LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085434.D
Acq On : 14 Mar 2016 17:42
Operator : UM/SJ
Sample : H1757-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-STOCKPICE-COMP1

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-BF030316.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	2.870	49	51	55	rVB	136294	181751	2.90%	0.380%
2	3.636	115	118	122	rBV	79035	134346	2.15%	0.281%
3	4.516	192	195	198	rBV	391003	450189	7.19%	0.941%
4	5.144	247	250	258	rVB	506403	905595	14.47%	1.892%
5	5.556	282	286	288	rBV	3401349	5009739	80.03%	10.467%
6	6.562	371	374	377	rVB	3462580	3953953	63.17%	8.261%
7	6.699	383	386	388	rBV	4460074	4779327	76.35%	9.986%
8	6.927	404	406	408	rBV	1116820	1083808	17.31%	2.264%
9	7.087	417	420	422	rBV	3690858	4316415	68.96%	9.018%
10	7.487	452	455	458	rBV	2652223	3349484	53.51%	6.998%
11	7.933	491	494	498	rBV3	50921	75600	1.21%	0.158%
12	8.207	516	518	522	rBV2	1650555	2152497	34.39%	4.497%
13	8.916	578	580	583	rBV	123560	140876	2.25%	0.294%
14	9.019	587	589	591	rBV	108382	92163	1.47%	0.193%
15	9.293	609	613	615	rBV	4844544	6259712	100.00%	13.079%
16	9.968	669	672	673	rVV	1536470	1543806	24.66%	3.225%
17	9.990	673	674	676	rVB	140745	158854	2.54%	0.332%
18	10.162	687	689	692	rBV	115695	128635	2.05%	0.269%
19	10.505	718	719	722	rVB2	61851	71136	1.14%	0.149%
20	10.756	738	741	744	rBV	3194990	3361109	53.69%	7.022%
21	11.008	760	763	769	rVB2	45597	118273	1.89%	0.247%
22	11.453	799	802	803	rBV	1349899	1507942	24.09%	3.151%
23	11.968	845	847	849	rBV	124708	126033	2.01%	0.263%
24	12.756	914	916	923	rBV	145967	159282	2.54%	0.333%
25	13.042	938	941	943	rBV	4857162	5361259	85.65%	11.201%
26	14.082	1030	1032	1035	rBV	867259	891000	14.23%	1.862%
27	15.545	1156	1160	1162	rBV	567946	860702	13.75%	1.798%
28	15.717	1169	1175	1177	rBV	191902	689109	11.01%	1.440%

Sum of corrected areas: 47862595

LSC Report - Integrated Chromatogram

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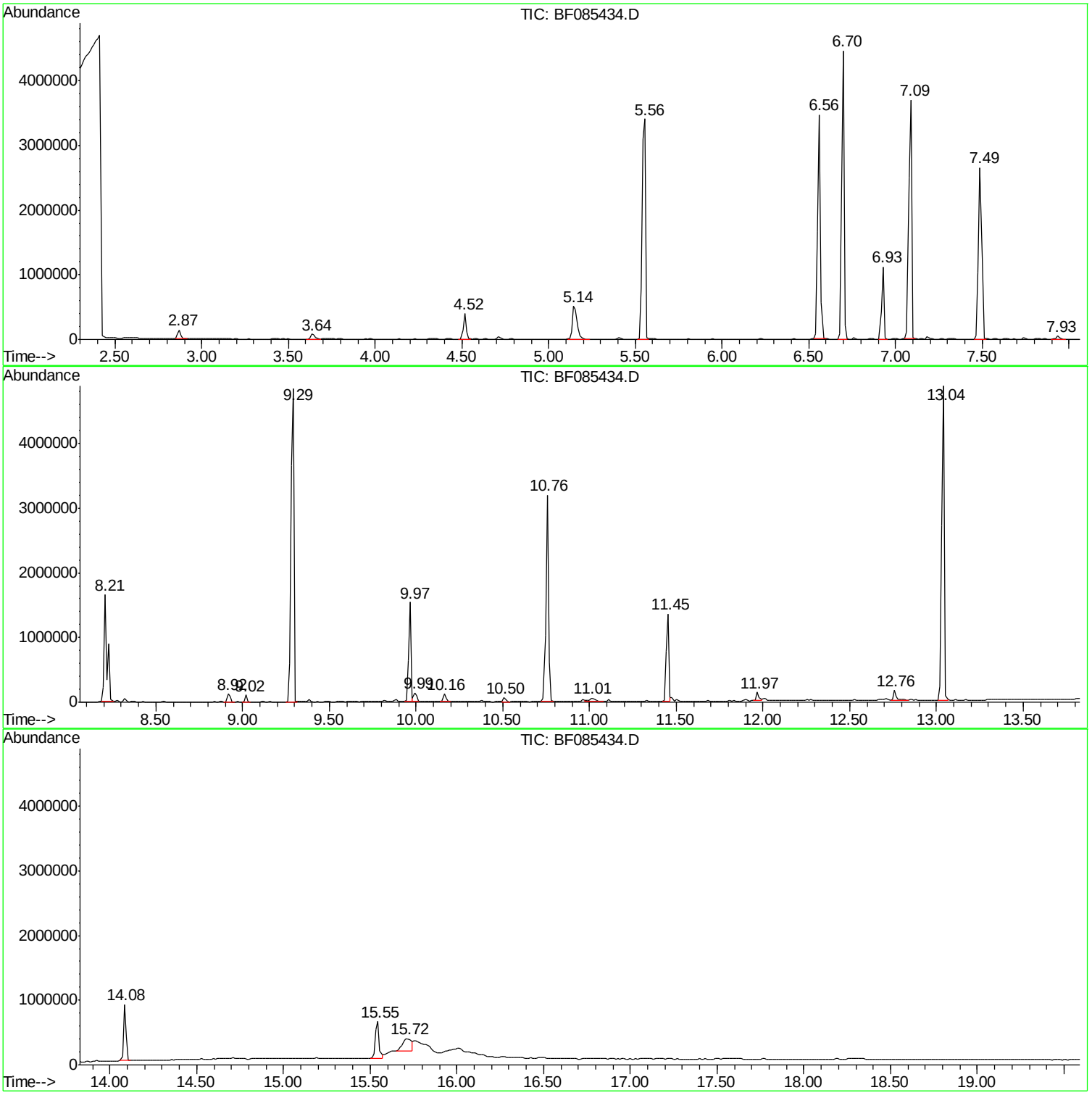
Sample : H1757-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-STOCKPICE-COMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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Data File : BF085434.D
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Operator : UM/SJ
Sample : H1757-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-STOCKPICE-COMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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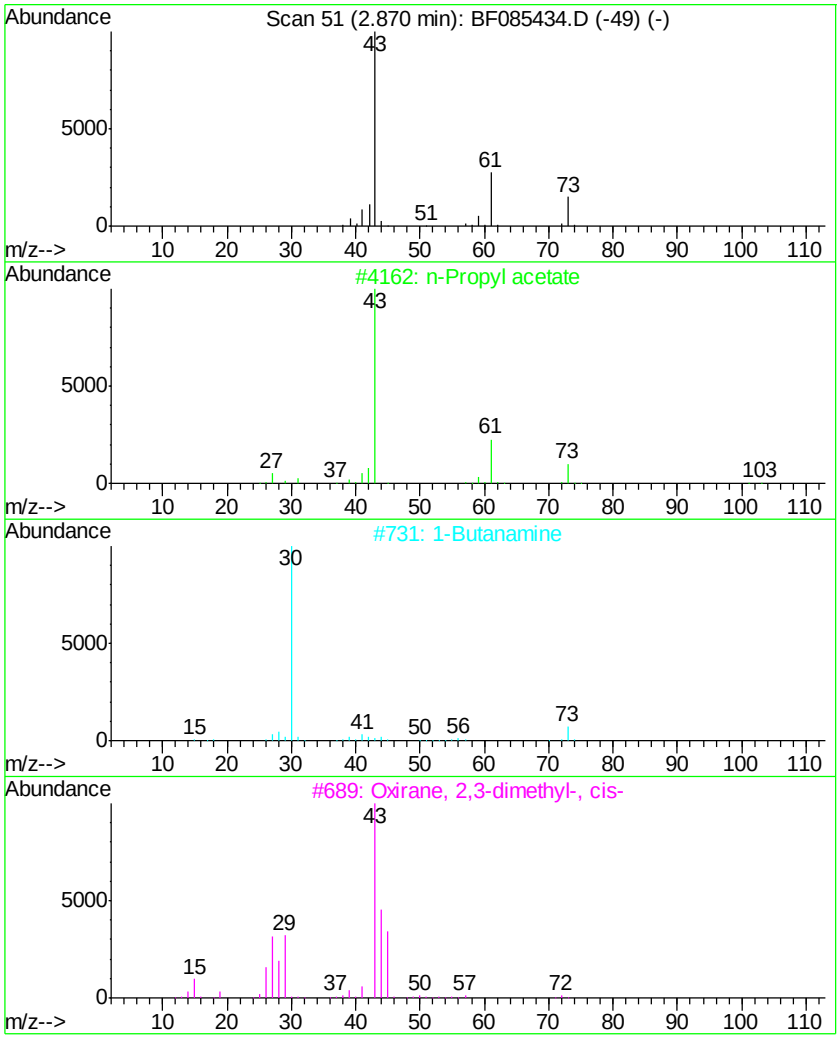
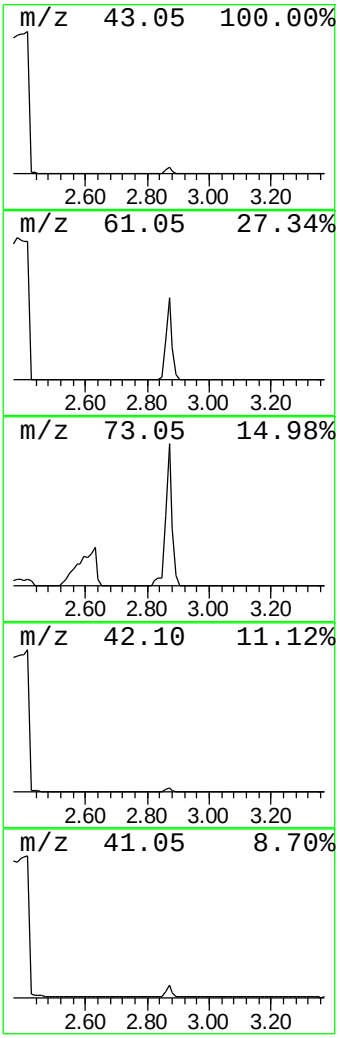
Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	3.35 ng	181751	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	9
3	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
4	Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	4
5	Pentane	72	C5H12	000109-66-0	4





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Acq On : 14 Mar 2016 17:42
Operator : UM/SJ
Sample : H1757-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-STOCKPICE-COMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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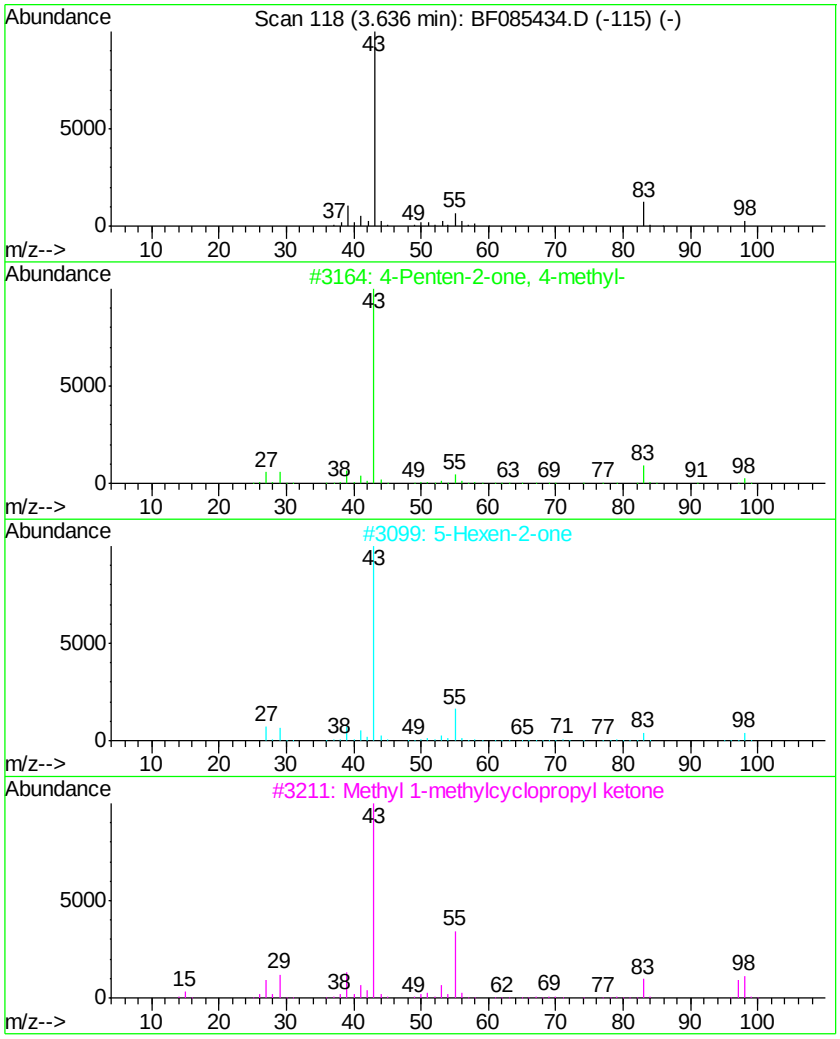
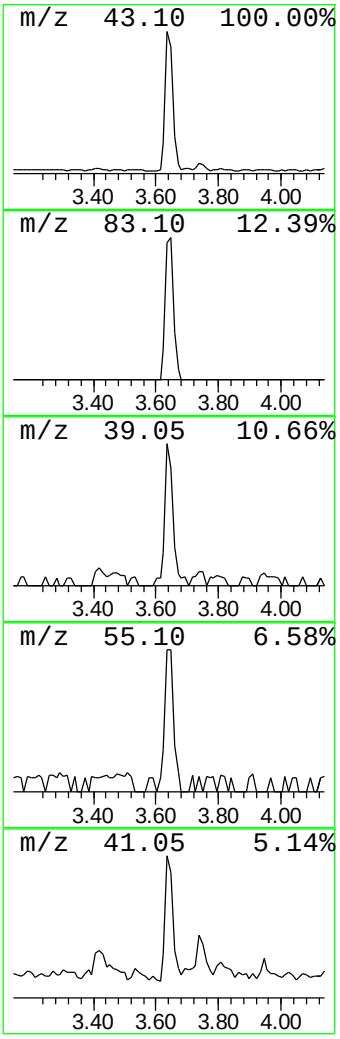
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.64	2.48 ng	134346	1,4-Dichlorobenzene-d4	6.93

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	38
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	30
4	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	28
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085434.D
Acq On : 14 Mar 2016 17:42
Operator : UM/SJ
Sample : H1757-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-STOCKPICE-COMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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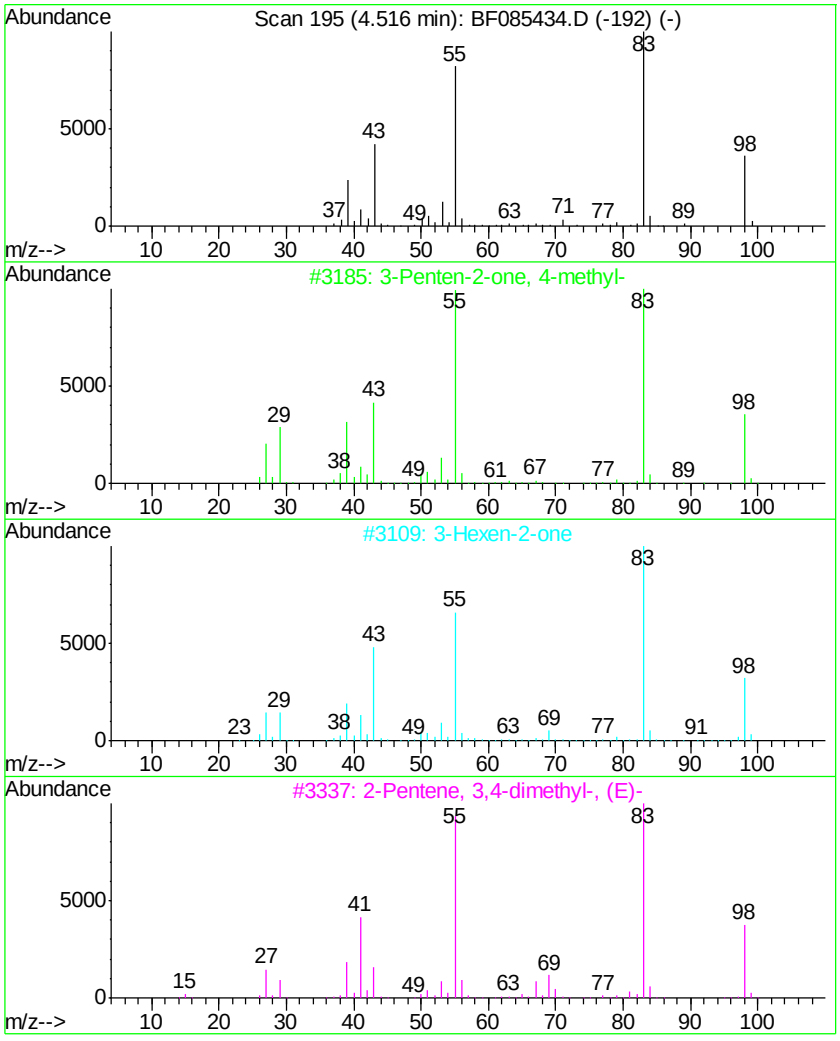
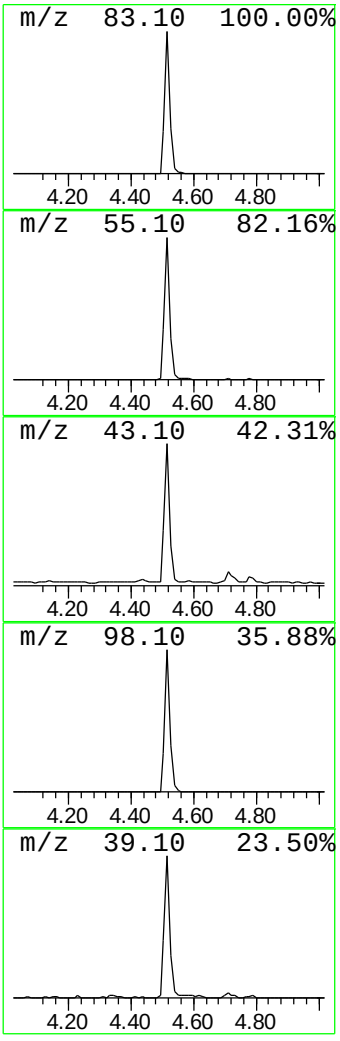
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	8.31 ng	450189	1,4-Dichlorobenzene-d4	6.93

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	87
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	86





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Data File : BF085434.D
Acq On : 14 Mar 2016 17:42
Operator : UM/SJ
Sample : H1757-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-STOCKPICE-COMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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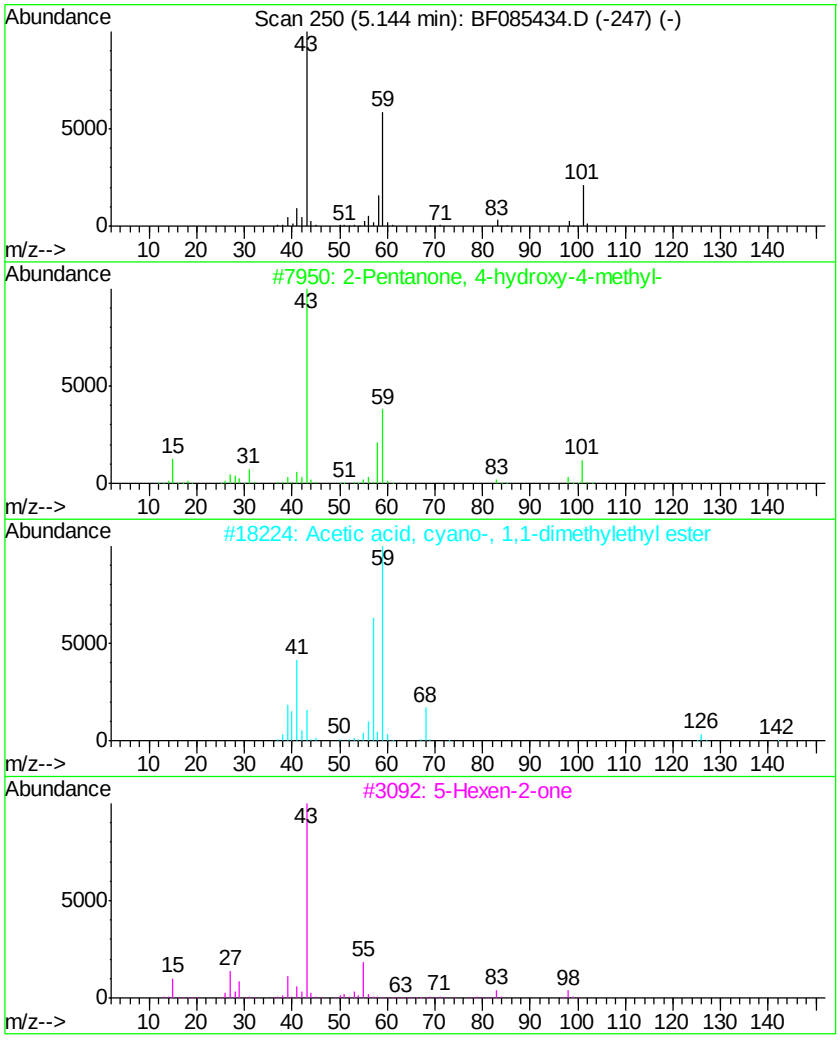
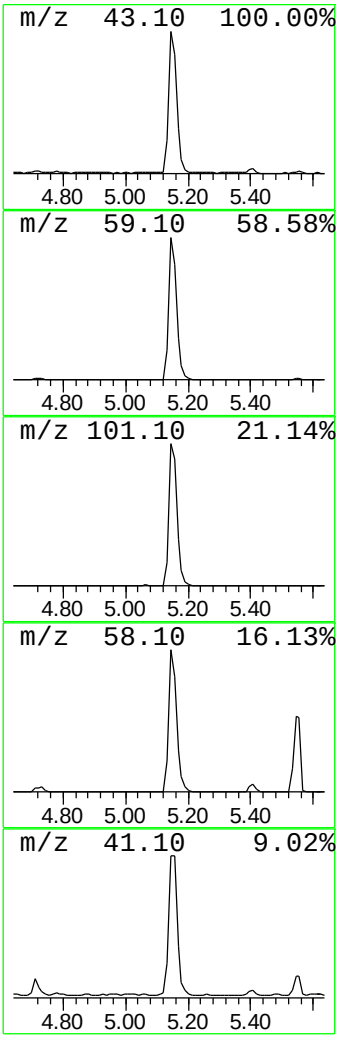
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	16.71 ng	905595	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Data File : BF085434.D
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Operator : UM/SJ
Sample : H1757-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRACK-D-STOCKPICE-COMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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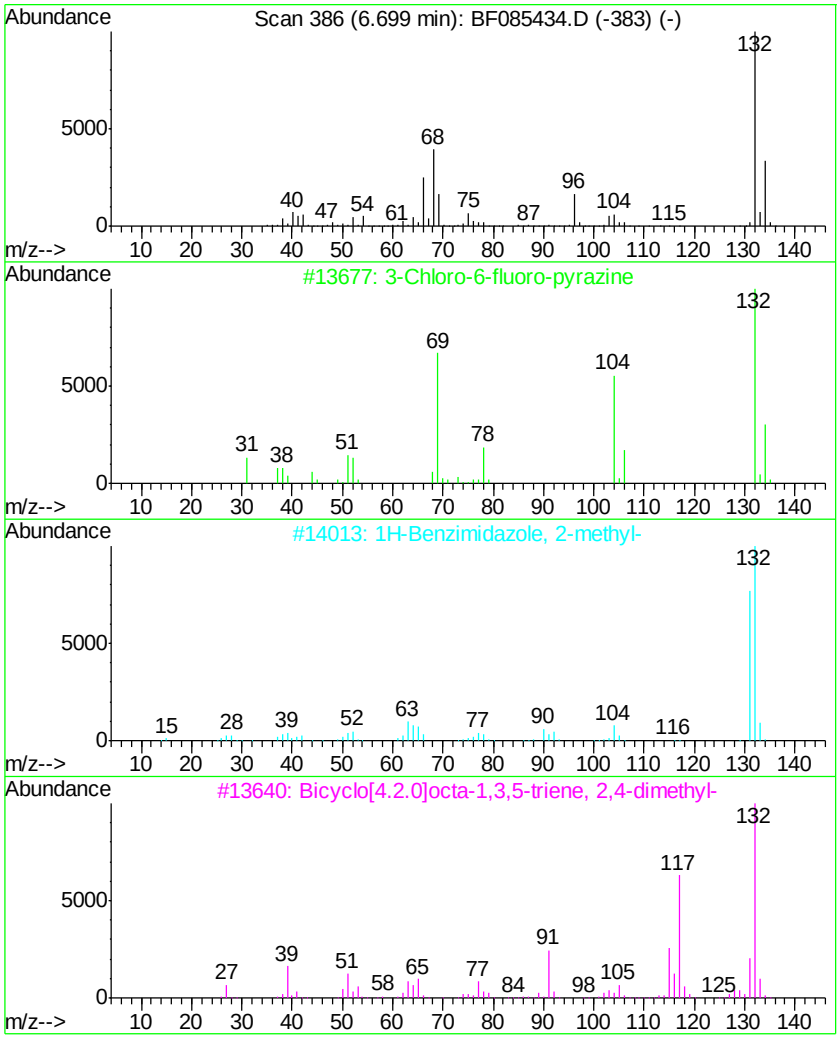
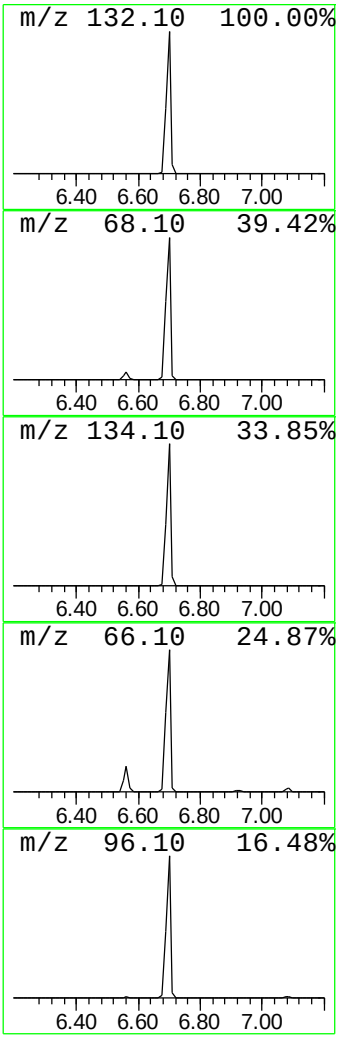
Peak Number 5 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	88.20 ng	4779330	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
Data File : BF085434.D
Acq On : 14 Mar 2016 17:42
Operator : UM/SJ
Sample : H1757-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-STOCKPICE-COMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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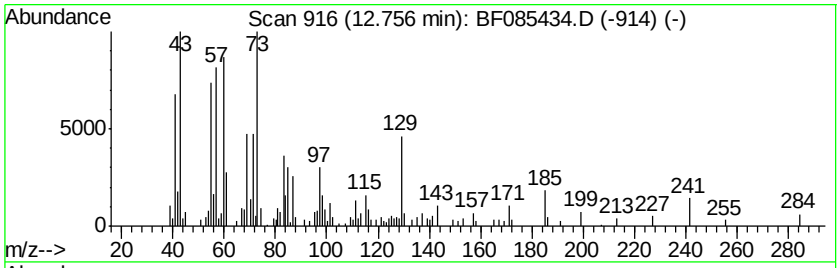
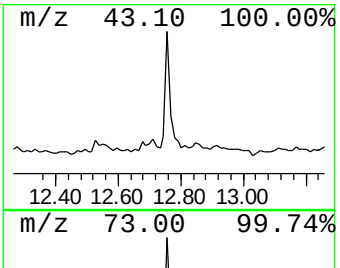
Peak Number 7 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	2.11 ng	159282	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	1-Hexacosanol	382	C26H54O	000506-52-5	18





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Instrument : BNA_F
ClientSampleId : TRACK-D-STOCKPICE-COMP1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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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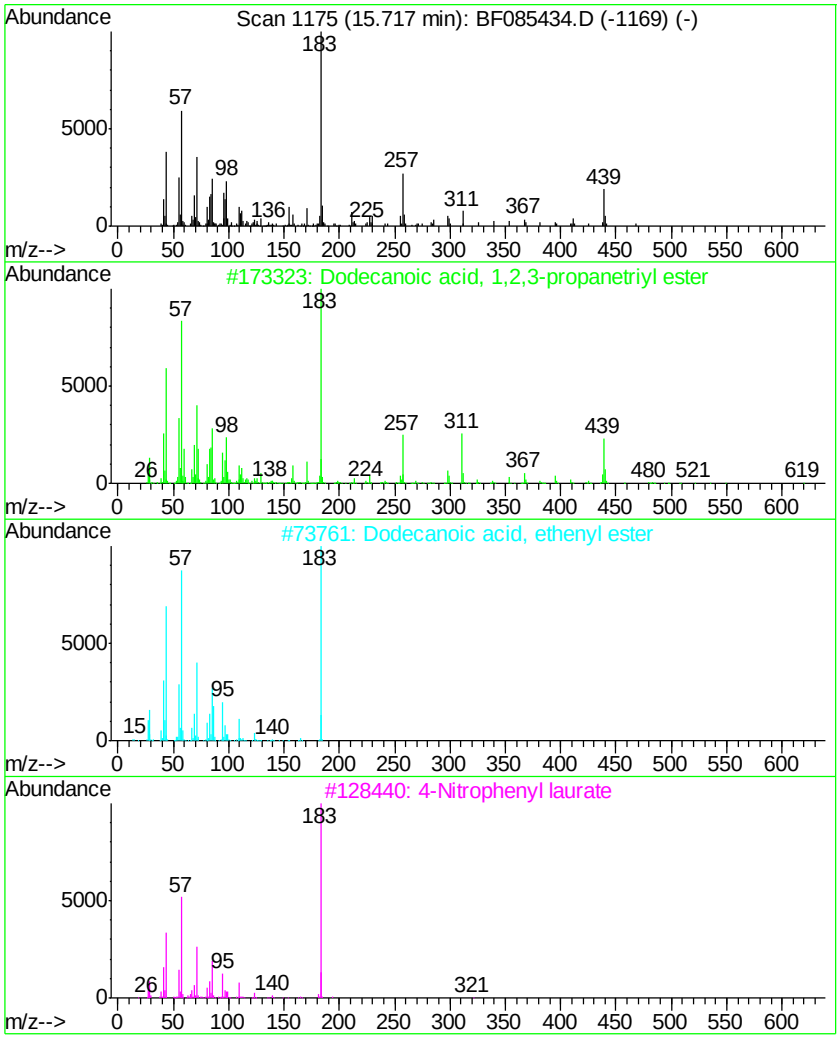
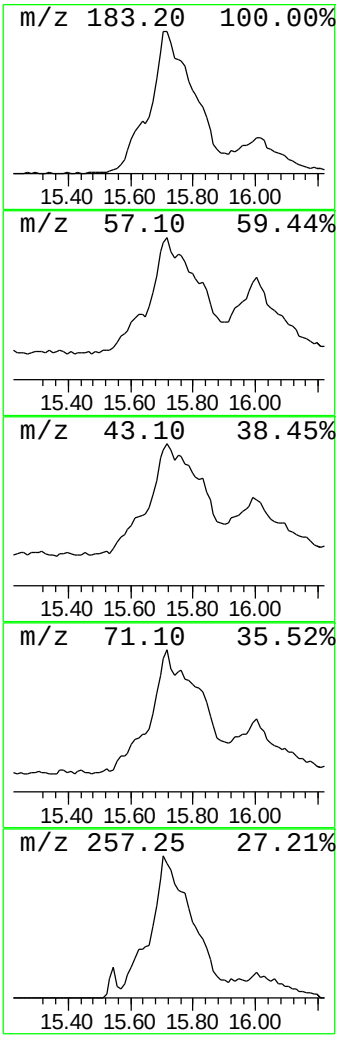
Peak Number 8 Dodecanoic acid, 1,2,3-prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	16.01 ng	689109	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid, 1,2,3-propanetr...	639	C39H74O6	000538-24-9	78
2	Dodecanoic acid, ethenyl ester	226	C14H26O2	002146-71-6	52
3	4-Nitrophenyl laurate	321	C18H27NO4	001956-11-2	46
4	3-Methyldiphenylamine	183	C13H13N	001205-64-7	38
5	2-Dibenzofuranamine	183	C12H9NO	003693-22-9	38





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
n-Propyl acetate	2.87	3.4	ng	181751	1	6.93	1083810	20.0
4-Penten-2-one, 4...	3.64	2.5	ng	134346	1	6.93	1083810	20.0
3-Penten-2-one, 4...	4.52	8.3	ng	450189	1	6.93	1083810	20.0
2-Pentanone, 4-hy...	5.14	16.7	ng	905595	1	6.93	1083810	20.0
unknown6.70	6.70	88.2	ng	4779330	1	6.93	1083810	20.0
Pentadecanoic acid	12.76	2.1	ng	159282	4	11.45	1507940	20.0
Dodecanoic acid, ...	15.72	16.0	ng	689109	6	15.55	860702	20.0