LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087694.D
Acq On : 5 Jun 2016 7:41
Operator : UM/SJ
Sample : H3344-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15

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_F\METHODS\8270-BF060416.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	1.770	15	16	21	rVB	343042	423700	7.81%	0.921%
2	1.907	26	28	47	rVB	2275047	4359051	80.32%	9.477%
3	2.147	47	49	91	rVB	100160	541783	9.98%	1.178%
4	3.827	193	196	199	rBV	950048	1466982	27.03%	3.189%
5	5.039	300	302	308	rVB	150499	177988	3.28%	0.387%
6	5.313	324	326	329	rVB	181783	191903	3.54%	0.417%
7	5.450	333	338	340	rBV	2081170	2172114	40.02%	4.722%
8	5.679	356	358	362	rBV2	1078930	1395206	25.71%	3.033%
9	6.399	418	421	424	rVB2	61482	128173	2.36%	0.279%
10	6.479	424	428	430	rBV	1392472	1317375	24.27%	2.864%
11	6.627	438	441	443	rVV	2777826	3188120	58.74%	6.931%
12	6.684	444	446	449	rVV	485605	544755	10.04%	1.184%
13	6.730	449	450	453	rVB	135424	107635	1.98%	0.234%
14	6.856	459	461	465	rVB	855713	758857	13.98%	1.650%
15	6.913	465	466	468	rBV	77814	92014	1.70%	0.200%
16	7.016	472	475	477	rVV	2751438	2881613	53.09%	6.265%
17	7.119	481	484	487	rVB	2017989	1981913	36.52%	4.309%
18	7.427	508	511	513	rVB	2137619	2628863	48.44%	5.715%
19	7.473	513	515	517	rBV	60806	58754	1.08%	0.128%
20	7.896	548	552	553	rBV3	233844	285967	5.27%	0.622%
21	7.930	553	555	559	rVV	164569	259013	4.77%	0.563%
22	8.170	571	576	578	rVV2	3846914	5427278	100.00%	11.799%
23	8.216	578	580	582	rVB	177607	146557	2.70%	0.319%
24	8.673	619	620	624	rVB	47949	69973	1.29%	0.152%
25	8.856	634	636	638	rBV	57189	55992	1.03%	0.122%
26	8.959	642	645	647	rVV	438642	457482	8.43%	0.995%
27	9.222	665	668	671	rVB	3078613	4122461	75.96%	8.963%
28	9.325	675	677	678	rVB	72885	69934	1.29%	0.152%
29	9.759	712	715	717	rVB	402141	360968	6.65%	0.785%
30	9.896	725	727	729	rBV	1225475	1113101	20.51%	2.420%
31	10.136	746	748	753	rBV	185270	185737	3.42%	0.404%
32	10.685	793	796	799	rBV	2191737	2520625	46.44%	5.480%
33	11.256	842	846	849	rBV3	25876	59504	1.10%	0.129%
34	11.382	854	857	859	rVB	1147861	1154595	21.27%	2.510%

LSC Area Percent Report

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Data File : BF087694.D
Acq On : 5 Jun 2016 7:41
Operator : UM/SJ
Sample : H3344-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15

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_F\METHODS\8270-BF060416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.971	993	996	998	rBV	3319532	3544456	65.31%	7.706%
36	14.011	1084	1087	1089	rBV	1147427	1019217	18.78%	2.216%
37	15.440	1209	1212	1215	rBV	620301	726986	13.40%	1.581%

Sum of corrected areas: 45996645

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
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Sample : H3344-06
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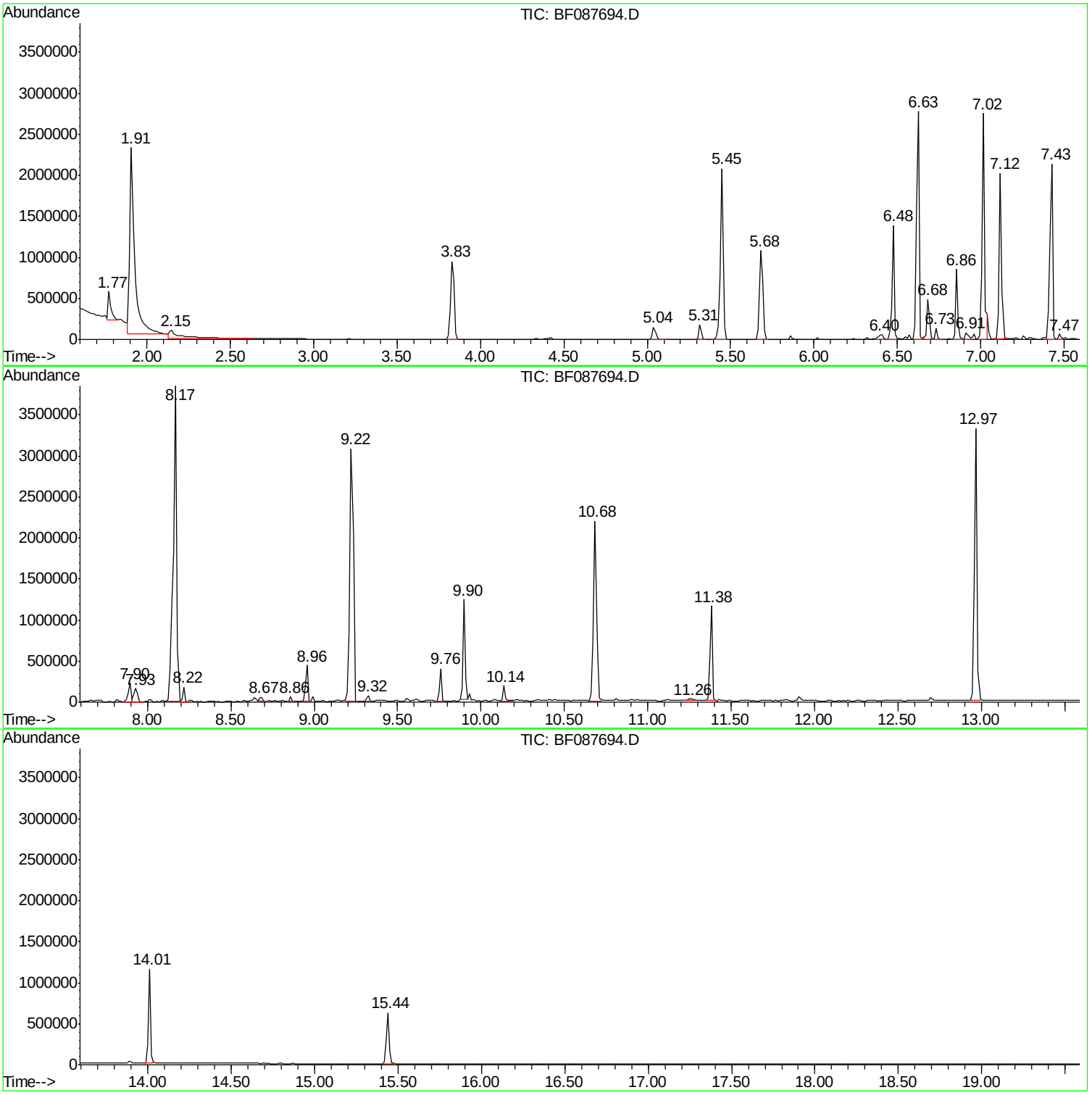
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
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Acq On : 5 Jun 2016 7:41
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Sample : H3344-06
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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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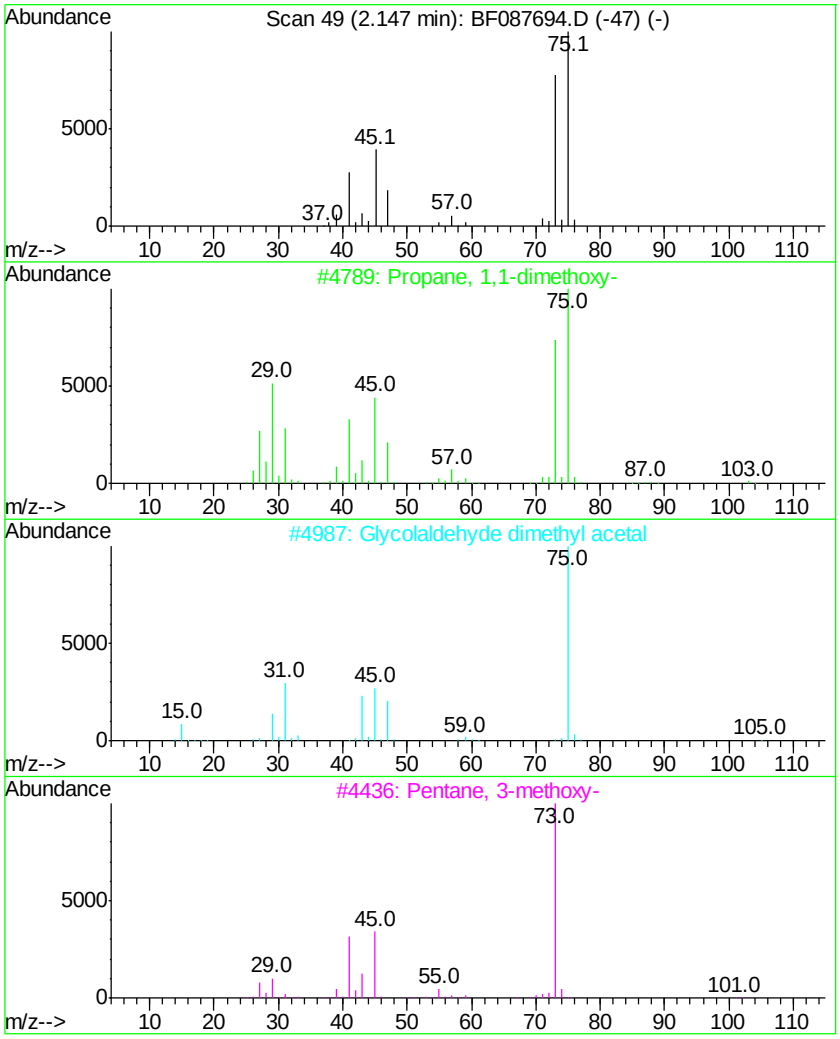
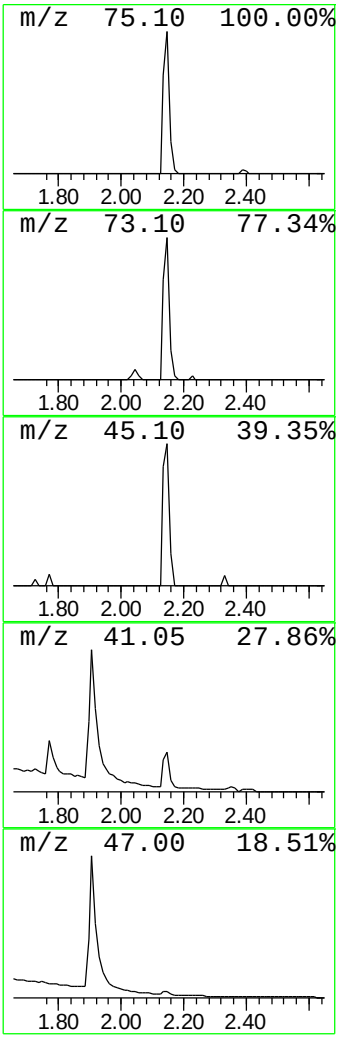
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	14.28 ng	541783	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	33
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
4	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	17
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087694.D
Acq On : 5 Jun 2016 7:41
Operator : UM/SJ
Sample : H3344-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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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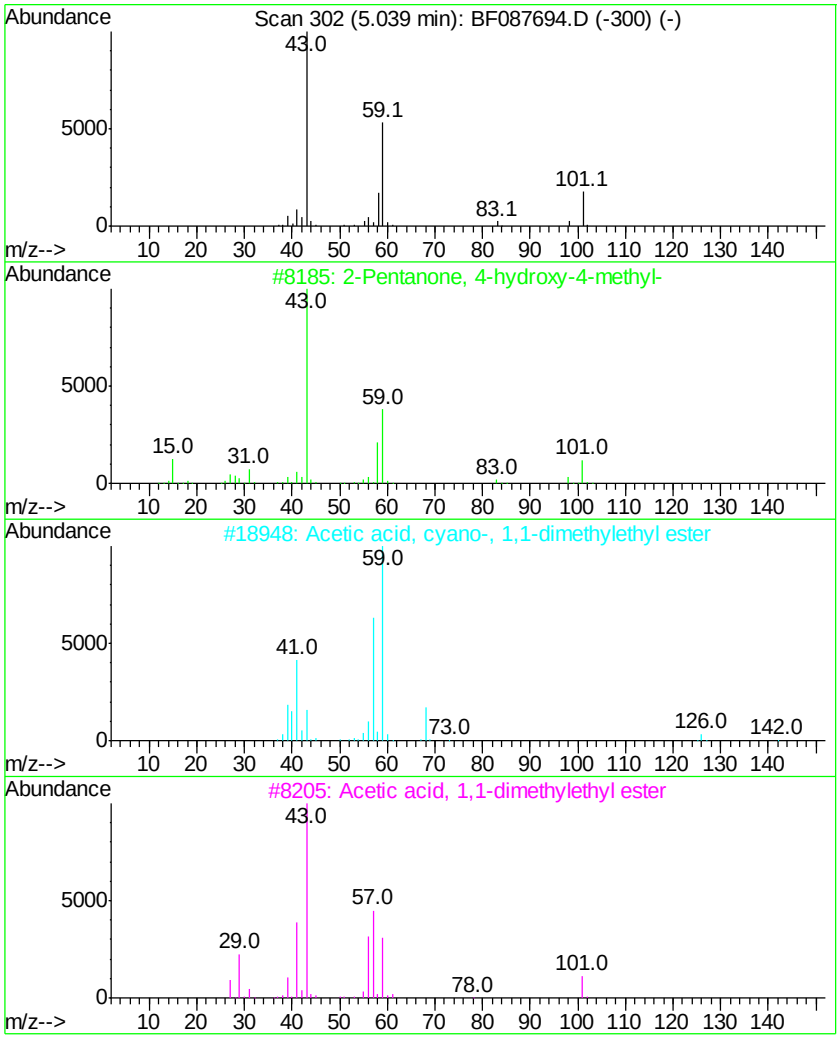
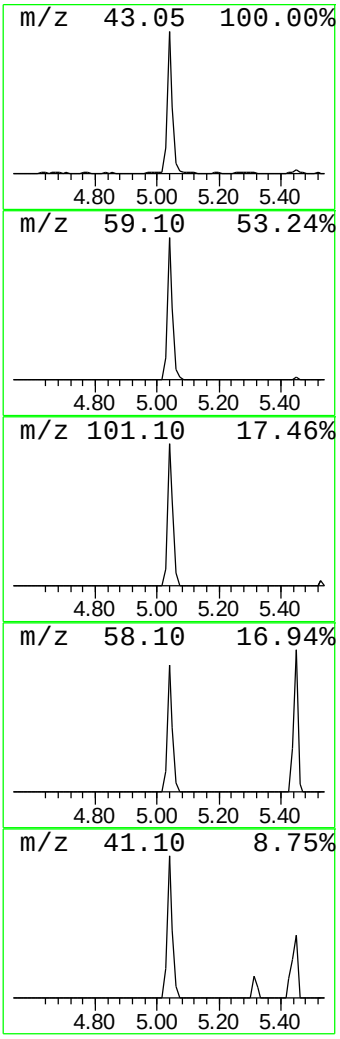
Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	4.69 ng	177988	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
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Operator : UM/SJ
Sample : H3344-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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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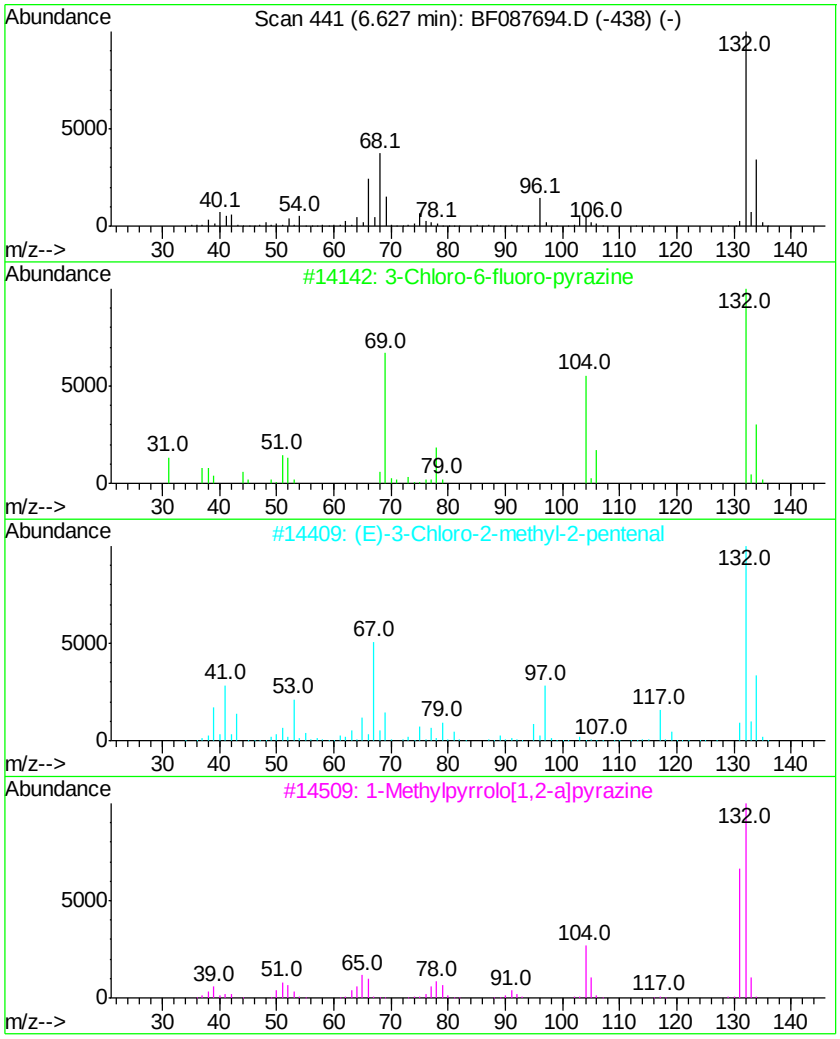
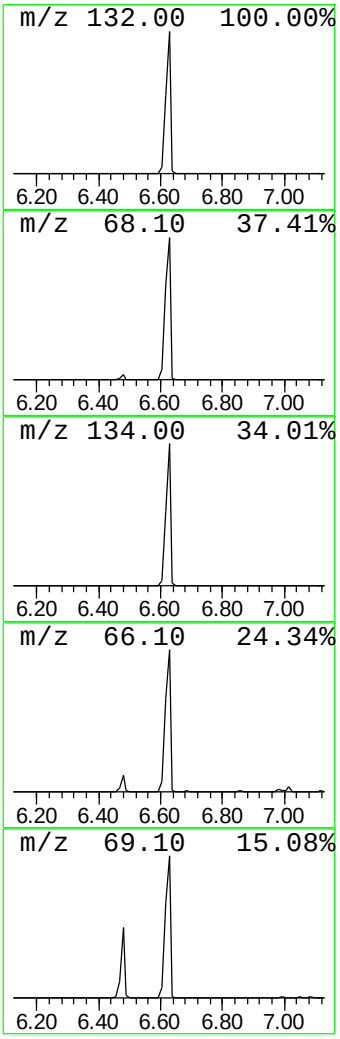
Peak Number 8 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	84.02 ng	3188120	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF060416\
Data File : BF087694.D
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Operator : UM/SJ
Sample : H3344-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.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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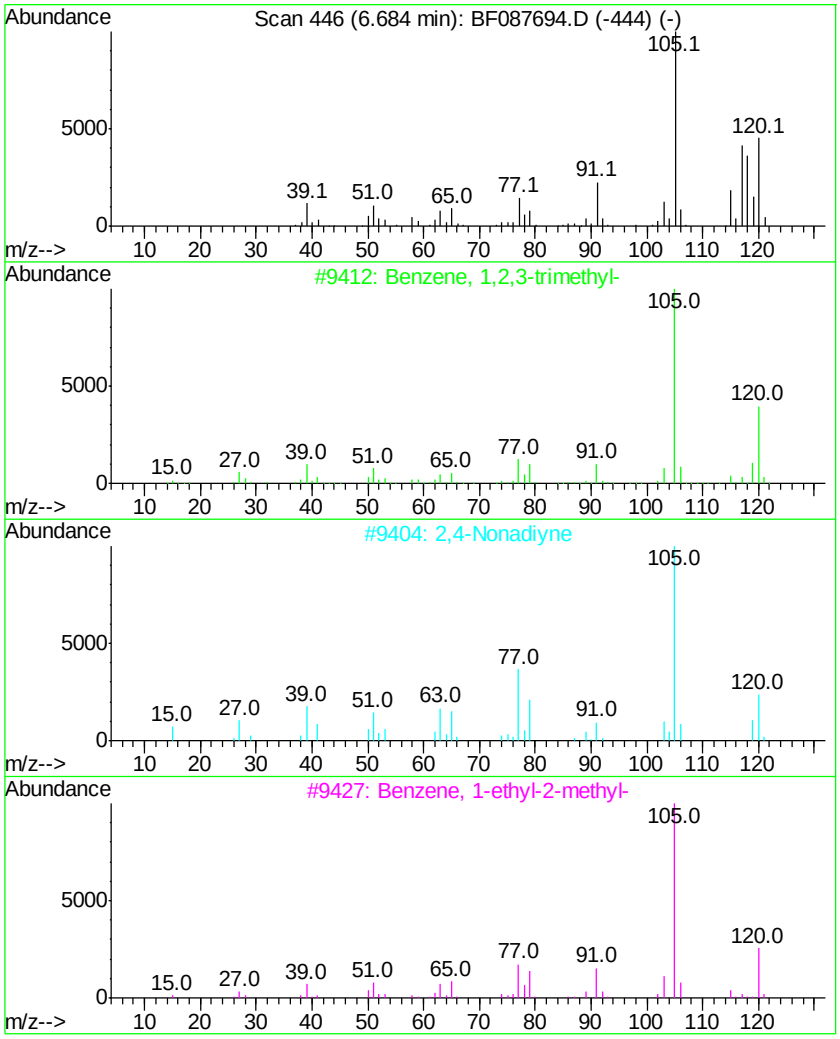
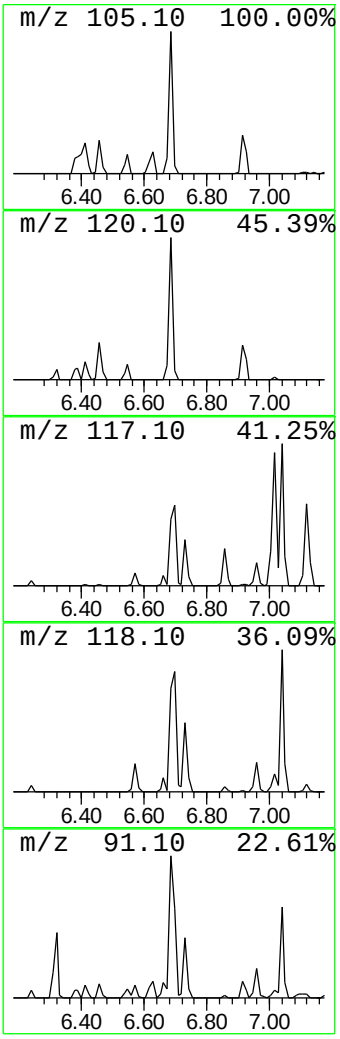
Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	14.36 ng	544755	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	55
2	2,4-Nonadiyne	120	C9H12	063621-15-8	50
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	50
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	50
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	50





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Sample : H3344-06
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

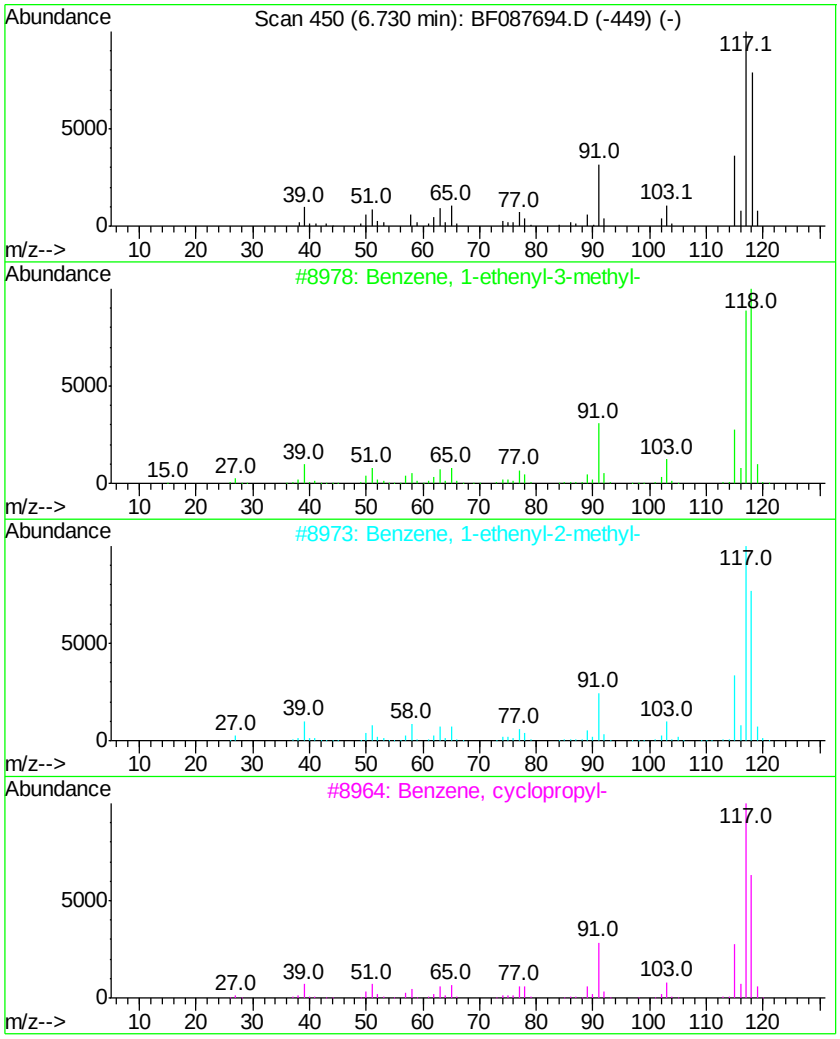
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

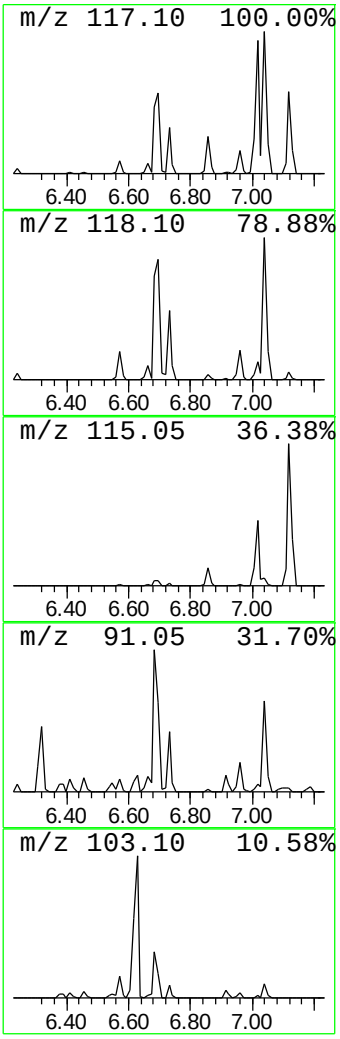
****

Peak Number 10 Benzene, 1-ethenyl-3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	2.84 ng	107635	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	95
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	93
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	93
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	93
5	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	93





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Sample : H3344-06
Misc :
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Instrument : BNA_F
ClientSampleId : MW-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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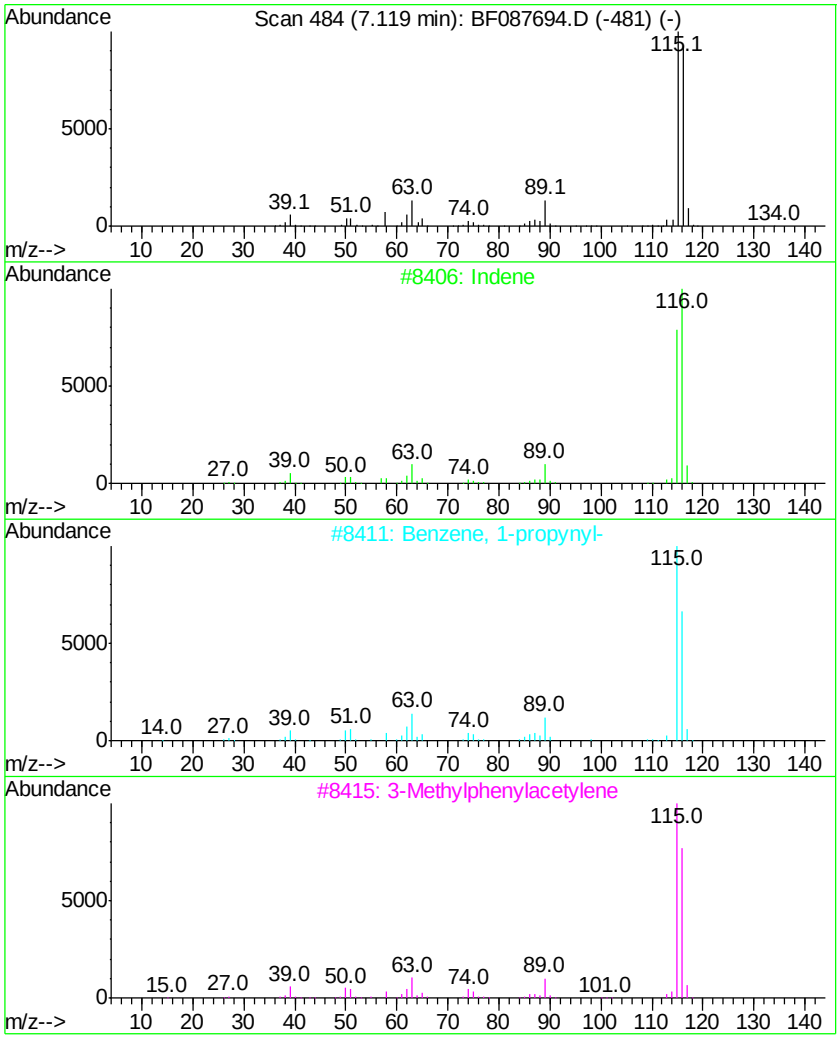
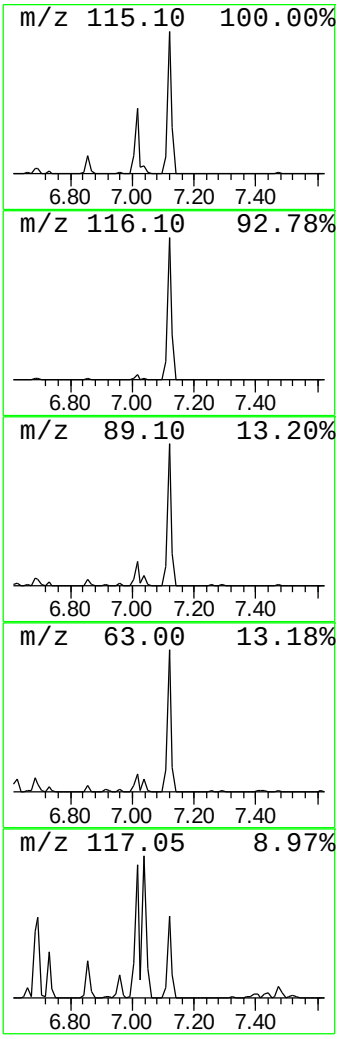
Peak Number 13 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	52.23 ng	1981910	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91





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Sample : H3344-06
Misc :
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Instrument : BNA_F
ClientSampleId : MW-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

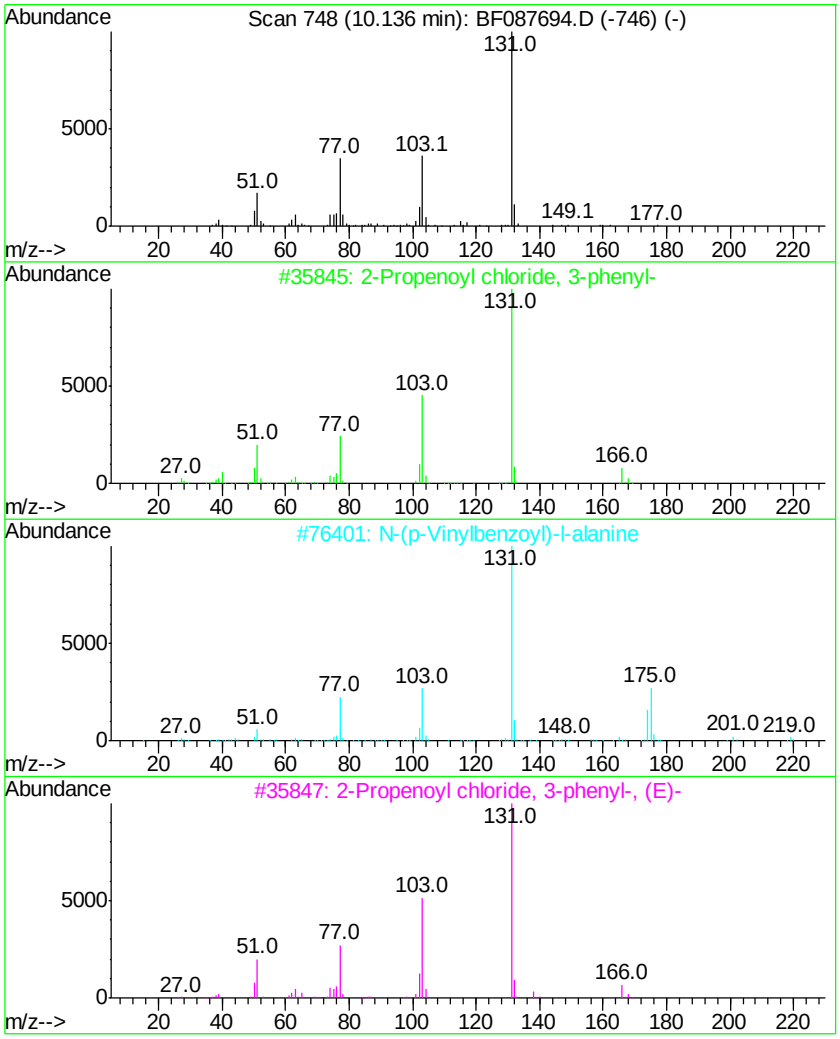
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

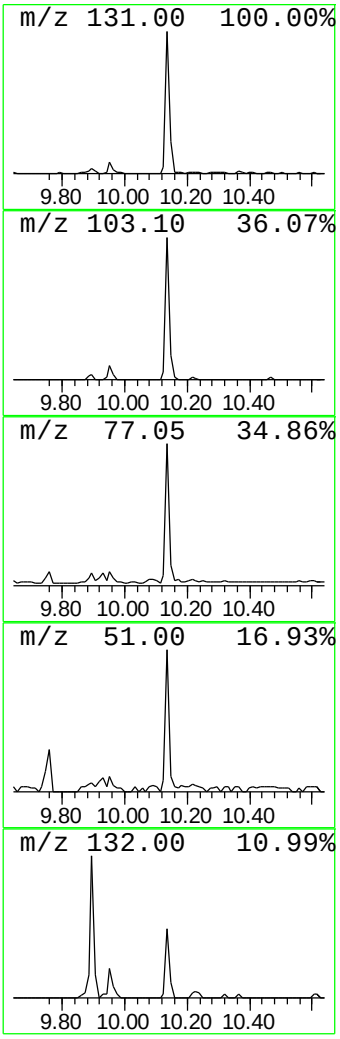
****

Peak Number 14 2-Propenoyl chloride, 3-phe... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	3.34 ng	185737	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoyl chloride, 3-phenyl-	166	C9H7ClO	000102-92-1	90
2	N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	83
3	2-Propenoyl chloride, 3-phenyl-,...	166	C9H7ClO	017082-09-6	78
4	6-Benzofuranylacetaldehyde	160	C10H8O2	1000301-98-1	78
5	Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
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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
Propane, 1,1-dime...	2.15	14.3	ng	541783	1	6.86	758857	20.0
2-Pentanone, 4-hy...	5.04	4.7	ng	177988	1	6.86	758857	20.0
unknown6.63	6.63	84.0	ng	3188120	1	6.86	758857	20.0
Benzene, 1,2,3-tr...	6.68	14.4	ng	544755	1	6.86	758857	20.0
Benzene, 1-etheny...	6.73	2.8	ng	107635	1	6.86	758857	20.0
Indene	7.12	52.2	ng	1981910	1	6.86	758857	20.0
2-Propenoyl chlor...	10.14	3.3	ng	185737	3	9.90	1113100	20.0