LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080748.D
Acq On : 31 Jul 2015 22:27
Operator : TP/UM
Sample : G3125-17
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-2(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	46146	66519	1.72%	0.180%
2	3.218	98	99	111	rBV	57800	173874	4.50%	0.471%
3	4.407	200	203	207	rBV	118051	161551	4.18%	0.438%
4	5.059	256	260	262	rBV	2224708	3556778	91.97%	9.635%
5	5.459	292	295	297	rBV	3726406	3669637	94.88%	9.940%
6	5.859	328	330	333	rBV	107819	123672	3.20%	0.335%
7	6.476	381	384	387	rBV	2964762	3694475	95.53%	10.008%
8	6.624	394	397	399	rBV	2730663	3867475	100.00%	10.476%
9	6.853	415	417	419	rBV	1003092	863168	22.32%	2.338%
10	7.013	428	431	433	rBV	1931685	2671616	69.08%	7.237%
11	7.413	463	466	468	rBV	2642158	2647370	68.45%	7.171%
12	7.493	468	473	481	rVB	60142	80876	2.09%	0.219%
13	8.133	526	529	531	rBV	1178642	1070382	27.68%	2.899%
14	9.207	620	623	626	rBV	3391466	3485898	90.13%	9.443%
15	9.608	655	658	660	rBV	585725	686549	17.75%	1.860%
16	9.882	680	682	685	rVB	1133125	1090207	28.19%	2.953%
17	10.670	748	751	753	rBV	2423792	2423344	62.66%	6.564%
18	10.796	760	762	765	rBV	54597	63228	1.63%	0.171%
19	11.242	799	801	802	rBV	79447	64645	1.67%	0.175%
20	11.368	809	812	814	rVB	1066157	1115941	28.85%	3.023%
21	11.665	836	838	840	rBV	76201	72277	1.87%	0.196%
22	11.905	856	859	861	rBV	190081	292150	7.55%	0.791%
23	12.076	871	874	876	rVV	38963	46119	1.19%	0.125%
24	12.156	878	881	883	rVB	571927	586192	15.16%	1.588%
25	12.682	925	927	933	rBV	175639	203702	5.27%	0.552%
26	12.945	948	950	953	rBV	2324144	2674918	69.16%	7.246%
27	13.997	1039	1042	1044	rBV	607891	788742	20.39%	2.137%
28	14.317	1069	1070	1081	rVB8	7883	44611	1.15%	0.121%
29	15.402	1162	1165	1168	rBV	414803	630745	16.31%	1.709%

Sum of corrected areas: 36916661

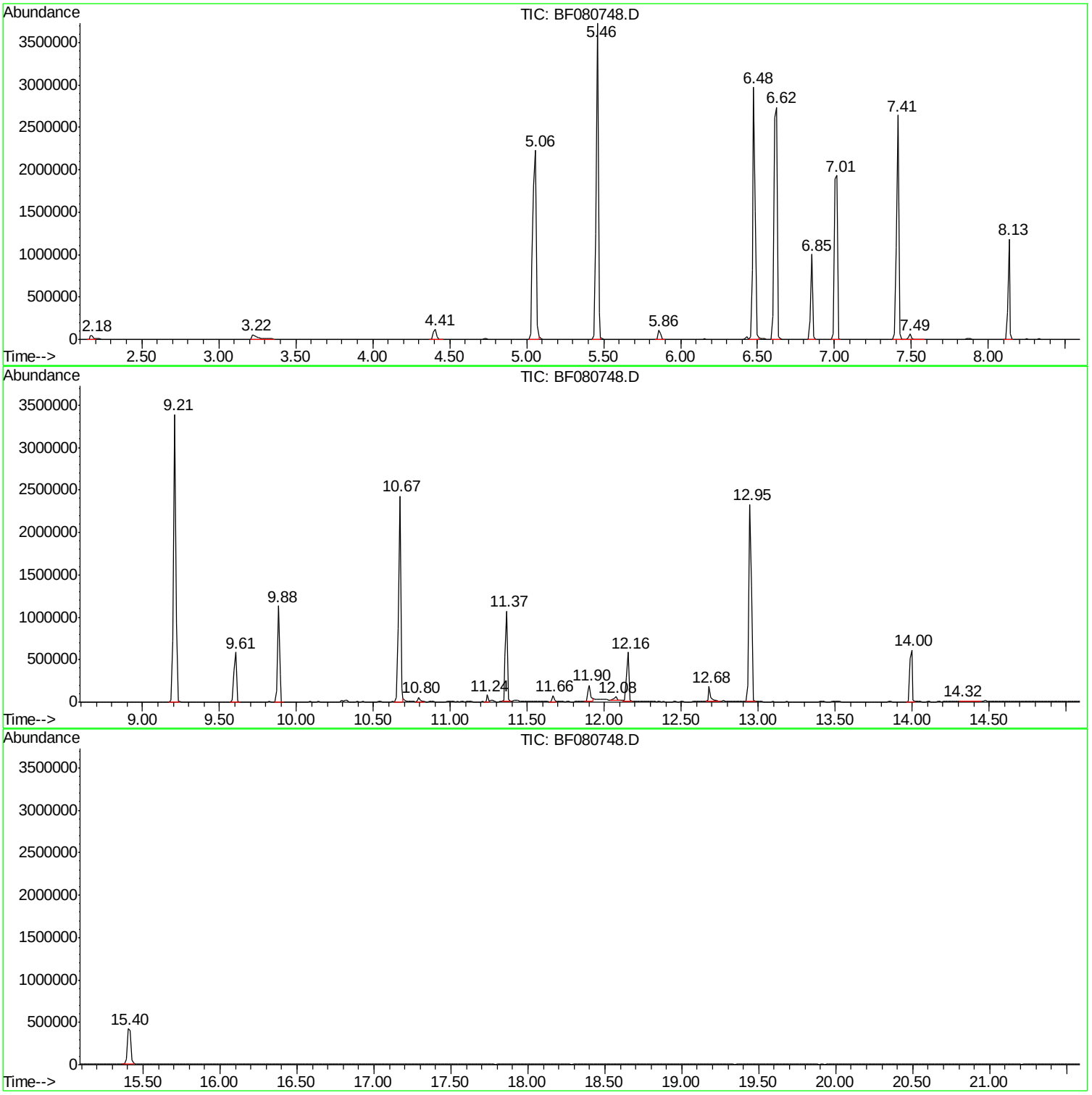
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080748.D
Acq On : 31 Jul 2015 22:27
Operator : TP/UM
Sample : G3125-17
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3RD-2(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

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080748.D
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Operator : TP/UM
Sample : G3125-17
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-2(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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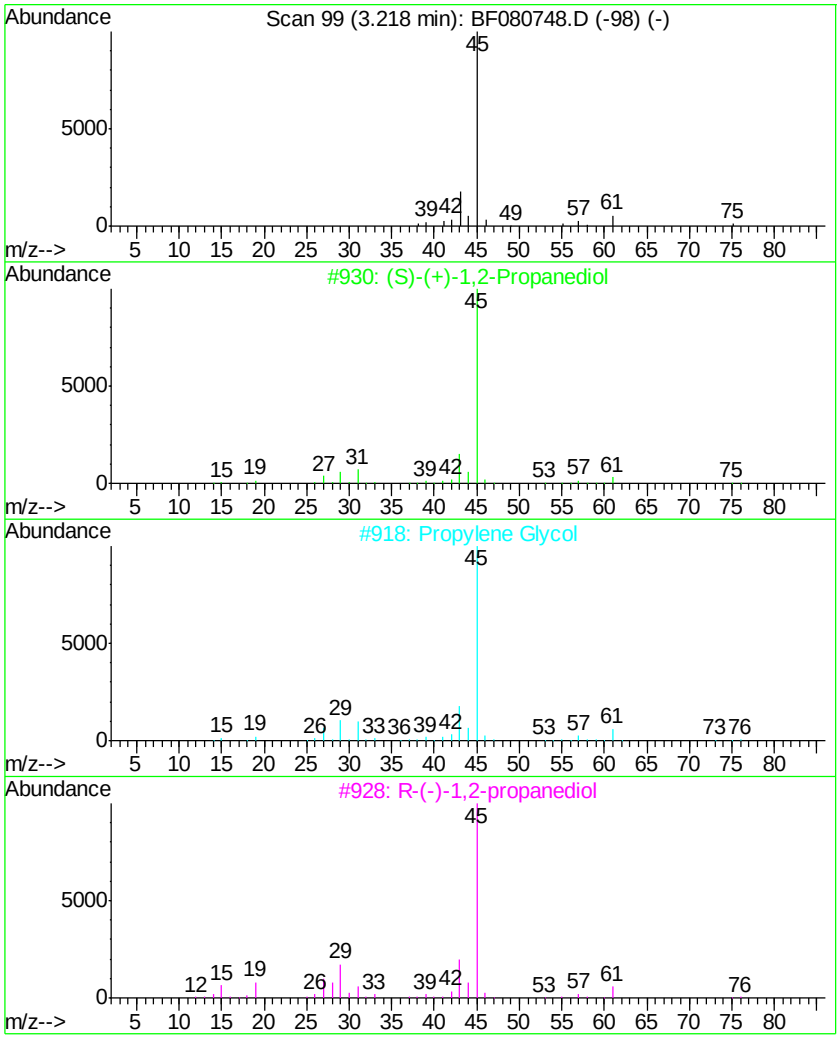
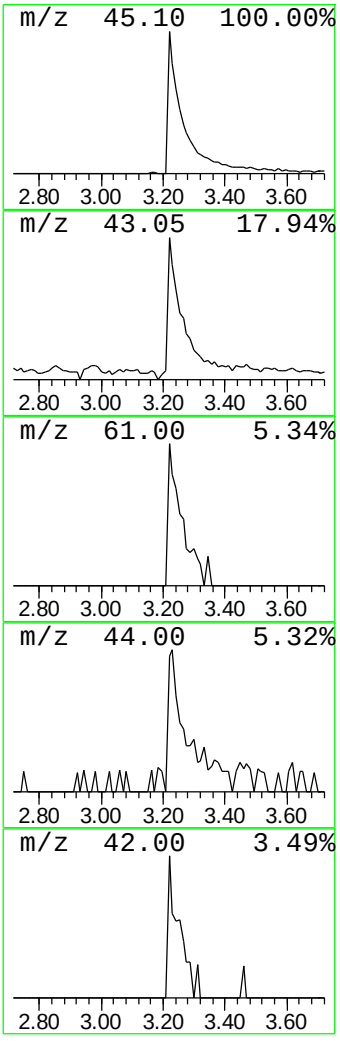
Peak Number 1 unknown3.22 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	4.03 ng	173874	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9
5	Formamide	45	CH3NO	000075-12-7	7





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Data File : BF080748.D
Acq On : 31 Jul 2015 22:27
Operator : TP/UM
Sample : G3125-17
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-2(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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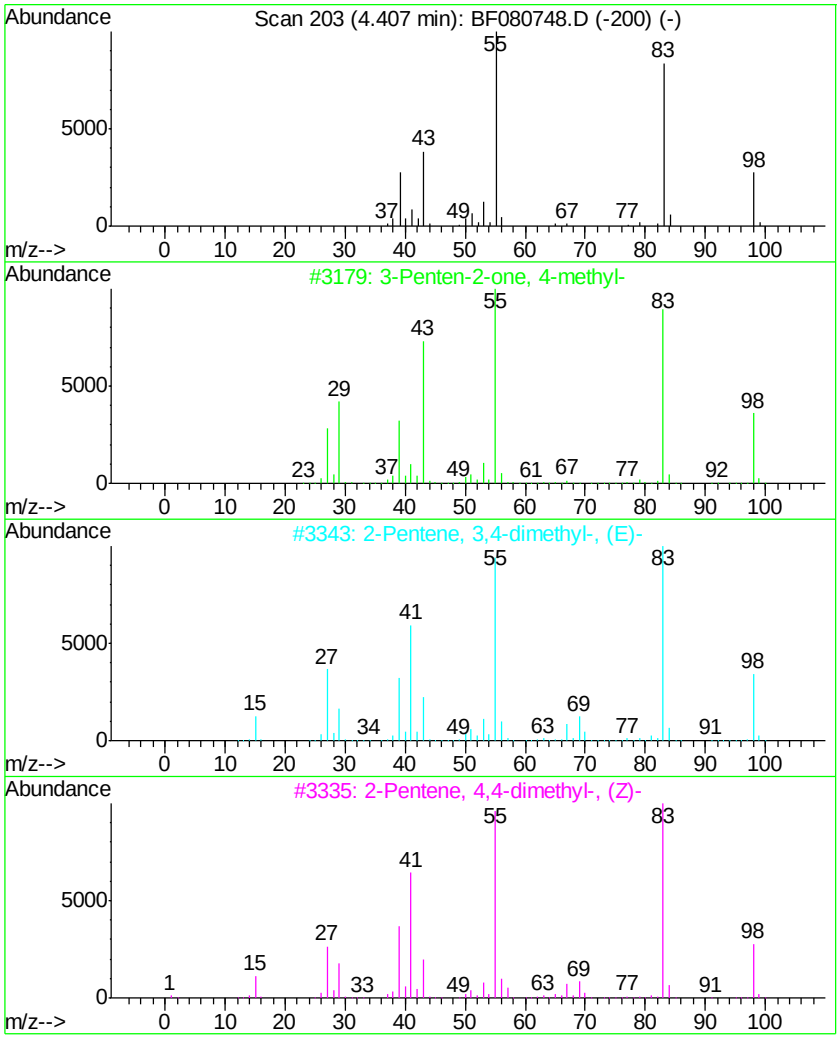
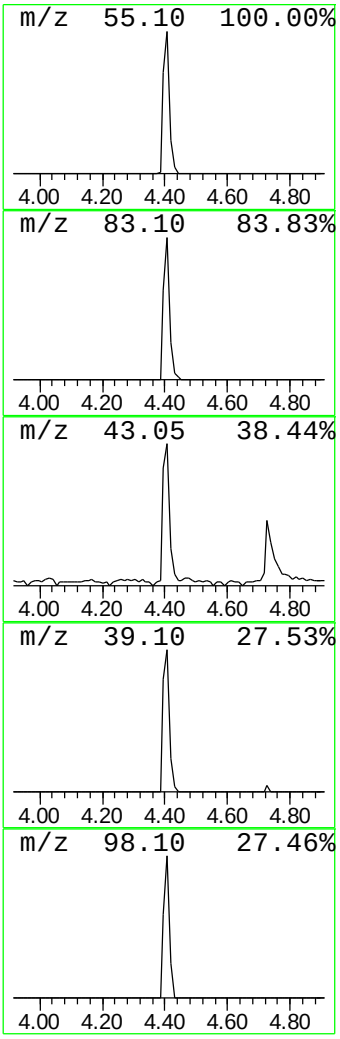
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	3.74 ng	161551	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	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
4	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080748.D
Acq On : 31 Jul 2015 22:27
Operator : TP/UM
Sample : G3125-17
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-2(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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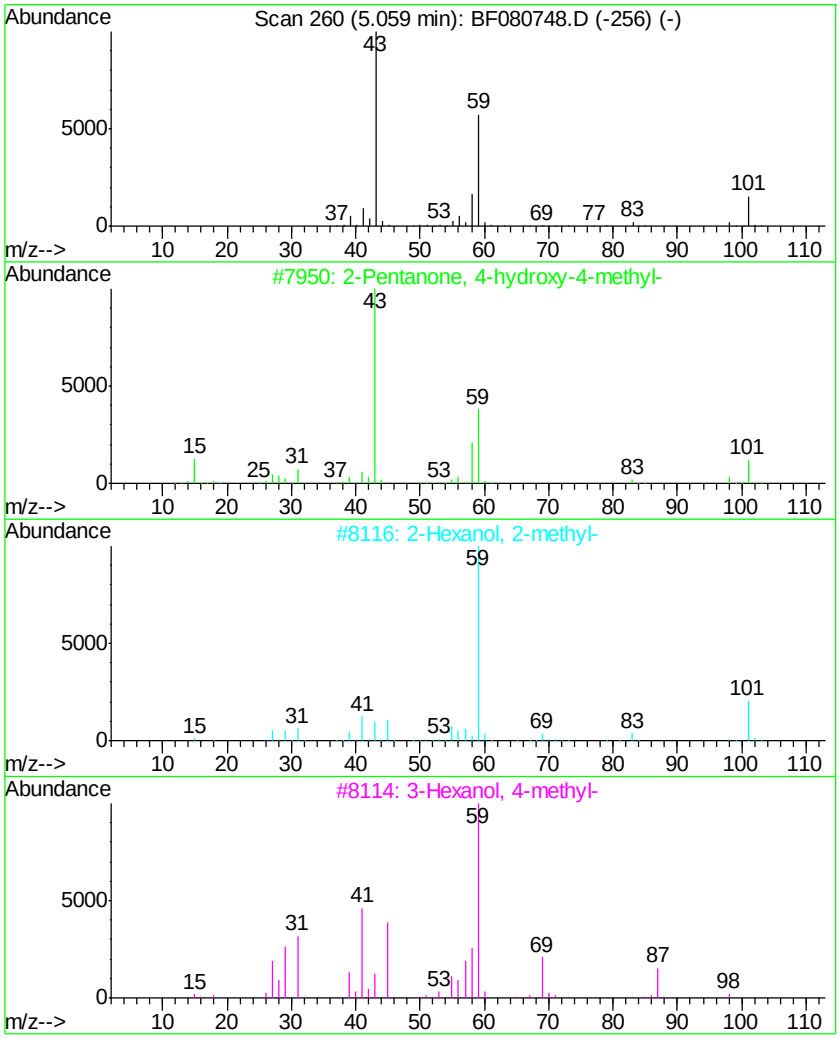
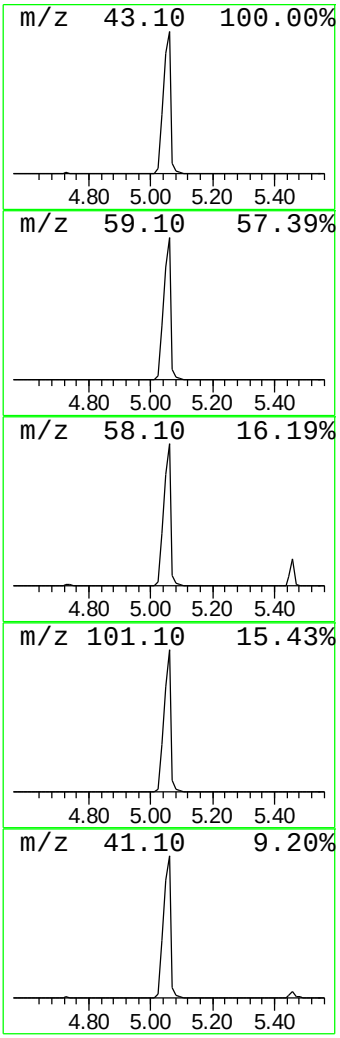
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	82.41 ng	3556780	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	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	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





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080748.D
Acq On : 31 Jul 2015 22:27
Operator : TP/UM
Sample : G3125-17
Misc :
ALS Vial : 40 Sample Multiplier: 1

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

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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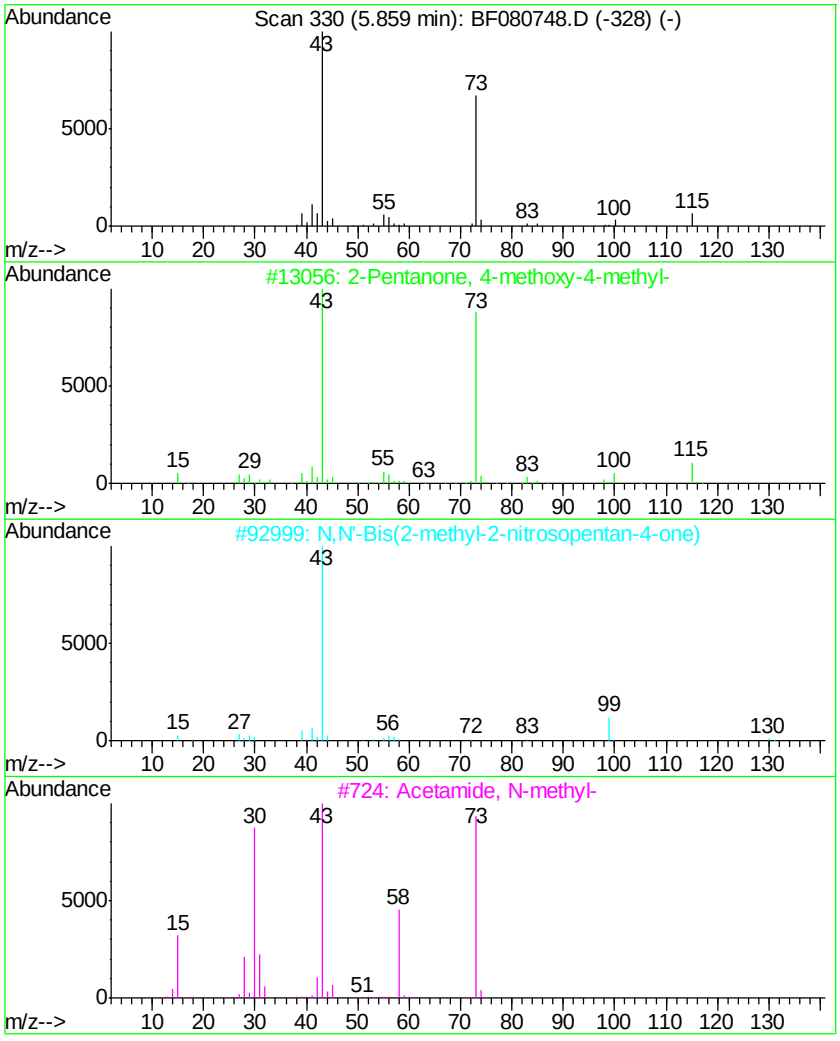
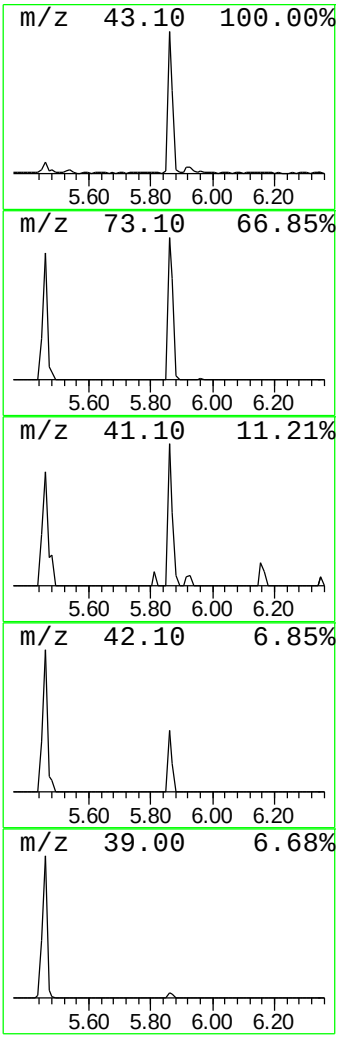
Peak Number 4 unknown5.86 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	2.87 ng	123672	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	83
2	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	23
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	16
4	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	16
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080748.D
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Sample : G3125-17
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-2(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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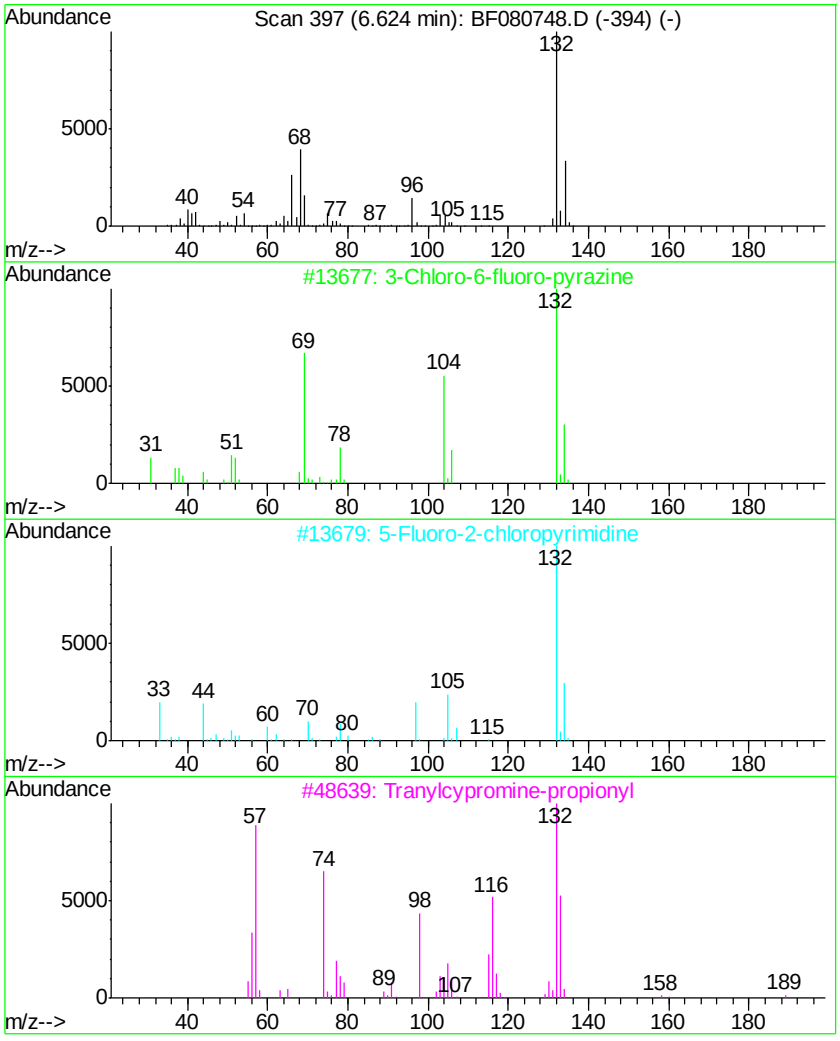
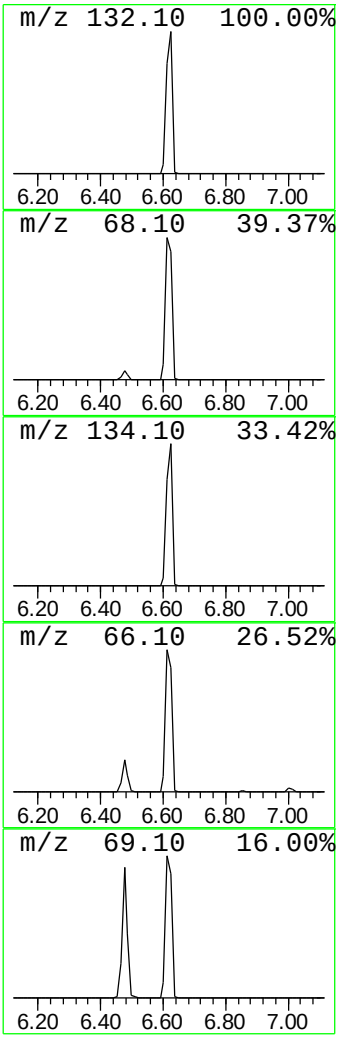
****

Peak Number 5 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	89.61 ng	3867480	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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
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Acq On : 31 Jul 2015 22:27
Operator : TP/UM
Sample : G3125-17
Misc :
ALS Vial : 40 Sample Multiplier: 1

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

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

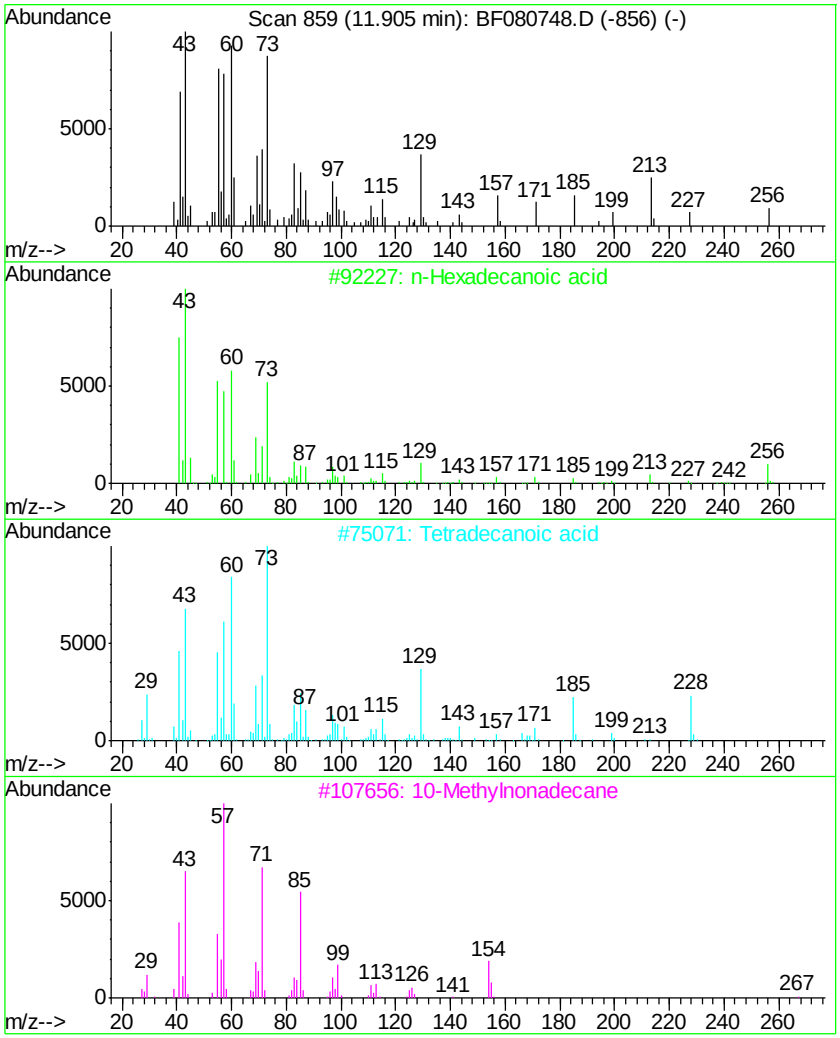
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

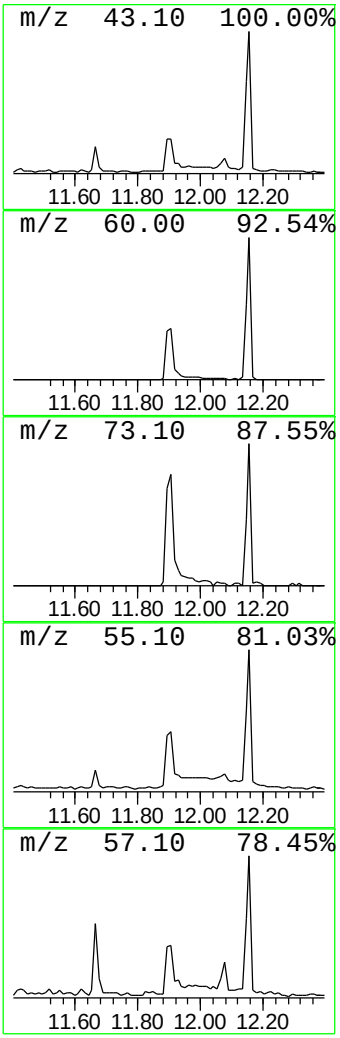
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	5.24 ng	292150	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	10-Methylnonadecane	282	C20H42	056862-62-5	11
4	Tetradecane	198	C14H30	000629-59-4	11
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	11





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Operator : TP/UM
Sample : G3125-17
Misc :
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Instrument : BNA_F
ClientSampleId : COFF-3RD-2(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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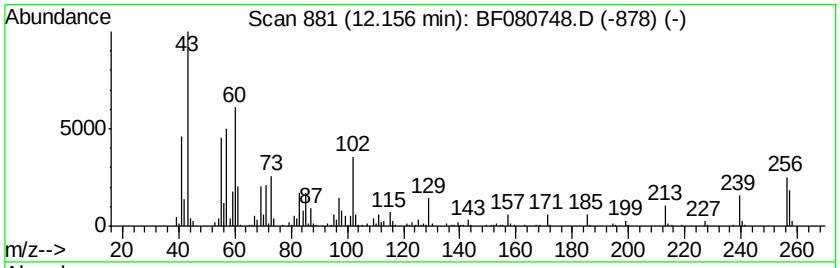
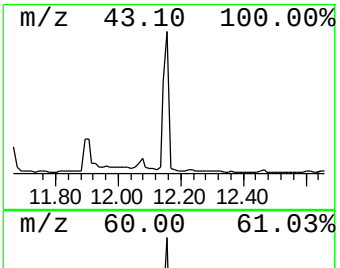
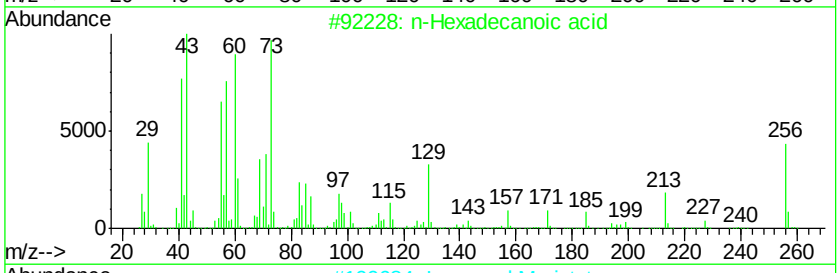
Peak Number 8 Isopropyl Myristate Concentration Rank 4

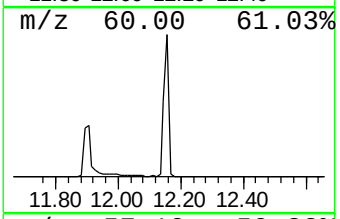
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	10.51 ng	586192	Phenanthrene-d10	11.37

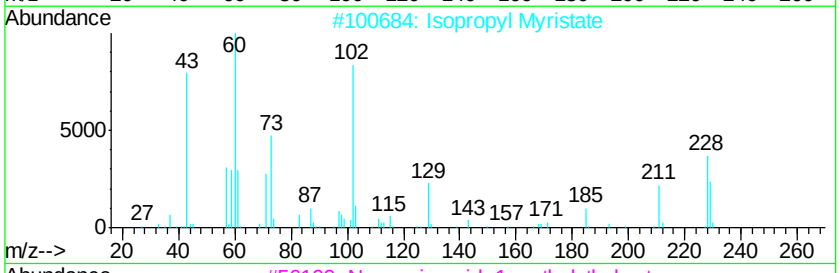
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60
2	Isopropyl Myristate	270	C17H34O2	000110-27-0	50
3	Nonanoic acid, 1-methylethyl ester	200	C12H24O2	028267-32-5	38
4	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	35
5	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	32

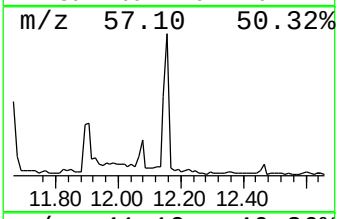


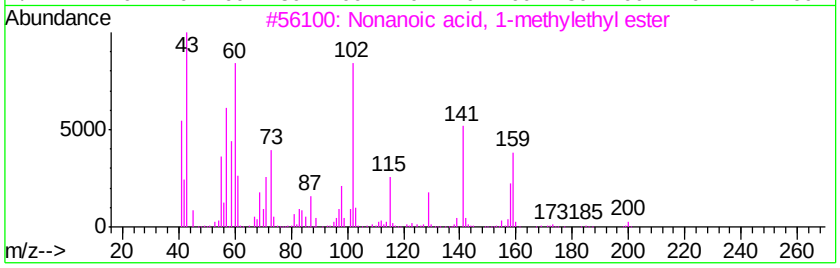


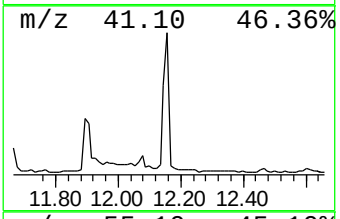


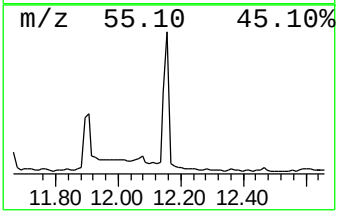












Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
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Operator : TP/UM
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF073015.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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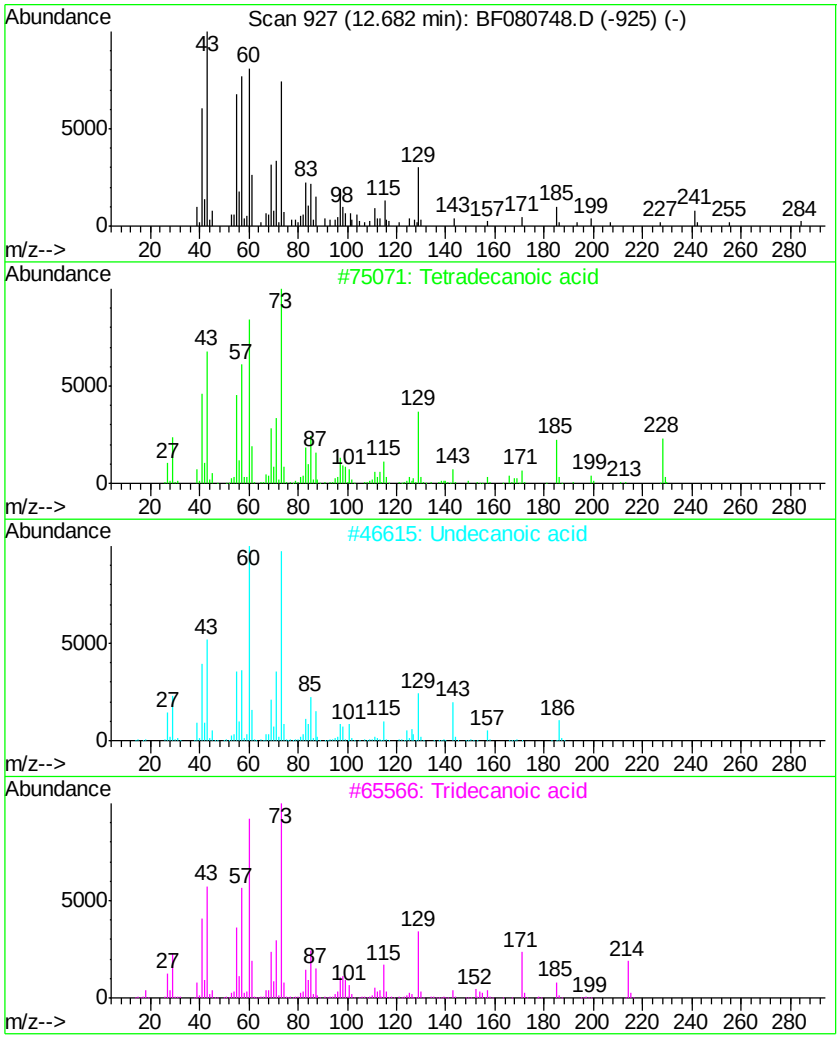
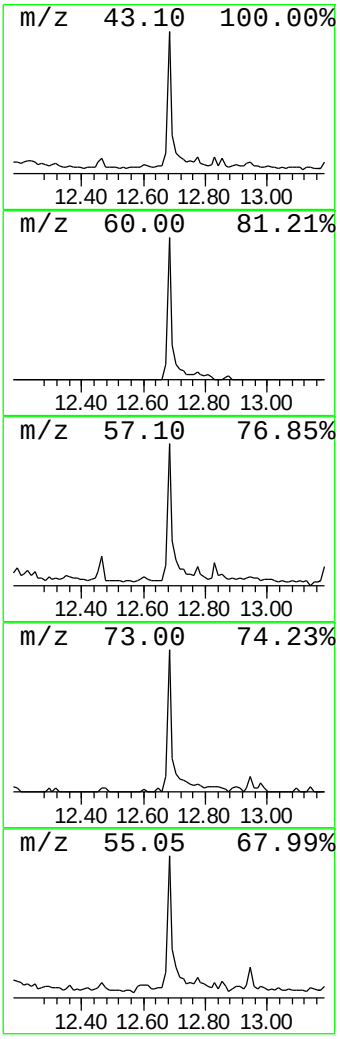
Peak Number 9 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.68	5.17 ng	203702	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
2	Undecanoic acid	186	C11H22O2	000112-37-8	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073115\
Data File : BF080748.D
Acq On : 31 Jul 2015 22:27
Operator : TP/UM
Sample : G3125-17
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3RD-2(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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.22	3.22	4.0	ng	173874	1	6.85	863168	20.0
3-Penten-2-one, 4...	4.41	3.7	ng	161551	1	6.85	863168	20.0
2-Pentanone, 4-hy...	5.06	82.4	ng	3556780	1	6.85	863168	20.0
unknown5.86	5.86	2.9	ng	123672	1	6.85	863168	20.0
unknown6.62	6.62	89.6	ng	3867480	1	6.85	863168	20.0
n-Hexadecanoic acid	11.90	5.2	ng	292150	4	11.37	1115940	20.0
Isopropyl Myristate	12.16	10.5	ng	586192	4	11.37	1115940	20.0
Tetradecanoic acid	12.68	5.2	ng	203702	5	14.00	788742	20.0