LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085518.D
Acq On : 18 Mar 2016 3:53
Operator : UM/SJ
Sample : H1774-18
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

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-BF031516.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	5.087	242	245	249	rBV	42998	74564	2.16%	0.240%
2	5.476	276	279	282	rBV	2496234	3078816	89.02%	9.905%
3	6.504	367	369	372	rBV	2213325	3458674	100.00%	11.127%
4	6.642	378	381	384	rBV	3031682	3169053	91.63%	10.195%
5	6.870	399	401	404	rBV	727730	755932	21.86%	2.432%
6	7.030	412	415	418	rBV	2703796	2540669	73.46%	8.173%
7	7.442	448	451	453	rBV	2224740	2305067	66.65%	7.416%
8	7.533	456	459	461	rVV	39725	56394	1.63%	0.181%
9	8.162	511	514	516	rBV	1214078	1063569	30.75%	3.422%
10	9.236	605	608	611	rBV	3123562	3448308	99.70%	11.093%
11	9.305	612	614	617	rVB2	37175	43984	1.27%	0.141%
12	9.636	640	643	644	rBV	500657	578235	16.72%	1.860%
13	9.853	658	662	664	rBV2	67624	100667	2.91%	0.324%
14	9.922	665	668	669	rBV	739164	1041776	30.12%	3.351%
15	10.345	704	705	707	rVB	125767	108418	3.13%	0.349%
16	10.562	721	724	728	rBV	42417	81464	2.36%	0.262%
17	10.699	733	736	739	rBV2	1469837	2204762	63.75%	7.093%
18	10.825	745	747	753	rBV	107835	169205	4.89%	0.544%
19	11.271	784	786	787	rBV	68349	69584	2.01%	0.224%
20	11.396	795	797	800	rBV	1133382	1014210	29.32%	3.263%
21	11.453	800	802	806	rVB2	18249	36052	1.04%	0.116%
22	11.922	841	843	855	rVB2	139445	208115	6.02%	0.670%
23	12.711	910	912	918	rBV	47873	61207	1.77%	0.197%
24	12.802	918	920	922	rBV	92373	86798	2.51%	0.279%
25	12.985	933	936	938	rBV	3085404	2803740	81.06%	9.020%
26	13.511	980	982	983	rBV	68023	55878	1.62%	0.180%
27	13.877	1011	1014	1025	rBV	558094	659504	19.07%	2.122%
28	14.037	1025	1028	1030	rBV	660259	766450	22.16%	2.466%
29	14.197	1040	1042	1045	rBV	32487	40276	1.16%	0.130%
30	14.505	1067	1069	1075	rBV	88788	120402	3.48%	0.387%
31	15.465	1150	1153	1156	rBV	546947	716353	20.71%	2.305%
32	15.968	1194	1197	1200	rBV2	39991	68987	1.99%	0.222%
33	16.437	1236	1238	1244	rVB	29352	57347	1.66%	0.184%
34	17.065	1288	1293	1294	rBV4	12902	39780	1.15%	0.128%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085518.D
Acq On : 18 Mar 2016 3:53
Operator : UM/SJ
Sample : H1774-18
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

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-BF031516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

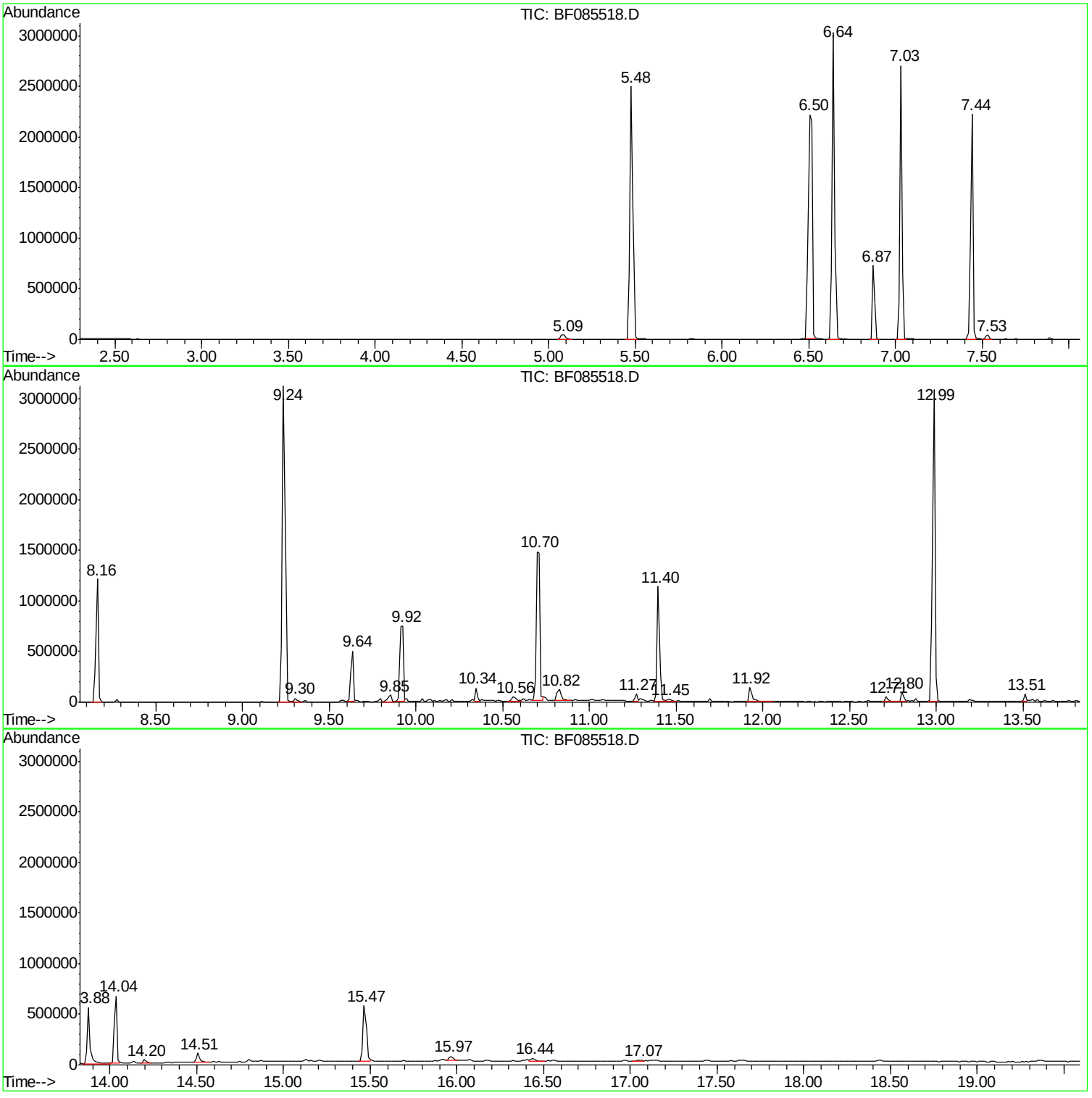
Sum of corrected areas: 31084240

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085518.D
Acq On : 18 Mar 2016 3:53
Operator : UM/SJ
Sample : H1774-18
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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\BF031716\
Data File : BF085518.D
Acq On : 18 Mar 2016 3:53
Operator : UM/SJ
Sample : H1774-18
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ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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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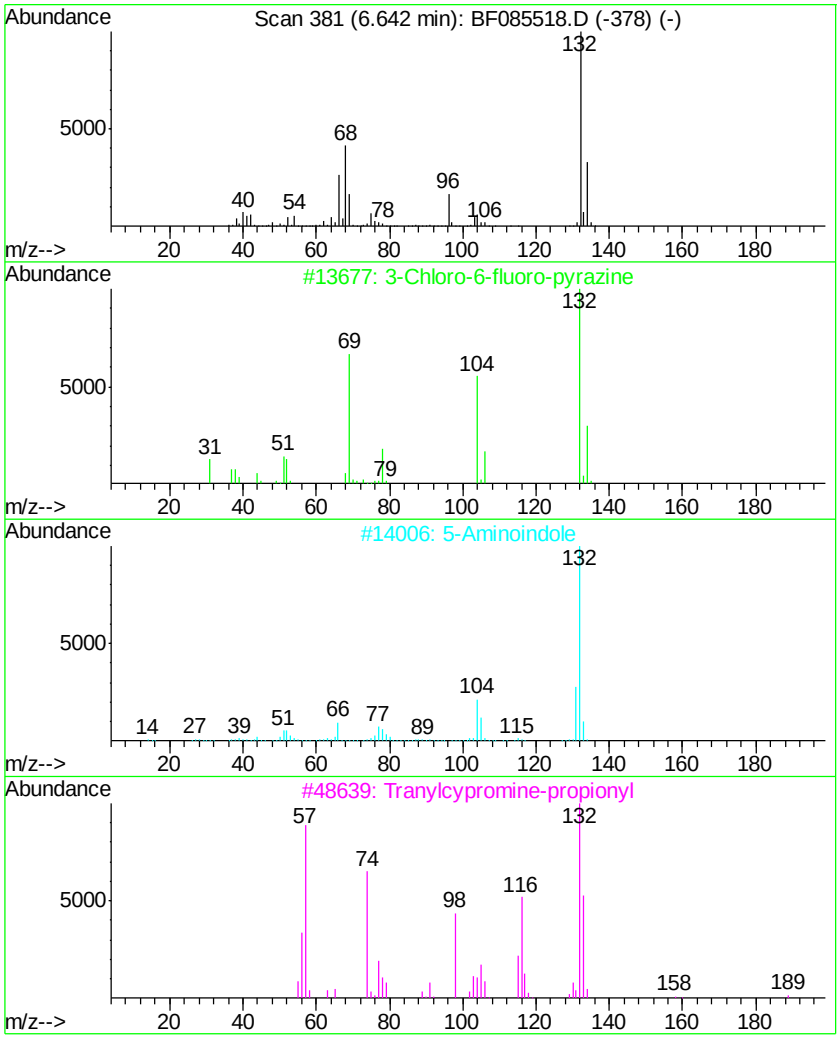
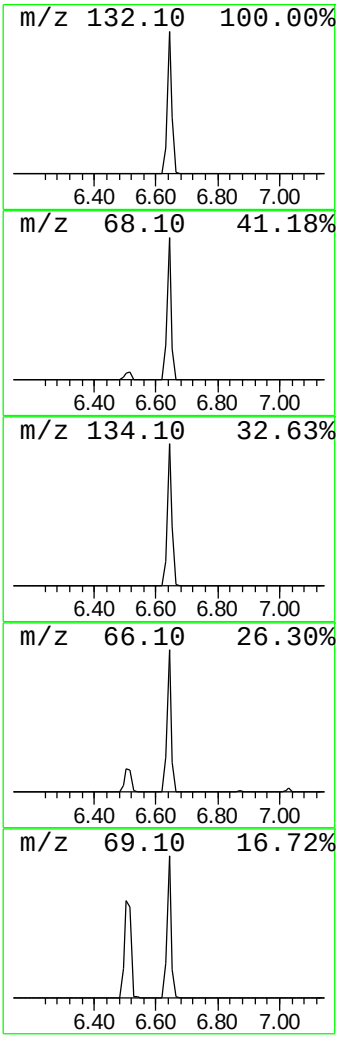
Peak Number 1 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	83.84 ng	3169050	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085518.D
Acq On : 18 Mar 2016 3:53
Operator : UM/SJ
Sample : H1774-18
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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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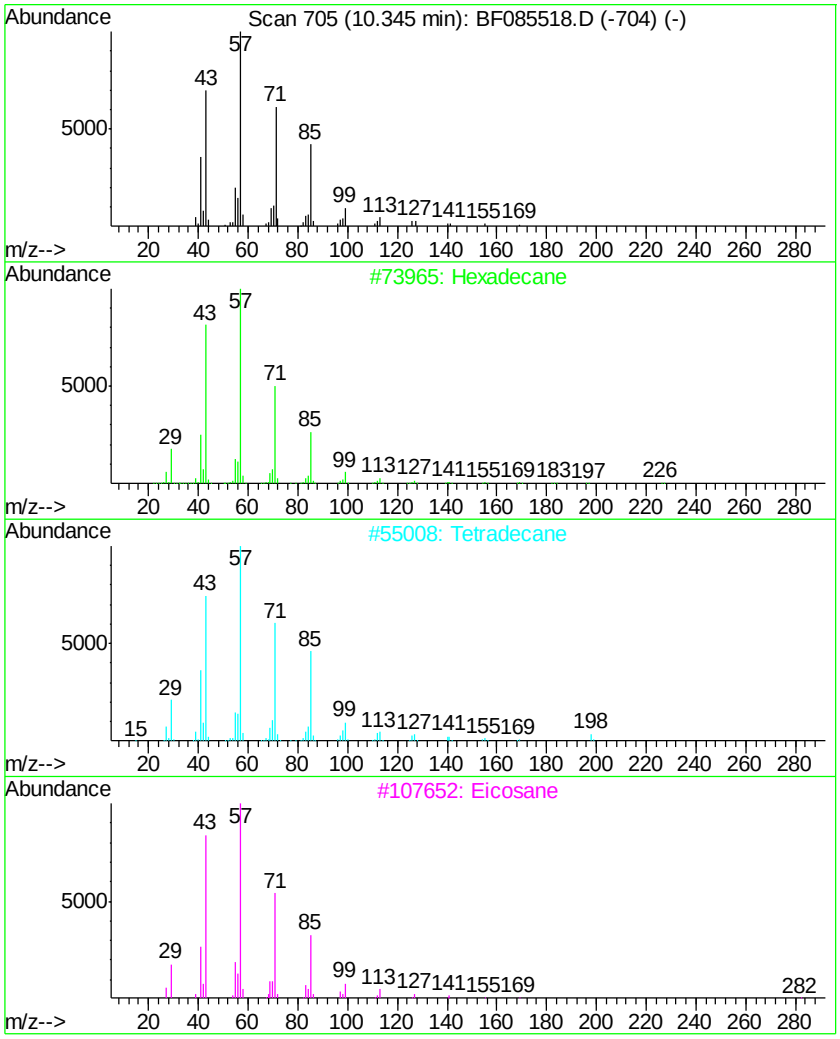
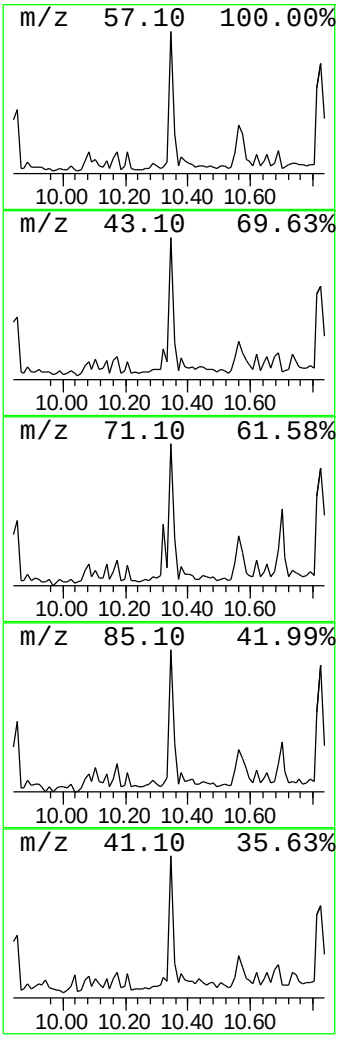
Peak Number 3 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.34	2.08 ng	108418	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetradecane	198	C14H30	000629-59-4	87
3	Eicosane	282	C20H42	000112-95-8	83
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085518.D
Acq On : 18 Mar 2016 3:53
Operator : UM/SJ
Sample : H1774-18
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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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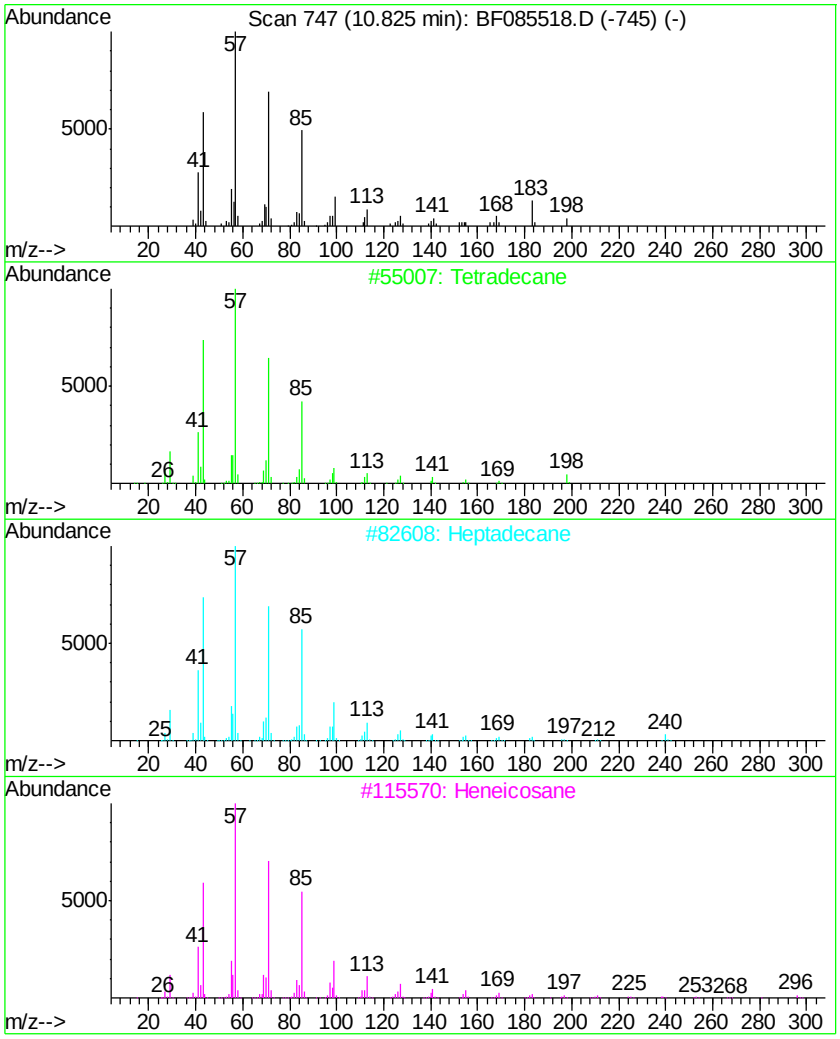
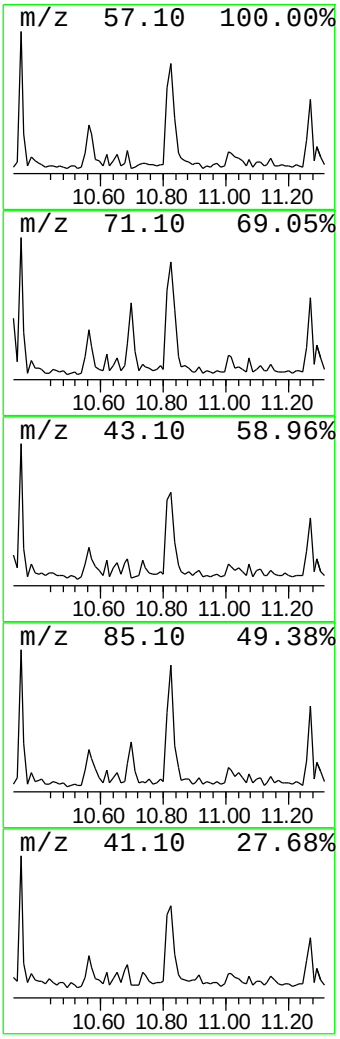
Peak Number 4 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.34 ng	169205	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	95
2	Heptadecane	240	C17H36	000629-78-7	87
3	Heneicosane	296	C21H44	000629-94-7	83
4	Octadecane	254	C18H38	000593-45-3	83
5	Tetracosane	338	C24H50	000646-31-1	83





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085518.D
Acq On : 18 Mar 2016 3:53
Operator : UM/SJ
Sample : H1774-18
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

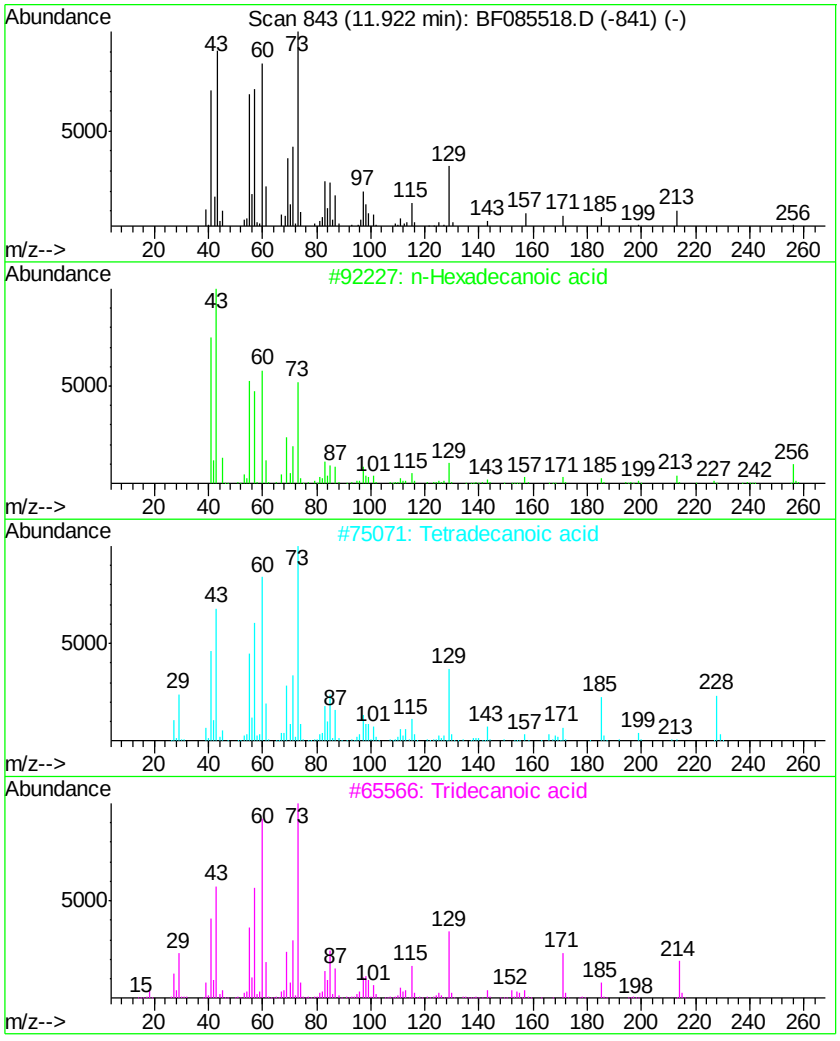
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

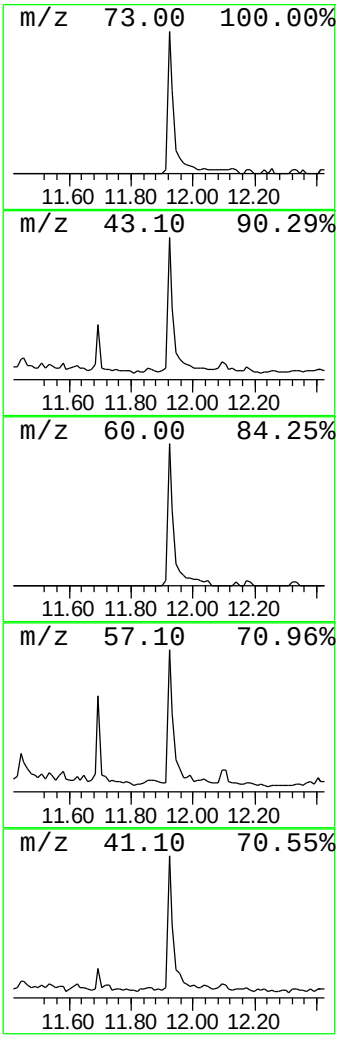
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.10 ng	208115	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	72
4	Undecane	156	C11H24	001120-21-4	18
5	Hexadecane	226	C16H34	000544-76-3	18





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Operator : UM/SJ
Sample : H1774-18
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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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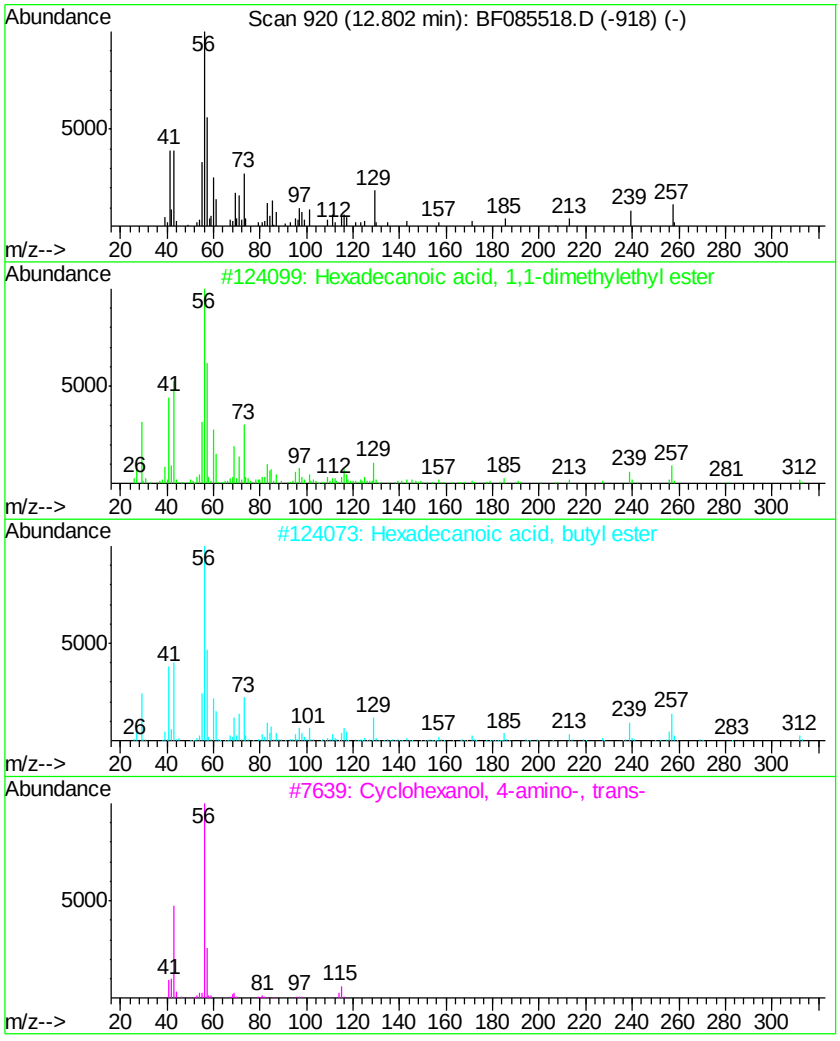
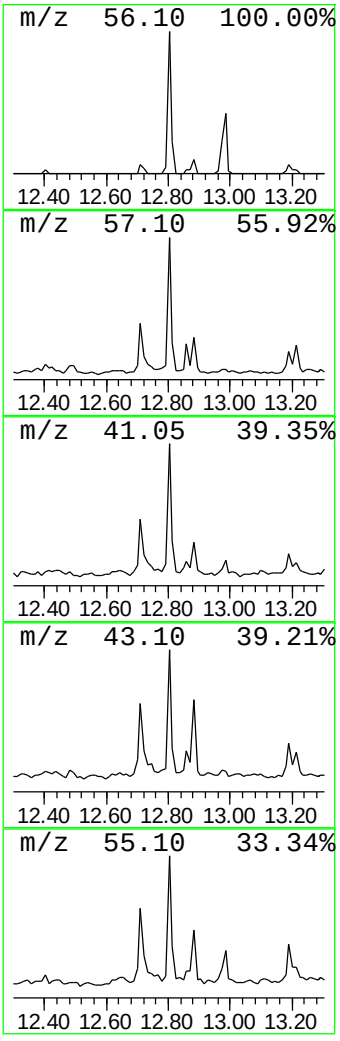
Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.26 ng	86798	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	87
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
3	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	35
5	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	35





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Acq On : 18 Mar 2016 3:53
Operator : UM/SJ
Sample : H1774-18
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

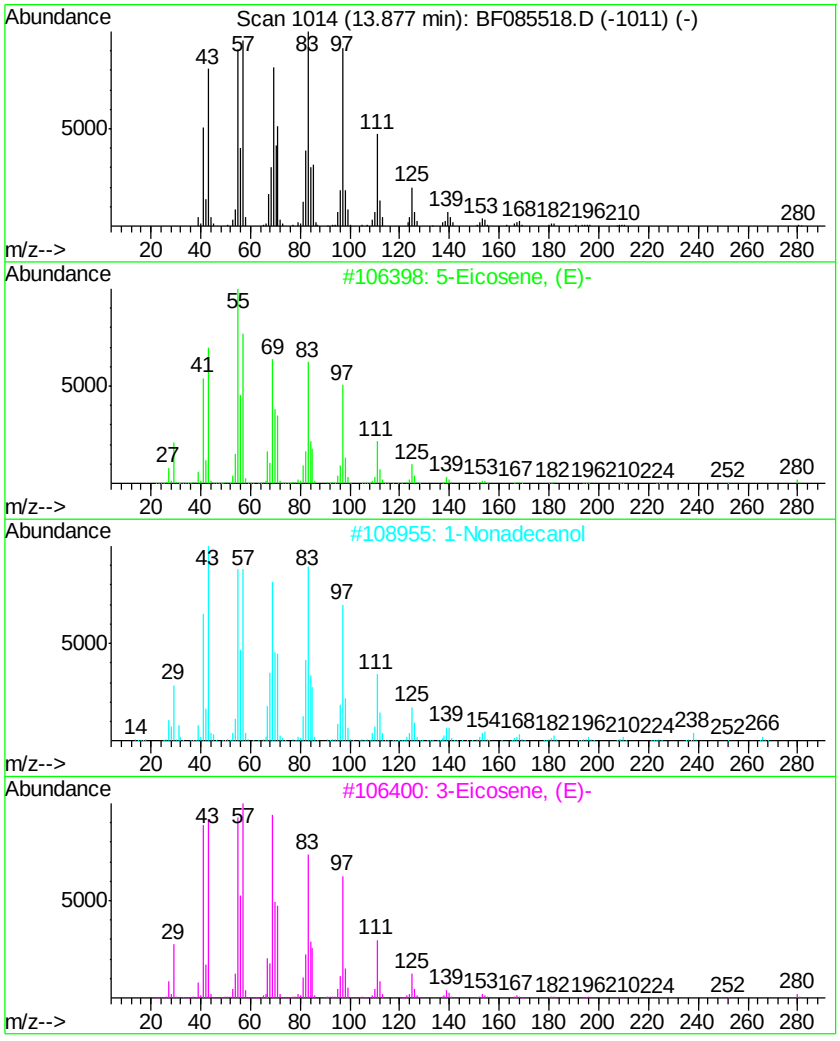
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

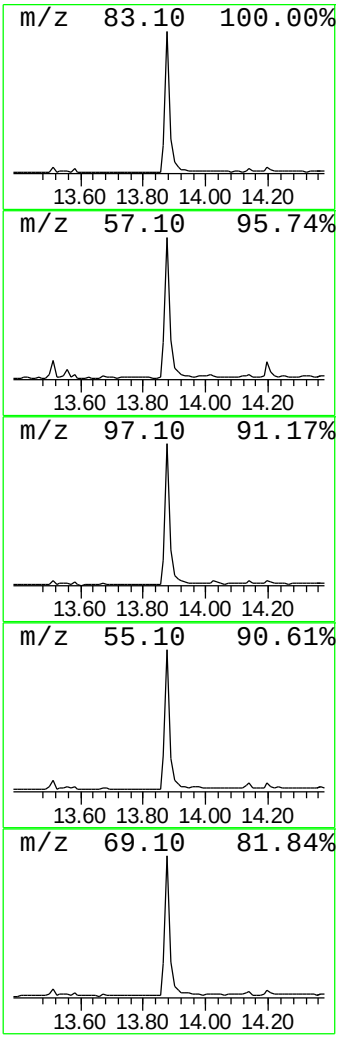
****

Peak Number 7 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	17.21 ng	659504	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Nonadecanol	284	C19H40O	001454-84-8	93
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Acq On : 18 Mar 2016 3:53
Operator : UM/SJ
Sample : H1774-18
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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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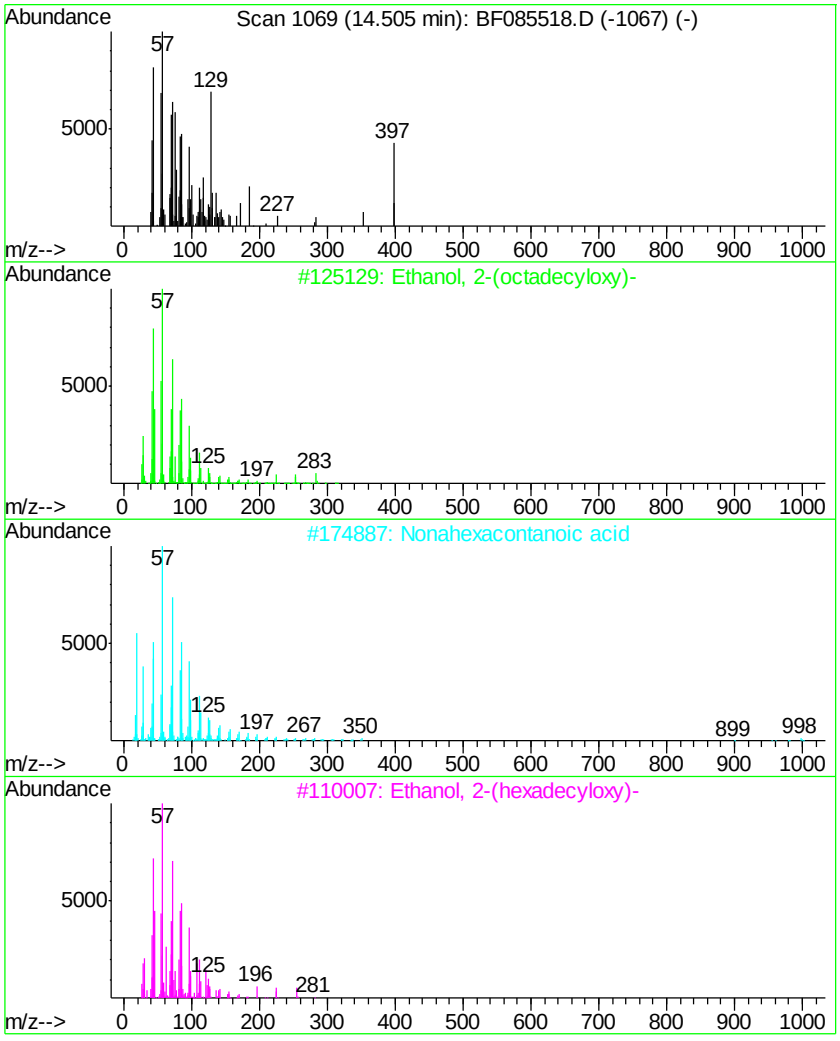
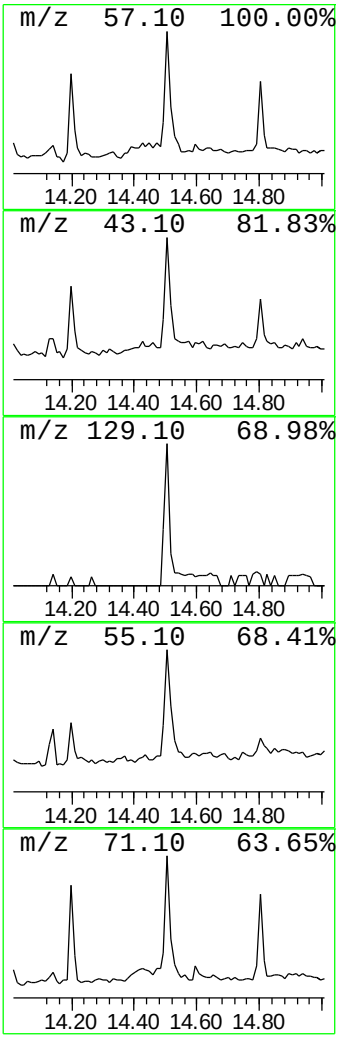
Peak Number 8 Ethanol, 2-(octadecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	3.14 ng	120402	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	50
2	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	49
3	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	43
4	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	41
5	17-Pentatriacontene	491	C35H70	006971-40-0	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085518.D
Acq On : 18 Mar 2016 3:53
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Sample : H1774-18
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.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
unknown6.64	6.64	83.8	ng	3169050	1	6.87	755932	20.0
Hexadecane	10.34	2.1	ng	108418	3	9.91	1041780	20.0
Tetradecane	10.82	3.3	ng	169205	4	11.40	1014210	20.0
n-Hexadecanoic acid	11.92	4.1	ng	208115	4	11.40	1014210	20.0
Hexadecanoic acid...	12.80	2.3	ng	86798	5	14.04	766450	20.0
5-Eicosene, (E)-	13.88	17.2	ng	659504	5	14.04	766450	20.0
Ethanol, 2-(octad...	14.51	3.1	ng	120402	5	14.04	766450	20.0