LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094703.D
Acq On : 29 Apr 2017 00:08
Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

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-BF041717.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	3.366	233	243	247	rBV2	19128	42735	1.31%	0.155%
2	3.942	337	341	349	rBV	452609	557207	17.03%	2.026%
3	4.331	403	407	420	rBV	3068054	3066988	93.71%	11.150%
4	4.713	469	472	478	rVB	33569	35233	1.08%	0.128%
5	5.401	584	589	592	rBV	2678570	3077589	94.04%	11.189%
6	5.525	605	610	614	rBV	3119264	3193853	97.59%	11.611%
7	5.772	648	652	656	rBV	691508	639083	19.53%	2.323%
8	5.948	677	682	685	rBV	2713893	2496043	76.27%	9.074%
9	6.425	757	763	766	rBV	1770677	1927569	58.90%	7.008%
10	7.260	901	905	909	rBV	908206	836589	25.56%	3.041%
11	8.583	1126	1130	1134	rVB	3296416	3272698	100.00%	11.898%
12	9.083	1212	1215	1219	rBV	235779	220085	6.72%	0.800%
13	9.395	1254	1268	1273	rBV2	848851	886166	27.08%	3.222%
14	9.989	1366	1369	1373	rVB	56278	51915	1.59%	0.189%
15	10.266	1411	1416	1419	rBV	37279	44596	1.36%	0.162%
16	10.371	1429	1434	1447	rBV	1406782	1607768	49.13%	5.845%
17	10.577	1465	1469	1470	rBV	61461	63311	1.93%	0.230%
18	10.595	1470	1472	1476	rVB	53863	55217	1.69%	0.201%
19	11.130	1560	1563	1565	rBV	39890	37074	1.13%	0.135%
20	11.166	1565	1569	1574	rVB	62018	73167	2.24%	0.266%
21	11.218	1574	1578	1581	rBV	711285	694071	21.21%	2.523%
22	11.248	1581	1583	1586	rVB	41033	37838	1.16%	0.138%
23	11.954	1699	1703	1718	rBV3	115623	205122	6.27%	0.746%
24	12.713	1829	1832	1838	rVB	91371	97531	2.98%	0.355%
25	12.983	1875	1878	1882	rVB	90266	102228	3.12%	0.372%
26	13.036	1884	1887	1893	rVB4	41884	50631	1.55%	0.184%
27	13.201	1910	1915	1918	rBV	2147960	2342161	71.57%	8.515%
28	14.371	2109	2114	2119	rVB2	82542	152903	4.67%	0.556%
29	14.471	2127	2131	2135	rBV	576041	610054	18.64%	2.218%
30	15.142	2242	2245	2251	rVB4	154707	206814	6.32%	0.752%
31	15.859	2364	2367	2377	rBV	146003	258852	7.91%	0.941%
32	16.101	2404	2408	2420	rVB2	443955	563446	17.22%	2.048%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094703.D
Acq On : 29 Apr 2017 00:08
Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

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-BF041717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 27506537

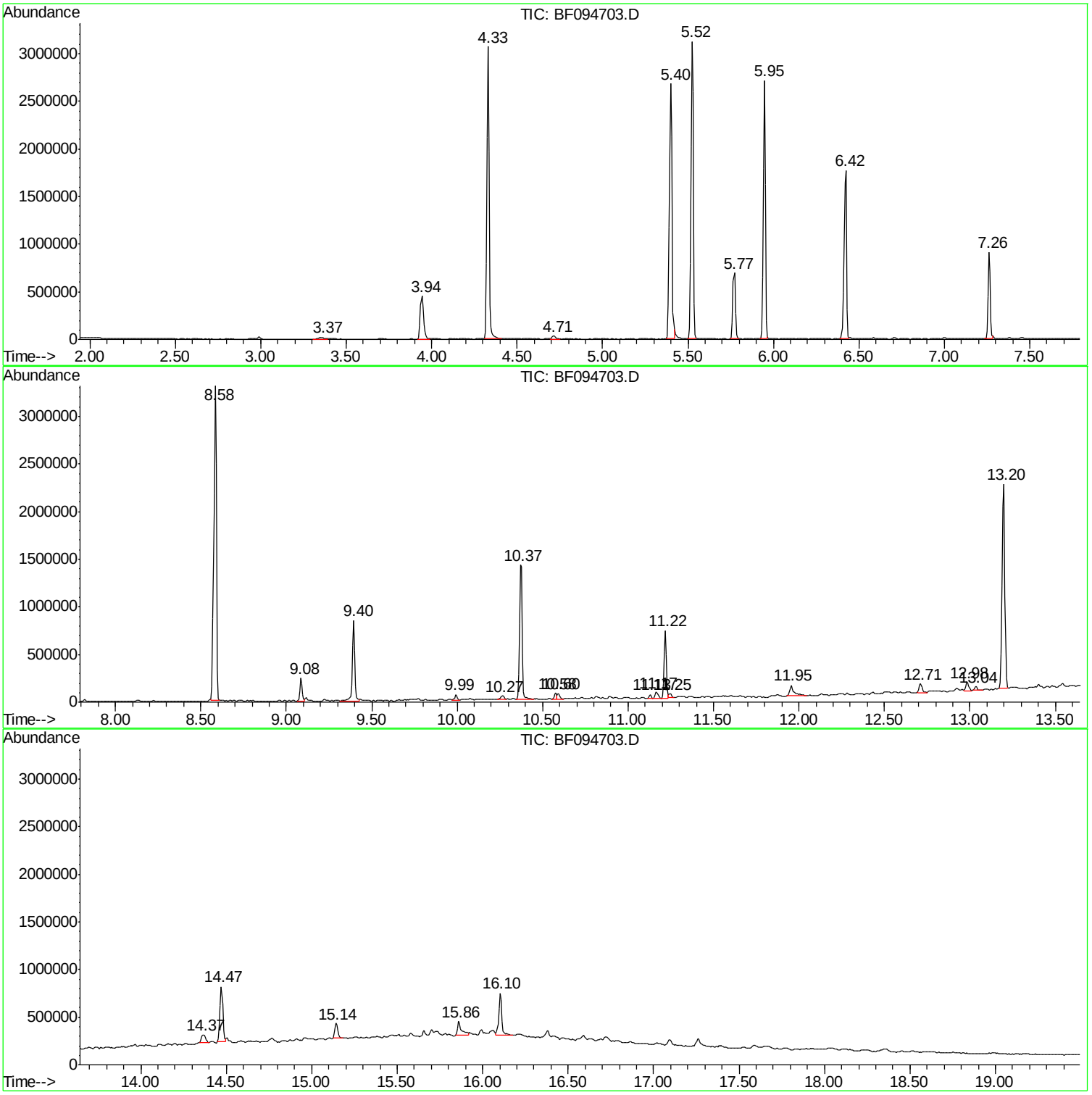
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094703.D
Acq On : 29 Apr 2017 00:08
Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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\BF042817\
Data File : BF094703.D
Acq On : 29 Apr 2017 00:08
Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

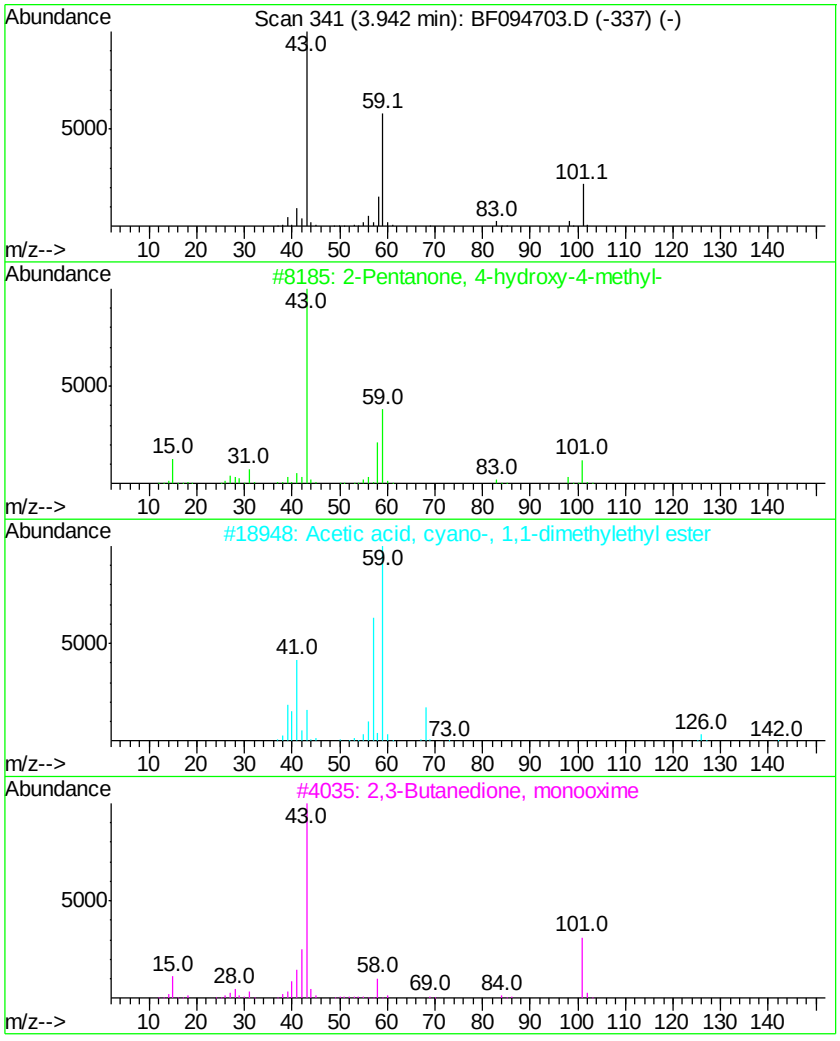
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

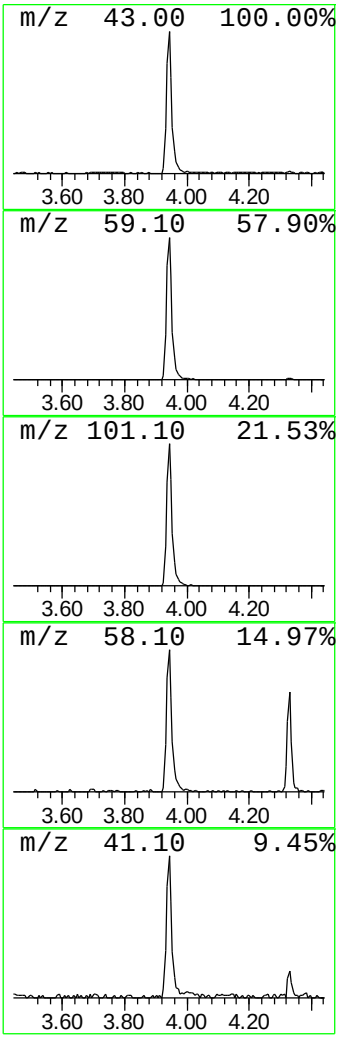
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	17.44 ng	557207	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094703.D
Acq On : 29 Apr 2017 00:08
Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

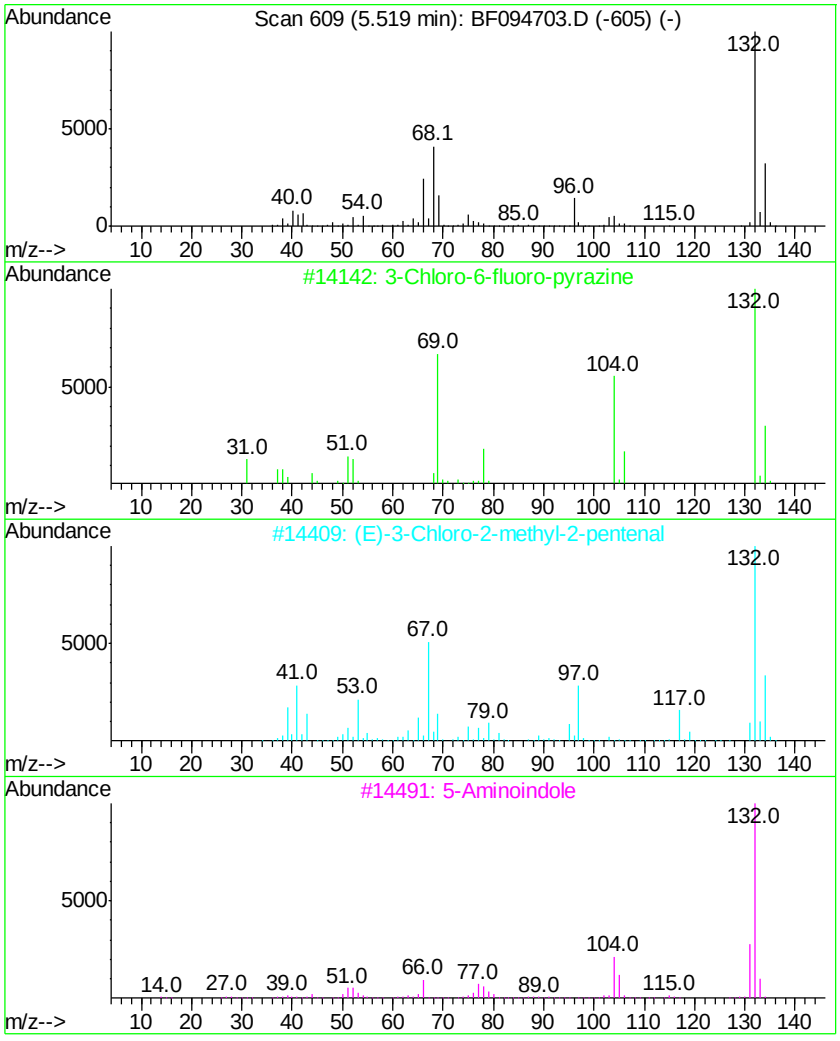
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

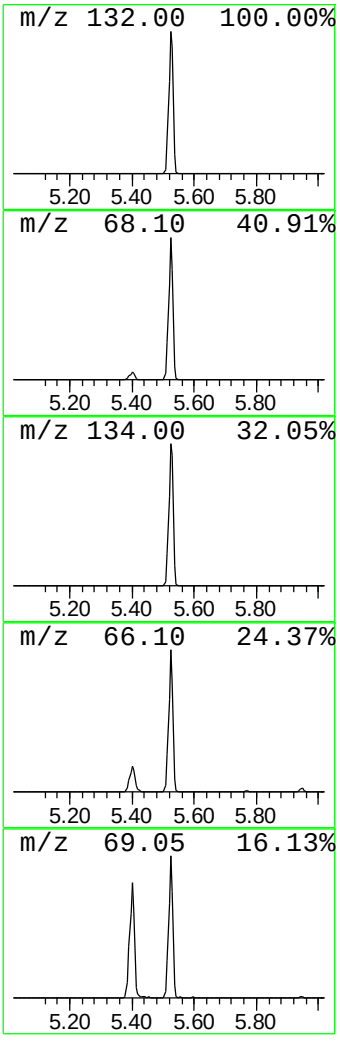
****

Peak Number 2 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	99.95 ng	3193850	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094703.D
Acq On : 29 Apr 2017 00:08
Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

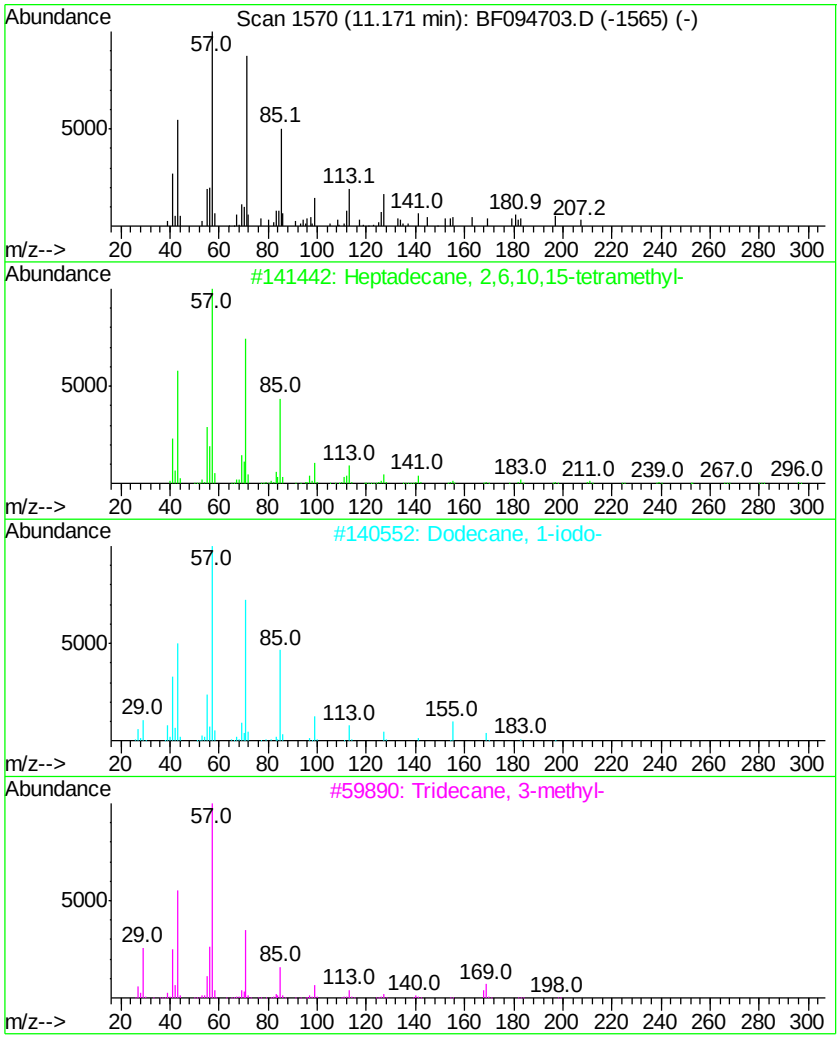
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

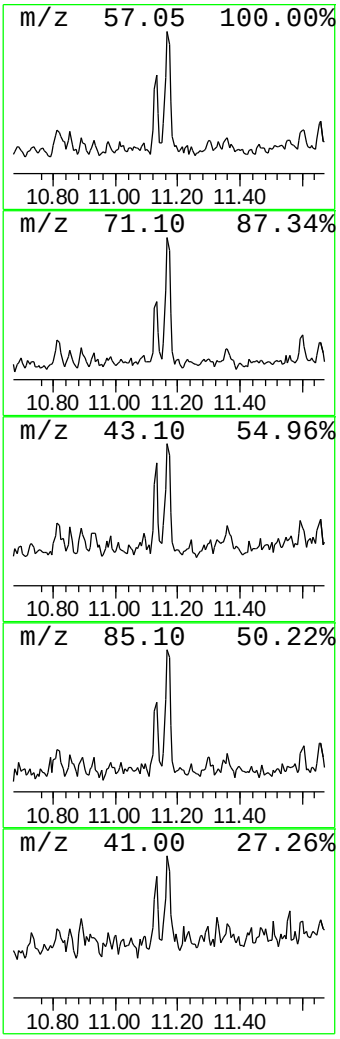
****

Peak Number 4 Heptadecane, 2,6,10,15-tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	2.11 ng	73167	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
3	Tridecane, 3-methyl-	198	C14H30	006418-41-3	72
4	l-Threitol, 2-O-nonyl-	248	C13H28O4	163776-15-6	53
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	52





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
Data File : BF094703.D
Acq On : 29 Apr 2017 00:08
Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

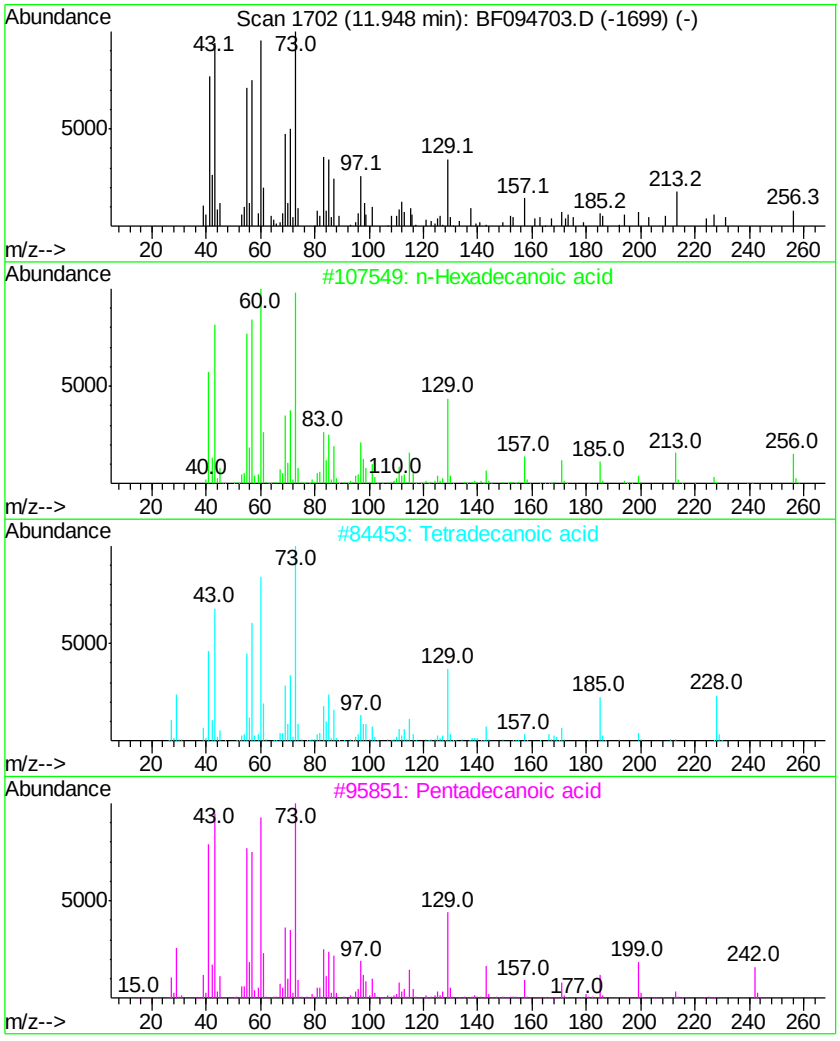
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

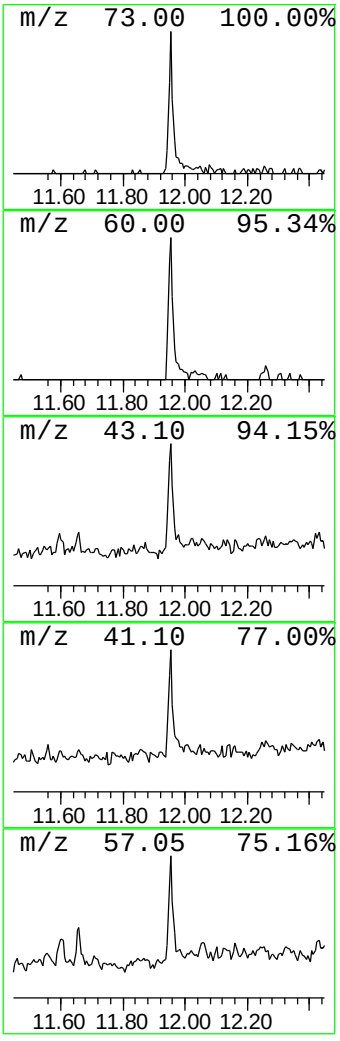
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	5.91 ng	205122	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042817\
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Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

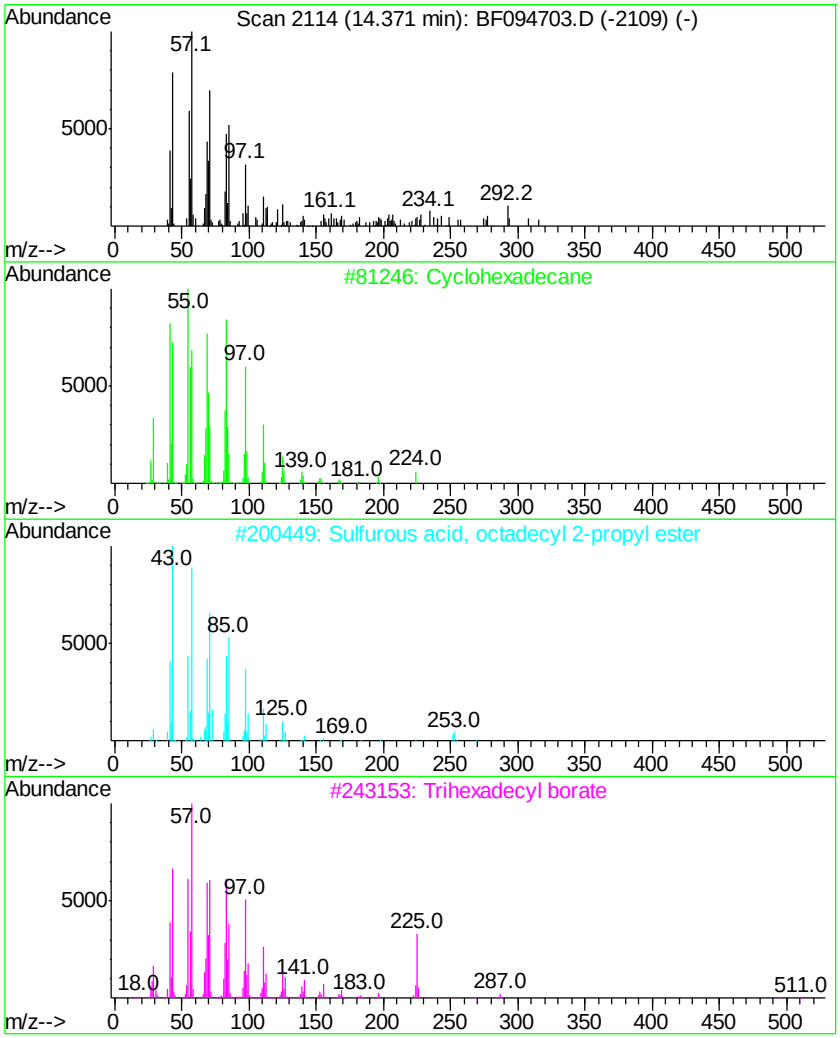
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

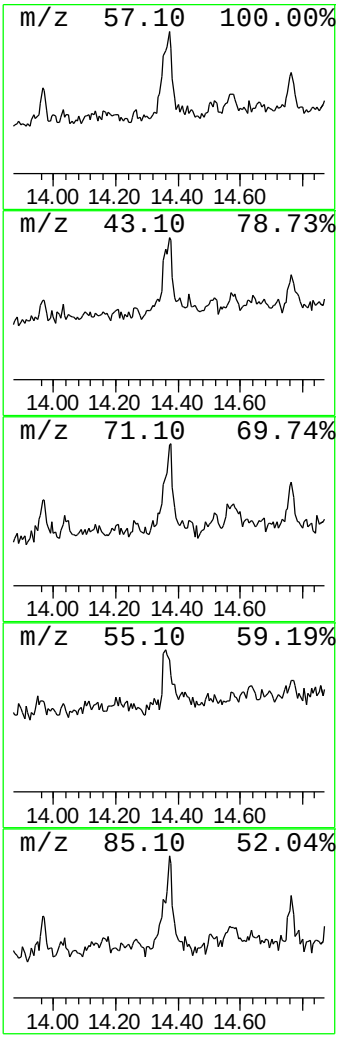
****

Peak Number 6 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	5.01 ng	152903	Chrysene-d12	14.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	93
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	74
3	Trihexadecyl borate	735	C48H99BO3	002665-11-4	49
4	Heptadecane	240	C17H36	000629-78-7	46
5	Tetradecane	198	C14H30	000629-59-4	46





Library Search Compound Report

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Acq On : 29 Apr 2017 00:08
Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

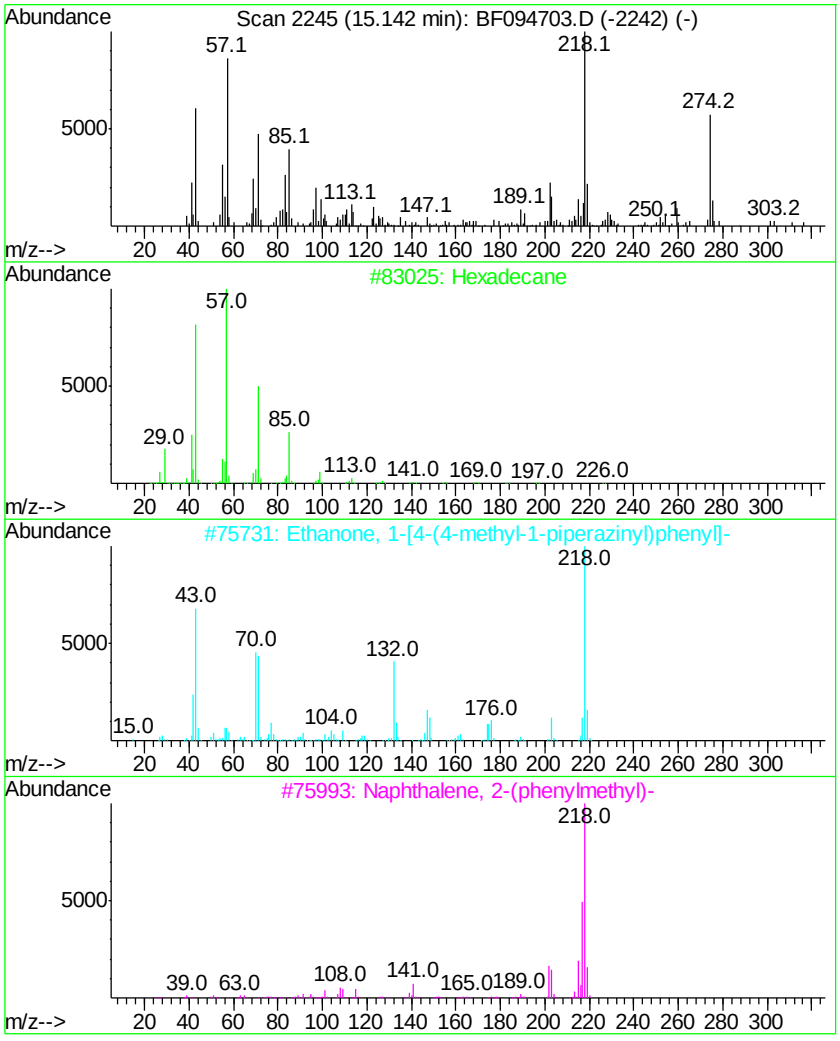
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

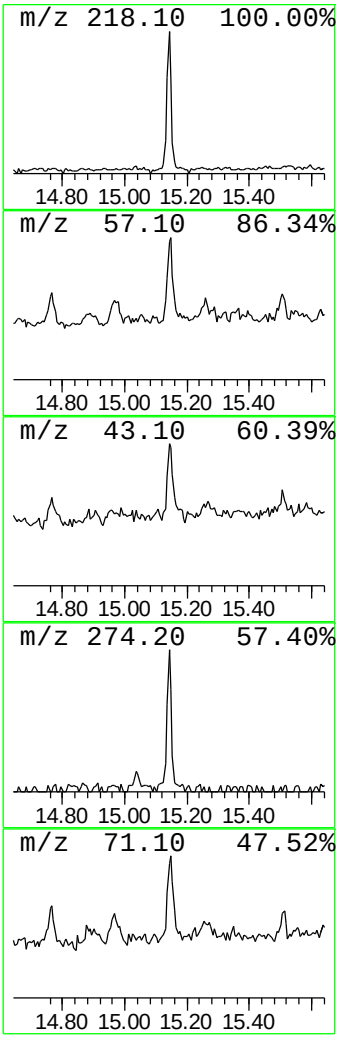
****

Peak Number 7 unknown15.14 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	6.78 ng	206814	Chrysene-d12	14.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	47
2	Ethanone, 1-[4-(4-methyl-1-piper...	218	C13H18N2O	026586-55-0	45
3	Naphthalene, 2-(phenylmethyl)-	218	C17H14	000613-59-2	38
4	4H-Benz[de]anthracene, 5,6-dihydro-	218	C17H14	004389-09-7	38
5	1H-Cyclopenta[l]phenanthrene, 2,...	218	C17H14	000723-98-8	38





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Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

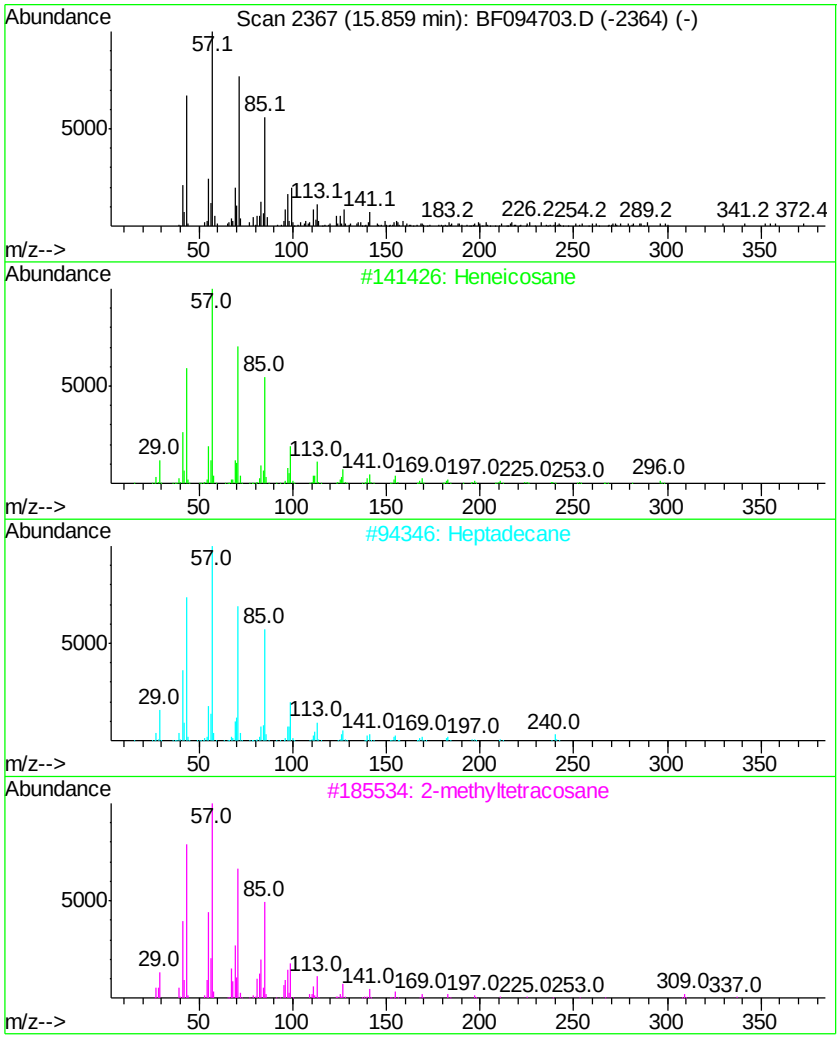
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

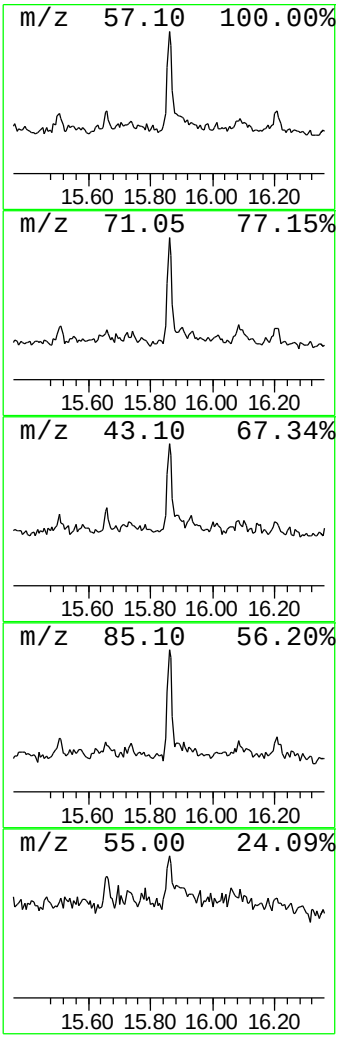
****

Peak Number 8 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	9.19 ng	258852	Perylene-d12	16.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Heptadecane	240	C17H36	000629-78-7	90
3	2-methyltetracosane	352	C25H52	1000376-72-6	90
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	90
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042817\
Data File : BF094703.D
Acq On : 29 Apr 2017 00:08
Operator : SJ/MA
Sample : I2895-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-01-2.0-3.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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
2-Pentanone, 4-hy...	3.94	17.4	ng	557207	1	5.77	639083	20.0
unknown5.52	5.52	100.0	ng	3193850	1	5.77	639083	20.0
Heptadecane, 2,6,...	11.17	2.1	ng	73167	4	11.22	694071	20.0
n-Hexadecanoic acid	11.95	5.9	ng	205122	4	11.22	694071	20.0
Cyclohexadecane	14.37	5.0	ng	152903	5	14.47	610054	20.0
unknown15.14	15.14	6.8	ng	206814	5	14.47	610054	20.0
Heneicosane	15.86	9.2	ng	258852	6	16.10	563446	20.0