

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051219\
 Data File : BM020299.D
 Acq On : 12 May 2019 15:31
 Operator : JU/SJ
 Sample : K2768-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P026-SS014-0206-01

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	5.346	395	401	410	rBV	1147804	1656626	60.68%	7.021%
2	6.928	663	670	684	rBV	1038216	1724734	63.18%	7.310%
3	7.293	725	732	748	rBV	1103607	1804032	66.08%	7.646%
4	7.763	805	812	819	rBV	204015	329068	12.05%	1.395%
5	8.081	859	866	876	rBV	817251	1320221	48.36%	5.595%
6	8.928	1003	1010	1027	rBV	596885	1047870	38.38%	4.441%
7	10.557	1280	1287	1300	rBV	214012	374402	13.71%	1.587%
8	13.028	1700	1707	1725	rBV	1130722	1769008	64.80%	7.497%
9	13.869	1844	1850	1860	rBV	129164	199210	7.30%	0.844%
10	14.410	1936	1942	1949	rBV2	325910	502353	18.40%	2.129%
11	15.904	2190	2196	2215	rBV	1151248	1743613	63.87%	7.390%
12	17.157	2403	2409	2417	rBV2	449232	680807	24.94%	2.885%
13	18.039	2554	2559	2570	rBV	179488	278431	10.20%	1.180%
14	18.321	2603	2607	2614	rBV4	60347	77991	2.86%	0.331%
15	19.321	2773	2777	2780	rBV2	52575	67368	2.47%	0.286%
16	19.357	2780	2783	2790	rVB6	21046	29370	1.08%	0.124%
17	19.586	2818	2822	2829	rVB	21870	33814	1.24%	0.143%
18	19.786	2850	2856	2868	rBV	2229900	2730064	100.00%	11.570%
19	20.062	2898	2903	2911	rBV3	91592	169362	6.20%	0.718%
20	20.345	2946	2951	2954	rBV	77232	91176	3.34%	0.386%
21	20.498	2974	2977	2982	rVB6	27601	41584	1.52%	0.176%
22	20.662	2998	3005	3011	rBV5	44229	70585	2.59%	0.299%
23	20.803	3026	3029	3035	rVB4	37500	46251	1.69%	0.196%
24	21.045	3066	3070	3080	rBV	693724	933655	34.20%	3.957%
25	21.127	3081	3084	3090	rVB3	38347	62445	2.29%	0.265%
26	21.345	3116	3121	3132	rBV	733478	1153968	42.27%	4.891%
27	21.486	3142	3145	3148	rBV4	34263	57880	2.12%	0.245%
28	21.668	3173	3176	3182	rVB7	49456	78751	2.88%	0.334%
29	21.921	3215	3219	3220	rBV	224566	254886	9.34%	1.080%
30	21.945	3220	3223	3233	rVB	672930	994354	36.42%	4.214%
31	22.386	3294	3298	3302	rBV3	83503	140546	5.15%	0.596%
32	22.627	3336	3339	3345	rVB3	87806	119372	4.37%	0.506%
33	22.903	3382	3386	3390	rBV	239731	349803	12.81%	1.483%
34	22.962	3391	3396	3403	rVB2	306672	543014	19.89%	2.301%

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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

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35	23.633	3504	3510	3522	rVB	552611	1087930	39.85%	4.611%
36	23.809	3536	3540	3547	rVB5	111212	200107	7.33%	0.848%
37	24.144	3592	3597	3605	rVB	171615	343706	12.59%	1.457%
38	24.244	3608	3614	3624	rVV	223958	487089	17.84%	2.064%

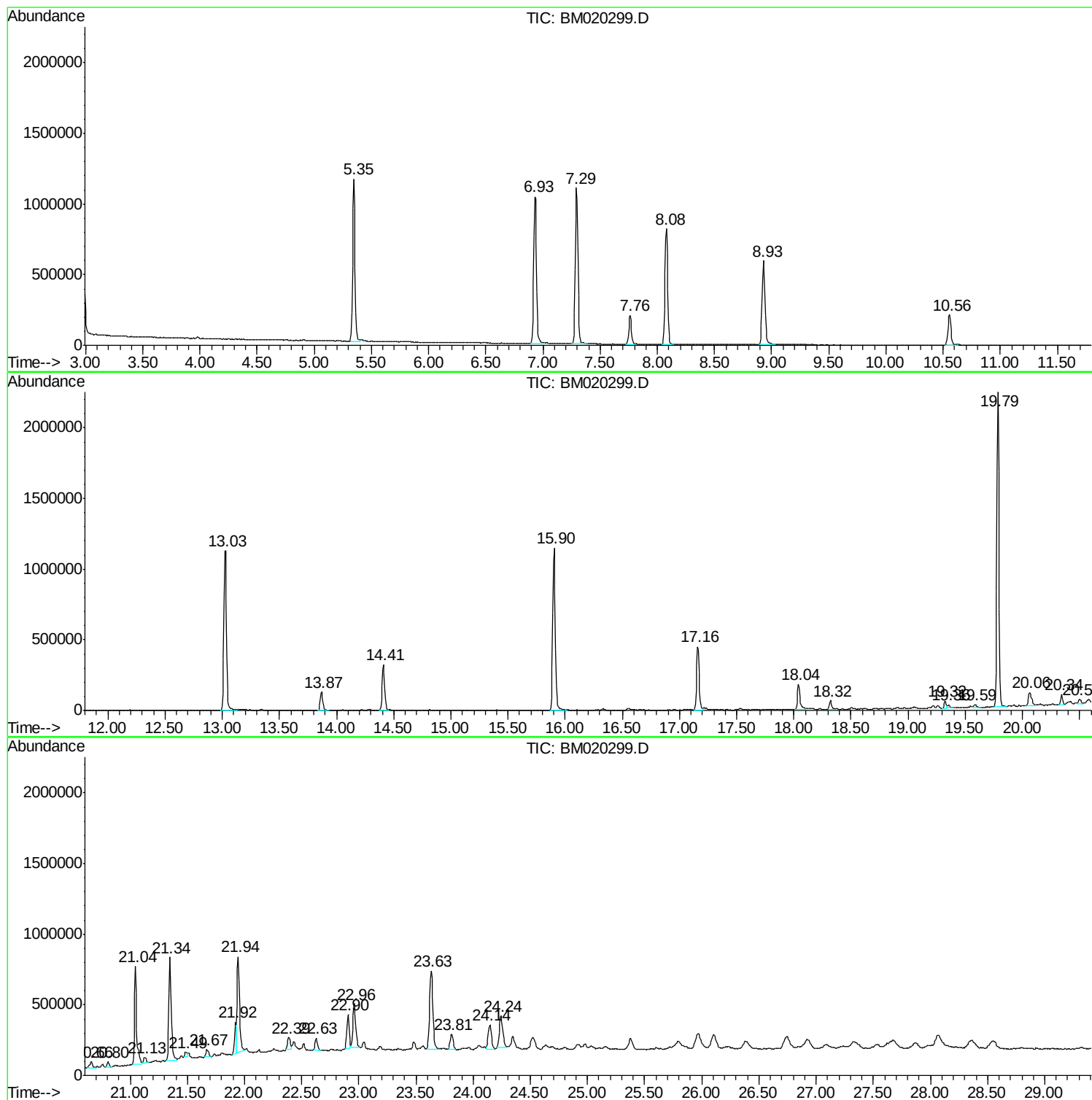
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM043019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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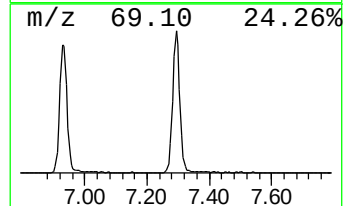
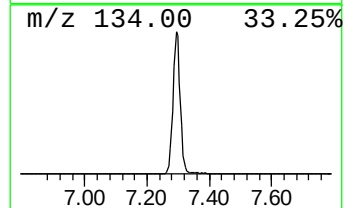
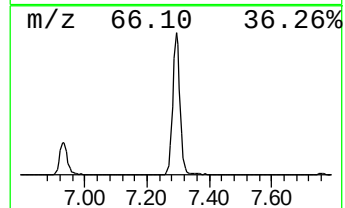
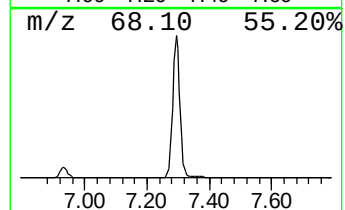
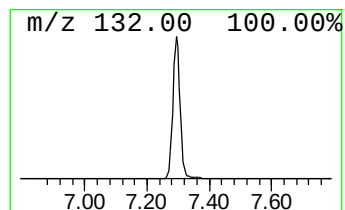
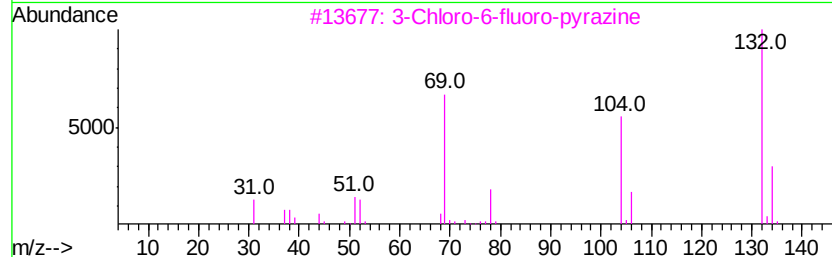
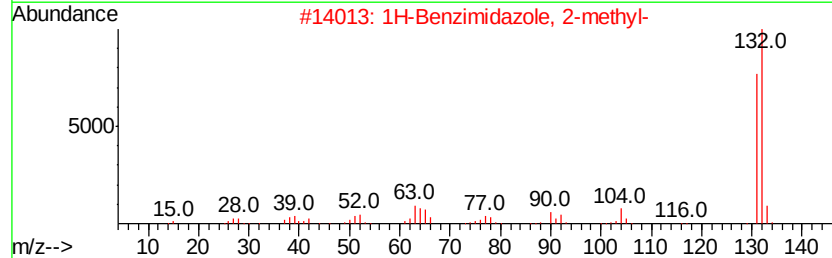
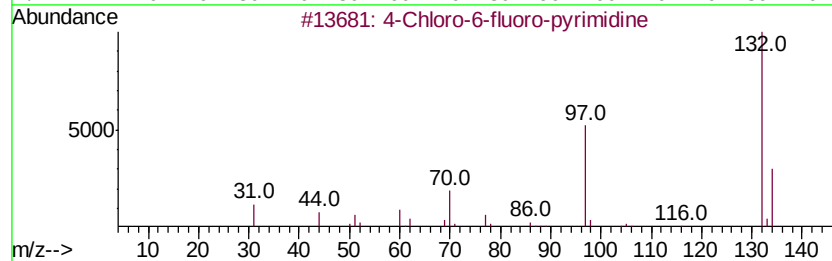
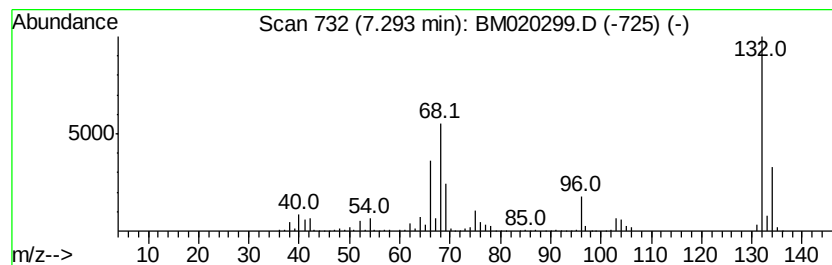
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	109.65 ng	1804030	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		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12



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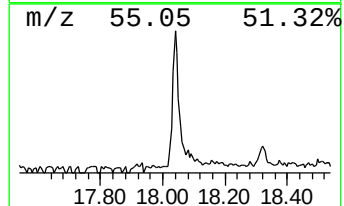
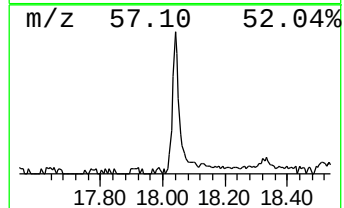
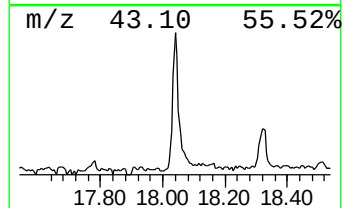
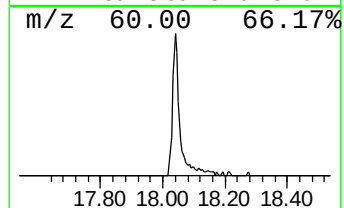
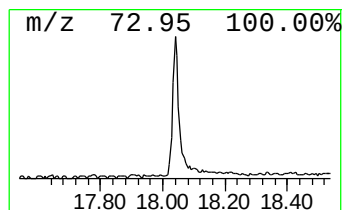
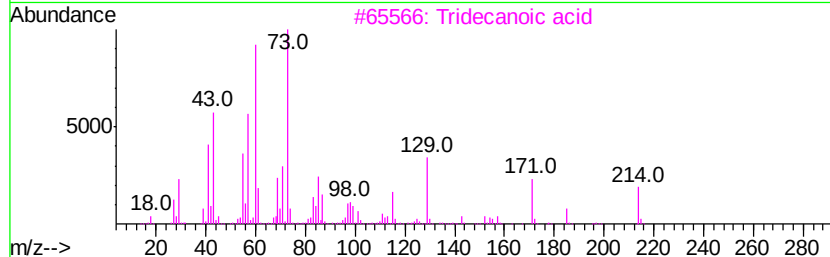
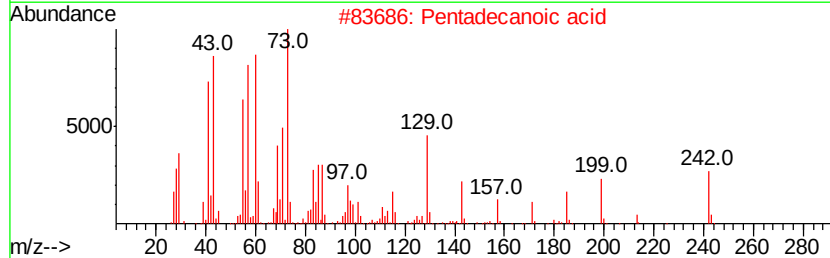
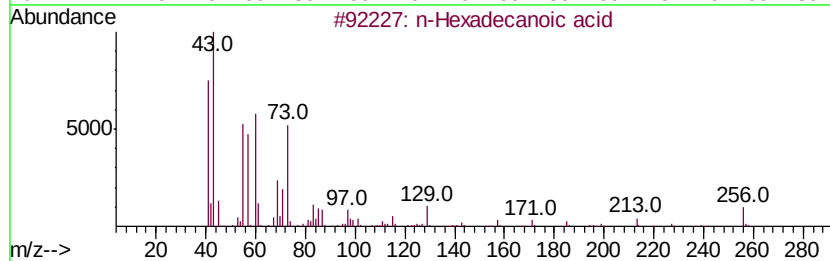
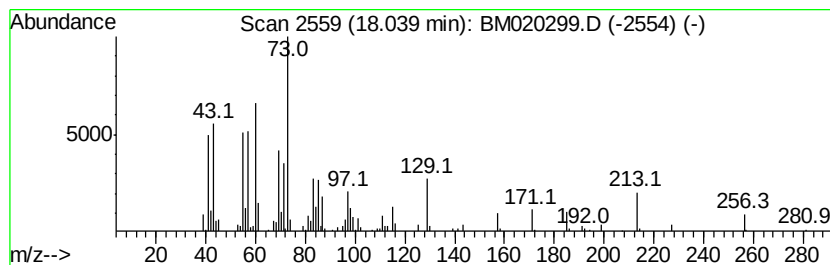
Instrument :
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.04	8.18 ng	278431	Phenanthrene-d10	17.16		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3		Tridecanoic acid	214	C13H26O2	000638-53-9	50
4		12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	43
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	43



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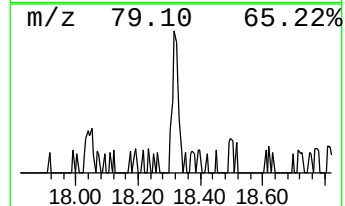
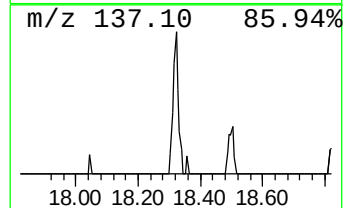
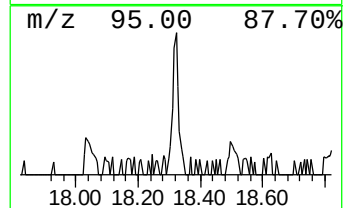
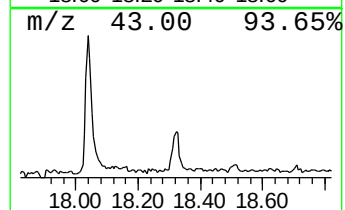
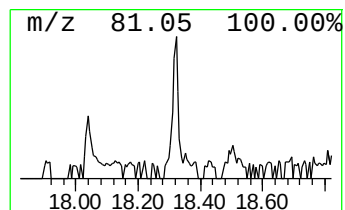
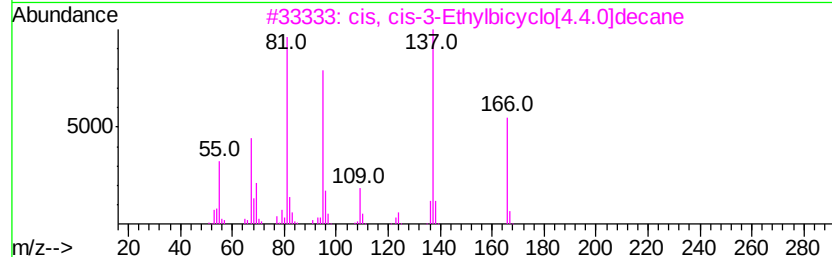
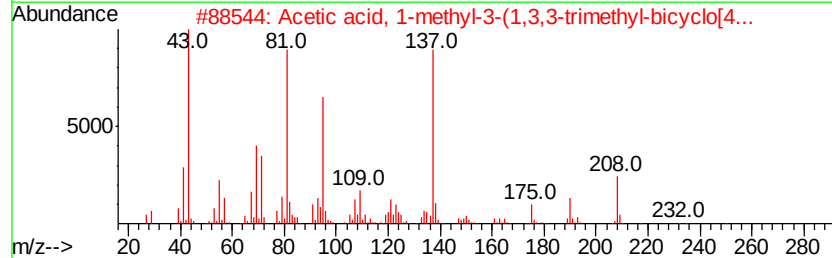
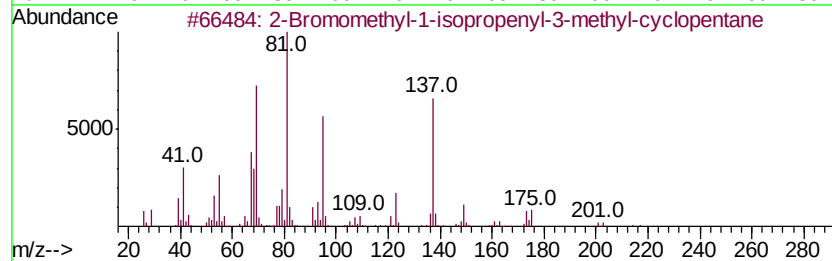
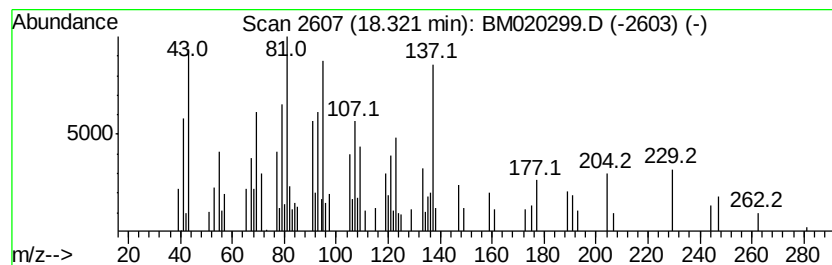
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Peak Number 4 2-Bromomethyl-1-isopropenyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.32	2.29 ng	77991	Phenanthrene-d10	17.16		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromomethyl-1-isopropenyl-3-me...	216	C10H17Br	1000187-07-8	50	
2	Acetic acid, 1-methyl-3-(1,3,3-t...	250	C16H26O2	1000192-22-3	50	
3	cis, cis-3-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-42-2	47	
4	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	38	
5	14-Oxatricyclo[9..2.1.0(1,10)]te...	262	C18H30O	1000193-06-8	38	



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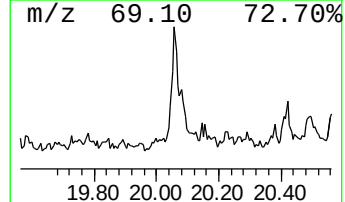
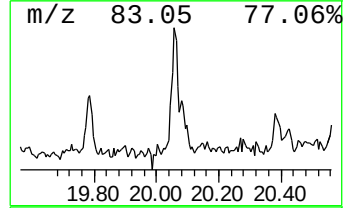
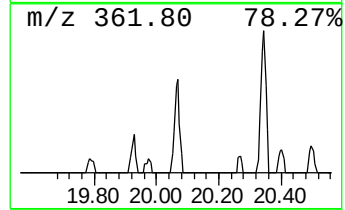
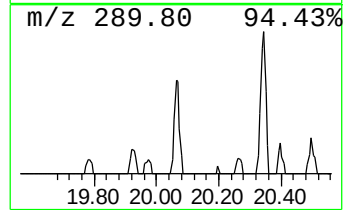
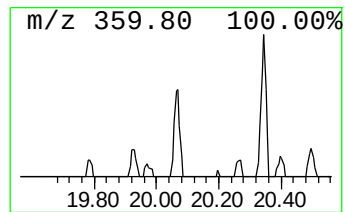
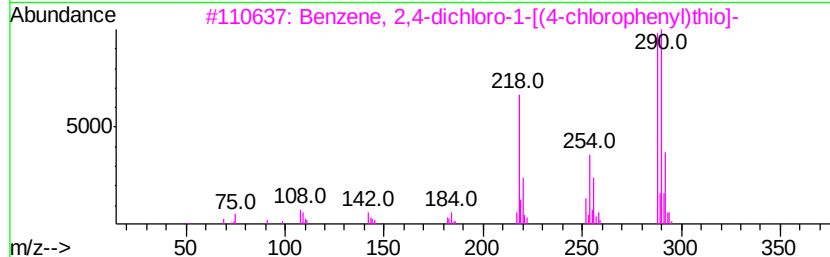
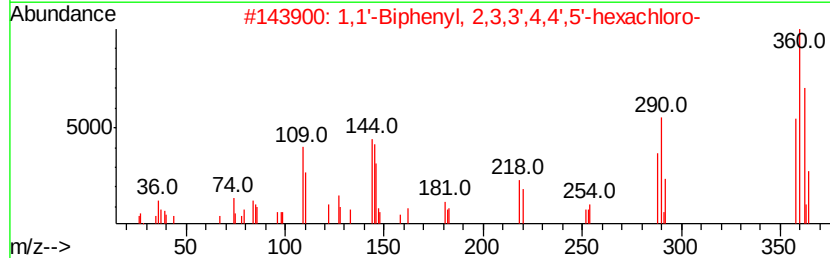
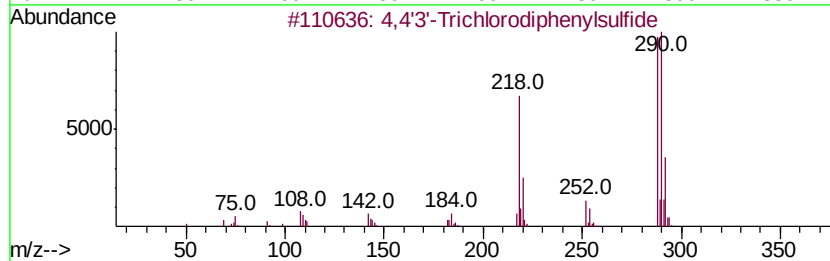
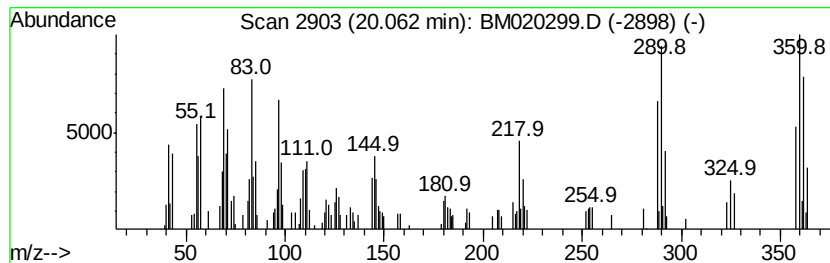
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4,4'3'-Trichlorodiphenylsul... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.06	2.94 ng	169362	Chrysene-d12		21.34	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4,4,3'-Trichlorodiphenylsulfide	288	C12H7Cl3S	1000283-58-7	74
2		1,1'-Biphenyl, 2,3,3',4,4',5'-he...	358	C12H4Cl6	069782-90-7	62
3		Benzene, 2,4-dichloro-1-[(4-chlo...	288	C12H7Cl3S	055759-88-1	25
4		3-Bromo-5,7-dichloro-1-methylnap...	288	C11H7BrCl2	055058-84-9	25
5		1,3-Butadiyne, 1,4-di(4-bromophe...	358	C16H8Br2	000959-88-6	22



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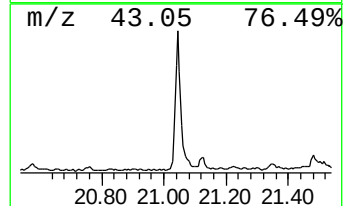
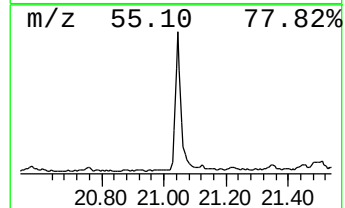
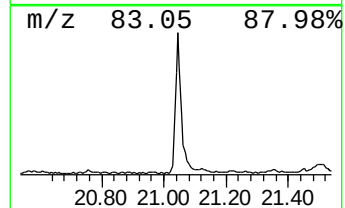
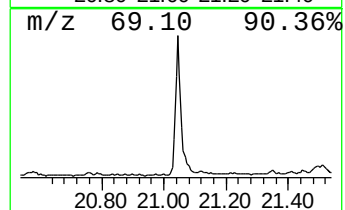
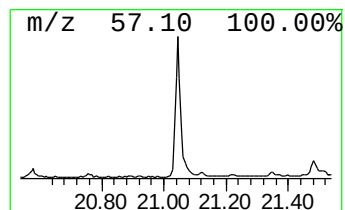
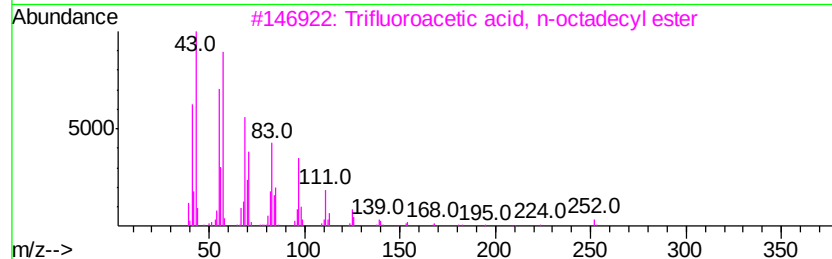
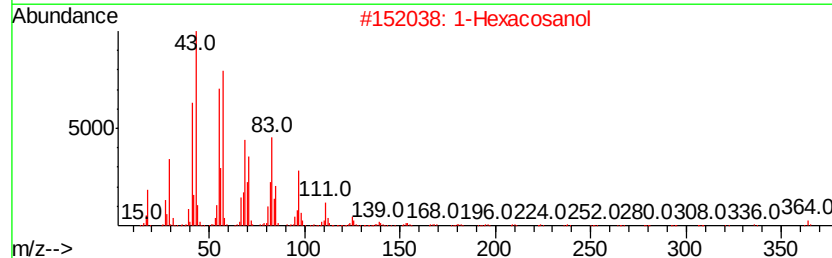
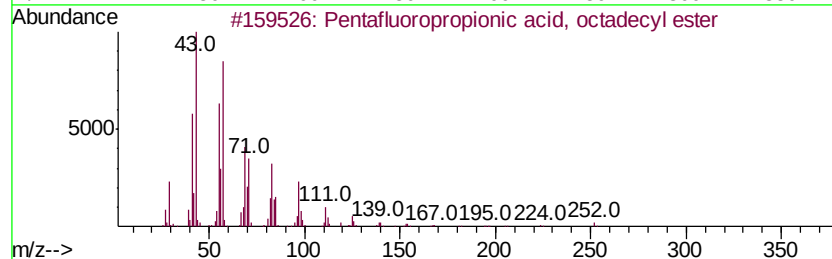
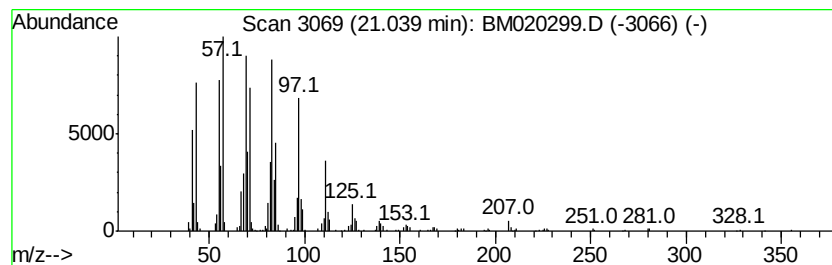
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	16.18 ng	933655	Chrysene-d12	21.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
2		1-Hexacosanol	382	C26H54O	000506-52-5	86
3		Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	83
4		1-Hexadecanol	242	C16H34O	036653-82-4	81
5		Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	74



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Acq On : 12 May 2019 15:31
Operator : JU/SJ
Sample : K2768-05
Misc :
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Instrument :
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ClientSampleId :
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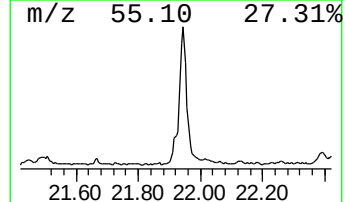
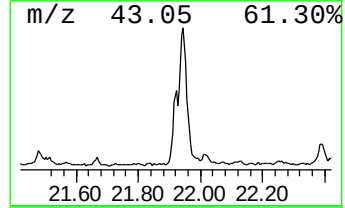
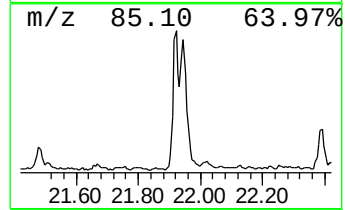
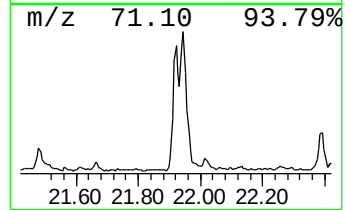
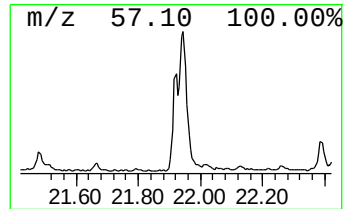
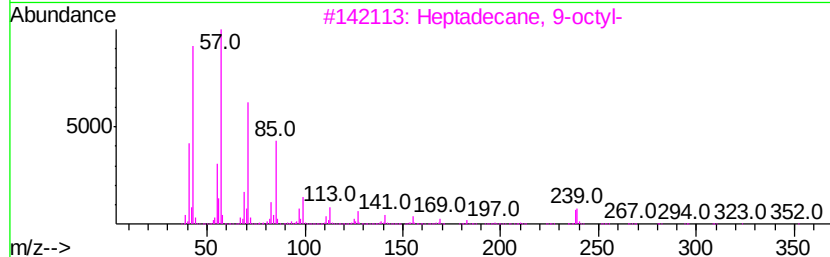
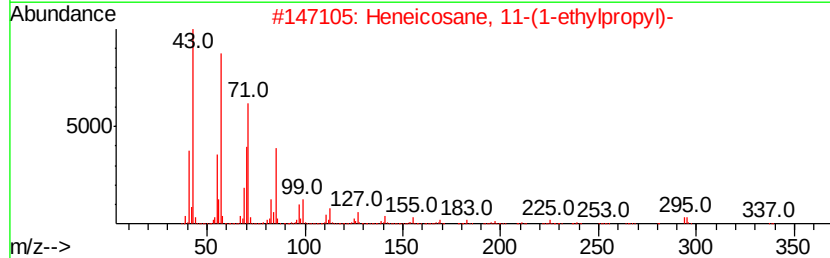
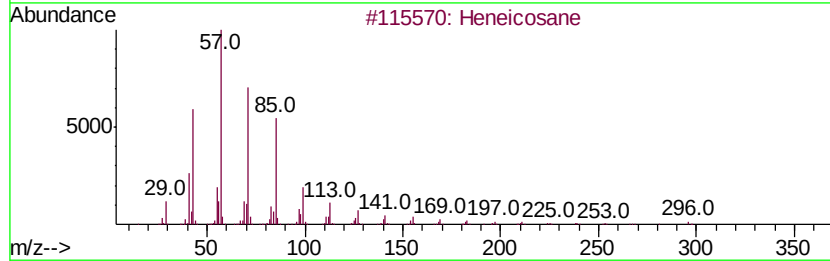
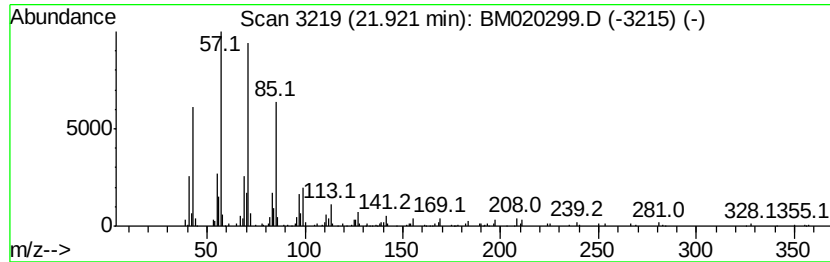
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.92	4.42 ng	254886	Chrysene-d12	21.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4		Octacosane	394	C28H58	000630-02-4	87
5		Nonacosane	408	C29H60	000630-03-5	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051219\
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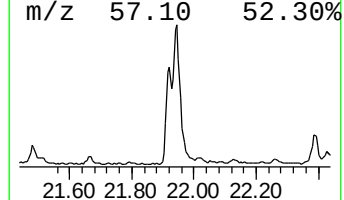
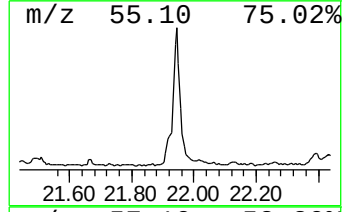
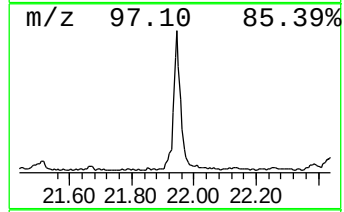
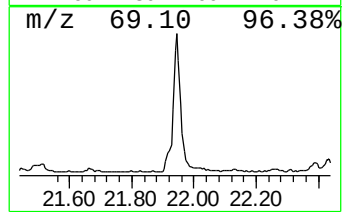
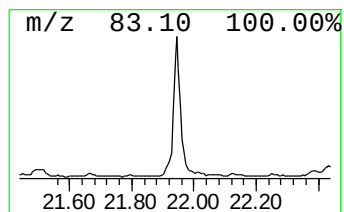
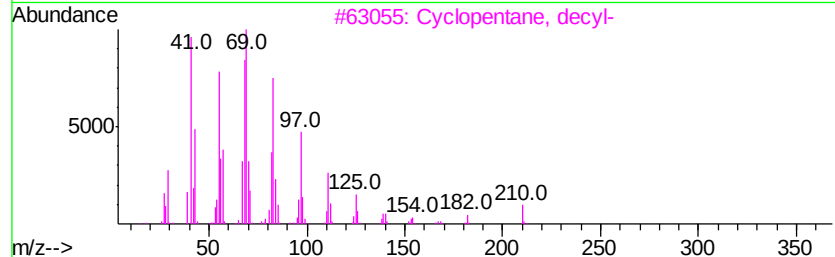
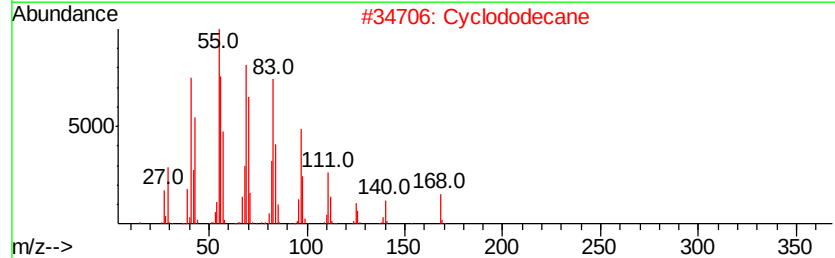
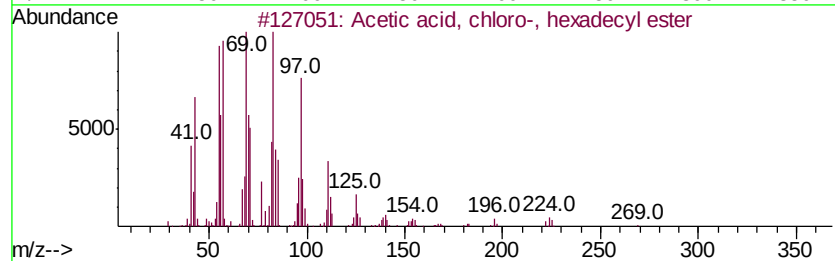
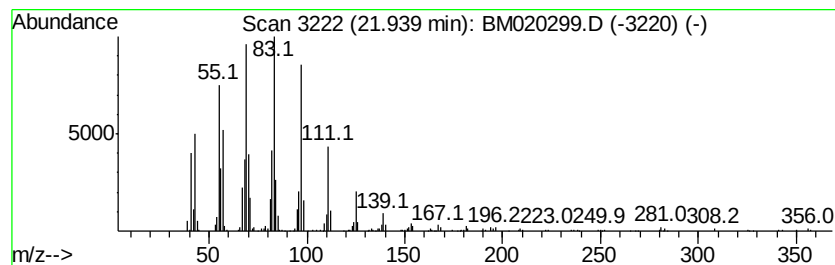
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Acetic acid, chloro-, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.94	17.23 ng	994354	Chrysene-d12	21.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	80
2		Cyclododecane	168	C12H24	000294-62-2	72
3		Cyclopentane, decyl-	210	C15H30	001795-21-7	58
4		1-Docosene	308	C22H44	001599-67-3	58
5		Cyclotetradecane	196	C14H28	000295-17-0	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051219\
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Sample : K2768-05
Misc :
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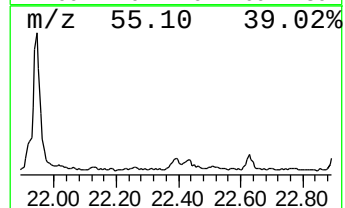
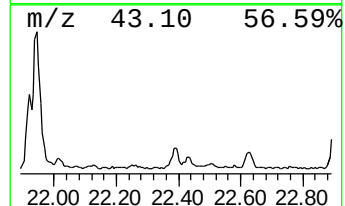
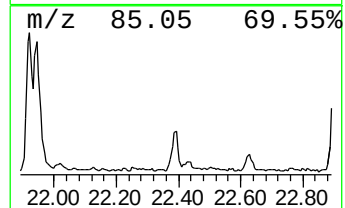
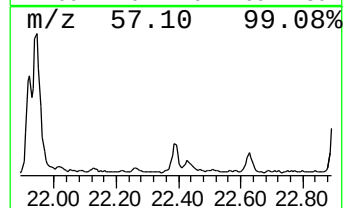
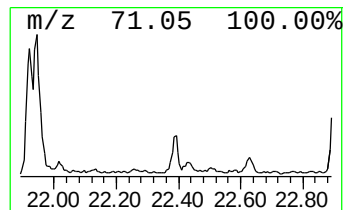
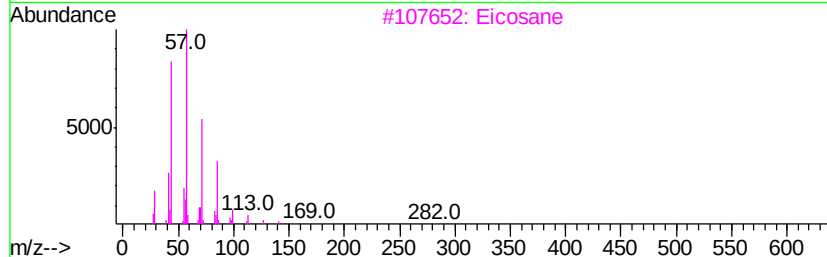
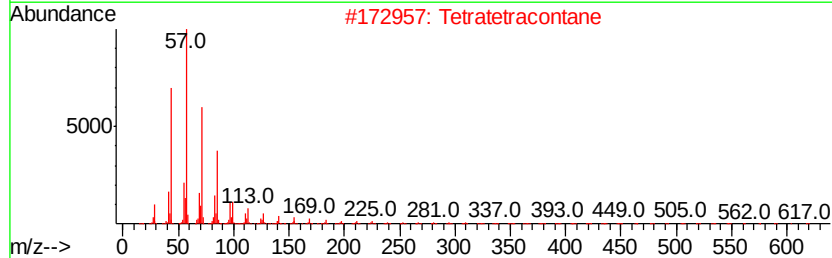
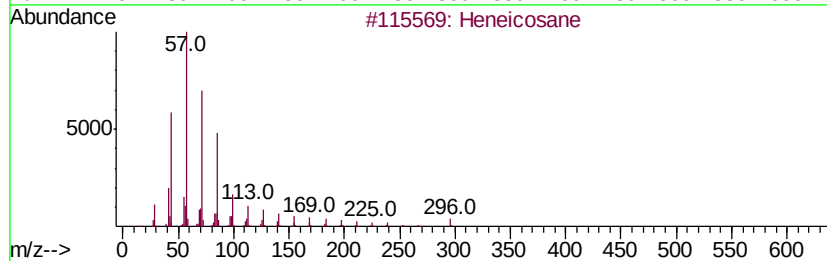
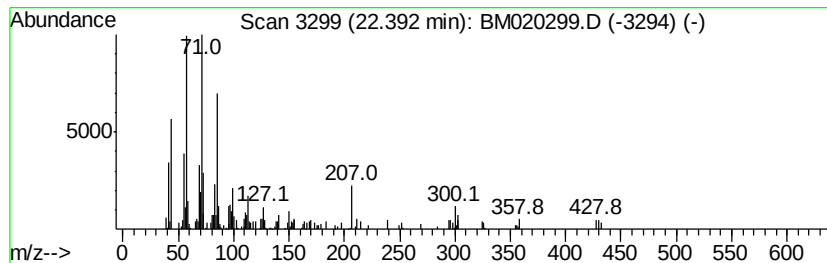
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratetracontane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	2.44 ng	140546	Chrysene-d12	21.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	83
2	Tetratetracontane	619 C44H90	007098-22-8	58
3	Eicosane	282 C20H42	000112-95-8	58
4	Tetracosane, 11-decyl-	479 C34H70	055429-84-0	52
5	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44	054833-48-6	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051219\
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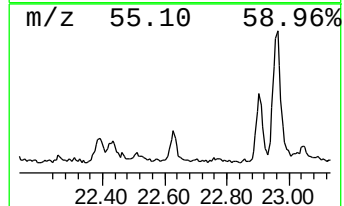
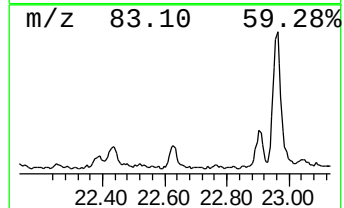
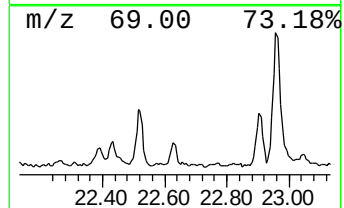
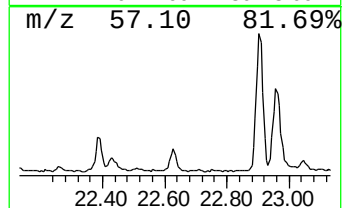
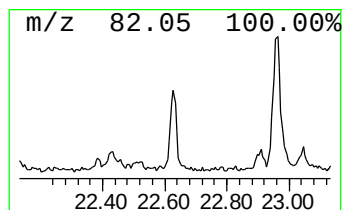
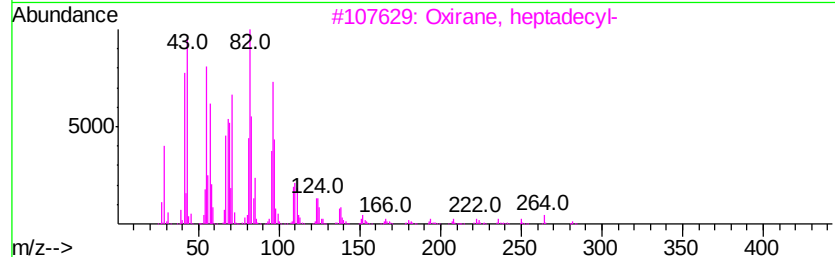
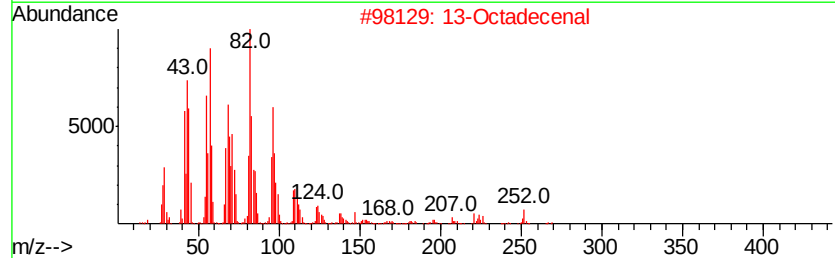
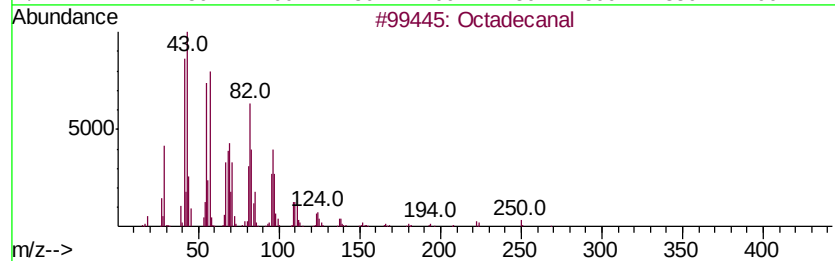
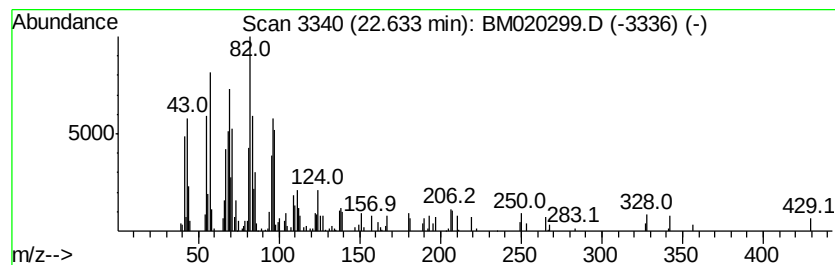
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD		R.T.
22.63	2.19 ng	119372	Perylene-d12		23.63
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	72
2	13-Octadecenal	266	C18H34O	056554-90-6	72
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	70
4	7-Octadecenal	266	C18H34O	056555-00-1	52
5	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051219\
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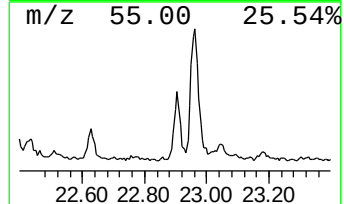
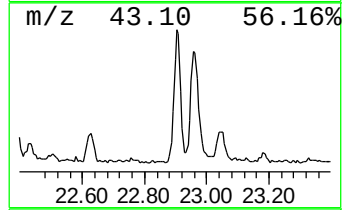
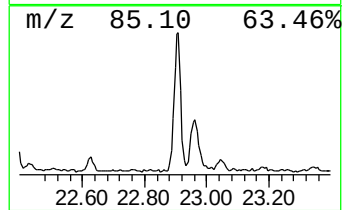
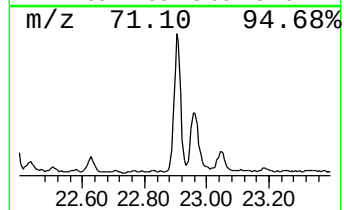
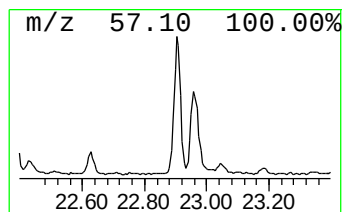
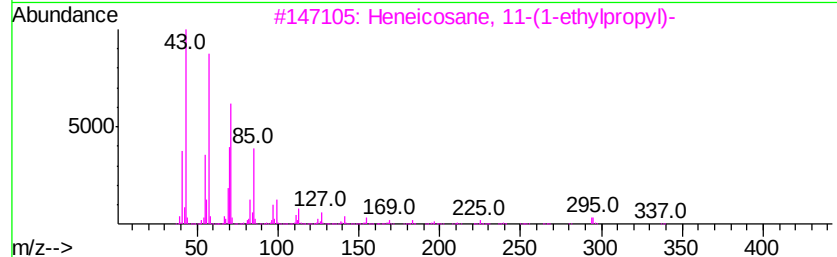
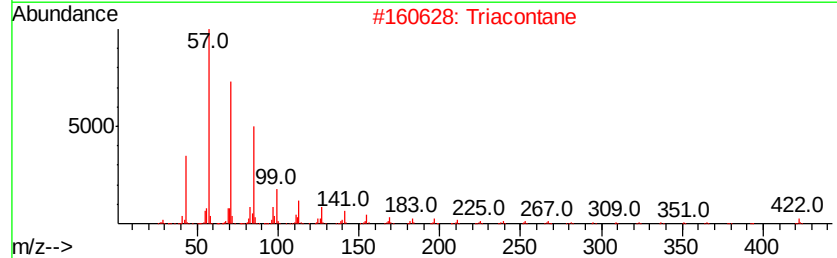
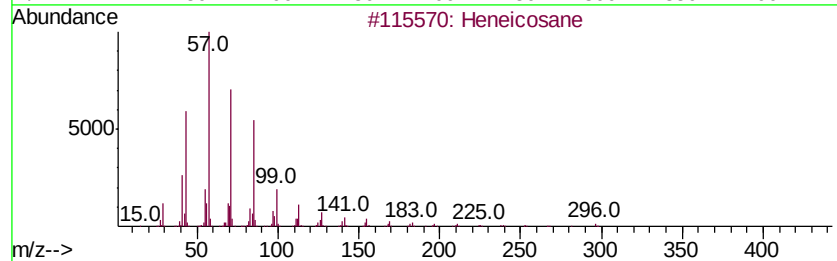
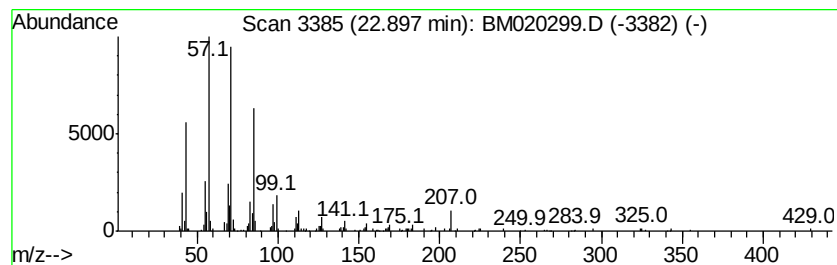
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.90	6.43 ng	349803	Perylene-d12	23.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Hexadecane	226	C16H34	000544-76-3	87
5	Octacosane	394	C28H58	000630-02-4	87



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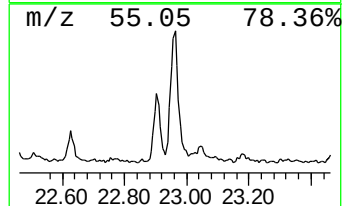
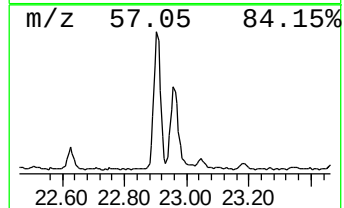
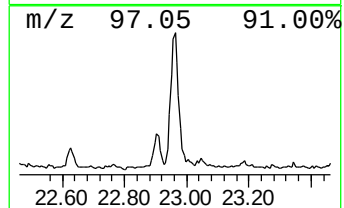
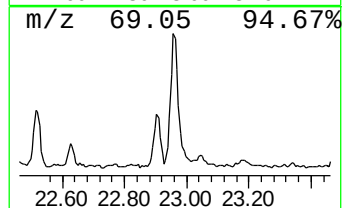
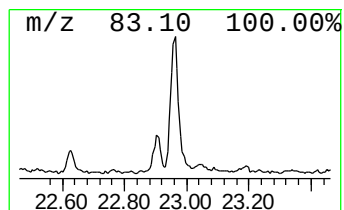
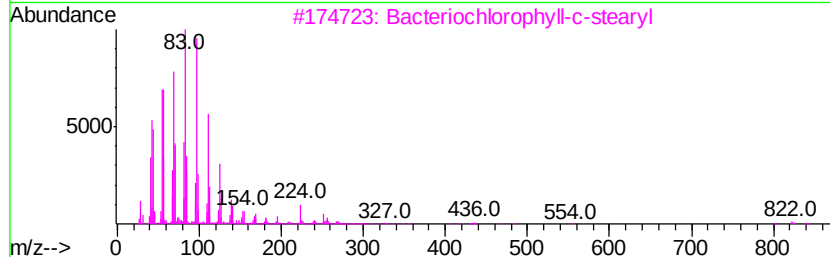
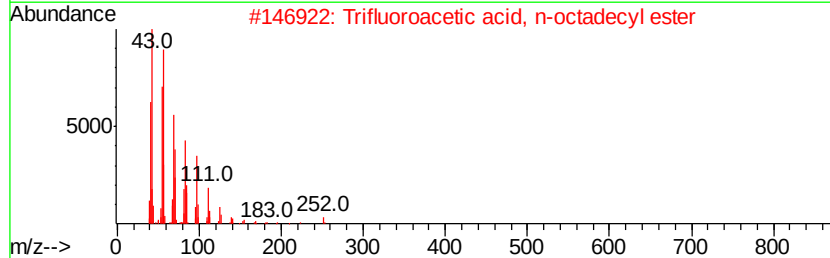
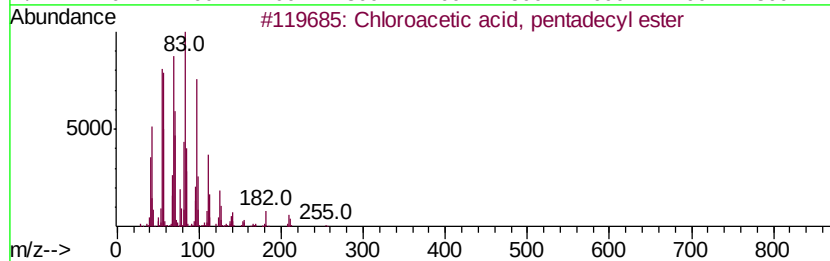
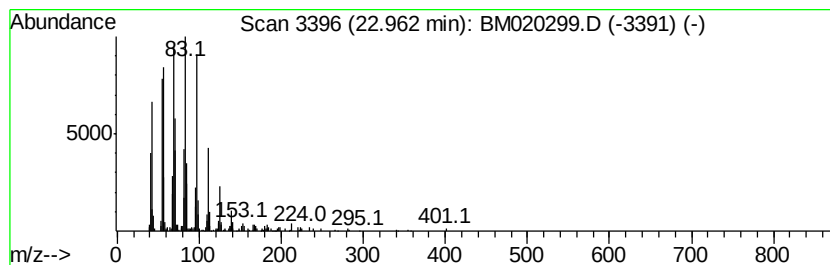
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Chloroacetic acid, pentadec... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.96	9.98 ng	543014	Perylene-d12	23.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	91
2		Trifluoroacetic acid, n-octadecyl ester	366	C20H37F3O2	079392-43-1	90
3		Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	90
4		17-Pentatriacontene	491	C35H70	006971-40-0	81
5		1-Docosene	308	C22H44	001599-67-3	76



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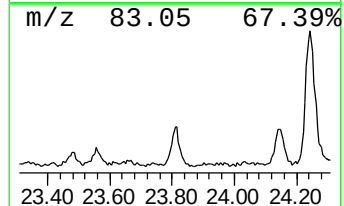
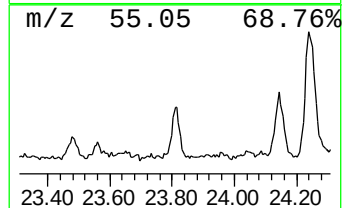
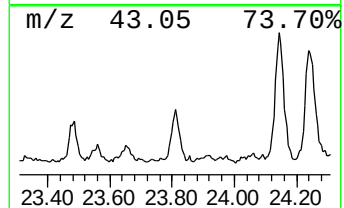
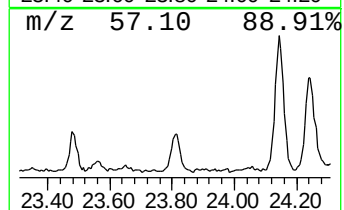
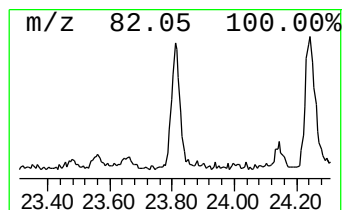
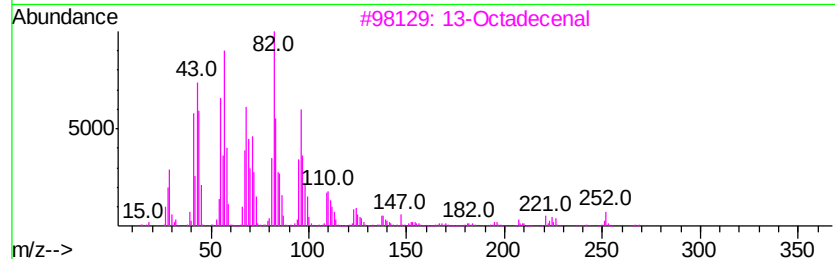
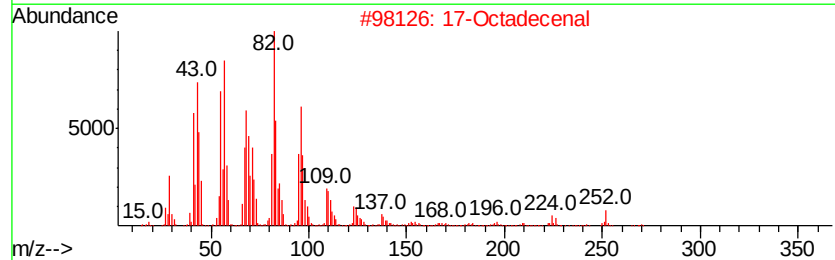
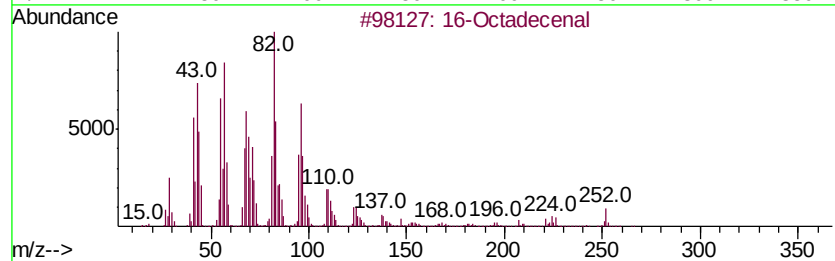
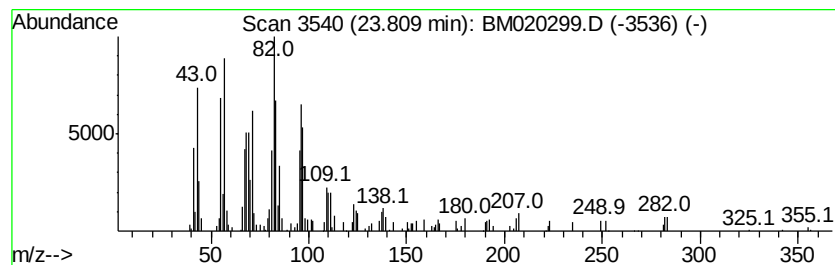
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TIC Integration Parameters: LSCINT.P

Peak Number 13 16-Octadecenal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
23.81	3.68 ng	200107	Perylene-d12		23.63
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenal	266	C18H34O	056554-87-1	94
2	17-Octadecenal	266	C18H34O	056554-86-0	94
3	13-Octadecenal	266	C18H34O	056554-90-6	91
4	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051219\
Data File : BM020299.D
Acq On : 12 May 2019 15:31
Operator : JU/SJ
Sample : K2768-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P026-SS014-0206-01

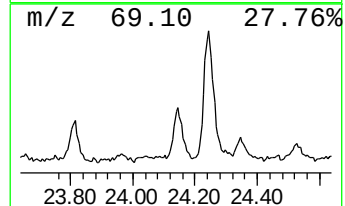
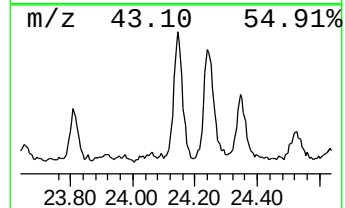
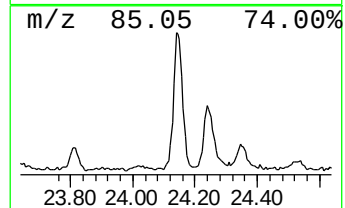
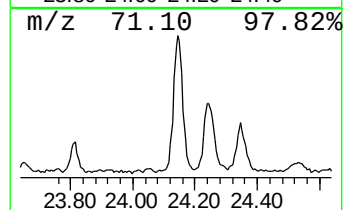
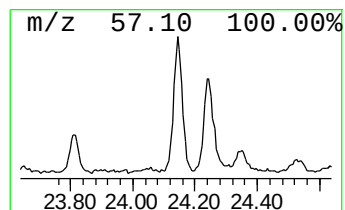
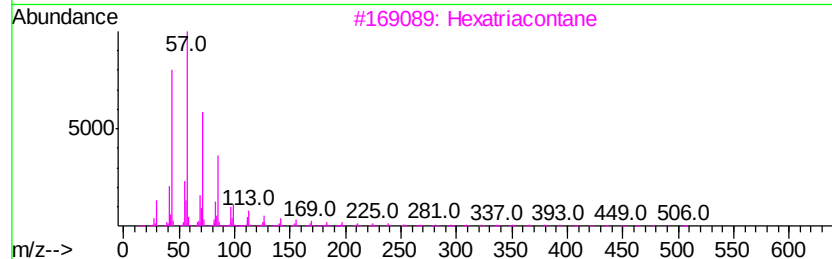
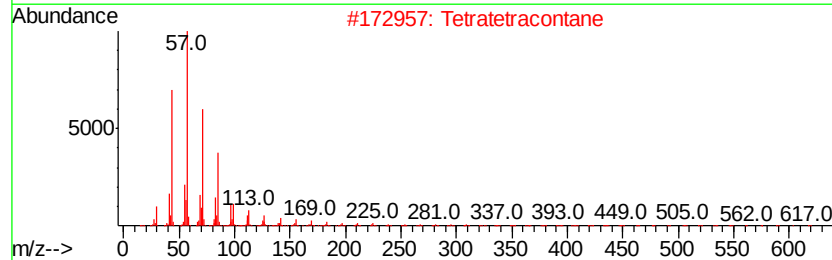
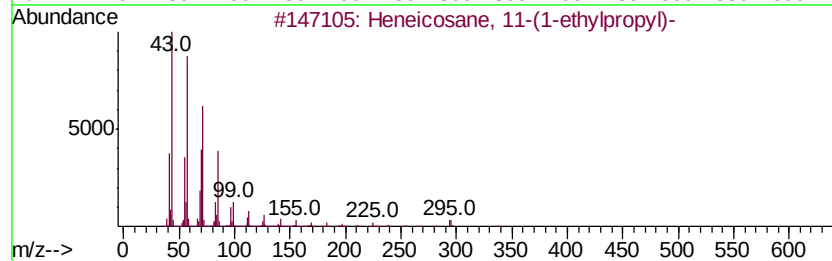
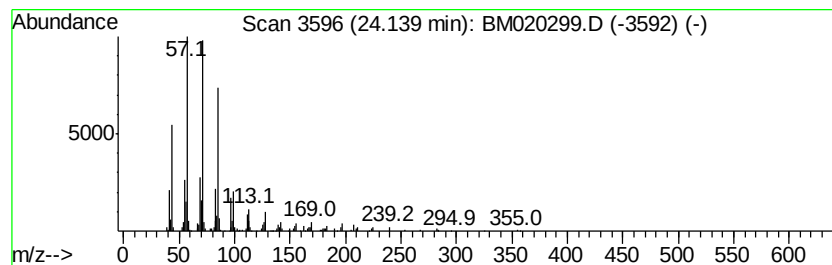
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Heneicosane, 11-(1-ethylpro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.14	6.32 ng	343706	Perylene-d12	23.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
2		Tetratetracontane	619	C44H90	007098-22-8	87
3		Hexatriacontane	507	C36H74	000630-06-8	86
4		Tricosane, 2-methyl-	338	C24H50	001928-30-9	86
5		Nonacosane	408	C29H60	000630-03-5	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051219\
Data File : BM020299.D
Acq On : 12 May 2019 15:31
Operator : JU/SJ
Sample : K2768-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

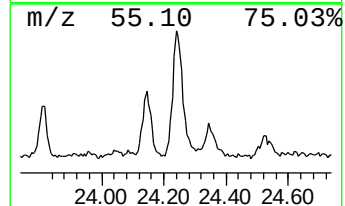
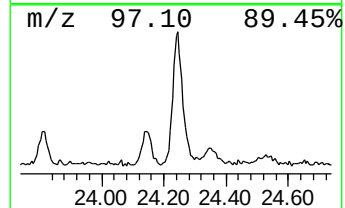
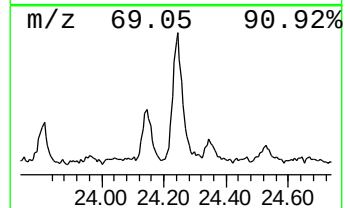
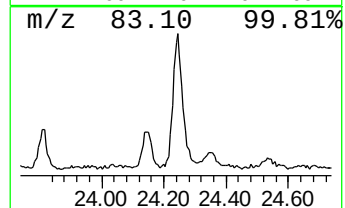
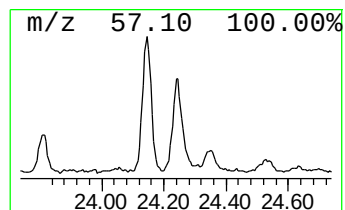
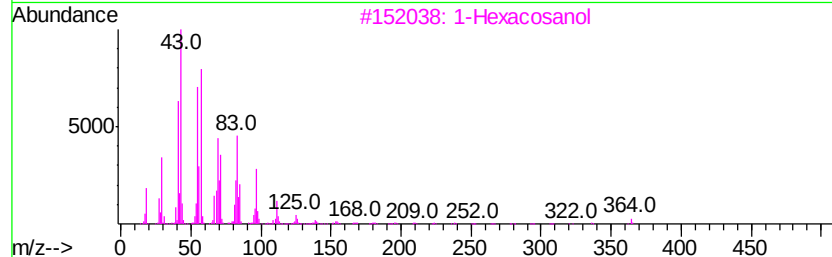
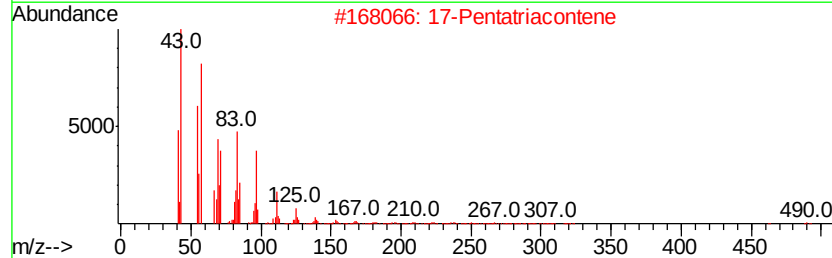
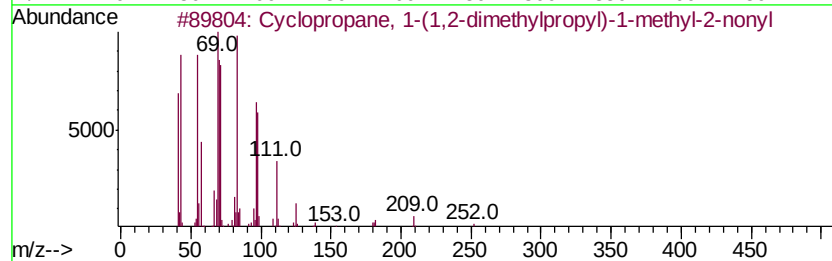
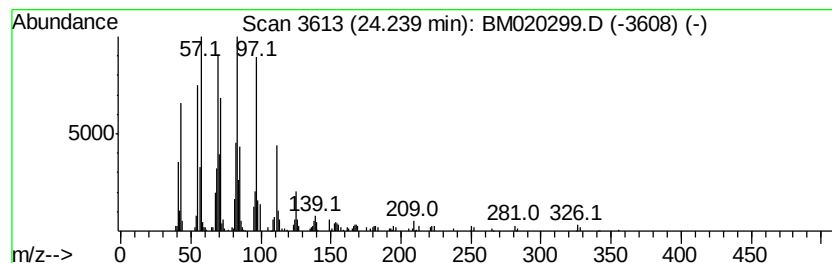
Instrument :
BNA_M
ClientSampleId :
P026-SS014-0206-01

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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 15 Cyclopropane, 1-(1,2-dimeth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.24	8.95 ng	487089	Perylene-d12	23.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1-(1,2-dimethylpro...	252	C18H36	041977-42-8	90
2	17-Pentatriacontene	491	C35H70	006971-40-0	81
3	1-Hexacosanol	382	C26H54O	000506-52-5	81
4	1-Docosene	308	C22H44	001599-67-3	68
5	Cyclotetracosane	336	C24H48	000297-03-0	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM051219\
 Data File : BM020299.D
 Acq On : 12 May 2019 15:31
 Operator : JU/SJ
 Sample : K2768-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P026-SS014-0206-01

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
unknown	7.29	109.7	ng	1804030	1	7.76	329068	20.0
n-Hexadecanoic acid	18.04	8.2	ng	278431	4	17.16	680807	20.0
2-Bromomethyl-1-i...	18.32	2.3	ng	77991	4	17.16	680807	20.0
4,4'3'-Trichlorod...	20.06	2.9	ng	169362	5	21.34	1153970	20.0
Pentafluoropropio...	21.04	16.2	ng	933655	5	21.34	1153970	20.0
Heneicosane	21.92	4.4	ng	254886	5	21.34	1153970	20.0
Acetic acid, chlo...	21.94	17.2	ng	994354	5	21.34	1153970	20.0
Tetratetracontane	22.39	2.4	ng	140546	5	21.34	1153970	20.0
Octadecanal	22.63	2.2	ng	119372	6	23.63	1087930	20.0
Triacontane	22.90	6.4	ng	349803	6	23.63	1087930	20.0
Chloroacetic acid...	22.96	10.0	ng	543014	6	23.63	1087930	20.0
16-Octadecenal	23.81	3.7	ng	200107	6	23.63	1087930	20.0
Heneicosane, 11-(...	24.14	6.3	ng	343706	6	23.63	1087930	20.0
Cyclopropane, 1-(...	24.24	8.9	ng	487089	6	23.63	1087930	20.0