LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062516\
Data File : BF088373.D
Acq On : 25 Jun 2016 13:22
Operator : UM/SJ
Sample : H3602-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

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-BF060716.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	1.701	8	10	61	rVB	1179252	2784795	14.81%	5.603%
2	5.153	310	312	336	rBV	1290908	2038283	10.84%	4.101%
3	6.227	404	406	413	rBV	1276161	1935733	10.29%	3.895%
4	6.330	413	415	418	rBV	1691016	1891546	10.06%	3.806%
5	6.559	433	435	445	rBV	380757	441546	2.35%	0.888%
6	6.719	447	449	451	rBV	1244291	1508256	8.02%	3.034%
7	7.142	483	486	488	rBV	1034672	1263714	6.72%	2.542%
8	7.850	545	548	550	rBV	506758	548459	2.92%	1.103%
9	8.925	639	642	645	rBV	1965969	2032613	10.81%	4.089%
10	9.325	675	677	681	rVB	269799	248465	1.32%	0.500%
11	9.588	698	700	703	rVV	624711	629042	3.35%	1.266%
12	10.376	767	769	772	rBV2	907758	1215292	6.46%	2.445%
13	10.616	787	790	792	rBV	299692	319000	1.70%	0.642%
14	11.062	827	829	839	rBV2	432886	620829	3.30%	1.249%
15	11.405	855	859	861	rBV	477141	646614	3.44%	1.301%
16	11.496	863	867	869	rBV	3874038	5648315	30.04%	11.364%
17	12.216	922	930	934	rBV2	4113085	18802845	100.00%	37.829%
18	12.285	934	936	938	rVB	2140491	2823728	15.02%	5.681%
19	12.662	966	969	971	rBV	944192	1312056	6.98%	2.640%
20	12.902	987	990	995	rVB	280578	509223	2.71%	1.025%
21	12.982	995	997	1002	rBV3	205280	556651	2.96%	1.120%
22	13.051	1002	1003	1009	rVV3	183042	445295	2.37%	0.896%
23	13.199	1013	1016	1022	rVV3	214674	397154	2.11%	0.799%
24	13.405	1031	1034	1039	rVB3	90664	198779	1.06%	0.400%
25	13.691	1057	1059	1066	rVB	350294	467823	2.49%	0.941%
26	15.051	1175	1178	1183	rBV	267191	418192	2.22%	0.841%

Sum of corrected areas: 49704248

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Misc :
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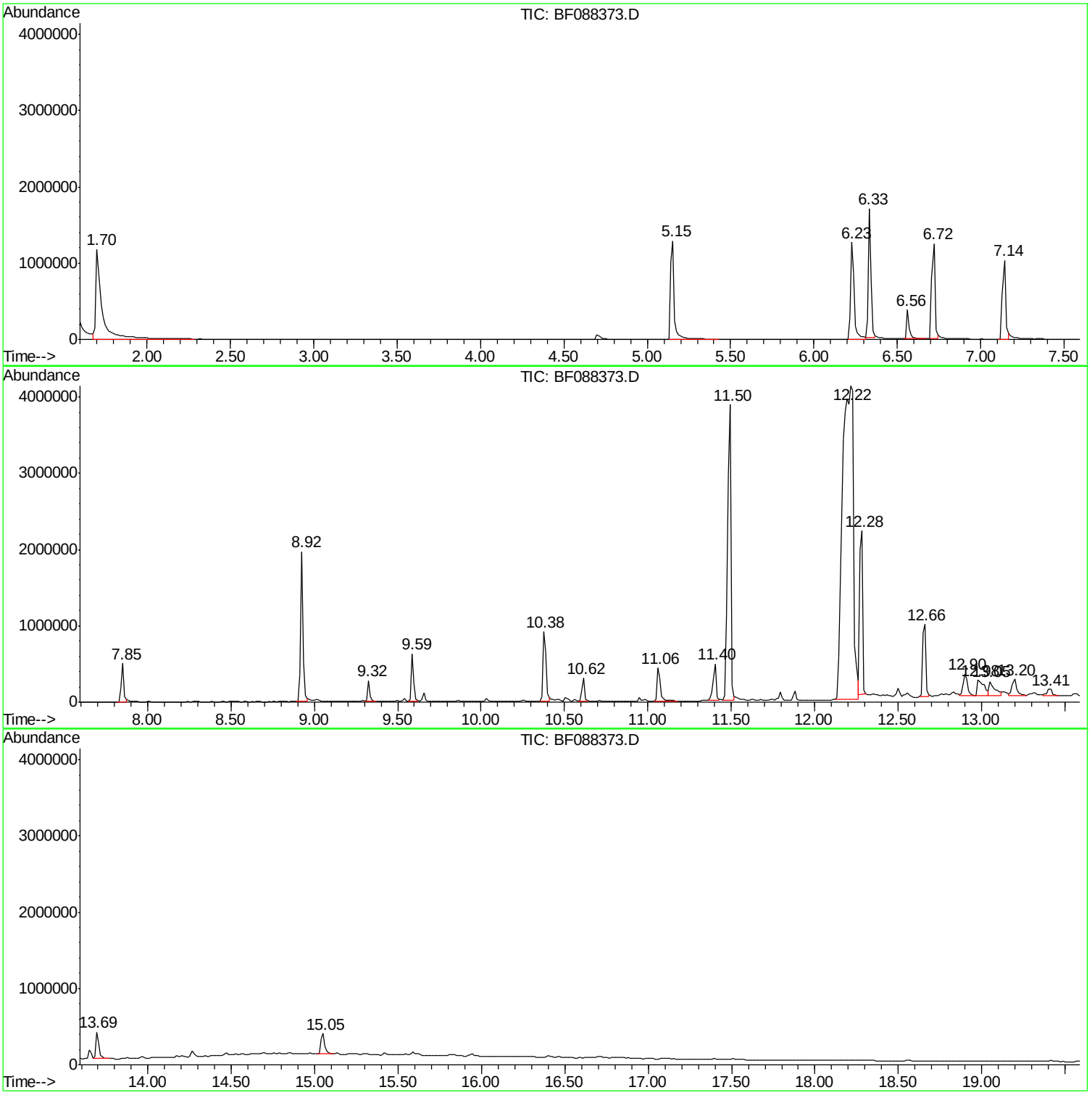
Instrument :
BNA_F
ClientSampleId :
P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062516\
Data File : BF088373.D
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Operator : UM/SJ
Sample : H3602-05
Misc :
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Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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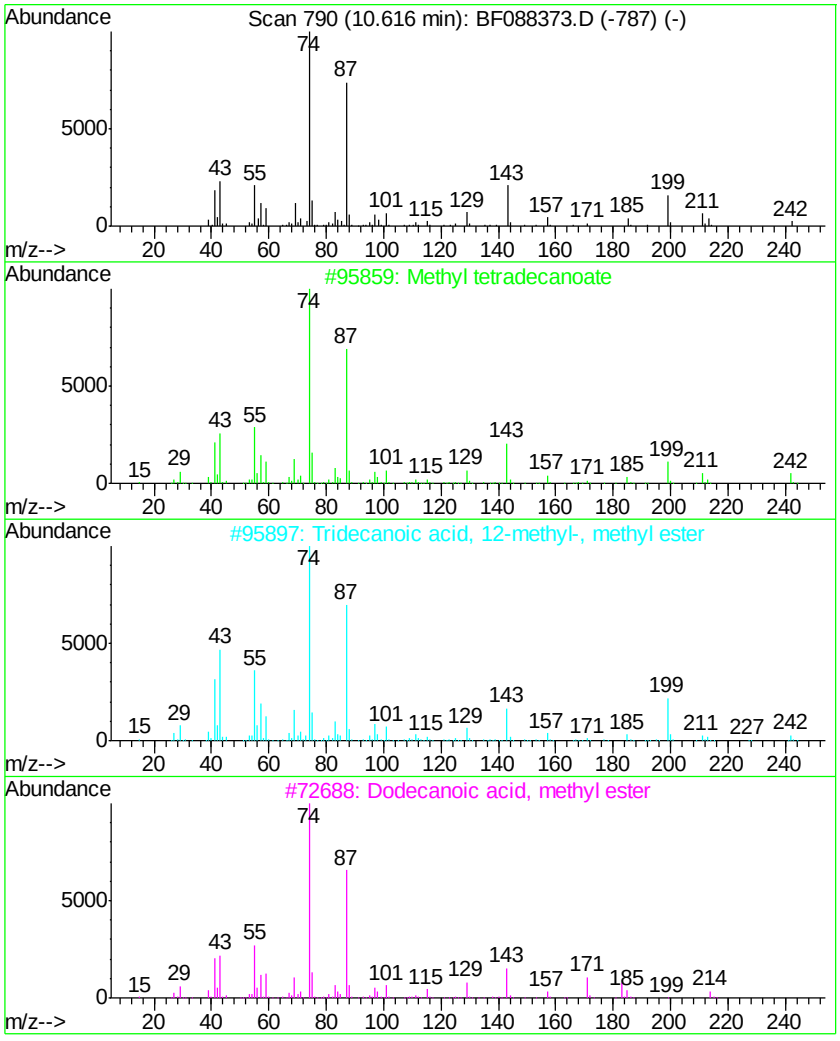
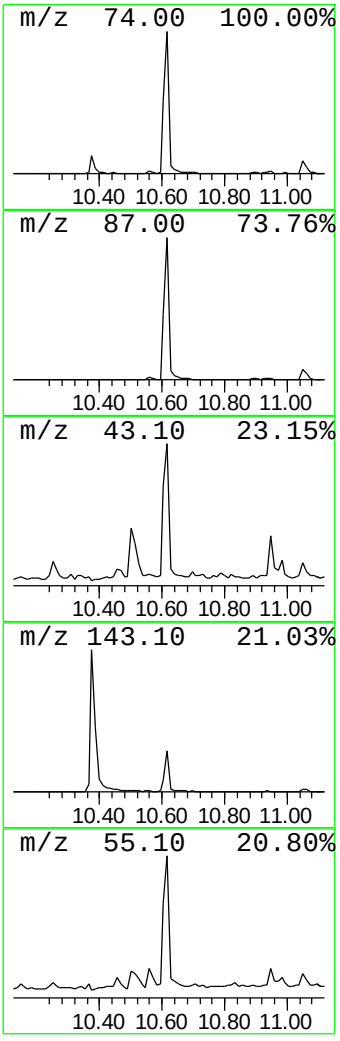
****

Peak Number 4 Methyl tetradecanoate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	10.28 ng	319000	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
2	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	89
3	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	80
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	72





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Data File : BF088373.D
Acq On : 25 Jun 2016 13:22
Operator : UM/SJ
Sample : H3602-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

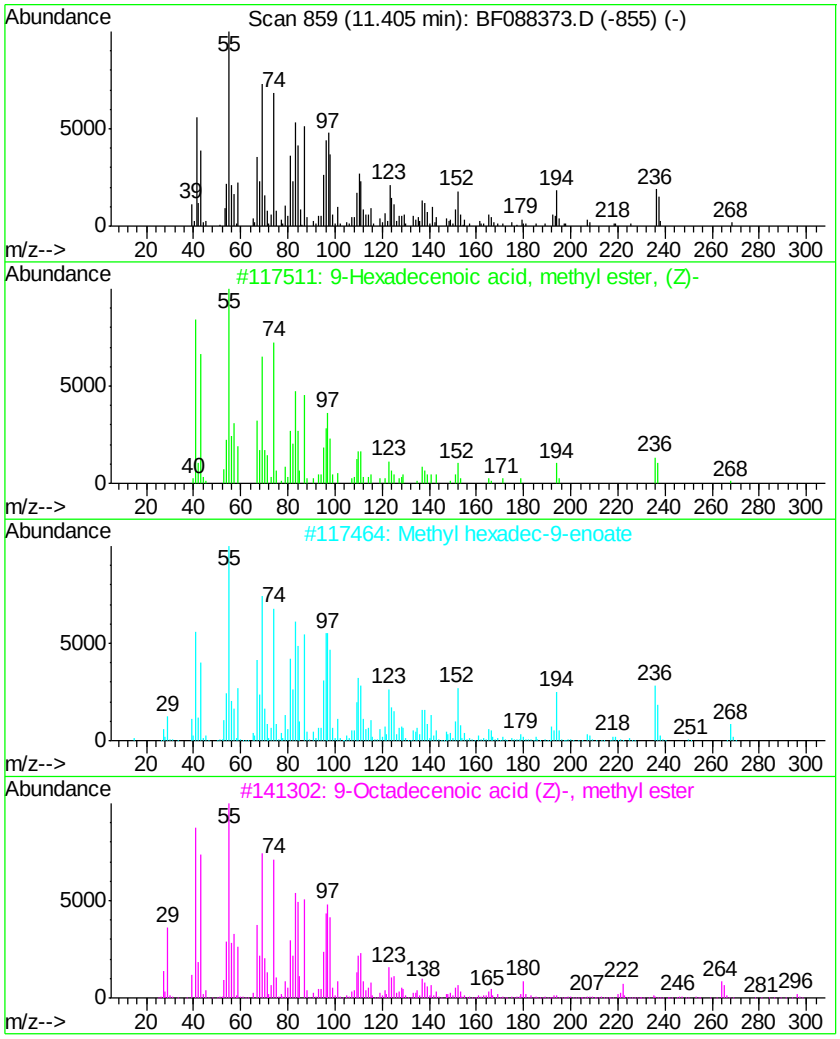
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

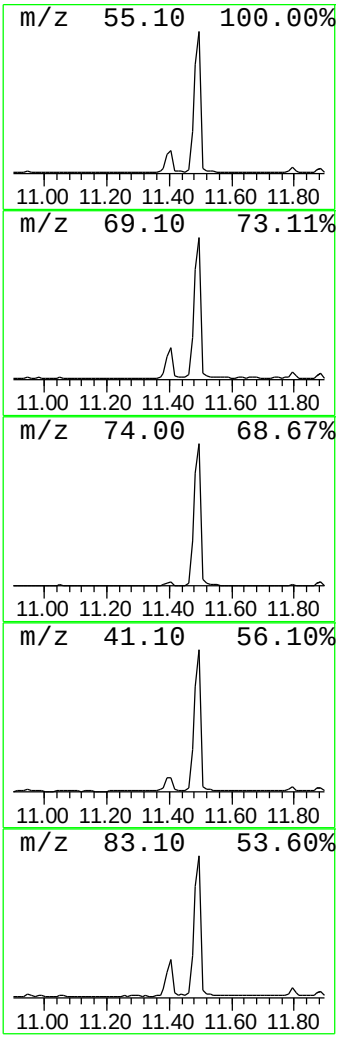
****

Peak Number 5 9-Hexadecenoic acid, methyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	20.83 ng	646614	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	99
2	Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	94
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
4	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	90
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062516\
Data File : BF088373.D
Acq On : 25 Jun 2016 13:22
Operator : UM/SJ
Sample : H3602-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

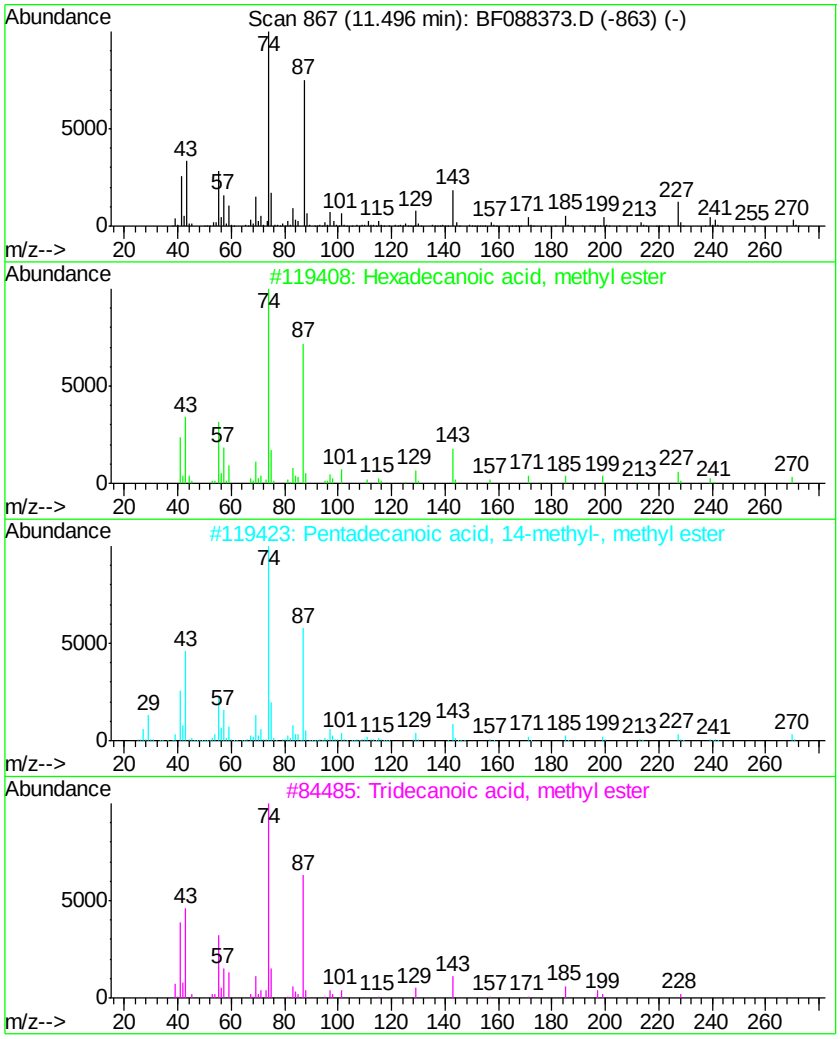
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

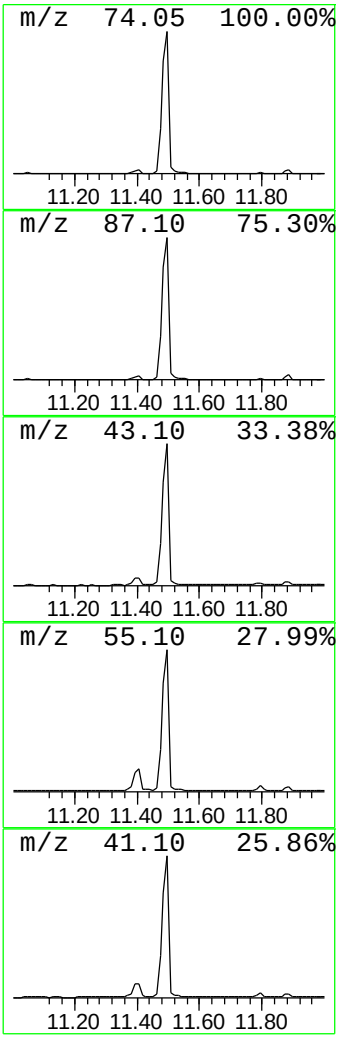
****

Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	181.96 ng	5648320	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062516\
Data File : BF088373.D
Acq On : 25 Jun 2016 13:22
Operator : UM/SJ
Sample : H3602-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

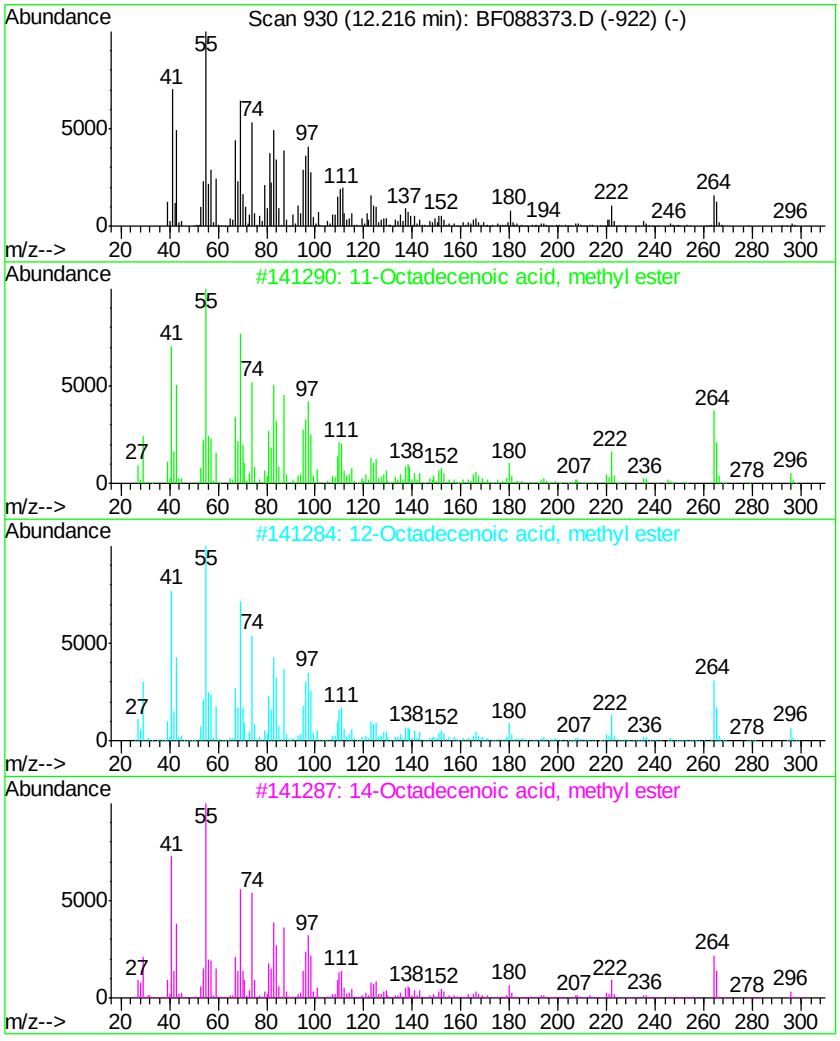
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

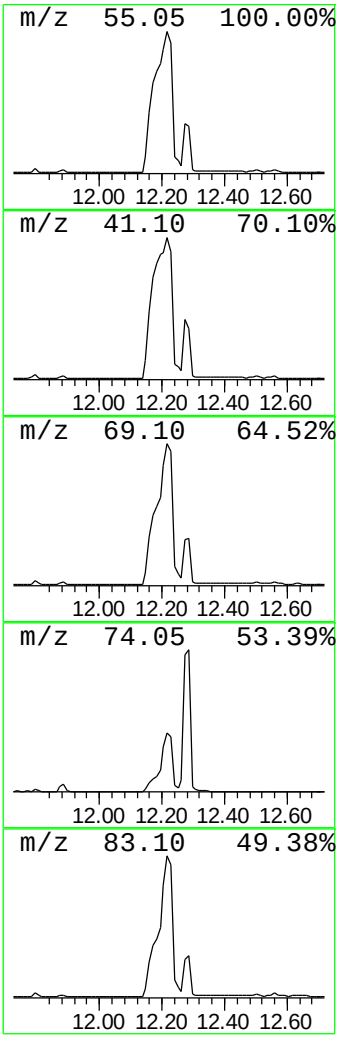
****

Peak Number 7 11-Octadecenoic acid, methy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.22	605.73 ng	18802800	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
4	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
5	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062516\
Data File : BF088373.D
Acq On : 25 Jun 2016 13:22
Operator : UM/SJ
Sample : H3602-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

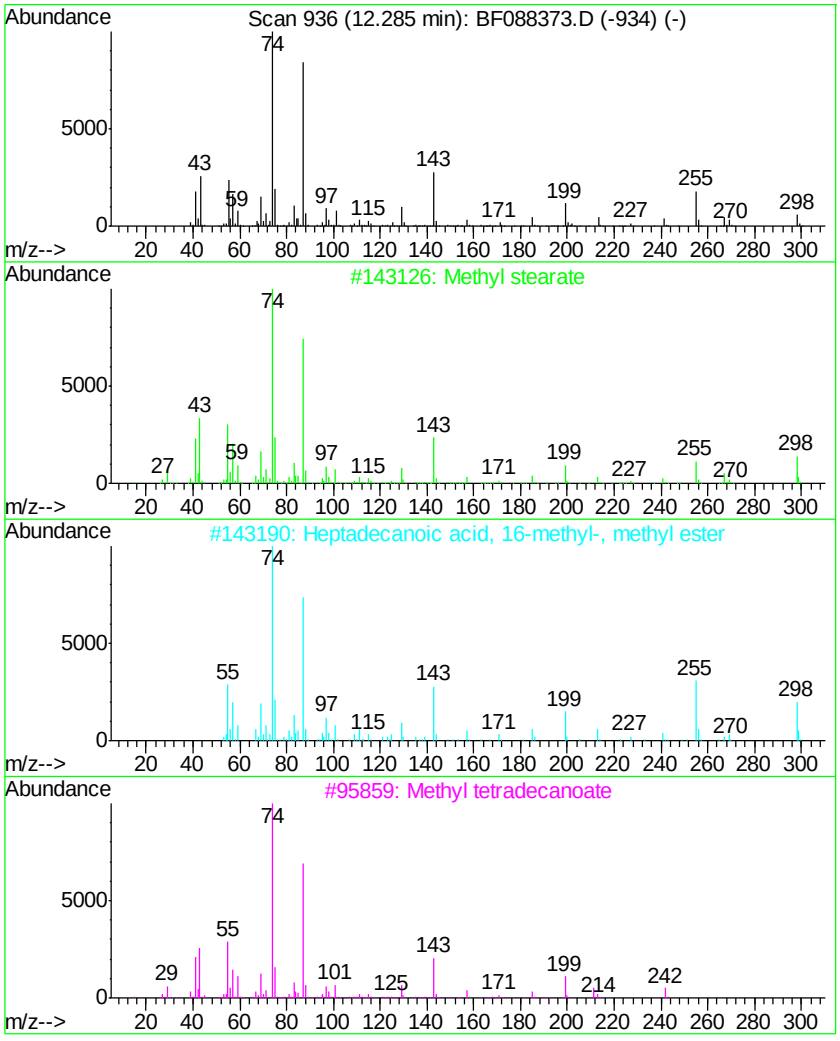
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

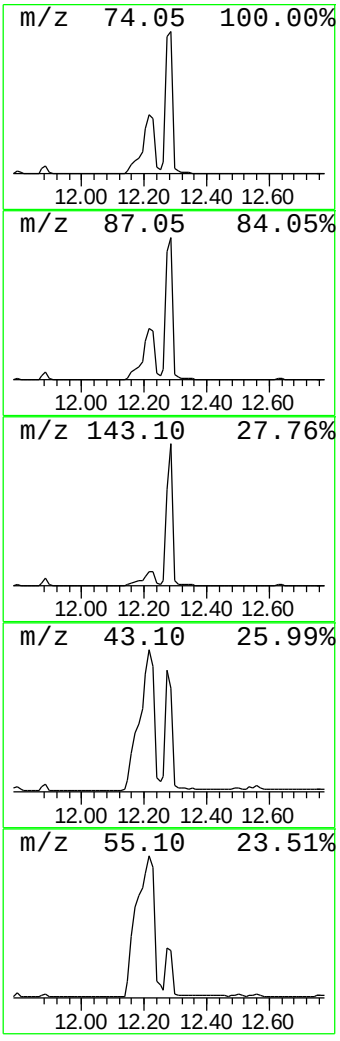
****

Peak Number 8 Methyl stearate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	90.97 ng	2823730	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
4	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	81





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Data File : BF088373.D
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Operator : UM/SJ
Sample : H3602-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

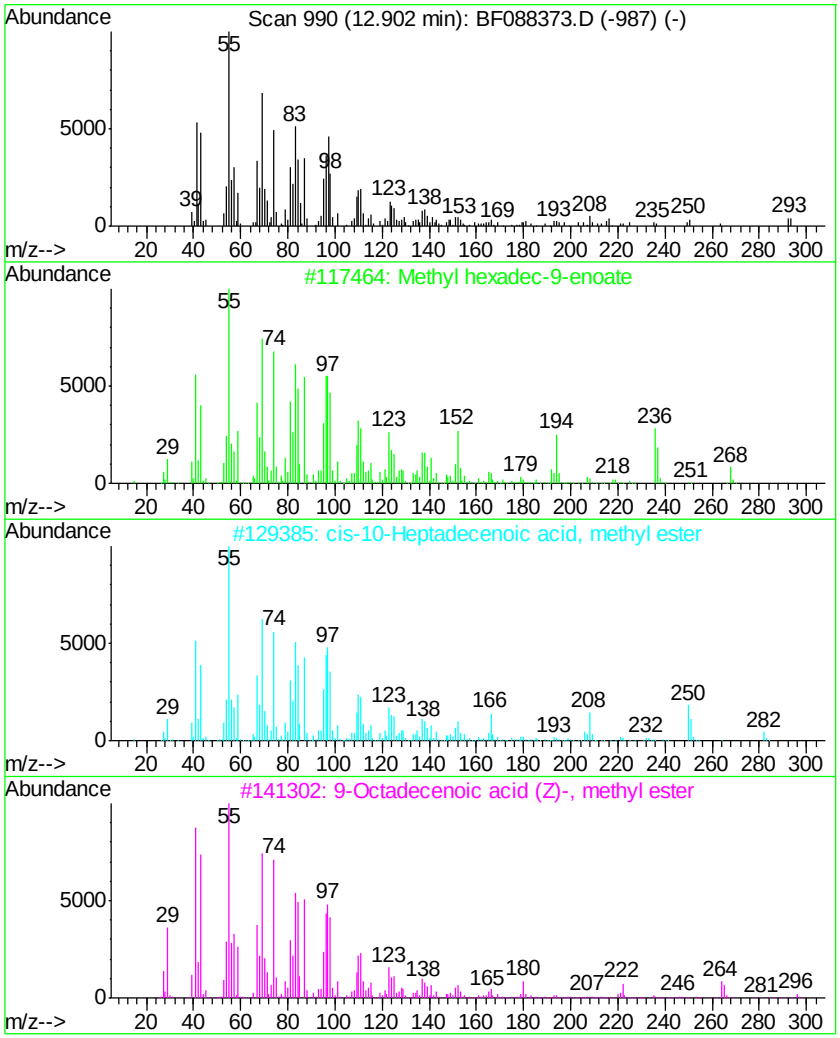
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

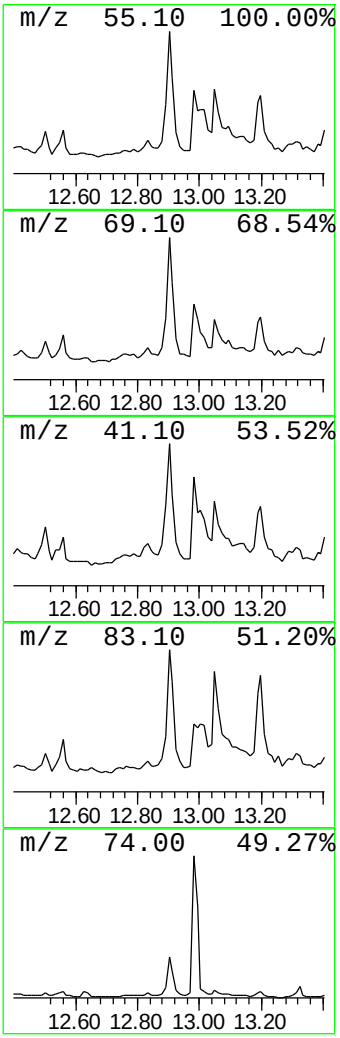
****

Peak Number 9 Methyl hexadec-9-enoate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.90	21.77 ng	509223	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl hexadec-9-enoate	268	C17H32O2	010030-74-7	91
2	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	91
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	90
4	Methyl 13-eicosenoate	324	C21H40O2	1000336-48-4	86
5	Methyl 9-heptadecenoate or 9-17:1	282	C18H34O2	1000336-38-0	80





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Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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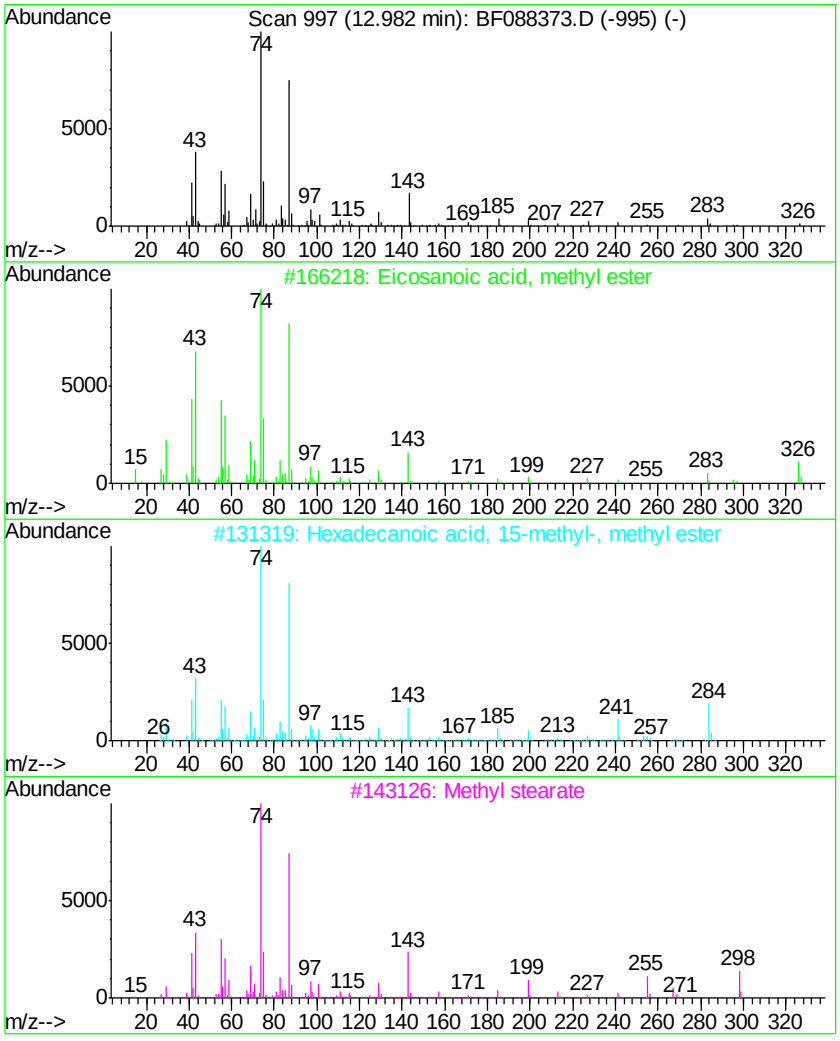
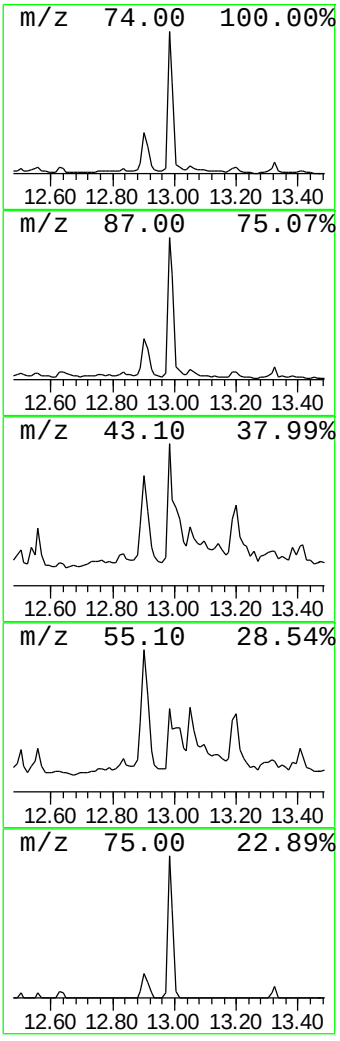
****

Peak Number 10 Eicosanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	23.80 ng	556651	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	96
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	94
3	Methyl stearate	298	C19H38O2	000112-61-8	91
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	90
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90





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Sample : H3602-05
Misc :
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Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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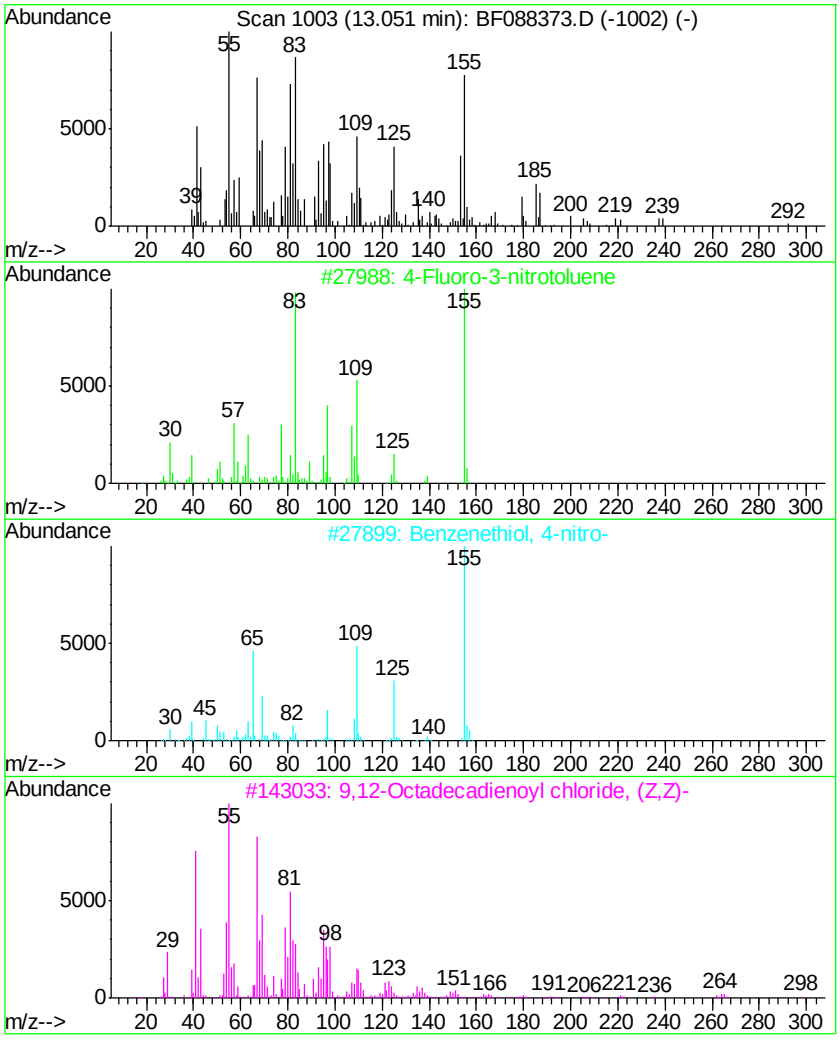
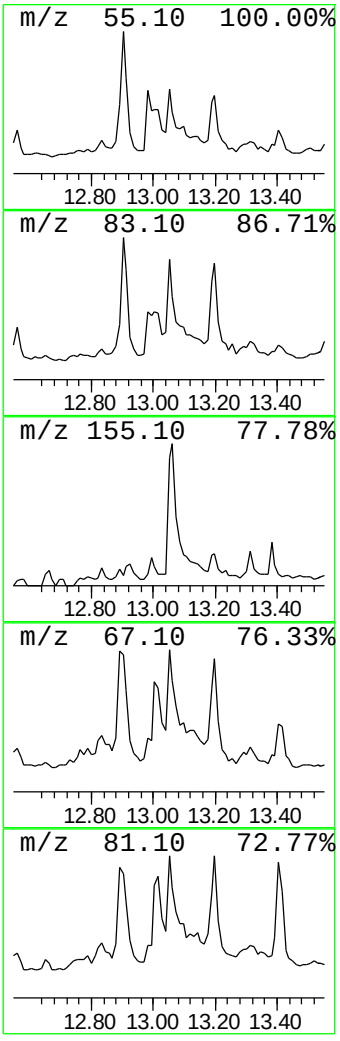
Peak Number 11 unknown13.05 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.05	19.04 ng	445295	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluoro-3-nitrotoluene	155	C7H6FNO2	000446-11-7	47
2	Benzenethiol, 4-nitro-	155	C6H5NO2S	001849-36-1	22
3	9,12-Octadecadienoyl chloride, (...	298	C18H31ClO	007459-33-8	22
4	(E)-But-2-enyl (E)-2-methylbut-2...	154	C9H14O2	1000373-71-7	22
5	3-Tetradecyne	194	C14H26	060212-32-0	22





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Sample : H3602-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

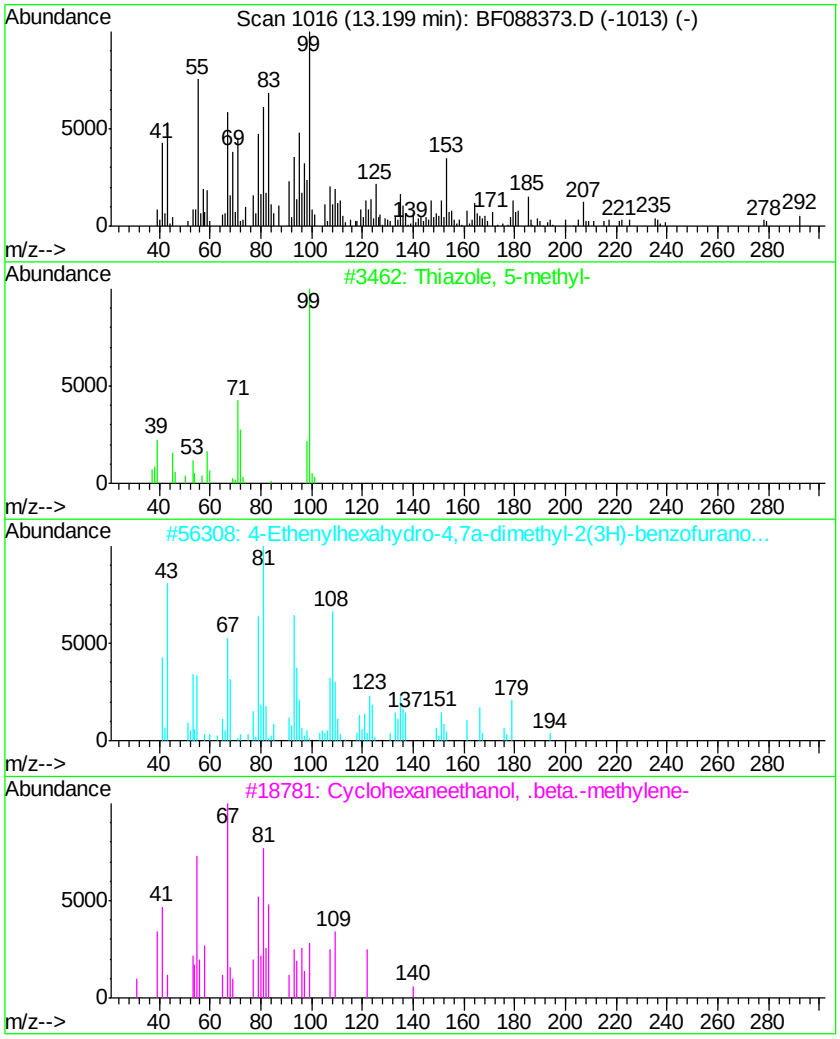
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

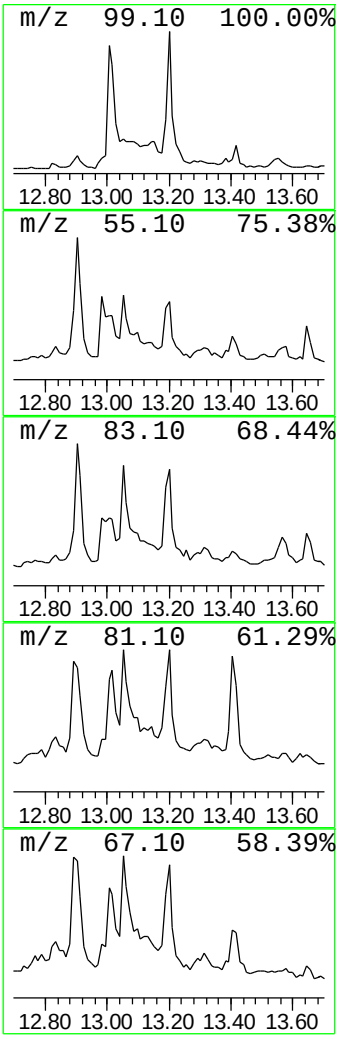
****

Peak Number 12 unknown13.20 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	16.98 ng	397154	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazole, 5-methyl-	99	C4H5NS	003581-89-3	30
2	4-Ethenylhexahydro-4,7a-dimethyl...	194	C12H18O2	086003-24-9	25
3	Cyclohexaneethanol, .beta.-methy...	140	C9H16O	007697-55-4	25
4	2-Propylthiazole	127	C6H9NS	017626-75-4	20
5	7-Oxabicyclo[4.1.0]heptane, 1-me...	168	C10H16O2	000096-08-2	18





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Data File : BF088373.D
Acq On : 25 Jun 2016 13:22
Operator : UM/SJ
Sample : H3602-05
Misc :
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Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

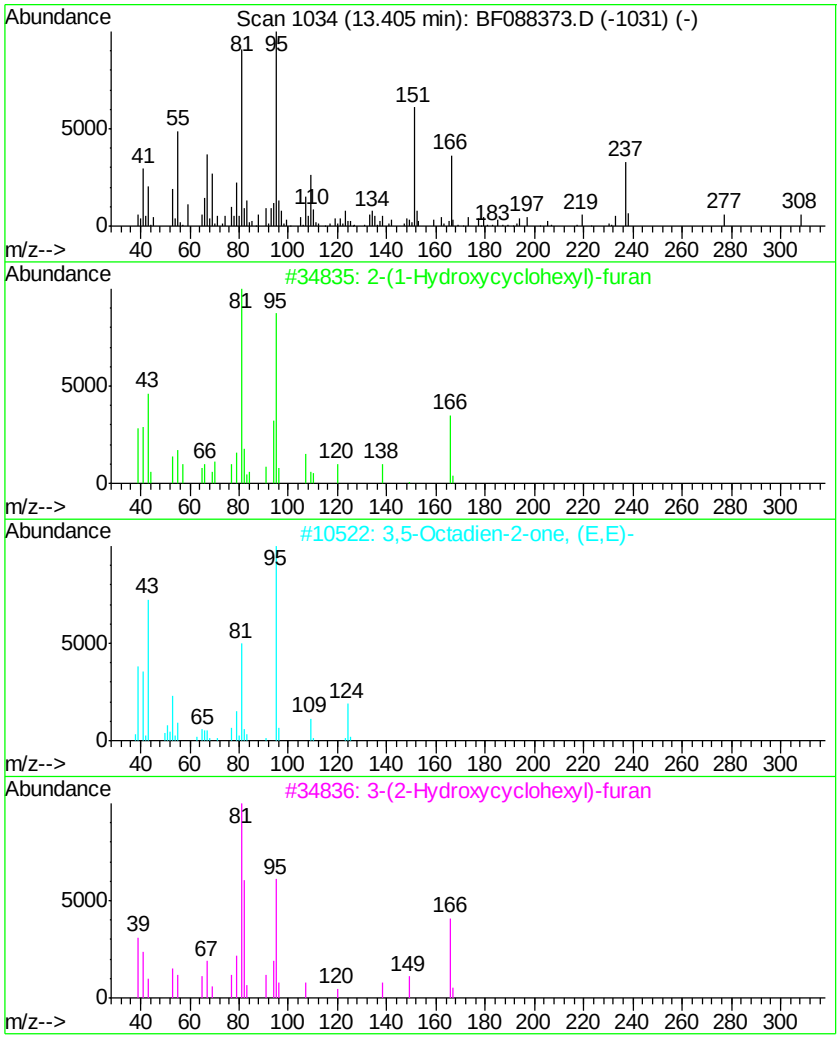
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

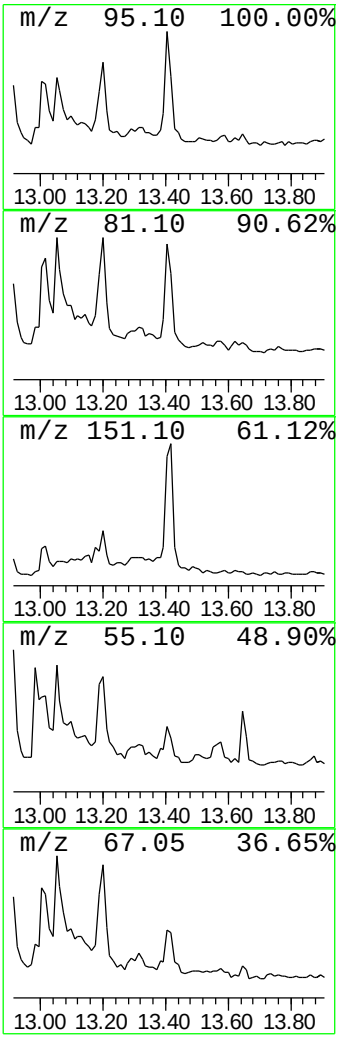
****

Peak Number 13 2-(1-Hydroxycyclohexyl)-furan Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	8.50 ng	198779	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(1-Hydroxycyclohexyl)-furan	166	C10H14O2	036169-67-2	58
2	3,5-Octadien-2-one, (E,E)-	124	C8H12O	030086-02-3	43
3	3-(2-Hydroxycyclohexyl)-furan	166	C10H14O2	118959-04-9	43
4	1,4 Benzodioxan-6-amine	151	C8H9NO2	022013-33-8	30
5	Furan-2-carboxamide, N-(5-chloro...	237	C11H8ClNO3	075748-60-6	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062516\
Data File : BF088373.D
Acq On : 25 Jun 2016 13:22
Operator : UM/SJ
Sample : H3602-05
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P8-B2(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Methyl tetradecan...	10.62	10.3	ng	319000	4	11.06	620829	20.0
9-Hexadecenoic ac...	11.40	20.8	ng	646614	4	11.06	620829	20.0
Hexadecanoic acid...	11.50	182.0	ng	5648320	4	11.06	620829	20.0
11-Octadecenoic a...	12.22	605.7	ng	18802800	4	11.06	620829	20.0
Methyl stearate	12.28	91.0	ng	2823730	4	11.06	620829	20.0
Methyl hexadec-9-...	12.90	21.8	ng	509223	5	13.69	467823	20.0
Eicosanoic acid, ...	12.98	23.8	ng	556651	5	13.69	467823	20.0
unknown13.05	13.05	19.0	ng	445295	5	13.69	467823	20.0
unknown13.20	13.20	17.0	ng	397154	5	13.69	467823	20.0
2-(1-Hydroxycyclo...	13.41	8.5	ng	198779	5	13.69	467823	20.0