

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101416\
 Data File : BF090596.D
 Acq On : 15 Oct 2016 9:23
 Operator : UM/SJ
 Sample : H5227-01 2X
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1

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-BF101316.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	5.103	239	242	253	rBV	455128	664746	23.90%	1.759%
2	5.514	276	278	281	rBV	1725358	2538901	91.28%	6.719%
3	6.543	366	368	378	rBV	1789816	2781426	100.00%	7.361%
4	6.680	378	380	383	rBV	2498736	2767071	99.48%	7.323%
5	6.920	399	401	412	rBV	1235476	1506293	54.16%	3.987%
6	7.069	412	414	417	rBV	1758592	1904480	68.47%	5.040%
7	7.183	423	424	434	rVB2	18745	53310	1.92%	0.141%
8	7.480	447	450	457	rBV	1444828	1680831	60.43%	4.448%
9	8.200	511	513	522	rBV	1621658	2090879	75.17%	5.534%
10	8.920	572	576	578	rBV	39305	41187	1.48%	0.109%
11	9.012	583	584	587	rBV	30489	38797	1.39%	0.103%
12	9.286	605	608	610	rBV	1519908	2094159	75.29%	5.542%
13	9.400	616	618	620	rVB2	33749	38420	1.38%	0.102%
14	9.618	635	637	640	rBV2	41261	59144	2.13%	0.157%
15	9.675	640	642	644	rVV	705194	613260	22.05%	1.623%
16	9.732	646	647	653	rVB3	21509	42218	1.52%	0.112%
17	9.823	653	655	657	rBV	72382	78441	2.82%	0.208%
18	9.892	660	661	663	rVB	57449	42794	1.54%	0.113%
19	9.961	665	667	669	rVV	2489963	2115976	76.08%	5.600%
20	9.995	669	670	675	rVB	182602	166614	5.99%	0.441%
21	10.166	683	685	687	rBV	58978	70782	2.54%	0.187%
22	10.201	687	688	691	rVB3	19664	31506	1.13%	0.083%
23	10.372	701	703	704	rBV	29390	48889	1.76%	0.129%
24	10.395	704	705	706	rVB	79774	54916	1.97%	0.145%
25	10.509	713	715	718	rBV	103269	111007	3.99%	0.294%
26	10.612	722	724	727	rVV	34828	60397	2.17%	0.160%
27	10.749	733	736	743	rBV	1262302	1345789	48.38%	3.562%
28	10.864	745	746	751	rVB2	98336	152577	5.49%	0.404%
29	11.058	760	763	764	rBV2	33627	37505	1.35%	0.099%
30	11.309	782	785	787	rBV2	41247	67342	2.42%	0.178%
31	11.344	787	788	791	rVB	53095	55402	1.99%	0.147%
32	11.446	795	797	802	rBV2	1507063	2246856	80.78%	5.946%
33	11.526	802	804	806	rVB	127123	143779	5.17%	0.381%
34	11.675	814	817	821	rBV3	65816	127615	4.59%	0.338%

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35	11.744	821	823	825	rVB	48158	47863	1.72%	0.127%
36	11.949	839	841	842	rBV	69913	68241	2.45%	0.181%
37	11.984	842	844	846	rVV	60659	96506	3.47%	0.255%
38	12.029	846	848	849	rVV2	34605	45349	1.63%	0.120%
39	12.064	849	851	855	rVB2	135219	210308	7.56%	0.557%
40	12.144	856	858	860	rBV2	18822	32691	1.18%	0.087%
41	12.246	865	867	868	rBV	38939	42637	1.53%	0.113%
42	12.395	877	880	881	rBV2	27450	39804	1.43%	0.105%
43	12.429	881	883	886	rVB3	29733	47523	1.71%	0.126%
44	12.498	887	889	891	rBV	68455	88831	3.19%	0.235%
45	12.532	891	892	895	rVV	45461	67869	2.44%	0.180%
46	12.589	895	897	901	rVV3	34293	67075	2.41%	0.178%
47	12.658	901	903	906	rBV	730525	762141	27.40%	2.017%
48	12.887	920	923	927	rBV	677558	886794	31.88%	2.347%
49	13.035	933	936	940	rBV	1442128	1517332	54.55%	4.016%
50	13.104	940	942	946	rVV3	60369	115819	4.16%	0.307%
51	13.218	948	952	954	rVV	124805	194041	6.98%	0.514%
52	13.287	956	958	959	rVV	84789	87333	3.14%	0.231%
53	13.321	959	961	965	rVV2	98754	145102	5.22%	0.384%
54	13.412	967	969	970	rVV	63119	64505	2.32%	0.171%
55	13.447	970	972	974	rVV	55405	79445	2.86%	0.210%
56	13.481	974	975	977	rVB	42025	39577	1.42%	0.105%
57	13.938	1013	1015	1020	rVB2	118054	196658	7.07%	0.520%
58	14.087	1025	1028	1035	rBV	1248945	2515602	90.44%	6.658%
59	15.127	1117	1119	1124	rBV	424057	1022092	36.75%	2.705%
60	15.424	1143	1145	1149	rVB	197363	356063	12.80%	0.942%
61	15.493	1149	1151	1154	rVV	347154	571489	20.55%	1.512%
62	15.561	1154	1157	1167	rVB	832822	1762236	63.36%	4.664%
63	16.258	1216	1218	1223	rVB2	115444	228241	8.21%	0.604%
64	17.001	1281	1283	1290	rVB2	111177	288641	10.38%	0.764%
65	17.436	1319	1321	1330	rVB	88230	223617	8.04%	0.592%

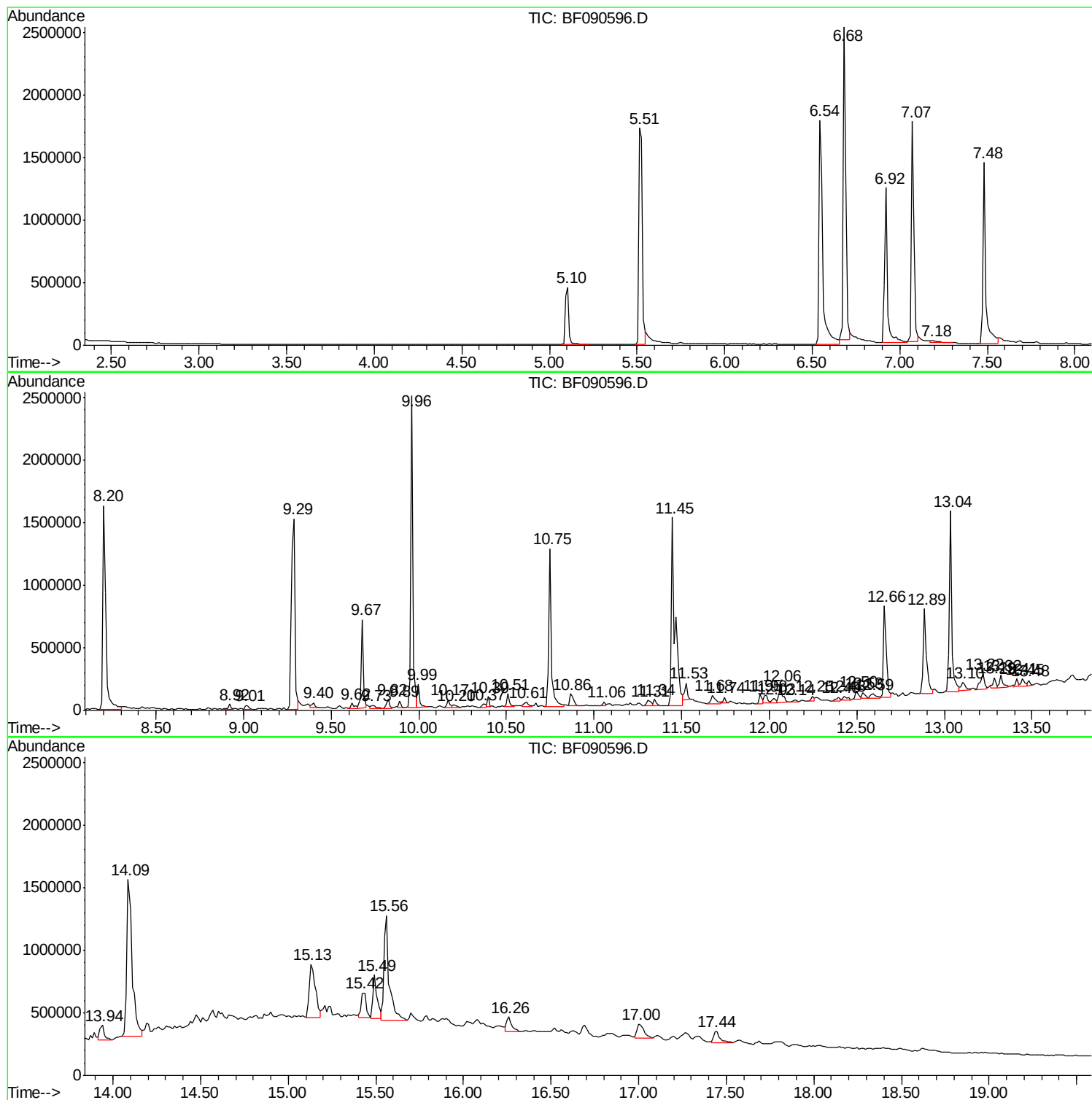
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ClientSampled :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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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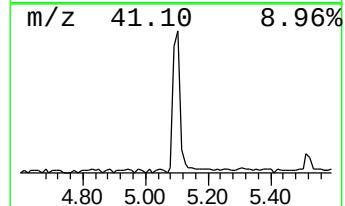
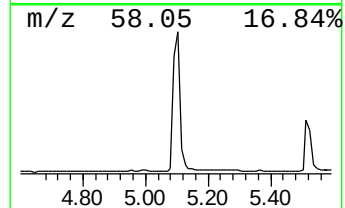
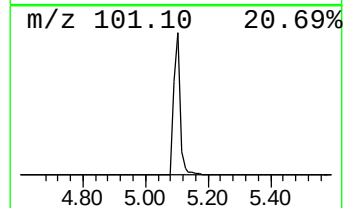
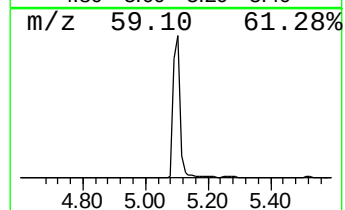
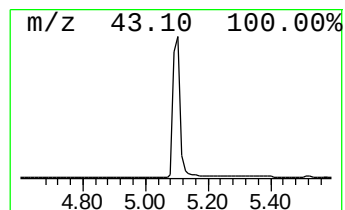
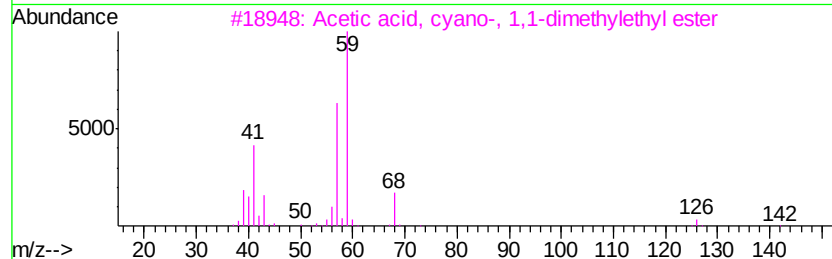
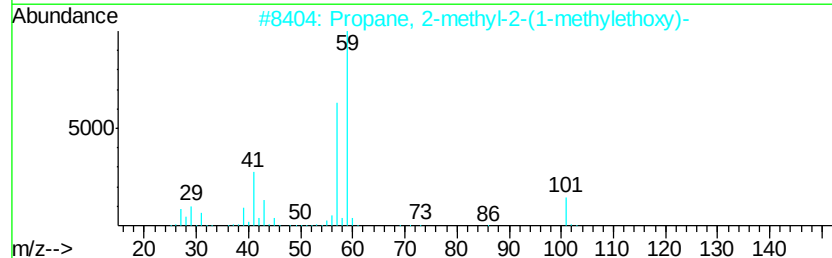
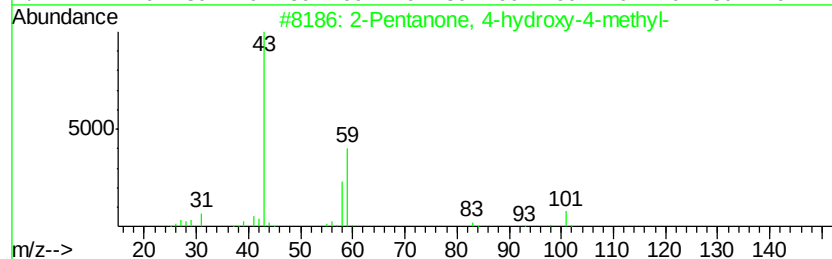
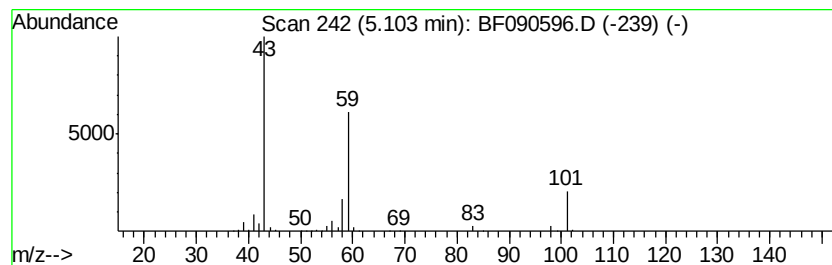
Instrument :
BNA_F
ClientSampleId :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.10	8.83 ng	664746	1,4-Dichlorobenzene-d4	6.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethv...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9



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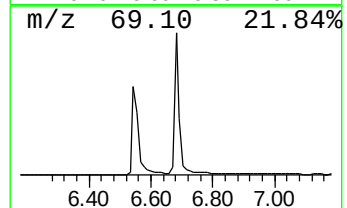
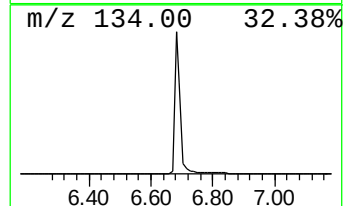
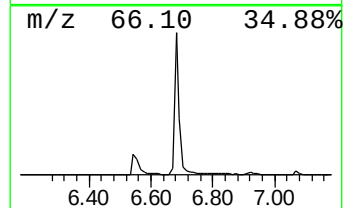
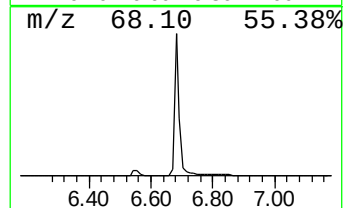
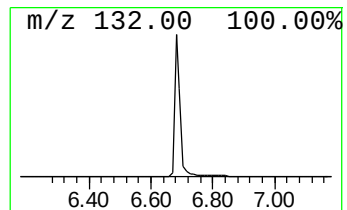
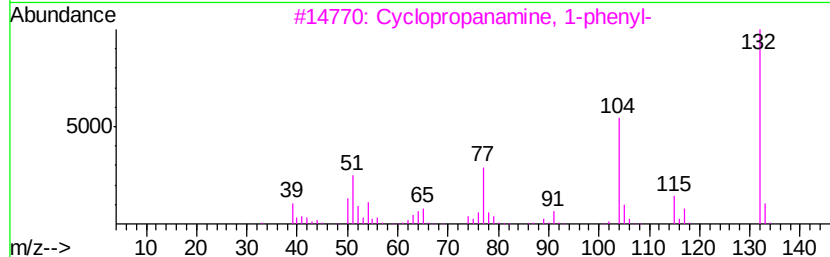
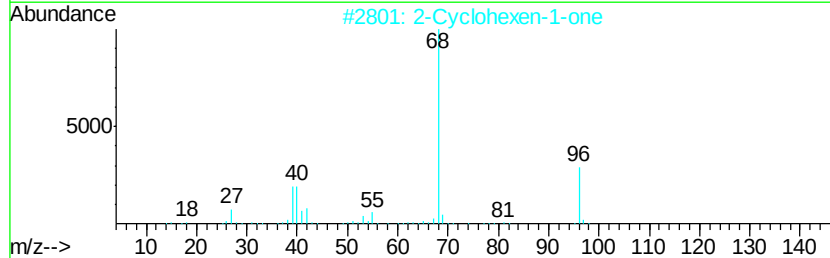
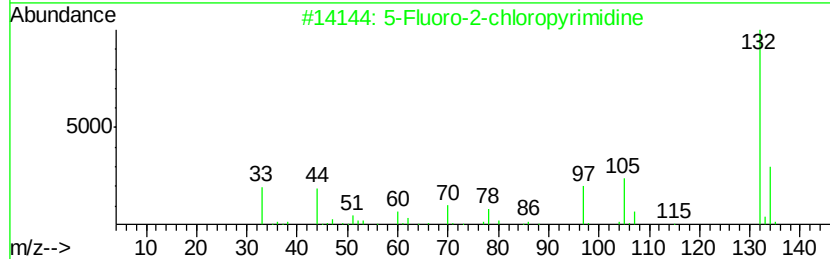
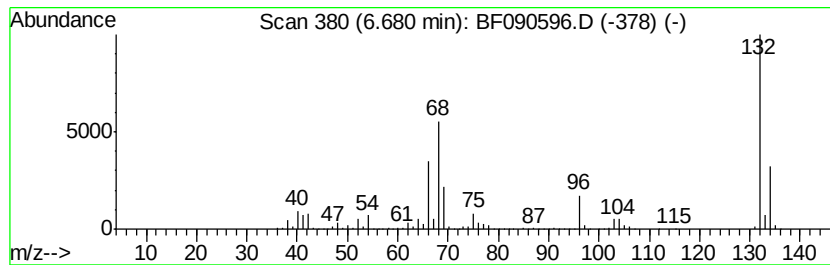
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	36.74 ng	2767070	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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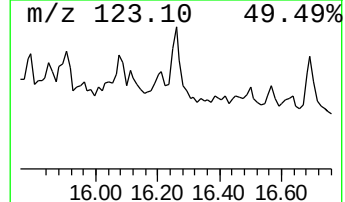
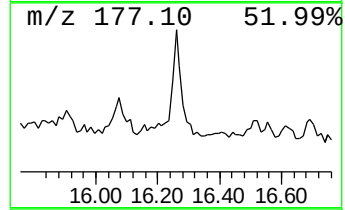
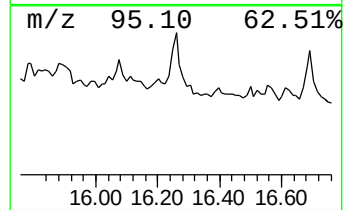
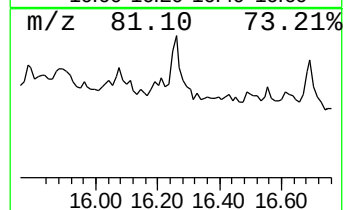
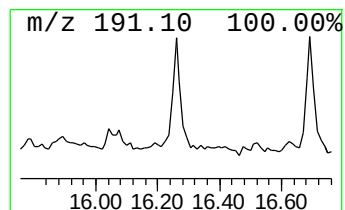
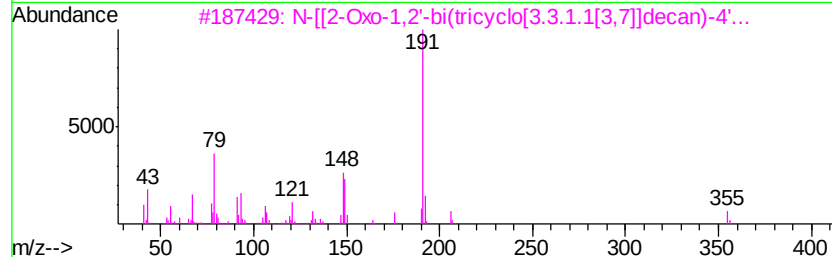
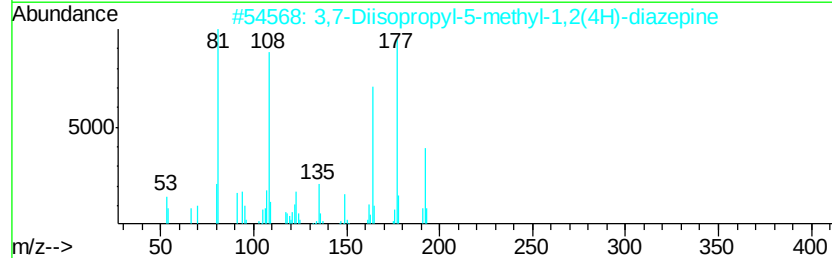
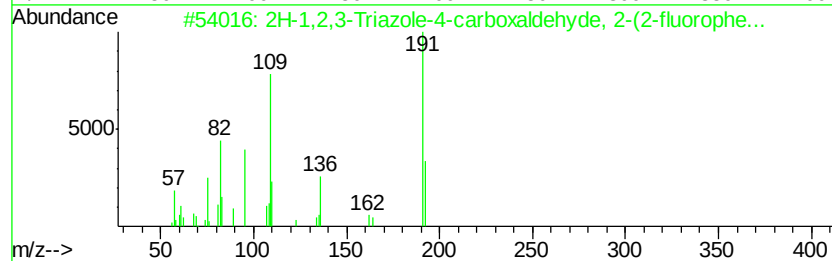
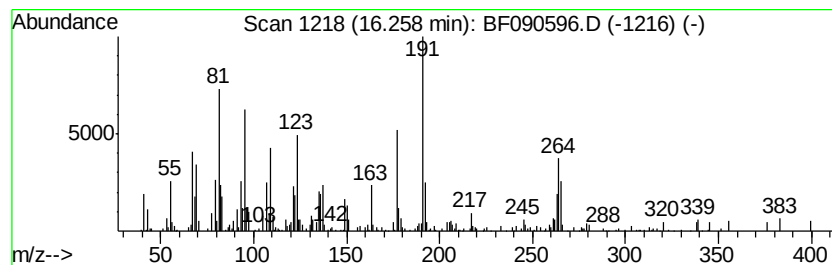
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Peak Number 5 unknown16.26 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.26	2.59 ng	228241	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	38
2		3,7-Diisopropyl-5-methyl-1,2(4H)...	192	C12H20N2	088829-71-4	30
3		N-[[2-Oxo-1,2'-bi(tricyclo[3.3.1...	355	C23H33N02	1000305-39-6	25
4		5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	15
5		1H-Pyrazole-4-acetic acid, 1-(4-...	264	C11H16N6O2	1000337-51-2	14



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	8.8	ng	664746	1	6.92	1506290	20.0
unknown6.68	6.68	36.7	ng	2767070	1	6.92	1506290	20.0
unknown16.26	16.26	2.6	ng	228241	6	15.56	1762240	20.0