

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
 Data File : BF080850.D
 Acq On : 4 Aug 2015 21:21
 Operator : TP/UM
 Sample : PB84692BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB84692BL

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-BF080415.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	4.373	198	200	204	rBB	141747	160623	8.63%	0.988%
2	5.024	254	257	260	rBV	1092318	1693773	90.96%	10.423%
3	5.436	290	293	295	rBV	1672697	1842675	98.96%	11.339%
4	5.836	326	328	330	rBB	104014	85057	4.57%	0.523%
5	6.453	379	382	384	rBV	1664660	1626290	87.34%	10.008%
6	6.590	391	394	396	rBV	1745745	1640703	88.11%	10.097%
7	6.819	412	414	417	rBB	398231	421456	22.63%	2.594%
8	6.979	426	428	430	rBB	1470365	1277248	68.59%	7.860%
9	7.379	461	463	466	rBB	867120	1076279	57.80%	6.623%
10	8.099	524	526	529	rBB	427079	529524	28.44%	3.259%
11	9.185	618	621	623	rBV	1597796	1862091	100.00%	11.459%
12	9.859	677	680	682	rBB	422054	542075	29.11%	3.336%
13	10.636	745	748	751	rBV	934610	952367	51.15%	5.861%
14	11.333	806	809	811	rBV	614133	514556	27.63%	3.166%
15	12.922	945	948	950	rBV	1358652	1401552	75.27%	8.625%
16	13.962	1036	1039	1041	rBV	371009	356102	19.12%	2.191%
17	15.368	1159	1162	1165	rBV	234855	267788	14.38%	1.648%

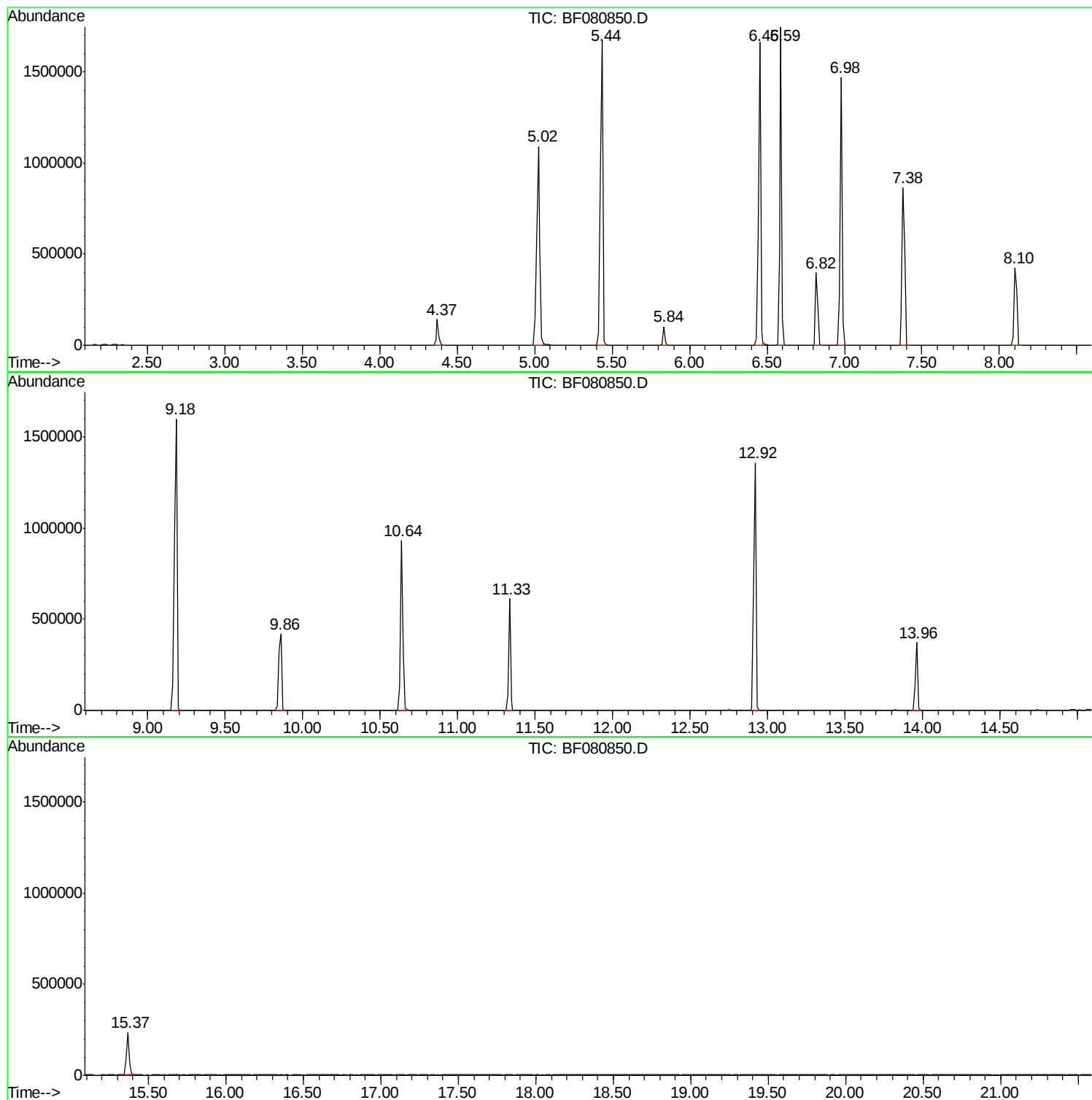
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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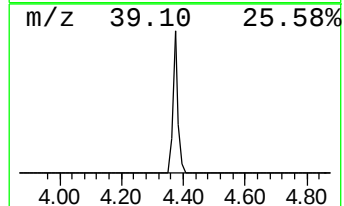
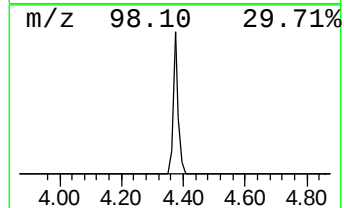
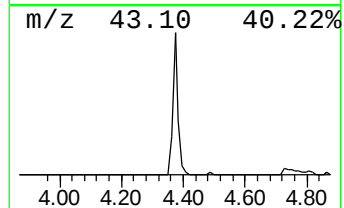
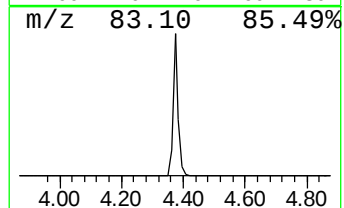
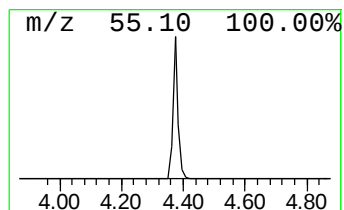
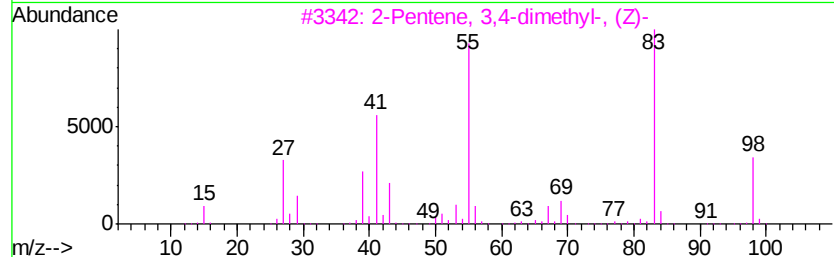
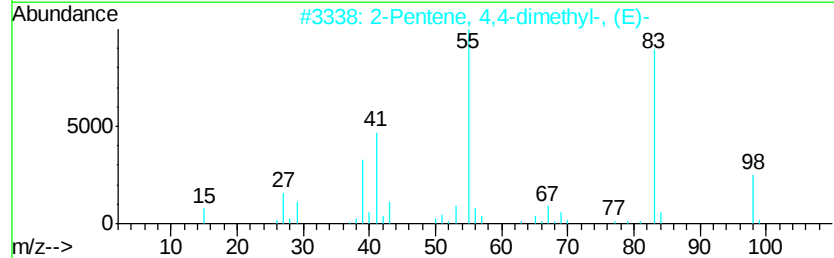
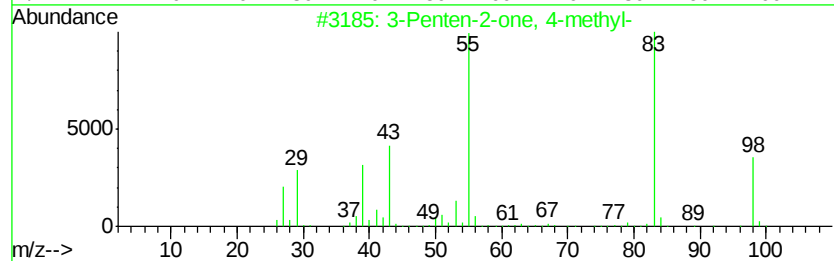
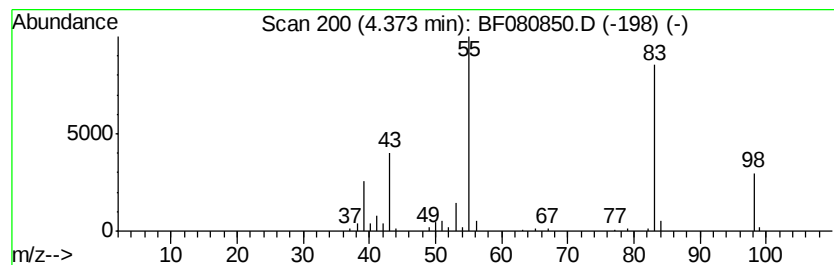
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	7.62 ng	160623	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
4			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	72
5			3-Hexen-2-one	98	C6H10O	000763-93-9	72



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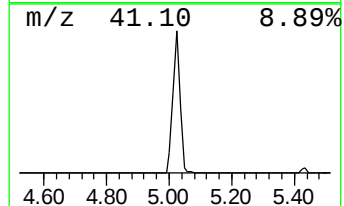
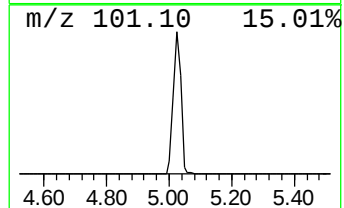
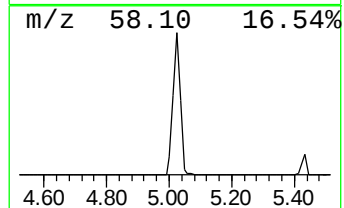
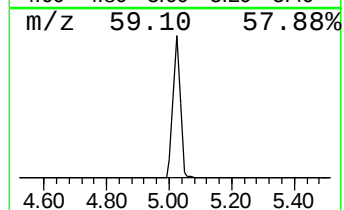
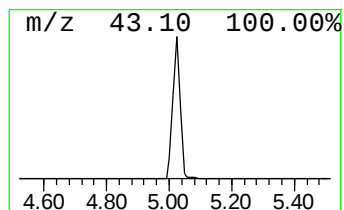
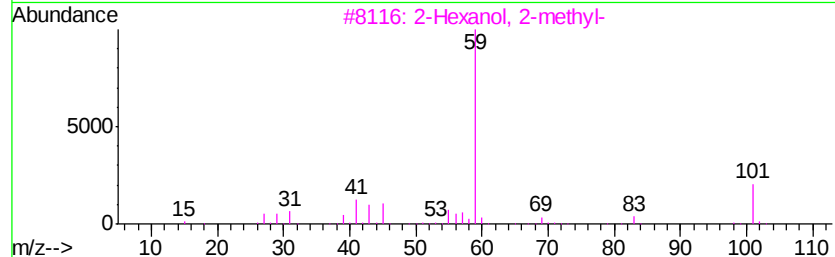
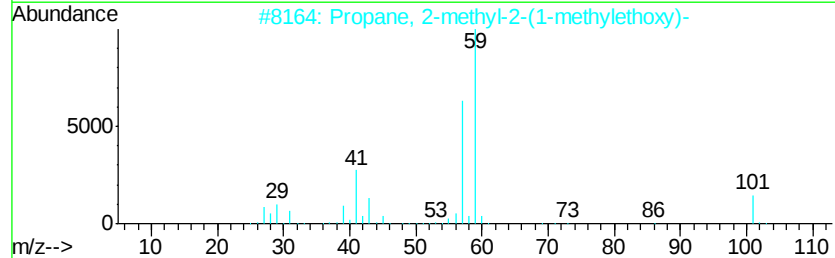
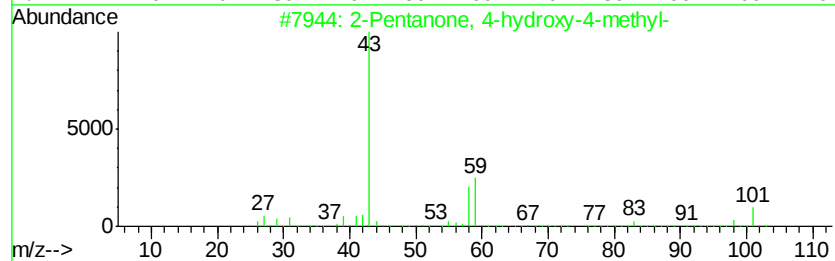
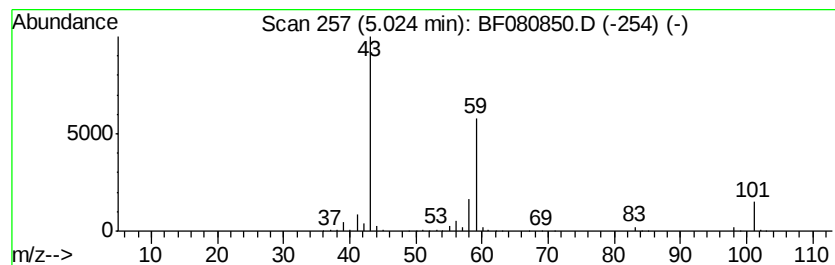
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	80.38 ng	1693770	1,4-Dichlorobenzene-d4	6.82

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	36
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
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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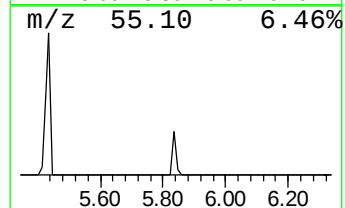
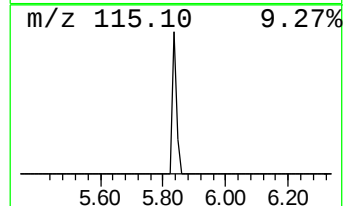
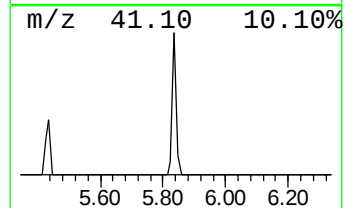
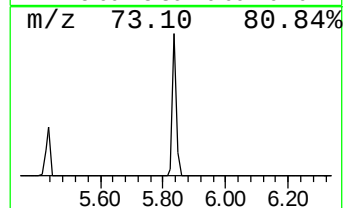
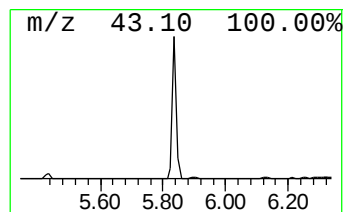
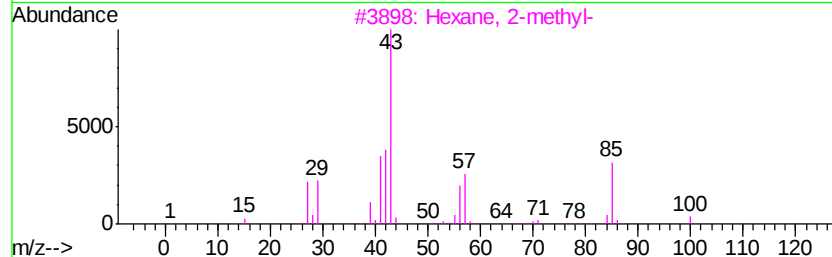
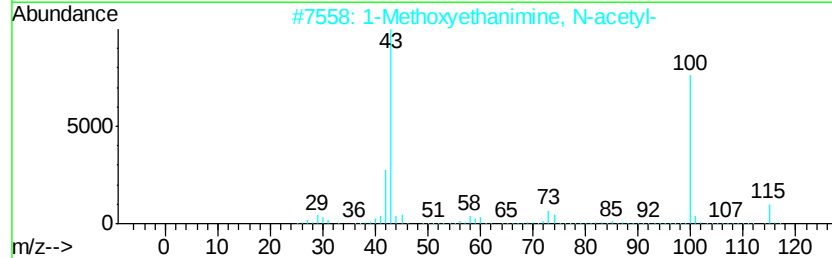
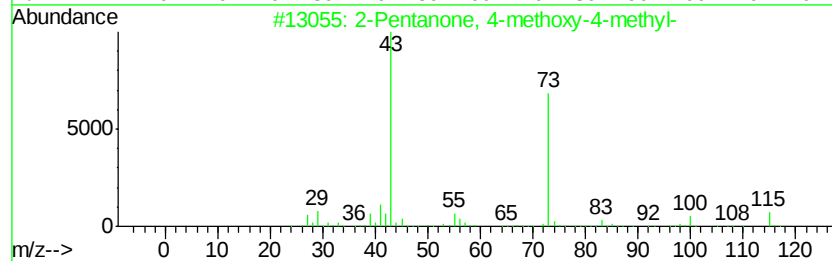
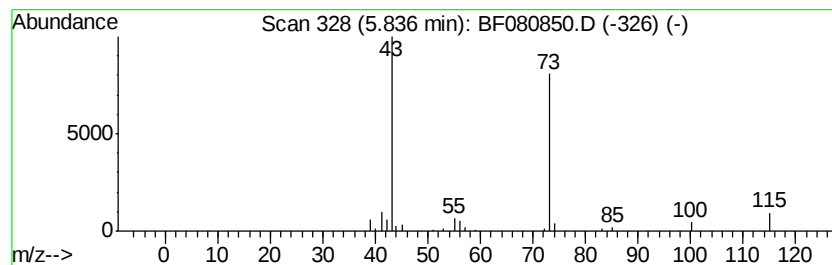
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.84	4.04 ng	85057	1,4-Dichlorobenzene-d4	6.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	28
3		Hexane, 2-methyl-	100	C7H16	000591-76-4	9
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5		Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	9



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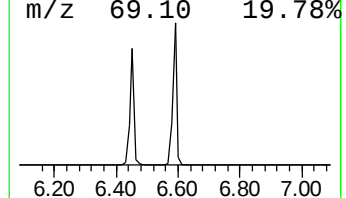
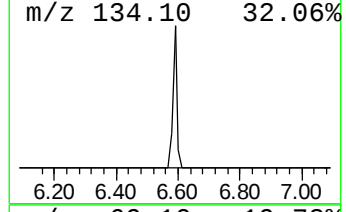
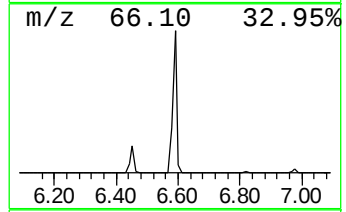
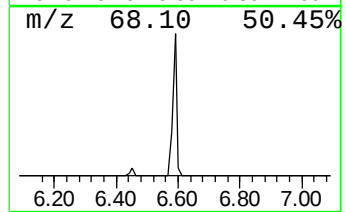
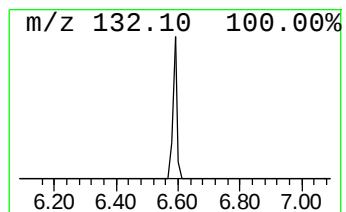
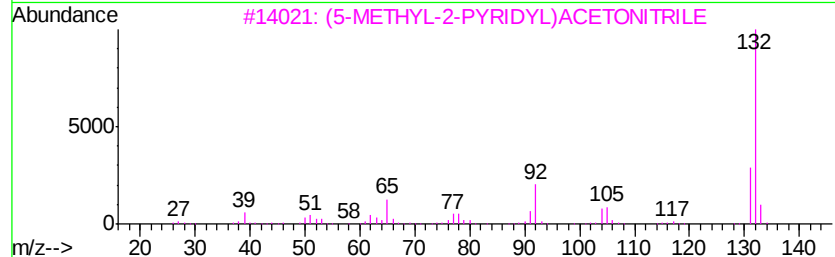
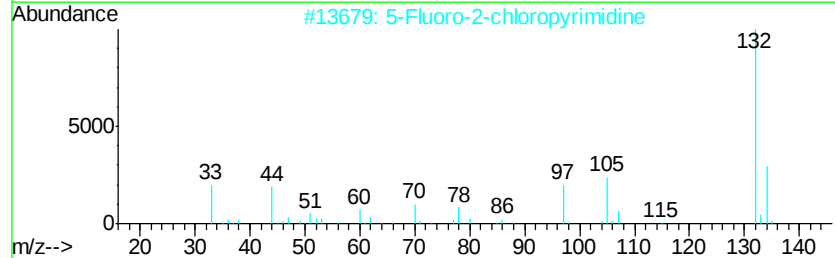
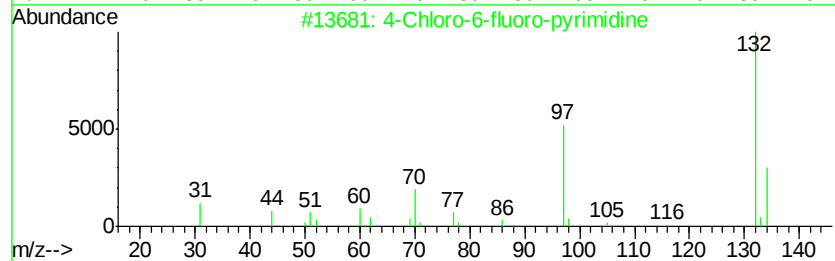
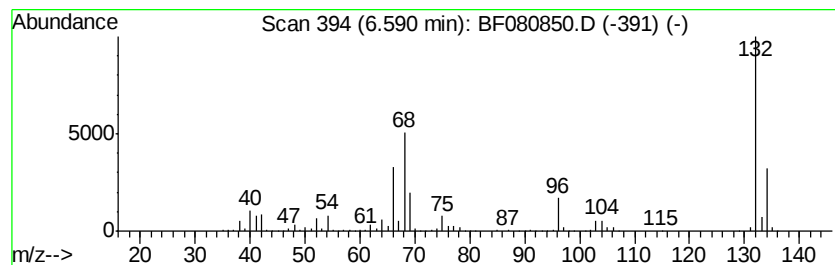
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Peak Number 4 unknown6.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	77.86 ng	1640700	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.37	7.6	ng	160623	1	6.82	421456	20.0
2-Pentanone, 4-hy...	5.02	80.4	ng	1693770	1	6.82	421456	20.0
2-Pentanone, 4-me...	5.84	4.0	ng	85057	1	6.82	421456	20.0
unknown6.59	6.59	77.9	ng	1640700	1	6.82	421456	20.0