

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011019\
 Data File : BF111986.D
 Acq On : 10 Jan 2019 14:44
 Operator : JU/SJ
 Sample : K1082-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-6

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-BF010719.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	2.175	11	15	17	rBV	34292	40223	1.33%	0.147%
2	5.093	507	511	520	rVB	139559	161183	5.32%	0.589%
3	5.510	577	582	585	rBV	2755655	2503071	82.64%	9.152%
4	6.516	748	753	756	rBV	2800169	2720194	89.80%	9.946%
5	6.651	771	776	779	rBV	3016794	2725056	89.96%	9.964%
6	6.698	782	784	790	rVB	33679	32181	1.06%	0.118%
7	6.875	810	814	821	rBV	903481	740719	24.45%	2.708%
8	7.034	837	841	844	rBV	2404145	2065034	68.17%	7.551%
9	7.434	904	909	912	rBV	1866742	1721522	56.83%	6.295%
10	8.157	1028	1032	1035	rBV	1070652	929893	30.70%	3.400%
11	9.234	1210	1215	1218	rBV	3295497	3029066	100.00%	11.075%
12	9.622	1277	1281	1284	rBV	795379	625479	20.65%	2.287%
13	9.910	1326	1330	1334	rBV	1130355	1070543	35.34%	3.914%
14	10.704	1460	1465	1468	rBV	2227702	2049401	67.66%	7.493%
15	10.828	1482	1486	1493	rVB2	23568	35324	1.17%	0.129%
16	11.398	1579	1583	1586	rBV	1282014	1072009	35.39%	3.920%
17	11.922	1668	1672	1679	rBV2	87233	95745	3.16%	0.350%
18	12.610	1786	1789	1792	rBV	112893	91391	3.02%	0.334%
19	12.839	1823	1828	1833	rBV2	77002	100541	3.32%	0.368%
20	12.980	1848	1852	1856	rBV	2817185	2770451	91.46%	10.130%
21	13.122	1873	1876	1879	rBV	47621	35455	1.17%	0.130%
22	13.457	1928	1933	1938	rVB7	26629	46452	1.53%	0.170%
23	13.551	1947	1949	1952	rVB	53491	39156	1.29%	0.143%
24	13.880	2000	2005	2011	rBV	126825	150495	4.97%	0.550%
25	14.039	2027	2032	2035	rBV	919259	834266	27.54%	3.050%
26	14.198	2056	2059	2063	rBV	101379	83683	2.76%	0.306%
27	14.504	2107	2111	2118	rVB	133315	130286	4.30%	0.476%
28	14.810	2160	2163	2167	rVB	127118	122028	4.03%	0.446%
29	15.151	2217	2221	2227	rBV	134052	148200	4.89%	0.542%
30	15.515	2278	2283	2296	rVB	648749	960119	31.70%	3.511%
31	15.980	2357	2362	2367	rVB	80480	120543	3.98%	0.441%
32	16.486	2444	2448	2455	rVB4	50493	99732	3.29%	0.365%

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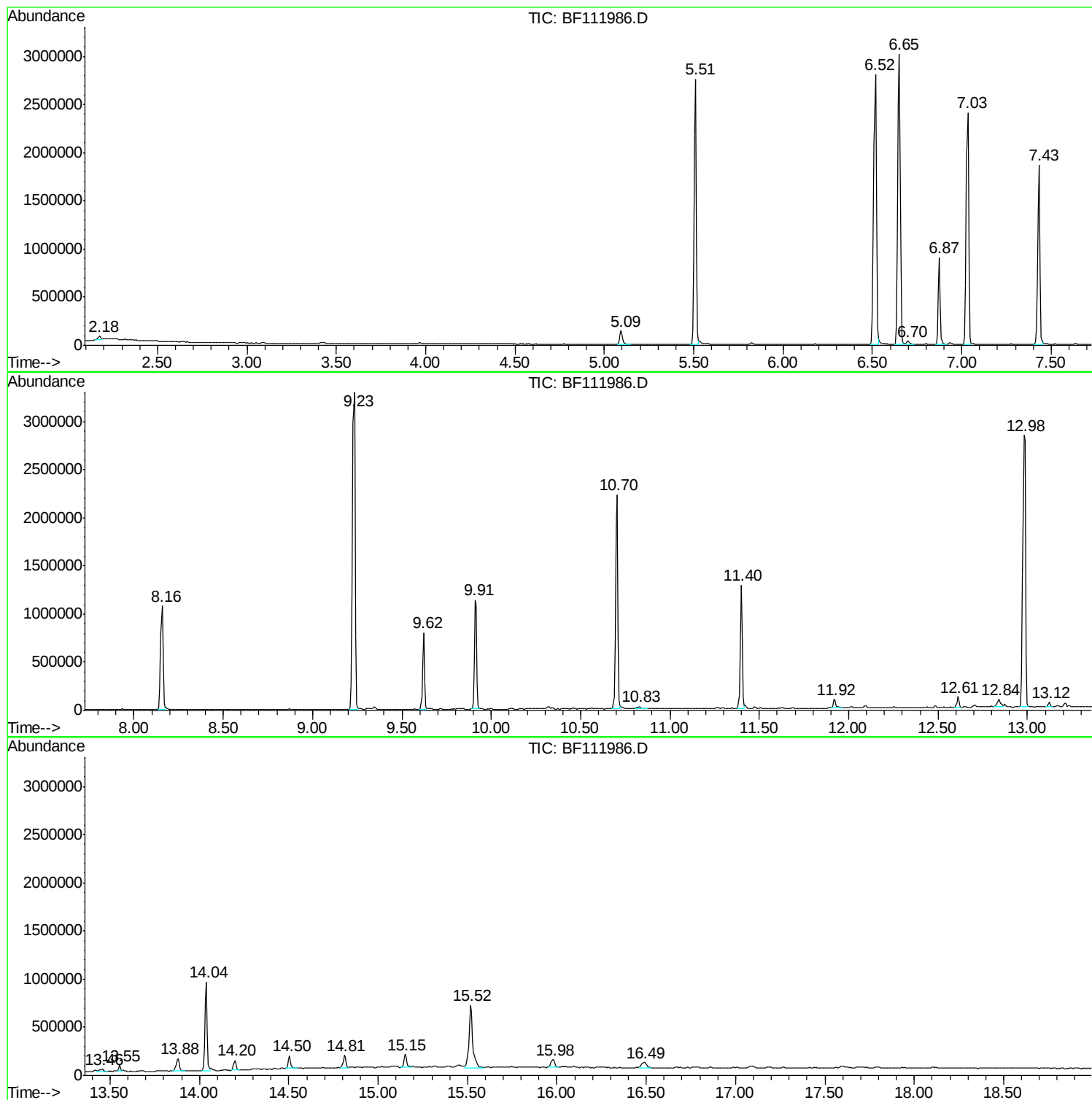
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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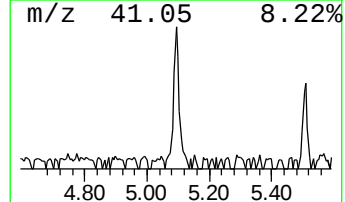
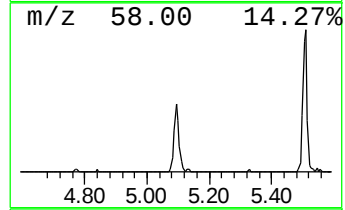
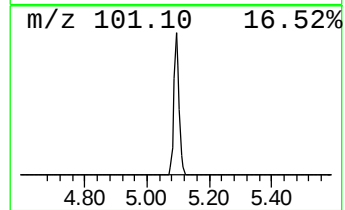
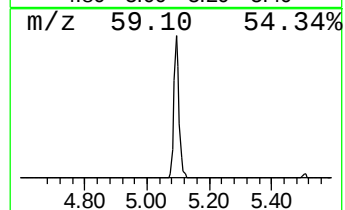
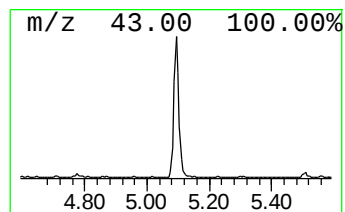
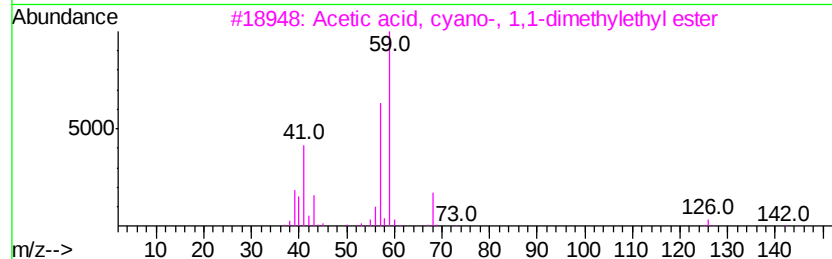
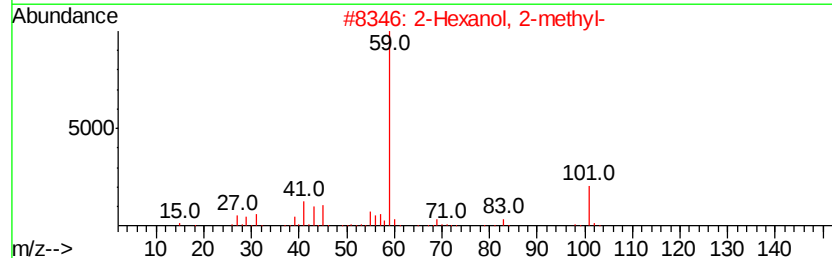
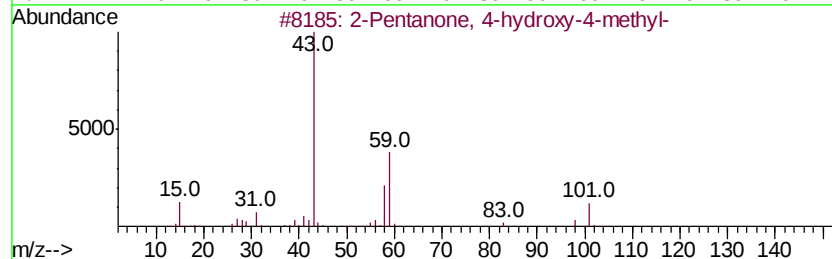
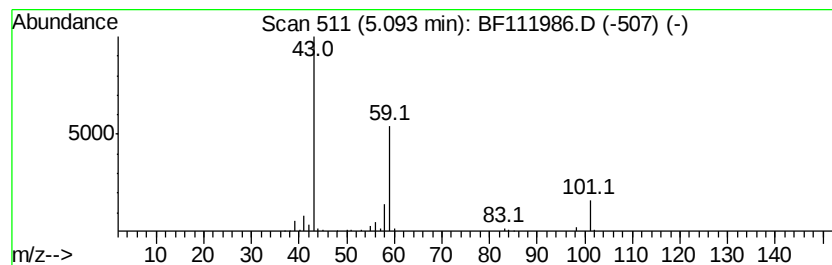
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	4.35 ng	161183	1,4-Dichlorobenzene-d4	6.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17	
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10	



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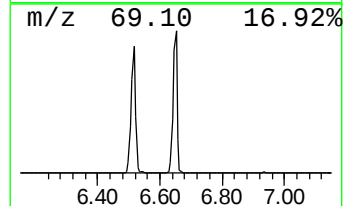
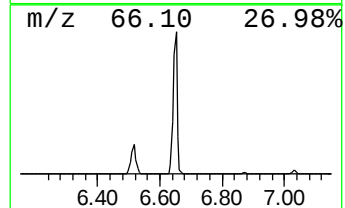
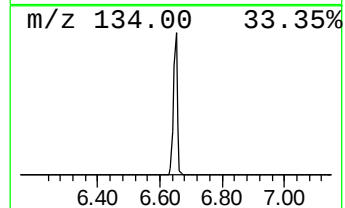
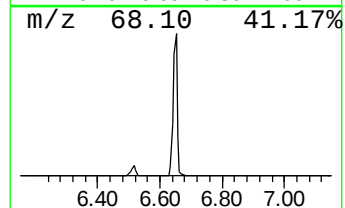
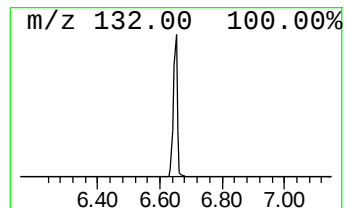
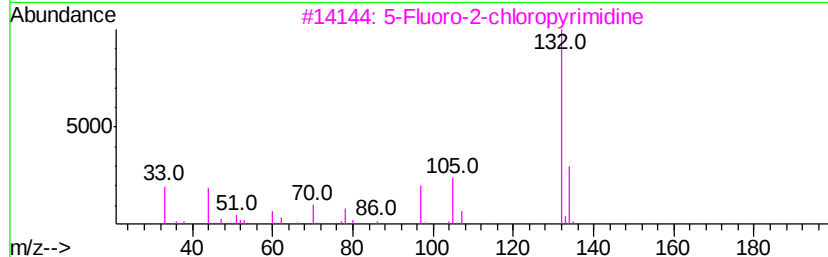
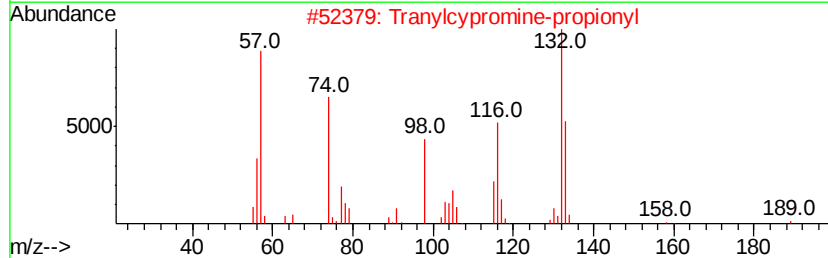
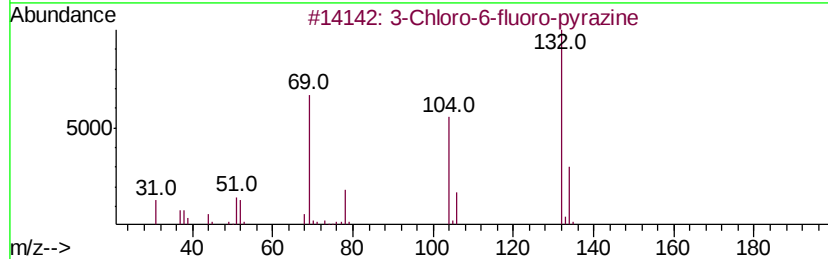
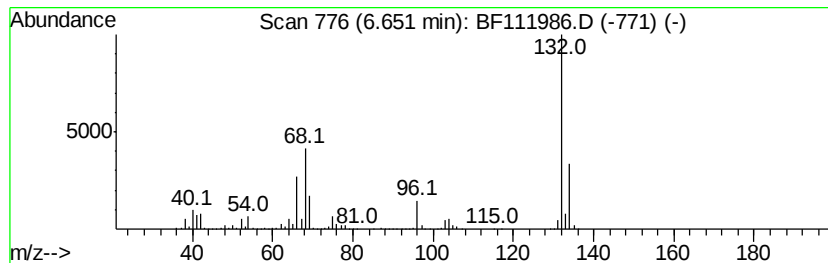
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	73.58 ng	2725060	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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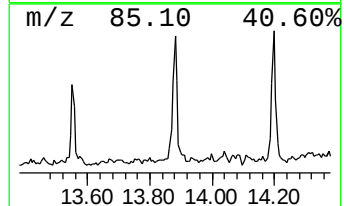
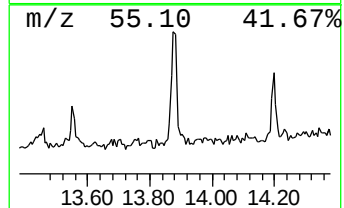
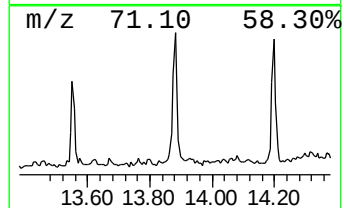
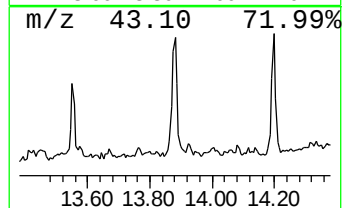
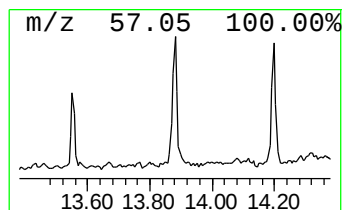
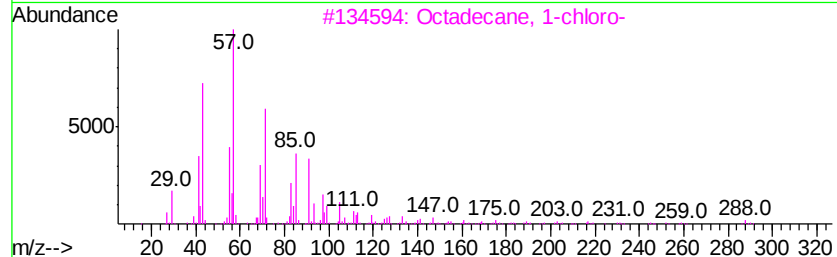
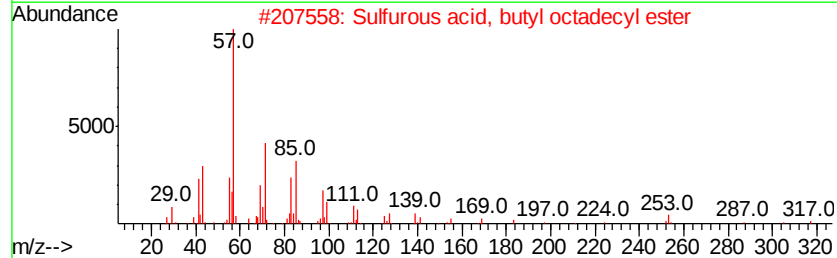
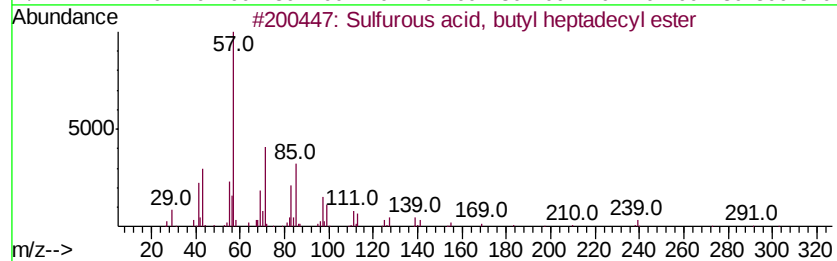
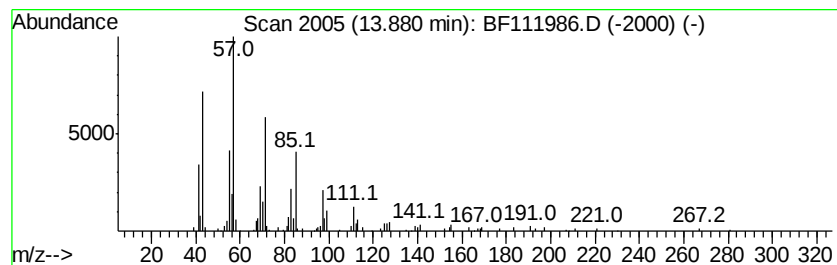
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Sulfurous acid, butyl hepta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	3.61 ng	150495	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
2		Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	90
3		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	90
4		Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	86
5		Tritetracontane	605	C43H88	007098-21-7	80



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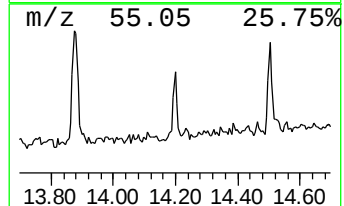
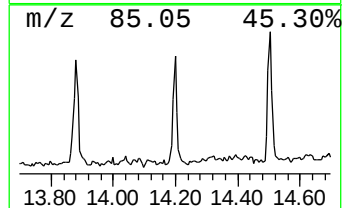
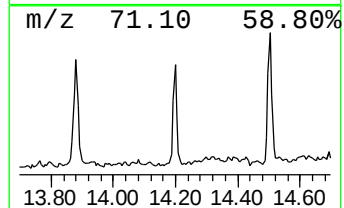
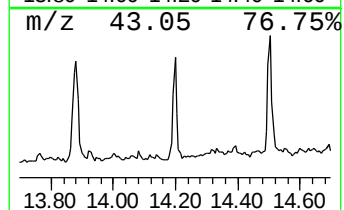
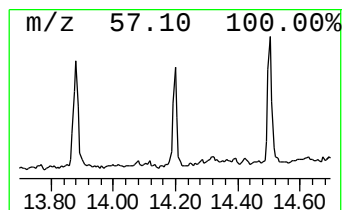
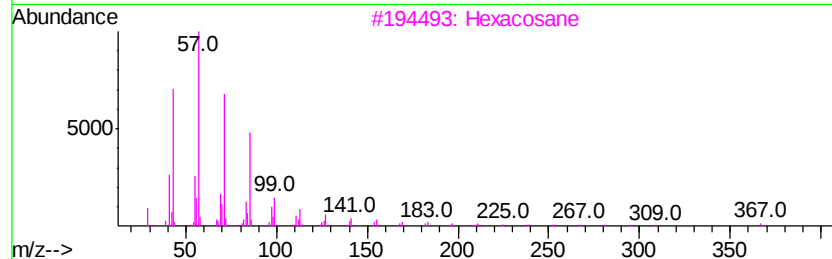
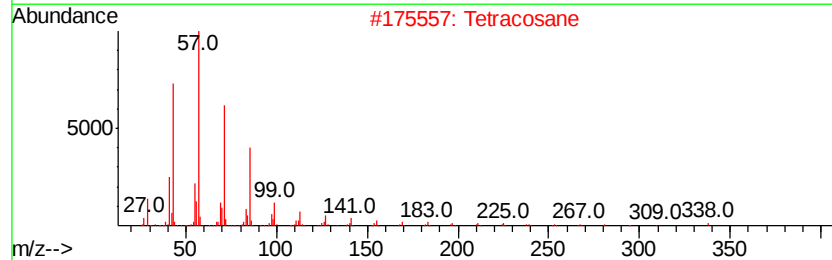
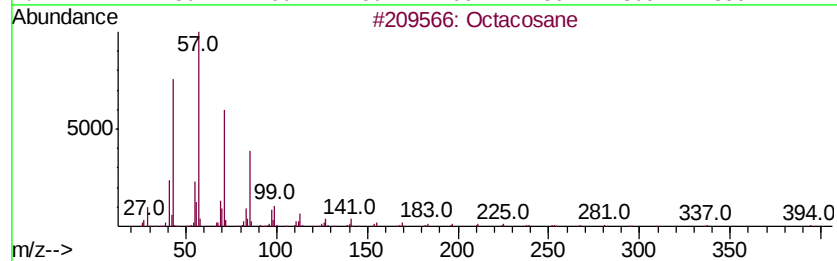
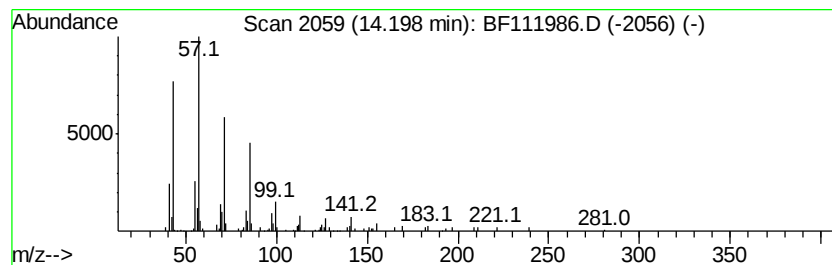
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	2.01 ng	83683	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Tetracosane	338	C24H50	000646-31-1	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Docosane	310	C22H46	000629-97-0	91
5		Heneicosane	296	C21H44	000629-94-7	91



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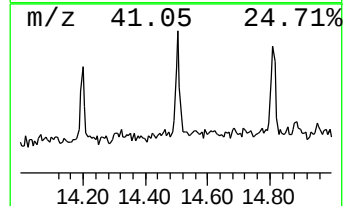
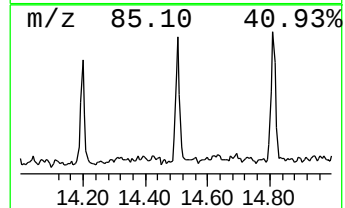
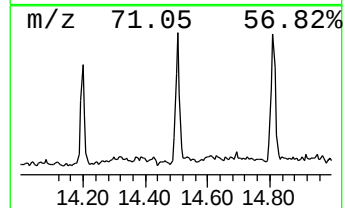
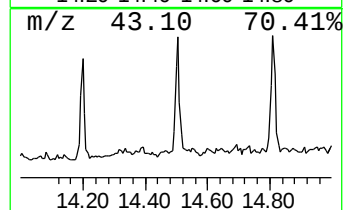
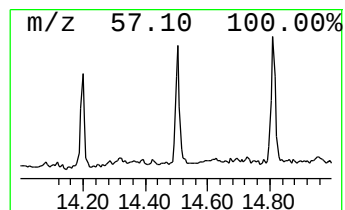
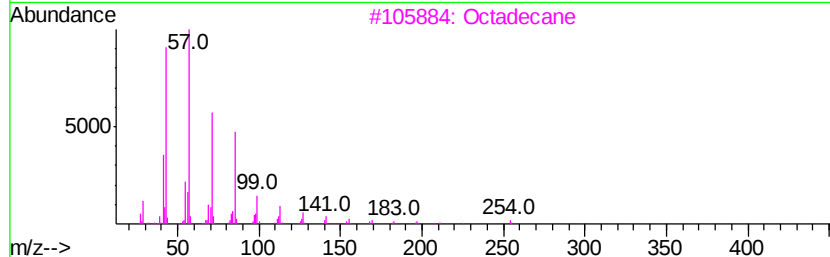
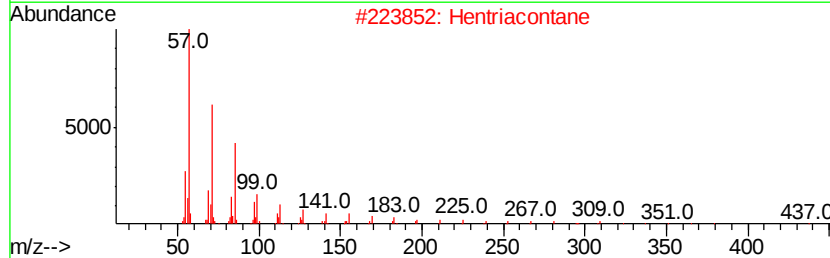
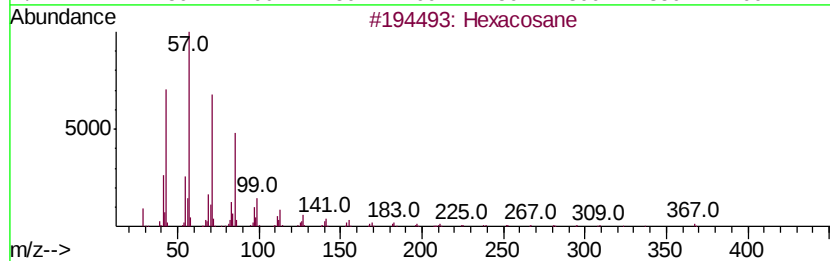
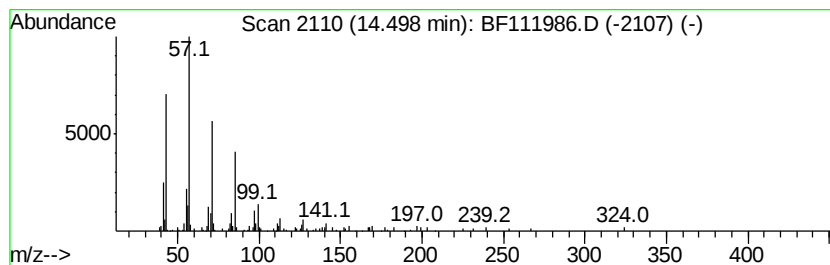
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.50	3.12 ng	130286	Chrysene-d12	14.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Hentriacontane		437	C31H64	000630-04-6	91
3	Octadecane		254	C18H38	000593-45-3	91
4	Hexatriacontane		507	C36H74	000630-06-8	90
5	2-methyloctacosane		408	C29H60	1000376-72-8	90



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Sample : K1082-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-6

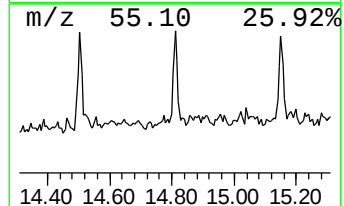
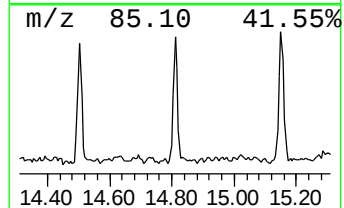
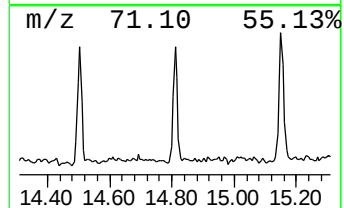
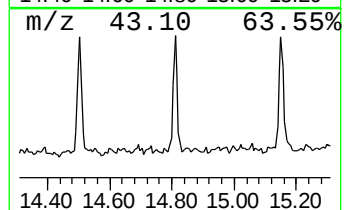
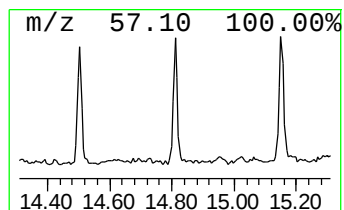
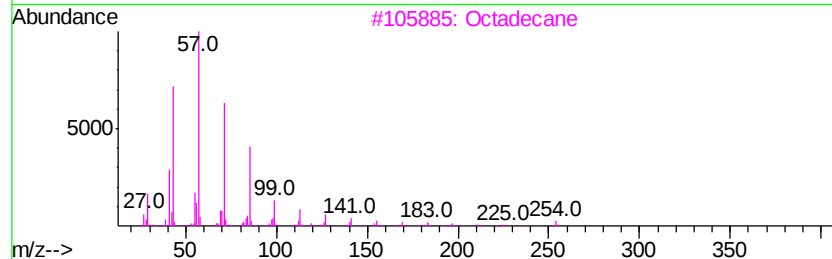
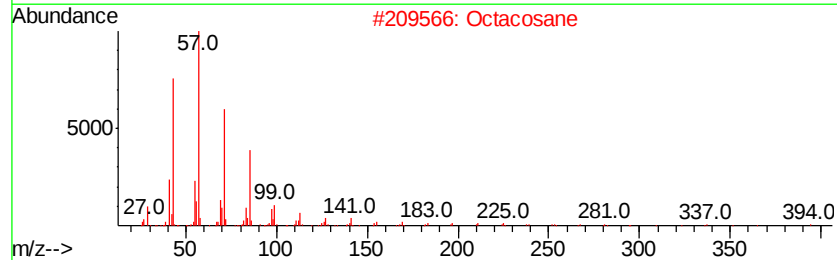
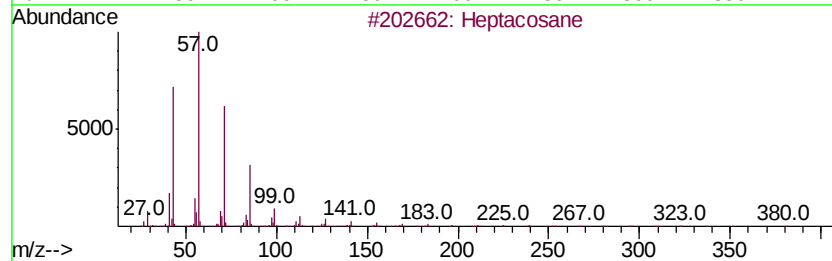
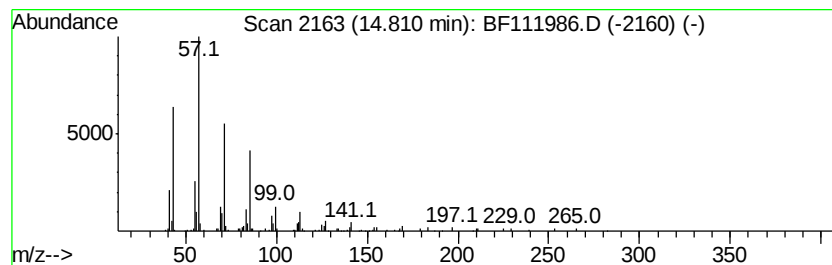
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.54 ng	122028	Perylene-d12	15.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	91
2		Octacosane	394	C28H58	000630-02-4	90
3		Octadecane	254	C18H38	000593-45-3	87
4		Heneicosane	296	C21H44	000629-94-7	83
5		Triacontane	422	C30H62	000638-68-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011019\
Data File : BF111986.D
Acq On : 10 Jan 2019 14:44
Operator : JU/SJ
Sample : K1082-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-6

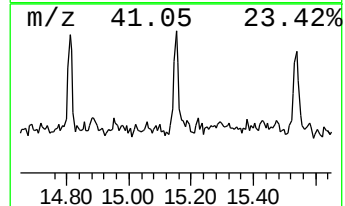
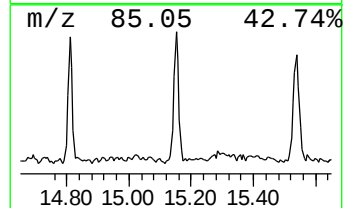
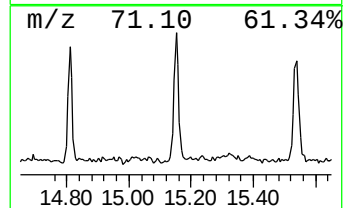
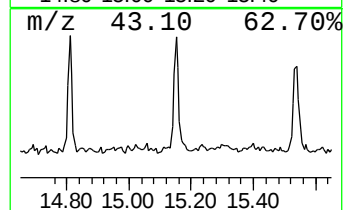
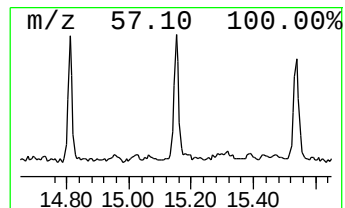
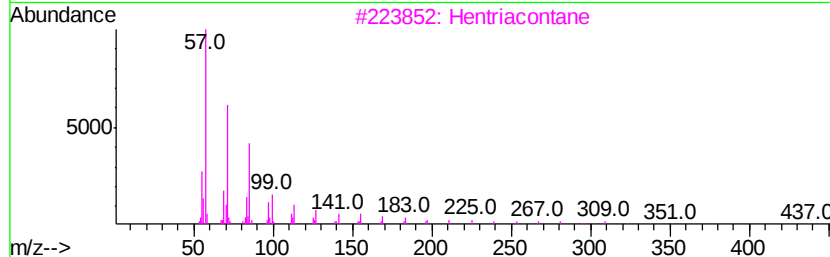
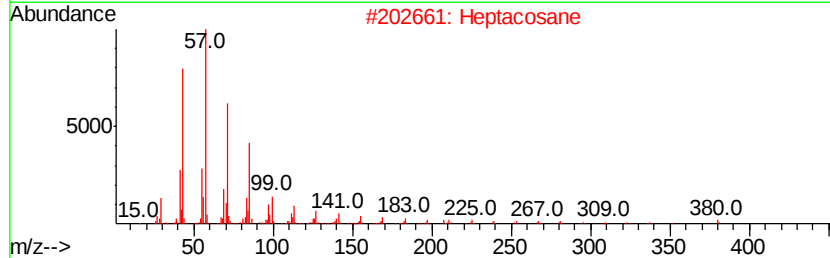
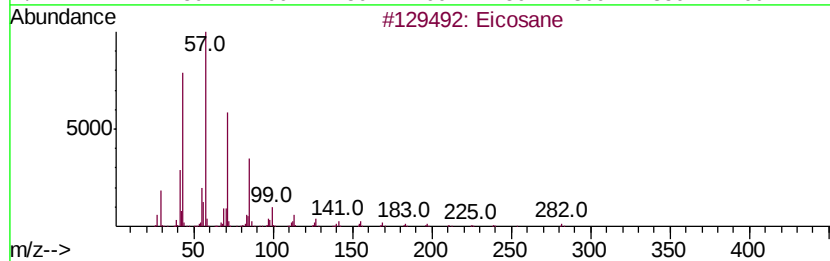
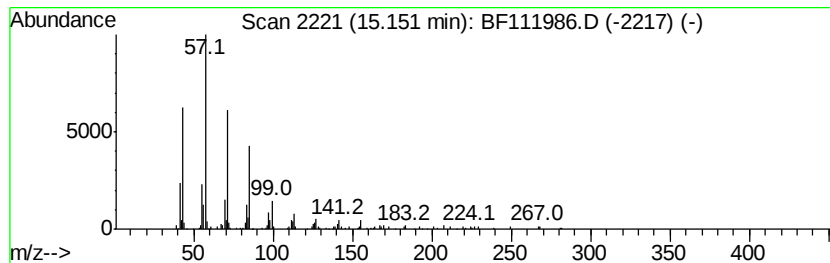
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.15	3.09 ng	148200	Perylene-d12	15.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	95
2	Heptacosane		380	C27H56	000593-49-7	91
3	Hentriacontane		437	C31H64	000630-04-6	90
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	90
5	Octacosane		394	C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011019\
Data File : BF111986.D
Acq On : 10 Jan 2019 14:44
Operator : JU/SJ
Sample : K1082-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-6

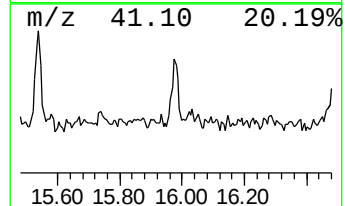
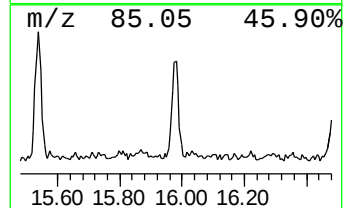
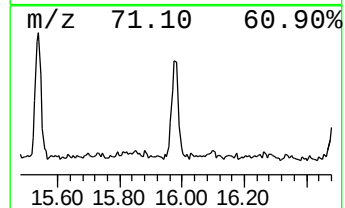
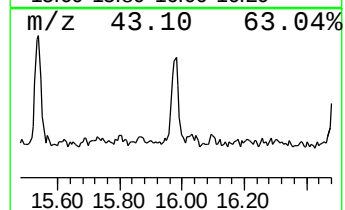
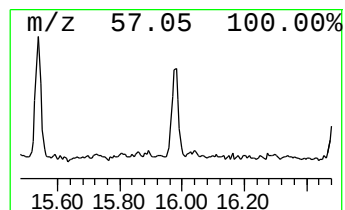
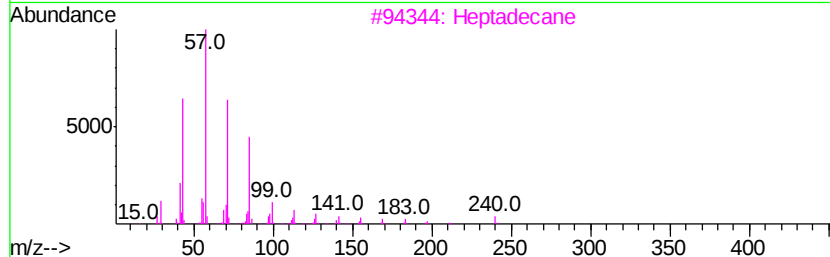
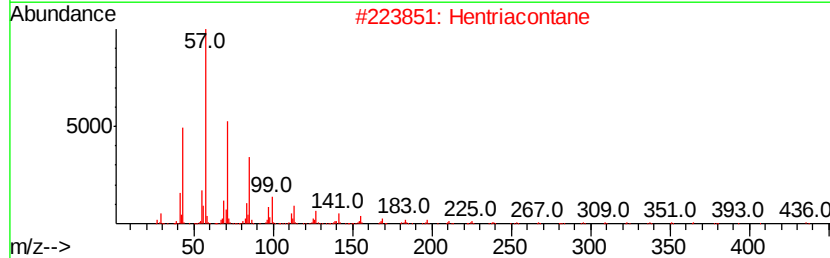
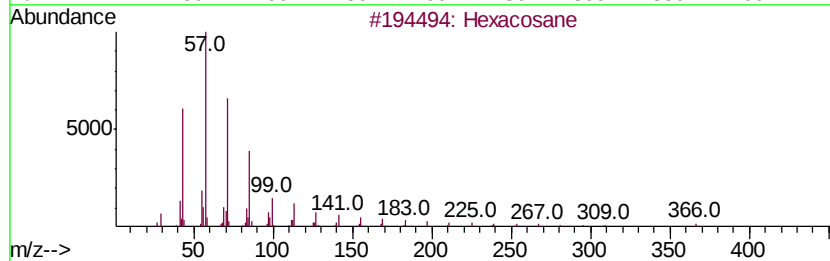
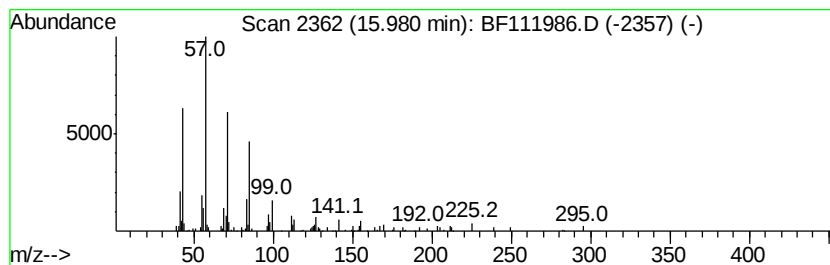
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.51 ng	120543	Perylene-d12	15.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Hentriacontane	437	C31H64	000630-04-6	86
3			Heptadecane	240	C17H36	000629-78-7	80
4			Octadecane	254	C18H38	000593-45-3	80
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011019\
Data File : BF111986.D
Acq On : 10 Jan 2019 14:44
Operator : JU/SJ
Sample : K1082-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-6

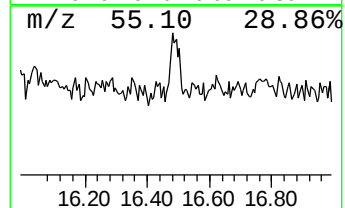
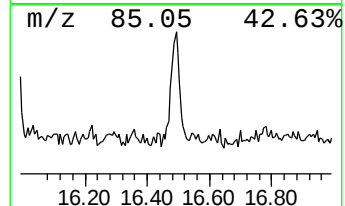
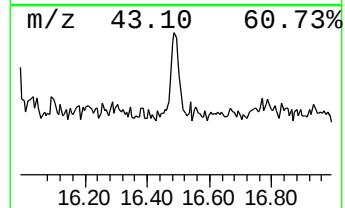
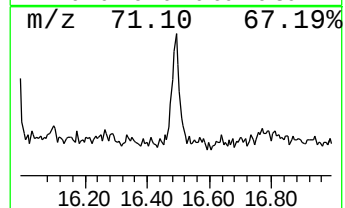
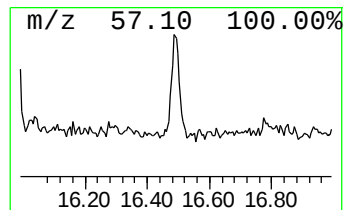
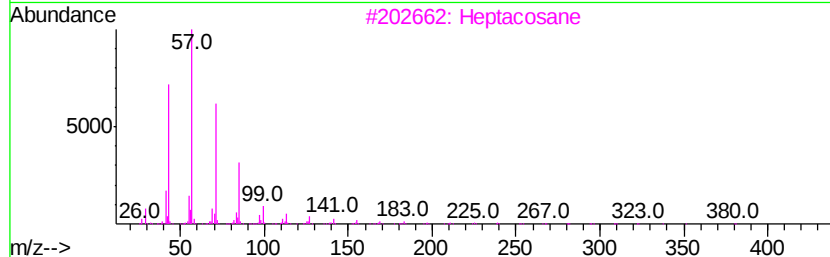
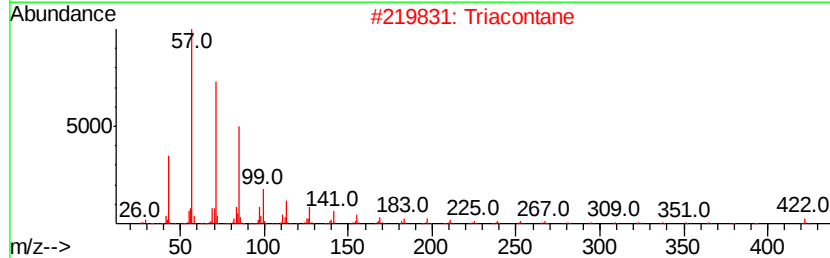
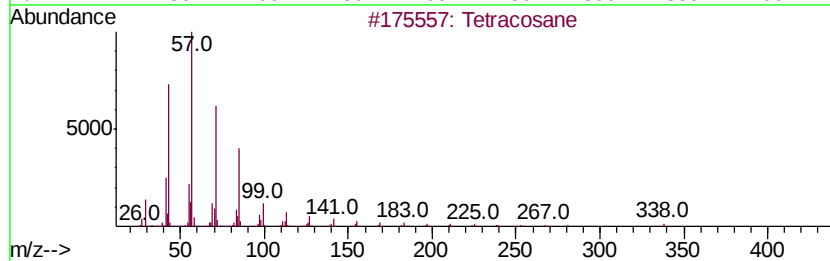
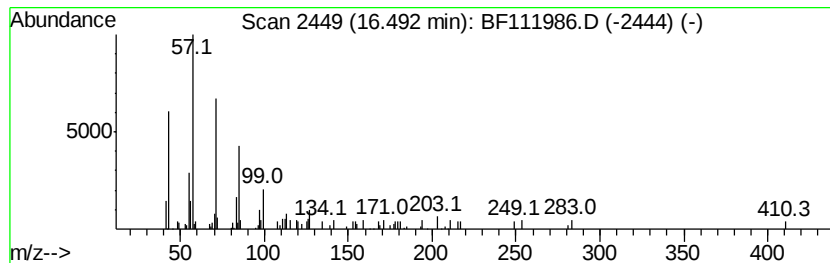
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.08 ng	99732	Perylene-d12	15.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	64
2			Triacontane	422	C30H62	000638-68-6	59
3			Heptacosane	380	C27H56	000593-49-7	59
4			Bacchotricuneatin c	342	C20H22O5	066563-30-2	55
5			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011019\
Data File : BF111986.D
Acq On : 10 Jan 2019 14:44
Operator : JU/SJ
Sample : K1082-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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
2-Pentanone, 4-hy...	5.09	4.3	ng	161183	1	6.87	740719	20.0
unknown6.65	6.65	73.6	ng	2725060	1	6.87	740719	20.0
Sulfurous acid, b...	13.88	3.6	ng	150495	5	14.04	834266	20.0
Octacosane	14.20	2.0	ng	83683	5	14.04	834266	20.0
Hexacosane	14.50	3.1	ng	130286	5	14.04	834266	20.0
Heptacosane	14.81	2.5	ng	122028	6	15.52	960119	20.0
Eicosane	15.15	3.1	ng	148200	6	15.52	960119	20.0
Hexacosane	15.98	2.5	ng	120543	6	15.52	960119	20.0
Tetracosane	16.49	2.1	ng	99732	6	15.52	960119	20.0