LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049861.D
Acq On : 16 Aug 2021 22:32
Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP1-1-6FT

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-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049861.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.138	11	17	32	rVB	135314	270916	20.31%	2.115%
2	5.106	347	352	360	rVB	46980	76450	5.73%	0.597%
3	5.588	427	434	444	rBV	509079	844217	63.29%	6.590%
4	6.193	534	537	547	rVB2	9746	16053	1.20%	0.125%
5	7.198	699	708	723	rVB	544399	966606	72.46%	7.545%
6	8.026	841	849	857	rBV	117206	211117	15.83%	1.648%
7	9.201	1040	1049	1057	rBV	345996	626126	46.94%	4.887%
8	10.605	1282	1288	1298	rBV	93977	176381	13.22%	1.377%
9	10.851	1322	1330	1337	rBV	165721	296882	22.26%	2.317%
10	13.301	1739	1747	1754	rBV	791632	1238520	92.85%	9.667%
11	14.682	1975	1982	1988	rBV	259834	401297	30.08%	3.132%
12	14.746	1988	1993	2001	rVB2	10782	17636	1.32%	0.138%
13	15.733	2155	2161	2169	rVB4	8278	15867	1.19%	0.124%
14	16.174	2229	2236	2244	rBV	709440	1099139	82.40%	8.580%
15	17.178	2399	2407	2412	rBV9	7141	17741	1.33%	0.138%
16	17.437	2445	2451	2455	rBV	287351	461706	34.61%	3.604%
17	17.478	2455	2458	2464	rVV	122122	171243	12.84%	1.337%
18	17.566	2468	2473	2478	rVB2	29095	48351	3.62%	0.377%
19	17.842	2516	2520	2524	rVB	11617	16351	1.23%	0.128%
20	18.089	2558	2562	2565	rVB	25889	31574	2.37%	0.246%
21	18.312	2596	2600	2605	rBV4	16733	24040	1.80%	0.188%
22	18.359	2605	2608	2613	rVB	21845	31995	2.40%	0.250%
23	18.512	2628	2634	2638	rBV2	24995	46009	3.45%	0.359%
24	18.805	2679	2684	2687	rBV2	15163	26763	2.01%	0.209%
25	18.852	2687	2692	2696	rVB8	14170	19324	1.45%	0.151%
26	19.223	2750	2755	2759	rBV8	14192	32083	2.41%	0.250%
27	19.487	2795	2800	2806	rBV	288146	408329	30.61%	3.187%
28	19.816	2851	2856	2857	rBV	47786	55212	4.14%	0.431%
29	19.851	2858	2862	2870	rVB	224716	323943	24.28%	2.529%
30	19.922	2870	2874	2880	rBV6	14894	27477	2.06%	0.214%
31	20.045	2889	2895	2900	rBV	1001737	1333952	100.00%	10.412%
32	20.086	2900	2902	2908	rVB3	15631	24051	1.80%	0.188%
33	20.162	2912	2915	2917	rBV4	13295	17686	1.33%	0.138%
34	20.339	2934	2945	2950	rBV	55115	117381	8.80%	0.916%
35	20.444	2957	2963	2967	rBV	44385	64954	4.87%	0.507%
36	20.503	2968	2973	2976	rVV3	18744	35701	2.68%	0.279%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049861.D
Acq On : 16 Aug 2021 22:32
Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP1-1-6FT

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-BG080321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.532	2976	2978	2983	rVB4	14843	19251	1.44%	0.150%
38	20.638	2993	2996	2999	rBV3	11120	15945	1.20%	0.124%
39	21.290	3103	3107	3111	rBV2	21358	32077	2.40%	0.250%
40	21.337	3111	3115	3119	rBV2	51758	82769	6.20%	0.646%
41	21.713	3171	3179	3184	rVV2	306759	684453	51.31%	5.343%
42	21.760	3184	3187	3199	rVB	104940	185361	13.90%	1.447%
43	22.124	3247	3249	3255	rVB3	19033	32086	2.41%	0.250%
44	22.459	3284	3306	3308	rBV3	323335	1243223	93.20%	9.704%
45	23.951	3553	3560	3566	rBV2	64371	184379	13.82%	1.439%
46	24.210	3598	3604	3609	rBV3	18257	41130	3.08%	0.321%
47	24.692	3680	3686	3693	rVB3	35268	92784	6.96%	0.724%
48	24.833	3704	3710	3719	rVB2	58949	158816	11.91%	1.240%
49	24.991	3727	3737	3745	rBV2	154925	445827	33.42%	3.480%

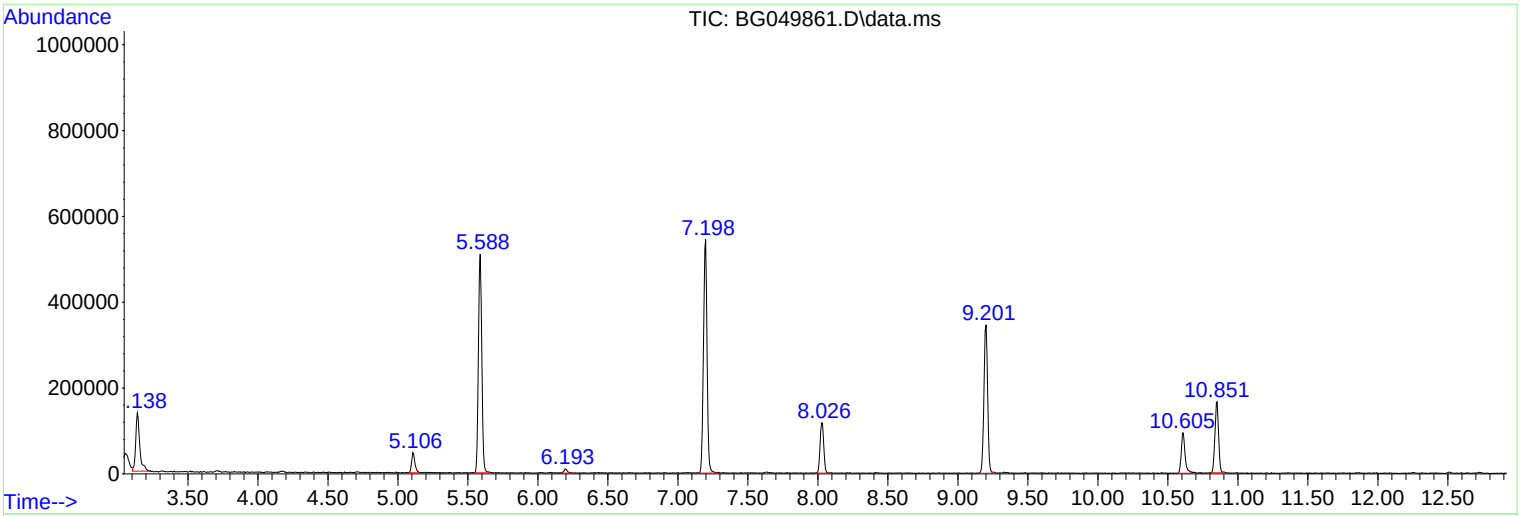
Sum of corrected areas: 12811174

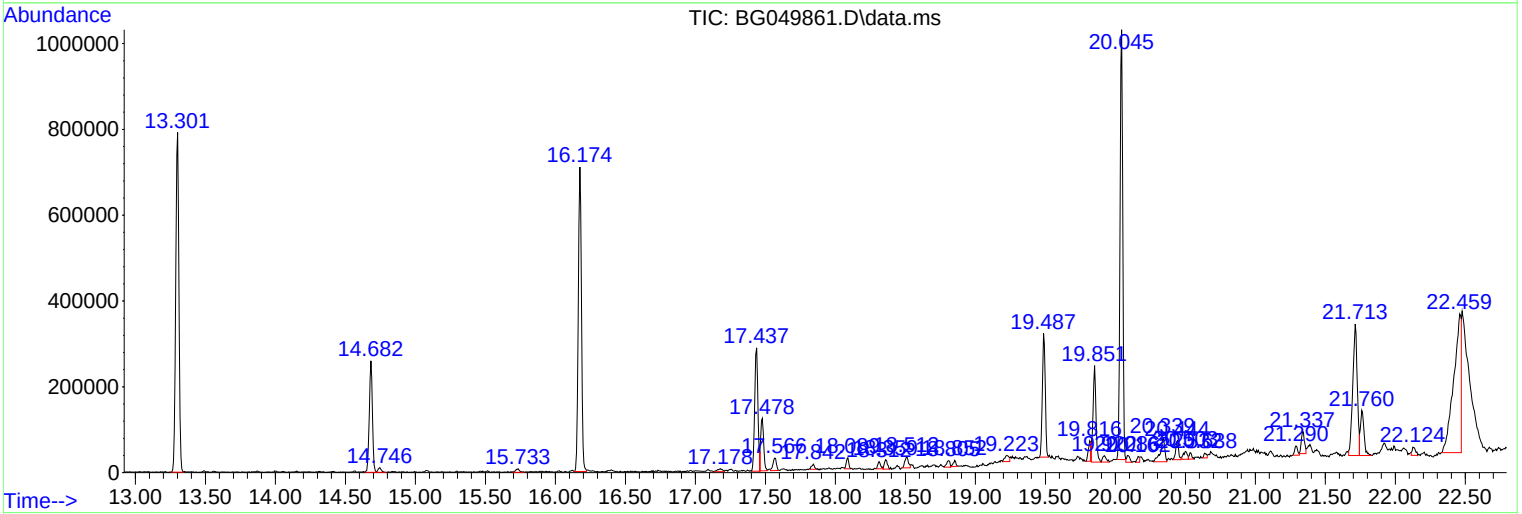
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049861.D
Acq On : 16 Aug 2021 22:32
Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

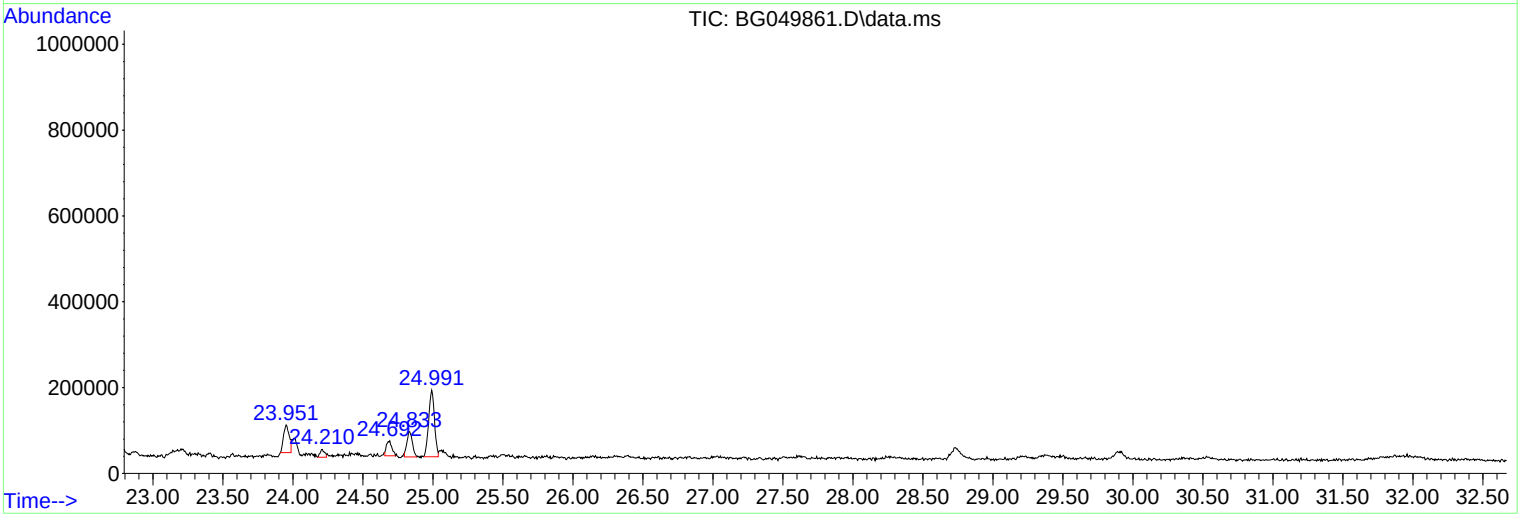
Instrument :
BNA_G
ClientSampleId :
TP1-1-6FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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_G\Data\BG081621\
Data File : BG049861.D
Acq On : 16 Aug 2021 22:32
Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP1-1-6FT

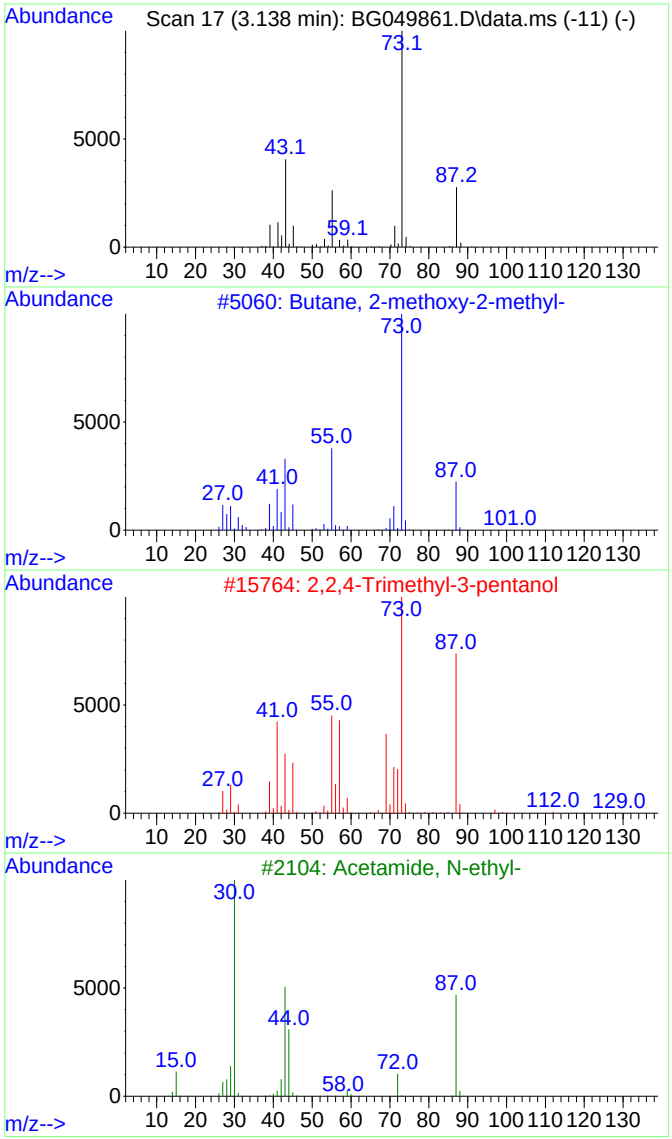
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

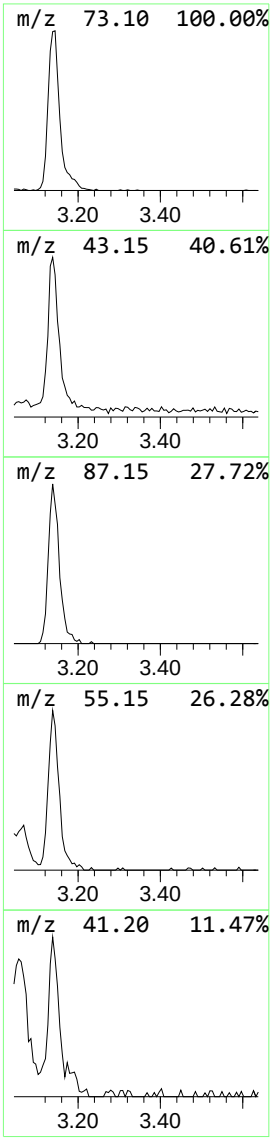
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.138	25.66 ng	270916	1,4-Dichlorobenzene-d4	8.026

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	25
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049861.D
Acq On : 16 Aug 2021 22:32
Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP1-1-6FT

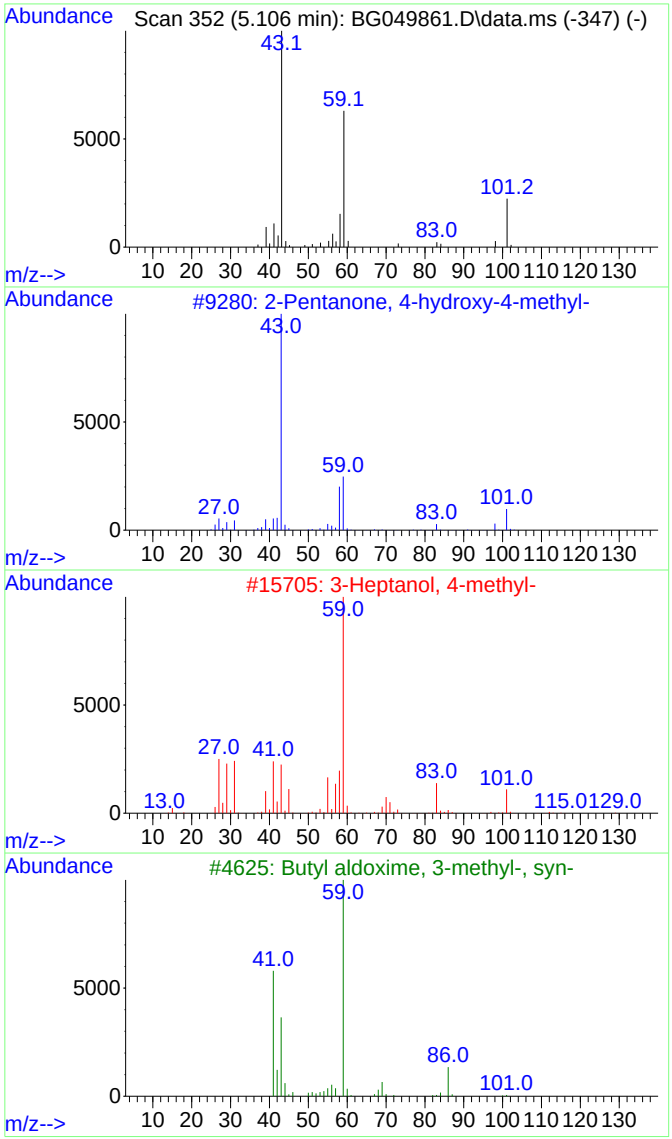
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

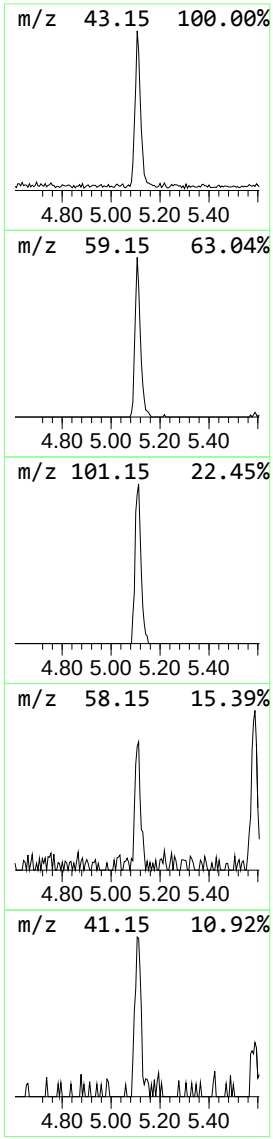
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.106	7.24 ng	76450	1,4-Dichlorobenzene-d4	8.026

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	36
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	1,2-Butanediol	90	C4H10O2	000584-03-2	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049861.D
Acq On : 16 Aug 2021 22:32
Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP1-1-6FT

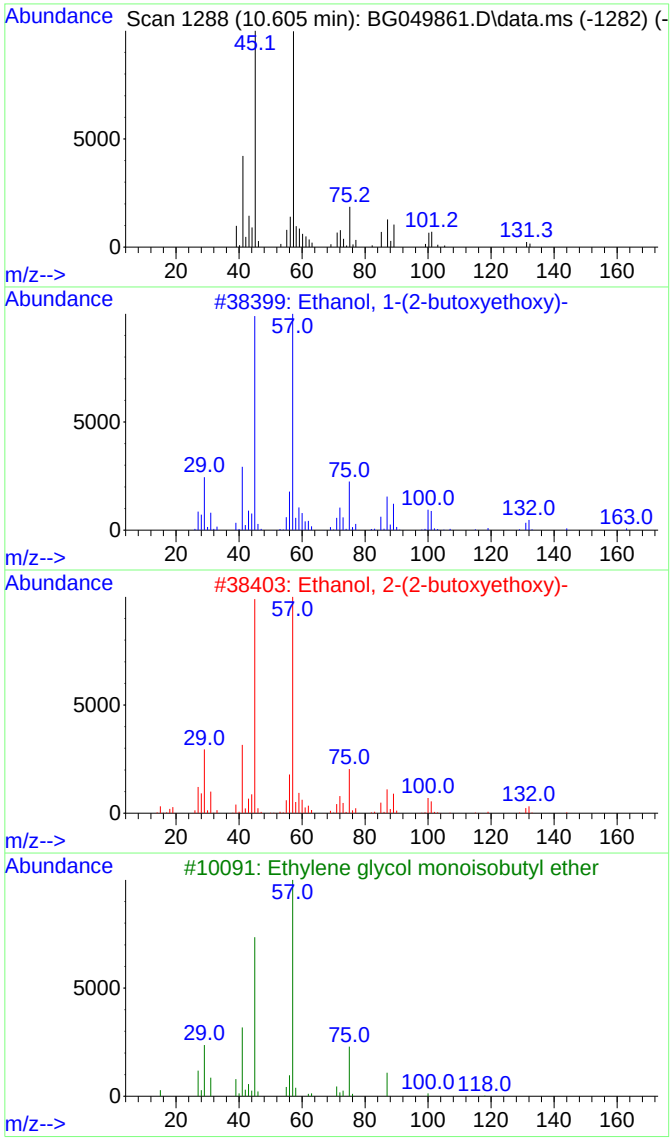
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

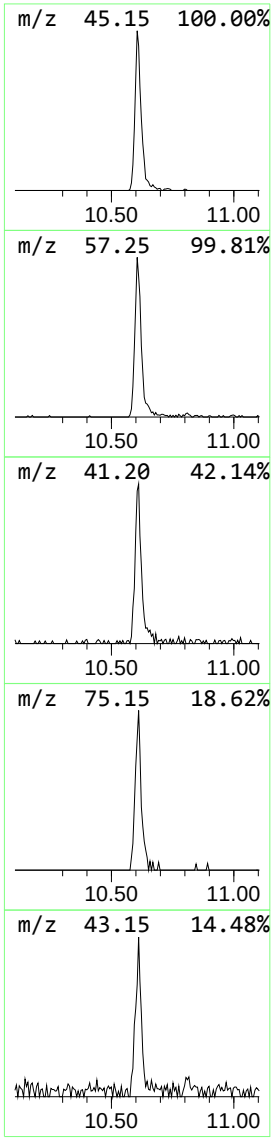
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.605	11.88 ng	176381	Naphthalene-d8	10.852

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049861.D
Acq On : 16 Aug 2021 22:32
Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP1-1-6FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

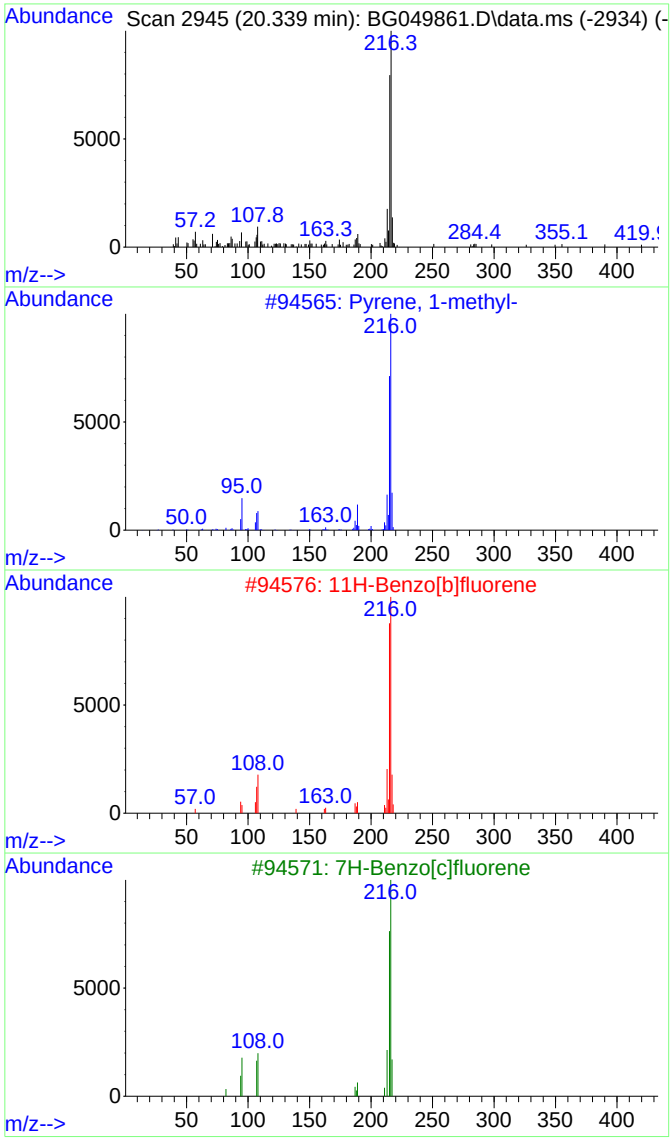
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

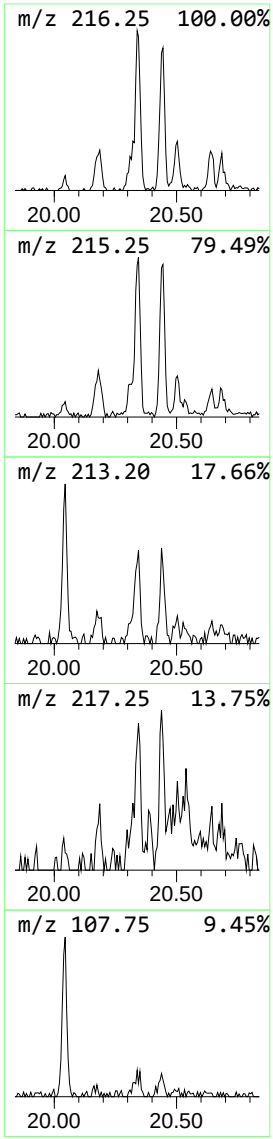
****

Peak Number 4 Pyrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.339	3.43 ng	117381	Chrysene-d12	21.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
3	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049861.D
Acq On : 16 Aug 2021 22:32
Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP1-1-6FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

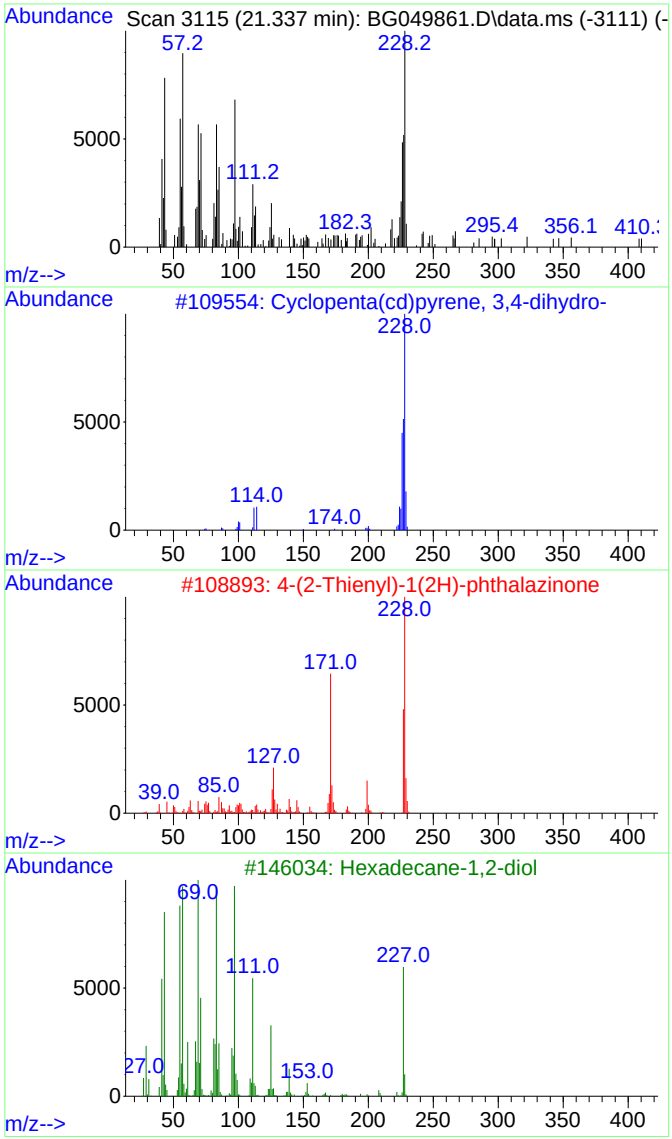
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

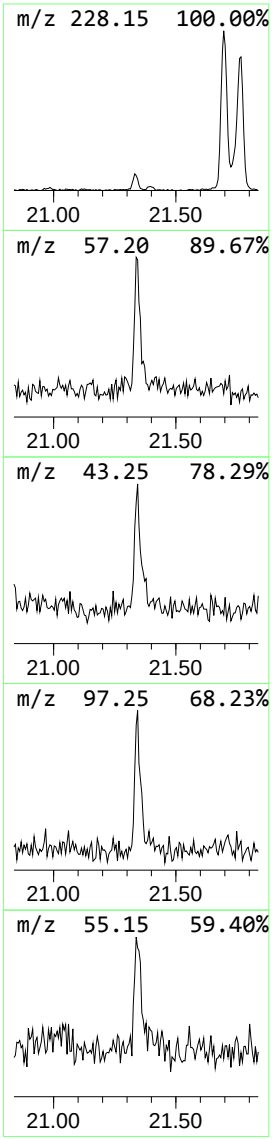
****

Peak Number 5 unknown21.337 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.337	2.42 ng	82769	Chrysene-d12	21.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	35
2	4-(2-Thienyl)-1(2H)-phthalazinone	228	C12H8N2OS	137382-45-7	30
3	Hexadecane-1,2-diol	258	C16H34O2	006920-24-7	30
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	25
5	Triphenylene	228	C18H12	000217-59-4	22





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Data File : BG049861.D
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Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP1-1-6FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

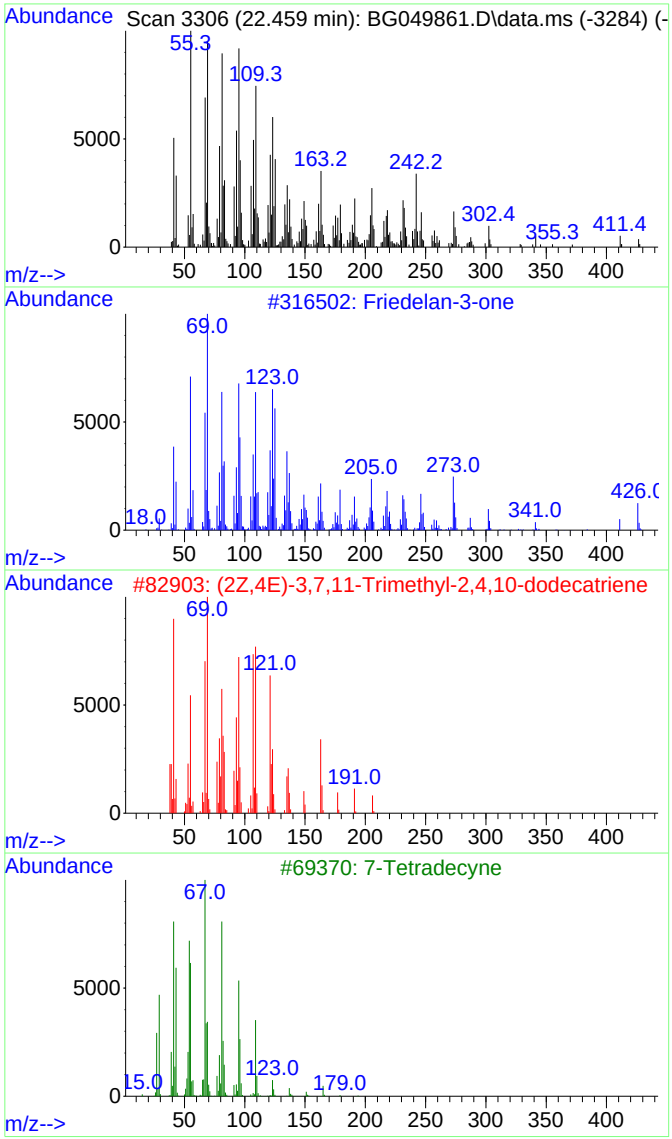
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

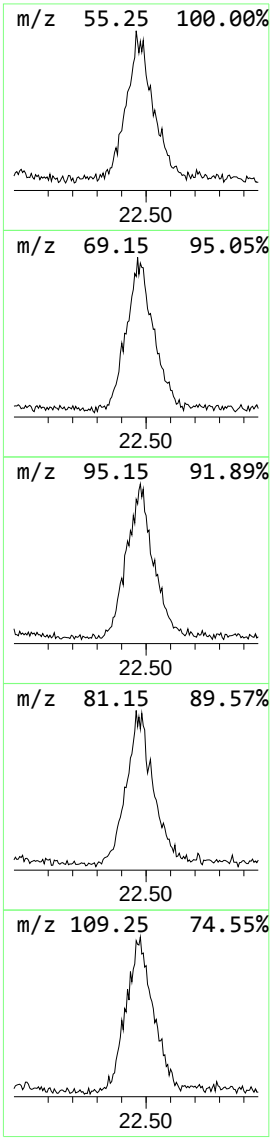
****

Peak Number 6 Friedelan-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.459	36.33 ng	1243220	Chrysene-d12	21.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Friedelan-3-one	426	C30H50O	000559-74-0	95
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	55
3	7-Tetradecyne	194	C14H26	035216-11-6	53
4	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	46
5	(-)-Neoclovene-(I), dihydro-	206	C15H26	1000152-82-1	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049861.D
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Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP1-1-6FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

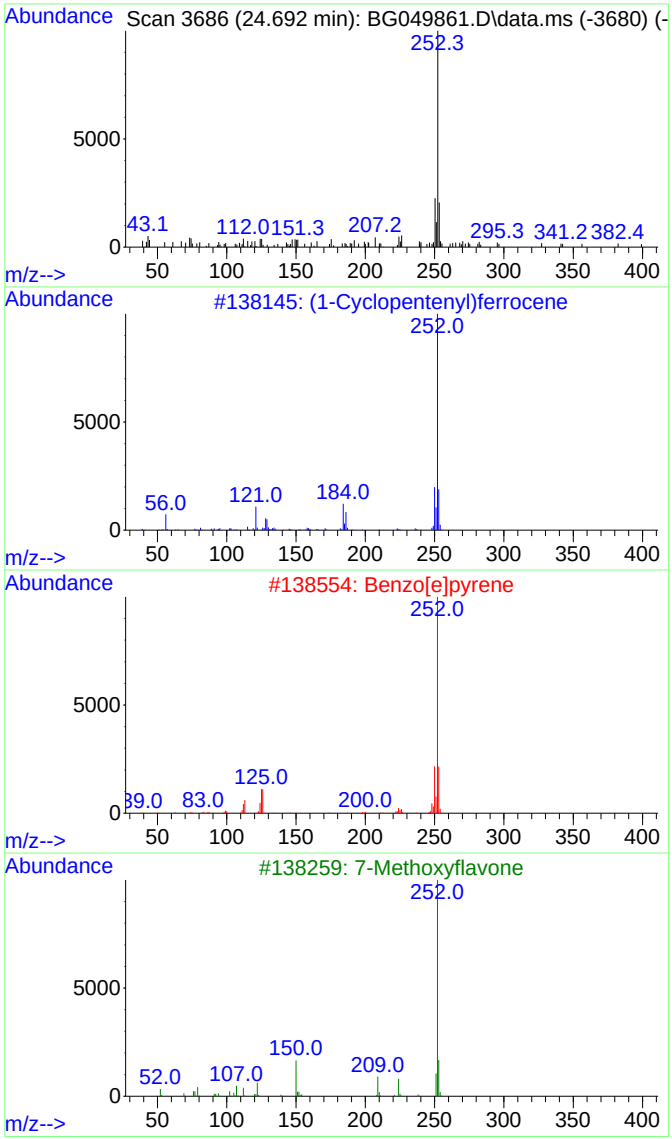
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

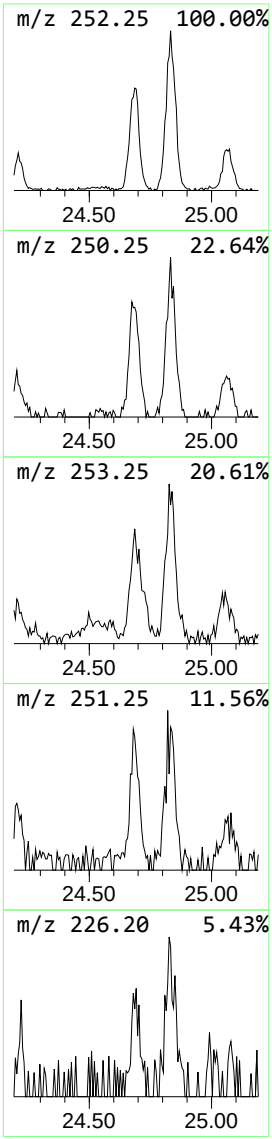
****

Peak Number 7 (1-Cyclopentenyl)ferrocene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.692	4.16 ng	92784	Perylene-d12	24.991

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	80
2	Benzo[e]pyrene	252	C20H12	000192-97-2	68
3	7-Methoxyflavone	252	C16H12O3	022395-22-8	64
4	Perylene	252	C20H12	000198-55-0	64
5	Benzo[a]pyrene	252	C20H12	000050-32-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG081621\
Data File : BG049861.D
Acq On : 16 Aug 2021 22:32
Operator : CG/JU
Sample : M3404-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP1-1-6FT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.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...	3.138	25.7	ng	270916	1	8.026	211117	20.0
2-Pentanone, 4-...	5.106	7.2	ng	76450	1	8.026	211117	20.0
Ethanol, 1-(2-b...	10.605	11.9	ng	176381	2	10.852	296882	20.0
Pyrene, 1-methyl-	20.339	3.4	ng	117381	5	21.713	684453	20.0
unknown21.337	21.337	2.4	ng	82769	5	21.713	684453	20.0
Friedelan-3-one	22.459	36.3	ng	1243220	5	21.713	684453	20.0
(1-Cyclopenteny...	24.692	4.2	ng	92784	6	24.991	445827	20.0