

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
 Data File : BF112879.D
 Acq On : 6 Mar 2019 3:52
 Operator : JU/SJ
 Sample : K1705-18
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-028-B004-022719

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	5.357	551	556	559	rBV	3754516	3690311	93.62%	10.337%
2	6.381	724	730	733	rBV	3730652	3845296	97.55%	10.771%
3	6.510	747	752	755	rBV	4127545	3941914	100.00%	11.042%
4	6.739	787	791	795	rBV	1120685	884470	22.44%	2.478%
5	6.898	814	818	821	rBV	3560400	3011354	76.39%	8.435%
6	7.298	881	886	889	rBV	2507420	2352995	59.69%	6.591%
7	8.022	1005	1009	1032	rBV	990973	1020808	25.90%	2.859%
8	9.098	1187	1192	1203	rBV	3644979	3408981	86.48%	9.549%
9	9.486	1255	1258	1265	rVB	195912	193756	4.92%	0.543%
10	9.769	1302	1306	1315	rBV2	1056472	1008248	25.58%	2.824%
11	10.557	1435	1440	1454	rBV	2331076	2348191	59.57%	6.578%
12	11.251	1554	1558	1560	rBV	969902	962647	24.42%	2.697%
13	11.268	1560	1561	1566	rVB	165087	131876	3.35%	0.369%
14	11.786	1645	1649	1659	rBV3	481024	519532	13.18%	1.455%
15	12.457	1759	1763	1767	rBV	239524	237506	6.03%	0.665%
16	12.568	1779	1782	1795	rBV3	195717	259295	6.58%	0.726%
17	12.680	1795	1801	1805	rBV	232481	254111	6.45%	0.712%
18	12.833	1822	1827	1830	rBV	3202414	3148124	79.86%	8.818%
19	13.074	1866	1868	1871	rVB2	48644	40044	1.02%	0.112%
20	13.115	1871	1875	1878	rBV	44209	44761	1.14%	0.125%
21	13.315	1903	1909	1914	rBV6	66084	89195	2.26%	0.250%
22	13.515	1940	1943	1948	rVB	41397	54935	1.39%	0.154%
23	13.621	1958	1961	1964	rBV3	29614	40871	1.04%	0.114%
24	13.733	1975	1980	1988	rVB3	274727	382361	9.70%	1.071%
25	13.874	1999	2004	2007	rBV	1302546	1364781	34.62%	3.823%
26	13.898	2007	2008	2014	rVB	130219	110782	2.81%	0.310%
27	14.057	2032	2035	2039	rBV	136606	124960	3.17%	0.350%
28	14.362	2083	2087	2094	rBV	244486	295454	7.50%	0.828%
29	14.656	2134	2137	2144	rVB	178213	182031	4.62%	0.510%
30	14.727	2147	2149	2152	rVB	47351	43798	1.11%	0.123%
31	14.792	2157	2160	2164	rVB	118516	119845	3.04%	0.336%
32	14.886	2173	2176	2179	rBV	70017	97409	2.47%	0.273%
33	14.974	2188	2191	2194	rBV	275412	333429	8.46%	0.934%
34	15.286	2239	2244	2248	rBV	625095	738548	18.74%	2.069%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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35	15.333	2249	2252	2256	rVB	145426	173640	4.40%	0.486%
36	15.739	2317	2321	2326	rBV	167592	243572	6.18%	0.682%

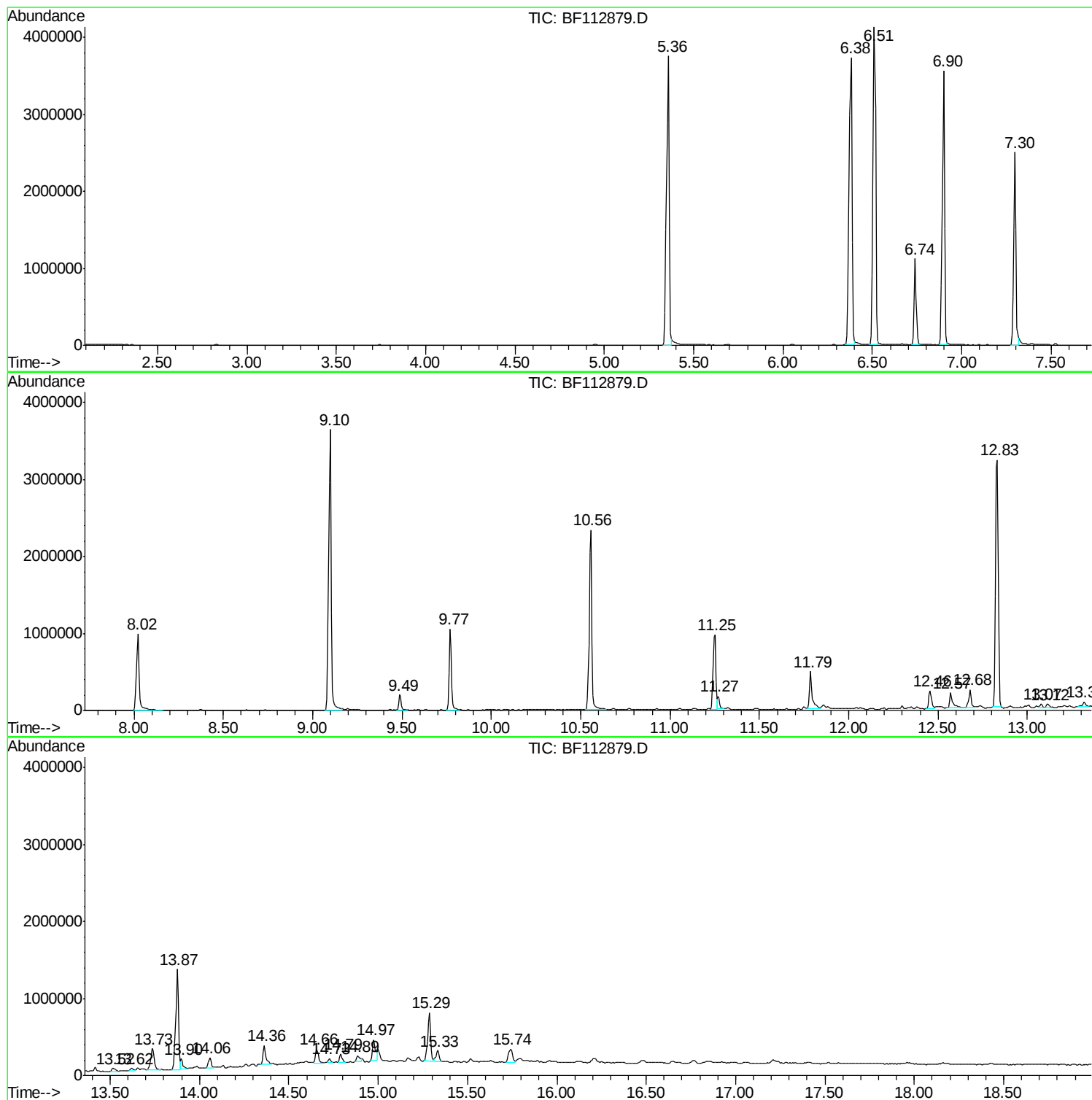
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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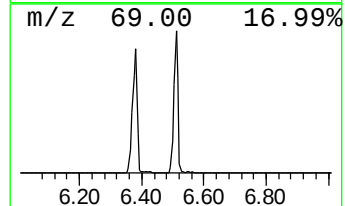
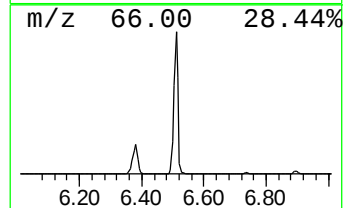
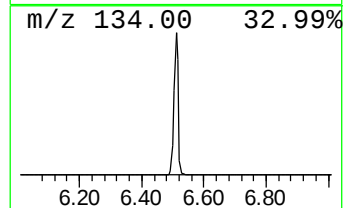
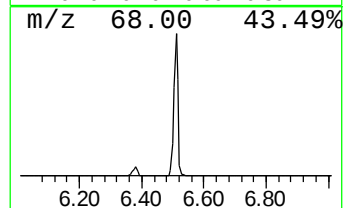
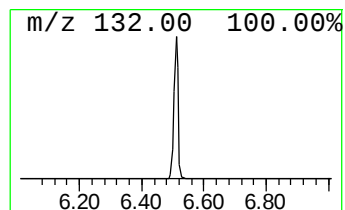
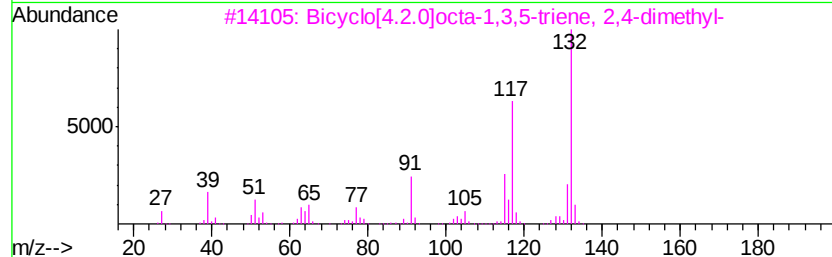
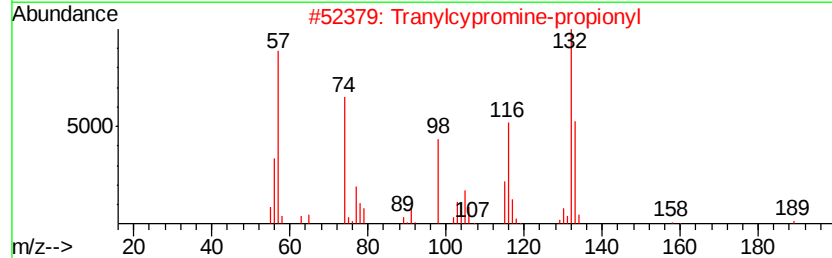
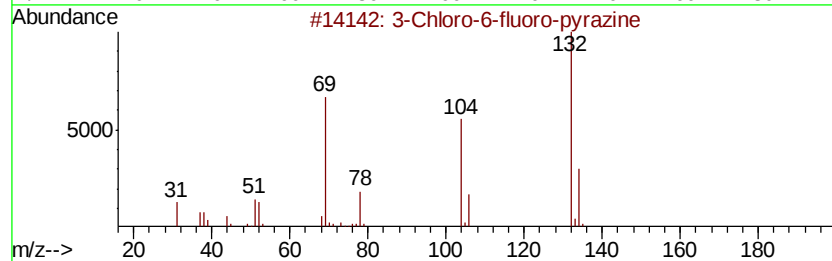
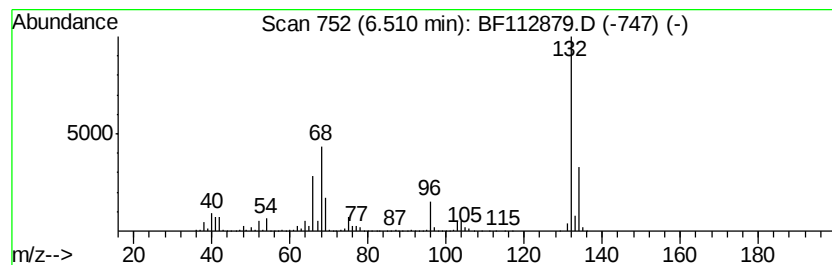
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	89.14 ng	3941910	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12	
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9	
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	



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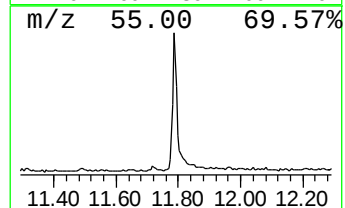
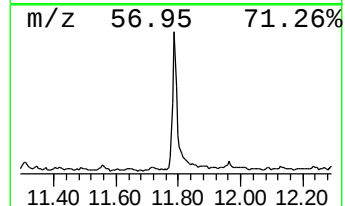
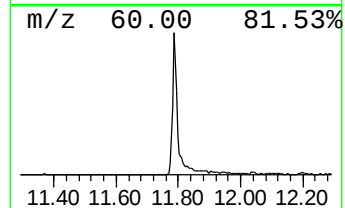
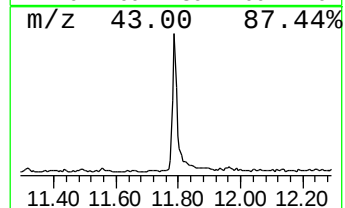
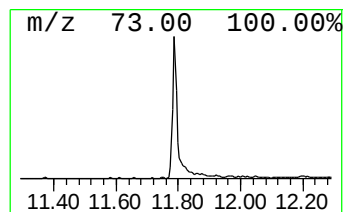
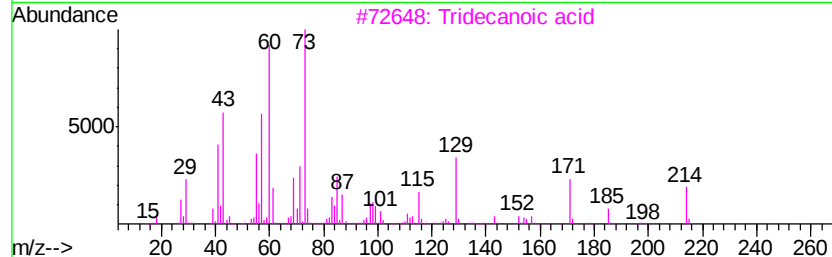
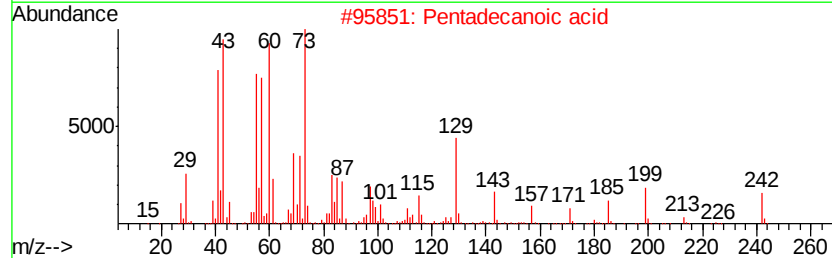
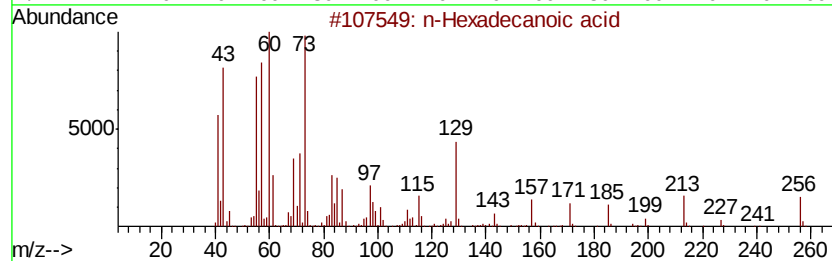
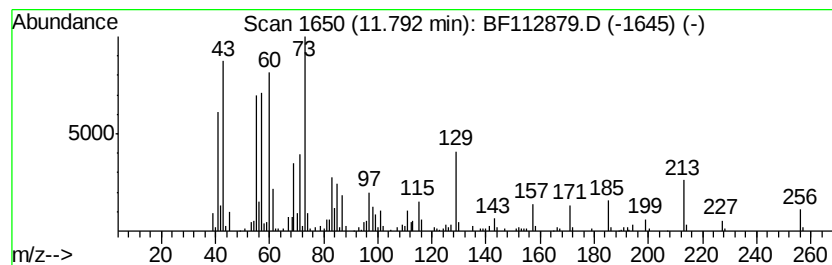
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	10.79 ng	519532	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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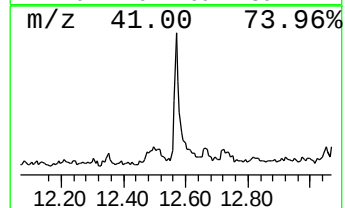
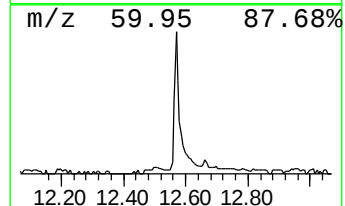
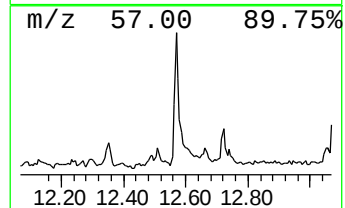
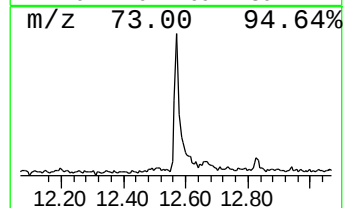
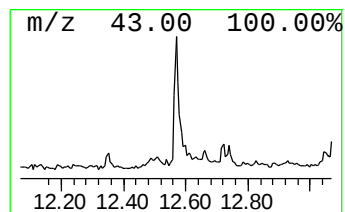
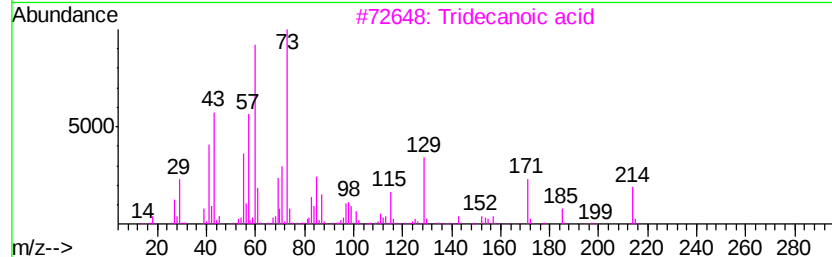
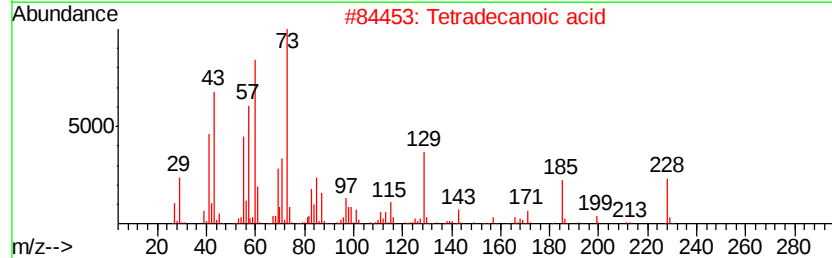
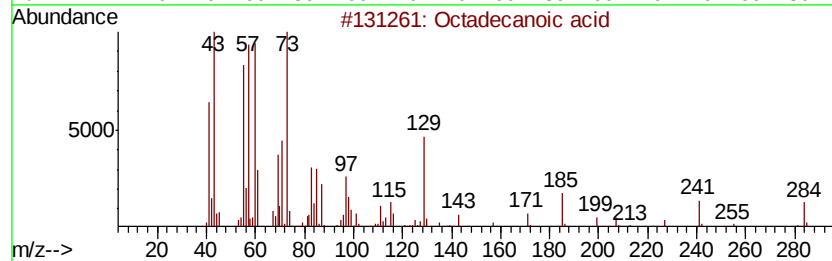
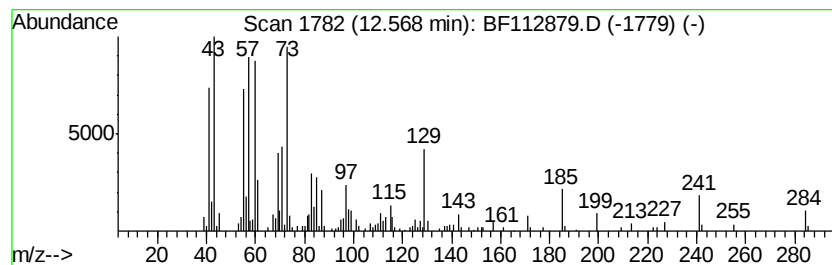
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.80 ng	259295	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	30
5		2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	20



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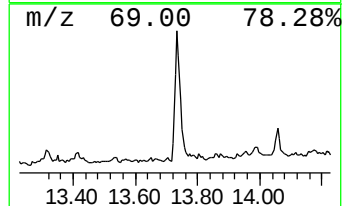
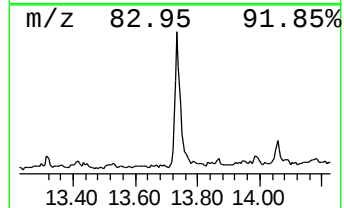
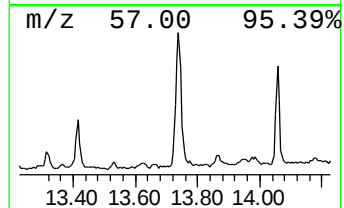
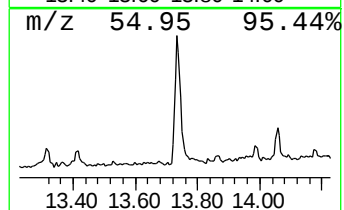
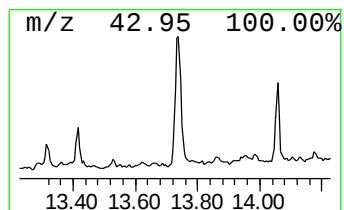
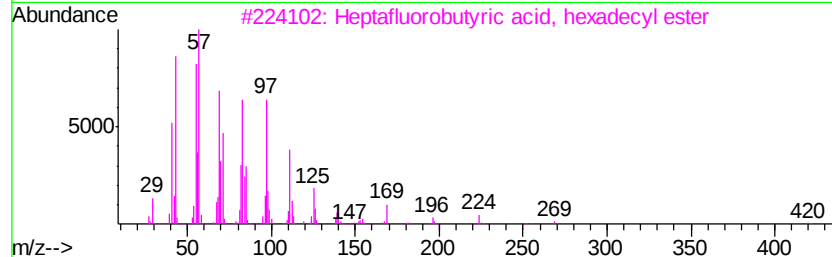
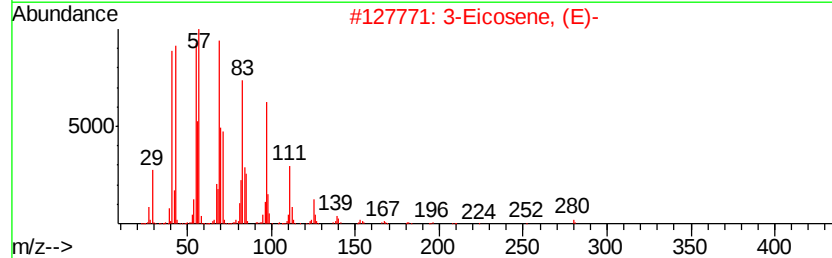
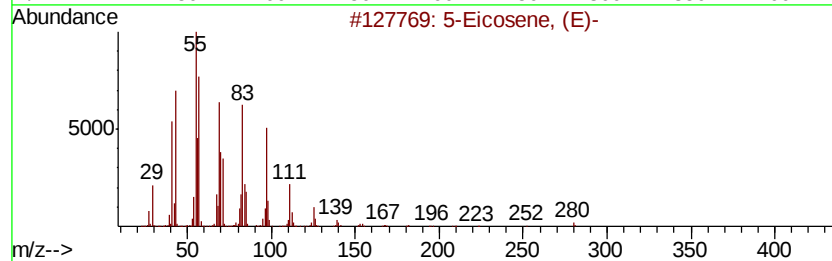
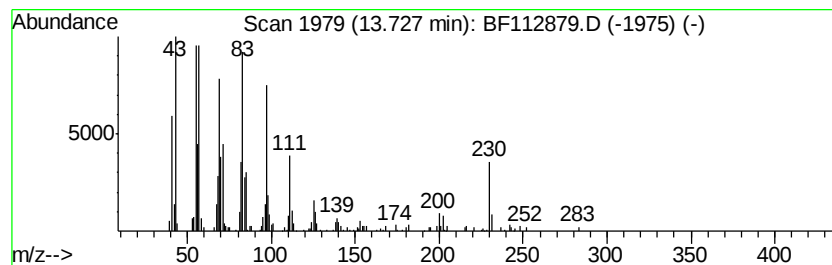
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	5.60 ng	382361	Chrysene-d12	13.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	5-Eicosene, (E)-	280 C20H40	074685-30-6	98
2	3-Eicosene, (E)-	280 C20H40	074685-33-9	96
3	Heptafluorobutyric acid, hexadec...	438 C20H33F7O2	006385-15-5	94
4	n-Tetracosanol-1	354 C24H50O	000506-51-4	94
5	Pentafluoropropionic acid, hexad...	388 C19H33F5O2	006222-07-7	94



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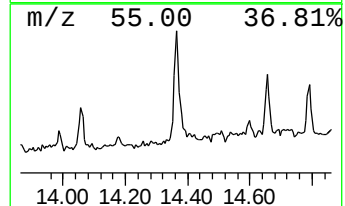
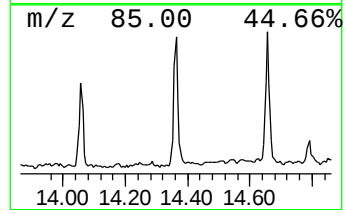
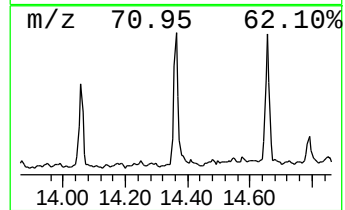
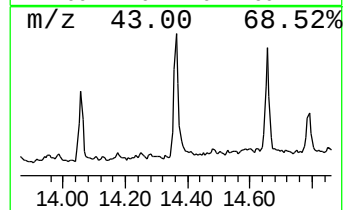
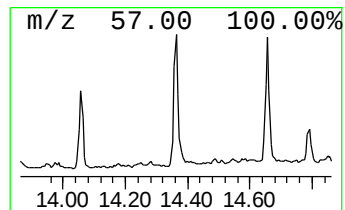
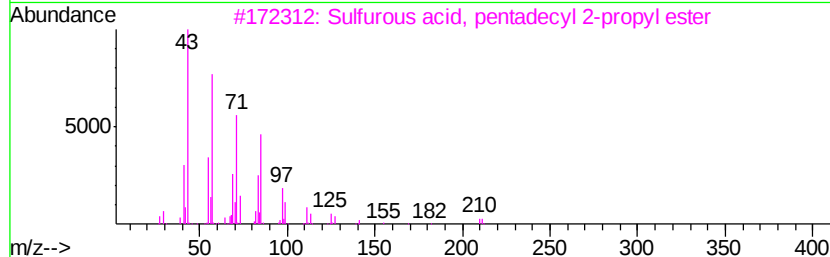
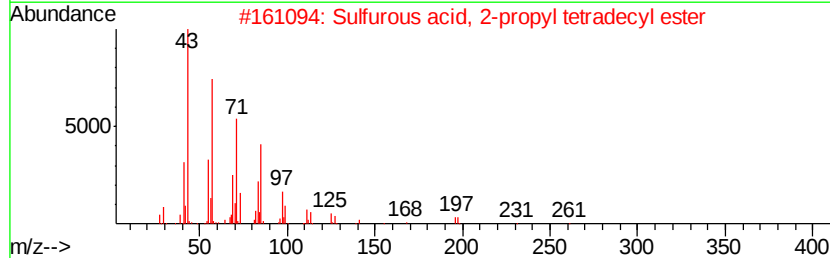
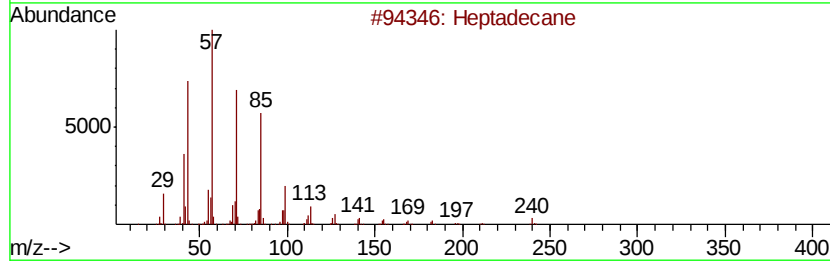
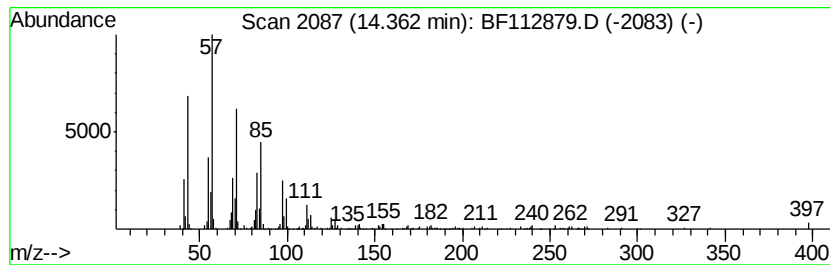
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	4.33 ng	295454	Chrysene-d12	13.87
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	93
2	Sulfurous acid, 2-propyl tetradec...	320 C17H36O3S	1000309-12-5	91
3	Sulfurous acid, pentadecyl 2-pro...	334 C18H38O3S	1000309-12-6	91
4	1-Octadecanesulphonyl chloride	352 C18H37ClO2S	1000342-70-4	91
5	Tritetracontane	605 C43H88	007098-21-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112879.D
Acq On : 6 Mar 2019 3:52
Operator : JU/SJ
Sample : K1705-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-B004-022719

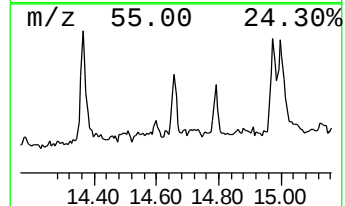
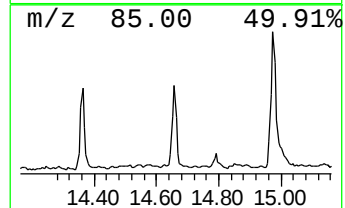
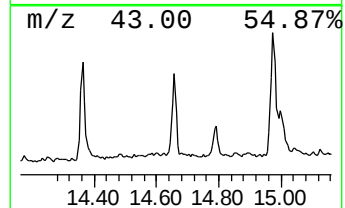
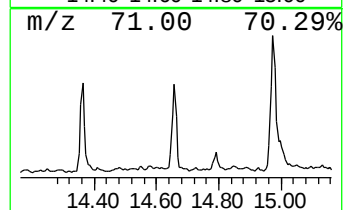
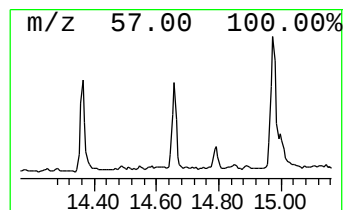
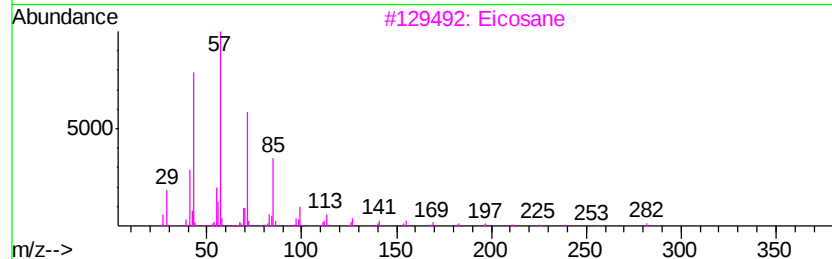
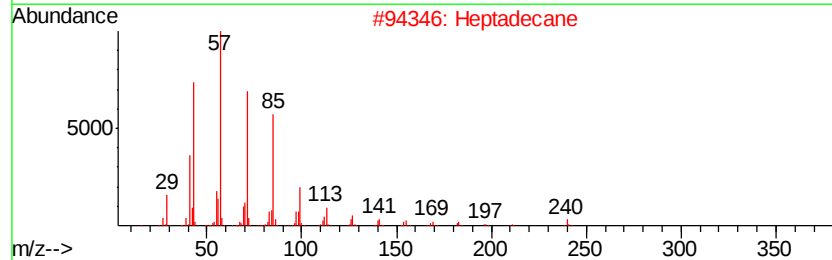
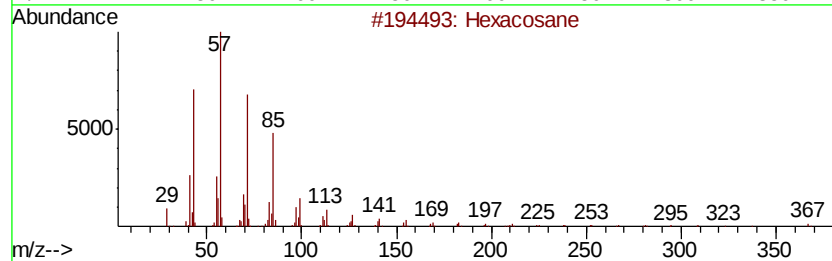
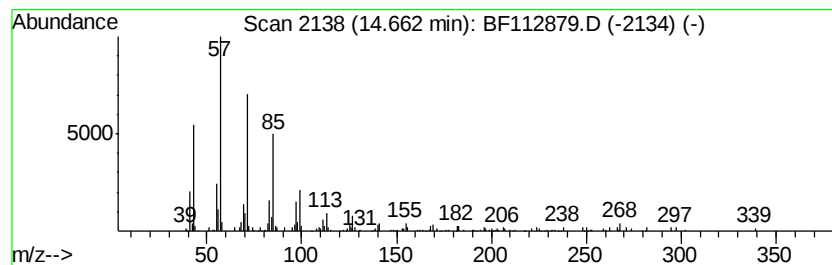
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	4.93 ng	182031	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Heptadecane	240	C17H36	000629-78-7	87
3		Eicosane	282	C20H42	000112-95-8	83
4		Docosane	310	C22H46	000629-97-0	80
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112879.D
Acq On : 6 Mar 2019 3:52
Operator : JU/SJ
Sample : K1705-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PST-028-B004-022719

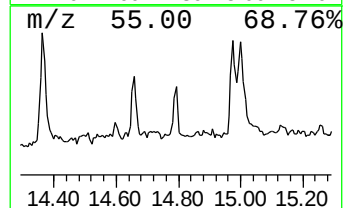
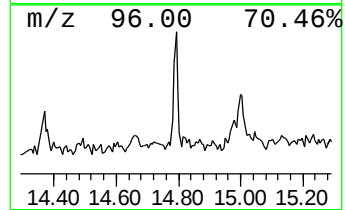
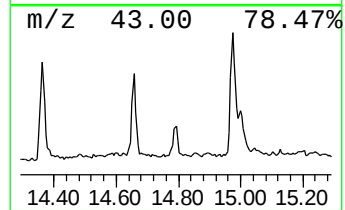
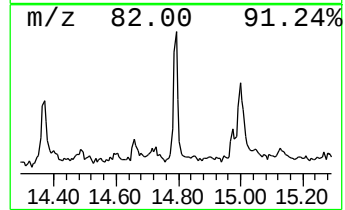
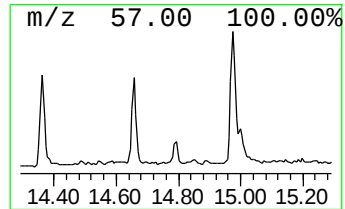
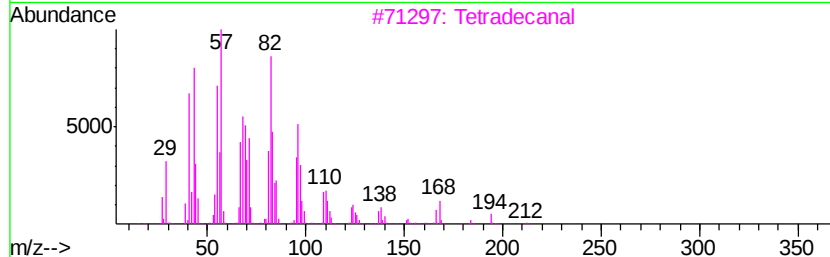
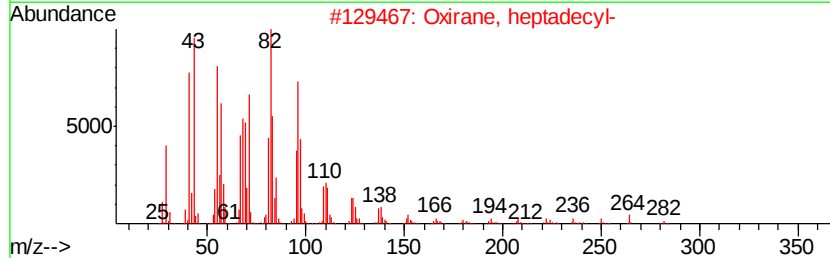
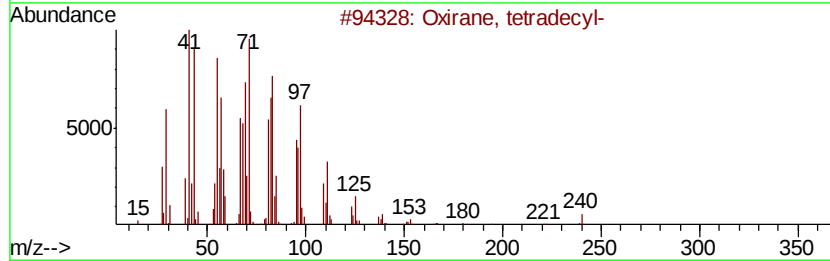
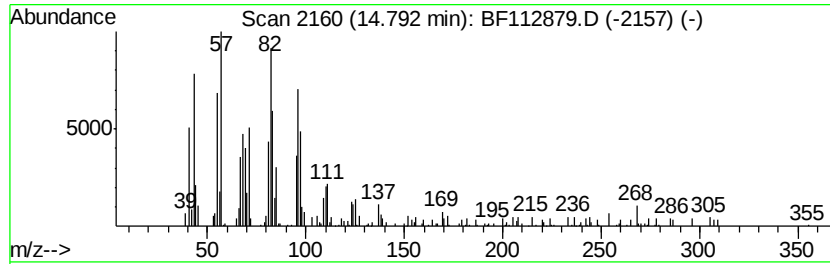
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, tetradecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	3.25 ng	119845	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	91
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	83
3		Tetradecanal	212	C14H28O	000124-25-4	80
4		1,19-Eicosadiene	278	C20H38	014811-95-1	76
5		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112879.D
Acq On : 6 Mar 2019 3:52
Operator : JU/SJ
Sample : K1705-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PST-028-B004-022719

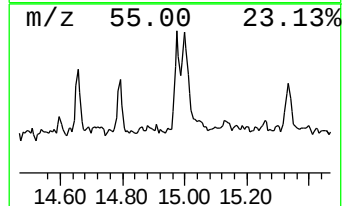
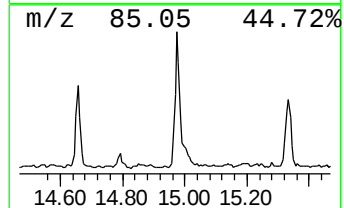
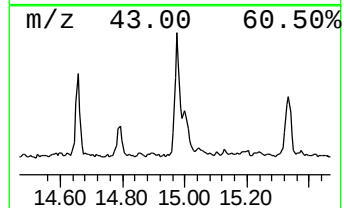
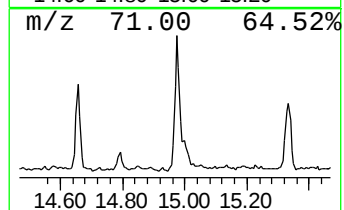
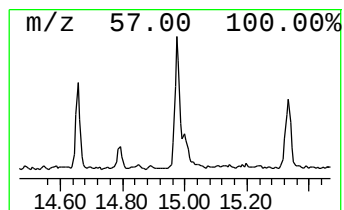
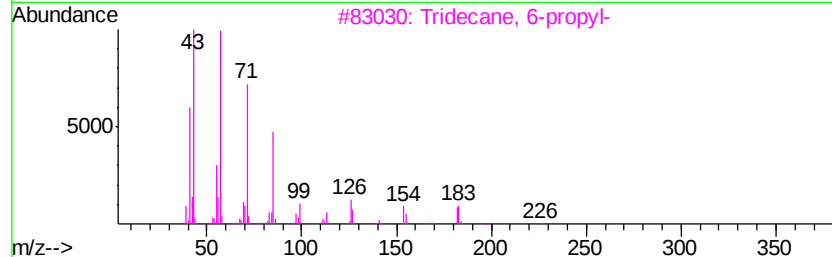
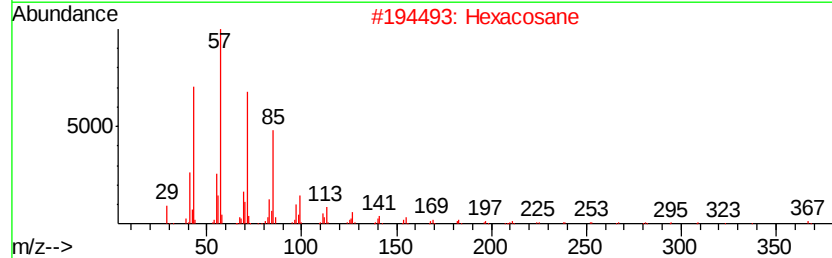
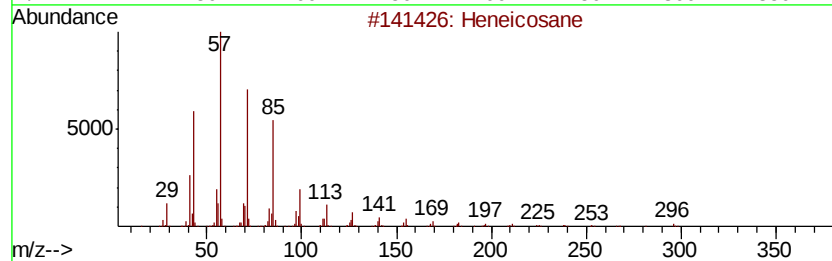
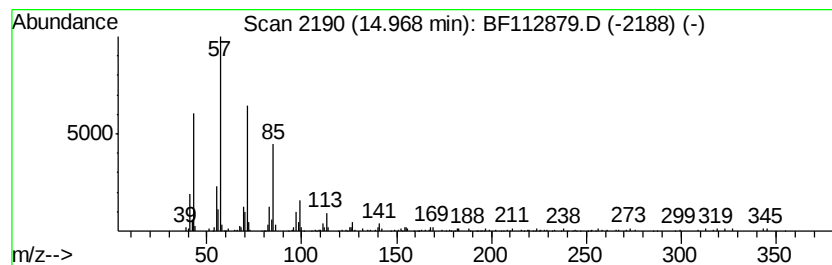
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	9.03 ng	333429	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Hexacosane		366	C26H54	000630-01-3	90
3	Tridecane, 6-propyl-		226	C16H34	055045-10-8	87
4	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	83
5	Octadecane		254	C18H38	000593-45-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030519\
Data File : BF112879.D
Acq On : 6 Mar 2019 3:52
Operator : JU/SJ
Sample : K1705-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-B004-022719

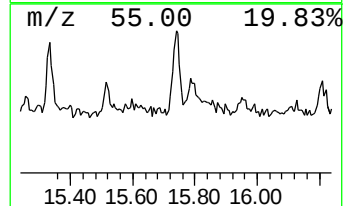
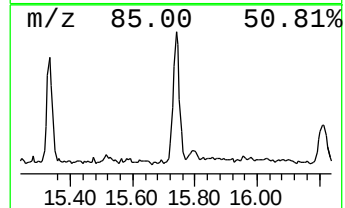
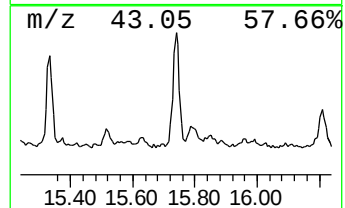
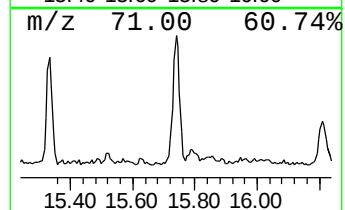
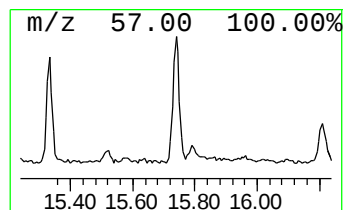
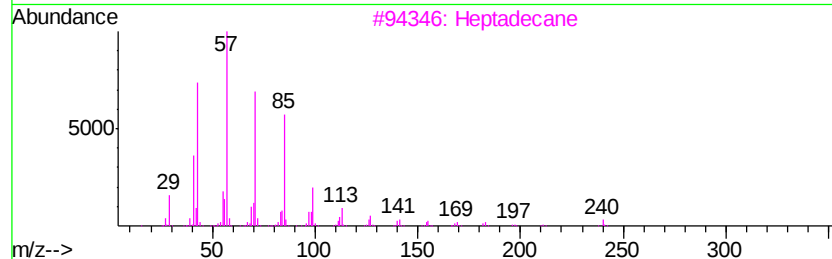
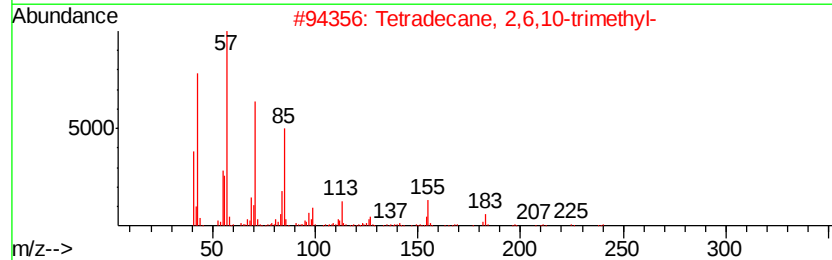
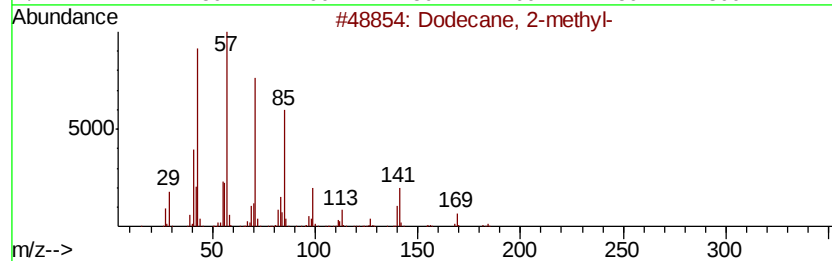
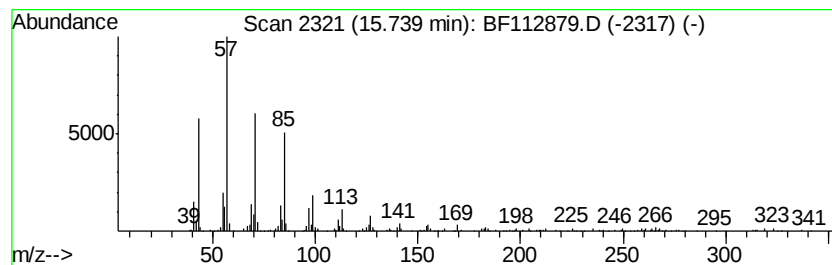
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dodecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	6.60 ng	243572	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87
3		Heptadecane	240	C17H36	000629-78-7	86
4		Pentacosane	352	C25H52	000629-99-2	86
5		Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030519\
Data File : BF112879.D
Acq On : 6 Mar 2019 3:52
Operator : JU/SJ
Sample : K1705-18
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.51	6.51	89.1	ng	3941910	1	6.74	884470	20.0
n-Hexadecanoic acid	11.79	10.8	ng	519532	4	11.25	962647	20.0
Octadecanoic acid	12.57	3.8	ng	259295	5	13.87	1364780	20.0
5-Eicosene, (E)-	13.73	5.6	ng	382361	5	13.87	1364780	20.0
Heptadecane	14.36	4.3	ng	295454	5	13.87	1364780	20.0
Hexacosane	14.66	4.9	ng	182031	6	15.29	738548	20.0
Oxirane, tetradecyl-	14.79	3.3	ng	119845	6	15.29	738548	20.0
Heneicosane	14.97	9.0	ng	333429	6	15.29	738548	20.0
Dodecane, 2-methyl-	15.74	6.6	ng	243572	6	15.29	738548	20.0