

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
 Data File : BF108972.D
 Acq On : 13 Sep 2018 18:49
 Operator : JU/SJ
 Sample : J4873-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NF-STONE

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	4.925	434	440	449	rVB	104056	127336	3.70%	0.424%
2	5.342	505	511	514	rBV	2723179	2887557	83.91%	9.606%
3	6.360	679	684	687	rBV	2769633	2970783	86.33%	9.883%
4	6.495	703	707	711	rBV	3022278	3014914	87.61%	10.029%
5	6.560	716	718	730	rVB	29889	35609	1.03%	0.118%
6	6.731	743	747	750	rBV	1010689	870936	25.31%	2.897%
7	6.883	769	773	777	rBV	2688614	2428892	70.58%	8.080%
8	7.289	837	842	845	rBV	2007496	1912582	55.58%	6.362%
9	8.007	960	964	968	rBV	1282627	1072847	31.18%	3.569%
10	9.089	1143	1148	1151	rBV	3509644	3441304	100.00%	11.448%
11	9.477	1210	1214	1217	rBV	809767	603967	17.55%	2.009%
12	9.760	1258	1262	1265	rBV	1361025	1144591	33.26%	3.808%
13	10.171	1329	1332	1336	rBV	32391	34596	1.01%	0.115%
14	10.542	1391	1395	1398	rBV	2137525	1855360	53.91%	6.172%
15	11.236	1509	1513	1516	rBV	1240268	1034941	30.07%	3.443%
16	11.777	1601	1605	1609	rBV	184088	173640	5.05%	0.578%
17	12.560	1735	1738	1741	rBV3	35654	36049	1.05%	0.120%
18	12.818	1778	1782	1786	rBV	2922406	2665836	77.47%	8.868%
19	13.742	1934	1939	1954	rBV	188071	447318	13.00%	1.488%
20	13.859	1955	1959	1963	rBV	1060153	954458	27.74%	3.175%
21	14.048	1988	1991	1994	rVB	43444	40938	1.19%	0.136%
22	14.354	2040	2043	2046	rBV	82563	73000	2.12%	0.243%
23	14.648	2090	2093	2097	rBV	108953	102553	2.98%	0.341%
24	14.718	2102	2105	2108	rVB	81097	72049	2.09%	0.240%
25	14.965	2143	2147	2152	rVB	141637	157548	4.58%	0.524%
26	15.271	2193	2199	2203	rBV	878960	1055143	30.66%	3.510%
27	15.324	2203	2208	2217	rVB	182784	233557	6.79%	0.777%
28	15.730	2272	2277	2284	rBV	180481	270391	7.86%	0.899%
29	15.806	2286	2290	2293	rBV6	27359	50235	1.46%	0.167%
30	16.201	2352	2357	2369	rVB2	108186	205796	5.98%	0.685%
31	16.753	2445	2451	2456	rVB2	44786	86303	2.51%	0.287%

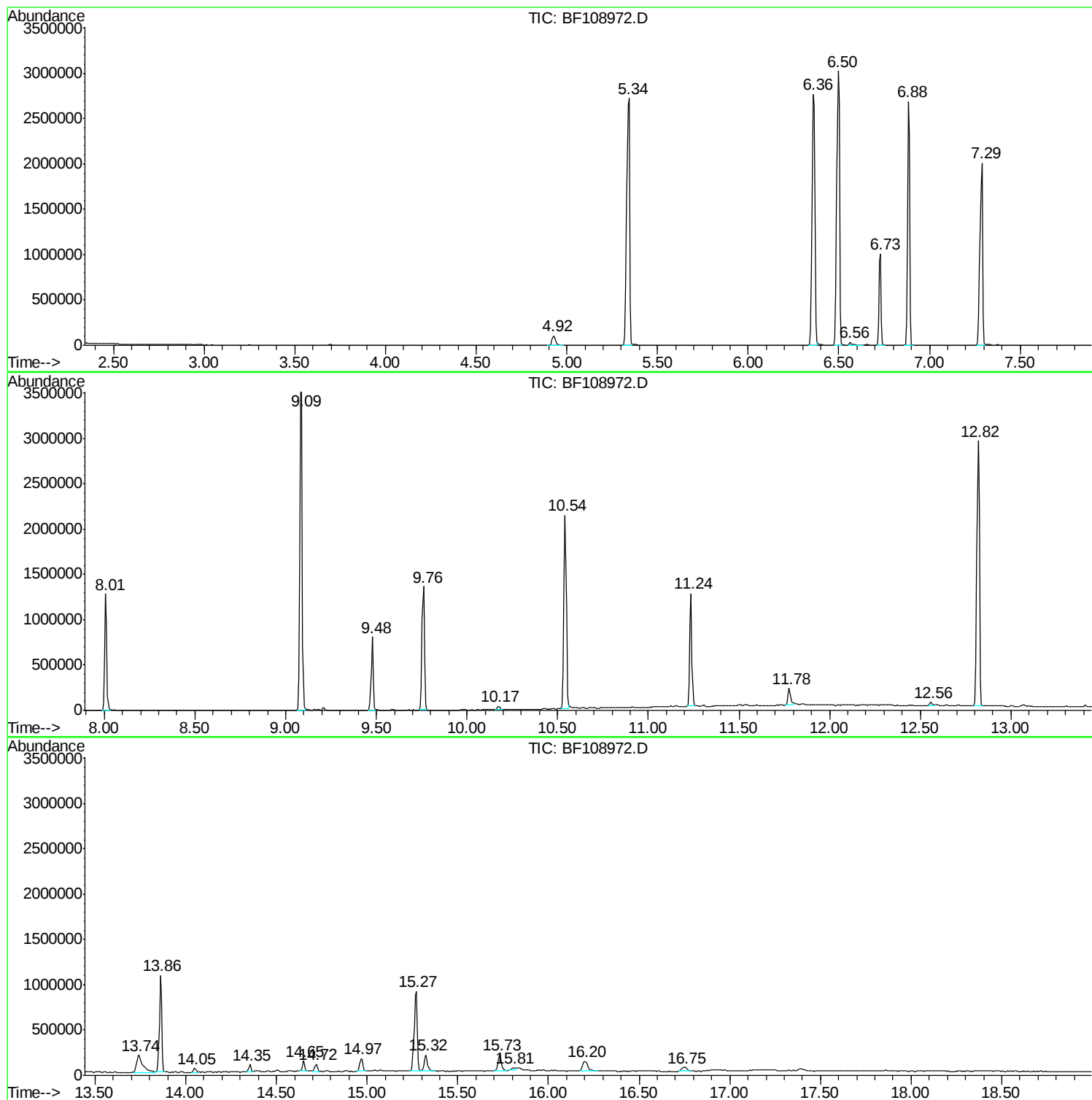
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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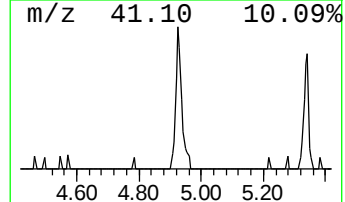
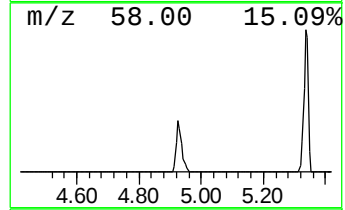
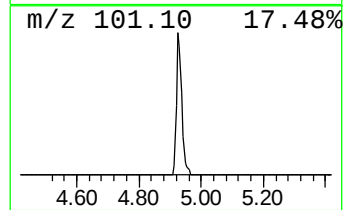
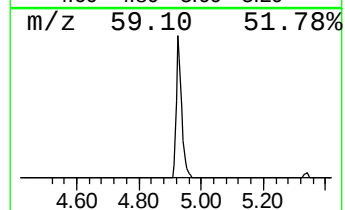
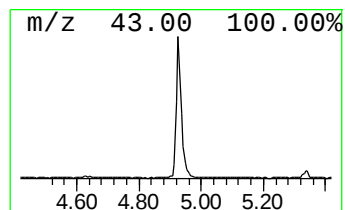
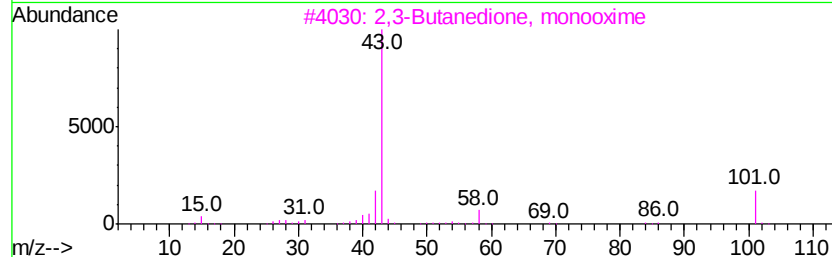
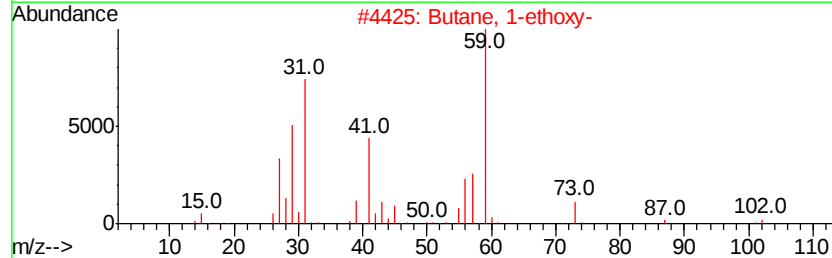
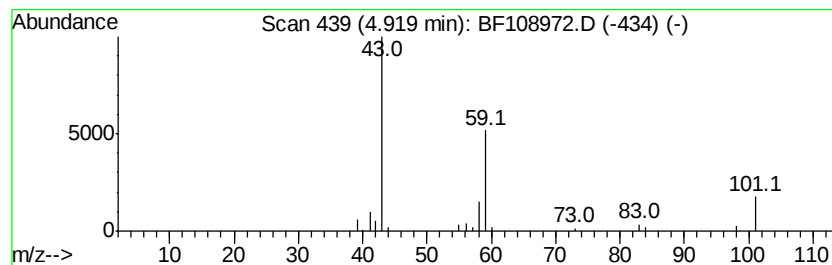
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.92 ng	127336	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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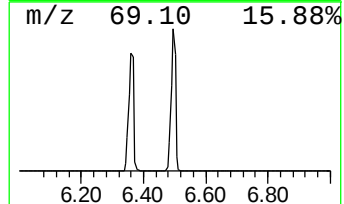
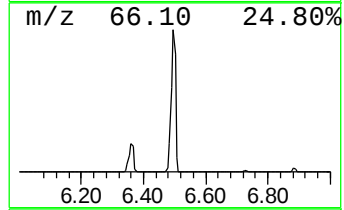
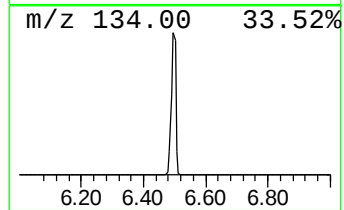
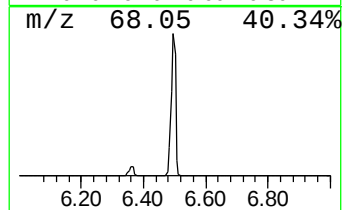
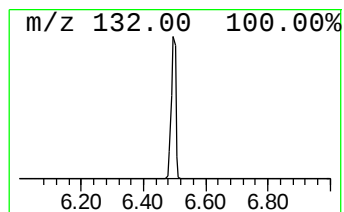
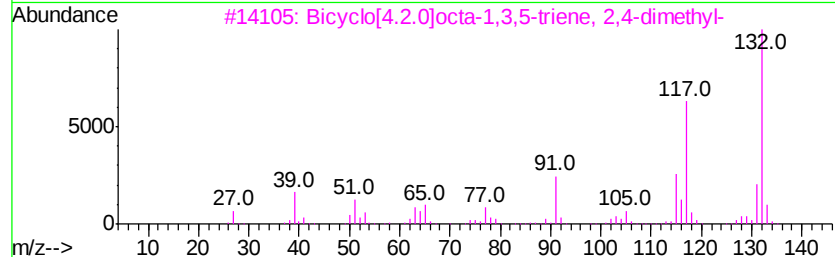
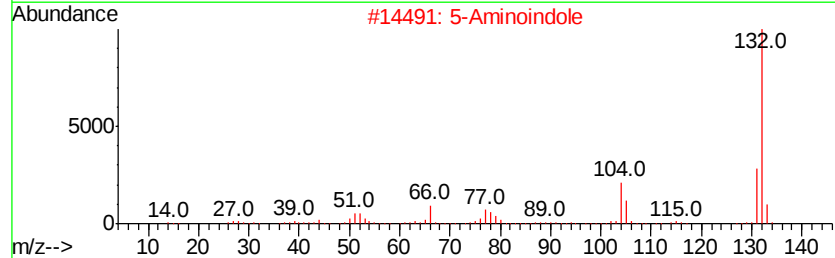
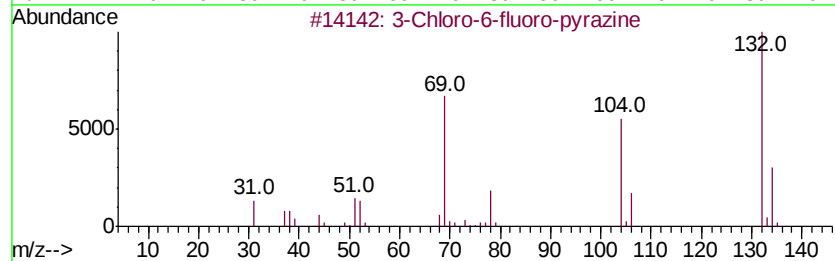
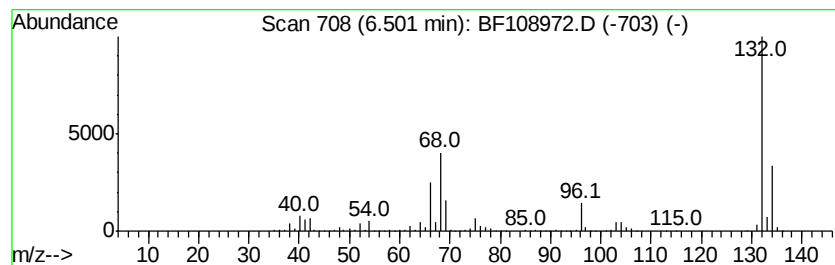
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	69.23 ng	3014910	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	25
2		5-Aminoindole	132	C8H8N2	005192-03-0	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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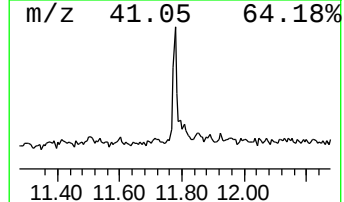
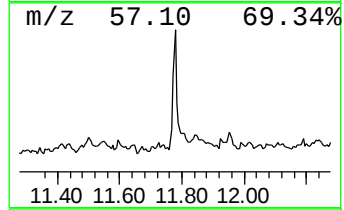
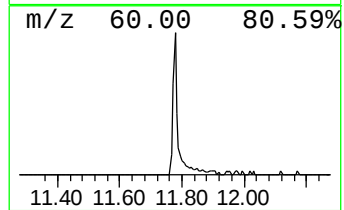
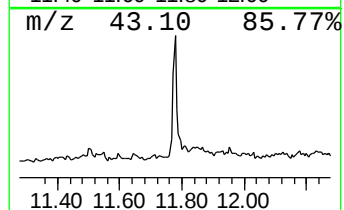
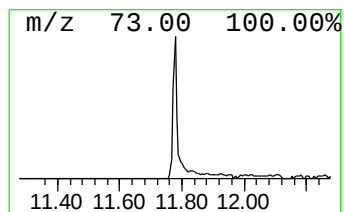
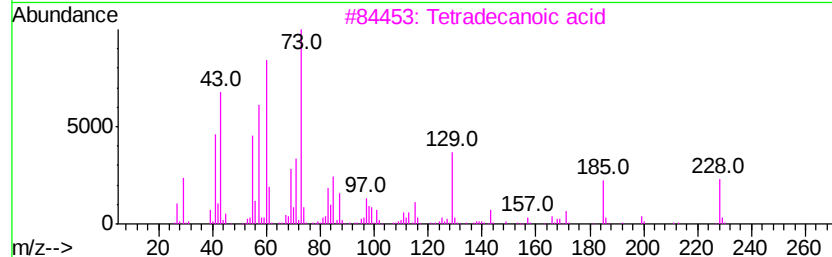
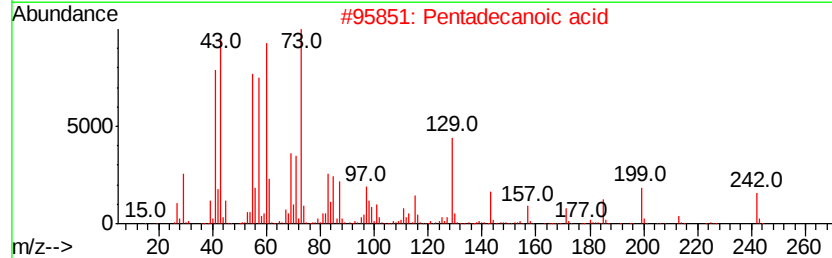
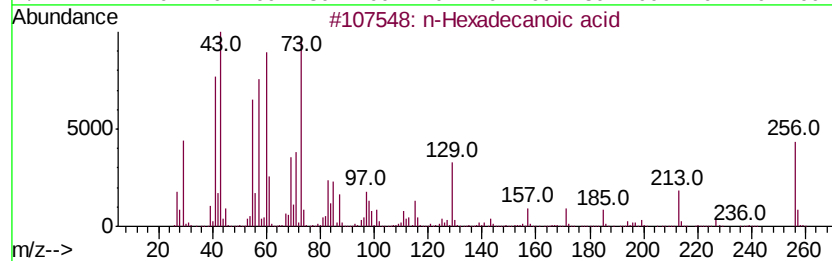
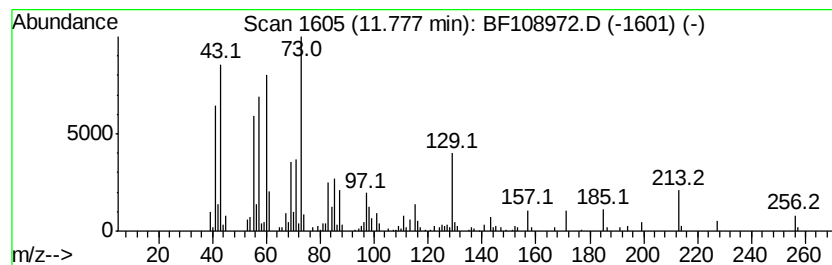
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	3.36 ng	173640	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53



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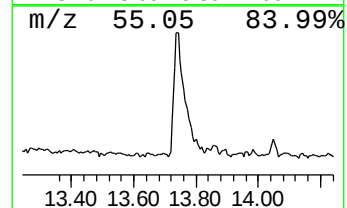
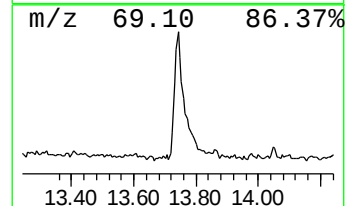
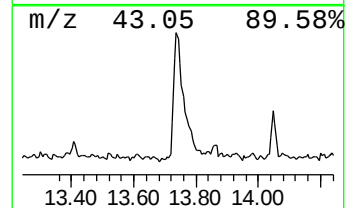
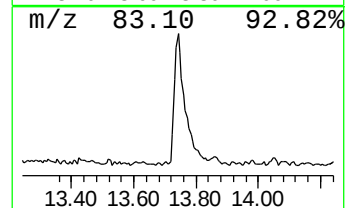
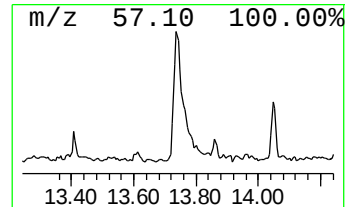
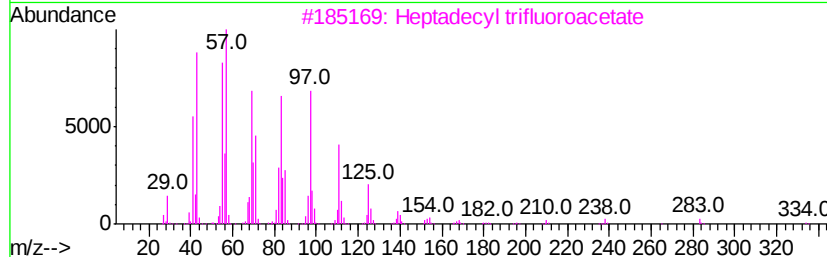
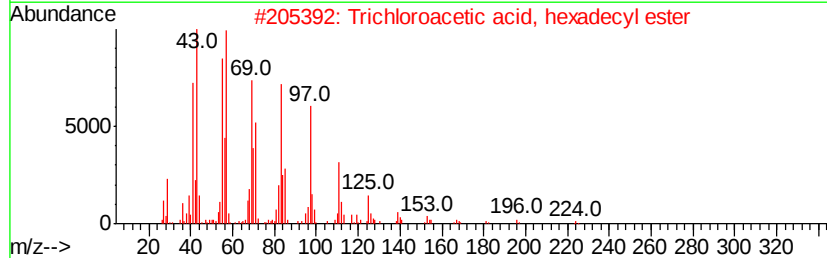
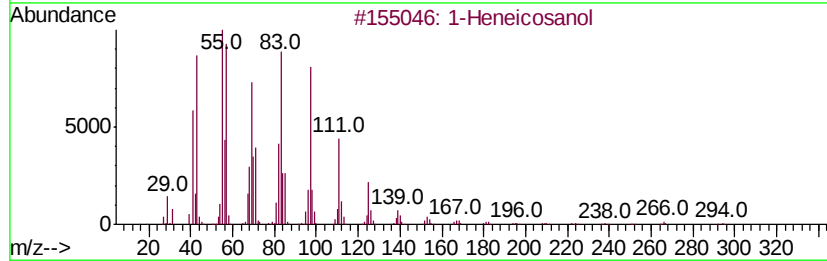
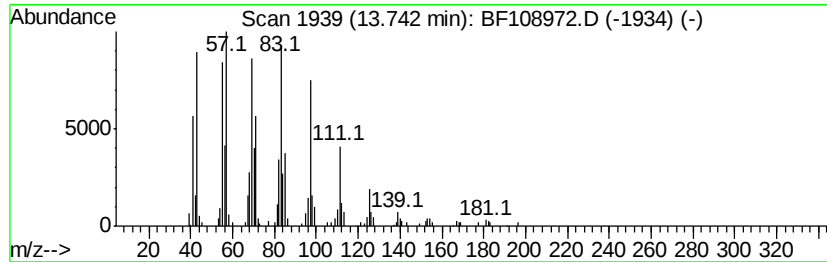
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Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	9.37 ng	447318	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	92
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



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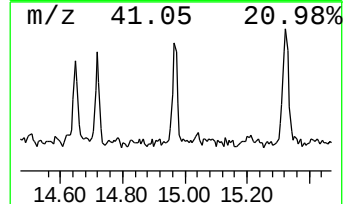
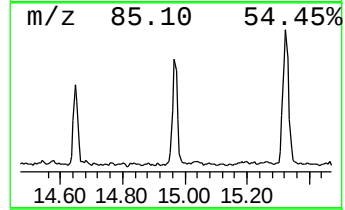
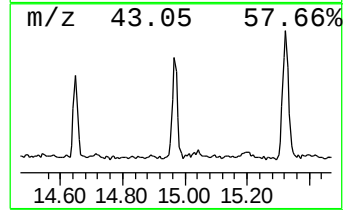
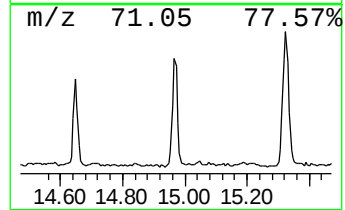
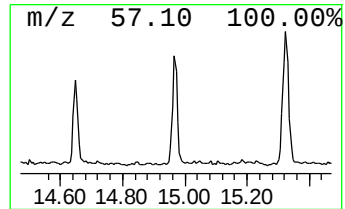
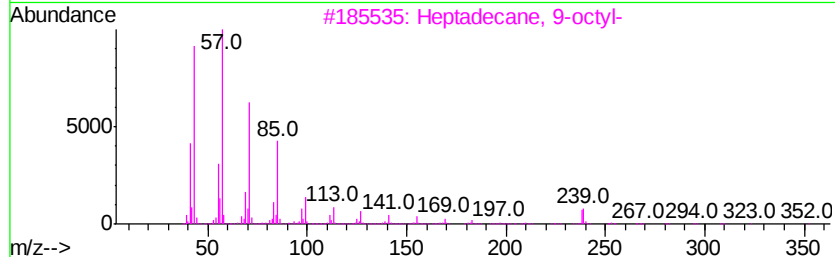
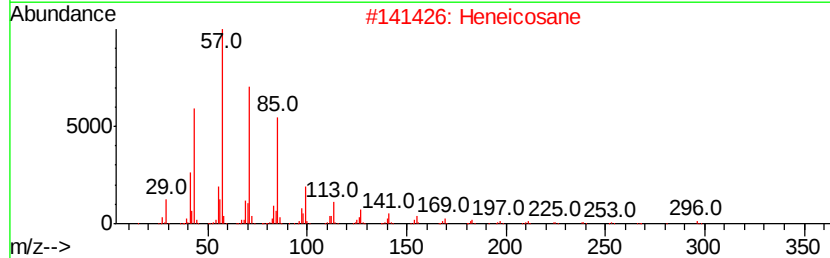
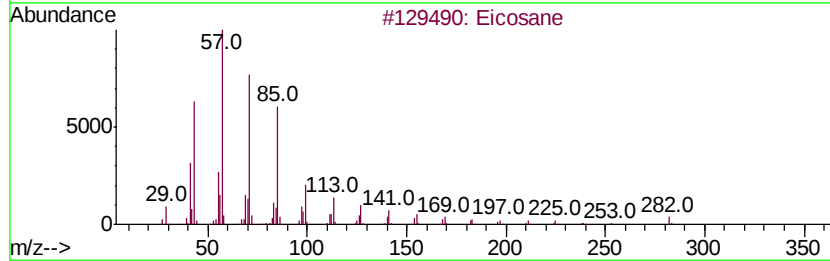
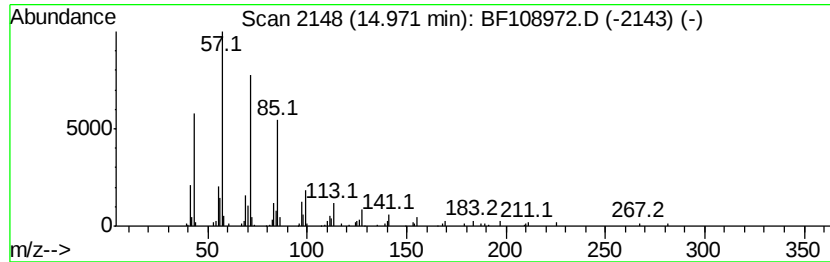
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Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.99 ng	157548	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	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Eicosane, 7-hexyl-		366	C26H54	055333-99-8	90
5	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	90



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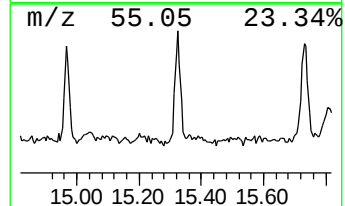
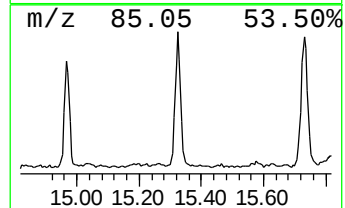
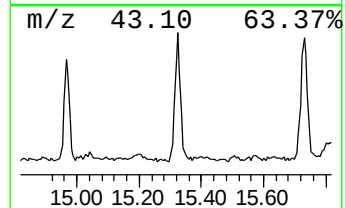
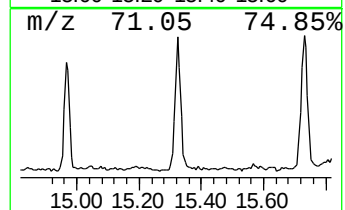
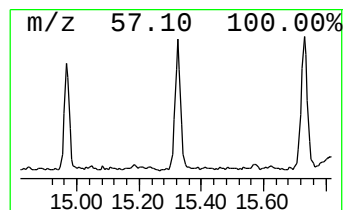
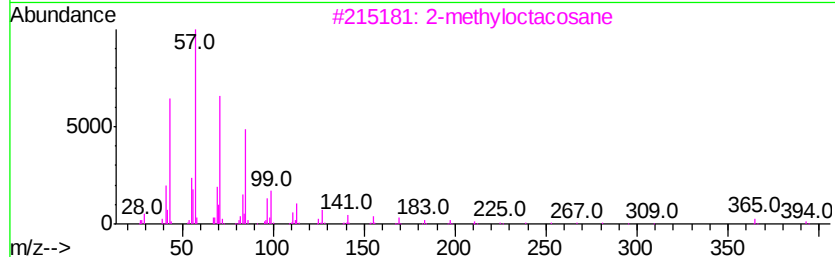
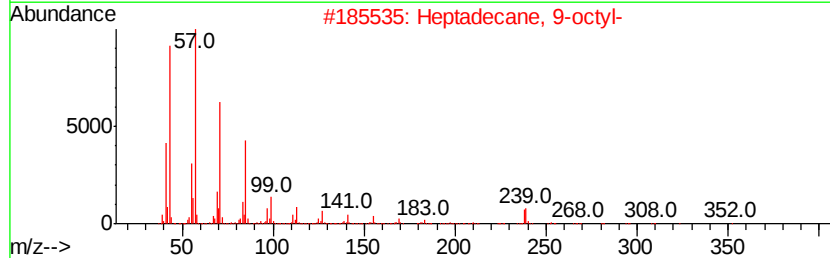
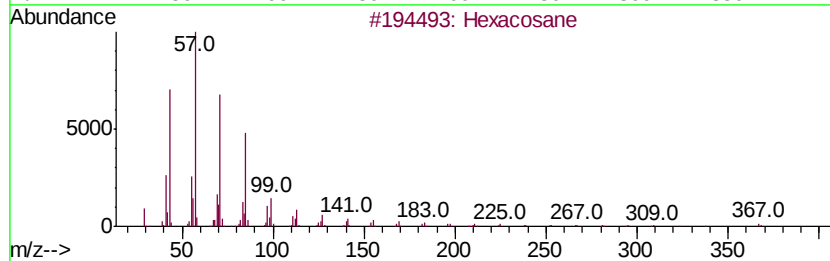
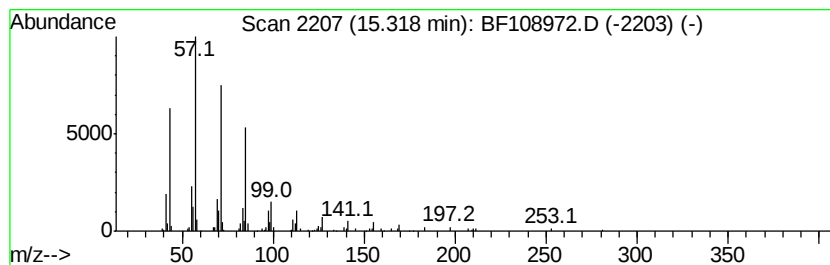
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	4.43 ng	233557	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	93
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Octacosane		394	C28H58	000630-02-4	91
5	triacontane		422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091318\
Data File : BF108972.D
Acq On : 13 Sep 2018 18:49
Operator : JU/SJ
Sample : J4873-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NF-STONE

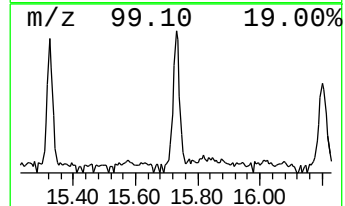
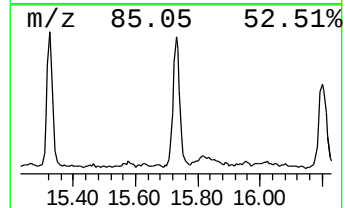
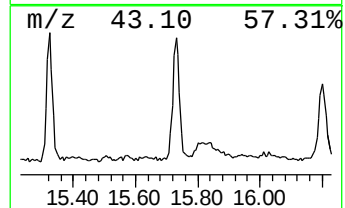
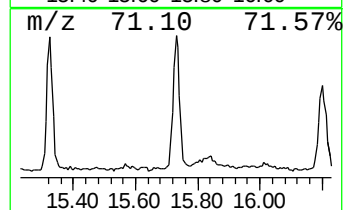
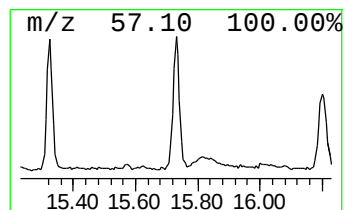
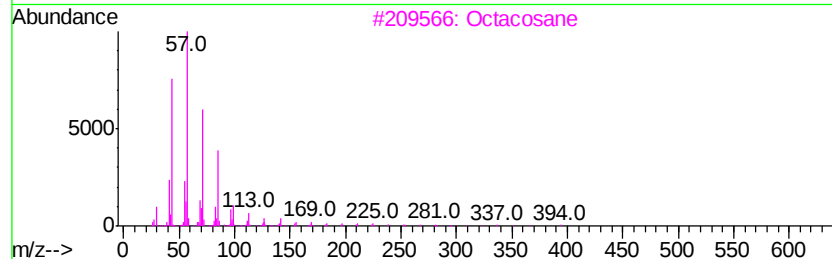
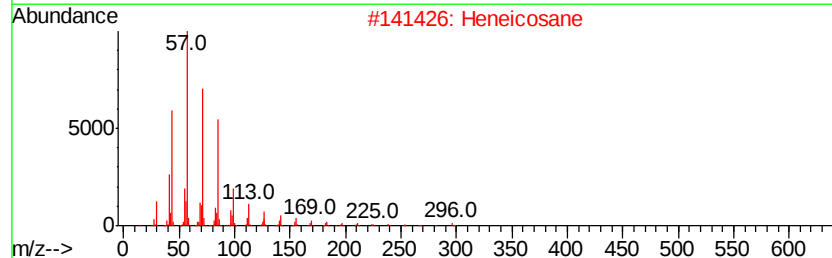
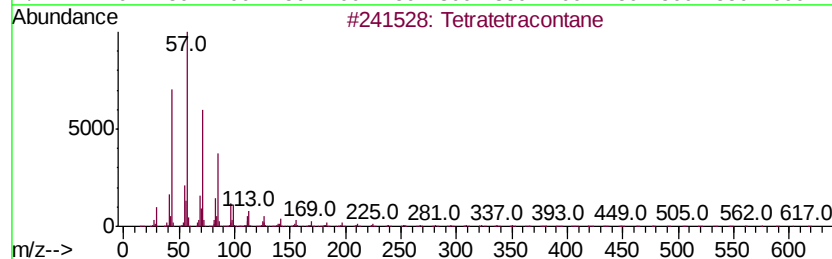
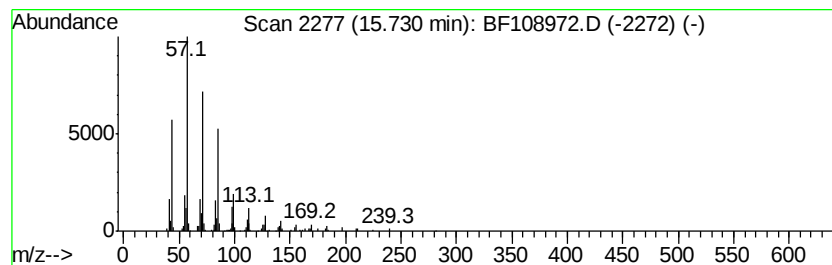
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetratetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	5.13 ng	270391	Perylene-d12	15.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Docosane	310	C22H46	000629-97-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091318\
Data File : BF108972.D
Acq On : 13 Sep 2018 18:49
Operator : JU/SJ
Sample : J4873-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NF-STONE

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...	4.92	2.9	ng	127336	1	6.73	870936	20.0
unknown6.50	6.50	69.2	ng	3014910	1	6.73	870936	20.0
n-Hexadecanoic acid	11.78	3.4	ng	173640	4	11.24	1034940	20.0
1-Heneicosanol	13.74	9.4	ng	447318	5	13.86	954458	20.0
Eicosane	14.97	3.0	ng	157548	6	15.27	1055140	20.0
Hexacosane	15.32	4.4	ng	233557	6	15.27	1055140	20.0
Tetratetracontane	15.73	5.1	ng	270391	6	15.27	1055140	20.0