

Data Path : Z:\HPCHEM1\BNA G\DATA\BG110716\
 Data File : BG024742.D
 Acq On : 7 Nov 2016 23:37
 Operator : UM/SJ
 Sample : H5543-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-109-17.5-18.0

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-BG102516.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	3.118	42	47	63	rVB	1897288	2853291	43.92%	7.162%
2	4.710	314	318	328	rVB	43453	76786	1.18%	0.193%
3	5.321	417	422	433	rVB	387272	630527	9.71%	1.583%
4	5.791	496	502	511	rBV	1507519	2480651	38.18%	6.226%
5	7.401	767	776	787	rBV	1532047	2725608	41.95%	6.841%
6	7.789	832	842	851	rBV	1428114	2584604	39.78%	6.487%
7	8.259	914	922	930	rBV	349845	631028	9.71%	1.584%
8	8.588	968	978	986	rBV	1043506	1872520	28.82%	4.700%
9	9.434	1113	1122	1130	rBV	876247	1657400	25.51%	4.160%
10	9.510	1130	1135	1146	rVB5	42412	92345	1.42%	0.232%
11	11.091	1396	1404	1413	rBV	439565	812452	12.51%	2.039%
12	13.500	1805	1814	1822	rVB	2204726	3543689	54.55%	8.895%
13	14.316	1945	1953	1959	rBV	709697	1043835	16.07%	2.620%
14	14.874	2042	2048	2056	rVB	753634	1219134	18.77%	3.060%
15	16.361	2292	2301	2310	rBV	2404475	3726259	57.36%	9.353%
16	16.525	2325	2329	2337	rBV3	46542	92902	1.43%	0.233%
17	17.618	2508	2515	2524	rBV	1030972	1665116	25.63%	4.179%
18	18.458	2655	2658	2667	rVB4	62755	91162	1.40%	0.229%
19	20.198	2948	2954	2960	rBV	4728466	6496527	100.00%	16.306%
20	21.490	3169	3174	3180	rBV5	125246	214207	3.30%	0.538%
21	21.913	3238	3246	3255	rVB	1488365	2570739	39.57%	6.453%
22	23.629	3532	3538	3546	rVB2	73265	174159	2.68%	0.437%
23	25.333	3818	3828	3841	rVB	814536	2585327	39.80%	6.489%

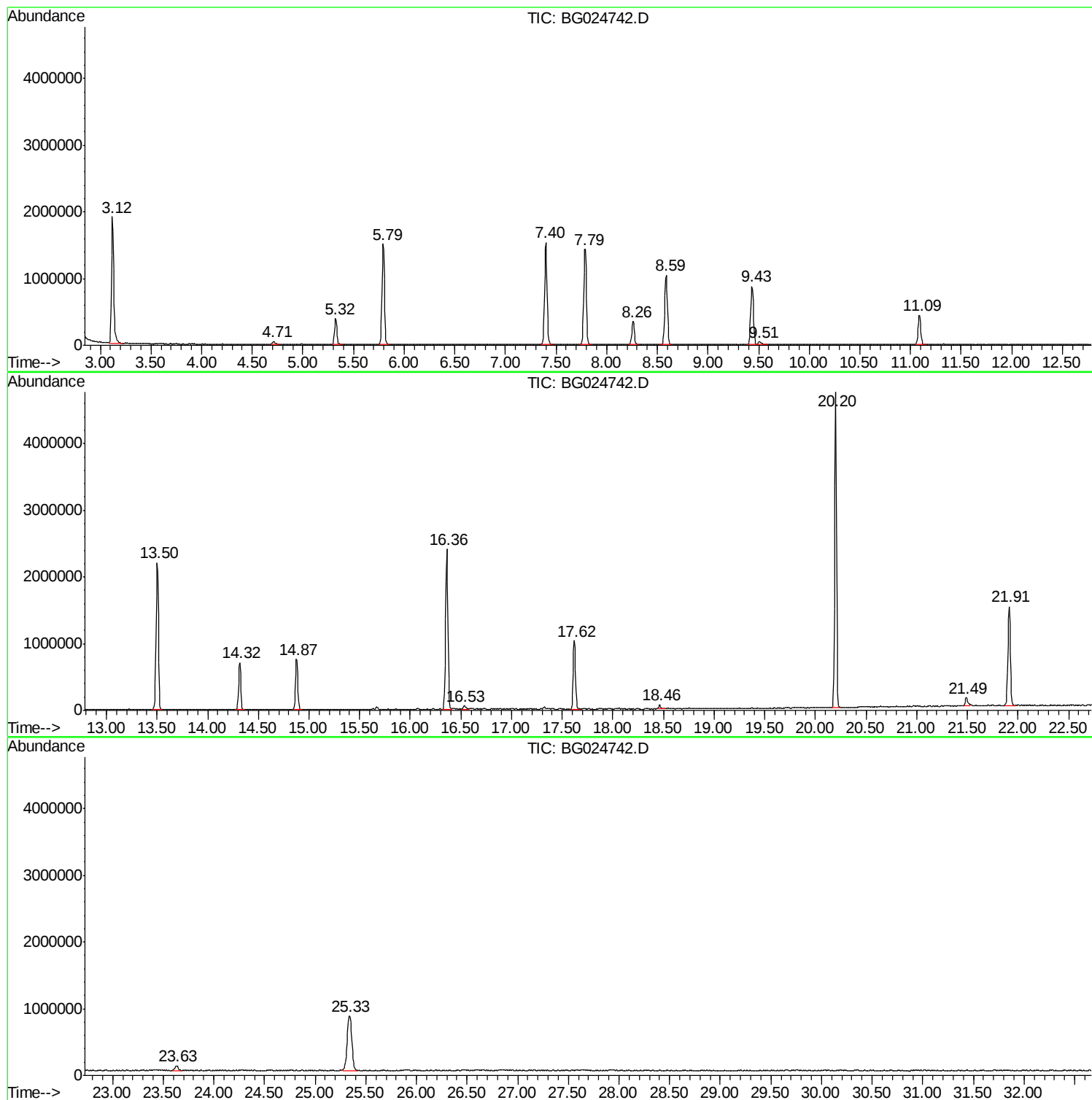
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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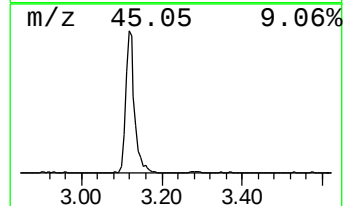
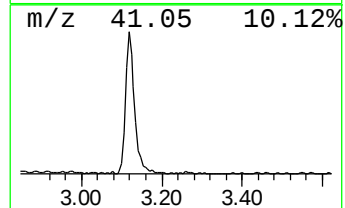
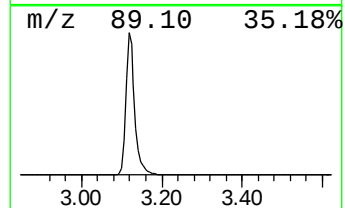
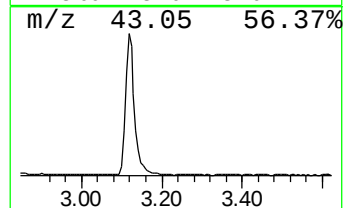
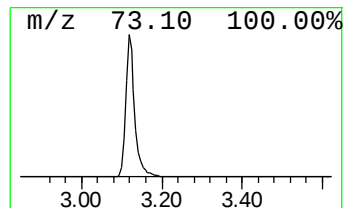
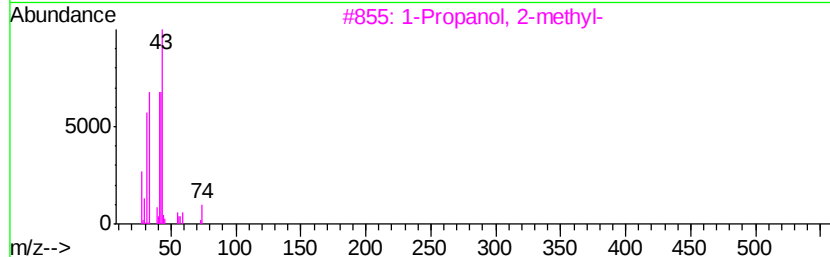
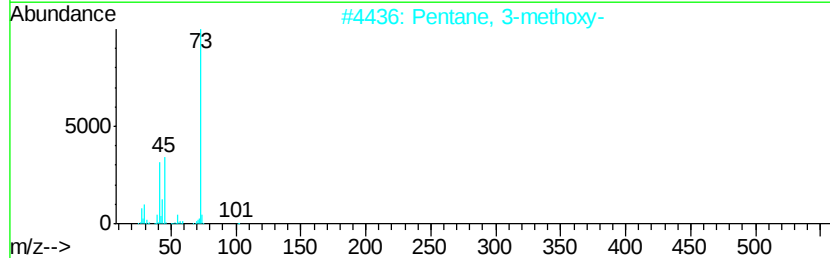
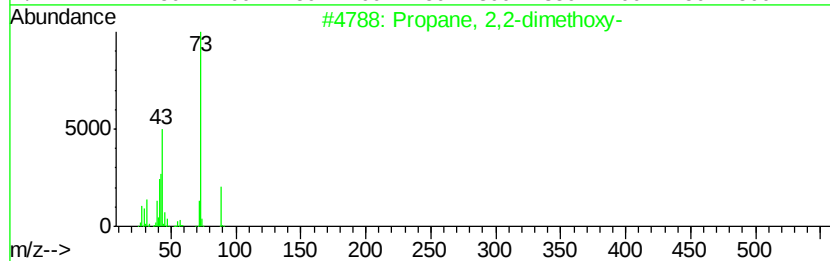
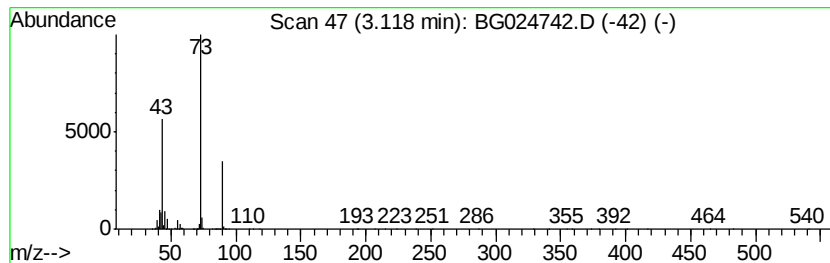
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	90.43 ng	2853290	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	43
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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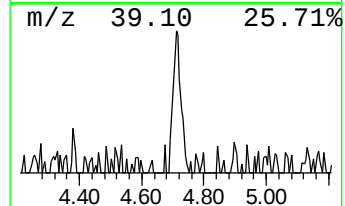
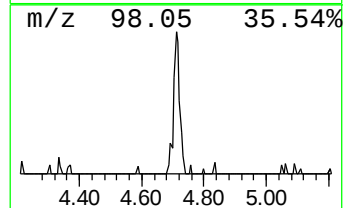
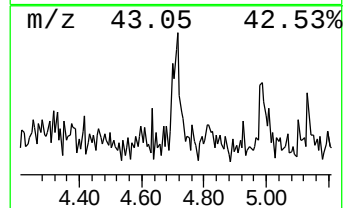
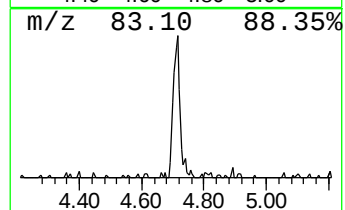
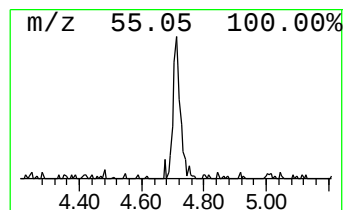
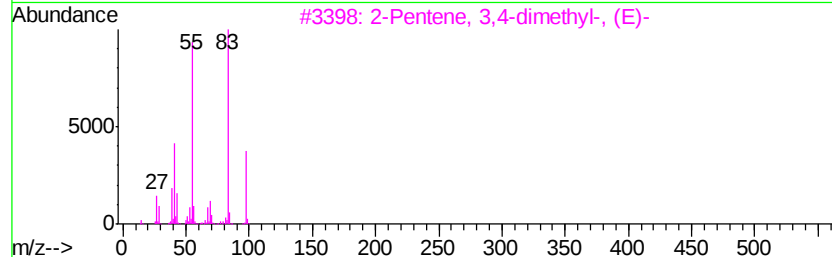
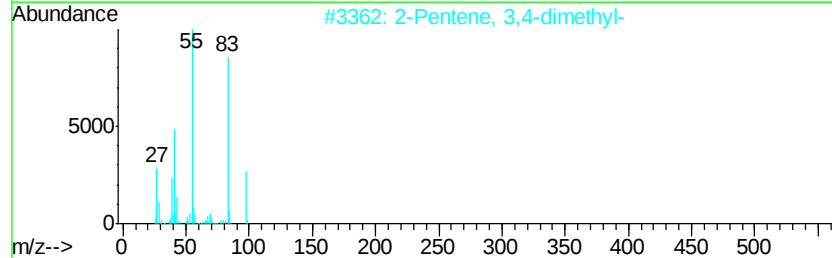
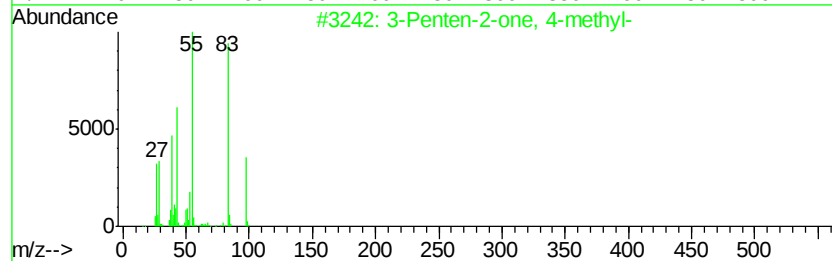
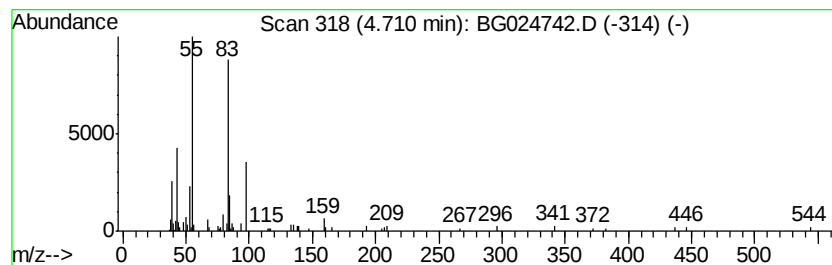
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	2.43 ng	76786	1,4-Dichlorobenzene-d4	8.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	72
2			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	59
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	59
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	59
5			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	59



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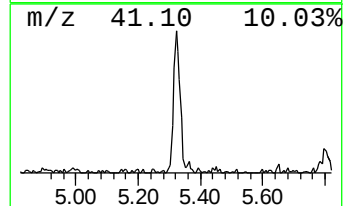
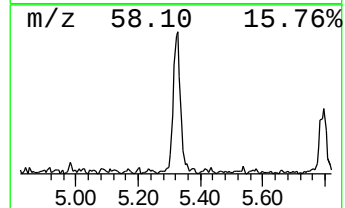
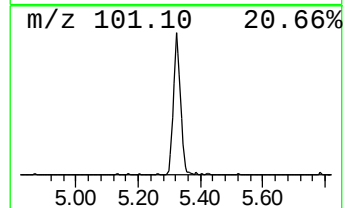
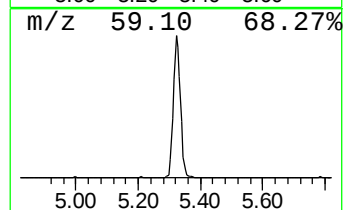
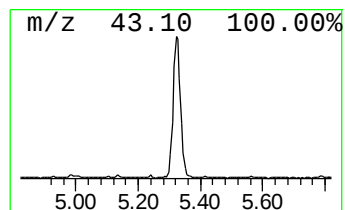
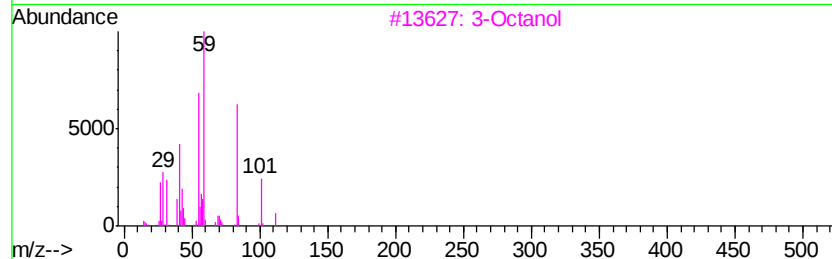
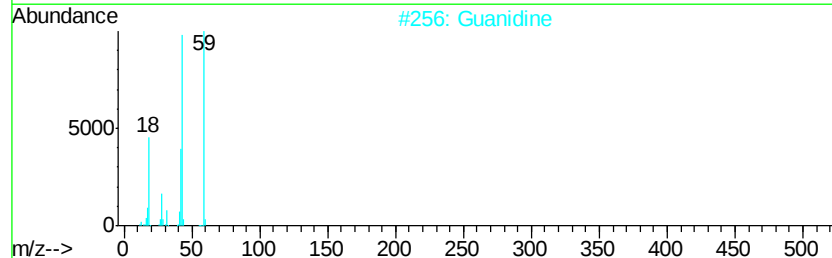
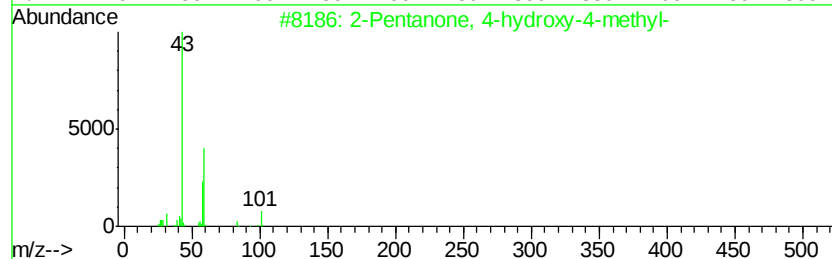
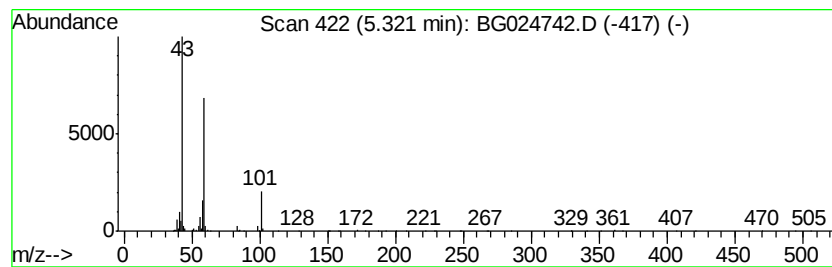
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	19.98 ng	630527	1,4-Dichlorobenzene-d4	8.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Guanidine	59	CH5N3	000113-00-8	47	
3	3-Octanol	130	C8H18O	000589-98-0	36	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
5	Tetraglyme	222	C10H22O5	000143-24-8	25	



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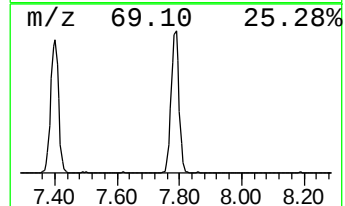
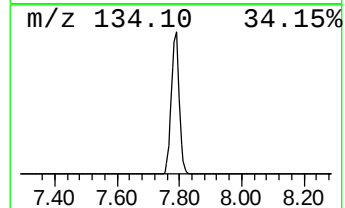
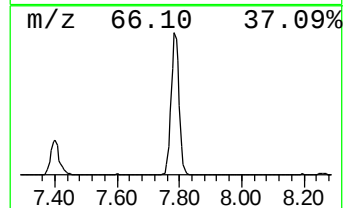
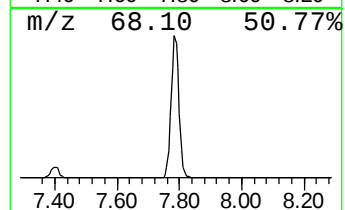
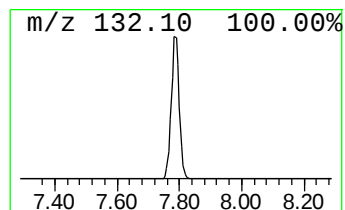
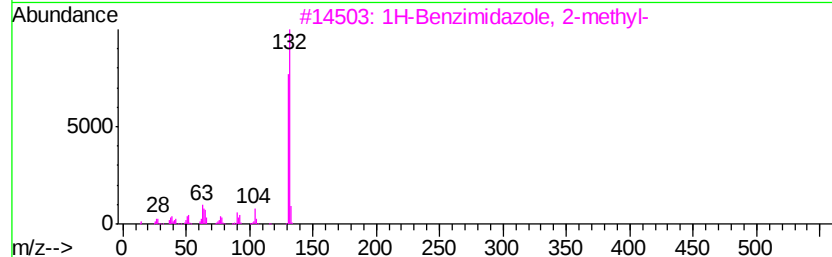
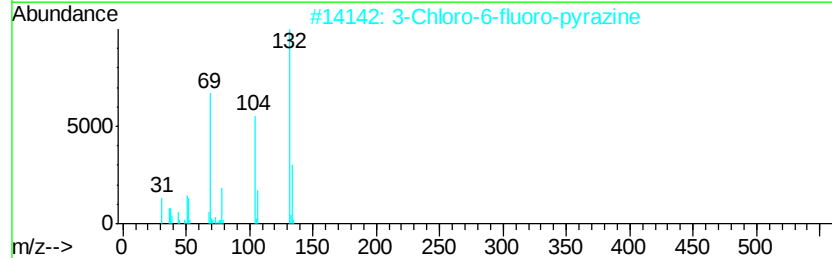
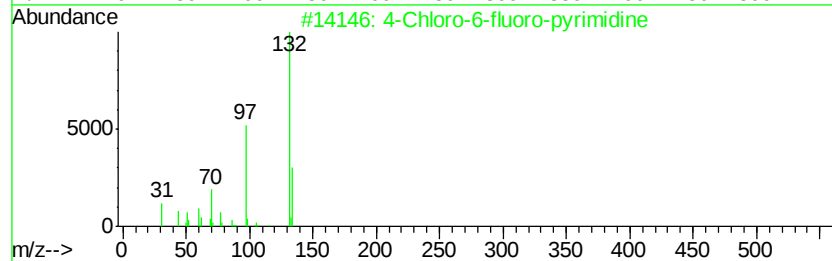
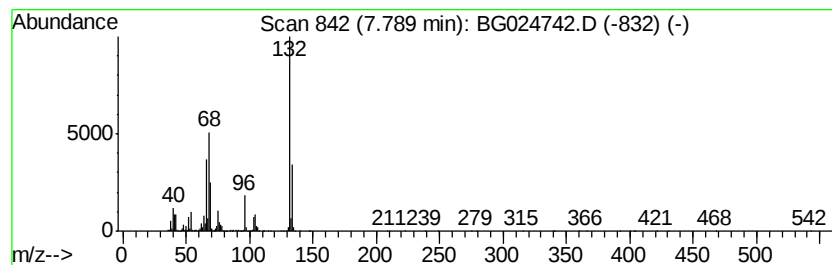
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	81.92 ng	2584600	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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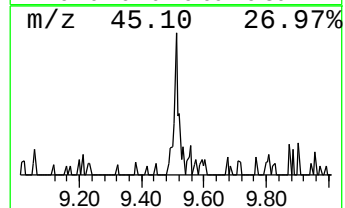
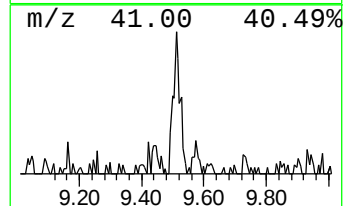
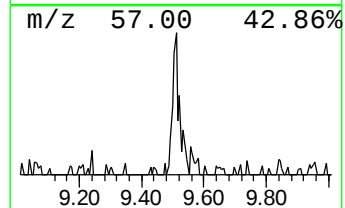
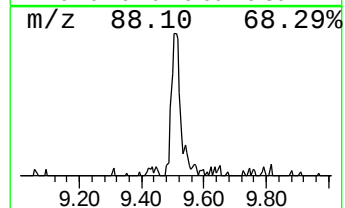
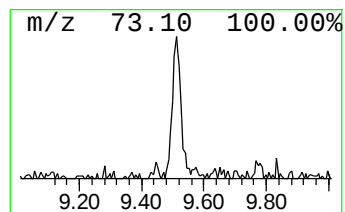
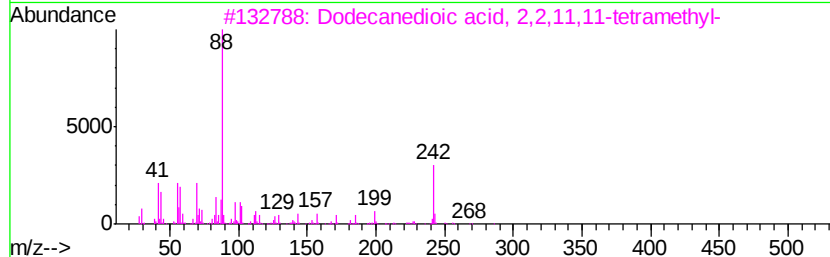
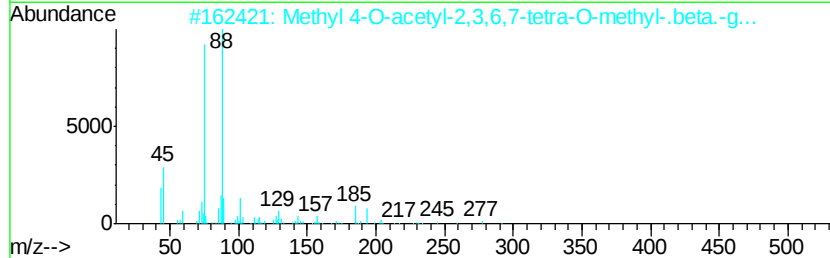
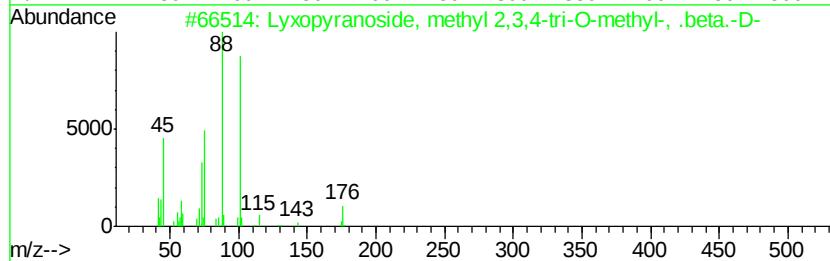
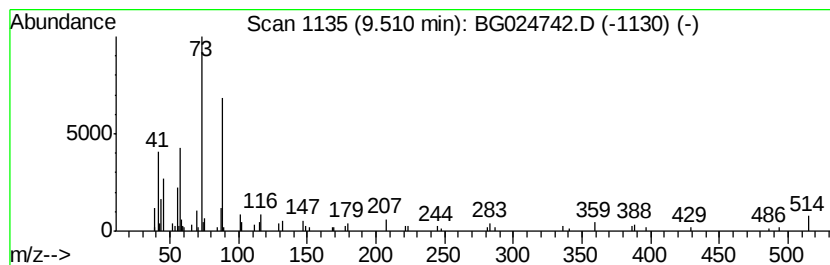
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown9.51 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.51	2.93 ng	92345	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Lvxopyranoside, methyl 2,3,4-tri...	206	C9H18O5	002876-84-8	36
2		Methyl 4-O-acetyl-2,3,6,7-tetra...	322	C14H26O8	084564-16-9	33
3		Dodecanedioic acid, 2,2,11,11-te...	286	C16H30O4	022092-64-4	25
4		Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	17
5		Dodecanoic acid, 2,6-dimethyl-, ...	242	C15H30O2	055955-75-4	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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3-Penten-2-one, 4...	4.71	2.4	ng	76786	1	8.26	631028	20.0
2-Pentanone, 4-hy...	5.32	20.0	ng	630527	1	8.26	631028	20.0
unknown7.79	7.79	81.9	ng	2584600	1	8.26	631028	20.0
unknown9.51	9.51	2.9	ng	92345	1	8.26	631028	20.0