LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091620\
Data File : BG046645.D
Acq On : 16 Sep 2020 18:01
Operator : CG/JU
Sample : L4021-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B14-1-3

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-BG082520.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	3.117	3	5	13	rVB	55075	74350	2.23%	0.442%
2	4.439	225	230	245	rVB	274641	384962	11.53%	2.287%
3	4.651	260	266	276	rVB	203229	314473	9.42%	1.868%
4	5.033	325	331	344	rBV	502191	742134	22.22%	4.409%
5	5.509	406	412	426	rBV	185762	303702	9.09%	1.804%
6	7.095	674	682	700	rBV	542505	1006526	30.14%	5.979%
7	7.918	815	822	830	rBV	219085	362594	10.86%	2.154%
8	9.075	1010	1019	1032	rBV	447047	821910	24.61%	4.882%
9	10.714	1291	1298	1312	rBV	290549	549679	16.46%	3.265%
10	13.170	1709	1716	1734	rBV	1342096	2155751	64.55%	12.806%
11	14.005	1852	1858	1869	rBV	84304	140261	4.20%	0.833%
12	14.551	1944	1951	1959	rBV	523407	805612	24.12%	4.786%
13	15.286	2071	2076	2084	rBV	95007	143124	4.29%	0.850%
14	16.043	2200	2205	2213	rBV3	32481	55775	1.67%	0.331%
15	17.295	2411	2418	2422	rBV	649180	979558	29.33%	5.819%
16	17.336	2422	2425	2432	rVB	126487	178877	5.36%	1.063%
17	18.170	2561	2567	2571	rBV	31905	51543	1.54%	0.306%
18	18.217	2571	2575	2580	rVB	33901	52819	1.58%	0.314%
19	18.358	2593	2599	2604	rBV2	39228	73875	2.21%	0.439%
20	18.400	2604	2606	2612	rVB2	26402	34714	1.04%	0.206%
21	19.228	2743	2747	2753	rVB2	20642	38458	1.15%	0.228%
22	19.345	2762	2767	2774	rVB	216893	306811	9.19%	1.823%
23	19.710	2819	2829	2838	rBV	226148	407356	12.20%	2.420%
24	19.910	2853	2863	2869	rBV	2509229	3339685	100.00%	19.839%
25	20.203	2902	2913	2922	rBV3	38097	118834	3.56%	0.706%
26	20.356	2936	2939	2944	rVB2	26715	36109	1.08%	0.215%
27	20.503	2960	2964	2967	rBV	20827	34188	1.02%	0.203%
28	21.202	3079	3083	3092	rVB3	191269	298882	8.95%	1.775%
29	21.543	3133	3141	3146	rBV	702538	1331725	39.88%	7.911%
30	21.584	3146	3148	3158	rVB	115102	170202	5.10%	1.011%
31	23.170	3415	3418	3424	rVB2	37772	66908	2.00%	0.397%
32	23.658	3495	3501	3508	rBV3	72881	208893	6.25%	1.241%
33	24.486	3636	3642	3650	rVB	57868	128180	3.84%	0.761%
34	24.633	3658	3667	3677	rBV2	398801	1115392	33.40%	6.626%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091620\
Data File : BG046645.D
Acq On : 16 Sep 2020 18:01
Operator : CG/JU
Sample : L4021-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B14-1-3

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-BG082520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

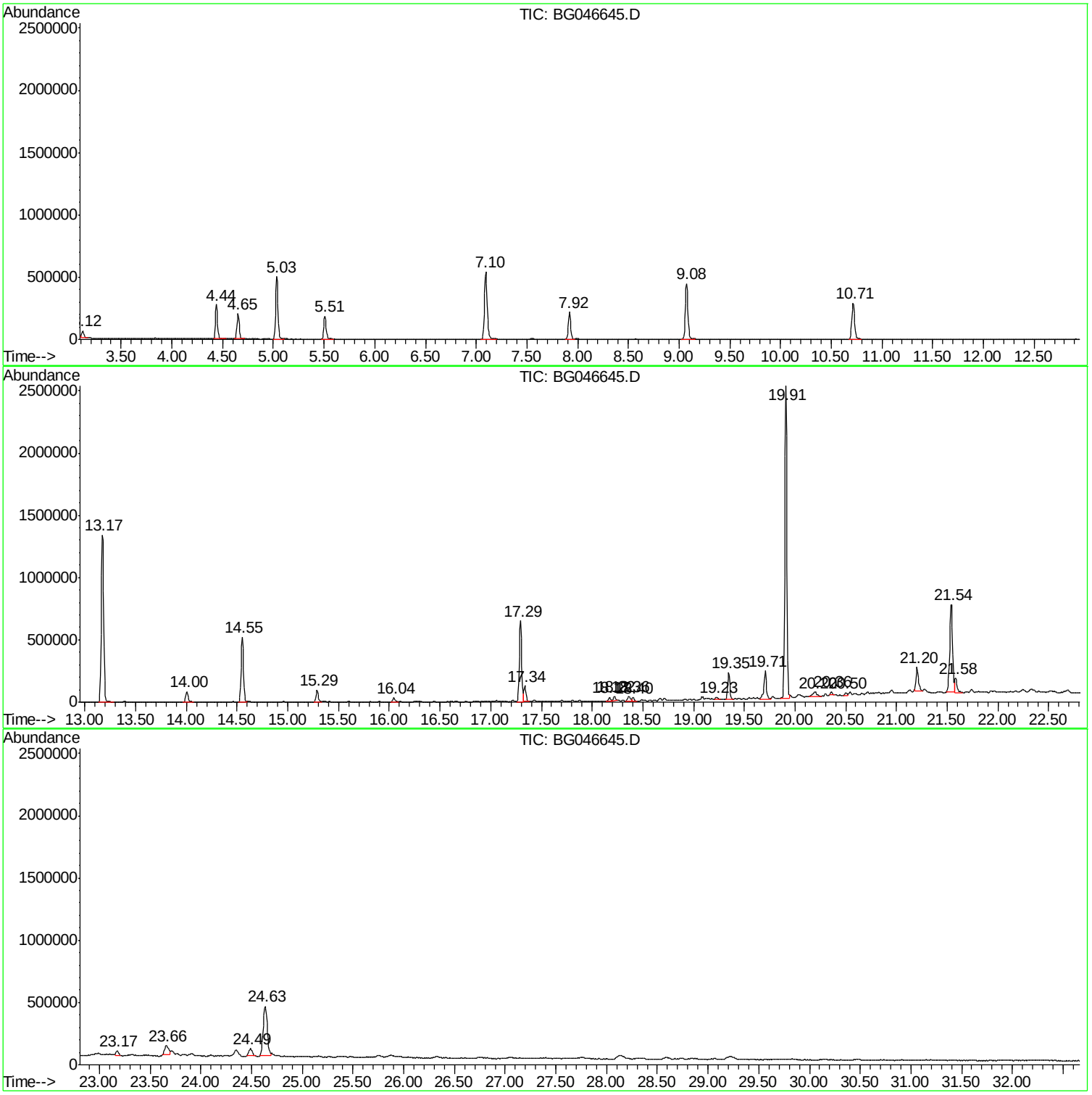
Sum of corrected areas: 16833862

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091620\
Data File : BG046645.D
Acq On : 16 Sep 2020 18:01
Operator : CG/JU
Sample : L4021-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B14-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082520.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\BG091620\
Data File : BG046645.D
Acq On : 16 Sep 2020 18:01
Operator : CG/JU
Sample : L4021-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B14-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

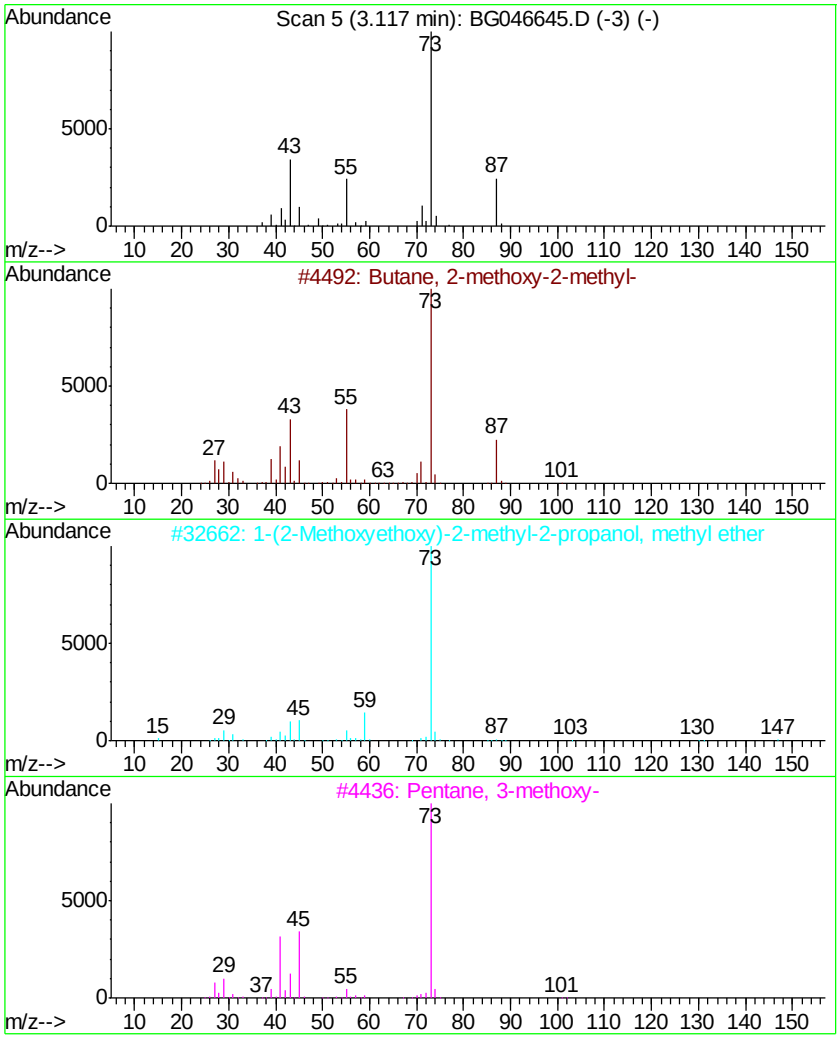
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

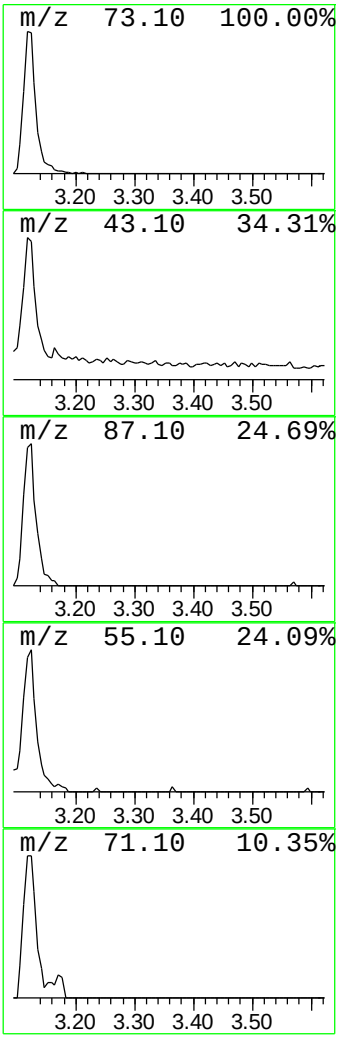
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	4.10 ng	74350	1,4-Dichlorobenzene-d4	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	25
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091620\
Data File : BG046645.D
Acq On : 16 Sep 2020 18:01
Operator : CG/JU
Sample : L4021-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B14-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

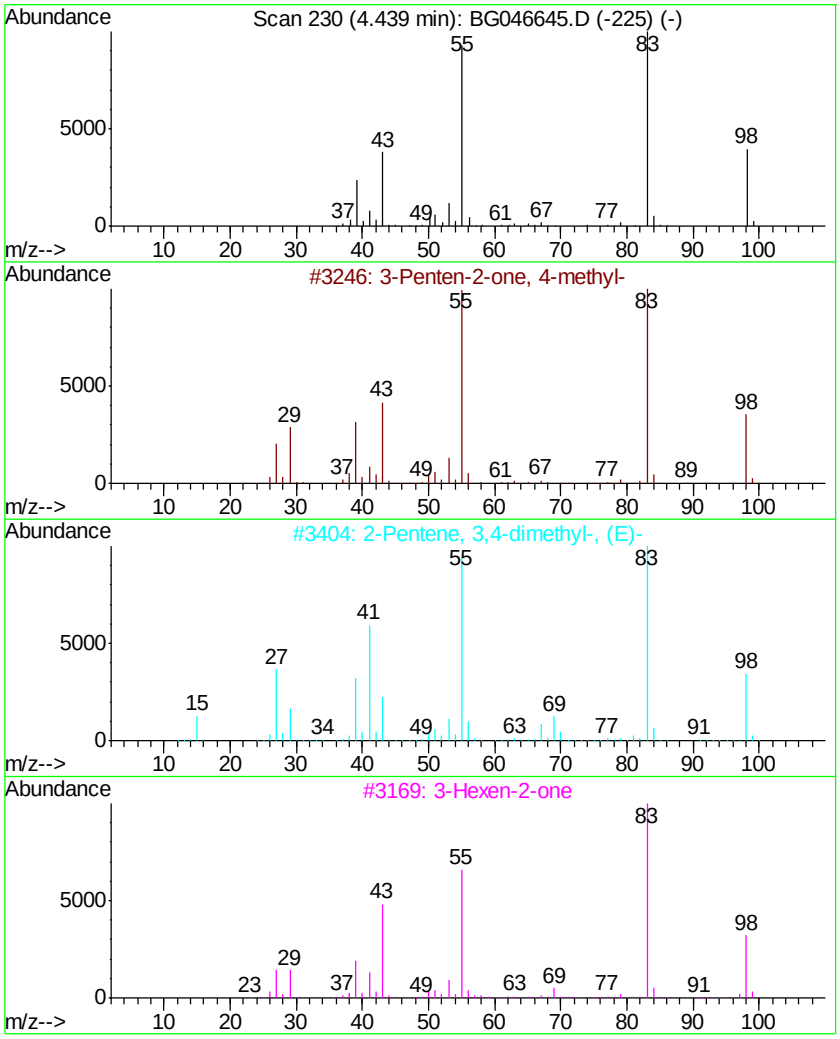
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

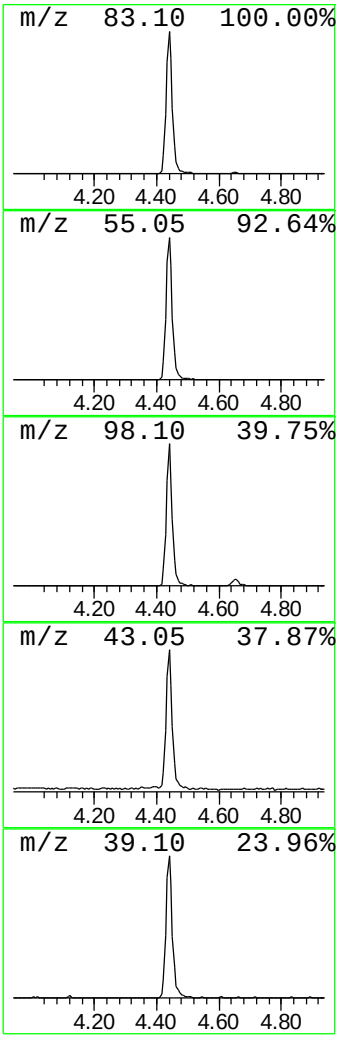
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.44	21.23 ng	384962	1,4-Dichlorobenzene-d4	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	90
4	Cyclohexane, methyl-	98	C7H14	000108-87-2	80
5	2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	78





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091620\
Data File : BG046645.D
Acq On : 16 Sep 2020 18:01
Operator : CG/JU
Sample : L4021-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B14-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

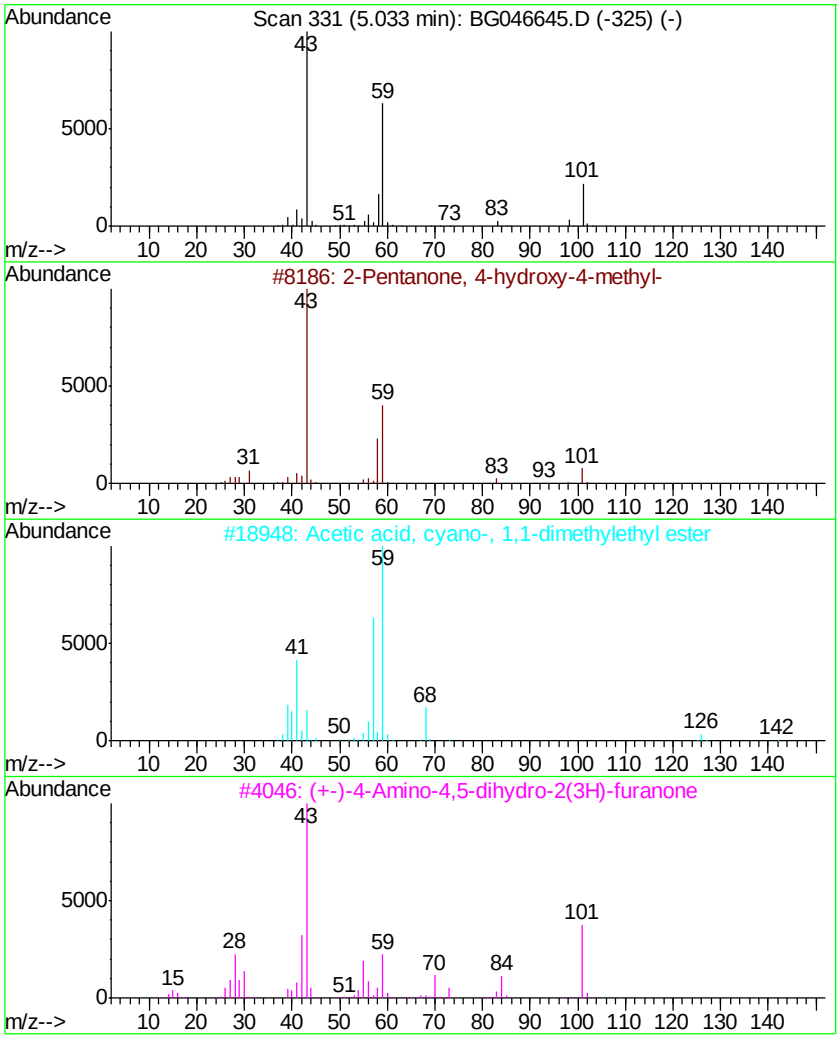
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

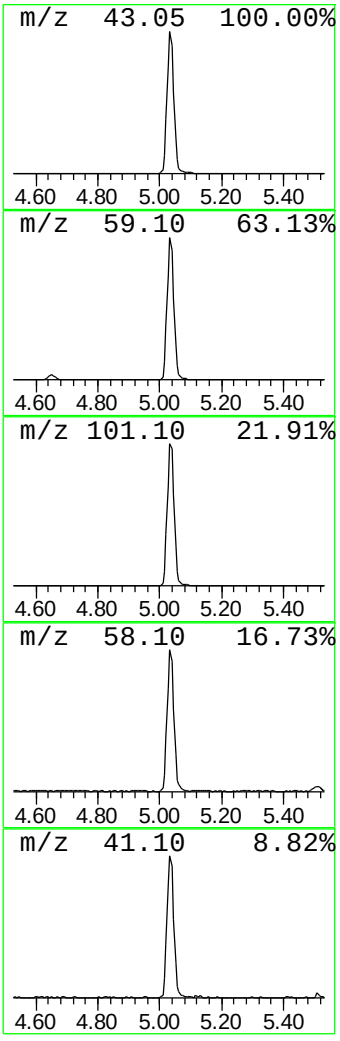
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	40.93 ng	742134	1,4-Dichlorobenzene-d4	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091620\
Data File : BG046645.D
Acq On : 16 Sep 2020 18:01
Operator : CG/JU
Sample : L4021-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B14-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

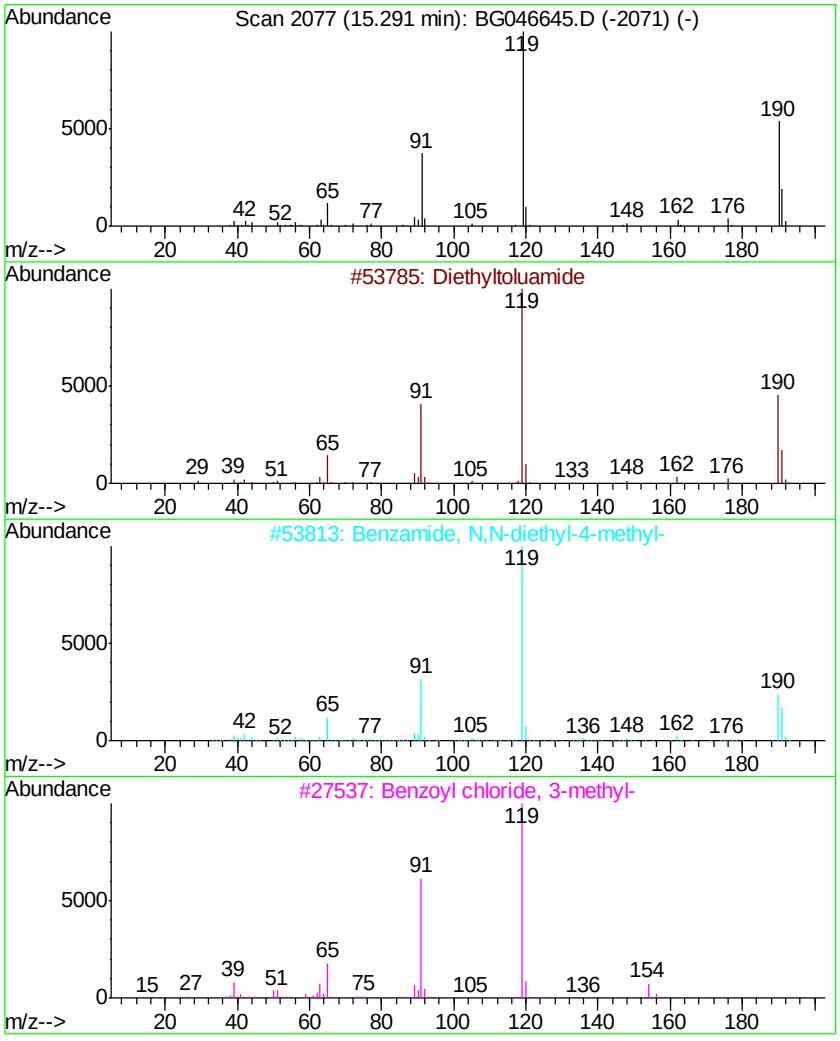
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

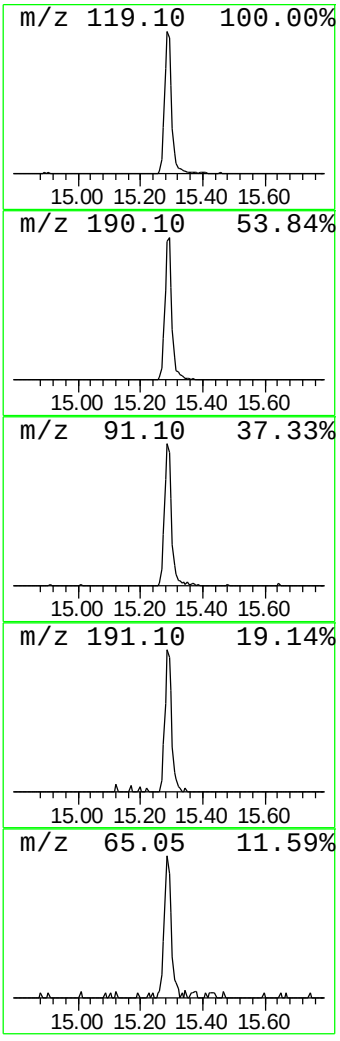
****

Peak Number 5 Diethyltoluamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	3.55 ng	143124	Acenaphthene-d10	14.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	87
3	Benzoyl chloride, 3-methyl-	154	C8H7ClO	001711-06-4	47
4	o-Toluic acid, 4-nitrophenyl ester	257	C14H11NO4	1000307-46-0	47
5	Benzoic acid, 3-methyl-, methyl ...	150	C9H10O2	000099-36-5	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091620\
Data File : BG046645.D
Acq On : 16 Sep 2020 18:01
Operator : CG/JU
Sample : L4021-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B14-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

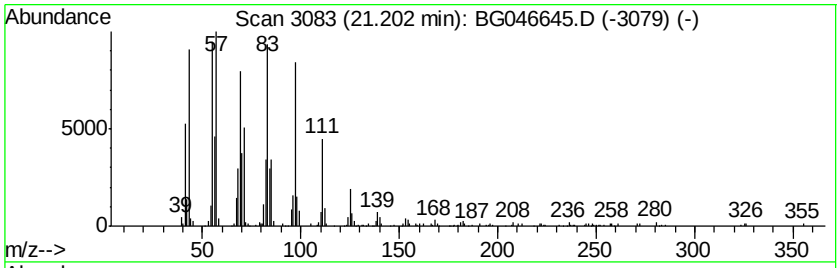
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

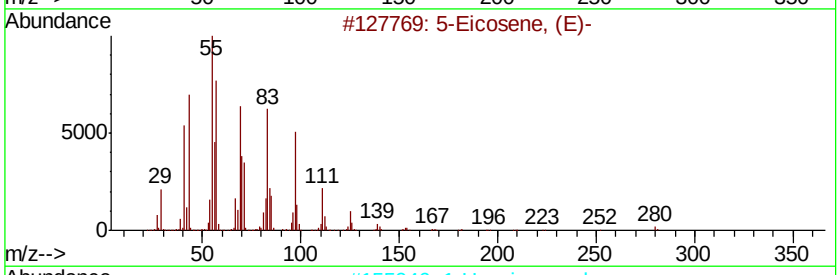
****

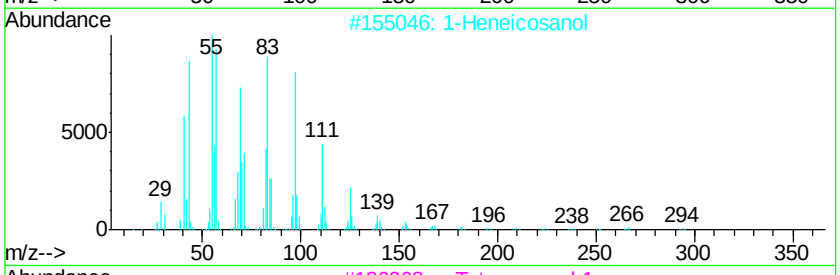
Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

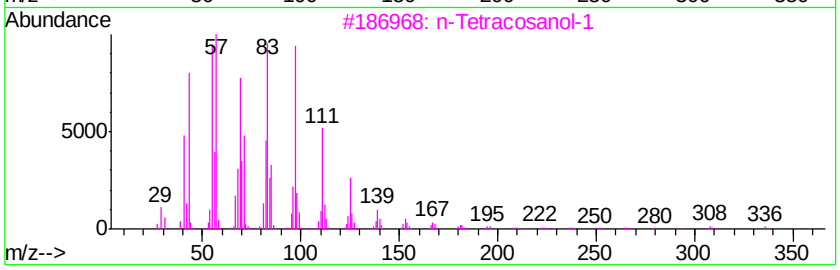
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.20	4.49 ng	298882	Chrysene-d12	21.54

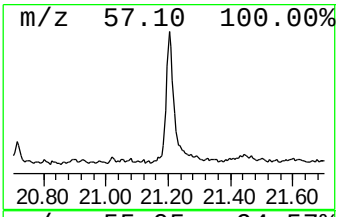
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93

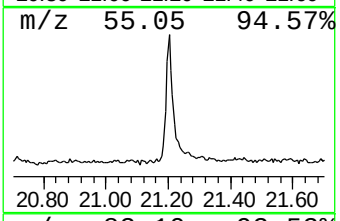


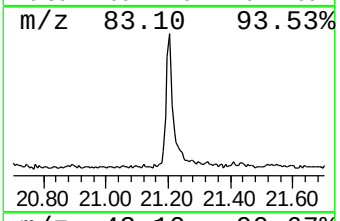


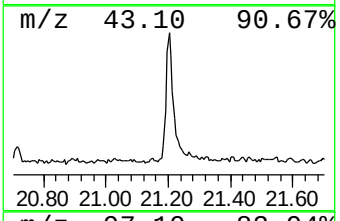


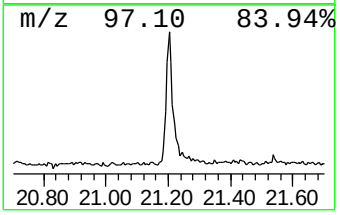












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG091620\
Data File : BG046645.D
Acq On : 16 Sep 2020 18:01
Operator : CG/JU
Sample : L4021-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B14-1-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082520.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...	3.12	4.1	ng	74350	1	7.92	362594	20.0
3-Penten-2-one, 4...	4.44	21.2	ng	384962	1	7.92	362594	20.0
2-Pentanone, 4-hy...	5.03	40.9	ng	742134	1	7.92	362594	20.0
Diethyltoluamide	15.29	3.5	ng	143124	3	14.55	805612	20.0
5-Eicosene, (E)-	21.20	4.5	ng	298882	5	21.54	1331730	20.0