

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012916\
 Data File : BF084652.D
 Acq On : 29 Jan 2016 23:10
 Operator : SJ/IZ
 Sample : H1273-11
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-B011(30-32)

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_F\METHODS\8270-BF012916.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	4.190	181	184	189	rVB	179665	271288	5.43%	0.579%
2	4.887	241	245	254	rBV	2440153	3568082	71.39%	7.611%
3	5.321	280	283	285	rBV	4547439	4402379	88.08%	9.390%
4	5.721	316	318	321	rBV	243309	213123	4.26%	0.455%
5	6.373	372	375	377	rBV	4544383	4982463	99.69%	10.628%
6	6.487	383	385	388	rBV	3731237	4406370	88.16%	9.399%
7	6.716	403	405	408	rBV	777353	1036268	20.73%	2.210%
8	6.876	417	419	422	rBV	3453940	3170854	63.44%	6.763%
9	7.287	452	455	458	rBV	2574344	2639557	52.81%	5.630%
10	8.007	516	518	520	rBV	1732947	1470473	29.42%	3.137%
11	8.042	520	521	523	rVB	71166	51043	1.02%	0.109%
12	9.093	610	613	615	rBV	4113505	4997977	100.00%	10.661%
13	9.482	645	647	649	rBV	505666	460829	9.22%	0.983%
14	9.699	665	666	669	rBV	56612	66579	1.33%	0.142%
15	9.756	669	671	674	rVV	1557110	1511651	30.25%	3.224%
16	10.202	708	710	712	rVB	134943	103810	2.08%	0.221%
17	10.419	726	729	732	rBV	39485	68138	1.36%	0.145%
18	10.545	737	740	743	rBV	3326090	3286874	65.76%	7.011%
19	10.671	750	751	756	rBV	113810	142096	2.84%	0.303%
20	11.116	788	790	792	rBV	50745	57240	1.15%	0.122%
21	11.242	798	801	803	rBV	1449865	1582656	31.67%	3.376%
22	11.791	846	849	851	rBV	52707	76017	1.52%	0.162%
23	12.831	937	940	942	rBV	4541458	4881760	97.67%	10.413%
24	13.768	1018	1022	1028	rBV2	83025	267186	5.35%	0.570%
25	13.871	1028	1031	1033	rVV	1717354	1663490	33.28%	3.548%
26	14.625	1095	1097	1101	rBV2	35708	55994	1.12%	0.119%
27	14.717	1103	1105	1107	rVV	52593	50689	1.01%	0.108%
28	15.254	1149	1152	1155	rBV	1238899	1397226	27.96%	2.980%

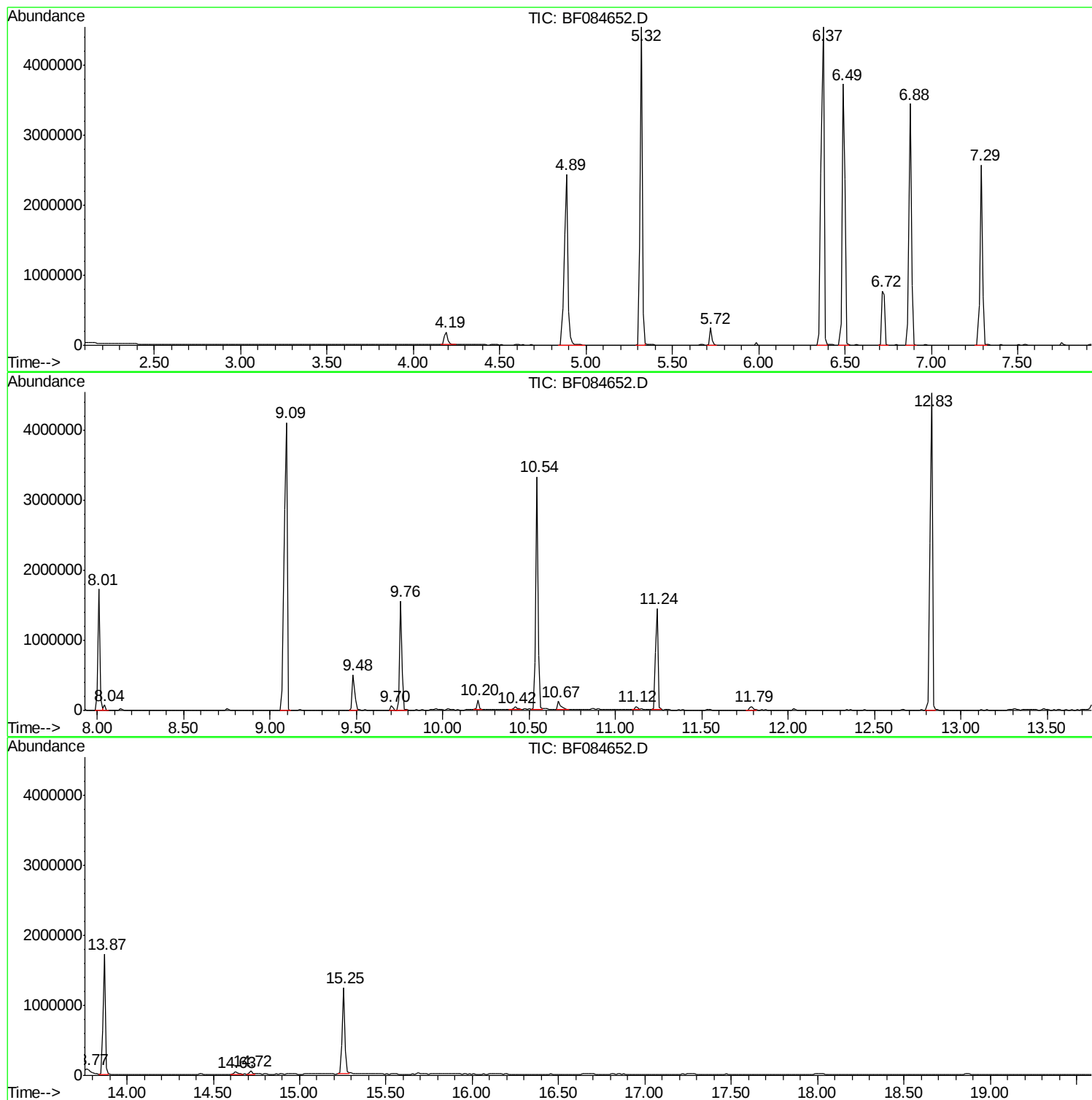
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ClientSampleId :
SUP-B011(30-32)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012916.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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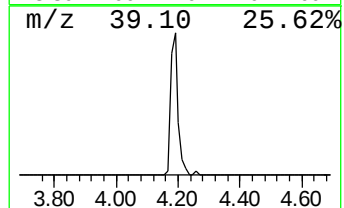
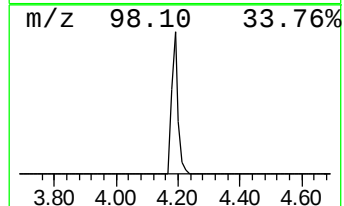
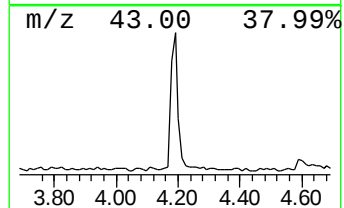
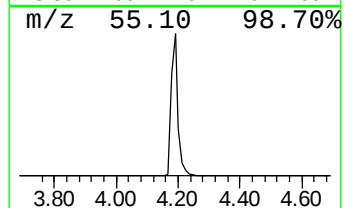
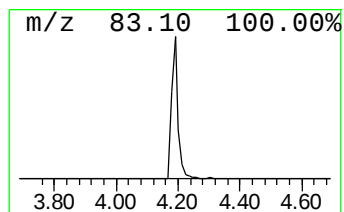
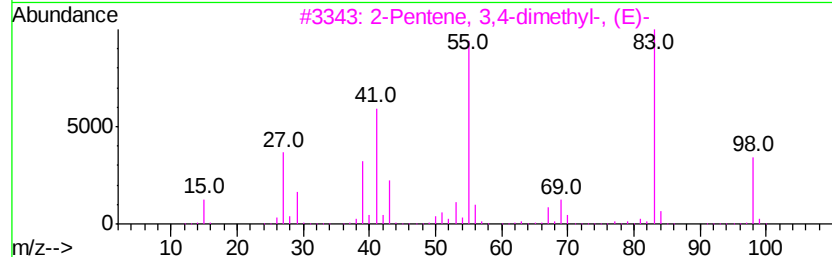
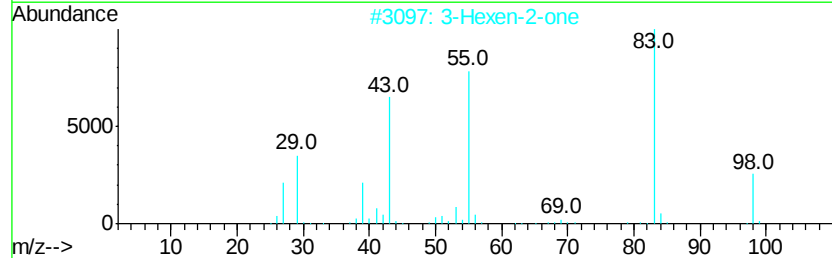
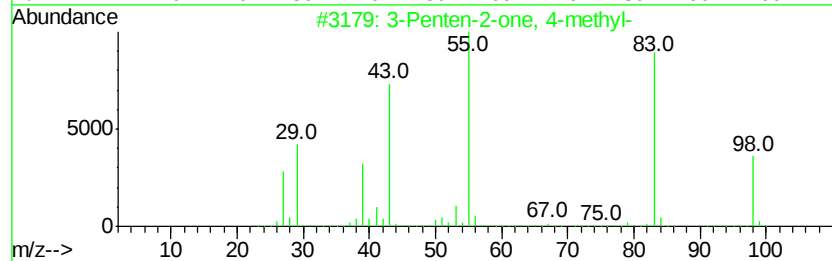
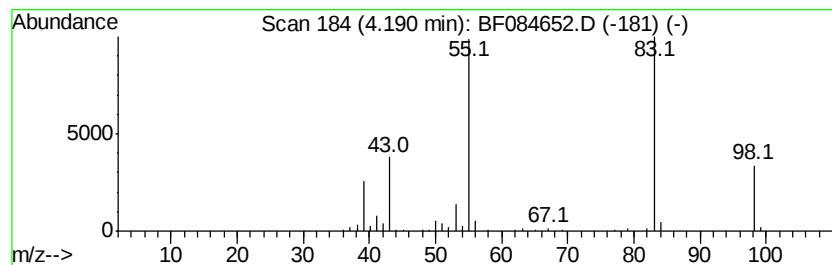
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	5.24 ng	271288	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
4			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	72
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72



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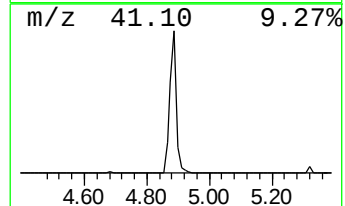
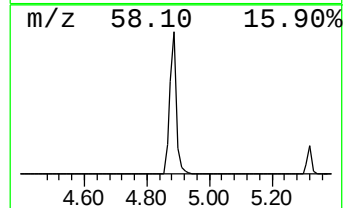
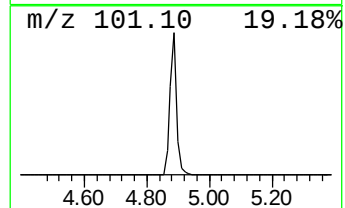
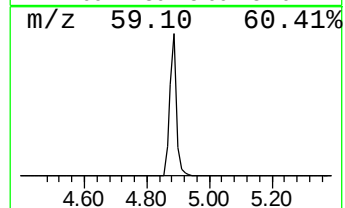
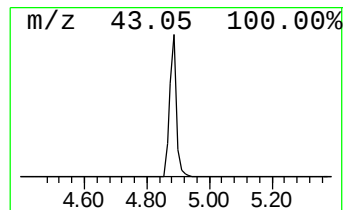
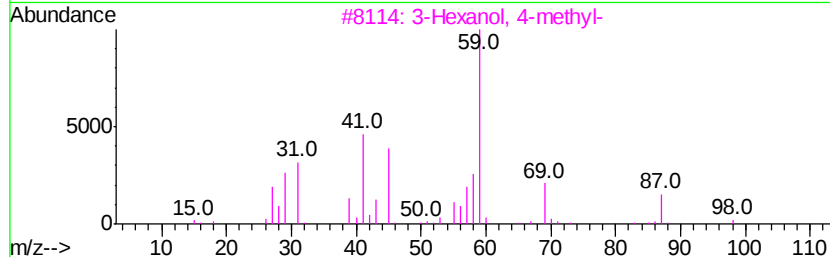
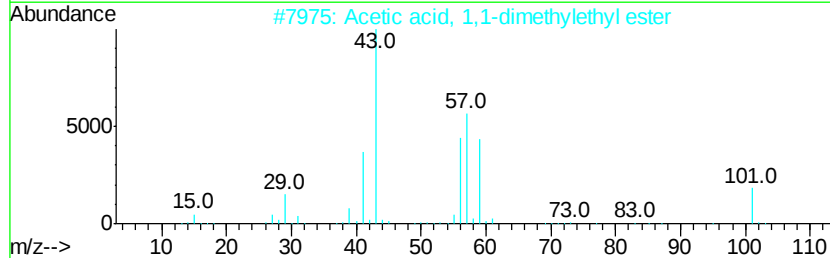
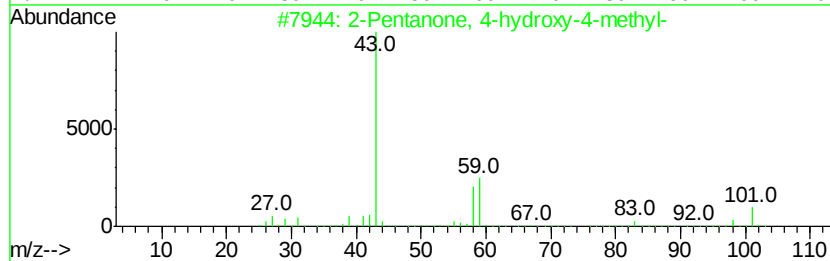
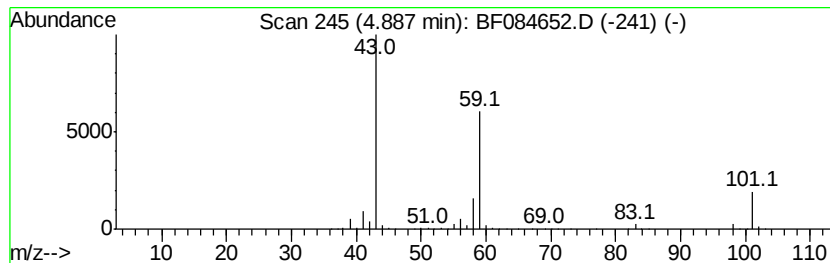
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	68.86 ng	3568080	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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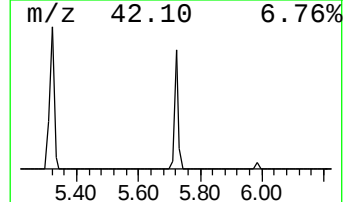
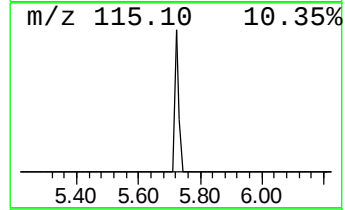
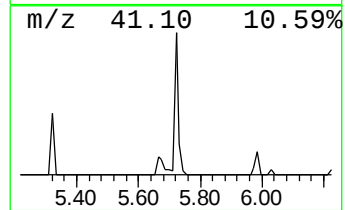
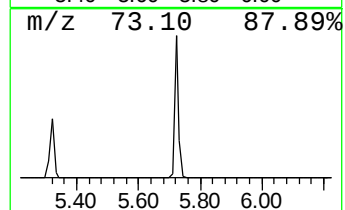
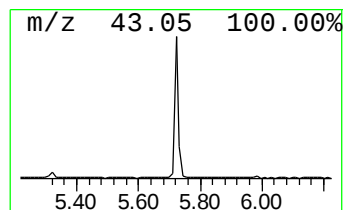
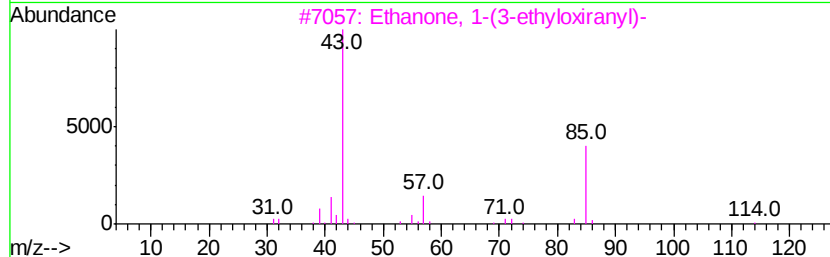
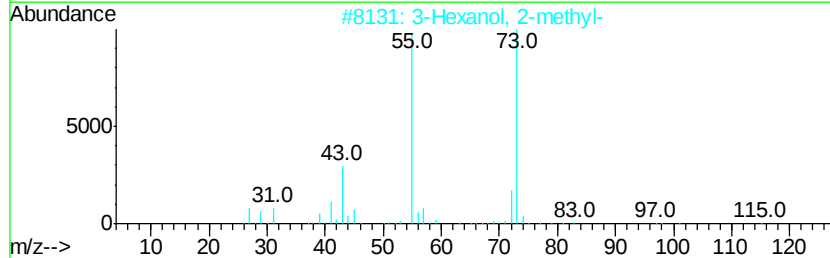
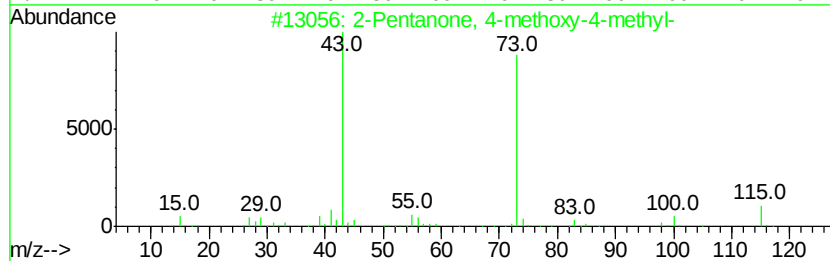
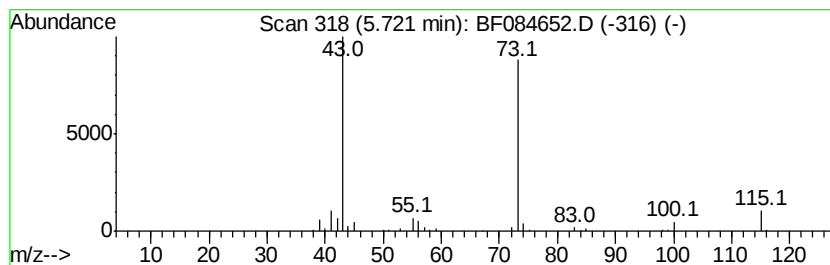
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	4.11 ng	213123	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
3			Ethanone, 1-(3-ethoxiran-1-yl)-	114	C6H10O2	017257-81-7	10
4			N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5			N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10



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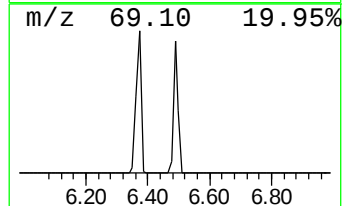
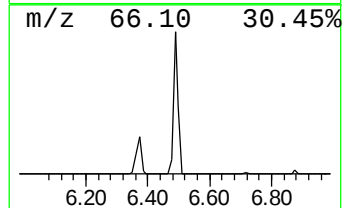
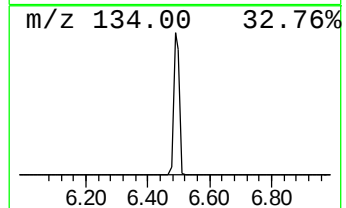
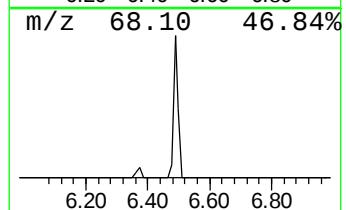
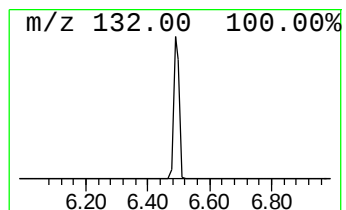
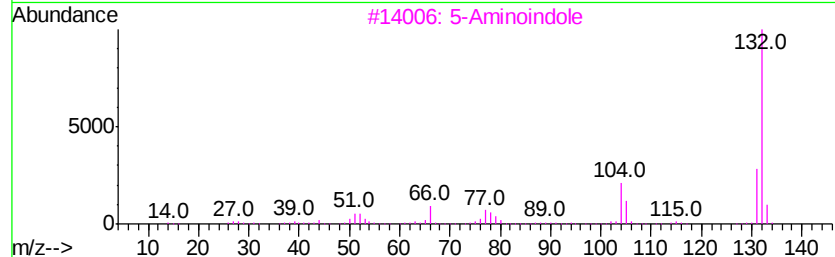
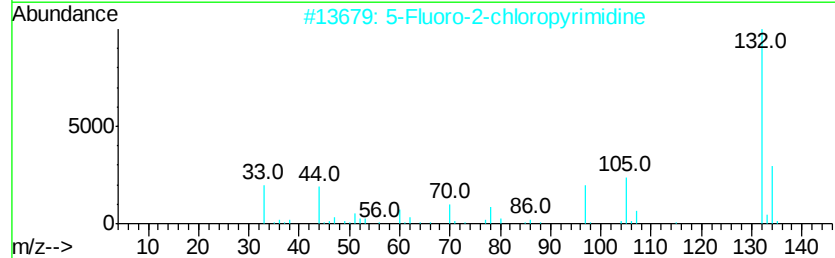
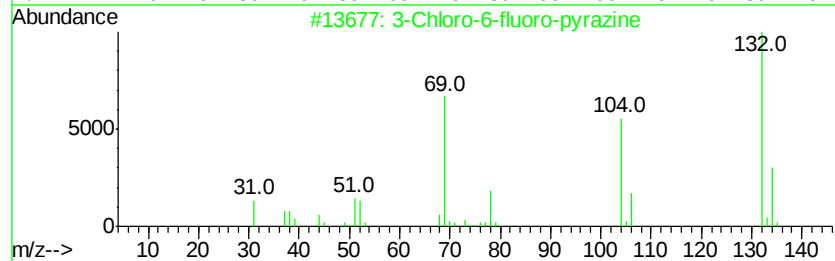
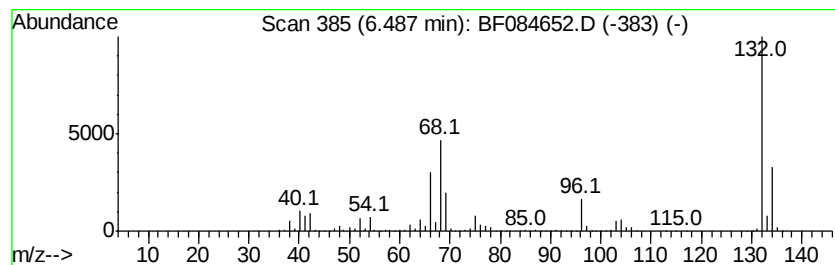
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Peak Number 4 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	85.04 ng	4406370	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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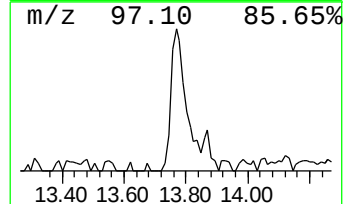
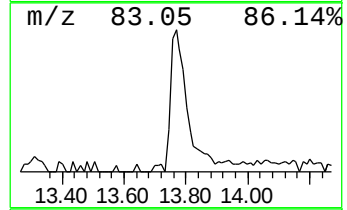
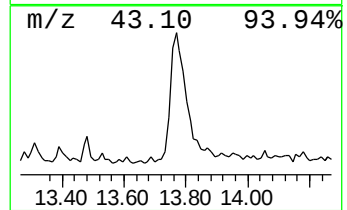
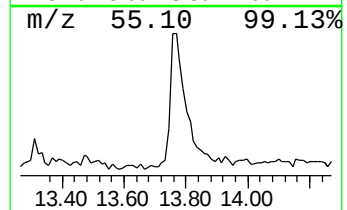
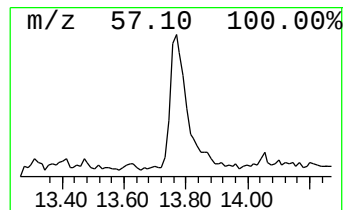
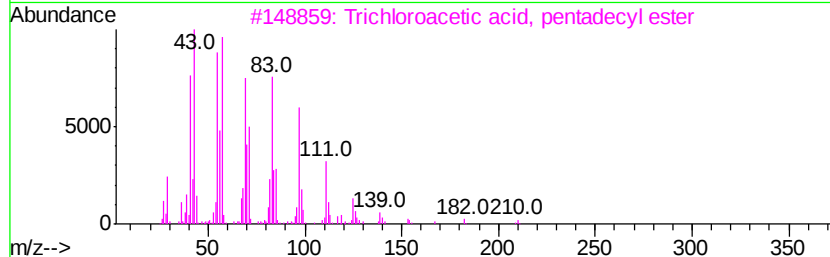
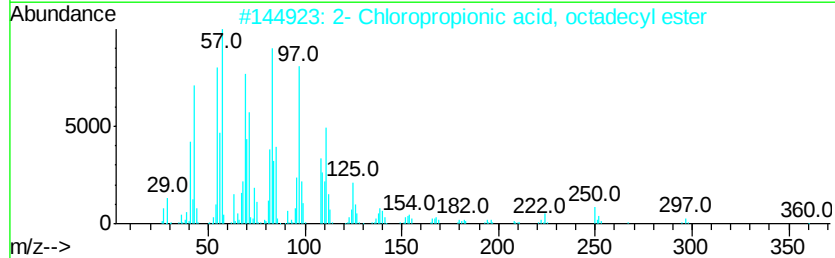
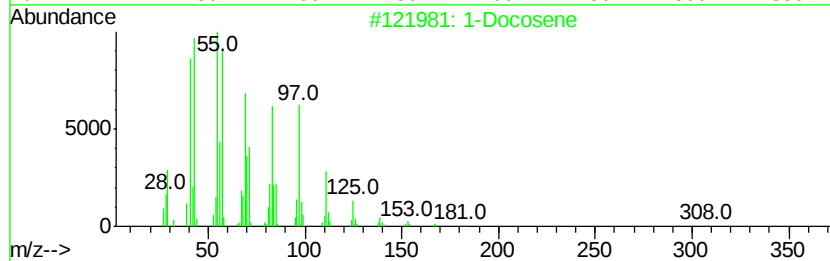
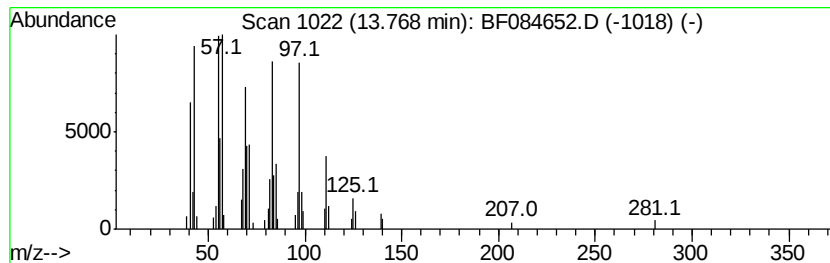
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	3.21 ng	267186	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	94
2	2- Chloropropionic acid, octadec...		360	C21H41ClO2	088104-31-8	94
3	Trichloroacetic acid, pentadecyl...		372	C17H31Cl3O2	074339-53-0	93
4	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	93
5	5-Eicosene, (E)-		280	C20H40	074685-30-6	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.19	5.2	ng	271288	1	6.73	1036270	20.0
2-Pentanone, 4-hy...	4.89	68.9	ng	3568080	1	6.73	1036270	20.0
2-Pentanone, 4-me...	5.72	4.1	ng	213123	1	6.73	1036270	20.0
unknown6.49	6.49	85.0	ng	4406370	1	6.73	1036270	20.0
1-Docosene	13.77	3.2	ng	267186	5	13.87	1663490	20.0