

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031519\
 Data File : BF113080.D
 Acq On : 15 Mar 2019 22:02
 Operator : JU/SJ
 Sample : K1901-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1(0.5-1.5)

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-BF022719.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	4.404	388	394	403	rBV	488406	619552	17.98%	2.007%
2	5.339	549	553	574	rVB	2275562	2171797	63.03%	7.035%
3	6.369	724	728	744	rBV	2520559	2429209	70.50%	7.869%
4	6.498	746	750	753	rBV	3097300	2597938	75.39%	8.415%
5	6.728	785	789	792	rBV	1011832	863697	25.06%	2.798%
6	6.881	811	815	819	rBV	2569673	2302572	66.82%	7.459%
7	7.286	879	884	896	rBV	2004214	1821761	52.87%	5.901%
8	7.510	918	922	931	rVB2	31220	40094	1.16%	0.130%
9	8.010	1003	1007	1029	rBV	1087188	1151324	33.41%	3.729%
10	9.080	1185	1189	1203	rBV	3260318	3445877	100.00%	11.162%
11	9.474	1253	1256	1262	rBV	203852	188909	5.48%	0.612%
12	9.757	1300	1304	1315	rBV	1239266	1191738	34.58%	3.860%
13	10.545	1434	1438	1449	rBV	1737850	1815551	52.69%	5.881%
14	11.233	1552	1555	1563	rBV	1359596	1391504	40.38%	4.507%
15	11.698	1630	1634	1638	rBV3	26098	36663	1.06%	0.119%
16	11.774	1643	1647	1656	rBV	608704	652264	18.93%	2.113%
17	11.945	1670	1676	1679	rBV2	36483	54937	1.59%	0.178%
18	12.333	1739	1742	1746	rVB	31628	35161	1.02%	0.114%
19	12.439	1757	1760	1764	rBV	105262	131426	3.81%	0.426%
20	12.557	1776	1780	1786	rBV	182294	254466	7.38%	0.824%
21	12.668	1796	1799	1802	rVB	91081	80981	2.35%	0.262%
22	12.815	1820	1824	1827	rBV	3634667	3348928	97.19%	10.848%
23	13.057	1859	1865	1868	rBV	63885	75799	2.20%	0.246%
24	13.398	1920	1923	1925	rBV	68725	59757	1.73%	0.194%
25	13.721	1974	1978	1988	rBV	284112	377815	10.96%	1.224%
26	13.862	1997	2002	2008	rBV	1206842	1270291	36.86%	4.115%
27	14.039	2029	2032	2038	rVB	122674	108915	3.16%	0.353%
28	14.339	2080	2083	2087	rBV	169124	154496	4.48%	0.500%
29	14.639	2130	2134	2141	rBV	201026	225521	6.54%	0.731%
30	14.704	2142	2145	2151	rVV	105255	104869	3.04%	0.340%
31	14.951	2184	2187	2192	rVB	203072	221623	6.43%	0.718%
32	15.268	2236	2241	2245	rBV	868480	1101846	31.98%	3.569%
33	15.304	2245	2247	2254	rVB	198941	244212	7.09%	0.791%
34	15.709	2312	2316	2321	rVB	147221	203041	5.89%	0.658%

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SB-1(0.5-1.5)

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

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35	16.174	2392	2395	2400	rVB	66705	96984	2.81%	0.314%
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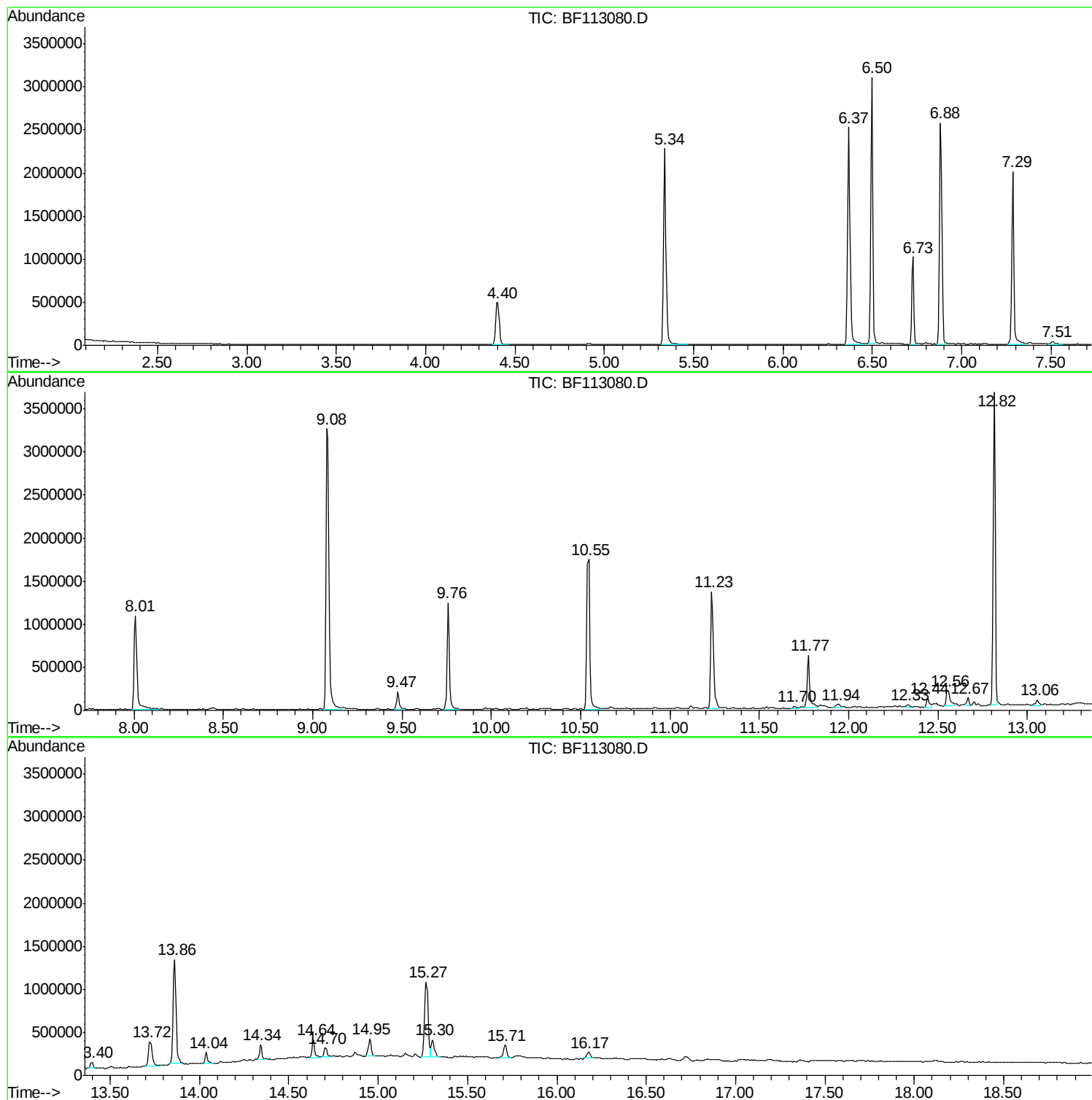
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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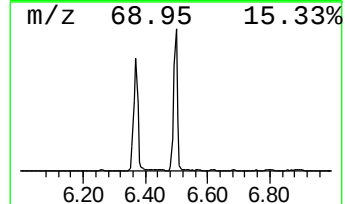
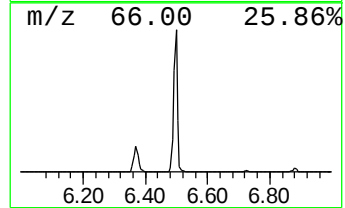
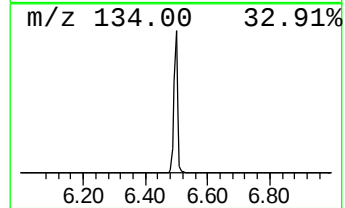
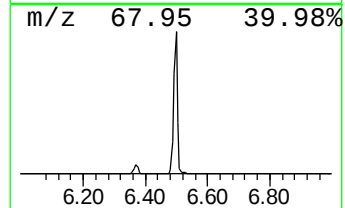
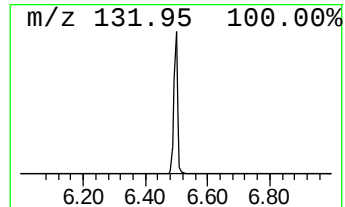
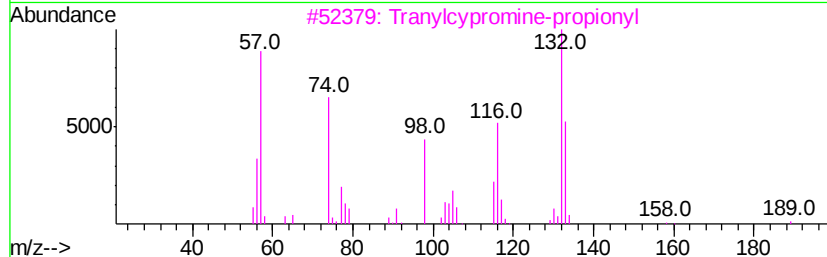
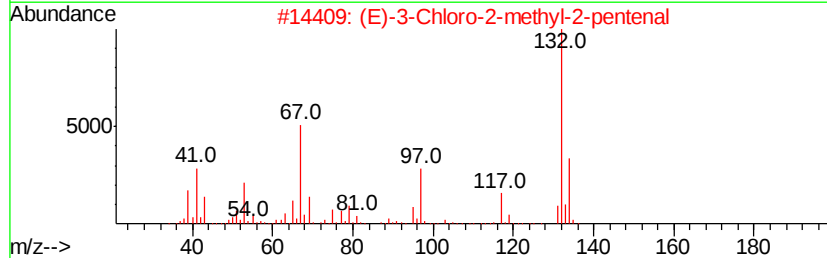
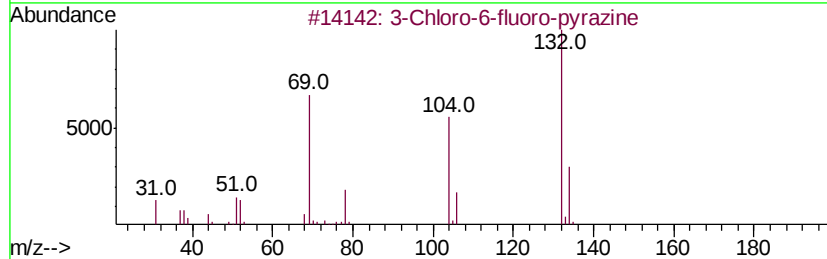
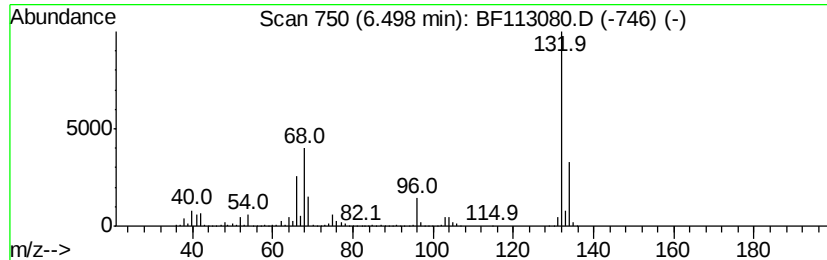
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	60.16 ng	2597940	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Xenon	132	Xe	007440-63-3	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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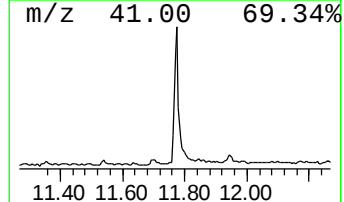
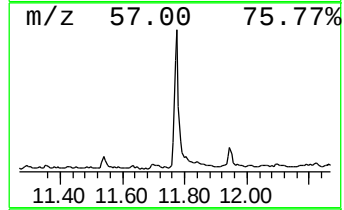
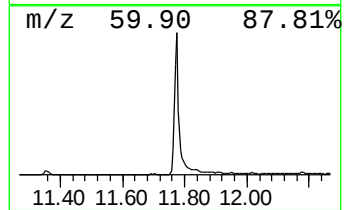
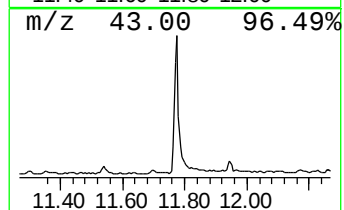
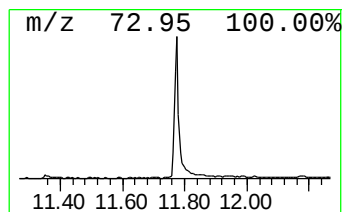
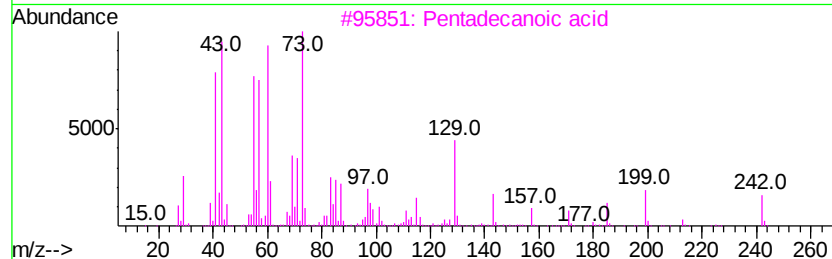
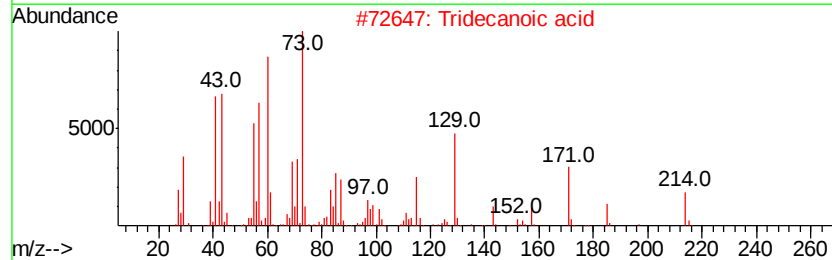
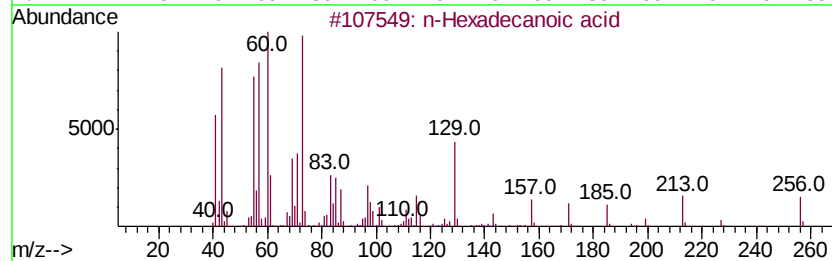
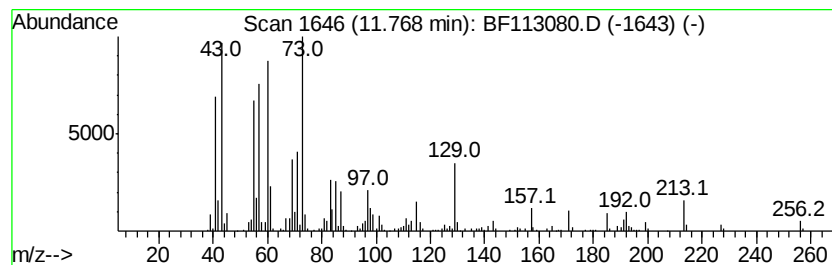
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	9.37 ng	652264	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



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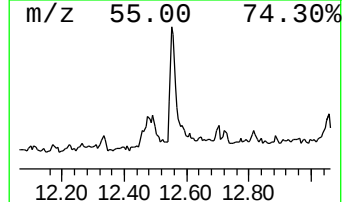
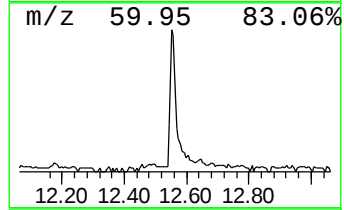
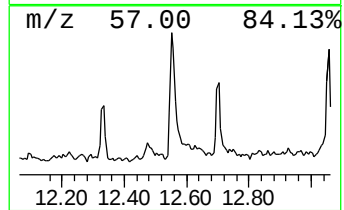
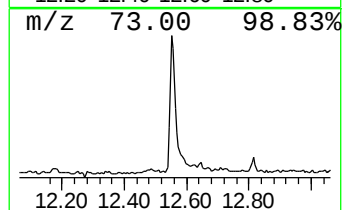
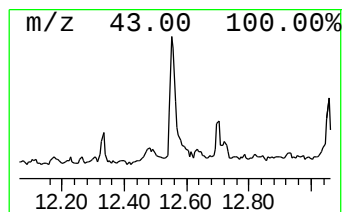
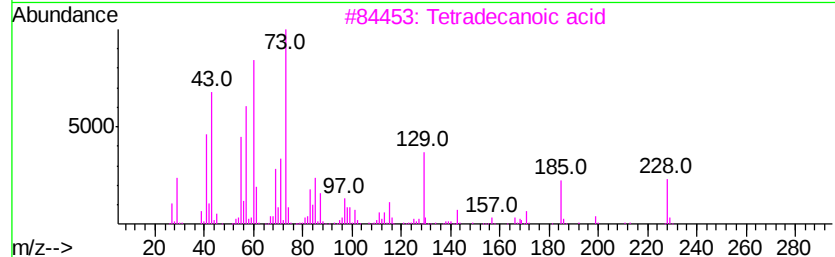
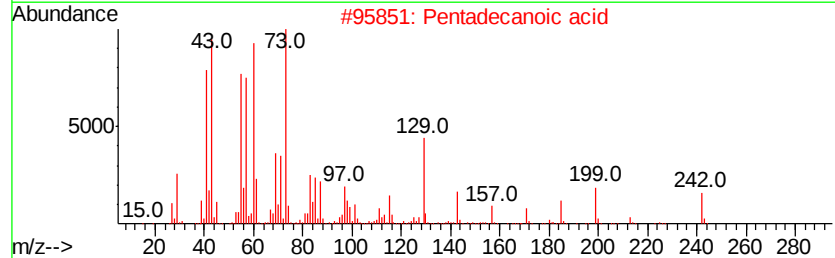
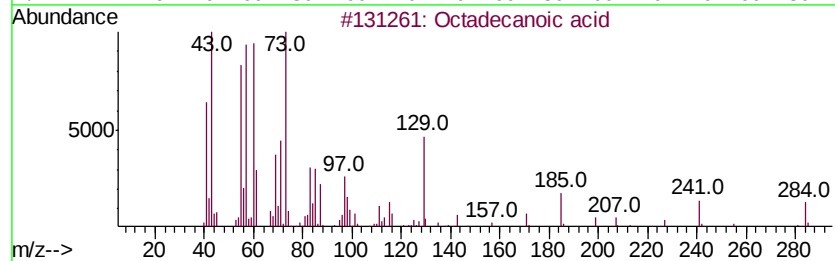
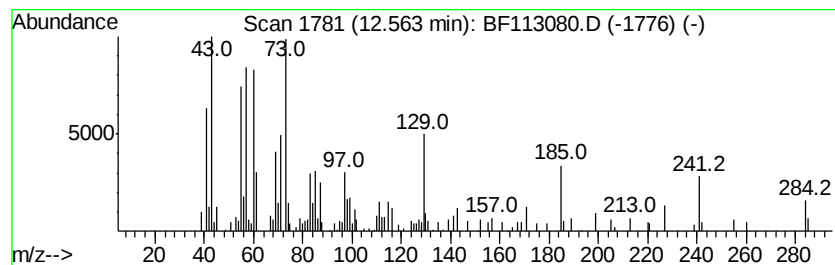
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	4.01 ng	254466	Chrysene-d12	13.86

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	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5		n-Decanoic acid	172	C10H20O2	000334-48-5	60



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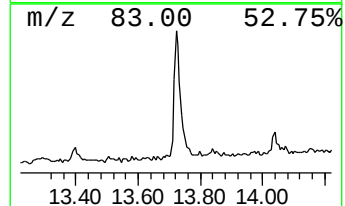
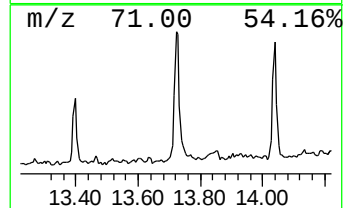
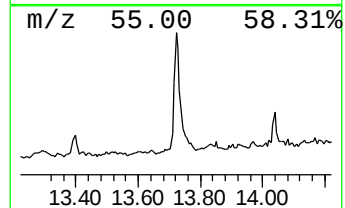
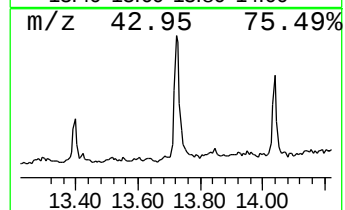
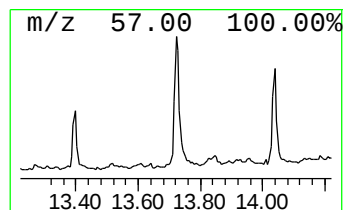
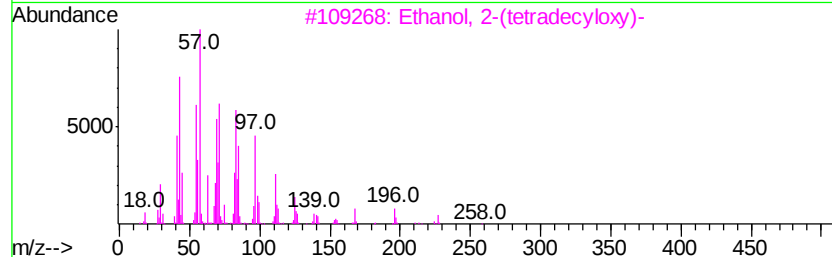
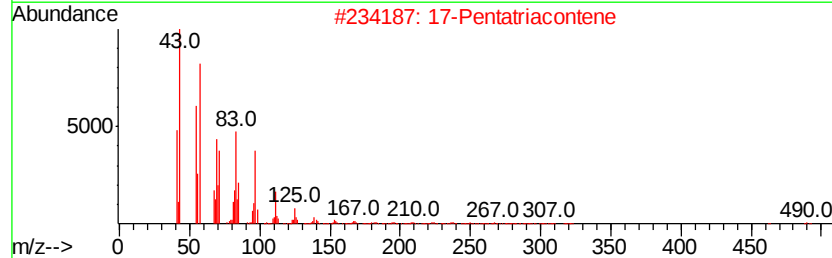
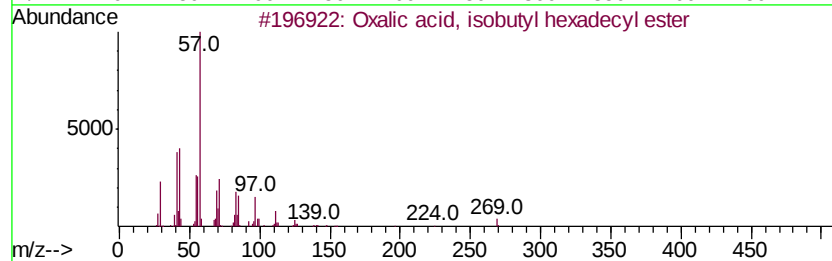
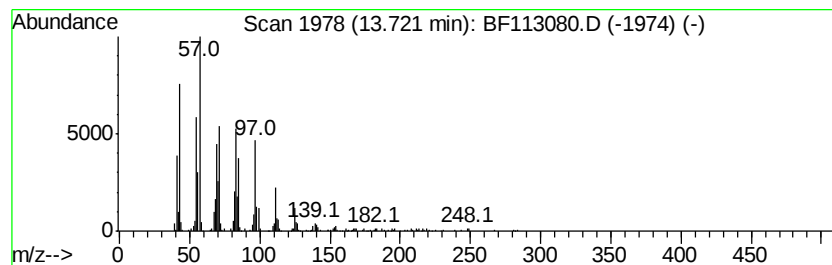
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxalic acid, isobutyl hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.95 ng	377815	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
4		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87



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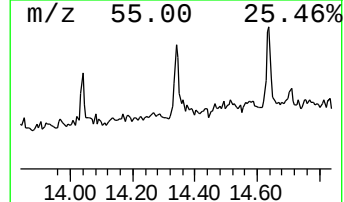
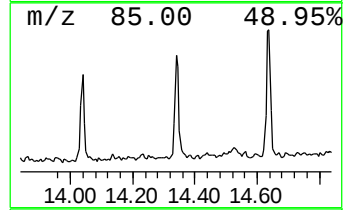
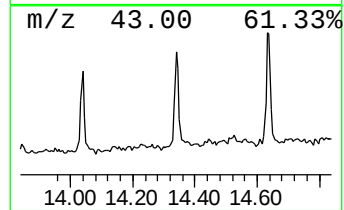
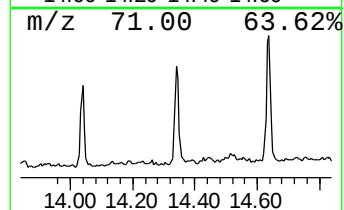
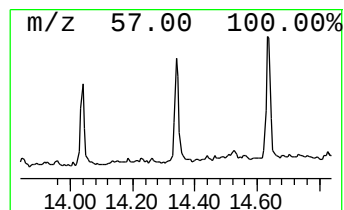
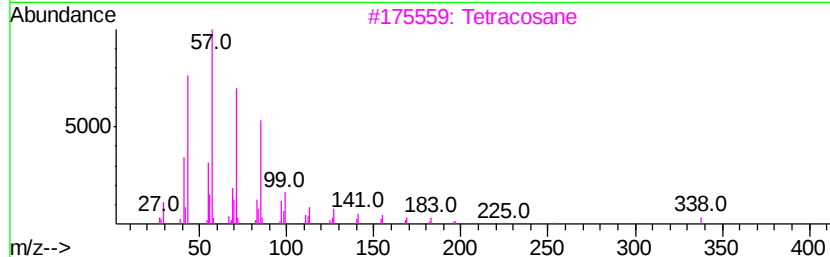
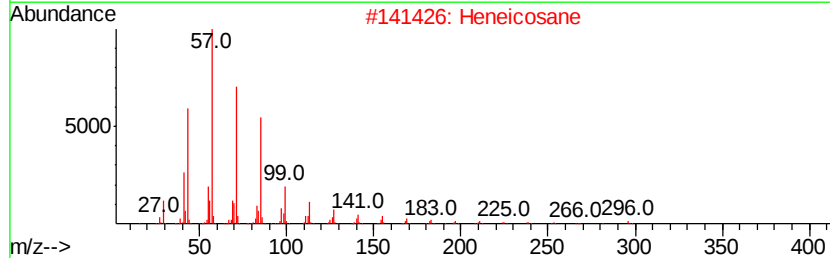
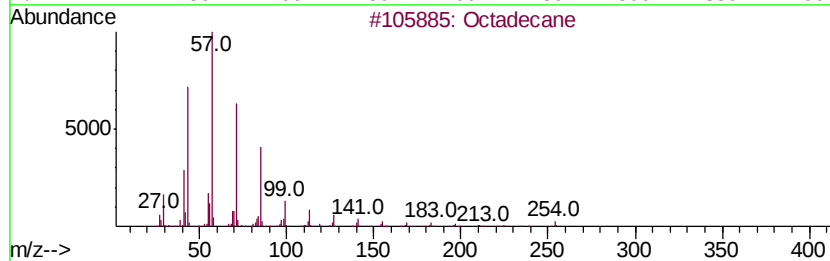
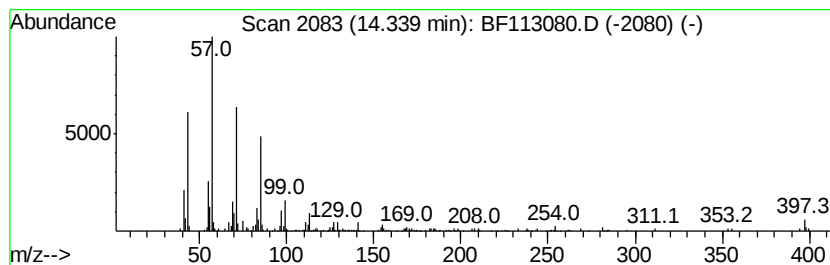
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Peak Number 7 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.43 ng	154496	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Heneicosane	296	C21H44	000629-94-7	87
3		Tetracosane	338	C24H50	000646-31-1	87
4		Octacosane	394	C28H58	000630-02-4	83
5		2-Bromo dodecane	248	C12H25Br	013187-99-0	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031519\
Data File : BF113080.D
Acq On : 15 Mar 2019 22:02
Operator : JU/SJ
Sample : K1901-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1(0.5-1.5)

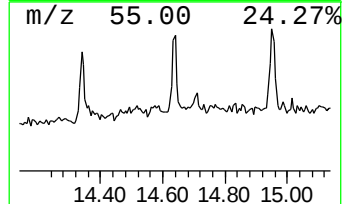
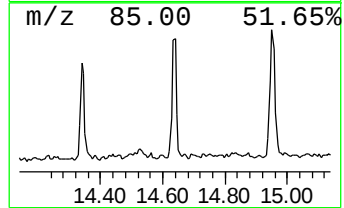
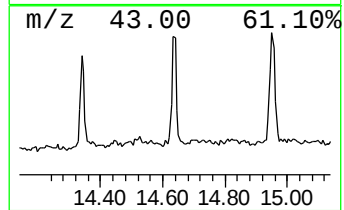
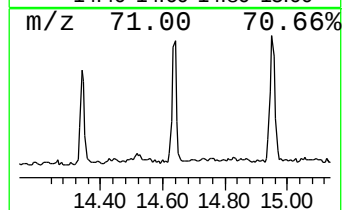
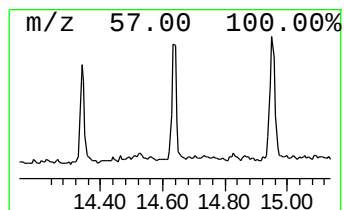
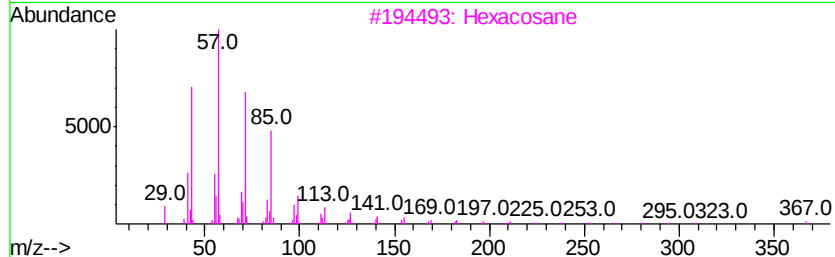
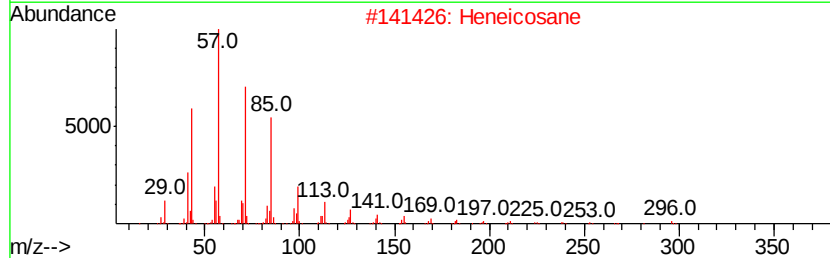
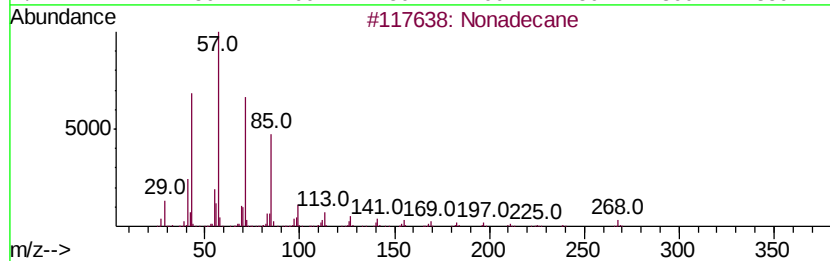
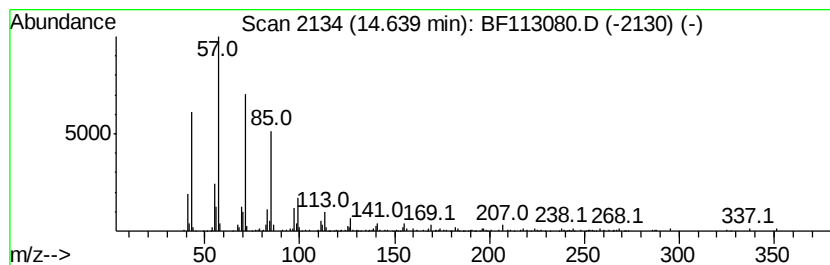
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.09 ng	225521	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	93
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		Eicosane	282	C20H42	000112-95-8	87
5		Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031519\
Data File : BF113080.D
Acq On : 15 Mar 2019 22:02
Operator : JU/SJ
Sample : K1901-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1(0.5-1.5)

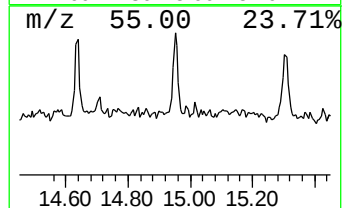
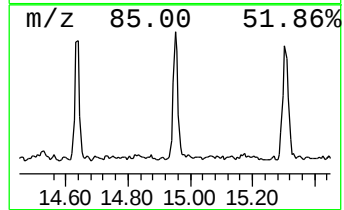
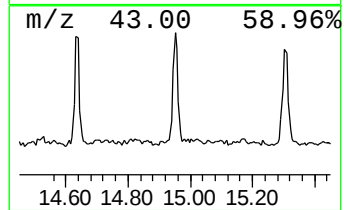
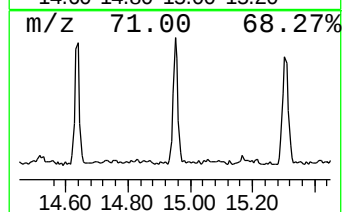
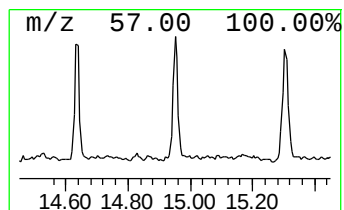
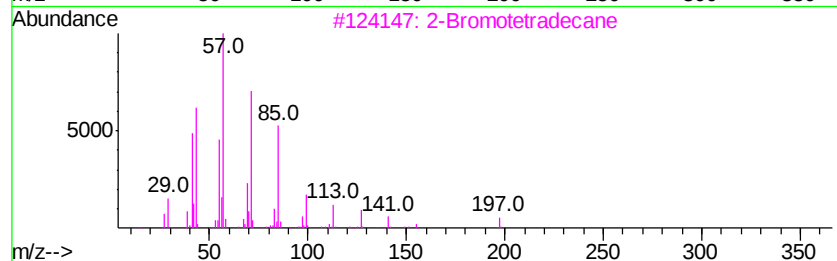
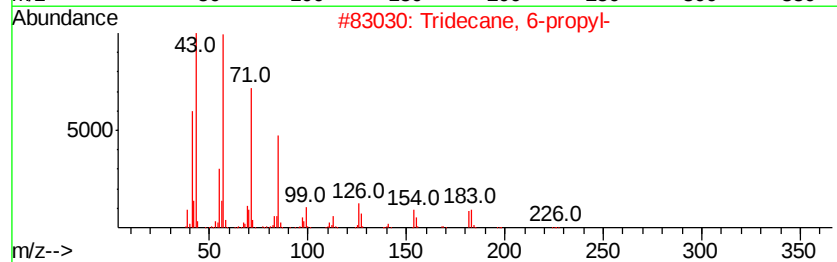
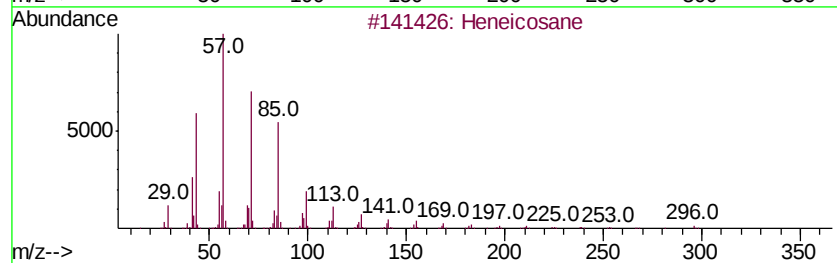
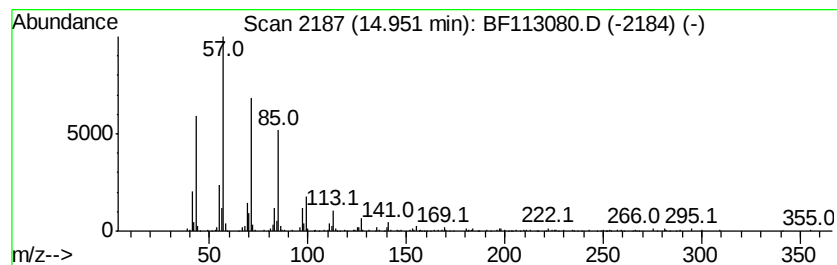
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	4.02 ng	221623	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Tridecane, 6-propyl-		226	C16H34	055045-10-8	86
3	2-Bromotetradecane		276	C14H29Br	074036-95-6	86
4	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	83
5	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031519\
Data File : BF113080.D
Acq On : 15 Mar 2019 22:02
Operator : JU/SJ
Sample : K1901-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1(0.5-1.5)

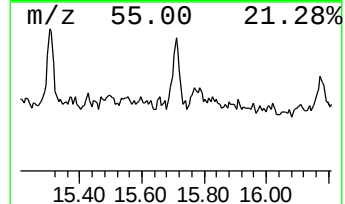
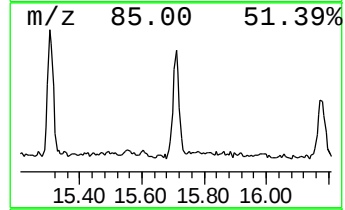
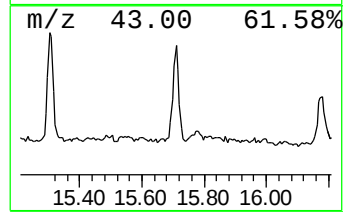
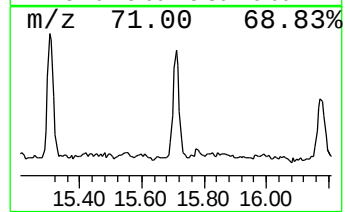
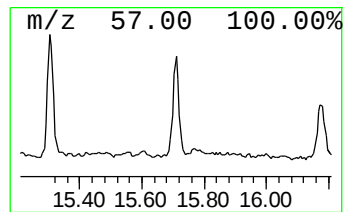
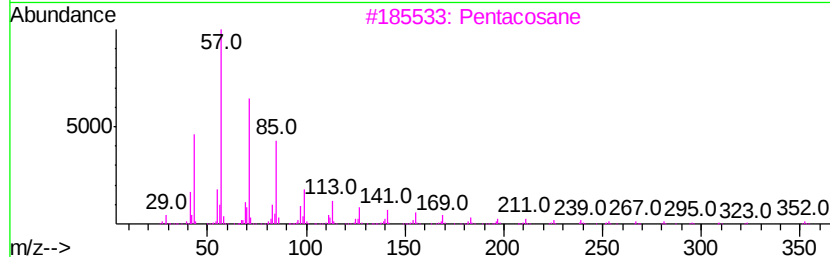
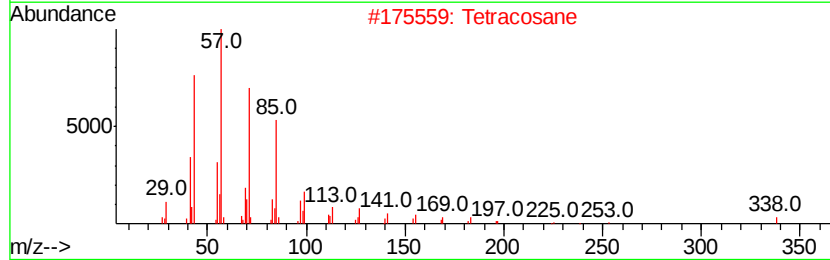
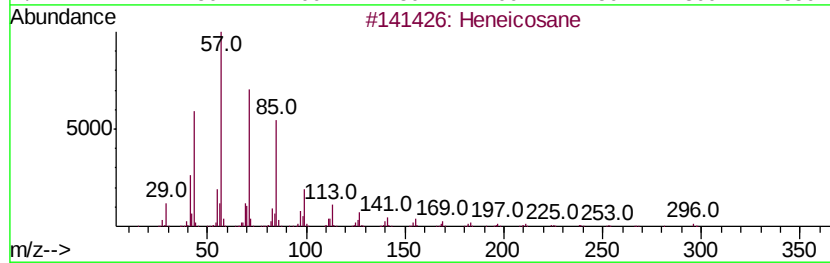
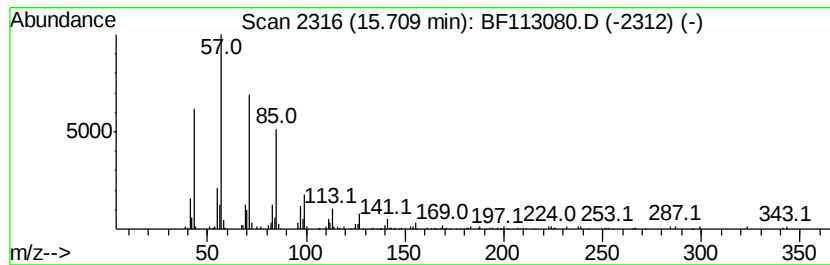
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.69 ng	203041	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Tetracosane	338	C24H50	000646-31-1	90
3			Pentacosane	352	C25H52	000629-99-2	87
4			Nonadecane	268	C19H40	000629-92-5	86
5			2-methyloctacosane	408	C29H60	1000376-72-8	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031519\
Data File : BF113080.D
Acq On : 15 Mar 2019 22:02
Operator : JU/SJ
Sample : K1901-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1(0.5-1.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.50	6.50	60.2	ng	2597940	1	6.73	863697	20.0
n-Hexadecanoic acid	11.77	9.4	ng	652264	4	11.23	1391500	20.0
Octadecanoic acid	12.56	4.0	ng	254466	5	13.86	1270290	20.0
Oxalic acid, isob...	13.72	6.0	ng	377815	5	13.86	1270290	20.0
Octadecane	14.34	2.4	ng	154496	5	13.86	1270290	20.0
Nonadecane	14.64	4.1	ng	225521	6	15.27	1101850	20.0
Heneicosane	14.95	4.0	ng	221623	6	15.27	1101850	20.0
Tetracosane	15.71	3.7	ng	203041	6	15.27	1101850	20.0