LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089750.D
Acq On : 17 Aug 2016 8:01
Operator : UM/SJ
Sample : H4429-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-7A-9-11

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-BF081616.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	1.667	5	7	16	rVV	2671964	4529639	17.04%	2.204%
2	1.792	16	18	28	rVV	12521176	26574944	100.00%	12.933%
3	1.930	28	30	65	rVB	1029282	5757002	21.66%	2.802%
4	4.856	283	286	295	rBV	2331162	3443145	12.96%	1.676%
5	5.290	321	324	326	rVB	12657458	15895520	59.81%	7.736%
6	5.850	371	373	375	rBV	216604	287699	1.08%	0.140%
7	6.159	397	400	402	rVB	754640	974491	3.67%	0.474%
8	6.341	412	416	418	rVB	10458083	15932825	59.95%	7.754%
9	6.467	424	427	429	rBV	14233951	15744843	59.25%	7.663%
10	6.696	445	447	449	rBV	5570677	4772559	17.96%	2.323%
11	6.856	458	461	462	rBV	13019412	11971202	45.05%	5.826%
12	6.879	462	463	466	rVV	1016077	840235	3.16%	0.409%
13	7.267	493	497	499	rBV	8907850	11204329	42.16%	5.453%
14	7.724	534	537	539	rBV2	447130	483049	1.82%	0.235%
15	7.987	557	560	562	rBV	6123450	6912769	26.01%	3.364%
16	9.073	651	655	657	rBV	11890433	18013660	67.78%	8.767%
17	9.462	686	689	691	rBV	4467424	3813232	14.35%	1.856%
18	9.736	710	713	715	rBV	8557437	7780160	29.28%	3.786%
19	10.525	778	782	784	rBV	8458164	11470005	43.16%	5.582%
20	10.662	792	794	800	rVB	381370	472973	1.78%	0.230%
21	11.210	839	842	845	rBV	8403892	7456372	28.06%	3.629%
22	11.759	888	890	902	rBV3	678797	1075075	4.05%	0.523%
23	12.548	957	959	965	rBV	242820	325084	1.22%	0.158%
24	12.811	978	982	984	rBV	12240144	16149639	60.77%	7.860%
25	13.748	1062	1064	1070	rVB	288651	456212	1.72%	0.222%
26	13.874	1073	1075	1078	rBV	6149762	7142887	26.88%	3.476%
27	15.371	1202	1206	1208	rBV	4131293	5995144	22.56%	2.918%

Sum of corrected areas: 205474694

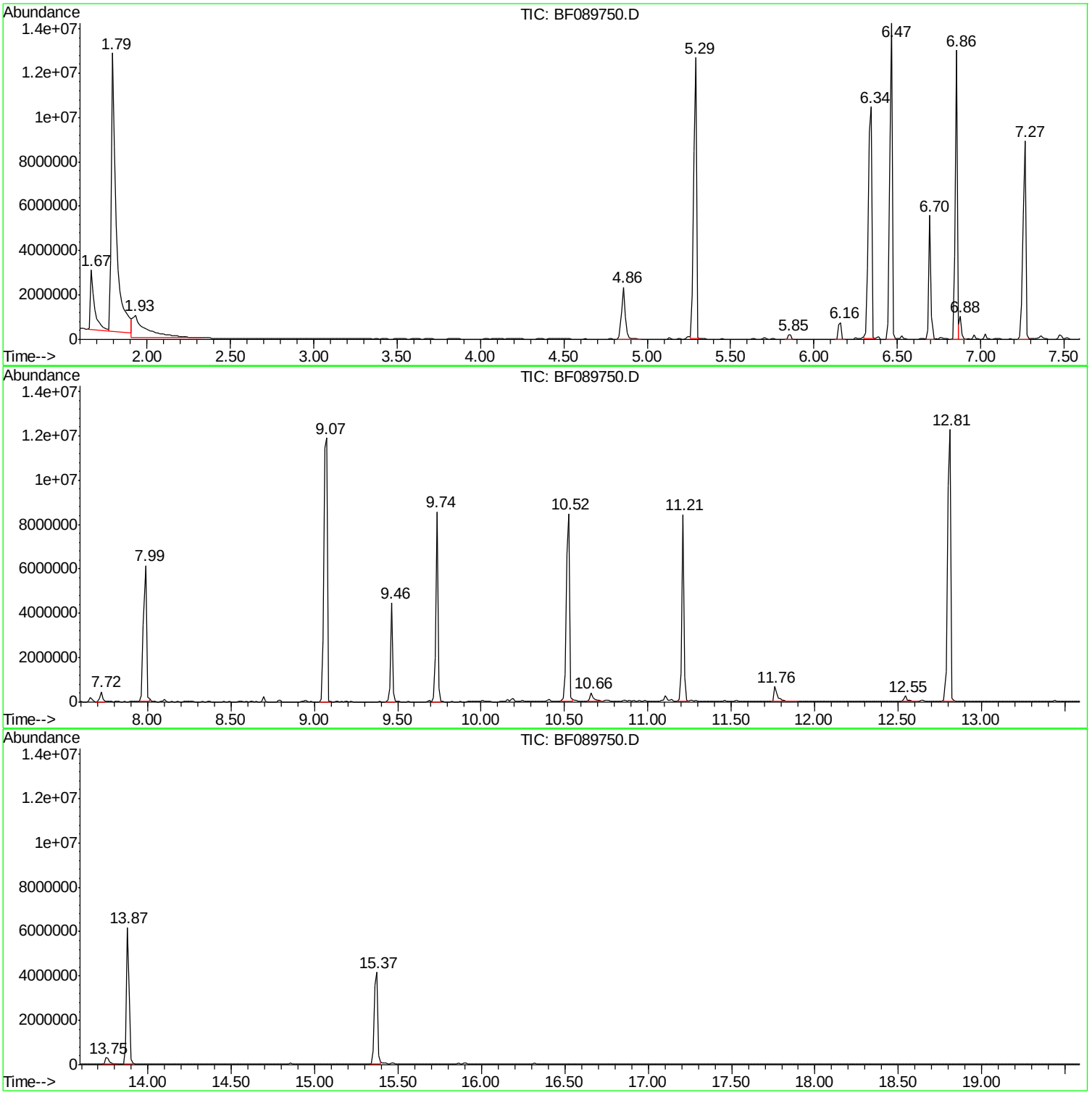
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089750.D
Acq On : 17 Aug 2016 8:01
Operator : UM/SJ
Sample : H4429-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-7A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089750.D
Acq On : 17 Aug 2016 8:01
Operator : UM/SJ
Sample : H4429-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-7A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

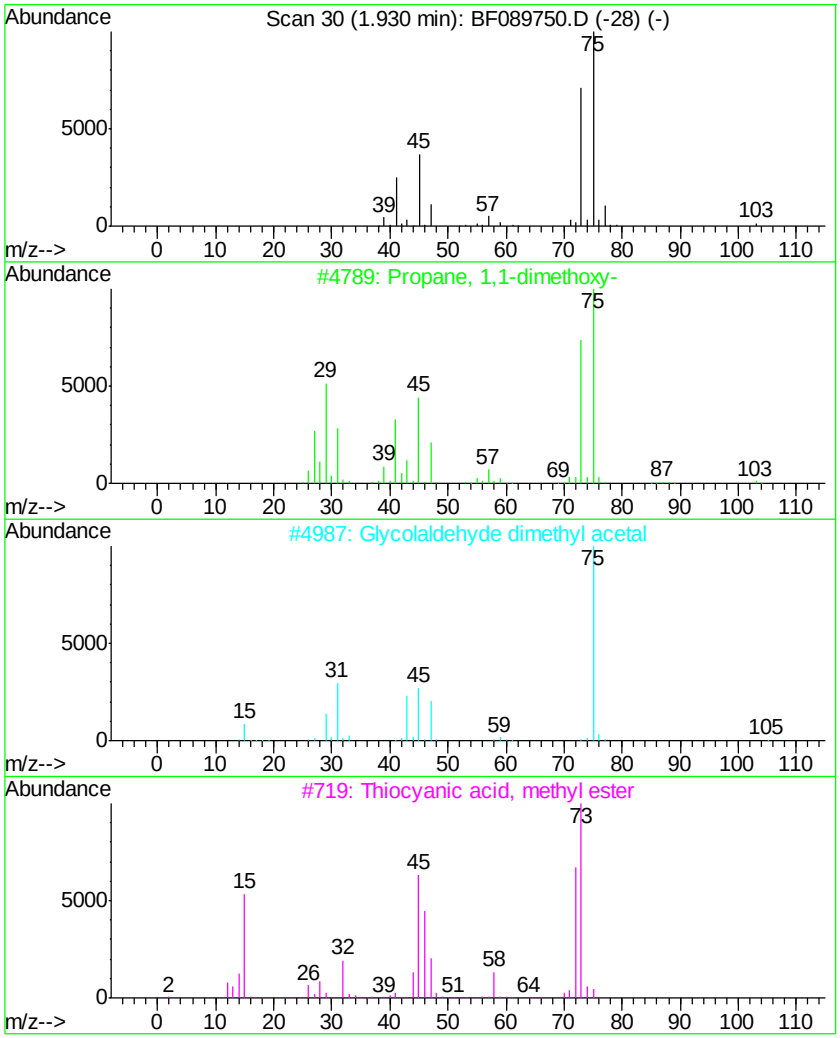
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

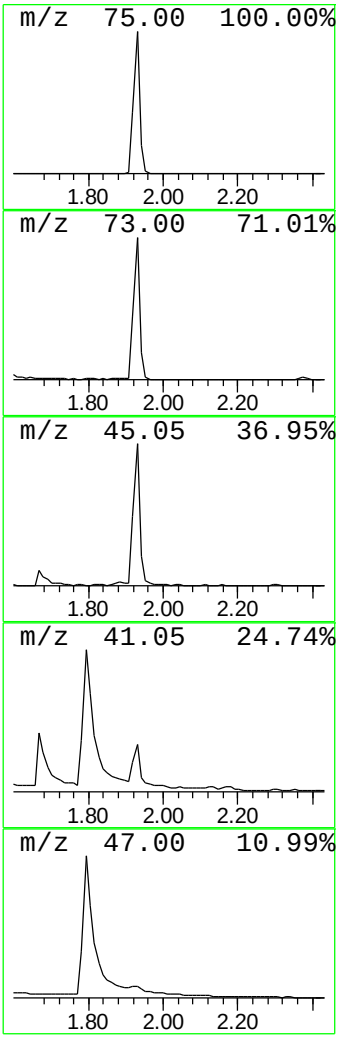
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.93	24.13 ng	5757000	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	36
3	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	10
4	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
5	tert-Butyldimethylsilanol	132	C6H16OSi	018173-64-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089750.D
Acq On : 17 Aug 2016 8:01
Operator : UM/SJ
Sample : H4429-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-7A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

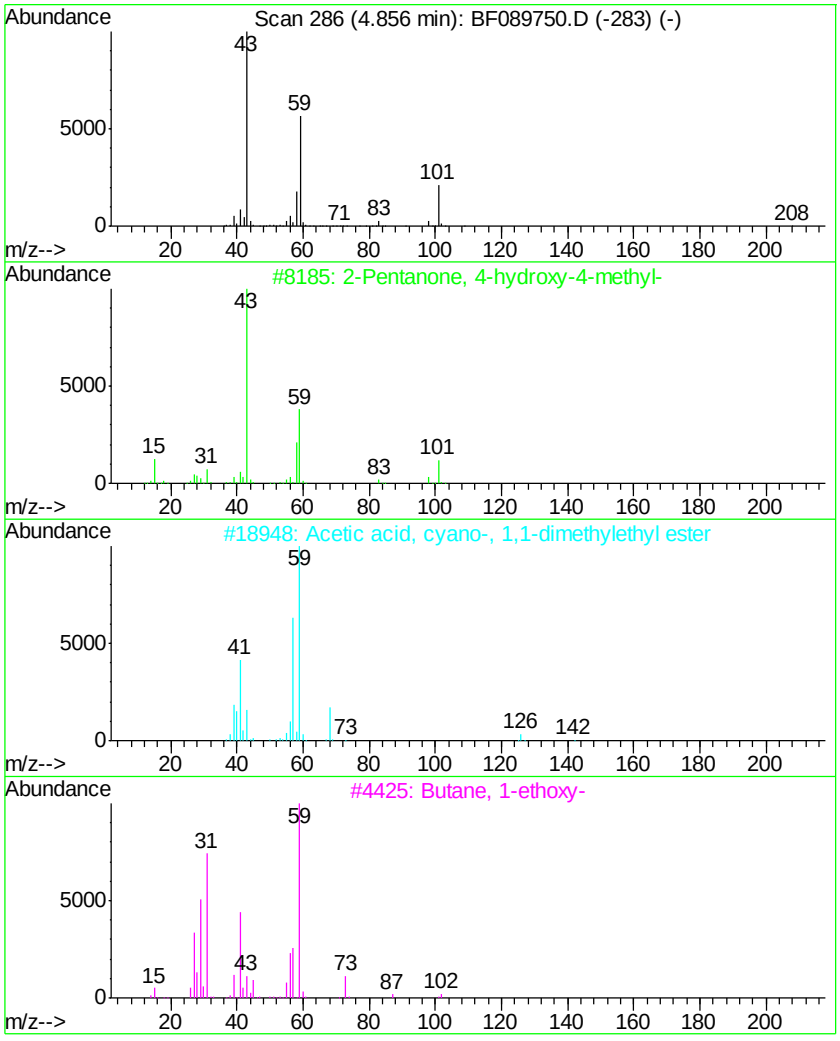
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

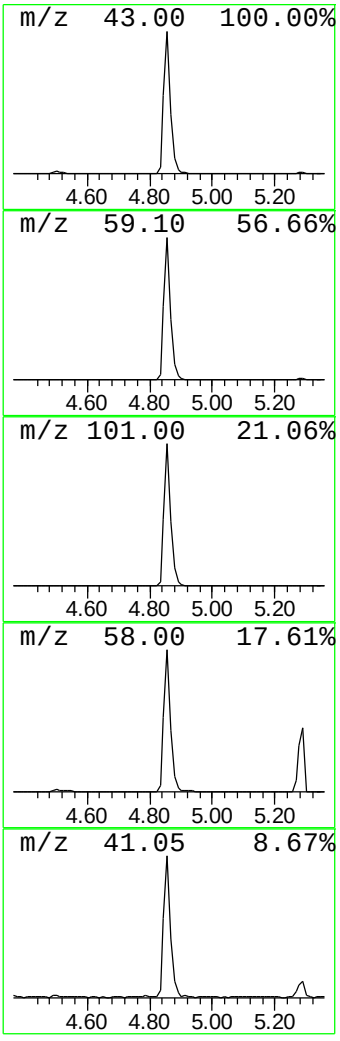
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	14.43 ng	3443150	1,4-Dichlorobenzene-d4	6.70

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	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089750.D
Acq On : 17 Aug 2016 8:01
Operator : UM/SJ
Sample : H4429-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-7A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

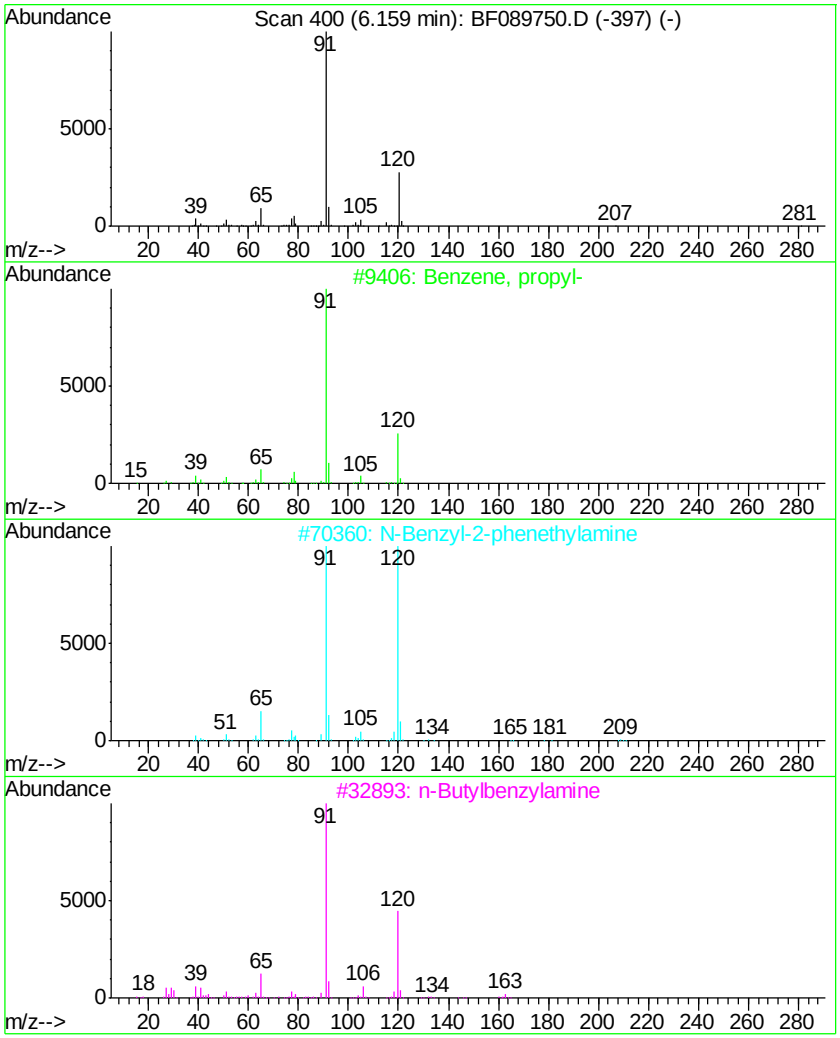
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

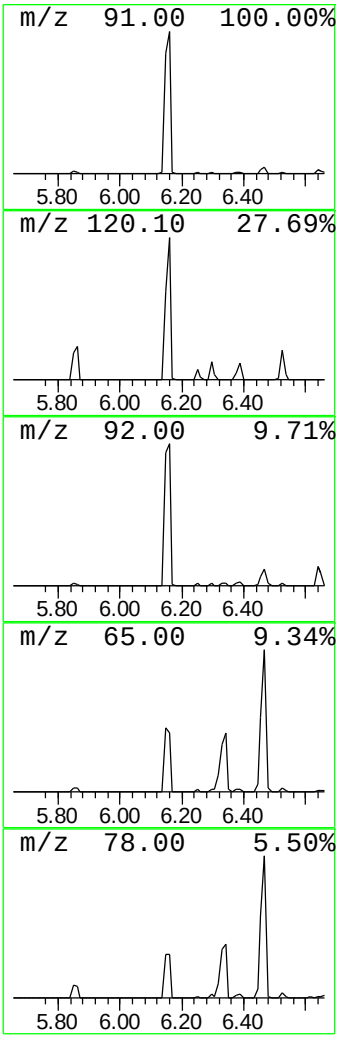
****

Peak Number 5 Benzene, propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	4.08 ng	974491	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	91
2	N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	74
3	n-Butylbenzylamine	163	C11H17N	002403-22-7	72
4	Propanenitrile, 3-[(phenylmethyl...	160	C10H12N2	000706-03-6	72
5	Phenethylamine, N-benzyl-p-chloro-	245	C15H16ClN	013622-43-0	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089750.D
Acq On : 17 Aug 2016 8:01
Operator : UM/SJ
Sample : H4429-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-7A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

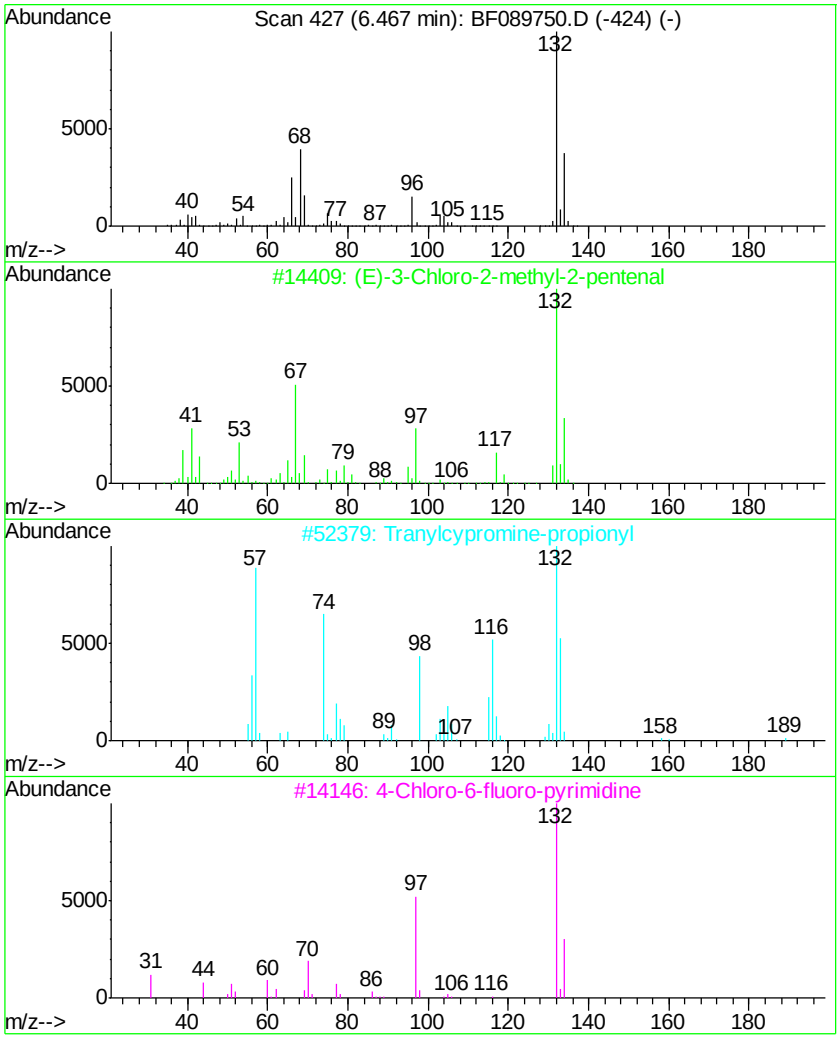
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

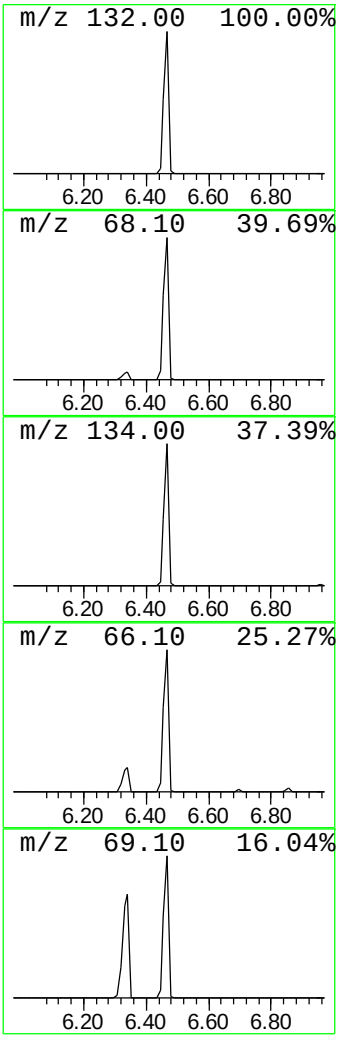
****

Peak Number 6 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	65.98 ng	15744800	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089750.D
Acq On : 17 Aug 2016 8:01
Operator : UM/SJ
Sample : H4429-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-7A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

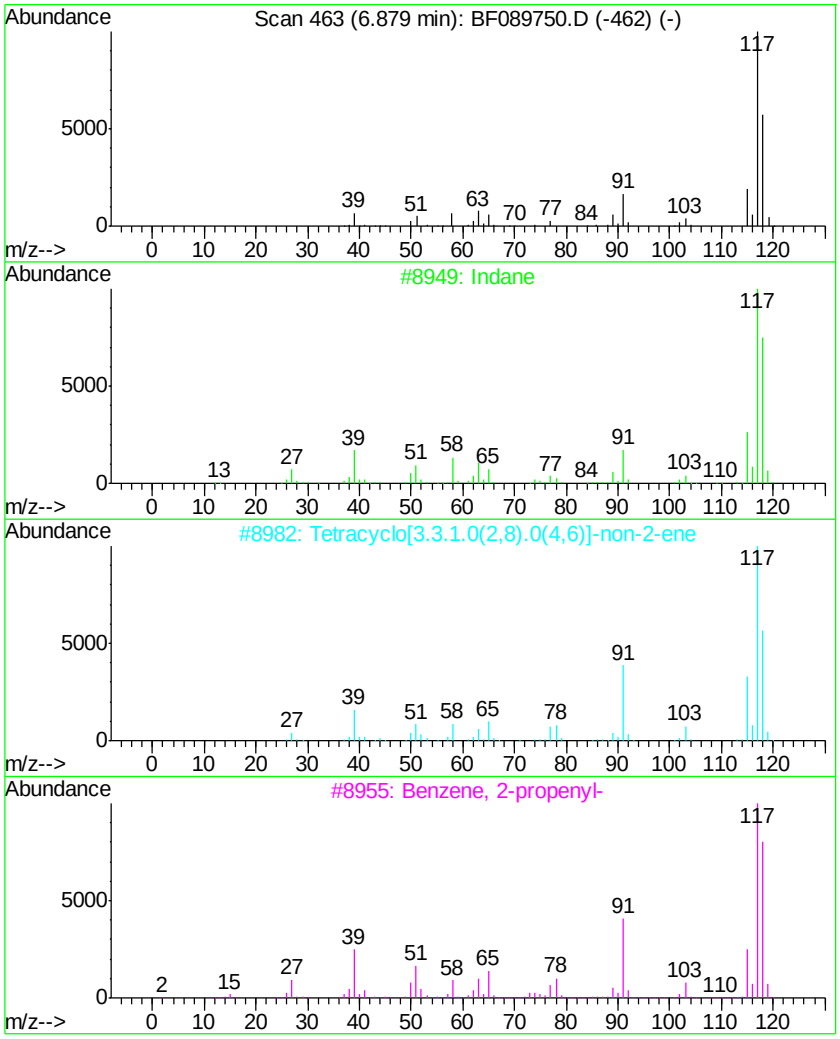
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

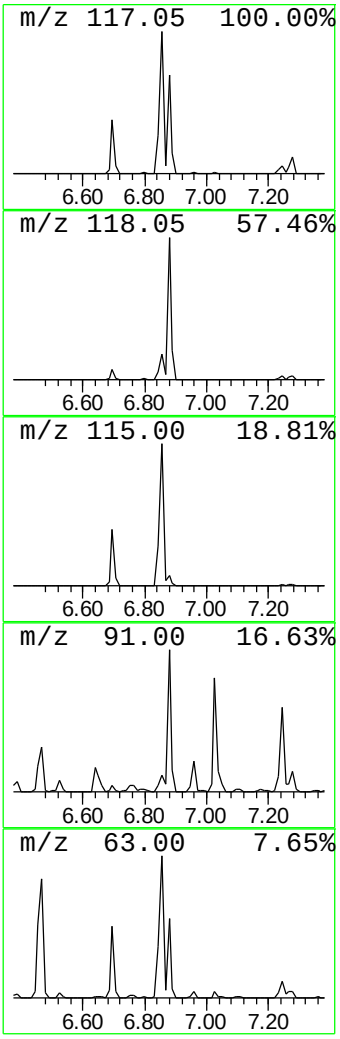
****

Peak Number 8 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	3.52 ng	840235	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	87
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	59
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	58
5	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081616\
Data File : BF089750.D
Acq On : 17 Aug 2016 8:01
Operator : UM/SJ
Sample : H4429-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LOCATION-7A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

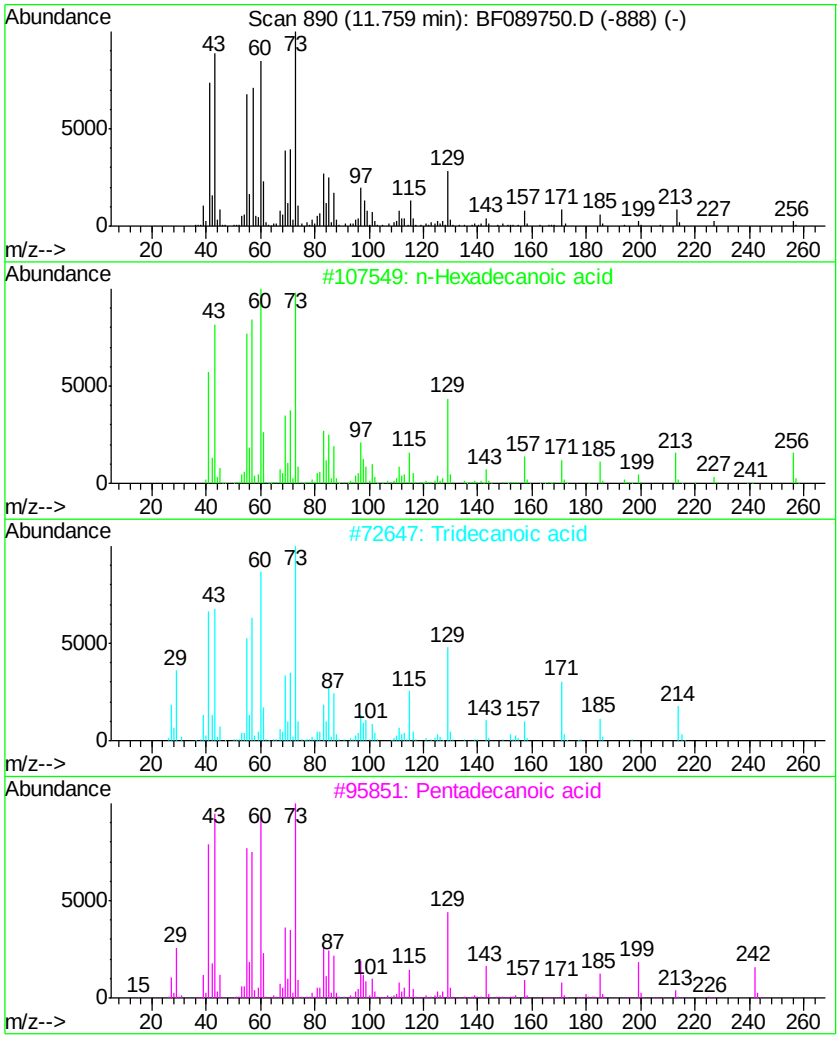
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

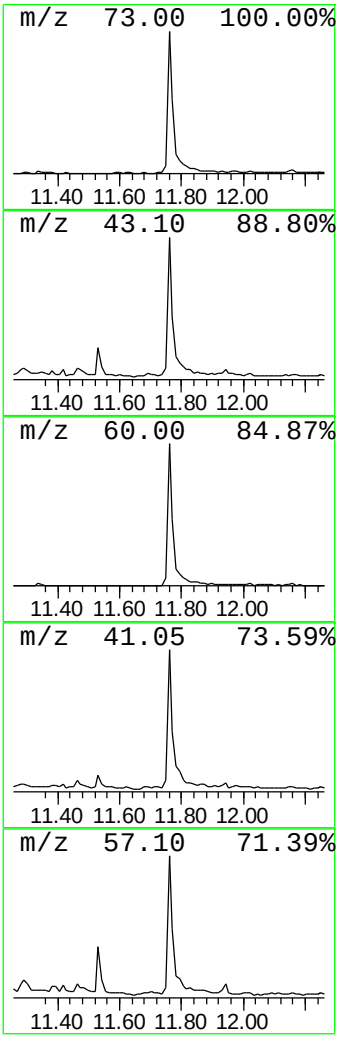
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	2.88 ng	1075080	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Dodecanoic acid	200	C12H24O2	000143-07-7	68
5	Isoamyl nitrite	117	C5H11NO2	000110-46-3	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081616\
Data File : BF089750.D
Acq On : 17 Aug 2016 8:01
Operator : UM/SJ
Sample : H4429-02
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LOCATION-7A-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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
Propane, 1,1-dime...	1.93	24.1	ng	5757000	1	6.70	4772560	20.0
2-Pentanone, 4-hy...	4.86	14.4	ng	3443150	1	6.70	4772560	20.0
Benzene, propyl-	6.16	4.1	ng	974491	1	6.70	4772560	20.0
unknown6.47	6.47	66.0	ng	15744800	1	6.70	4772560	20.0
Indane	6.88	3.5	ng	840235	1	6.70	4772560	20.0
n-Hexadecanoic acid	11.76	2.9	ng	1075080	4	11.21	7456370	20.0