

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030117\
 Data File : BF093304.D
 Acq On : 1 Mar 2017 22:08
 Operator : SJ/MA
 Sample : I2012-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P-8

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-BF013017.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	3.230	97	100	113	rVB	723530	1588045	4.30%	2.362%
2	4.373	188	200	202	rBV	6860057	36964745	100.00%	54.979%
3	5.002	249	255	257	rBV	4457433	10603913	28.69%	15.772%
4	6.807	410	413	415	rBV	700695	868123	2.35%	1.291%
5	6.956	424	426	429	rBV	2237828	2240551	6.06%	3.332%
6	7.127	439	441	444	rBV	636642	786680	2.13%	1.170%
7	7.367	460	462	465	rBV	1346373	1868782	5.06%	2.779%
8	8.088	523	525	536	rVB	1192052	1216413	3.29%	1.809%
9	9.162	616	619	622	rBV	3093854	3263905	8.83%	4.855%
10	9.836	676	678	681	rBV	1056799	1333201	3.61%	1.983%
11	11.322	806	808	814	rBV	1081822	1520109	4.11%	2.261%
12	12.911	944	947	950	rBV	2779338	2975047	8.05%	4.425%
13	13.974	1037	1040	1042	rBV	819479	1161958	3.14%	1.728%
14	15.391	1161	1164	1167	rBV	681784	843101	2.28%	1.254%

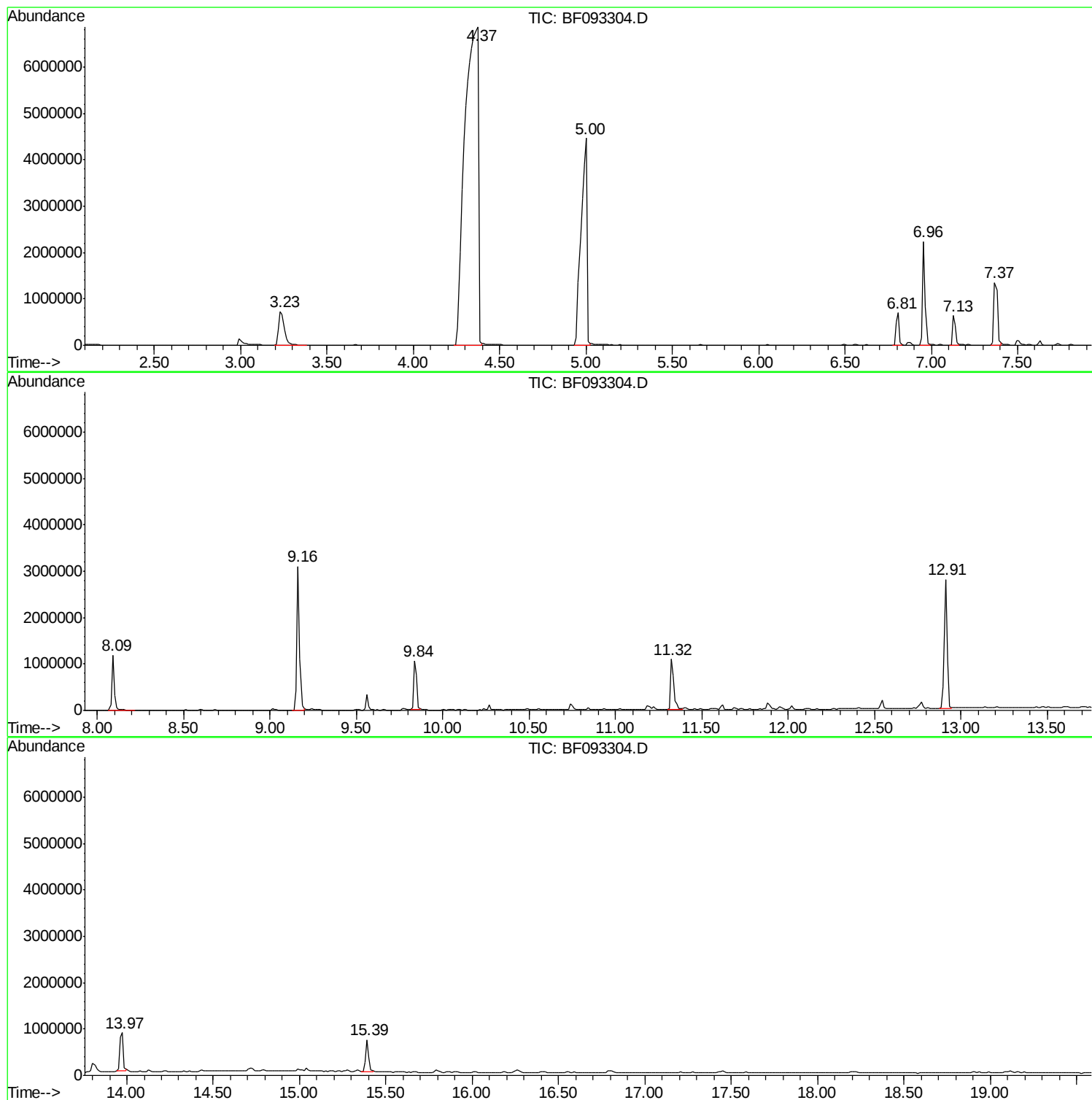
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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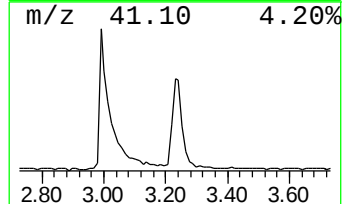
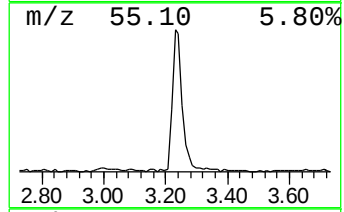
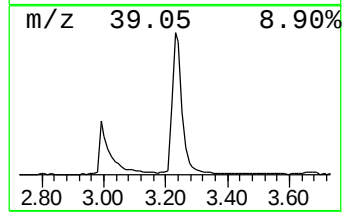
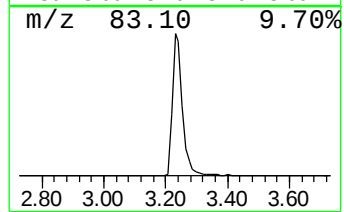
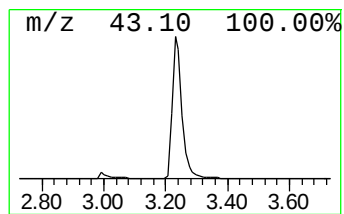
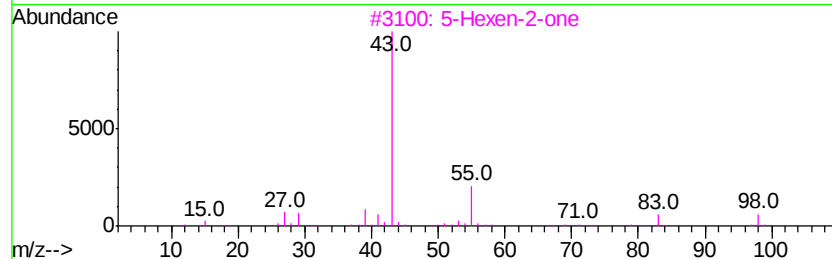
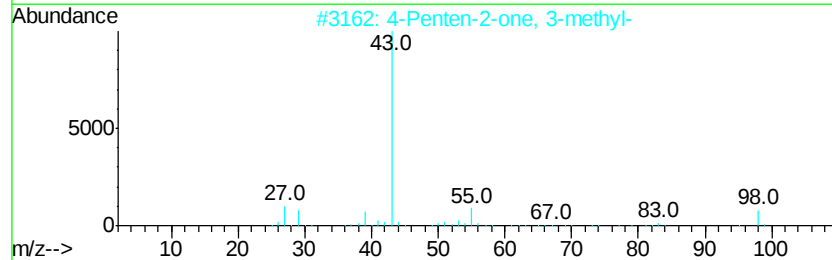
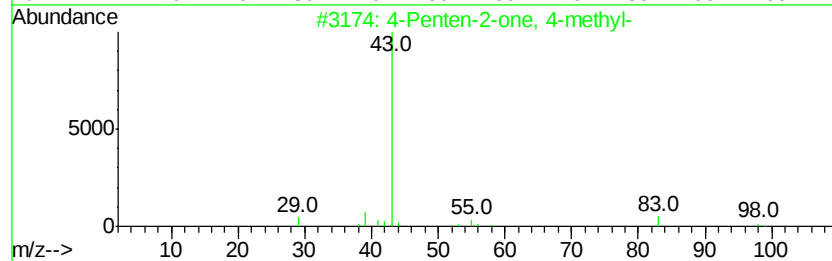
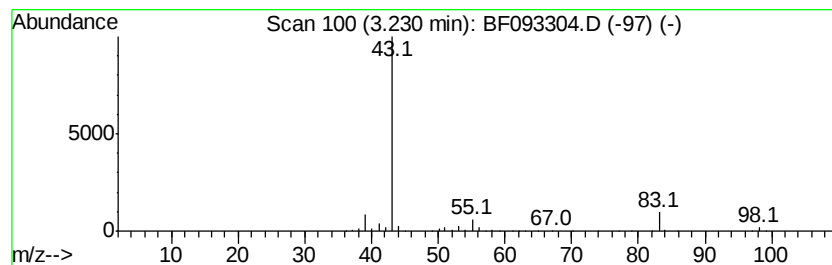
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	36.59 ng	1588050	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
3		5-Hexen-2-one	98	C6H10O	000109-49-9	40
4		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	28
5		4-Hexen-2-one	98	C6H10O	025659-22-7	9



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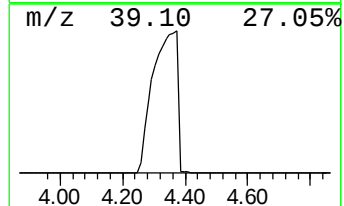
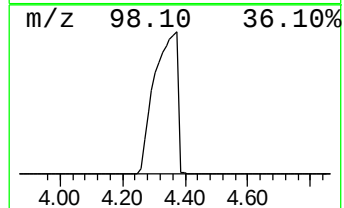
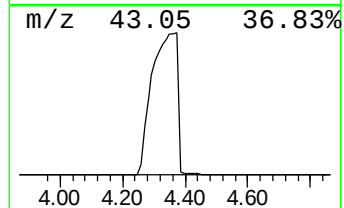
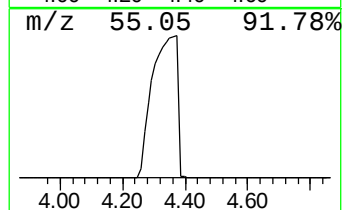
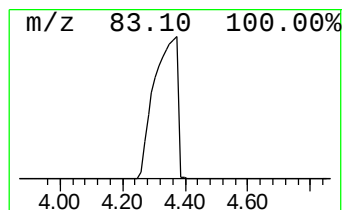
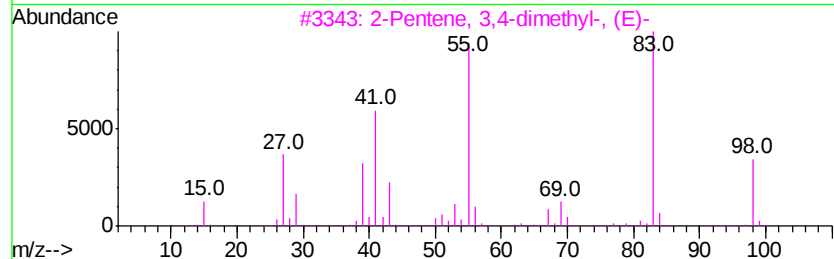
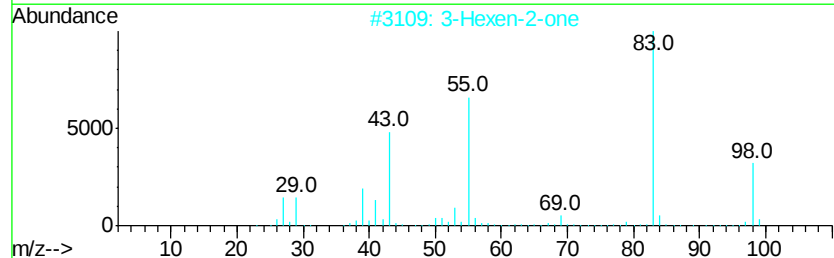
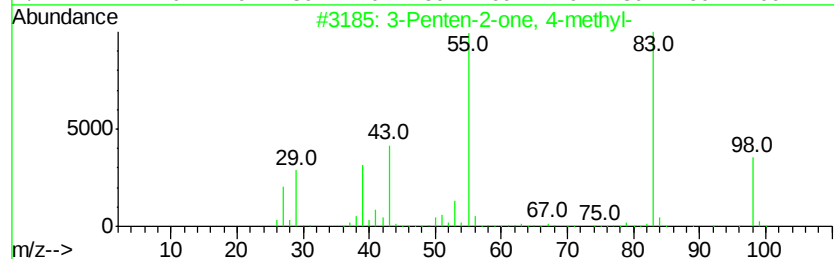
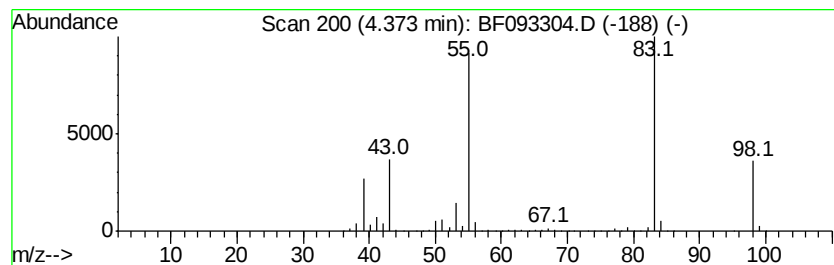
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	851.60 ng	36964700	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
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, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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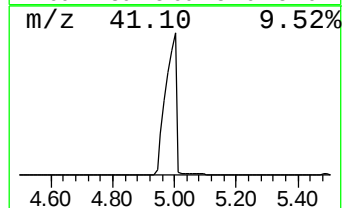
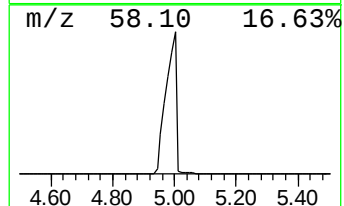
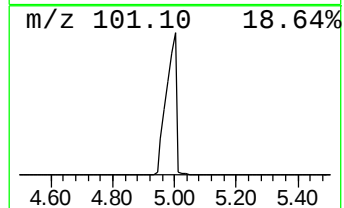
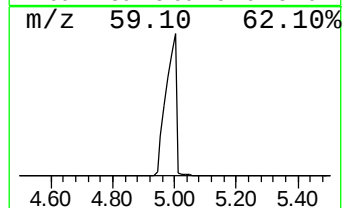
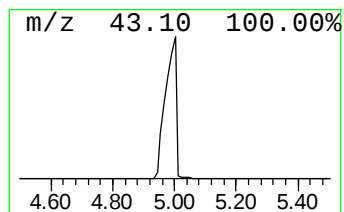
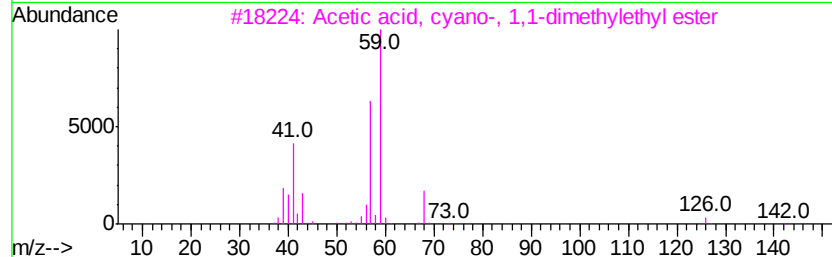
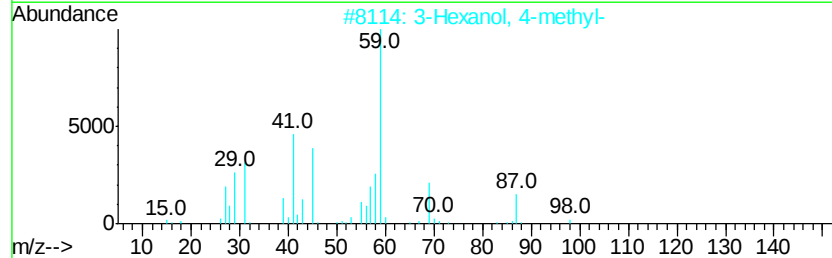
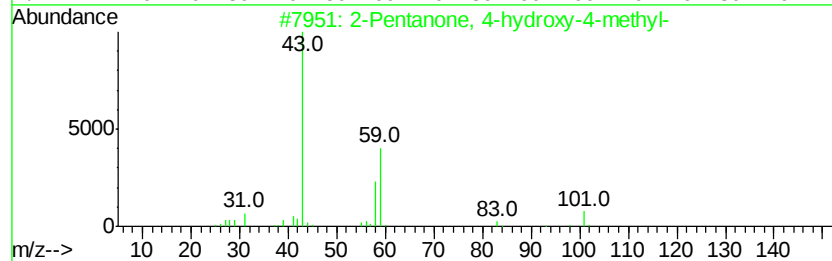
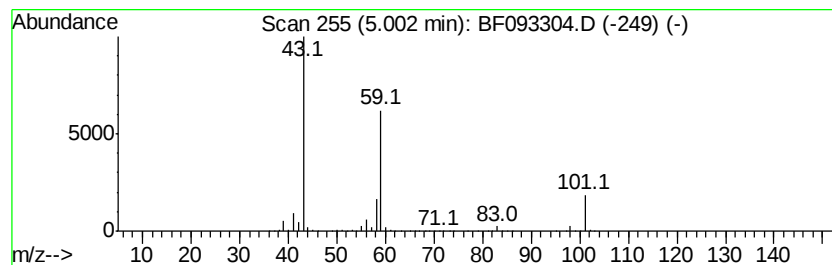
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	244.30 ng	10603900	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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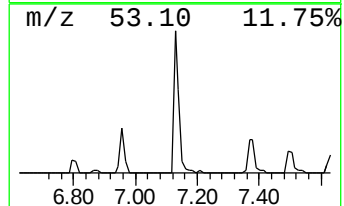
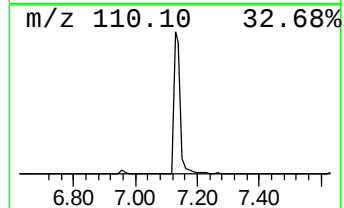
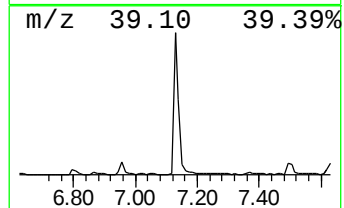
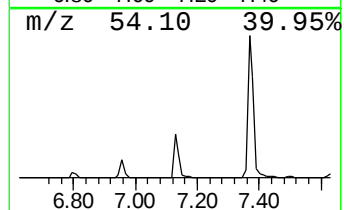
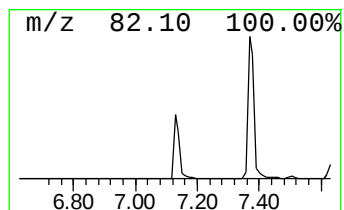
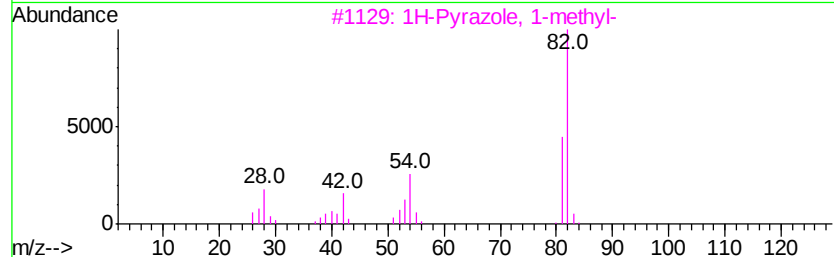
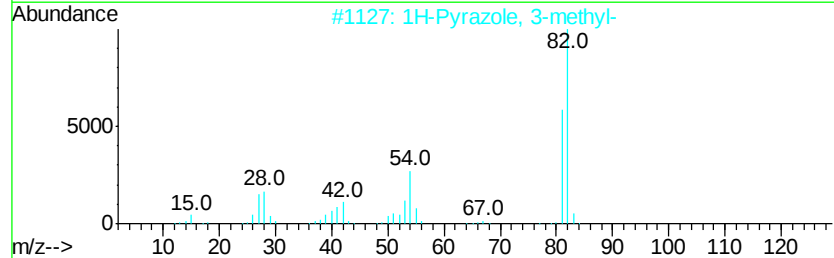
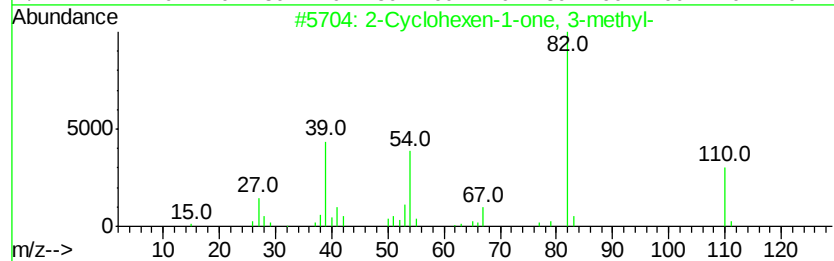
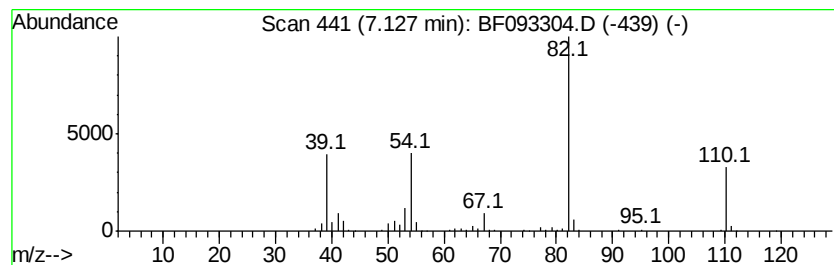
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Peak Number 5 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	18.12 ng	786680	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2		1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	50
3		1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	38
4		Betazole	111	C5H9N3	000105-20-4	25
5		1-Propene, 3-azido-	83	C3H5N3	000821-13-6	16



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	3.23	36.6	ng	1588050	1	6.81	868123	20.0
3-Penten-2-one, 4...	4.37	851.6	ng	36964700	1	6.81	868123	20.0
2-Pentanone, 4-hy...	5.00	244.3	ng	10603900	1	6.81	868123	20.0
2-Cyclohexen-1-on...	7.13	18.1	ng	786680	1	6.81	868123	20.0