LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
Data File : BF089103.D
Acq On : 19 Jul 2016 1:39
Operator : UM/SJ
Sample : H4044-11
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : F9-B1(6-12)C

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-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	1.633	3	4	13	rVB	178558	279068	11.57%	2.228%
2	1.747	13	14	66	rVB	1239652	2411555	100.00%	19.255%
3	4.776	277	279	284	rBB	46372	74816	3.10%	0.597%
4	5.233	317	319	322	rBV	883113	1105721	45.85%	8.828%
5	5.896	375	377	379	rBB	100210	110031	4.56%	0.879%
6	6.296	409	412	415	rBV	866484	1148019	47.60%	9.166%
7	6.410	420	422	425	rBV	1053418	1104682	45.81%	8.820%
8	6.479	426	428	431	rBV	56434	45925	1.90%	0.367%
9	6.639	440	442	444	rBB	338575	292113	12.11%	2.332%
10	6.730	448	450	451	rBB	21206	26949	1.12%	0.215%
11	6.799	454	456	458	rBV	1034863	891282	36.96%	7.116%
12	7.210	489	492	494	rBV	746471	689791	28.60%	5.508%
13	7.930	552	555	557	rBV	437358	383798	15.91%	3.064%
14	9.005	647	649	652	rVB	1221473	1072045	44.45%	8.560%
15	9.405	682	684	686	rBB	244667	211276	8.76%	1.687%
16	9.679	705	708	710	rBV	337660	338272	14.03%	2.701%
17	10.456	774	776	779	rBV2	442609	507077	21.03%	4.049%
18	10.594	786	788	793	rVB	26404	29033	1.20%	0.232%
19	11.154	834	837	838	rBV	284349	287968	11.94%	2.299%
20	12.148	923	924	927	rBV	36991	29747	1.23%	0.238%
21	12.582	959	962	964	rBV2	22567	30091	1.25%	0.240%
22	12.731	973	975	978	rVB	811004	801780	33.25%	6.402%
23	13.645	1053	1055	1058	rVB2	43406	49042	2.03%	0.392%
24	13.771	1064	1066	1071	rVB	307083	328992	13.64%	2.627%
25	14.571	1134	1136	1139	rBV3	16177	37627	1.56%	0.300%
26	14.765	1151	1153	1157	rBV2	18180	34278	1.42%	0.274%
27	15.131	1183	1185	1188	rBV	168141	203474	8.44%	1.625%

Sum of corrected areas: 12524452

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BNA_F
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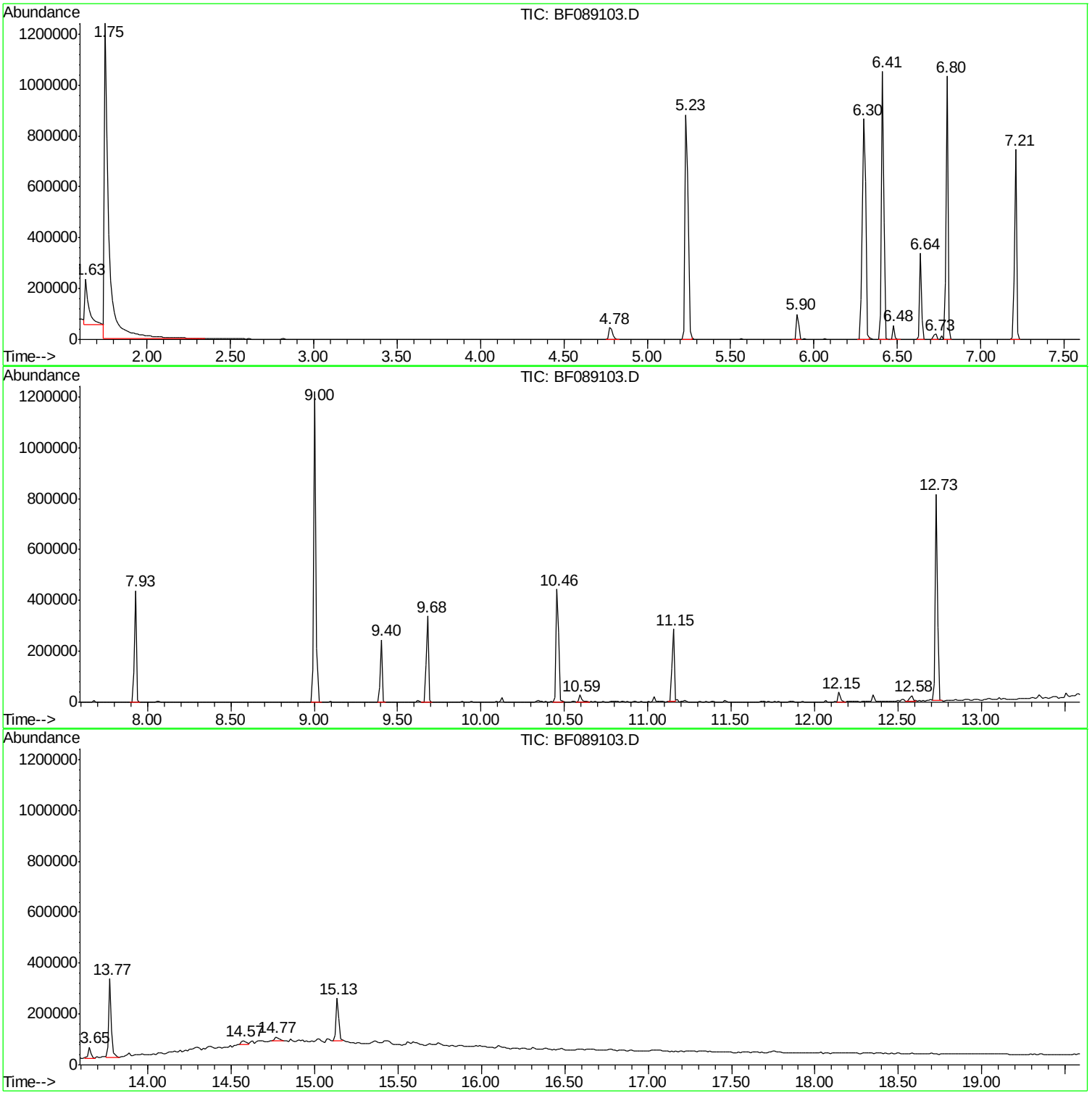
F9-B1(6-12)C

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



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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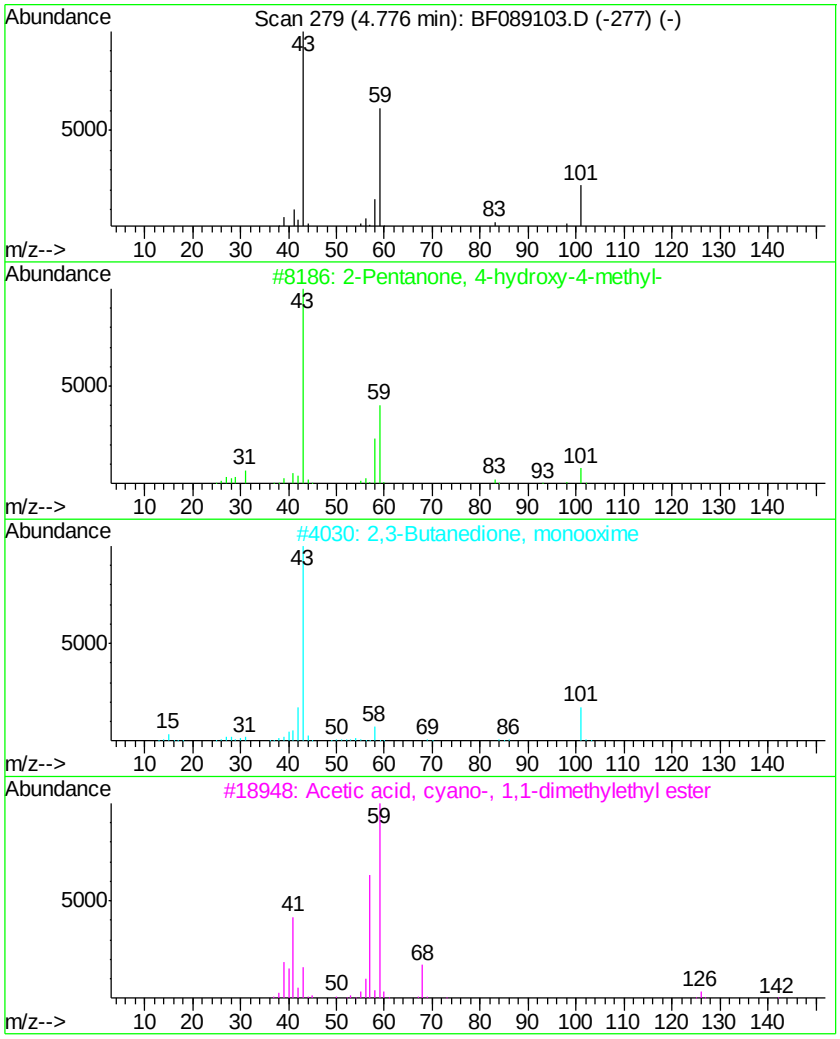
TIC Integration Parameters: LSCINT.P

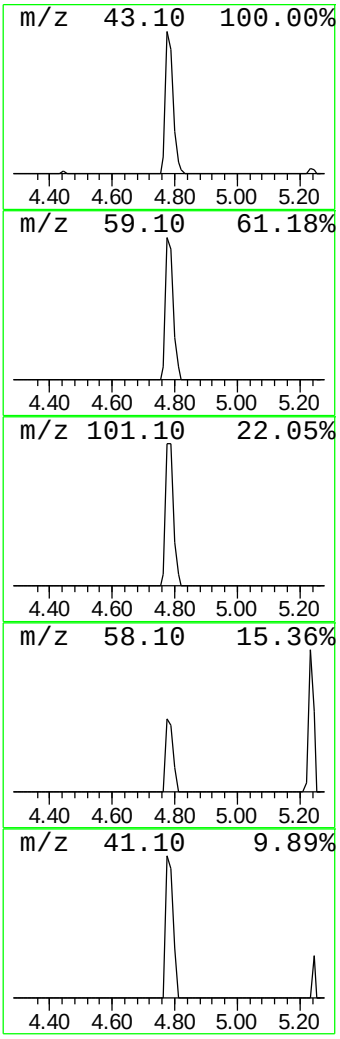
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	5.12 ng	74816	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	10
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071816\
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Operator : UM/SJ
Sample : H4044-11
Misc :
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Instrument : BNA_F
ClientSampleId : F9-B1(6-12)C

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

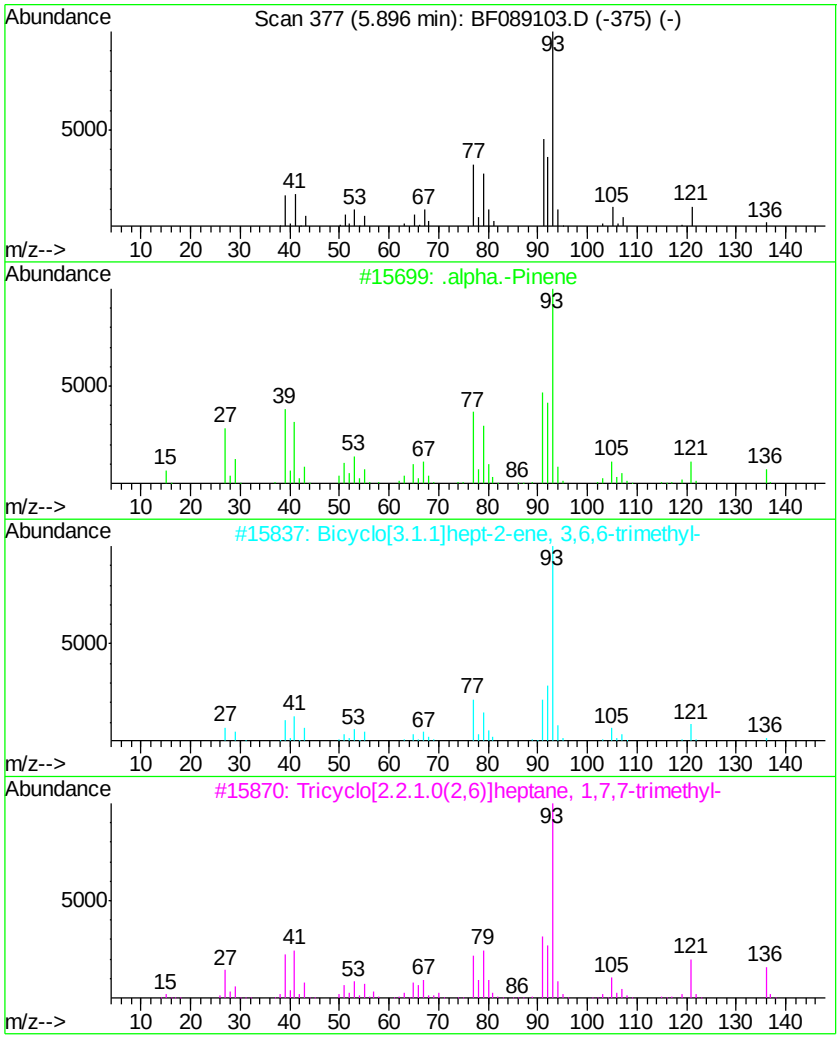
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

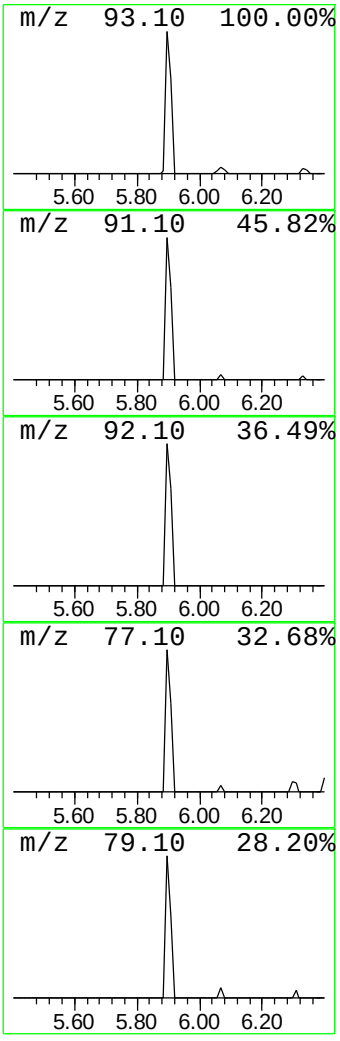
****

Peak Number 4 .alpha.-Pinene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.90	7.53 ng	110031	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	94
2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
3	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4	(+)-3-Carene	136	C10H16	000498-15-7	87
5	3-Carene	136	C10H16	013466-78-9	86





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Instrument : BNA_F
ClientSampleId : F9-B1(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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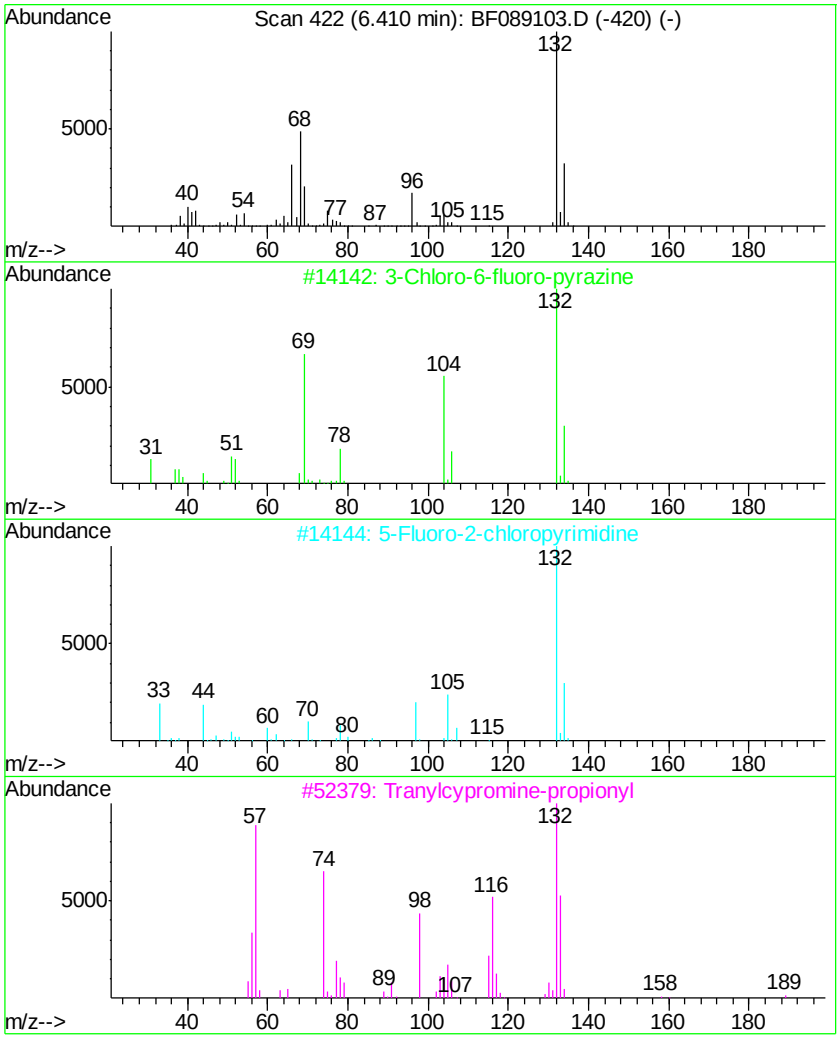
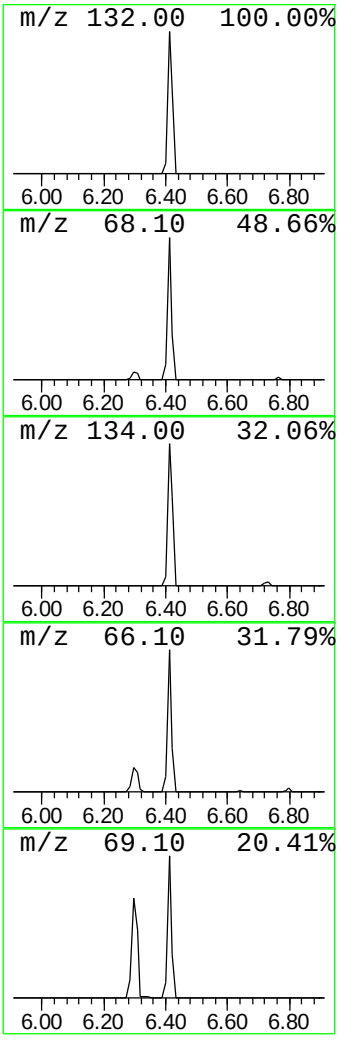
****

Peak Number 5 unknown6.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	75.63 ng	1104680	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : F9-B1(6-12)C

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

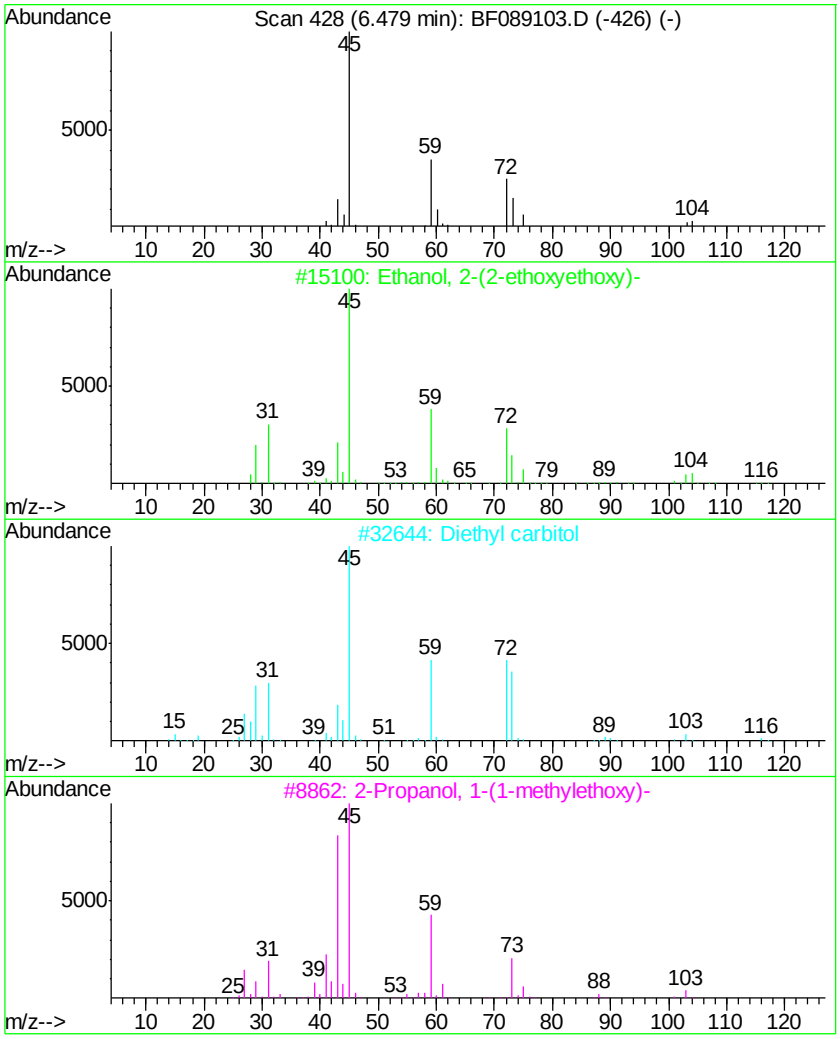
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

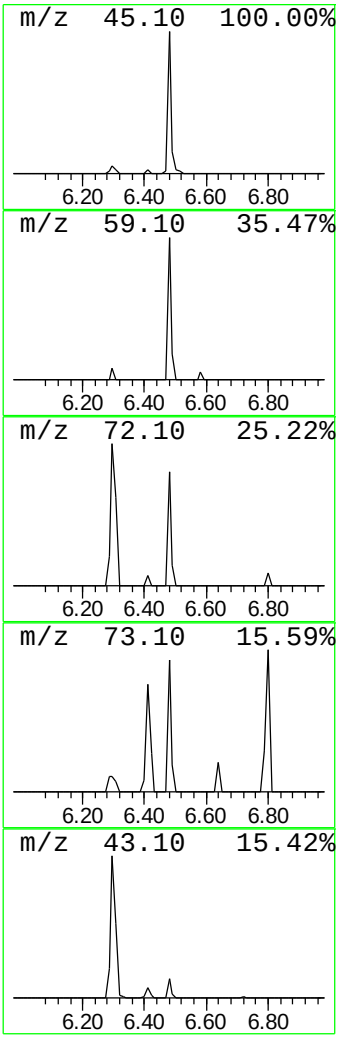
****

Peak Number 6 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	3.14 ng	45925	1,4-Dichlorobenzene-d4	6.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5	Ethyl ether	74	C4H10O	000060-29-7	33





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Instrument : BNA_F
ClientSampleId : F9-B1(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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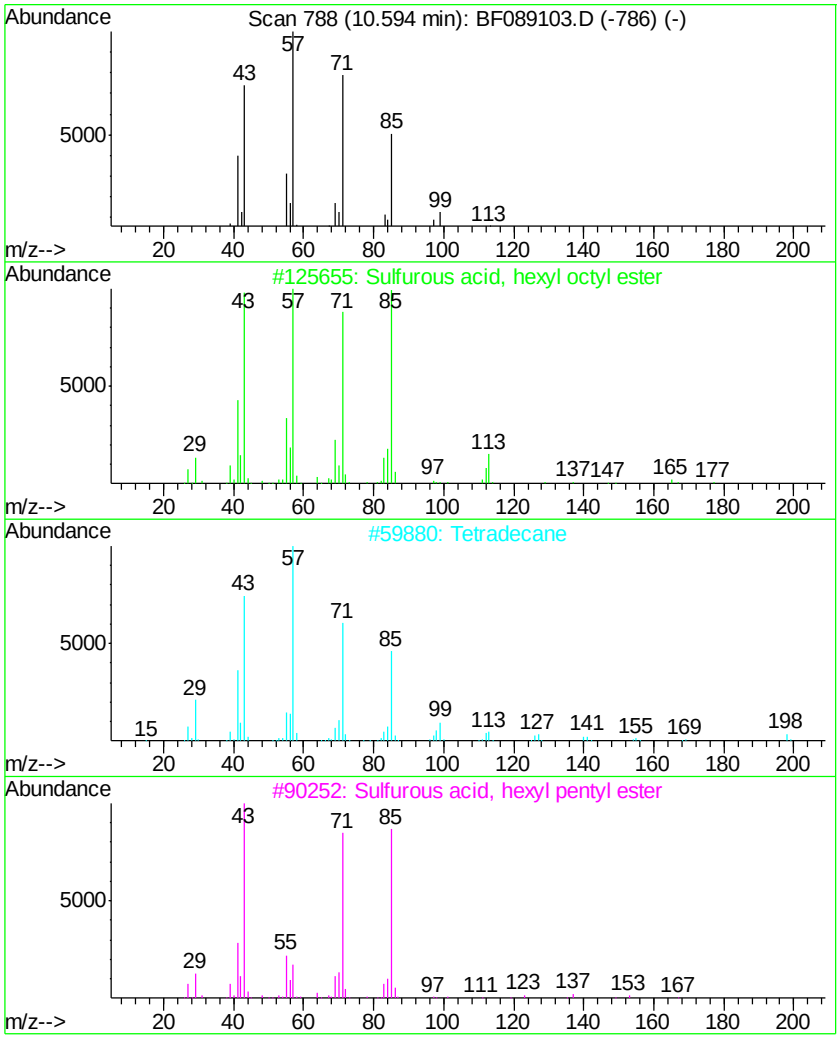
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

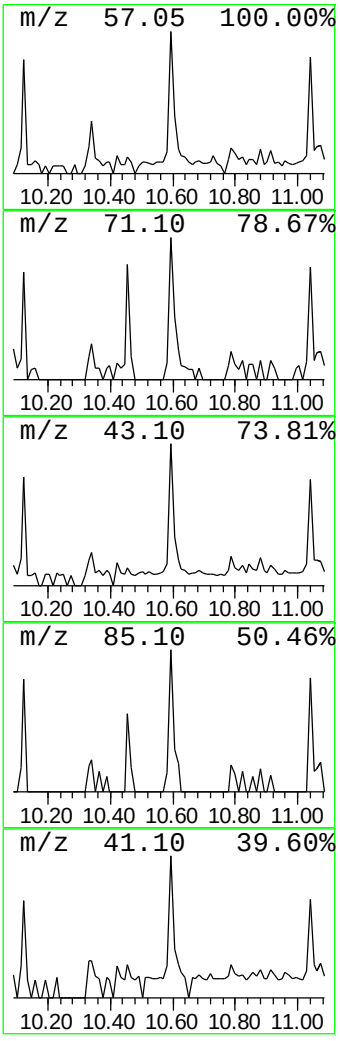
****

Peak Number 8 Sulfurous acid, hexyl octyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	2.02 ng	29033	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	78
2	Tetradecane	198	C14H30	000629-59-4	72
3	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	64
4	3-Ethyl-3-methylheptane	142	C10H22	017302-01-1	59
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	53





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

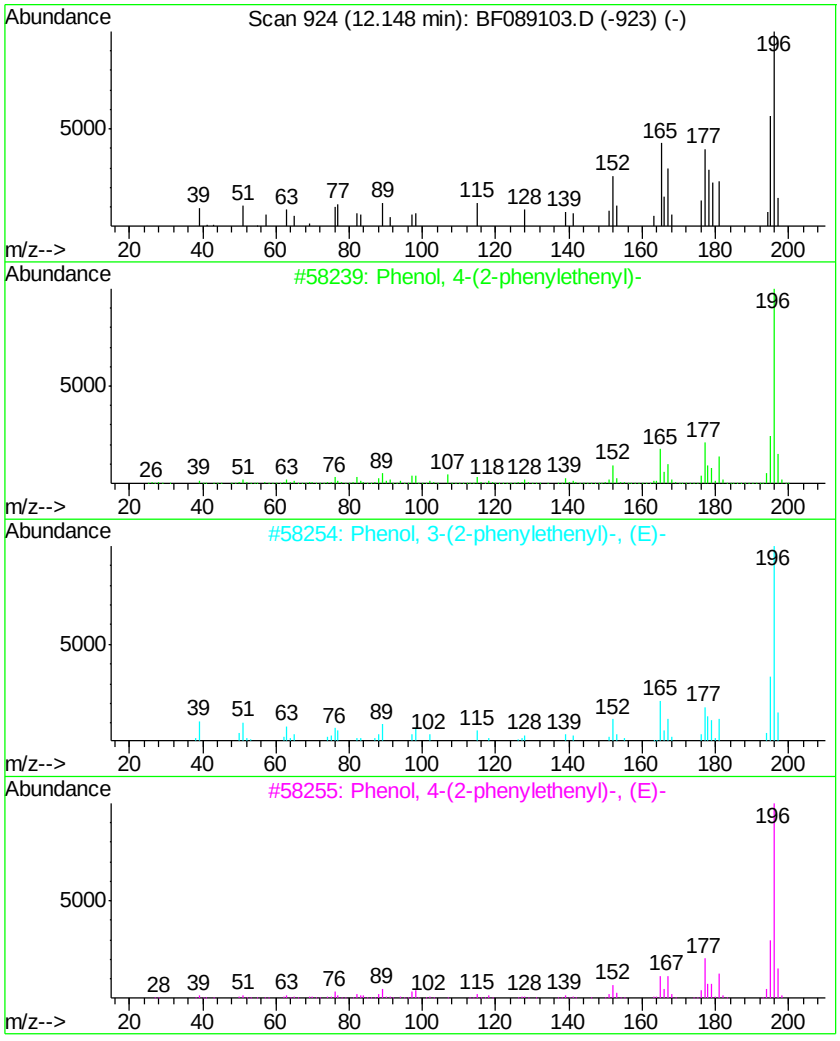
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

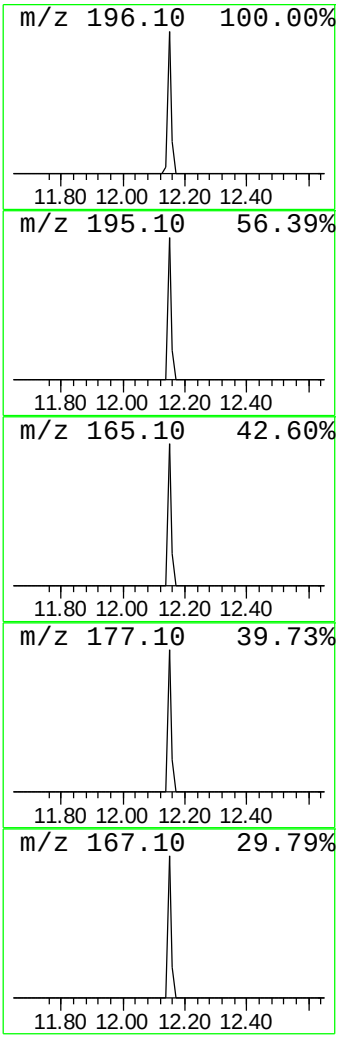
****

Peak Number 9 Phenol, 4-(2-phenylethenyl)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	2.07 ng	29747	Phenanthrene-d10	11.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(2-phenylethenyl)-	196	C14H12O	003839-46-1	93
2	Phenol, 3-(2-phenylethenyl)-, (E)-	196	C14H12O	017861-18-6	93
3	Phenol, 4-(2-phenylethenyl)-, (E)-	196	C14H12O	006554-98-9	76
4	Dibenz[c,e]oxepin, 5,7-dihydro-	196	C14H12O	001136-22-7	55
5	Methanone, diphenyl-, hydrazone	196	C13H12N2	005350-57-2	49





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TIC Library : C:\Database\NIST11.L
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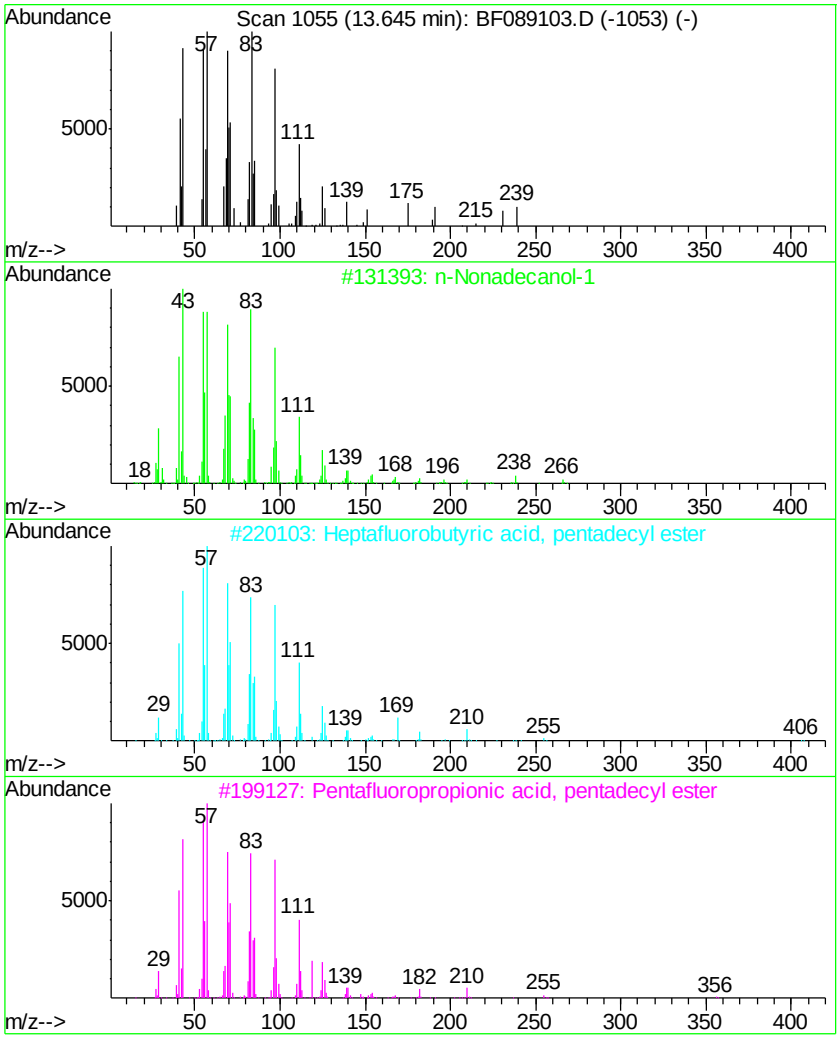
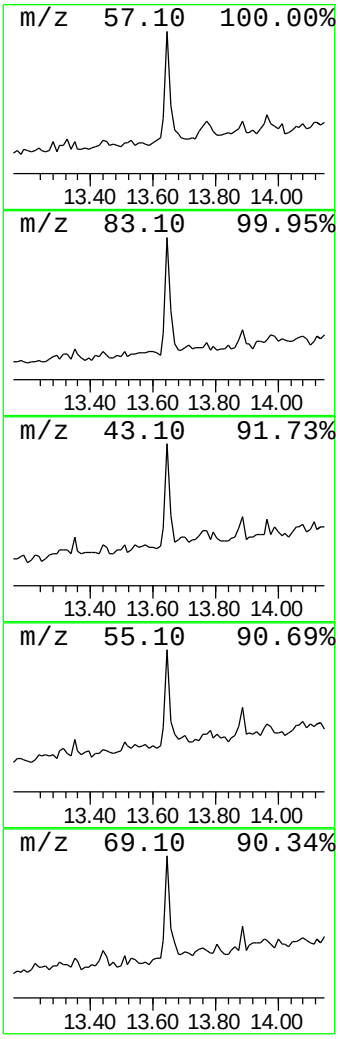
****

Peak Number 10 n-Nonadecanol-1 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	2.98 ng	49042	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





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ClientSampleId : F9-B1(6-12)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
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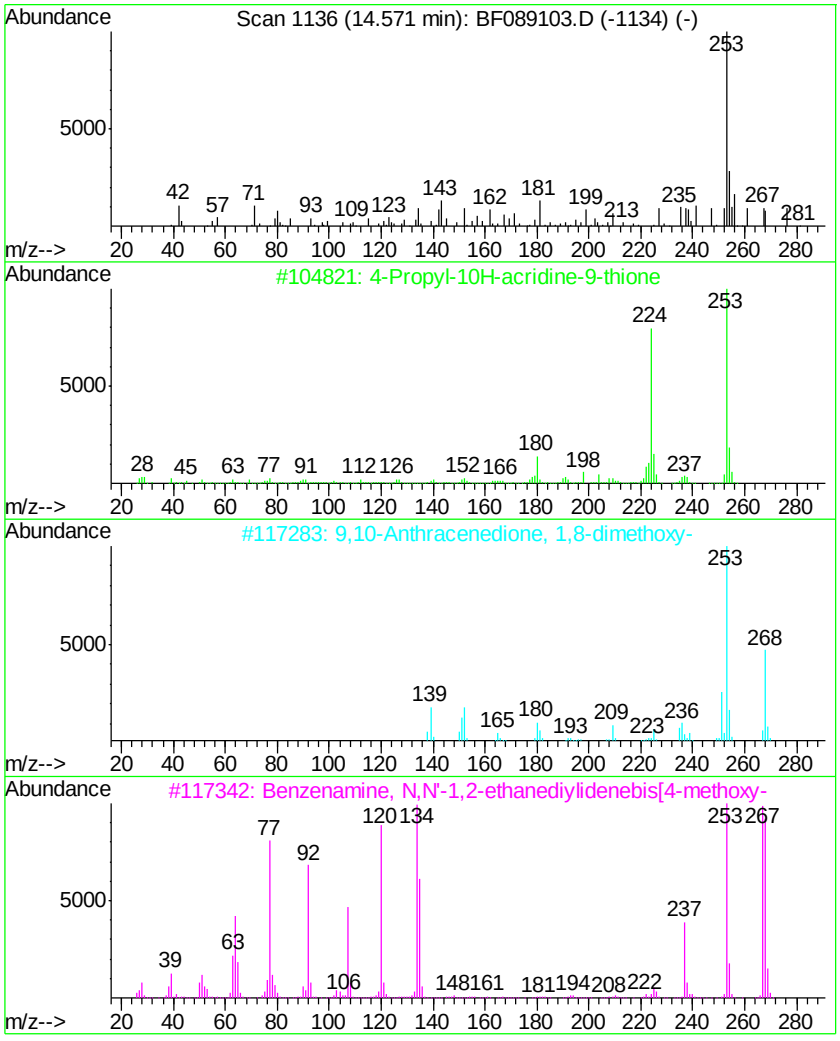
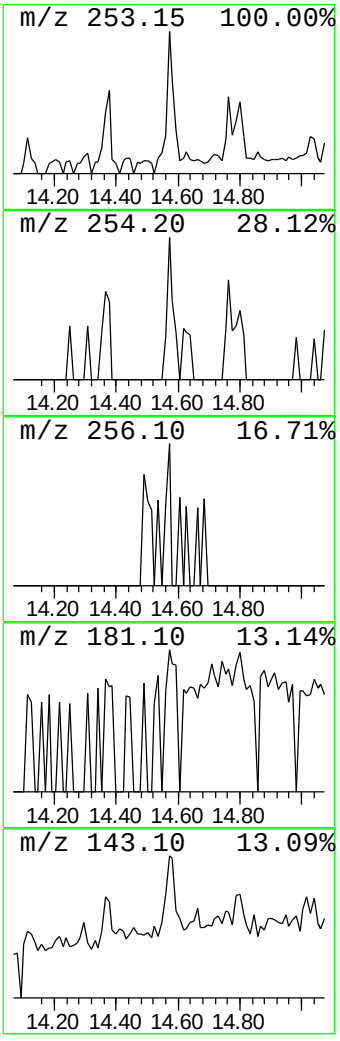
****

Peak Number 11 4-Propyl-10H-acridine-9-thione Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.70 ng	37627	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Propyl-10H-acridine-9-thione	253	C16H15NS	1000211-07-8	52
2	9,10-Anthracenedione, 1,8-dimeth...	268	C16H12O4	006407-55-2	38
3	Benzenamine, N,N'-1,2-ethanediyl...	268	C16H16N2O2	024764-91-8	38
4	1,3-Diphenyl-4H-1,2,4-triazoline...	253	C14H11N3S	005055-73-2	37
5	Benzenamine, 2,4,6-trimethyl-N-(...	253	C18H23N	1000327-29-3	36





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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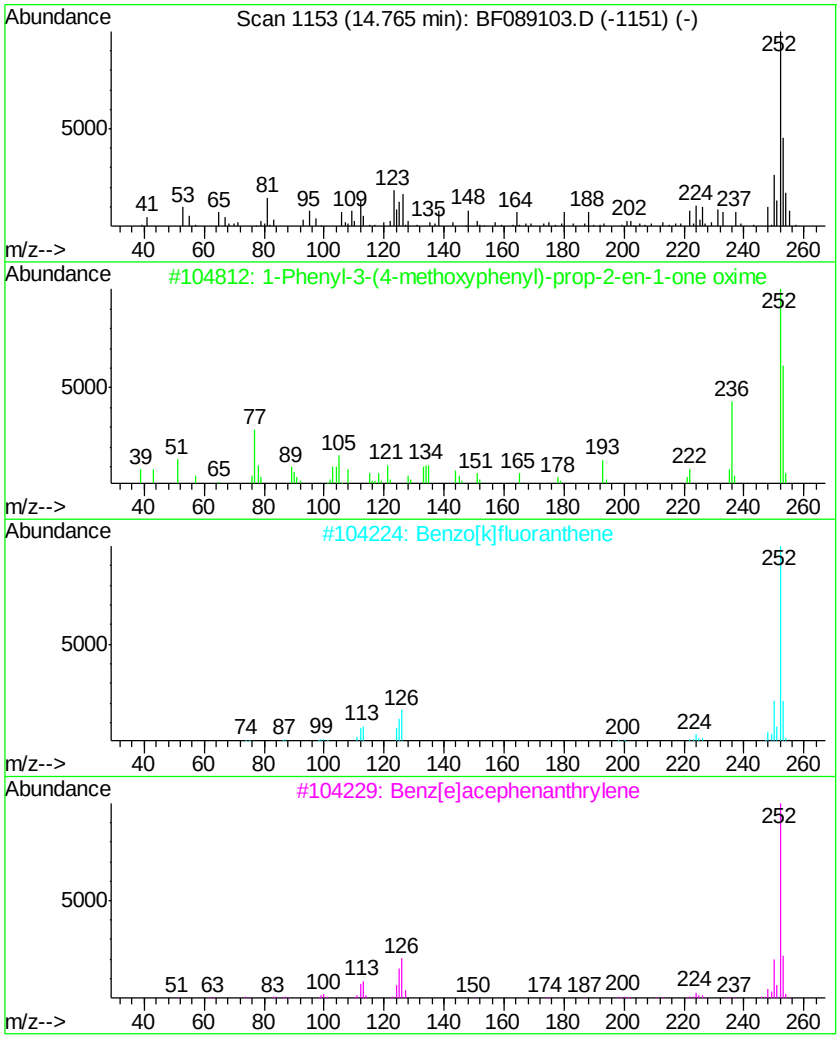
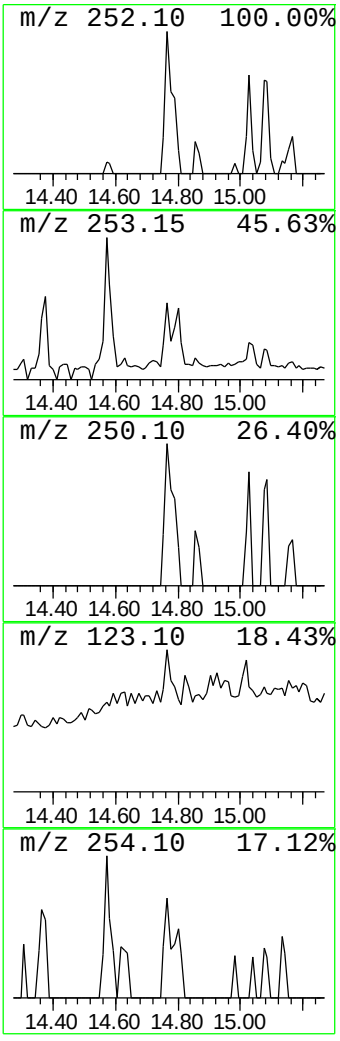
****

Peak Number 12 1-Phenyl-3-(4-methoxyphenyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	3.37 ng	34278	Perylene-d12	15.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-3-(4-methoxyphenyl)-pro...	253	C16H15NO2	1000148-25-2	50
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	49
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	47
4	Benzo[b]naphtho[2,3-d]thiophene,...	252	C17H16S	024964-06-5	47
5	Perylene	252	C20H12	000198-55-0	47





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.78	5.1	ng	74816	1	6.64	292113	20.0
.alpha.-Pinene	5.90	7.5	ng	110031	1	6.64	292113	20.0
unknown6.41	6.41	75.6	ng	1104680	1	6.64	292113	20.0
Ethanol, 2-(2-eth...	6.48	3.1	ng	45925	1	6.64	292113	20.0
Sulfurous acid, h...	10.59	2.0	ng	29033	4	11.15	287968	20.0
Phenol, 4-(2-phen...	12.15	2.1	ng	29747	4	11.15	287968	20.0
n-Nonadecanol-1	13.65	3.0	ng	49042	5	13.77	328992	20.0
4-Propyl-10H-acri...	14.57	3.7	ng	37627	6	15.13	203474	20.0
1-Phenyl-3-(4-met...	14.77	3.4	ng	34278	6	15.13	203474	20.0