

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080620\
 Data File : BF121220.D
 Acq On : 7 Aug 2020 00:13
 Operator : JU/CG
 Sample : L3575-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-0D015-03-016

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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	3.428	220	228	240	rBV	875536	1624877	5.36%	3.005%
2	4.451	380	402	404	rBV2	5219190	30319620	100.00%	56.066%
3	5.051	490	504	506	rBV	3499528	9559642	31.53%	17.677%
4	6.798	797	801	808	rBV	724299	701049	2.31%	1.296%
5	7.122	852	856	864	rBV	866226	780067	2.57%	1.442%
6	7.357	892	896	900	rBV	1384815	1214030	4.00%	2.245%
7	7.481	914	917	925	rBV	463692	406834	1.34%	0.752%
8	7.616	936	940	948	rVB	446344	425489	1.40%	0.787%
9	8.081	1012	1019	1027	rBV	959389	982055	3.24%	1.816%
10	9.157	1198	1202	1205	rBV	2455380	2331927	7.69%	4.312%
11	9.833	1313	1317	1330	rBV	1066395	1009068	3.33%	1.866%
12	11.322	1566	1570	1578	rBV	968745	994596	3.28%	1.839%
13	12.910	1835	1840	1843	rBV	2304483	2118928	6.99%	3.918%
14	13.963	2016	2019	2023	rBV	775327	805775	2.66%	1.490%
15	15.415	2262	2266	2275	rBV	571289	804481	2.65%	1.488%

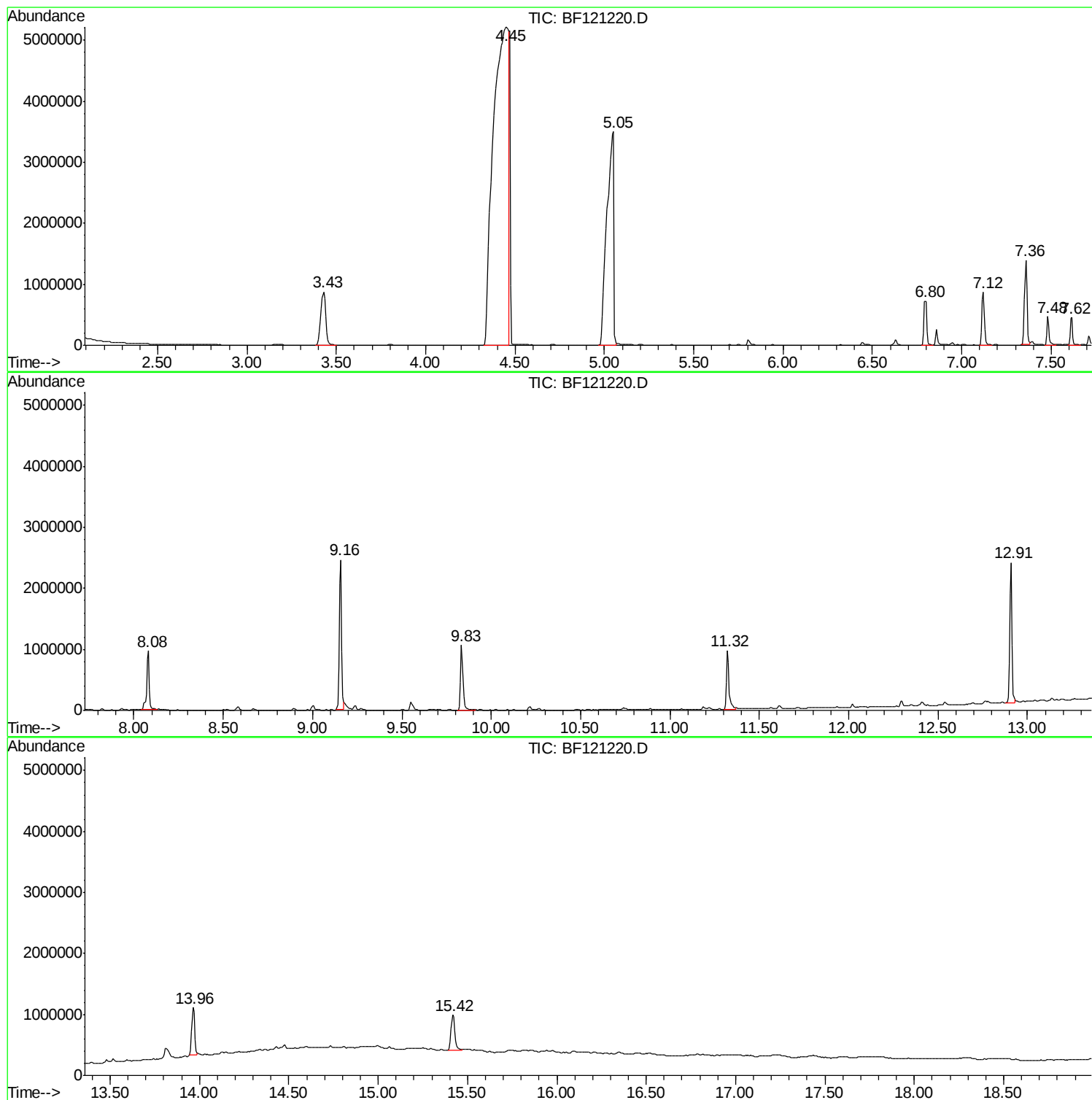
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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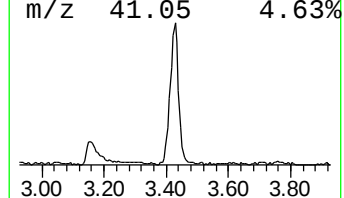
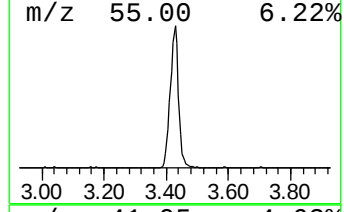
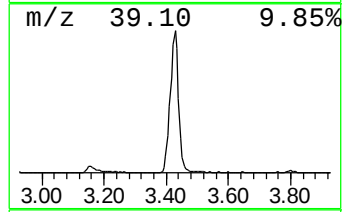
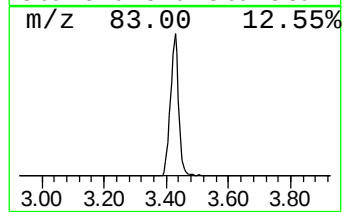
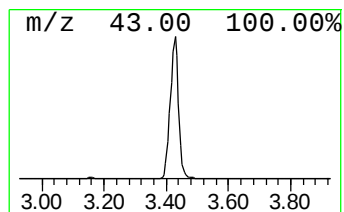
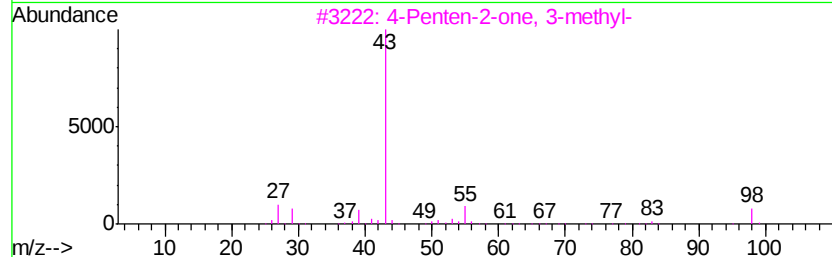
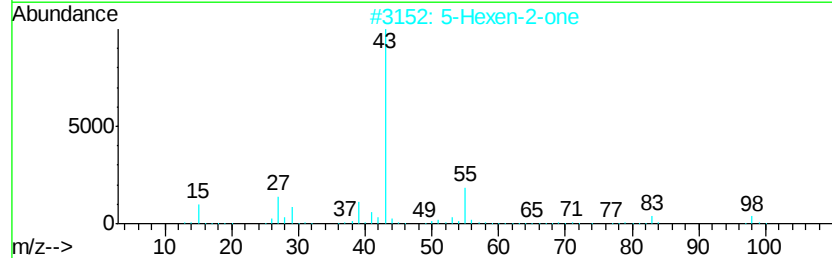
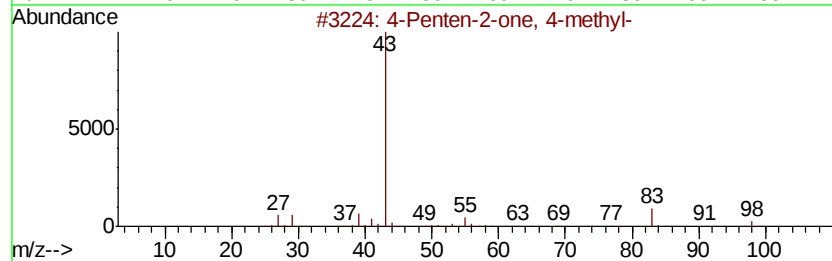
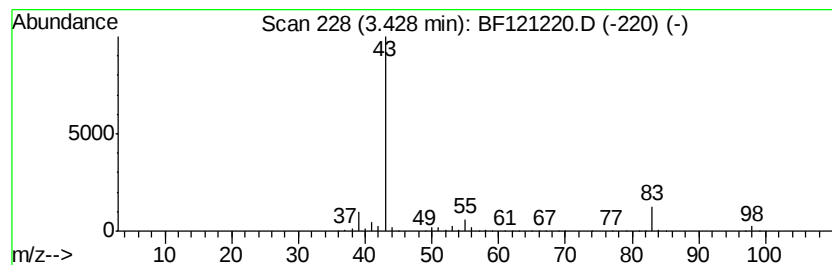
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.43	46.36 ng	1624880	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2			5-Hexen-2-one	98	C6H10O	000109-49-9	38
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	36
4			2-Pentanone, 3-methyl-	98	C6H10O	004359-77-7	23
5			Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	16



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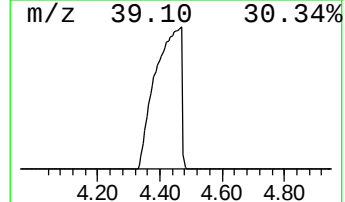
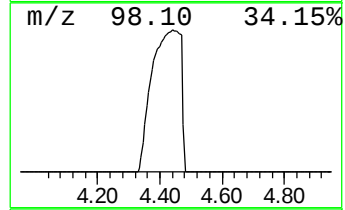
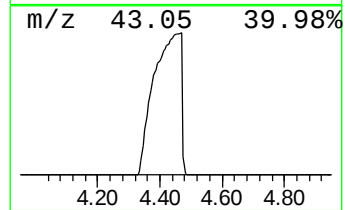
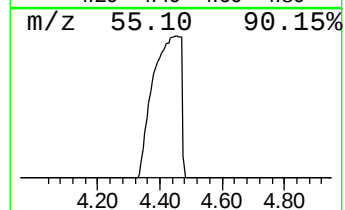
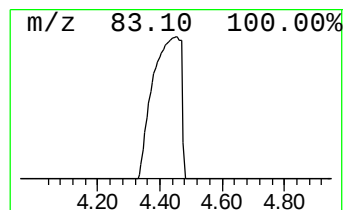
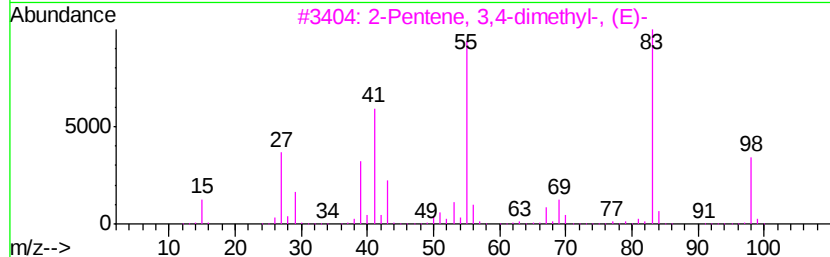
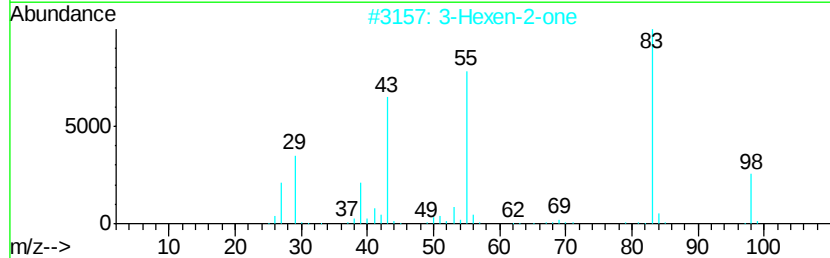
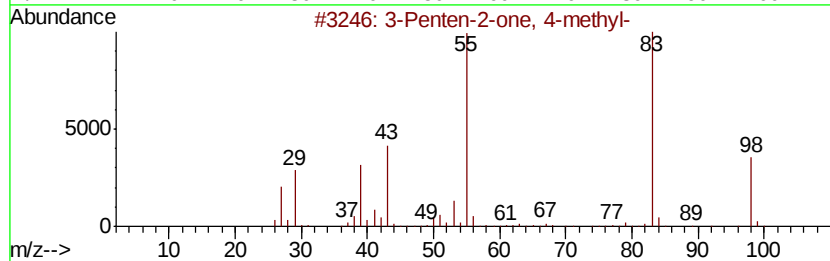
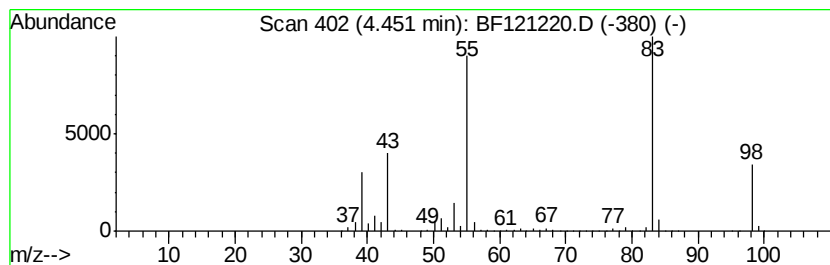
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	864.98 ng	30319600	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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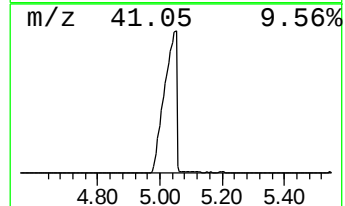
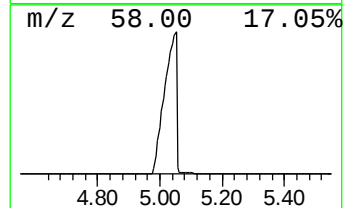
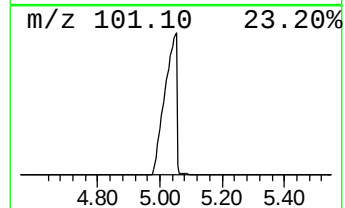
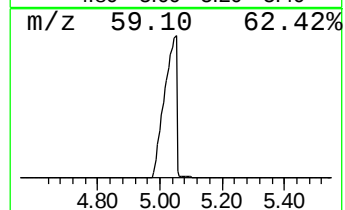
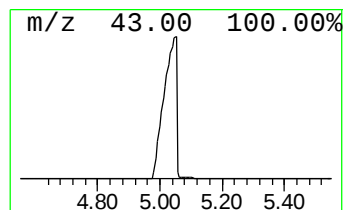
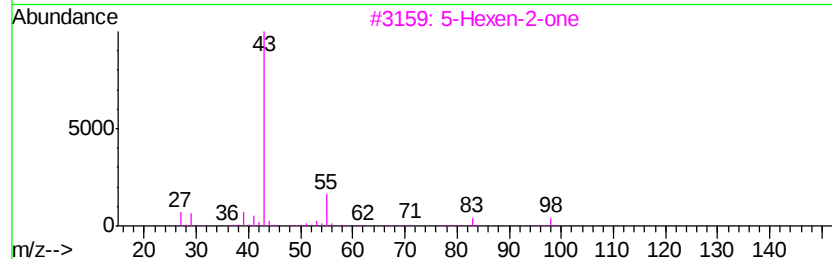
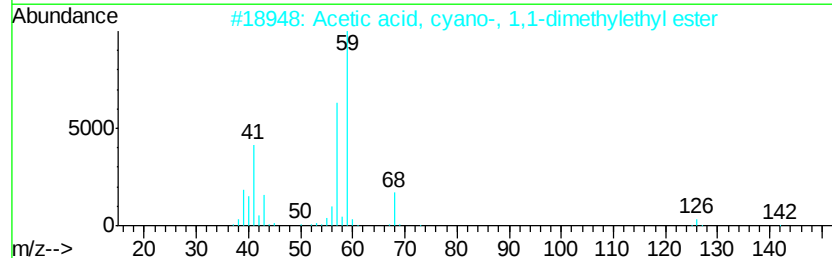
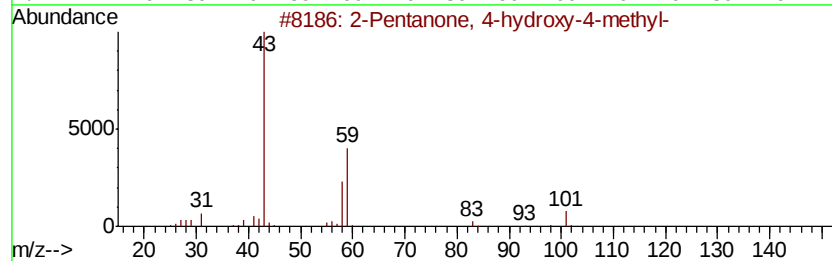
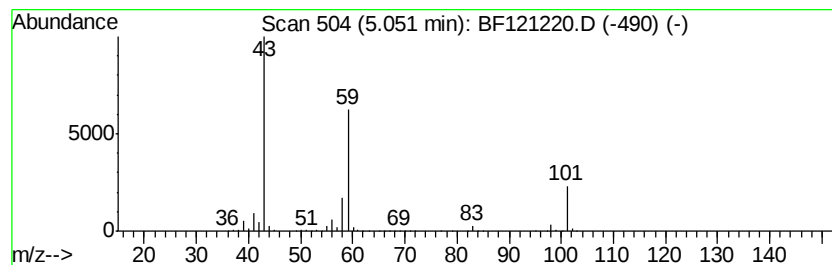
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	272.72 ng	9559640	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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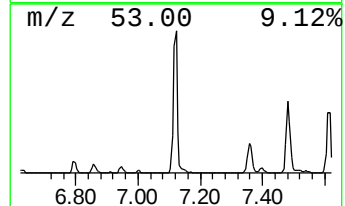
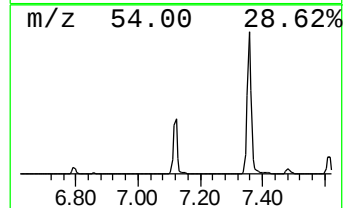
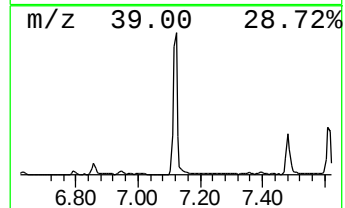
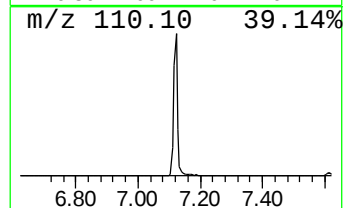
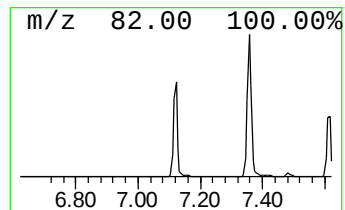
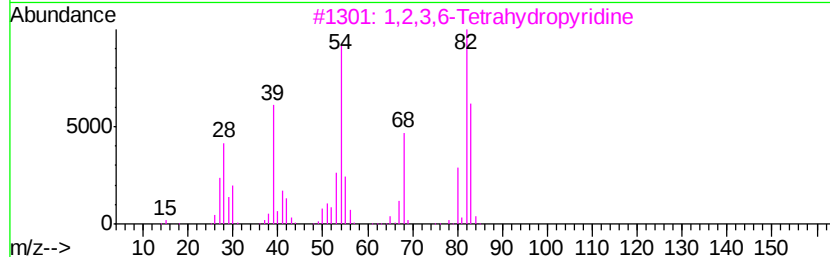
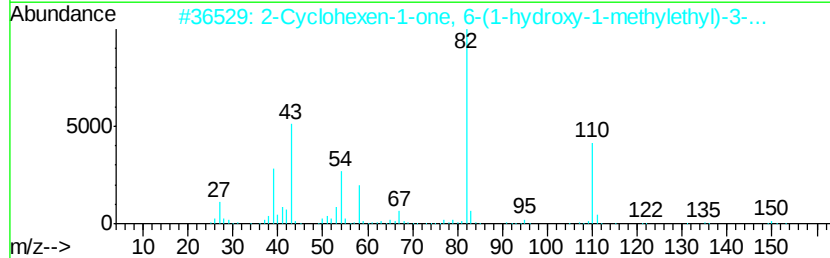
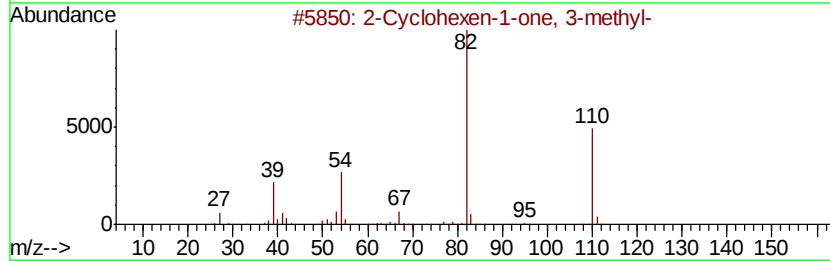
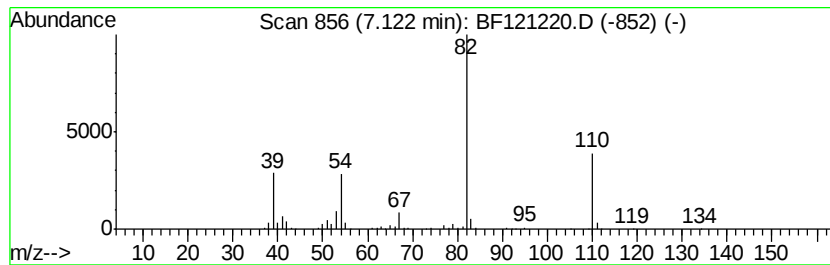
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.12	22.25 ng	780067	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	64
3	1,2,3,6-Tetrahdropvridine	83	C5H9N	000694-05-3	53
4	Betazole	111	C5H9N3	000105-20-4	43
5	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	33



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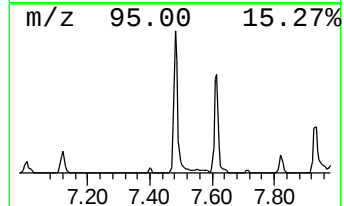
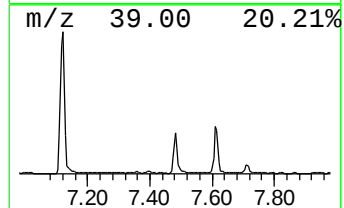
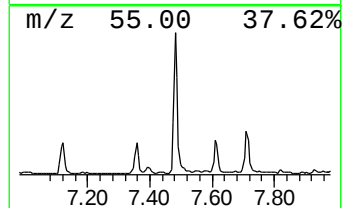
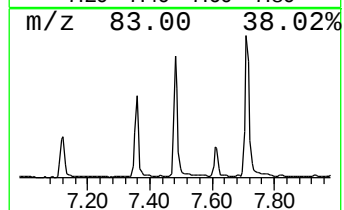
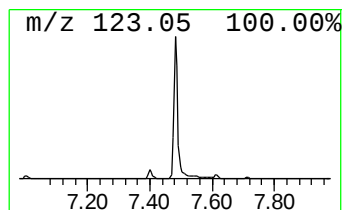
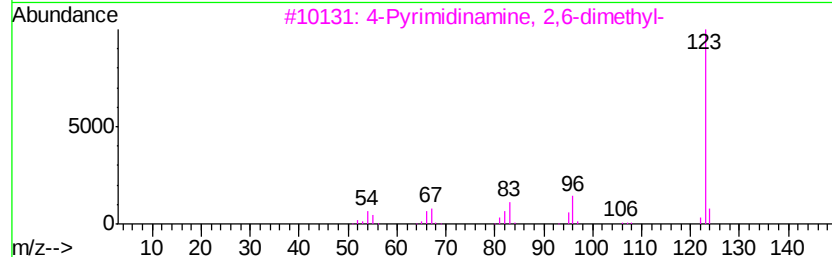
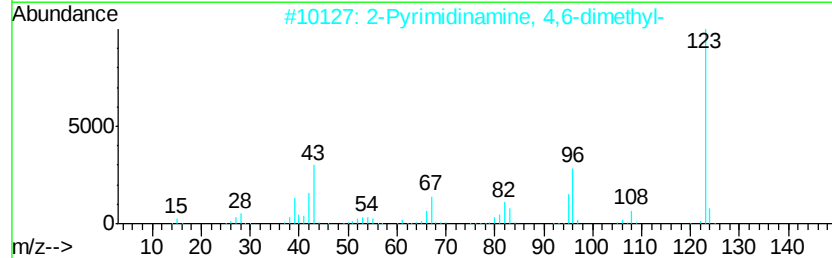
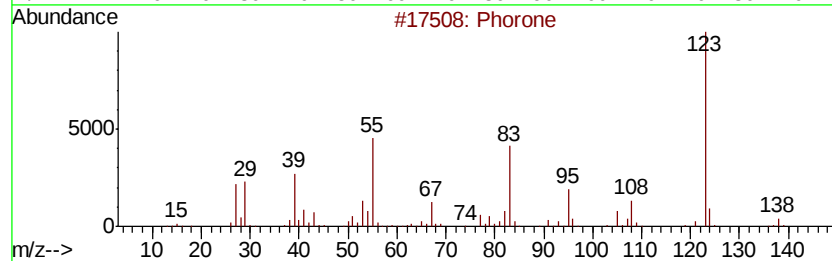
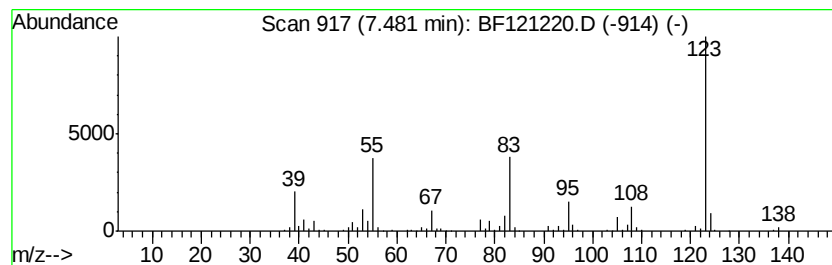
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phorone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	8.29 ng	406834	Naphthalene-d8	8.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phorone		138	C9H14O	000504-20-1	90
2	2-Pyrimidinamine, 4,6-dimethyl-		123	C6H9N3	000767-15-7	59
3	4-Pyrimidinamine, 2,6-dimethyl-		123	C6H9N3	000461-98-3	53
4	1,3-Benzenediol, 4-ethyl-		138	C8H10O2	002896-60-8	53
5	2-Cyclopenten-1-one, 3,4,5,5-tet...		138	C9H14O	090611-02-2	53



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	3.43	46.4	ng	1624880	1	6.80	701049	20.0
3-Penten-2-one, 4...	4.45	865.0	ng	30319600	1	6.80	701049	20.0
2-Pentanone, 4-hy...	5.05	272.7	ng	9559640	1	6.80	701049	20.0
2-Cyclohexen-1-on...	7.12	22.3	ng	780067	1	6.80	701049	20.0
Phorone	7.48	8.3	ng	406834	2	8.08	982055	20.0