LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG121517\
Data File : BG031607.D
Acq On : 16 Dec 2017 3:06
Operator : SJ/JU
Sample : I6884-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-20171211

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:\HPCHEM1\BNA_G\METHODS\8270-BG121117.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	4.560	210	216	231	rVB	340151	544319	7.93%	2.058%
2	5.177	313	321	334	rBV	1739122	2719140	39.59%	10.279%
3	5.659	397	403	427	rBV	325766	672768	9.80%	2.543%
4	7.269	670	677	688	rBV	320547	621014	9.04%	2.348%
5	7.633	732	739	757	rBV	623738	1277469	18.60%	4.829%
6	8.097	811	818	828	rBV	228364	400546	5.83%	1.514%
7	8.420	866	873	883	rBV	888588	1581362	23.03%	5.978%
8	8.514	883	889	896	rVB3	53650	93432	1.36%	0.353%
9	8.749	922	929	940	rBV	96644	186398	2.71%	0.705%
10	9.266	1009	1017	1038	rBV	613957	1198985	17.46%	4.533%
11	10.912	1288	1297	1304	rBV	289329	601720	8.76%	2.275%
12	10.964	1304	1306	1317	rVB2	51206	94850	1.38%	0.359%
13	13.344	1704	1711	1733	rBV	2222190	3608720	52.55%	13.642%
14	14.725	1939	1946	1959	rBV2	515099	932362	13.58%	3.525%
15	16.229	2196	2202	2216	rBV2	97596	260922	3.80%	0.986%
16	17.469	2403	2413	2427	rBV2	795855	1378982	20.08%	5.213%
17	19.690	2785	2791	2804	rBV	194371	358463	5.22%	1.355%
18	20.060	2848	2854	2867	rBV	4994539	6867763	100.00%	25.963%
19	21.740	3132	3140	3156	rBV2	906735	1667415	24.28%	6.304%
20	25.019	3686	3698	3720	rBV2	454928	1385575	20.18%	5.238%

Sum of corrected areas: 26452205

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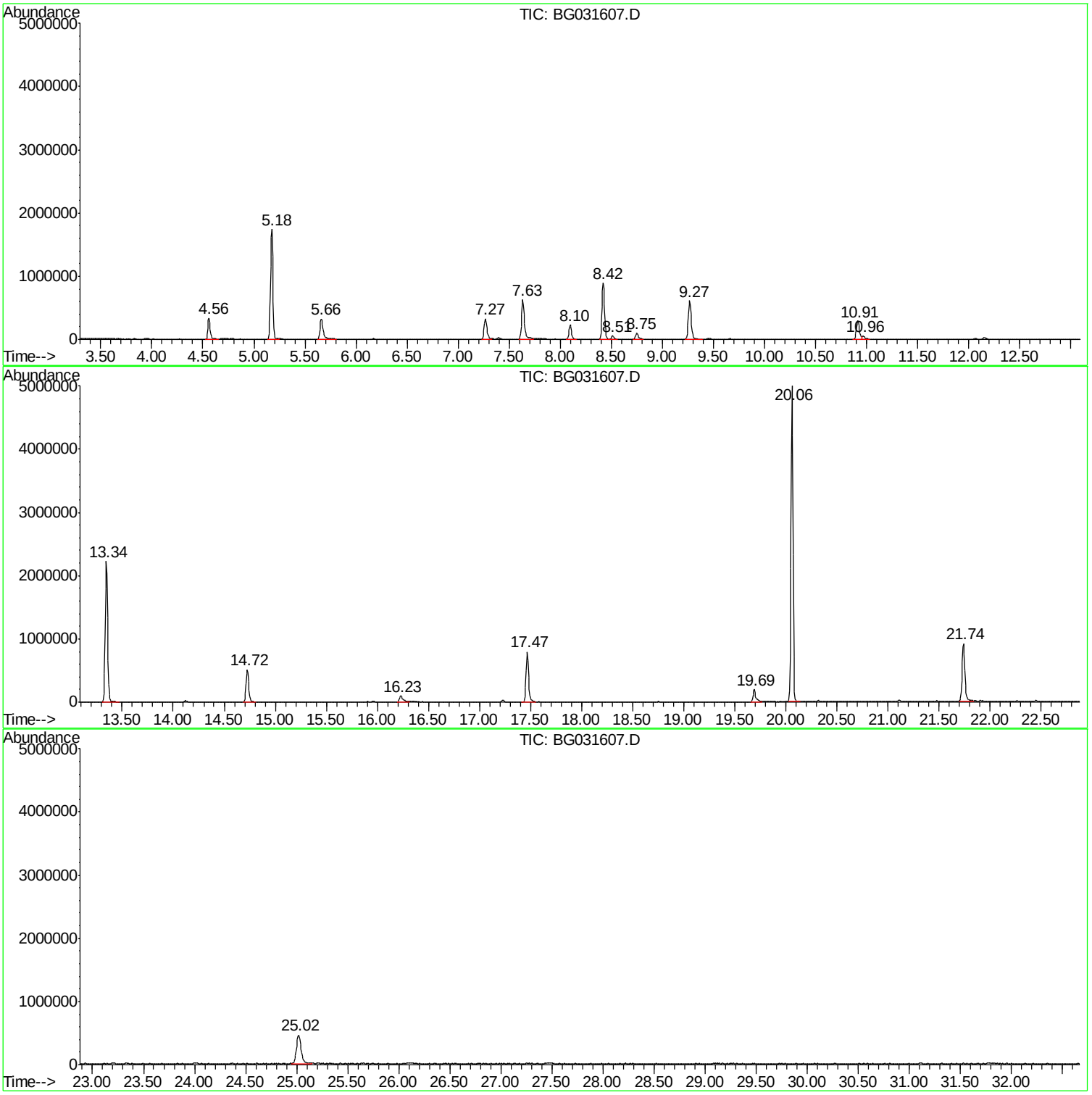
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-20171211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG121117.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

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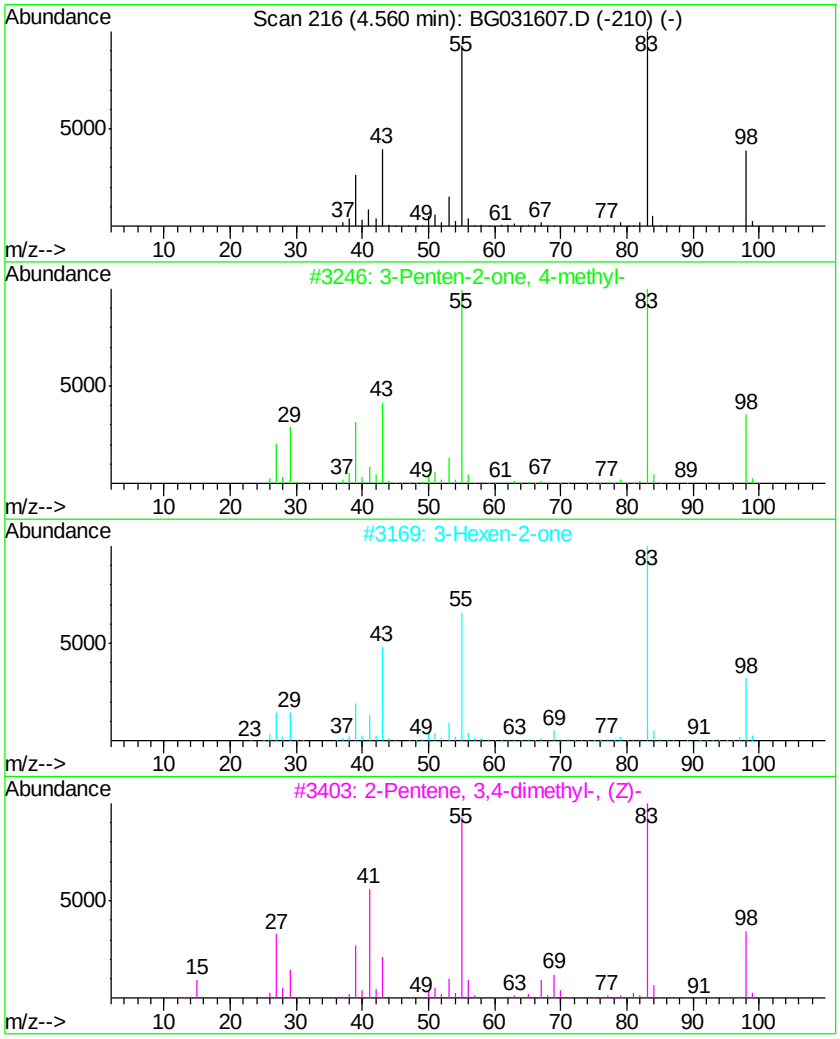
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

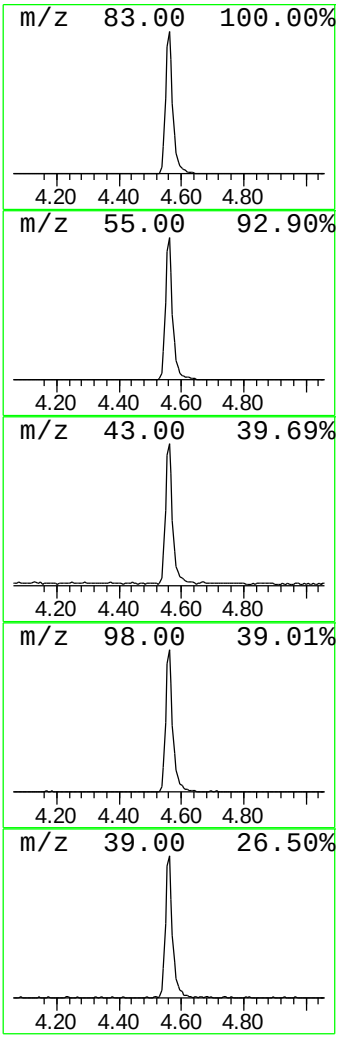
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	27.18 ng	544319	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





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Data File : BG031607.D
Acq On : 16 Dec 2017 3:06
Operator : SJ/JU
Sample : I6884-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-20171211

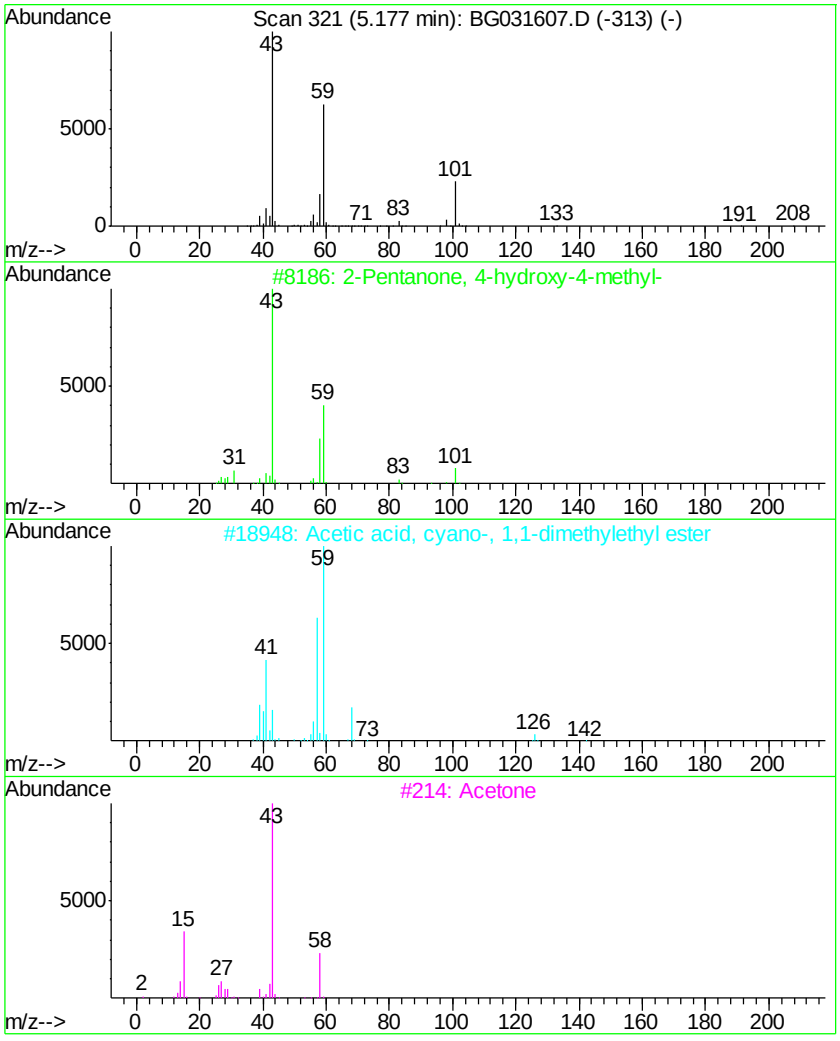
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG121117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

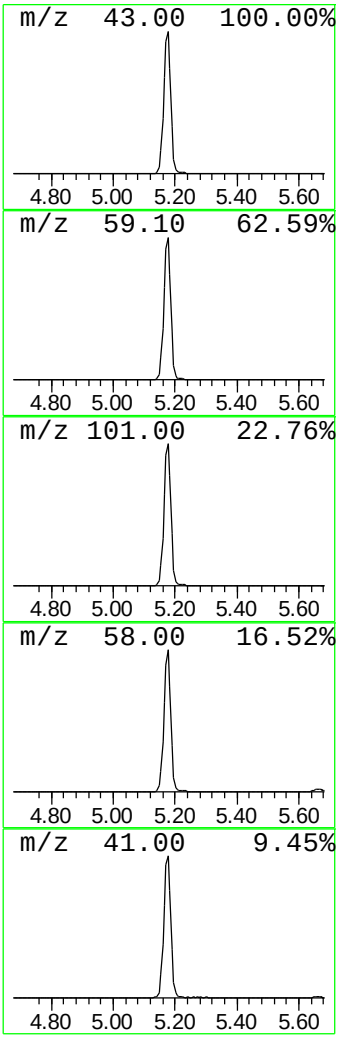
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	135.77 ng	2719140	1,4-Dichlorobenzene-d4	8.10

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	25
3	Acetone	58	C3H6O	000067-64-1	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Acq On : 16 Dec 2017 3:06
Operator : SJ/JU
Sample : I6884-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-20171211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG121117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

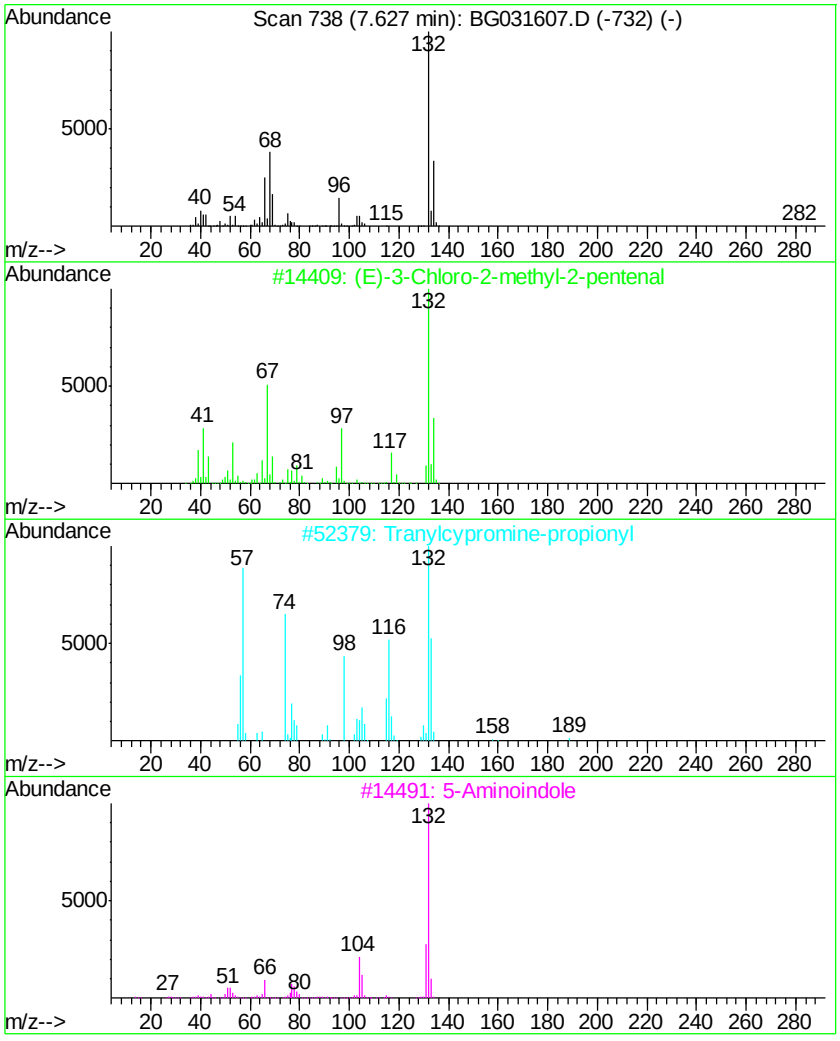
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

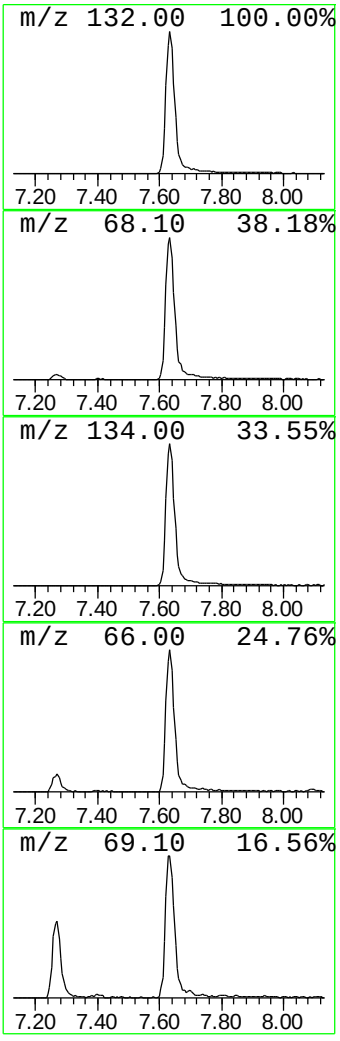
****

Peak Number 3 unknown7.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	63.79 ng	1277470	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : I6884-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-20171211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG121117.M
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TIC Library : C:\Database\NIST11.L
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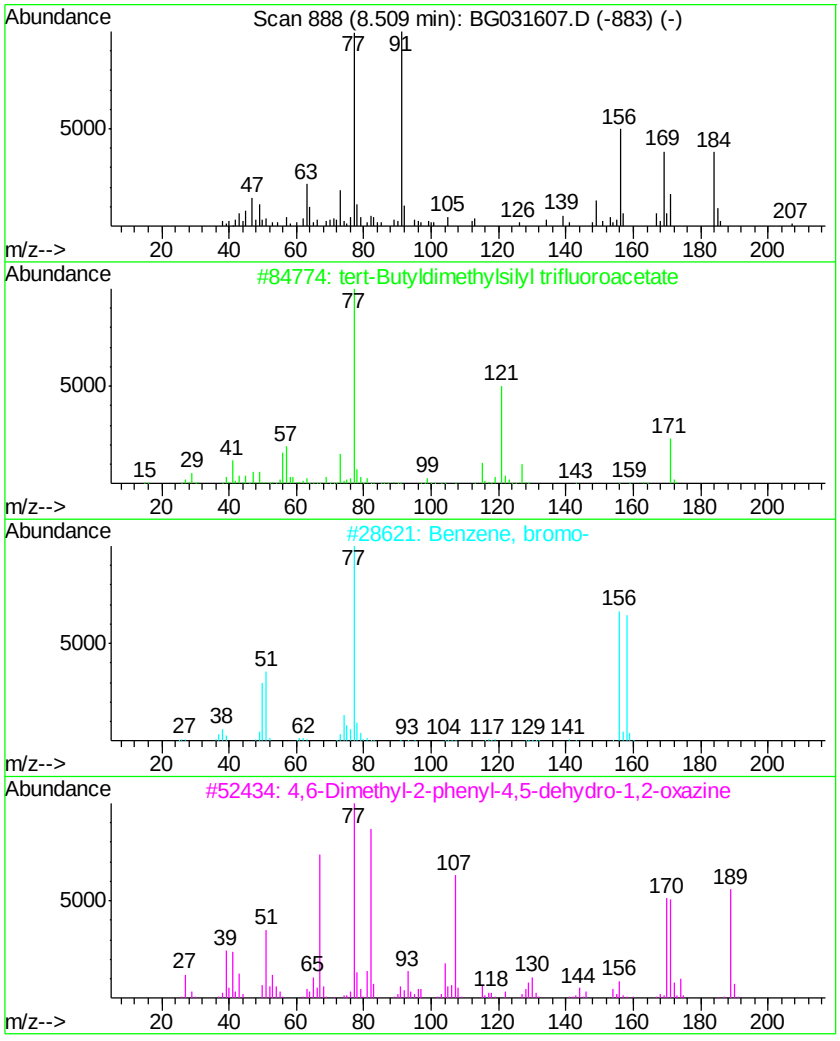
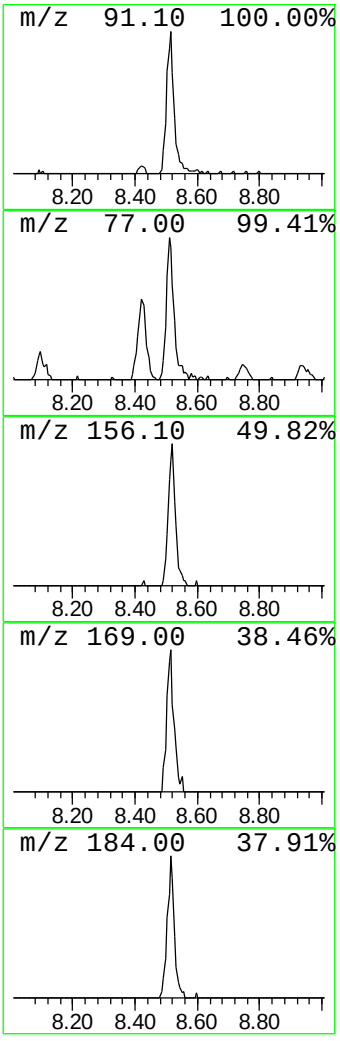
Peak Number 5 unknown8.51 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.51	4.67 ng	93432	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	tert-Butyldimethylsilyl trifluor...	228	C8H15F3O2Si	1000366-60-3	38
2	Benzene, bromo-	156	C6H5Br	000108-86-1	35
3	4,6-Dimethyl-2-phenyl-4,5-dehydr...	189	C12H15NO	177420-38-1	16
4	tert-Butyldimethylfluorosilane	134	C6H15FSi	1000366-62-3	16
5	Trimethylsilyl trifluoroacetate	186	C5H9F3O2Si	000400-53-3	16





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG121517\
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Operator : SJ/JU
Sample : I6884-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-20171211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG121117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

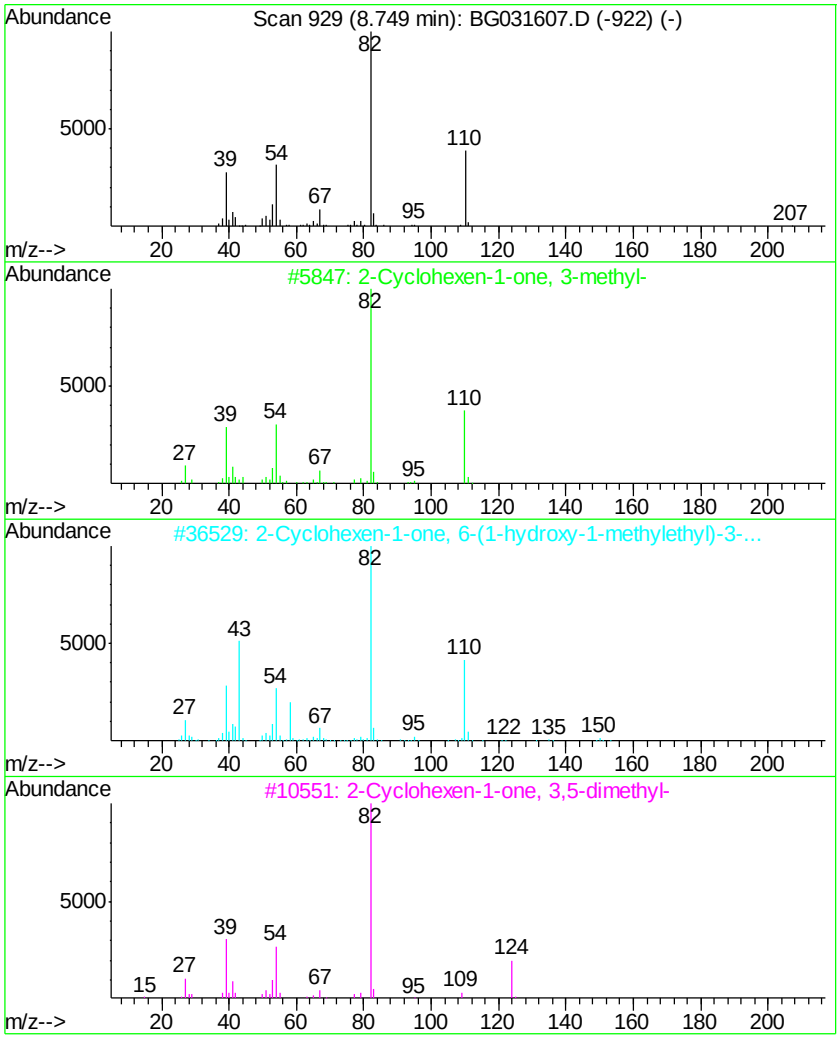
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

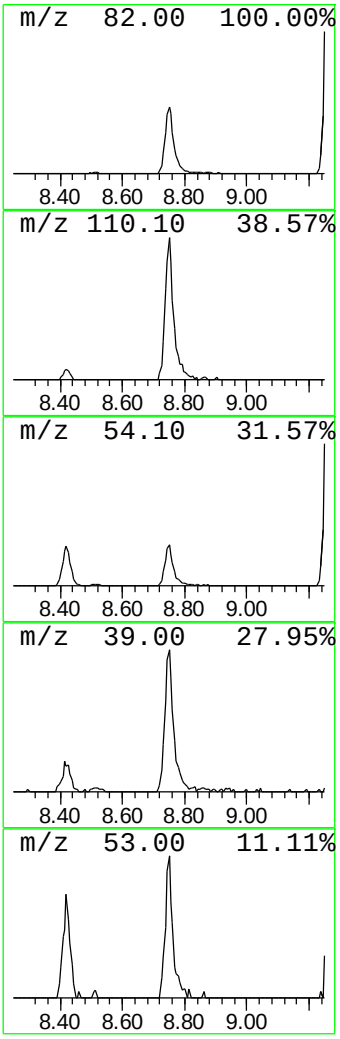
****

Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.75	9.31 ng	186398	1,4-Dichlorobenzene-d4	8.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	64
3	2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	59
4	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	53
5	1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	38





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ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FB-20171211

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG121117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

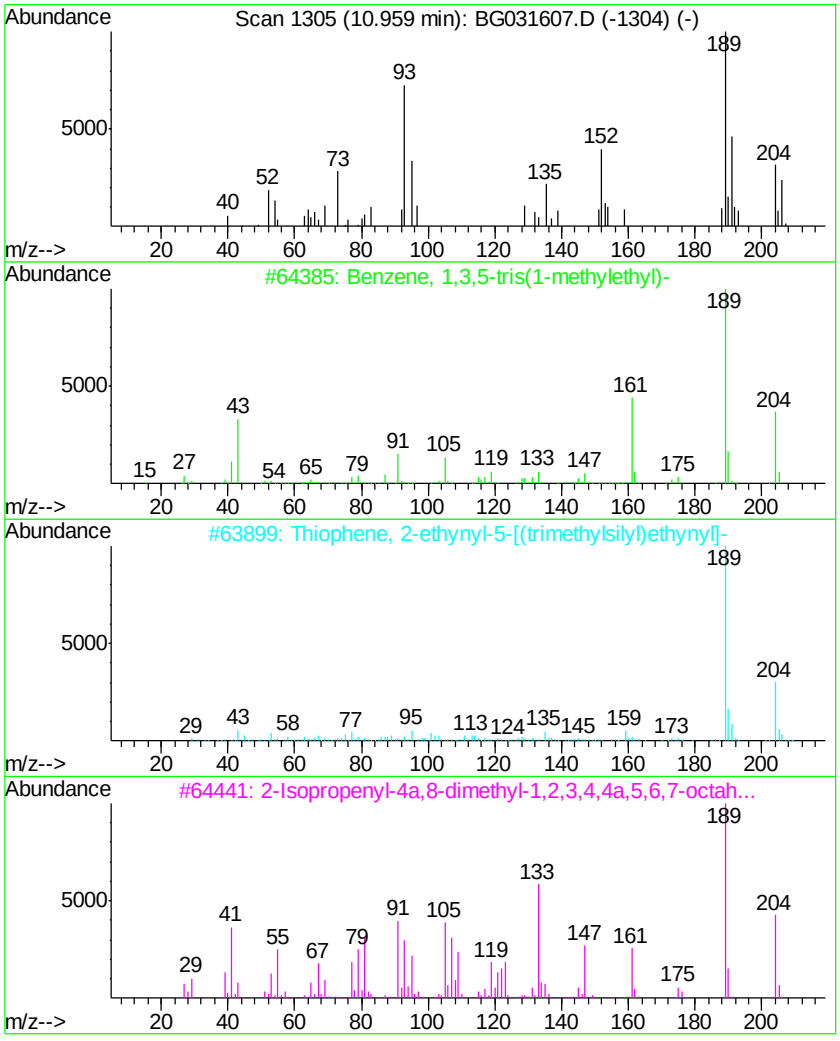
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

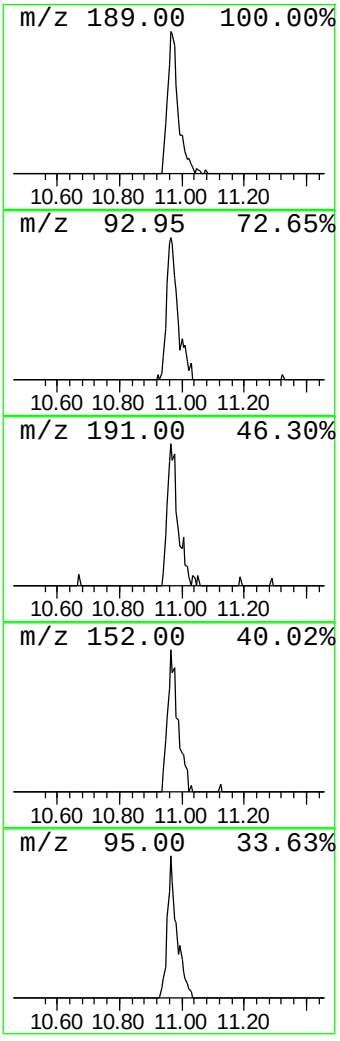
****

Peak Number 7 unknown10.96 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	3.15 ng	94850	Naphthalene-d8	10.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3,5-tris(1-methylethyl)-	204	C15H24	000717-74-8	25
2	Thiophene, 2-ethynyl-5-[(trimeth...	204	C11H12SSi	182323-29-1	25
3	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000192-43-5	23
4	3-Acetyl-2,5-dimethylbenzo(b)thi...	204	C12H12OS	006179-04-0	17
5	1,3,4-Thiadiazole, 2-isopropyl-5...	204	C11H12N2S	050834-84-9	17





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.56	27.2	ng	544319	1	8.10	400546	20.0
2-Pentanone, 4-hy...	5.18	135.8	ng	2719140	1	8.10	400546	20.0
unknown7.63	7.63	63.8	ng	1277470	1	8.10	400546	20.0
unknown8.51	8.51	4.7	ng	93432	1	8.10	400546	20.0
2-Cyclohexen-1-on...	8.75	9.3	ng	186398	1	8.10	400546	20.0
unknown10.96	10.96	3.1	ng	94850	2	10.91	601720	20.0