

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071715\
 Data File : BG017944.D
 Acq On : 18 Jul 2015 2:12
 Operator : TP/UM
 Sample : G2977-02
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FLATBUSH-S-GW

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-BG071715.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	2.789	12	17	25	rVV	68331	119219	1.91%	0.421%
2	2.860	25	29	43	rVB	1432155	1901857	30.51%	6.717%
3	4.147	242	248	254	rBV	58941	79633	1.28%	0.281%
4	4.734	342	348	356	rBV	365128	494528	7.93%	1.747%
5	5.192	419	426	433	rBV	539673	772706	12.39%	2.729%
6	6.761	686	693	702	rBV	346248	541293	8.68%	1.912%
7	7.120	747	754	765	rBV	958781	1481536	23.77%	5.232%
8	7.584	827	833	843	rBV	327353	508288	8.15%	1.795%
9	7.901	880	887	895	rVB	1263815	1991441	31.94%	7.033%
10	8.735	1022	1029	1038	rBV	977702	1606866	25.78%	5.675%
11	10.363	1297	1306	1314	rBV	471772	791081	12.69%	2.794%
12	12.860	1724	1731	1738	rBV	2770327	4095607	65.70%	14.464%
13	14.241	1959	1966	1974	rVB2	729995	1110121	17.81%	3.921%
14	15.739	2213	2221	2233	rBV	1299931	1956159	31.38%	6.909%
15	16.996	2428	2435	2441	rBV	916660	1314160	21.08%	4.641%
16	17.913	2586	2591	2598	rBV2	102317	174878	2.81%	0.618%
17	19.205	2806	2811	2822	rBV2	70378	127186	2.04%	0.449%
18	19.646	2879	2886	2897	rBV	4670463	6234084	100.00%	22.017%
19	20.921	3099	3103	3110	rBV2	77264	118968	1.91%	0.420%
20	21.191	3144	3149	3161	rVB	1097155	1465889	23.51%	5.177%
21	23.412	3519	3527	3537	rBV2	764210	1429583	22.93%	5.049%

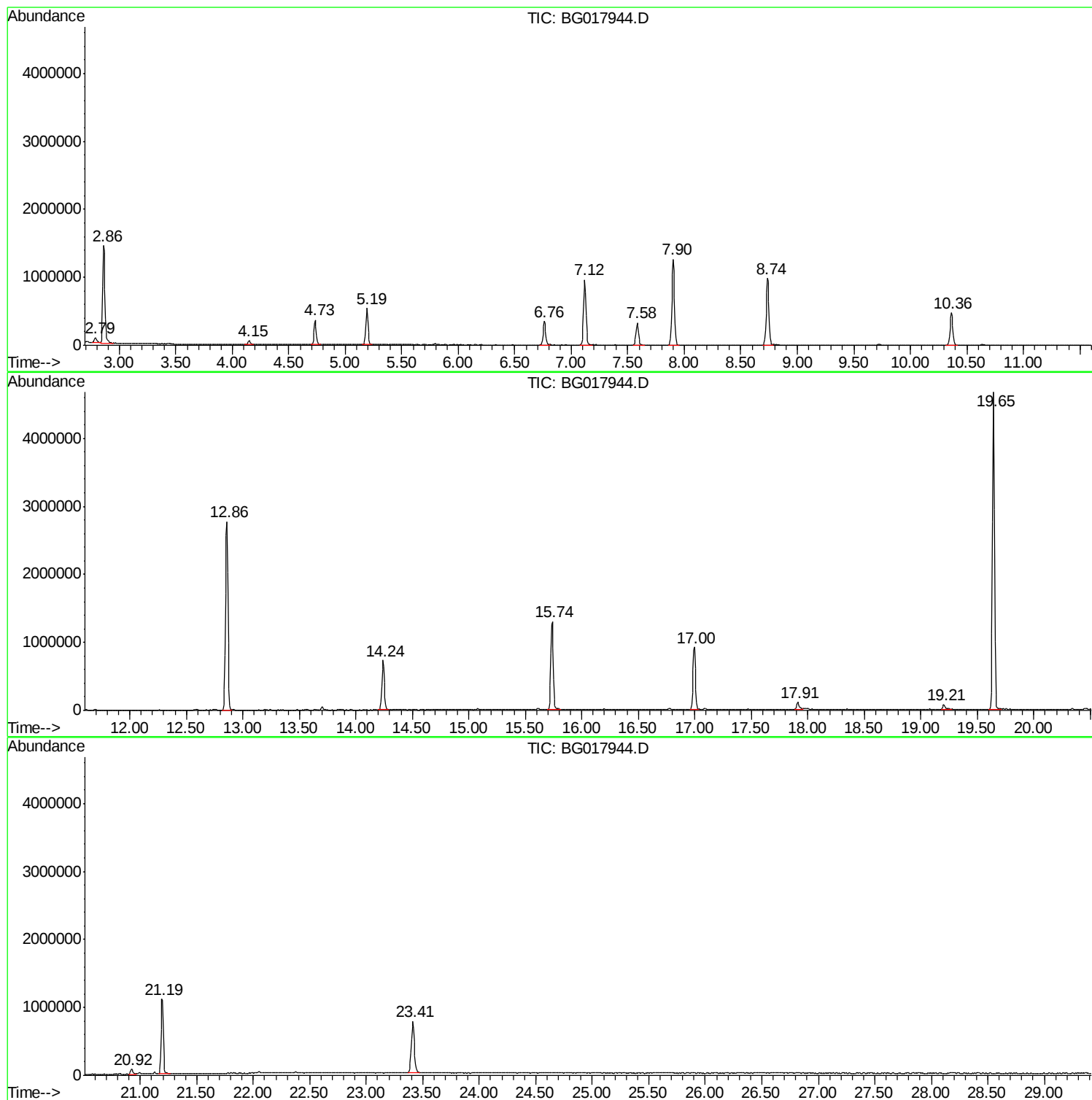
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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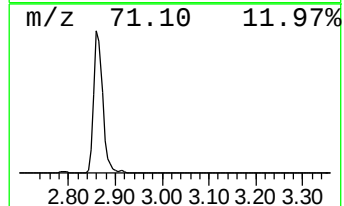
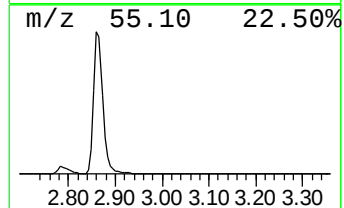
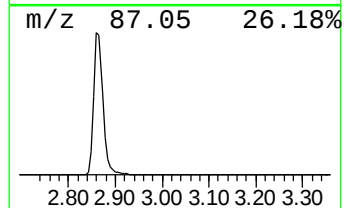
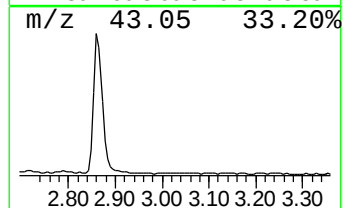
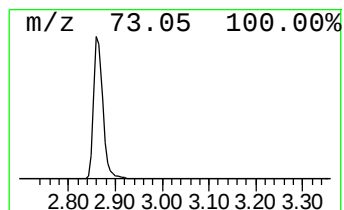
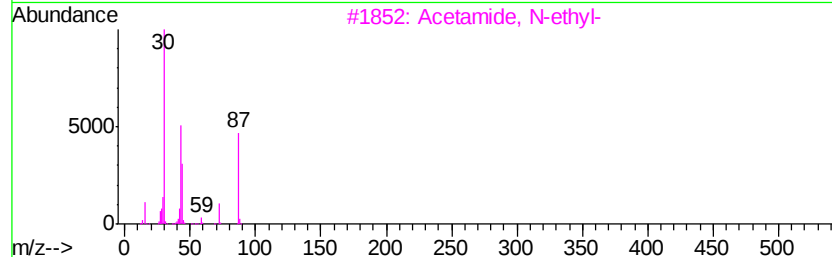
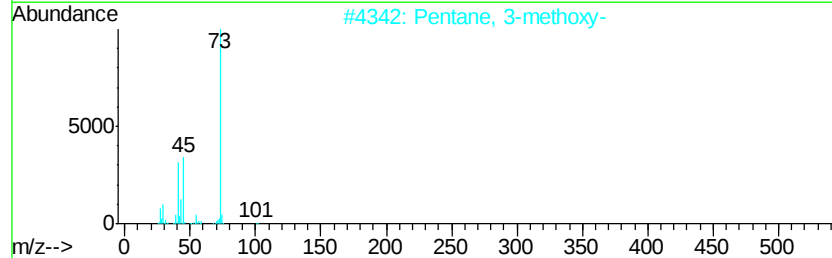
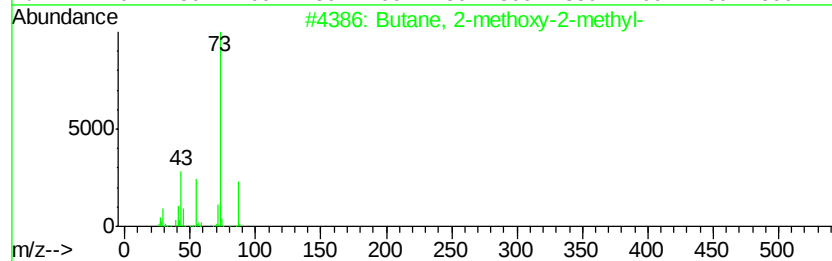
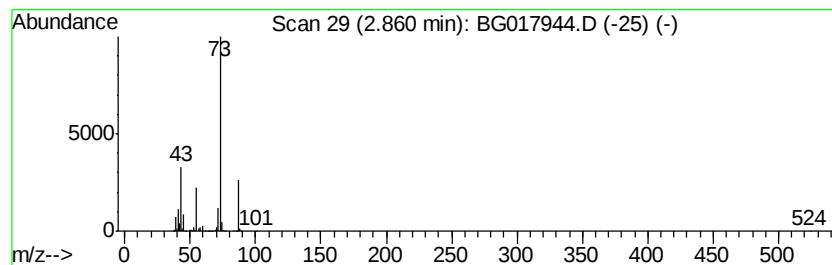
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	74.83 ng	1901860	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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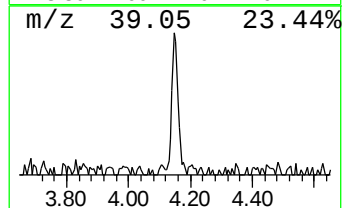
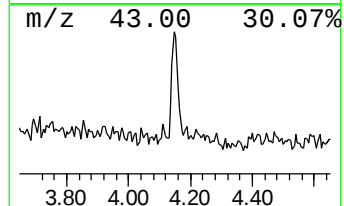
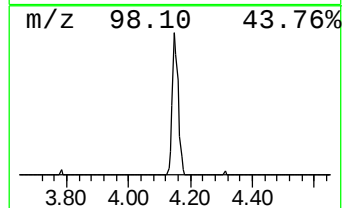
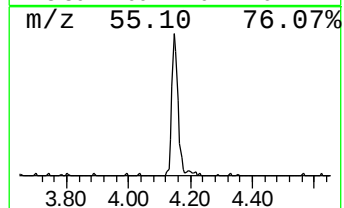
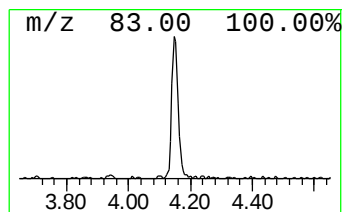
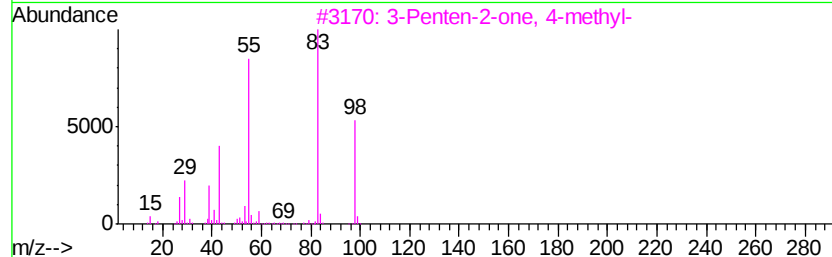
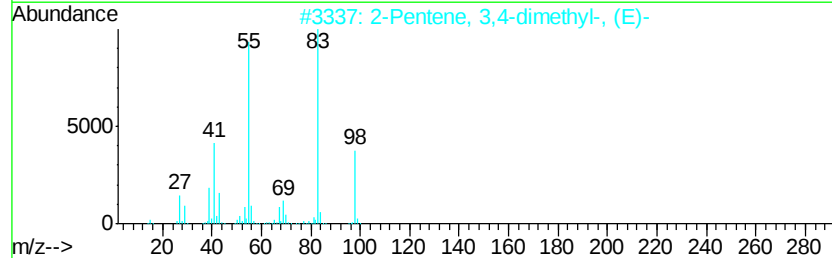
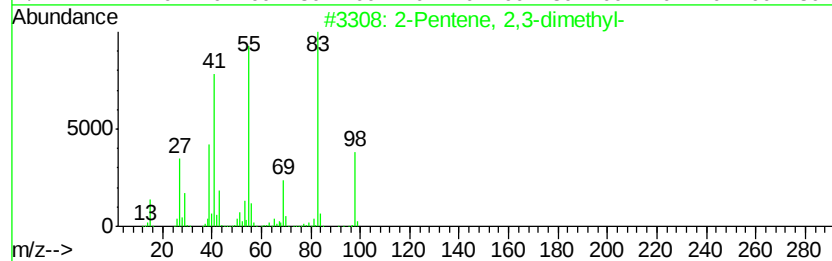
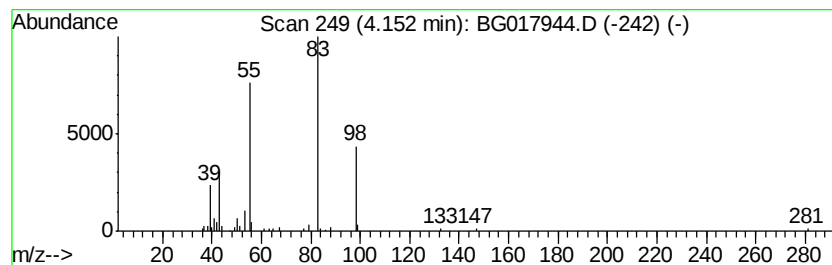
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentene, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.15	3.13 ng	79633	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	86
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
3		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	78
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	64
5		Cyclohexane, methyl-	98	C7H14	000108-87-2	56



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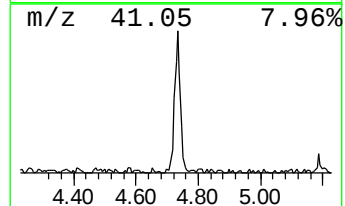
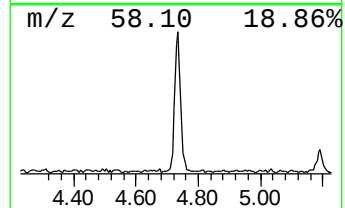
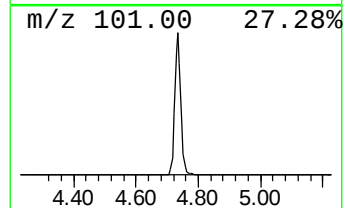
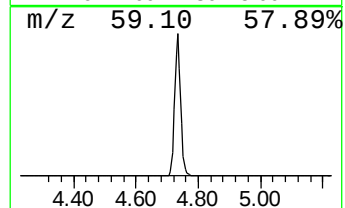
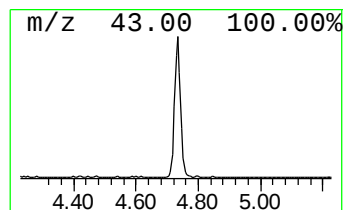
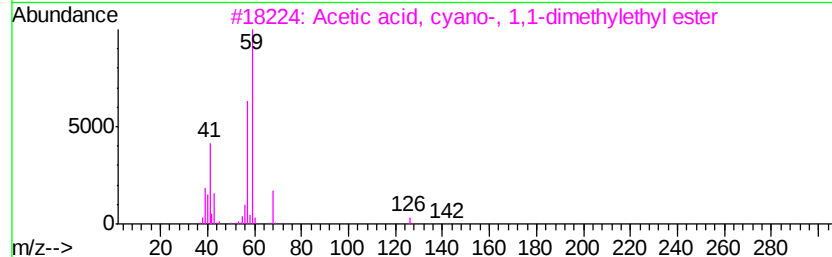
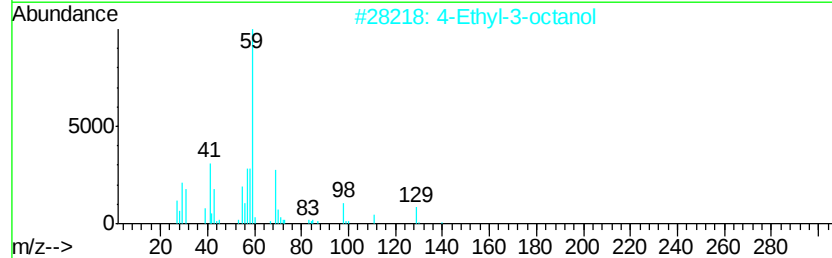
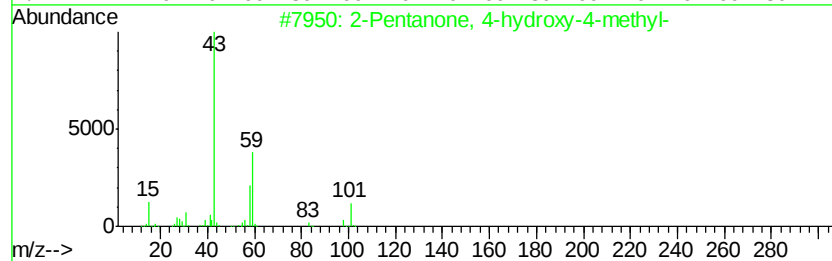
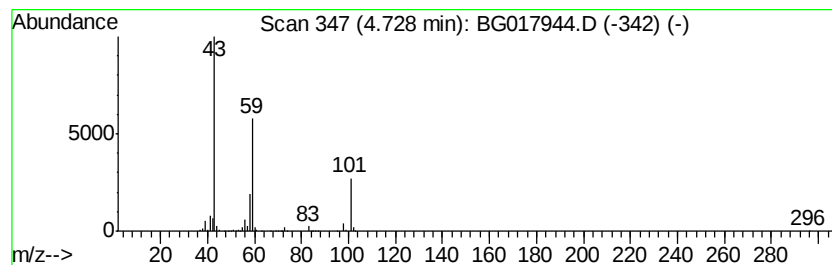
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	19.46 ng	494528	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		4-Ethyl-3-octanol	158	C10H22O	019781-26-1	25
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	17
5		Acetone	58	C3H6O	000067-64-1	10



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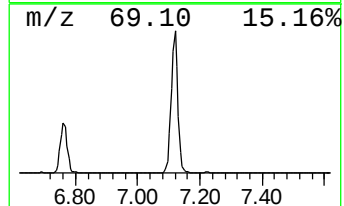
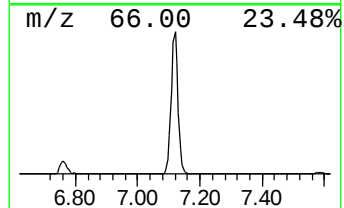
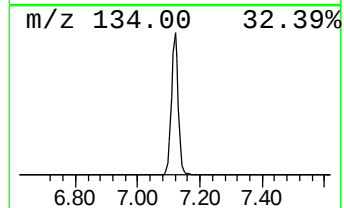
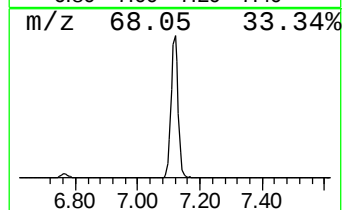
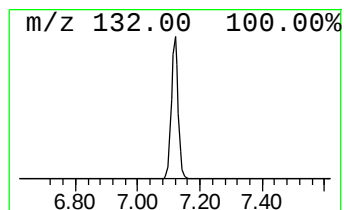
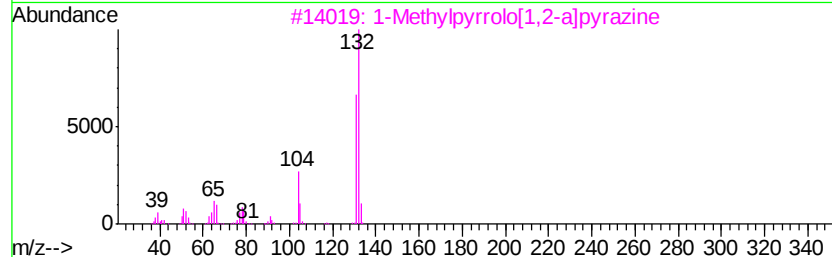
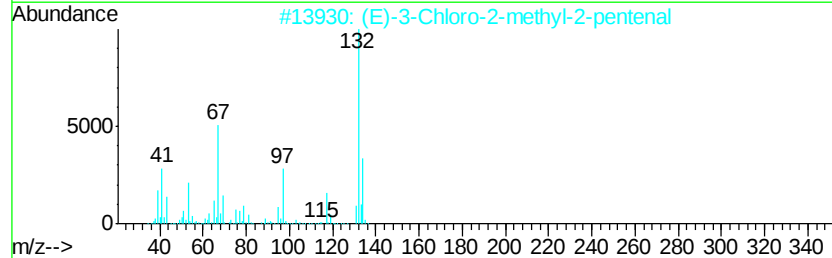
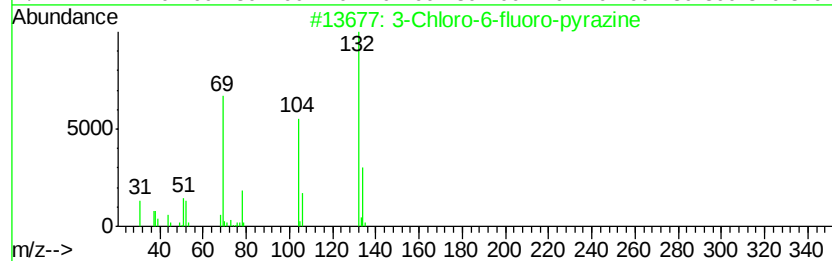
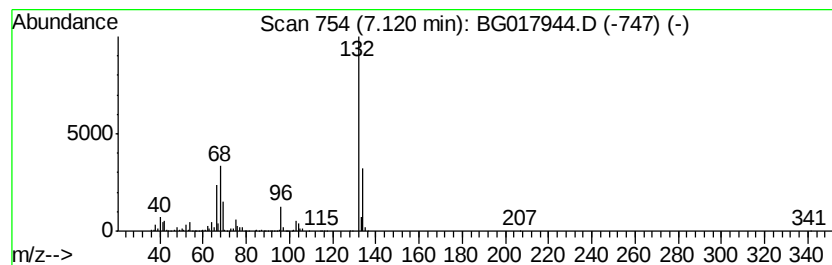
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown7.12 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	58.30 ng	1481540	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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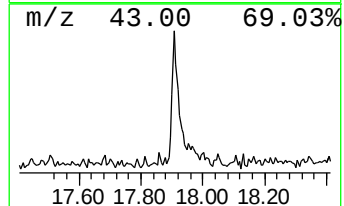
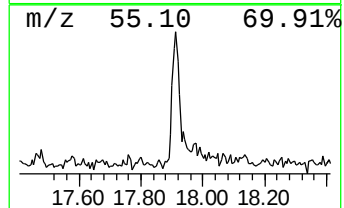
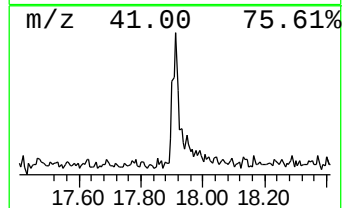
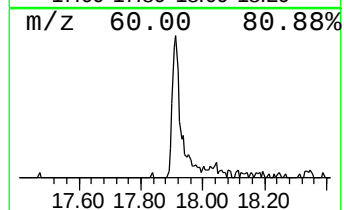
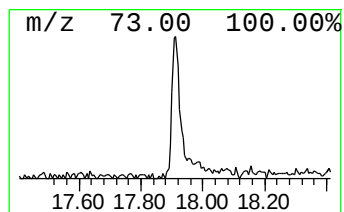
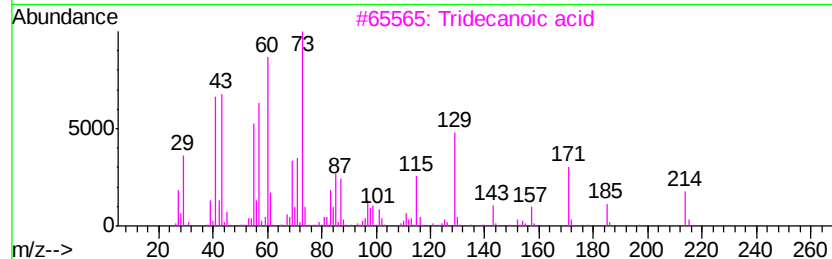
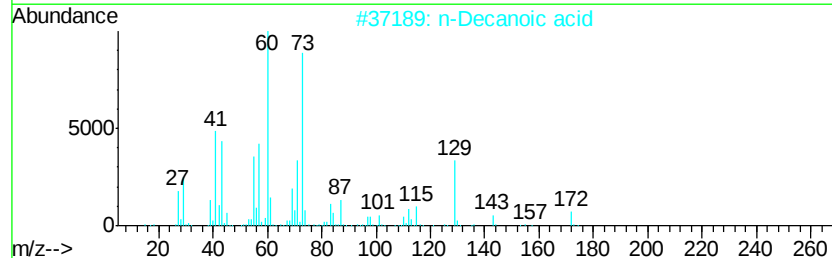
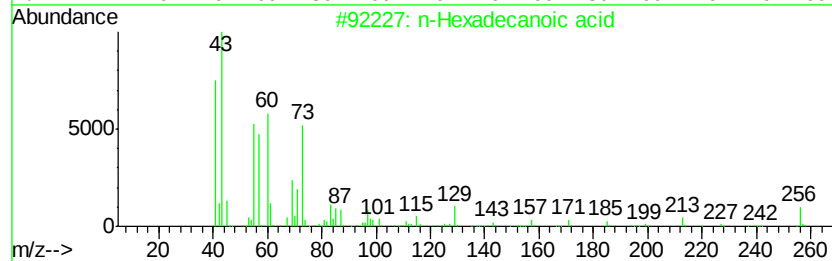
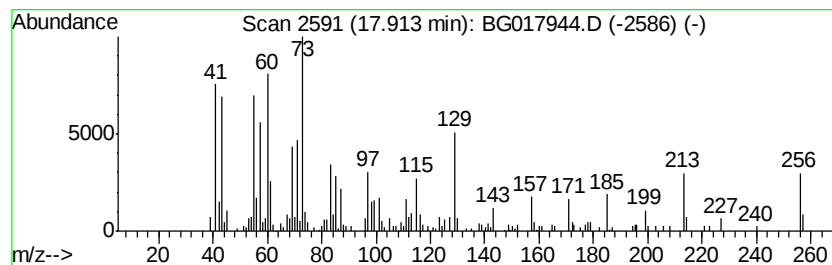
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	2.66 ng	174878	Phenanthrene-d10	17.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		n-Decanoic acid	172	C10H20O2	000334-48-5	70
3		Tridecanoic acid	214	C13H26O2	000638-53-9	64
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5		Heptadecane	240	C17H36	000629-78-7	15



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.86	74.8	ng	1901860	1	7.58	508288	20.0
2-Pentene, 2,3-di...	4.15	3.1	ng	79633	1	7.58	508288	20.0
2-Pentanone, 4-hy...	4.73	19.5	ng	494528	1	7.58	508288	20.0
unknown7.12	7.12	58.3	ng	1481540	1	7.58	508288	20.0
n-Hexadecanoic acid	17.91	2.7	ng	174878	4	17.00	1314160	20.0