LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086232.D
Acq On : 15 Apr 2016 22:38
Operator : UM/SJ
Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE-4-7-16

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-BF041516.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	2.167	4	7	17	rVB	121359	250917	3.07%	0.424%
2	5.081	259	262	265	rVB	165281	250427	3.06%	0.424%
3	5.481	294	297	300	rBV	3516053	3525526	43.10%	5.963%
4	6.510	384	387	389	rBV	2924545	2425583	29.65%	4.103%
5	6.659	397	400	402	rBV	5918888	5990979	73.24%	10.134%
6	6.887	418	420	423	rBV	1414214	1714303	20.96%	2.900%
7	7.047	431	434	437	rBV	5085883	5659898	69.19%	9.574%
8	7.459	466	470	472	rBV	4869946	5734187	70.10%	9.699%
9	7.687	486	490	494	rBV3	51924	100389	1.23%	0.170%
10	7.779	494	498	500	rVV2	52382	83967	1.03%	0.142%
11	7.939	510	512	514	rVB	105290	163185	1.99%	0.276%
12	8.099	521	526	527	rBV3	111202	280359	3.43%	0.474%
13	8.179	527	533	535	rVV	2800259	2957167	36.15%	5.002%
14	8.213	535	536	538	rVV	207623	148768	1.82%	0.252%
15	8.305	541	544	546	rBV3	75807	194109	2.37%	0.328%
16	8.350	546	548	549	rVV2	92468	160726	1.96%	0.272%
17	8.385	549	551	552	rVV	205751	226990	2.77%	0.384%
18	8.430	552	555	558	rVV3	83246	207171	2.53%	0.350%
19	8.499	559	561	563	rVB	265072	237827	2.91%	0.402%
20	8.545	563	565	567	rBV2	68246	107539	1.31%	0.182%
21	8.636	571	573	575	rVB2	105623	124245	1.52%	0.210%
22	8.693	575	578	580	rBV2	105158	181620	2.22%	0.307%
23	8.750	580	583	586	rVV4	118381	205136	2.51%	0.347%
24	8.796	586	587	589	rVB2	103351	103271	1.26%	0.175%
25	8.876	589	594	596	rBV3	123037	306506	3.75%	0.518%
26	8.945	596	600	603	rVB2	182835	336398	4.11%	0.569%
27	9.025	605	607	609	rVB	108641	125126	1.53%	0.212%
28	9.093	612	613	616	rVB2	75143	110911	1.36%	0.188%
29	9.196	621	622	624	rVB	103910	95206	1.16%	0.161%
30	9.265	624	628	630	rBV	5629058	8180314	100.00%	13.837%
31	9.333	633	634	639	rVB3	130402	206325	2.52%	0.349%
32	9.516	646	650	651	rBV2	72958	152954	1.87%	0.259%
33	9.539	651	652	655	rVV3	85256	127381	1.56%	0.215%
34	9.608	655	658	660	rVV2	58276	140086	1.71%	0.237%

LSC Area Percent Report

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Data File : BF086232.D
Acq On : 15 Apr 2016 22:38
Operator : UM/SJ
Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE-4-7-16

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-BF041516.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.653	660	662	664	rVB	115086	153151	1.87%	0.259%
36	9.928	684	686	689	rBV	1869558	2383732	29.14%	4.032%
37	10.442	730	731	732	rBV	107830	86887	1.06%	0.147%
38	10.716	752	755	758	rBV2	3425437	4199898	51.34%	7.104%
39	10.842	765	766	773	rVB	121397	155568	1.90%	0.263%
40	11.288	803	805	807	rBV	126157	120934	1.48%	0.205%
41	11.413	813	816	818	rBV	2564993	2215650	27.09%	3.748%
42	11.951	860	863	871	rBV2	174702	335540	4.10%	0.568%
43	12.728	929	931	937	rBV	177063	265629	3.25%	0.449%
44	13.002	952	955	958	rBV	5002027	5554197	67.90%	9.395%
45	13.894	1032	1033	1038	rVB2	91503	132150	1.62%	0.224%
46	14.042	1044	1046	1049	rBV	1454344	1464182	17.90%	2.477%
47	15.482	1169	1172	1175	rBV	988544	1237317	15.13%	2.093%

Sum of corrected areas: 59120331

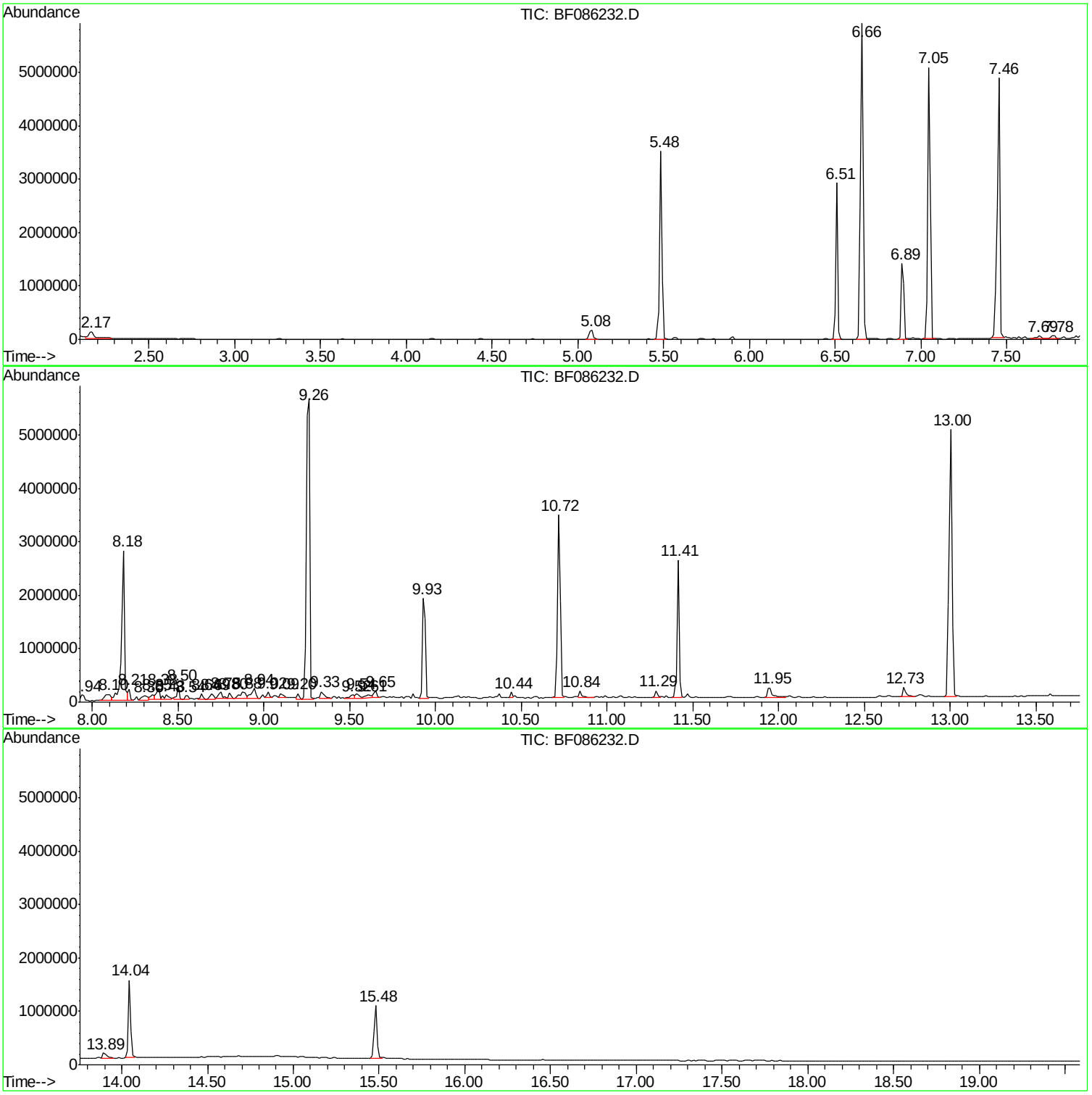
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086232.D
Acq On : 15 Apr 2016 22:38
Operator : UM/SJ
Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLIND-DUPLICATE-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086232.D
Acq On : 15 Apr 2016 22:38
Operator : UM/SJ
Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

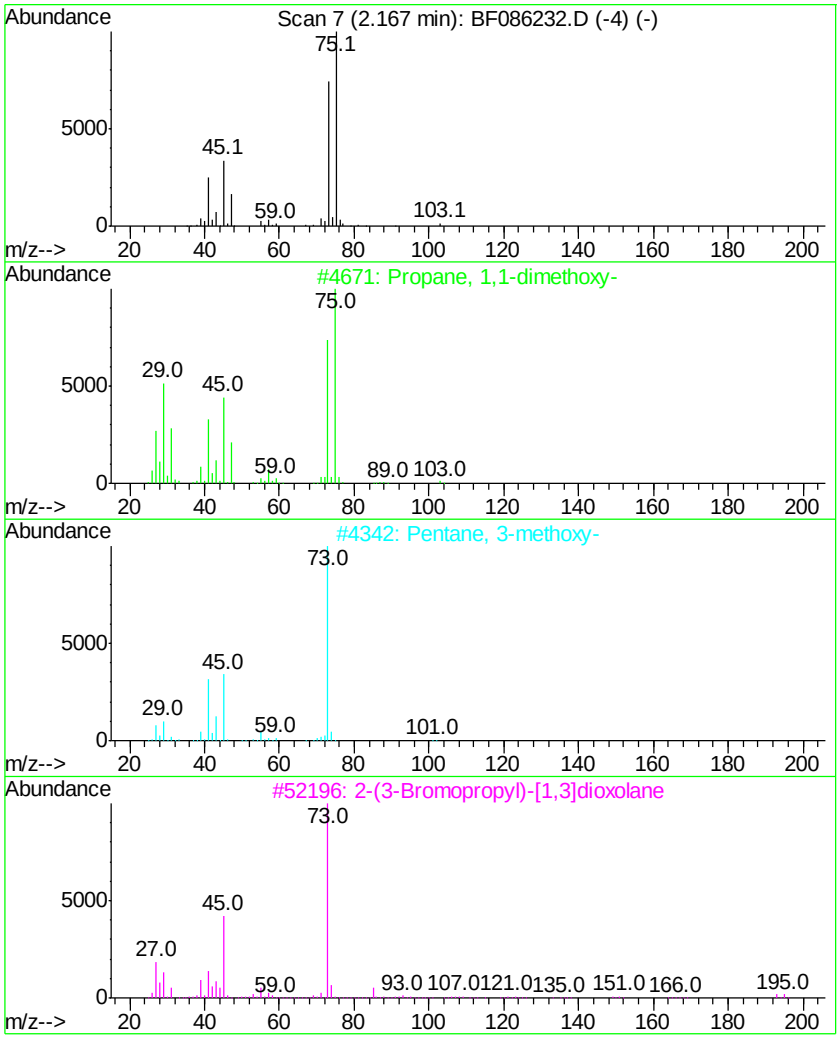
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

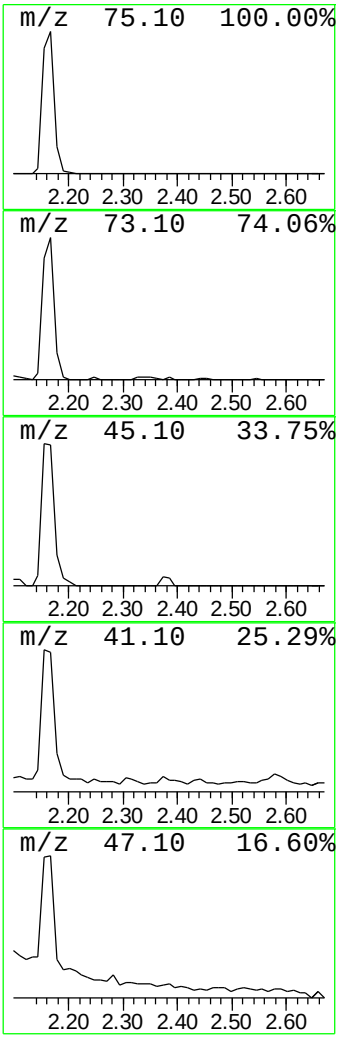
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	2.93 ng	250917	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3	2-(3-Bromopropyl)-[1,3]dioxolane	194	C6H11BrO2	062563-07-9	10
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086232.D
Acq On : 15 Apr 2016 22:38
Operator : UM/SJ
Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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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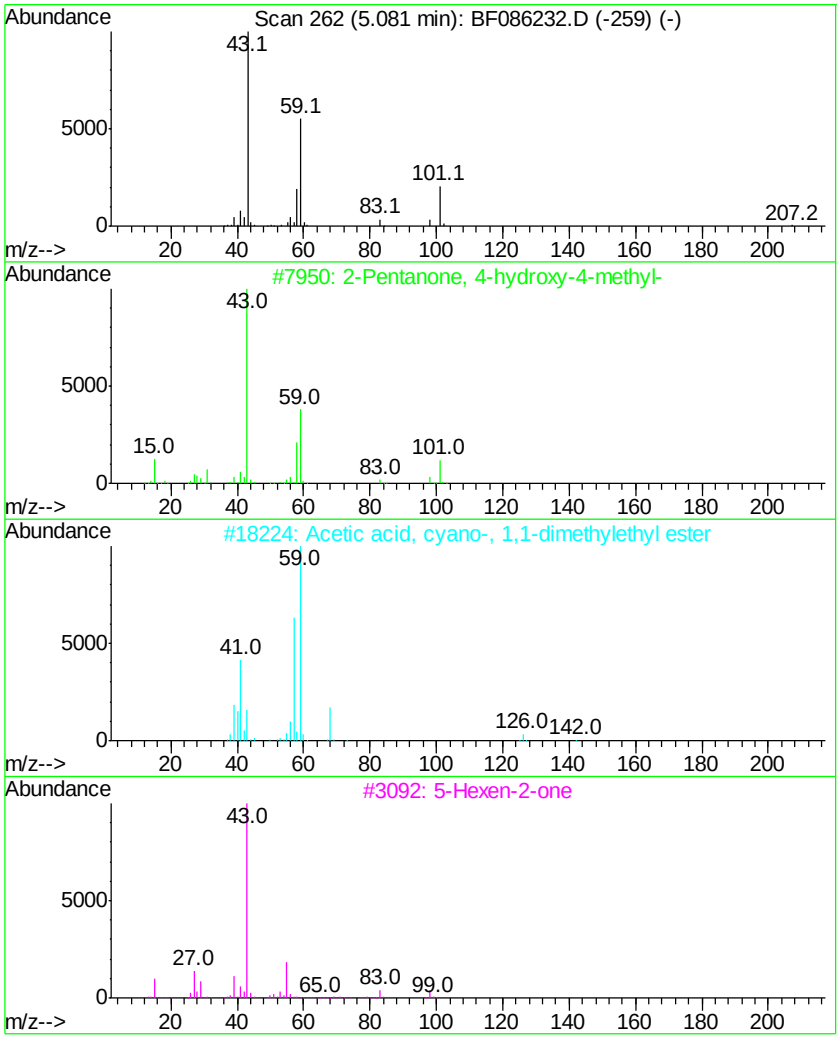
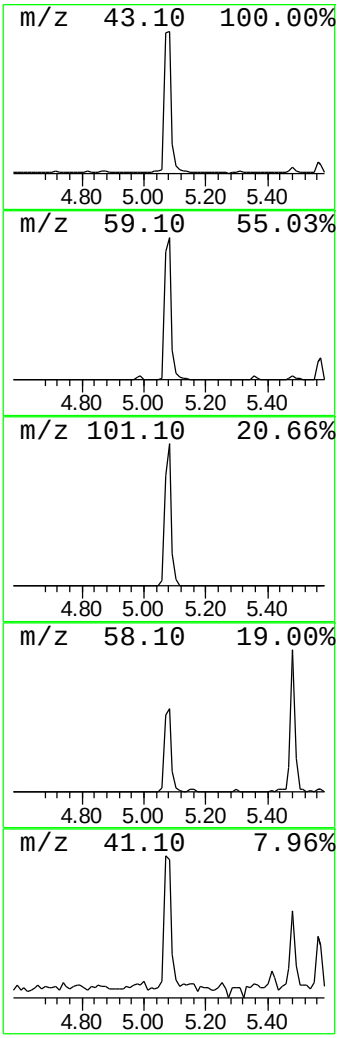
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	2.92 ng	250427	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086232.D
Acq On : 15 Apr 2016 22:38
Operator : UM/SJ
Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLIND-DUPLICATE-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

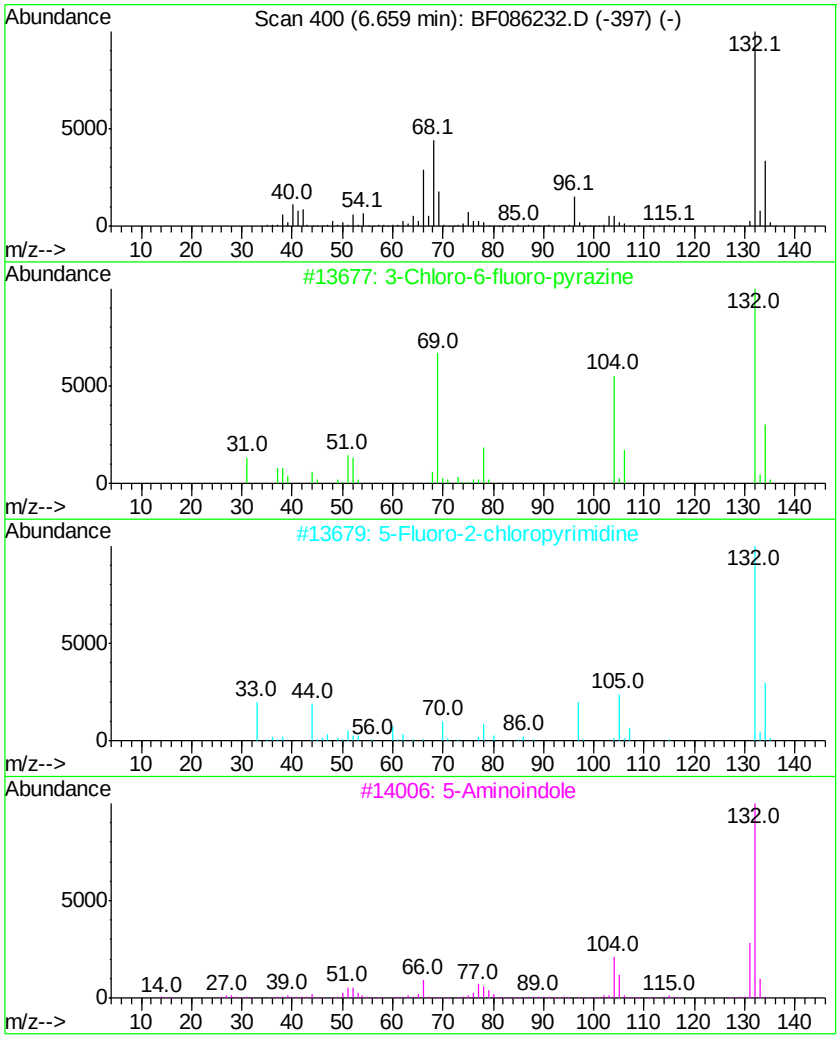
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

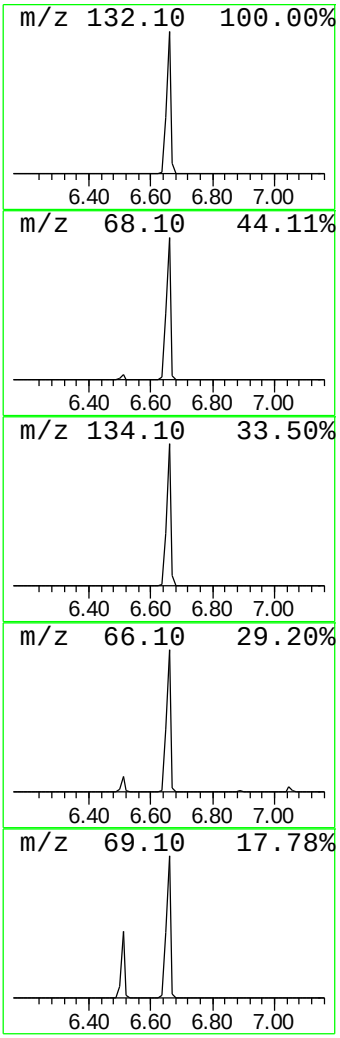
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	69.89 ng	5990980	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





Library Search Compound Report

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Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLIND-DUPLICATE-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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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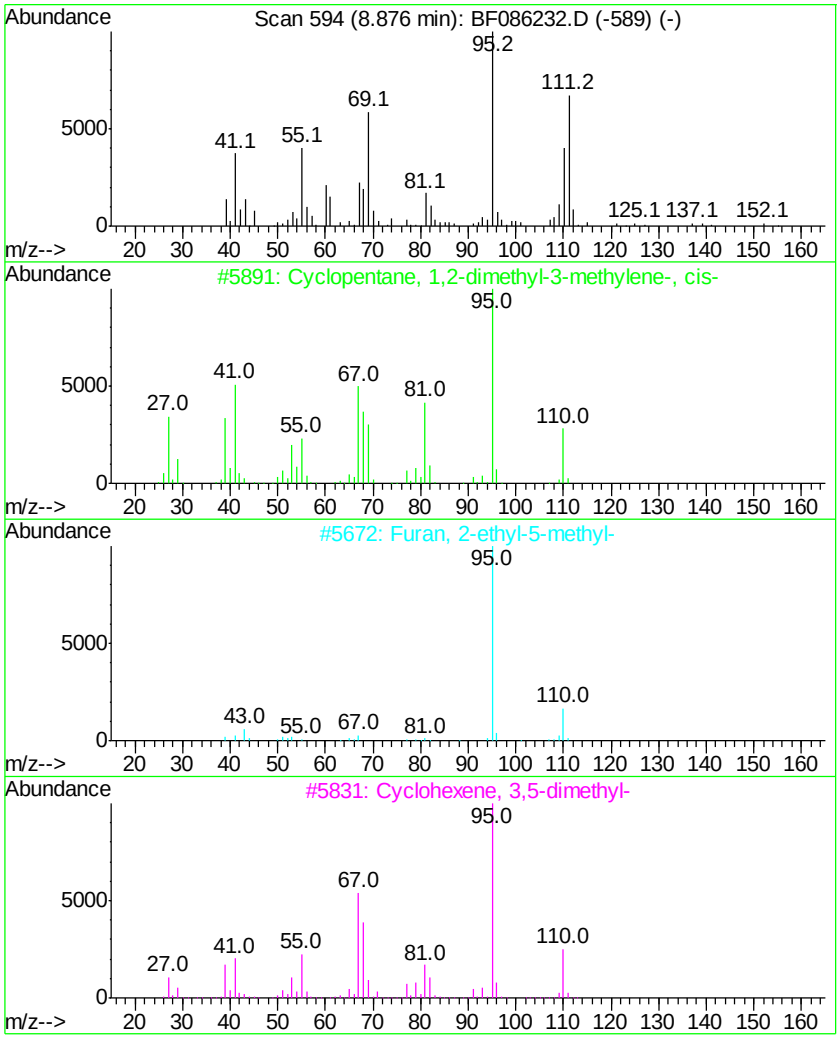
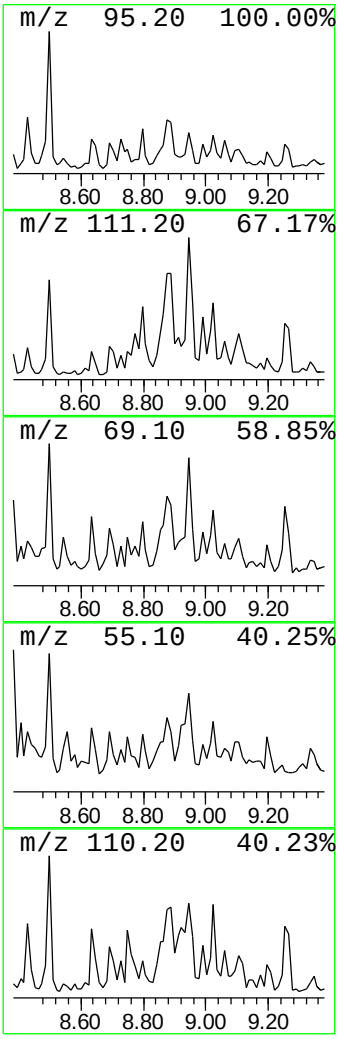
Peak Number 5 Cyclopentane, 1,2-dimethyl-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	2.07 ng	306506	Naphthalene-d8	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	091884-67-2	50
2	Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	47
3	Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	47
4	Cyclopentane, 1,2-dimethyl-3-met...	110	C8H14	1000150-99-3	47
5	2-Furanecarboxylic acid, 3,5-dim...	222	C13H18O3	1000278-87-2	47





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Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

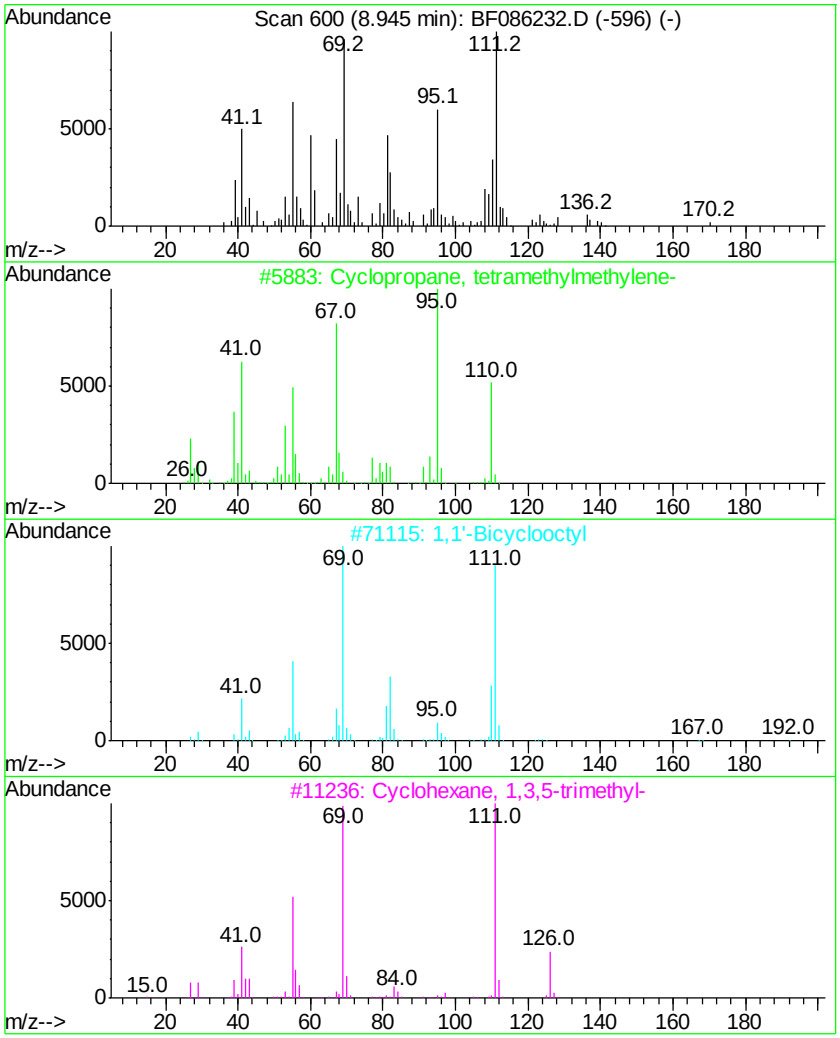
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

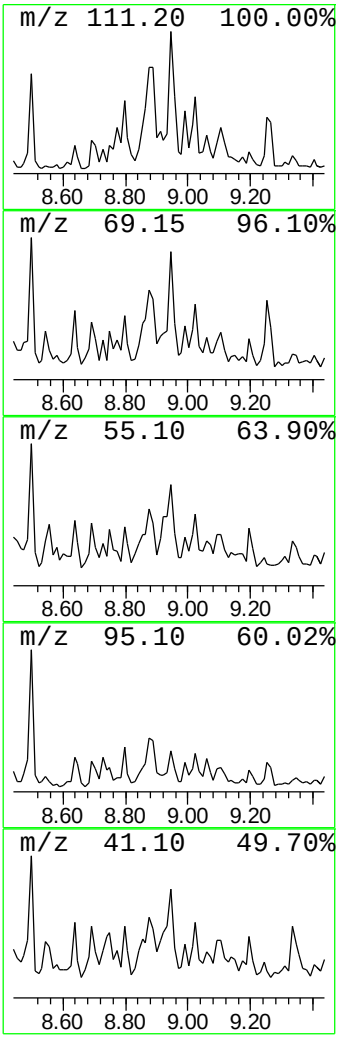
****

Peak Number 6 Cyclopropane, tetramethylme... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.94	2.28 ng	336398	Naphthalene-d8	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, tetramethylmethylene-	110	C8H14	054376-39-5	64
2	1,1'-Bicyclooctyl	222	C16H30	006708-17-4	47
3	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	43
4	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	35
5	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	35





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Data File : BF086232.D
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Operator : UM/SJ
Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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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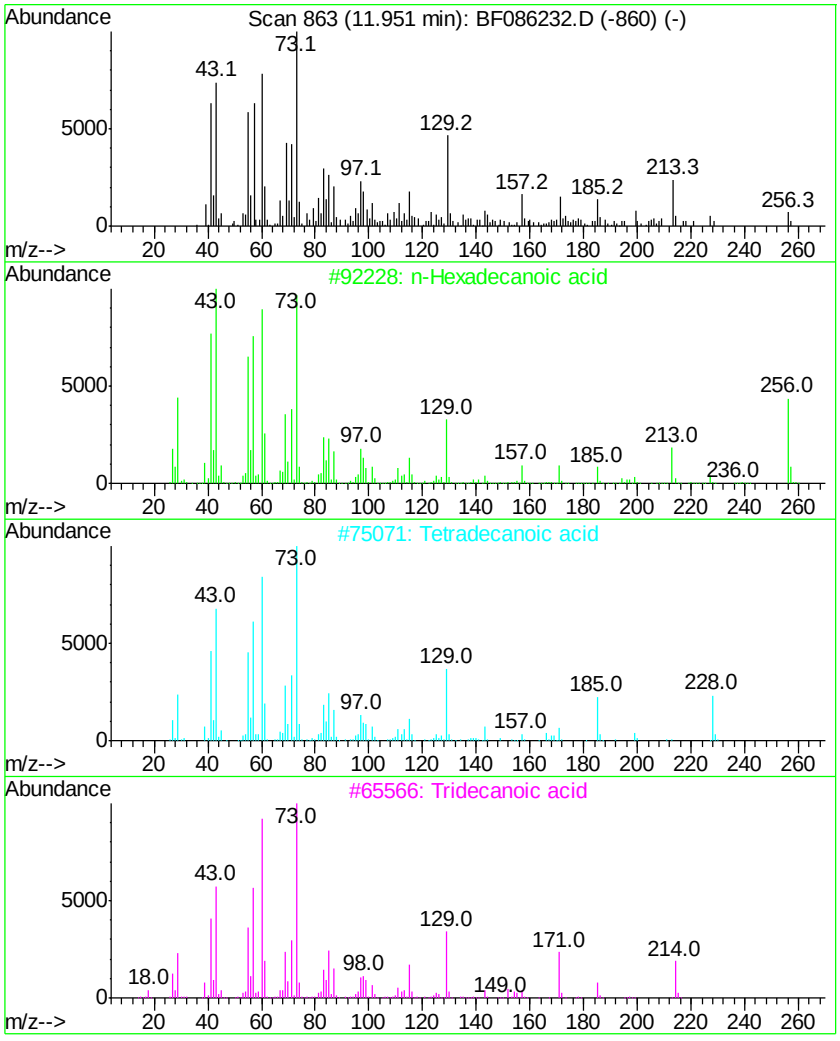
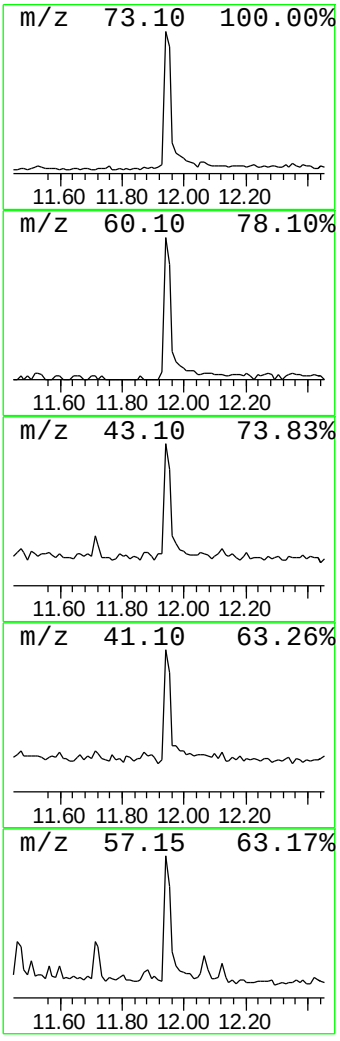
Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	3.03 ng	335540	Phenanthrene-d10	11.41

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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	80





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Operator : UM/SJ
Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

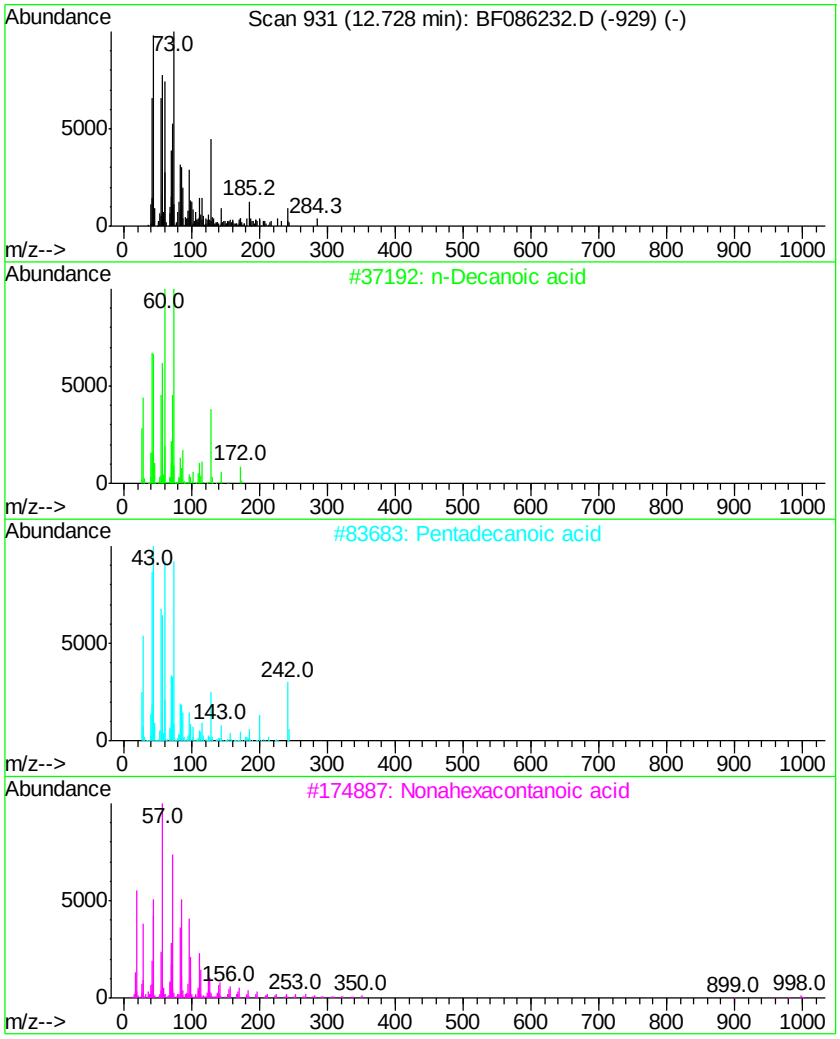
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

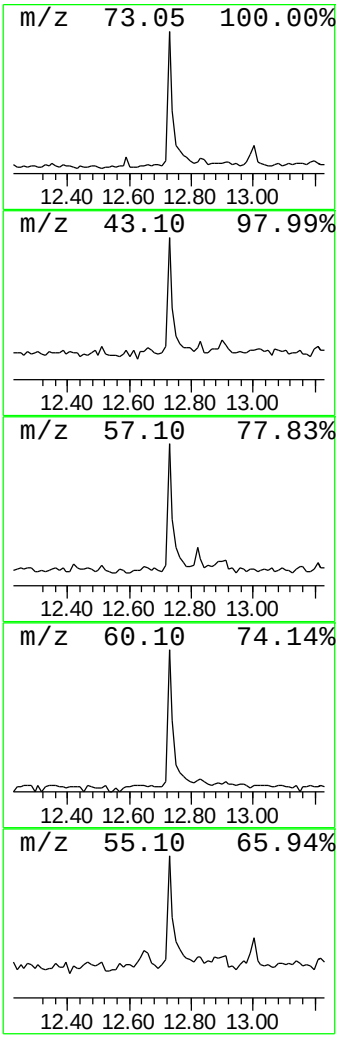
****

Peak Number 8 n-Decanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	3.63 ng	265629	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	76
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
3	Nonahexacontanoic acid	999	C69H138O2	040710-32-5	18
4	Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	18
5	Dodecane	170	C12H26	000112-40-3	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
Data File : BF086232.D
Acq On : 15 Apr 2016 22:38
Operator : UM/SJ
Sample : H2402-08
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BLIND-DUPLICATE-4-7-16

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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
Propane, 1,1-dime...	2.17	2.9	ng	250917	1	6.89	1714300	20.0
2-Pentanone, 4-hy...	5.08	2.9	ng	250427	1	6.89	1714300	20.0
unknown6.66	6.66	69.9	ng	5990980	1	6.89	1714300	20.0
Cyclopentane, 1,2...	8.88	2.1	ng	306506	2	8.18	2957170	20.0
Cyclopropane, tet...	8.94	2.3	ng	336398	2	8.18	2957170	20.0
n-Hexadecanoic acid	11.95	3.0	ng	335540	4	11.41	2215650	20.0
n-Decanoic acid	12.73	3.6	ng	265629	5	14.04	1464180	20.0