

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063016\
 Data File : BF088558.D
 Acq On : 1 Jul 2016 5:11
 Operator : UM/SJ
 Sample : H3747-02
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D9-B2(0-11)C

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-BF063016.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	1.690	5	9	11	rVB	5111789	7698043	100.00%	20.924%
2	1.736	11	13	23	rVB	273760	602151	7.82%	1.637%
3	1.873	23	25	41	rVB	2007639	3390670	44.05%	9.216%
4	2.078	41	43	71	rVB4	104180	395079	5.13%	1.074%
5	3.084	129	131	146	rBV	69776	186880	2.43%	0.508%
6	5.004	296	299	303	rBV	138873	209228	2.72%	0.569%
7	5.416	332	335	338	rBV	2461225	2527067	32.83%	6.869%
8	6.445	422	425	428	rBV	1942412	2970811	38.59%	8.075%
9	6.582	434	437	440	rBV	2281199	2664181	34.61%	7.242%
10	6.822	455	458	460	rBV	853696	839321	10.90%	2.281%
11	6.970	469	471	474	rVB	1694840	2114032	27.46%	5.746%
12	7.382	504	507	509	rBV	1947255	1890426	24.56%	5.138%
13	8.102	568	570	572	rVB	1292231	1085984	14.11%	2.952%
14	9.176	662	664	667	rVB	2299982	2864654	37.21%	7.787%
15	9.576	696	699	701	rBV	159363	182939	2.38%	0.497%
16	9.851	721	723	726	rBV	1084132	1093592	14.21%	2.973%
17	10.639	789	792	794	rBV	1460851	1419684	18.44%	3.859%
18	11.336	850	853	855	rVB	892448	992342	12.89%	2.697%
19	12.914	989	991	993	rBV	1888097	1930989	25.08%	5.249%
20	13.828	1069	1071	1074	rBV	124468	210187	2.73%	0.571%
21	13.954	1080	1082	1085	rVB	737285	781682	10.15%	2.125%
22	15.360	1203	1205	1208	rVB	516362	739923	9.61%	2.011%

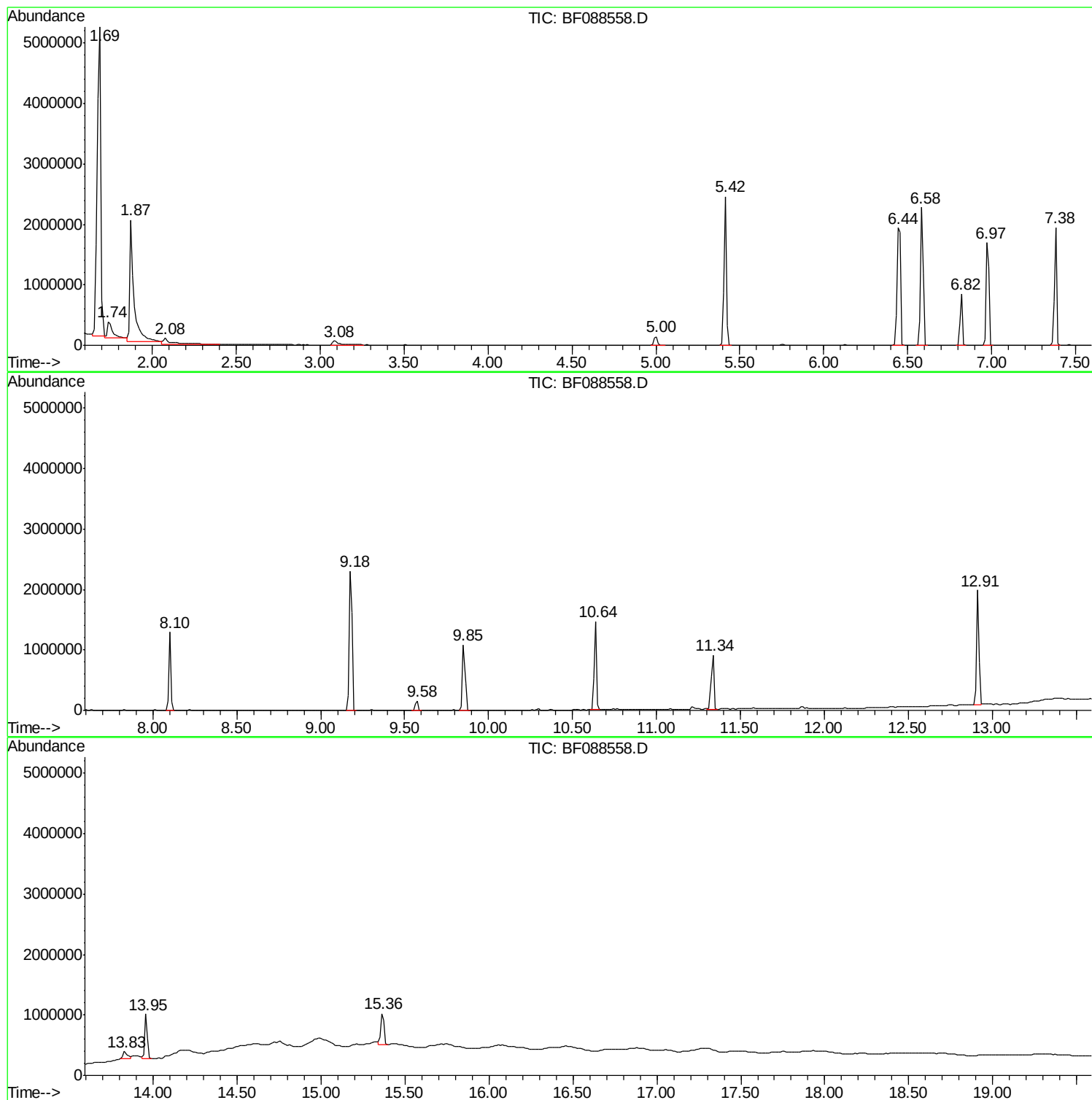
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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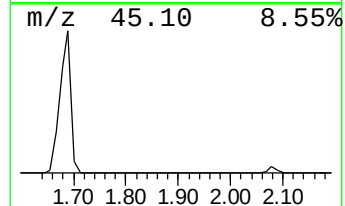
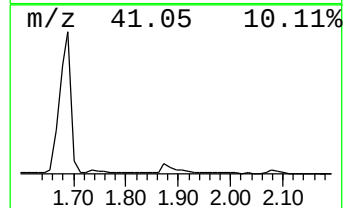
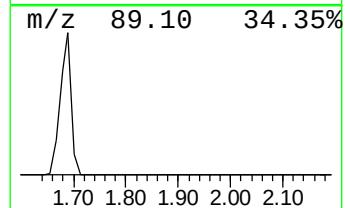
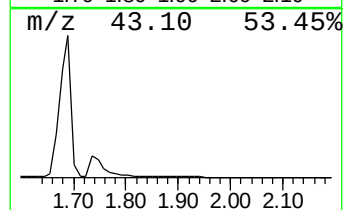
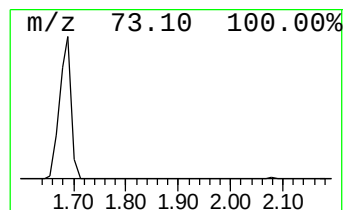
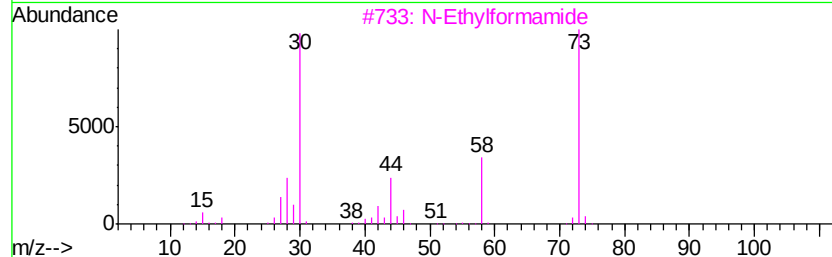
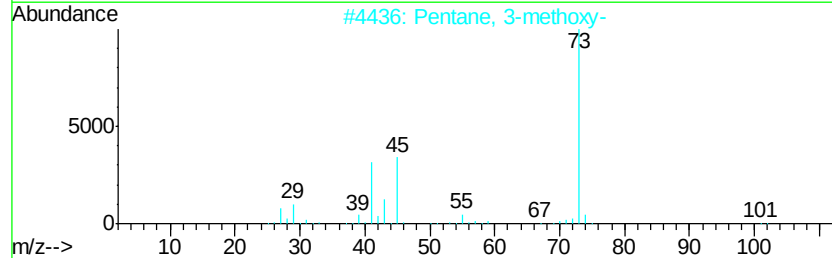
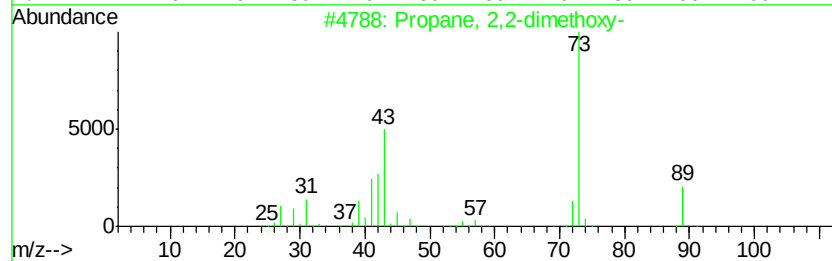
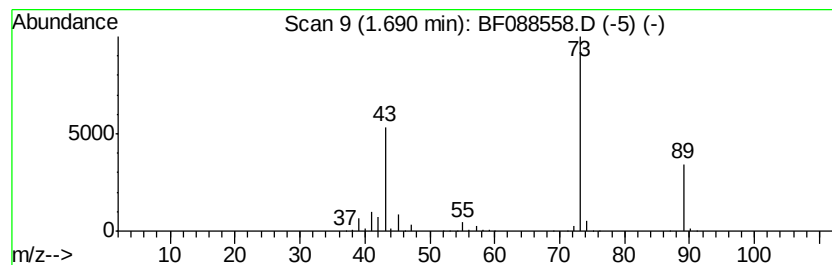
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.69	183.44 ng	7698040	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9



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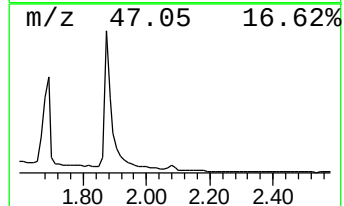
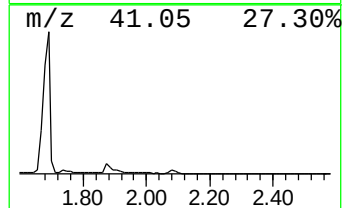
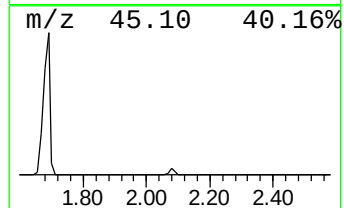
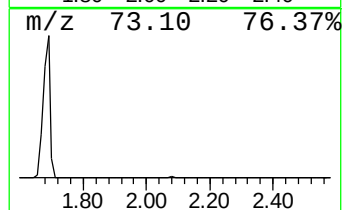
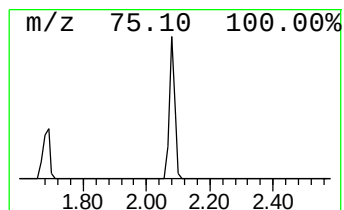
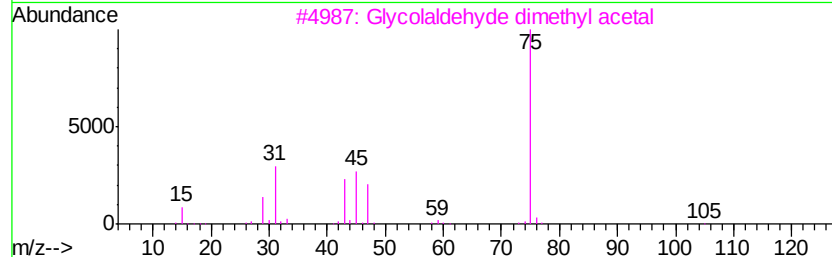
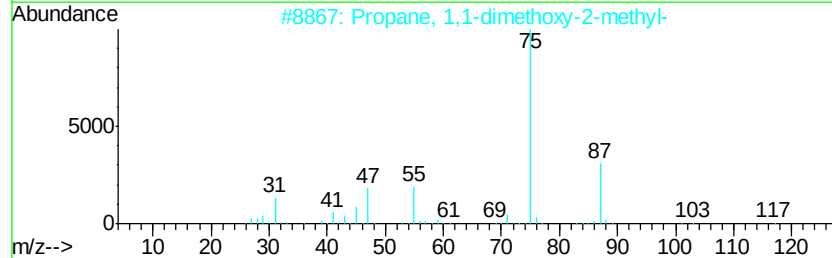
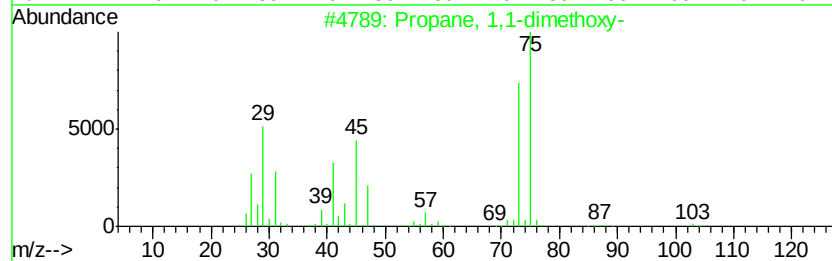
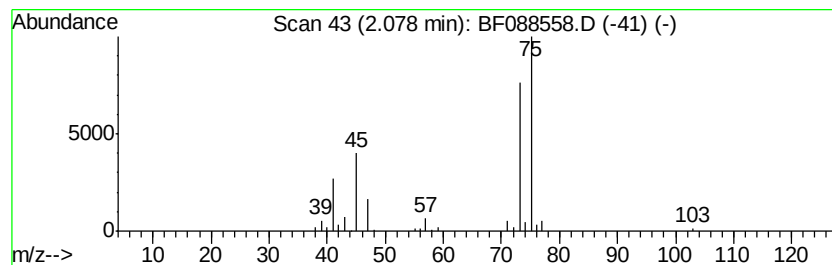
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Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.08	9.41 ng	395079	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2		Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	37
3		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	33
4		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	28
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27



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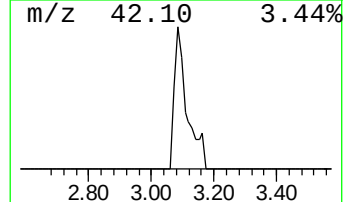
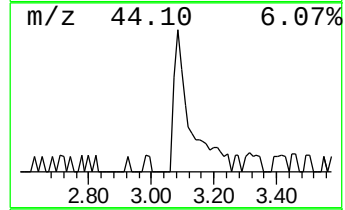
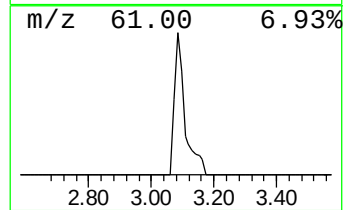
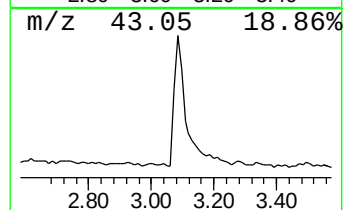
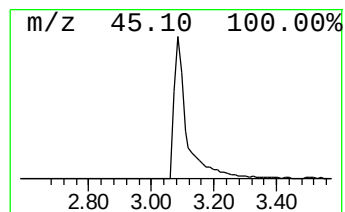
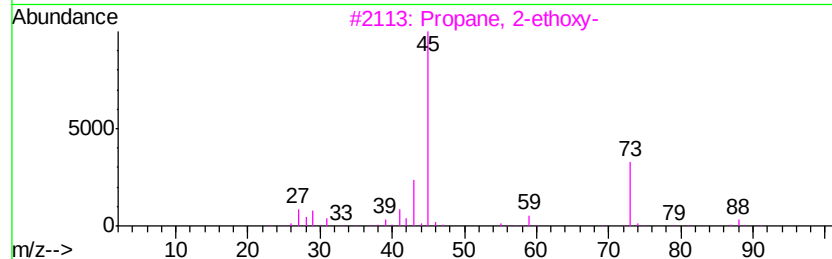
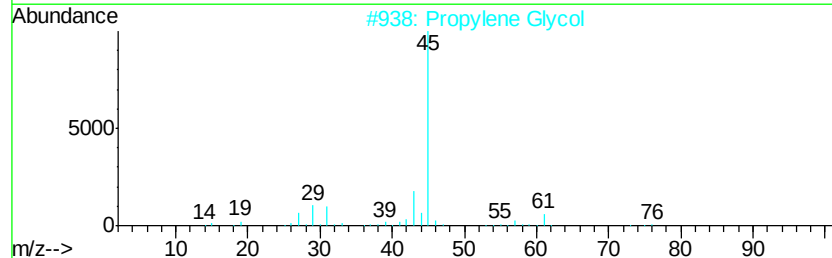
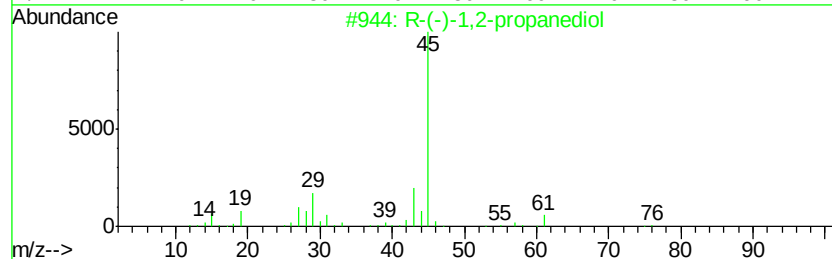
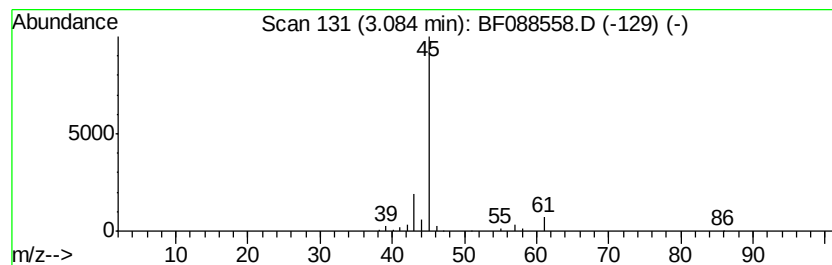
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Peak Number 5 unknown3.08 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.08	4.45 ng	186880	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9
4	2-Pentanol	88	C5H12O	006032-29-7	9
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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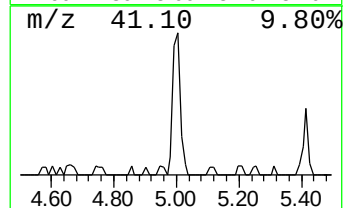
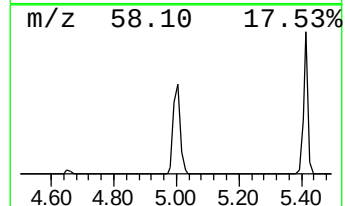
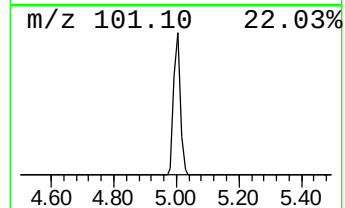
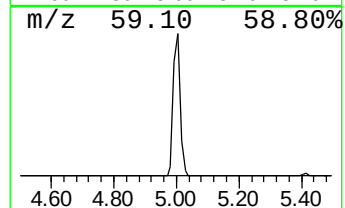
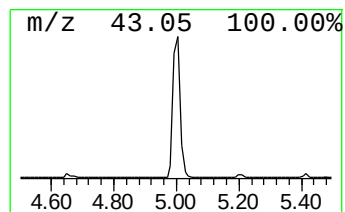
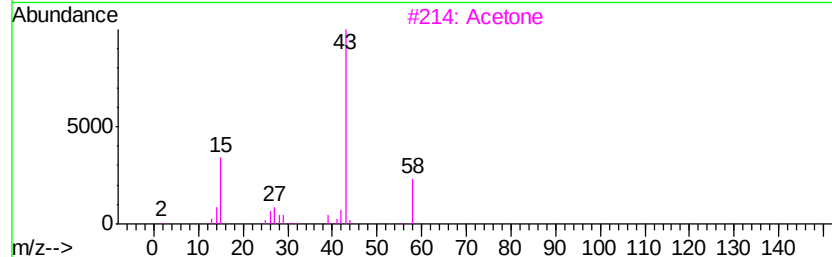
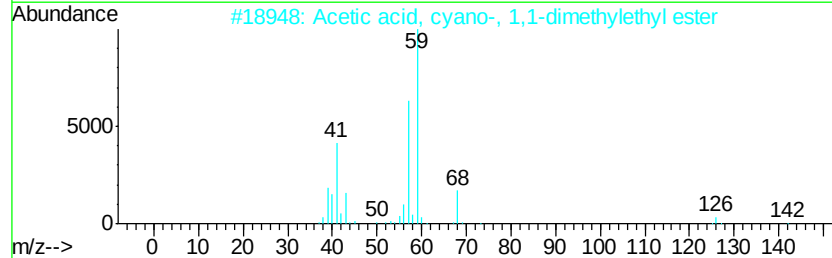
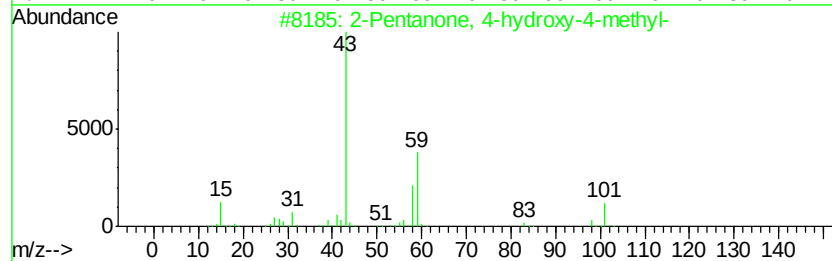
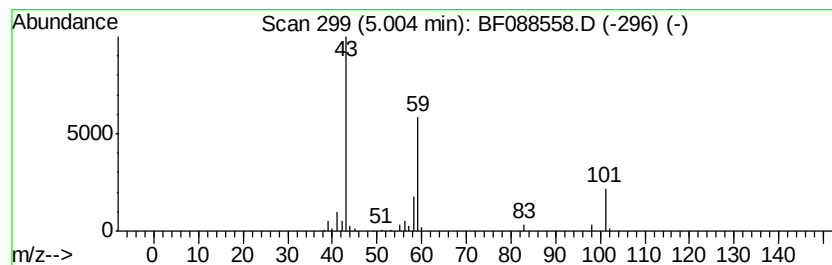
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Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.99 ng	209228	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Acetone	58	C3H6O	000067-64-1	10
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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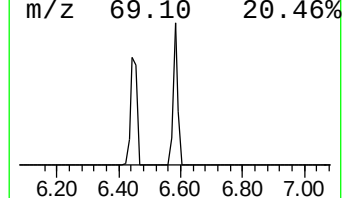
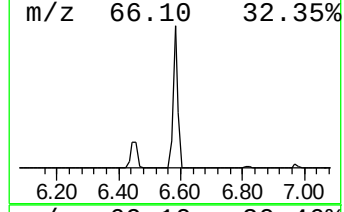
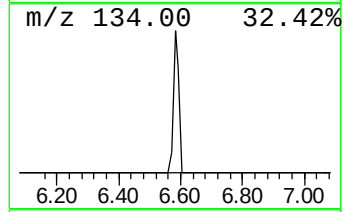
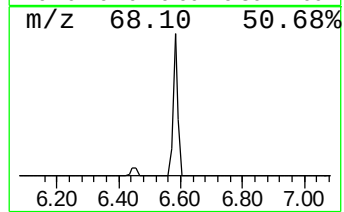
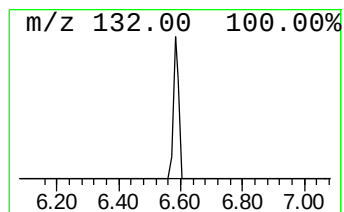
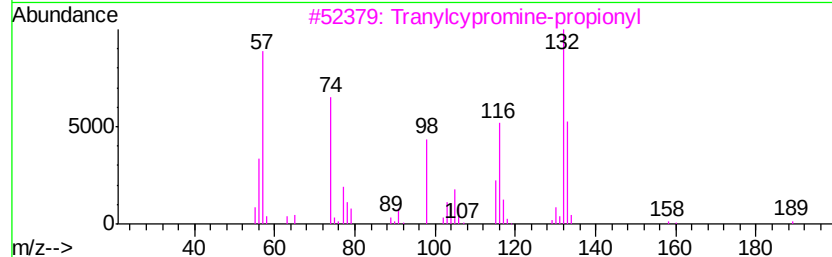
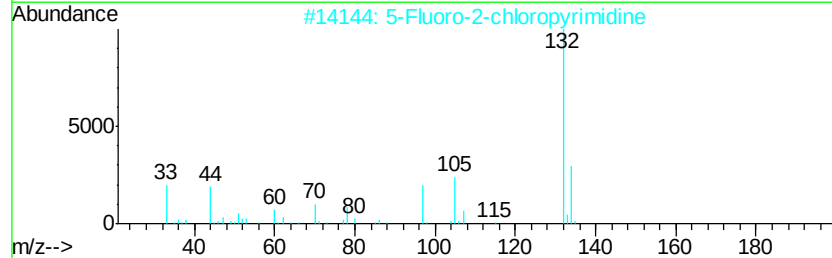
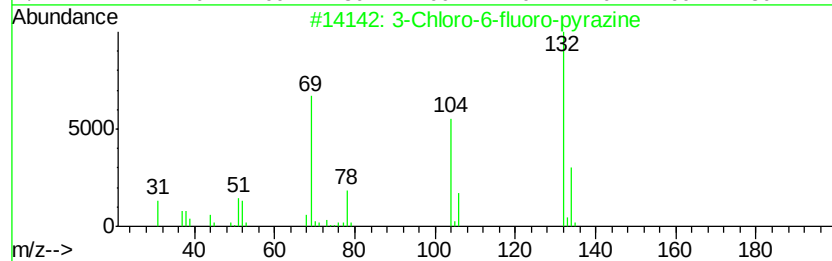
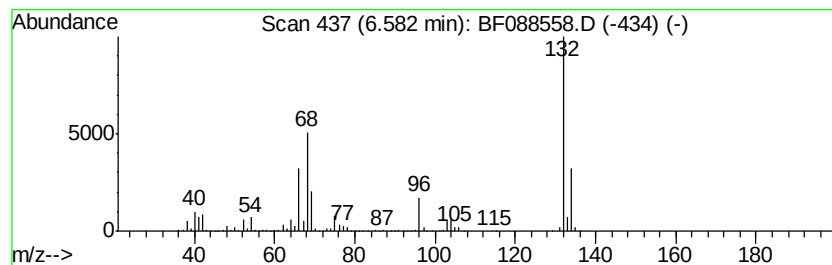
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TIC Library : C:\Database\NIST11.L
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Peak Number 7 unknown6.58 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	63.48 ng	2664180	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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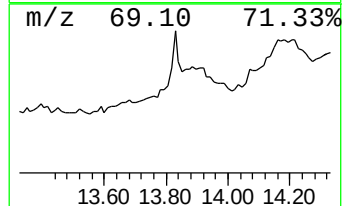
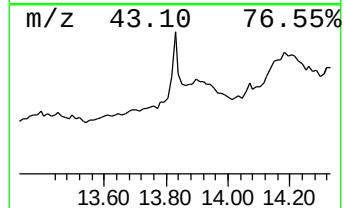
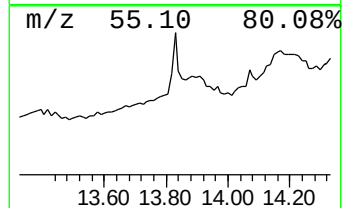
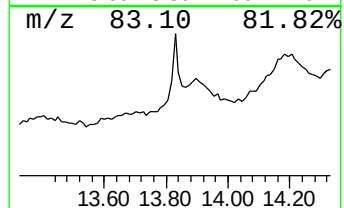
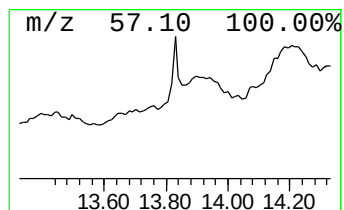
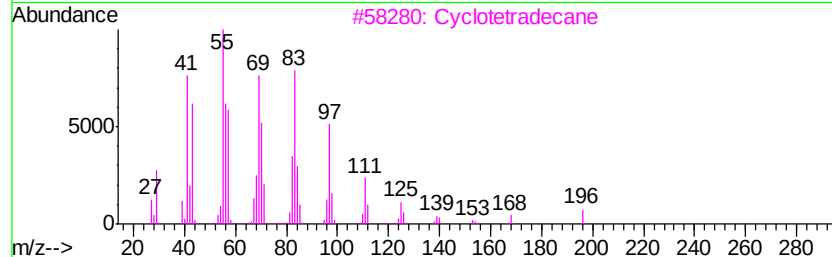
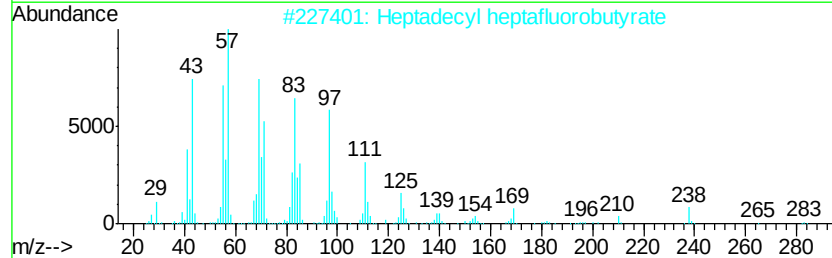
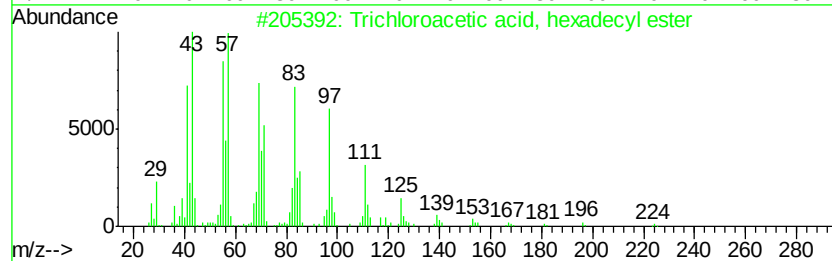
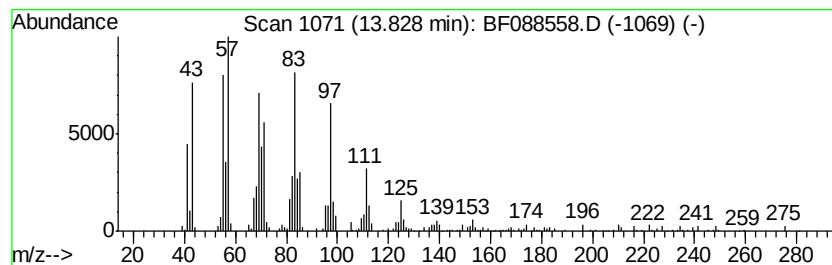
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.38 ng	210187	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3		Cyclotetradecane	196	C14H28	000295-17-0	93
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF063016\
Data File : BF088558.D
Acq On : 1 Jul 2016 5:11
Operator : UM/SJ
Sample : H3747-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D9-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.69	183.4	ng	7698040	1	6.82	839321	20.0
Propane, 1,1-dime...	2.08	9.4	ng	395079	1	6.82	839321	20.0
unknown3.08	3.08	4.5	ng	186880	1	6.82	839321	20.0
2-Pentanone, 4-hy...	5.00	5.0	ng	209228	1	6.82	839321	20.0
unknown6.58	6.58	63.5	ng	2664180	1	6.82	839321	20.0
Trichloroacetic a...	13.83	5.4	ng	210187	5	13.95	781682	20.0