

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
 Data File : BF092142.D
 Acq On : 9 Jan 2017 17:27
 Operator : UM/SJ
 Sample : PB95818BL
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB95818BL

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-BF122116.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	4.081	189	192	203	rBV	107192	204648	3.40%	0.376%
2	4.790	251	254	264	rBV	1950710	3097801	51.50%	5.692%
3	5.247	291	294	297	rBV	5304482	5897700	98.05%	10.836%
4	6.299	383	386	389	rBV	4041650	5038850	83.77%	9.258%
5	6.401	392	395	398	rVV	4592188	6014976	100.00%	11.051%
6	6.630	412	415	417	rBV	1499178	1456964	24.22%	2.677%
7	6.790	426	429	431	rBV	3499943	4588270	76.28%	8.430%
8	7.202	461	465	467	rBV	3694261	4118669	68.47%	7.567%
9	7.910	524	527	530	rBV	1360331	1842869	30.64%	3.386%
10	8.996	618	622	625	rBV	4776875	5604237	93.17%	10.297%
11	9.670	677	681	683	rBV	1285913	1740488	28.94%	3.198%
12	10.459	746	750	752	rBV	3293095	3777775	62.81%	6.941%
13	11.145	807	810	812	rBV	2046215	1866698	31.03%	3.430%
14	12.734	946	949	952	rVB	4738048	5555879	92.37%	10.208%
15	13.774	1037	1040	1042	rBV	1854609	1750343	29.10%	3.216%
16	14.997	1139	1147	1157	rBV2	48105	222357	3.70%	0.409%
17	15.145	1157	1160	1162	rBV	1190174	1650013	27.43%	3.032%

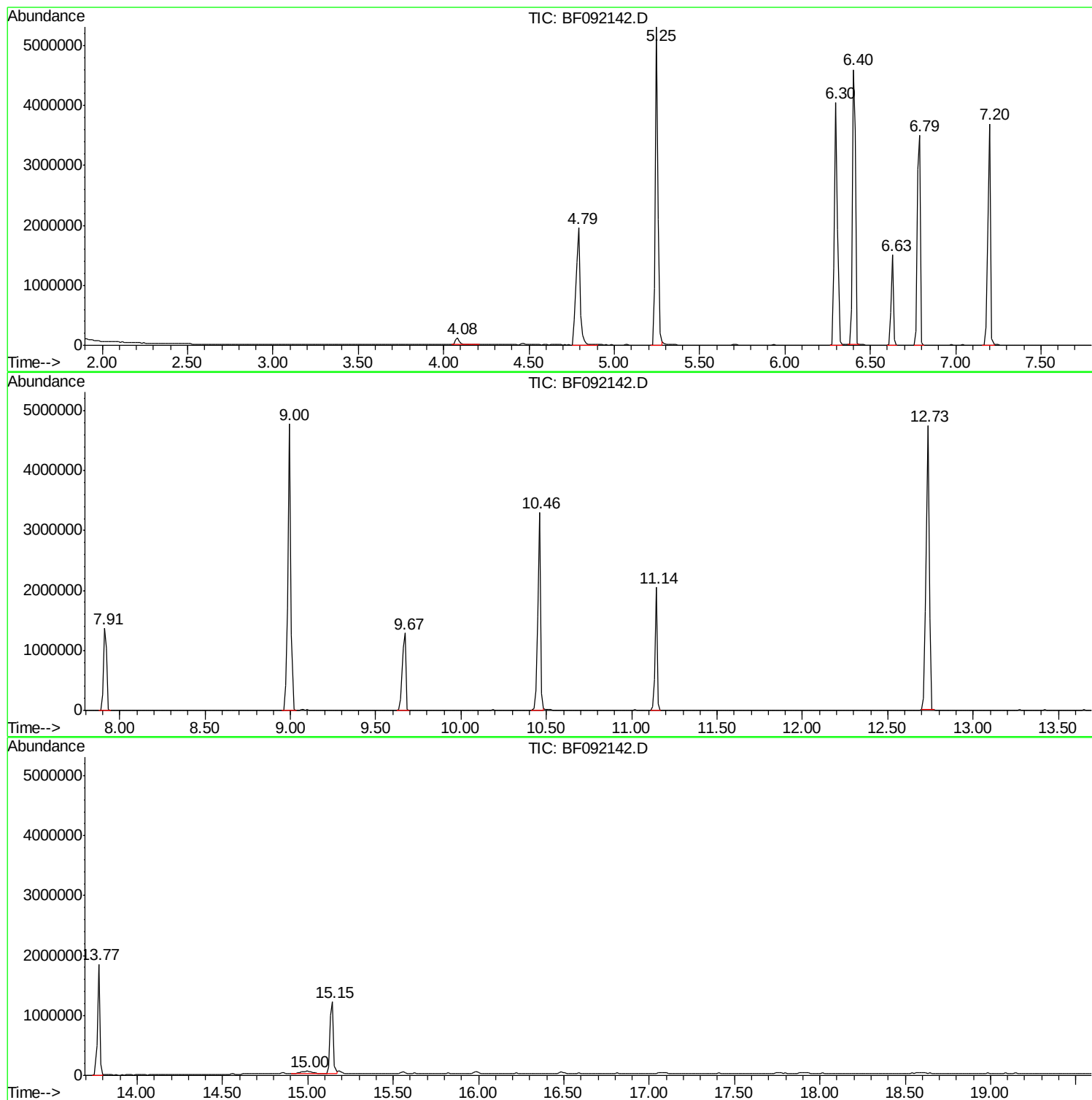
Sum of corrected areas: 54428537

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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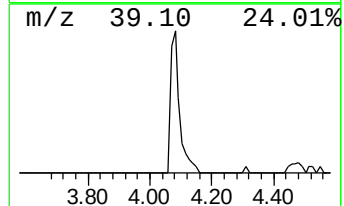
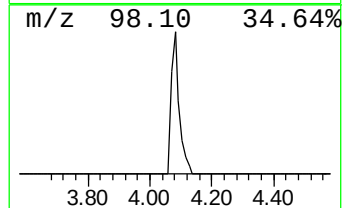
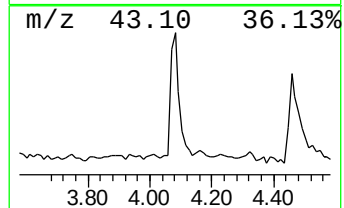
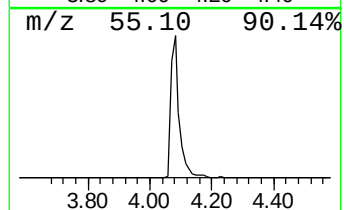
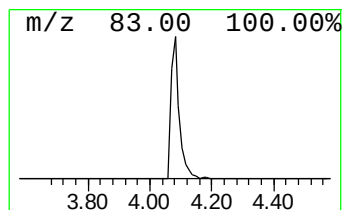
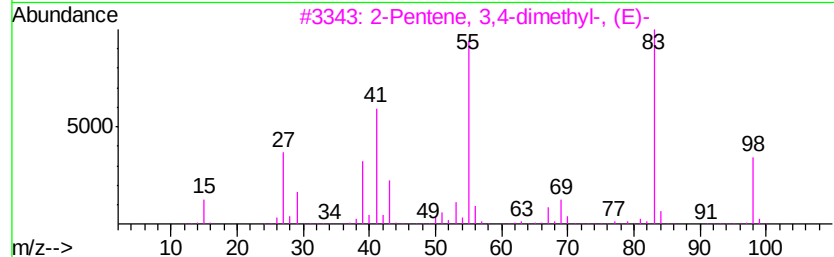
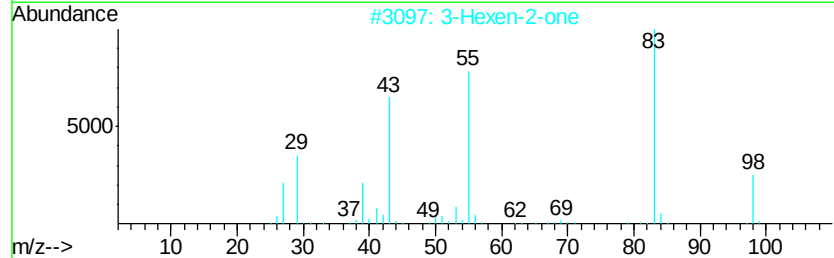
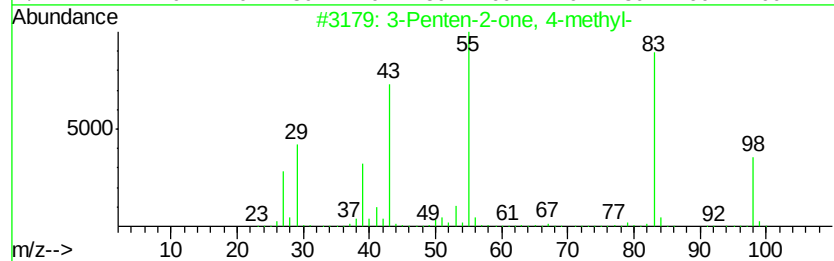
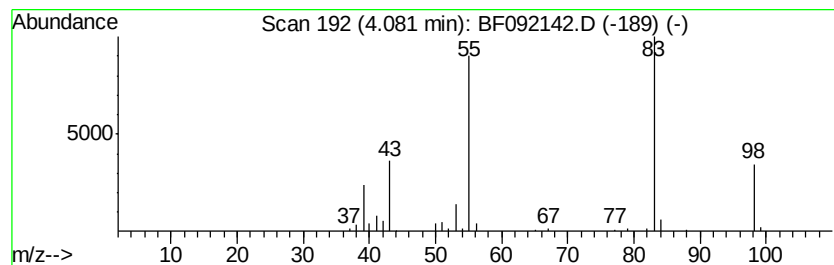
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.08	2.81 ng	204648	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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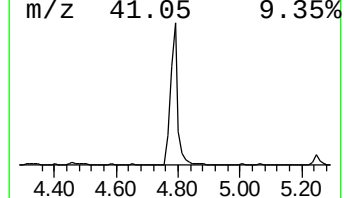
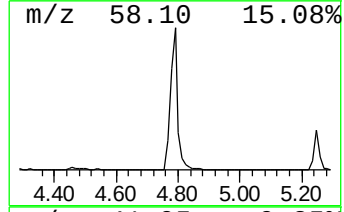
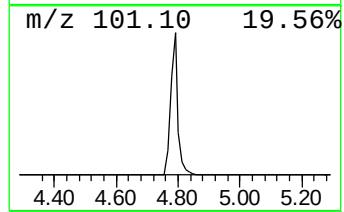
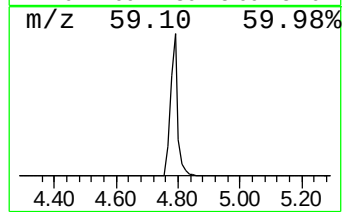
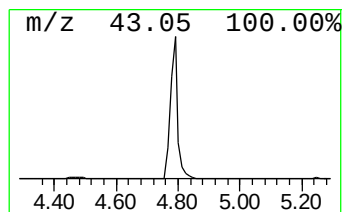
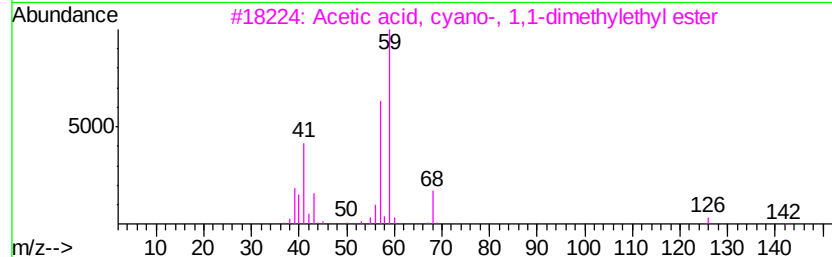
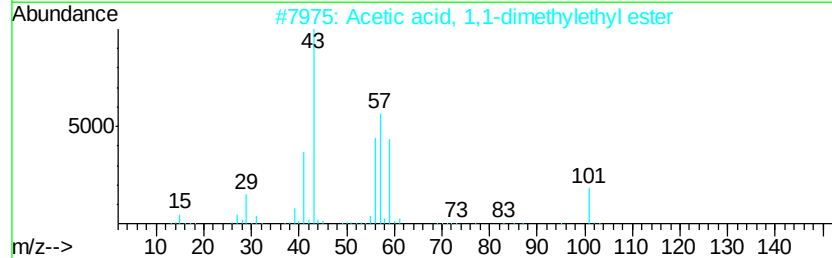
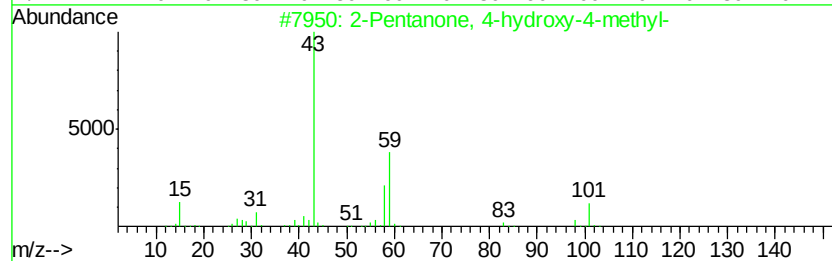
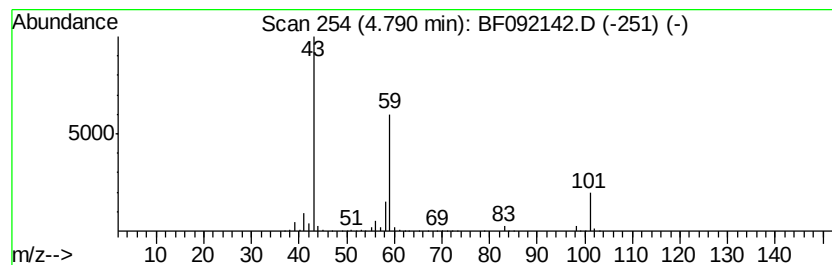
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	42.52 ng	3097800	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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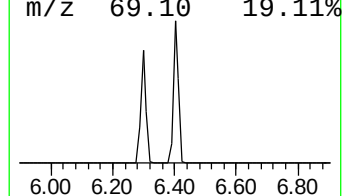
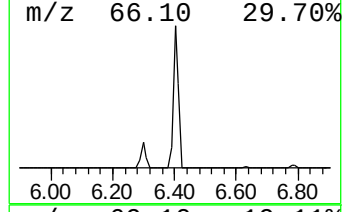
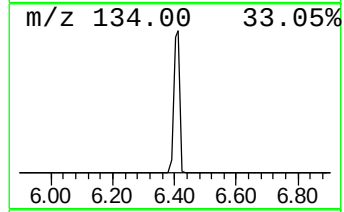
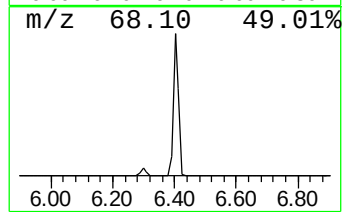
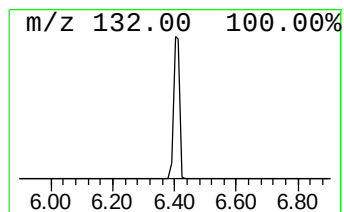
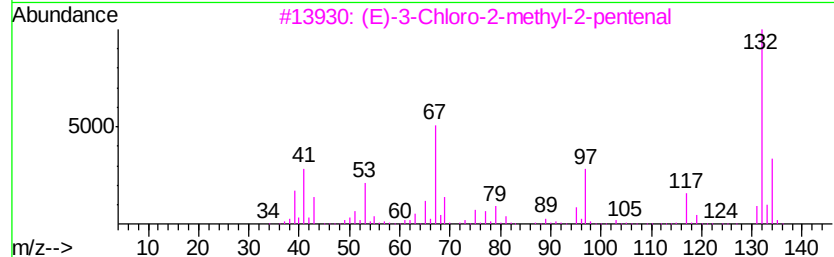
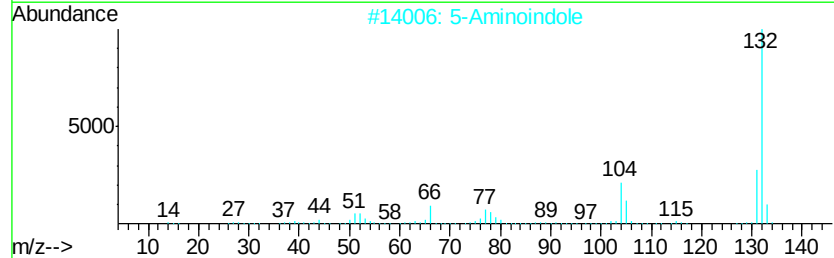
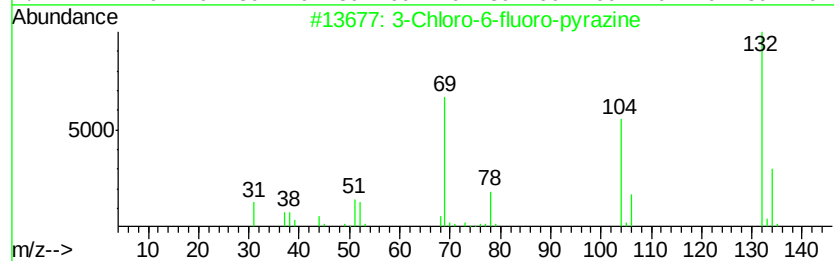
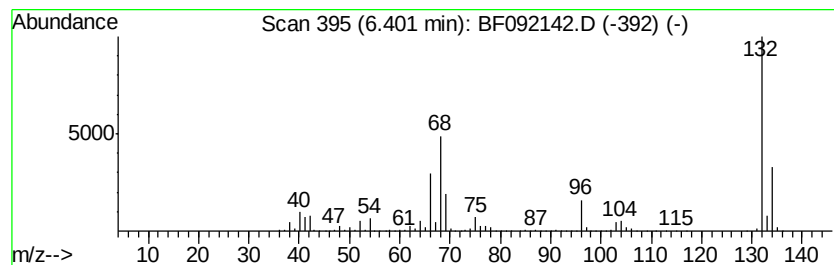
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Peak Number 3 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	82.57 ng	6014980	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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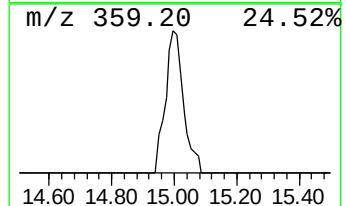
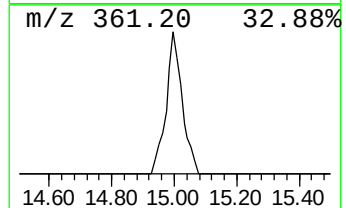
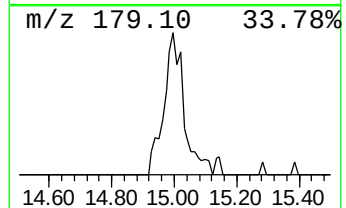
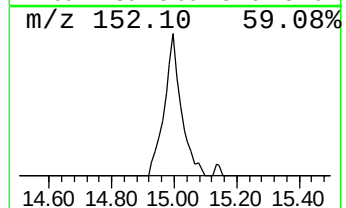
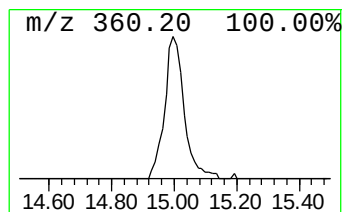
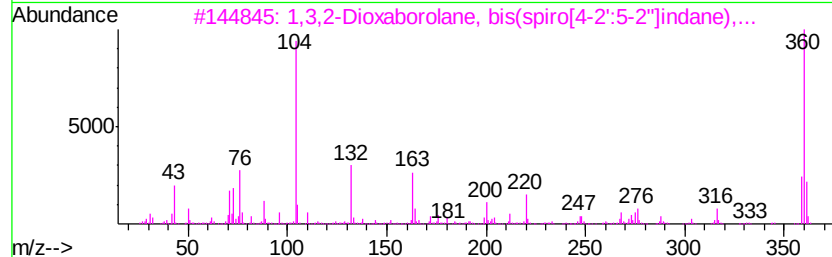
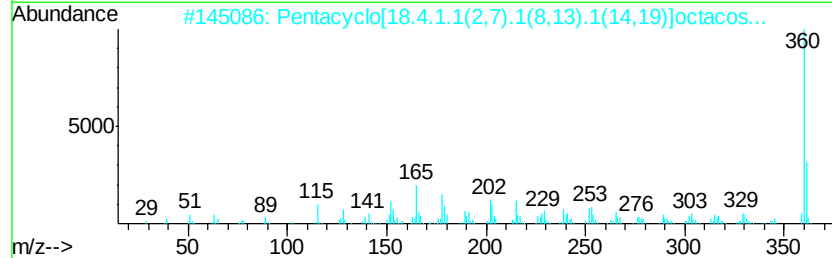
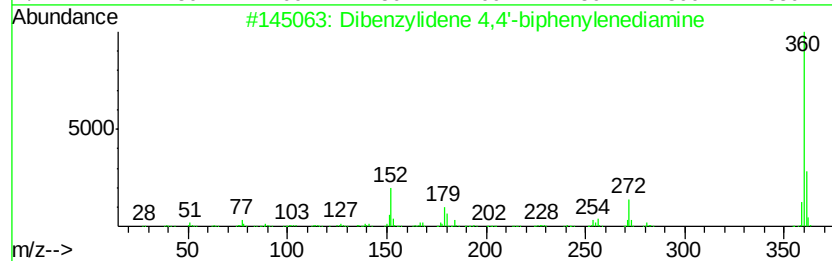
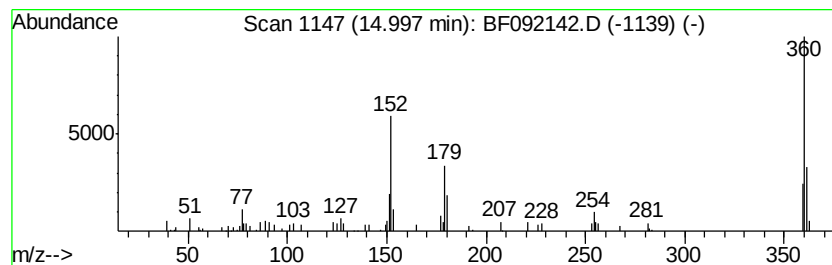
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Peak Number 5 Dibenzylidene 4,4'-biphenyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.70 ng	222357	Perylene-d12	15.15
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Dibenzylidene 4,4'-biphenylenedi...	360 C26H20N2	006311-48-4 90
2		Pentacyclo[18.4.1.1(2,7).1(8,13)...]	360 C28H24	101077-60-5 43
3		1,3,2-Dioxaborolane, bis(spiro[4...]	360 C20H13B06	1000150-23-7 43
4		1,10-Phenanthroline, 2,9-dimethy...	360 C26H20N2	004733-39-5 43
5		Benzaldehyde, 4-hydroxy-3,5-dime...	360 C18H20N2O6	014414-32-5 43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.08	2.8	ng	204648	1	6.63	1456960	20.0
2-Pentanone, 4-hy...	4.79	42.5	ng	3097800	1	6.63	1456960	20.0
unknown6.40	6.40	82.6	ng	6014980	1	6.63	1456960	20.0
Dibenzylidene 4,4...	15.00	2.7	ng	222357	6	15.15	1650010	20.0