

Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\
 Data File : BM010175.D
 Acq On : 24 May 2017 11:51
 Operator : SJ/MA
 Sample : PB99209BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB99209BL

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_M\METHODS\8270-BM051917.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	4.451	228	232	247	rBV	3135492	4183058	50.27%	8.789%
2	5.075	332	338	349	rBV	5691476	7652102	91.96%	16.078%
3	5.534	410	416	426	rBV	1384854	1948902	23.42%	4.095%
4	6.134	512	518	528	rBV	373896	549825	6.61%	1.155%
5	7.140	682	689	697	rBV	1194069	1875024	22.53%	3.940%
6	7.492	742	749	761	rVB	1287829	2022433	24.30%	4.249%
7	7.951	820	827	837	rVB	516598	809770	9.73%	1.701%
8	8.275	875	882	893	rBV	1544455	2566689	30.84%	5.393%
9	9.139	1021	1029	1039	rBV	1072695	1747168	21.00%	3.671%
10	10.757	1295	1304	1313	rBV	556641	951516	11.43%	1.999%
11	13.204	1713	1720	1732	rBV	3056934	4470503	53.72%	9.393%
12	14.586	1948	1955	1966	rVB2	843086	1265343	15.21%	2.659%
13	16.074	2202	2208	2222	rBV	1552980	2107541	25.33%	4.428%
14	17.327	2415	2421	2429	rBV	1163737	1642419	19.74%	3.451%
15	19.927	2858	2863	2870	rBV	6606250	8321317	100.00%	17.485%
16	21.486	3123	3128	3134	rBV	2078497	2667164	32.05%	5.604%
17	23.850	3524	3530	3537	rVB2	1462493	2811697	33.79%	5.908%

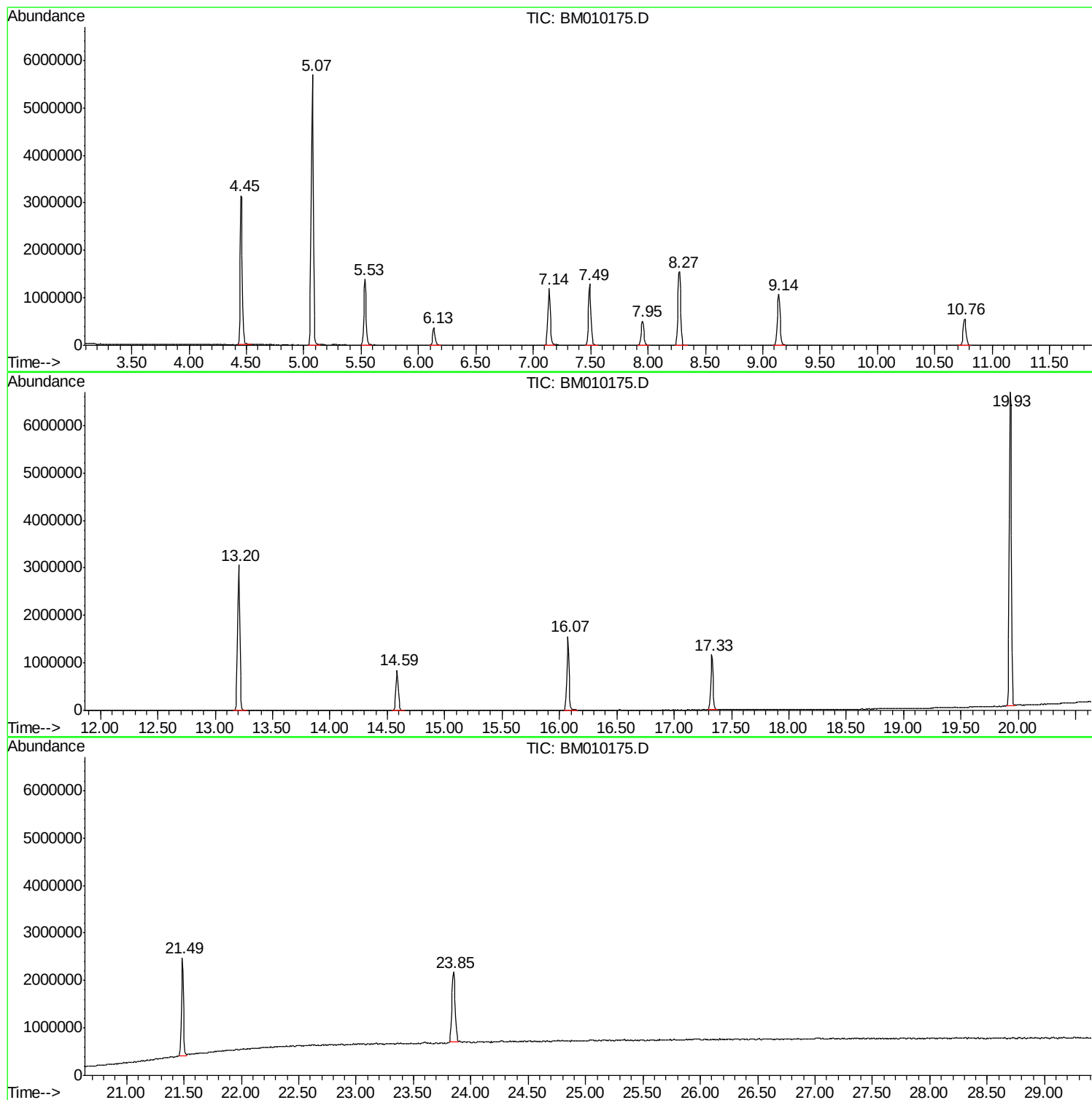
Sum of corrected areas: 47592471

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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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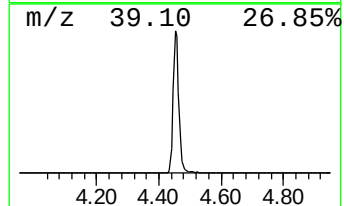
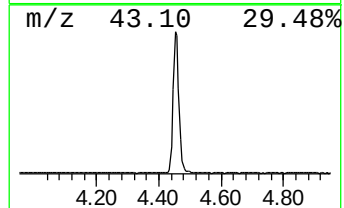
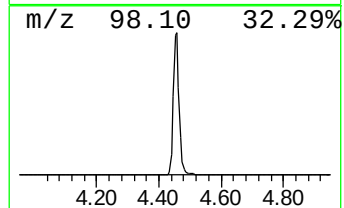
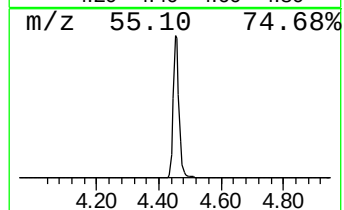
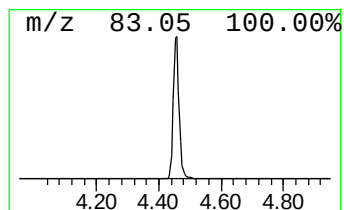
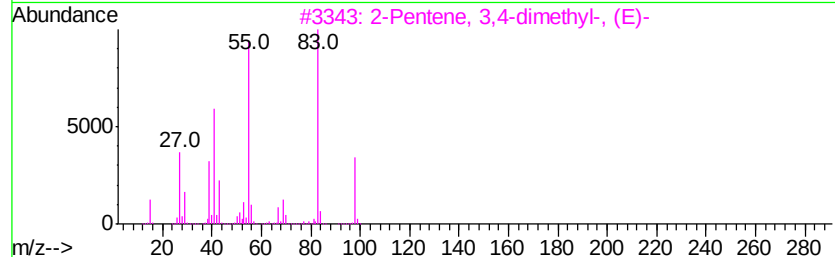
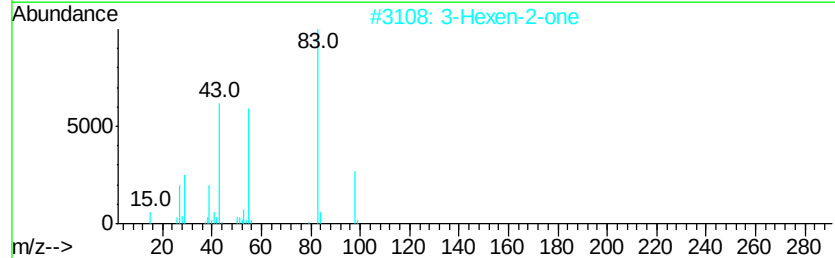
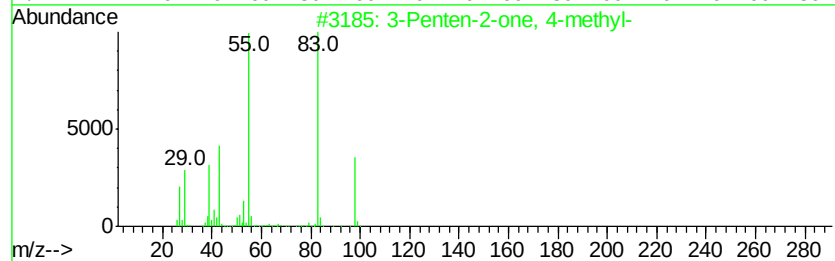
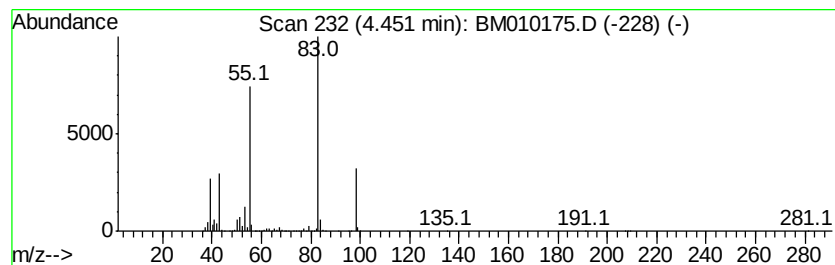
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	103.32 ng	4183060	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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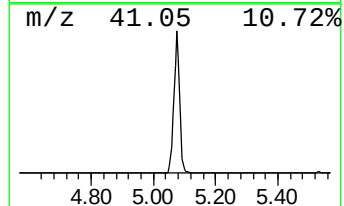
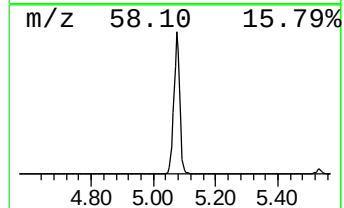
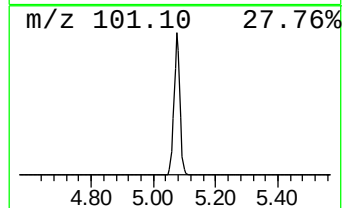
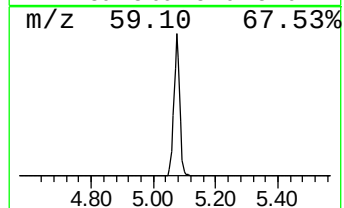
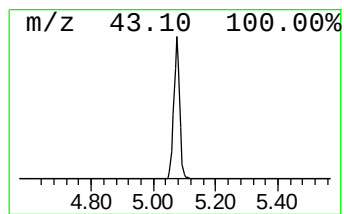
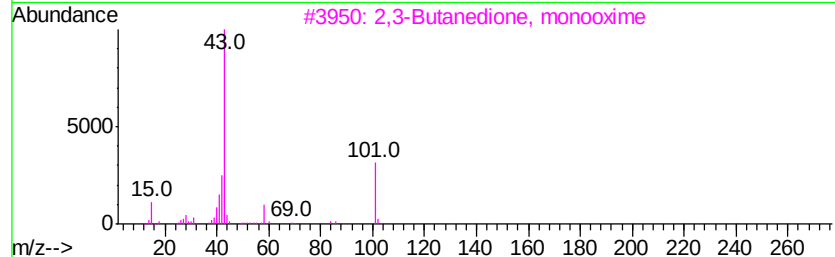
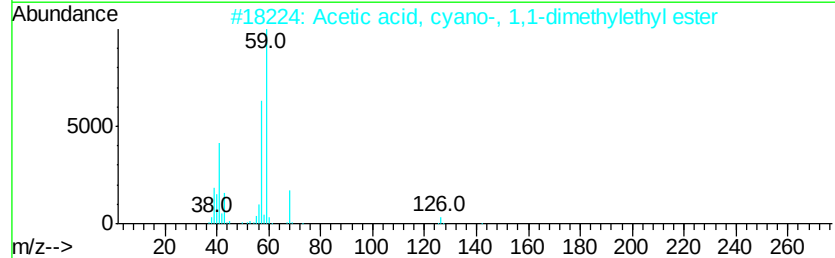
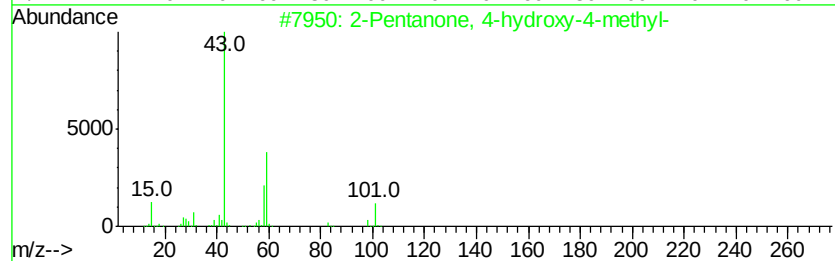
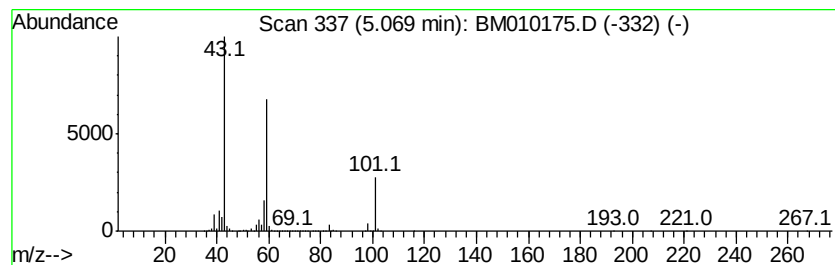
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	188.99 ng	7652100	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12



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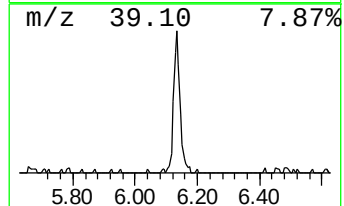
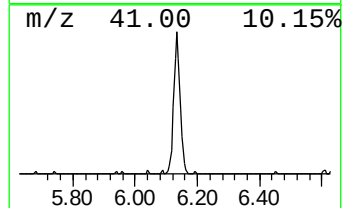
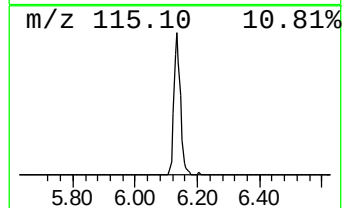
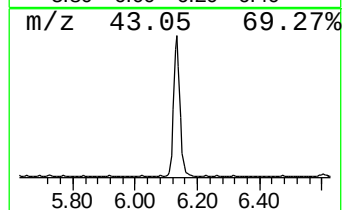
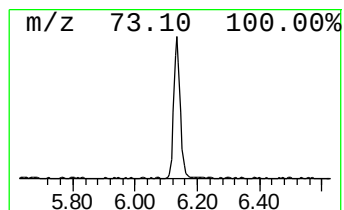
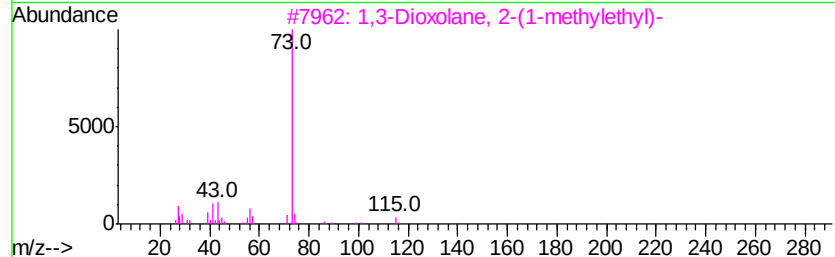
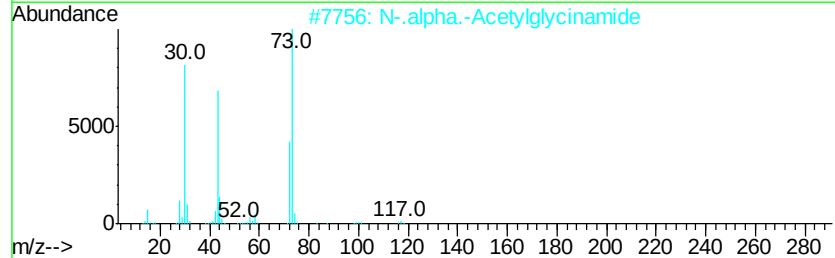
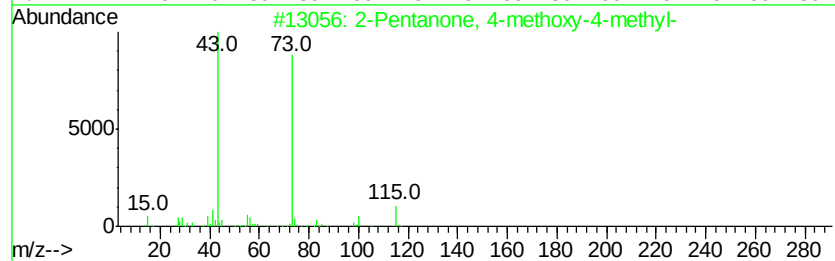
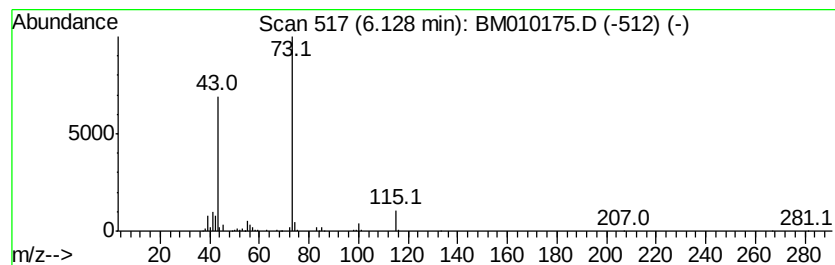
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.13	13.58 ng	549825	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		N-.alpha.-Acetylglucynamide	116	C4H8N2O2	002620-63-5	38
3		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	25
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5		N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



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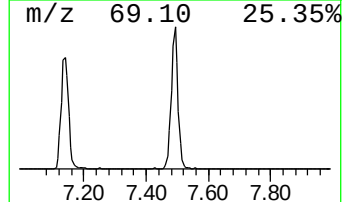
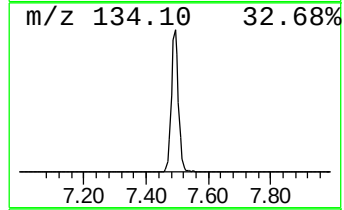
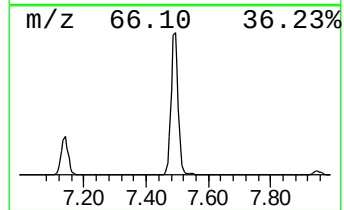
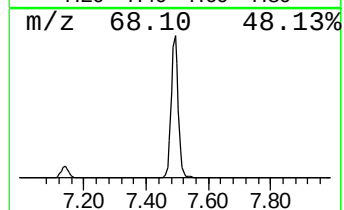
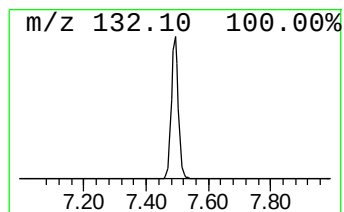
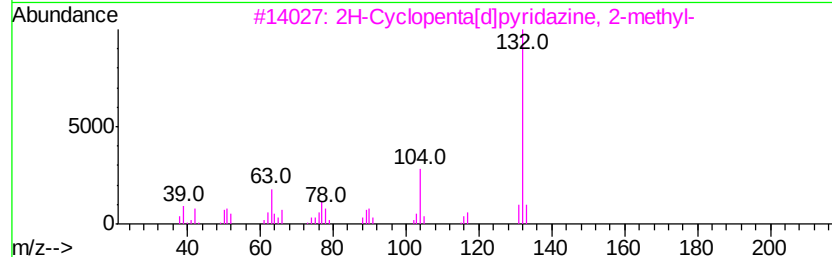
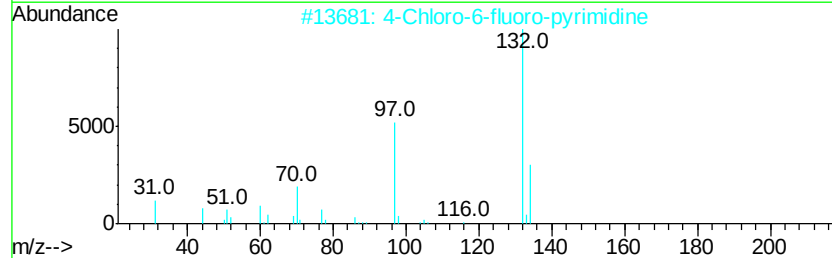
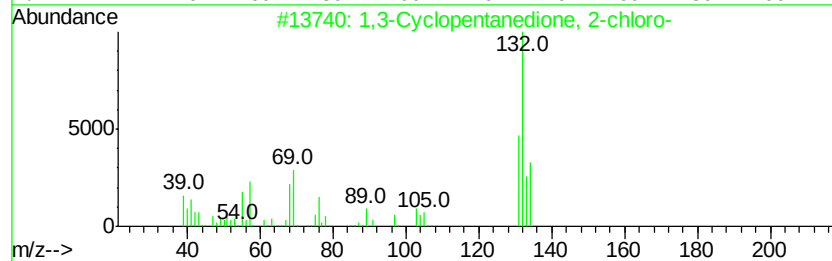
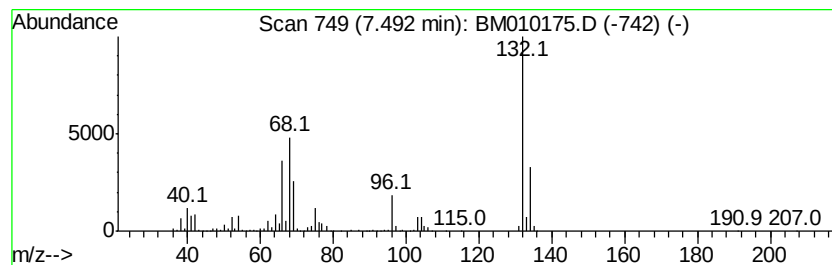
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Peak Number 4 unknown7.49 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.49	49.95 ng	2022430	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.45	103.3	ng	4183060	1	7.95	809770	20.0
2-Pentanone, 4-hy...	5.07	189.0	ng	7652100	1	7.95	809770	20.0
2-Pentanone, 4-me...	6.13	13.6	ng	549825	1	7.95	809770	20.0
unknown7.49	7.49	50.0	ng	2022430	1	7.95	809770	20.0