LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096956.D
Acq On : 21 Jul 2017 20:55
Operator : SJ/JU
Sample : I4352-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-001-A

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-BF071317.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	4.722	462	465	476	rBV	228460	336894	11.58%	1.478%
2	5.169	536	541	544	rBV	2660030	2806195	96.44%	12.307%
3	6.216	714	719	734	rBV	2526591	2909744	100.00%	12.761%
4	6.328	734	738	742	rBV	2664236	2682207	92.18%	11.763%
5	6.557	773	777	781	rBV	816943	715800	24.60%	3.139%
6	6.710	799	803	807	rBV	2096095	2046720	70.34%	8.976%
7	7.122	868	873	876	rBV	1825184	1706385	58.64%	7.484%
8	7.839	990	995	998	rBV	1003083	927589	31.88%	4.068%
9	8.916	1173	1178	1181	rBV	2718957	2546034	87.50%	11.166%
10	9.310	1242	1245	1248	rBV	312925	234877	8.07%	1.030%
11	9.586	1287	1292	1295	rBV	902088	854555	29.37%	3.748%
12	10.033	1365	1368	1372	rVB	51125	45231	1.55%	0.198%
13	10.251	1399	1405	1408	rBV	30562	37108	1.28%	0.163%
14	10.369	1421	1425	1429	rBV	1229649	1148489	39.47%	5.037%
15	10.504	1445	1448	1456	rBV	76288	98317	3.38%	0.431%
16	10.951	1520	1524	1527	rBV	42847	35954	1.24%	0.158%
17	11.057	1538	1542	1545	rBV	682383	607561	20.88%	2.665%
18	12.263	1744	1747	1752	rBV	41226	36000	1.24%	0.158%
19	12.486	1781	1785	1790	rVB	36541	39717	1.36%	0.174%
20	12.645	1807	1812	1815	rBV	1572270	1491214	51.25%	6.540%
21	13.221	1906	1910	1917	rVB7	14366	35251	1.21%	0.155%
22	13.551	1960	1966	1972	rBV	152525	196694	6.76%	0.863%
23	13.686	1985	1989	1992	rBV	657187	649229	22.31%	2.847%
24	14.186	2071	2074	2083	rVB	60009	68616	2.36%	0.301%
25	15.051	2216	2221	2226	rVB	433772	507731	17.45%	2.227%
26	15.568	2307	2309	2310	rBV2	53057	37059	1.27%	0.163%

Sum of corrected areas: 22801171

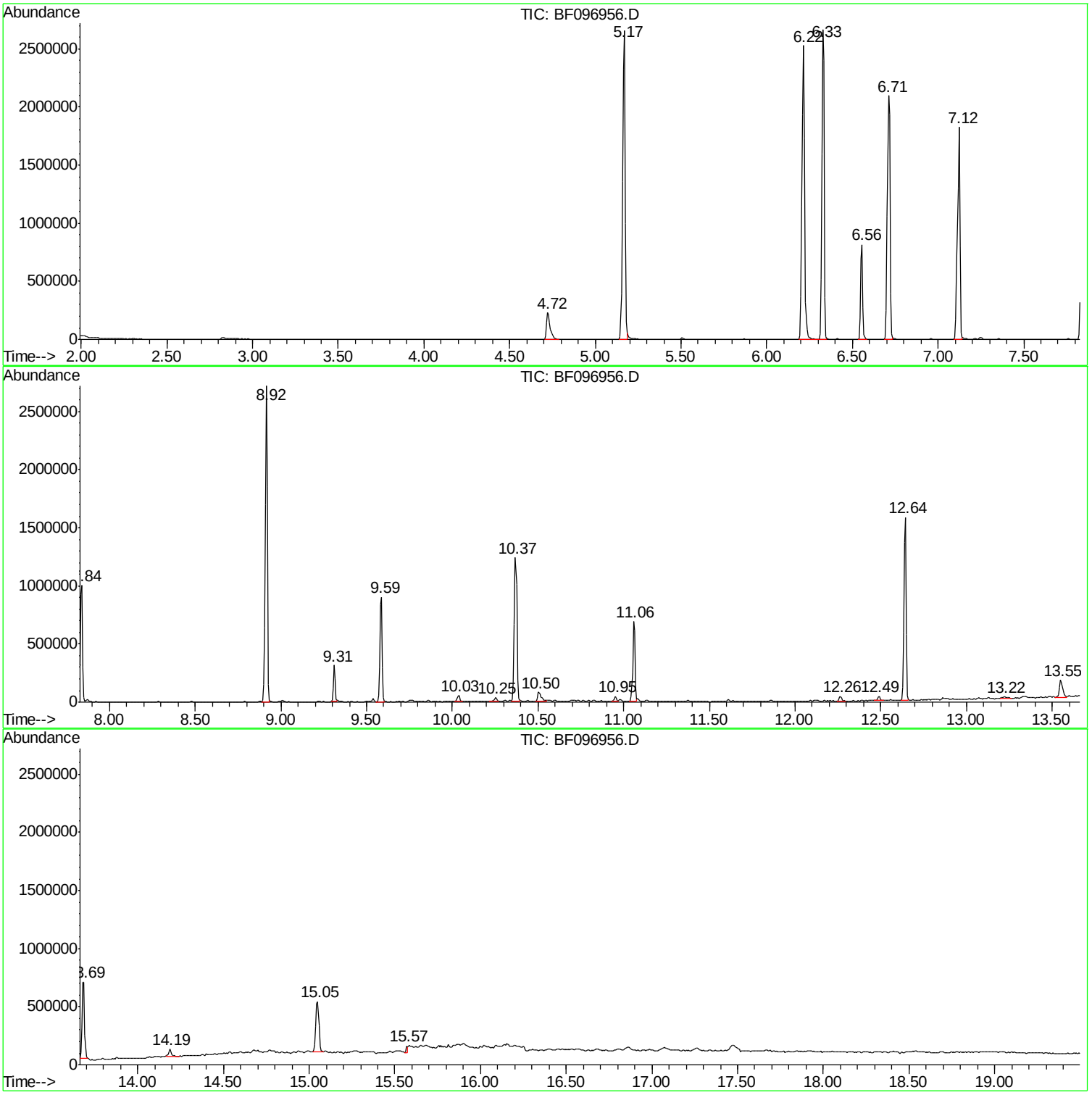
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096956.D
Acq On : 21 Jul 2017 20:55
Operator : SJ/JU
Sample : I4352-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-001-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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\BF072117\
Data File : BF096956.D
Acq On : 21 Jul 2017 20:55
Operator : SJ/JU
Sample : I4352-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-001-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

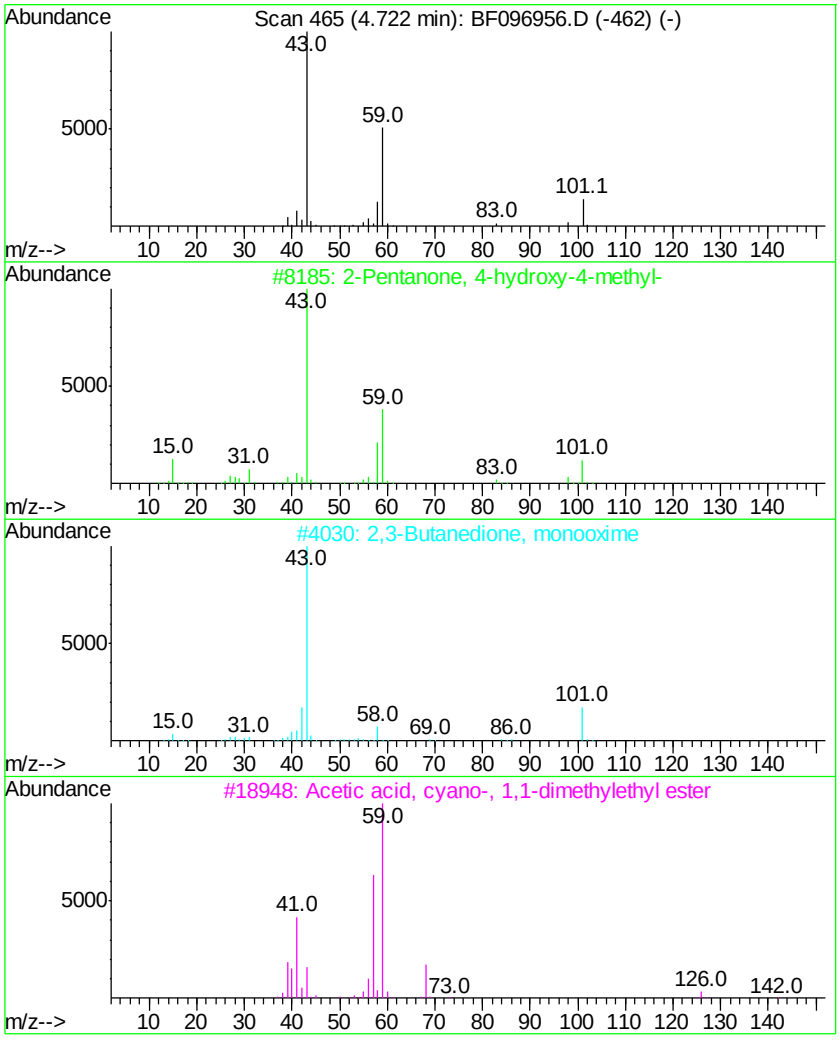
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

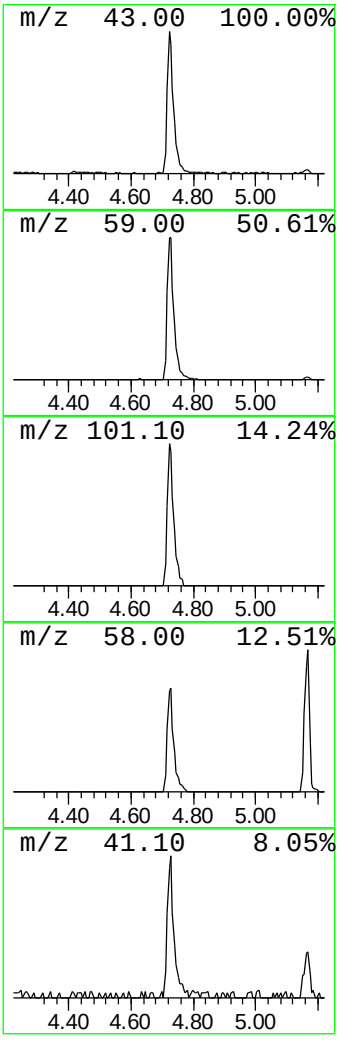
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	9.41 ng	336894	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
4	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096956.D
Acq On : 21 Jul 2017 20:55
Operator : SJ/JU
Sample : I4352-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-001-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

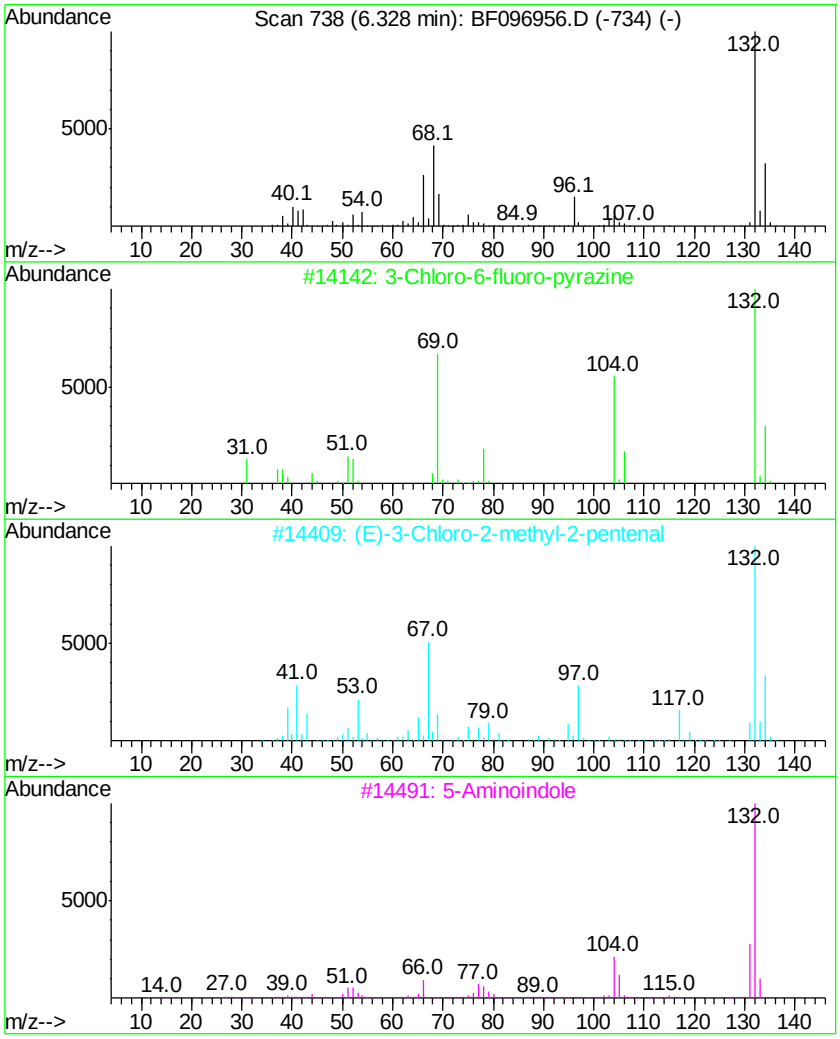
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

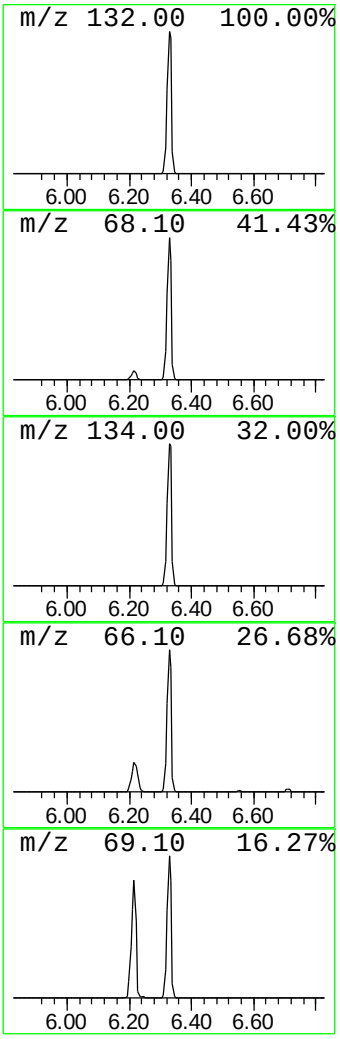
****

Peak Number 2 unknown6.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	74.94 ng	2682210	1,4-Dichlorobenzene-d4	6.56

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	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096956.D
Acq On : 21 Jul 2017 20:55
Operator : SJ/JU
Sample : I4352-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-001-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

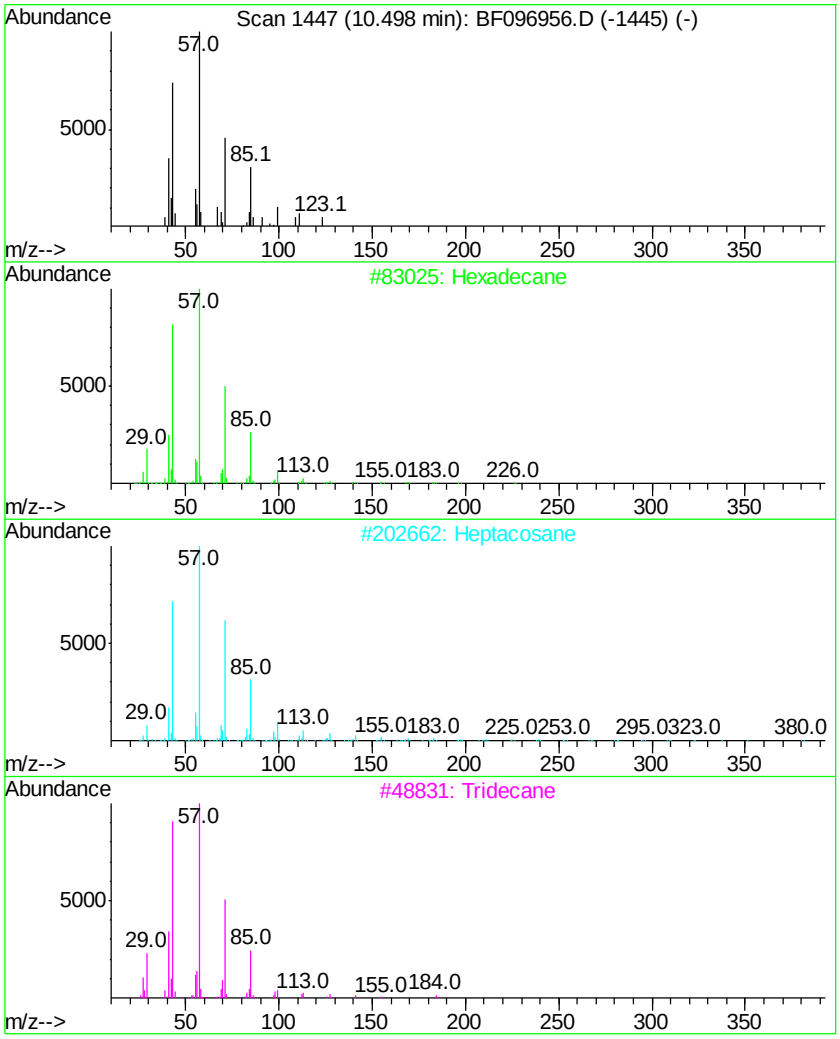
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

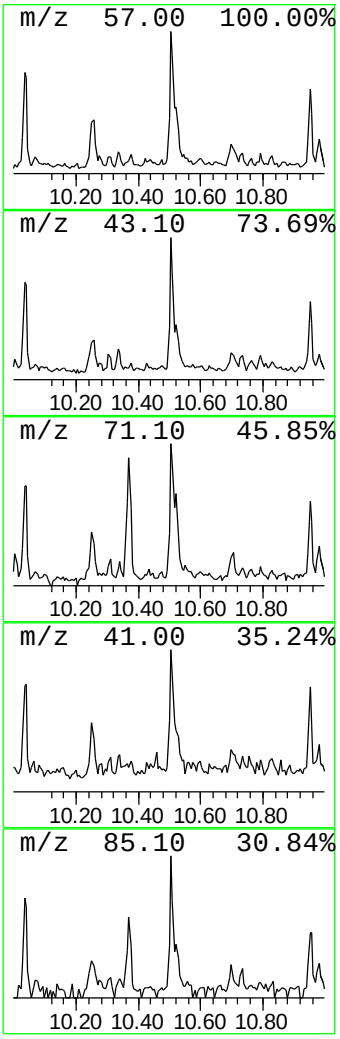
****

Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	3.24 ng	98317	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Heptacosane	380	C27H56	000593-49-7	80
3	Tridecane	184	C13H28	000629-50-5	78
4	Eicosane	282	C20H42	000112-95-8	72
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096956.D
Acq On : 21 Jul 2017 20:55
Operator : SJ/JU
Sample : I4352-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-001-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

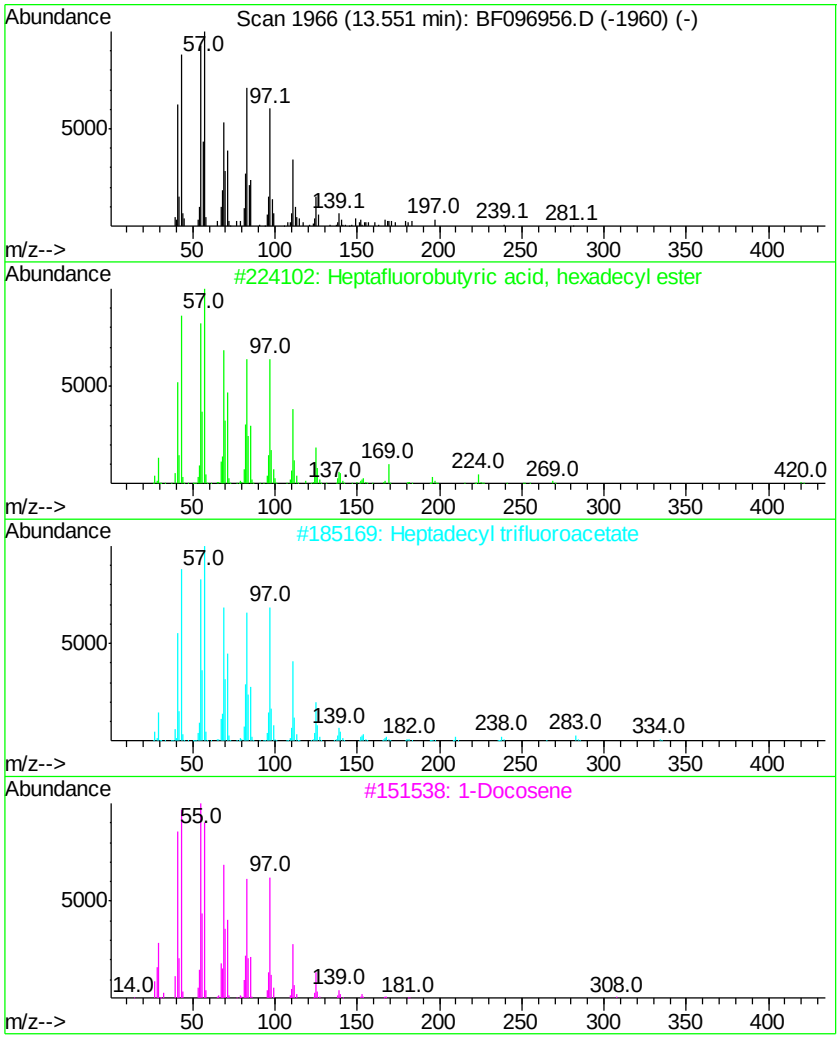
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

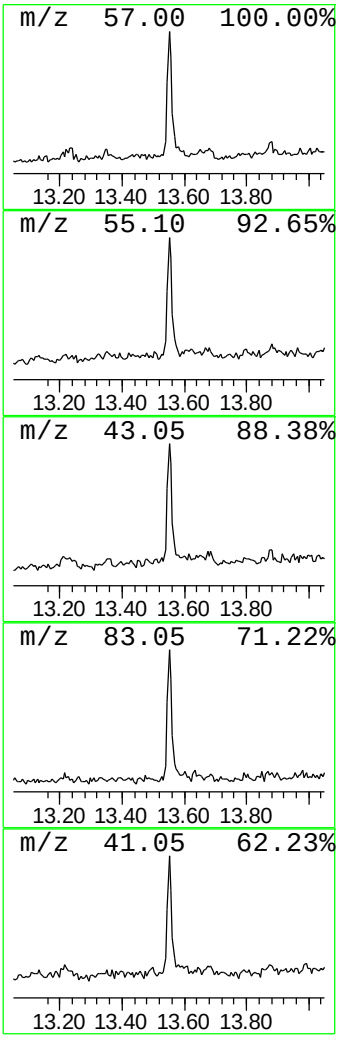
****

Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	6.06 ng	196694	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3	1-Docosene	308	C22H44	001599-67-3	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096956.D
Acq On : 21 Jul 2017 20:55
Operator : SJ/JU
Sample : I4352-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-001-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

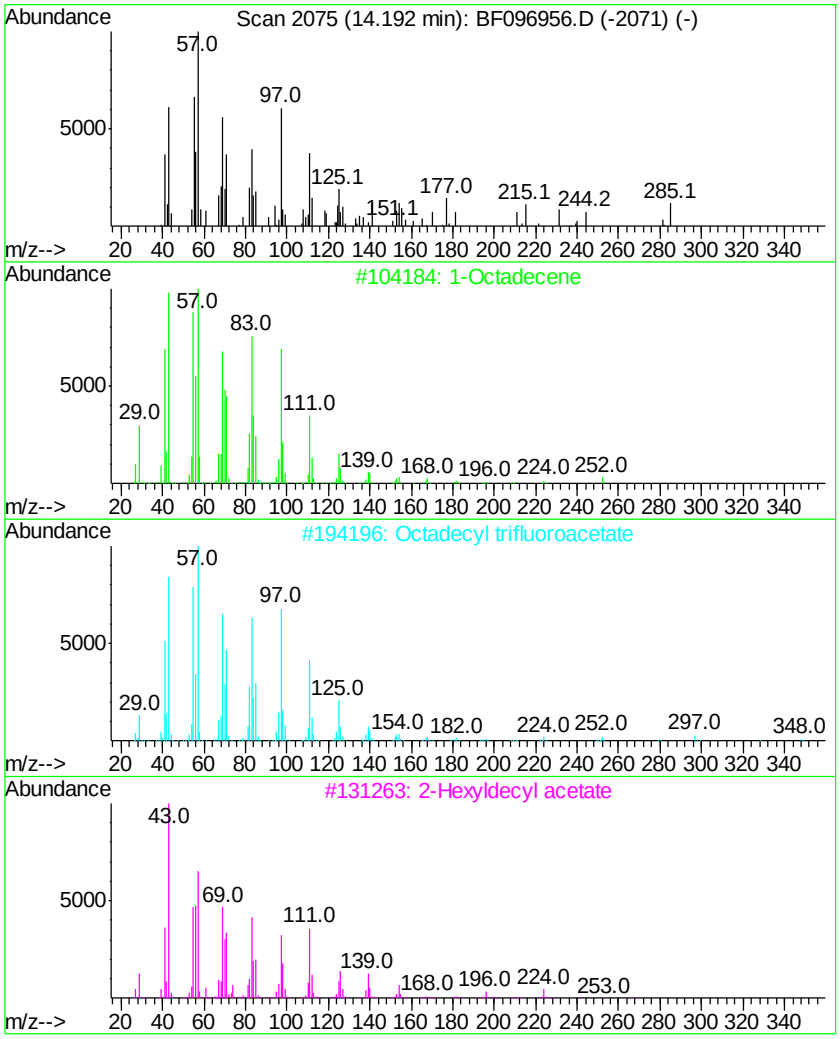
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

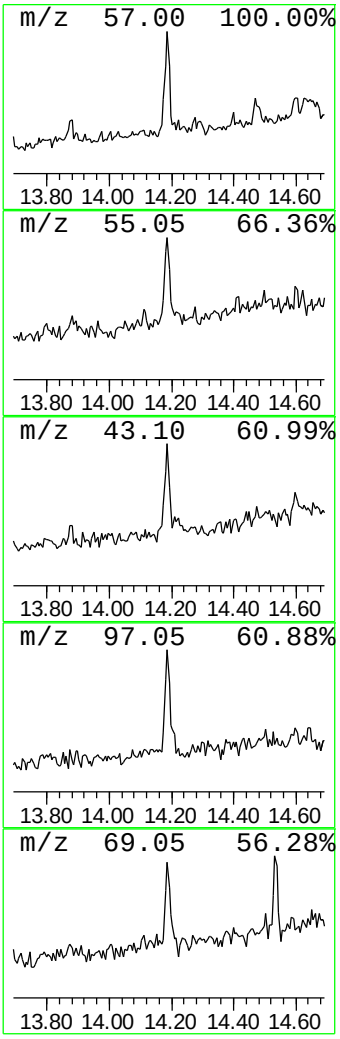
****

Peak Number 6 1-Octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.11 ng	68616	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	83
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	83
3	2-Hexyldecyl acetate	284	C18H36O2	082409-75-4	80
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096956.D
Acq On : 21 Jul 2017 20:55
Operator : SJ/JU
Sample : I4352-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-001-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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
2-Pentanone, 4-hy...	4.72	9.4	ng	336894	1	6.56	715800	20.0
unknown6.33	6.33	74.9	ng	2682210	1	6.56	715800	20.0
Hexadecane	10.50	3.2	ng	98317	4	11.06	607561	20.0
Heptafluorobutyri...	13.55	6.1	ng	196694	5	13.69	649229	20.0
1-Octadecene	14.19	2.1	ng	68616	5	13.69	649229	20.0