LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032816\
Data File : BF085830.D
Acq On : 29 Mar 2016 4:45
Operator : UM/SJ
Sample : H1942-12
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-932SCOMP

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-BF032416.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	5	10	18	rVB2	10957	44548	1.35%	0.152%
2	2.618	27	29	41	rVB	111436	168849	5.13%	0.576%
3	3.373	92	95	103	rBV	70741	149839	4.56%	0.511%
4	4.356	178	181	192	rBV	1611225	2130042	64.77%	7.264%
5	4.561	197	199	203	rVV	26328	36458	1.11%	0.124%
6	4.641	203	206	208	rVB	42016	50619	1.54%	0.173%
7	5.007	236	238	252	rBV	315679	536871	16.32%	1.831%
8	5.430	272	275	277	rBV	2292870	2864121	87.09%	9.767%
9	6.459	362	365	367	rBV	2373414	2701148	82.13%	9.212%
10	6.584	373	376	379	rBV	2819431	2757389	83.84%	9.403%
11	6.813	394	396	399	rBV	793141	699110	21.26%	2.384%
12	6.973	408	410	412	rBV	2741502	2494364	75.84%	8.506%
13	7.327	438	441	443	rBV	79672	93795	2.85%	0.320%
14	7.385	443	446	448	rBV	2078588	2097981	63.79%	7.155%
15	8.105	506	509	513	rBV2	683487	1169139	35.55%	3.987%
16	8.813	569	571	574	rBV	83441	74199	2.26%	0.253%
17	8.916	577	580	582	rBV	41893	40254	1.22%	0.137%
18	9.179	600	603	605	rBV	3430798	3288794	100.00%	11.216%
19	9.853	660	662	664	rBV	1044604	916726	27.87%	3.126%
20	9.888	664	665	667	rVB	96808	71294	2.17%	0.243%
21	10.059	678	680	683	rBV	42761	38945	1.18%	0.133%
22	10.402	709	710	713	rVB	50590	39538	1.20%	0.135%
23	10.642	729	731	734	rBV	1711608	1837327	55.87%	6.266%
24	11.339	790	792	793	rBV	952938	847682	25.77%	2.891%
25	11.362	793	794	796	rVB	57032	42018	1.28%	0.143%
26	12.745	913	915	918	rBV	68058	61108	1.86%	0.208%
27	12.928	928	931	933	rBV	2539603	2974542	90.44%	10.144%
28	13.968	1020	1022	1025	rBV	537195	539954	16.42%	1.841%
29	15.385	1144	1146	1153	rBV	344704	482277	14.66%	1.645%
30	16.985	1284	1286	1290	rBV5	38289	74232	2.26%	0.253%

Sum of corrected areas: 29323163

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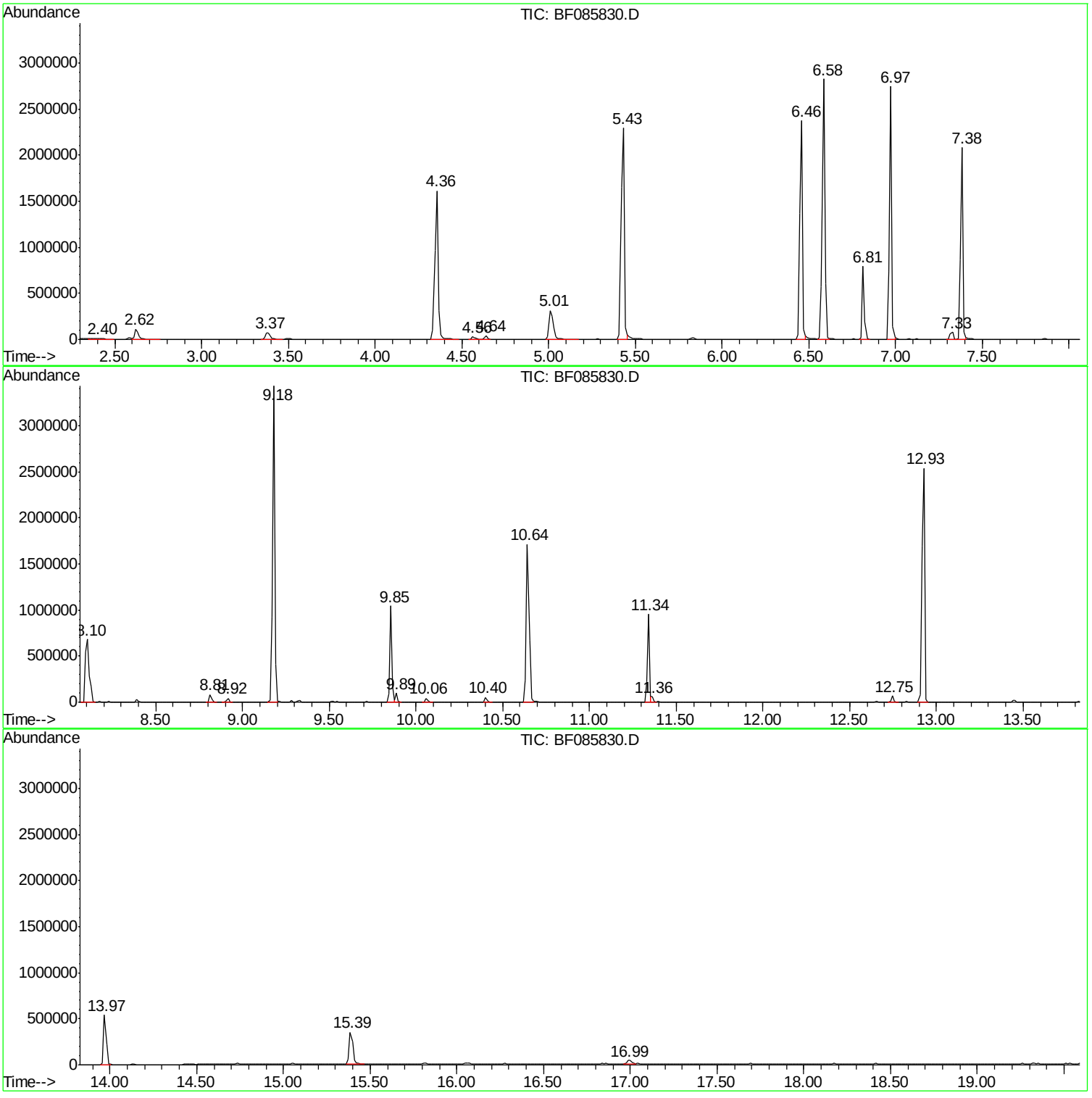
Instrument :
BNA_F
ClientSampleId :
B-932SCOMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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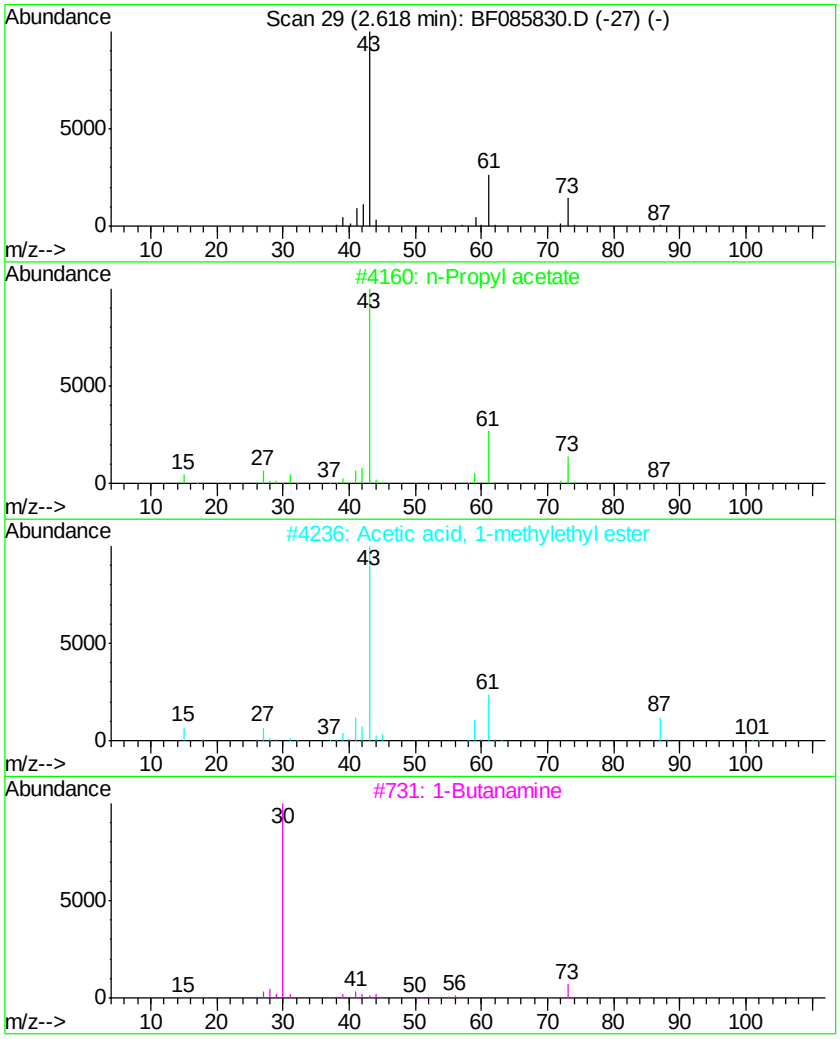
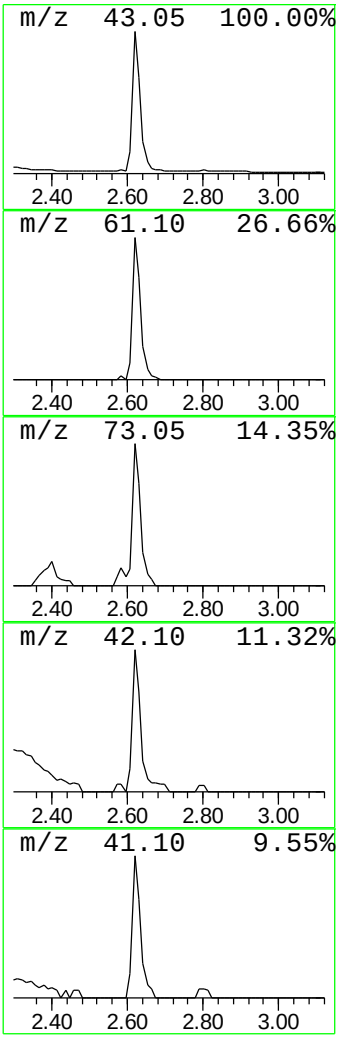
Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.62	4.83 ng	168849	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	38
3	1-Butanamine	73	C4H11N	000109-73-9	9
4	Pentane	72	C5H12	000109-66-0	5
5	Isobutylamine	73	C4H11N	000078-81-9	4





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Instrument : BNA_F
ClientSampleId : B-932SCOMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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TIC Integration Parameters: LSCINT.P

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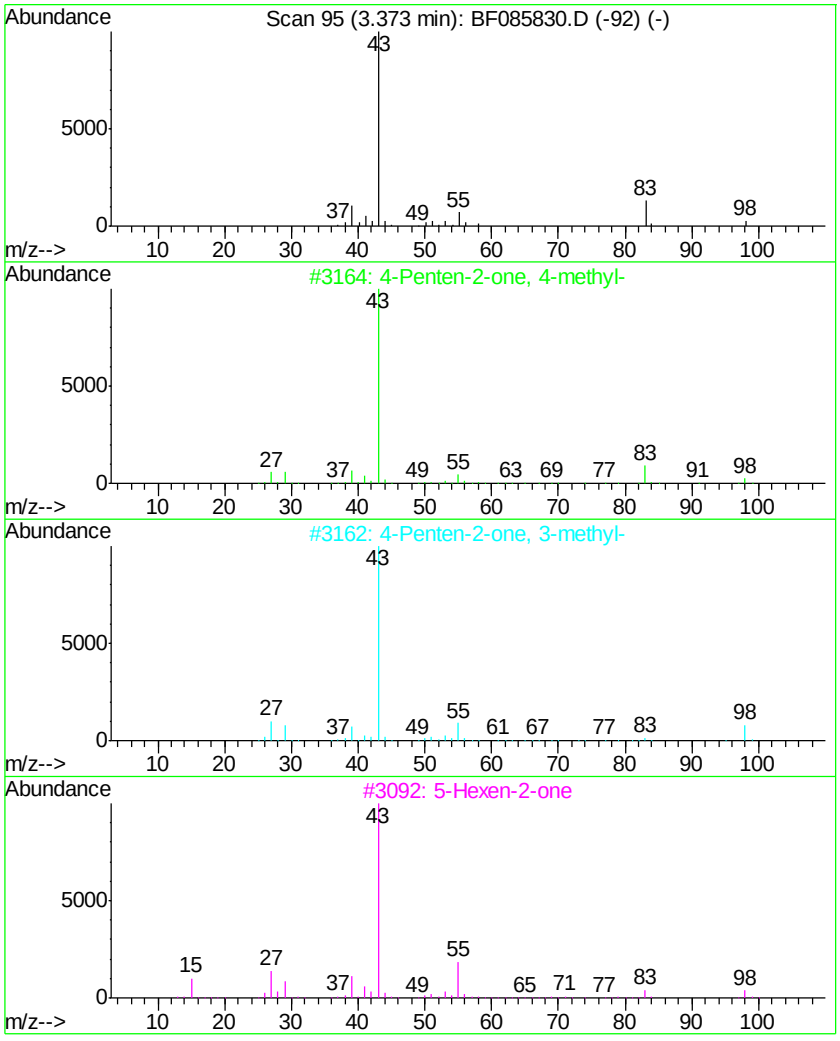
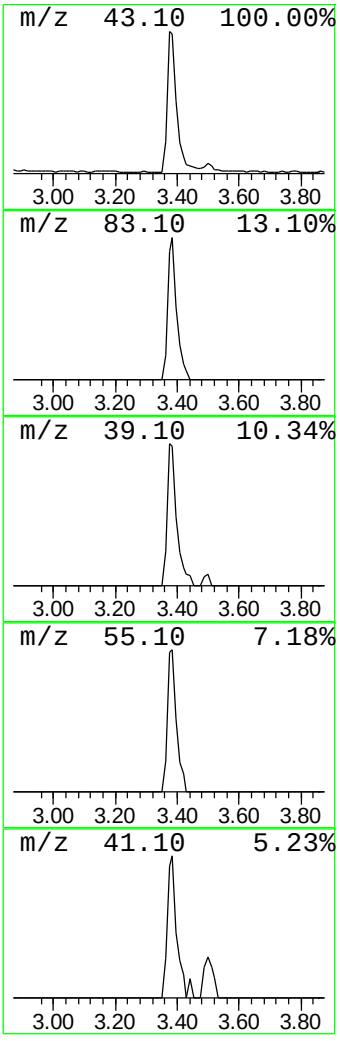
Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.37	4.29 ng	149839	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
3	5-Hexen-2-one	98	C6H10O	000109-49-9	50
4	2-Vinylethyl acetate	114	C6H10O2	001576-84-7	23
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	23





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Operator : UM/SJ
Sample : H1942-12
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-932SCOMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.M
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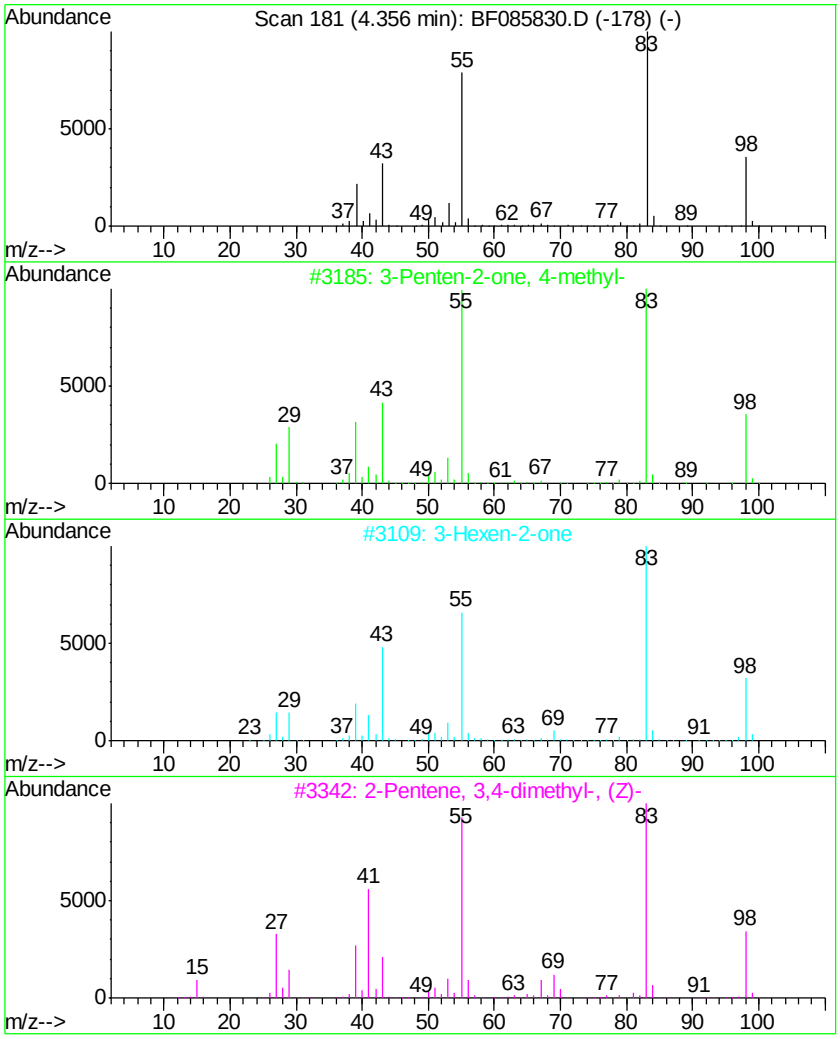
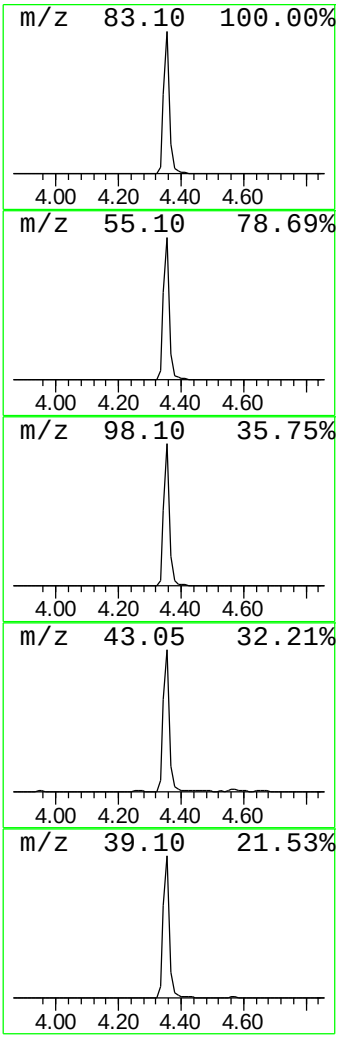
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	60.94 ng	2130040	1,4-Dichlorobenzene-d4	6.81

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-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78





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Instrument : BNA_F
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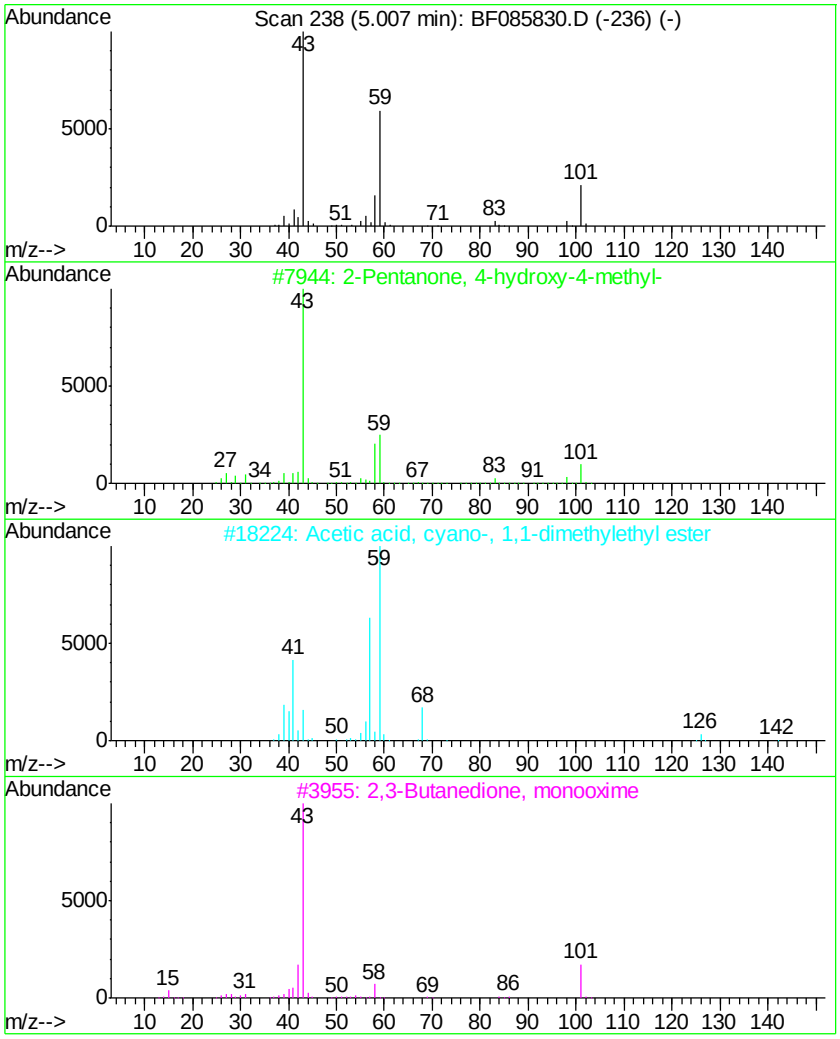
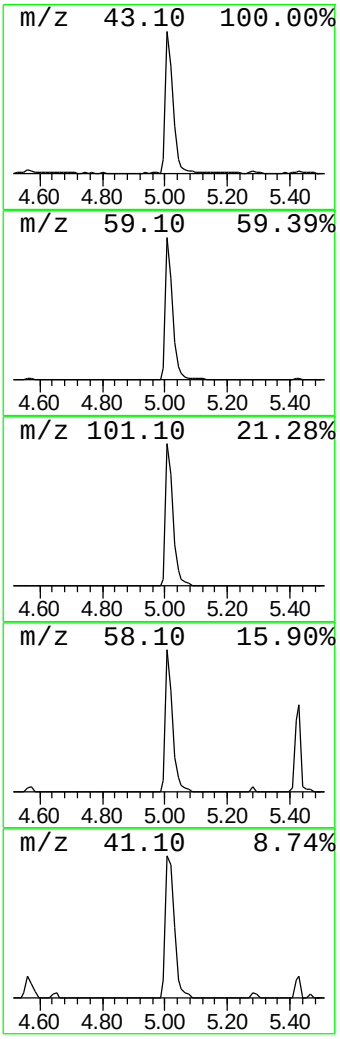
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	15.36 ng	536871	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	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Instrument : BNA_F
ClientSampleId : B-932SCOMP

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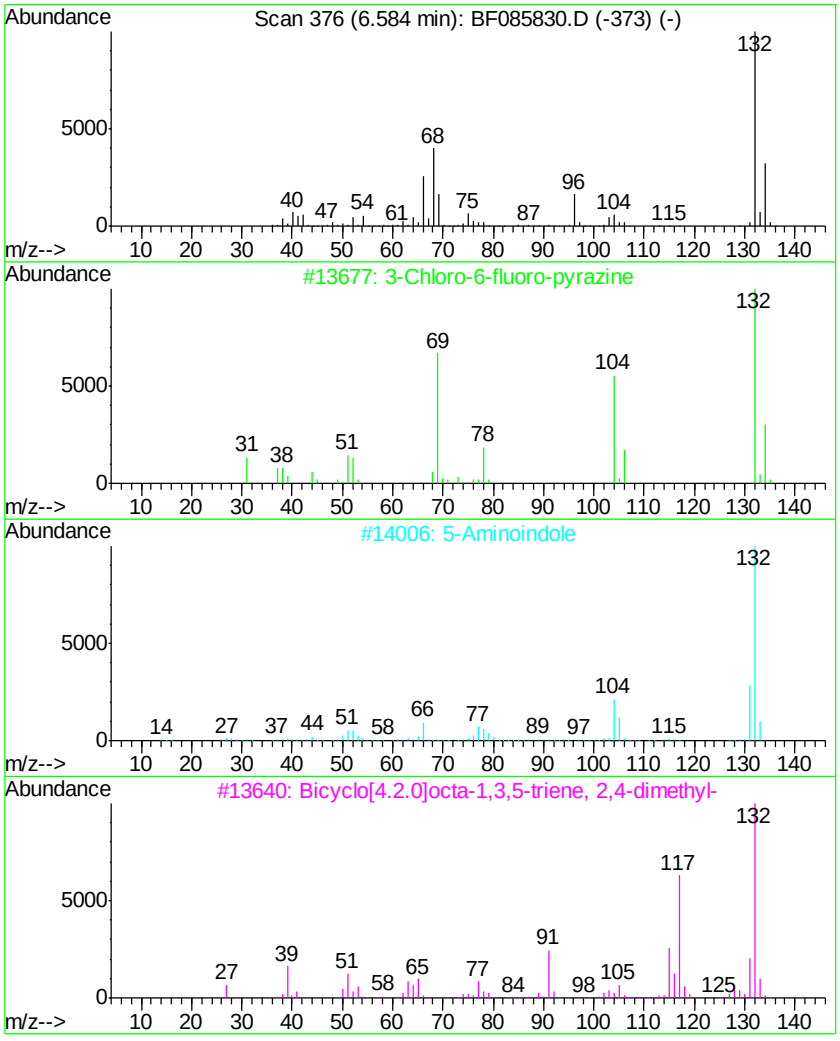
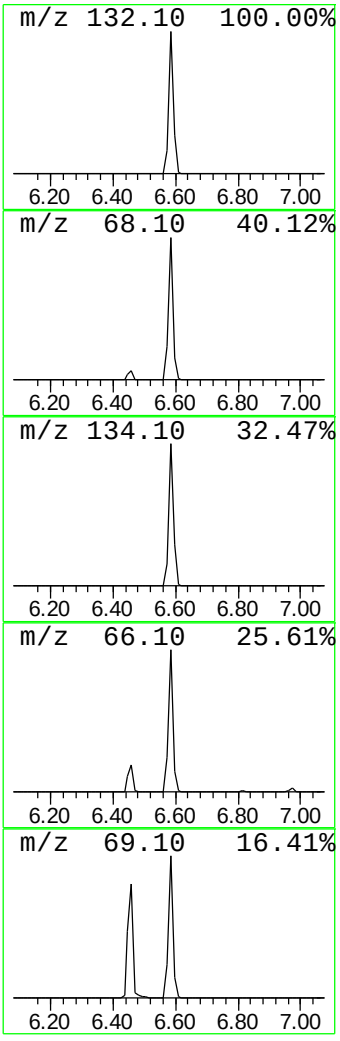
Peak Number 5 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	78.88 ng	2757390	1,4-Dichlorobenzene-d4	6.81

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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TIC Library : C:\DATABASE\NIST02.L
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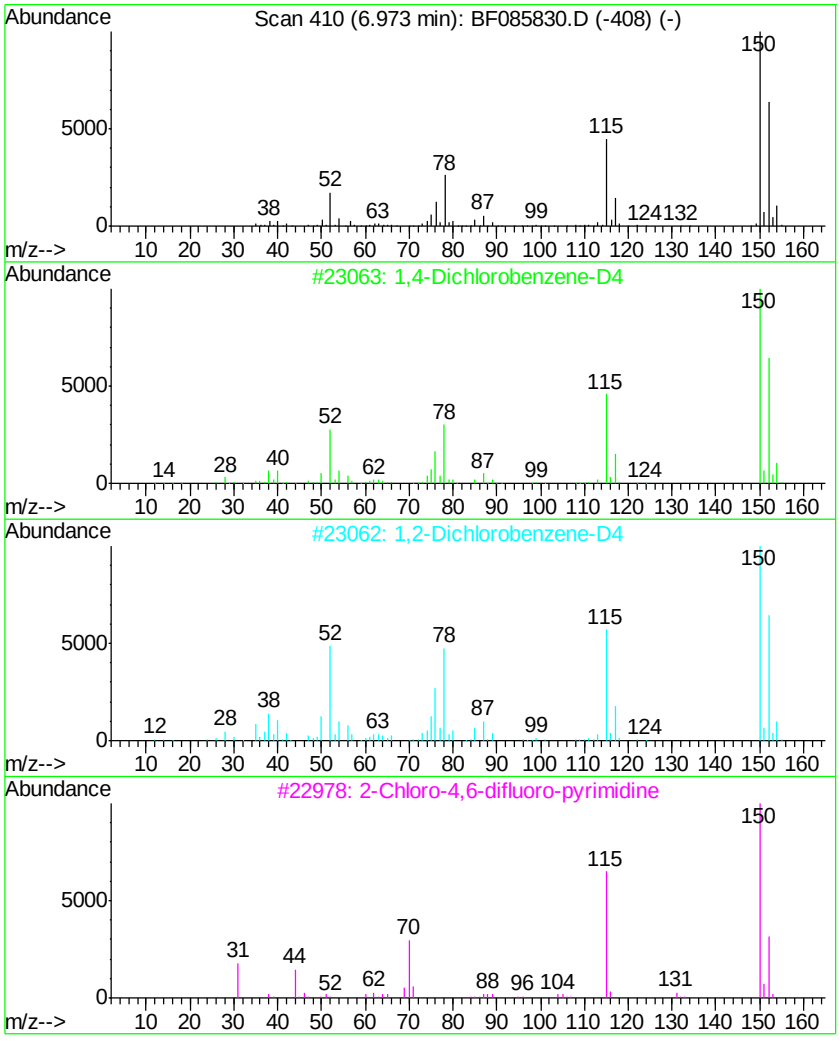
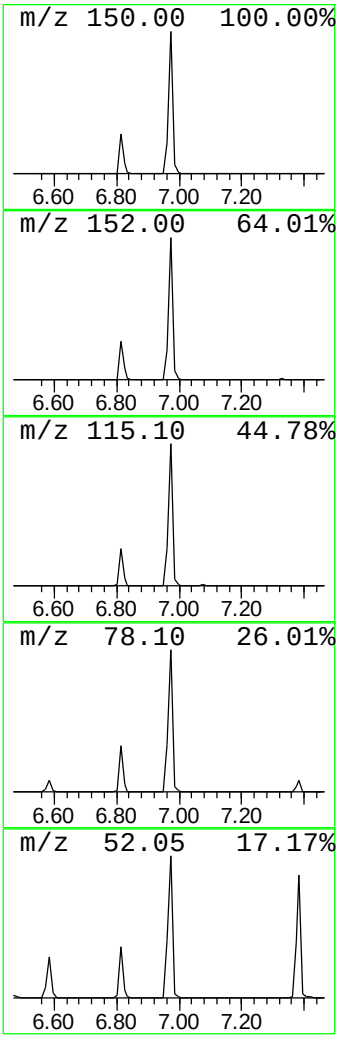
Peak Number 6 2-Chloro-4,6-difluoro-pyrim... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.97	71.36 ng	2494360	1,4-Dichlorobenzene-d4	6.81

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	50
4	9-Borabicyclo[3.3.1]nonane, 9-et...	150	C10H19B	052102-17-7	22
5	But-2-yne-1,4-diol, o,o'-bis(3-n...	384	C18H12N2O8	055709-58-5	17





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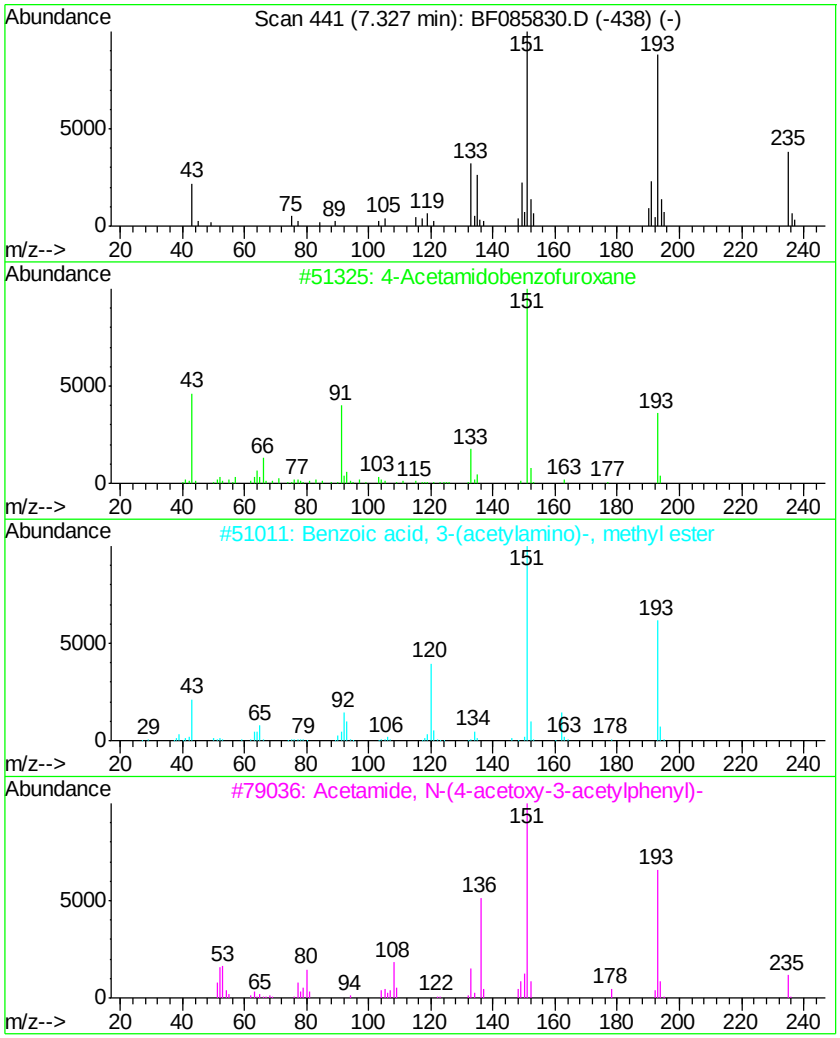
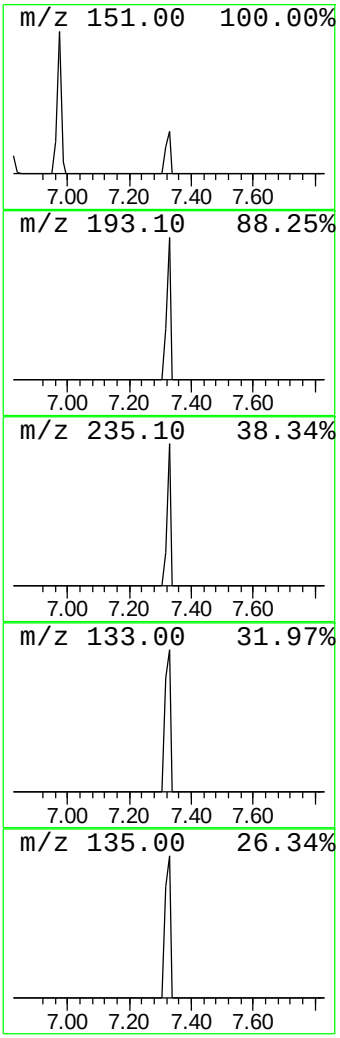
Peak Number 7 unknown7.33 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	2.68 ng	93795	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Acetamidobenzofuroxane	193	C8H7N3O3	010199-72-1	47
2	Benzoic acid, 3-(acetylamino)-, ...	193	C10H11NO3	052189-36-3	43
3	Acetamide, N-(4-acetoxy-3-acetyl...	235	C12H13NO4	1000280-82-8	40
4	Acetamide, N-9-phenanthrenyl-	235	C16H13NO	004235-09-0	38
5	1-Acetyl-5-methyl-3-(5-nitro-2-f...	235	C10H9N3O4	016239-91-1	35





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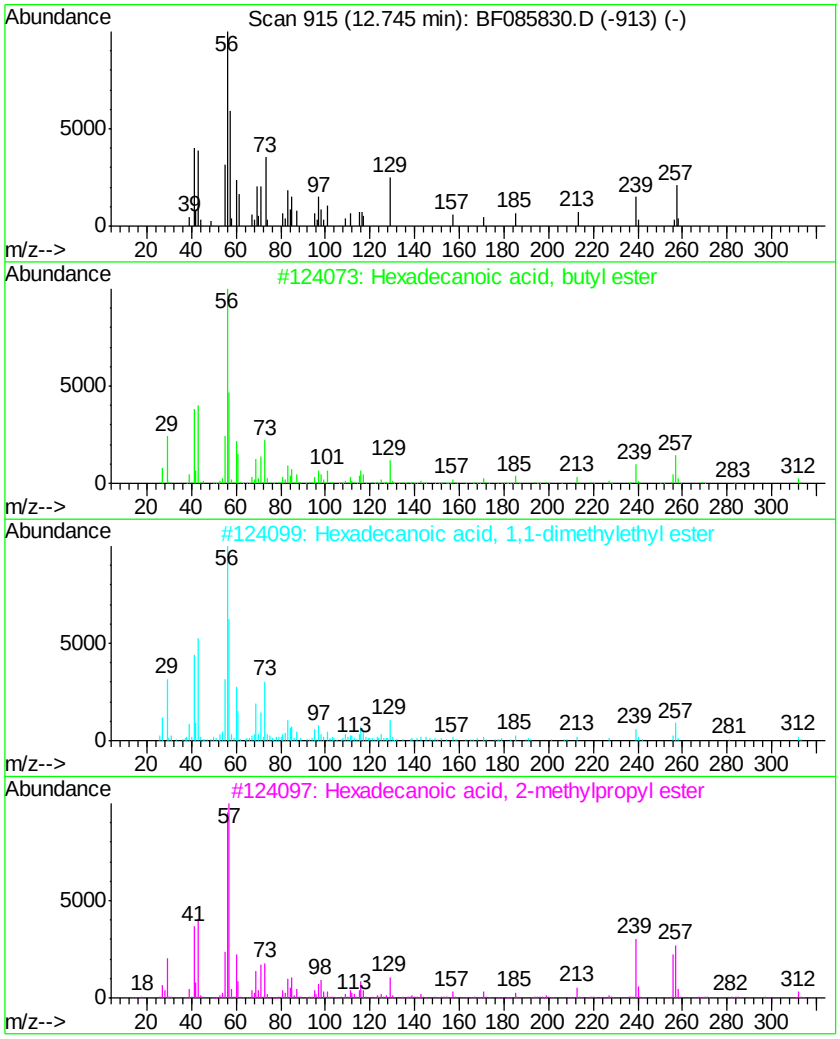
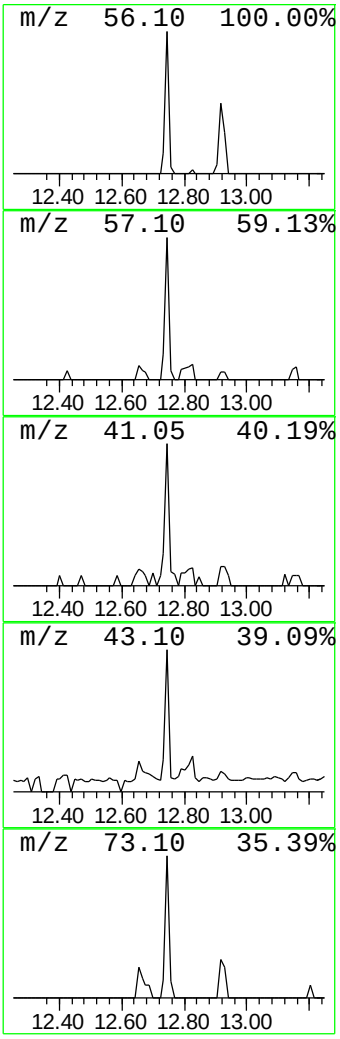
Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	2.26 ng	61108	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	45
4	Nipecotic acid	129	C6H11NO2	000498-95-3	38
5	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	27





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032416.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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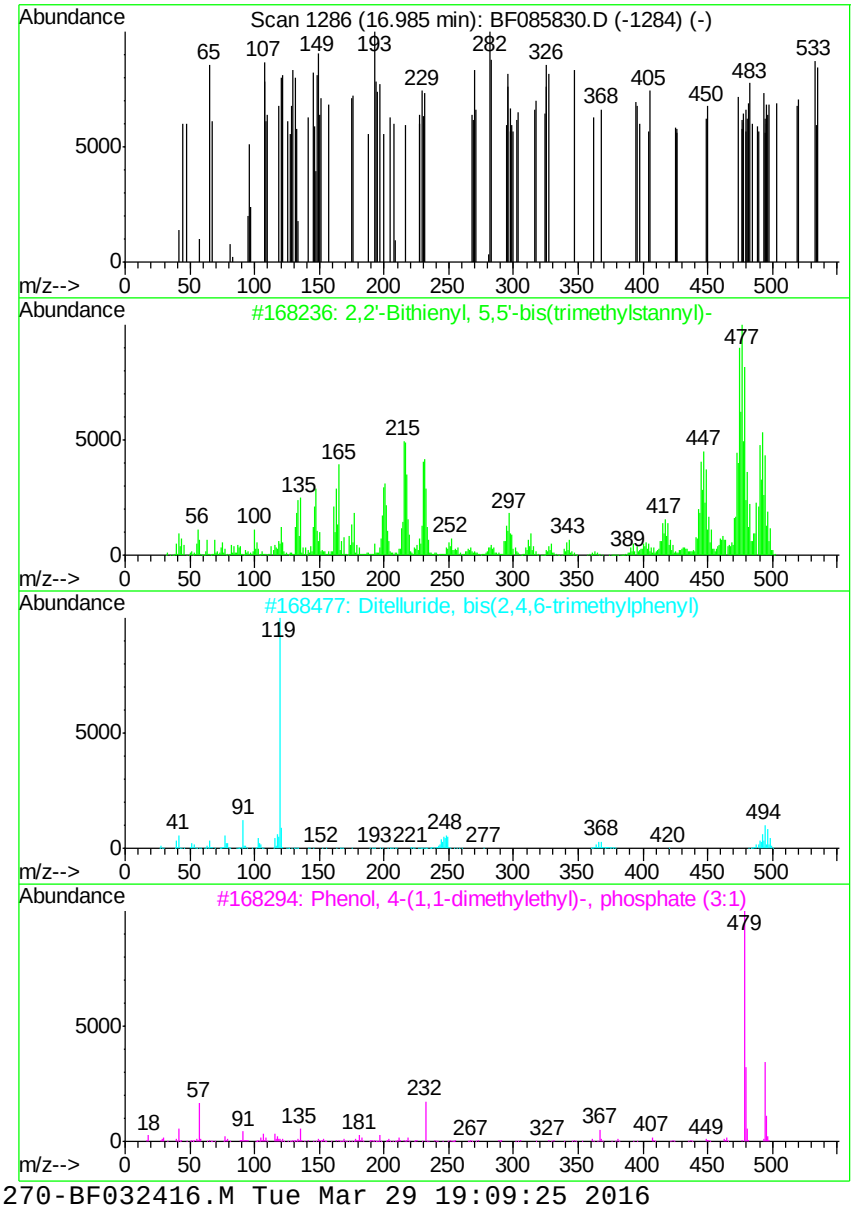
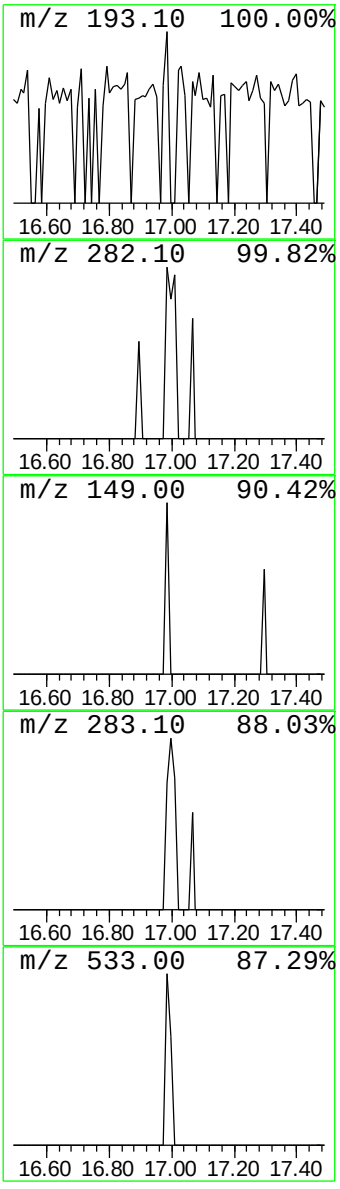
Peak Number 9 2,2'-Bithienyl, 5,5'-bis(tr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.99	3.08 ng	74232	Perylene-d12	15.39

Hit# of 3	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-Bithienyl, 5,5'-bis(trimeth...	494	C14H22S2Sn2	143367-56-0	53
2	Ditelluride, bis(2,4,6-trimethyl...	498	C18H22Te2	092720-46-2	2
3	Phenol, 4-(1,1-dimethylethyl)-, ...	494	C30H39O4P	000078-33-1	1





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.62	4.8	ng	168849	1	6.81	699110	20.0
4-Penten-2-one, 4...	3.37	4.3	ng	149839	1	6.81	699110	20.0
3-Penten-2-one, 4...	4.36	60.9	ng	2130040	1	6.81	699110	20.0
2-Pentanone, 4-hy...	5.01	15.4	ng	536871	1	6.81	699110	20.0
unknown6.58	6.58	78.9	ng	2757390	1	6.81	699110	20.0
2-Chloro-4,6-difl...	6.97	71.4	ng	2494360	1	6.81	699110	20.0
unknown7.33	7.33	2.7	ng	93795	1	6.81	699110	20.0
Hexadecanoic acid...	12.75	2.3	ng	61108	5	13.97	539954	20.0
2,2'-Bithienyl, 5...	16.99	3.1	ng	74232	6	15.39	482277	20.0