

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020817\
 Data File : BF092865.D
 Acq On : 8 Feb 2017 20:46
 Operator : SJ/MA
 Sample : I1741-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 020617-PR-E-U-M

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-BF013017.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	4.407	201	203	214	rVB	169868	232465	5.42%	0.813%
2	5.059	258	260	263	rBV	996483	1061115	24.75%	3.711%
3	5.493	295	298	300	rBV	1058302	1018421	23.75%	3.562%
4	5.893	331	333	335	rBV	187004	168286	3.92%	0.589%
5	6.522	386	388	394	rVB2	792505	751367	17.52%	2.628%
6	6.659	398	400	402	rBV	2334934	1965331	45.83%	6.874%
7	6.887	418	420	423	rBV	828623	823294	19.20%	2.880%
8	7.047	432	434	437	rBV	3218345	2881574	67.20%	10.079%
9	7.459	467	470	472	rBV	2635726	2599718	60.63%	9.093%
10	8.179	530	533	535	rBV	1297812	1171196	27.31%	4.096%
11	9.253	624	627	630	rBV	4514257	4287997	100.00%	14.998%
12	9.642	659	661	663	rBV	58792	66166	1.54%	0.231%
13	9.928	684	686	689	rBV	1367256	1268895	29.59%	4.438%
14	10.362	720	724	726	rBV	103152	101186	2.36%	0.354%
15	10.579	740	743	746	rBV	31229	44187	1.03%	0.155%
16	10.716	753	755	758	rBV2	1397018	1558389	36.34%	5.451%
17	10.831	763	765	770	rVB	126642	152787	3.56%	0.534%
18	11.276	803	804	810	rVB	67427	100792	2.35%	0.353%
19	11.413	814	816	819	rBV	1327232	1258763	29.36%	4.403%
20	13.002	952	955	958	rBV	3674367	4233111	98.72%	14.806%
21	13.905	1031	1034	1043	rBV	44292	114505	2.67%	0.400%
22	14.054	1044	1047	1049	rBV	1459012	1322313	30.84%	4.625%
23	15.505	1170	1174	1178	rBV	777253	1196226	27.90%	4.184%
24	15.940	1209	1212	1217	rBV	41136	62588	1.46%	0.219%
25	16.431	1252	1255	1259	rBV	33340	63507	1.48%	0.222%
26	17.003	1301	1305	1309	rBV	22267	43231	1.01%	0.151%
27	17.677	1362	1364	1370	rVB2	17638	43790	1.02%	0.153%

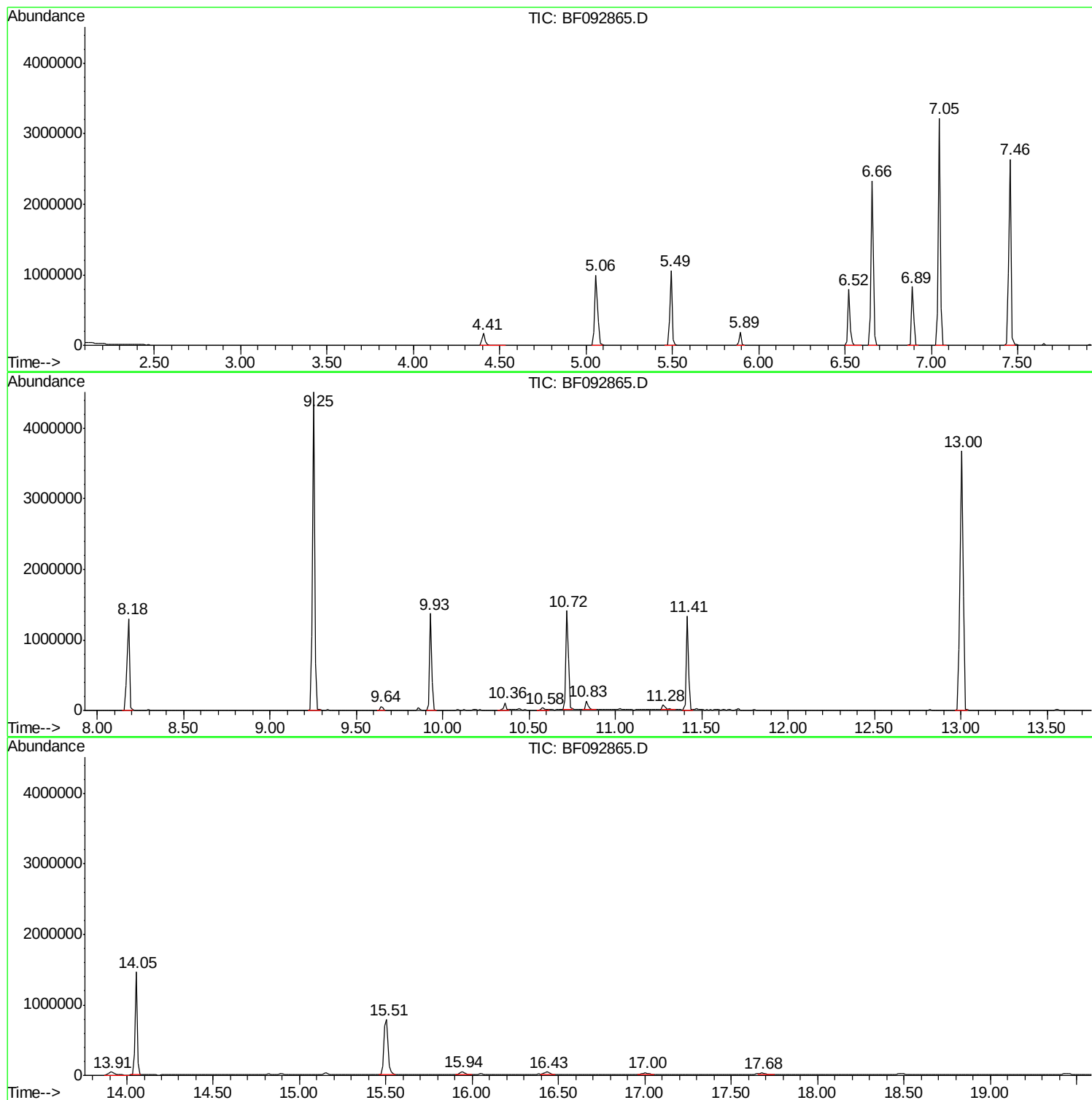
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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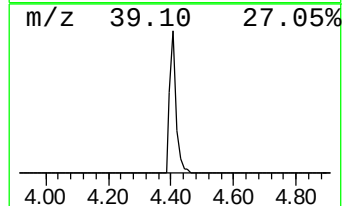
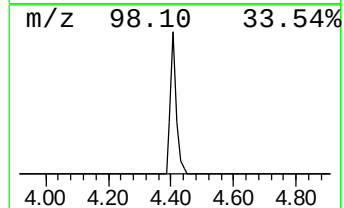
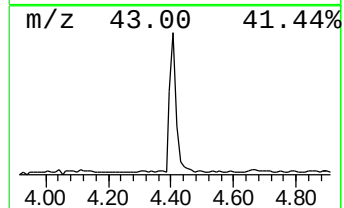
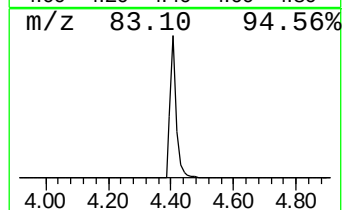
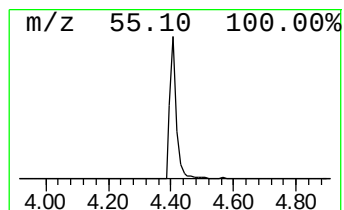
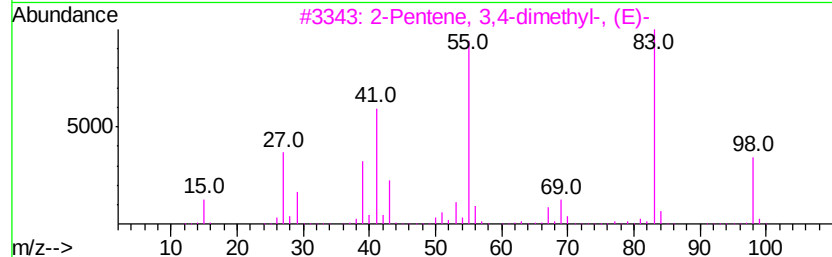
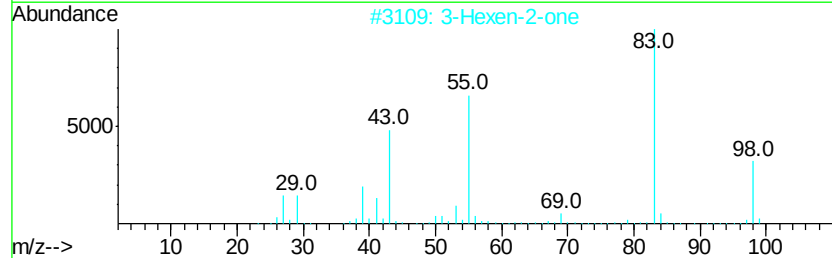
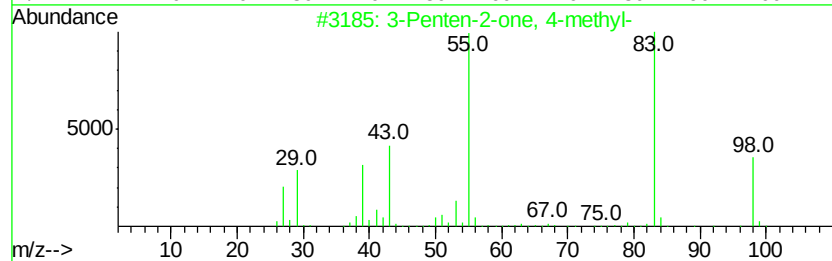
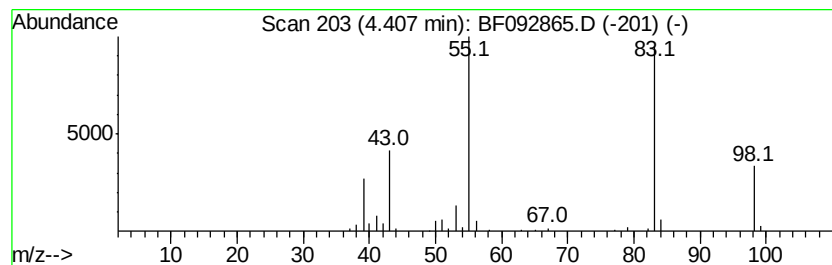
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.41	5.65 ng	232465	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			3-Hexen-2-one	98	C6H10O	000763-93-9	87
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	83
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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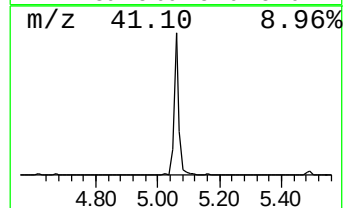
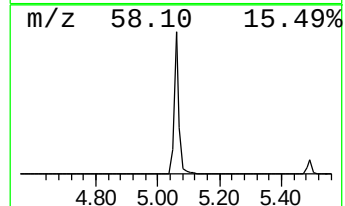
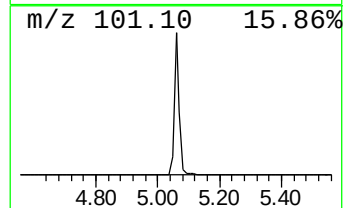
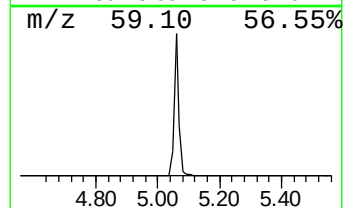
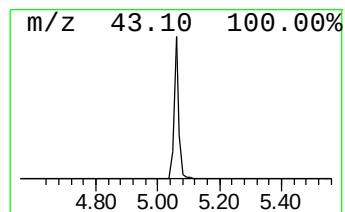
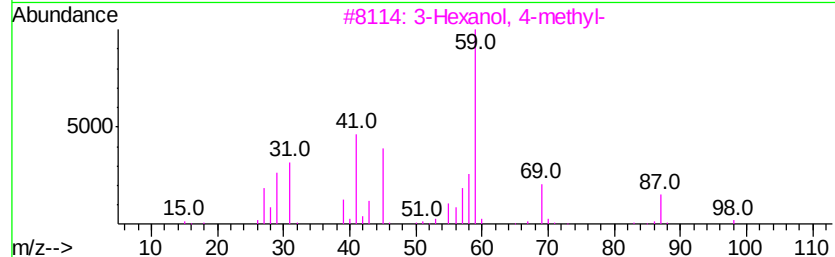
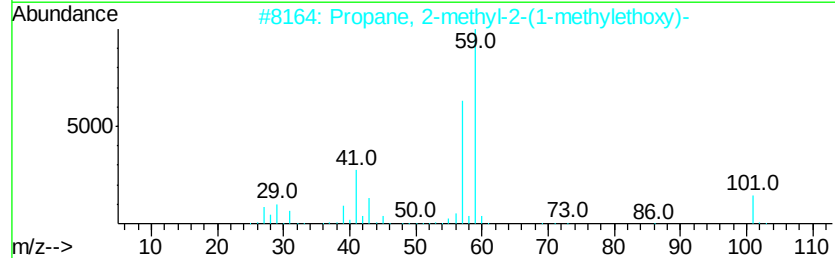
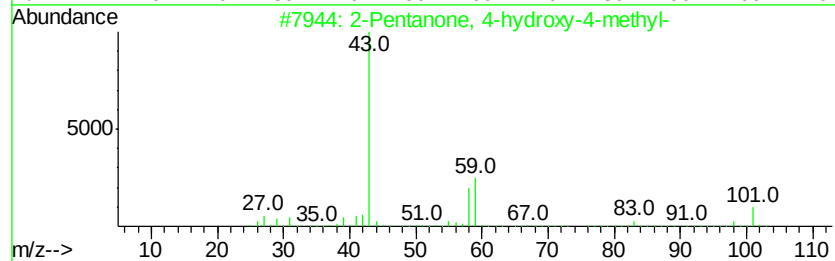
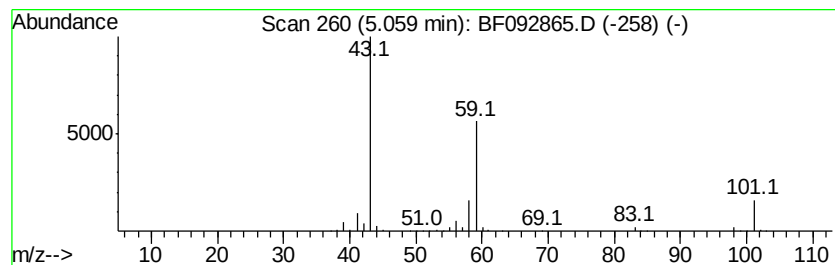
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	25.78 ng	1061120	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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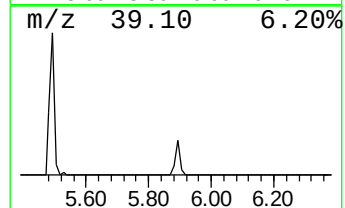
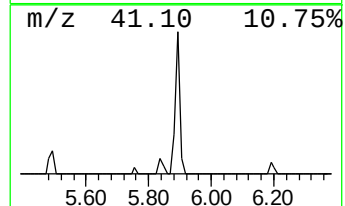
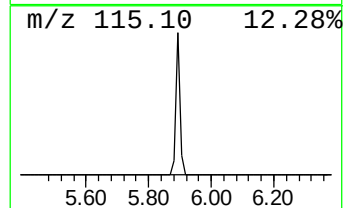
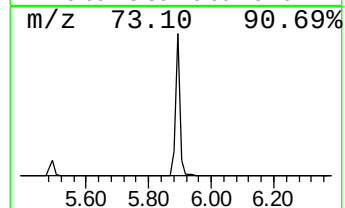
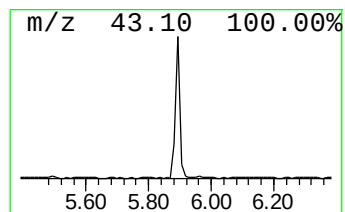
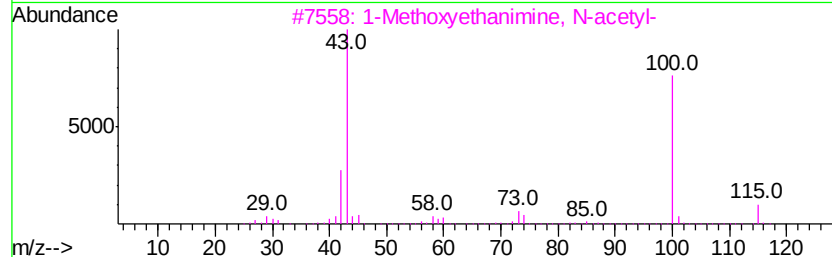
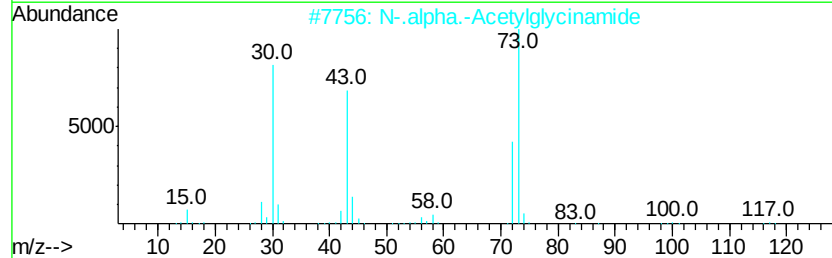
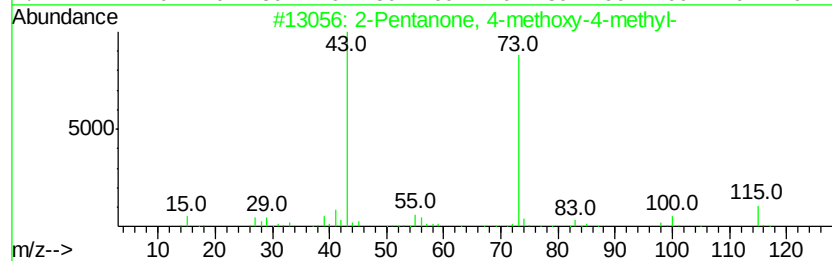
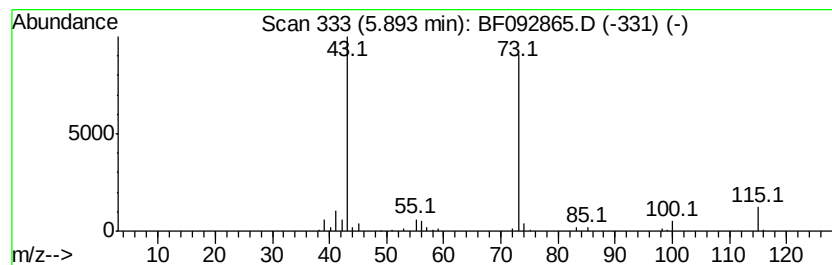
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.09 ng	168286	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglucynamide	116	C4H8N2O2	002620-63-5	38
3			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	28
4			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10



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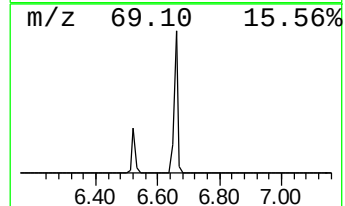
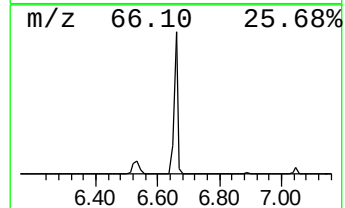
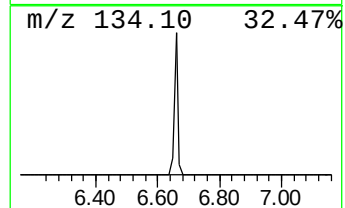
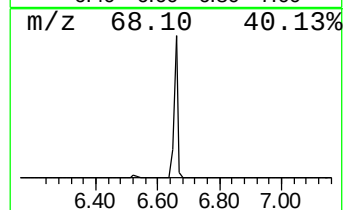
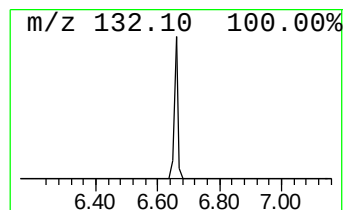
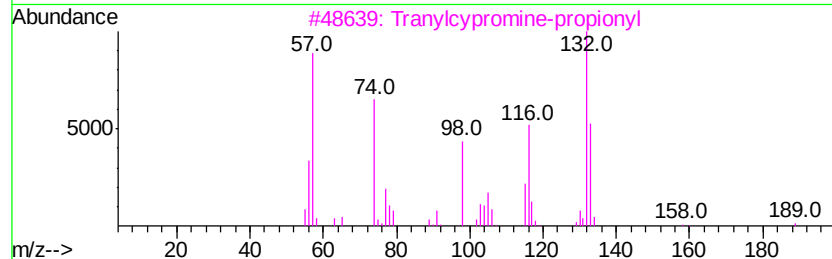
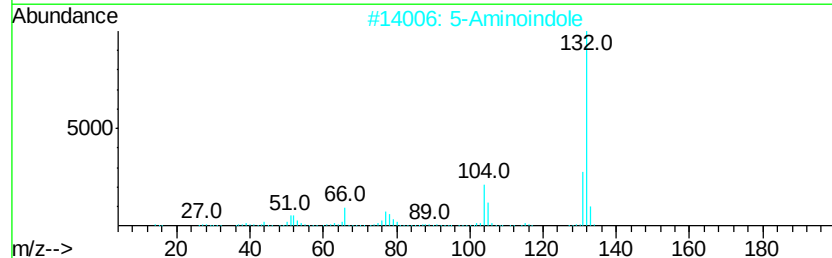
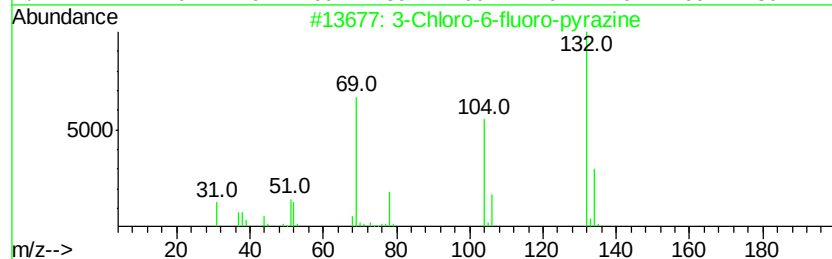
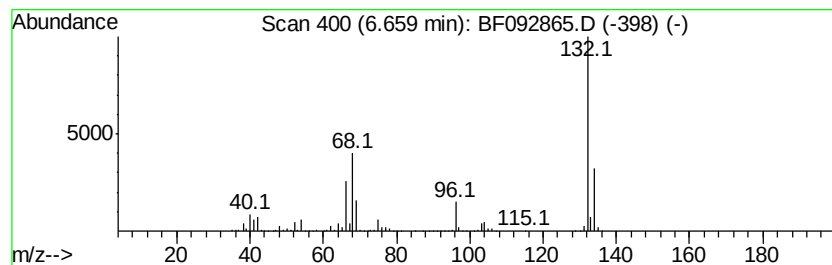
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	47.74 ng	1965330	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	Tranvlcypromine-propionyl			189	C12H15NO	1000123-86-3	10
4	Imidazole, 4,5-dicyano-1-methyl-			132	C6H4N4	019485-35-9	9
5	Benzene, 1,3,5-trifluoro-			132	C6H3F3	000372-38-3	9



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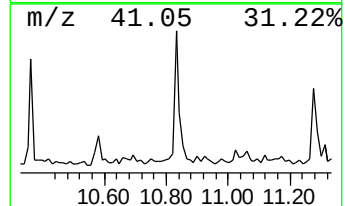
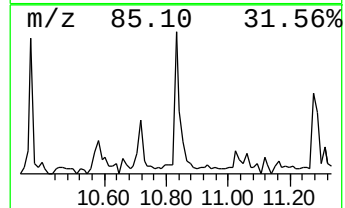
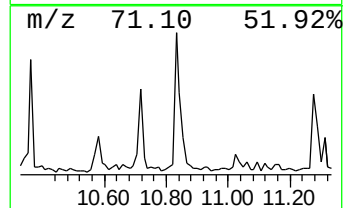
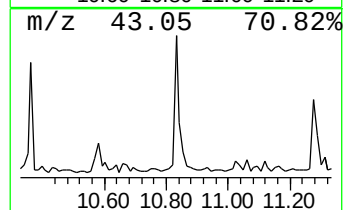
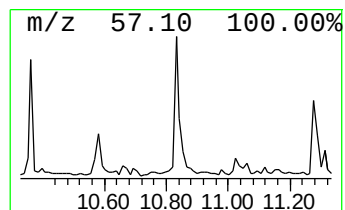
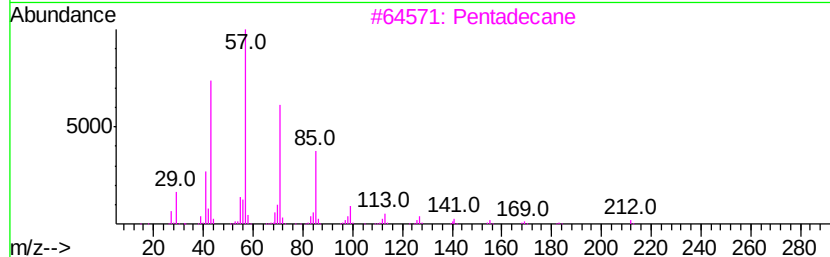
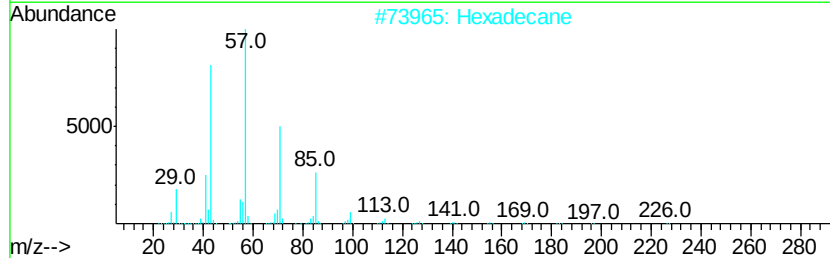
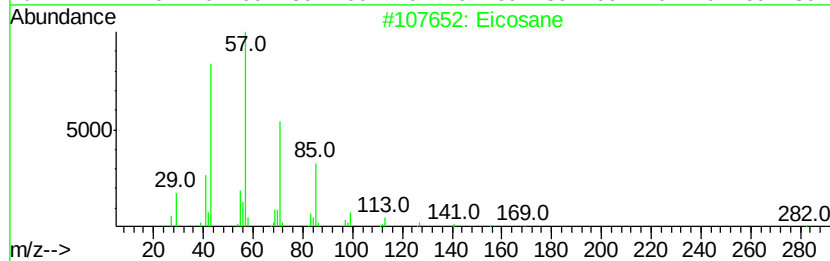
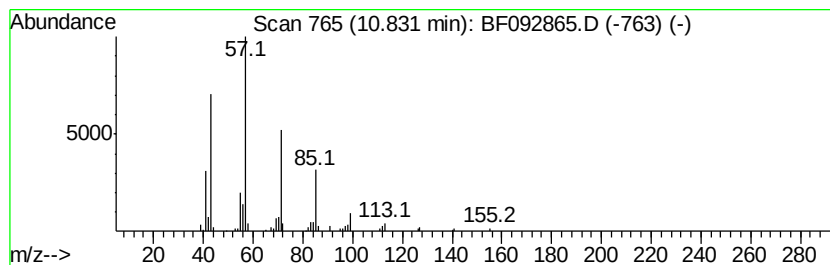
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.		
10.83	2.43 ng	152787	Phenanthrene-d10		11.41		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Hexadecane	226	C16H34	000544-76-3	91
3			Pentadecane	212	C15H32	000629-62-9	90
4			Tetradecane	198	C14H30	000629-59-4	86
5			Tridecane	184	C13H28	000629-50-5	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.41	5.7	ng	232465	1	6.89	823294	20.0
2-Pentanone, 4-hy...	5.06	25.8	ng	1061120	1	6.89	823294	20.0
2-Pentanone, 4-me...	5.89	4.1	ng	168286	1	6.89	823294	20.0
unknown6.66	6.66	47.7	ng	1965330	1	6.89	823294	20.0
Eicosane	10.83	2.4	ng	152787	4	11.41	1258760	20.0