LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

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-BF032122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127633.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.104	127	139	148	rBV2	26263	61358	2.00%	0.268%
2	4.328	344	347	356	rBV	63281	87368	2.84%	0.382%
3	4.434	363	365	373	rVB	31549	44147	1.44%	0.193%
4	5.010	458	463	469	rBV	22351	36209	1.18%	0.158%
5	5.063	469	472	477	rVV	21604	42455	1.38%	0.186%
6	5.110	477	480	487	rVV3	25771	39295	1.28%	0.172%
7	5.175	488	491	506	rVB	134133	161020	5.24%	0.704%
8	5.457	536	539	548	rBV	1043345	1272552	41.38%	5.564%
9	5.522	548	550	564	rVB	83738	120361	3.91%	0.526%
10	6.104	646	649	655	rBV	28899	37889	1.23%	0.166%
11	6.410	698	701	710	rBV2	65030	137991	4.49%	0.603%
12	6.475	710	712	729	rVB	715605	856605	27.86%	3.745%
13	6.628	734	738	746	rVB4	23023	55643	1.81%	0.243%
14	6.834	769	773	779	rBV	612311	580324	18.87%	2.537%
15	6.881	779	781	788	rVV	65841	77653	2.53%	0.340%
16	6.998	798	801	805	rBV	48283	56845	1.85%	0.249%
17	7.069	809	813	821	rVV	84787	128766	4.19%	0.563%
18	7.192	828	834	842	rBV3	48139	79454	2.58%	0.347%
19	7.251	842	844	852	rVB	95426	88117	2.87%	0.385%
20	7.404	866	870	880	rVB	2025223	1852129	60.23%	8.098%
21	7.804	933	938	944	rBV	34062	47445	1.54%	0.207%
22	8.004	968	972	978	rBV4	22141	42040	1.37%	0.184%
23	8.116	986	991	1001	rBV	885405	814478	26.49%	3.561%
24	8.322	1022	1026	1031	rBV2	31809	42775	1.39%	0.187%
25	8.392	1034	1038	1051	rVB2	104908	185287	6.03%	0.810%
26	8.716	1090	1093	1109	rVB	815023	730878	23.77%	3.196%
27	8.863	1113	1118	1123	rVB	61436	61925	2.01%	0.271%
28	8.933	1127	1130	1133	rBV	57879	50293	1.64%	0.220%
29	9.128	1159	1163	1169	rBV	56630	56945	1.85%	0.249%
30	9.186	1169	1173	1177	rBV	3037801	2938104	95.55%	12.846%
31	9.298	1189	1192	1196	rVB	48648	46645	1.52%	0.204%
32	9.451	1215	1218	1219	rBV	44296	31751	1.03%	0.139%
33	9.469	1219	1221	1225	rVB	86997	78856	2.56%	0.345%
34	9.786	1272	1275	1281	rBV	44365	48465	1.58%	0.212%
35	9.869	1286	1289	1297	rBV	1035603	885475	28.80%	3.872%
36	10.669	1421	1425	1438	rBV	2135379	2076643	67.53%	9.080%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

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-BF032122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	11.363	1540	1543	1552	rBV	1119995	949639	30.88%	4.152%
38	11.880	1626	1631	1646	rBV	492923	704077	22.90%	3.078%
39	12.680	1759	1767	1786	rBV	1622652	2537494	82.52%	11.095%
40	12.951	1808	1813	1816	rBV	3233195	3074951	100.00%	13.445%
41	13.863	1963	1968	1981	rVB4	63548	173140	5.63%	0.757%
42	14.015	1991	1994	2003	rBV	853484	802027	26.08%	3.507%
43	14.827	2129	2132	2140	rVB	37053	49239	1.60%	0.215%
44	15.498	2243	2246	2260	rVB	452969	626558	20.38%	2.739%

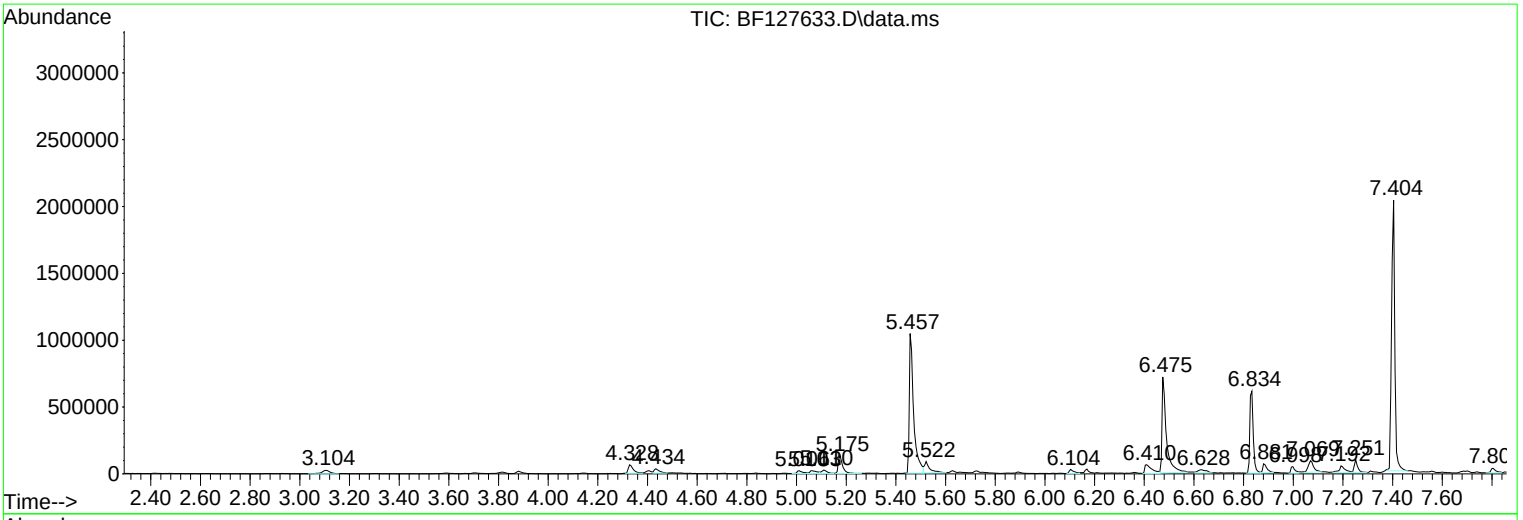
Sum of corrected areas: 22871311

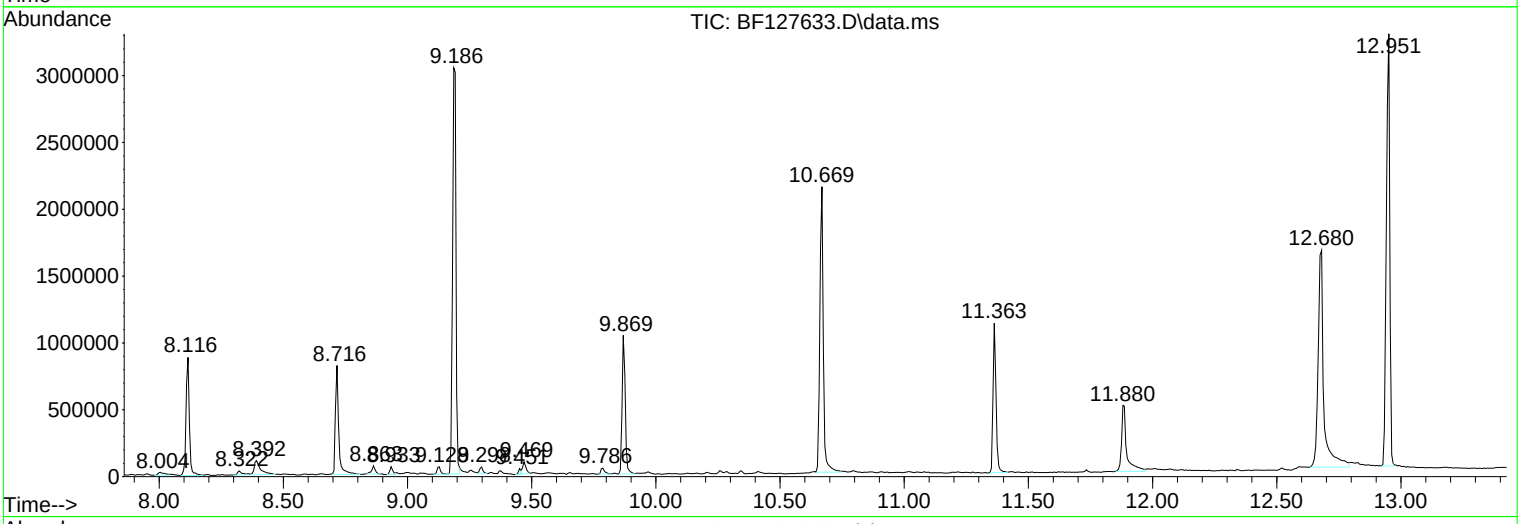
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

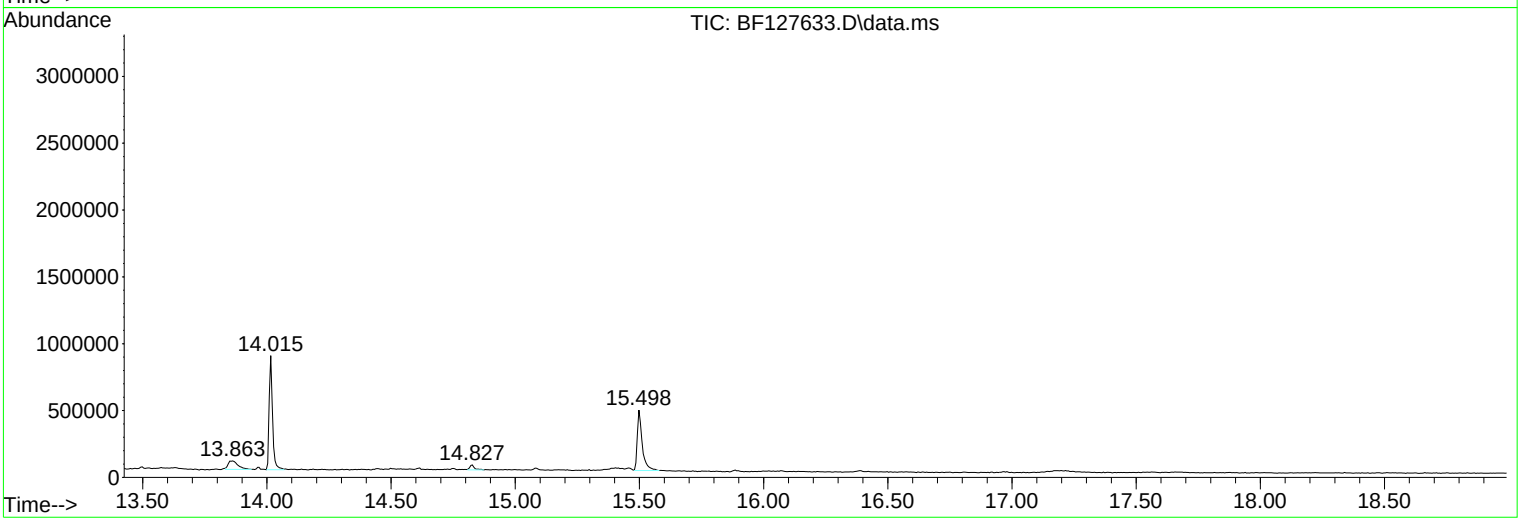
Instrument :
BNA_F
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

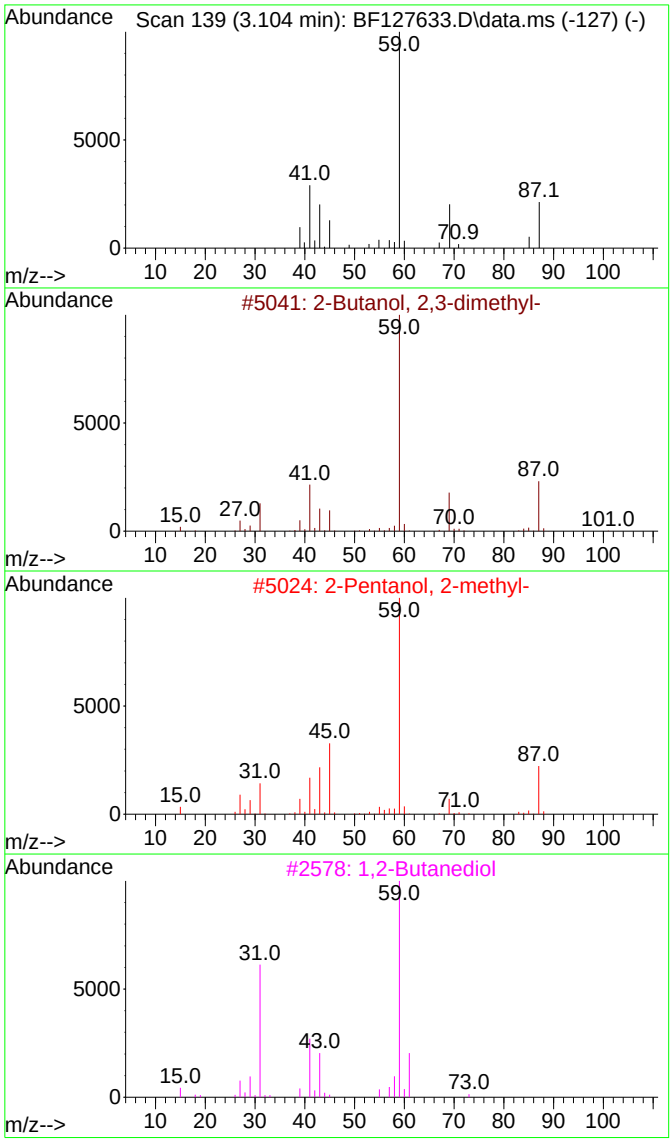
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

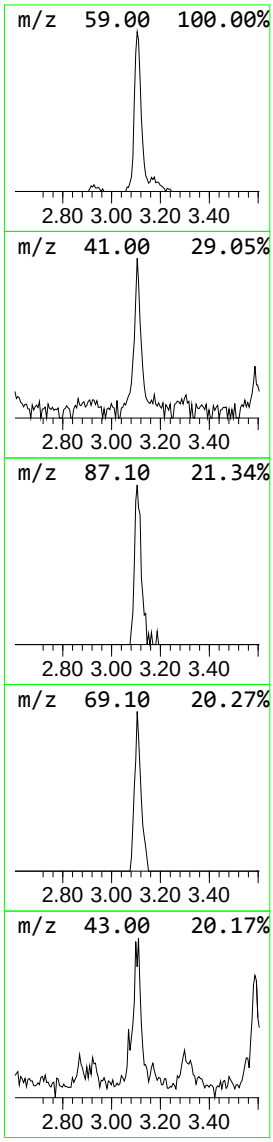
****

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.104	2.11 ng	61358	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	78
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
3	1,2-Butanediol	90	C4H10O2	000584-03-2	36
4	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	36
5	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

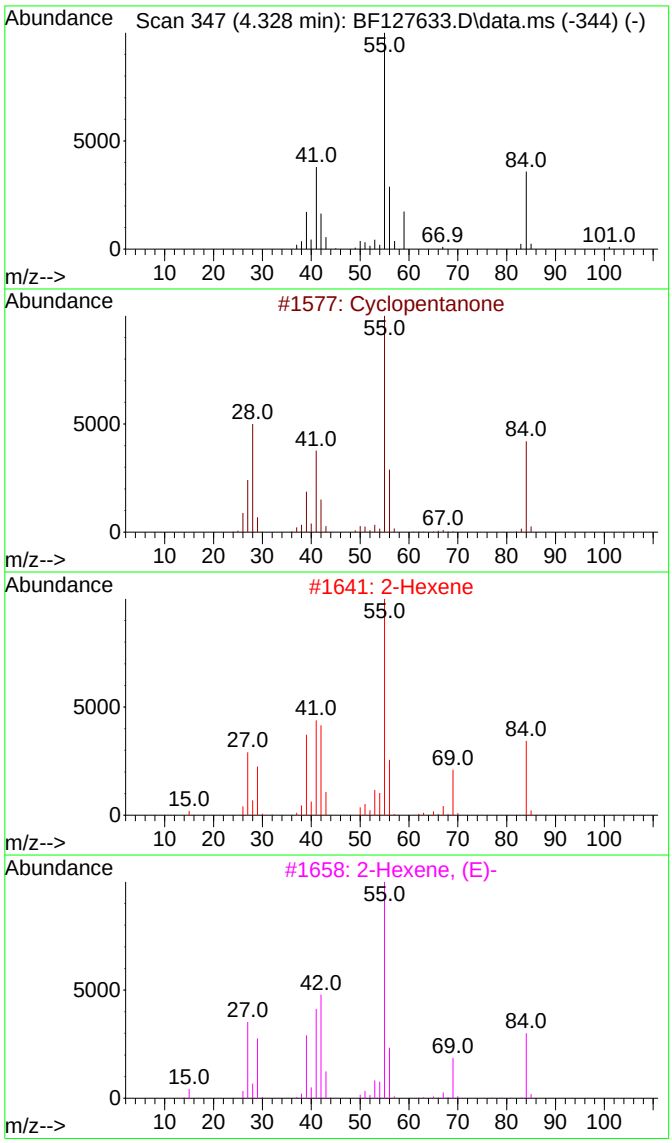
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

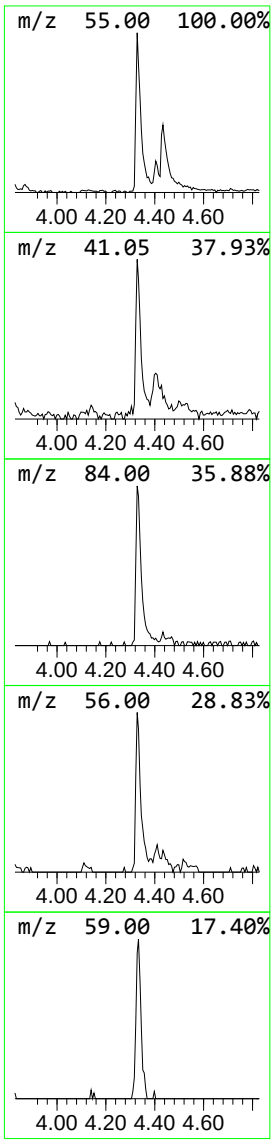
****

Peak Number 2 Cyclopentanone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.328	3.01 ng	87368	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	87
2	2-Hexene	84	C6H12	000592-43-8	50
3	2-Hexene, (E)-	84	C6H12	004050-45-7	50
4	2-Hexene, (Z)-	84	C6H12	007688-21-3	49
5	Tricyclohexanone triperoxide	300	C15H24O6	1000357-14-9	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

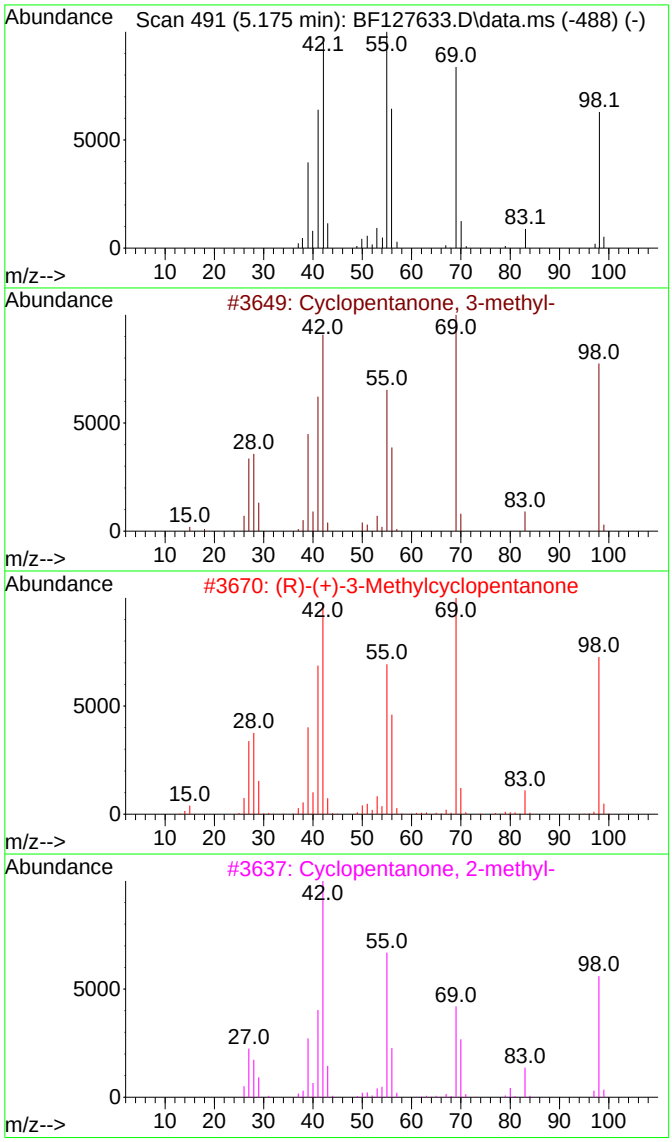
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

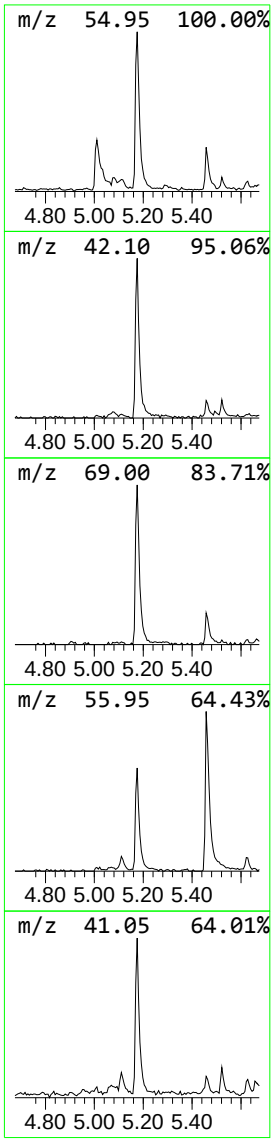
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentanone, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	5.55 ng	161020	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	90
2	(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	90
3	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	59
4	Cycloheptane	98	C7H14	000291-64-5	47
5	6-Oxabicyclo[3.1.0]hexan-2-one	98	C5H6O2	006705-52-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

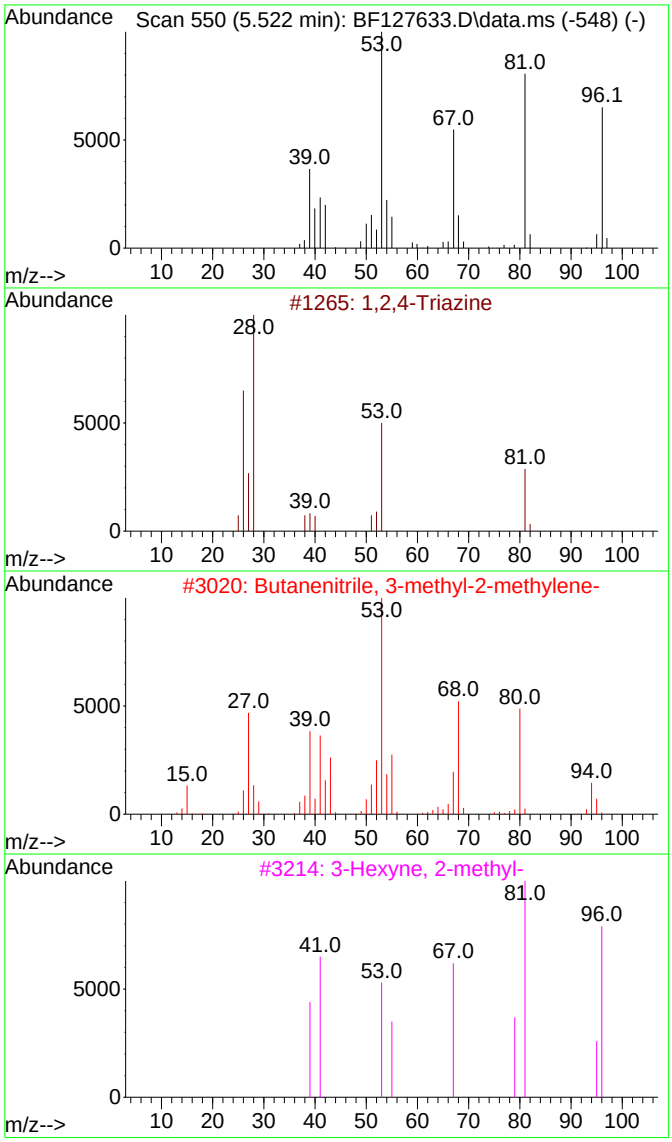
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

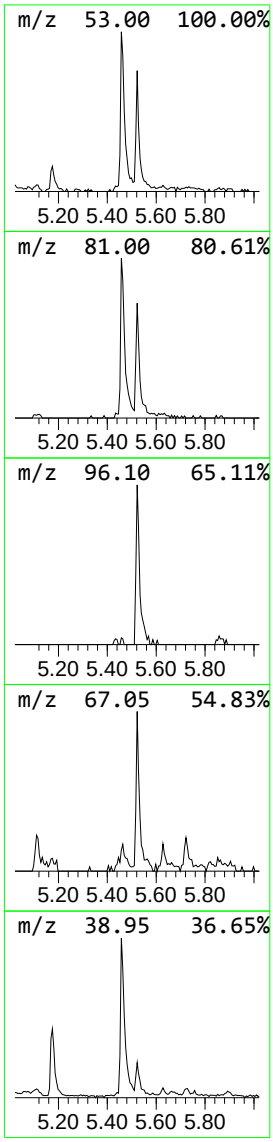
****

Peak Number 4 1,2,4-Triazine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.522	4.15 ng	120361	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Triazine	81	C3H3N3	000290-38-0	59
2	Butanenitrile, 3-methyl-2-methyl...	95	C6H9N	002813-69-6	53
3	3-Hexyne, 2-methyl-	96	C7H12	036566-80-0	43
4	1,4-Hexadiene, 5-methyl-	96	C7H12	000763-88-2	35
5	1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

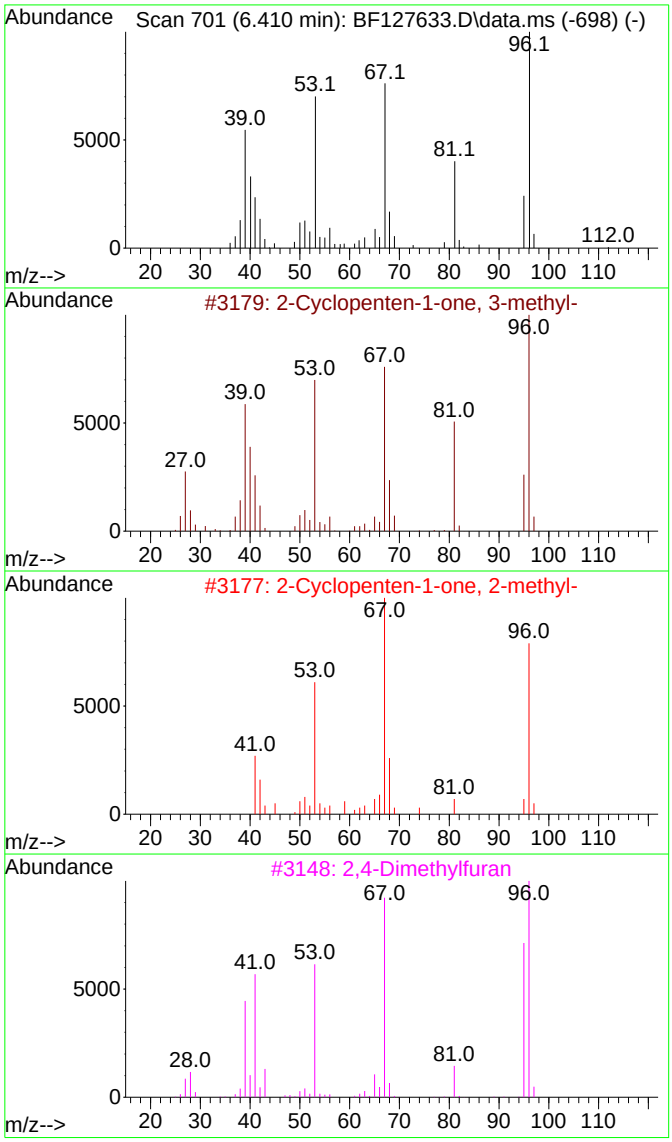
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

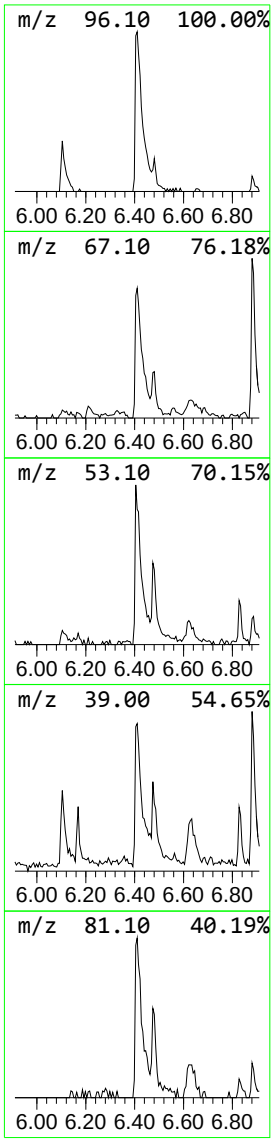
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Cyclopenten-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.410	4.76 ng	137991	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	002758-18-1	96
2	2-Cyclopenten-1-one, 2-methyl-	96	C6H8O	001120-73-6	86
3	2,4-Dimethylfuran	96	C6H8O	003710-43-8	86
4	Isoprene	68	C5H8	000078-79-5	58
5	1-Butyne, 3-methyl-	68	C5H8	000598-23-2	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

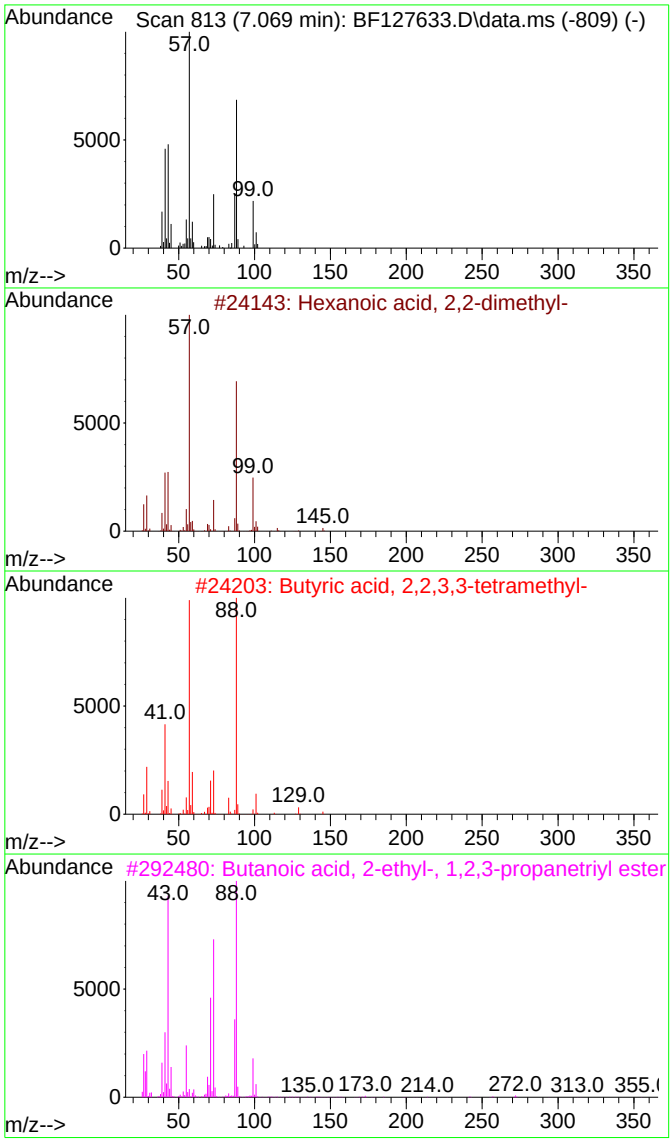
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

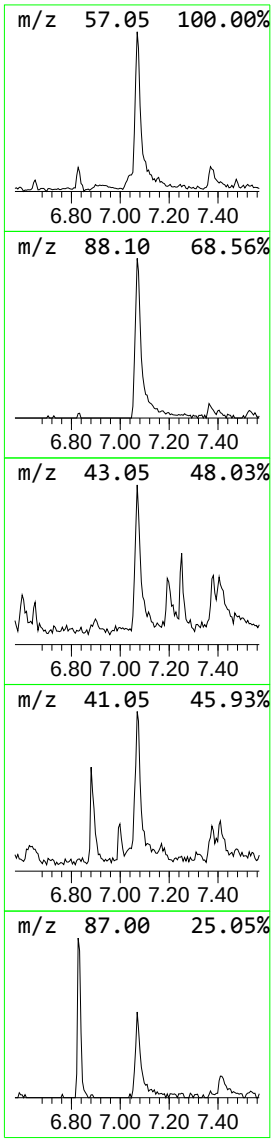
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Hexanoic acid, 2,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	4.44 ng	128766	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	53
2	Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	38
3	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	38
4	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	37
5	Acetic acid, diethyl-	116	C6H12O2	000088-09-5	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
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Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

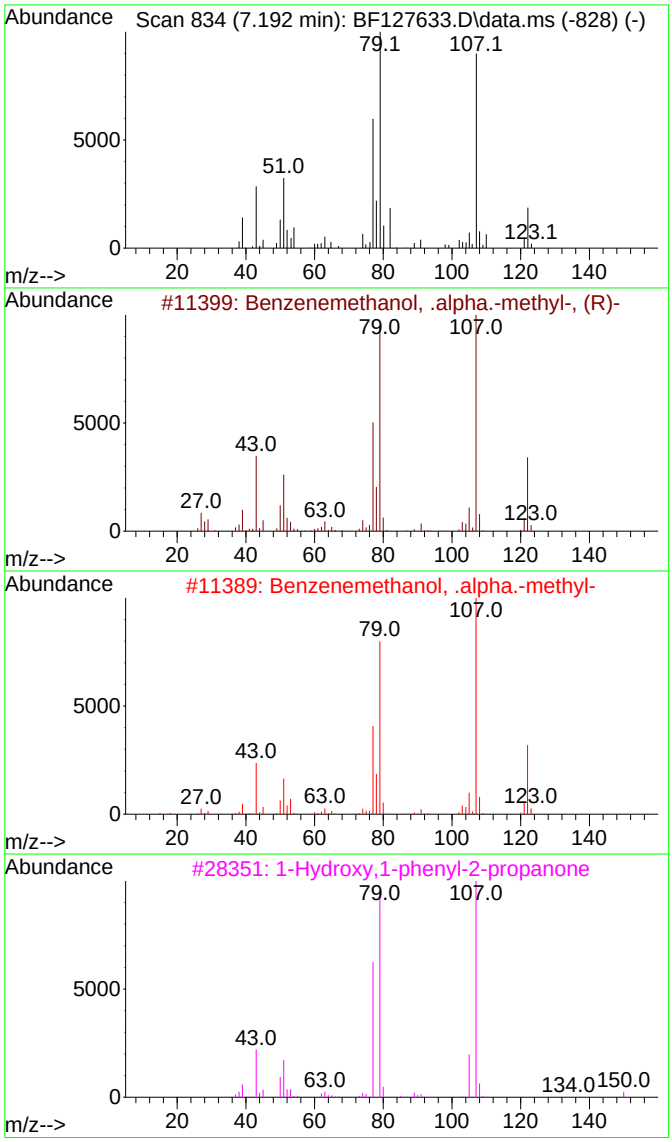
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

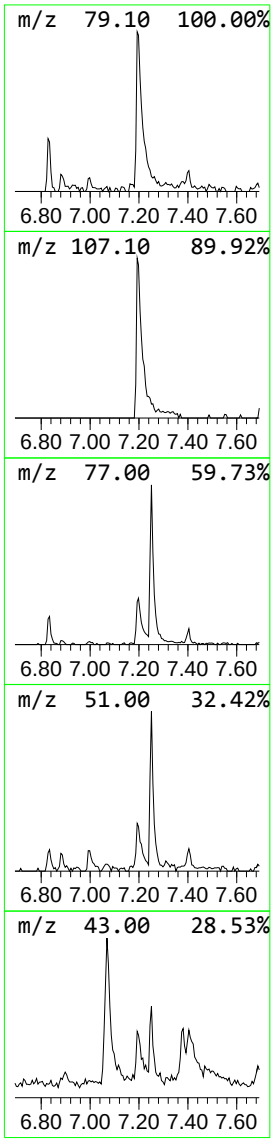
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzenemethanol, .alpha.-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.192	2.74 ng	79454	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, .alpha.-methyl-...	122	C8H10O	001517-69-7	96
2	Benzenemethanol, .alpha.-methyl-	122	C8H10O	000098-85-1	95
3	1-Hydroxy,1-phenyl-2-propanone	150	C9H10O2	1000222-86-8	64
4	Benzenemethanol, .alpha.-2-prope...	148	C10H12O	000936-58-3	59
5	4,4-Dimethylcyclohexadienone	122	C8H10O	001073-14-9	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040422\
Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

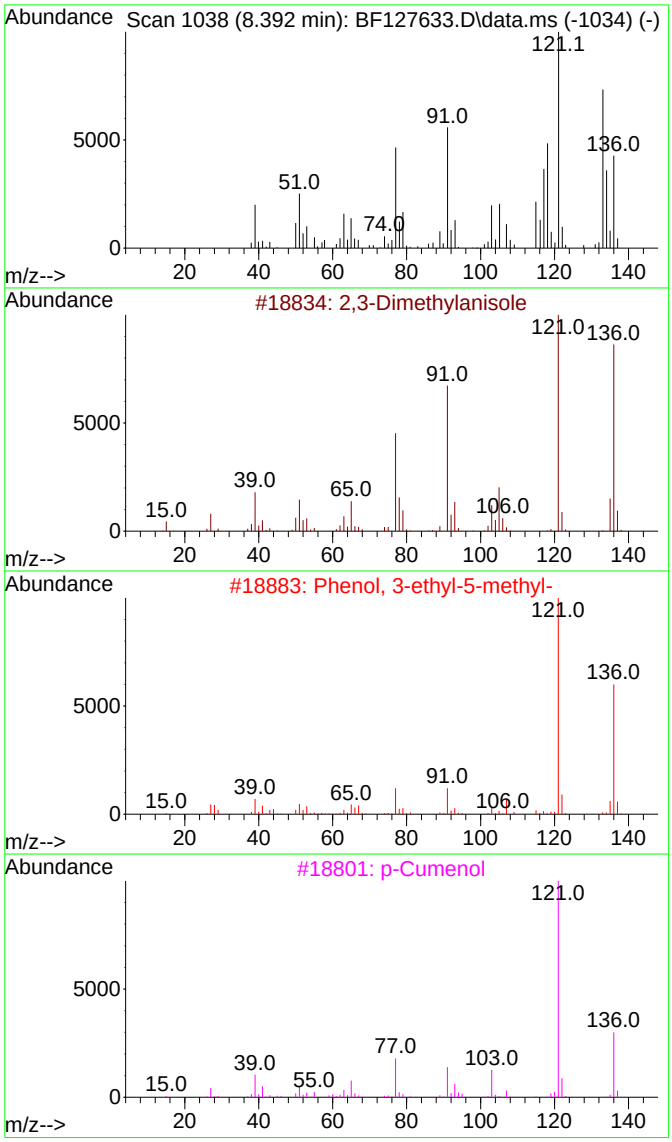
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

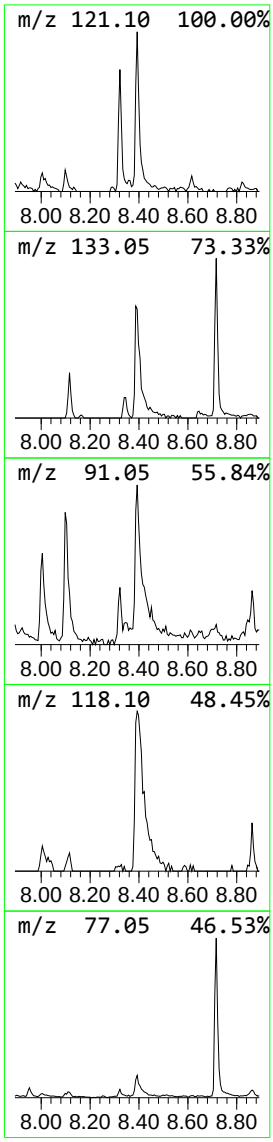
****

Peak Number 9 unknown8.392 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.392	4.55 ng	185287	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dimethylanisole	136	C9H12O	002944-49-2	45
2	Phenol, 3-ethyl-5-methyl-	136	C9H12O	000698-71-5	45
3	p-Cumenol	136	C9H12O	000099-89-8	43
4	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	43
5	2-Ethylphenol, methyl ether	136	C9H12O	1000333-44-2	42





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Data File : BF127633.D
Acq On : 04 Apr 2022 15:43
Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

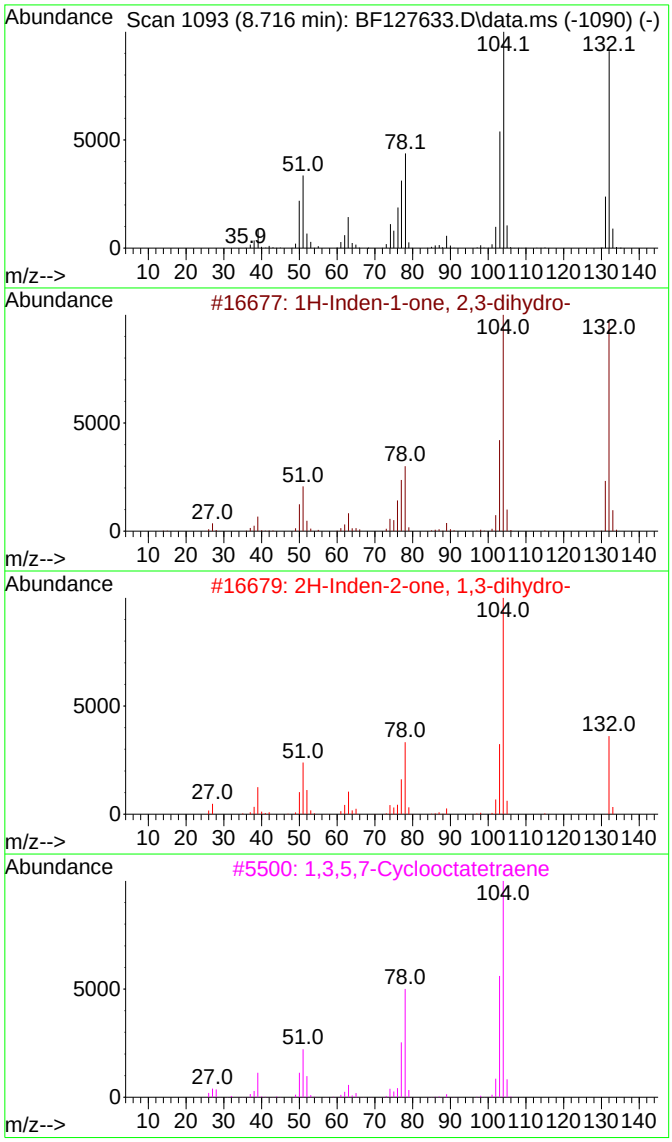
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

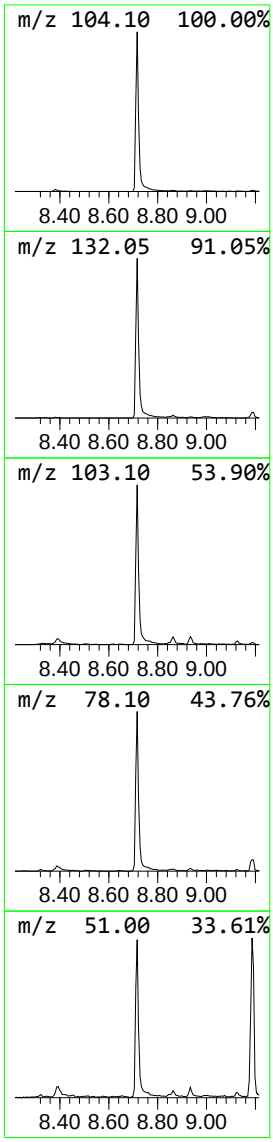
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.716	17.95 ng	730878	Naphthalene-d8	8.116

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	96
2	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	68
3	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	64
4	Styrene	104	C8H8	000100-42-5	64
5	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	60





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

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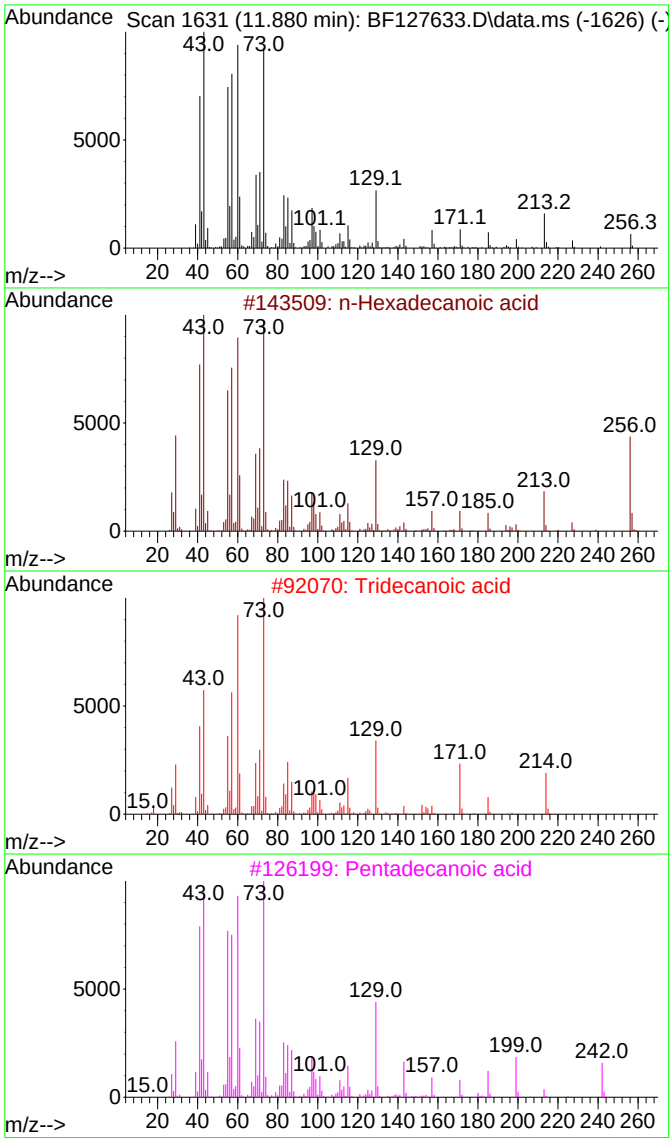
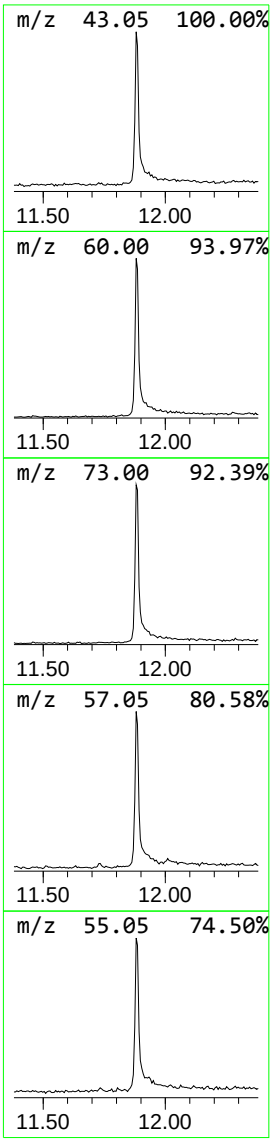
Peak Number 11 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	14.83 ng	704077	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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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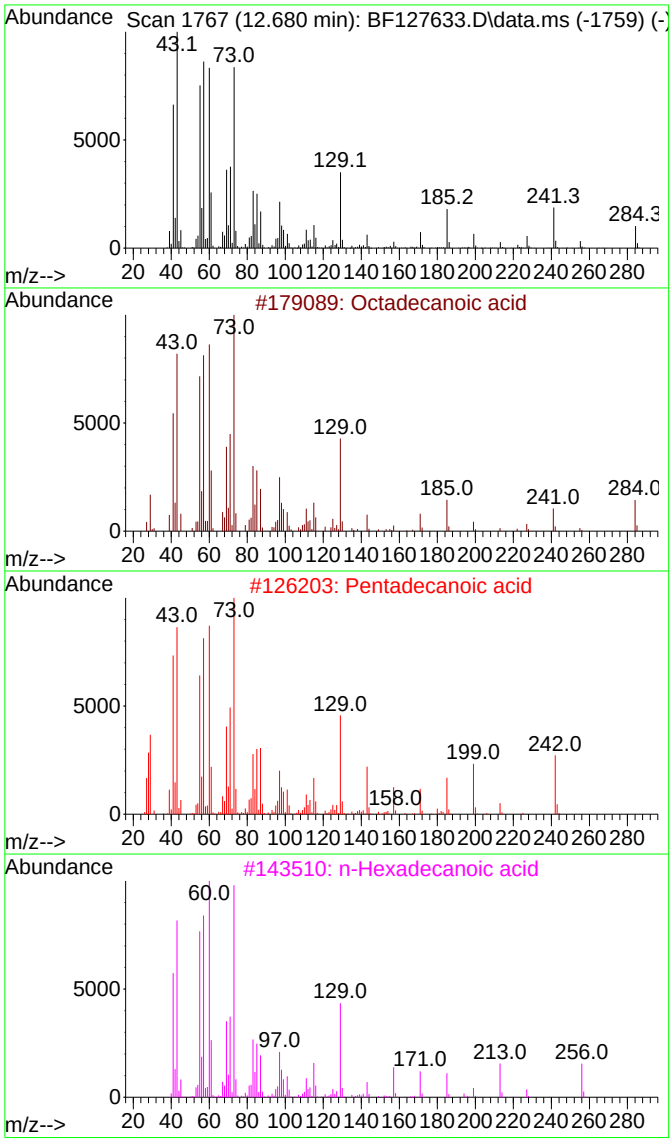
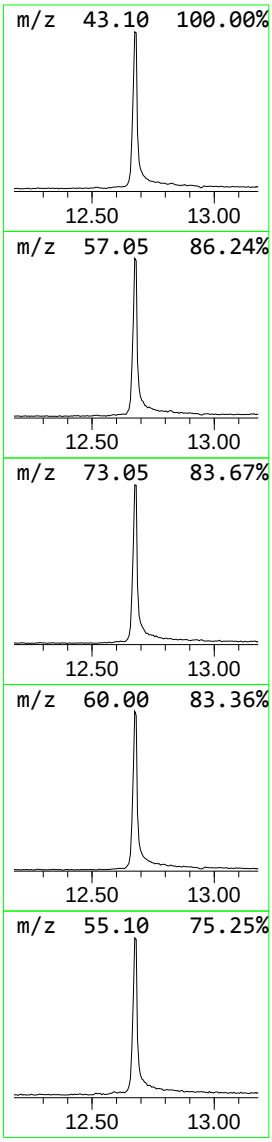
Peak Number 12 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	53.44 ng	2537490	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





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Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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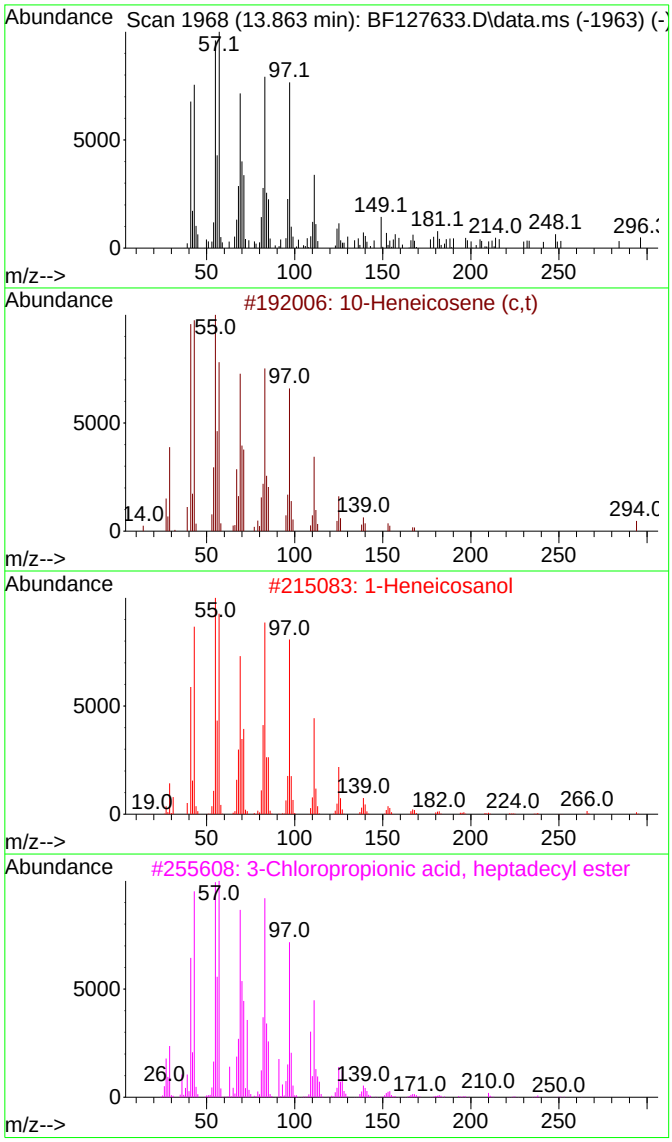
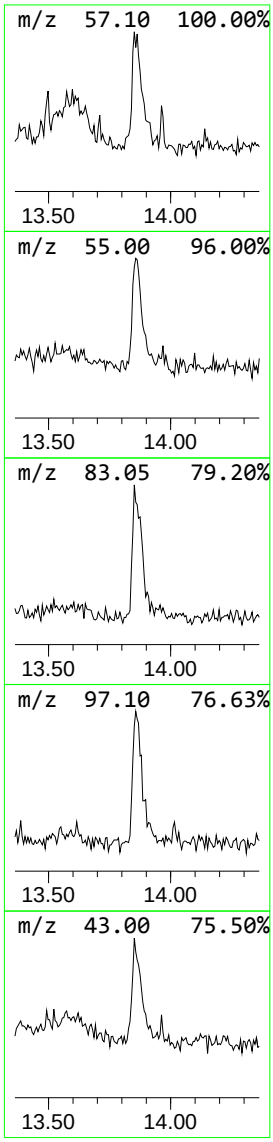
Peak Number 13 10-Heneicosene (c,t) Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	4.32 ng	173140	Chrysene-d12	14.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Heneicosene (c,t)	294	C21H42	095008-11-0	87
2	1-Heneicosanol	312	C21H44O	015594-90-8	87
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	83
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83





Tentatively Identified Compound (LSC) summary

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Data File : BF127633.D
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Operator : CG\JU
Sample : N2249-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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
2-Butanol, 2,3-...	3.104	2.1	ng	61358	1	6.834	580324	20.0
Cyclopentanone	4.328	3.0	ng	87368	1	6.834	580324	20.0
Cyclopentanone,...	5.175	5.5	ng	161020	1	6.834	580324	20.0
1,2,4-Triazine	5.522	4.2	ng	120361	1	6.834	580324	20.0
2-Cyclopenten-1...	6.410	4.8	ng	137991	1	6.834	580324	20.0
Hexanoic acid, ...	7.069	4.4	ng	128766	1	6.834	580324	20.0
Benzenemethanol...	7.192	2.7	ng	79454	1	6.834	580324	20.0
unknown8.392	8.392	4.5	ng	185287	2	8.116	814478	20.0
1H-Inden-1-one,...	8.716	17.9	ng	730878	2	8.116	814478	20.0
n-Hexadecanoic ...	11.880	14.8	ng	704077	4	11.363	949639	20.0
Octadecanoic acid	12.680	53.4	ng	2537490	4	11.363	949639	20.0
10-Heneicosene ...	13.863	4.3	ng	173140	5	14.015	802027	20.0