LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100920\
Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

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-BF091020.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	5.375	556	559	582	rBV	1943709	2253087	99.75%	18.059%
2	6.404	729	734	752	rBV	1914280	2258745	100.00%	18.104%
3	6.598	763	767	780	rBV	54779	105811	4.68%	0.848%
4	6.757	790	794	801	rBV	723795	585395	25.92%	4.692%
5	7.322	886	890	903	rBV	1573187	1450663	64.22%	11.627%
6	8.039	1008	1012	1018	rBV	751955	635250	28.12%	5.092%
7	8.481	1085	1087	1093	rBV2	120953	126261	5.59%	1.012%
8	8.539	1093	1097	1100	rBV2	79540	107447	4.76%	0.861%
9	8.575	1100	1103	1105	rBV3	102582	131598	5.83%	1.055%
10	8.663	1115	1118	1120	rBV3	69231	81761	3.62%	0.655%
11	8.781	1135	1138	1140	rBV2	181191	195558	8.66%	1.567%
12	8.804	1140	1142	1147	rVV4	102063	141127	6.25%	1.131%
13	8.922	1159	1162	1165	rBV2	331479	345178	15.28%	2.767%
14	9.033	1177	1181	1183	rBV	392526	499109	22.10%	4.000%
15	9.057	1183	1185	1188	rVV2	214390	248132	10.99%	1.989%
16	9.116	1191	1195	1199	rVV	2307765	2221304	98.34%	17.804%
17	9.157	1199	1202	1204	rBV2	327701	359645	15.92%	2.883%
18	15.368	2254	2258	2263	rVB	591608	730313	32.33%	5.854%

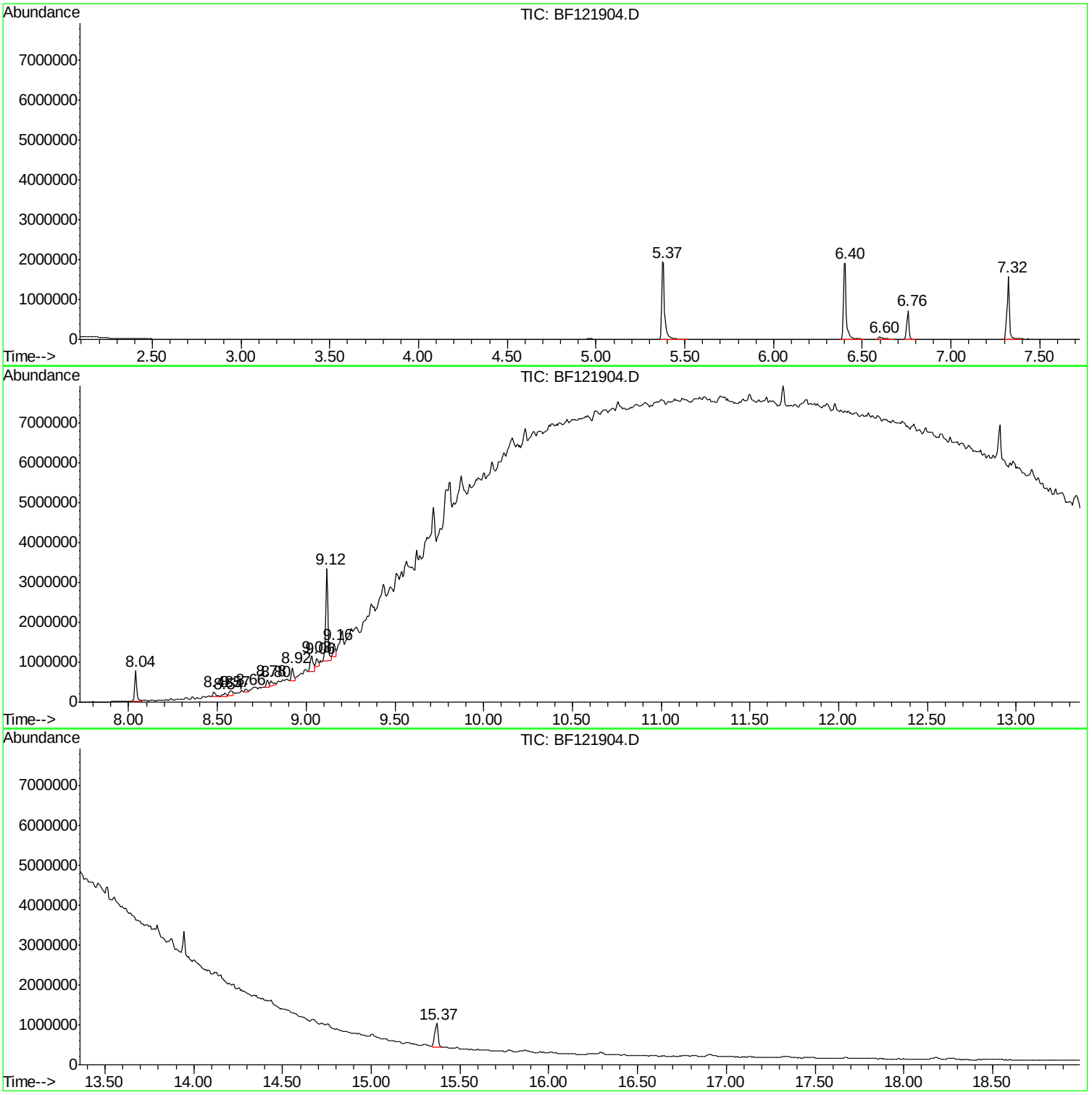
Sum of corrected areas: 12476384

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100920\
Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.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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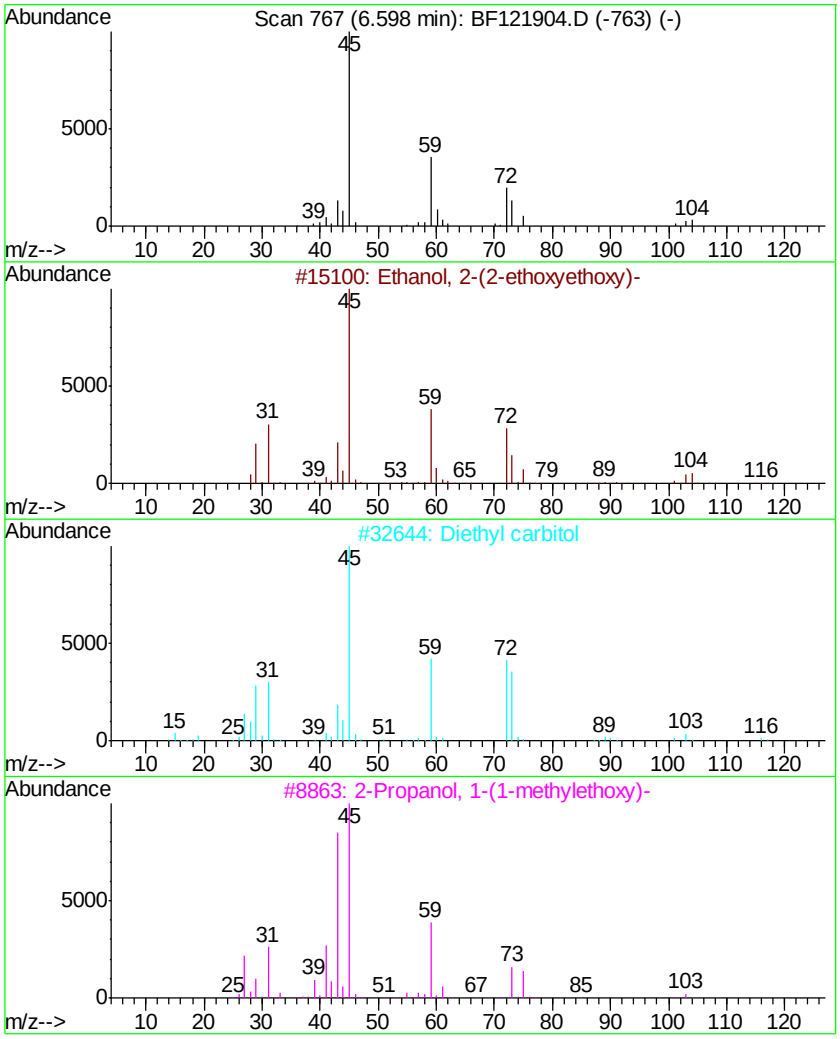
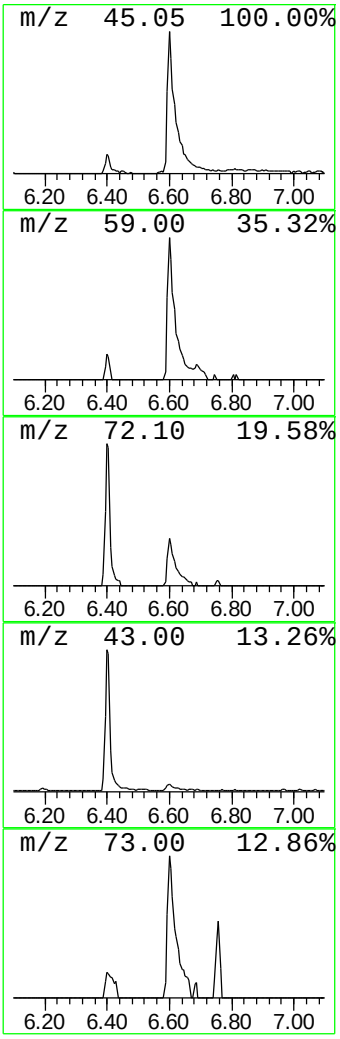
Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	3.62 ng	105811	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	78
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	37





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100920\
Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

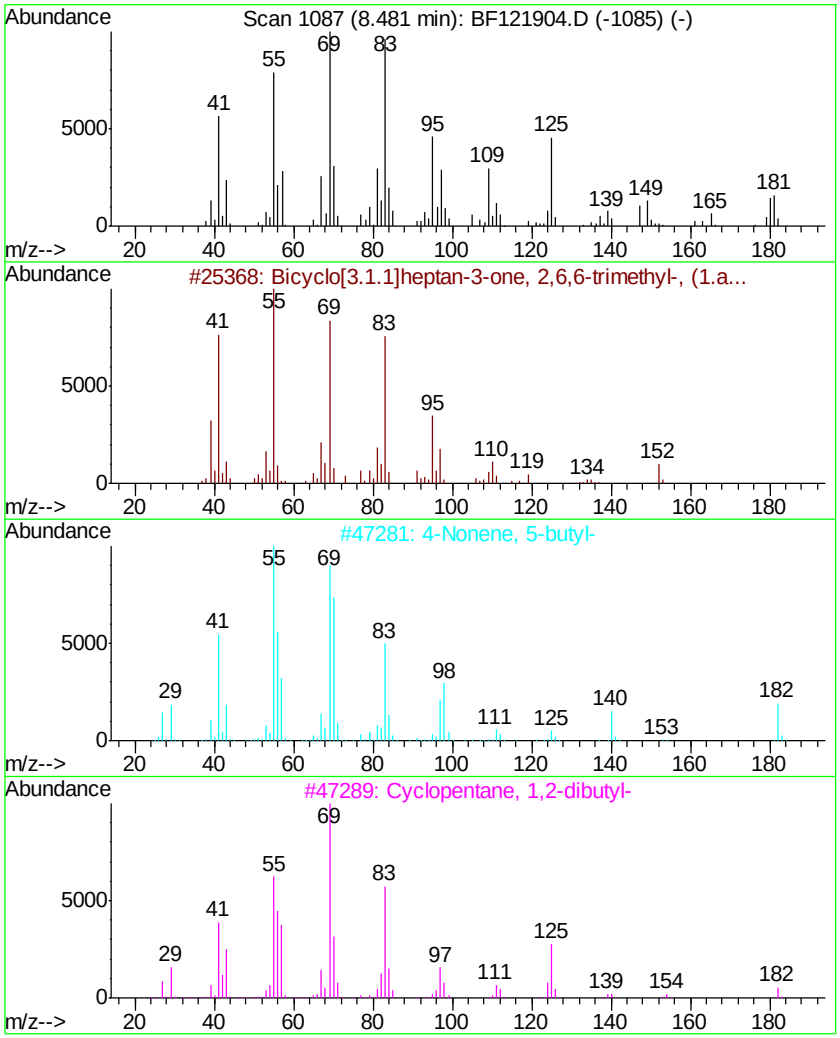
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

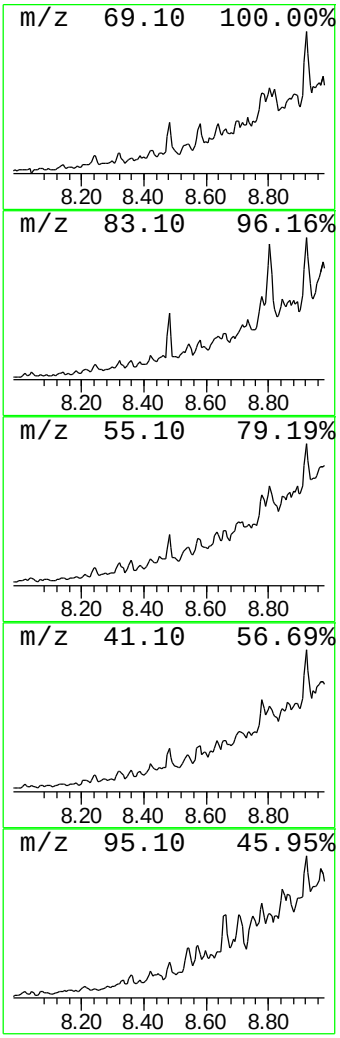
****

Peak Number 2 Bicyclo[3.1.1]heptan-3-one,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.48	3.98 ng	126261	Naphthalene-d8	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	015358-88-0	70
2	4-Nonene, 5-butyl-	182	C13H26	007367-38-6	38
3	Cyclopentane, 1,2-dibutyl-	182	C13H26	062199-52-4	38
4	2,6-Octadienal, 3,7-dimethyl-, (Z)-	152	C10H16O	000106-26-3	30
5	2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	27





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100920\
Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

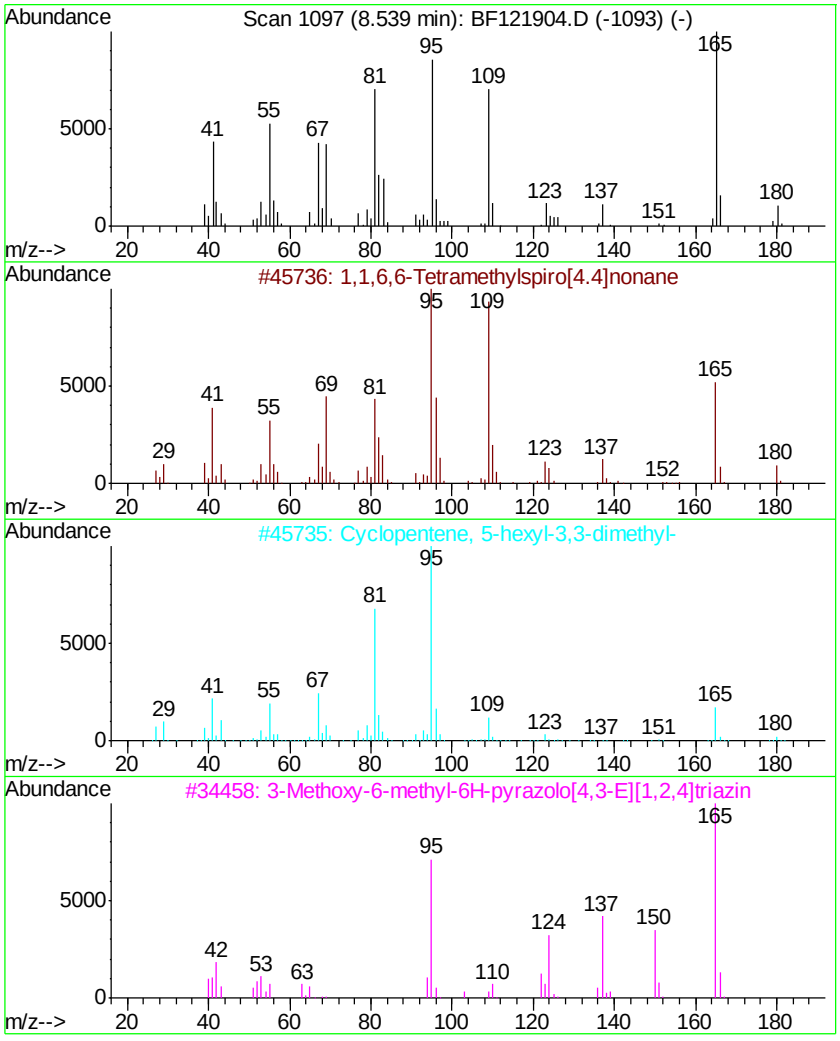
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

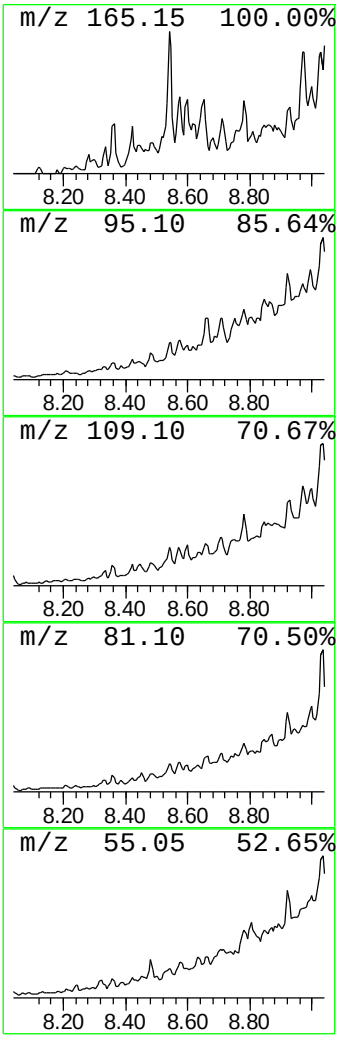
****

Peak Number 3 1,1,6,6-Tetramethylspiro[4.... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.54	3.38 ng	107447	Naphthalene-d8	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,6,6-Tetramethylspiro[4.4]nonane	180	C13H24	074054-92-5	58
2	Cyclopentene, 5-hexyl-3,3-dimethyl-	180	C13H24	061142-66-3	58
3	3-Methoxy-6-methyl-6H-pyrazolo[4...	165	C6H7N5O	037526-57-1	50
4	cis,cis- and cis,trans-1,9-dimet...	166	C12H22	1000111-72-5	46
5	trans,trans-1,7-Dimethylspiro[4....	166	C12H22	1000111-72-6	46





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Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

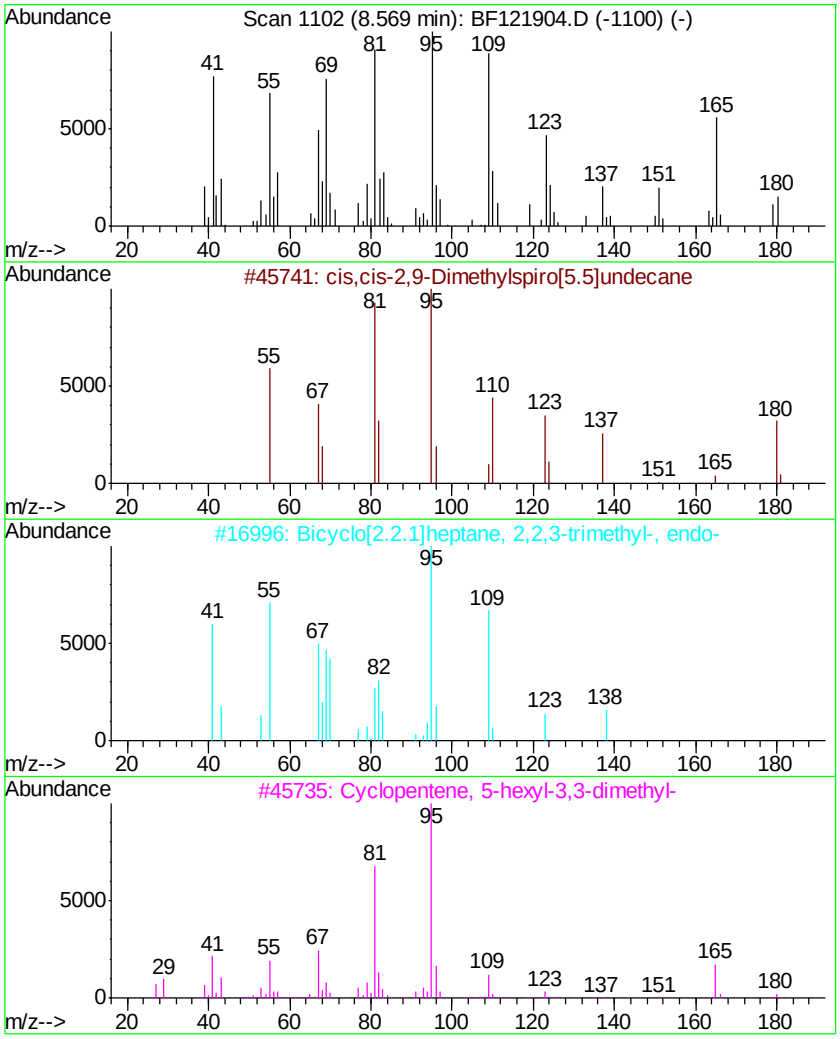
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

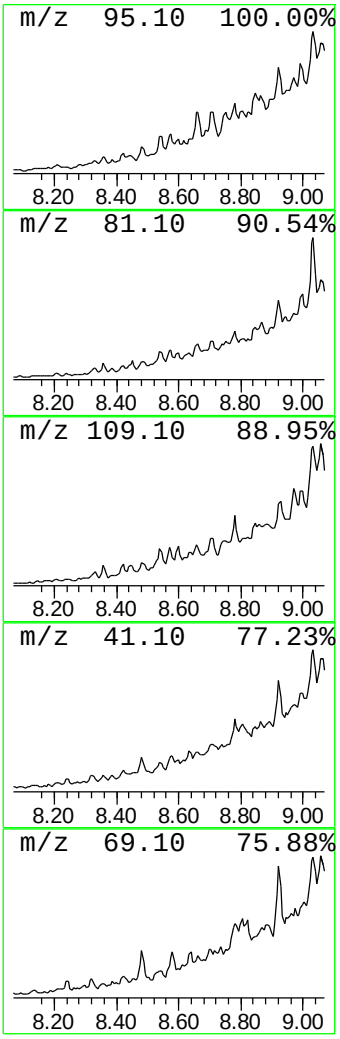
****

Peak Number 4 unknown8.57 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.57	4.14 ng	131598	Naphthalene-d8	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,cis-2,9-Dimethylspiro[5.5]un...	180	C13H24	095472-51-8	49
2	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	42
3	Cyclopentene, 5-hexyl-3,3-dimethyl-	180	C13H24	061142-66-3	41
4	Cyclohexane, (2-ethyl-1-methylbu...	180	C13H24	074810-41-6	38
5	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100920\
Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

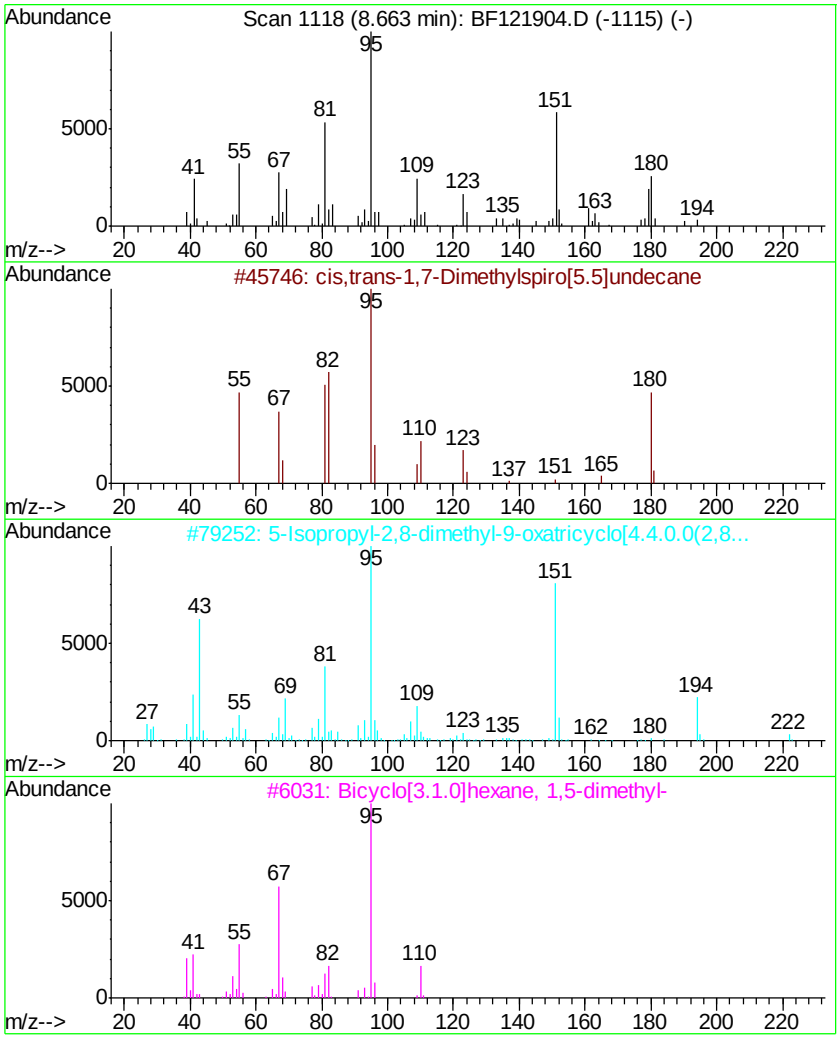
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

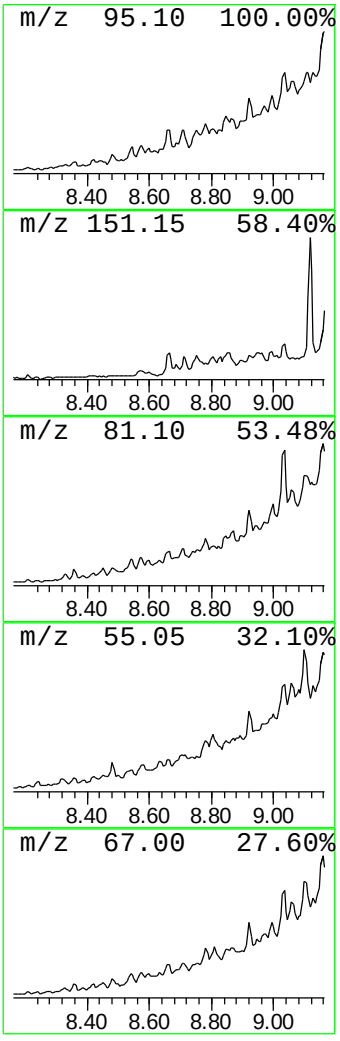
****

Peak Number 5 cis,trans-1,7-Dimethylspiro... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.66	2.57 ng	81761	Naphthalene-d8	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis,trans-1,7-Dimethylspiro[5.5]...	180	C13H24	1000111-73-1	52
2	5-Isopropyl-2,8-dimethyl-9-oxatr...	222	C14H22O2	1000185-23-8	47
3	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	38
4	6-(5-Methyl-furan-2-yl)-hexan-2-one	180	C11H16O2	1000185-87-5	38
5	Silane, diethyldifluoro-	124	C4H10F2Si	000358-06-5	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100920\
Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

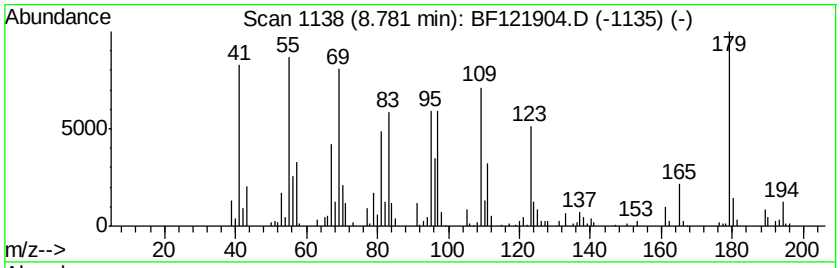
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

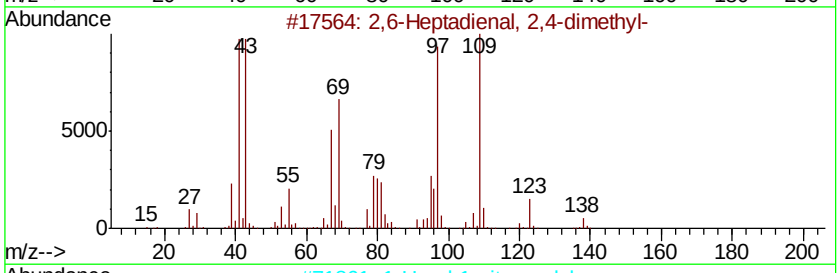
****

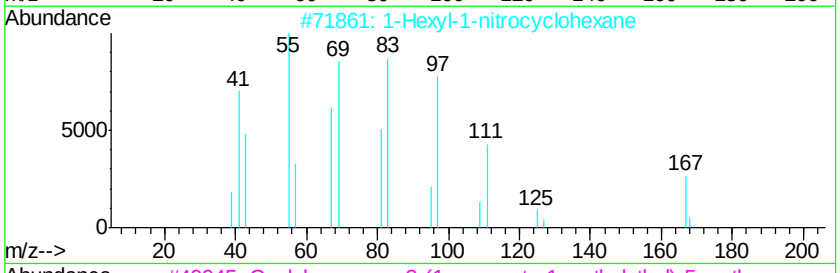
Peak Number 6 unknown8.78 Concentration Rank 4

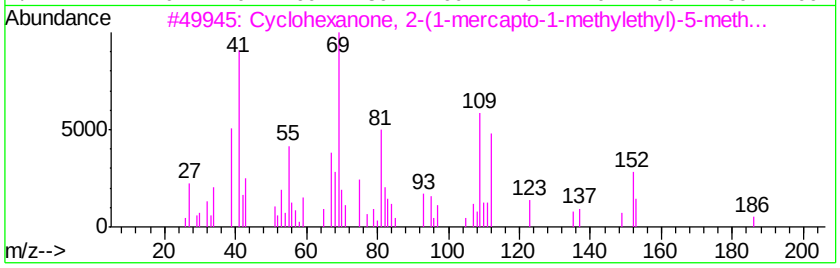
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.78	6.16 ng	195558	Naphthalene-d8	8.04

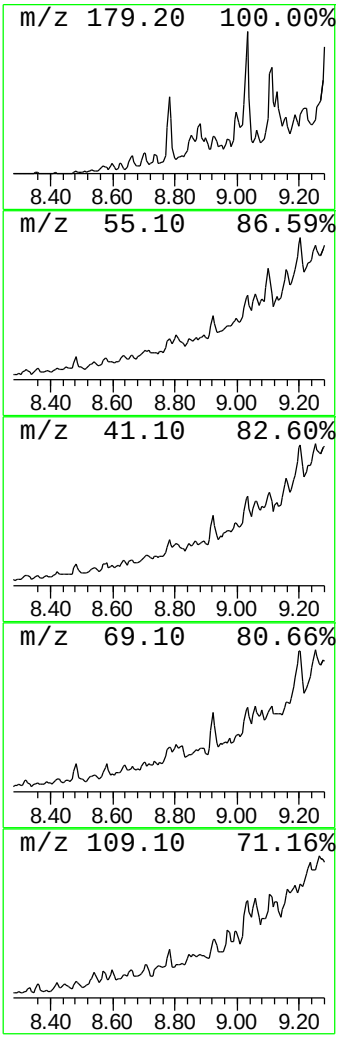
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	35
2	1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	30
3	Cyclohexanone, 2-(1-mercapto-1-m...	186	C10H18OS	033281-91-3	27
4	Benzoic acid, 4-nitroso-, ethyl ...	179	C9H9NO3	007476-79-1	25
5	7-Tetradecanol	214	C14H30O	003981-79-1	22











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Acq On : 9 Oct 2020 14:07
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Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

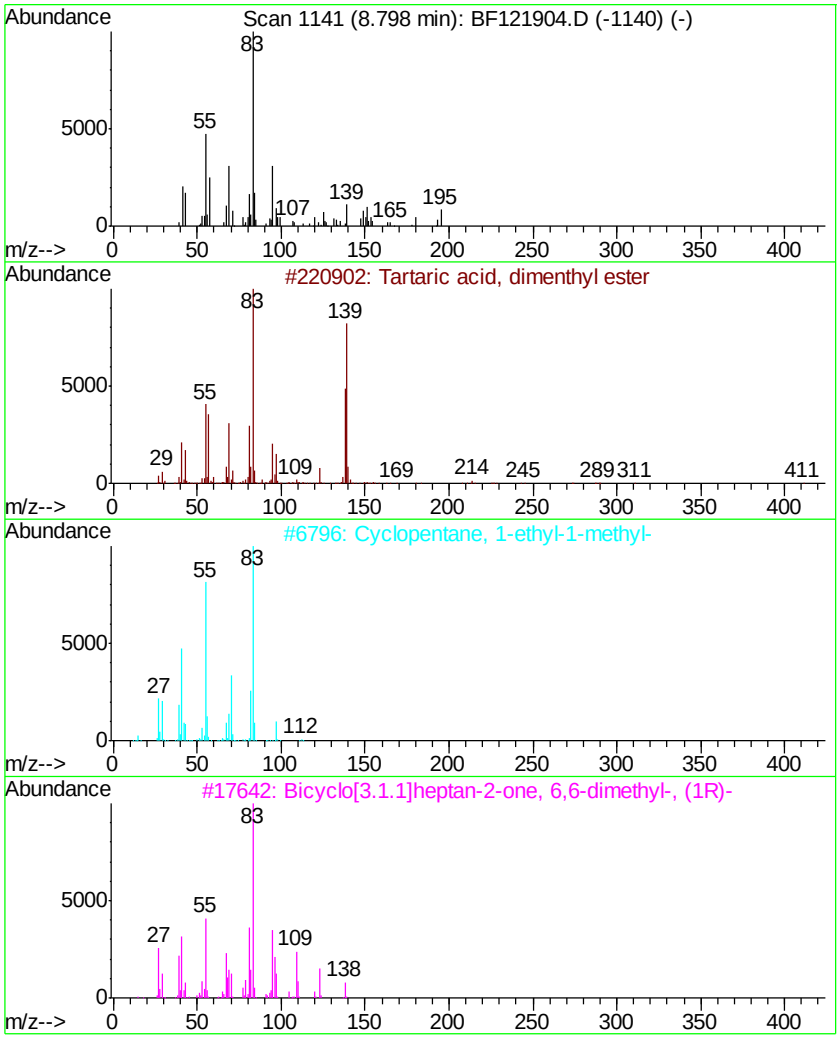
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

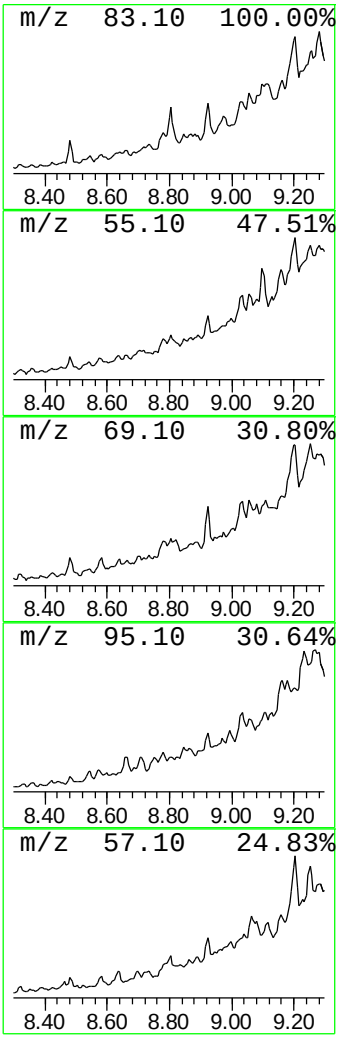
****

Peak Number 7 Tartaric acid, dimenthyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	4.44 ng	141127	Naphthalene-d8	8.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tartaric acid, dimenthyl ester	426	C24H42O6	1000149-89-9	53
2	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	50
3	Bicyclo[3.1.1]heptan-2-one, 6,6-...	138	C9H14O	038651-65-9	50
4	Oxalic acid, 1-menthyl pentadecy...	438	C27H50O4	1000314-98-2	50
5	N-Isopropoxy-2-carbomenthyloxyaz...	283	C16H29NO3	060999-69-1	50





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

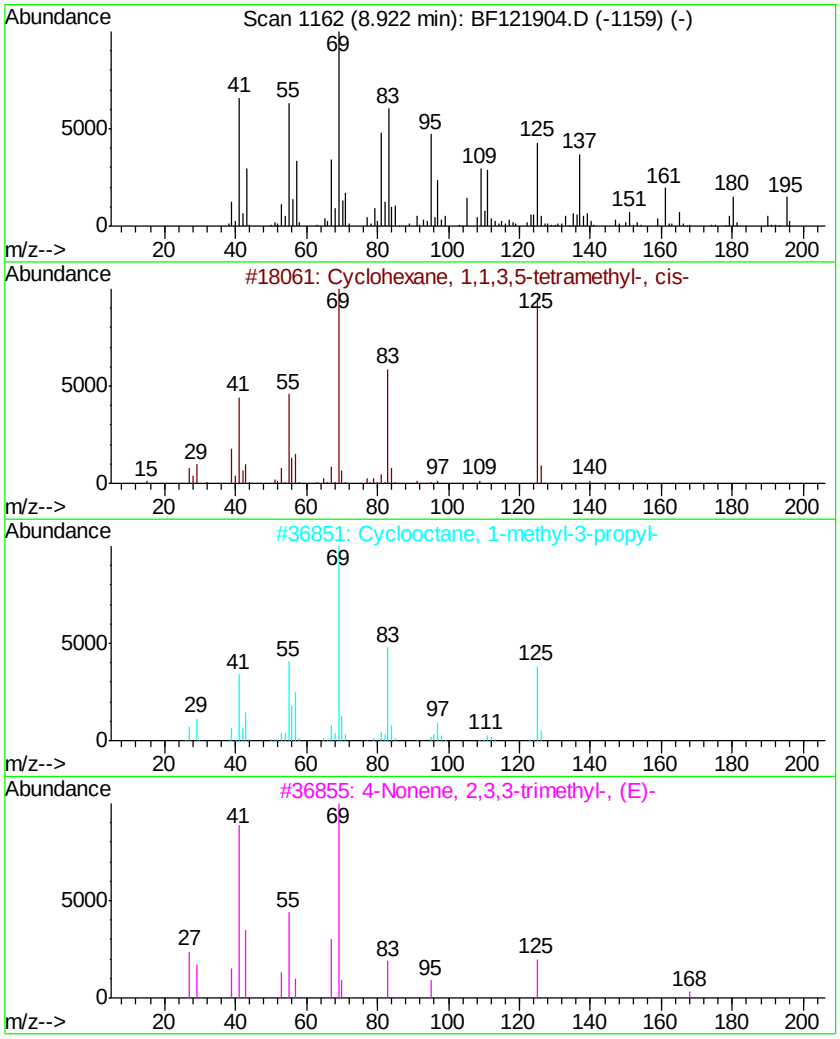
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

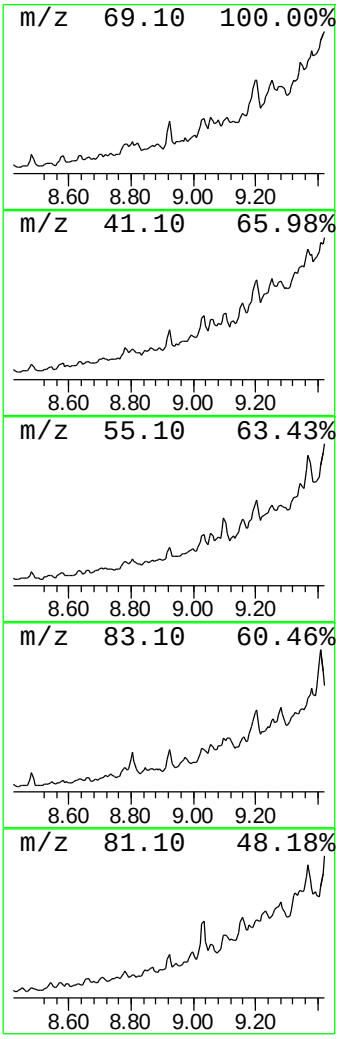
****

Peak Number 8 unknown8.92 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.92	19.20 ng	345178	Acenaphthene-d10	9.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	38
2	Cyclooctane, 1-methyl-3-propyl-	168	C12H24	255885-37-1	35
3	4-Nonene, 2,3,3-trimethyl-, (E)-	168	C12H24	063830-67-1	35
4	Triallylsilane	152	C9H16Si	001116-62-7	35
5	Cyclohexane, 1-ethyl-2-propyl-	154	C11H22	062238-33-9	27





Library Search Compound Report

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Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

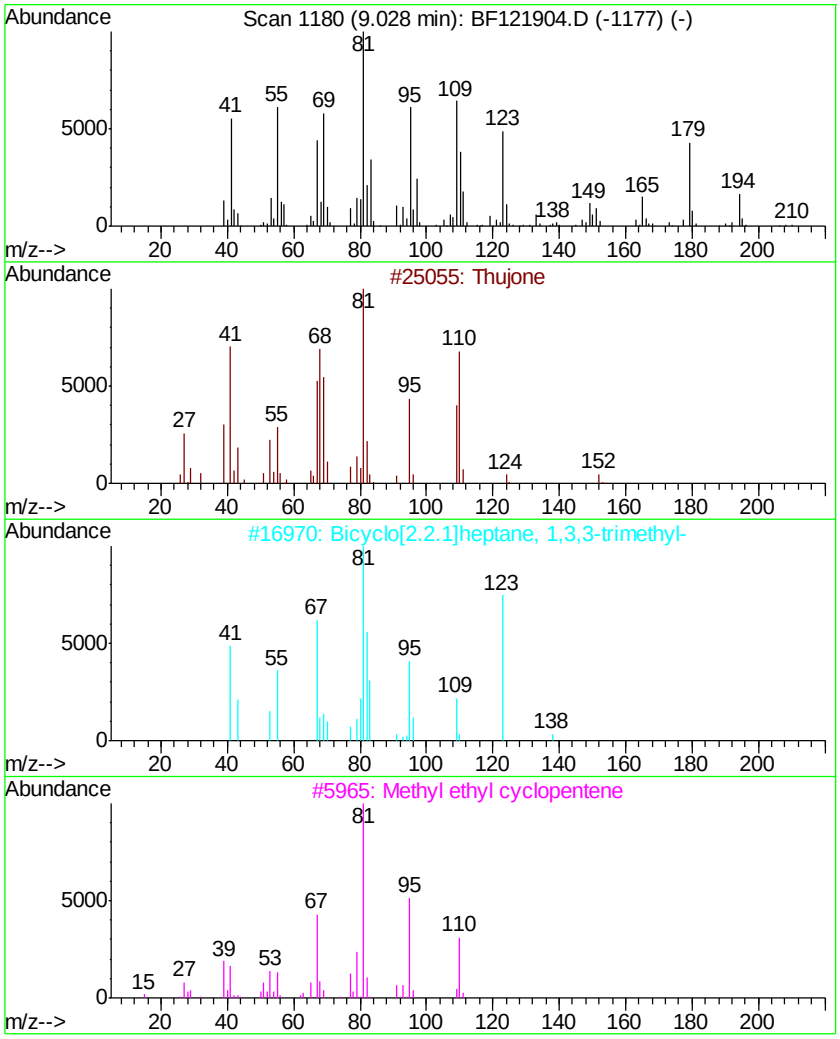
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

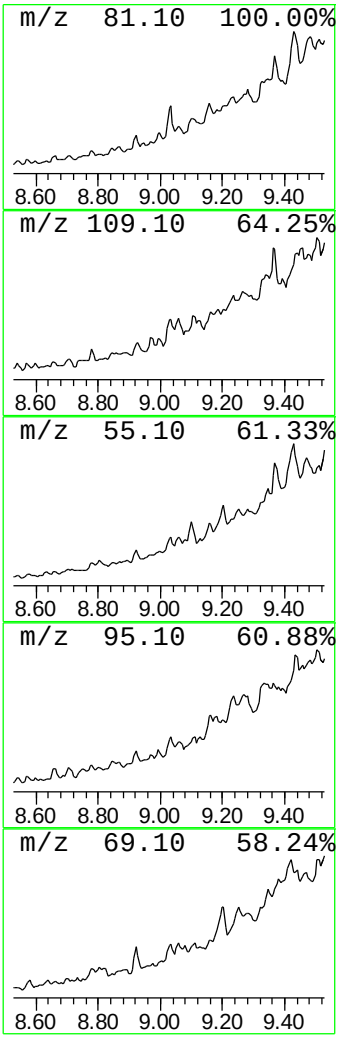
****

Peak Number 9 Thujone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.03	27.76 ng	499109	Acenaphthene-d10	9.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thujone	152	C10H16O	000546-80-5	55
2	Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	50
3	Methyl ethyl cyclopentene	110	C8H14	019780-56-4	46
4	Cyclohexane, ethylidene-	110	C8H14	001003-64-1	38
5	Cyclohexene, 3-ethyl-	110	C8H14	002808-71-1	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100920\
Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

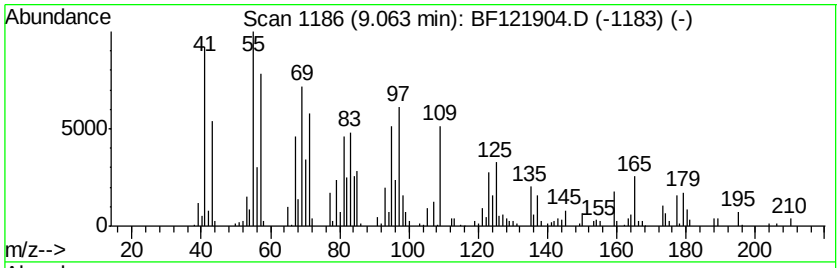
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

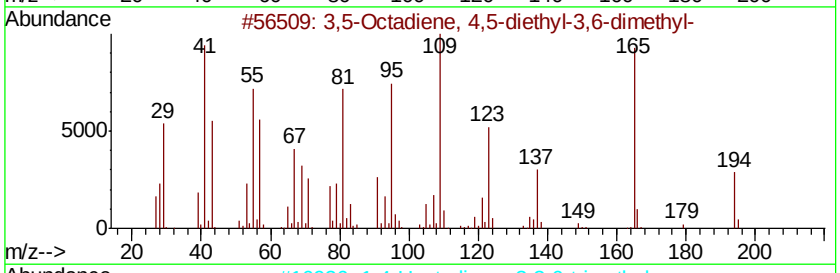
****

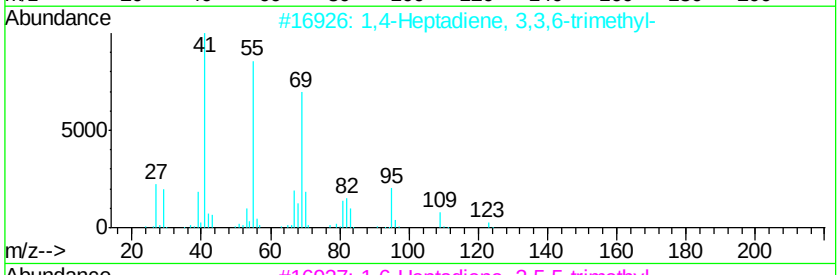
Peak Number 10 unknown9.06 Concentration Rank 3

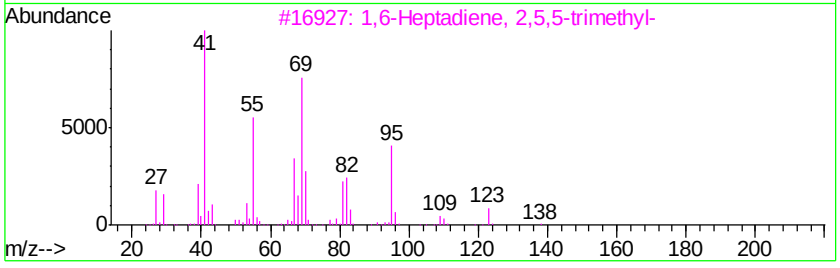
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.06	13.80 ng	248132	Acenaphthene-d10	9.80

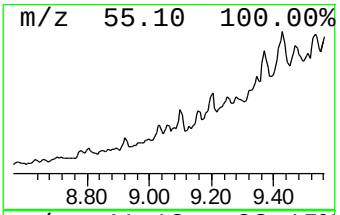
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Octadiene, 4,5-diethyl-3,6-d...	194	C14H26	061233-79-2	42
2	1,4-Heptadiene, 3,3,6-trimethyl-	138	C10H18	074498-89-8	38
3	1,6-Heptadiene, 2,5,5-trimethyl-	138	C10H18	062238-28-2	27
4	2R-Acetoxymethyl-1,3,5-trimethyl...	282	C17H30O3	1000144-12-6	27
5	1-Heptanol, 7-bromo-	194	C7H15BrO	010160-24-4	27

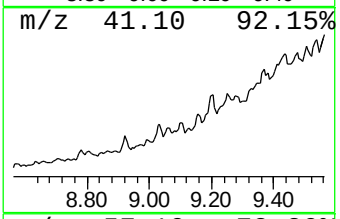


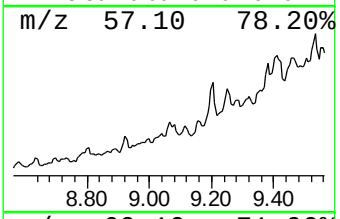


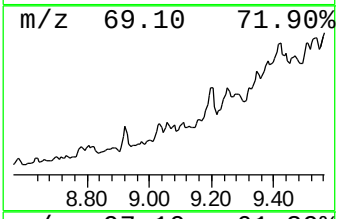


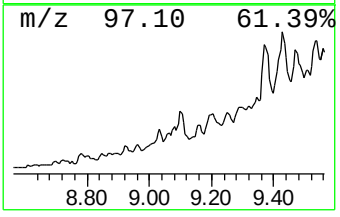












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100920\
Data File : BF121904.D
Acq On : 9 Oct 2020 14:07
Operator : JU/CG
Sample : L4317-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 11991

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
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
Ethanol, 2-(2-eth...	6.60	3.6	ng	105811	1	6.76	585395	20.0
Bicyclo[3.1.1]hep...	8.48	4.0	ng	126261	2	8.04	635250	20.0
1,1,6,6-Tetrameth...	8.54	3.4	ng	107447	2	8.04	635250	20.0
unknown8.57	8.57	4.1	ng	131598	2	8.04	635250	20.0
cis,trans-1,7-Dim...	8.66	2.6	ng	81761	2	8.04	635250	20.0
unknown8.78	8.78	6.2	ng	195558	2	8.04	635250	20.0
Tartaric acid, di...	8.80	4.4	ng	141127	2	8.04	635250	20.0
unknown8.92	8.92	19.2	ng	345178	3	9.80	359645	20.0
Thujone	9.03	27.8	ng	499109	3	9.80	359645	20.0
unknown9.06	9.06	13.8	ng	248132	3	9.80	359645	20.0