LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

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-BG121218.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	3.176	11	15	27	rVB	30209	49395	1.87%	0.418%
2	5.138	344	349	357	rVB	17781	32349	1.22%	0.274%
3	5.608	421	429	437	rBV	226673	384634	14.56%	3.254%
4	7.212	691	702	716	rVB	167344	340250	12.88%	2.879%
5	7.582	754	765	778	rBV	414035	741655	28.07%	6.275%
6	8.053	839	845	849	rBV	77894	143498	5.43%	1.214%
7	8.094	849	852	861	rVB	57481	91026	3.44%	0.770%
8	8.376	892	900	910	rBV	337337	597949	22.63%	5.059%
9	9.233	1038	1046	1057	rBV	304227	564197	21.35%	4.773%
10	9.404	1061	1075	1089	rVV2	119354	409188	15.49%	3.462%
11	10.068	1184	1188	1197	rVB3	14517	31915	1.21%	0.270%
12	10.156	1197	1203	1217	rBV	23089	61353	2.32%	0.519%
13	10.620	1275	1282	1288	rBV2	27666	53935	2.04%	0.456%
14	10.685	1288	1293	1305	rVB2	23377	50540	1.91%	0.428%
15	10.873	1312	1325	1338	rBV	117235	253961	9.61%	2.149%
16	11.590	1441	1447	1459	rVB8	9233	27560	1.04%	0.233%
17	12.071	1520	1529	1540	rBV2	53344	106903	4.05%	0.904%
18	13.311	1733	1740	1748	rBV	991791	1525151	57.72%	12.904%
19	14.134	1875	1880	1886	rBV	28081	41662	1.58%	0.352%
20	14.692	1968	1975	1983	rBV2	215558	354882	13.43%	3.002%
21	16.184	2221	2229	2243	rBV2	926884	1446964	54.76%	12.242%
22	17.442	2436	2443	2451	rBV	295402	474129	17.94%	4.011%
23	18.293	2583	2588	2596	rBV6	18794	34406	1.30%	0.291%
24	20.044	2879	2886	2891	rBV	1927382	2642373	100.00%	22.356%
25	21.319	3098	3103	3107	rBV4	25372	44809	1.70%	0.379%
26	21.719	3164	3171	3179	rBV2	300761	534410	20.22%	4.521%
27	22.465	3294	3298	3303	rVB2	16718	26604	1.01%	0.225%
28	23.164	3412	3417	3423	rVB	22280	42881	1.62%	0.363%
29	23.294	3434	3439	3444	rVB7	16164	31209	1.18%	0.264%
30	23.975	3549	3555	3562	rVB2	26719	54696	2.07%	0.463%
31	24.933	3710	3718	3721	rBV6	20701	46679	1.77%	0.395%
32	25.015	3723	3732	3748	rVB2	176855	523746	19.82%	4.431%
33	26.073	3904	3912	3922	rVB5	17613	54673	2.07%	0.463%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

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-BG121218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

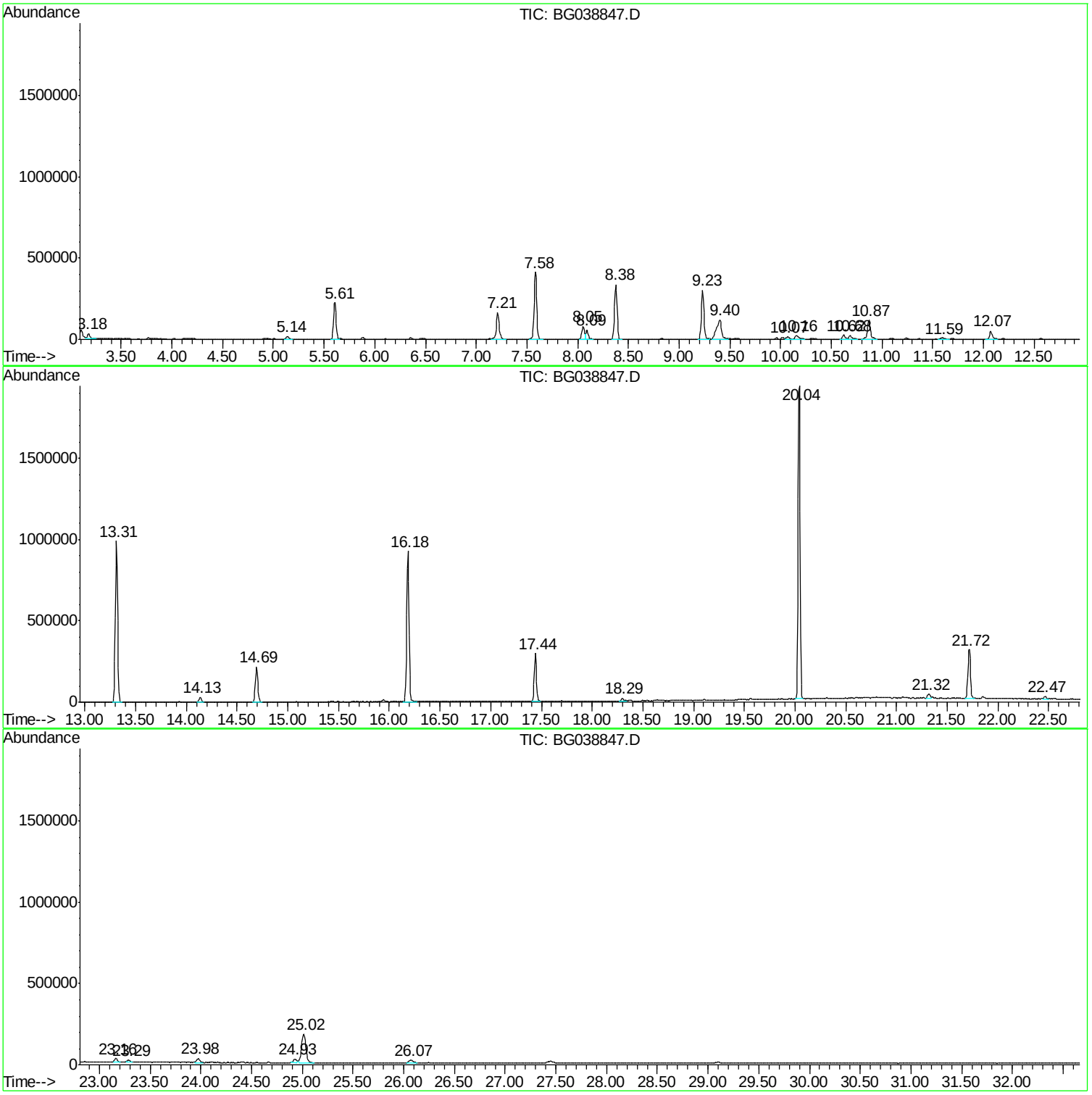
Sum of corrected areas: 11819582

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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 G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

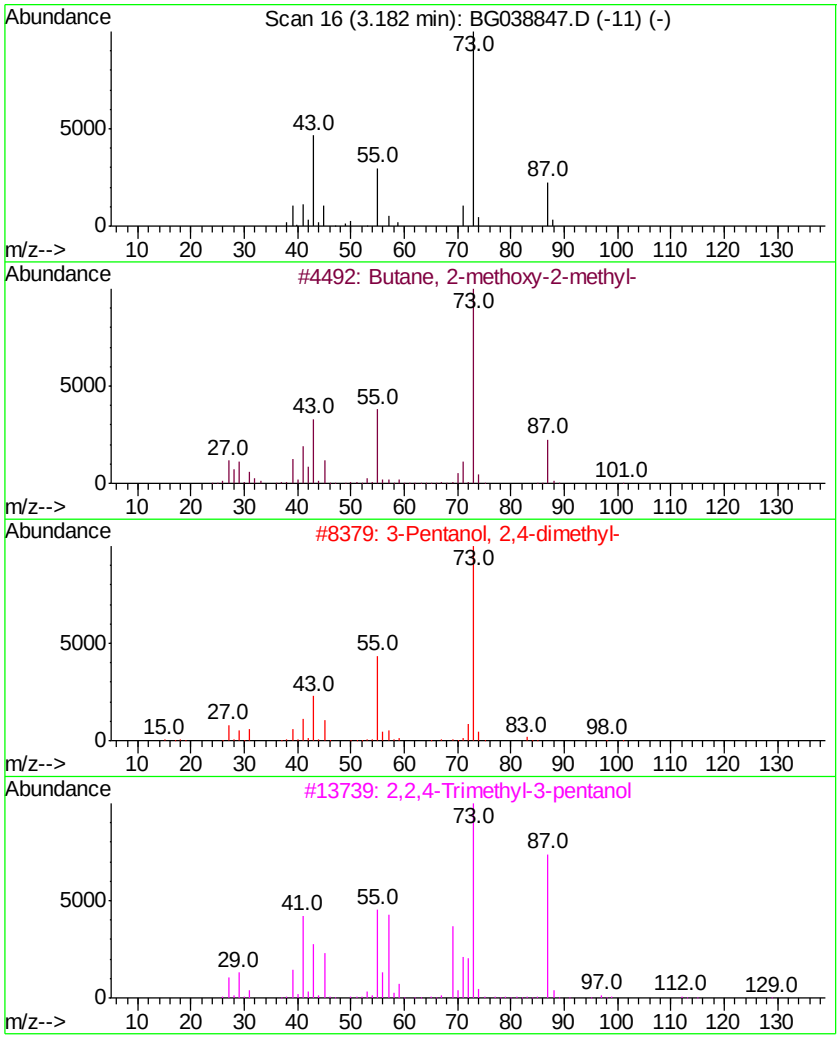
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

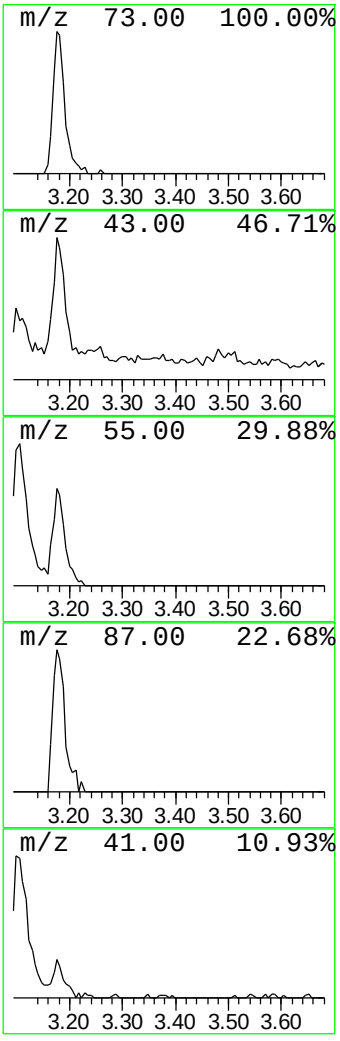
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	6.88 ng	49395	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
4	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

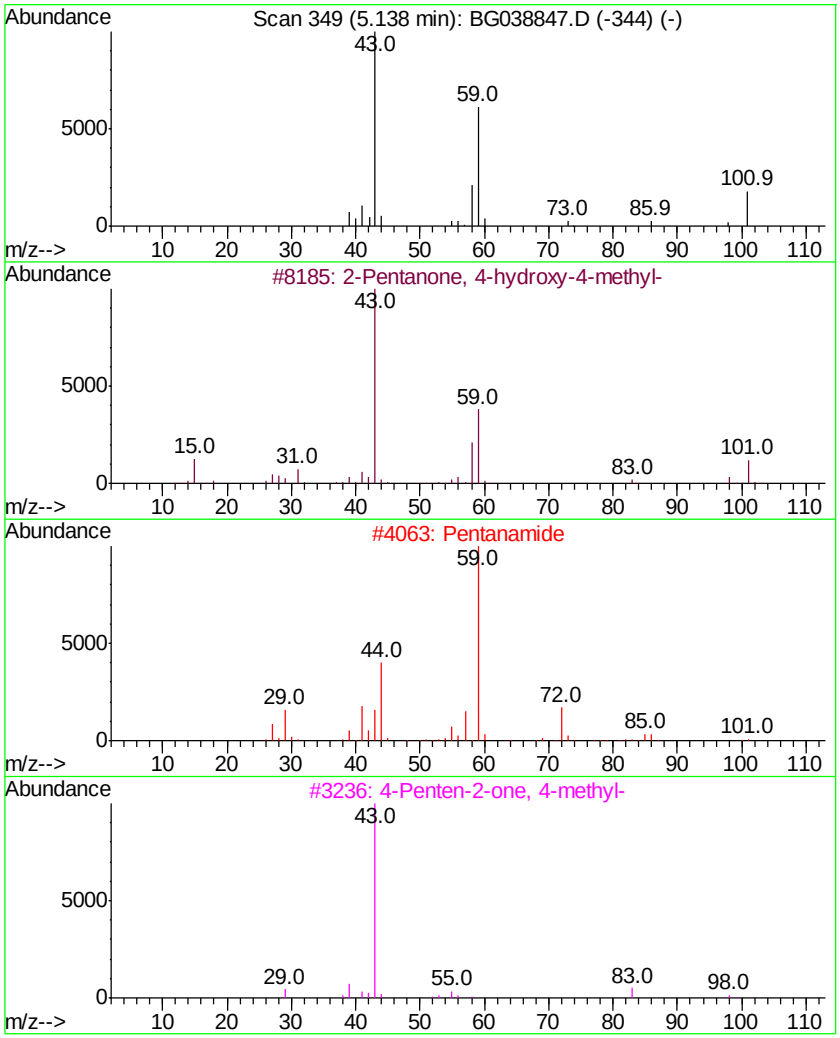
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

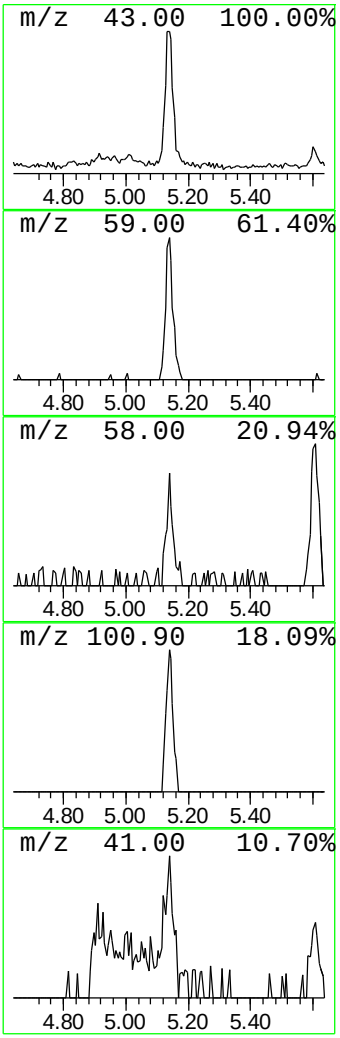
****

Peak Number 2 unknown5.14 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	4.51 ng	32349	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Pentanamide	101	C5H11NO	000626-97-1	17
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	1,6:2,3-Dianhydro-4-O-acetyl-.be...	186	C8H10O5	1000139-89-8	9
5	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

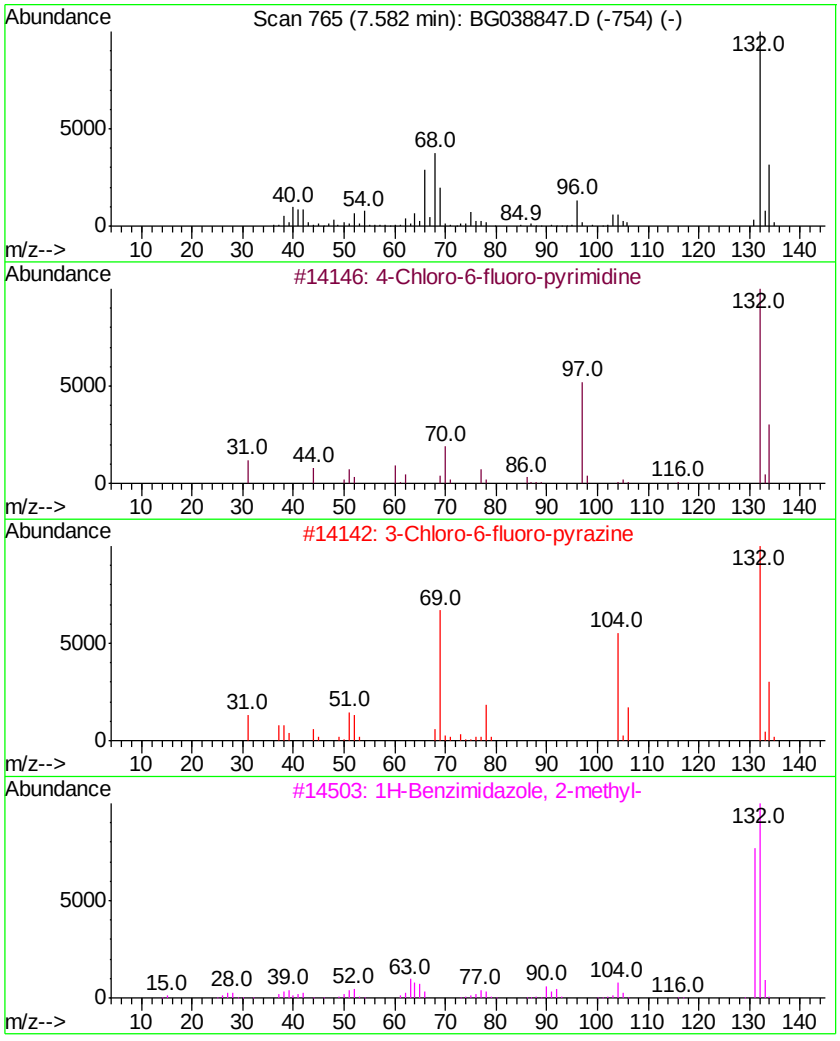
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

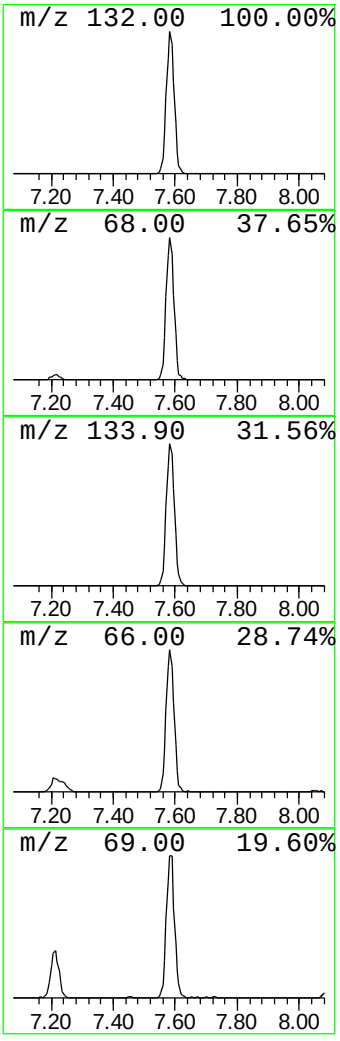
****

Peak Number 3 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	103.37 ng	741655	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	30
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

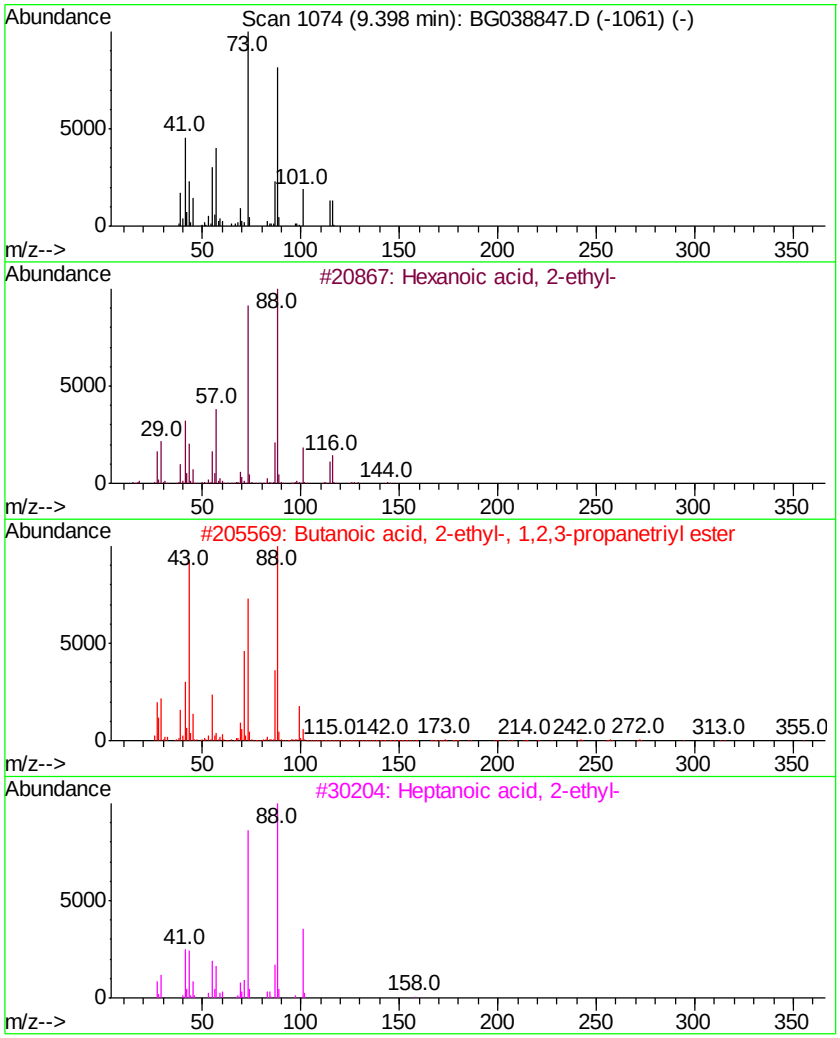
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

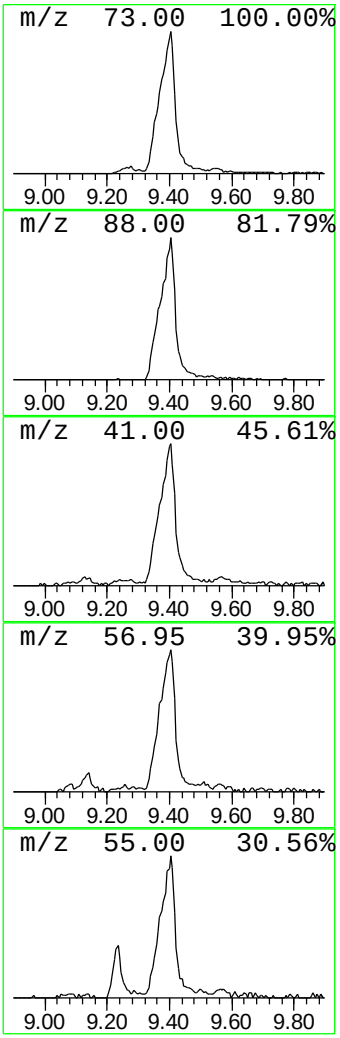
****

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.40	57.03 ng	409188	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
4	1,4-Dioxane	88	C4H8O2	000123-91-1	43
5	Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	42





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

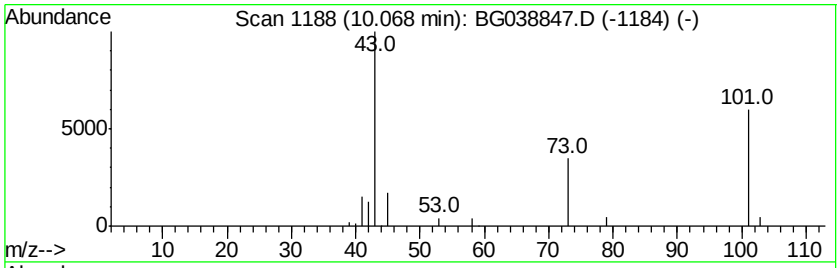
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

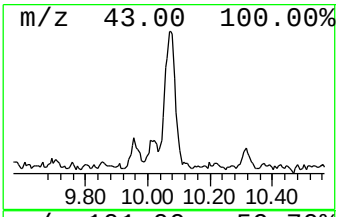
****

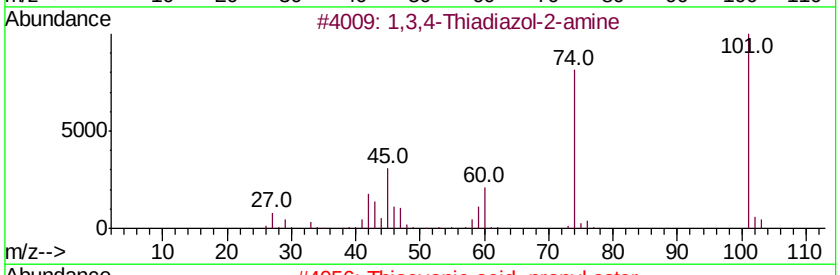
Peak Number 6 unknown10.07 Concentration Rank 9

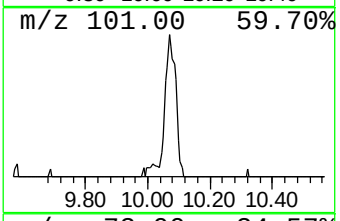
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.07	2.51 ng	31915	Naphthalene-d8	10.87

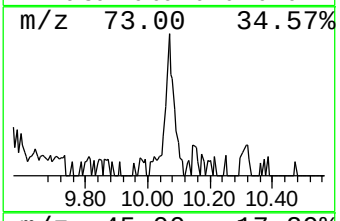
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4-Thiadiazol-2-amine	101	C2H3N3S	004005-51-0	43
2	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
3	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	7
4	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	7
5	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	7

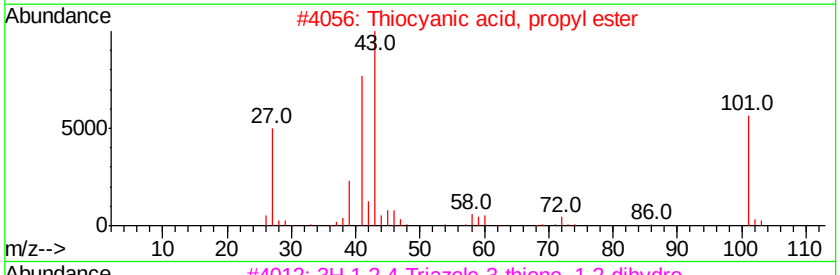


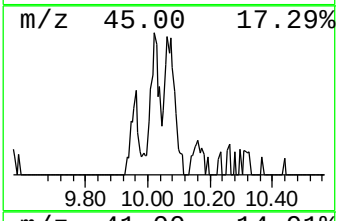


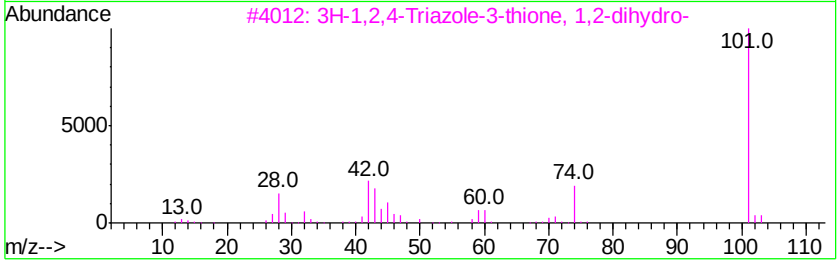


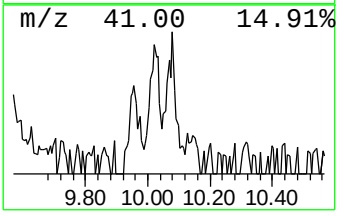












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Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

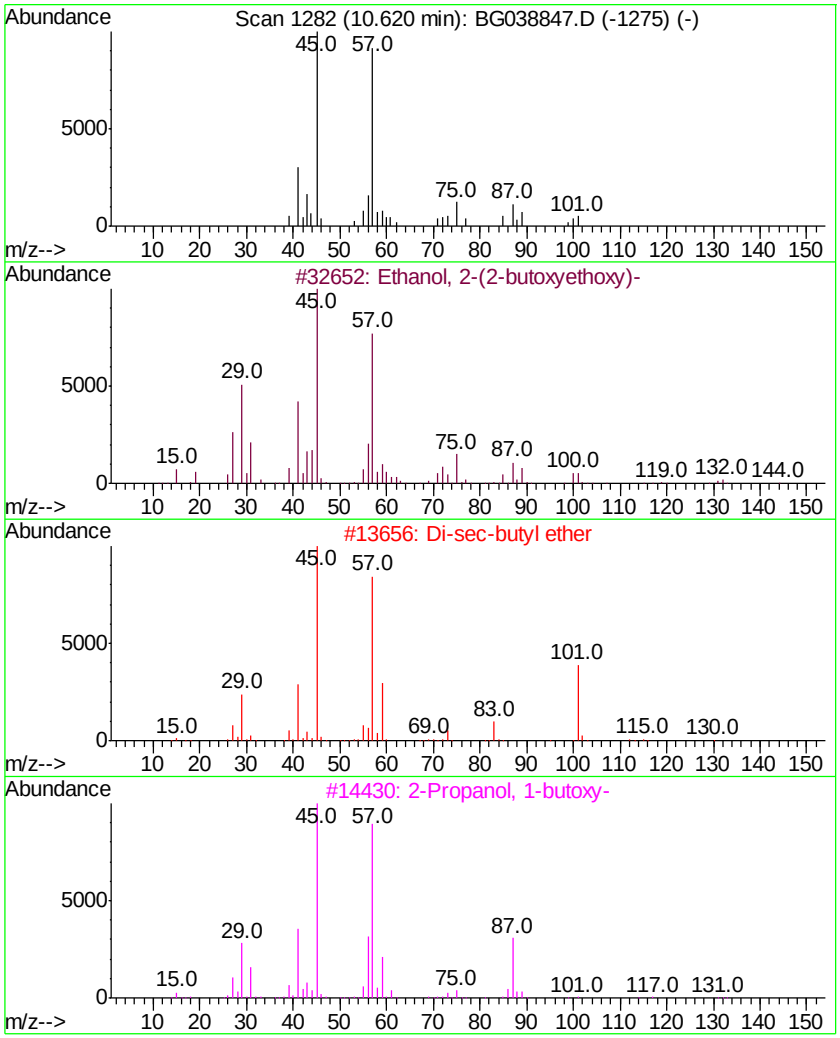
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

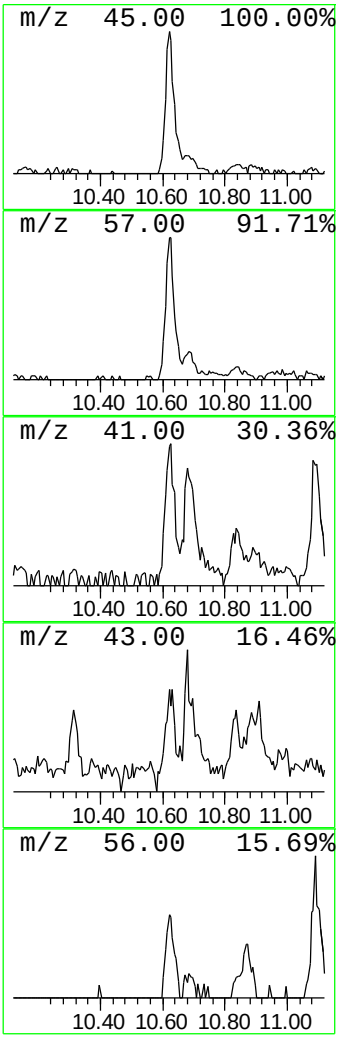
****

Peak Number 7 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	4.25 ng	53935	Naphthalene-d8	10.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2	Di-sec-butyl ether	130	C8H18O	006863-58-7	53
3	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	50
4	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
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Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

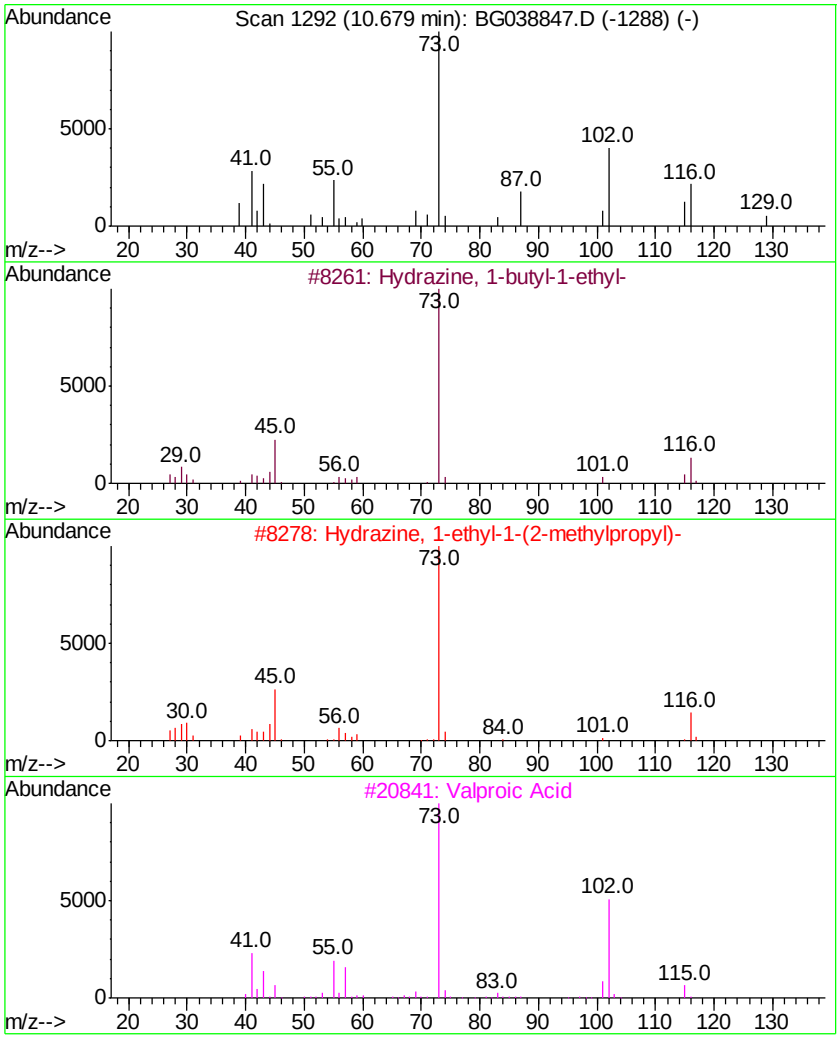
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

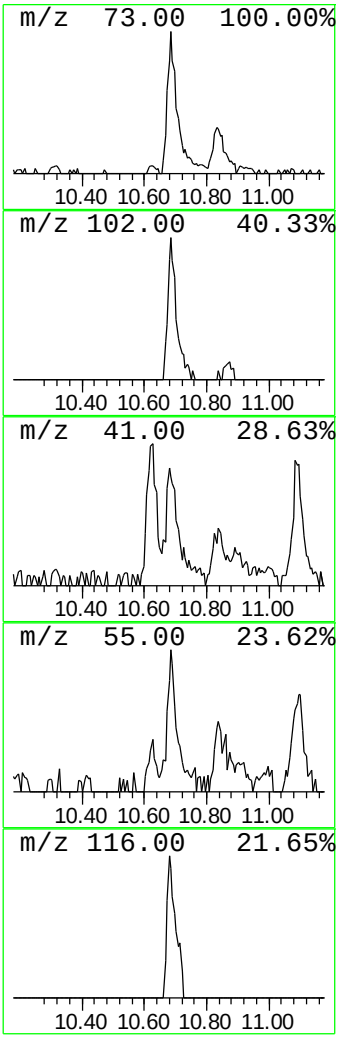
****

Peak Number 8 unknown10.68 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	3.98 ng	50540	Naphthalene-d8	10.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1-butyl-1-ethyl-	116	C6H16N2	052728-56-0	46
2	Hydrazine, 1-ethyl-1-(2-methylpr...	116	C6H16N2	067398-35-0	35
3	Valproic Acid	144	C8H16O2	000099-66-1	23
4	Urea, butyl-	116	C5H12N2O	000592-31-4	12
5	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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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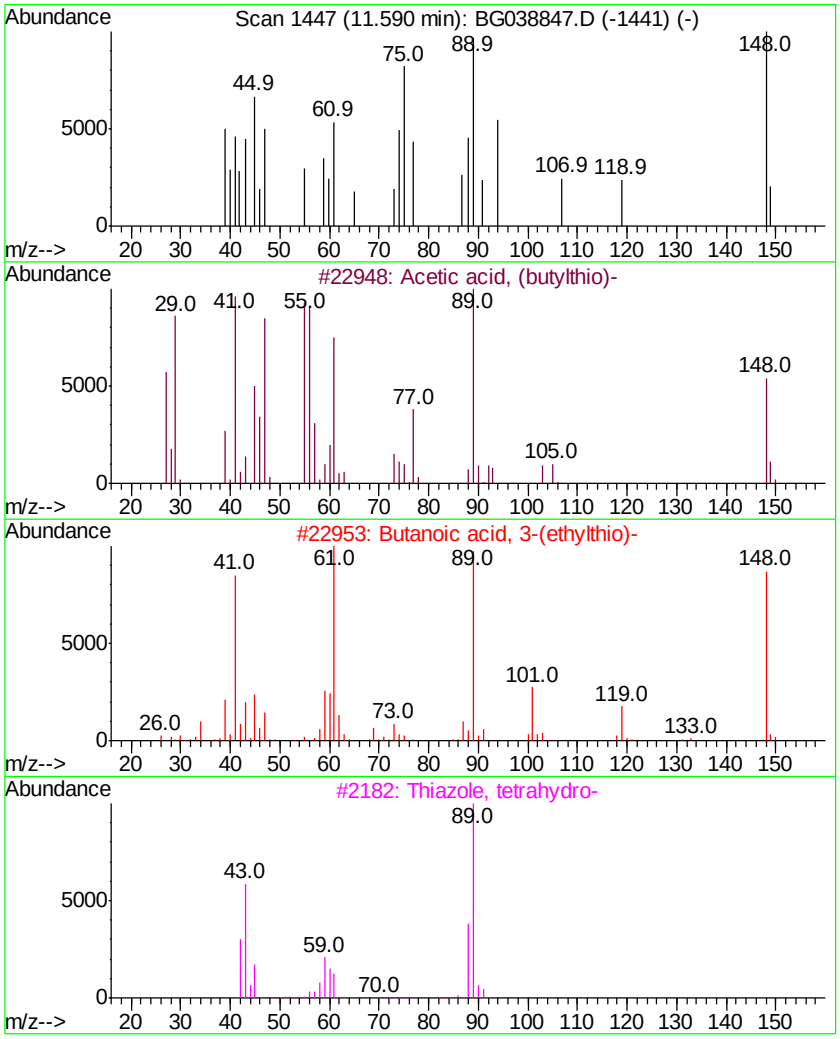
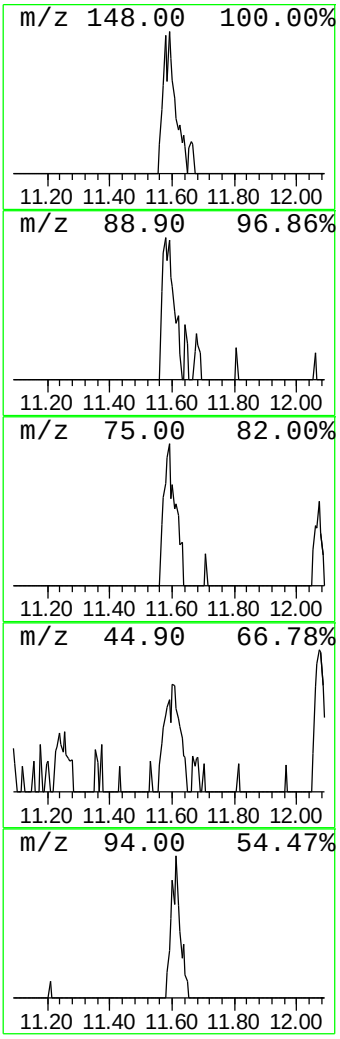
Peak Number 9 Acetic acid, (butylthio)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	2.17 ng	27560	Naphthalene-d8	10.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, (butylthio)-	148	C6H12O2S	020600-61-7	53
2	Butanoic acid, 3-(ethylthio)-	148	C6H12O2S	089534-40-7	47
3	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	43
4	2-Diisopropylsilyloxypropane	174	C9H22OSi	119968-53-5	25
5	1-Dimethyl(isopropyl)silyloxypen...	188	C10H24OSi	1000278-82-0	25





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Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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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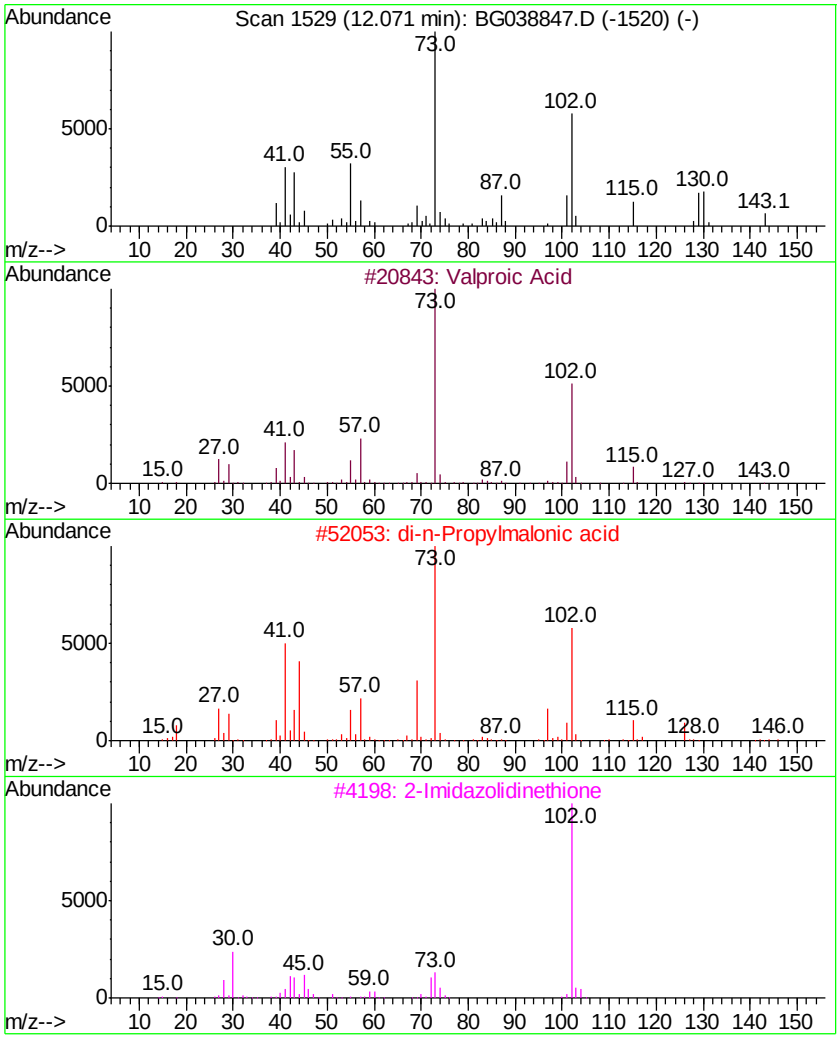
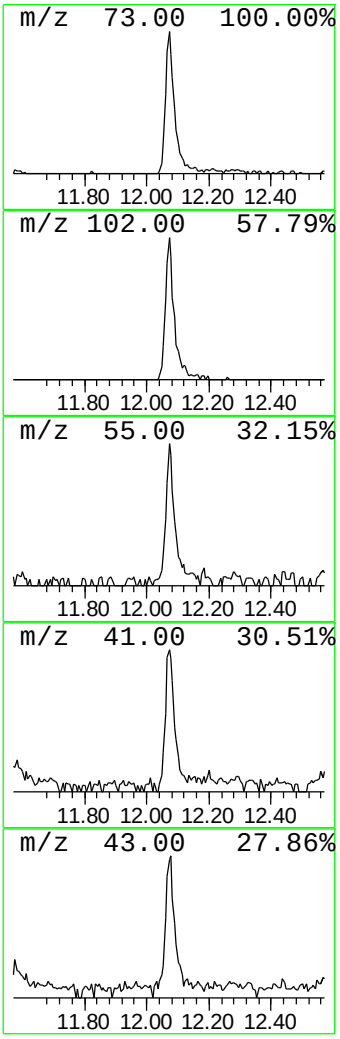
Peak Number 10 Valproic Acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	8.42 ng	106903	Naphthalene-d8	10.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Valproic Acid	144	C8H16O2	000099-66-1	53
2	di-n-Propylmalonic acid	188	C9H16O4	001636-27-7	50
3	2-Imidazolidinethione	102	C3H6N2S	000096-45-7	27
4	Aziridine-2-carbothioamide	102	C3H6N2S	1000189-98-7	23
5	N,N-Dimethyltrimethylsilamine	117	C5H15NSi	002083-91-2	16





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Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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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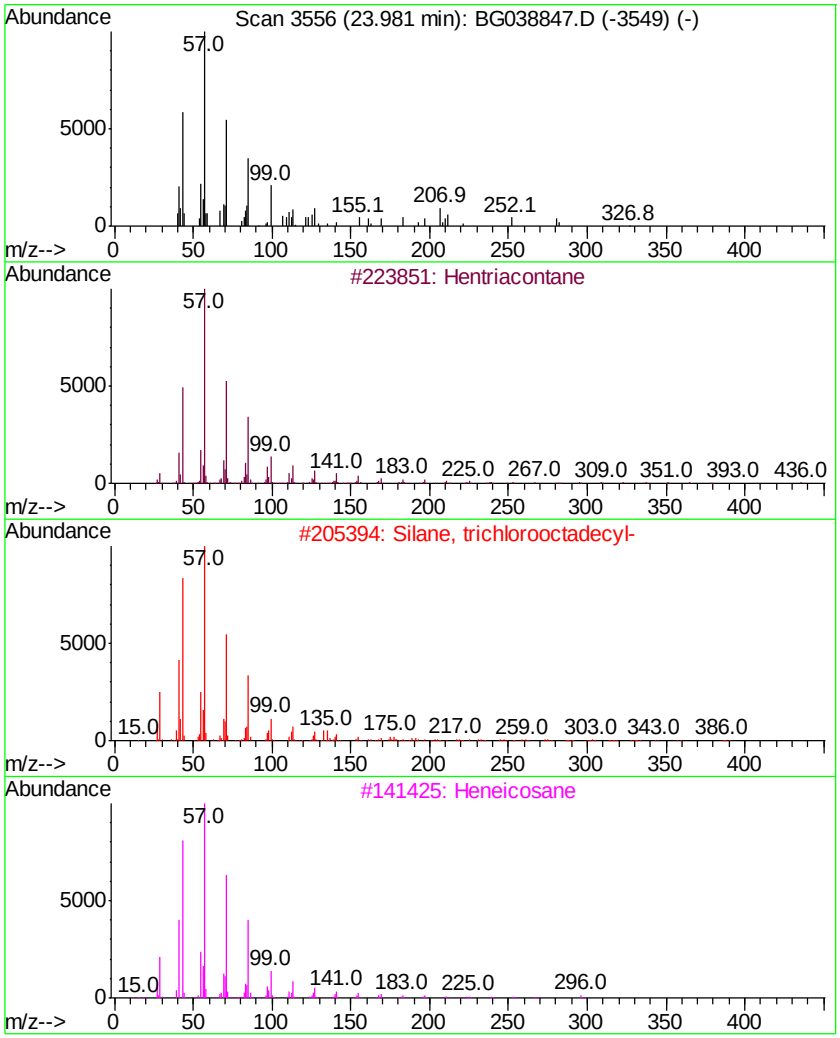
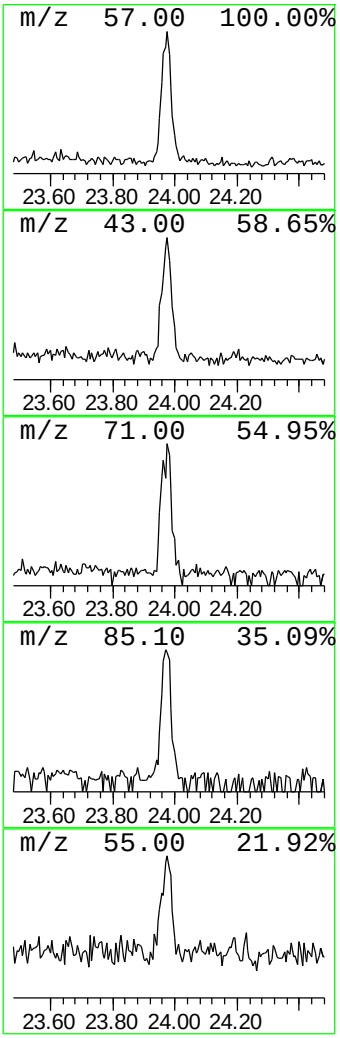
Peak Number 11 Hentriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.98	2.09 ng	54696	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	80
2	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	80
3	Heneicosane	296	C21H44	000629-94-7	80
4	Heptadecane	240	C17H36	000629-78-7	72
5	Hexacosane	366	C26H54	000630-01-3	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG122718\
Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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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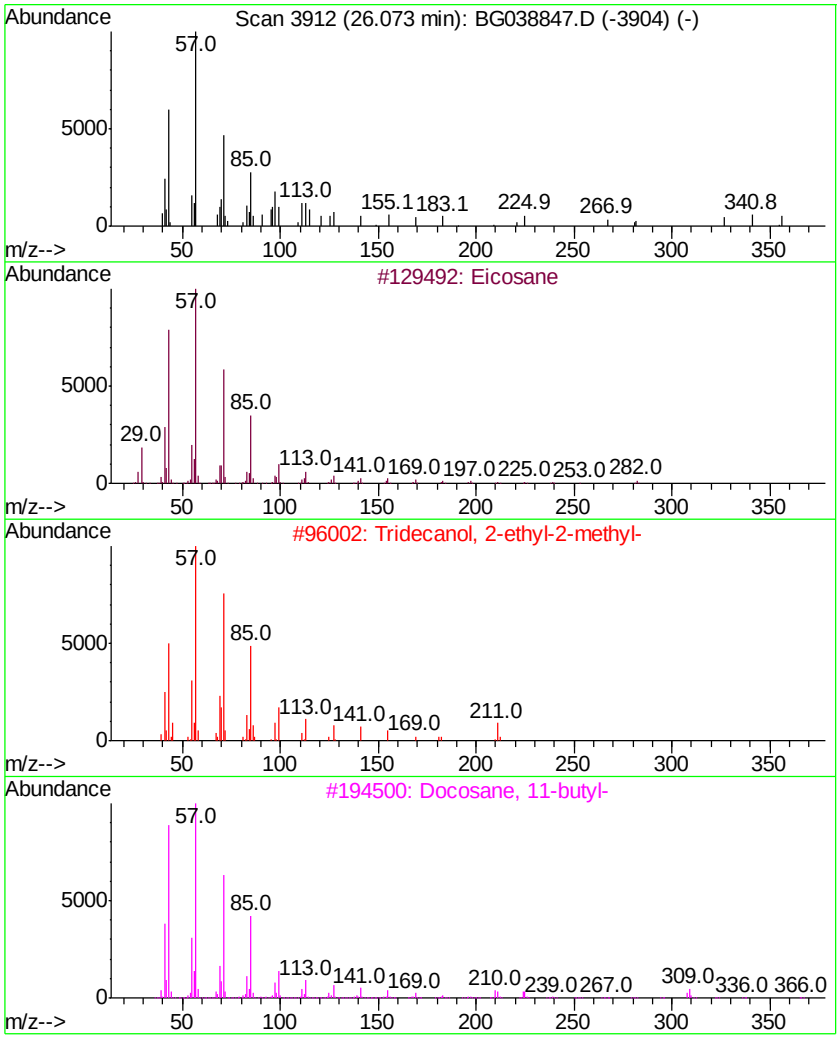
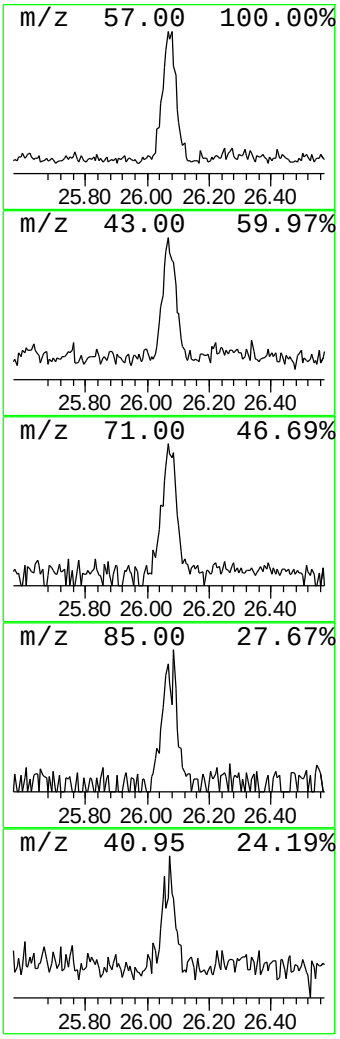
Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.07	2.09 ng	54673	Perylene-d12	25.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	60
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	58
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	58
4	Hentriacontane	437	C31H64	000630-04-6	58
5	Docosane, 11-decyl-	451	C32H66	055401-55-3	58





Tentatively Identified Compound (LSC) summary

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Data File : BG038847.D
Acq On : 27 Dec 2018 17:22
Operator : JU/SJ
Sample : J6533-07
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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-methoxy...	3.18	6.9	ng	49395	1	8.05	143498	20.0
unknown5.14	5.14	4.5	ng	32349	1	8.05	143498	20.0
unknown7.58	7.58	103.4	ng	741655	1	8.05	143498	20.0
Hexanoic acid, 2-...	9.40	57.0	ng	409188	1	8.05	143498	20.0
unknown10.07	10.07	2.5	ng	31915	2	10.87	253961	20.0
Ethanol, 2-(2-but...	10.62	4.3	ng	53935	2	10.87	253961	20.0
unknown10.68	10.68	4.0	ng	50540	2	10.87	253961	20.0
Acetic acid, (but...	11.59	2.2	ng	27560	2	10.87	253961	20.0
Valproic Acid	12.07	8.4	ng	106903	2	10.87	253961	20.0
Hentriacontane	23.98	2.1	ng	54696	6	25.01	523746	20.0
Eicosane	26.07	2.1	ng	54673	6	25.01	523746	20.0