

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
 Data File : BF097796.D
 Acq On : 17 Aug 2017 19:58
 Operator : SJ/JU
 Sample : I4817-01 5X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-03-081517

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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	4.957	484	488	495	rVB	84723	87014	8.18%	0.719%
2	5.369	554	558	562	rBV	827258	741854	69.72%	6.130%
3	6.392	728	732	736	rBV	873769	742283	69.76%	6.134%
4	6.539	753	757	760	rBV	836651	747534	70.25%	6.177%
5	6.775	793	797	800	rBV	1029140	797580	74.96%	6.591%
6	6.928	819	823	827	rBV	681857	545957	51.31%	4.511%
7	7.334	888	892	895	rBV	499236	420350	39.50%	3.474%
8	7.416	902	906	911	rVB	12753	13156	1.24%	0.109%
9	8.057	1010	1015	1018	rBV	1218303	976571	91.78%	8.070%
10	8.657	1114	1117	1120	rBV	25137	20811	1.96%	0.172%
11	9.133	1194	1198	1201	rBV	778609	629608	59.17%	5.203%
12	9.222	1210	1213	1217	rBV	36213	32602	3.06%	0.269%
13	9.528	1262	1265	1269	rBV	108121	95341	8.96%	0.788%
14	9.751	1300	1303	1307	rVB	39938	33412	3.14%	0.276%
15	9.810	1309	1313	1317	rVB	1006831	826626	77.69%	6.831%
16	10.245	1384	1387	1390	rVB	39336	34814	3.27%	0.288%
17	10.469	1421	1425	1428	rBV	20237	20427	1.92%	0.169%
18	10.592	1442	1446	1451	rBV	360570	297025	27.91%	2.454%
19	10.722	1465	1468	1476	rVB	47754	60101	5.65%	0.497%
20	11.169	1541	1544	1547	rBV	41170	32830	3.09%	0.271%
21	11.198	1547	1549	1555	rVB	19156	17597	1.65%	0.145%
22	11.292	1561	1565	1568	rBV	870894	691247	64.96%	5.712%
23	11.598	1614	1617	1619	rBV	33702	27147	2.55%	0.224%
24	11.698	1630	1634	1637	rBV	360693	314128	29.52%	2.596%
25	11.898	1665	1668	1672	rBV6	10107	18764	1.76%	0.155%
26	12.004	1682	1686	1689	rBV	25644	21740	2.04%	0.180%
27	12.380	1746	1750	1752	rBV	1271081	1064048	100.00%	8.793%
28	12.404	1752	1754	1757	rVB	819462	639983	60.15%	5.288%
29	12.486	1765	1768	1773	rVB2	145003	138207	12.99%	1.142%
30	12.727	1806	1809	1812	rBV2	36259	36645	3.44%	0.303%
31	12.763	1813	1815	1818	rVB	27026	22722	2.14%	0.188%
32	12.874	1831	1834	1838	rBV	543818	475830	44.72%	3.932%
33	13.063	1861	1866	1868	rBV6	27567	41776	3.93%	0.345%
34	13.121	1874	1876	1880	rVB4	30226	31430	2.95%	0.260%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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35	13.210	1889	1891	1893	rBV3	17838	13893	1.31%	0.115%
36	13.274	1900	1902	1904	rBV3	19494	21259	2.00%	0.176%
37	13.321	1908	1910	1915	rVV5	28600	29605	2.78%	0.245%
38	13.463	1932	1934	1938	rVB2	26818	24675	2.32%	0.204%
39	13.927	2009	2013	2016	rBV	807369	761053	71.52%	6.289%
40	15.357	2252	2256	2260	rVB	482858	553899	52.06%	4.577%

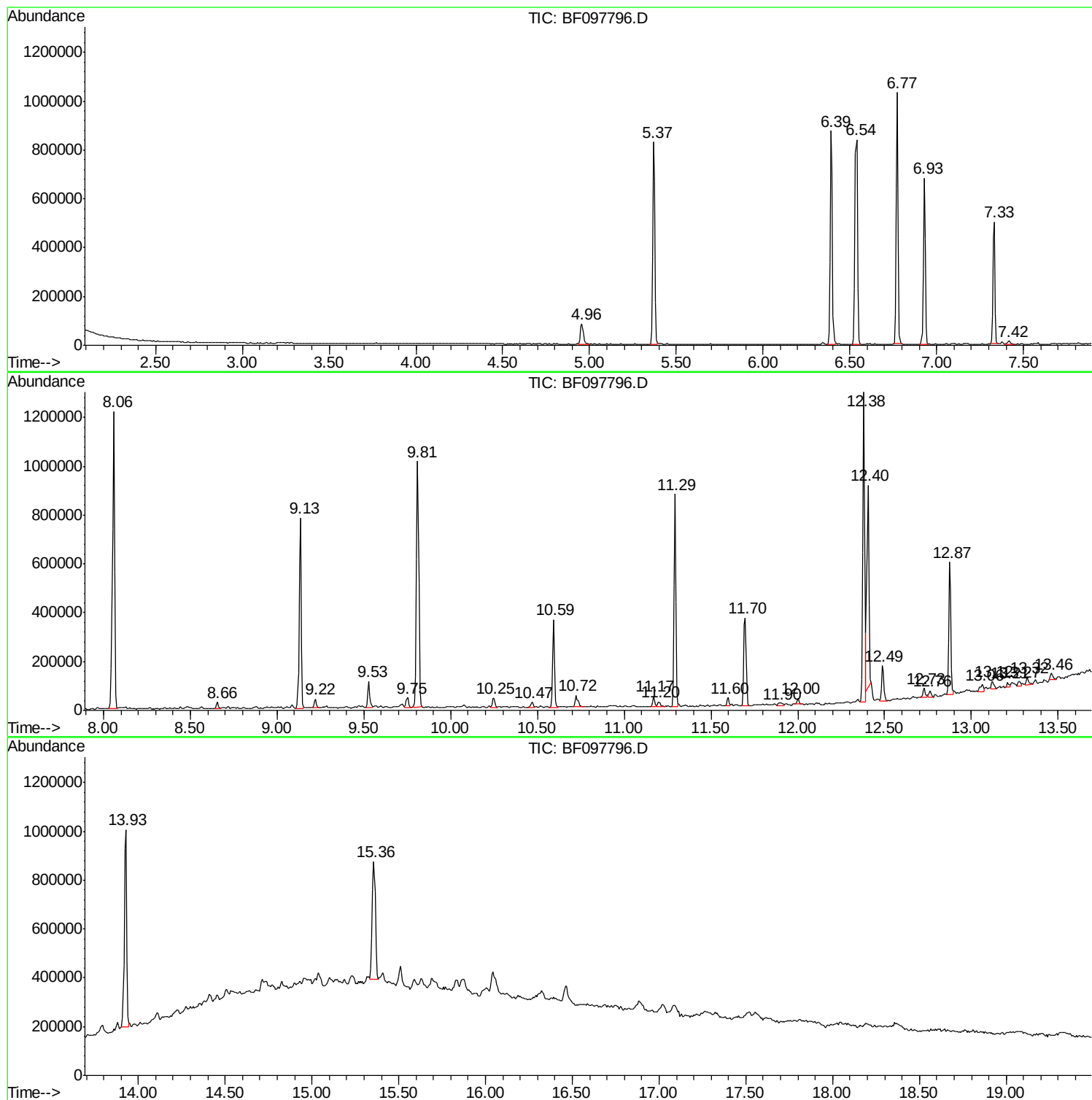
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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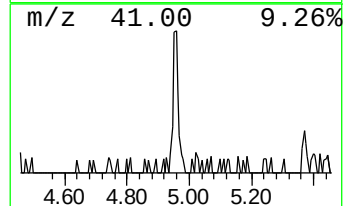
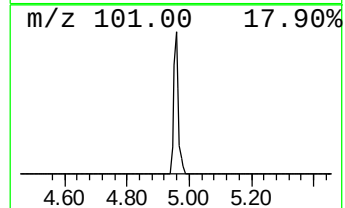
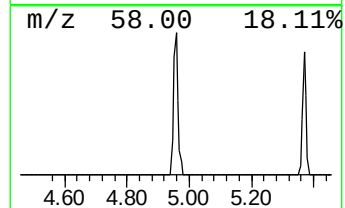
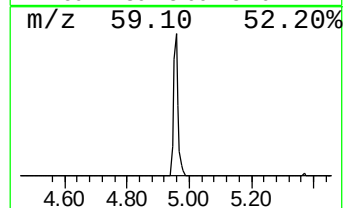
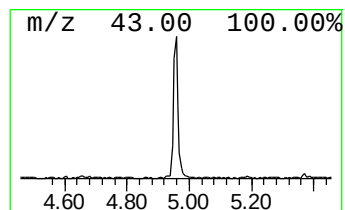
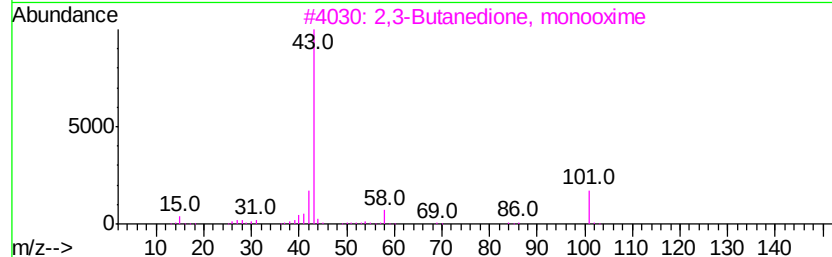
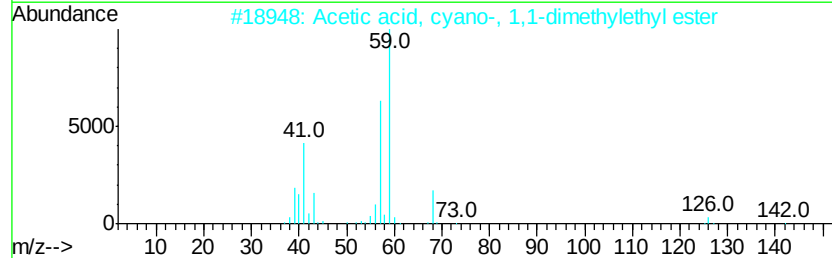
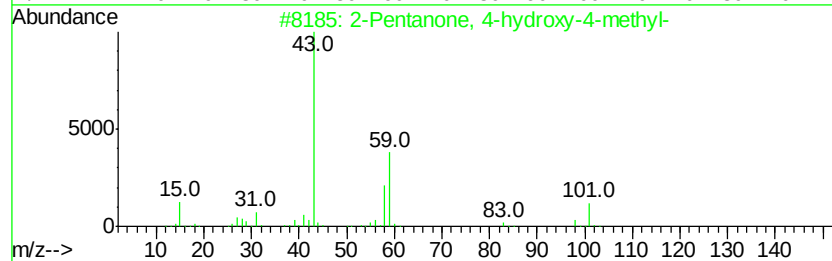
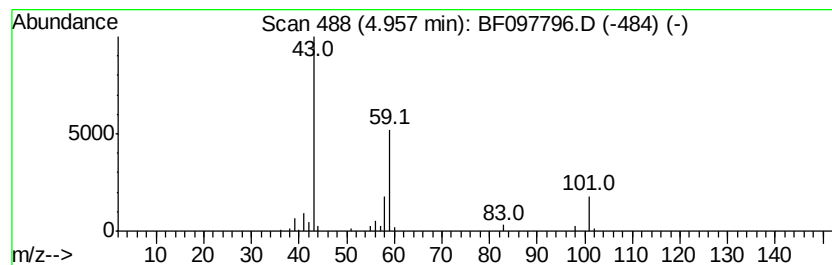
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	2.18 ng	87014	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		5-Hexen-2-one	98	C6H10O	000109-49-9	14
5		Acetone	58	C3H6O	000067-64-1	9



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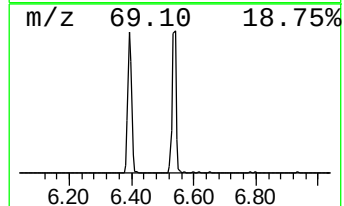
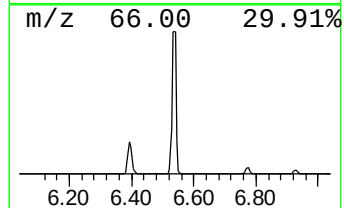
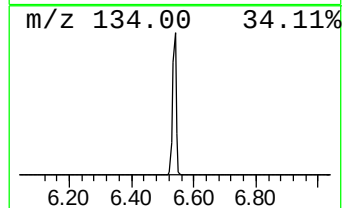
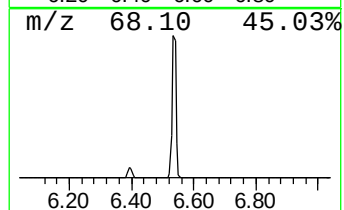
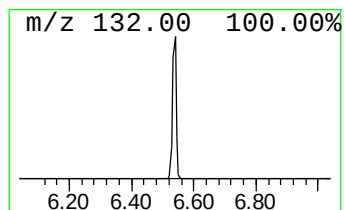
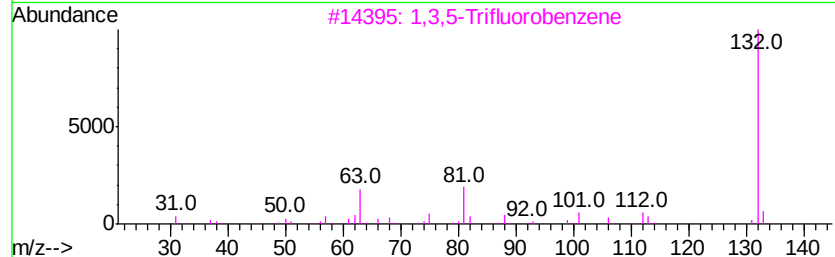
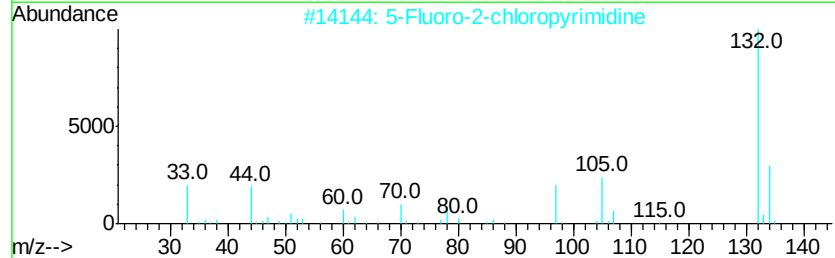
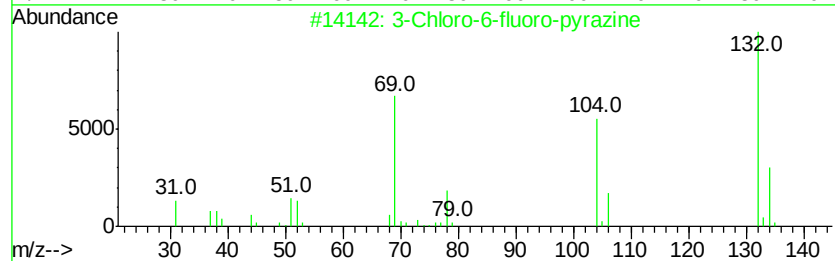
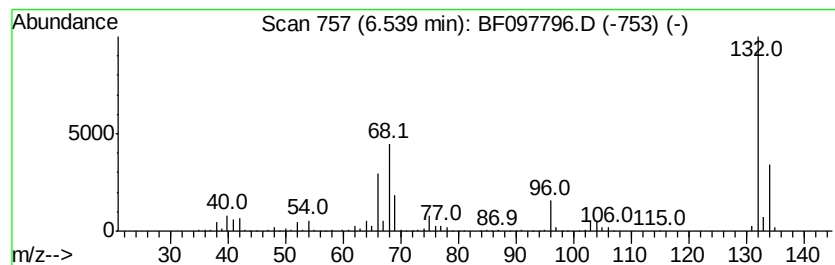
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	18.75 ng	747534	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
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		Xenon	132	Xe	007440-63-3	9



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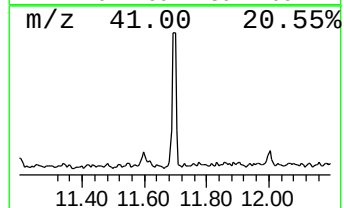
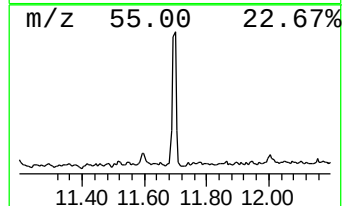
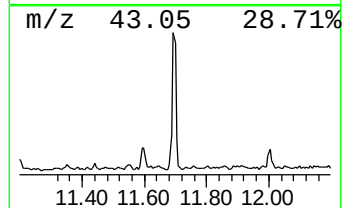
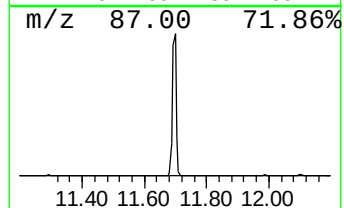
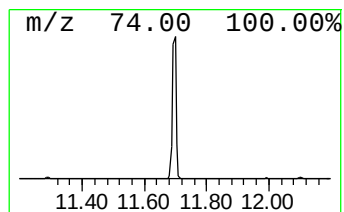
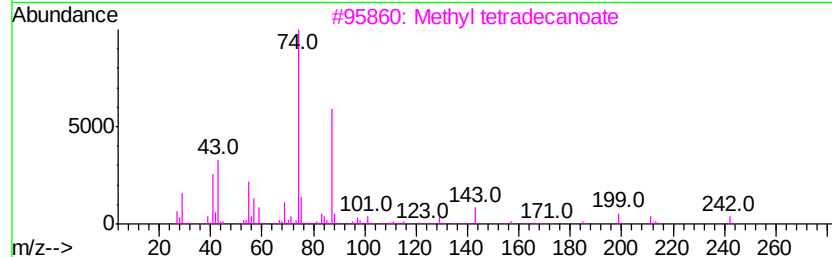
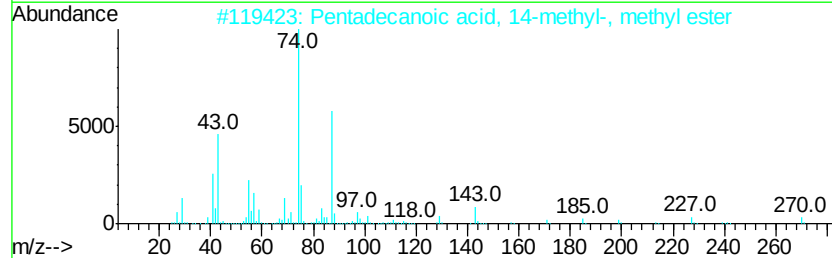
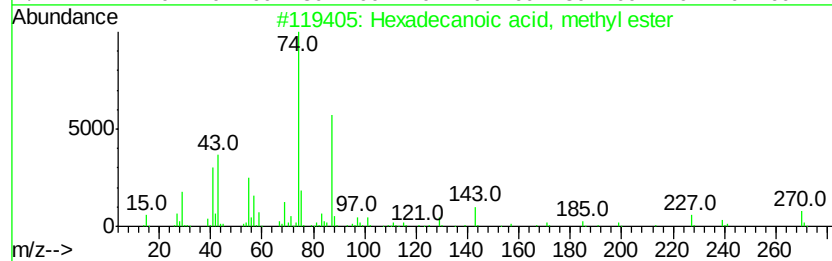
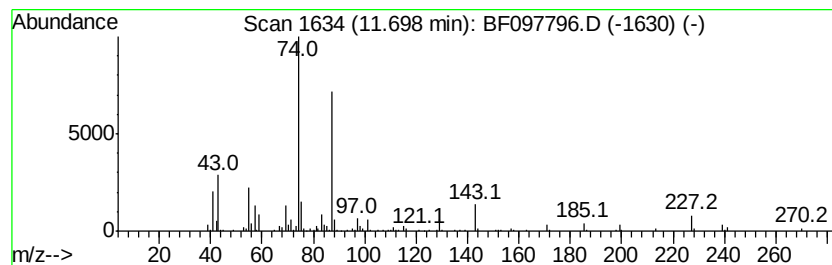
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	9.09 ng	314128	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	95
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87



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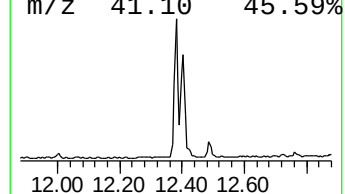
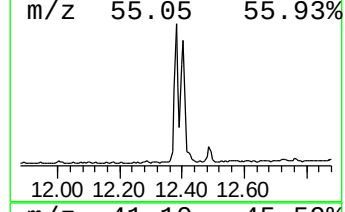
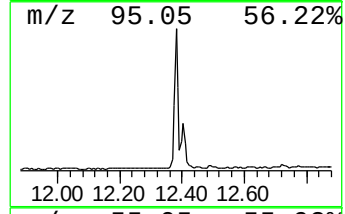
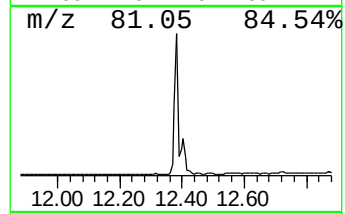
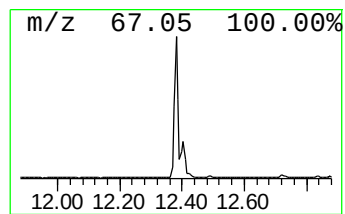
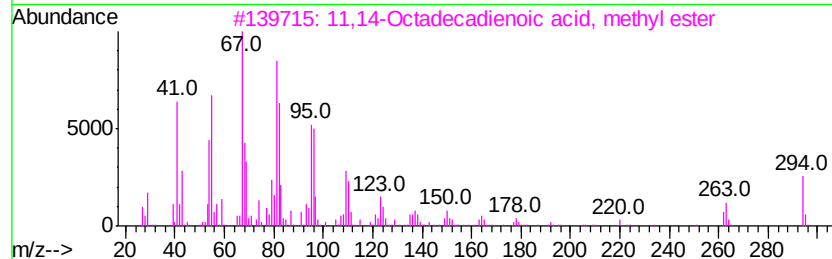
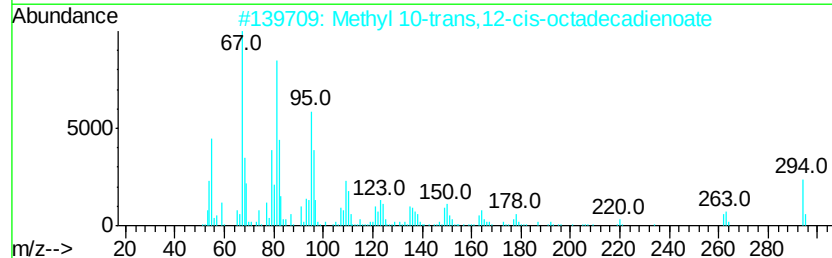
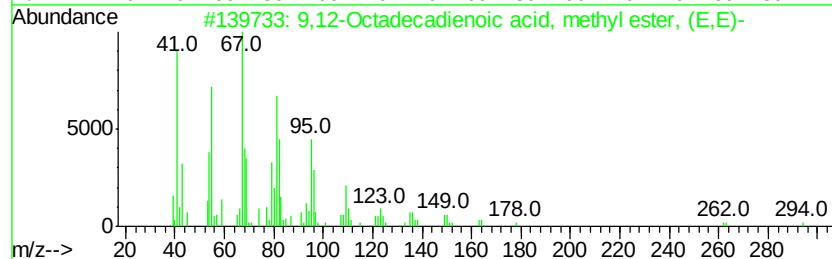
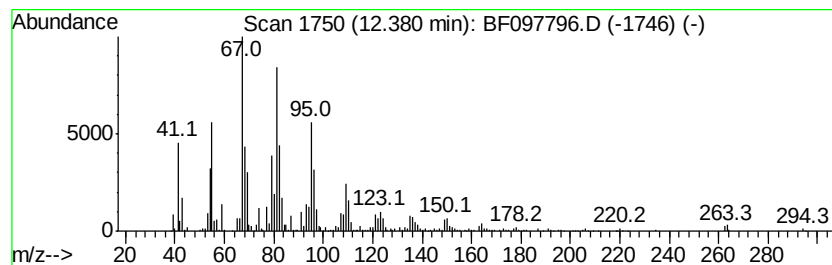
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	30.79 ng	1064050	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
3		11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98
4		Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	95
5		10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	95



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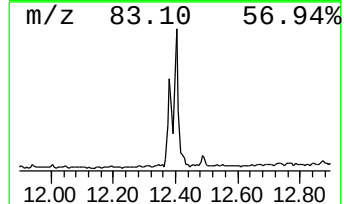
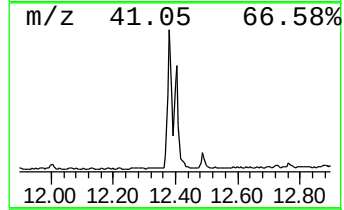
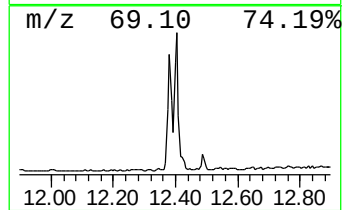
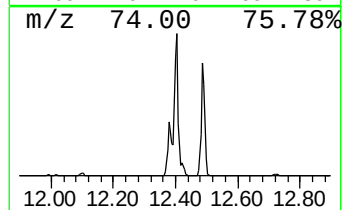
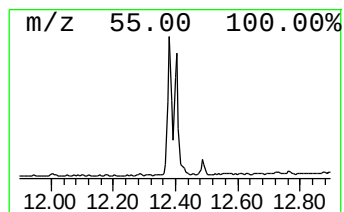
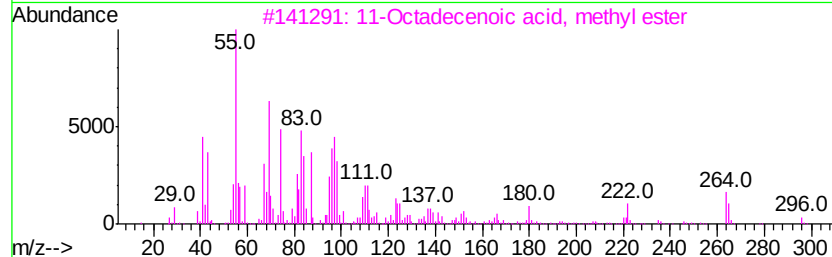
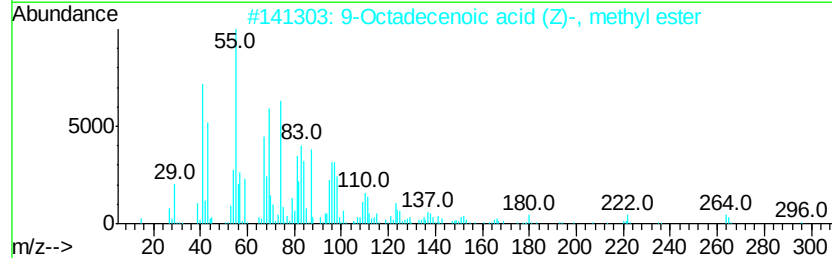
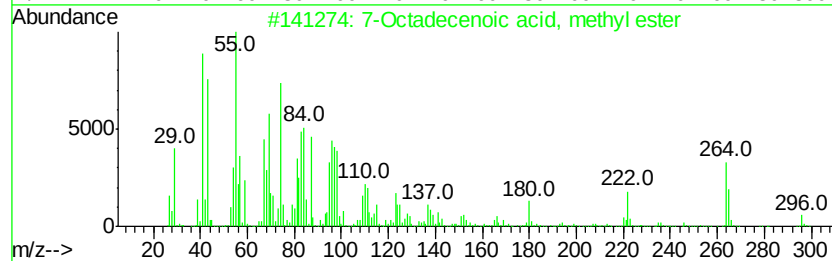
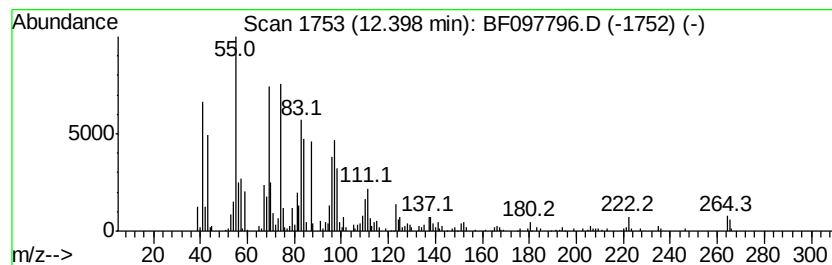
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Peak Number 6 7-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	18.52 ng	639983	Phenanthrene-d10	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	97
2		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	96
3		11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	96
4		cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	95
5		9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081717\
Data File : BF097796.D
Acq On : 17 Aug 2017 19:58
Operator : SJ/JU
Sample : I4817-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

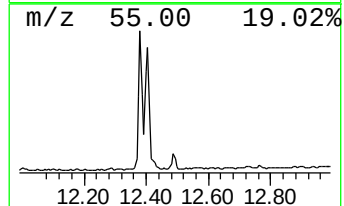
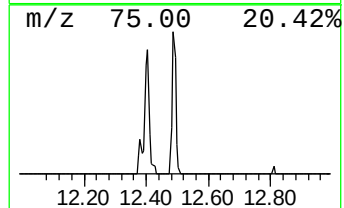
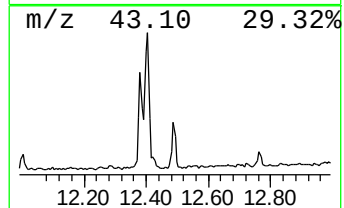
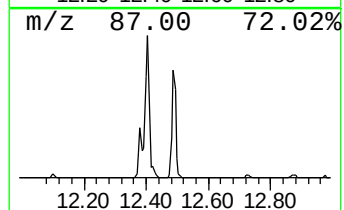
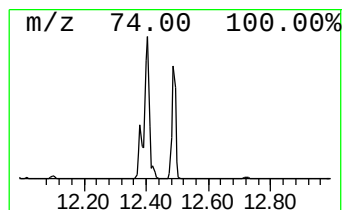
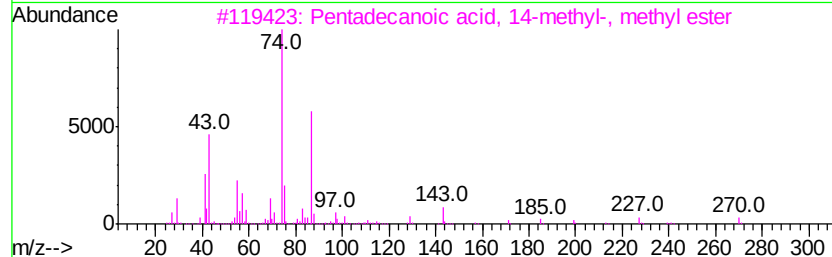
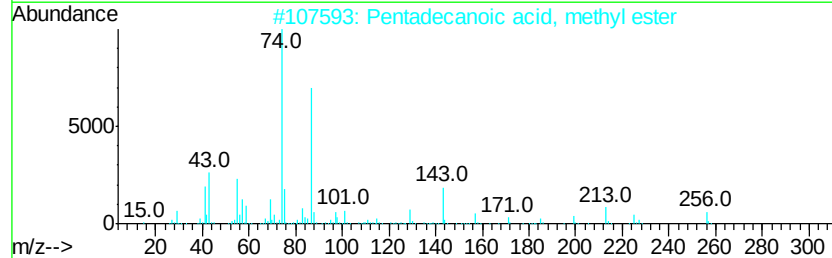
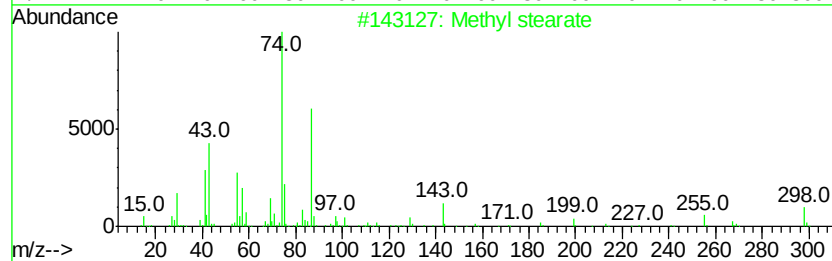
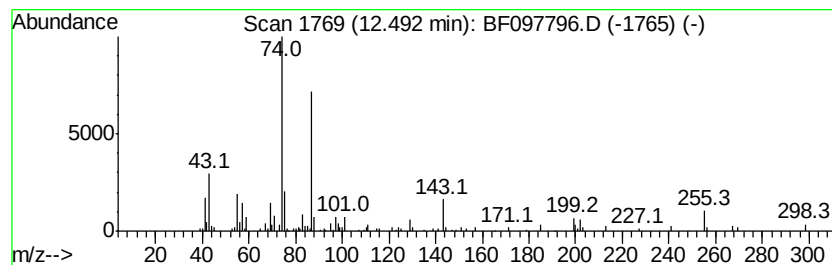
Instrument :
BNA_F
ClientSampleId :
SU-03-081517

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.49	4.00 ng	138207	Phenanthrene-d10	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	96
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	93
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081717\
Data File : BF097796.D
Acq On : 17 Aug 2017 19:58
Operator : SJ/JU
Sample : I4817-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-081517

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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...	4.96	2.2	ng	87014	1	6.77	797580	20.0
unknown6.54	6.54	18.8	ng	747534	1	6.77	797580	20.0
Hexadecanoic acid...	11.70	9.1	ng	314128	4	11.29	691247	20.0
9,12-Octadecadien...	12.38	30.8	ng	1064050	4	11.29	691247	20.0
7-Octadecenoic ac...	12.40	18.5	ng	639983	4	11.29	691247	20.0
Methyl stearate	12.49	4.0	ng	138207	4	11.29	691247	20.0