LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012418\
Data File : BF102401.D
Acq On : 24 Jan 2018 20:33
Operator : SJ/JU
Sample : J1250-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AB-17(0-2)

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-BF012218.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	4.910	477	480	487	rVB	62973	86995	3.60%	0.398%
2	5.328	546	551	554	rBV	2340357	2305300	95.38%	10.538%
3	6.357	721	726	743	rBV	2365053	2417036	100.00%	11.049%
4	6.486	743	748	751	rBV	2642262	2363856	97.80%	10.805%
5	6.716	783	787	793	rBV	763014	657310	27.19%	3.005%
6	6.869	809	813	816	rBV	2148785	1830117	75.72%	8.366%
7	7.281	879	883	886	rBV	1639895	1423723	58.90%	6.508%
8	7.998	1001	1005	1019	rVB	890968	842965	34.88%	3.853%
9	8.557	1095	1100	1103	rBV	220385	193191	7.99%	0.883%
10	9.075	1183	1188	1191	rBV	2381273	2258052	93.42%	10.322%
11	9.469	1251	1255	1264	rBV	505580	444326	18.38%	2.031%
12	9.745	1299	1302	1312	rVB	850561	847400	35.06%	3.874%
13	10.463	1420	1424	1431	rBV	1081104	906984	37.52%	4.146%
14	10.539	1433	1437	1448	rVB	1271997	1175022	48.61%	5.371%
15	10.651	1453	1456	1460	rBV	25557	26300	1.09%	0.120%
16	11.233	1552	1555	1568	rVB	850953	750696	31.06%	3.432%
17	12.815	1820	1824	1828	rBV	1654007	1606785	66.48%	7.345%
18	13.709	1973	1976	1988	rBV	264398	308853	12.78%	1.412%
19	13.868	1999	2003	2012	rVB	695505	705873	29.20%	3.227%
20	15.298	2241	2246	2252	rBV	552398	674013	27.89%	3.081%
21	15.774	2325	2327	2334	rVB6	35604	51683	2.14%	0.236%

Sum of corrected areas: 21876480

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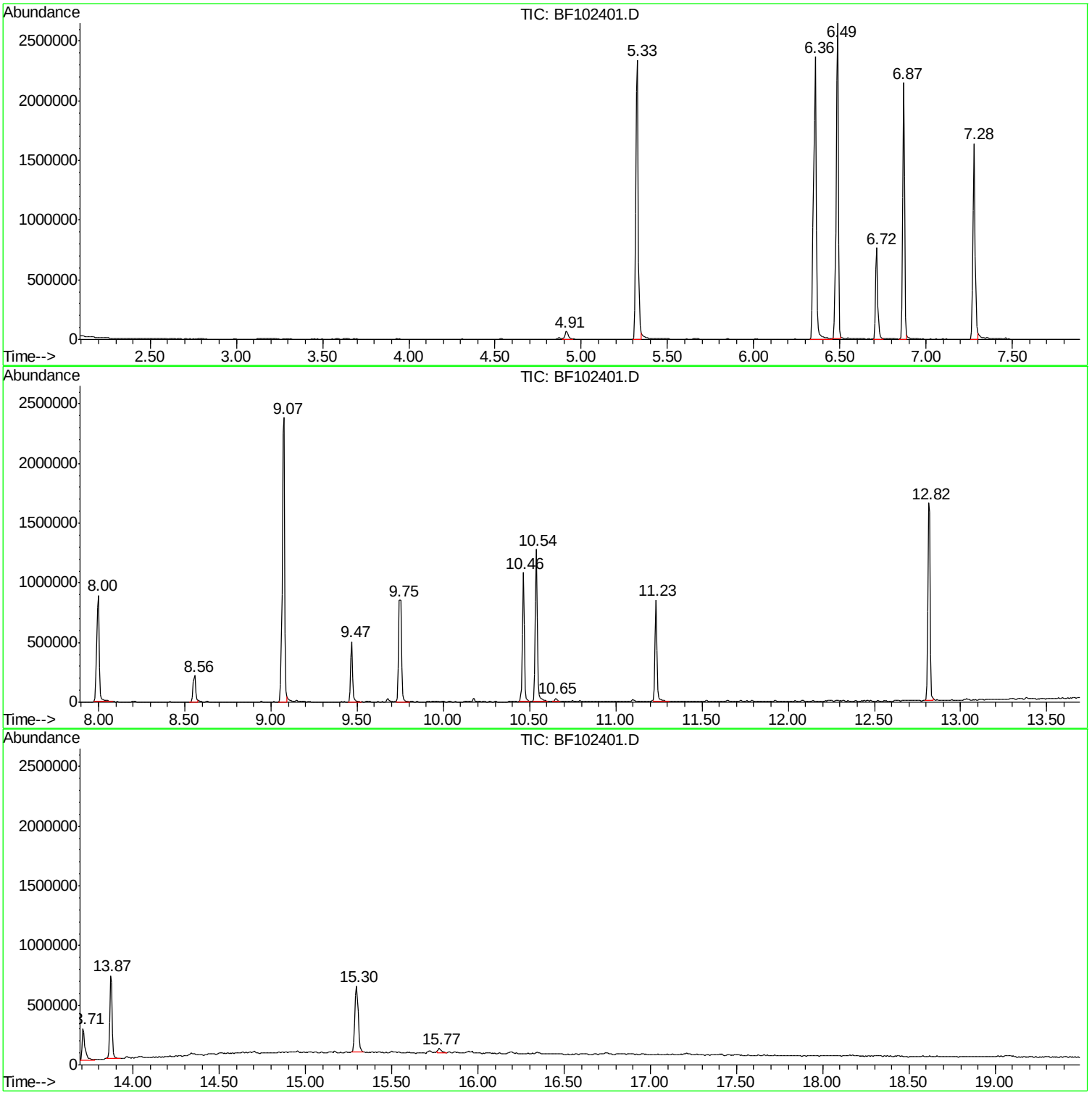
Instrument :
BNA_F
ClientSampleId :
AB-17(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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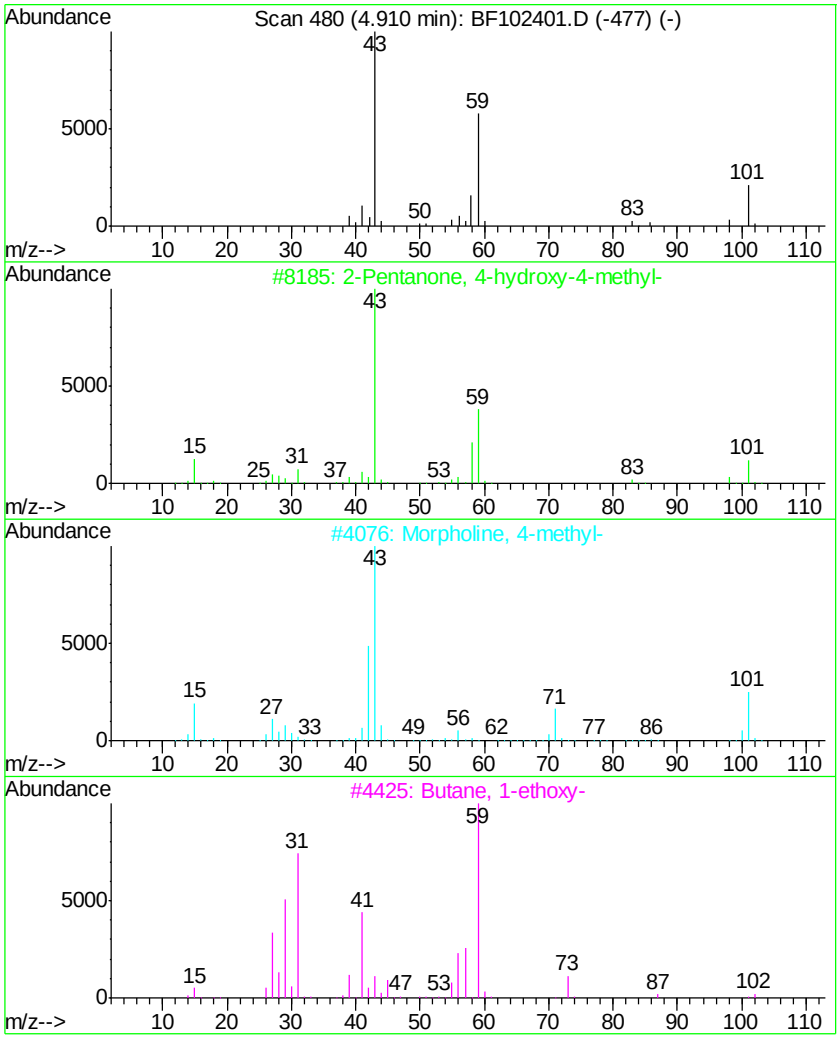
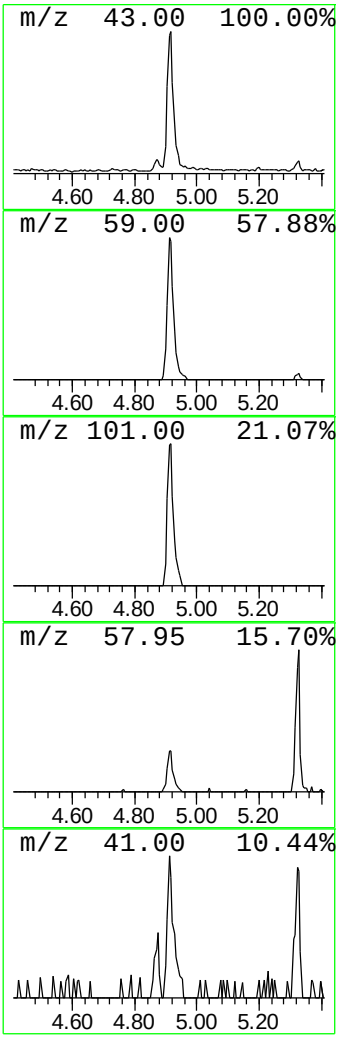
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	2.65 ng	86995	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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ClientSampleId : AB-17(0-2)

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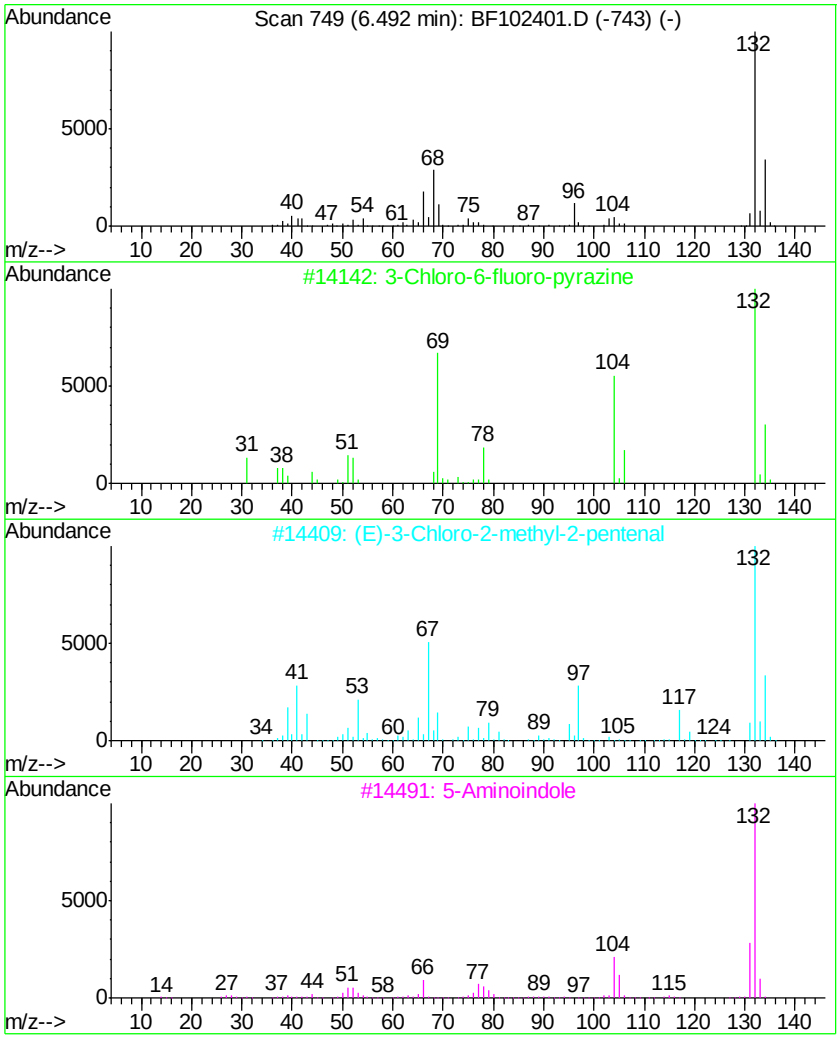
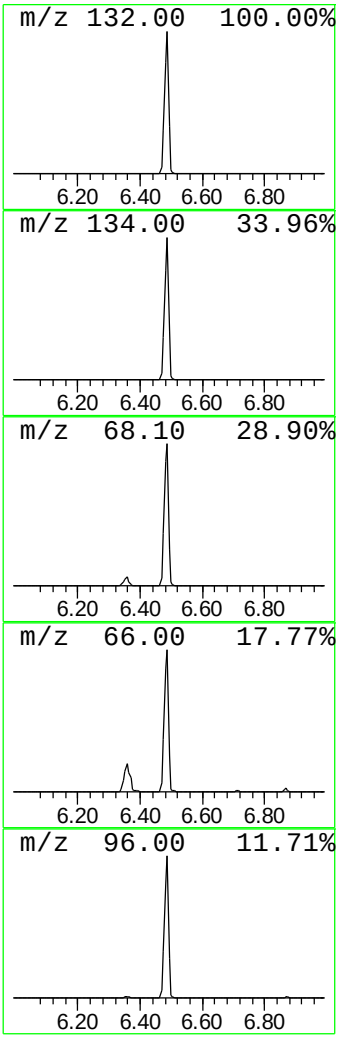
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	71.93 ng	2363860	1,4-Dichlorobenzene-d4	6.72

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Instrument : BNA_F
ClientSampleId : AB-17(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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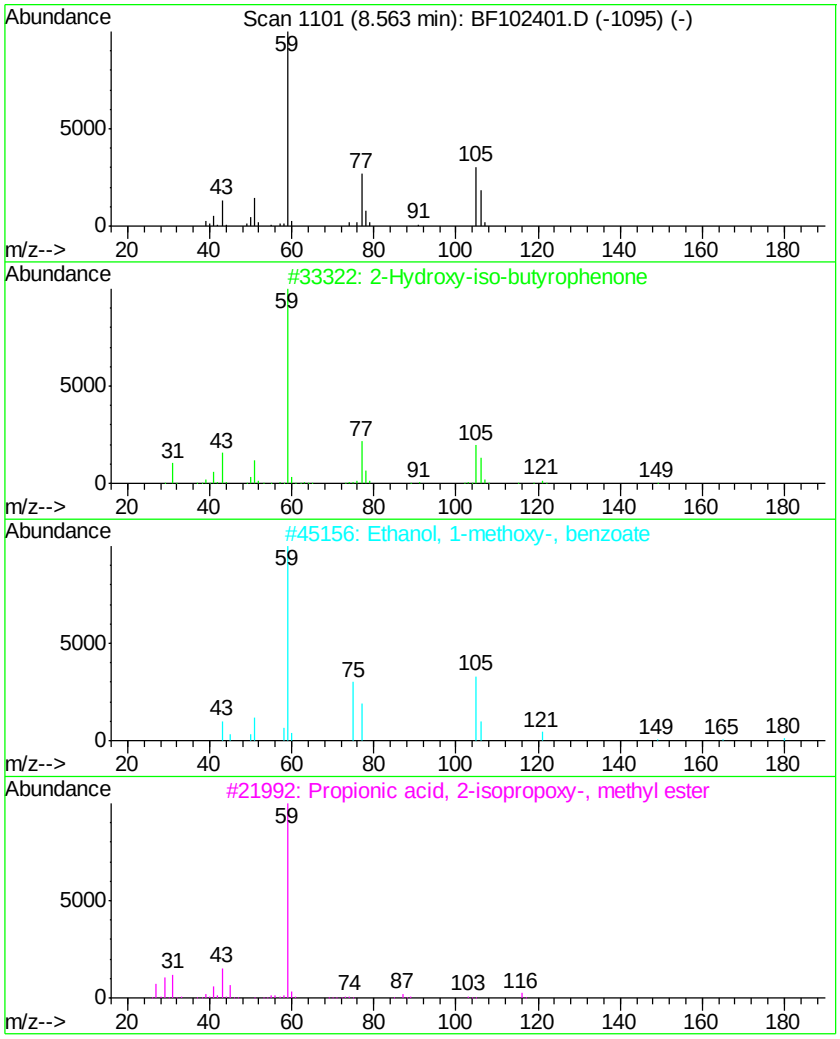
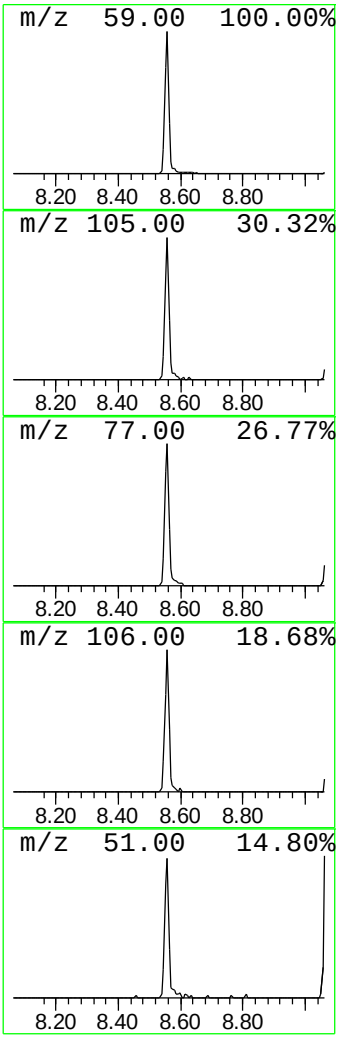
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.56	4.58 ng	193191	Naphthalene-d8	8.00

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	9
3	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
5	Guanidine	59	CH5N3	000113-00-8	7





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Instrument : BNA_F
ClientSampleId : AB-17(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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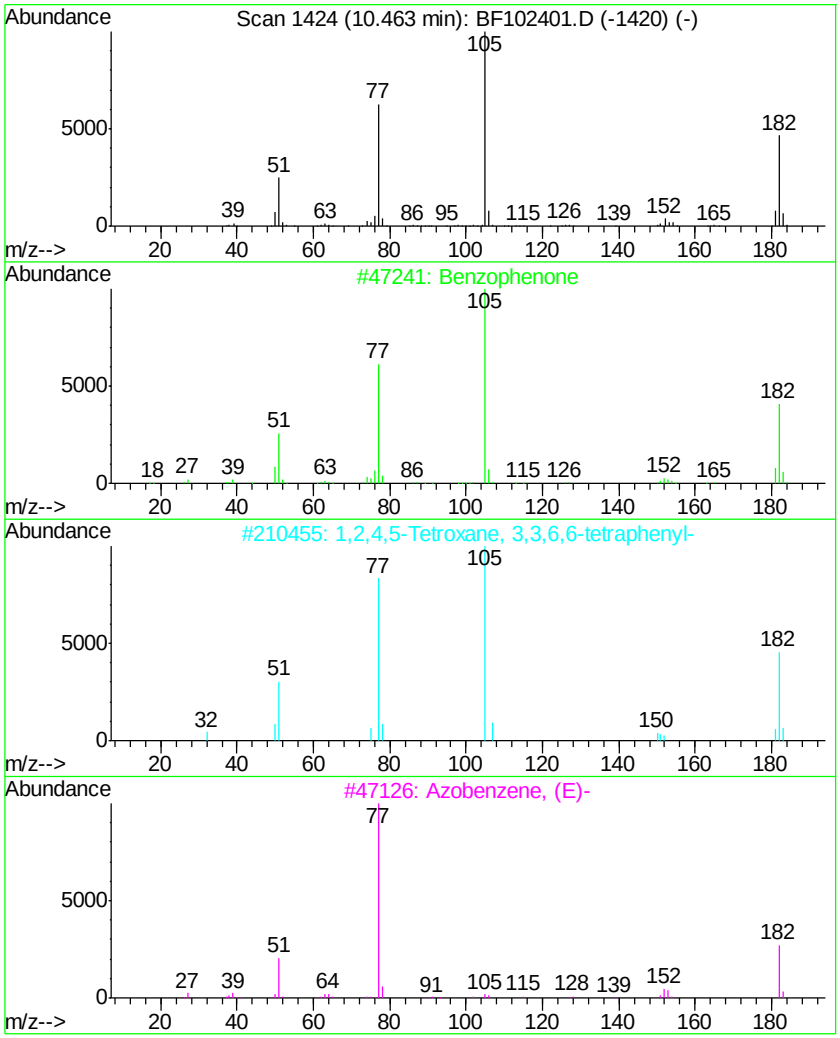
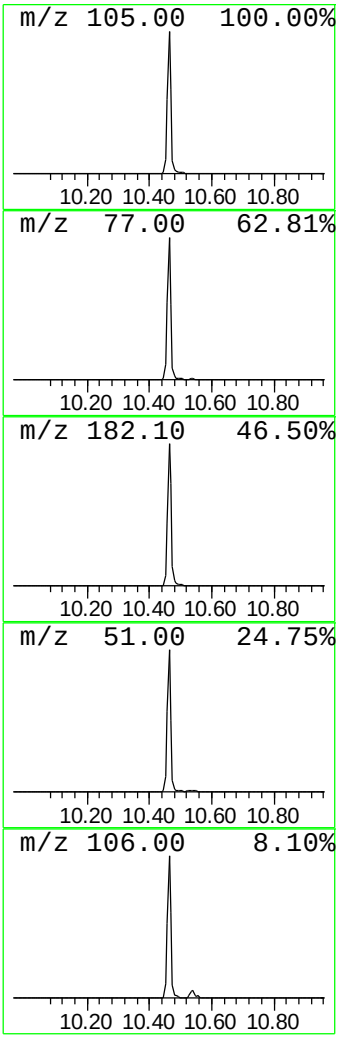
Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.46	21.41 ng	906984	Acenaphthene-d10	9.75

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	Azobenzene, (E)-	182	C12H10N2	017082-12-1	59
4	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
5	5-[N-Benzoylaminomethyl]tetrazole	203	C9H9N5O	1000227-36-3	47





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Acq On : 24 Jan 2018 20:33
Operator : SJ/JU
Sample : J1250-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : AB-17(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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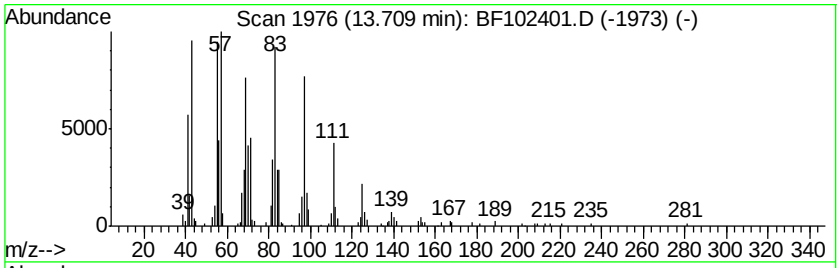
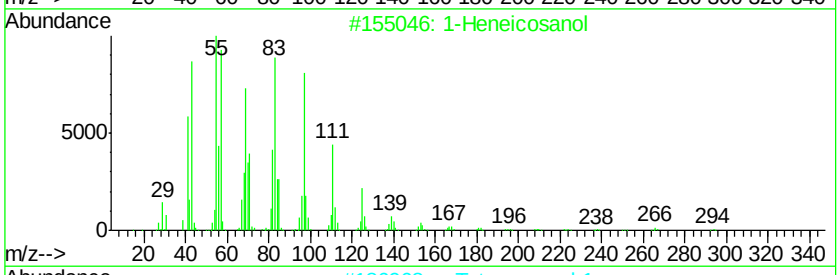
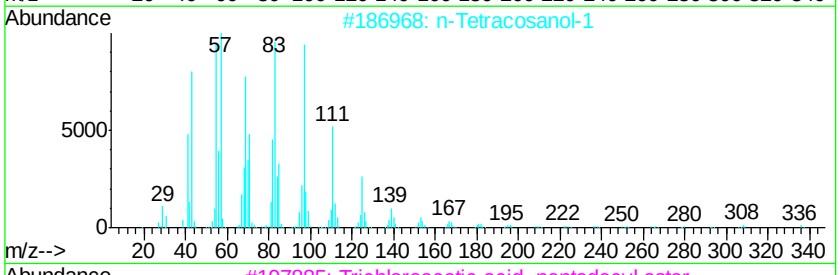
Peak Number 6 1-Heneicosanol Concentration Rank 4

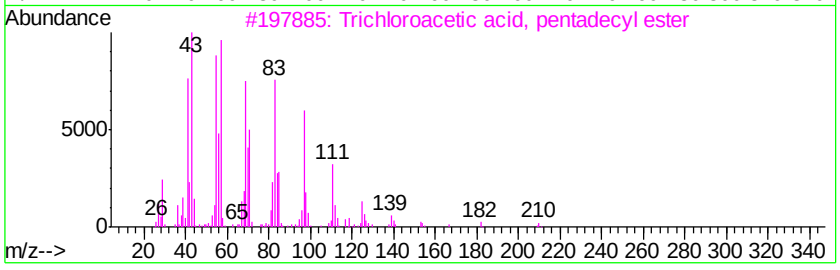
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	8.75 ng	308853	Chrysene-d12	13.87

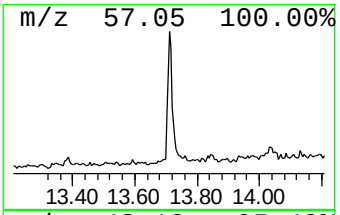
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93

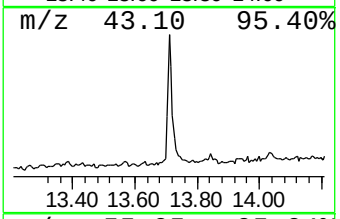


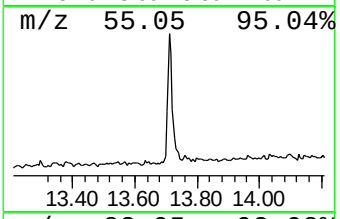


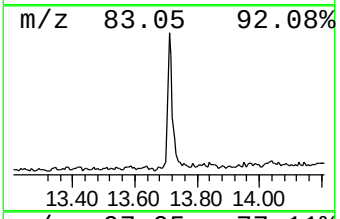


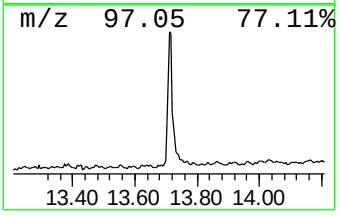












Tentatively Identified Compound (LSC) summary

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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...	4.91	2.6	ng	86995	1	6.72	657310	20.0
unknown6.49	6.49	71.9	ng	2363860	1	6.72	657310	20.0
2-Hydroxy-iso-but...	8.56	4.6	ng	193191	2	8.00	842965	20.0
Benzophenone	10.46	21.4	ng	906984	3	9.75	847400	20.0
1-Heneicosanol	13.71	8.8	ng	308853	5	13.87	705873	20.0