

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
 Data File : BM018918.D
 Acq On : 25 Feb 2019 18:00
 Operator : JU/SJ
 Sample : K1597-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-25

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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	5.287	367	374	391	rBV	4805996	6895332	33.64%	5.373%
2	6.869	634	643	664	rBV	4572790	7372793	35.97%	5.745%
3	7.228	696	704	717	rBV	4708731	7541898	36.79%	5.877%
4	7.693	776	783	790	rBV	829188	1341133	6.54%	1.045%
5	8.004	829	836	848	rVB	3278739	5227436	25.50%	4.073%
6	8.857	974	981	995	rBV	2539812	4222404	20.60%	3.290%
7	10.475	1249	1256	1264	rBV	999722	1689856	8.24%	1.317%
8	12.957	1670	1678	1698	rBV	5591956	8046253	39.25%	6.270%
9	13.804	1817	1822	1835	rBV	275270	439267	2.14%	0.342%
10	14.339	1907	1913	1924	rBV2	1309170	2053158	10.02%	1.600%
11	15.839	2161	2168	2185	rBV	4829795	6983411	34.07%	5.442%
12	17.092	2376	2381	2387	rBV2	1561691	2305170	11.25%	1.796%
13	17.998	2523	2535	2560	rBV	8504531	15194449	74.12%	11.840%
14	19.127	2723	2727	2728	rBV	236906	269062	1.31%	0.210%
15	19.157	2729	2732	2740	rVB3	267055	487223	2.38%	0.380%
16	19.286	2745	2754	2772	rVV	12741661	20499448	100.00%	15.974%
17	19.727	2824	2829	2838	rVB	8329995	10053841	49.04%	7.834%
18	20.992	3040	3044	3056	rBV	639929	916330	4.47%	0.714%
19	21.292	3090	3095	3103	rBV	2124170	2706243	13.20%	2.109%
20	21.427	3114	3118	3123	rBV	908229	947680	4.62%	0.738%
21	21.862	3187	3192	3195	rBV	1914031	2638875	12.87%	2.056%
22	22.321	3266	3270	3278	rVB	2737269	3566122	17.40%	2.779%
23	22.827	3351	3356	3364	rBV	2872501	4284695	20.90%	3.339%
24	23.397	3447	3453	3465	rVB	2572240	4444821	21.68%	3.463%
25	23.539	3472	3477	3492	rVB2	1465893	2986083	14.57%	2.327%
26	24.044	3557	3563	3572	rVB	1782133	3419235	16.68%	2.664%
27	24.791	3685	3690	3699	rVB2	847425	1801221	8.79%	1.404%

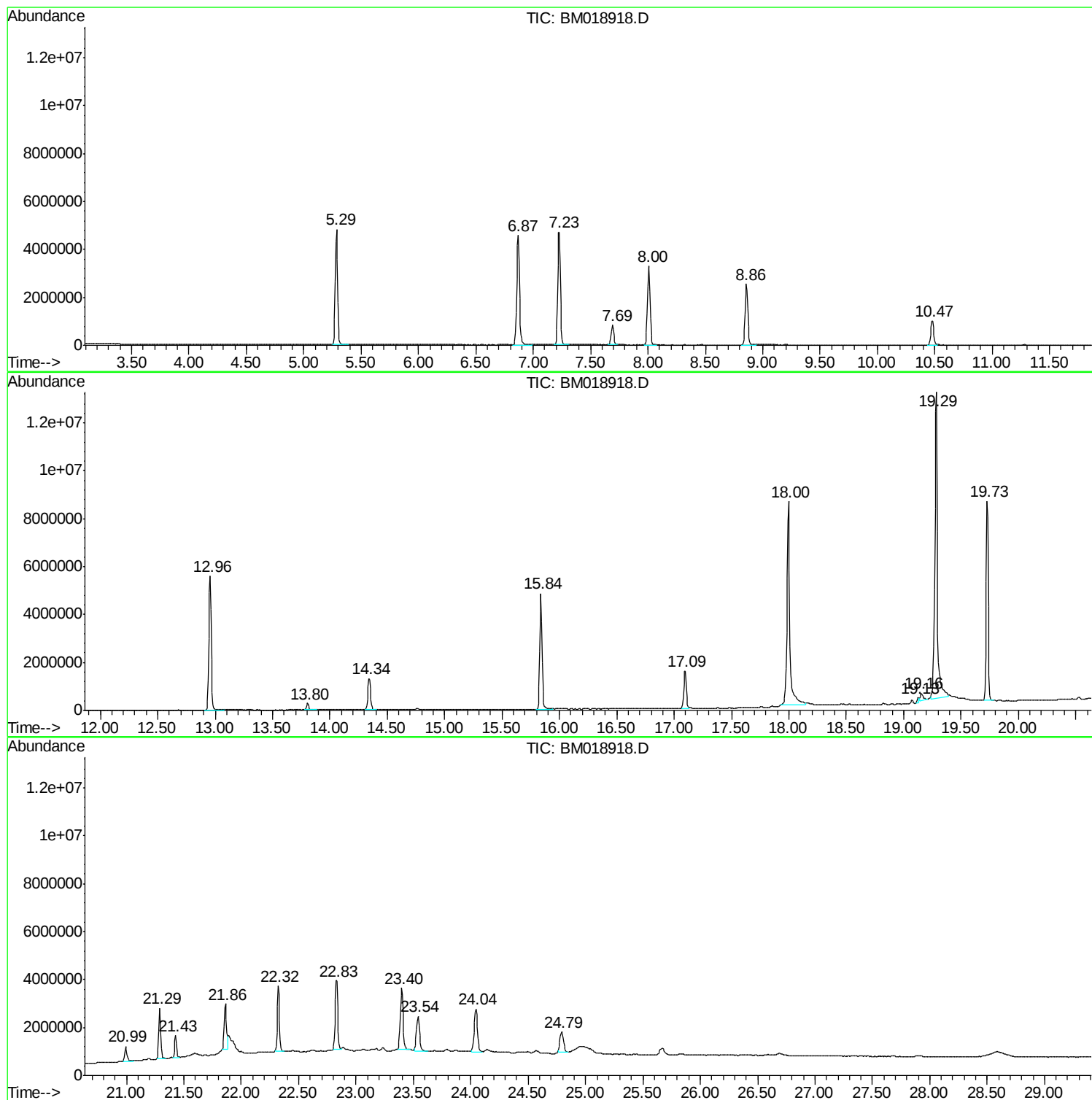
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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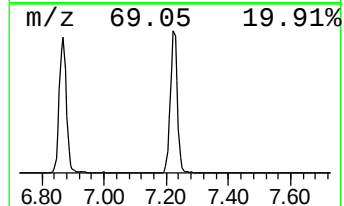
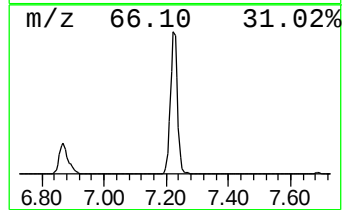
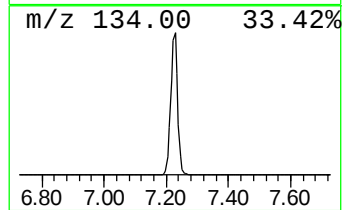
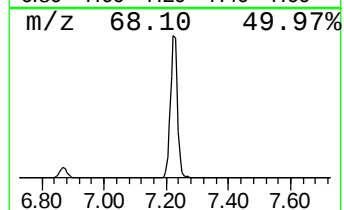
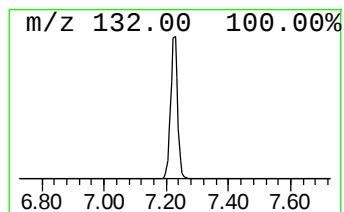
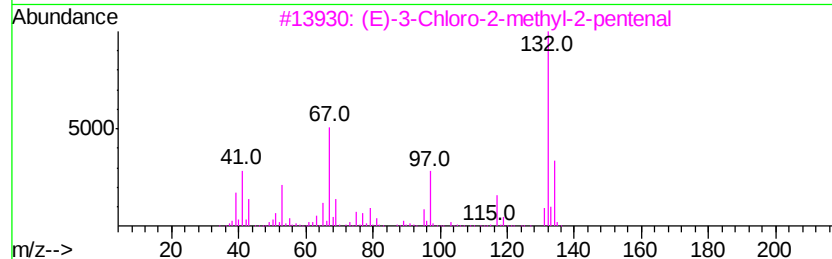
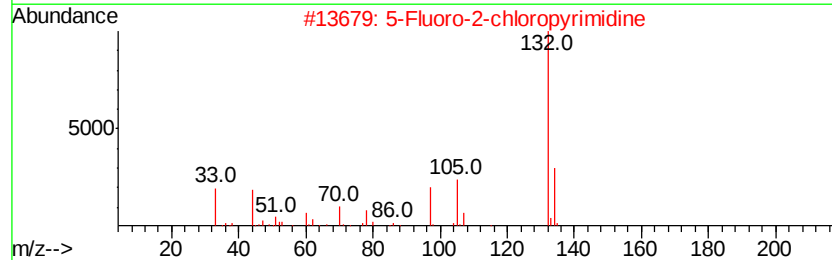
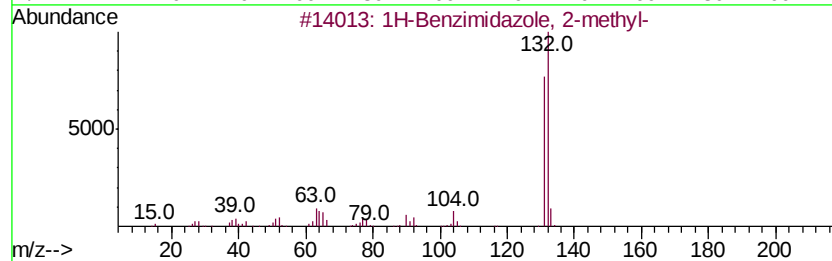
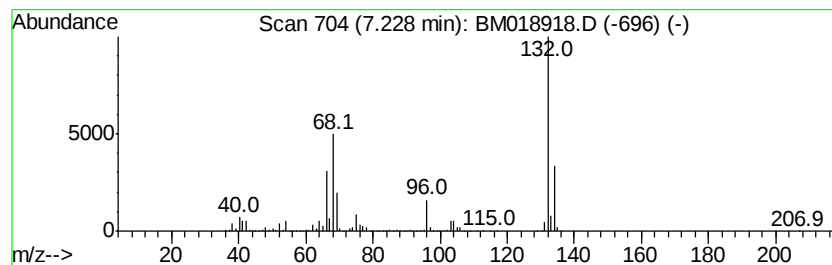
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.23 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	112.47 ng	7541900	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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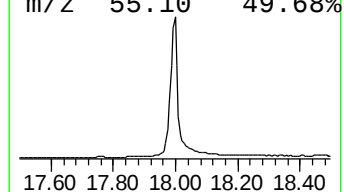
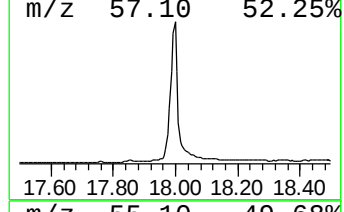
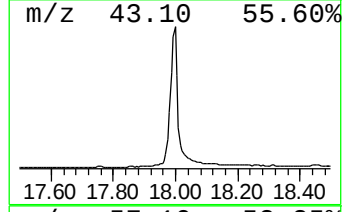
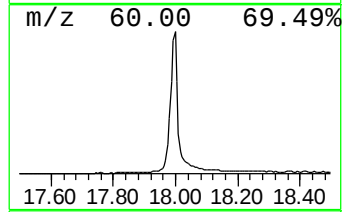
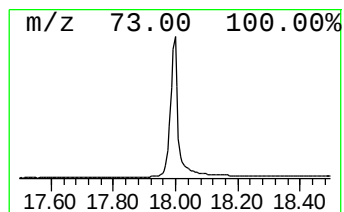
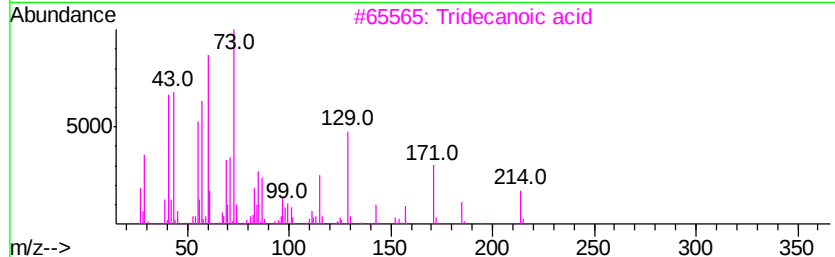
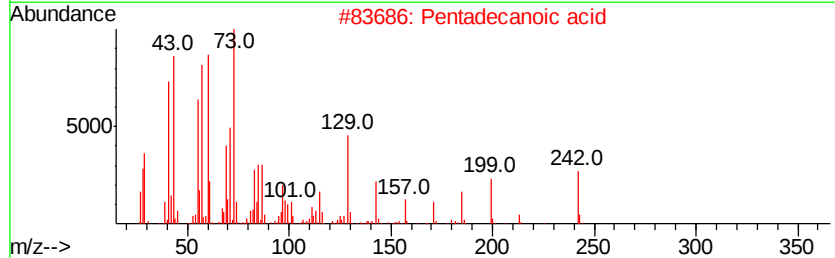
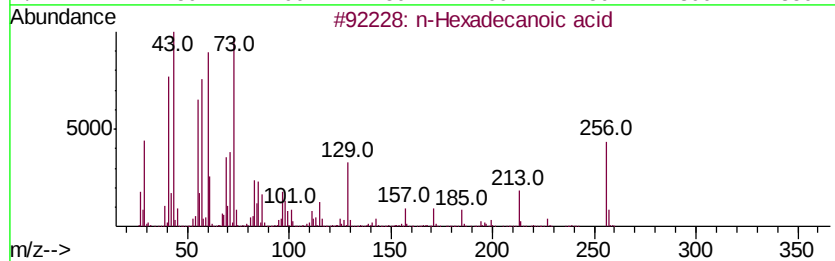
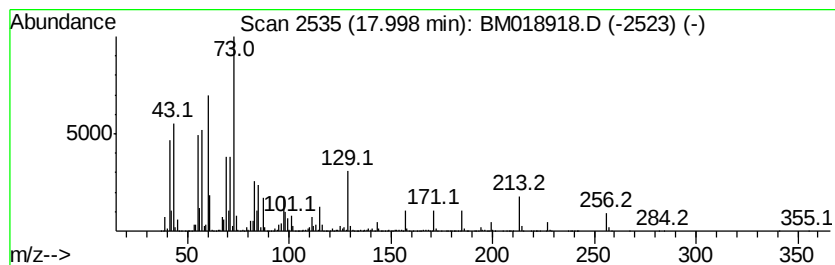
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.00	131.83 ng	15194400	Phenanthrene-d10	17.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	60
4		Tetradecane	198	C14H30	000629-59-4	18
5		Dodecane	170	C12H26	000112-40-3	18



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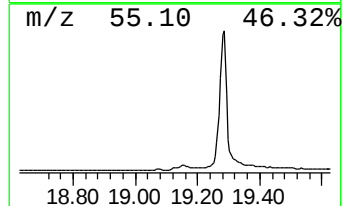
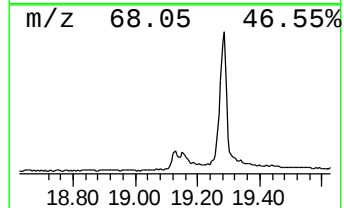
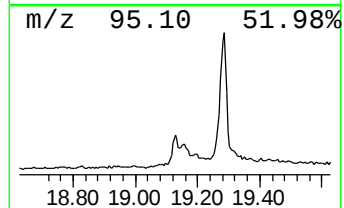
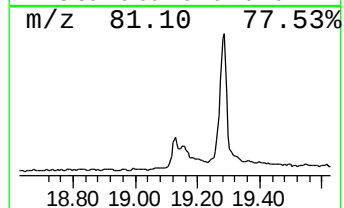
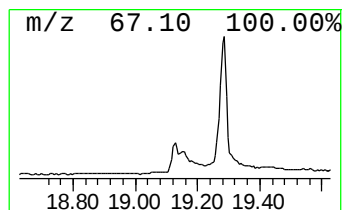
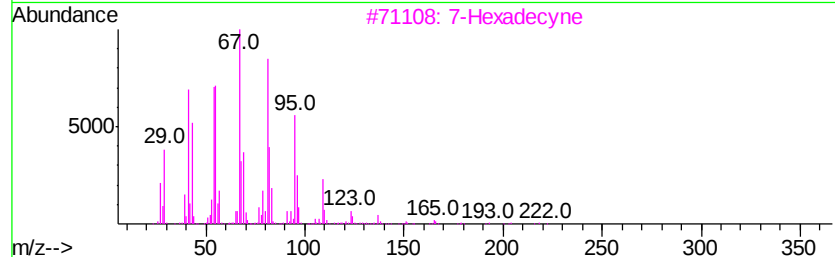
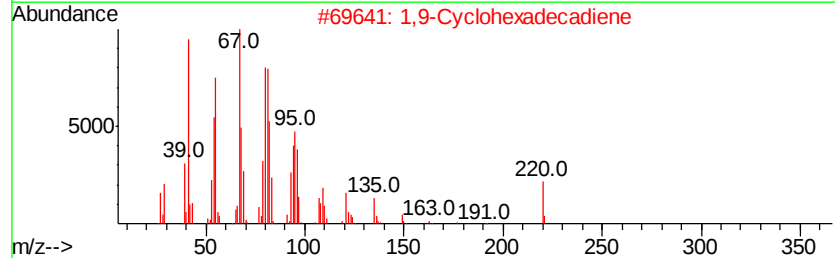
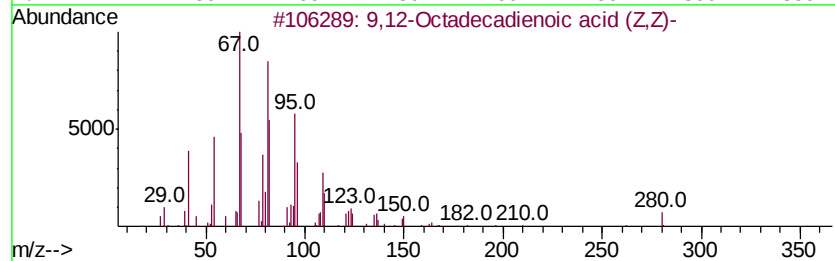
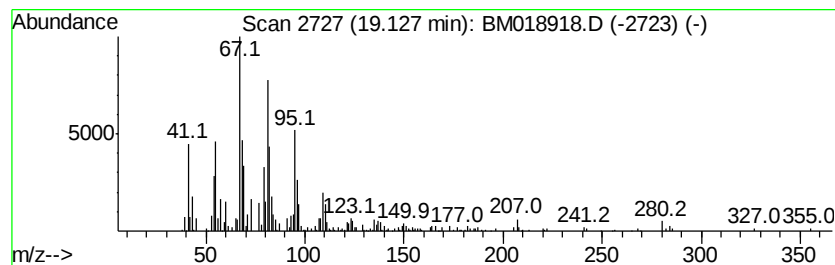
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Peak Number 4 9,12-Octadecadienoic acid (... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.13	2.33 ng	269062	Phenanthrene-d10	17.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	93
2		1,9-Cyclohexadecadiene	220	C16H28	004277-06-9	87
3		7-Hexadecyne	222	C16H30	074685-28-2	86
4		3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	81
5		Cycloundecene, 1-methyl-	166	C12H22	088828-82-4	80



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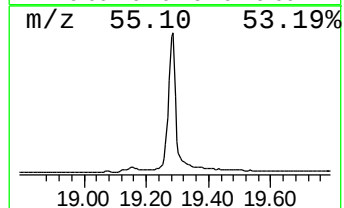
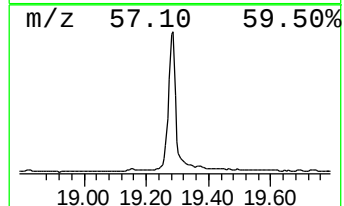
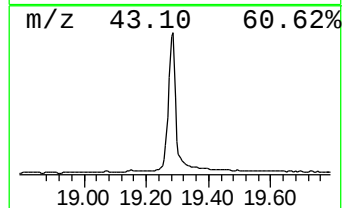
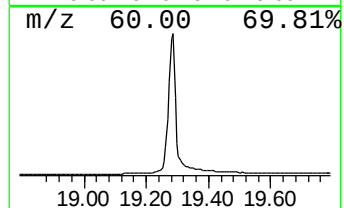
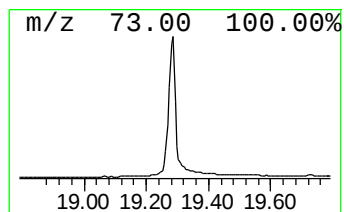
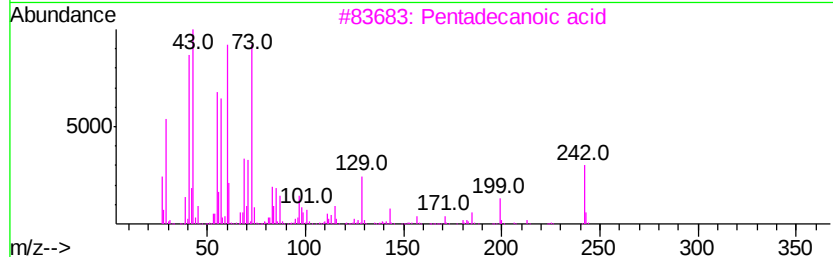
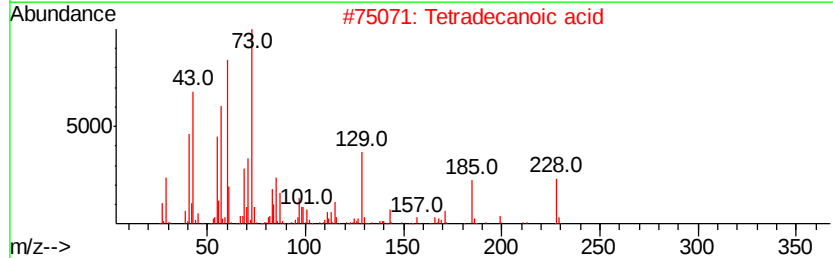
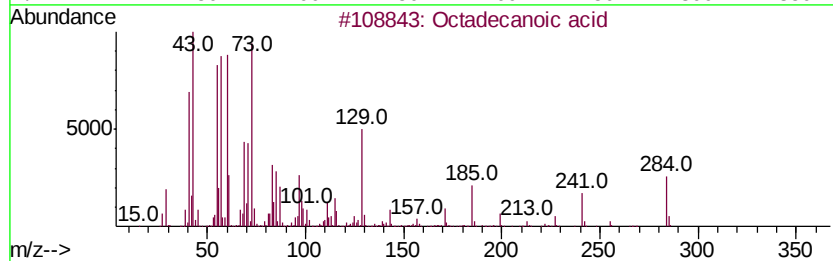
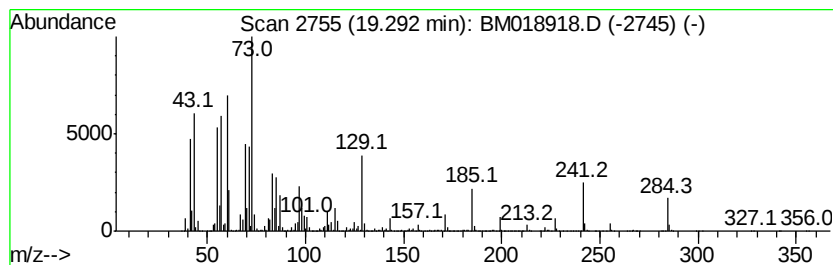
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Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.29	151.50 ng	20499400	Chrysene-d12	21.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
5		d-Glucitol, 4-O-nonyl-	308	C15H32O6	132591-06-1	27



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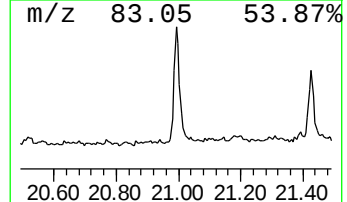
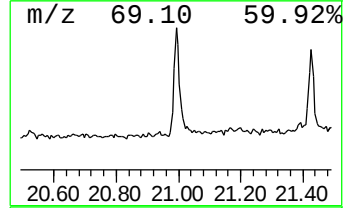
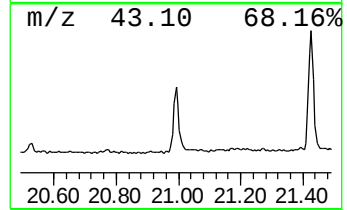
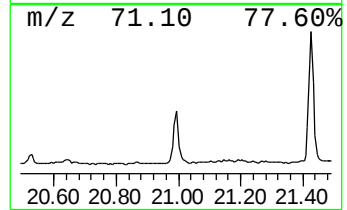
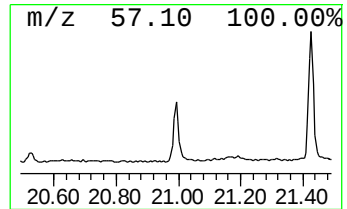
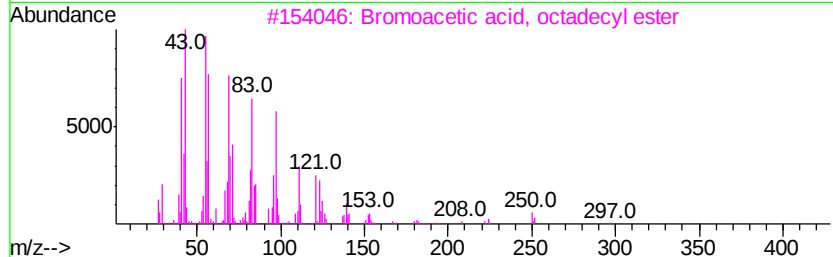
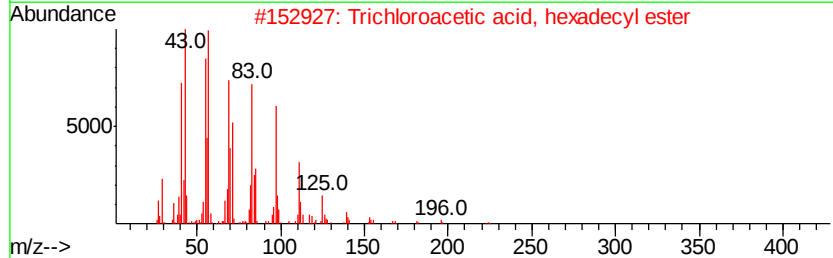
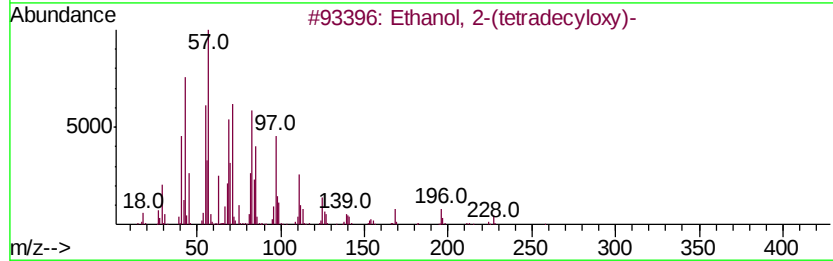
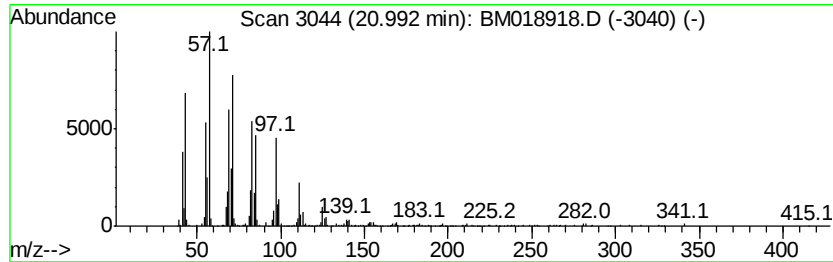
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.99	6.77 ng	916330	Chrysene-d12	21.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	68
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	58
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	58
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	58
5	10-Heneicosene (c,t)	294	C21H42	095008-11-0	58



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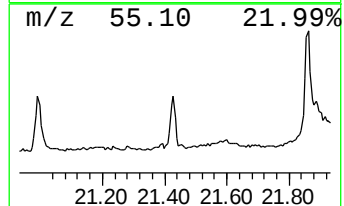
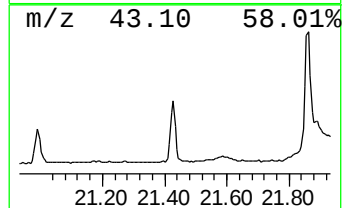
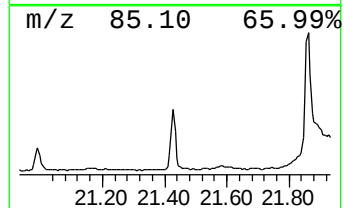
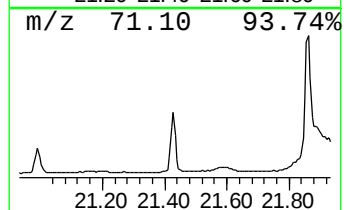
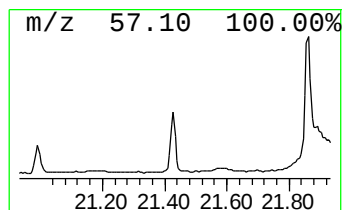
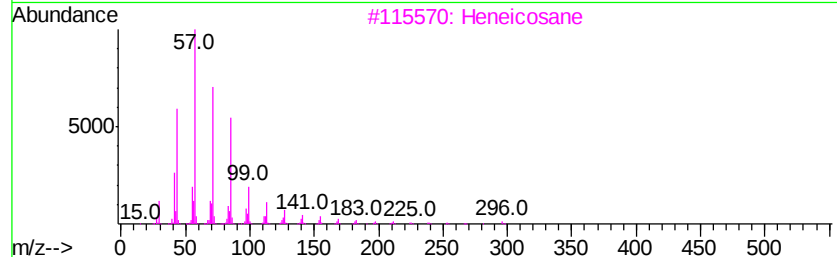
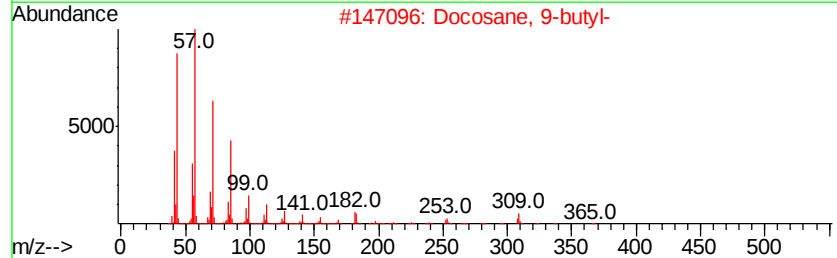
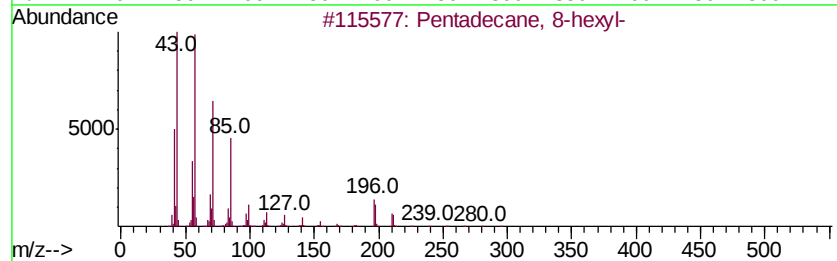
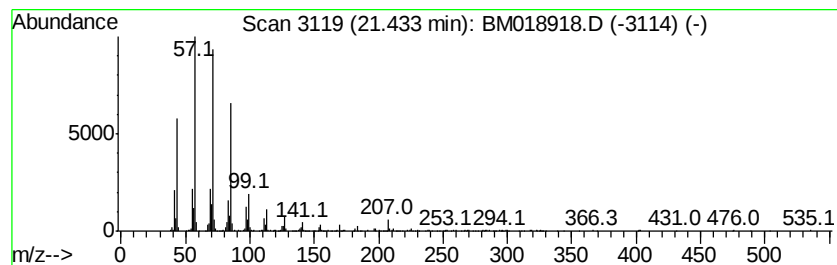
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ClientSampleId :
TP-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecane, 8-hexyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.43	7.00 ng	947680	Chrysene-d12	21.29		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2		Docosane, 9-butyl-	366	C26H54	055282-14-9	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	90
5		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
Data File : BM018918.D
Acq On : 25 Feb 2019 18:00
Operator : JU/SJ
Sample : K1597-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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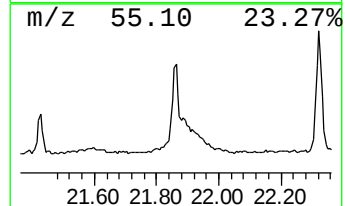
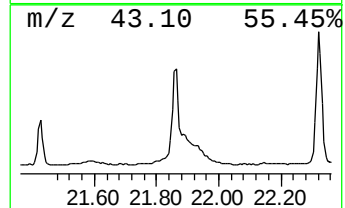
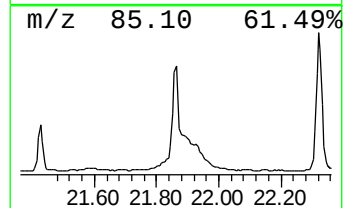
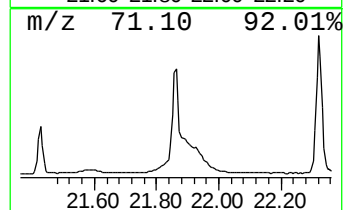
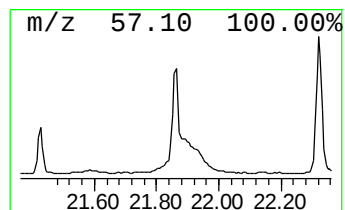
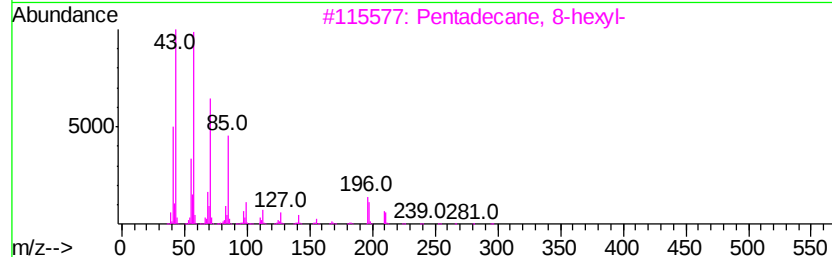
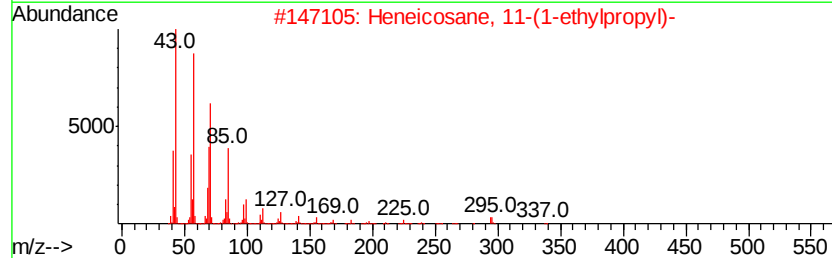
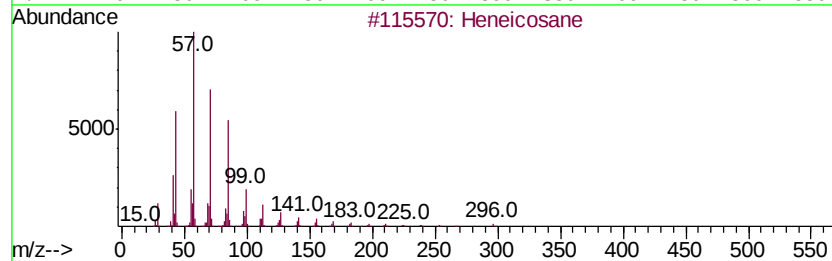
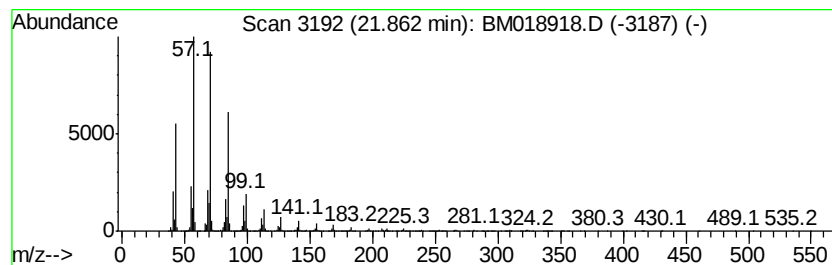
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.86	19.50 ng	2638880	Chrysene-d12	21.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	91
3	Pentadecane, 8-hexyl-		296	C21H44	013475-75-7	90
4	Octadecane, 2-methyl-		268	C19H40	001560-88-9	90
5	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
Data File : BM018918.D
Acq On : 25 Feb 2019 18:00
Operator : JU/SJ
Sample : K1597-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-25

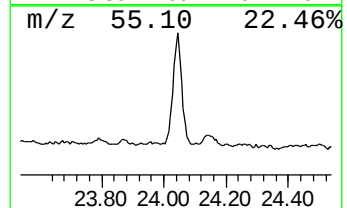
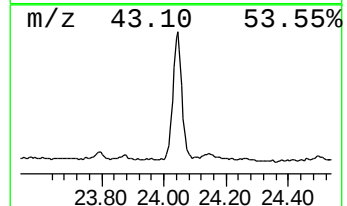
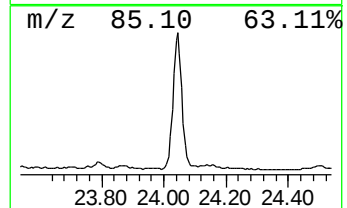
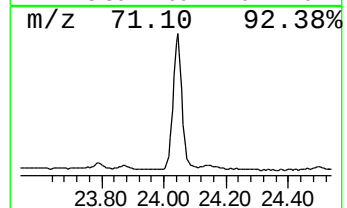
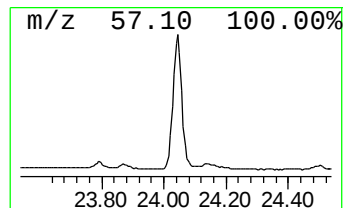
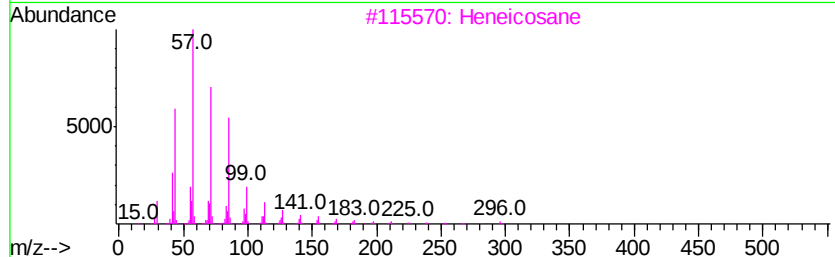
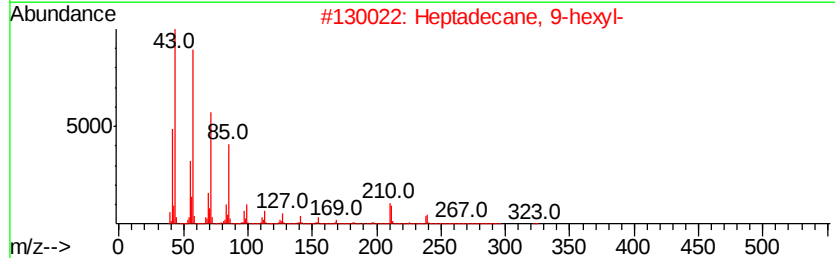
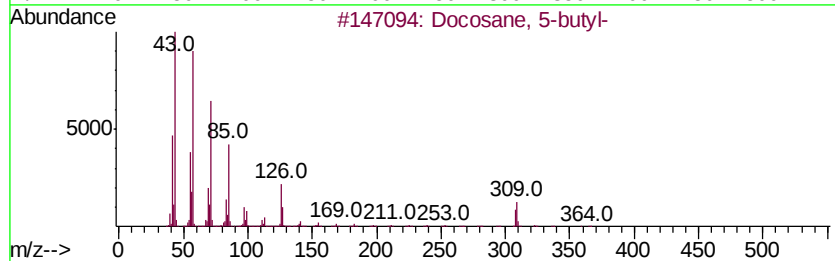
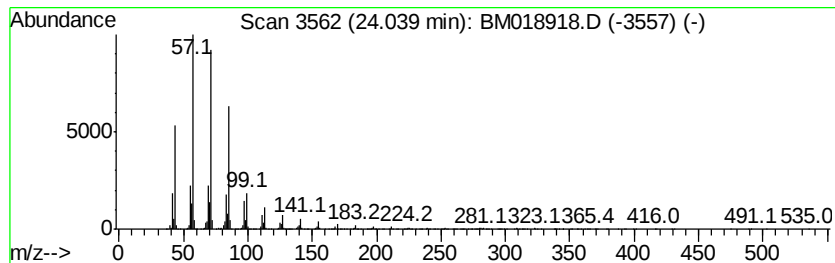
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Docosane, 5-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.04	22.90 ng	3419240	Perylene-d12	23.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 5-butyl-	366	C26H54	055282-16-1	93
2		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Docosane, 9-butyl-	366	C26H54	055282-14-9	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022519\
 Data File : BM018918.D
 Acq On : 25 Feb 2019 18:00
 Operator : JU/SJ
 Sample : K1597-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-25

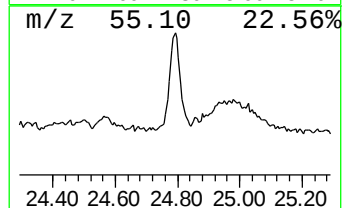
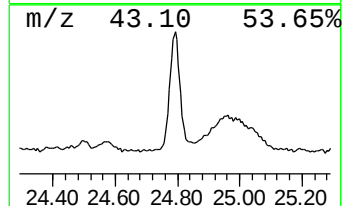
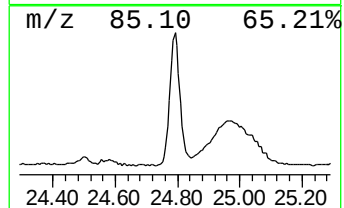
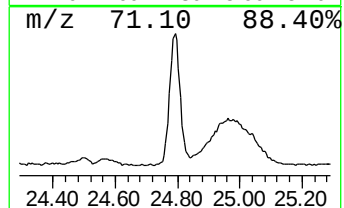
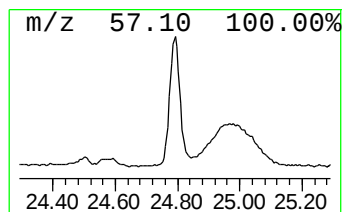
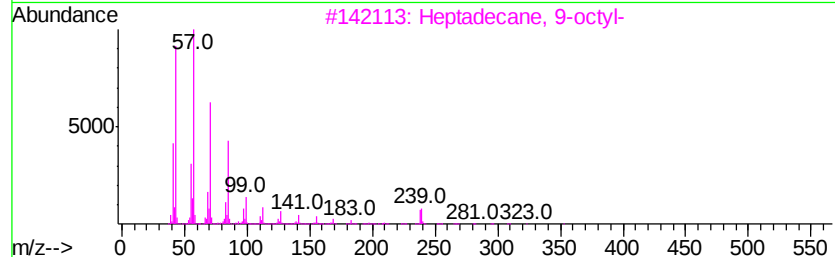
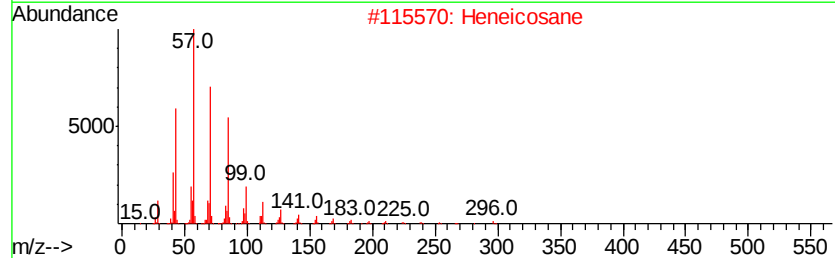
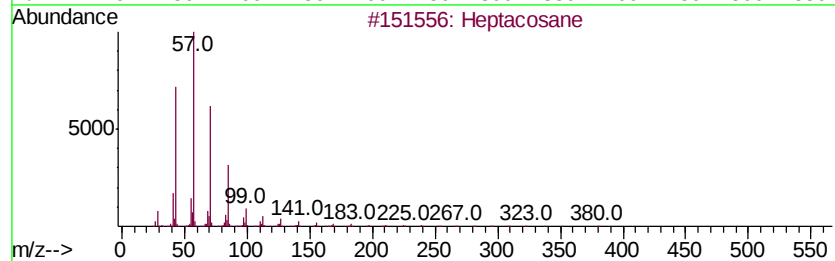
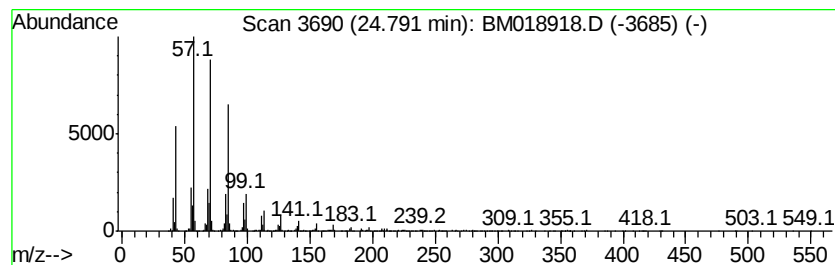
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 14 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.79	12.06 ng	1801220	Perylene-d12	23.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	90
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM022519\
Data File : BM018918.D
Acq On : 25 Feb 2019 18:00
Operator : JU/SJ
Sample : K1597-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM021119.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
unknown7.23	7.23	112.5	ng	7541900	1	7.69	1341130	20.0
n-Hexadecanoic acid	18.00	131.8	ng	15194400	4	17.09	2305170	20.0
9,12-Octadecadien...	19.13	2.3	ng	269062	4	17.09	2305170	20.0
Octadecanoic acid	19.29	151.5	ng	20499400	5	21.29	2706240	20.0
Ethanol, 2-(tetra...	20.99	6.8	ng	916330	5	21.29	2706240	20.0
Pentadecane, 8-he...	21.43	7.0	ng	947680	5	21.29	2706240	20.0
Heneicosane	21.86	19.5	ng	2638880	5	21.29	2706240	20.0
Docosane, 5-butyl-	24.04	22.9	ng	3419240	6	23.54	2986080	20.0
Heptacosane	24.79	12.1	ng	1801220	6	23.54	2986080	20.0