LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096560.D
Acq On : 7 Jul 2017 15:42
Operator : SJ/MA
Sample : I4064-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PET-BF005-01

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-BF070117.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	4.887	471	476	485	rBV	399780	501084	19.89%	2.213%
2	5.310	543	548	551	rBV	2569445	2471353	98.10%	10.915%
3	6.333	717	722	736	rVB	2460459	2519252	100.00%	11.126%
4	6.463	740	744	748	rBV	2408312	2423730	96.21%	10.704%
5	6.692	780	783	787	rBV	755872	683343	27.12%	3.018%
6	6.851	806	810	814	rBV	2014356	1776087	70.50%	7.844%
7	7.257	873	879	882	rBV	1564154	1558241	61.85%	6.882%
8	7.975	997	1001	1005	rBV	1047862	931748	36.99%	4.115%
9	9.057	1179	1185	1188	rBV	2335096	2391209	94.92%	10.561%
10	9.445	1246	1251	1254	rBV	228925	184879	7.34%	0.817%
11	9.727	1294	1299	1303	rBV2	1150184	1007672	40.00%	4.450%
12	10.174	1372	1375	1378	rVB	45879	36733	1.46%	0.162%
13	10.510	1428	1432	1436	rBV	1360779	1402018	55.65%	6.192%
14	10.645	1451	1455	1462	rVB	54436	55006	2.18%	0.243%
15	11.204	1546	1550	1554	rBV	1049524	910288	36.13%	4.020%
16	12.792	1815	1820	1823	rBV	2088140	1919832	76.21%	8.479%
17	13.692	1970	1973	1984	rBV	131956	141310	5.61%	0.624%
18	13.833	1993	1997	2001	rBV	737696	654325	25.97%	2.890%
19	14.592	2122	2126	2134	rBV	411320	428642	17.01%	1.893%
20	14.686	2139	2142	2146	rVB	42941	42719	1.70%	0.189%
21	15.233	2230	2235	2240	rBV	460348	540067	21.44%	2.385%
22	15.286	2240	2244	2248	rVB2	23879	32633	1.30%	0.144%
23	15.686	2308	2312	2316	rBV4	19257	30132	1.20%	0.133%

Sum of corrected areas: 22642303

LSC Report - Integrated Chromatogram

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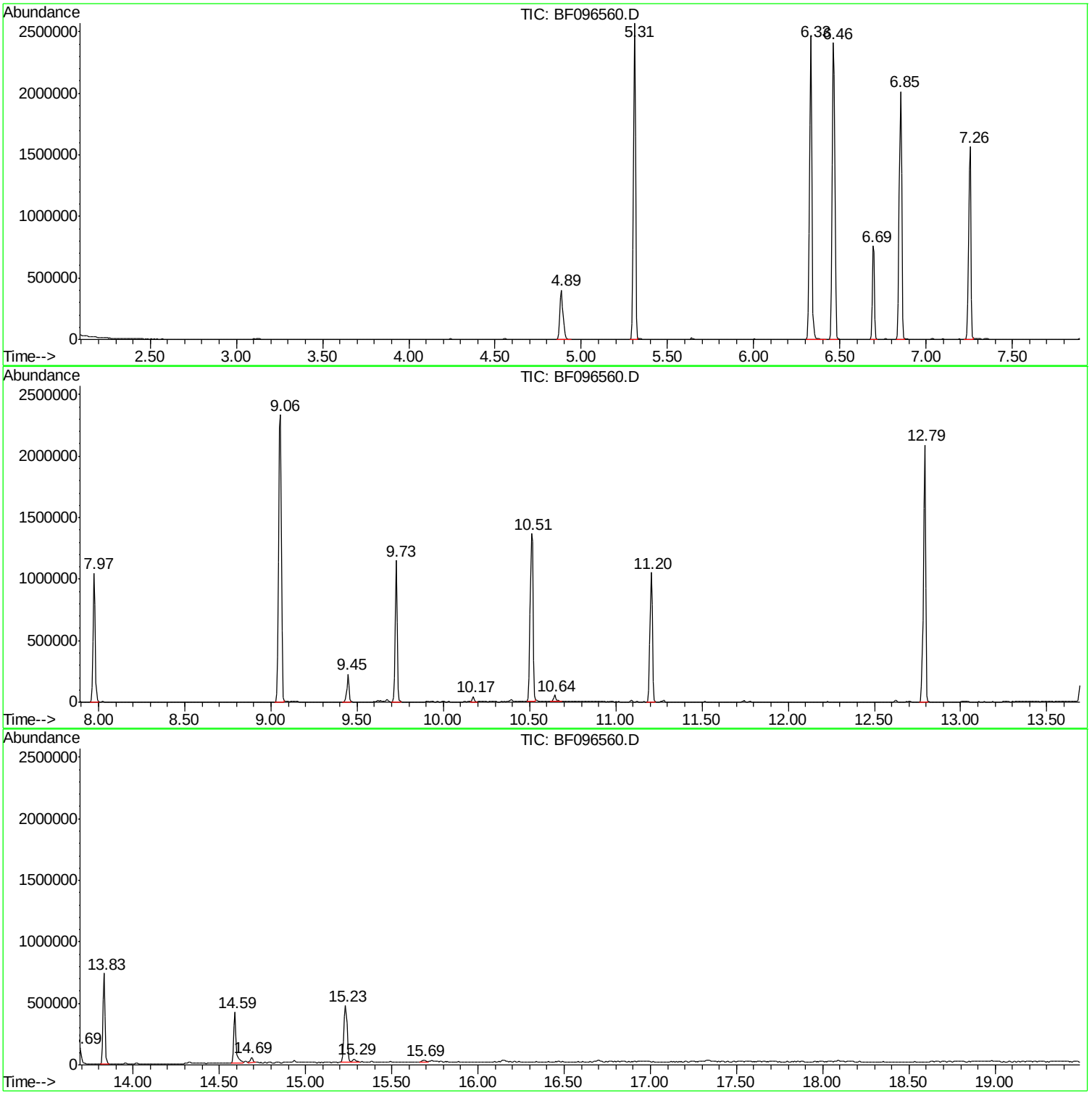
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PET-BF005-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF096560.D
Acq On : 7 Jul 2017 15:42
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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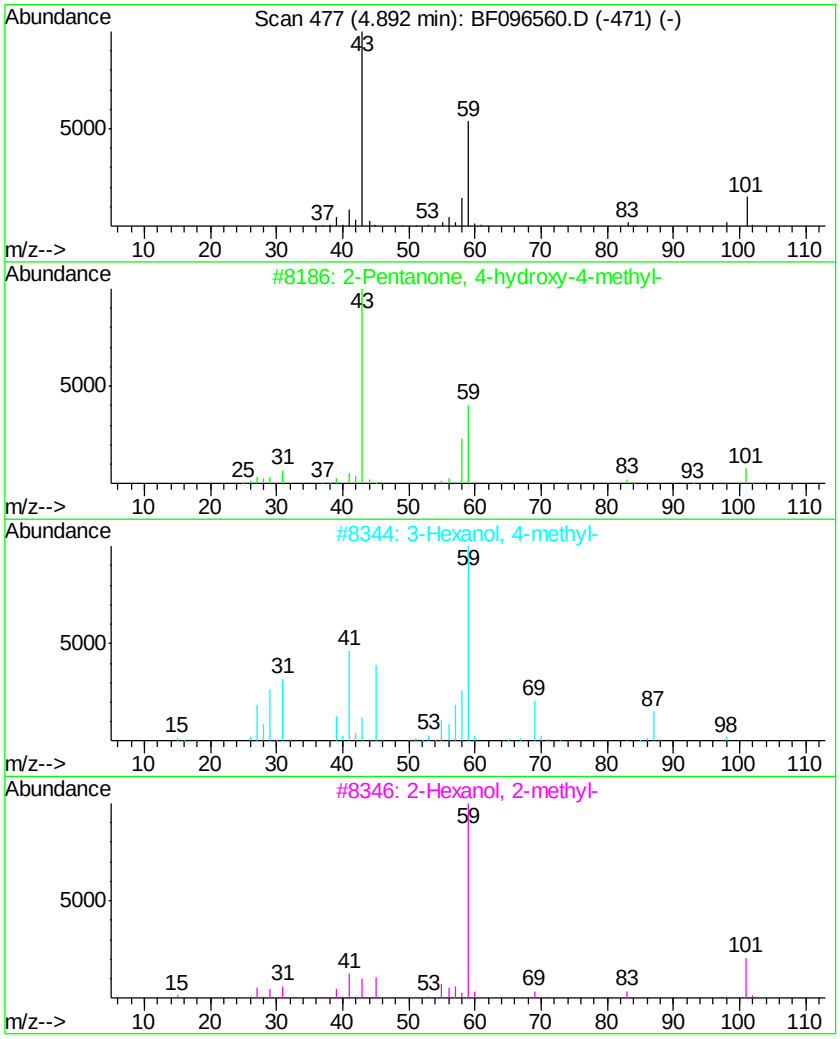
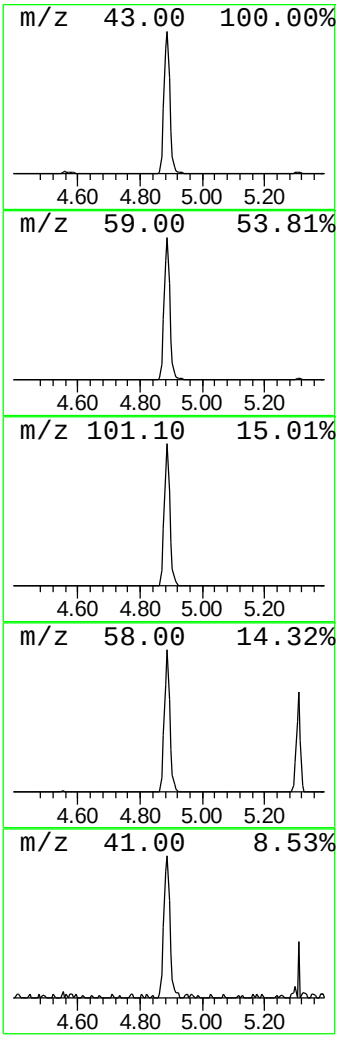
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	14.67 ng	501084	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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096560.D
Acq On : 7 Jul 2017 15:42
Operator : SJ/MA
Sample : I4064-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PET-BF005-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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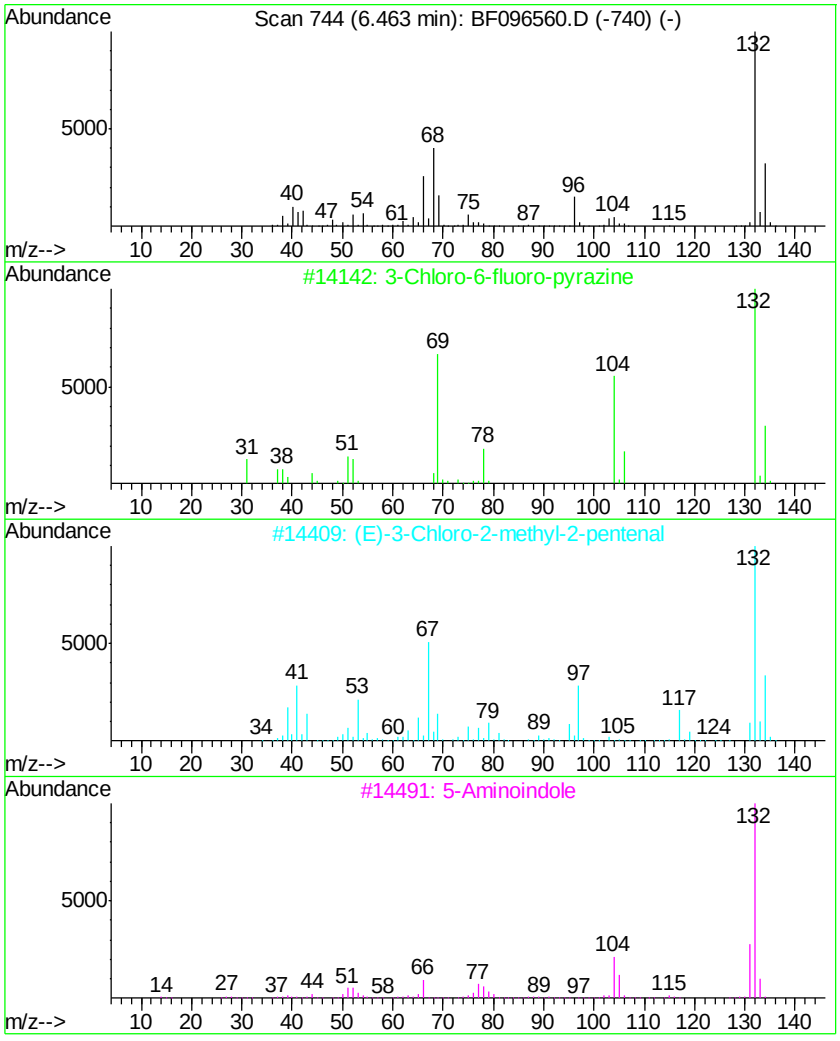
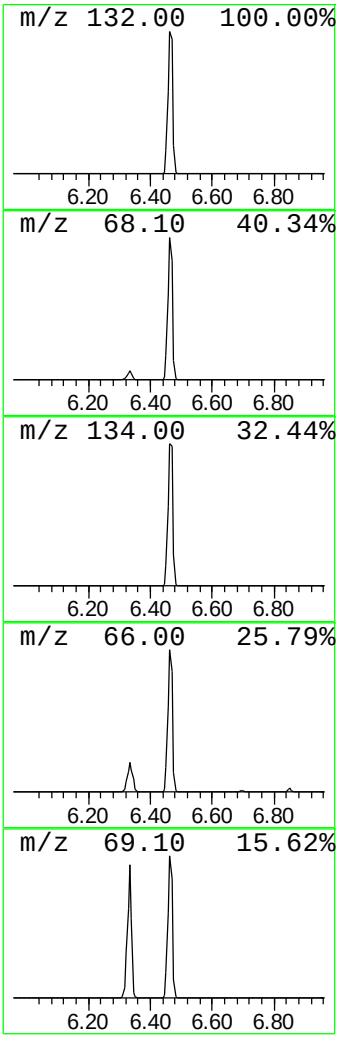
Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	70.94 ng	2423730	1,4-Dichlorobenzene-d4	6.70

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Operator : SJ/MA
Sample : I4064-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PET-BF005-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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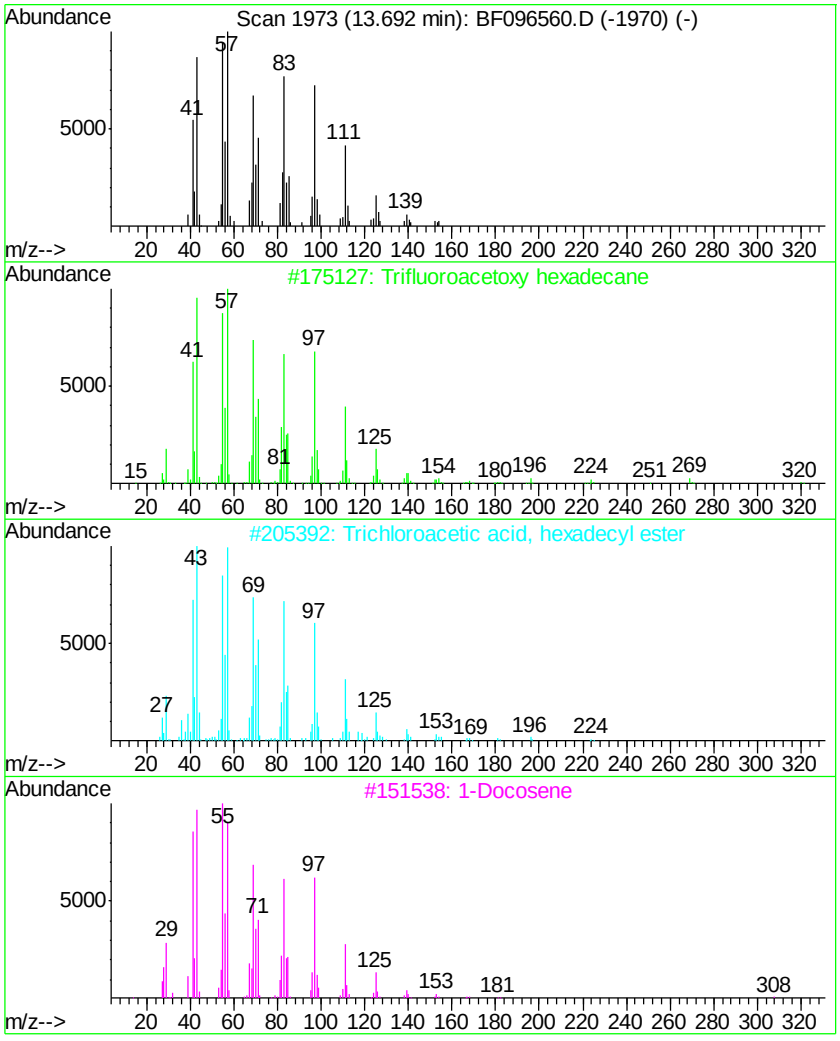
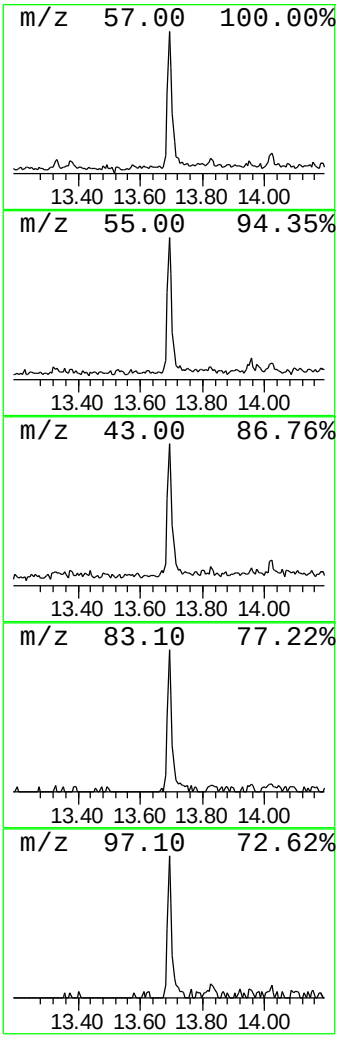
Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	4.32 ng	141310	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Docosene	308	C22H44	001599-67-3	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Octacosanol	410	C28H58O	000557-61-9	91





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Sample : I4064-08
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PET-BF005-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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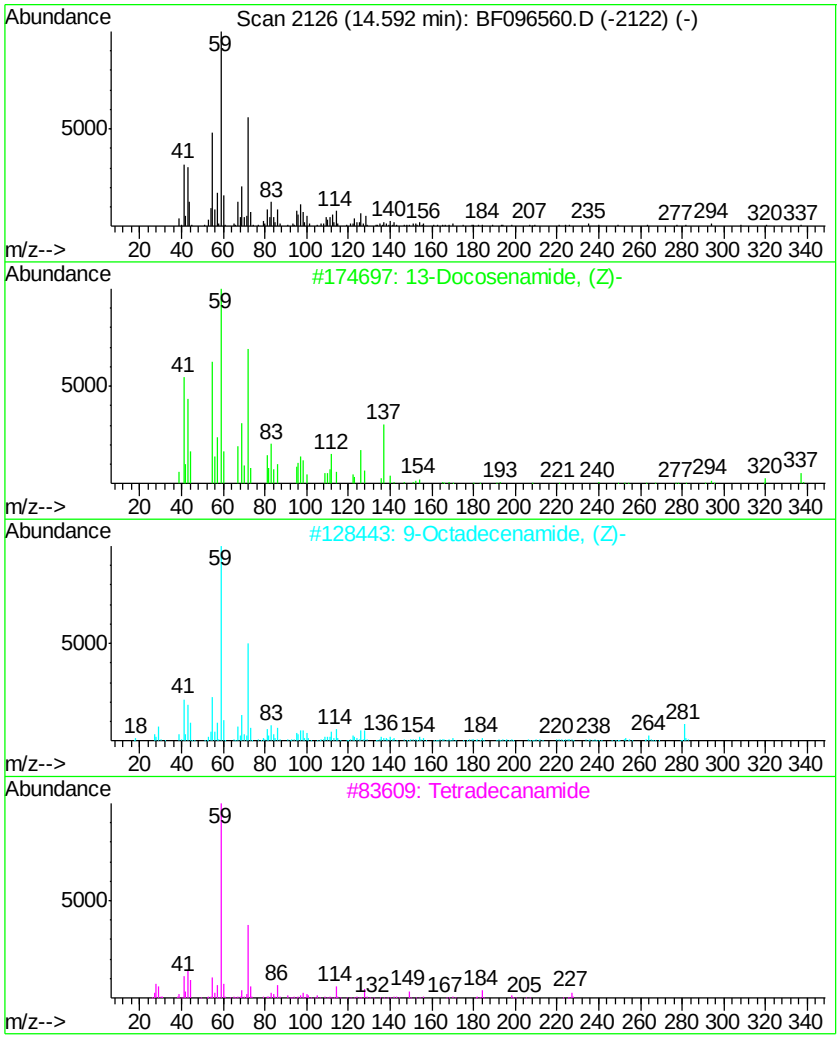
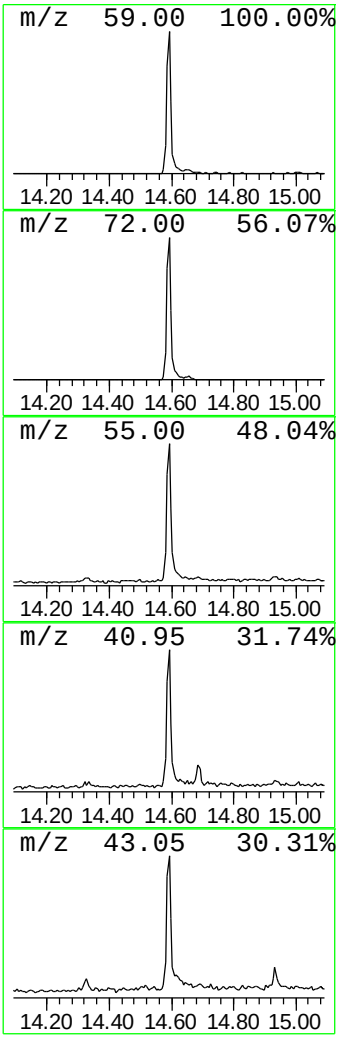
Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	15.87 ng	428642	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
3	Tetradecanamide	227	C14H29NO	000638-58-4	78
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	64
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	43





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_F
ClientSampleId : PET-BF005-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.89	14.7	ng	501084	1	6.70	683343	20.0
unknown6.46	6.46	70.9	ng	2423730	1	6.70	683343	20.0
Trifluoroacetoxy ...	13.69	4.3	ng	141310	5	13.83	654325	20.0
13-Docosenamide, ...	14.59	15.9	ng	428642	6	15.23	540067	20.0