LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081339.D
Acq On : 2 Sep 2015 10:17
Operator : UM/IZ
Sample : G3479-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-8(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-BF090115.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	4.444	247	250	264	rVB	602336	1259658	57.68%	7.163%
2	4.936	291	293	296	rBV	1445830	1778304	81.44%	10.112%
3	6.056	388	391	393	rBV	1817043	2183695	100.00%	12.417%
4	6.159	397	400	402	rVV	1379231	1887997	86.46%	10.736%
5	6.387	418	420	422	rBV	438381	382797	17.53%	2.177%
6	6.547	431	434	436	rBV	977083	1278246	58.54%	7.269%
7	6.959	468	470	473	rBV	871866	1116244	51.12%	6.347%
8	7.679	530	533	535	rBV	470176	490741	22.47%	2.791%
9	8.753	625	627	630	rBV	1321570	1734863	79.45%	9.865%
10	9.165	660	663	665	rBV	298882	308498	14.13%	1.754%
11	9.416	683	685	687	rVB	618343	545688	24.99%	3.103%
12	9.885	724	726	727	rVB	24769	22760	1.04%	0.129%
13	10.193	751	753	756	rBV2	905102	1053315	48.24%	5.990%
14	10.353	765	767	771	rBV	39687	59597	2.73%	0.339%
15	10.788	804	805	807	rBV	34511	46847	2.15%	0.266%
16	10.879	811	813	815	rBV	650119	536120	24.55%	3.049%
17	11.222	840	843	845	rVB	34118	43911	2.01%	0.250%
18	11.451	861	863	867	rBV2	54728	65316	2.99%	0.371%
19	11.531	867	870	874	rVB2	13321	21841	1.00%	0.124%
20	11.622	875	878	880	rBV	37859	33299	1.52%	0.189%
21	12.319	937	939	942	rBV	62478	59311	2.72%	0.337%
22	12.468	949	952	954	rBV	1619508	1551250	71.04%	8.821%
23	13.028	998	1001	1003	rBV	33522	41862	1.92%	0.238%
24	13.394	1030	1033	1039	rBV	128461	275200	12.60%	1.565%
25	13.485	1039	1041	1044	rVV	483402	425389	19.48%	2.419%
26	14.800	1153	1156	1158	rBV	311850	322166	14.75%	1.832%
27	15.245	1193	1195	1206	rVB2	18379	60870	2.79%	0.346%

Sum of corrected areas: 17585785

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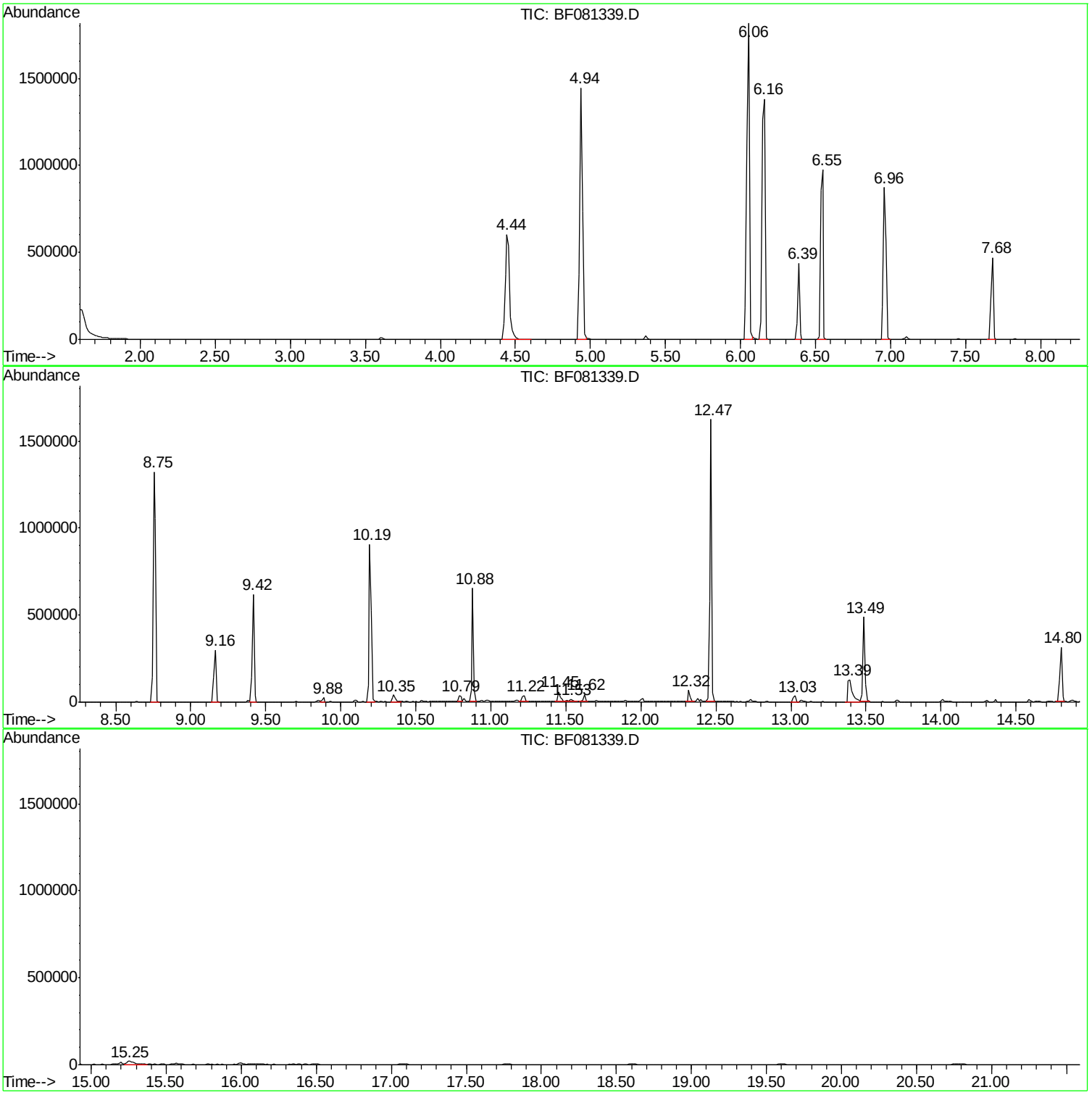
Instrument : BNA_F
ClientSampleId : COFF-3-8(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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Sample : G3479-15
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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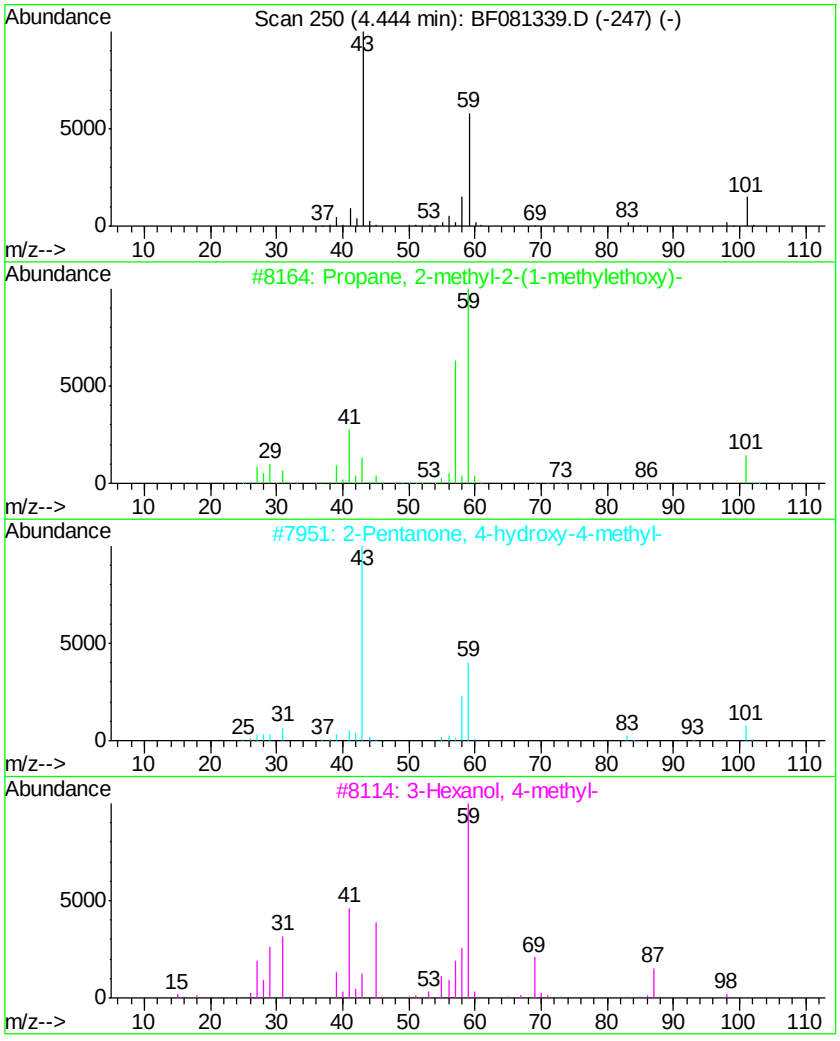
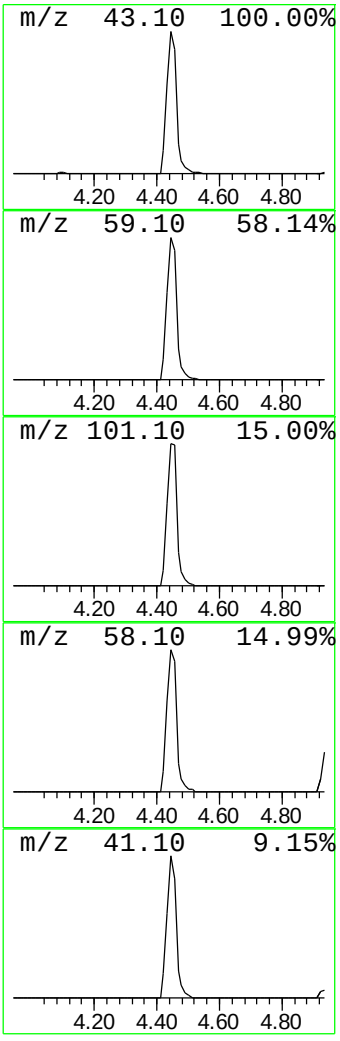
Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	65.81 ng	1259660	1,4-Dichlorobenzene-d4	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





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Operator : UM/IZ
Sample : G3479-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-8(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

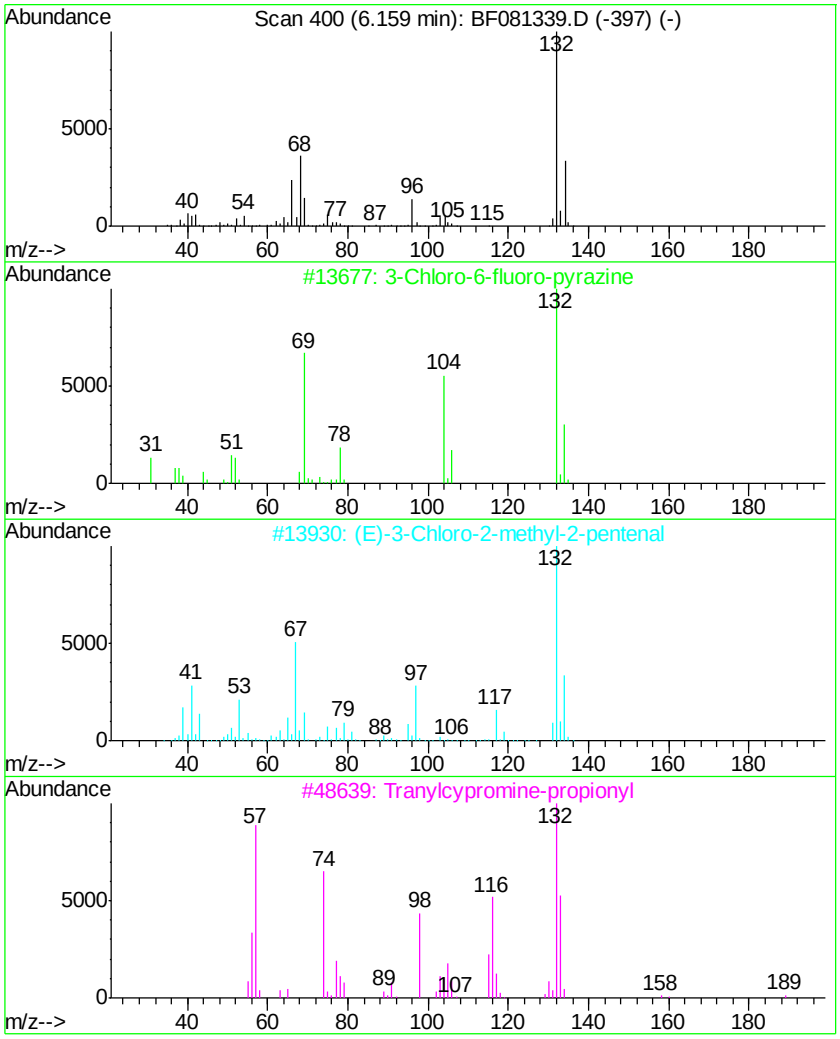
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

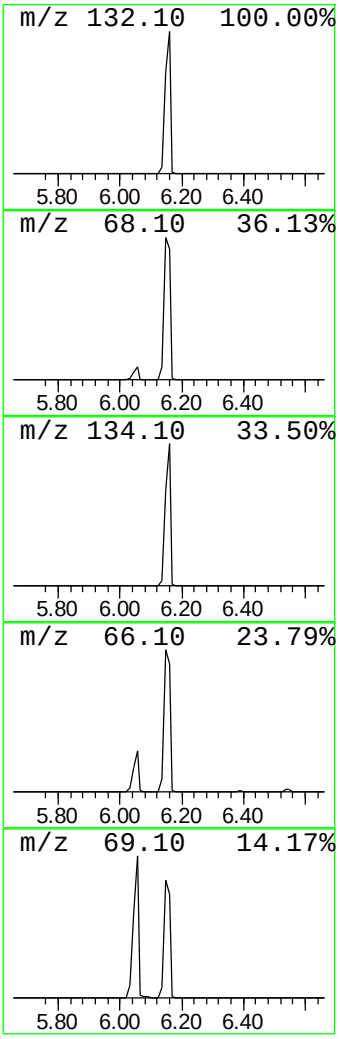
****

Peak Number 2 unknown6.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	98.64 ng	1888000	1,4-Dichlorobenzene-d4	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
Data File : BF081339.D
Acq On : 2 Sep 2015 10:17
Operator : UM/IZ
Sample : G3479-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-8(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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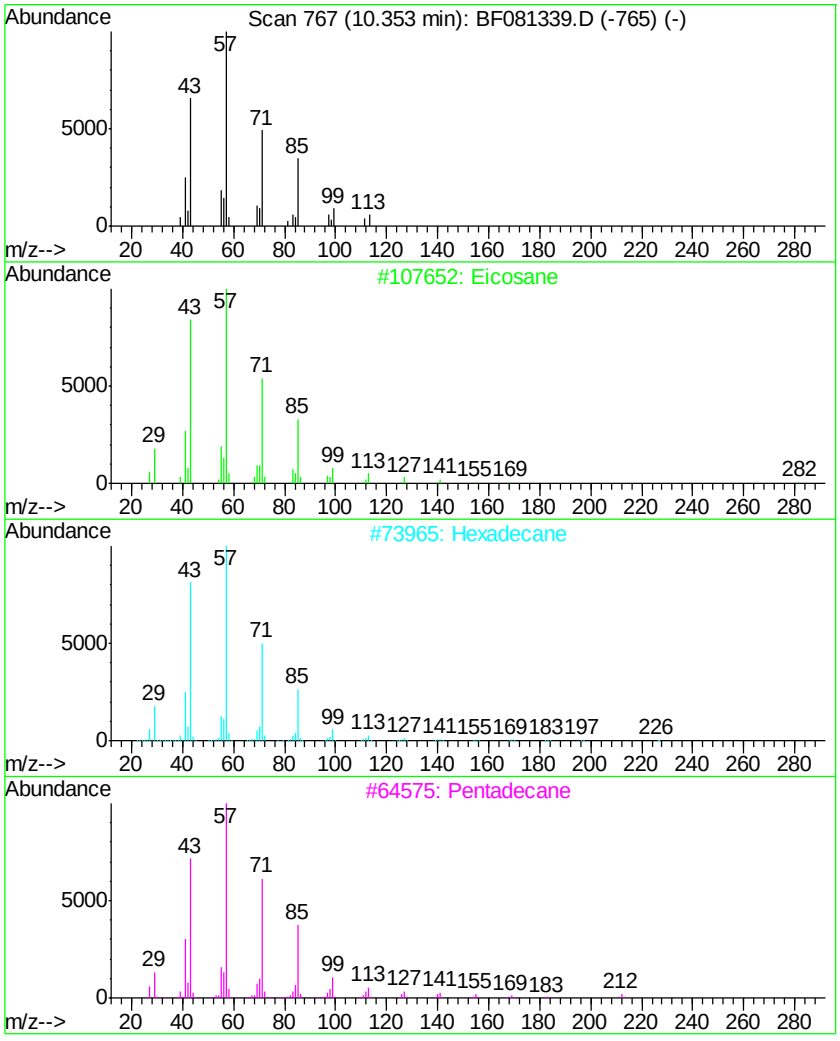
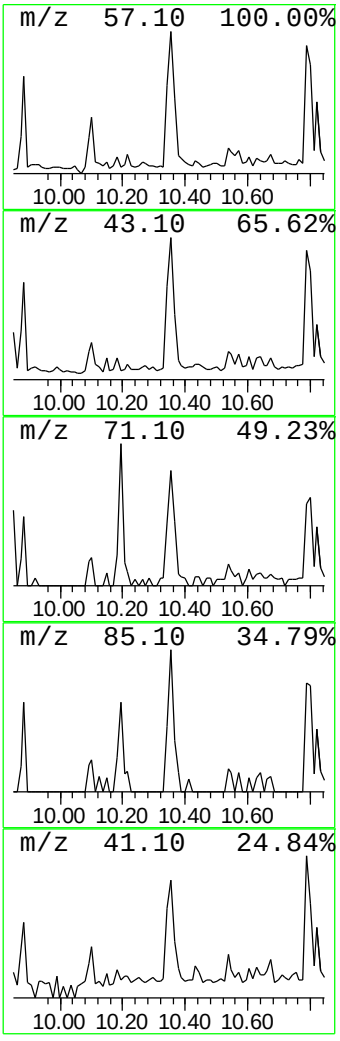
Peak Number 4 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.22 ng	59597	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Hexadecane	226	C16H34	000544-76-3	83
3	Pentadecane	212	C15H32	000629-62-9	72
4	Tridecane	184	C13H28	000629-50-5	64
5	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	59





Library Search Compound Report

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Data File : BF081339.D
Acq On : 2 Sep 2015 10:17
Operator : UM/IZ
Sample : G3479-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-8(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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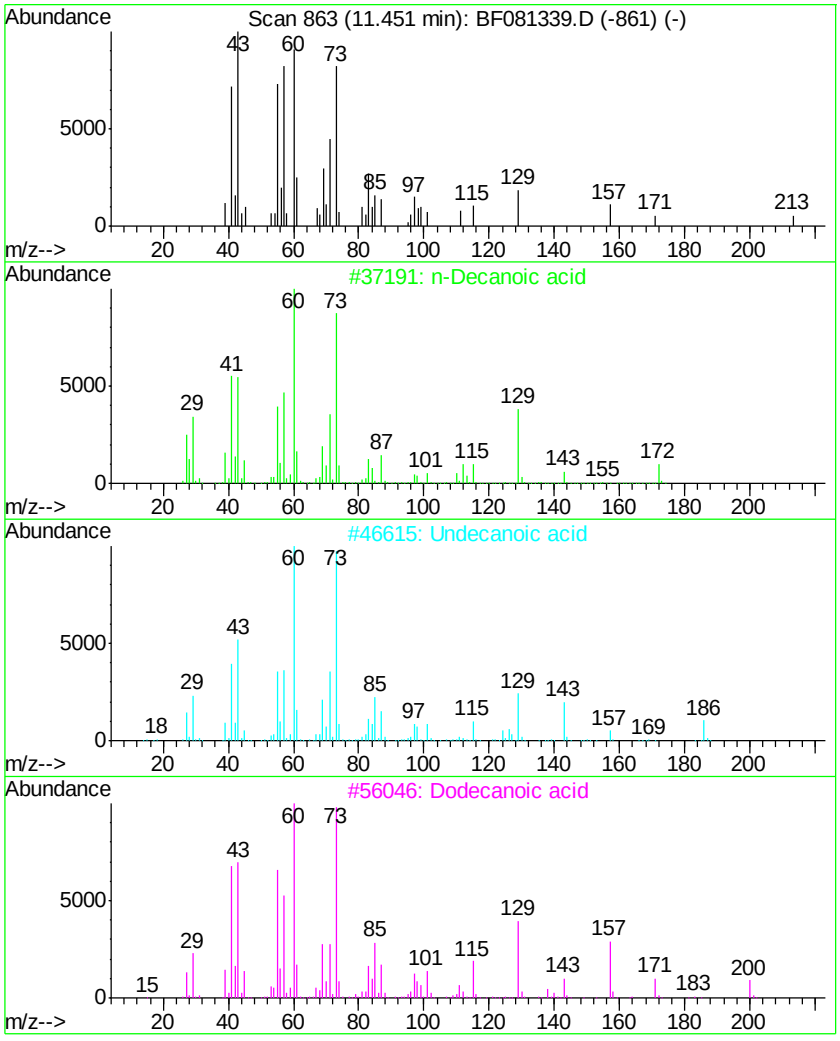
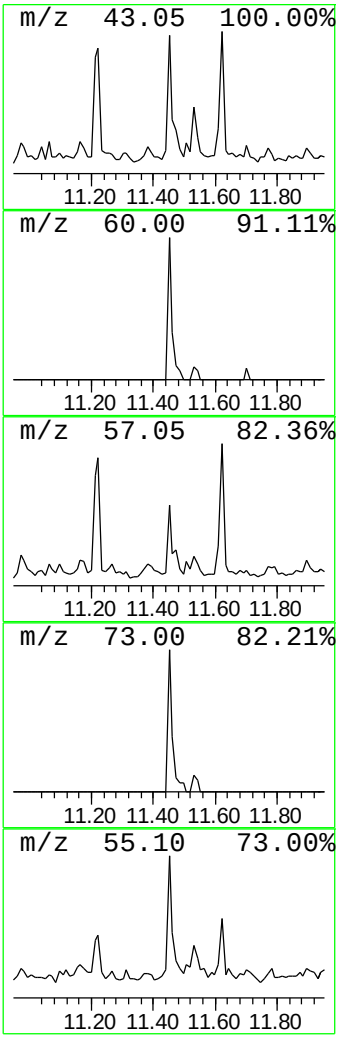
Peak Number 5 n-Decanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	2.44 ng	65316	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	64
2	Undecanoic acid	186	C11H22O2	000112-37-8	59
3	Dodecanoic acid	200	C12H24O2	000143-07-7	59
4	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	53
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47





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Data File : BF081339.D
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Operator : UM/IZ
Sample : G3479-15
Misc :
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Instrument : BNA_F
ClientSampleId : COFF-3-8(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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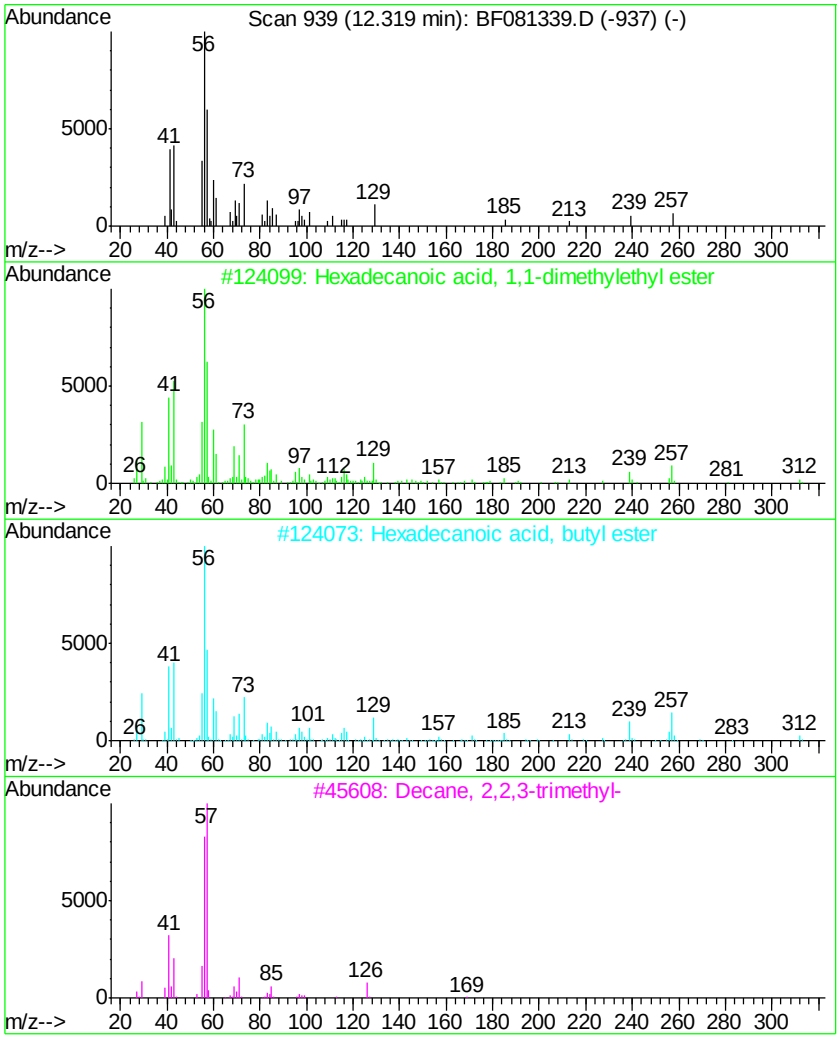
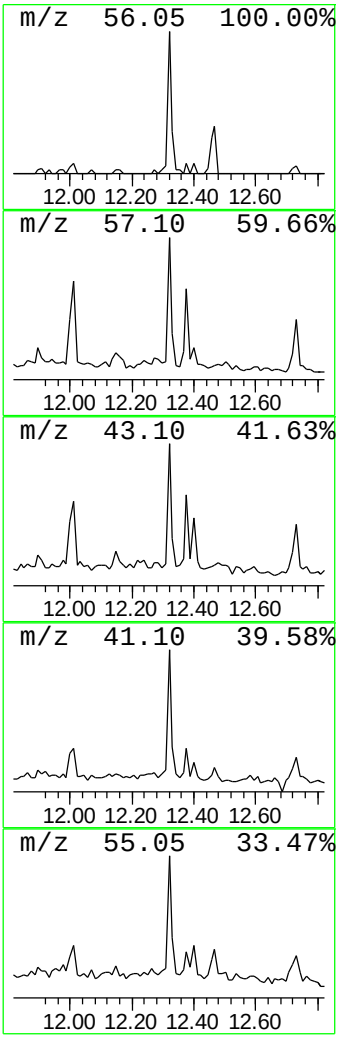
Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	2.79 ng	59311	Chrysene-d12	13.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
3	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	38
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	37
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35





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Acq On : 2 Sep 2015 10:17
Operator : UM/IZ
Sample : G3479-15
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-8(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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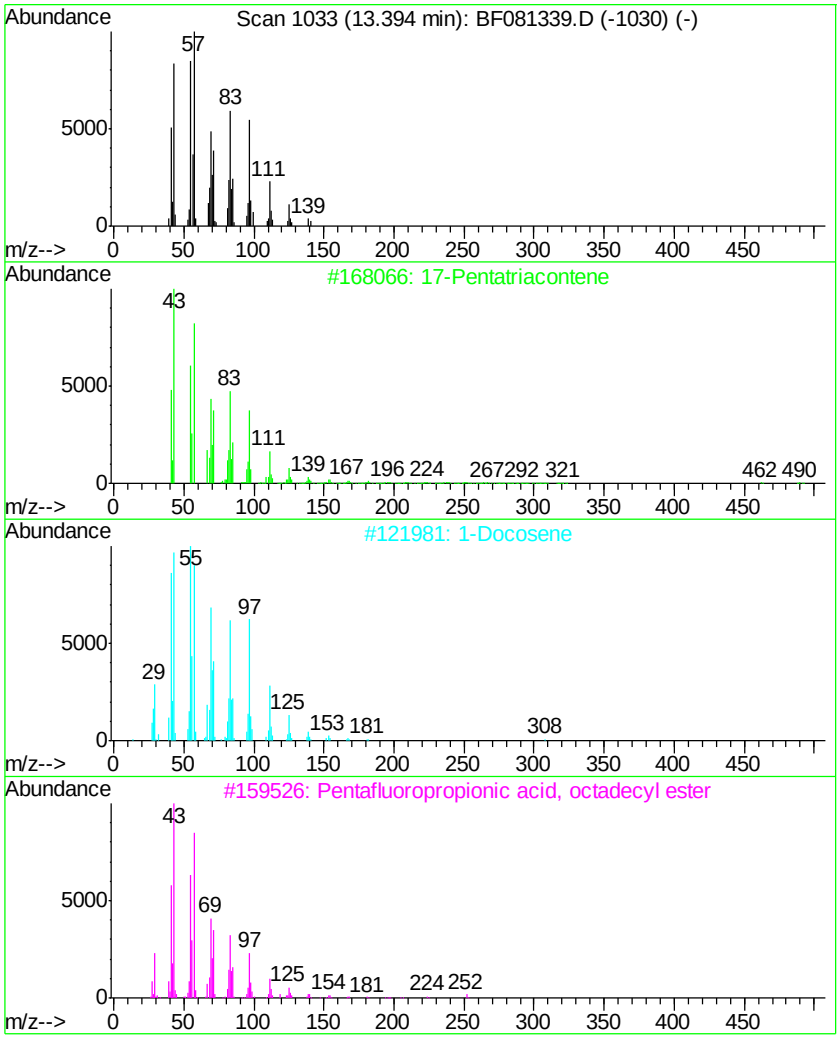
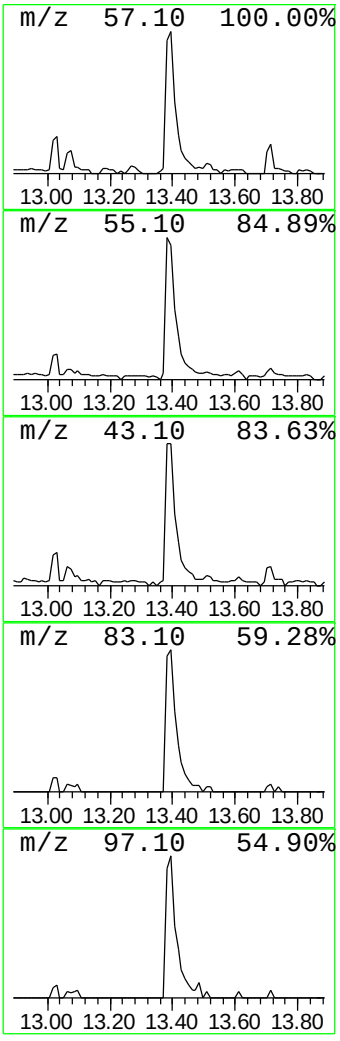
Peak Number 7 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	12.94 ng	275200	Chrysene-d12	13.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	90
2	1-Docosene	308	C22H44	001599-67-3	87
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	87
4	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	86
5	1-Hexacosanol	382	C26H54O	000506-52-5	83





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Sample : G3479-15
Misc :
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Instrument : BNA_F
ClientSampleId : COFF-3-8(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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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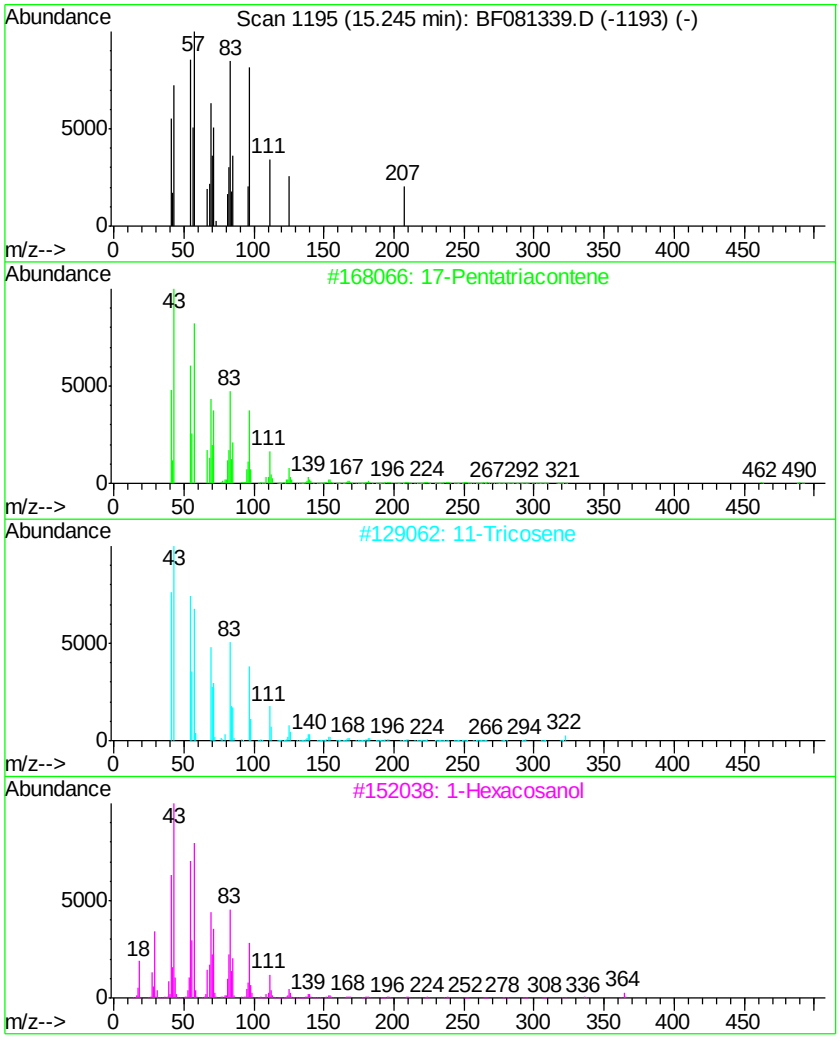
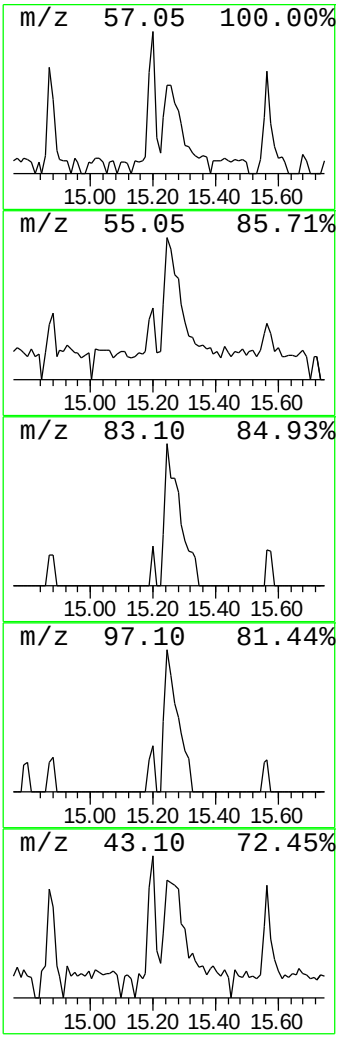
Peak Number 8 11-Tricosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	3.78 ng	60870	Perylene-d12	14.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	80
2	11-Tricosene	322	C23H46	052078-56-5	64
3	1-Hexacosanol	382	C26H54O	000506-52-5	46
4	1-Tetracosanol	354	C24H50O	000506-51-4	46
5	1-Eicosanol	298	C20H42O	000629-96-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090215\
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Acq On : 2 Sep 2015 10:17
Operator : UM/IZ
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Misc :
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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
Propane, 2-methyl...	4.44	65.8	ng	1259660	1	6.39	382797	20.0
unknown6.16	6.16	98.6	ng	1888000	1	6.39	382797	20.0
Eicosane	10.35	2.2	ng	59597	4	10.88	536120	20.0
n-Decanoic acid	11.45	2.4	ng	65316	4	10.88	536120	20.0
Hexadecanoic acid...	12.32	2.8	ng	59311	5	13.49	425389	20.0
17-Pentatriacontene	13.39	12.9	ng	275200	5	13.49	425389	20.0
11-Tricosene	15.25	3.8	ng	60870	6	14.80	322166	20.0