

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100617\
 Data File : BF099183.D
 Acq On : 7 Oct 2017 8:26
 Operator : SJ/JU
 Sample : I5675-03
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RI-MW-3-GW

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-BF092317.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	2.158	7	12	24	rVB	677795	854725	22.38%	3.110%
2	5.087	507	510	518	rVB	229974	275562	7.22%	1.003%
3	5.487	574	578	581	rBV	2084986	1843131	48.27%	6.706%
4	6.493	745	749	752	rBV	1470233	1199115	31.40%	4.363%
5	6.634	769	773	777	rBV	2912674	2938941	76.96%	10.692%
6	6.863	808	812	815	rBV	1095160	839810	21.99%	3.055%
7	7.022	834	839	842	rBV	2929230	2649020	69.37%	9.638%
8	7.175	863	865	874	rVB	43574	43117	1.13%	0.157%
9	7.428	903	908	911	rBV	1998096	2190891	57.37%	7.971%
10	8.145	1026	1030	1033	rBV	1338647	1161804	30.42%	4.227%
11	8.339	1060	1063	1066	rBV2	49784	40491	1.06%	0.147%
12	8.387	1068	1071	1074	rVB	87416	67076	1.76%	0.244%
13	9.139	1196	1199	1203	rBV	45014	40815	1.07%	0.148%
14	9.222	1207	1213	1216	rBV	3960370	3818675	100.00%	13.893%
15	9.392	1239	1242	1247	rVB4	39543	41617	1.09%	0.151%
16	9.610	1276	1279	1282	rVB	65322	50612	1.33%	0.184%
17	9.669	1282	1289	1295	rVB5	37080	64548	1.69%	0.235%
18	9.757	1298	1304	1311	rBV	56429	67868	1.78%	0.247%
19	9.898	1324	1328	1332	rBV2	1432397	1228425	32.17%	4.469%
20	9.928	1332	1333	1337	rVB	71581	46405	1.22%	0.169%
21	10.051	1349	1354	1357	rBV4	20726	40778	1.07%	0.148%
22	10.104	1359	1363	1367	rVV	130152	130138	3.41%	0.473%
23	10.216	1378	1382	1385	rBV3	73588	74364	1.95%	0.271%
24	10.257	1387	1389	1392	rVV	49775	40374	1.06%	0.147%
25	10.322	1397	1400	1403	rVB2	65675	57056	1.49%	0.208%
26	10.510	1429	1432	1434	rBV	47489	46158	1.21%	0.168%
27	10.598	1442	1447	1453	rVB4	22962	48176	1.26%	0.175%
28	10.692	1453	1463	1466	rBV	1888008	1950101	51.07%	7.095%
29	10.792	1477	1480	1481	rBV2	43159	38311	1.00%	0.139%
30	10.980	1507	1512	1516	rBV3	23828	44077	1.15%	0.160%
31	11.386	1577	1581	1584	rBV	1263613	1044168	27.34%	3.799%
32	11.498	1597	1600	1605	rVB2	38036	43859	1.15%	0.160%
33	11.616	1618	1620	1623	rVB	96646	75920	1.99%	0.276%
34	12.969	1846	1850	1854	rBV	2640043	2637074	69.06%	9.594%

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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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.127	1874	1877	1883	rBV	53200	54025	1.41%	0.197%
36	13.851	1997	2000	2005	rBV	33013	41528	1.09%	0.151%
37	14.021	2025	2029	2033	rBV	733138	661645	17.33%	2.407%
38	15.498	2275	2280	2289	rVB	602722	743735	19.48%	2.706%
39	15.933	2348	2354	2361	rBV2	38057	61327	1.61%	0.223%
40	16.433	2435	2439	2447	rVB	41663	71551	1.87%	0.260%
41	17.027	2535	2540	2547	rVB3	28892	58370	1.53%	0.212%
42	17.733	2654	2660	2669	rVB7	24625	60914	1.60%	0.222%

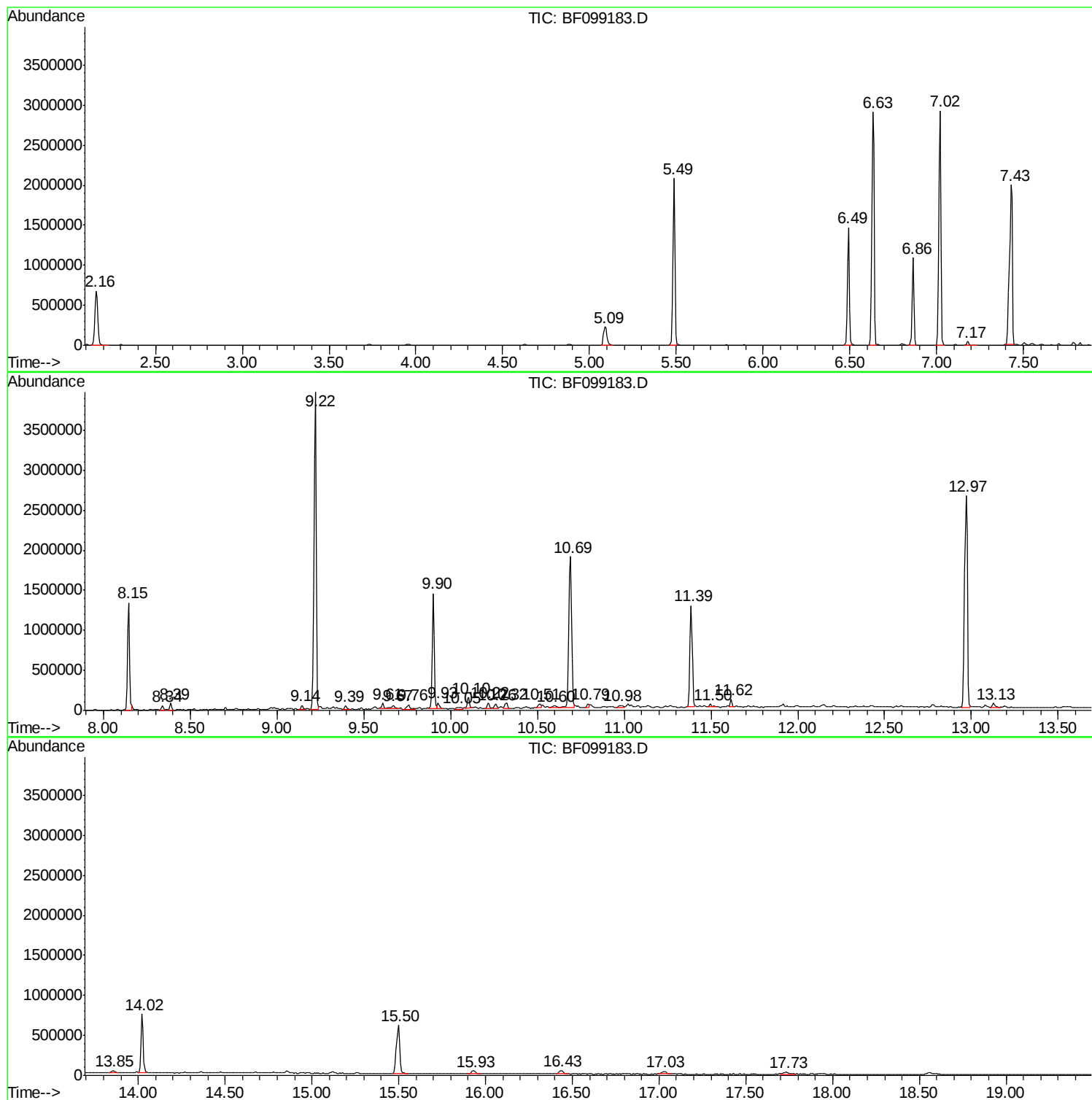
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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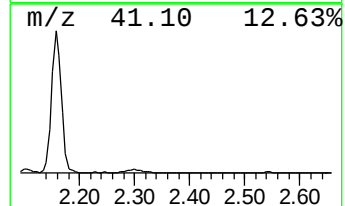
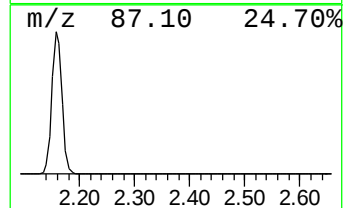
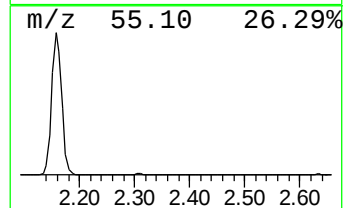
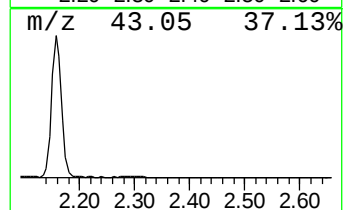
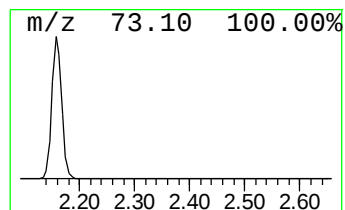
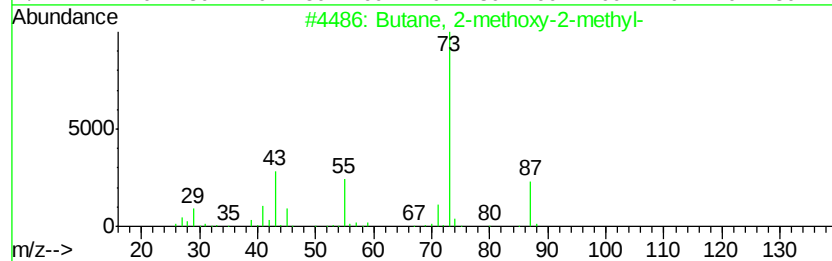
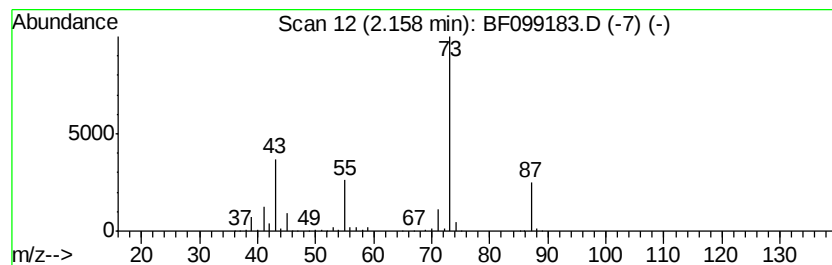
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	20.36 ng	854725	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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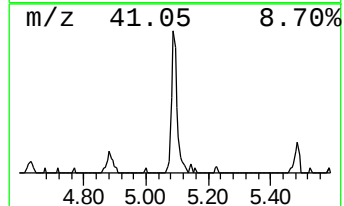
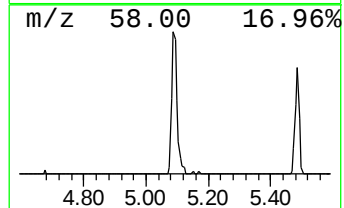
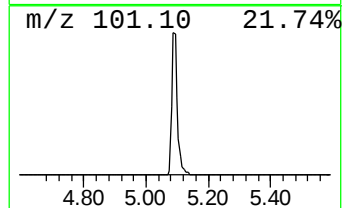
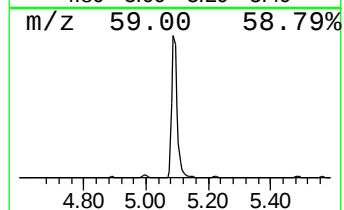
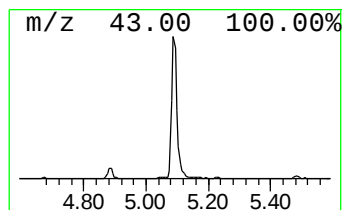
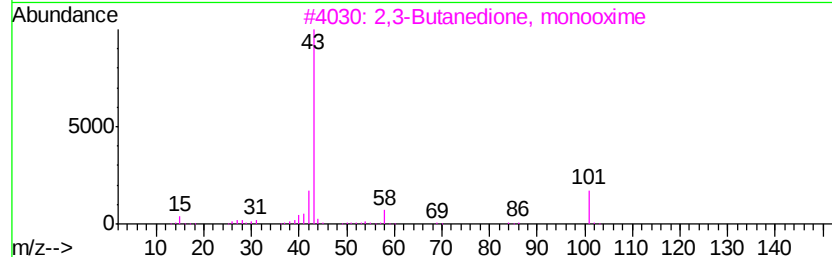
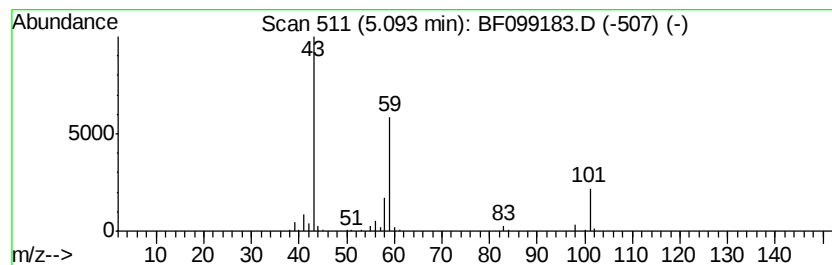
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	6.56 ng	275562	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			1,2-Butanediol	90	C4H10O2	000584-03-2	9



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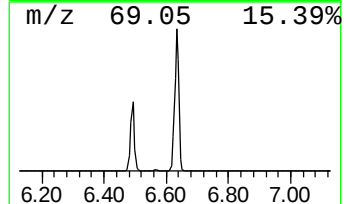
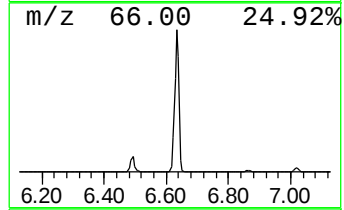
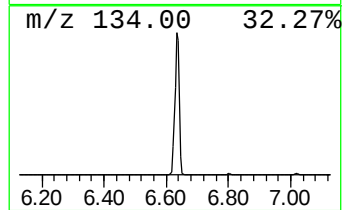
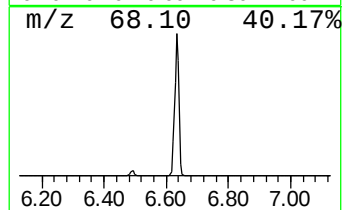
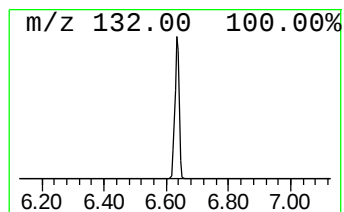
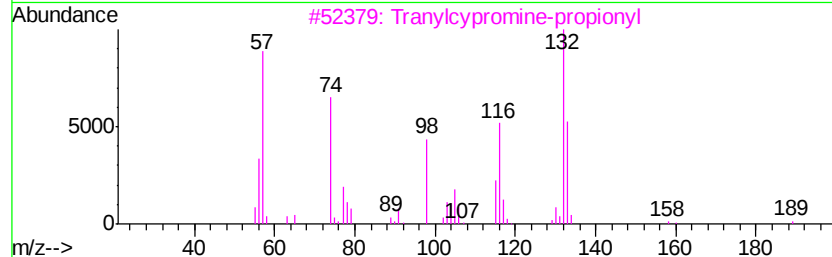
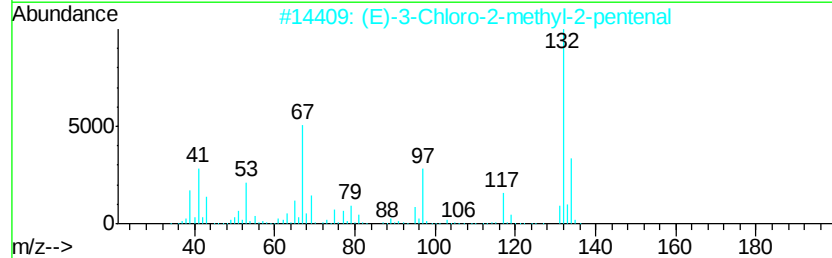
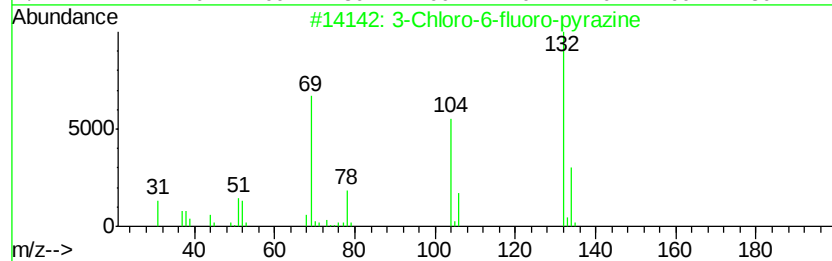
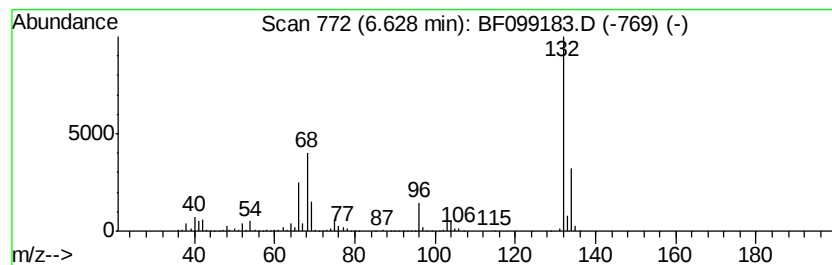
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	69.99 ng	2938940	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.16	20.4	ng	854725	1	6.86	839810	20.0
2-Pentanone, 4-hy...	5.09	6.6	ng	275562	1	6.86	839810	20.0
unknown6.63	6.63	70.0	ng	2938940	1	6.86	839810	20.0