

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF043016\
 Data File : BF086522.D
 Acq On : 30 Apr 2016 14:30
 Operator : UM/SJ
 Sample : PB90147BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90147BL

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-BF042716.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	4.270	187	191	193	rBV	2555081	3762010	42.66%	8.341%
2	4.956	246	251	254	rBV	3791808	8819324	100.00%	19.553%
3	5.367	284	287	289	rBV	2687532	2848132	32.29%	6.315%
4	5.767	320	322	325	rBV	577730	503071	5.70%	1.115%
5	6.407	375	378	380	rBV	2029600	2834877	32.14%	6.285%
6	6.533	387	389	391	rBV	2900026	2815289	31.92%	6.242%
7	6.761	407	409	412	rBV	809434	873468	9.90%	1.937%
8	6.922	420	423	425	rBV	3296032	3025188	34.30%	6.707%
9	7.333	456	459	461	rBV	2336103	2598211	29.46%	5.760%
10	8.053	519	522	524	rBV	1167324	1165679	13.22%	2.584%
11	9.127	613	616	619	rBV	3665233	3999940	45.35%	8.868%
12	9.802	672	675	678	rBV	1441555	1365913	15.49%	3.028%
13	10.590	741	744	746	rBV	1815520	1969485	22.33%	4.367%
14	11.288	802	805	807	rBV	974979	1311158	14.87%	2.907%
15	12.876	941	944	946	rBV	3500452	4654368	52.77%	10.319%
16	13.916	1032	1035	1049	rBV	998048	1445951	16.40%	3.206%
17	15.311	1154	1157	1170	rBV	714085	1111874	12.61%	2.465%

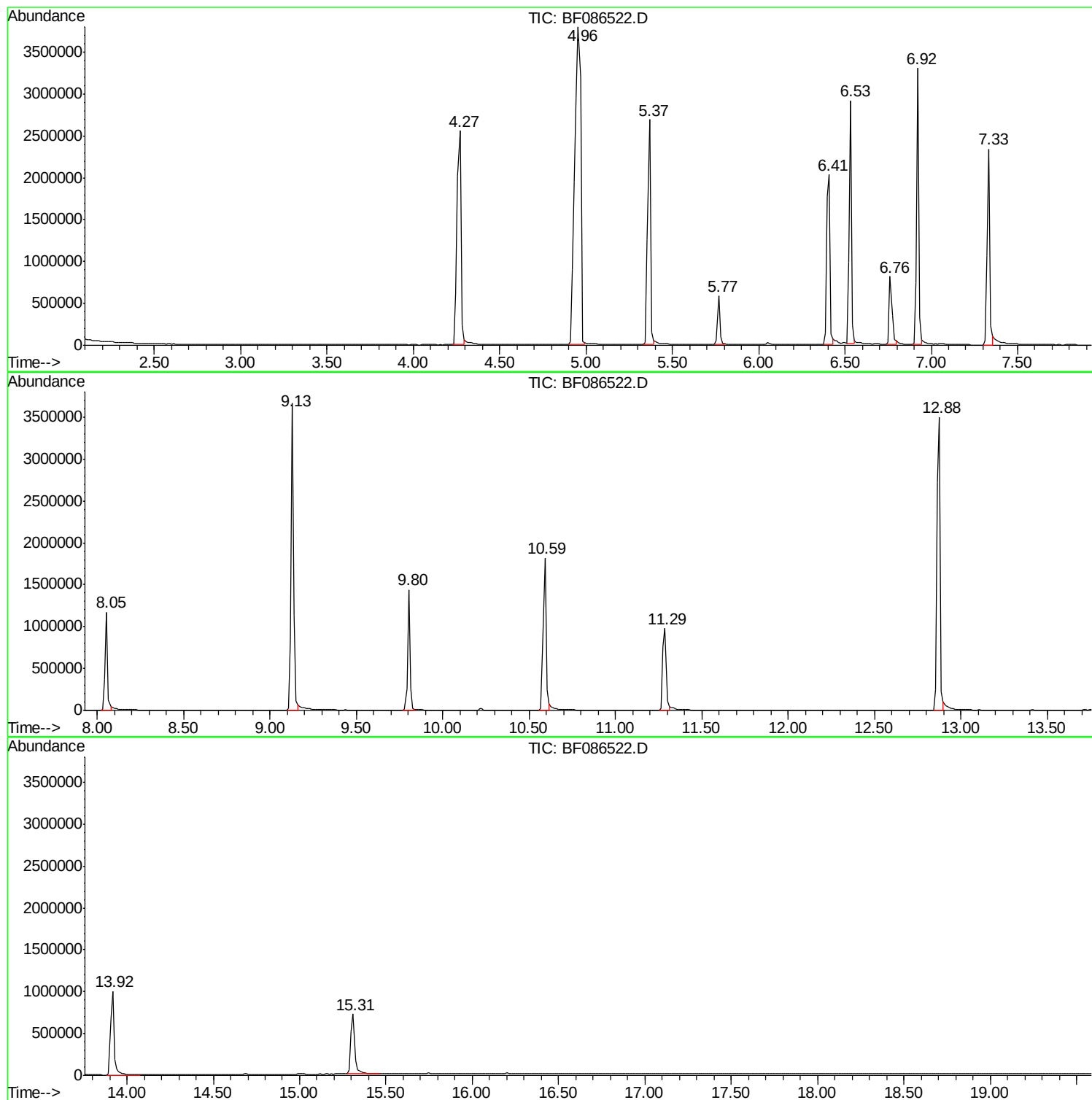
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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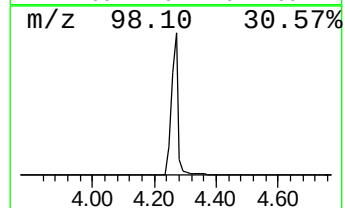
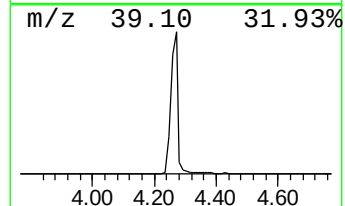
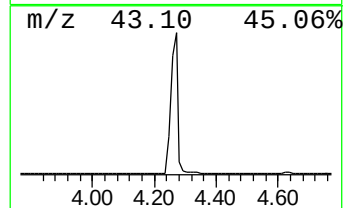
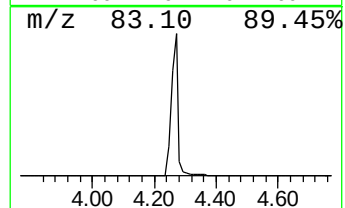
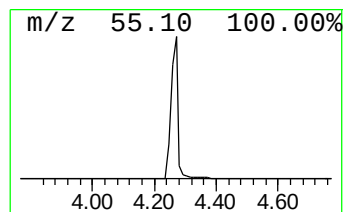
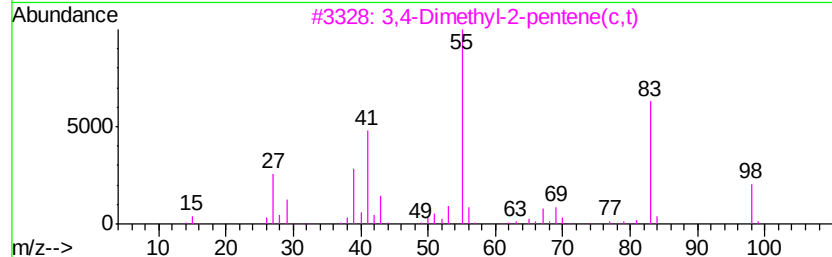
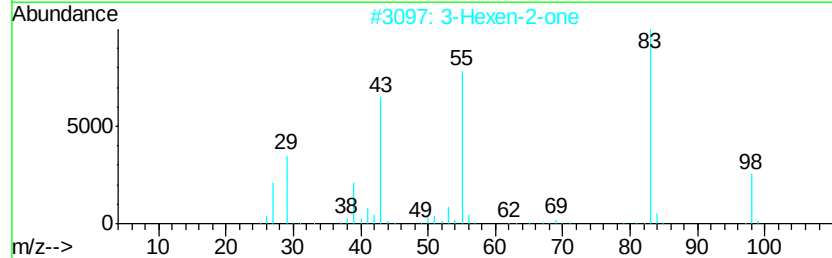
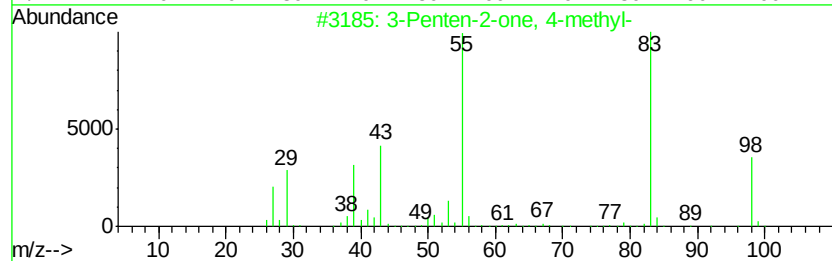
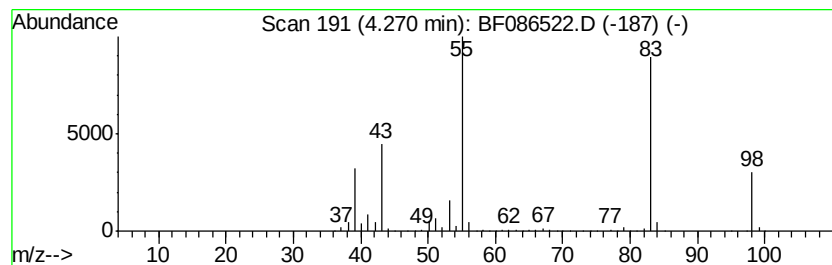
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	86.14 ng	3762010	1,4-Dichlorobenzene-d4	6.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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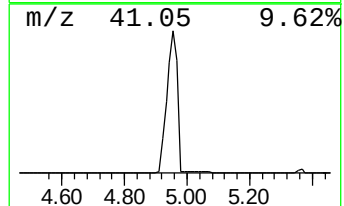
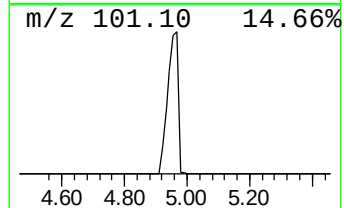
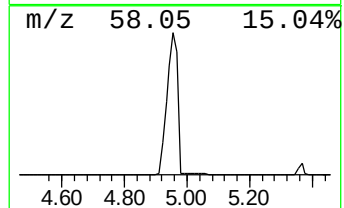
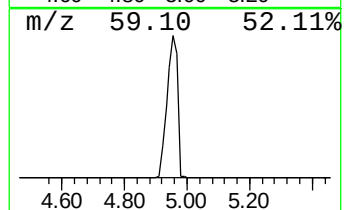
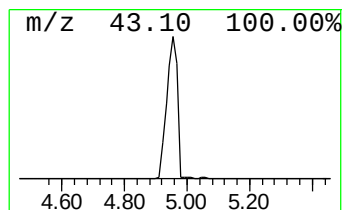
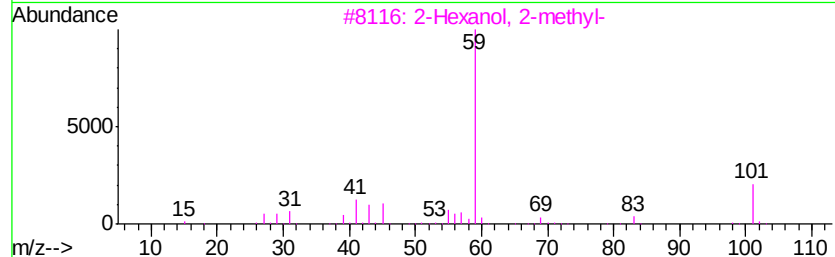
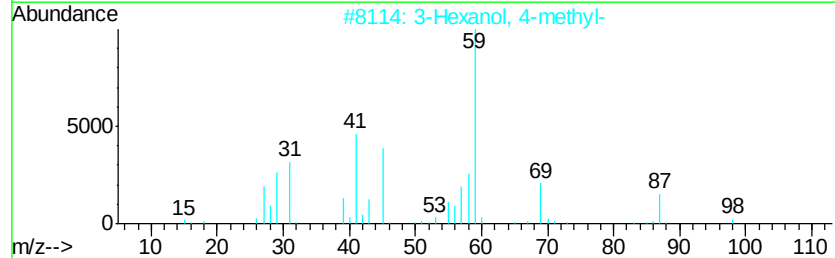
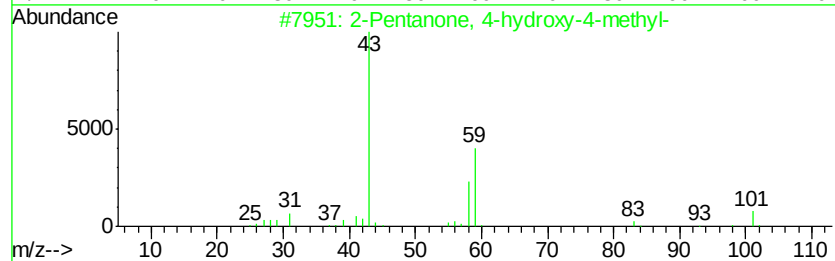
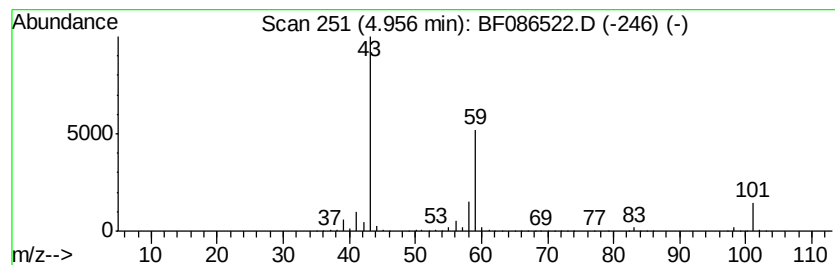
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	201.94 ng	8819320	1,4-Dichlorobenzene-d4	6.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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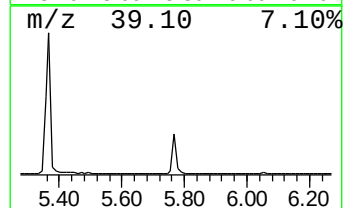
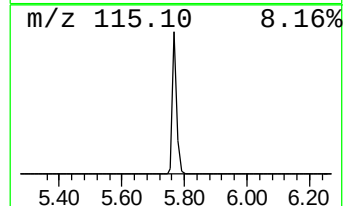
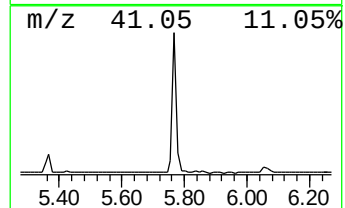
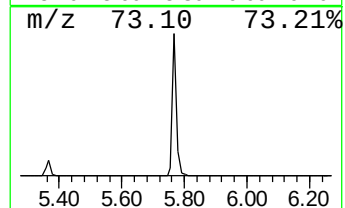
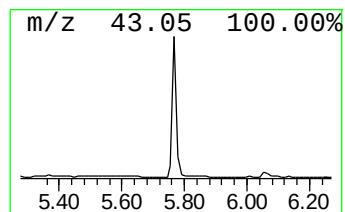
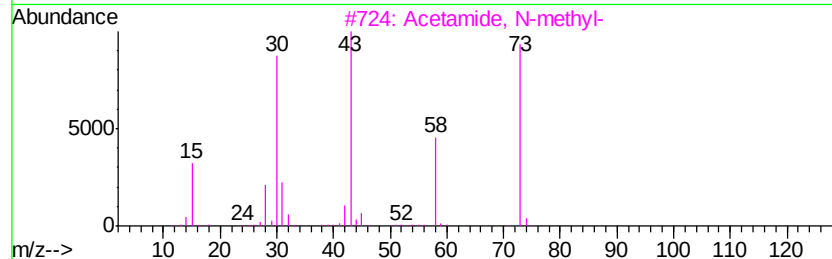
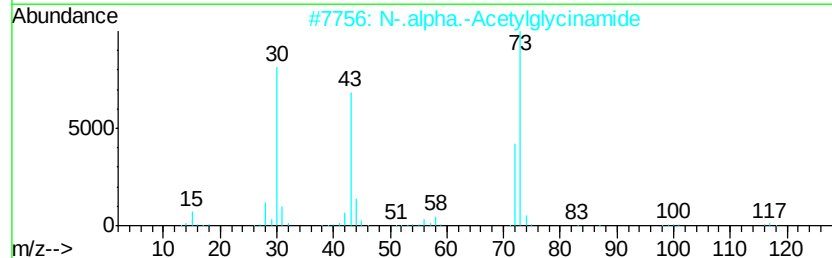
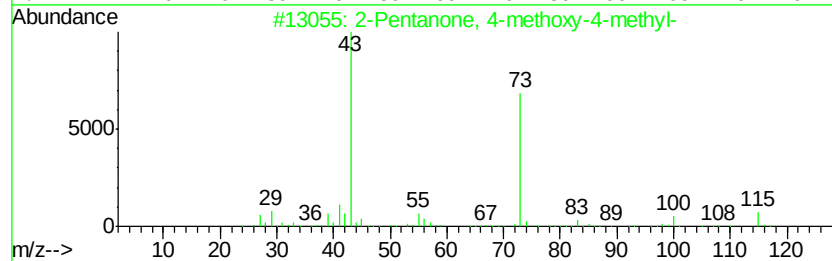
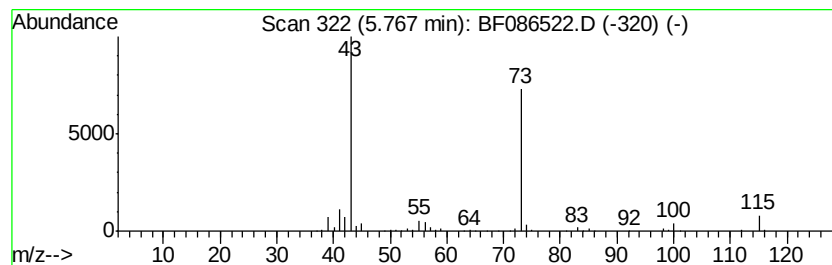
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Peak Number 3 unknown5.77 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	11.52 ng	503071	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	12
5		N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12



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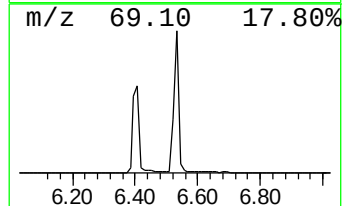
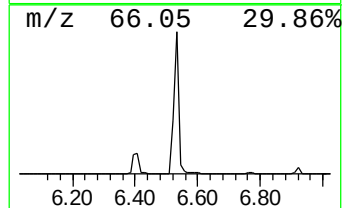
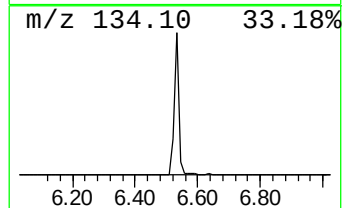
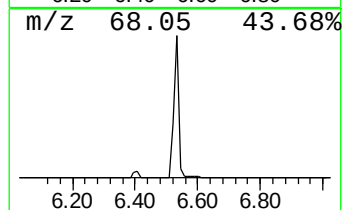
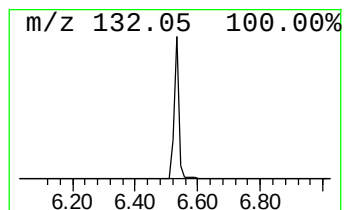
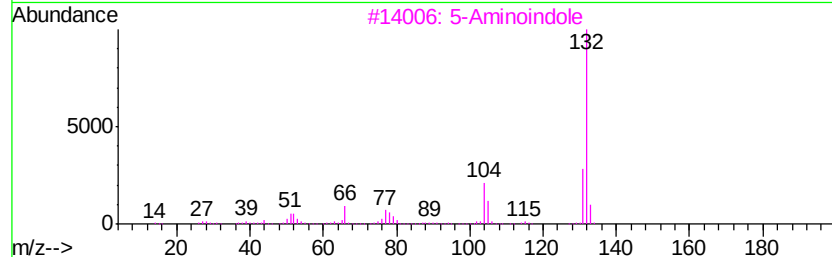
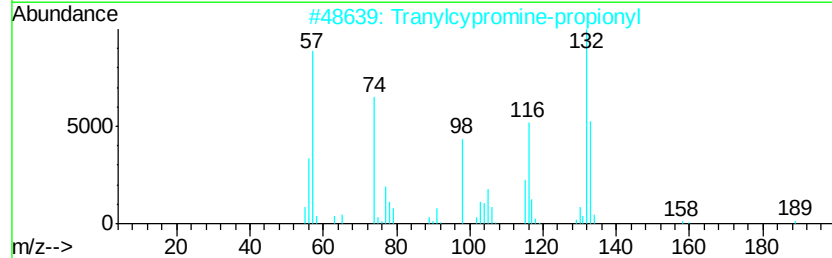
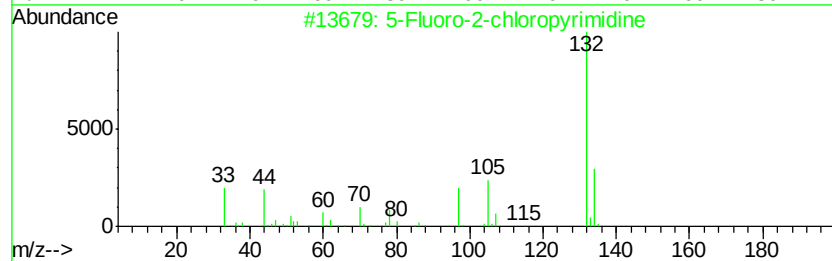
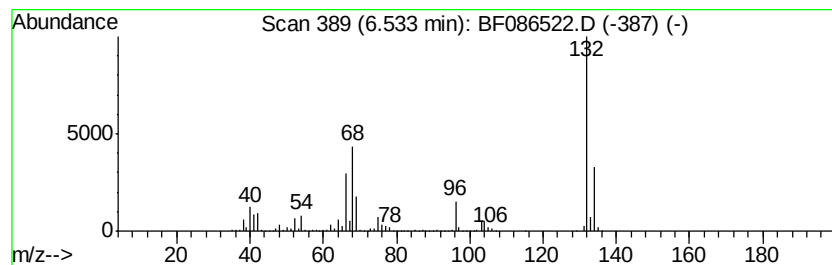
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Peak Number 4 unknown6.53 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	64.46 ng	2815290	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.27	86.1	ng	3762010	1	6.76	873468	20.0
2-Pentanone, 4-hy...	4.96	201.9	ng	8819320	1	6.76	873468	20.0
unknown5.77	5.77	11.5	ng	503071	1	6.76	873468	20.0
unknown6.53	6.53	64.5	ng	2815290	1	6.76	873468	20.0