LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
Data File : BF101455.D
Acq On : 15 Dec 2017 20:48
Operator : SJ/JU
Sample : I6889-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1(0-3)

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	2.116	3	5	19	rVB	213828	305471	6.61%	0.786%
2	5.045	499	503	524	rBV	544447	943043	20.41%	2.427%
3	5.445	566	571	597	rBV	3553792	4359636	94.36%	11.219%
4	5.781	625	628	639	rBV	28724	62827	1.36%	0.162%
5	6.457	738	743	758	rBV	3393684	4620069	100.00%	11.889%
6	6.587	761	765	769	rBV	3765369	3986662	86.29%	10.259%
7	6.816	800	804	811	rBV	1167466	1139292	24.66%	2.932%
8	6.969	826	830	844	rBV	3136597	3133226	67.82%	8.063%
9	7.386	896	901	918	rBV	2555521	2829247	61.24%	7.281%
10	8.098	1018	1022	1038	rVB	1383470	1495100	32.36%	3.848%
11	8.657	1113	1117	1125	rBV	200916	213370	4.62%	0.549%
12	9.175	1199	1205	1215	rBV	3803139	3884151	84.07%	9.996%
13	9.569	1268	1272	1282	rVB	415412	434124	9.40%	1.117%
14	9.851	1316	1320	1329	rVB2	1543923	1474917	31.92%	3.796%
15	10.569	1438	1442	1451	rBV	597114	577936	12.51%	1.487%
16	10.651	1451	1456	1470	rBV	2017670	2294186	49.66%	5.904%
17	11.345	1570	1574	1583	rBV	1394721	1372987	29.72%	3.533%
18	11.863	1658	1662	1670	rBV3	151300	186215	4.03%	0.479%
19	12.563	1778	1781	1785	rBV	56033	63271	1.37%	0.163%
20	12.645	1792	1795	1803	rBV4	48830	60651	1.31%	0.156%
21	12.798	1815	1821	1827	rBV2	55065	93505	2.02%	0.241%
22	12.927	1839	1843	1847	rBV	2888166	2825733	61.16%	7.272%
23	13.810	1989	1993	2005	rBV	327630	453003	9.81%	1.166%
24	13.951	2014	2017	2020	rVB	72216	66790	1.45%	0.172%
25	13.992	2020	2024	2034	rBV	991174	1082716	23.44%	2.786%
26	15.468	2267	2275	2285	rVB	637413	900395	19.49%	2.317%

Sum of corrected areas: 38858523

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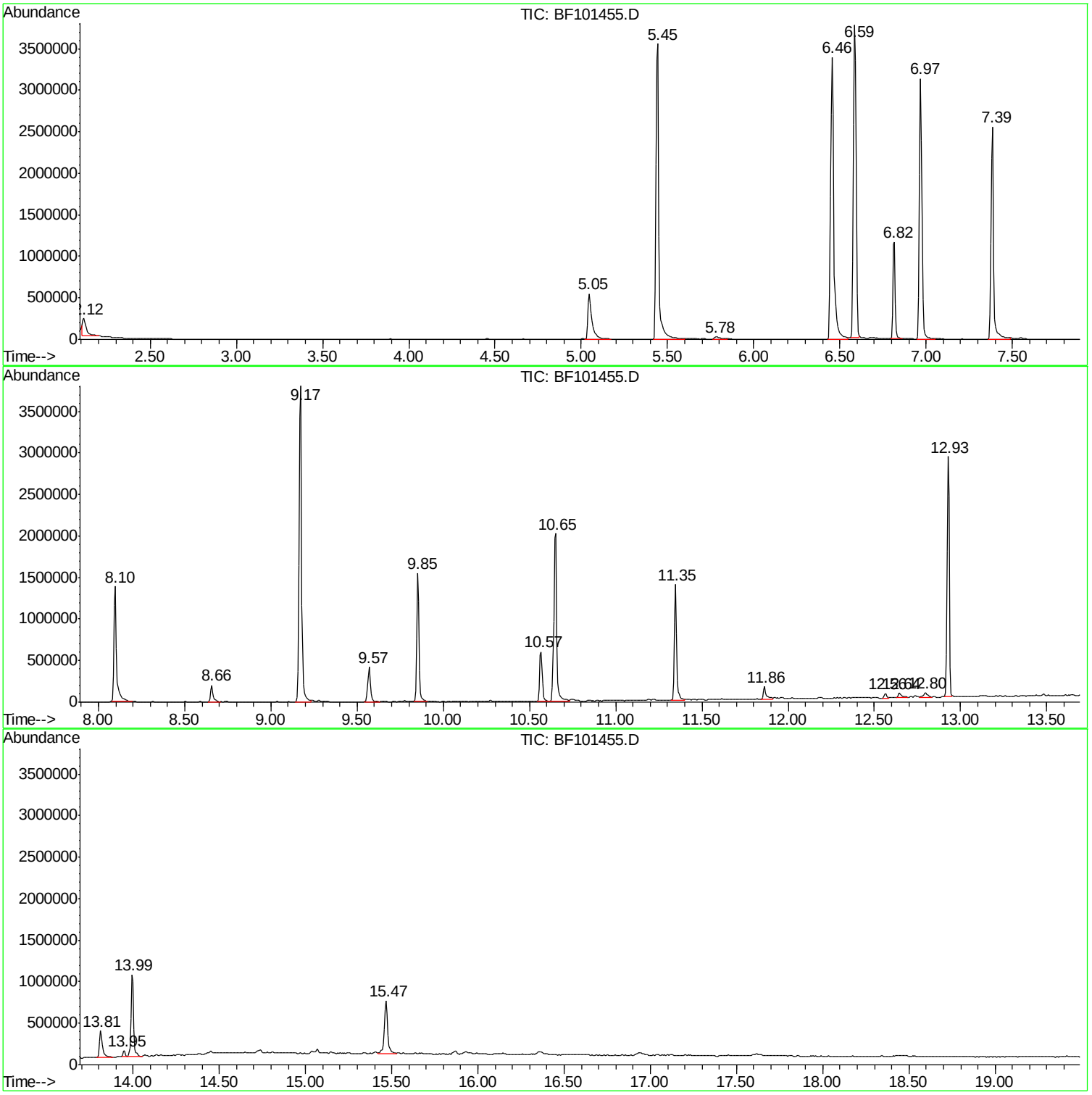
Instrument :
BNA_F
ClientSampleId :
T-1(0-3)

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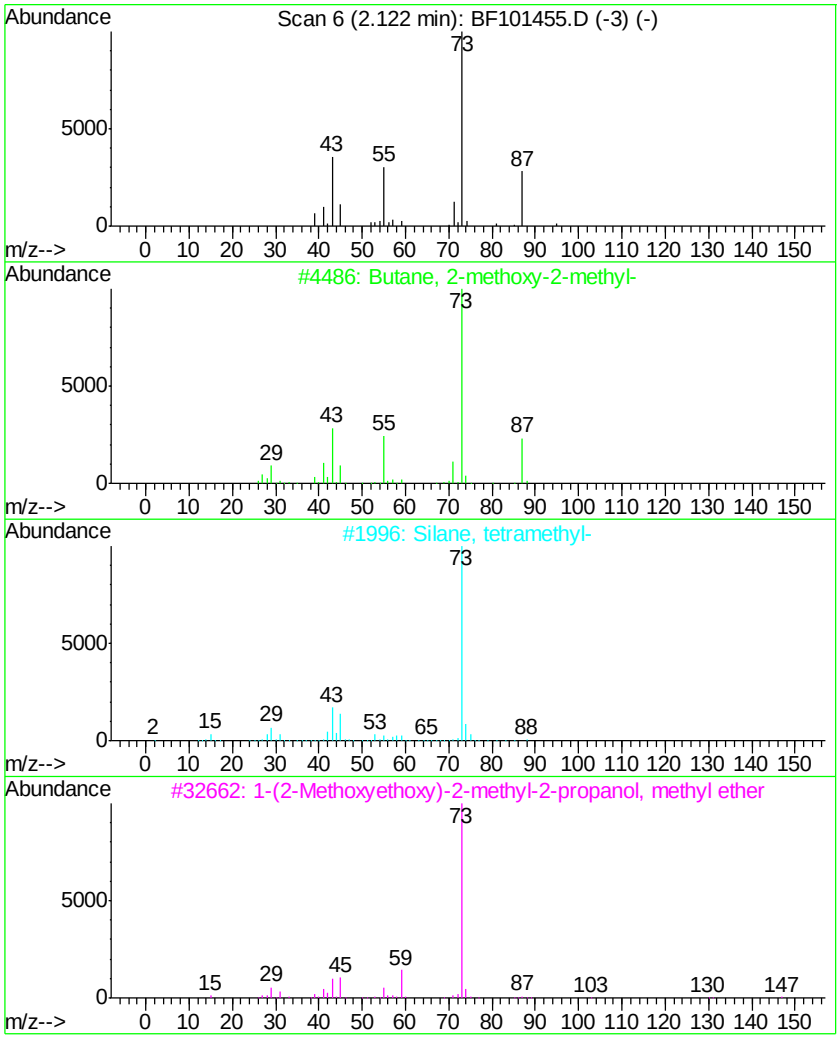
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

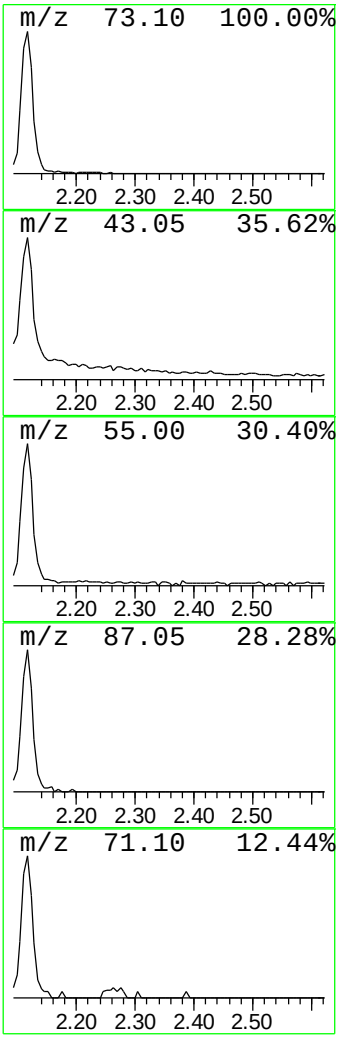
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	5.36 ng	305471	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
3	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1(0-3)

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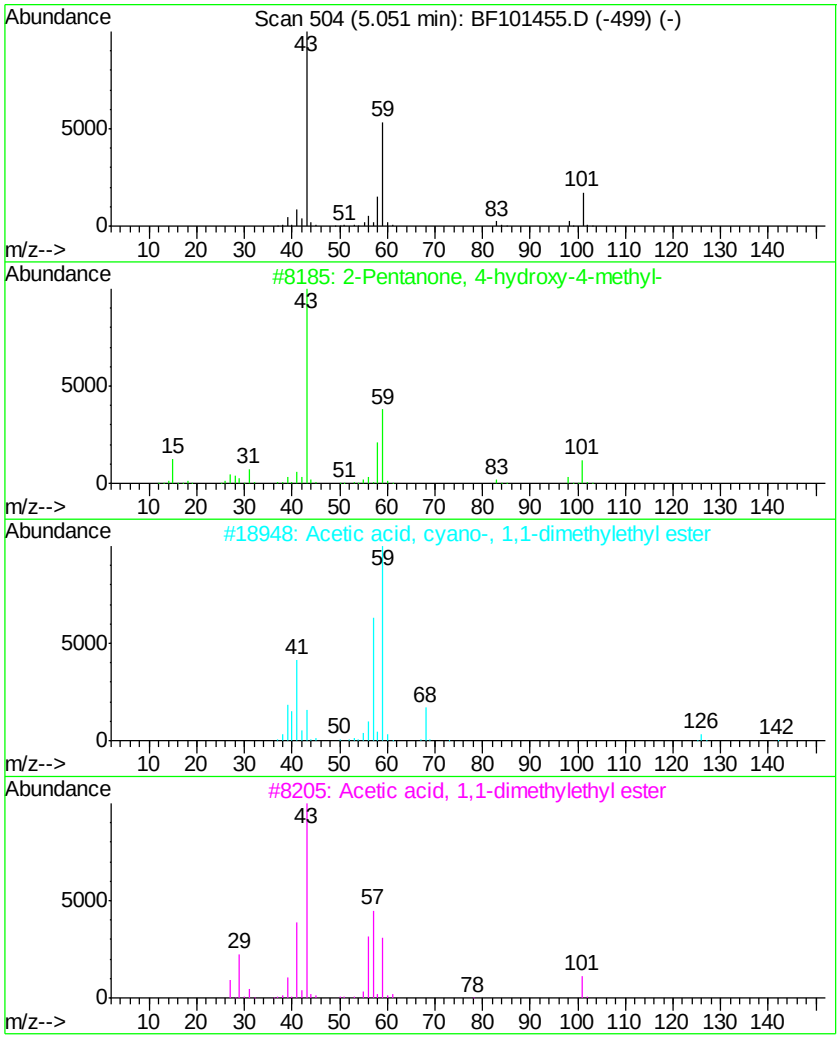
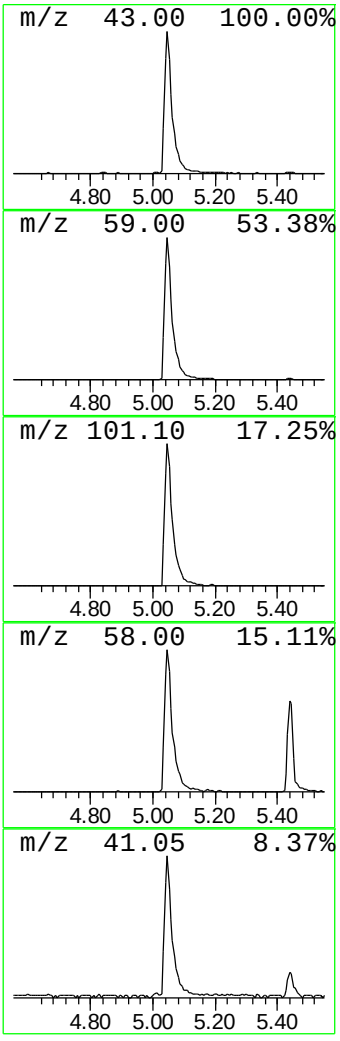
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	16.55 ng	943043	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121517\
Data File : BF101455.D
Acq On : 15 Dec 2017 20:48
Operator : SJ/JU
Sample : I6889-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1(0-3)

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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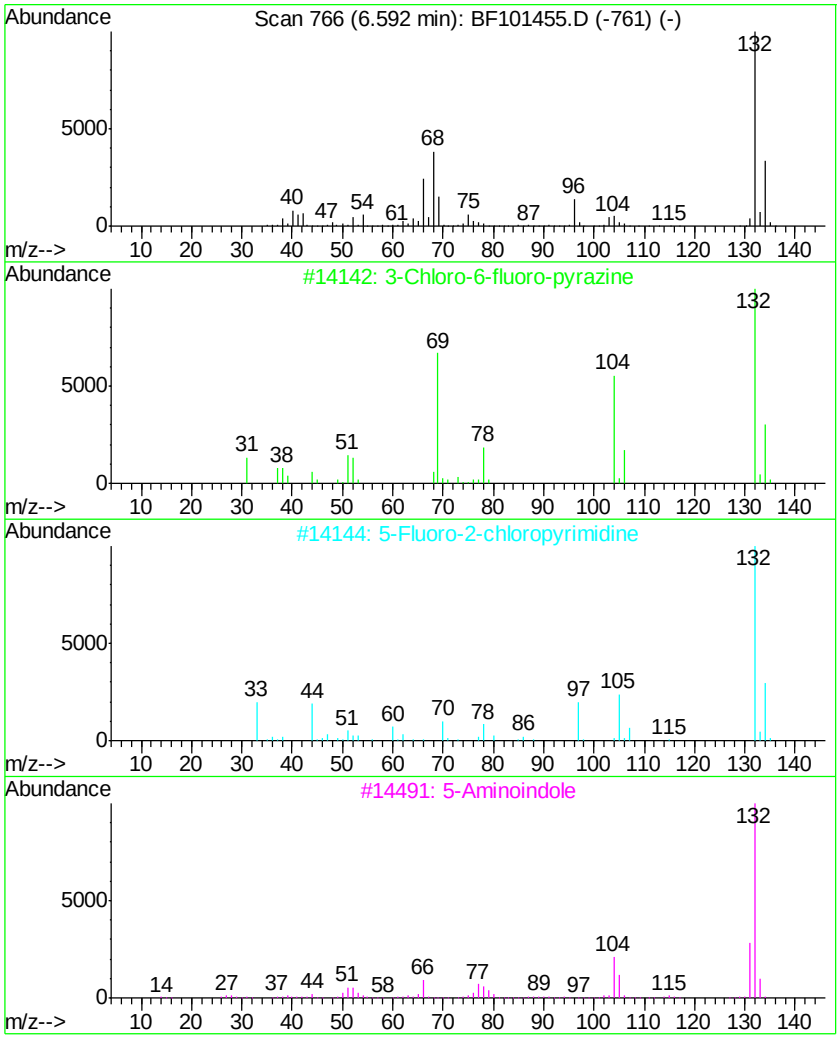
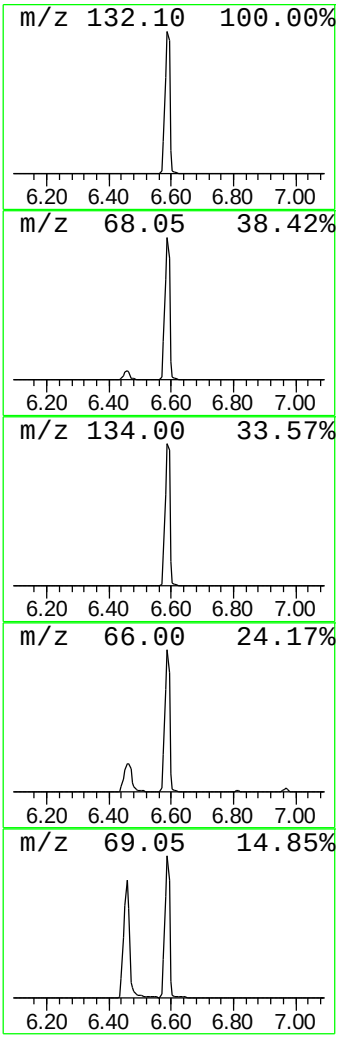
Peak Number 3 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	69.98 ng	3986660	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Operator : SJ/JU
Sample : I6889-04
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T-1(0-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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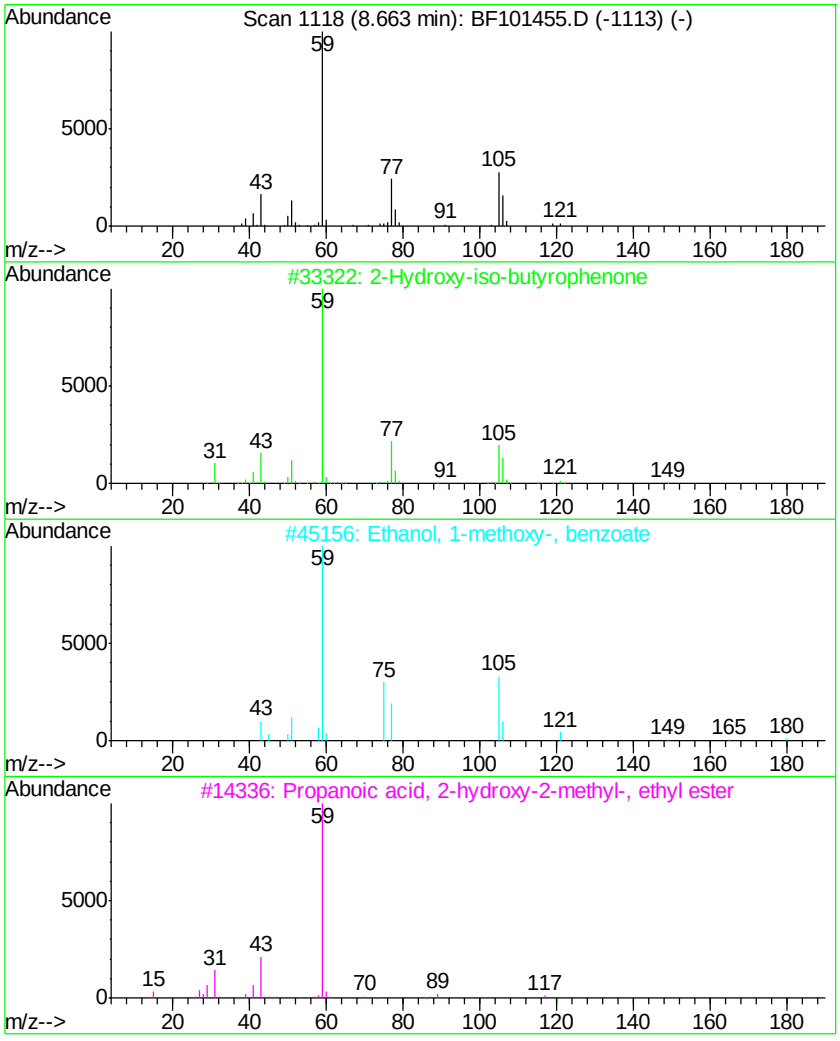
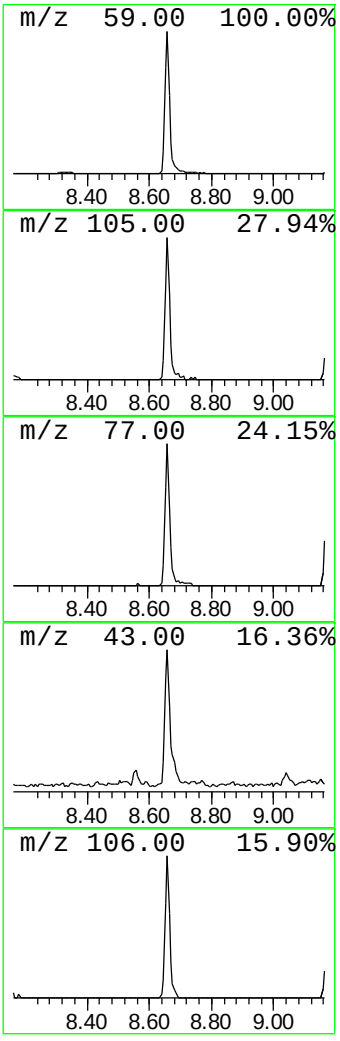
Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	2.85 ng	213370	Naphthalene-d8	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
4	Guanidine	59	CH5N3	000113-00-8	7
5	Acetamide	59	C2H5NO	000060-35-5	5





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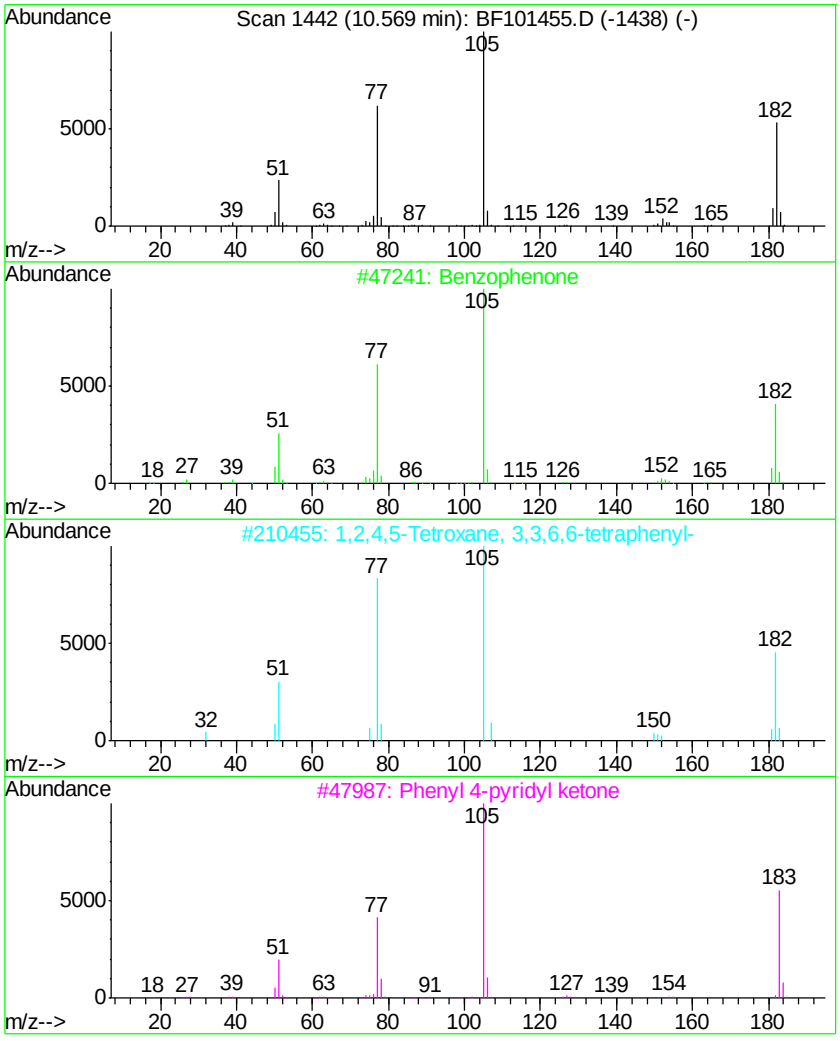
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

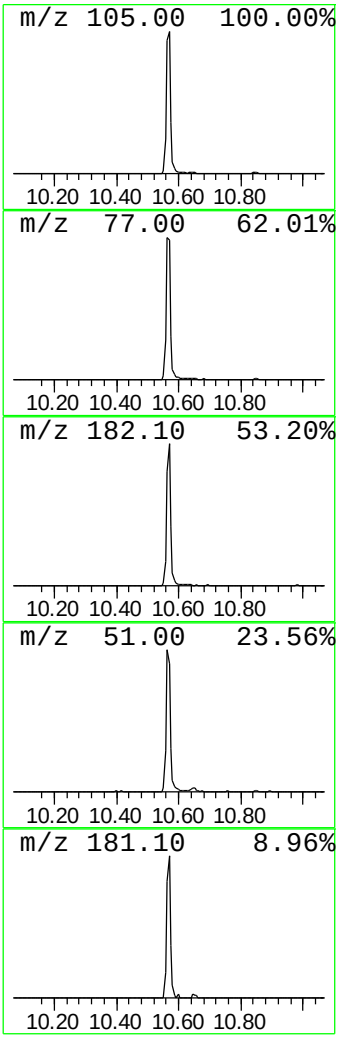
****

Peak Number 6 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	7.84 ng	577936	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





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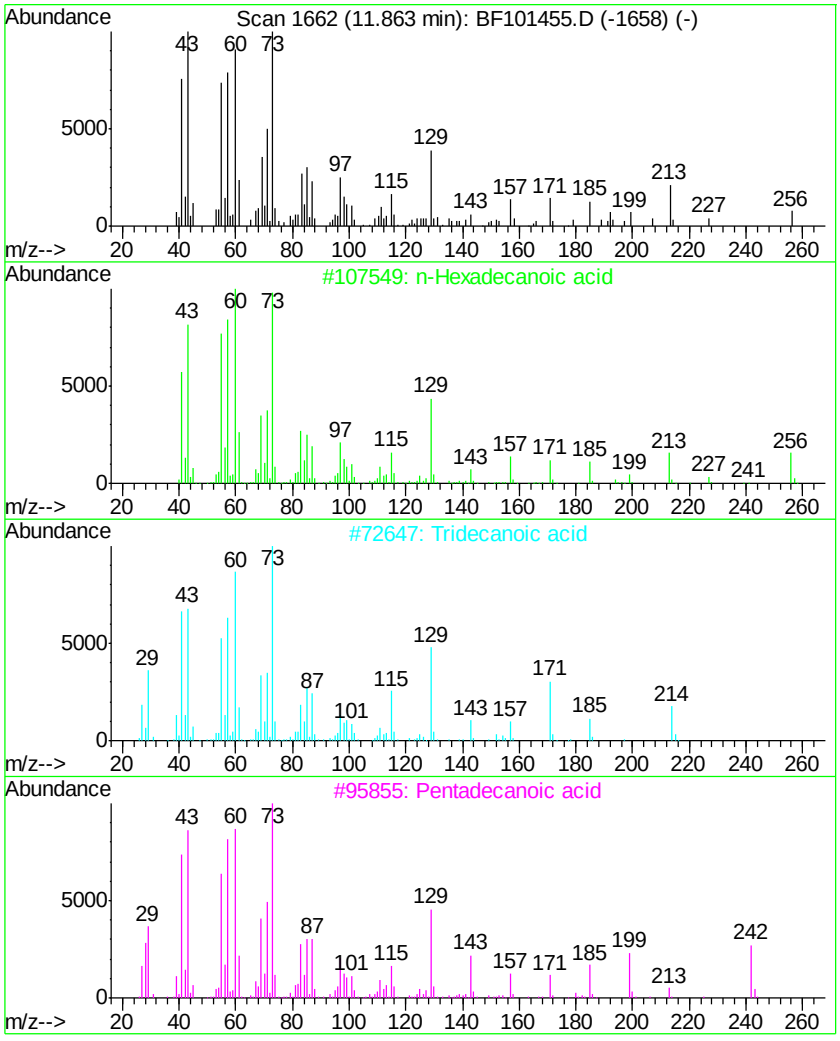
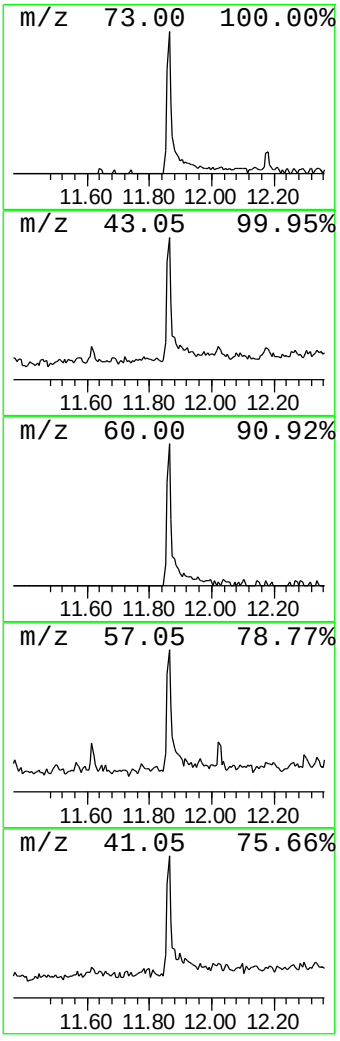
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.71 ng	186215	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Nonanoic acid	158	C9H18O2	000112-05-0	38





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

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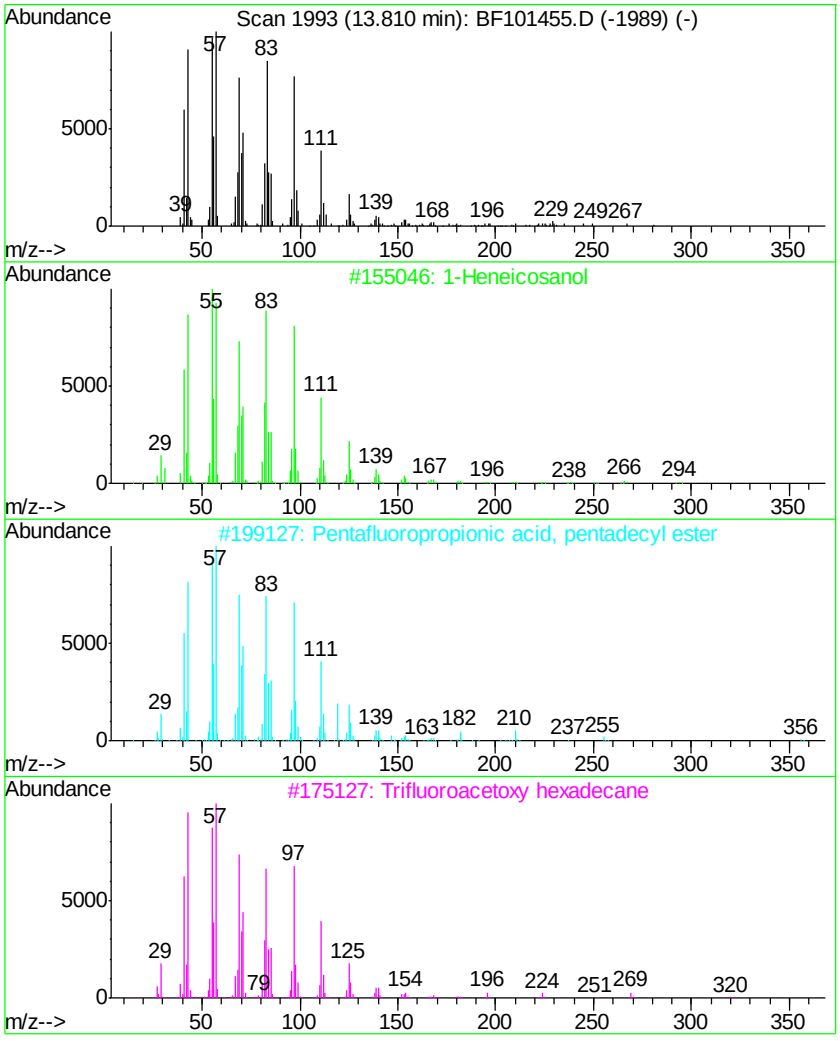
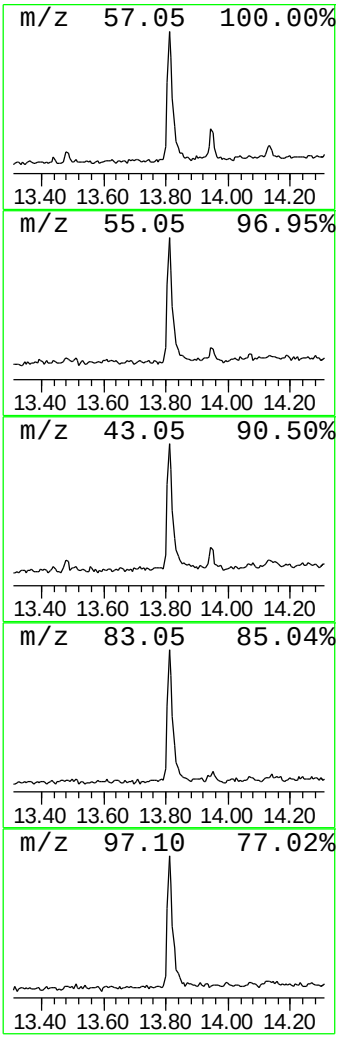
Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	8.37 ng	453003	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.12	5.4	ng	305471	1	6.82	1139290	20.0
2-Pentanone, 4-hy...	5.05	16.6	ng	943043	1	6.82	1139290	20.0
unknown6.59	6.59	70.0	ng	3986660	1	6.82	1139290	20.0
2-Hydroxy-iso-but...	8.66	2.9	ng	213370	2	8.10	1495100	20.0
Benzophenone	10.57	7.8	ng	577936	3	9.85	1474920	20.0
n-Hexadecanoic acid	11.86	2.7	ng	186215	4	11.35	1372990	20.0
1-Heneicosanol	13.81	8.4	ng	453003	5	13.99	1082720	20.0