

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
 Data File : BM018839.D
 Acq On : 18 Feb 2019 15:35
 Operator : JU/SJ
 Sample : K1508-15
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 M-13-D

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-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	4.857	296	301	313	rVB	273427	407940	2.35%	0.324%
2	5.298	369	376	393	rBV	5830498	8282875	47.66%	6.579%
3	6.881	638	645	658	rBV	5604047	8998620	51.78%	7.147%
4	7.239	698	706	720	rBV	6043903	9178497	52.81%	7.290%
5	7.704	778	785	793	rBV	1484253	2255100	12.98%	1.791%
6	8.022	831	839	850	rBV	4189984	6523741	37.54%	5.182%
7	8.875	975	984	1001	rBV	3221007	5381660	30.97%	4.275%
8	10.492	1251	1259	1274	rBV	1828464	3133632	18.03%	2.489%
9	12.968	1673	1680	1695	rBV	8035518	11880552	68.36%	9.436%
10	13.821	1816	1825	1840	rBV	414985	695562	4.00%	0.552%
11	14.357	1909	1916	1934	rBV2	2585735	4054894	23.33%	3.221%
12	15.851	2161	2170	2196	rBV	6474330	9493731	54.63%	7.541%
13	17.103	2377	2383	2395	rBV2	3218251	4862647	27.98%	3.862%
14	17.997	2529	2535	2560	rBV	2215315	3260382	18.76%	2.590%
15	19.280	2748	2753	2763	rBV	1140572	1634738	9.41%	1.298%
16	19.739	2825	2831	2840	rVB	14648742	17378755	100.00%	13.804%
17	20.533	2963	2966	2970	rBV	241433	258766	1.49%	0.206%
18	20.997	3041	3045	3058	rBV	2136690	2989645	17.20%	2.375%
19	21.297	3091	3096	3105	rBV	4201535	5316612	30.59%	4.223%
20	21.438	3116	3120	3127	rBV	1271909	1392431	8.01%	1.106%
21	21.868	3189	3193	3207	rBV	1835432	2502438	14.40%	1.988%
22	22.333	3268	3272	3280	rVB	2328084	3016692	17.36%	2.396%
23	22.844	3354	3359	3365	rVB	2062056	2945051	16.95%	2.339%
24	23.415	3450	3456	3464	rVB	1664992	2748639	15.82%	2.183%
25	23.556	3473	3480	3494	rVB	2350026	4319558	24.86%	3.431%
26	24.062	3560	3566	3573	rVB	1083577	1985835	11.43%	1.577%
27	24.815	3688	3694	3701	rVB	486117	1001075	5.76%	0.795%

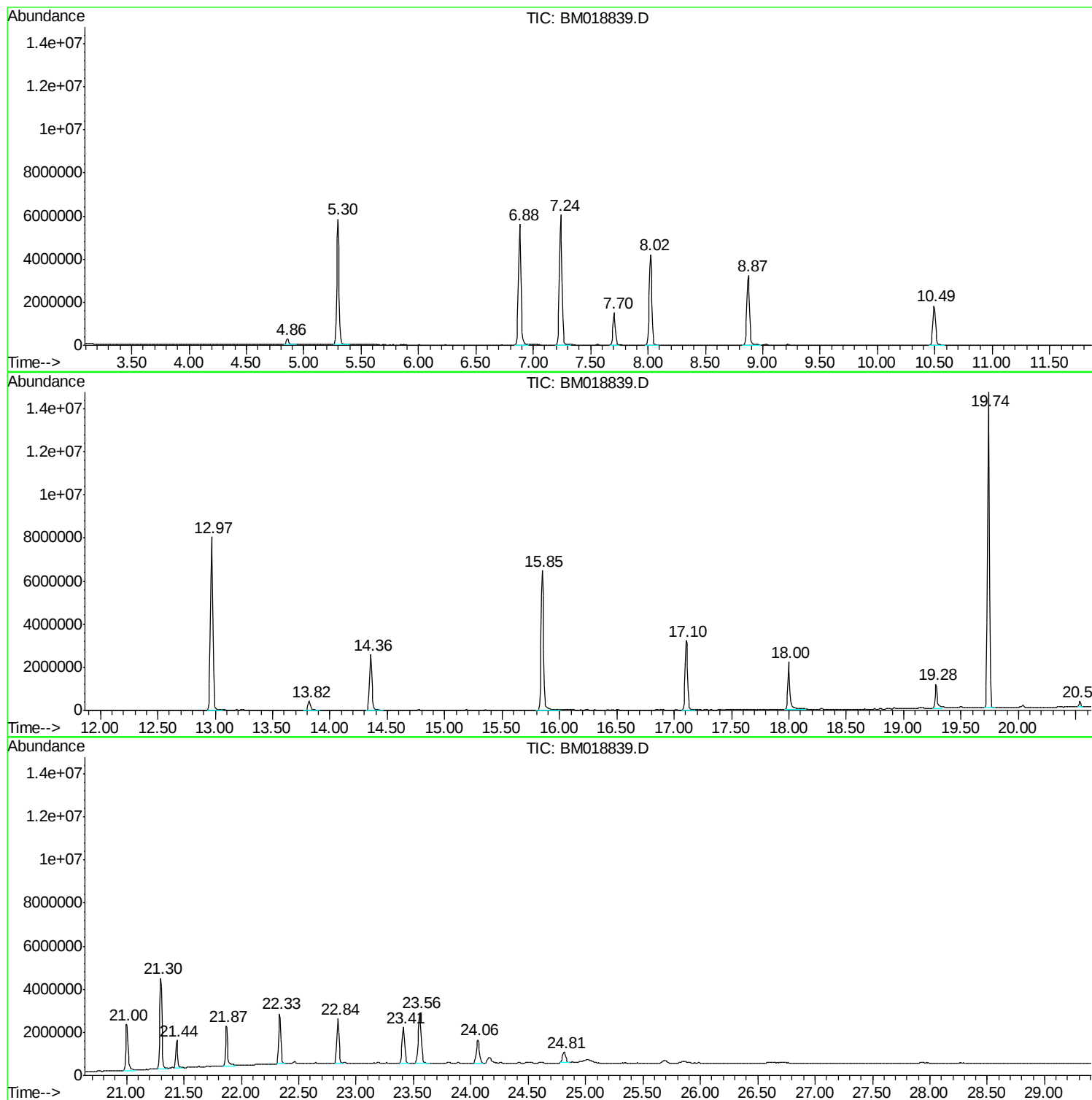
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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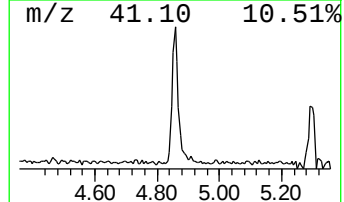
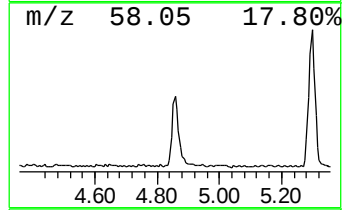
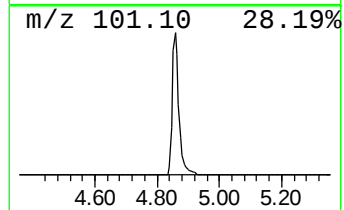
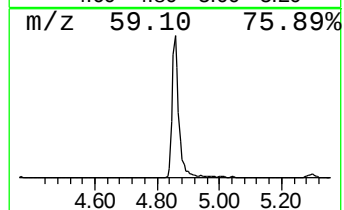
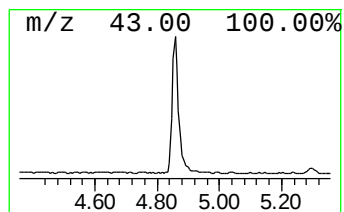
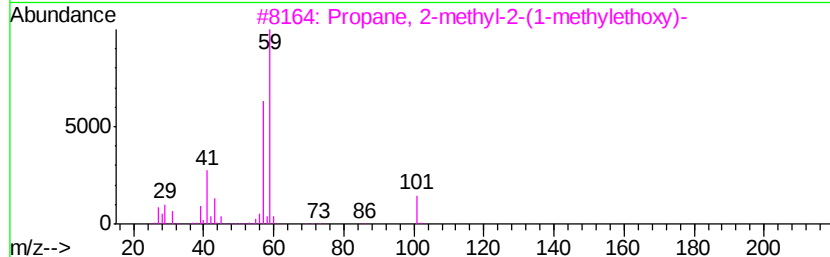
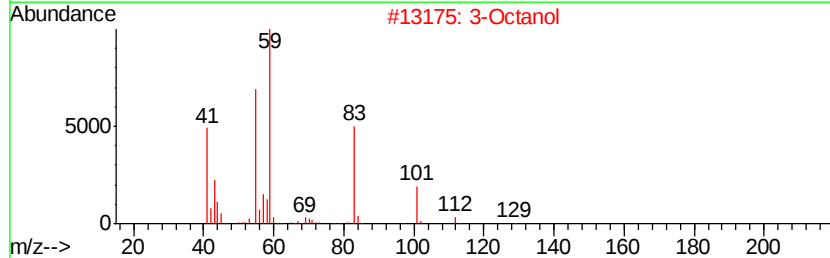
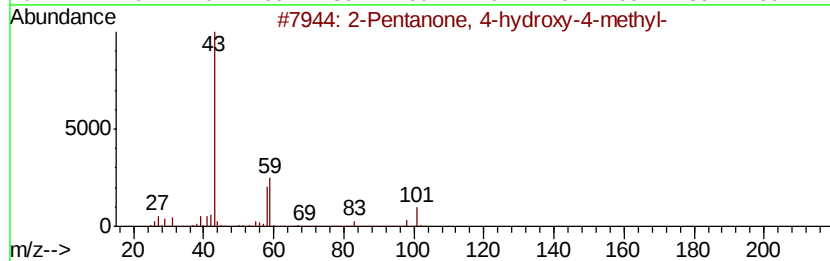
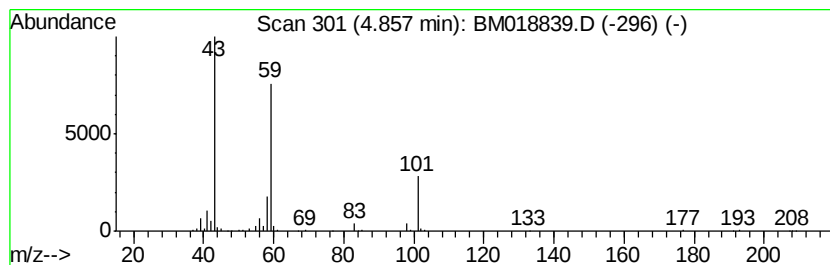
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	3.62 ng	407940	1,4-Dichlorobenzene-d4	7.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			3-Octanol	130	C8H18O	020296-29-1	38
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	36
5			Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	33



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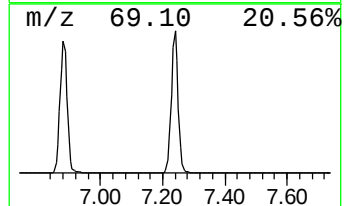
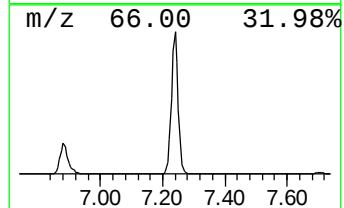
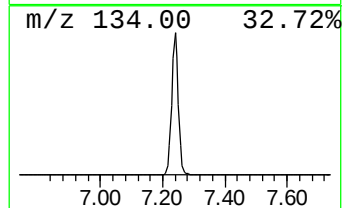
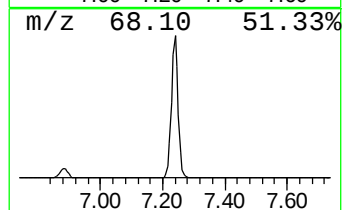
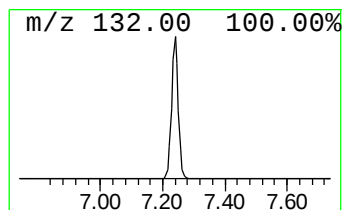
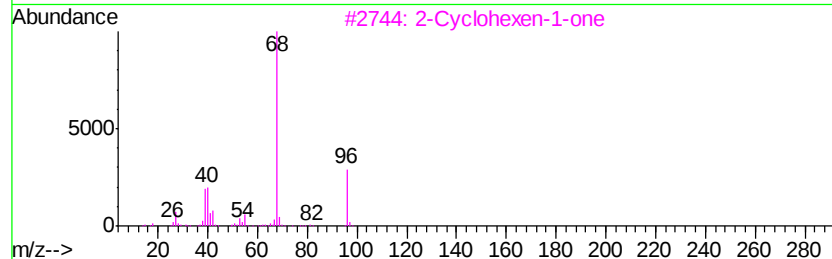
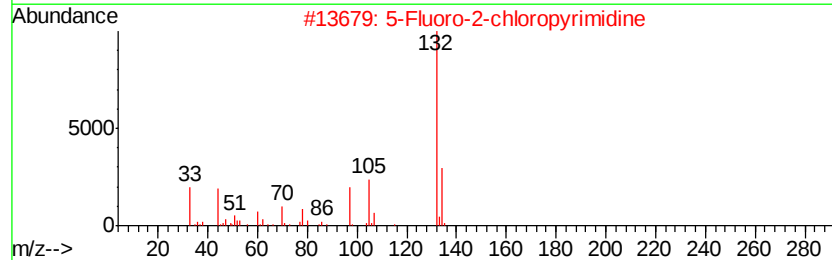
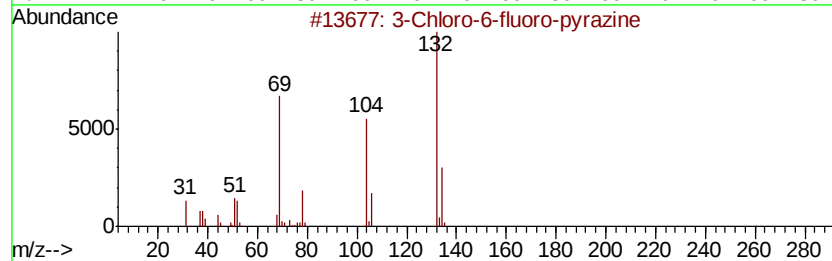
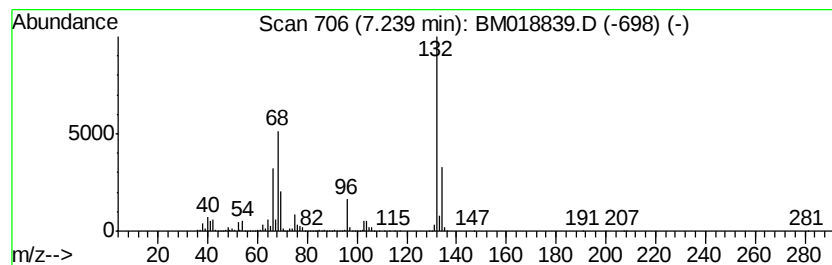
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Peak Number 2 unknown7.24 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.24	81.40 ng	9178500	1,4-Dichlorobenzene-d4	7.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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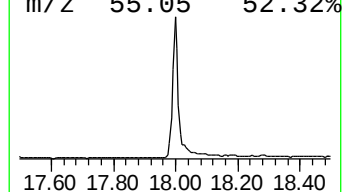
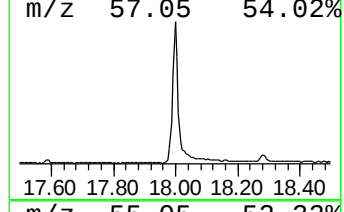
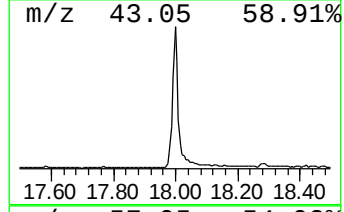
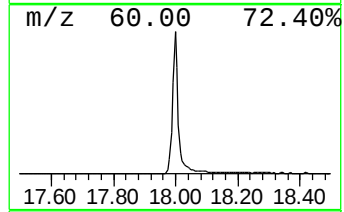
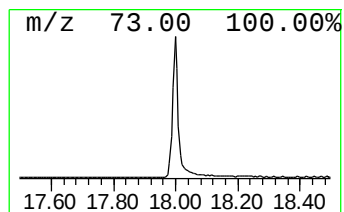
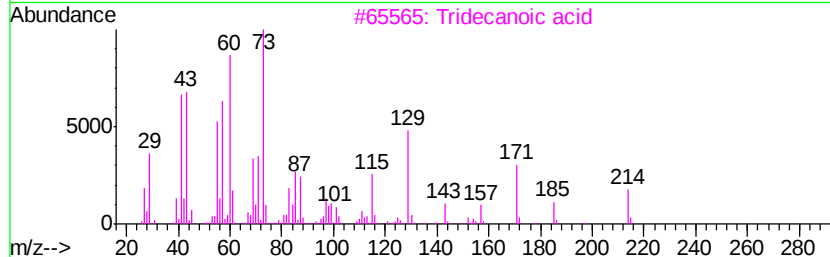
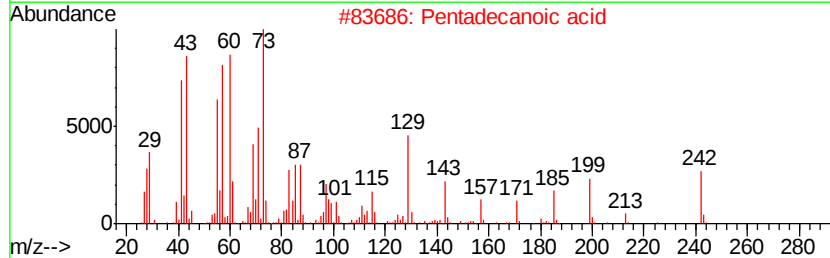
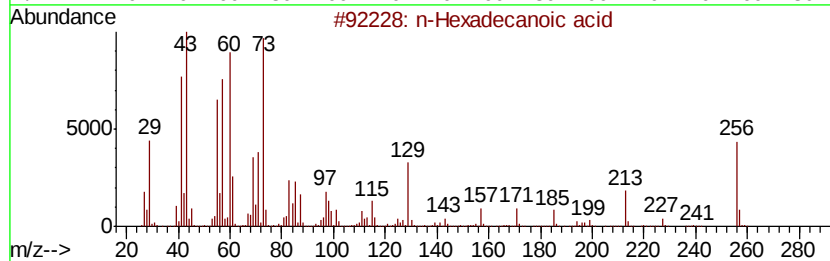
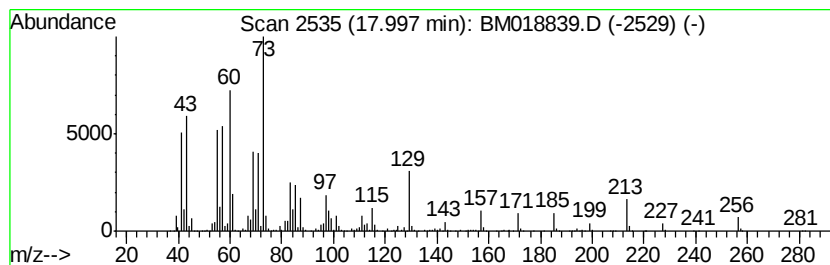
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.00	13.41 ng	3260380	Phenanthrene-d10	17.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3		Tridecanoic acid	214	C13H26O2	000638-53-9	47
4		Tridecane	184	C13H28	000629-50-5	18
5		Hexadecane	226	C16H34	000544-76-3	18



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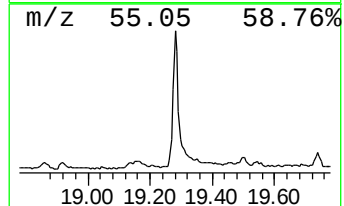
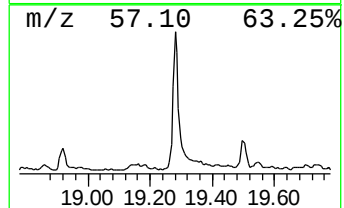
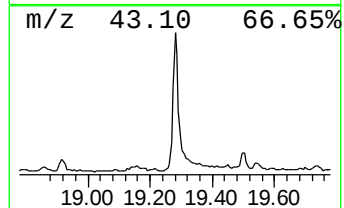
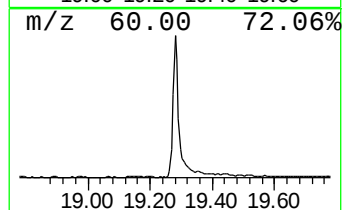
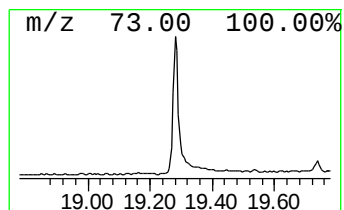
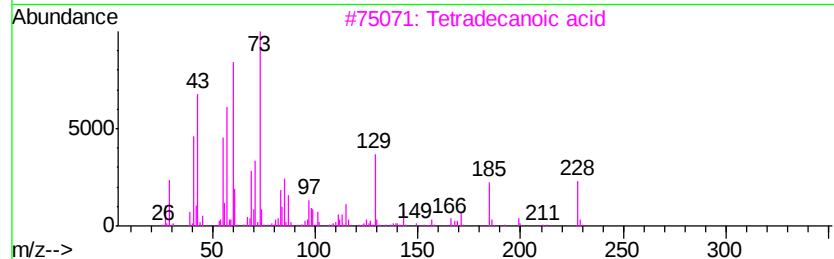
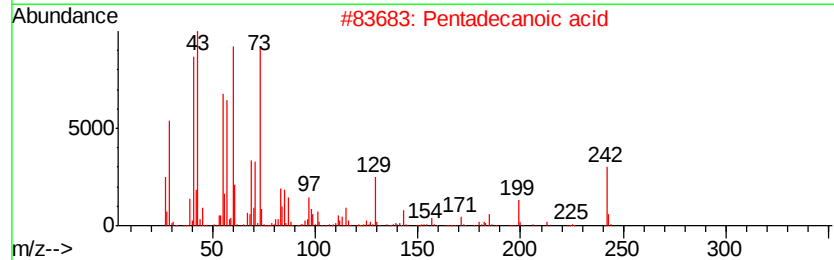
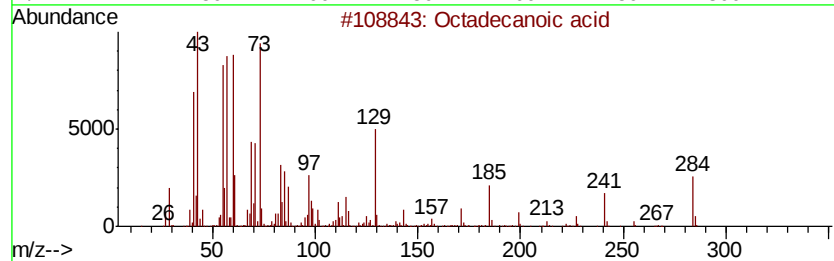
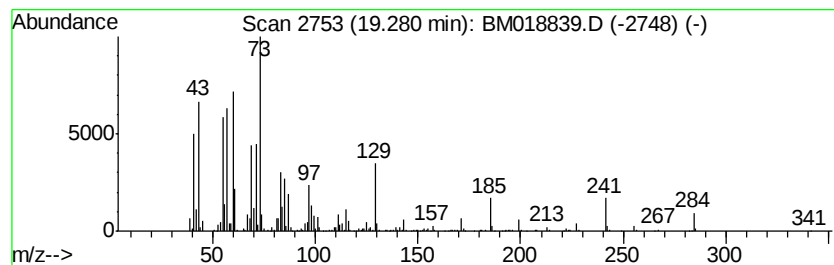
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Peak Number 5 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.28	6.15 ng	1634740	Chrysene-d12	21.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
5		Eicosane	282	C20H42	000112-95-8	18



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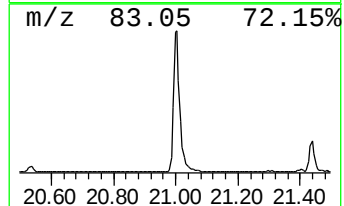
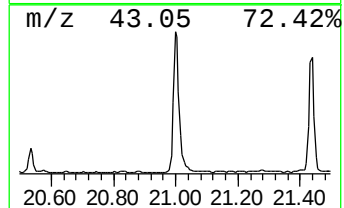
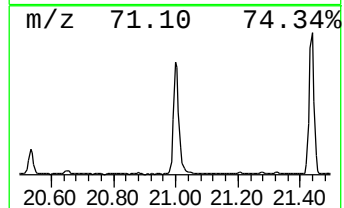
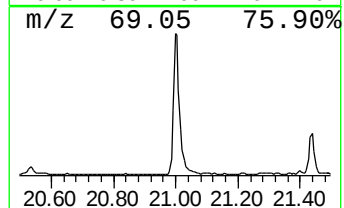
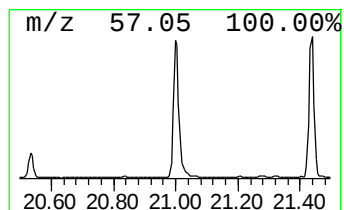
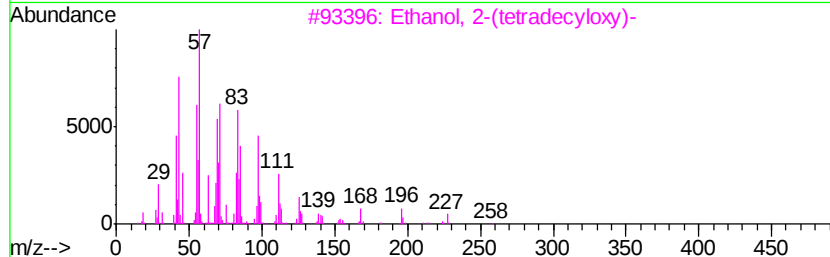
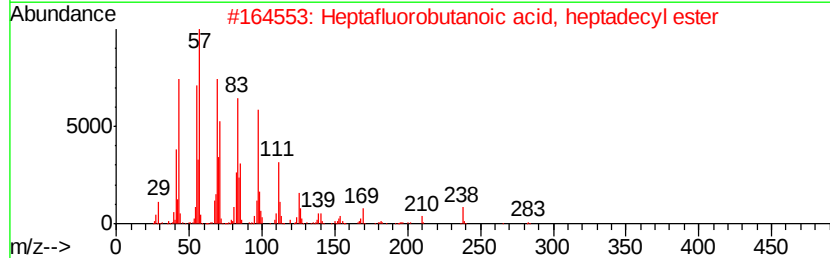
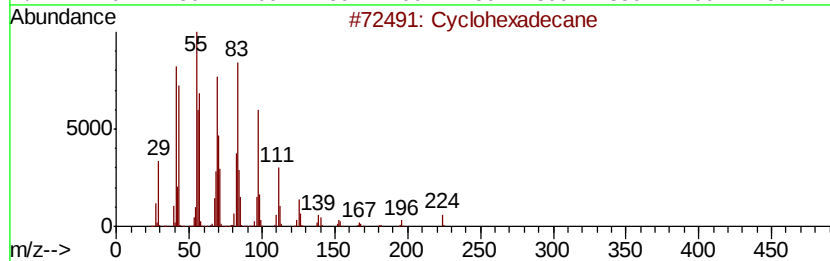
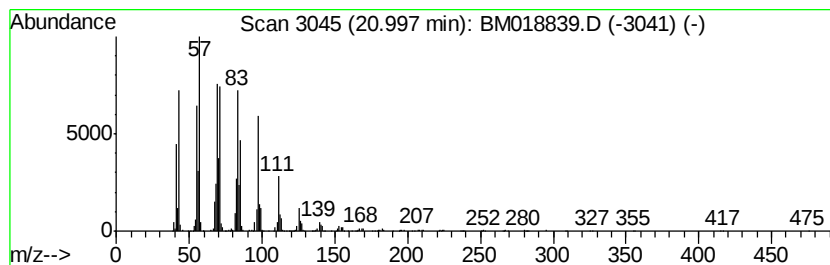
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.00	11.25 ng	2989650	Chrysene-d12	21.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 84
2		Heptafluorobutanoic acid, heptad...	452 C21H35F7O2	1000282-97-3 74
3		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 70
4		1-Octadecanol	270 C18H38O	000112-92-5 70
5		Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0 64



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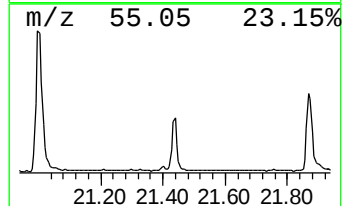
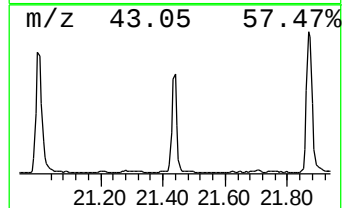
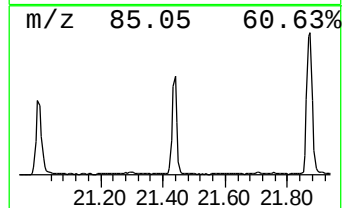
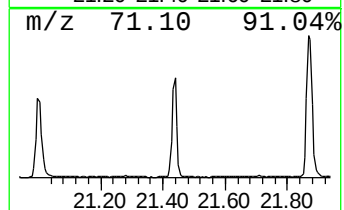
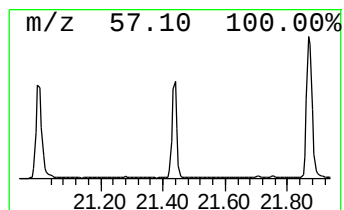
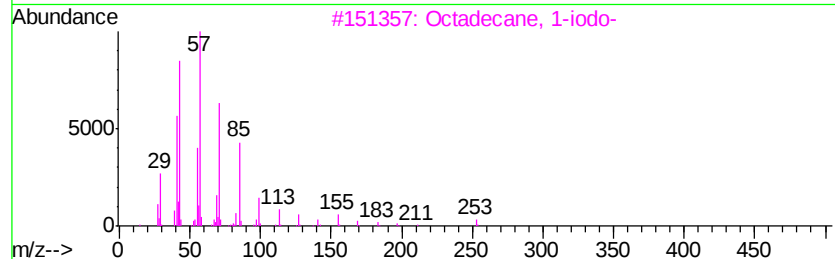
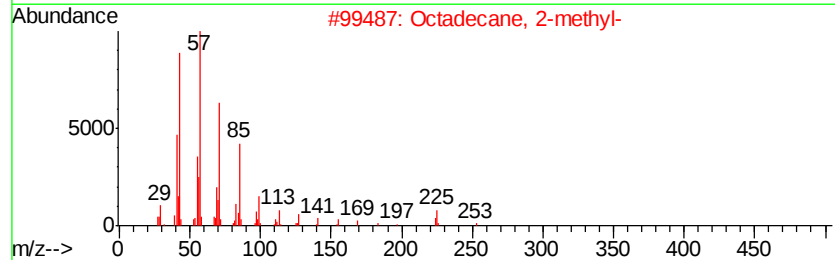
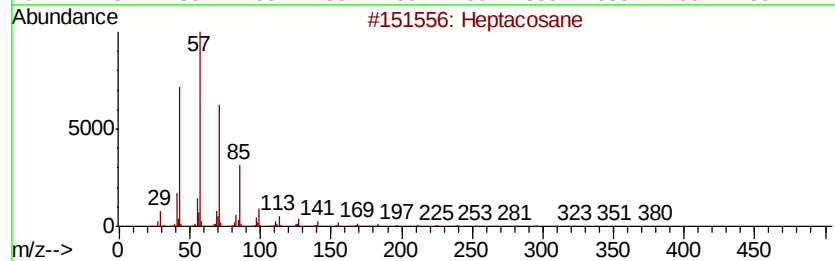
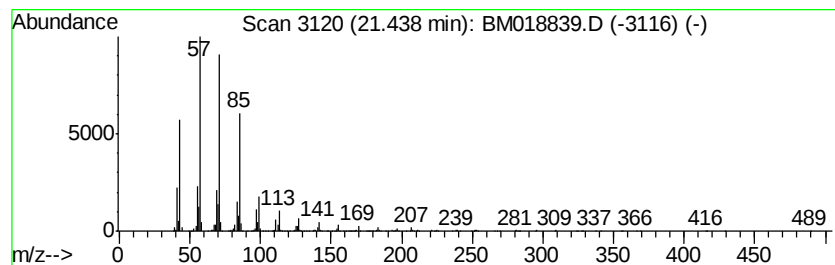
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.44	5.24 ng	1392430	Chrysene-d12	21.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	90
2		Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
3		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4		Tetradecane	198	C14H30	000629-59-4	87
5		Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
Data File : BM018839.D
Acq On : 18 Feb 2019 15:35
Operator : JU/SJ
Sample : K1508-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
M-13-D

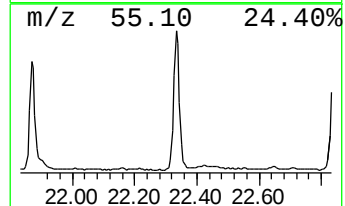
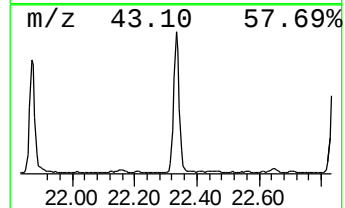
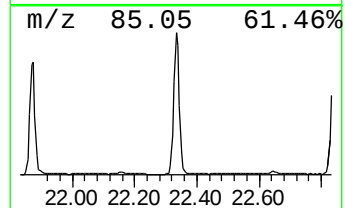
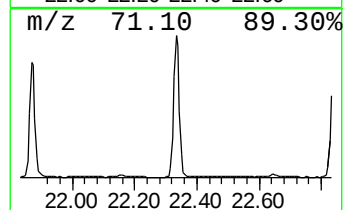
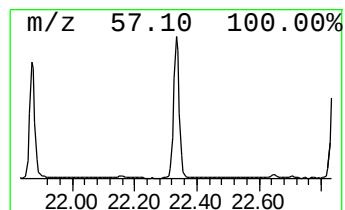
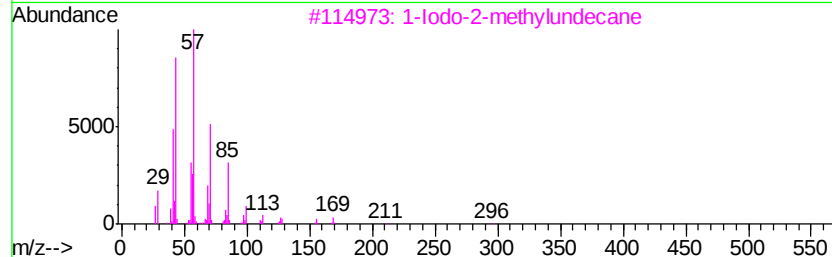
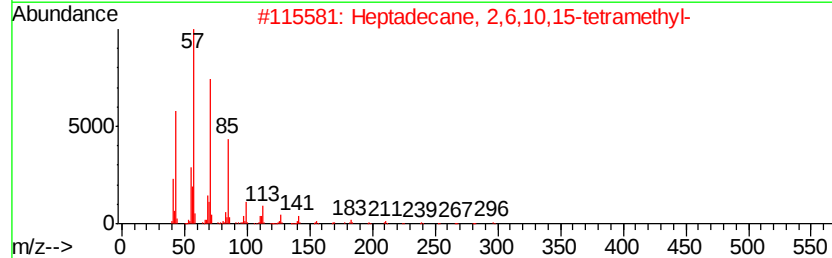
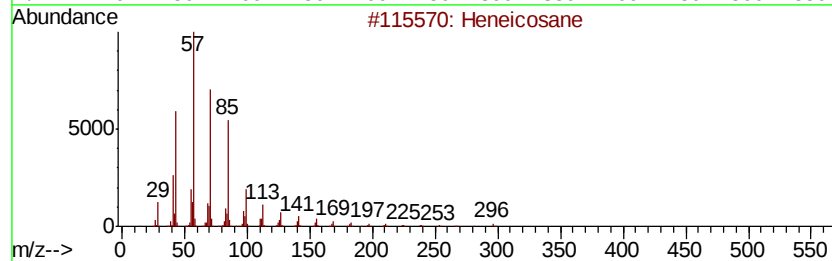
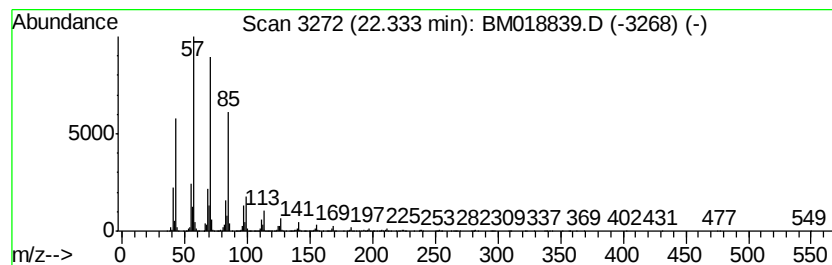
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.33	11.35 ng	3016690	Chrysene-d12	21.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	95
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	94
3	1-Iodo-2-methylundecane		296	C12H25I	073105-67-6	94
4	Eicosane, 10-methyl-		296	C21H44	054833-23-7	93
5	Heptacosane		380	C27H56	000593-49-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM021819\
Data File : BM018839.D
Acq On : 18 Feb 2019 15:35
Operator : JU/SJ
Sample : K1508-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
M-13-D

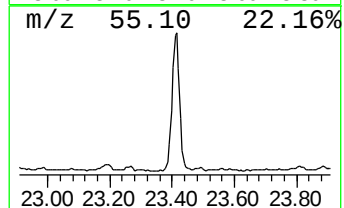
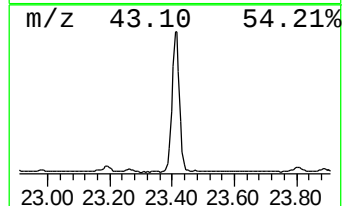
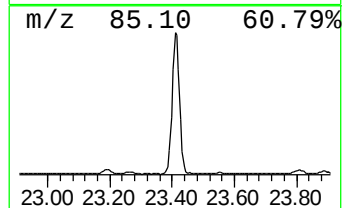
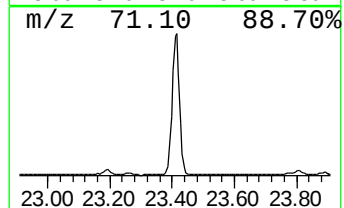
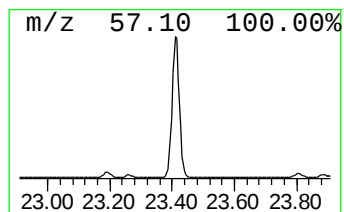
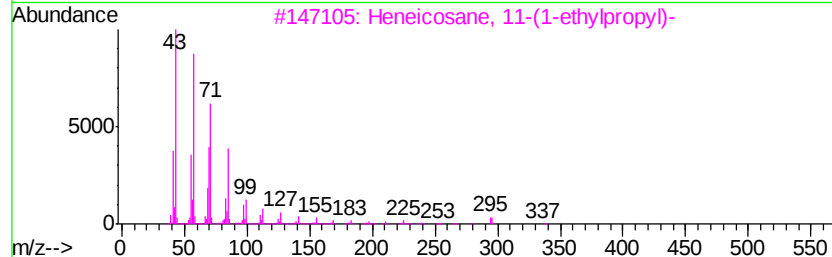
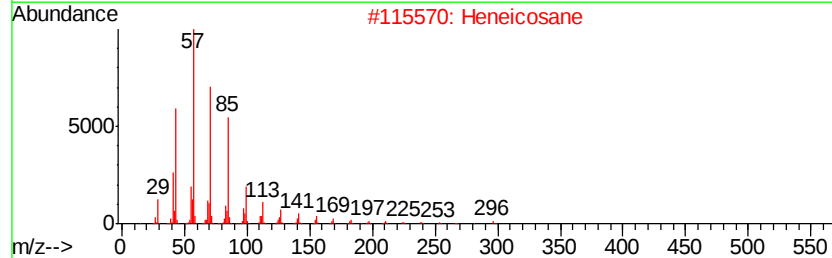
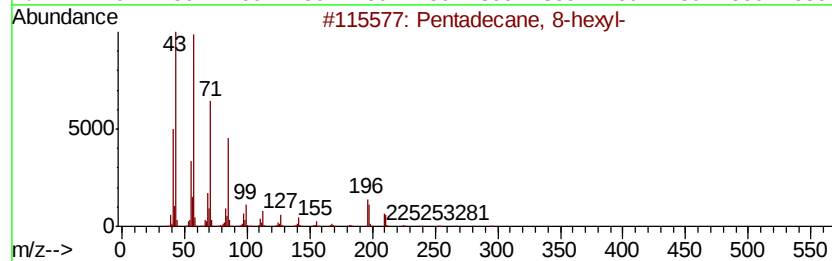
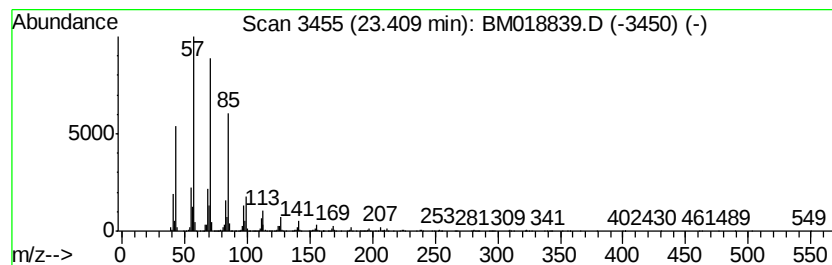
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentadecane, 8-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.41	12.73 ng	2748640	Perylene-d12	23.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4		Heptacosane	380	C27H56	000593-49-7	87
5		2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM021819\
Data File : BM018839.D
Acq On : 18 Feb 2019 15:35
Operator : JU/SJ
Sample : K1508-15
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
M-13-D

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
2-Pentanone, 4-hy...	4.86	3.6	ng	407940	1	7.70	2255100	20.0
unknown7.24	7.24	81.4	ng	9178500	1	7.70	2255100	20.0
n-Hexadecanoic acid	18.00	13.4	ng	3260380	4	17.10	4862650	20.0
Octadecanoic acid	19.28	6.2	ng	1634740	5	21.30	5316610	20.0
Cyclohexadecane	21.00	11.3	ng	2989650	5	21.30	5316610	20.0
Heptacosane	21.44	5.2	ng	1392430	5	21.30	5316610	20.0
Heneicosane	22.33	11.4	ng	3016690	5	21.30	5316610	20.0
Pentadecane, 8-he...	23.41	12.7	ng	2748640	6	23.56	4319560	20.0