LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106475.D
Acq On : 15 Jun 2018 6:23
Operator : JU/SJ
Sample : J3475-02
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-M

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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	5.196	482	486	491	rBV	84815	87600	2.79%	0.432%
2	5.613	554	557	570	rVB	1173764	1129359	35.92%	5.564%
3	6.607	723	726	736	rBV	868665	798644	25.40%	3.935%
4	6.743	745	749	753	rBV	1955818	1751344	55.70%	8.629%
5	6.966	783	787	790	rBV	860248	671669	21.36%	3.309%
6	7.125	809	814	817	rBV	2580501	2355882	74.92%	11.607%
7	7.531	877	883	886	rBV	1948265	1880124	59.79%	9.263%
8	8.248	1001	1005	1008	rBV	937315	750073	23.85%	3.696%
9	8.801	1095	1099	1102	rBV	112060	89492	2.85%	0.441%
10	9.325	1183	1188	1191	rBV	2908612	2905763	92.41%	14.316%
11	9.713	1250	1254	1262	rBV	276174	234132	7.45%	1.154%
12	10.007	1301	1304	1308	rVB	800009	694498	22.09%	3.422%
13	10.666	1413	1416	1420	rVB	98702	74190	2.36%	0.366%
14	10.719	1421	1425	1428	rVB	307779	249796	7.94%	1.231%
15	10.795	1434	1438	1442	rBV	1268580	1145639	36.43%	5.644%
16	11.495	1554	1557	1561	rBV	840516	720119	22.90%	3.548%
17	12.889	1790	1794	1797	rBV	101583	84586	2.69%	0.417%
18	13.083	1823	1827	1831	rBV	3049654	3144439	100.00%	15.492%
19	13.595	1910	1914	1917	rBV	82064	64579	2.05%	0.318%
20	13.971	1974	1978	1981	rBV2	29695	35936	1.14%	0.177%
21	14.148	2004	2008	2011	rBV	902701	821663	26.13%	4.048%
22	15.683	2263	2269	2275	rBV	454059	572307	18.20%	2.820%
23	16.148	2344	2348	2354	rVB2	21246	35062	1.12%	0.173%

Sum of corrected areas: 20296896

LSC Report - Integrated Chromatogram

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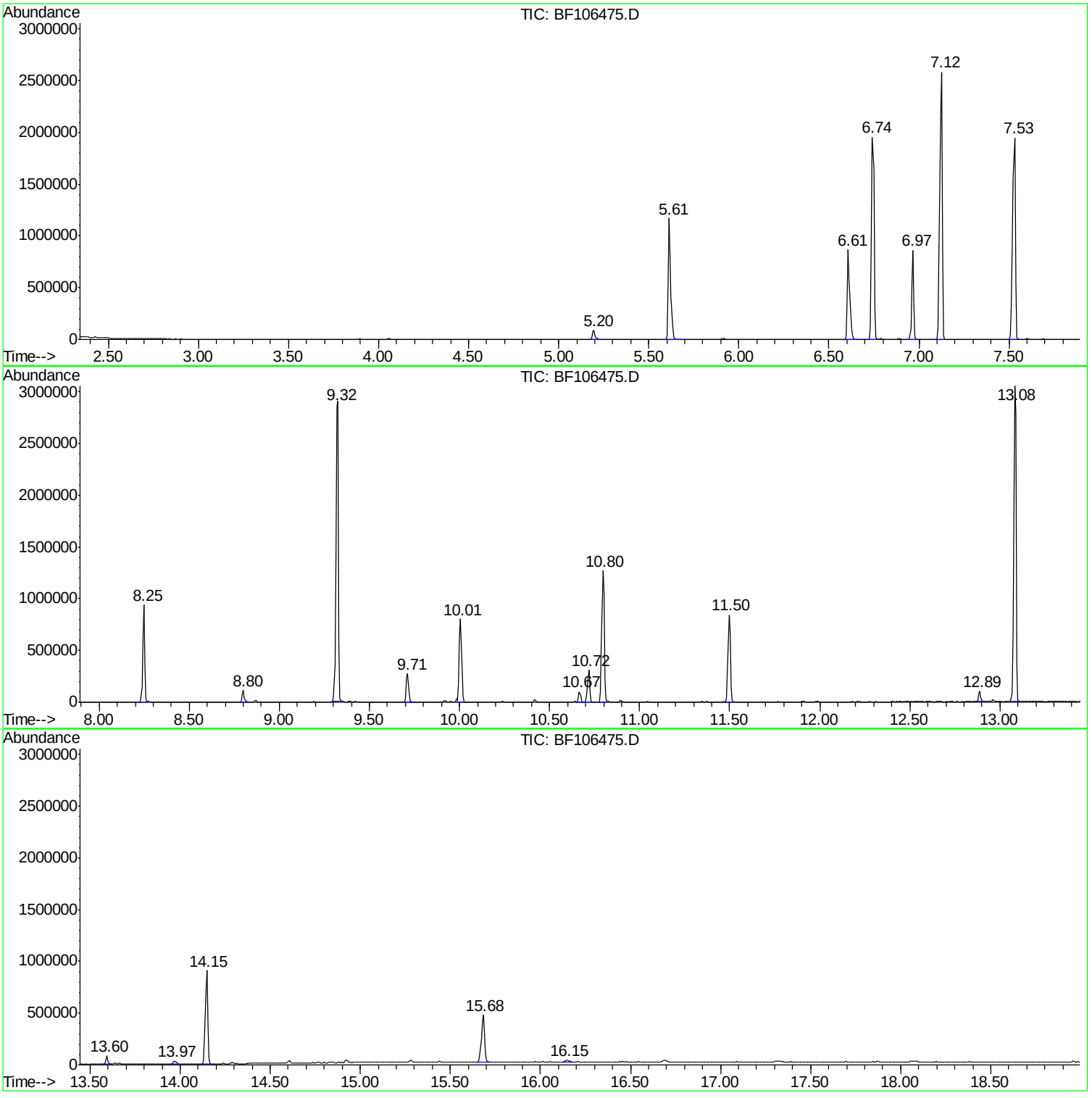
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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ClientSampleId : 061218-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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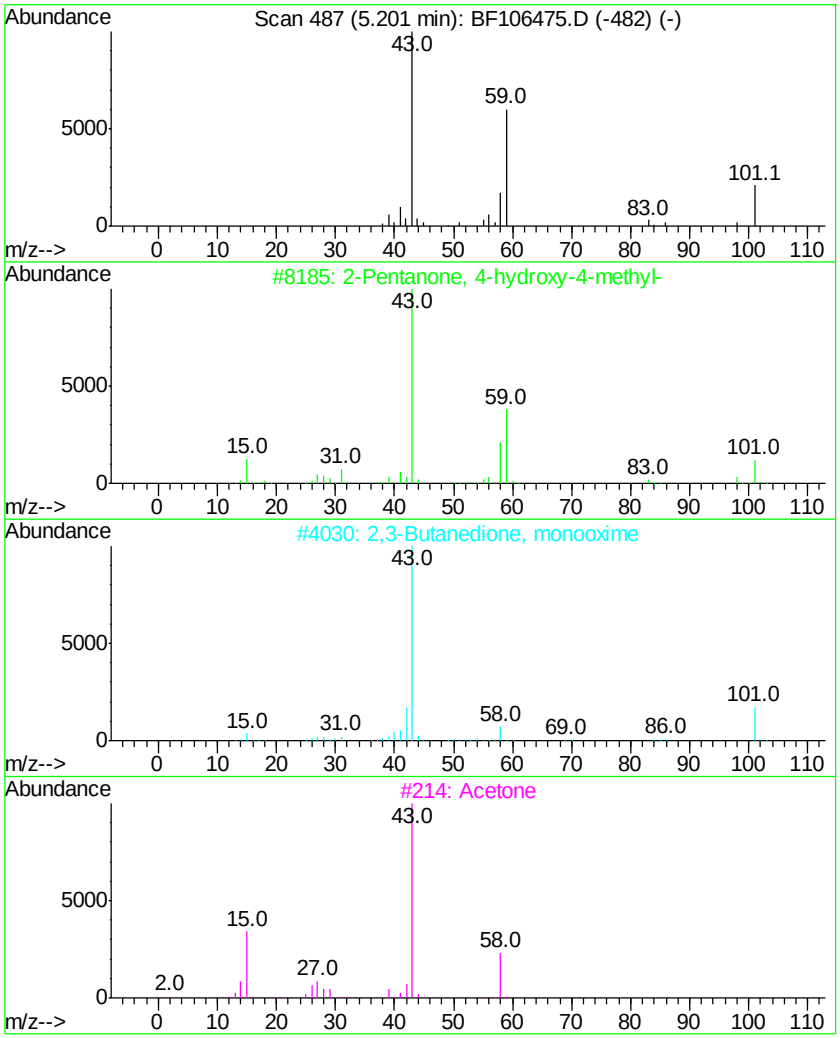
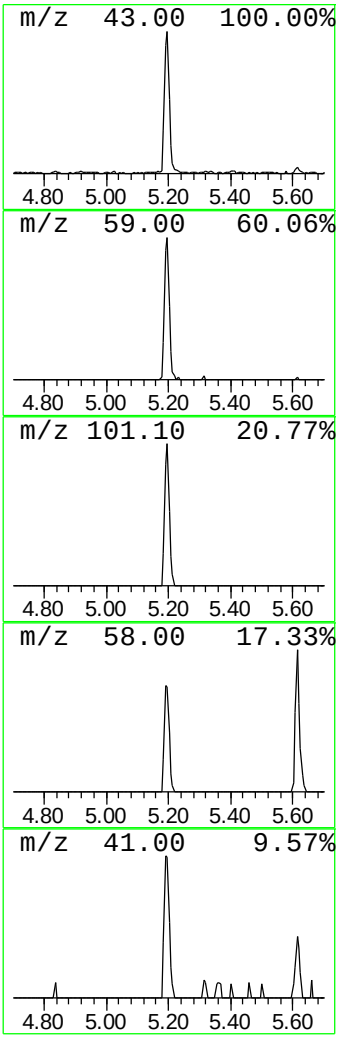
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.61 ng	87600	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetone	58	C3H6O	000067-64-1	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





Library Search Compound Report

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Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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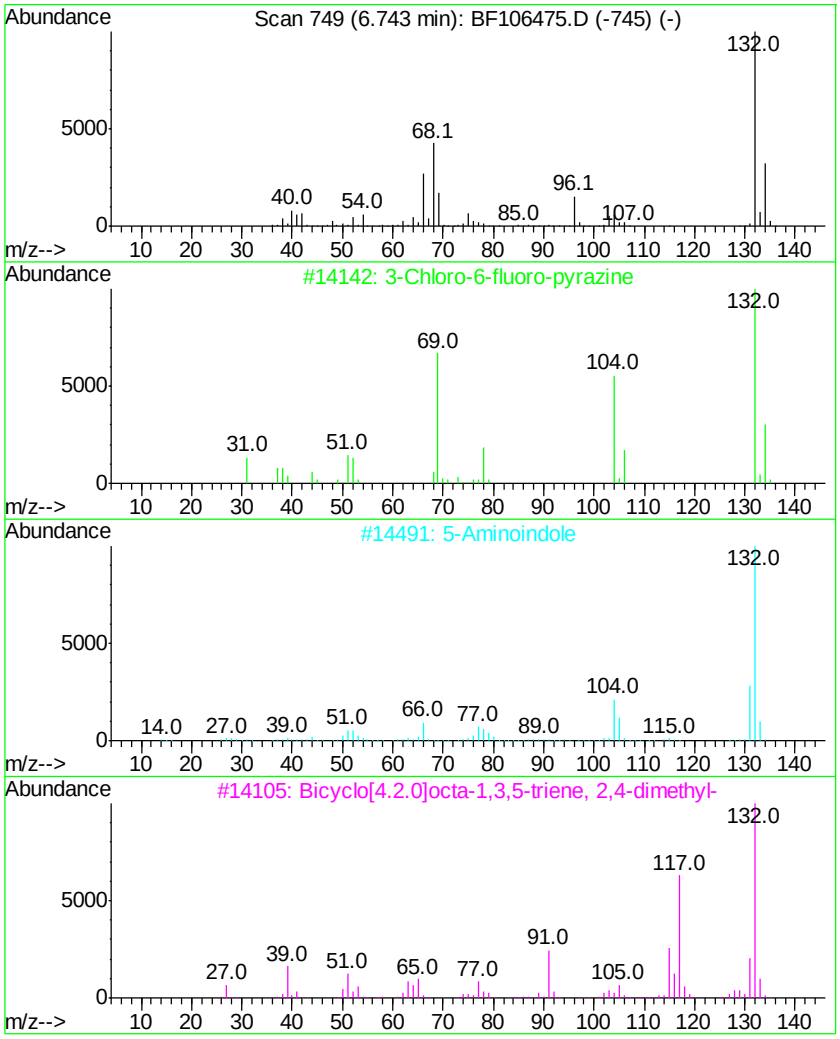
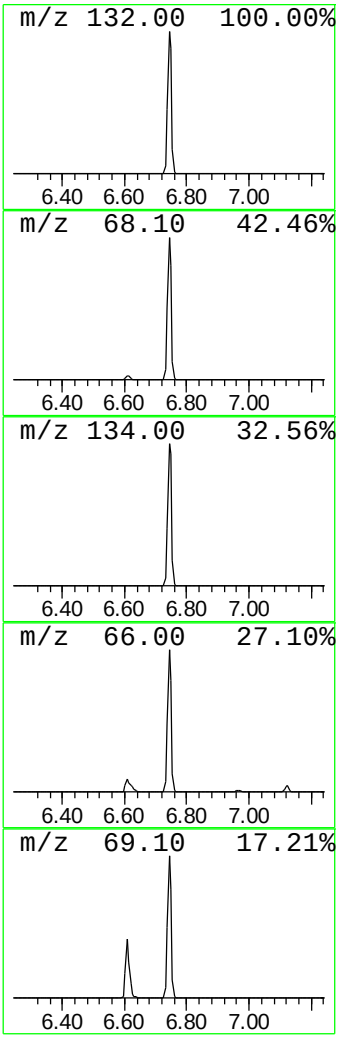
Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	52.15 ng	1751340	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J3475-02
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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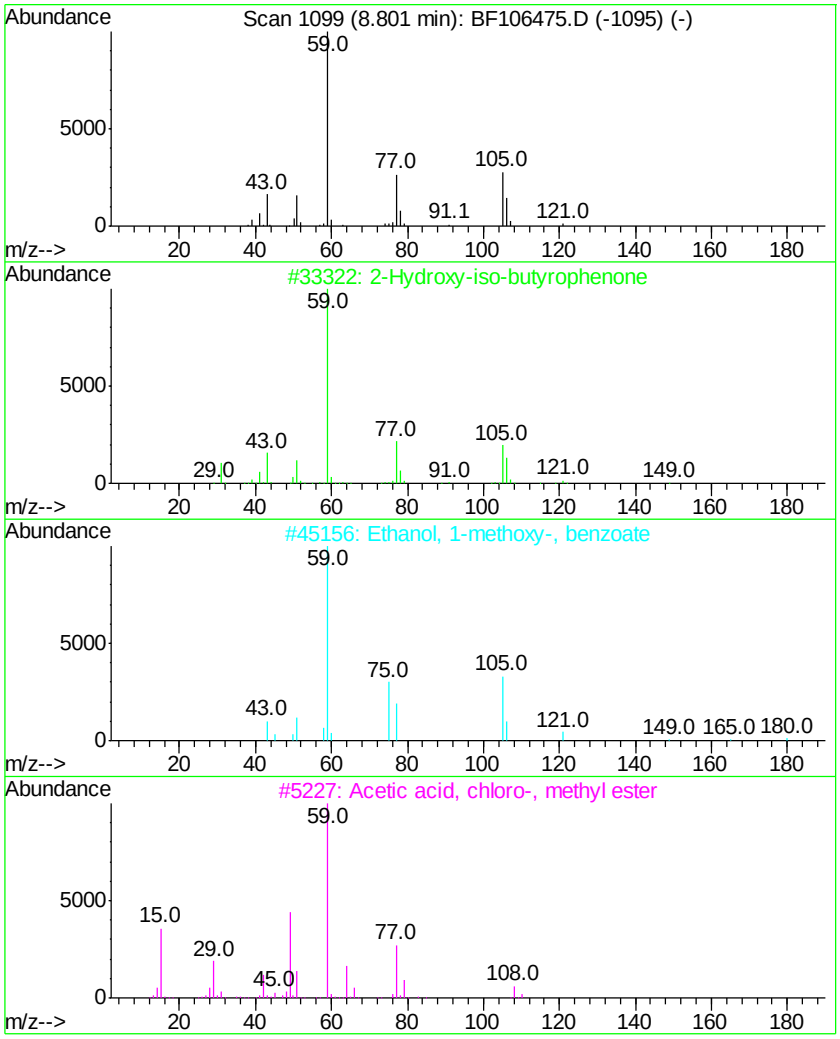
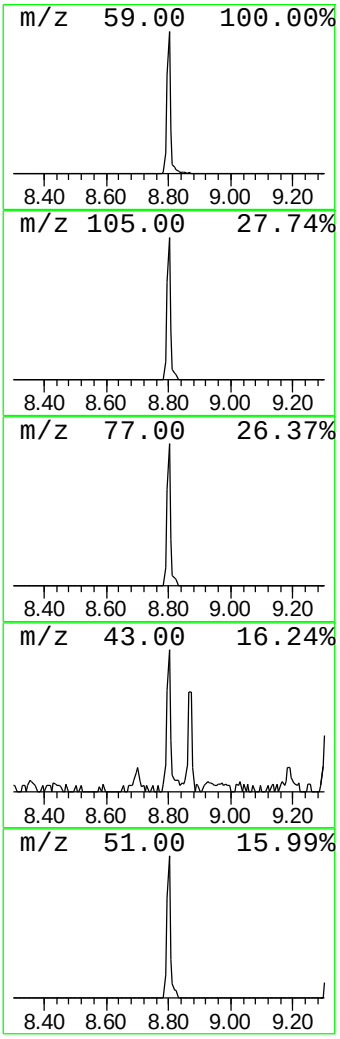
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	2.39 ng	89492	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	72
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	9
4	Guanidine	59	CH5N3	000113-00-8	7
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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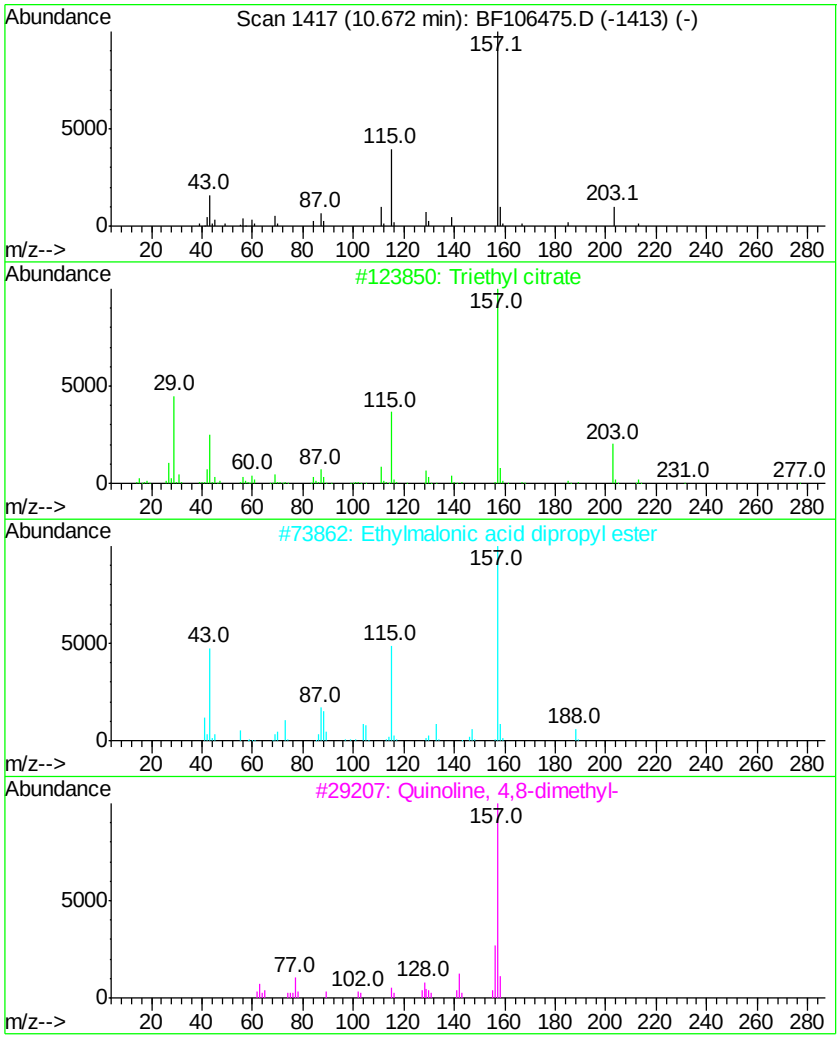
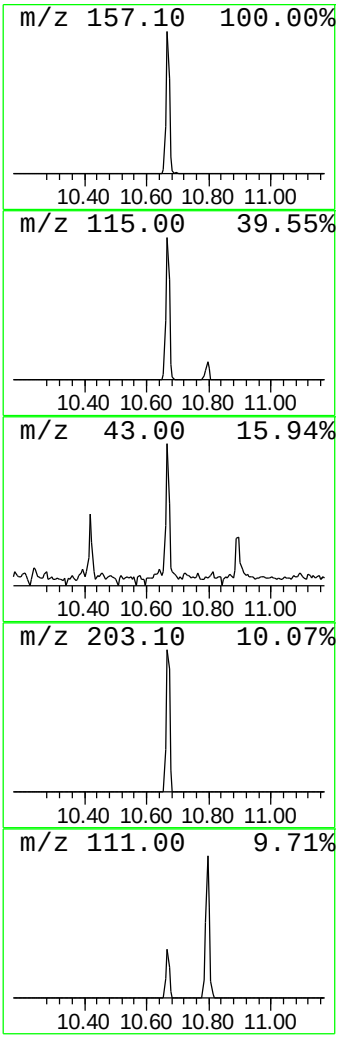
Peak Number 5 Triethyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.14 ng	74190	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	91
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	64
3	Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	40
4	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	36
5	3-Chloro2-fluorobenzoic acid, 3-...	370	C21H32ClFO2	1000338-64-6	36





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Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061218-DBRI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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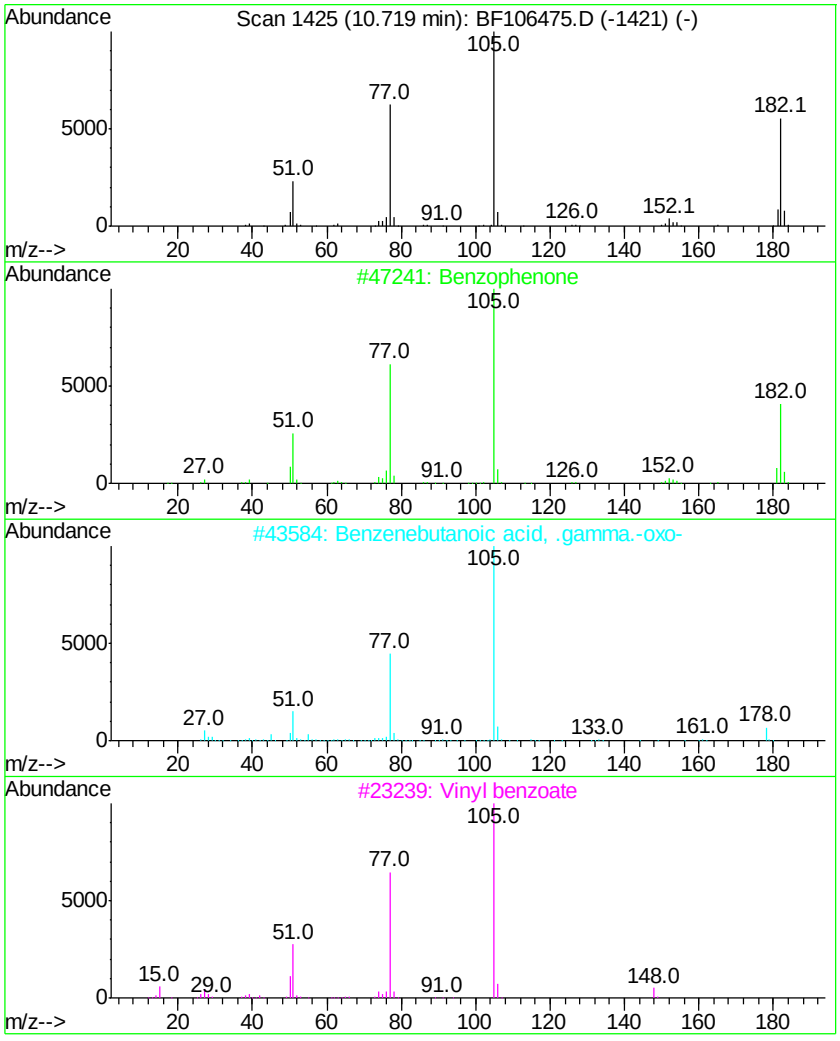
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

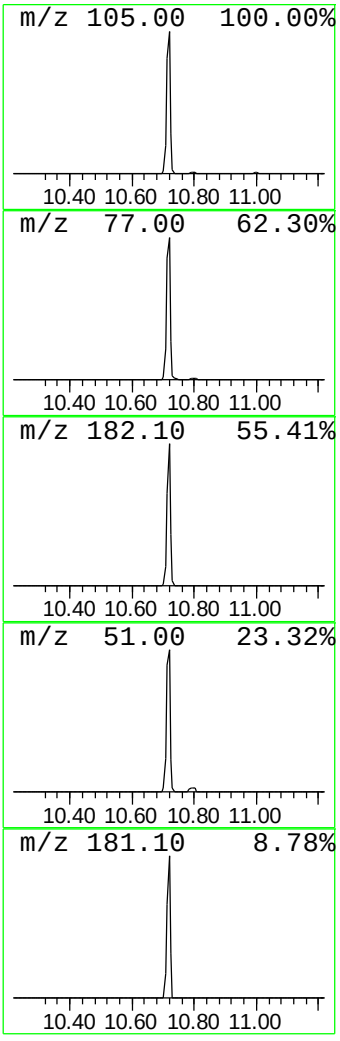
****

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	7.19 ng	249796	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	Benzoic acid, 3,5-difluophenyl e...	234	C13H8F2O2	1000357-79-5	47
5	Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47





Library Search Compound Report

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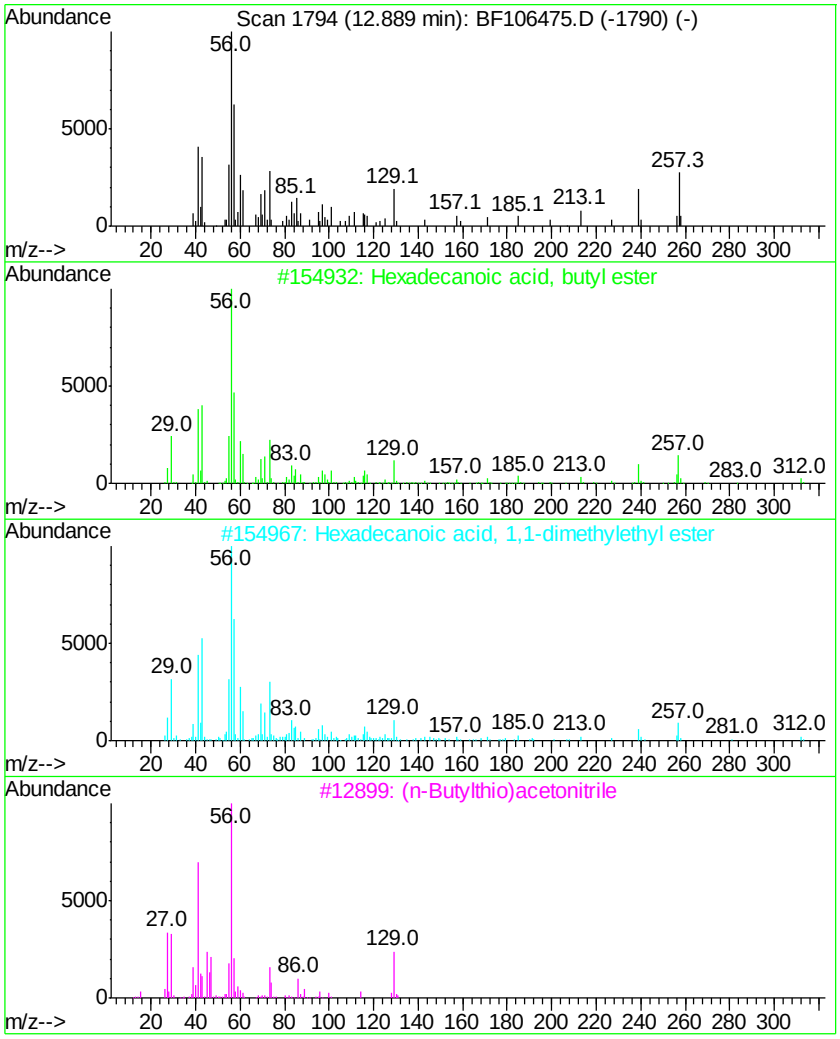
TIC Integration Parameters: LSCINT.P

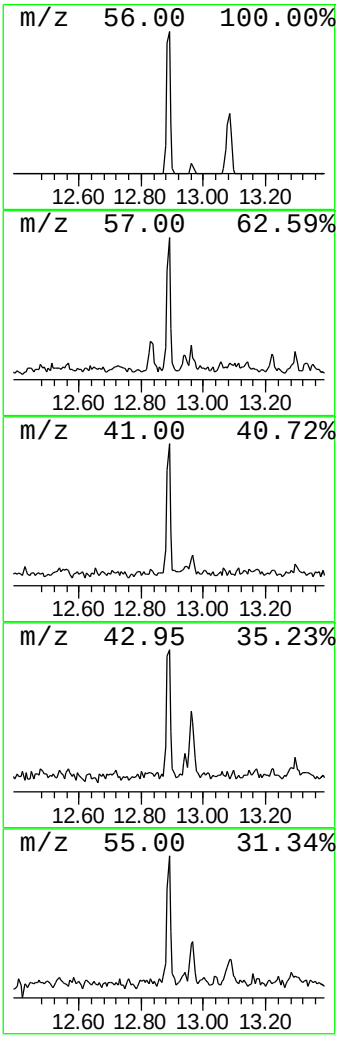
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	2.06 ng	84586	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3	(n-Butylthio)acetonitrile	129	C6H11NS	071037-08-6	38
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	35





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...	5.20	2.6	ng	87600	1	6.97	671669	20.0
unknown6.74	6.74	52.1	ng	1751340	1	6.97	671669	20.0
2-Hydroxy-iso-but...	8.80	2.4	ng	89492	2	8.25	750073	20.0
Triethyl citrate	10.67	2.1	ng	74190	3	10.01	694498	20.0
Benzophenone	10.72	7.2	ng	249796	3	10.01	694498	20.0
Hexadecanoic acid...	12.89	2.1	ng	84586	5	14.15	821663	20.0