LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
Data File : BP020626.D
Acq On : 14 Jun 2024 15:21
Operator : MA/JU
Sample : P2878-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
348

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_P\Methods\8270E-BP052924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP020626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.022	3	6	23	rVB	1617496	2396015	27.07%	5.538%
2	5.375	398	406	415	rBV	2429631	3717868	42.01%	8.594%
3	6.928	662	670	684	rBV	2161048	3777761	42.69%	8.732%
4	7.752	802	810	817	rBV	931489	1507008	17.03%	3.483%
5	8.893	997	1004	1012	rBV	1519240	2556936	28.89%	5.910%
6	10.522	1269	1281	1285	rBV	1220978	2095466	23.68%	4.844%
7	10.569	1285	1289	1295	rVB	464915	752207	8.50%	1.739%
8	12.169	1557	1561	1569	rVB	295524	585402	6.61%	1.353%
9	12.304	1581	1584	1591	rBV6	127273	338005	3.82%	0.781%
10	12.398	1595	1600	1608	rBV2	534997	1503322	16.99%	3.475%
11	12.569	1624	1629	1635	rBV9	339494	606448	6.85%	1.402%
12	12.904	1683	1686	1690	rBV2	442707	640433	7.24%	1.480%
13	12.993	1696	1701	1709	rVB	3848838	5862256	66.24%	13.550%
14	13.063	1709	1713	1715	rBV2	637245	984623	11.13%	2.276%
15	13.651	1810	1813	1817	rBV3	1409036	2209809	24.97%	5.108%
16	13.793	1835	1837	1840	rBV3	1175449	1313041	14.84%	3.035%
17	23.316	3452	3456	3467	rVB	4016148	8849883	100.00%	20.456%
18	25.063	3748	3753	3763	rVB	1470575	3566253	40.30%	8.243%

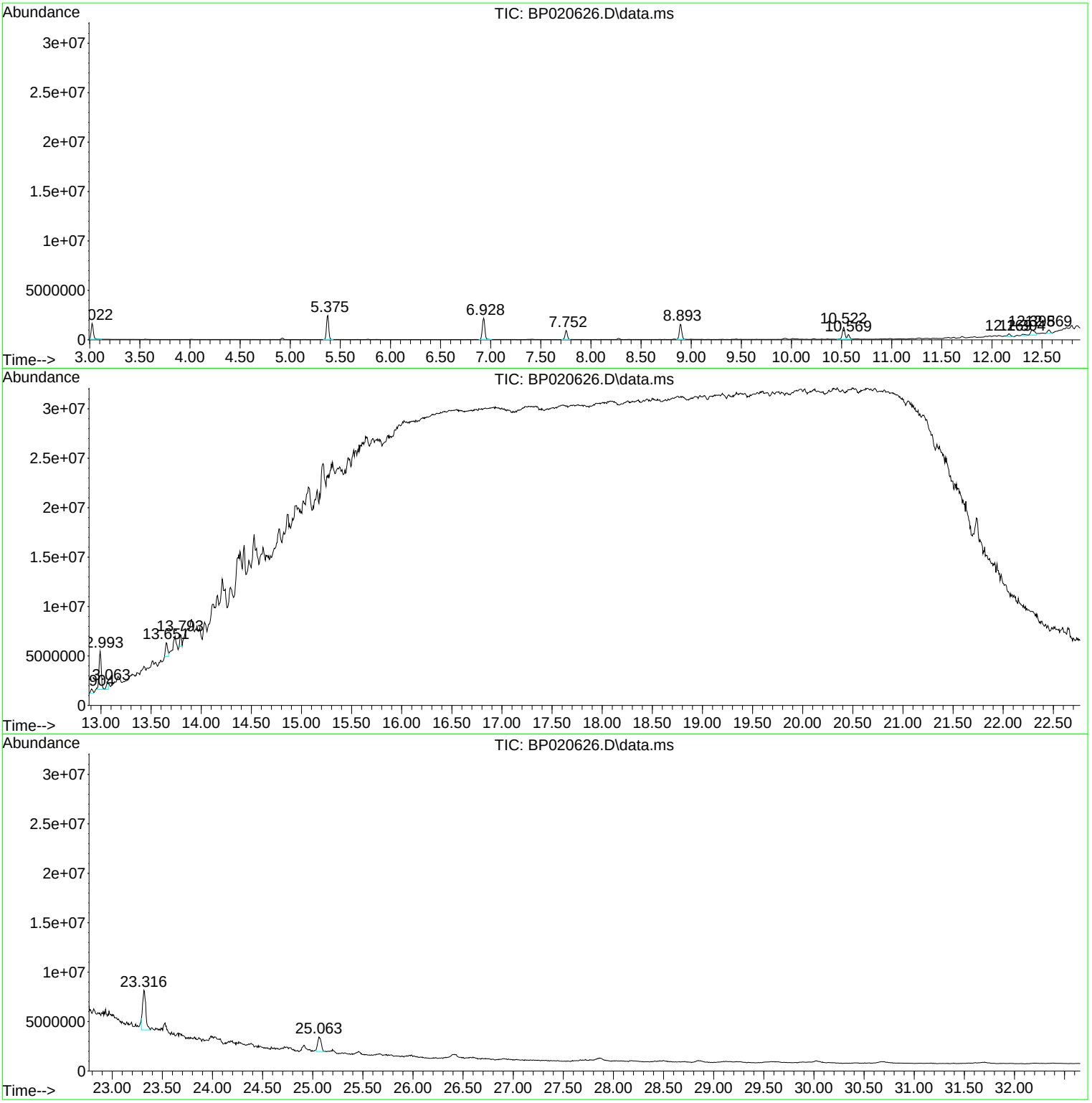
Sum of corrected areas: 43262736

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
Data File : BP020626.D
Acq On : 14 Jun 2024 15:21
Operator : MA/JU
Sample : P2878-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
348

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
Data File : BP020626.D
Acq On : 14 Jun 2024 15:21
Operator : MA/JU
Sample : P2878-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
348

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

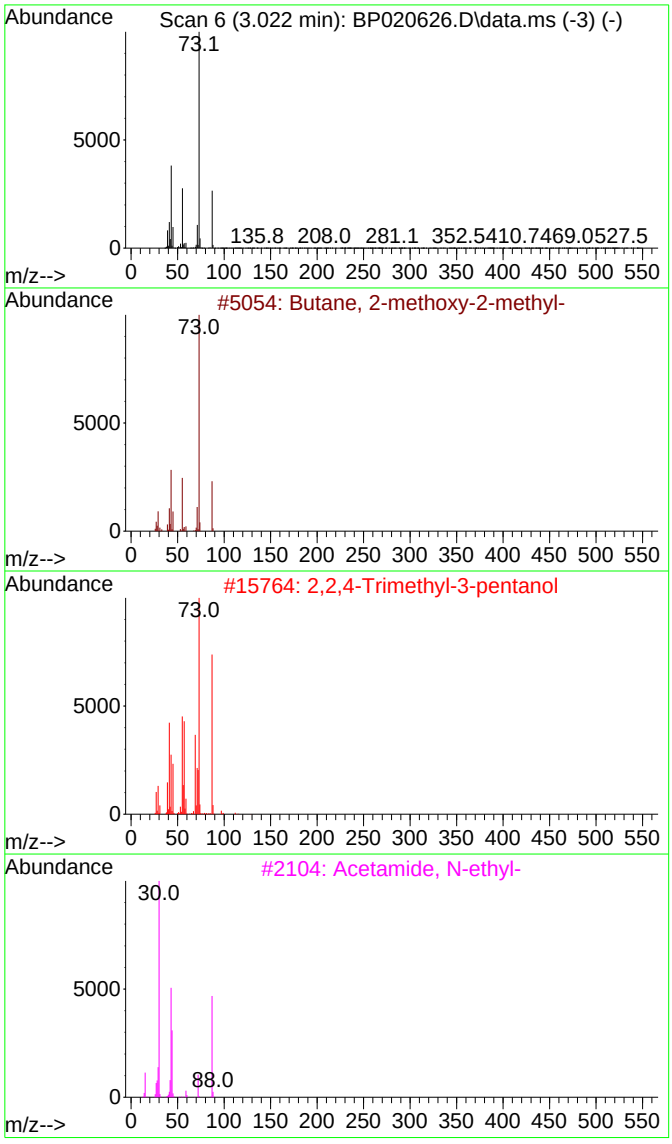
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

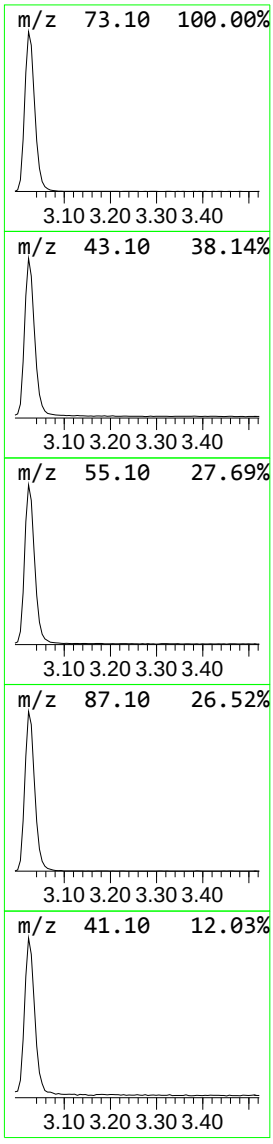
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.022	31.80 ng	2396020	1,4-Dichlorobenzene-d4	7.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BP020626.D
Acq On : 14 Jun 2024 15:21
Operator : MA/JU
Sample : P2878-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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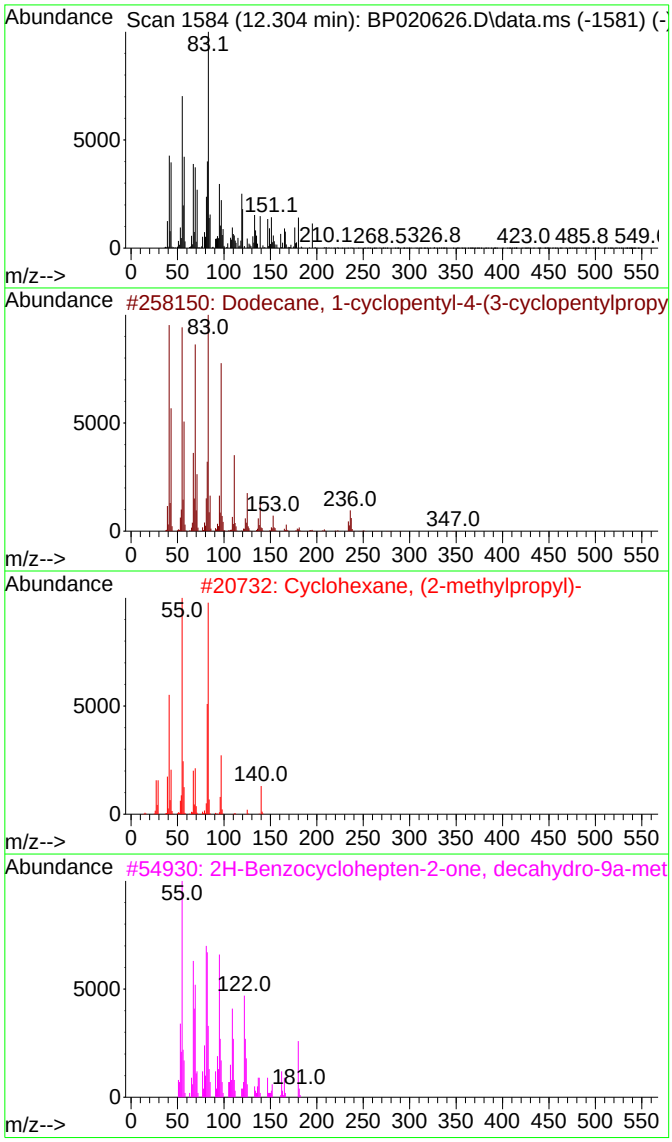
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

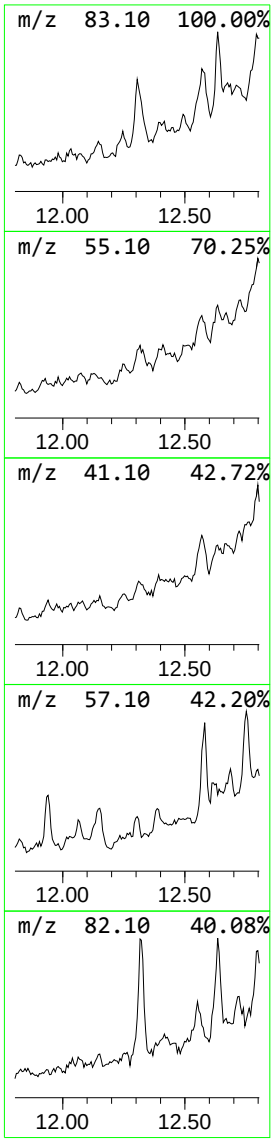
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Dodecane, 1-cyclopentyl-4-(... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	3.23 ng	338005	Naphthalene-d8	10.522

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-cyclopentyl-4-(3-cyc...	348	C25H48	007225-68-5	50
2	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	43
3	2H-Benzocyclohepten-2-one, decah...	180	C12H20O	055103-67-8	41
4	1-Benzenesulfinate-4-methyl, 2-(...	294	C17H26O2S	098147-48-9	38
5	N-Phenyl-4-piperidinamine	176	C11H16N2	023056-29-3	38





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Data File : BP020626.D
Acq On : 14 Jun 2024 15:21
Operator : MA/JU
Sample : P2878-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
348

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

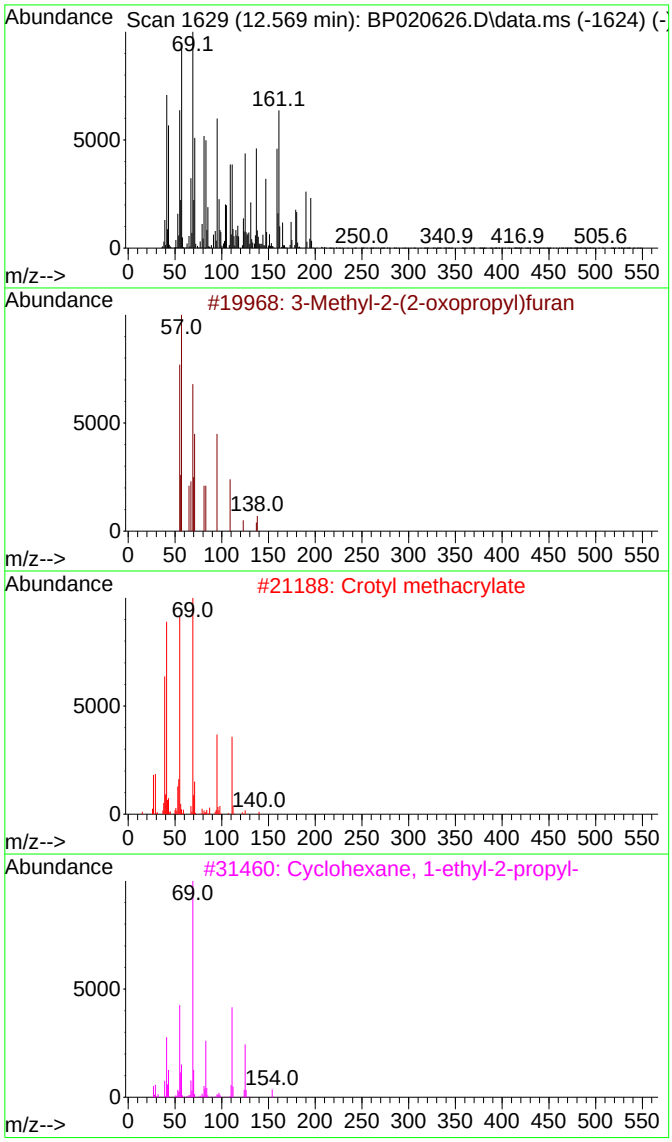
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

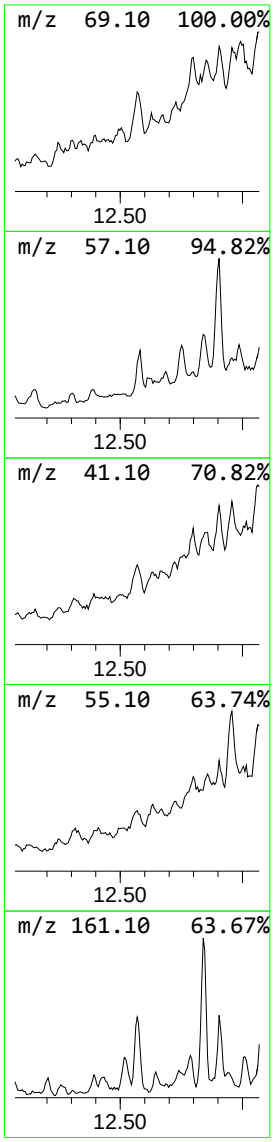
****

Peak Number 3 unknown12.569 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	9.24 ng	606448	Acenaphthene-d10	14.393

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-2-(2-oxopropyl)furan	138	C8H10O2	087773-62-4	38
2	Crotyl methacrylate	140	C8H12O2	007376-45-6	27
3	Cyclohexane, 1-ethyl-2-propyl-	154	C11H22	062238-33-9	27
4	Neral	152	C10H16O	000106-26-3	22
5	Cyclohexane, 1-ethyl-2,3-dimethyl-	140	C10H20	007058-05-1	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
Data File : BP020626.D
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Operator : MA/JU
Sample : P2878-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
348

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

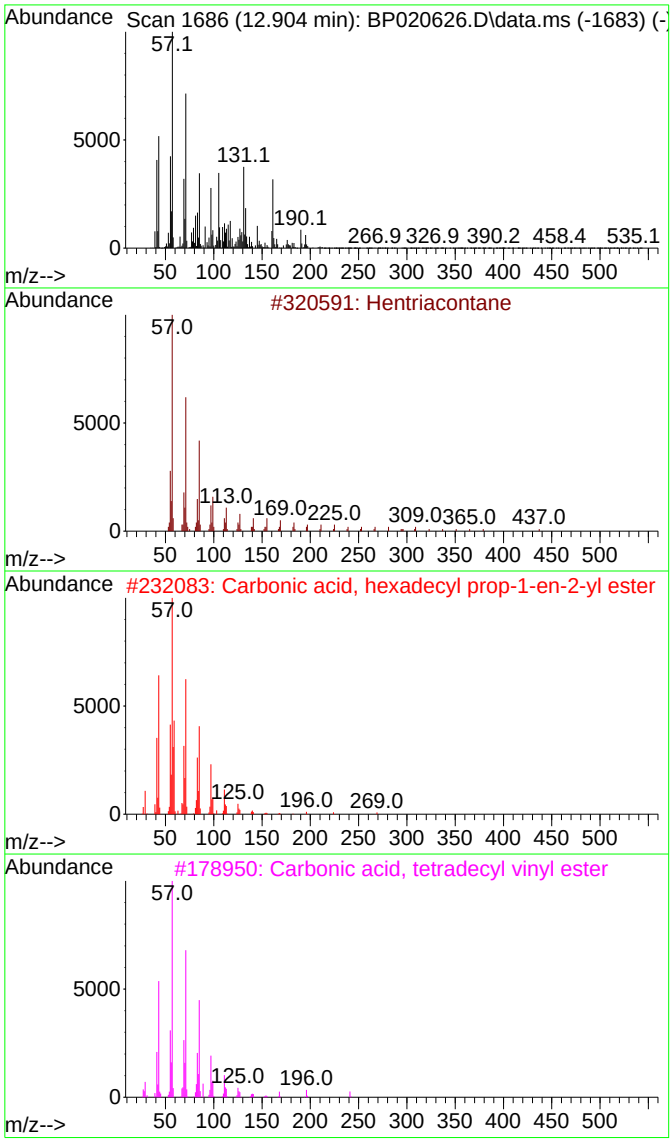
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

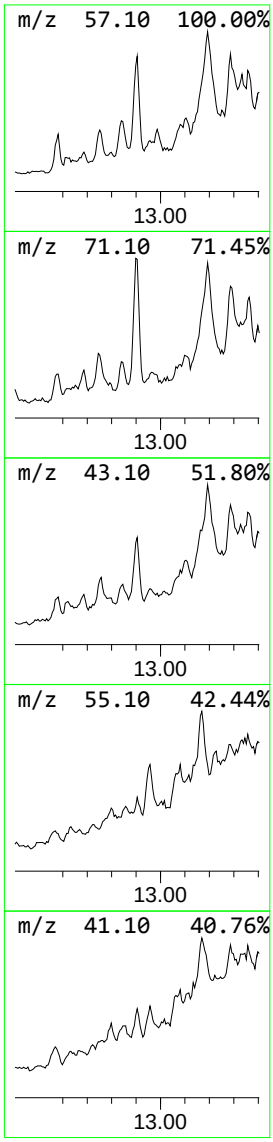
****

Peak Number 4 unknown12.904 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.904	9.75 ng	640433	Acenaphthene-d10	14.393

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	43
2	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	43
3	Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	38
4	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	38
5	Tetratetracontane	619	C44H90	007098-22-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
Data File : BP020626.D
Acq On : 14 Jun 2024 15:21
Operator : MA/JU
Sample : P2878-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
348

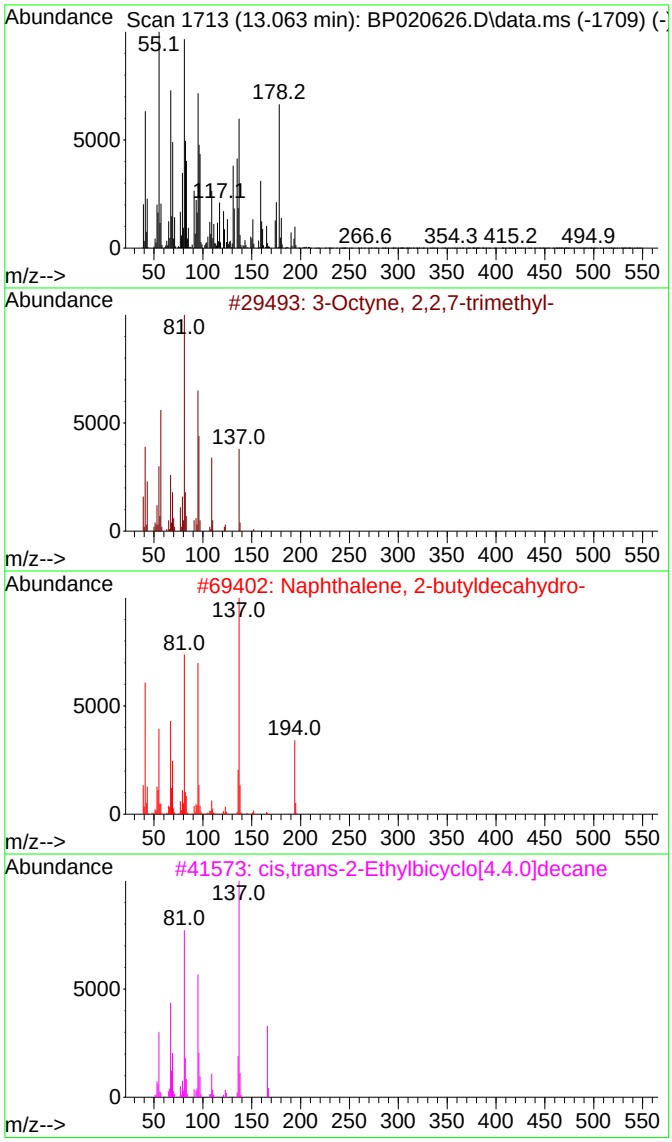
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

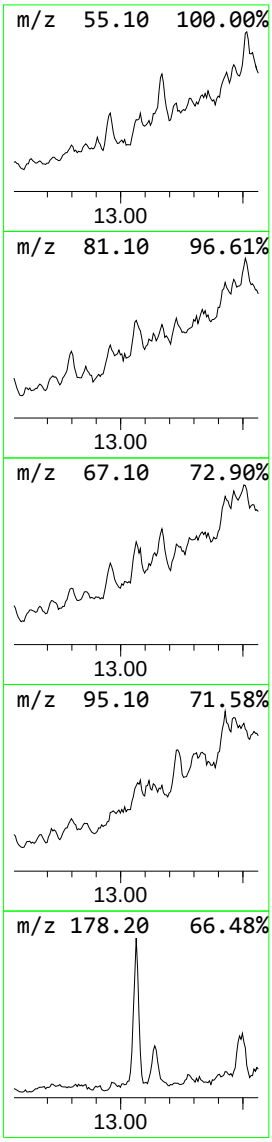
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Octyne, 2,2,7-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.063	15.00 ng	984623	Acenaphthene-d10	14.393

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	50
2	Naphthalene, 2-butyldecahydro-	194	C14H26	006305-52-8	41
3	cis,trans-2-Ethylbicyclo[4.4.0]d...	166	C12H22	066660-38-6	35
4	Bicyclo[4.1.0]heptane, 2-methyl-...	180	C13H24	055937-92-3	35
5	Perhydrophenalene, (3a.alpha., 6...	178	C13H22	040250-64-4	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
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Instrument :
BNA_P
ClientSampleId :
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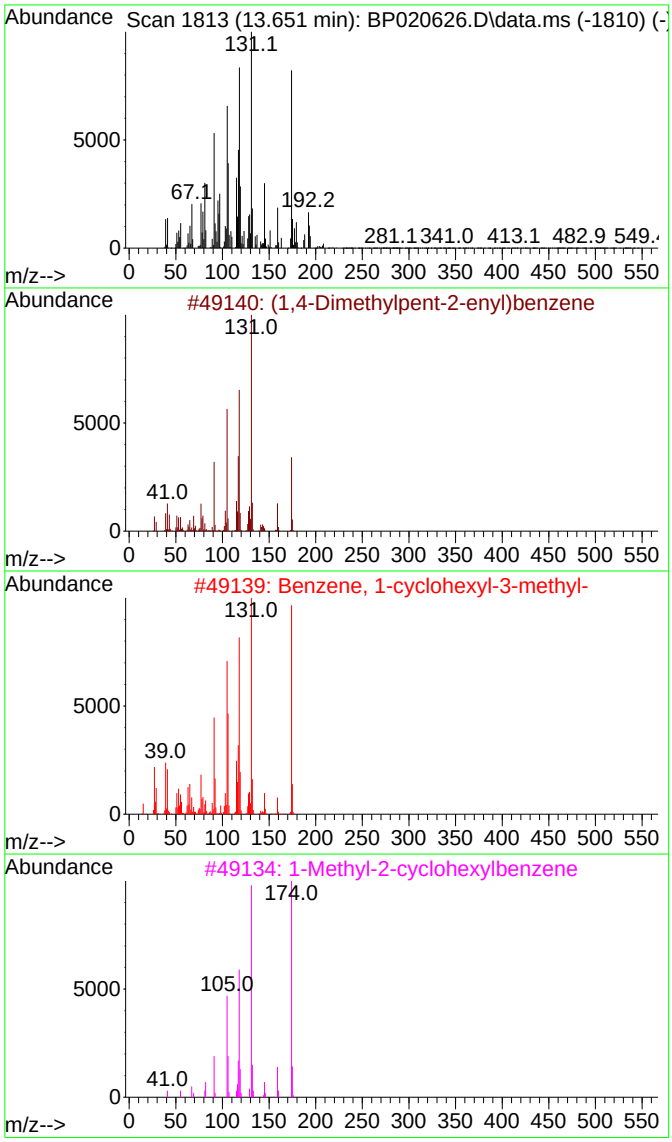
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

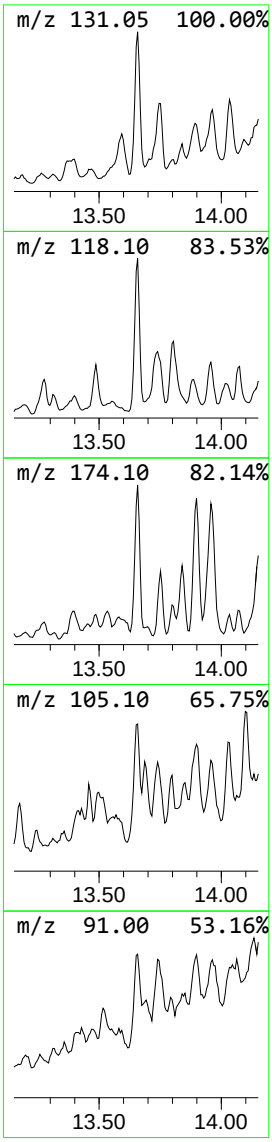
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (1,4-Dimethylpent-2-enyl)be... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.651	33.66 ng	2209810	Acenaphthene-d10	14.393

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,4-Dimethylpent-2-enyl)benzene	174	C13H18	1000184-97-9	93
2	Benzene, 1-cyclohexyl-3-methyl-	174	C13H18	004575-46-6	89
3	1-Methyl-2-cyclohexylbenzene	174	C13H18	004501-35-3	76
4	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	70
5	2-Pentanone, 3-(phenylmethylene)-	174	C12H14O	003437-89-6	38





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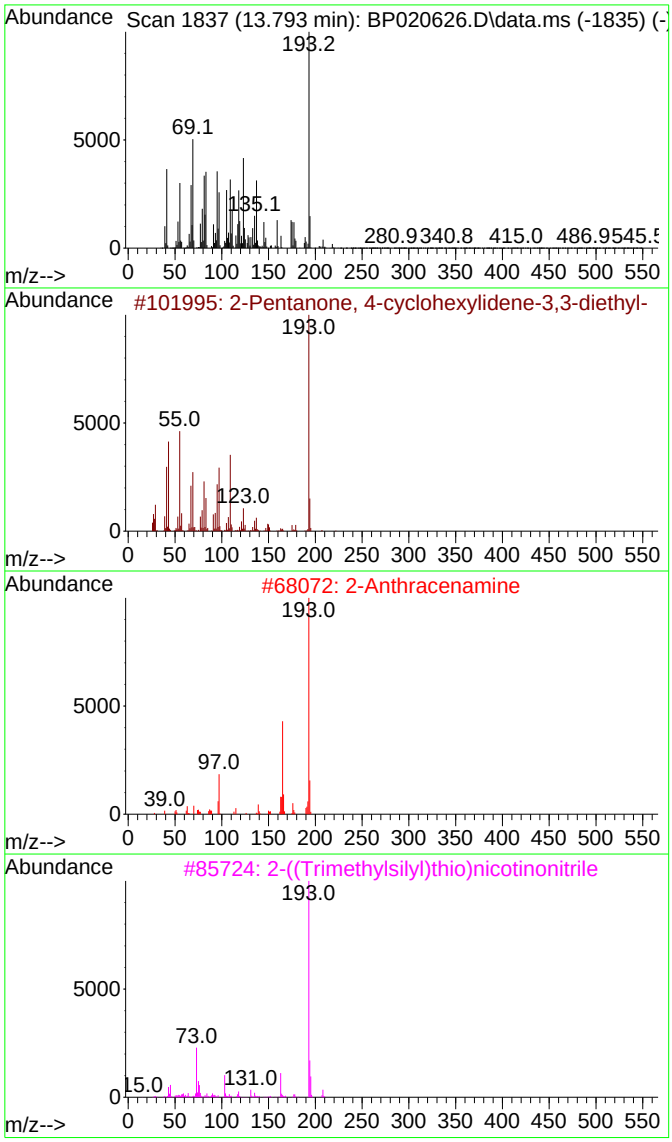
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

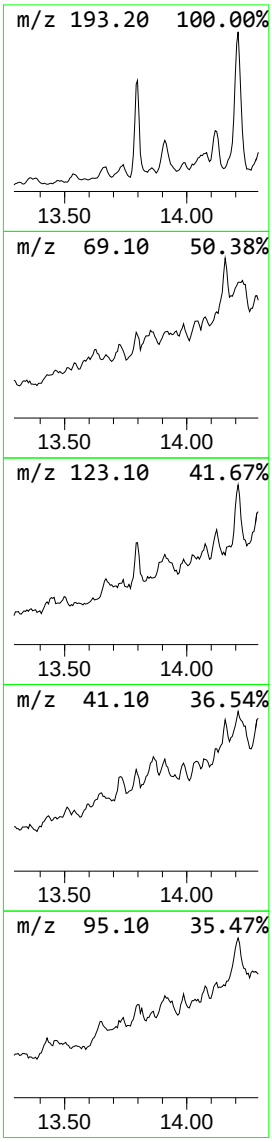
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Pentanone, 4-cyclohexylid... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.793	20.00 ng	1313040	Acenaphthene-d10	14.393

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	50
2	2-Anthracenamine	193	C14H11N	000613-13-8	35
3	2-((Trimethylsilyl)thio)nicotino...	208	C9H12N2SSi	1000474-02-5	30
4	benzoxazole, 5,6-dimethoxy-2-met...	193	C10H11NO3	1000395-98-9	27
5	Trisiloxane, 1,1,3,3,5,5-hexamet...	208	C6H20O2Si3	001189-93-1	27





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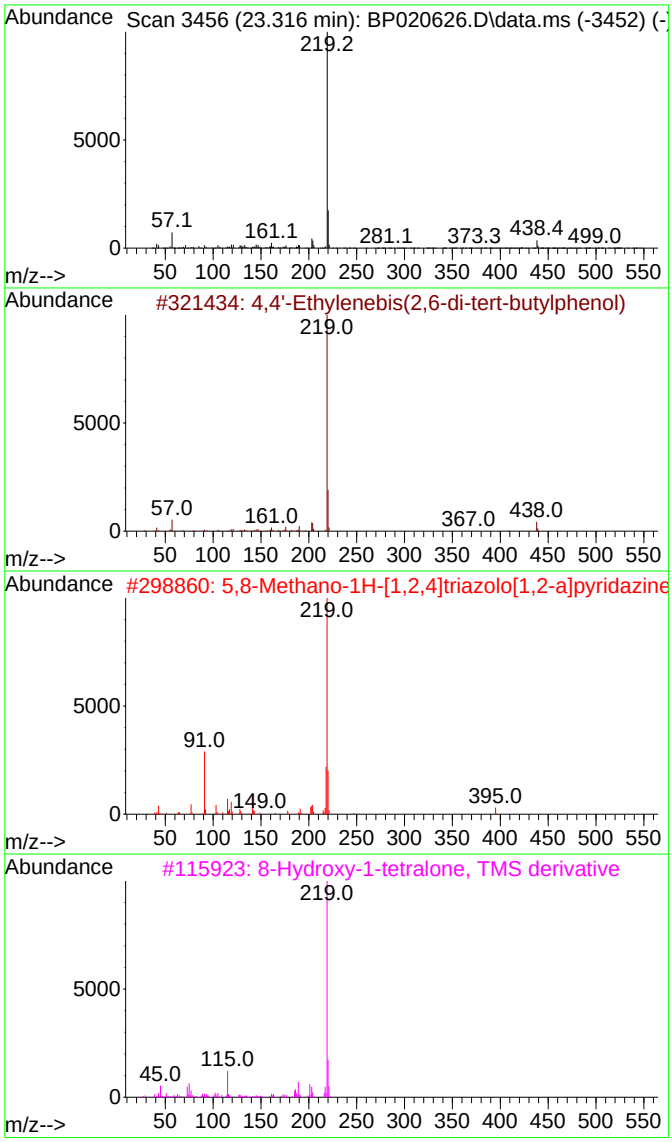
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

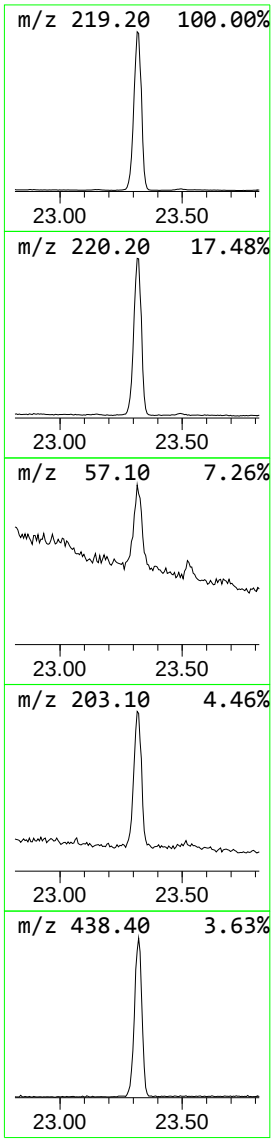
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4,4'-Ethylenebis(2,6-di-ter... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.316	20.00 ng	8849880	Chrysene-d12	21.733

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Ethylenebis(2,6-di-tert-but...	438	C30H46O2	001516-94-5	94
2	5,8-Methano-1H-[1,2,4]triazolo[1...	395	C25H21N3O2	1000142-91-6	78
3	8-Hydroxy-1-tetralone, TMS deriv...	234	C13H18O2Si	1000161-48-8	72
4	2-Methyl-4-phenylquinoline	219	C16H13N	001721-92-2	72
5	Propanohydrazide, N2-(3,5-di-ter...	382	C24H34N2O2	304870-86-8	72





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.022	31.8	ng	2396020	1	7.752	1507010	20.0
Dodecane, 1-cyc...	12.304	3.2	ng	338005	2	10.522	2095470	20.0
unknown12.569	12.569	9.2	ng	606448	3	14.393	1313040	20.0
unknown12.904	12.904	9.8	ng	640433	3	14.393	1313040	20.0
3-Octyne, 2,2,7...	13.063	15.0	ng	984623	3	14.393	1313040	20.0
(1,4-Dimethylpe...	13.651	33.7	ng	2209810	3	14.393	1313040	20.0
2-Pentanone, 4-...	13.793	20.0	ng	1313040	3	14.393	1313040	20.0
4,4'-Ethylenebi...	23.316	20.0	ng	8849880	5	21.733	8849880	20.0