LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080752.D
Acq On : 1 Aug 2015 00:31
Operator : TP/UM
Sample : G3127-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-4(0-2)

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-BF073015.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	2.178	5	8	10	rBV	57612	77360	1.55%	0.190%
2	3.253	99	102	115	rBV	20677	85366	1.71%	0.209%
3	4.407	201	203	207	rVB	131395	172377	3.45%	0.423%
4	5.059	256	260	268	rBV	2580539	3959474	79.29%	9.712%
5	5.459	292	295	298	rBV	3591368	4181333	83.74%	10.256%
6	5.859	328	330	333	rBV	115301	142009	2.84%	0.348%
7	6.487	381	385	387	rBV	3449455	4993363	100.00%	12.248%
8	6.624	394	397	399	rBV	3780311	4711371	94.35%	11.556%
9	6.853	415	417	419	rBV	1019147	877674	17.58%	2.153%
10	7.013	428	431	433	rBV	2485169	3098820	62.06%	7.601%
11	7.413	463	466	468	rBV	2835727	2882230	57.72%	7.070%
12	8.133	526	529	531	rBV	1208878	1090931	21.85%	2.676%
13	9.208	620	623	626	rBV	3441821	3816938	76.44%	9.362%
14	9.608	655	658	660	rBV	459812	551829	11.05%	1.354%
15	9.882	680	682	685	rVB	1178163	1111346	22.26%	2.726%
16	10.671	748	751	753	rBV	3043180	3004532	60.17%	7.370%
17	10.796	759	762	767	rVB	62515	77636	1.55%	0.190%
18	11.242	798	801	802	rBV	69393	56737	1.14%	0.139%
19	11.368	809	812	814	rBV	1017860	1100568	22.04%	2.699%
20	11.894	856	858	871	rVB	143346	218169	4.37%	0.535%
21	12.156	878	881	883	rVB	111109	124312	2.49%	0.305%
22	12.682	924	927	933	rBV	34734	54517	1.09%	0.134%
23	12.945	948	950	953	rBV	2720293	3108864	62.26%	7.625%
24	13.985	1039	1041	1044	rBV	579108	692123	13.86%	1.698%
25	15.402	1162	1165	1168	rBV	413852	579930	11.61%	1.422%

Sum of corrected areas: 40769809

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BNA_F
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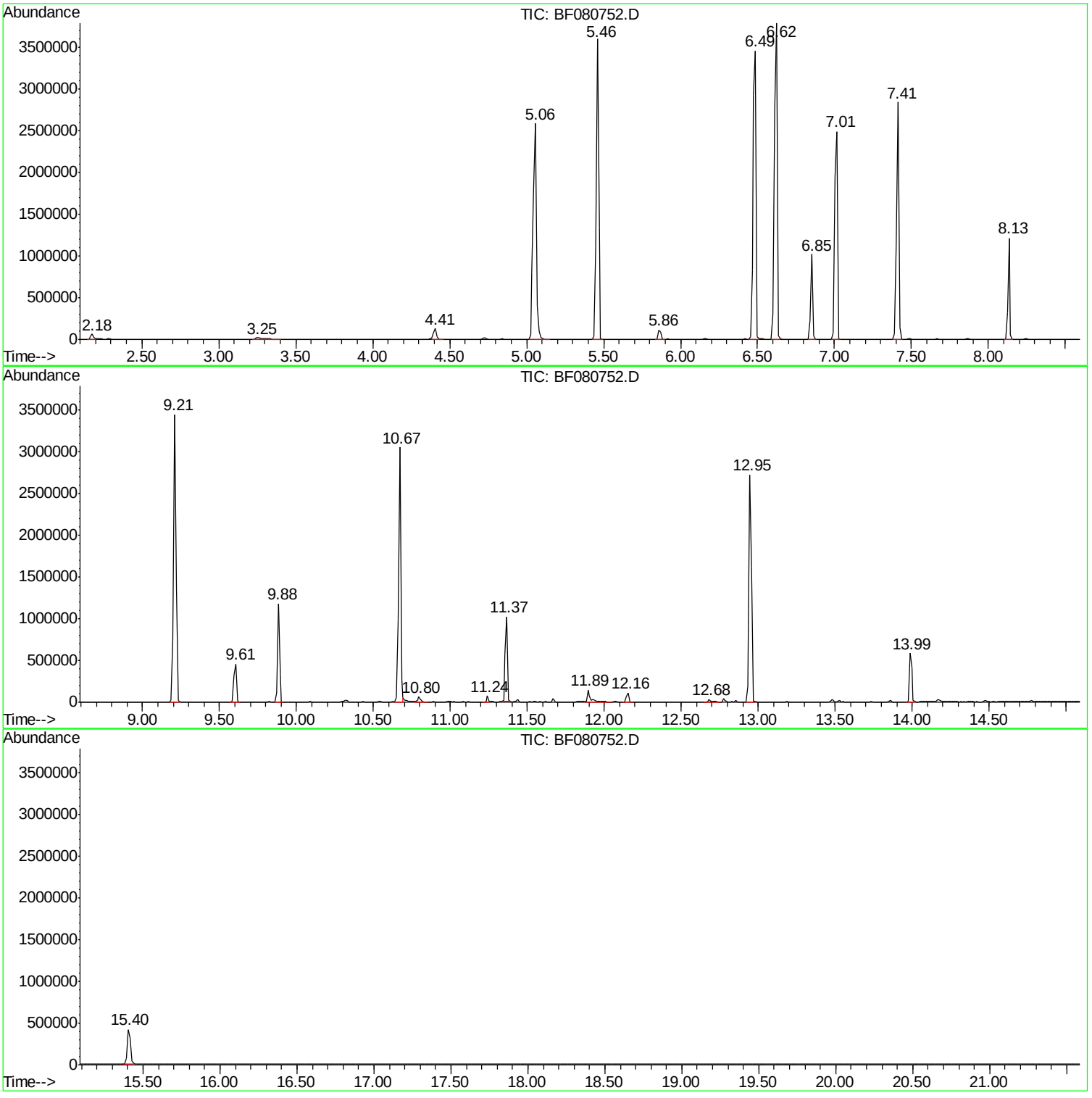
COFF-3RD-4(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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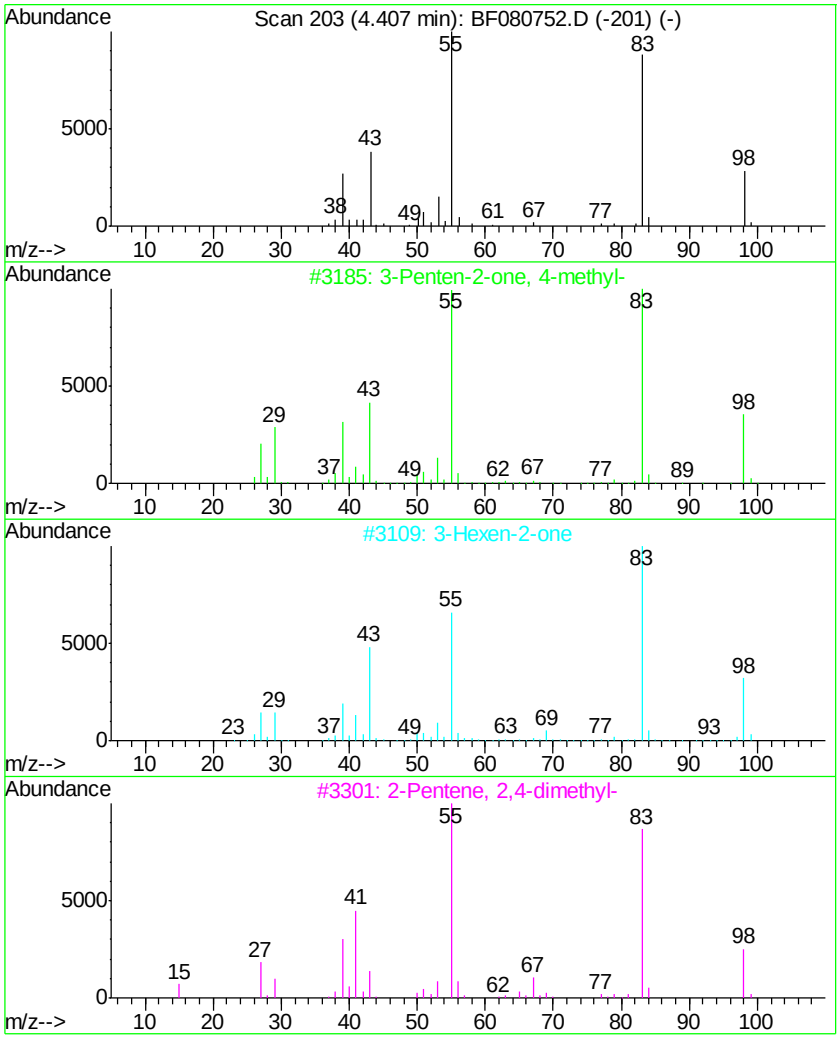
TIC Integration Parameters: LSCINT.P

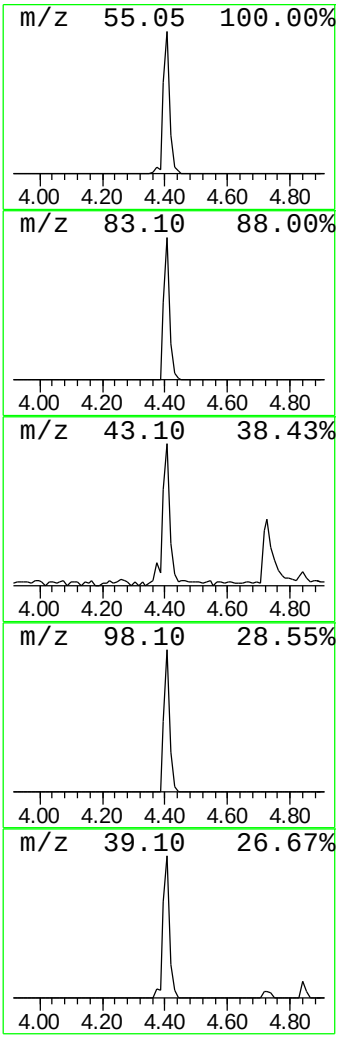
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	3.93 ng	172377	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72





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Operator : TP/UM
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Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-4(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.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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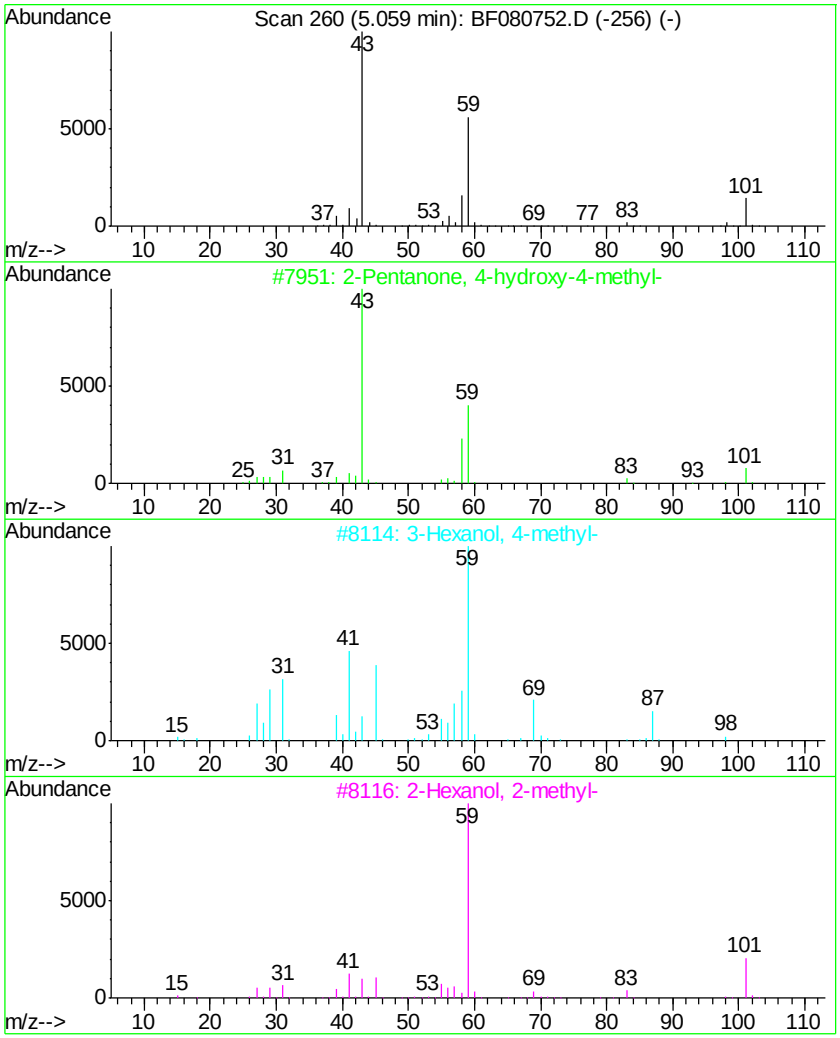
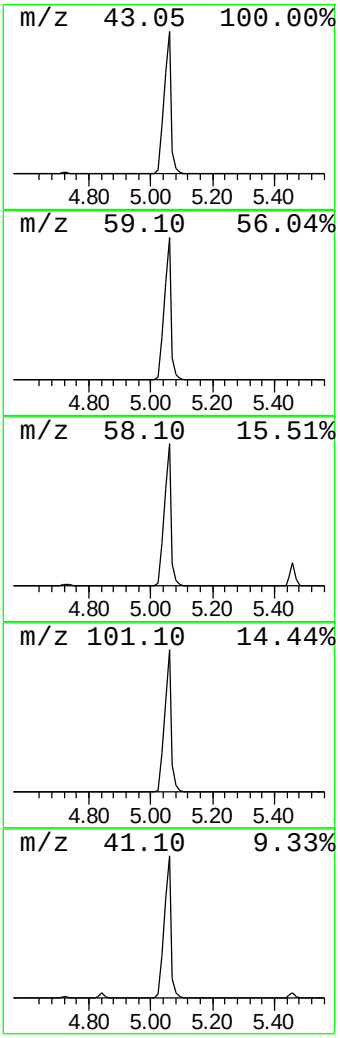
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	90.23 ng	3959470	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17





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Data File : BF080752.D
Acq On : 1 Aug 2015 00:31
Operator : TP/UM
Sample : G3127-01
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-4(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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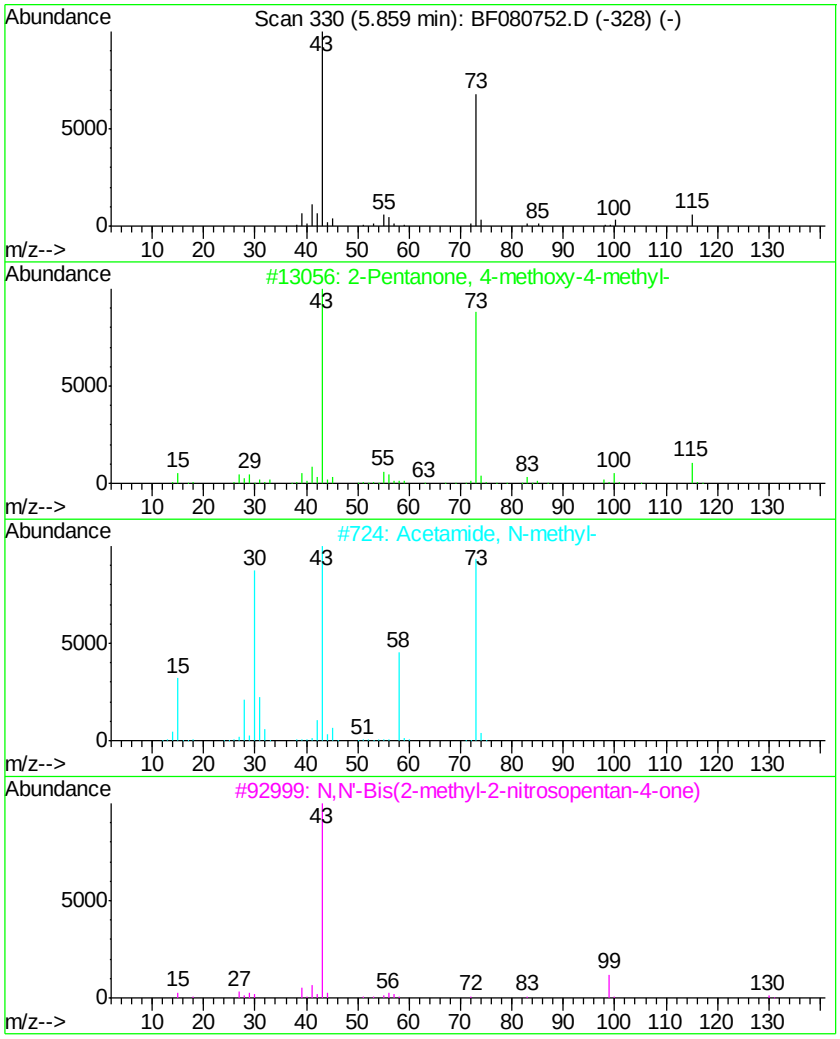
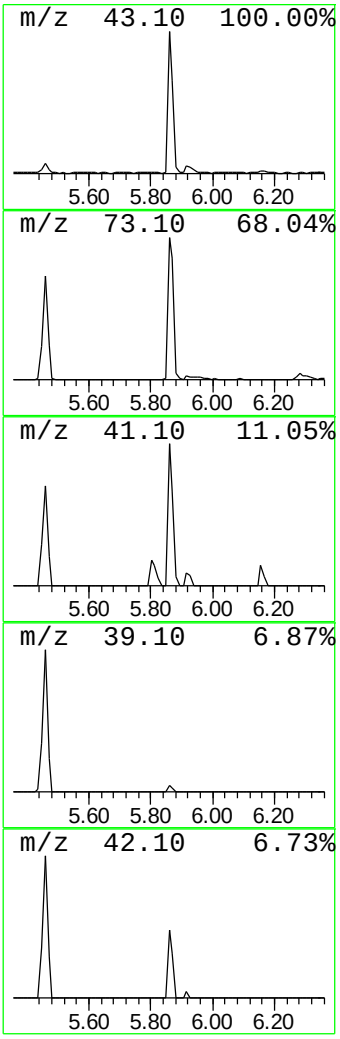
Peak Number 3 unknown5.86 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	3.24 ng	142009	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
3	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	12
4	1,3-Dioxolane, 2-ethenyl-	100	C5H8O2	003984-22-3	9
5	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9





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Misc :
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Instrument : BNA_F
ClientSampleId : COFF-3RD-4(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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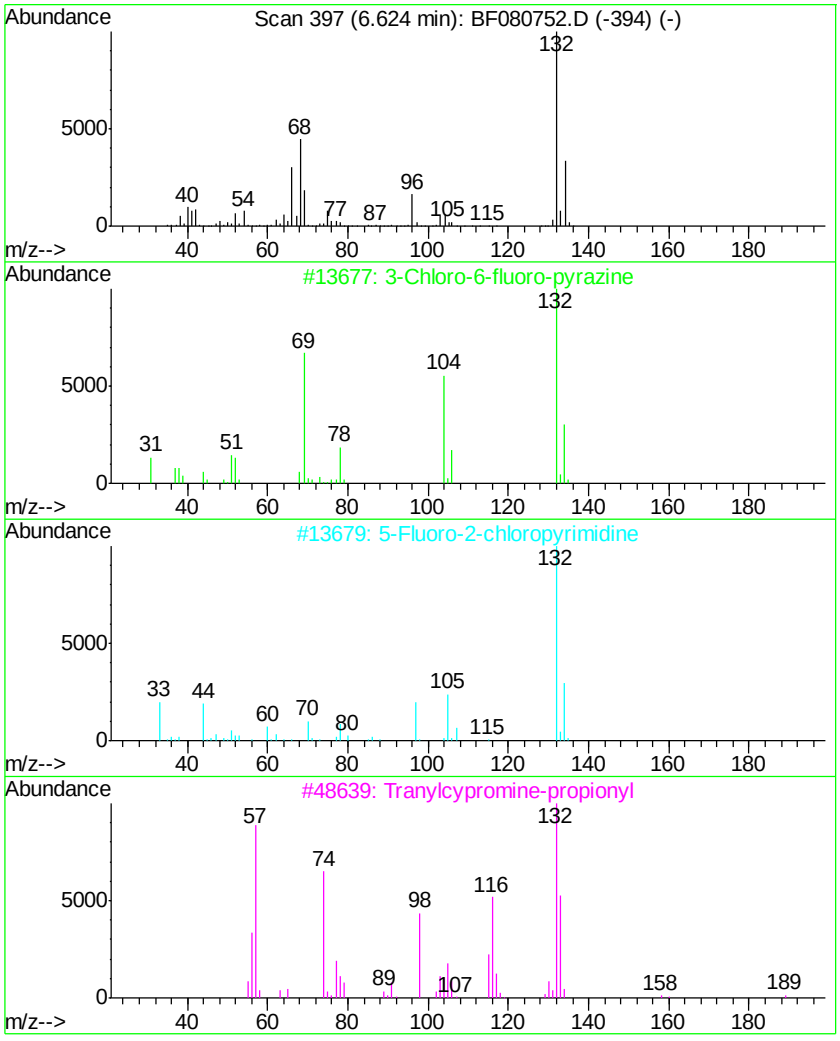
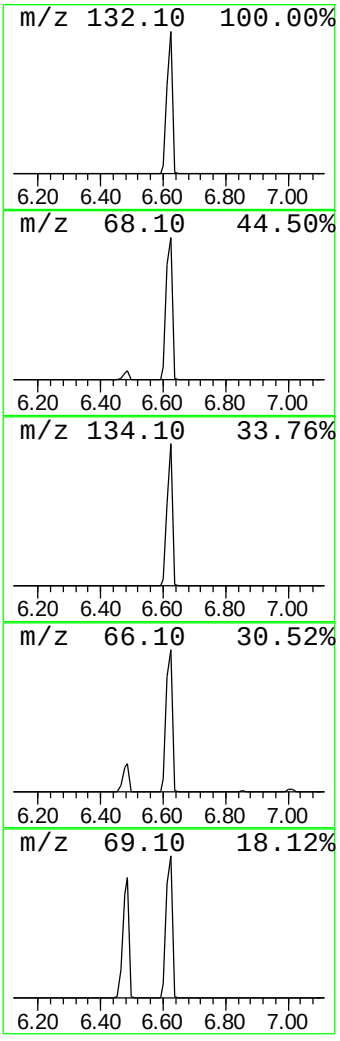
Peak Number 4 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	107.36 ng	4711370	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : COFF-3RD-4(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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TIC Library : C:\DATABASE\NIST02.L
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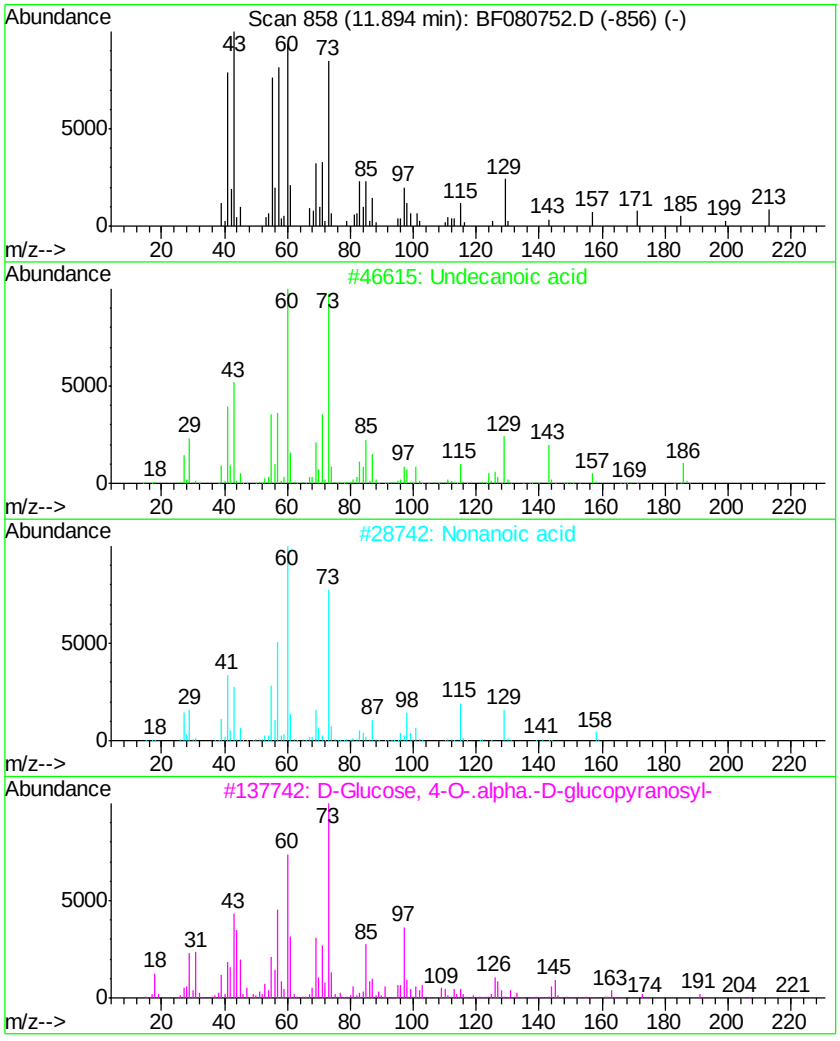
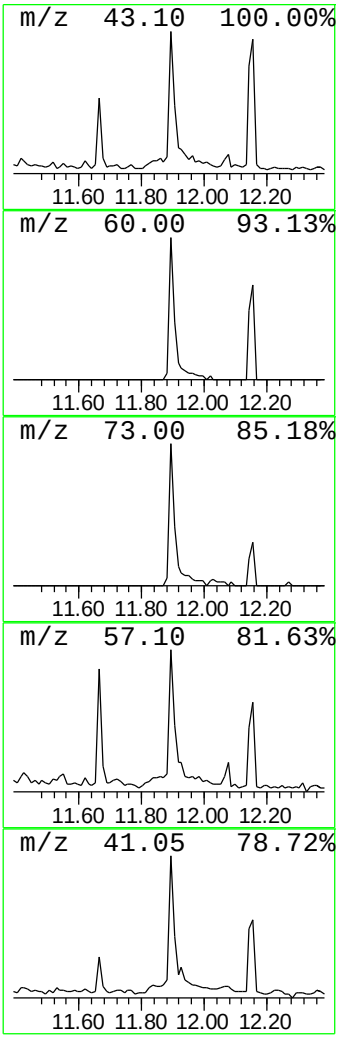
****

Peak Number 6 Undecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	3.96 ng	218169	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	Nonanoic acid	158	C9H18O2	000112-05-0	47
3	D-Glucose, 4-O-.alpha.-D-glucopy...	342	C12H22O11	000069-79-4	43
4	Heptanoic acid	130	C7H14O2	000111-14-8	38
5	4-Propionyloxytridecane	256	C16H32O2	1000245-62-6	27





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ClientSampleId : COFF-3RD-4(0-2)

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

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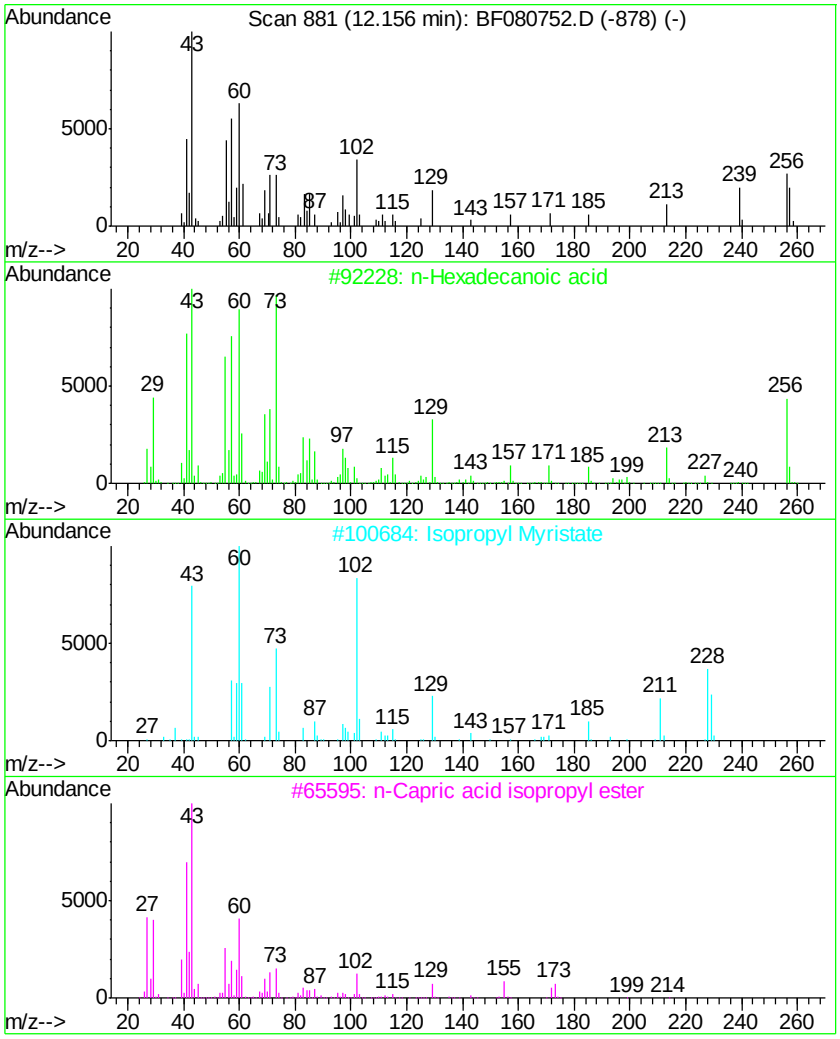
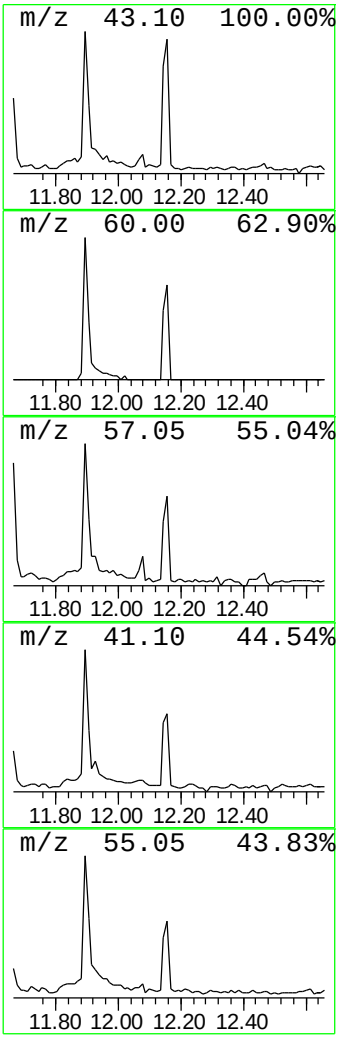
Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	2.26 ng	124312	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Isopropyl Myristate	270	C17H34O2	000110-27-0	47
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	37
4	Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	32
5	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	32





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.41	3.9	ng	172377	1	6.85	877674	20.0
2-Pentanone, 4-hy...	5.06	90.2	ng	3959470	1	6.85	877674	20.0
unknown5.86	5.86	3.2	ng	142009	1	6.85	877674	20.0
unknown6.62	6.62	107.4	ng	4711370	1	6.85	877674	20.0
Undecanoic acid	11.89	4.0	ng	218169	4	11.37	1100570	20.0
n-Hexadecanoic acid	12.16	2.3	ng	124312	4	11.37	1100570	20.0