LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

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-BF060416.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	1.770	14	16	19	rBV	562910	1103578	31.97%	3.270%
2	1.895	25	27	31	rBV	1592844	2970263	86.05%	8.801%
3	2.684	93	96	97	rBV	33365	49400	1.43%	0.146%
4	2.718	97	99	102	rVB	74462	110834	3.21%	0.328%
5	3.473	162	165	172	rVB	131616	226348	6.56%	0.671%
6	4.318	236	239	242	rVB	54977	69244	2.01%	0.205%
7	4.398	244	246	249	rBV	331426	459184	13.30%	1.361%
8	4.616	262	265	269	rVB2	23508	42240	1.22%	0.125%
9	5.050	300	303	308	rBV	207153	385327	11.16%	1.142%
10	5.461	336	339	341	rBV	2382068	2497978	72.37%	7.401%
11	6.490	426	429	431	rVB	2070129	2729458	79.07%	8.087%
12	6.616	437	440	443	rBV	2233966	2846023	82.45%	8.432%
13	6.787	453	455	458	rVV2	110698	101615	2.94%	0.301%
14	6.844	458	460	464	rVB2	526198	830078	24.05%	2.459%
15	7.004	471	474	477	rVB	2301800	2152848	62.37%	6.379%
16	7.142	484	486	488	rVB2	26737	34522	1.00%	0.102%
17	7.416	507	510	512	rBV	1824047	2027815	58.75%	6.008%
18	7.564	521	523	526	rBV	57895	62974	1.82%	0.187%
19	8.079	565	568	570	rVB	666981	820017	23.76%	2.430%
20	8.136	570	573	575	rBV	914632	996557	28.87%	2.953%
21	8.296	585	587	589	rVB	299596	262982	7.62%	0.779%
22	9.210	664	667	670	rBV	3068911	3328955	96.44%	9.863%
23	9.816	717	720	724	rBV	89262	162290	4.70%	0.481%
24	9.885	724	726	728	rVB	1025586	941192	27.27%	2.789%
25	10.285	758	761	766	rBV3	13922	37508	1.09%	0.111%
26	10.673	792	795	798	rBV	1986909	2243953	65.01%	6.649%
27	11.371	853	856	858	rBV	982931	1053191	30.51%	3.120%
28	11.896	900	902	904	rBV	67538	83027	2.41%	0.246%
29	12.685	969	971	977	rBV	67090	96313	2.79%	0.285%
30	12.959	992	995	997	rBV	3226478	3451761	100.00%	10.227%
31	13.999	1083	1086	1088	rBV	1069835	1049560	30.41%	3.110%
32	14.639	1140	1142	1144	rVB	35824	45406	1.32%	0.135%
33	15.417	1207	1210	1213	rBV	309124	431932	12.51%	1.280%
34	15.977	1254	1259	1262	rBV	13533	46603	1.35%	0.138%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

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-BF060416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 33750976

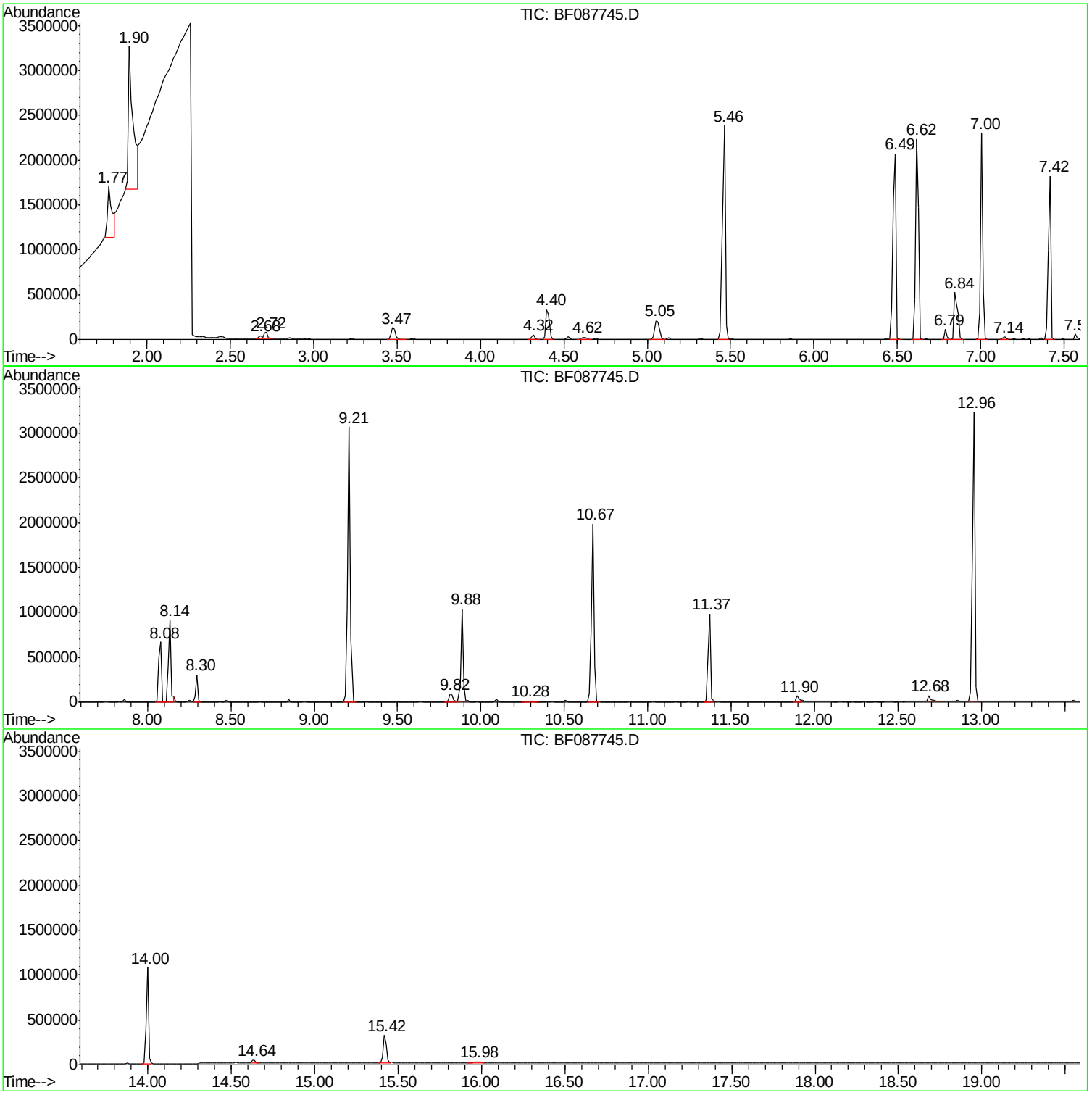
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

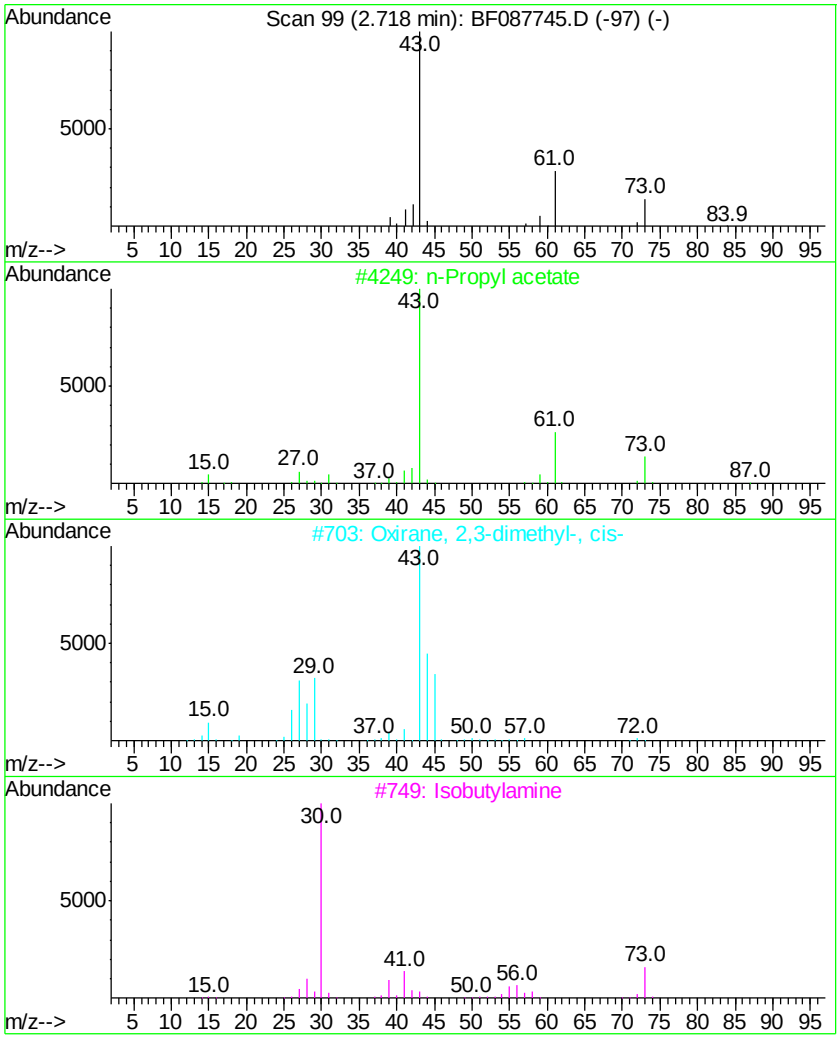
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

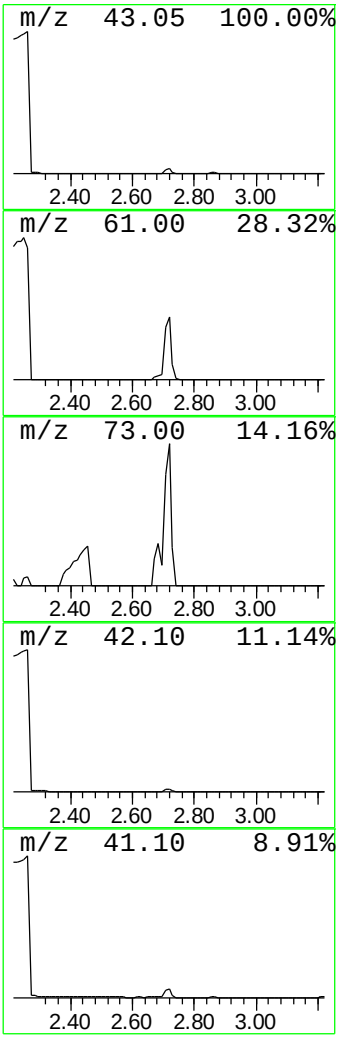
****

Peak Number 3 n-Propyl acetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.72	2.67 ng	110834	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
3	Isobutylamine	73	C4H11N	000078-81-9	7
4	1-Butanamine	73	C4H11N	000109-73-9	5
5	Butane, 2-methyl-	72	C5H12	000078-78-4	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

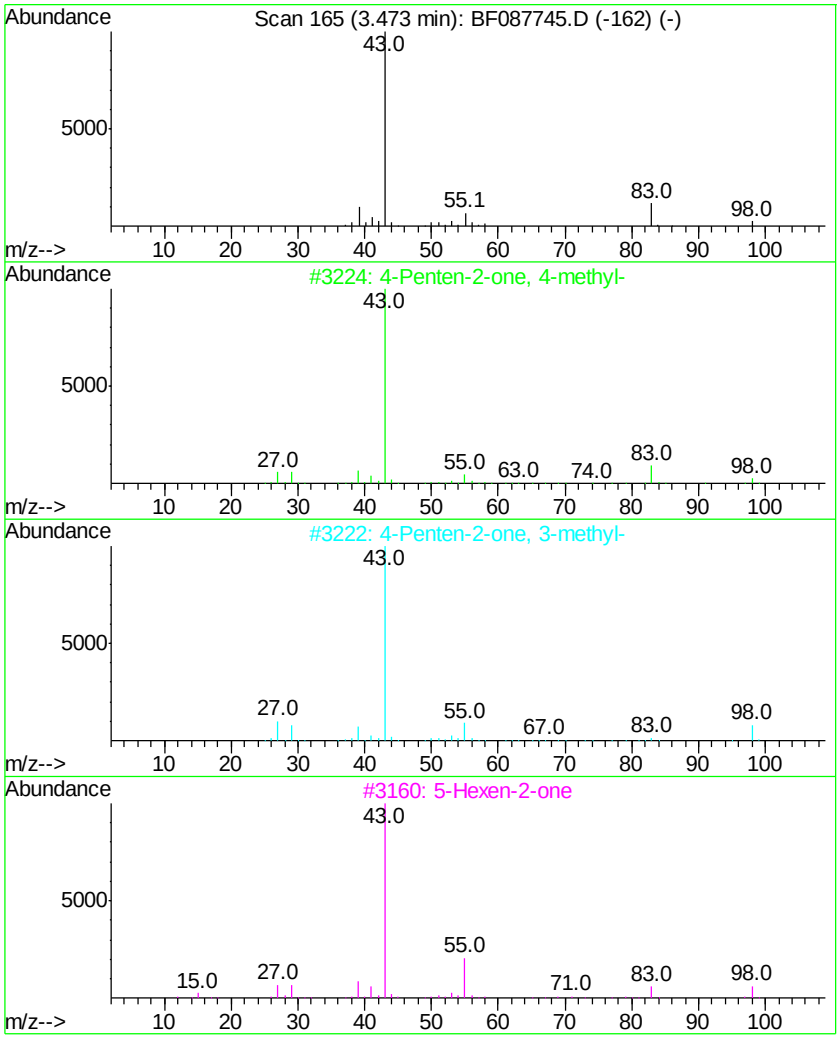
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

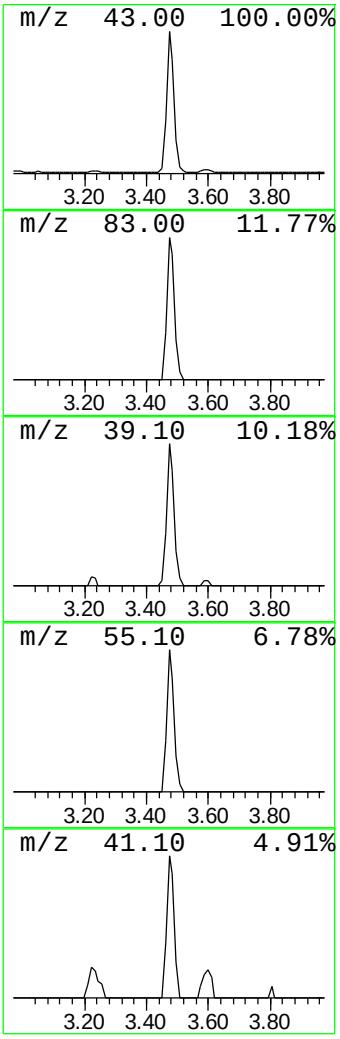
****

Peak Number 4 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.47	5.45 ng	226348	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	43
3	5-Hexen-2-one	98	C6H10O	000109-49-9	28
4	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	17
5	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

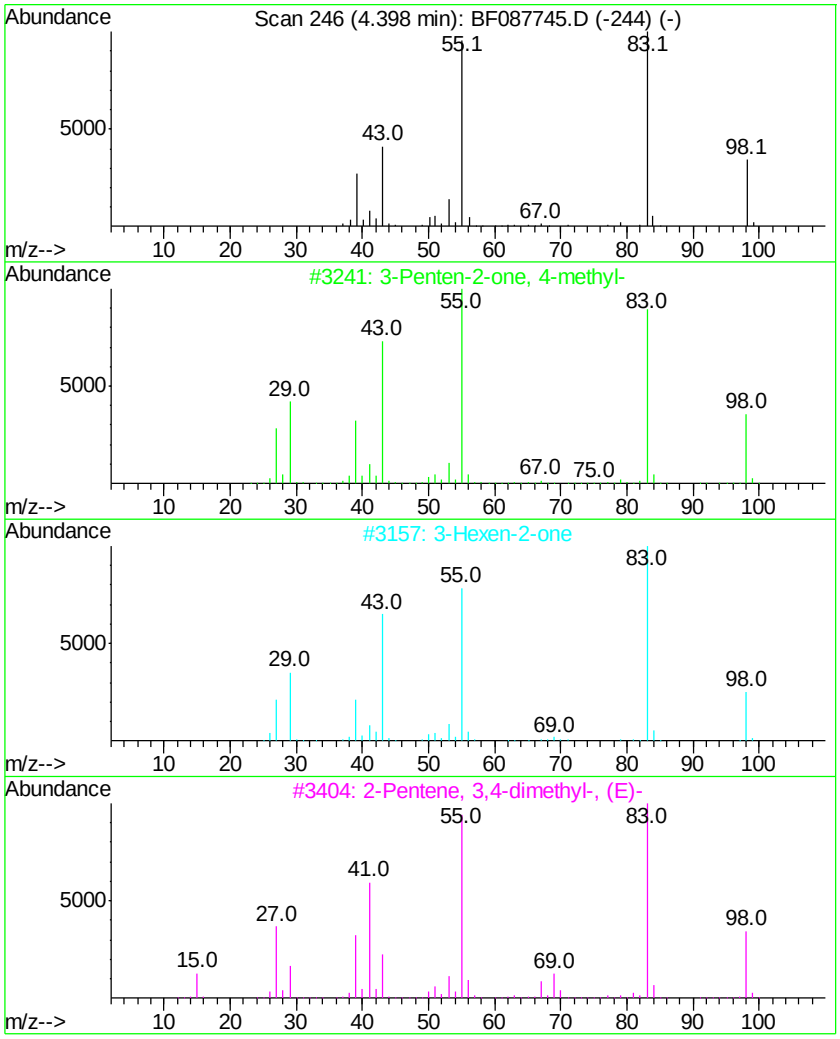
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

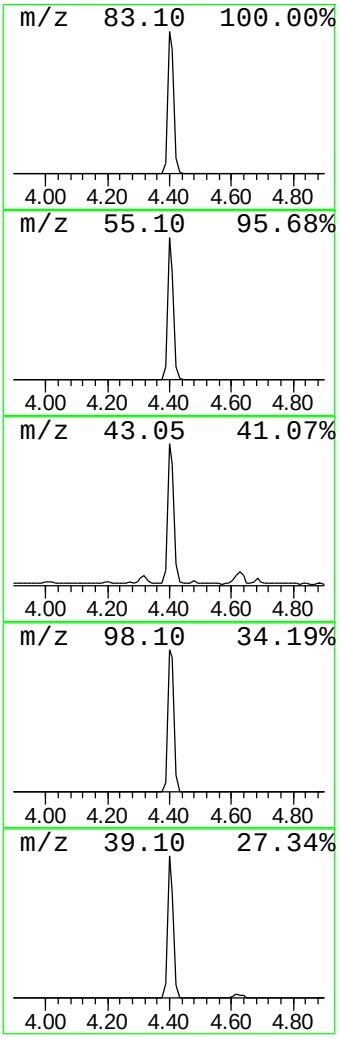
****

Peak Number 5 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	11.06 ng	459184	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

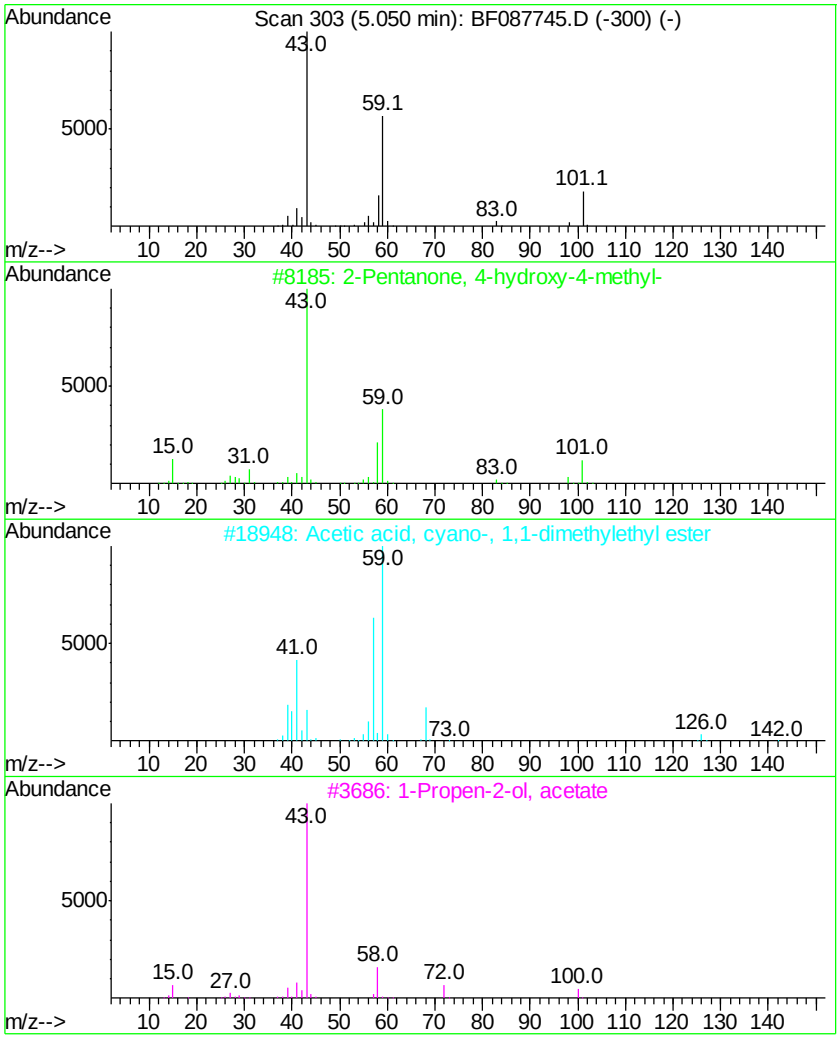
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

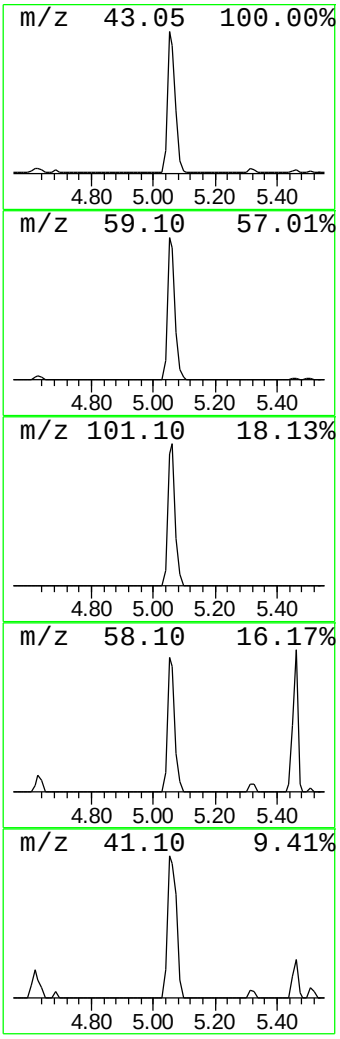
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	9.28 ng	385327	1,4-Dichlorobenzene-d4	6.84

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	32
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

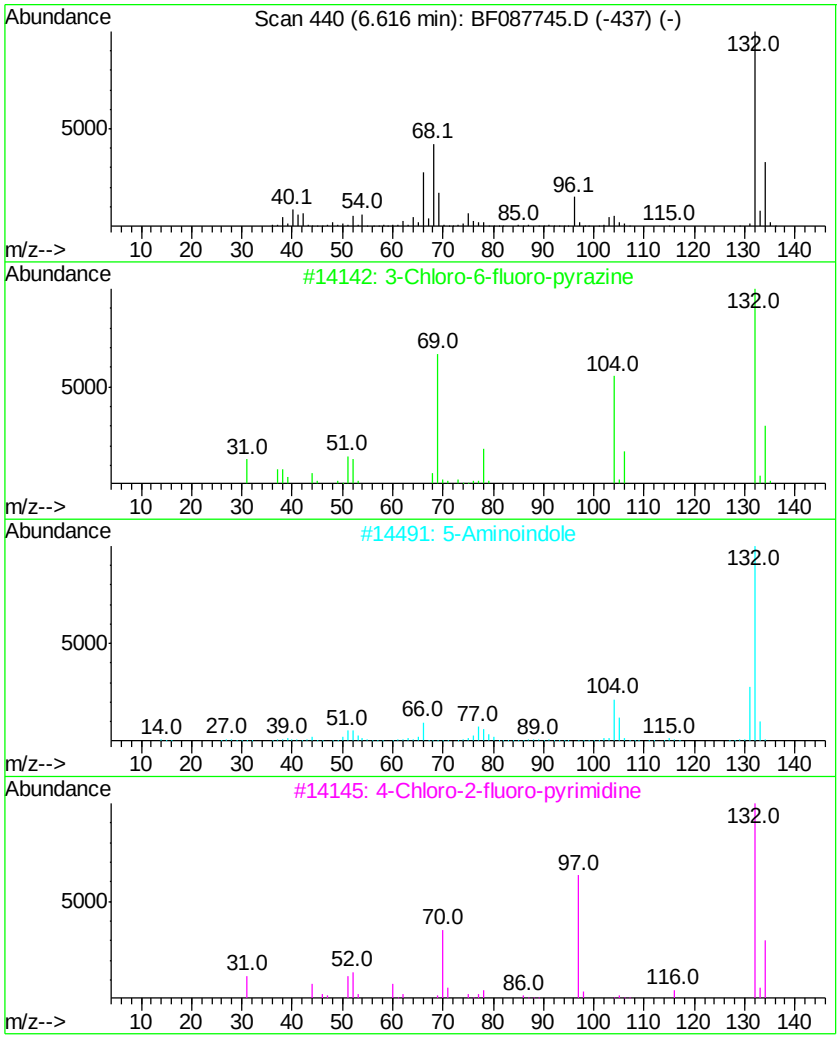
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

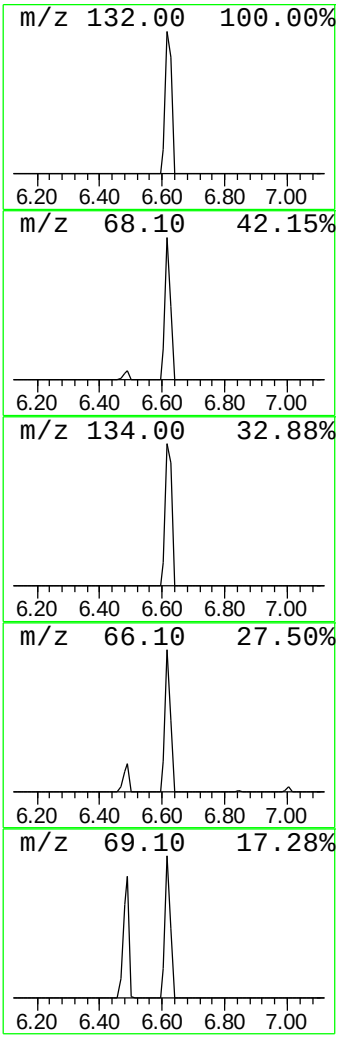
****

Peak Number 7 unknown6.62 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	68.57 ng	2846020	1,4-Dichlorobenzene-d4	6.84

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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

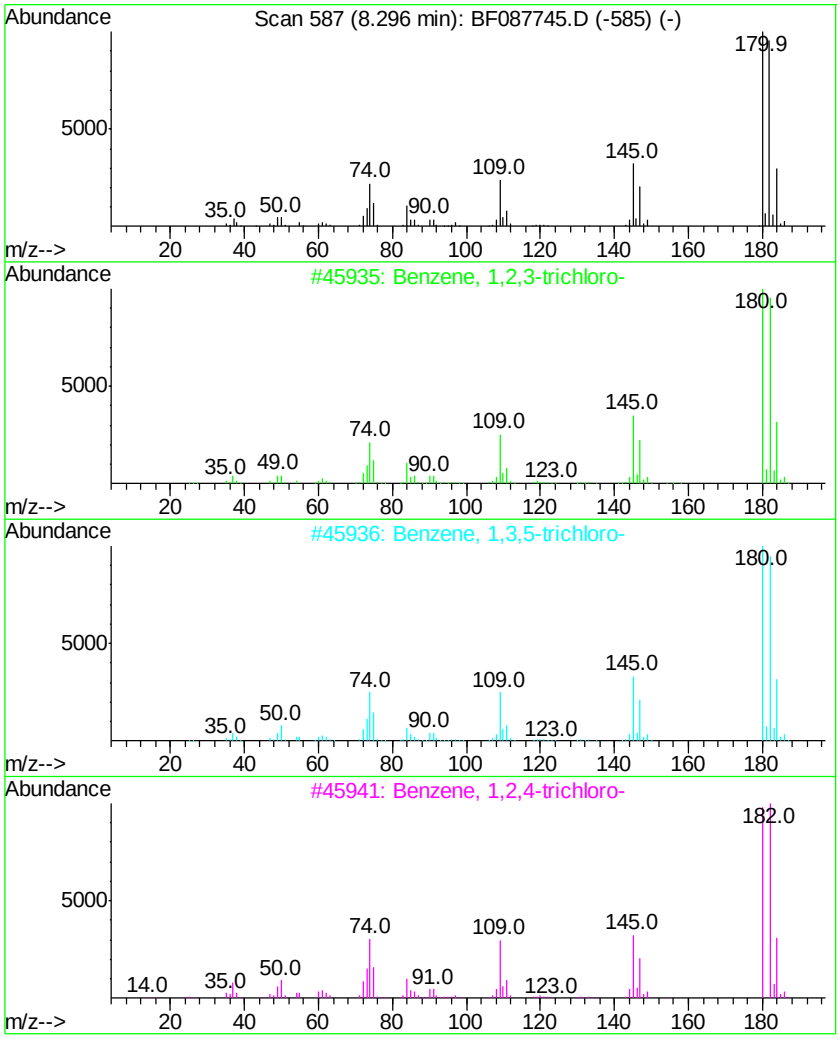
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

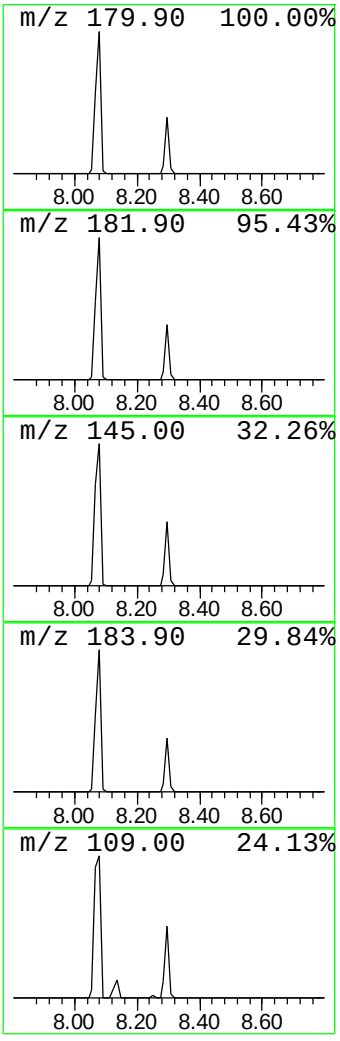
****

Peak Number 9 Benzene, 1,2,3-trichloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.30	5.28 ng	262982	Naphthalene-d8	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	99
2	Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
3	Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	97
4	Benzene, 1-chloro-3-(trifluorome...	180	C7H4ClF3	000098-15-7	27
5	5-Benzofurazancarboxylic acid, 1...	180	C7H4N2O4	006086-24-4	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

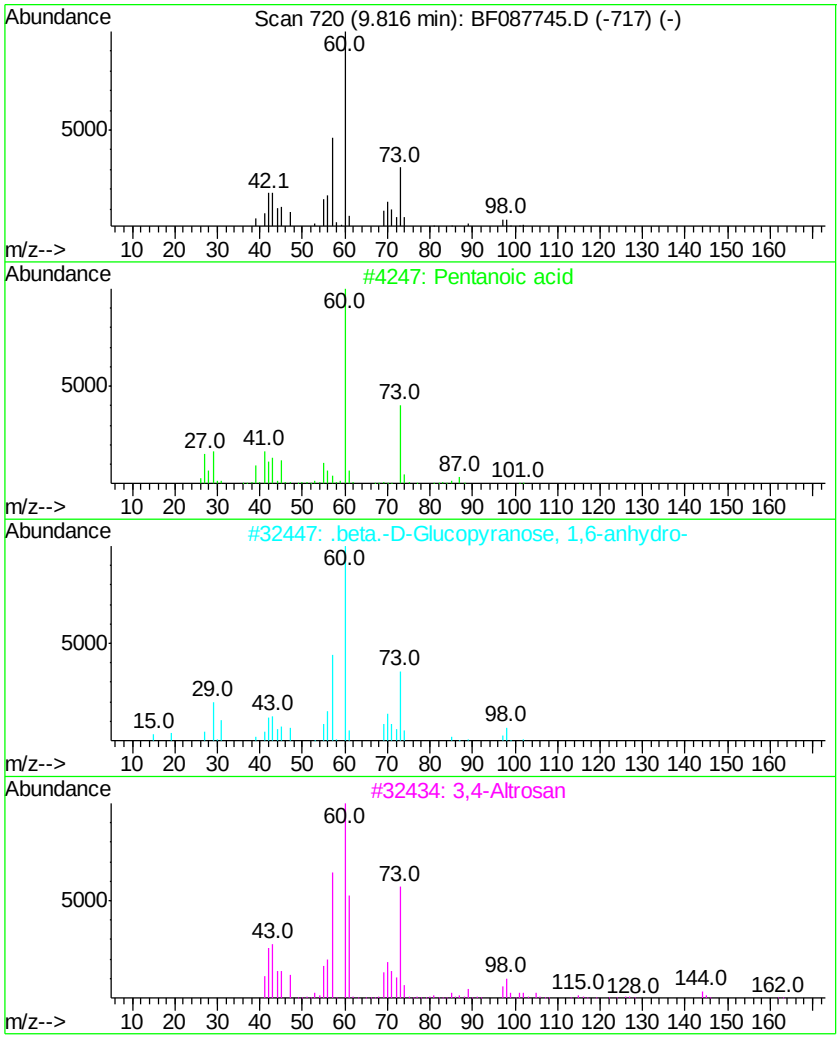
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

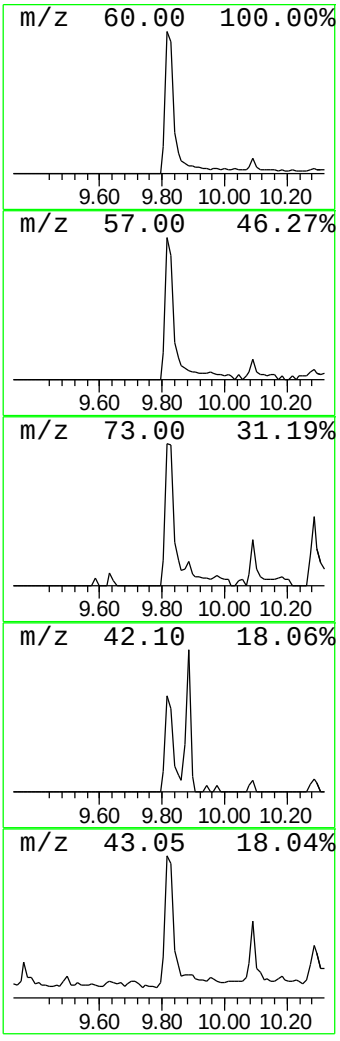
****

Peak Number 10 Pentanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.82	3.45 ng	162290	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	50
2	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	50
3	3,4-Altrosan	162	C6H10O5	1000129-76-4	42
4	Methyl-4-azido-4-desoxy.beta.l-a...	189	C6H11N3O4	1000312-10-3	40
5	Heptanoic acid	130	C7H14O2	000111-14-8	39





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

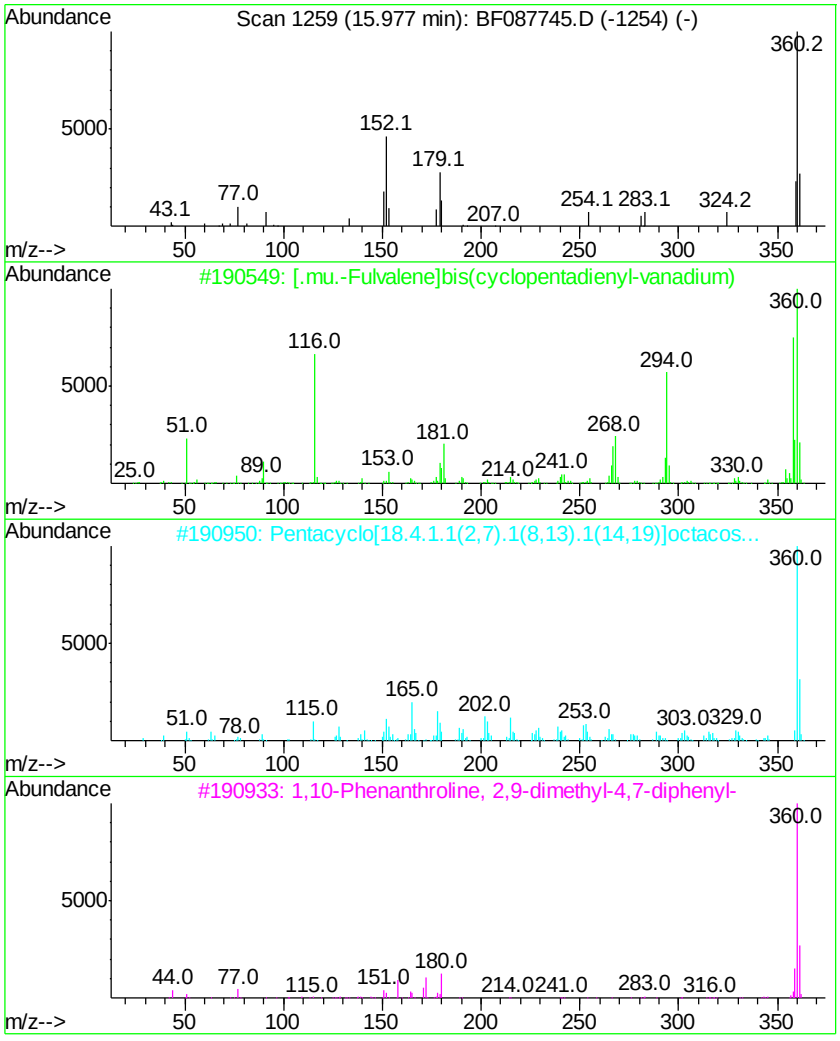
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

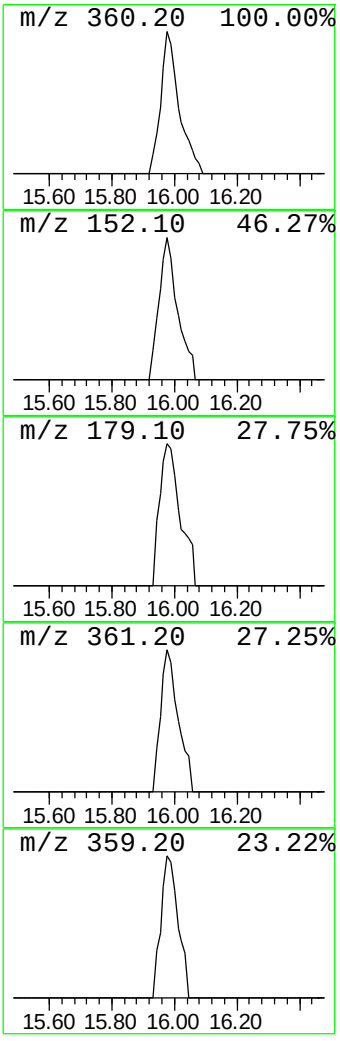
****

Peak Number 11 unknown15.98 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.16 ng	46603	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[.mu.-Fulvalene]bis(cyclopentadi...	360	C20H18V2	1000163-45-2	38
2	Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	9
3	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	9
4	Benzo[1,2-b:4,3-b']dipyrrole-1,8...	360	C18H20N2O6	174832-71-4	5
5	Melatonin, pentafluoropropionyl ...	360	C16H13F5N2O2	066012-87-1	5





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060616\
Data File : BF087745.D
Acq On : 6 Jun 2016 11:44
Operator : UM/SJ
Sample : H3372-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HSR-WC-49-060116

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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
n-Propyl acetate	2.72	2.7	ng	110834	1	6.84	830078	20.0
4-Penten-2-one, 4...	3.47	5.5	ng	226348	1	6.84	830078	20.0
3-Penten-2-one, 4...	4.40	11.1	ng	459184	1	6.84	830078	20.0
2-Pentanone, 4-hy...	5.05	9.3	ng	385327	1	6.84	830078	20.0
unknown6.62	6.62	68.6	ng	2846020	1	6.84	830078	20.0
Benzene, 1,2,3-tr...	8.30	5.3	ng	262982	2	8.14	996557	20.0
Pentanoic acid	9.82	3.5	ng	162290	3	9.88	941192	20.0
unknown15.98	15.98	2.2	ng	46603	6	15.42	431932	20.0