LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061615\
Data File : BF080009.D
Acq On : 17 Jun 2015 3:04
Operator : TP/IZ
Sample : G2474-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-3

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-BF061115.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	4.984	164	166	170	rVB3	14653	18821	1.15%	0.202%
2	5.133	176	179	181	rBV	51799	53894	3.29%	0.578%
3	5.567	214	217	220	rBV	138919	132111	8.05%	1.416%
4	5.956	249	251	254	rBV	355807	329087	20.06%	3.528%
5	6.356	284	286	289	rVB2	17256	22208	1.35%	0.238%
6	6.573	303	305	309	rBV	36526	48147	2.94%	0.516%
7	6.950	335	338	340	rBV	247042	234827	14.32%	2.518%
8	7.110	350	352	355	rVB	424339	533030	32.50%	5.715%
9	7.350	371	373	375	rBV	362796	301216	18.36%	3.229%
10	7.510	385	387	389	rBV	989338	794209	48.42%	8.515%
11	7.910	419	422	424	rBV	565143	602790	36.75%	6.463%
12	8.642	484	486	488	rBV	510230	415689	25.34%	4.457%
13	9.590	566	569	573	rBV	35735	34734	2.12%	0.372%
14	9.716	578	580	582	rVB	1759298	1393379	84.95%	14.939%
15	10.105	612	614	616	rVB	104902	81161	4.95%	0.870%
16	10.413	639	641	643	rBV	558354	472868	28.83%	5.070%
17	11.031	693	695	699	rVB	19323	24918	1.52%	0.267%
18	11.122	699	703	705	rBV	47108	41572	2.53%	0.446%
19	11.202	708	710	712	rBV2	460771	496921	30.30%	5.328%
20	11.922	771	773	775	rBV	502134	507096	30.92%	5.437%
21	13.591	917	919	922	rBV	1252927	1640207	100.00%	17.585%
22	14.642	1008	1011	1016	rBV	51391	75662	4.61%	0.811%
23	14.860	1027	1030	1033	rBV	537316	544979	33.23%	5.843%
24	16.734	1191	1194	1203	rBV	320994	527594	32.17%	5.657%

Sum of corrected areas: 9327120

LSC Report - Integrated Chromatogram

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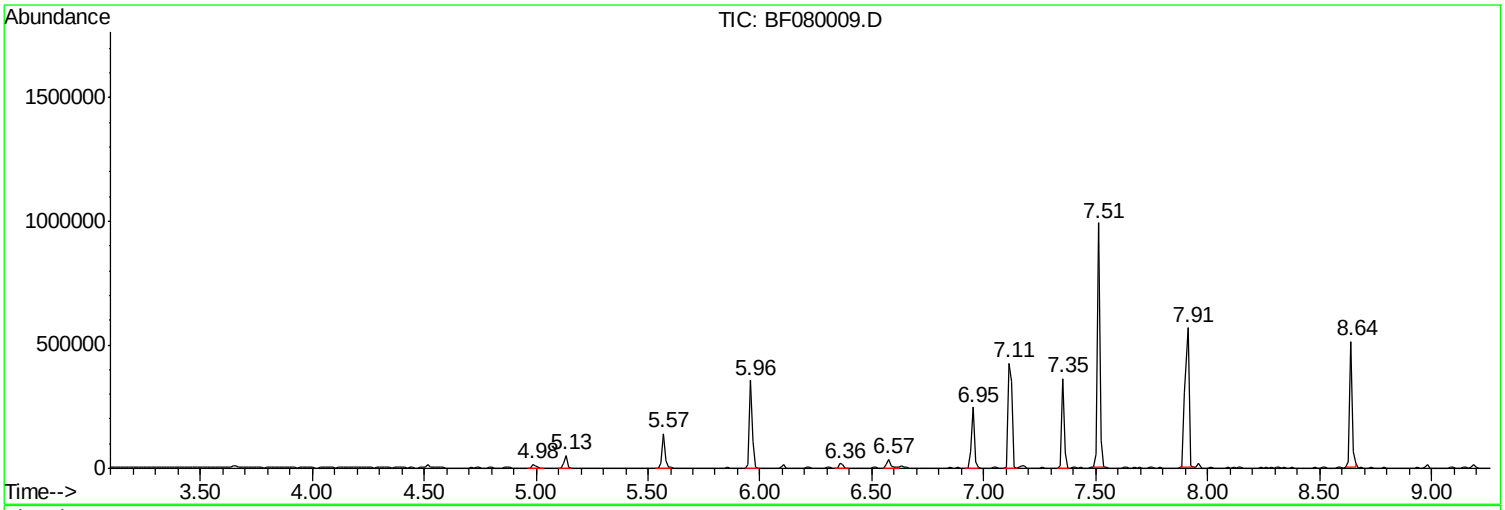
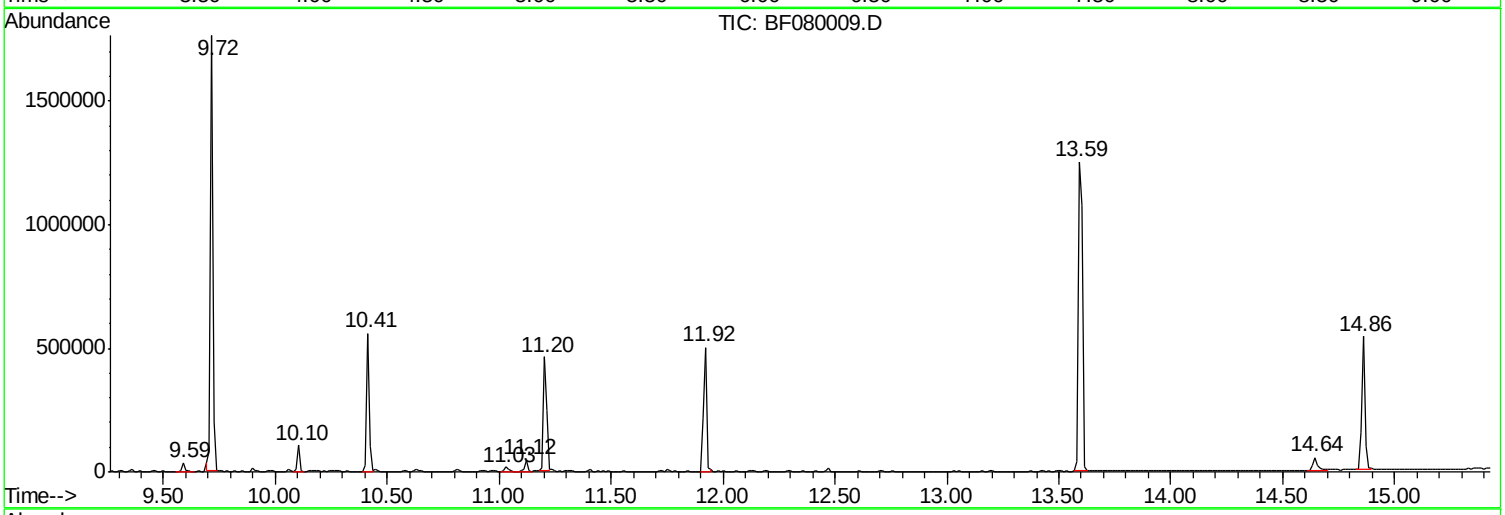
ALS Vial : 19 Sample Multiplier: 1

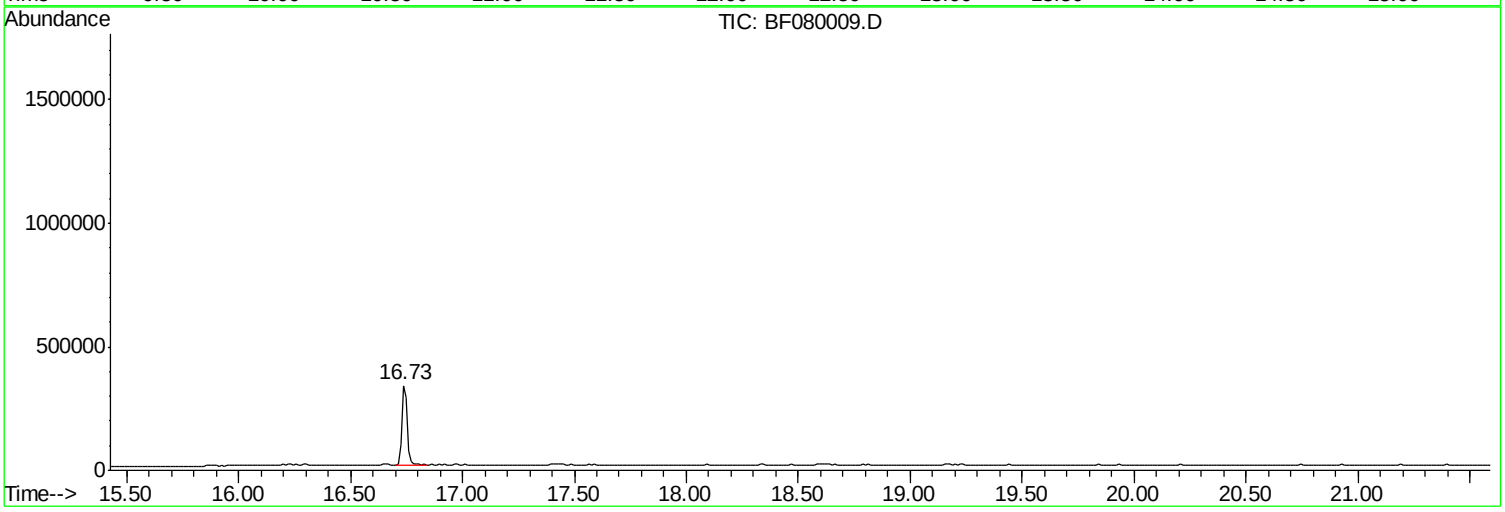
Instrument :
BNA_F
ClientSampleId :
C-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Library Search Compound Report

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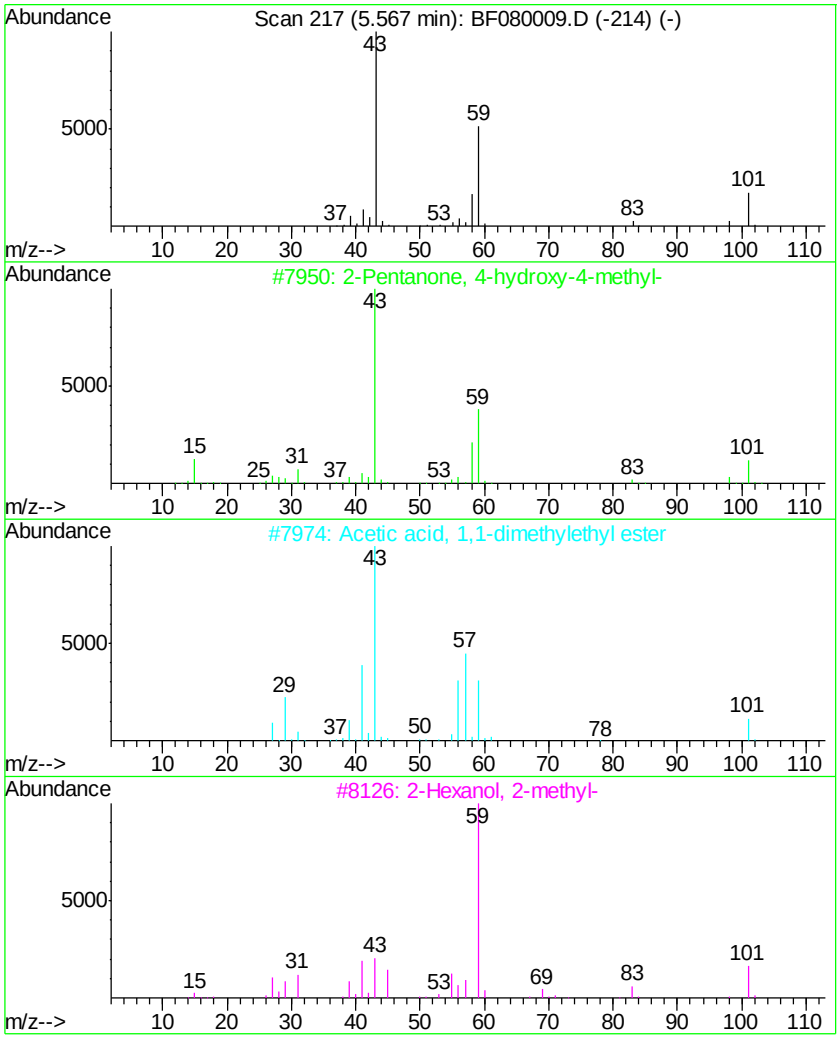
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

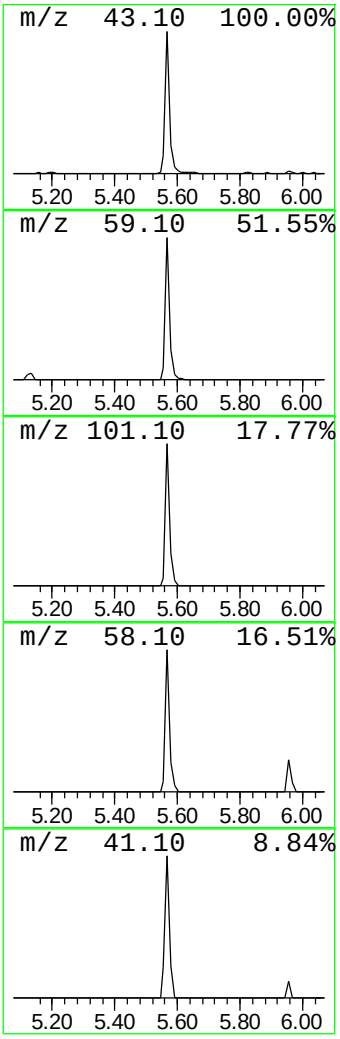
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.57	8.77 ng	132111	1,4-Dichlorobenzene-d4	7.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





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Instrument :
BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

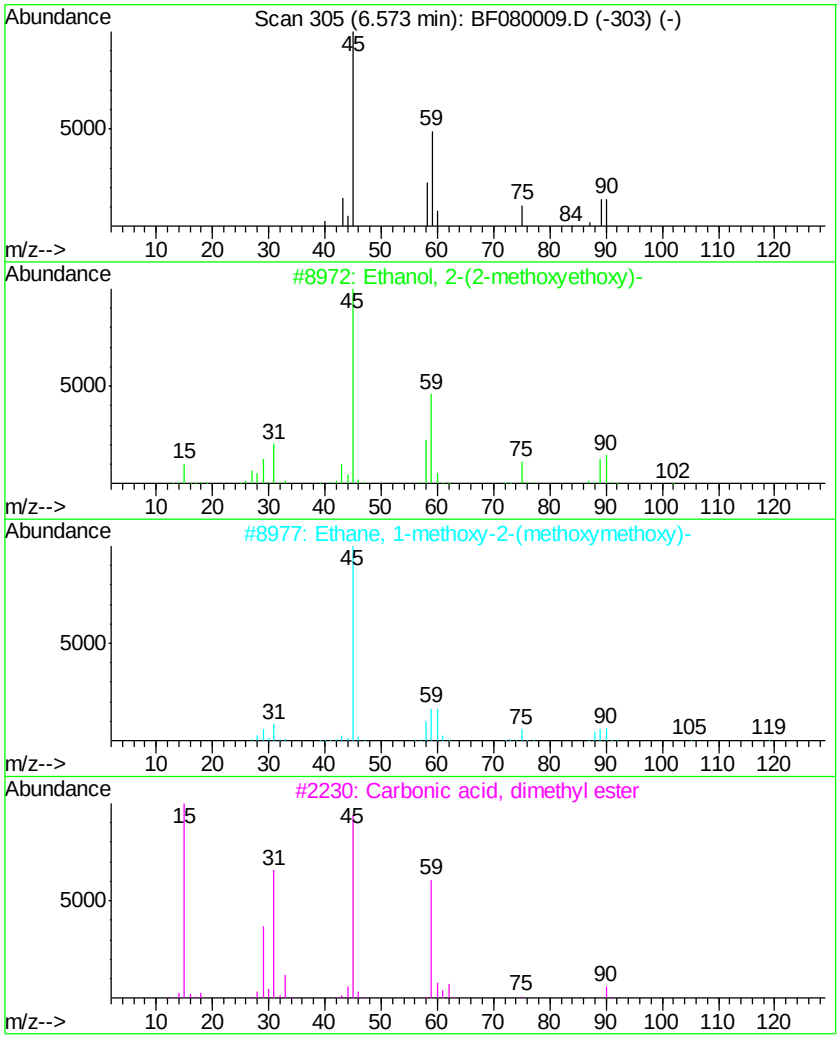
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

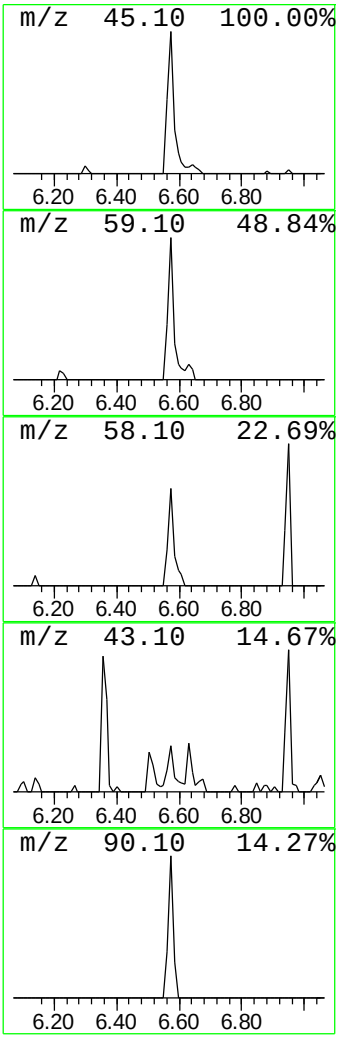
****

Peak Number 3 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	3.20 ng	48147	1,4-Dichlorobenzene-d4	7.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	83
2	Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	9
3	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	9
4	Acetic acid, hydroxy-, methyl ester	90	C3H6O3	000096-35-5	7
5	Ethane, 1,2-dimethoxy-	90	C4H10O2	000110-71-4	5





Library Search Compound Report

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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
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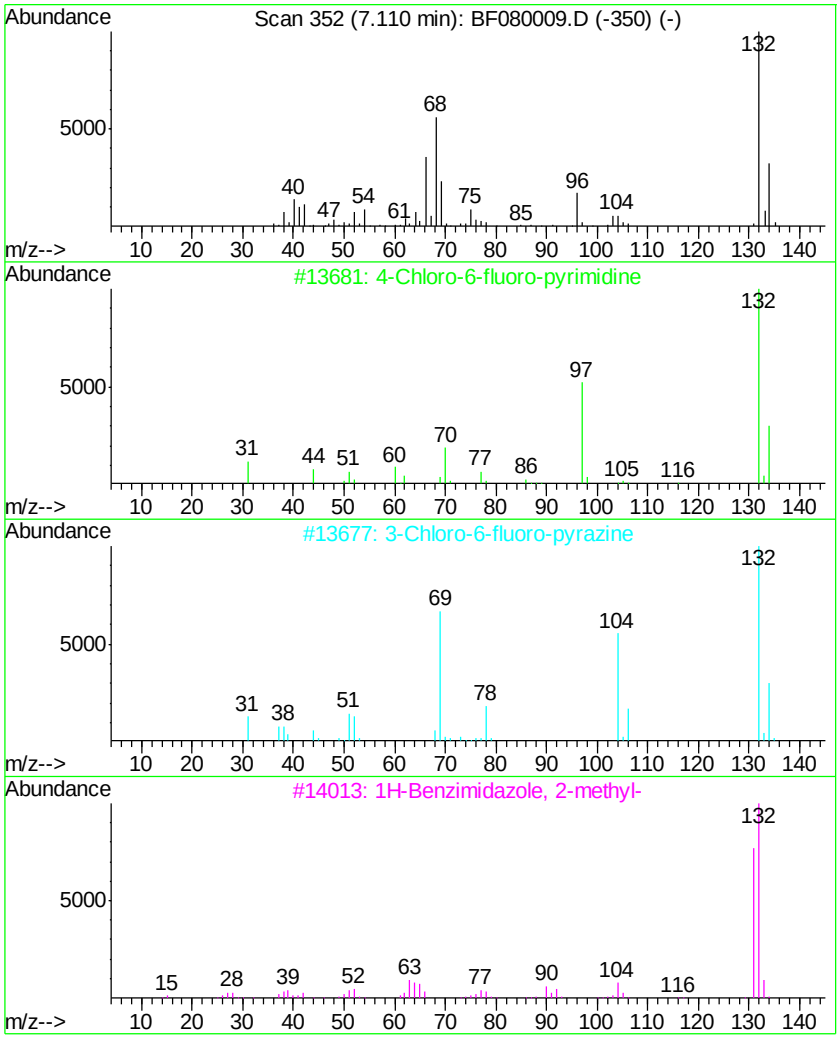
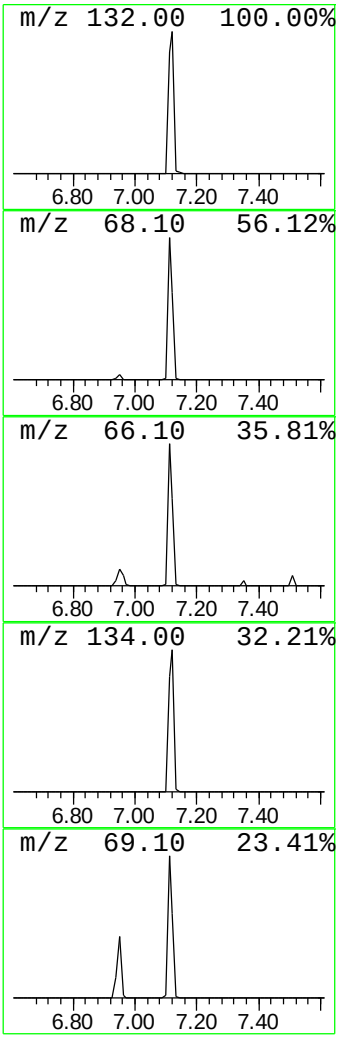
****

Peak Number 4 unknown7.11 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.11	35.39 ng	533030	1,4-Dichlorobenzene-d4	7.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
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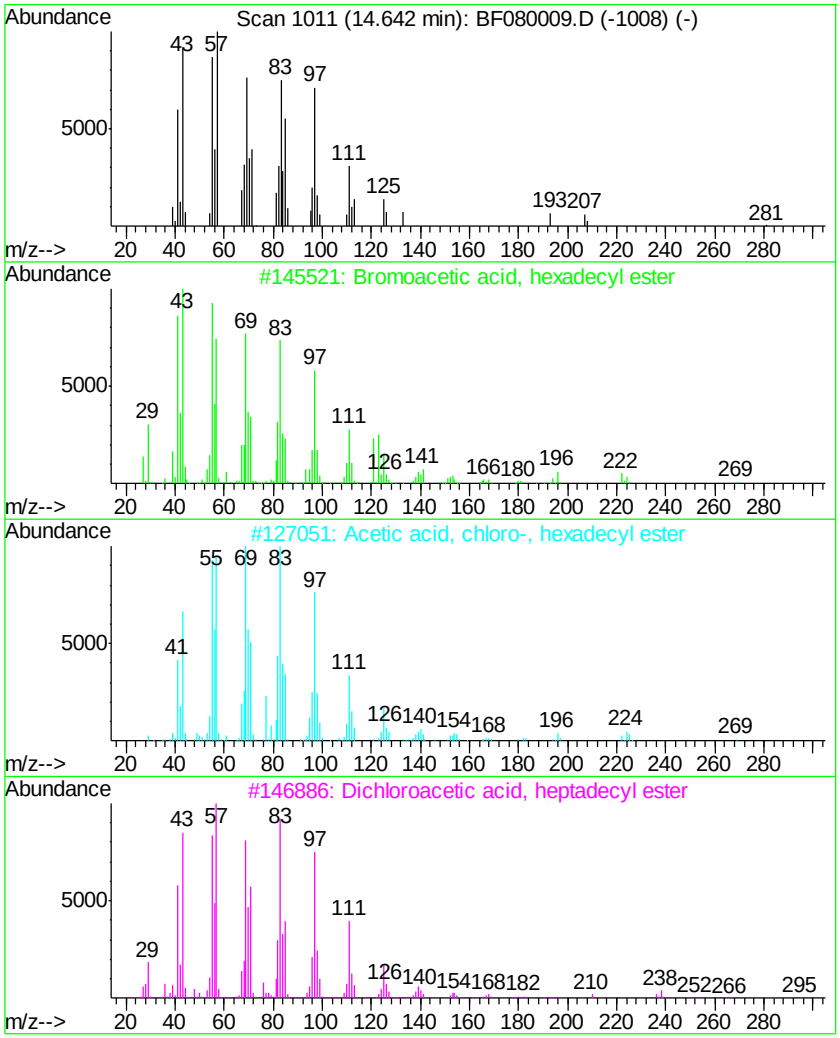
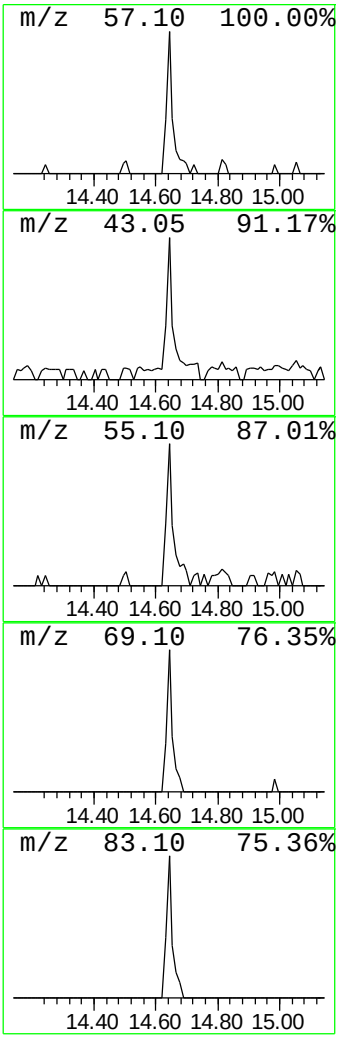
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Bromoacetic acid, hexadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.78 ng	75662	Chrysene-d12	14.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	1-Nonadecene	266	C19H38	018435-45-5	90
5	1-Nonadecanol	284	C19H40O	001454-84-8	90





Tentatively Identified Compound (LSC) summary

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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...	5.57	8.8	ng	132111	1	7.35	301216	20.0
Ethanol, 2-(2-met...	6.57	3.2	ng	48147	1	7.35	301216	20.0
unknown7.11	7.11	35.4	ng	533030	1	7.35	301216	20.0
Bromoacetic acid,...	14.64	2.8	ng	75662	5	14.86	544979	20.0