LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG100317\
Data File : BG029029.D
Acq On : 4 Oct 2017 7:10
Operator : SJ/JU
Sample : I5517-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LIP-16

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-BG091217.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	4.135	88	93	102	rVB	42465	62220	3.56%	0.619%
2	4.740	190	196	206	rBV	465279	719537	41.12%	7.156%
3	4.846	208	214	225	rBV	136258	283608	16.21%	2.821%
4	5.809	372	378	394	rVB	191267	353725	20.22%	3.518%
5	7.325	628	636	644	rBV	300249	517118	29.55%	5.143%
6	7.408	644	650	664	rVB2	53707	150043	8.57%	1.492%
7	7.772	705	712	726	rBV	365225	695761	39.76%	6.920%
8	8.236	783	791	799	rVB	113143	194351	11.11%	1.933%
9	8.565	838	847	856	rBV	408303	728369	41.63%	7.244%
10	9.411	982	991	1003	rBV	333736	648770	37.08%	6.453%
11	9.775	1045	1053	1062	rBV	69874	124606	7.12%	1.239%
12	11.062	1265	1272	1279	rBV	134089	262097	14.98%	2.607%
13	12.267	1470	1477	1483	rBV2	39366	59369	3.39%	0.590%
14	12.831	1567	1573	1579	rBV3	14521	31886	1.82%	0.317%
15	12.889	1581	1583	1591	rVB5	9171	18801	1.07%	0.187%
16	13.483	1677	1684	1694	rBV	970336	1505429	86.03%	14.973%
17	14.235	1807	1812	1818	rBV3	15900	21351	1.22%	0.212%
18	14.311	1820	1825	1830	rBV3	11068	18651	1.07%	0.186%
19	14.864	1912	1919	1926	rBV2	77366	134427	7.68%	1.337%
20	16.350	2166	2172	2186	rBV	684638	1193245	68.19%	11.868%
21	17.613	2380	2387	2396	rBV2	218409	385814	22.05%	3.837%
22	18.477	2529	2534	2539	rBV6	21540	49515	2.83%	0.492%
23	20.204	2822	2828	2838	rBV	1321357	1749813	100.00%	17.403%
24	21.932	3115	3122	3131	rBV3	68417	145900	8.34%	1.451%

Sum of corrected areas: 10054406

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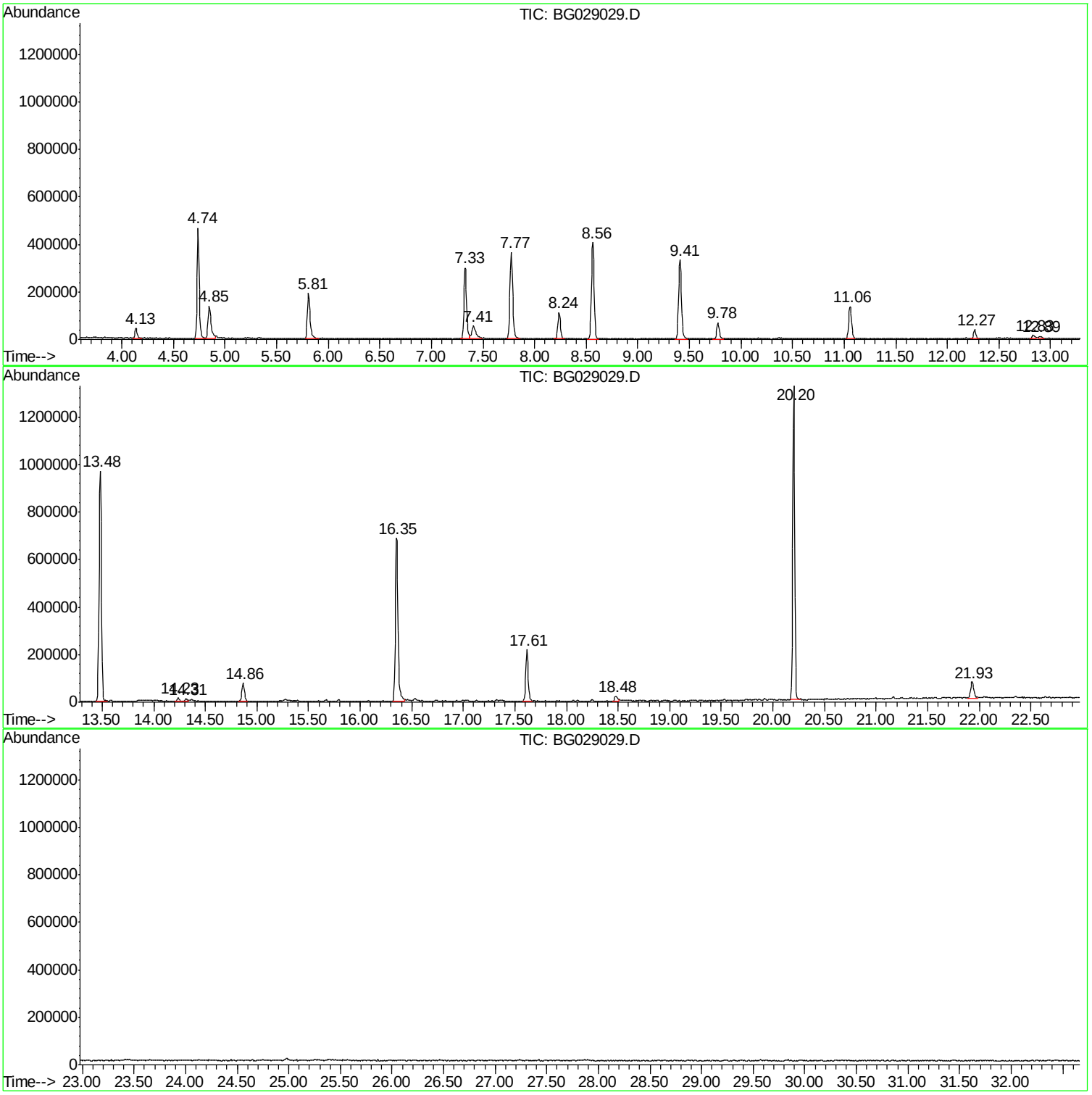
Instrument : BNA_G
ClientSampleId : LIP-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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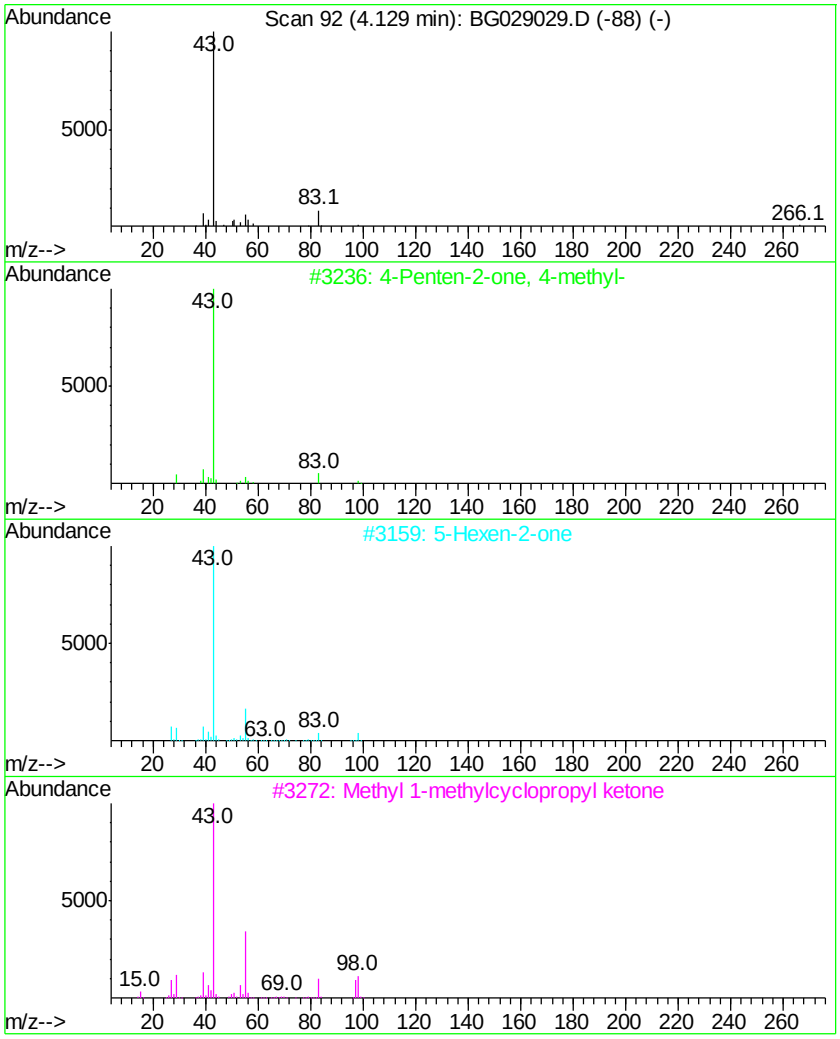
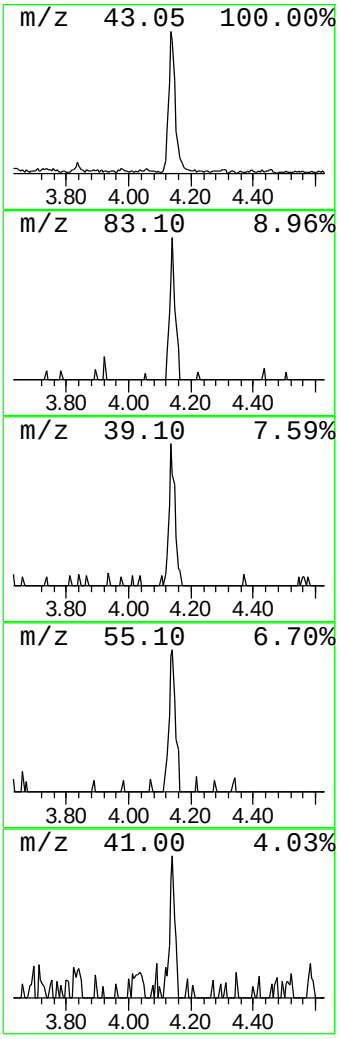
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.13	6.40 ng	62220	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	58
2	5-Hexen-2-one	98	C6H10O	000109-49-9	49
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	46
4	3-Methylpenta-1,4-diene-3-ol	98	C6H10O	000918-86-5	9
5	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9





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

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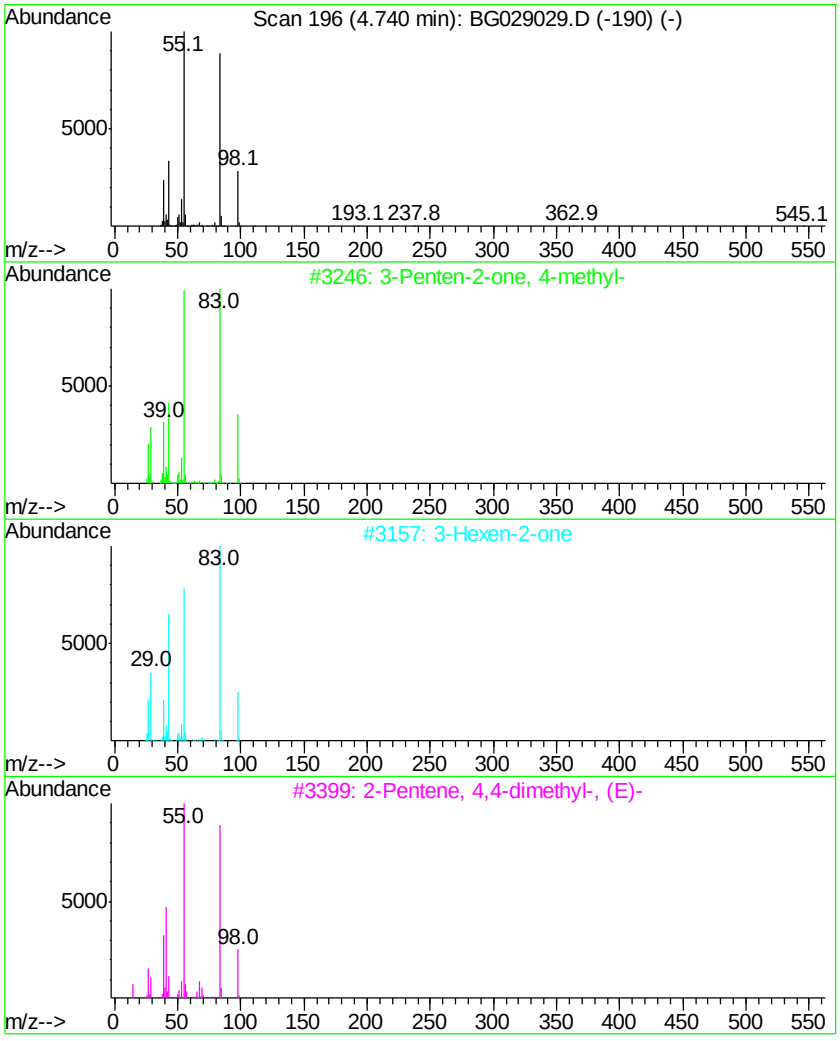
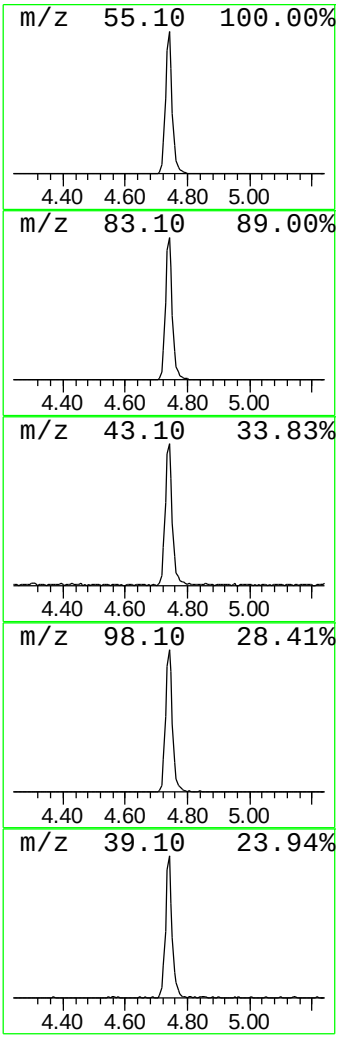
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	74.05 ng	719537	1,4-Dichlorobenzene-d4	8.24

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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Sample : I5517-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LIP-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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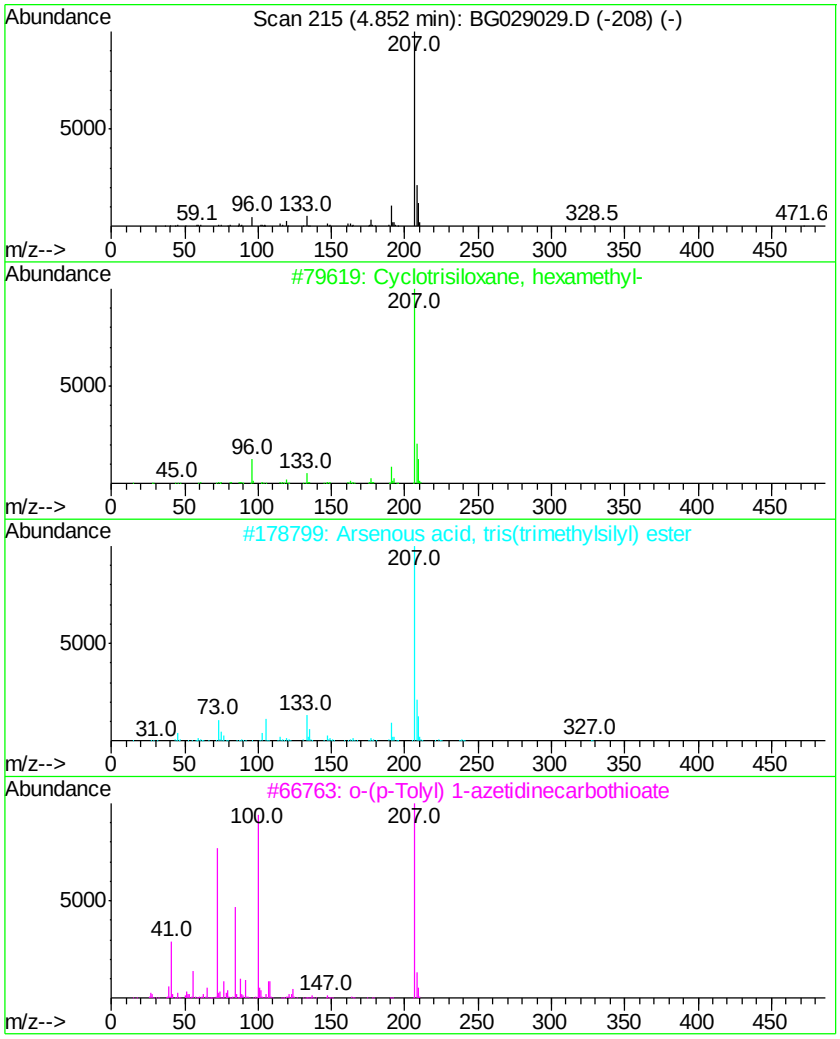
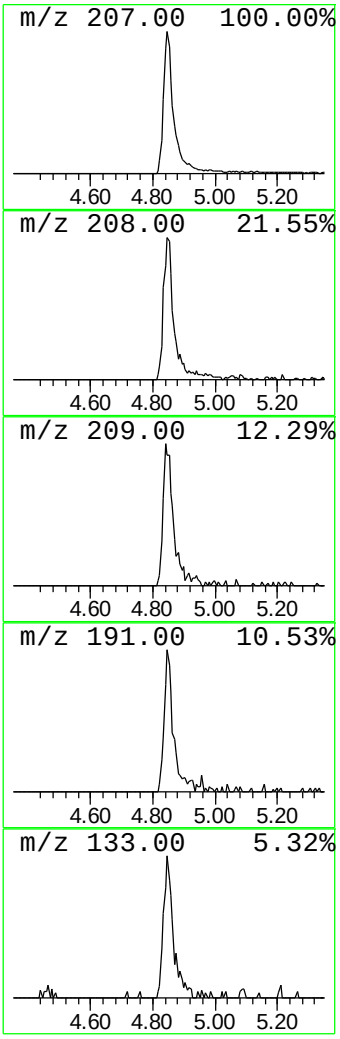
****

Peak Number 3 Cyclotrisiloxane, hexamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	29.19 ng	283608	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	90
2	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	56
3	o-(p-Tolyl) 1-azetidinecarbothioate	207	C11H13NOS	010560-24-4	45
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	42
5	4-Cyclohexene-1,2-dicarboximide,...	207	C12H17NO2	028916-00-9	42





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ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LIP-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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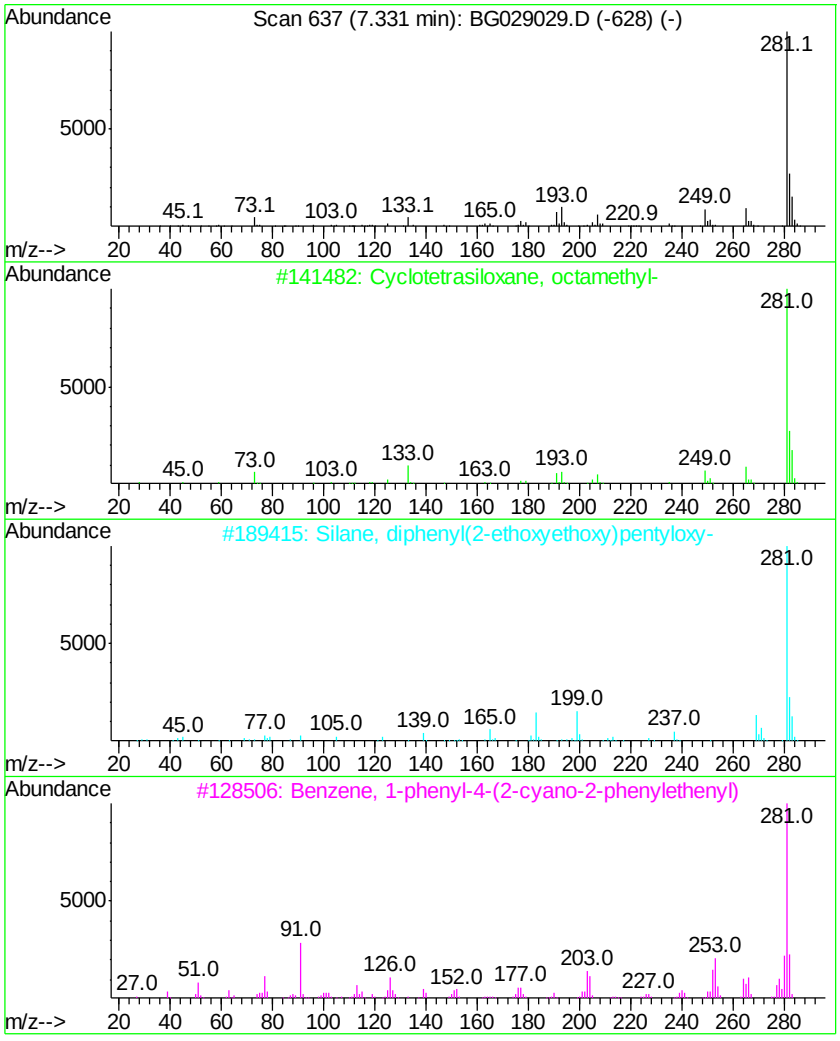
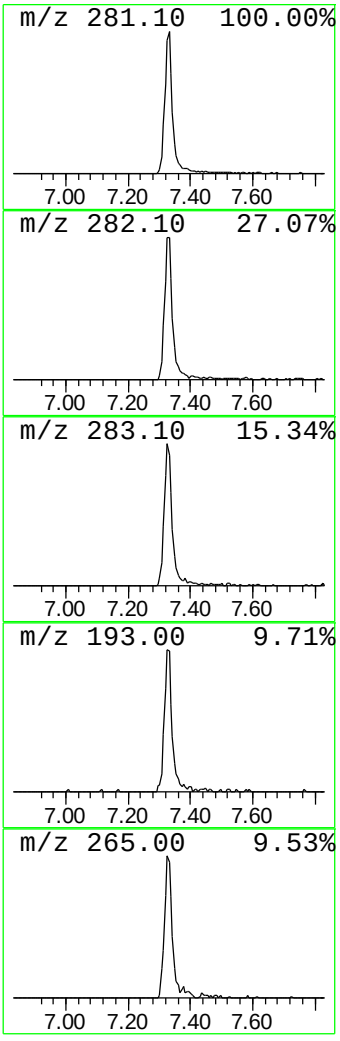
Peak Number 4 Cyclotetrasiloxane, octamet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	53.21 ng	517118	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetrasiloxane, octamethyl-	296	C8H24O4Si4	000556-67-2	91
2	Silane, diphenyl(2-ethoxyethoxy)...	358	C21H30O3Si	1000367-66-1	59
3	Benzene, 1-phenyl-4-(2-cyano-2-p...	281	C21H15N	027869-56-3	59
4	trans-4-(2-(5-Nitro-2-furyl)vinyl...	281	C15H11N3O3	000847-10-9	40
5	trans-4-Dimethylamino-4'-methoxy...	281	C18H19NO2	052119-37-6	38





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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LIP-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
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TIC Library : C:\Database\NIST11.L
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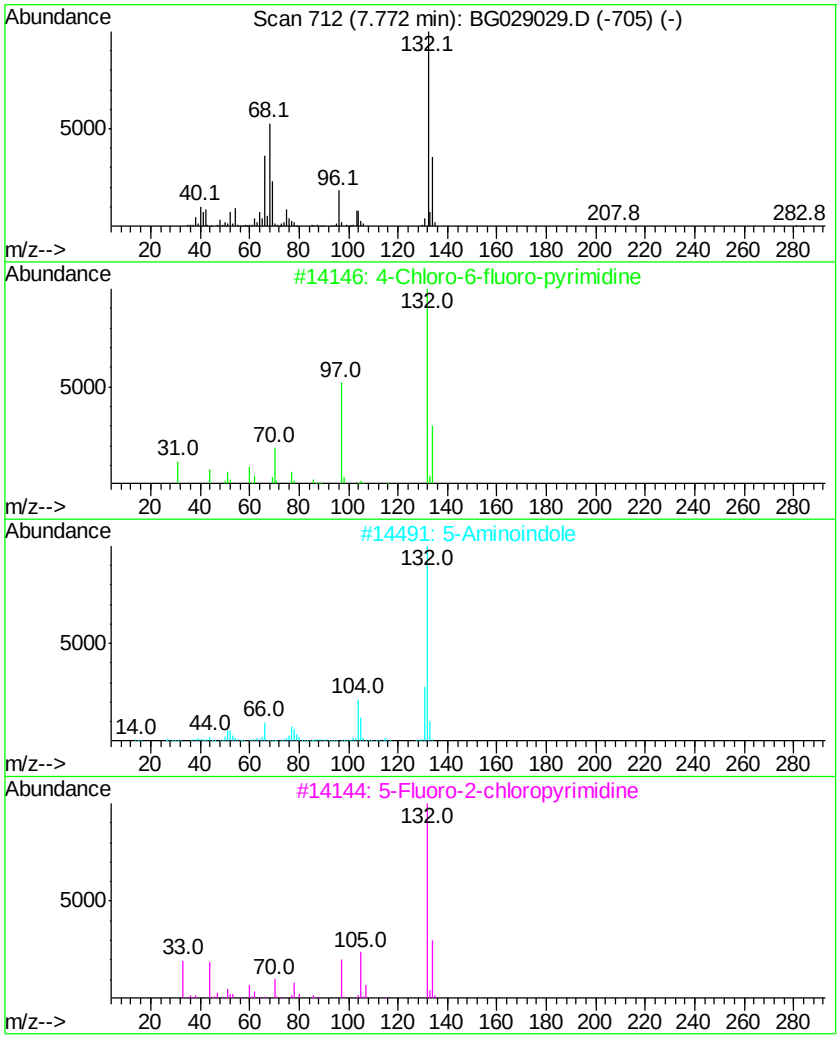
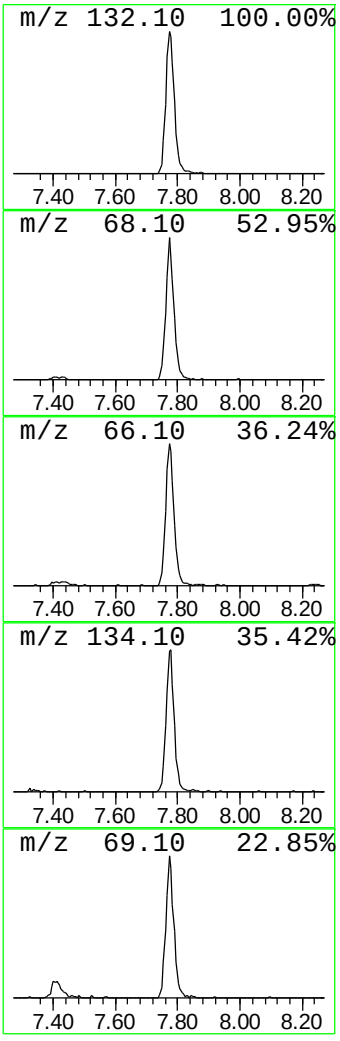
****

Peak Number 5 unknown7.77 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.77	71.60 ng	695761	1,4-Dichlorobenzene-d4	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG100317\
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Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LIP-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

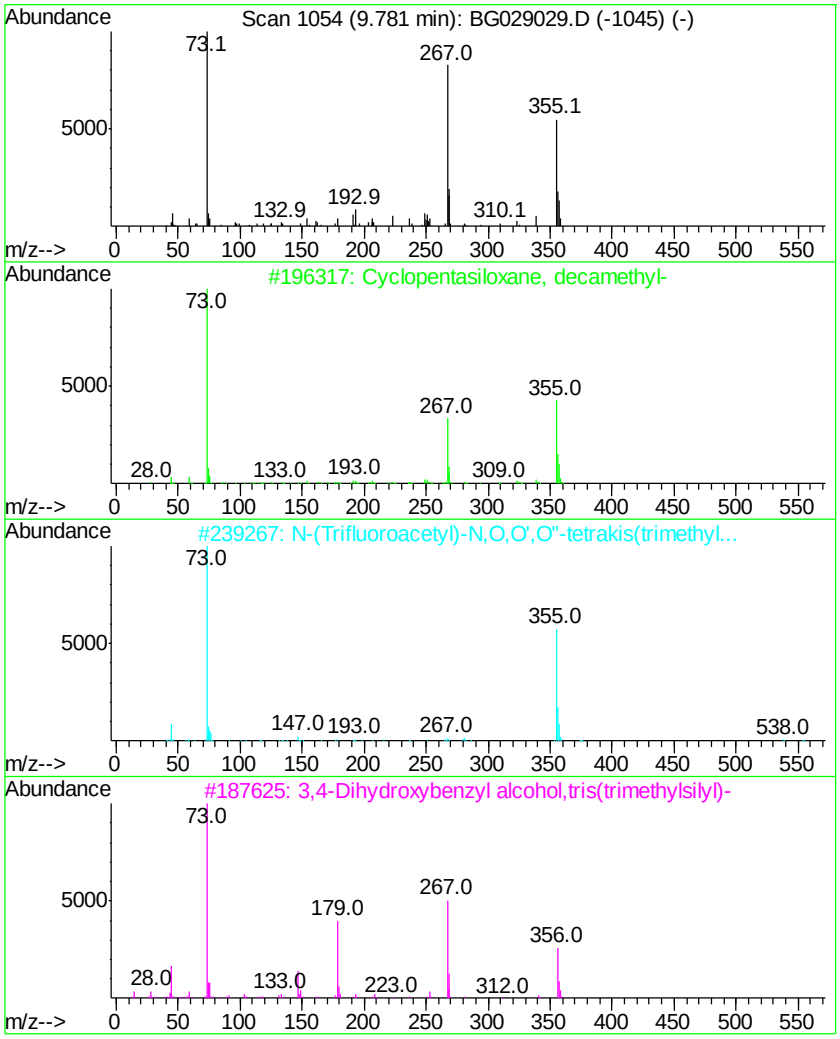
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

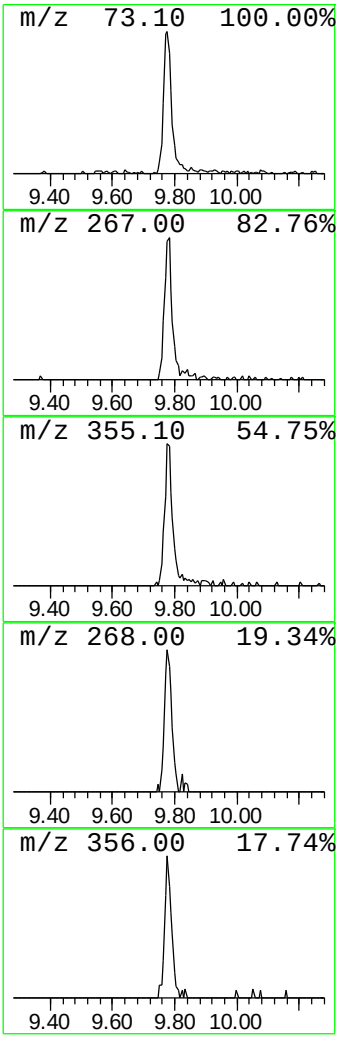
****

Peak Number 7 Cyclopentasiloxane, decamet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.78	9.51 ng	124606	Naphthalene-d8	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	64
2	N-(Trifluoroacetyl)-N,O,O',O''-t...	553	C22H42F3NO4Si4	1000072-26-7	47
3	3,4-Dihydroxybenzyl alcohol,tris...	356	C16H32O3Si3	068595-79-9	46
4	Benzeneethanamine, N-[(pentafluo...	563	C24H34F5NO3Si3	055429-13-5	43
5	Benzoic acid, 2,6-bis[(trimethyl...	370	C16H30O4Si3	003782-85-2	43





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Instrument : BNA_G
ClientSampleId : LIP-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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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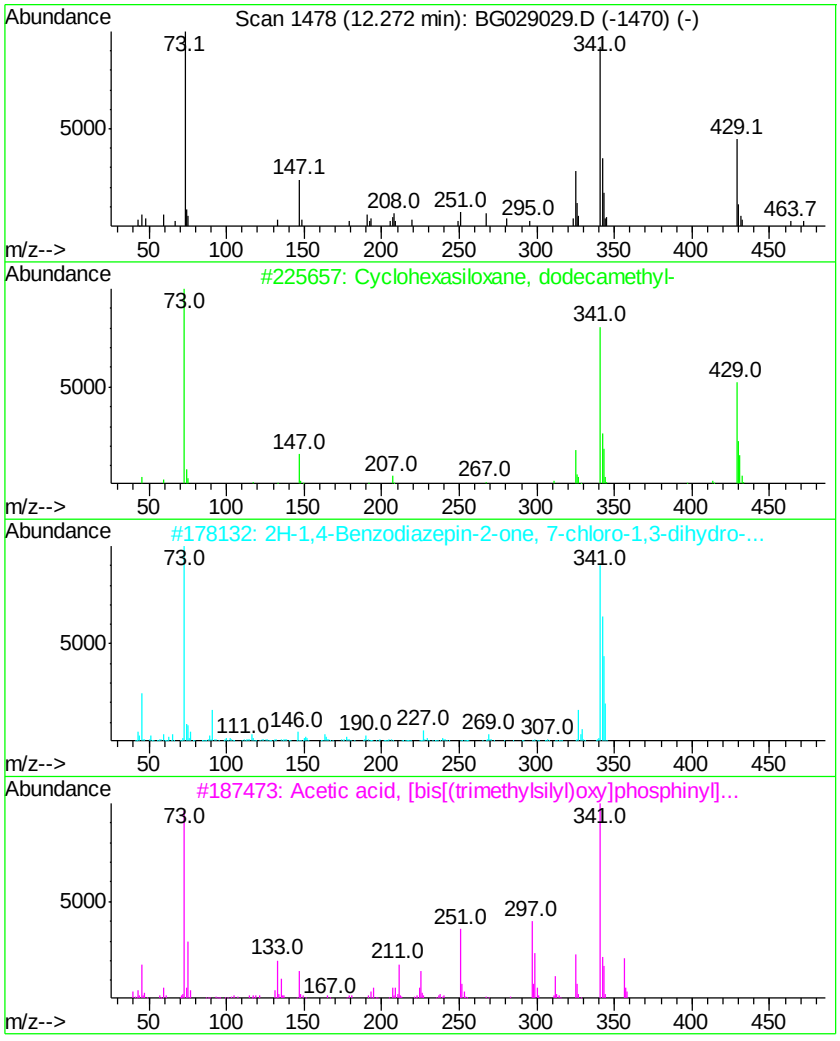
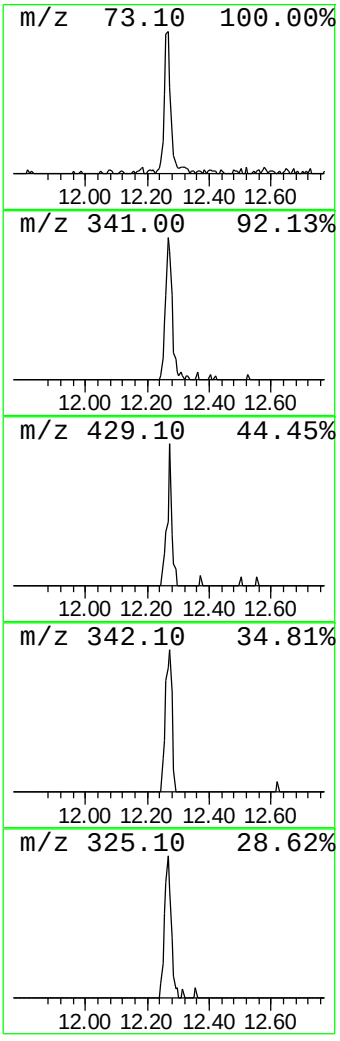
Peak Number 8 Cyclohexasiloxane, dodecame... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	4.53 ng	59369	Naphthalene-d8	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	83
2	2H-1,4-Benzodiazepin-2-one, 7-ch...	342	C18H19ClN2OSi	055299-24-6	32
3	Acetic acid, [bis[(trimethylsilv...	356	C11H29O5PSi3	053044-27-2	28
4	5-[4-(Dimethylamino)benzylidenea...	341	C21H19N5	299928-54-4	27
5	Cobalt, .eta.-5-cyclopentadienyl...	341	C22H18Co	1000161-22-8	27





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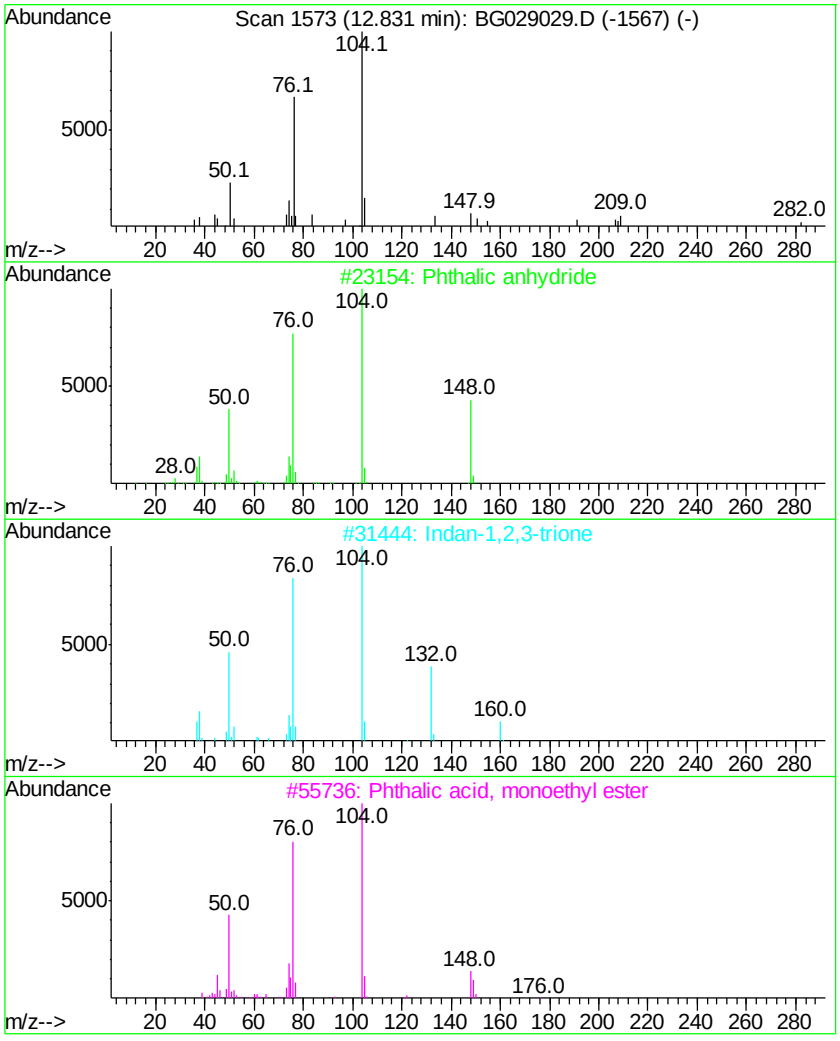
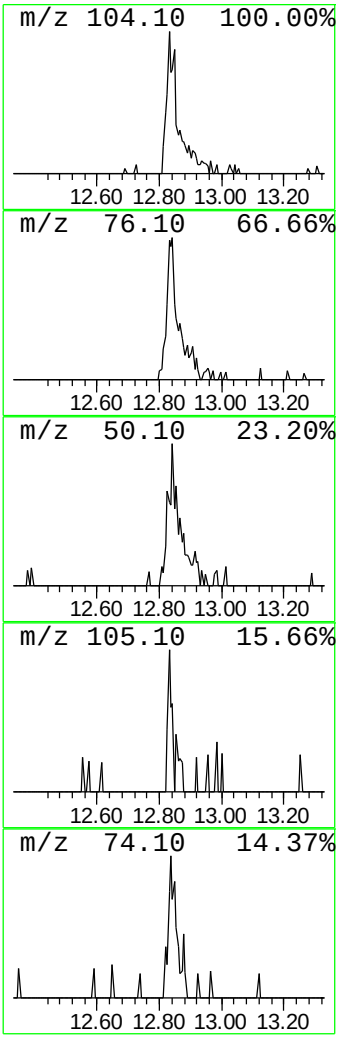
****

Peak Number 9 Phthalic anhydride Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	2.43 ng	31886	Naphthalene-d8	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	64
2	Indan-1,2,3-trione	160	C9H4O3	000938-24-9	64
3	Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	59
4	Ninhydrin	178	C9H6O4	000485-47-2	50
5	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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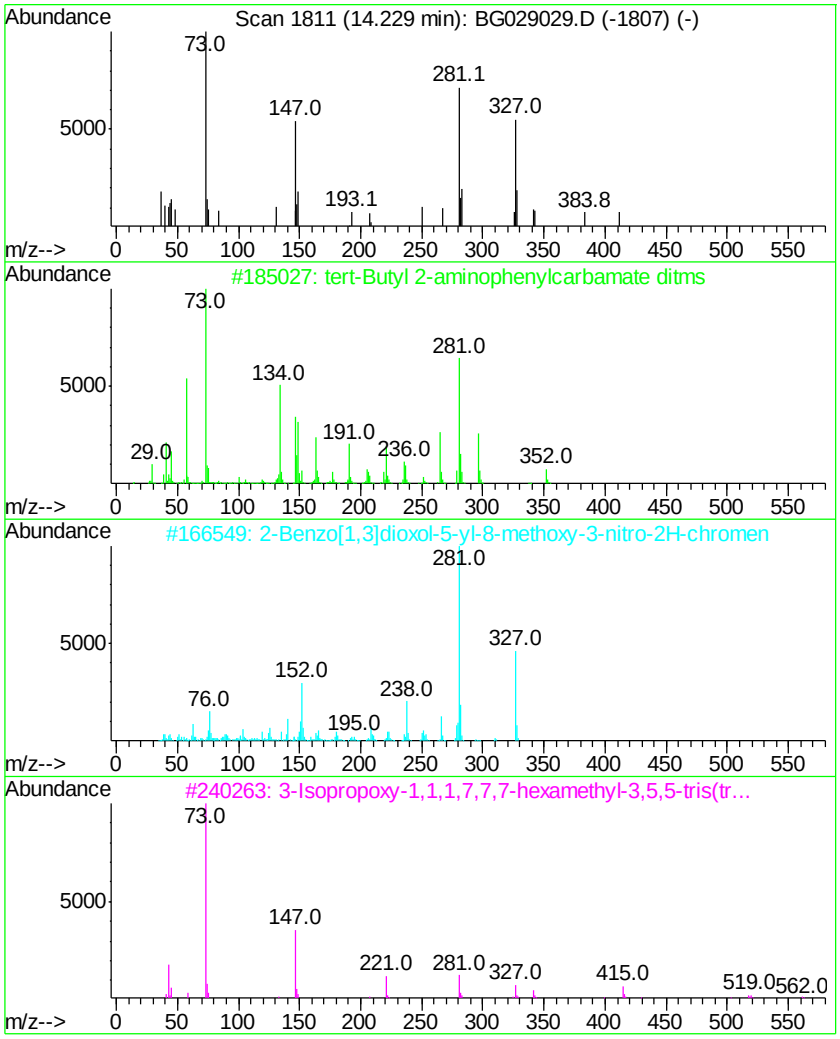
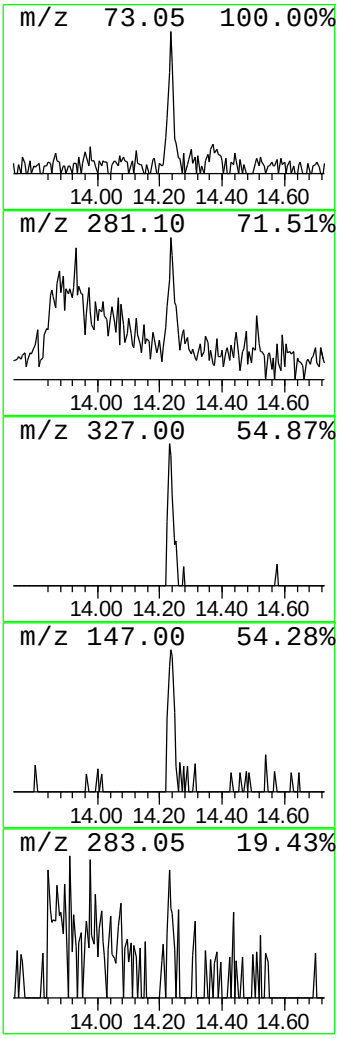
Peak Number 10 unknown14.23 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	3.18 ng	21351	Acenaphthene-d10	14.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	tert-Butyl 2-aminophenylcarbamat...	352	C17H32N2O2Si2	1000332-06-9	38
2	2-Benzo[1,3]dioxol-5-yl-8-methox...	327	C17H13NO6	1000275-63-1	38
3	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	35
4	3,6-Bis(N-dimethylamino)-9-ethyl...	281	C18H23N3	057103-04-5	27
5	Ethyl 4-[[(E)-(2-nitrophenyl)met...	298	C16H14N2O4	057707-09-2	27





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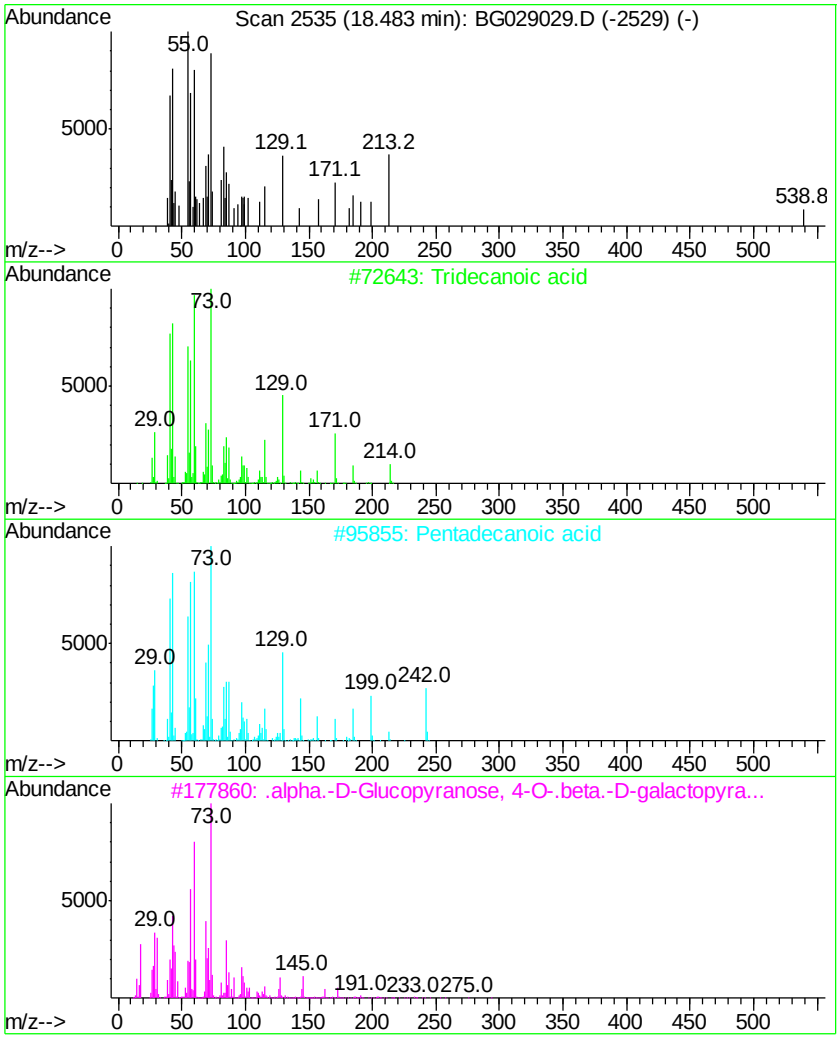
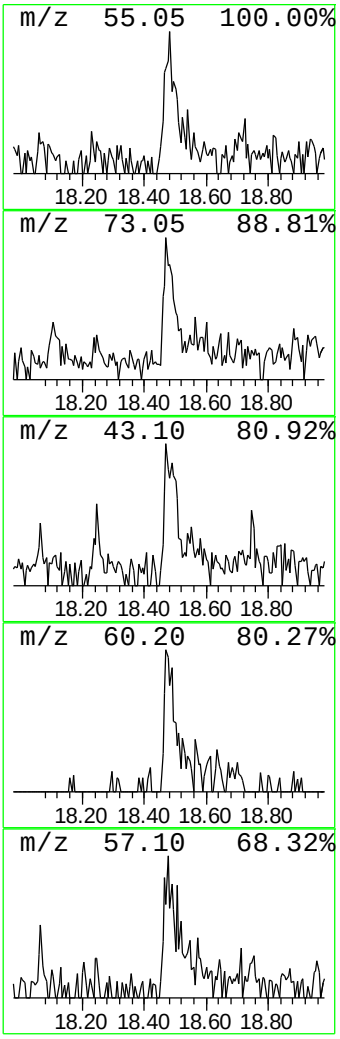
Peak Number 11 Tridecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.48	2.57 ng	49515	Phenanthrene-d10	17.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	53
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
3	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38
4	Undecanoic acid	186	C11H22O2	000112-37-8	38
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG100317\
Data File : BG029029.D
Acq On : 4 Oct 2017 7:10
Operator : SJ/JU
Sample : I5517-03
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : LIP-16

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.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
4-Penten-2-one, 4...	4.13	6.4	ng	62220	1	8.24	194351	20.0
3-Penten-2-one, 4...	4.74	74.0	ng	719537	1	8.24	194351	20.0
Cyclotrisiloxane,...	4.85	29.2	ng	283608	1	8.24	194351	20.0
Cyclotetrasiloxan...	7.33	53.2	ng	517118	1	8.24	194351	20.0
unknown7.77	7.77	71.6	ng	695761	1	8.24	194351	20.0
Cyclopentasiloxan...	9.78	9.5	ng	124606	2	11.06	262097	20.0
Cyclohexasiloxane...	12.27	4.5	ng	59369	2	11.06	262097	20.0
Phthalic anhydride	12.83	2.4	ng	31886	2	11.06	262097	20.0
unknown14.23	14.23	3.2	ng	21351	3	14.86	134427	20.0
Tridecanoic acid	18.48	2.6	ng	49515	4	17.61	385814	20.0