

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040216\
 Data File : BF085989.D
 Acq On : 2 Apr 2016 4:30
 Operator : UM/SJ
 Sample : PB89385BL
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB89385BL

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-BF040216.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	3.241	98	101	113	rBV	186416	371040	9.31%	1.489%
2	4.281	188	192	195	rBV	2045746	3984936	100.00%	15.997%
3	4.944	247	250	266	rBV	656821	869462	21.82%	3.490%
4	5.367	285	287	307	rBV	1311636	1548742	38.86%	6.217%
5	5.779	321	323	331	rVB	36104	44198	1.11%	0.177%
6	6.407	376	378	387	rBV	1520886	1495062	37.52%	6.002%
7	6.533	387	389	392	rBV	1411729	1602561	40.22%	6.433%
8	6.773	407	410	421	rBV	644528	605807	15.20%	2.432%
9	6.922	421	423	426	rBV	1603485	1859319	46.66%	7.464%
10	7.333	457	459	462	rBV	1072947	1423621	35.73%	5.715%
11	8.053	520	522	525	rBV	803120	815970	20.48%	3.276%
12	9.128	614	616	619	rBV	2131890	2692410	67.56%	10.808%
13	9.802	673	675	678	rBV	693213	879476	22.07%	3.531%
14	10.591	742	744	747	rBV2	863040	1104941	27.73%	4.436%
15	11.288	803	805	808	rBV	1080663	972506	24.40%	3.904%
16	12.877	941	944	946	rBV	3194693	3154685	79.17%	12.664%
17	13.928	1034	1036	1038	rBV	824301	928169	23.29%	3.726%
18	15.334	1156	1159	1166	rBV	350215	557704	14.00%	2.239%

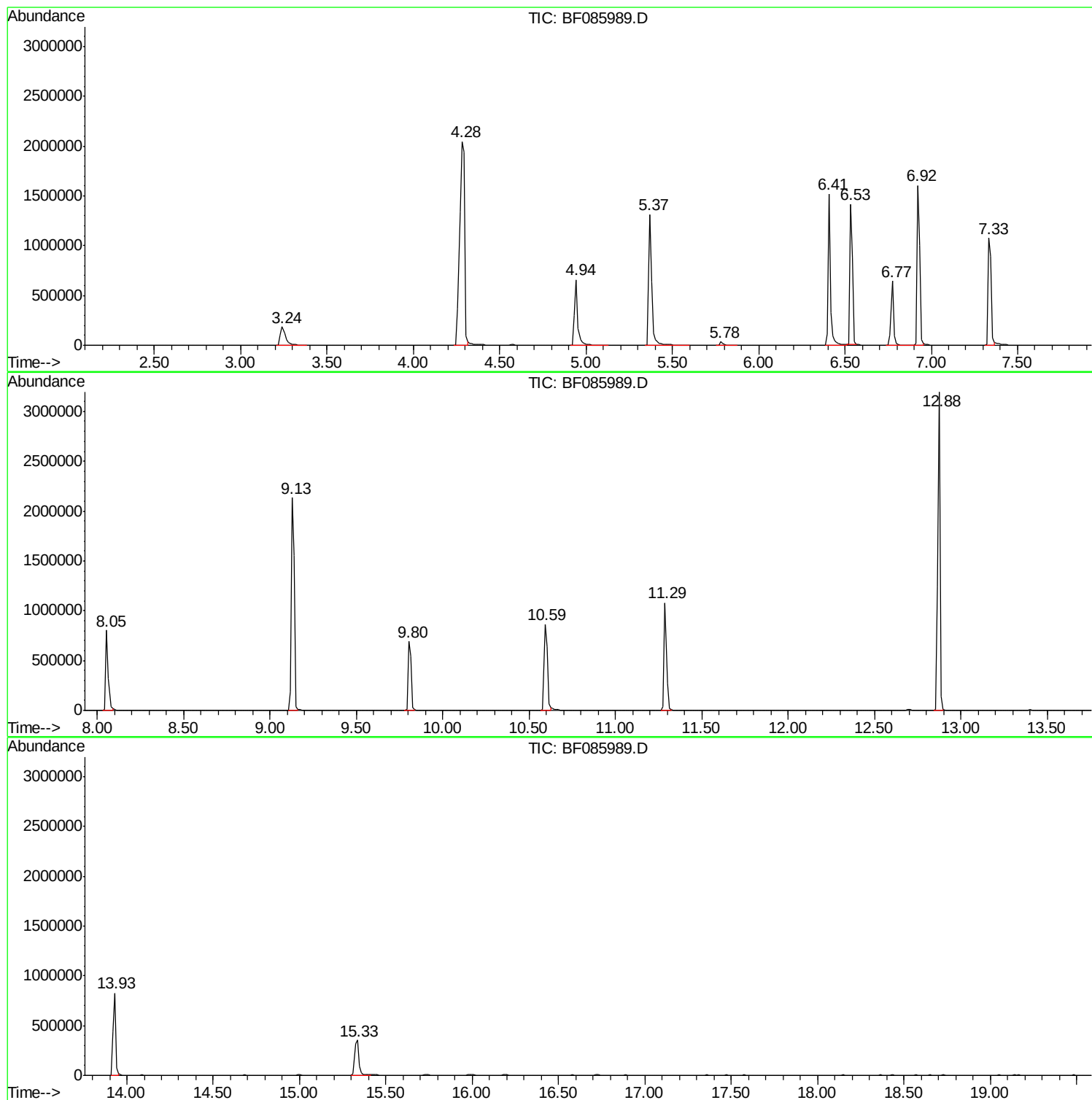
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040216.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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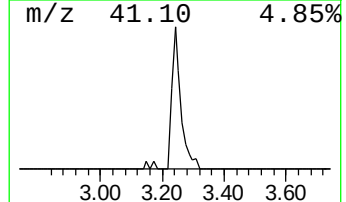
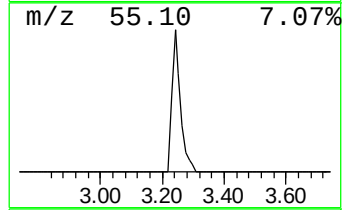
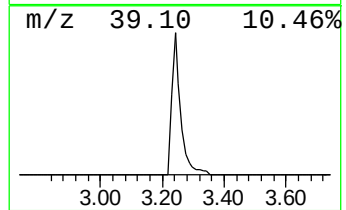
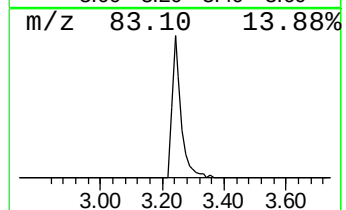
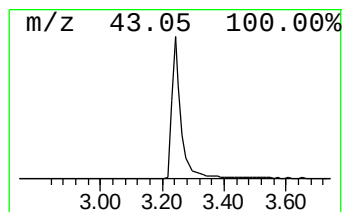
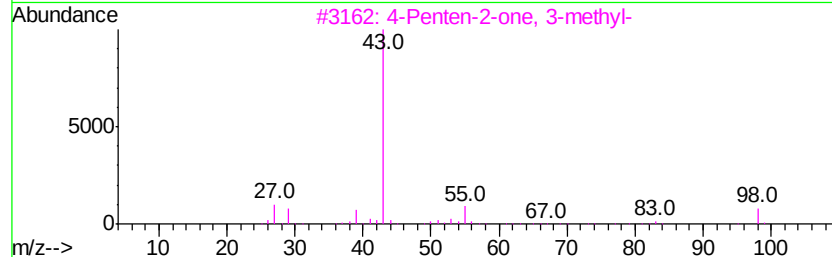
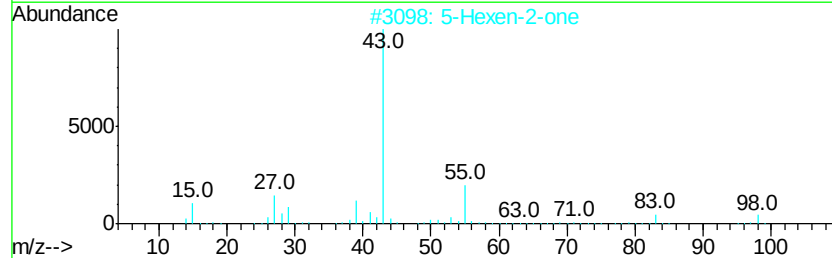
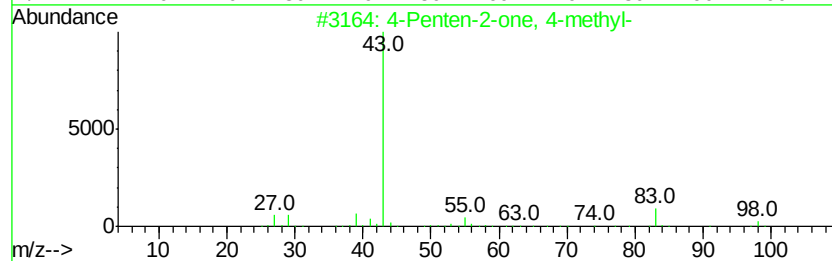
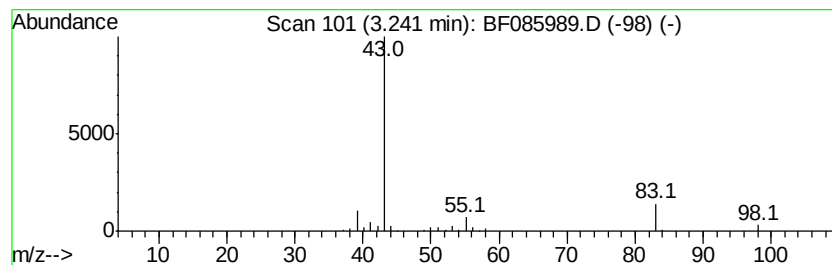
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.24	12.25 ng	371040	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2		5-Hexen-2-one	98	C6H10O	000109-49-9	50
3		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	37
4		2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17
5		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	12



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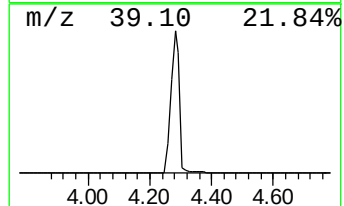
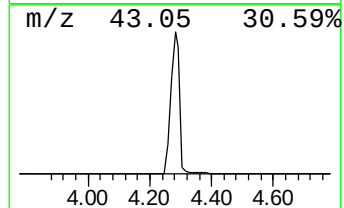
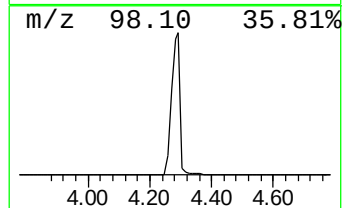
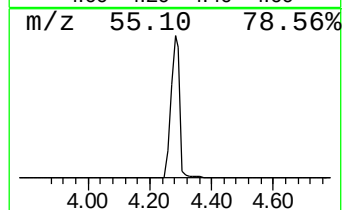
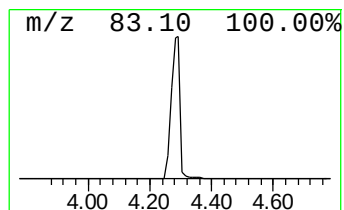
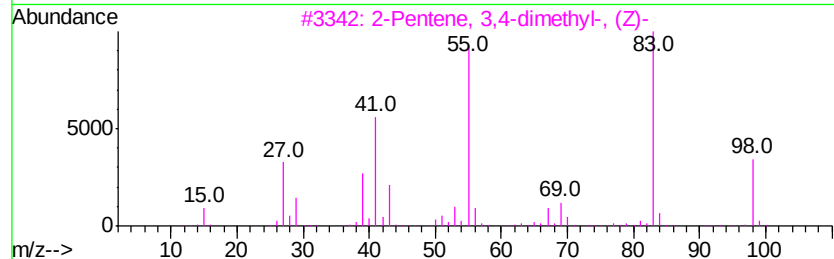
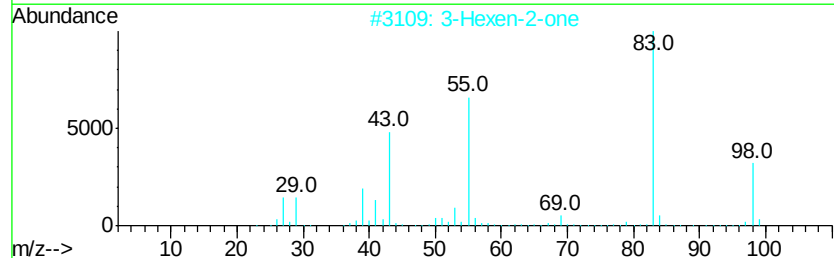
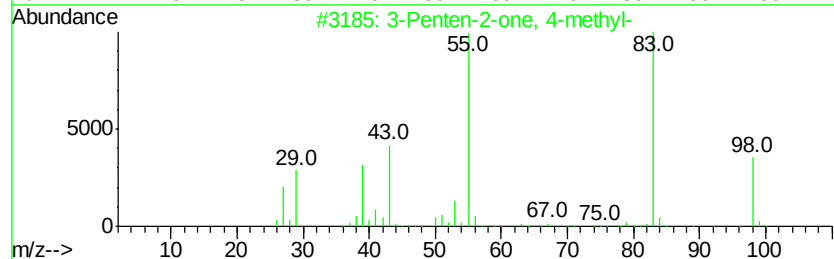
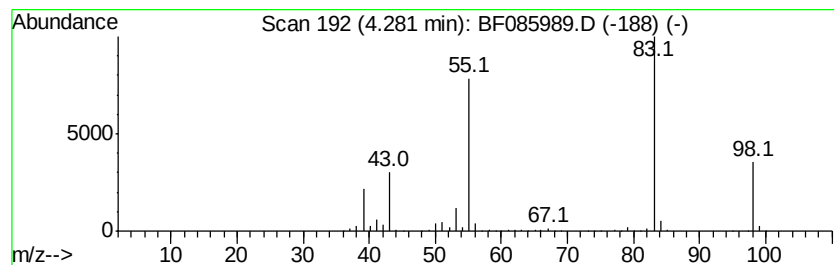
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	131.56 ng	3984940	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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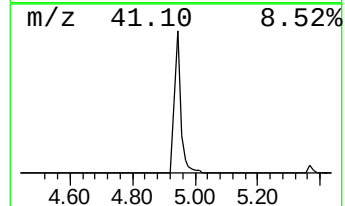
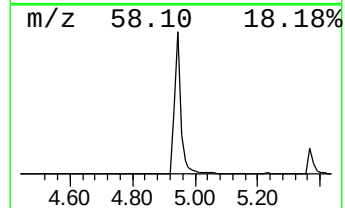
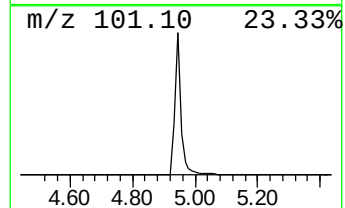
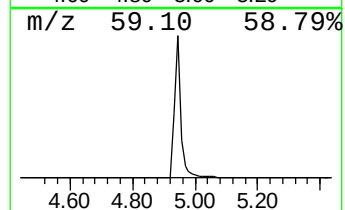
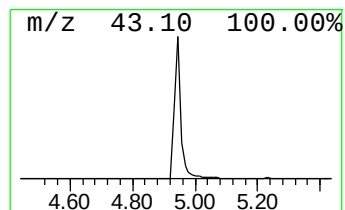
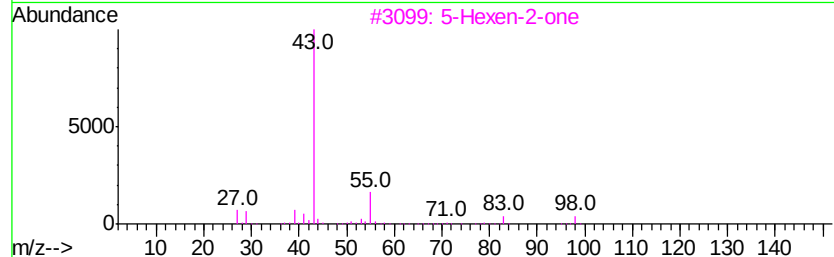
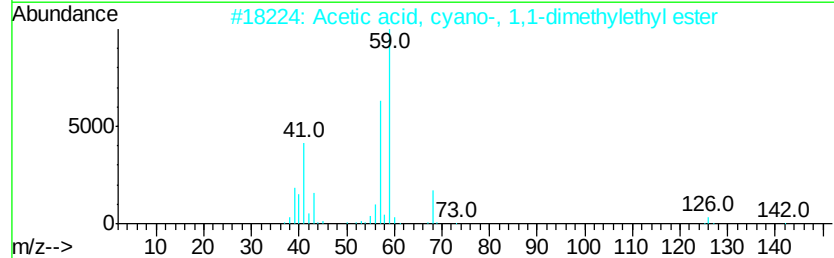
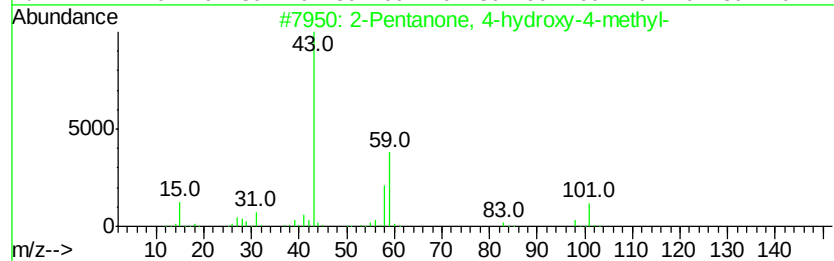
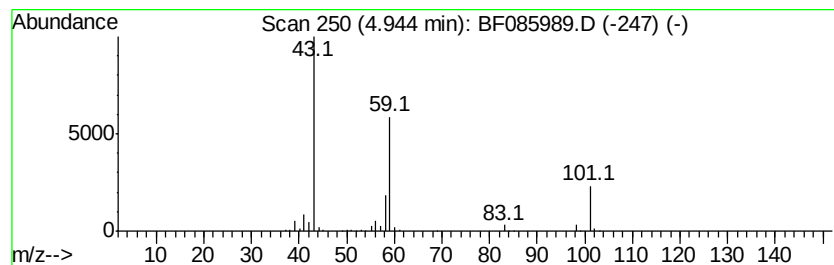
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	28.70 ng	869462	1,4-Dichlorobenzene-d4	6.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
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			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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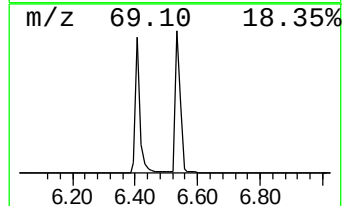
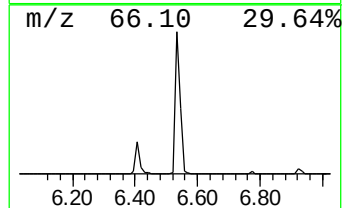
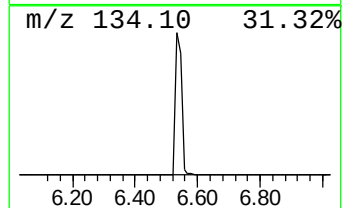
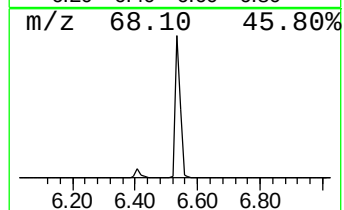
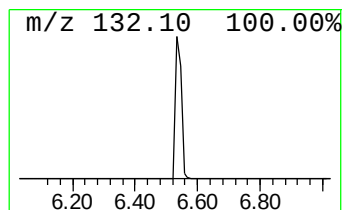
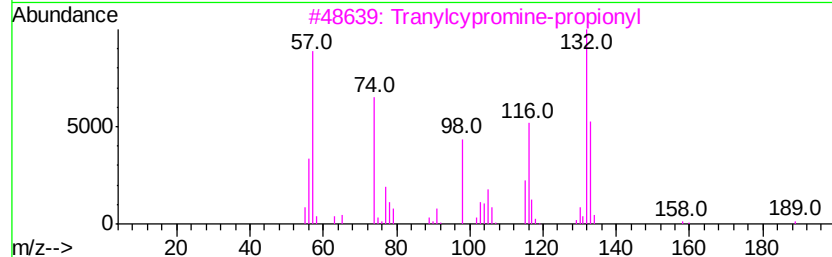
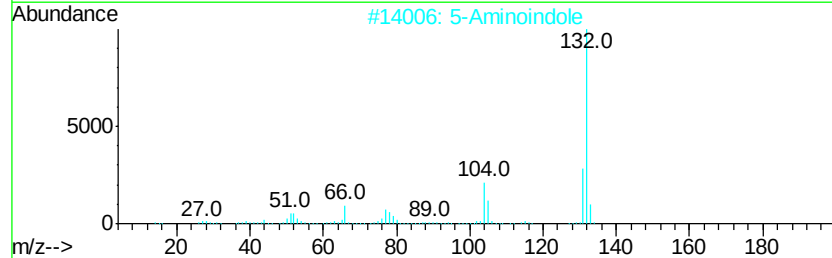
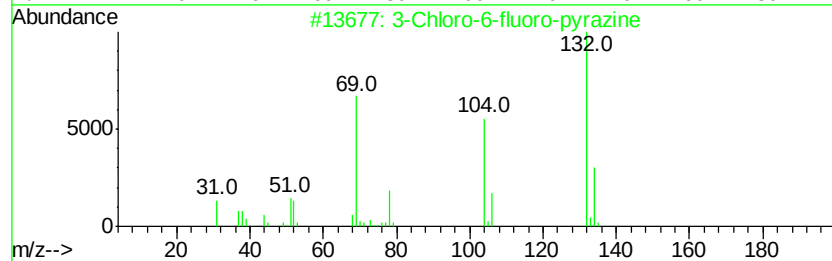
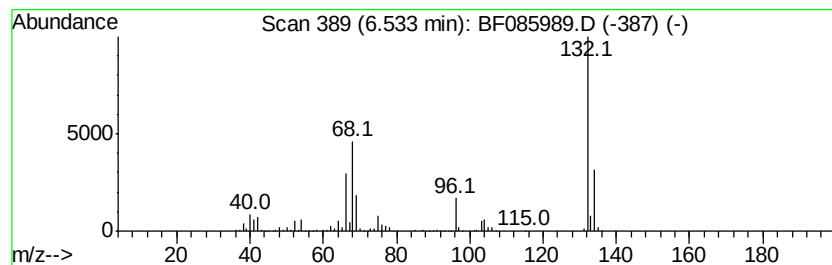
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Peak Number 4 unknown6.53 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	52.91 ng	1602560	1,4-Dichlorobenzene-d4	6.77

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



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Penten-2-one, 4...	3.24	12.3	ng	371040	1	6.77	605807	20.0
3-Penten-2-one, 4...	4.28	131.6	ng	3984940	1	6.77	605807	20.0
2-Pentanone, 4-hy...	4.94	28.7	ng	869462	1	6.77	605807	20.0
unknown6.53	6.53	52.9	ng	1602560	1	6.77	605807	20.0