LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102517\
Data File : BF099846.D
Acq On : 26 Oct 2017 7:31
Operator : SJ/JU
Sample : I6057-05
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 101917-SIDI-F-D-B

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	4.998	492	495	514	rBV	58321	84140	3.86%	0.602%
2	5.410	562	565	589	rBV	496877	604930	27.78%	4.330%
3	6.434	736	739	758	rBV	359156	448530	20.60%	3.210%
4	6.563	758	761	772	rVB	1269663	1086626	49.90%	7.777%
5	6.792	797	800	811	rBV	470803	394365	18.11%	2.823%
6	6.945	823	826	844	rBV	1586667	1488241	68.34%	10.652%
7	7.363	893	897	916	rBV	1248296	1087434	49.94%	7.783%
8	8.075	1015	1018	1037	rBV	656766	545534	25.05%	3.905%
9	8.639	1111	1114	1121	rBV	69657	65187	2.99%	0.467%
10	9.157	1197	1202	1205	rBV	2409096	2177666	100.00%	15.586%
11	9.557	1267	1270	1278	rBB	39413	37091	1.70%	0.265%
12	9.833	1312	1317	1329	rVB	669832	624521	28.68%	4.470%
13	10.510	1429	1432	1436	rBV	73288	56736	2.61%	0.406%
14	10.551	1436	1439	1443	rBV	380303	278564	12.79%	1.994%
15	10.633	1449	1453	1465	rBV	845262	776215	35.64%	5.556%
16	10.886	1493	1496	1500	rBV	46879	35118	1.61%	0.251%
17	10.933	1500	1504	1507	rBV	172437	182915	8.40%	1.309%
18	10.969	1507	1510	1511	rBV	28711	26767	1.23%	0.192%
19	11.327	1568	1571	1579	rBV	641657	593957	27.27%	4.251%
20	12.363	1743	1747	1756	rBV	63329	72214	3.32%	0.517%
21	12.721	1805	1808	1814	rVB	44446	39012	1.79%	0.279%
22	12.915	1837	1841	1845	rBV	2047418	2090250	95.99%	14.960%
23	13.427	1925	1928	1933	rVB2	34014	31085	1.43%	0.222%
24	13.980	2019	2022	2030	rBV	635348	574638	26.39%	4.113%
25	15.451	2263	2272	2279	rBV	374562	508870	23.37%	3.642%
26	15.851	2334	2340	2345	rBV2	19061	28828	1.32%	0.206%
27	16.345	2418	2424	2430	rBV3	16622	32484	1.49%	0.232%

Sum of corrected areas: 13971918

LSC Report - Integrated Chromatogram

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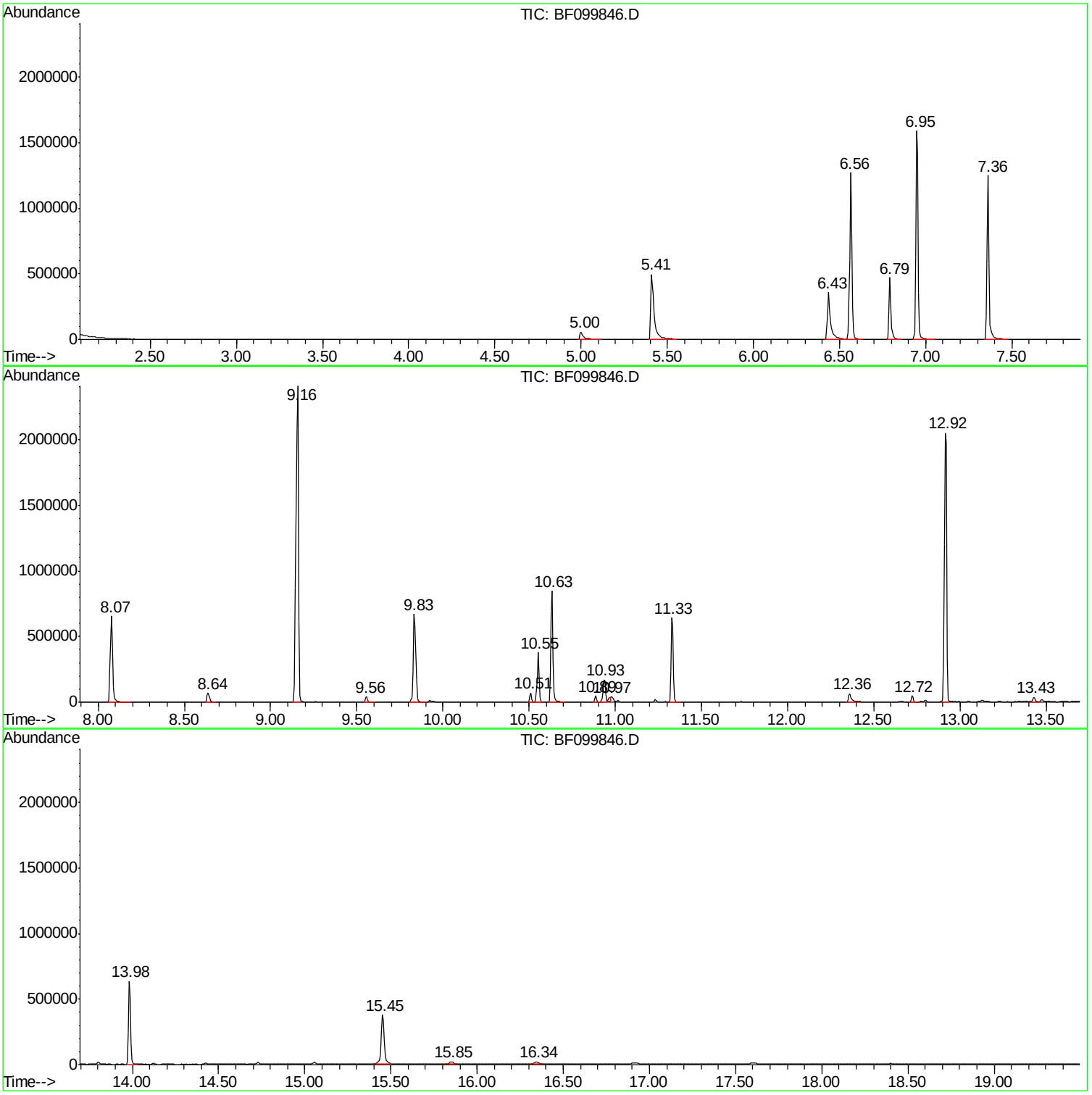
Instrument :
BNA_F
ClientSampleId :
101917-SIDI-F-D-B

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



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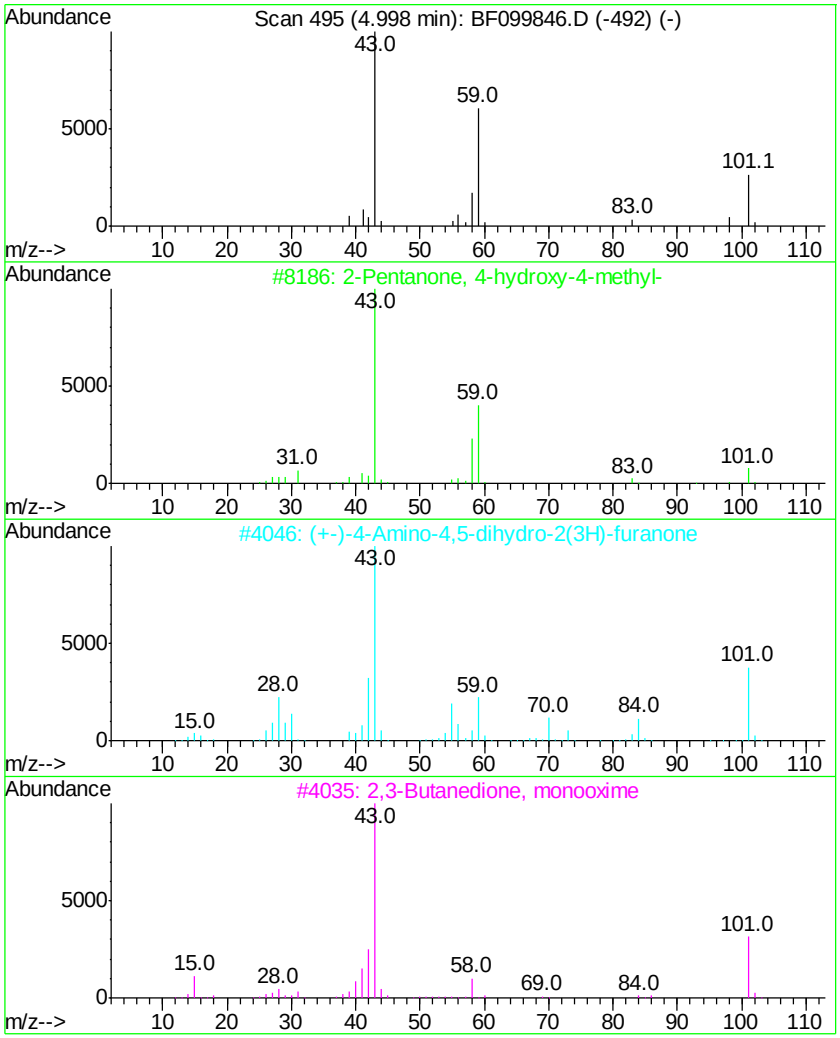
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

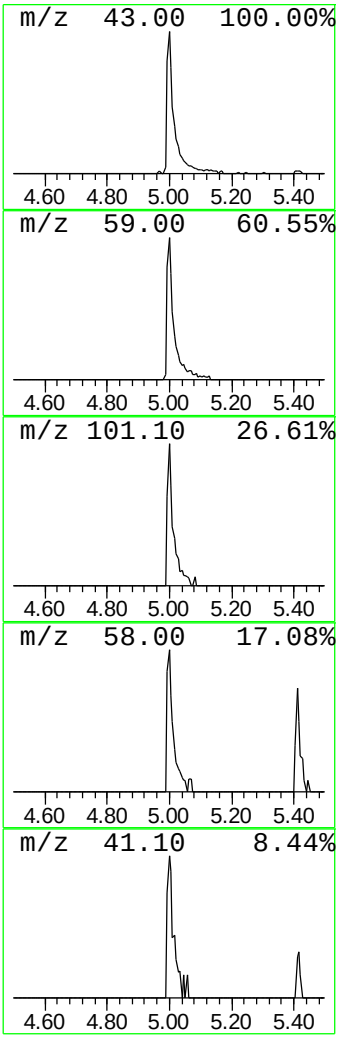
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.27 ng	84140	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	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : I6057-05
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 101917-SIDI-F-D-B

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

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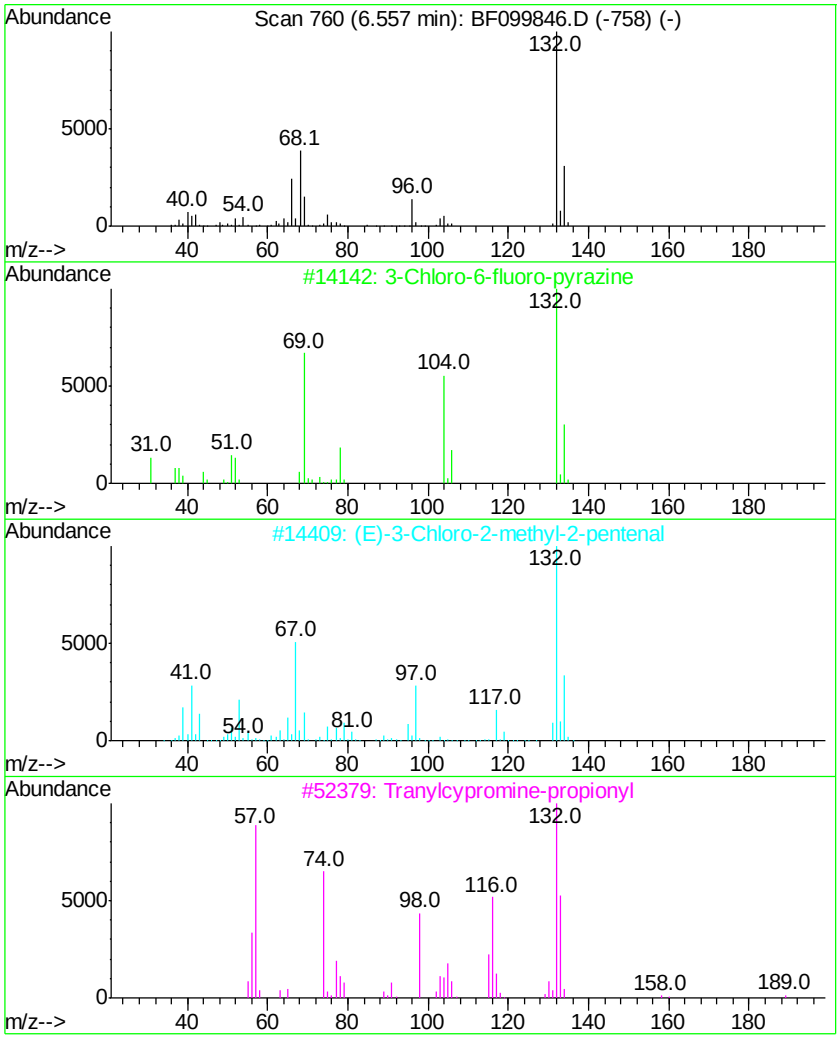
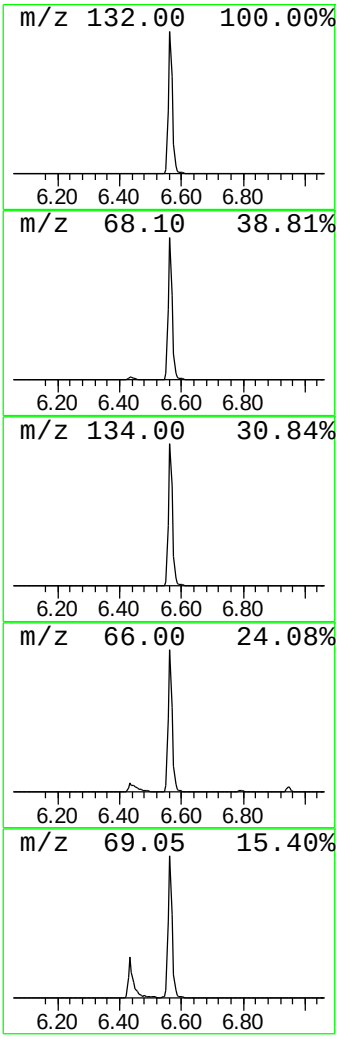
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	55.11 ng	1086630	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Data File : BF099846.D
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Operator : SJ/JU
Sample : I6057-05
Misc :
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Instrument : BNA_F
ClientSampleId : 101917-SIDI-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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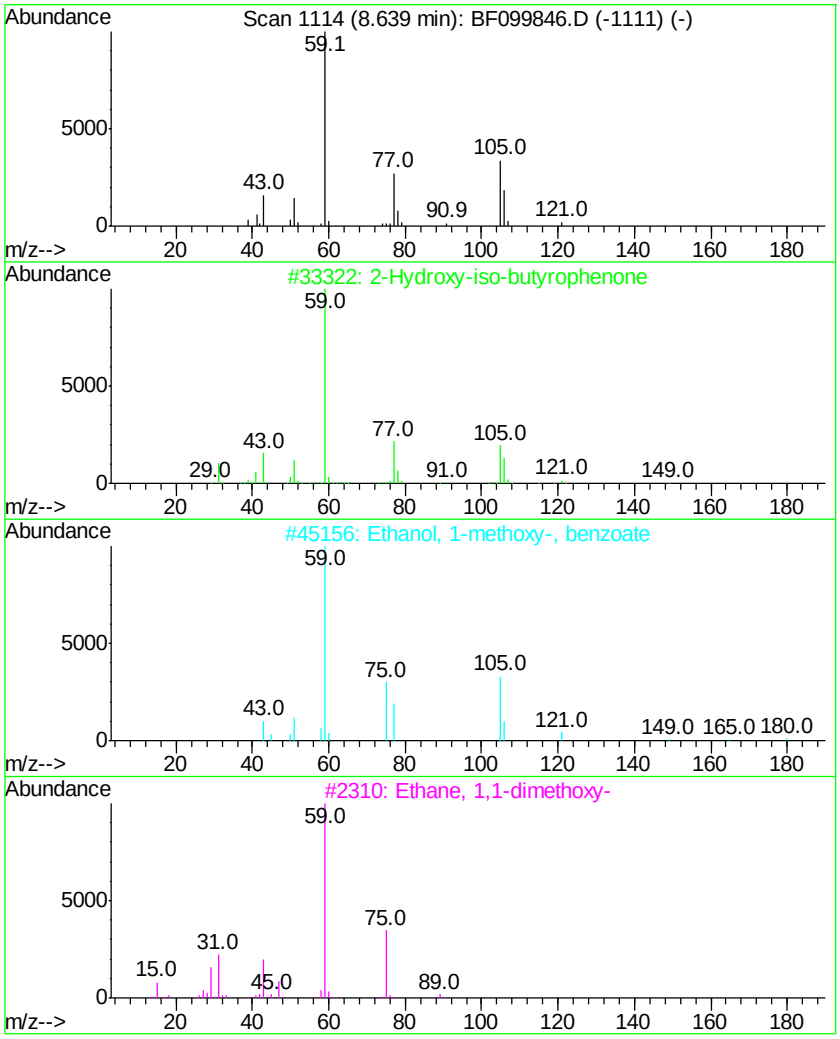
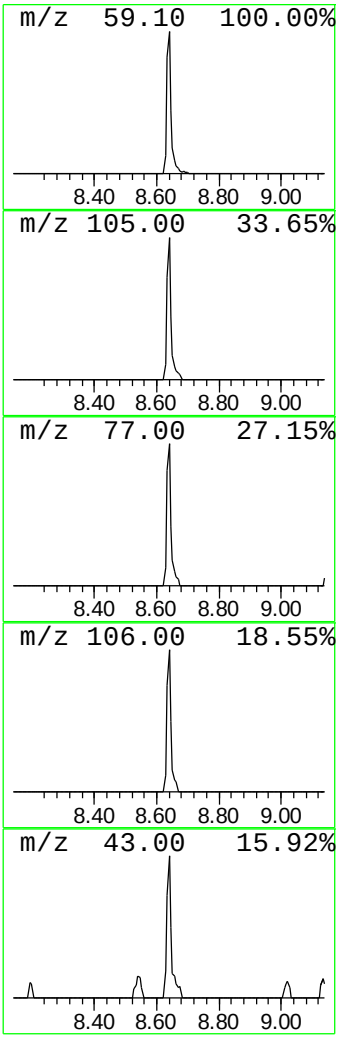
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.64	2.39 ng	65187	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	78
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	50
3	Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	9
4	Guanidine	59	CH5N3	000113-00-8	7
5	Acetamide	59	C2H5NO	000060-35-5	5





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : 101917-SIDI-F-D-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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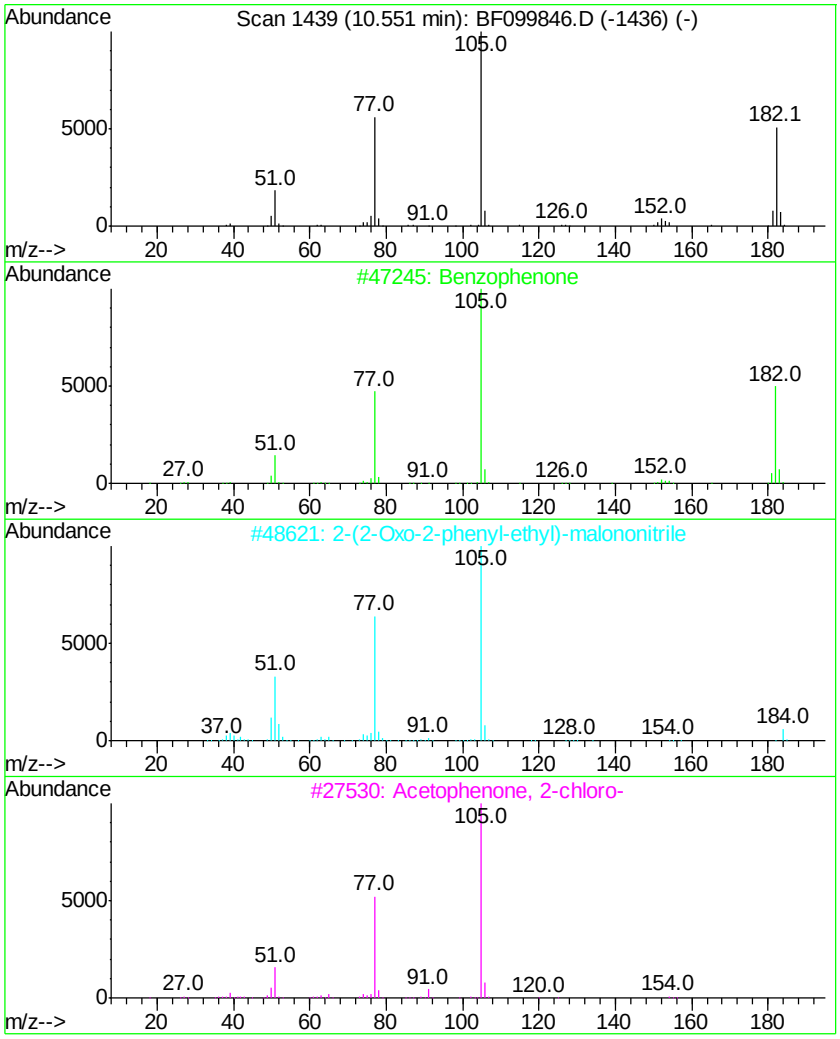
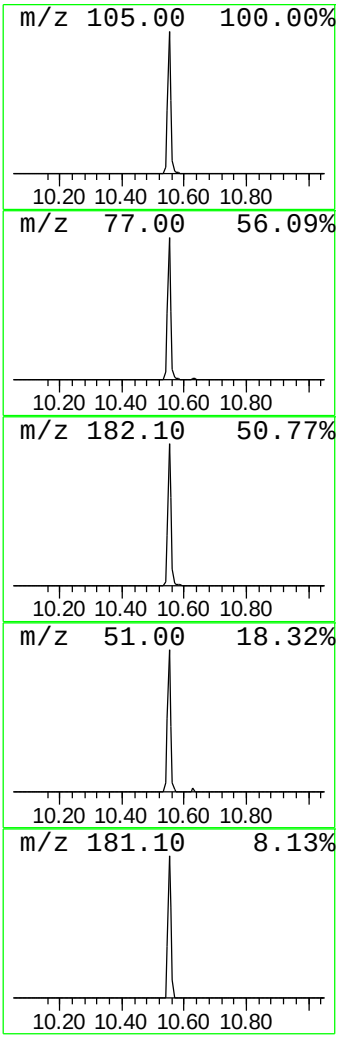
Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	8.92 ng	278564	Acenaphthene-d10	9.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	46
4	Benzoyl bromide	184	C7H5BrO	000618-32-6	43
5	Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	43





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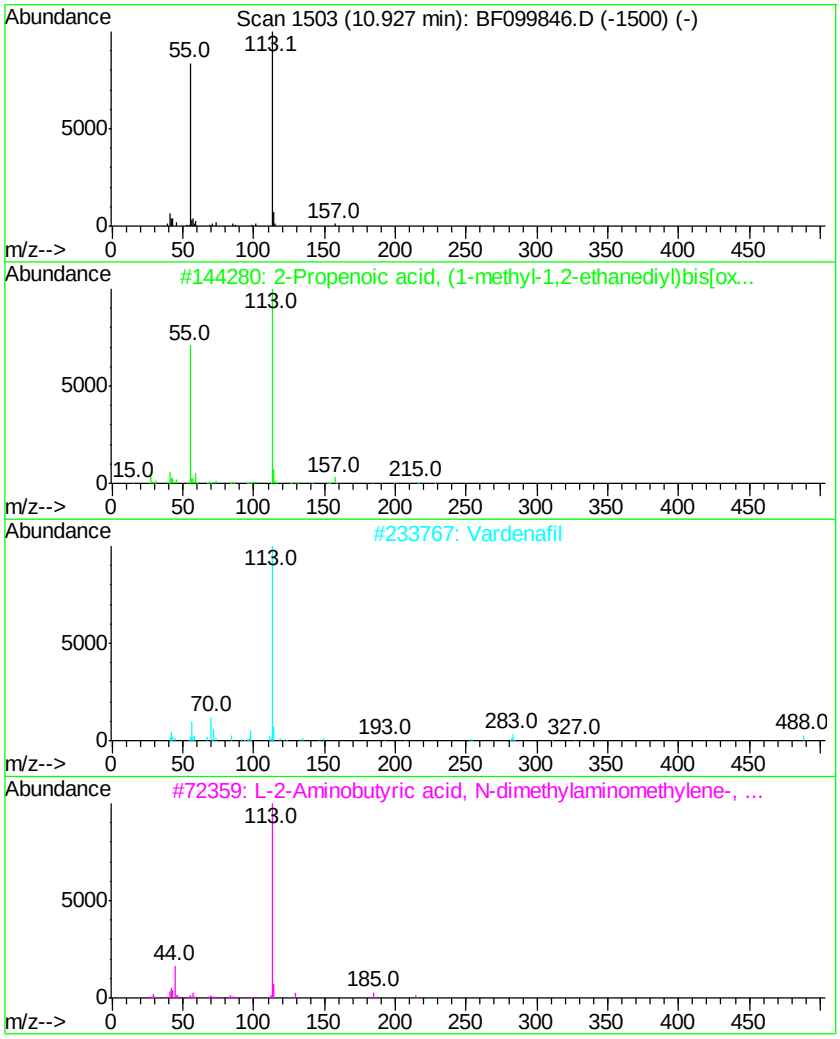
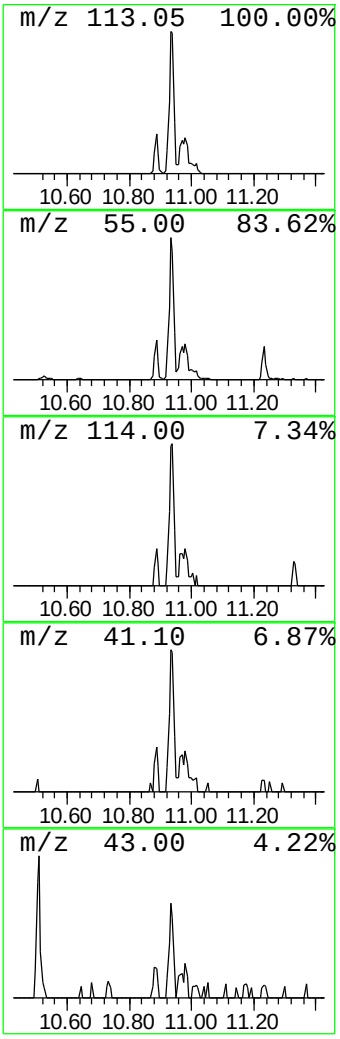
****

Peak Number 6 2-Propenoic acid, (1-methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	6.16 ng	182915	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, (1-methyl-1,2-...	300	C15H24O6	042978-66-5	78
2	Vardenafil	488	C23H32N6O4S	224785-90-4	36
3	L-2-Aminobutyric acid, N-dimethy...	214	C11H22N2O2	1000375-52-5	36
4	Caprolactam	113	C6H11NO	000105-60-2	9
5	Propanedioic acid, 2-propenyl-, ...	172	C8H12O4	040637-56-7	9





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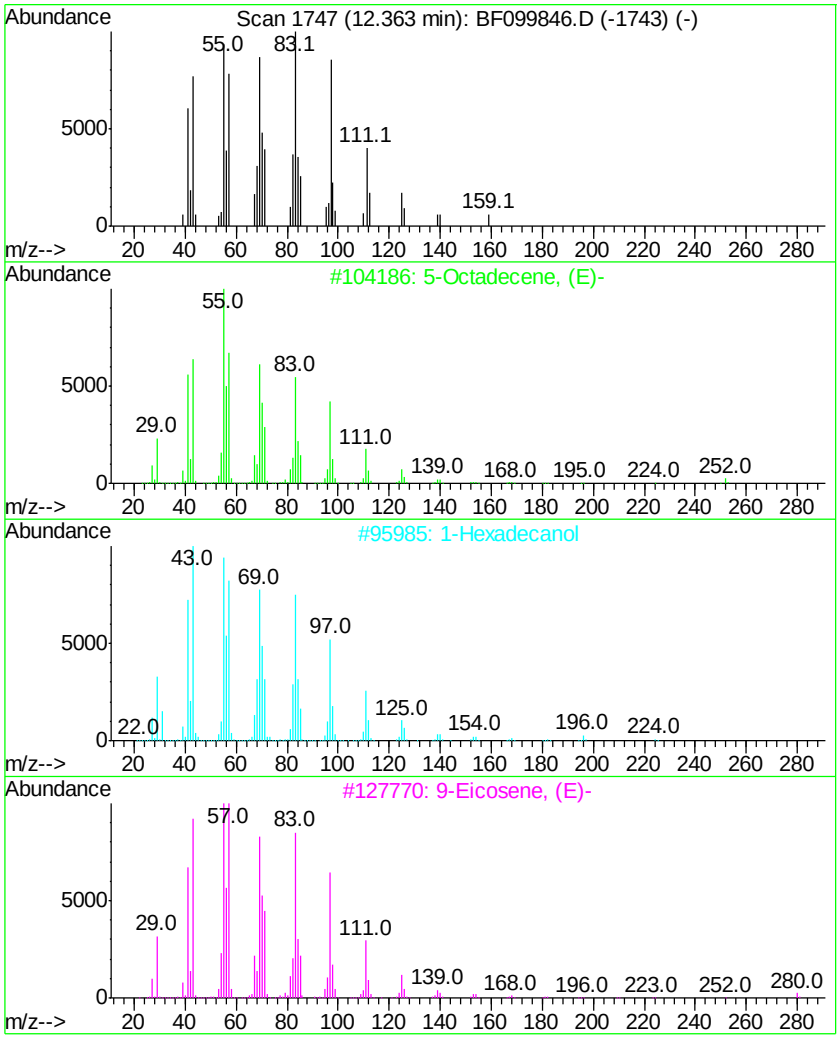
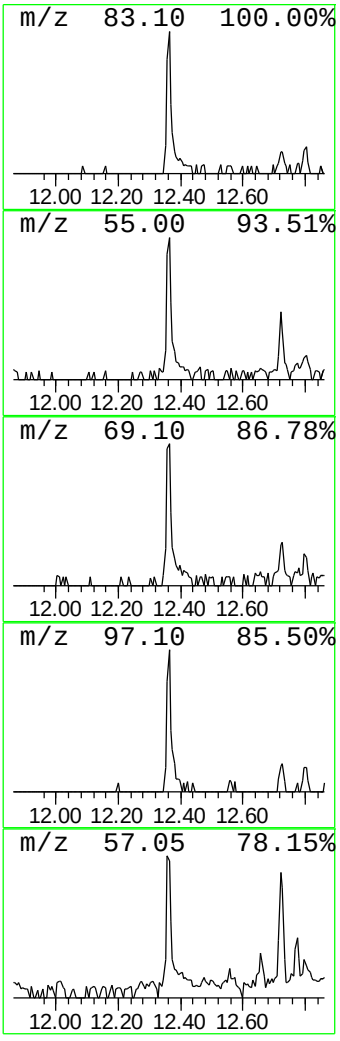
Peak Number 7 5-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	2.43 ng	72214	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	11-Tricosene	322	C23H46	052078-56-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Tentatively Identified Compound (LSC) summary

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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...	5.00	4.3	ng	84140	1	6.79	394365	20.0
unknown6.56	6.56	55.1	ng	1086630	1	6.79	394365	20.0
2-Hydroxy-iso-but...	8.64	2.4	ng	65187	2	8.07	545534	20.0
Benzophenone	10.55	8.9	ng	278564	3	9.83	624521	20.0
2-Propenoic acid,...	10.93	6.2	ng	182915	4	11.33	593957	20.0
5-Octadecene, (E)-	12.36	2.4	ng	72214	4	11.33	593957	20.0