LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060517\
Data File : BG027232.D
Acq On : 6 Jun 2017 3:46
Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

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-BG060517.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	3.982	10	50	53	rBV2	430174	2905187	6.58%	2.142%
2	4.470	112	133	136	rBV	194193	811527	1.84%	0.598%
3	5.439	175	298	301	rVB	2320507	44119549	100.00%	32.524%
4	5.886	336	374	377	rBV	1039207	7268837	16.48%	5.358%
5	6.039	377	400	403	rVB	804797	4012671	9.09%	2.958%
6	6.156	413	420	427	rBV	625869	1124049	2.55%	0.829%
7	6.362	427	455	458	rVV	548801	2851073	6.46%	2.102%
8	7.684	652	680	682	rBV	348754	1634879	3.71%	1.205%
9	7.719	682	686	697	rVB2	453745	962514	2.18%	0.710%
10	8.113	744	753	763	rVB	1068989	2100578	4.76%	1.548%
11	8.900	879	887	895	rBV	845844	1580137	3.58%	1.165%
12	9.311	914	957	969	rBV2	1170389	6365880	14.43%	4.693%
13	9.740	1017	1030	1042	rVB	740018	1457611	3.30%	1.075%
14	10.721	1168	1197	1203	rBV3	419046	2073670	4.70%	1.529%
15	11.391	1303	1311	1317	rVV	319088	628604	1.42%	0.463%
16	12.073	1390	1427	1440	rBV	1526165	9698807	21.98%	7.150%
17	12.519	1495	1503	1511	rBV	361797	670597	1.52%	0.494%
18	13.354	1598	1645	1658	rBV	3380508	25185967	57.09%	18.566%
19	13.783	1711	1718	1726	rVB	2170848	3600287	8.16%	2.654%
20	15.152	1945	1951	1969	rVV2	573908	1187673	2.69%	0.876%
21	16.421	2161	2167	2172	rVV	338588	550598	1.25%	0.406%
22	16.491	2172	2179	2191	rVV	956966	1866826	4.23%	1.376%
23	16.632	2192	2203	2210	rVB2	1992404	3868039	8.77%	2.851%
24	17.901	2412	2419	2425	rBV2	629218	1062116	2.41%	0.783%
25	18.753	2558	2564	2585	rBV	497701	790514	1.79%	0.583%
26	20.011	2773	2778	2791	rBV	412842	663923	1.50%	0.489%
27	20.481	2852	2858	2865	rBV	3056674	4285121	9.71%	3.159%
28	22.290	3159	3166	3177	rVB	597766	1189675	2.70%	0.877%
29	25.998	3787	3797	3812	rVB3	342764	1136864	2.58%	0.838%

Sum of corrected areas: 135653773

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060517\
Data File : BG027232.D
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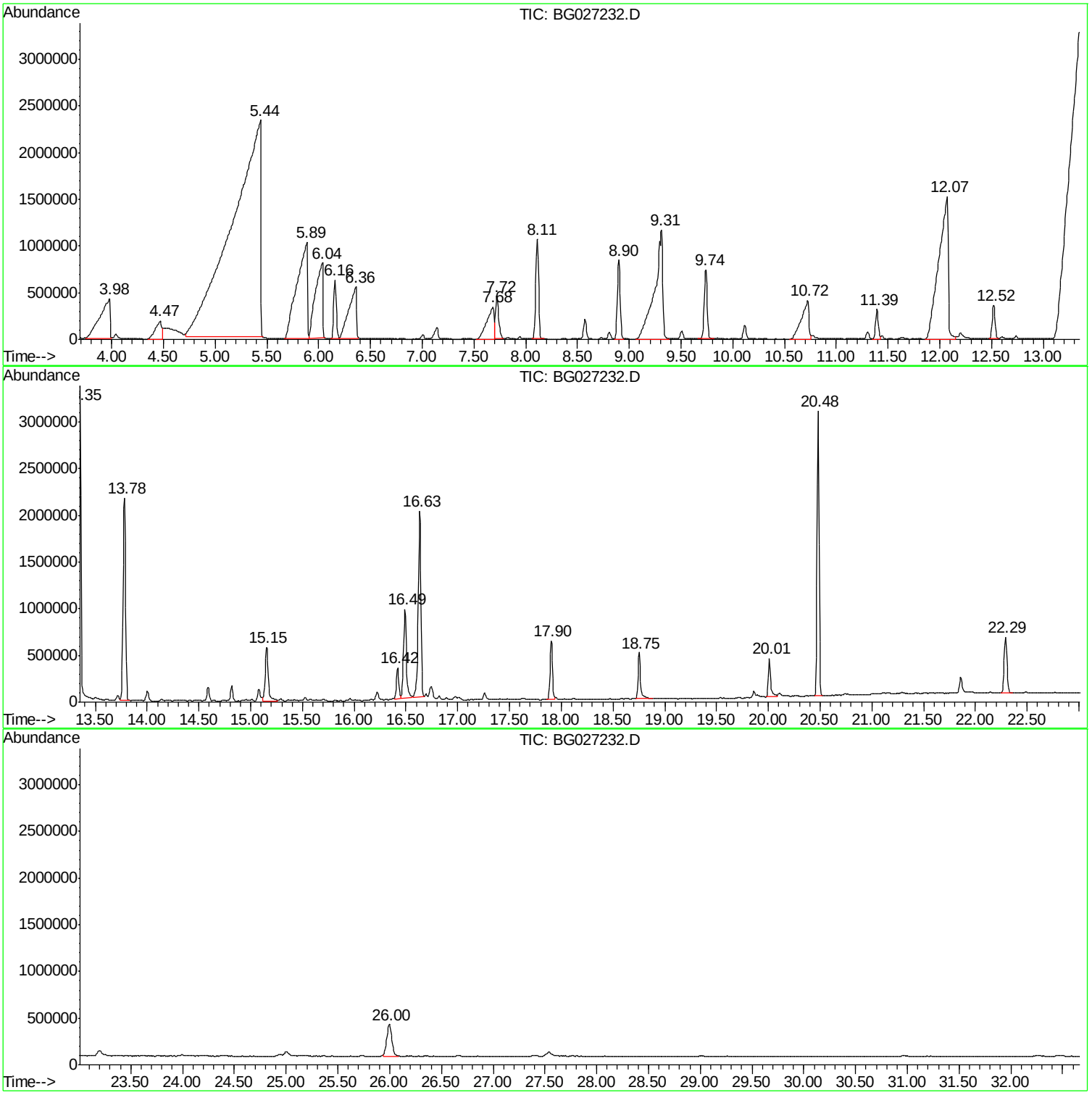
Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.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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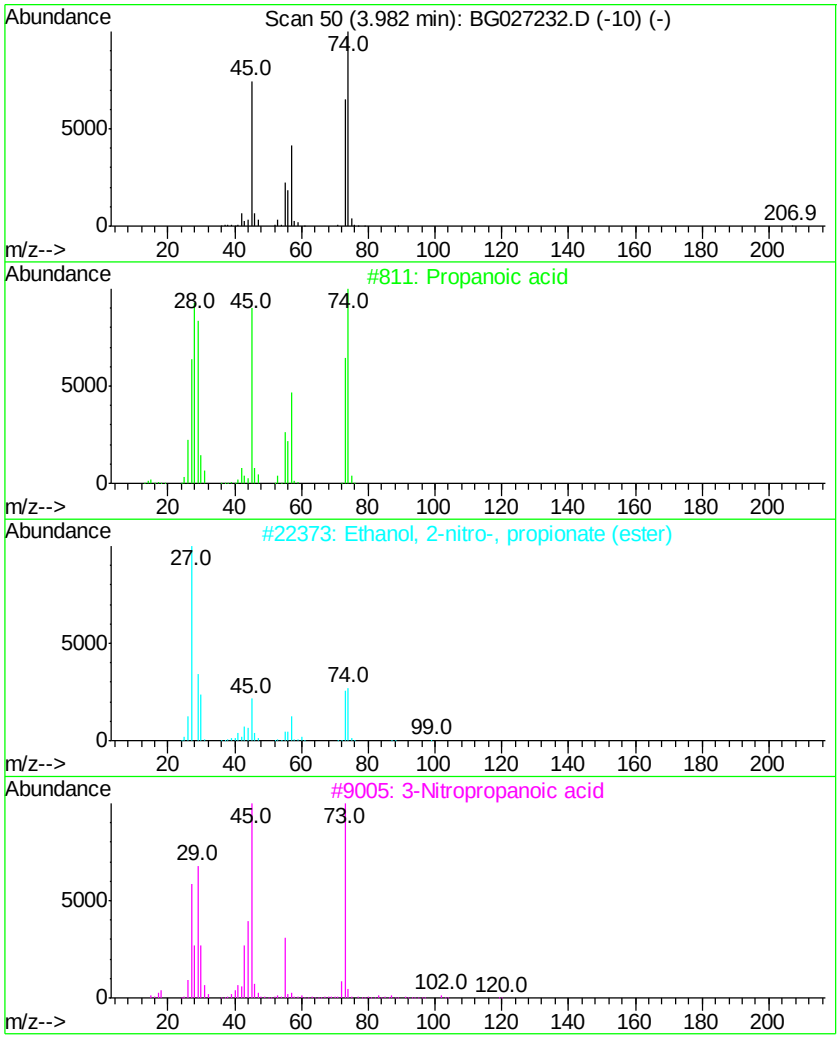
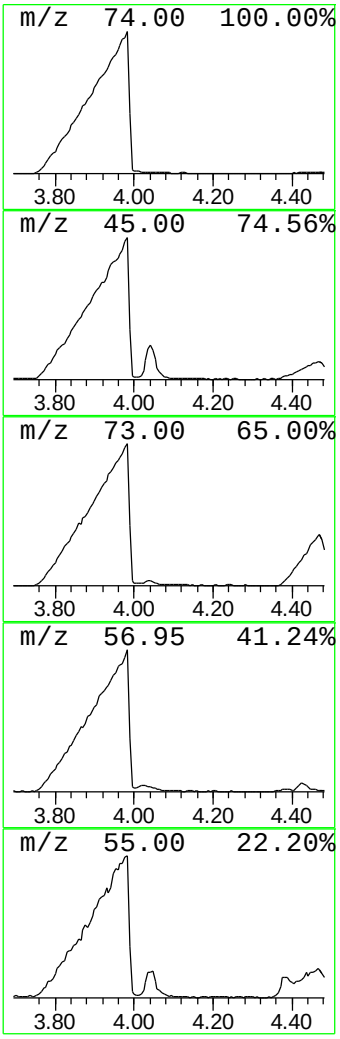
****

Peak Number 1 Propanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.98	36.77 ng	2905190	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid	74	C3H6O2	000079-09-4	91
2	Ethanol, 2-nitro-, propionate (e...	147	C5H9NO4	005390-28-3	64
3	3-Nitropropanoic acid	119	C3H5NO4	000504-88-1	23
4	Ethyl ether	74	C4H10O	000060-29-7	9
5	Propanoic acid, 2-hydroxy-, ethy...	118	C5H10O3	000687-47-8	9





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Data File : BG027232.D
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Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

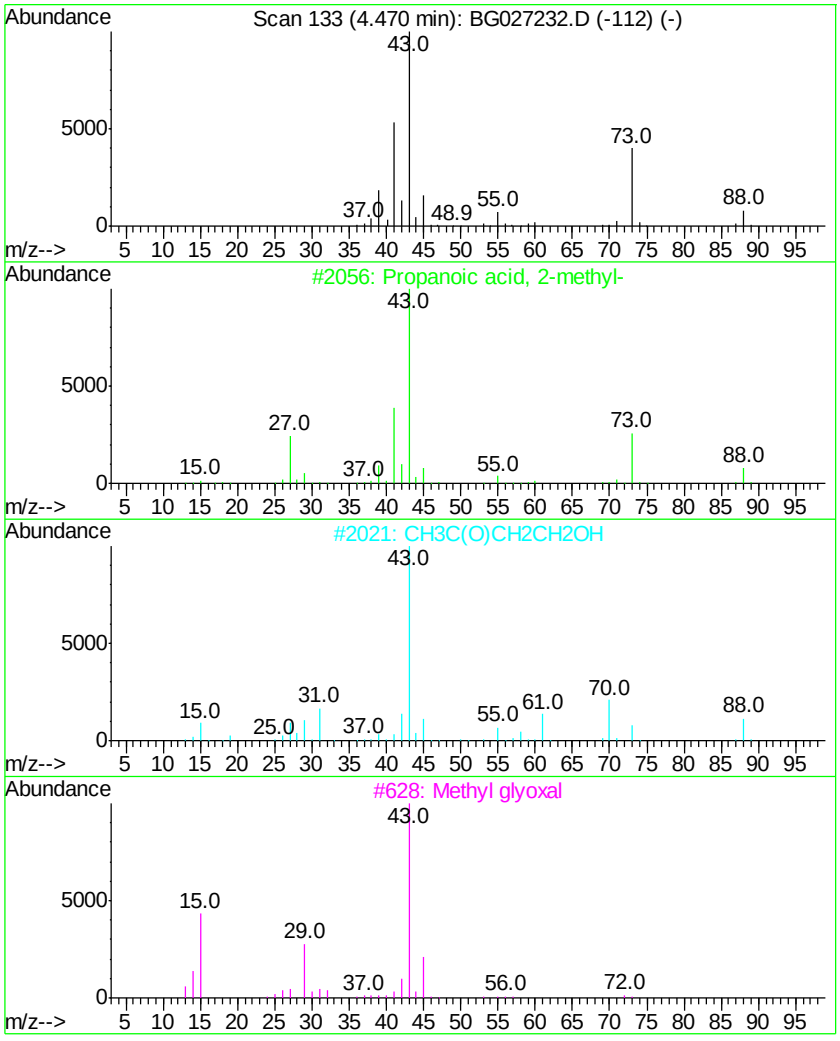
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

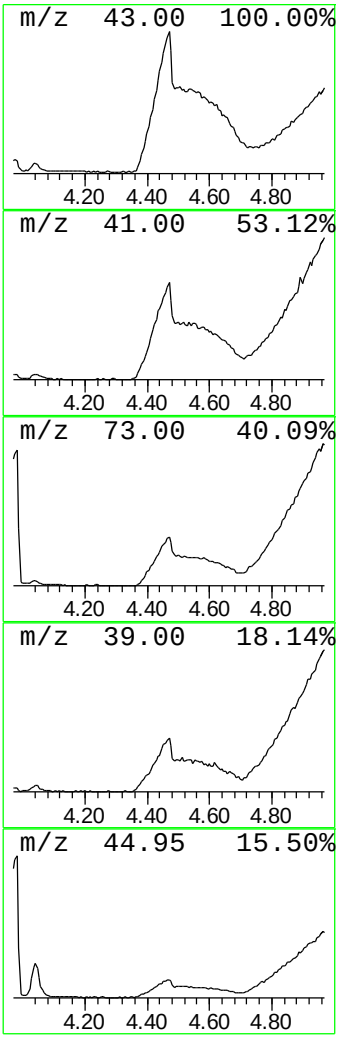
****

Peak Number 2 Propanoic acid, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	10.27 ng	811527	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	90
2	CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	59
3	Methyl glyoxal	72	C3H4O2	000078-98-8	37
4	Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	32
5	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	12





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060517\
Data File : BG027232.D
Acq On : 6 Jun 2017 3:46
Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

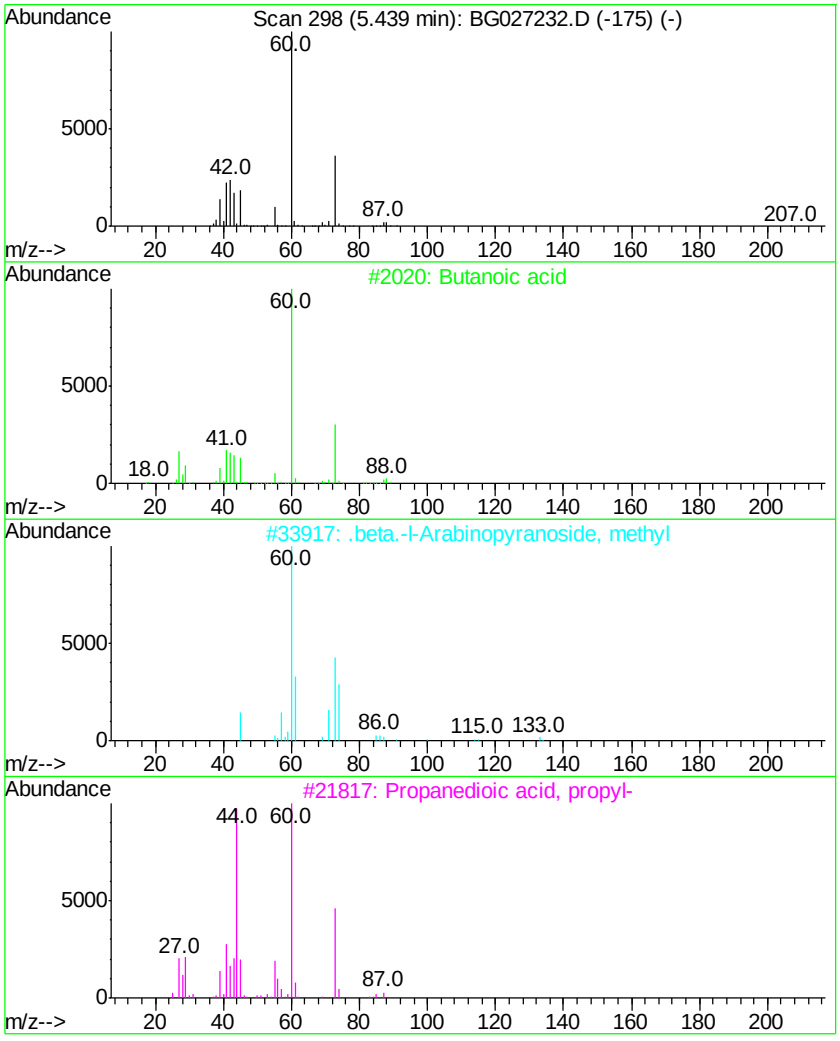
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

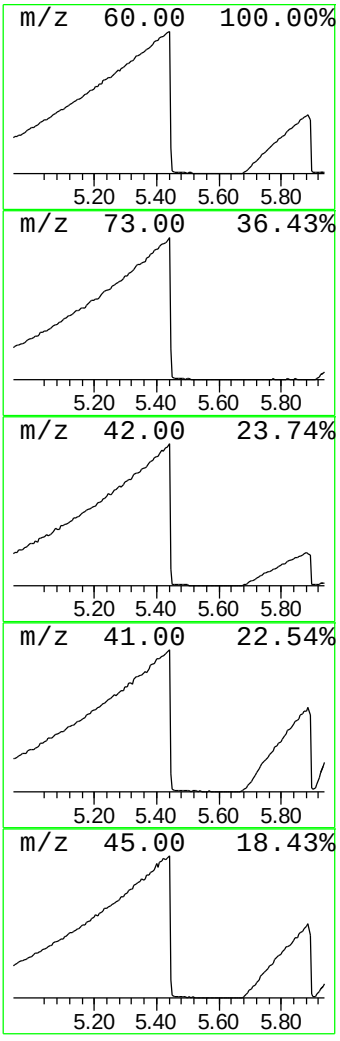
****

Peak Number 3 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.44	558.43 ng	44119500	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	86
2	.beta.-l-Arabinopyranoside, methyl	164	C6H12O5	001825-00-9	9
3	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	9
4	Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	9
5	Hexanoic acid	116	C6H12O2	000142-62-1	9





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Acq On : 6 Jun 2017 3:46
Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

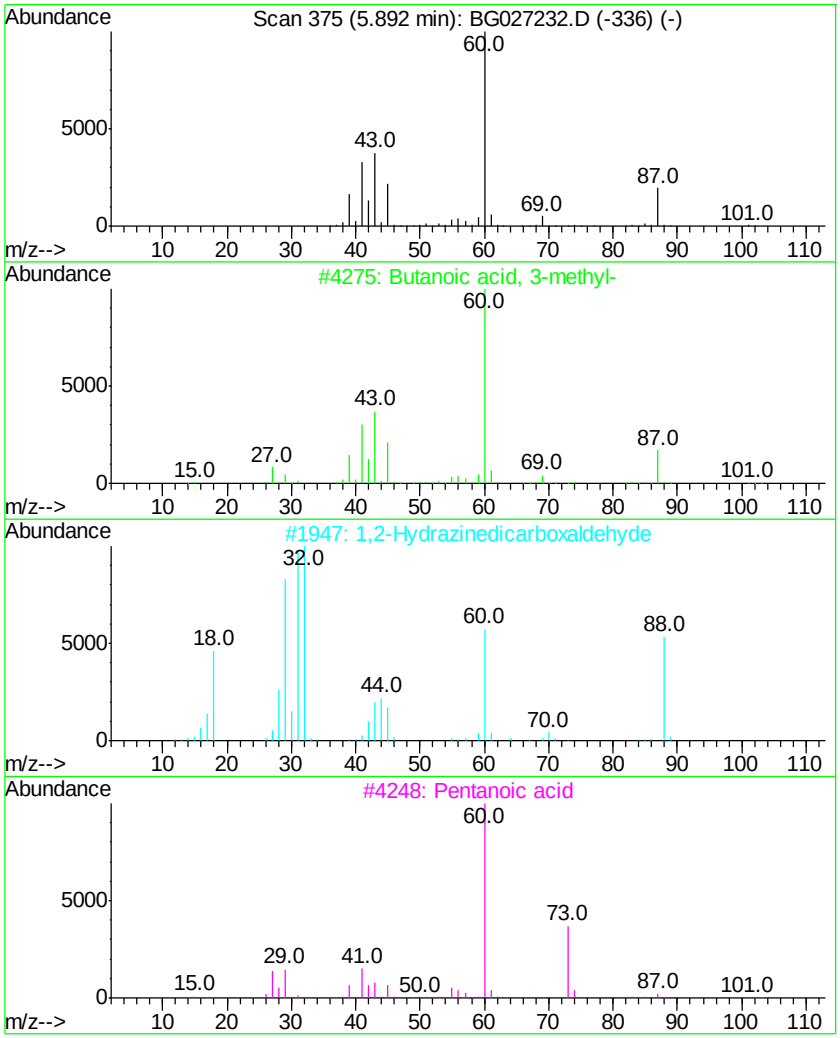
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

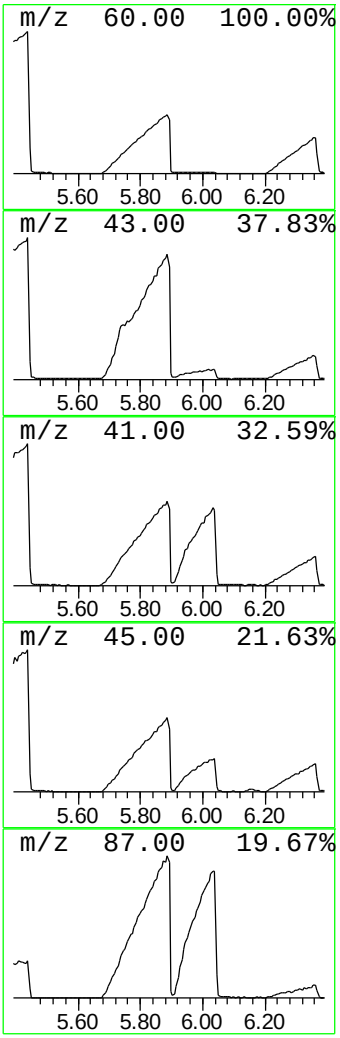
****

Peak Number 4 Butanoic acid, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	92.00 ng	7268840	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	39
3	Pentanoic acid	102	C5H10O2	000109-52-4	38
4	Formic acid hydrazide	60	CH4N2O	000624-84-0	9
5	Heptanoic acid	130	C7H14O2	000111-14-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060517\
Data File : BG027232.D
Acq On : 6 Jun 2017 3:46
Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

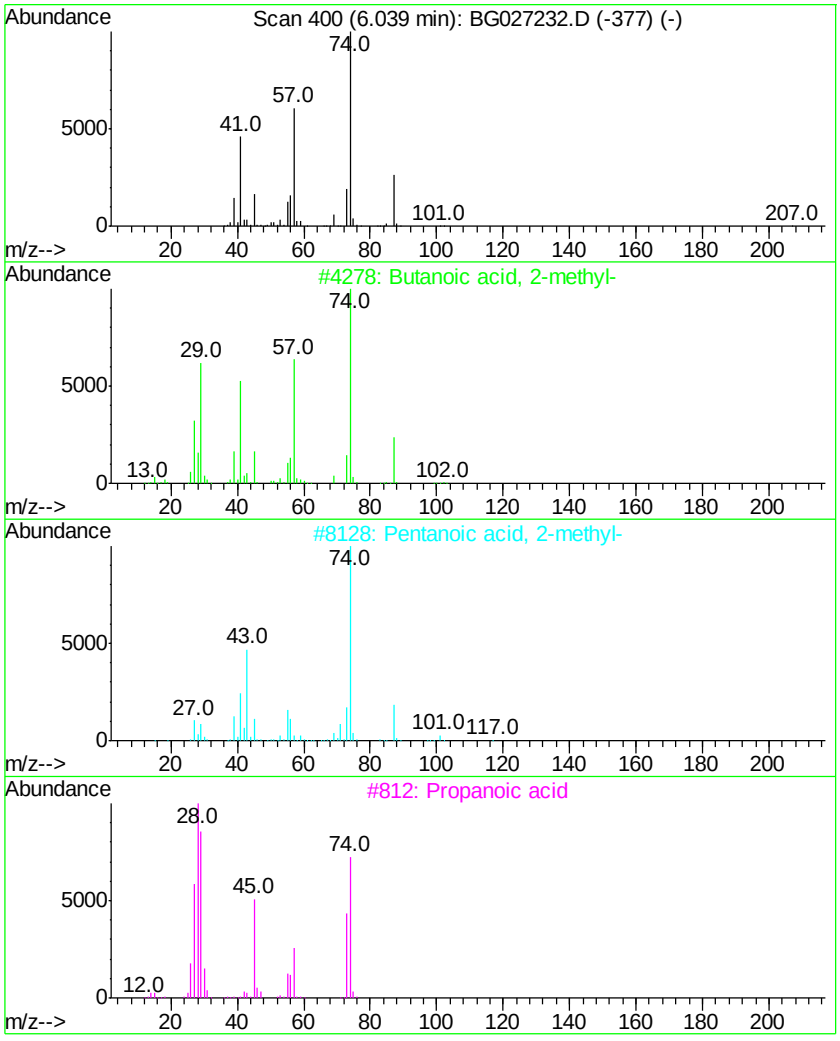
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

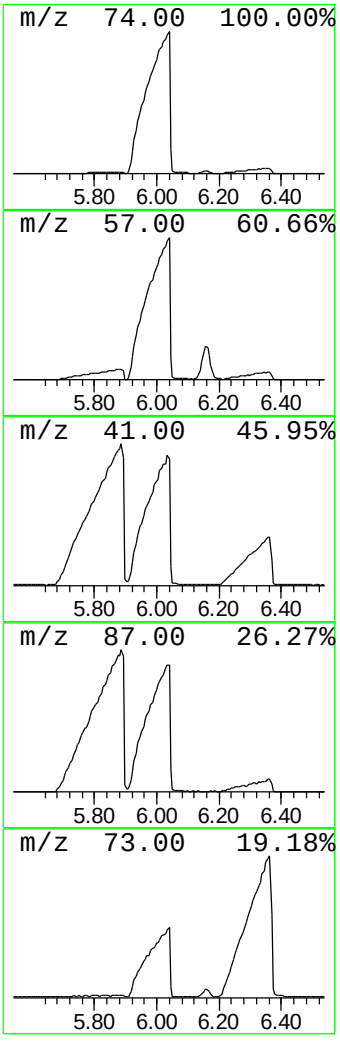
****

Peak Number 5 Butanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.04	50.79 ng	4012670	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	87
2	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	78
3	Propanoic acid	74	C3H6O2	000079-09-4	28
4	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	9
5	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	9





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Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

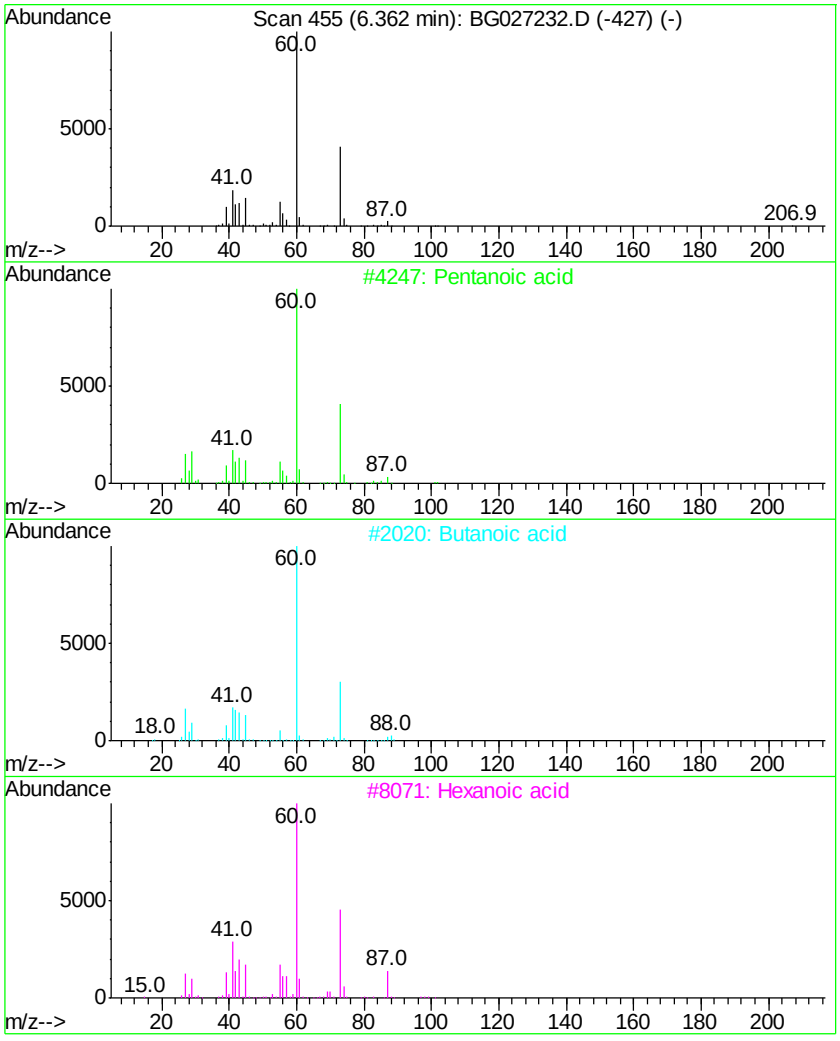
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

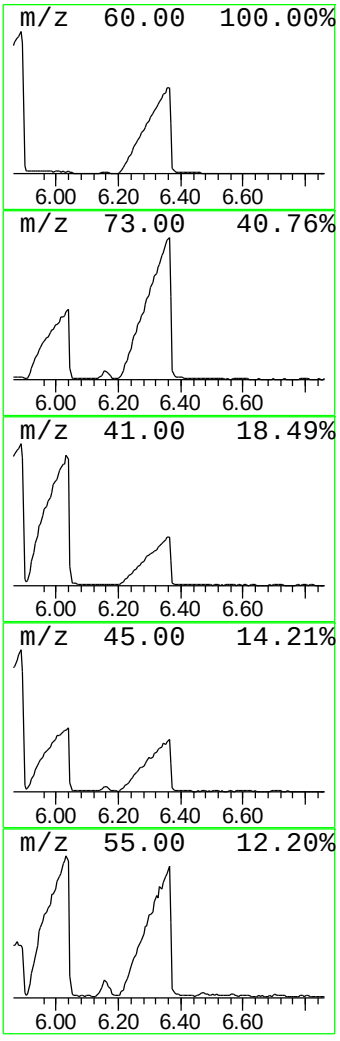
****

Peak Number 6 Pentanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	36.09 ng	2851070	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	90
2	Butanoic acid	88	C4H8O2	000107-92-6	83
3	Hexanoic acid	116	C6H12O2	000142-62-1	56
4	.beta.-Methyl xyloside	164	C6H12O5	1000130-04-0	40
5	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	40





Data Path : Z:\HPCHEM1\BNA G\DATA\BG060517\
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Operator : SJ/MA
Sample : I3393-01
Misc :
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Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

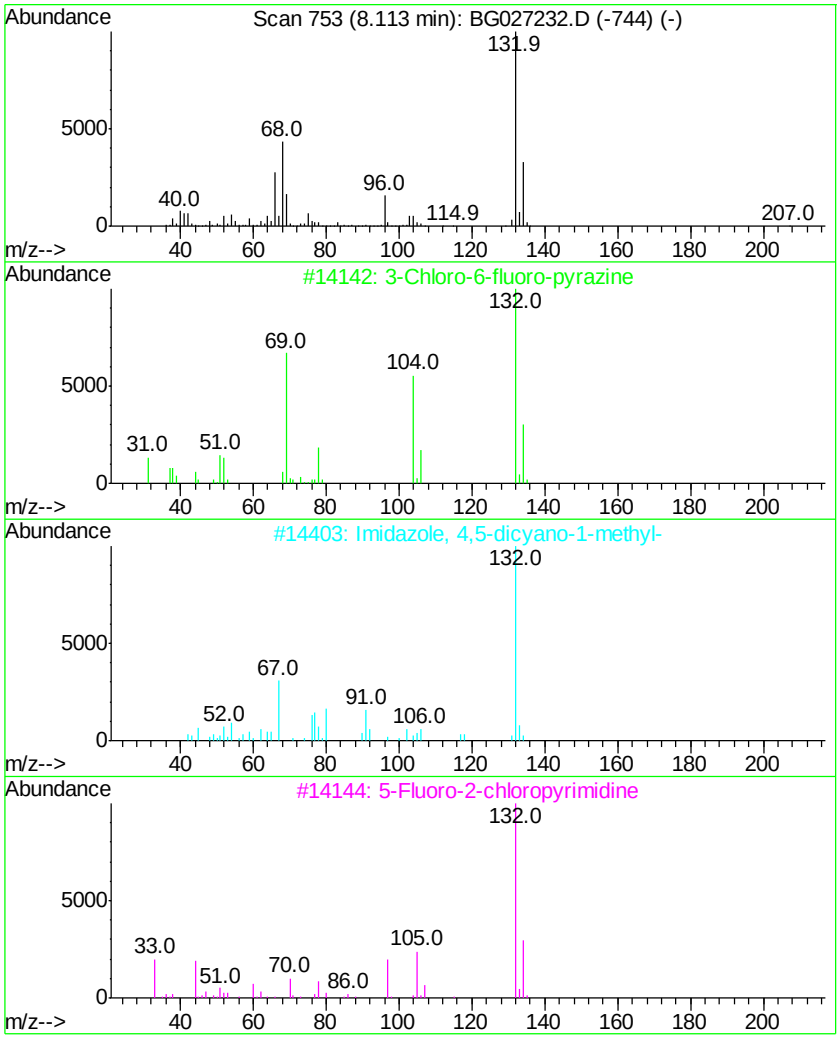
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

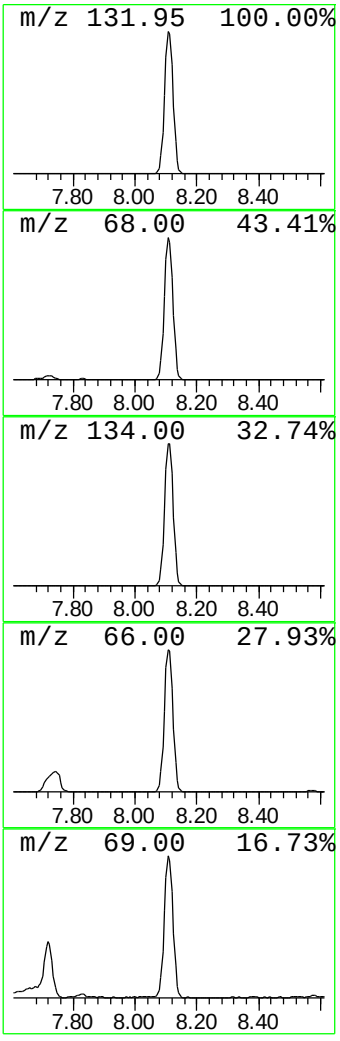
****

Peak Number 7 unknown8.11 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.11	26.59 ng	2100580	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	14
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Sample : I3393-01
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
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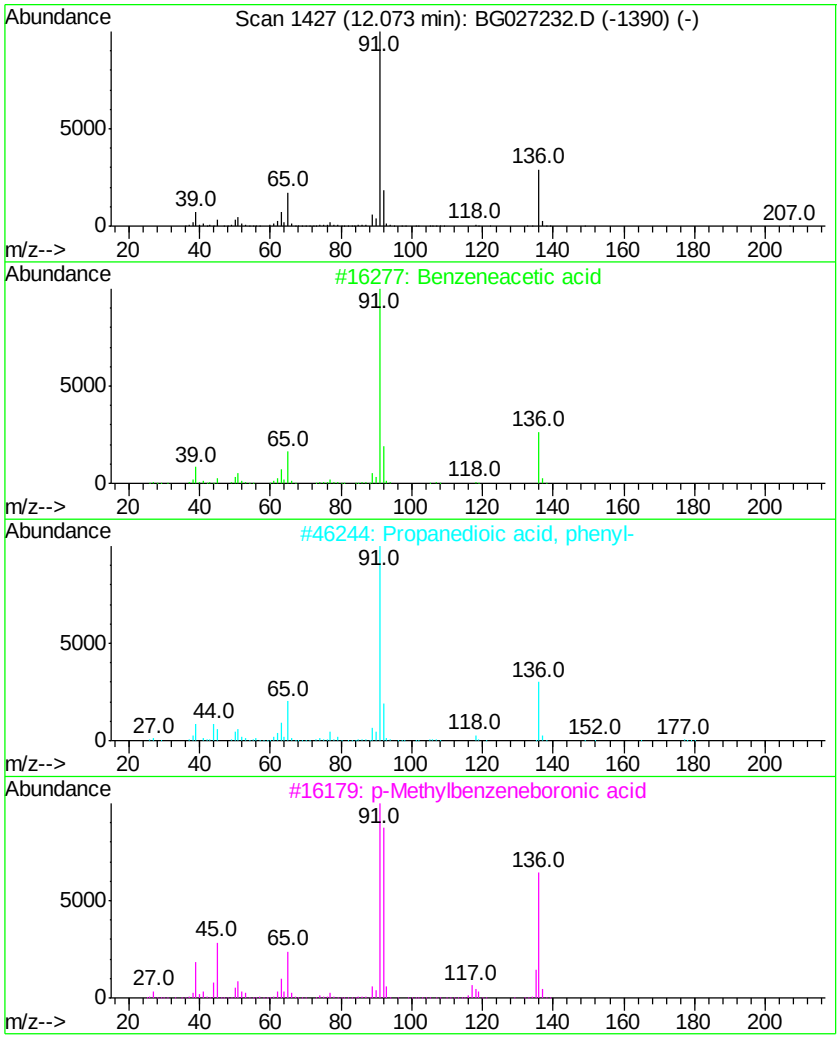
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

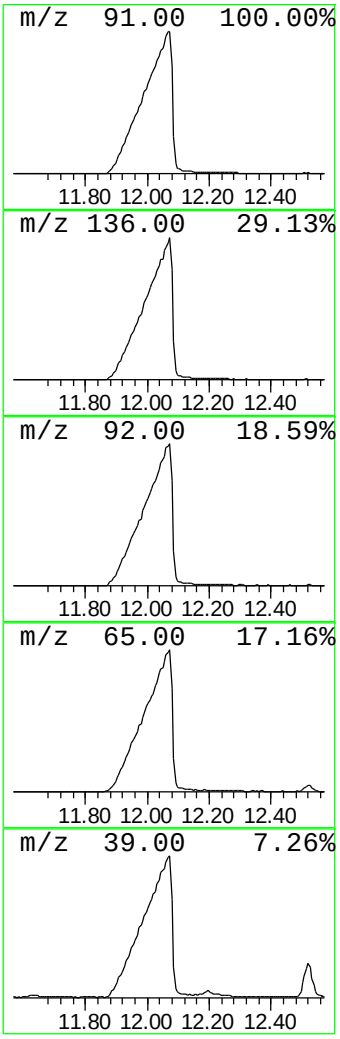
****

Peak Number 9 Benzeneacetic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.07	308.58 ng	9698810	Naphthalene-d8	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2	Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	83
3	p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	64
4	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	64
5	Benzene, (2-methoxyethyl)-	136	C9H12O	003558-60-9	64





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Sample : I3393-01
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Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

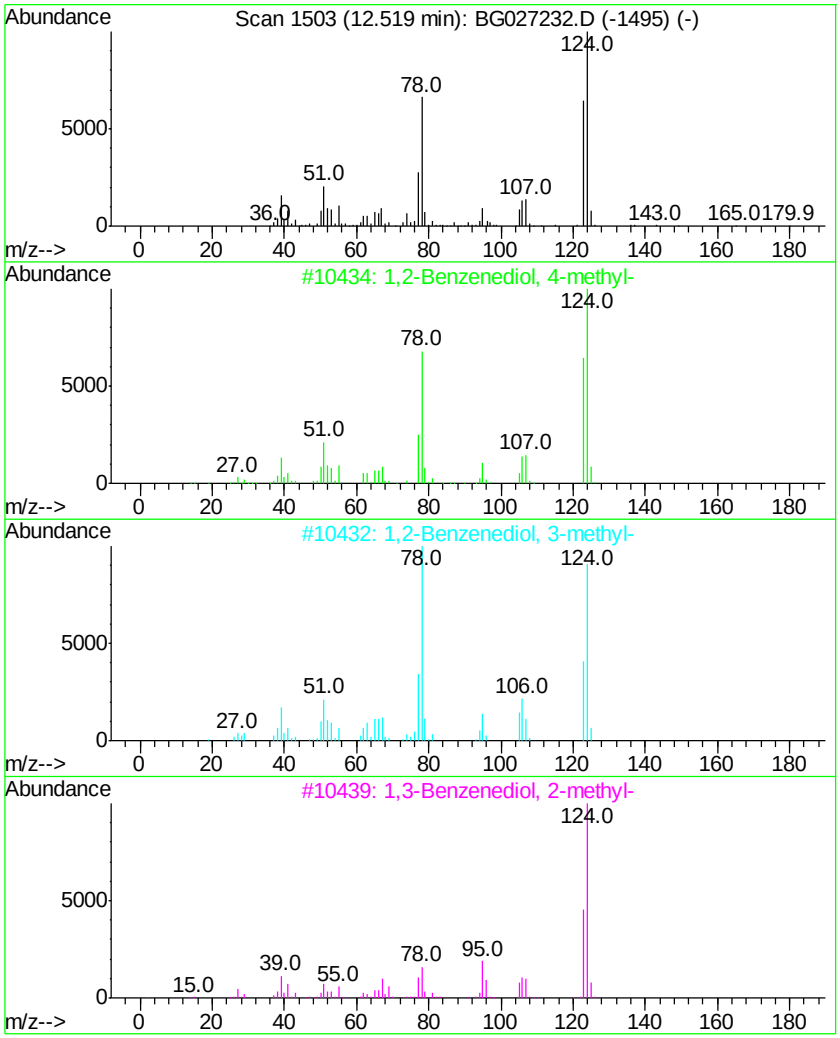
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

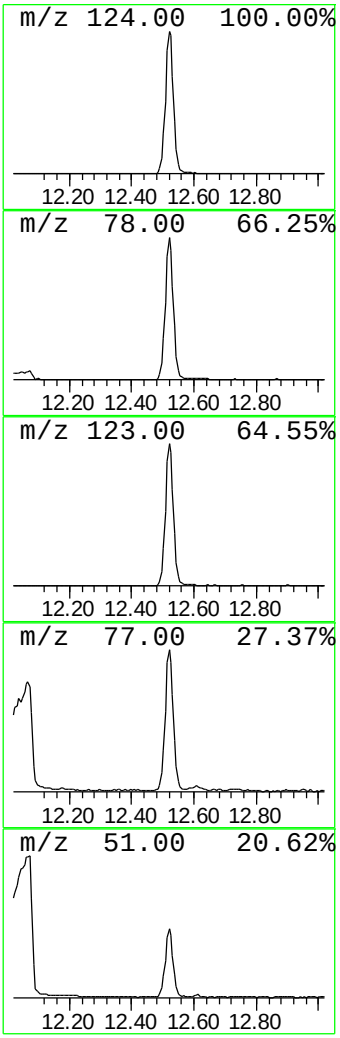
****

Peak Number 10 1,2-Benzenediol, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	21.34 ng	670597	Naphthalene-d8	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	96
2	1,2-Benzenediol, 3-methyl-	124	C7H8O2	000488-17-5	94
3	1,3-Benzenediol, 2-methyl-	124	C7H8O2	000608-25-3	58
4	Orcinol	124	C7H8O2	000504-15-4	53
5	Salicyl alcohol	124	C7H8O2	000090-01-7	50





Data Path : Z:\HPCHEM1\BNA G\DATA\BG060517\
Data File : BG027232.D
Acq On : 6 Jun 2017 3:46
Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

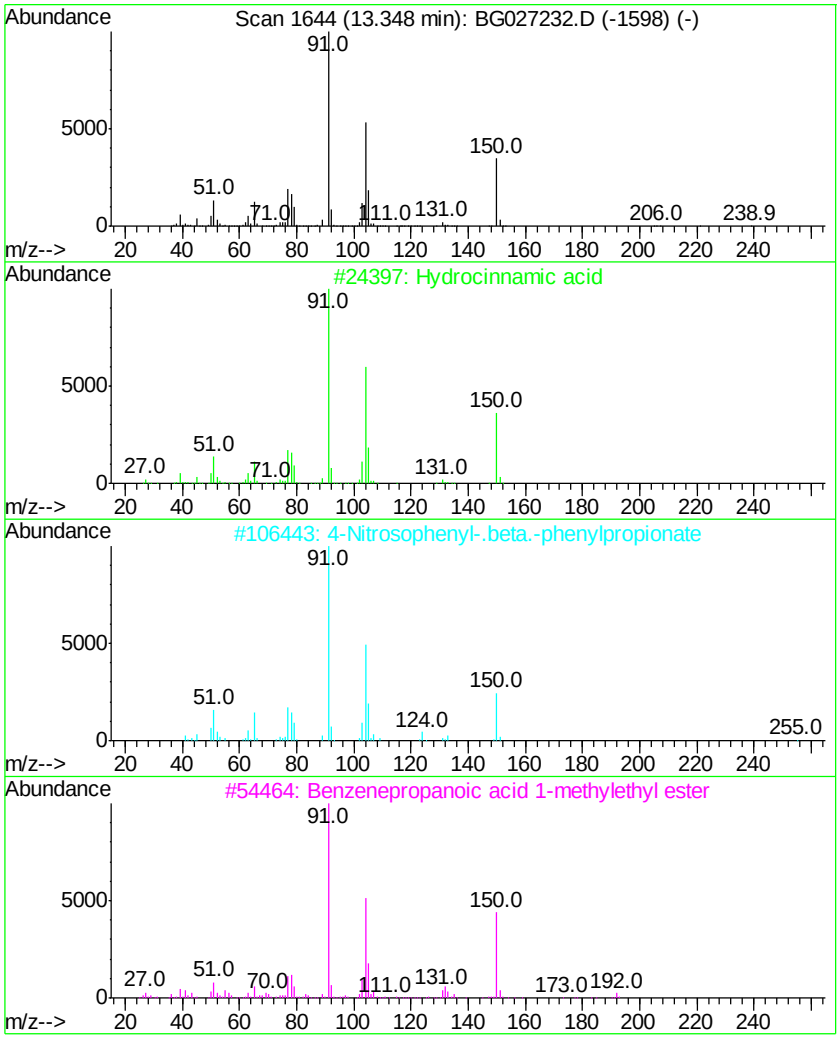
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

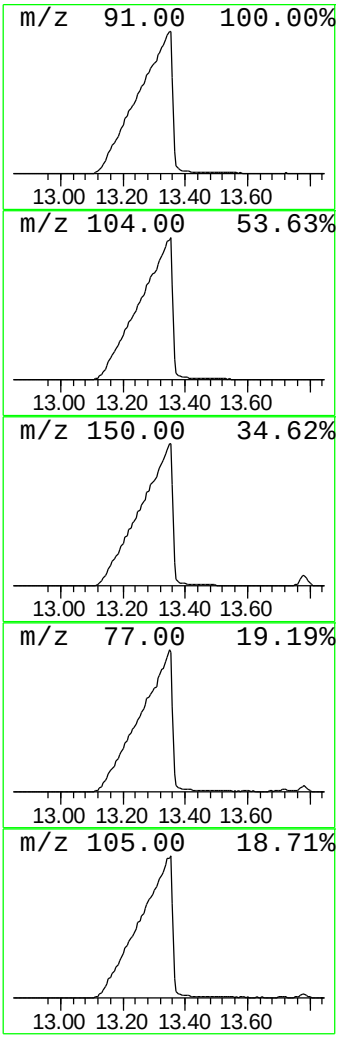
****

Peak Number 11 Hydrocinnamic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	424.12 ng	25186000	Acenaphthene-d10	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	96
2	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	90
3	Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	78
4	Acetic acid, trifluoro-, 2-phenyl...	218	C10H9F3O2	055419-66-4	58
5	Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	53





Data Path : Z:\HPCHEM1\BNA G\DATA\BG060517\
Data File : BG027232.D
Acq On : 6 Jun 2017 3:46
Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.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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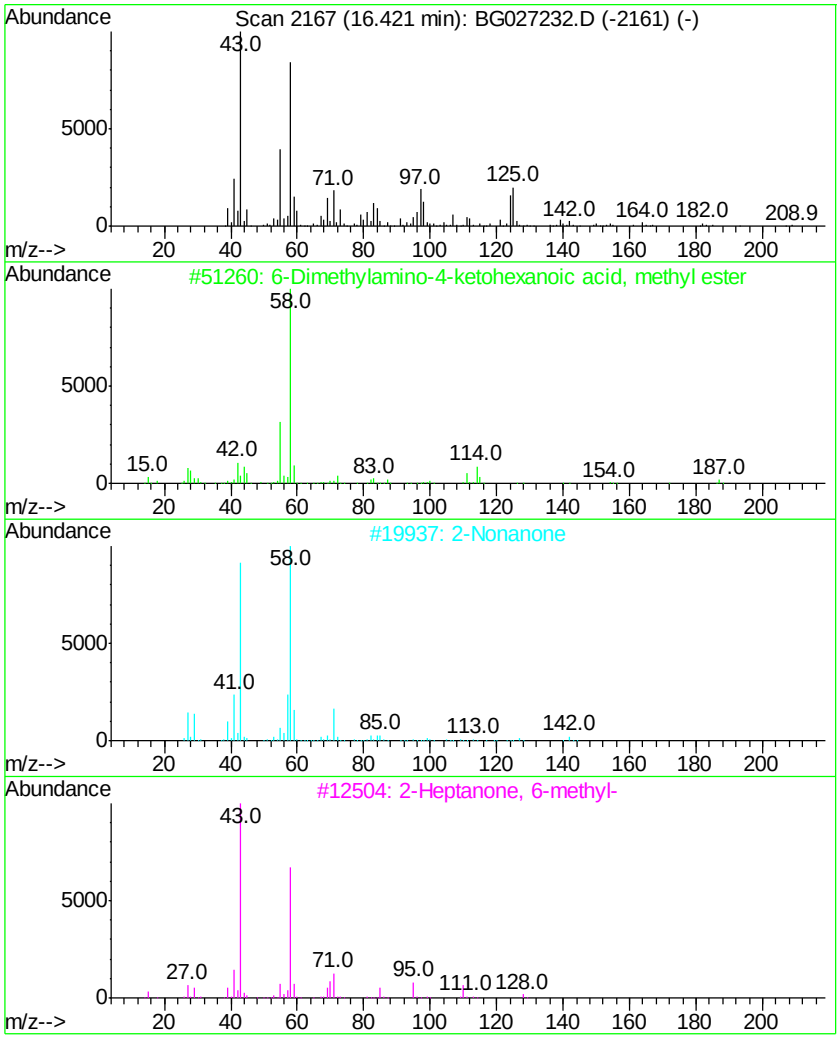
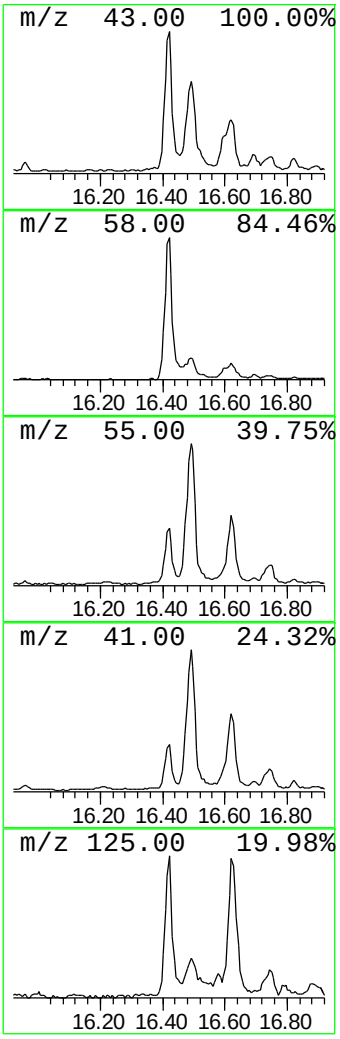
Peak Number 12 unknown16.42 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.42	9.27 ng	550598	Acenaphthene-d10	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Dimethylamino-4-ketohexanoic a...	187	C9H17NO3	1000353-25-7	47
2	2-Nonanone	142	C9H18O	000821-55-6	46
3	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	43
4	2-Heptanone	114	C7H14O	000110-43-0	43
5	Pholedrine	165	C10H15NO	000370-14-9	43





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Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
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TIC Library : C:\DATABASE\NIST11.L
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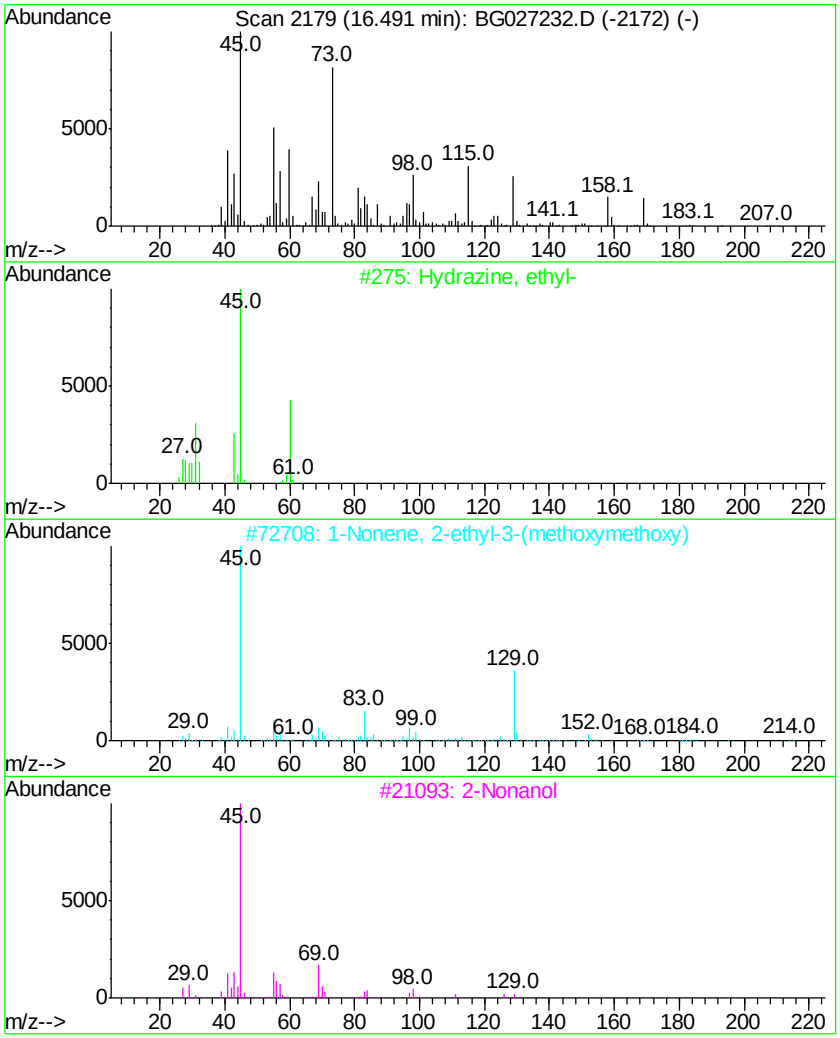
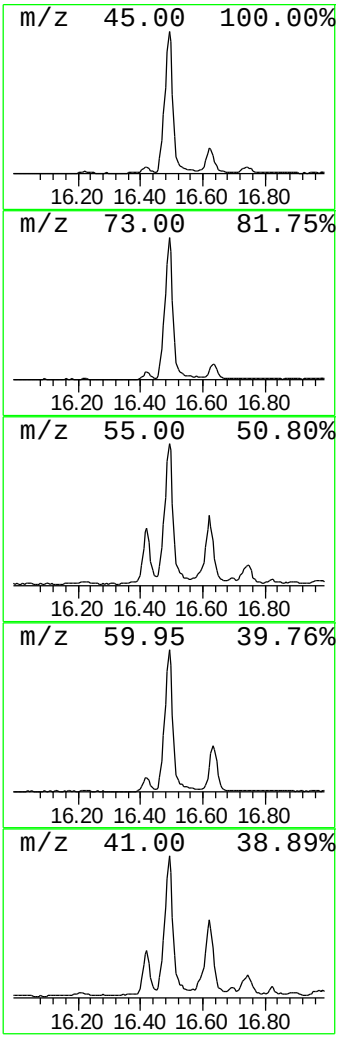
Peak Number 13 unknown16.49 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	31.44 ng	1866830	Acenaphthene-d10	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	43
2	1-Nonene, 2-ethyl-3-(methoxymeth...	214	C13H26O2	1000197-21-7	35
3	2-Nonanol	144	C9H20O	000628-99-9	35
4	2-Ethoxypentane	116	C7H16O	001817-89-6	27
5	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	27





Data Path : Z:\HPCHEM1\BNA G\DATA\BG060517\
Data File : BG027232.D
Acq On : 6 Jun 2017 3:46
Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.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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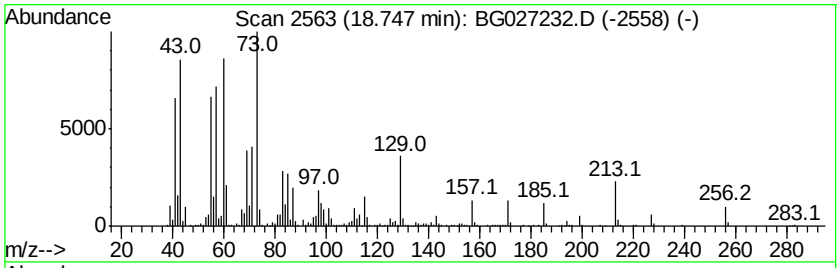
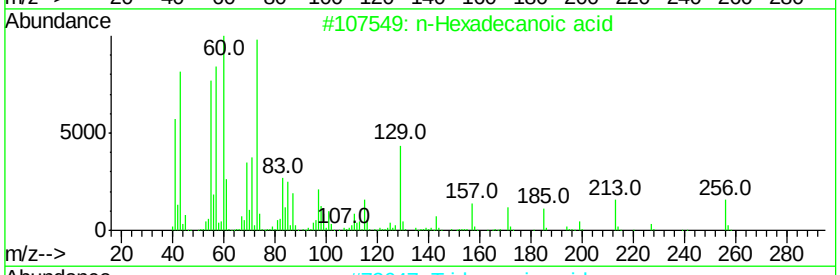
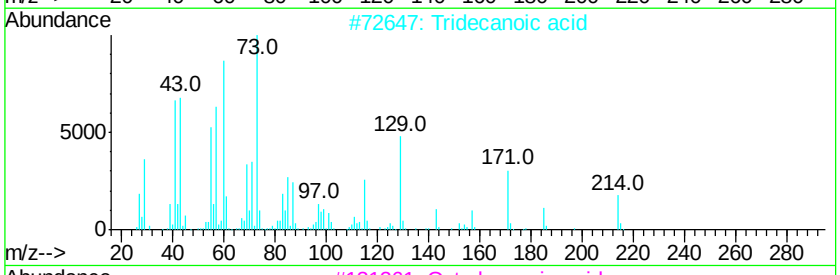
Peak Number 14 n-Hexadecanoic acid Concentration Rank 12

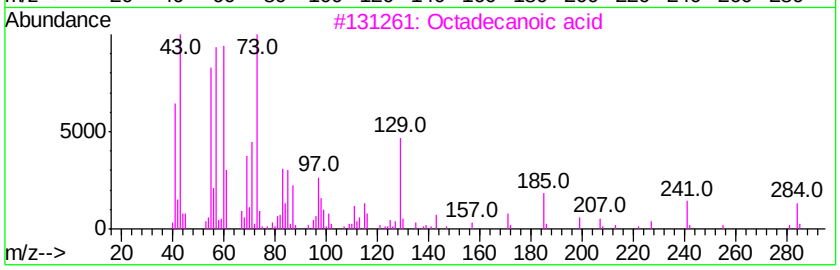
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.75	14.89 ng	790514	Phenanthrene-d10	17.90

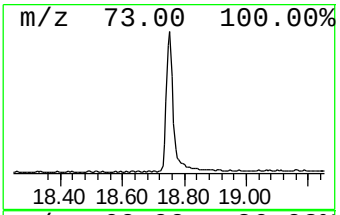
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	93

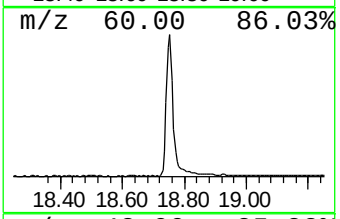


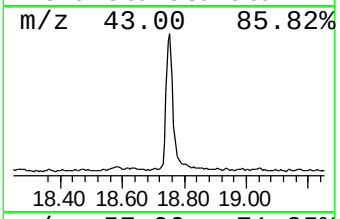


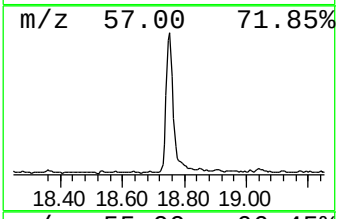


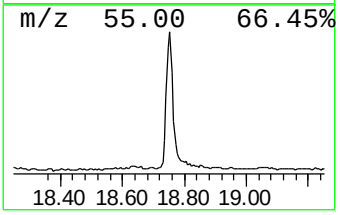












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG060517\
Data File : BG027232.D
Acq On : 6 Jun 2017 3:46
Operator : SJ/MA
Sample : I3393-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TW-01

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

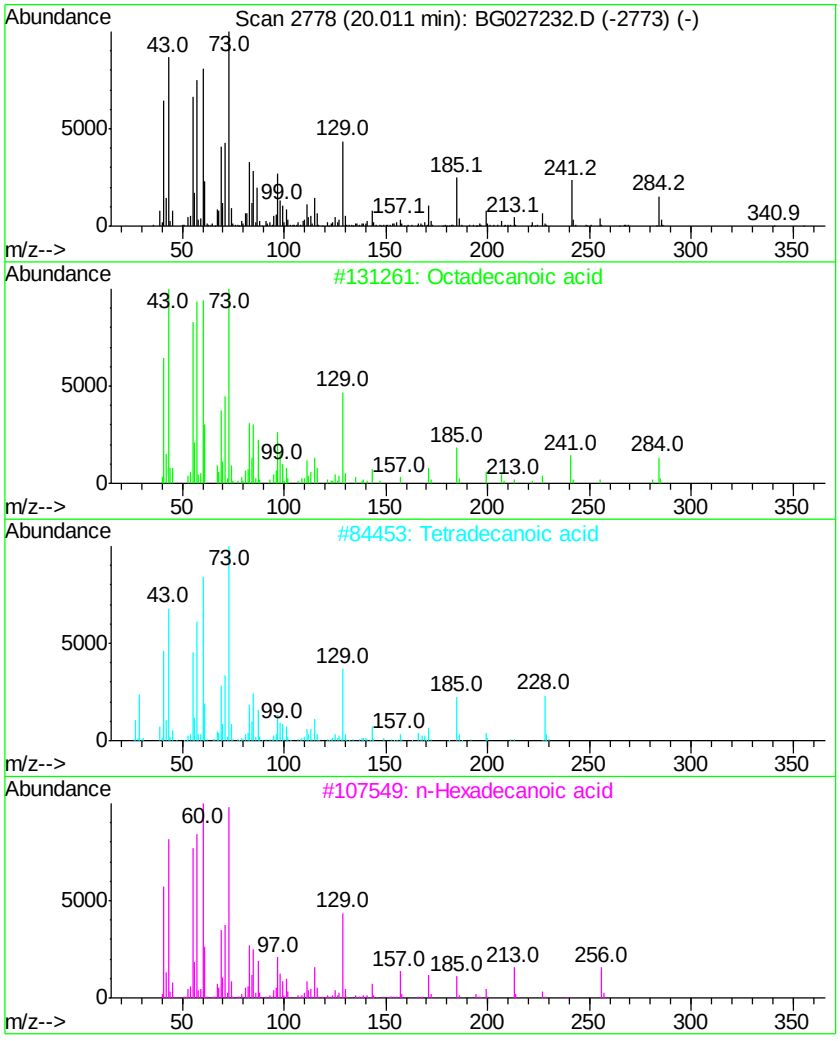
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

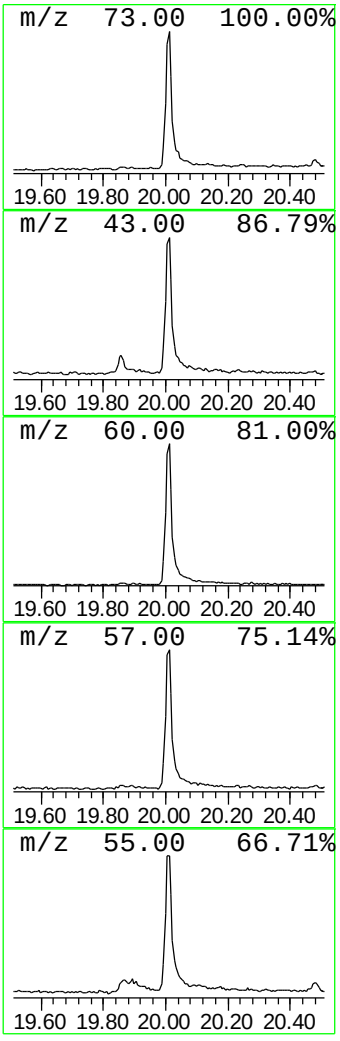
****

Peak Number 15 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.01	12.50 ng	663923	Phenanthrene-d10	17.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060517\
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanoic acid	3.98	36.8	ng	2905190	1	8.57	1580140	20.0
Propanoic acid, 2...	4.47	10.3	ng	811527	1	8.57	1580140	20.0
Butanoic acid	5.44	558.4	ng	44119500	1	8.57	1580140	20.0
Butanoic acid, 3-...	5.89	92.0	ng	7268840	1	8.57	1580140	20.0
Butanoic acid, 2-...	6.04	50.8	ng	4012670	1	8.57	1580140	20.0
Pentanoic acid	6.36	36.1	ng	2851070	1	8.57	1580140	20.0
unknown8.11	8.11	26.6	ng	2100580	1	8.57	1580140	20.0
Benzeneacetic acid	12.07	308.6	ng	9698810	2	11.39	628604	20.0
1,2-Benzenediol, ...	12.52	21.3	ng	670597	2	11.39	628604	20.0
Hydrocinnamic acid	13.35	424.1	ng	25186000	3	15.15	1187670	20.0
unknown16.42	16.42	9.3	ng	550598	3	15.15	1187670	20.0
unknown16.49	16.49	31.4	ng	1866830	3	15.15	1187670	20.0
n-Hexadecanoic acid	18.75	14.9	ng	790514	4	17.90	1062120	20.0
Octadecanoic acid	20.01	12.5	ng	663923	4	17.90	1062120	20.0