

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
 Data File : BF091516.D
 Acq On : 8 Dec 2016 21:35
 Operator : UM/SJ
 Sample : H5886-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 URSMW-13

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-BF112916.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	4.996	234	237	240	rBV	354203	456371	11.68%	1.491%
2	5.419	271	274	276	rBV	2190598	2040405	52.22%	6.665%
3	6.447	362	364	367	rVB	1111328	1503277	38.47%	4.910%
4	6.584	374	376	379	rBV	2636724	2786357	71.31%	9.101%
5	6.813	394	396	399	rBV	825463	924046	23.65%	3.018%
6	6.882	401	402	408	rVV	85326	117074	3.00%	0.382%
7	6.973	408	410	412	rVB	2319513	2098104	53.70%	6.853%
8	7.384	443	446	448	rBV	2071617	2063054	52.80%	6.739%
9	8.013	498	501	502	rBV2	33456	45898	1.17%	0.150%
10	8.104	506	509	511	rBV	1580483	1395682	35.72%	4.559%
11	8.482	538	542	545	rBV5	24199	60099	1.54%	0.196%
12	8.585	548	551	553	rVB	41300	67553	1.73%	0.221%
13	8.630	553	555	557	rBV2	30020	45141	1.16%	0.147%
14	8.676	557	559	561	rVB	44969	51143	1.31%	0.167%
15	8.722	561	563	567	rBV4	19767	56398	1.44%	0.184%
16	8.813	570	571	573	rBV2	25416	48202	1.23%	0.157%
17	8.962	582	584	586	rVB2	44501	74857	1.92%	0.245%
18	9.053	588	592	594	rBV4	46939	87992	2.25%	0.287%
19	9.087	594	595	598	rBV3	32257	60613	1.55%	0.198%
20	9.179	601	603	606	rBV	3272004	3219966	82.41%	10.517%
21	9.282	608	612	615	rBV5	52465	138764	3.55%	0.453%
22	9.350	616	618	623	rBV5	36889	94194	2.41%	0.308%
23	9.430	623	625	626	rBV	37985	54979	1.41%	0.180%
24	9.488	628	630	631	rBV	55479	60399	1.55%	0.197%
25	9.670	644	646	648	rBV3	49160	103335	2.64%	0.338%
26	9.705	648	649	653	rVV3	43164	104848	2.68%	0.342%
27	9.773	653	655	658	rVV4	37494	94188	2.41%	0.308%
28	9.853	660	662	665	rVB	1550095	1421650	36.38%	4.644%
29	10.116	684	685	687	rBV	71328	81514	2.09%	0.266%
30	10.208	691	693	694	rVV2	63651	68738	1.76%	0.225%
31	10.413	710	711	713	rBV2	57090	62785	1.61%	0.205%
32	10.596	725	727	729	rBV	162455	188790	4.83%	0.617%
33	10.642	729	731	734	rVV	2375691	2357914	60.34%	7.702%
34	11.339	789	792	794	rBV	1585851	1447431	37.04%	4.728%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.888	837	840	843	rVB2	135886	196991	5.04%	0.643%
36	12.665	906	908	911	rVB	182947	166959	4.27%	0.545%
37	12.836	919	923	924	rBV4	137220	413068	10.57%	1.349%
38	12.928	928	931	933	rVV	3663308	3907401	100.00%	12.763%
39	13.968	1020	1022	1025	rVB	1389150	1268127	32.45%	4.142%
40	15.385	1143	1146	1149	rBV	979192	1181048	30.23%	3.858%

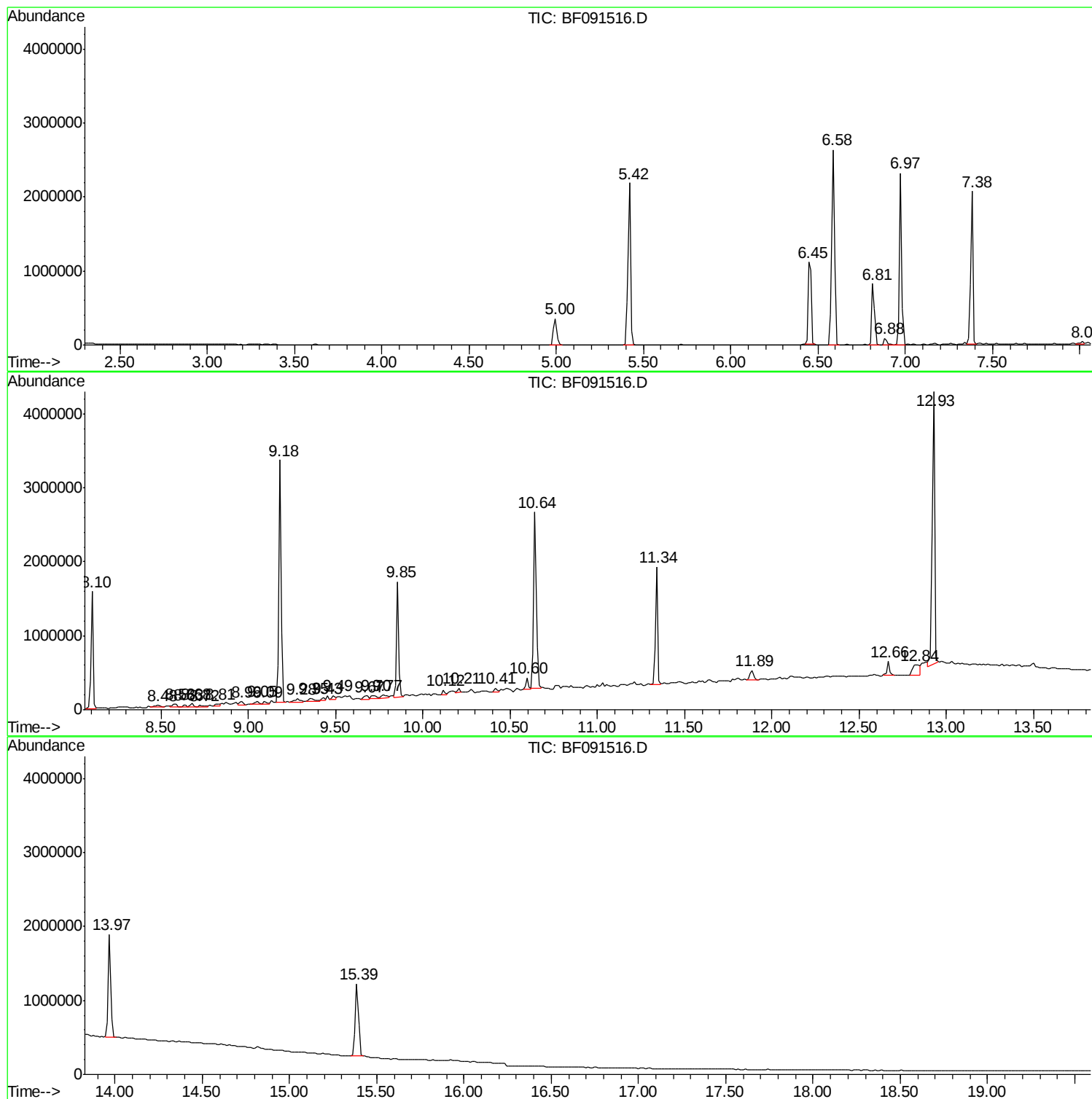
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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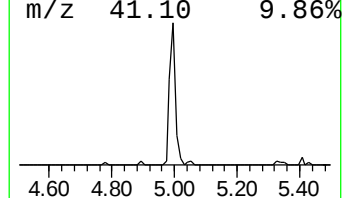
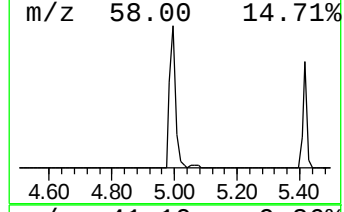
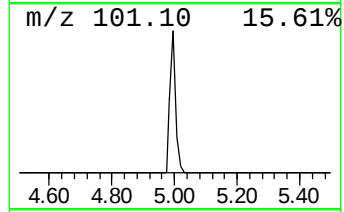
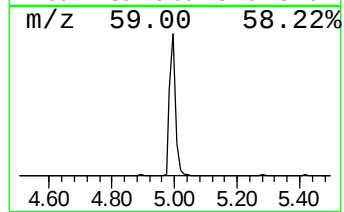
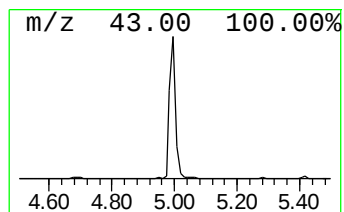
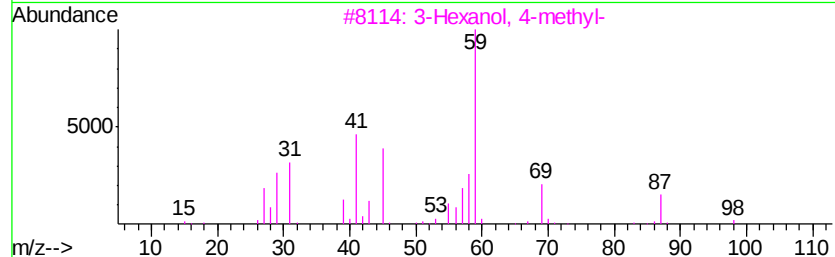
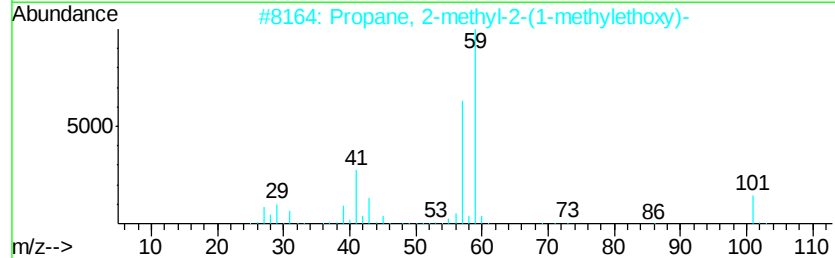
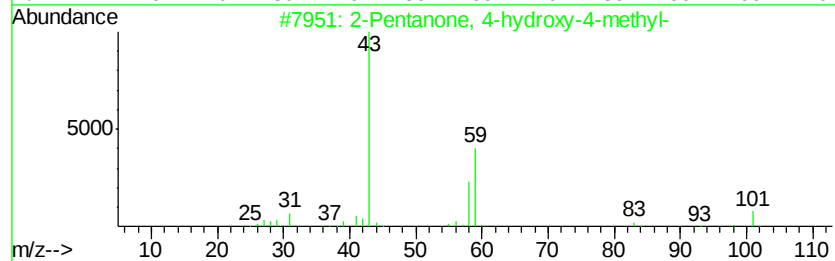
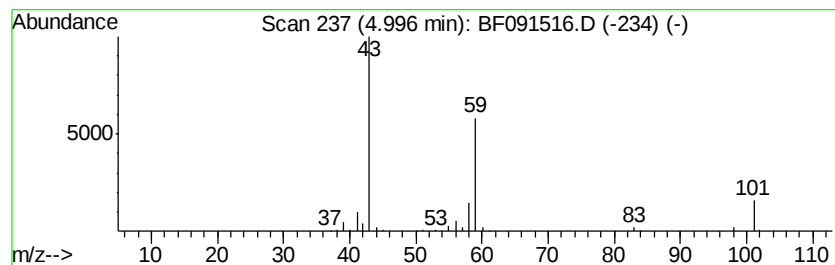
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	9.88 ng	456371	1,4-Dichlorobenzene-d4	6.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32	



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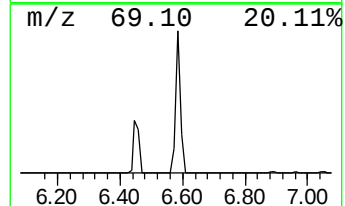
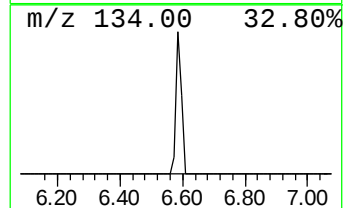
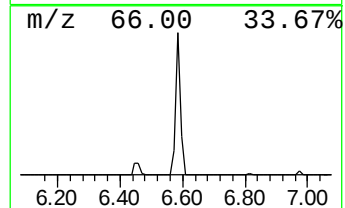
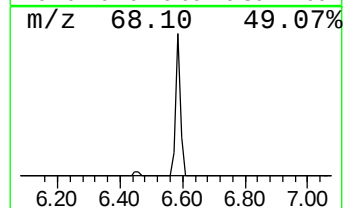
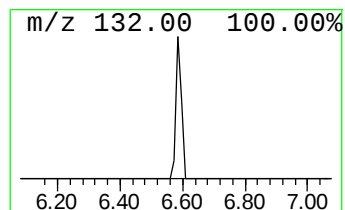
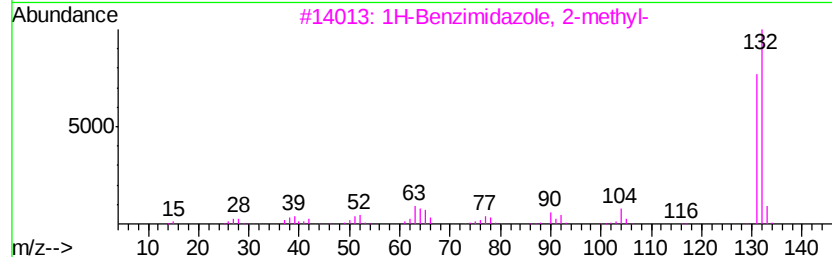
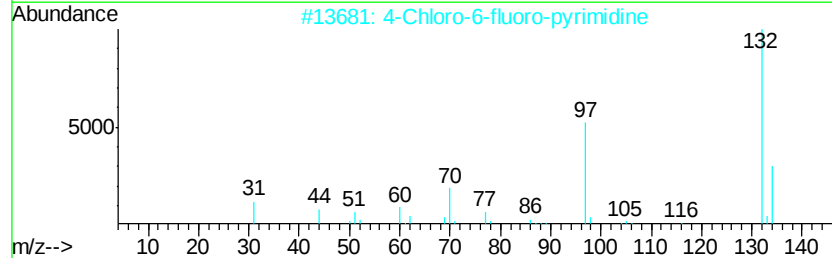
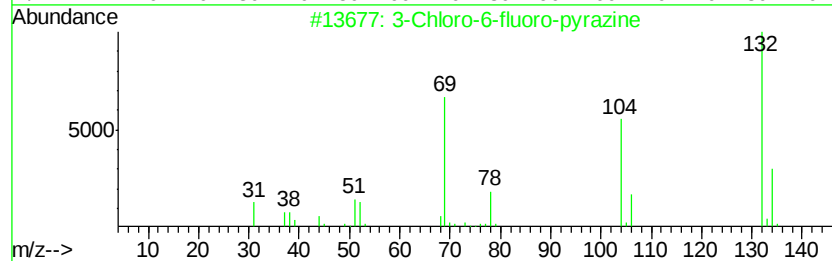
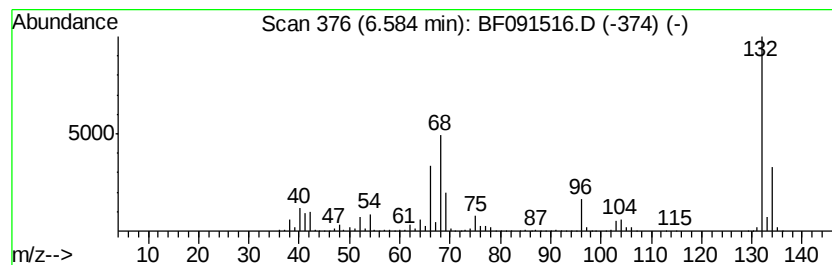
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	60.31 ng	2786360	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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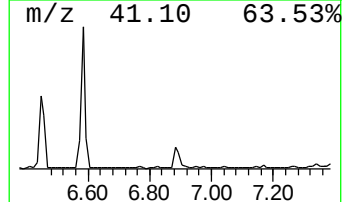
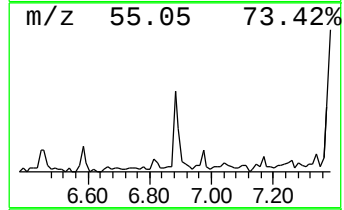
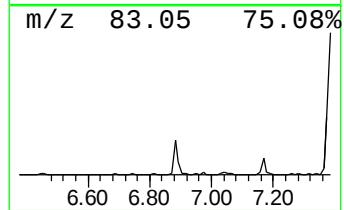
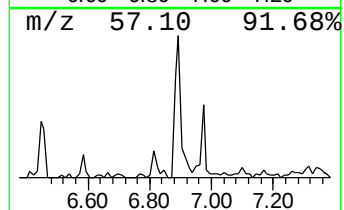
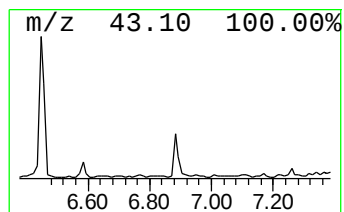
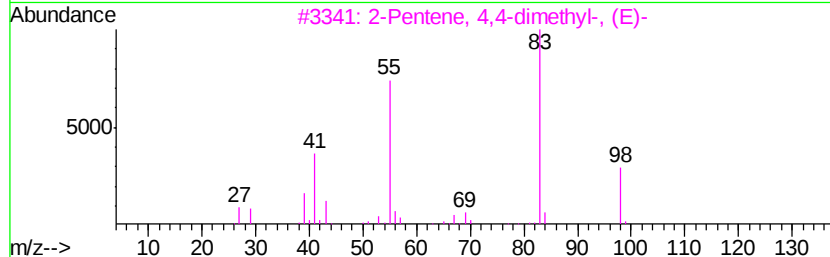
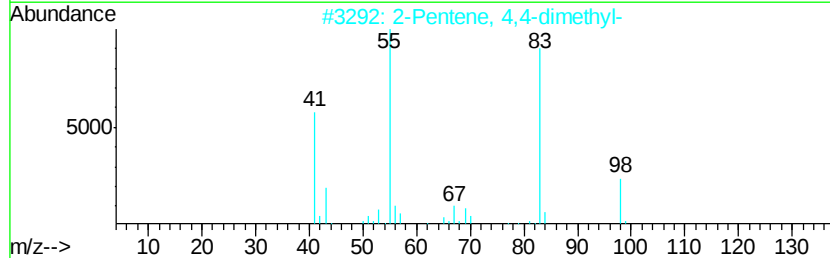
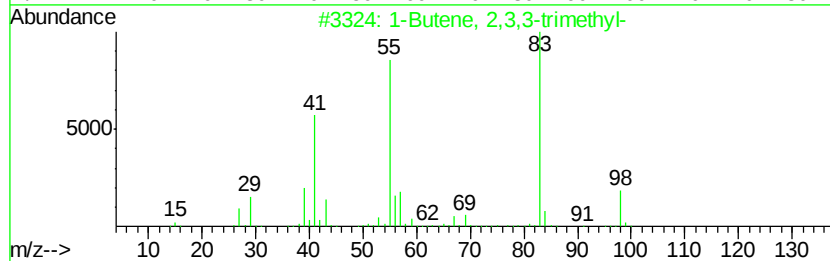
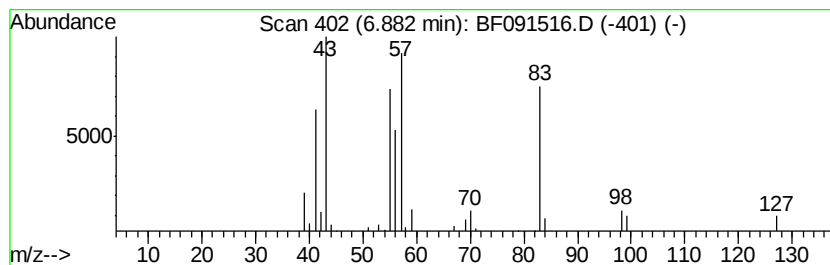
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Butene, 2,3,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	2.53 ng	117074	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	52
2			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	47
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	47
4			2-Chloro-2,4-dimethylpentane	134	C7H15Cl	035951-33-8	47
5			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	46



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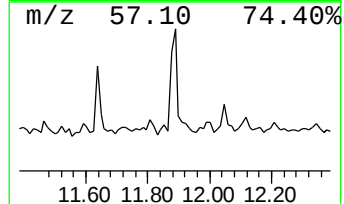
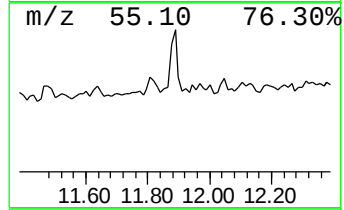
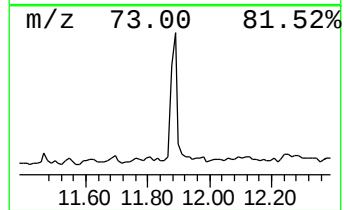
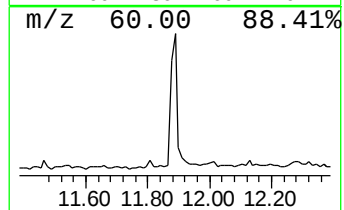
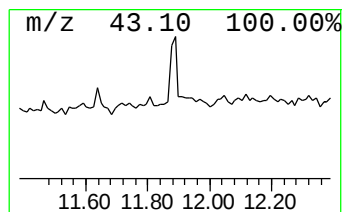
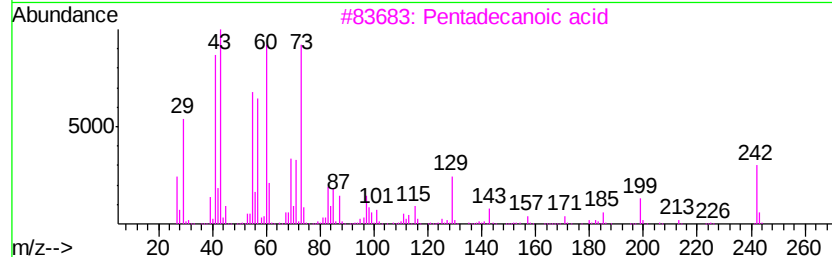
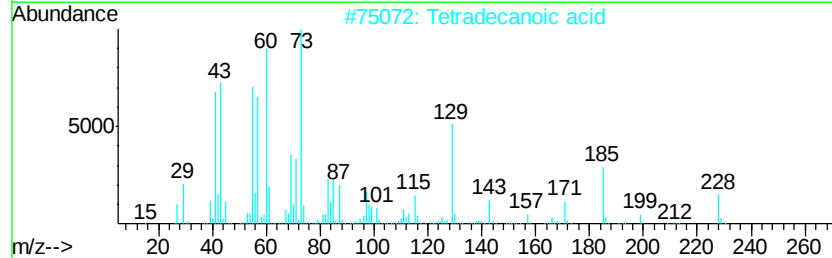
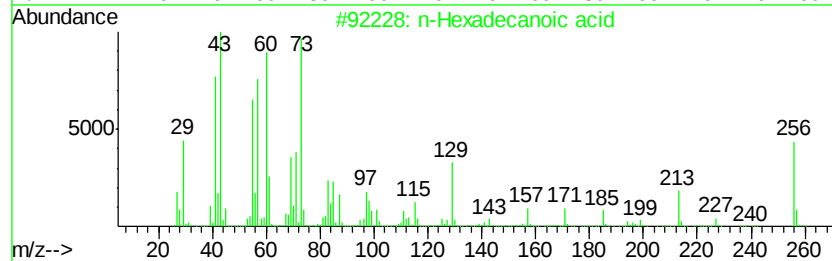
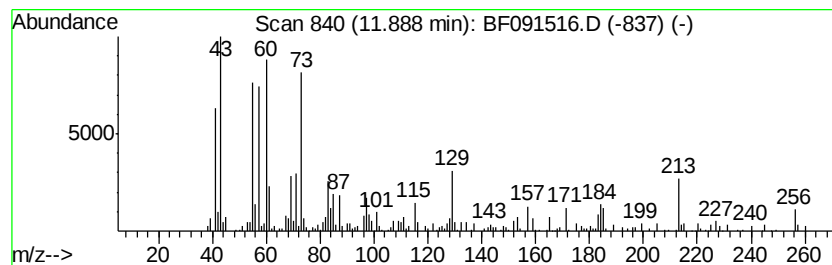
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	2.72 ng	196991	Phenanthrene-d10	11.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4		Dodecanoic acid	200	C12H24O2	000143-07-7	53
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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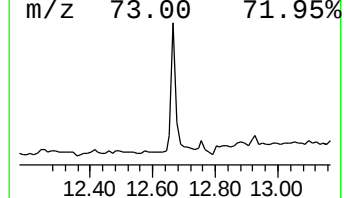
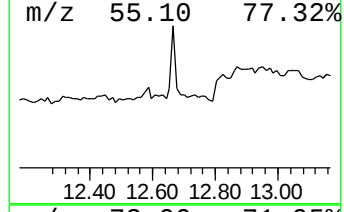
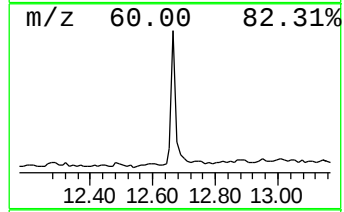
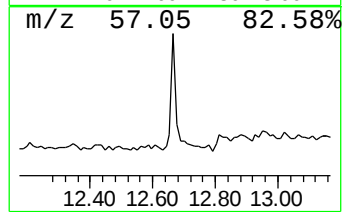
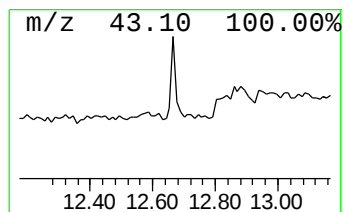
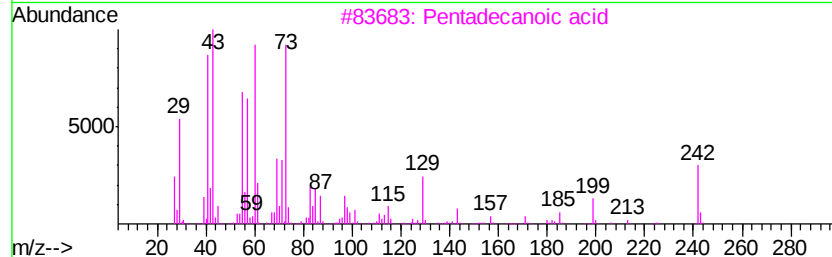
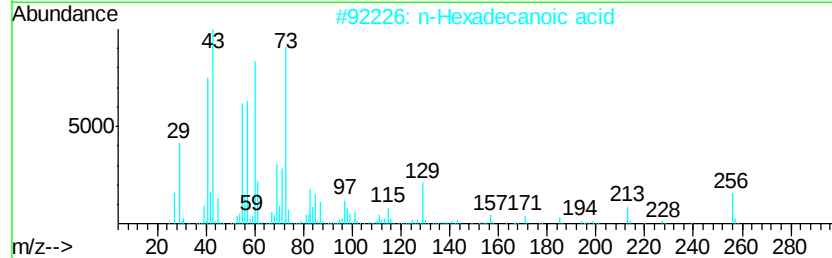
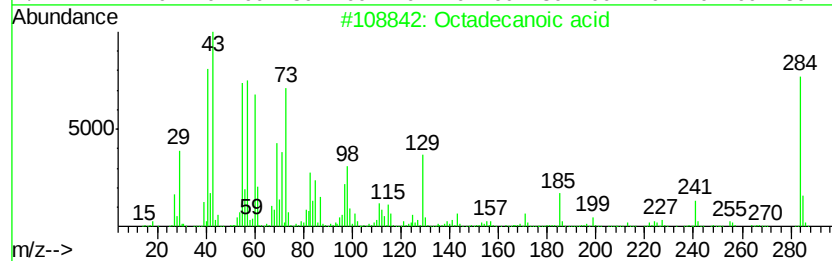
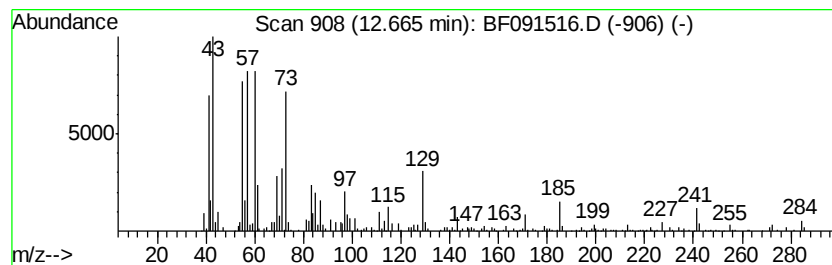
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.67	2.63 ng	166959	Chrysene-d12		13.97
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
Data File : BF091516.D
Acq On : 8 Dec 2016 21:35
Operator : UM/SJ
Sample : H5886-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

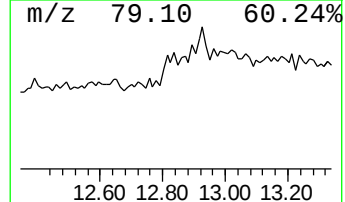
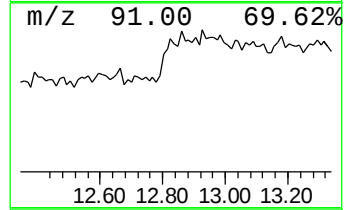
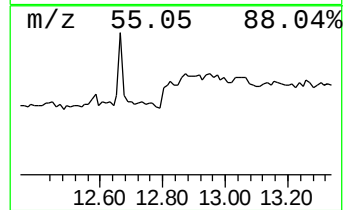
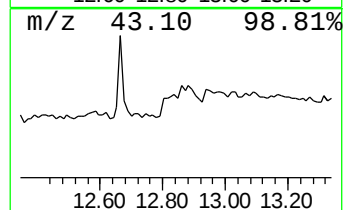
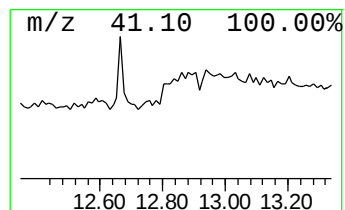
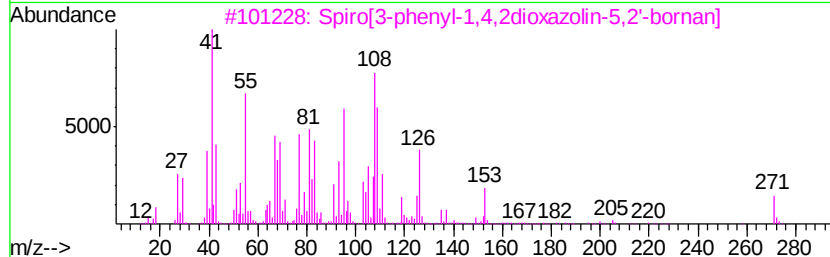
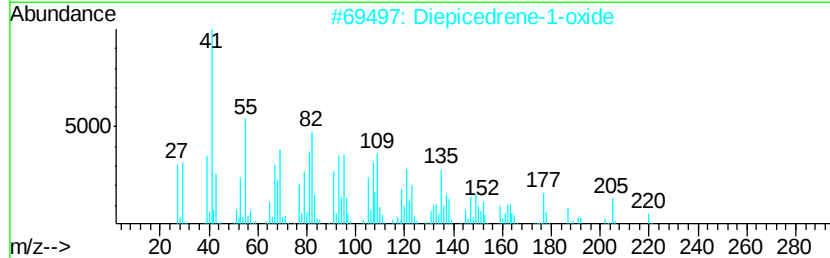
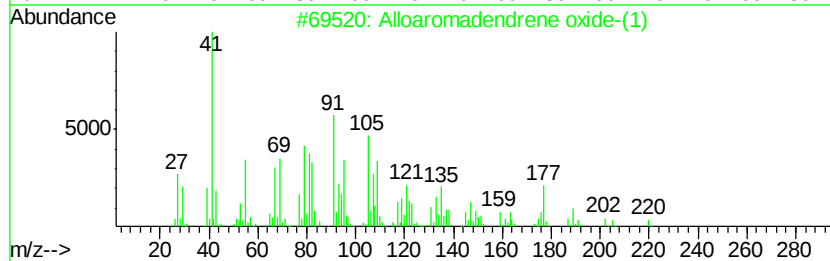
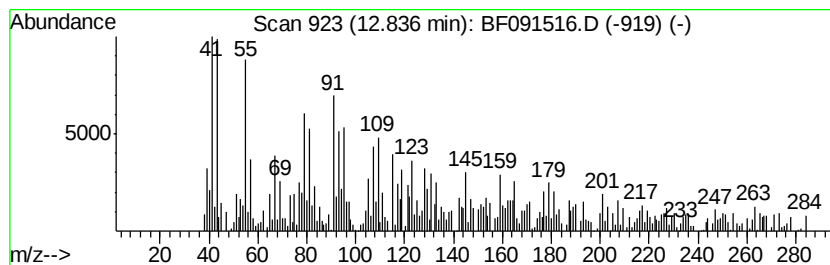
Instrument :
BNA_F
ClientSampleId :
URSMW-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Alloaromadendrene oxide-(1) Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.84	6.51 ng	413068	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Alloaromadendrene oxide-(1)	220	C15H24O	1000156-12-8	70
2	Diepicedrene-1-oxide	220	C15H24O	1000156-11-0	52
3	Spiro[3-phenyl-1,4,2dioxazolin-5...	271	C17H21NO2	287488-39-5	38
4	cis-Z-.alpha.-Bisabolene epoxide	220	C15H24O	1000131-71-2	38
5	3-Buten-2-ol, 2-methyl-4-(1,3,3-...	224	C14H24O2	072294-84-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120816\
Data File : BF091516.D
Acq On : 8 Dec 2016 21:35
Operator : UM/SJ
Sample : H5886-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
URSMW-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112916.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
2-Pentanone, 4-hy...	5.00	9.9	ng	456371	1	6.81	924046	20.0
unknown6.58	6.58	60.3	ng	2786360	1	6.81	924046	20.0
1-Butene, 2,3,3-t...	6.88	2.5	ng	117074	1	6.81	924046	20.0
n-Hexadecanoic acid	11.89	2.7	ng	196991	4	11.34	1447430	20.0
Octadecanoic acid	12.67	2.6	ng	166959	5	13.97	1268130	20.0
Alloaromadendrene...	12.84	6.5	ng	413068	5	13.97	1268130	20.0