LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032116\
Data File : BF085650.D
Acq On : 22 Mar 2016 6:40
Operator : UM/SJ
Sample : H1837-06
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-11B

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-BF031816.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	2.401	8	10	19	rVB2	16201	43133	1.29%	0.150%
2	2.664	31	33	38	rVB	123387	168399	5.02%	0.584%
3	3.441	98	101	108	rBV	35171	67238	2.01%	0.233%
4	4.390	181	184	187	rBV	1539011	2249897	67.10%	7.802%
5	4.596	200	202	207	rVB	31486	43306	1.29%	0.150%
6	5.041	238	241	247	rBV	388756	649890	19.38%	2.254%
7	5.453	274	277	279	rBV	2613380	2733508	81.53%	9.479%
8	6.481	364	367	369	rBV	2365828	2753292	82.12%	9.548%
9	6.607	376	378	381	rVB	2438815	2989499	89.16%	10.367%
10	6.836	396	398	401	rBV	552360	751144	22.40%	2.605%
11	6.996	410	412	415	rBV	2366027	2450746	73.09%	8.498%
12	7.407	445	448	450	rBV	1927686	1973759	58.87%	6.844%
13	8.127	508	511	512	rBV	1157151	1066697	31.81%	3.699%
14	8.836	571	573	576	rBV	61966	59206	1.77%	0.205%
15	9.202	602	605	608	rBV	3276788	3352852	100.00%	11.627%
16	9.876	662	664	666	rBV	1025224	950230	28.34%	3.295%
17	9.910	666	667	669	rVB	101181	75368	2.25%	0.261%
18	10.665	730	733	736	rBV	1625039	1716253	51.19%	5.951%
19	11.362	792	794	796	rBV	901933	817633	24.39%	2.835%
20	12.951	930	933	935	rBV	2374192	2668235	79.58%	9.253%
21	13.991	1022	1024	1027	rBV	637974	635215	18.95%	2.203%
22	15.420	1146	1149	1155	rBV	494539	621923	18.55%	2.157%

Sum of corrected areas: 28837423

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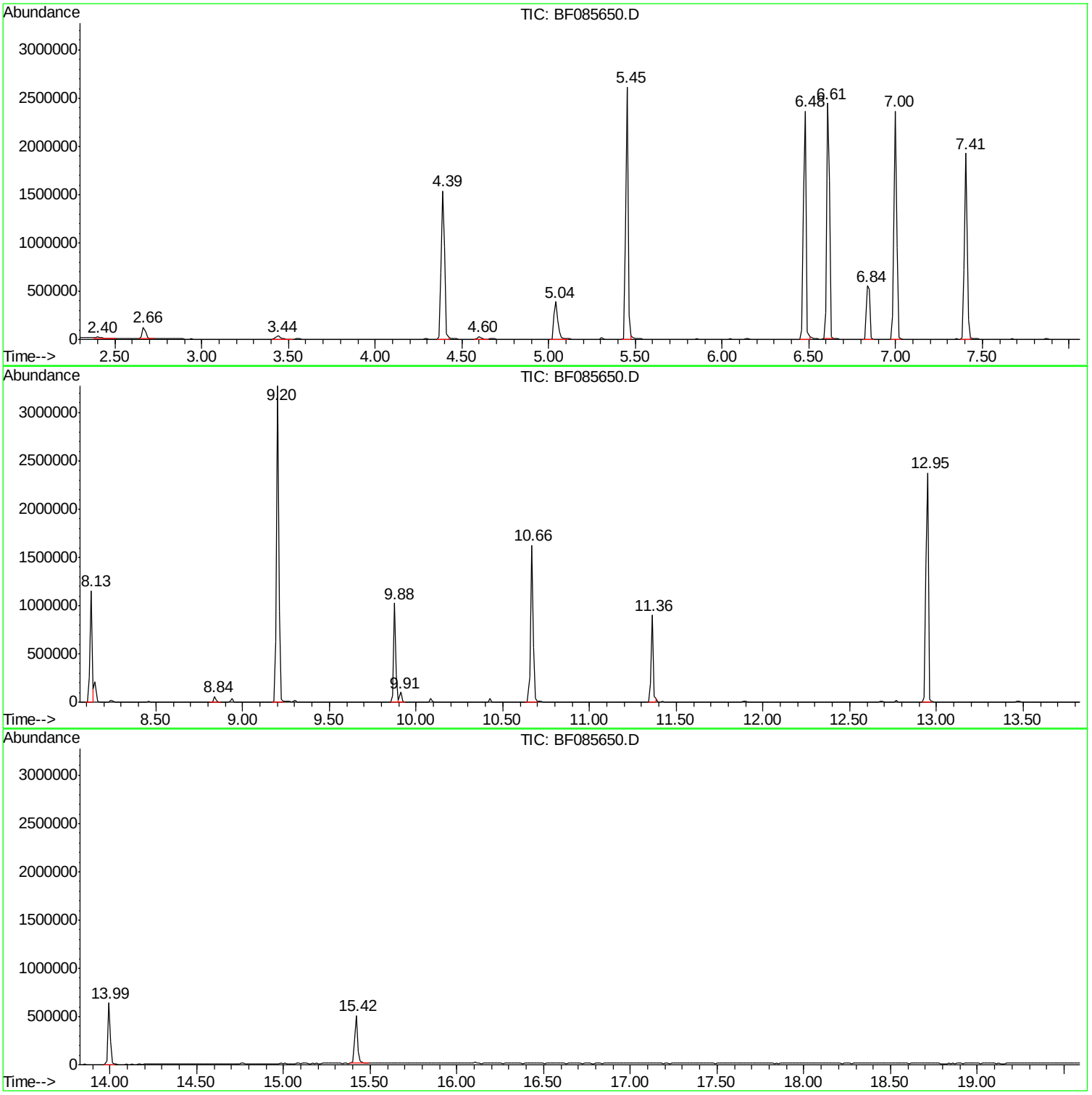
ClientSampleId :
TRACK-D-GRID-11B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.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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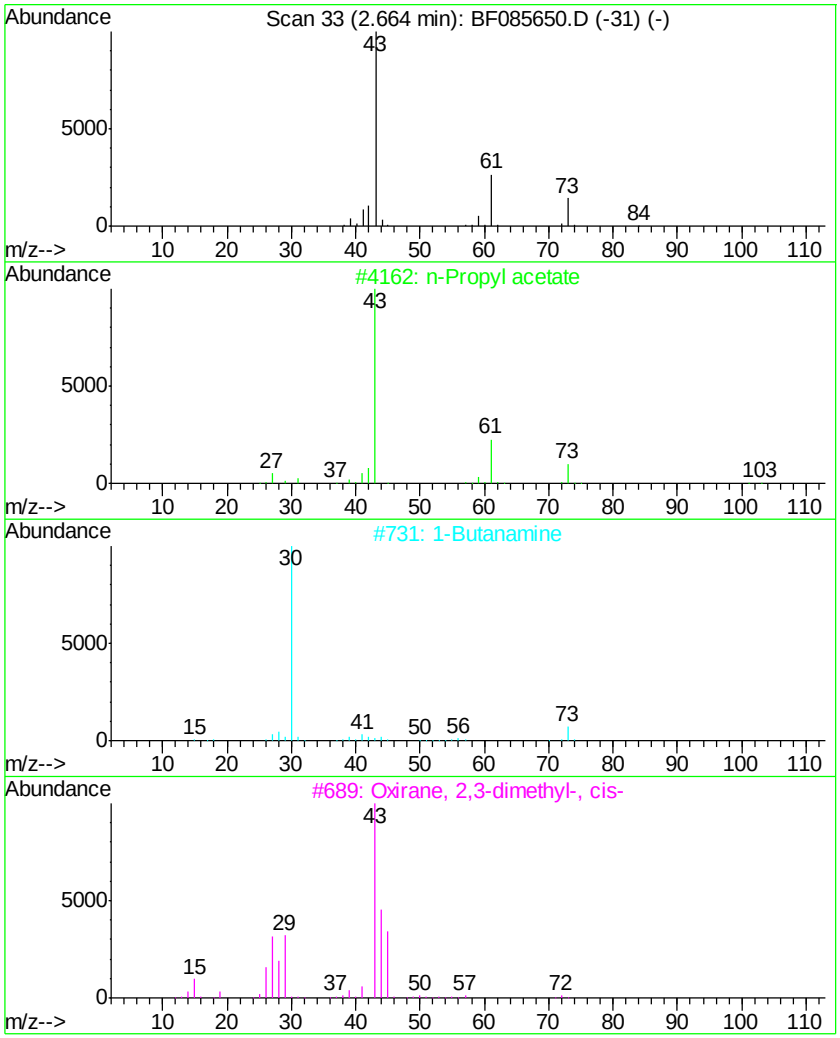
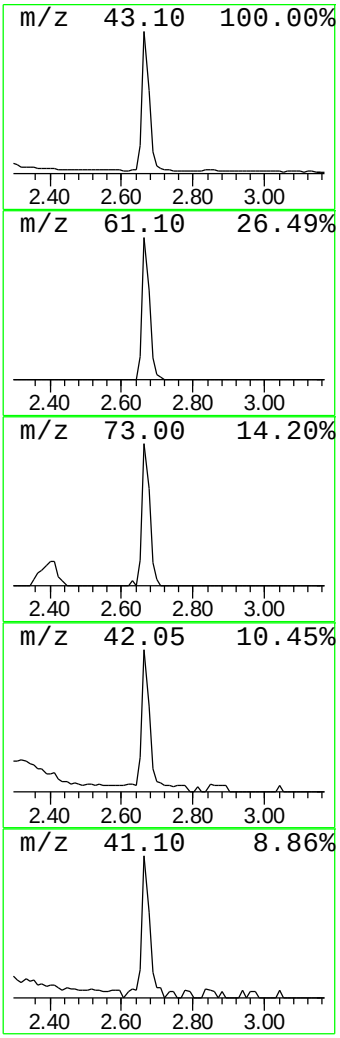
Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.66	4.48 ng	168399	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	9
3	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	4





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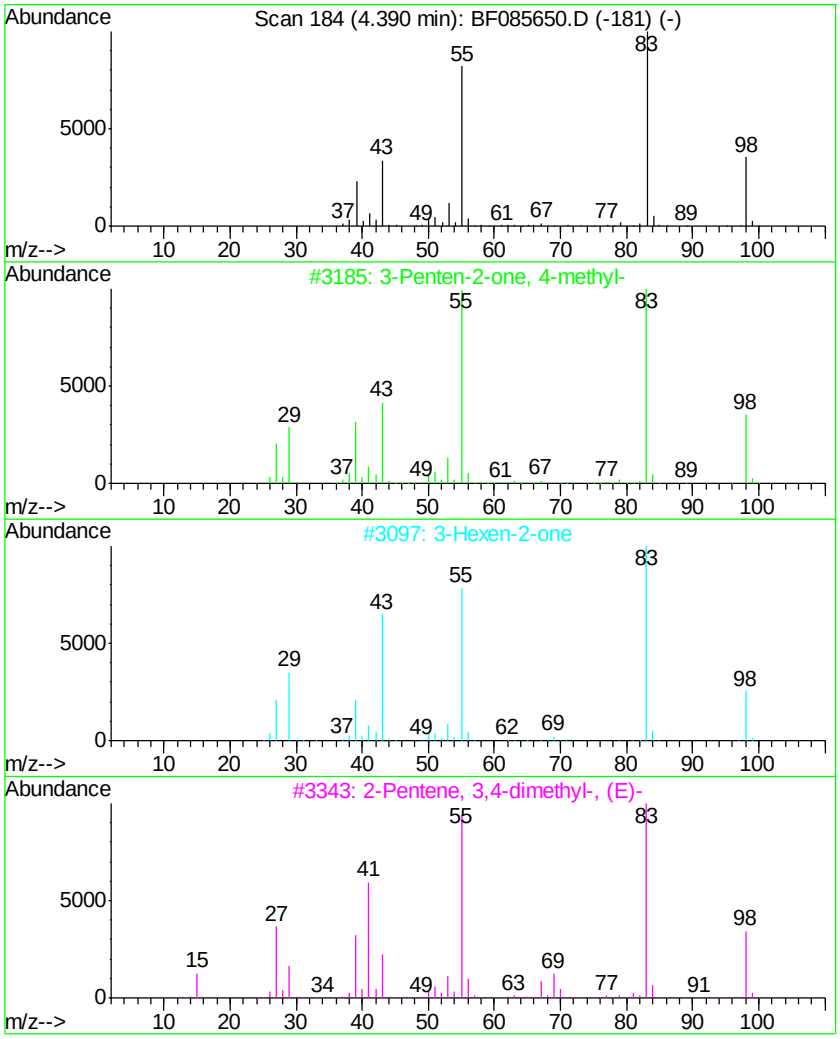
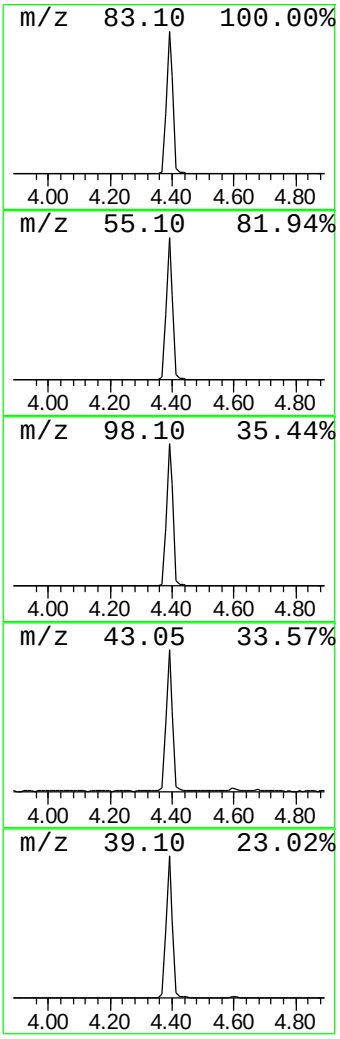
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	59.91 ng	2249900	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





Library Search Compound Report

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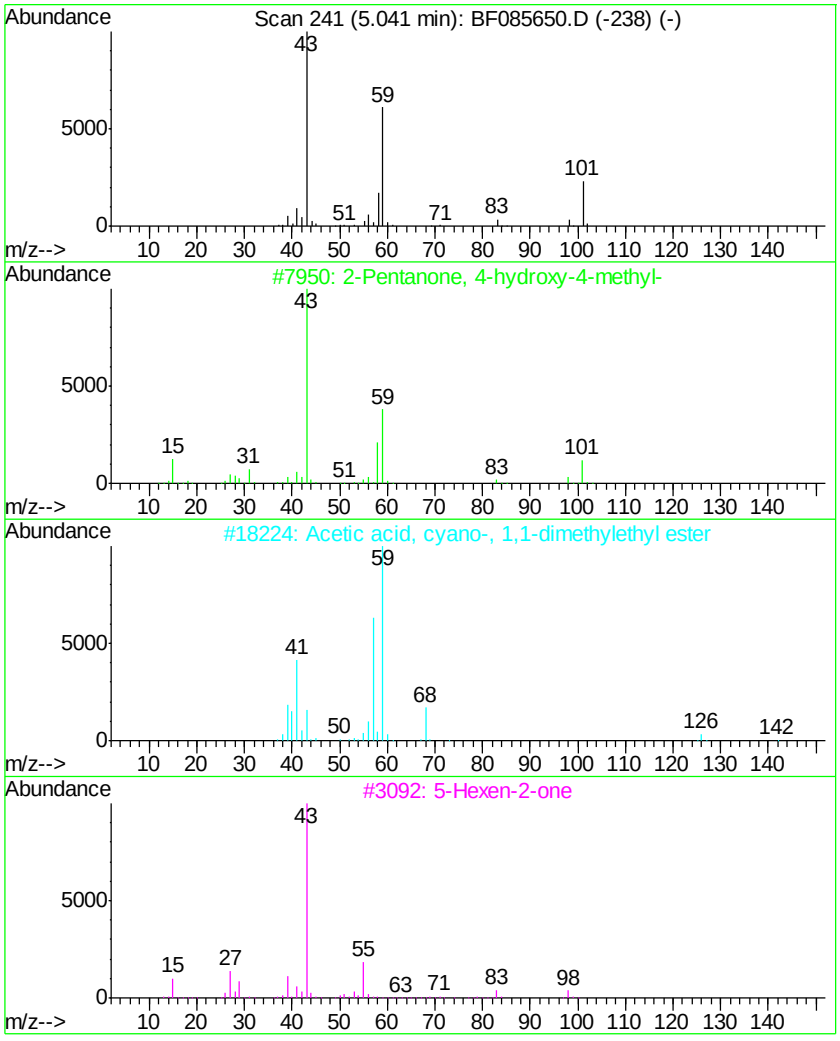
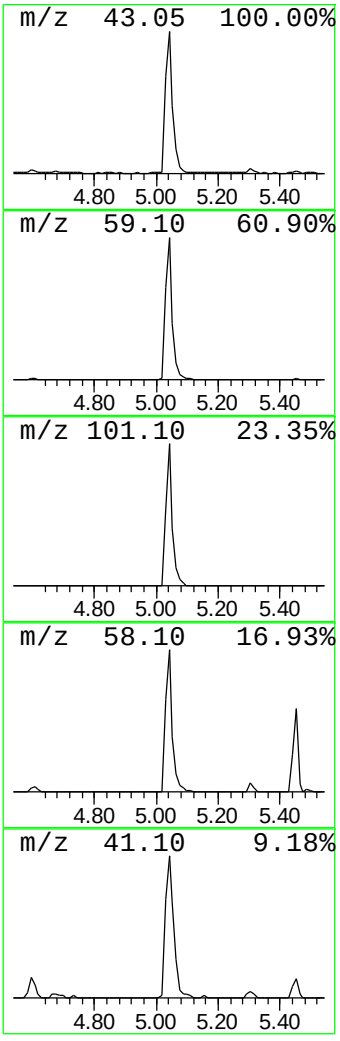
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	17.30 ng	649890	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_F
ClientSampleId : TRACK-D-GRID-11B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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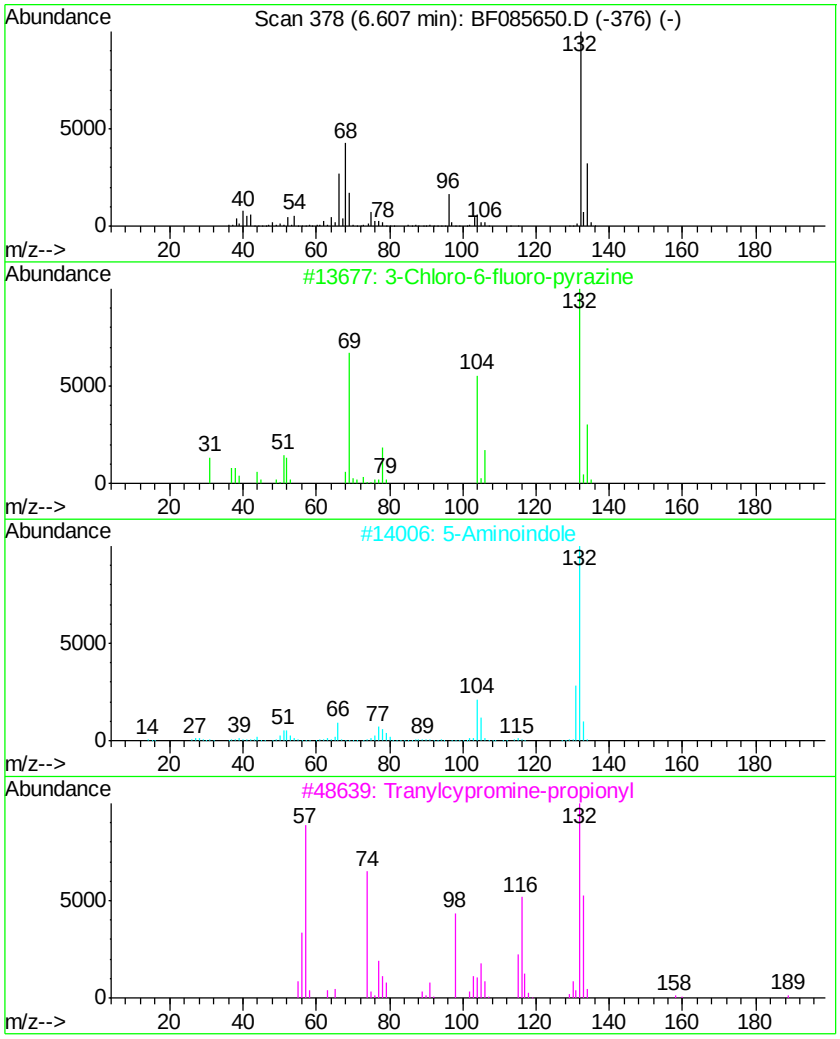
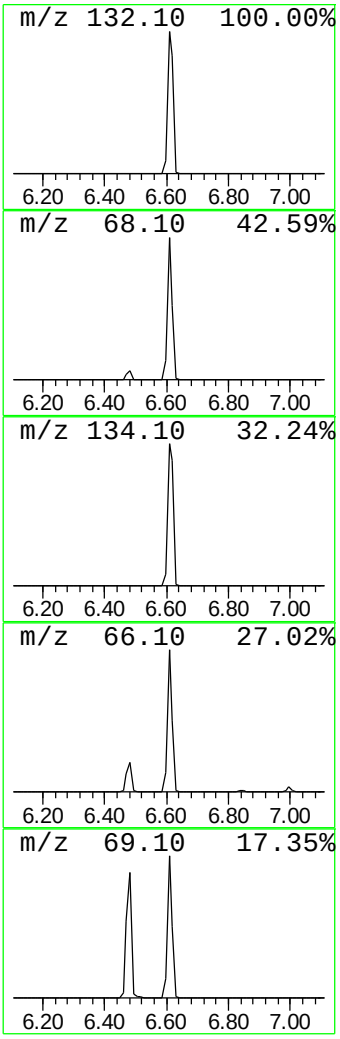
Peak Number 4 3-Chloro-6-fluoro-pyrazine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	79.60 ng	2989500	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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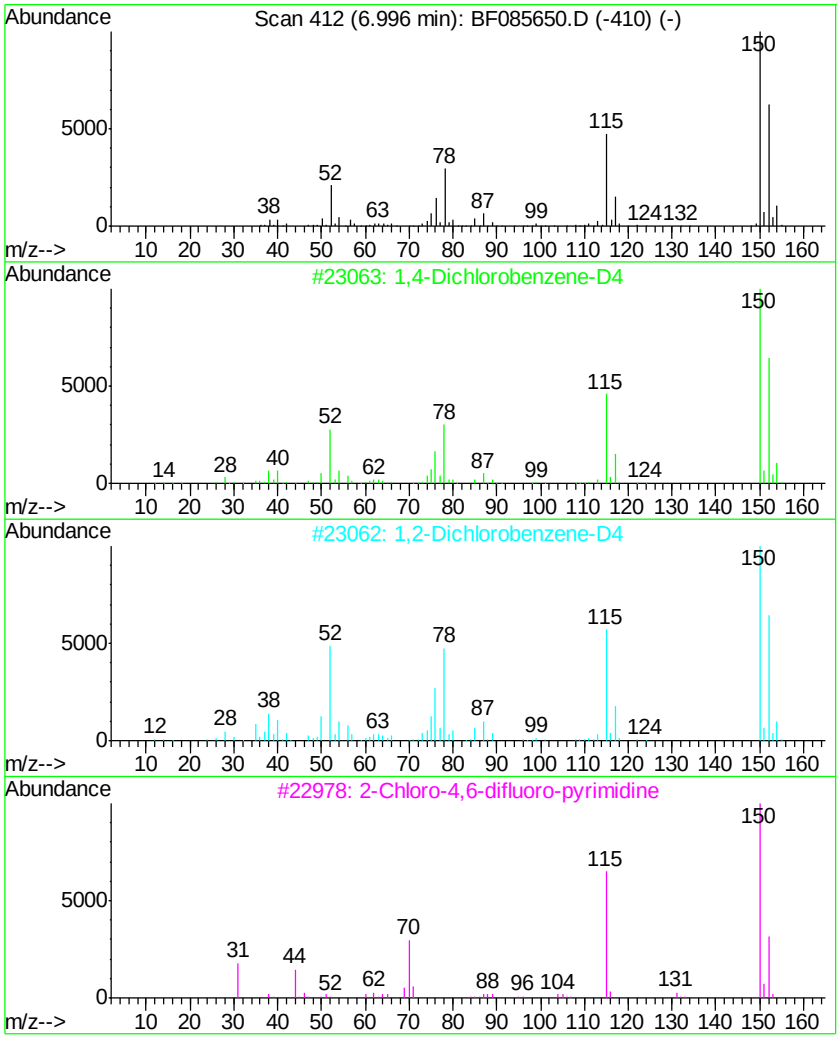
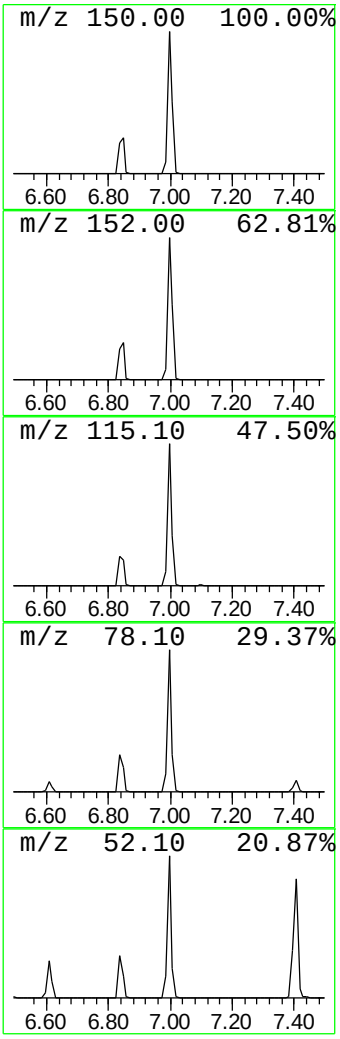
Peak Number 5 1,4-Dichlorobenzene-D4 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.00	65.25 ng	2450750	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	94
2	1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	91
3	2-Chloro-4,6-difluoro-pyrimidine	150	C4HClF2N2	038953-30-9	38
4	9-Borabicyclo[3.3.1]nonane, 9-et...	150	C10H19B	052102-17-7	38
5	2,3,5-Tri-O-p-nitrobenzoyl-.alph...	606	C27H18N4O13	1000129-91-5	10





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.66	4.5	ng	168399	1	6.85	751144	20.0
3-Penten-2-one, 4...	4.39	59.9	ng	2249900	1	6.85	751144	20.0
2-Pentanone, 4-hy...	5.04	17.3	ng	649890	1	6.85	751144	20.0
3-Chloro-6-fluoro...	6.61	79.6	ng	2989500	1	6.85	751144	20.0
1,4-Dichlorobenze...	7.00	65.3	ng	2450750	1	6.85	751144	20.0