LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122217\
Data File : BF101681.D
Acq On : 23 Dec 2017 5:00
Operator : SJ/JU
Sample : I6971-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-S

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-BF121417.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	5.010	494	497	509	rBV	45742	89306	2.07%	0.316%
2	5.410	562	565	596	rBV	1008253	1671722	38.80%	5.919%
3	6.428	735	738	756	rBV	720857	1141419	26.49%	4.041%
4	6.557	756	760	767	rBV	2585807	2565131	59.54%	9.082%
5	6.787	795	799	807	rBV	1107646	1060165	24.61%	3.754%
6	6.940	821	825	847	rBV	3102356	3300131	76.60%	11.684%
7	7.357	892	896	917	rBV	2475508	2911787	67.58%	10.309%
8	8.069	1013	1017	1035	rBV	1399040	1358466	31.53%	4.810%
9	9.145	1195	1200	1203	rBV	4398884	4308431	100.00%	15.254%
10	9.822	1312	1315	1327	rVB2	1419518	1350113	31.34%	4.780%
11	10.616	1446	1450	1464	rBV	1558006	1685081	39.11%	5.966%
12	11.316	1565	1569	1577	rBV	1221971	1211428	28.12%	4.289%
13	12.698	1801	1804	1808	rBV	234138	192475	4.47%	0.681%
14	12.898	1833	1838	1841	rBV	3307775	3192969	74.11%	11.305%
15	13.404	1920	1924	1929	rBV2	191127	157463	3.65%	0.558%
16	13.780	1984	1988	2000	rBV2	91545	147190	3.42%	0.521%
17	13.963	2015	2019	2029	rBV	938604	918877	21.33%	3.253%
18	14.092	2038	2041	2047	rBV	49981	45122	1.05%	0.160%
19	14.698	2140	2144	2147	rVB	48124	46482	1.08%	0.165%
20	15.021	2195	2199	2207	rBV	39958	52303	1.21%	0.185%
21	15.427	2263	2268	2279	rVB	606111	837963	19.45%	2.967%

Sum of corrected areas: 28244024

LSC Report - Integrated Chromatogram

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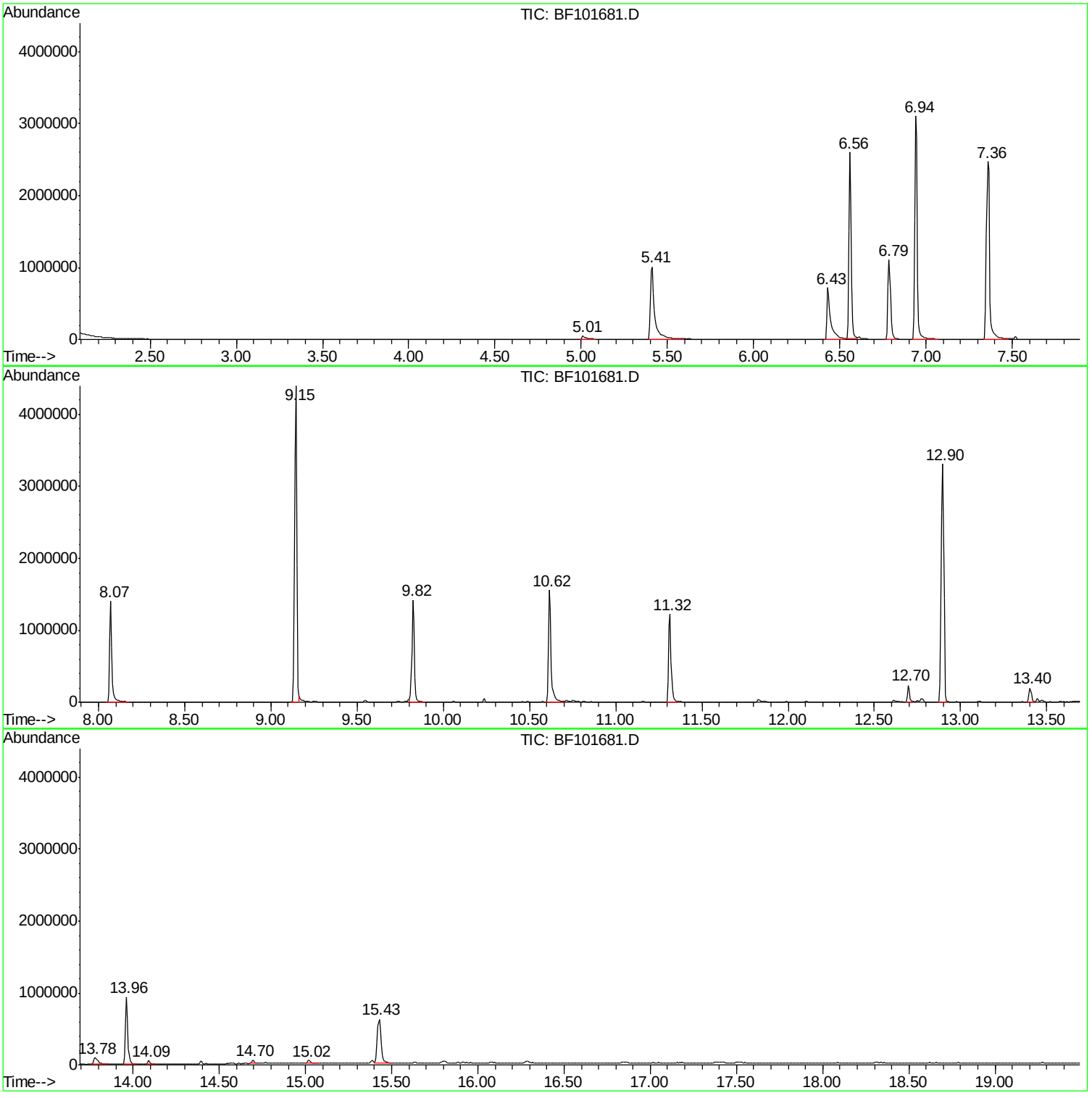
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
121517-TIFR-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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\BF122217\
Data File : BF101681.D
Acq On : 23 Dec 2017 5:00
Operator : SJ/JU
Sample : I6971-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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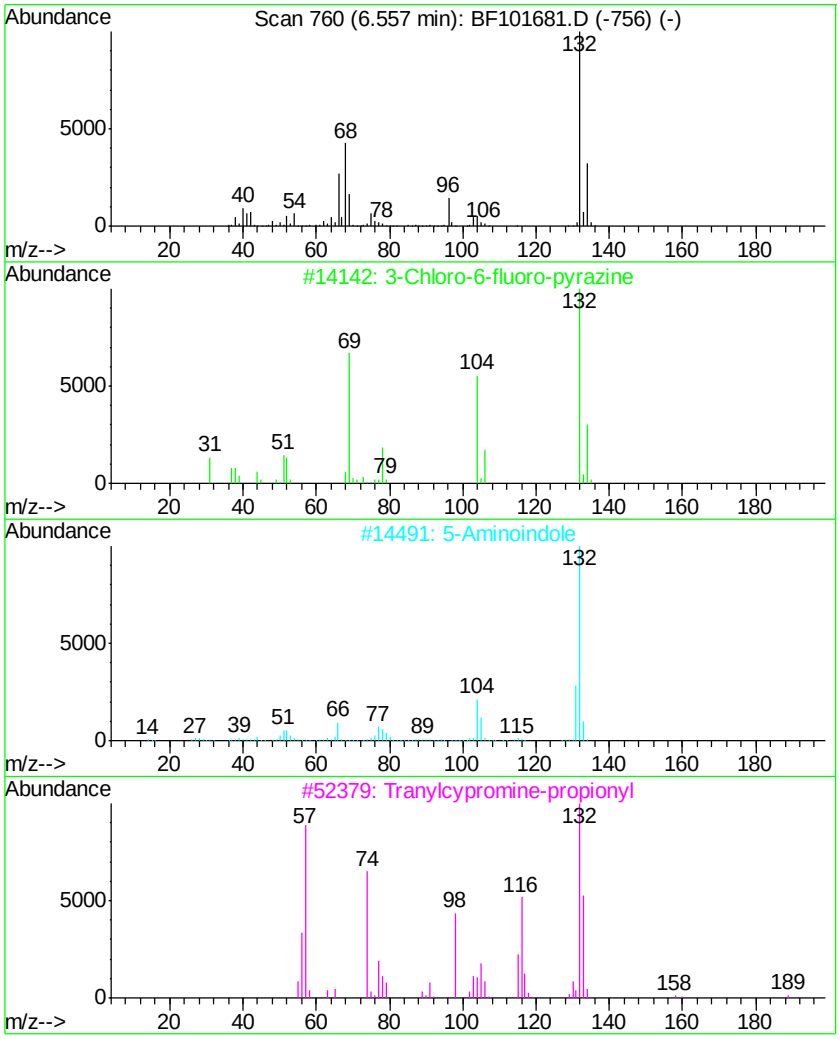
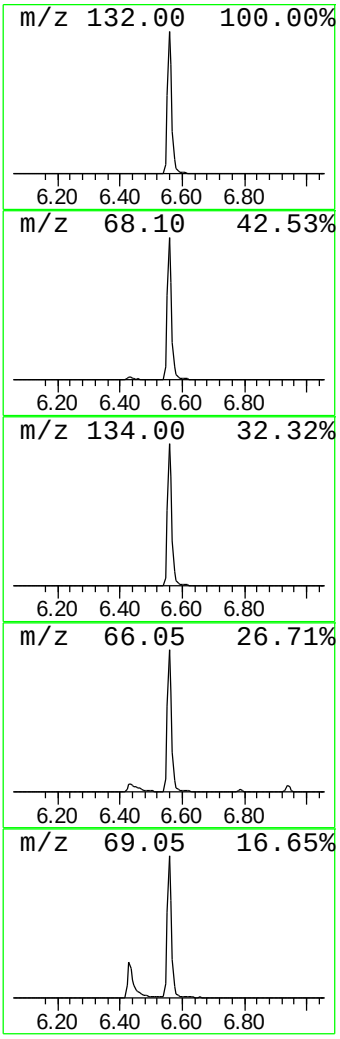
Peak Number 1 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	48.39 ng	2565130	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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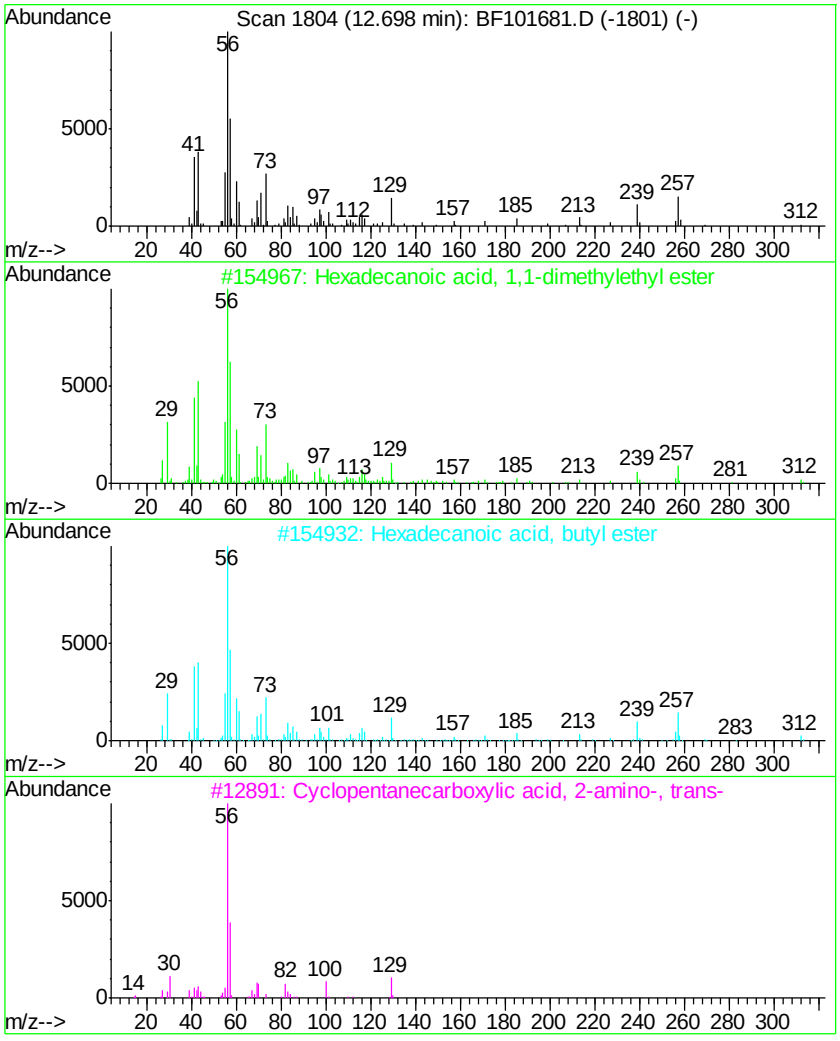
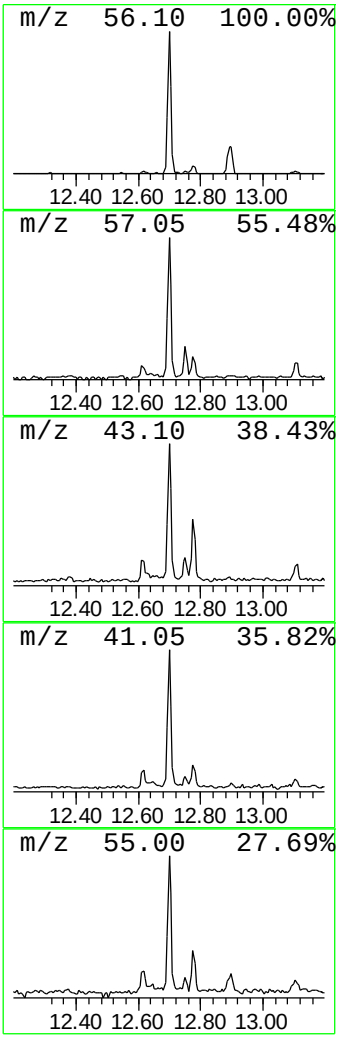
Peak Number 3 Hexadecanoic acid, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	4.19 ng	192475	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	60
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	38
5	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38





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Operator : SJ/JU
Sample : I6971-17
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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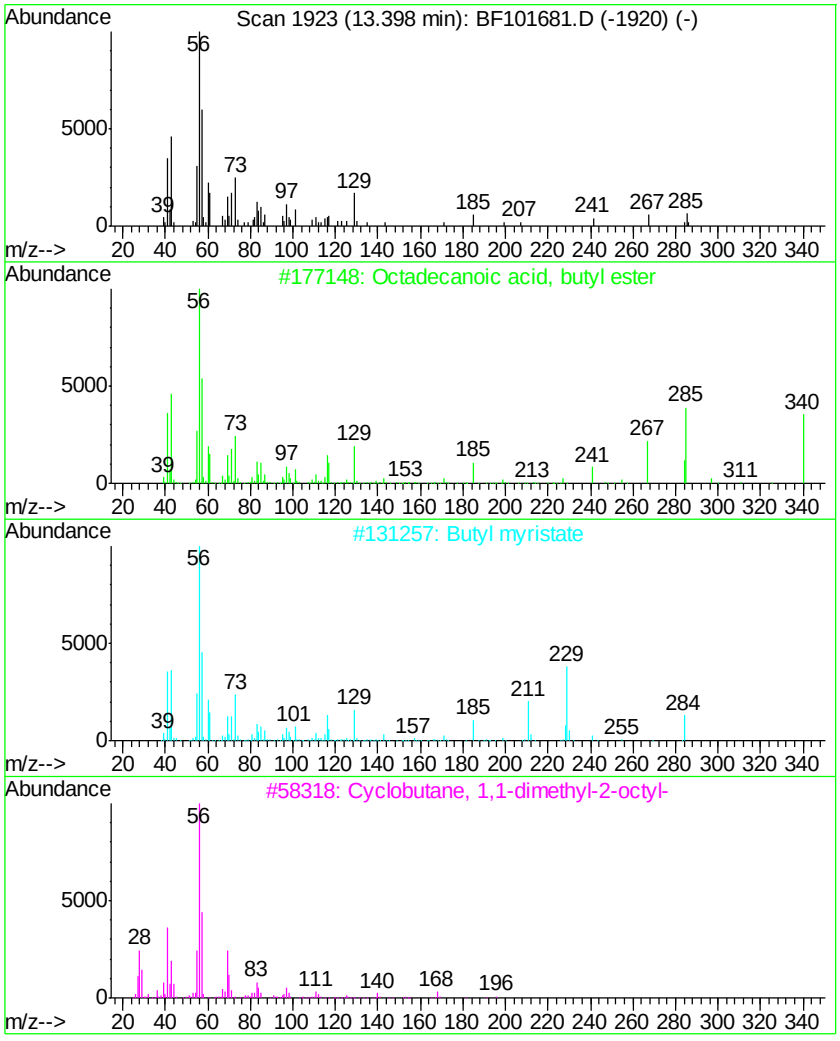
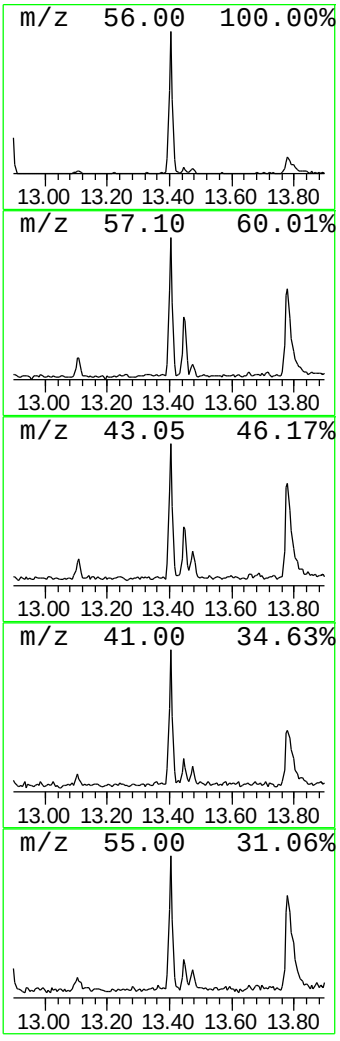
Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	3.43 ng	157463	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2	Butyl myristate	284	C18H36O2	000110-36-1	86
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	38





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Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 121517-TIFR-E-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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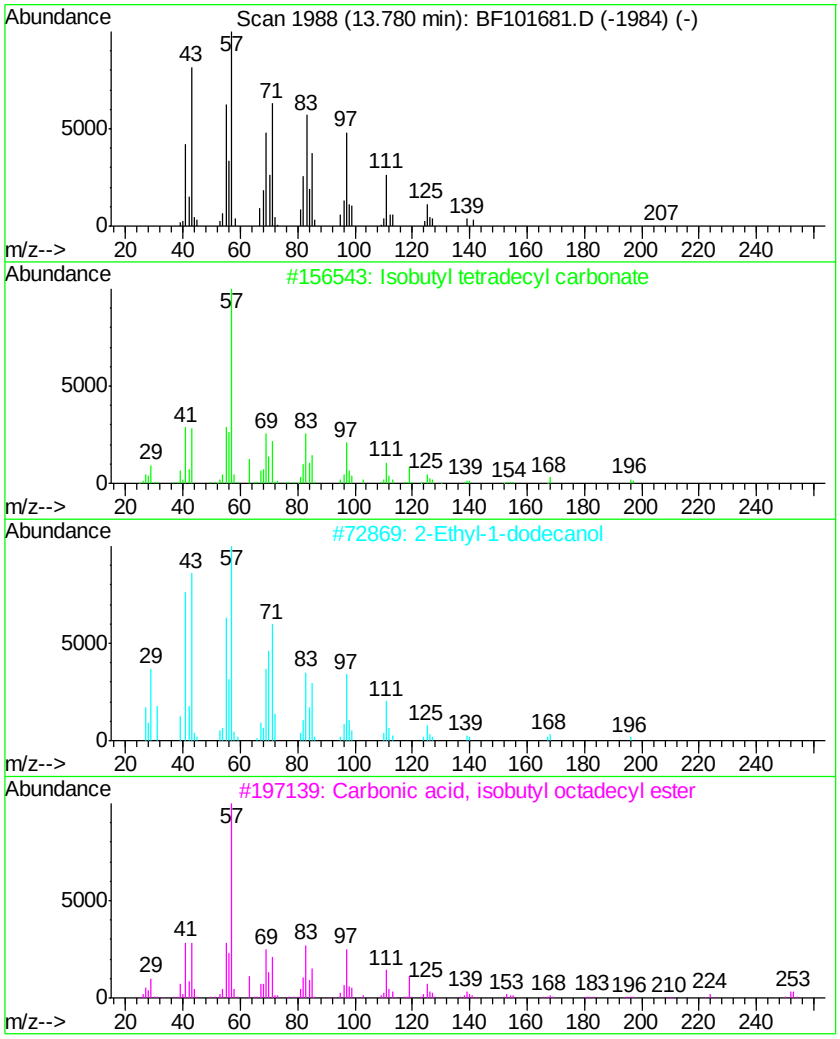
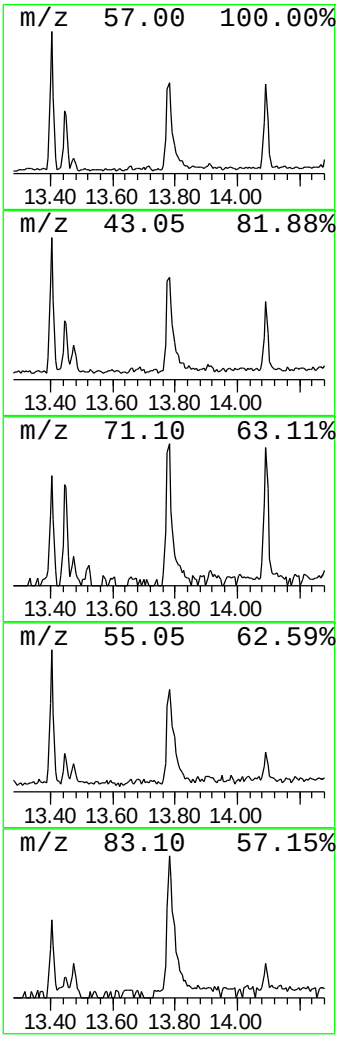
Peak Number 5 Isobutyl tetradecyl carbonate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	3.20 ng	147190	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	90
2	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	87
3	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	86
4	17-Pentatriacontene	491	C35H70	006971-40-0	83
5	1-Eicosanol	298	C20H42O	000629-96-9	81





Tentatively Identified Compound (LSC) summary

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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
unknown6.56	6.56	48.4	ng	2565130	1	6.79	1060170	20.0
Hexadecanoic acid...	12.70	4.2	ng	192475	5	13.96	918877	20.0
Octadecanoic acid...	13.40	3.4	ng	157463	5	13.96	918877	20.0
Isobutyl tetradec...	13.78	3.2	ng	147190	5	13.96	918877	20.0