LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

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\8270-BP010820.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	2.952	24	28	34	rVB	51430	58850	2.53%	0.453%
2	4.805	337	343	352	rVB	155839	216270	9.30%	1.666%
3	5.264	415	421	431	rBV	718453	1001838	43.08%	7.715%
4	6.834	680	688	704	rBV	755008	1181849	50.82%	9.102%
5	7.175	738	746	762	rBV	721220	1136521	48.88%	8.753%
6	7.634	817	824	833	rVB	147017	224095	9.64%	1.726%
7	7.952	871	878	896	rVB	562540	892403	38.38%	6.873%
8	8.781	1011	1019	1033	rBV	453115	746436	32.10%	5.748%
9	10.410	1289	1296	1310	rBV	157963	270751	11.64%	2.085%
10	12.899	1712	1719	1741	rBV	1062104	1587764	68.28%	12.228%
11	13.751	1859	1864	1872	rBV2	13477	24505	1.05%	0.189%
12	14.281	1947	1954	1967	rBV2	233915	355137	15.27%	2.735%
13	15.781	2203	2209	2222	rBV	860202	1227920	52.81%	9.456%
14	17.040	2415	2423	2439	rBV	264906	405898	17.46%	3.126%
15	19.634	2858	2864	2879	rBV	1908946	2325347	100.00%	17.908%
16	20.898	3074	3079	3087	rBV3	47704	94409	4.06%	0.727%
17	21.145	3116	3121	3132	rBV	312304	427719	18.39%	3.294%
18	22.222	3299	3304	3317	rBV3	95870	180176	7.75%	1.388%
19	22.363	3325	3328	3332	rVB	19075	23342	1.00%	0.180%
20	22.751	3390	3394	3399	rBV	46129	63710	2.74%	0.491%
21	23.333	3488	3493	3495	rBV	42415	66578	2.86%	0.513%
22	23.374	3495	3500	3513	rVB	208160	405706	17.45%	3.124%
23	23.986	3600	3604	3611	rVB3	35813	67735	2.91%	0.522%

Sum of corrected areas: 12984959

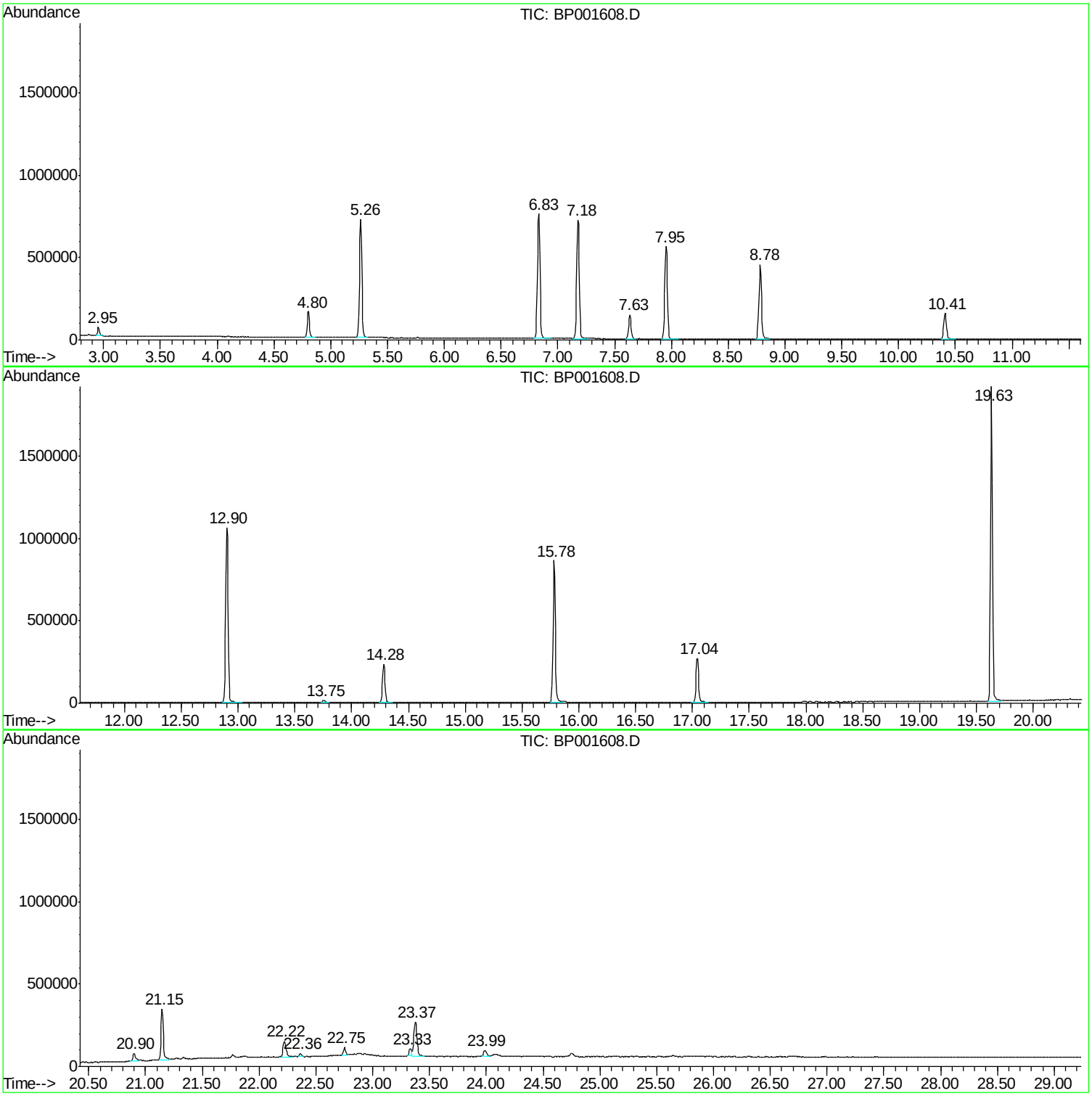
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

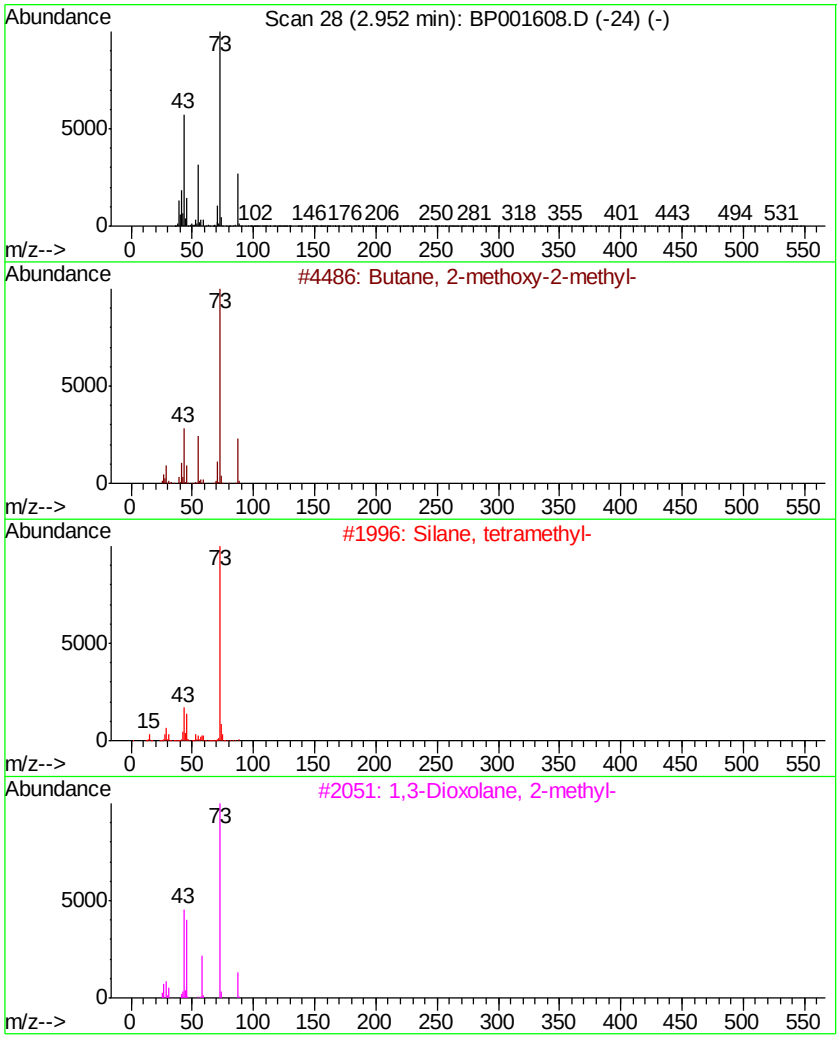
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

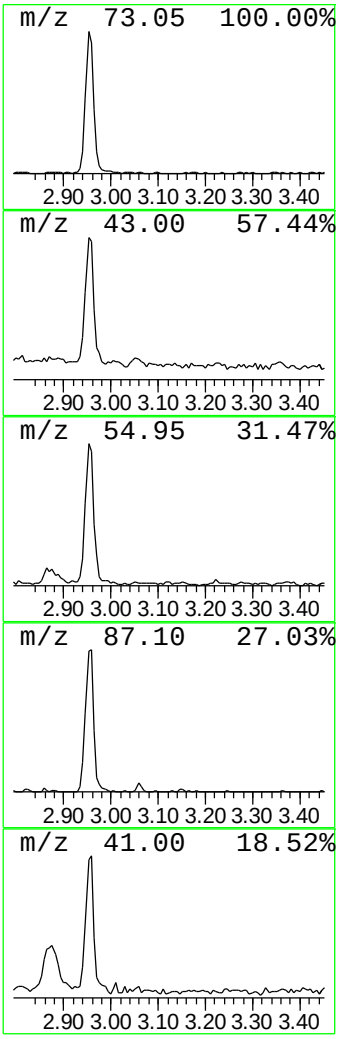
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.95	5.25 ng	58850	1,4-Dichlorobenzene-d4	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	17
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	12
5	4-Penten-2-ol, acetate	128	C7H12O2	1000352-31-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

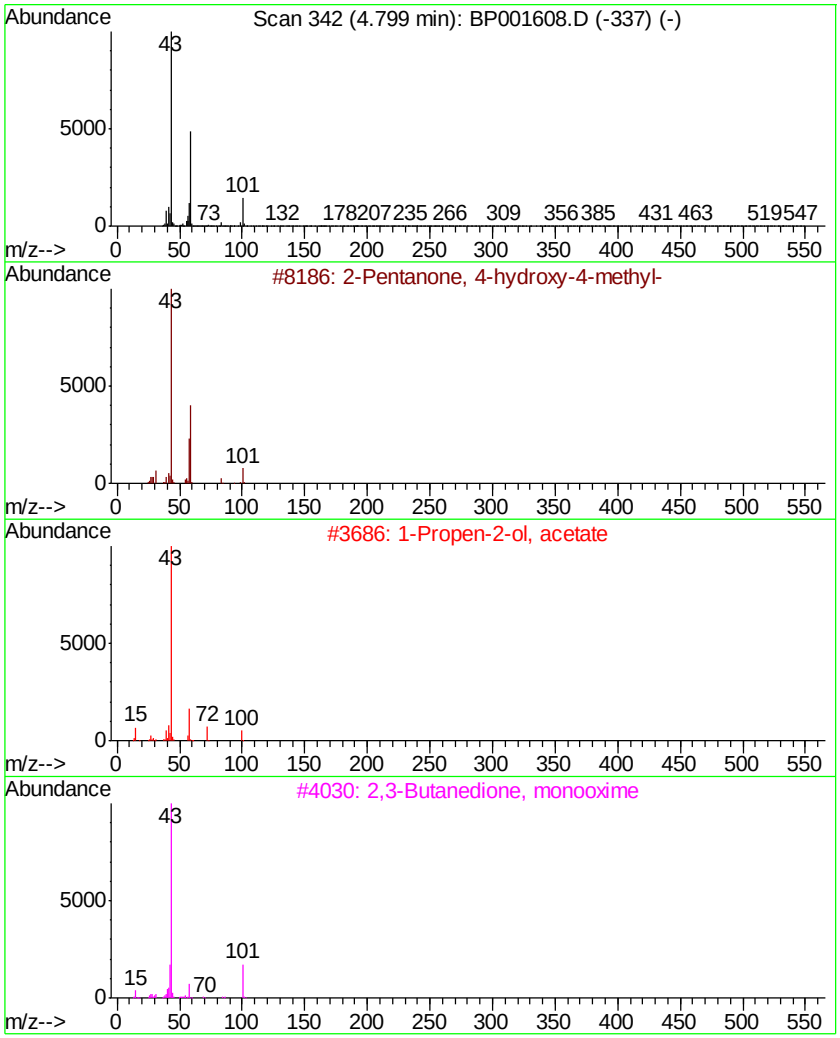
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

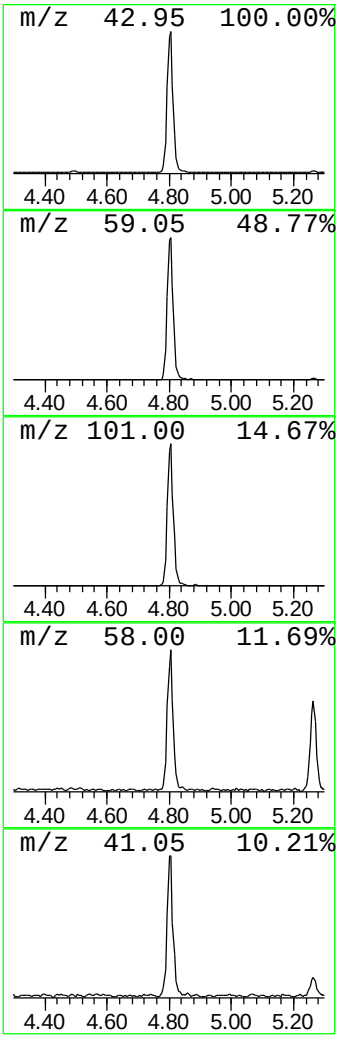
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	19.30 ng	216270	1,4-Dichlorobenzene-d4	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	22
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Allyl acetate	100	C5H8O2	000591-87-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

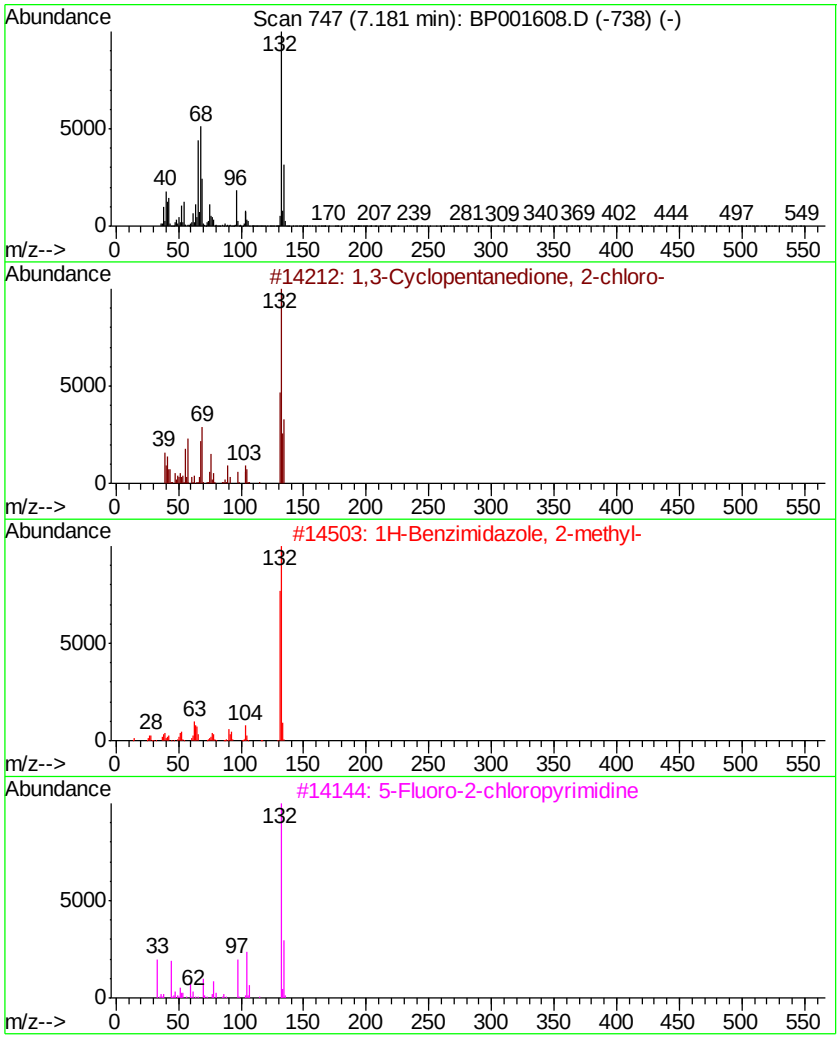
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

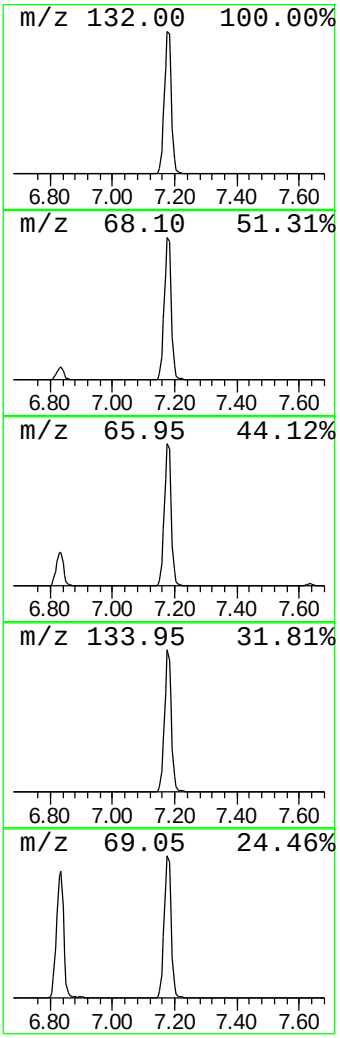
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown7.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.18	101.43 ng	1136520	1,4-Dichlorobenzene-d4	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	16
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4	3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

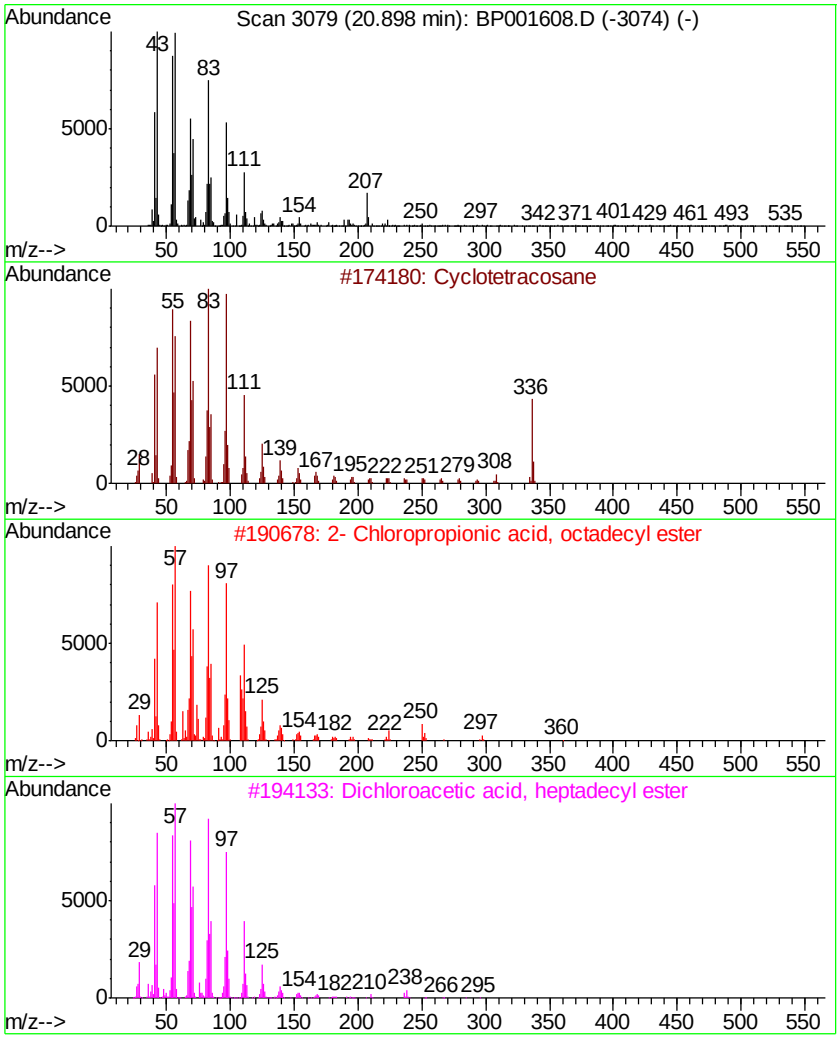
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

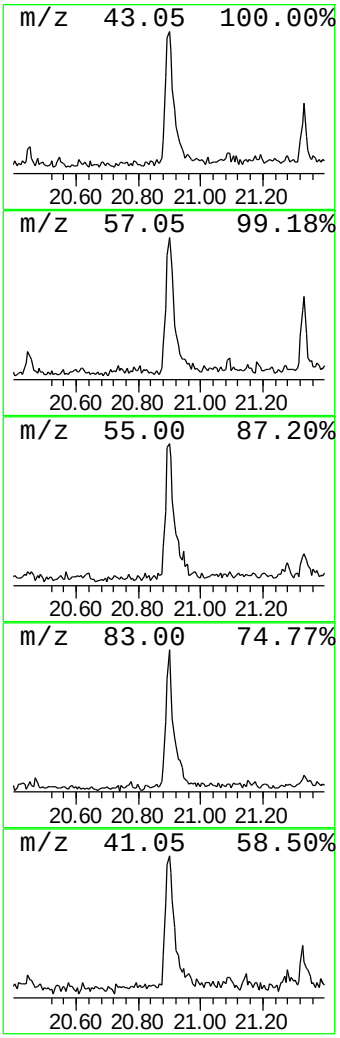
****

Peak Number 5 Cyclotetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.90	4.41 ng	94409	Chrysene-d12	21.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	95
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

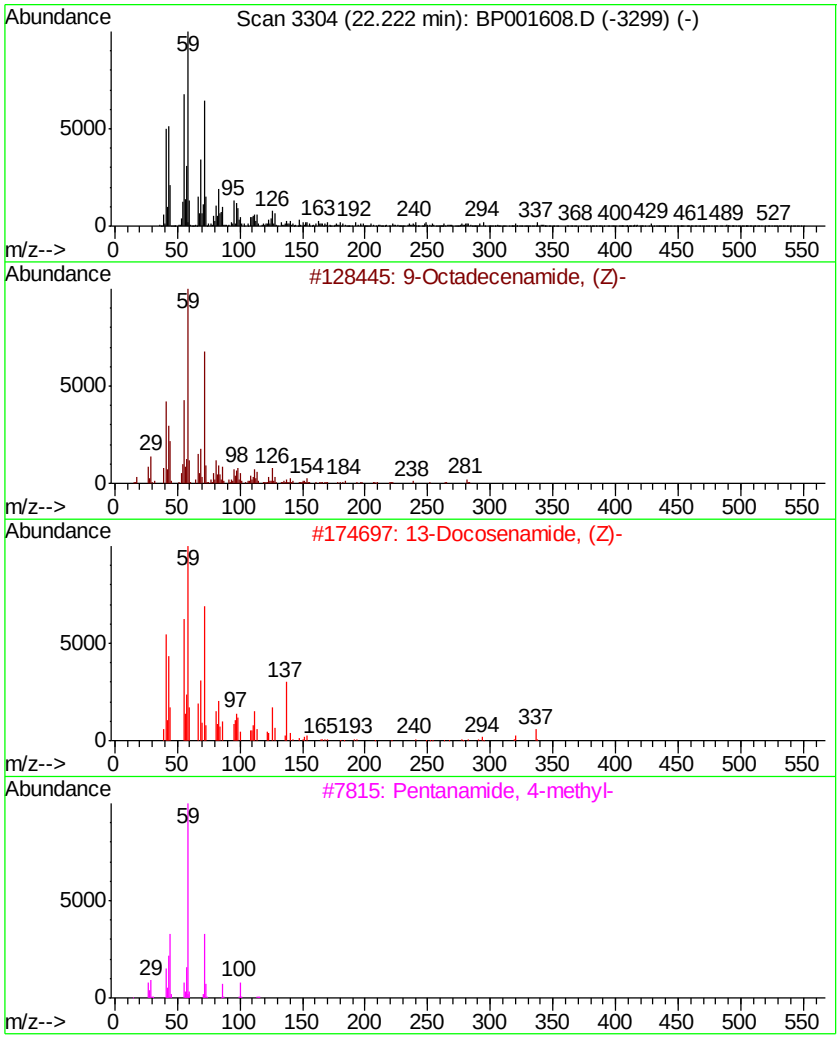
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

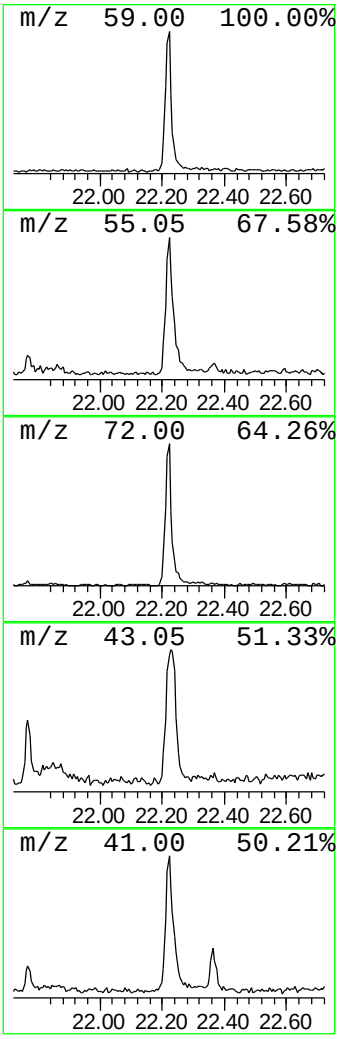
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.22	8.42 ng	180176	Chrysene-d12	21.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53
4	2-Methyl-2-decanol	172	C11H24O	003396-02-9	47
5	4-Cyclohexylbutyramide	169	C10H19NO	004441-62-7	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

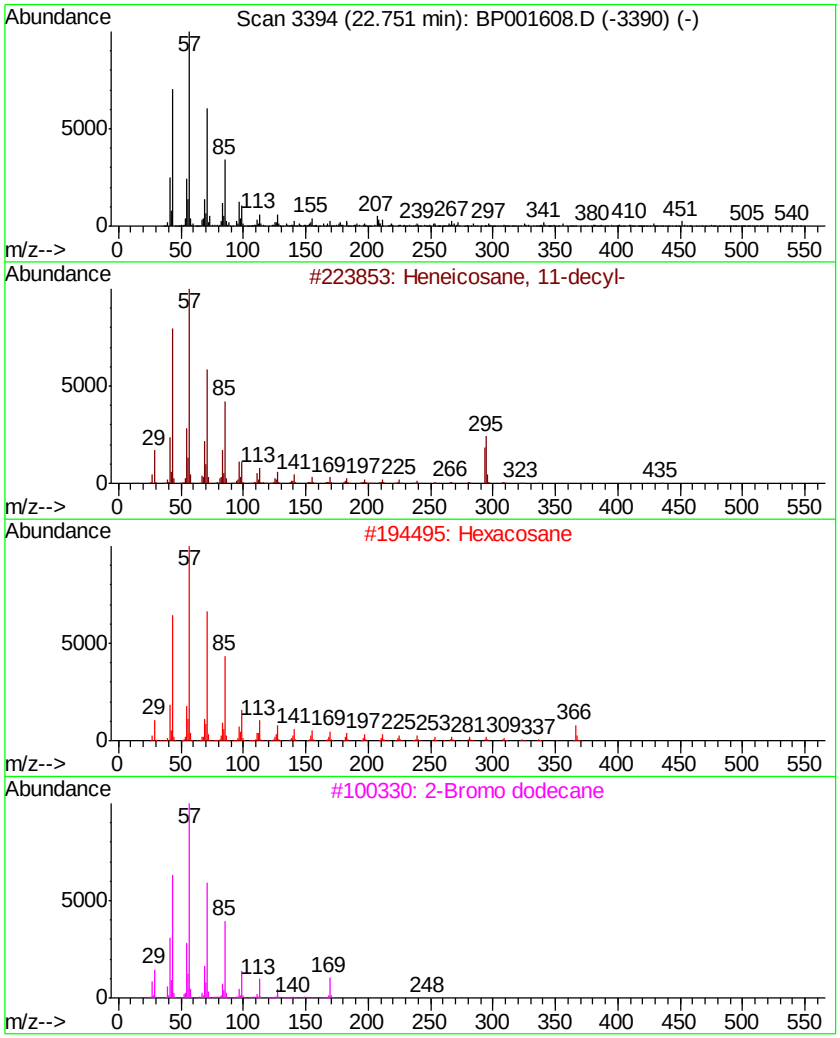
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

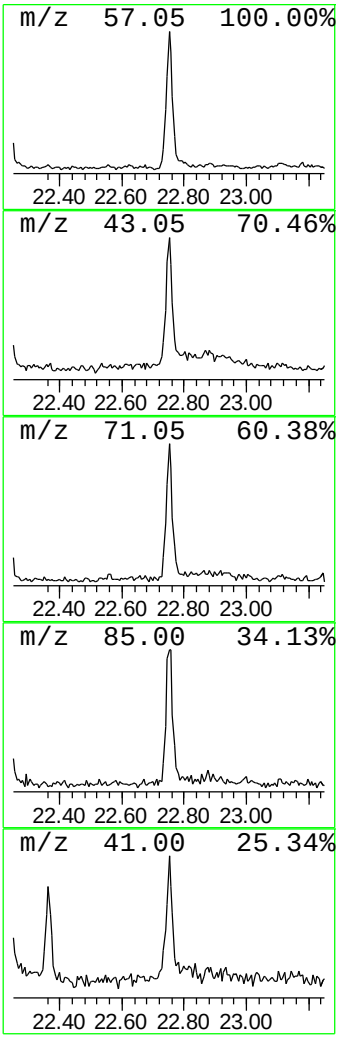
****

Peak Number 7 Heneicosane, 11-decyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.75	3.14 ng	63710	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	97
2	Hexacosane	366	C26H54	000630-01-3	90
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	87
4	Tricosane, 2-methyl-	338	C24H50	001928-30-9	87
5	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

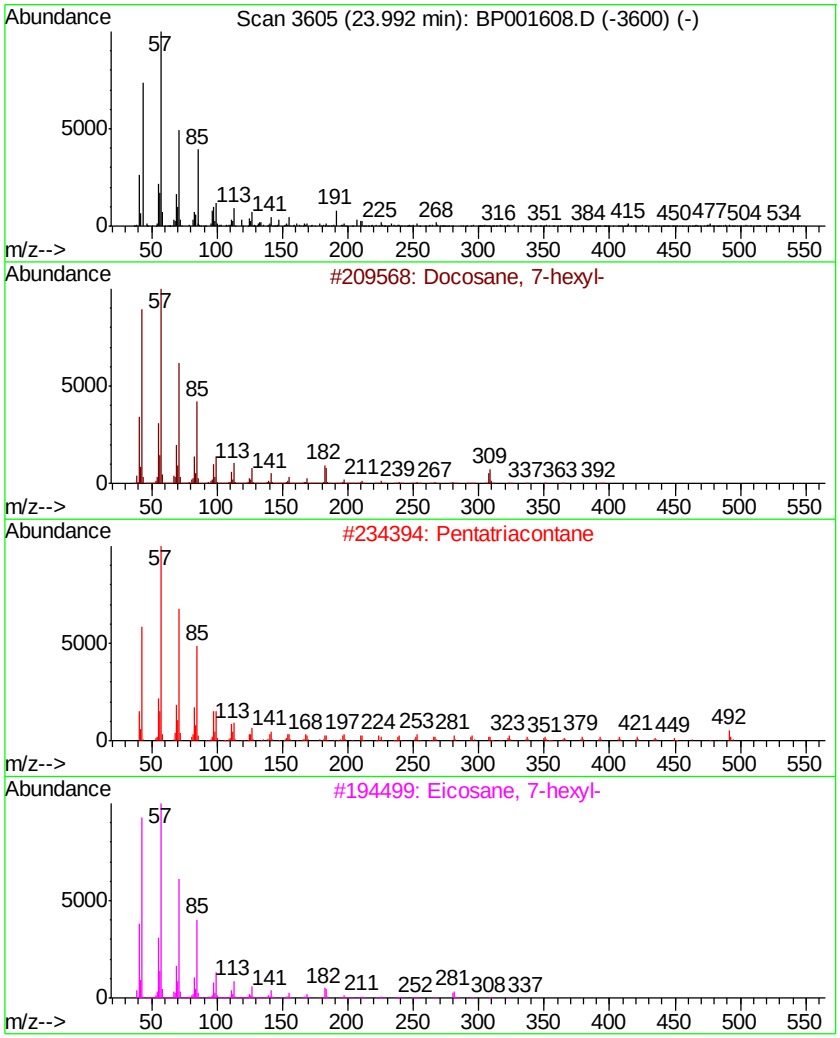
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

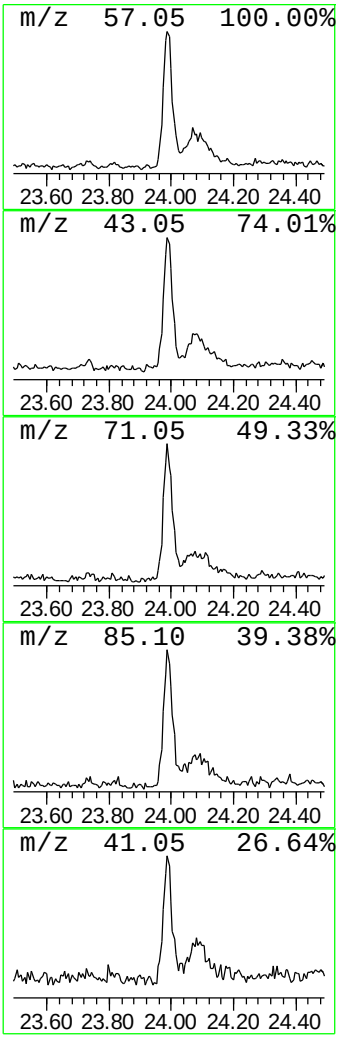
****

Peak Number 8 Docosane, 7-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	3.34 ng	67735	Perylene-d12	23.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
2	Pentatriacontane	493	C35H72	000630-07-9	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP011520\
Data File : BP001608.D
Acq On : 15 Jan 2020 14:36
Operator : JU
Sample : PB126101BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PB126101BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-methoxy...	2.95	5.3	ng	58850	1	7.63	224095	20.0
2-Pentanone, 4-hy...	4.80	19.3	ng	216270	1	7.63	224095	20.0
unknown7.18	7.18	101.4	ng	1136520	1	7.63	224095	20.0
Cyclotetracosane	20.90	4.4	ng	94409	5	21.15	427719	20.0
9-Octadecenamide,...	22.22	8.4	ng	180176	5	21.15	427719	20.0
Heneicosane, 11-d...	22.75	3.1	ng	63710	6	23.37	405706	20.0
Docosane, 7-hexyl-	23.99	3.3	ng	67735	6	23.37	405706	20.0