

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032719\
 Data File : BF113328.D
 Acq On : 27 Mar 2019 13:57
 Operator : JU/SJ
 Sample : K2102-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TT-001-IDWSO-20190325

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_F\METHODS\8270-BF032519.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	5.316	545	549	575	rBV	2799008	3009715	85.78%	9.594%
2	6.345	720	724	742	rBV	2894729	3241732	92.39%	10.333%
3	6.475	742	746	749	rBV	3447040	3085339	87.94%	9.835%
4	6.698	781	784	794	rVB	1045256	985671	28.09%	3.142%
5	6.857	807	811	821	rBV	2809731	2458535	70.07%	7.837%
6	7.263	875	880	883	rBV	2130105	1913488	54.54%	6.099%
7	7.981	998	1002	1018	rBV	1215895	1269743	36.19%	4.047%
8	9.057	1181	1185	1198	rBV	3686160	3508597	100.00%	11.184%
9	9.451	1248	1252	1260	rBV	206856	222723	6.35%	0.710%
10	9.733	1296	1300	1312	rBV	1491762	1402467	39.97%	4.470%
11	10.516	1429	1433	1448	rBV	1757172	1821444	51.91%	5.806%
12	11.210	1547	1551	1566	rVB	1607996	1502146	42.81%	4.788%
13	11.751	1635	1643	1652	rBV3	65994	132444	3.77%	0.422%
14	12.527	1771	1775	1788	rBV	136821	265430	7.57%	0.846%
15	12.792	1815	1820	1823	rBV	3401226	3209237	91.47%	10.230%
16	13.774	1977	1987	1993	rBV6	81421	318293	9.07%	1.015%
17	13.839	1994	1998	2009	rVB	1053766	1190546	33.93%	3.795%
18	14.010	2024	2027	2030	rBV	60020	51452	1.47%	0.164%
19	14.310	2075	2078	2083	rVB	90218	86467	2.46%	0.276%
20	14.604	2125	2128	2132	rVB	126216	121149	3.45%	0.386%
21	14.916	2177	2181	2186	rBV	144438	170175	4.85%	0.542%
22	15.239	2231	2236	2239	rBV	771004	1060984	30.24%	3.382%
23	15.663	2303	2308	2314	rVB	130889	195483	5.57%	0.623%
24	16.121	2381	2386	2396	rBV2	76430	148463	4.23%	0.473%

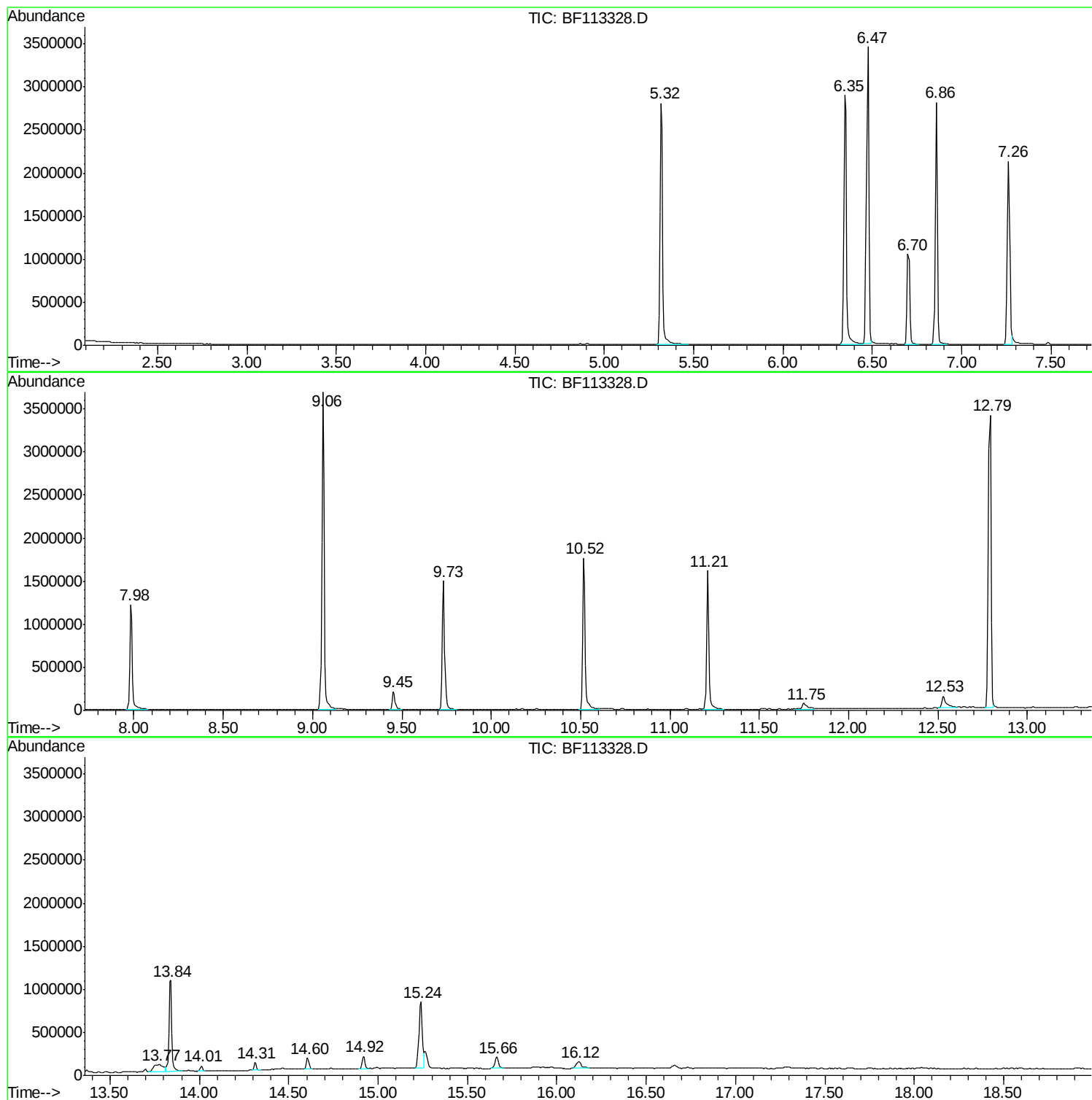
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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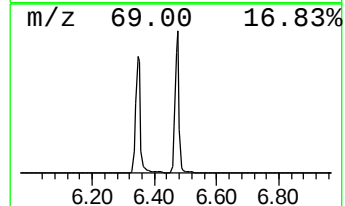
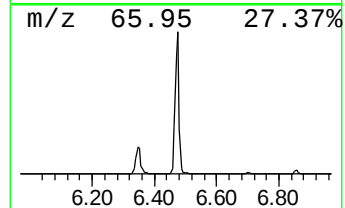
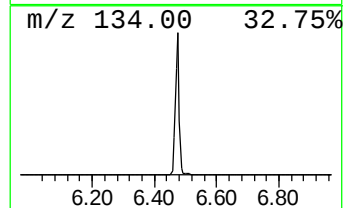
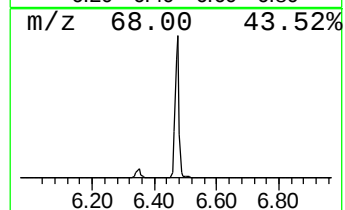
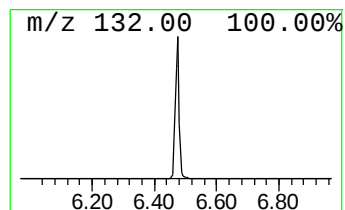
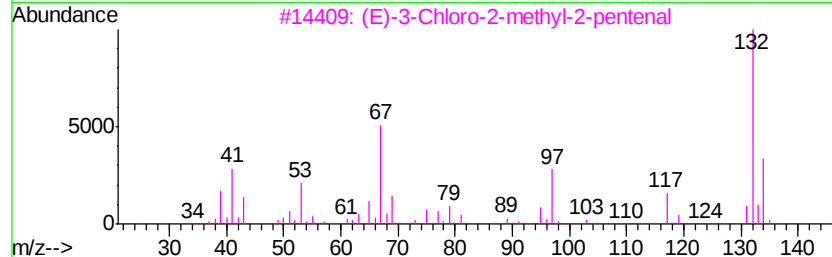
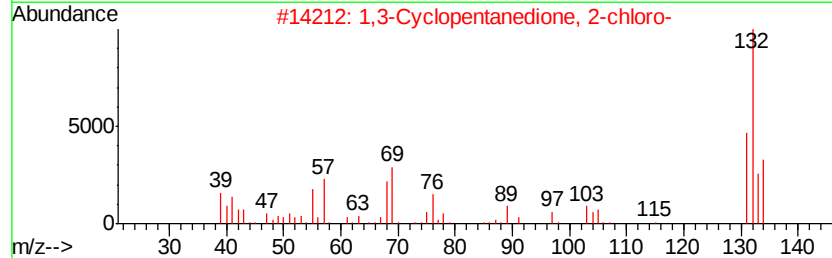
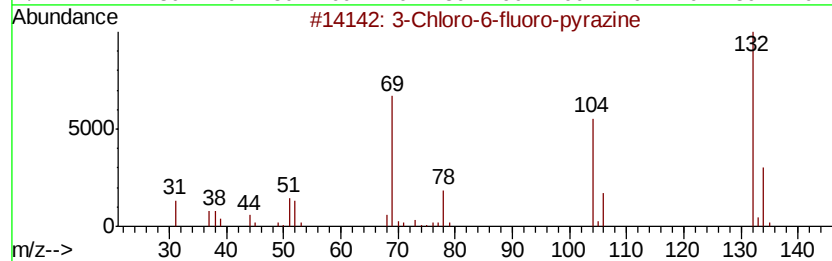
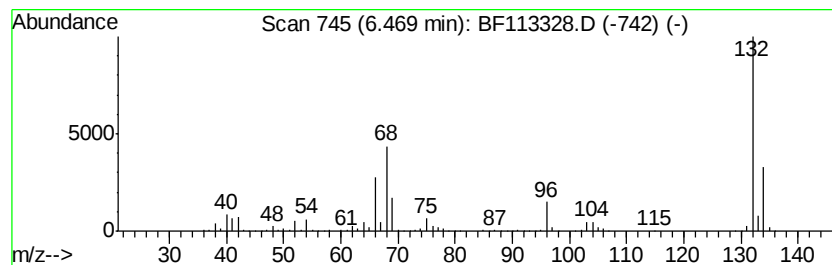
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	62.60 ng	3085340	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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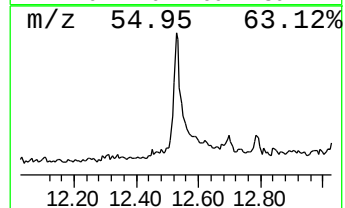
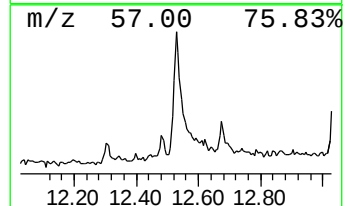
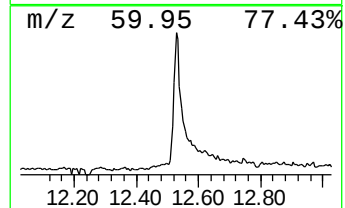
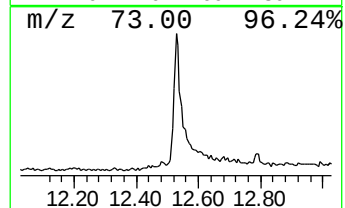
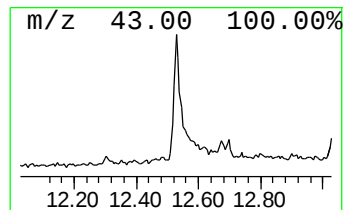
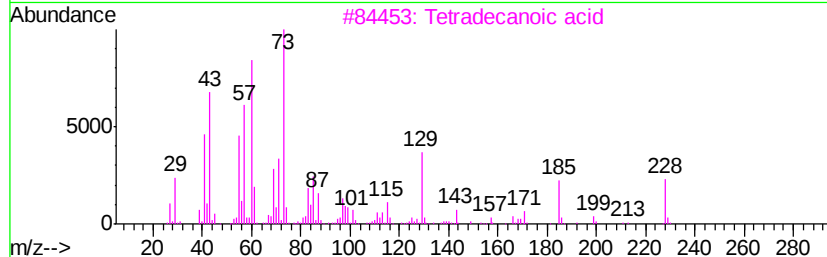
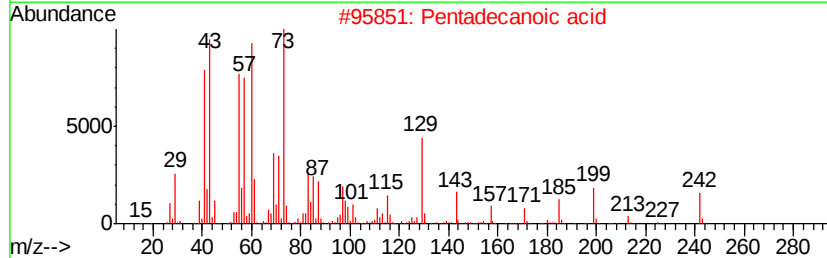
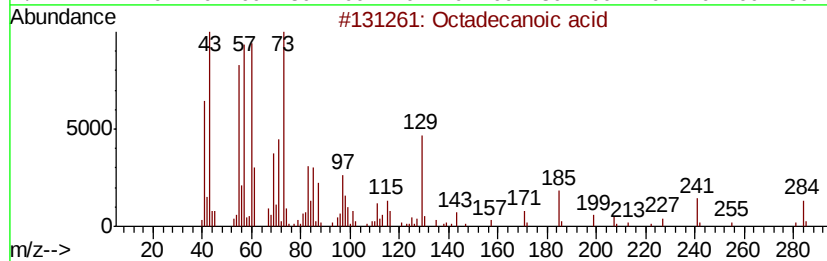
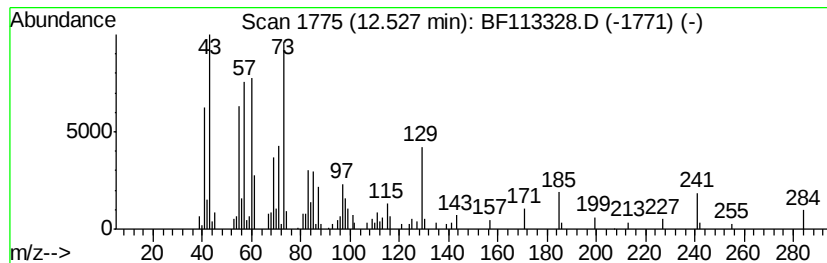
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.53	4.46 ng	265430	Chrysene-d12	13.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	46
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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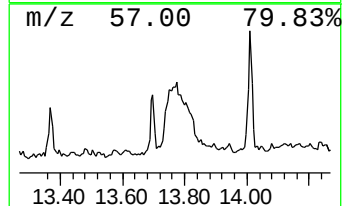
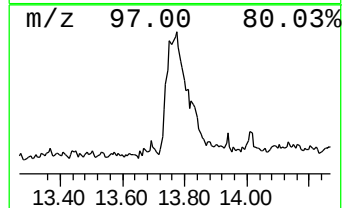
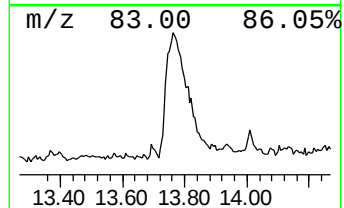
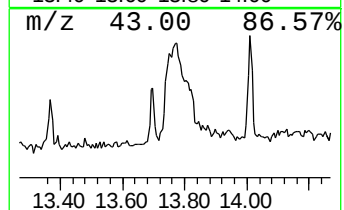
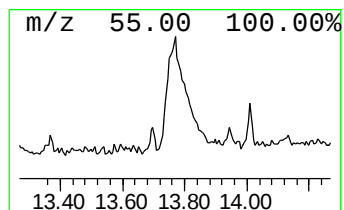
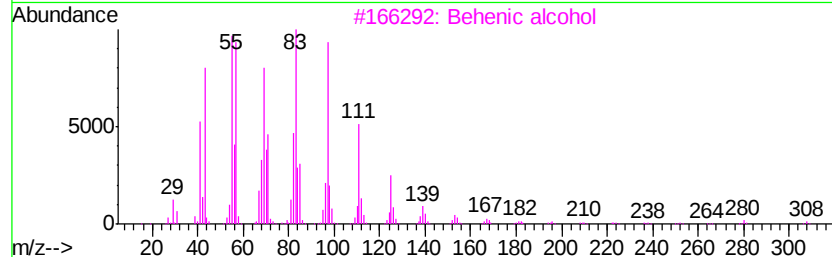
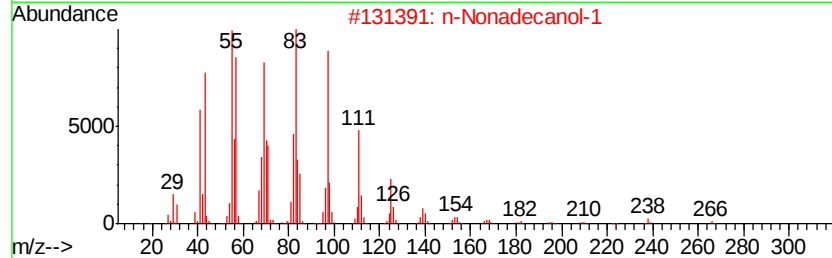
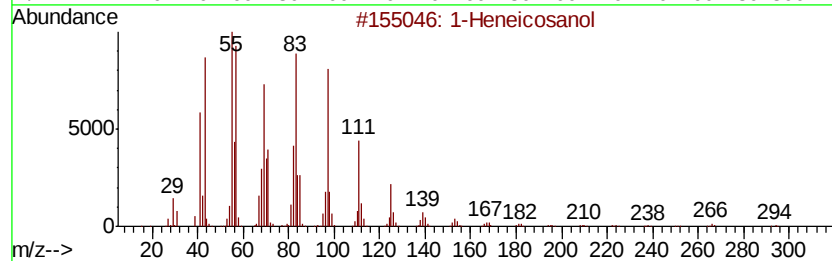
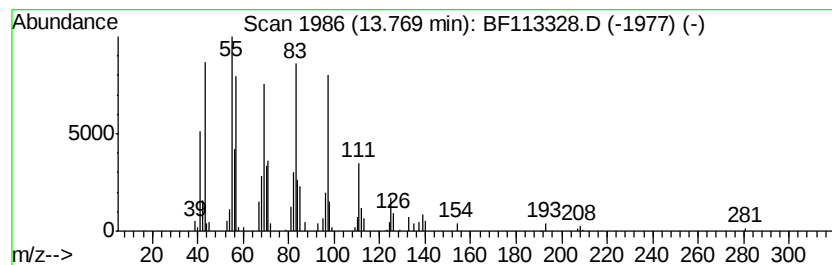
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Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.77	5.35 ng	318293	Chrysene-d12		13.84
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	1-Hexadecanol	242	C16H34O	036653-82-4	95
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	91



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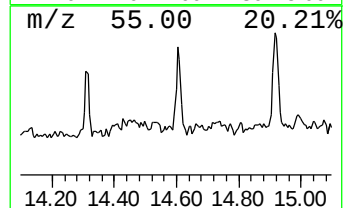
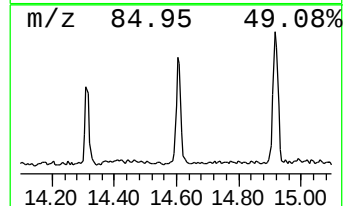
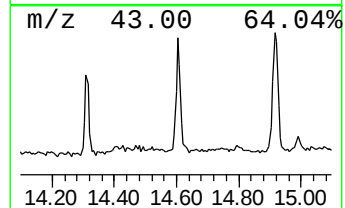
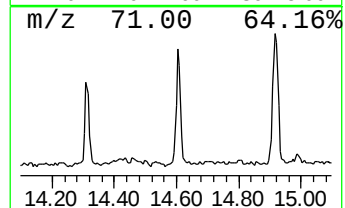
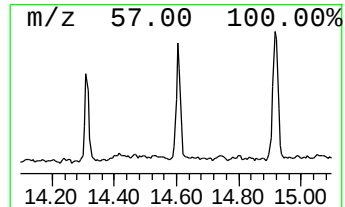
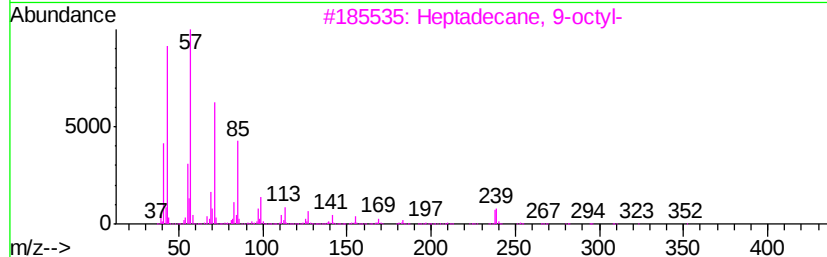
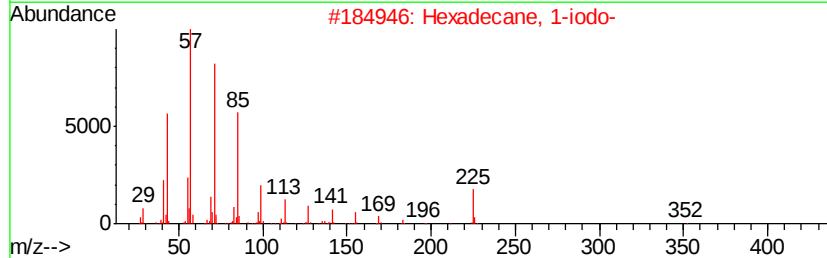
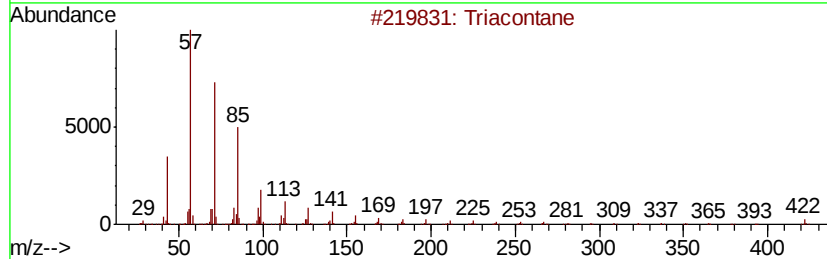
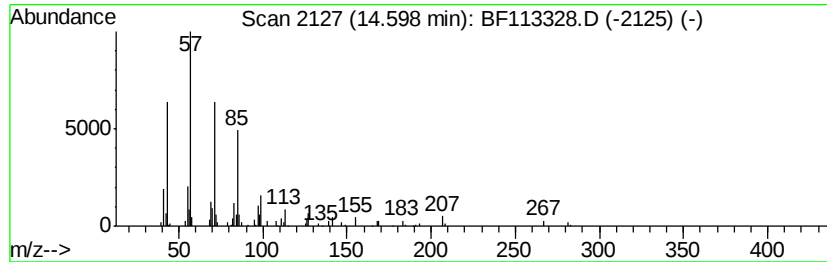
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Peak Number 5 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.28 ng	121149	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	91
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Hentriacontane	437	C31H64	000630-04-6	91
5		Eicosane	282	C20H42	000112-95-8	91



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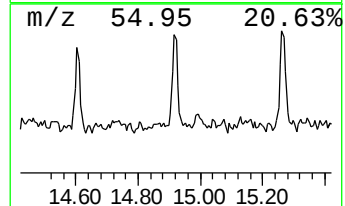
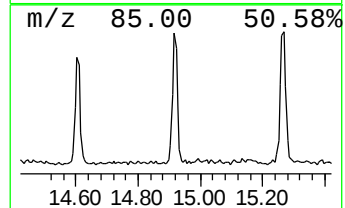
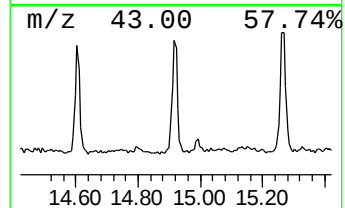
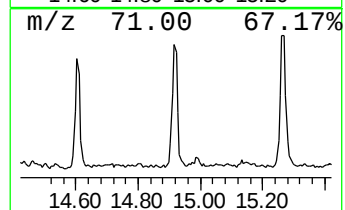
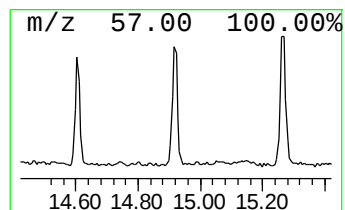
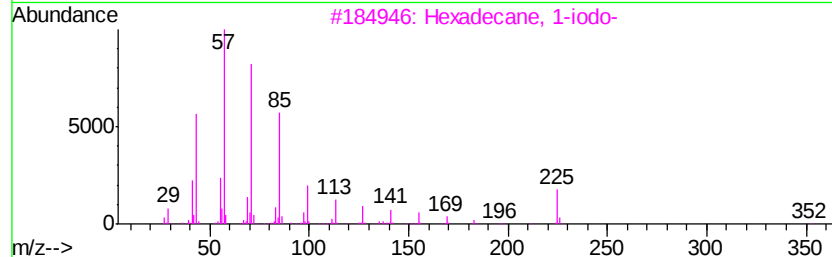
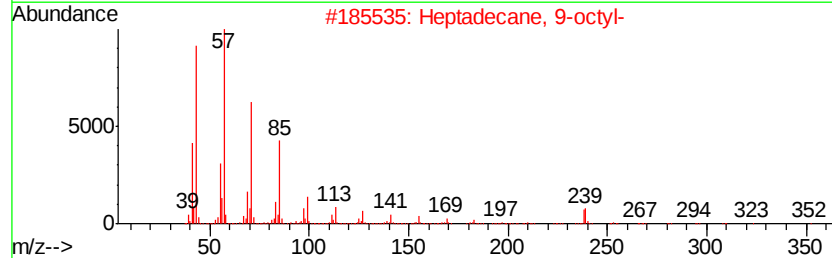
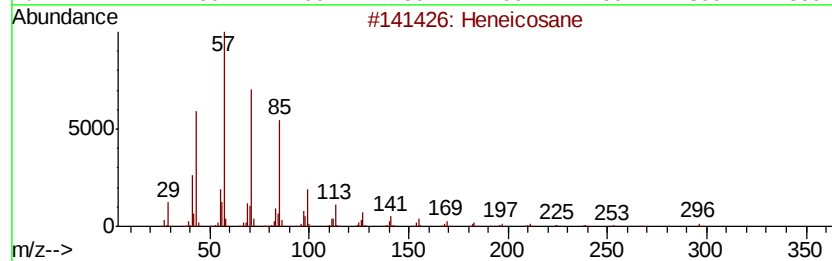
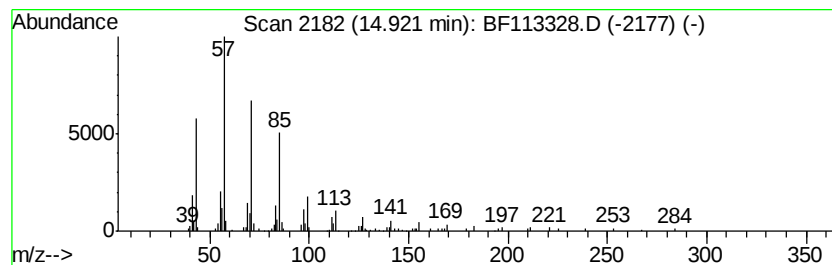
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	3.21 ng	170175	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	Hexadecane, 1-iodo-		352	C16H33I	000544-77-4	87
4	Docosane		310	C22H46	000629-97-0	87
5	Heptadecane		240	C17H36	000629-78-7	87



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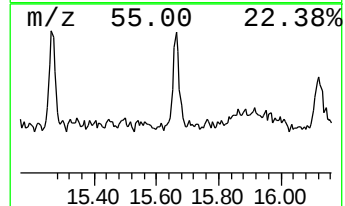
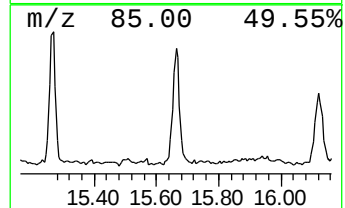
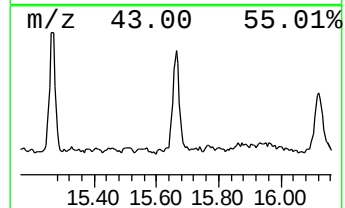
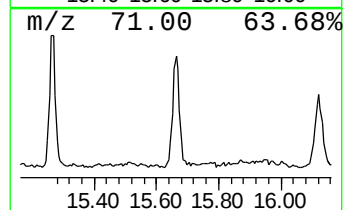
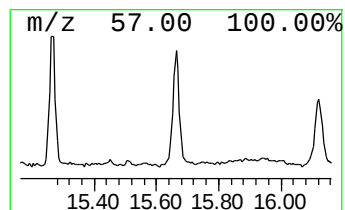
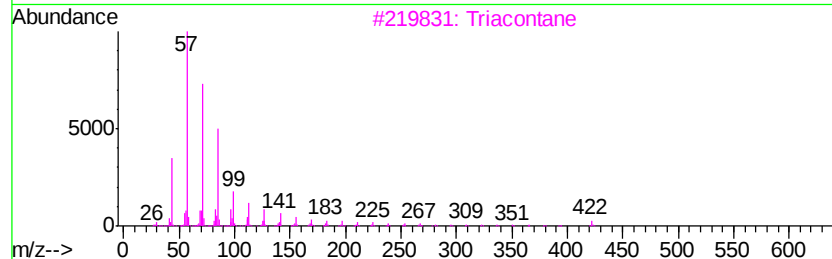
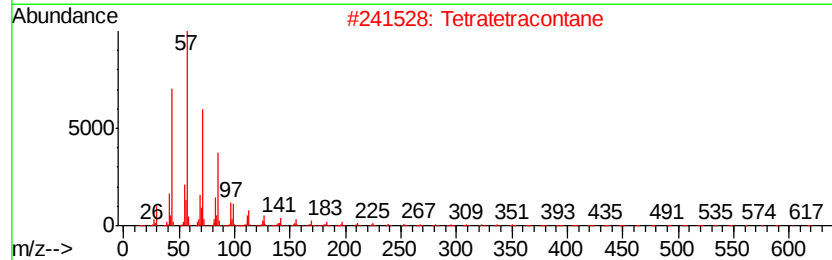
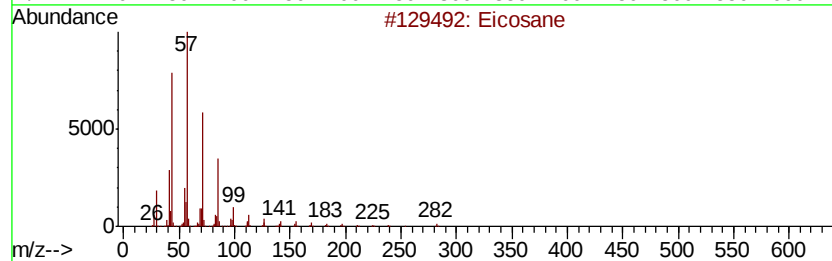
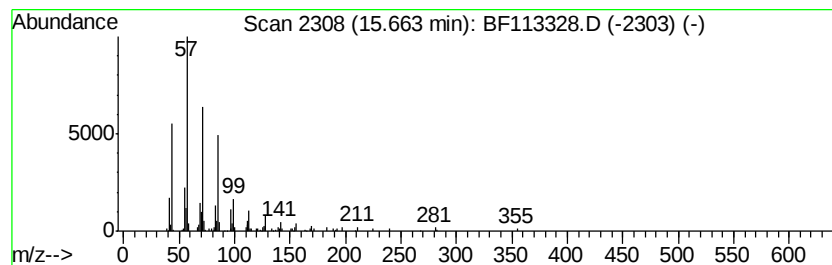
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	3.68 ng	195483	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		Triacontane	422	C30H62	000638-68-6	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF032719\
Data File : BF113328.D
Acq On : 27 Mar 2019 13:57
Operator : JU/SJ
Sample : K2102-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TT-001-IDWSO-20190325

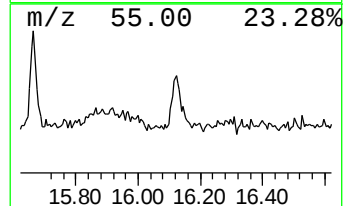
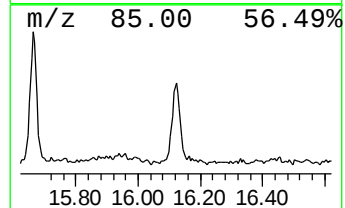
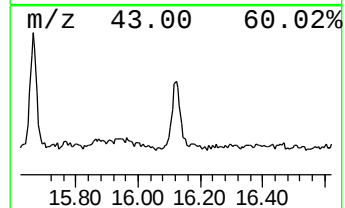
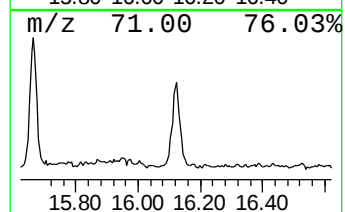
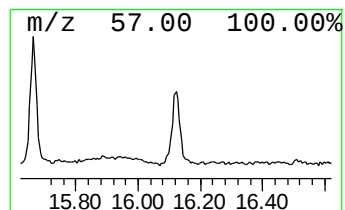
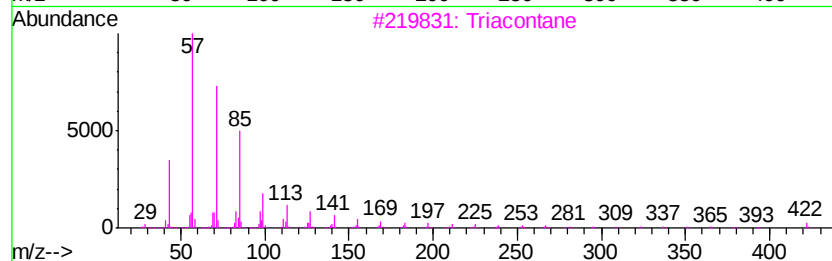
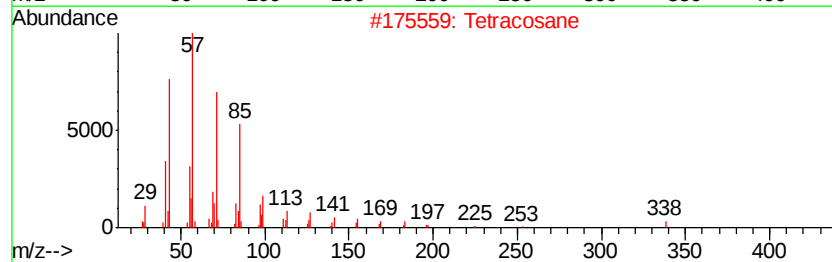
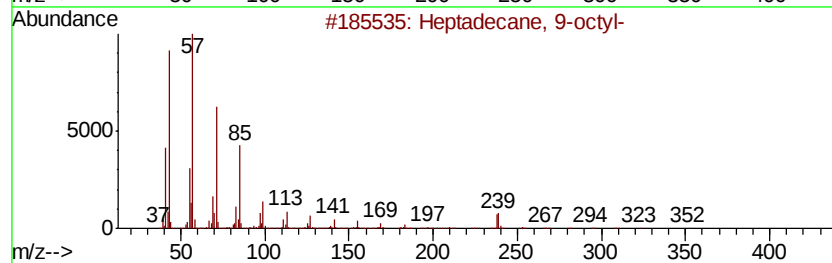
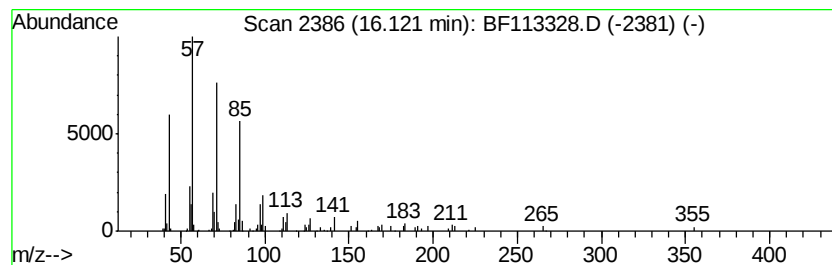
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	2.80 ng	148463	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032719\
Data File : BF113328.D
Acq On : 27 Mar 2019 13:57
Operator : JU/SJ
Sample : K2102-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TT-001-IDWSO-20190325

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.47	6.47	62.6	ng	3085340	1	6.70	985671	20.0
Octadecanoic acid	12.53	4.5	ng	265430	5	13.84	1190550	20.0
1-Heneicosanol	13.77	5.3	ng	318293	5	13.84	1190550	20.0
Triacontane	14.60	2.3	ng	121149	6	15.24	1060980	20.0
Heneicosane	14.92	3.2	ng	170175	6	15.24	1060980	20.0
Eicosane	15.66	3.7	ng	195483	6	15.24	1060980	20.0
Heptadecane, 9-oc...	16.12	2.8	ng	148463	6	15.24	1060980	20.0