LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016429.D
Acq On : 15 Apr 2015 18:44
Operator : TP/IZ
Sample : PB82798BL
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB82798BL

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-BG040615.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	2.758	7	12	23	rVB3	47810	92724	2.71%	0.353%
2	4.180	249	254	266	rBV	337046	429309	12.54%	1.636%
3	4.791	351	358	370	rBV	2192101	3109627	90.86%	11.854%
4	5.273	433	440	448	rBV	839282	1198513	35.02%	4.569%
5	5.860	535	540	546	rBV	119938	170737	4.99%	0.651%
6	6.877	704	713	720	rBV	899243	1371581	40.08%	5.228%
7	7.212	762	770	780	rBV	886831	1384999	40.47%	5.279%
8	7.670	841	848	856	rBV	304828	466371	13.63%	1.778%
9	7.740	856	860	869	rVB2	26264	41305	1.21%	0.157%
10	7.987	895	902	909	rBV	816829	1295978	37.87%	4.940%
11	8.827	1035	1045	1055	rBV	663215	1053129	30.77%	4.014%
12	10.455	1315	1322	1331	rBV	461186	775634	22.66%	2.957%
13	12.934	1737	1744	1753	rBV	1978692	2759509	80.63%	10.519%
14	14.315	1972	1979	1987	rBV2	804907	1203583	35.17%	4.588%
15	15.807	2227	2233	2240	rVB	979225	1346022	39.33%	5.131%
16	17.059	2441	2446	2451	rBV	892419	1211717	35.41%	4.619%
17	18.933	2761	2765	2768	rBV5	81593	145154	4.24%	0.553%
18	19.685	2888	2893	2898	rVB	2774789	3422402	100.00%	13.046%
19	20.543	3036	3039	3049	rVB2	177659	371420	10.85%	1.416%
20	20.778	3076	3079	3086	rBV2	142348	236359	6.91%	0.901%
21	20.849	3088	3091	3095	rBV2	185517	287676	8.41%	1.097%
22	21.142	3138	3141	3144	rBV	173507	216576	6.33%	0.826%
23	21.236	3153	3157	3161	rVB	1029042	1235241	36.09%	4.709%
24	21.765	3242	3247	3254	rVB	663775	1285923	37.57%	4.902%
25	23.469	3533	3537	3546	rVB2	656395	1122124	32.79%	4.277%

Sum of corrected areas: 26233613

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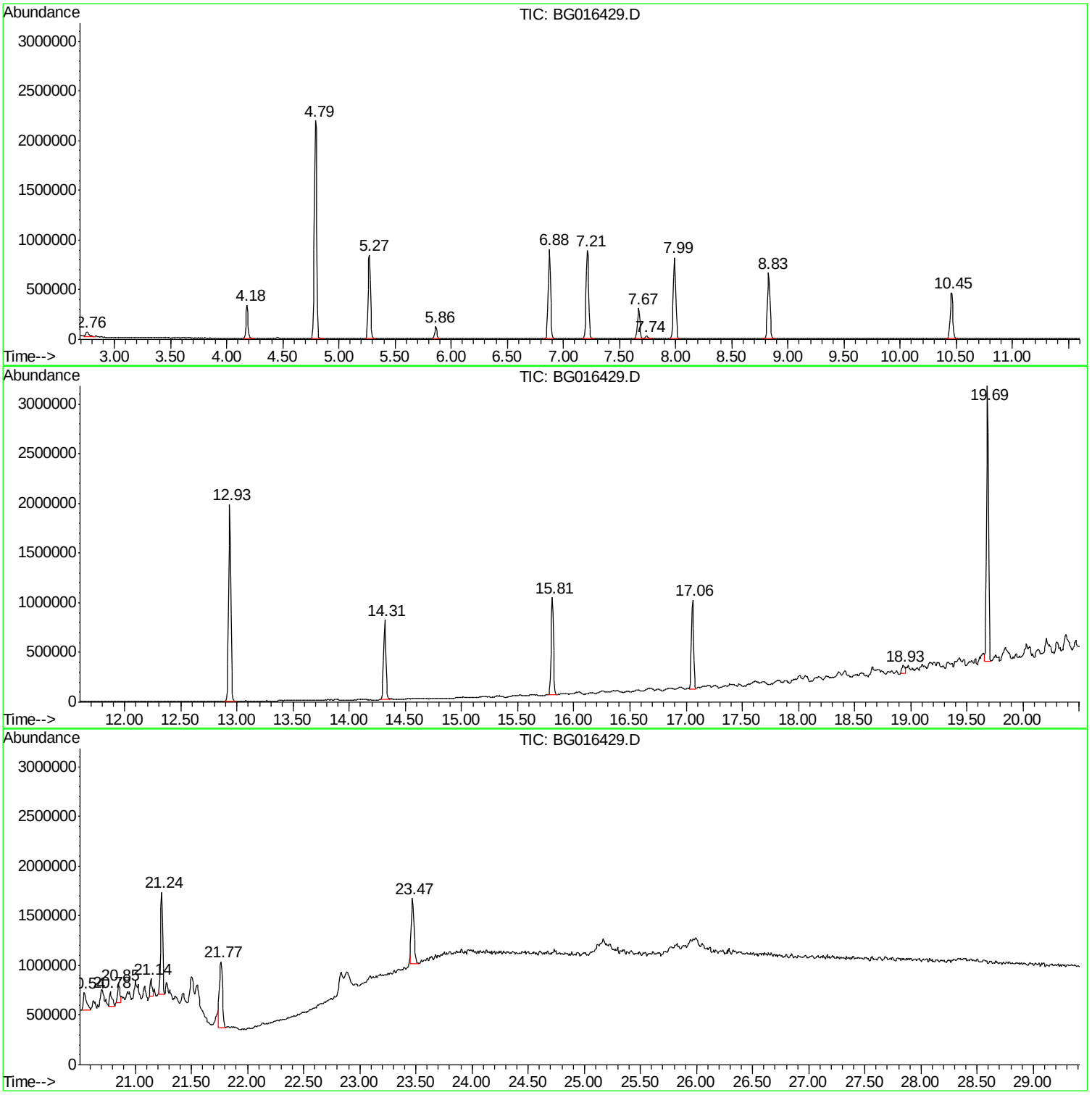
ClientSampleId : PB82798BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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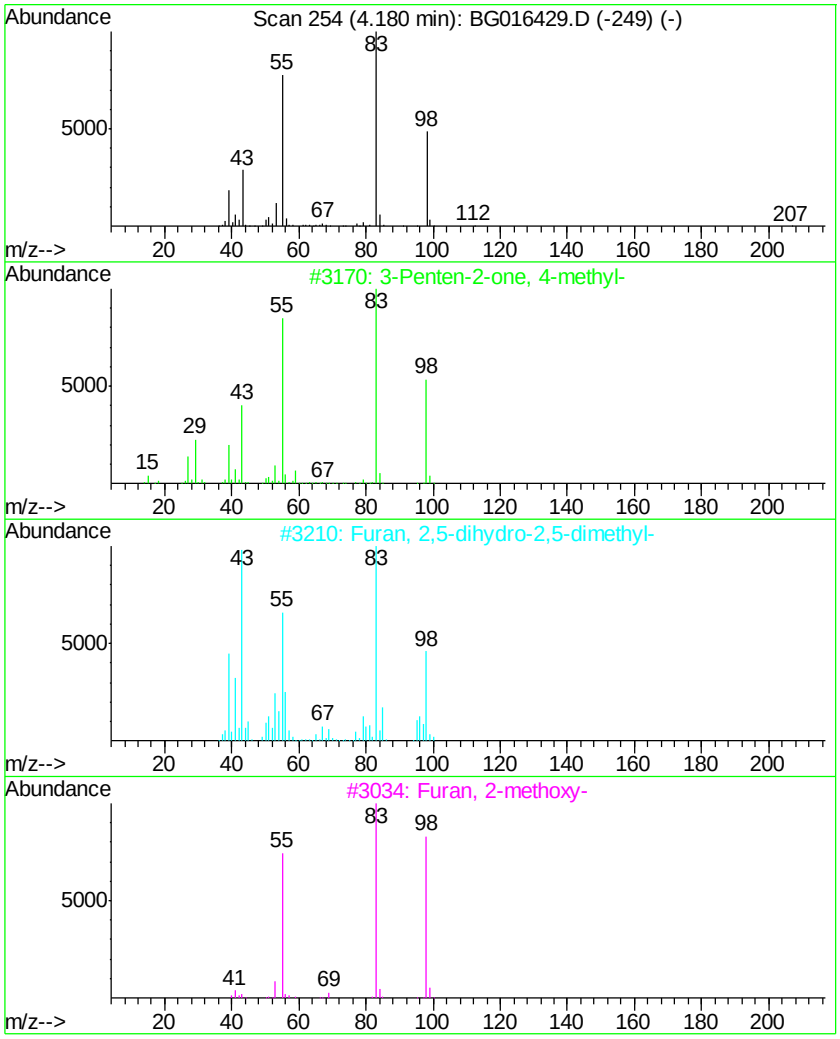
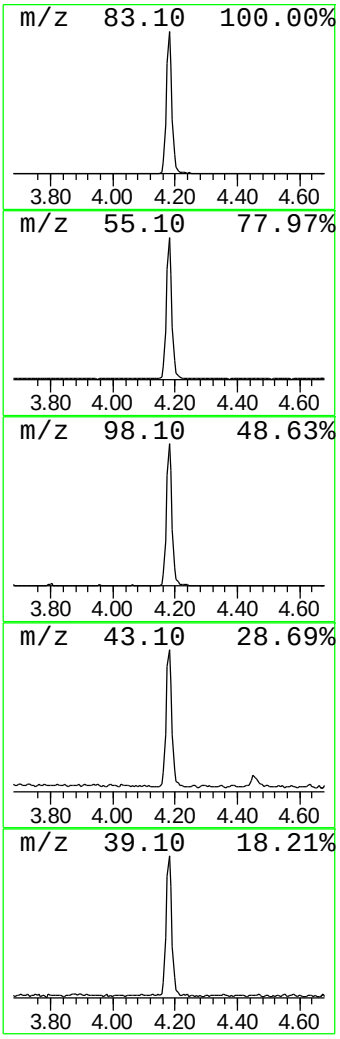
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	18.41 ng	429309	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	Furan, 2,5-dihydro-2,5-dimethyl-	98	C6H10O	059242-27-2	80
3	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
5	Cyclohexane, methyl-	98	C7H14	000108-87-2	72





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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TIC Integration Parameters: LSCINT.P

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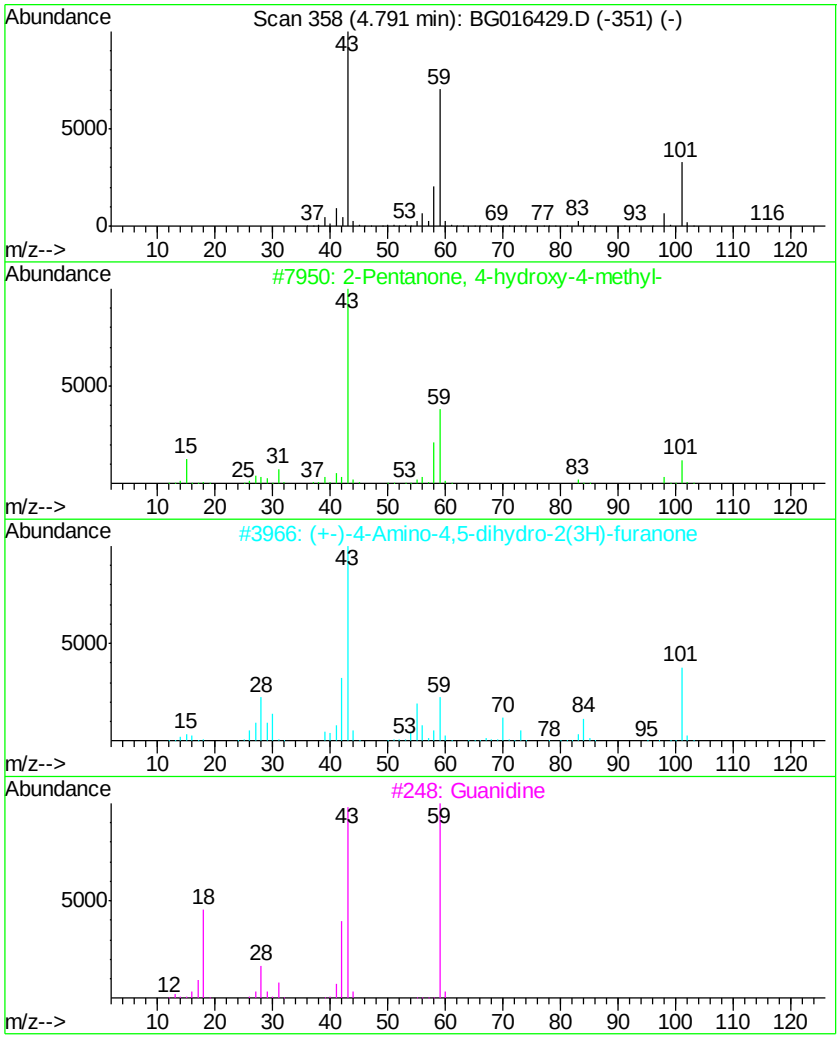
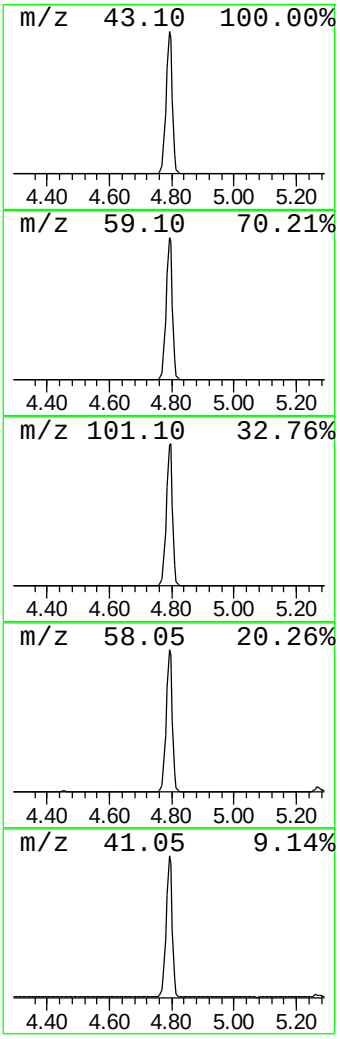
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	133.35 ng	3109630	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38
3	Guanidine	59	CH5N3	000113-00-8	38
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





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Sample : PB82798BL
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Instrument : BNA_G
ClientSampleId : PB82798BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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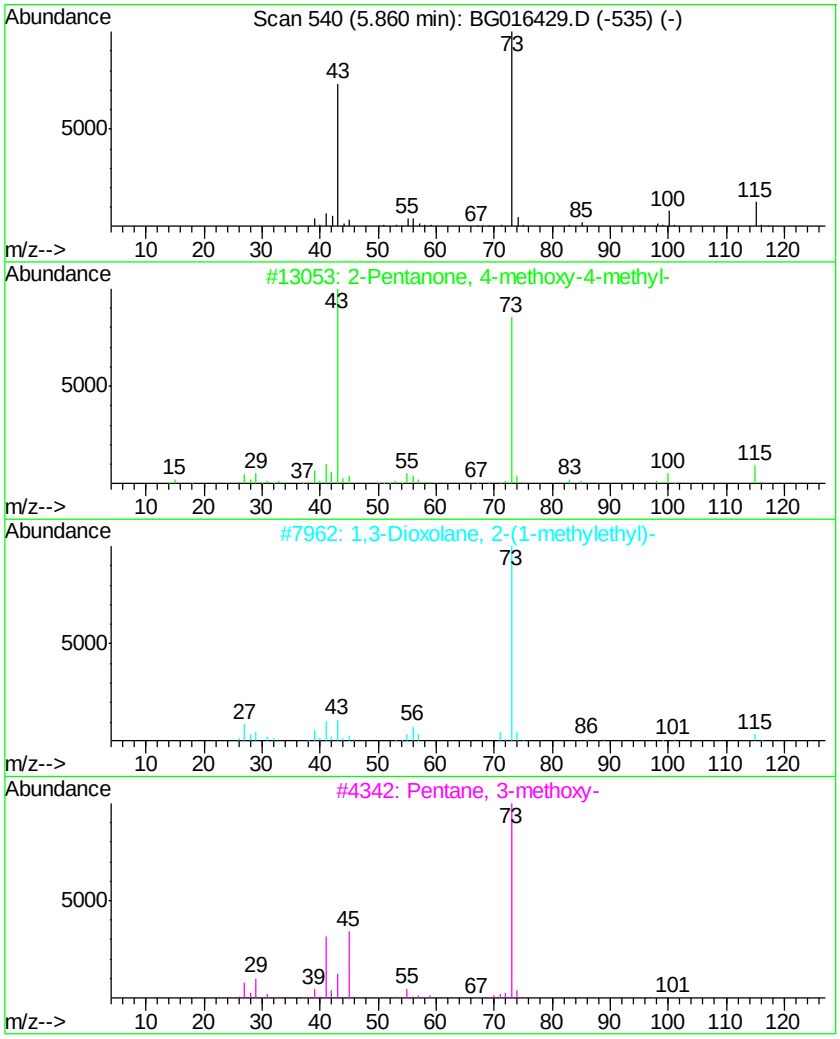
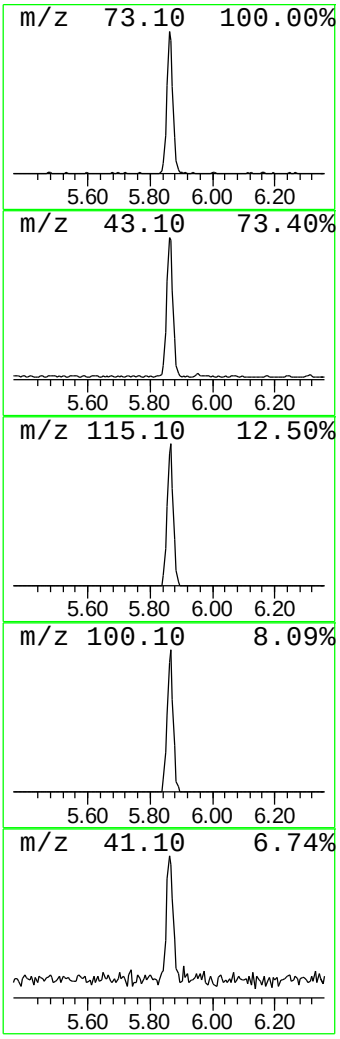
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.86	7.32 ng	170737	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
4	Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
5	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	9





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Sample : PB82798BL
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB82798BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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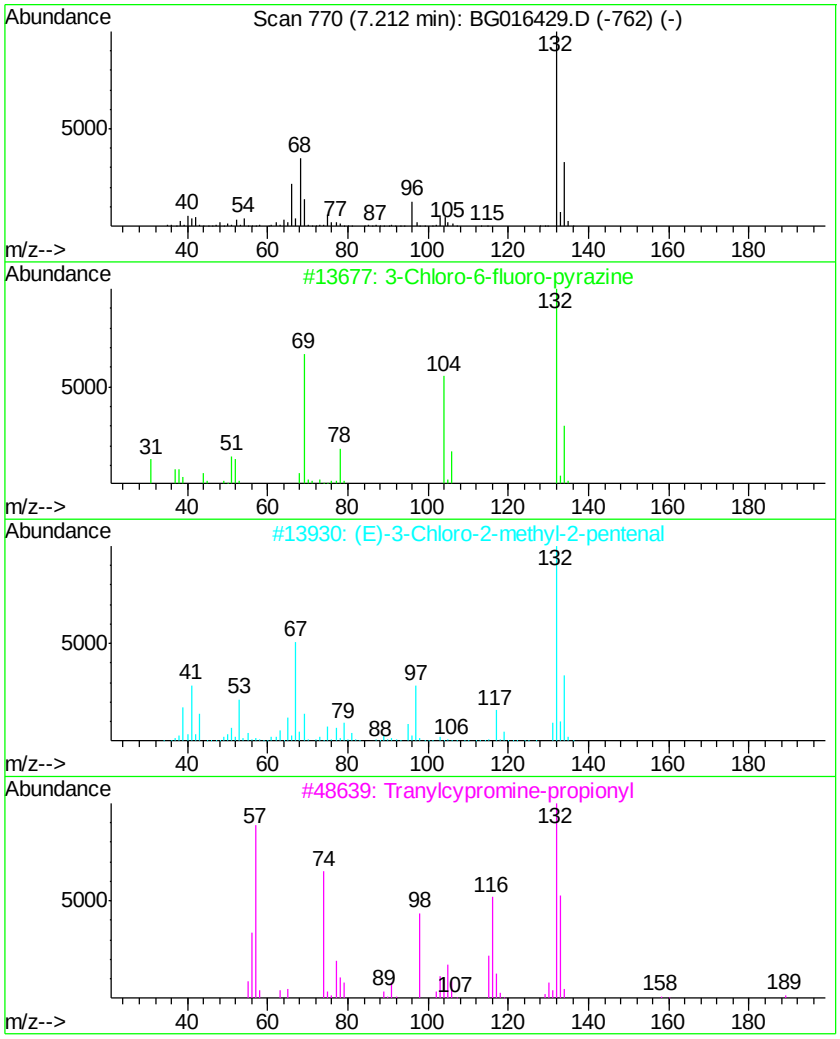
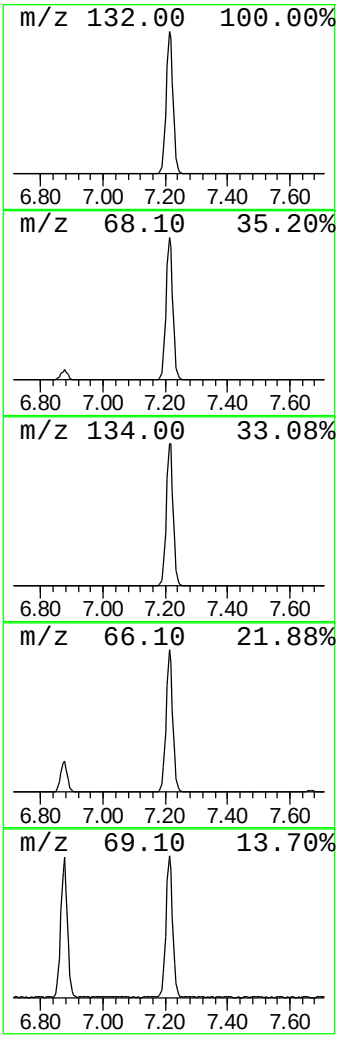
****

Peak Number 5 unknown7.21 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	59.39 ng	1385000	1,4-Dichlorobenzene-d4	7.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9





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Instrument : BNA_G
ClientSampleId : PB82798BL

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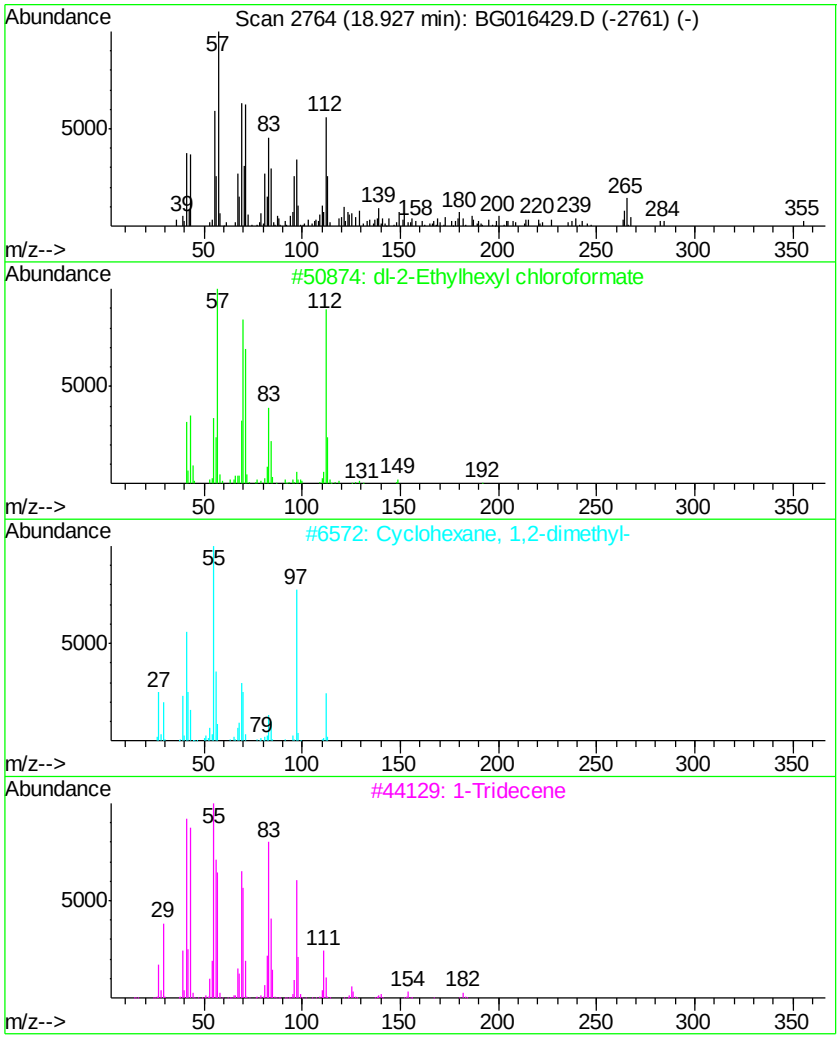
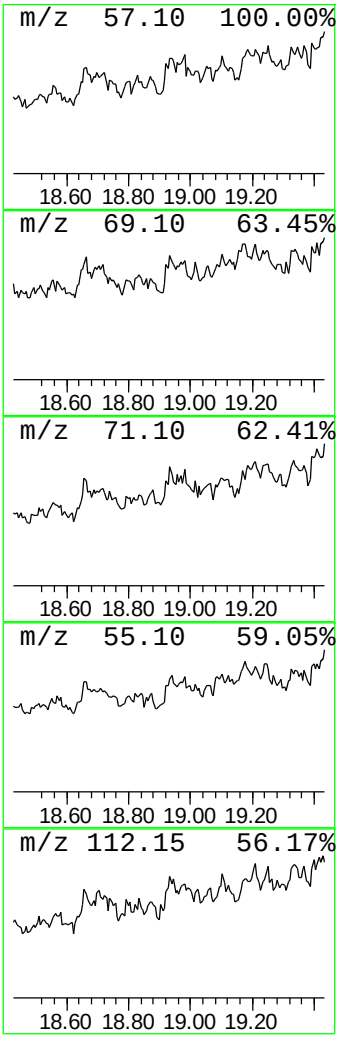
Peak Number 7 unknown18.93 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.93	2.40 ng	145154	Phenanthrene-d10	17.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-2-Ethylhexyl chloroformate	192	C9H17ClO2	024468-13-1	43
2	Cyclohexane, 1,2-dimethyl-	112	C8H16	000583-57-3	27
3	1-Tridecene	182	C13H26	002437-56-1	25
4	Cyclohexanone, 4-methyl-	112	C7H12O	000589-92-4	22
5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	014073-97-3	22





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Sample : PB82798BL
Misc :
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Instrument : BNA_G
ClientSampleId : PB82798BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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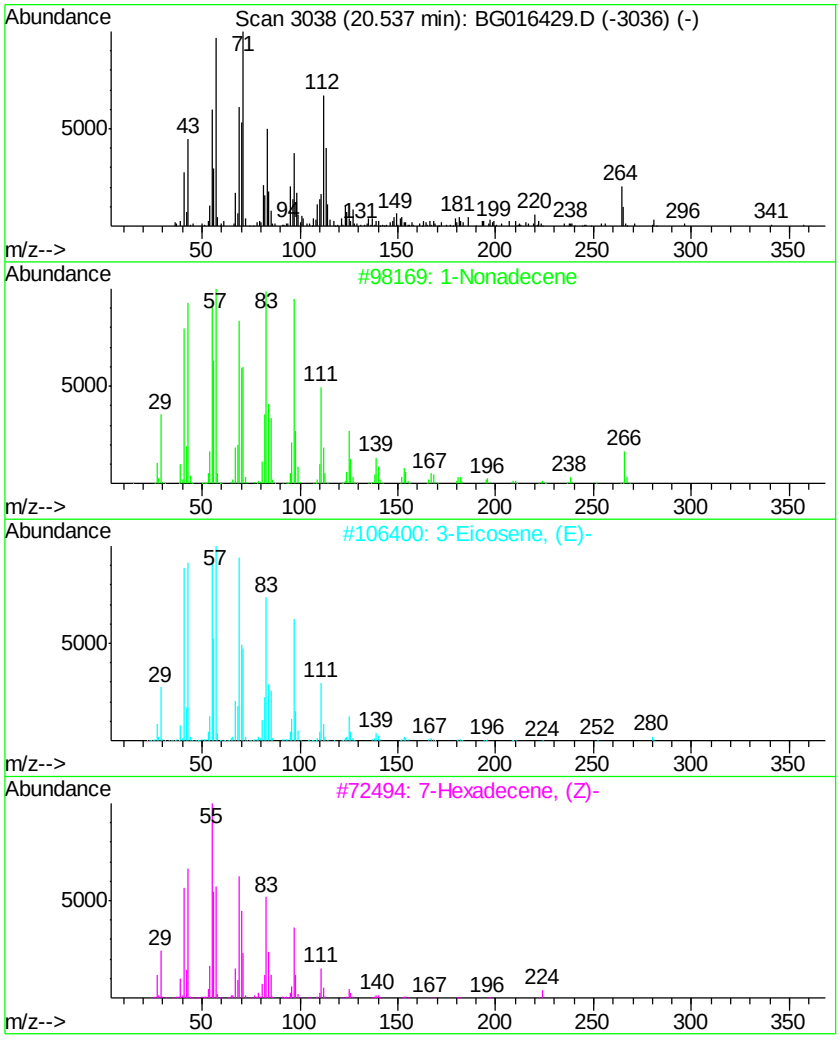
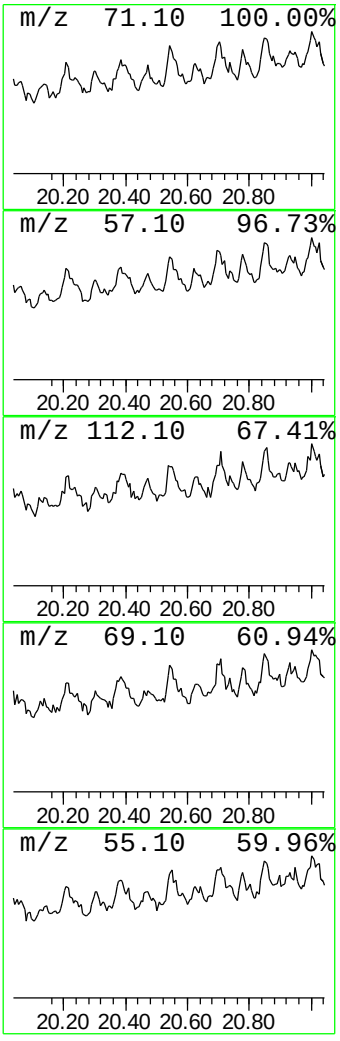
Peak Number 8 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.54	6.01 ng	371420	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	50
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	38
3	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	38
4	1-Tetradecanol	214	C14H30O	000112-72-1	38
5	Cyclododecane	168	C12H24	000294-62-2	35





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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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TIC Library : C:\DATABASE\NIST02.L
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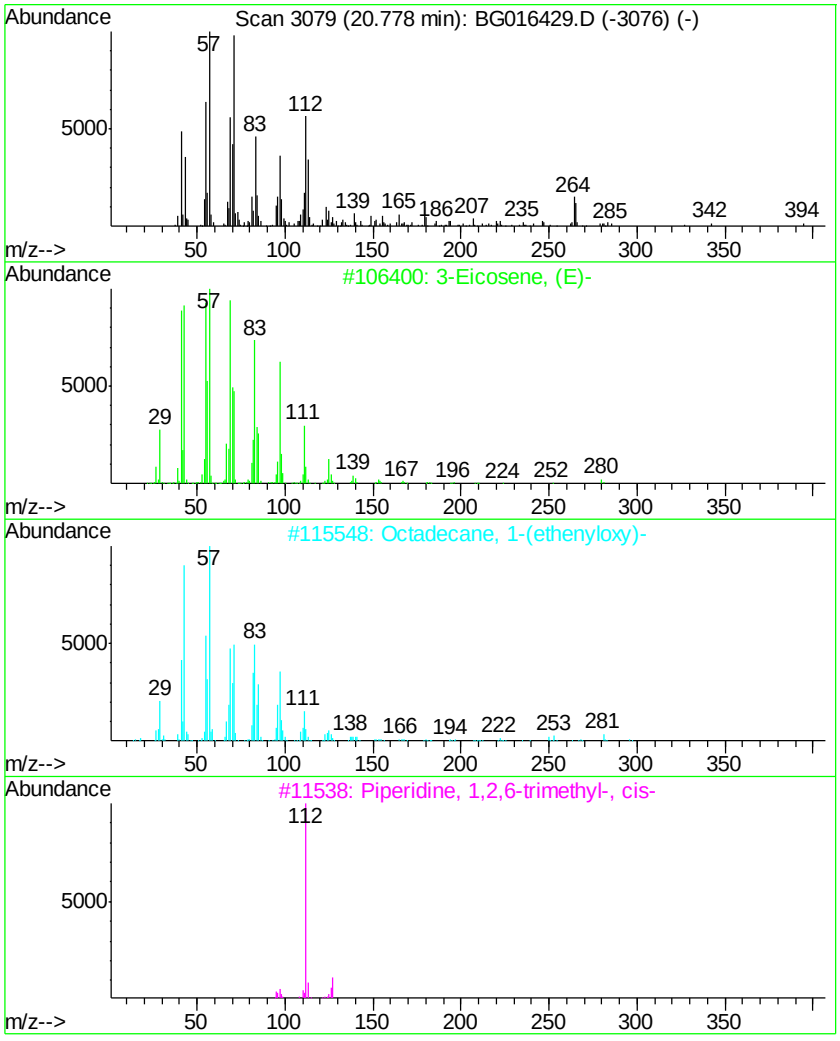
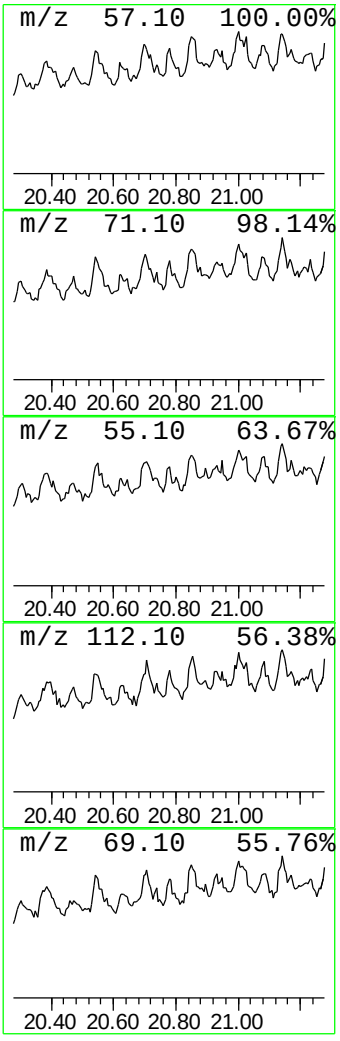
Peak Number 9 unknown20.78 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	3.83 ng	236359	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	46
2	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	38
3	Piperidine, 1,2,6-trimethyl-, cis-	127	C8H17N	002439-13-6	38
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	35
5	Cyclohexane, 1,2-dimethyl-	112	C8H16	000583-57-3	35





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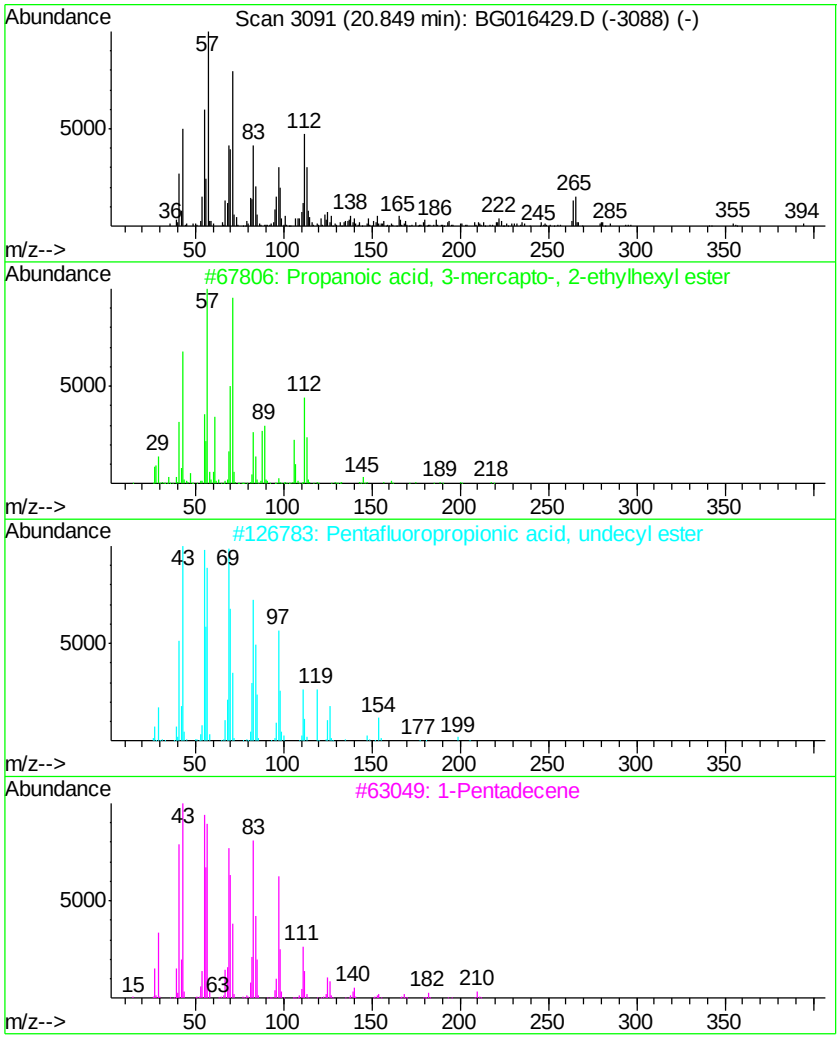
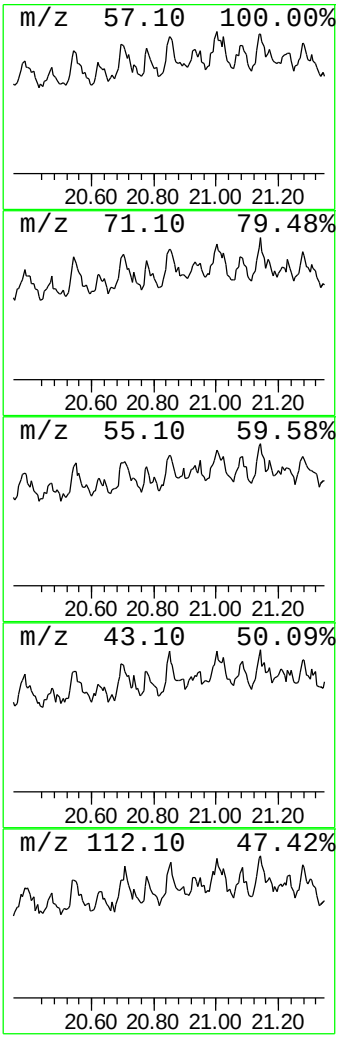
Peak Number 10 Propanoic acid, 3-mercapto-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	4.66 ng	287676	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 3-mercapto-, 2-e...	218	C11H22O2S	050448-95-8	52
2	Pentafluoropropionic acid, undec...	318	C14H23F5O2	1000283-04-0	41
3	1-Pentadecene	210	C15H30	013360-61-7	38
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	38
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	30





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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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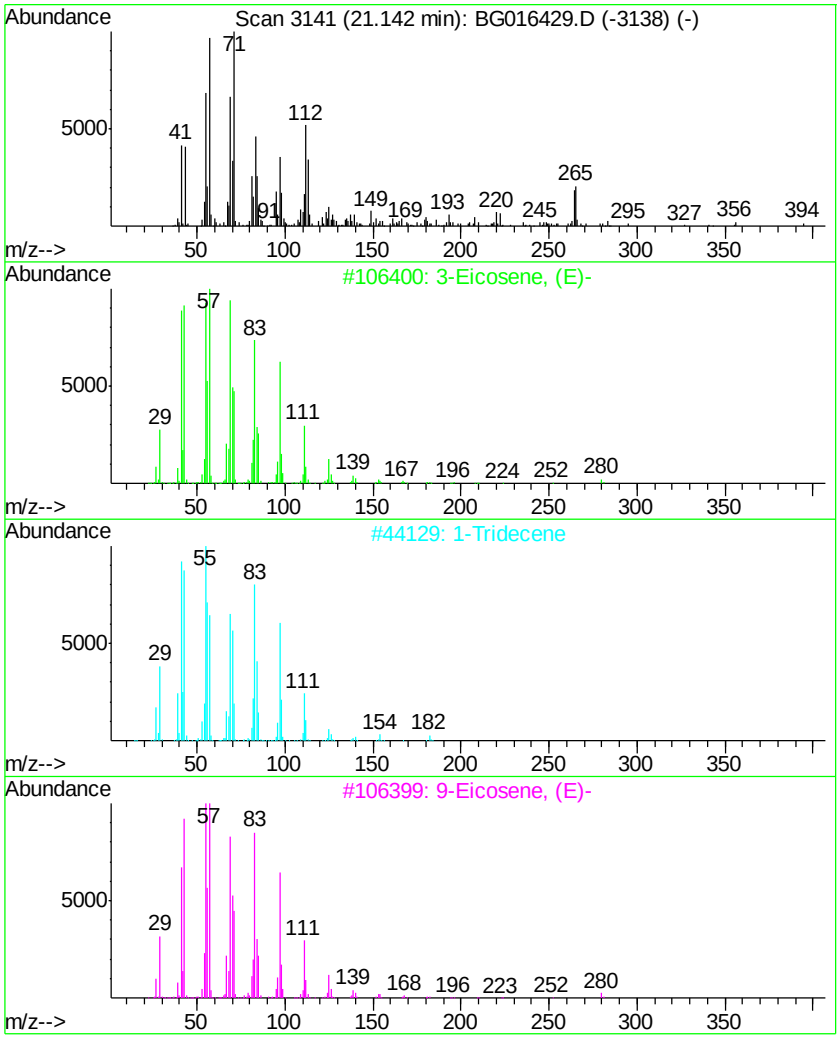
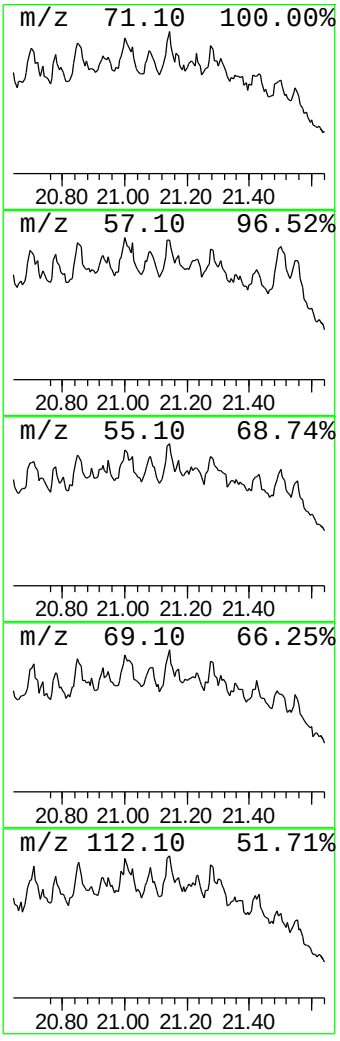
Peak Number 11 3-Eicosene, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.14	3.51 ng	216576	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	51
2	1-Tridecene	182	C13H26	002437-56-1	51
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	50
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	47
5	Oleic Acid	282	C18H34O2	000112-80-1	30





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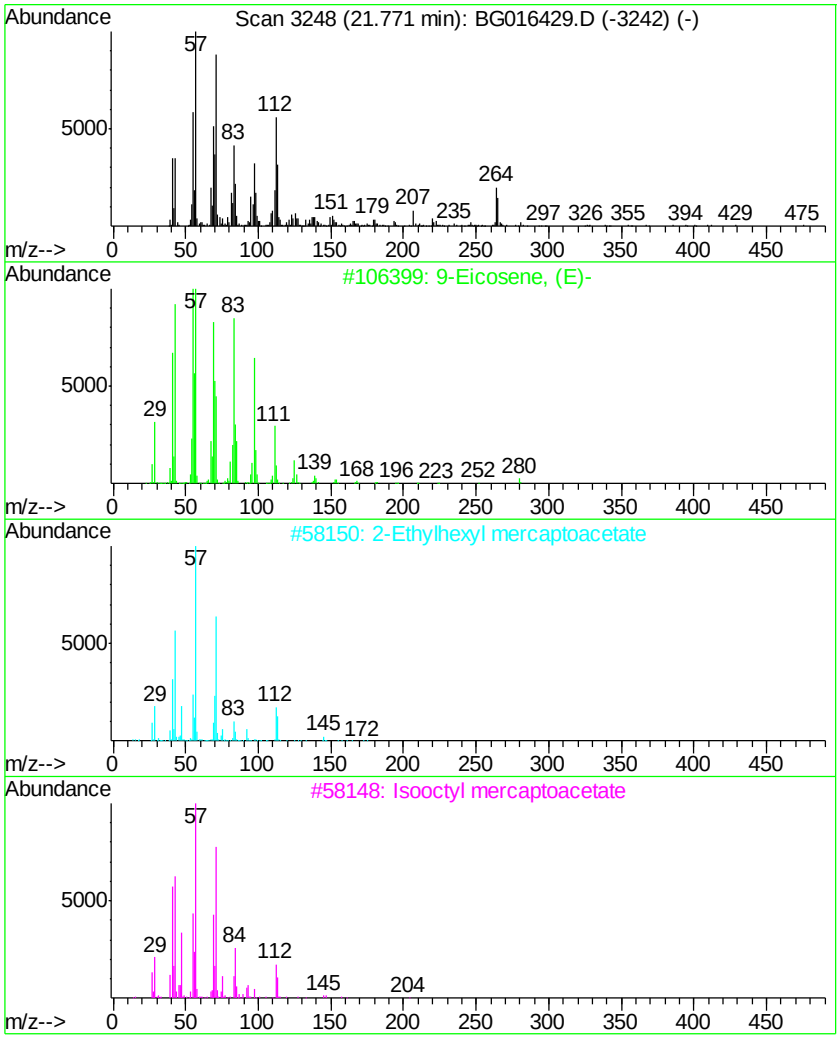
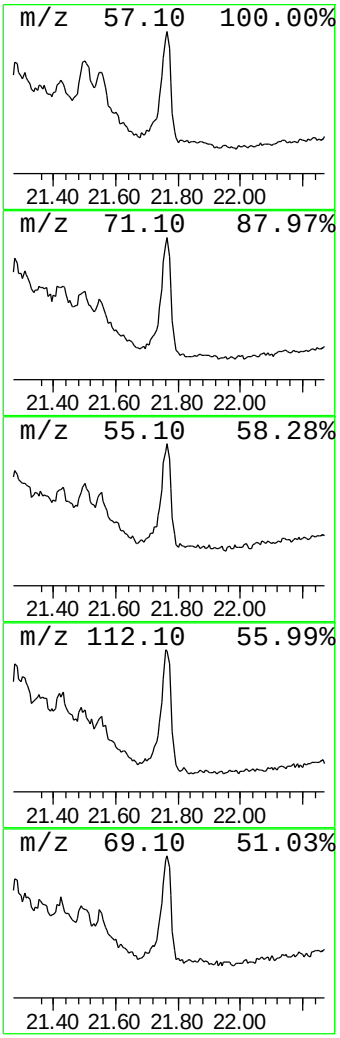
****

Peak Number 12 9-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.77	20.82 ng	1285920	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	52
2	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	47
3	Isooctyl mercaptoacetate	204	C10H20O2S	025103-09-7	43
4	Oleic Acid	282	C18H34O2	000112-80-1	38
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016429.D
Acq On : 15 Apr 2015 18:44
Operator : TP/IZ
Sample : PB82798BL
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PB82798BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.18	18.4	ng	429309	1	7.67	466371	20.0
2-Pentanone, 4-hy...	4.79	133.3	ng	3109630	1	7.67	466371	20.0
2-Pentanone, 4-me...	5.86	7.3	ng	170737	1	7.67	466371	20.0
unknown7.21	7.21	59.4	ng	1385000	1	7.67	466371	20.0
unknown18.93	18.93	2.4	ng	145154	4	17.06	1211720	20.0
1-Nonadecene	20.54	6.0	ng	371420	5	21.24	1235240	20.0
unknown20.78	20.78	3.8	ng	236359	5	21.24	1235240	20.0
Propanoic acid, 3...	20.85	4.7	ng	287676	5	21.24	1235240	20.0
3-Eicosene, (E)-	21.14	3.5	ng	216576	5	21.24	1235240	20.0
9-Eicosene, (E)-	21.77	20.8	ng	1285920	5	21.24	1235240	20.0