LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096553.D
Acq On : 7 Jul 2017 12:31
Operator : SJ/MA
Sample : I4064-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PET-BF001-01

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	486	rVB	436547	613538	20.66%	2.391%
2	5.316	543	549	552	rBV	2910514	2909641	97.95%	11.339%
3	6.340	717	723	727	rBV	2540247	2658643	89.50%	10.360%
4	6.469	740	745	748	rBV	2665455	2566740	86.41%	10.002%
5	6.698	780	784	787	rBV	691746	612024	20.60%	2.385%
6	6.851	806	810	814	rBV	1954902	1901788	64.02%	7.411%
7	7.257	873	879	882	rBV	1713273	1651909	55.61%	6.437%
8	7.981	997	1002	1005	rBV	894613	866658	29.18%	3.377%
9	9.057	1179	1185	1188	rBV	3072274	2970409	100.00%	11.575%
10	9.445	1247	1251	1254	rBV	276966	224190	7.55%	0.874%
11	9.728	1295	1299	1303	rBV	1138865	1049523	35.33%	4.090%
12	10.175	1372	1375	1378	rVB	68977	51334	1.73%	0.200%
13	10.392	1407	1412	1415	rBV3	22492	30745	1.04%	0.120%
14	10.516	1428	1433	1436	rBV	1767059	1721472	57.95%	6.708%
15	10.645	1452	1455	1463	rBV	76587	77691	2.62%	0.303%
16	11.204	1546	1550	1554	rBV	1044071	989573	33.31%	3.856%
17	11.745	1638	1642	1646	rBV	69100	65605	2.21%	0.256%
18	12.792	1815	1820	1824	rBV	2383426	2639214	88.85%	10.285%
19	13.692	1970	1973	1981	rBV	212953	222335	7.48%	0.866%
20	13.833	1993	1997	2001	rBV	855775	793541	26.71%	3.092%
21	14.592	2122	2126	2134	rBV	424179	408674	13.76%	1.593%
22	14.686	2139	2142	2146	rBV2	41072	47996	1.62%	0.187%
23	15.233	2230	2235	2240	rBV	499638	588191	19.80%	2.292%

Sum of corrected areas: 25661434

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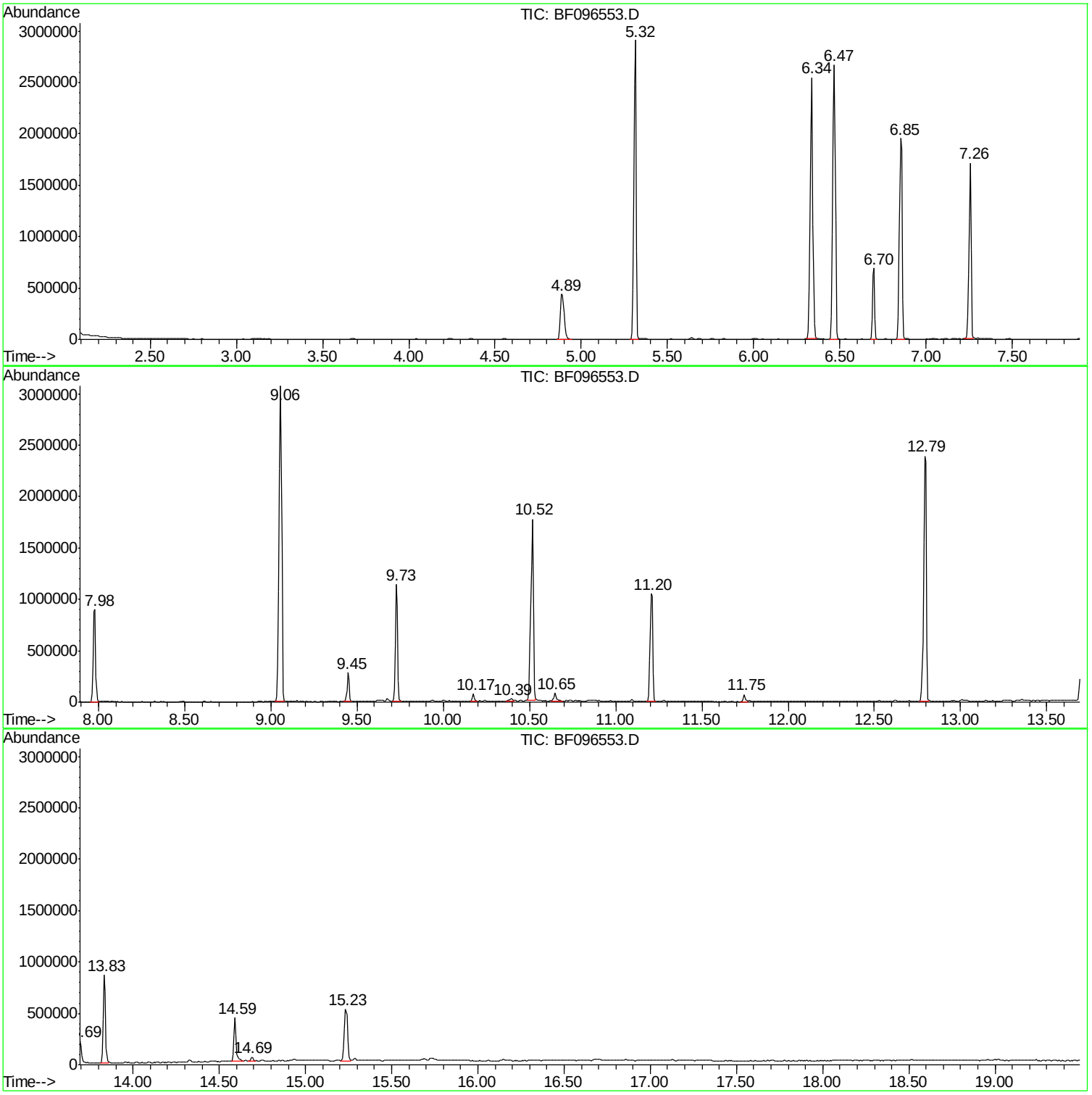
Instrument :
BNA_F
ClientSampleId :
PET-BF001-01

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096553.D
Acq On : 7 Jul 2017 12:31
Operator : SJ/MA
Sample : I4064-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PET-BF001-01

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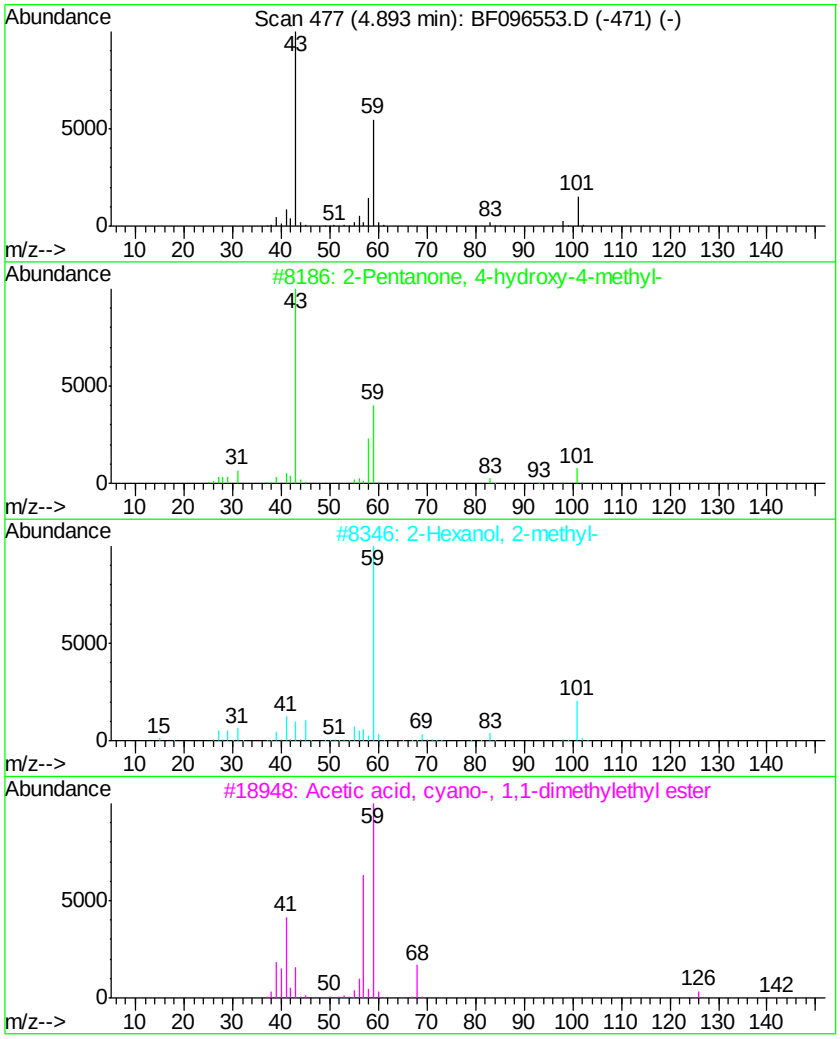
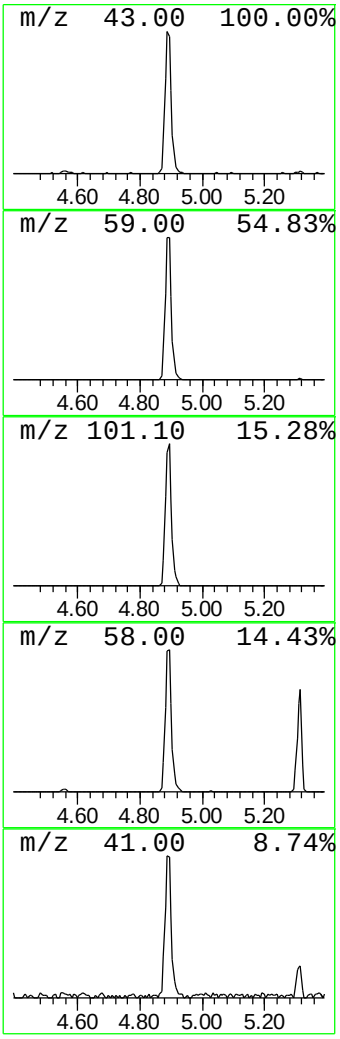
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	20.05 ng	613538	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	56
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





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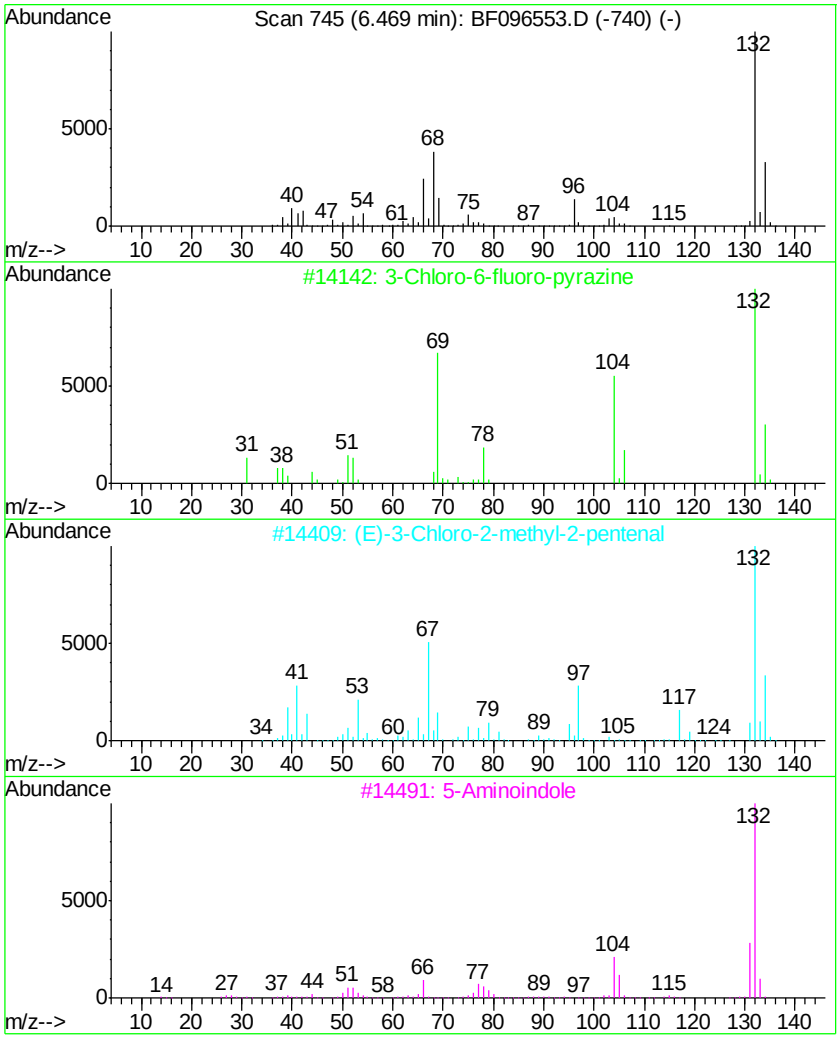
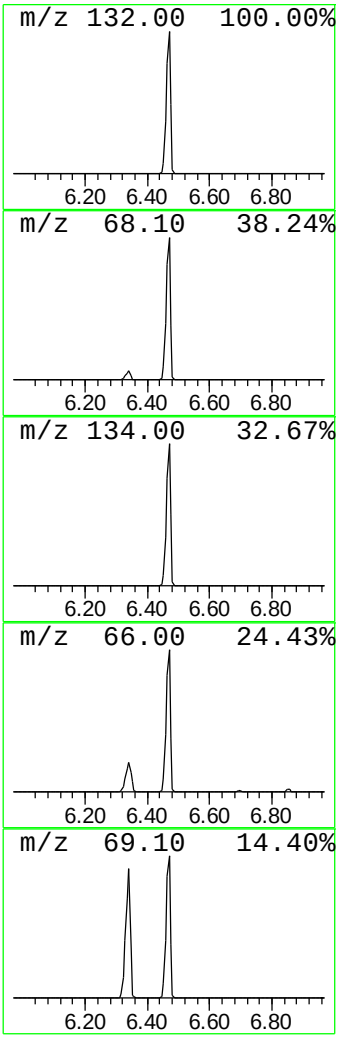
Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	83.88 ng	2566740	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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Acq On : 7 Jul 2017 12:31
Operator : SJ/MA
Sample : I4064-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PET-BF001-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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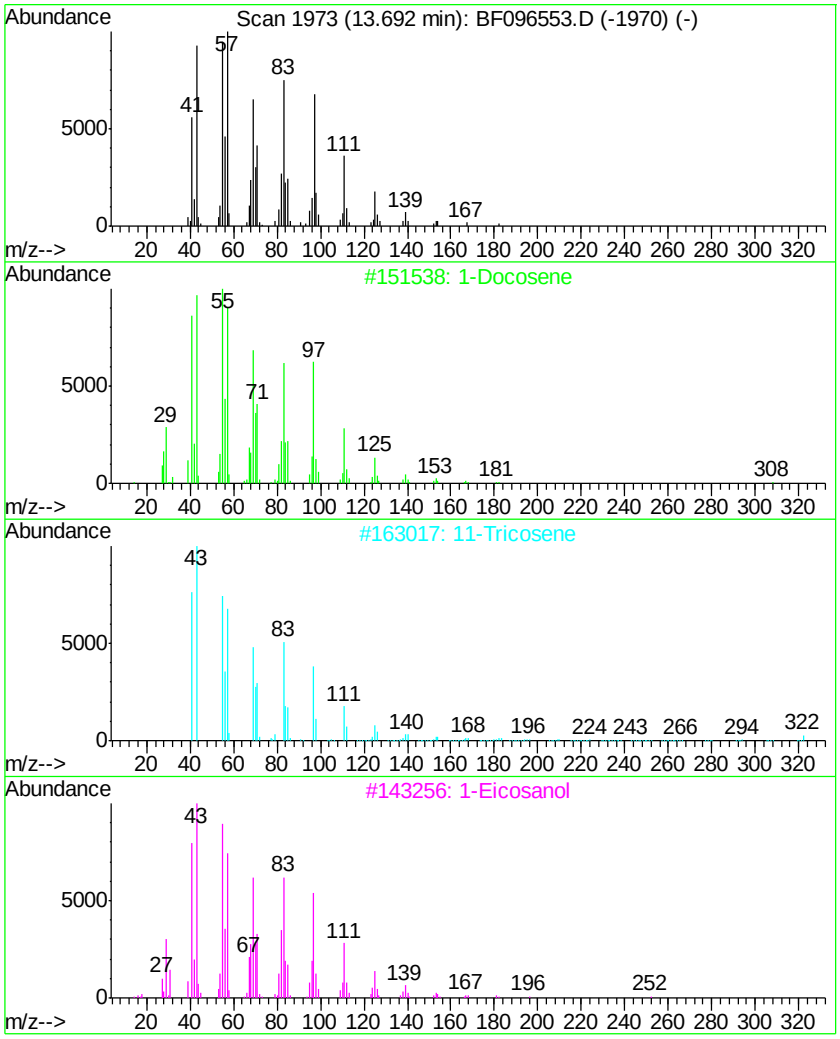
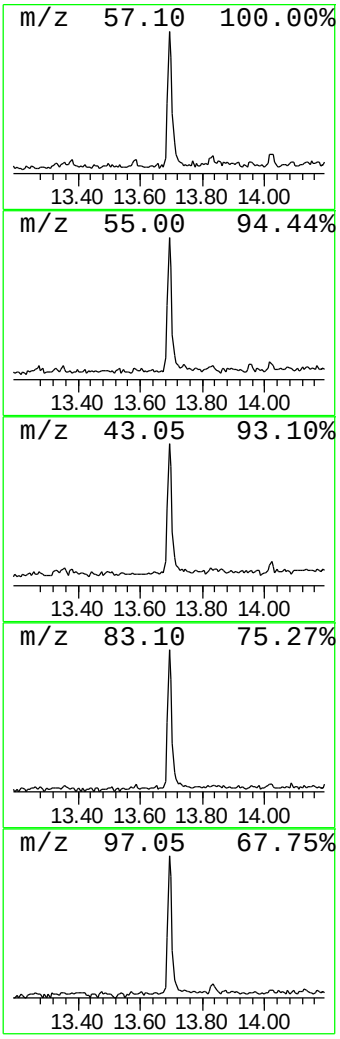
Peak Number 4 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	5.60 ng	222335	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	11-Tricosene	322	C23H46	052078-56-5	91
3	1-Eicosanol	298	C20H42O	000629-96-9	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	1-Octadecanol	270	C18H38O	000112-92-5	90





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Sample : I4064-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PET-BF001-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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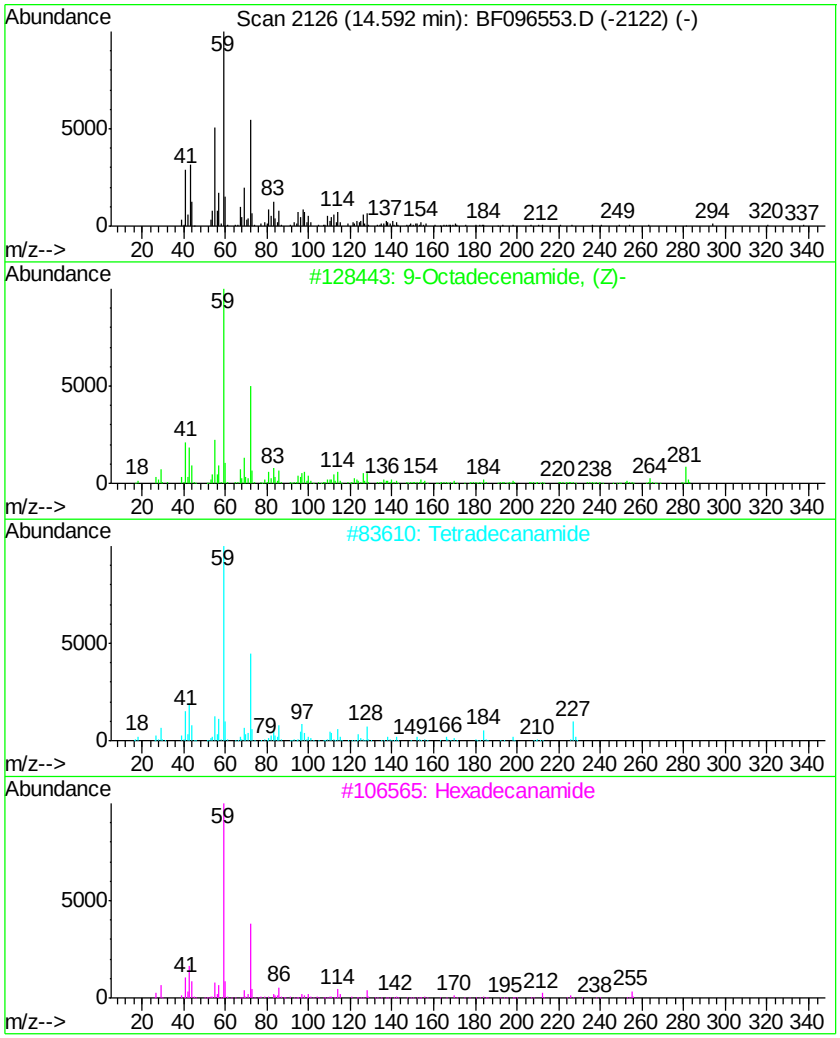
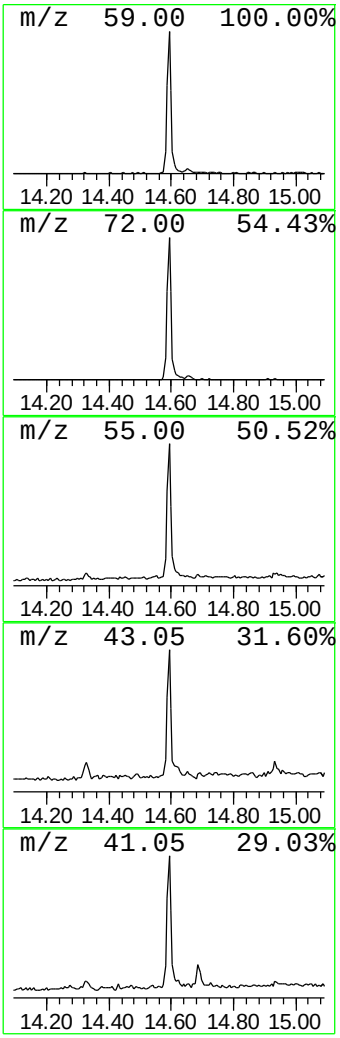
Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	13.90 ng	408674	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Tetradecanamide	227	C14H29NO	000638-58-4	86
3	Hexadecanamide	255	C16H33NO	000629-54-9	78
4	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	72
5	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	20.1	ng	613538	1	6.70	612024	20.0
unknown6.47	6.47	83.9	ng	2566740	1	6.70	612024	20.0
1-Docosene	13.69	5.6	ng	222335	5	13.83	793541	20.0
9-Octadecenamide,...	14.59	13.9	ng	408674	6	15.23	588191	20.0