LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100932.D
Acq On : 28 Nov 2017 14:28
Operator : SJ/JU
Sample : I6578-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BBR-2-E(0-1)

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-BF110817.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	5.081	505	509	518	rBV	163815	237035	11.07%	1.463%
2	5.481	571	577	580	rBV	1635876	1631718	76.20%	10.073%
3	6.492	743	749	752	rBV	1590266	1749730	81.71%	10.802%
4	6.633	767	773	776	rBV	1717003	1788094	83.50%	11.039%
5	6.857	808	811	815	rVB	499199	383732	17.92%	2.369%
6	7.016	834	838	841	rBV	1625728	1368289	63.90%	8.447%
7	7.422	902	907	910	rBV	1009093	1088965	50.85%	6.723%
8	8.139	1025	1029	1032	rBV	620723	482471	22.53%	2.978%
9	8.692	1120	1123	1126	rBV	117645	87946	4.11%	0.543%
10	9.216	1207	1212	1215	rBV	2375576	2141422	100.00%	13.220%
11	9.604	1275	1278	1288	rBV	105844	78446	3.66%	0.484%
12	9.892	1323	1327	1339	rVB	584896	509268	23.78%	3.144%
13	10.610	1445	1449	1452	rBV	468957	411867	19.23%	2.543%
14	10.686	1457	1462	1465	rBV	1126235	1038357	48.49%	6.410%
15	11.380	1577	1580	1583	rBV	523498	417061	19.48%	2.575%
16	11.898	1665	1668	1676	rVB2	85807	81372	3.80%	0.502%
17	12.592	1783	1786	1789	rBV	68703	59324	2.77%	0.366%
18	12.686	1798	1802	1805	rBV2	58641	62795	2.93%	0.388%
19	12.821	1820	1825	1833	rBV	74163	89317	4.17%	0.551%
20	12.968	1842	1850	1853	rBV	1527849	1533611	71.62%	9.468%
21	13.404	1922	1924	1926	rBV2	29909	26355	1.23%	0.163%
22	13.857	1998	2001	2006	rBV3	43357	51800	2.42%	0.320%
23	14.021	2025	2029	2032	rBV	448987	429902	20.08%	2.654%
24	15.498	2276	2280	2287	rVB	351486	449630	21.00%	2.776%

Sum of corrected areas: 16198507

LSC Report - Integrated Chromatogram

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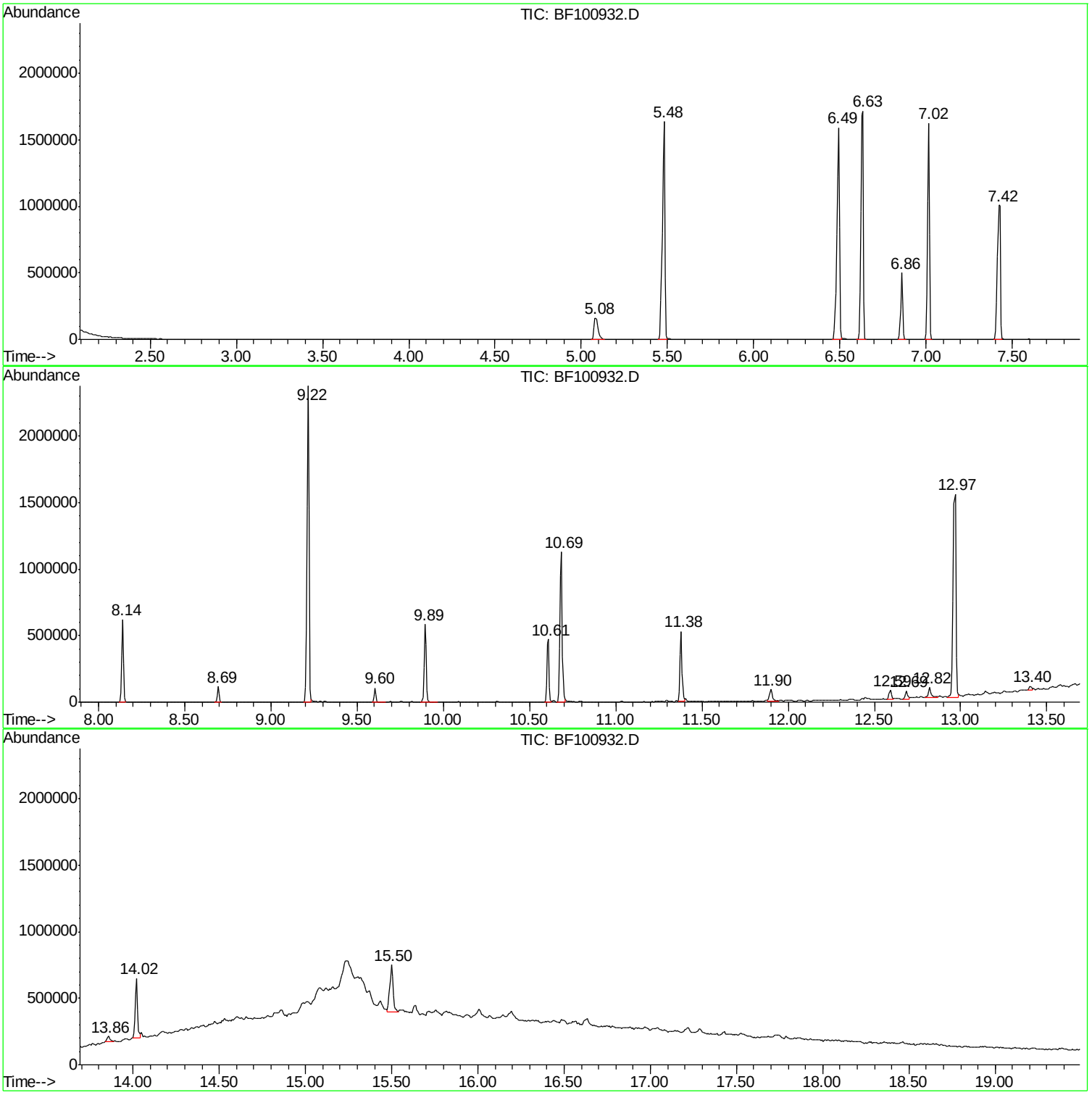
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BBR-2-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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\BF112817\
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Operator : SJ/JU
Sample : I6578-04
Misc :
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Instrument : BNA_F
ClientSampleId : BBR-2-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

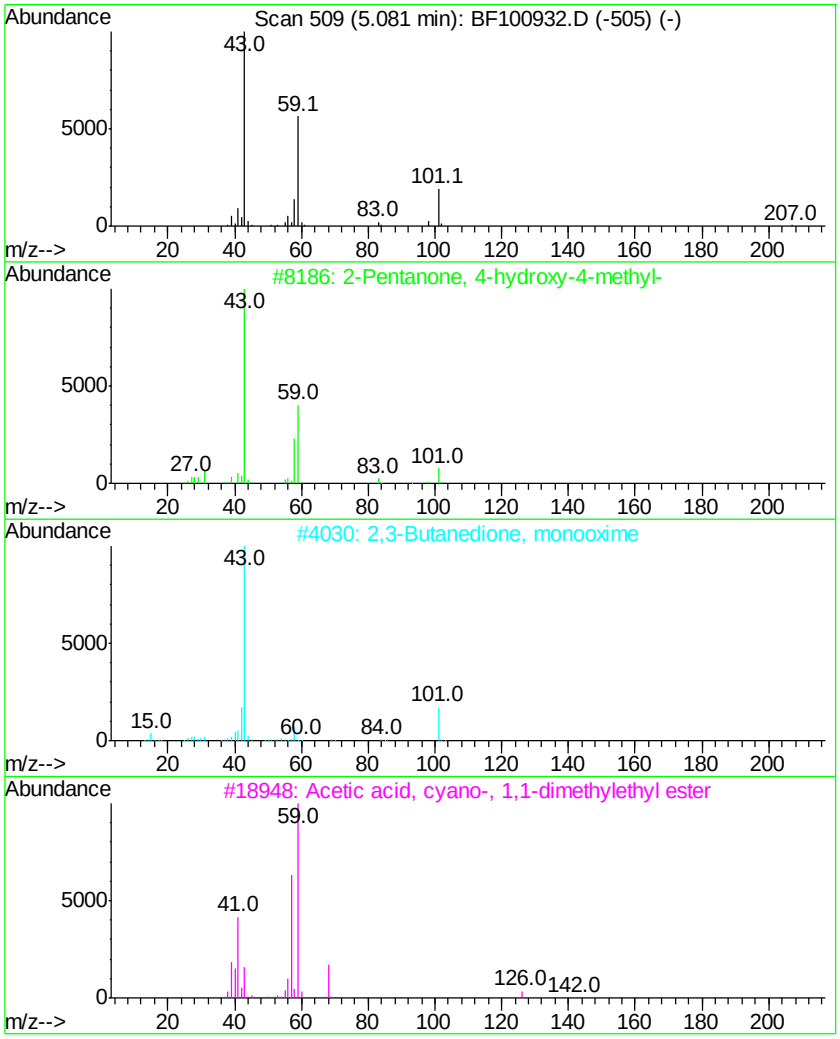
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

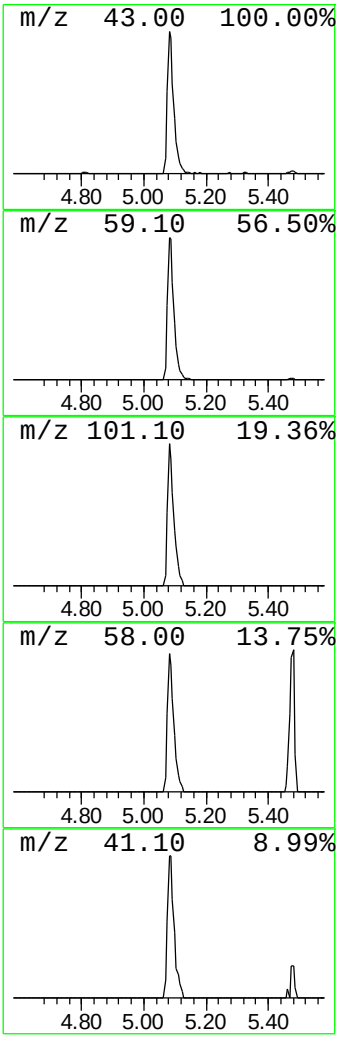
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	12.35 ng	237035	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Operator : SJ/JU
Sample : I6578-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BBR-2-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

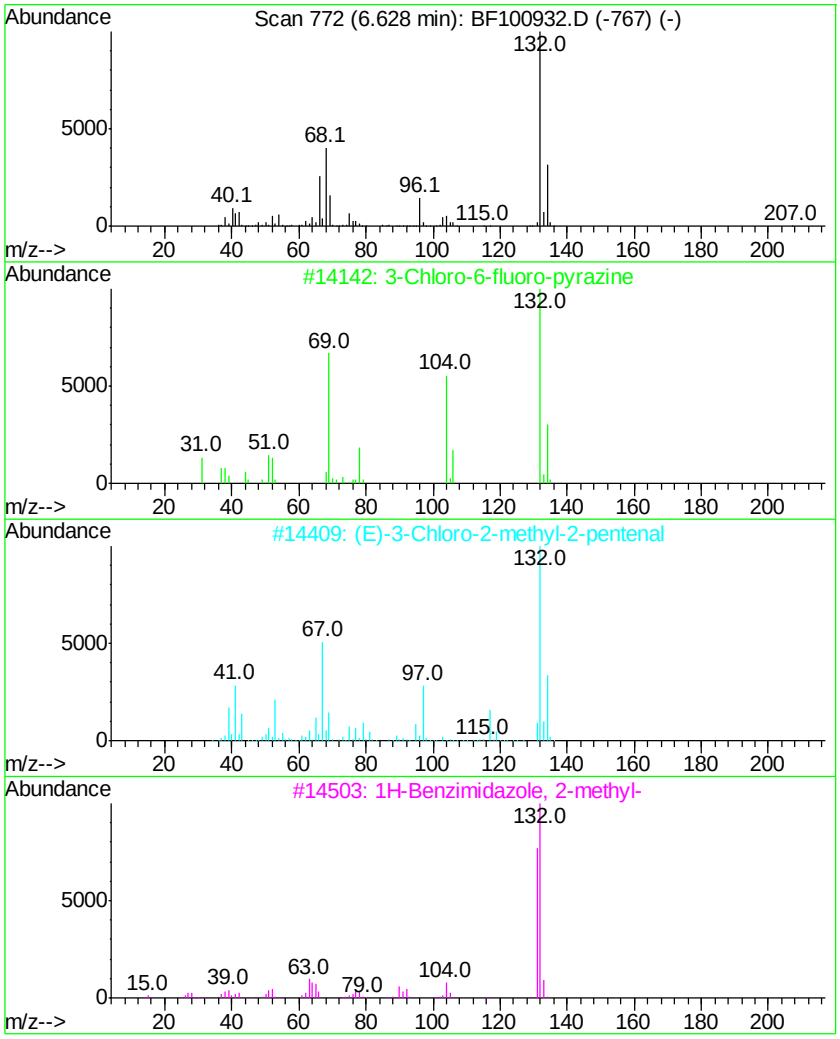
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

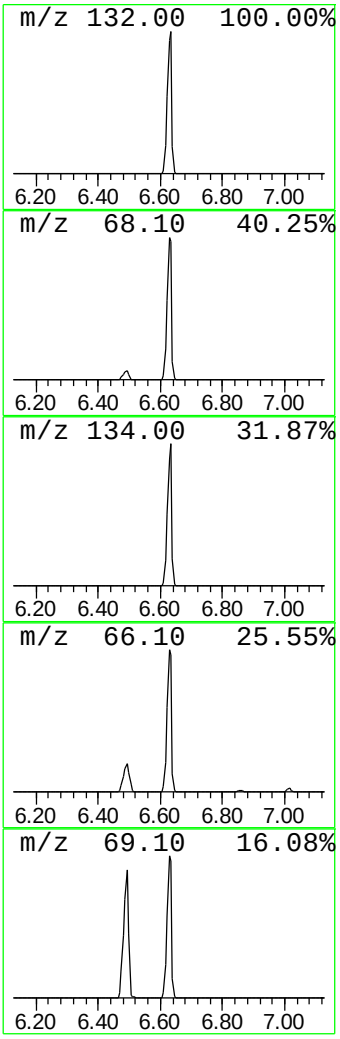
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	93.19 ng	1788090	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Operator : SJ/JU
Sample : I6578-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BBR-2-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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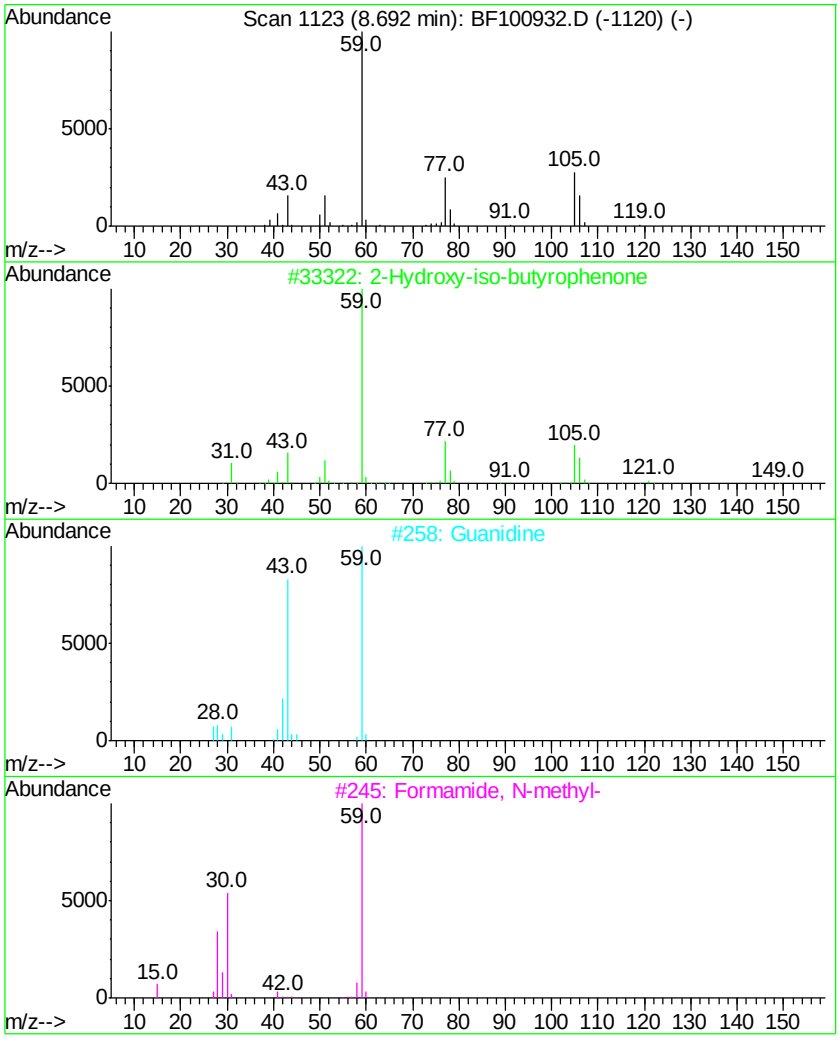
TIC Integration Parameters: LSCINT.P

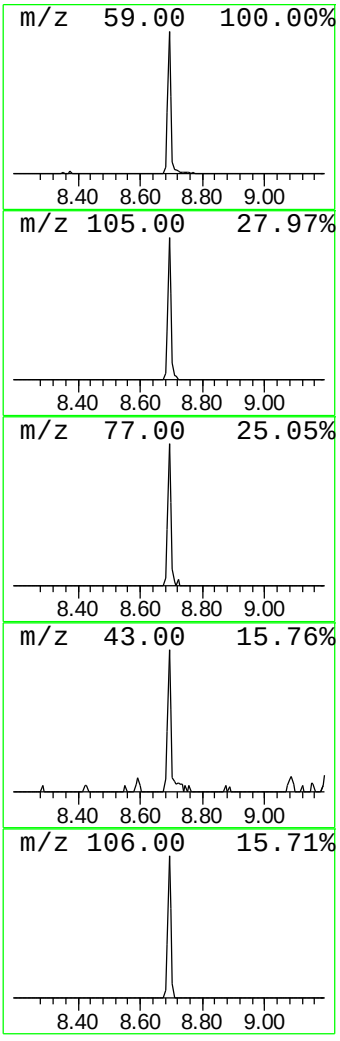
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	3.65 ng	87946	Naphthalene-d8	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Guanidine	59	CH5N3	000113-00-8	7
3	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
4	Acetamide	59	C2H5NO	000060-35-5	5
5	Propylamine	59	C3H9N	000107-10-8	4





Library Search Compound Report

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Operator : SJ/JU
Sample : I6578-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BBR-2-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
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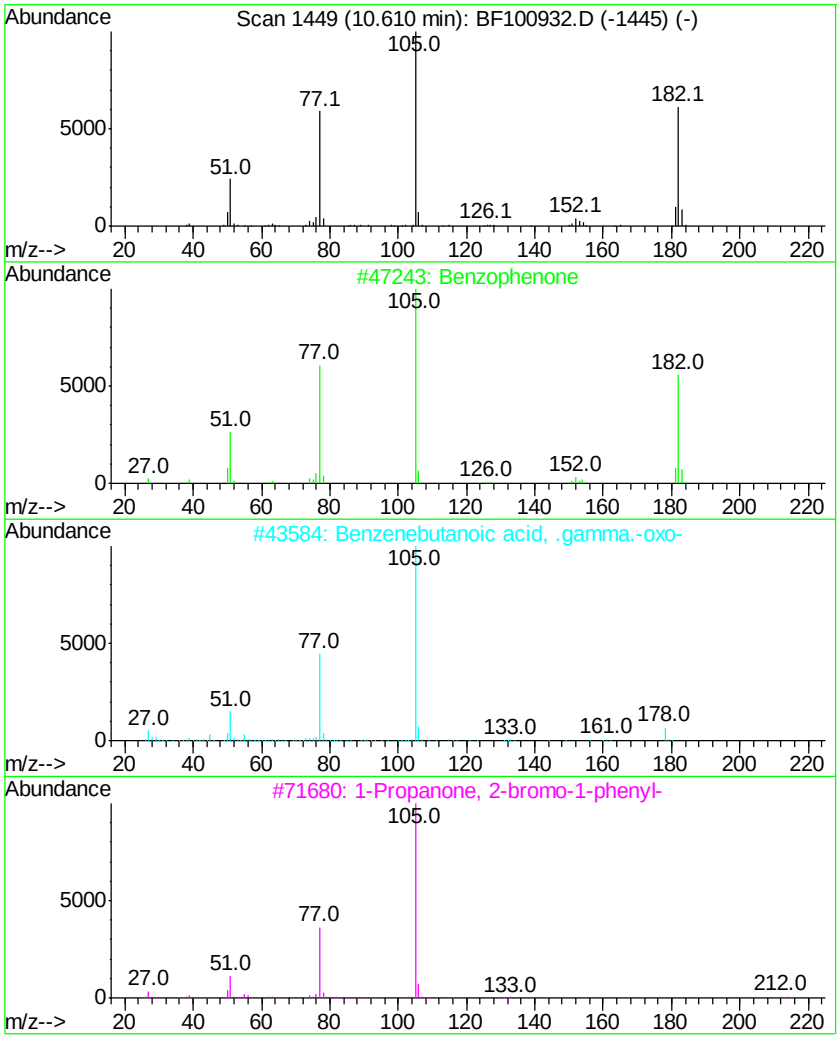
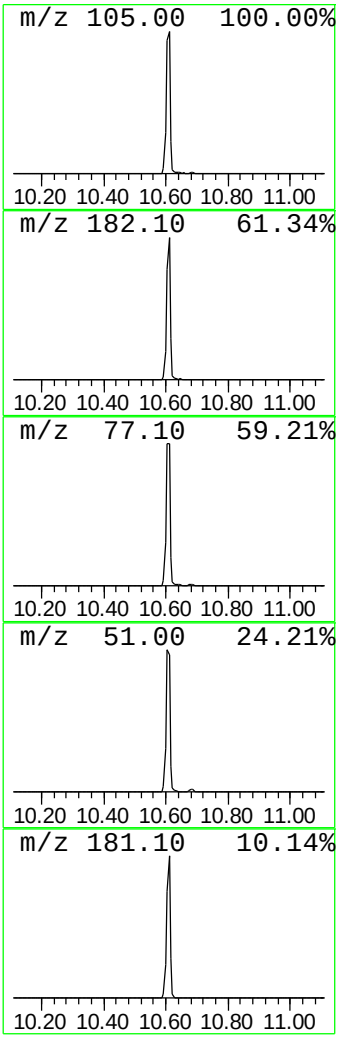
Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.61	16.17 ng	411867	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47





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Sample : I6578-04
Misc :
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Instrument : BNA_F
ClientSampleId : BBR-2-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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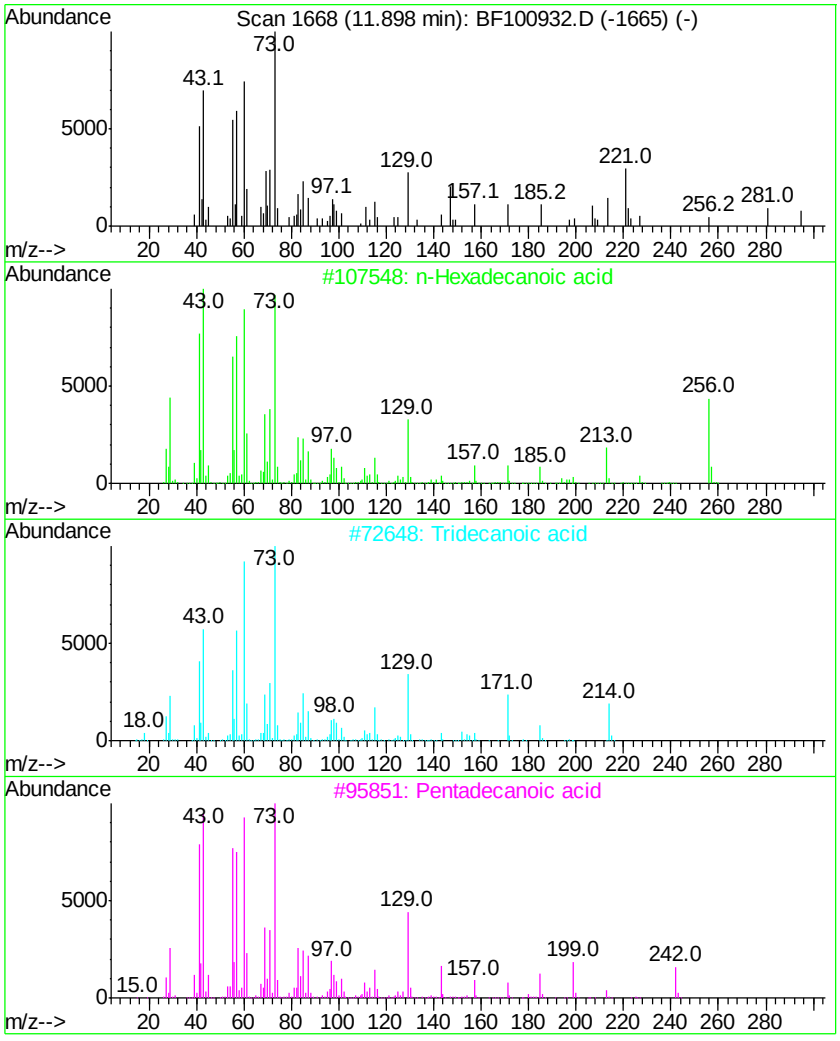
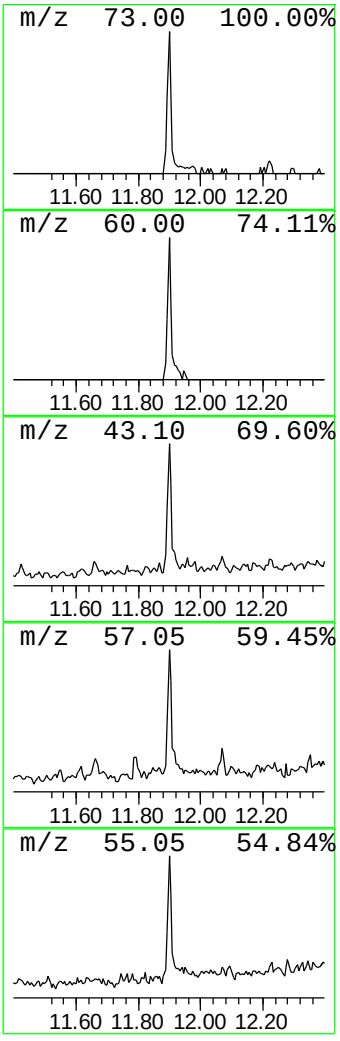
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.90 ng	81372	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	62
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Instrument : BNA_F
ClientSampleId : BBR-2-E(0-1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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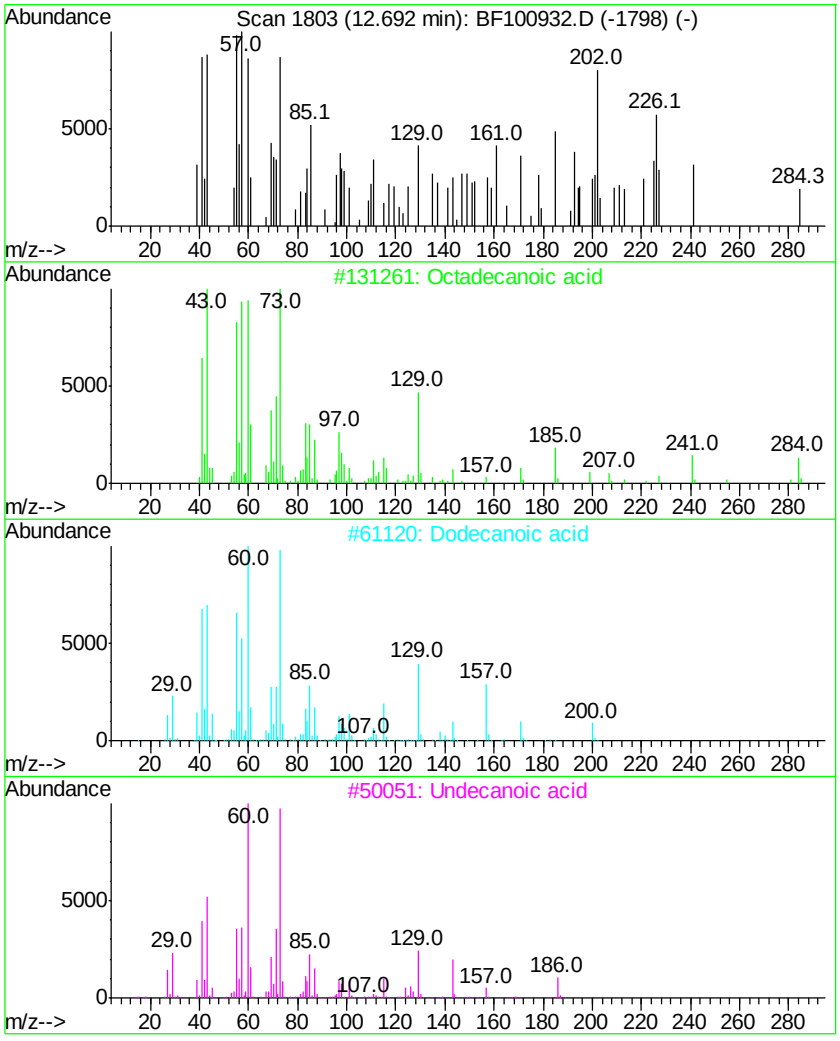
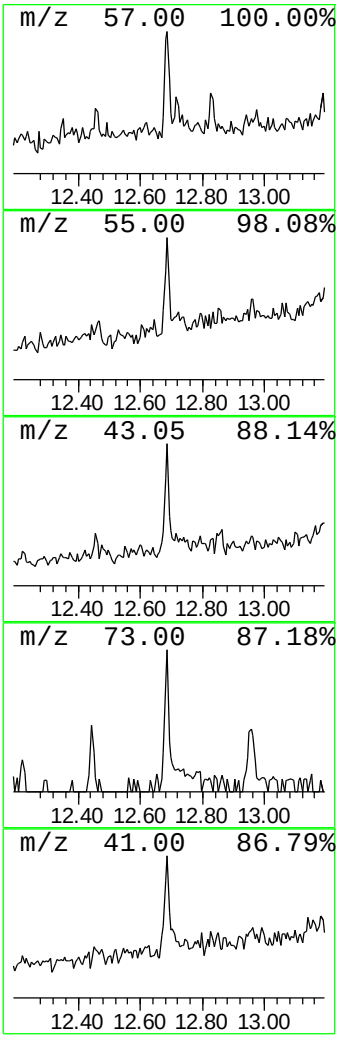
****

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	3.01 ng	62795	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Dodecanoic acid	200	C12H24O2	000143-07-7	70
3	Undecanoic acid	186	C11H22O2	000112-37-8	55
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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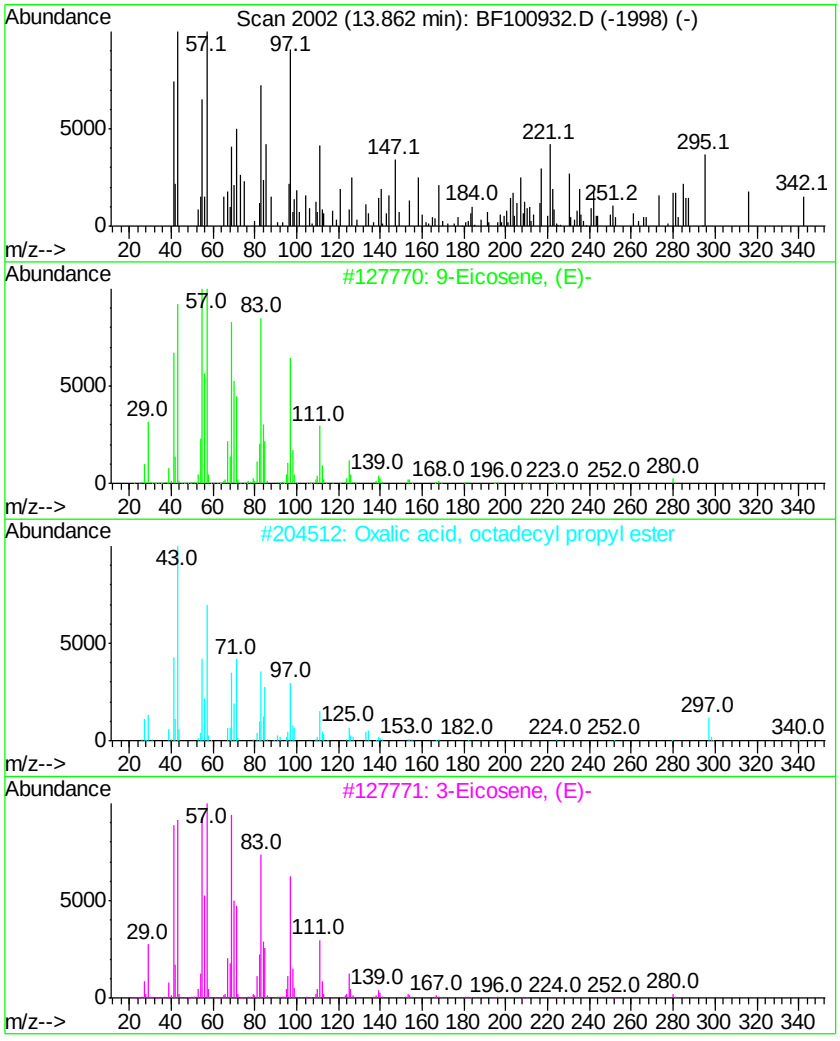
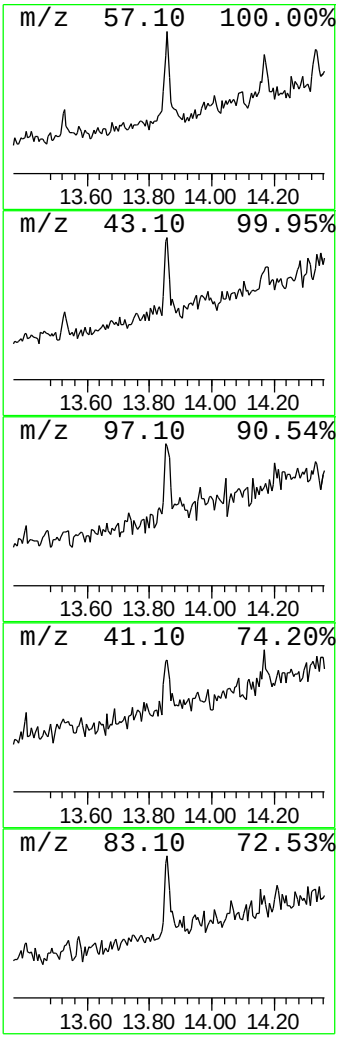
Peak Number 8 9-Eicosene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	2.41 ng	51800	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	64
2	Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	62
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	58
4	17-Pentatriacontene	491	C35H70	006971-40-0	58
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	58





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...	5.08	12.4	ng	237035	1	6.86	383732	20.0
unknown6.63	6.63	93.2	ng	1788090	1	6.86	383732	20.0
2-Hydroxy-iso-but...	8.69	3.6	ng	87946	2	8.14	482471	20.0
Benzophenone	10.61	16.2	ng	411867	3	9.89	509268	20.0
n-Hexadecanoic acid	11.90	3.9	ng	81372	4	11.38	417061	20.0
Octadecanoic acid	12.69	3.0	ng	62795	4	11.38	417061	20.0
9-Eicosene, (E)-	13.86	2.4	ng	51800	5	14.02	429902	20.0