LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087032.D
Acq On : 14 May 2016 21:08
Operator : UM/SJ
Sample : PB90536BL
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB90536BL

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-BF050916.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	1.735	11	13	45	rVB	1883212	3565494	73.93%	8.206%
2	4.021	211	213	224	rBV	320643	567965	11.78%	1.307%
3	4.753	274	277	291	rBV	1288600	2133287	44.23%	4.910%
4	5.210	315	317	320	rBV	3523303	3854067	79.91%	8.870%
5	5.610	350	352	361	rVB	68254	78523	1.63%	0.181%
6	6.284	408	411	413	rBV	3233993	4477850	92.84%	10.306%
7	6.387	417	420	422	rBV	4094463	4433892	91.93%	10.205%
8	6.604	437	439	442	rBV	714476	913191	18.93%	2.102%
9	6.764	450	453	456	rBV	3372696	3155656	65.43%	7.263%
10	7.187	487	490	492	rBV	2660982	3013891	62.49%	6.936%
11	7.896	550	552	565	rBV	1233113	1226144	25.42%	2.822%
12	8.982	644	647	649	rBV	3988597	4823037	100.00%	11.100%
13	9.645	702	705	708	rBV	1393467	1301324	26.98%	2.995%
14	10.433	771	774	777	rBV	2578500	2649094	54.93%	6.097%
15	11.119	832	834	837	rBV	1190136	1262372	26.17%	2.905%
16	12.548	956	959	961	rBV	76618	102329	2.12%	0.236%
17	12.708	970	973	976	rBV	4036676	4032738	83.61%	9.281%
18	13.245	1018	1020	1022	rBV	79892	67358	1.40%	0.155%
19	13.748	1061	1064	1076	rBV	992078	974738	20.21%	2.243%
20	15.108	1180	1183	1192	rBV	667395	817143	16.94%	1.881%

Sum of corrected areas: 43450093

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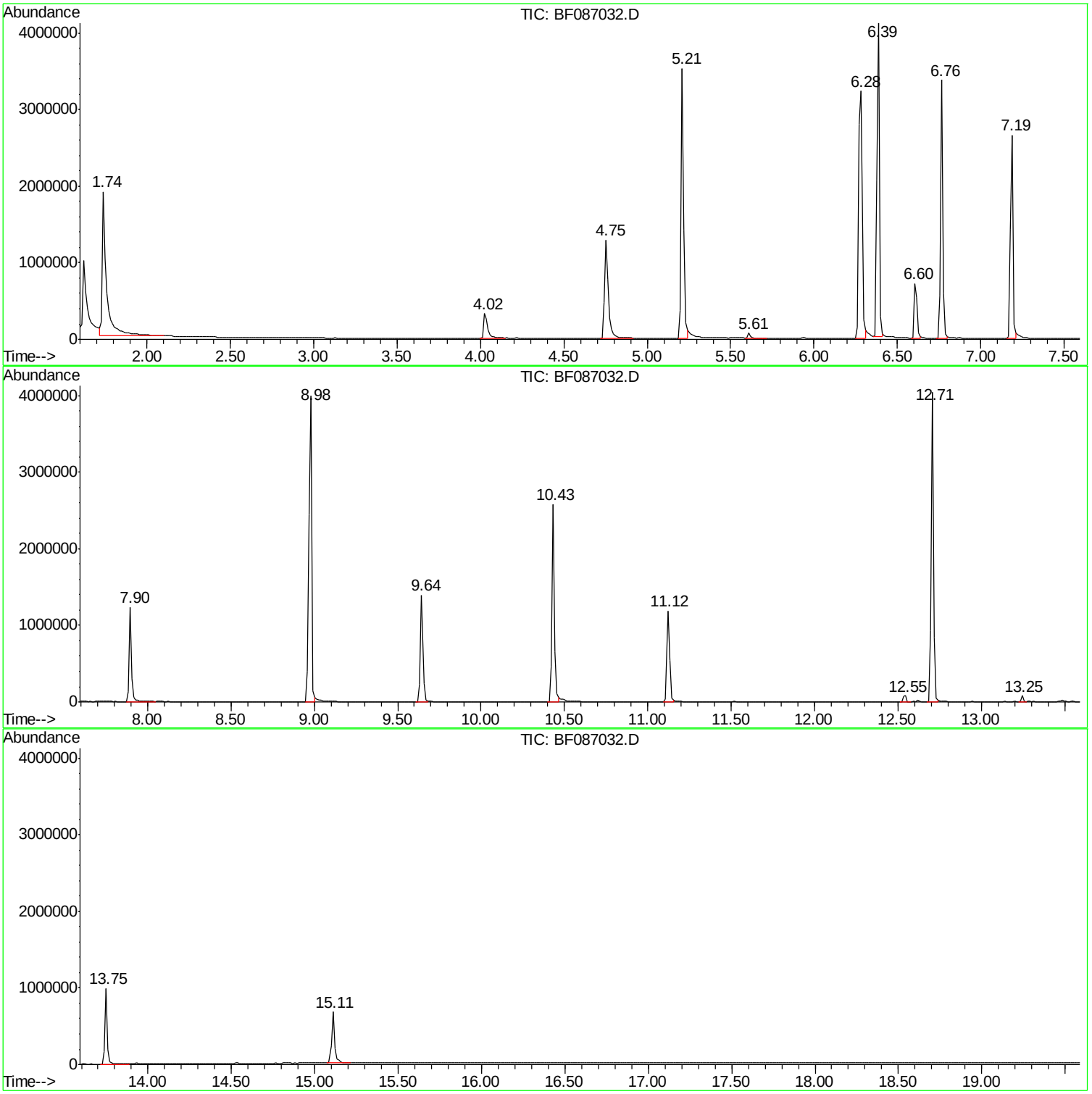
Instrument :
BNA_F
ClientSampleId :
PB90536BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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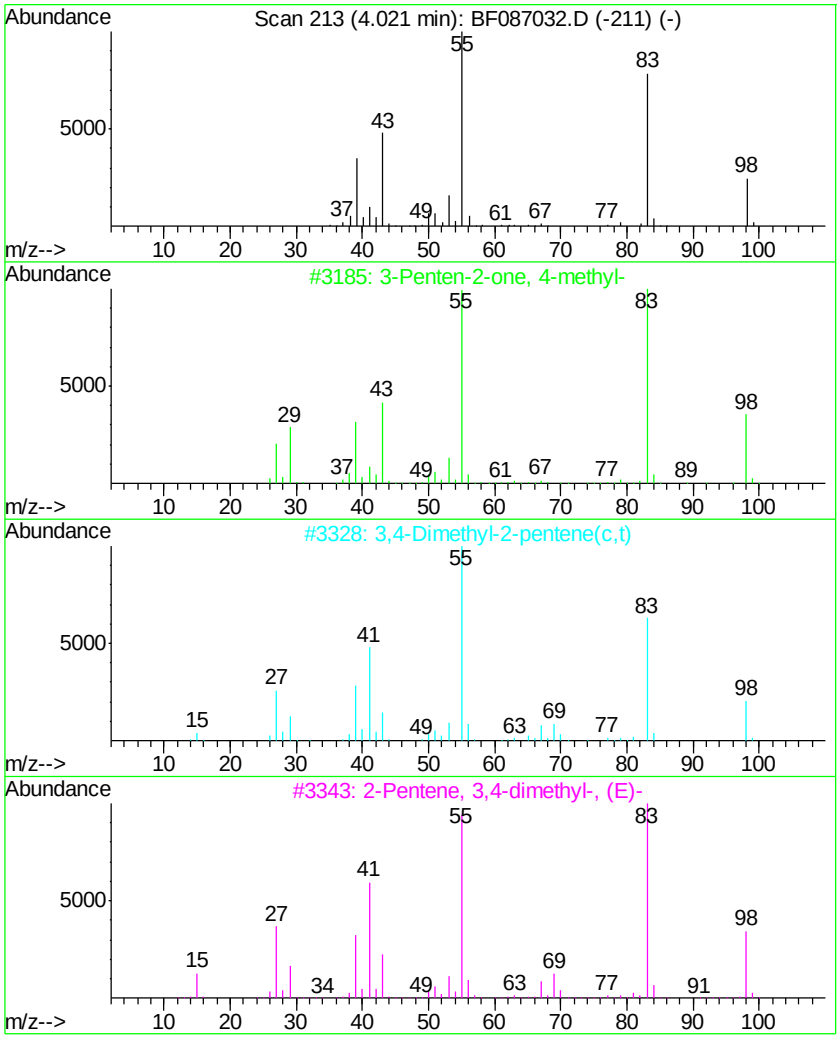
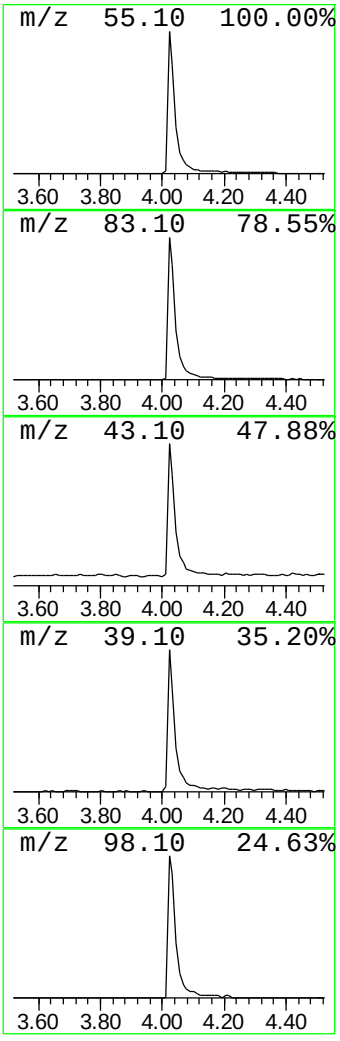
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.02	12.44 ng	567965	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4	3-Hexen-2-one	98	C6H10O	000763-93-9	80
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087032.D
Acq On : 14 May 2016 21:08
Operator : UM/SJ
Sample : PB90536BL
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB90536BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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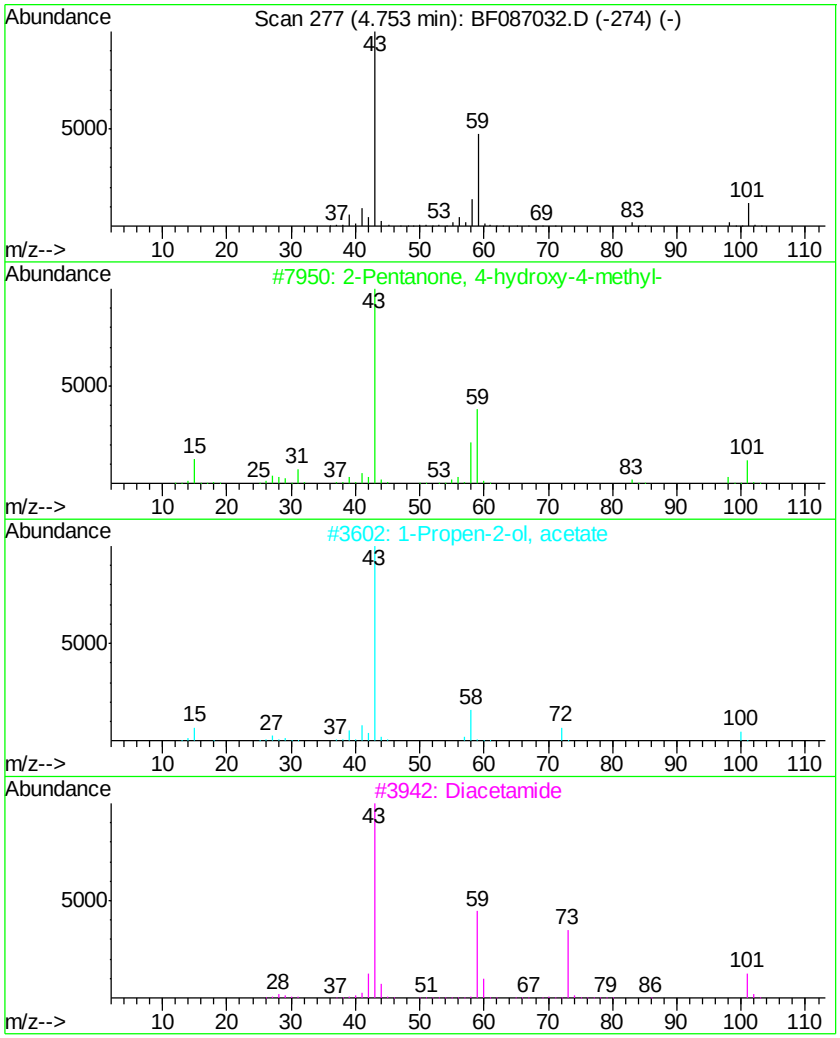
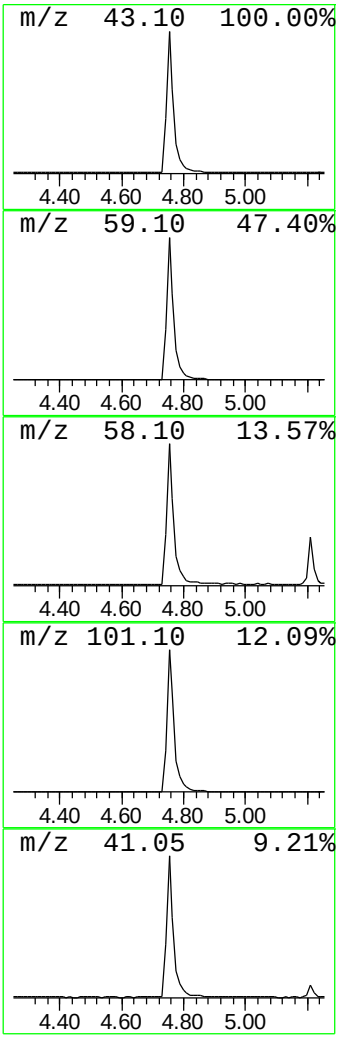
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	46.72 ng	2133290	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane	58	C4H10	000106-97-8	9





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Misc :
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Instrument : BNA_F
ClientSampleId : PB90536BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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TIC Library : C:\DATABASE\NIST02.L
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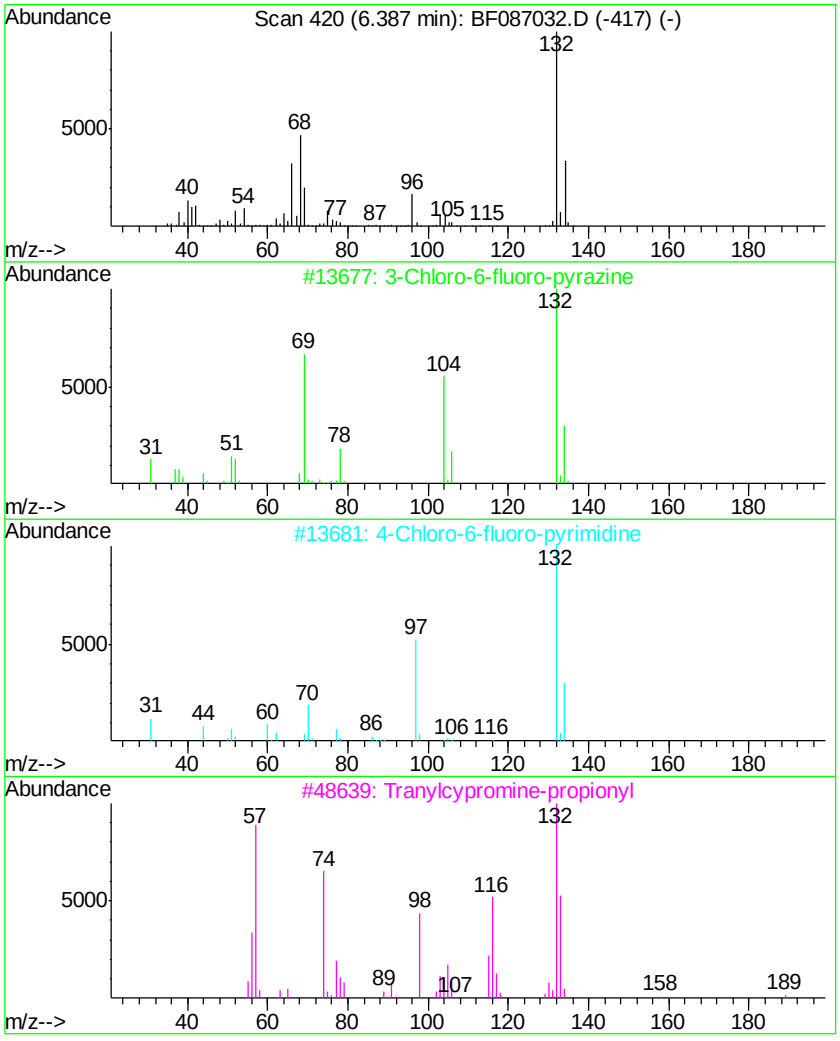
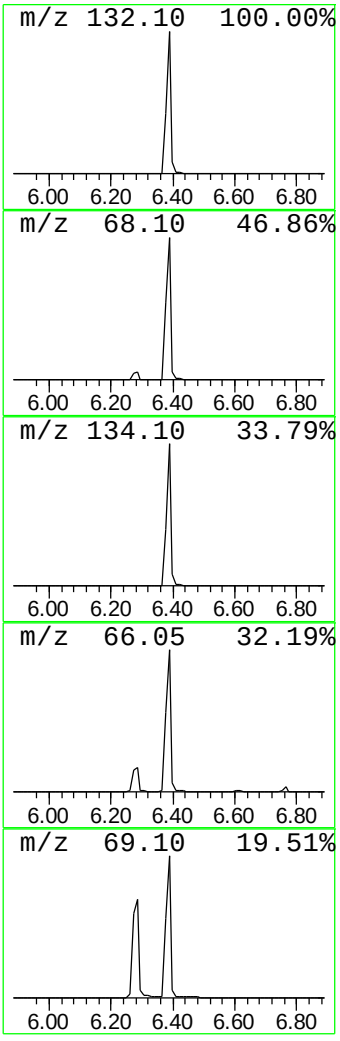
Peak Number 4 unknown6.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	97.11 ng	4433890	1,4-Dichlorobenzene-d4	6.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16





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Instrument : BNA_F
ClientSampleId : PB90536BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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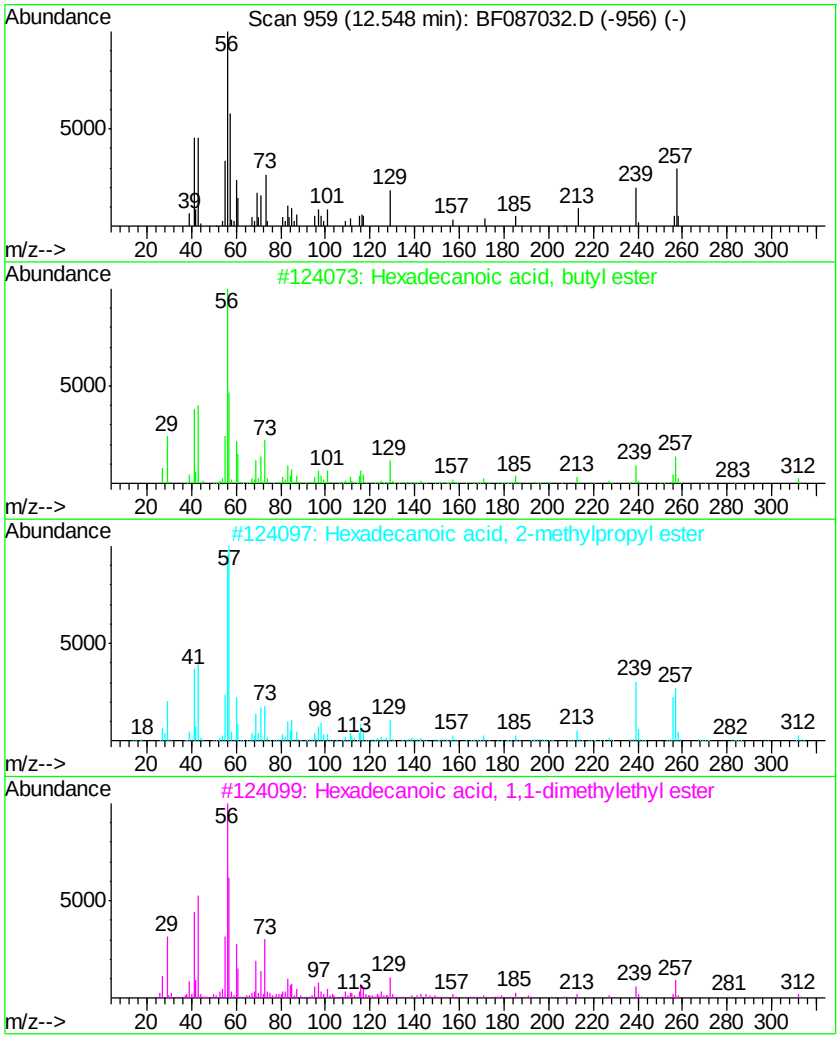
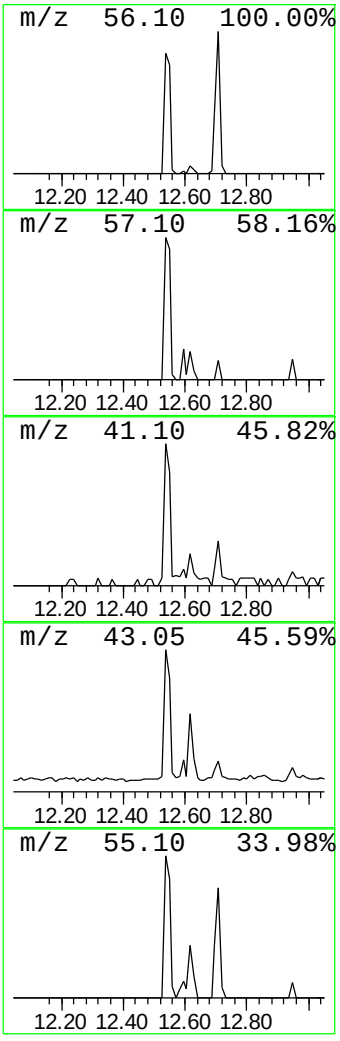
Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	2.10 ng	102329	Chrysene-d12	13.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	81
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	72
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	68
4	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27





Tentatively Identified Compound (LSC) summary

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Acq On : 14 May 2016 21:08
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Sample : PB90536BL
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.02	12.4	ng	567965	1	6.60	913191	20.0
2-Pentanone, 4-hy...	4.75	46.7	ng	2133290	1	6.60	913191	20.0
unknown6.39	6.39	97.1	ng	4433890	1	6.60	913191	20.0
Hexadecanoic acid...	12.55	2.1	ng	102329	5	13.75	974738	20.0