

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111516\
 Data File : BF091170.D
 Acq On : 15 Nov 2016 10:46
 Operator : UM/SJ
 Sample : H5643-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1-111016

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	1.744	3	5	29	rVB	3022342	8334191	100.00%	16.558%
2	2.030	29	30	33	rVV2	115690	162619	1.95%	0.323%
3	2.076	33	34	42	rVV	64053	96670	1.16%	0.192%
4	2.178	42	43	46	rVB	73411	84600	1.02%	0.168%
5	4.762	267	269	281	rBV	375965	564061	6.77%	1.121%
6	5.219	307	309	326	rBV	2276669	2564841	30.77%	5.096%
7	6.282	400	402	410	rBV	1535259	1715601	20.59%	3.408%
8	6.407	410	413	415	rBV	3419828	4462668	53.55%	8.866%
9	6.636	431	433	442	rVB	837921	957726	11.49%	1.903%
10	6.785	444	446	449	rBV	3255549	4044322	48.53%	8.035%
11	7.207	480	483	485	rBV	3185796	3337802	40.05%	6.631%
12	7.916	543	545	548	rBV	1051917	1320864	15.85%	2.624%
13	8.465	589	593	595	rVB	95195	158242	1.90%	0.314%
14	9.002	637	640	642	rBV	5641085	5614921	67.37%	11.155%
15	9.402	673	675	682	rVB	94987	89041	1.07%	0.177%
16	9.665	696	698	701	rBV	1494494	1573207	18.88%	3.125%
17	10.465	765	768	770	rBV	3139586	4110117	49.32%	8.166%
18	11.151	825	828	830	rBV	1568492	1638002	19.65%	3.254%
19	12.739	964	967	969	rBV	5906901	6814848	81.77%	13.539%
20	13.780	1055	1058	1060	rBV	1323643	1534855	18.42%	3.049%
21	15.140	1175	1177	1180	rBV	894581	1155439	13.86%	2.296%

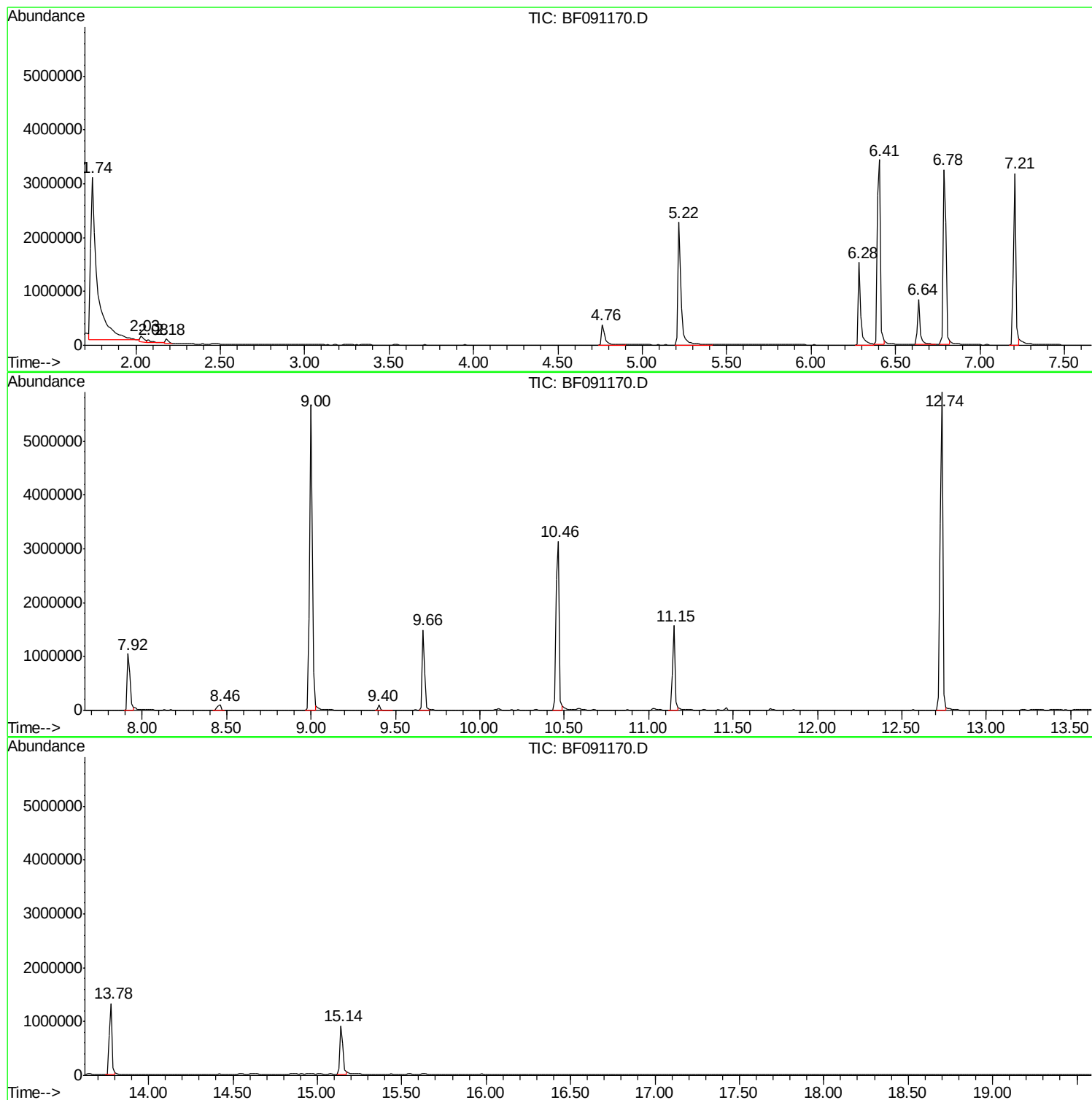
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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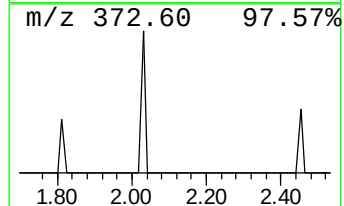
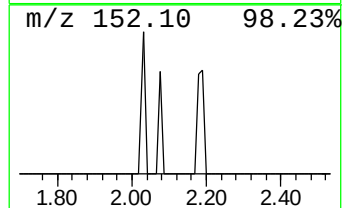
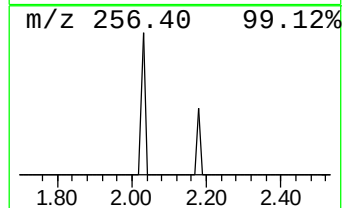
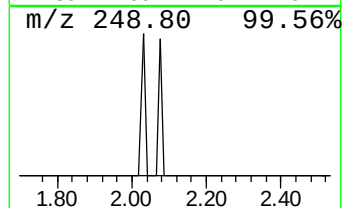
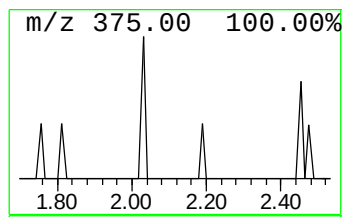
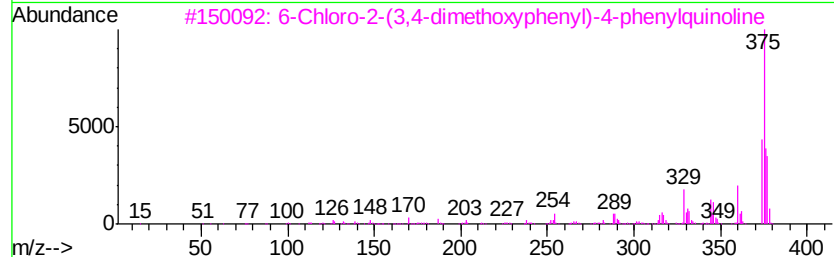
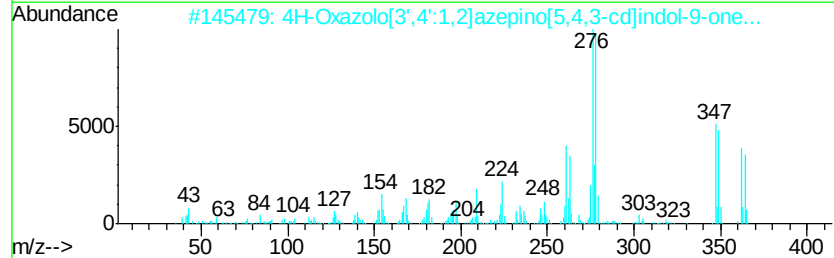
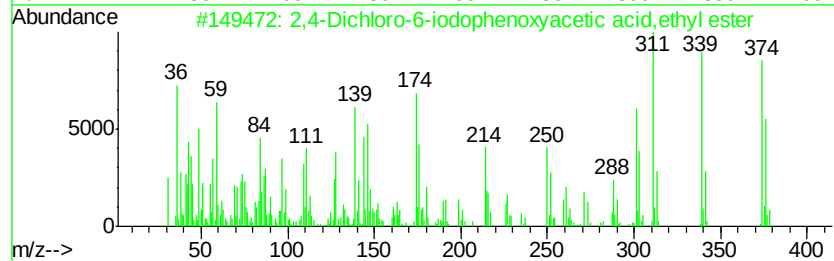
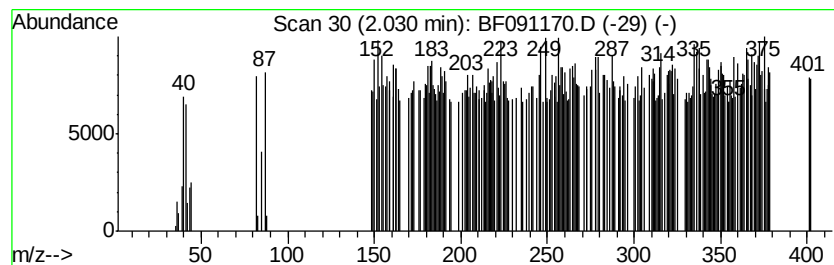
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4-Dichloro-6-iodophenoxya... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.03	3.40 ng	162619	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dichloro-6-iodophenoxyacetic...	374	C10H9Cl2IO3	1000281-36-6	90
2			4H-Oxazolo[3',4':1,2]azepino[5,4...	362	C17H19BrN2O2	1000276-61-6	58
3			6-Chloro-2-(3,4-dimethoxyphenyl)...	375	C23H18ClNO2	021923-47-7	35
4			N-[(4,6-Dimethoxynaphthalen-1-yl...	375	C19H15Cl2NO3	1000256-82-3	27
5			3,6-Dibromo-1,2:4,5-benzenetetra...	374	C10Br2O6	024848-78-0	25



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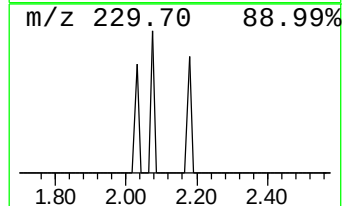
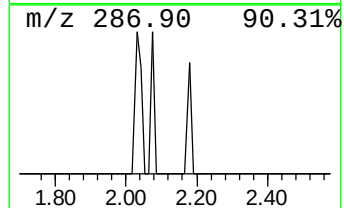
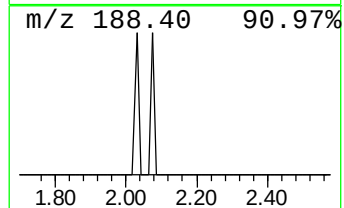
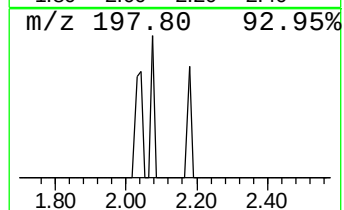
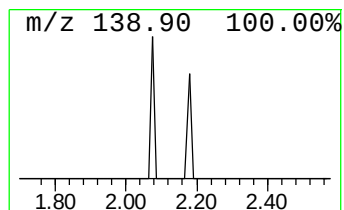
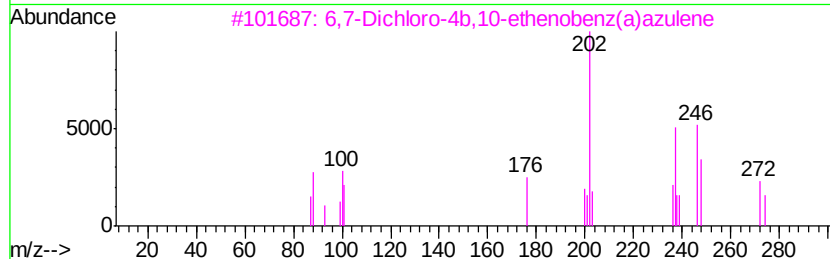
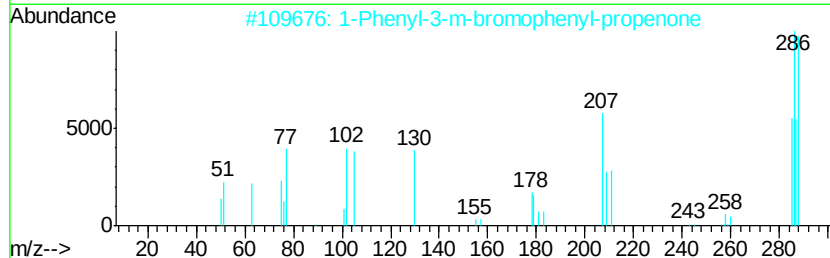
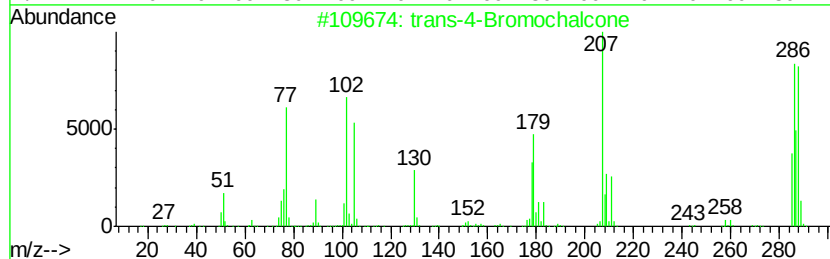
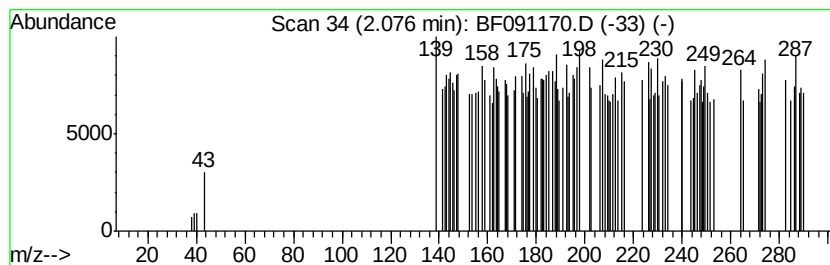
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown2.08 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.08	2.02 ng	96670	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-4-Bromochalcone	286	C15H11BrO	022966-09-2	20
2		1-Phenyl-3-m-bromophenyl-propenone	286	C15H11BrO	1000148-60-7	18
3		6,7-Dichloro-4b,10-ethenobenz(a)...	272	C16H10Cl2	110190-25-5	14
4		2,5-Dimethyl-4,6-dibenzyl-pyridine	287	C21H21N	036063-39-5	14
5		Mercury(II) chloride	272	Cl2Hg	007487-94-7	10



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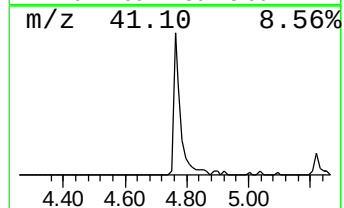
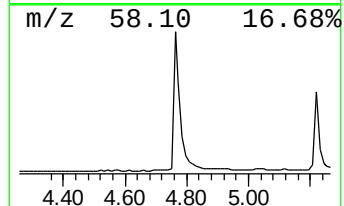
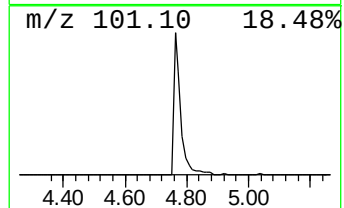
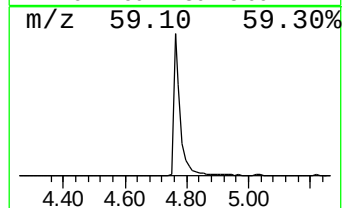
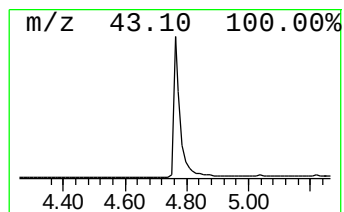
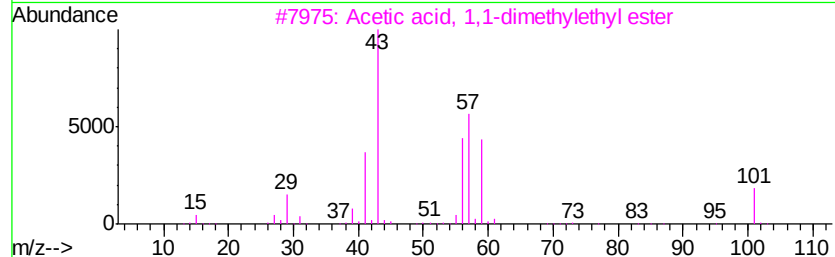
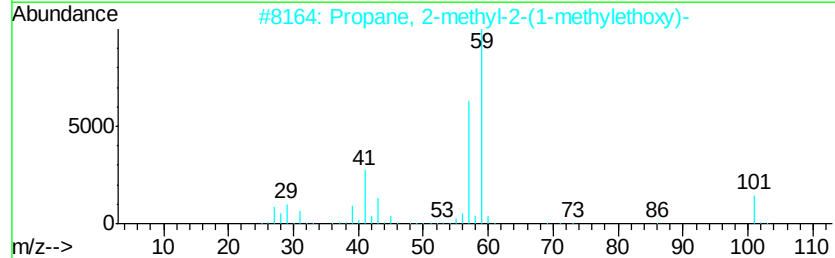
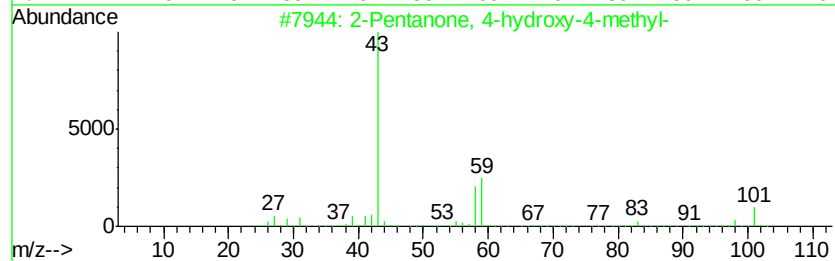
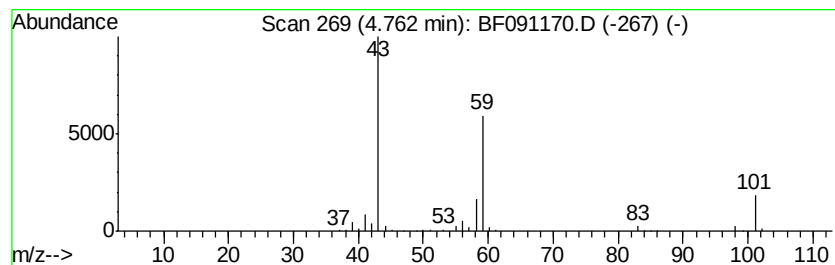
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	11.78 ng	564061	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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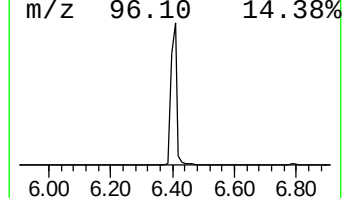
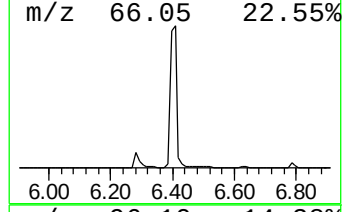
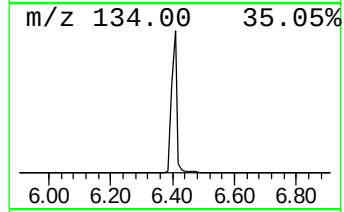
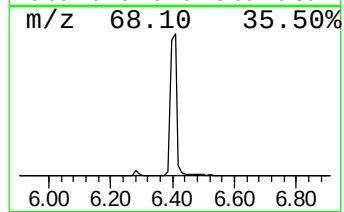
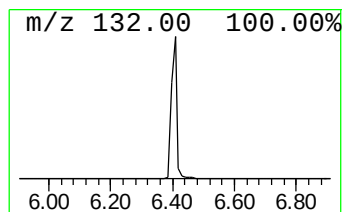
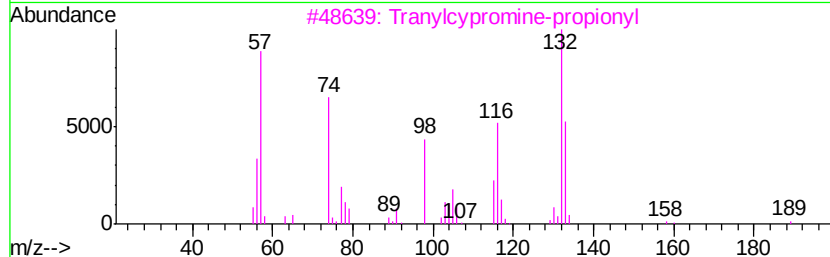
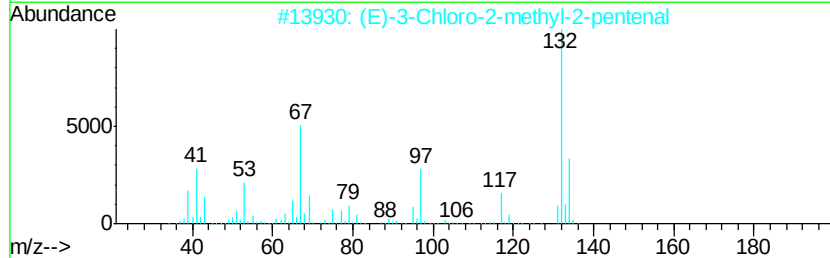
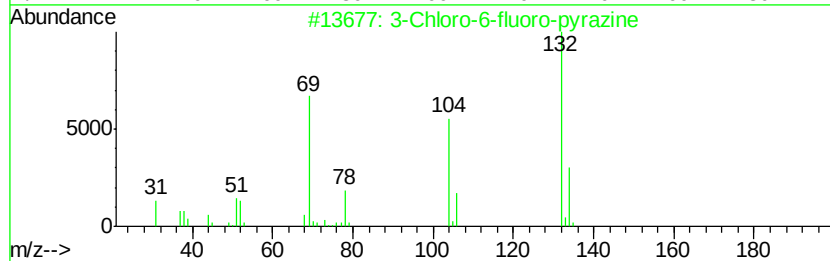
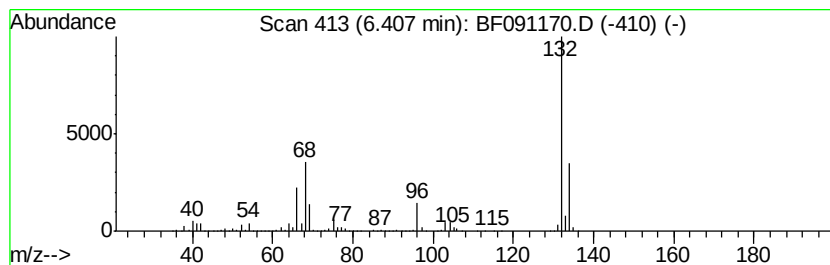
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Peak Number 5 unknown6.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	93.19 ng	4462670	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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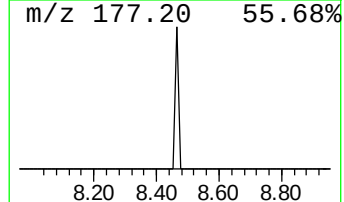
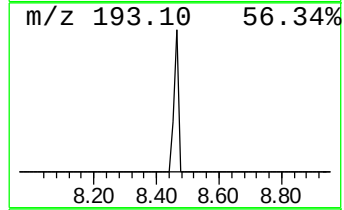
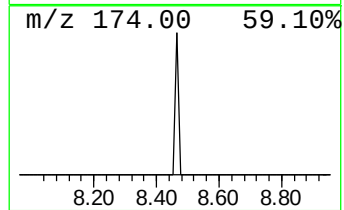
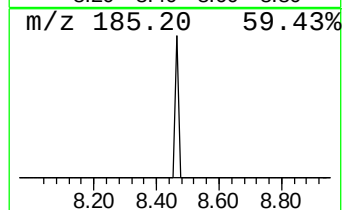
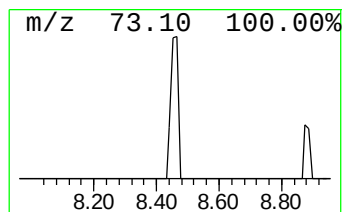
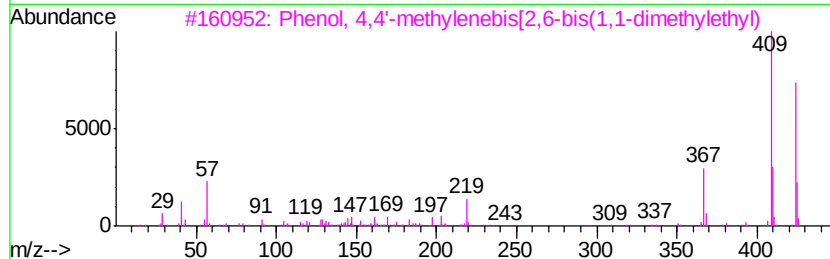
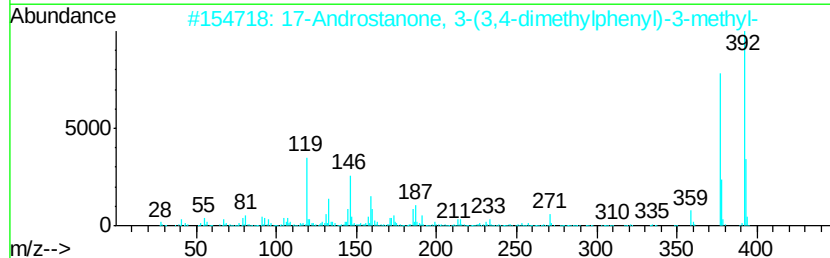
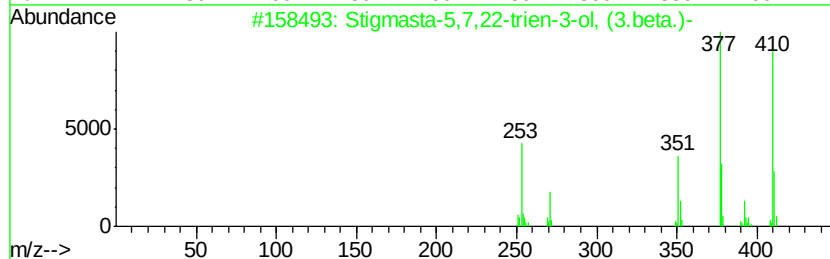
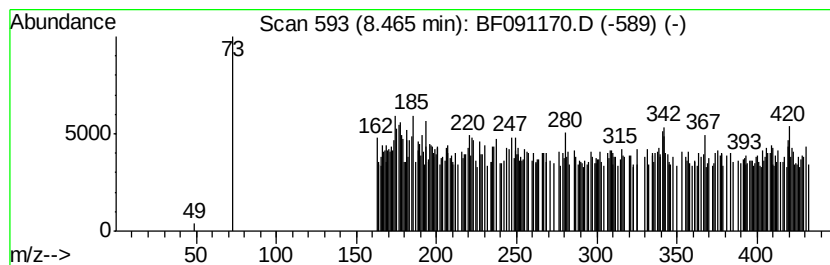
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown8.46 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	2.40 ng	158242	Napthalene-d8	7.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Stigmasta-5,7,22-trien-3-ol, (3....	410	C29H46O	000481-19-6	10
2		17-Androstanone, 3-(3,4-dimethyl...	392	C28H40O	1000197-51-6	9
3		Phenol, 4,4'-methylenebis[2,6-bi...	424	C29H44O2	000118-82-1	9
4		22-Desoxycarpesterol	546	C37H54O3	040129-53-1	9
5		2,4-Diamino-6,7-bis[4-chlorobenz...	410	C20H16Cl2N6	049647-21-4	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4-Dichloro-6-io...	2.03	3.4	ng	162619	1	6.64	957726	20.0
unknown2.08	2.08	2.0	ng	96670	1	6.64	957726	20.0
2-Pentanone, 4-hy...	4.76	11.8	ng	564061	1	6.64	957726	20.0
unknown6.41	6.41	93.2	ng	4462670	1	6.64	957726	20.0
unknown8.46	8.46	2.4	ng	158242	2	7.92	1320860	20.0