

Data Path : Z:\HPCHEM1\BNA G\DATA\BG022716\
 Data File : BG021128.D
 Acq On : 27 Feb 2016 23:37
 Operator : UM/SJ
 Sample : PB88567BL
 Misc :
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB88567BL

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-BG022616.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	3.085	38	42	52	rVB	41559	53237	8.52%	2.089%
2	4.653	305	309	315	rVB	7062	10730	1.72%	0.421%
3	5.258	405	412	419	rBV	98688	147952	23.69%	5.805%
4	5.717	484	490	499	rVB	78524	123166	19.72%	4.832%
5	7.309	754	761	769	rBB	83946	139516	22.34%	5.474%
6	7.697	819	827	833	rBB	77221	131023	20.98%	5.141%
7	8.167	901	907	913	rBB	23142	36939	5.91%	1.449%
8	8.490	956	962	969	rBB	83695	138996	22.25%	5.453%
9	9.330	1097	1105	1112	rBB	70618	126042	20.18%	4.945%
10	10.975	1378	1385	1392	rBB	33202	56636	9.07%	2.222%
11	13.402	1791	1798	1804	rBB	191874	288173	46.14%	11.306%
12	14.771	2025	2031	2037	rBB2	52299	83364	13.35%	3.271%
13	16.246	2277	2282	2288	rBB	121399	172066	27.55%	6.751%
14	17.509	2491	2497	2503	rBB2	80905	124397	19.92%	4.881%
15	20.094	2932	2937	2946	rVB	497097	624571	100.00%	24.504%
16	20.823	3056	3061	3065	rBV3	4375	6408	1.03%	0.251%
17	21.769	3215	3222	3229	rVB	97201	152745	24.46%	5.993%
18	25.047	3770	3780	3792	rVB2	47479	132863	21.27%	5.213%

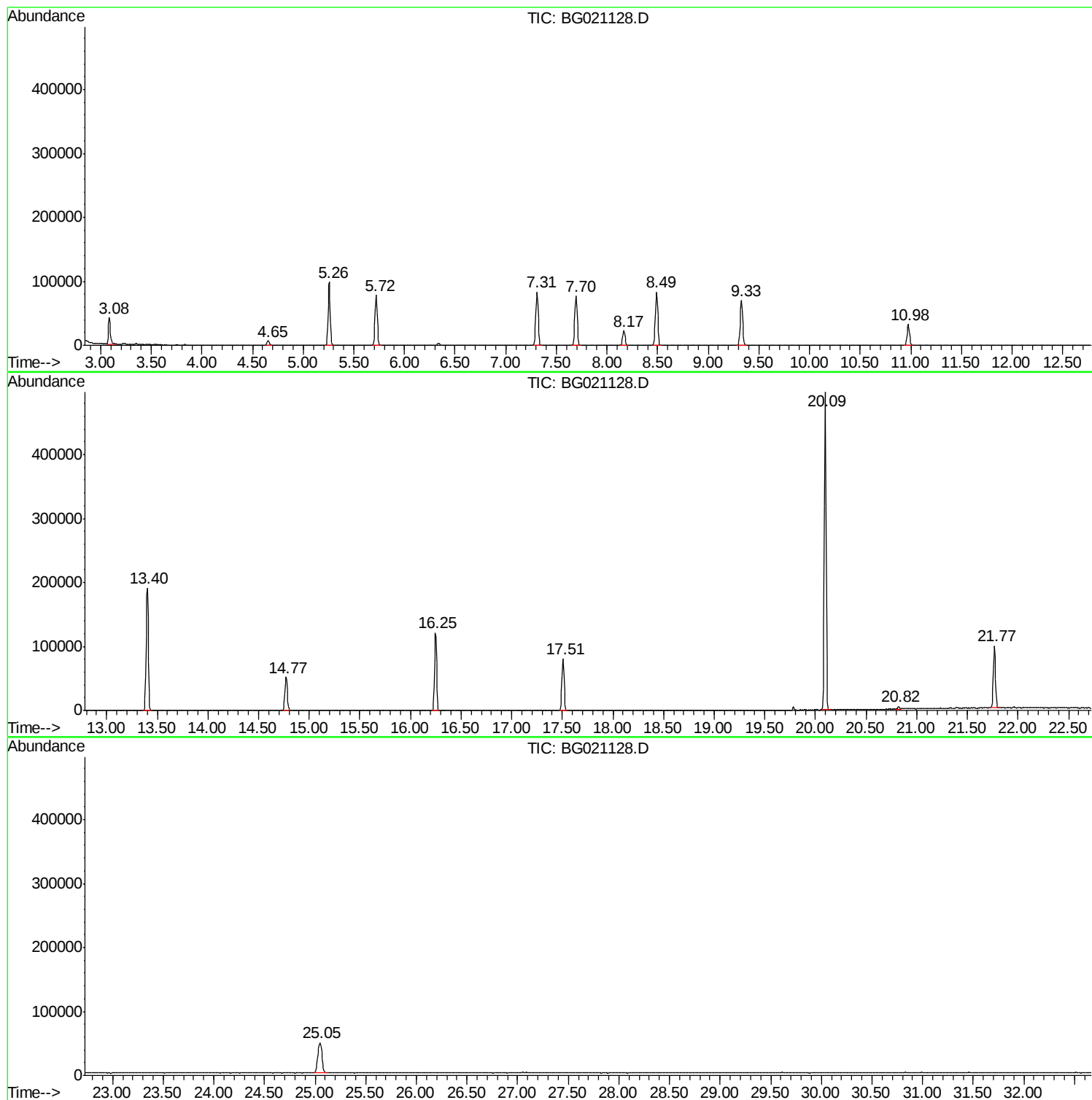
Sum of corrected areas: 2548824

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022616.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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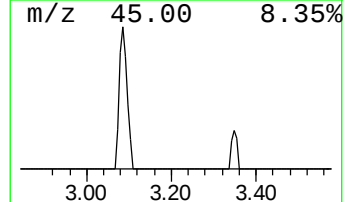
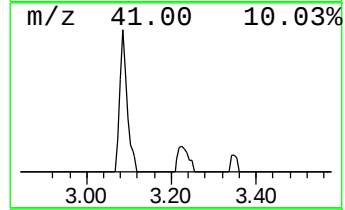
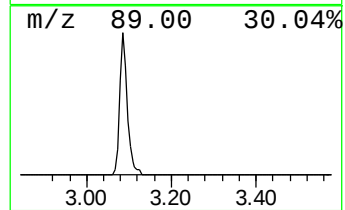
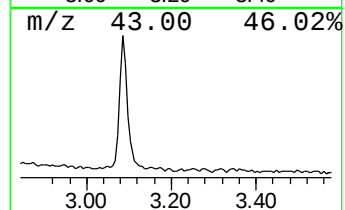
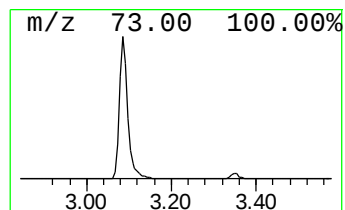
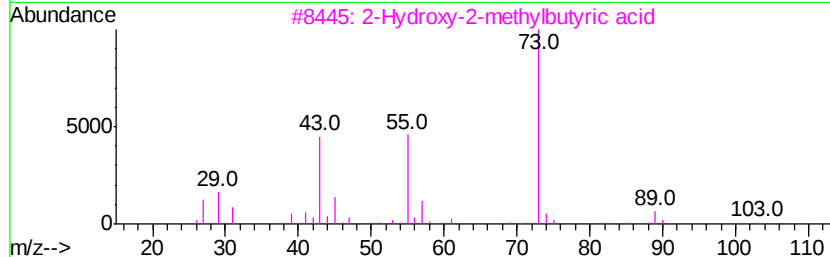
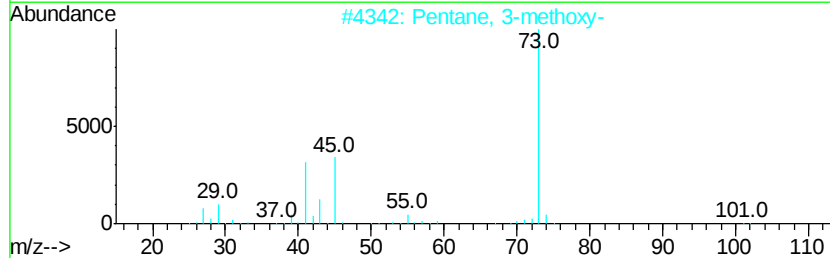
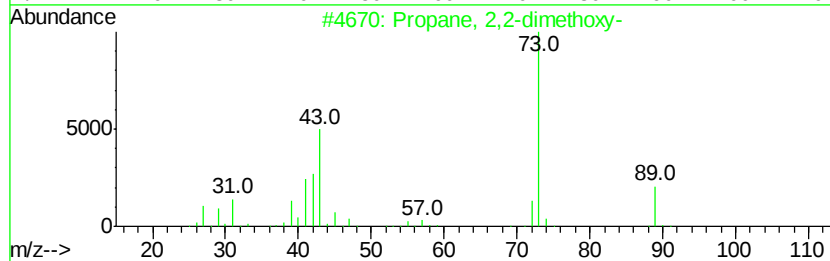
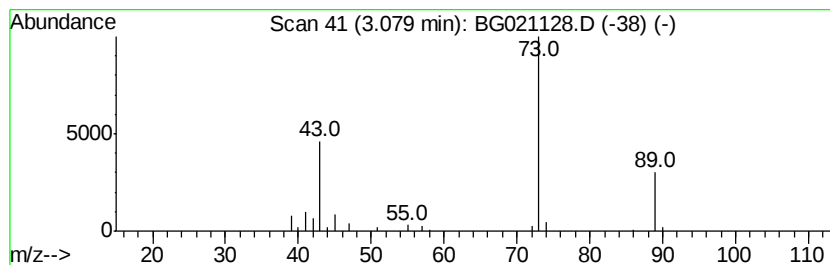
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.08	28.82 ng	53237	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9



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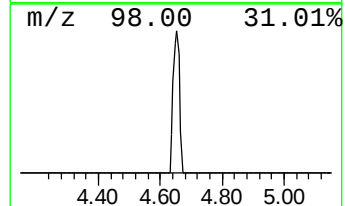
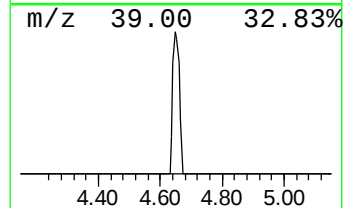
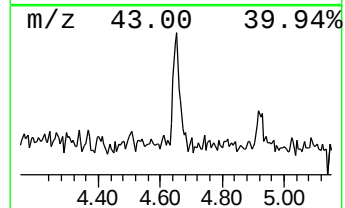
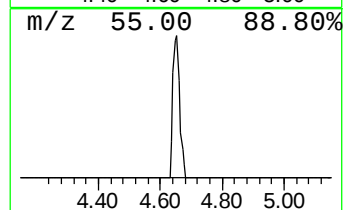
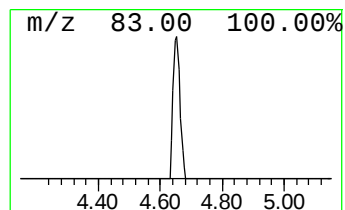
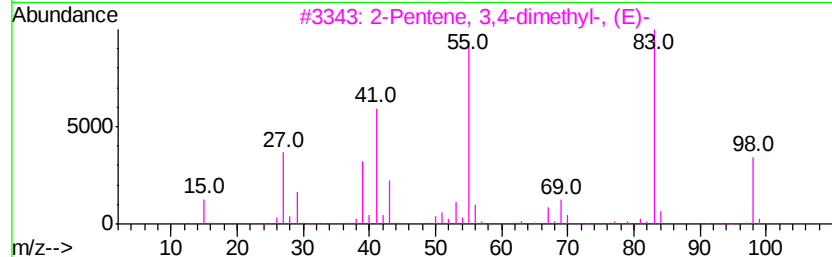
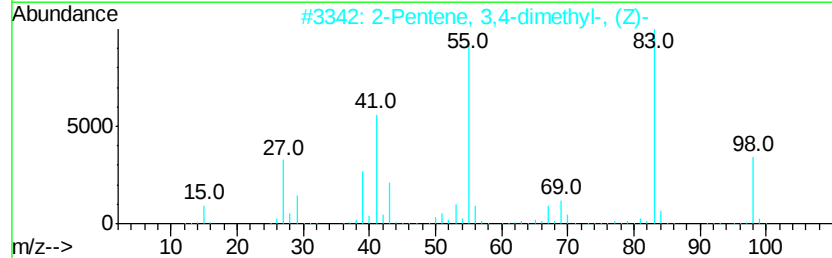
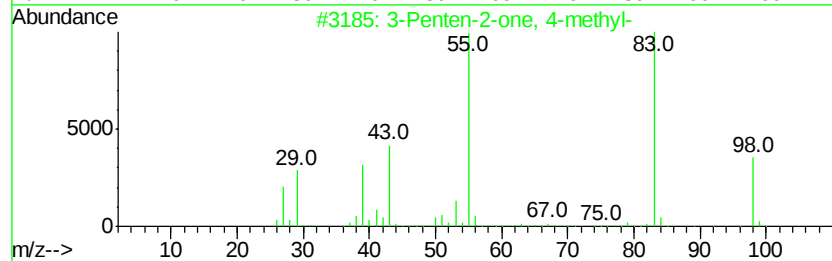
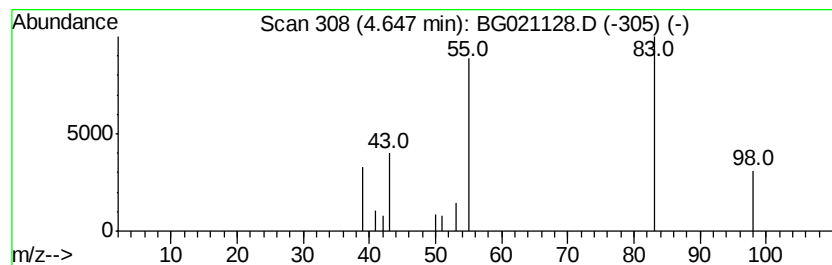
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TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	5.81 ng	10730	1,4-Dichlorobenzene-d4	8.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	83
4			3-Hexen-2-one	98	C6H10O	000763-93-9	83
5			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78



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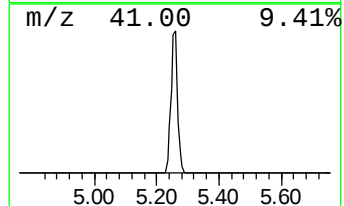
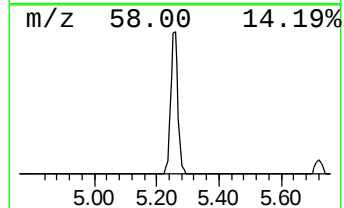
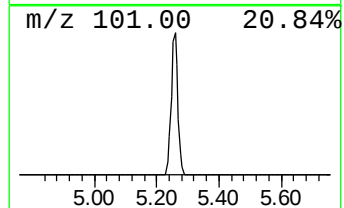
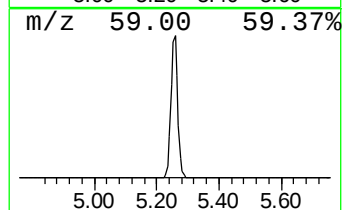
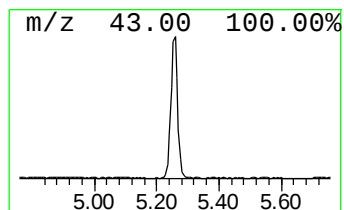
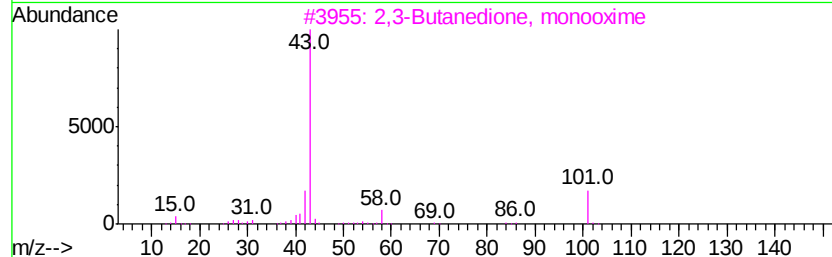
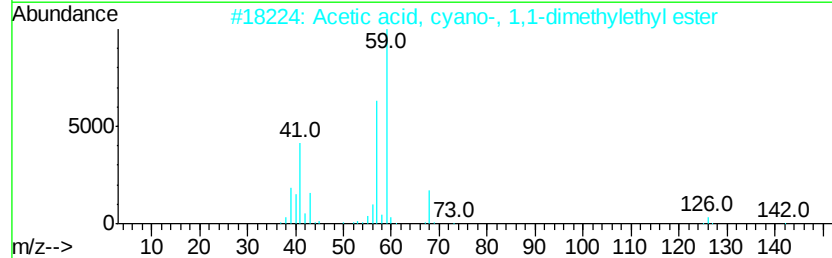
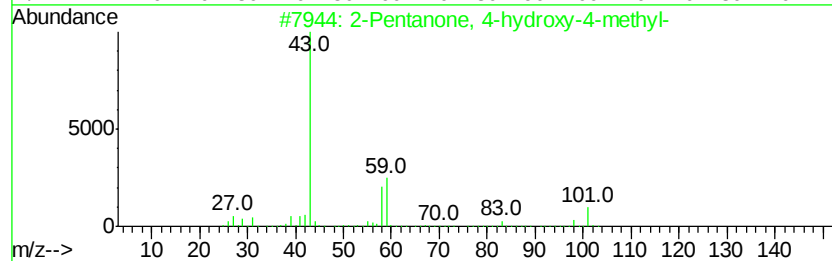
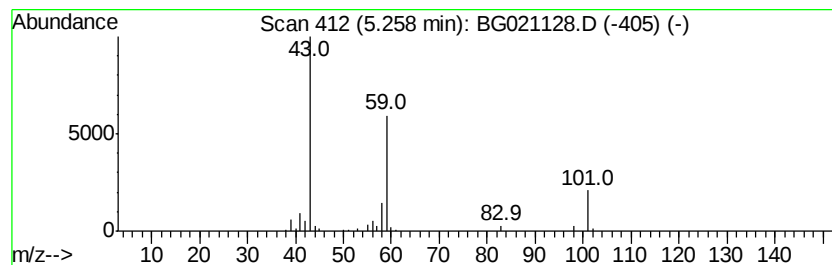
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	80.11 ng	147952	1,4-Dichlorobenzene-d4	8.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9



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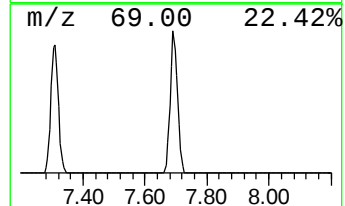
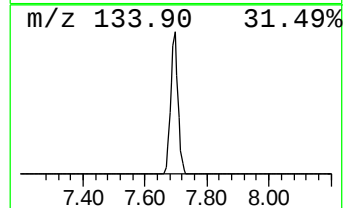
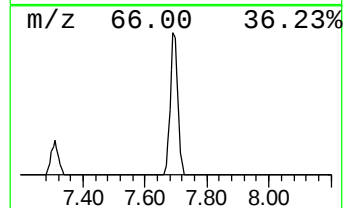
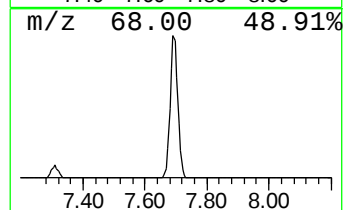
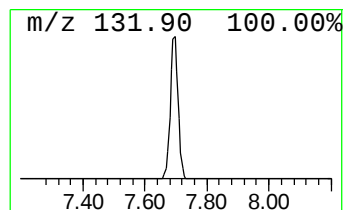
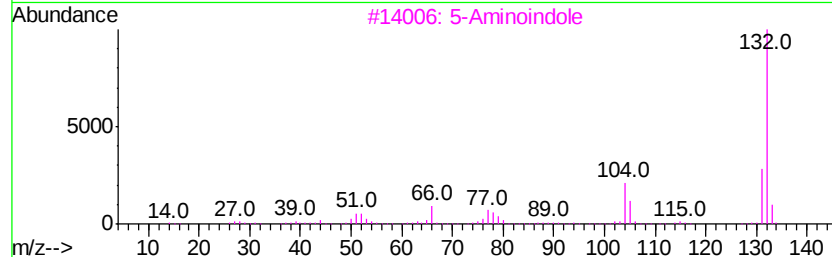
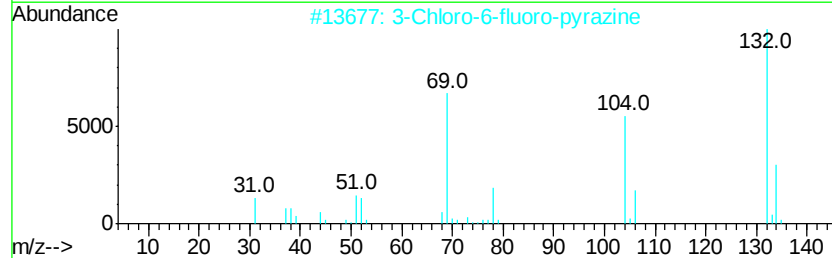
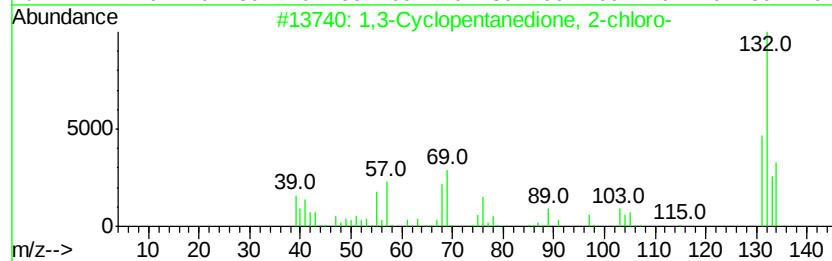
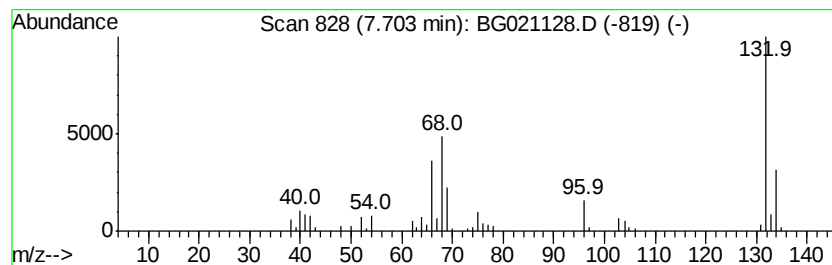
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Peak Number 4 unknown7.70 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	70.94 ng	131023	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	3.08	28.8	ng	53237	1	8.17	36939	20.0
3-Penten-2-one, 4...	4.65	5.8	ng	10730	1	8.17	36939	20.0
2-Pentanone, 4-hy...	5.26	80.1	ng	147952	1	8.17	36939	20.0
unknown7.70	7.70	70.9	ng	131023	1	8.17	36939	20.0