

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
 Data File : BF087691.D
 Acq On : 5 Jun 2016 6:10
 Operator : UM/SJ
 Sample : H3344-03
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-9

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	268342	333668	8.13%	0.960%
2	1.907	26	28	46	rVB	2031566	3766299	91.78%	10.835%
3	2.136	46	48	68	rVB	94734	285467	6.96%	0.821%
4	3.827	192	196	199	rVB	272662	387426	9.44%	1.115%
5	5.039	300	302	306	rBV	121066	149654	3.65%	0.431%
6	5.313	324	326	329	rVB	56904	56808	1.38%	0.163%
7	5.450	335	338	340	rBV	1739131	1732639	42.22%	4.985%
8	5.690	355	359	361	rVB2	163020	239634	5.84%	0.689%
9	6.479	425	428	430	rBV	1170938	1124717	27.41%	3.236%
10	6.627	438	441	443	rBV	2479387	3084621	75.17%	8.874%
11	6.685	443	446	449	rVB	73845	84328	2.05%	0.243%
12	6.856	459	461	465	rVB	891307	770010	18.76%	2.215%
13	7.016	472	475	477	rBV	2835608	2874057	70.03%	8.268%
14	7.119	482	484	486	rBV	551784	484995	11.82%	1.395%
15	7.428	507	511	513	rVB	2034248	2635626	64.22%	7.582%
16	7.896	548	552	553	rBV3	63490	100892	2.46%	0.290%
17	7.930	553	555	559	rVB	45680	87567	2.13%	0.252%
18	8.148	571	574	577	rBV2	880317	1253379	30.54%	3.606%
19	8.296	585	587	591	rVB	45892	51676	1.26%	0.149%
20	8.673	619	620	624	rVB	30368	45611	1.11%	0.131%
21	8.959	642	645	647	rBV	170737	191676	4.67%	0.551%
22	9.222	665	668	671	rVB	3250112	4103787	100.00%	11.806%
23	9.611	700	702	705	rBV	65875	71872	1.75%	0.207%
24	9.759	712	715	717	rBV	142280	147440	3.59%	0.424%
25	9.896	724	727	729	rBV	1263370	1161310	28.30%	3.341%
26	10.685	793	796	799	rBV	2247078	2481086	60.46%	7.138%
27	10.811	804	807	811	rVB	35325	42001	1.02%	0.121%
28	11.382	854	857	859	rBV	1024093	1204264	29.35%	3.465%
29	11.908	901	903	905	rBV	91581	96063	2.34%	0.276%
30	12.697	970	972	979	rBV	141222	169860	4.14%	0.489%
31	12.799	979	981	983	rVB	80360	83722	2.04%	0.241%
32	12.971	993	996	998	rBV	3312470	3527388	85.95%	10.148%
33	13.497	1040	1042	1044	rBV	48727	52707	1.28%	0.152%
34	13.897	1074	1077	1082	rBV2	22906	45458	1.11%	0.131%

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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 >
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35	14.011	1084	1087	1089	rBV	1161039	1057771	25.78%	3.043%
36	15.440	1209	1212	1215	rBV	609073	774118	18.86%	2.227%

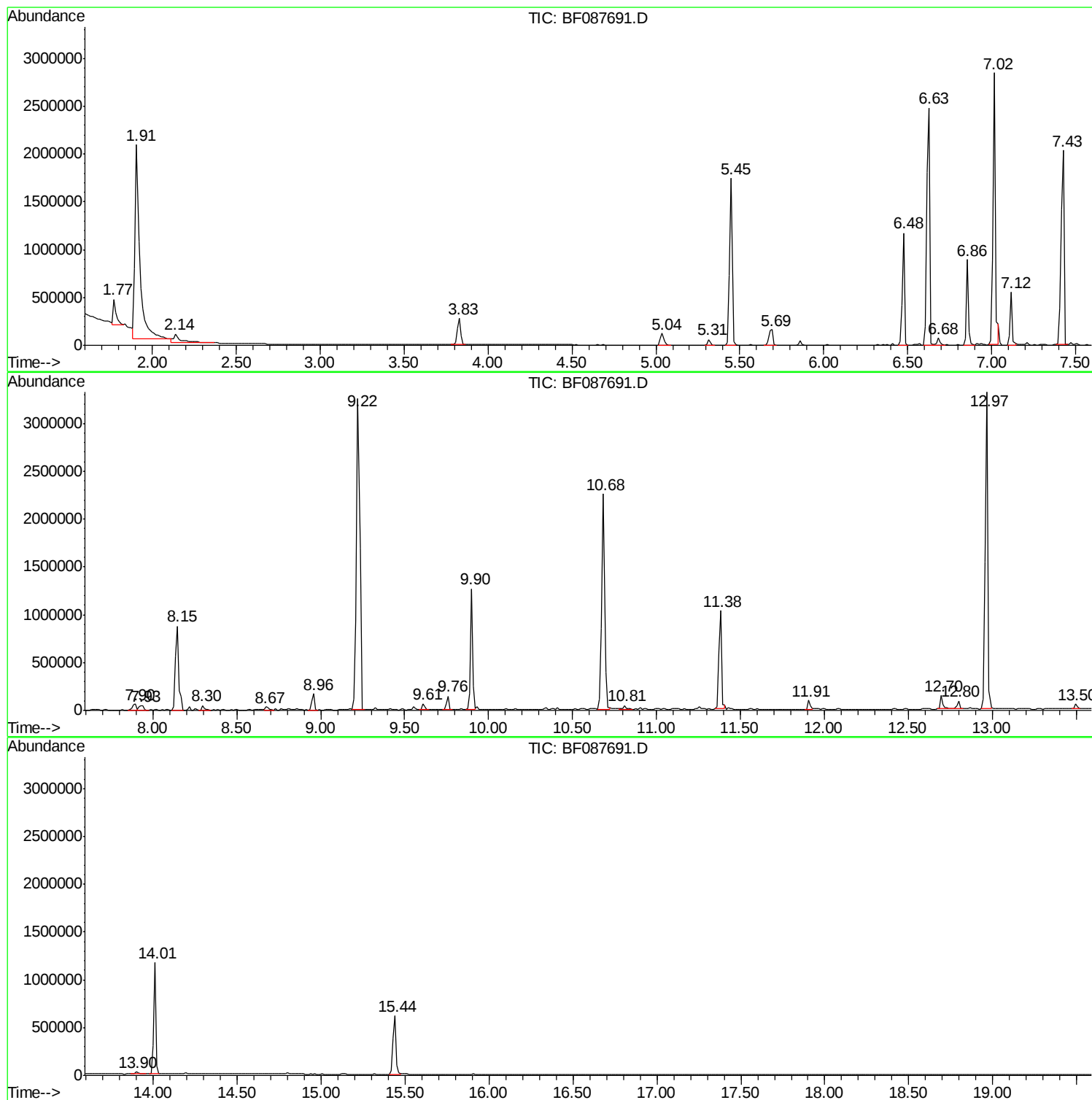
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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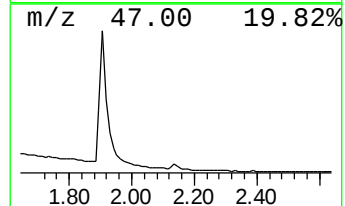
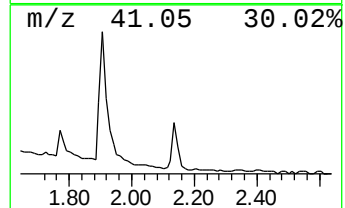
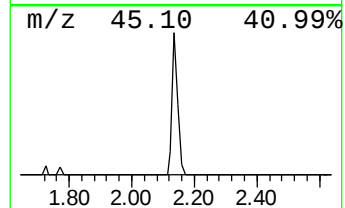
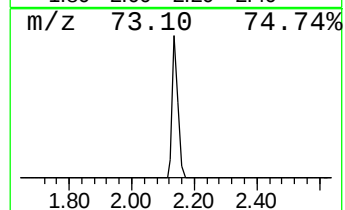
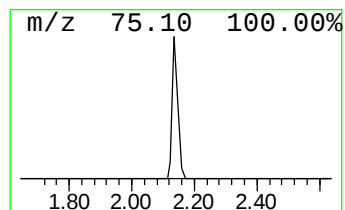
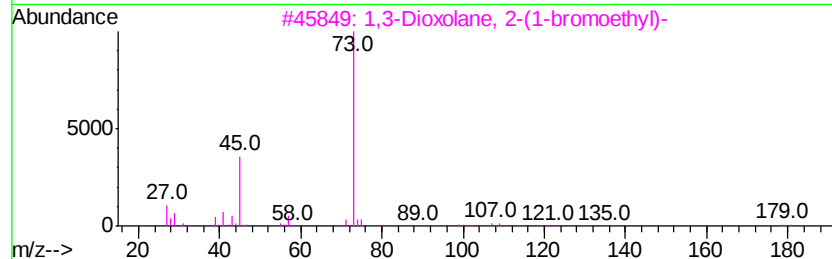
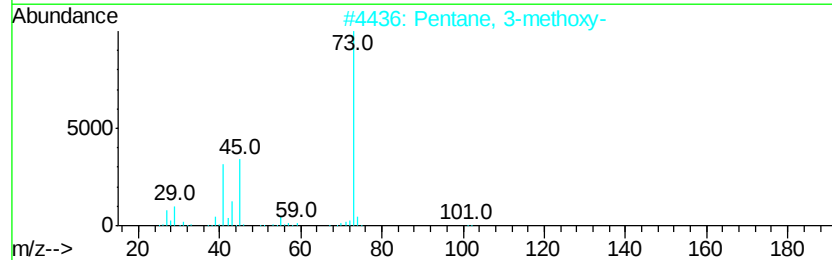
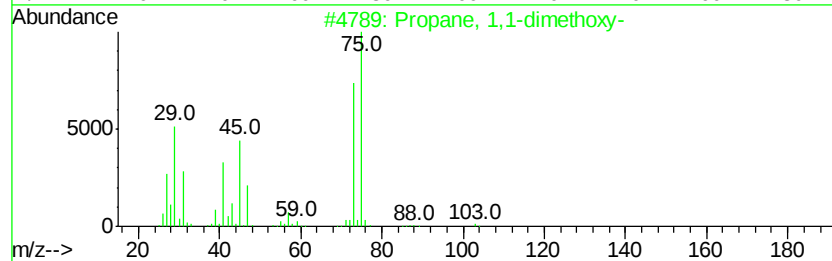
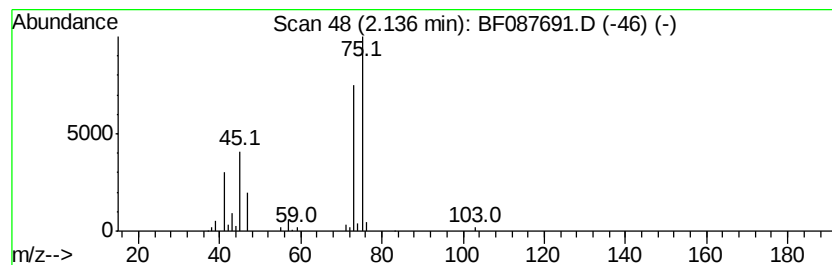
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060416.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	7.41 ng	285467	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
3		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9
4		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5		Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9



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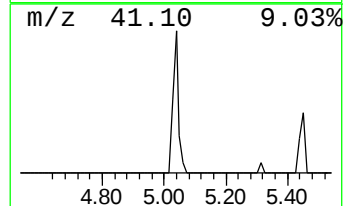
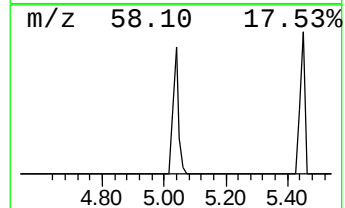
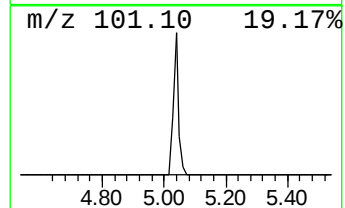
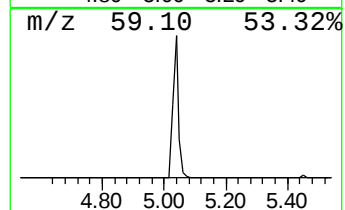
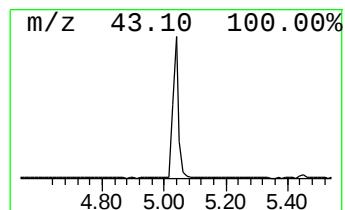
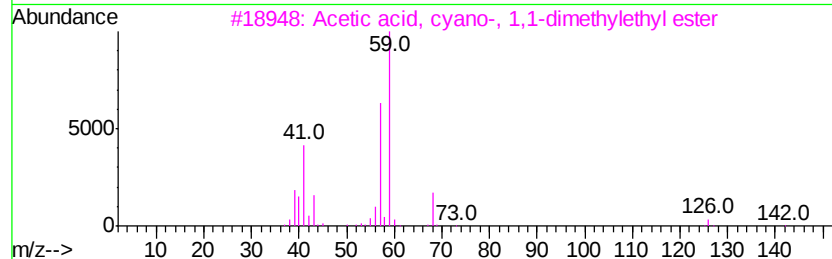
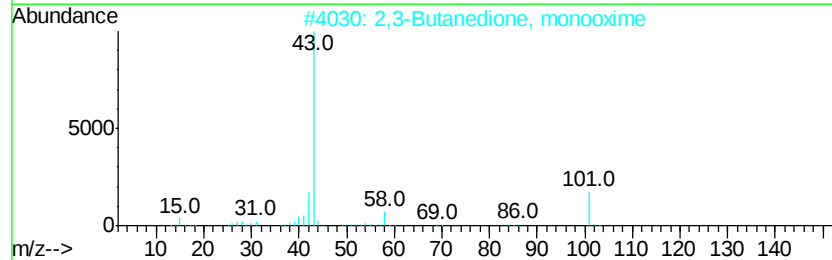
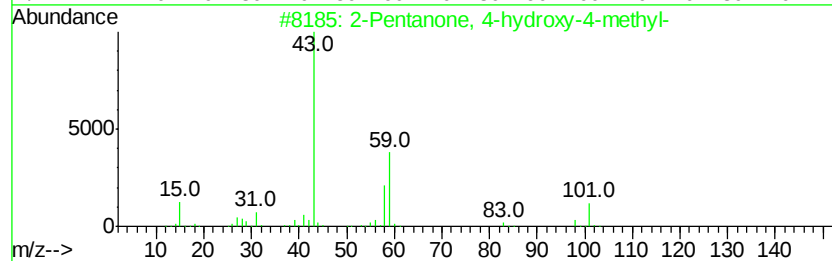
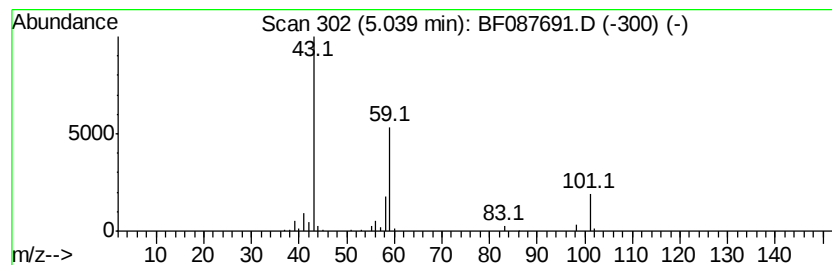
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	3.89 ng	149654	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	53		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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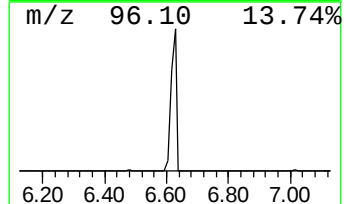
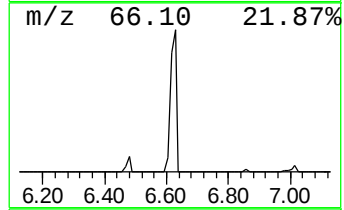
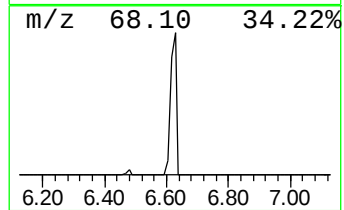
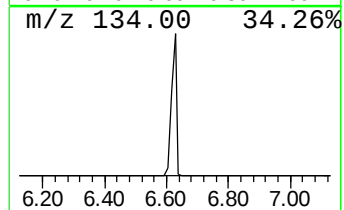
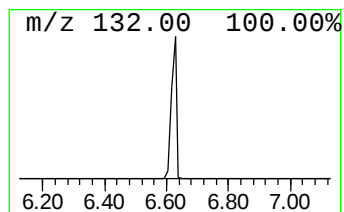
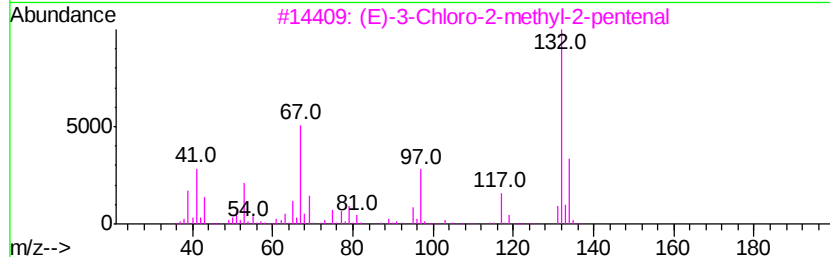
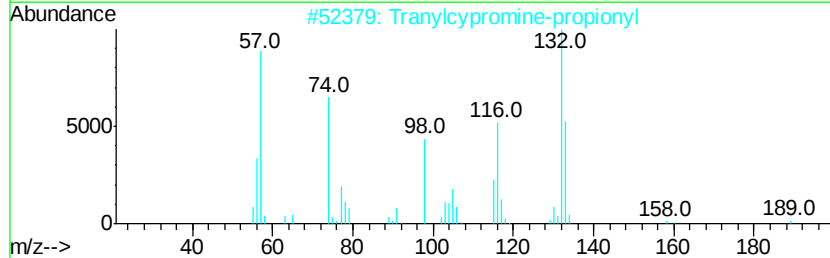
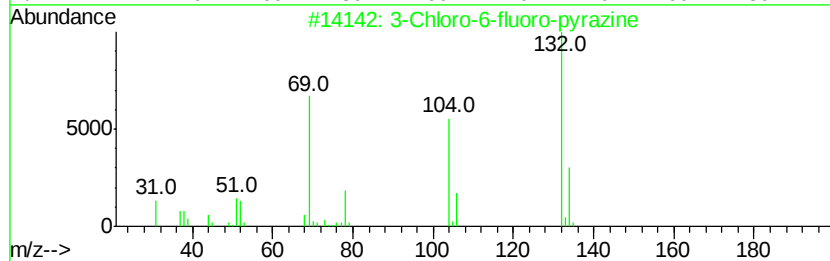
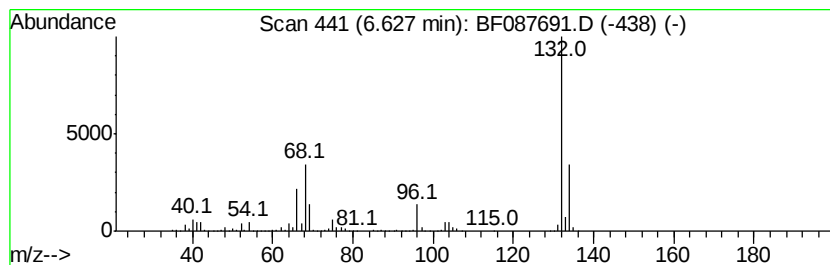
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	80.12 ng	3084620	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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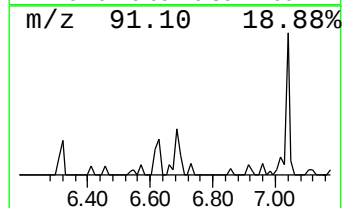
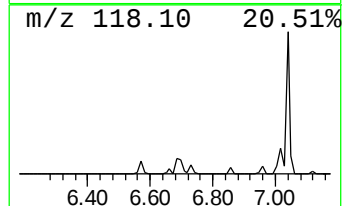
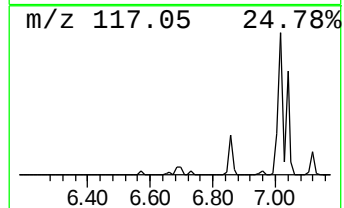
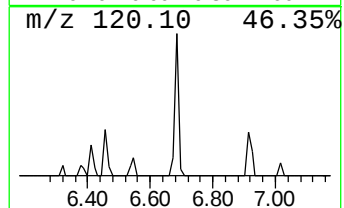
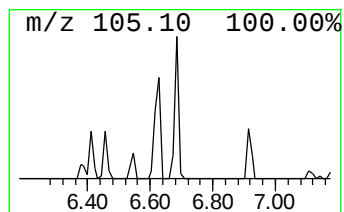
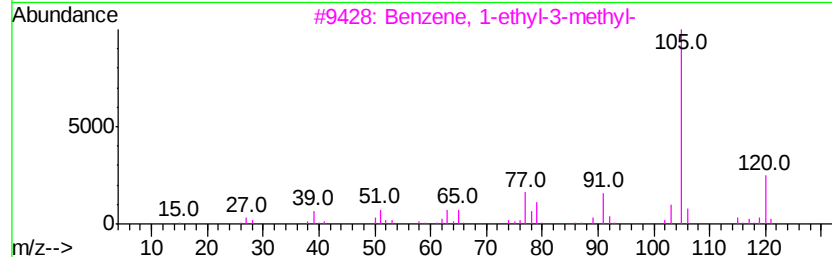
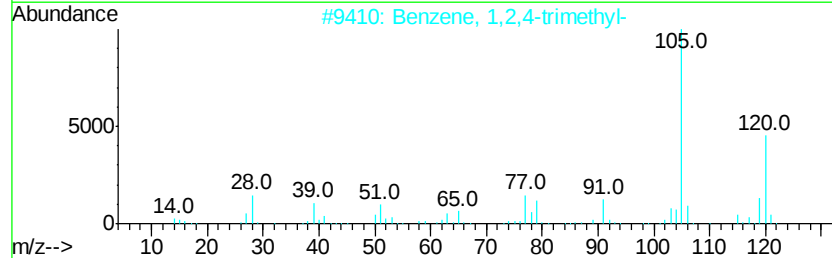
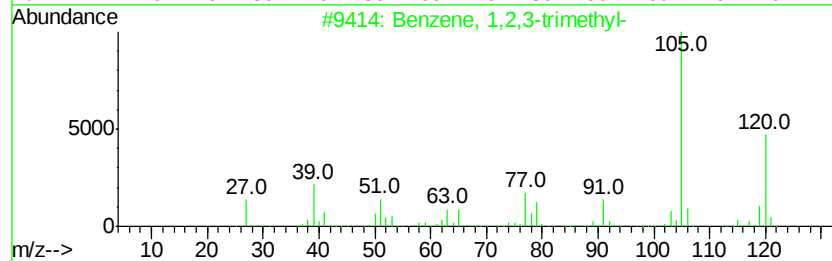
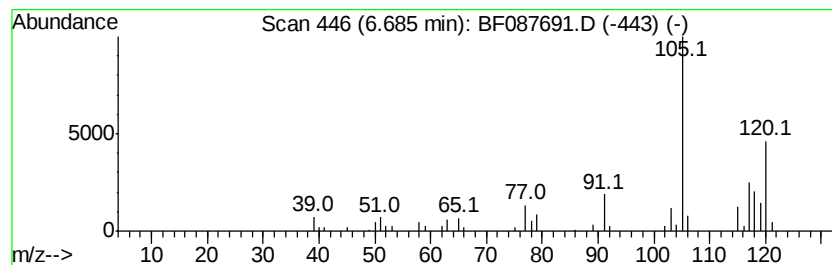
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1,2,3-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	2.19 ng	84328	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	64
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	60
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	60
4		Mesitylene	120	C9H12	000108-67-8	60
5		2,4-Nonadiyne	120	C9H12	063621-15-8	60



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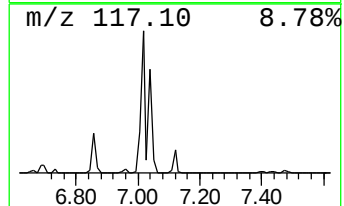
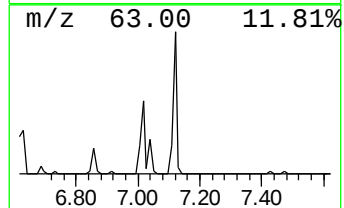
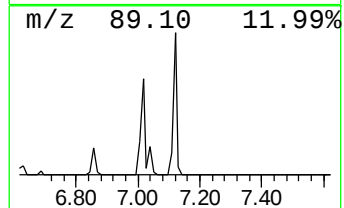
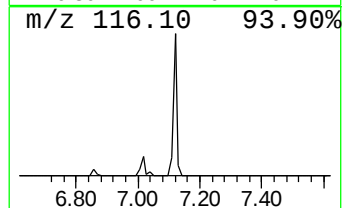
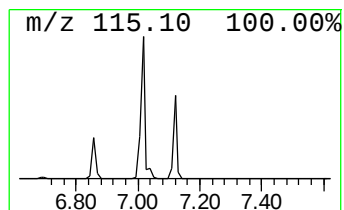
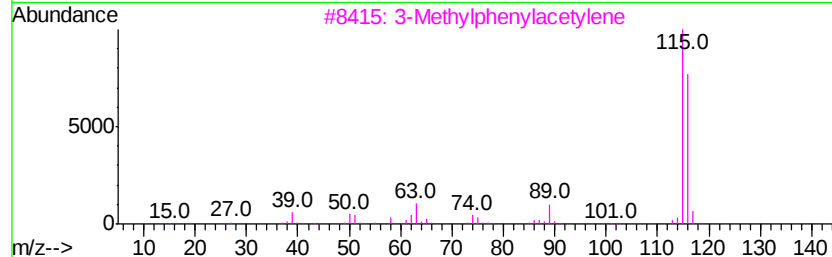
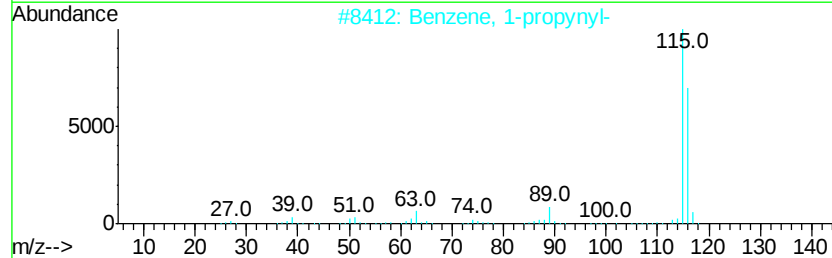
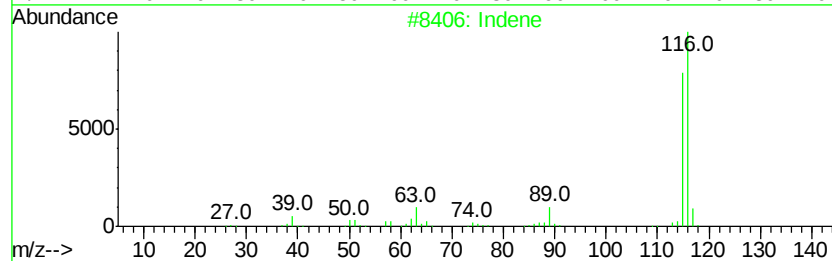
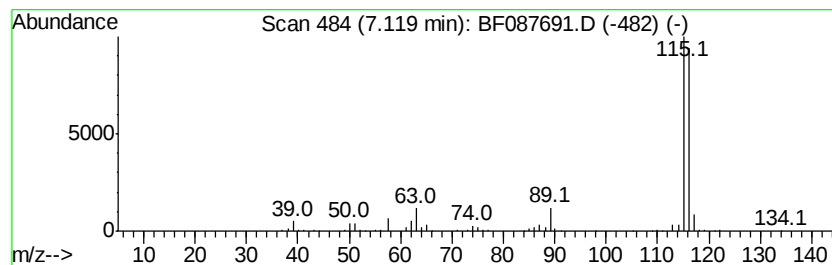
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Peak Number 10 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	12.60 ng	484995	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indene	116	C9H8	000095-13-6	97
2		Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3		3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4		Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5		2-Methylphenylacetylene	116	C9H8	000766-47-2	91



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ClientSampleId :
MW-9

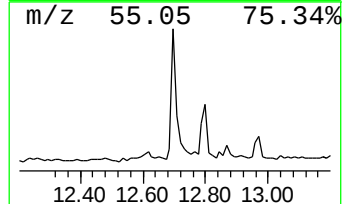
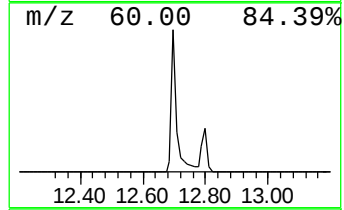
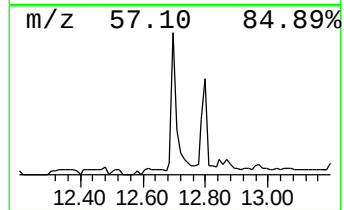
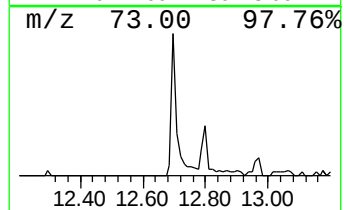
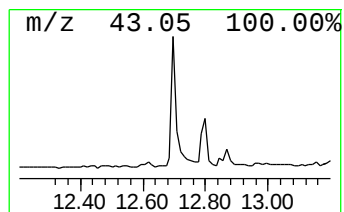
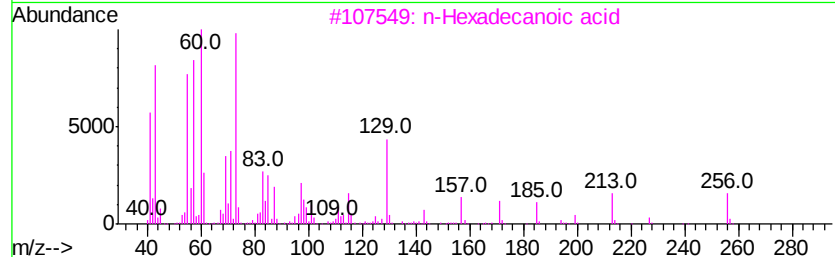
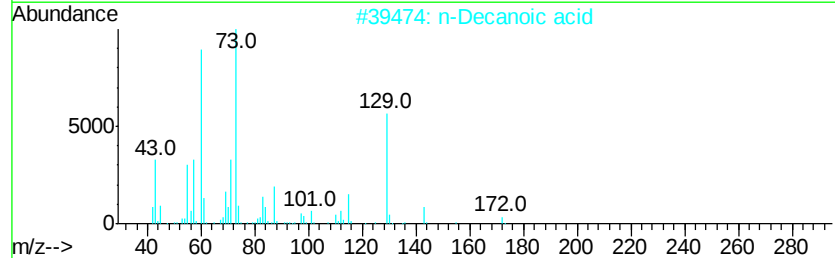
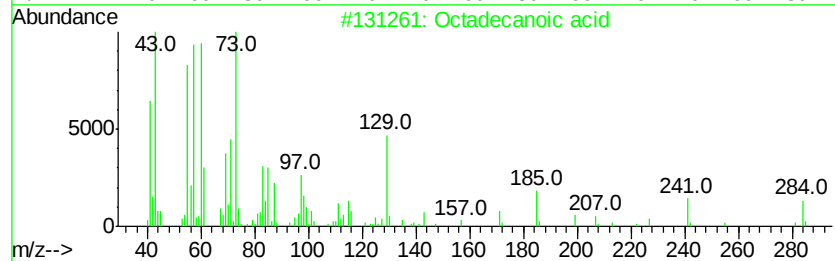
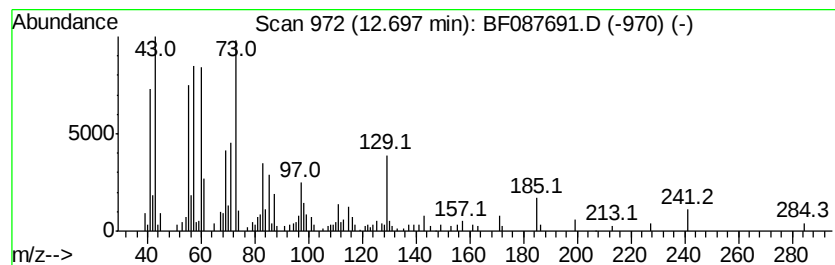
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	3.21 ng	169860	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Decanoic acid	172	C10H20O2	000334-48-5	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
Data File : BF087691.D
Acq On : 5 Jun 2016 6:10
Operator : UM/SJ
Sample : H3344-03
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-9

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.14	7.4	ng	285467	1	6.86	770010	20.0
2-Pentanone, 4-hy...	5.04	3.9	ng	149654	1	6.86	770010	20.0
unknown6.63	6.63	80.1	ng	3084620	1	6.86	770010	20.0
Benzene, 1,2,3-tr...	6.68	2.2	ng	84328	1	6.86	770010	20.0
Indene	7.12	12.6	ng	484995	1	6.86	770010	20.0
Octadecanoic acid	12.70	3.2	ng	169860	5	14.01	1057770	20.0