

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101215\
 Data File : BF082218.D
 Acq On : 12 Oct 2015 13:19
 Operator : UM/IZ
 Sample : G3959-02
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FB

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 1 % 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-BF101015.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	4.994	248	250	259	rVB	293422	347929	9.71%	1.701%
2	5.417	285	287	290	rBV	892783	943434	26.34%	4.613%
3	6.457	376	378	381	rBV	533282	570082	15.92%	2.787%
4	6.594	388	390	393	rBV	1720904	1836188	51.27%	8.978%
5	6.835	409	411	413	rBV	413486	482934	13.48%	2.361%
6	6.983	422	424	427	rBV	1505243	1951242	54.48%	9.541%
7	7.406	458	461	463	rBV	1454987	1635389	45.66%	7.996%
8	8.115	521	523	526	rBV	586045	642200	17.93%	3.140%
9	9.200	615	618	620	rBV	3188095	3102830	86.64%	15.171%
10	9.875	675	677	680	rBV	913482	819929	22.89%	4.009%
11	10.675	744	747	749	rBV2	1303206	1933346	53.98%	9.453%
12	11.361	805	807	810	rBV	878977	816530	22.80%	3.992%
13	11.886	849	853	855	rBV	51505	54996	1.54%	0.269%
14	12.195	878	880	884	rBV	40565	48234	1.35%	0.236%
15	12.961	944	947	949	rBV	2523668	3581477	100.00%	17.512%
16	13.635	1004	1006	1008	rBV	136790	116903	3.26%	0.572%
17	14.001	1036	1038	1041	rBV	846345	832101	23.23%	4.069%
18	15.441	1161	1164	1173	rBV	547352	736127	20.55%	3.599%

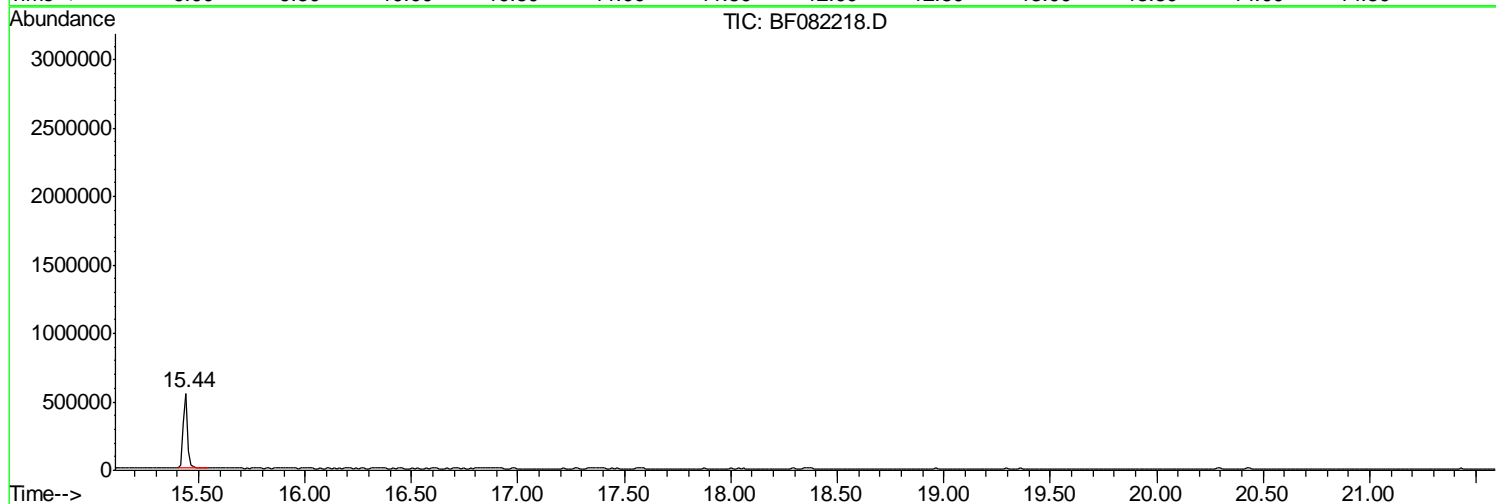
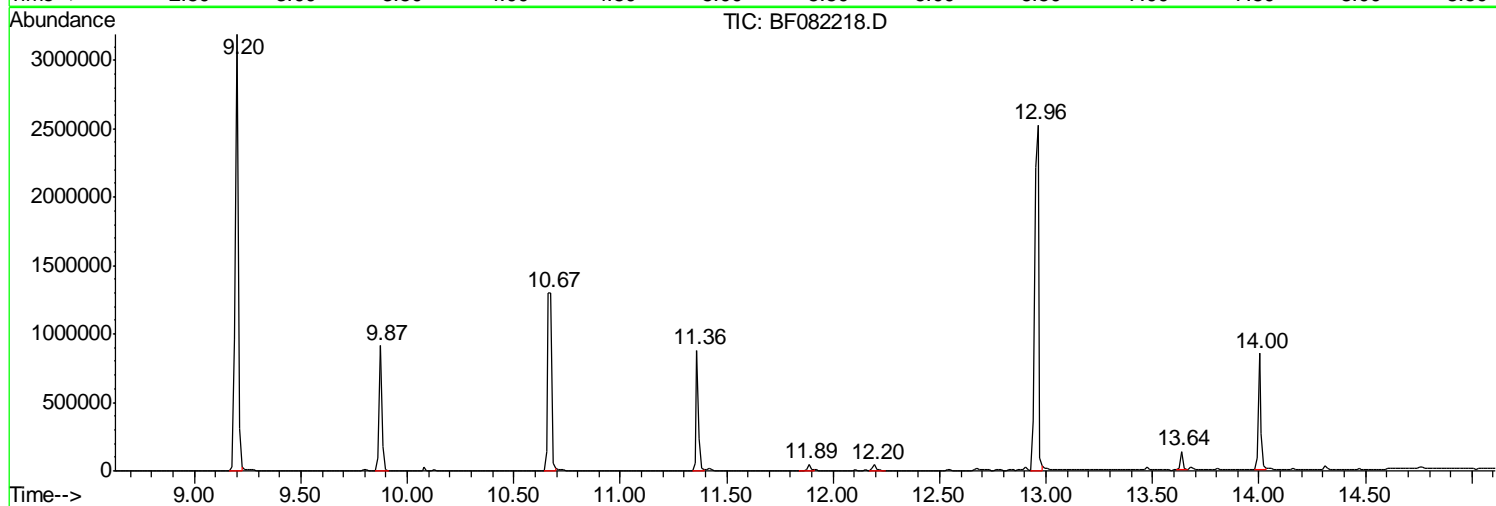
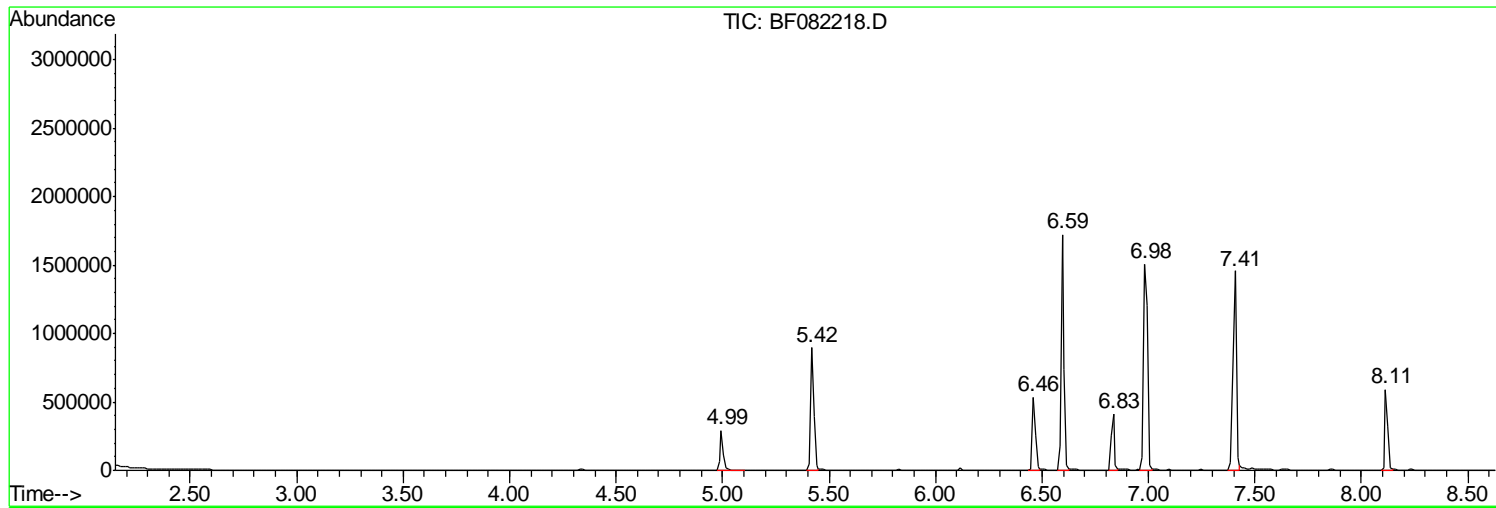
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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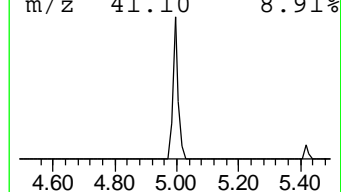
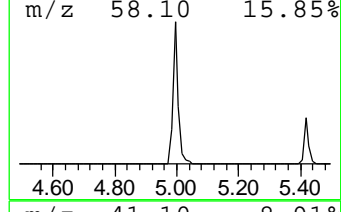
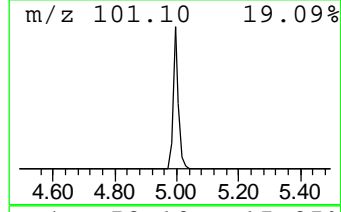
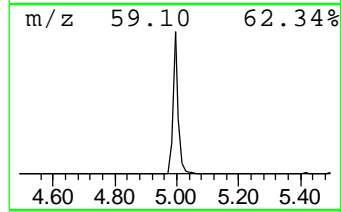
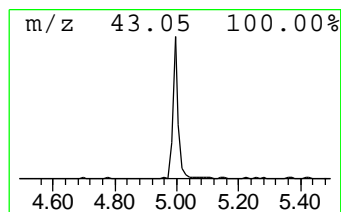
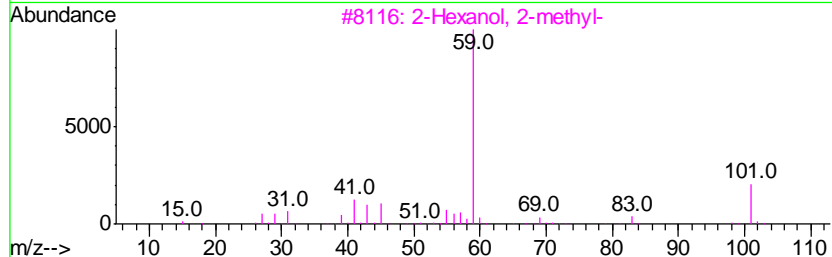
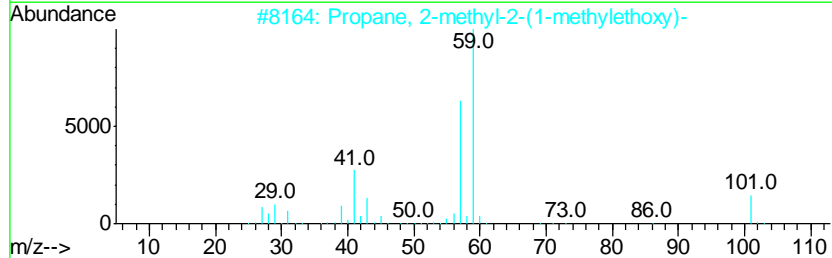
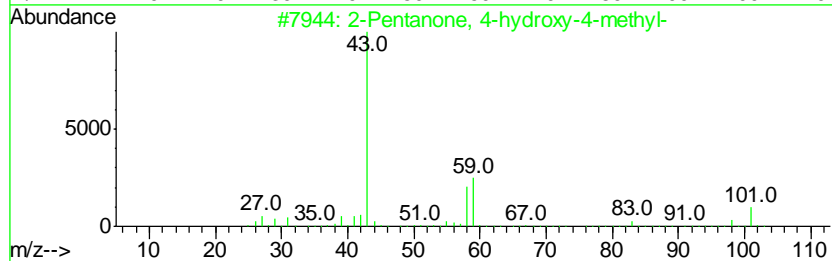
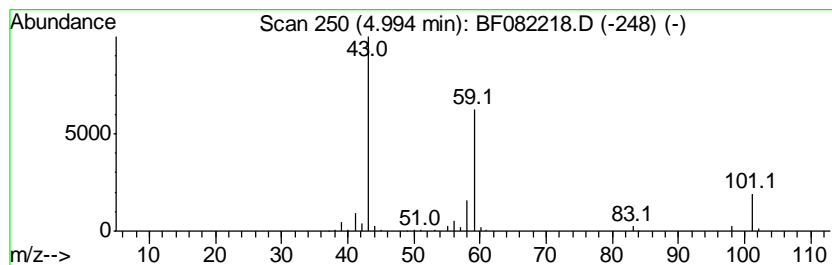
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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	14.41 ng	347929	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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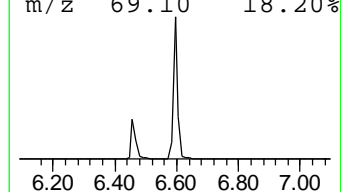
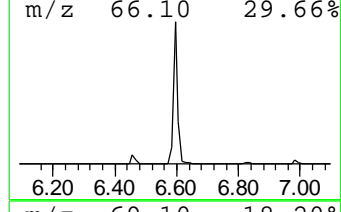
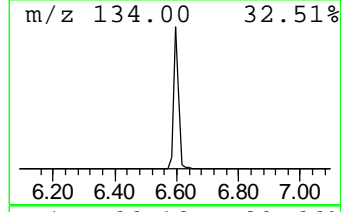
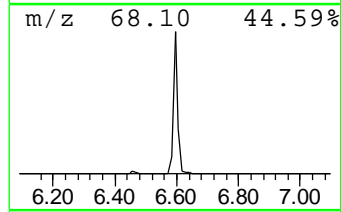
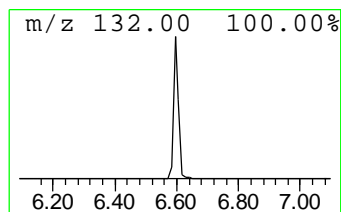
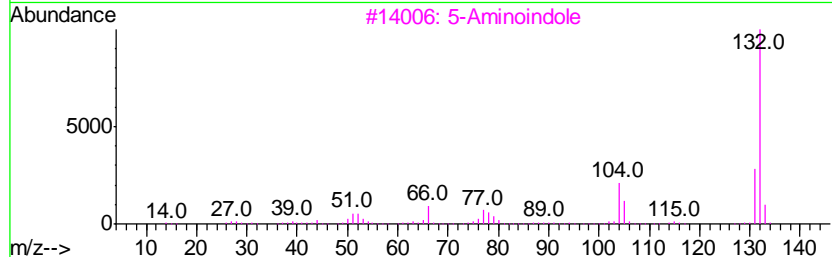
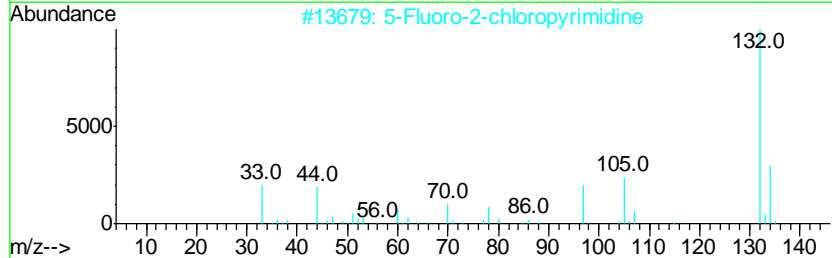
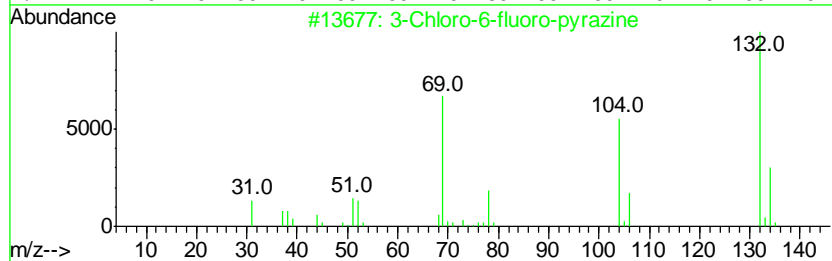
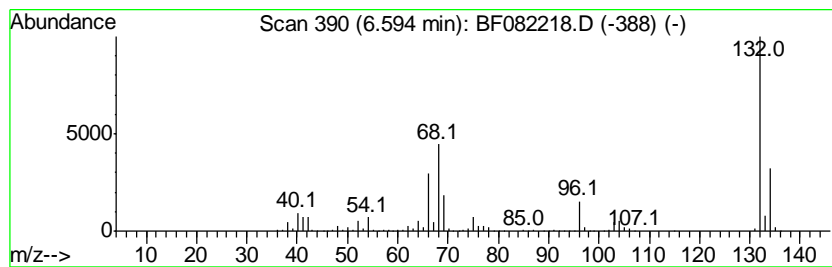
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 TIC Integration Parameters: LSCINT.P

 Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	76.04 ng	1836190	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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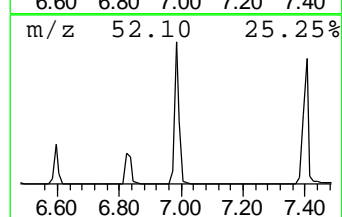
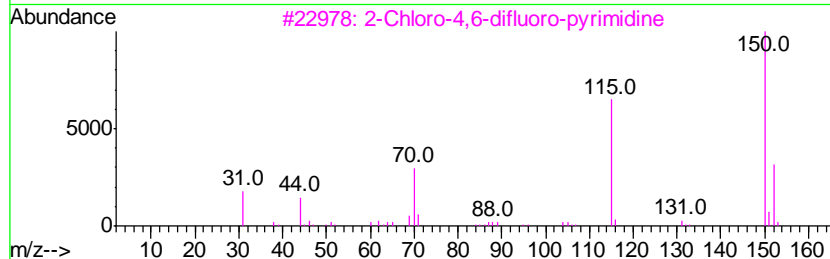
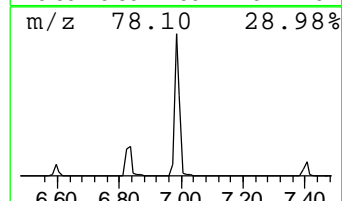
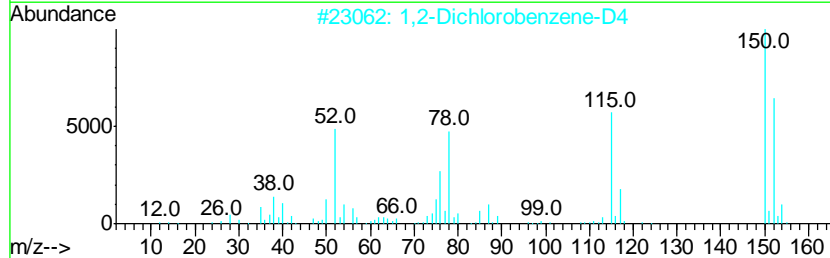
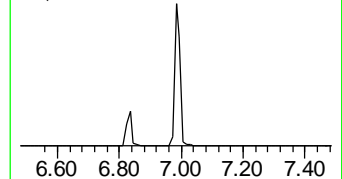
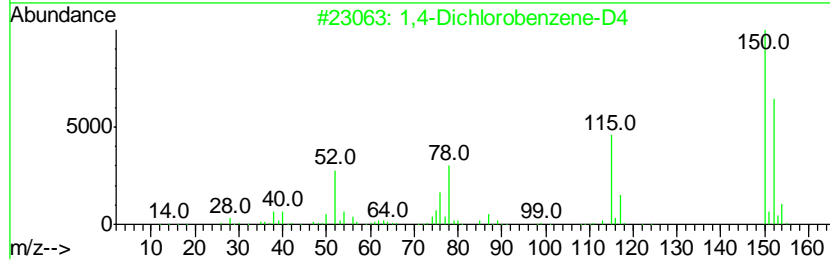
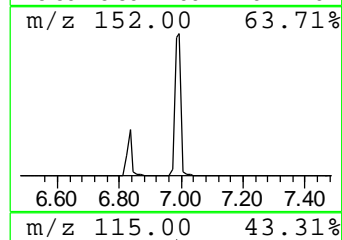
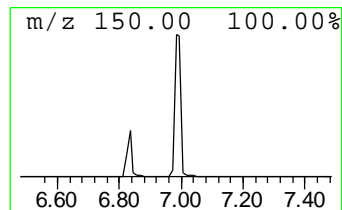
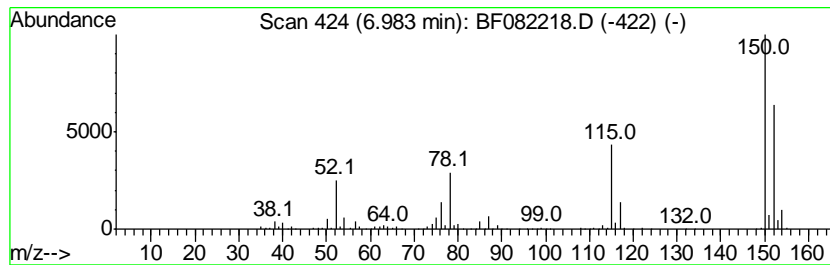
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 Peak Number 3 1,4-Dichlorobenzene-D4 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	80.81 ng	1951240	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	95
2		1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94
3		2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	35
4		2-Bromo-2'-nitroacetophenone	243	C8H6BrNO3	006851-99-6	14
5		2-Bromo-3'-nitroacetophenone	243	C8H6BrNO3	002227-64-7	10



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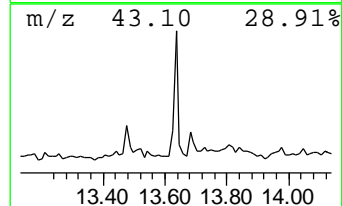
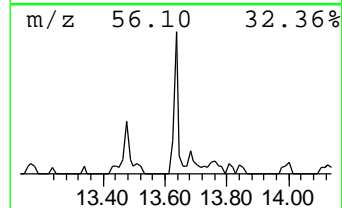
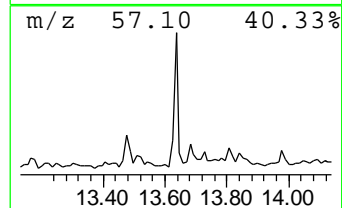
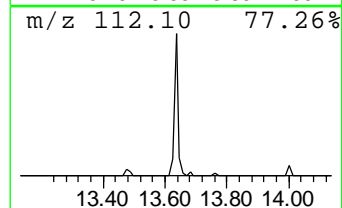
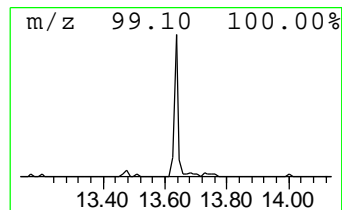
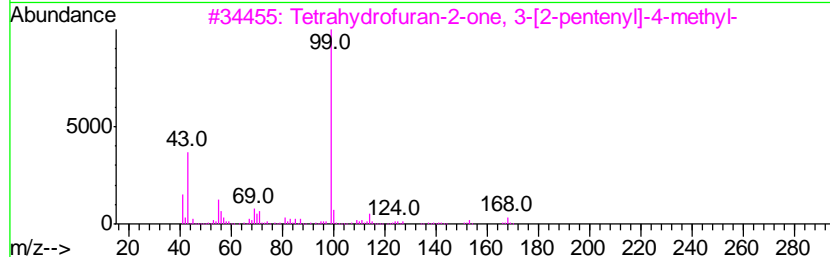
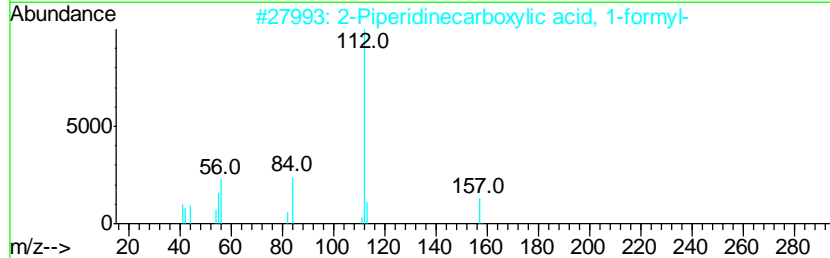
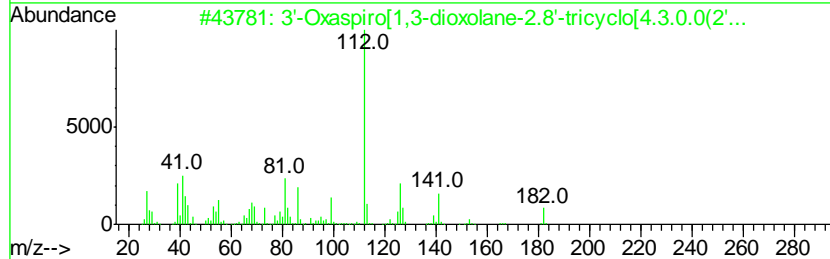
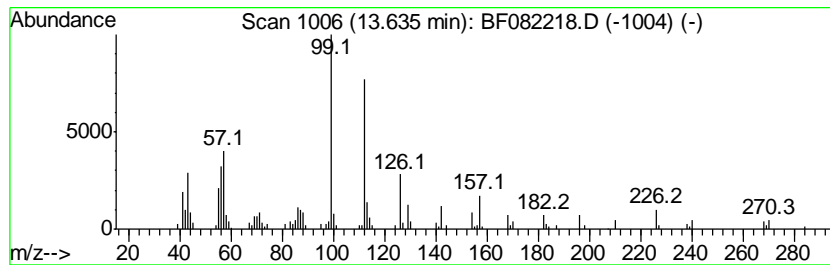
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 TIC Integration Parameters: LSCINT.P

 Peak Number 4 3'-Oxaspiro[1,3-dioxolane-2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	2.81 ng	116903	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3'-Oxaspiro[1,3-dioxolane-2.8'-t...	182	C10H14O3	1000150-55-1	30
2		2-Piperidinecarboxylic acid, 1-f...	157	C7H11NO3	054966-20-0	27
3		Tetrahydrofuran-2-one, 3-[2-pent...	168	C10H16O2	1000132-08-6	25
4		4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	25
5		1,4-Dioxaspiro[4.5]decane	142	C8H14O2	000177-10-6	25



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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...	4.99	14.4	ng	347929	1	6.83	482934	20.0
3-Chloro-6-fluoro...	6.59	76.0	ng	1836190	1	6.83	482934	20.0
1,4-Dichlorobenze...	6.98	80.8	ng	1951240	1	6.83	482934	20.0
3'-Oxaspiro[1,3-d...	13.64	2.8	ng	116903	5	14.00	832101	20.0