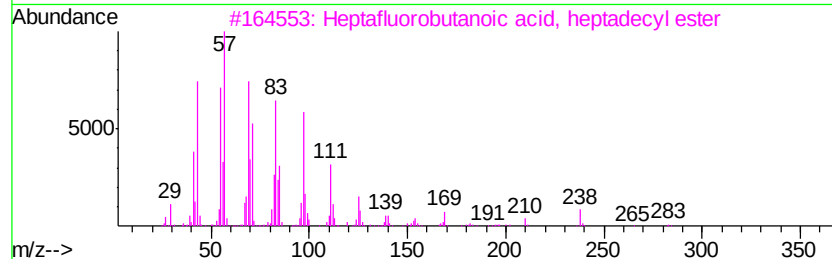
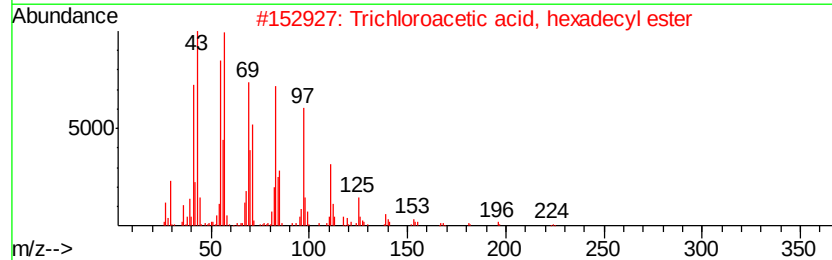
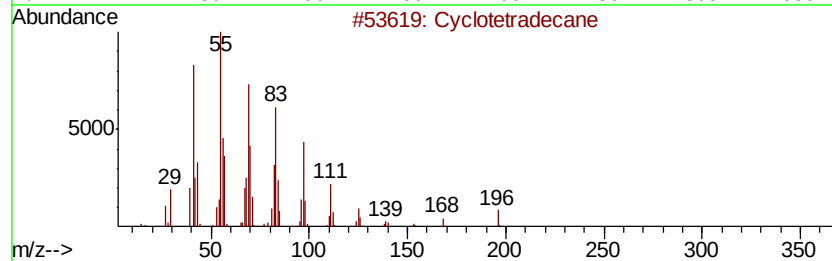
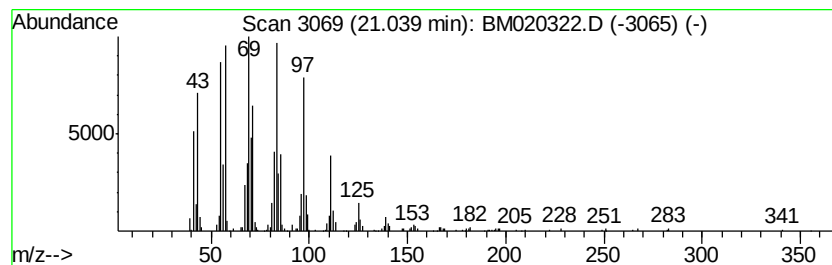
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Peak Number 4 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.04	15.62 ng	560632	Chrysene-d12	21.34	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	93
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
4	1-Tetracosanol	354	C24H50O	000506-51-4	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



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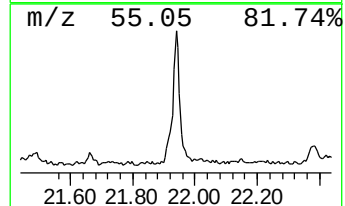
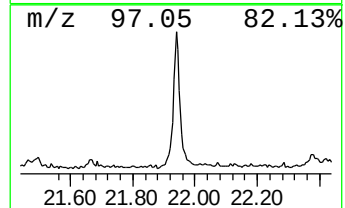
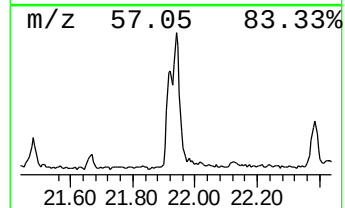
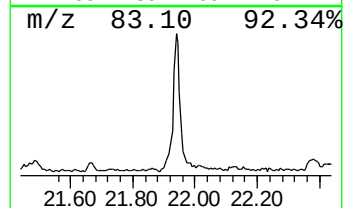
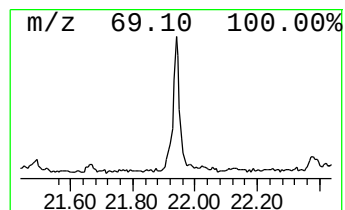
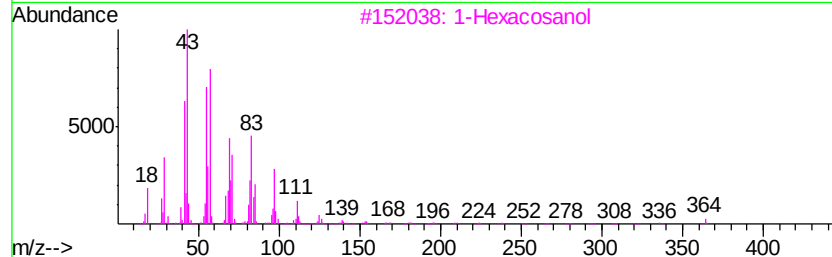
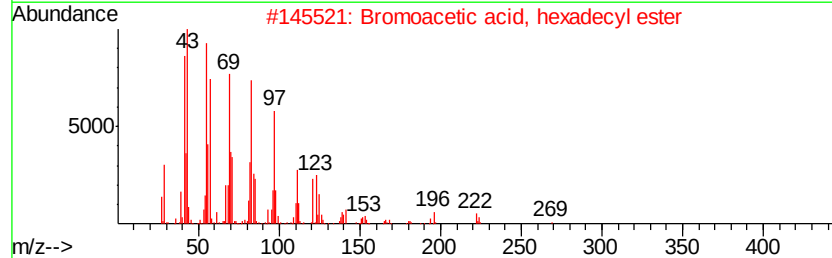
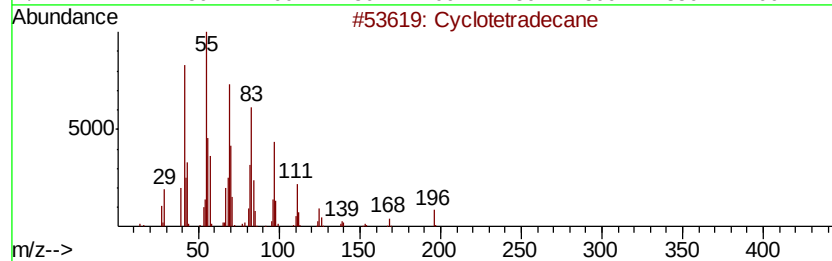
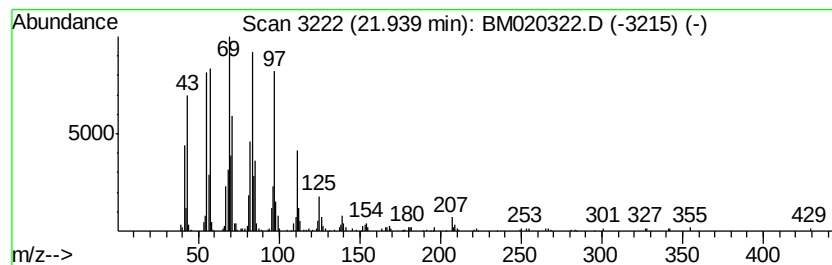
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Peak Number 5 Bromoacetic acid, hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.94	14.89 ng	534247	Chrysene-d12	21.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclotetradecane	196	C14H28	000295-17-0	93
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
3		1-Hexacosanol	382	C26H54O	000506-52-5	87
4		1-Tetracosanol	354	C24H50O	000506-51-4	87
5		Isoheptadecanol	256	C17H36O	057289-07-3	86



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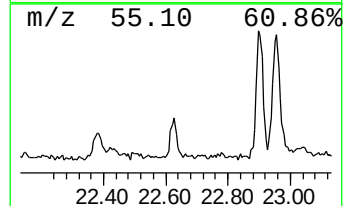
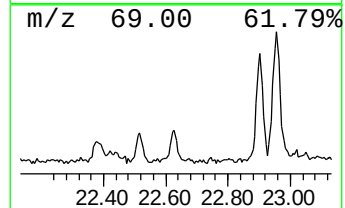
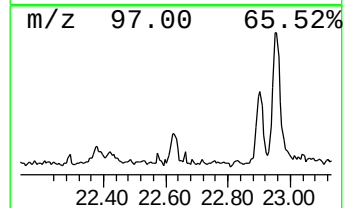
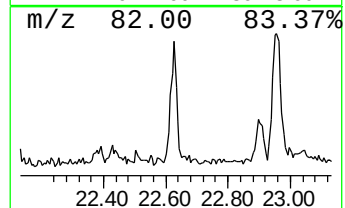
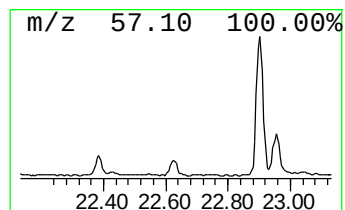
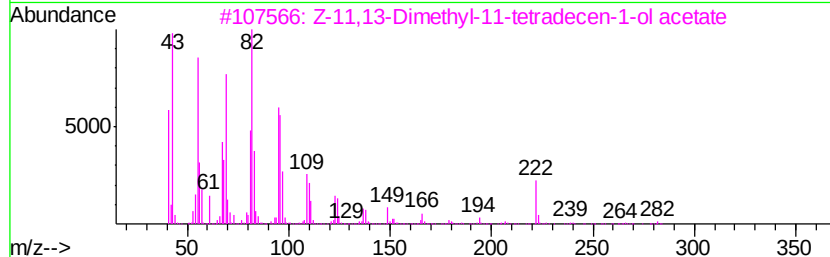
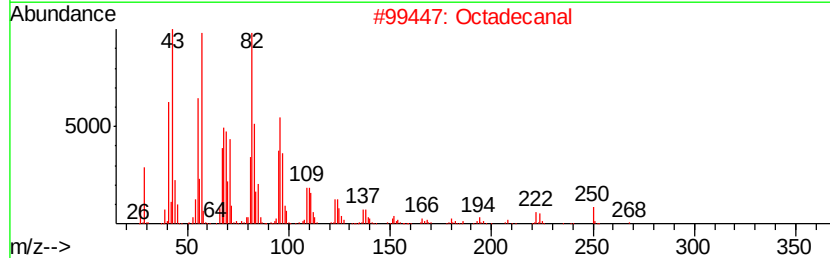
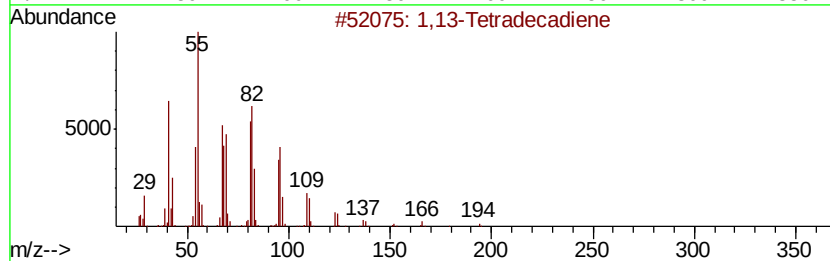
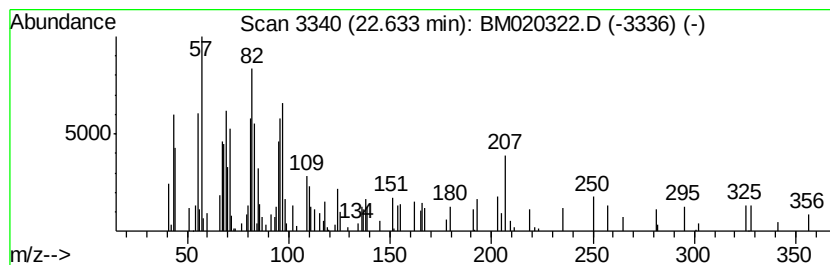
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Peak Number 6 1,13-Tetradecadiene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
22.63	3.37 ng	106722	Perylene-d12	23.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,13-Tetradecadiene		194	C14H26	021964-49-8	64
2	Octadecanal		268	C18H36O	000638-66-4	64
3	Z-11,13-Dimethyl-11-tetradecen-1...		282	C18H34O2	1000131-36-6	58
4	Pentadecanal-		226	C15H30O	002765-11-9	58
5	E-11(13-Methyl)tetradecen-1-ol a...		268	C17H32O2	1000130-80-4	52



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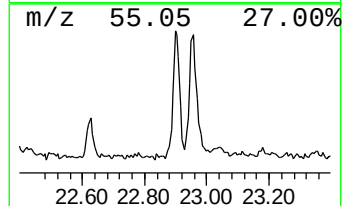
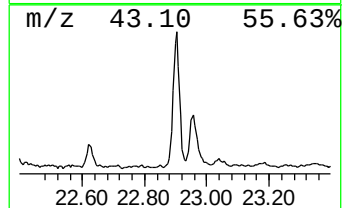
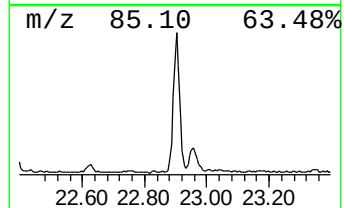
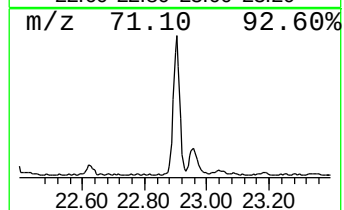
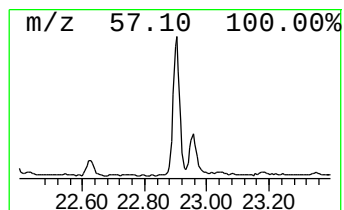
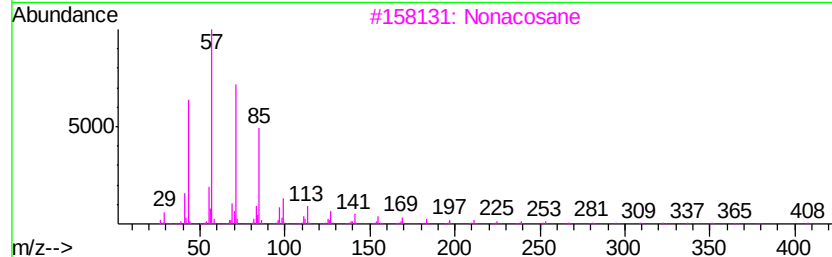
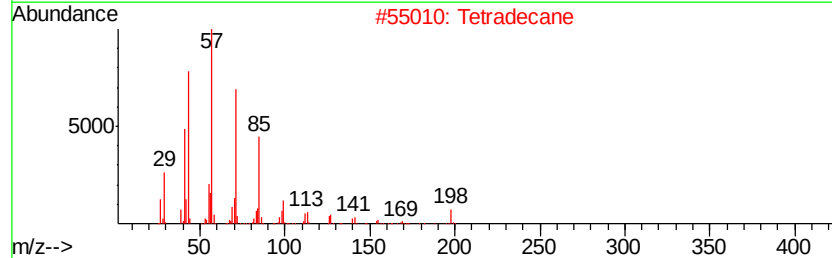
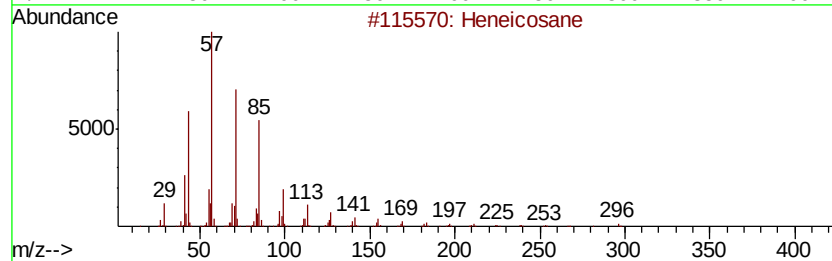
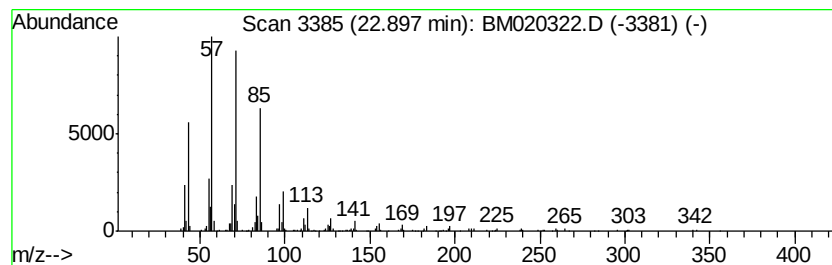
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.90	13.72 ng	434669	Perylene-d12	23.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Tetradecane		198	C14H30	000629-59-4	90
3	Nonacosane		408	C29H60	000630-03-5	86
4	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	86
5	Heptacosane		380	C27H56	000593-49-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
 Data File : BM020322.D
 Acq On : 13 May 2019 18:45
 Operator : JU/SJ
 Sample : K2769-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P026-SS017-0002-01

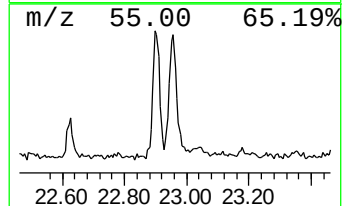
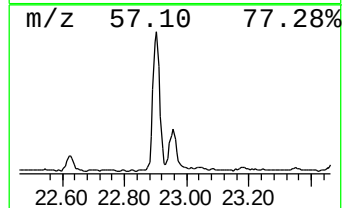
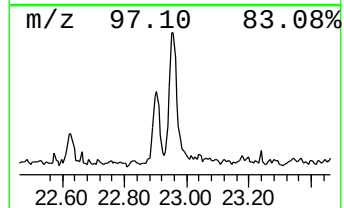
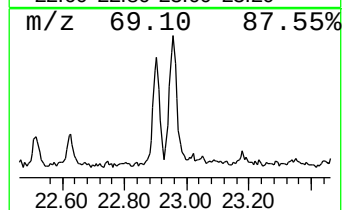
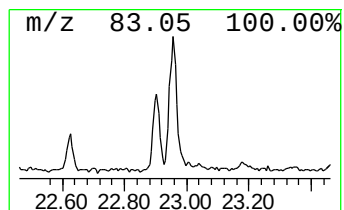
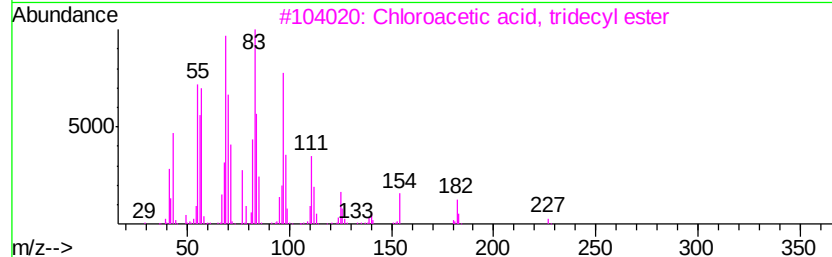
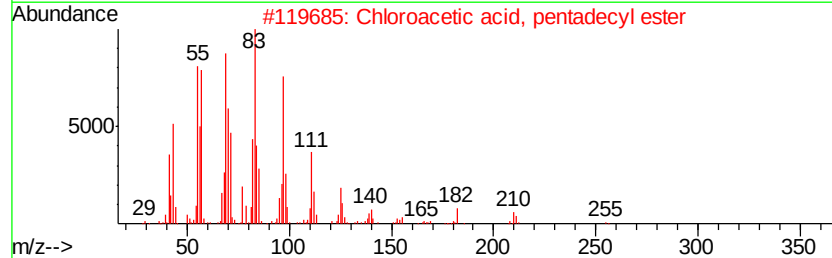
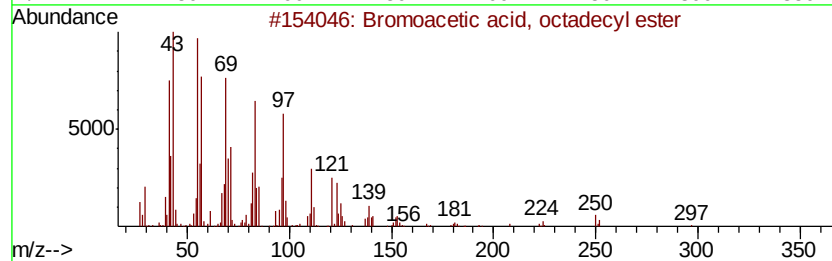
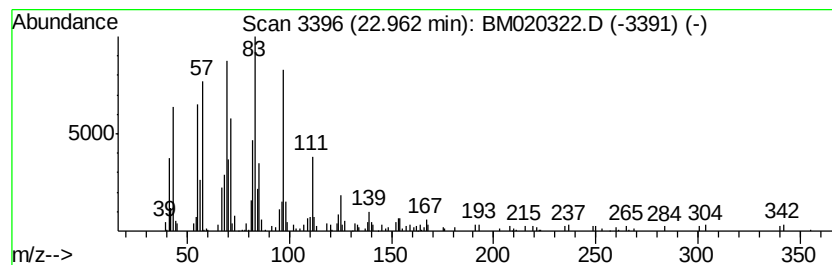
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 8 Bromoacetic acid, octadecyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.96	10.17 ng	322219	Perylene-d12	23.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	87
3		Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	86
4		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	76
5		1-Eicosanol	298	C20H42O	000629-96-9	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
Data File : BM020322.D
Acq On : 13 May 2019 18:45
Operator : JU/SJ
Sample : K2769-01
Misc :
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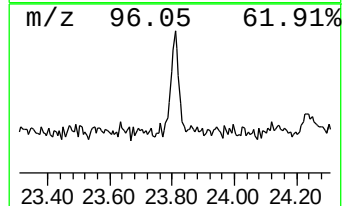
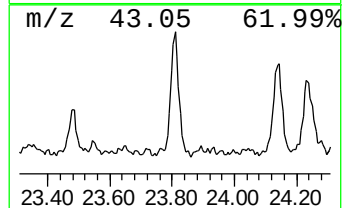
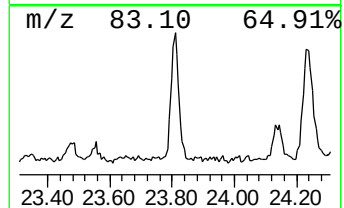
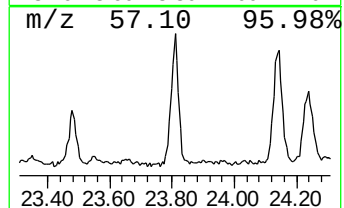
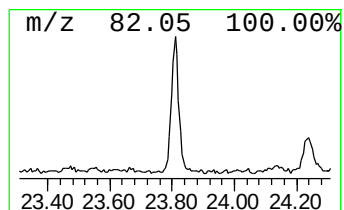
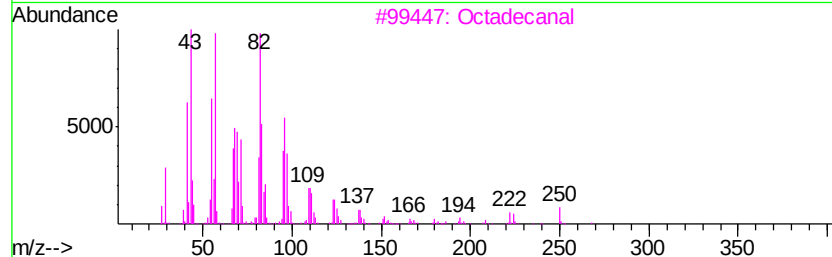
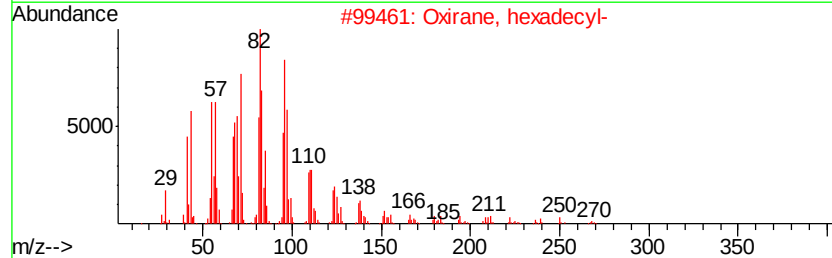
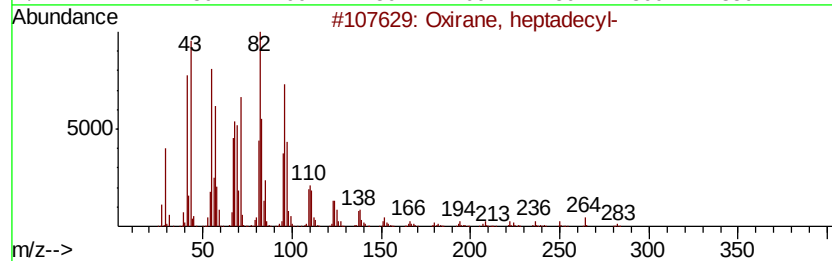
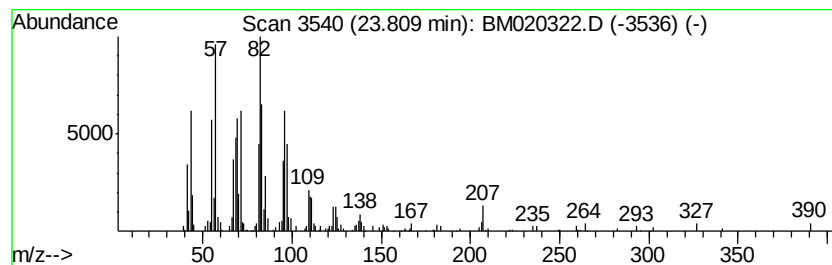
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Oxirane, heptadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.81	8.87 ng	280930	Perylene-d12	23.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
3	Octadecanal	268	C18H36O	000638-66-4	91
4	Tetradecanal	212	C14H28O	000124-25-4	86
5	12-Octadecenal	266	C18H34O	056554-91-7	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
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Sample : K2769-01
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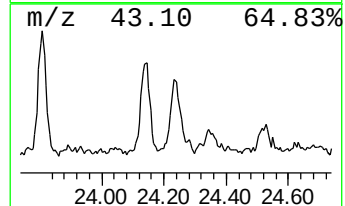
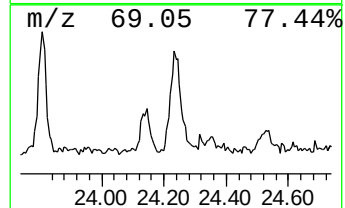
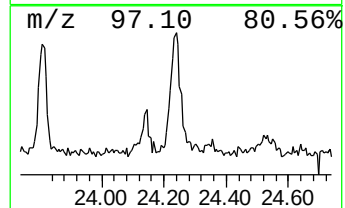
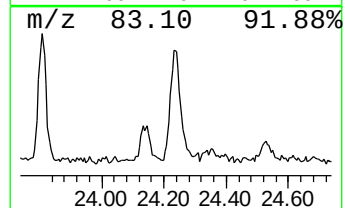
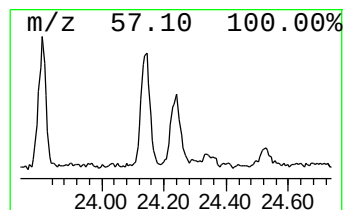
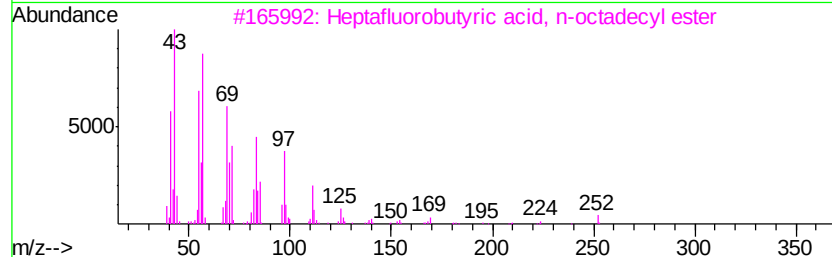
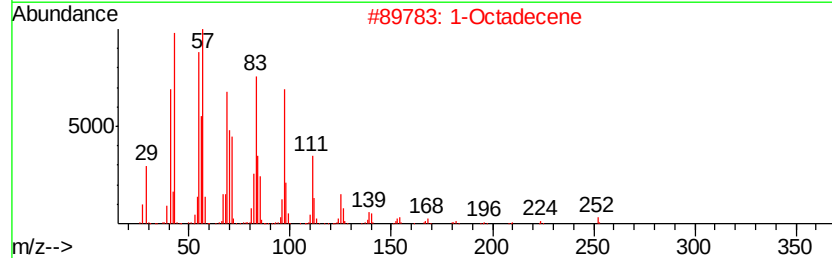
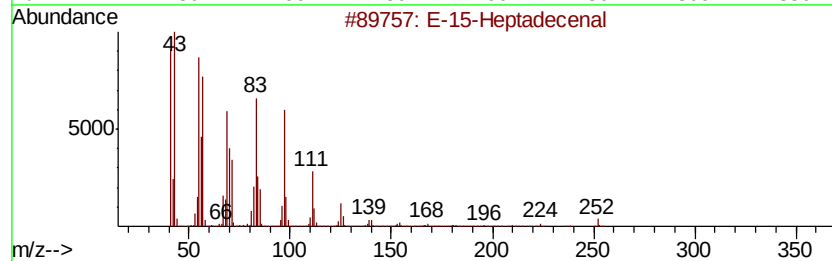
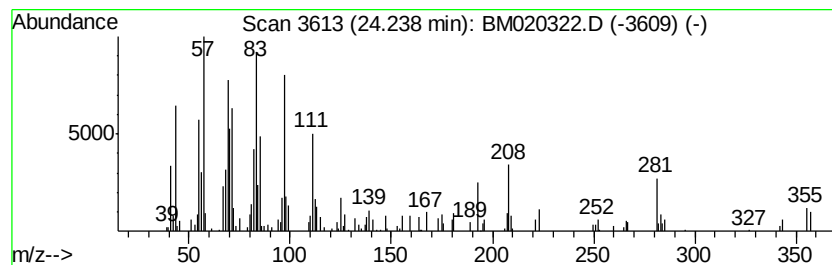
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 E-15-Heptadecenal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.24	5.95 ng	188415	Perylene-d12	23.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	70
2	1-Octadecene	252	C18H36	000112-88-9	70
3	Heptafluorobutvric acid, n-octad...	466	C22H37F7O2	000400-57-7	68
4	1-Nonadecene	266	C19H38	018435-45-5	68
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
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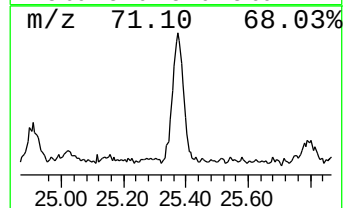
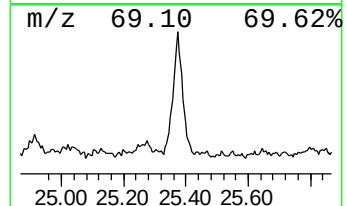
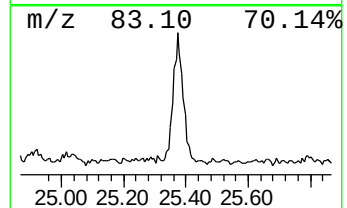
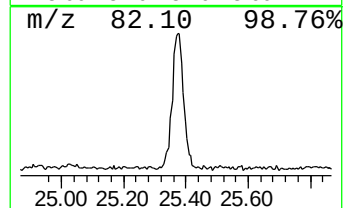
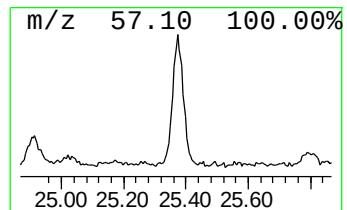
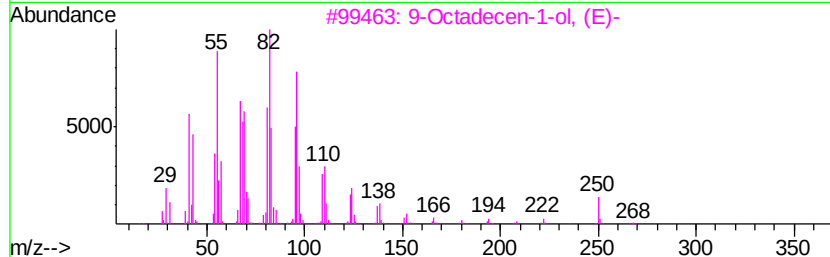
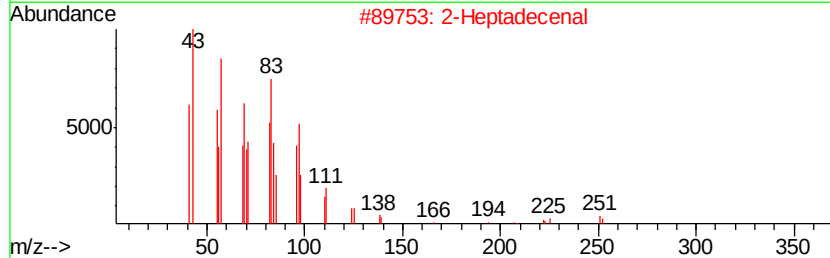
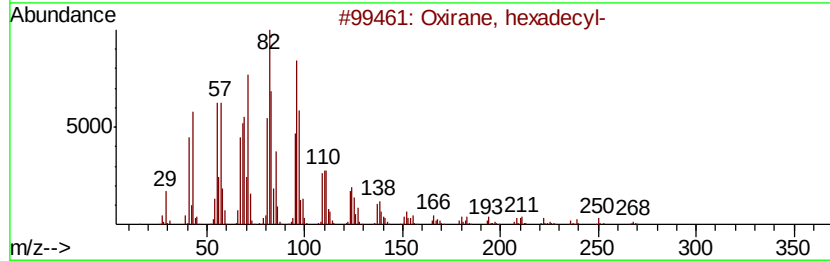
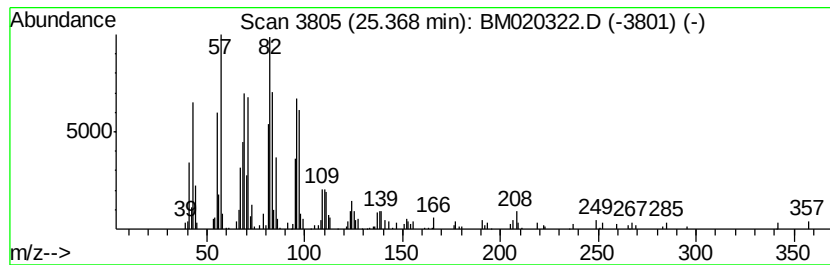
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.37	13.36 ng	423134	Perylene-d12	23.63
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Oxirane, hexadecyl-	268 C18H36O	007390-81-0 95
2		2-Heptadecenal	252 C17H32O	1000143-48-6 90
3		9-Octadecen-1-ol, (E)-	268 C18H36O	000506-42-3 90
4		Z-2-Octadecen-1-ol	268 C18H36O	1000131-11-0 83
5		Oxirane, heptadecyl-	282 C19H38O	067860-04-2 74



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
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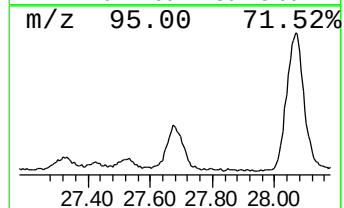
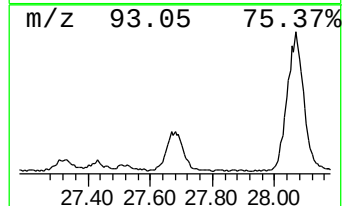
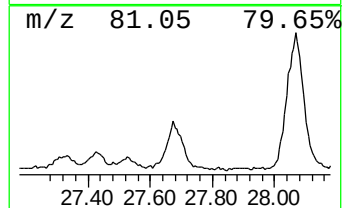
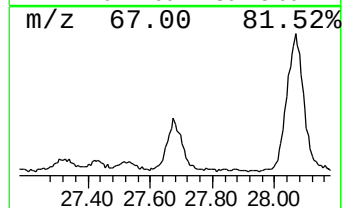
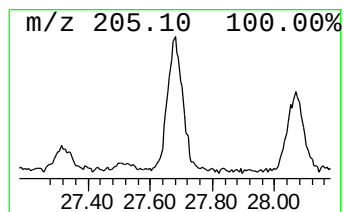
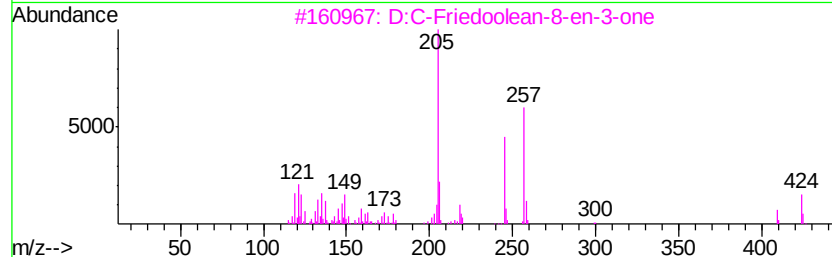
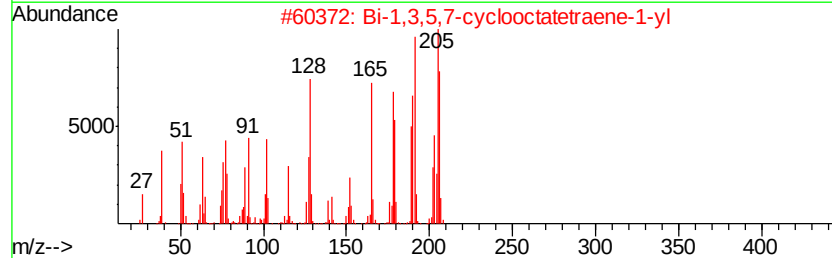
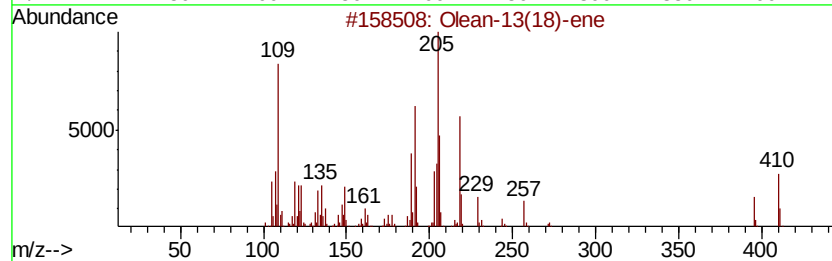
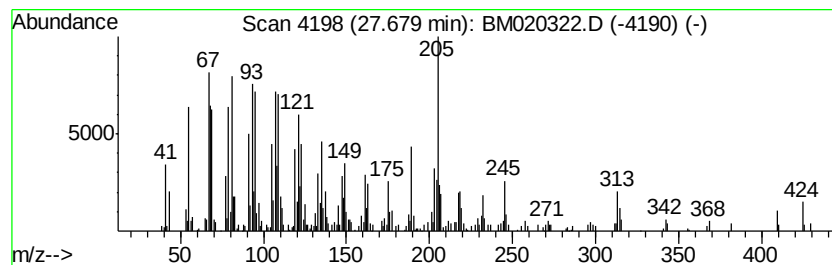
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Olean-13(18)-ene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
27.68	33.88 ng	1073300	Perylene-d12	23.63		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Olean-13(18)-ene	410	C30H50	003399-27-7	62
2		Bi-1,3,5,7-cyclooctatetraene-1-yl	206	C16H14	006715-22-6	60
3		D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	53
4		Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	49
5		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051319\
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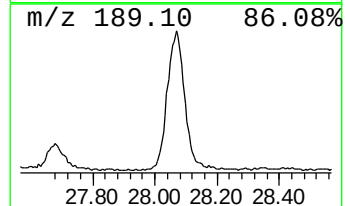
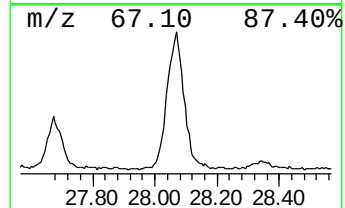
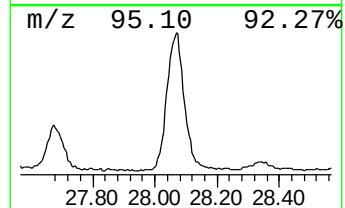
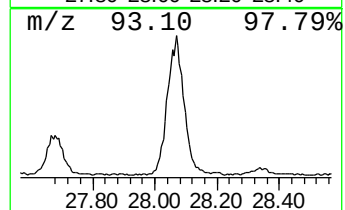
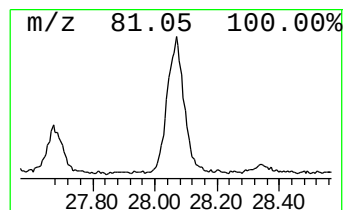
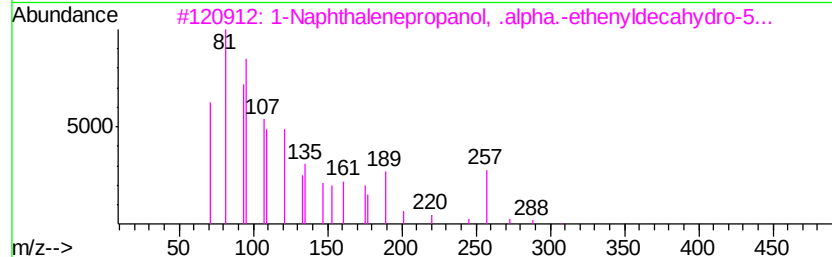
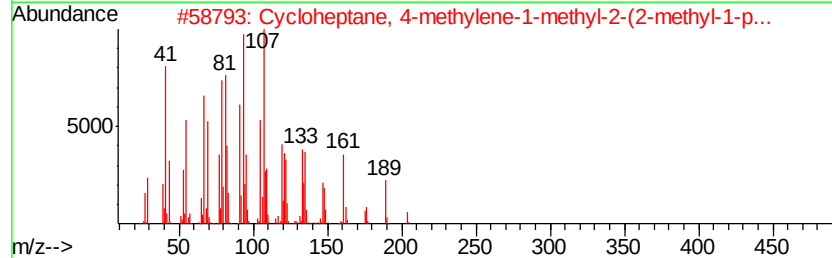
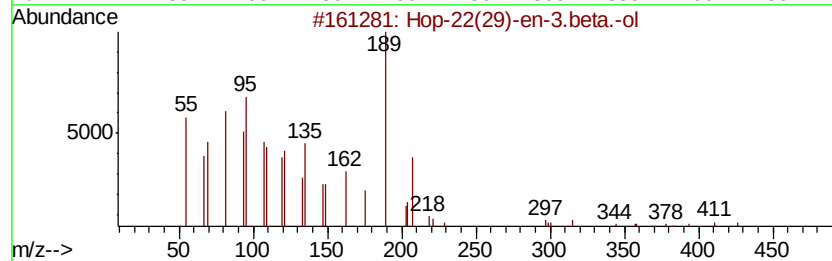
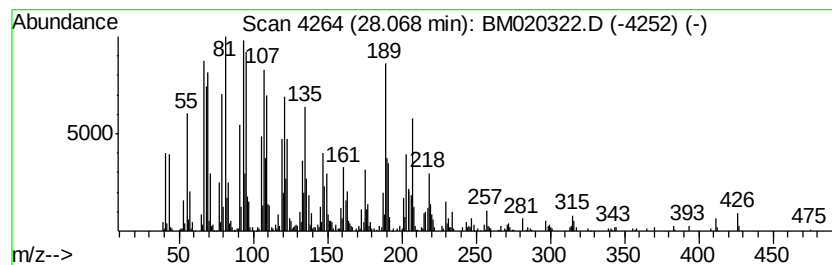
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Hop-22(29)-en-3.beta.-ol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.07	117.45 ng	3721150	Perylene-d12	23.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	89
2	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	60
3	1-Naphthalenepropanol, .alpha.-e...	306	C20H34O2	003650-30-4	45
4	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	42
5	6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	41



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM051319\
Data File : BM020322.D
Acq On : 13 May 2019 18:45
Operator : JU/SJ
Sample : K2769-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.29	7.29	108.5	ng	1396090	1	7.76	257386	20.0
n-Hexadecanoic acid	18.04	4.6	ng	136445	4	17.16	588987	20.0
Cyclotetradecane	21.04	15.6	ng	560632	5	21.34	717657	20.0
Bromoacetic acid,...	21.94	14.9	ng	534247	5	21.34	717657	20.0
1,13-Tetradecadiene	22.63	3.4	ng	106722	6	23.63	633653	20.0
Heneicosane	22.90	13.7	ng	434669	6	23.63	633653	20.0
Bromoacetic acid,...	22.96	10.2	ng	322219	6	23.63	633653	20.0
Oxirane, heptadecyl-	23.81	8.9	ng	280930	6	23.63	633653	20.0
E-15-Heptadecenal	24.24	6.0	ng	188415	6	23.63	633653	20.0
Oxirane, hexadecyl-	25.37	13.4	ng	423134	6	23.63	633653	20.0
Olean-13(18)-ene	27.68	33.9	ng	1073300	6	23.63	633653	20.0
Hop-22(29)-en-3.b...	28.07	117.5	ng	3721150	6	23.63	633653	20.0