LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100587.D
Acq On : 15 Nov 2017 14:50
Operator : SJ/JU
Sample : I6422-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EPE-110-3(0-5)

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	2.193	16	18	24	rVB3	21579	29977	1.27%	0.143%
2	5.110	510	514	524	rVB	407979	494098	20.91%	2.351%
3	5.504	576	581	584	rBV	2327009	2301628	97.40%	10.949%
4	6.510	746	752	756	rBV	2260442	2363098	100.00%	11.242%
5	6.651	771	776	779	rBV	2466386	2321746	98.25%	11.045%
6	6.881	812	815	819	rBV	859088	736745	31.18%	3.505%
7	7.039	838	842	845	rBV	2072654	1766901	74.77%	8.405%
8	7.445	906	911	914	rBV	1618615	1464657	61.98%	6.968%
9	8.163	1029	1033	1036	rBV	1166412	931314	39.41%	4.430%
10	8.716	1123	1127	1130	rBV	139733	104859	4.44%	0.499%
11	9.239	1211	1216	1219	rBV	2527561	2175032	92.04%	10.347%
12	9.627	1278	1282	1285	rBV	215222	161600	6.84%	0.769%
13	9.922	1328	1332	1335	rVB	988095	923736	39.09%	4.394%
14	10.627	1448	1452	1455	rBV	285202	220371	9.33%	1.048%
15	10.704	1461	1465	1469	rBV	1329077	1154773	48.87%	5.493%
16	11.404	1580	1584	1587	rBV	883888	728871	30.84%	3.467%
17	11.916	1665	1671	1676	rBV3	72829	81665	3.46%	0.388%
18	12.615	1787	1790	1796	rVB	29976	28816	1.22%	0.137%
19	12.792	1817	1820	1825	rVB	56539	46600	1.97%	0.222%
20	12.845	1825	1829	1832	rBV	22105	25795	1.09%	0.123%
21	12.986	1849	1853	1856	rBV	1503992	1334859	56.49%	6.350%
22	13.868	2000	2003	2015	rBV	139818	176591	7.47%	0.840%
23	14.010	2024	2027	2029	rBV	32782	37815	1.60%	0.180%
24	14.039	2029	2032	2036	rVB	787403	703288	29.76%	3.346%
25	15.515	2278	2283	2289	rVB	555450	706013	29.88%	3.359%

Sum of corrected areas: 21020848

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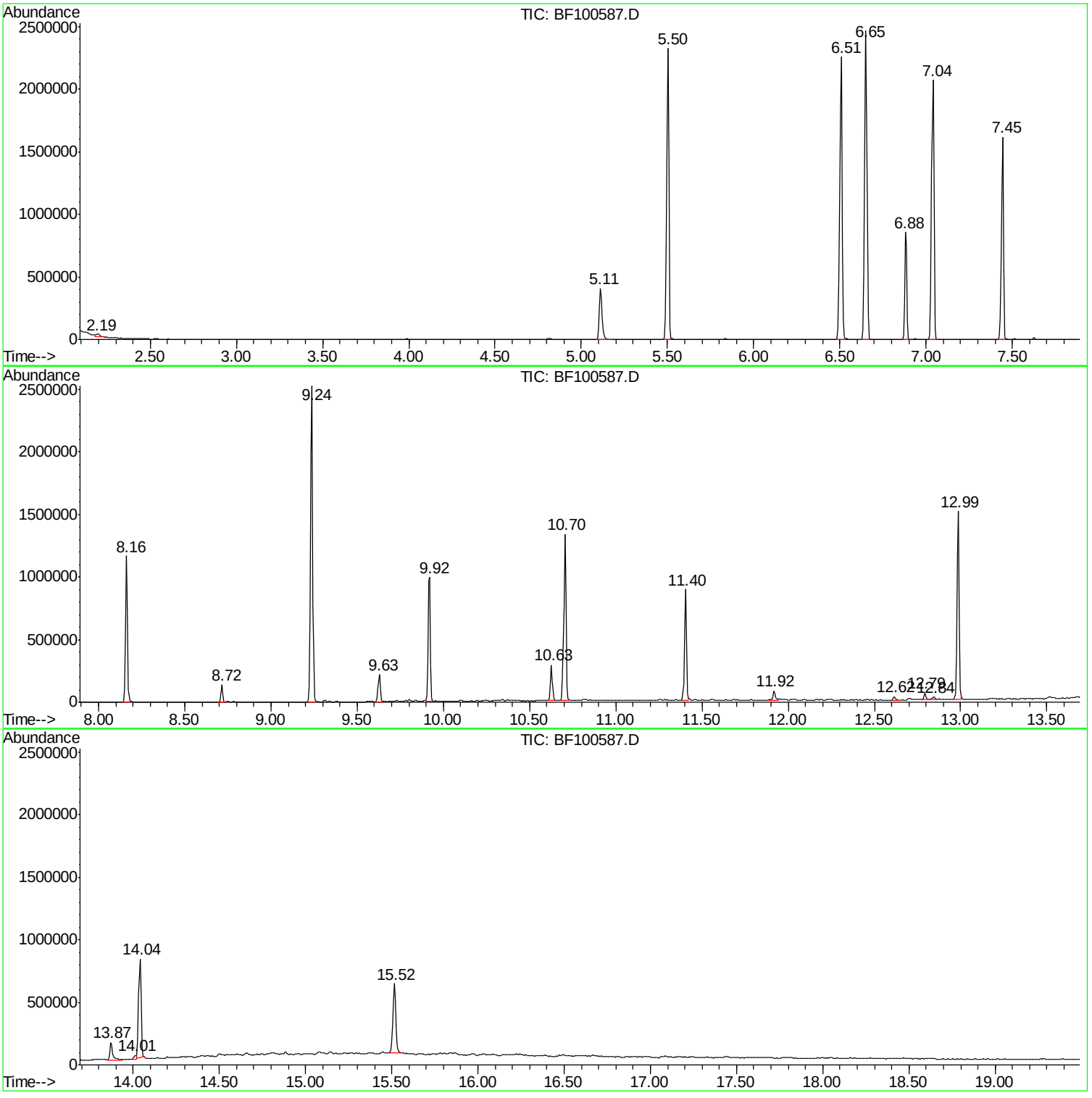
EPE-110-3(0-5)

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

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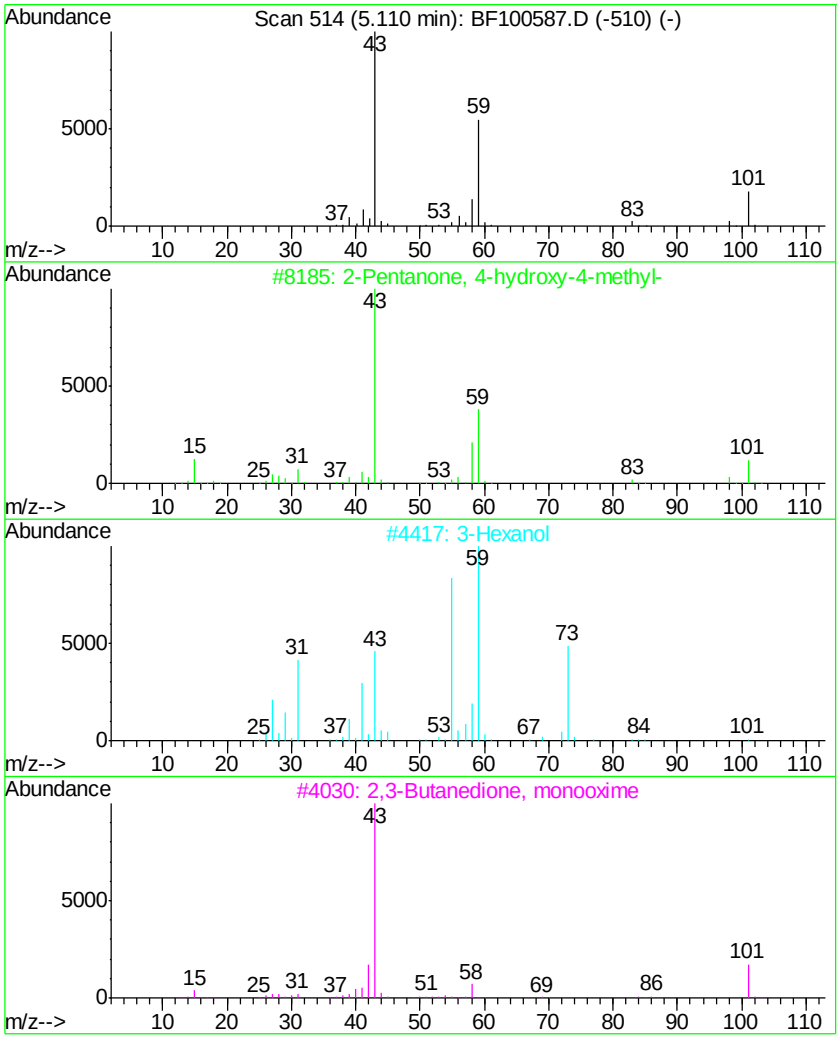
TIC Integration Parameters: LSCINT.P

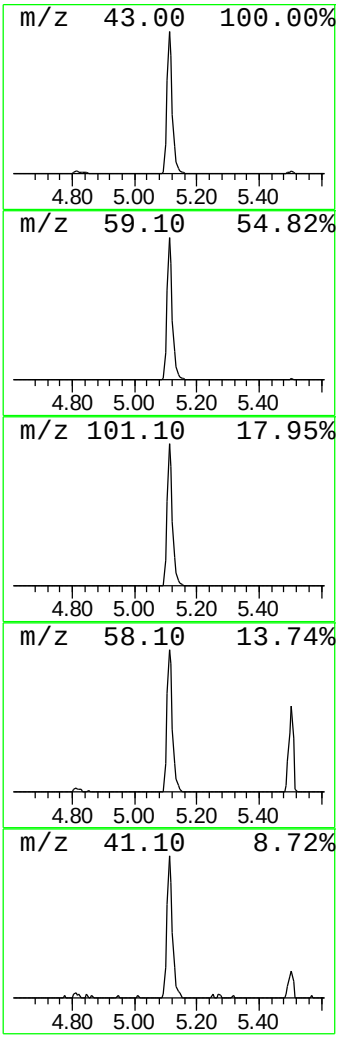
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	13.41 ng	494098	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Instrument : BNA_F
ClientSampleId : EPE-110-3(0-5)

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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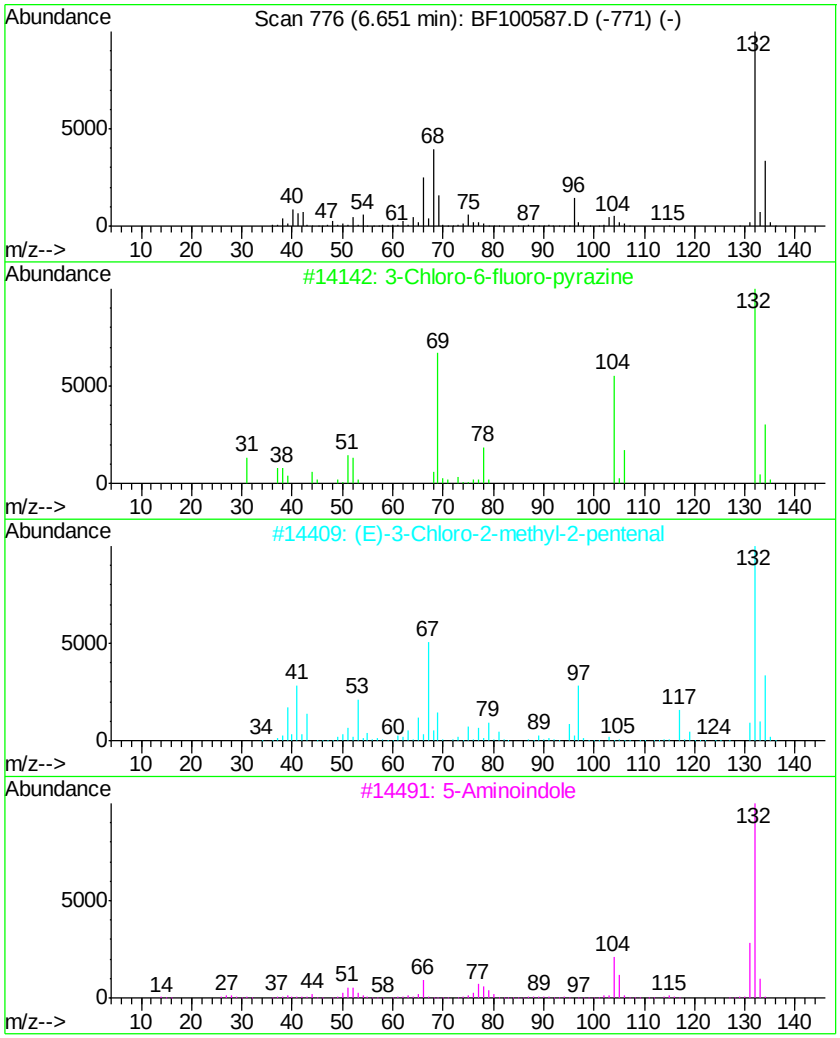
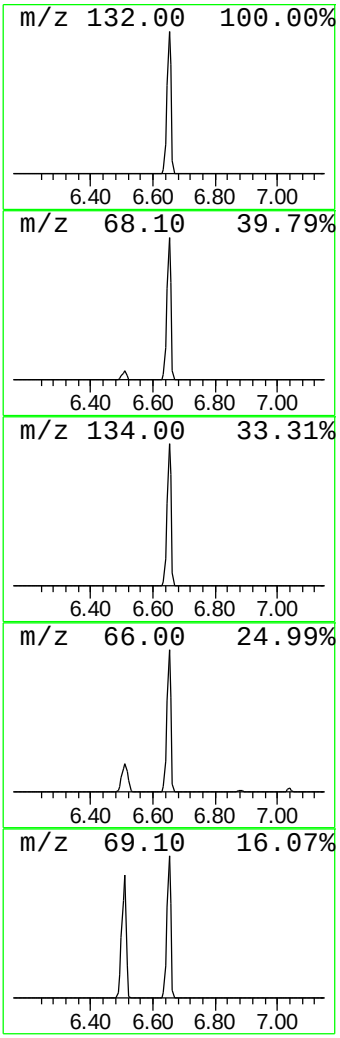
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	63.03 ng	2321750	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Misc :
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Instrument : BNA_F
ClientSampleId : EPE-110-3(0-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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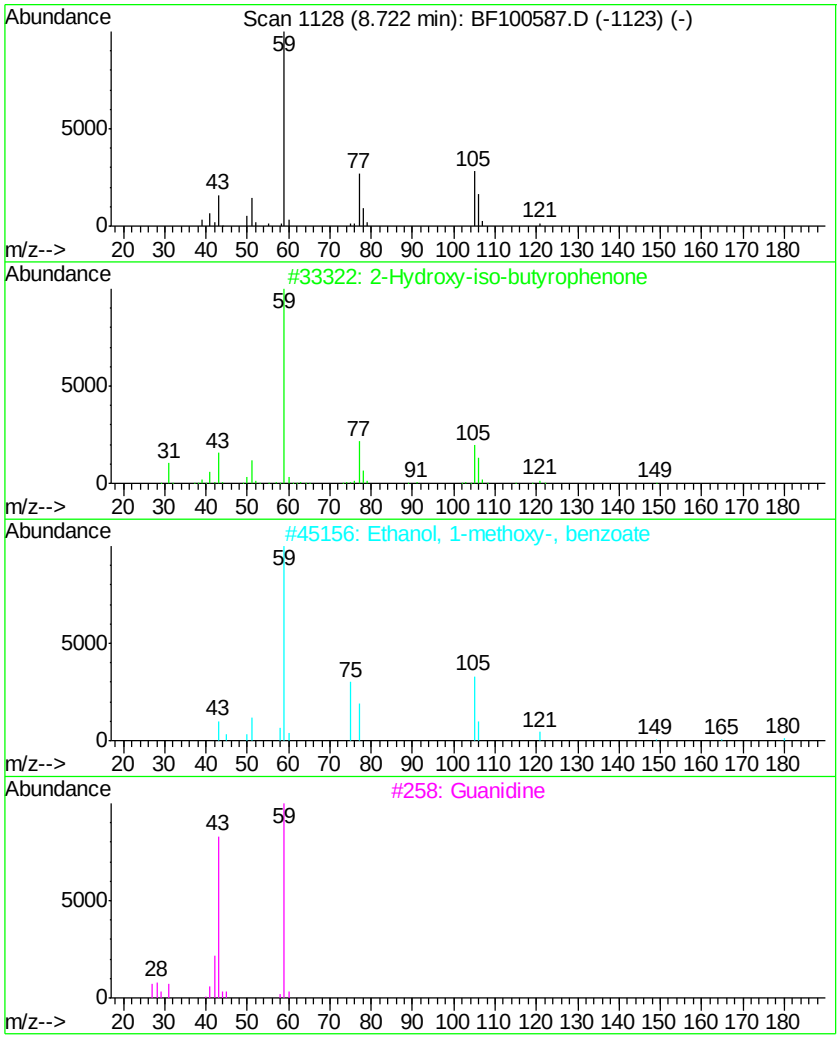
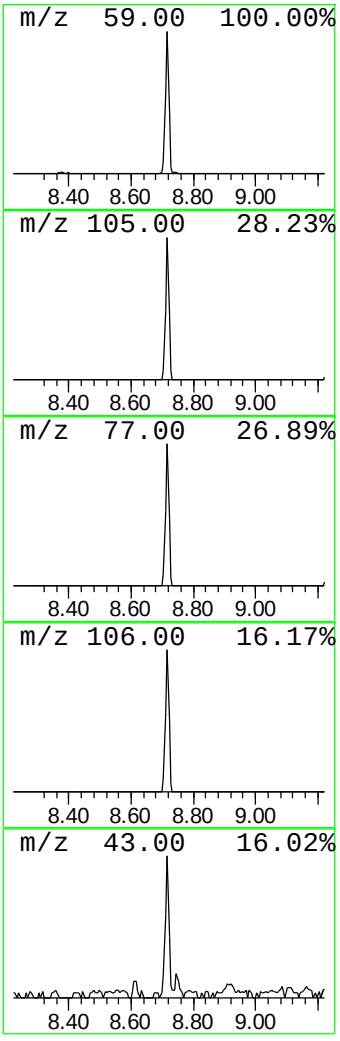
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.25 ng	104859	Naphthalene-d8	8.16

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	Guanidine	59	CH5N3	000113-00-8	7
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
5	Acetamide	59	C2H5NO	000060-35-5	5





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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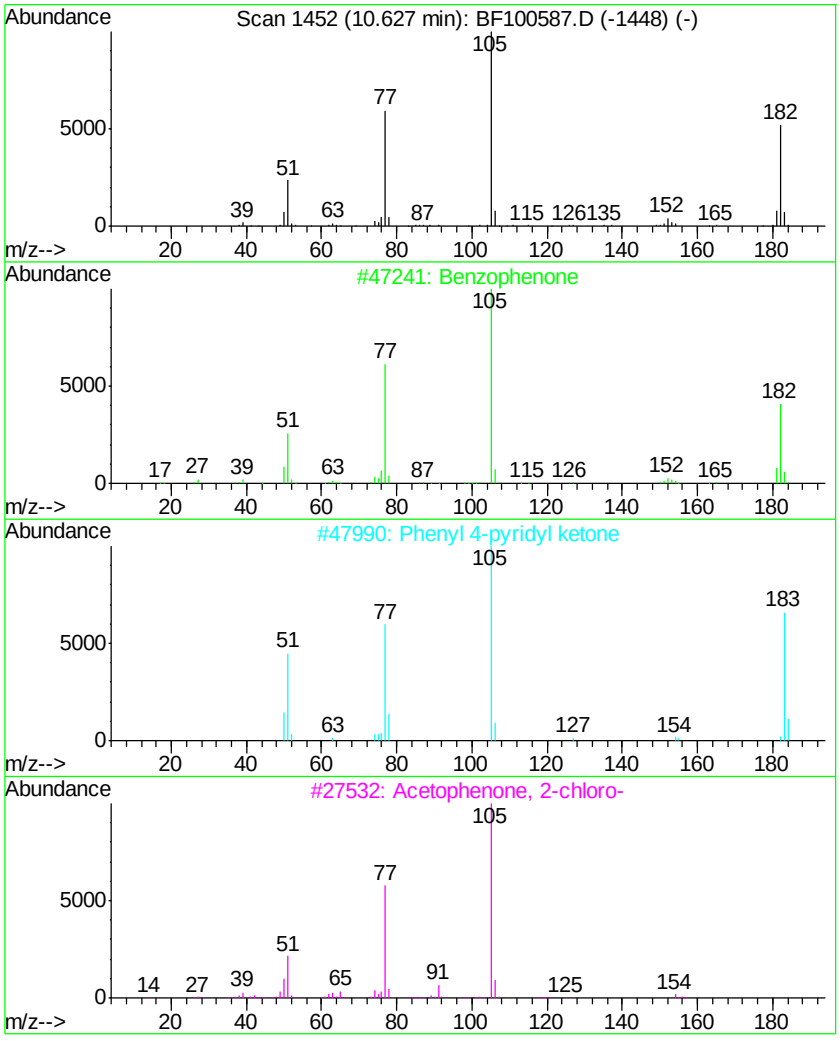
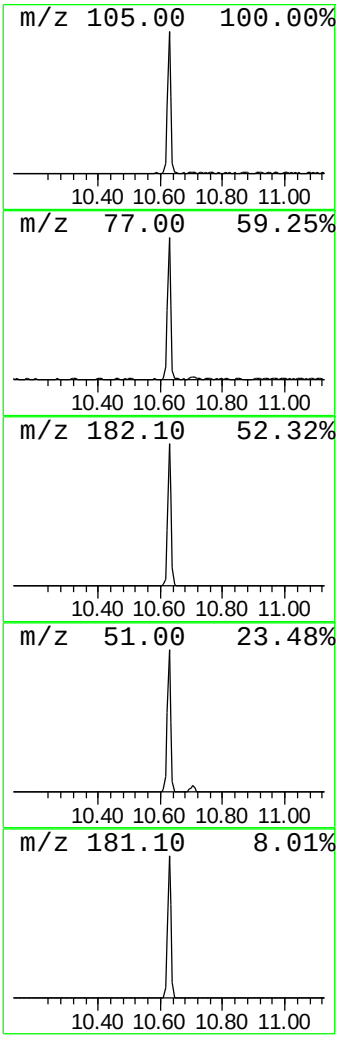
Peak Number 5 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	4.77 ng	220371	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





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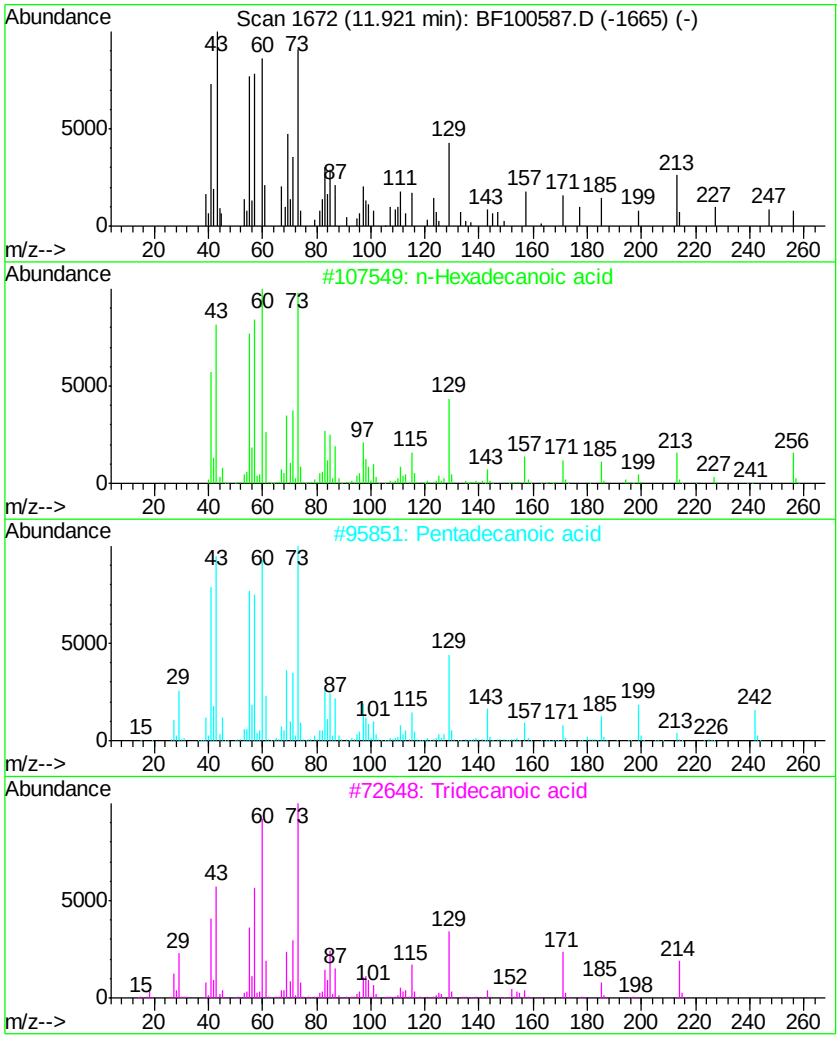
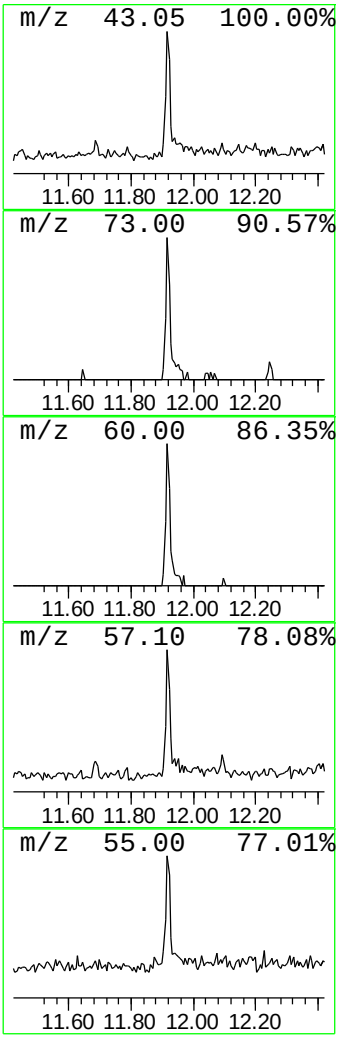
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.24 ng	81665	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59





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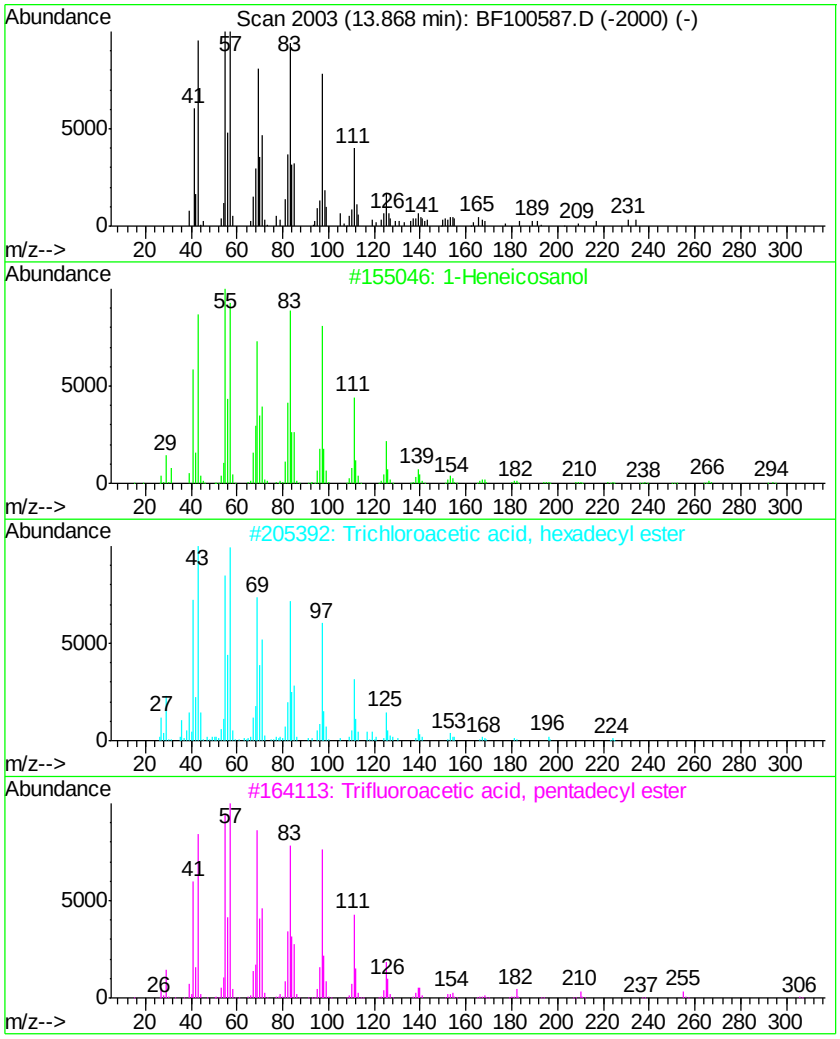
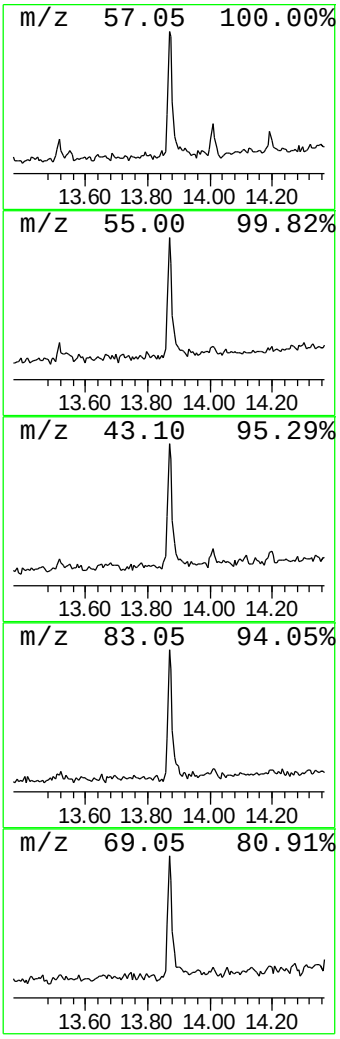
Peak Number 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	5.02 ng	176591	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





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...	5.11	13.4	ng	494098	1	6.88	736745	20.0
unknown6.65	6.65	63.0	ng	2321750	1	6.88	736745	20.0
2-Hydroxy-iso-but...	8.72	2.3	ng	104859	2	8.16	931314	20.0
Benzophenone	10.63	4.8	ng	220371	3	9.92	923736	20.0
n-Hexadecanoic acid	11.92	2.2	ng	81665	4	11.40	728871	20.0
1-Heneicosanol	13.87	5.0	ng	176591	5	14.04	703288	20.0