

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
 Data File : BF108980.D
 Acq On : 13 Sep 2018 22:25
 Operator : JU/SJ
 Sample : J4875-08
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 091118-DBRI-F-U-B

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-BF090518.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	4.907	434	437	448	rVB	147786	157001	3.50%	0.528%
2	5.331	505	509	513	rBV	1481085	1312698	29.27%	4.414%
3	6.354	679	683	690	rBV	1148318	911953	20.33%	3.067%
4	6.495	702	707	710	rBV	2708221	2311110	51.52%	7.772%
5	6.725	743	746	750	rBV	1000943	843814	18.81%	2.837%
6	6.884	769	773	777	rBV	3271543	3040719	67.79%	10.225%
7	7.290	836	842	845	rBV	2728925	2634400	58.73%	8.859%
8	8.007	960	964	968	rBV	1328829	1054672	23.51%	3.547%
9	9.089	1143	1148	1151	rBV	4901809	4485462	100.00%	15.083%
10	9.478	1210	1214	1217	rBV	452864	345669	7.71%	1.162%
11	9.760	1258	1262	1265	rBV	1344477	1201902	26.80%	4.042%
12	10.436	1374	1377	1381	rVB	85238	68795	1.53%	0.231%
13	10.542	1390	1395	1398	rBV	2203775	1932396	43.08%	6.498%
14	11.236	1509	1513	1516	rBV	1417266	1173538	26.16%	3.946%
15	11.772	1601	1604	1608	rBV	99398	105055	2.34%	0.353%
16	12.824	1778	1783	1786	rBV	4306184	4240321	94.53%	14.259%
17	13.066	1821	1824	1827	rBV	64791	51633	1.15%	0.174%
18	13.407	1879	1882	1885	rBV	88633	72748	1.62%	0.245%
19	13.736	1934	1938	1952	rBV	192365	330501	7.37%	1.111%
20	13.860	1955	1959	1963	rVV	1135029	972222	21.67%	3.269%
21	14.048	1986	1991	1995	rBV	147998	132449	2.95%	0.445%
22	14.354	2039	2043	2047	rBV	165883	140132	3.12%	0.471%
23	14.648	2089	2093	2097	rBV	200450	207618	4.63%	0.698%
24	14.718	2102	2105	2109	rVB	185000	170516	3.80%	0.573%
25	14.966	2143	2147	2151	rBV	173275	188932	4.21%	0.635%
26	15.265	2193	2198	2203	rBV	867655	969630	21.62%	3.261%
27	15.324	2203	2208	2215	rVB	155978	189921	4.23%	0.639%
28	15.730	2272	2277	2282	rBV	131949	179756	4.01%	0.604%
29	16.195	2349	2356	2367	rBV	86983	168074	3.75%	0.565%
30	16.748	2443	2450	2457	rBV2	44266	88012	1.96%	0.296%
31	17.389	2555	2559	2568	rVB5	26974	56450	1.26%	0.190%

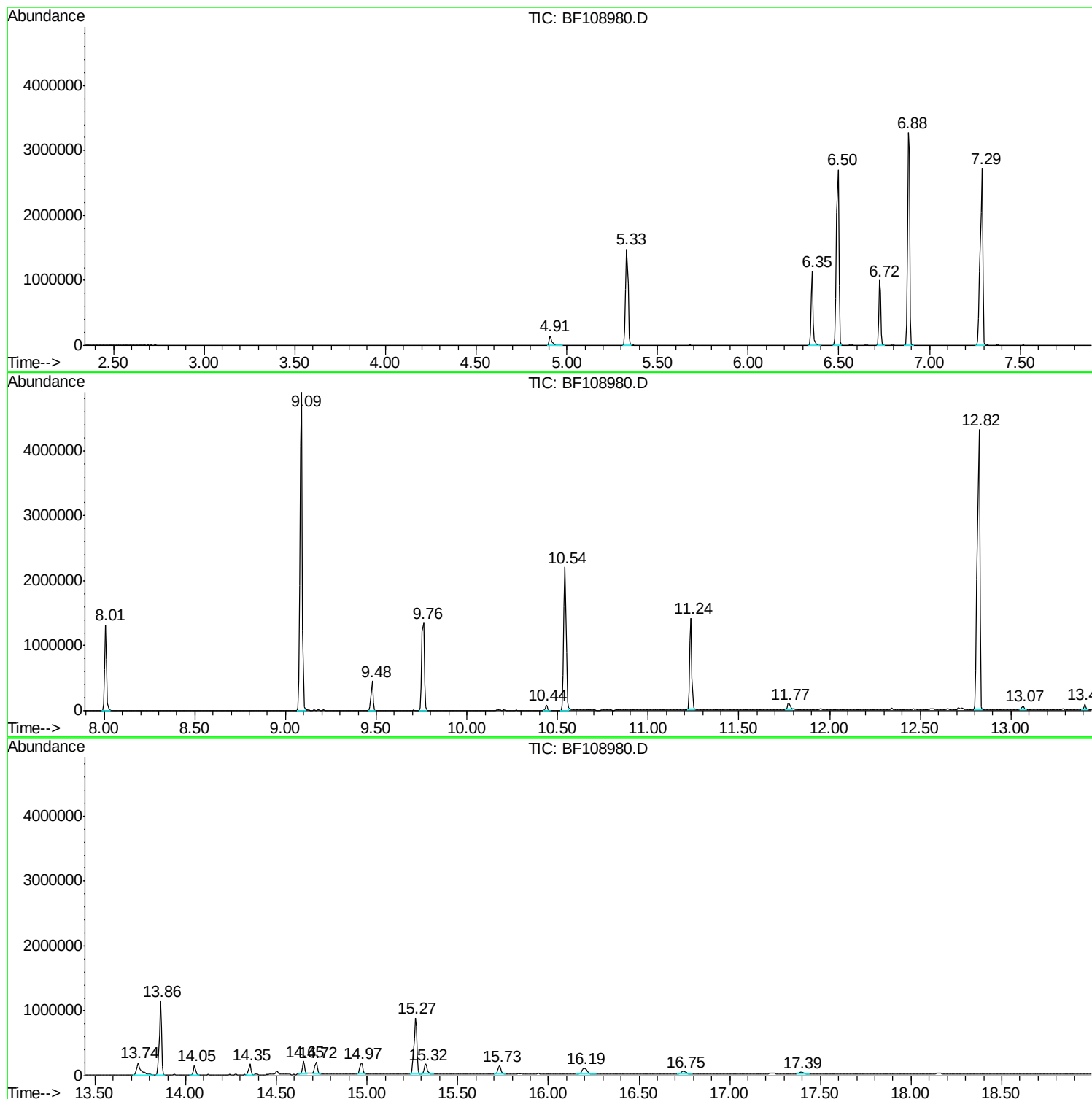
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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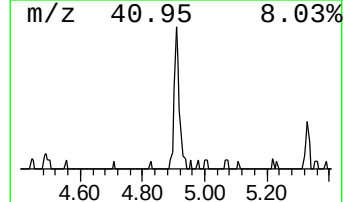
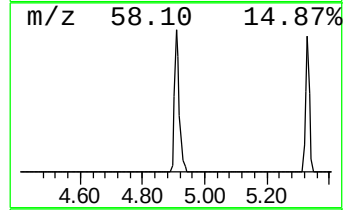
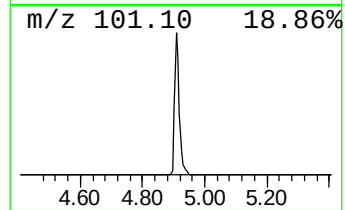
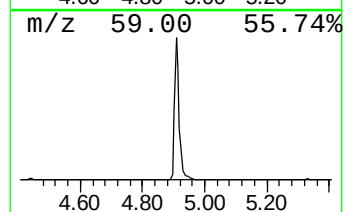
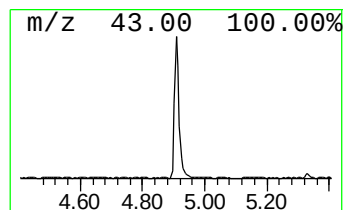
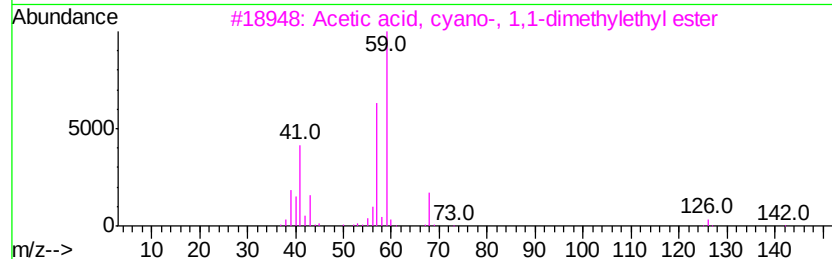
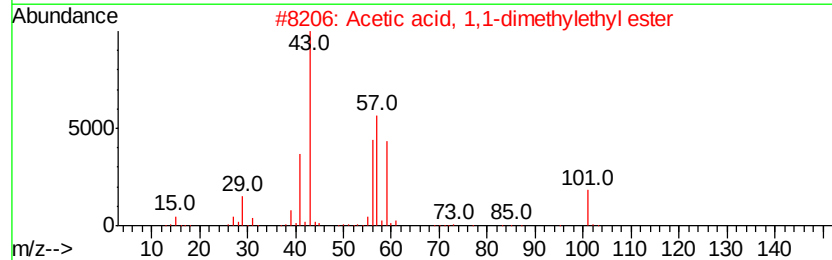
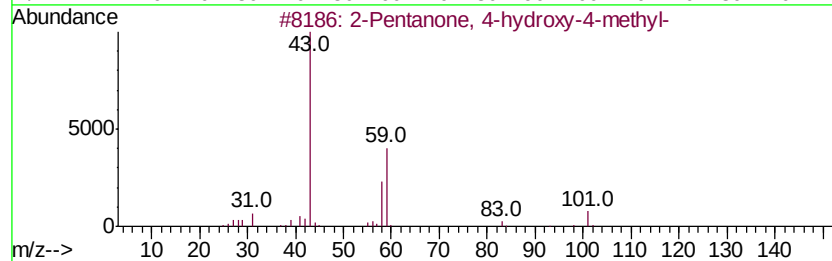
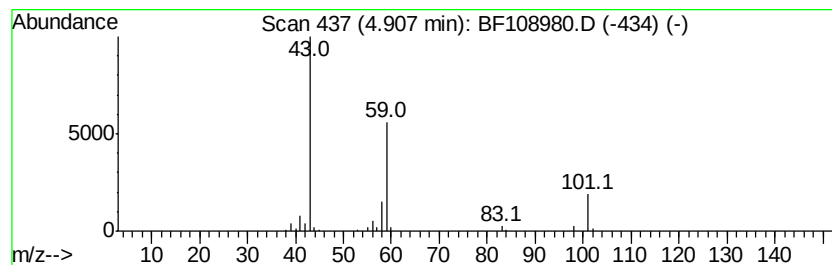
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	3.72 ng	157001	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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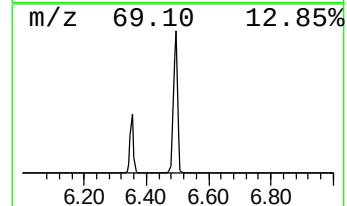
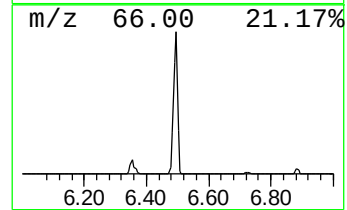
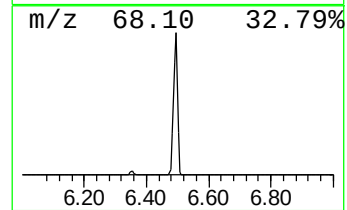
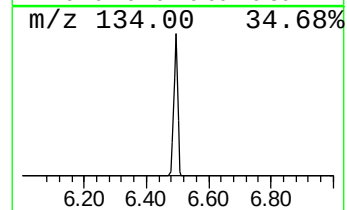
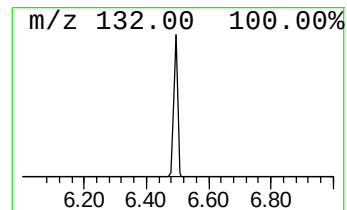
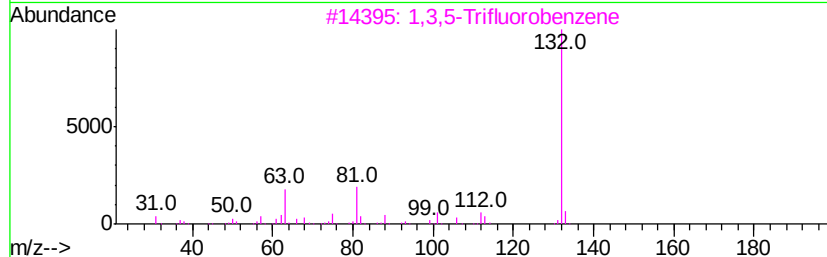
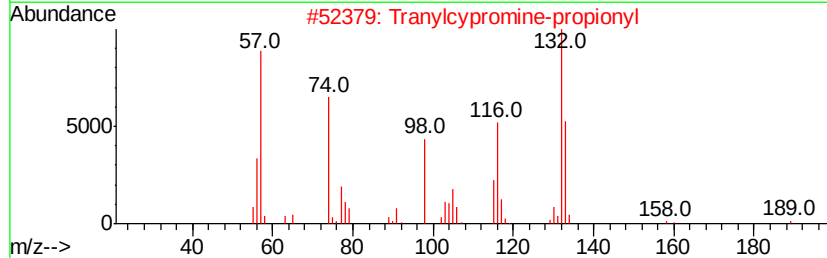
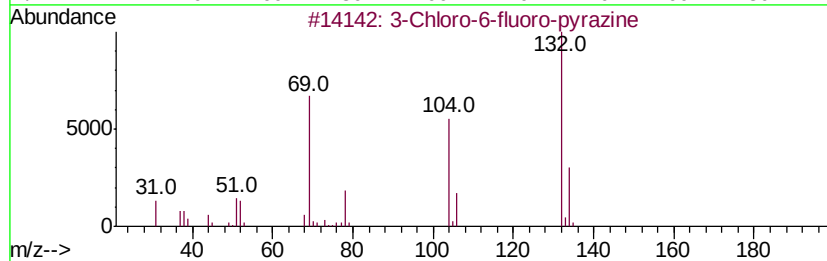
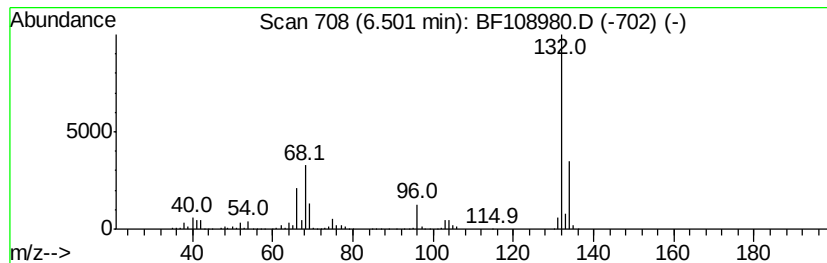
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Peak Number 2 unknown6.50 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	54.78 ng	2311110	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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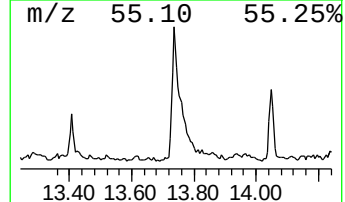
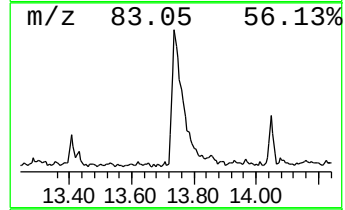
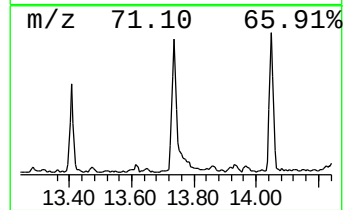
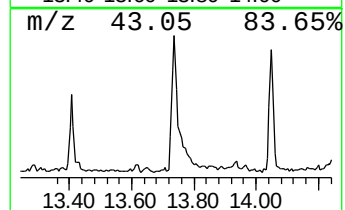
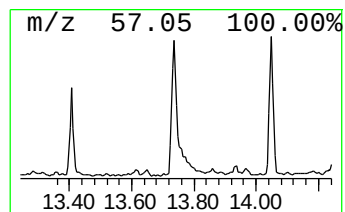
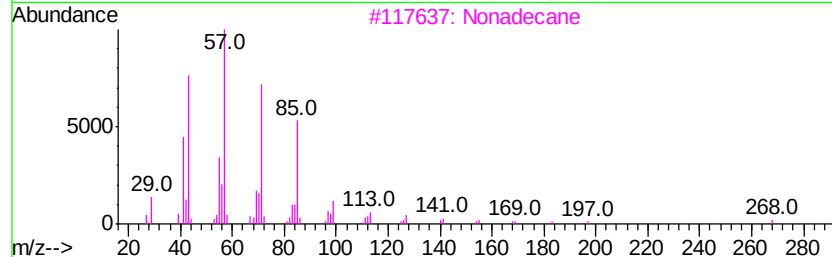
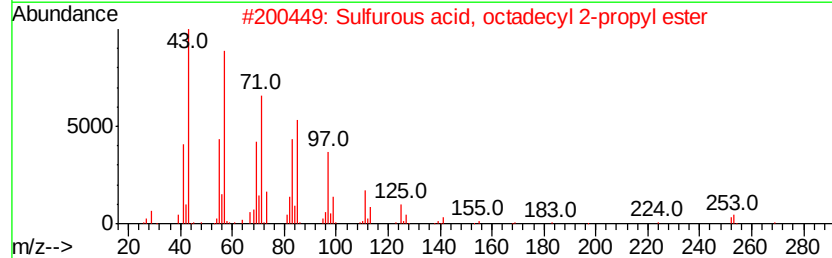
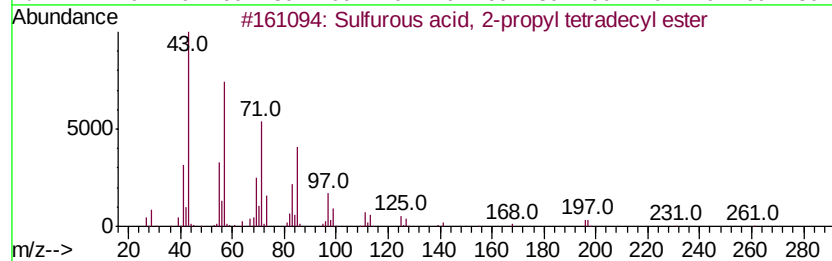
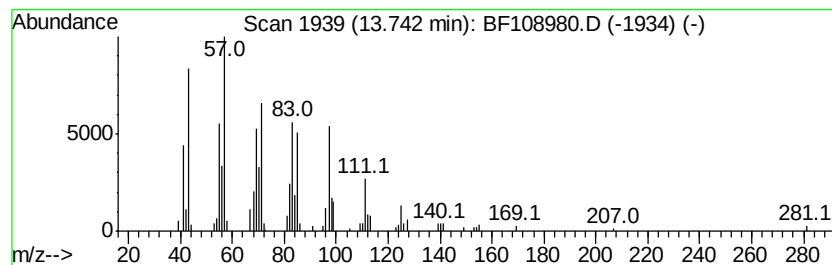
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Peak Number 4 Sulfurous acid, 2-propyl te... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.74	6.80 ng	330501	Chrysene-d12		13.86
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	91
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
3	Nonadecane	268	C19H40	000629-92-5	74
4	Tetradecane	198	C14H30	000629-59-4	62
5	Pentadecane	212	C15H32	000629-62-9	62



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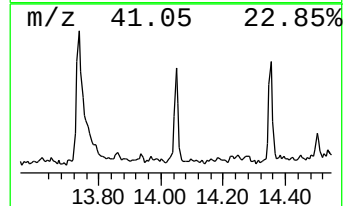
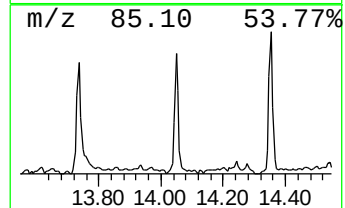
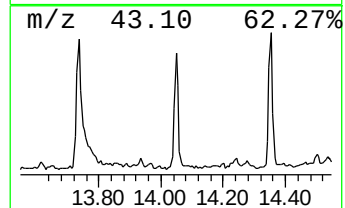
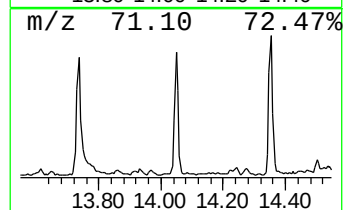
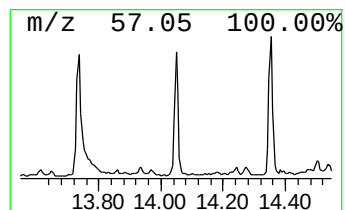
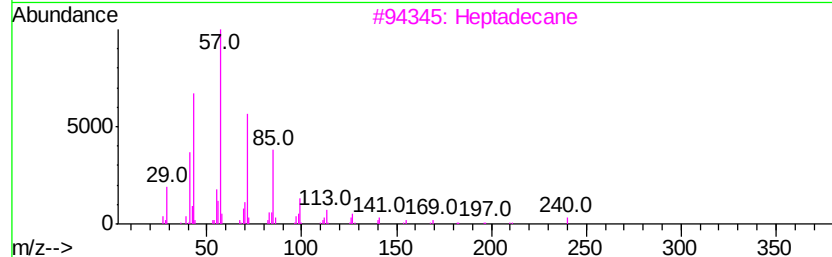
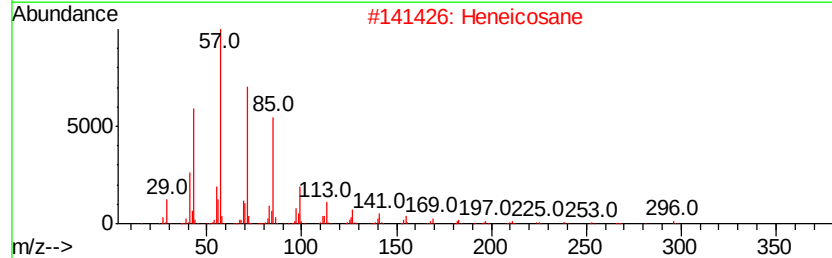
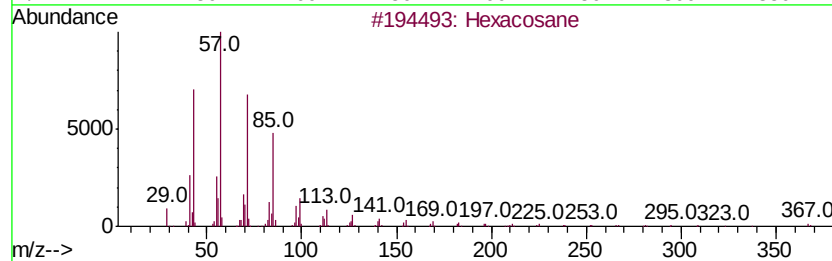
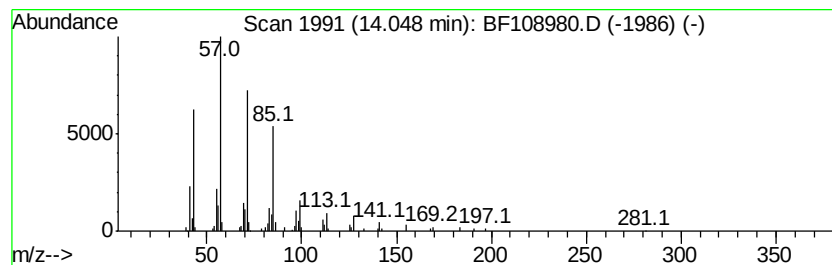
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Peak Number 5 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	2.72 ng	132449	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Heptadecane		240	C17H36	000629-78-7	90
4	Octadecane		254	C18H38	000593-45-3	90
5	2-Bromotetradecane		276	C14H29Br	074036-95-6	86



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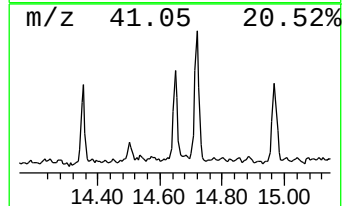
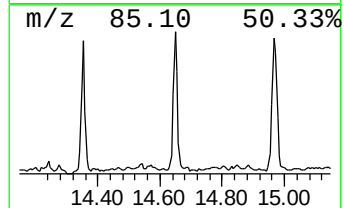
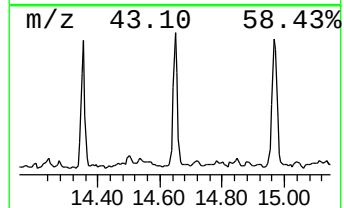
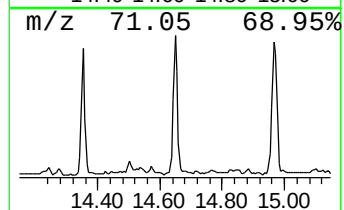
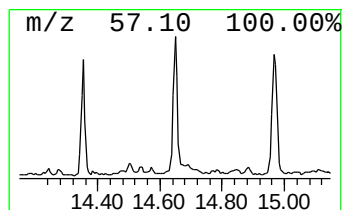
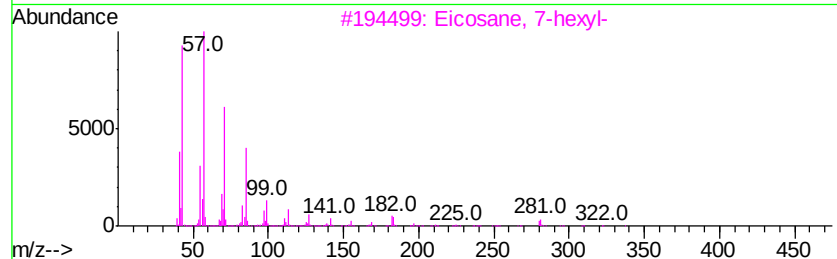
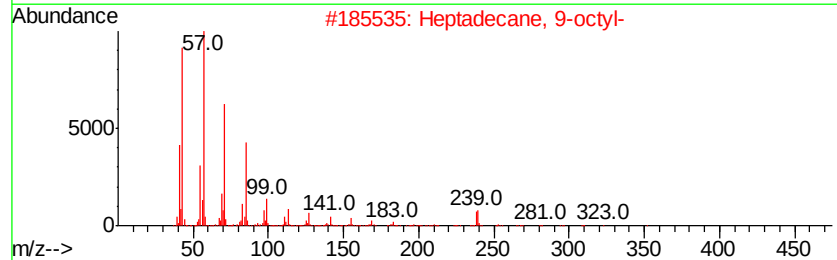
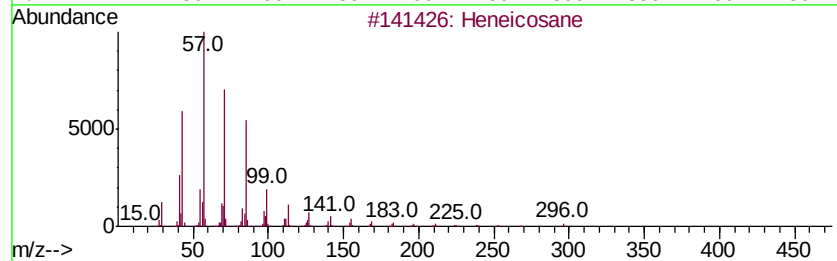
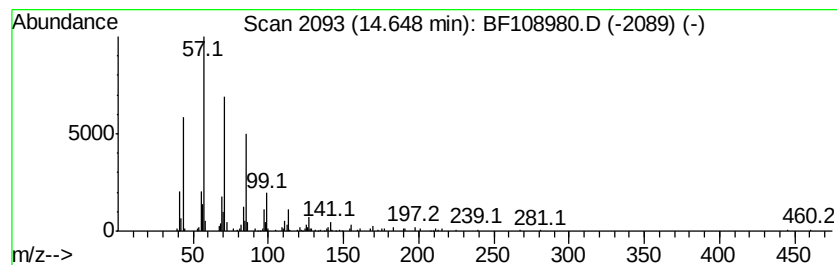
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 Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	4.28 ng	207618	Perylene-d12	15.27

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	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	91
4	Octacosane		394	C28H58	000630-02-4	90
5	Hexacosane		366	C26H54	000630-01-3	90



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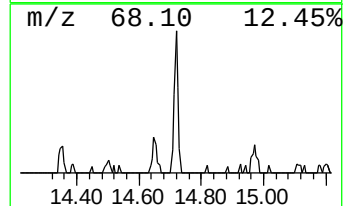
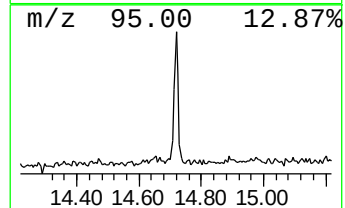
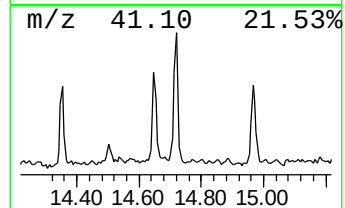
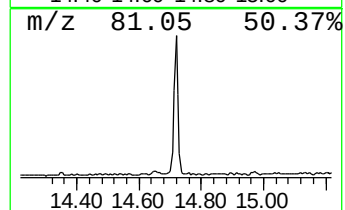
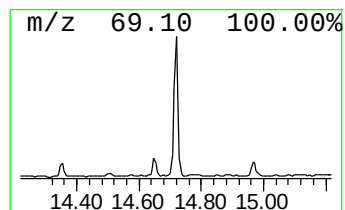
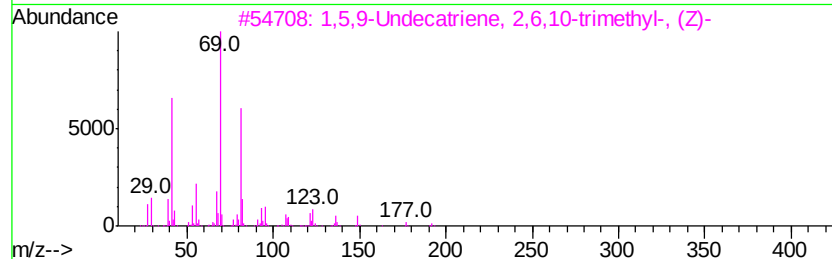
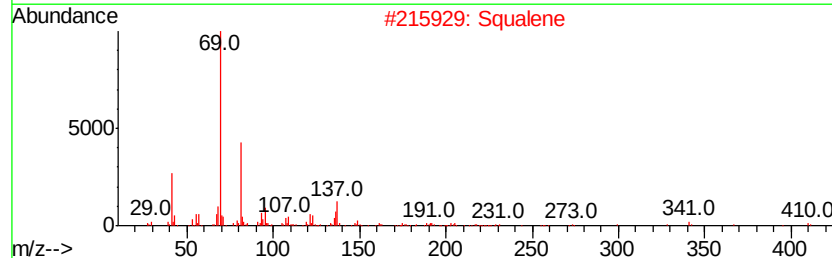
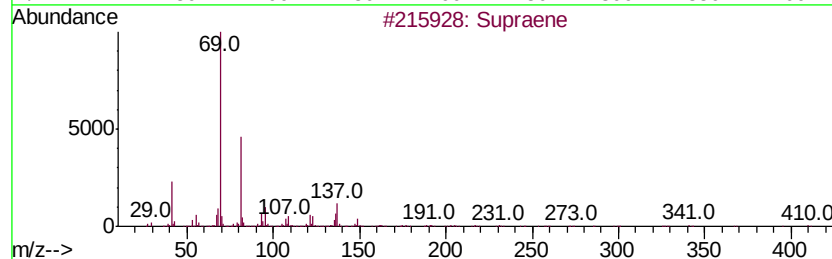
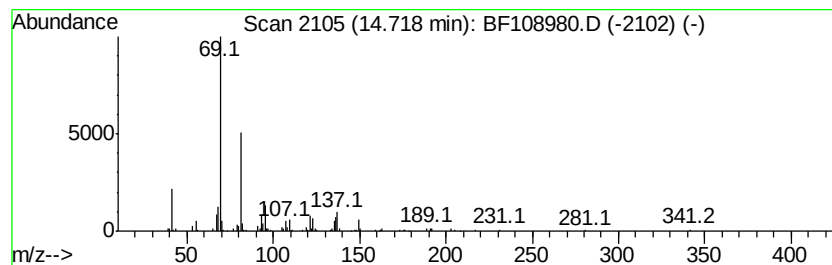
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.52 ng	170516	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	91
2	Squalene		410	C30H50	000111-02-4	90
3	1,5,9-Undecatriene, 2,6,10-trime...		192	C14H24	062951-96-6	87
4	1,6-Octadiene, 3,5-dimethyl-, tr...		138	C10H18	074630-87-8	53
5	1,5,9-Decatriene, 2,3,5,8-tetram...		192	C14H24	230646-72-7	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
Data File : BF108980.D
Acq On : 13 Sep 2018 22:25
Operator : JU/SJ
Sample : J4875-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091118-DBRI-F-U-B

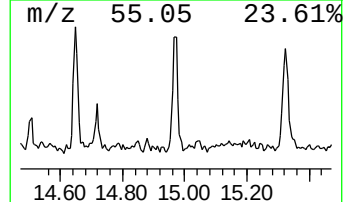
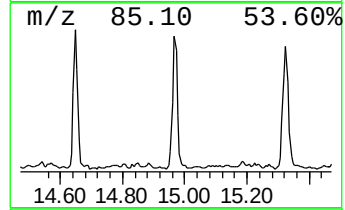
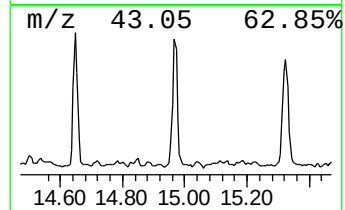
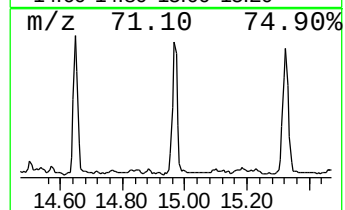
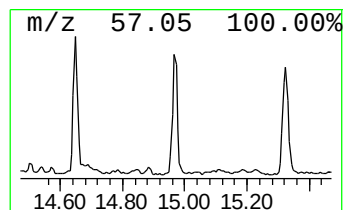
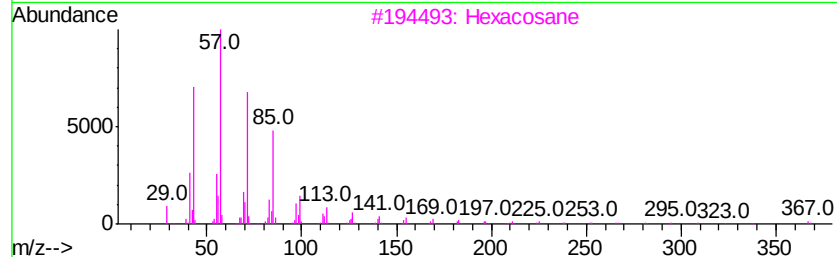
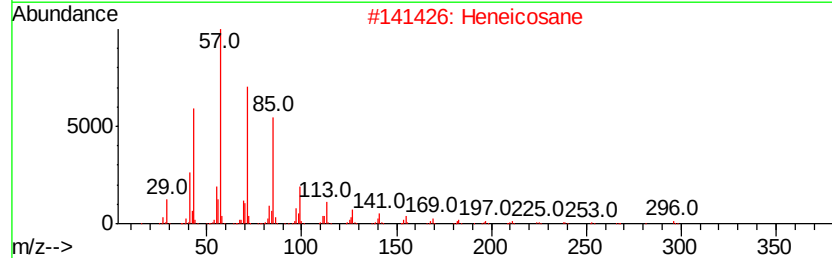
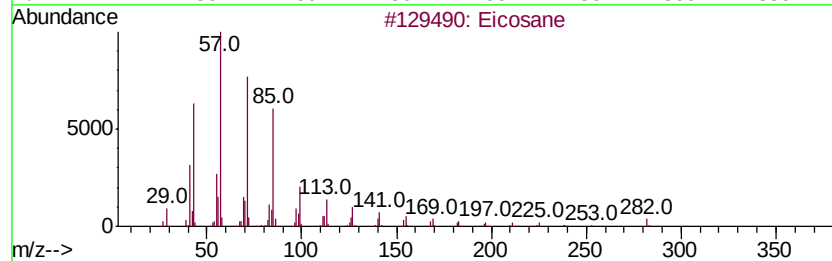
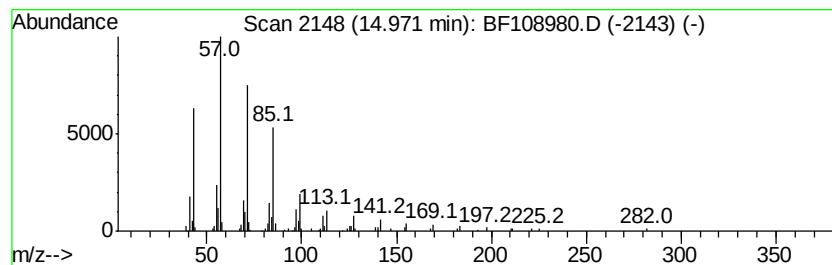
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
14.97	3.90 ng	188932	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	97
2	Heneicosane		296	C21H44	000629-94-7	91
3	Hexacosane		366	C26H54	000630-01-3	91
4	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	90
5	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
Data File : BF108980.D
Acq On : 13 Sep 2018 22:25
Operator : JU/SJ
Sample : J4875-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091118-DBRI-F-U-B

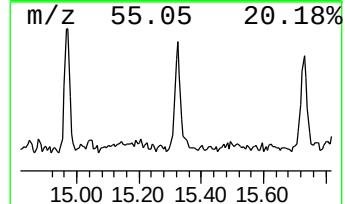
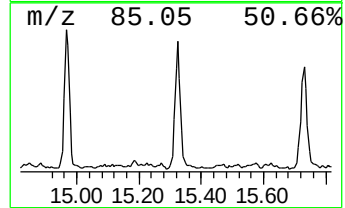
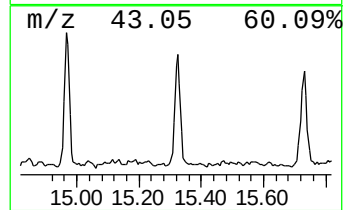
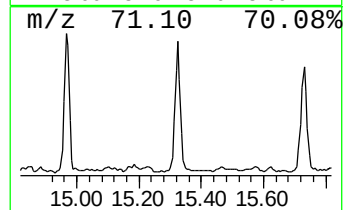
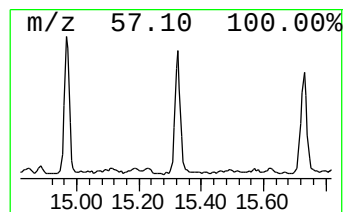
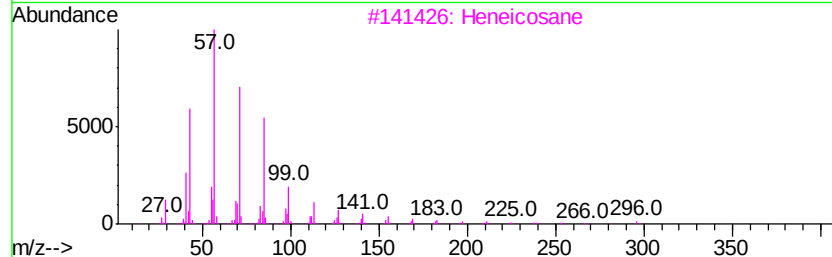
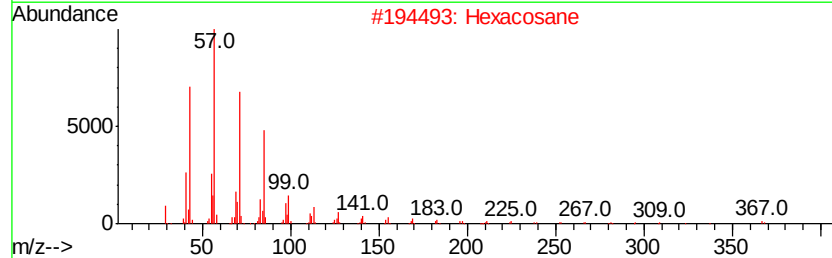
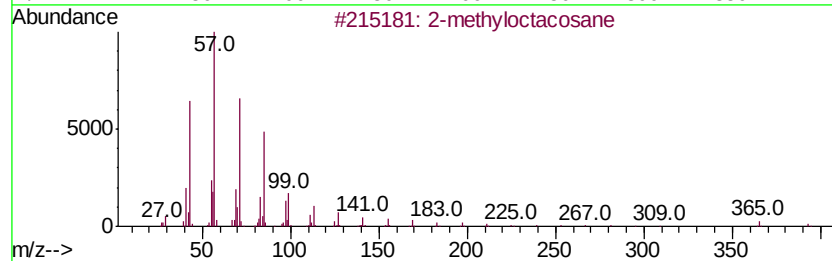
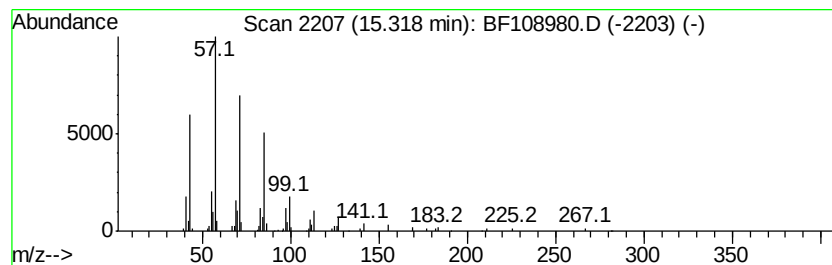
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	3.92 ng	189921	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
5		Octadecane	254	C18H38	000593-45-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
Data File : BF108980.D
Acq On : 13 Sep 2018 22:25
Operator : JU/SJ
Sample : J4875-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
091118-DBRI-F-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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...	4.91	3.7	ng	157001	1	6.72	843814	20.0
unknown6.50	6.50	54.8	ng	2311110	1	6.72	843814	20.0
Sulfurous acid, 2...	13.74	6.8	ng	330501	5	13.86	972222	20.0
Hexacosane	14.05	2.7	ng	132449	5	13.86	972222	20.0
Heneicosane	14.65	4.3	ng	207618	6	15.27	969630	20.0
Supraene	14.72	3.5	ng	170516	6	15.27	969630	20.0
Eicosane	14.97	3.9	ng	188932	6	15.27	969630	20.0
2-methyloctacosane	15.32	3.9	ng	189921	6	15.27	969630	20.0