LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082416\
Data File : BF089871.D
Acq On : 24 Aug 2016 13:50
Operator : UM/SJ
Sample : H4551-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AST-2

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-BF081916.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	1.655	4	6	14	rBV	640918	1134400	9.83%	1.054%
2	1.770	14	16	21	rVV	4443220	7551707	65.43%	7.016%
3	1.838	21	22	58	rVB	718196	2592114	22.46%	2.408%
4	4.799	278	281	291	rBV	1789061	3039196	26.33%	2.824%
5	5.244	317	320	323	rBV	8062821	9796694	84.88%	9.102%
6	5.667	355	357	359	rVB	99112	121786	1.06%	0.113%
7	6.307	410	413	415	rBV	8635248	9547354	82.72%	8.871%
8	6.433	421	424	426	rBV	10235691	10231150	88.64%	9.506%
9	6.662	442	444	447	rBV	2113740	2195921	19.03%	2.040%
10	6.822	456	458	461	rBV	8949865	8168176	70.77%	7.589%
11	7.233	491	494	496	rBV	6621961	6468916	56.05%	6.010%
12	7.953	554	557	559	rBV	3509847	3015237	26.12%	2.802%
13	9.039	649	652	654	rBV	10669779	11541830	100.00%	10.724%
14	9.428	684	686	689	rBV	1934699	1927365	16.70%	1.791%
15	9.702	708	710	712	rBV	3823266	3316926	28.74%	3.082%
16	10.159	748	750	751	rVB	143208	115533	1.00%	0.107%
17	10.491	776	779	781	rBV	6321362	6695335	58.01%	6.221%
18	10.628	789	791	797	rVB	235823	268304	2.32%	0.249%
19	11.176	837	839	842	rBV	3651702	3318954	28.76%	3.084%
20	11.736	886	888	891	rBV2	120204	166172	1.44%	0.154%
21	12.776	976	979	981	rBV	8325650	9978767	86.46%	9.271%
22	13.737	1060	1063	1067	rBV3	71800	233127	2.02%	0.217%
23	13.839	1069	1072	1080	rVB2	3133368	3761837	32.59%	3.495%
24	14.800	1154	1156	1159	rBV	116976	159522	1.38%	0.148%
25	15.314	1198	1201	1204	rBV	1834171	2282999	19.78%	2.121%

Sum of corrected areas: 107629322

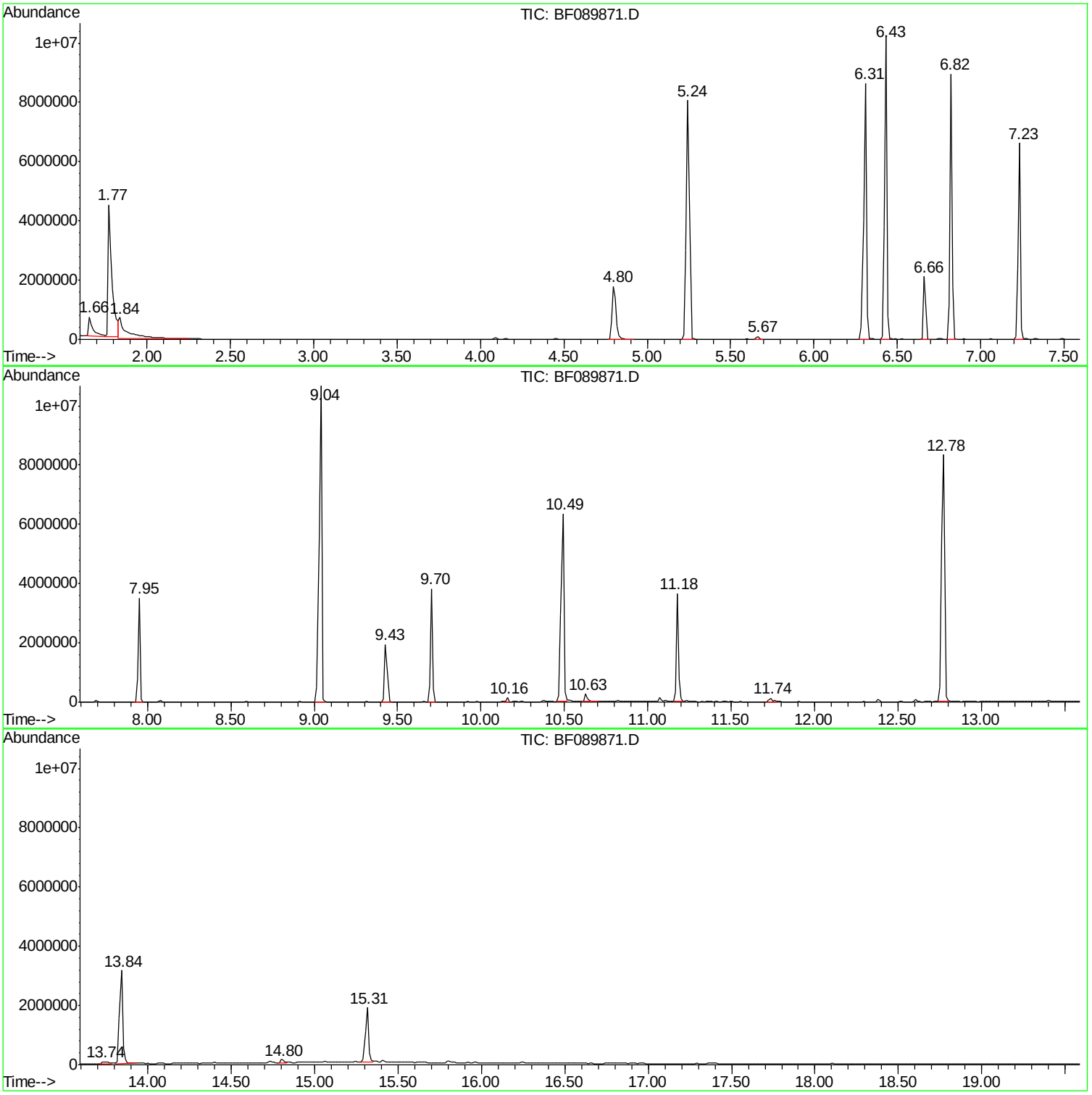
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082416\
Data File : BF089871.D
Acq On : 24 Aug 2016 13:50
Operator : UM/SJ
Sample : H4551-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AST-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.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\BF082416\
Data File : BF089871.D
Acq On : 24 Aug 2016 13:50
Operator : UM/SJ
Sample : H4551-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AST-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

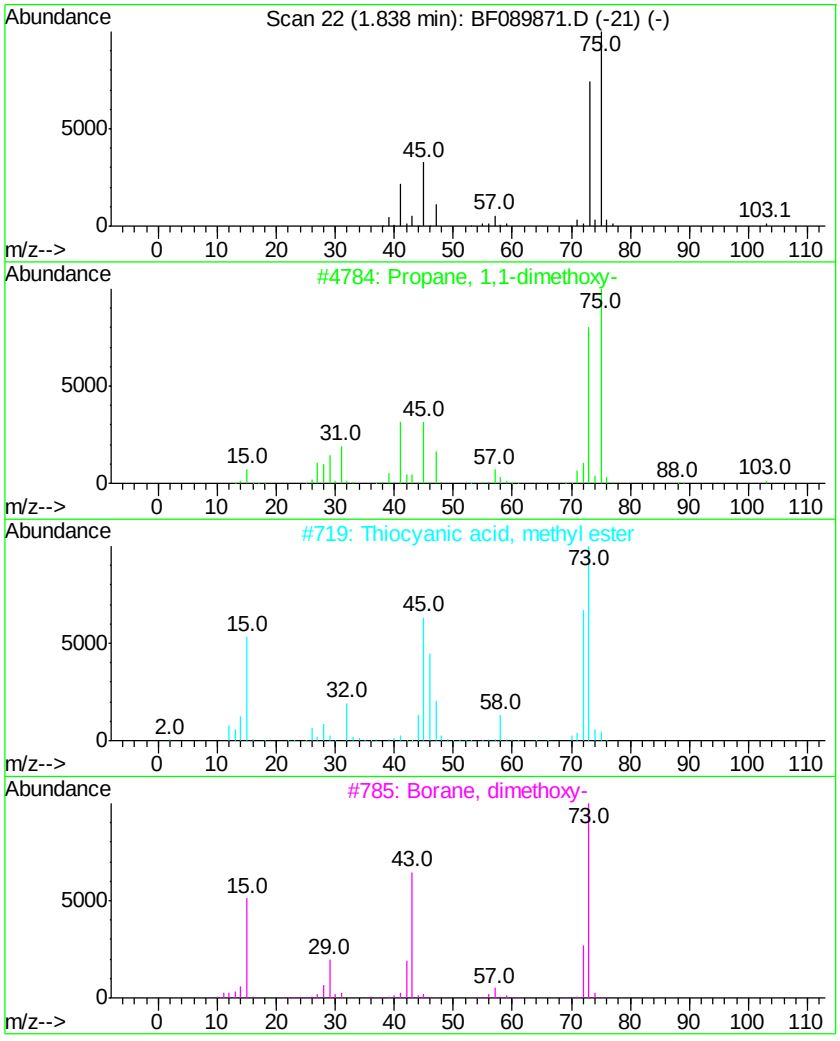
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

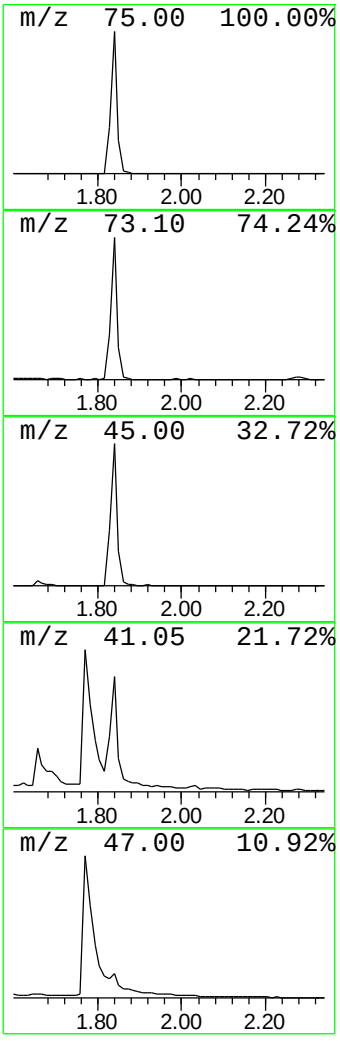
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.84	23.61 ng	2592110	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	22
3	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
4	Acetic acid, (aminooxy)-	91	C2H5NO3	000645-88-5	9
5	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082416\
Data File : BF089871.D
Acq On : 24 Aug 2016 13:50
Operator : UM/SJ
Sample : H4551-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AST-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

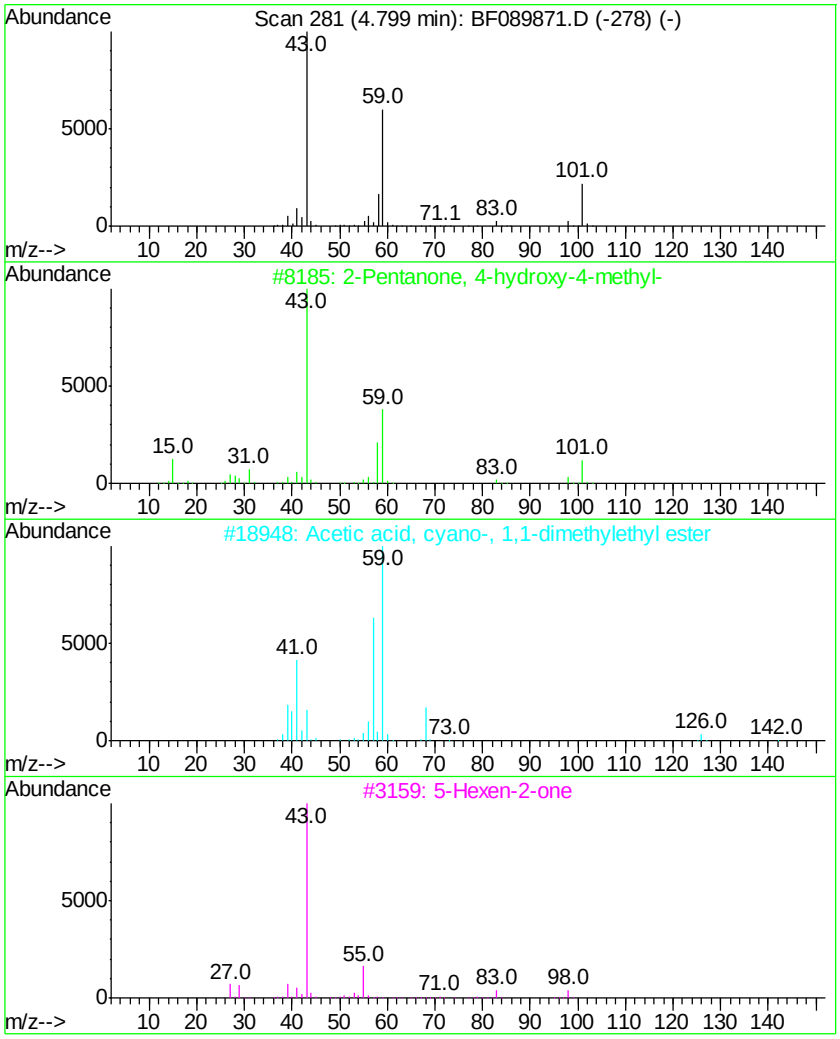
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

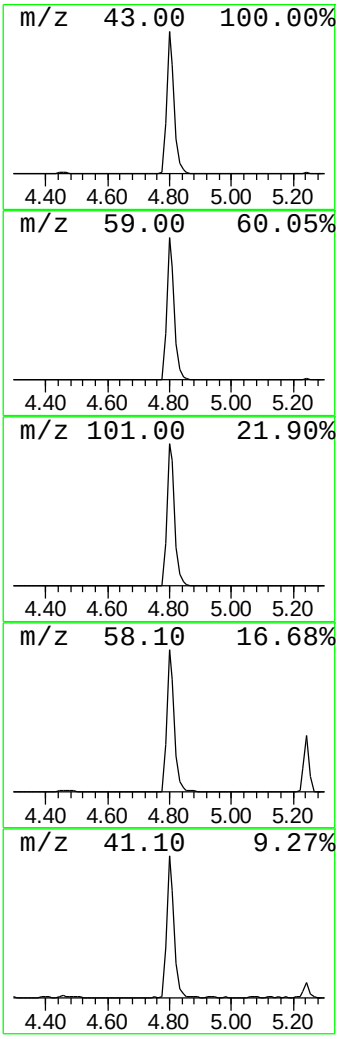
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	27.68 ng	3039200	1,4-Dichlorobenzene-d4	6.66

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	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF082416\
Data File : BF089871.D
Acq On : 24 Aug 2016 13:50
Operator : UM/SJ
Sample : H4551-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AST-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

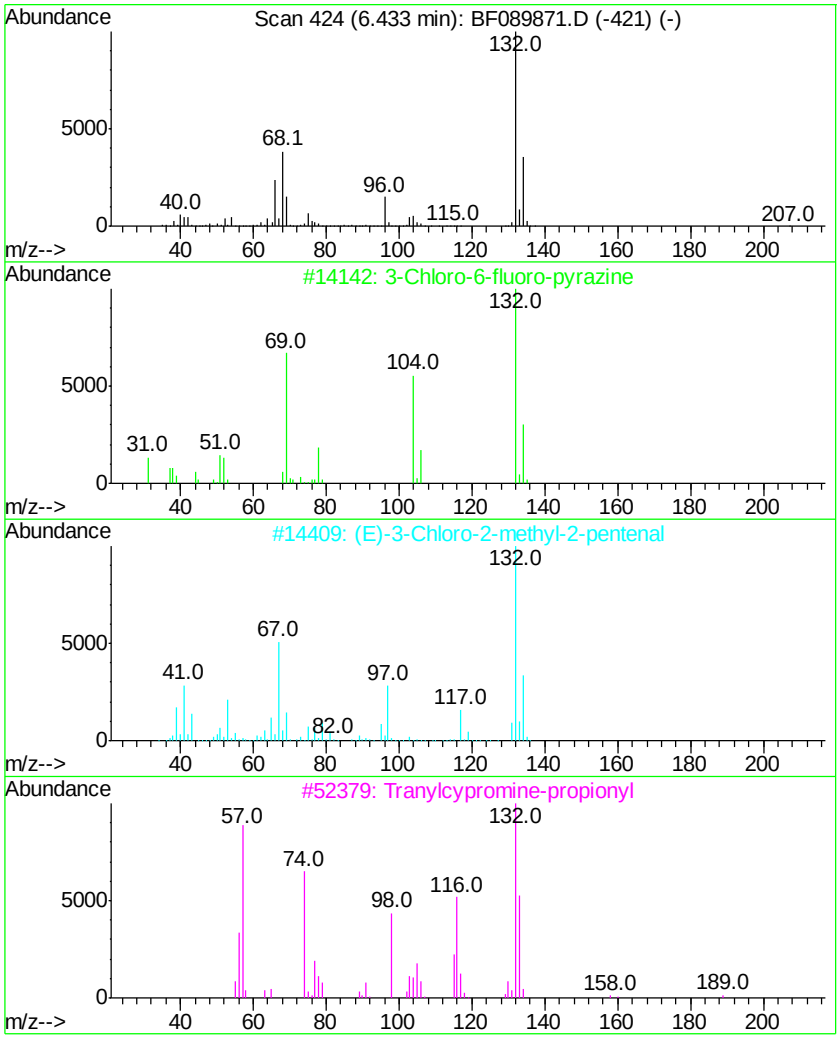
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

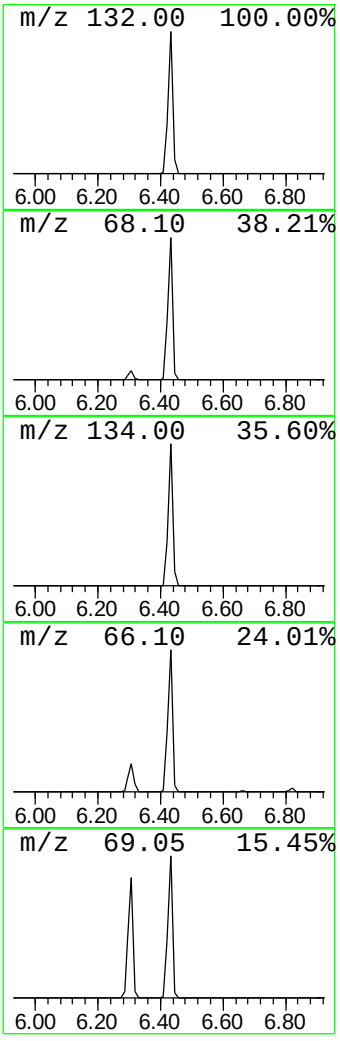
****

Peak Number 5 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	93.18 ng	10231200	1,4-Dichlorobenzene-d4	6.66

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Amphetaminil	250	C17H18N2	017590-01-1	10
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082416\
Data File : BF089871.D
Acq On : 24 Aug 2016 13:50
Operator : UM/SJ
Sample : H4551-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AST-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.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...	1.84	23.6	ng	2592110	1	6.66	2195920	20.0
2-Pentanone, 4-hy...	4.80	27.7	ng	3039200	1	6.66	2195920	20.0
unknown6.43	6.43	93.2	ng	10231200	1	6.66	2195920	20.0