LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092521\
Data File : BF125655.D
Acq On : 25 Sep 2021 14:25
Operator : JU/CG
Sample : M3908-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUB-SLAB-04-(6-8)

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-BF092421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125655.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	20	rVB	1006485	1286943	31.12%	4.507%
2	5.104	505	513	522	rVB	101053	125223	3.03%	0.439%
3	5.504	576	581	584	rBV	3081715	3033296	73.34%	10.623%
4	6.504	746	751	754	rBV	3191336	3178024	76.84%	11.130%
5	6.887	812	816	819	rBV	1154435	883009	21.35%	3.093%
6	7.445	906	911	914	rBV	2281150	2034696	49.19%	7.126%
7	8.063	1013	1016	1023	rBV	276618	242774	5.87%	0.850%
8	8.169	1030	1034	1037	rVB	1422848	1216733	29.42%	4.261%
9	9.245	1212	1217	1220	rBV	4536564	4136066	100.00%	14.485%
10	9.922	1328	1332	1335	rBV	1736369	1397531	33.79%	4.894%
11	10.704	1461	1465	1469	rBV	2478752	2298496	55.57%	8.050%
12	11.404	1581	1584	1589	rBV	1576137	1320566	31.93%	4.625%
13	11.933	1671	1674	1676	rBV	316005	294885	7.13%	1.033%
14	12.716	1805	1807	1810	rBV3	207778	199749	4.83%	0.700%
15	12.992	1850	1854	1857	rBV	3624859	3129281	75.66%	10.959%
16	14.045	2030	2033	2036	rVB	995474	792627	19.16%	2.776%
17	15.492	2276	2279	2281	rBV2	253614	311583	7.53%	1.091%
18	15.521	2281	2284	2288	rVB	772911	882029	21.33%	3.089%
19	15.686	2309	2312	2316	rVB2	319461	433426	10.48%	1.518%
20	16.257	2405	2409	2416	rVB2	332430	640580	15.49%	2.243%
21	16.698	2479	2484	2492	rVB	382794	715632	17.30%	2.506%

Sum of corrected areas: 28553149

LSC Report - Integrated Chromatogram

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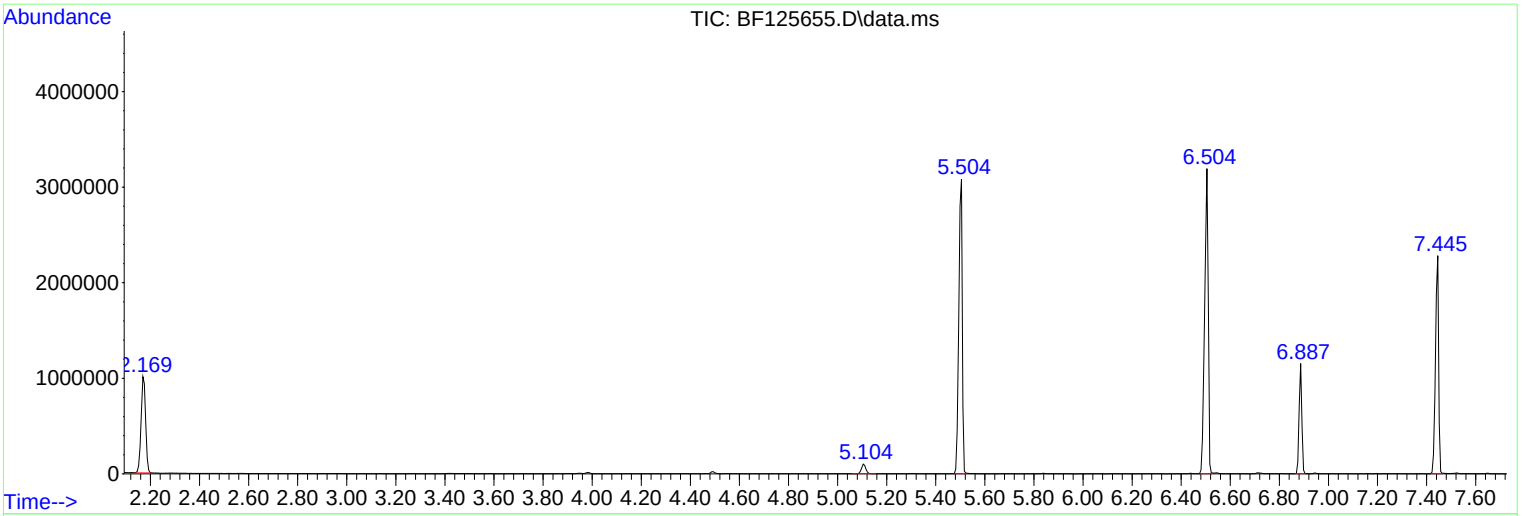
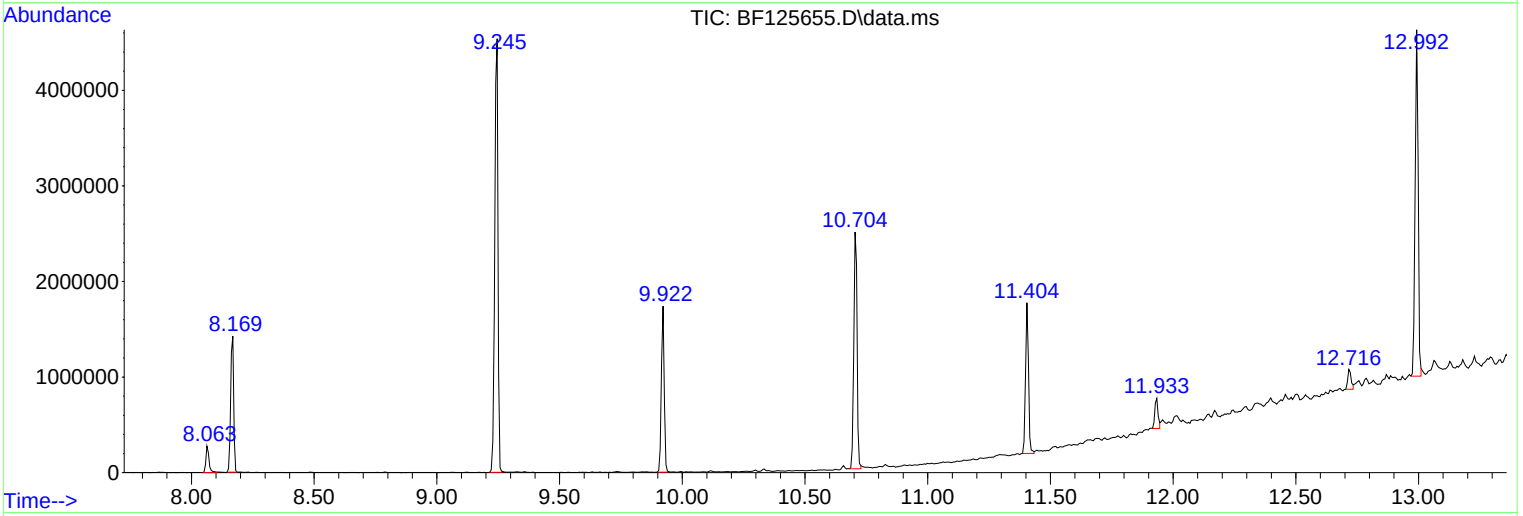
Sample : M3908-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

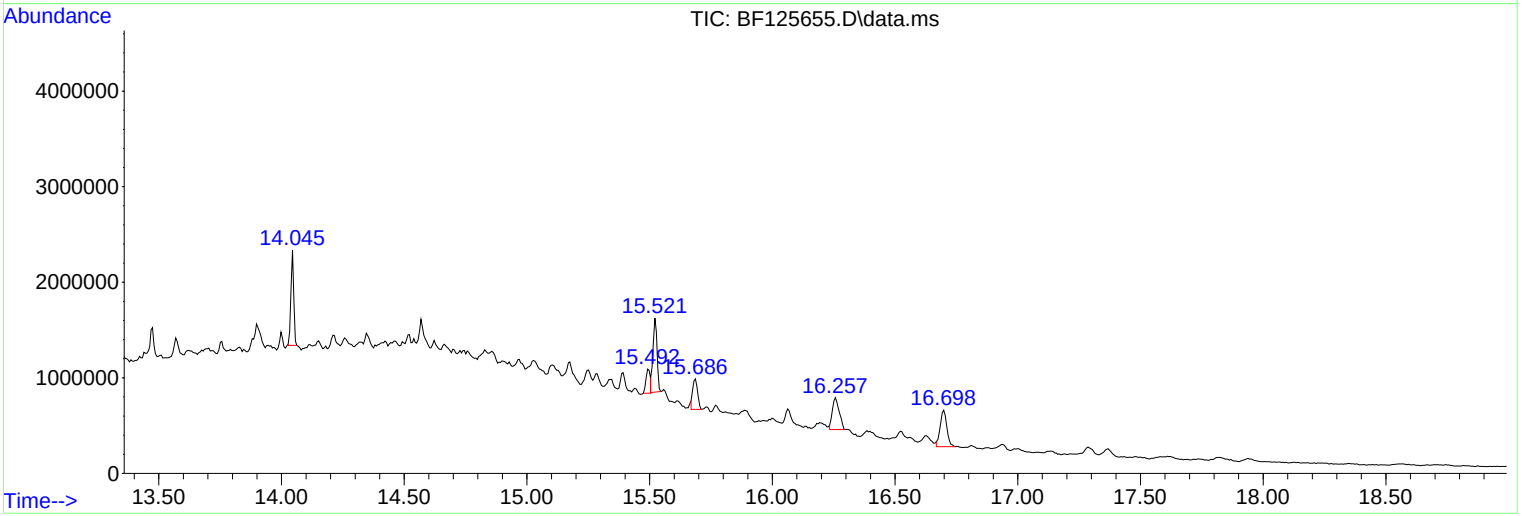
Instrument :
BNA_F
ClientSampleId :
SUB-SLAB-04-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.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 : BF125655.D
Acq On : 25 Sep 2021 14:25
Operator : JU/CG
Sample : M3908-02
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Instrument : BNA_F
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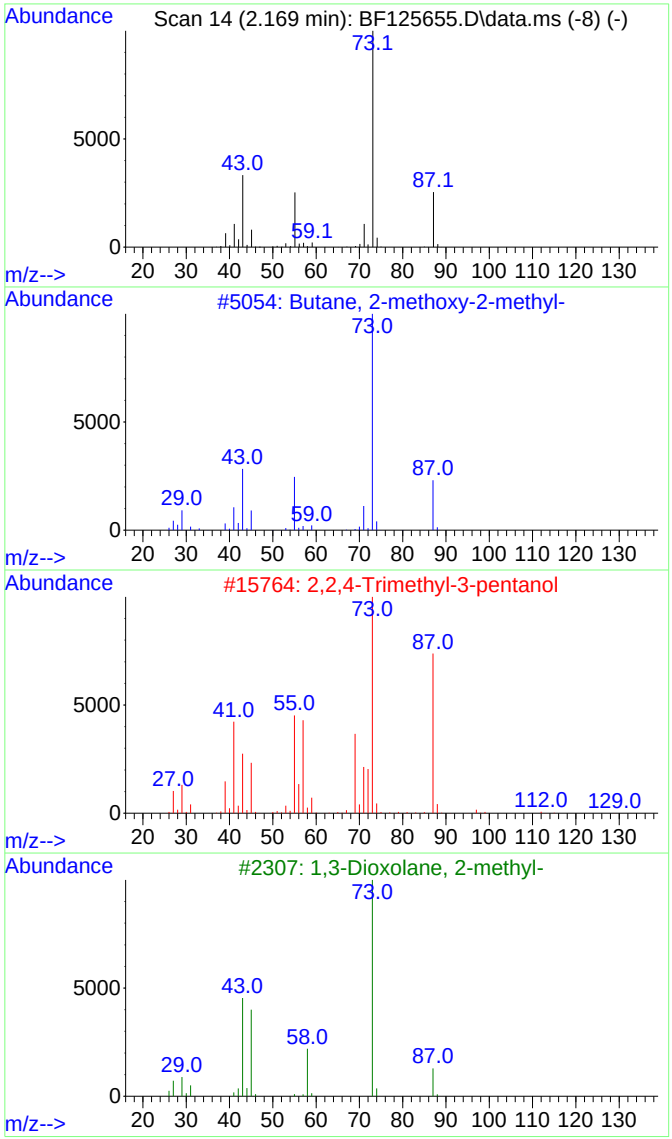
TIC Integration Parameters: LSCINT.P

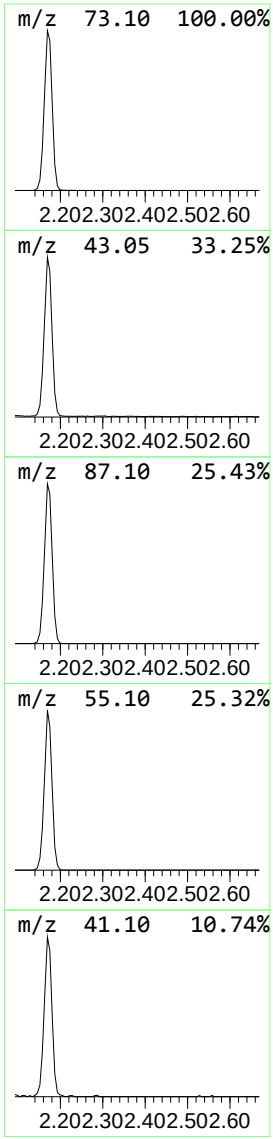
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	29.15 ng	1286940	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Sample : M3908-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUB-SLAB-04-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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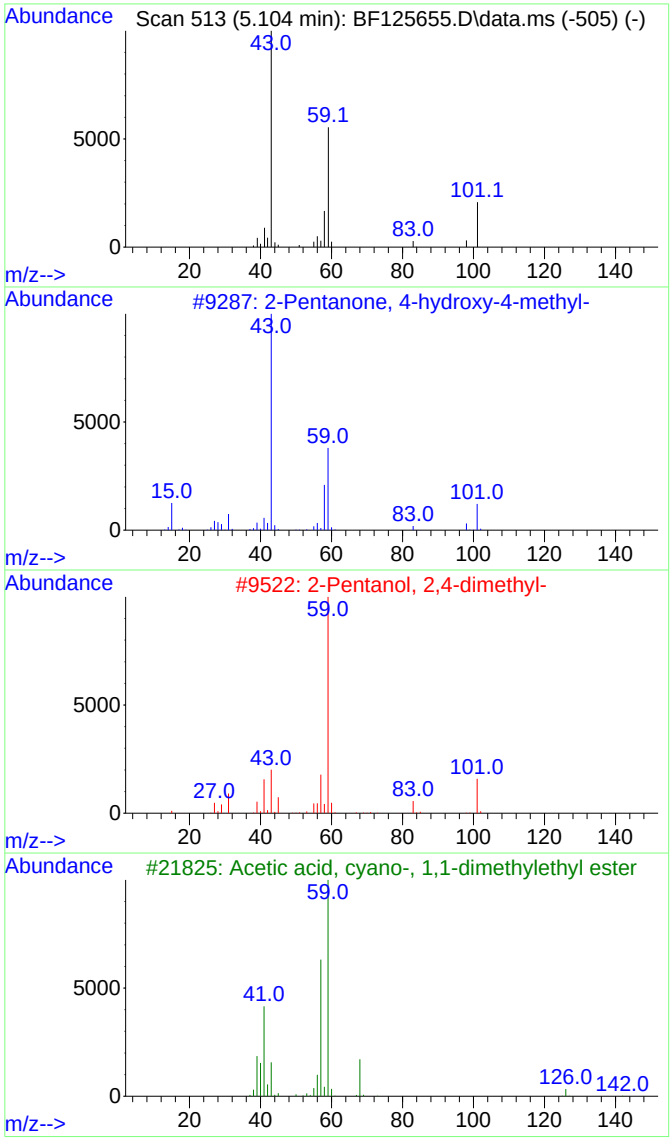
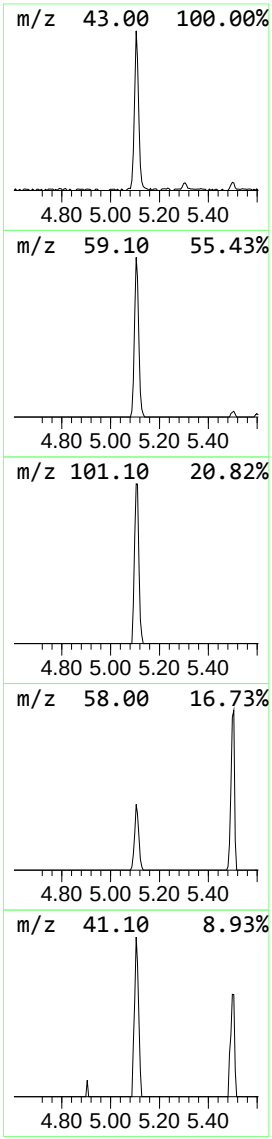
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	2.84 ng	125223	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Sample : M3908-02
Misc :
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Instrument : BNA_F
ClientSampleId : SUB-SLAB-04-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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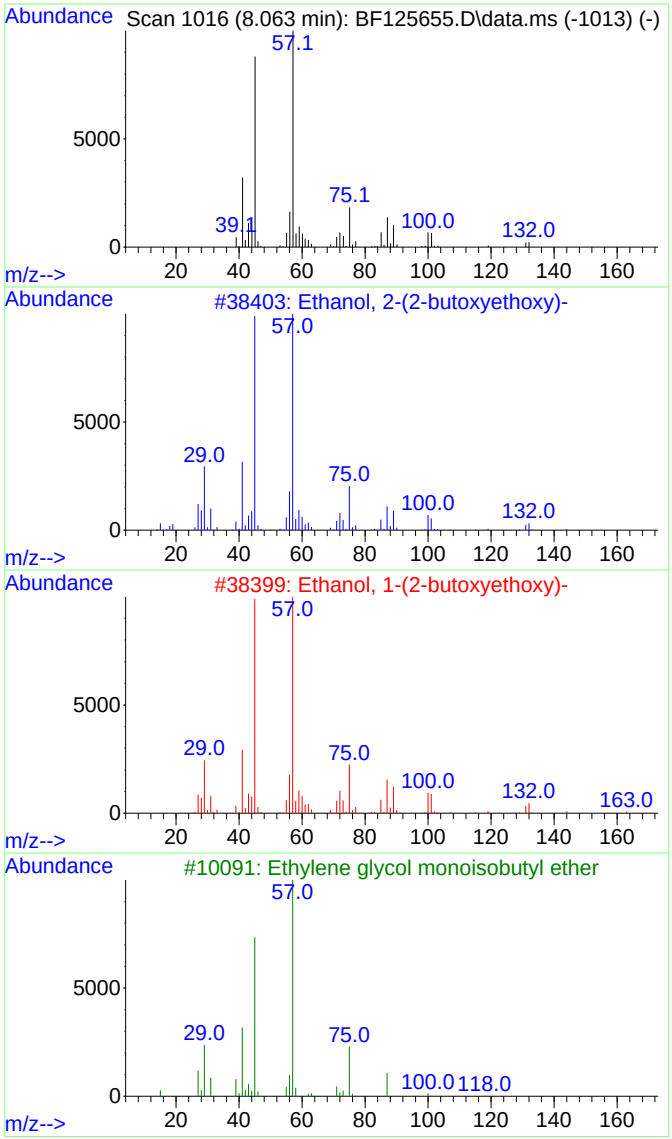
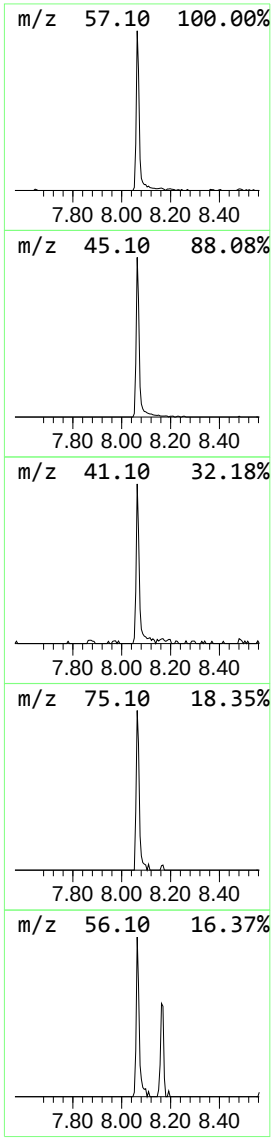
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.063	3.99 ng	242774	Naphthalene-d8	8.169

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	58
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56





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Sample : M3908-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
SUB-SLAB-04-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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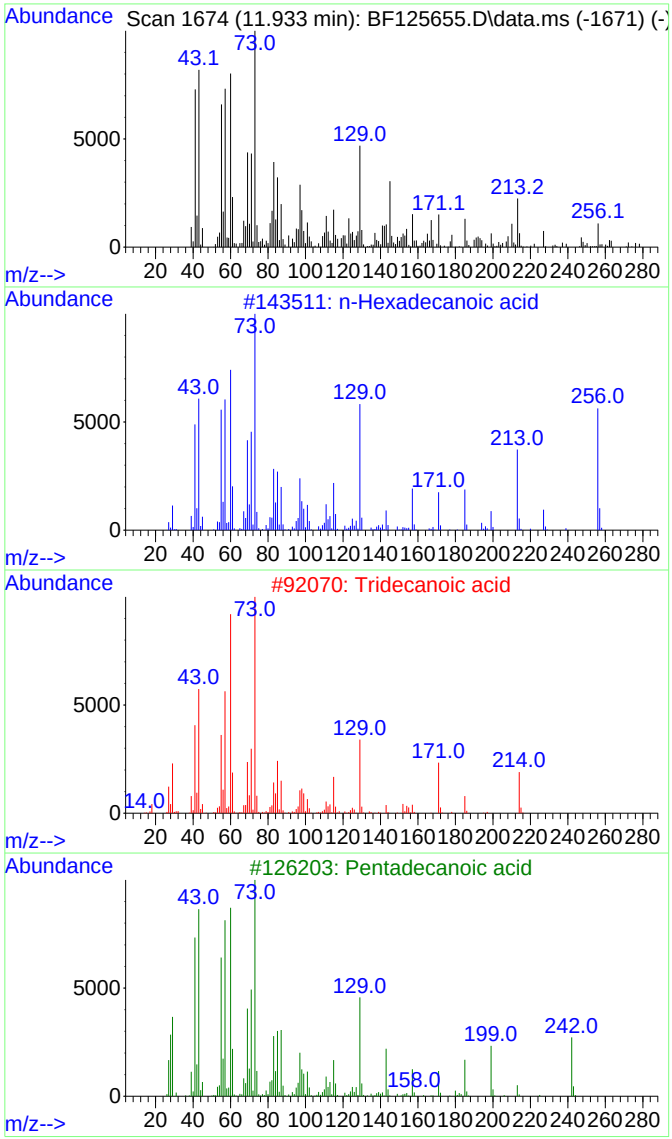
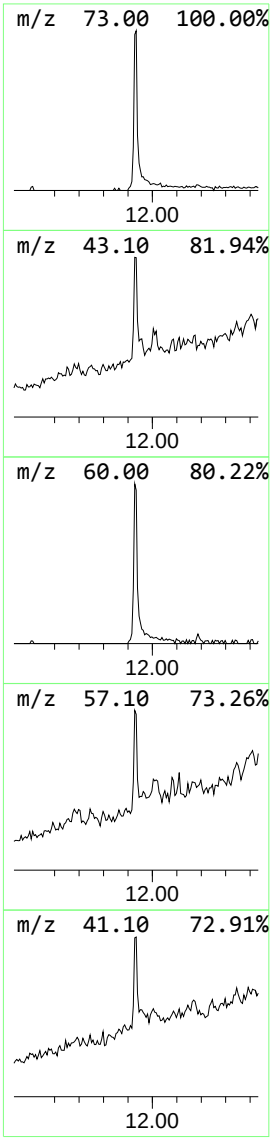
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.47 ng	294885	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
4	1-(Ethenesulfonyl)dodecane	260	C14H28O2S	030719-66-5	44
5	Ethyl .alpha.-hydroxymyristate	272	C16H32O3	129086-73-3	40





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Sample : M3908-02
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUB-SLAB-04-(6-8)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

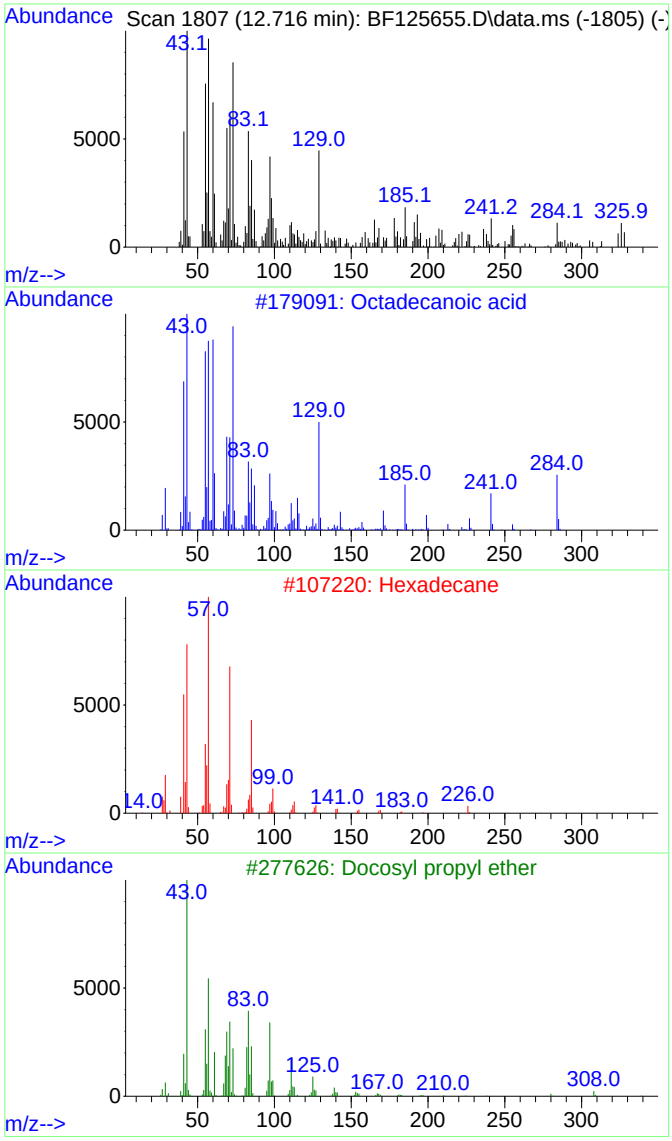
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

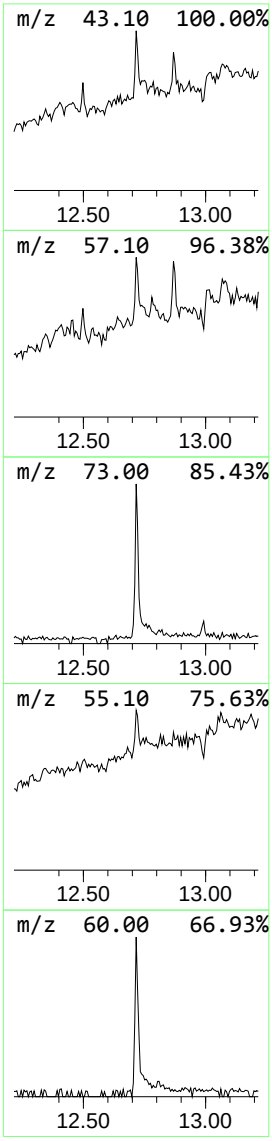
****

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	3.03 ng	199749	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Hexadecane	226	C16H34	000544-76-3	56
3	Docosyl propyl ether	368	C25H52O	1000406-28-2	46
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	44
5	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	41





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SUB-SLAB-04-(6-8)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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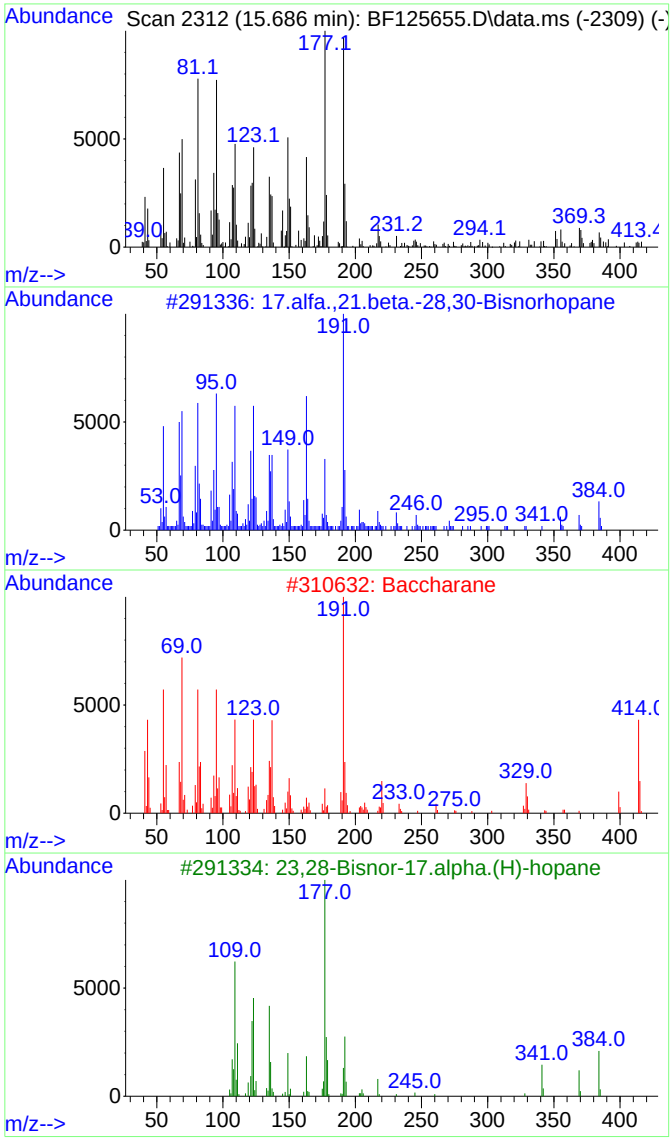
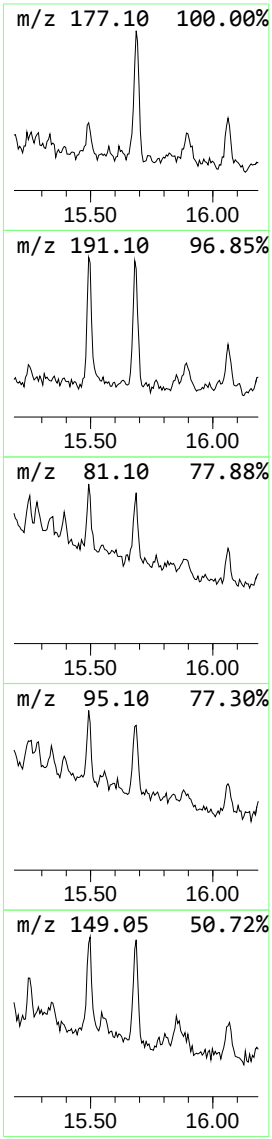
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 17.alfa.,21.beta.-28,30-Bis... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.686	9.83 ng	433426	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17.alfa.,21.beta.-28,30-Bisnorho...	384	C28H48	1000360-26-1	70
2	Baccharane	414	C30H54	036441-74-4	64
3	23,28-Bisnor-17.alpha.(H)-hopane	384	C28H48	1000101-35-1	60
4	17.alpha.H-Trisnorhopane	370	C27H46	053584-59-1	45
5	Acetamide, N-benzothiazol-2-yl-2...	370	C16H14N6O3S	1000303-47-0	41





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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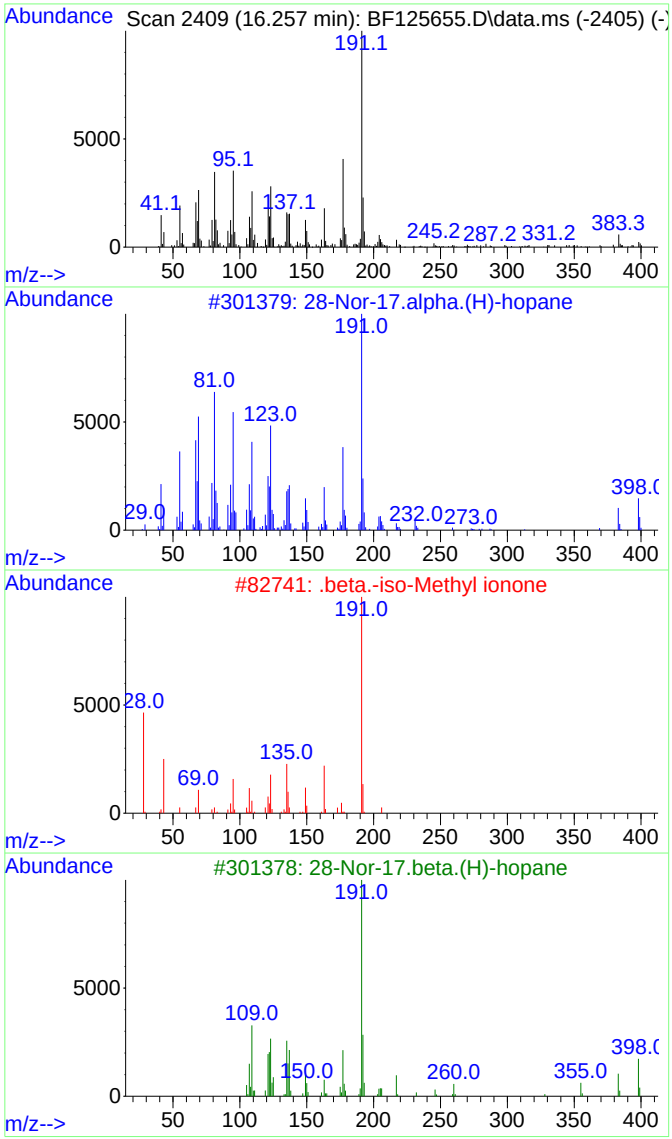
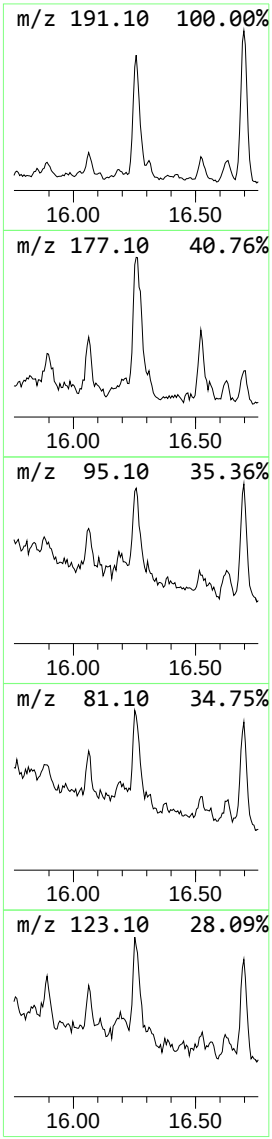
****

Peak Number 7 28-Nor-17.alpha.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.257	14.53 ng	640580	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	64
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	46
3	28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	41
4	(7S,7aR,13aS)-9-Methoxy-4,4,7,7a...	344	C22H32O3	1000482-45-3	38
5	4-(3H-Imidazo[4,5-b]pyridin-2-yl...	342	C15H18N8S	1000276-08-2	35





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TIC Library : C:\Database\NIST20.L
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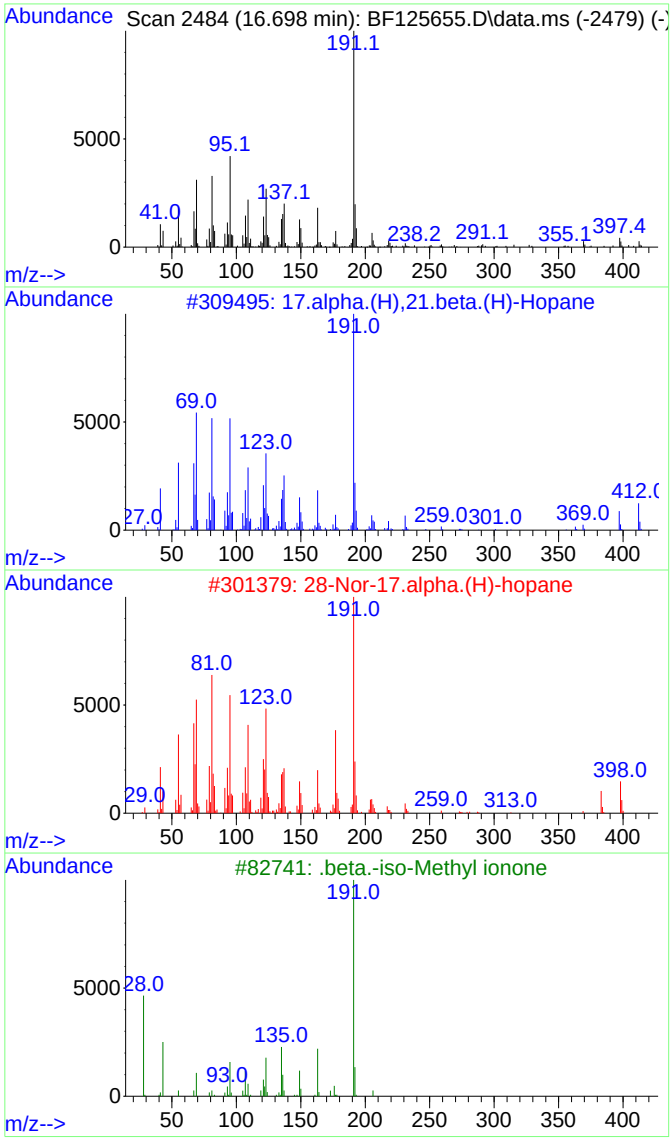
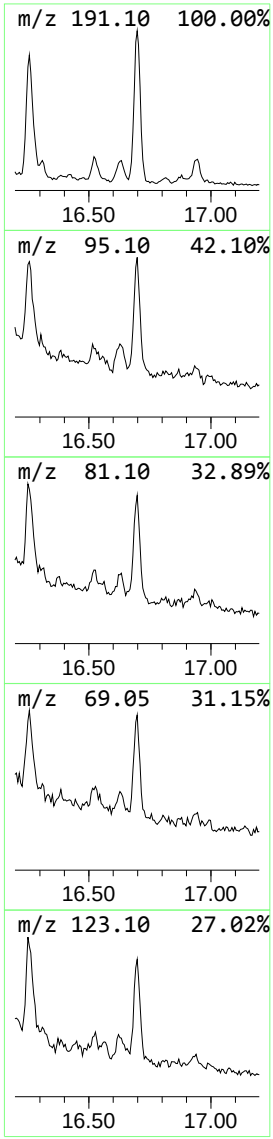
****
Peak Number 8 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.698	16.23 ng	715632	Perylene-d12	15.521

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	93
2	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	78
3	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	53
4	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	53
5	1-(2-Fluorobenzyl)-3-piperidinam...	278	C16H23FN2O	1546741-98-3	43





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092421.M
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
Butane, 2-metho...	2.169	29.1	ng	1286940	1	6.887	883009	20.0
2-Pentanone, 4-...	5.104	2.8	ng	125223	1	6.887	883009	20.0
Ethanol, 2-(2-b...	8.063	4.0	ng	242774	2	8.169	1216730	20.0
n-Hexadecanoic ...	11.933	4.5	ng	294885	4	11.404	1320570	20.0
Octadecanoic acid	12.716	3.0	ng	199749	4	11.404	1320570	20.0
17.alfa.,21.bet...	15.686	9.8	ng	433426	6	15.521	882029	20.0
28-Nor-17.alpha...	16.257	14.5	ng	640580	6	15.521	882029	20.0
17.alpha.(H),21...	16.698	16.2	ng	715632	6	15.521	882029	20.0