

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082517\
 Data File : BF098040.D
 Acq On : 25 Aug 2017 19:50
 Operator : SJ/JU
 Sample : I4947-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ELIZABETH-RO-COMP-A

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	4.293	371	375	382	rBV	156578	187453	5.80%	0.617%
2	4.940	481	485	494	rVB	381265	527144	16.30%	1.734%
3	5.351	549	555	558	rBV	2901235	3021049	93.44%	9.937%
4	6.375	723	729	732	rBV	2867836	3233274	100.00%	10.635%
5	6.510	747	752	755	rBV	2798690	2989487	92.46%	9.833%
6	6.740	787	791	794	rBV	1616870	1389301	42.97%	4.570%
7	6.798	797	801	804	rVB	120639	102551	3.17%	0.337%
8	6.892	813	817	820	rBV	2171089	1915529	59.24%	6.301%
9	7.304	881	887	890	rBV	1775488	1931988	59.75%	6.355%
10	8.022	1004	1009	1012	rBV	1924982	1818810	56.25%	5.983%
11	8.098	1019	1022	1026	rBV2	32296	33121	1.02%	0.109%
12	9.098	1186	1192	1195	rBV	1981220	1931548	59.74%	6.353%
13	9.181	1200	1206	1215	rVV5	27047	44862	1.39%	0.148%
14	9.492	1254	1259	1262	rBV	548987	462583	14.31%	1.522%
15	9.710	1293	1296	1300	rVB	36551	33997	1.05%	0.112%
16	9.775	1300	1307	1310	rBV	2017783	1937600	59.93%	6.373%
17	10.557	1435	1440	1444	rBV	1811821	1854214	57.35%	6.099%
18	10.680	1458	1461	1469	rBV	42977	48419	1.50%	0.159%
19	11.128	1534	1537	1540	rBV2	45079	38871	1.20%	0.128%
20	11.257	1553	1559	1562	rBV	2062835	1956638	60.52%	6.436%
21	12.839	1823	1828	1831	rBV	2015720	1966341	60.82%	6.468%
22	13.069	1865	1867	1870	rBV2	32233	36869	1.14%	0.121%
23	13.198	1887	1889	1892	rBV3	32876	32949	1.02%	0.108%
24	13.527	1943	1945	1950	rBV6	31164	50499	1.56%	0.166%
25	13.886	2001	2006	2009	rBV	1670443	1596506	49.38%	5.251%
26	14.727	2146	2149	2153	rVB	85910	87384	2.70%	0.287%
27	15.304	2241	2247	2252	rBV	962373	1173105	36.28%	3.859%

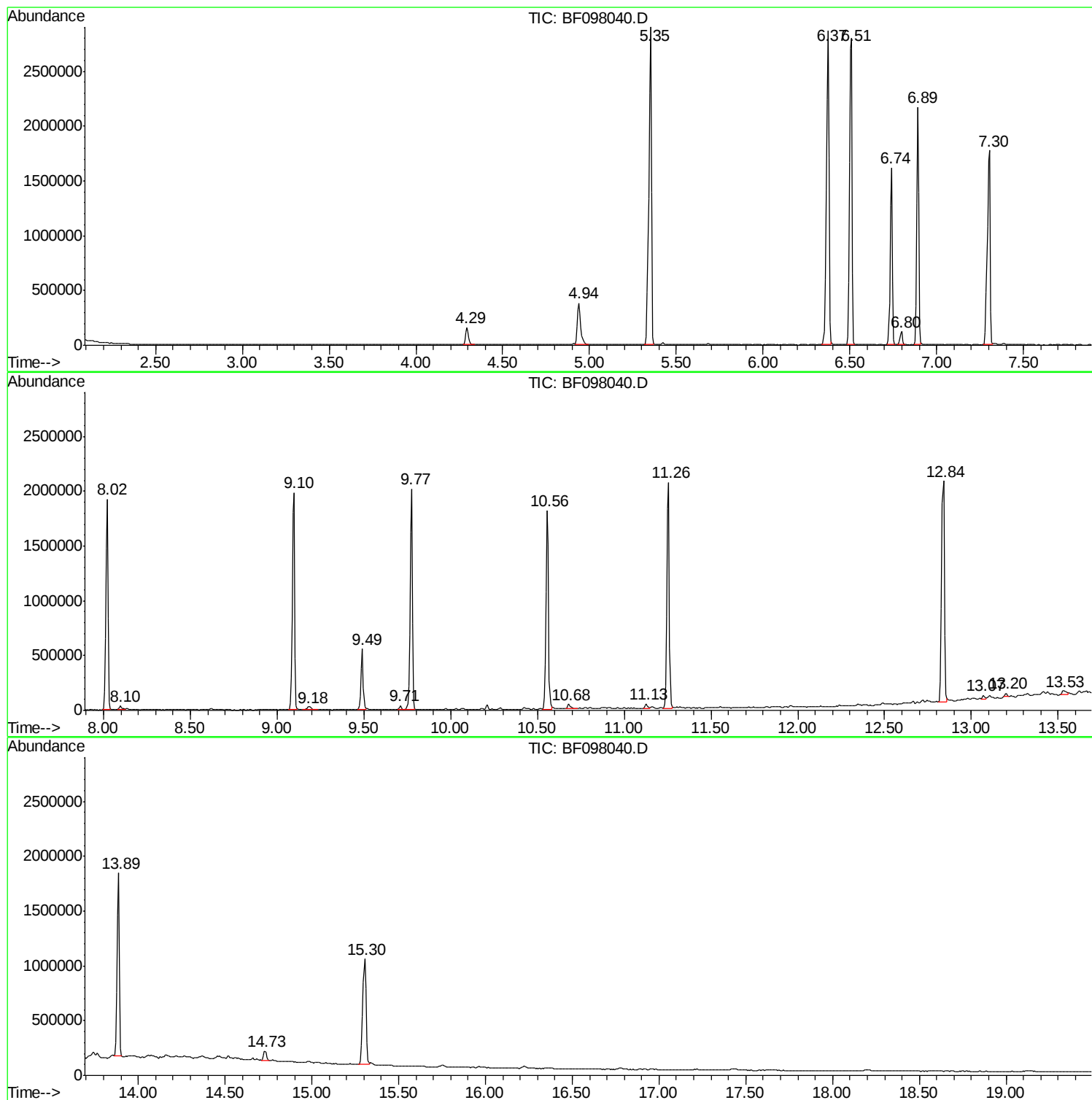
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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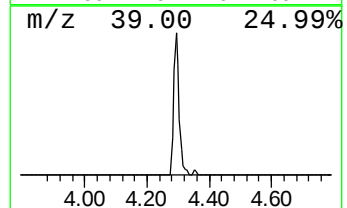
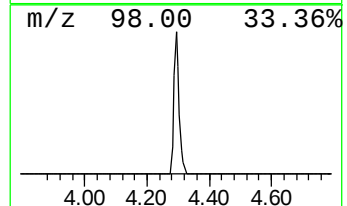
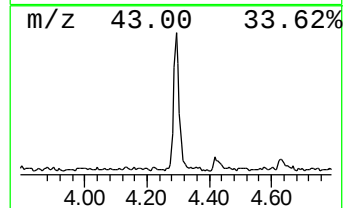
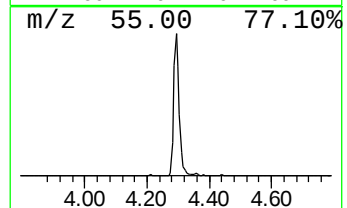
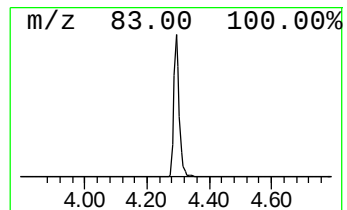
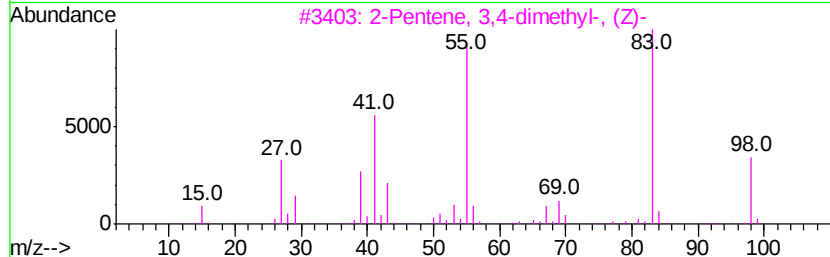
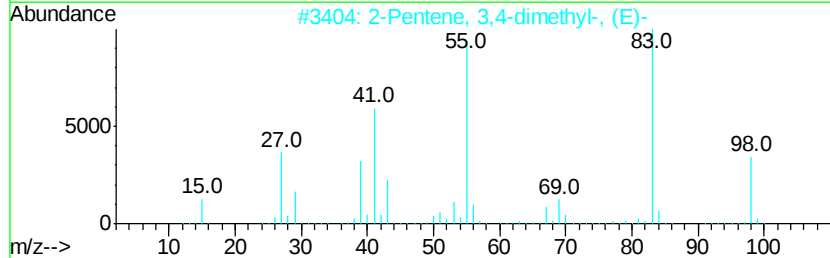
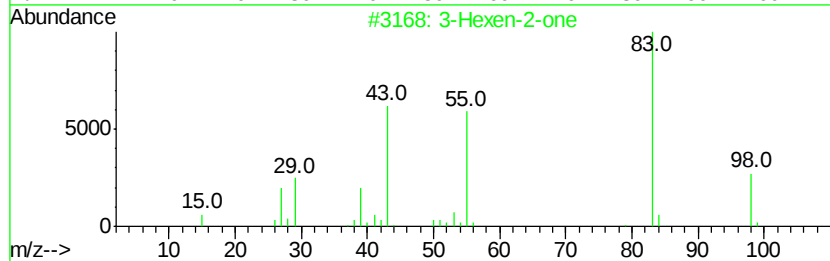
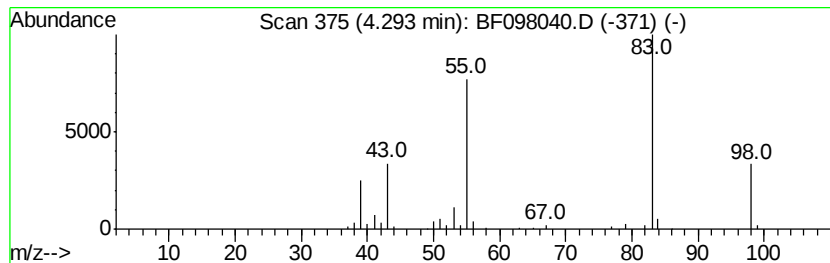
Instrument :
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ClientSampleId :
ELIZABETH-RO-COMP-A

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

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.29	2.70 ng	187453	1,4-Dichlorobenzene-d4	6.74	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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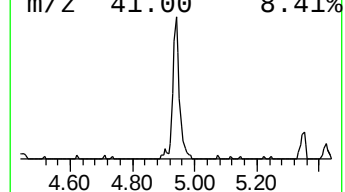
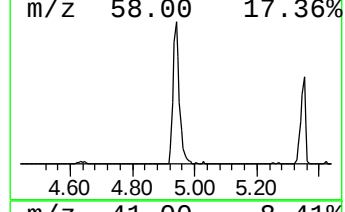
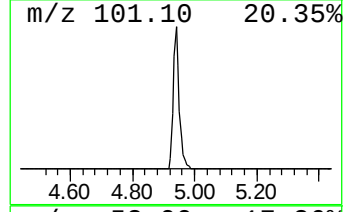
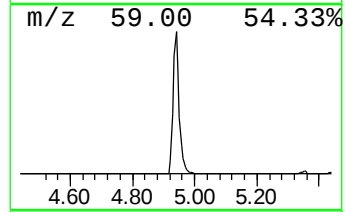
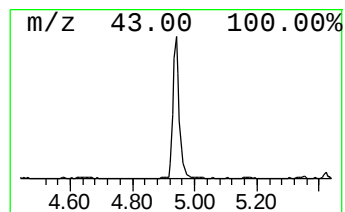
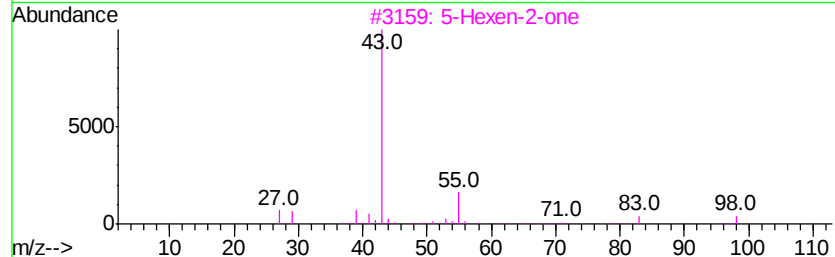
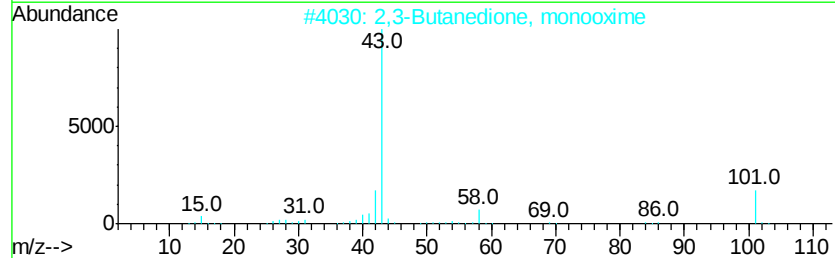
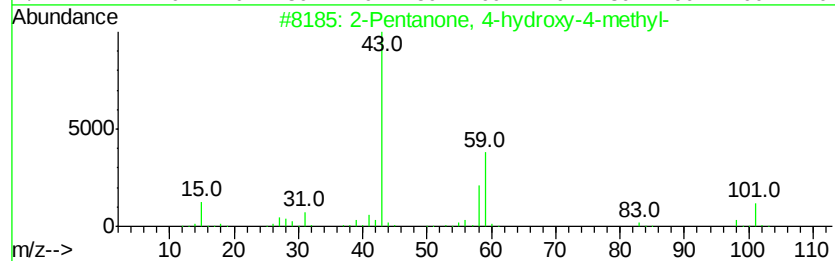
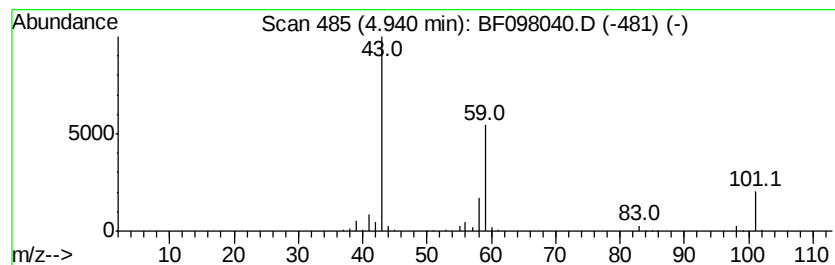
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	7.59 ng	527144	1,4-Dichlorobenzene-d4	6.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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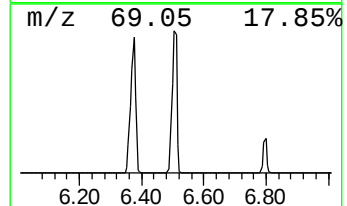
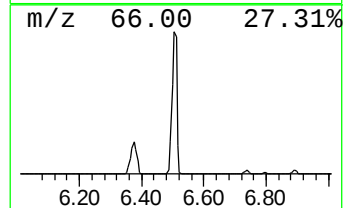
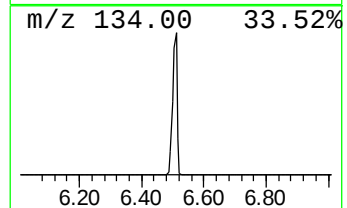
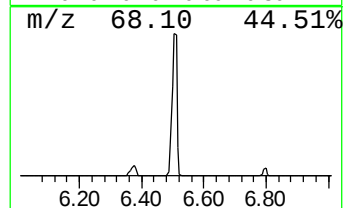
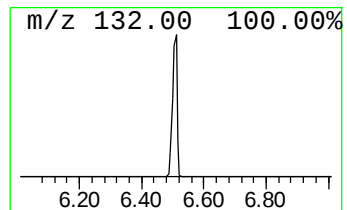
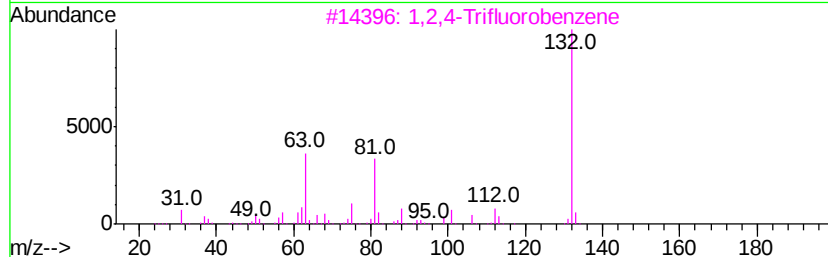
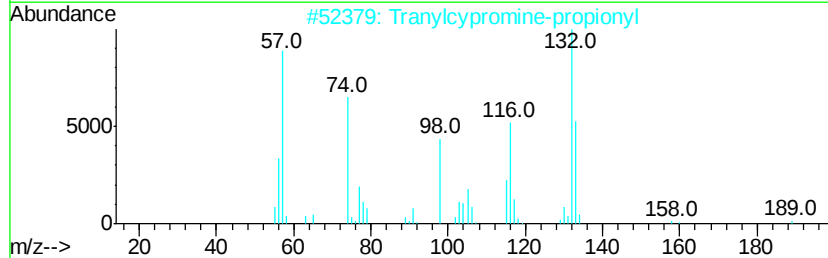
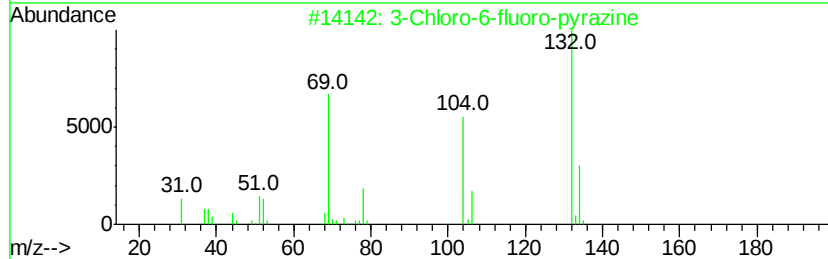
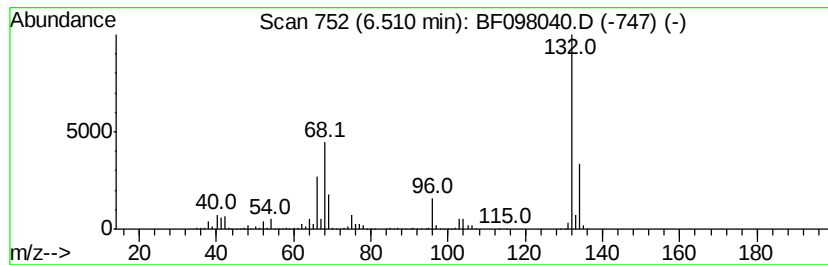
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Peak Number 3 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	43.04 ng	2989490	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.29	2.7	ng	187453	1	6.74	1389300	20.0
2-Pentanone, 4-hy...	4.94	7.6	ng	527144	1	6.74	1389300	20.0
unknown6.51	6.51	43.0	ng	2989490	1	6.74	1389300	20.0