

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011117\
 Data File : BG025475.D
 Acq On : 11 Jan 2017 16:00
 Operator : UM/SJ
 Sample : I1098-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP3-COMP13

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_G\METHODS\8270-BG122116.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	2.931	14	16	18	rVB	7746647	5421334	70.07%	13.904%
2	3.578	121	126	134	rBV	83023	119092	1.54%	0.305%
3	4.647	303	308	313	rBV	94543	149583	1.93%	0.384%
4	5.264	407	413	421	rVB2	552241	891817	11.53%	2.287%
5	5.740	487	494	512	rBV	1361752	2367494	30.60%	6.072%
6	7.361	758	770	780	rBV	1266714	2387998	30.86%	6.124%
7	7.731	824	833	844	rBV	1451584	2604008	33.66%	6.678%
8	8.202	903	913	921	rBV	253472	441812	5.71%	1.133%
9	8.525	959	968	977	rBV	1067162	1914525	24.74%	4.910%
10	9.383	1107	1114	1126	rBV	910800	1760082	22.75%	4.514%
11	11.028	1387	1394	1402	rBV	284208	580585	7.50%	1.489%
12	13.448	1798	1806	1816	rBV	2465652	3907396	50.50%	10.021%
13	14.829	2032	2041	2048	rBV	501817	846552	10.94%	2.171%
14	16.316	2286	2294	2307	rBV	2110085	3571193	46.16%	9.159%
15	17.573	2501	2508	2520	rBV	662866	1134829	14.67%	2.910%
16	20.152	2940	2947	2958	rBV	5646922	7737055	100.00%	19.843%
17	21.862	3231	3238	3248	rBV	919370	1602545	20.71%	4.110%
18	25.264	3807	3817	3833	rVB2	480486	1554067	20.09%	3.986%

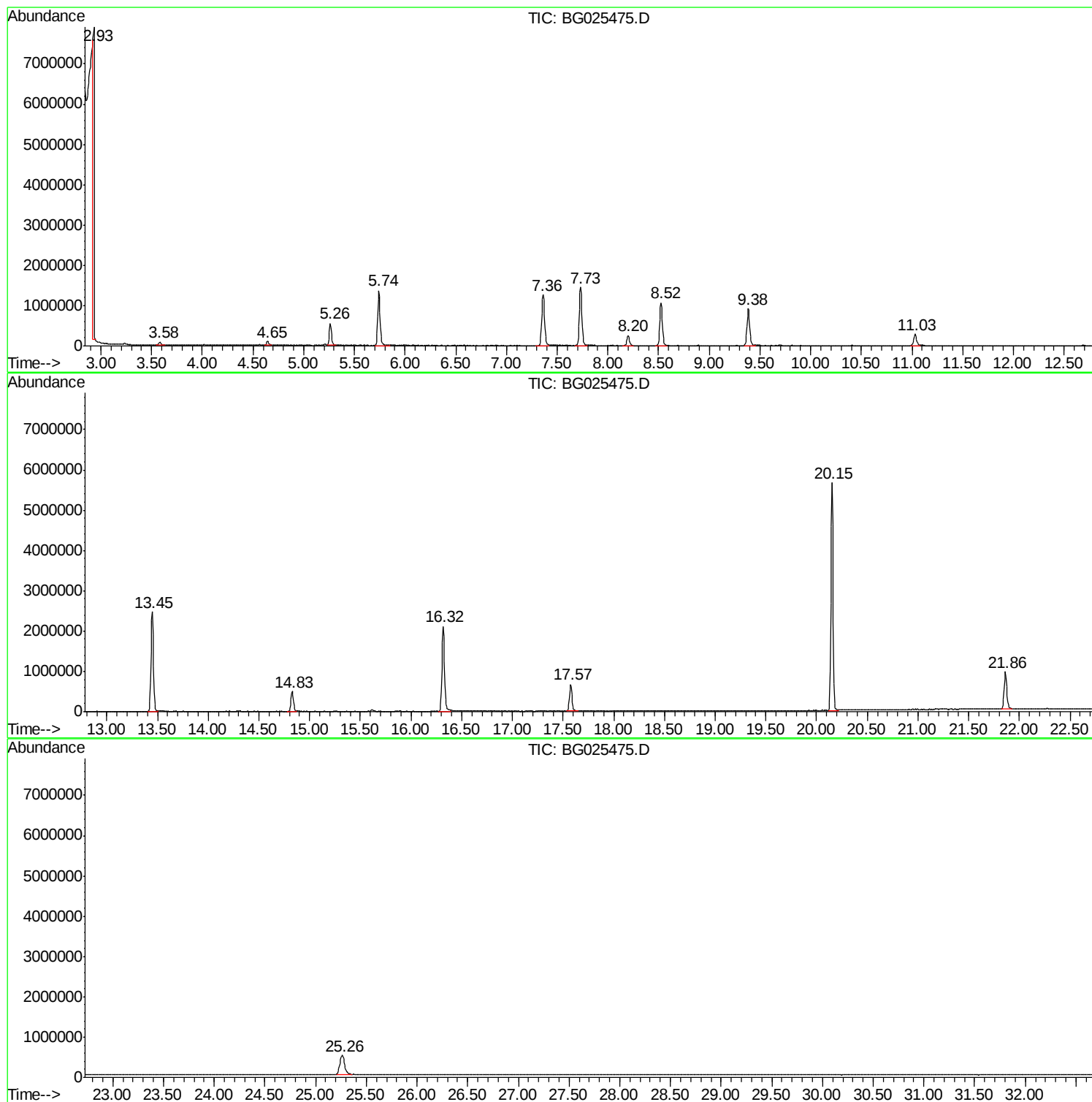
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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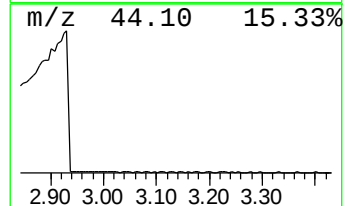
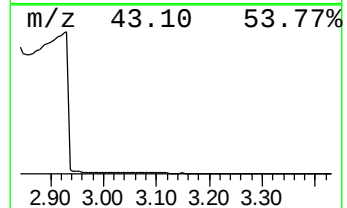
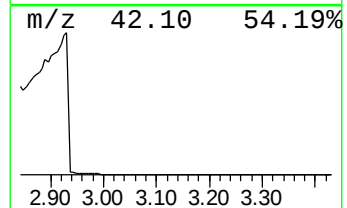
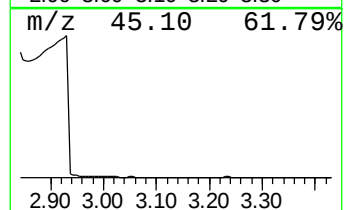
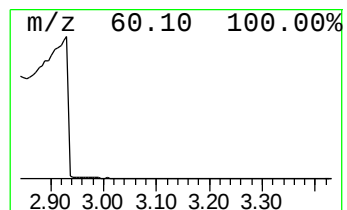
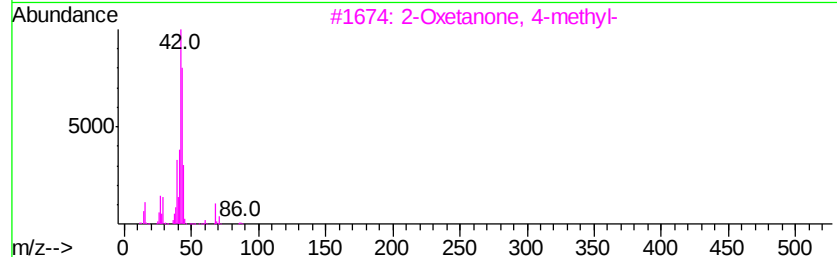
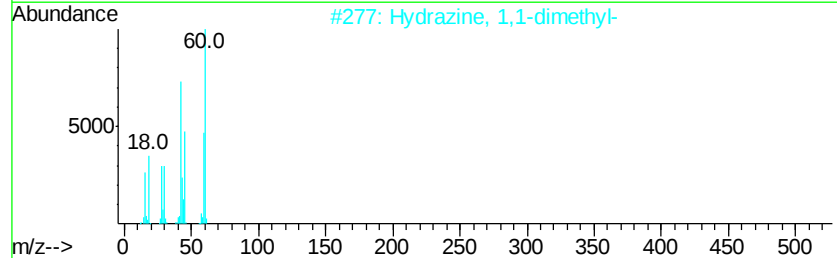
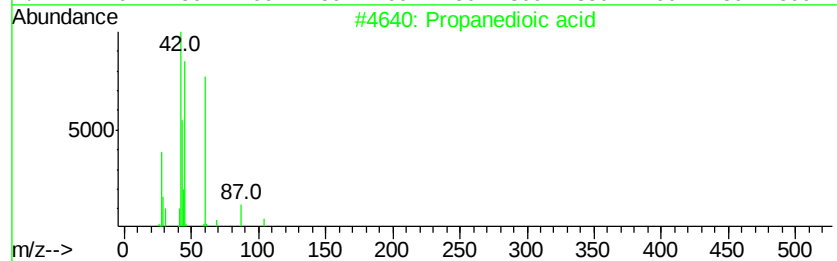
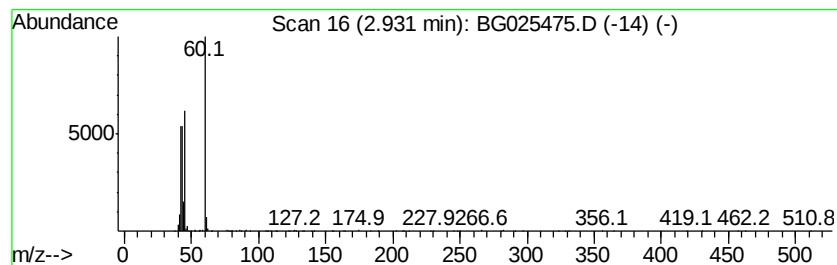
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanedioic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	245.41 ng	5421330	1,4-Dichlorobenzene-d4	8.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanedioic acid	104	C3H4O4	000141-82-2	78
2		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	58
3		2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9
4		Propylene Glycol	76	C3H8O2	000057-55-6	9
5		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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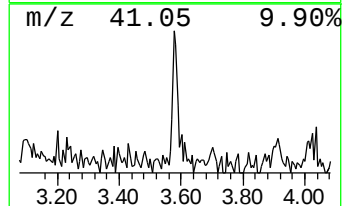
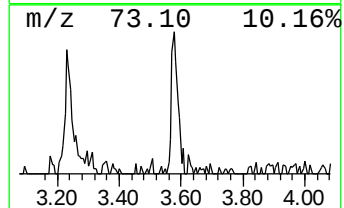
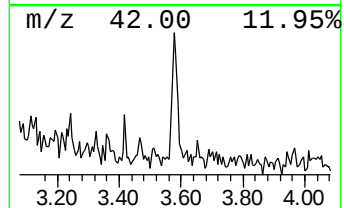
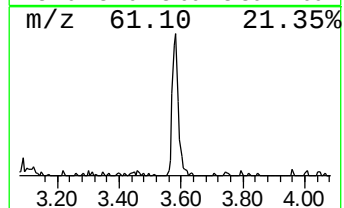
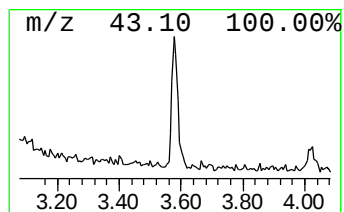
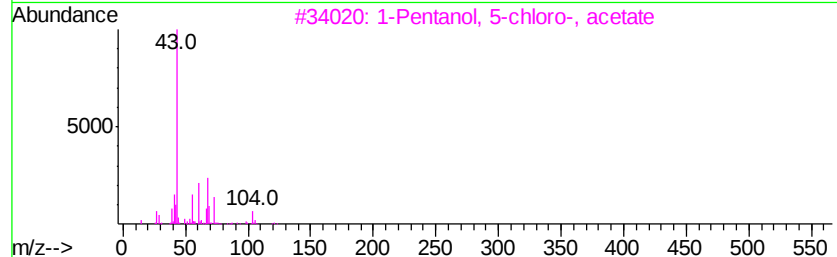
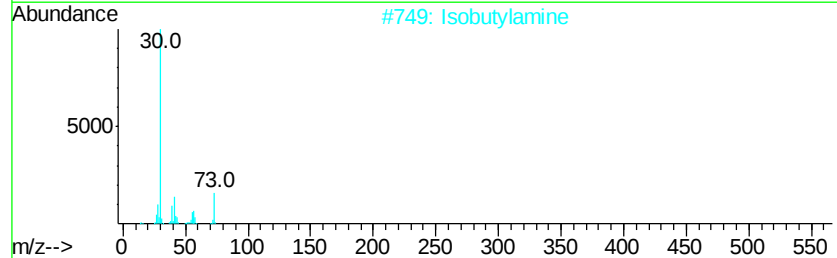
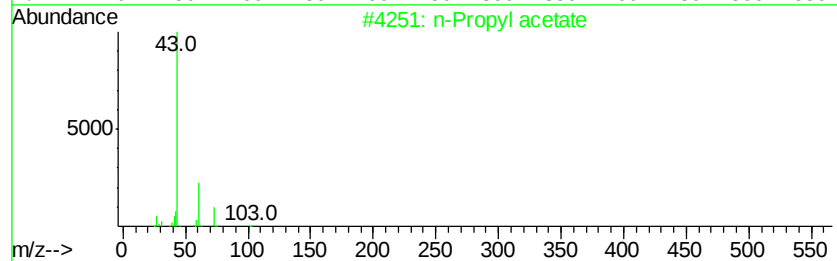
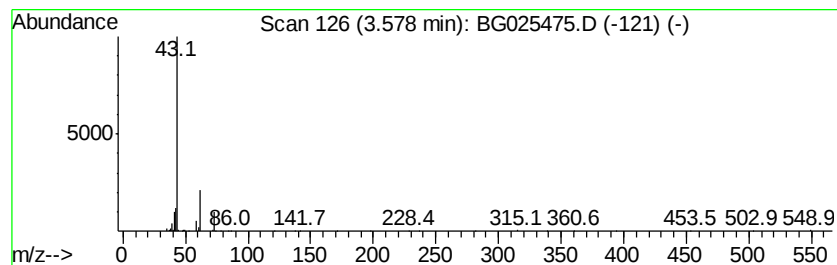
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.58	5.39 ng	119092	1,4-Dichlorobenzene-d4	8.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	64
2		Isobutylamine	73	C4H11N	000078-81-9	5
3		1-Pentanol, 5-chloro-, acetate	164	C7H13ClO2	020395-28-2	4
4		5-Bromo-n-amyl acetate	208	C7H13BrO2	015848-22-3	4
5		Acetic acid, 8-chlorooctyl ester	206	C10H19ClO2	021727-90-2	4



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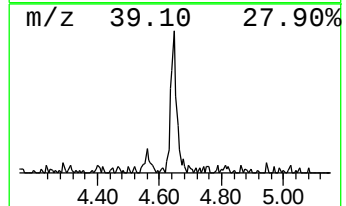
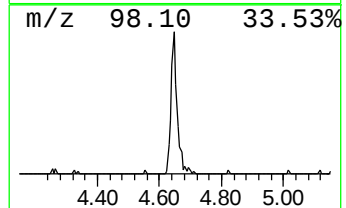
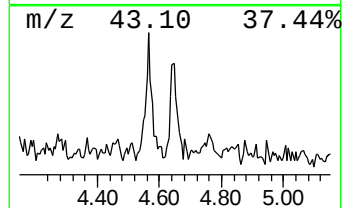
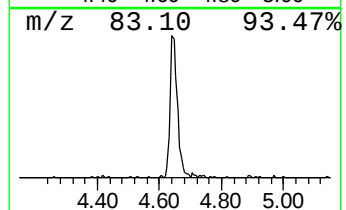
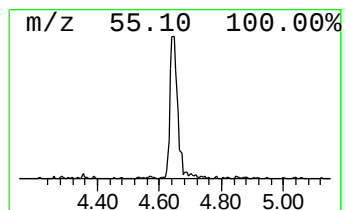
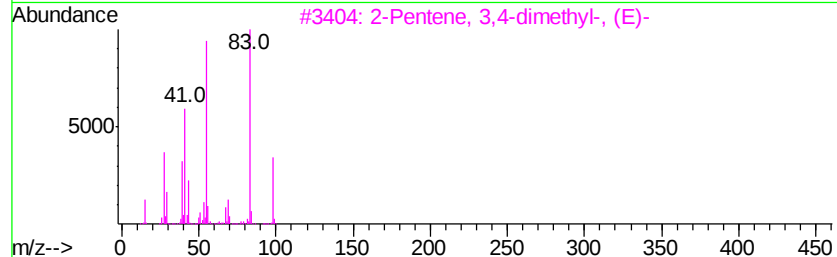
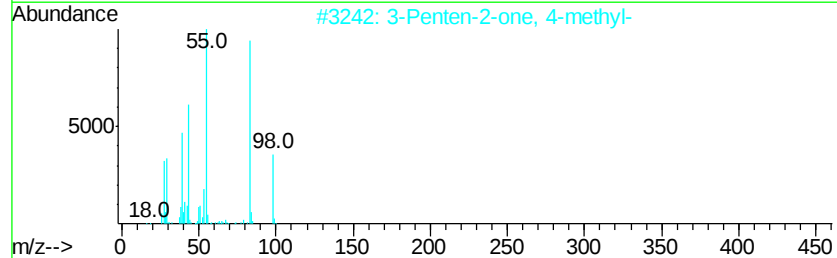
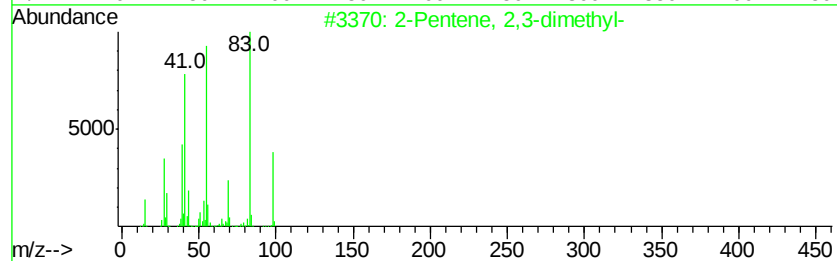
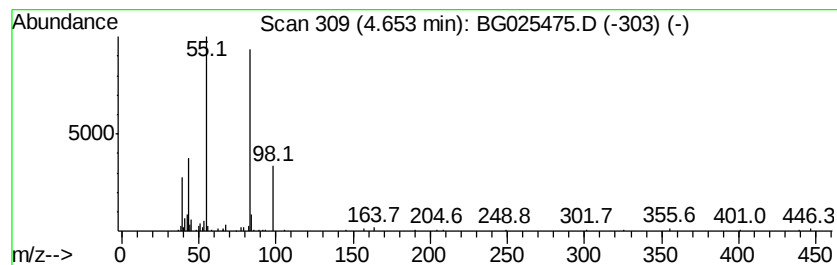
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Peak Number 3 2-Pentene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	6.77 ng	149583	1,4-Dichlorobenzene-d4	8.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	78
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	58
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	53
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	42



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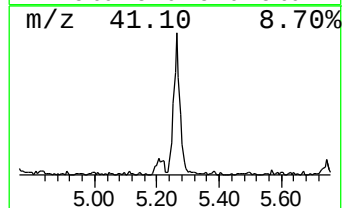
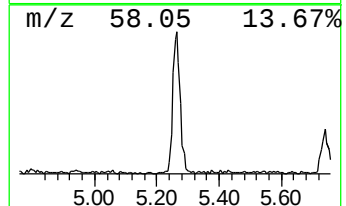
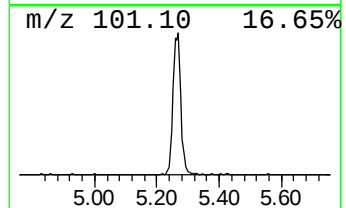
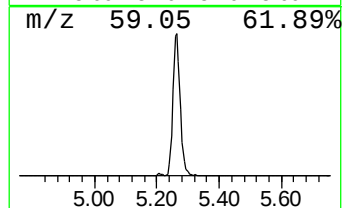
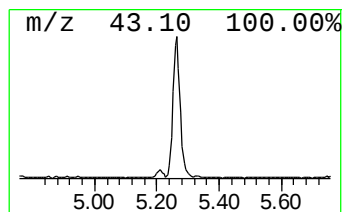
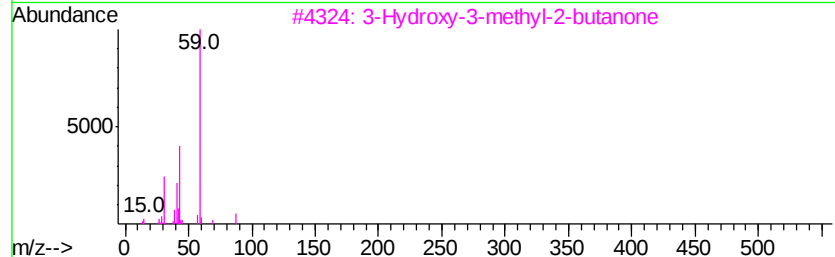
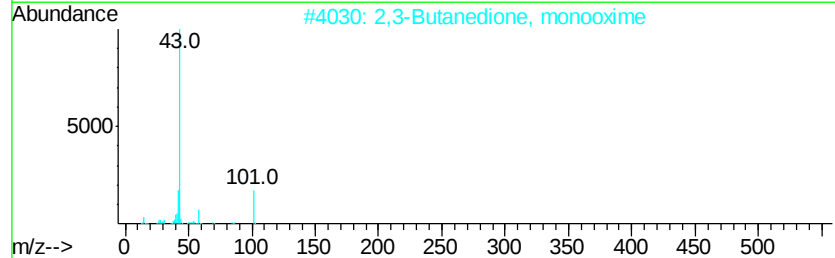
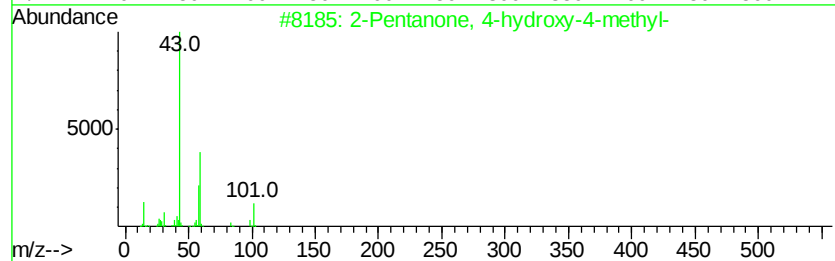
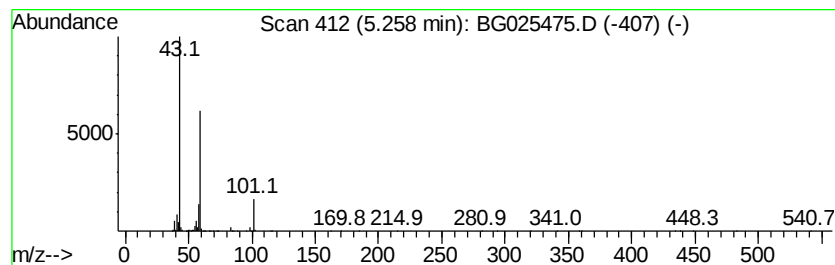
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	40.37 ng	891817	1,4-Dichlorobenzene-d4	8.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4		1,2-Butanediol	90	C4H10O2	000584-03-2	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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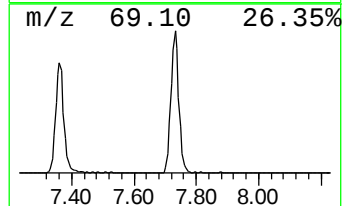
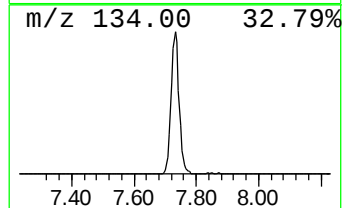
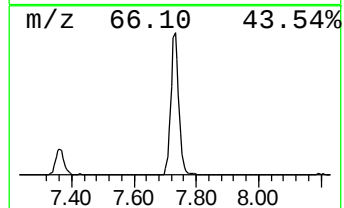
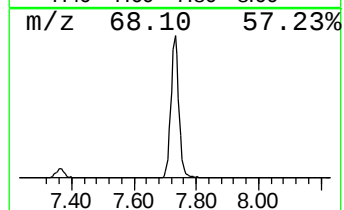
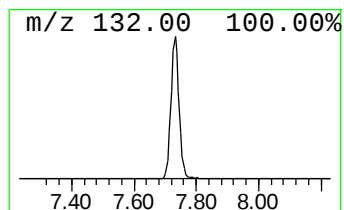
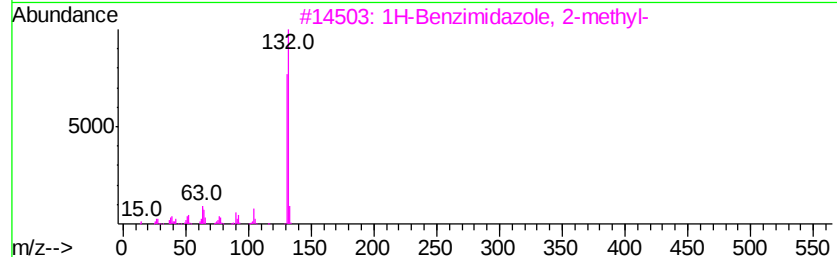
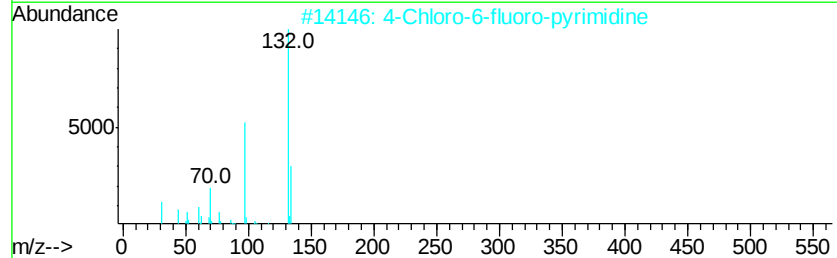
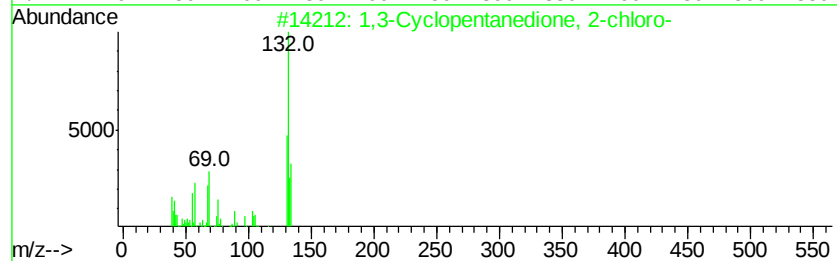
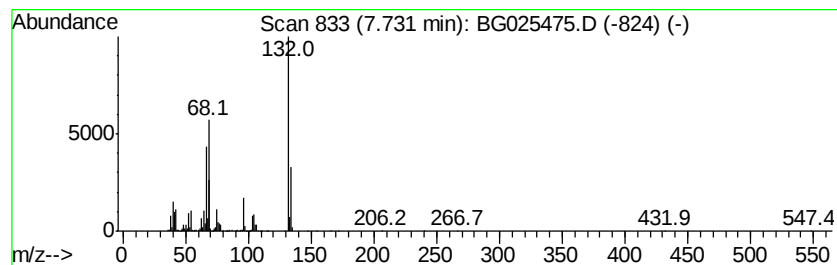
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Peak Number 5 unknown7.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	117.88 ng	2604010	1,4-Dichlorobenzene-d4	8.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	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
Propanedioic acid	2.93	245.4	ng	5421330	1	8.20	441812	20.0
n-Propyl acetate	3.58	5.4	ng	119092	1	8.20	441812	20.0
2-Pentene, 2,3-di...	4.65	6.8	ng	149583	1	8.20	441812	20.0
2-Pentanone, 4-hy...	5.26	40.4	ng	891817	1	8.20	441812	20.0
unknown7.73	7.73	117.9	ng	2604010	1	8.20	441812	20.0