

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
 Data File : BG023116.D
 Acq On : 15 Jul 2016 16:47
 Operator : UM/SJ
 Sample : H4016-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 C5-18

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	2.899	6	10	29	rVB	380554	888418	11.12%	1.740%
2	3.040	29	34	46	rBV	2241263	3019451	37.78%	5.915%
3	3.187	54	59	72	rVV	274144	541205	6.77%	1.060%
4	5.220	400	405	414	rVB	239343	374882	4.69%	0.734%
5	5.695	479	486	496	rBV	1683999	2809635	35.15%	5.504%
6	7.305	753	760	771	rBV	2021091	3557375	44.51%	6.969%
7	7.681	813	824	836	rBV	1817380	3230433	40.42%	6.329%
8	8.151	896	904	911	rVB	373267	647481	8.10%	1.268%
9	8.480	952	960	968	rVB	1240060	2191068	27.42%	4.292%
10	9.326	1095	1104	1115	rBV	1274653	2296609	28.74%	4.499%
11	10.977	1378	1385	1392	rBV	576668	1059001	13.25%	2.075%
12	12.423	1624	1631	1639	rBV2	473444	771215	9.65%	1.511%
13	13.416	1791	1800	1807	rBV	3466446	5627899	70.42%	11.025%
14	14.238	1933	1940	1946	rBV	1003037	1469301	18.38%	2.878%
15	14.797	2028	2035	2044	rBV2	1061280	1816586	22.73%	3.559%
16	16.124	2255	2261	2266	rBV7	51172	81857	1.02%	0.160%
17	16.289	2282	2289	2302	rBV	3117284	4951490	61.95%	9.700%
18	16.483	2317	2322	2325	rBV	60735	82665	1.03%	0.162%
19	17.552	2497	2504	2513	rBV	1460164	2235251	27.97%	4.379%
20	18.416	2647	2651	2660	rBV3	143178	213703	2.67%	0.419%
21	20.155	2939	2947	2954	rBV	5812389	7992205	100.00%	15.657%
22	21.483	3166	3173	3179	rBV	64385	193517	2.42%	0.379%
23	21.853	3230	3236	3247	rBV2	1435362	2573507	32.20%	5.042%
24	25.231	3799	3811	3825	rBV2	726766	2419955	30.28%	4.741%

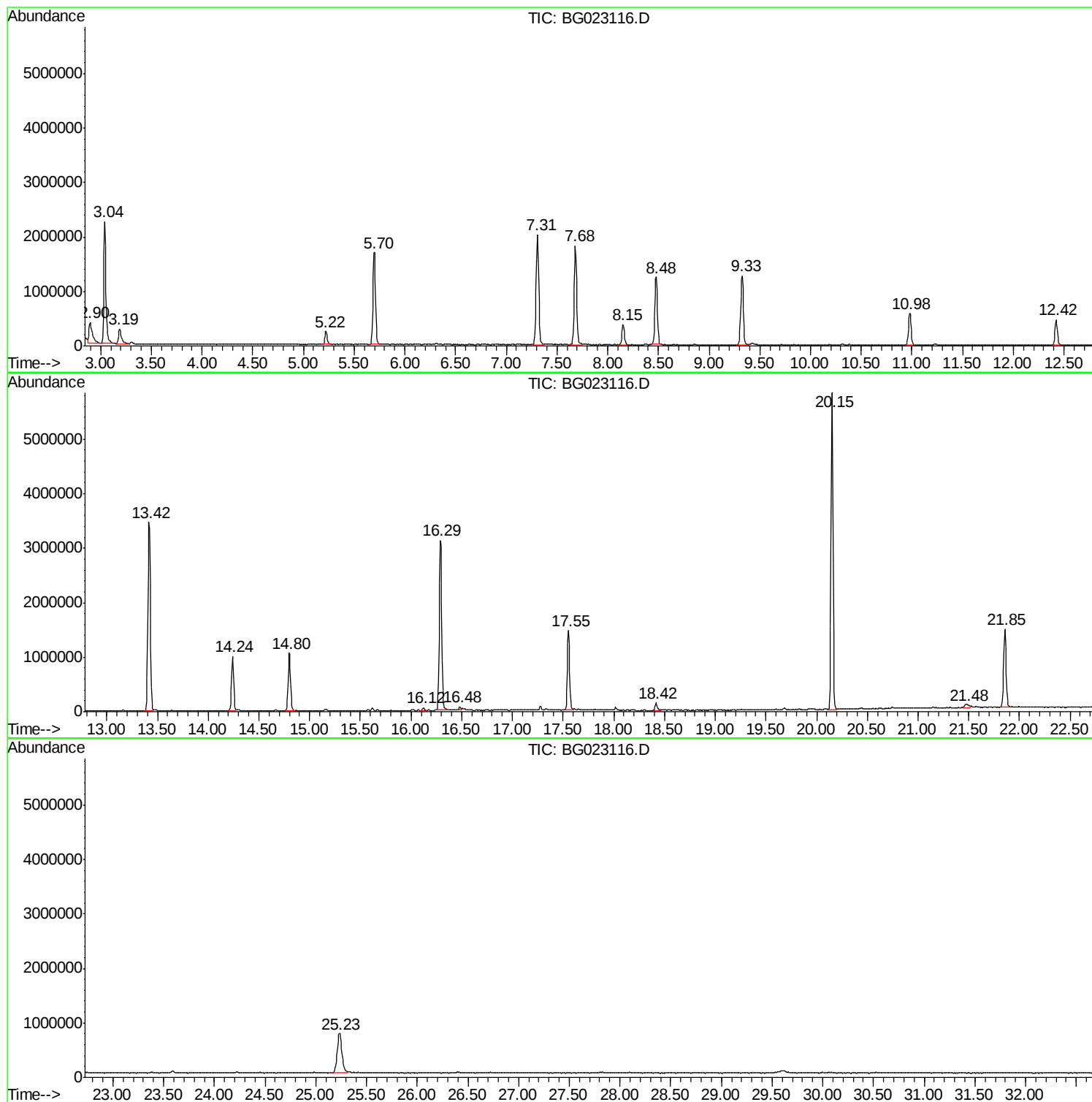
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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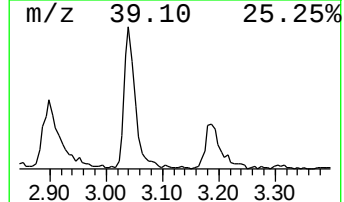
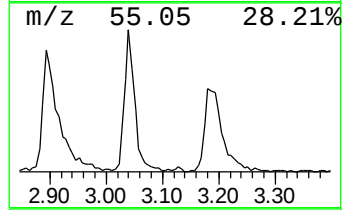
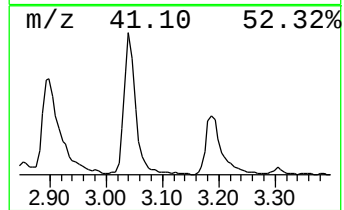
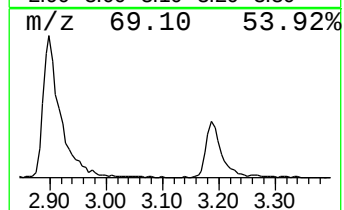
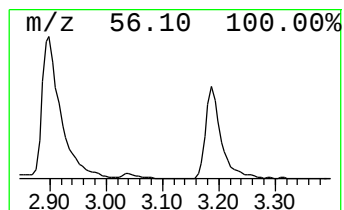
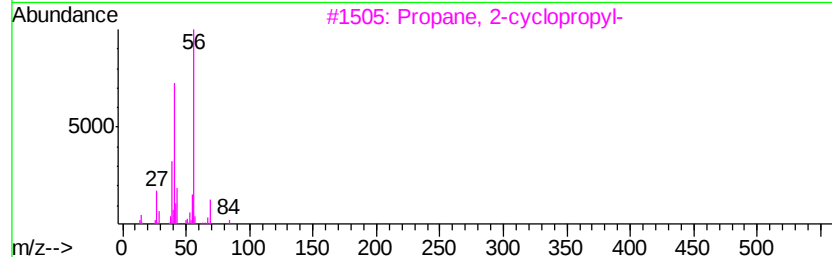
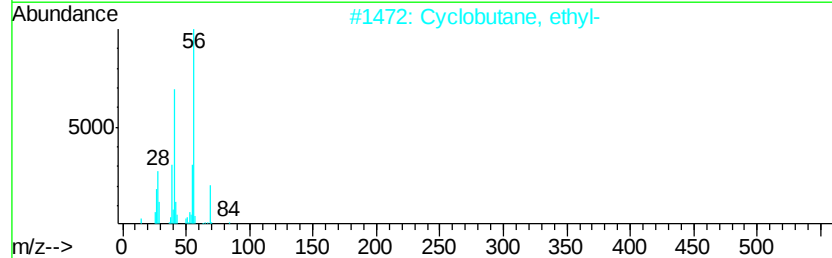
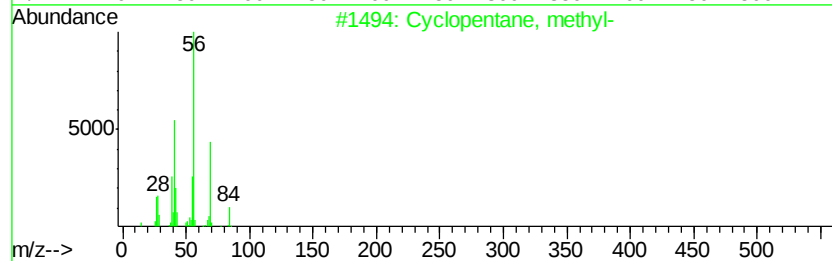
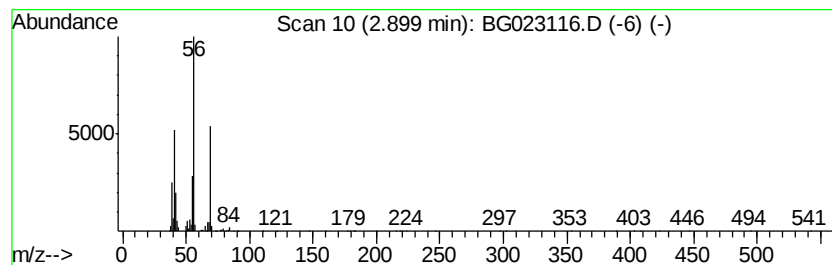
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	27.44 ng	888418	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	72
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	58
3		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	53
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
5		Cyclobutane	56	C4H8	000287-23-0	47



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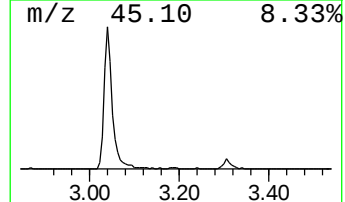
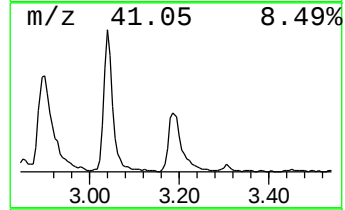
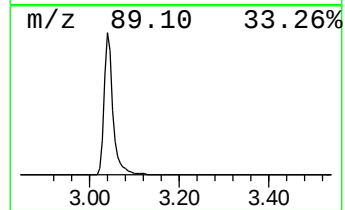
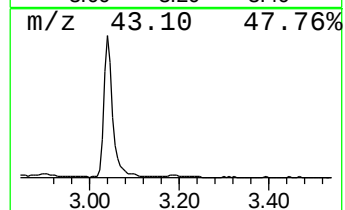
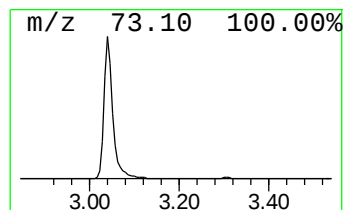
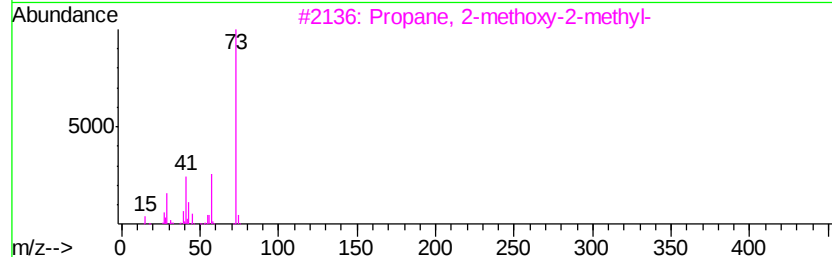
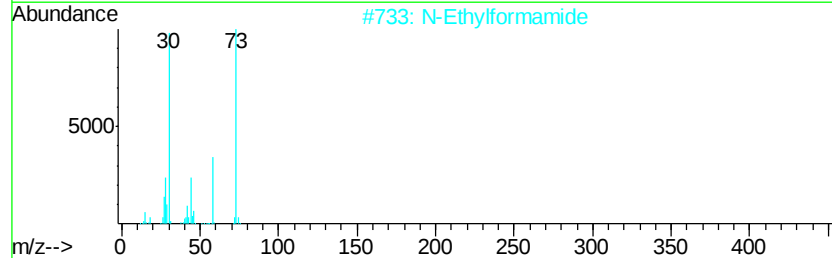
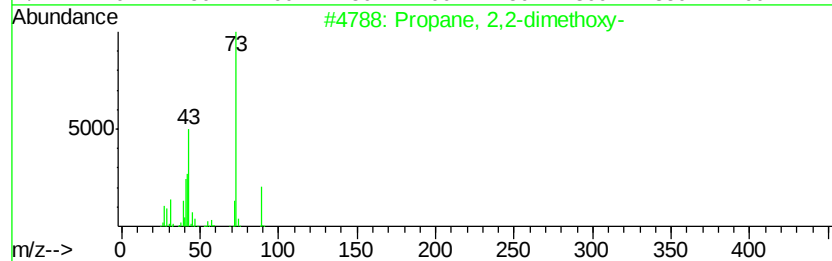
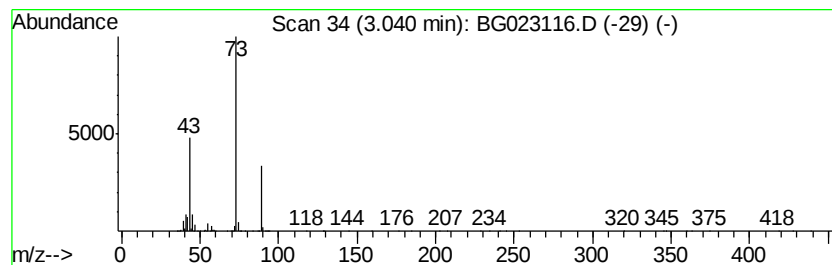
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	93.27 ng	3019450	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	56
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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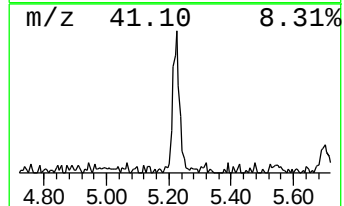
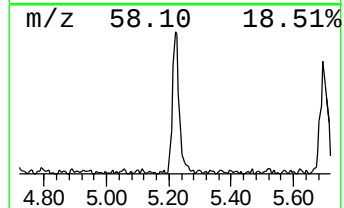
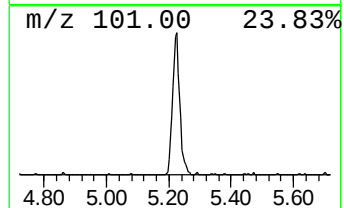
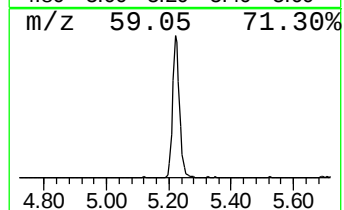
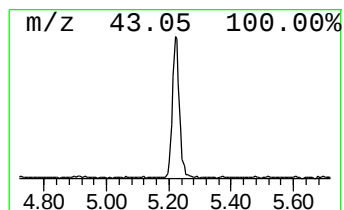
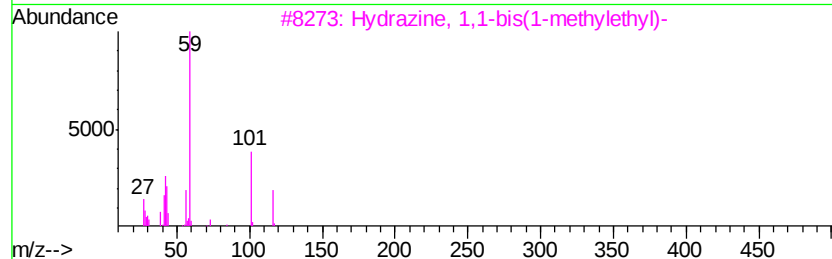
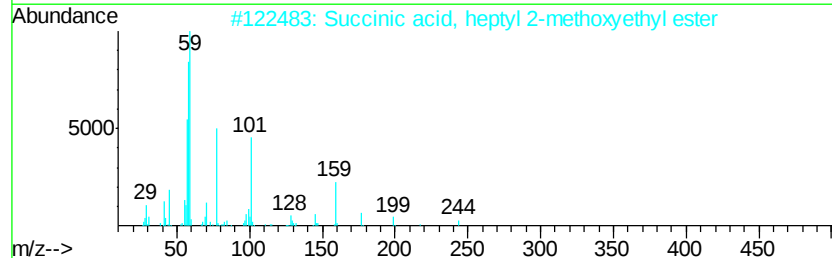
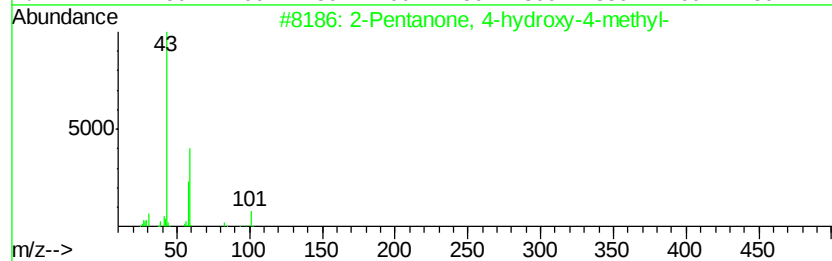
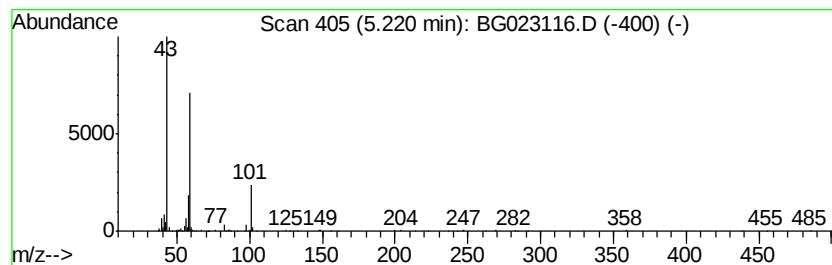
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Peak Number 4 unknown5.22 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	11.58 ng	374882	1,4-Dichlorobenzene-d4	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	38
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



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Instrument :
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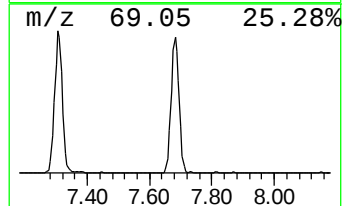
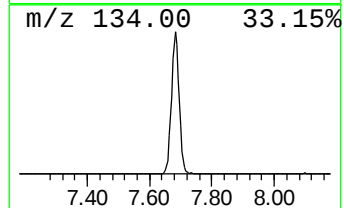
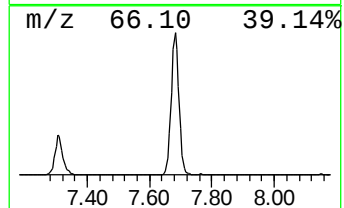
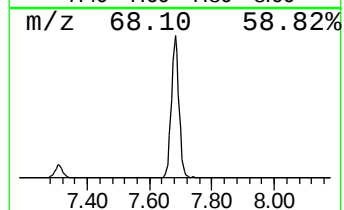
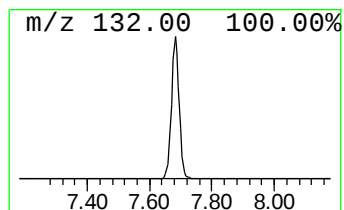
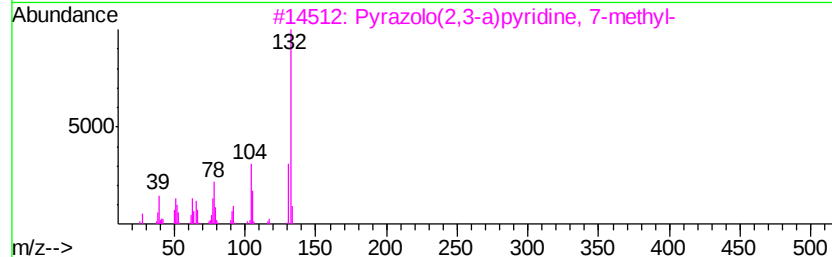
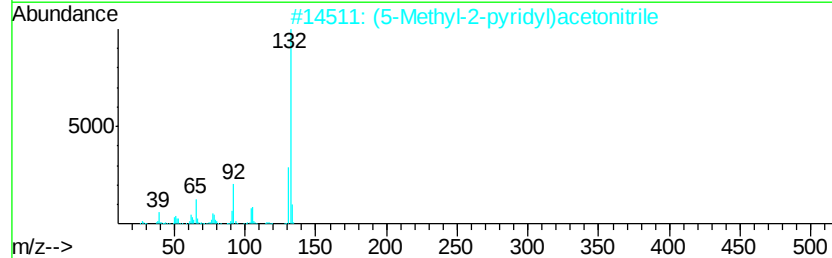
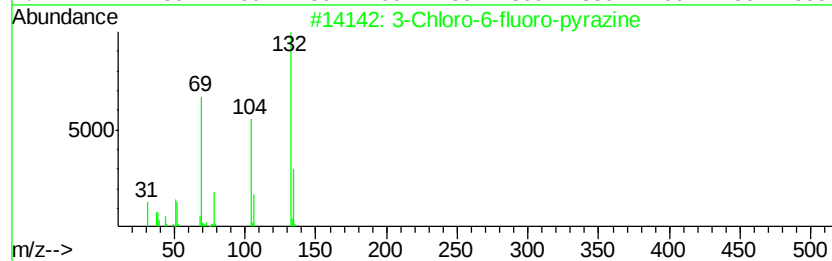
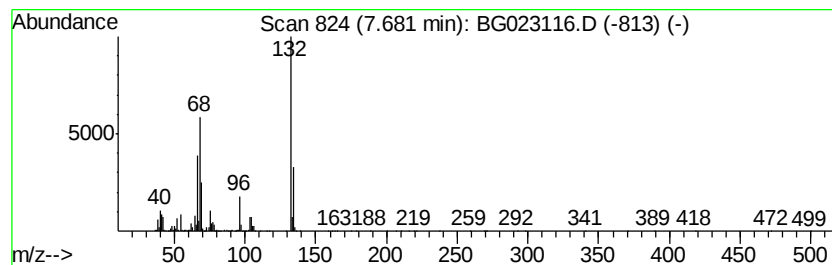
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Peak Number 5 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	99.78 ng	3230430	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
3		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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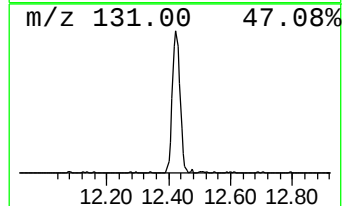
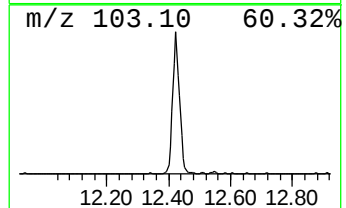
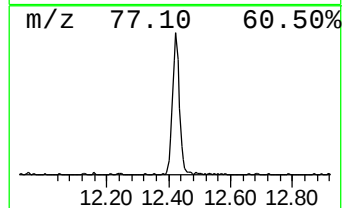
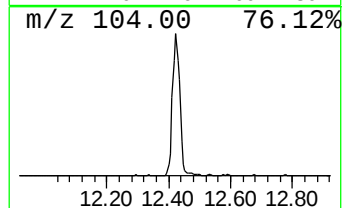
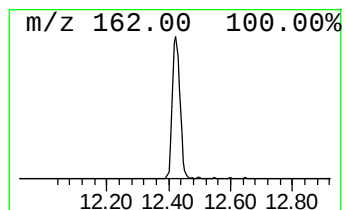
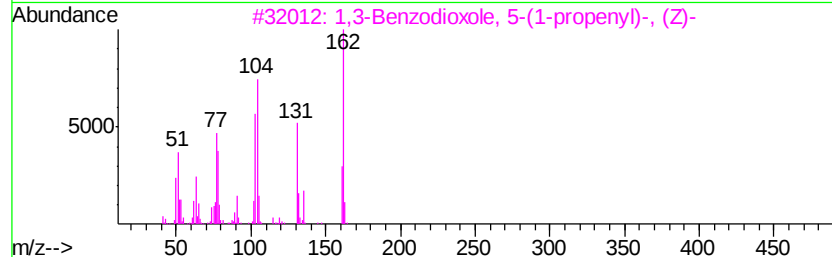
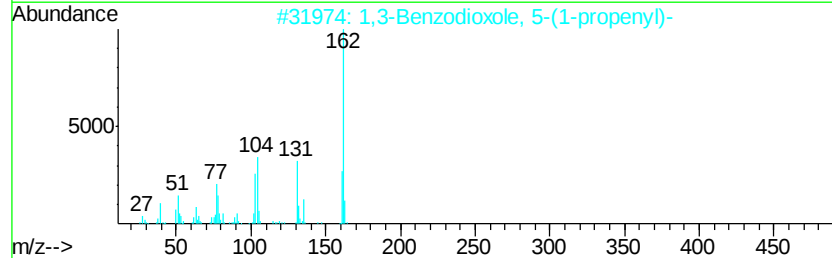
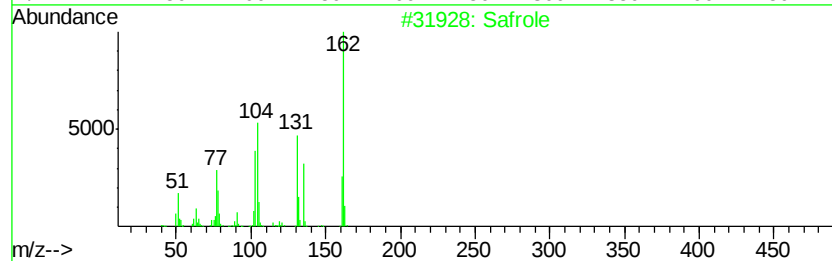
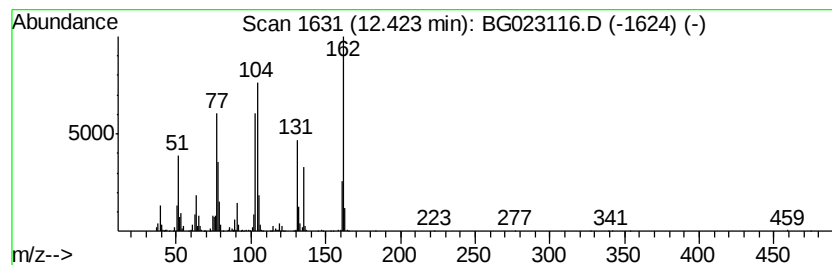
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Peak Number 7 Safrole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	14.57 ng	771215	Naphthalene-d8	10.98
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Safrole		162 C10H10O2	000094-59-7 97
2	1,3-Benzodioxole, 5-(1-propenyl)-		162 C10H10O2	000120-58-1 97
3	1,3-Benzodioxole, 5-(1-propenyl)...		162 C10H10O2	017627-76-8 96
4	Benzene, 1,2-(methylenedioxy)-4-...		162 C10H10O2	004043-71-4 95
5	Sydnone, 3-phenyl-		162 C8H6N2O2	000120-06-9 58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclopentane, met...	2.90	27.4	ng	888418	1	8.15	647481	20.0
Propane, 2,2-dime...	3.04	93.3	ng	3019450	1	8.15	647481	20.0
unknown5.22	5.22	11.6	ng	374882	1	8.15	647481	20.0
unknown7.68	7.68	99.8	ng	3230430	1	8.15	647481	20.0
Safrole	12.42	14.6	ng	771215	2	10.98	1059000	20.0