

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
 Data File : BF087898.D
 Acq On : 11 Jun 2016 3:25
 Operator : UM/SJ
 Sample : H3440-03
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PW-03

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-BF060716.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	1.747	12	14	23	rVB	248468	520810	9.39%	1.842%
2	1.872	23	25	92	rVB	2411117	5547027	100.00%	19.620%
3	4.970	295	296	301	rBV	54967	78992	1.42%	0.279%
4	5.404	331	334	336	rVB	1373486	1371309	24.72%	4.850%
5	5.964	381	383	385	rBB	61520	61878	1.12%	0.219%
6	6.444	422	425	427	rVB	971696	953914	17.20%	3.374%
7	6.581	434	437	439	rBV	2132546	2343977	42.26%	8.291%
8	6.764	449	453	455	rBV2	90681	111923	2.02%	0.396%
9	6.810	455	457	459	rBV	783450	628746	11.33%	2.224%
10	6.970	468	471	472	rBV	2351616	2146970	38.70%	7.594%
11	6.993	472	473	475	rVB	90662	65307	1.18%	0.231%
12	7.061	478	479	481	rBV2	60165	55734	1.00%	0.197%
13	7.153	484	487	489	rBV2	107912	163131	2.94%	0.577%
14	7.381	502	507	509	rBV	1885979	2384334	42.98%	8.433%
15	7.462	512	514	516	rBV	81706	69593	1.25%	0.246%
16	7.507	516	518	520	rVB	81559	72417	1.31%	0.256%
17	7.587	523	525	527	rVB	324556	269505	4.86%	0.953%
18	7.747	537	539	541	rVV2	75093	104029	1.88%	0.368%
19	7.839	544	547	549	rBV	719400	642665	11.59%	2.273%
20	8.033	563	564	567	rBV2	49379	58993	1.06%	0.209%
21	8.102	567	570	571	rVV	694874	809700	14.60%	2.864%
22	8.147	571	574	576	rVV2	152871	212338	3.83%	0.751%
23	8.296	585	587	589	rBV2	99223	89539	1.61%	0.317%
24	8.342	589	591	592	rVV	78160	73768	1.33%	0.261%
25	8.376	592	594	598	rVV3	38215	88715	1.60%	0.314%
26	8.479	602	603	605	rVB	82527	74992	1.35%	0.265%
27	8.570	605	611	612	rBV	68701	86760	1.56%	0.307%
28	8.764	626	628	629	rVV	108311	146506	2.64%	0.518%
29	9.016	646	650	651	rBV3	31948	71127	1.28%	0.252%
30	9.176	661	664	666	rVB	3006472	2633357	47.47%	9.314%
31	9.565	697	698	702	rVB	218497	185287	3.34%	0.655%
32	9.747	712	714	718	rVB4	53795	95204	1.72%	0.337%
33	9.850	720	723	725	rBV	755645	792051	14.28%	2.801%
34	10.628	789	791	794	rBV2	1043675	1381300	24.90%	4.886%

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Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.325	850	852	854 rBV	727479	596856	10.76%	2.111%
36	12.913	988	991	993 rBV	1919257	2303610	41.53%	8.148%
37	13.954	1079	1082	1084 rBV	534601	575101	10.37%	2.034%
38	15.359	1202	1205	1207 rBV	342776	405222	7.31%	1.433%

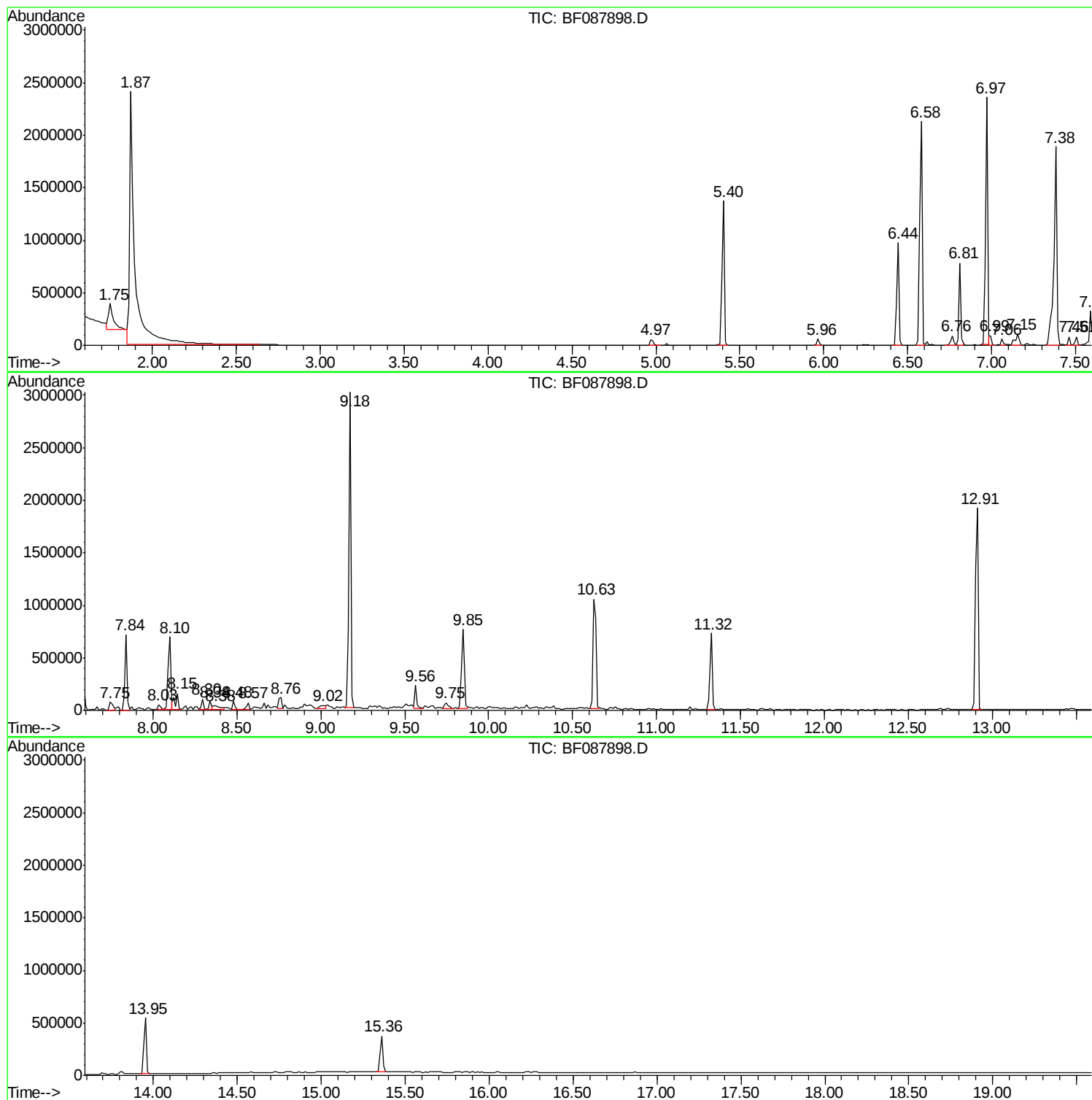
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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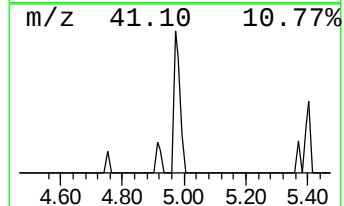
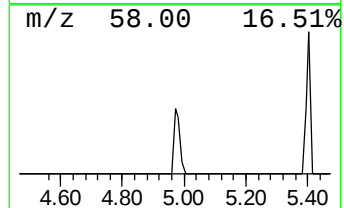
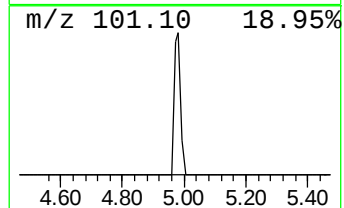
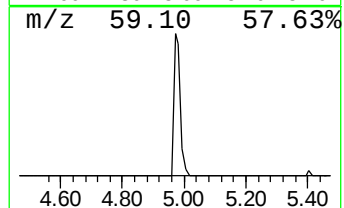
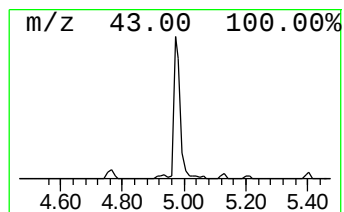
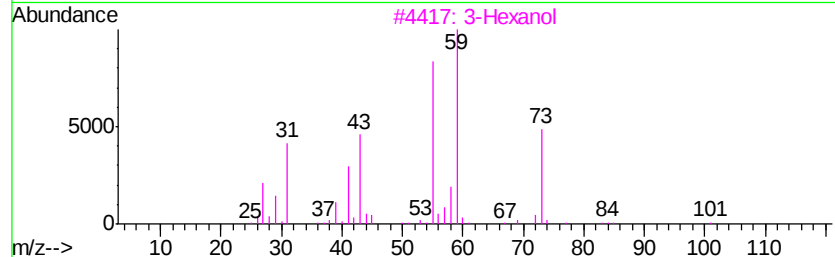
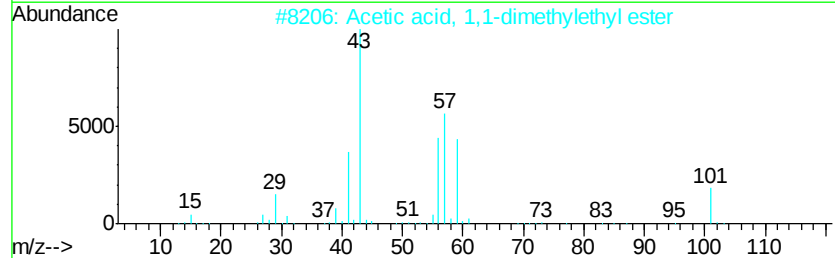
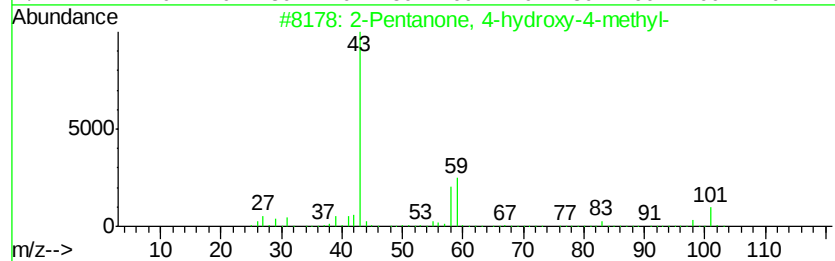
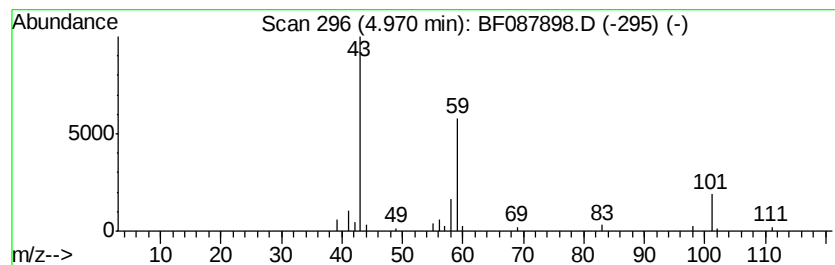
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	2.51 ng	78992	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	3-Hexanol	102	C6H14O	000623-37-0	33		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		



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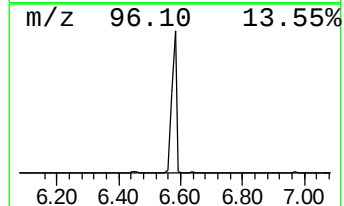
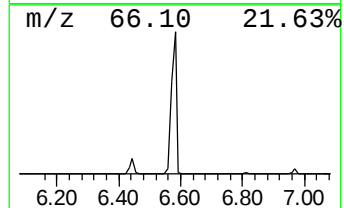
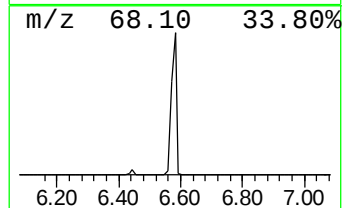
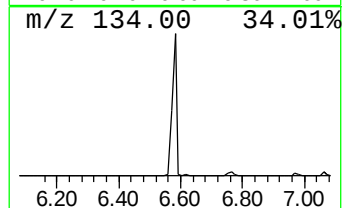
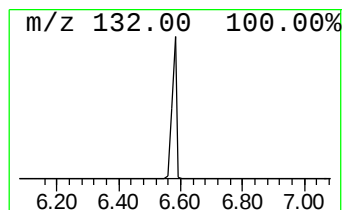
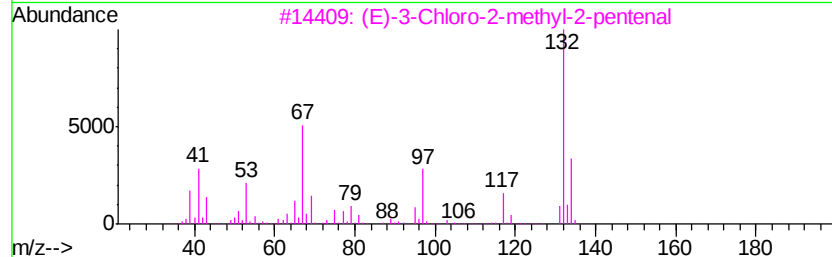
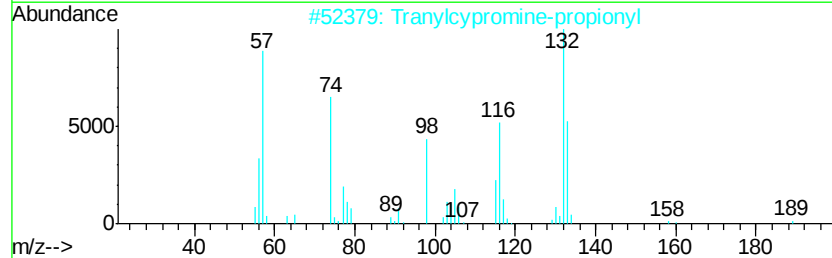
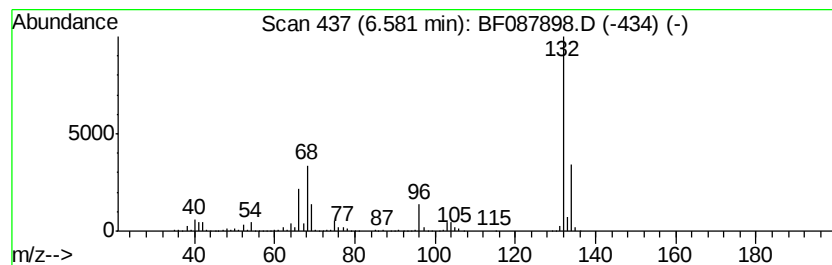
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown6.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	74.56 ng	2343980	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Xenon	132	Xe	007440-63-3	9	
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	



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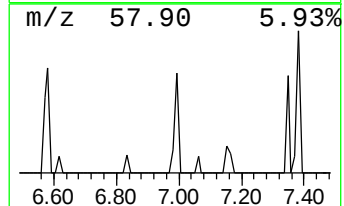
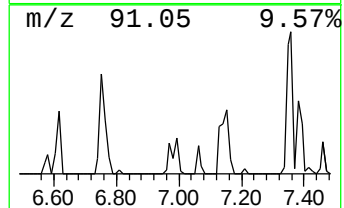
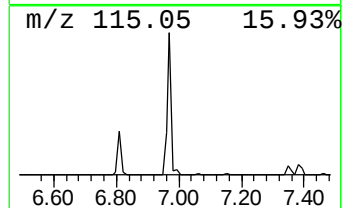
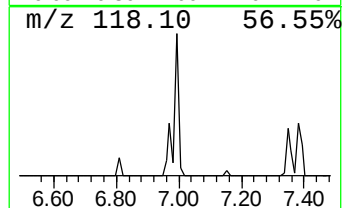
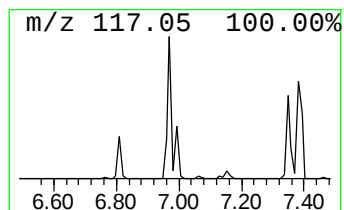
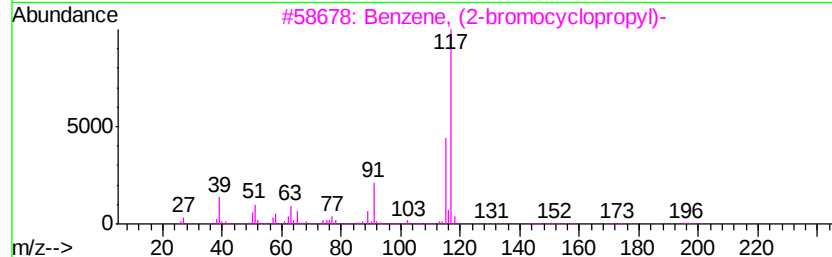
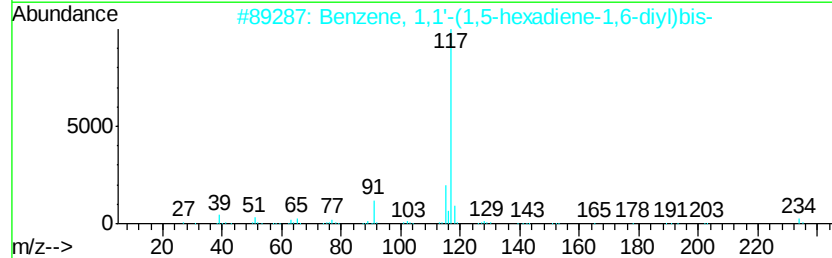
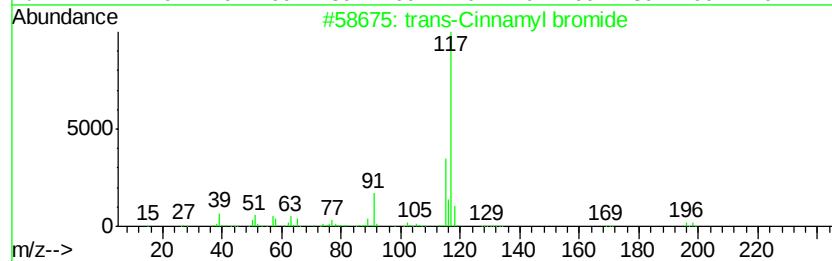
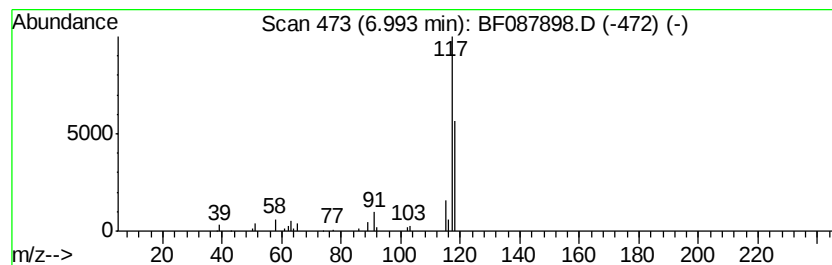
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.99 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.99	2.08 ng	65307	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	47
2		Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	42
3		Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	28
4		Benzaldehyde, 4-(1-phenyl-2-prop...	238	C16H14O2	1000277-56-1	28
5		Deltacyclene	118	C9H10	007785-10-6	10



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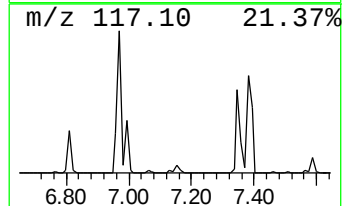
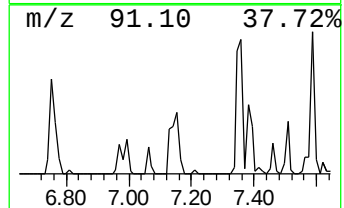
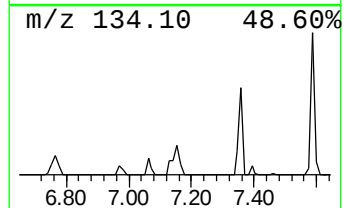
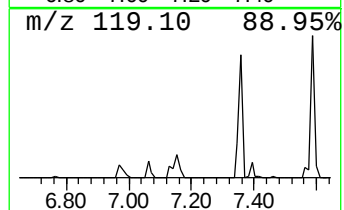
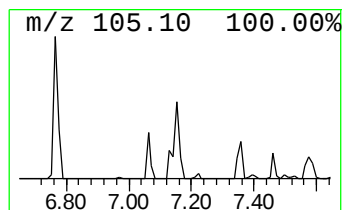
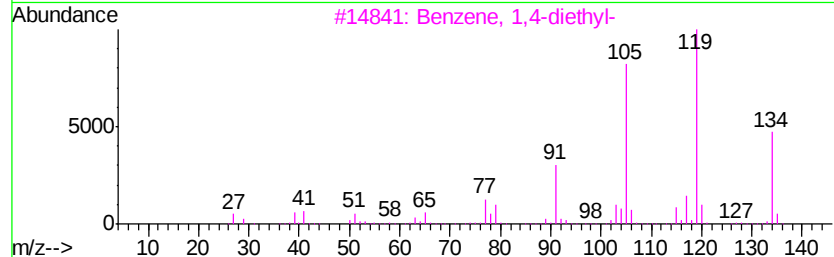
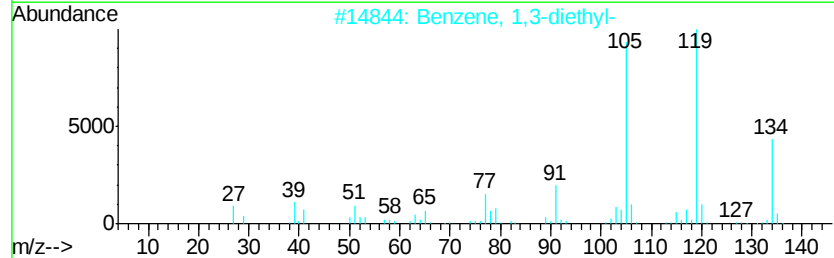
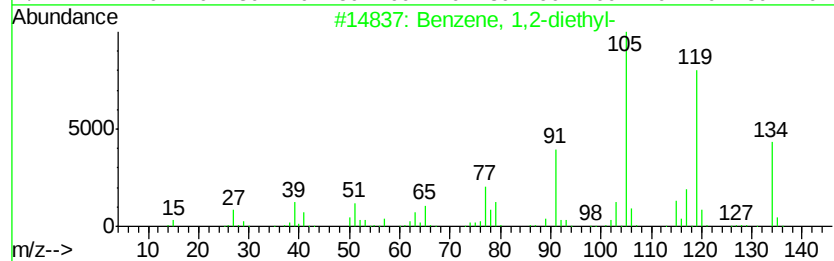
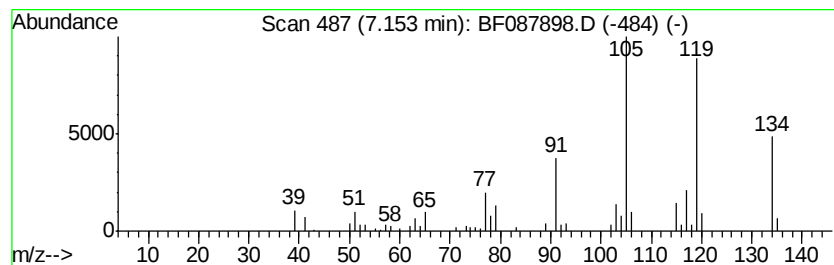
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 Benzene, 1,2-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.15	5.19 ng	163131	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	98
2			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	93
3			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	93
4			o-Cymene	134	C10H14	000527-84-4	81
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	74



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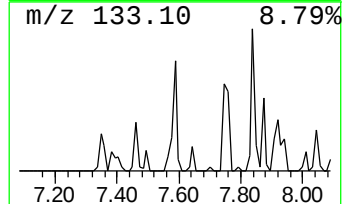
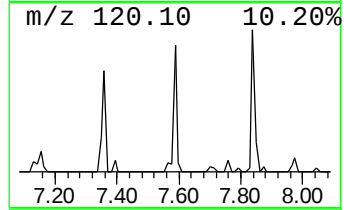
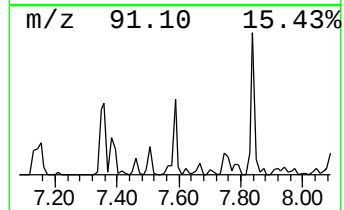
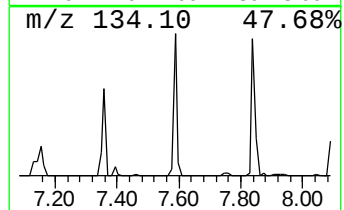
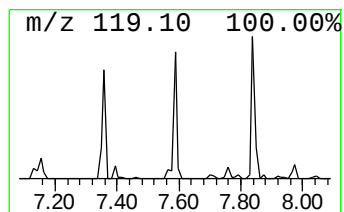
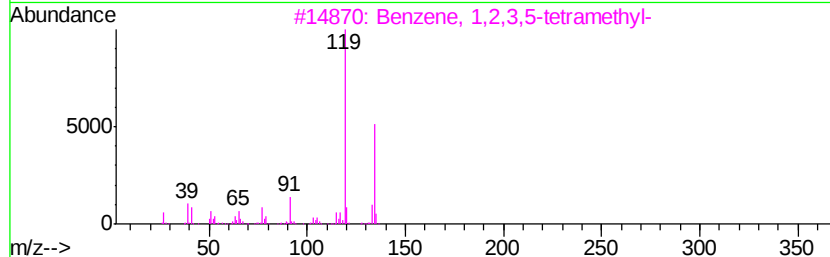
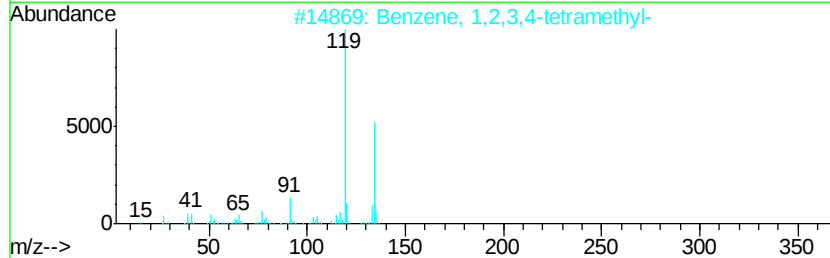
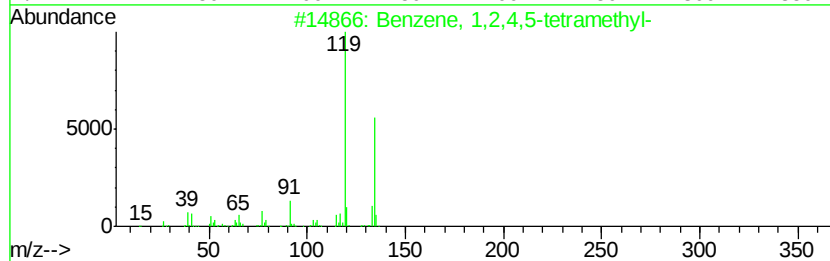
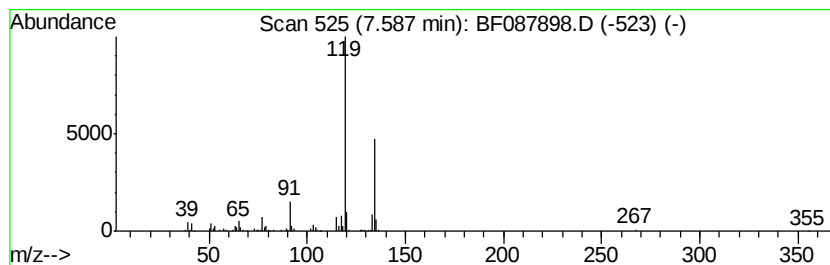
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Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	6.66 ng	269505	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2		Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
3		Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91
5		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	91



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ClientSampleId :
PW-03

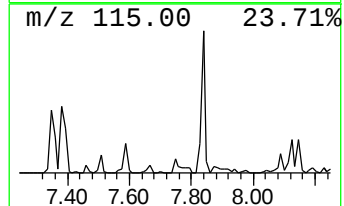
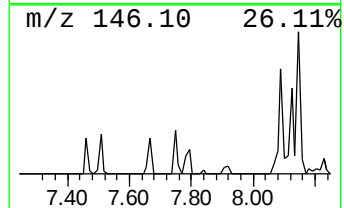
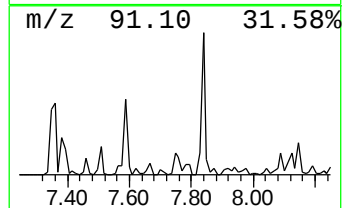
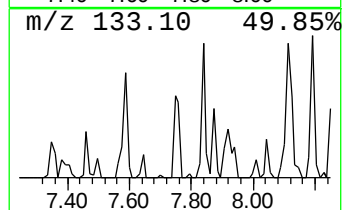
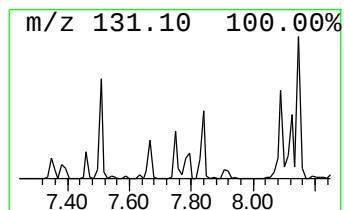
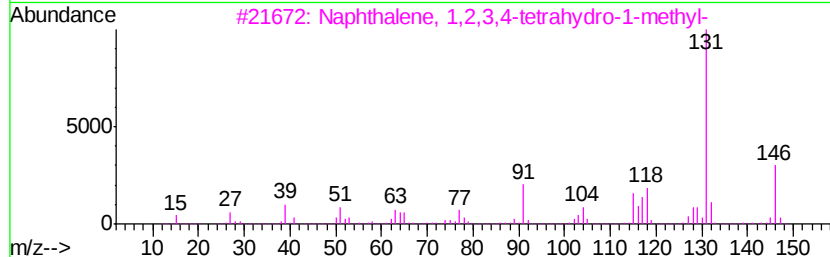
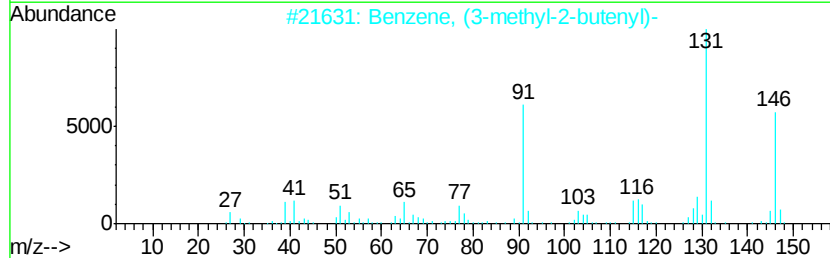
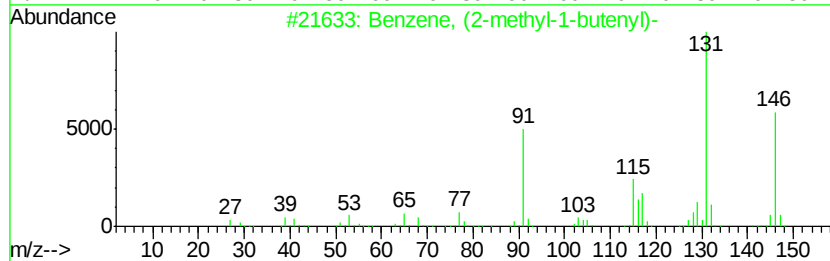
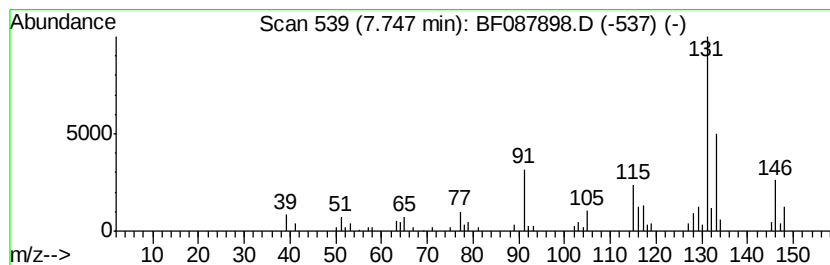
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzene, (2-methyl-1-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	2.57 ng	104029	Naphthalene-d8	8.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	91
2		Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	86
3		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	86
4		Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	70
5		Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
Data File : BF087898.D
Acq On : 11 Jun 2016 3:25
Operator : UM/SJ
Sample : H3440-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

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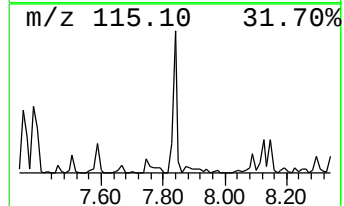
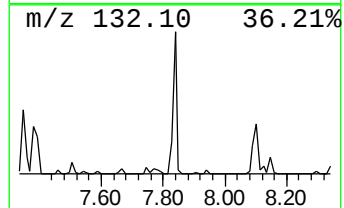
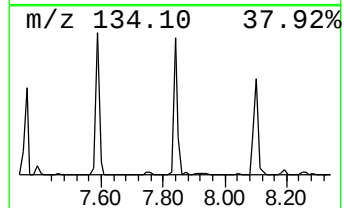
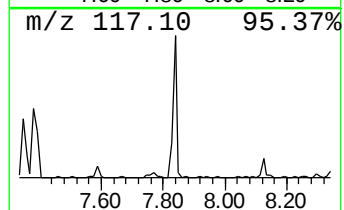
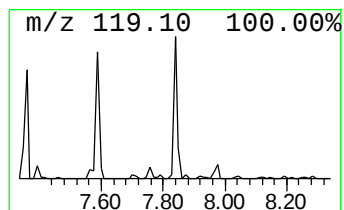
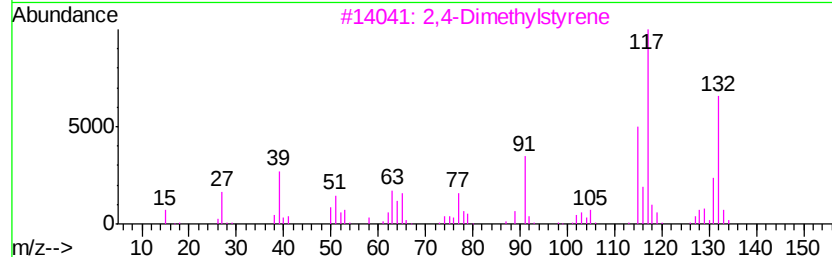
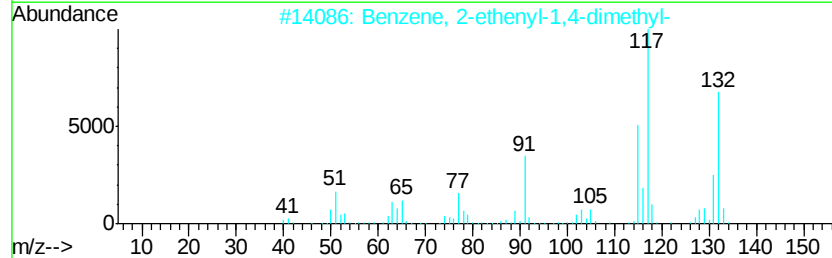
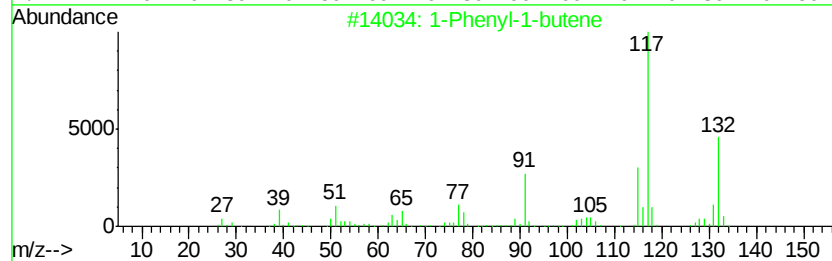
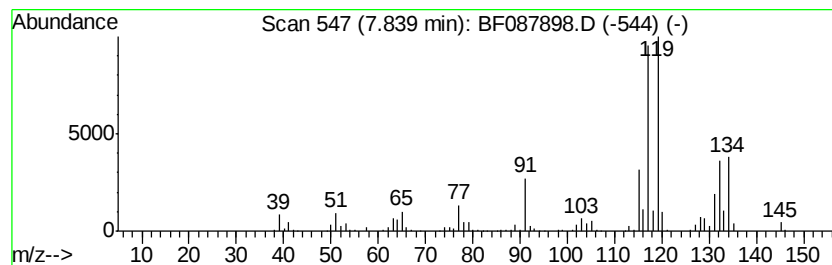
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Phenyl-1-butene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.84	15.87 ng	642665	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenyl-1-butene	132	C10H12	000824-90-8	90
2		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	86
3		2,4-Dimethylstyrene	132	C10H12	002234-20-0	80
4		Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70
5		Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	55



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
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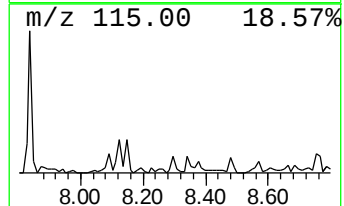
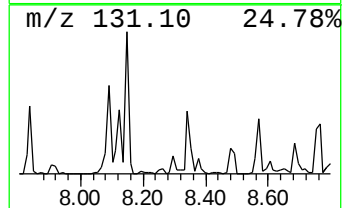
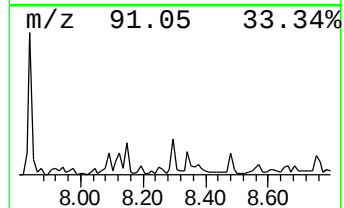
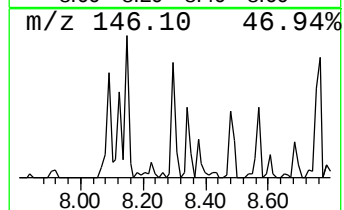
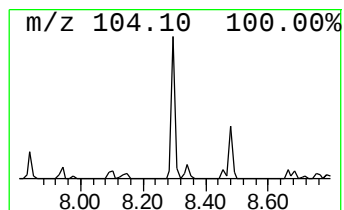
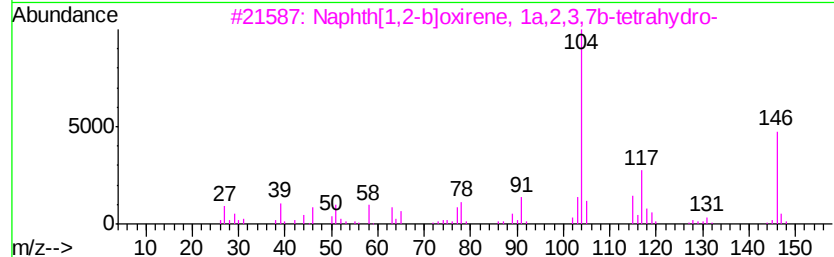
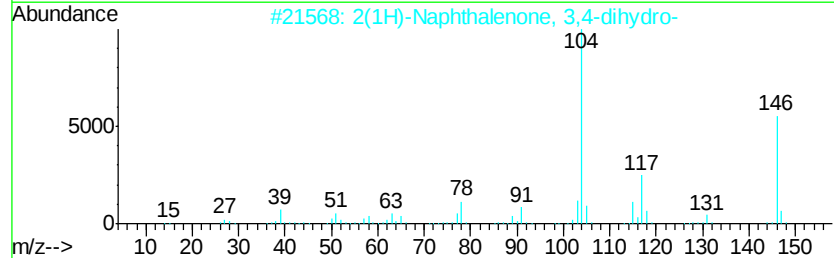
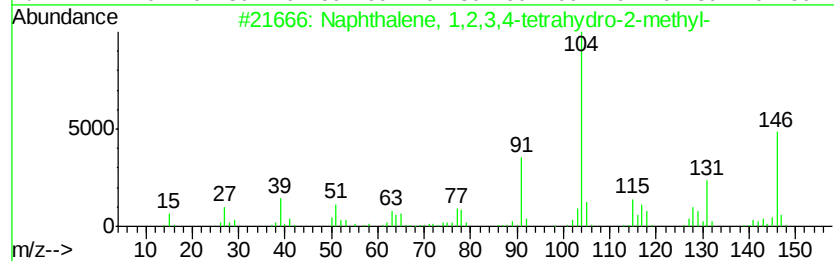
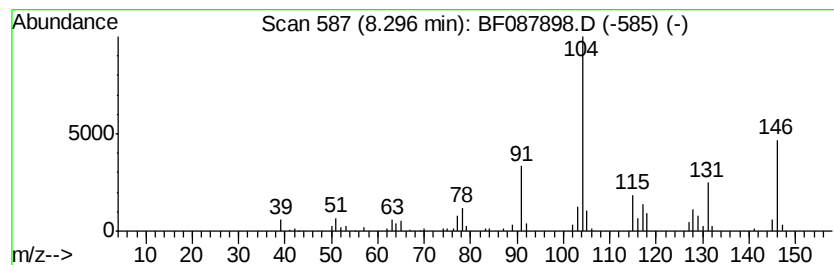
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Naphthalene, 1,2,3,4-tetra... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.30	2.21 ng	89539	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	93
2		2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	68
3		Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	58
4		2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	38
5		Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087898.D
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ClientSampleId :
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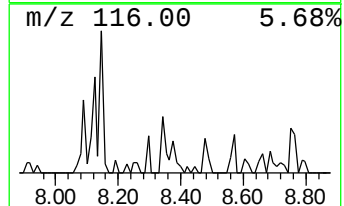
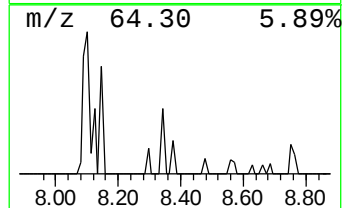
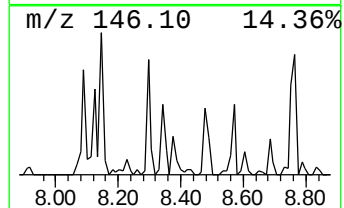
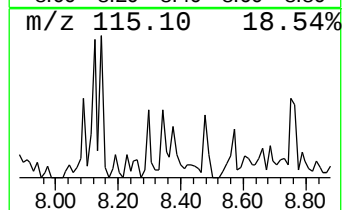
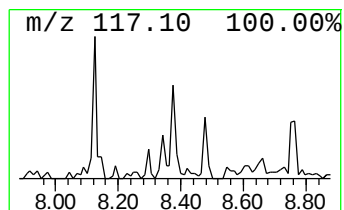
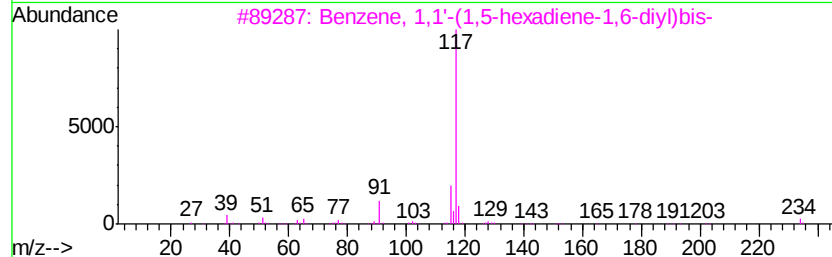
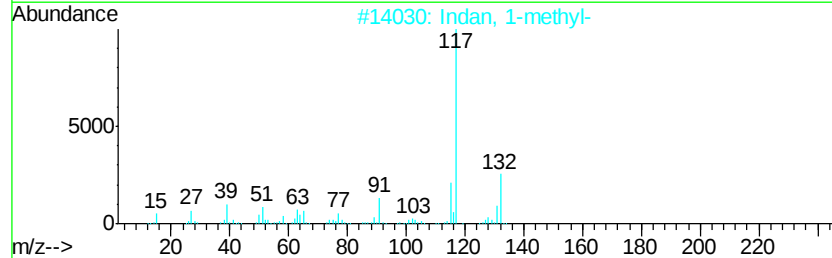
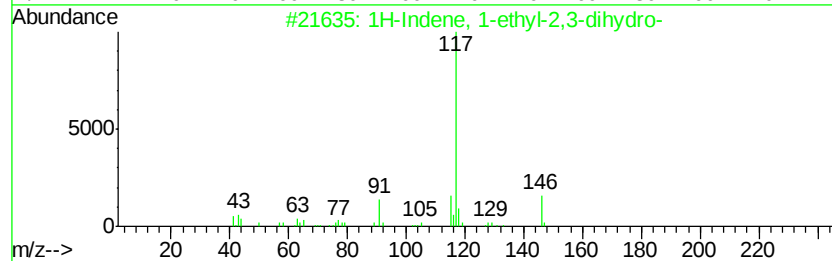
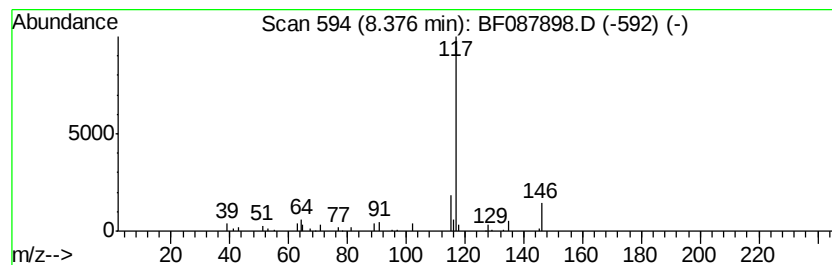
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 1H-Indene, 1-ethyl-2,3-dihydro... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	2.19 ng	88715	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 1-ethyl-2,3-dihydro-	146	C11H14	004830-99-3	72
2		Indan, 1-methyl-	132	C10H12	000767-58-8	39
3		Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	36
4		Indole	117	C8H7N	000120-72-9	33
5		Benzene, 1-pentenyl-	146	C11H14	000826-18-6	9



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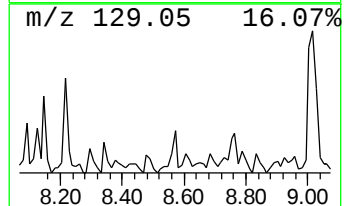
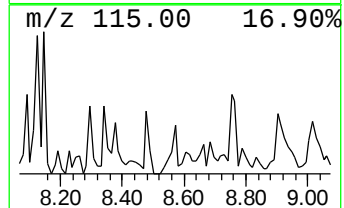
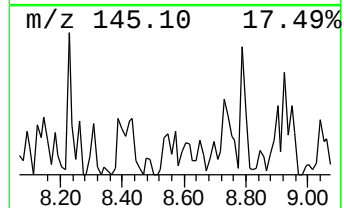
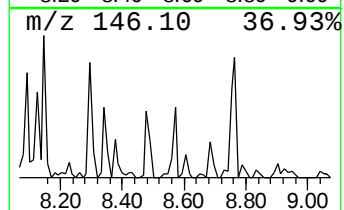
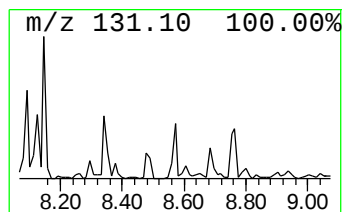
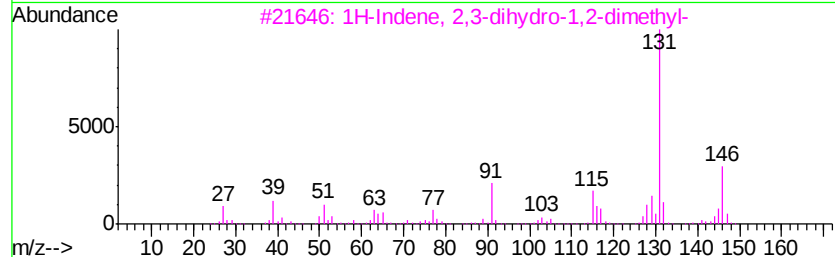
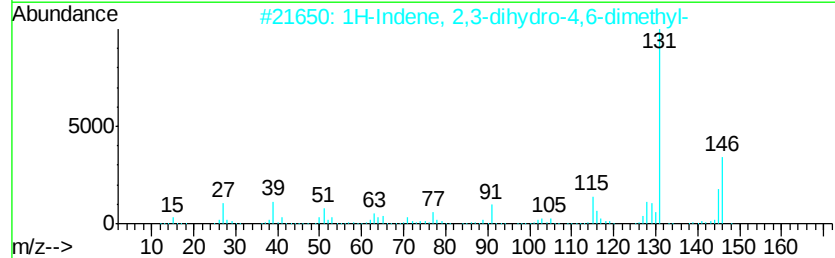
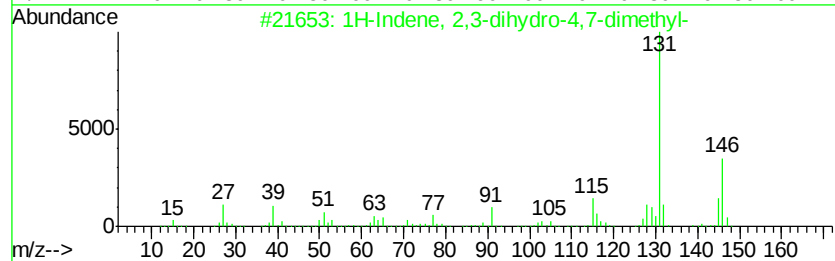
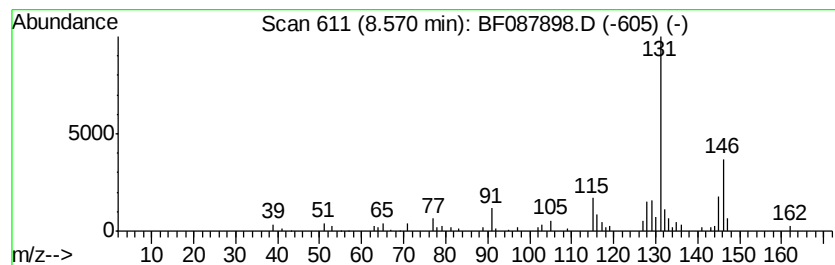
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.57	2.14 ng	86760	Naphthalene-d8	8.10

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	96
2			1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	94
3			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	93
4			Benzene, (3-methyl-2-butenvl)-	146	C11H14	004489-84-3	90
5			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
Data File : BF087898.D
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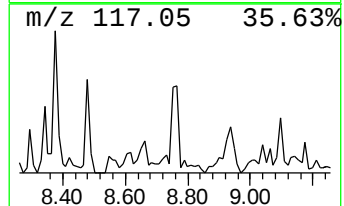
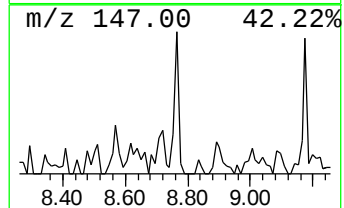
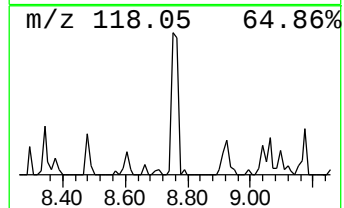
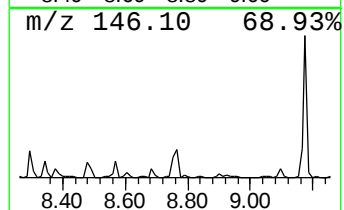
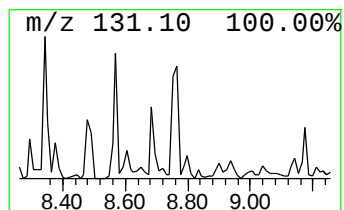
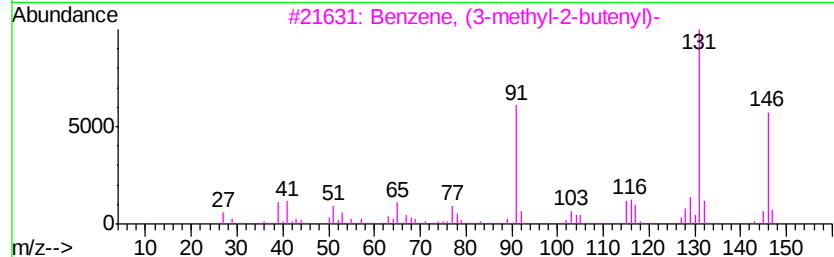
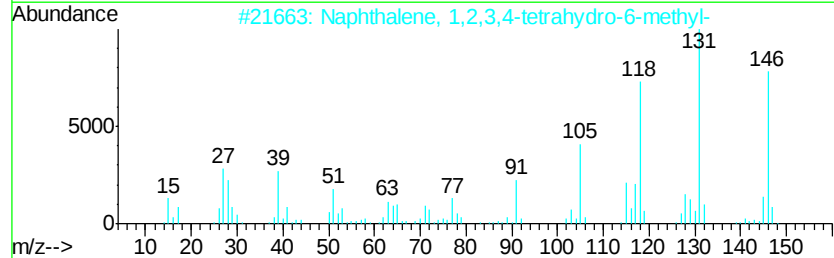
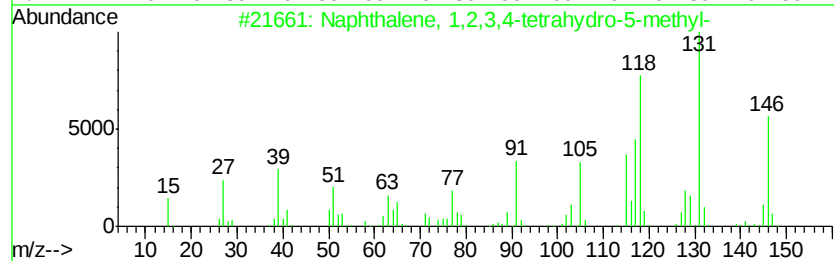
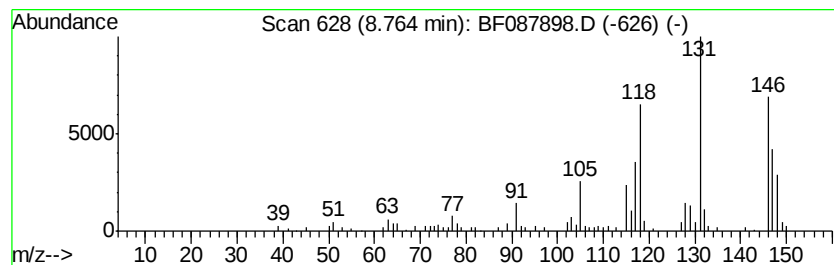
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Naphthalene, 1,2,3,4-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	3.62 ng	146506	Naphthalene-d8	8.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	93
2		Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	70
3		Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	60
4		1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	60
5		Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061016\
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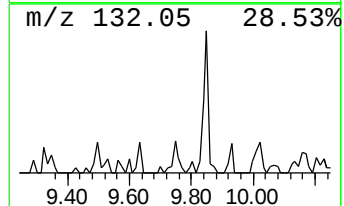
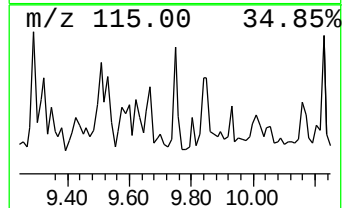
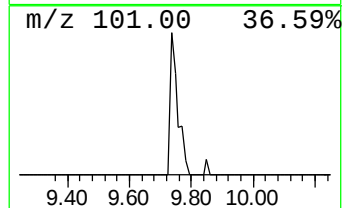
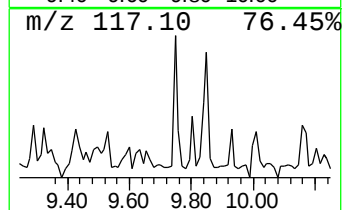
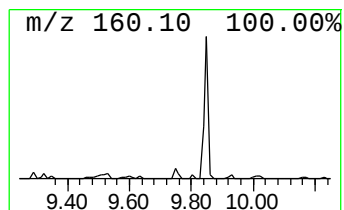
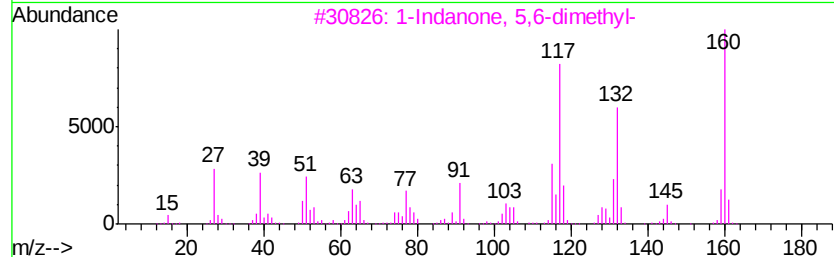
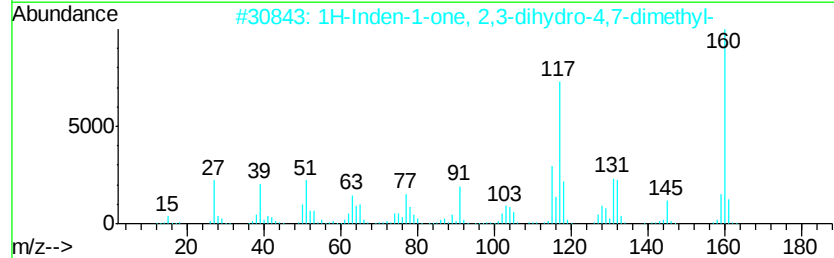
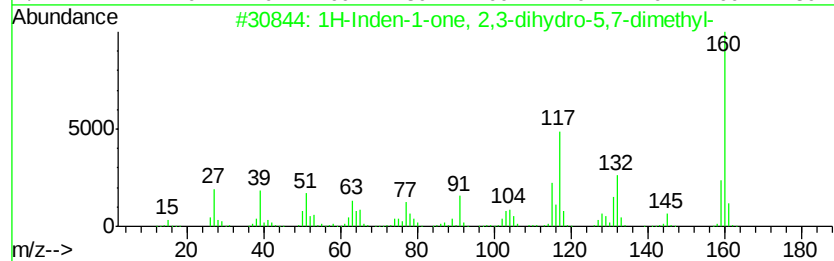
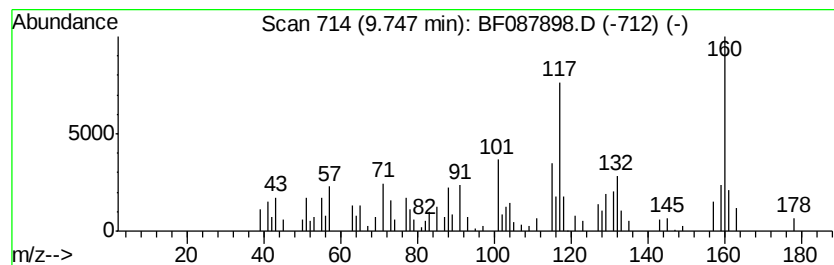
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 1H-Inden-1-one, 2,3-dihydro... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	2.40 ng	95204	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Inden-1-one, 2,3-dihydro-5,7-...	160	C11H12O	006682-69-5	76
2		1H-Inden-1-one, 2,3-dihydro-4,7-...	160	C11H12O	005037-60-5	58
3		1-Indanone, 5,6-dimethyl-	160	C11H12O	016440-97-4	52
4		Benzene, 1-ethenyl-4-(2-methylpr...	160	C12H16	063444-56-4	49
5		Bicyclo[4.2.1]nona-2,4,7-triene,...	160	C11H12O	1000141-51-6	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061016\
Data File : BF087898.D
Acq On : 11 Jun 2016 3:25
Operator : UM/SJ
Sample : H3440-03
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PW-03

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
2-Pentanone, 4-hy...	4.97	2.5	ng	78992	1	6.81	628746	20.0
unknown6.58	6.58	74.6	ng	2343980	1	6.81	628746	20.0
unknown6.99	6.99	2.1	ng	65307	1	6.81	628746	20.0
Benzene, 1,2-diet...	7.15	5.2	ng	163131	1	6.81	628746	20.0
Benzene, 1,2,4,5-...	7.59	6.7	ng	269505	2	8.10	809700	20.0
Benzene, (2-methy...	7.75	2.6	ng	104029	2	8.10	809700	20.0
1-Phenyl-1-butene	7.84	15.9	ng	642665	2	8.10	809700	20.0
Naphthalene, 1,2,...	8.30	2.2	ng	89539	2	8.10	809700	20.0
1H-Indene, 1-ethy...	8.38	2.2	ng	88715	2	8.10	809700	20.0
1H-Indene, 2,3-di...	8.57	2.1	ng	86760	2	8.10	809700	20.0
Naphthalene, 1,2,...	8.76	3.6	ng	146506	2	8.10	809700	20.0
1H-Inden-1-one, 2...	9.75	2.4	ng	95204	3	9.85	792051	20.0