

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070815\
 Data File : BF080387.D
 Acq On : 8 Jul 2015 14:54
 Operator : TP/UM
 Sample : PB84381BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84381BL

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-BF070615.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	2.190	7	9	15	rVB	29280	36472	2.27%	0.317%
2	2.407	26	28	31	rVB	14884	20320	1.26%	0.177%
3	4.807	236	238	243	rBB	97835	105021	6.54%	0.912%
4	5.413	288	291	293	rBV	526502	615521	38.31%	5.347%
5	5.813	324	326	328	rBV	1030894	916351	57.04%	7.961%
6	6.213	359	361	364	rVB	55440	45612	2.84%	0.396%
7	6.807	411	413	416	rBV	646716	884779	55.07%	7.686%
8	6.967	425	427	430	rBV	923124	924214	57.53%	8.029%
9	7.207	446	448	450	rVB	284141	224333	13.96%	1.949%
10	7.367	459	462	464	rBV	906182	777937	48.42%	6.758%
11	7.767	495	497	499	rVB	527336	546439	34.01%	4.747%
12	8.499	558	561	563	rBB	353473	294779	18.35%	2.561%
13	9.573	653	655	657	rBV	1627862	1249024	77.75%	10.851%
14	10.259	713	715	718	rBV	252315	322258	20.06%	2.800%
15	11.059	783	785	787	rBV	760457	725785	45.18%	6.305%
16	11.768	845	847	850	rBV2	280663	365565	22.76%	3.176%
17	12.351	890	898	900	rBV	10149	27711	1.72%	0.241%
18	13.082	955	962	964	rBV	34716	74955	4.67%	0.651%
19	13.345	976	985	988	rBV2	41535	132522	8.25%	1.151%
20	13.505	996	999	1002	rVB	1733301	1606517	100.00%	13.956%
21	14.065	1046	1048	1051	rBV	46487	54848	3.41%	0.476%
22	14.157	1053	1056	1058	rVV	47287	58561	3.65%	0.509%
23	14.191	1058	1059	1062	rVB	31049	32939	2.05%	0.286%
24	14.545	1086	1090	1092	rBV	20106	32362	2.01%	0.281%
25	14.591	1092	1094	1096	rVV	22643	37099	2.31%	0.322%
26	14.637	1096	1098	1101	rVB	81755	87504	5.45%	0.760%
27	14.808	1109	1113	1122	rBV2	456509	793603	49.40%	6.894%
28	15.631	1182	1185	1193	rVB	18049	25283	1.57%	0.220%
29	16.180	1231	1233	1234	rBV	27900	36138	2.25%	0.314%
30	16.214	1234	1236	1240	rVB	28006	35682	2.22%	0.310%
31	16.614	1270	1271	1275	rVB	11897	18115	1.13%	0.157%
32	16.694	1275	1278	1283	rBV	261428	402879	25.08%	3.500%

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Peak separation: 5

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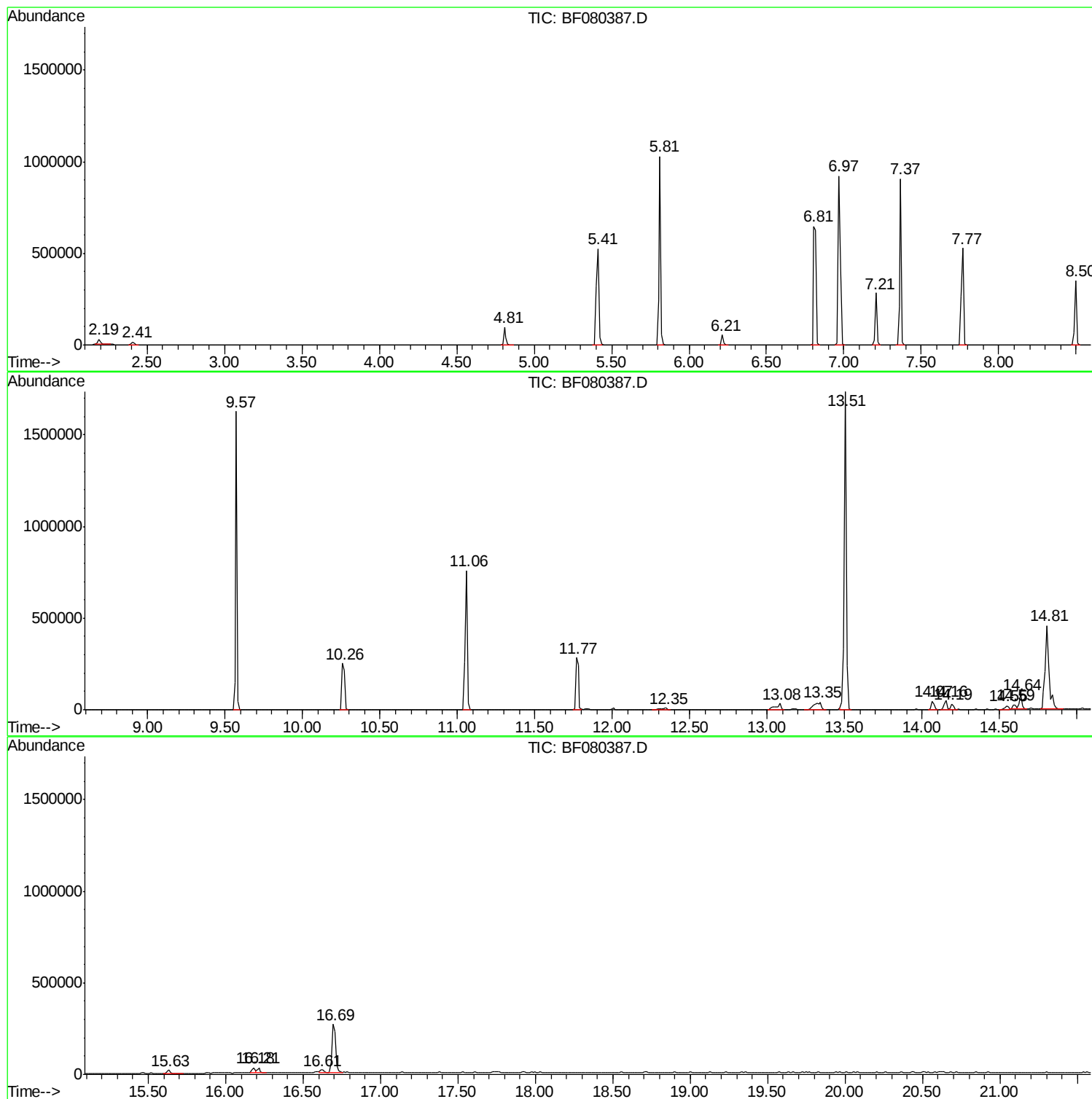
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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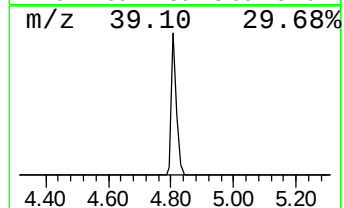
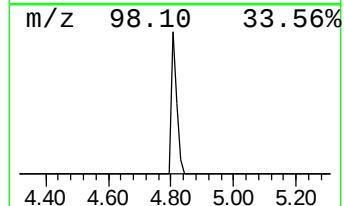
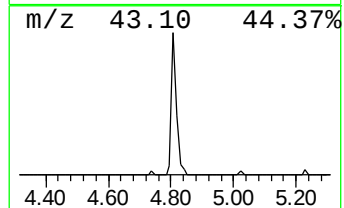
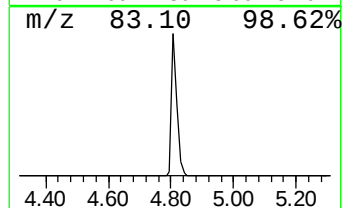
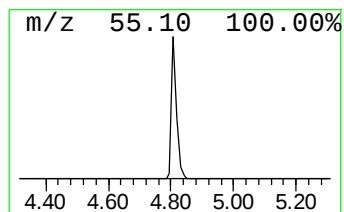
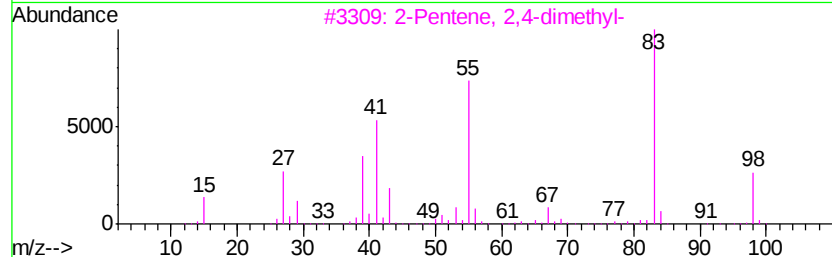
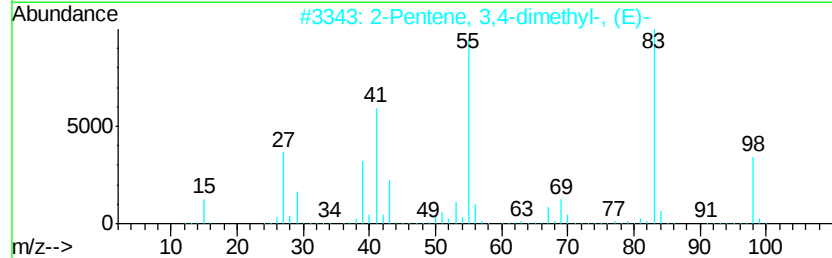
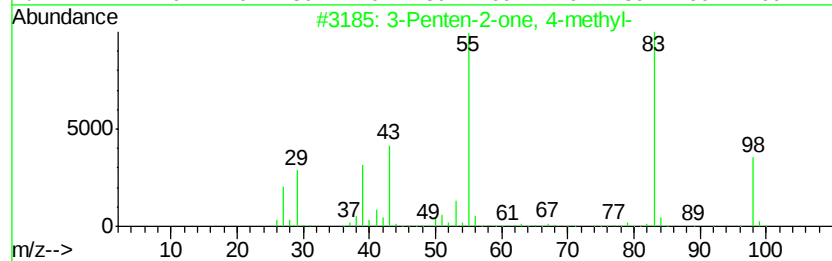
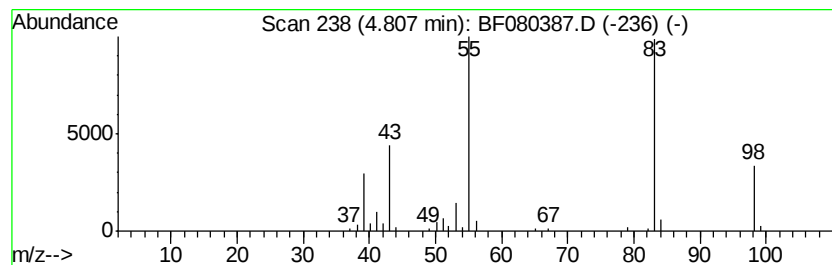
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	9.36 ng	105021	1,4-Dichlorobenzene-d4	7.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4			3-Hexen-2-one	98	C6H10O	000763-93-9	87
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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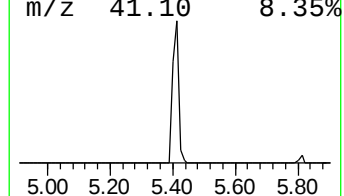
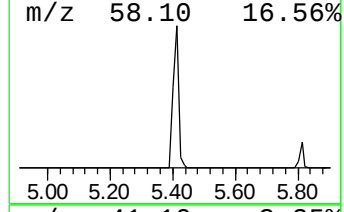
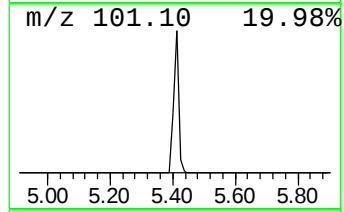
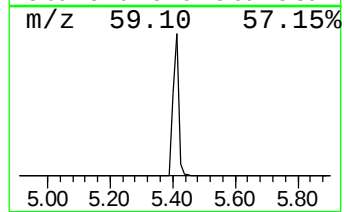
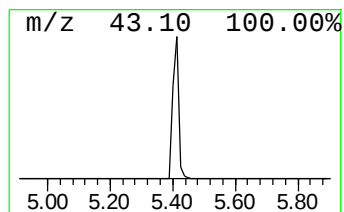
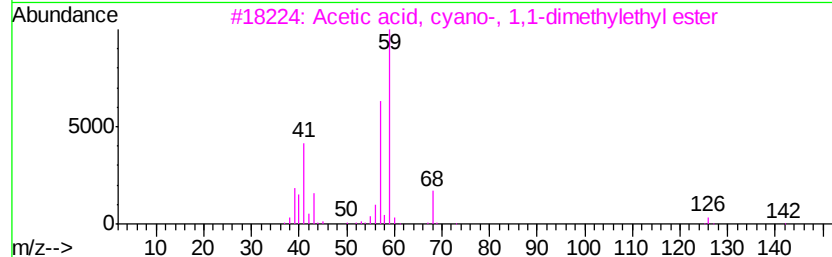
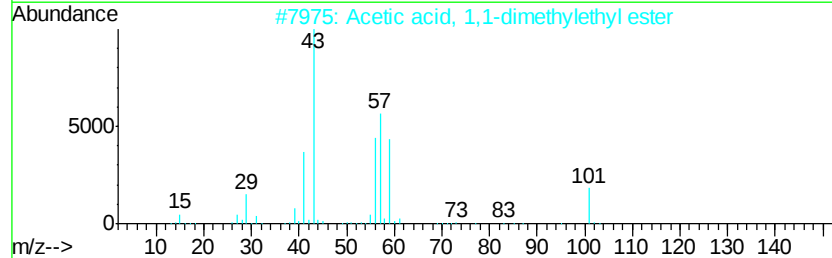
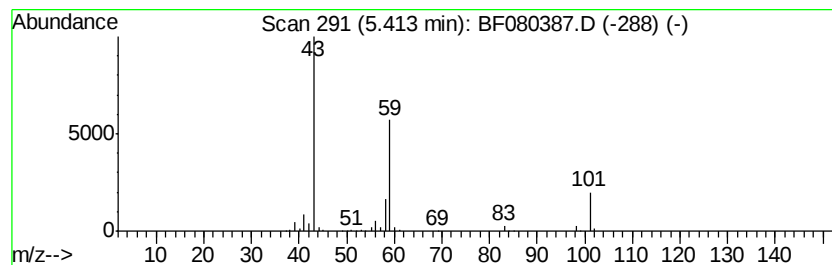
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.41	54.88 ng	615521	1,4-Dichlorobenzene-d4	7.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Acetone	58	C3H6O	000067-64-1	9



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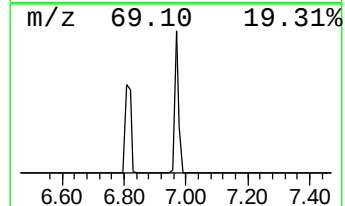
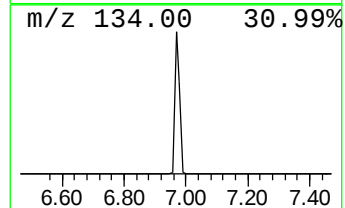
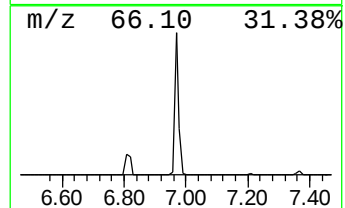
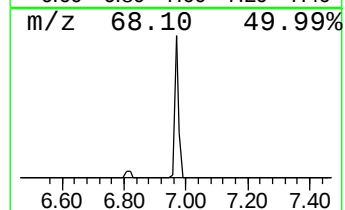
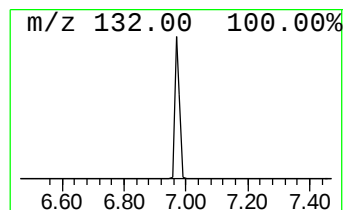
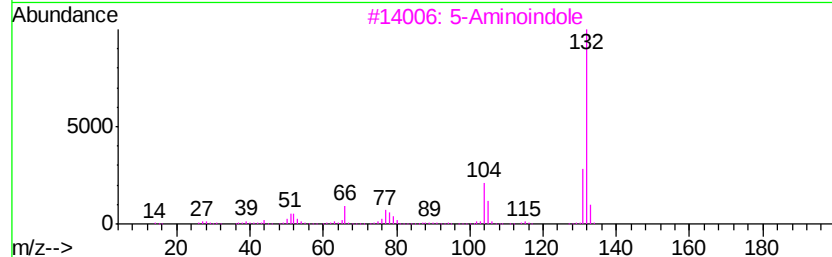
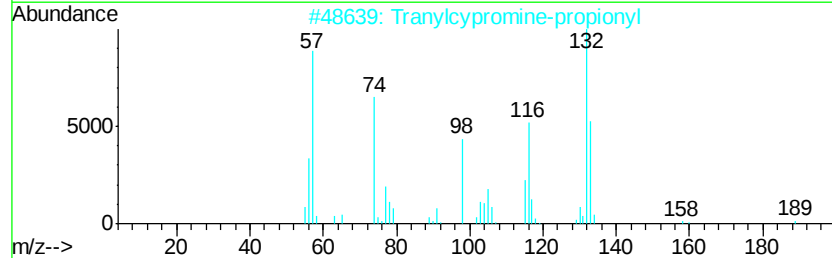
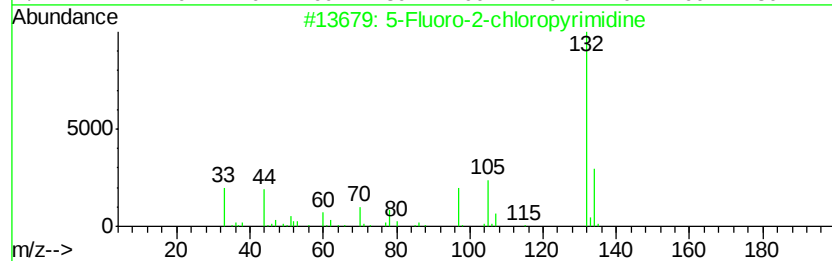
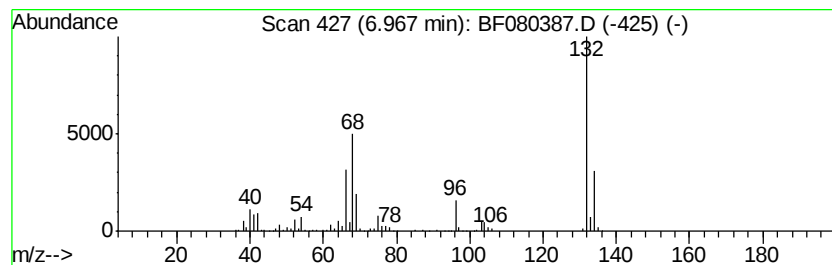
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.97 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.97	82.40 ng	924214	1,4-Dichlorobenzene-d4	7.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		1,2,3-Trifluorobenzene	132	C6H3F3	001489-53-8	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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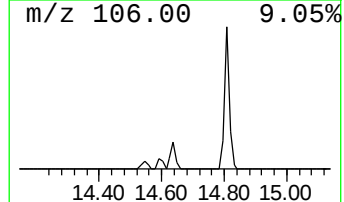
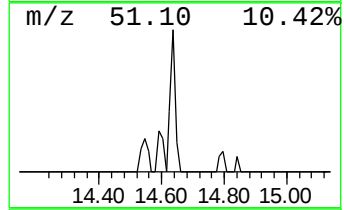
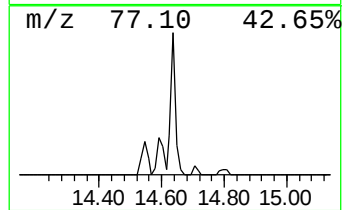
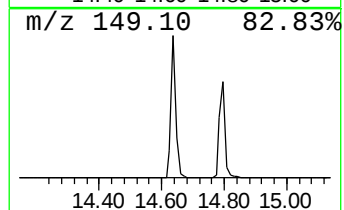
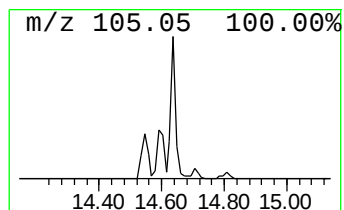
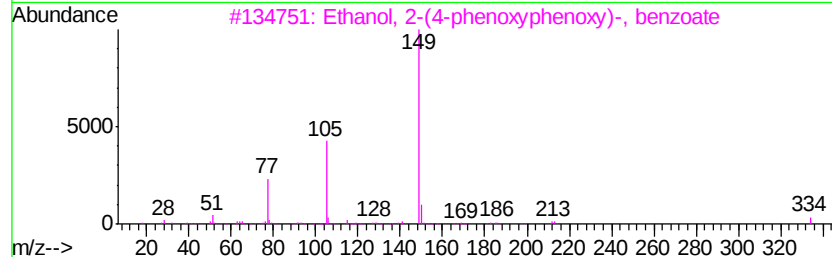
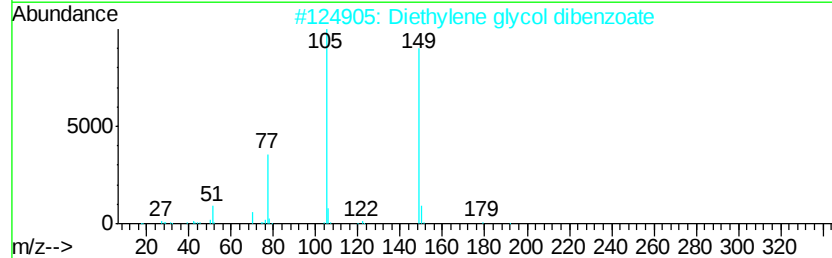
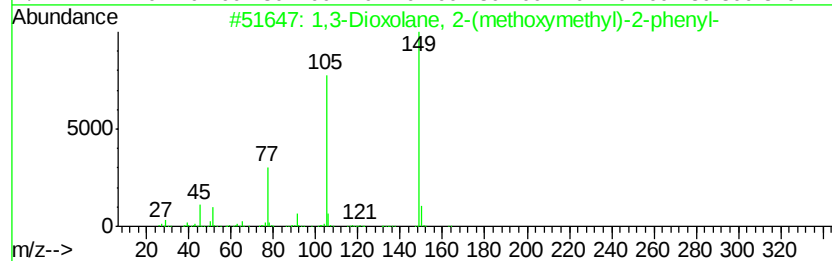
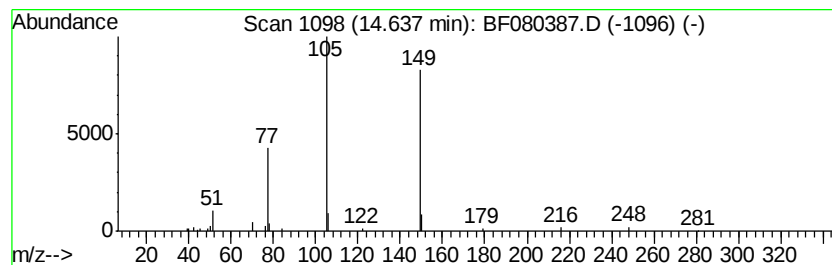
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.21 ng	87504	Chrysene-d12	14.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
2		Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
3		Ethanol, 2-(4-phenoxyphenoxy)-, ...	334	C21H18O4	055191-59-8	56
4		1,3,4-Oxadiazin-6-one, 5-isoprop...	216	C12H12N2O2	173973-78-9	38
5		1-Propanone, 2,2-dichloro-3-hydr...	218	C9H8Cl2O2	054824-08-7	35



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.81	9.4	ng	105021	1	7.21	224333	20.0
2-Pentanone, 4-hy...	5.41	54.9	ng	615521	1	7.21	224333	20.0
unknown6.97	6.97	82.4	ng	924214	1	7.21	224333	20.0
1,3-Dioxolane, 2-...	14.64	2.2	ng	87504	5	14.81	793603	20.0