

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM032119\
 Data File : BM019302.D
 Acq On : 21 Mar 2019 22:09
 Operator : JU/SJ
 Sample : K2004-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-19B(13.5-14.5)

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-BM031119.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	5.234	375	382	404	rBV	3624050	5257035	54.68%	6.412%
2	6.816	644	651	667	rBV	3851729	6394269	66.50%	7.800%
3	7.163	703	710	724	rBV	3914935	6274608	65.26%	7.654%
4	7.628	782	789	796	rBV	729849	1118535	11.63%	1.364%
5	7.946	835	843	853	rBV	2715183	4306855	44.79%	5.253%
6	8.798	980	988	1003	rBV	2188374	3614860	37.60%	4.409%
7	9.887	1166	1173	1184	rBV	64334	144566	1.50%	0.176%
8	10.410	1255	1262	1269	rBV	1014690	1682020	17.49%	2.052%
9	12.898	1678	1685	1700	rBV	6260245	8980159	93.40%	10.954%
10	13.233	1734	1742	1748	rBV	64701	128520	1.34%	0.157%
11	13.751	1824	1830	1836	rBV	428846	611270	6.36%	0.746%
12	14.286	1914	1921	1936	rVB2	1647724	2481245	25.81%	3.027%
13	15.786	2170	2176	2189	rBV	4956425	7211750	75.01%	8.797%
14	16.827	2348	2353	2362	rVB4	62812	113263	1.18%	0.138%
15	17.045	2383	2390	2399	rBV	1759126	2620824	27.26%	3.197%
16	17.933	2536	2541	2552	rBV	399280	630914	6.56%	0.770%
17	19.221	2757	2760	2770	rBV	115471	213444	2.22%	0.260%
18	19.686	2833	2839	2846	rBV	6705845	8246499	85.77%	10.059%
19	20.662	3002	3005	3011	rBV	111500	109349	1.14%	0.133%
20	20.874	3037	3041	3049	rBV2	248365	367641	3.82%	0.448%
21	20.951	3050	3054	3063	rVV	699789	1137693	11.83%	1.388%
22	21.245	3100	3104	3114	rBV	1640524	2035751	21.17%	2.483%
23	21.568	3155	3159	3163	rBV3	216519	276019	2.87%	0.337%
24	21.809	3198	3200	3203	rBV	127873	137784	1.43%	0.168%
25	21.845	3203	3206	3214	rVB2	247028	398133	4.14%	0.486%
26	23.474	3477	3483	3493	rVB	1106748	2111929	21.97%	2.576%
27	26.656	4014	4024	4039	rVB2	1789942	5762147	59.93%	7.029%
28	27.044	4079	4090	4113	rVB2	2540966	9614811	100.00%	11.728%

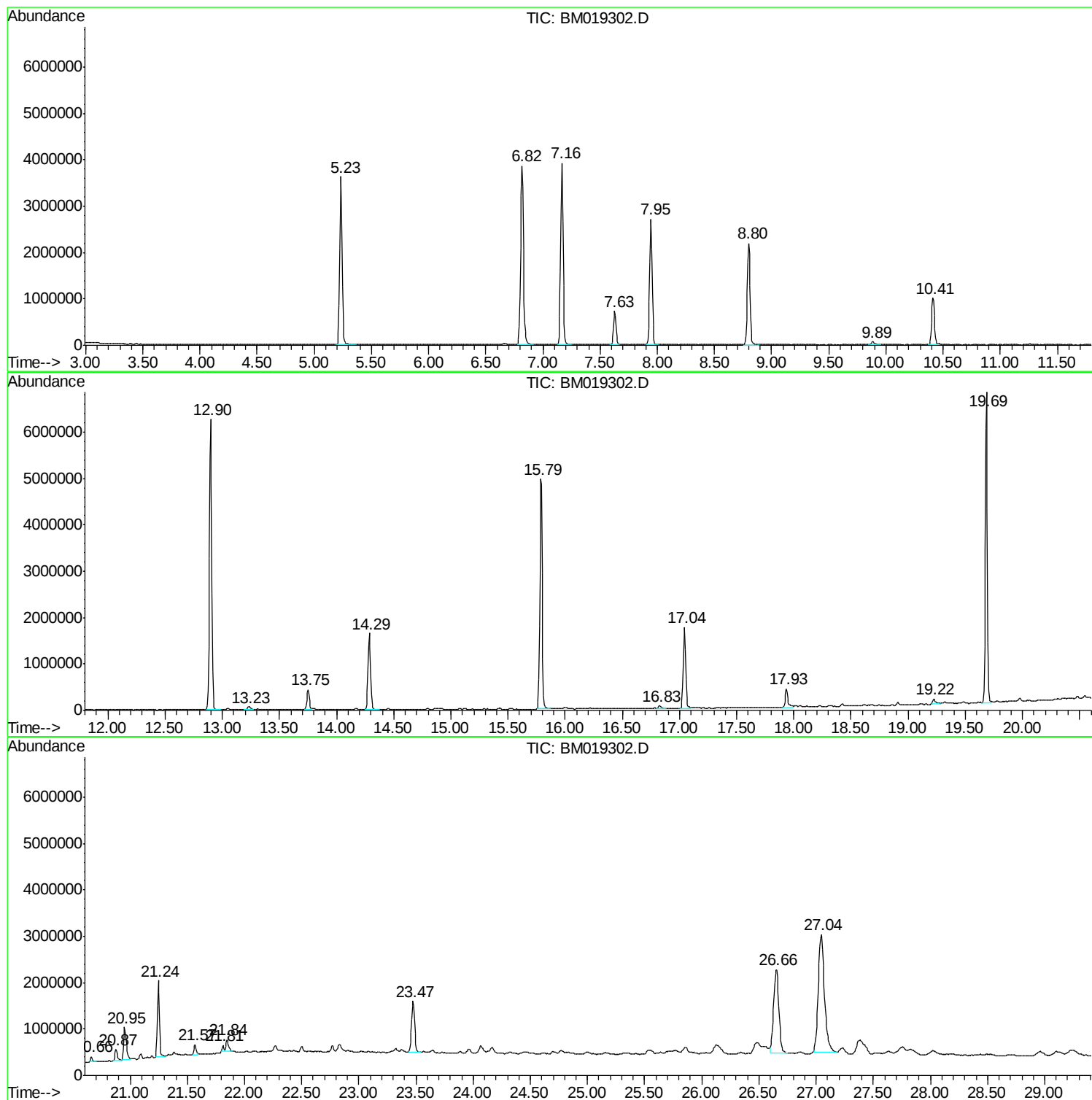
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ClientSampleId :
SB-19B(13.5-14.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM031119.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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ClientSampled :
SB-19B(13.5-14.5)

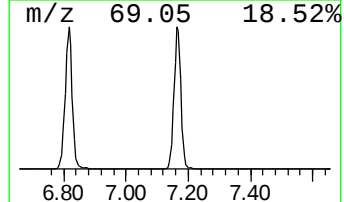
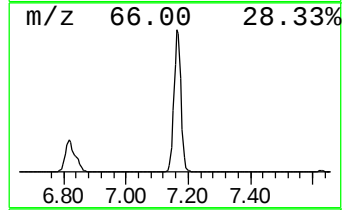
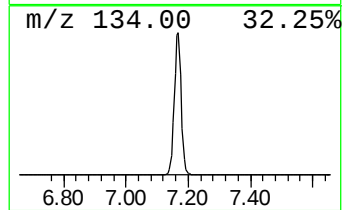
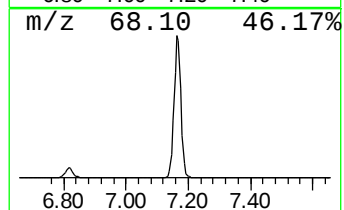
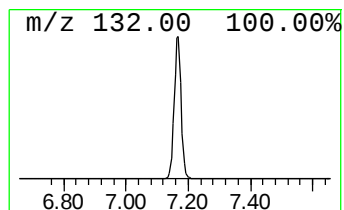
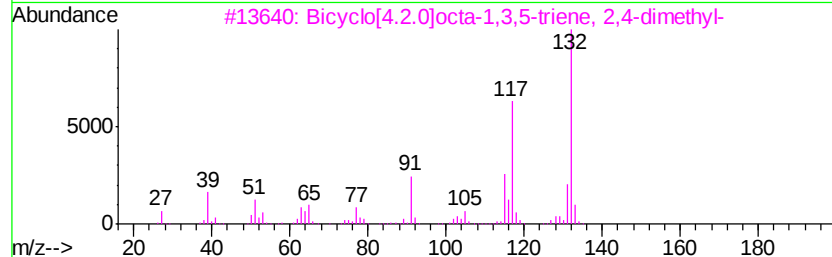
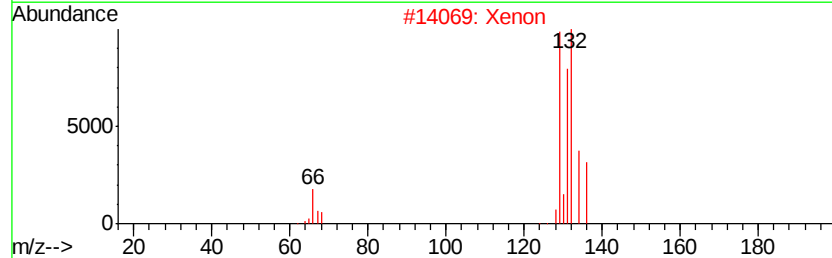
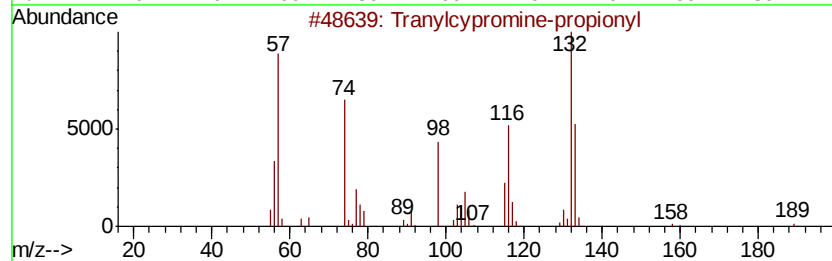
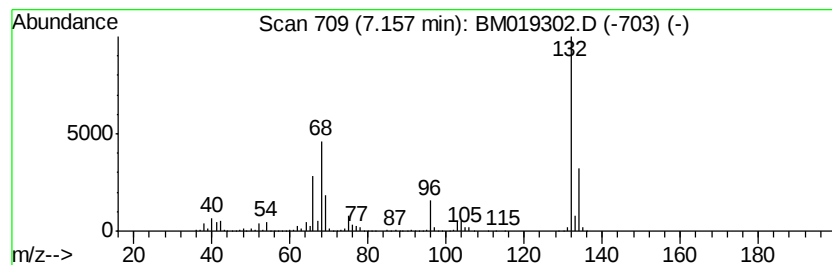
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	112.19 ng	6274610	1,4-Dichlorobenzene-d4	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Xenon	132	Xe	007440-63-3	9
3		Bicvclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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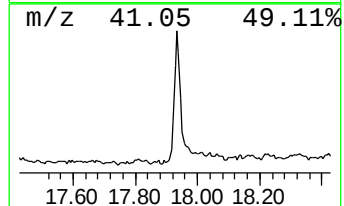
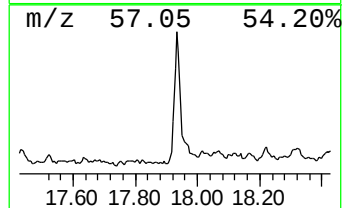
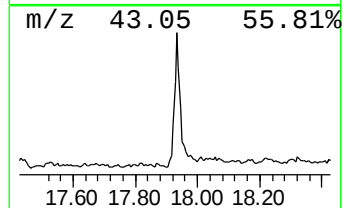
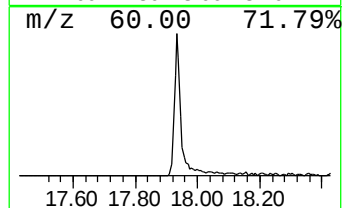
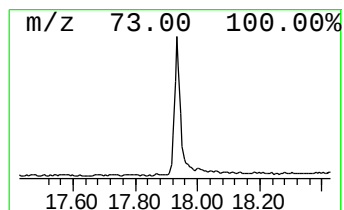
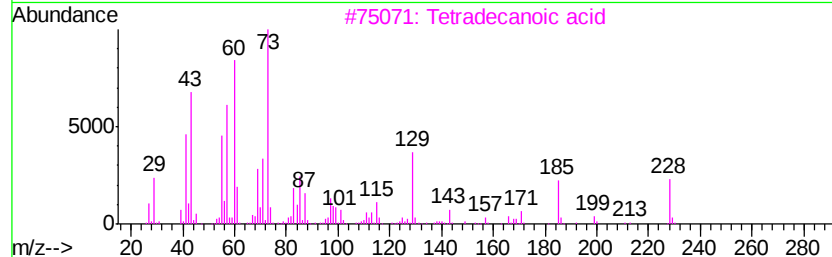
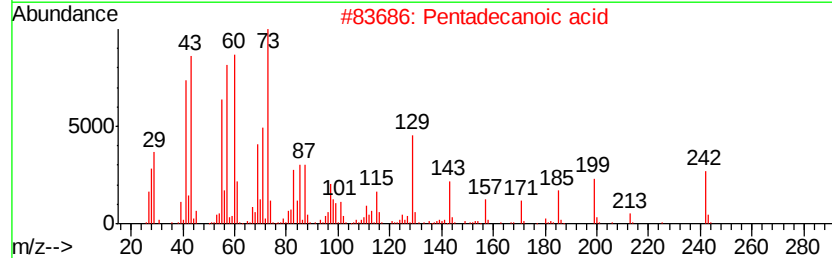
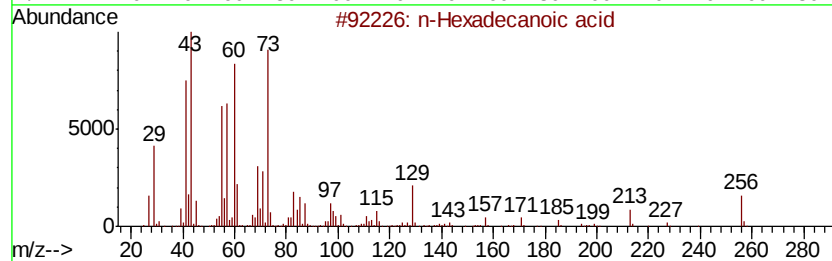
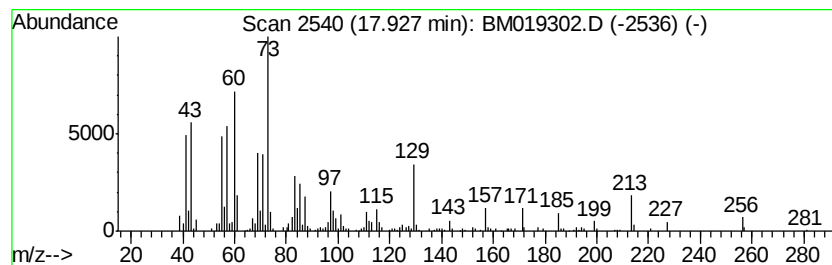
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.93	4.81 ng	630914	Phenanthrene-d10		17.04	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4		12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	43
5		Tridecanoic acid	214	C13H26O2	000638-53-9	43



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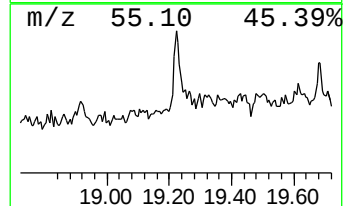
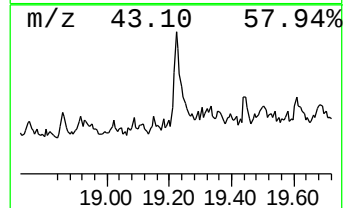
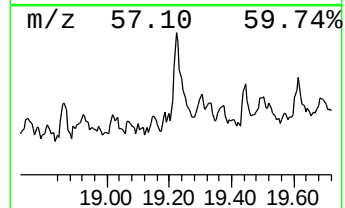
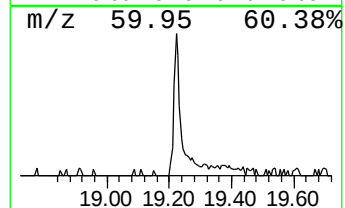
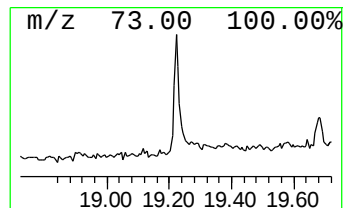
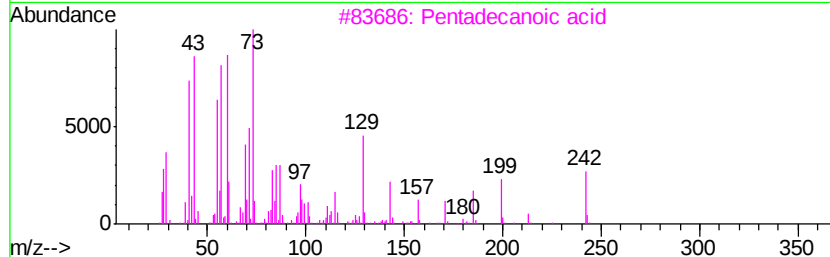
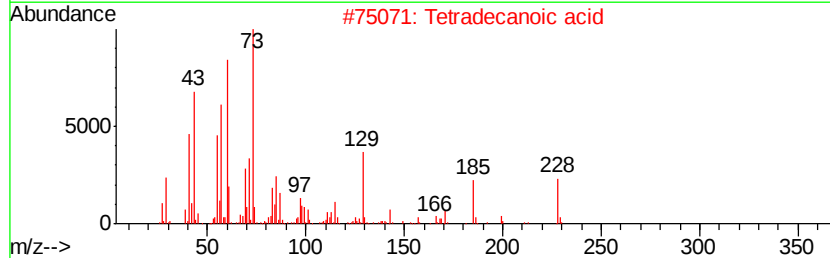
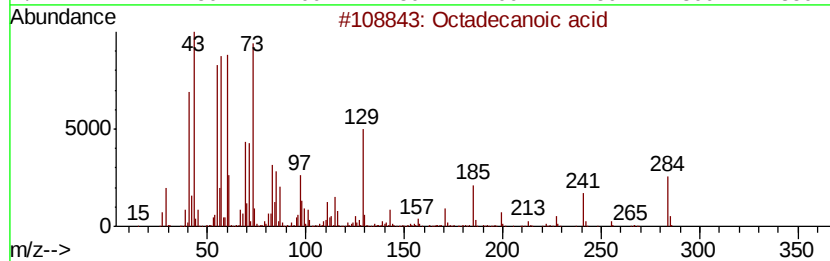
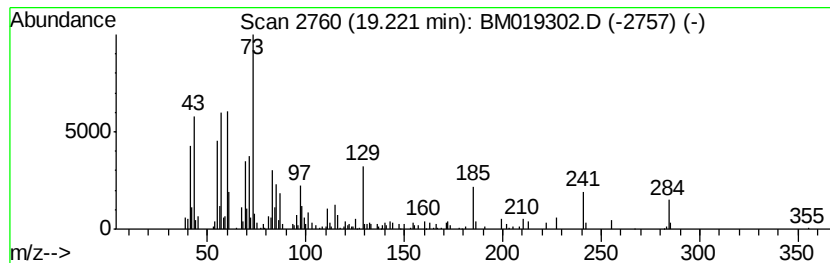
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Peak Number 4 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.22	2.10 ng	213444	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	47
4		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	42
5		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	37



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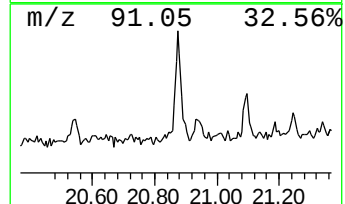
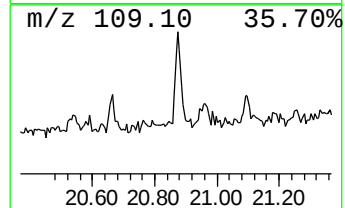
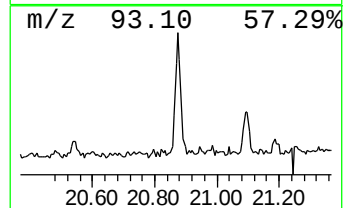
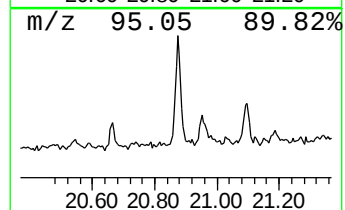
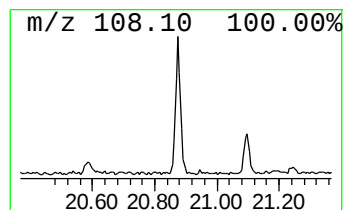
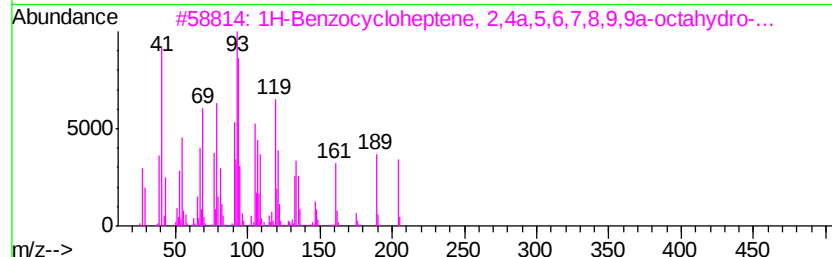
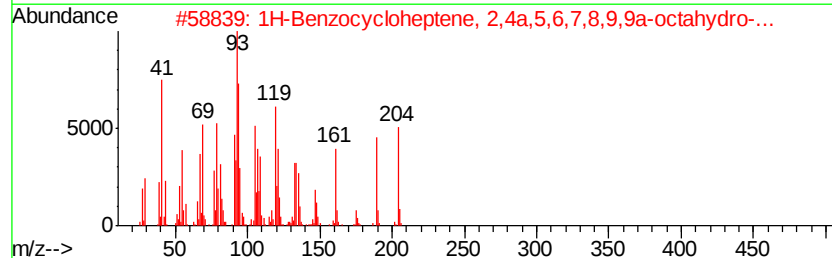
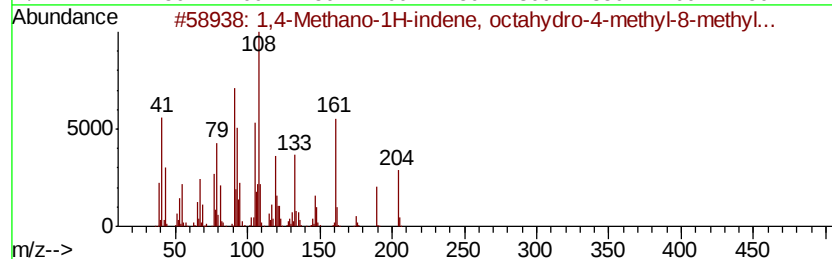
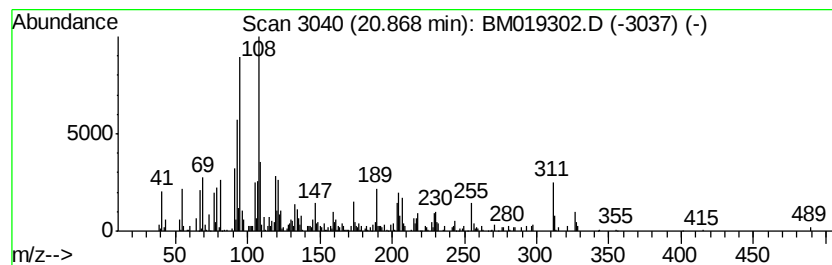
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Peak Number 5 unknown20.87 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	3.61 ng	367641	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Methano-1H-indene, octahydro...	204	C15H24	003650-28-0	47
2		1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	42
3		1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	080923-88-2	30
4		(E,E,E)-2,4,6-Octatriene	108	C8H12	015192-80-0	27
5		2,3-Dimethyl-cyclohexa-1,3-diene	108	C8H12	004430-91-5	27



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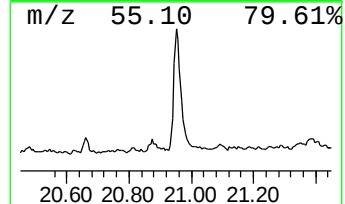
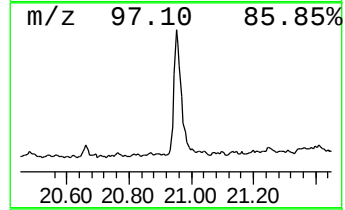
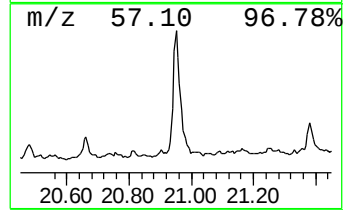
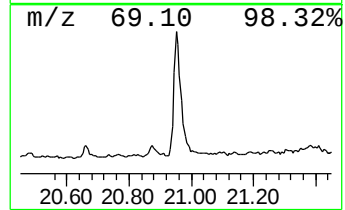
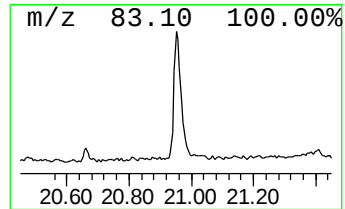
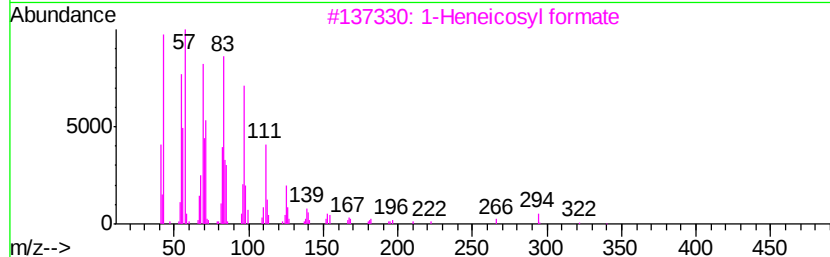
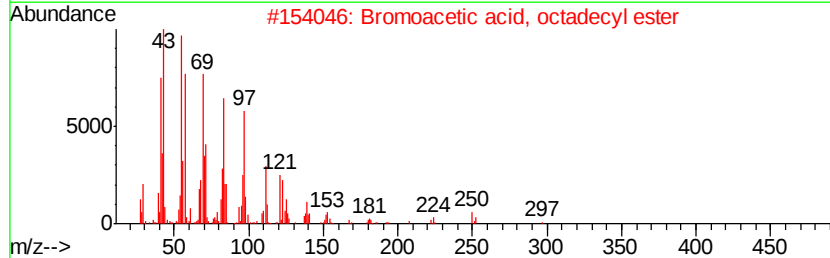
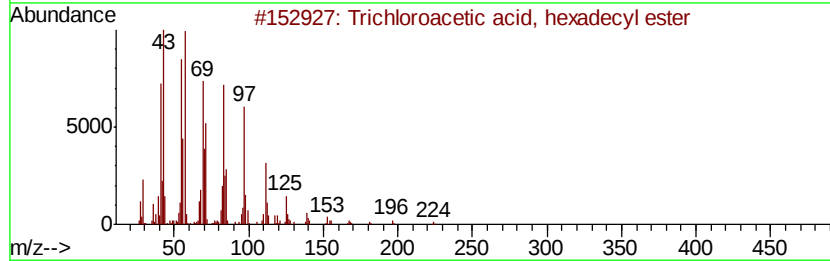
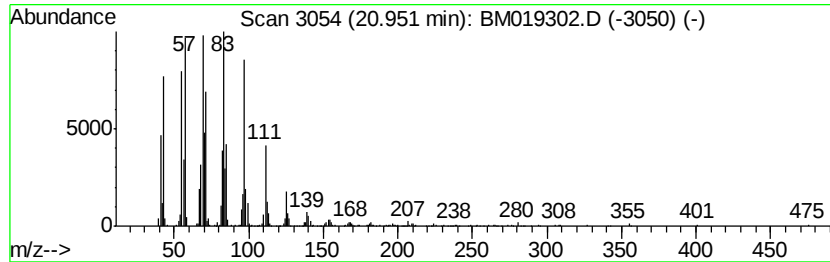
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	11.18 ng	1137690	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5		1-Hexadecanol	242	C16H34O	036653-82-4	90



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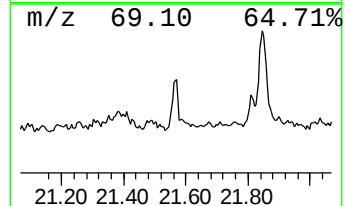
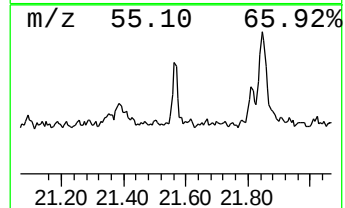
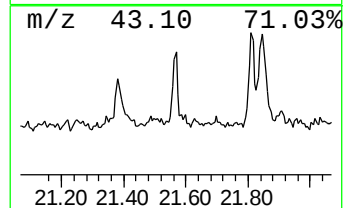
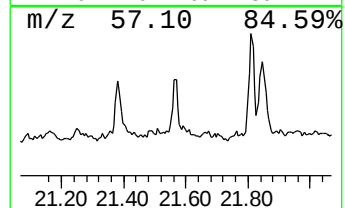
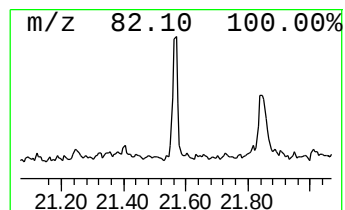
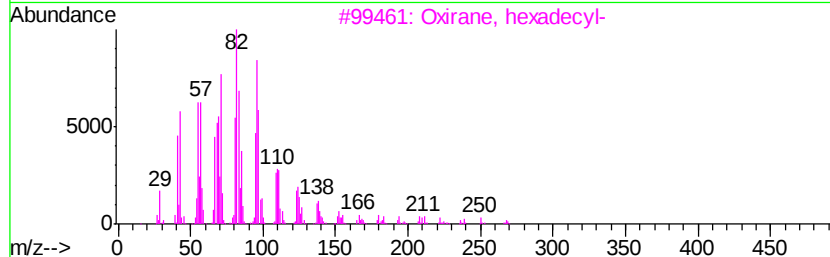
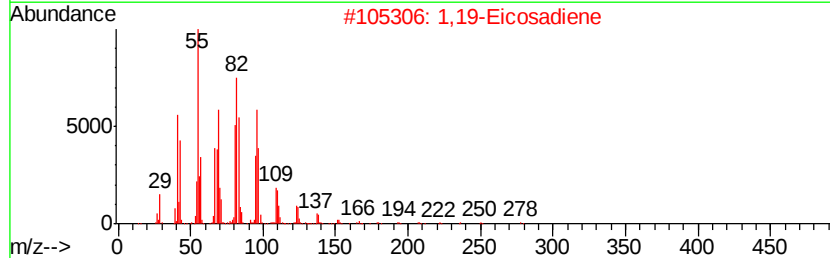
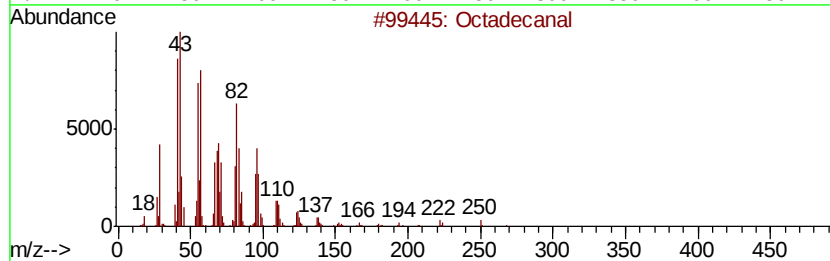
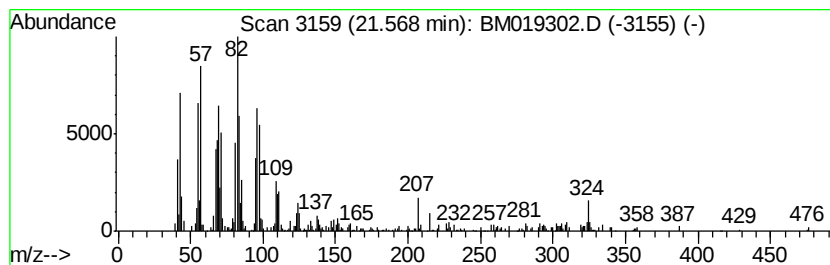
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.57	2.71 ng	276019	Chrysene-d12	21.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanal	268	C18H36O	000638-66-4	90
2		1,19-Eicosadiene	278	C20H38	014811-95-1	89
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
4		17-Octadecenal	266	C18H34O	056554-86-0	83
5		1,22-Docosanediol	342	C22H46O2	022513-81-1	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM032119\
Data File : BM019302.D
Acq On : 21 Mar 2019 22:09
Operator : JU/SJ
Sample : K2004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

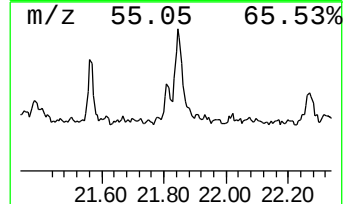
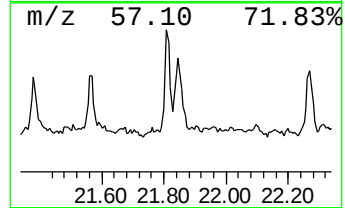
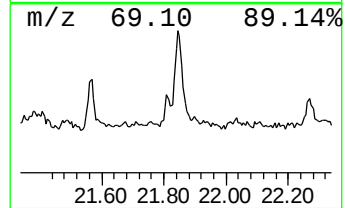
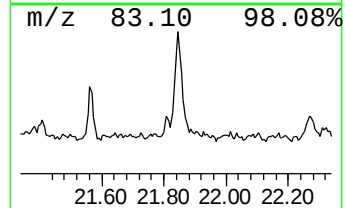
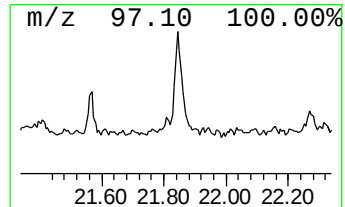
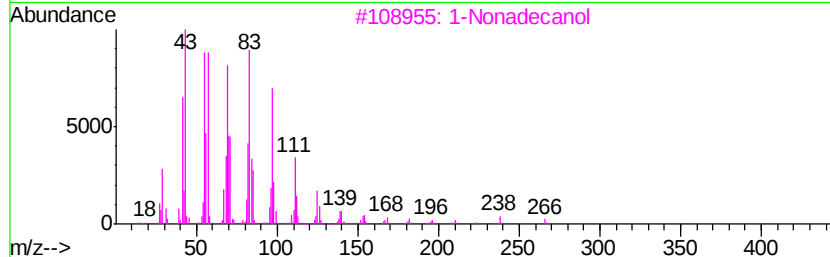
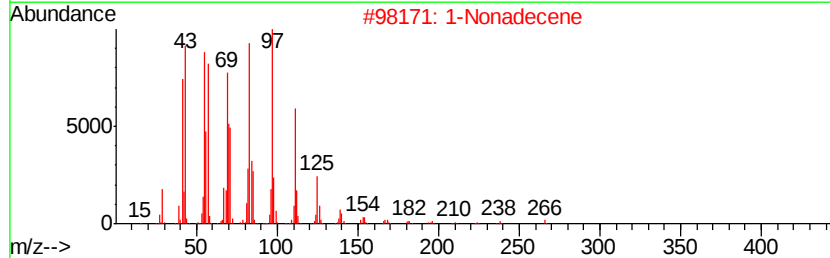
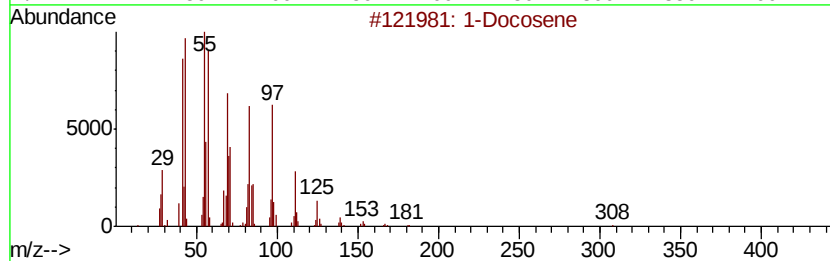
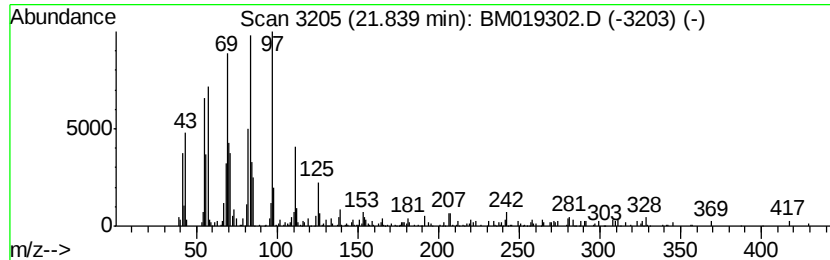
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ClientSampleId :
SB-19B(13.5-14.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.84	3.91 ng	398133	Chrysene-d12	21.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosene	308 C22H44	001599-67-3	86
2	1-Nonadecene	266 C19H38	018435-45-5	81
3	1-Nonadecanol	284 C19H40O	001454-84-8	80
4	1-Heptadecene	238 C17H34	006765-39-5	80
5	1-Octadecanol	270 C18H38O	000112-92-5	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM032119\
Data File : BM019302.D
Acq On : 21 Mar 2019 22:09
Operator : JU/SJ
Sample : K2004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

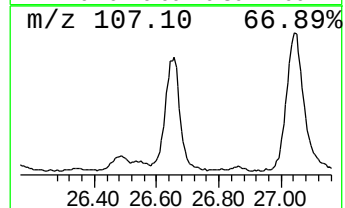
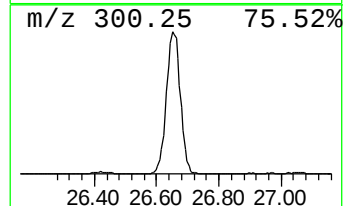
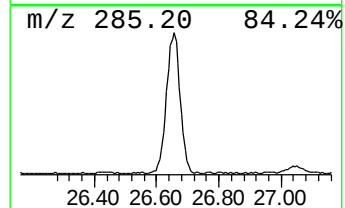
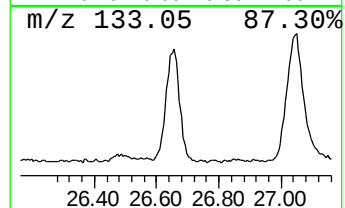
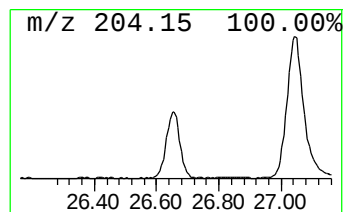
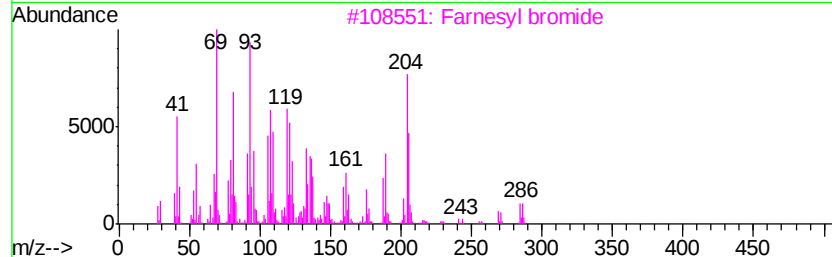
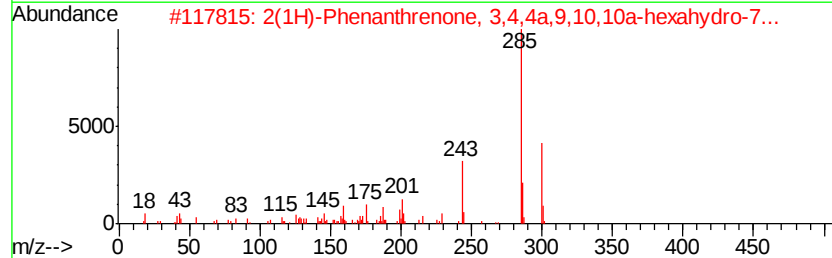
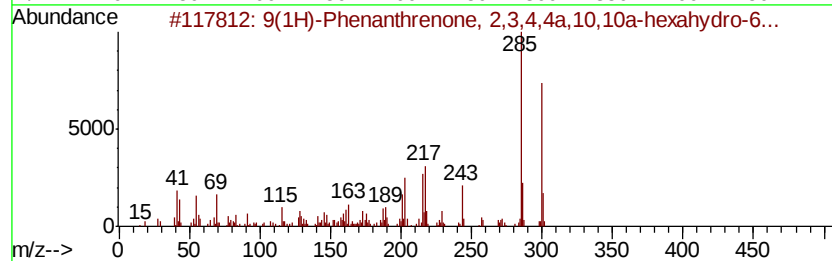
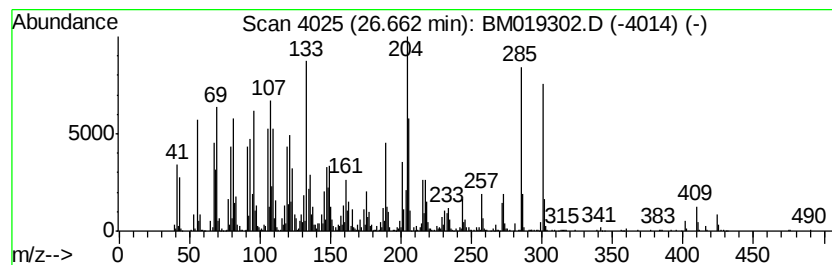
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ClientSampleId :
SB-19B(13.5-14.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM031119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9(1H)-Phenanthrene, 2,3,4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
26.66	54.57 ng	5762150	Perylene-d12	23.47		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9(1H)-Phenanthrenone,	2,3,4,4a,1...	300	C20H28O2	000511-05-7	56
2	2(1H)-Phenanthrenone,	3,4,4a,9,1...	300	C20H28O2	006755-93-7	41
3	Farnesyl bromide		284	C15H25Br	006874-67-5	38
4	1,3-Dimethyl-5-(propen-1-yl)adam...		204	C15H24	057040-48-9	38
5	1,1,4a-Trimethyl-5,6-dimethylene...		204	C15H24	1000193-60-8	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM032119\
Data File : BM019302.D
Acq On : 21 Mar 2019 22:09
Operator : JU/SJ
Sample : K2004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-19B(13.5-14.5)

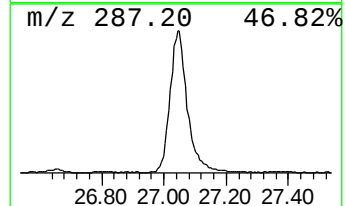
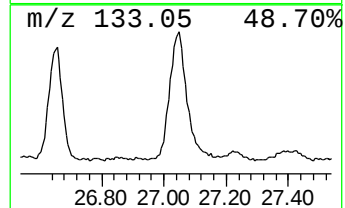
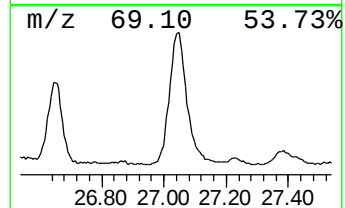
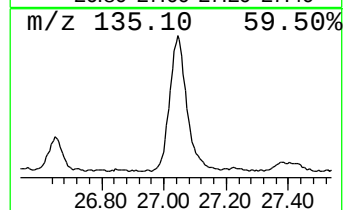
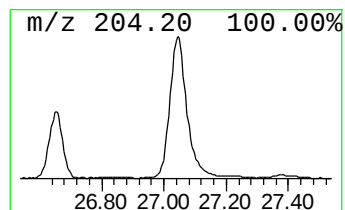
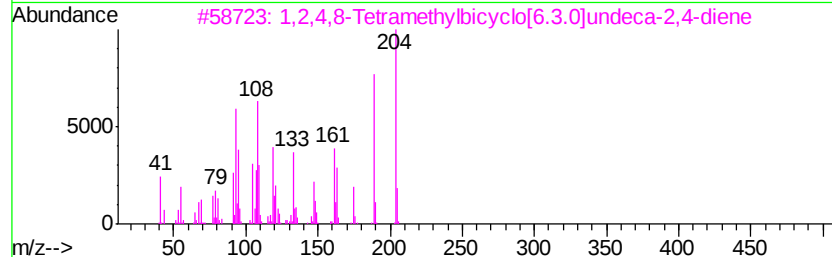
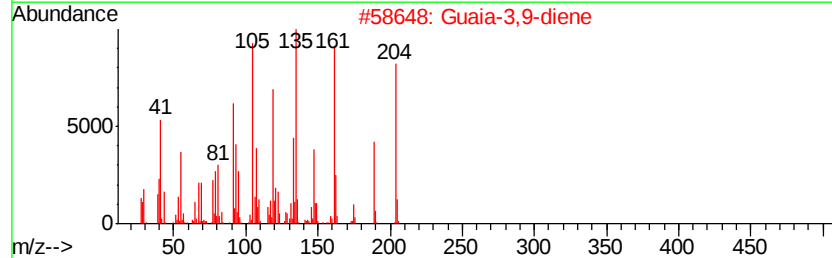
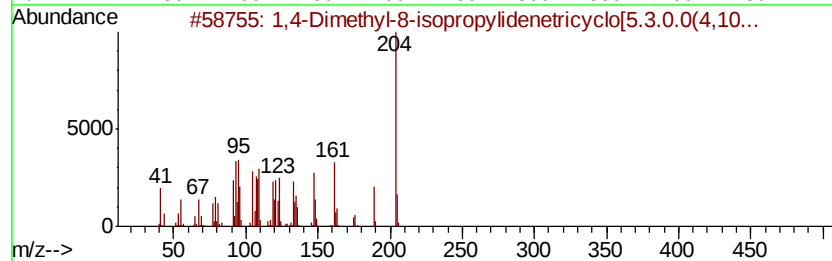
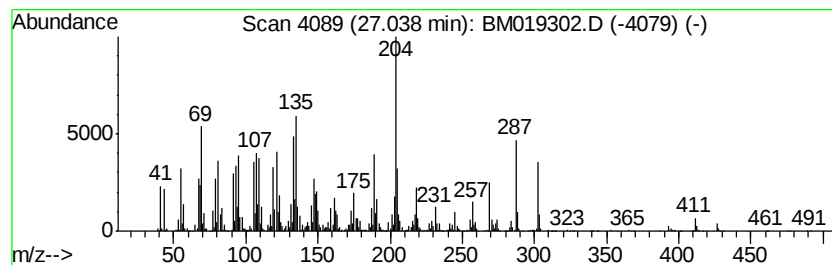
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown27.04 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.04	91.05 ng	9614810	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	49
2		Guaia-3,9-diene	204	C15H24	000489-83-8	47
3		1,2,4,8-Tetramethylbicyclo[6.3.0]...	204	C15H24	137235-51-9	45
4		1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	43
5		2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	41



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM032119\
Data File : BM019302.D
Acq On : 21 Mar 2019 22:09
Operator : JU/SJ
Sample : K2004-08
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-19B(13.5-14.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM031119.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
unknown7.16	7.16	112.2	ng	6274610	1	7.63	1118540	20.0
n-Hexadecanoic acid	17.93	4.8	ng	630914	4	17.04	2620820	20.0
Octadecanoic acid	19.22	2.1	ng	213444	5	21.24	2035750	20.0
unknown20.87	20.87	3.6	ng	367641	5	21.24	2035750	20.0
Trichloroacetic a...	20.95	11.2	ng	1137690	5	21.24	2035750	20.0
Octadecanal	21.57	2.7	ng	276019	5	21.24	2035750	20.0
1-Docosene	21.84	3.9	ng	398133	5	21.24	2035750	20.0
9(1H)-Phenanthren...	26.66	54.6	ng	5762150	6	23.47	2111930	20.0
unknown27.04	27.04	91.0	ng	9614810	6	23.47	2111930	20.0