

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121616\
 Data File : BF091674.D
 Acq On : 16 Dec 2016 15:57
 Operator : UM/SJ
 Sample : PB95362BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB95362BL

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-BF120916.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	4.281	189	192	200	rVB	168429	213109	2.72%	0.332%
2	4.956	248	251	259	rBV	1502347	2151643	27.51%	3.355%
3	5.378	285	288	291	rBV	4611554	6004358	76.76%	9.364%
4	6.419	375	379	381	rBV	5830561	6581199	84.14%	10.263%
5	6.544	387	390	392	rBV	6179520	6305530	80.61%	9.833%
6	6.773	407	410	412	rBV	1645669	1457939	18.64%	2.274%
7	6.933	421	424	426	rBV	4673196	5180513	66.23%	8.079%
8	7.333	456	459	462	rBV	3231226	4104147	52.47%	6.400%
9	8.053	519	522	525	rBV	1750801	2063077	26.38%	3.217%
10	9.139	613	617	619	rBV	6840978	7822016	100.00%	12.198%
11	9.813	672	676	678	rBV	1901296	2330239	29.79%	3.634%
12	10.602	741	745	747	rBV	3815903	5004780	63.98%	7.805%
13	11.288	802	805	808	rBV	2632894	2398832	30.67%	3.741%
14	12.876	941	944	947	rBV	6184053	7758057	99.18%	12.098%
15	13.916	1033	1035	1038	rBV	2297950	2329981	29.79%	3.634%
16	15.322	1155	1158	1161	rBV	1852058	2278059	29.12%	3.553%
17	15.642	1181	1186	1194	rBV2	36145	141148	1.80%	0.220%

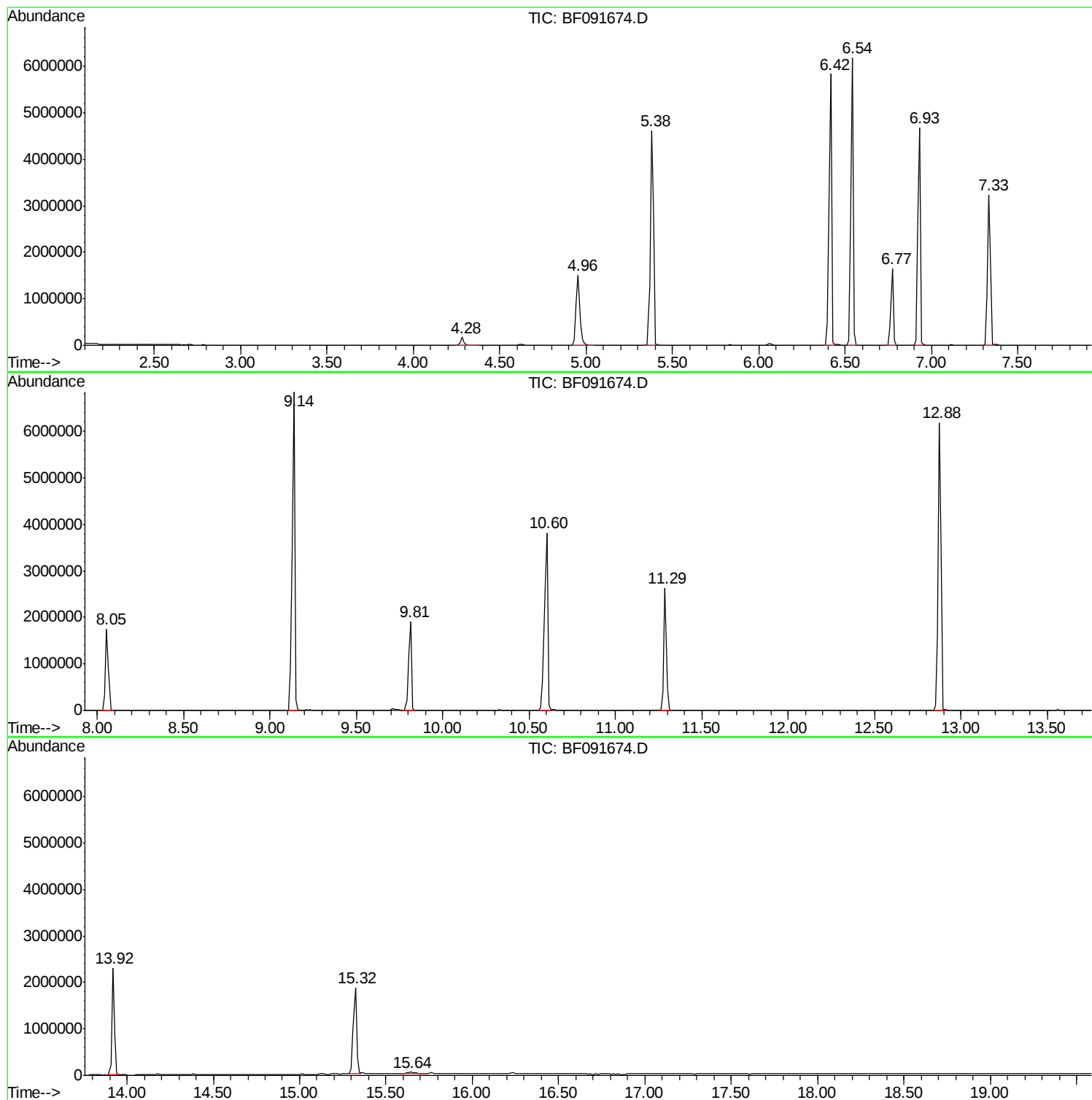
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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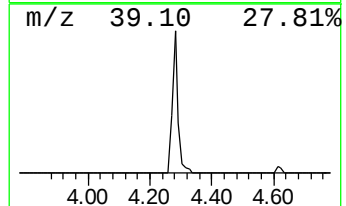
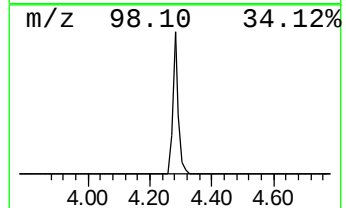
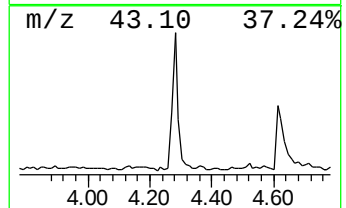
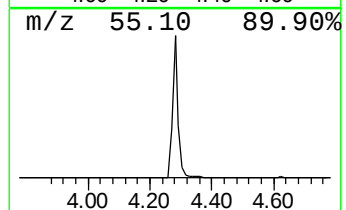
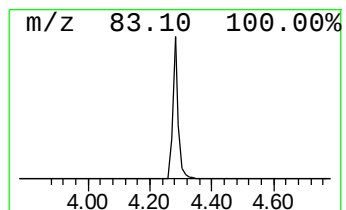
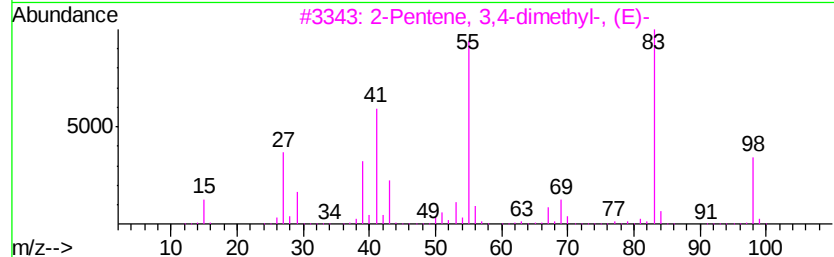
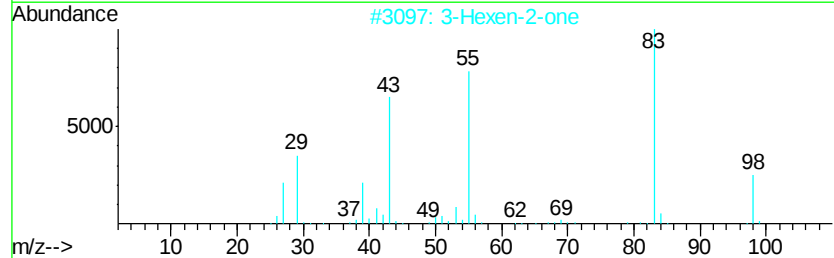
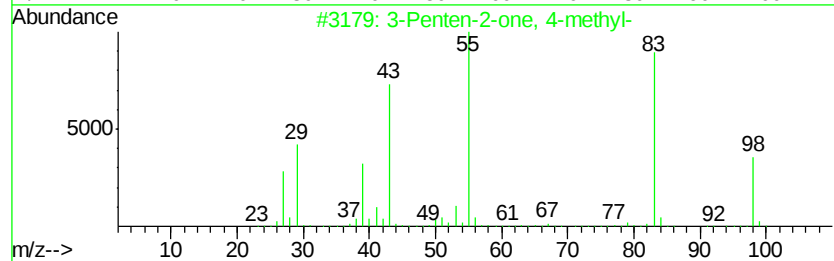
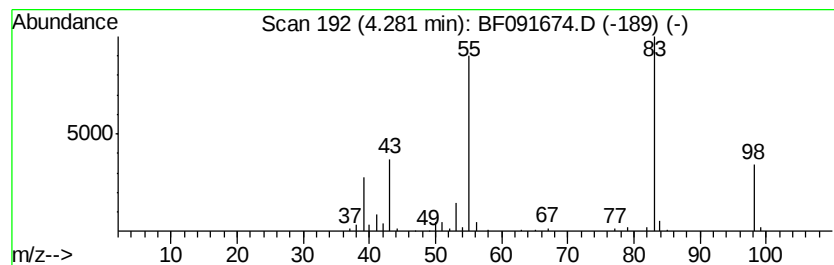
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.28	2.92 ng	213109	1,4-Dichlorobenzene-d4	6.77

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	90
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86



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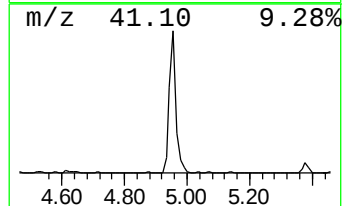
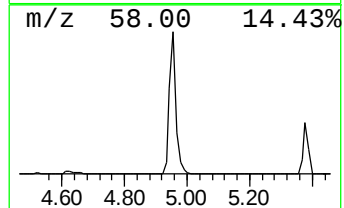
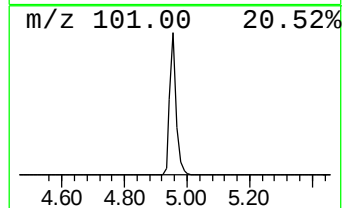
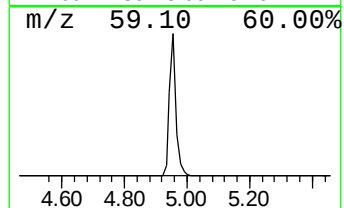
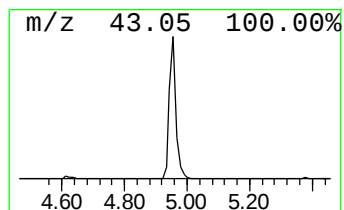
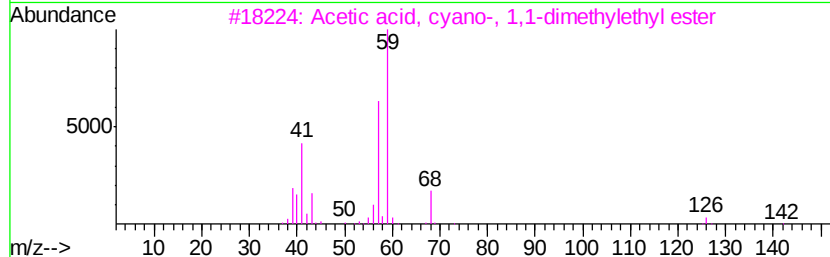
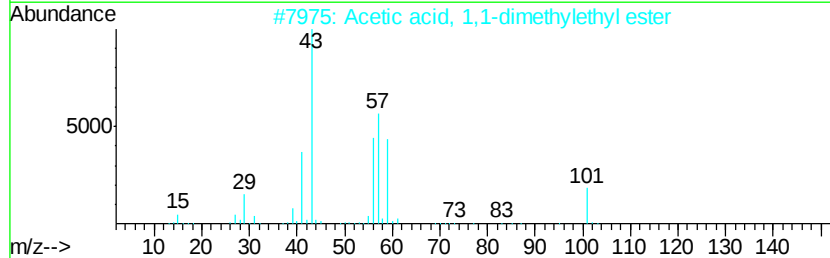
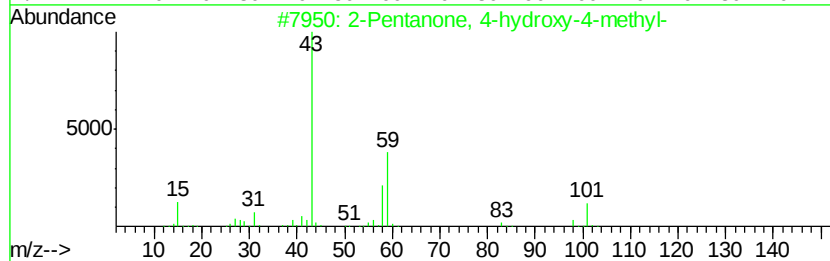
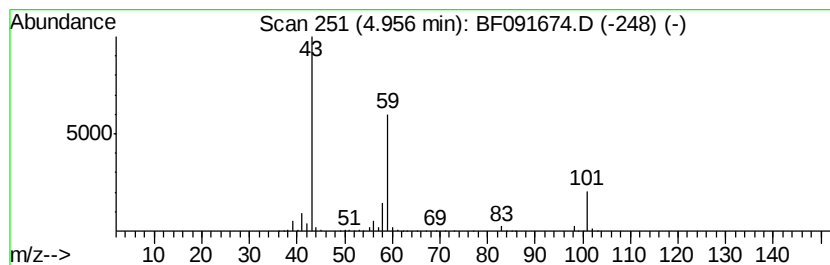
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	29.52 ng	2151640	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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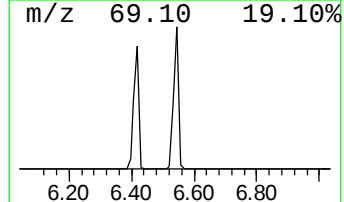
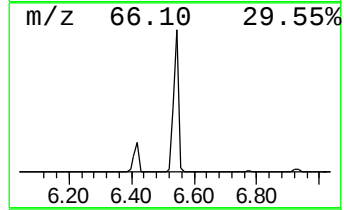
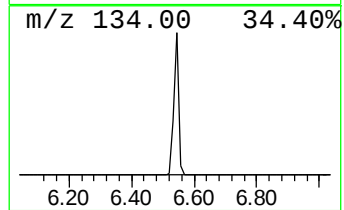
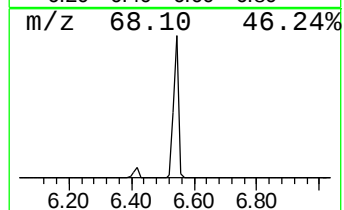
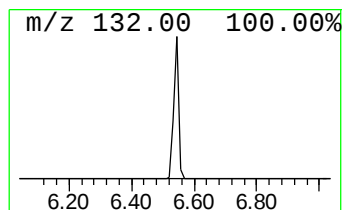
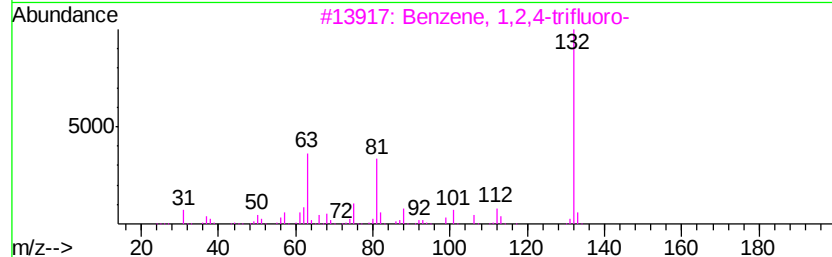
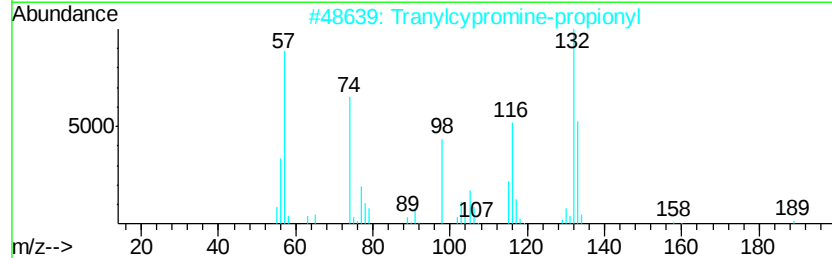
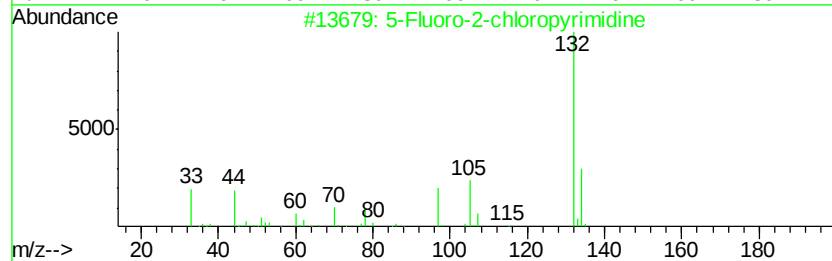
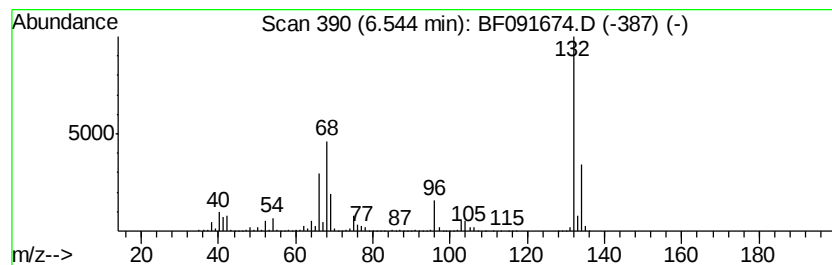
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Peak Number 3 unknown6.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	86.50 ng	6305530	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.28	2.9	ng	213109	1	6.77	1457940	20.0
2-Pentanone, 4-hy...	4.96	29.5	ng	2151640	1	6.77	1457940	20.0
unknown6.54	6.54	86.5	ng	6305530	1	6.77	1457940	20.0