

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
 Data File : BM026631.D
 Acq On : 01 Jul 2020 11:16
 Operator : JU/CG
 Sample : L3153-16
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP2-C

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-BM060520.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	4.992	352	358	372	rBV	1925638	2663435	53.36%	7.528%
2	6.563	614	625	641	rBV	1917773	2893655	57.97%	8.179%
3	7.357	753	760	769	rBV	395885	614795	12.32%	1.738%
4	7.669	806	813	826	rBV	1500816	2265434	45.39%	6.403%
5	8.504	948	955	976	rBV	1193368	1922476	38.52%	5.434%
6	10.110	1221	1228	1241	rBV	481977	792320	15.87%	2.239%
7	12.621	1648	1655	1668	rBV	2611173	3642161	72.97%	10.294%
8	13.486	1796	1802	1813	rBV	321116	469315	9.40%	1.326%
9	14.015	1878	1892	1900	rBV	664885	1037225	20.78%	2.932%
10	15.521	2140	2148	2161	rBV	2051974	2877043	57.64%	8.132%
11	16.774	2355	2361	2371	rVB	750430	1082864	21.69%	3.061%
12	16.856	2371	2375	2380	rBV3	42218	57589	1.15%	0.163%
13	17.709	2515	2520	2526	rBV	80463	115786	2.32%	0.327%
14	18.456	2643	2647	2651	rBV	44079	52202	1.05%	0.148%
15	19.339	2793	2797	2803	rBV	312064	385871	7.73%	1.091%
16	19.433	2807	2813	2818	rBV	4267210	4991414	100.00%	14.108%
17	19.856	2881	2885	2889	rVB	47288	51379	1.03%	0.145%
18	20.291	2955	2959	2964	rVB	162932	193951	3.89%	0.548%
19	20.562	3001	3005	3011	rBV	259582	286439	5.74%	0.810%
20	20.739	3031	3035	3045	rBV	476751	670509	13.43%	1.895%
21	20.986	3072	3077	3082	rBV	1023937	1212757	24.30%	3.428%
22	21.186	3107	3111	3118	rBV3	64624	97291	1.95%	0.275%
23	21.350	3137	3139	3144	rVB3	49902	51126	1.02%	0.145%
24	21.615	3177	3184	3191	rBV2	346541	711982	14.26%	2.012%
25	22.021	3251	3253	3257	rVB	98963	104817	2.10%	0.296%
26	22.233	3286	3289	3295	rVB	147381	174368	3.49%	0.493%
27	22.485	3328	3332	3336	rBV	560211	737380	14.77%	2.084%
28	22.533	3336	3340	3349	rVB	255025	432577	8.67%	1.223%
29	22.997	3416	3419	3424	rVB	122758	176732	3.54%	0.500%
30	23.068	3425	3431	3438	rVV2	740615	1245187	24.95%	3.519%
31	23.280	3463	3467	3474	rVB	245969	350821	7.03%	0.992%
32	23.580	3513	3518	3525	rVB	604770	999826	20.03%	2.826%
33	23.662	3527	3532	3543	rVB2	254676	554542	11.11%	1.567%
34	24.638	3694	3698	3705	rVB	168047	309719	6.21%	0.875%

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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SP2-C

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	25.797	3889	3895	3909	rVB3	357406	1156184	23.16%	3.268%
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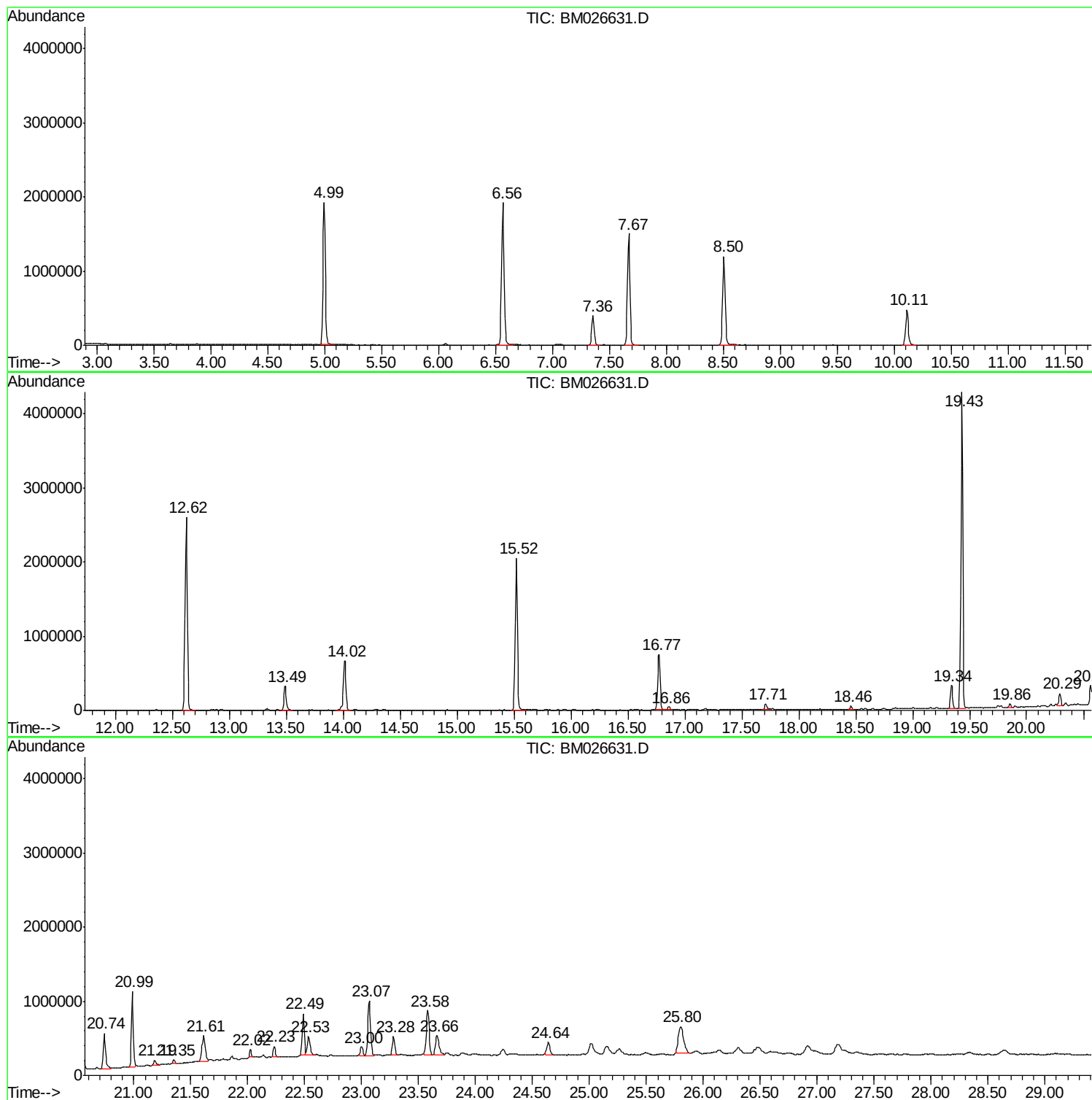
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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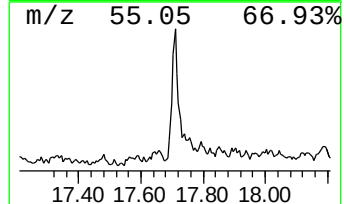
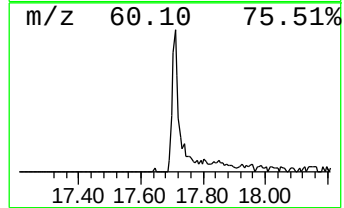
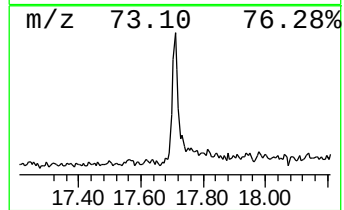
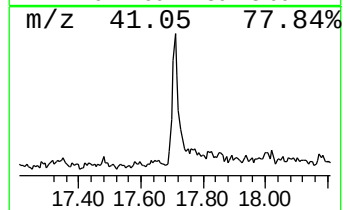
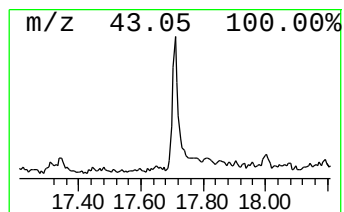
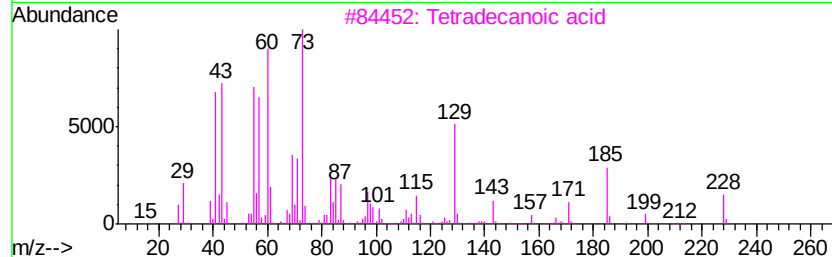
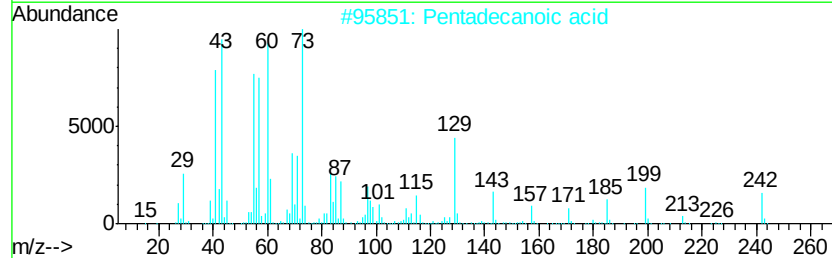
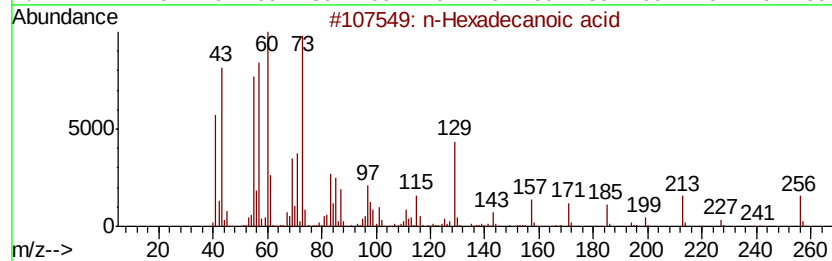
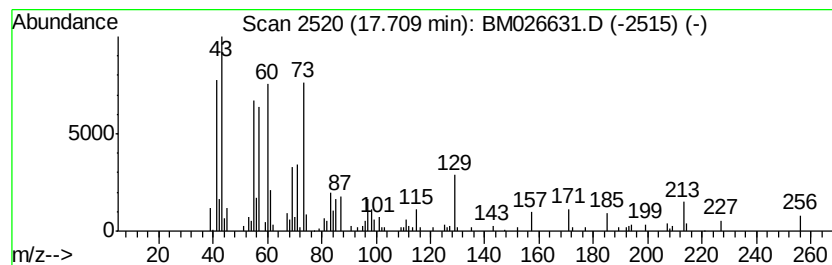
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.71	2.14 ng	115786	Phenanthrene-d10	16.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Tridecanoic acid	214	C13H26O2	000638-53-9	76
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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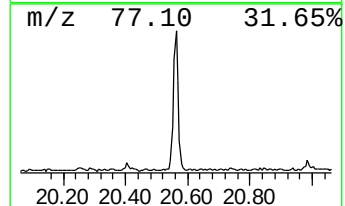
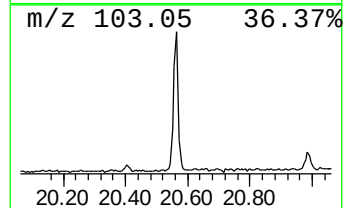
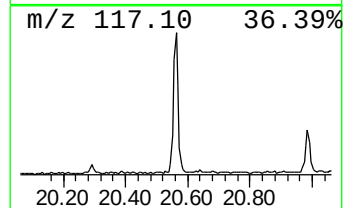
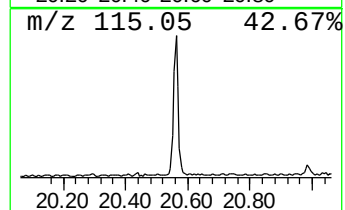
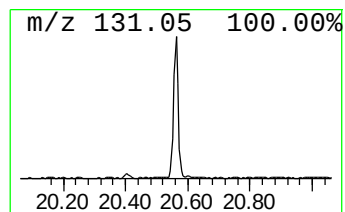
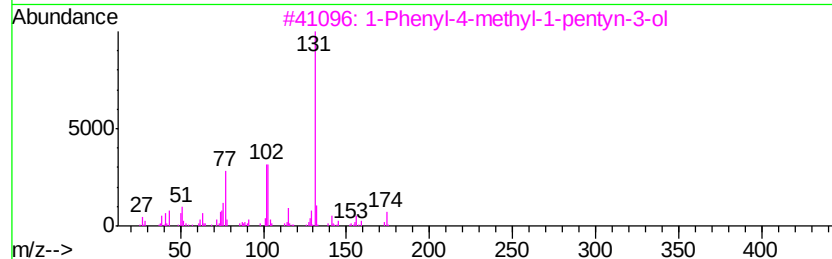
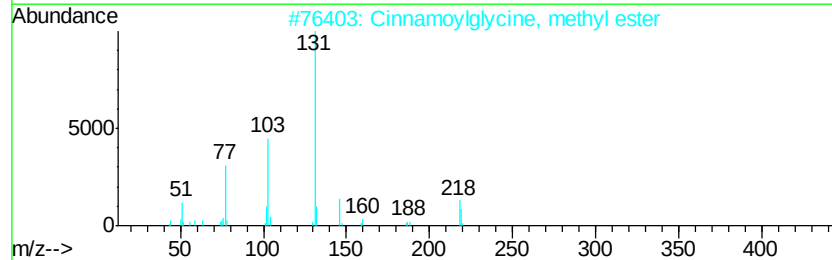
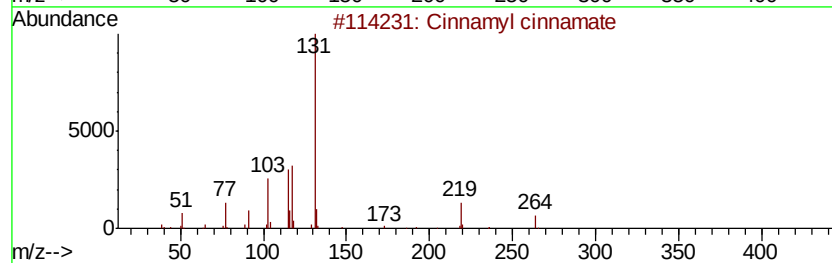
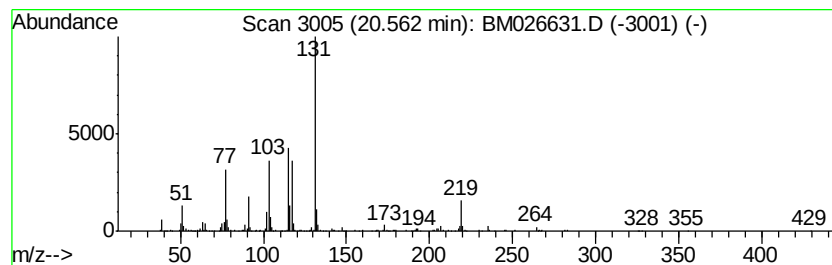
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cinnamyl cinnamate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.56	4.72 ng	286439	Chrysene-d12	20.99
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Cinnamyl cinnamate	264 C18H16O2	000122-69-0	64
2	Cinnamoylglycine, methyl ester	219 C12H13NO3	040778-04-9	49
3	1-Phenyl-4-methyl-1-pentyn-3-ol	174 C12H14O	005923-02-4	47
4	1-Penten-3-one, 4-methyl-1-phenyl-	174 C12H14O	003160-32-5	47
5	trans-1-Cinnamoylimidazole	198 C12H10N2O	001138-15-4	47



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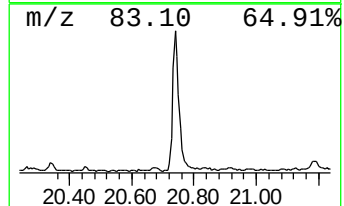
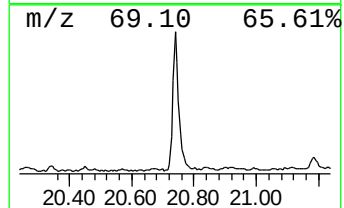
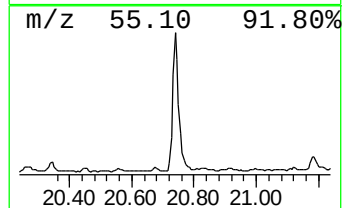
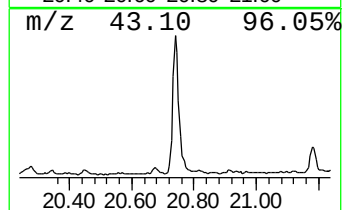
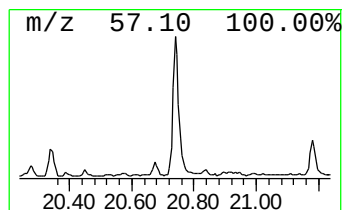
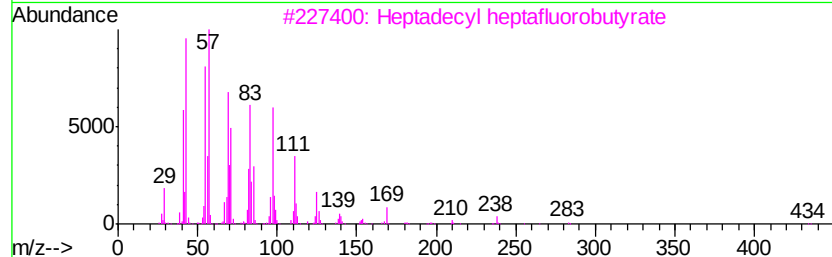
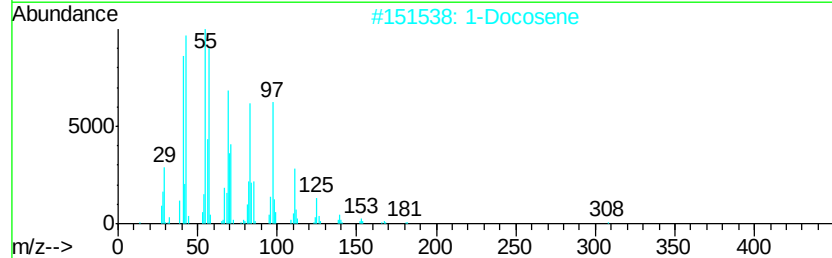
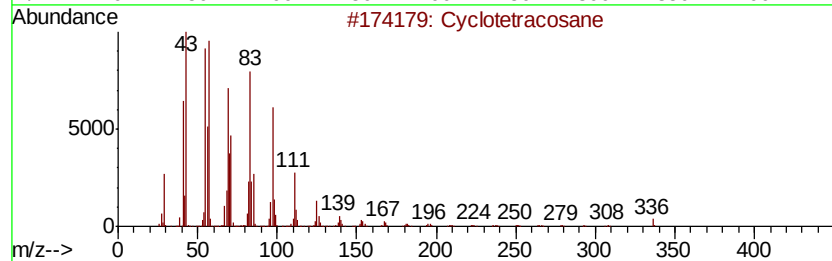
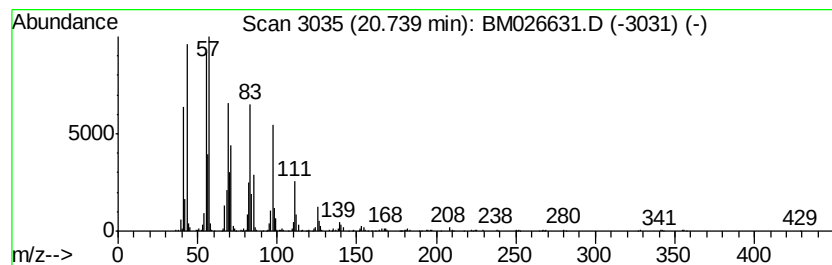
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclotetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.74	11.06 ng	670509	Chrysene-d12	20.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetracosane	336	C24H48	000297-03-0	95
2		1-Docosene	308	C22H44	001599-67-3	95
3		Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	94
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94



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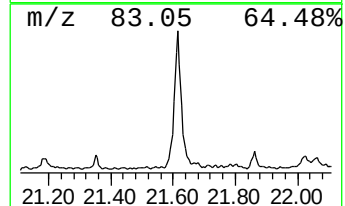
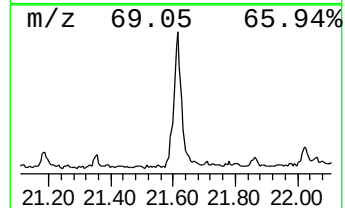
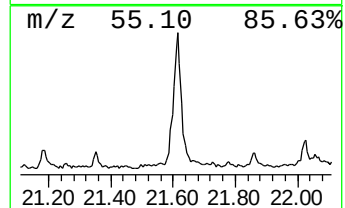
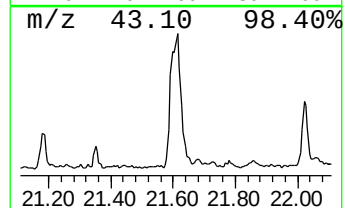
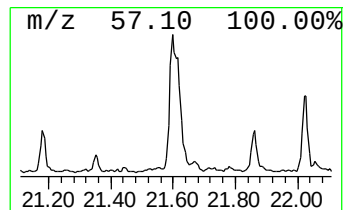
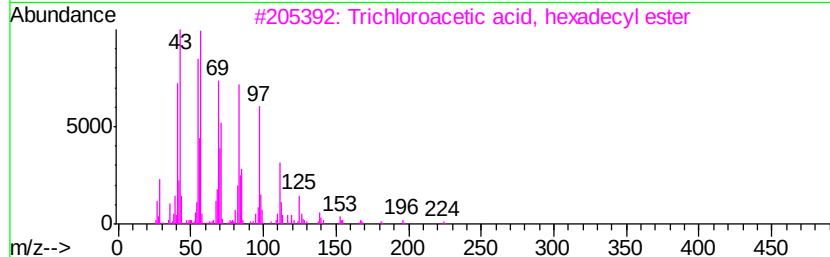
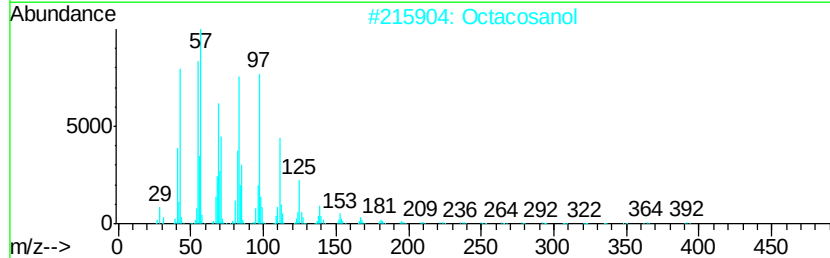
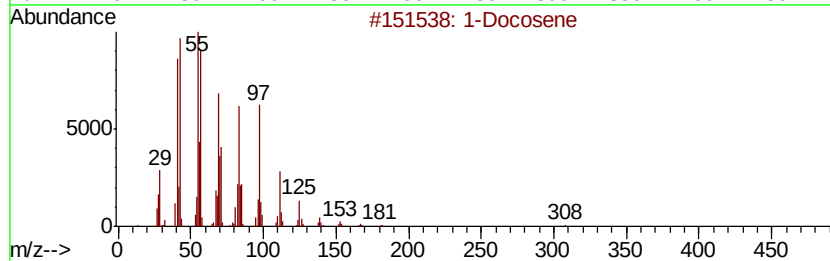
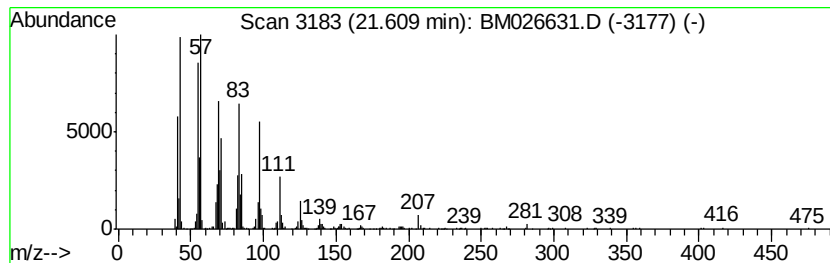
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.61	11.74 ng	711982	Chrysene-d12	20.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	95
2		Octacosanol	410	C28H58O	000557-61-9	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
4		Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
5		1-Heptacosanol	396	C27H56O	002004-39-9	91



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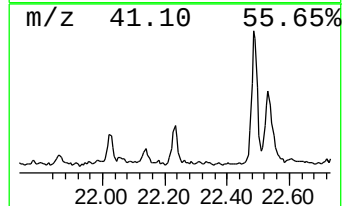
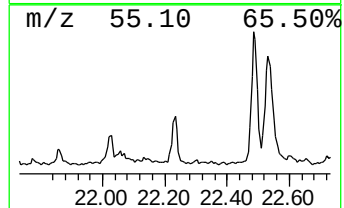
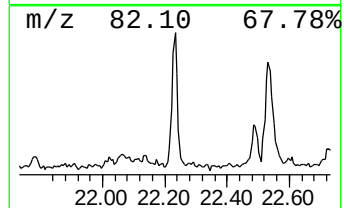
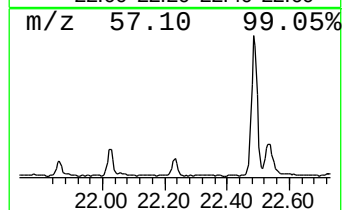
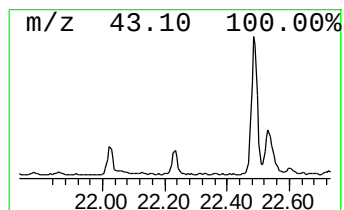
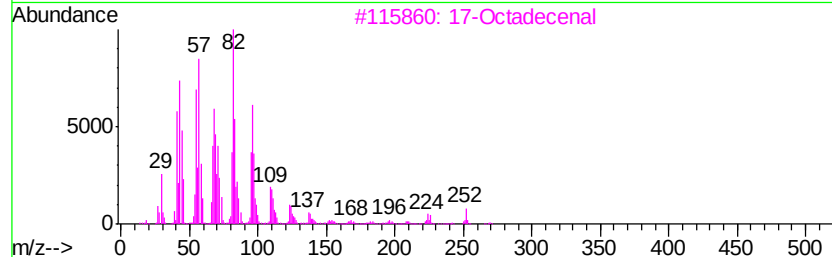
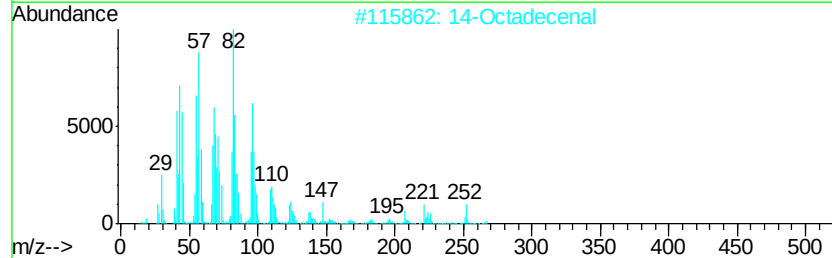
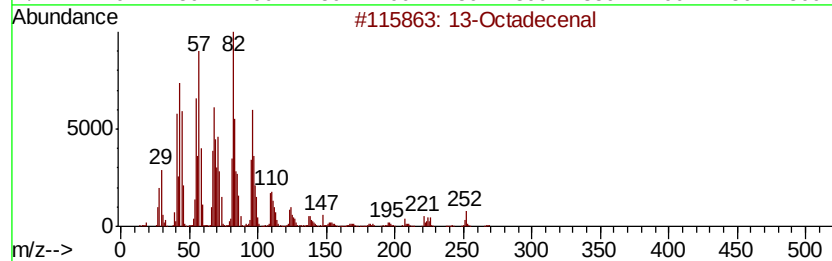
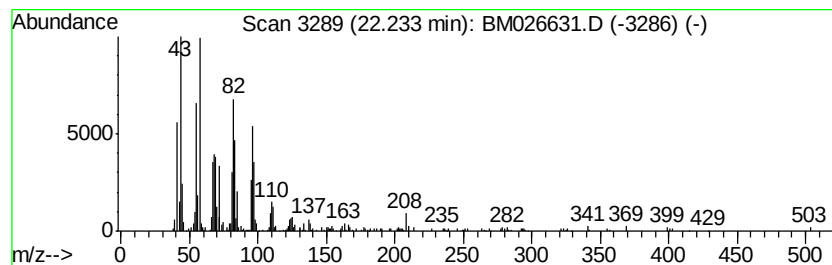
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 8 13-Octadecenal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.23	2.80 ng	174368	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Octadecenal	266	C18H34O	056554-90-6	93
2		14-Octadecenal	266	C18H34O	056554-89-3	90
3		17-Octadecenal	266	C18H34O	056554-86-0	87
4		1,19-Eicosadiene	278	C20H38	014811-95-1	83
5		Octadecanal	268	C18H36O	000638-66-4	80



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ClientSampleId :
SP2-C

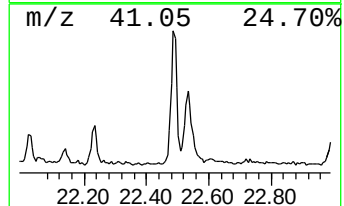
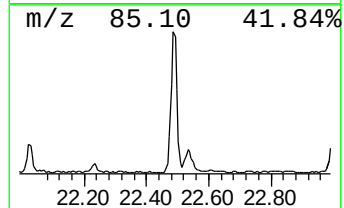
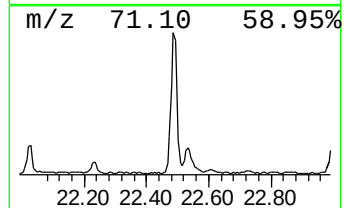
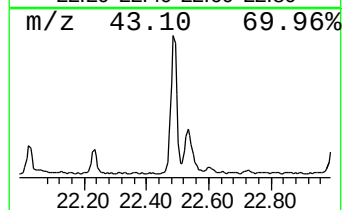
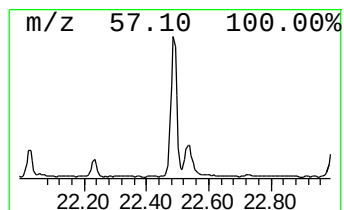
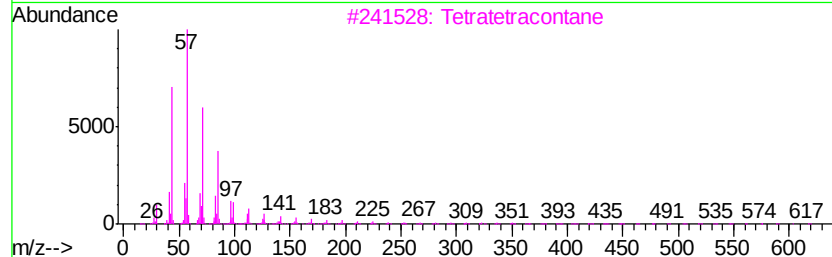
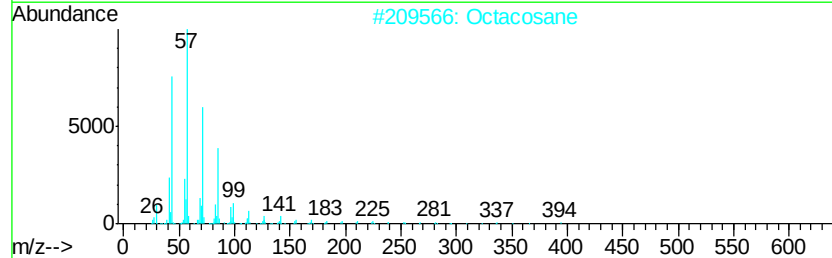
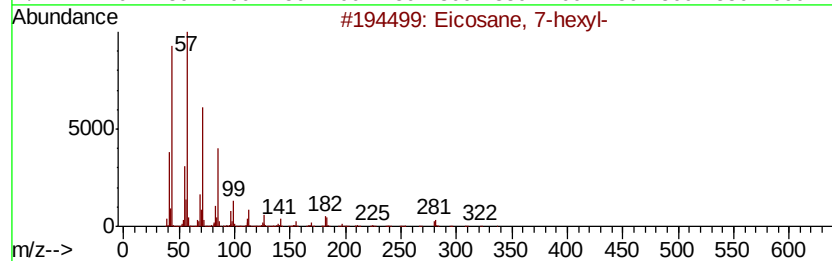
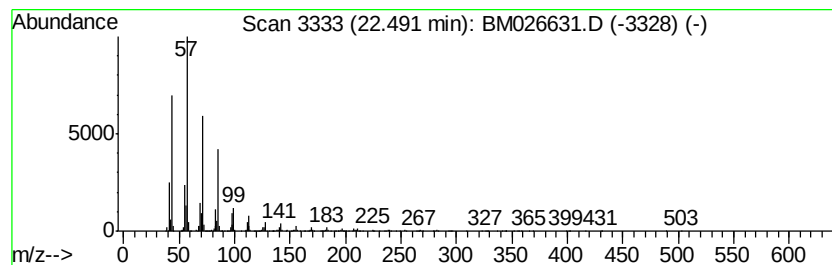
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.49	11.84 ng	737380	Perylene-d12	23.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91	
2	Octacosane	394	C28H58	000630-02-4	91	
3	Tetratetracontane	619	C44H90	007098-22-8	91	
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91	
5	Heptacosane	380	C27H56	000593-49-7	91	



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026631.D
Acq On : 01 Jul 2020 11:16
Operator : JU/CG
Sample : L3153-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP2-C

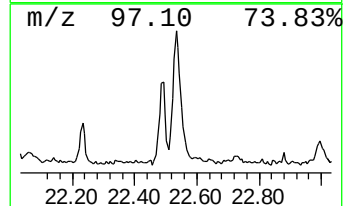
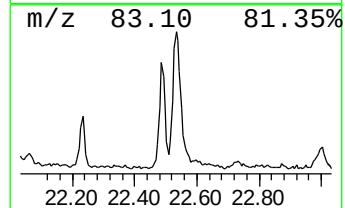
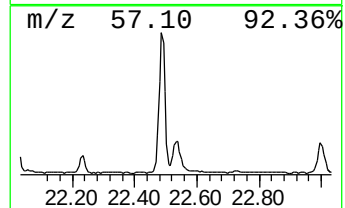
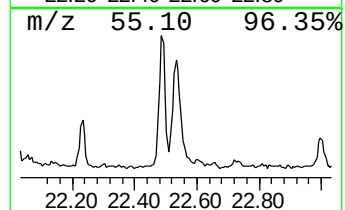
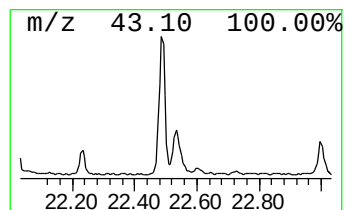
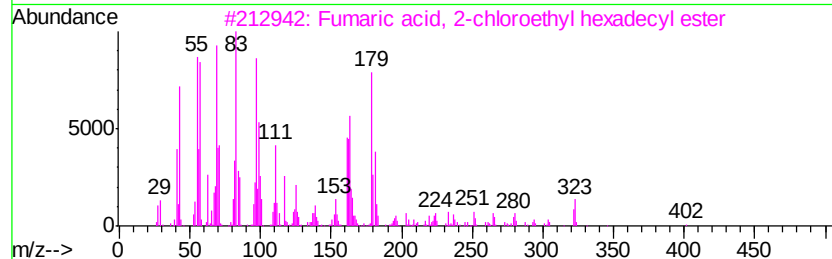
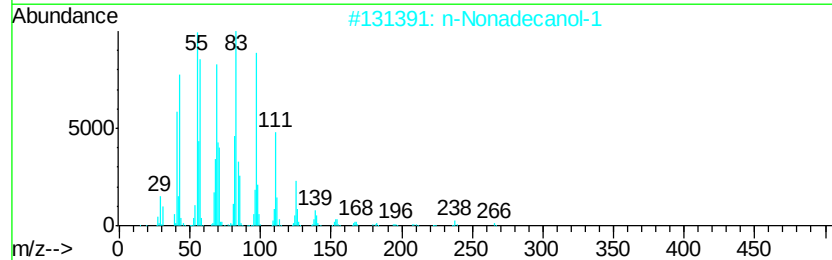
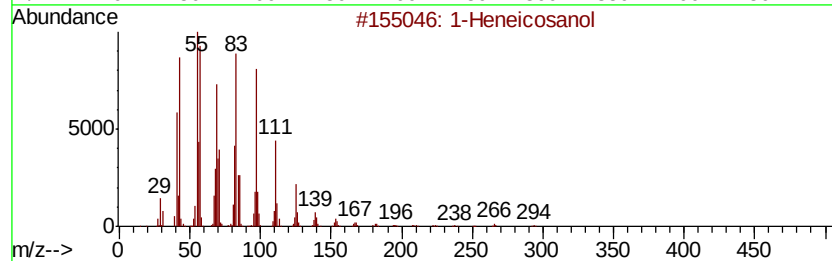
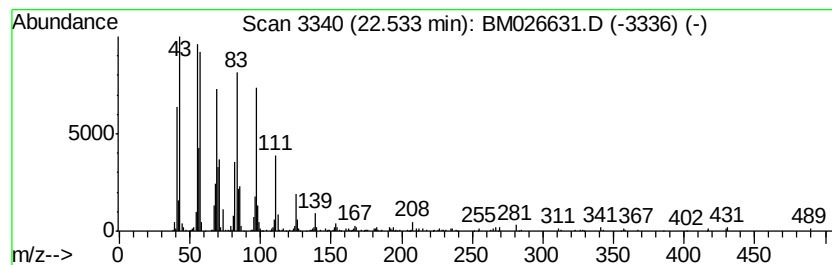
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.53	6.95 ng	432577	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3		Fumaric acid, 2-chloroethyl hexa...	402	C22H39ClO4	1000330-62-2	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
5		1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
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ClientSampleId :
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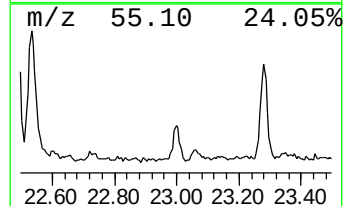
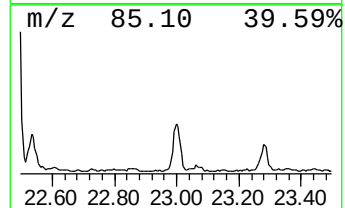
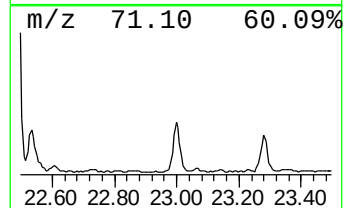
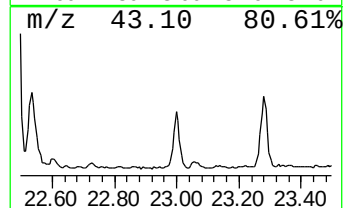
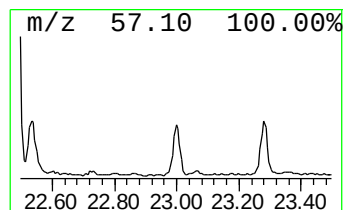
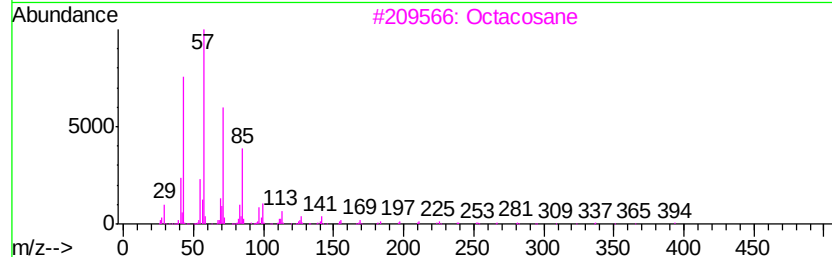
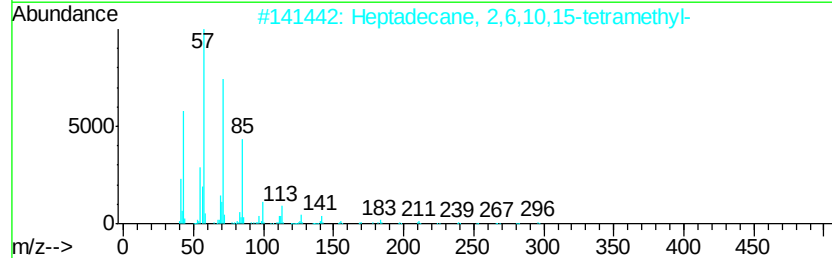
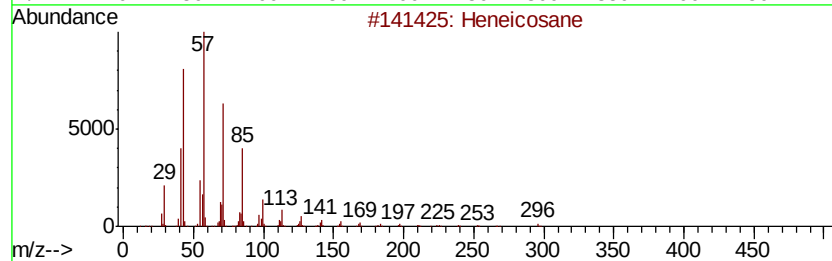
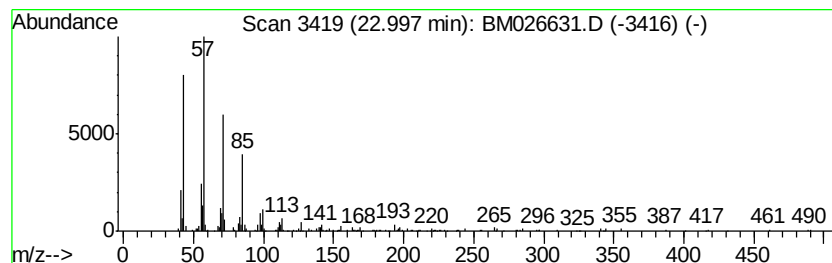
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.00	2.84 ng	176732	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	93
2		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3		Octacosane	394	C28H58	000630-02-4	90
4		Heptacosane	380	C27H56	000593-49-7	87
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026631.D
Acq On : 01 Jul 2020 11:16
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Sample : L3153-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

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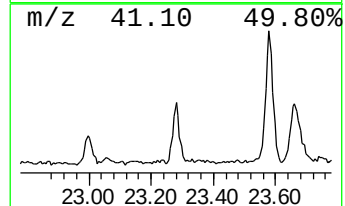
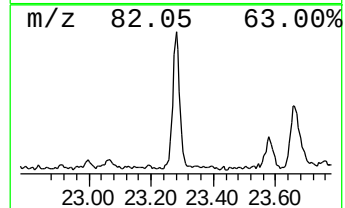
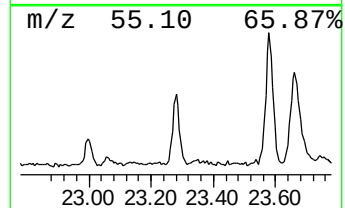
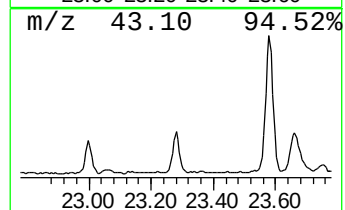
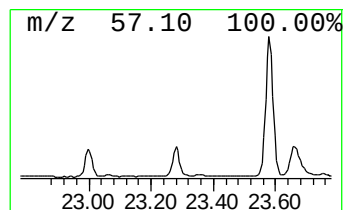
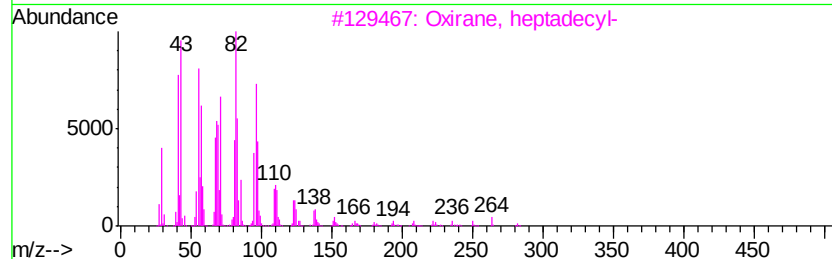
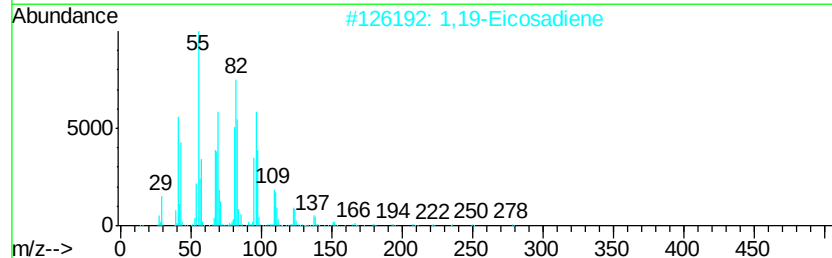
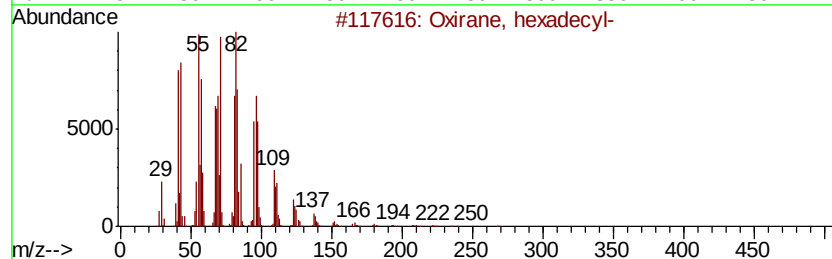
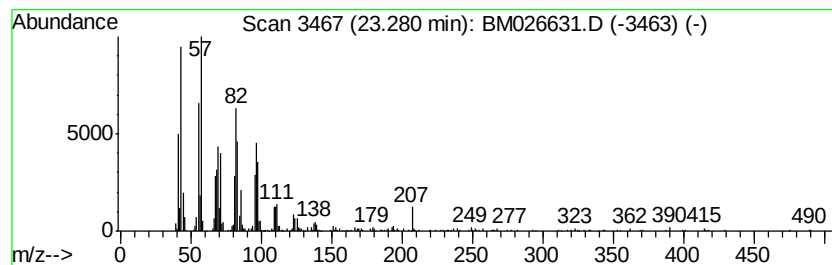
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Oxirane, hexadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.28	5.63 ng	350821	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
2		1,19-Eicosadiene	278	C20H38	014811-95-1	70
3		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	62
4		(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	58
5		Pentadecanal-	226	C15H30O	002765-11-9	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
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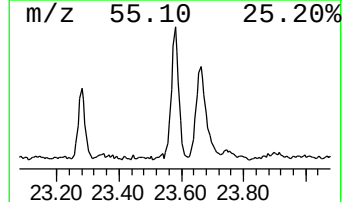
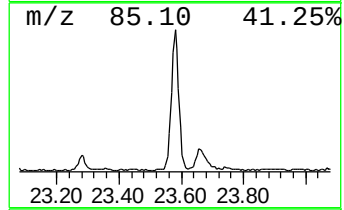
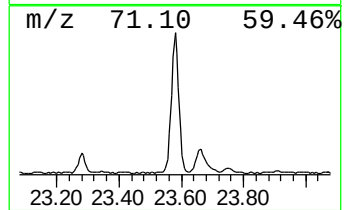
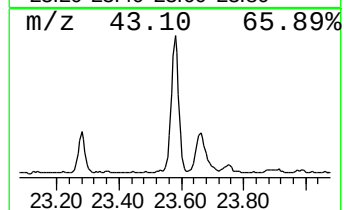
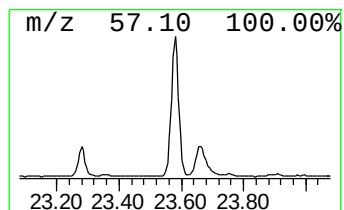
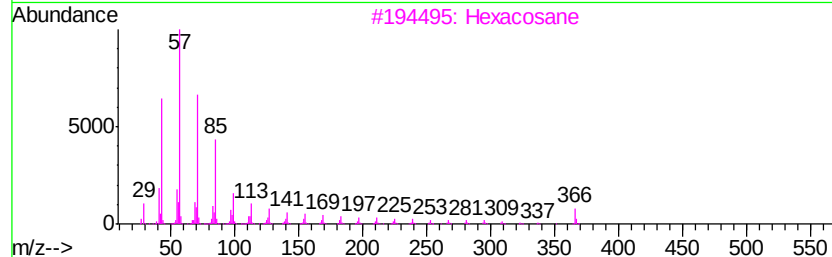
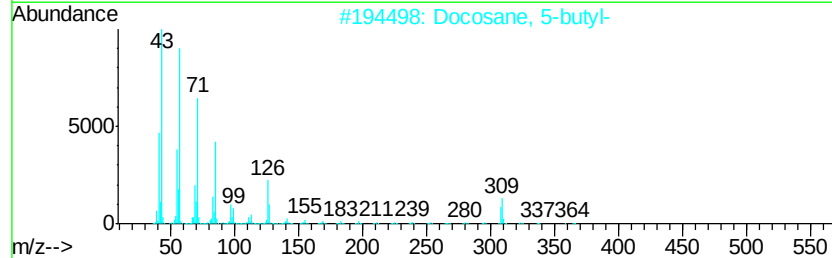
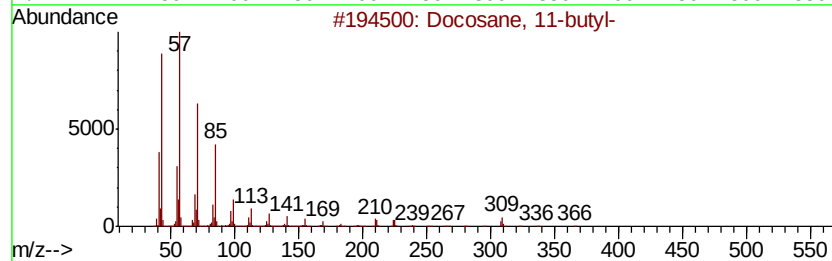
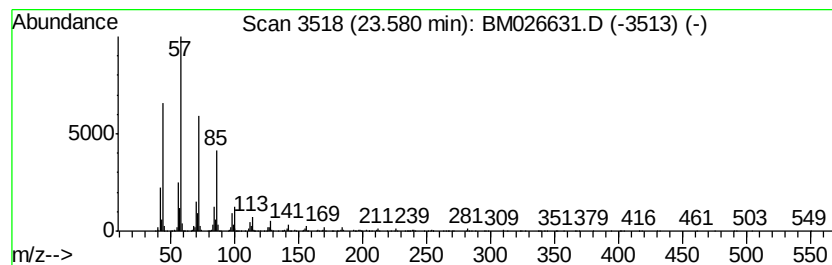
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 13 Docosane, 11-butyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.58	16.06 ng	999826	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 11-butyl-	366	C26H54	013475-76-8	95
2		Docosane, 5-butyl-	366	C26H54	055282-16-1	93
3		Hexacosane	366	C26H54	000630-01-3	93
4		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
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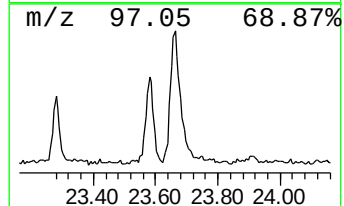
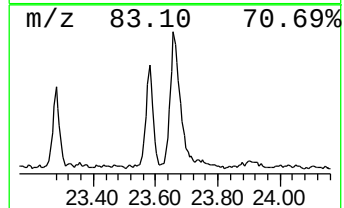
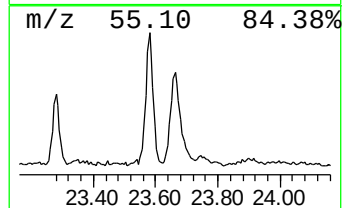
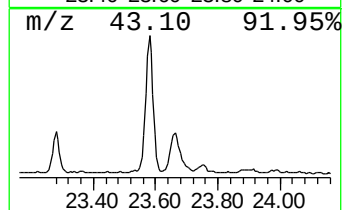
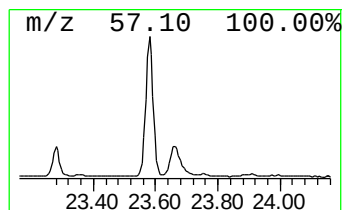
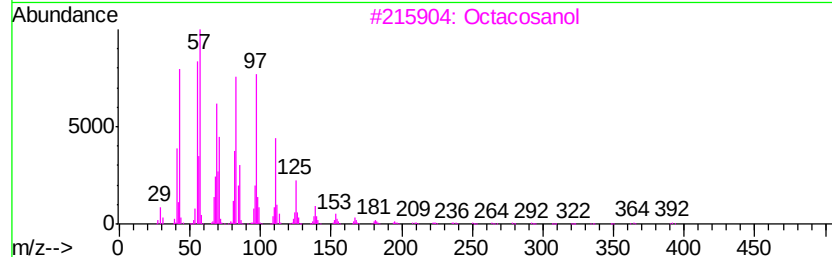
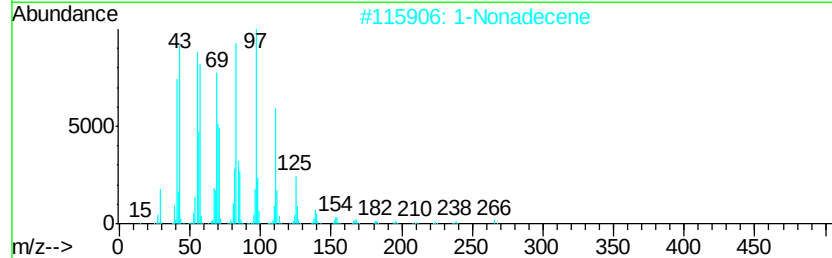
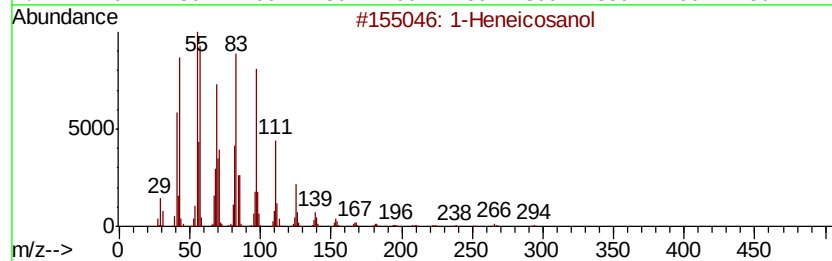
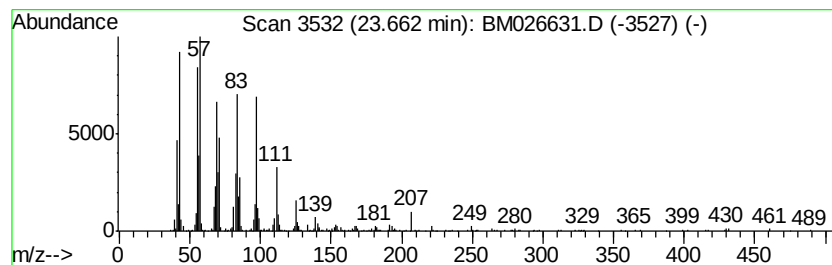
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.66	8.91 ng	554542	Perylene-d12	23.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8 93
2		1-Nonadecene	266 C19H38	018435-45-5 93
3		Octacosanol	410 C28H58O	000557-61-9 93
4		1-Heptacosanol	396 C27H56O	002004-39-9 90
5		Pentafluoropropionic acid, hepta...	402 C20H35F5O2	959218-78-1 90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026631.D
Acq On : 01 Jul 2020 11:16
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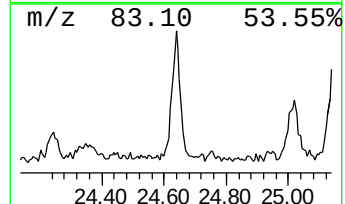
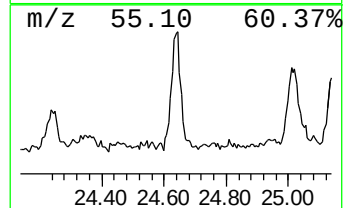
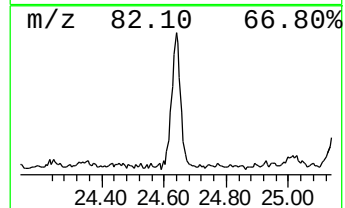
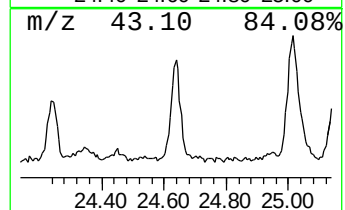
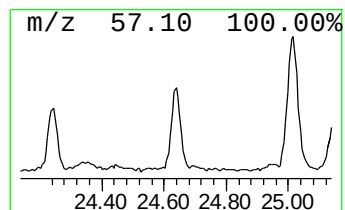
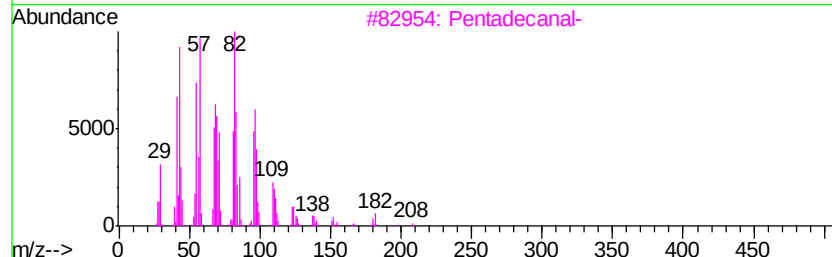
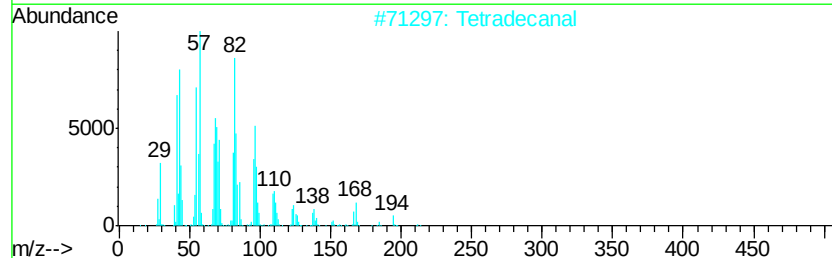
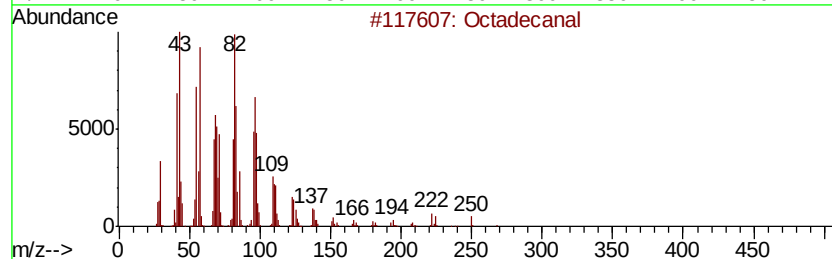
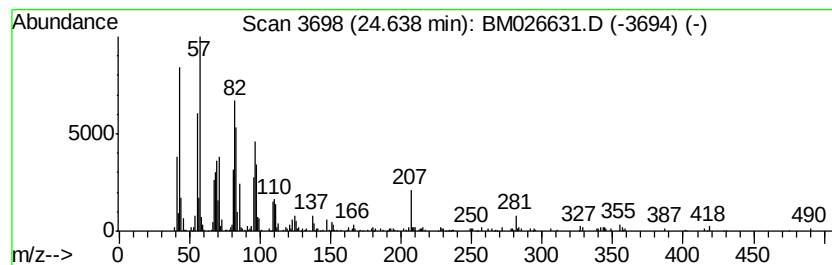
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Octadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.64	4.97 ng	309719	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanal	268	C18H36O	000638-66-4	93
2		Tetradecanal	212	C14H28O	000124-25-4	93
3		Pentadecanal-	226	C15H30O	002765-11-9	90
4		17-Octadecenal	266	C18H34O	056554-86-0	86
5		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM070120\
Data File : BM026631.D
Acq On : 01 Jul 2020 11:16
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Sample : L3153-16
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SP2-C

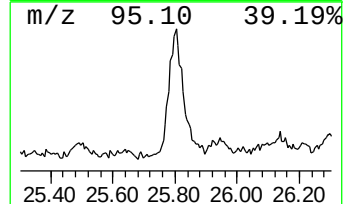
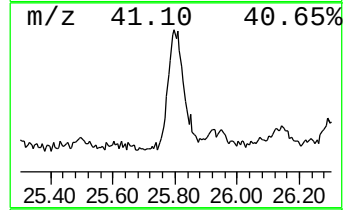
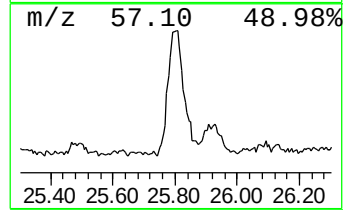
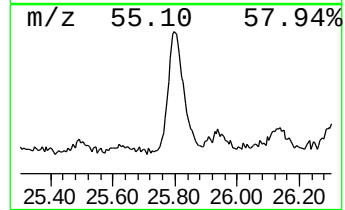
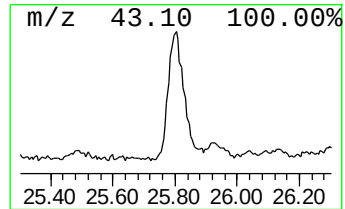
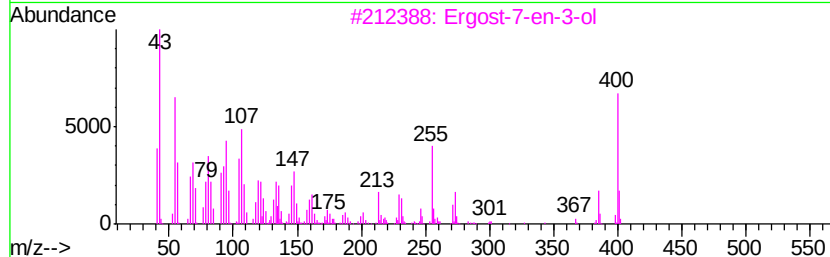
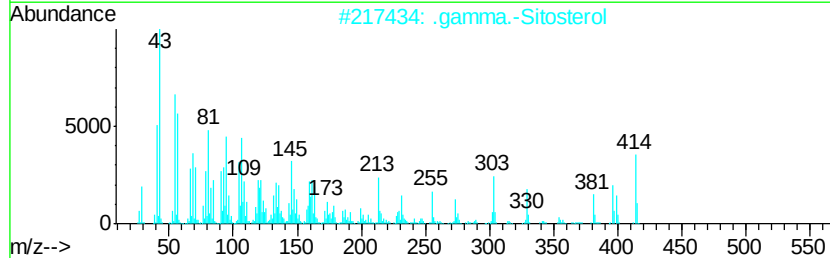
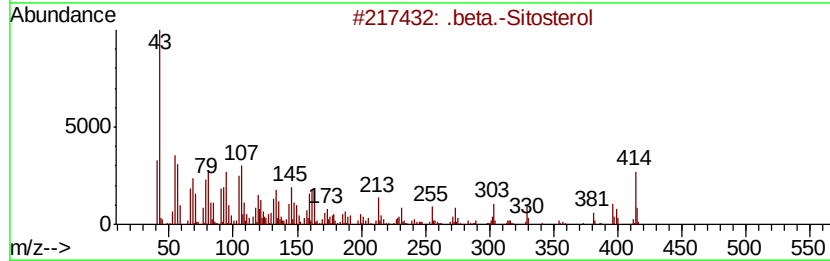
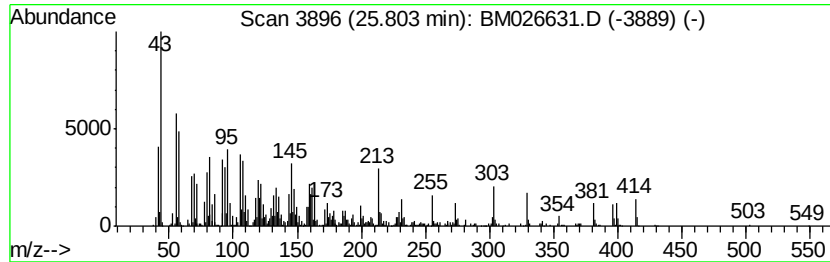
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 .beta.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.80	18.57 ng	1156180	Perylene-d12	23.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.beta.-Sitosterol	414	C29H50O	000083-46-5	89
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	60
3		Ergost-7-en-3-ol	400	C28H48O	116179-22-7	55
4		.alpha.-Ergosterol	400	C28H48O	000632-32-6	38
5		Isocholesteryl methyl ether	400	C28H48O	029944-53-4	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM070120\
 Data File : BM026631.D
 Acq On : 01 Jul 2020 11:16
 Operator : JU/CG
 Sample : L3153-16
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP2-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM060520.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
n-Hexadecanoic acid	17.71	2.1 ng		115786	4	16.77	1082860	20.0
Cinnamyl cinnamate	20.56	4.7 ng		286439	5	20.99	1212760	20.0
Cyclotetracosane	20.74	11.1 ng		670509	5	20.99	1212760	20.0
1-Docosene	21.61	11.7 ng		711982	5	20.99	1212760	20.0
13-Octadecenal	22.23	2.8 ng		174368	6	23.07	1245190	20.0
Eicosane, 7-hexyl-	22.49	11.8 ng		737380	6	23.07	1245190	20.0
1-Heneicosanol	22.53	7.0 ng		432577	6	23.07	1245190	20.0
Heneicosane	23.00	2.8 ng		176732	6	23.07	1245190	20.0
Oxirane, hexadecyl-	23.28	5.6 ng		350821	6	23.07	1245190	20.0
Docosane, 11-butyl-	23.58	16.1 ng		999826	6	23.07	1245190	20.0
1-Nonadecene	23.66	8.9 ng		554542	6	23.07	1245190	20.0
Octadecanal	24.64	5.0 ng		309719	6	23.07	1245190	20.0
.beta.-Sitosterol	25.80	18.6 ng		1156180	6	23.07	1245190	20.0