LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF033016\
Data File : BF085885.D
Acq On : 30 Mar 2016 14:43
Operator : UM/SJ
Sample : PB89280BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB89280BL

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-BF032416.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	3.281	84	87	100	rBV	148072	294412	10.75%	1.315%
2	3.704	121	124	131	rVB	18061	36117	1.32%	0.161%
3	4.298	173	176	188	rBV	805809	1136180	41.48%	5.073%
4	4.973	232	235	237	rBV	814690	1047216	38.24%	4.676%
5	5.396	270	272	285	rBV	1610741	1566811	57.21%	6.996%
6	5.796	305	307	310	rBV	43528	50522	1.84%	0.226%
7	6.436	360	363	365	rBV	1635642	1676241	61.20%	7.485%
8	6.561	372	374	377	rBV	1897092	1630241	59.52%	7.280%
9	6.790	392	394	397	rBV	471638	600911	21.94%	2.683%
10	6.950	406	408	411	rBV	2091383	1853156	67.66%	8.275%
11	7.362	442	444	447	rBV	1461357	1416068	51.70%	6.323%
12	7.522	457	458	467	rVB2	70380	117410	4.29%	0.524%
13	8.082	505	507	510	rBV	952647	825186	30.13%	3.685%
14	8.219	516	519	524	rBV	20086	33473	1.22%	0.149%
15	9.156	598	601	604	rBV	2213411	2689978	98.22%	12.012%
16	9.785	652	656	658	rBV	228763	374545	13.68%	1.672%
17	9.830	658	660	663	rVB	639763	878488	32.08%	3.923%
18	10.253	695	697	705	rBV	20777	42976	1.57%	0.192%
19	10.619	727	729	732	rBV2	891137	1160155	42.36%	5.180%
20	11.316	788	790	793	rBV	959114	895169	32.68%	3.997%
21	12.905	926	929	931	rBV	2957429	2738781	100.00%	12.230%
22	13.956	1018	1021	1023	rBV	889345	807441	29.48%	3.605%
23	15.374	1142	1145	1150	rBV	354708	523382	19.11%	2.337%

Sum of corrected areas: 22394859

LSC Report - Integrated Chromatogram

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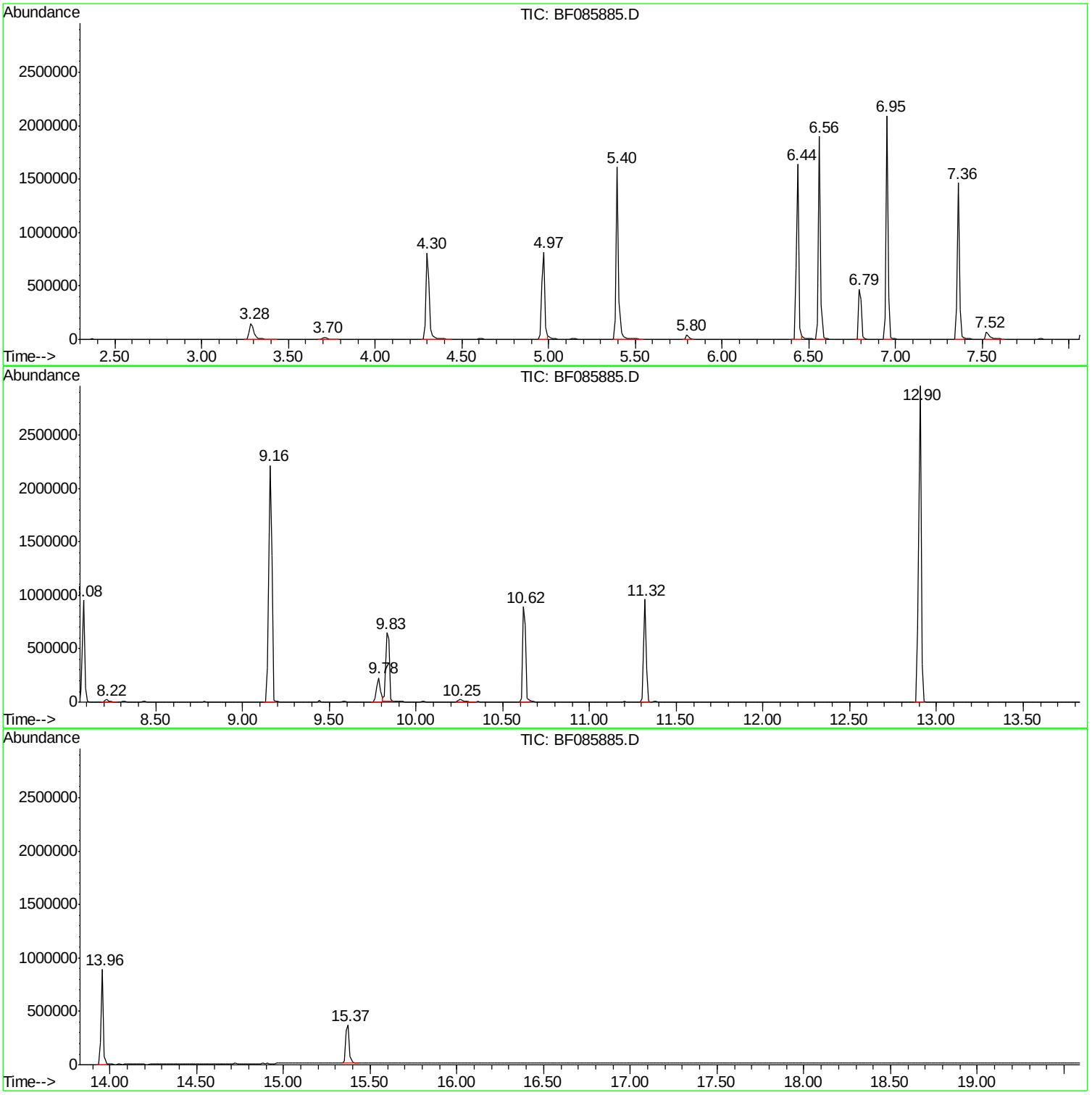
Instrument : BNA_F
ClientSampleId : PB89280BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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Operator : UM/SJ
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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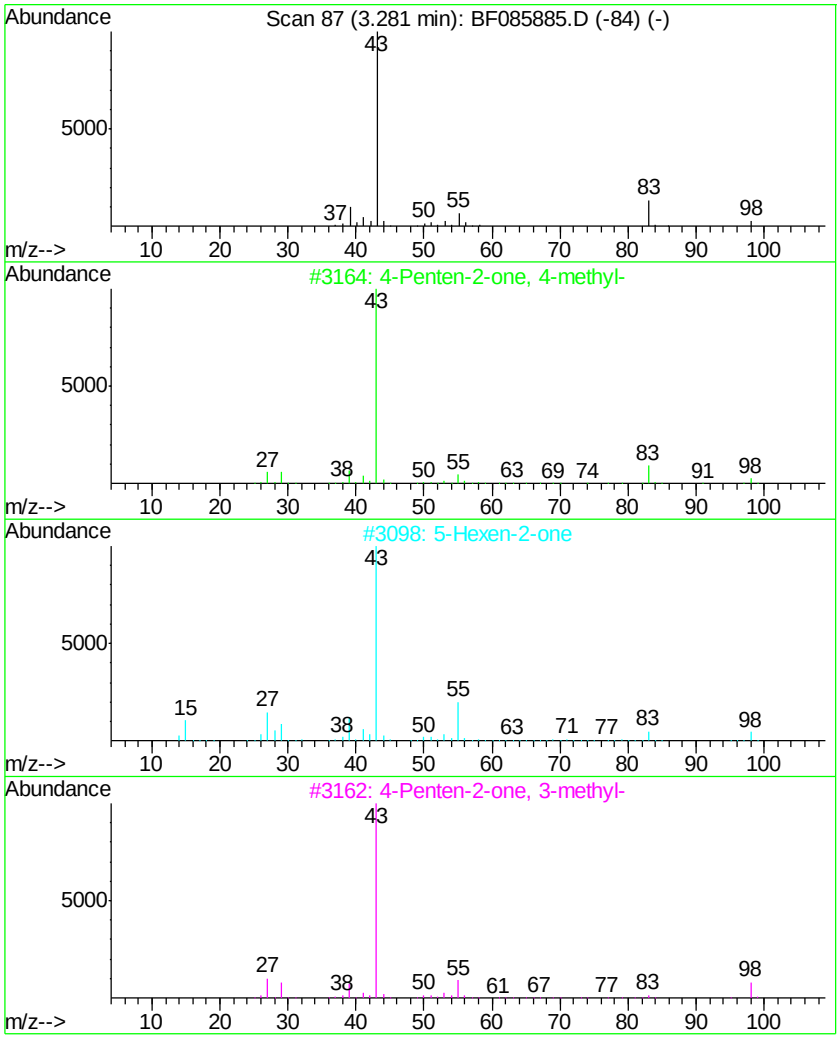
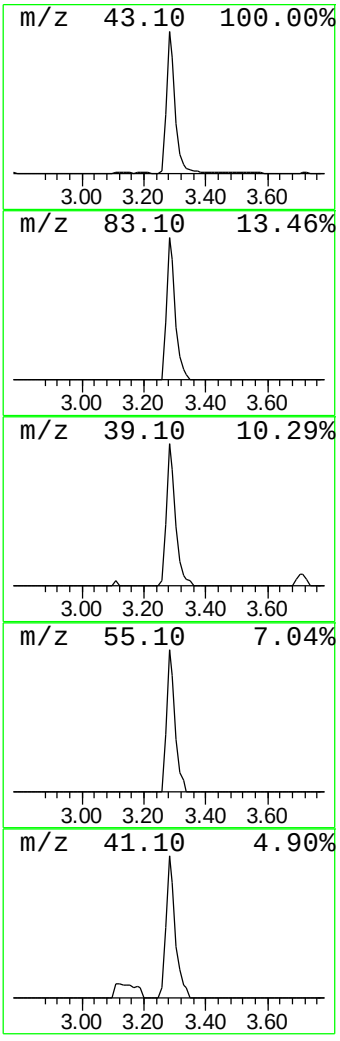
Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	9.80 ng	294412	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	5-Hexen-2-one	98	C6H10O	000109-49-9	50
3	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	47
4	2-Vinylethyl acetate	114	C6H10O2	001576-84-7	23
5	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	16





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Data File : BF085885.D
Acq On : 30 Mar 2016 14:43
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Sample : PB89280BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB89280BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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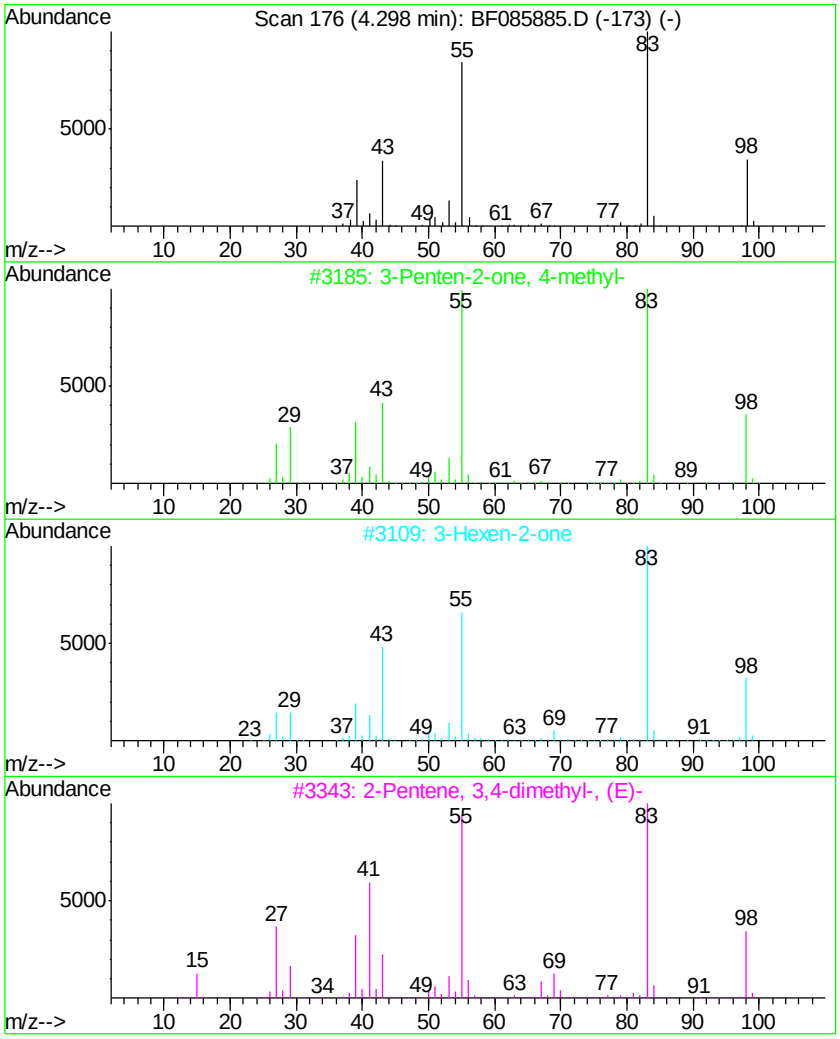
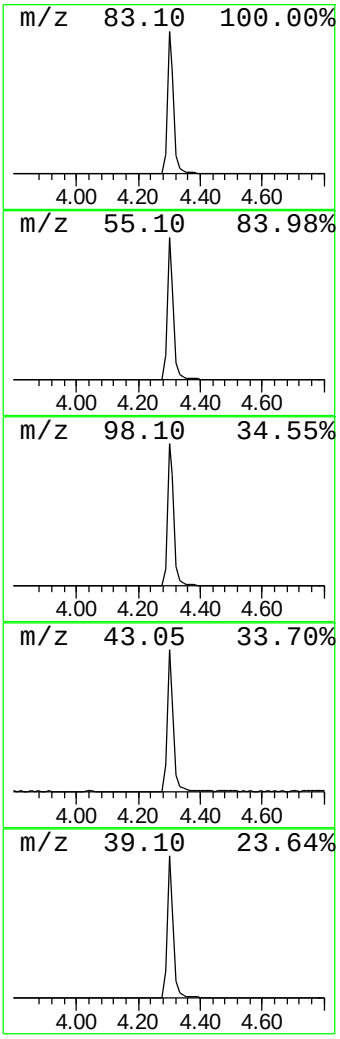
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	37.82 ng	1136180	1,4-Dichlorobenzene-d4	6.80

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	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80





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Data File : BF085885.D
Acq On : 30 Mar 2016 14:43
Operator : UM/SJ
Sample : PB89280BL
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB89280BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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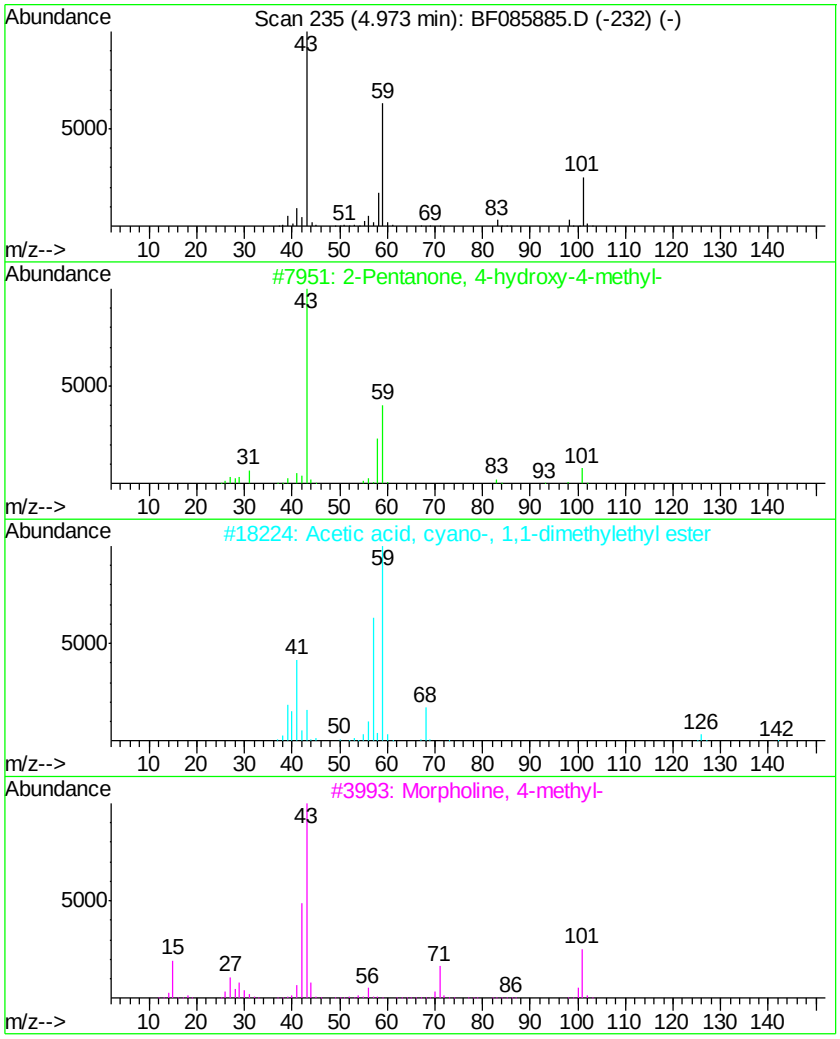
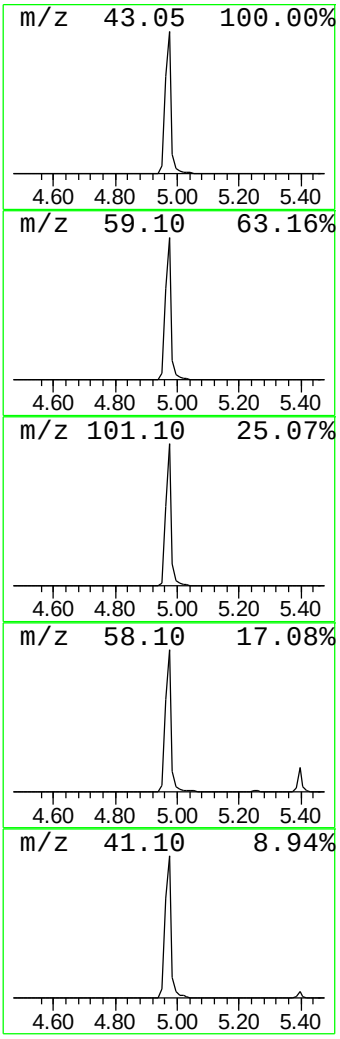
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	34.85 ng	1047220	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Sample : PB89280BL
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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB89280BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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TIC Integration Parameters: LSCINT.P

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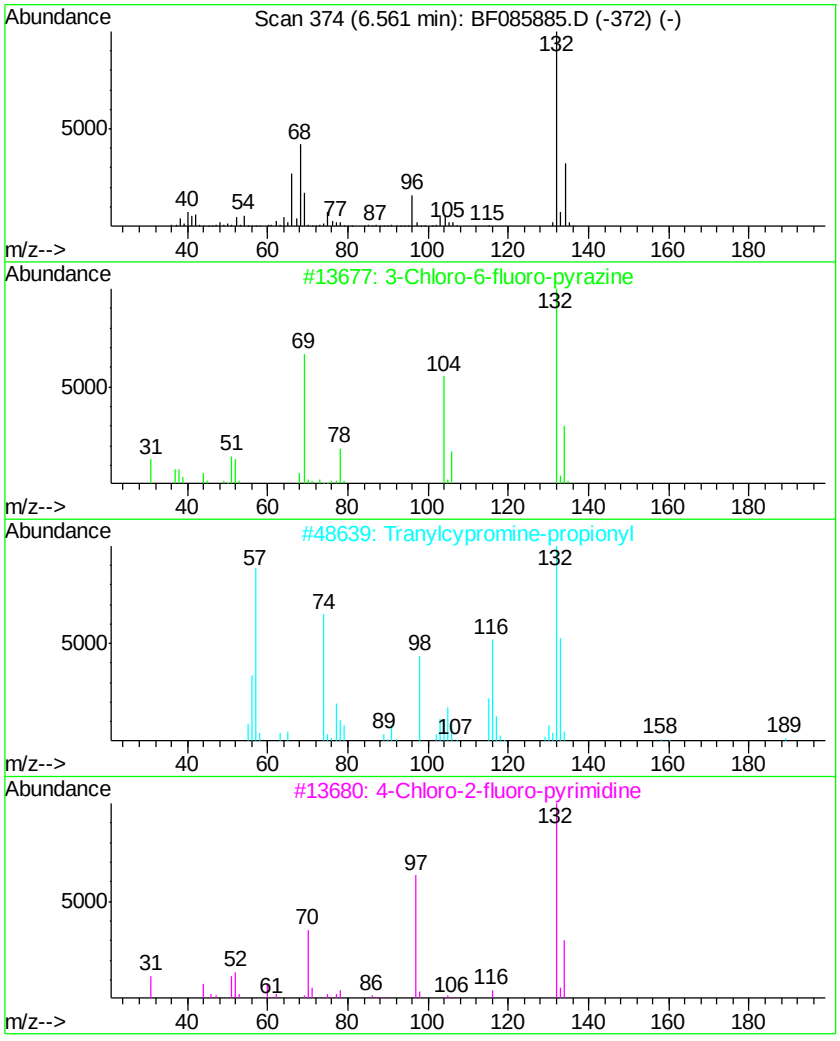
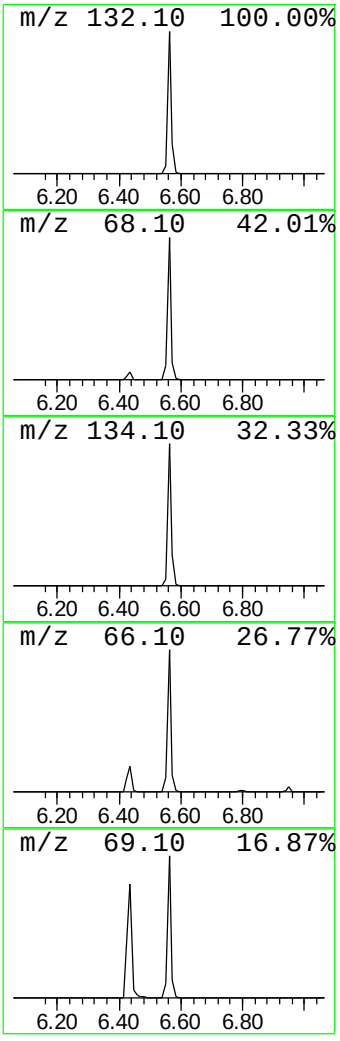
Peak Number 4 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	54.26 ng	1630240	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Misc :
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Instrument : BNA_F
ClientSampleId : PB89280BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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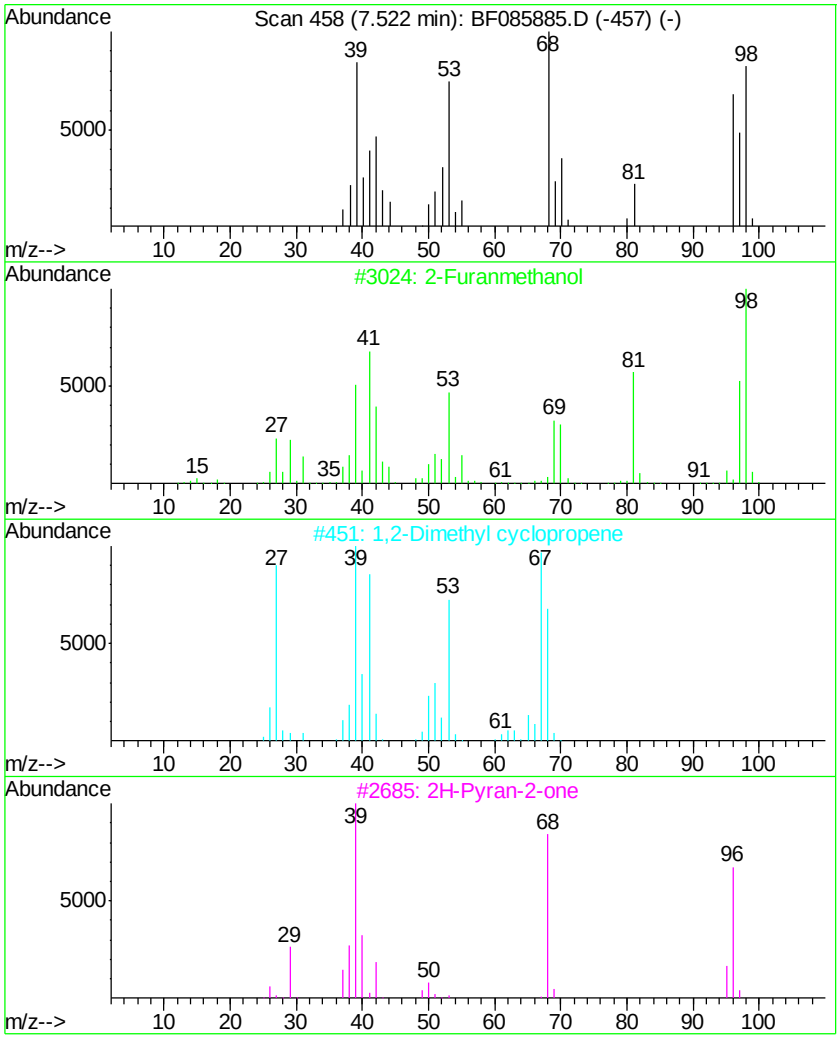
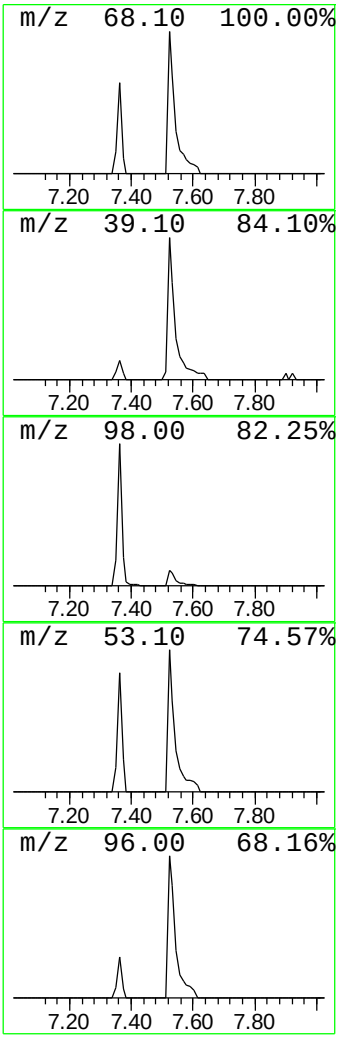
Peak Number 6 2-Furanmethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.52	2.85 ng	117410	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furanmethanol	98	C5H6O2	000098-00-0	70
2	1,2-Dimethyl cyclopropene	68	C5H8	014309-32-1	50
3	2H-Pyran-2-one	96	C5H4O2	000504-31-4	45
4	1,2-Butadiene, 3-methyl-	68	C5H8	000598-25-4	35
5	Bicyclo[3.1.0]hexan-3-one	96	C6H8O	001755-04-0	35





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
4-Penten-2-one, 4...	3.28	9.8	ng	294412	1	6.80	600911	20.0
3-Penten-2-one, 4...	4.30	37.8	ng	1136180	1	6.80	600911	20.0
2-Pentanone, 4-hy...	4.97	34.9	ng	1047220	1	6.80	600911	20.0
unknown6.56	6.56	54.3	ng	1630240	1	6.80	600911	20.0
2-Furanmethanol	7.52	2.9	ng	117410	2	8.08	825186	20.0