

Data Path : V:\HPCHEM1\BNA G\DATA\BG070916\
 Data File : BG022961.D
 Acq On : 9 Jul 2016 12:05
 Operator : UM/SJ
 Sample : PB91974BL
 Misc :
 ALS Vial : 56 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB91974BL

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_G\METHODS\8270-BG070816.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	3.040	29	34	42	rBV	241403	311336	3.37%	0.668%
2	4.615	296	302	313	rVB	1558604	2326514	25.17%	4.990%
3	5.226	399	406	417	rBV	3090762	4904595	53.06%	10.519%
4	5.696	476	486	499	rBV	1153826	1918828	20.76%	4.115%
5	6.313	585	591	597	rBV	231150	363744	3.94%	0.780%
6	7.306	753	760	768	rBV	1349139	2250100	24.34%	4.826%
7	7.682	817	824	835	rVB	1208796	2083112	22.54%	4.468%
8	8.152	895	904	914	rVB2	318395	581388	6.29%	1.247%
9	8.475	952	959	967	rBV	1258792	2192601	23.72%	4.703%
10	9.321	1096	1103	1115	rVB	1153582	2100121	22.72%	4.504%
11	10.978	1378	1385	1392	rVB	494030	861192	9.32%	1.847%
12	13.416	1791	1800	1807	rBV	3423887	5315835	57.51%	11.401%
13	14.797	2027	2035	2042	rBV3	904706	1506633	16.30%	3.231%
14	16.289	2278	2289	2303	rBV	2170073	3581334	38.75%	7.681%
15	17.552	2498	2504	2514	rVB2	1329462	2048892	22.17%	4.394%
16	19.832	2888	2892	2896	rBV	205289	235437	2.55%	0.505%
17	20.155	2941	2947	2953	rBV	6918593	9242895	100.00%	19.824%
18	20.866	3063	3068	3074	rBV3	154081	174697	1.89%	0.375%
19	21.847	3228	3235	3243	rBV2	1409965	2415690	26.14%	5.181%
20	25.202	3795	3806	3817	rBV2	729403	2210810	23.92%	4.742%

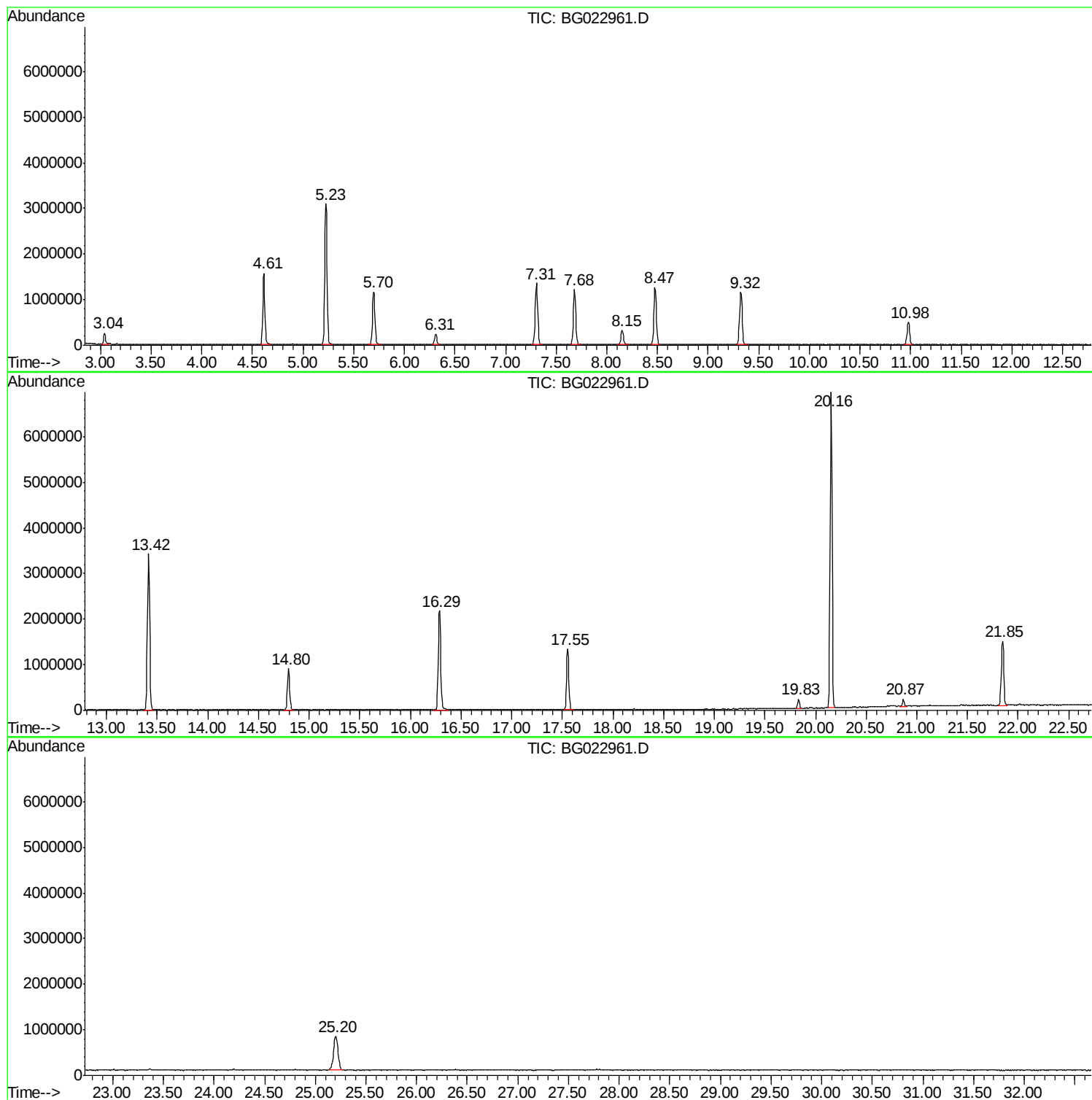
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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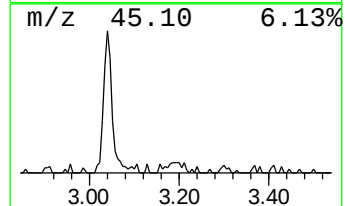
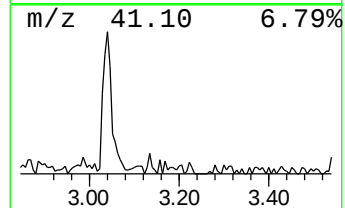
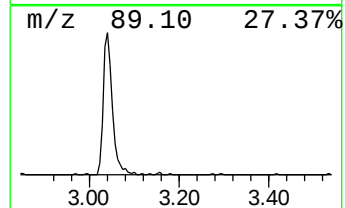
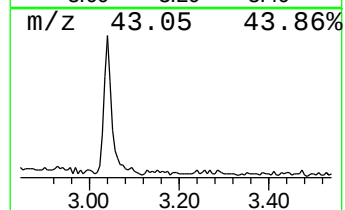
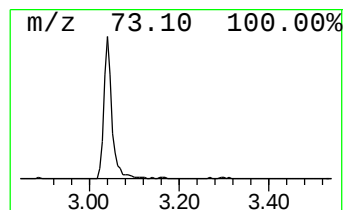
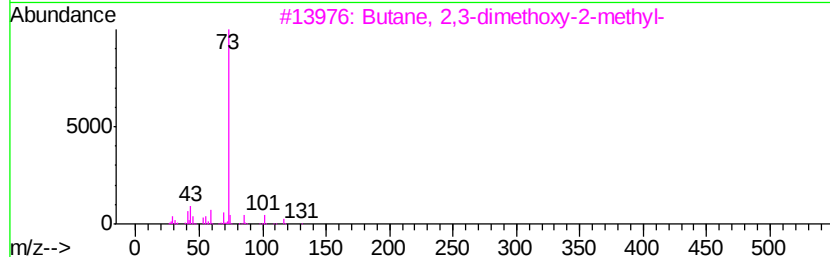
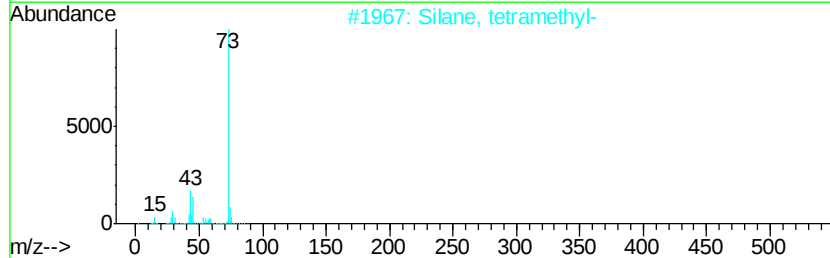
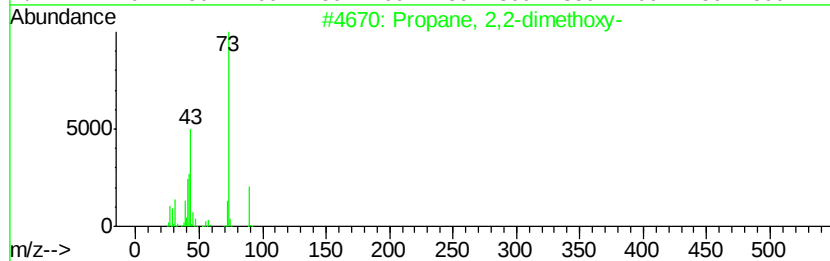
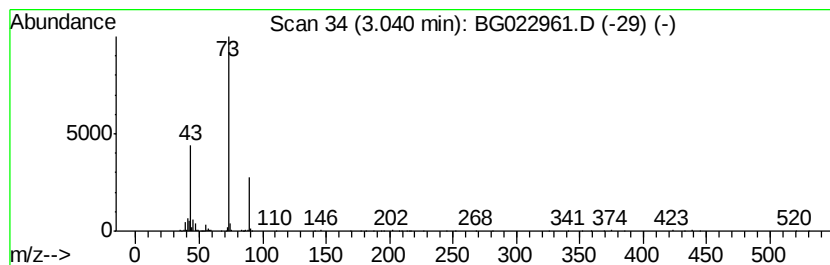
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.04 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	10.71 ng	311336	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	25
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3		Butane, 2,3-dimethoxy-2-methyl-	132	C7H16O2	074421-00-4	9
4		2,2'-Trimethylenebis-1,3-dioxolane	188	C9H16O4	006543-04-0	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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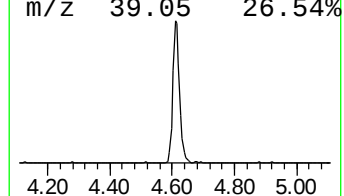
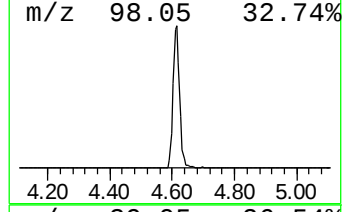
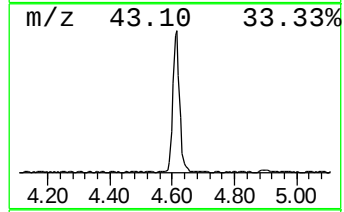
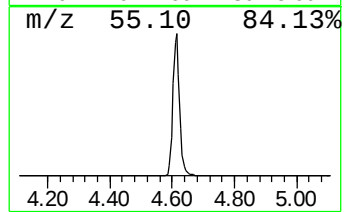
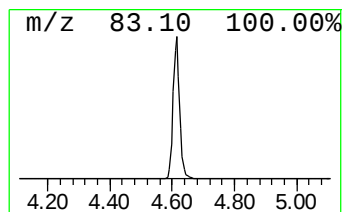
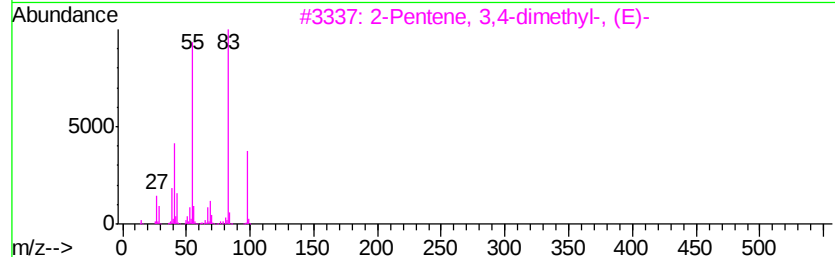
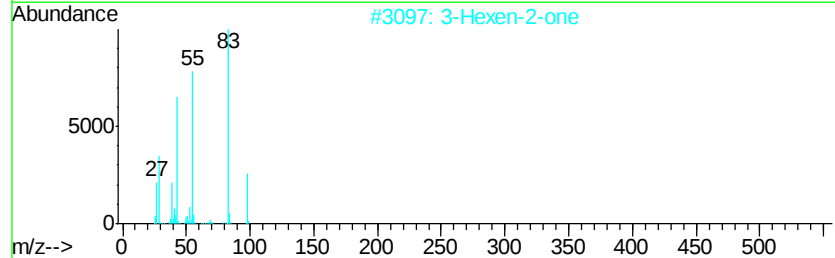
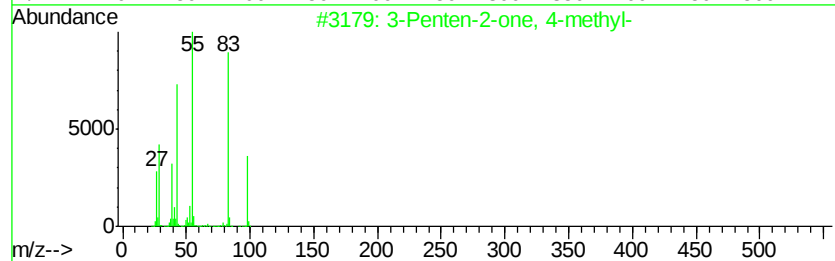
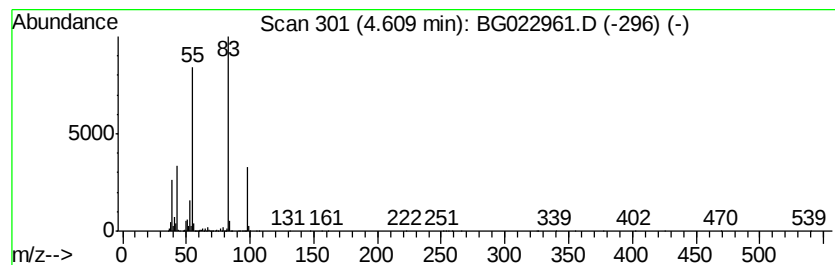
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	80.03 ng	2326510	1,4-Dichlorobenzene-d4	8.15

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			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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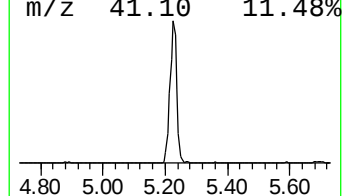
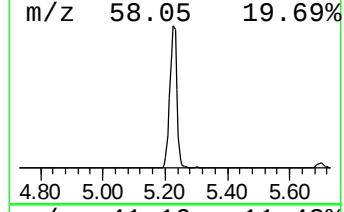
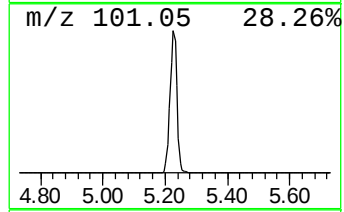
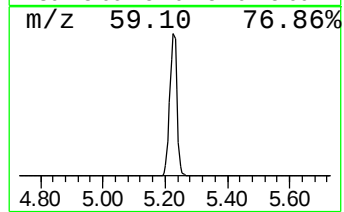
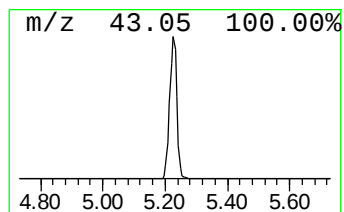
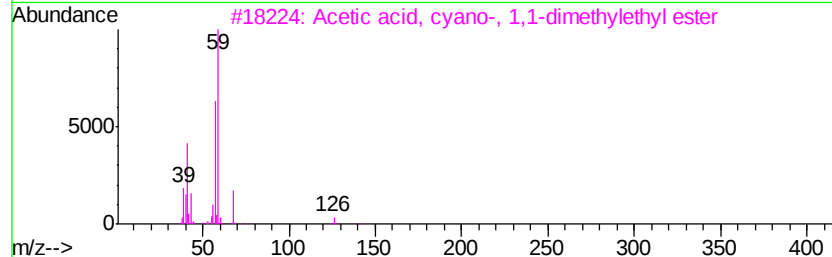
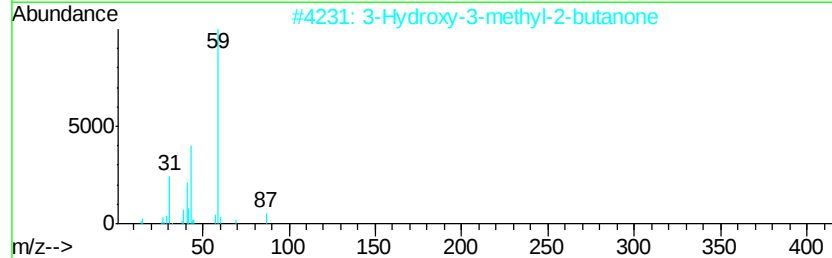
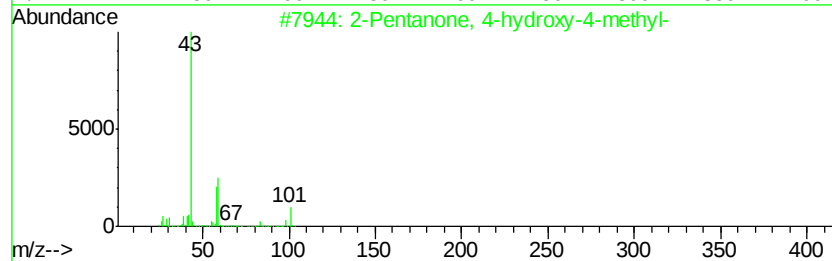
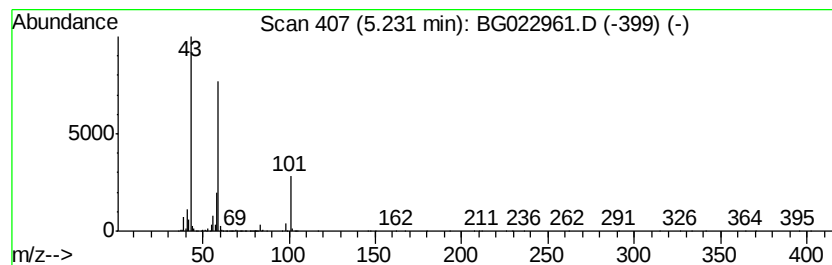
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	168.72 ng	4904600	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Acetone	58	C3H6O	000067-64-1	10
5		Guanidine	59	CH5N3	000113-00-8	9



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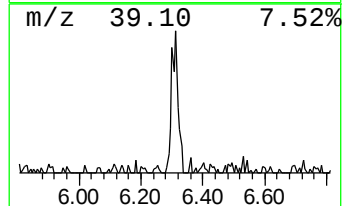
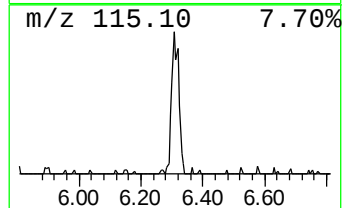
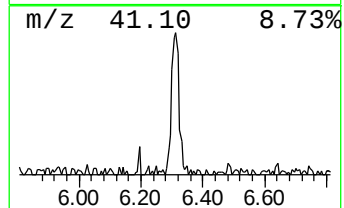
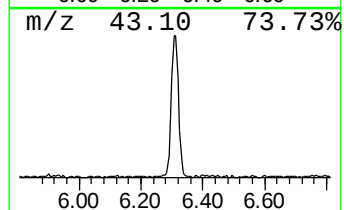
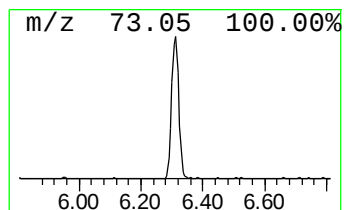
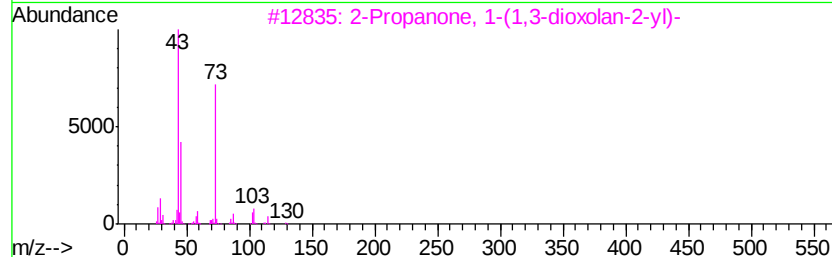
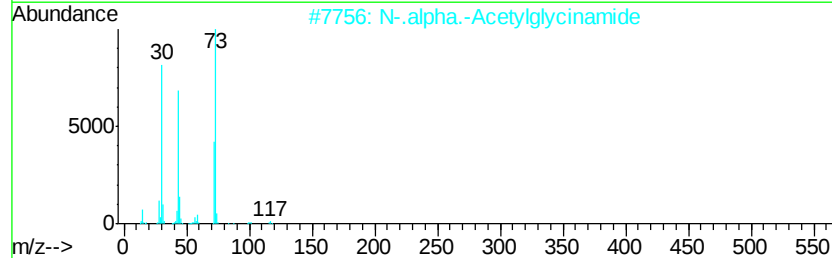
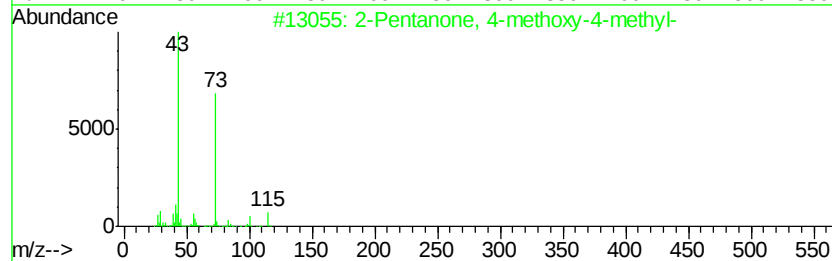
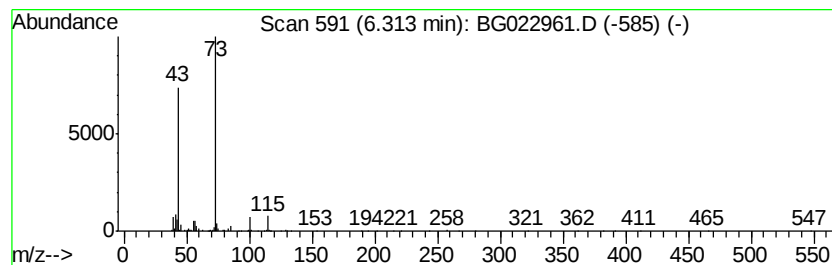
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.31	12.51 ng	363744	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	59
2		N-.alpha.-Acetylglucineamide	116	C4H8N2O2	002620-63-5	28
3		2-Propanone, 1-(1,3-dioxolan-2-yl)-	130	C6H10O3	000767-04-4	9
4		N-trimethylsilylaziridine	115	C5H13NSi	002116-90-7	9
5		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9



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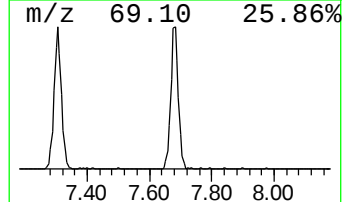
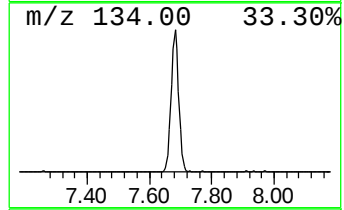
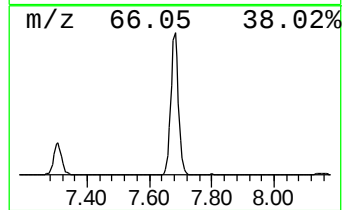
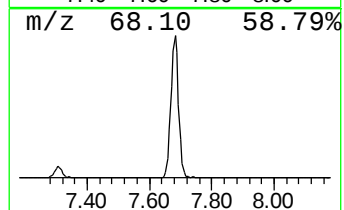
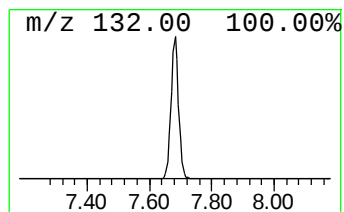
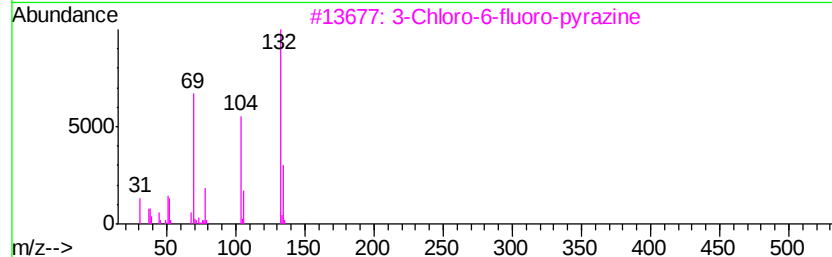
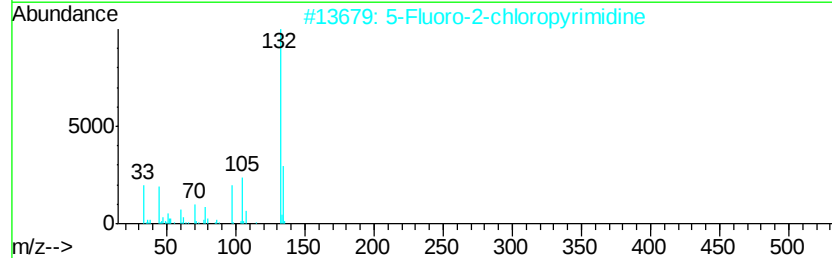
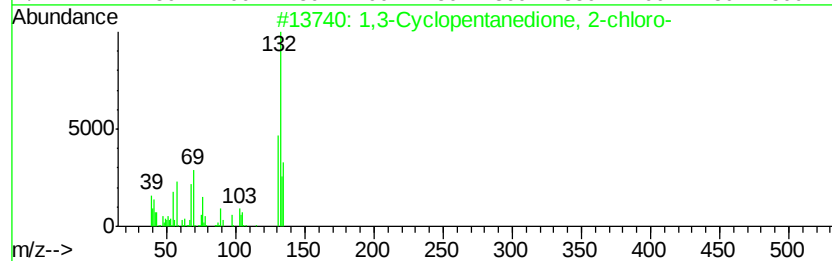
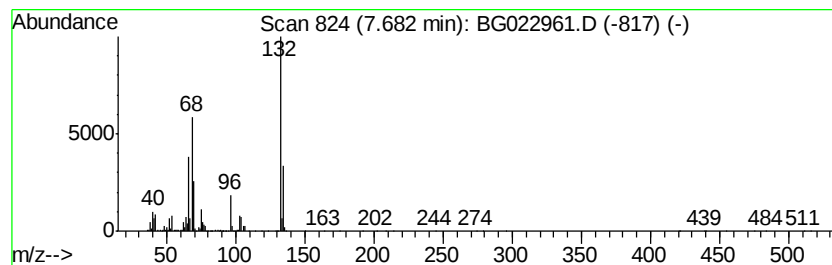
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Peak Number 5 unknown7.68 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	71.66 ng	2083110	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	32
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.04	3.04	10.7	ng	311336	1	8.15	581388	20.0
3-Penten-2-one, 4...	4.61	80.0	ng	2326510	1	8.15	581388	20.0
2-Pentanone, 4-hy...	5.23	168.7	ng	4904600	1	8.15	581388	20.0
2-Pentanone, 4-me...	6.31	12.5	ng	363744	1	8.15	581388	20.0
unknown7.68	7.68	71.7	ng	2083110	1	8.15	581388	20.0