LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093377.D
Acq On : 3 Mar 2017 23:46
Operator : SJ/MA
Sample : I2100-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-252657

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-BF013017.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	5.207	270	273	276	rBV	6297623	9641003	6.96%	2.397%
2	5.356	280	286	299	rVV2	8186507	28782949	20.79%	7.157%
3	5.607	305	308	311	rVV	7647469	15300988	11.05%	3.805%
4	6.441	379	381	385	rBV2	1355335	2169795	1.57%	0.540%
5	6.556	388	391	393	rVV	3853579	3937739	2.84%	0.979%
6	6.944	422	425	427	rBV	3496996	4138619	2.99%	1.029%
7	7.367	457	462	465	rBV3	2766961	6890724	4.98%	1.713%
8	7.687	476	490	493	rBV	1759086	10581893	7.64%	2.631%
9	8.899	593	596	598	rBV	4126494	4410757	3.19%	1.097%
10	9.162	616	619	620	rBV	3134405	5025324	3.63%	1.250%
11	9.539	622	652	654	rVV2	7906695	138465190	100.00%	34.431%
12	9.573	654	655	657	rVB	2070406	1552234	1.12%	0.386%
13	9.836	672	678	680	rBV	1255850	2231804	1.61%	0.555%
14	10.648	745	749	752	rBV2	1952356	3362126	2.43%	0.836%
15	10.728	752	756	768	rBV2	5964936	13456429	9.72%	3.346%
16	11.322	805	808	809	rBV	1569060	1619631	1.17%	0.403%
17	12.888	943	945	948	rBV	1992987	2773788	2.00%	0.690%
18	13.356	980	986	991	rVB2	2258454	8786645	6.35%	2.185%
19	14.008	1039	1043	1047	rVB2	3601870	10784763	7.79%	2.682%
20	14.602	1090	1095	1100	rVB	1925669	5218976	3.77%	1.298%
21	15.162	1138	1144	1147	rBV	5571864	17963732	12.97%	4.467%
22	15.940	1201	1212	1231	rVB3	6190910	40405674	29.18%	10.047%
23	16.923	1284	1298	1311	rVB5	5861552	43571419	31.47%	10.834%
24	18.168	1397	1407	1421	rVB	4418096	21082797	15.23%	5.242%

Sum of corrected areas: 402154999

LSC Report - Integrated Chromatogram

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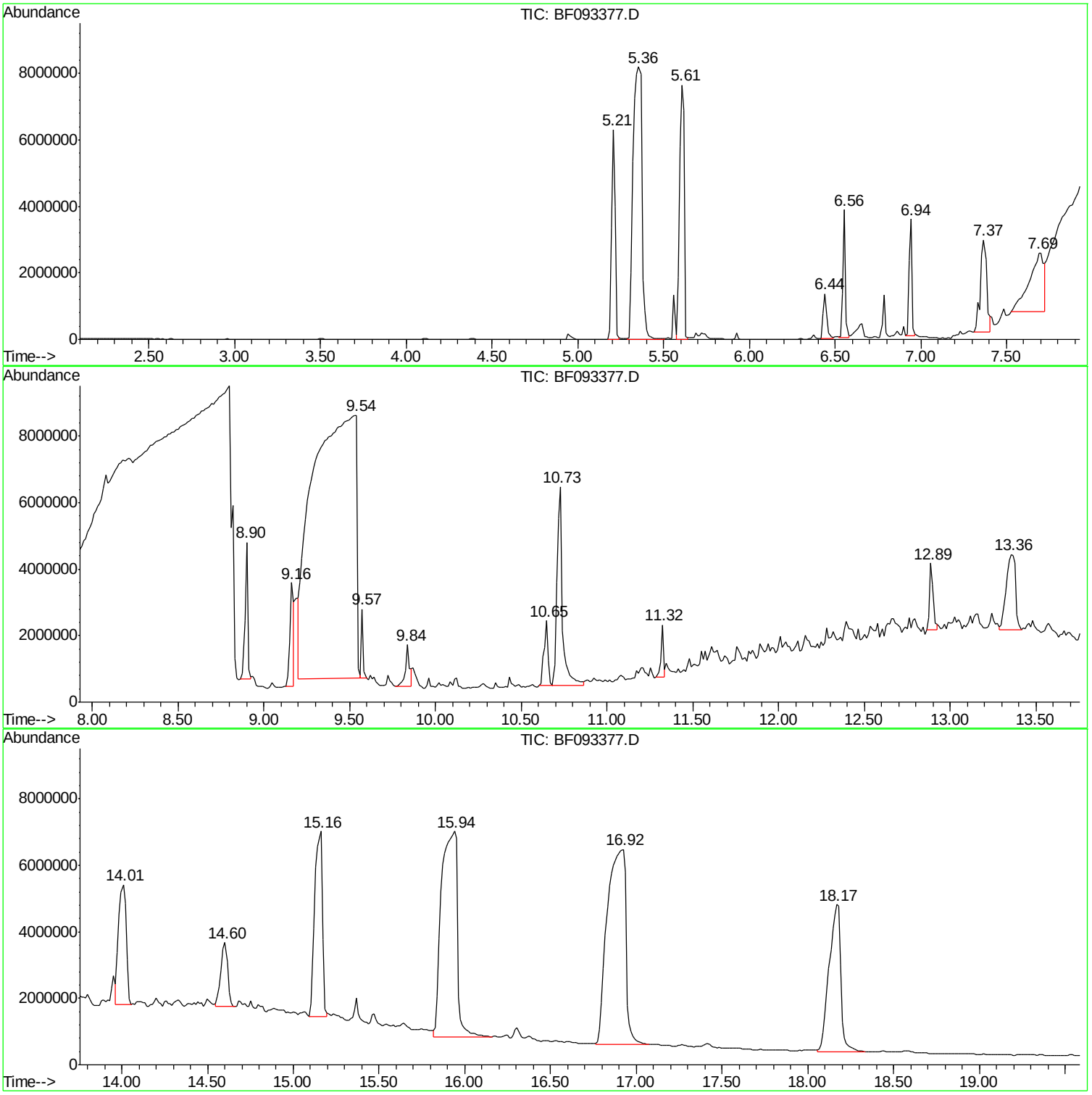
Instrument :
BNA_F
ClientSampleId :
FRAC-TANK-252657

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST02.L
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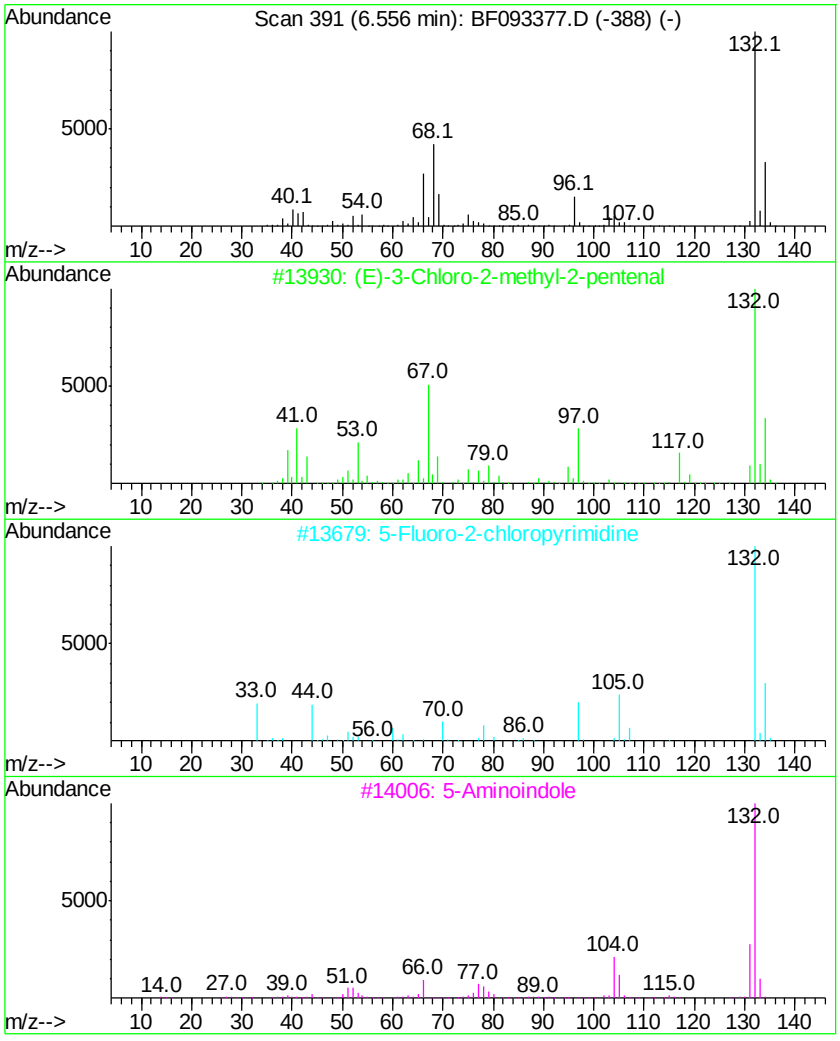
Peak Number 3 unknown6.56 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	19.03 ng	3937740	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



m/z 132.10 100.00%
m/z 68.10 42.21%
m/z 134.10 32.65%
m/z 66.05 27.09%
m/z 69.05 16.25%

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Instrument : BNA_F
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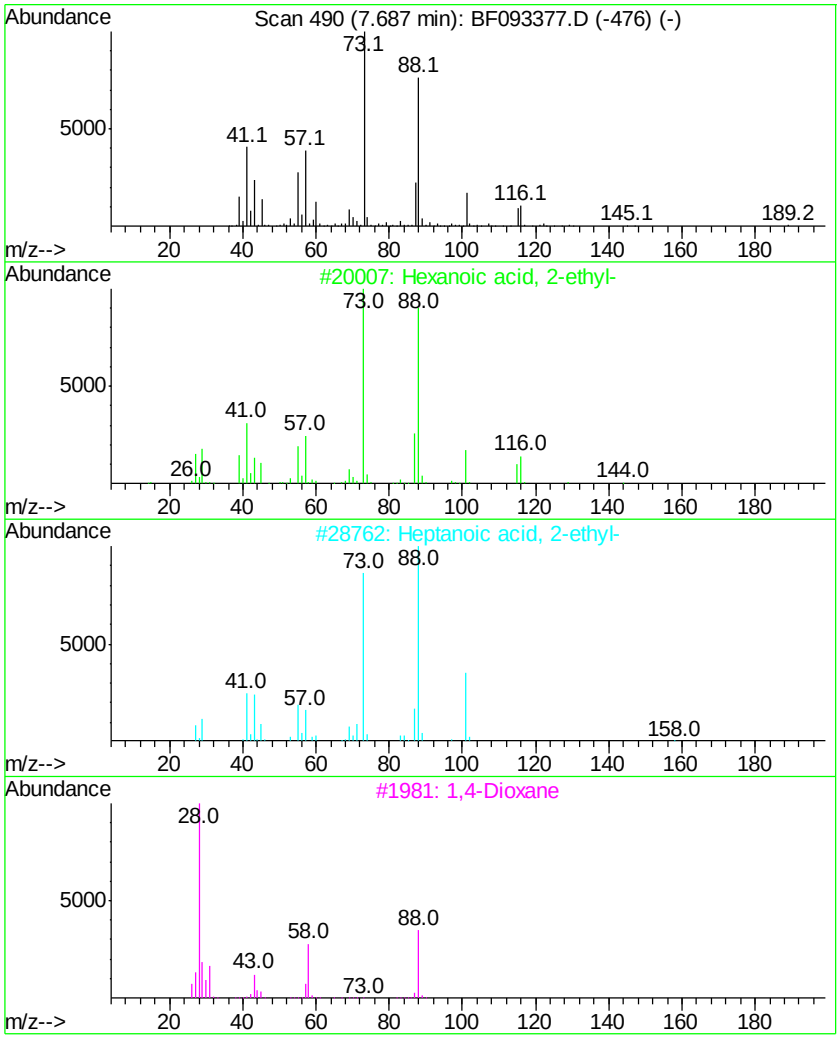
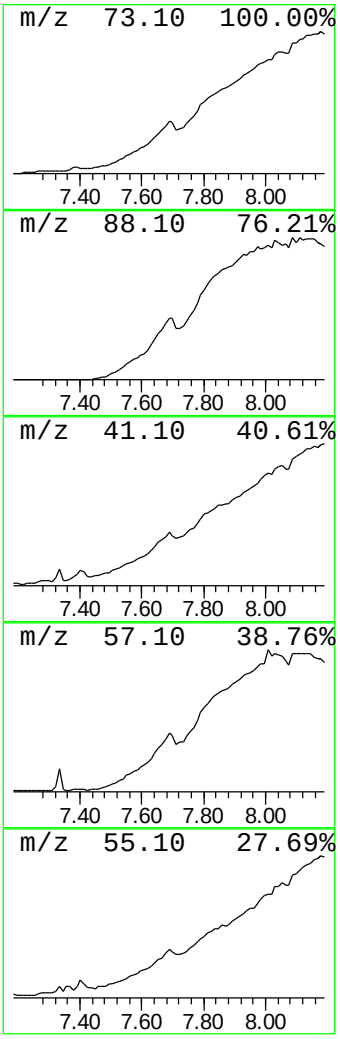
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	20.00 ng	10581900	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
2	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3	1,4-Dioxane	88	C4H8O2	000123-91-1	43
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
5	Methyl (R)-(-)-3-hydroxy-2-methy...	118	C5H10O3	072657-23-9	38





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ClientSampleId : FRAC-TANK-252657

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TIC Library : C:\DATABASE\NIST02.L
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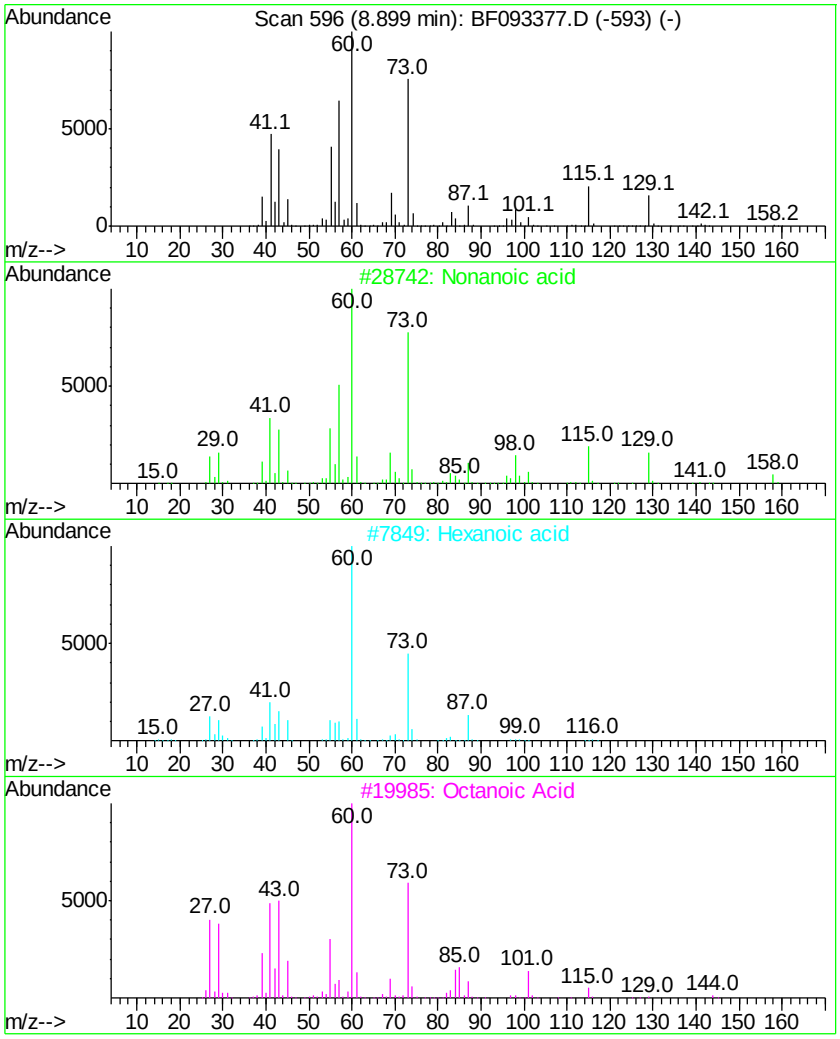
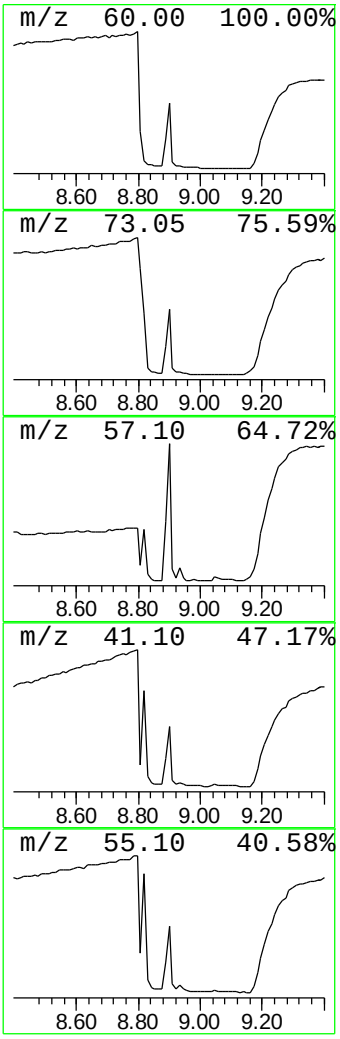
Peak Number 6 Nonanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	8.34 ng	4410760	Naphthalene-d8	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	83
2	Hexanoic acid	116	C6H12O2	000142-62-1	58
3	Octanoic Acid	144	C8H16O2	000124-07-2	53
4	Pentanoic acid	102	C5H10O2	000109-52-4	50
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	46





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Sample : I2100-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-252657

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TIC Library : C:\DATABASE\NIST02.L
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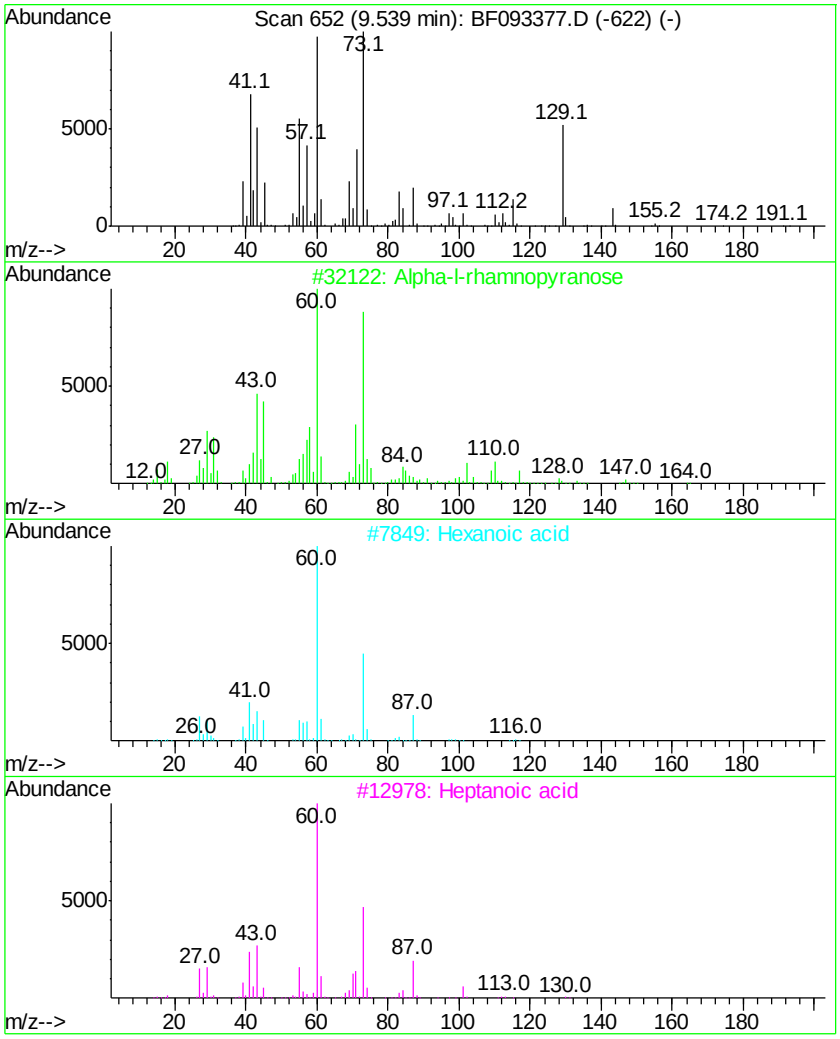
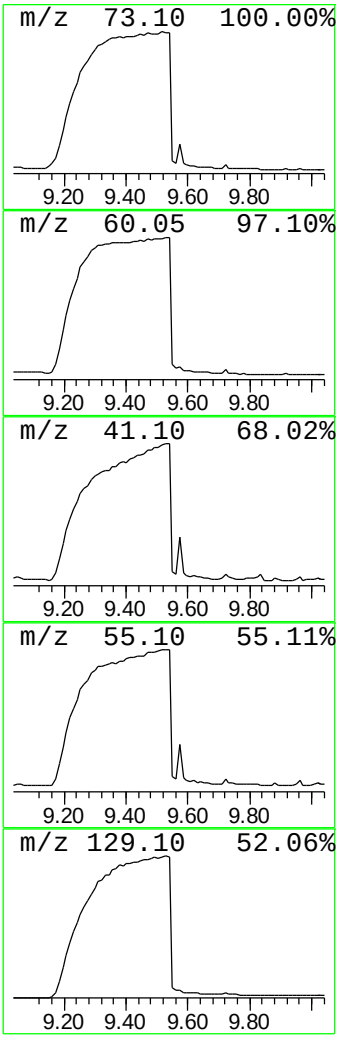
Peak Number 7 Alpha-l-rhamnopyranose Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	1240.84 ng	138465000	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Alpha-l-rhamnopyranose	164	C6H12O5	035810-56-1	50
2	Hexanoic acid	116	C6H12O2	000142-62-1	43
3	Heptanoic acid	130	C7H14O2	000111-14-8	43
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	43
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38





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Sample : I2100-01
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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-252657

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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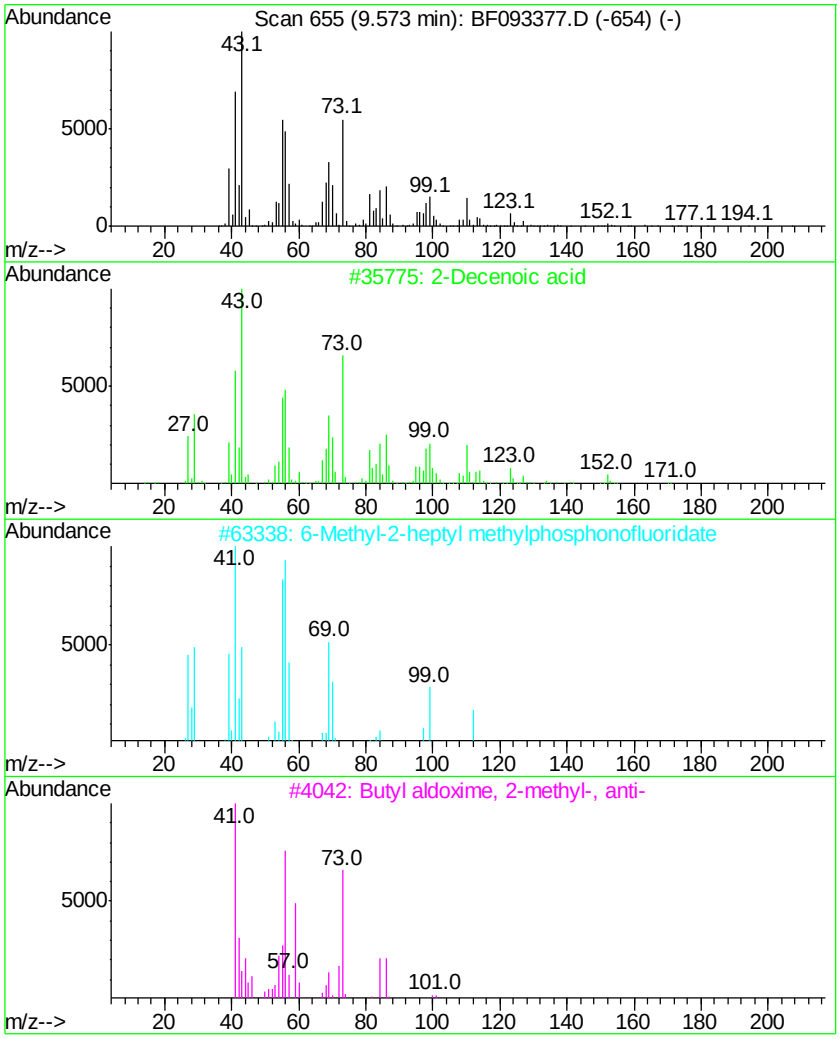
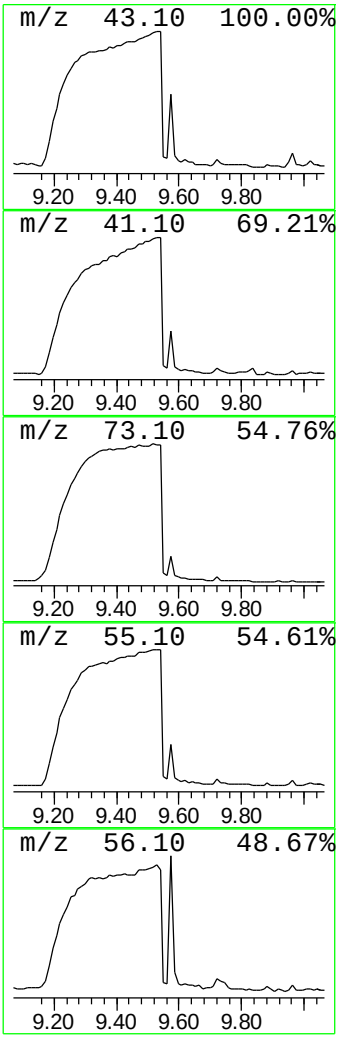
Peak Number 8 2-Decenoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	13.91 ng	1552230	Acenaphthene-d10	9.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decenoic acid	170	C10H18O2	003913-85-7	72
2	6-Methyl-2-heptyl methylphosphon...	210	C9H20FO2P	159395-76-3	43
3	Butyl aldoxime, 2-methyl-, anti-	101	C5H11NO	049805-55-2	35
4	1-Decanol	158	C10H22O	000112-30-1	35
5	cis-1-Methyl-2-propylcyclohexane	140	C10H20	1000113-64-3	35





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Instrument : BNA_F
ClientSampleId : FRAC-TANK-252657

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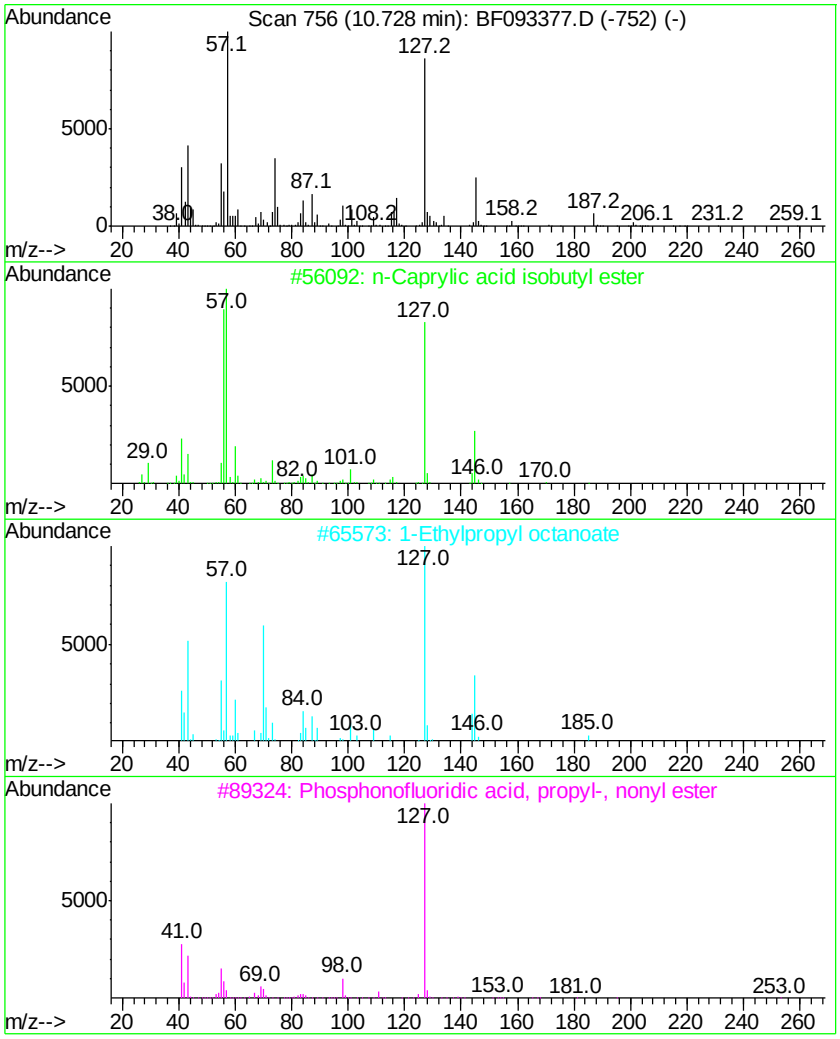
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

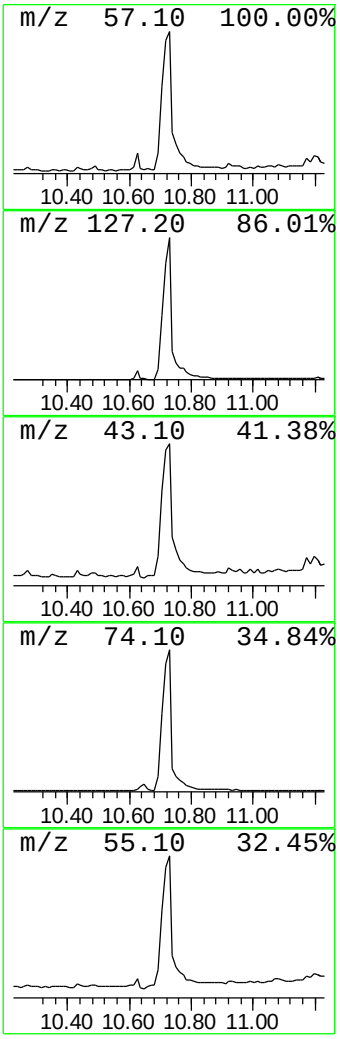
****

Peak Number 9 unknown10.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	166.17 ng	13456400	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Caprylic acid isobutyl ester	200	C12H24O2	005461-06-3	42
2	1-Ethylpropyl octanoate	214	C13H26O2	005457-67-0	40
3	Phosphonofluoridic acid, propyl-...	252	C12H26FO2P	333416-21-0	38
4	Octanoic acid, 2-pentyl ester	214	C13H26O2	055193-30-1	38
5	Nonanoic acid, 2-oxo-, methyl ester	186	C10H18O3	056275-54-8	38





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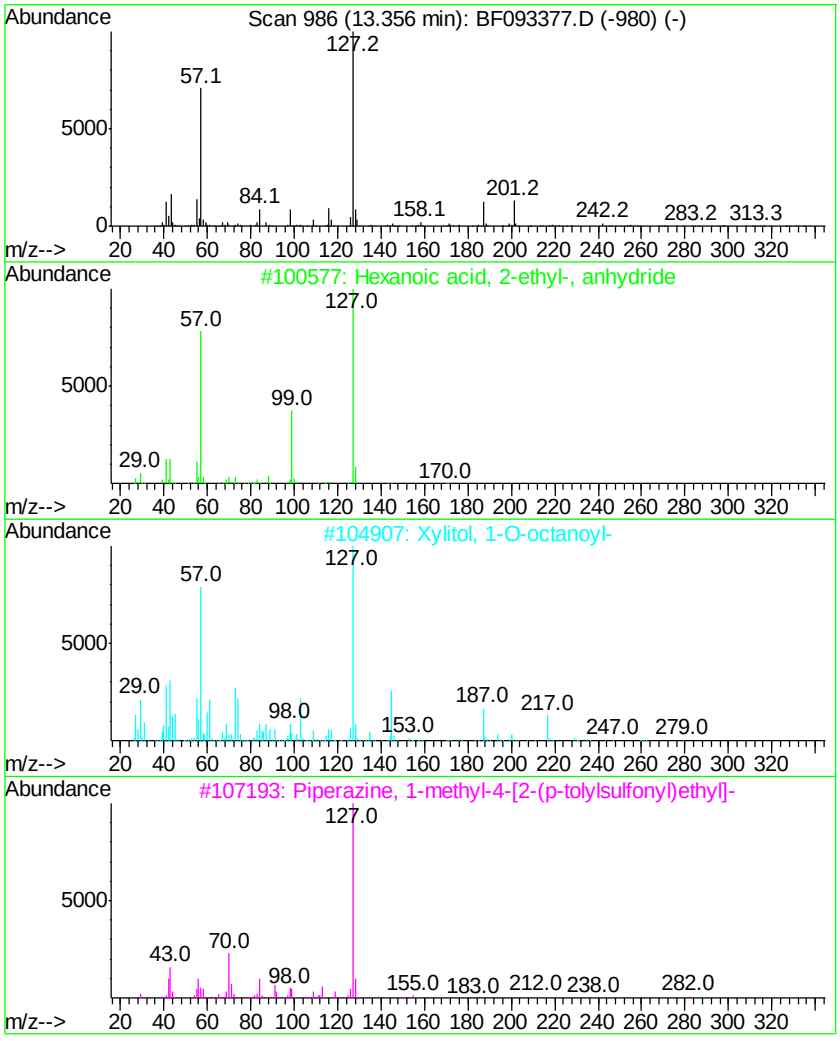
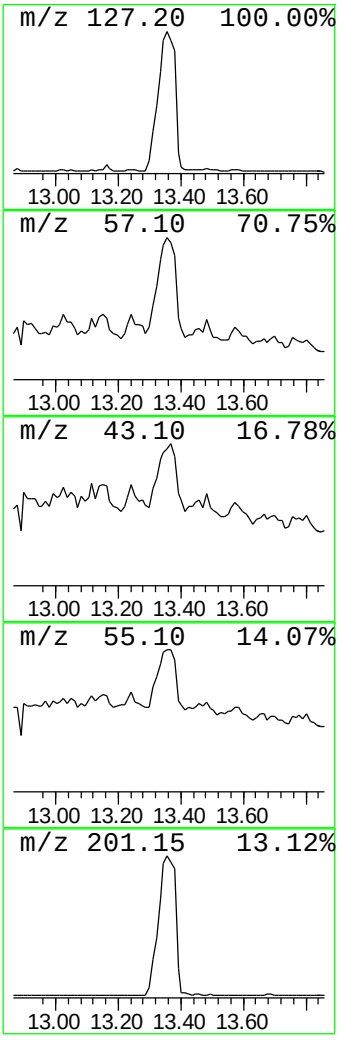
Peak Number 10 Hexanoic acid, 2-ethyl-, an... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	16.29 ng	8786650	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-, anhydride	270	C16H30O3	036765-89-6	50
2	Xylitol, 1-O-octanoyl-	278	C13H26O6	1000155-88-7	39
3	Piperazine, 1-methyl-4-[2-(p-tol...	282	C14H22N2O2S	016191-68-7	36
4	Octanoic acid, 2-pentadecyl ester	354	C23H46O2	1000280-63-0	34
5	Octanoic acid, 1-methyltridecyl ...	340	C22H44O2	055193-79-8	34





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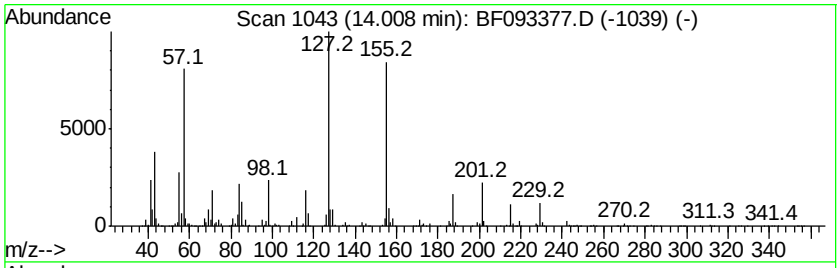
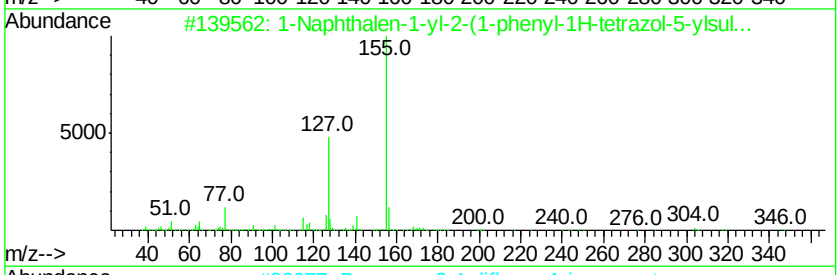
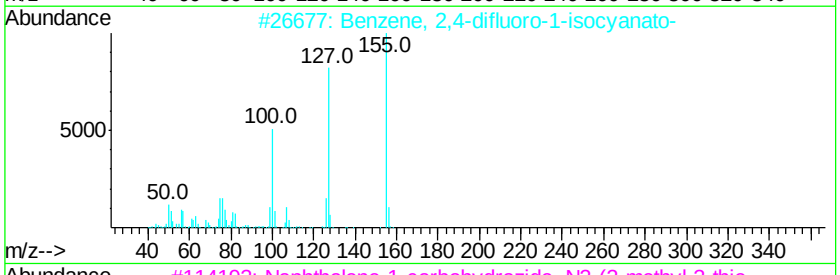
Peak Number 11 unknown14.01 Concentration Rank 10

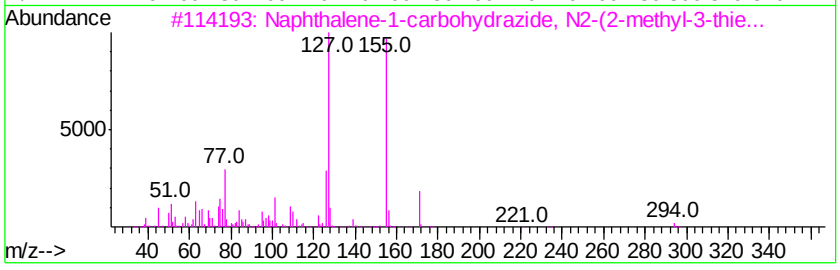
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	20.00 ng	10784800	Chrysene-d12	13.95

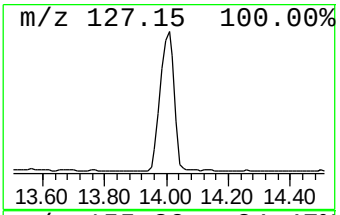
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalen-1-yl-2-(1-phenyl-1H...	346	C19H14N4OS	1000295-34-4	47
2	Benzene, 2,4-difluoro-1-isocyanato-	155	C7H3F2NO	059025-55-7	47
3	Naphthalene-1-carbohydrazide, N2...	294	C17H14N2OS	1000263-63-0	47
4	4-Cyanocinnoline	155	C9H5N3	016470-90-9	47
5	Naphthalene-1-carboxamide, N-(1,...	238	C13H10N4O	1000259-81-8	38

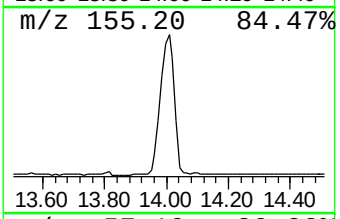


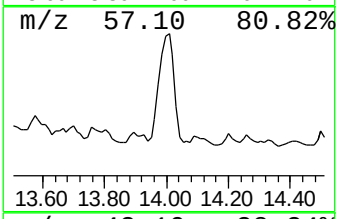


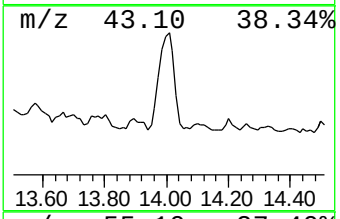


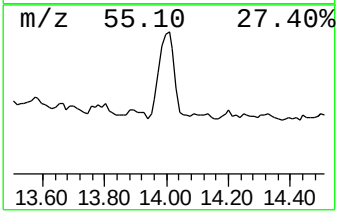












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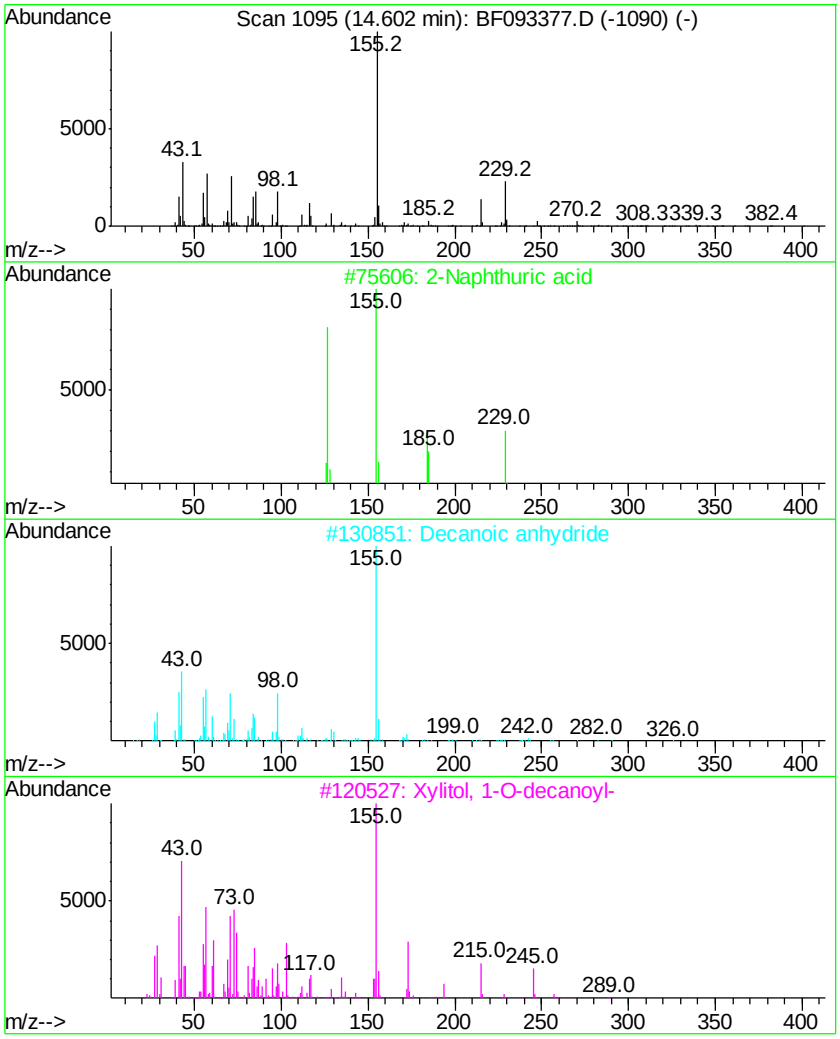
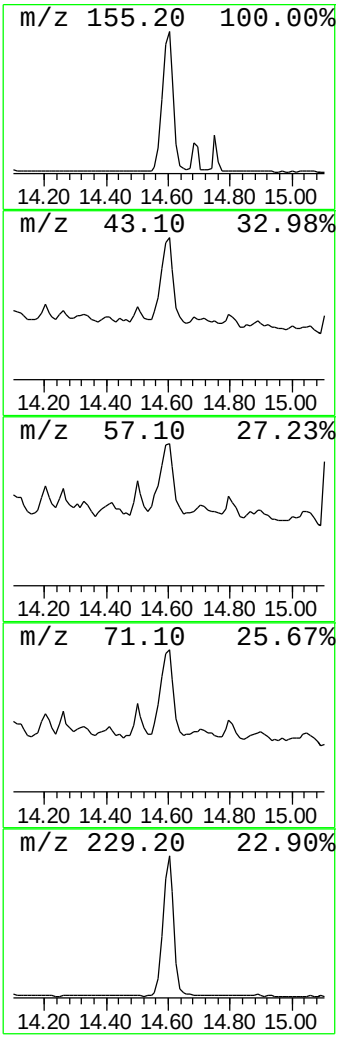
Peak Number 12 2-Naphthuric acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	9.68 ng	5218980	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Naphthuric acid	229	C13H11NO3	069826-63-7	78
2	Decanoic anhydride	326	C20H38O3	002082-76-0	62
3	Xylitol, 1-O-decanoyl-	306	C15H30O6	1000155-78-0	50
4	2,4,6-TRIBROMOPHENYL DECANOATE	482	C16H21Br3O2	1000233-09-1	50
5	Methanol, (phenylsulfonyl)-, 4-m...	326	C14H14O5S2	031081-06-8	38





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Data File : BF093377.D
Acq On : 3 Mar 2017 23:46
Operator : SJ/MA
Sample : I2100-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-252657

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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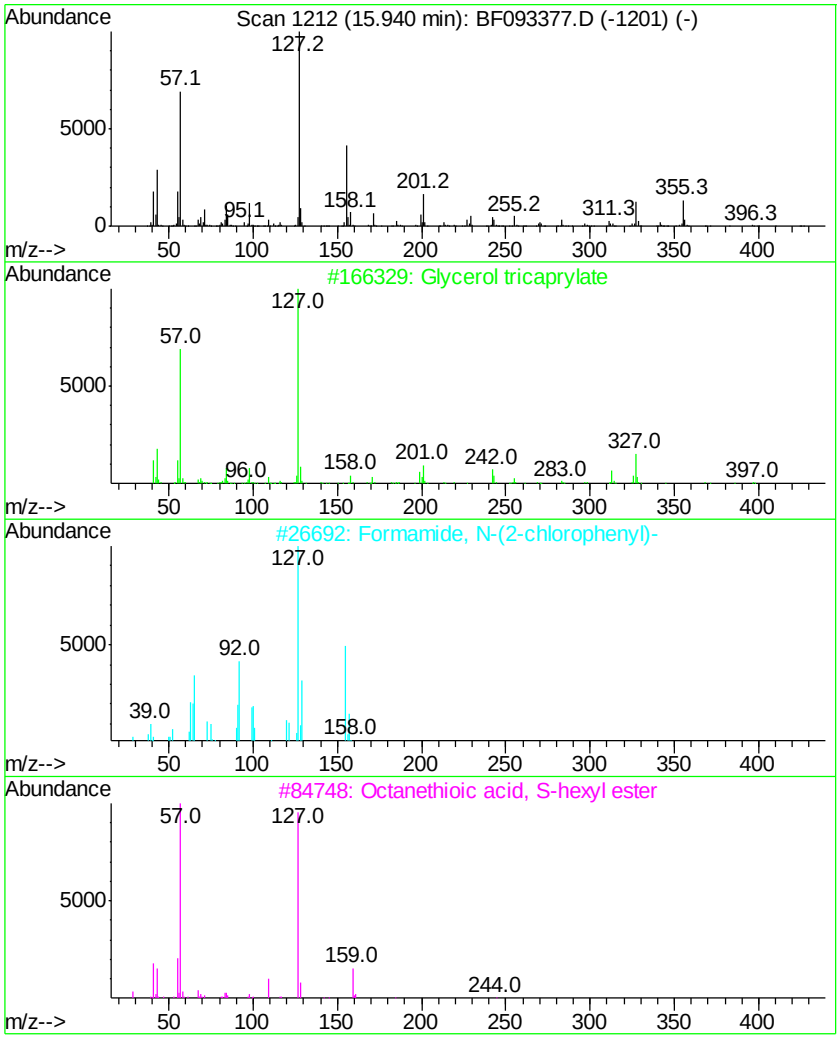
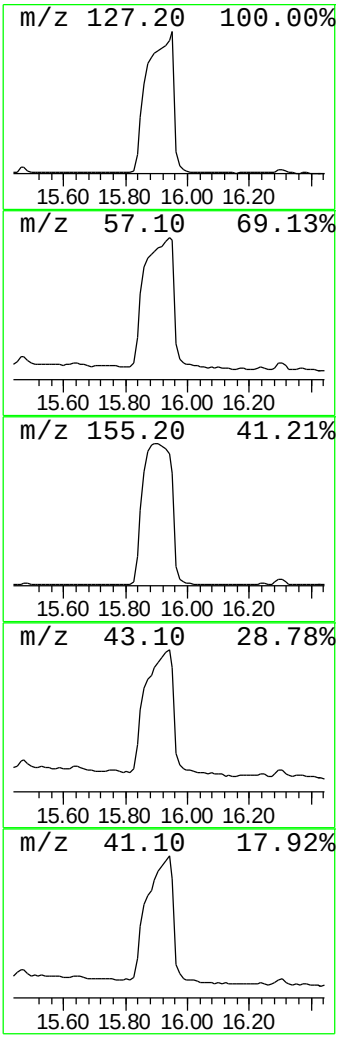
Peak Number 14 Glycerol tricaprylate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	44.99 ng	40405700	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glycerol tricaprylate	470	C27H50O6	000538-23-8	53
2	Formamide, N-(2-chlorophenyl)-	155	C7H6ClNO	002596-93-2	42
3	Octanethioic acid, S-hexyl ester	244	C14H28OS	055590-85-7	38
4	Hexanoic acid, 2-ethyl-, anhydride	270	C16H30O3	036765-89-6	35
5	3,7-Dimethyloctyl isopropylphosp...	266	C13H28FO2P	1000298-27-5	32





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030317\
Data File : BF093377.D
Acq On : 3 Mar 2017 23:46
Operator : SJ/MA
Sample : I2100-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-252657

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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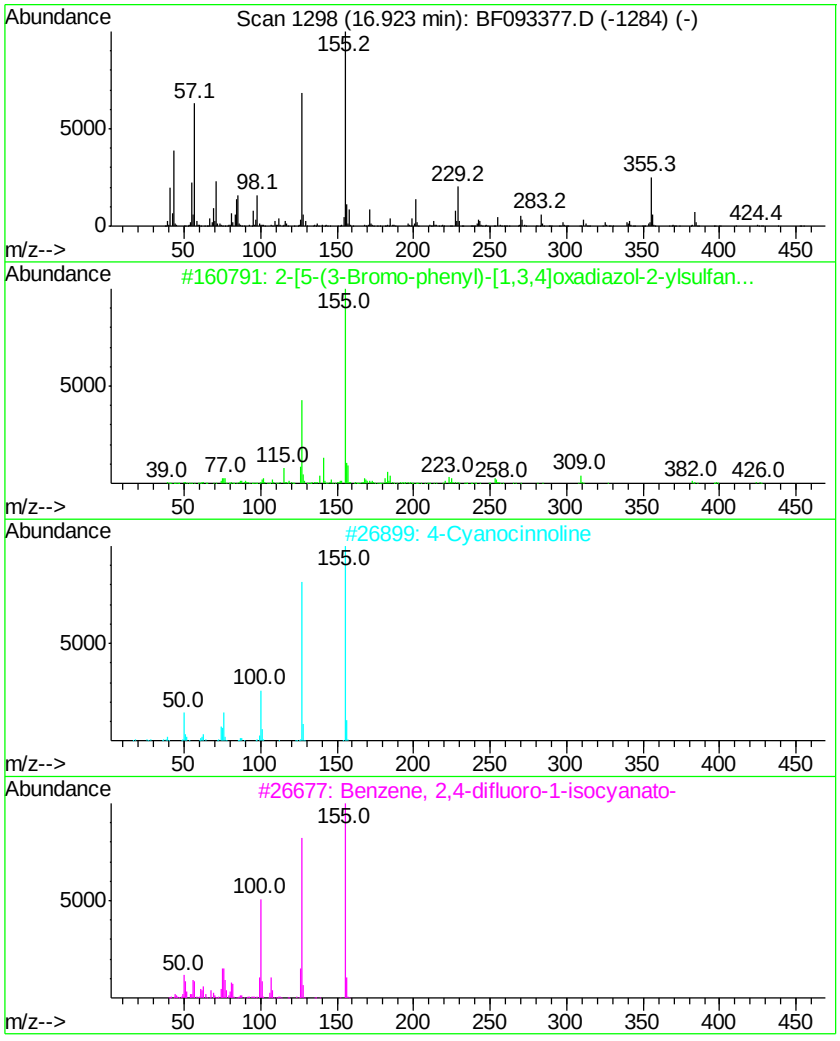
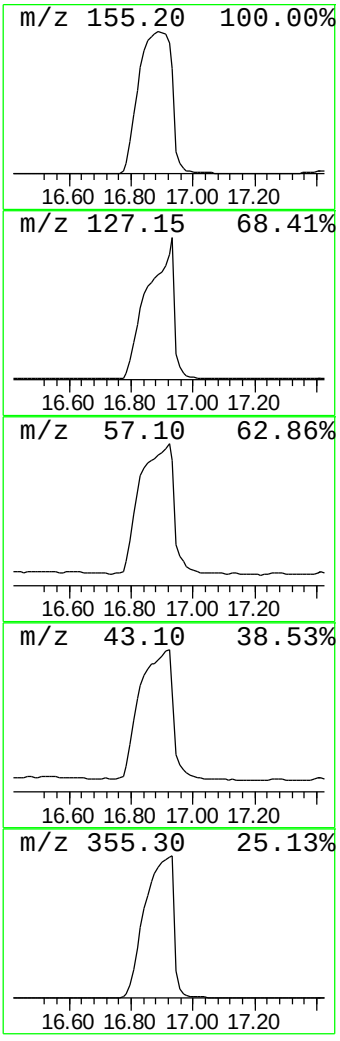
Peak Number 15 unknown16.92 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.92	48.51 ng	43571400	Perylene-d12	15.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[5-(3-Bromo-phenyl)-[1,3,4]oxa...	424	C20H13BrN2O2S	1000275-09-0	47
2	4-Cyanocinnoline	155	C9H5N3	016470-90-9	47
3	Benzene, 2,4-difluoro-1-isocyanato-	155	C7H3F2NO	059025-55-7	47
4	1-Naphthanilide	247	C17H13NO	006833-19-8	38
5	Pyridine, 4-phenyl-	155	C11H9N	000939-23-1	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030317\
Data File : BF093377.D
Acq On : 3 Mar 2017 23:46
Operator : SJ/MA
Sample : I2100-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FRAC-TANK-252657

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.56	6.56	19.0	ng	3937740	1	6.78	4138620	20.0
Hexanoic acid, 2-...	7.69	20.0	ng	10581900	2	8.08	10581900	20.0
Nonanoic acid	8.90	8.3	ng	4410760	2	8.08	10581900	20.0
Alpha-l-rhamnopyr...	9.54	1240.8	ng	138465000	3	9.87	2231800	20.0
2-Decenoic acid	9.57	13.9	ng	1552230	3	9.87	2231800	20.0
unknown10.73	10.73	166.2	ng	13456400	4	11.32	1619630	20.0
Hexanoic acid, 2-...	13.36	16.3	ng	8786650	5	13.95	10784800	20.0
unknown14.01	14.01	20.0	ng	10784800	5	13.95	10784800	20.0
2-Naphthuric acid	14.60	9.7	ng	5218980	5	13.95	10784800	20.0
Glycerol tricapry...	15.94	45.0	ng	40405700	6	15.37	17963700	20.0
unknown16.92	16.92	48.5	ng	43571400	6	15.37	17963700	20.0