LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099813.D
Acq On : 25 Oct 2017 15:10
Operator : SJ/JU
Sample : I6064-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11989-COMP

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-BF102317.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	5.016	495	498	519	rBV	212214	361603	14.16%	1.651%
2	5.422	563	567	585	rBV	1986790	2158615	84.51%	9.855%
3	6.439	736	740	758	rBV	1978373	2257532	88.38%	10.306%
4	6.569	758	762	765	rBV	2432551	2218978	86.87%	10.130%
5	6.792	797	800	809	rBV	582068	481483	18.85%	2.198%
6	6.951	823	827	842	rBV	1864021	1787670	69.99%	8.161%
7	7.363	893	897	900	rBV	1402337	1370802	53.67%	6.258%
8	8.075	1015	1018	1029	rBV	834018	699681	27.39%	3.194%
9	8.633	1110	1113	1124	rBB	160166	134927	5.28%	0.616%
10	9.157	1197	1202	1205	rBV	2779784	2554277	100.00%	11.661%
11	9.263	1217	1220	1224	rVB	102973	91764	3.59%	0.419%
12	9.551	1266	1269	1274	rBV	153300	115571	4.52%	0.528%
13	9.833	1314	1317	1321	rBV	836070	799383	31.30%	3.649%
14	10.557	1436	1440	1443	rBV	717996	620556	24.29%	2.833%
15	10.633	1449	1453	1457	rBV	1551264	1512306	59.21%	6.904%
16	11.327	1568	1571	1574	rBV	956968	819254	32.07%	3.740%
17	11.351	1574	1575	1580	rVB	37025	30735	1.20%	0.140%
18	11.851	1655	1660	1668	rBV4	58694	78848	3.09%	0.360%
19	12.551	1775	1779	1782	rBV	62768	56604	2.22%	0.258%
20	12.780	1813	1818	1821	rBV	51303	49996	1.96%	0.228%
21	12.921	1837	1842	1845	rBV	2321908	2370383	92.80%	10.821%
22	13.798	1987	1991	1998	rBV	153153	166745	6.53%	0.761%
23	13.980	2018	2022	2026	rBV	728386	646048	25.29%	2.949%
24	15.451	2265	2272	2286	rVB	405114	520940	20.39%	2.378%

Sum of corrected areas: 21904701

LSC Report - Integrated Chromatogram

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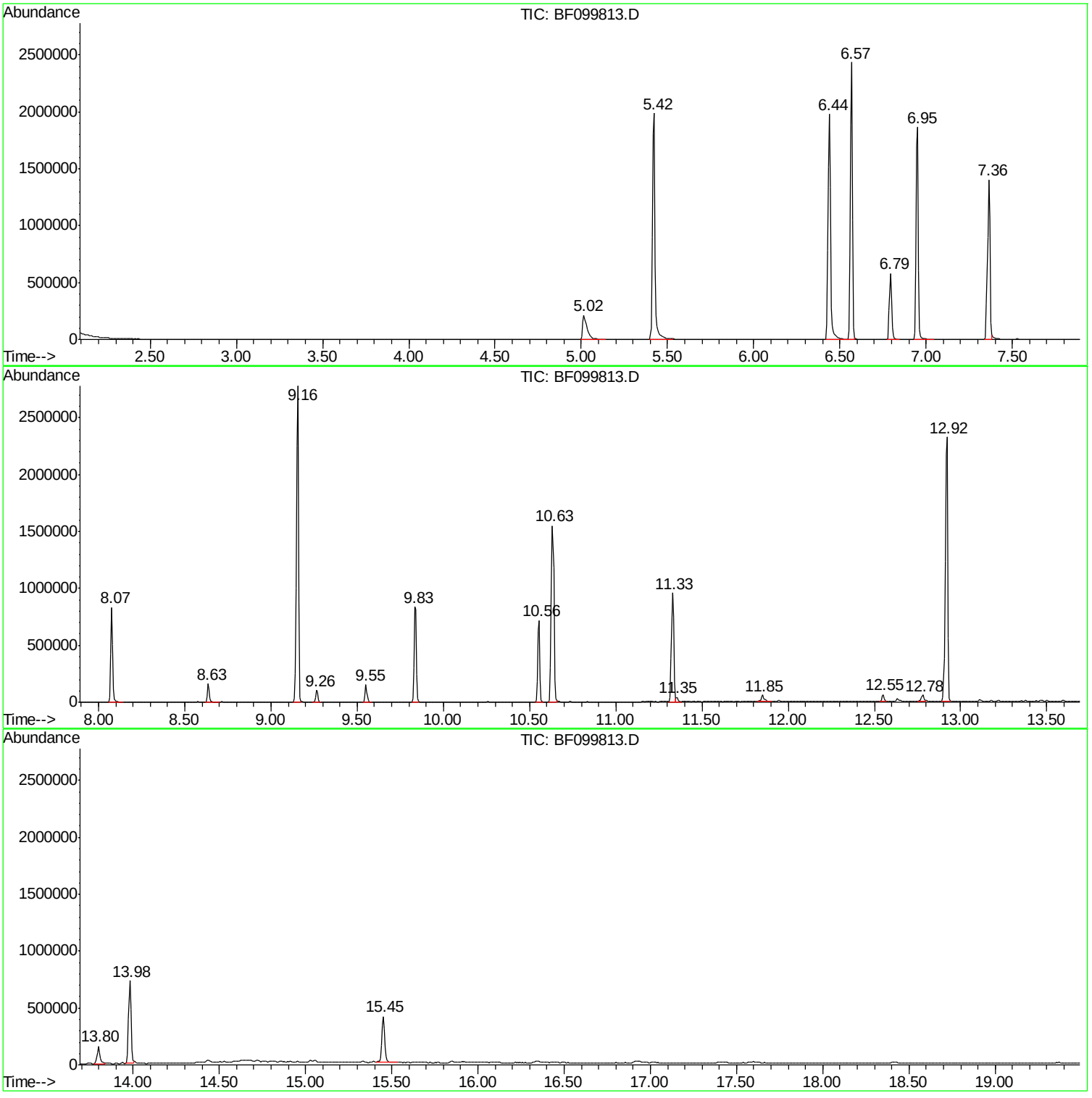
Instrument : BNA_F
ClientSampleId : 72-11989-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099813.D
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Operator : SJ/JU
Sample : I6064-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11989-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

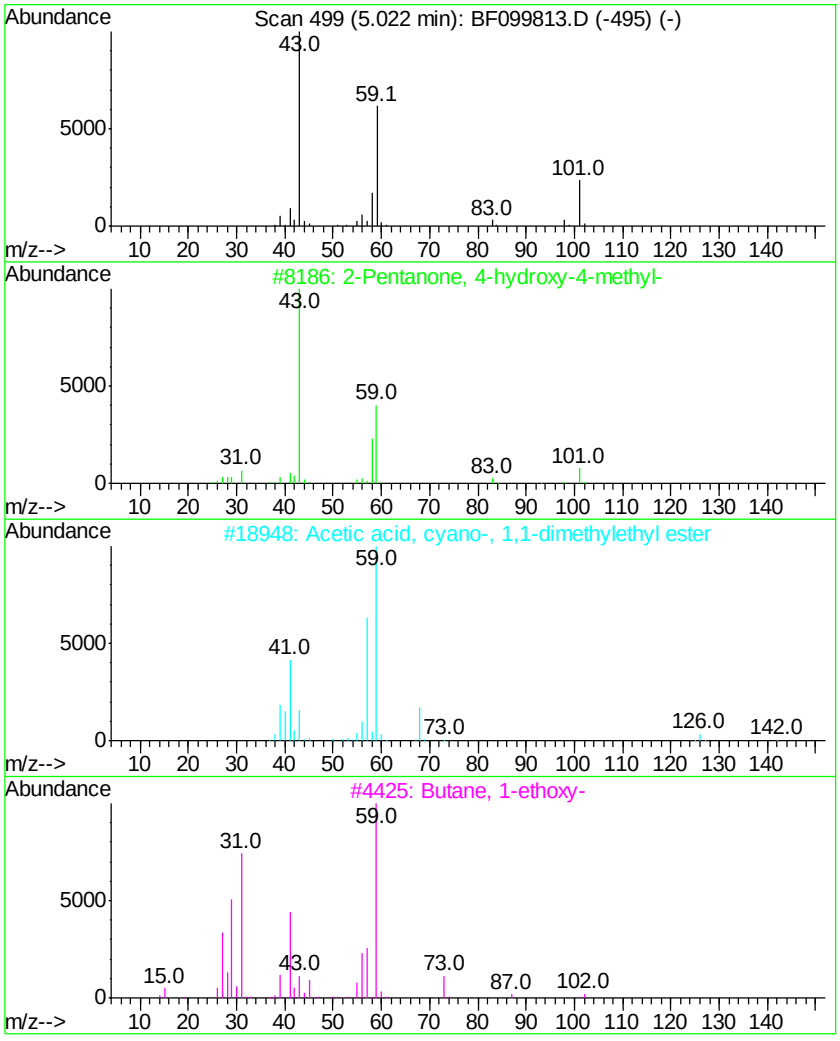
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

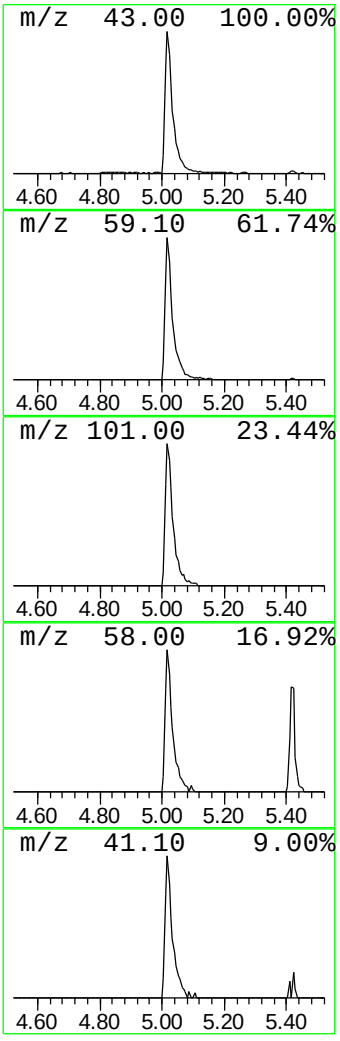
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	15.02 ng	361603	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Data File : BF099813.D
Acq On : 25 Oct 2017 15:10
Operator : SJ/JU
Sample : I6064-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11989-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

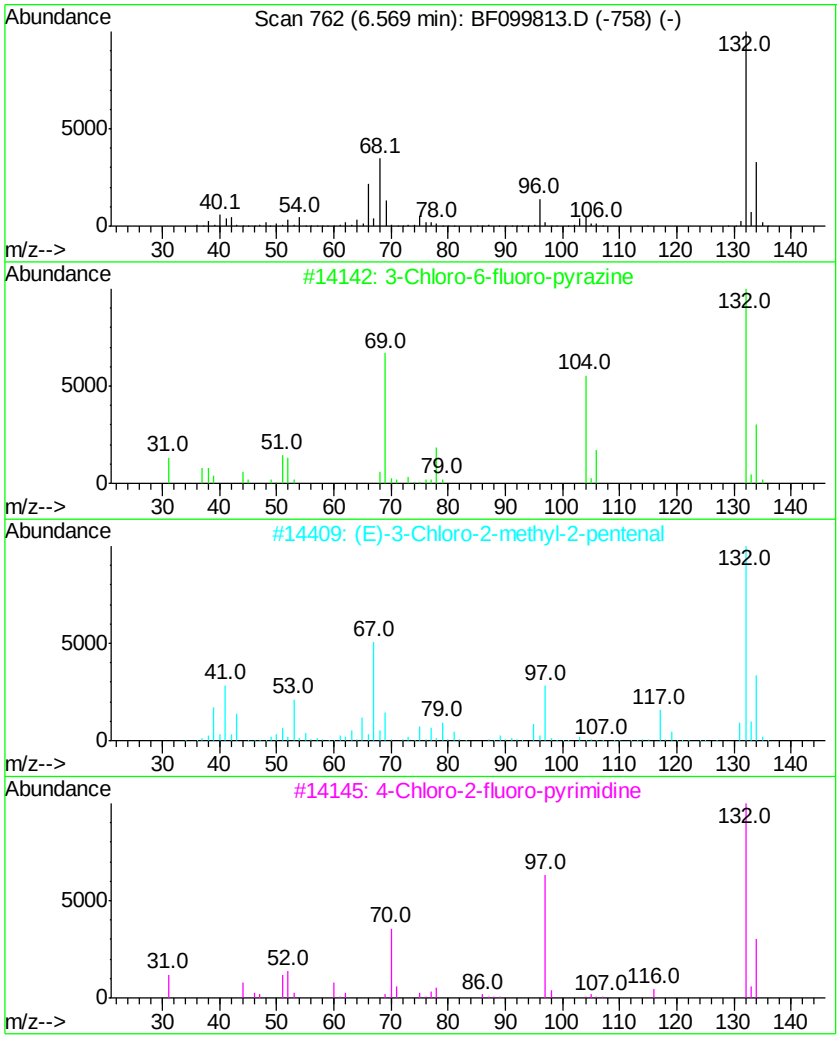
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

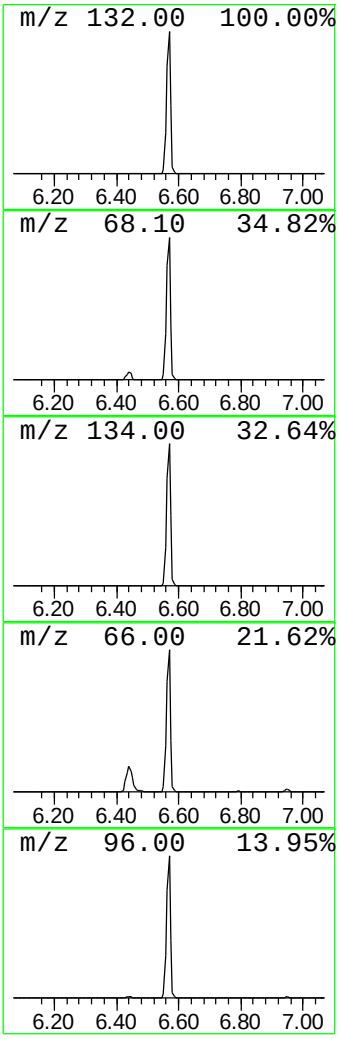
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	92.17 ng	2218980	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Data File : BF099813.D
Acq On : 25 Oct 2017 15:10
Operator : SJ/JU
Sample : I6064-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11989-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

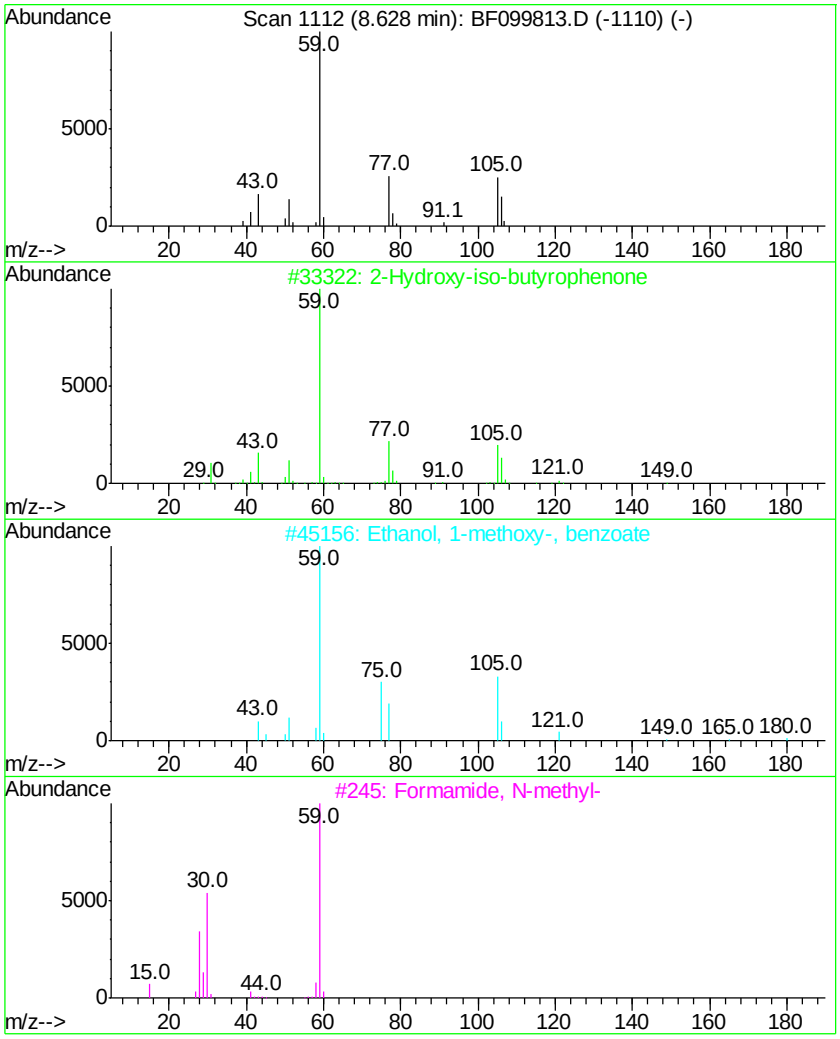
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

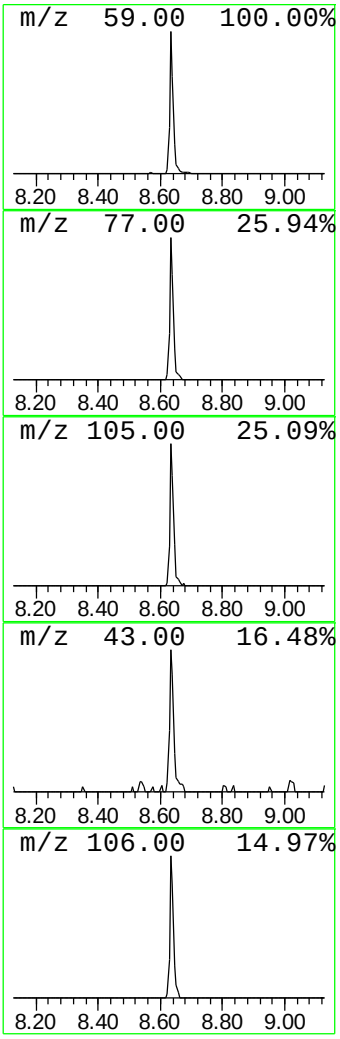
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	3.86 ng	134927	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
4	Guanidine	59	CH5N3	000113-00-8	7
5	Acetamide	59	C2H5NO	000060-35-5	5





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099813.D
Acq On : 25 Oct 2017 15:10
Operator : SJ/JU
Sample : I6064-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 72-11989-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

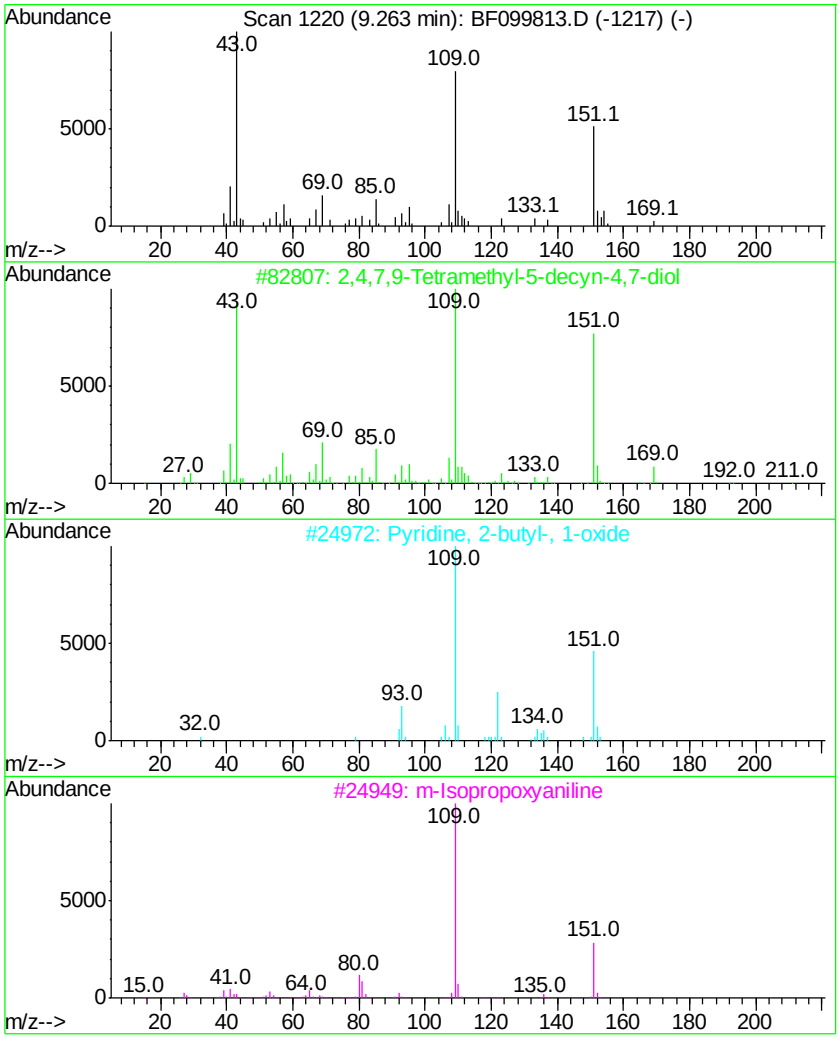
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

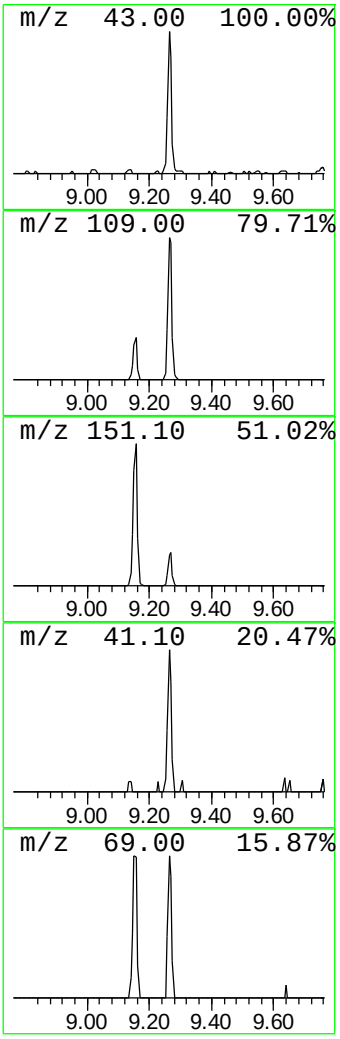
****

Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.26	2.30 ng	91764	Acenaphthene-d10	9.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
4	(4-Fluorophenyl) methanol, ethyl...	154	C9H11FO	1000374-63-4	47
5	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	43





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Sample : I6064-04
Misc :
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Instrument : BNA_F
ClientSampleId : 72-11989-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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TIC Library : C:\DATABASE\NIST11.L
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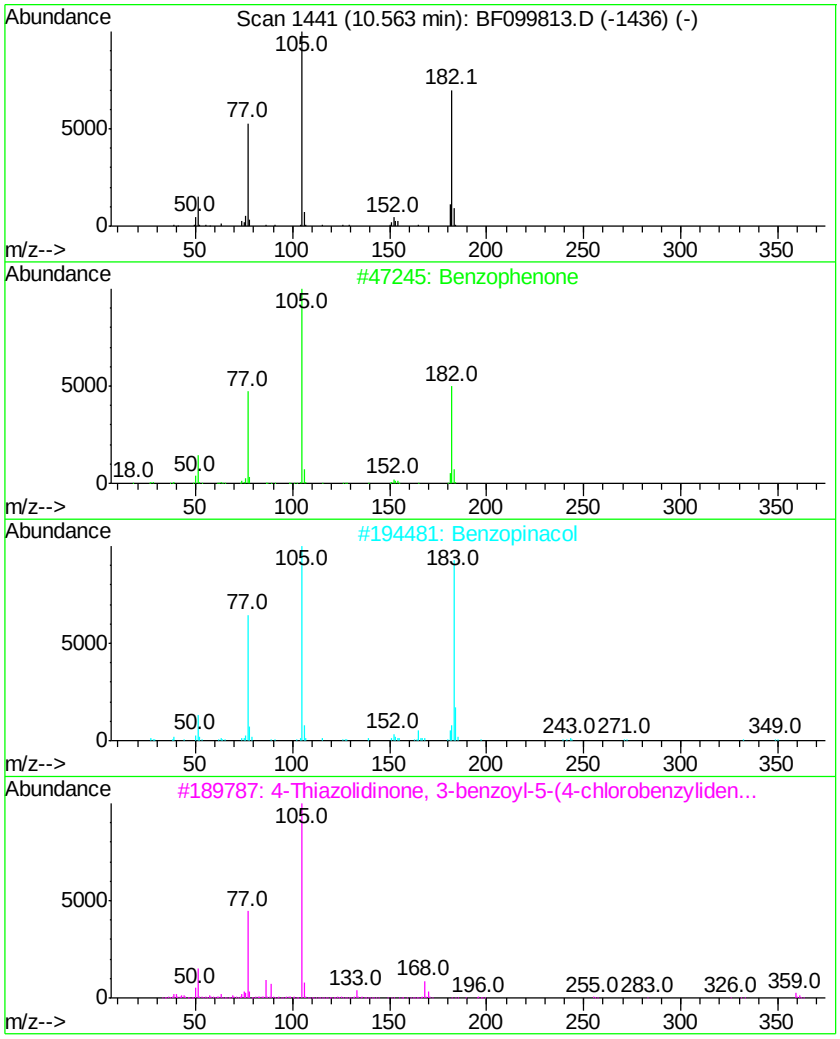
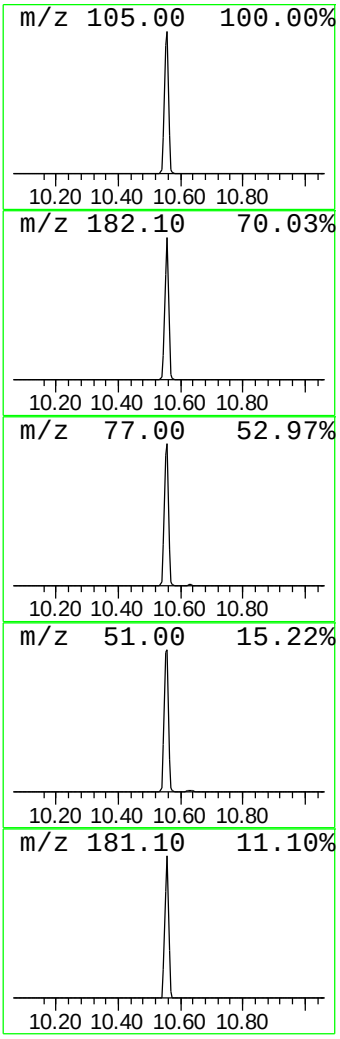
****

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	15.53 ng	620556	Acenaphthene-d10	9.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzopinacol	366	C26H22O2	000464-72-2	50
3	4-Thiazolidinone, 3-benzoyl-5-(4...	359	C17H10ClNO2S2	349498-40-4	43
4	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	43
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	43





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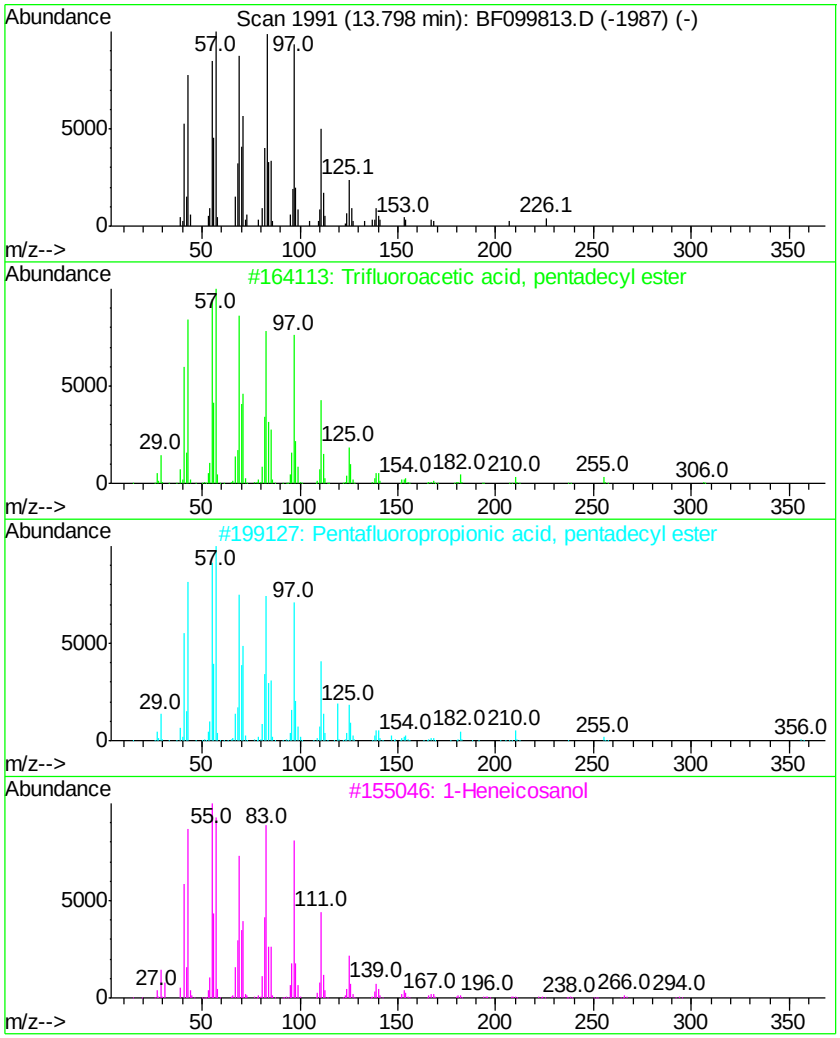
TIC Integration Parameters: LSCINT.P

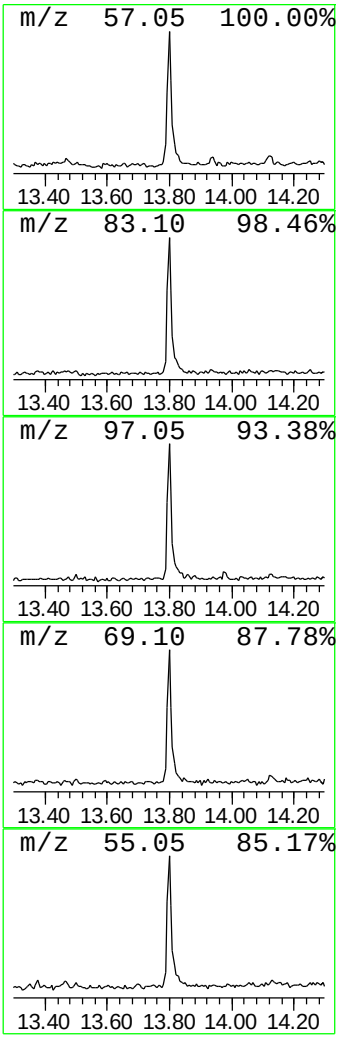
****

Peak Number 7 Trifluoroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	5.16 ng	166745	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	95





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
2-Pentanone, 4-hy...	5.02	15.0	ng	361603	1	6.79	481483	20.0
unknown6.57	6.57	92.2	ng	2218980	1	6.79	481483	20.0
2-Hydroxy-iso-but...	8.63	3.9	ng	134927	2	8.07	699681	20.0
2,4,7,9-Tetrameth...	9.26	2.3	ng	91764	3	9.83	799383	20.0
Benzophenone	10.56	15.5	ng	620556	3	9.83	799383	20.0
Trifluoroacetic a...	13.80	5.2	ng	166745	5	13.98	646048	20.0