

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032717\
 Data File : BF093960.D
 Acq On : 27 Mar 2017 23:41
 Operator : SJ/MA
 Sample : I2409-07
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-5

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-BF032217.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	4.069	367	371	379	rVB	176128	179331	3.70%	0.534%
2	4.463	434	438	442	rBV	1964423	1812340	37.44%	5.395%
3	5.528	614	619	622	rBV	1232788	1128087	23.31%	3.358%
4	5.681	639	645	648	rBV	3208962	3271868	67.59%	9.739%
5	5.934	684	688	692	rBV	1010797	962069	19.88%	2.864%
6	6.004	696	700	712	rVB6	29834	54796	1.13%	0.163%
7	6.116	712	719	723	rBV	2971582	3009984	62.18%	8.960%
8	6.586	792	799	802	rBV	2313489	2594901	53.61%	7.724%
9	6.792	828	834	838	rBV3	52354	64396	1.33%	0.192%
10	6.963	859	863	870	rBV2	84012	141328	2.92%	0.421%
11	7.139	889	893	899	rVB3	55980	67882	1.40%	0.202%
12	7.233	902	909	915	rBV5	65069	120986	2.50%	0.360%
13	7.439	939	944	948	rVB	1358396	1351080	27.91%	4.022%
14	7.898	1016	1022	1028	rBV6	24633	48957	1.01%	0.146%
15	8.769	1160	1170	1173	rBV	4321170	4840483	100.00%	14.409%
16	9.263	1250	1254	1257	rBV	121426	121378	2.51%	0.361%
17	9.498	1292	1294	1301	rVB4	51747	69576	1.44%	0.207%
18	9.586	1301	1309	1313	rBV2	1468124	1561338	32.26%	4.648%
19	9.751	1333	1337	1338	rBV	47315	55193	1.14%	0.164%
20	9.863	1353	1356	1359	rBV	57416	60005	1.24%	0.179%
21	9.904	1360	1363	1369	rVB6	37379	56631	1.17%	0.169%
22	10.133	1397	1402	1406	rBV	499266	486742	10.06%	1.449%
23	10.174	1406	1409	1412	rVB	63372	61265	1.27%	0.182%
24	10.451	1449	1456	1459	rBV3	28420	58666	1.21%	0.175%
25	10.563	1467	1475	1478	rBV	2288088	2742033	56.65%	8.162%
26	10.757	1505	1508	1514	rBV	75983	99290	2.05%	0.296%
27	10.921	1532	1536	1539	rBV3	38726	51973	1.07%	0.155%
28	11.316	1600	1603	1606	rVB	62567	55913	1.16%	0.166%
29	11.410	1614	1619	1623	rBV	1489680	1431989	29.58%	4.263%
30	11.751	1674	1677	1681	rBV	137582	133405	2.76%	0.397%
31	12.139	1740	1743	1751	rBV3	57686	102588	2.12%	0.305%
32	13.257	1929	1933	1937	rBV	187234	181403	3.75%	0.540%
33	13.392	1950	1956	1960	rBV	3452481	4315818	89.16%	12.847%
34	14.115	2076	2079	2084	rBV2	73825	84206	1.74%	0.251%

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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-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.545	2149	2152	2158	rVB	123006	138658	2.86%	0.413%
36	14.662	2167	2172	2176	rBV	1139388	1187778	24.54%	3.536%
37	16.298	2445	2450	2454	rBV	730410	890046	18.39%	2.649%

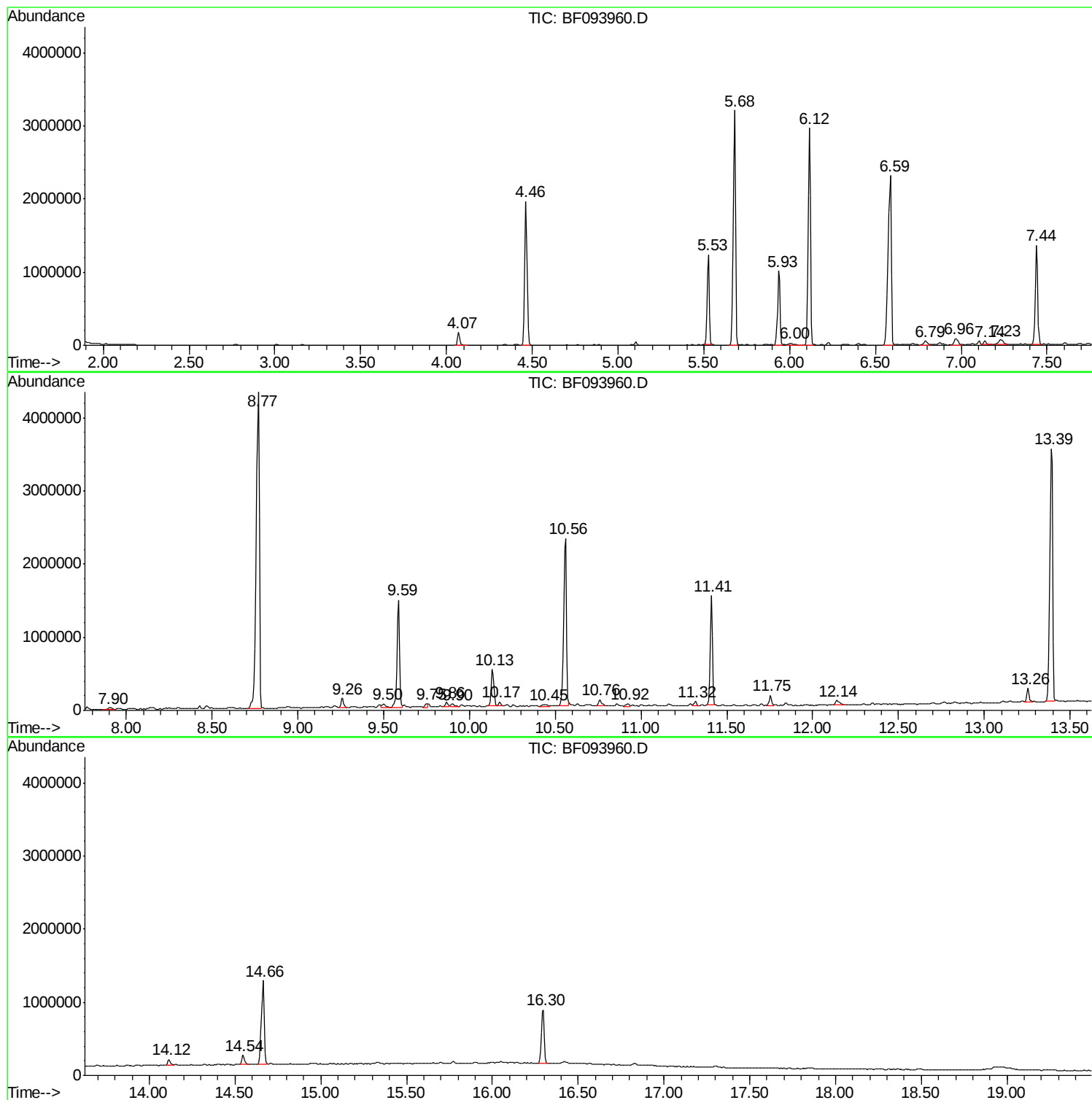
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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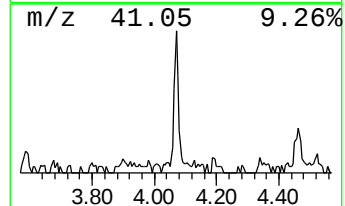
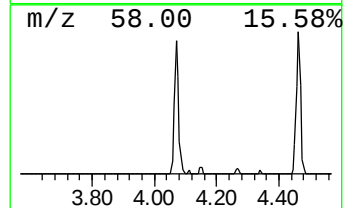
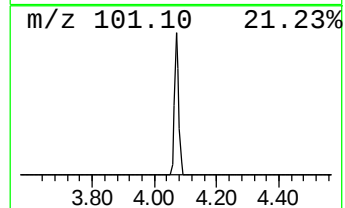
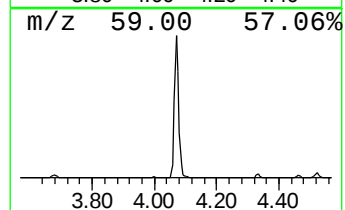
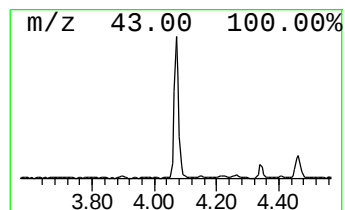
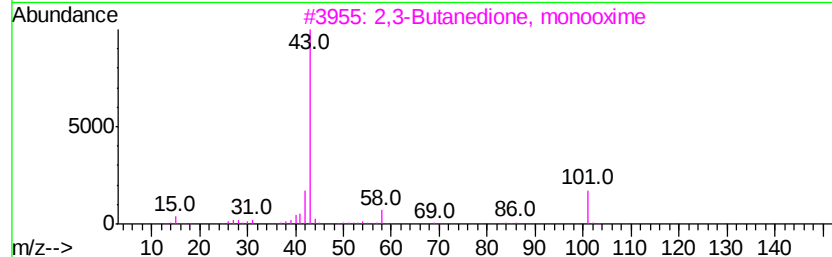
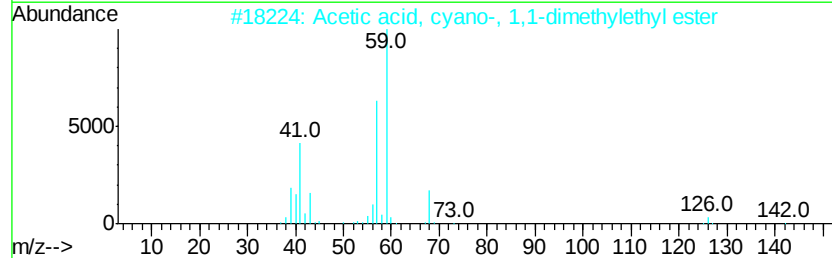
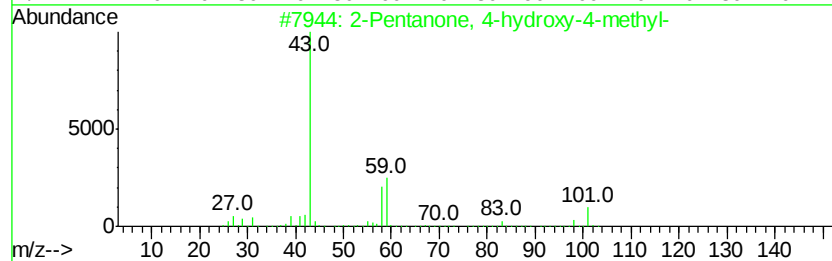
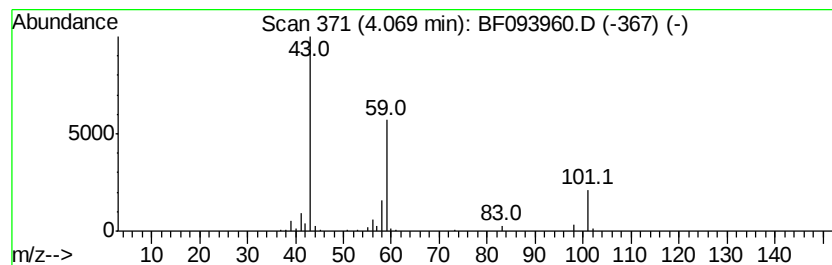
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.07	3.73 ng	179331	1,4-Dichlorobenzene-d4	5.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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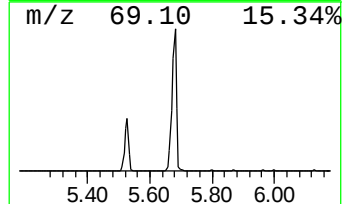
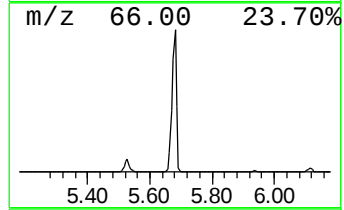
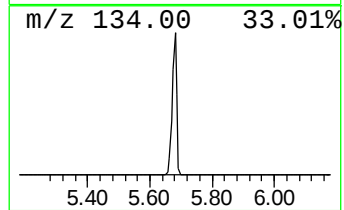
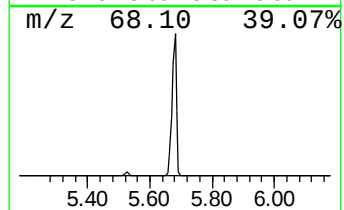
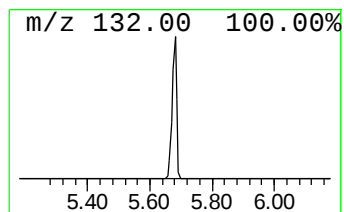
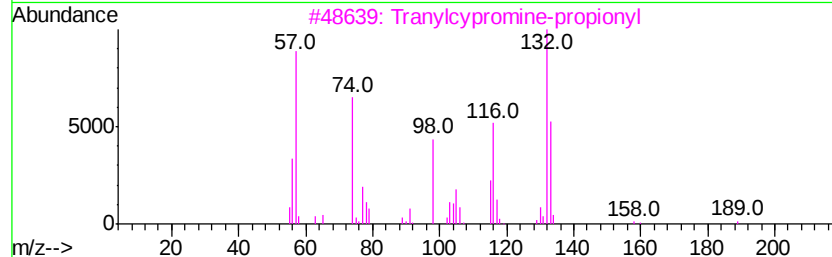
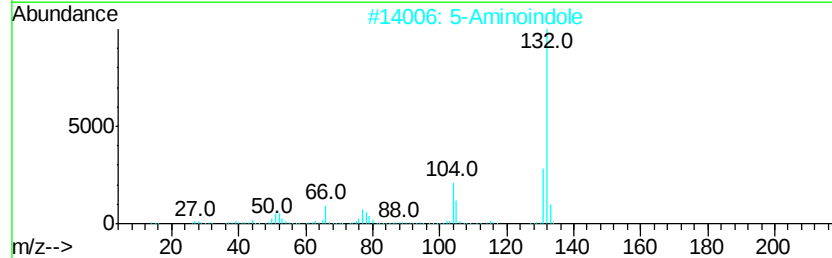
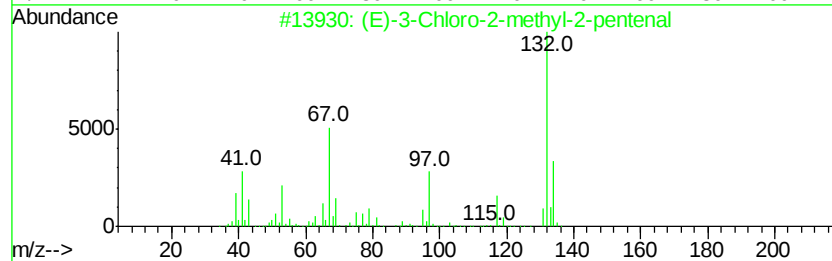
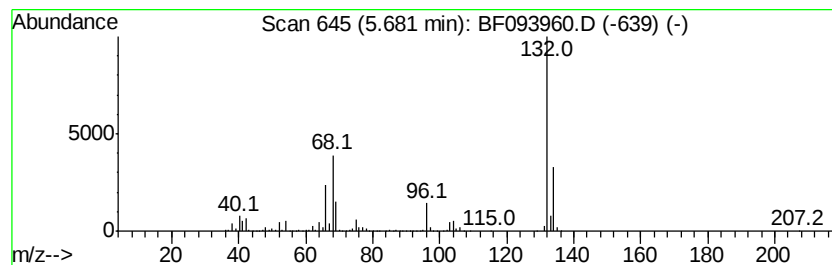
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	68.02 ng	3271870	1,4-Dichlorobenzene-d4	5.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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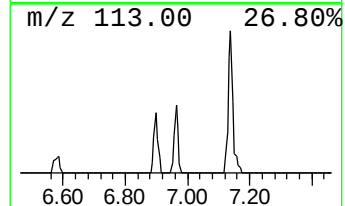
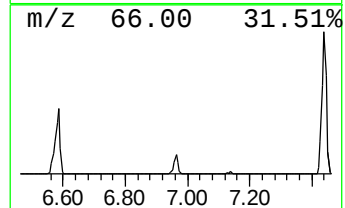
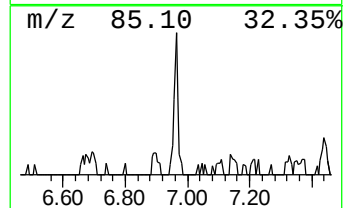
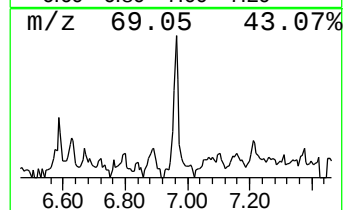
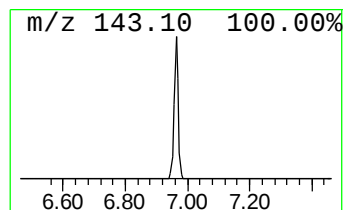
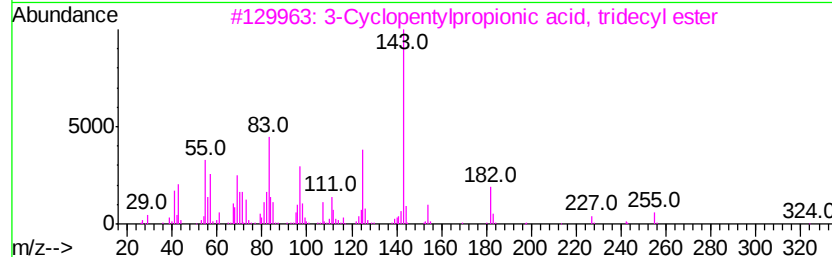
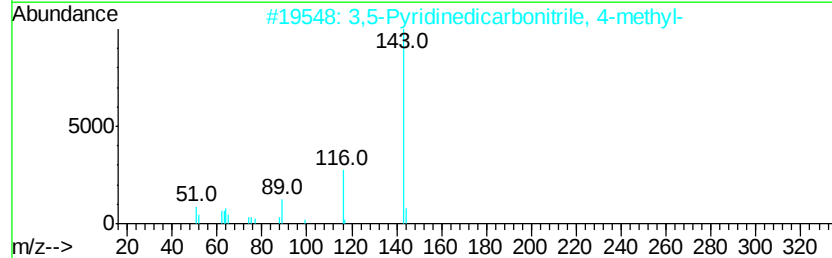
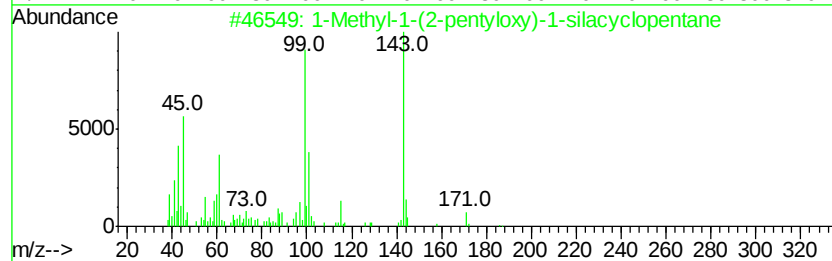
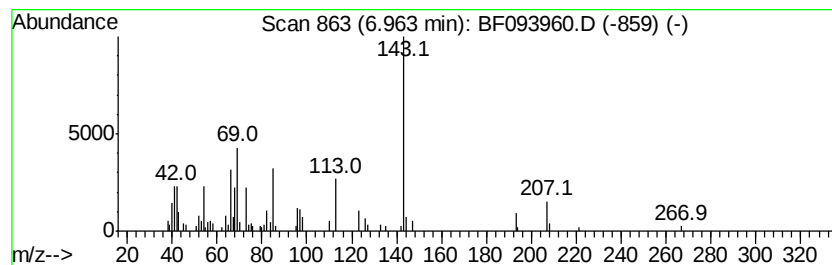
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.96 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	2.09 ng	141328	Naphthalene-d8	7.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-1-(2-pentyl-oxo)-1-silacyclopentane	186	C10H22OSi	1000216-95-9	14		
2	3,5-Pyridinedicarbonitrile, 4-methyl-	143	C8H5N3	004574-75-8	14		
3	3-Cyclopentylpropionic acid, triethyl ester	324	C21H40O2	1000292-33-7	12		
4	3-Aminophthalonitrile	143	C8H5N3	058632-96-5	10		
5	(3H,6H)Thieno[3,4-c]isoxazole, 3-methyl-	143	C6H9NOS	1000115-56-0	9		



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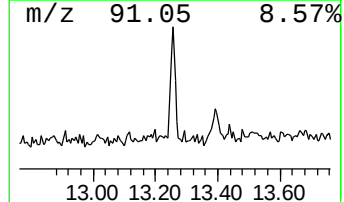
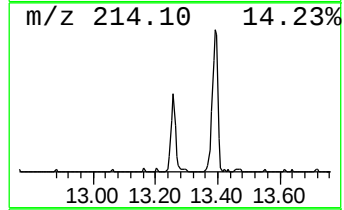
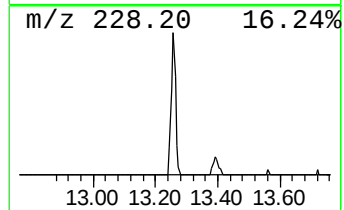
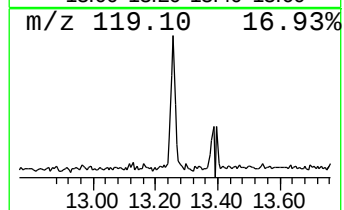
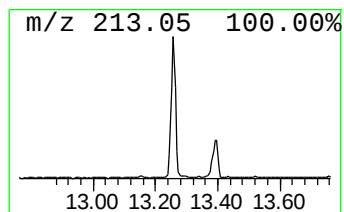
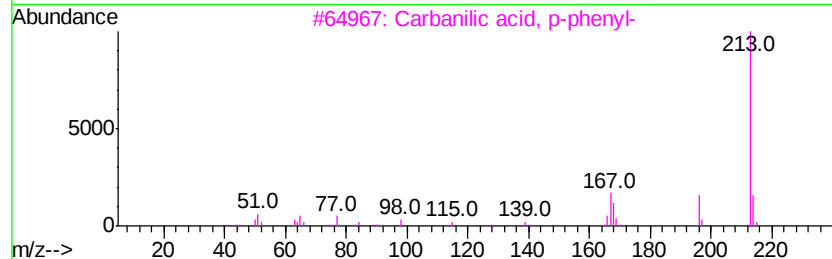
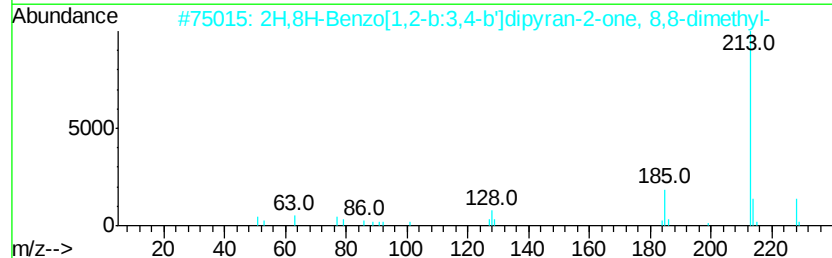
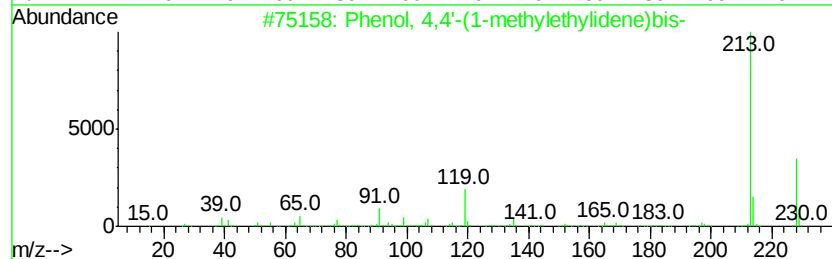
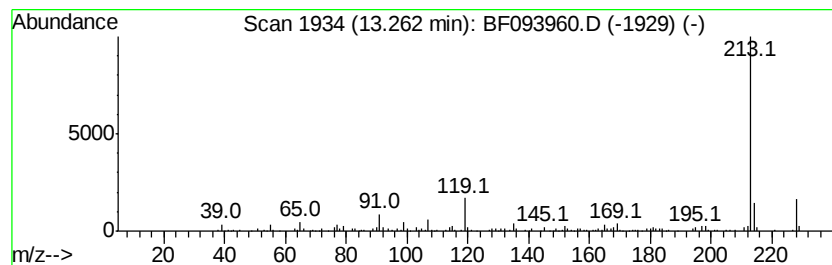
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	3.05 ng	181403	Chrysene-d12	14.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97	
2	2H,8H-Benzo[1,2-b:3,4-b']dipyr...	228	C14H12O3	000523-59-1	53	
3	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52	
4	1,4-Naphthalenedione, 2-(1-buten...	228	C14H12O3	029366-43-6	50	
5	Carbamic acid, [1,1'-biphenyl]-3...	213	C13H11NO2	055030-29-0	50	



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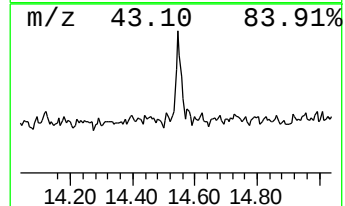
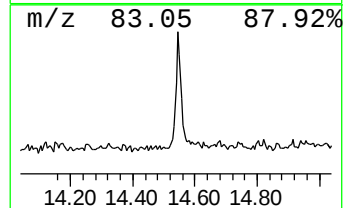
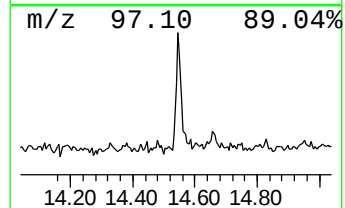
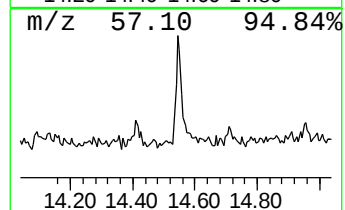
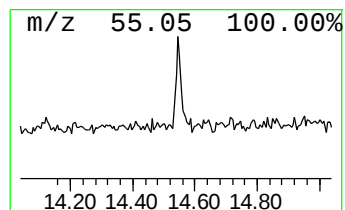
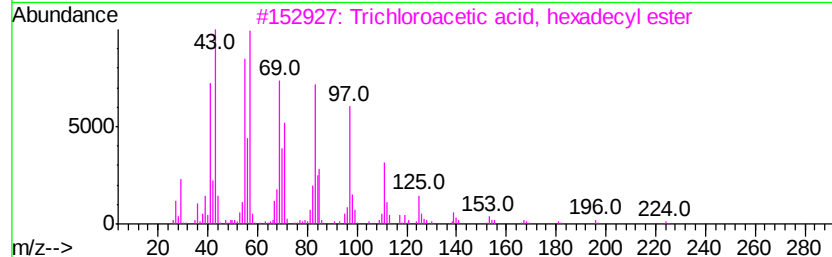
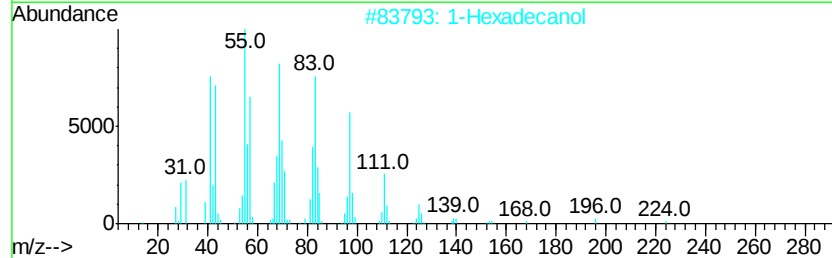
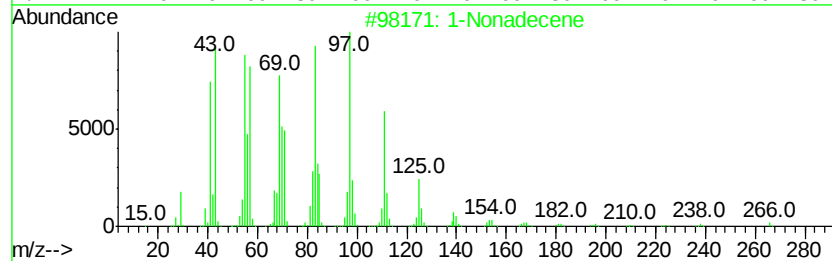
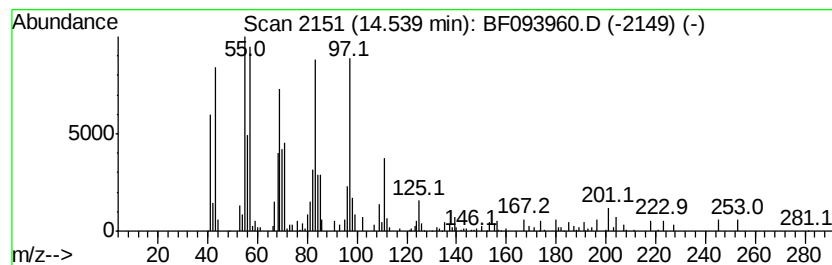
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	2.33 ng	138658	Chrysene-d12	14.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	91
2	1-Hexadecanol		242	C16H34O	036653-82-4	87
3	Trichloroacetic acid, hexadecyl ...		386	C18H33Cl3O2	074339-54-1	81
4	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	81
5	Bromoacetic acid, pentadecyl ester		348	C17H33BrO2	131143-01-6	76



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032717\
Data File : BF093960.D
Acq On : 27 Mar 2017 23:41
Operator : SJ/MA
Sample : I2409-07
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.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...	4.07	3.7	ng	179331	1	5.93	962069	20.0
unknown5.68	5.68	68.0	ng	3271870	1	5.93	962069	20.0
unknown6.96	6.96	2.1	ng	141328	2	7.44	1351080	20.0
Phenol, 4,4'-(1-m...	13.26	3.0	ng	181403	5	14.66	1187780	20.0
1-Nonadecene	14.54	2.3	ng	138658	5	14.66	1187780	20.0