

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051716\
 Data File : BF087119.D
 Acq On : 17 May 2016 23:25
 Operator : UM/SJ
 Sample : PB90651TB
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB90651TB

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-BF051716.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	1.724	10	12	60	rVB	3460208	7988404	71.51%	14.347%
2	3.998	207	211	214	rBV	3386126	6810325	60.97%	12.231%
3	4.764	271	278	280	rBV	4351483	11170719	100.00%	20.062%
4	5.187	313	315	328	rBV	2315656	2445042	21.89%	4.391%
5	5.587	348	350	352	rBV	600834	738750	6.61%	1.327%
6	6.250	406	408	416	rBV	1854965	2345416	21.00%	4.212%
7	6.364	416	418	420	rBV	2373593	2426023	21.72%	4.357%
8	6.593	435	438	440	rBV	737336	899818	8.06%	1.616%
9	6.742	449	451	454	rBV	2565801	2571860	23.02%	4.619%
10	7.164	485	488	490	rBV	2309146	2275439	20.37%	4.087%
11	7.873	548	550	553	rBV	863203	1162410	10.41%	2.088%
12	8.959	642	645	647	rBV	3817635	3774552	33.79%	6.779%
13	9.622	701	703	706	rBV	1011967	1332162	11.93%	2.393%
14	10.411	770	772	775	rBV2	1282761	1718317	15.38%	3.086%
15	11.108	830	833	835	rBV	1340758	1439378	12.89%	2.585%
16	12.696	969	972	974	rBV	3308978	4292880	38.43%	7.710%
17	13.737	1060	1063	1065	rBV	874439	1265721	11.33%	2.273%
18	15.085	1178	1181	1188	rBV	825794	1023055	9.16%	1.837%

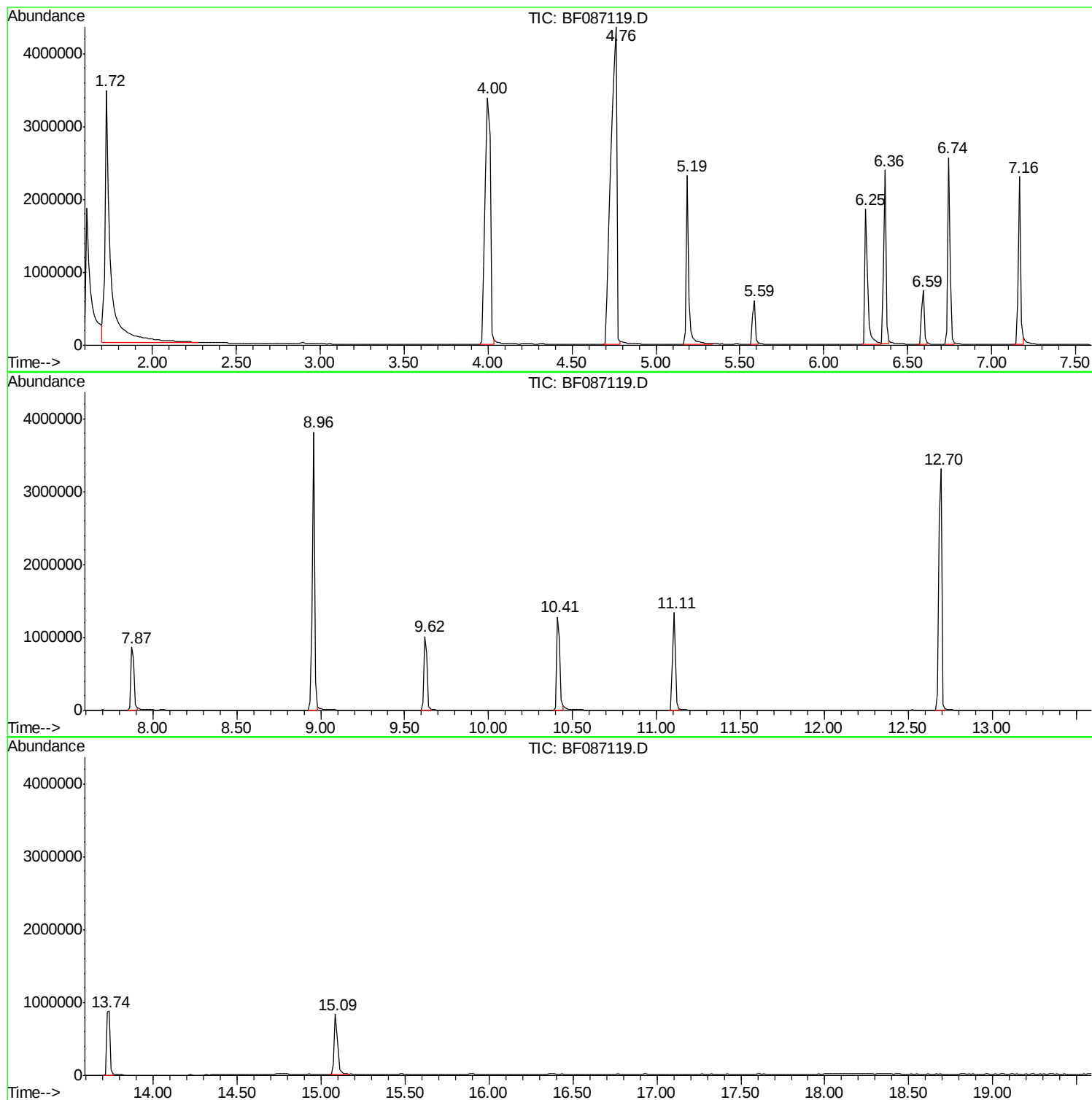
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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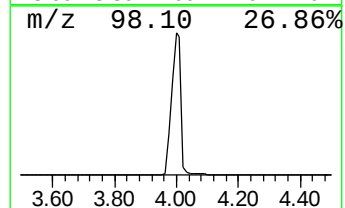
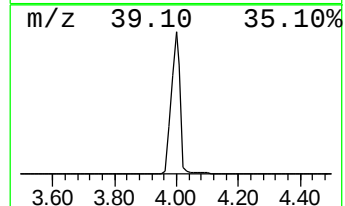
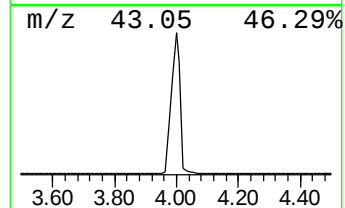
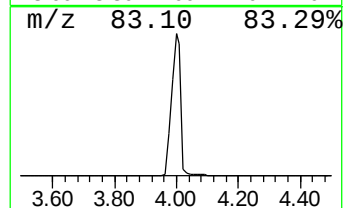
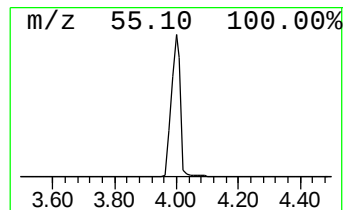
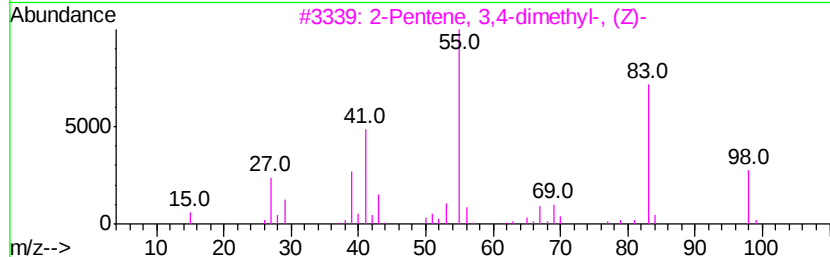
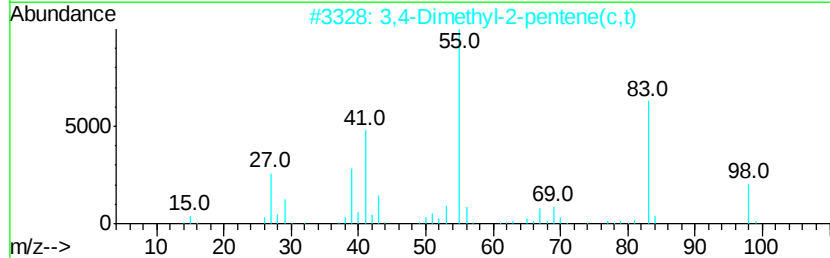
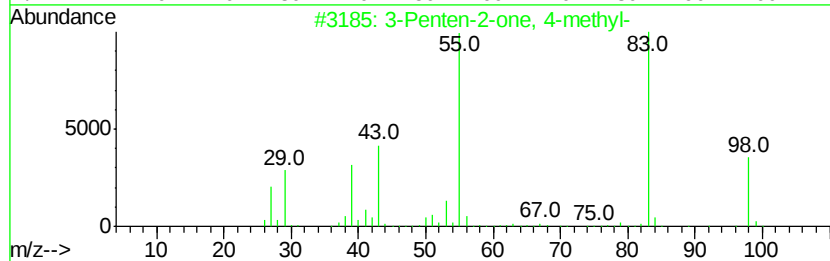
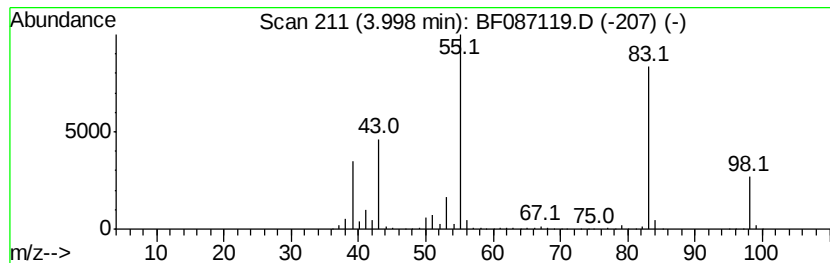
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	151.37 ng	6810330	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		3-Hexen-2-one	98	C6H10O	000763-93-9	80
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78



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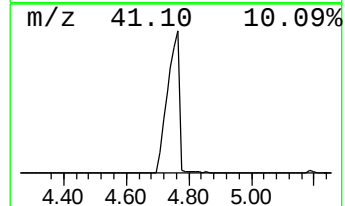
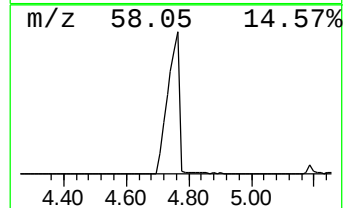
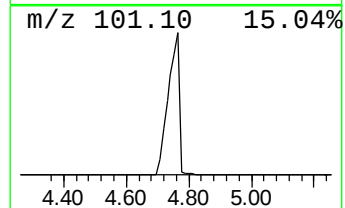
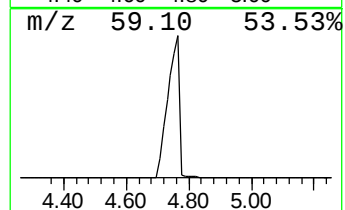
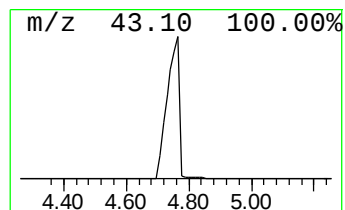
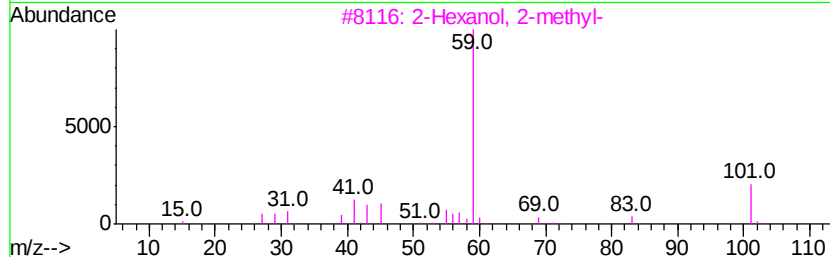
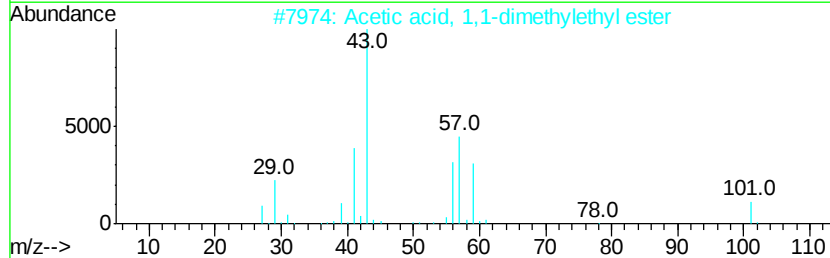
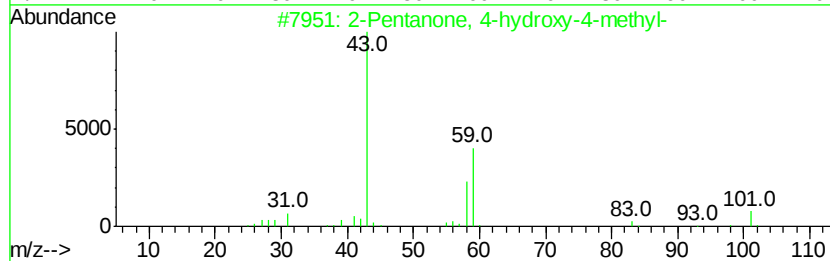
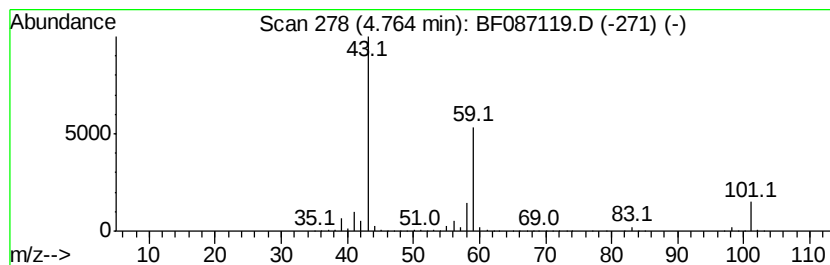
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	248.29 ng	11170700	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
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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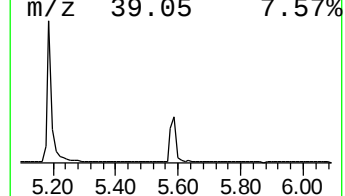
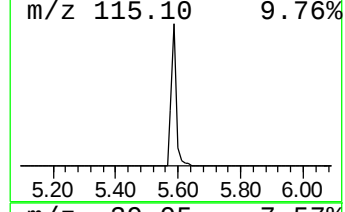
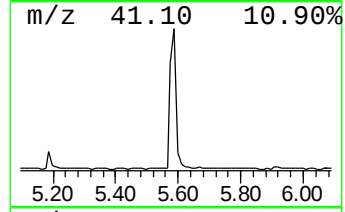
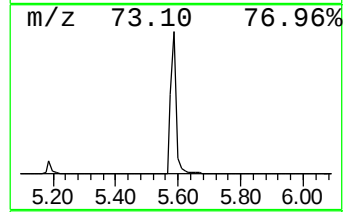
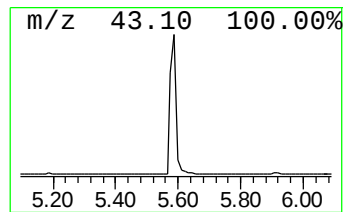
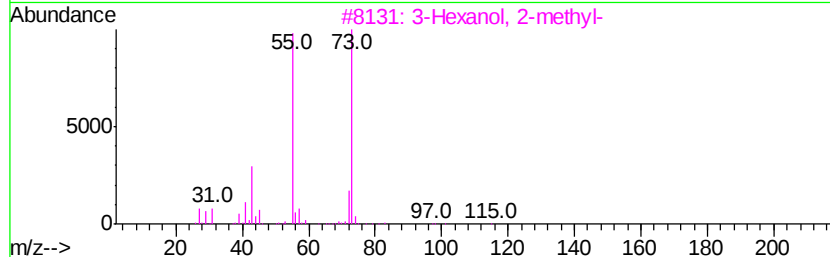
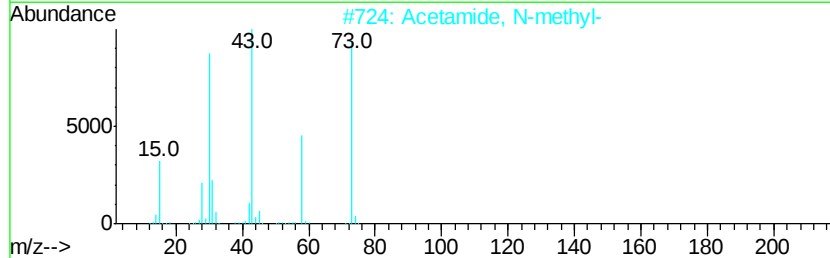
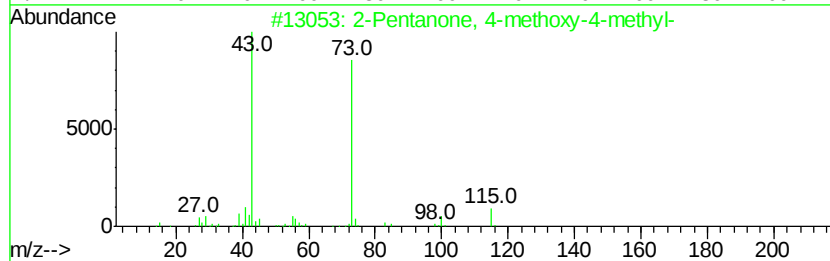
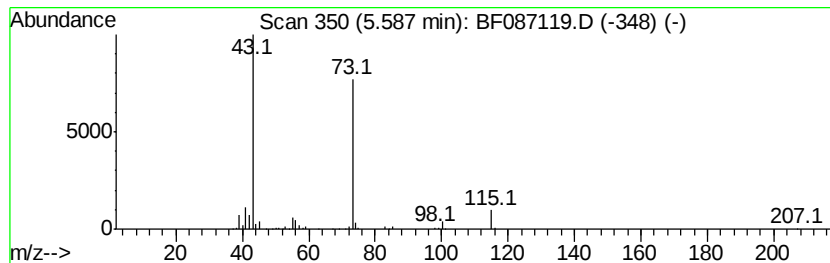
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	16.42 ng	738750	1,4-Dichlorobenzene-d4	6.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83	
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25	
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17	
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	12	
5	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10	



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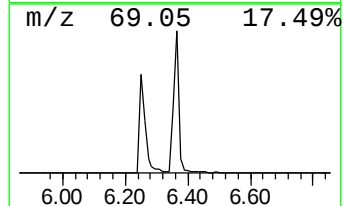
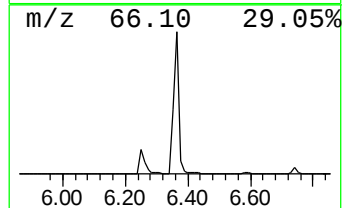
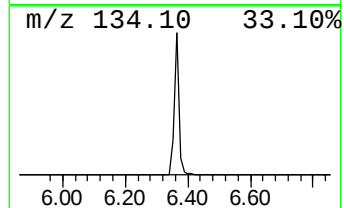
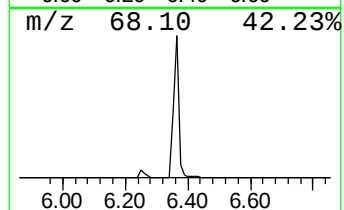
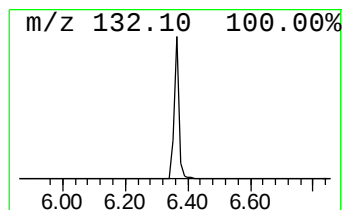
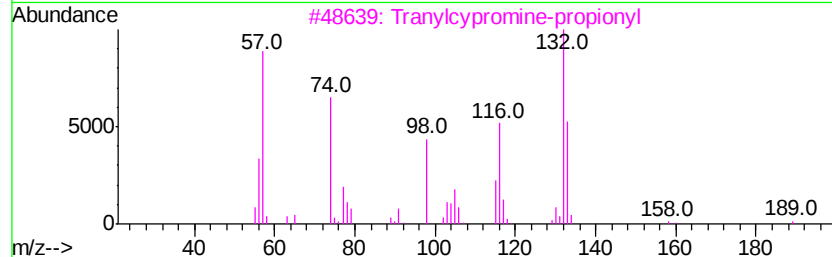
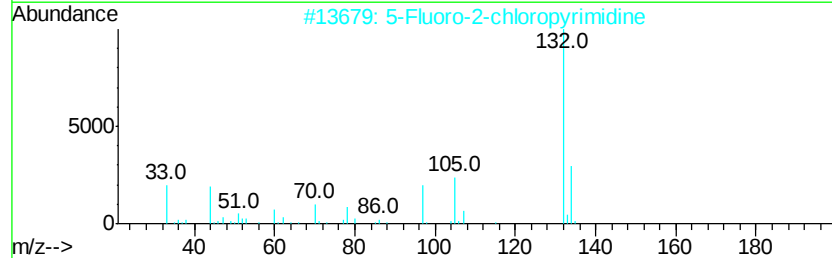
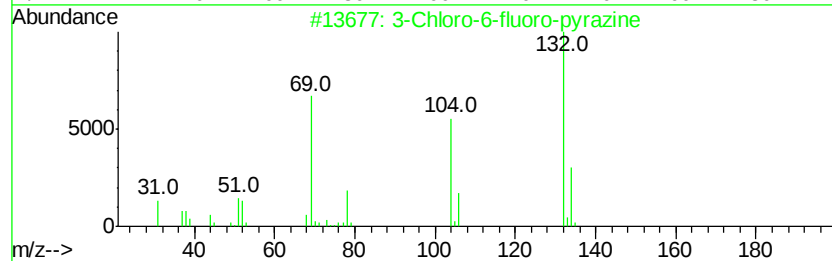
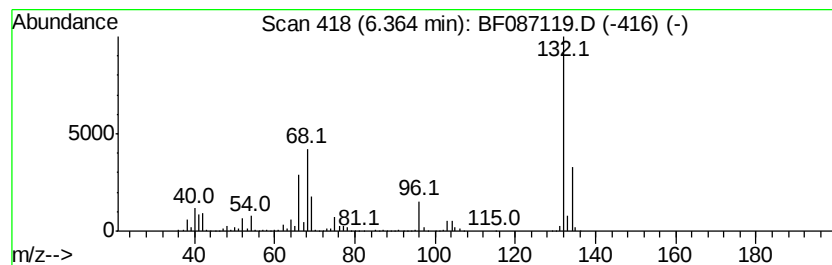
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Peak Number 5 unknown6.36 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	53.92 ng	2426020	1,4-Dichlorobenzene-d4	6.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	16
3	Tranvlcvpromine-propionyl			189	C12H15NO	1000123-86-3	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE			132	C8H8N2	1000241-93-9	10
5	Benzene, 1,2,4-trifluoro-			132	C6H3F3	000367-23-7	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.00	151.4	ng	6810330	1	6.59	899818	20.0
2-Pentanone, 4-hy...	4.76	248.3	ng	11170700	1	6.59	899818	20.0
2-Pentanone, 4-me...	5.59	16.4	ng	738750	1	6.59	899818	20.0
unknown6.36	6.36	53.9	ng	2426020	1	6.59	899818	20.0