LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099948.D
Acq On : 29 Oct 2017 7:27
Operator : SJ/JU
Sample : I6100-03
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-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	4.999	493	495	508	rBV	79955	118924	4.21%	0.714%
2	5.410	562	565	597	rBV	628685	821000	29.06%	4.927%
3	6.428	736	738	755	rBV	406280	552093	19.54%	3.313%
4	6.557	757	760	767	rVB	1604455	1471708	52.10%	8.832%
5	6.787	796	799	808	rBV	653395	591010	20.92%	3.547%
6	6.940	821	825	846	rBB	2124810	2071634	73.34%	12.433%
7	7.357	892	896	899	rBV	1526259	1461676	51.74%	8.772%
8	8.069	1013	1017	1035	rBV	841471	786965	27.86%	4.723%
9	8.628	1109	1112	1123	rBB	80955	76829	2.72%	0.461%
10	9.145	1195	1200	1203	rBV	2843187	2824820	100.00%	16.953%
11	9.539	1264	1267	1276	rBV	107717	87829	3.11%	0.527%
12	9.822	1309	1315	1327	rVB	905003	806697	28.56%	4.841%
13	10.492	1425	1429	1433	rBV	94461	74588	2.64%	0.448%
14	10.533	1433	1436	1443	rVB	336948	260430	9.22%	1.563%
15	10.616	1446	1450	1462	rBV	802634	747533	26.46%	4.486%
16	11.310	1565	1568	1576	rBV	610804	593383	21.01%	3.561%
17	12.698	1801	1804	1808	rBV	213315	177862	6.30%	1.067%
18	12.775	1815	1817	1820	rVB	39992	32969	1.17%	0.198%
19	12.898	1833	1838	1841	rBV	1901022	1822109	64.50%	10.935%
20	13.404	1921	1924	1927	rBV	153566	117986	4.18%	0.708%
21	13.774	1984	1987	1997	rBV	52042	57775	2.05%	0.347%
22	13.963	2015	2019	2026	rBV	561333	523499	18.53%	3.142%
23	15.421	2263	2267	2278	rVB	361439	491010	17.38%	2.947%
24	16.286	2409	2414	2422	rBV2	18221	31059	1.10%	0.186%
25	16.845	2503	2509	2517	rBV5	14104	29072	1.03%	0.174%
26	17.521	2616	2624	2632	rVB7	13030	32015	1.13%	0.192%

Sum of corrected areas: 16662475

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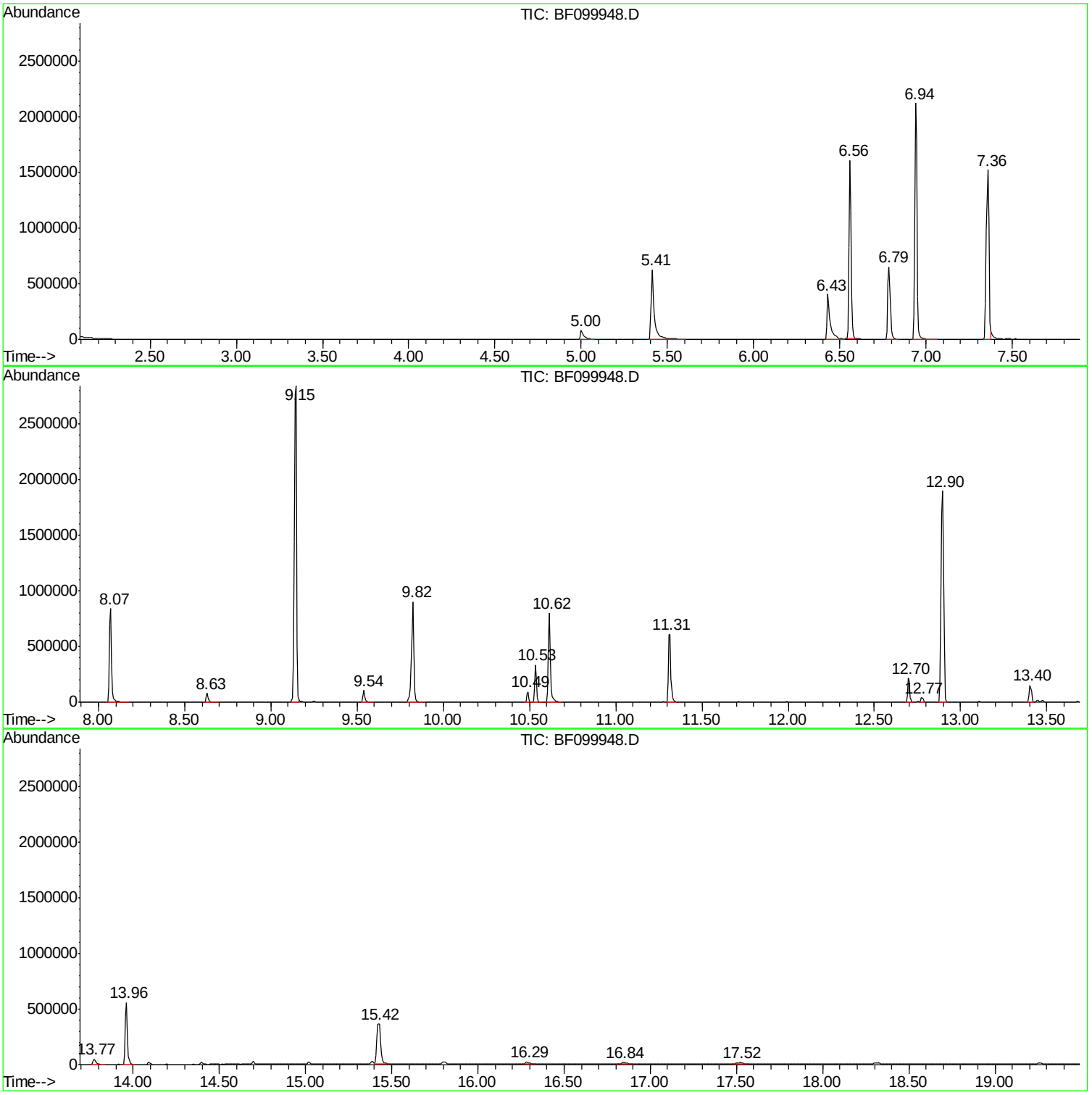
102317-TIDO-F-U-B

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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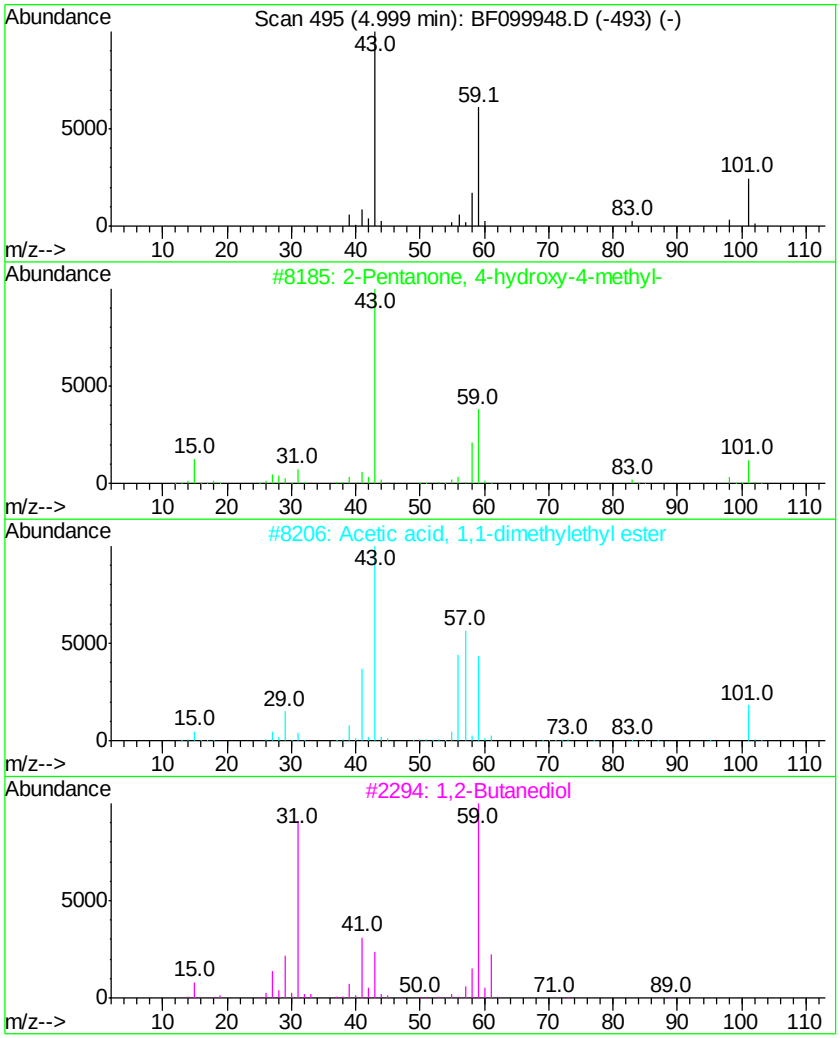
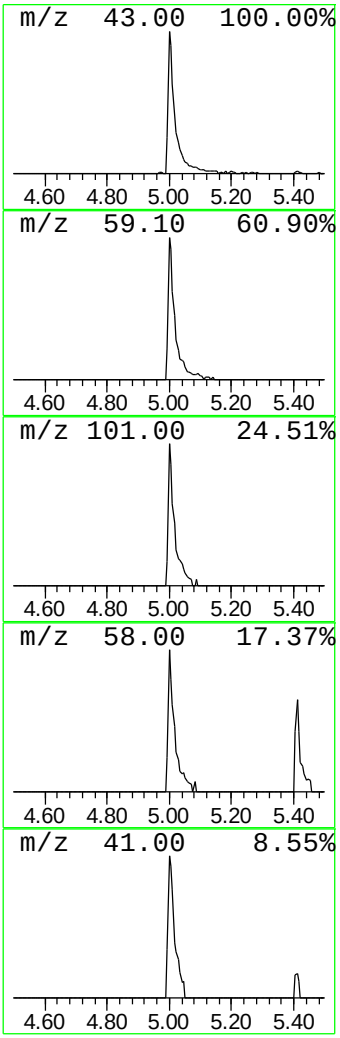
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.02 ng	118924	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	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,2-Butanediol	90	C4H10O2	000584-03-2	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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Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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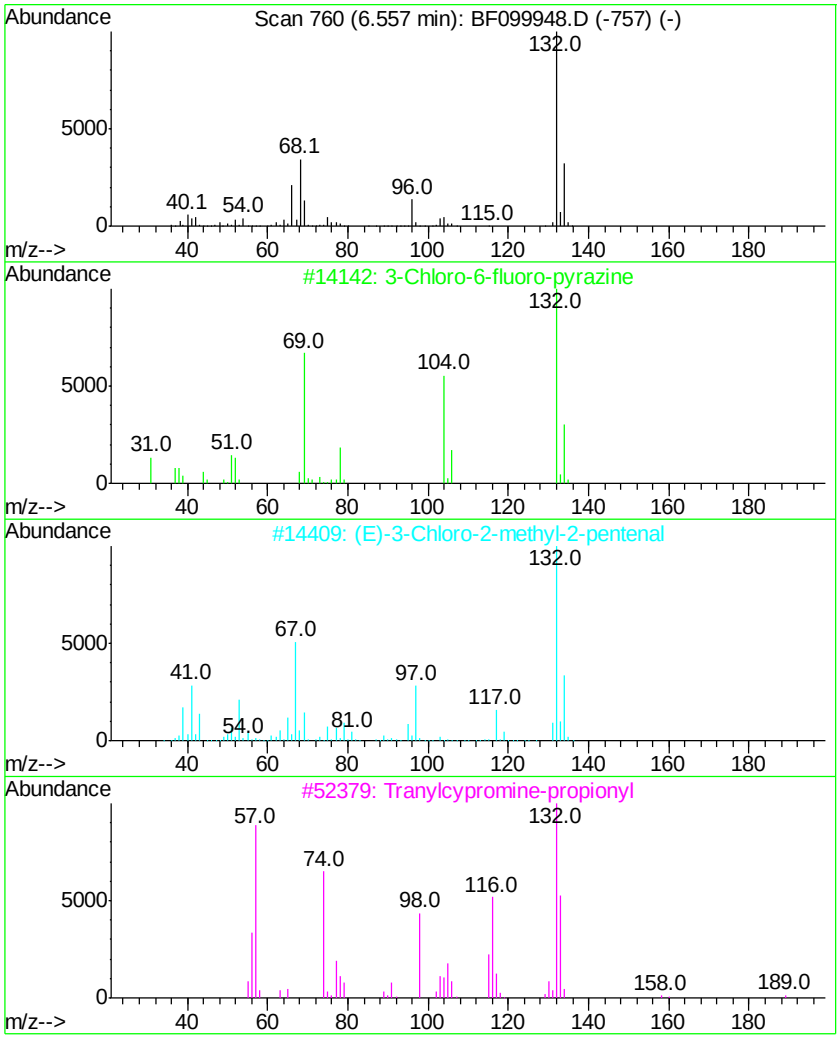
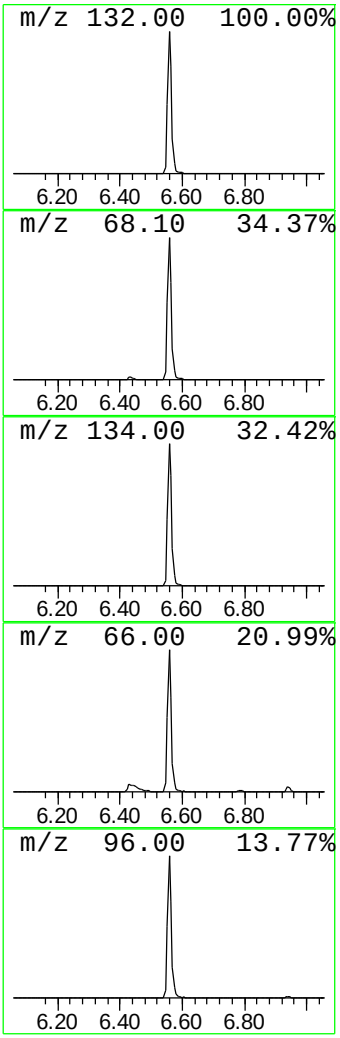
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	49.80 ng	1471710	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Misc :
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Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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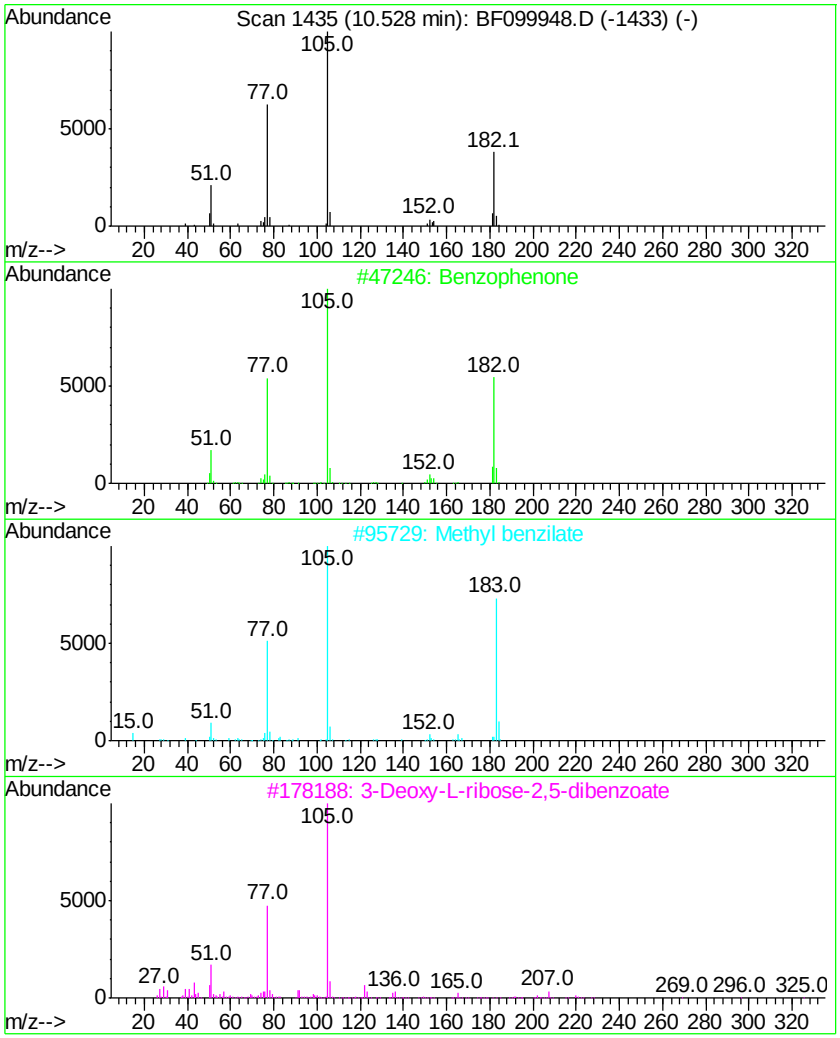
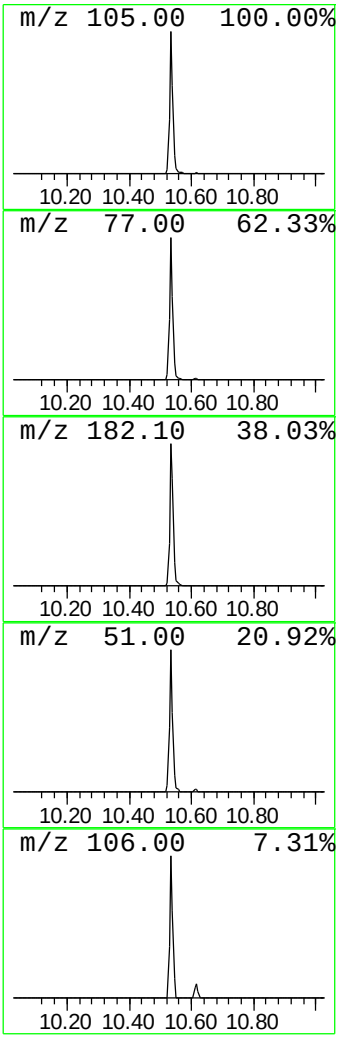
Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	6.46 ng	260430	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Methyl benzilate	242	C15H14O3	000076-89-1	47
3	3-Deoxy-L-ribose-2,5-dibenzoate	342	C19H18O6	1000194-12-7	43
4	Vinyl benzoate	148	C9H8O2	000769-78-8	43
5	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	43





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Misc :
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Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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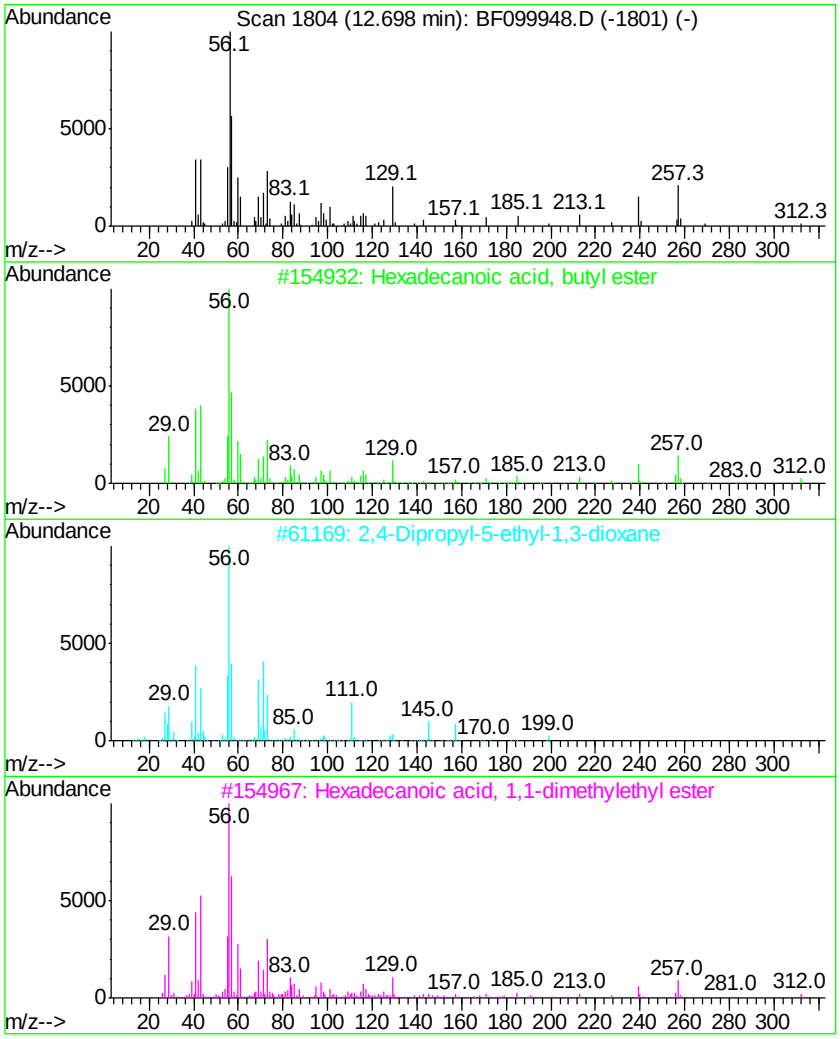
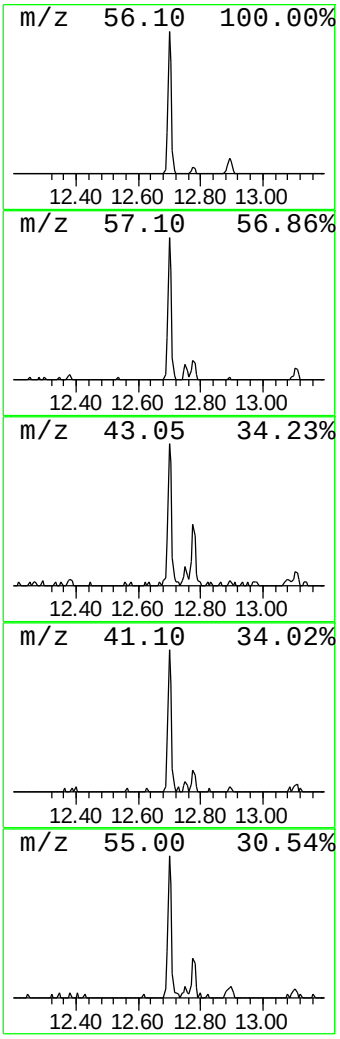
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	6.80 ng	177862	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	96
2	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	43
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	41
4	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





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Instrument : BNA_F
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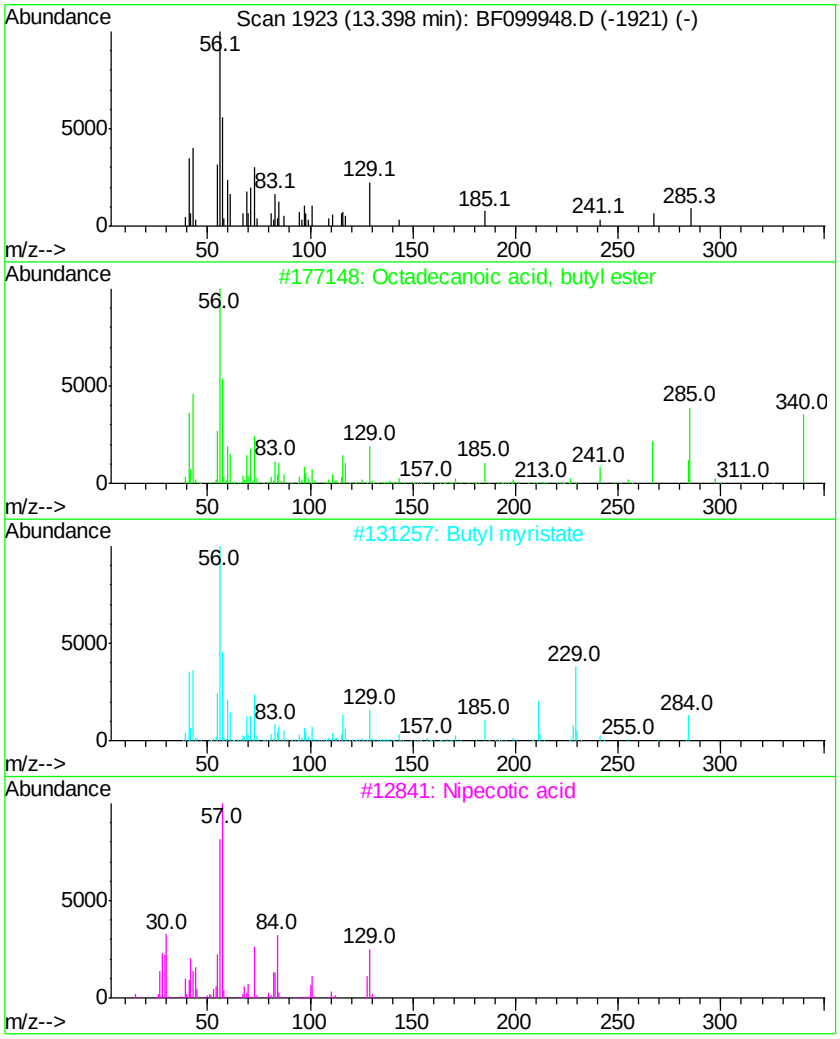
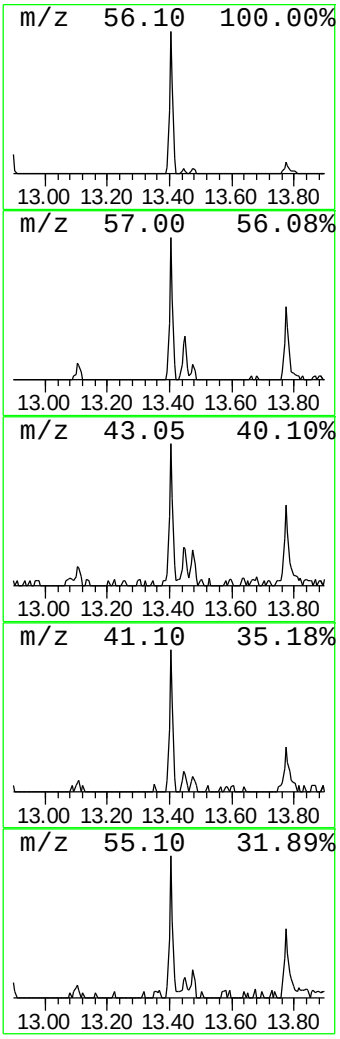
Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	4.51 ng	117986	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	83
2	Butyl myristate	284	C18H36O2	000110-36-1	64
3	Nipecotic acid	129	C6H11NO2	000498-95-3	37
4	2-Methyl-1-octadecene	266	C19H38	061868-20-0	35
5	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	32





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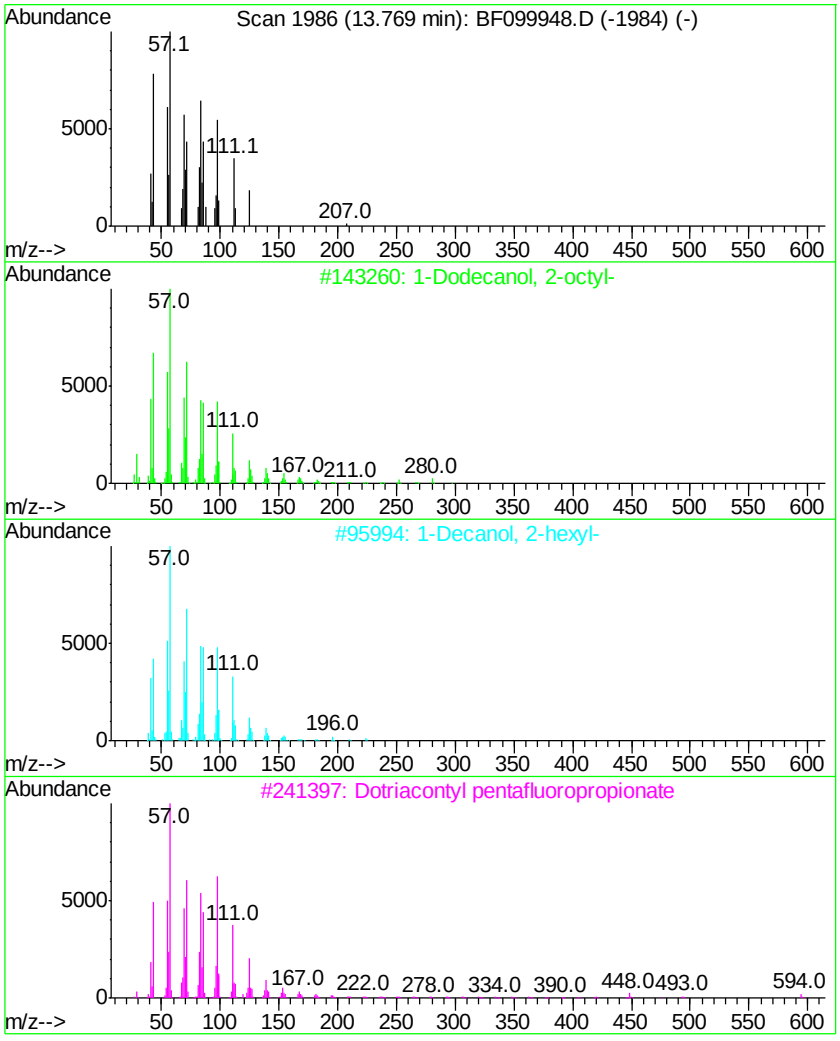
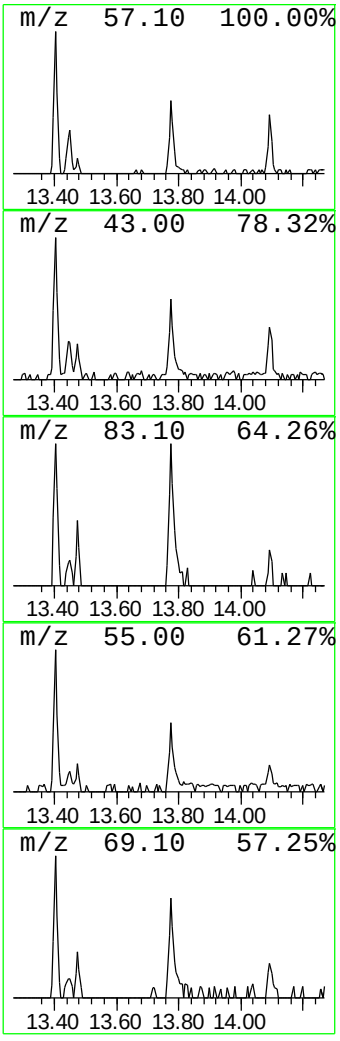
Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.21 ng	57775	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
3	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	90
4	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87
5	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	74





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.00	4.0	ng	118924	1	6.79	591010	20.0
unknown6.56	6.56	49.8	ng	1471710	1	6.79	591010	20.0
Benzophenone	10.53	6.5	ng	260430	3	9.82	806697	20.0
Hexadecanoic acid...	12.70	6.8	ng	177862	5	13.96	523499	20.0
Octadecanoic acid...	13.40	4.5	ng	117986	5	13.96	523499	20.0
1-Dodecanol, 2-oc...	13.77	2.2	ng	57775	5	13.96	523499	20.0