

Data Path : Z:\HPCHEM1\BNA G\DATA\BG051115\
 Data File : BG017059.D
 Acq On : 11 May 2015 18:36
 Operator : TP/IZ
 Sample : G2177-20
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PS-30A(20-25)

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-BG050515.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	2.717	3	5	24	rVB	3623811	4428909	100.00%	20.268%
2	2.858	24	29	38	rVB	100916	177912	4.02%	0.814%
3	2.935	38	42	47	rBV	126255	156138	3.53%	0.715%
4	4.862	365	370	377	rBV	55156	78537	1.77%	0.359%
5	5.344	445	452	463	rVB	840080	1204329	27.19%	5.511%
6	6.948	718	725	735	rVB	884504	1371554	30.97%	6.277%
7	7.294	777	784	791	rBV	853887	1319152	29.79%	6.037%
8	7.753	855	862	869	rBV	250809	389017	8.78%	1.780%
9	8.070	908	916	924	rBV	547933	890099	20.10%	4.073%
10	8.910	1052	1059	1066	rBV	505341	829050	18.72%	3.794%
11	10.549	1330	1338	1346	rVB	331460	545917	12.33%	2.498%
12	13.023	1752	1759	1768	rBV	1164790	1700819	38.40%	7.783%
13	13.863	1897	1902	1907	rBV	44387	67152	1.52%	0.307%
14	14.404	1988	1994	2004	rVB2	507813	747533	16.88%	3.421%
15	15.896	2241	2248	2258	rBV	1160964	1622962	36.64%	7.427%
16	17.147	2455	2461	2469	rVB2	677382	977701	22.08%	4.474%
17	18.046	2609	2614	2618	rBV2	61611	81413	1.84%	0.373%
18	19.780	2903	2909	2914	rBV	2346332	2785758	62.90%	12.748%
19	21.043	3120	3124	3129	rBV3	52630	84347	1.90%	0.386%
20	21.331	3168	3173	3178	rBV	954800	1153467	26.04%	5.279%
21	22.523	3372	3376	3381	rBV	99638	135007	3.05%	0.618%
22	23.616	3555	3562	3573	rVB2	563597	1104943	24.95%	5.057%

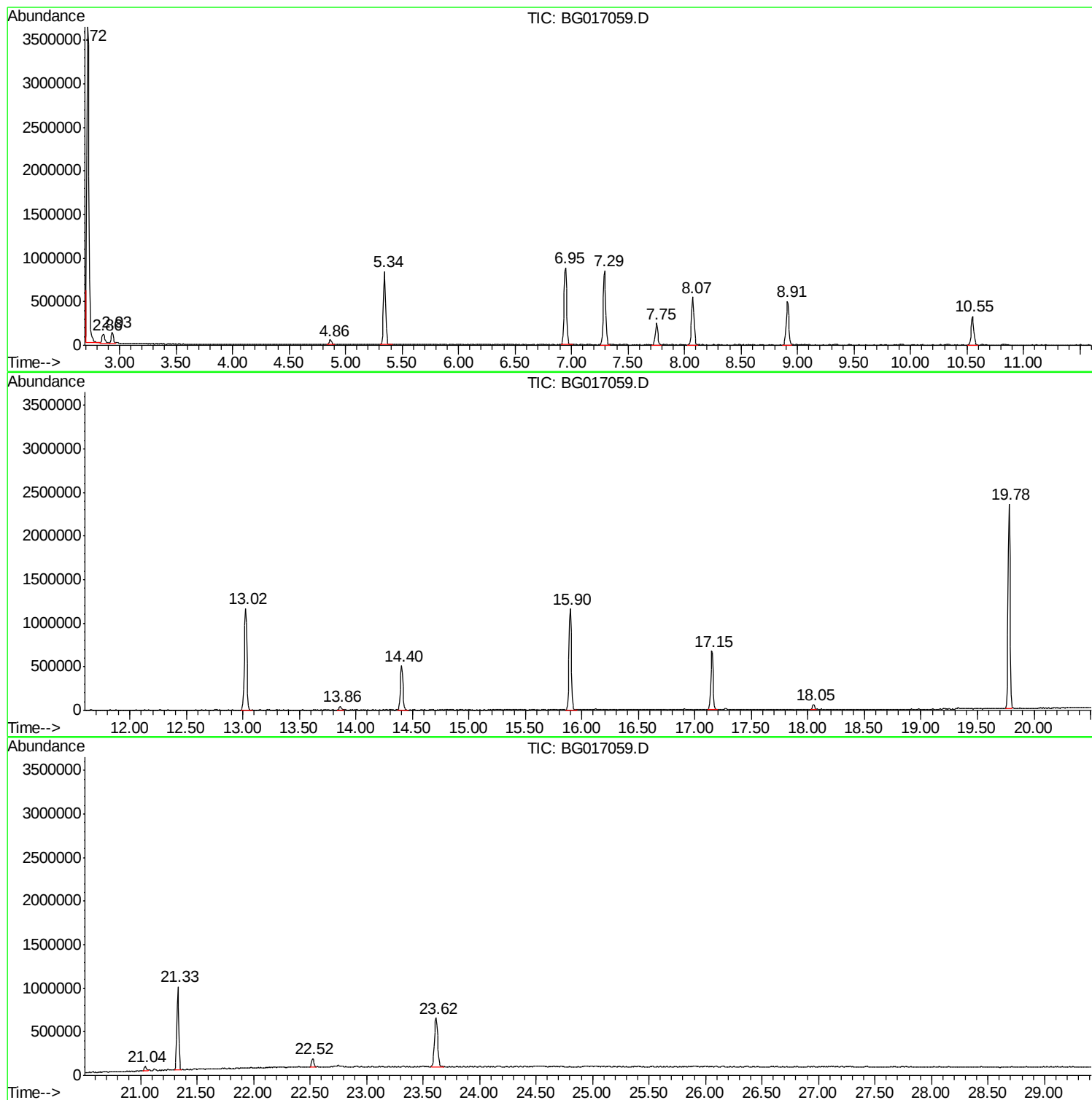
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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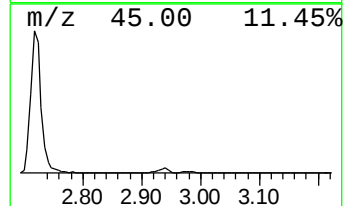
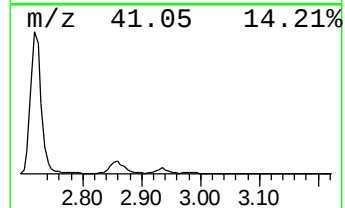
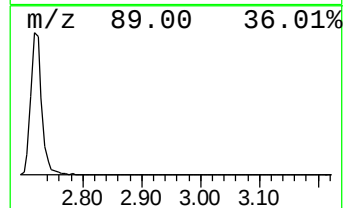
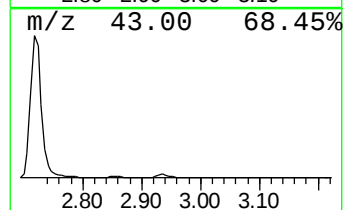
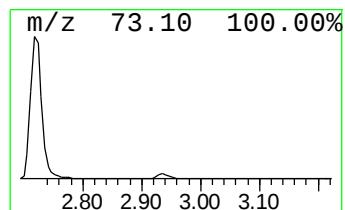
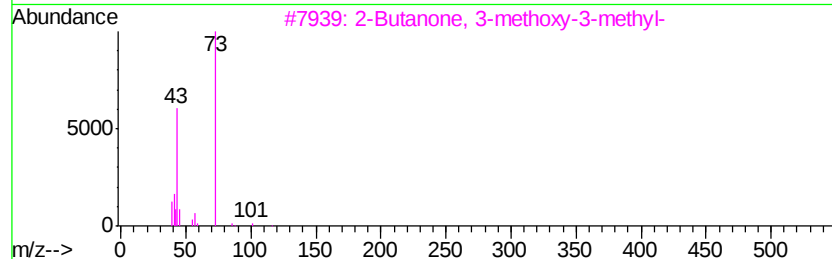
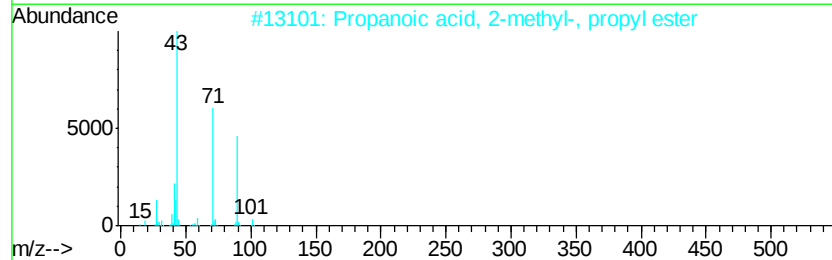
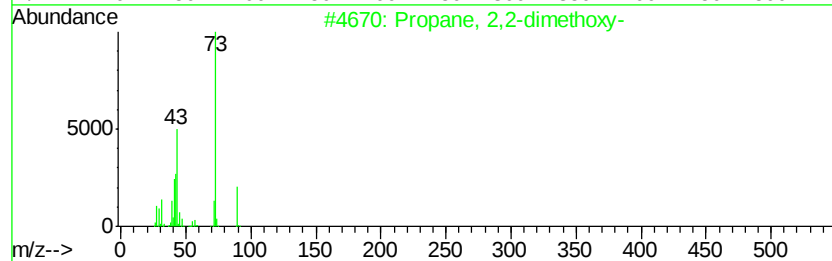
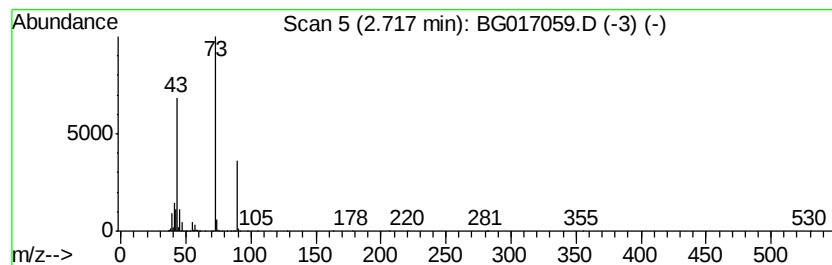
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.72	227.70 ng	4428910	1,4-Dichlorobenzene-d4	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	39
2		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	38
3		2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	28
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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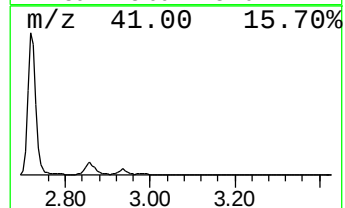
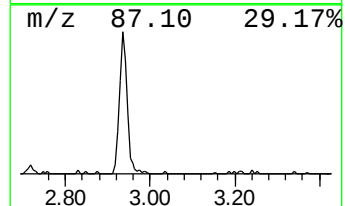
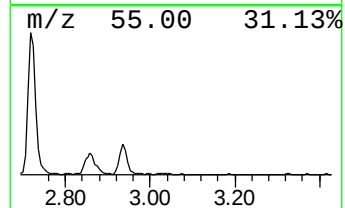
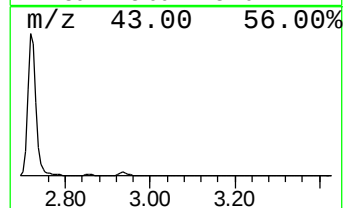
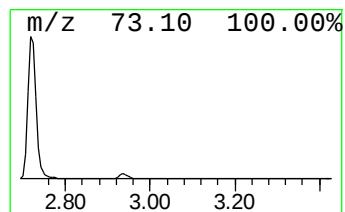
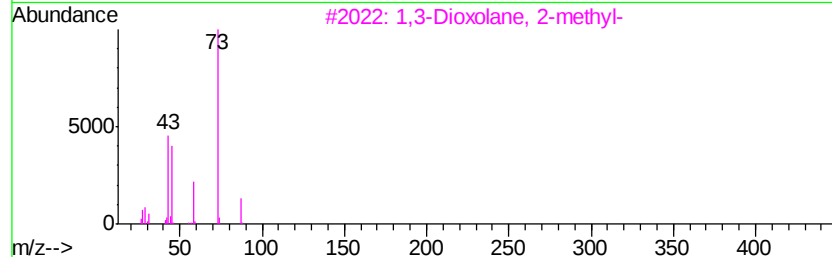
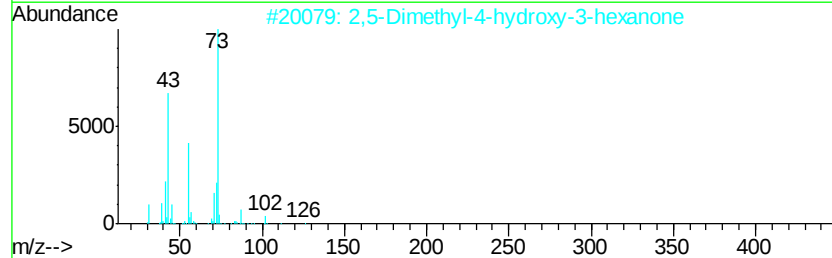
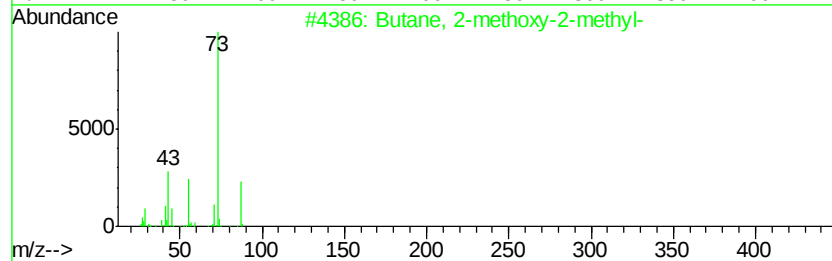
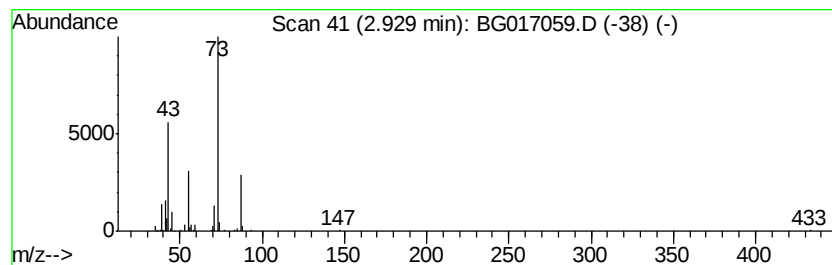
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	8.03 ng	156138	1,4-Dichlorobenzene-d4	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	43
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9



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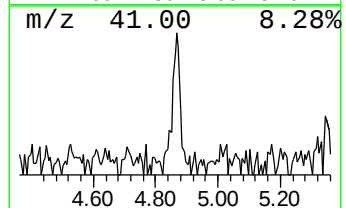
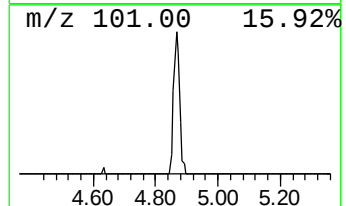
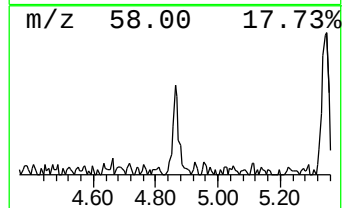
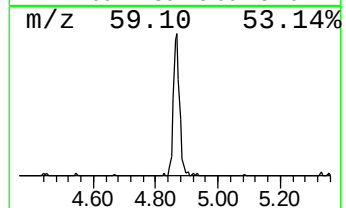
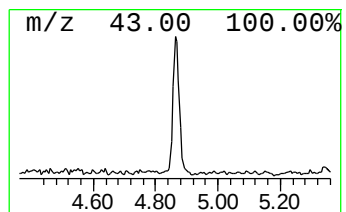
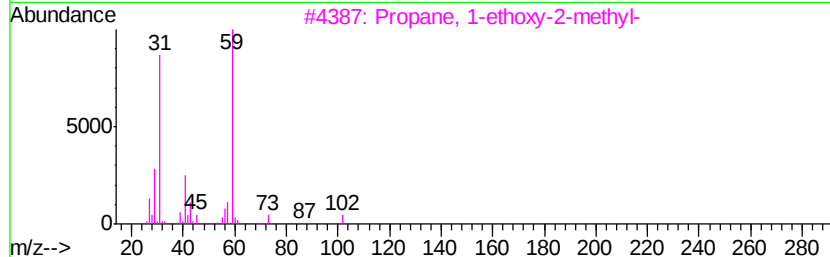
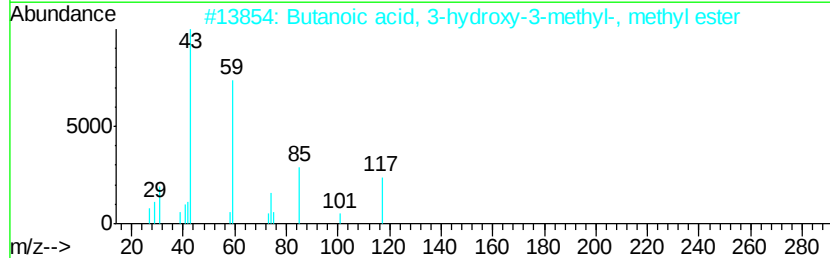
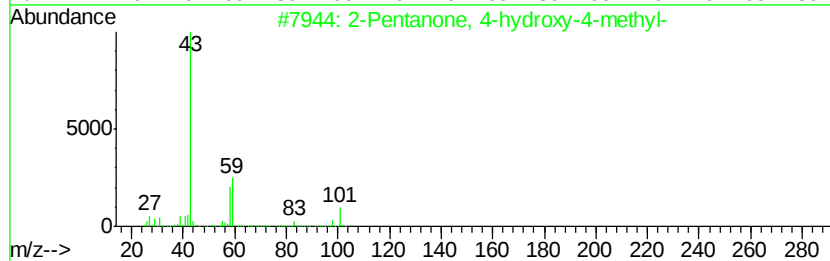
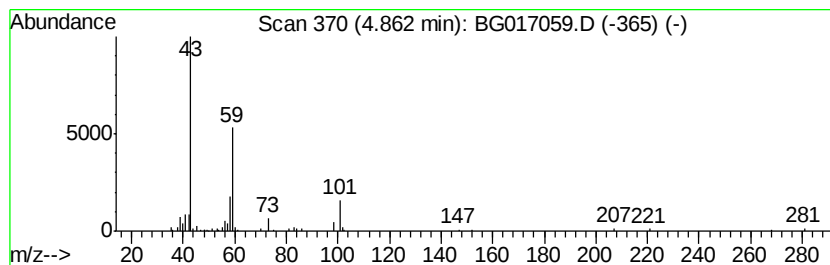
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	4.04 ng	78537	1,4-Dichlorobenzene-d4	7.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	59
2	Butanoic acid, 3-hydroxy-3-methyl-	132	C6H12O3		006149-45-7	38
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O		000627-02-1	30
4	2-Butanol, 1-methoxy-	104	C5H12O2		053778-73-7	25
5	2-[5-(1-Hydroxy-1-methylethyl)-2...	218	C11H22O4		1000190-33-6	25



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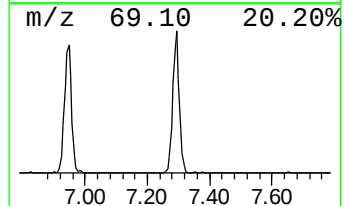
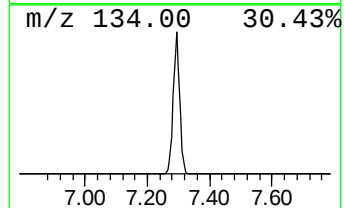
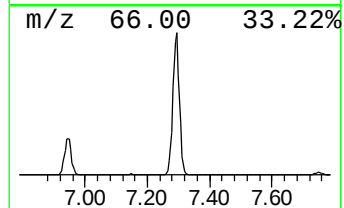
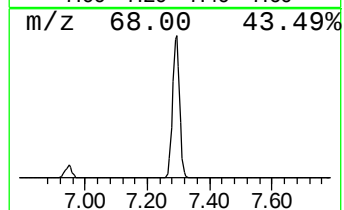
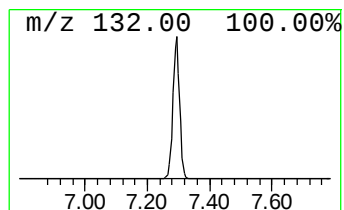
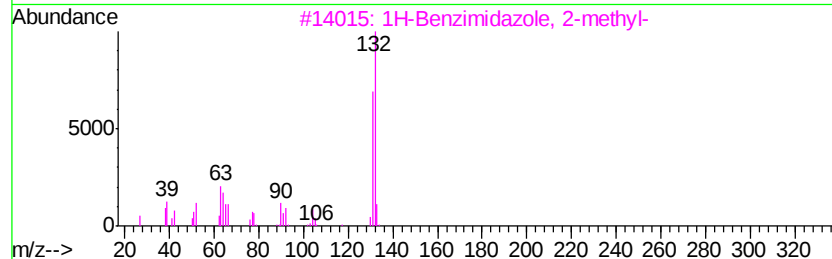
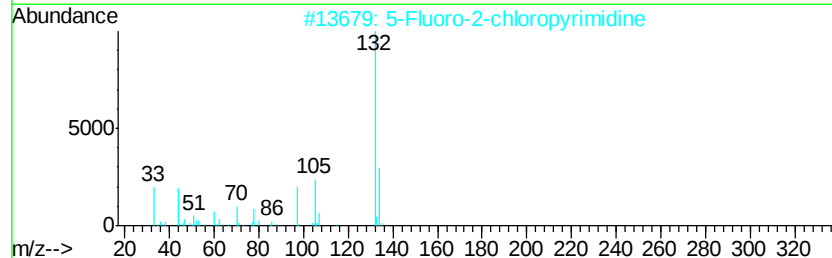
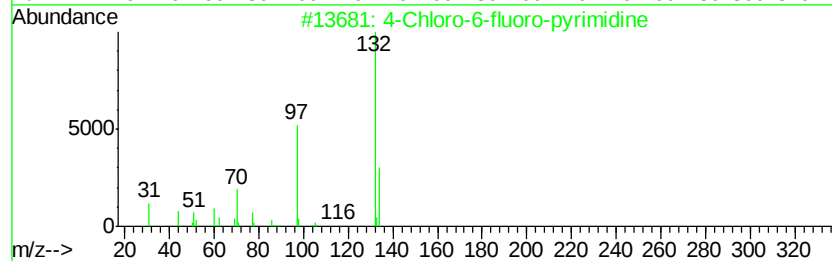
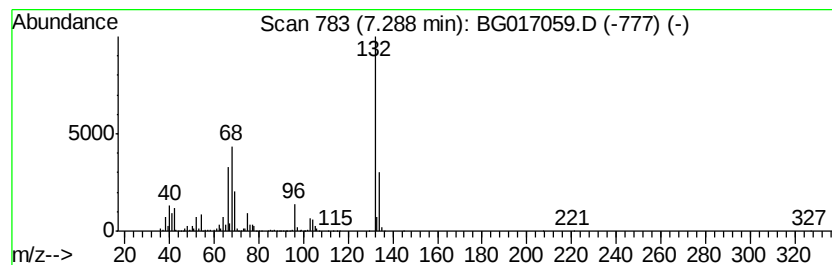
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown7.29 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	67.82 ng	1319150	1,4-Dichlorobenzene-d4	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4		Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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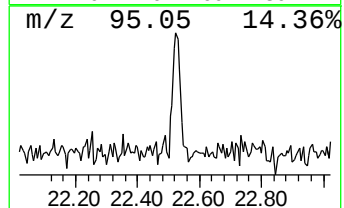
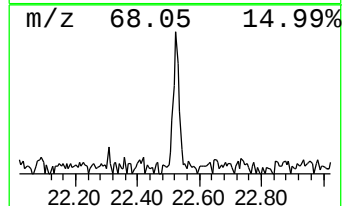
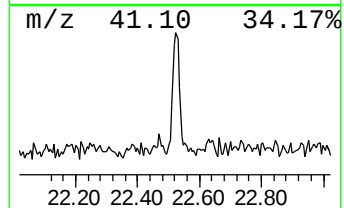
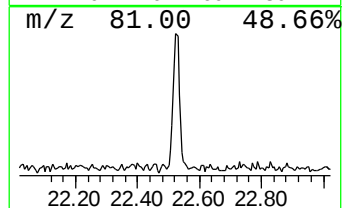
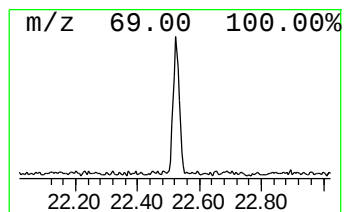
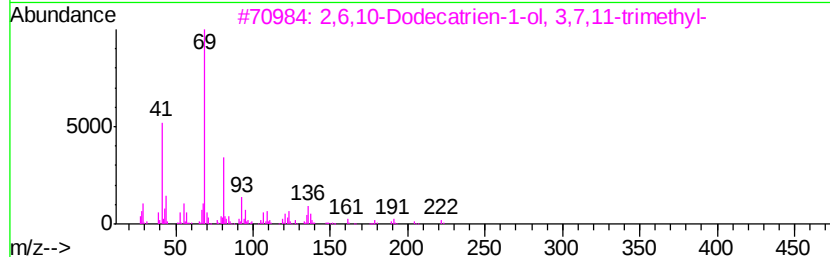
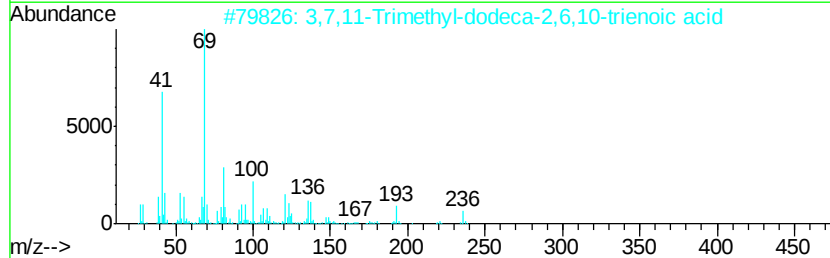
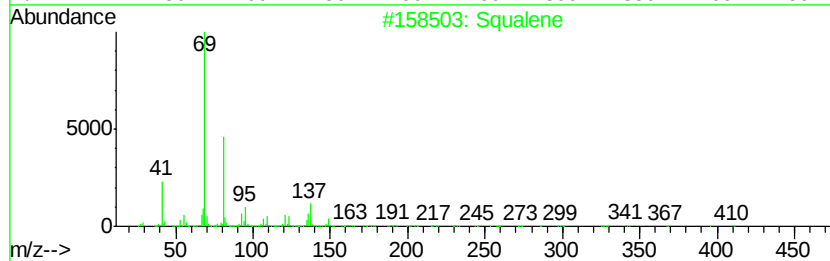
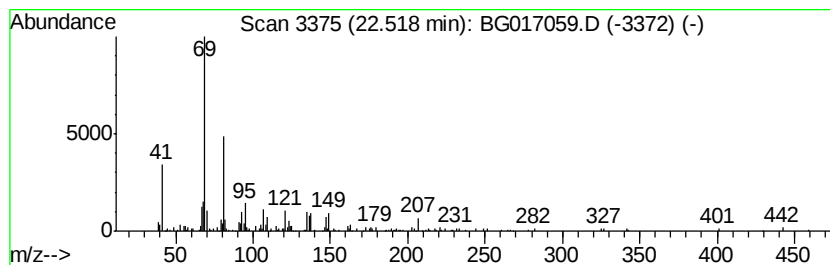
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Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.52	2.44 ng	135007	Perylene-d12	23.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	83
2	3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	72
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
4	2,6-Octadien-1-ol, 3,7-dimethyl-...	182	C11H18O2	000105-86-2	59
5	1,6-Octadien-3-ol, 3,7-dimethyl-...	182	C11H18O2	000115-99-1	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.72	2.72	227.7	ng	4428910	1	7.75	389017	20.0
Butane, 2-methoxy...	2.93	8.0	ng	156138	1	7.75	389017	20.0
2-Pentanone, 4-hy...	4.86	4.0	ng	78537	1	7.75	389017	20.0
unknown7.29	7.29	67.8	ng	1319150	1	7.75	389017	20.0
Squalene	22.52	2.4	ng	135007	6	23.62	1104940	20.0