

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
 Data File : BM018616.D
 Acq On : 17 Jan 2019 16:23
 Operator : JU/SJ
 Sample : K1139-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S-4

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-BM010919.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	4.881	300	305	314	rVB	275435	396112	3.77%	0.382%
2	5.328	375	381	389	rBV	4835564	6945351	66.14%	6.700%
3	6.916	643	651	669	rBV	4799700	7531606	71.72%	7.265%
4	7.275	705	712	722	rBV	5181915	8052002	76.68%	7.767%
5	7.740	784	791	797	rBV	1592513	2447526	23.31%	2.361%
6	8.057	837	845	853	rVB	3405610	5388622	51.32%	5.198%
7	8.904	980	989	999	rBV	2865125	4844706	46.14%	4.673%
8	10.528	1258	1265	1272	rBV	1963918	3270222	31.14%	3.154%
9	13.004	1679	1686	1697	rBV	5318453	7663944	72.98%	7.393%
10	13.845	1823	1829	1837	rBV	1271686	1792657	17.07%	1.729%
11	14.263	1894	1900	1910	rVB3	57155	145213	1.38%	0.140%
12	14.386	1914	1921	1930	rBV2	2654798	4015616	38.24%	3.873%
13	15.880	2166	2175	2185	rBV	4610720	6783235	64.60%	6.543%
14	17.139	2382	2389	2394	rBV	3020385	4220170	40.19%	4.071%
15	17.180	2394	2396	2400	rVB	148866	165029	1.57%	0.159%
16	18.027	2533	2540	2551	rBV2	1221163	1970068	18.76%	1.900%
17	18.204	2565	2570	2574	rBV3	70626	134811	1.28%	0.130%
18	18.933	2689	2694	2700	rBV2	88233	174794	1.66%	0.169%
19	19.198	2731	2739	2744	rBV	396485	638524	6.08%	0.616%
20	19.251	2745	2748	2753	rVB2	87200	114706	1.09%	0.111%
21	19.310	2753	2758	2763	rBV	504154	707438	6.74%	0.682%
22	19.562	2798	2801	2809	rVB	367972	559842	5.33%	0.540%
23	19.768	2831	2836	2851	rVB	8513611	10500957	100.00%	10.129%
24	19.886	2853	2856	2866	rVB4	61904	145937	1.39%	0.141%
25	21.027	3046	3050	3061	rBV3	978011	1281233	12.20%	1.236%
26	21.333	3095	3102	3106	rBV	3341146	4662260	44.40%	4.497%
27	21.368	3106	3108	3115	rVB	350338	422830	4.03%	0.408%
28	21.468	3122	3125	3129	rVB	235358	245225	2.34%	0.237%
29	21.909	3196	3200	3209	rVB	632098	915008	8.71%	0.883%
30	22.374	3275	3279	3286	rBV	1236336	1710006	16.28%	1.649%
31	22.509	3298	3302	3314	rVB	429278	716684	6.82%	0.691%
32	22.892	3362	3367	3377	rBV2	1716319	3072746	29.26%	2.964%
33	23.468	3459	3465	3479	rVB2	1856997	3615811	34.43%	3.488%
34	23.609	3482	3489	3502	rVB	1993083	4020550	38.29%	3.878%

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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

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35	24.121	3570	3576	3585	rVB	1453812	2773509	26.41%	2.675%
36	24.880	3700	3705	3714	rVB	774901	1624531	15.47%	1.567%

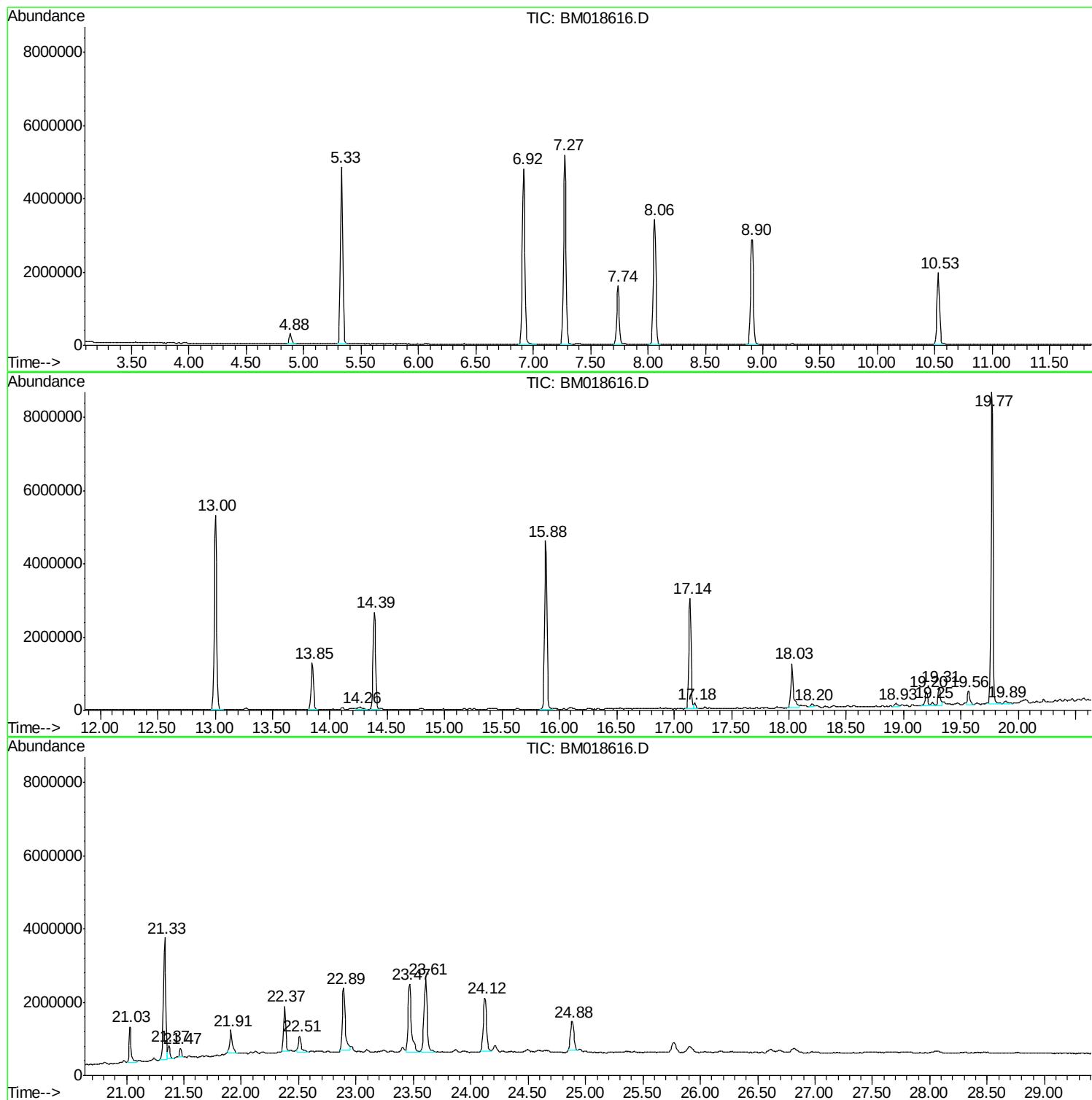
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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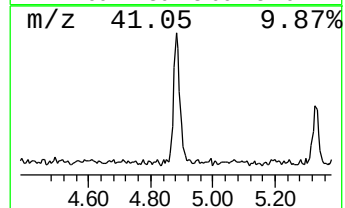
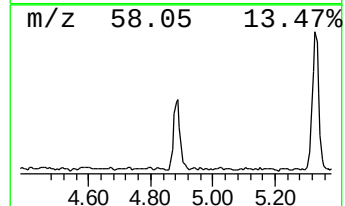
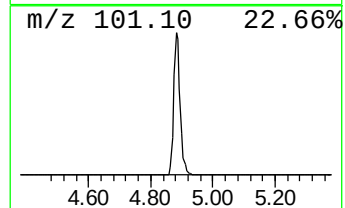
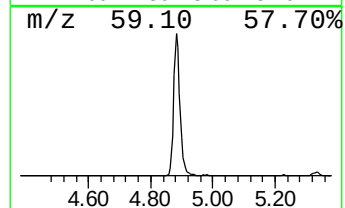
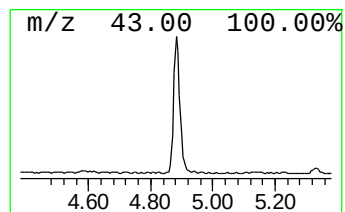
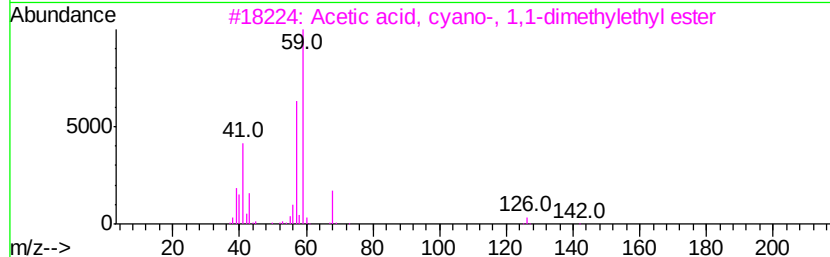
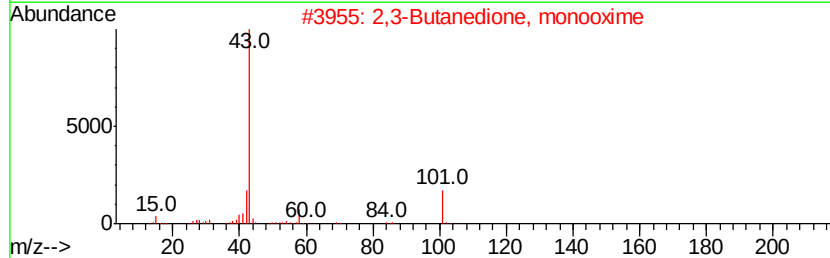
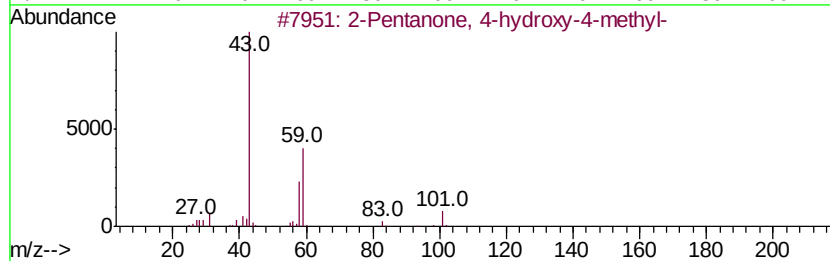
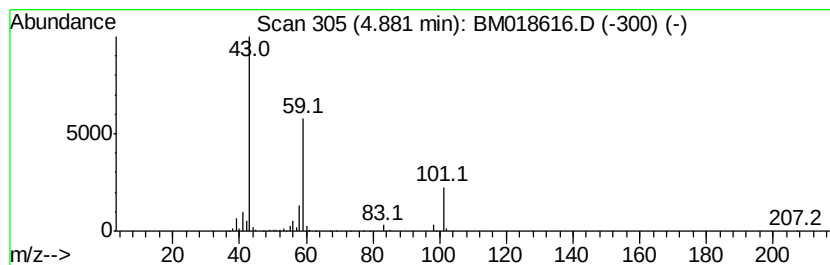
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	3.24 ng	396112	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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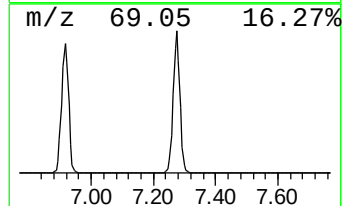
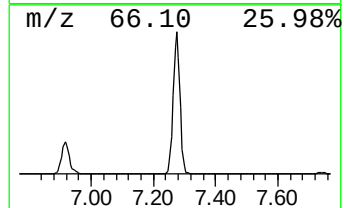
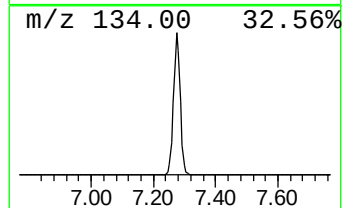
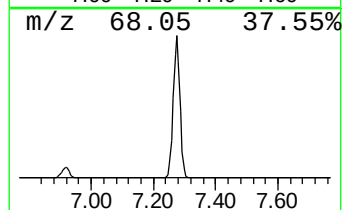
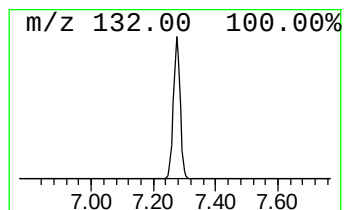
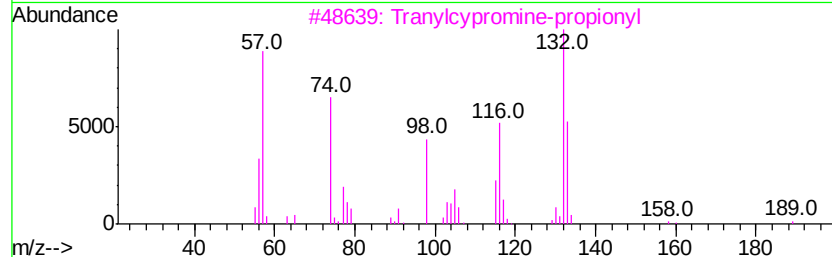
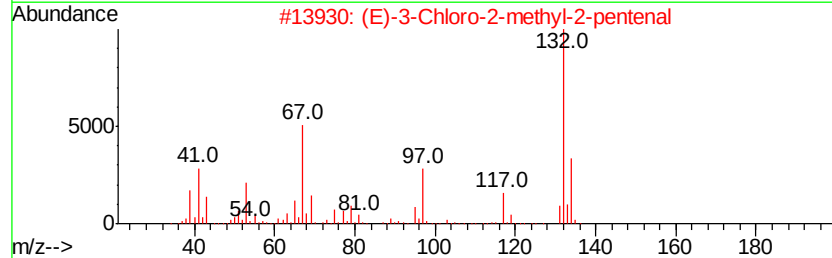
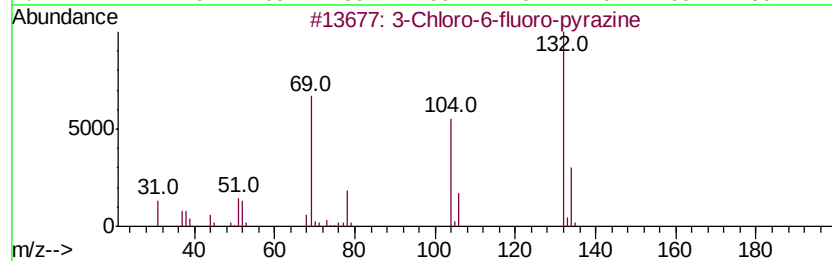
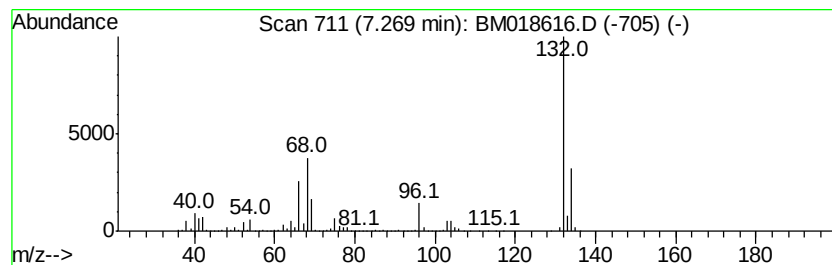
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	65.80 ng	8052000	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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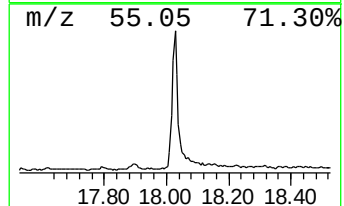
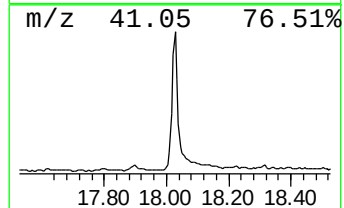
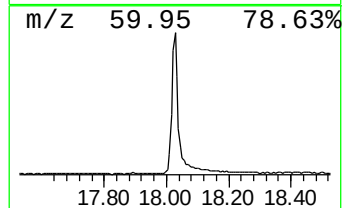
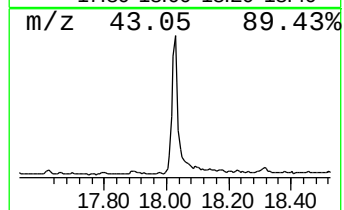
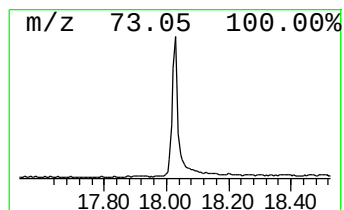
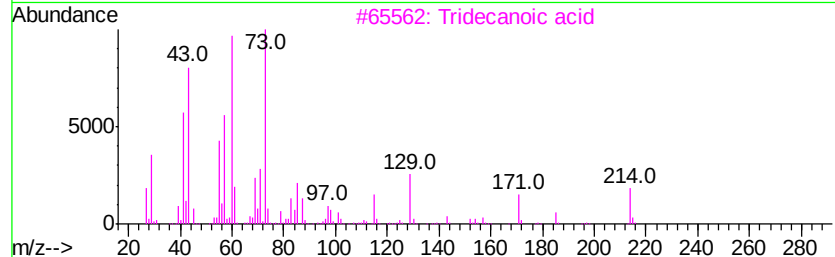
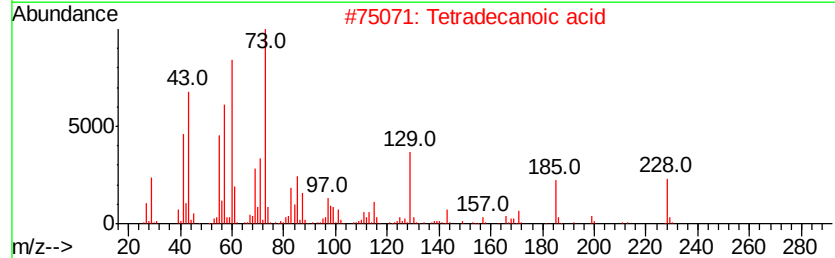
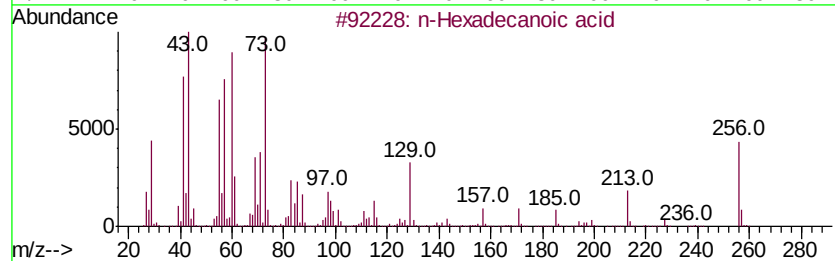
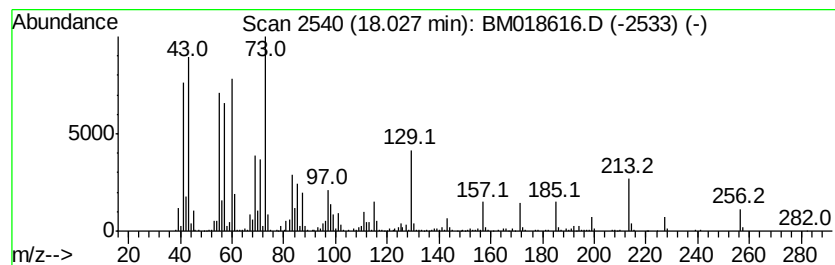
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.03	9.34 ng	1970070	Phenanthrene-d10	17.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	91
4		Undecanoic acid	186	C11H22O2	000112-37-8	72
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	68



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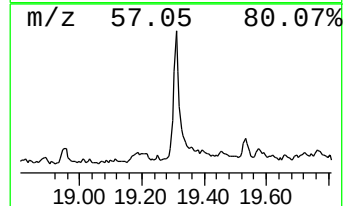
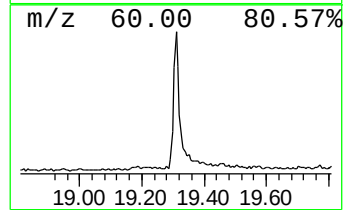
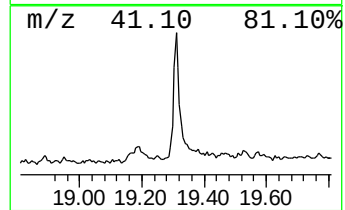
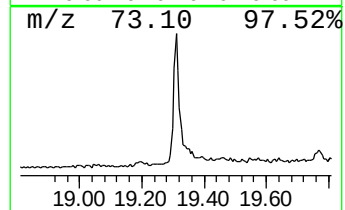
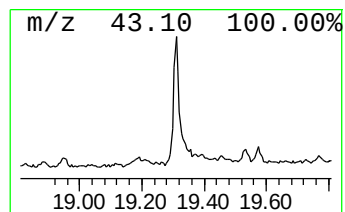
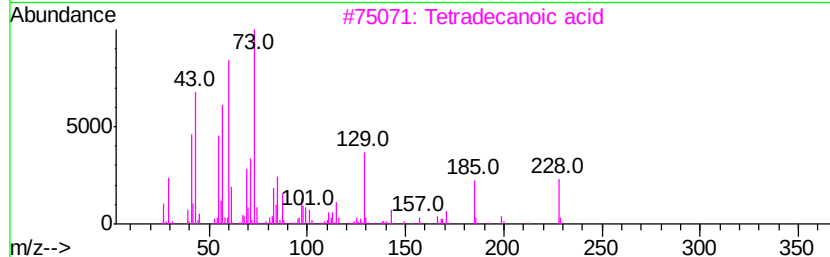
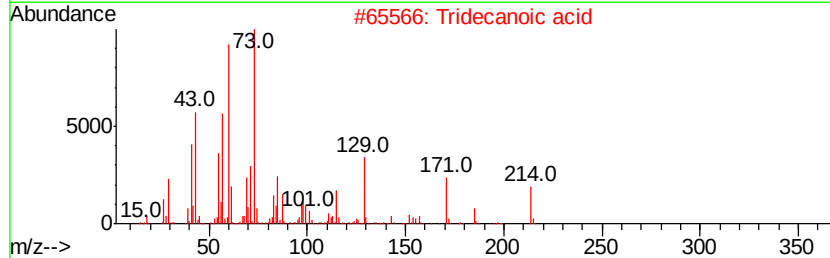
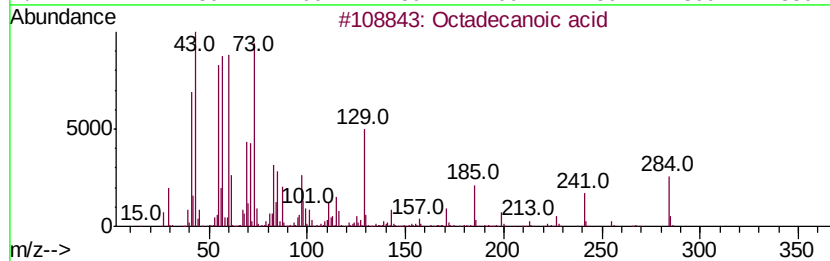
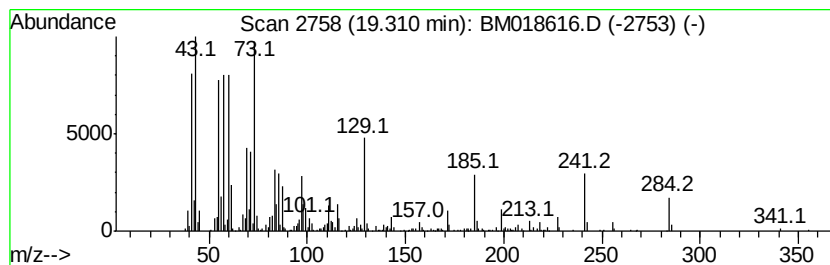
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.31	3.03 ng	707438	Chrysene-d12	21.33		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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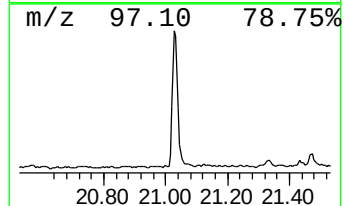
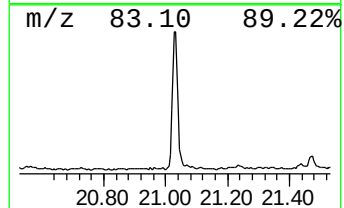
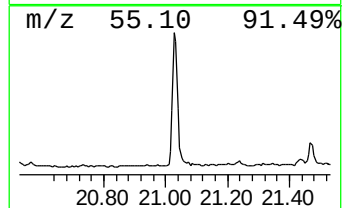
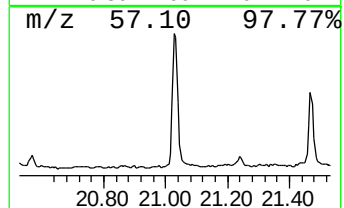
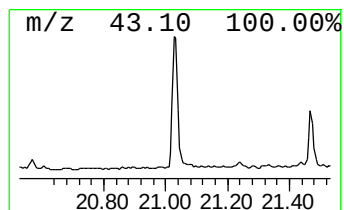
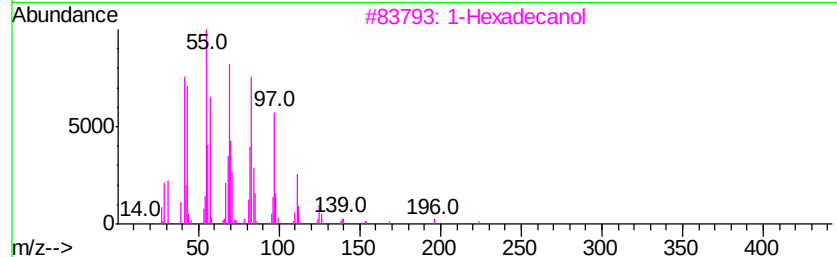
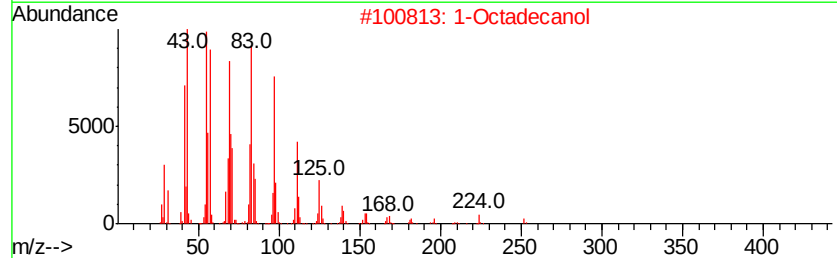
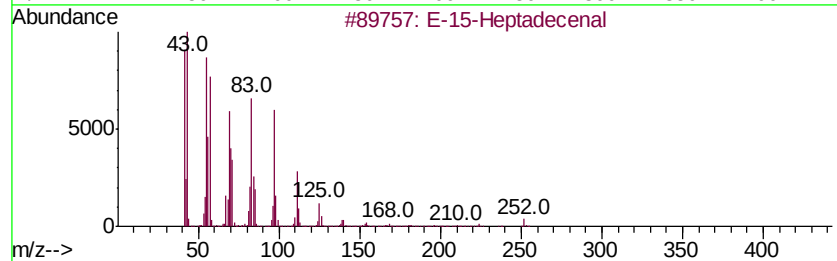
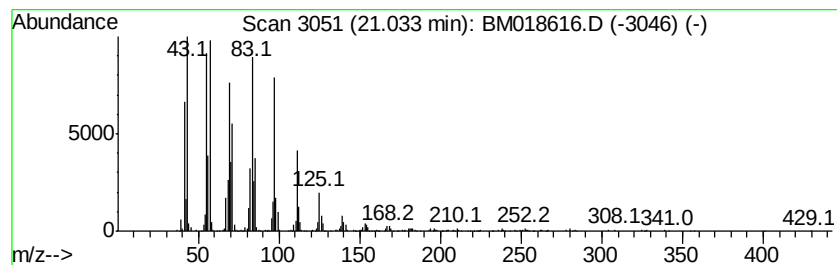
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Peak Number 7 E-15-Heptadecenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	5.50 ng	1281230	Chrysene-d12	21.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	97	
2	1-Octadecanol	270	C18H38O	000112-92-5	90	
3	1-Hexadecanol	242	C16H34O	036653-82-4	87	
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81	
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	81	



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Operator : JU/SJ
Sample : K1139-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-4

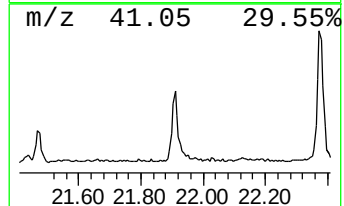
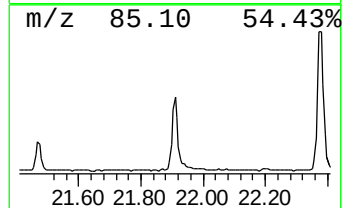
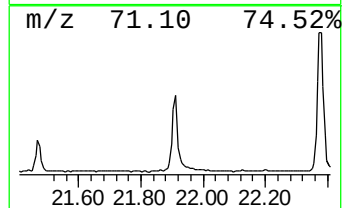
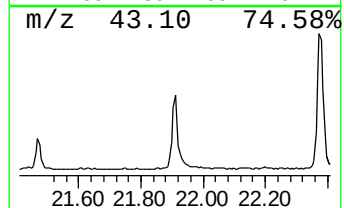
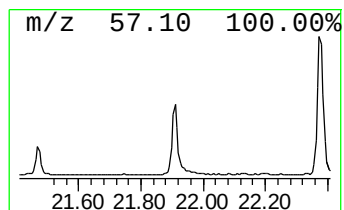
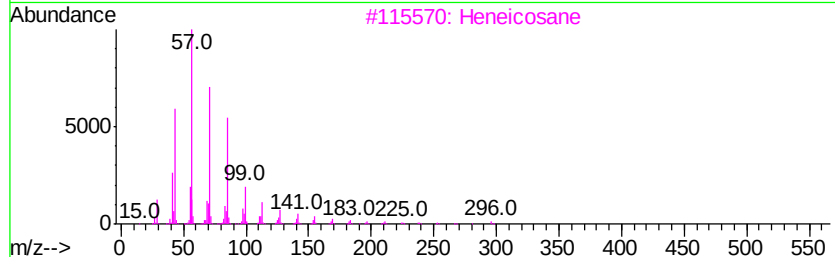
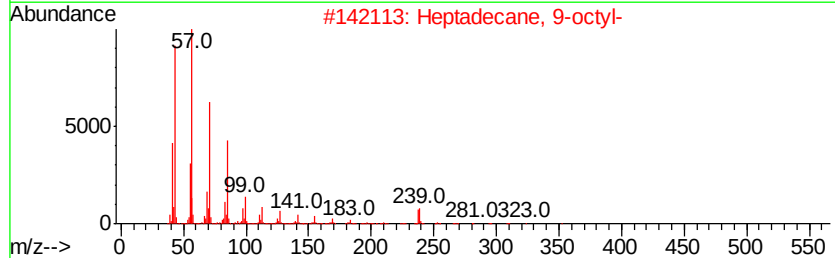
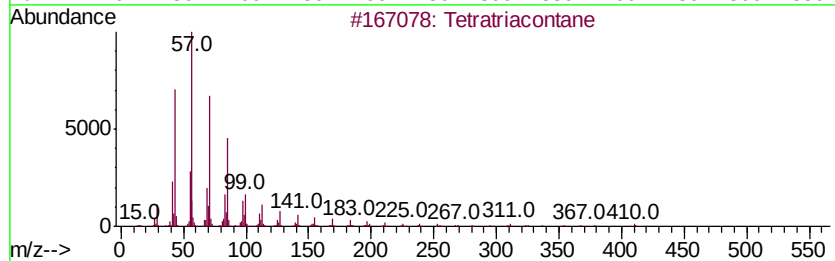
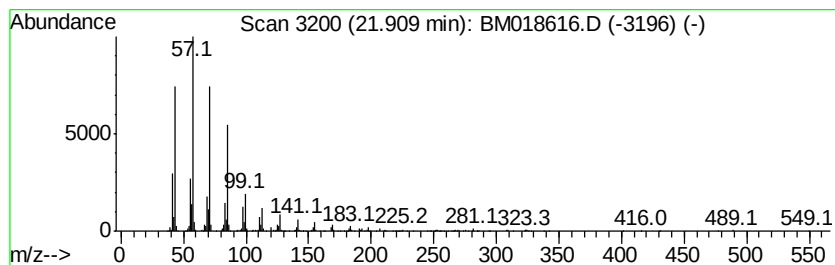
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.91	3.93 ng	915008	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratriacontane	479	C34H70	014167-59-0	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
5		Eicosane	282	C20H42	000112-95-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018616.D
Acq On : 17 Jan 2019 16:23
Operator : JU/SJ
Sample : K1139-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

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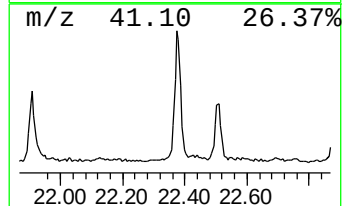
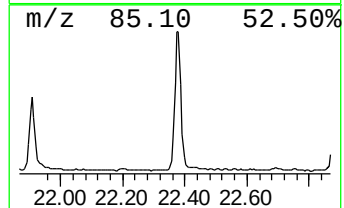
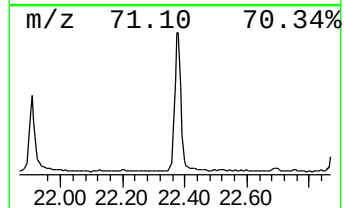
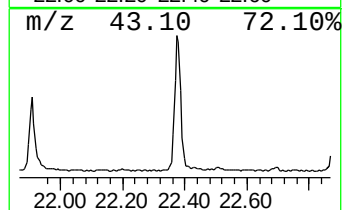
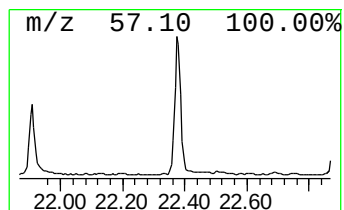
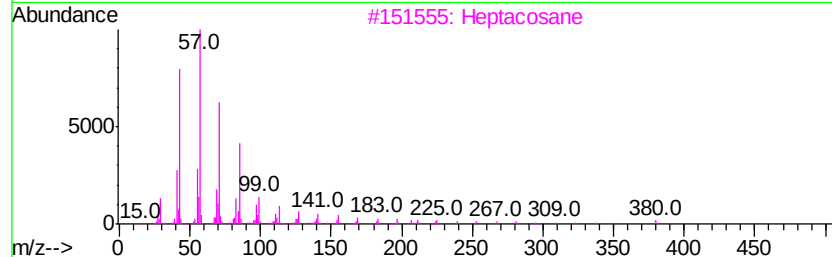
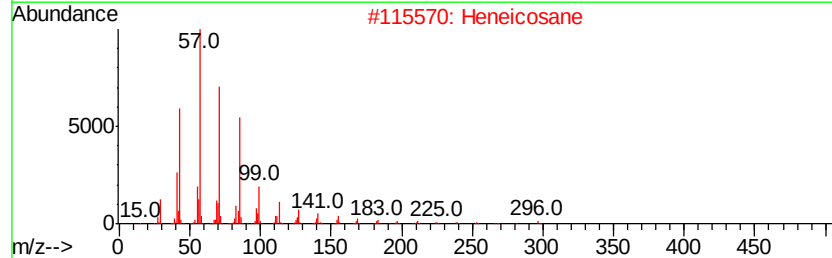
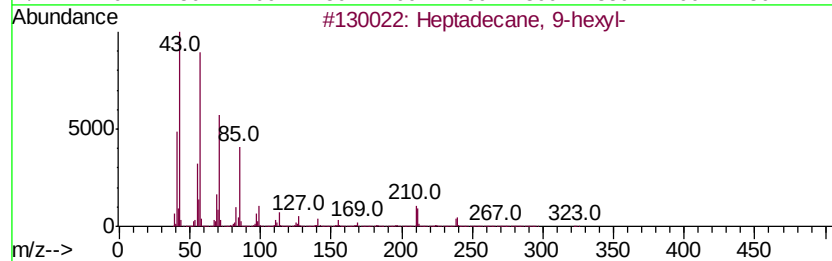
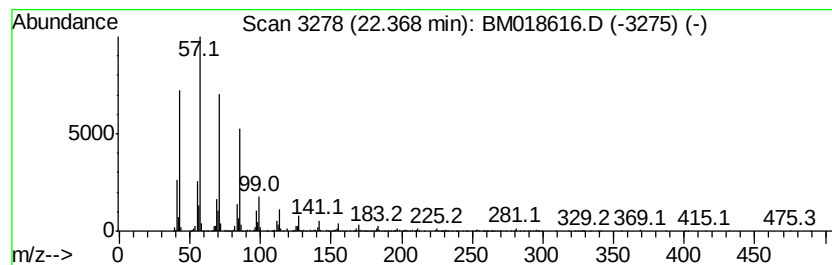
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane, 9-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	7.34 ng	1710010	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018616.D
Acq On : 17 Jan 2019 16:23
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Sample : K1139-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

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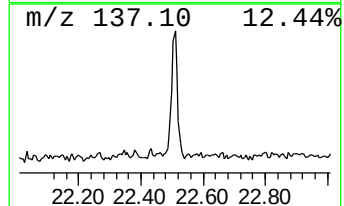
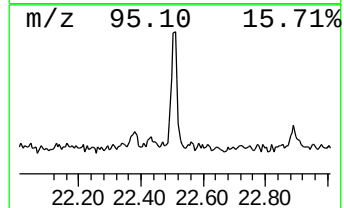
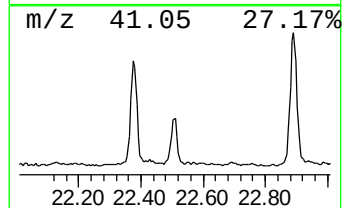
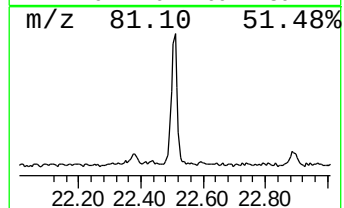
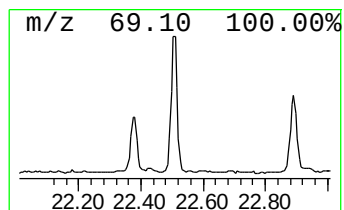
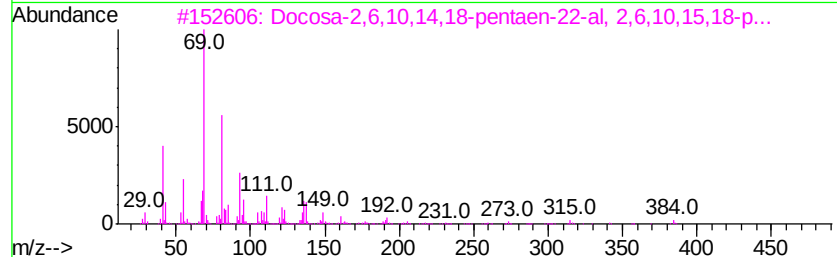
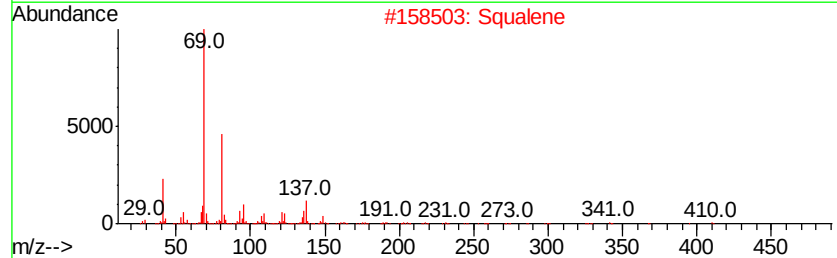
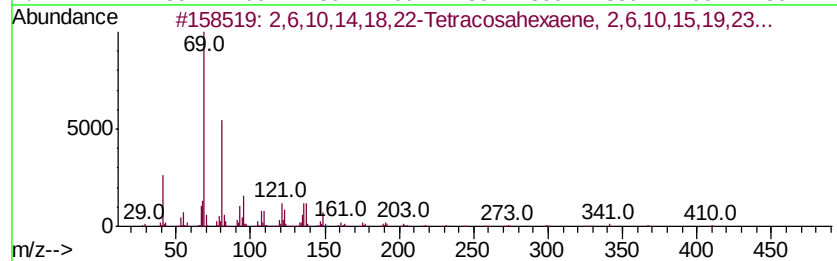
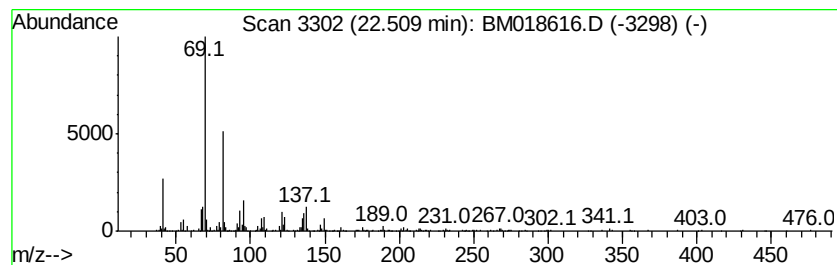
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	3.57 ng	716684	Perylene-d12	23.61

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90		
2	Squalene	410	C30H50	007683-64-9	87		
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72		
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72		
5	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64		



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018616.D
Acq On : 17 Jan 2019 16:23
Operator : JU/SJ
Sample : K1139-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

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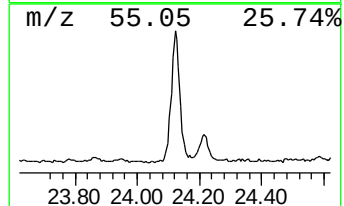
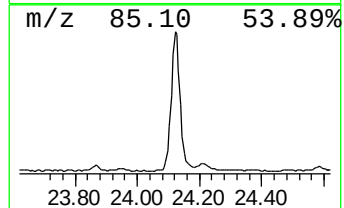
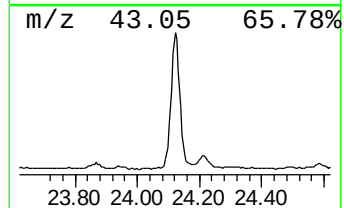
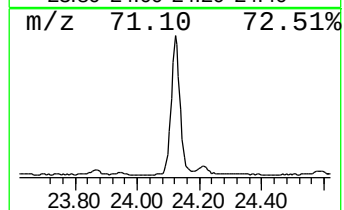
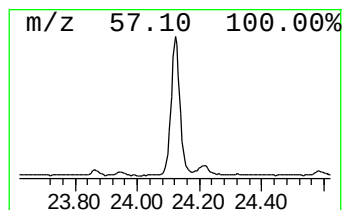
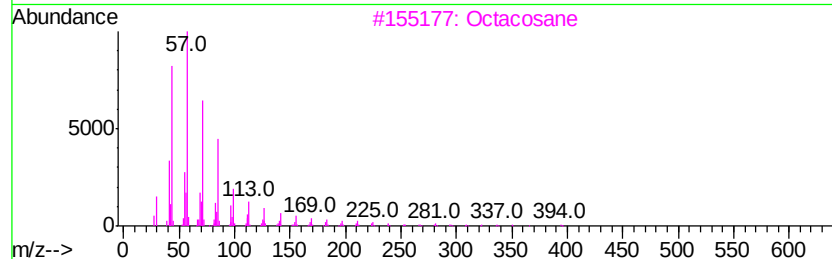
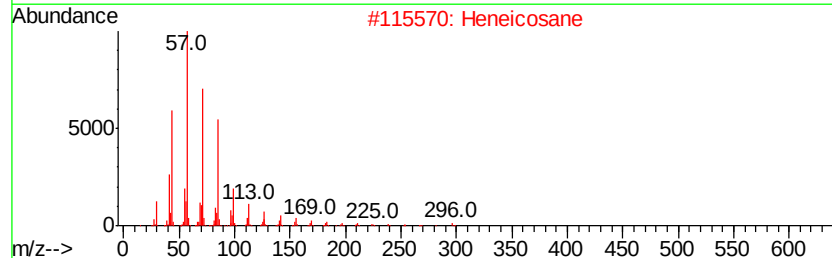
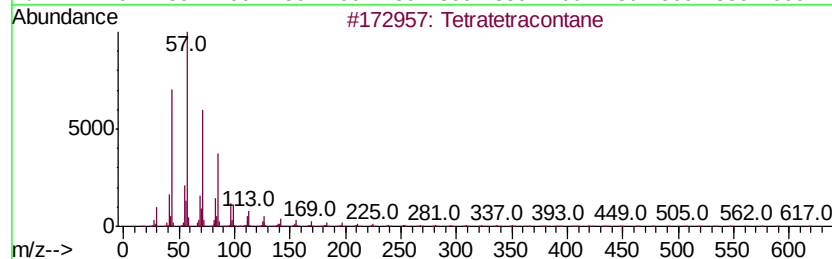
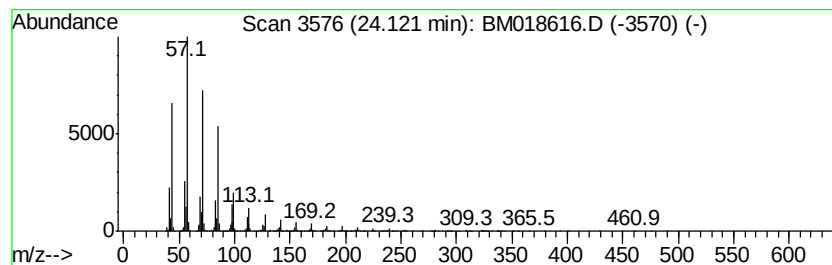
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetratetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.12	13.80 ng	2773510	Perylene-d12	23.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Docosane, 11-decyl-	451	C32H66	055401-55-3	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011719\
Data File : BM018616.D
Acq On : 17 Jan 2019 16:23
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Sample : K1139-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

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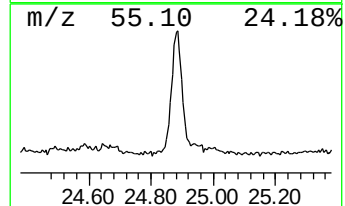
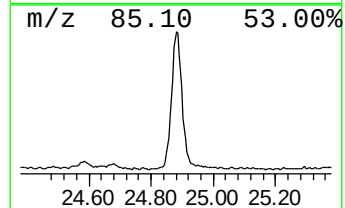
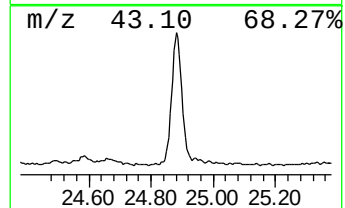
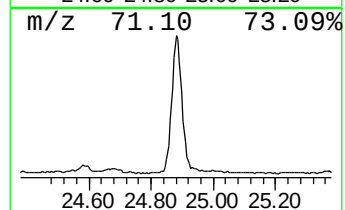
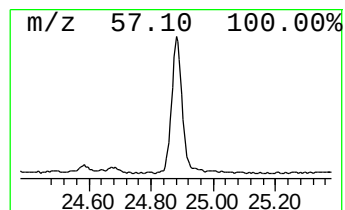
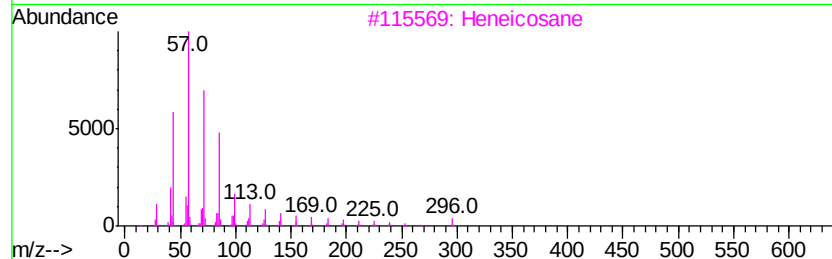
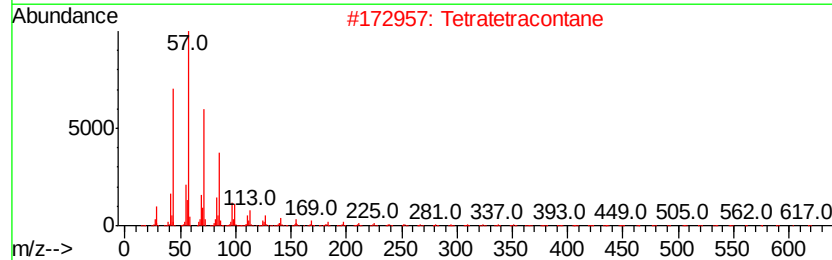
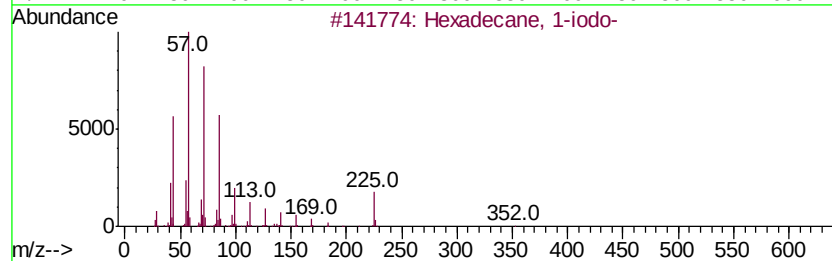
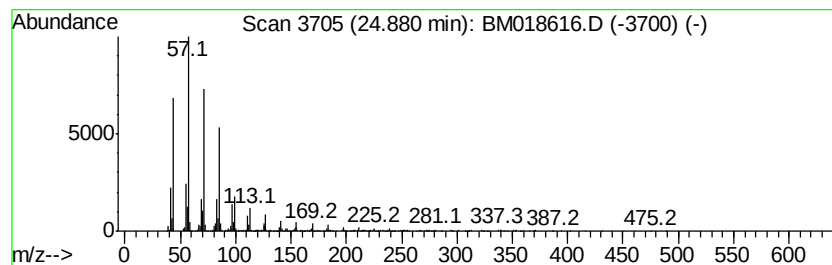
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexadecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.88	8.08 ng	1624530	Perylene-d12	23.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	97
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Docosane, 11-decyl-	451	C32H66	055401-55-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM011719\
Data File : BM018616.D
Acq On : 17 Jan 2019 16:23
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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
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unknown7.27	7.27	65.8	ng	8052000	1	7.74	2447530	20.0
n-Hexadecanoic acid	18.03	9.3	ng	1970070	4	17.14	4220170	20.0
Octadecanoic acid	19.31	3.0	ng	707438	5	21.33	4662260	20.0
E-15-Heptadecenal	21.03	5.5	ng	1281230	5	21.33	4662260	20.0
Tetratriacontane	21.91	3.9	ng	915008	5	21.33	4662260	20.0
Heptadecane, 9-he...	22.37	7.3	ng	1710010	5	21.33	4662260	20.0
2,6,10,14,18,22-T...	22.51	3.6	ng	716684	6	23.61	4020550	20.0
Tetratetracontane	24.12	13.8	ng	2773510	6	23.61	4020550	20.0
Hexadecane, 1-iodo-	24.88	8.1	ng	1624530	6	23.61	4020550	20.0