LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080921\
Data File : BF125018.D
Acq On : 10 Aug 2021 00:18
Operator : JU/CG
Sample : M3308-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-325

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-BF080421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125018.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.440	566	570	573	rBV	118253	94156	59.91%	8.734%
2	6.457	739	743	746	rBV	107568	96401	61.33%	8.943%
3	6.822	802	805	808	rBB	34653	26981	17.17%	2.503%
4	7.386	897	901	904	rBB	70379	59078	37.59%	5.480%
5	8.104	1020	1023	1026	rBV	46106	33044	21.02%	3.065%
6	9.098	1188	1192	1194	rBV4	16466	22655	14.41%	2.102%
7	9.122	1194	1196	1200	rVB2	21709	21537	13.70%	1.998%
8	9.180	1202	1206	1209	rVV	131873	108392	68.96%	10.055%
9	9.222	1210	1213	1215	rBV3	17644	20262	12.89%	1.880%
10	9.257	1216	1219	1222	rVV4	22346	32423	20.63%	3.008%
11	9.498	1257	1260	1262	rBV4	28898	35007	22.27%	3.247%
12	9.569	1270	1272	1274	rBV2	43112	44926	28.58%	4.168%
13	9.616	1278	1280	1289	rVB8	57606	104322	66.37%	9.678%
14	9.733	1297	1300	1303	rBV5	50000	84342	53.66%	7.824%
15	9.775	1305	1307	1310	rVB2	99278	110828	70.51%	10.281%
16	9.869	1321	1323	1329	rVB	161881	157173	100.00%	14.580%
17	15.457	2270	2273	2277	rVB	21502	26456	16.83%	2.454%

Sum of corrected areas: 1077983

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Misc :
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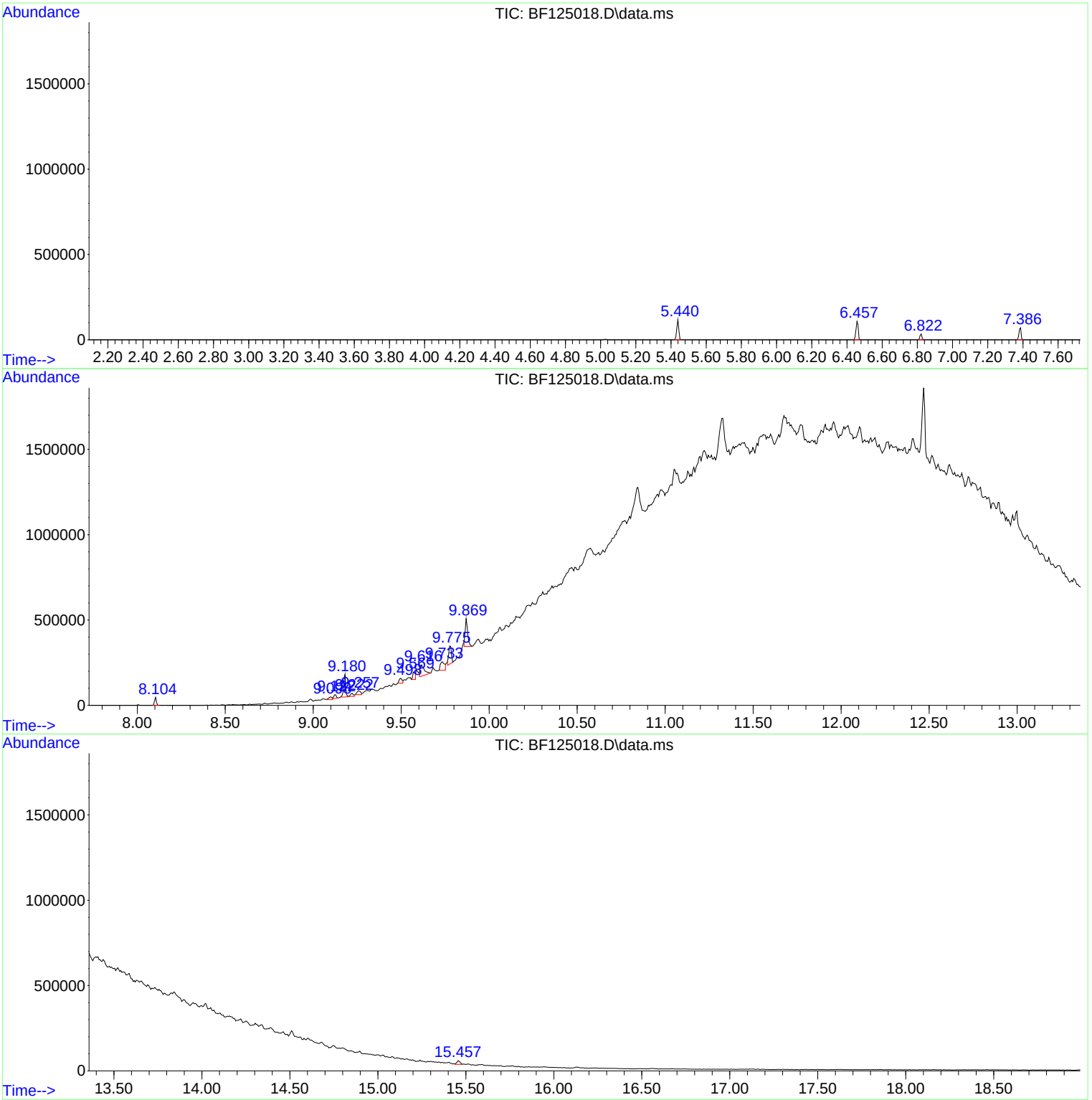
Instrument :
BNA_F
ClientSampleId :
ETGI-325

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Data File : BF125018.D
Acq On : 10 Aug 2021 00:18
Operator : JU/CG
Sample : M3308-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-325

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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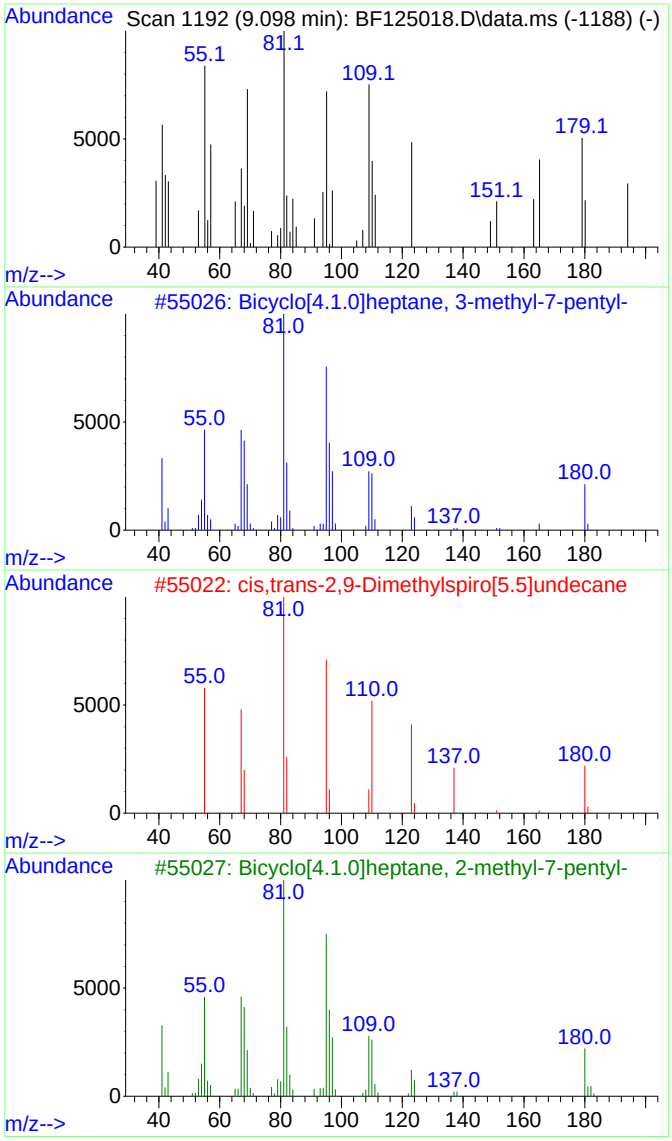
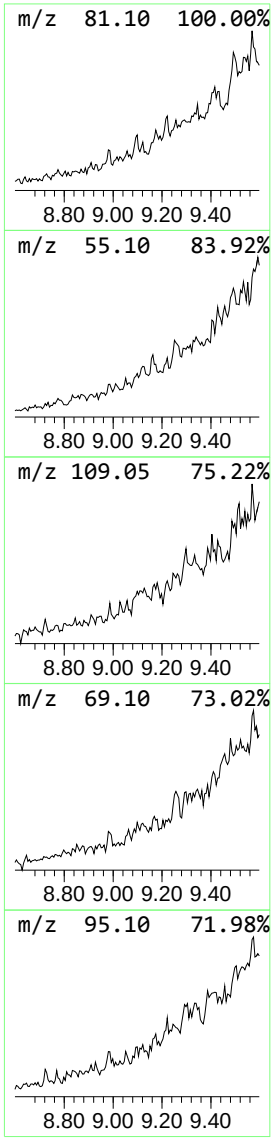
Peak Number 1 unknown9.098 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.098	2.88 ng	22655	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.1.0]heptane, 3-methyl-...	180	C13H24	041977-48-4	41
2	cis,trans-2,9-Dimethylspiro[5.5]...	180	C13H24	095530-74-8	41
3	Bicyclo[4.1.0]heptane, 2-methyl-...	180	C13H24	055937-92-3	38
4	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	38
5	2(1H)-Naphthalenone, octahydro-4...	180	C12H20O	000941-19-5	25





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Data File : BF125018.D
Acq On : 10 Aug 2021 00:18
Operator : JU/CG
Sample : M3308-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-325

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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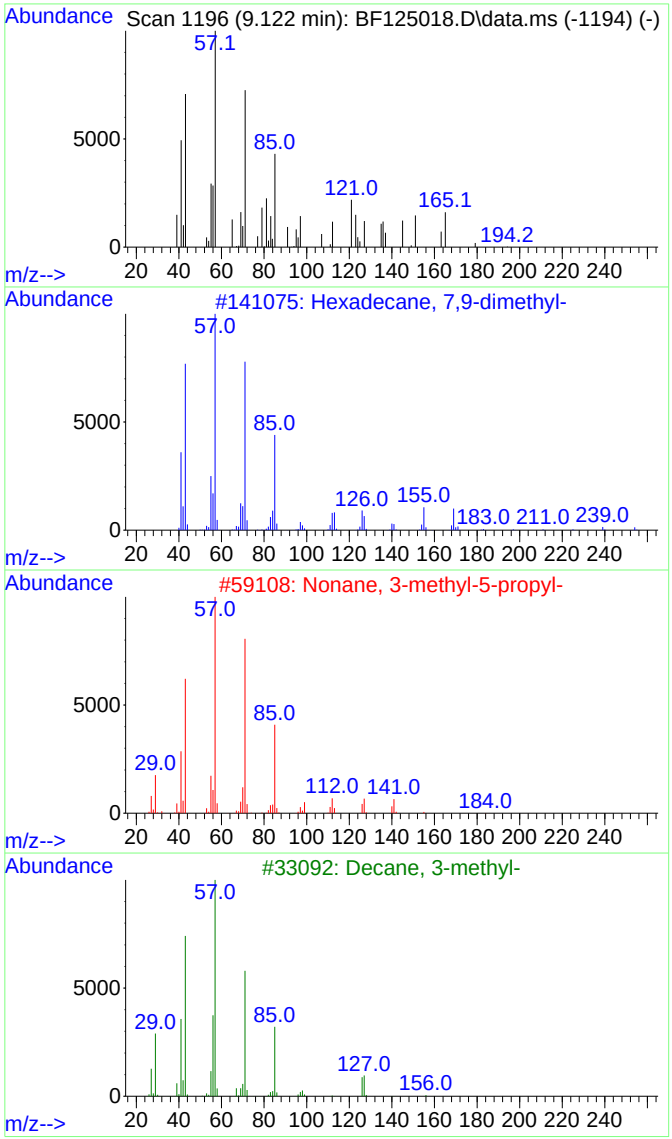
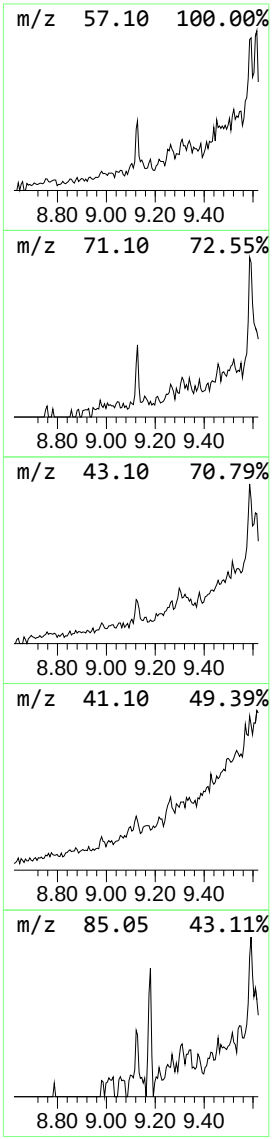
Peak Number 2 unknown9.122 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.122	2.74 ng	21537	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	47
2	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	47
3	Decane, 3-methyl-	156	C11H24	013151-34-3	43
4	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	43
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	38





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Operator : JU/CG
Sample : M3308-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-325

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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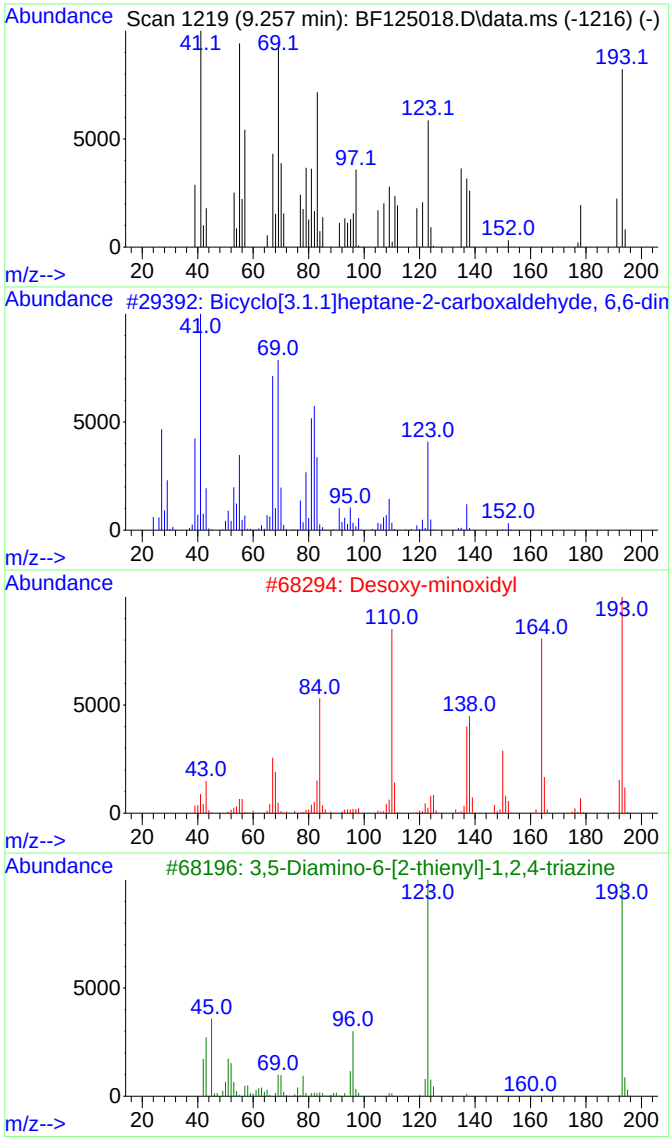
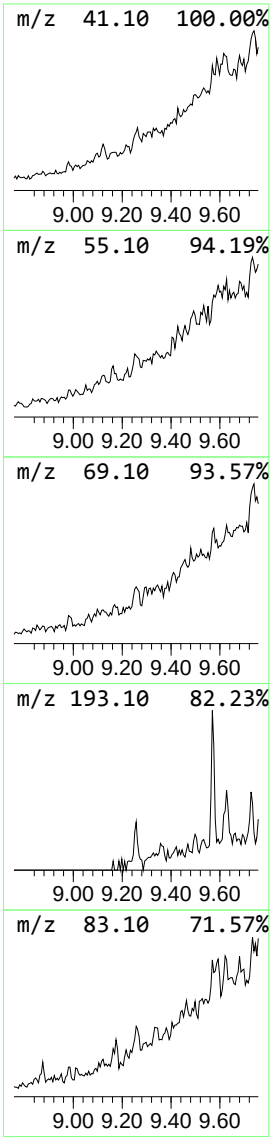
Peak Number 3 unknown9.257 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	4.13 ng	32423	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptane-2-carboxal...	152	C10H16O	004764-14-1	30
2	Desoxy-minoxidyl	193	C9H15N5	024867-26-3	25
3	3,5-Diamino-6-[2-thienyl]-1,2,4-...	193	C7H7N5S	058848-66-1	22
4	2-Heptene, 4-methyl-, (E)-	112	C8H16	066225-17-0	18
5	1,2-Oxazino[2,3-b]isoquinoline, ...	193	C12H19NO	1000196-68-0	18





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Sample : M3308-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-325

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

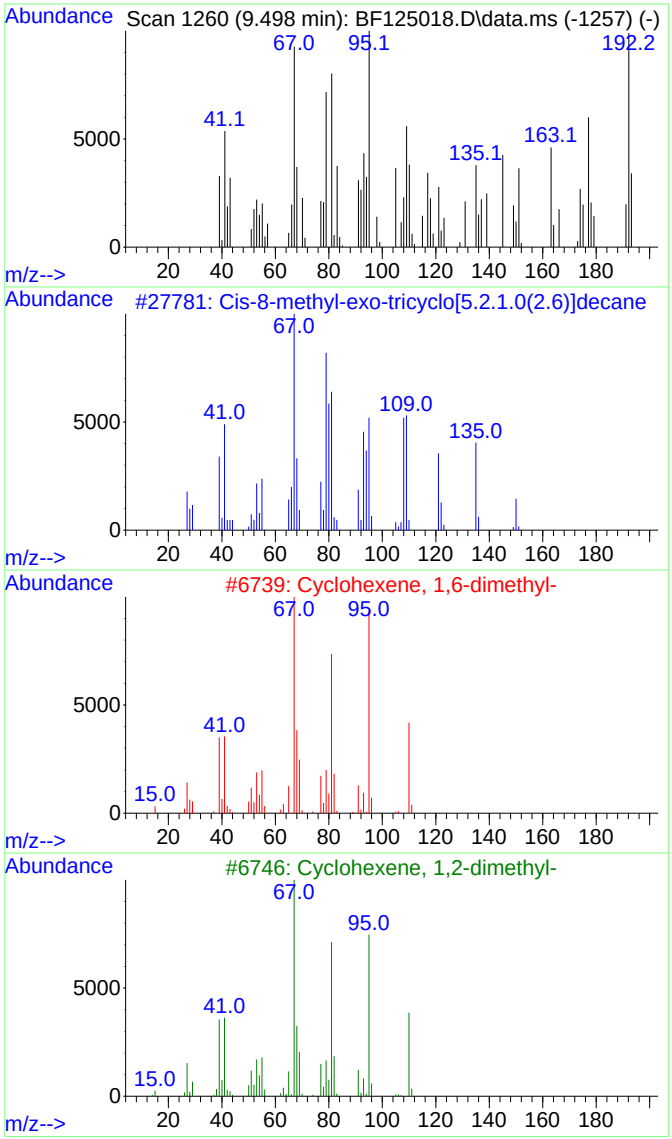
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

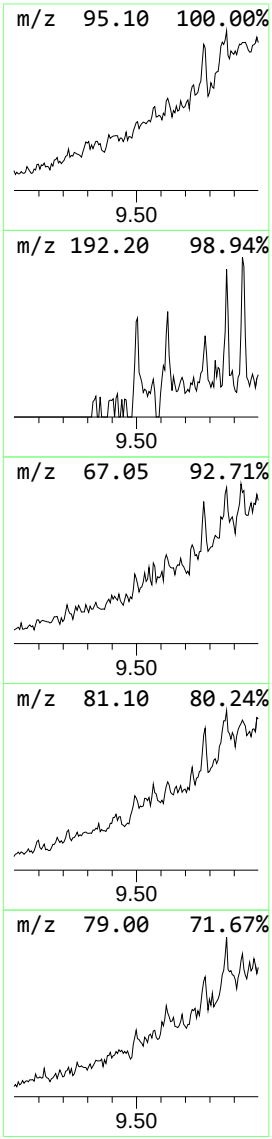
****

Peak Number 4 Cis-8-methyl-exo-tricyclo[5... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.498	4.45 ng	35007	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cis-8-methyl-exo-tricyclo[5.2.1....	150	C11H18	1000215-29-3	55
2	Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	46
3	Cyclohexene, 1,2-dimethyl-	110	C8H14	001674-10-8	41
4	Tricyclo[5.2.1.0(2,6)]decane, 4-...	150	C11H18	1000150-03-4	38
5	3-Tetradecyne	194	C14H26	060212-32-0	35





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Data File : BF125018.D
Acq On : 10 Aug 2021 00:18
Operator : JU/CG
Sample : M3308-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-325

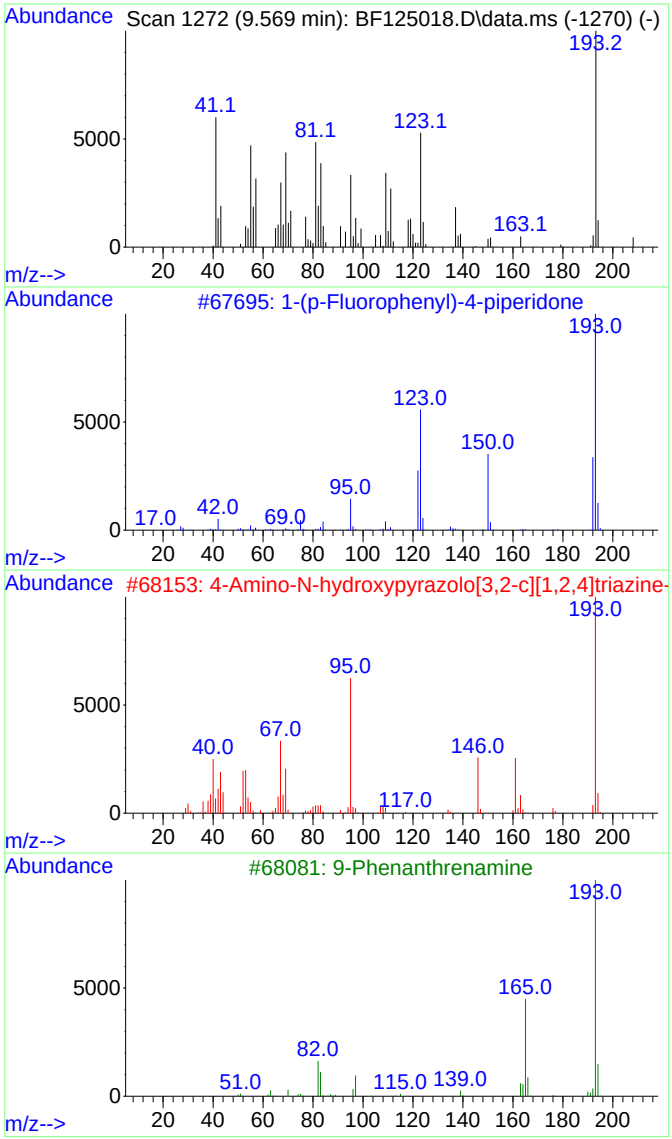
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

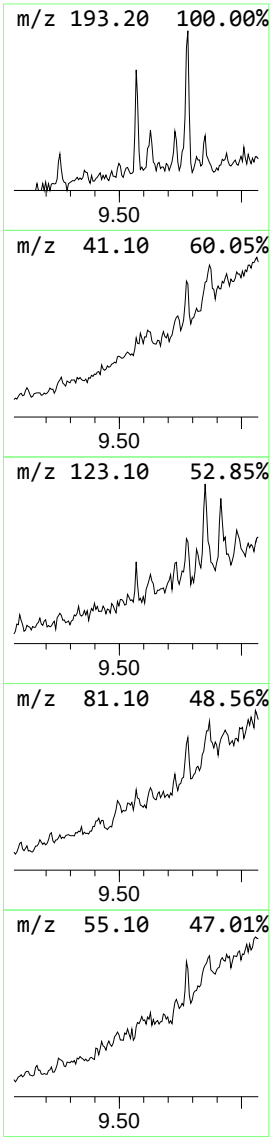
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-(p-Fluorophenyl)-4-piperi... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.569	5.72 ng	44926	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	50
2	4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	35
3	9-Phenanthrenamine	193	C14H11N	000947-73-9	30
4	[1,2,4]Triazolo[1,5-a]pyrimidin-...	193	C8H11N5O	1000351-50-1	27
5	3-pyridinamine, 2-(1H-1,2,4-tria...	193	C7H7N5S	1000400-27-7	27





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Operator : JU/CG
Sample : M3308-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ETGI-325

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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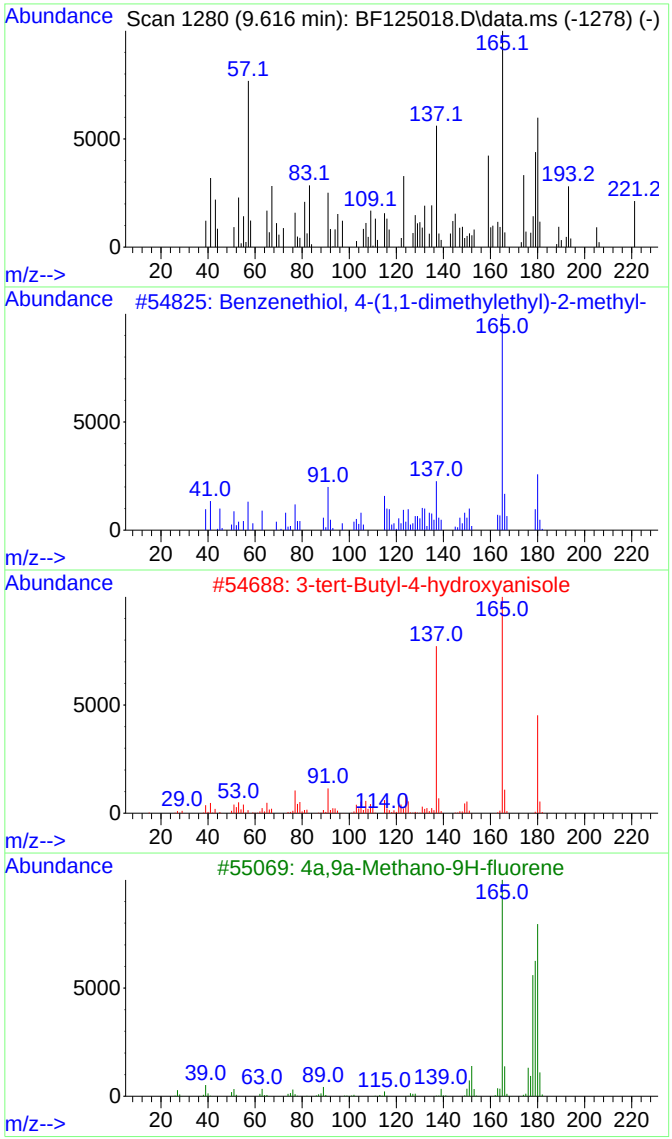
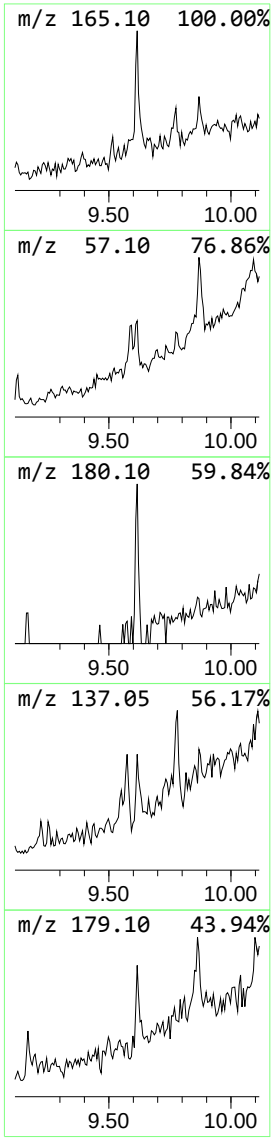
Peak Number 6 unknown9.616 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.616	13.27 ng	104322	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenethiol, 4-(1,1-dimethyleth...	180	C11H16S	015570-10-2	46
2	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	41
3	4a,9a-Methano-9H-fluorene	180	C14H12	019540-84-2	41
4	Ethylene, 1,1-diphenyl-	180	C14H12	000530-48-3	38
5	3H-Benz[e]indene, 2-methyl-	180	C14H12	150096-60-9	38





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ETGI-325

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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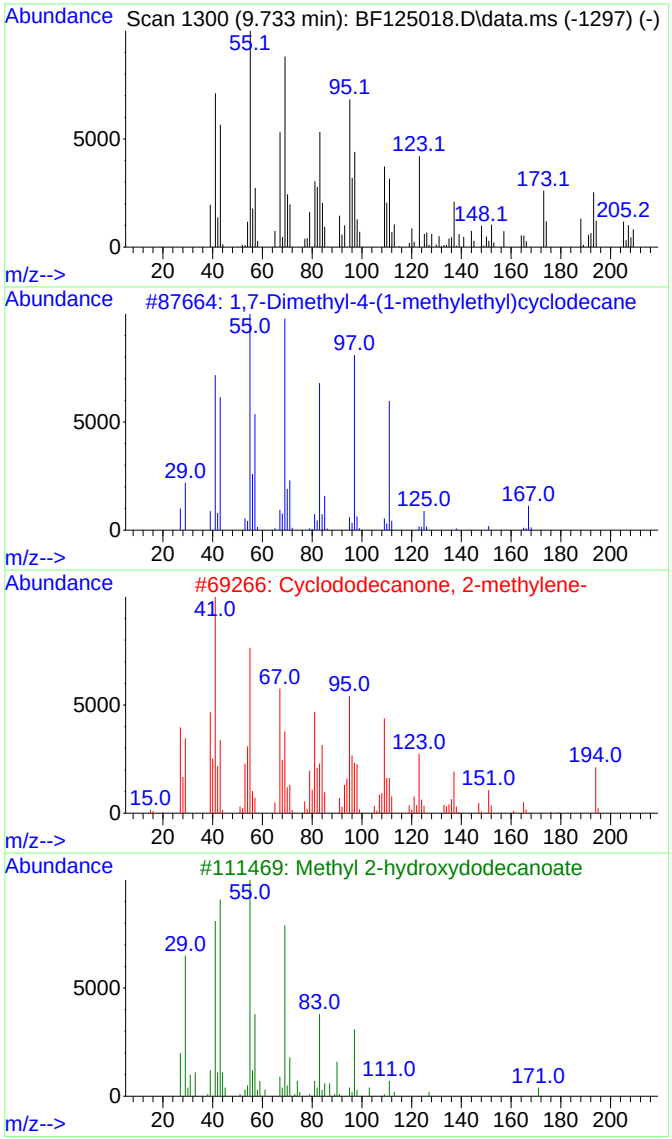
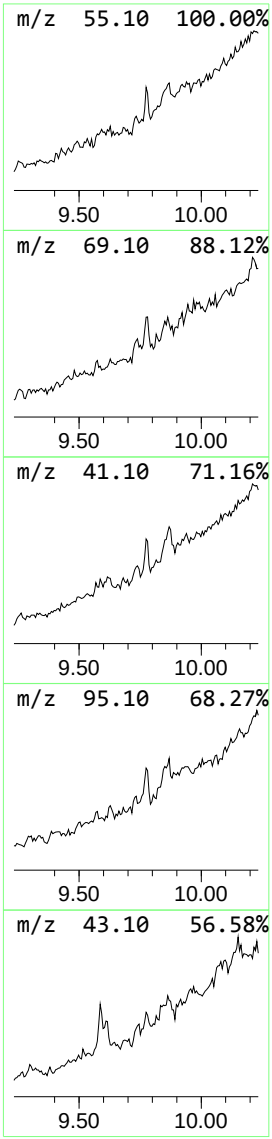
Peak Number 7 unknown9.733 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.733	10.73 ng	84342	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	35
2	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	35
3	Methyl 2-hydroxydodecanoate	230	C13H26O3	051067-85-7	35
4	Spiro[2,4,5,6,7,7a-hexahydro-2-o...	208	C12H16O3	1000197-10-9	27
5	Cyclooctane, methyl-	126	C9H18	001502-38-1	27





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BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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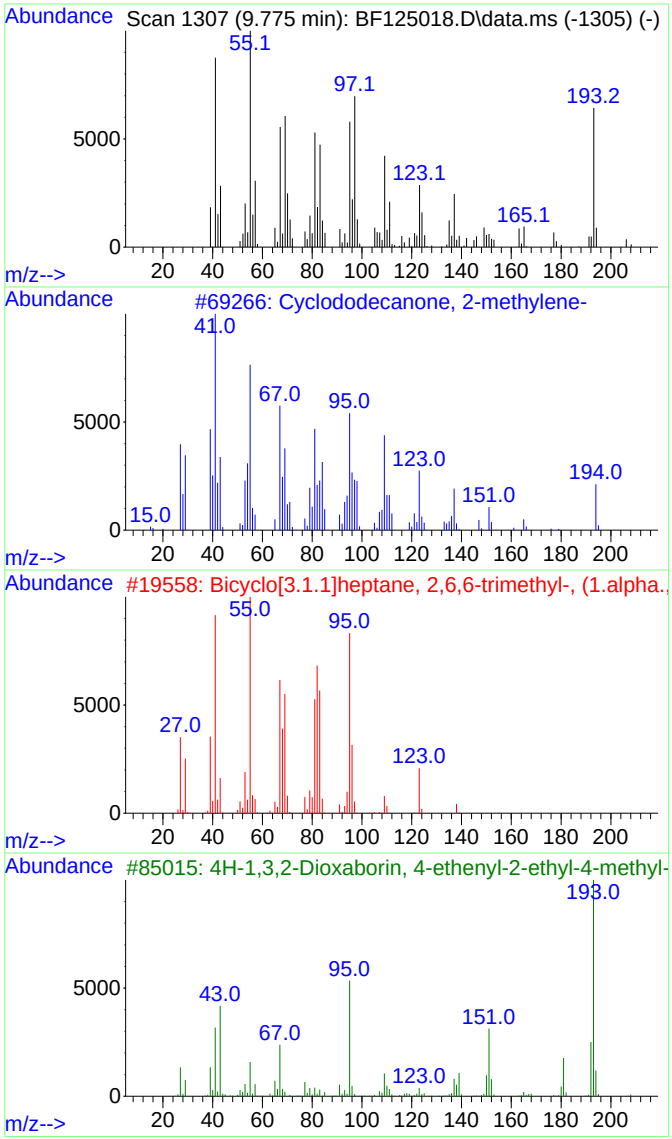
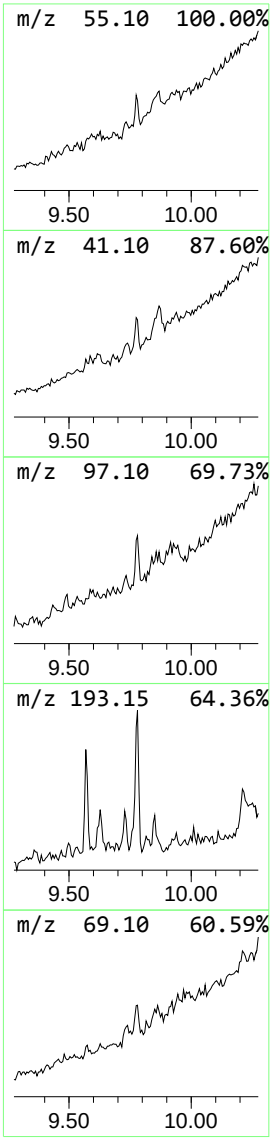
Peak Number 8 unknown9.775 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.775	14.10 ng	110828	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	47
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	006876-13-7	43
3	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	42
4	1-Hexylbicyclo[2.2.2]octane	194	C14H26	1000435-94-2	38
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	35





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown9.098	9.098	2.9	ng	22655	3	9.869	157173	20.0
unknown9.122	9.122	2.7	ng	21537	3	9.869	157173	20.0
unknown9.257	9.257	4.1	ng	32423	3	9.869	157173	20.0
Cis-8-methyl-ex...	9.498	4.5	ng	35007	3	9.869	157173	20.0
1-(p-Fluorophen...	9.569	5.7	ng	44926	3	9.869	157173	20.0
unknown9.616	9.616	13.3	ng	104322	3	9.869	157173	20.0
unknown9.733	9.733	10.7	ng	84342	3	9.869	157173	20.0
unknown9.775	9.775	14.1	ng	110828	3	9.869	157173	20.0