LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG080318\
Data File : BG036099.D
Acq On : 3 Aug 2018 18:14
Operator : JU/SJ
Sample : J4303-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-A05

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_G\METHODS\8270-BG071218.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	5.133	307	314	324	rBV2	27263	49113	1.55%	0.410%
2	5.603	387	394	408	rBV	266148	465434	14.66%	3.889%
3	7.189	655	664	682	rBV	174725	366995	11.56%	3.066%
4	7.553	719	726	739	rBV	470925	859695	27.08%	7.183%
5	8.023	800	806	813	rBV	97517	164396	5.18%	1.374%
6	8.346	854	861	868	rBV	417520	734220	23.13%	6.135%
7	9.127	989	994	997	rBV	24902	37566	1.18%	0.314%
8	9.186	997	1004	1017	rVB	335243	672285	21.18%	5.617%
9	10.226	1174	1181	1189	rVB2	37853	69040	2.17%	0.577%
10	10.825	1273	1283	1296	rBV	110552	244079	7.69%	2.039%
11	12.364	1539	1545	1551	rBV5	20237	33541	1.06%	0.280%
12	13.269	1691	1699	1706	rBV	924907	1503911	47.37%	12.566%
13	13.956	1808	1816	1824	rBV	11786	39681	1.25%	0.332%
14	14.097	1835	1840	1848	rBV	31165	58804	1.85%	0.491%
15	14.644	1923	1933	1940	rBV2	194798	345078	10.87%	2.883%
16	15.243	2029	2035	2040	rBV6	30496	71314	2.25%	0.596%
17	15.348	2048	2053	2056	rBV3	35283	53303	1.68%	0.445%
18	16.136	2180	2187	2199	rBV	850945	1395853	43.97%	11.663%
19	17.387	2395	2400	2409	rBV	292150	473077	14.90%	3.953%
20	19.995	2838	2844	2853	rBV	2436842	3174719	100.00%	26.526%
21	21.652	3119	3126	3138	rBV	350019	610963	19.24%	5.105%
22	24.847	3660	3670	3686	rBV2	171156	545359	17.18%	4.557%

Sum of corrected areas: 11968426

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG080318\
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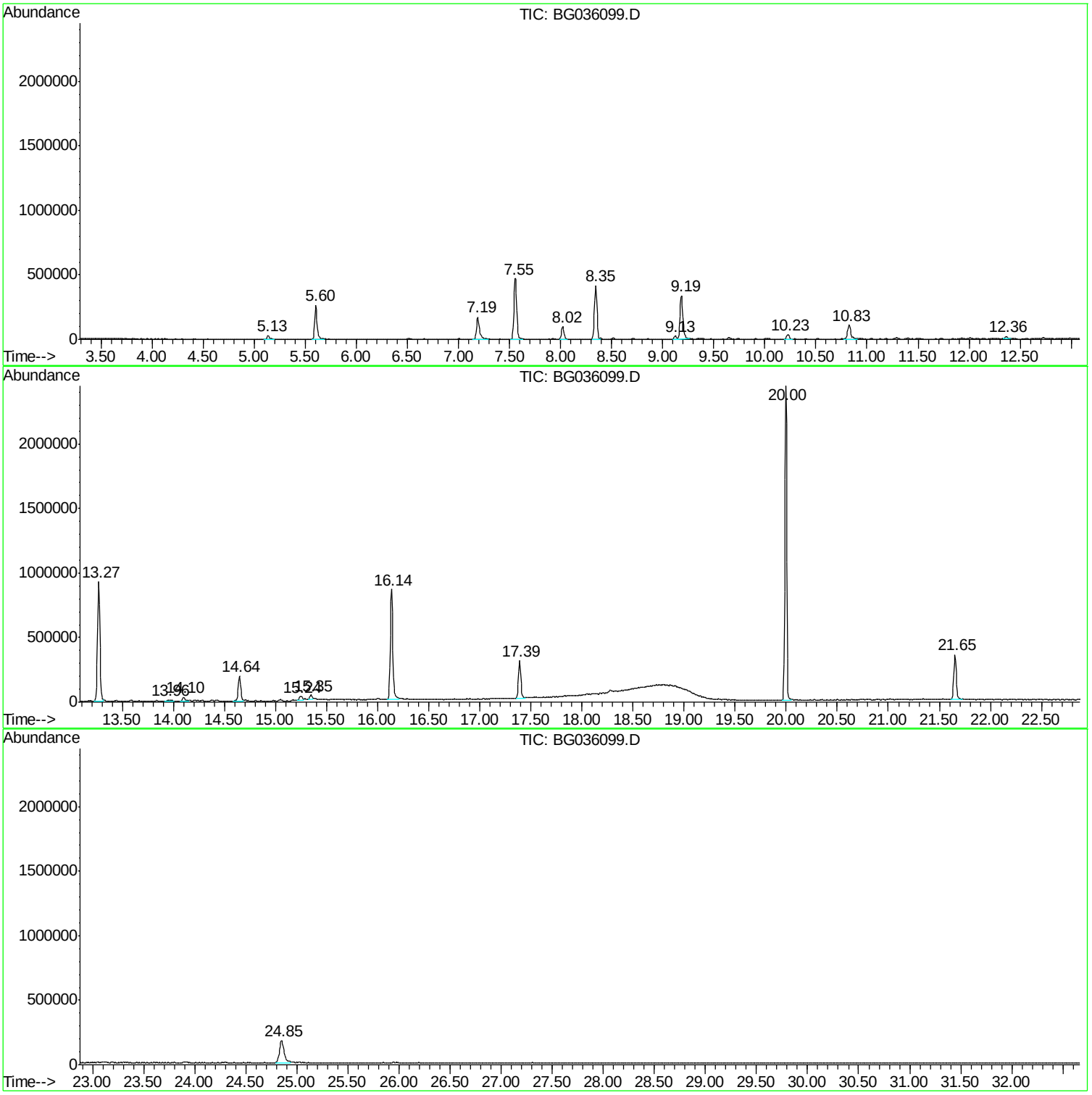
Operator : JU/SJ
Sample : J4303-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-A05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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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Data File : BG036099.D
Acq On : 3 Aug 2018 18:14
Operator : JU/SJ
Sample : J4303-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-A05

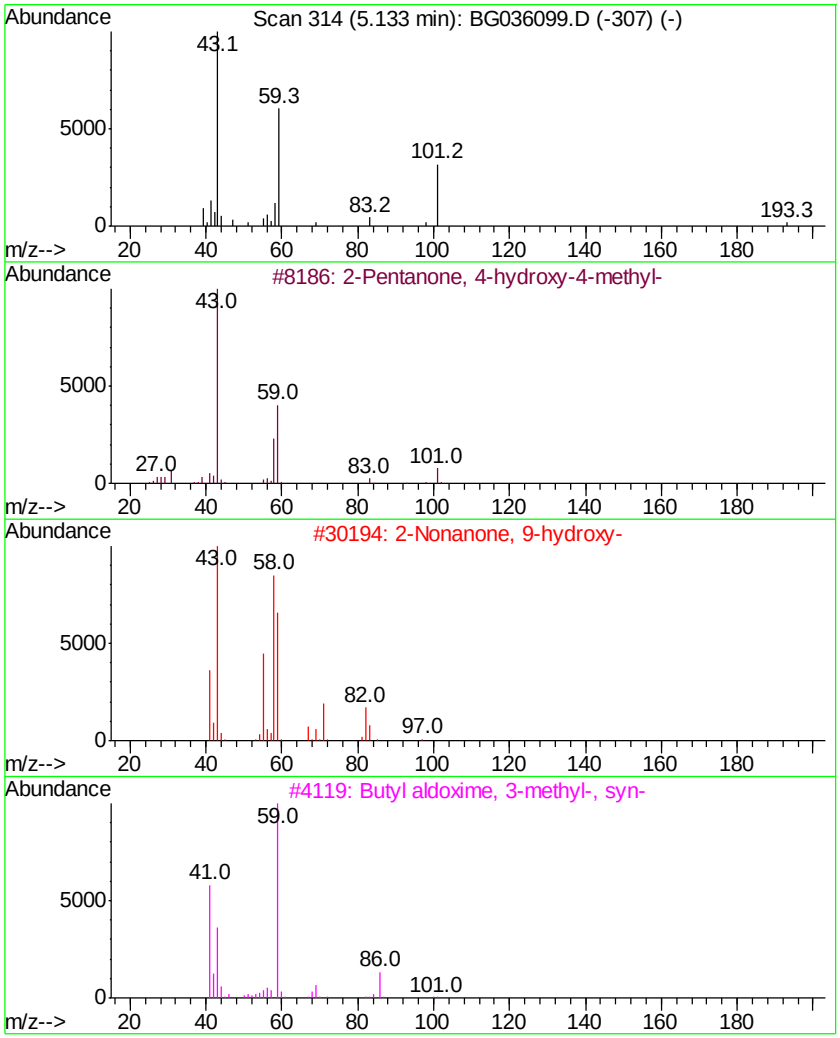
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

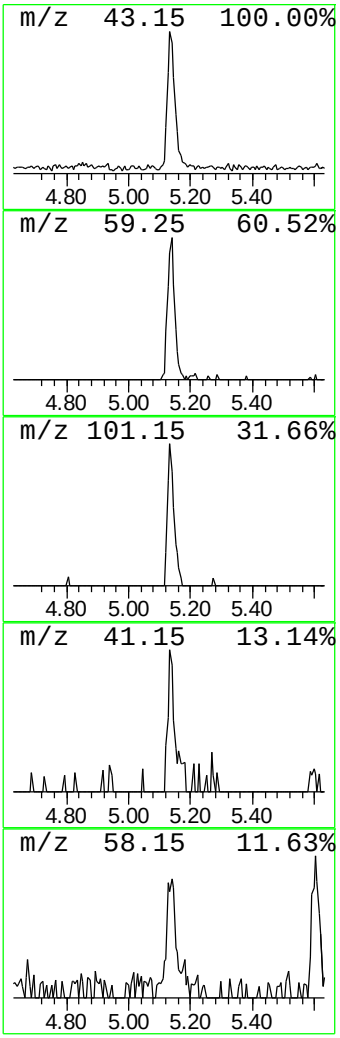
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	5.97 ng	49113	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

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Data File : BG036099.D
Acq On : 3 Aug 2018 18:14
Operator : JU/SJ
Sample : J4303-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-A05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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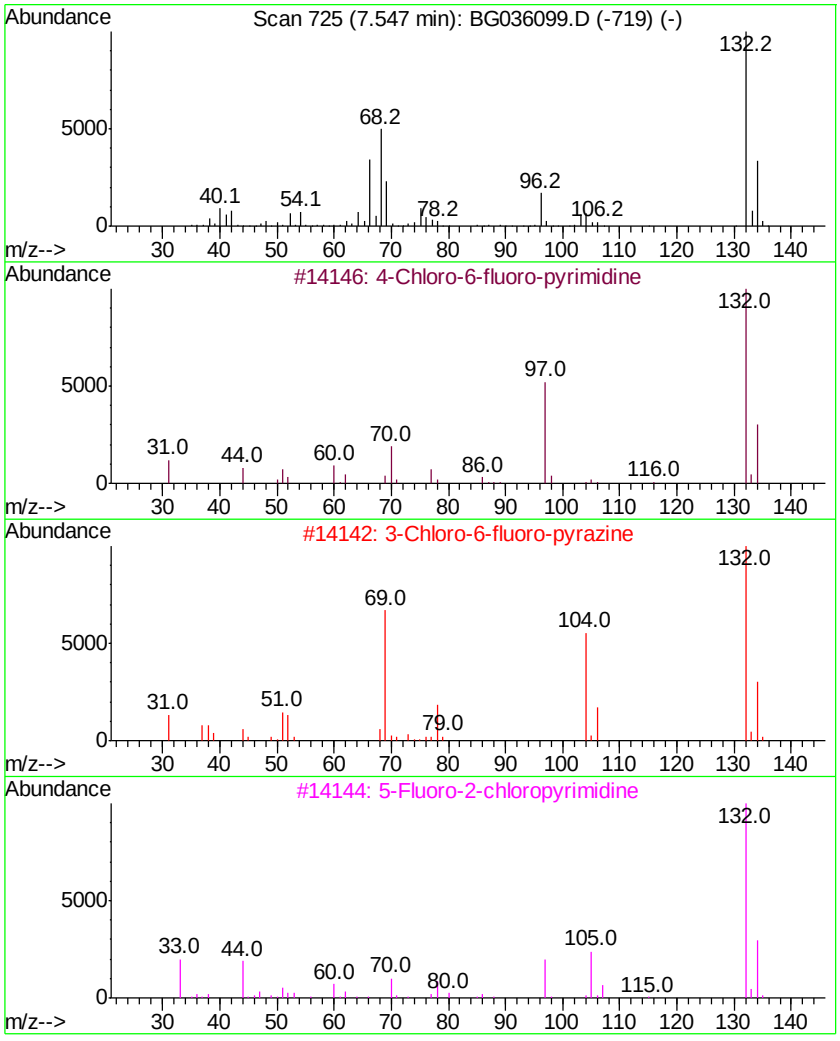
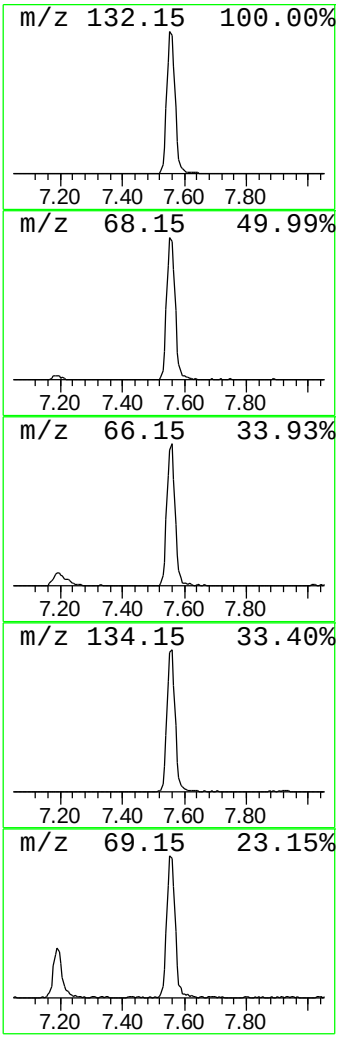
****

Peak Number 2 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	104.59 ng	859695	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	14
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12





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Data File : BG036099.D
Acq On : 3 Aug 2018 18:14
Operator : JU/SJ
Sample : J4303-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-A05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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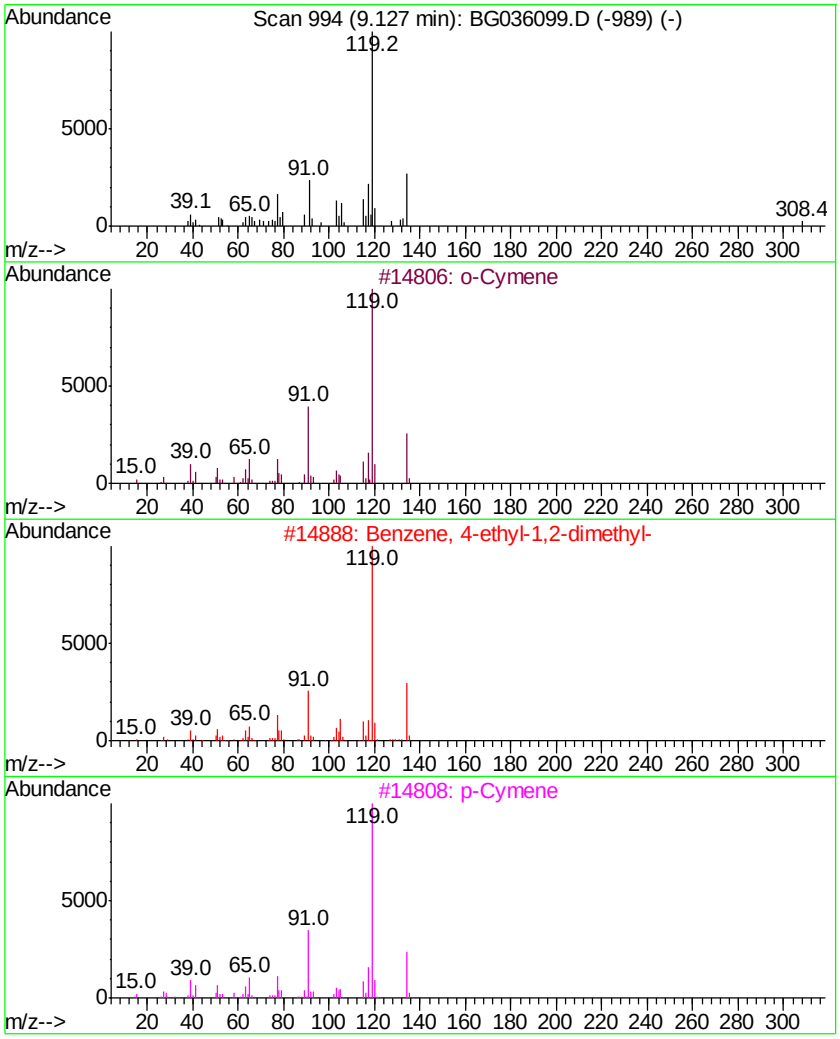
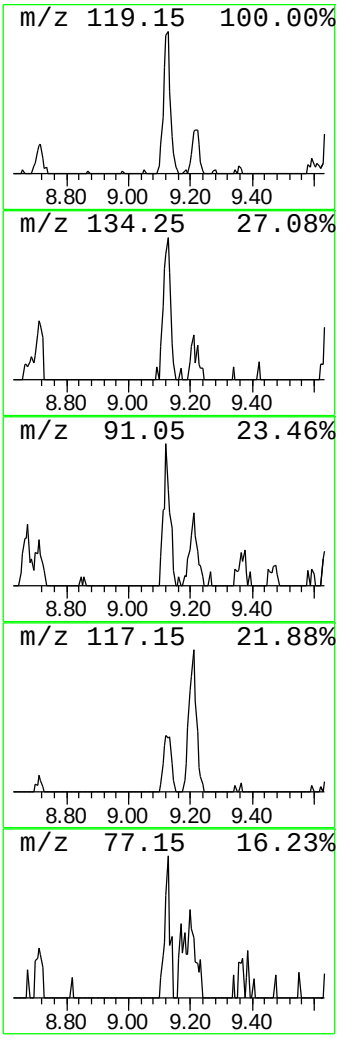
****

Peak Number 4 o-Cymene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.13	4.57 ng	37566	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	90
2	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	87
3	p-Cymene	134	C10H14	000099-87-6	83
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	81
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	81





Library Search Compound Report

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Data File : BG036099.D
Acq On : 3 Aug 2018 18:14
Operator : JU/SJ
Sample : J4303-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-A05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

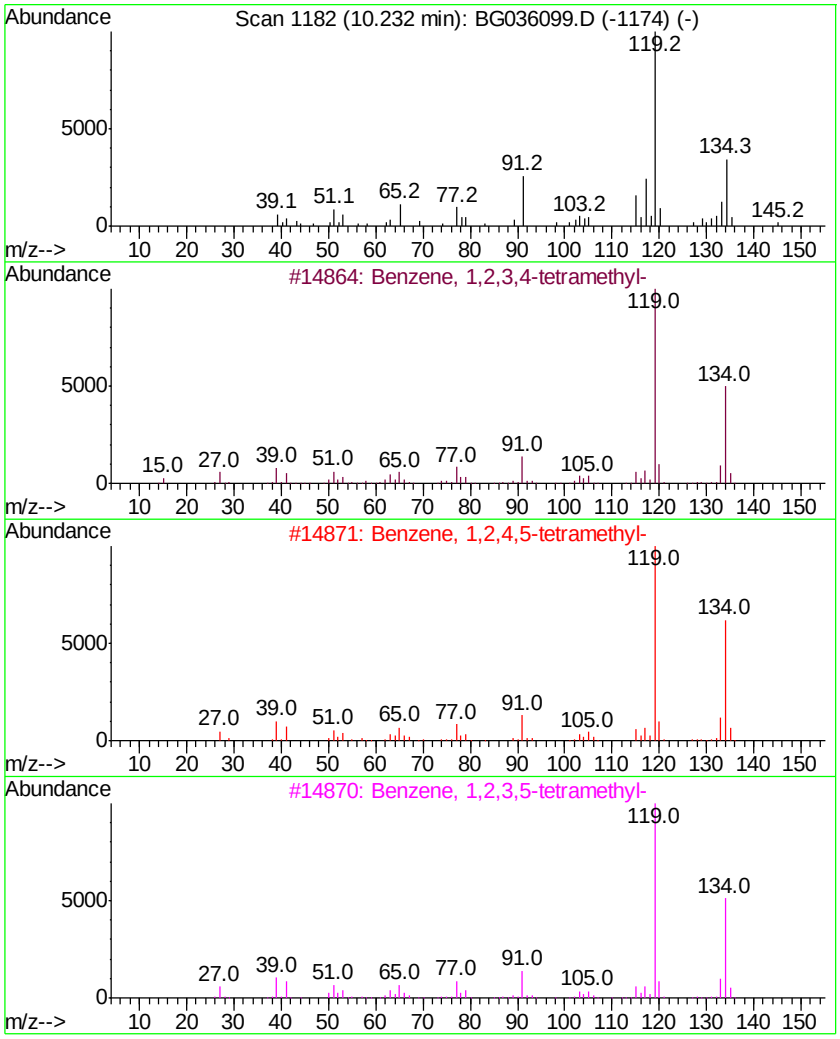
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

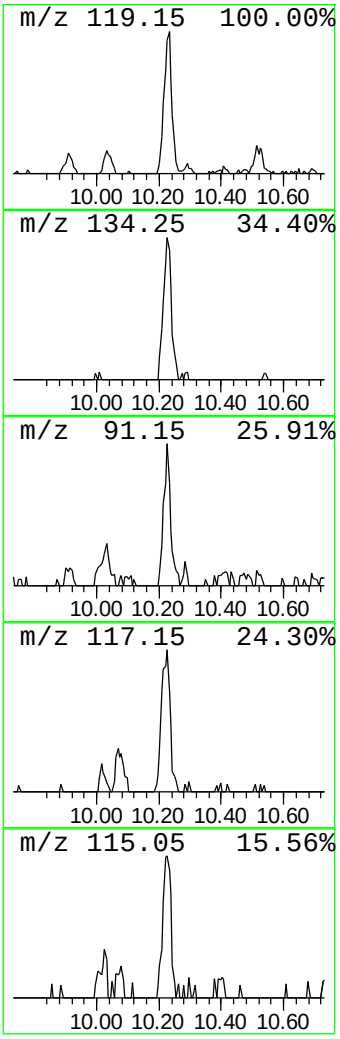
****

Peak Number 5 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.23	5.66 ng	69040	Naphthalene-d8	10.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	81
2	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	81
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	81
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	74
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	74





Library Search Compound Report

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Operator : JU/SJ
Sample : J4303-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-A05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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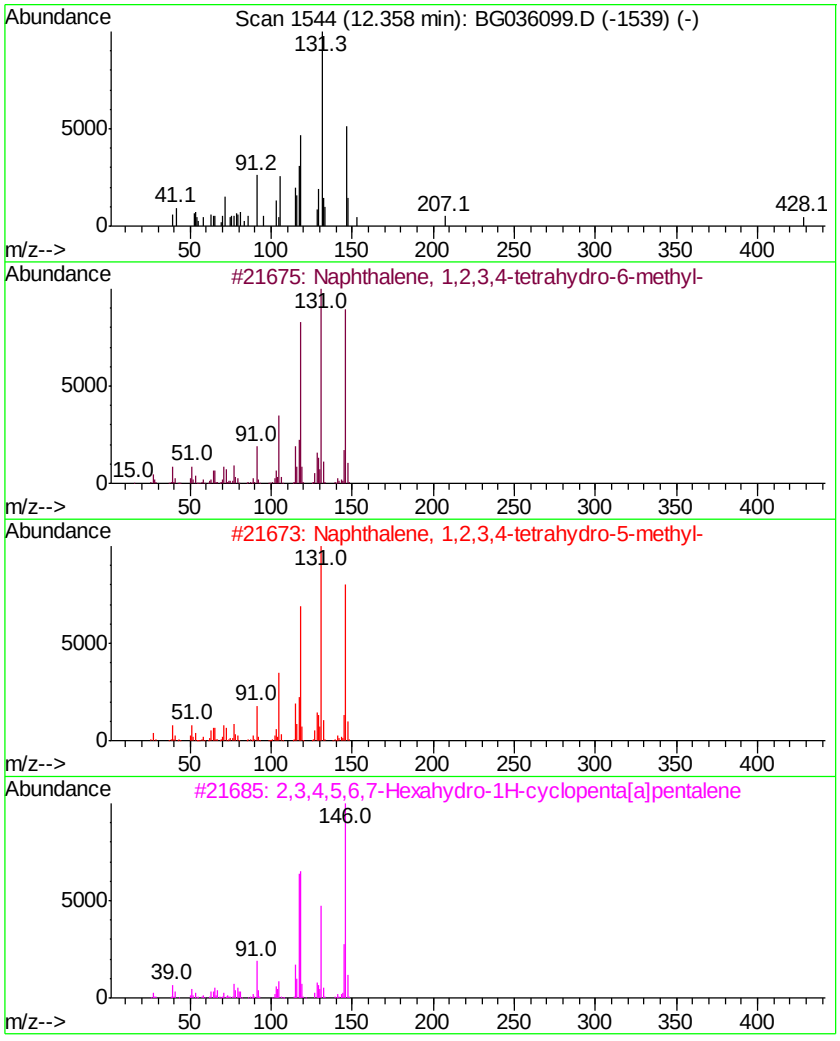
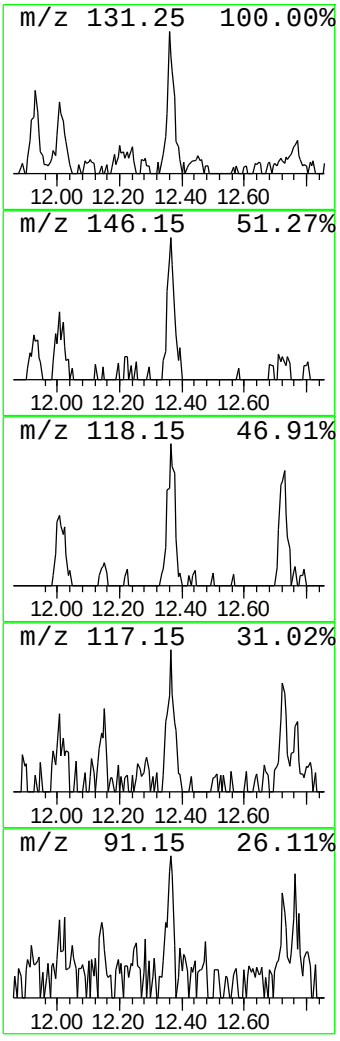
****

Peak Number 6 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	2.75 ng	33541	Naphthalene-d8	10.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	76
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	74
3	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1000189-31-0	49
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	49
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	49





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : MW-A05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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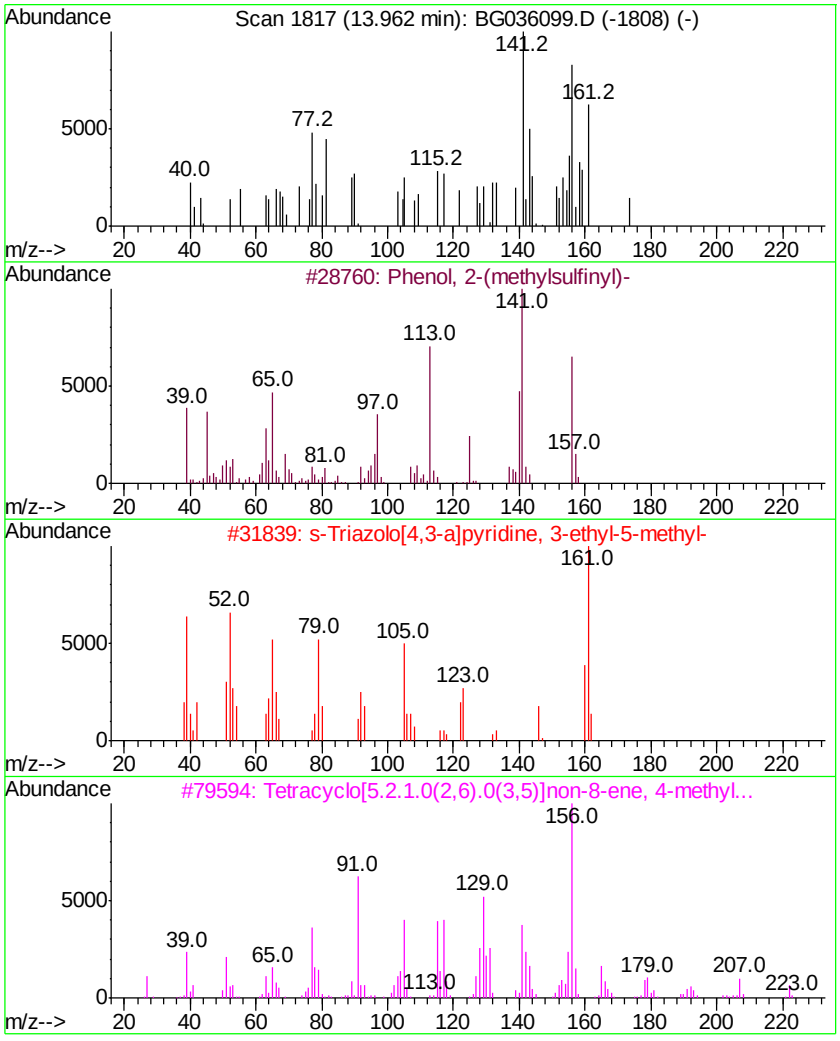
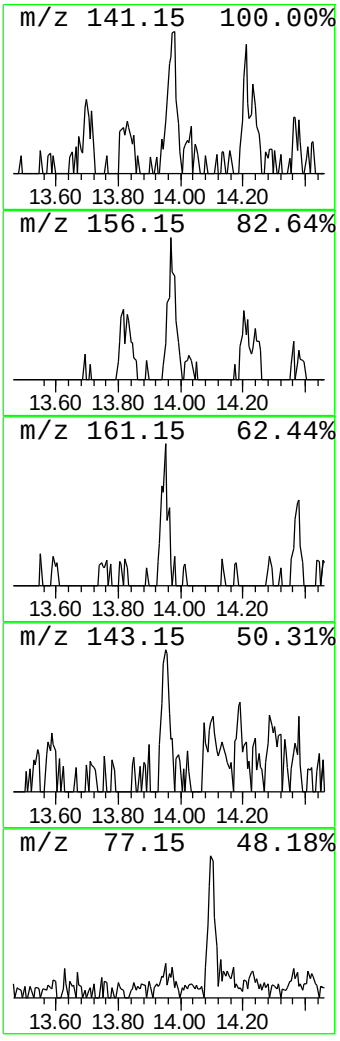
****

Peak Number 7 unknown13.96 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	2.30 ng	39681	Acenaphthene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(methylsulfinyl)-	156	C7H8O2S	001074-02-8	27
2	s-Triazolo[4,3-a]pyridine, 3-eth...	161	C9H11N3	004919-18-0	12
3	Tetracyclo[5.2.1.0(2,6).0(3,5)]n...	222	C17H18	1000154-17-8	10
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	10
5	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	10





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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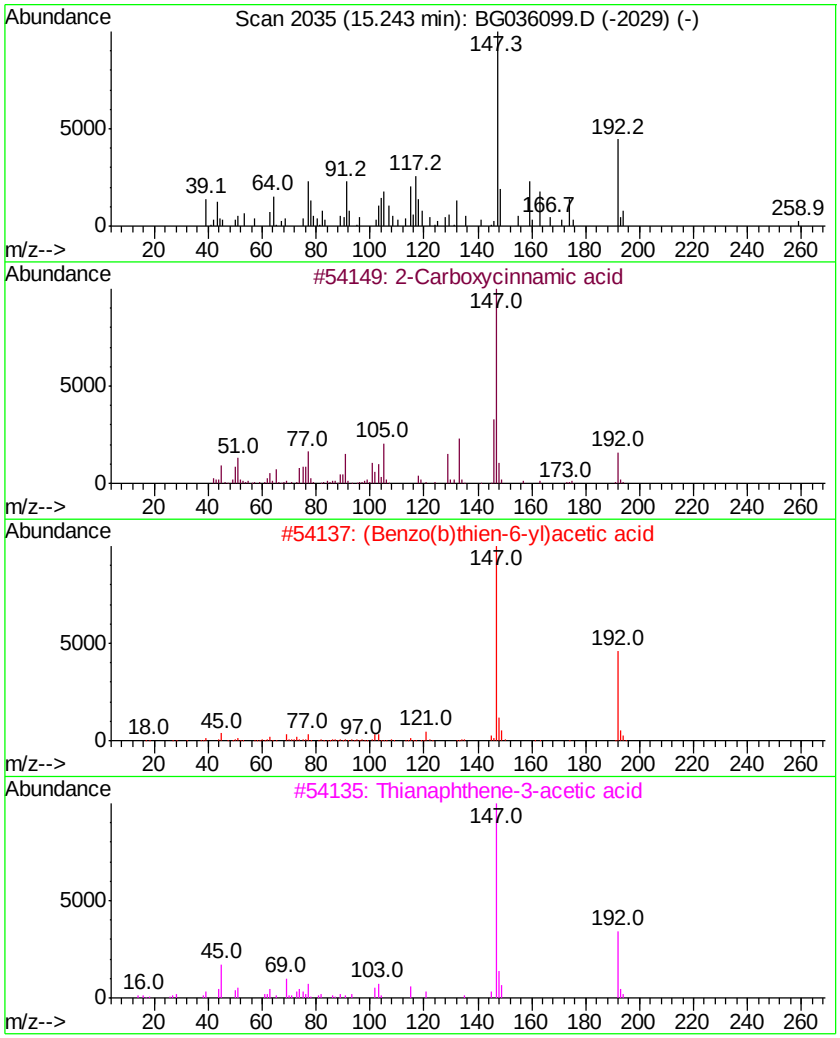
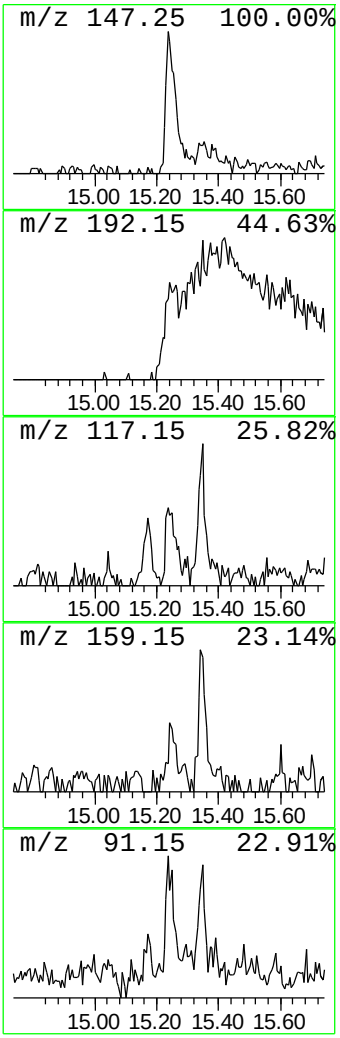
****

Peak Number 8 unknown15.24 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	4.13 ng	71314	Acenaphthene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Carboxycinnamic acid	192	C10H8O4	000612-40-8	43
2	(Benzo(b)thien-6-yl)acetic acid	192	C10H8O2S	006177-87-3	43
3	Thianaphthene-3-acetic acid	192	C10H8O2S	001131-09-5	38
4	2H-Indazol-3-amine, 2-methyl-	147	C8H9N3	097990-19-7	38
5	1,3-Benzenediol, o-propargyloxyc...	192	C10H8O4	1000330-77-2	37





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TIC Library : C:\Database\NIST11.L
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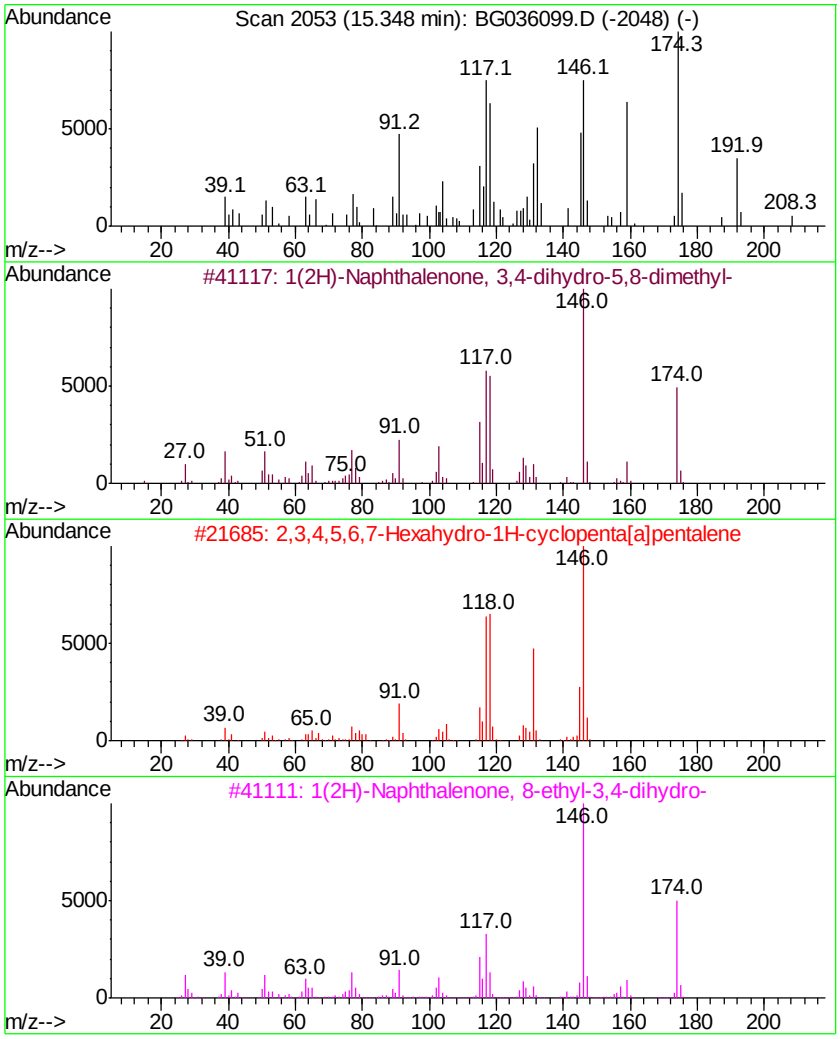
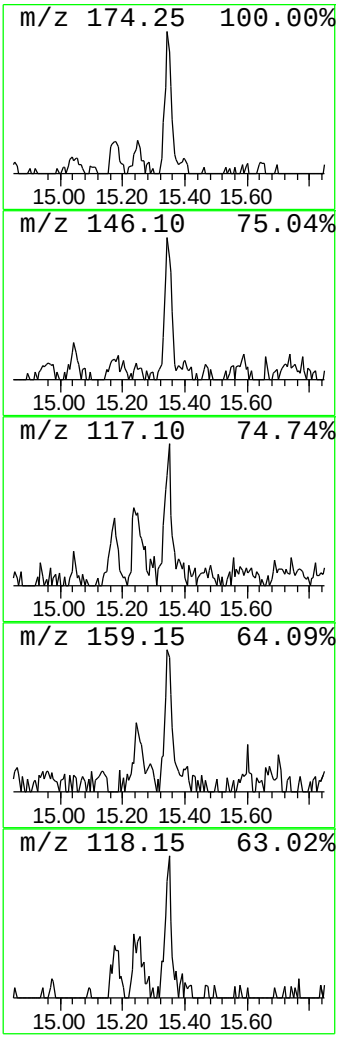
****

Peak Number 9 1(2H)-Naphthalenone, 3,4-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.35	3.09 ng	53303	Acenaphthene-d10	14.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Naphthalenone, 3,4-dihydro...	174	C12H14O	005037-63-8	64
2	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1000189-31-0	55
3	1(2H)-Naphthalenone, 8-ethyl-3,4...	174	C12H14O	051015-33-9	52
4	1(2H)-Naphthalenone, 3,4-dihydro...	174	C12H14O	019550-57-3	50
5	7-Methylindan-1-one	146	C10H10O	039627-61-7	45





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...	5.13	6.0	ng	49113	1	8.02	164396	20.0
unknown7.55	7.55	104.6	ng	859695	1	8.02	164396	20.0
o-Cymene	9.13	4.6	ng	37566	1	8.02	164396	20.0
Benzene, 1,2,3,4-...	10.23	5.7	ng	69040	2	10.83	244079	20.0
Naphthalene, 1,2,...	12.36	2.8	ng	33541	2	10.83	244079	20.0
unknown13.96	13.96	2.3	ng	39681	3	14.64	345078	20.0
unknown15.24	15.24	4.1	ng	71314	3	14.64	345078	20.0
1(2H)-Naphthaleno...	15.35	3.1	ng	53303	3	14.64	345078	20.0