LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087717.D
Acq On : 5 Jun 2016 19:51
Operator : UM/SJ
Sample : H3379-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

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	11	16	18	rBV	4280637	8043198	100.00%	20.641%
2	1.907	26	28	48	rVB	1394700	2871761	35.70%	7.370%
3	2.158	48	50	64	rVB	88763	178305	2.22%	0.458%
4	5.062	301	304	312	rBV	206410	317730	3.95%	0.815%
5	5.462	336	339	341	rBV	2567093	2867630	35.65%	7.359%
6	6.490	425	429	431	rBV	2443669	2863825	35.61%	7.349%
7	6.627	438	441	443	rBV	2865862	3070001	38.17%	7.878%
8	6.856	459	461	464	rBV	809250	692561	8.61%	1.777%
9	7.016	472	475	477	rBV	2642924	2446679	30.42%	6.279%
10	7.427	507	511	513	rBV	1781854	2295964	28.55%	5.892%
11	8.148	571	574	576	rBV	738355	926740	11.52%	2.378%
12	9.222	665	668	671	rBV	2998239	3164790	39.35%	8.122%
13	9.611	700	702	705	rBV	204160	264862	3.29%	0.680%
14	9.896	724	727	730	rVB	1150326	1042031	12.96%	2.674%
15	10.685	793	796	799	rBV	2006238	2130528	26.49%	5.468%
16	11.382	854	857	859	rBV	1047409	1057649	13.15%	2.714%
17	12.799	978	981	983	rVB	170285	172623	2.15%	0.443%
18	12.971	993	996	998	rBV	2800427	2950457	36.68%	7.572%
19	13.497	1040	1042	1045	rBV	105755	105846	1.32%	0.272%
20	14.011	1084	1087	1089	rBV	945595	859665	10.69%	2.206%
21	15.440	1209	1212	1215	rBV	536797	644004	8.01%	1.653%

Sum of corrected areas: 38966849

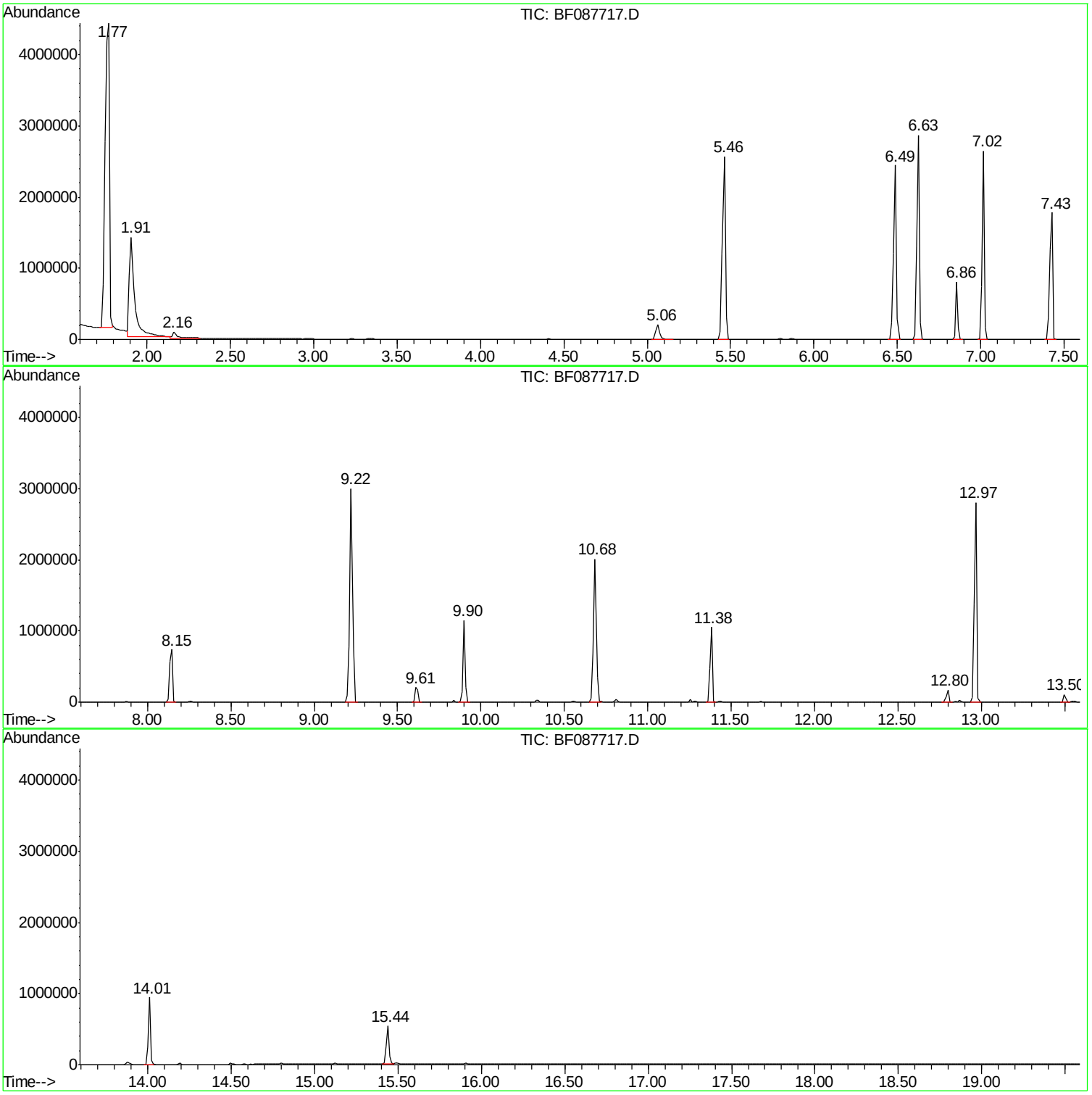
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087717.D
Acq On : 5 Jun 2016 19:51
Operator : UM/SJ
Sample : H3379-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087717.D
Acq On : 5 Jun 2016 19:51
Operator : UM/SJ
Sample : H3379-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

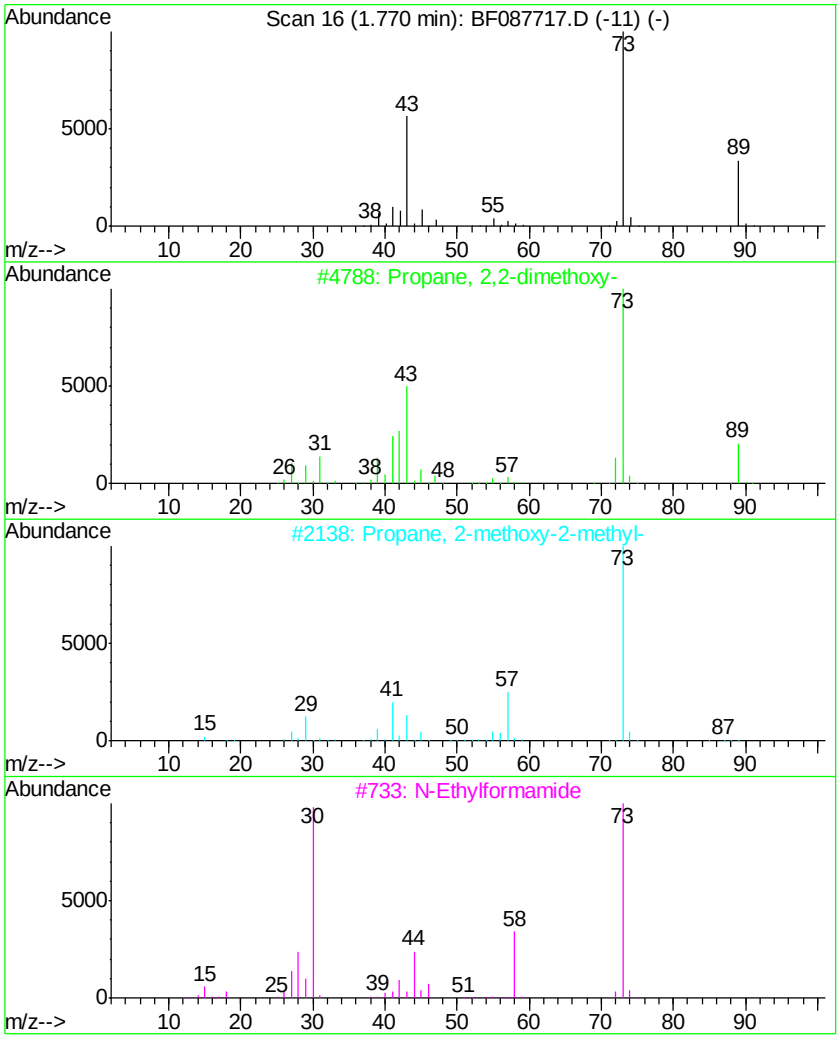
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

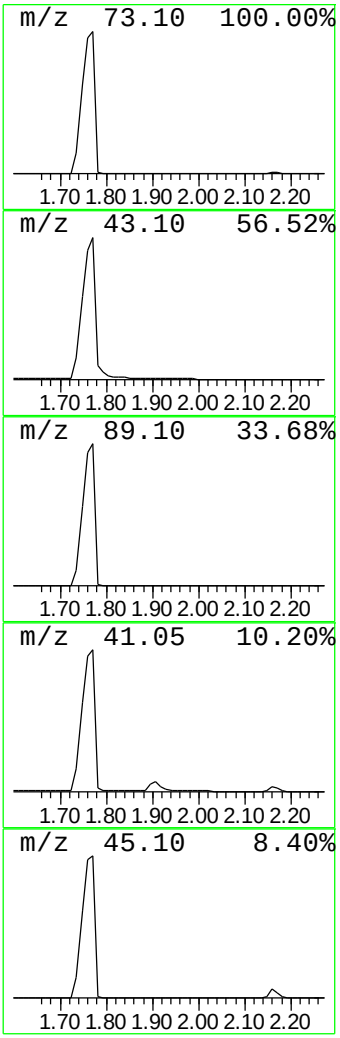
****

Peak Number 1 unknown1.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.77	232.27 ng	8043200	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	17
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
5	1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087717.D
Acq On : 5 Jun 2016 19:51
Operator : UM/SJ
Sample : H3379-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

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

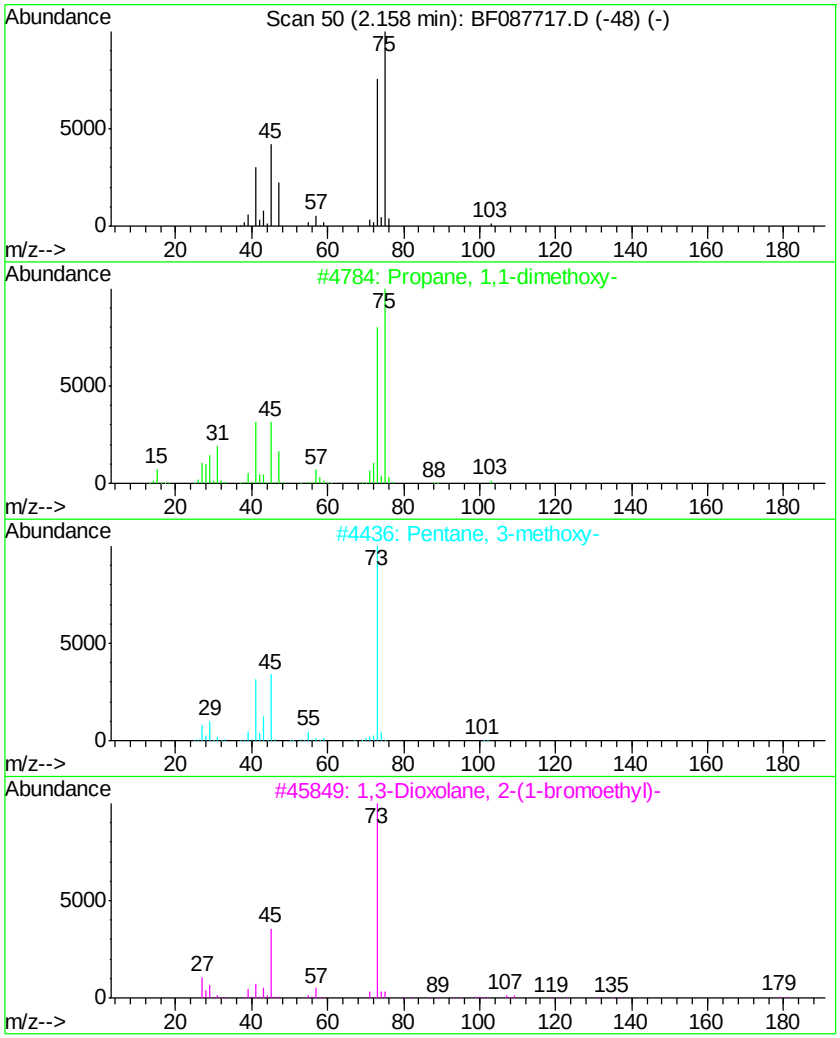
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

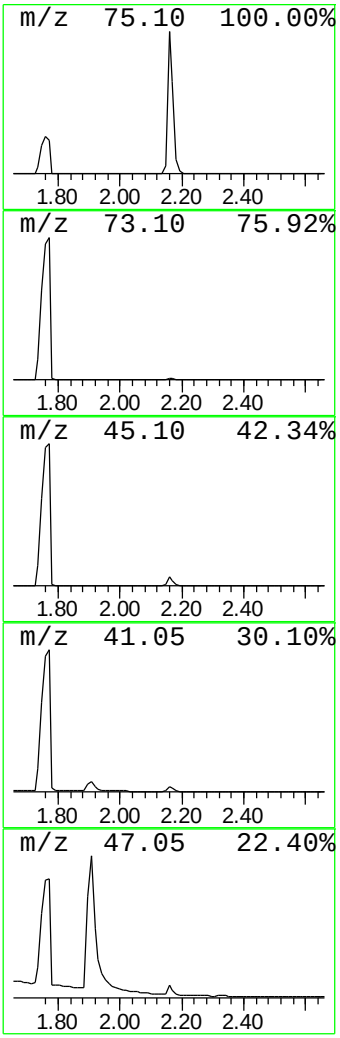
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	5.15 ng	178305	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
3	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
4	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
5	.beta.-D-Glucopyranoside, methyl...	176	C7H12O5	003056-46-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
Data File : BF087717.D
Acq On : 5 Jun 2016 19:51
Operator : UM/SJ
Sample : H3379-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

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

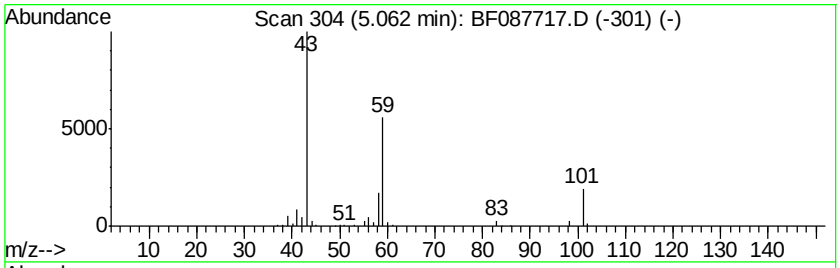
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

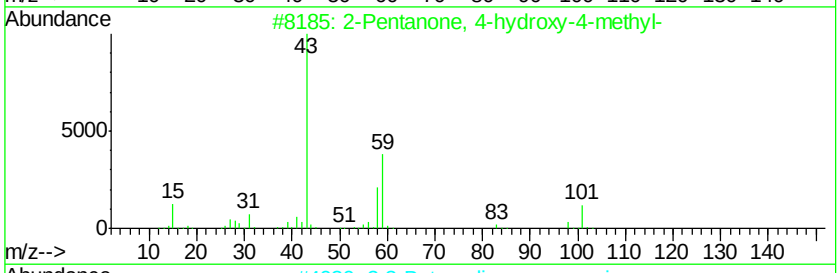
****

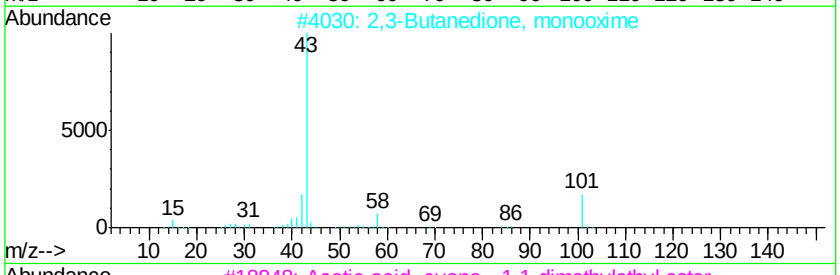
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

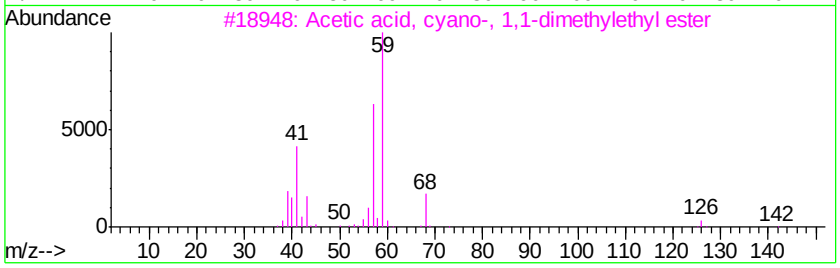
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	9.18 ng	317730	1,4-Dichlorobenzene-d4	6.86

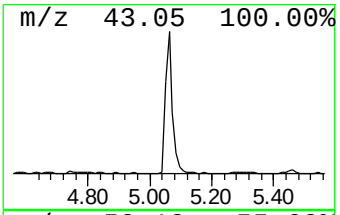
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9

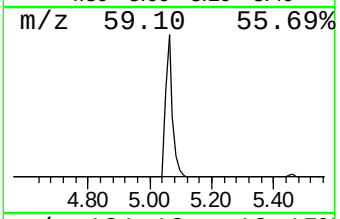


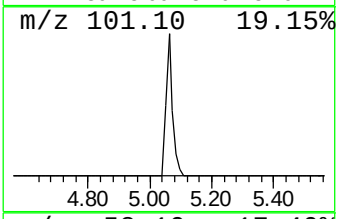


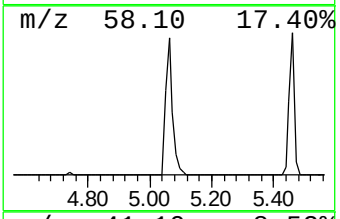


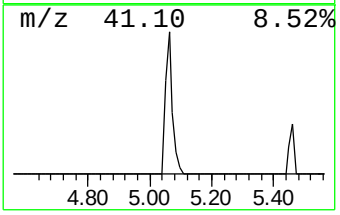












Data Path : Z:\HPCHEM1\BNA F\DATA\BF060516\
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Sample : H3379-01
Misc :
ALS Vial : 56 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1

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

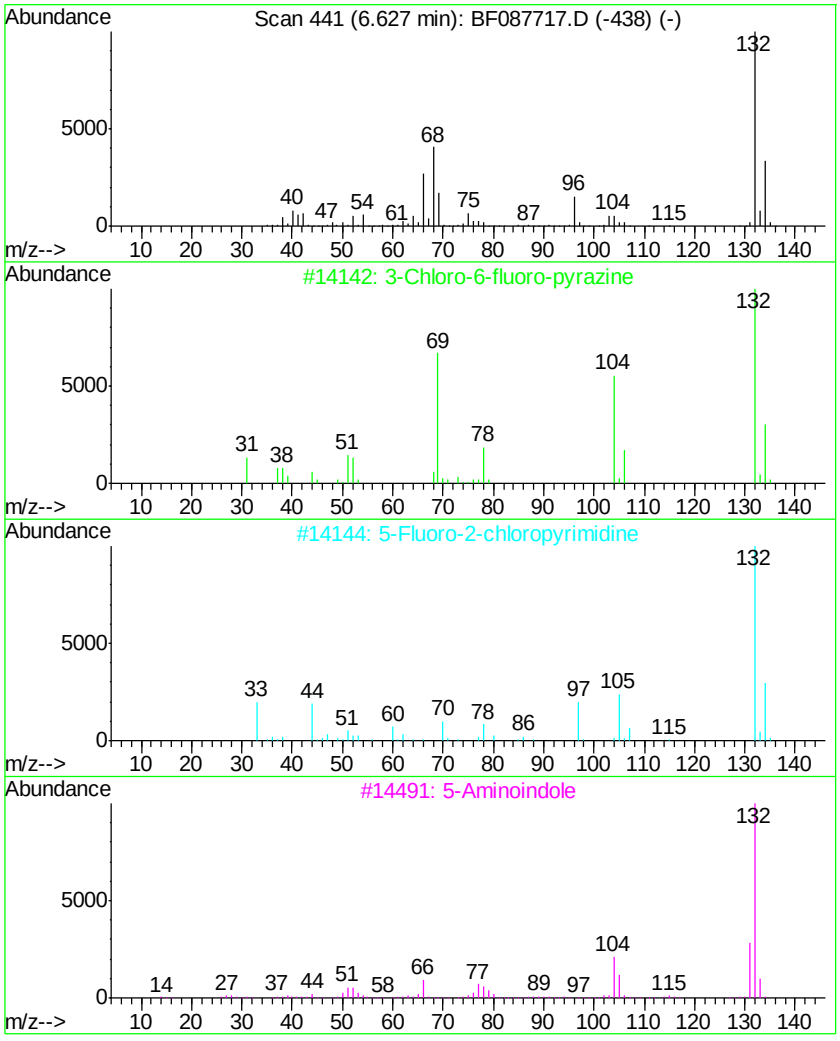
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

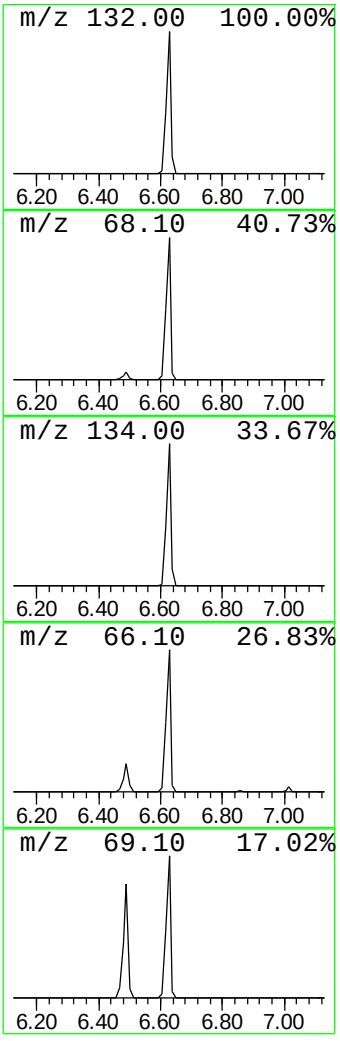
****

Peak Number 5 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	88.66 ng	3070000	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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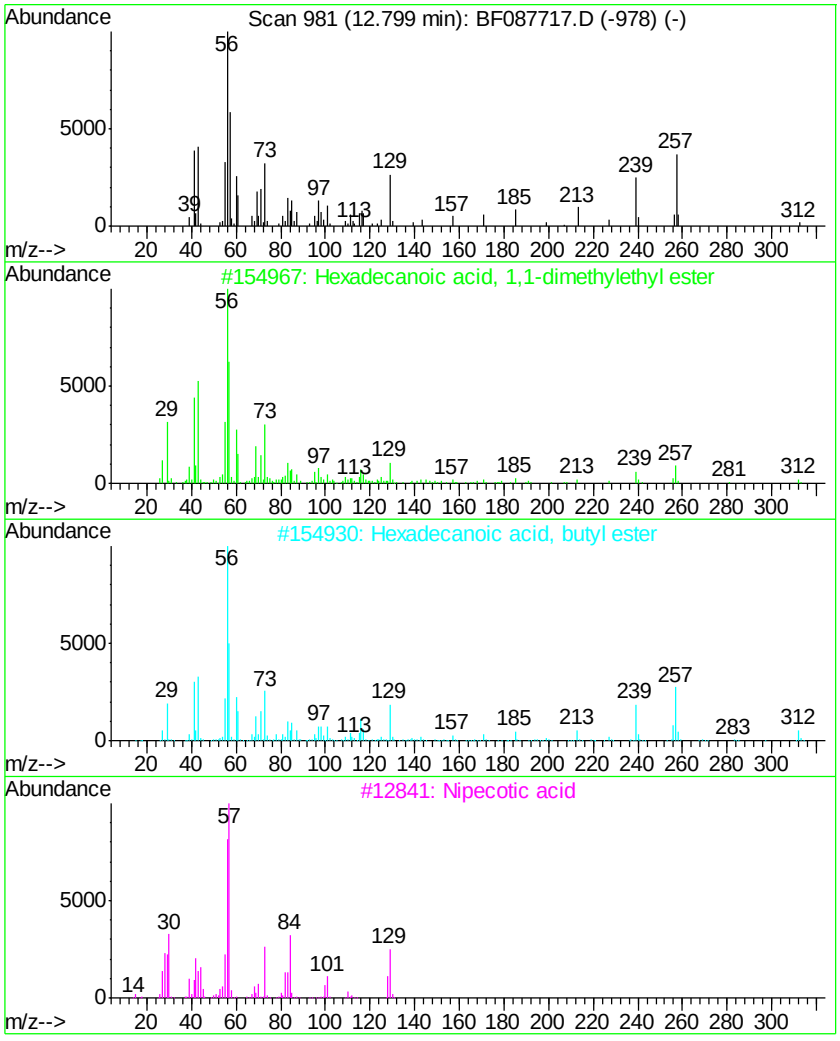
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

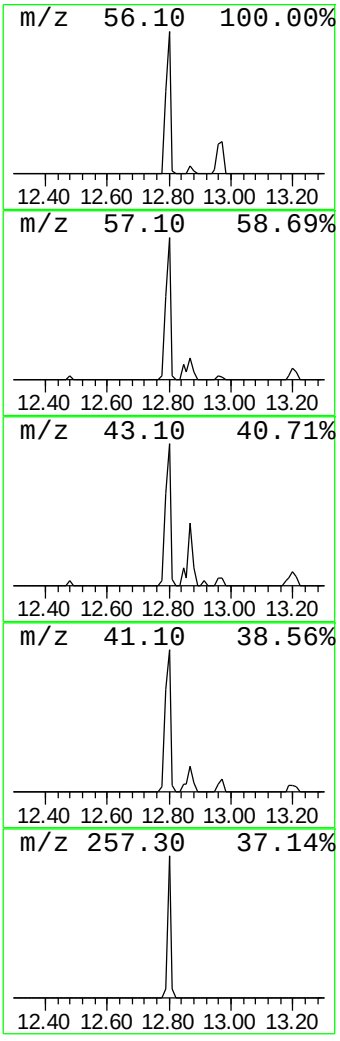
****

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	4.02 ng	172623	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Nipecotic acid	129	C6H11NO2	000498-95-3	47
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	38
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	25





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

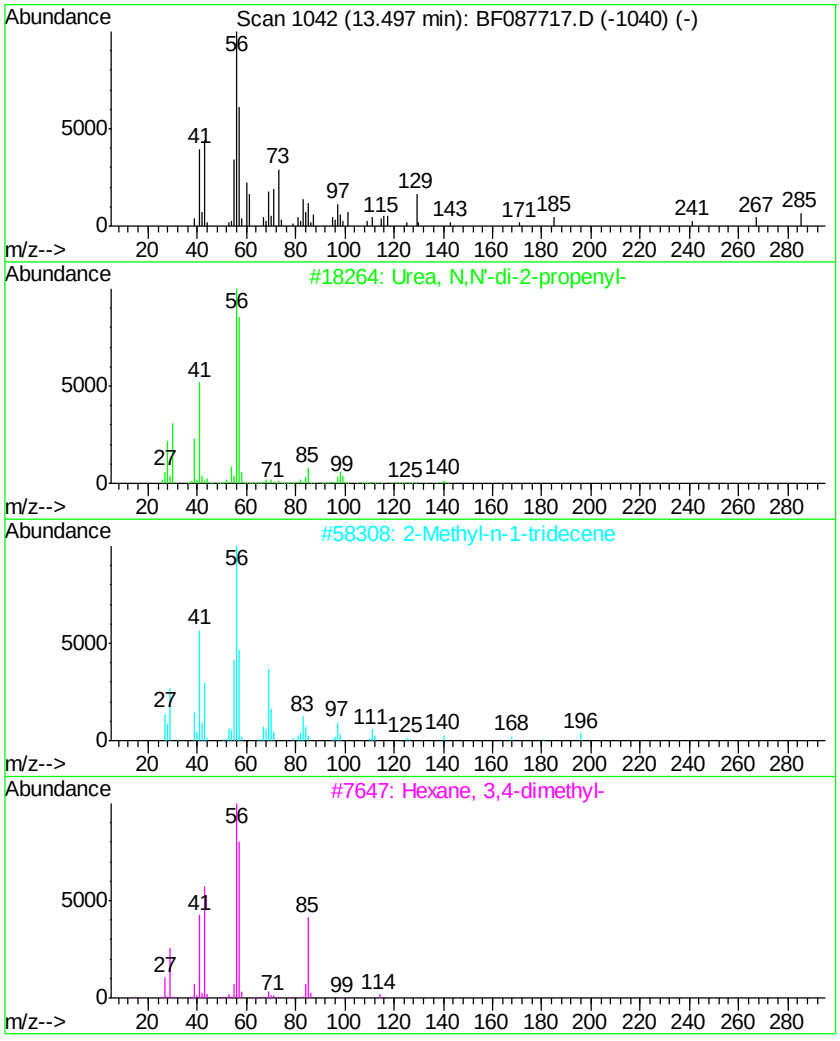
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

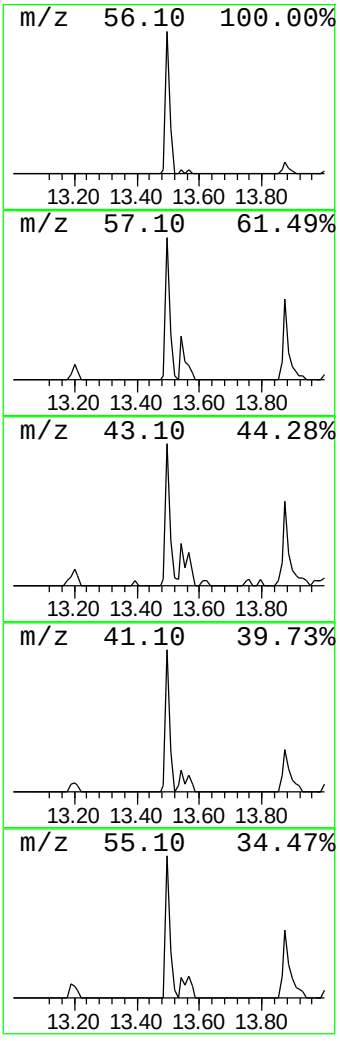
****

Peak Number 8 unknown13.50 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.46 ng	105846	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
2	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
3	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	38
4	Cyclohexanamine	99	C6H13N	000108-91-8	38
5	2-Methyl-1-octadecene	266	C19H38	061868-20-0	37





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.77	1.77	232.3	ng	8043200	1	6.86	692561	20.0
Propane, 1,1-dime...	2.16	5.2	ng	178305	1	6.86	692561	20.0
2-Pentanone, 4-hy...	5.06	9.2	ng	317730	1	6.86	692561	20.0
unknown6.63	6.63	88.7	ng	3070000	1	6.86	692561	20.0
Hexadecanoic acid...	12.80	4.0	ng	172623	5	14.01	859665	20.0
unknown13.50	13.50	2.5	ng	105846	5	14.01	859665	20.0