

Data Path : U:\HPCHEM1\BNA_F\DATA\BF082117\
 Data File : BF097912.D
 Acq On : 21 Aug 2017 18:27
 Operator : SJ/JU
 Sample : PB101660BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB101660BL

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-BF081517.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	4.316	375	379	386	rVB	82545	98786	2.55%	0.297%
2	4.957	483	488	501	rVB	583530	898207	23.20%	2.698%
3	5.369	552	558	561	rBV	3332013	3617357	93.44%	10.867%
4	6.386	725	731	734	rBV	3332297	3648987	94.26%	10.962%
5	6.516	748	753	757	rBV	3106232	3516024	90.82%	10.562%
6	6.745	788	792	796	rBV	993597	792992	20.48%	2.382%
7	6.904	814	819	822	rBV	2949002	2737286	70.71%	8.223%
8	7.310	882	888	891	rBV	2150132	2348245	60.66%	7.054%
9	8.028	1005	1010	1014	rBV	1099854	1039195	26.84%	3.122%
10	9.110	1187	1194	1197	rBV	3562253	3871356	100.00%	11.630%
11	9.780	1303	1308	1312	rBV	1183989	1103930	28.52%	3.316%
12	10.569	1435	1442	1445	rBV	2170996	2336783	60.36%	7.020%
13	11.263	1554	1560	1563	rBV	1397849	1172384	30.28%	3.522%
14	12.674	1797	1800	1804	rBV	63129	56428	1.46%	0.170%
15	12.857	1824	1831	1834	rBV	3463668	3834973	99.06%	11.521%
16	13.380	1913	1920	1924	rBV	56688	53284	1.38%	0.160%
17	13.892	2001	2007	2011	rBV	1248473	1209701	31.25%	3.634%
18	15.315	2243	2249	2253	rBV	760326	952177	24.60%	2.860%

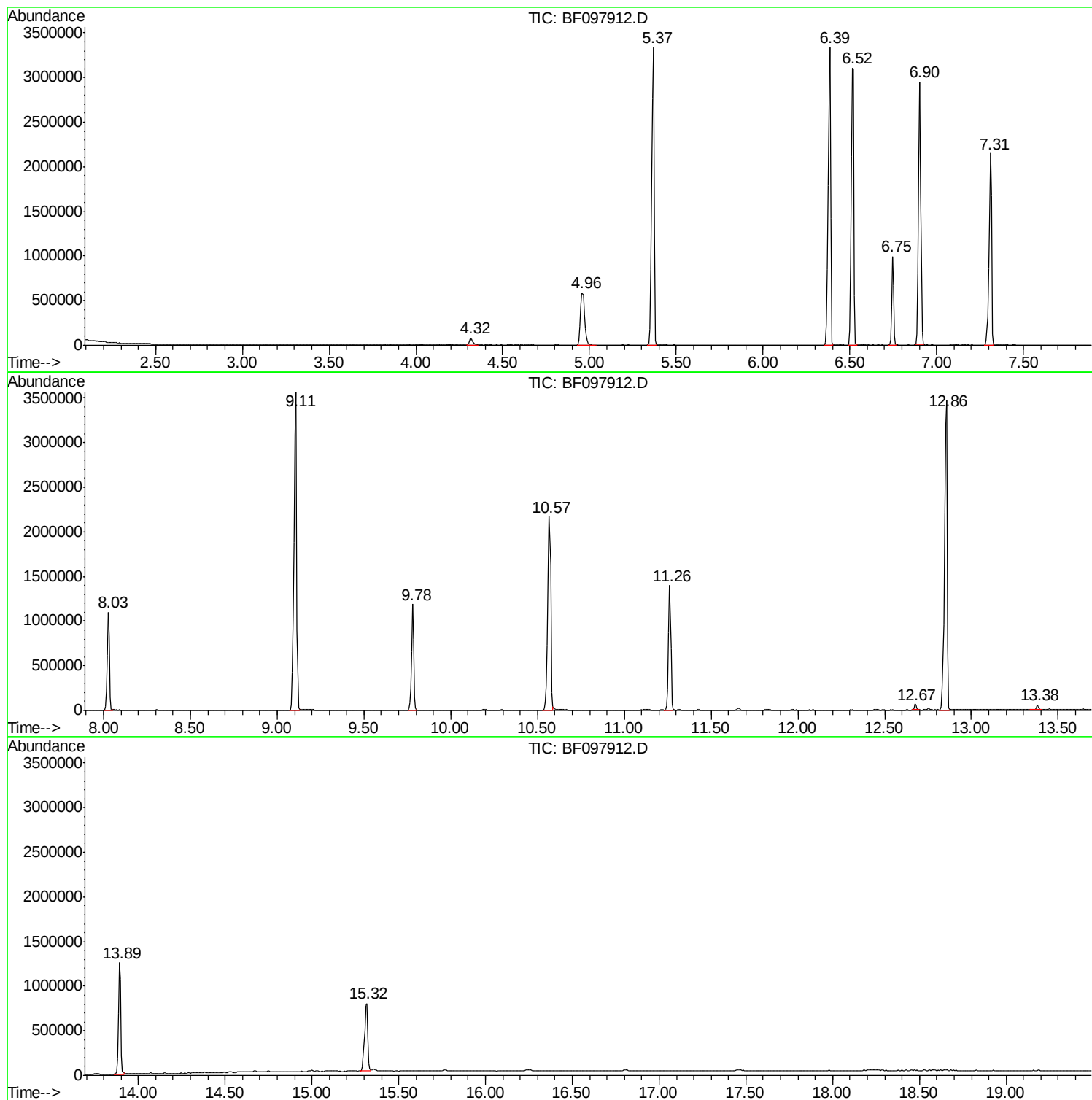
Sum of corrected areas: 33288095

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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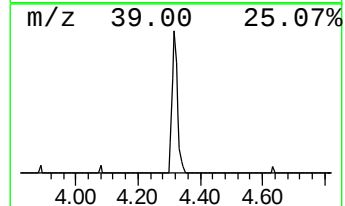
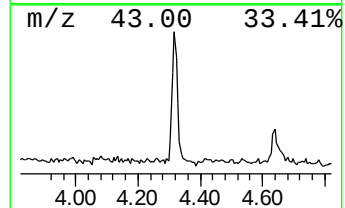
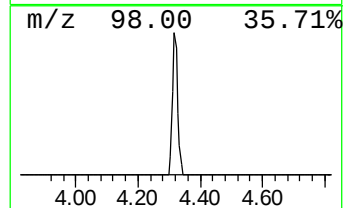
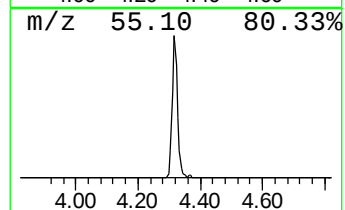
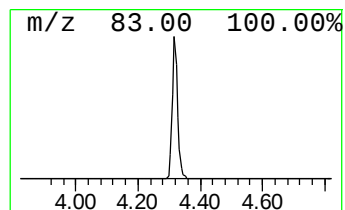
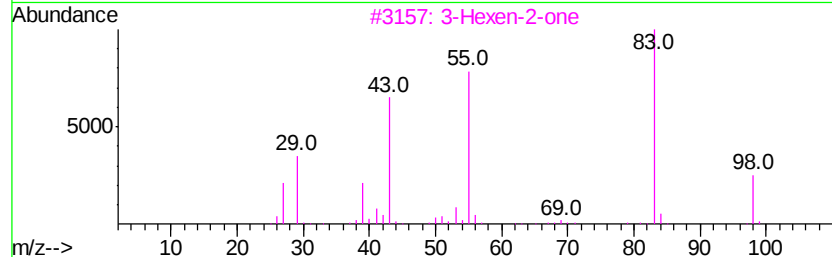
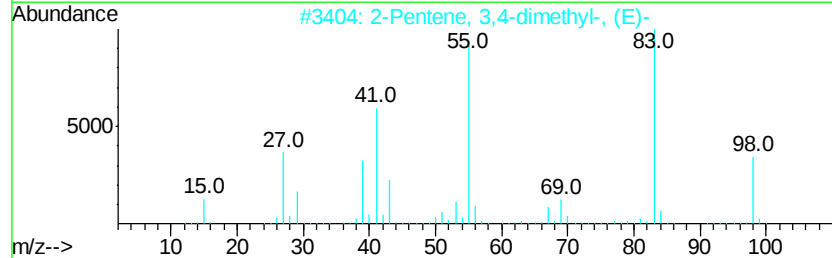
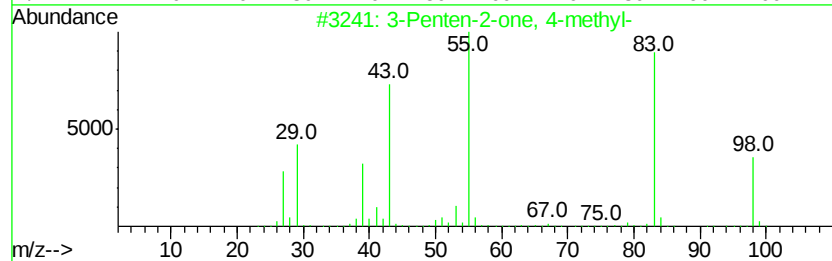
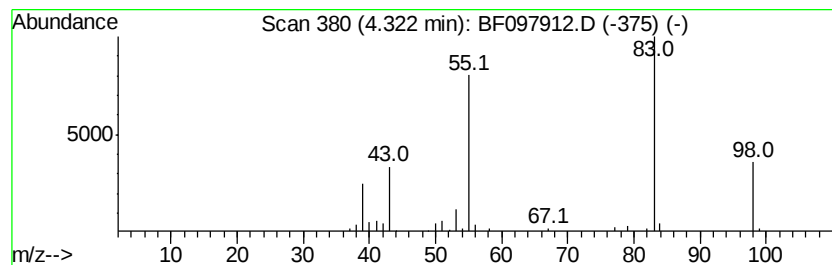
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	2.49 ng	98786	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3		3-Hexen-2-one	98	C6H10O	000763-93-9	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	90
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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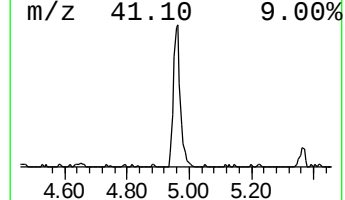
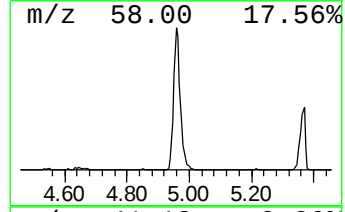
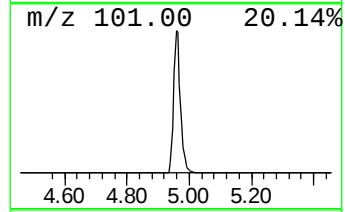
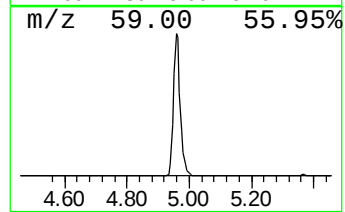
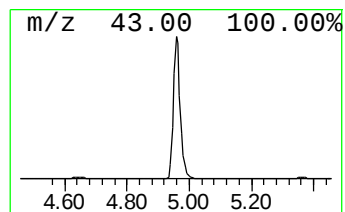
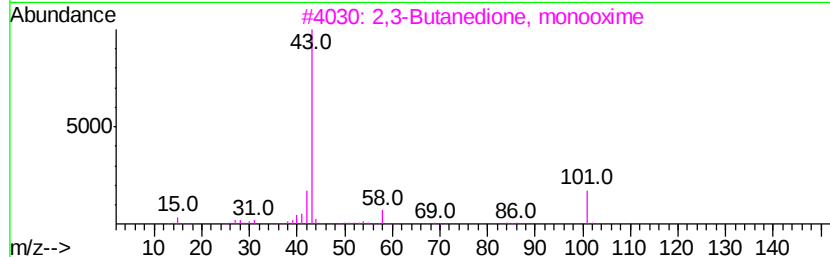
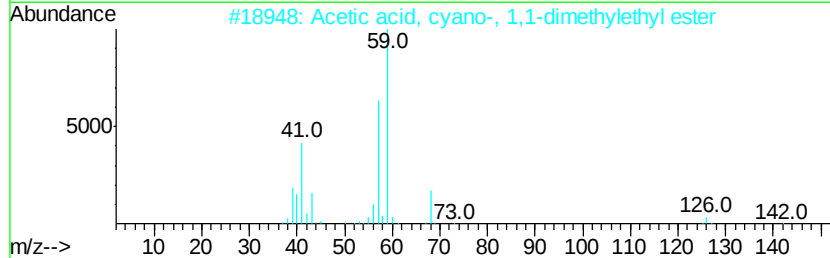
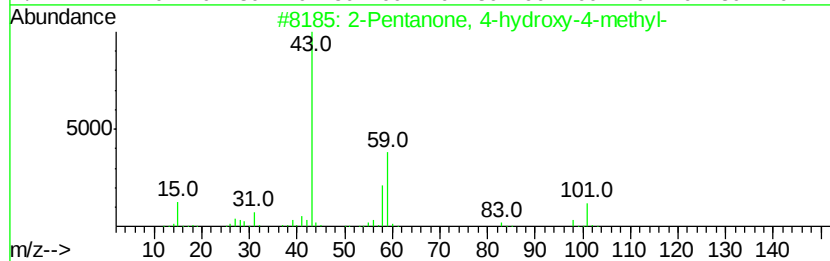
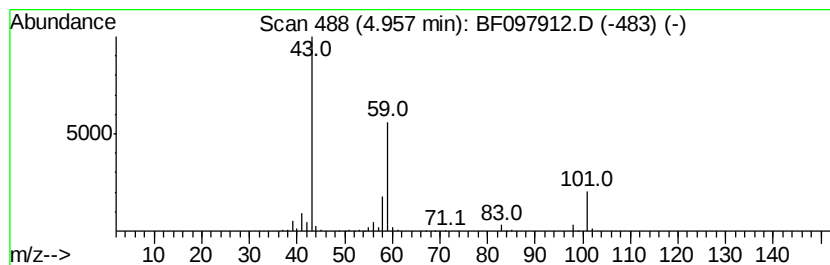
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	22.65 ng	898207	1,4-Dichlorobenzene-d4	6.75

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	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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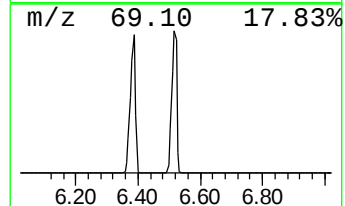
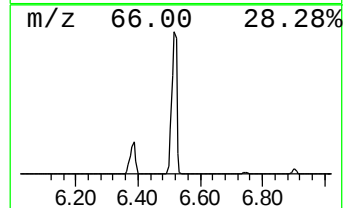
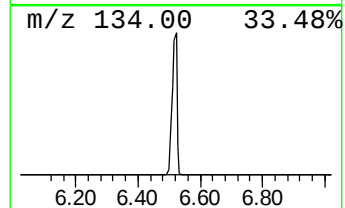
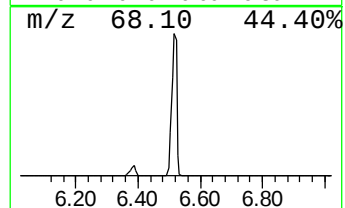
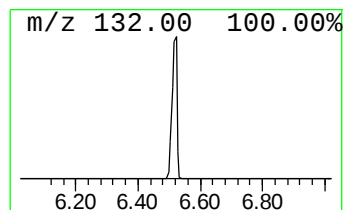
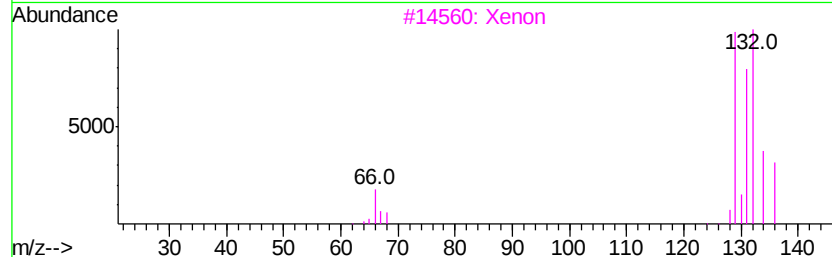
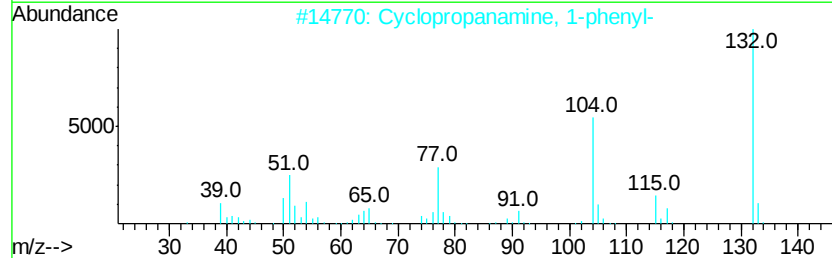
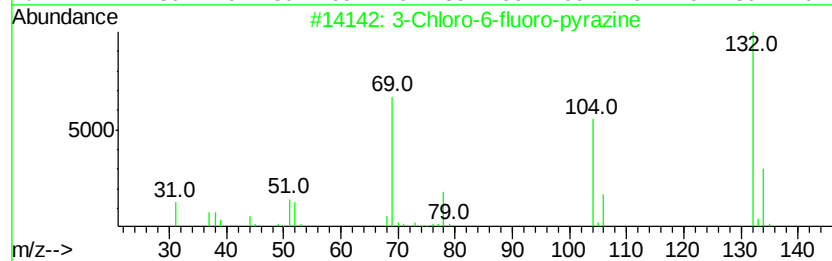
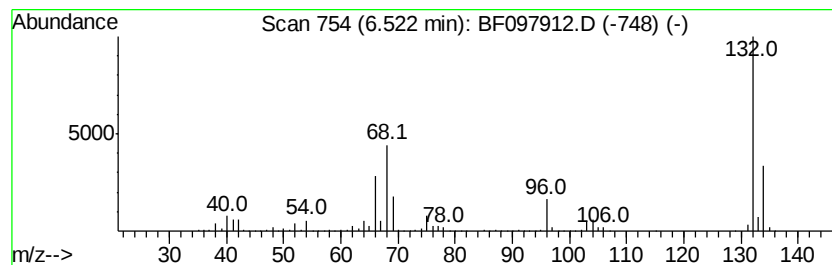
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Peak Number 3 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	88.68 ng	3516020	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
3		Xenon	132	Xe	007440-63-3	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.32	2.5	ng	98786	1	6.75	792992	20.0
2-Pentanone, 4-hy...	4.96	22.6	ng	898207	1	6.75	792992	20.0
unknown6.52	6.52	88.7	ng	3516020	1	6.75	792992	20.0