

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110916\
 Data File : BF091132.D
 Acq On : 9 Nov 2016 18:56
 Operator : UM/SJ
 Sample : H5579-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW-3

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-BF110316.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	1.755	4	6	54	rVB	2635287	8741994	100.00%	16.424%
2	4.796	269	272	281	rBV	264325	424959	4.86%	0.798%
3	5.241	309	311	329	rBV	2384964	2579153	29.50%	4.846%
4	6.304	402	404	412	rBV	1576631	1697832	19.42%	3.190%
5	6.419	412	414	417	rBV	3514919	4160745	47.59%	7.817%
6	6.647	432	434	437	rBV	785180	1053480	12.05%	1.979%
7	6.807	445	448	456	rBV	3879394	4035320	46.16%	7.582%
8	7.230	482	485	487	rBV	2815105	3343129	38.24%	6.281%
9	7.436	499	503	504	rBV	80614	90414	1.03%	0.170%
10	7.619	514	519	522	rVB2	48503	102537	1.17%	0.193%
11	7.676	522	524	527	rBV2	236605	354332	4.05%	0.666%
12	7.939	544	547	550	rVV	1649550	1756112	20.09%	3.299%
13	7.996	550	552	554	rVV	98025	160976	1.84%	0.302%
14	8.419	586	589	590	rBV2	63066	95768	1.10%	0.180%
15	8.602	601	605	607	rBV4	64820	98690	1.13%	0.185%
16	8.659	607	610	612	rBV	83938	120379	1.38%	0.226%
17	8.750	615	618	620	rBV	412412	425685	4.87%	0.800%
18	9.025	638	642	644	rBV	6021996	6643585	76.00%	12.482%
19	9.287	662	665	667	rBV	64937	107573	1.23%	0.202%
20	9.356	669	671	672	rBV	108864	142882	1.63%	0.268%
21	9.470	679	681	686	rVB3	45534	106387	1.22%	0.200%
22	9.687	697	700	703	rBV	2038243	1895097	21.68%	3.560%
23	10.488	766	770	772	rBV2	2740160	4133765	47.29%	7.766%
24	10.602	779	780	784	rVB2	51777	88583	1.01%	0.166%
25	11.173	827	830	832	rBV	1297456	1712703	19.59%	3.218%
26	12.762	966	969	971	rBV	5557783	6709630	76.75%	12.606%
27	13.802	1057	1060	1062	rBV	1037761	1403018	16.05%	2.636%
28	15.174	1177	1180	1187	rBV	788467	1040864	11.91%	1.956%

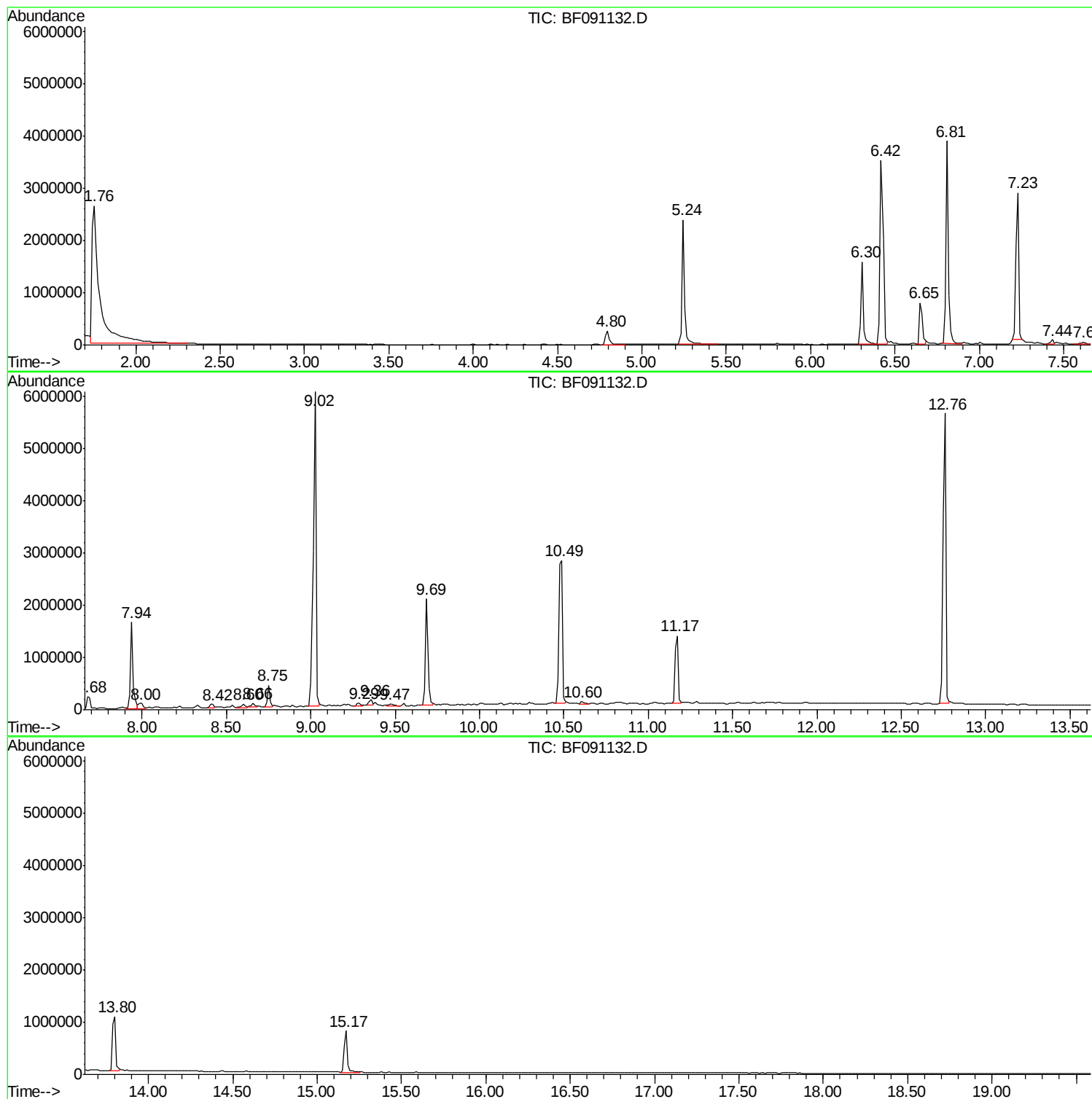
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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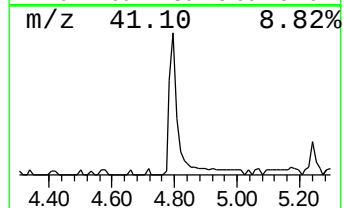
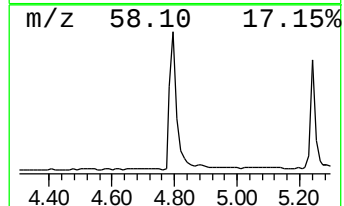
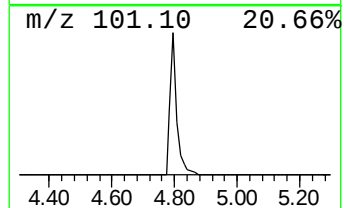
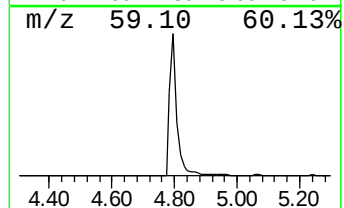
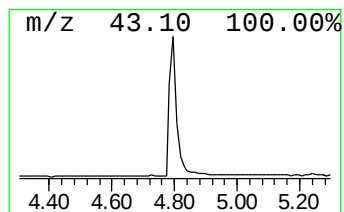
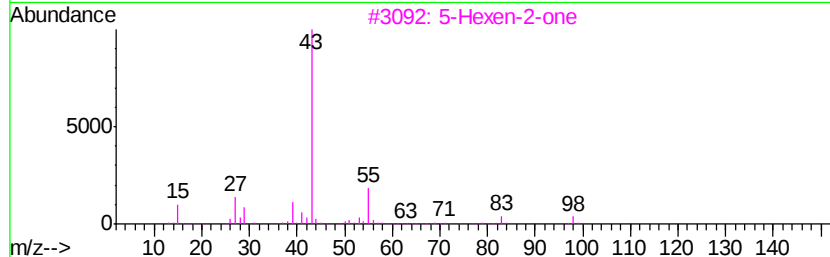
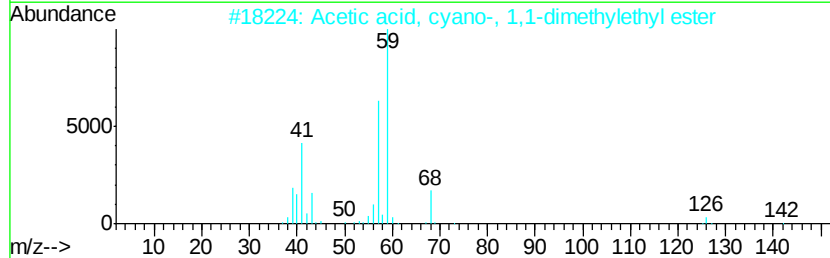
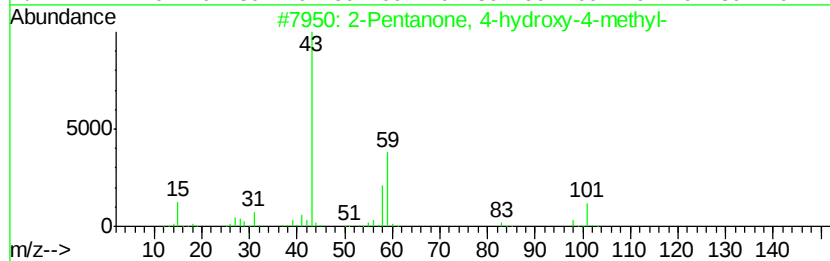
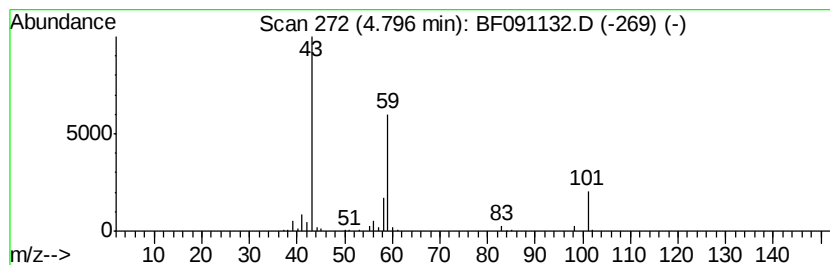
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	8.07 ng	424959	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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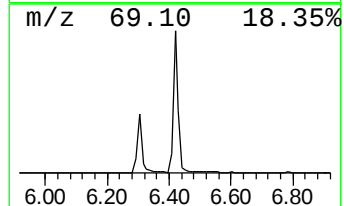
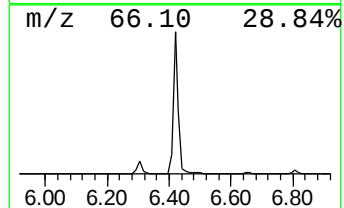
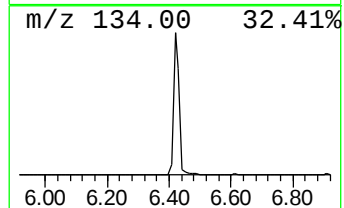
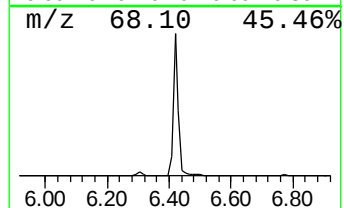
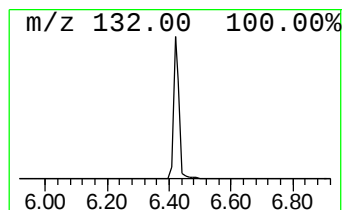
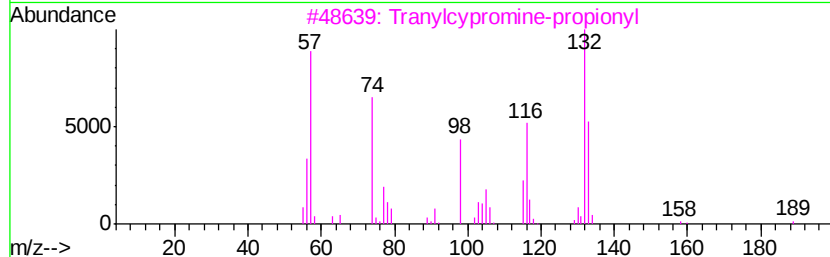
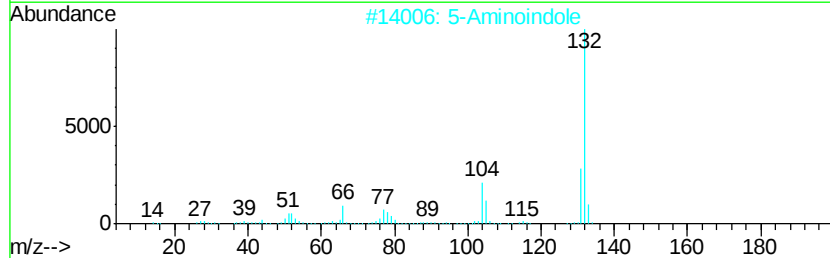
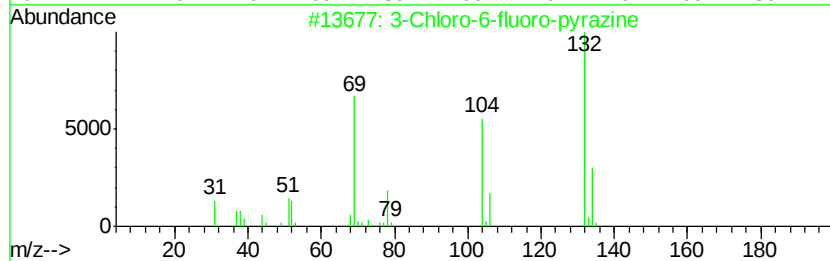
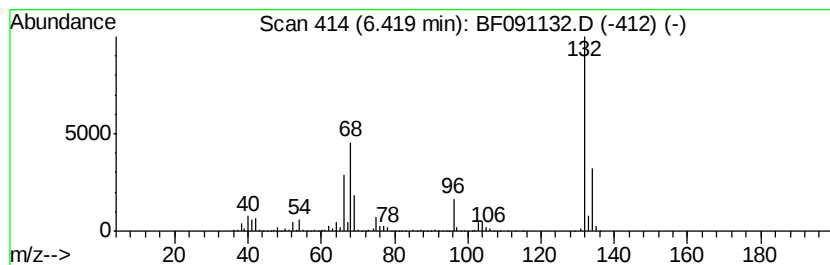
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Peak Number 3 unknown6.42 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	78.99 ng	4160750	1,4-Dichlorobenzene-d4	6.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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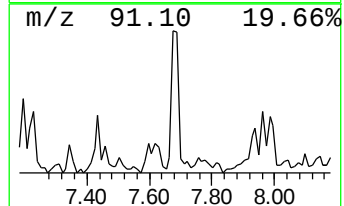
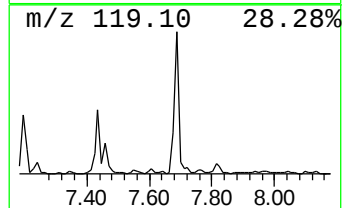
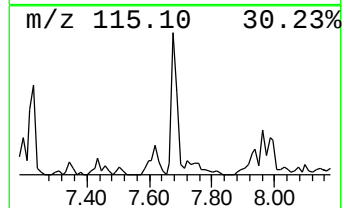
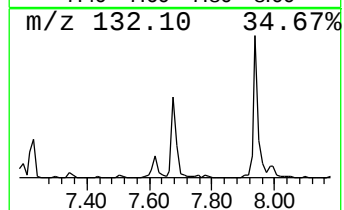
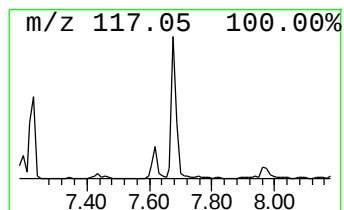
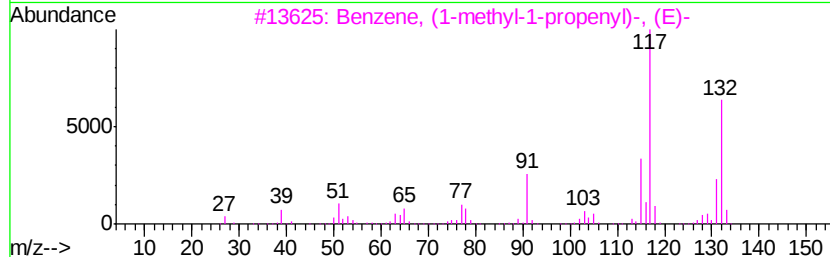
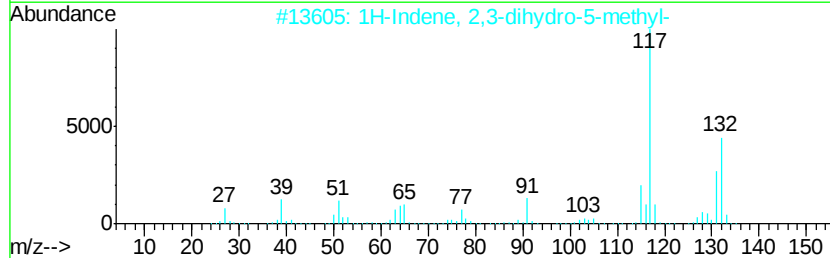
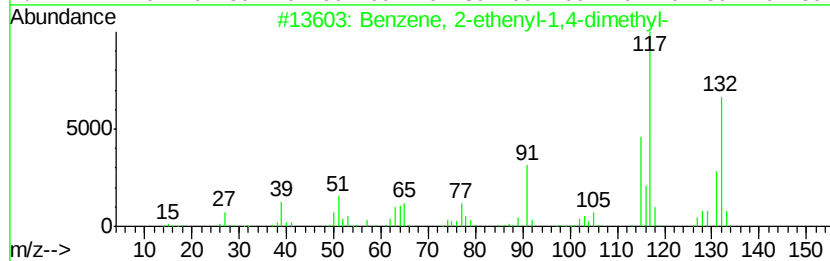
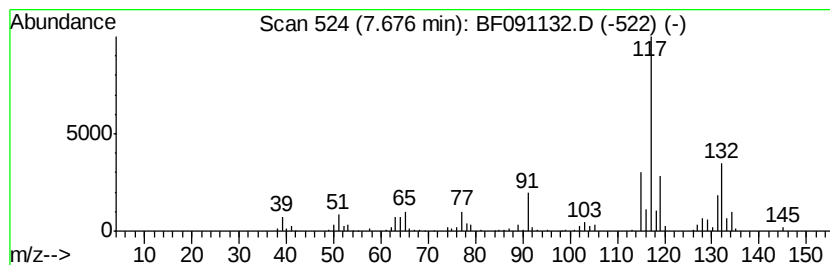
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Peak Number 5 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	4.04 ng	354332	Naphthalene-d8	7.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
3		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
4		3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5		Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83



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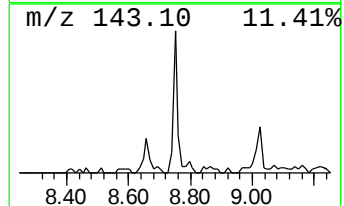
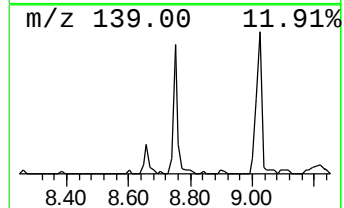
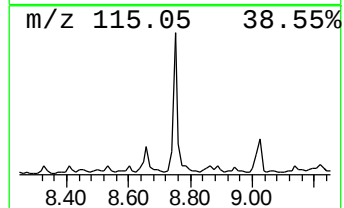
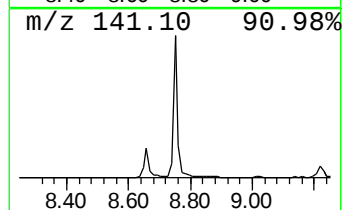
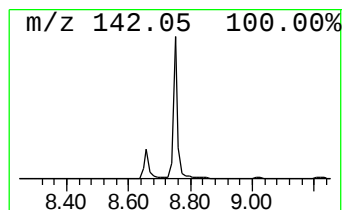
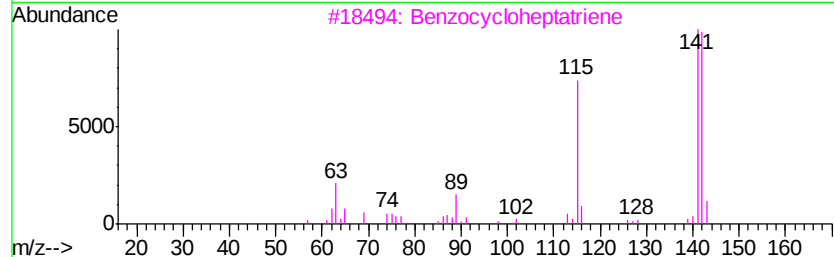
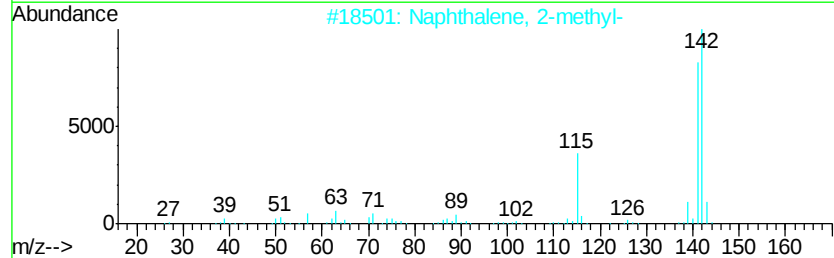
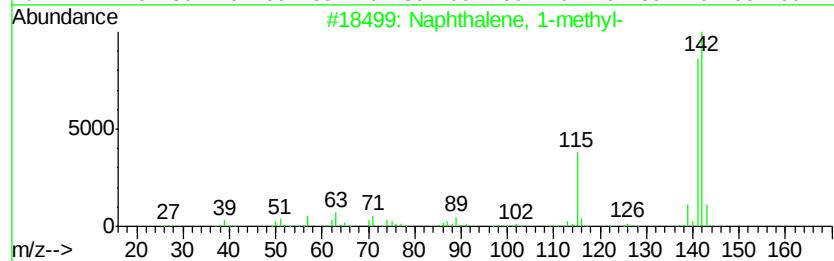
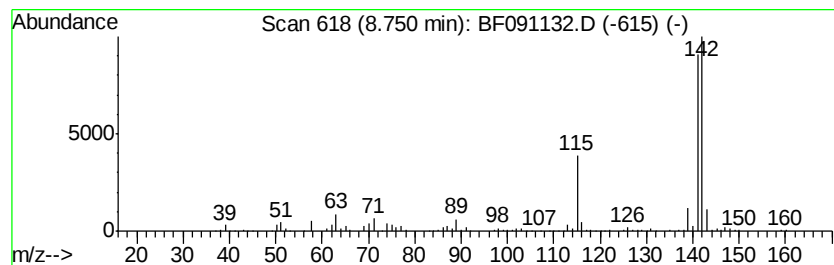
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Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.75	4.85 ng	425685	Naphthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		Benzocycloheptatriene	142	C11H10	000264-09-5	94
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	8.1	ng	424959	1	6.65	1053480	20.0
unknown6.42	6.42	79.0	ng	4160750	1	6.65	1053480	20.0
Benzene, 2-etheny...	7.68	4.0	ng	354332	2	7.94	1756110	20.0
Naphthalene, 1-me...	8.75	4.8	ng	425685	2	7.94	1756110	20.0