

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
 Data File : BM019079.D
 Acq On : 08 Mar 2019 18:29
 Operator : JU/SJ
 Sample : K1807-31
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-13

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	5.263	364	370	384	rBV	1633250	2447513	78.66%	9.119%
2	6.845	632	639	656	rBV	1590632	2612778	83.97%	9.734%
3	7.204	692	700	712	rBV	1675598	2694601	86.60%	10.039%
4	7.669	772	779	787	rBV	442698	685178	22.02%	2.553%
5	7.986	826	833	841	rBV	1134406	1832414	58.89%	6.827%
6	8.839	970	978	992	rBV	802757	1500740	48.23%	5.591%
7	10.457	1244	1253	1265	rBV	476239	839229	26.97%	3.127%
8	12.933	1667	1674	1696	rBV	1624585	2578349	82.87%	9.606%
9	13.792	1811	1820	1832	rBV	98197	184002	5.91%	0.686%
10	14.204	1882	1890	1904	rBV2	86610	252006	8.10%	0.939%
11	14.321	1904	1910	1921	rVB2	581647	944968	30.37%	3.521%
12	15.821	2159	2165	2178	rBV	1248971	2020074	64.92%	7.526%
13	17.080	2373	2379	2393	rBV	627207	1031653	33.16%	3.844%
14	17.962	2524	2529	2541	rBV	128102	238091	7.65%	0.887%
15	19.250	2744	2748	2757	rBV2	66600	115975	3.73%	0.432%
16	19.709	2821	2826	2837	rBV	2480515	3111397	100.00%	11.592%
17	20.974	3037	3041	3047	rBV	119155	174995	5.62%	0.652%
18	21.274	3087	3092	3103	rBV	913981	1282562	41.22%	4.778%
19	21.839	3186	3188	3196	rVB3	97574	128072	4.12%	0.477%
20	22.297	3263	3266	3270	rBV	162441	209712	6.74%	0.781%
21	22.803	3349	3352	3359	rVB2	171483	237826	7.64%	0.886%
22	23.368	3445	3448	3455	rVB	180230	275326	8.85%	1.026%
23	23.515	3468	3473	3490	rVB2	684315	1443401	46.39%	5.378%

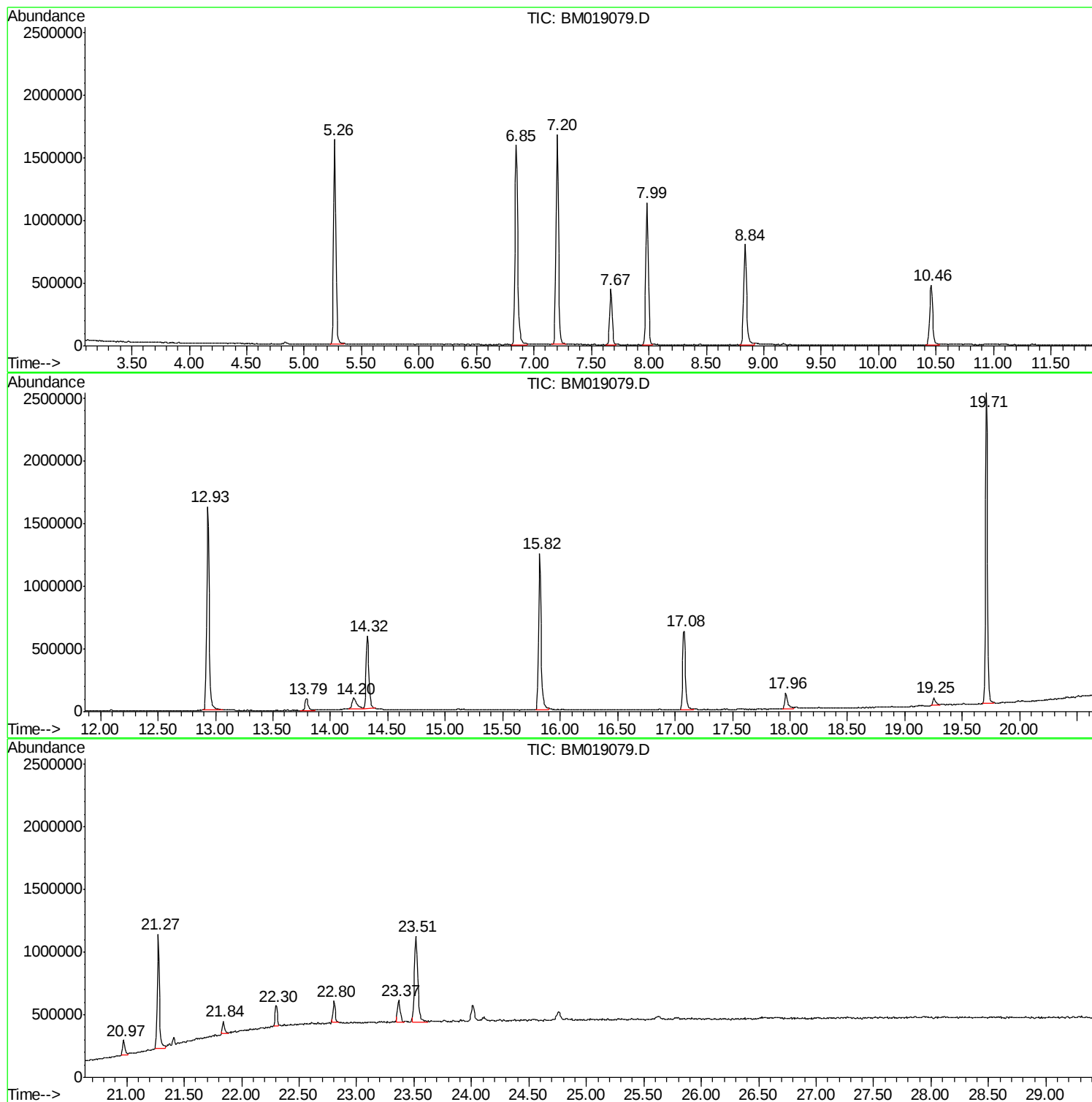
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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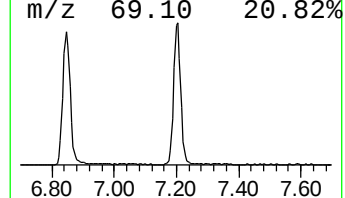
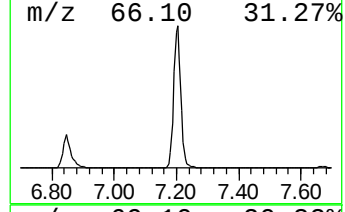
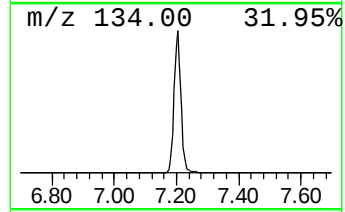
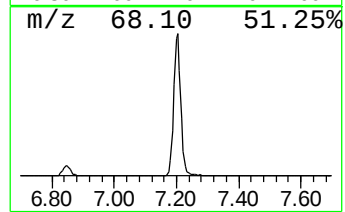
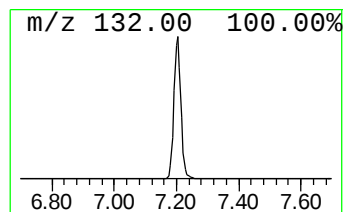
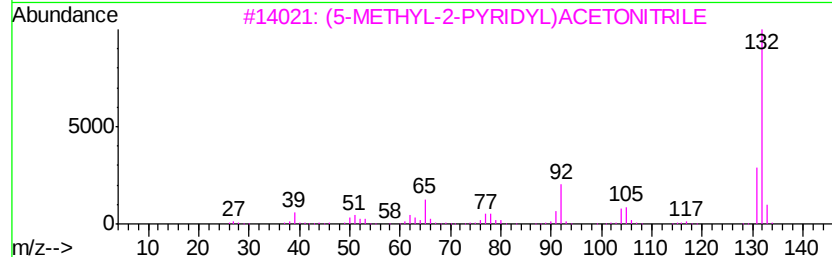
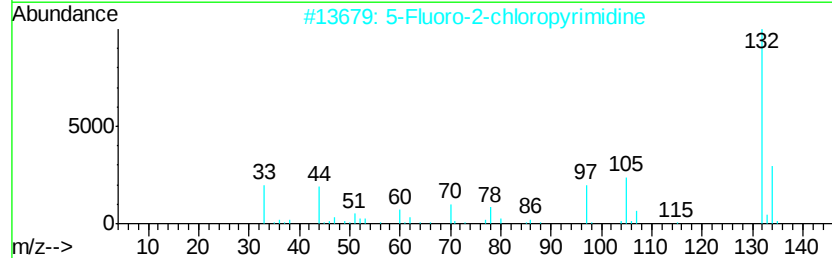
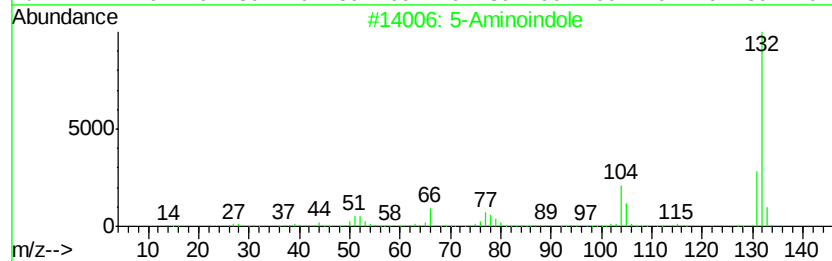
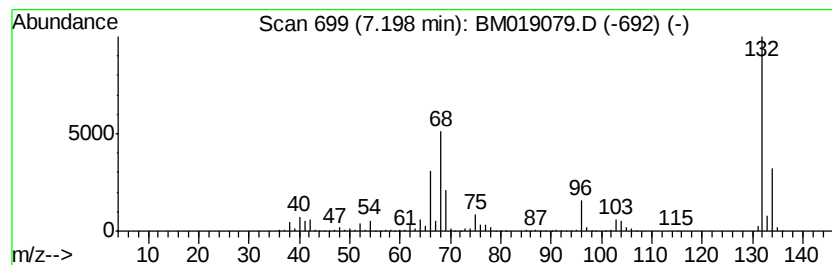
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	78.65 ng	2694600	1,4-Dichlorobenzene-d4	7.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Aminoindole	132	C8H8N2	005192-03-0	22
2			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3			(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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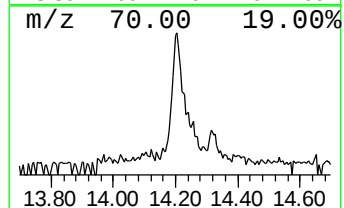
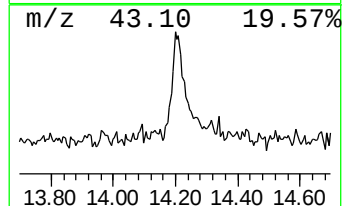
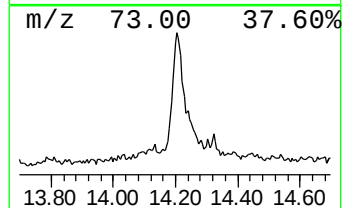
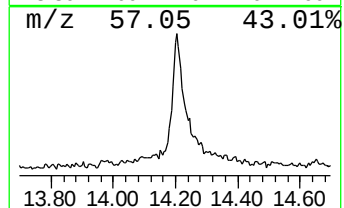
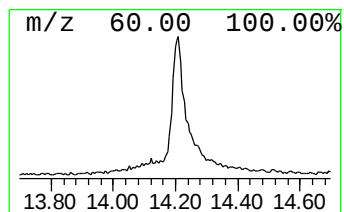
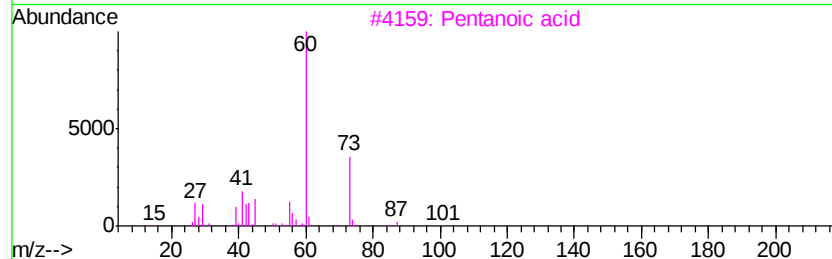
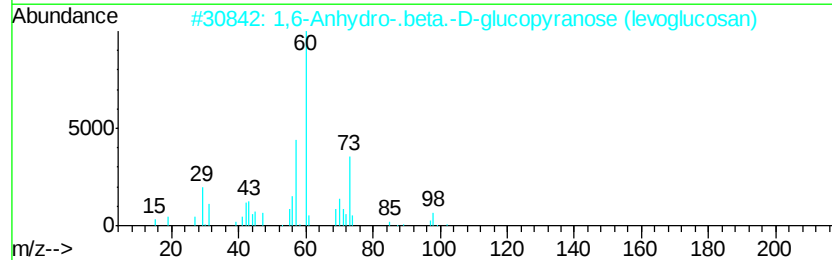
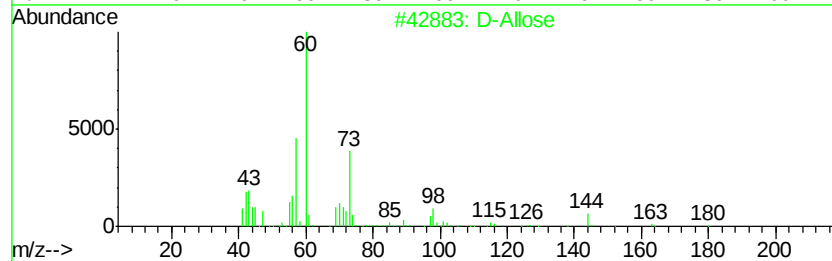
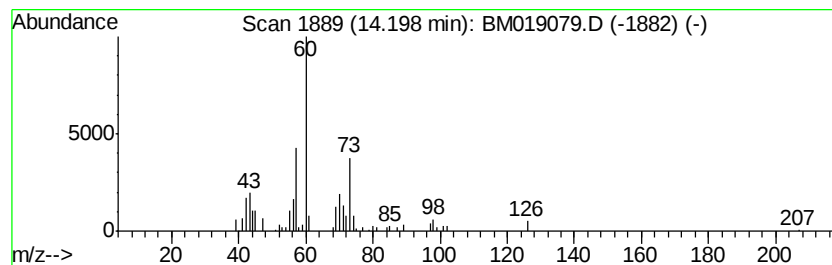
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Peak Number 3 D-Allose Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	5.33 ng	252006	Acenaphthene-d10	14.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	D-Allose	180	C6H12O6	002595-97-3	72
2		1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	72
3		Pentanoic acid	102	C5H10O2	000109-52-4	50
4		Hexanoic acid	116	C6H12O2	000142-62-1	50
5		Thietane, 2,4-dimethyl-	102	C5H10S	043044-24-2	46



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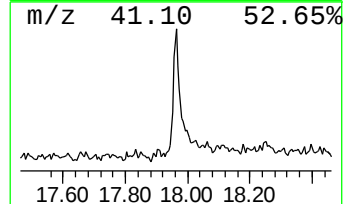
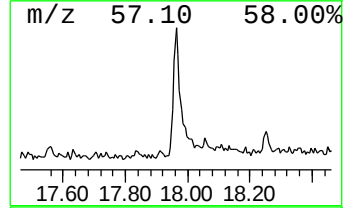
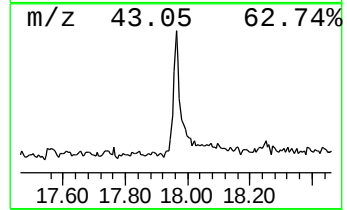
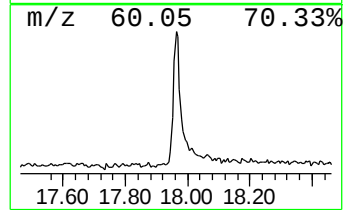
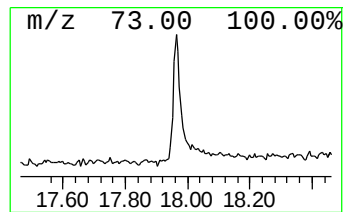
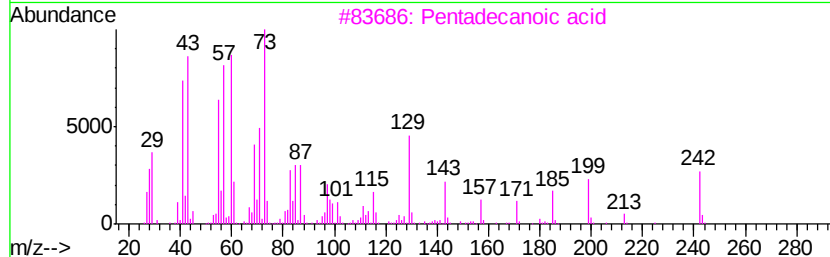
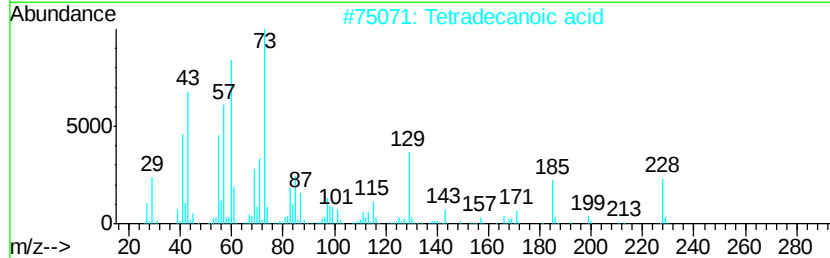
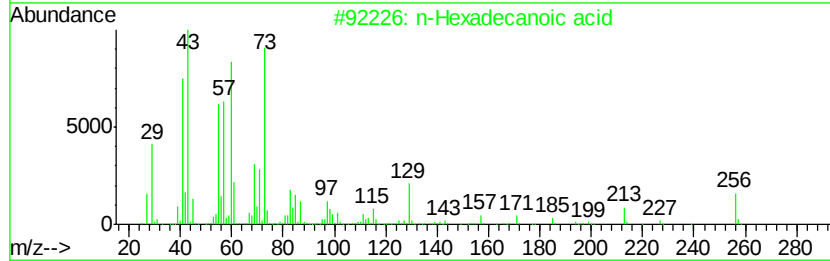
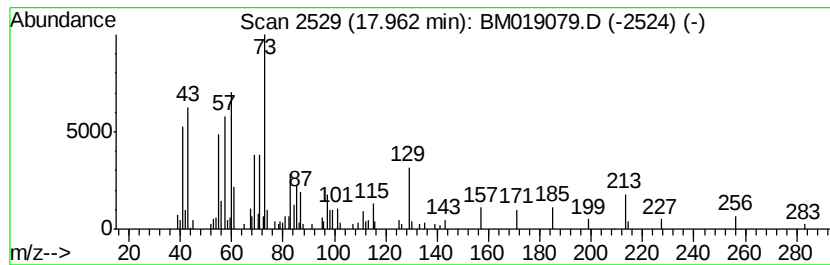
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.96	4.62 ng	238091	Phenanthrene-d10	17.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Undecanoic acid	186	C11H22O2	000112-37-8	52
5	Tridecane	184	C13H28	000629-50-5	18



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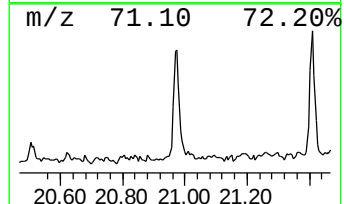
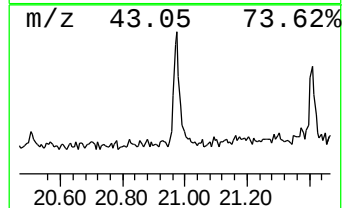
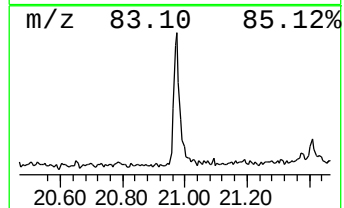
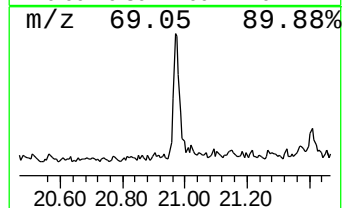
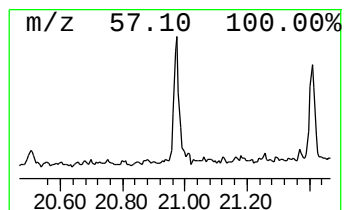
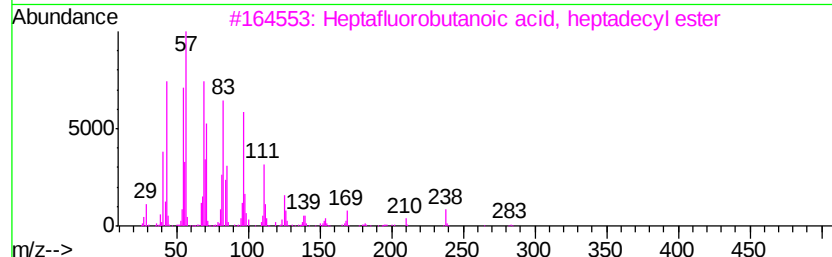
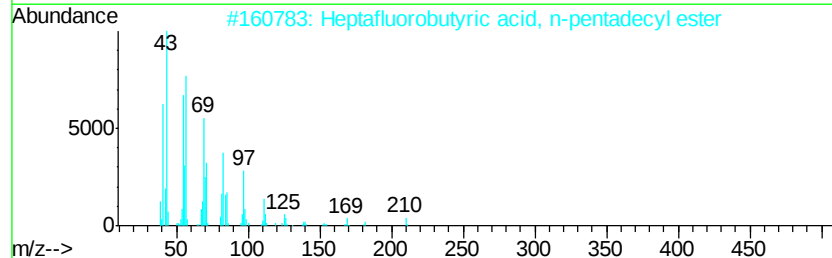
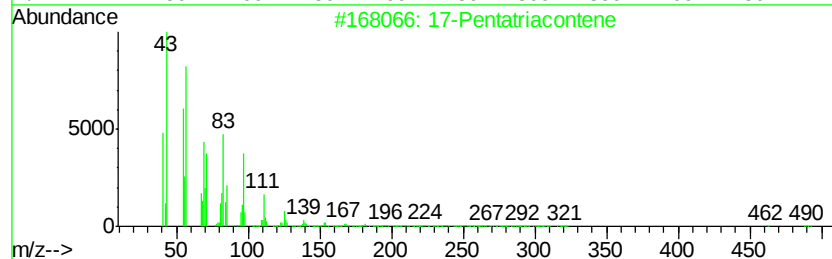
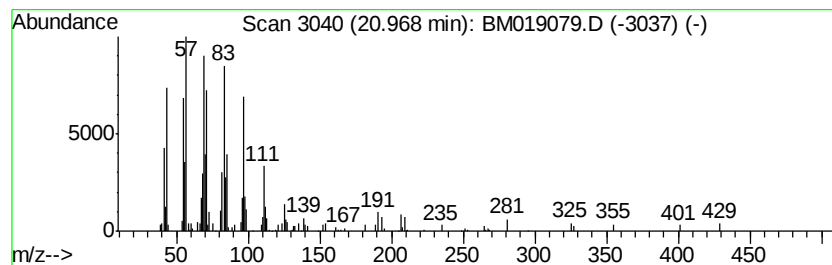
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Peak Number 5 17-Pentatriacontene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.97	2.73 ng	174995	Chrysene-d12	21.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	91
2		Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90
4		1-Heptadecanol	256	C17H36O	001454-85-9	83
5		Isoheptadecanol	256	C17H36O	057289-07-3	74



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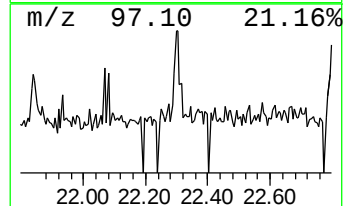
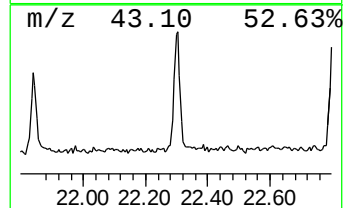
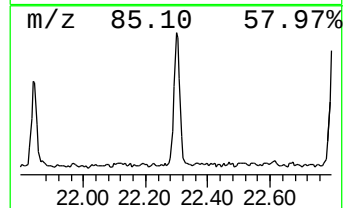
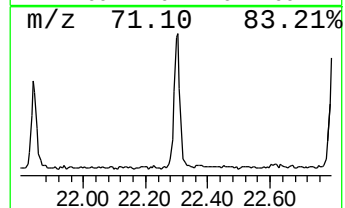
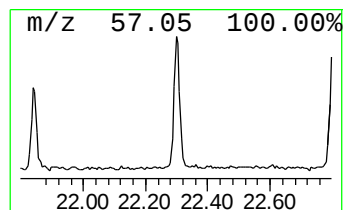
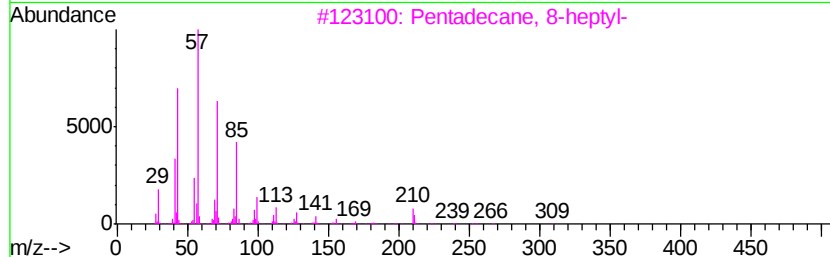
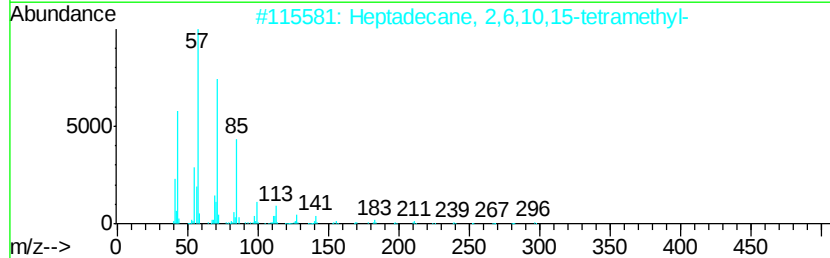
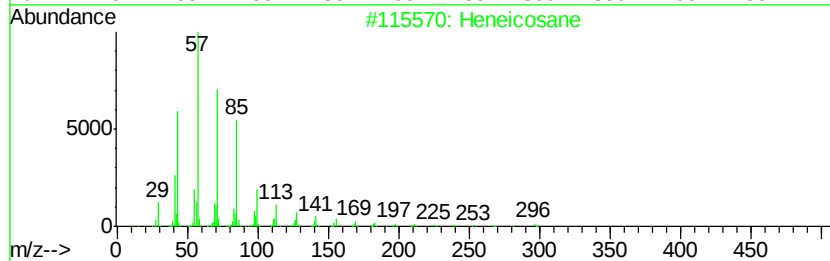
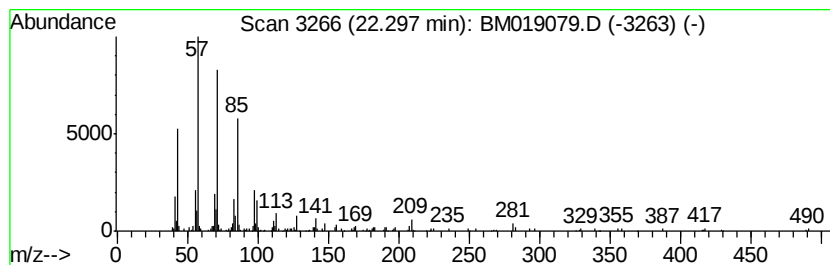
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.30	3.27 ng	209712	Chrysene-d12	21.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	96
2	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	91
3	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	80
4	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	80
5	Docosane		310	C22H46	000629-97-0	80



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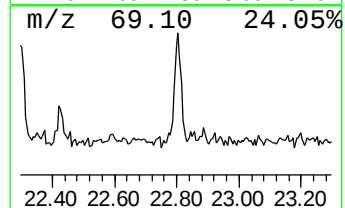
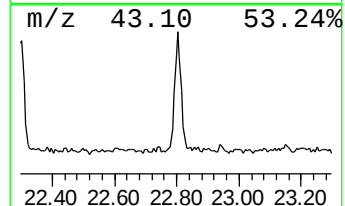
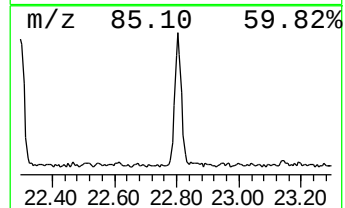
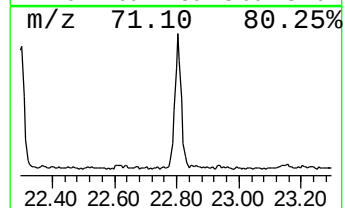
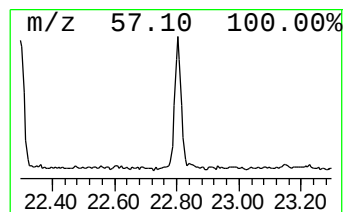
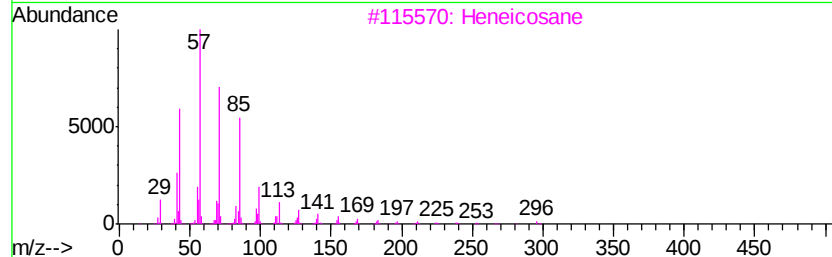
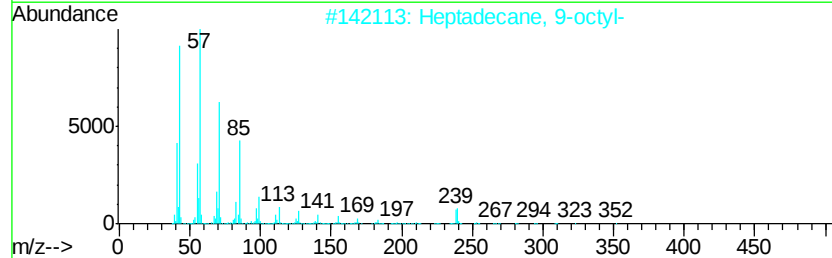
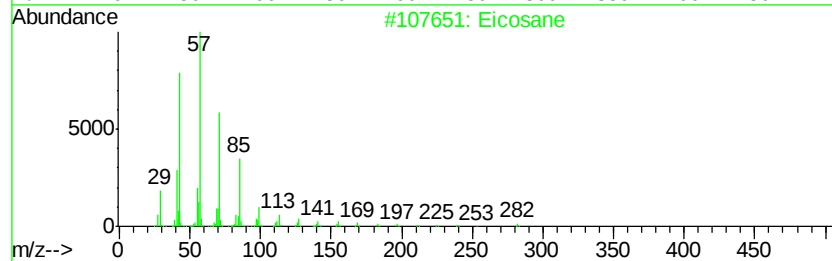
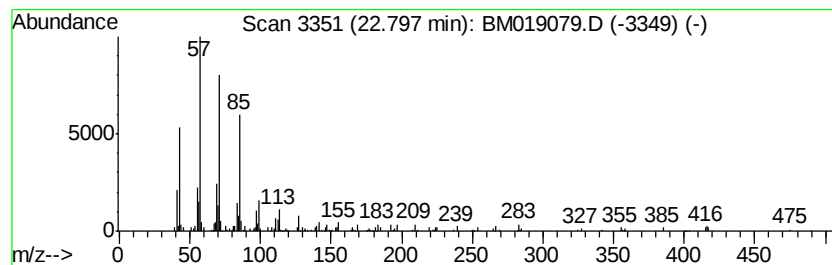
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.80	3.30 ng	237826	Perylene-d12	23.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Nonacosane	408	C29H60	000630-03-5	87
5		Octadecane	254	C18H38	000593-45-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019079.D
Acq On : 08 Mar 2019 18:29
Operator : JU/SJ
Sample : K1807-31
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-13

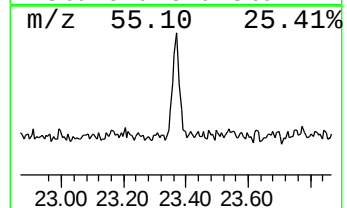
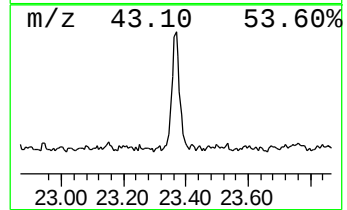
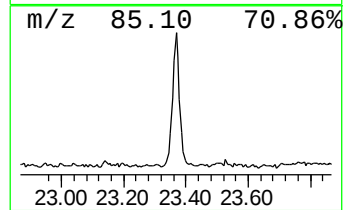
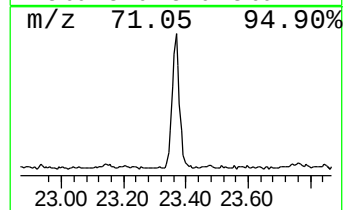
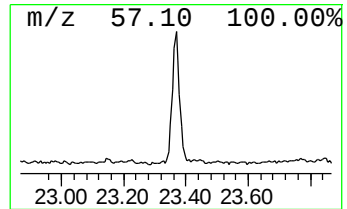
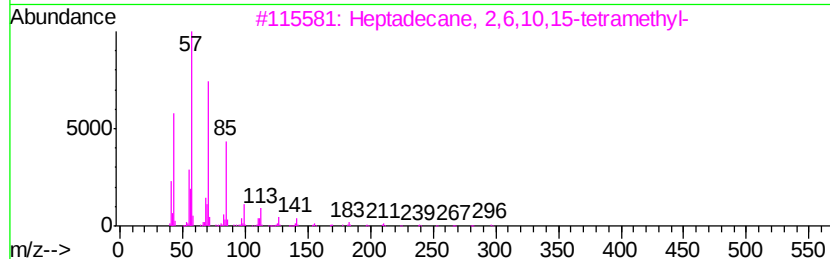
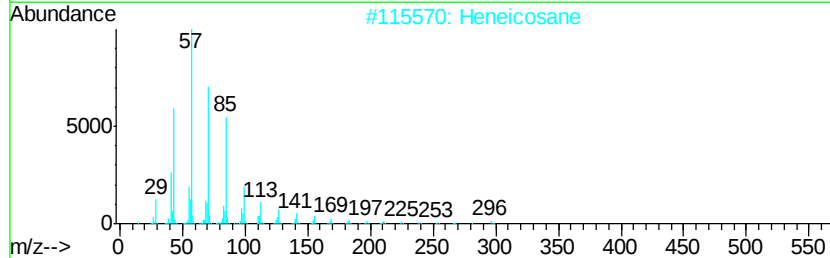
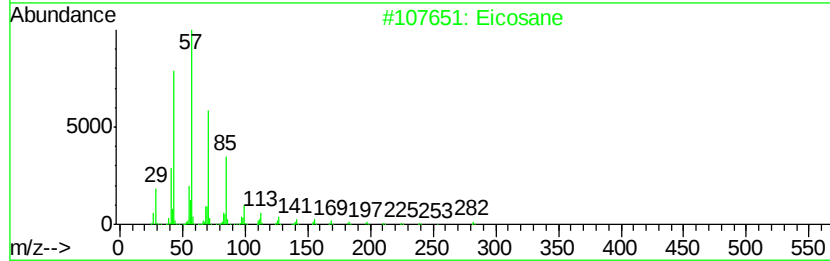
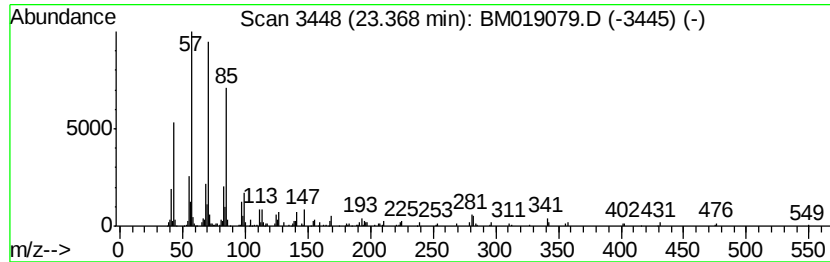
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown23.37 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.37	3.81 ng	275326	Perylene-d12	23.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Heneicosane	296	C21H44	000629-94-7	81
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	74
4		Tetracosane	338	C24H50	000646-31-1	72
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM030819\
Data File : BM019079.D
Acq On : 08 Mar 2019 18:29
Operator : JU/SJ
Sample : K1807-31
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP-13

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
unknown7.20	7.20	78.7	ng	2694600	1	7.67	685178	20.0
D-Allose	14.20	5.3	ng	252006	3	14.32	944968	20.0
n-Hexadecanoic acid	17.96	4.6	ng	238091	4	17.08	1031650	20.0
17-Pentatriacontene	20.97	2.7	ng	174995	5	21.27	1282560	20.0
Heneicosane	22.30	3.3	ng	209712	5	21.27	1282560	20.0
Eicosane	22.80	3.3	ng	237826	6	23.51	1443400	20.0
unknown23.37	23.37	3.8	ng	275326	6	23.51	1443400	20.0