

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110716\
 Data File : BF091066.D
 Acq On : 7 Nov 2016 19:55
 Operator : UM/SJ
 Sample : H5543-07
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-112-0.5-1.0

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-BF110316.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	1.767	5	7	29	rVB	2181064	4918188	94.36%	10.433%
2	2.064	31	33	48	rVB2	89566	251474	4.82%	0.533%
3	4.819	272	274	282	rBV	332974	624413	11.98%	1.325%
4	5.264	311	313	316	rBV	2967087	4320921	82.90%	9.166%
5	6.327	403	406	409	rBV2	3151100	5211913	100.00%	11.056%
6	6.442	414	416	419	rBV	3625838	4321644	82.92%	9.168%
7	6.670	434	436	442	rBV	1070898	1037618	19.91%	2.201%
8	6.830	447	450	452	rBV	3925337	3638816	69.82%	7.719%
9	7.242	483	486	488	rBV	1899341	1872453	35.93%	3.972%
10	7.345	494	495	503	rVB2	61977	111458	2.14%	0.236%
11	7.962	546	549	551	rBV	1367872	1405976	26.98%	2.983%
12	8.968	635	637	641	rBV	168387	245363	4.71%	0.521%
13	9.048	641	644	646	rBV	3627111	4451365	85.41%	9.443%
14	9.436	676	678	681	rBV	835547	1013684	19.45%	2.150%
15	9.711	700	702	705	rBV	1414860	1322878	25.38%	2.806%
16	10.156	740	741	743	rVB	72161	58529	1.12%	0.124%
17	10.374	757	760	763	rBV	32165	55055	1.06%	0.117%
18	10.499	769	771	774	rBV	1211868	1356062	26.02%	2.877%
19	10.636	781	783	787	rBV2	78695	148838	2.86%	0.316%
20	11.082	820	822	823	rBV	62753	76559	1.47%	0.162%
21	11.196	829	832	833	rBV	1253594	1185828	22.75%	2.516%
22	11.219	833	834	836	rVV	179454	151816	2.91%	0.322%
23	11.265	836	838	842	rVB2	31790	60583	1.16%	0.129%
24	11.436	850	853	856	rBV2	57864	106325	2.04%	0.226%
25	11.802	883	885	889	rVB	46692	81620	1.57%	0.173%
26	12.248	922	924	926	rBV	37215	59498	1.14%	0.126%
27	12.328	930	931	935	rBV2	36065	84702	1.63%	0.180%
28	12.408	935	938	940	rBV	282042	393373	7.55%	0.834%
29	12.625	954	957	960	rBV	315570	447774	8.59%	0.950%
30	12.785	968	971	973	rBV	4211320	3886709	74.57%	8.245%
31	13.688	1048	1050	1053	rBV2	282195	311821	5.98%	0.661%
32	13.825	1059	1062	1068	rBV2	1166467	1776630	34.09%	3.769%
33	13.940	1070	1072	1073	rBV	110265	168598	3.23%	0.358%
34	14.671	1134	1136	1139	rVB	272479	356171	6.83%	0.756%

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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-BF110316.M
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35	14.831	1148	1150	1156	rVB	291176	628934	12.07%	1.334%
36	15.208	1181	1183	1186	rBV	749269	996242	19.11%	2.113%

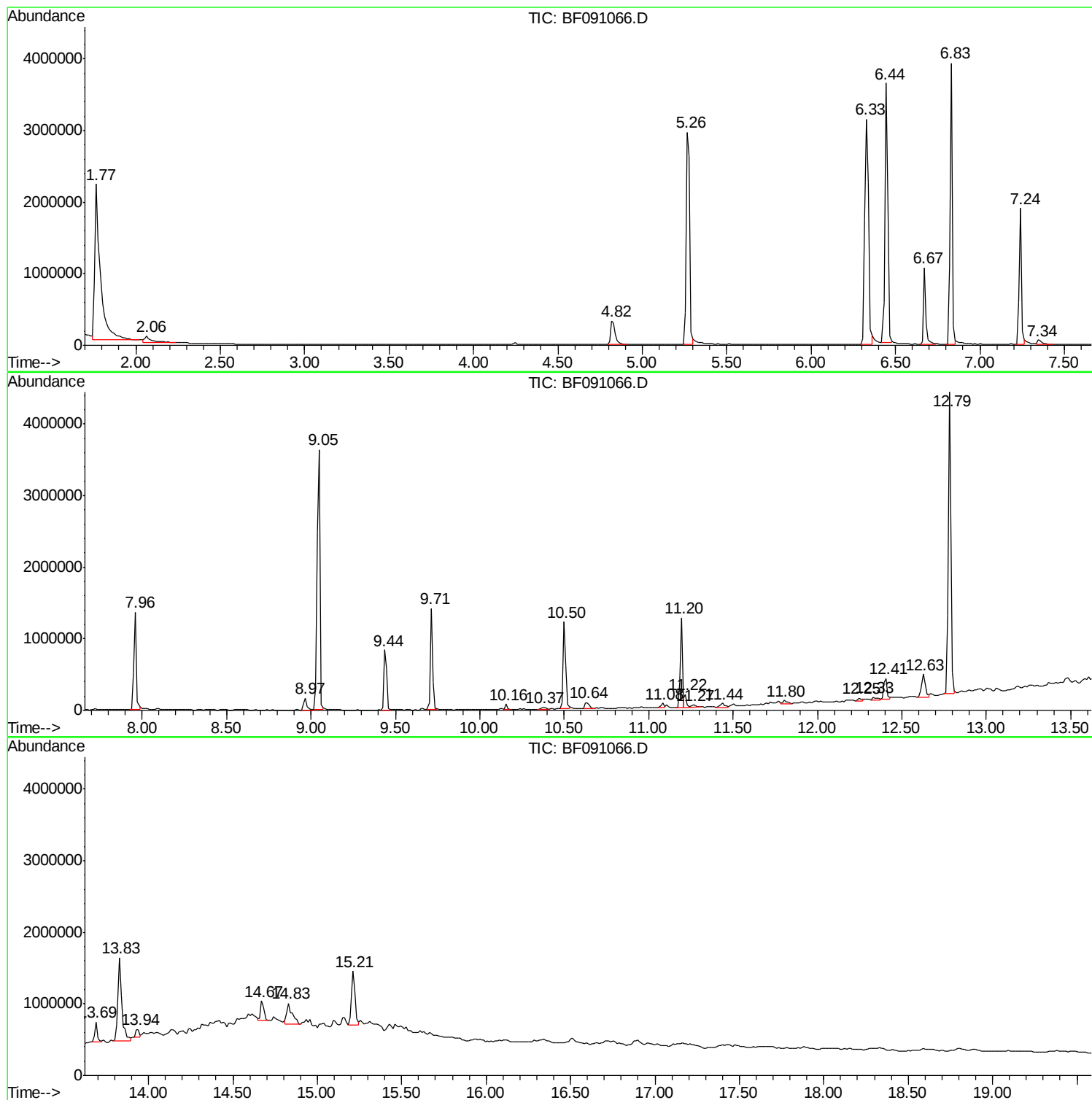
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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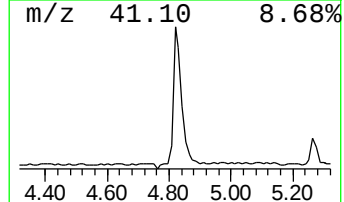
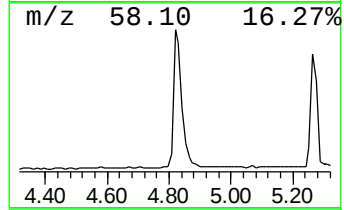
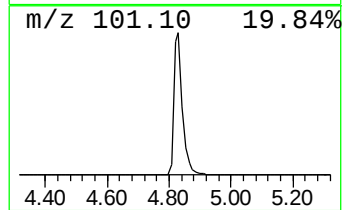
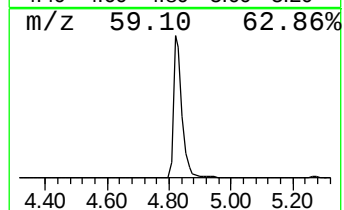
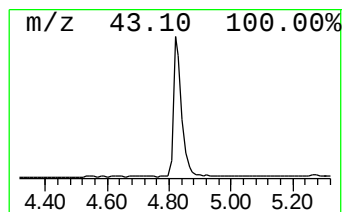
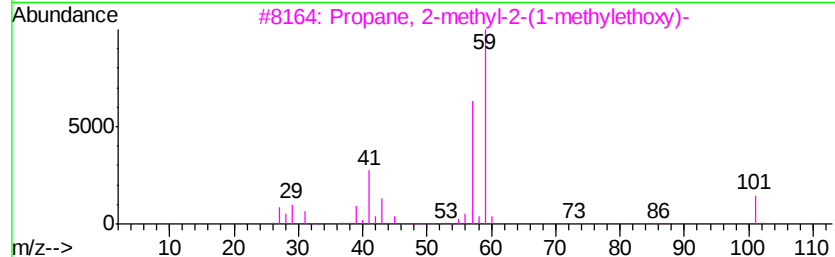
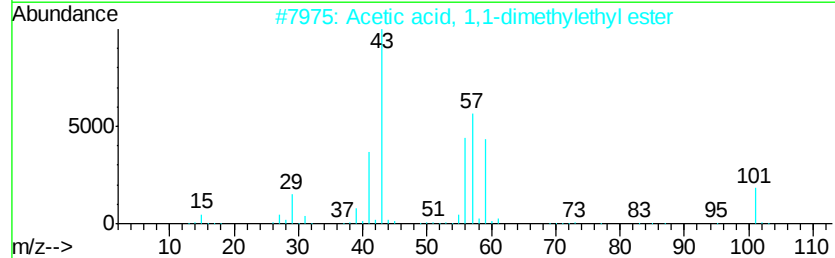
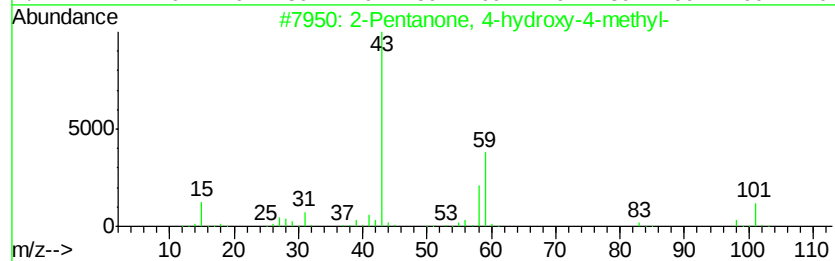
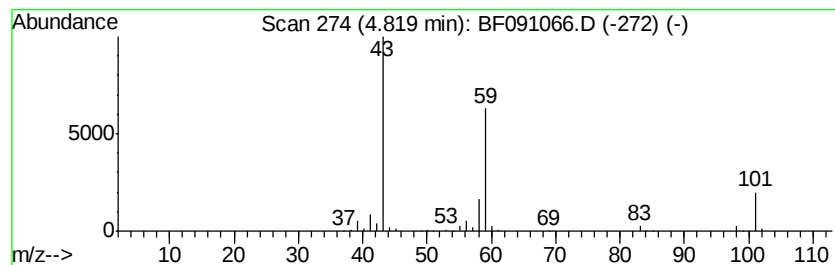
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	12.04 ng	624413	1,4-Dichlorobenzene-d4	6.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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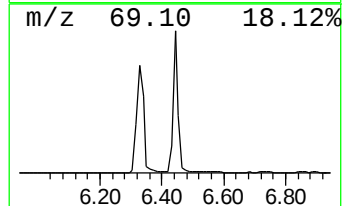
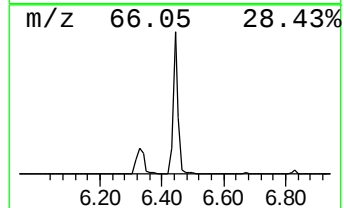
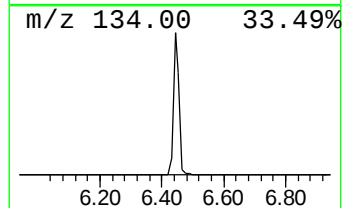
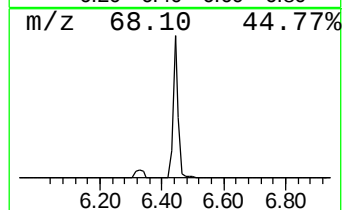
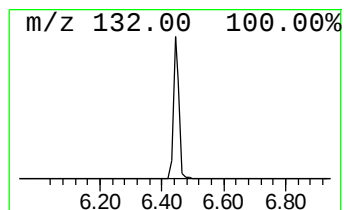
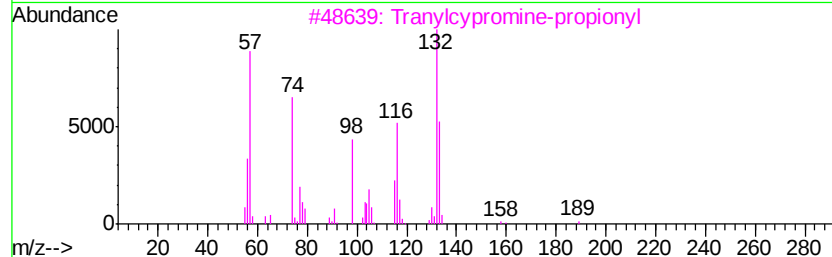
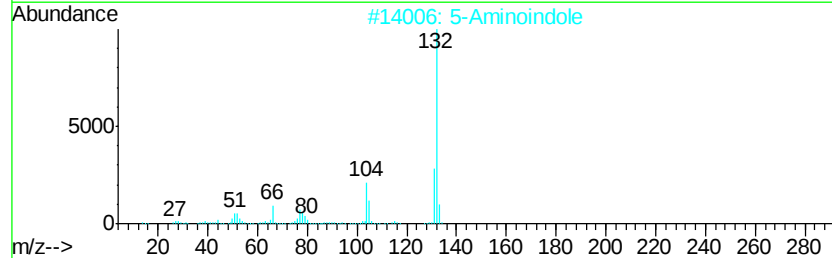
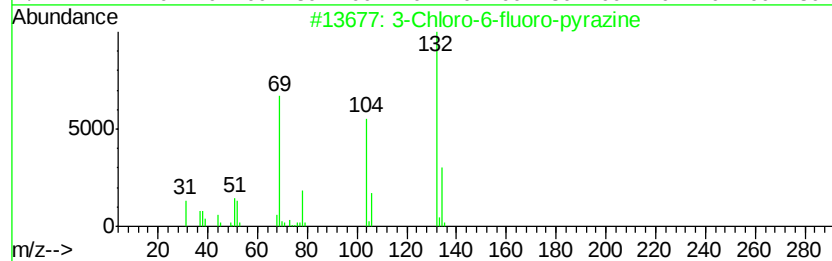
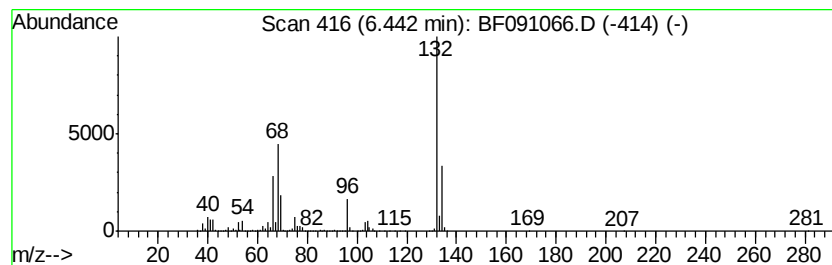
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	83.30 ng	4321640	1,4-Dichlorobenzene-d4	6.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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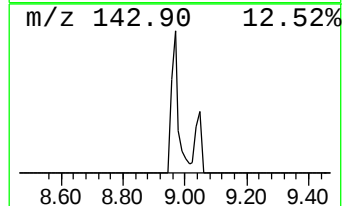
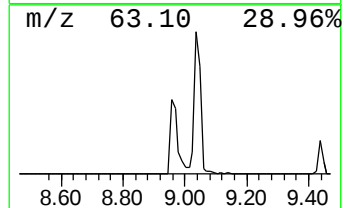
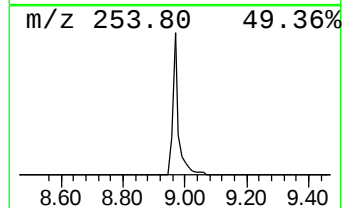
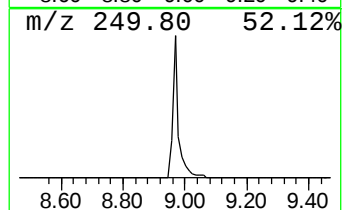
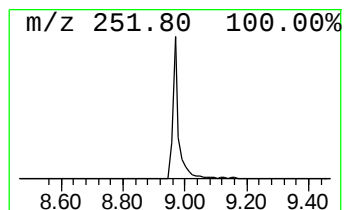
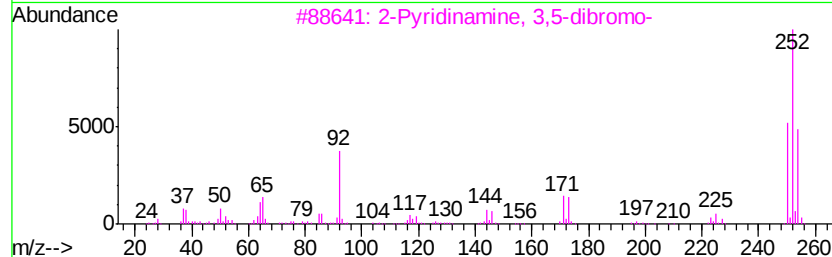
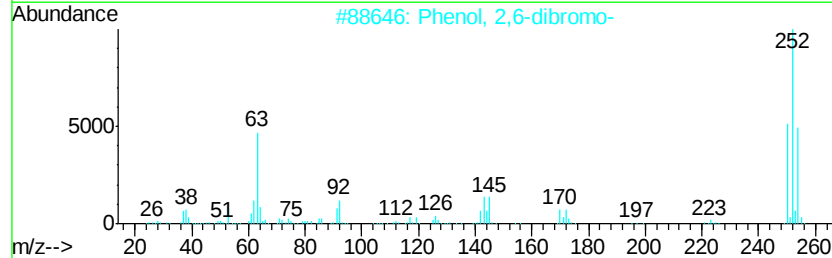
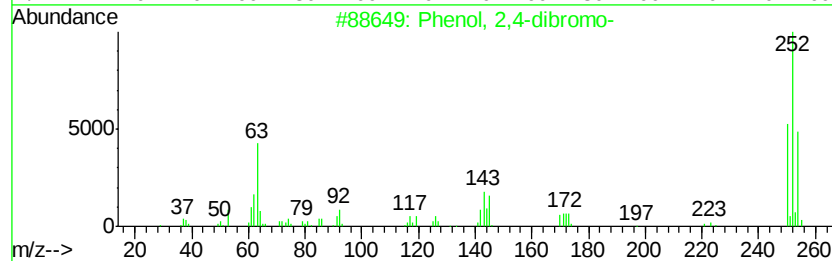
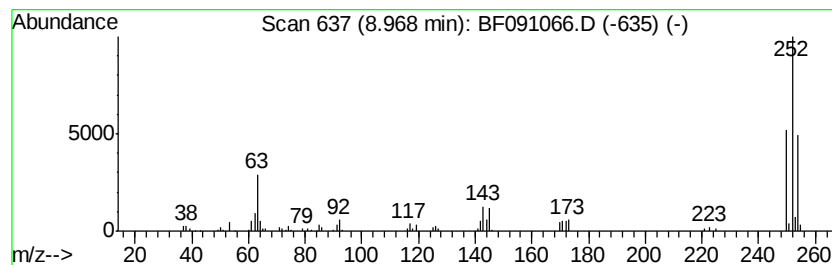
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 2,4-dibromo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
8.97	3.71 ng	245363	Acenaphthene-d10		9.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,4-dibromo-	250	C6H4Br2O	000615-58-7	99
2			Phenol, 2,6-dibromo-	250	C6H4Br2O	000608-33-3	98
3			2-Pyridinamine, 3,5-dibromo-	250	C5H4Br2N2	035486-42-1	58
4			7-Chloro-6-methoxy-4-methyl-8-ni...	252	C11H9ClN2O3	1000213-13-0	32
5			Benzene, pentachloro-	248	C6HCl5	000608-93-5	13



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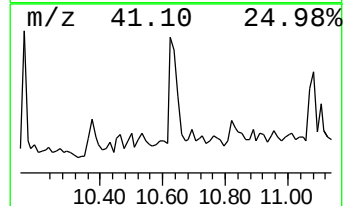
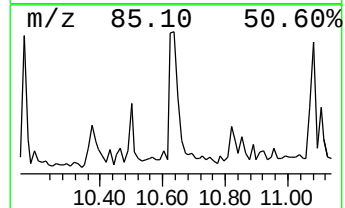
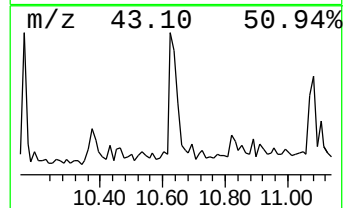
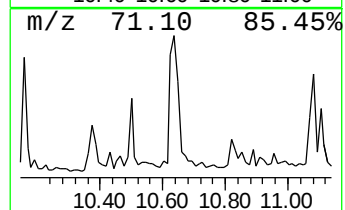
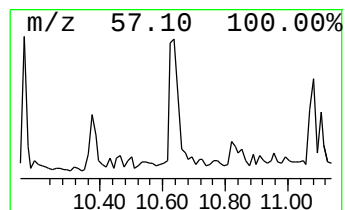
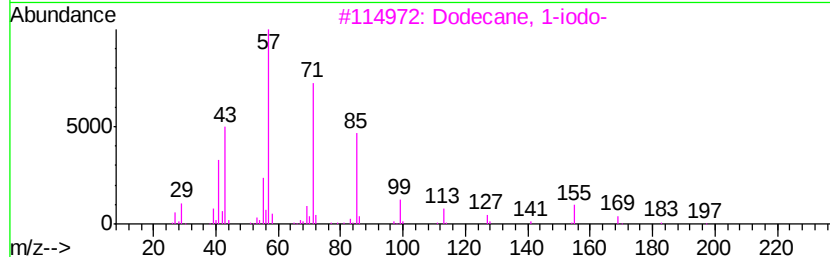
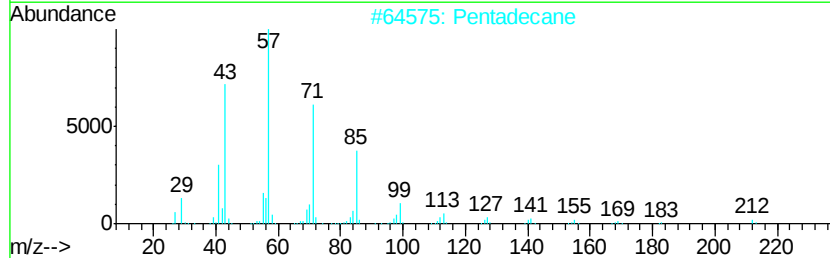
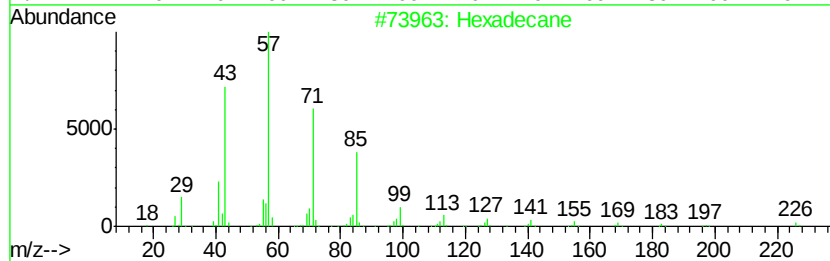
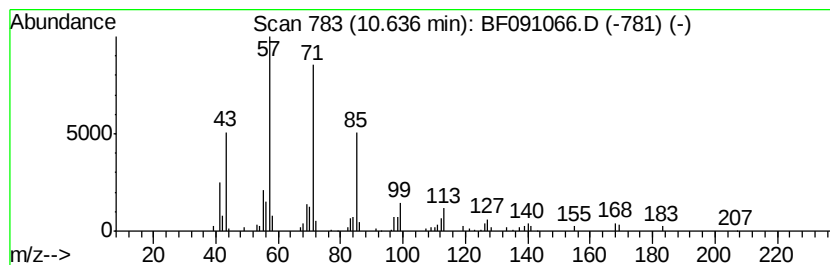
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	2.51 ng	148838	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	90
2	Pentadecane		212	C15H32	000629-62-9	86
3	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86
4	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	86
5	Tridecane, 4-methyl-		198	C14H30	026730-12-1	86



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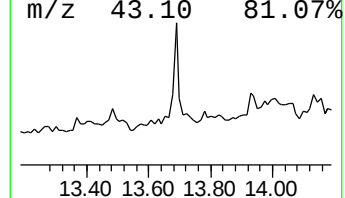
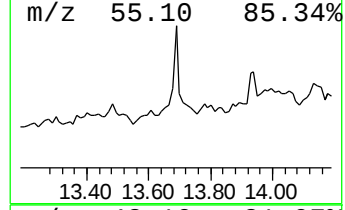
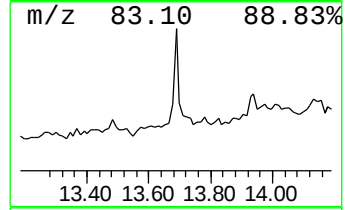
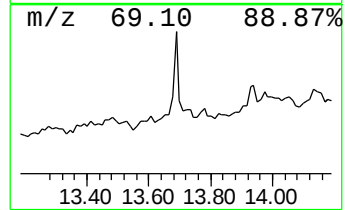
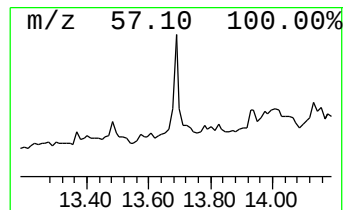
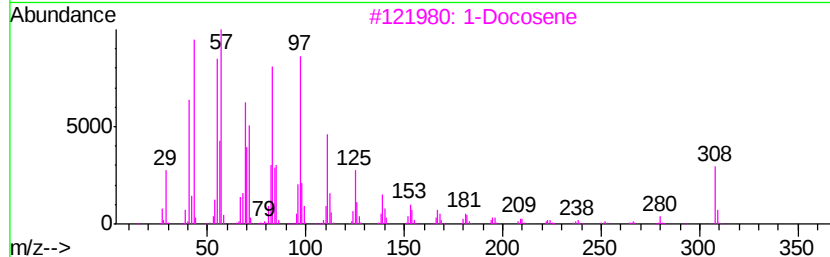
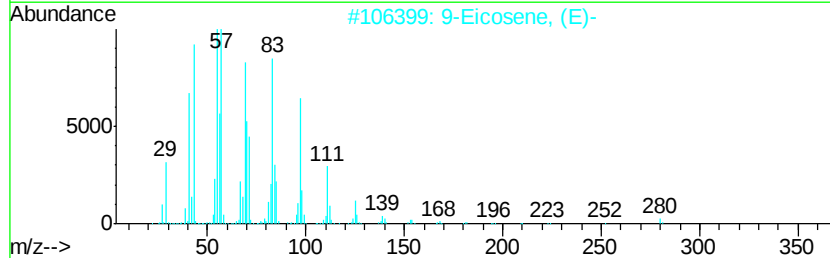
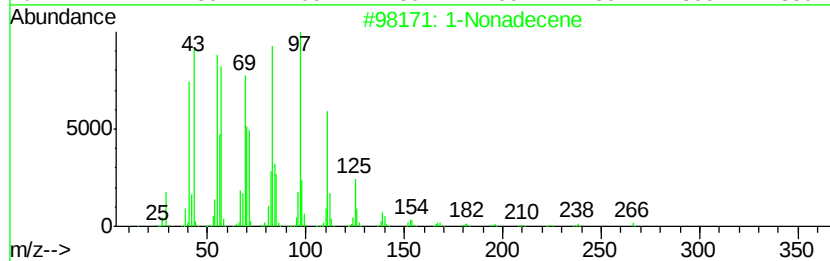
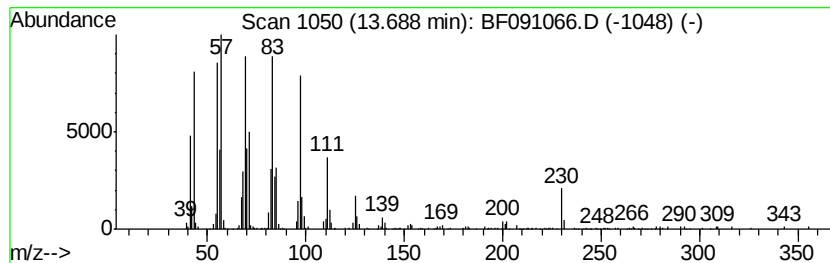
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 8 1-Nonadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.69	3.51 ng	311821	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	95
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	94
3	1-Docosene	308	C22H44	001599-67-3	92
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110716\
Data File : BF091066.D
Acq On : 7 Nov 2016 19:55
Operator : UM/SJ
Sample : H5543-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-112-0.5-1.0

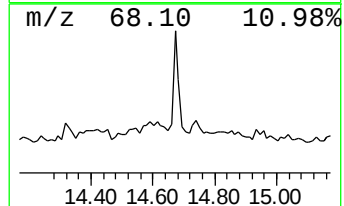
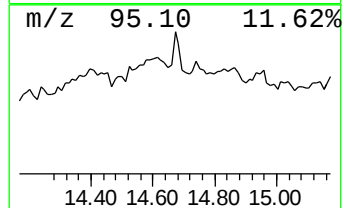
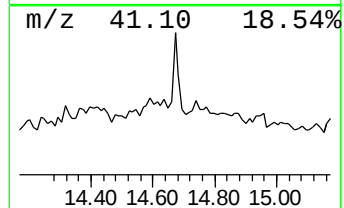
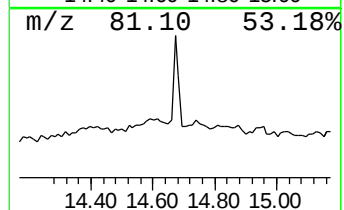
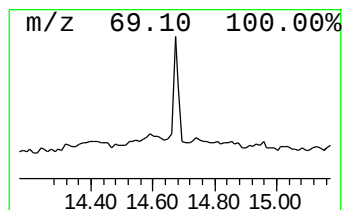
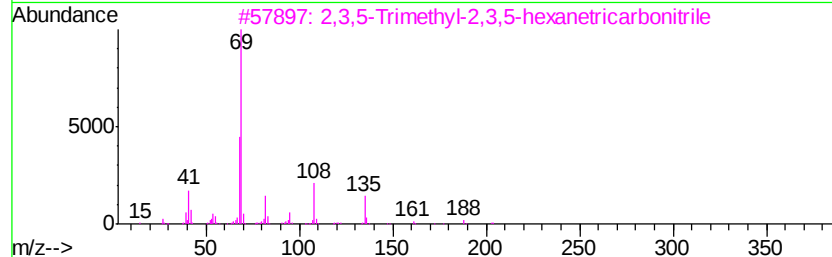
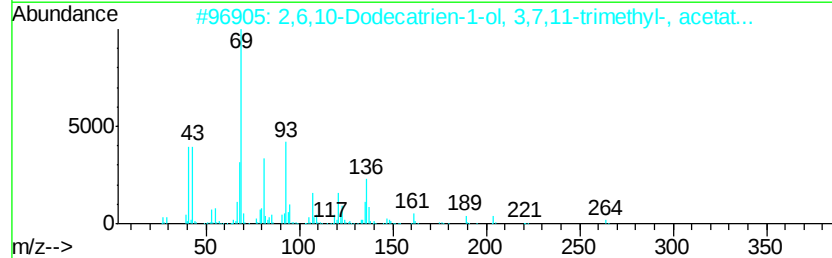
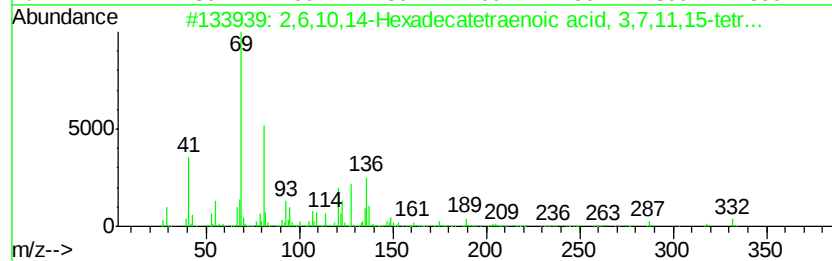
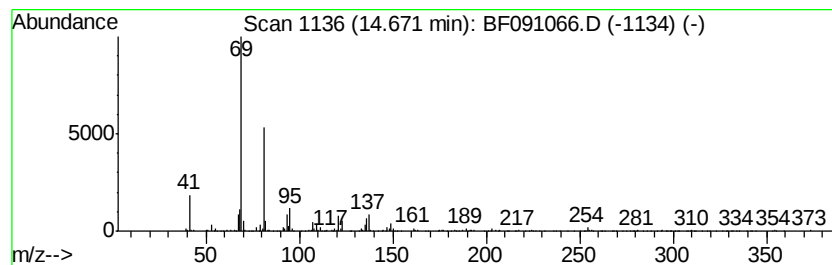
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,6,10,14-Hexadecatetraenoi... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	7.15 ng	356171	Perylene-d12	15.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
2		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
3		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59
4		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	53
5		1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110716\
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Sample : H5543-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-112-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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...	4.82	12.0	ng	624413	1	6.67	1037620	20.0
unknown6.44	6.44	83.3	ng	4321640	1	6.67	1037620	20.0
Phenol, 2,4-dibromo-	8.97	3.7	ng	245363	3	9.71	1322880	20.0
Hexadecane	10.64	2.5	ng	148838	4	11.20	1185830	20.0
1-Nonadecene	13.69	3.5	ng	311821	5	13.83	1776630	20.0
2,6,10,14-Hexadec...	14.67	7.2	ng	356171	6	15.21	996242	20.0