LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106469.D
Acq On : 15 Jun 2018 3:44
Operator : JU/SJ
Sample : J3474-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-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	5.195	483	486	494	rVB	93321	92448	3.15%	0.503%
2	5.619	554	558	568	rVB	1019888	1108922	37.76%	6.034%
3	6.613	723	727	735	rBV	712205	767746	26.14%	4.178%
4	6.748	746	750	753	rBV	1790441	1663800	56.66%	9.054%
5	6.966	783	787	790	rBV	825101	632286	21.53%	3.441%
6	7.125	810	814	817	rVB	2543236	2232816	76.03%	12.150%
7	7.531	878	883	886	rBV	1852362	1753137	59.70%	9.540%
8	8.248	1001	1005	1008	rBV	867845	685830	23.35%	3.732%
9	9.325	1183	1188	1191	rBV	2893395	2643031	90.00%	14.382%
10	9.713	1249	1254	1259	rBV	78610	68105	2.32%	0.371%
11	10.007	1297	1304	1312	rVB	737642	637216	21.70%	3.467%
12	10.666	1414	1416	1419	rBV	108772	79481	2.71%	0.433%
13	10.795	1434	1438	1442	rBV	1103730	1014753	34.55%	5.522%
14	10.895	1452	1455	1464	rBV	31364	32429	1.10%	0.176%
15	11.495	1554	1557	1561	rBV	732068	645954	22.00%	3.515%
16	13.083	1823	1827	1830	rBV	3067617	2936712	100.00%	15.980%
17	13.965	1974	1977	1982	rBV4	25084	33419	1.14%	0.182%
18	14.148	2004	2008	2011	rBV	843581	743512	25.32%	4.046%
19	15.001	2150	2153	2161	rVB	60789	68958	2.35%	0.375%
20	15.677	2263	2268	2279	rBV	380427	536383	18.26%	2.919%

Sum of corrected areas: 18376938

LSC Report - Integrated Chromatogram

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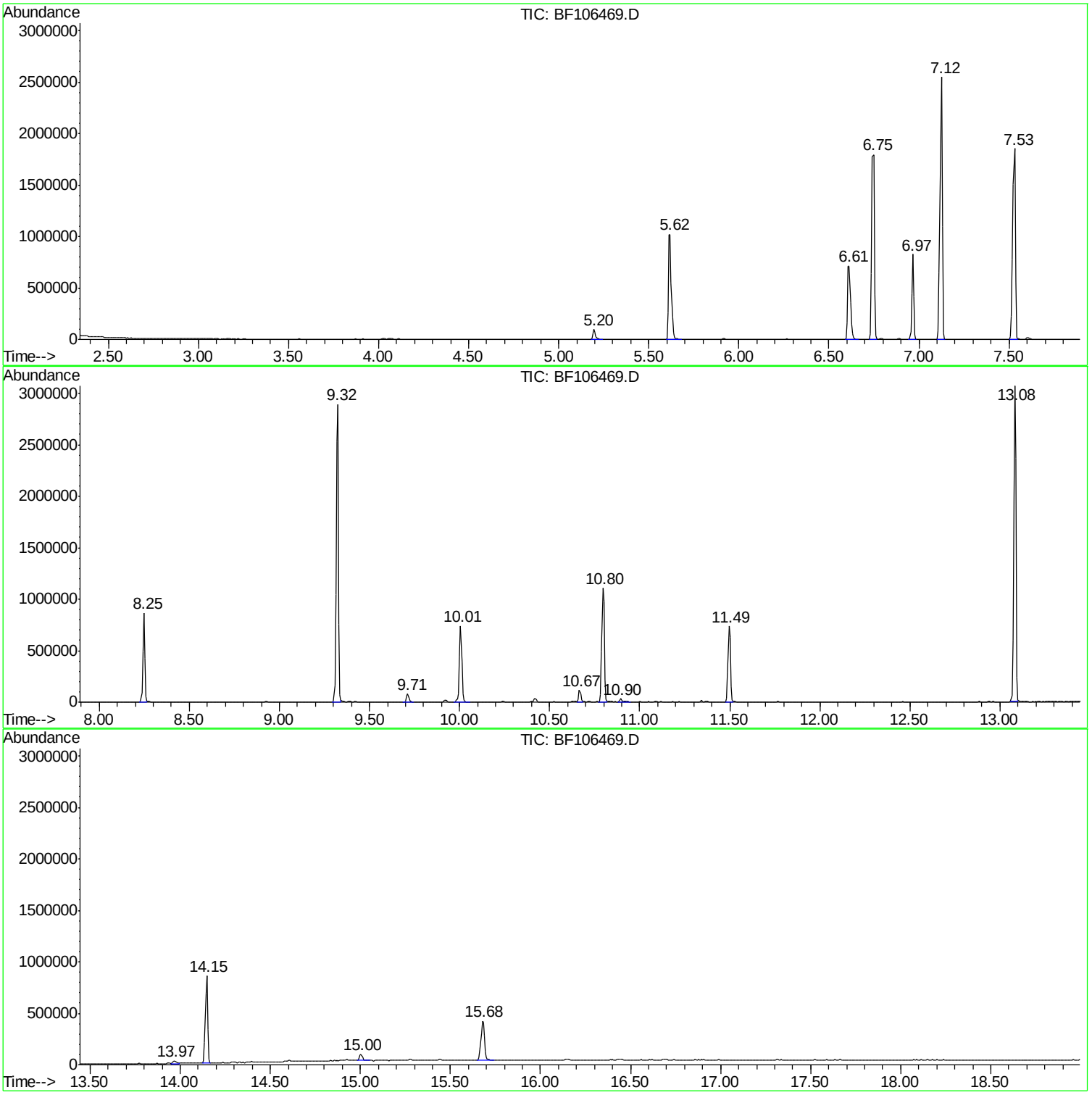
Sample : J3474-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
061118-DBRI-E-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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106469.D
Acq On : 15 Jun 2018 3:44
Operator : JU/SJ
Sample : J3474-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-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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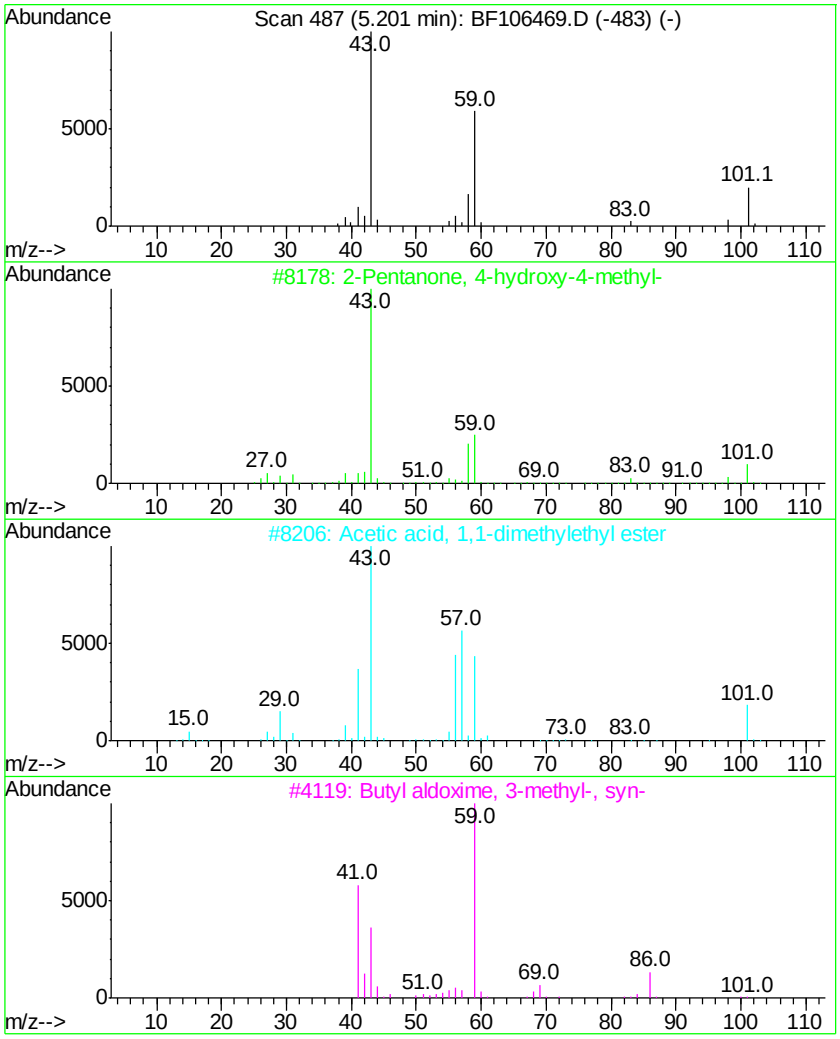
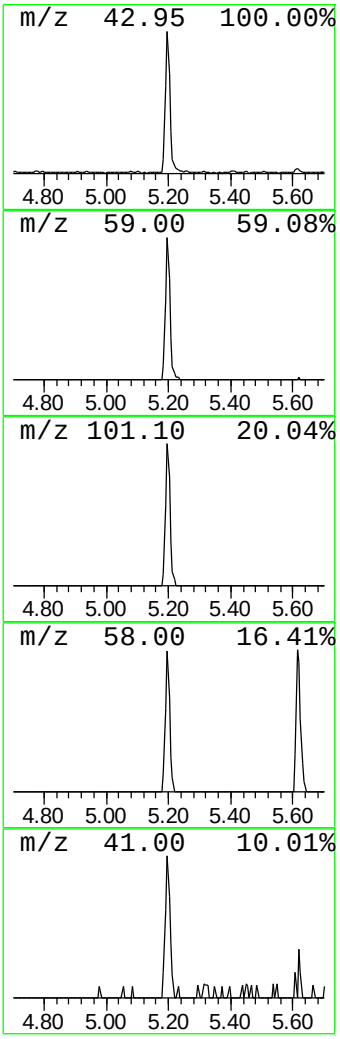
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.92 ng	92448	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	12





Library Search Compound Report

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Operator : JU/SJ
Sample : J3474-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-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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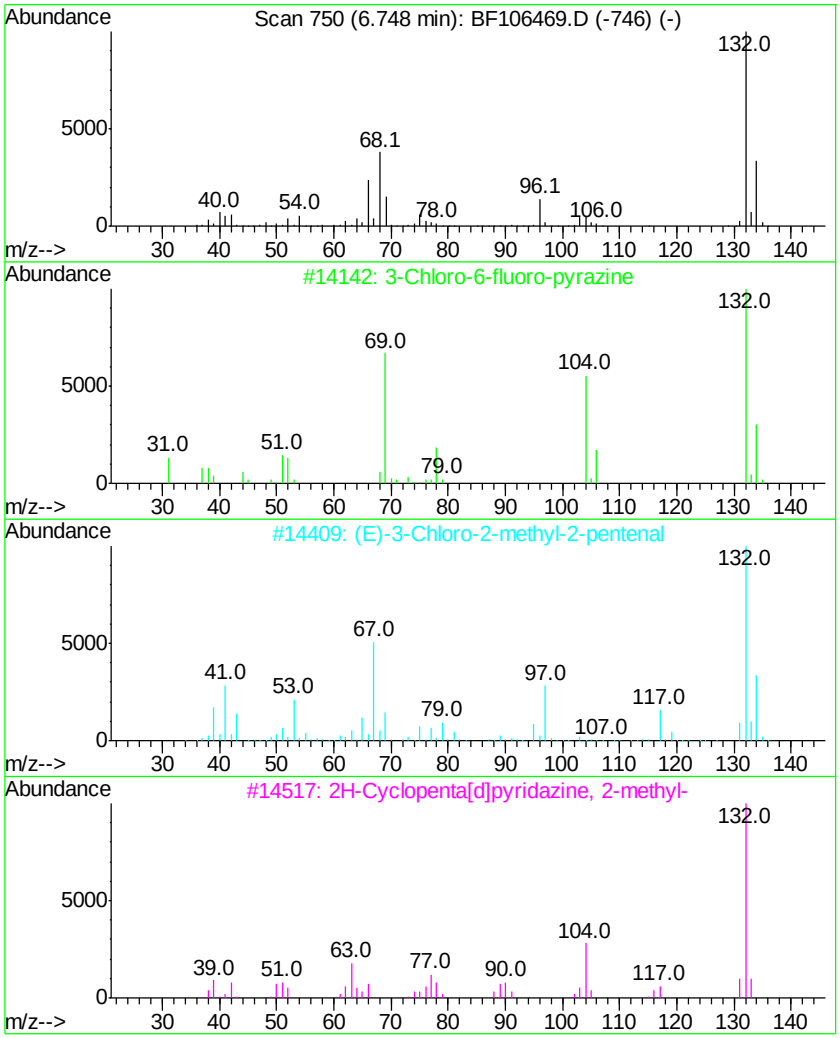
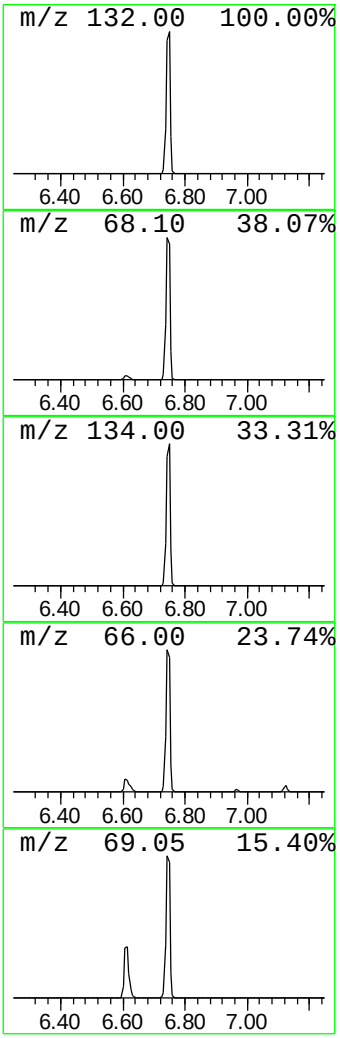
Peak Number 2 unknown6.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	52.63 ng	1663800	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	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061418\
Data File : BF106469.D
Acq On : 15 Jun 2018 3:44
Operator : JU/SJ
Sample : J3474-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-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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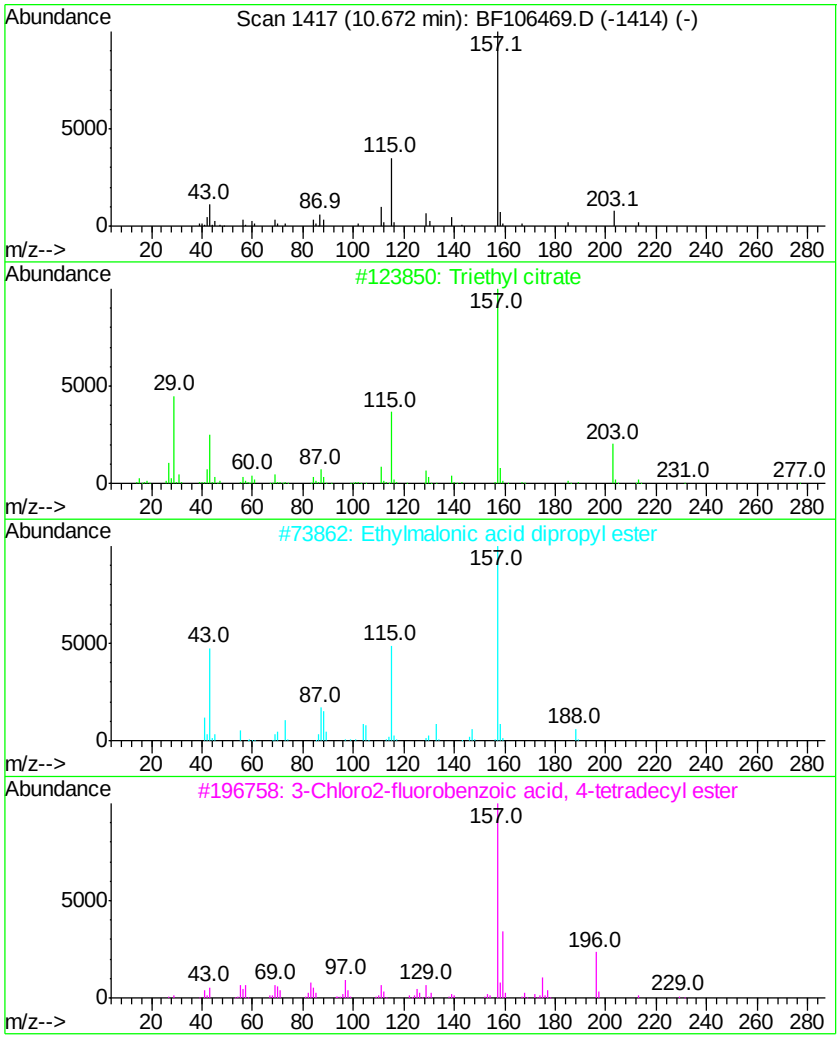
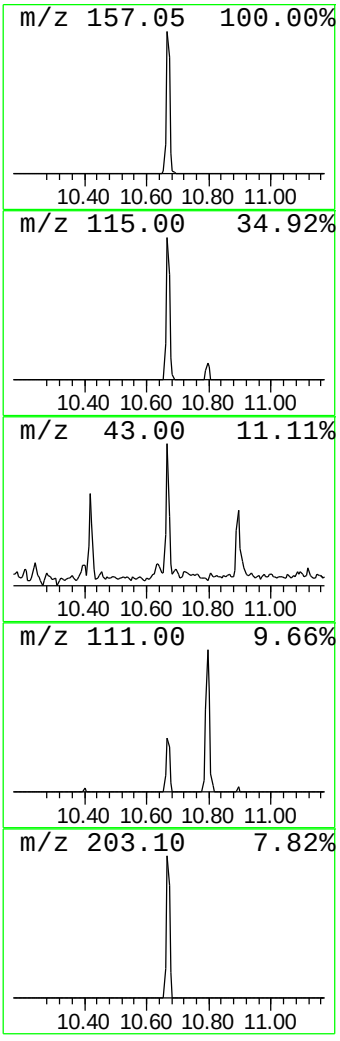
Peak Number 4 Triethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	2.49 ng	79481	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	3-Chloro2-fluorobenzoic acid, 4-...	370	C21H32ClFO2	1000338-64-7	40
4	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-79-9	38
5	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	38





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Sample : J3474-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 061118-DBRI-E-D-M

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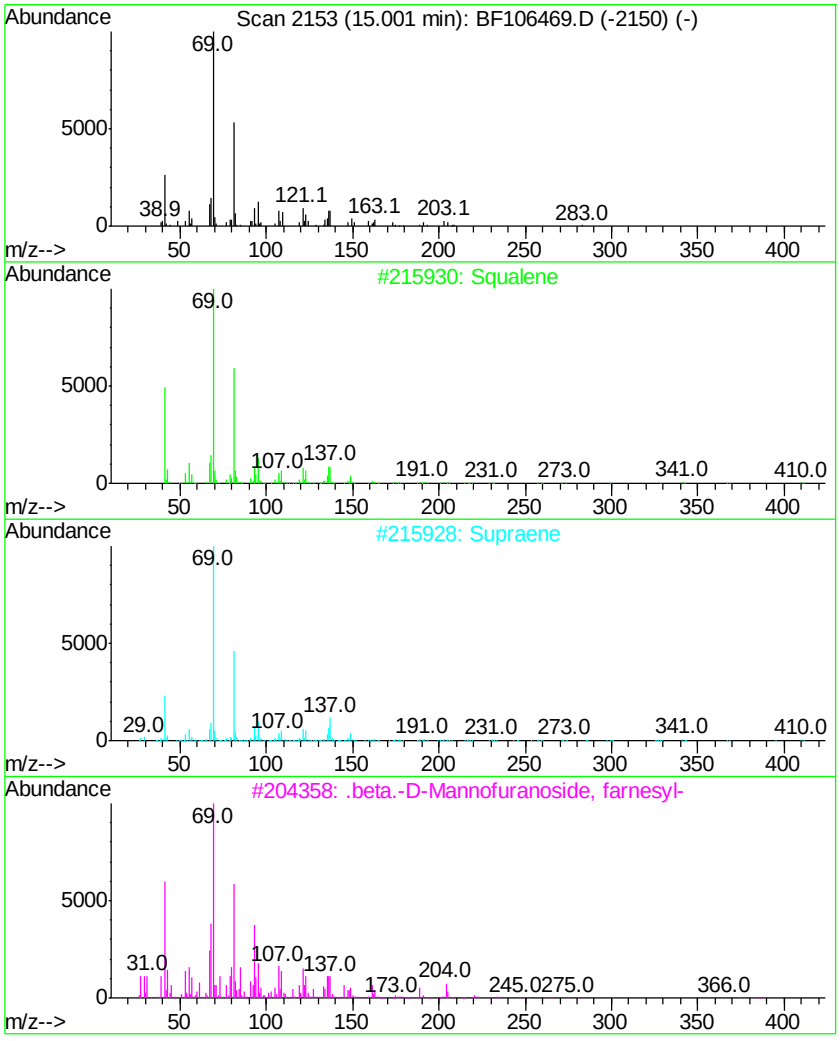
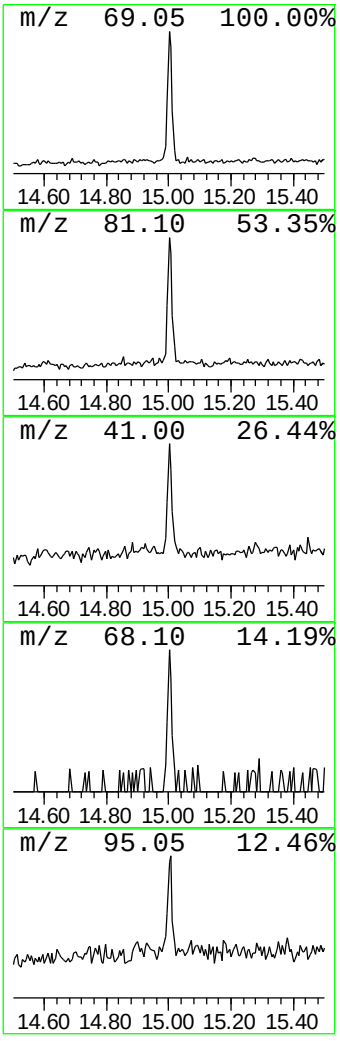
Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.57 ng	68958	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	.beta.-D-Mannofuranoside, farnesyl-	384	C21H36O6	1000155-15-5	83
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	74





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	2.9	ng	92448	1	6.97	632286	20.0
unknown6.75	6.75	52.6	ng	1663800	1	6.97	632286	20.0
Triethyl citrate	10.67	2.5	ng	79481	3	10.01	637216	20.0
Squalene	15.00	2.6	ng	68958	6	15.68	536383	20.0