LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\
Data File : BF096314.D
Acq On : 30 Jun 2017 1:38
Operator : SJ/MA
Sample : I3882-13 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G54-0-1.5

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-BF062717.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	4.322	375	380	389	rVB	54575	67740	9.14%	1.161%
2	4.951	484	487	498	rVB	217850	218627	29.51%	3.747%
3	5.375	556	559	565	rVB	157637	135548	18.29%	2.323%
4	6.057	667	675	677	rBV5	6728	11416	1.54%	0.196%
5	6.392	728	732	740	rVB	327775	288649	38.96%	4.947%
6	6.534	753	756	759	rBV	248848	196464	26.51%	3.367%
7	6.769	793	796	800	rBV	685924	585177	78.97%	10.029%
8	6.928	819	823	827	rVB	292404	232787	31.42%	3.989%
9	7.322	886	890	894	rBV	218700	167390	22.59%	2.869%
10	8.051	1010	1014	1018	rBV	895319	740970	100.00%	12.699%
11	8.492	1085	1089	1092	rBV	7845	8731	1.18%	0.150%
12	8.657	1113	1117	1120	rBV	18214	15720	2.12%	0.269%
13	9.128	1193	1197	1200	rBV	384121	290561	39.21%	4.980%
14	9.222	1210	1213	1217	rBV2	21651	20030	2.70%	0.343%
15	9.522	1260	1264	1266	rBV	53129	45491	6.14%	0.780%
16	9.692	1290	1293	1297	rVB3	12983	16318	2.20%	0.280%
17	9.751	1300	1303	1306	rVB	25545	19833	2.68%	0.340%
18	9.804	1308	1312	1316	rBV2	726219	614775	82.97%	10.536%
19	10.251	1385	1388	1390	rVB	22221	19214	2.59%	0.329%
20	10.469	1422	1425	1429	rVB4	12883	12805	1.73%	0.219%
21	10.586	1442	1445	1448	rVB4	12248	9470	1.28%	0.162%
22	10.722	1465	1468	1469	rBV	25978	21906	2.96%	0.375%
23	10.739	1469	1471	1475	rVB	18615	15898	2.15%	0.272%
24	11.169	1541	1544	1547	rBV2	19612	16993	2.29%	0.291%
25	11.198	1547	1549	1554	rVV3	11433	10874	1.47%	0.186%
26	11.245	1554	1557	1560	rVB3	7916	8791	1.19%	0.151%
27	11.286	1560	1564	1566	rBV	605908	508057	68.57%	8.707%
28	11.310	1566	1568	1571	rVB	45143	35221	4.75%	0.604%
29	11.357	1571	1576	1580	rBV3	13959	15323	2.07%	0.263%
30	11.592	1614	1616	1619	rBV2	17916	15459	2.09%	0.265%
31	11.816	1652	1654	1658	rVB3	15573	13359	1.80%	0.229%
32	11.898	1665	1668	1670	rBV3	16130	16990	2.29%	0.291%
33	11.998	1683	1685	1690	rVB3	15372	15213	2.05%	0.261%
34	12.163	1709	1713	1716	rBV5	6854	11113	1.50%	0.190%

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.339	1740	1743	1746	rBV5	9165	11506	1.55%	0.197%
36	12.386	1749	1751	1754	rVB	12944	13159	1.78%	0.226%
37	12.492	1766	1769	1772	rVB	66268	55375	7.47%	0.949%
38	12.721	1801	1808	1810	rBV	63156	73411	9.91%	1.258%
39	12.868	1829	1833	1836	rBV	248217	230094	31.05%	3.943%
40	13.116	1872	1875	1879	rBV6	20014	25904	3.50%	0.444%
41	13.157	1879	1882	1886	rBV5	16165	26013	3.51%	0.446%
42	13.315	1907	1909	1913	rBV5	15986	22769	3.07%	0.390%
43	13.351	1913	1915	1919	rVV4	23179	27218	3.67%	0.466%
44	13.457	1930	1933	1935	rBV4	19640	23577	3.18%	0.404%
45	13.915	2007	2011	2014	rBV	611183	551866	74.48%	9.458%
46	15.339	2250	2253	2257	rVB	301722	351257	47.41%	6.020%

Sum of corrected areas: 5835062

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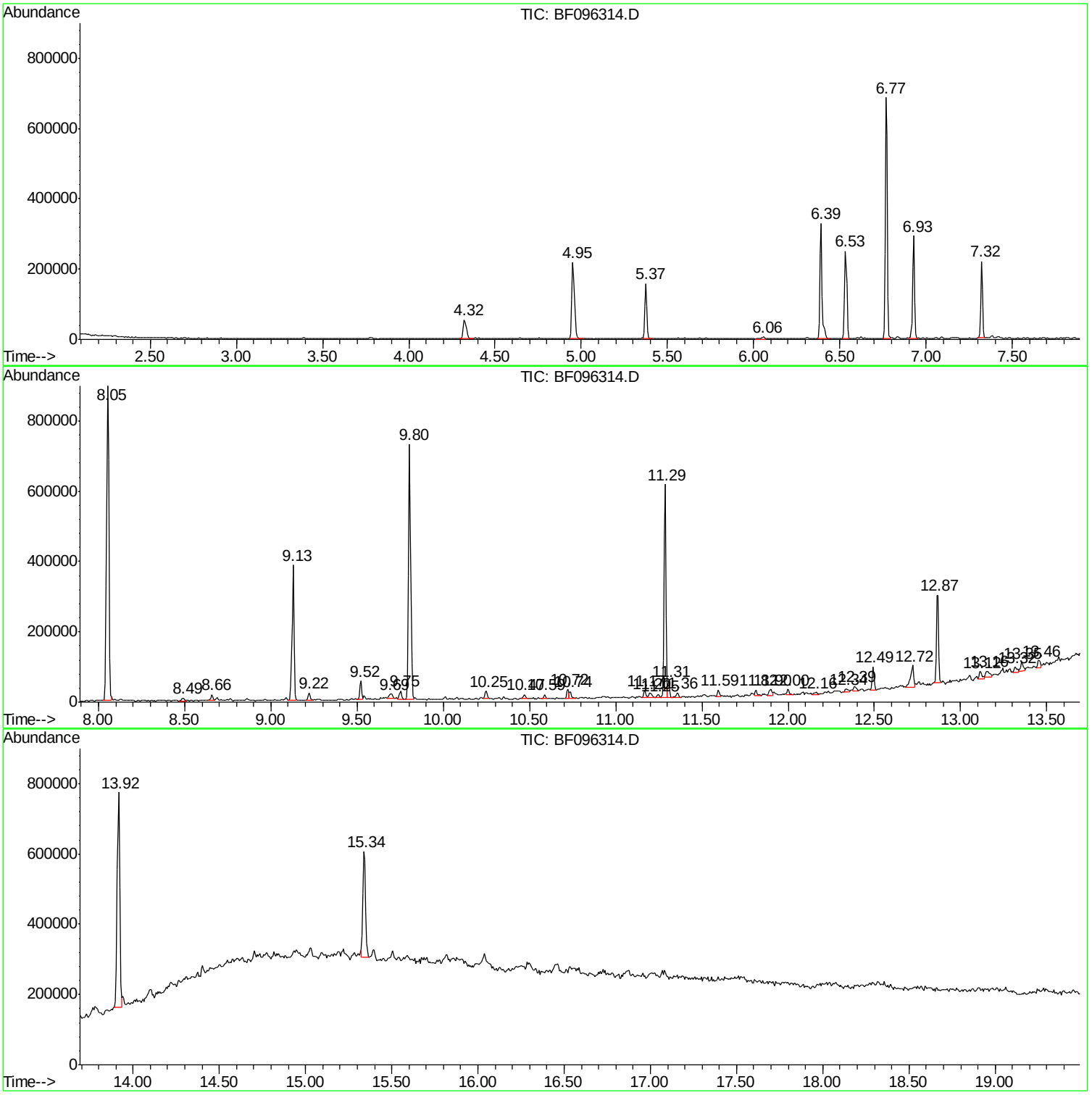
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF096314.D
Acq On : 30 Jun 2017 1:38
Operator : SJ/MA
Sample : I3882-13 5X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G54-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

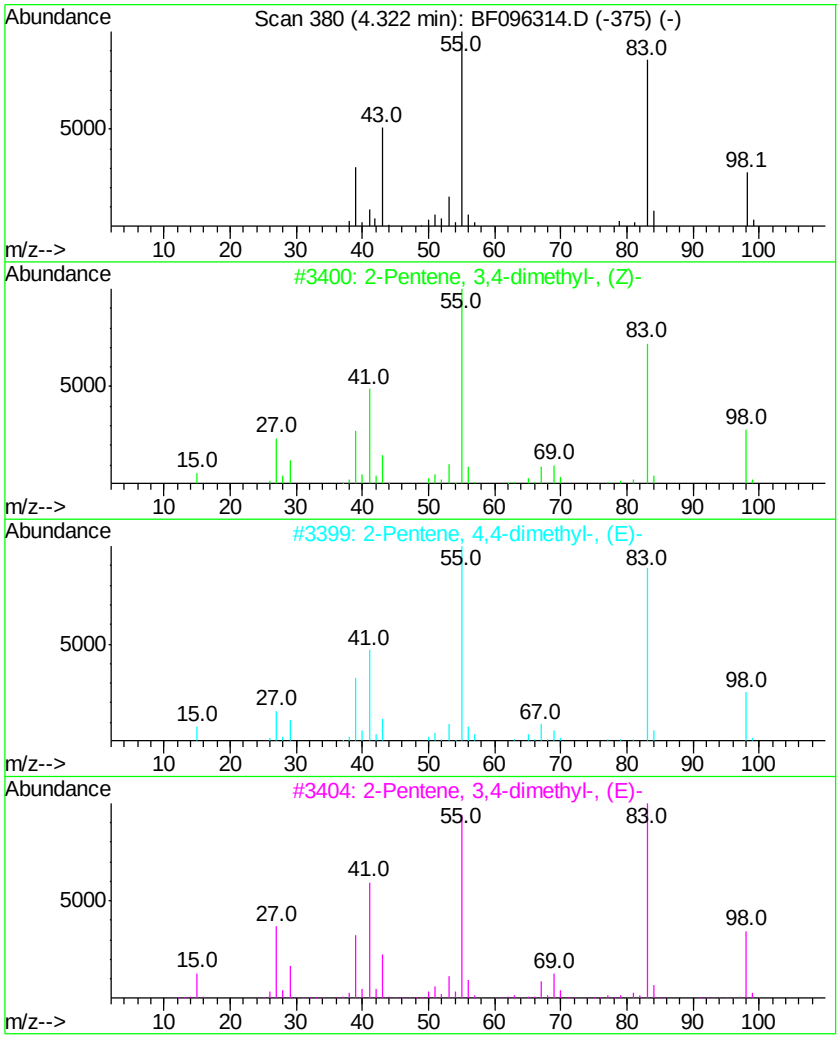
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

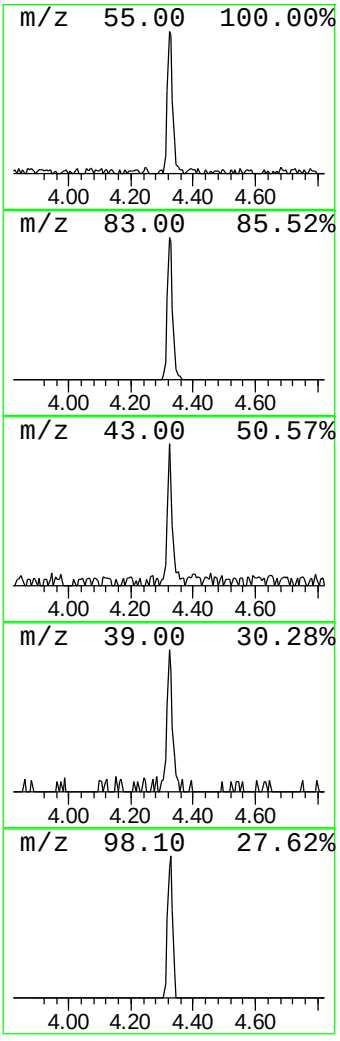
****

Peak Number 1 2-Pentene, 3,4-dimethyl-, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	2.32 ng	67740	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
2	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86





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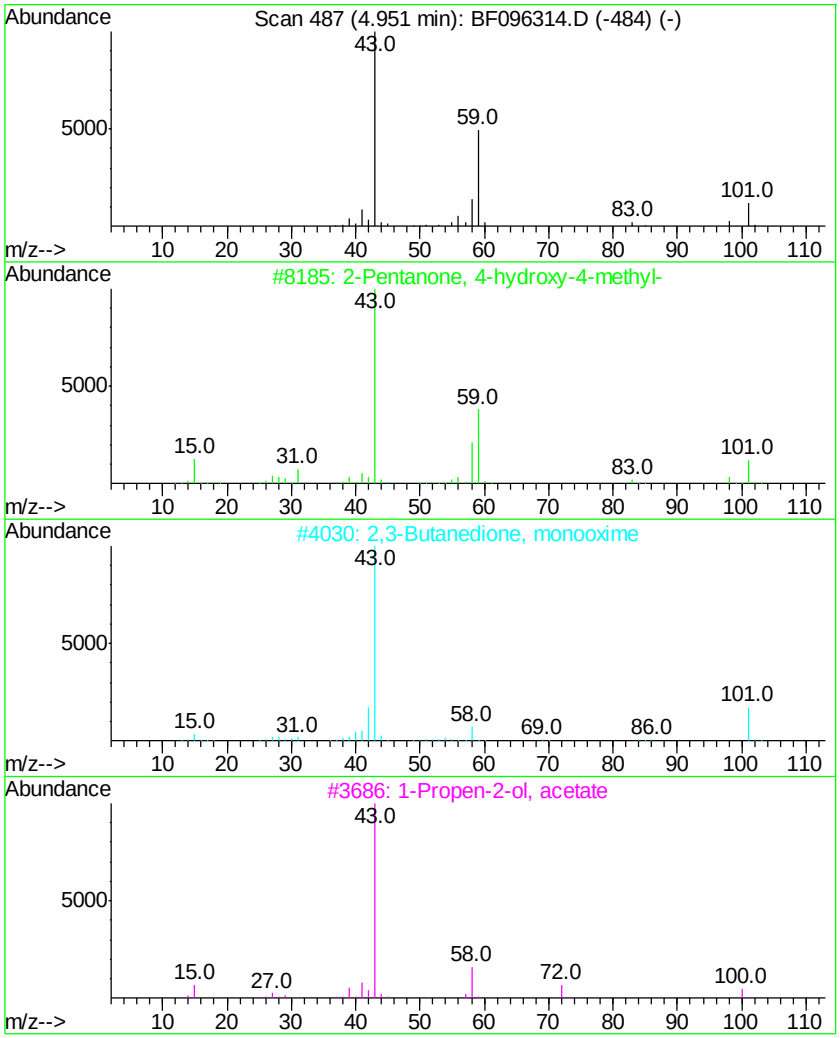
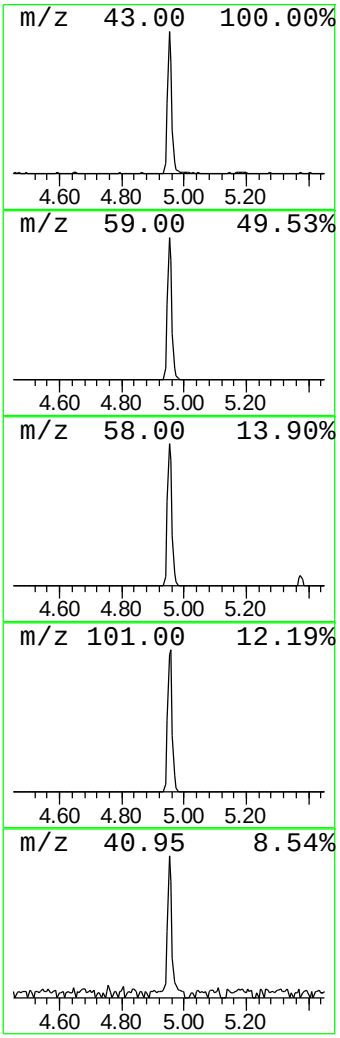
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	7.47 ng	218627	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9
5	Butanoic acid, 4-amino-3-hydroxy...	119	C4H9NO3	000924-49-2	9





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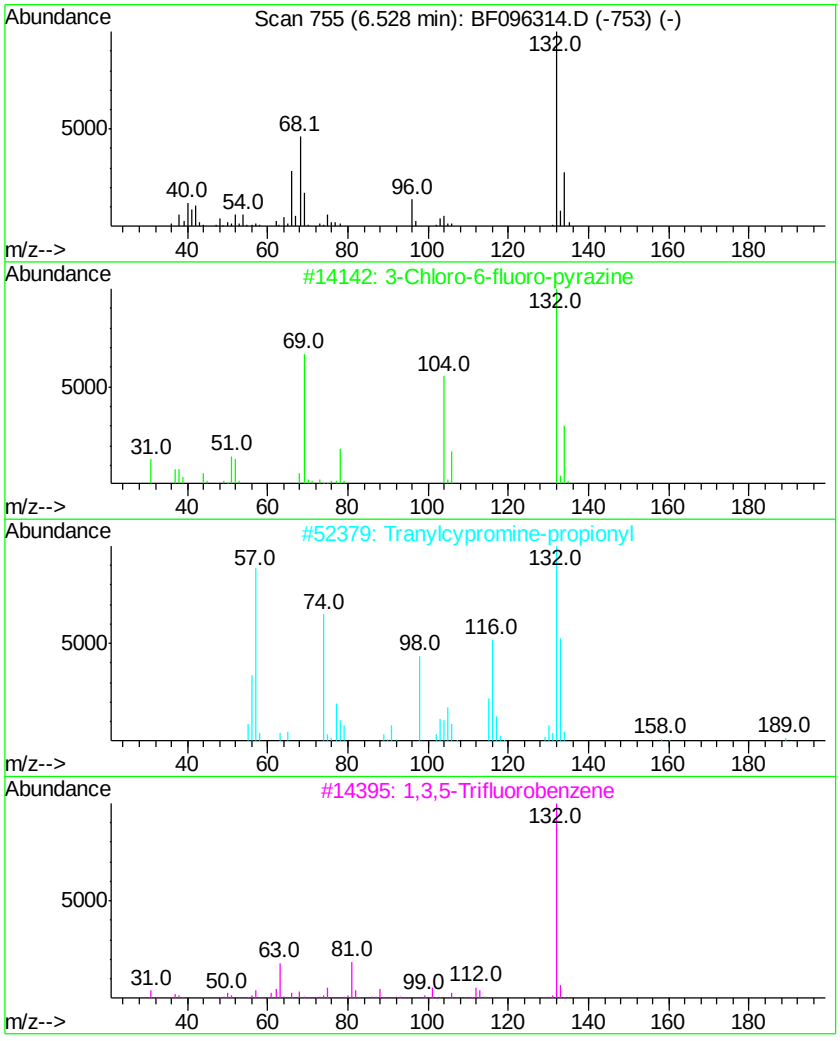
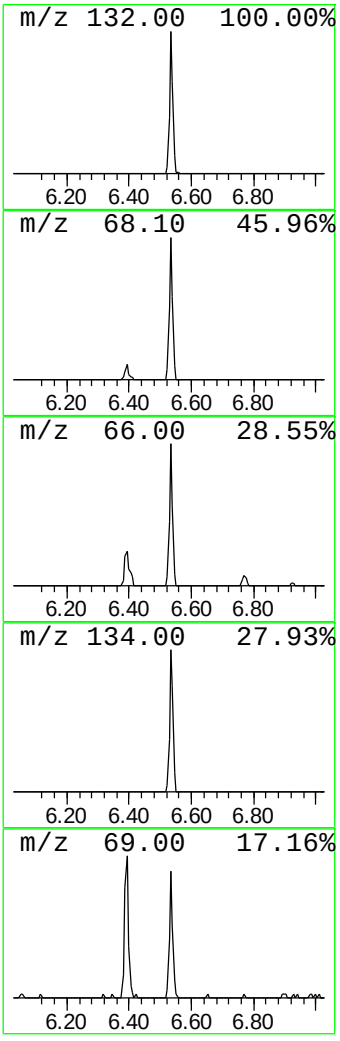
Peak Number 3 unknown6.53 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	6.71 ng	196464	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentene, 3,4-di...	4.32	2.3	ng	67740	1	6.77	585177	20.0
2-Pentanone, 4-hy...	4.95	7.5	ng	218627	1	6.77	585177	20.0
unknown6.53	6.53	6.7	ng	196464	1	6.77	585177	20.0