LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048990.D
Acq On : 15 Jun 2021 23:28
Operator : CG/JU
Sample : M2672-20
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(84-88)

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_G\METHODS\8270-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048990.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.160	15	21	35	rVB	61021	109975	2.67%	0.816%
2	3.278	37	41	48	rVB2	41121	61173	1.48%	0.454%
3	5.663	440	447	455	rBV	499908	849716	20.62%	6.306%
4	7.267	709	720	730	rBV	534264	937564	22.76%	6.957%
5	8.113	856	864	870	rBV	111747	191443	4.65%	1.421%
6	9.277	1055	1062	1072	rBV	318175	586843	14.24%	4.355%
7	10.940	1337	1345	1352	rVB	142876	259175	6.29%	1.923%
8	13.378	1752	1760	1768	rBV	896989	1384920	33.61%	10.277%
9	14.753	1988	1994	2002	rBV2	239950	393675	9.56%	2.921%
10	16.157	2227	2233	2239	rBV2	55683	77604	1.88%	0.576%
11	16.245	2239	2248	2258	rBV	1172441	1834512	44.53%	13.613%
12	17.502	2453	2462	2469	rBV	350296	561992	13.64%	4.170%
13	17.620	2478	2482	2488	rBV3	38016	50783	1.23%	0.377%
14	18.384	2606	2612	2620	rBV2	64374	96915	2.35%	0.719%
15	19.653	2824	2828	2834	rBV	46295	61879	1.50%	0.459%
16	20.117	2900	2907	2917	rVB	3096032	4119972	100.00%	30.573%
17	20.793	3015	3022	3030	rBV	175030	255781	6.21%	1.898%
18	21.427	3126	3130	3135	rBV	54330	83134	2.02%	0.617%
19	21.680	3169	3173	3183	rVB	69661	109062	2.65%	0.809%
20	21.797	3186	3193	3203	rVB2	361986	647110	15.71%	4.802%
21	23.020	3396	3401	3407	rVB6	38667	68286	1.66%	0.507%
22	23.325	3449	3453	3458	rBV8	24150	51650	1.25%	0.383%
23	25.129	3749	3760	3774	rBV2	214349	682569	16.57%	5.065%

Sum of corrected areas: 13475733

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
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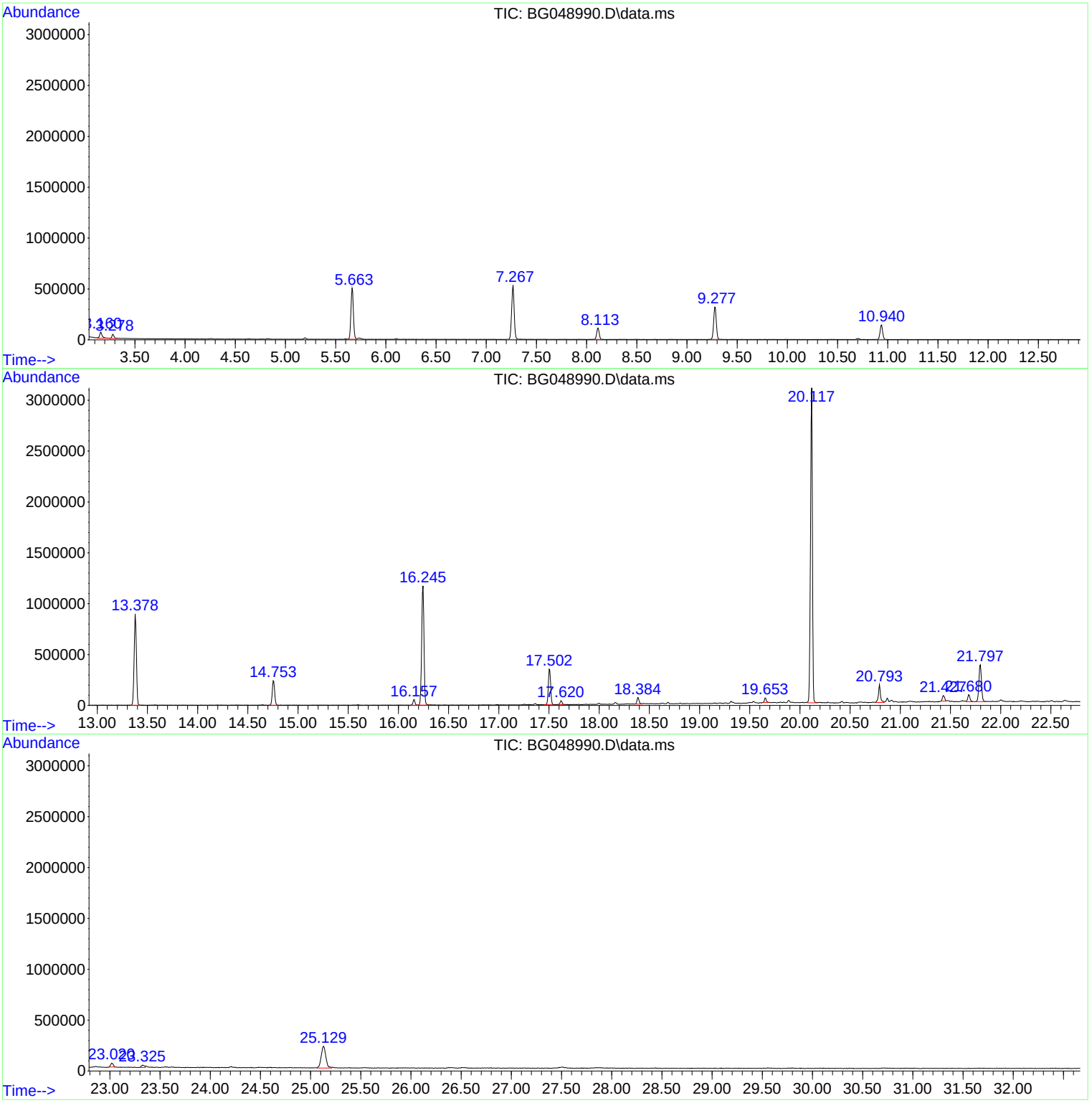
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
17-B6(84-88)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048990.D
Acq On : 15 Jun 2021 23:28
Operator : CG/JU
Sample : M2672-20
Misc :
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Instrument : BNA_G
ClientSampleId : 17-B6(84-88)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

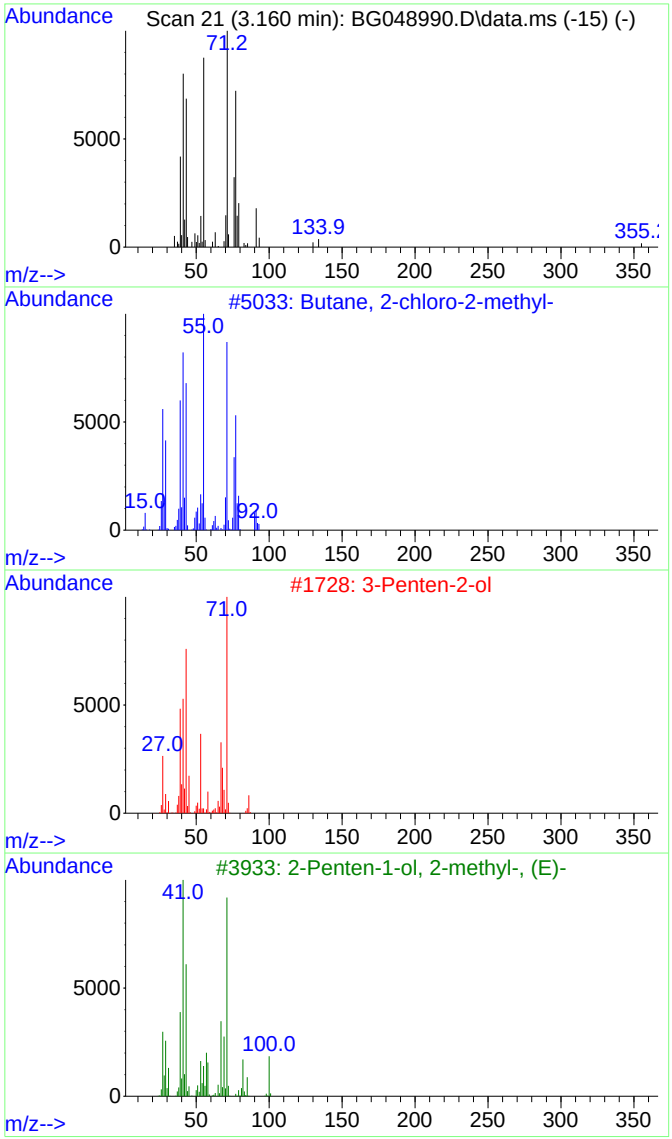
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

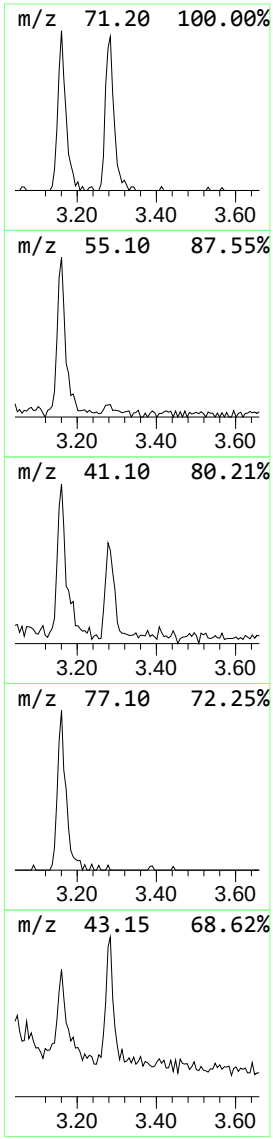
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.160	11.49 ng	109975	1,4-Dichlorobenzene-d4	8.113

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	59
2	3-Penten-2-ol	86	C5H10O	001569-50-2	32
3	2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	23
4	Tetrahydrofurfuryl acrylate	156	C8H12O3	002399-48-6	22
5	2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	22





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Data File : BG048990.D
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Sample : M2672-20
Misc :
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Instrument : BNA_G
ClientSampleId : 17-B6(84-88)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

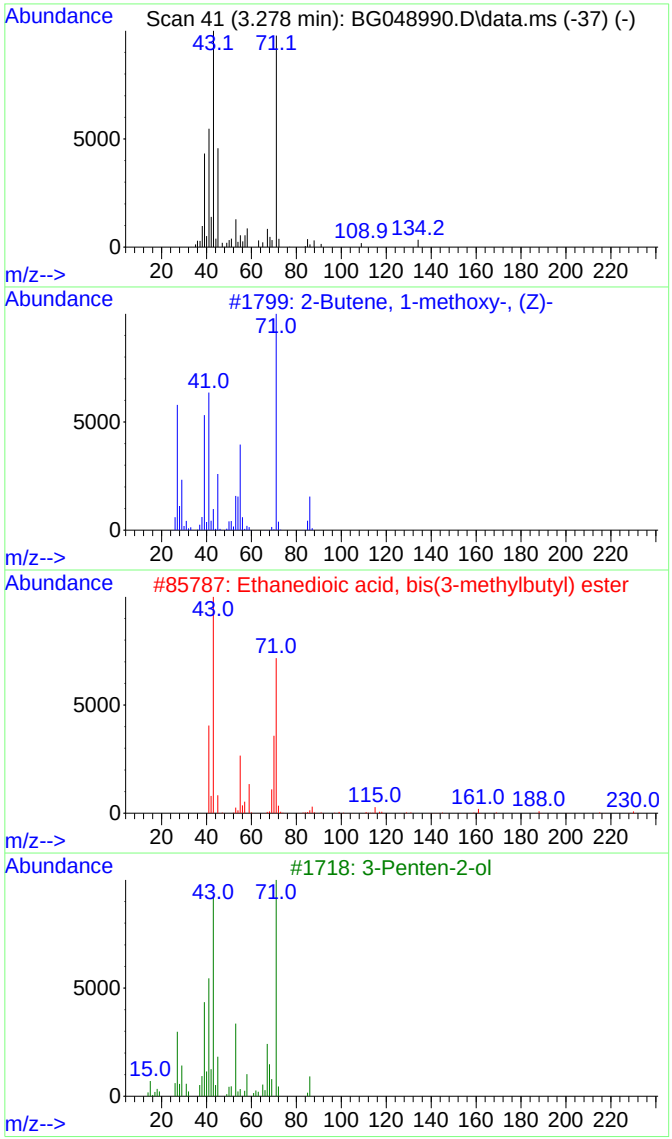
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

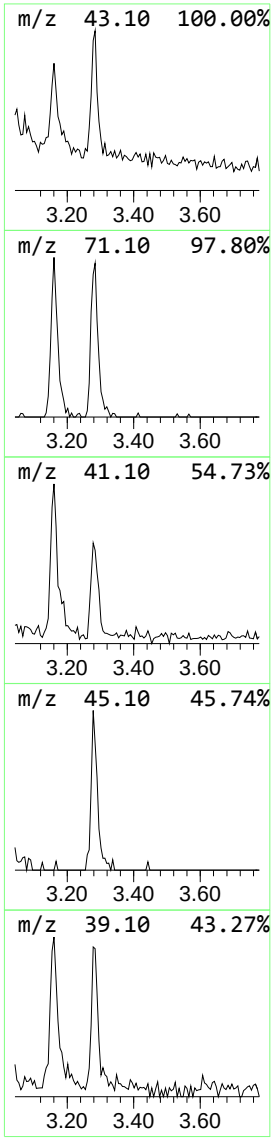
****

Peak Number 2 2-Butene, 1-methoxy-, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.278	6.39 ng	61173	1,4-Dichlorobenzene-d4	8.113

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	64
2	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	47
3	3-Penten-2-ol	86	C5H10O	001569-50-2	42
4	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	40
5	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048990.D
Acq On : 15 Jun 2021 23:28
Operator : CG/JU
Sample : M2672-20
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(84-88)

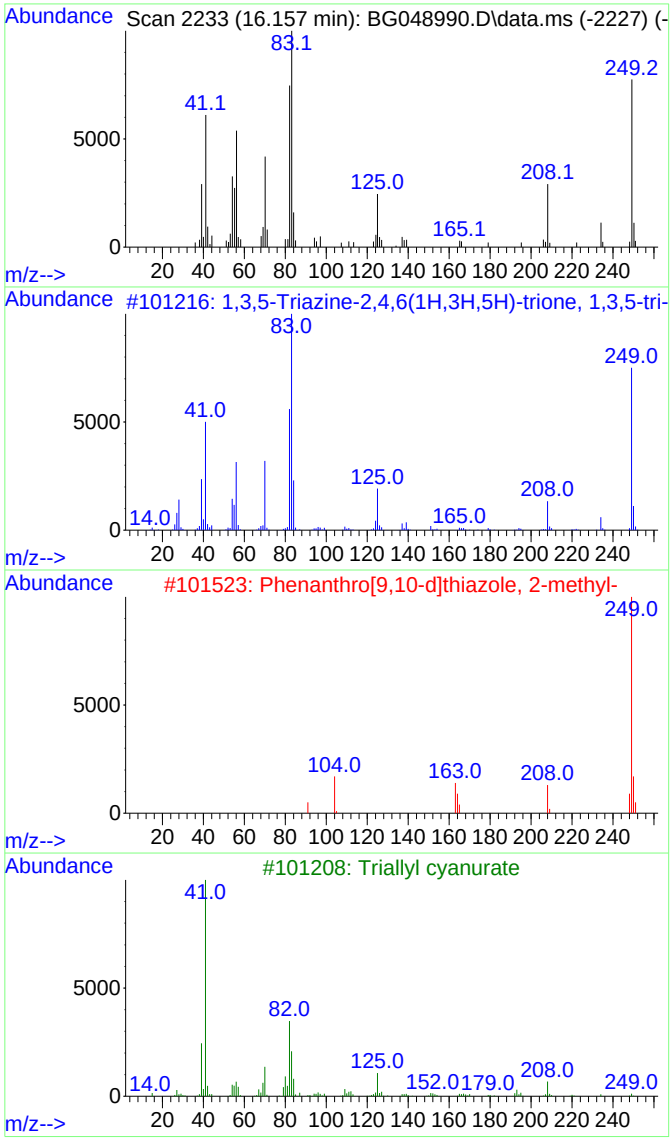
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

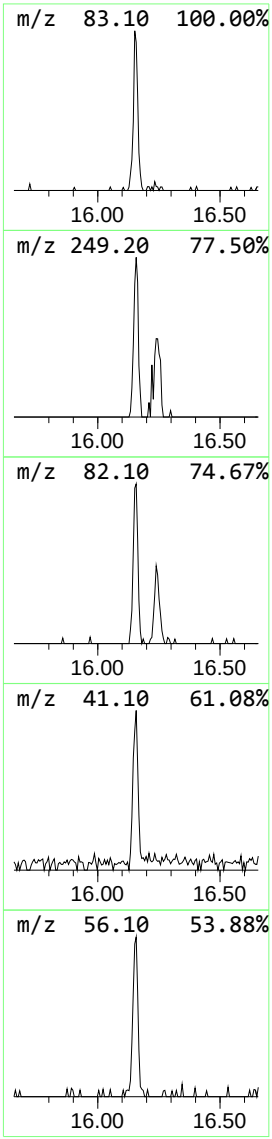
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.157	2.76 ng	77604	Phenanthrene-d10	17.508

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	93
2	Phenanthro[9,10-d]thiazole, 2-me...	249	C16H11NS	021639-90-7	50
3	Triallyl cyanurate	249	C12H15N3O3	000101-37-1	27
4	Cyclohexane, hexyl-	168	C12H24	004292-75-5	27
5	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	27





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Instrument : BNA_G
ClientSampleId : 17-B6(84-88)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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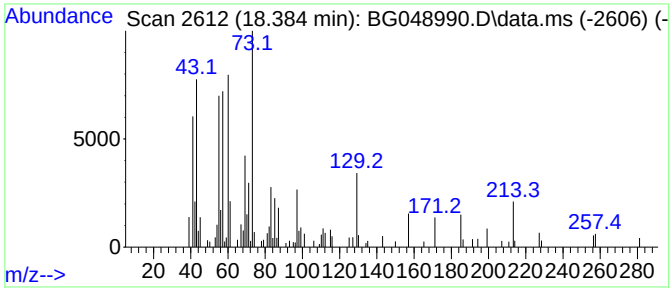
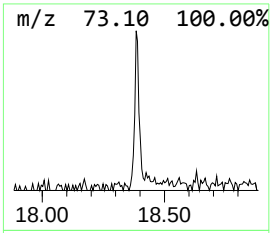
****

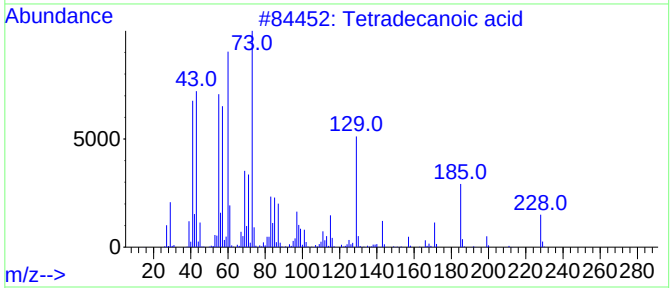
Peak Number 4 Tetradecanoic acid Concentration Rank 4

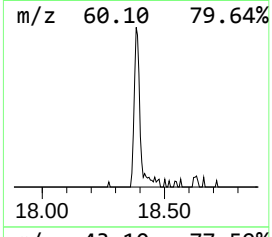
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.384	3.45 ng	96915	Phenanthrene-d10	17.508

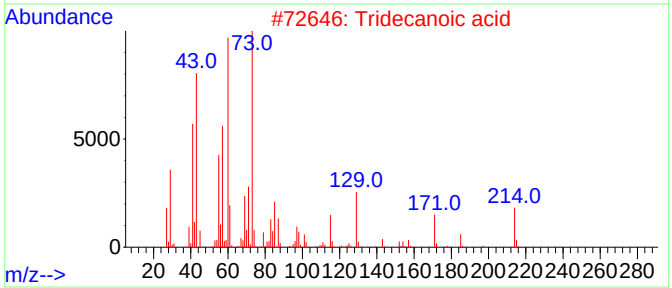
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	53
5	Undecanoic acid	186	C11H22O2	000112-37-8	53

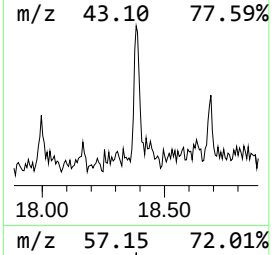


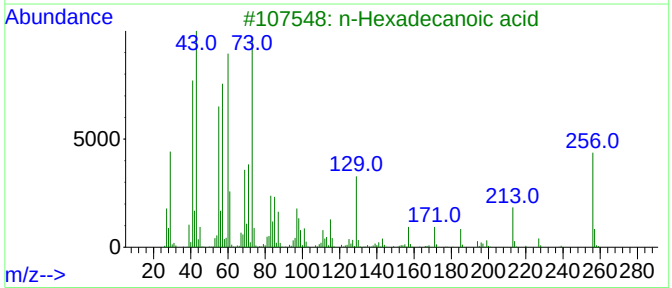


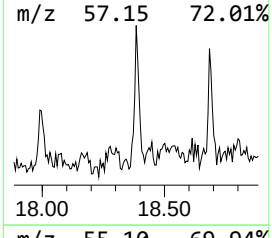


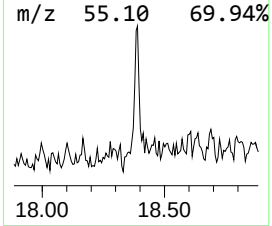












Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061521\
Data File : BG048990.D
Acq On : 15 Jun 2021 23:28
Operator : CG/JU
Sample : M2672-20
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 17-B6(84-88)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

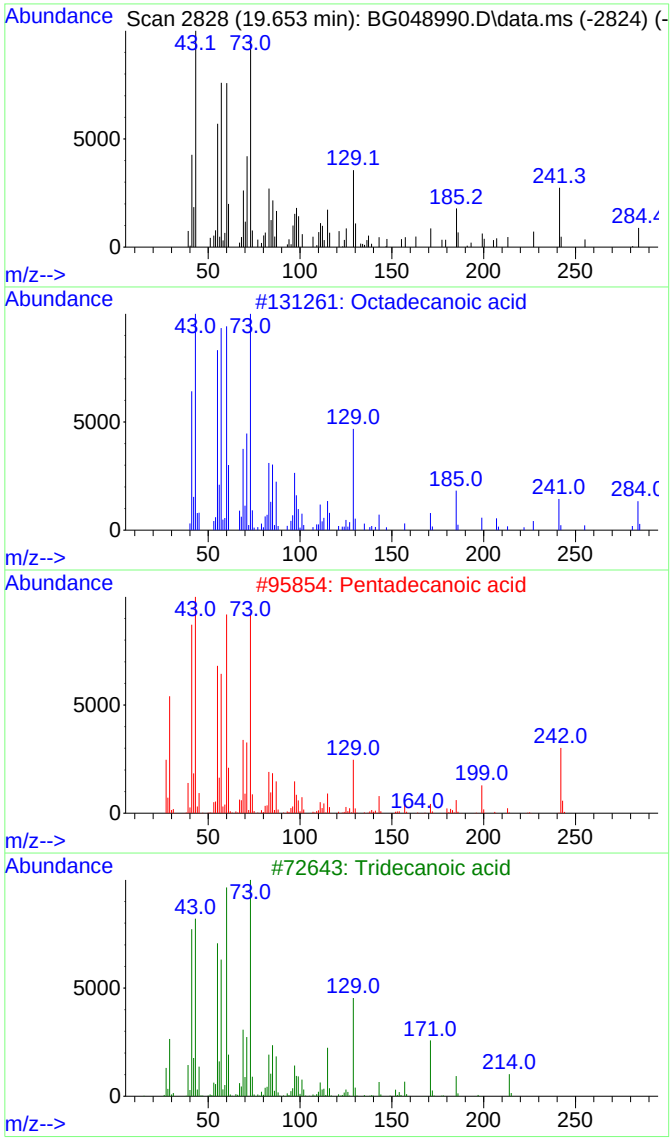
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

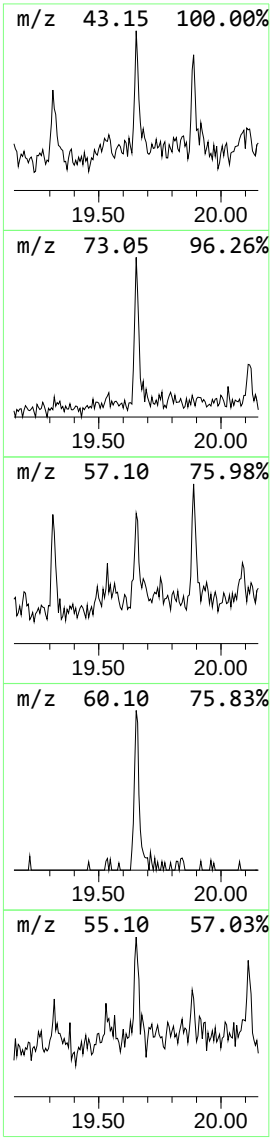
****

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.653	2.20 ng	61879	Phenanthrene-d10	17.508

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58





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ClientSampleId :
17-B6(84-88)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
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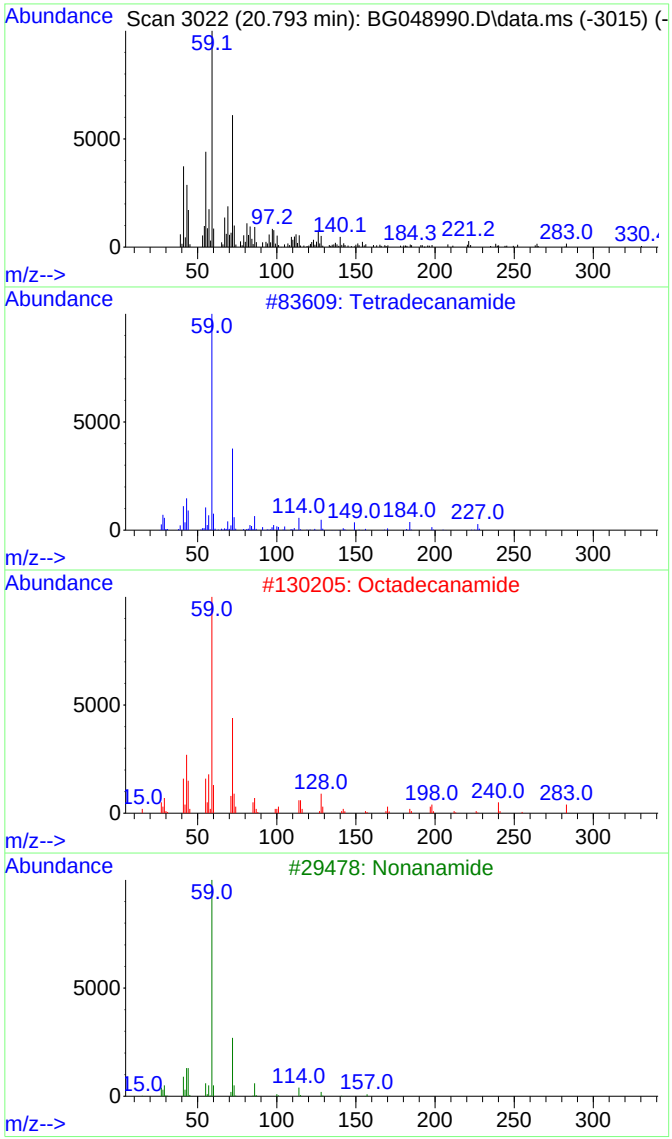
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

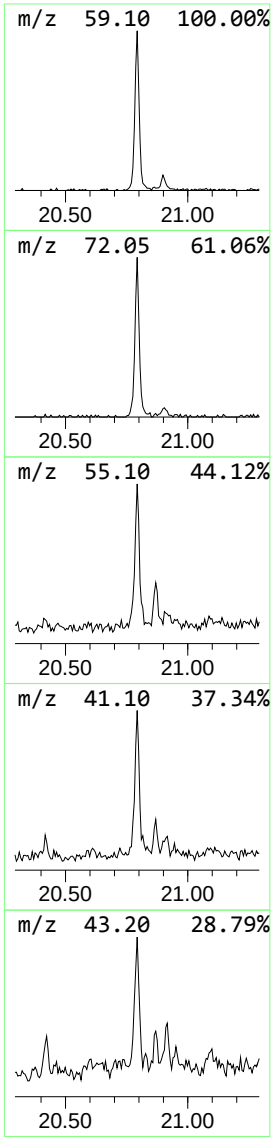
****

Peak Number 6 Tetradecanamide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.793	7.91 ng	255781	Chrysene-d12	21.797

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	72
2	Octadecanamide	283	C18H37NO	000124-26-5	64
3	Nonanamide	157	C9H19NO	001120-07-6	64
4	Octanamide	143	C8H17NO	000629-01-6	64
5	Dodecanamide	199	C12H25NO	001120-16-7	64





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ClientSampleId :
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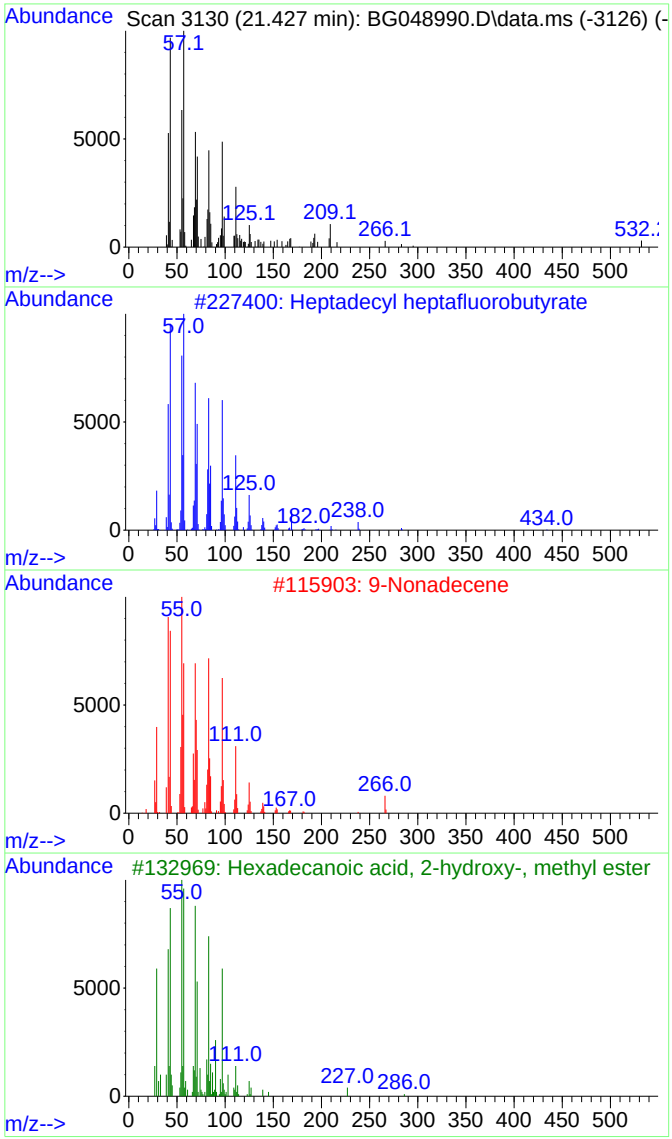
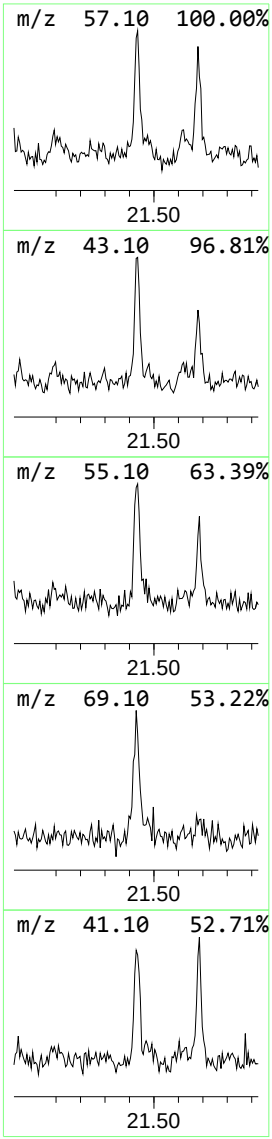
****
Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.427	2.57 ng	83134	Chrysene-d12	21.797

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	72
2	9-Nonadecene	266	C19H38	031035-07-1	64
3	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	58
4	1-Octadecanol	270	C18H38O	000112-92-5	58
5	Cyclotetradecane	196	C14H28	000295-17-0	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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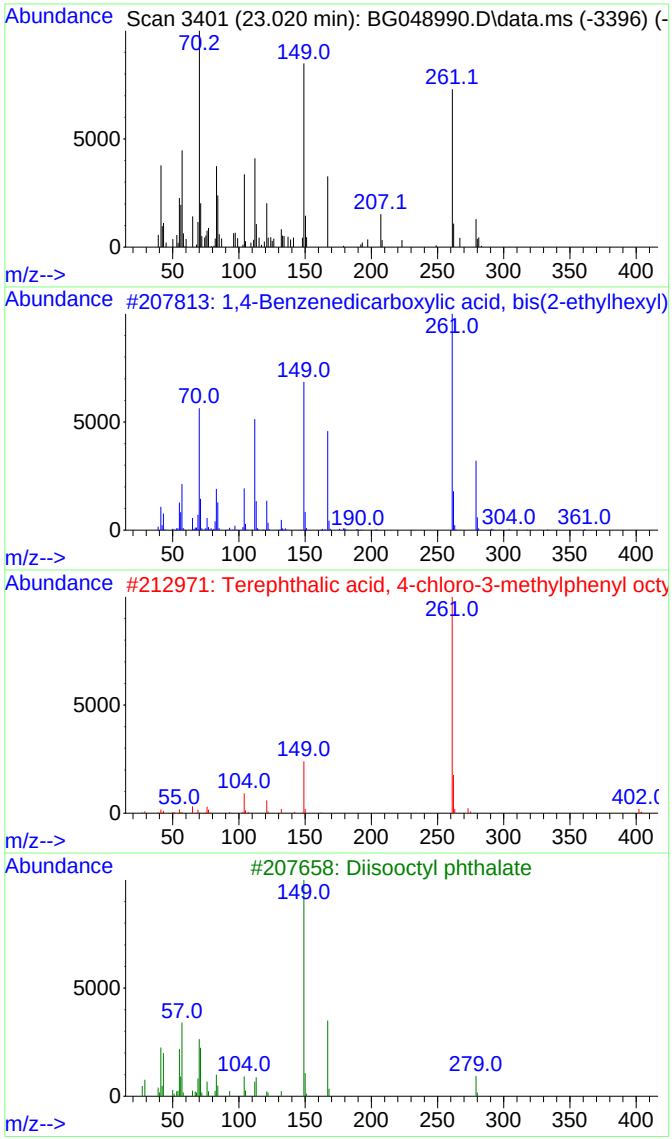
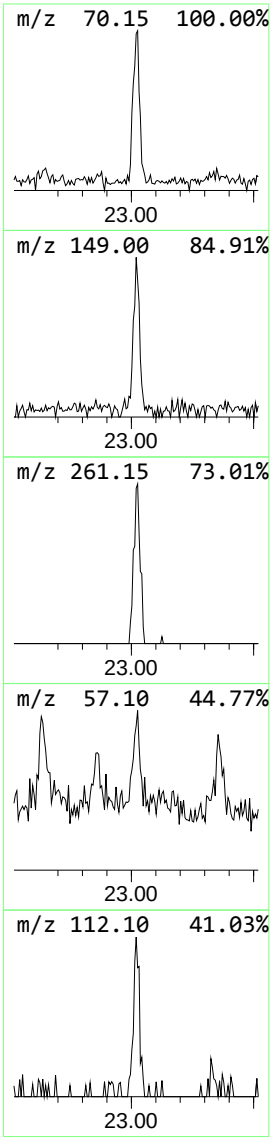
****

Peak Number 8 1,4-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.020	2.11 ng	68286	Chrysene-d12	21.797

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	50
2	Terephthalic acid, 4-chloro-3-me...	402	C23H27ClO4	1000323-70-4	35
3	Diisooctyl phthalate	390	C24H38O4	000131-20-4	35
4	Terephthalic acid, phenyl octyl ...	354	C22H26O4	1000324-06-6	35
5	Phthalic acid, 3,5-difluoropheny...	348	C19H18F2O4	1000315-54-1	27





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
ClientSampleId : 17-B6(84-88)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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
Butane, 2-chlor...	3.160	11.5	ng	109975	1	8.113	191443	20.0
2-Butene, 1-met...	3.278	6.4	ng	61173	1	8.113	191443	20.0
1,3,5-Triazine-...	16.157	2.8	ng	77604	4	17.508	561992	20.0
Tetradecanoic acid	18.384	3.5	ng	96915	4	17.508	561992	20.0
Octadecanoic acid	19.653	2.2	ng	61879	4	17.508	561992	20.0
Tetradecanamide	20.793	7.9	ng	255781	5	21.797	647110	20.0
Heptadecyl hept...	21.427	2.6	ng	83134	5	21.797	647110	20.0
1,4-Benzenedica...	23.020	2.1	ng	68286	5	21.797	647110	20.0