

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101715\
 Data File : BF082321.D
 Acq On : 16 Oct 2015 12:49
 Operator : UM/IZ
 Sample : PB86109BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB86109BL

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-BF101015.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	4.354	191	194	201	rBV	36477	46274	1.86%	0.284%
2	5.017	249	252	255	rBV	698335	990585	39.87%	6.079%
3	5.451	287	290	292	rBV	969361	1393393	56.08%	8.551%
4	5.840	322	324	326	rVB	33876	28826	1.16%	0.177%
5	6.480	378	380	383	rBV	1226332	1274543	51.30%	7.822%
6	6.606	389	391	394	rBV	1210232	1408737	56.70%	8.645%
7	6.846	409	412	414	rBV	251915	349501	14.07%	2.145%
8	6.994	423	425	428	rBV	1342354	1170781	47.12%	7.185%
9	7.406	459	461	464	rBV	775089	819774	33.00%	5.031%
10	8.126	522	524	527	rBV	479978	467003	18.80%	2.866%
11	9.212	616	619	621	rBV	1672865	1890032	76.07%	11.599%
12	9.818	669	672	676	rBV	59153	95115	3.83%	0.584%
13	9.886	676	678	680	rBV	687028	600115	24.15%	3.683%
14	10.675	745	747	750	rBV	1151916	1212646	48.81%	7.442%
15	11.372	806	808	811	rBV	713955	634709	25.55%	3.895%
16	11.898	851	854	856	rBV	43725	63703	2.56%	0.391%
17	12.686	920	923	928	rBV	20984	33395	1.34%	0.205%
18	12.984	946	949	951	rBV	1905541	2484511	100.00%	15.247%
19	14.104	1045	1047	1050	rBV	677632	703383	28.31%	4.317%
20	15.692	1183	1186	1189	rBV	472001	601980	24.23%	3.694%
21	15.738	1189	1190	1194	rVB	18498	25630	1.03%	0.157%

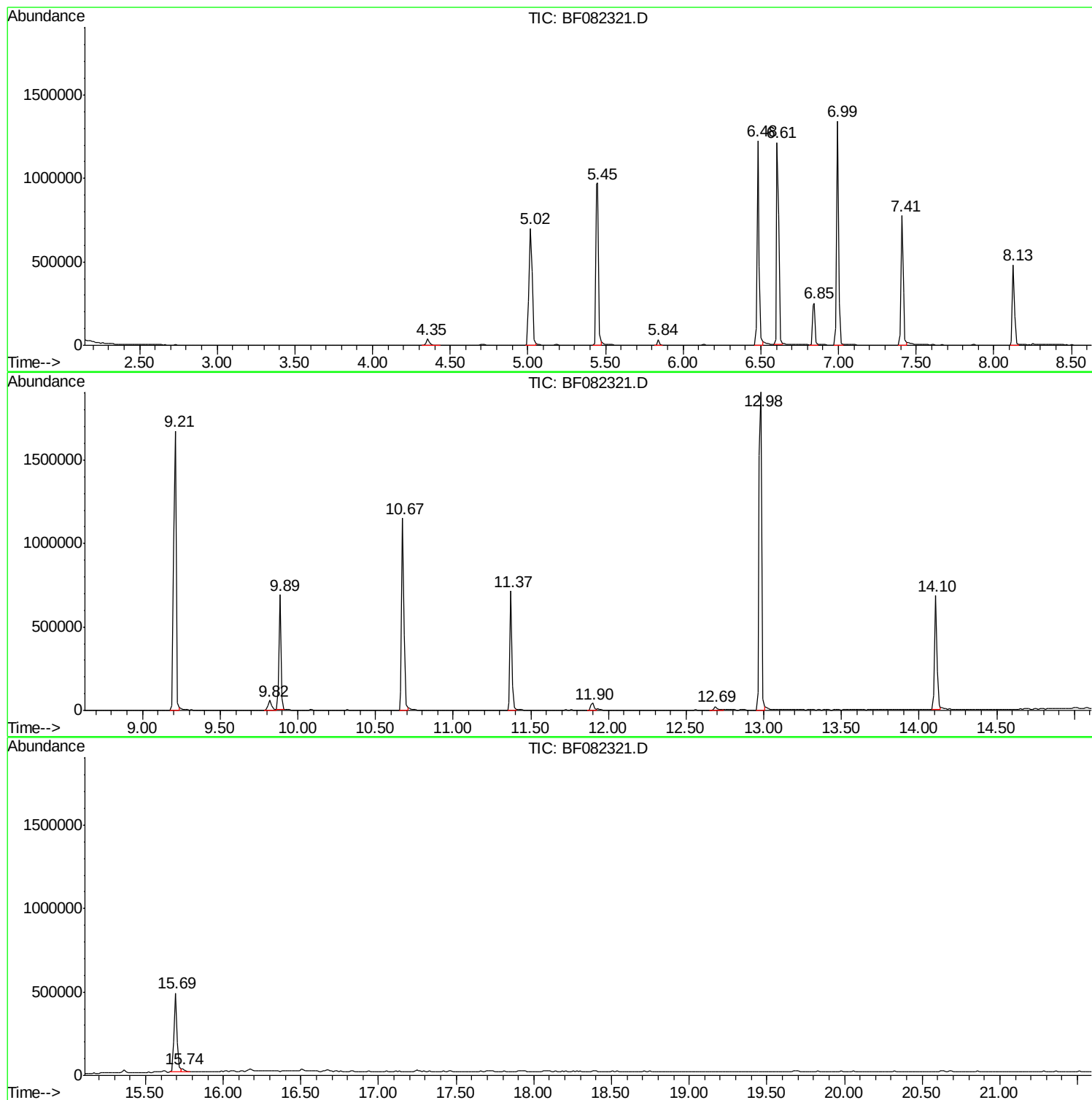
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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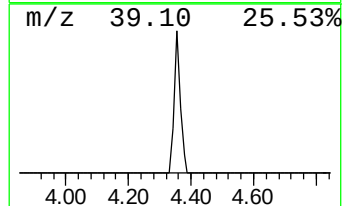
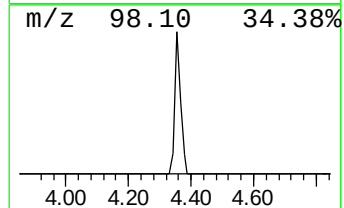
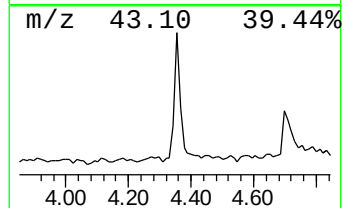
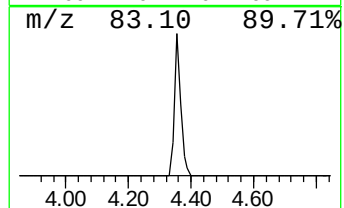
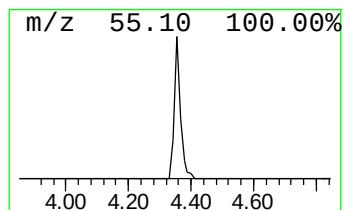
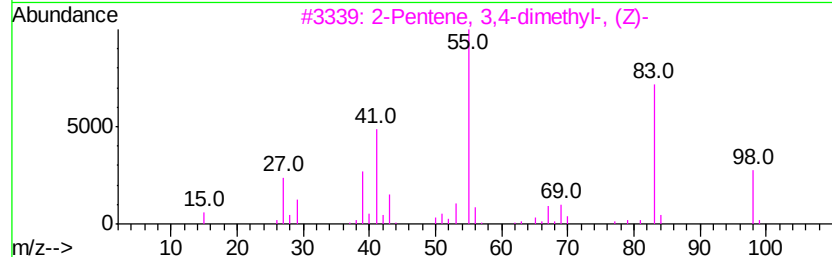
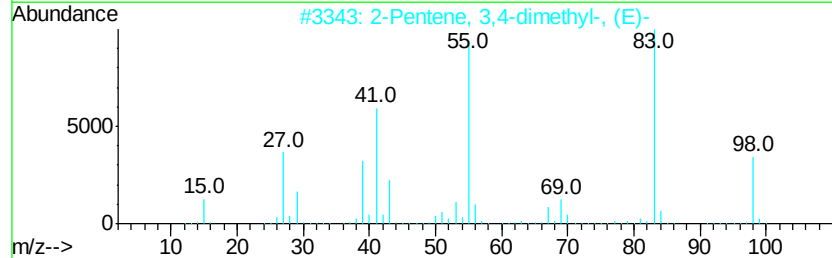
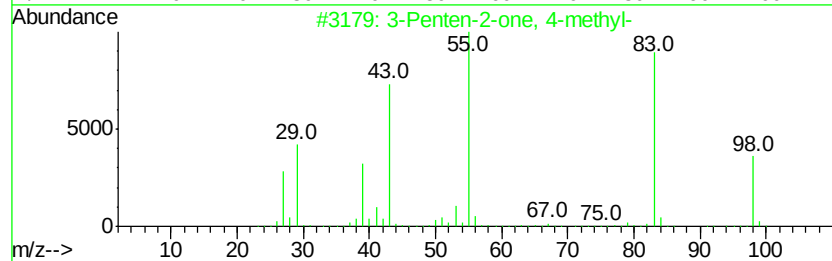
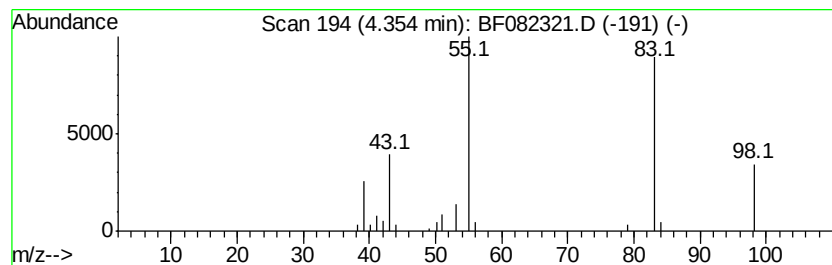
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.35	2.65 ng	46274	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
4		3-Hexen-2-one	98	C6H10O	000763-93-9	80
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72



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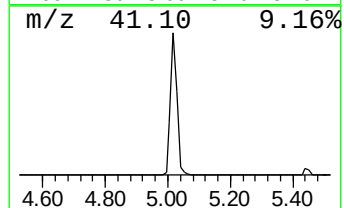
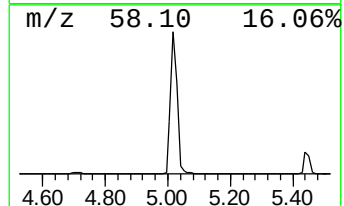
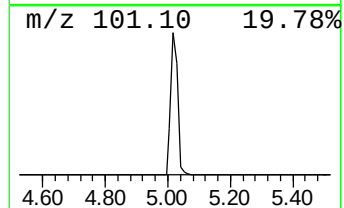
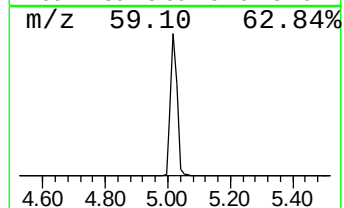
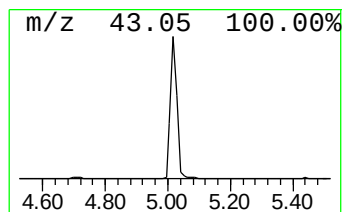
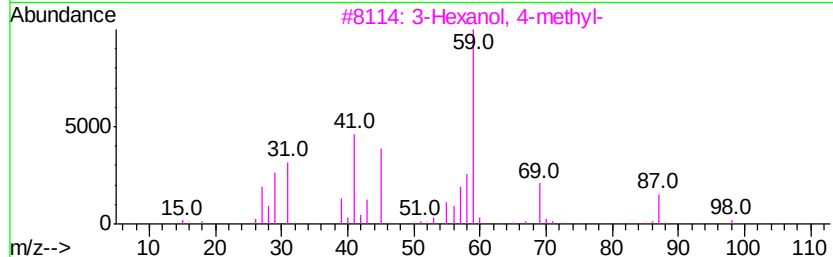
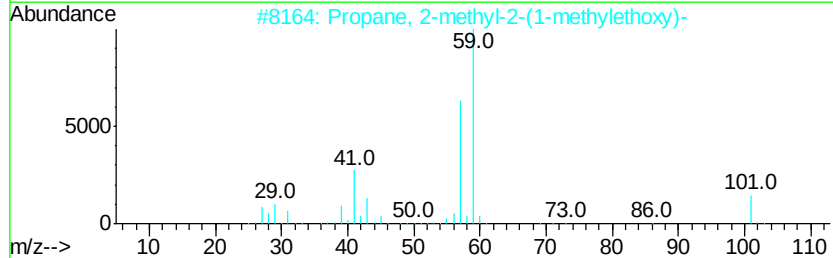
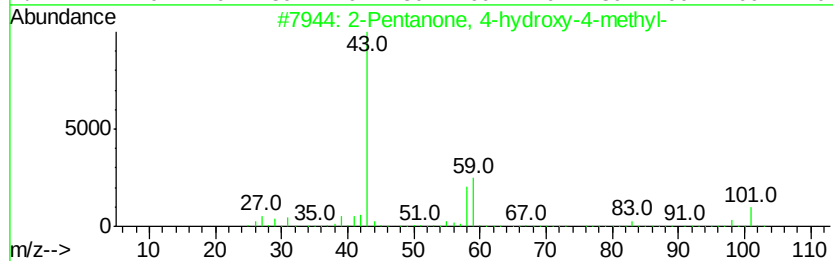
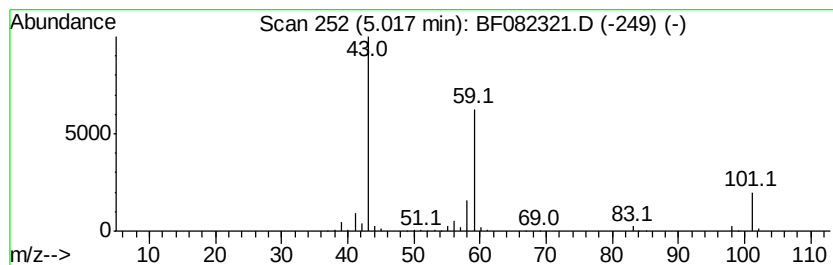
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	56.69 ng	990585	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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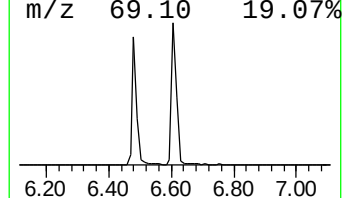
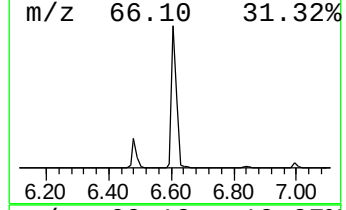
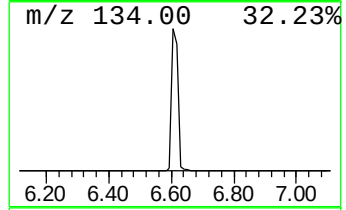
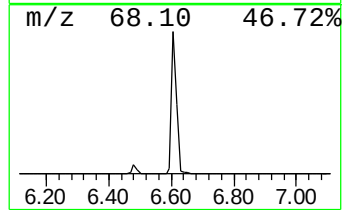
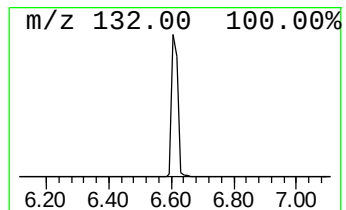
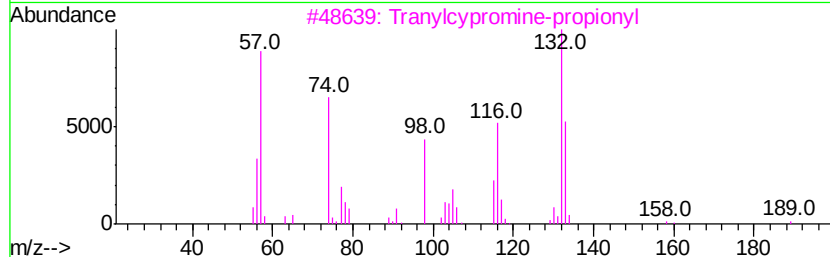
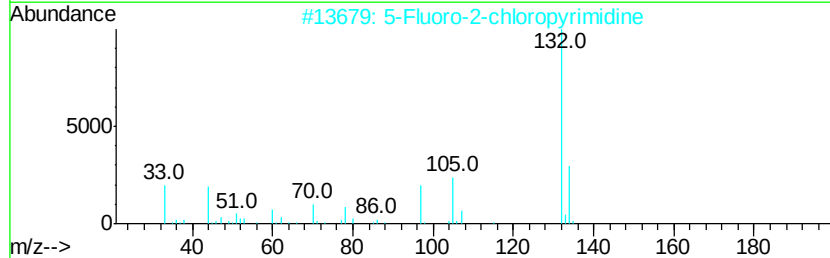
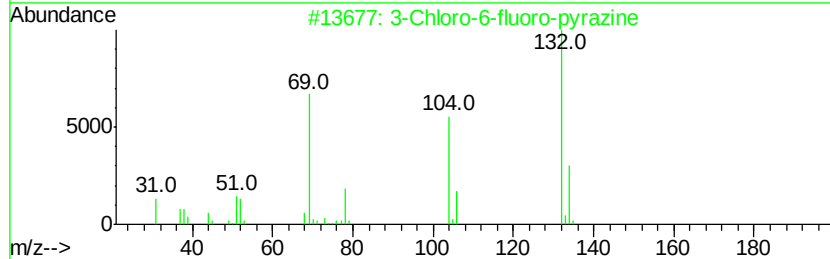
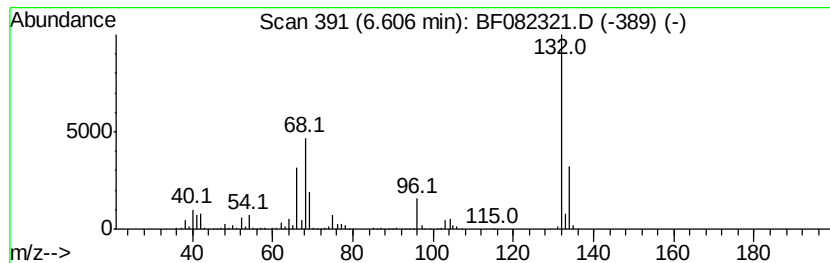
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Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	80.61 ng	1408740	1,4-Dichlorobenzene-d4	6.85

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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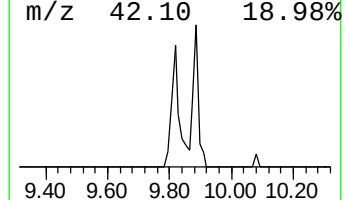
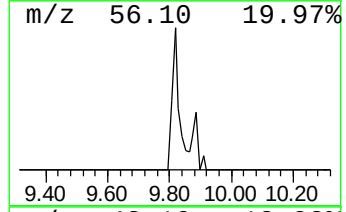
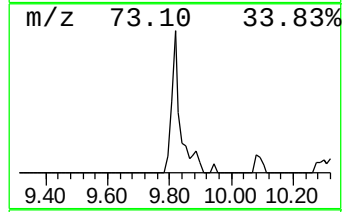
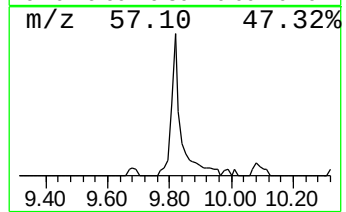
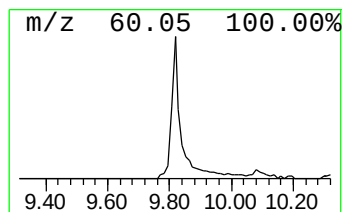
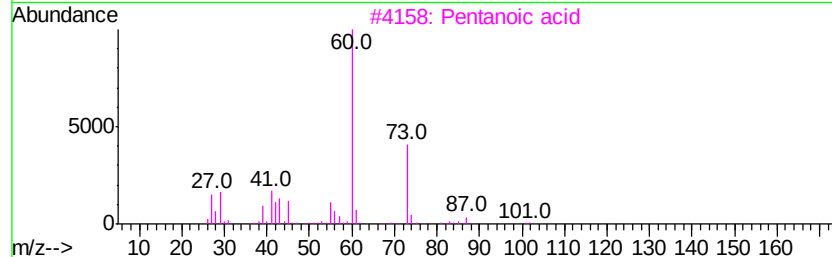
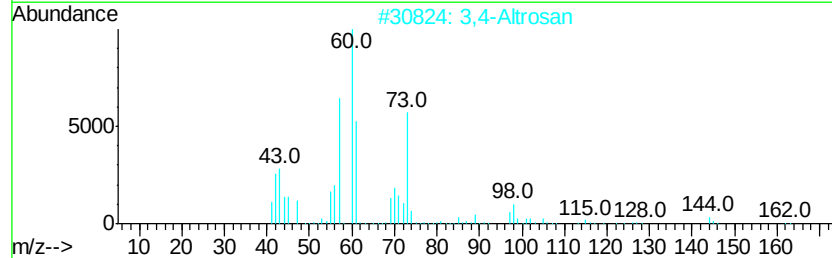
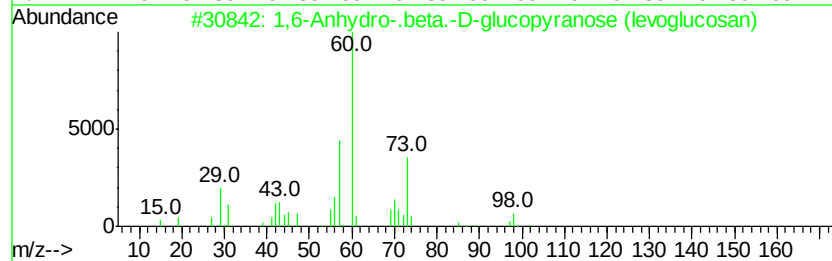
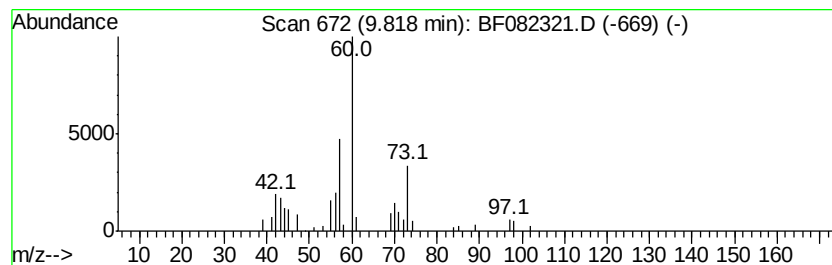
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Peak Number 5 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	3.17 ng	95115	Acenaphthene-d10	9.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	72
2		3,4-Altrosan	162	C6H10O5	1000129-76-4	59
3		Pentanoic acid	102	C5H10O2	000109-52-4	47
4		Heptanoic acid	130	C7H14O2	000111-14-8	42
5		Ethyl .beta.-d-ribose	178	C7H14O5	1000126-95-4	33



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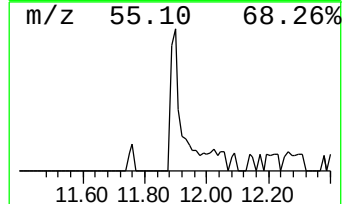
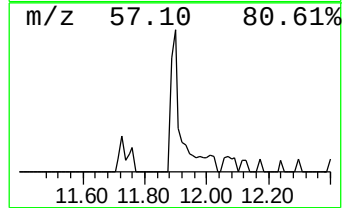
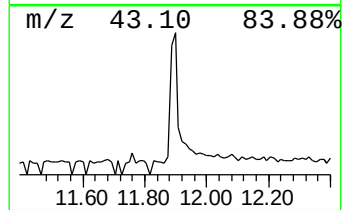
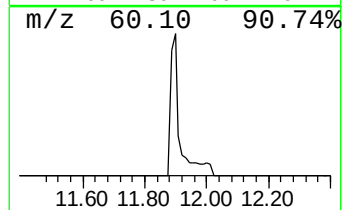
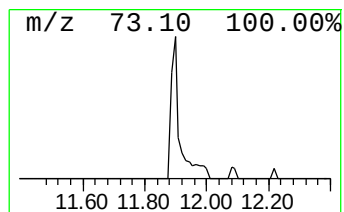
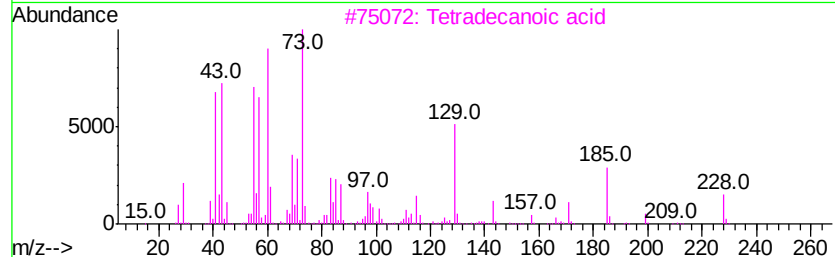
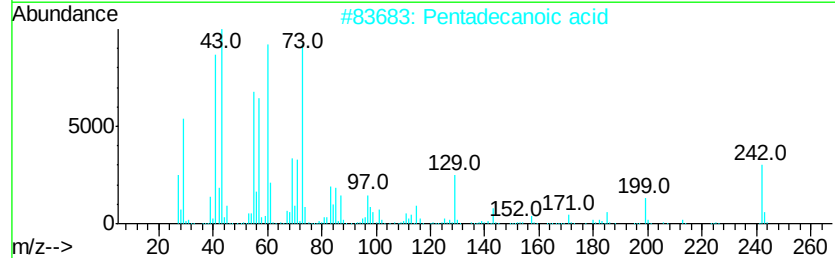
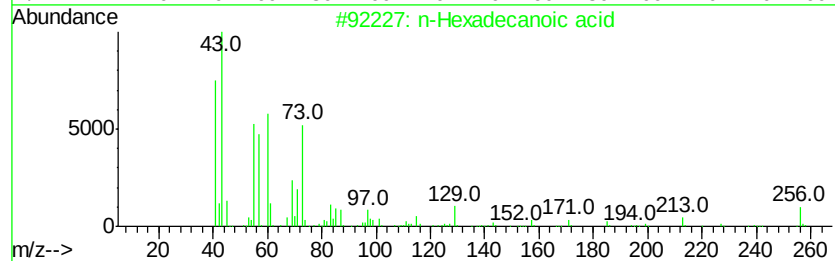
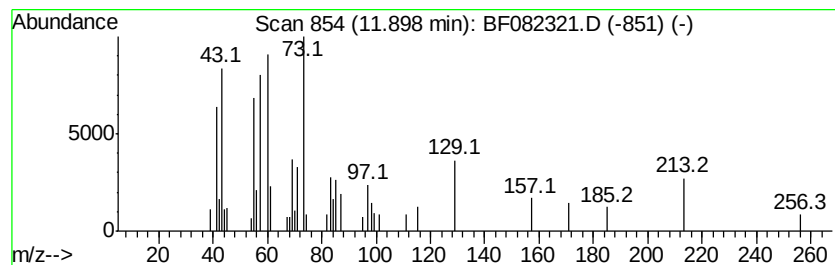
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.01 ng	63703	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.35	2.6	ng	46274	1	6.85	349501	20.0
2-Pentanone, 4-hy...	5.02	56.7	ng	990585	1	6.85	349501	20.0
unknown6.61	6.61	80.6	ng	1408740	1	6.85	349501	20.0
1,6-Anhydro-.beta...	9.82	3.2	ng	95115	3	9.89	600115	20.0
n-Hexadecanoic acid	11.90	2.0	ng	63703	4	11.37	634709	20.0