

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
 Data File : BF092935.D
 Acq On : 14 Feb 2017 11:16
 Operator : SJ/MA
 Sample : I1799-04
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-2

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-BF013017.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	3.824	148	152	155	rBV	308107	497713	9.73%	1.355%
2	5.047	257	259	268	rBV	544026	594012	11.61%	1.617%
3	5.322	281	283	286	rVB	148980	143692	2.81%	0.391%
4	5.470	294	296	299	rVB	1540855	2073135	40.53%	5.644%
5	5.699	314	316	319	rBV	570044	561923	10.98%	1.530%
6	6.396	375	377	379	rBV	252665	212161	4.15%	0.578%
7	6.430	379	380	382	rVB	95168	67822	1.33%	0.185%
8	6.476	382	384	385	rBV	157880	133902	2.62%	0.365%
9	6.510	385	387	390	rVV2	1545237	1468716	28.71%	3.998%
10	6.556	390	391	393	rVB	128011	111653	2.18%	0.304%
11	6.647	396	399	401	rBV	3690739	3509654	68.61%	9.554%
12	6.704	401	404	406	rVB	337958	380886	7.45%	1.037%
13	6.876	417	419	421	rBV	1150311	957769	18.72%	2.607%
14	6.933	421	424	427	rVV2	141012	142516	2.79%	0.388%
15	7.036	430	433	435	rVV	3559552	3438258	67.21%	9.360%
16	7.196	445	447	452	rVB	60547	61531	1.20%	0.168%
17	7.447	466	469	471	rVB	2783780	3053974	59.70%	8.314%
18	7.642	483	486	488	rBV2	35731	53321	1.04%	0.145%
19	7.905	506	509	510	rBV	39512	56985	1.11%	0.155%
20	8.156	529	531	534	rBV	923408	1306035	25.53%	3.555%
21	9.242	623	626	628	rBV	4547417	5115616	100.00%	13.926%
22	9.630	658	660	662	rBV	220736	178999	3.50%	0.487%
23	9.916	682	685	687	rVB	1456868	1429977	27.95%	3.893%
24	10.339	721	722	724	rVB	114714	110067	2.15%	0.300%
25	10.556	739	741	744	rBV	37749	61957	1.21%	0.169%
26	10.705	751	754	756	rBV	2508719	2638237	51.57%	7.182%
27	10.819	762	764	768	rVB	120775	196945	3.85%	0.536%
28	11.265	801	803	804	rBV	129191	133532	2.61%	0.364%
29	11.391	812	814	817	rBV	1101332	1402768	27.42%	3.819%
30	11.688	838	840	842	rBV	96490	78485	1.53%	0.214%
31	12.797	935	937	939	rBV	136936	155082	3.03%	0.422%
32	12.979	950	953	956	rBV	3733814	4042879	79.03%	11.006%
33	13.882	1029	1032	1039	rBV2	64016	132451	2.59%	0.361%
34	14.031	1042	1045	1047	rBV	1246848	1266337	24.75%	3.447%

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35	14.282	1062	1067	1073	rVB3	19811	56198	1.10%	0.153%
36	15.460	1167	1170	1173	rBV	647690	909141	17.77%	2.475%

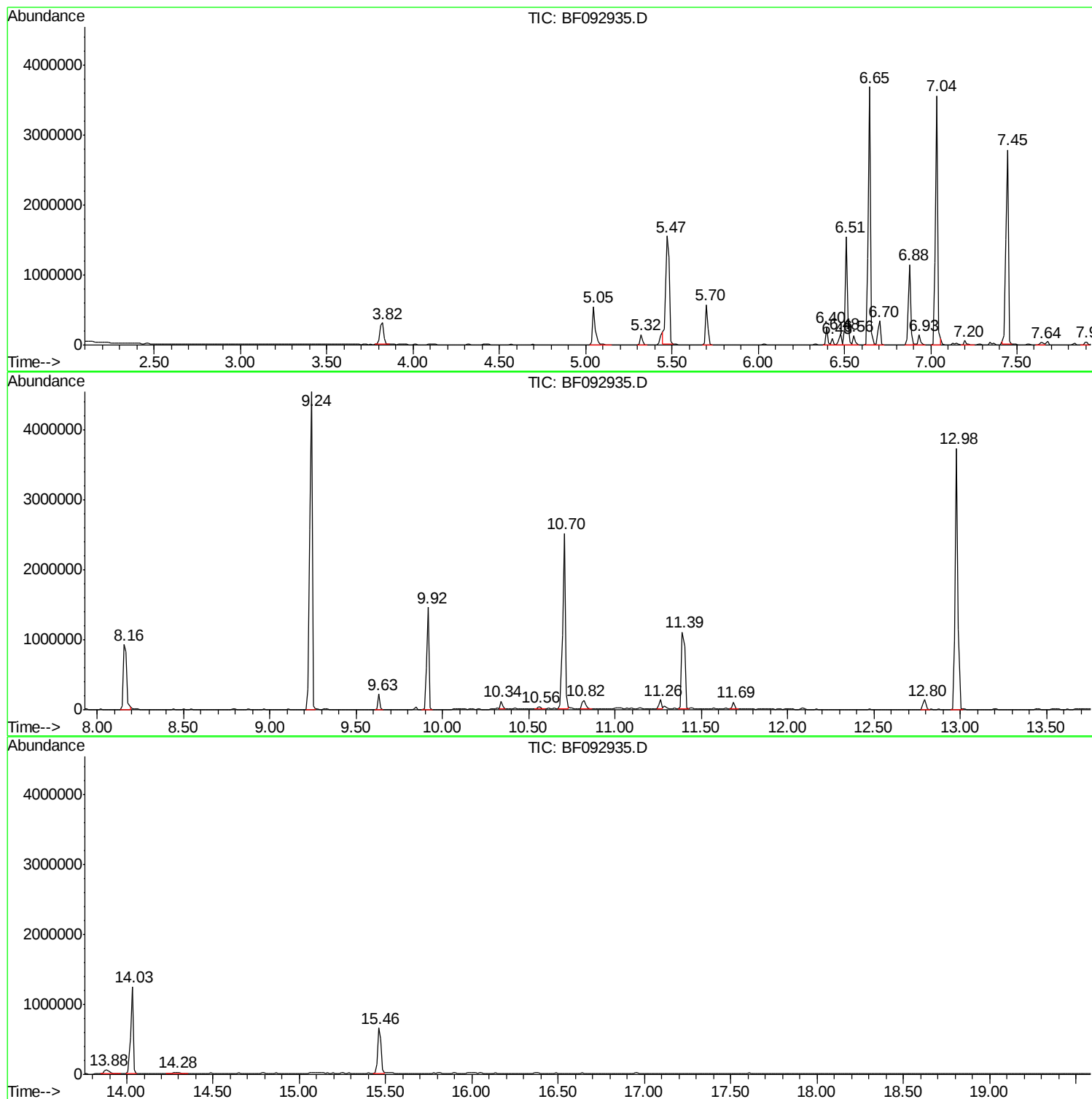
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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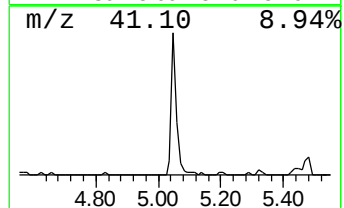
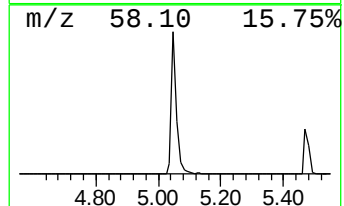
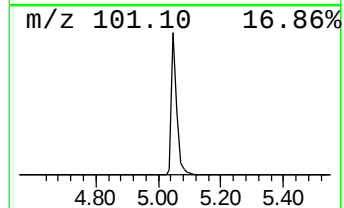
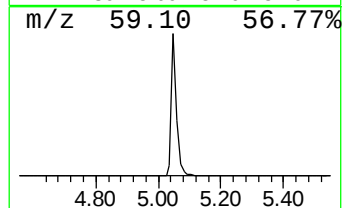
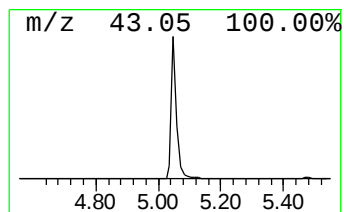
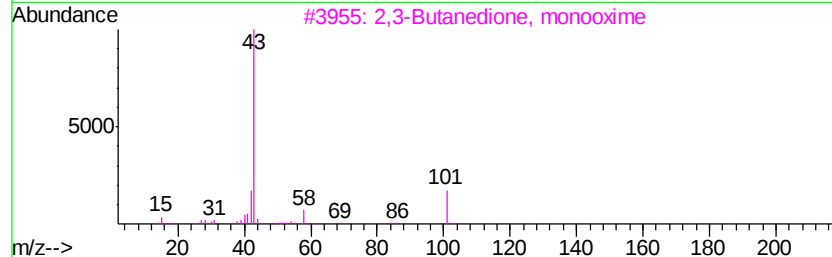
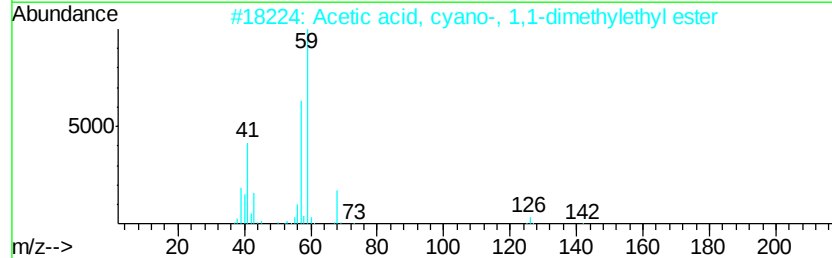
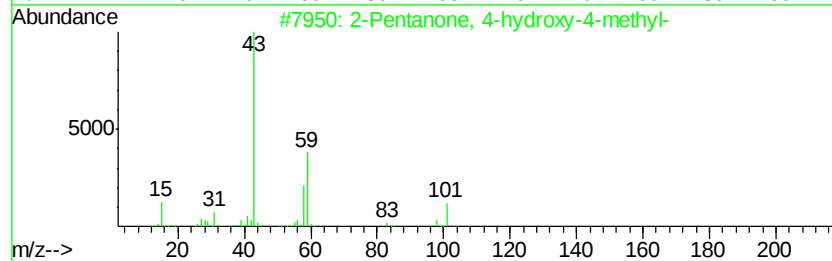
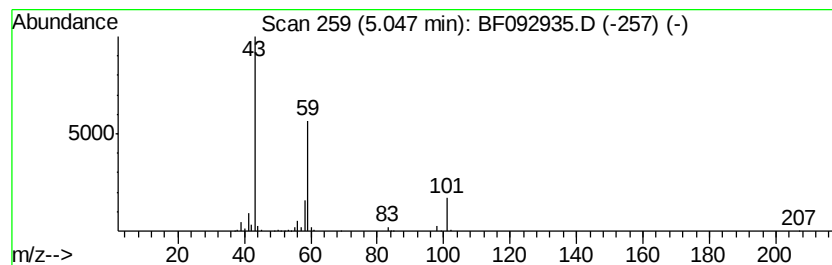
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	12.40 ng	594012	1,4-Dichlorobenzene-d4	6.88

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-dimethy...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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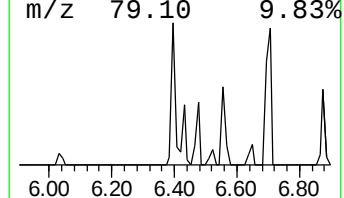
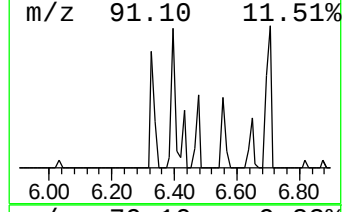
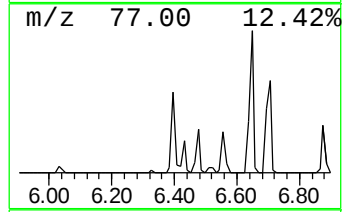
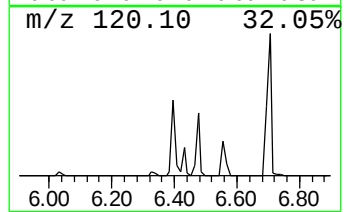
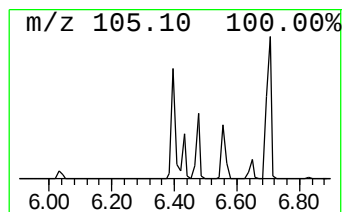
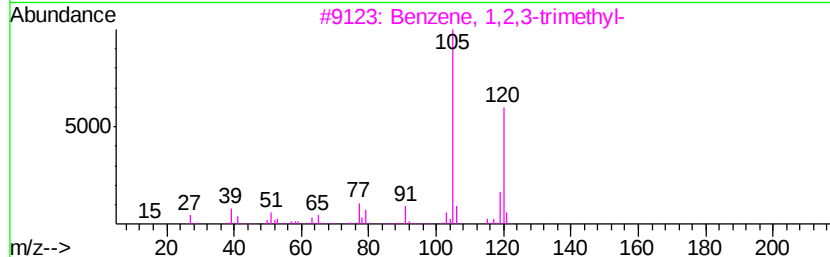
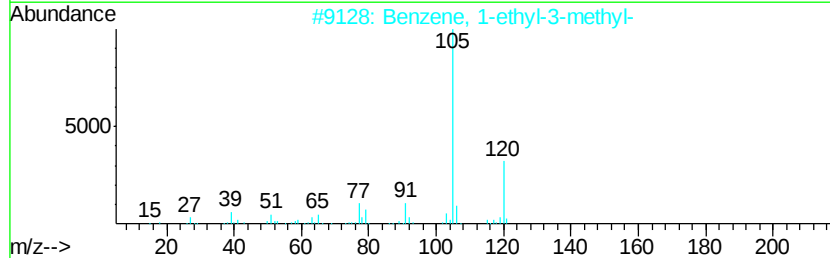
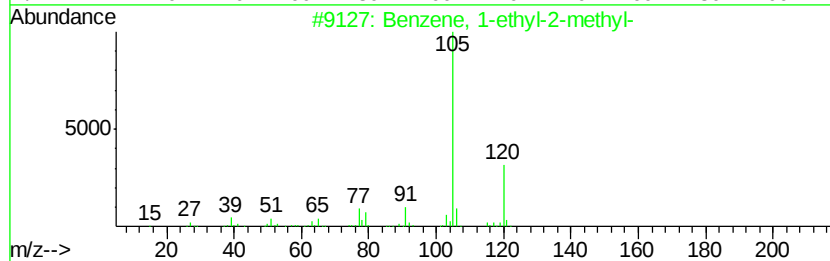
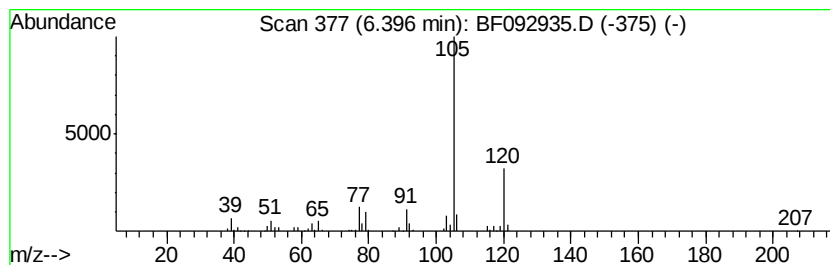
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	4.43 ng	212161	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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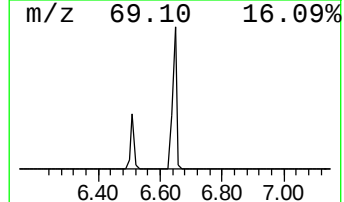
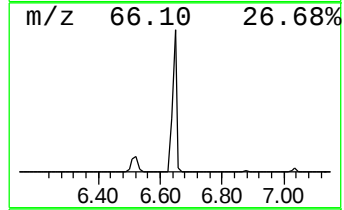
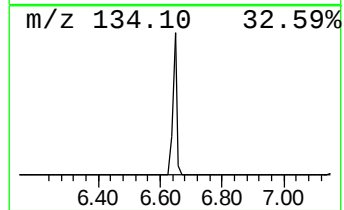
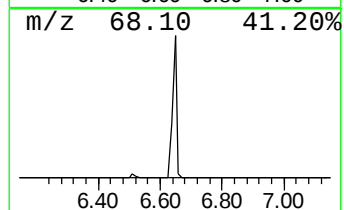
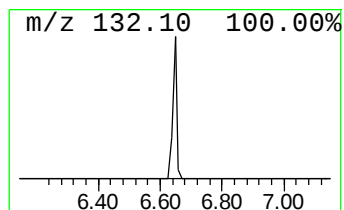
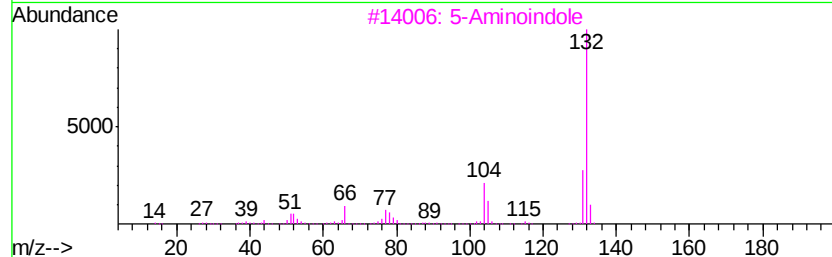
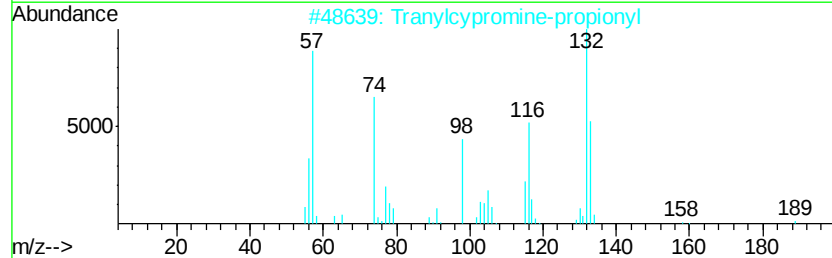
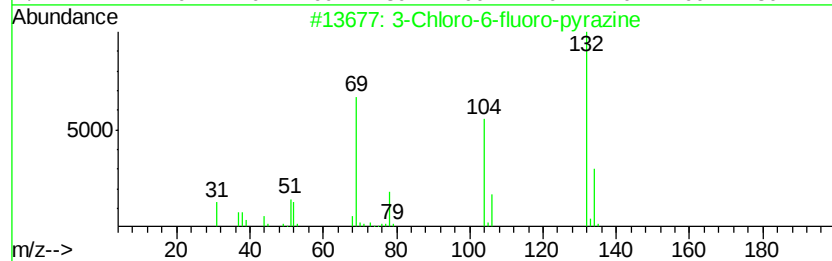
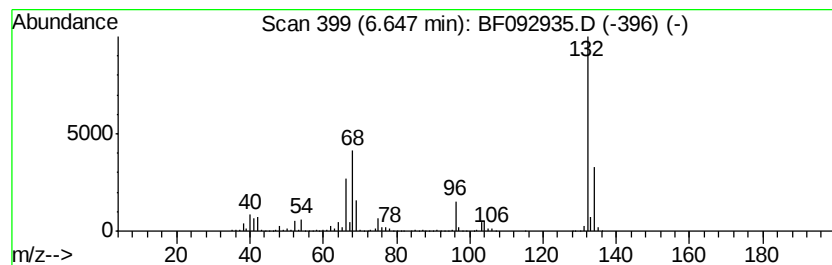
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	73.29 ng	3509650	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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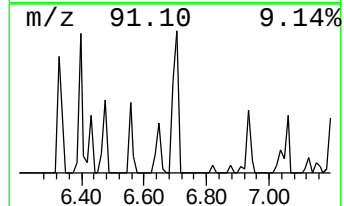
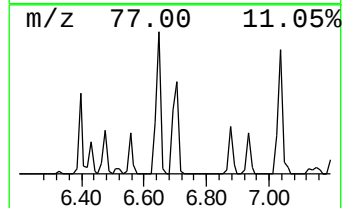
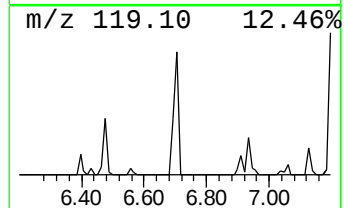
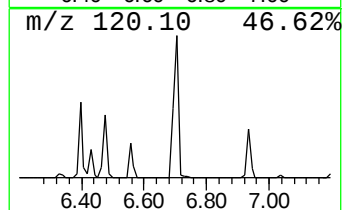
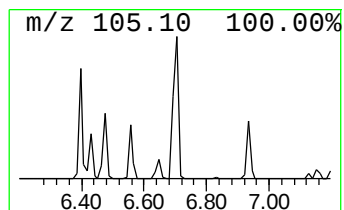
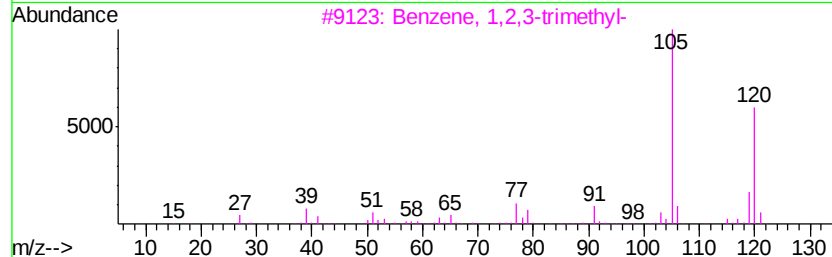
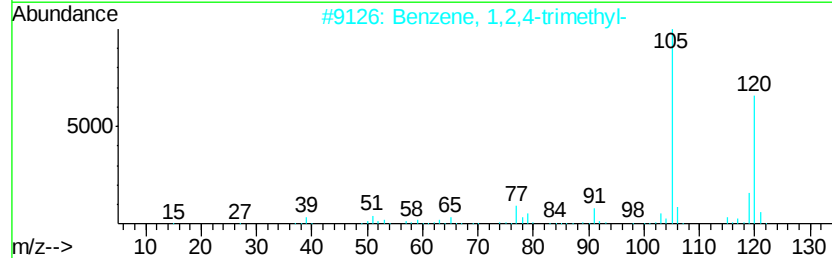
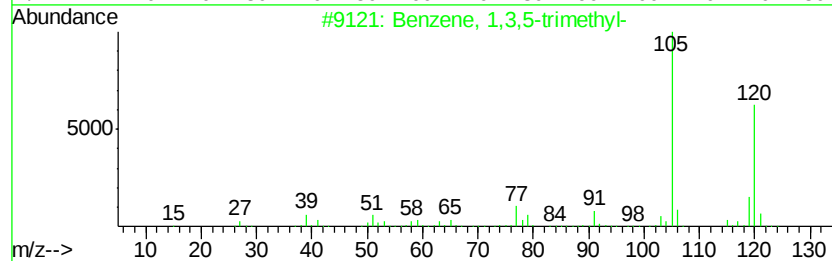
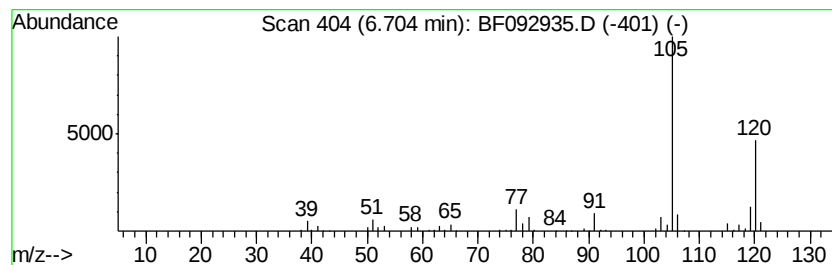
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 Benzene, 1,3,5-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	7.95 ng	380886	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	95
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	93
4		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



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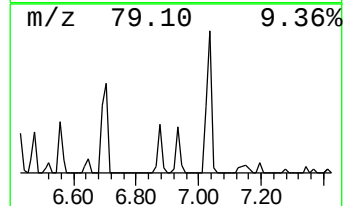
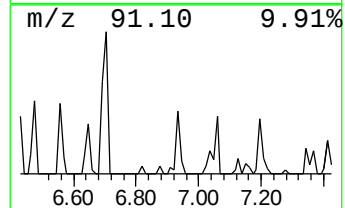
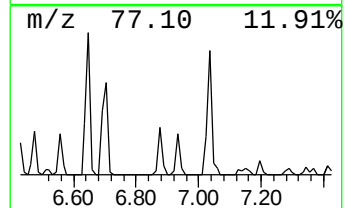
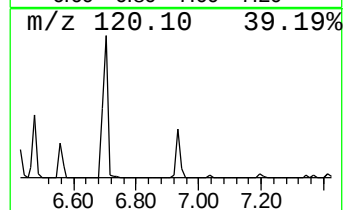
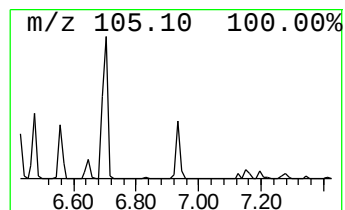
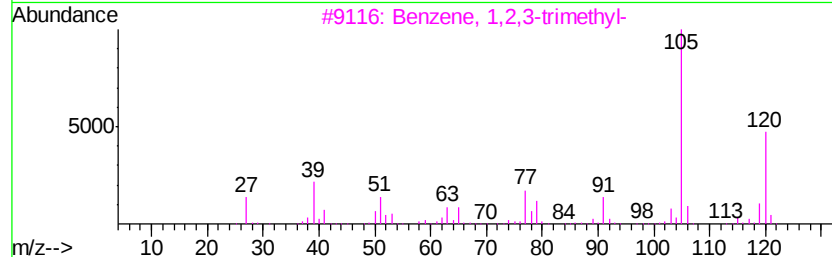
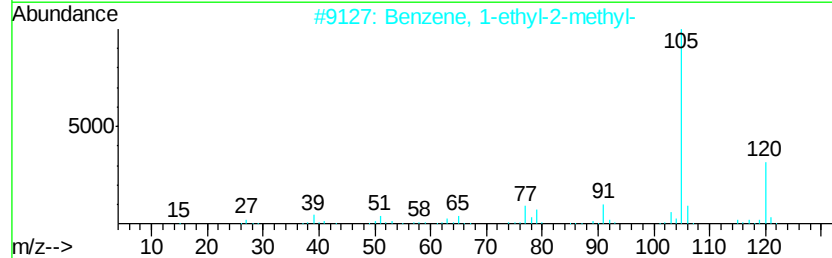
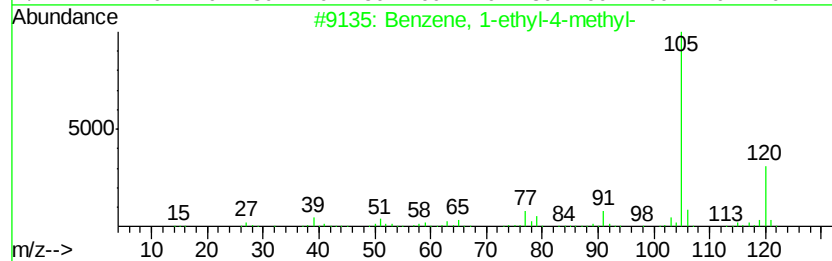
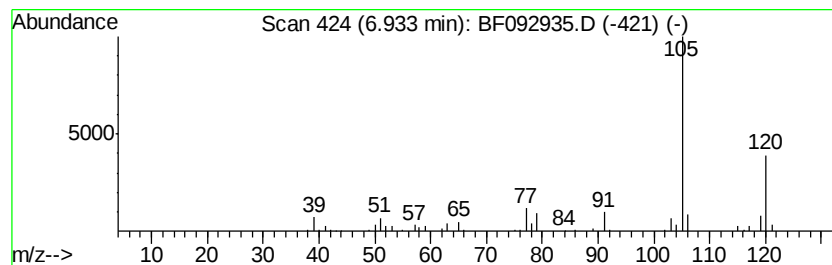
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TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1-ethyl-4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	2.98 ng	142516	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092935.D
Acq On : 14 Feb 2017 11:16
Operator : SJ/MA
Sample : I1799-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

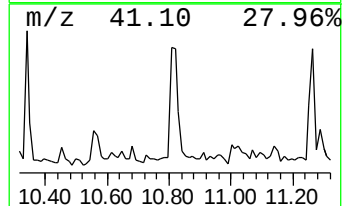
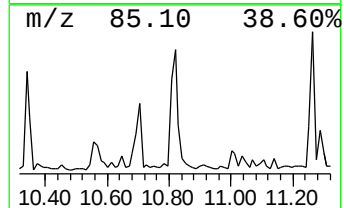
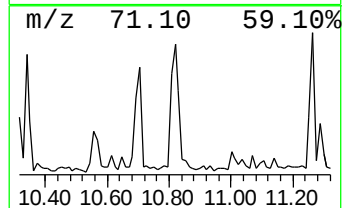
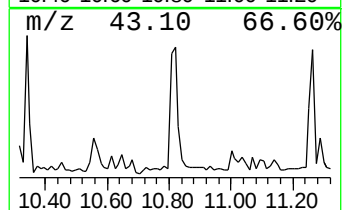
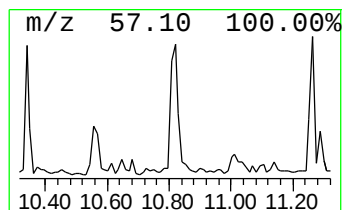
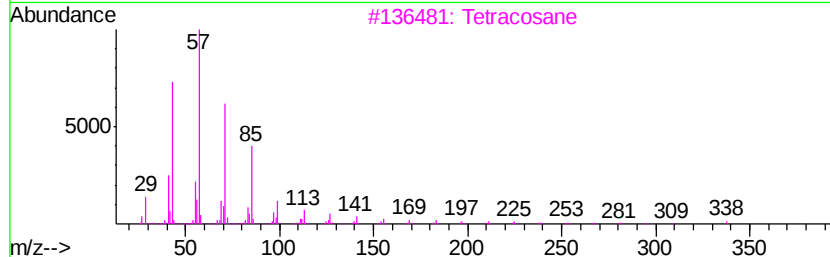
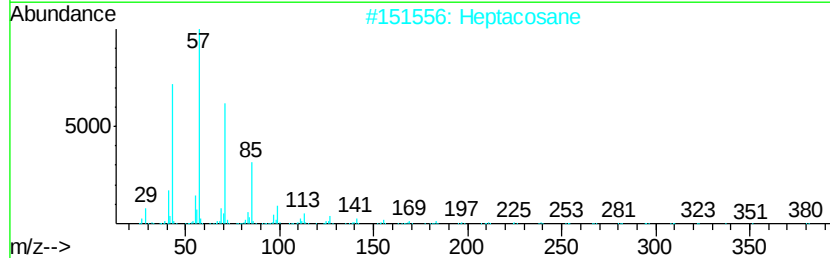
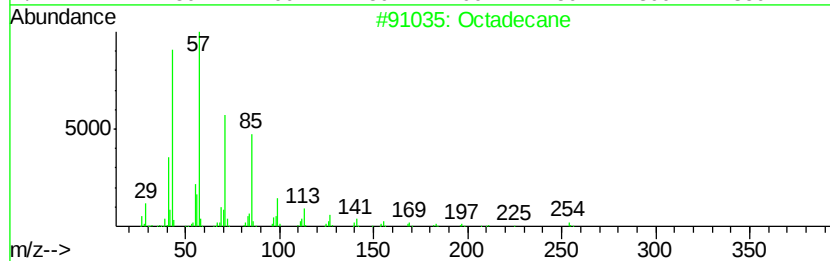
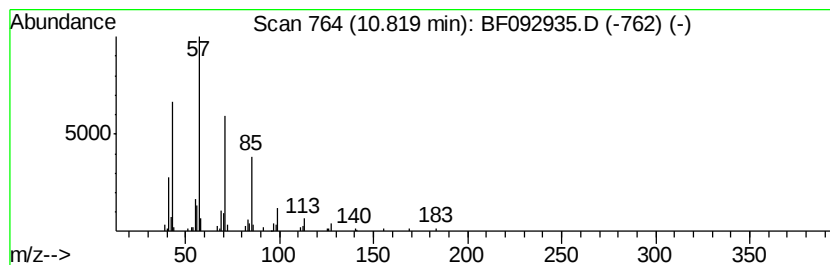
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	2.81 ng	196945	Phenanthrene-d10	11.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
5			Hexadecane	226	C16H34	000544-76-3	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092935.D
Acq On : 14 Feb 2017 11:16
Operator : SJ/MA
Sample : I1799-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

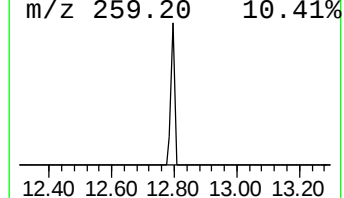
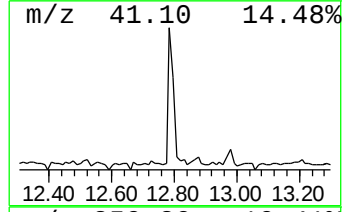
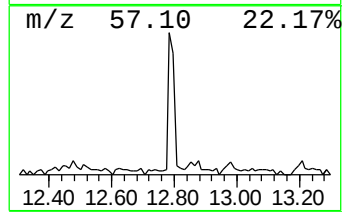
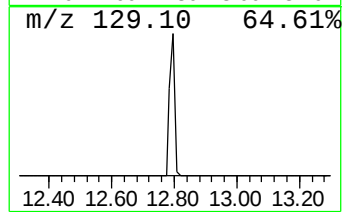
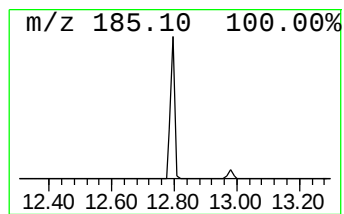
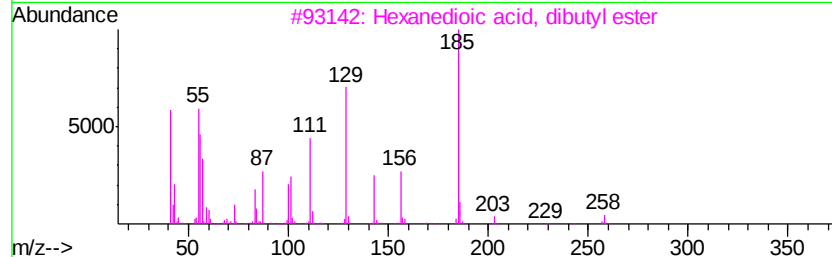
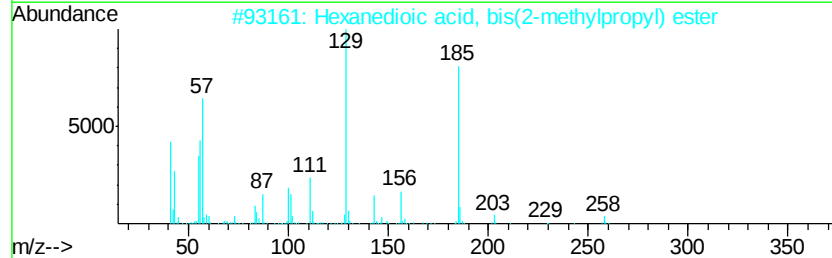
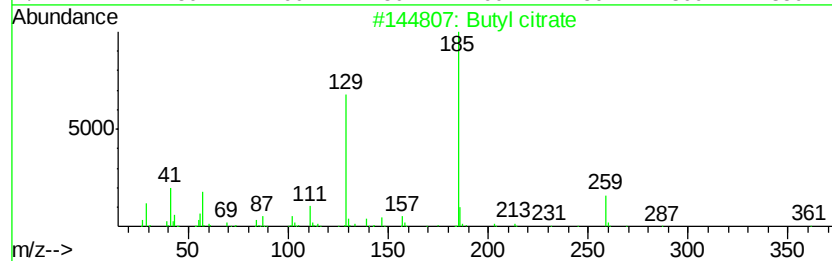
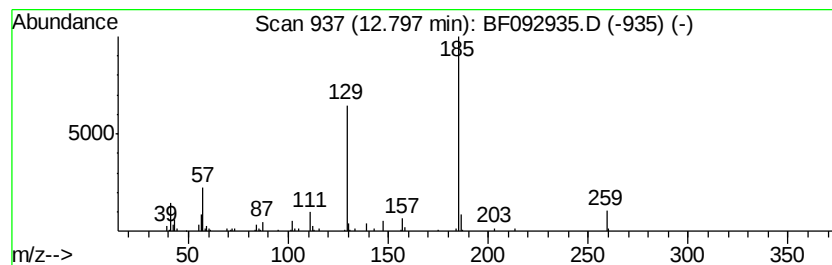
Instrument :
BNA_F
ClientSampleId :
SW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Butyl citrate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.45 ng	155082	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	91
2	Hexanedioic acid, bis(2-methylpr...	258 C14H26O4	000141-04-8	72
3	Hexanedioic acid, dibutyl ester	258 C14H26O4	000105-99-7	38
4	2-Bromo-3-methylaniline	185 C7H8BrN	1000289-33-5	38
5	Butanedioic acid, 2,3-dimethyl-,...	258 C14H26O4	056051-57-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092935.D
Acq On : 14 Feb 2017 11:16
Operator : SJ/MA
Sample : I1799-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

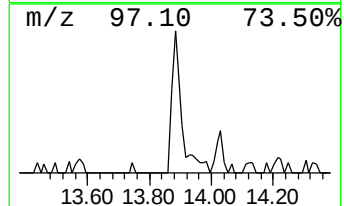
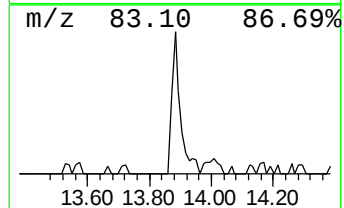
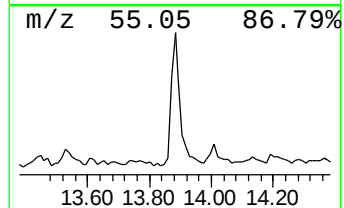
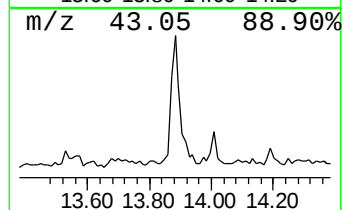
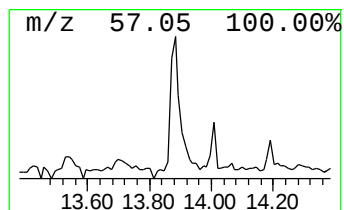
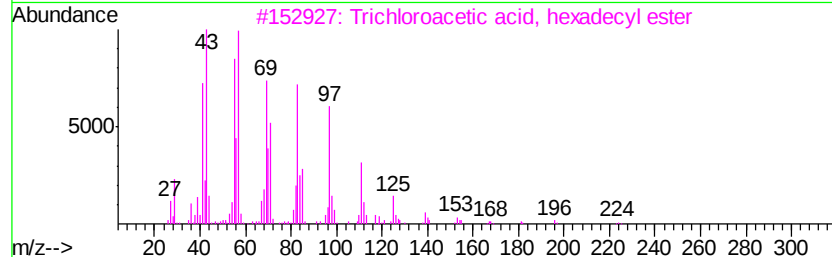
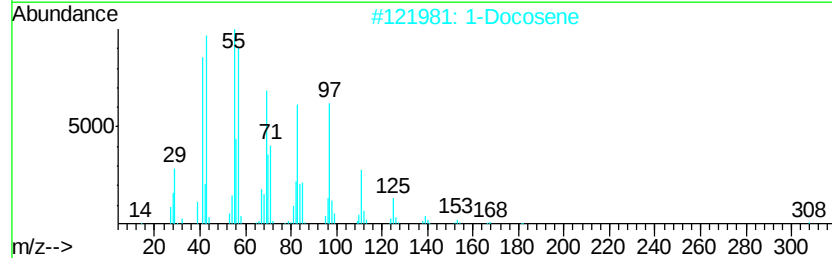
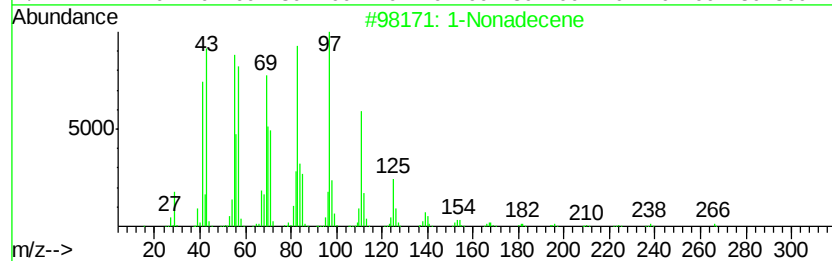
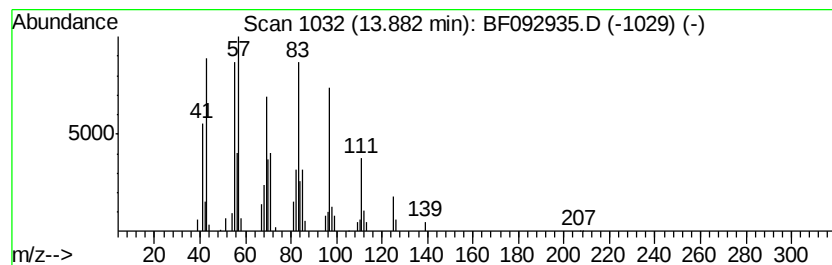
Instrument :
BNA_F
ClientSampleId :
SW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 1-Nonadecene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	2.09 ng	132451	Chrysene-d12	14.03
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene	266 C19H38	018435-45-5	91
2	1-Docosene	308 C22H44	001599-67-3	91
3	Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1	87
4	Dichloroacetic acid, tetradecyl ...	324 C16H30Cl2O2	083005-02-1	83
5	17-Pentatriacontene	491 C35H70	006971-40-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021417\
Data File : BF092935.D
Acq On : 14 Feb 2017 11:16
Operator : SJ/MA
Sample : I1799-04
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SW-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	12.4	ng	594012	1	6.88	957769	20.0
Benzene, 1-ethyl-...	6.40	4.4	ng	212161	1	6.88	957769	20.0
unknown6.65	6.65	73.3	ng	3509650	1	6.88	957769	20.0
Benzene, 1,3,5-tr...	6.70	8.0	ng	380886	1	6.88	957769	20.0
Benzene, 1-ethyl-...	6.93	3.0	ng	142516	1	6.88	957769	20.0
Octadecane	10.82	2.8	ng	196945	4	11.39	1402770	20.0
Butyl citrate	12.80	2.5	ng	155082	5	14.03	1266340	20.0
1-Nonadecene	13.88	2.1	ng	132451	5	14.03	1266340	20.0