LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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	1.655	5	6	14	rVB	267435	411050	10.61%	1.797%
2	1.770	14	16	71	rVB	1643618	3872738	100.00%	16.928%
3	4.821	281	283	288	rBV	75133	108313	2.80%	0.473%
4	5.256	319	321	324	rBV	1205117	1728221	44.63%	7.554%
5	5.896	376	377	381	rBV2	35192	57836	1.49%	0.253%
6	6.319	411	414	417	rBV	1534319	1626888	42.01%	7.111%
7	6.433	422	424	427	rVV	1679951	1718480	44.37%	7.512%
8	6.662	443	444	447	rVB2	475114	512669	13.24%	2.241%
9	6.822	456	458	460	rVV	1679204	1473103	38.04%	6.439%
10	6.936	466	468	473	rVB	26492	46739	1.21%	0.204%
11	7.233	492	494	497	rVV	1051301	1012066	26.13%	4.424%
12	7.587	521	525	528	rBV3	26261	51599	1.33%	0.226%
13	7.953	554	557	559	rVV	738768	705000	18.20%	3.082%
14	8.388	592	595	599	rVB	74160	104484	2.70%	0.457%
15	8.982	645	647	648	rVB	74992	60715	1.57%	0.265%
16	9.028	648	651	654	rBV	2122135	1989962	51.38%	8.698%
17	9.119	655	659	661	rBV4	16464	40604	1.05%	0.177%
18	9.428	682	686	688	rBV	752370	701994	18.13%	3.069%
19	9.645	703	705	707	rBV	46039	53899	1.39%	0.236%
20	9.702	707	710	712	rVB	636187	773127	19.96%	3.379%
21	10.136	747	748	756	rVB	78879	87656	2.26%	0.383%
22	10.353	764	767	770	rBV	68249	103260	2.67%	0.451%
23	10.491	776	779	781	rBV	947674	1235691	31.91%	5.401%
24	10.616	788	790	794	rBV	102804	188512	4.87%	0.824%
25	11.051	827	828	830	rBV2	39568	56187	1.45%	0.246%
26	11.085	830	831	834	rVB	54957	47396	1.22%	0.207%
27	11.176	837	839	841	rVV	882481	792926	20.47%	3.466%
28	12.582	961	962	968	rVB2	49908	107464	2.77%	0.470%
29	12.754	975	977	980	rBV	1607173	1711172	44.19%	7.480%
30	13.291	1022	1024	1025	rBV	50681	41588	1.07%	0.182%
31	13.714	1058	1061	1066	rBV3	18817	70497	1.82%	0.308%
32	13.805	1066	1069	1071	rBV	586333	650175	16.79%	2.842%
33	14.571	1132	1136	1139	rBV2	30947	51187	1.32%	0.224%
34	14.640	1139	1142	1144	rVB	86796	96340	2.49%	0.421%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.177	1187	1189	1196	rVB	394683	505031	13.04%	2.208%
36	15.760	1238	1240	1248	rVB4	15357	38884	1.00%	0.170%
37	16.457	1298	1301	1303	rBV	24881	43836	1.13%	0.192%

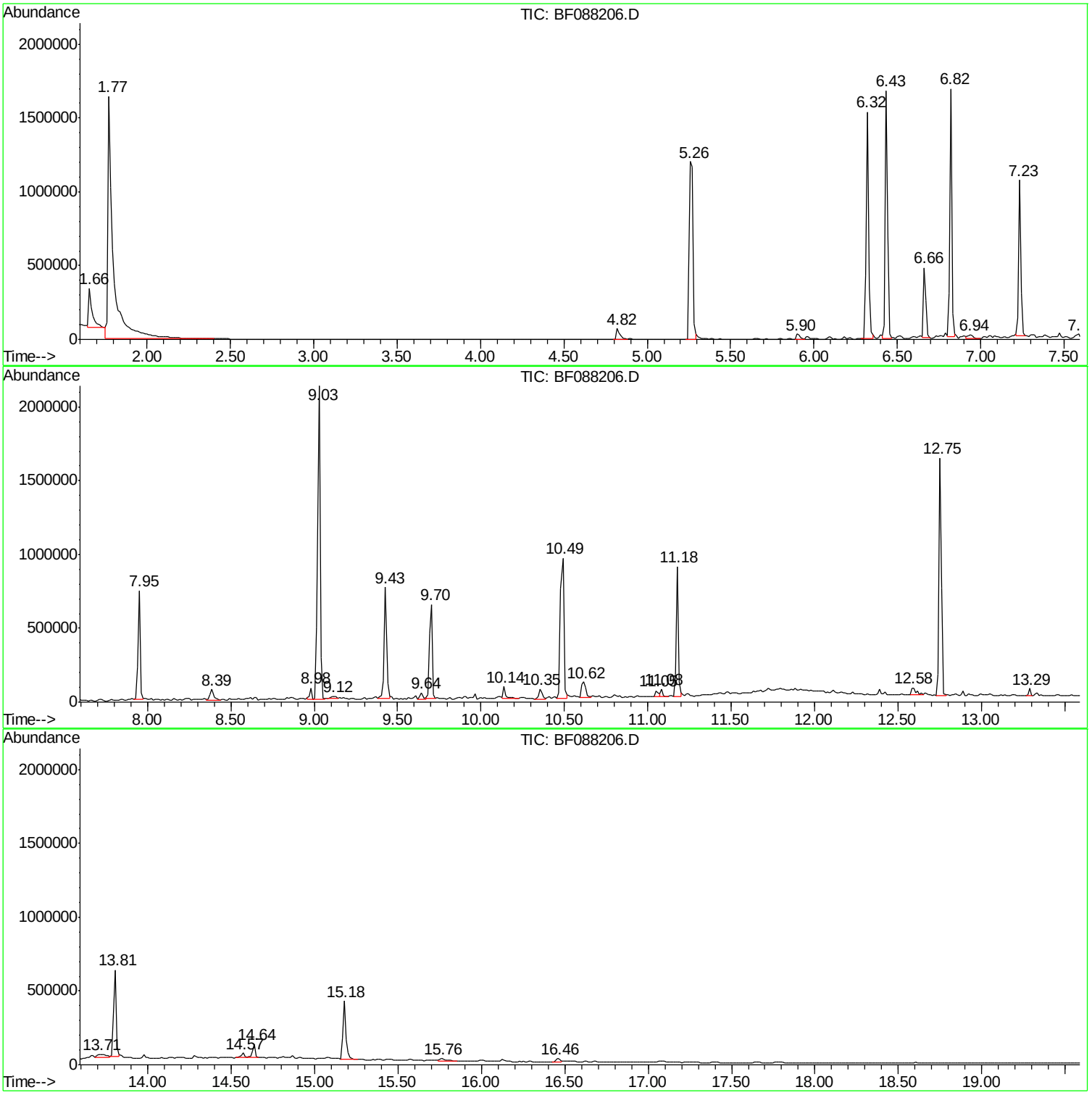
Sum of corrected areas: 22877289

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

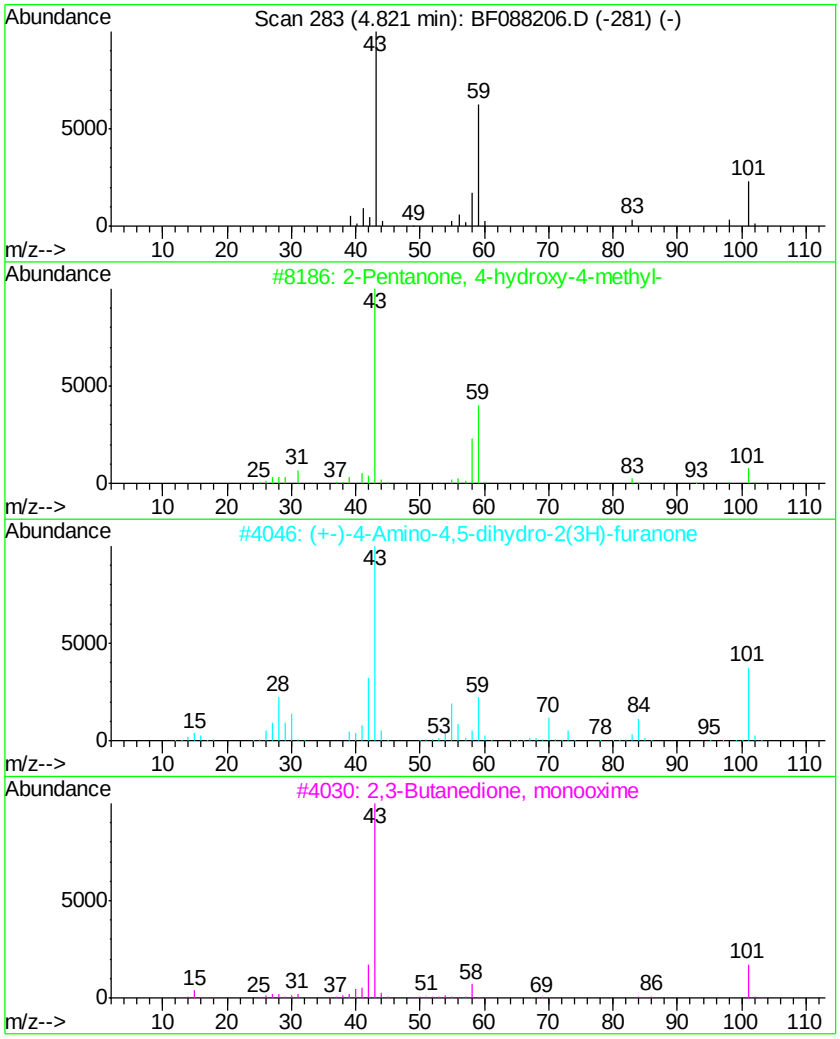
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

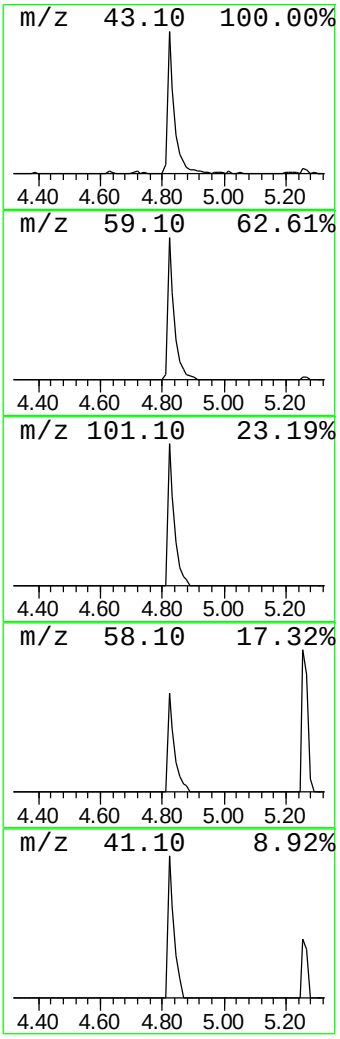
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	4.23 ng	108313	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

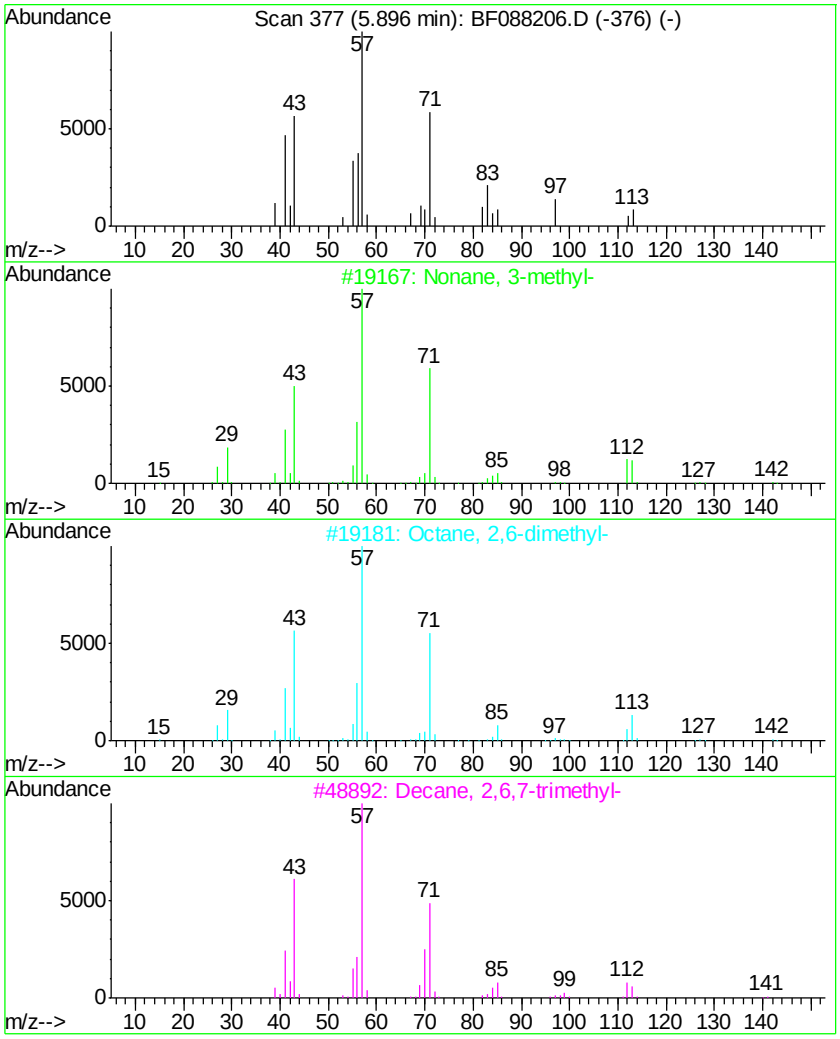
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

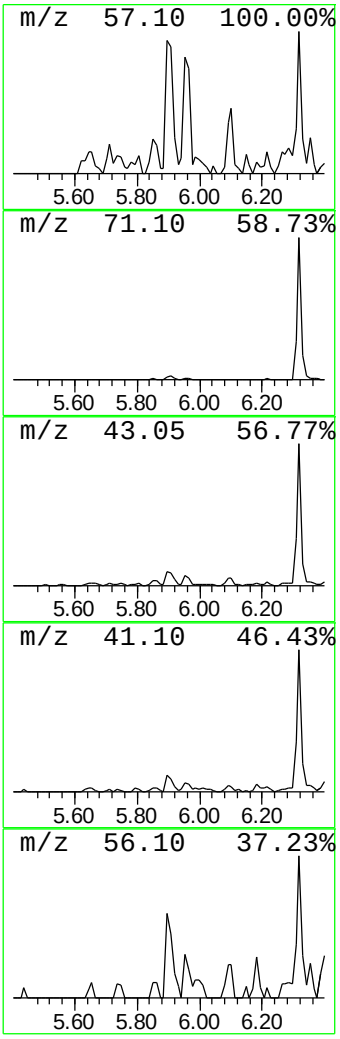
****

Peak Number 4 Nonane, 3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.90	2.26 ng	57836	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	53
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	53
3	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	53
4	Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	50
5	Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

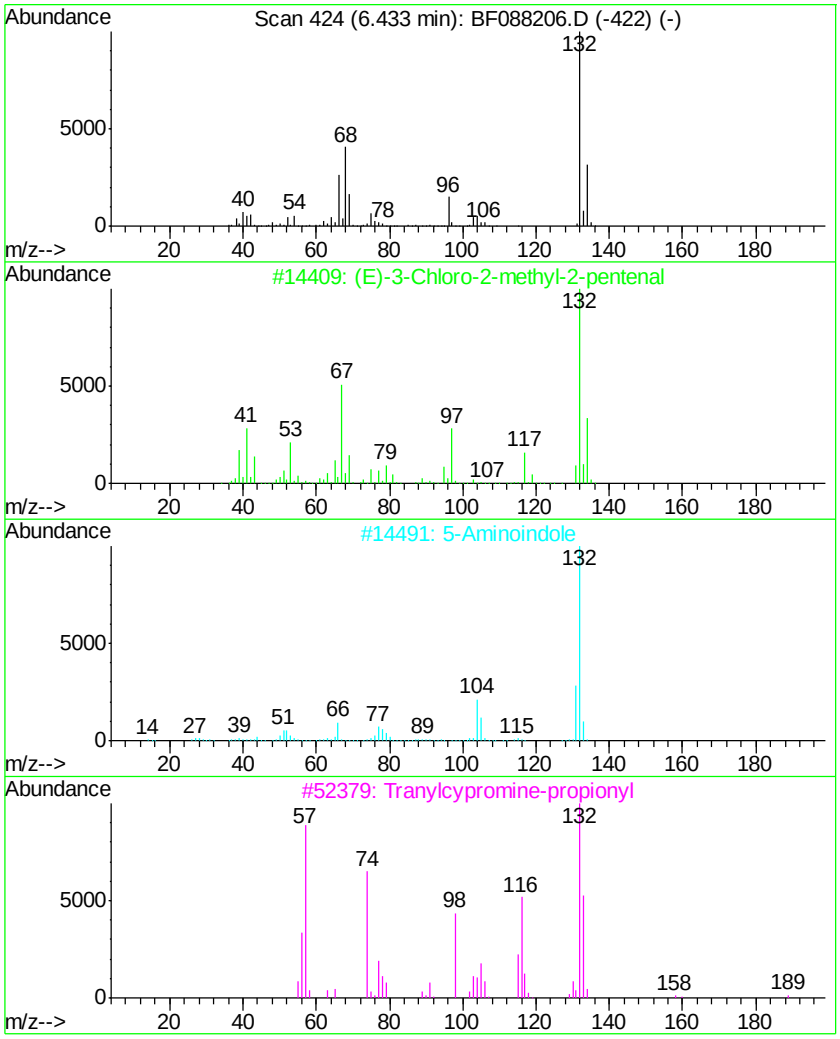
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

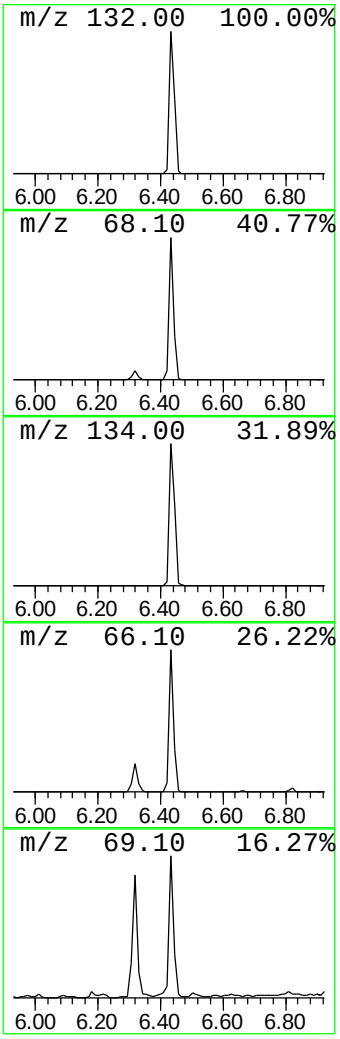
****

Peak Number 5 unknown6.43 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	67.04 ng	1718480	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

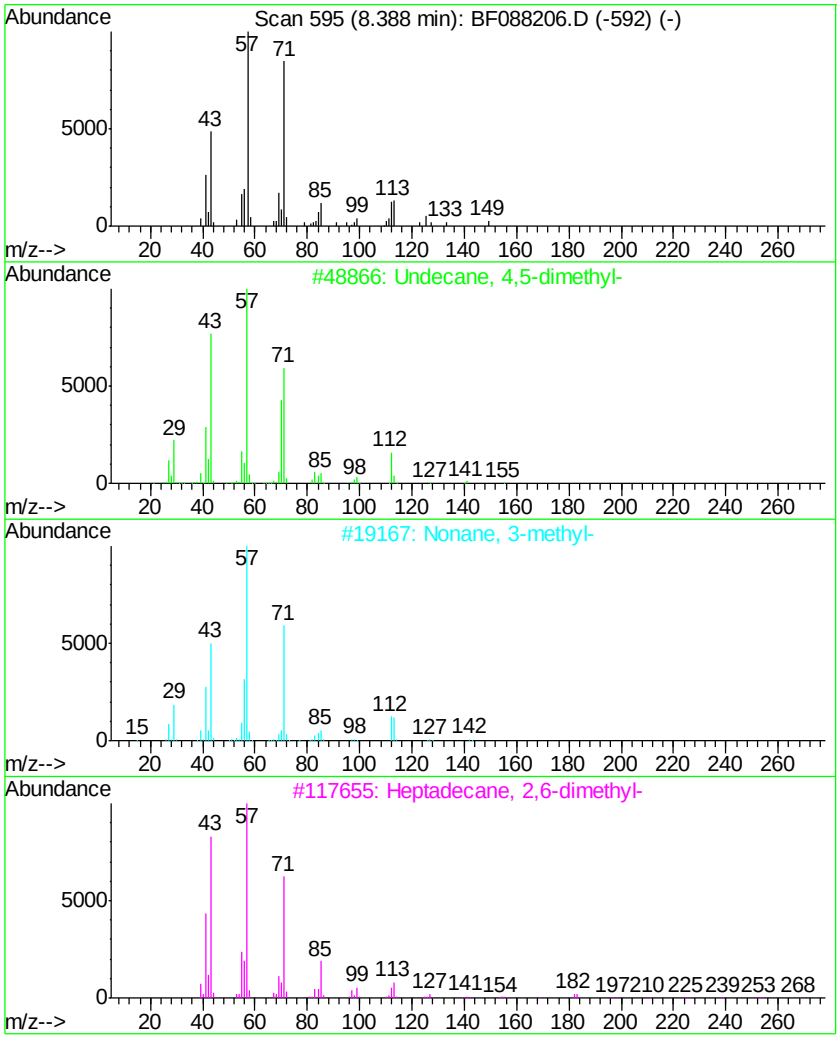
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

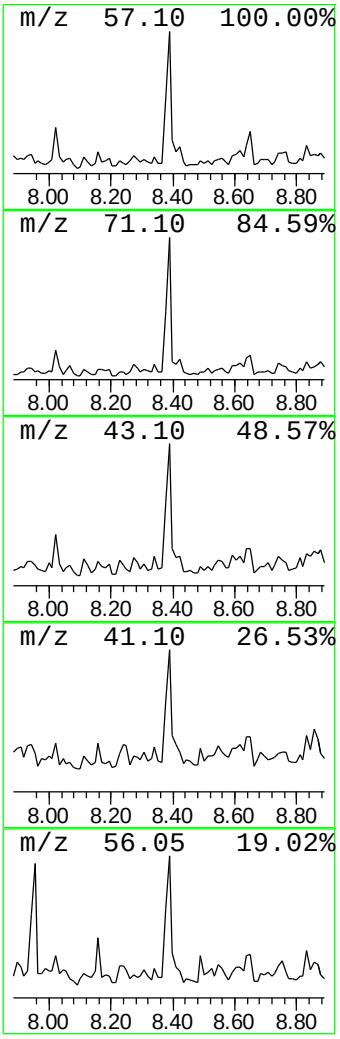
****

Peak Number 7 Undecane, 4,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.39	2.96 ng	104484	Naphthalene-d8	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	72
2	Nonane, 3-methyl-	142	C10H22	005911-04-6	72
3	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	64
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	59
5	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

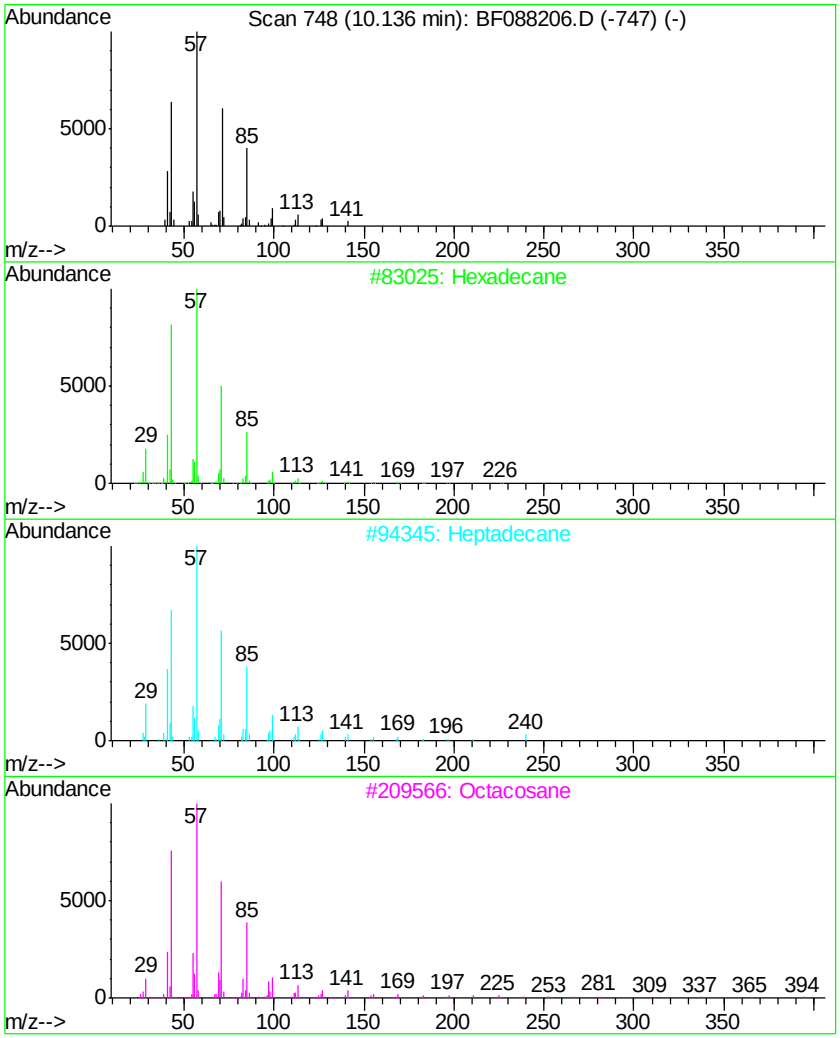
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

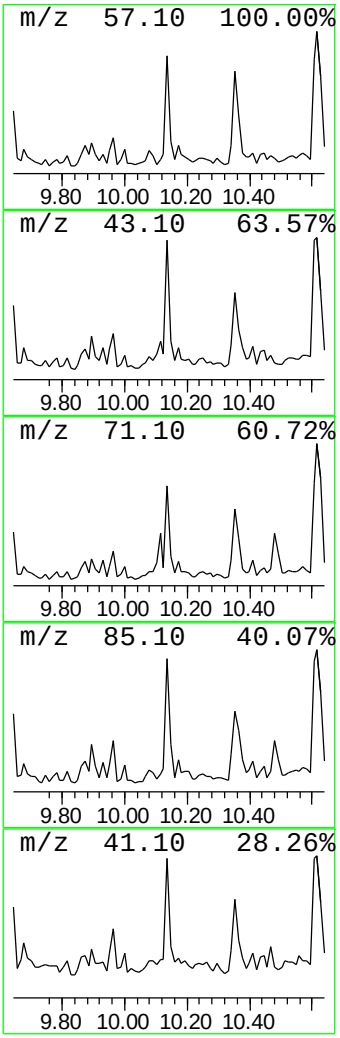
****

Peak Number 8 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	2.27 ng	87656	Acenaphthene-d10	9.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptadecane	240	C17H36	000629-78-7	90
3	Octacosane	394	C28H58	000630-02-4	86
4	Pentadecane	212	C15H32	000629-62-9	86
5	Tetradecane	198	C14H30	000629-59-4	80





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Acq On : 21 Jun 2016 8:30
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Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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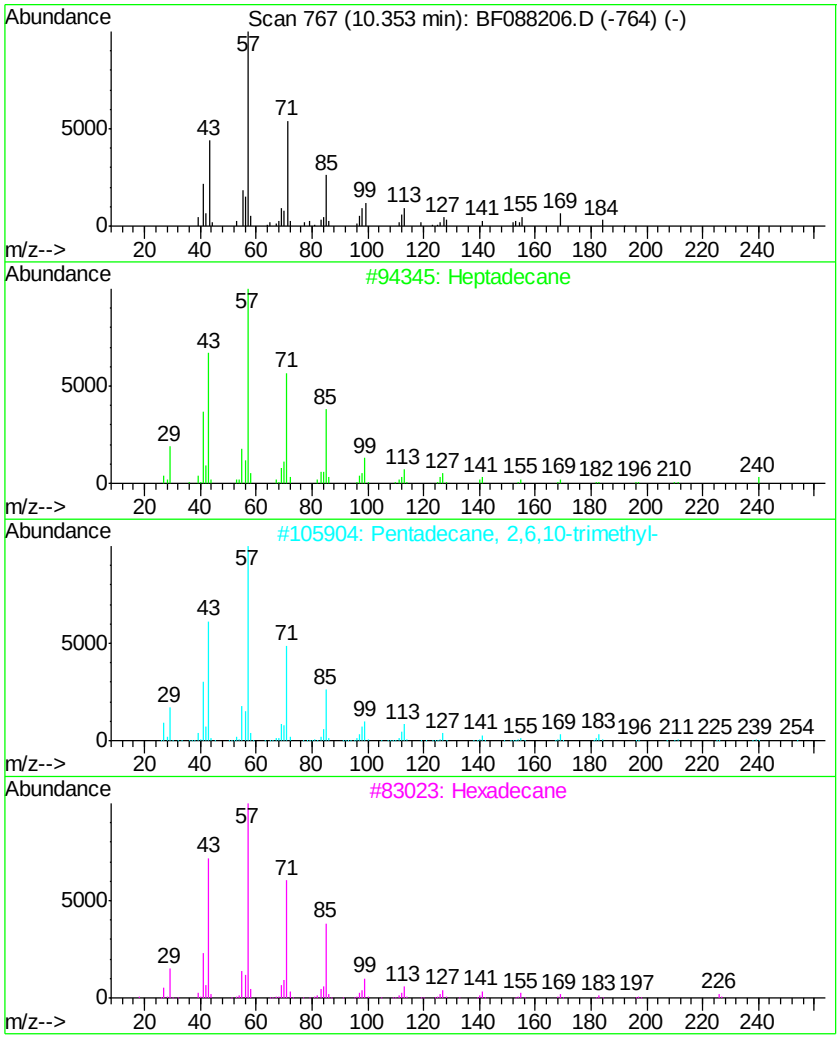
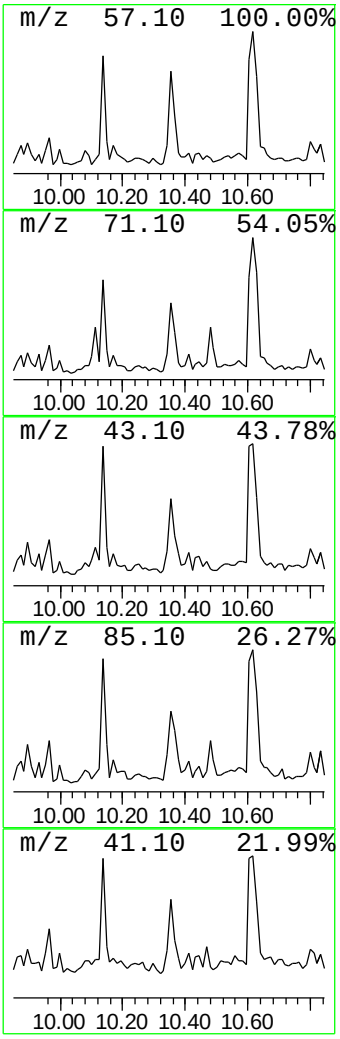
****

Peak Number 9 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.67 ng	103260	Acenaphthene-d10	9.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
3	Hexadecane	226	C16H34	000544-76-3	72
4	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	70
5	Tetracosane	338	C24H50	000646-31-1	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
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Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

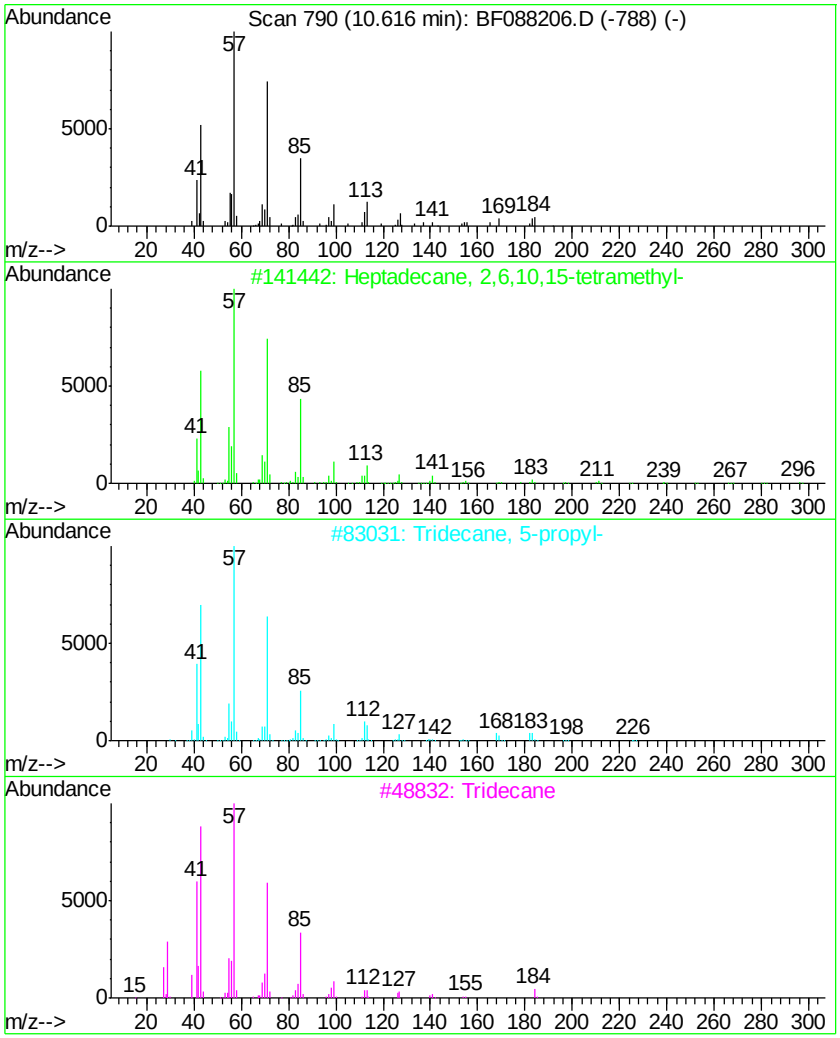
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

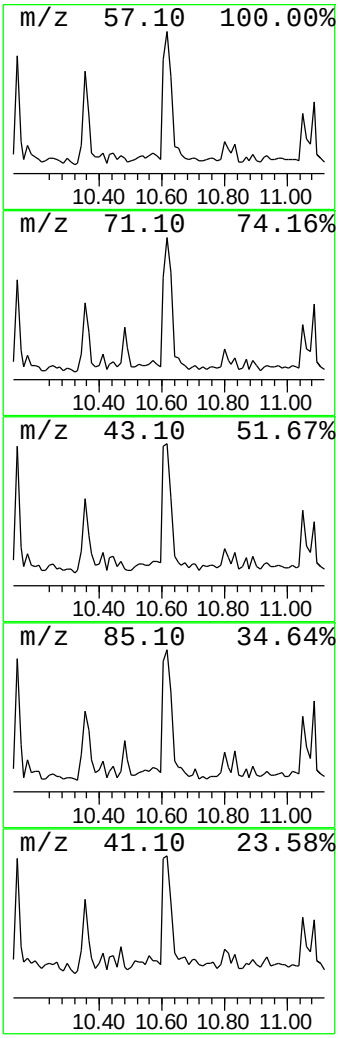
****

Peak Number 10 Heptadecane, 2,6,10,15-tetr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	4.75 ng	188512	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	86
3	Tridecane	184	C13H28	000629-50-5	86
4	Eicosane	282	C20H42	000112-95-8	86
5	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	86





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Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

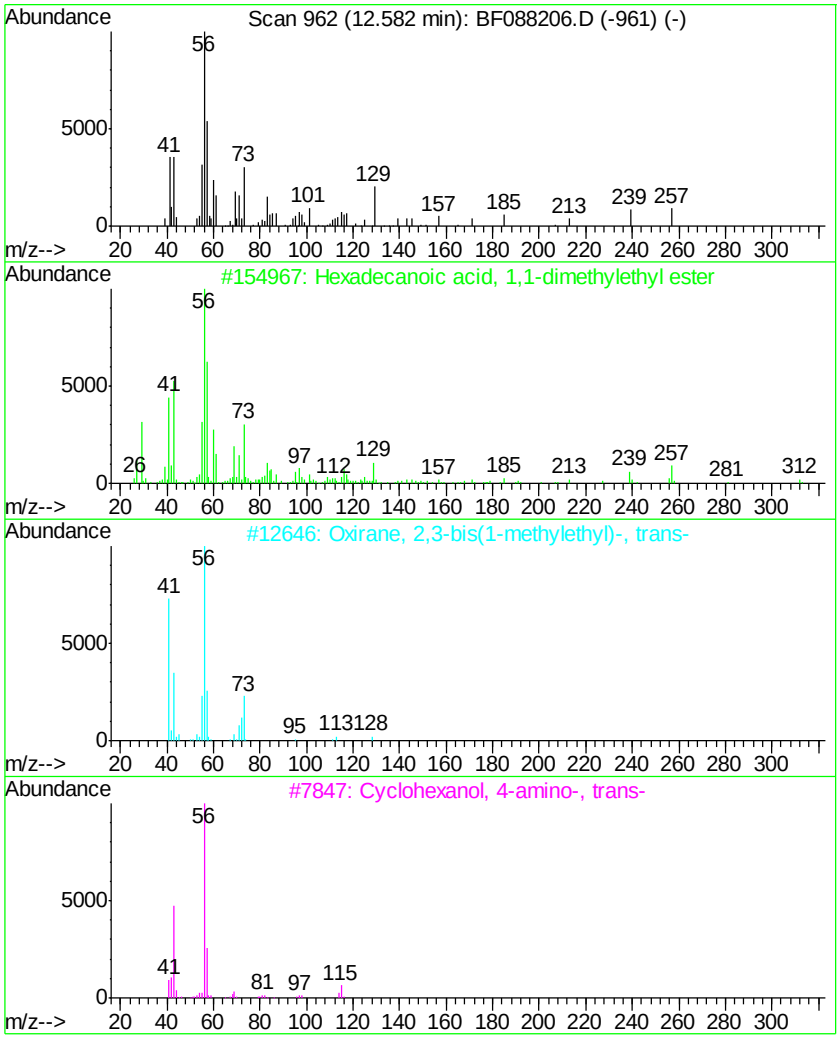
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

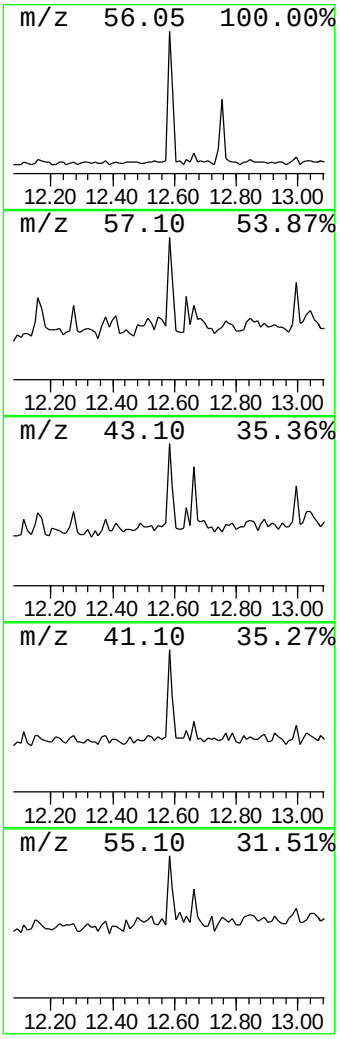
****

Peak Number 11 Hexadecanoic acid, 1,1-dime... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	3.31 ng	107464	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	81
2	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	43
3	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

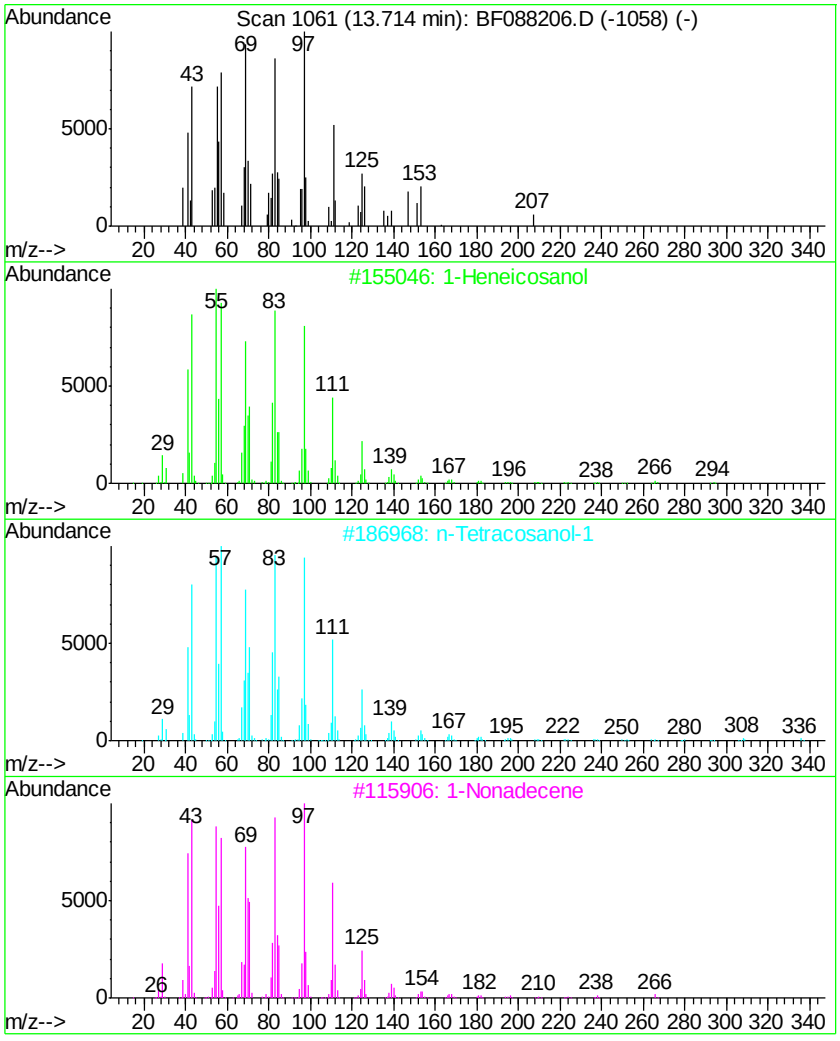
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

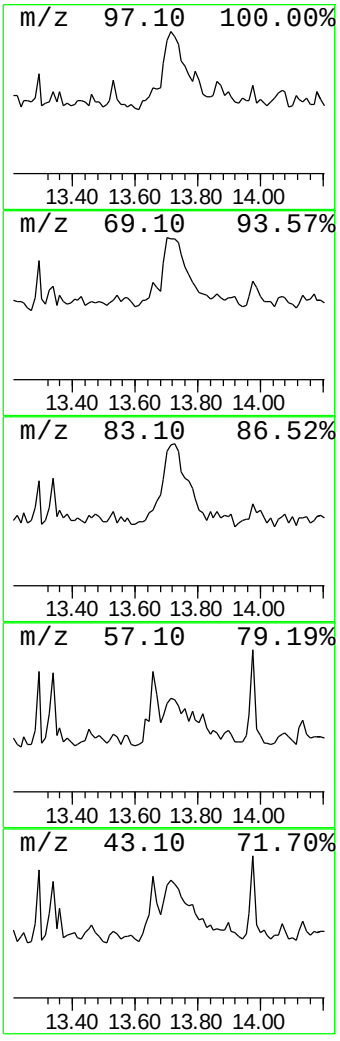
****

Peak Number 12 1-Heneicosanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	2.17 ng	70497	Chrysene-d12	13.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	72
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	58
3	1-Nonadecene	266	C19H38	018435-45-5	58
4	Behenic alcohol	326	C22H46O	000661-19-8	58
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	58





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Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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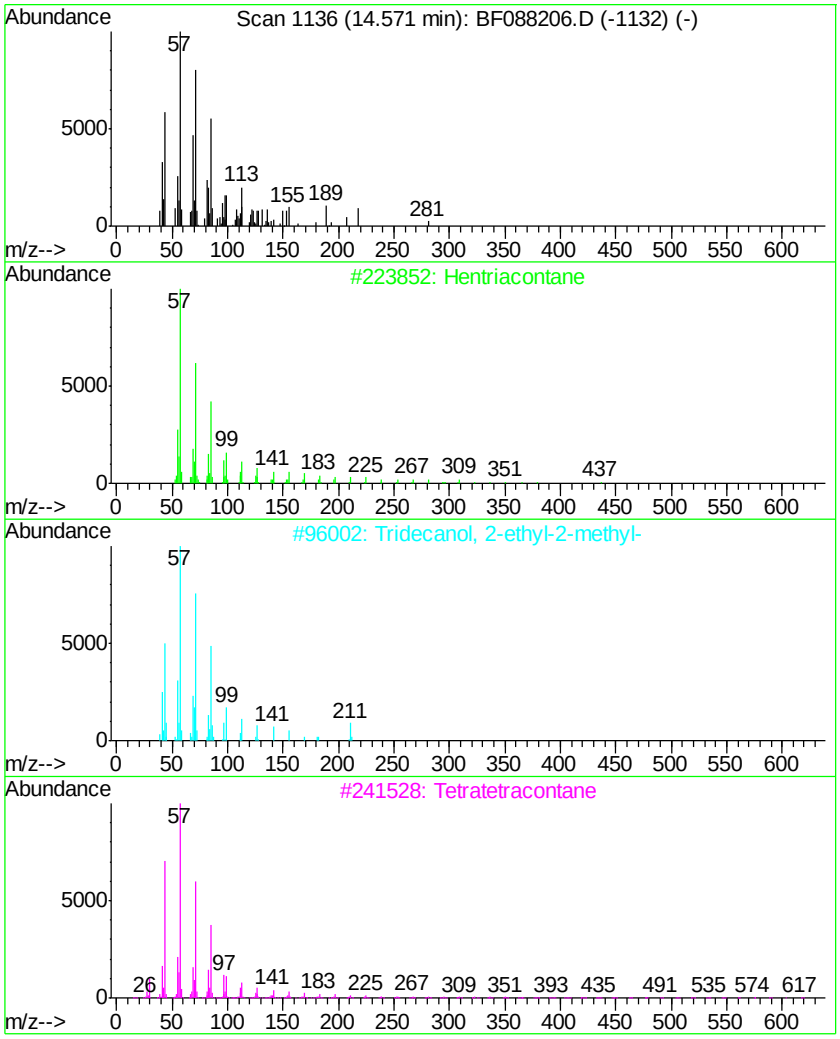
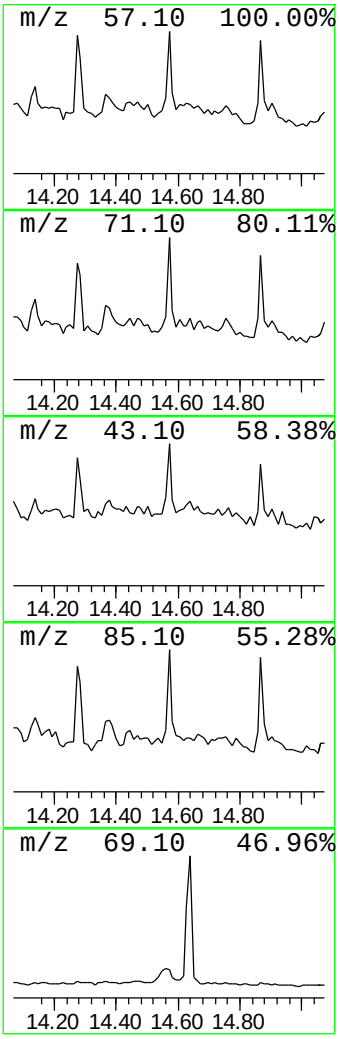
Peak Number 13 Hentriacontane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.03 ng	51187	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	64
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	59
3	Tetratetracontane	619	C44H90	007098-22-8	58
4	Hexadecane	226	C16H34	000544-76-3	58
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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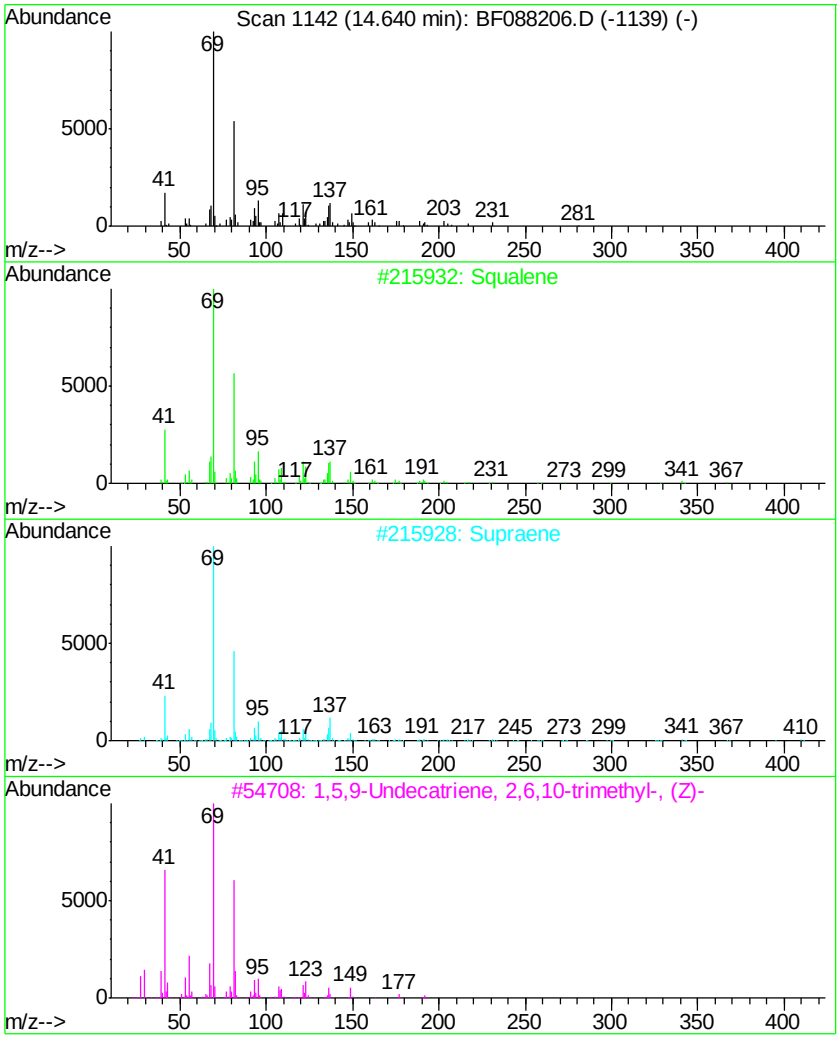
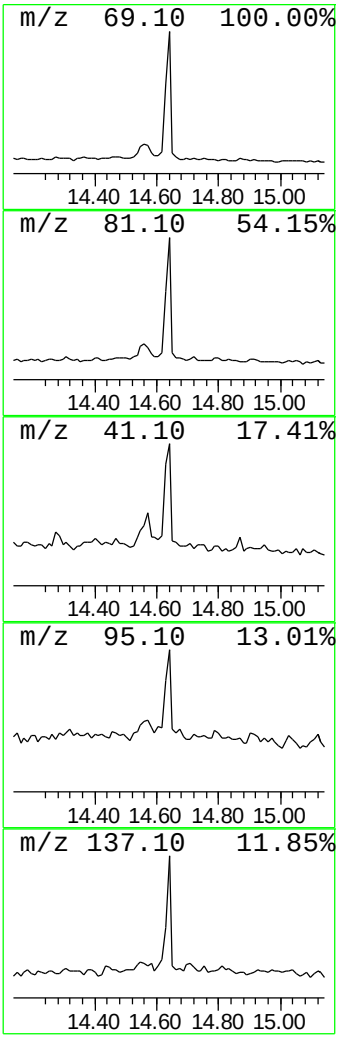
Peak Number 14 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.82 ng	96340	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	trans-Farnesol	222	C15H26O	000106-28-5	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062016\
Data File : BF088206.D
Acq On : 21 Jun 2016 8:30
Operator : UM/SJ
Sample : H3580-17
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B1(0-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
2-Pentanone, 4-hy...	4.82	4.2	ng	108313	1	6.66	512669	20.0
Nonane, 3-methyl-	5.90	2.3	ng	57836	1	6.66	512669	20.0
unknown6.43	6.43	67.0	ng	1718480	1	6.66	512669	20.0
Undecane, 4,5-dim...	8.39	3.0	ng	104484	2	7.95	705000	20.0
Hexadecane	10.14	2.3	ng	87656	3	9.70	773127	20.0
Heptadecane	10.35	2.7	ng	103260	3	9.70	773127	20.0
Heptadecane, 2,6,...	10.62	4.8	ng	188512	4	11.18	792926	20.0
Hexadecanoic acid...	12.58	3.3	ng	107464	5	13.81	650175	20.0
1-Heneicosanol	13.71	2.2	ng	70497	5	13.81	650175	20.0
Hentriacontane	14.57	2.0	ng	51187	6	15.18	505031	20.0
Squalene	14.64	3.8	ng	96340	6	15.18	505031	20.0