

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
 Data File : BF091607.D
 Acq On : 15 Dec 2016 1:48
 Operator : UM/SJ
 Sample : H6007-02 5X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-5-0-5

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-BF120916.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	3.664	135	138	144	rVB	36759	63471	2.55%	0.248%
2	4.270	189	191	195	rBV	467100	595281	23.89%	2.328%
3	4.944	248	250	253	rBV	1543912	2049411	82.24%	8.015%
4	5.390	287	289	291	rVB	72136	79365	3.18%	0.310%
5	6.430	377	380	383	rBV	931607	909787	36.51%	3.558%
6	6.556	389	391	394	rVB	237698	225966	9.07%	0.884%
7	6.796	409	412	414	rBV	1884282	1852938	74.36%	7.247%
8	6.865	415	418	420	rVV	37512	34937	1.40%	0.137%
9	6.945	423	425	428	rBV	1119912	1087876	43.66%	4.255%
10	7.356	458	461	463	rBV	932220	861444	34.57%	3.369%
11	8.076	522	524	527	rBV	2332381	2348443	94.24%	9.184%
12	9.162	616	619	621	rBV	1156065	1502030	60.27%	5.874%
13	9.242	624	626	630	rVV	17698	29829	1.20%	0.117%
14	9.413	639	641	645	rBV3	12953	28470	1.14%	0.111%
15	9.550	651	653	657	rBV	157052	153594	6.16%	0.601%
16	9.699	663	666	669	rBV	19154	43445	1.74%	0.170%
17	9.779	671	673	675	rVB	20020	24979	1.00%	0.098%
18	9.836	675	678	680	rBV	2582877	2491972	100.00%	9.746%
19	10.031	693	695	697	rVB3	23310	29606	1.19%	0.116%
20	10.156	703	706	709	rBV5	18170	46888	1.88%	0.183%
21	10.248	712	714	715	rBV	36913	56910	2.28%	0.223%
22	10.271	715	716	718	rVB	58881	46245	1.86%	0.181%
23	10.373	724	725	729	rVB3	22821	30904	1.24%	0.121%
24	10.488	733	735	738	rVB	26585	42678	1.71%	0.167%
25	10.751	756	758	762	rVB	81092	143079	5.74%	0.560%
26	10.819	762	764	767	rBV3	13915	25778	1.03%	0.101%
27	10.956	772	776	781	rVB7	17904	50754	2.04%	0.198%
28	11.196	792	797	798	rBV	70533	101086	4.06%	0.395%
29	11.219	798	799	802	rVB	41280	52320	2.10%	0.205%
30	11.311	805	807	811	rVV	1860635	2086664	83.74%	8.161%
31	11.391	811	814	815	rVB2	51544	73824	2.96%	0.289%
32	11.551	825	828	829	rBV2	20316	34678	1.39%	0.136%
33	11.619	832	834	835	rVV	60563	51092	2.05%	0.200%
34	11.814	849	851	852	rBV	34024	33747	1.35%	0.132%

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35	11.848	852	854	855 rVB	35631	45809	1.84%	0.179%
36	11.882	855	857	859 rVB	497106	426746	17.12%	1.669%
37	11.928	859	861	866 rVB2	61924	108922	4.37%	0.426%
38	12.031	866	870	873 rBV2	30999	92379	3.71%	0.361%
39	12.111	875	877	878 rBV	37905	35961	1.44%	0.141%
40	12.259	887	890	891 rBV2	26566	47649	1.91%	0.186%
41	12.294	891	893	896 rVV2	28804	59004	2.37%	0.231%
42	12.362	897	899	901 rVV	65227	81986	3.29%	0.321%
43	12.454	905	907	909 rBV3	23541	43191	1.73%	0.169%
44	12.522	911	913	915 rVV	473675	405969	16.29%	1.588%
45	12.568	915	917	920 rVV3	23474	43024	1.73%	0.168%
46	12.625	920	922	923 rBV2	26230	34242	1.37%	0.134%
47	12.751	930	933	935 rBV	434990	479596	19.25%	1.876%
48	12.865	942	943	944 rBV	36201	39454	1.58%	0.154%
49	12.899	944	946	948 rVV	1232731	1092892	43.86%	4.274%
50	12.968	950	952	954 rBV2	39927	78085	3.13%	0.305%
51	13.082	960	962	963 rVB	63868	66562	2.67%	0.260%
52	13.185	969	971	974 rBV2	74234	137725	5.53%	0.539%
53	13.277	977	979	980 rVB	50556	50287	2.02%	0.197%
54	13.345	983	985	986 rBV2	60750	51922	2.08%	0.203%
55	13.391	986	989	991 rBV	664332	807288	32.40%	3.157%
56	13.585	1004	1006	1008 rBV	62137	85891	3.45%	0.336%
57	13.688	1013	1015	1019 rBV4	63973	186969	7.50%	0.731%
58	13.951	1035	1038	1039 rBV	1661699	1973816	79.21%	7.719%
59	14.957	1124	1126	1131 rVB	180276	379535	15.23%	1.484%
60	15.368	1159	1162	1164 rBV	778378	1173344	47.08%	4.589%
61	15.505	1172	1174	1178 rVB2	166989	252059	10.11%	0.986%

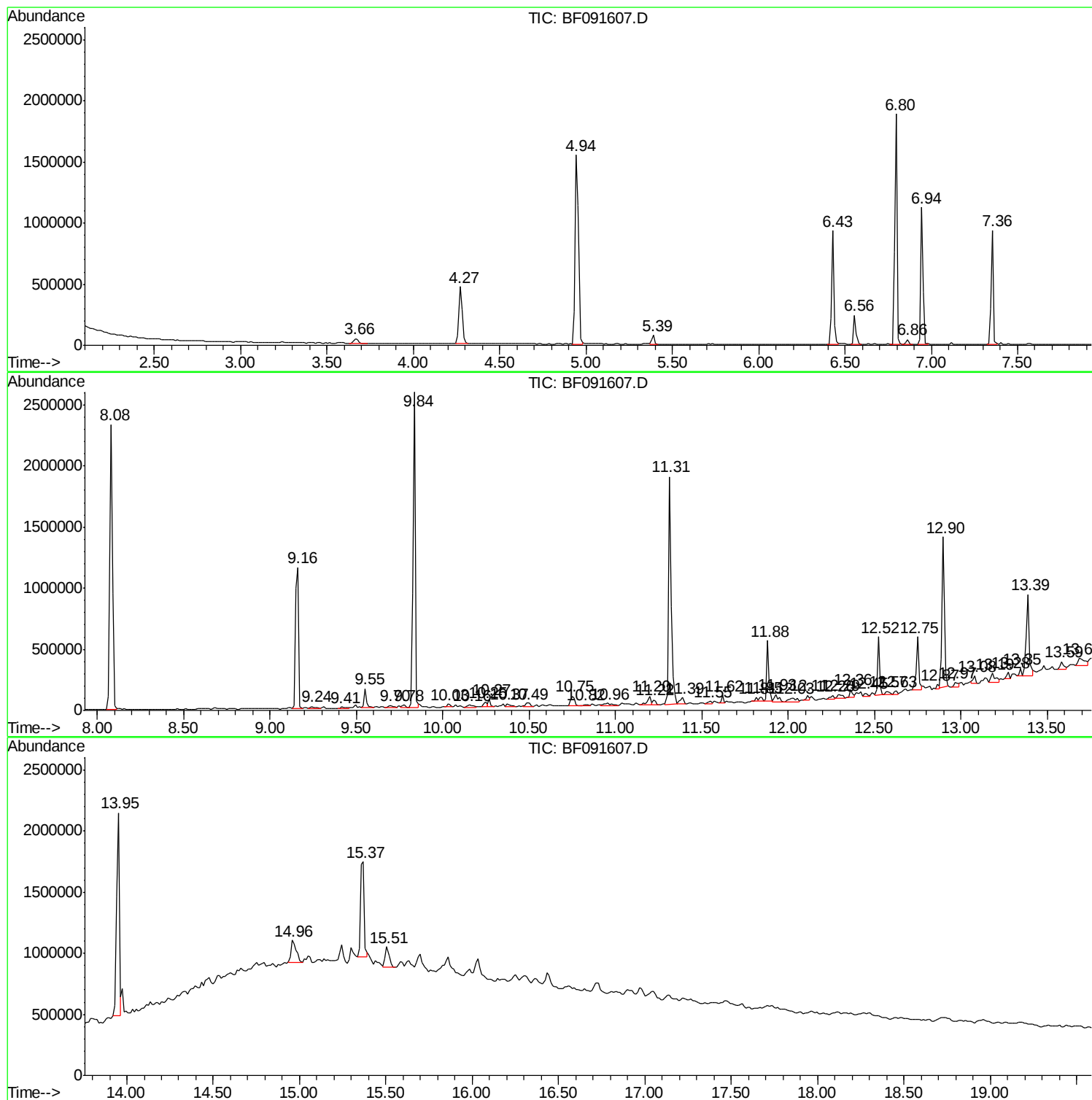
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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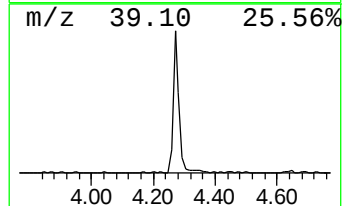
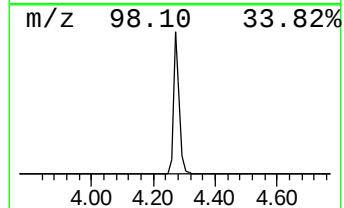
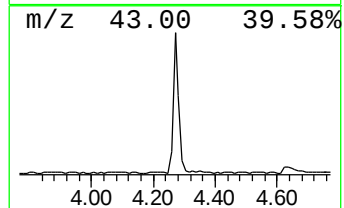
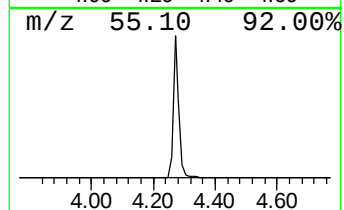
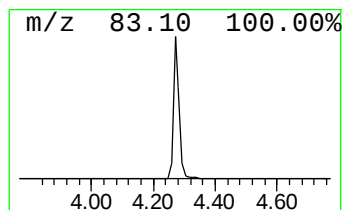
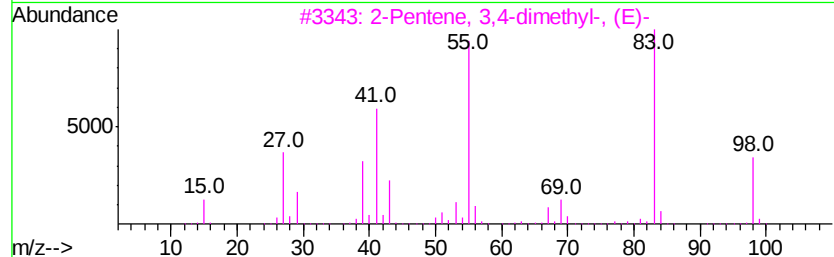
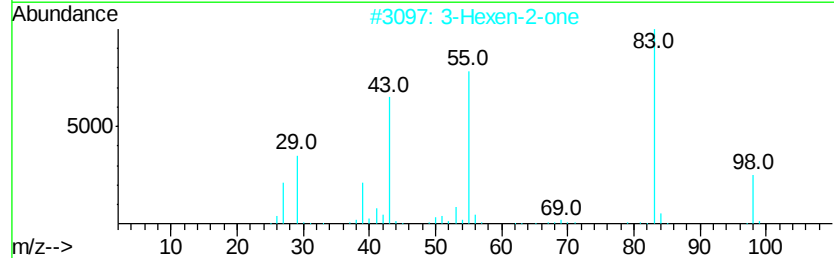
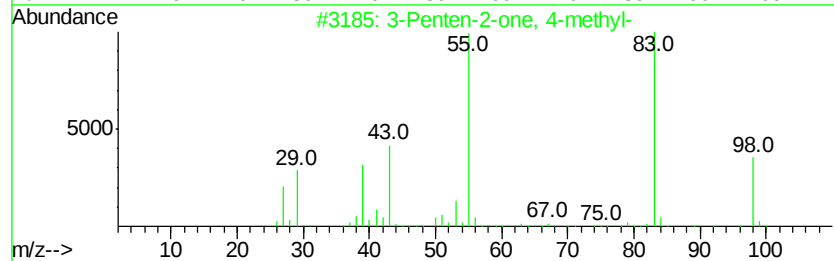
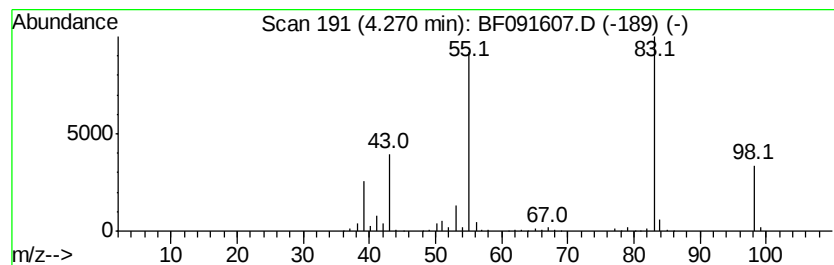
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	6.43 ng	595281	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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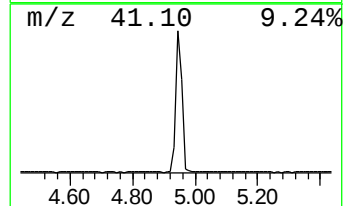
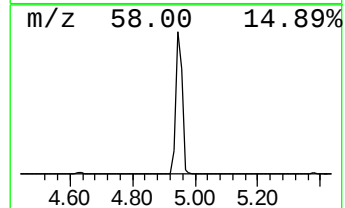
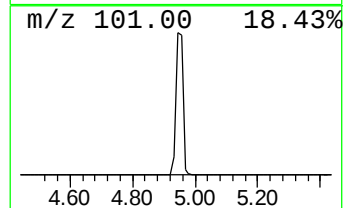
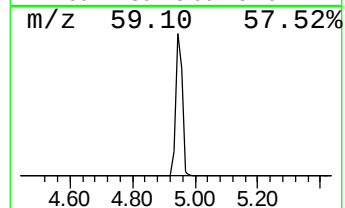
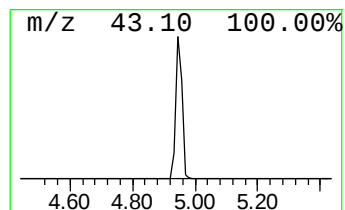
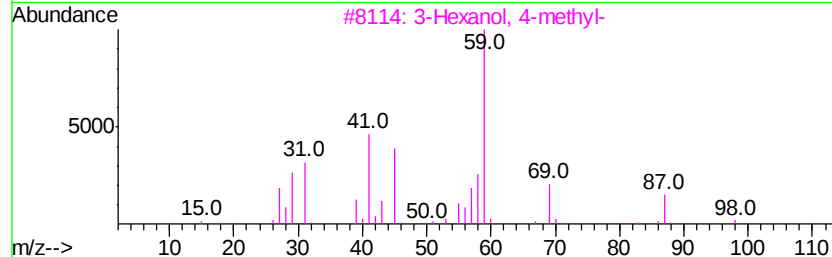
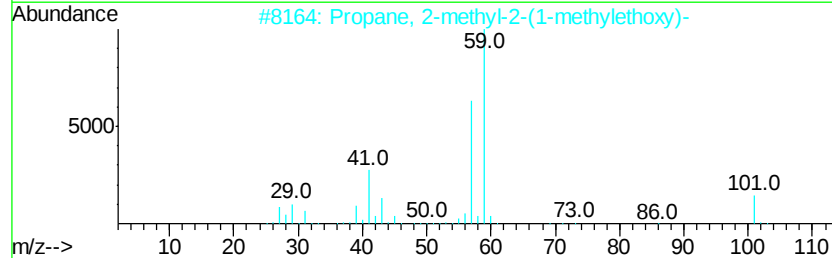
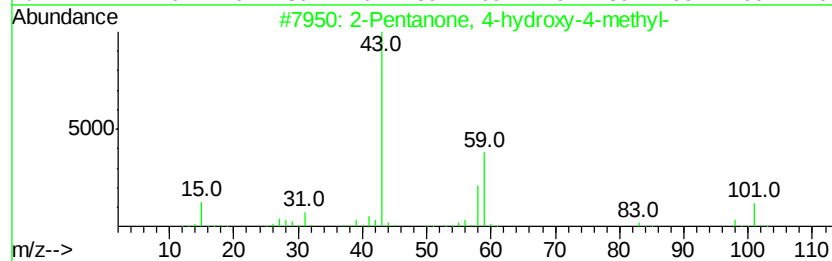
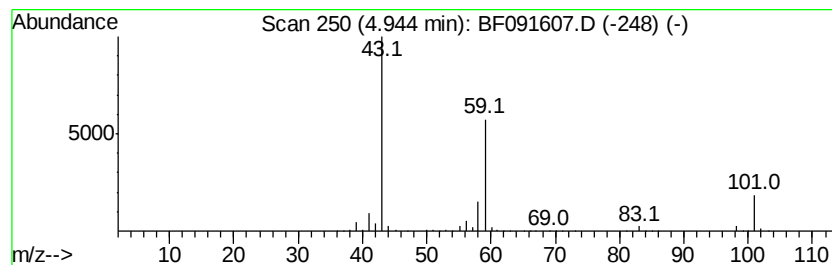
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	22.12 ng	2049410	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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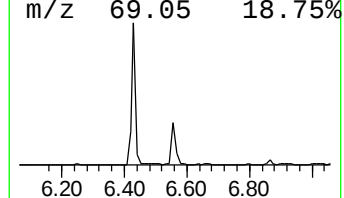
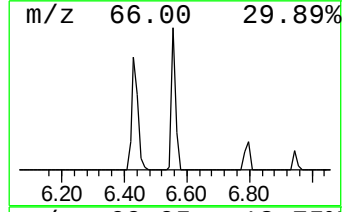
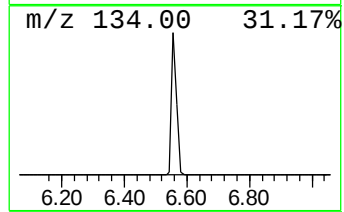
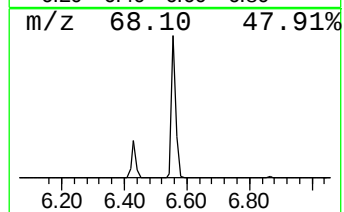
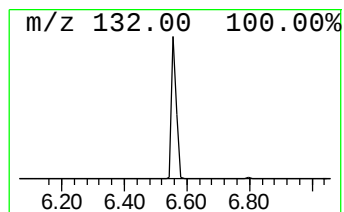
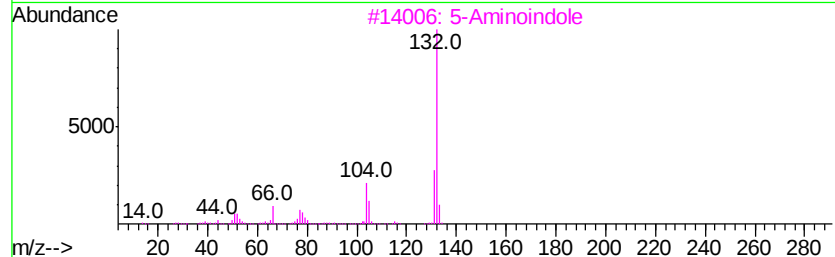
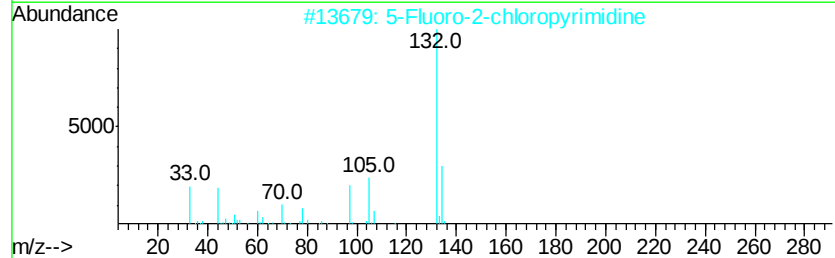
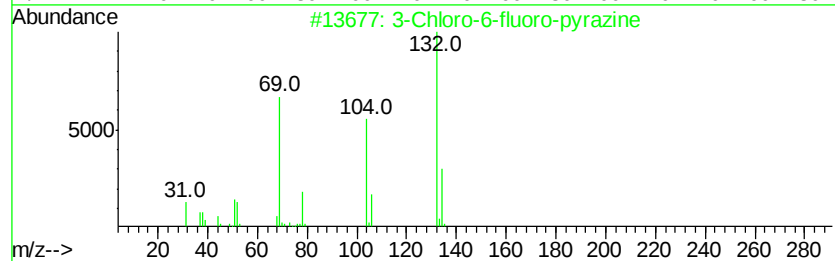
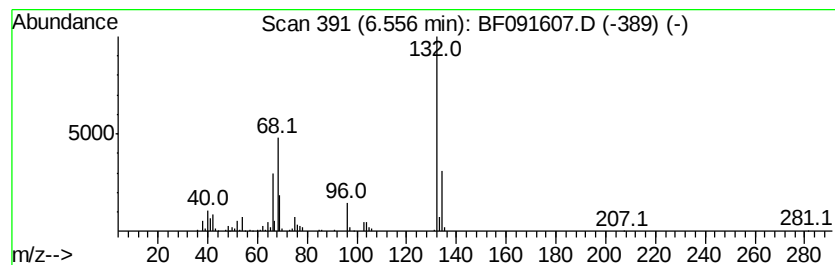
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.56 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	2.44 ng	225966	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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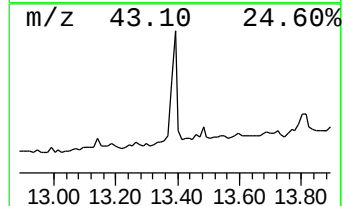
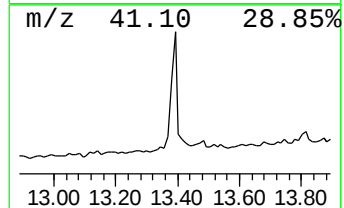
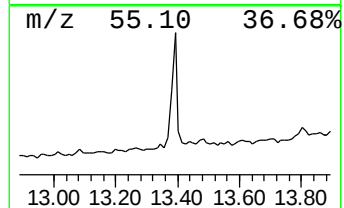
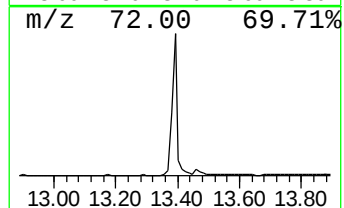
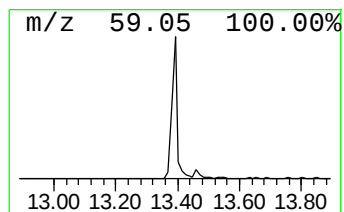
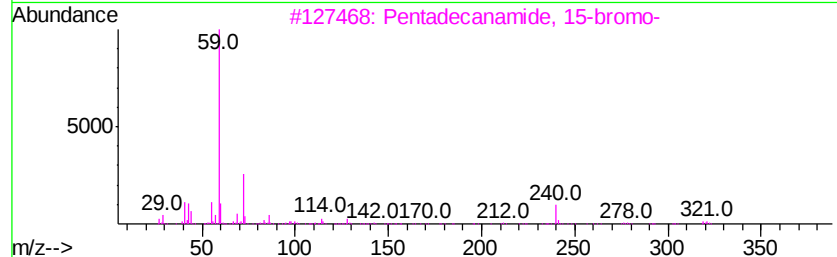
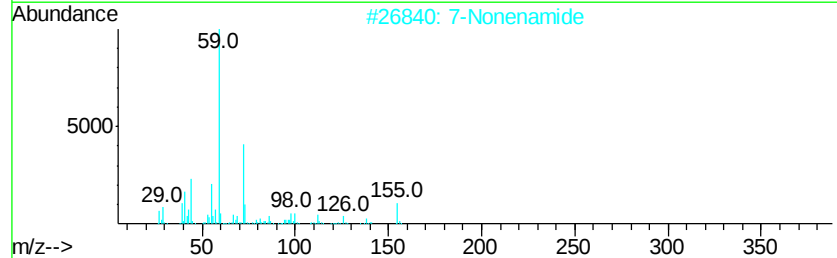
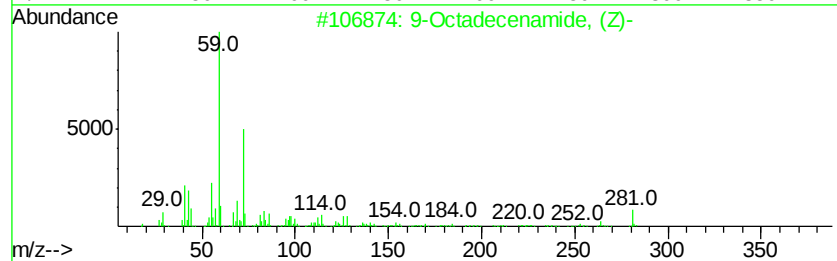
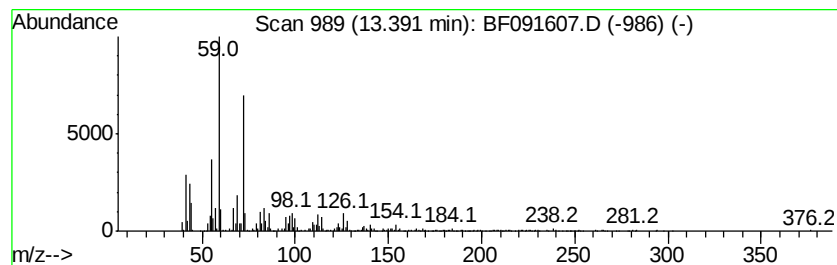
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	8.18 ng	807288	Chrysene-d12	13.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		7-Nonenamide	155	C9H17NO	090949-53-4	72
3		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
5		Octadecanamide	283	C18H37NO	000124-26-5	59



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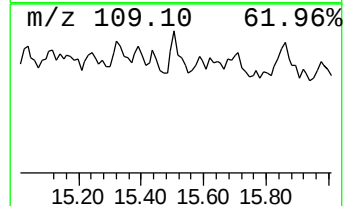
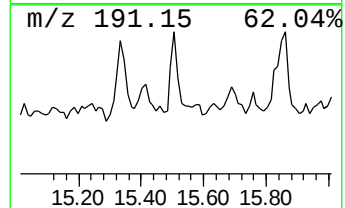
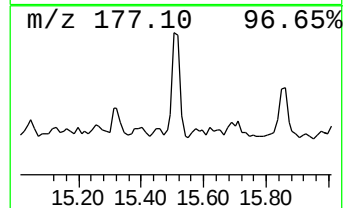
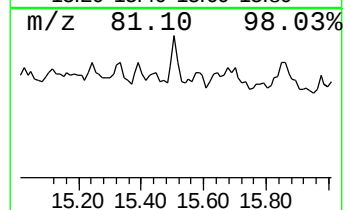
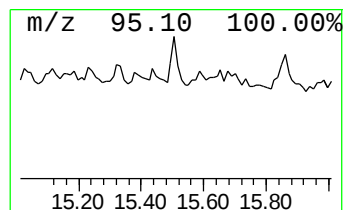
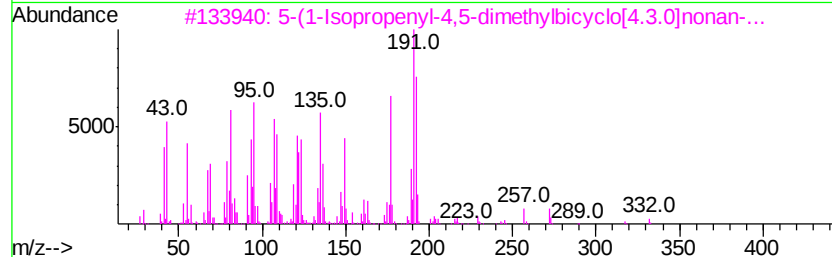
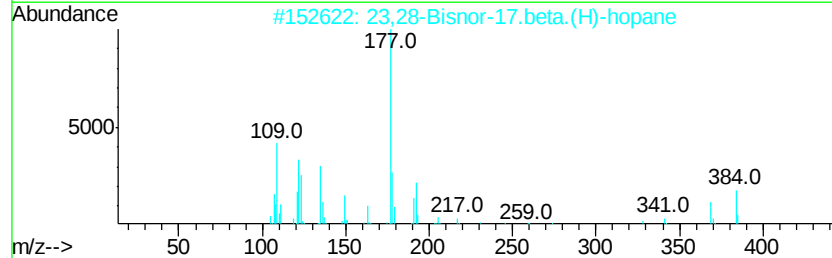
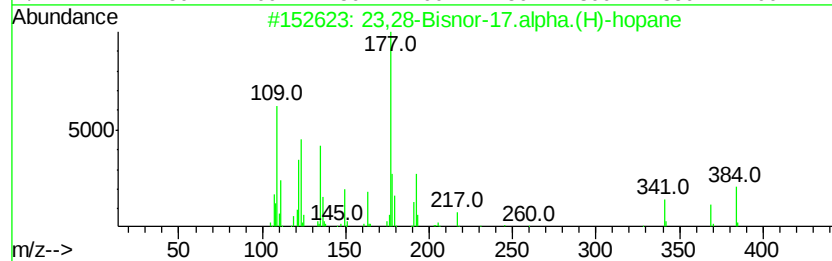
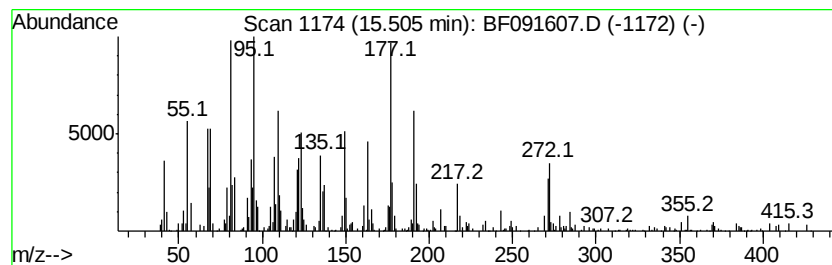
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 23,28-Bisnor-17.alpha.(H)-h... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	4.30 ng	252059	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	23,28-Bisnor-17.alpha.(H)-hopane	384	C28H48	1000101-35-1	70
2		23,28-Bisnor-17.beta.(H)-hopane	384	C28H48	1000101-35-0	70
3		5-(1-Isopropenyl-4,5-dimethylbicyclo[4.3.0]nonan-...	332	C22H36O2	1000195-69-8	43
4		2-Buten-1-one, 1-(2,6,6-trimethyl-...	192	C13H20O	035044-68-9	35
5		2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121416\
Data File : BF091607.D
Acq On : 15 Dec 2016 1:48
Operator : UM/SJ
Sample : H6007-02 5X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-5-0-5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.27	6.4	ng	595281	1	6.80	1852940	20.0
2-Pentanone, 4-hy...	4.94	22.1	ng	2049410	1	6.80	1852940	20.0
unknown6.56	6.56	2.4	ng	225966	1	6.80	1852940	20.0
9-Octadecenamide, ...	13.39	8.2	ng	807288	5	13.95	1973820	20.0
23,28-Bisnor-17.a...	15.51	4.3	ng	252059	6	15.37	1173340	20.0