LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009971.D
Acq On : 10 May 2017 15:21
Operator : SJ/MA
Sample : I3058-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DUP-0398-170508

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_M\METHODS\8270-BM050517.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	4.422	222	227	234	rBV	333024	477934	4.98%	1.248%
2	4.899	301	308	319	rBV	146380	224084	2.33%	0.585%
3	5.093	335	341	351	rVB2	85686	132597	1.38%	0.346%
4	5.357	379	386	403	rVB	985442	1482620	15.44%	3.871%
5	6.951	650	657	671	rBV	606604	1008890	10.50%	2.634%
6	7.304	710	717	730	rBV	1846374	2907152	30.27%	7.591%
7	7.769	789	796	806	rBV	356017	567816	5.91%	1.483%
8	8.087	842	850	863	rVB	1521108	2448152	25.49%	6.392%
9	8.940	988	995	1005	rBV	1486372	2473904	25.76%	6.460%
10	10.563	1263	1271	1277	rBV	443660	740864	7.71%	1.934%
11	13.033	1683	1691	1700	rBV	3577829	5067328	52.76%	13.231%
12	13.880	1828	1835	1840	rBV	166714	239583	2.49%	0.626%
13	14.422	1921	1927	1938	rVB2	658978	992358	10.33%	2.591%
14	15.357	2080	2086	2094	rBV5	61519	127863	1.33%	0.334%
15	15.921	2176	2182	2196	rBV2	3286038	4870710	50.71%	12.718%
16	16.463	2266	2274	2281	rBV2	149559	228603	2.38%	0.597%
17	17.174	2389	2395	2402	rBV	862992	1262328	13.14%	3.296%
18	17.545	2451	2458	2466	rBV2	125594	196067	2.04%	0.512%
19	18.915	2687	2691	2698	rBV2	174661	238726	2.49%	0.623%
20	19.804	2836	2842	2850	rBV	8551892	9605164	100.00%	25.080%
21	21.056	3051	3055	3060	rVB5	120213	154769	1.61%	0.404%
22	21.362	3103	3107	3112	rBV	1226592	1581503	16.47%	4.129%
23	23.662	3492	3498	3506	rVB	679829	1269056	13.21%	3.314%

Sum of corrected areas: 38298071

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009971.D
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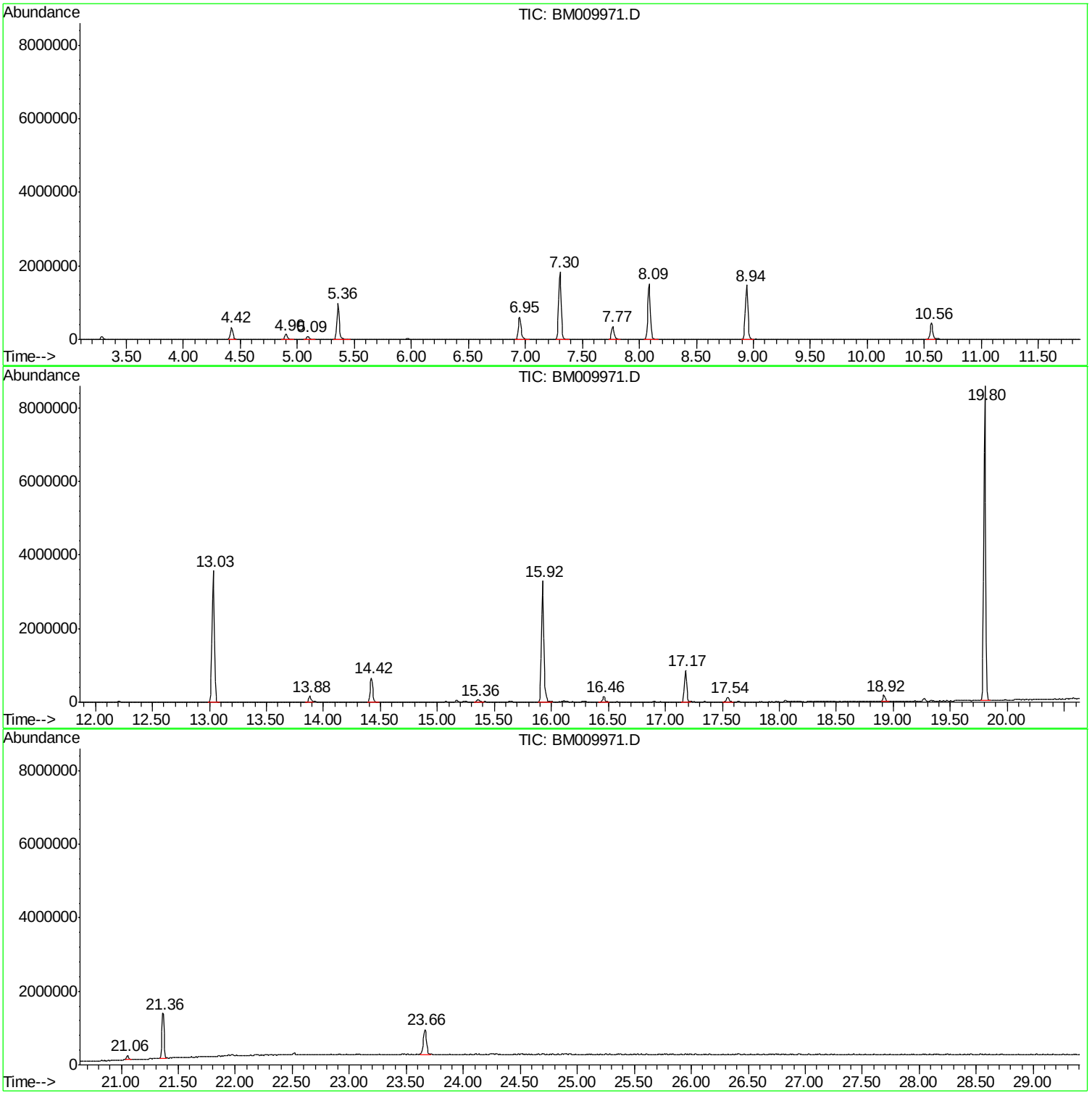
Operator : SJ/MA
Sample : I3058-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DUP-0398-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009971.D
Acq On : 10 May 2017 15:21
Operator : SJ/MA
Sample : I3058-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DUP-0398-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

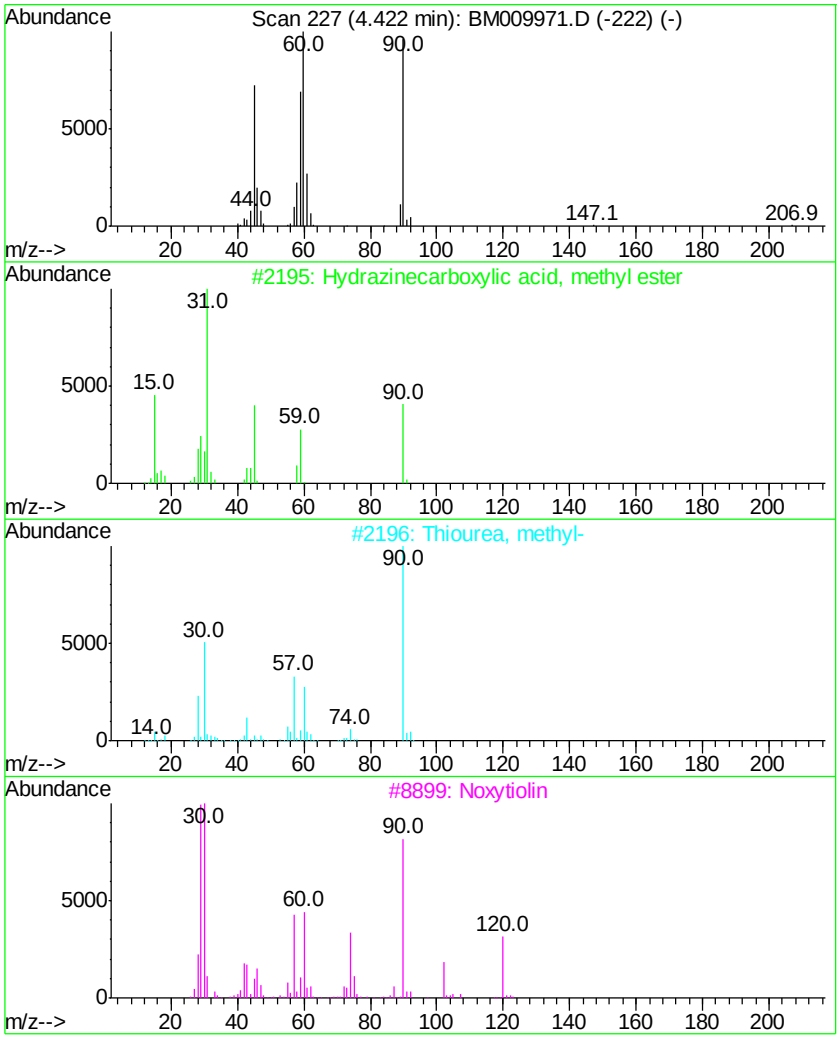
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

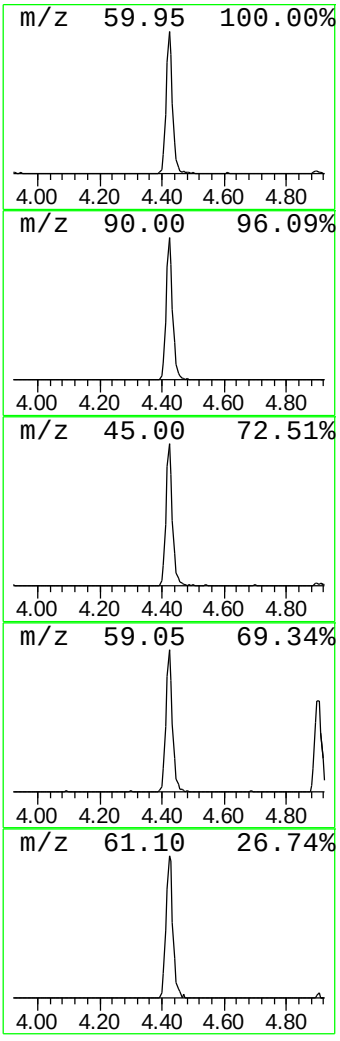
****

Peak Number 1 Hydrazinecarboxylic acid, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	16.83 ng	477934	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	59
2	Thiourea, methyl-	90	C2H6N2S	000598-52-7	47
3	Noxytiolin	120	C3H8N2OS	015599-39-0	42
4	1-Cyano-N-fluoroformimidoyl fluo...	90	C2F2N2	014011-05-3	40
5	2,3-Dimercaptopropan-1-ol	124	C3H8OS2	000059-52-9	38





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Data File : BM009971.D
Acq On : 10 May 2017 15:21
Operator : SJ/MA
Sample : I3058-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DUP-0398-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

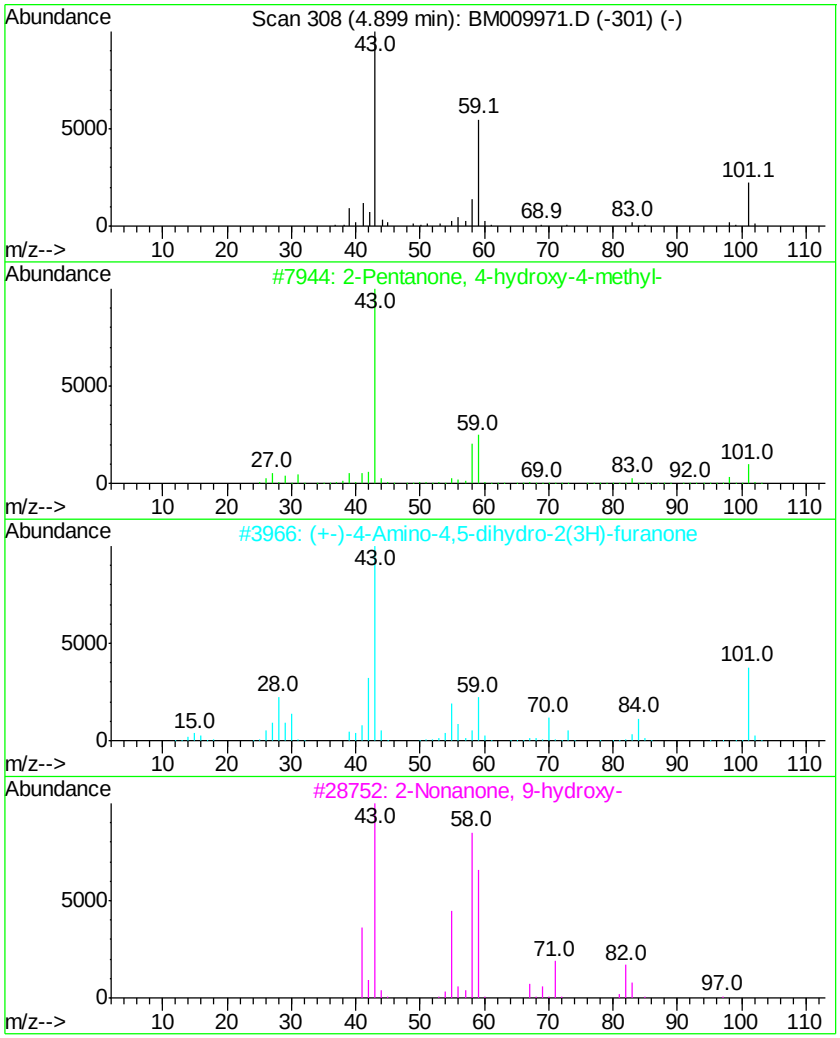
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

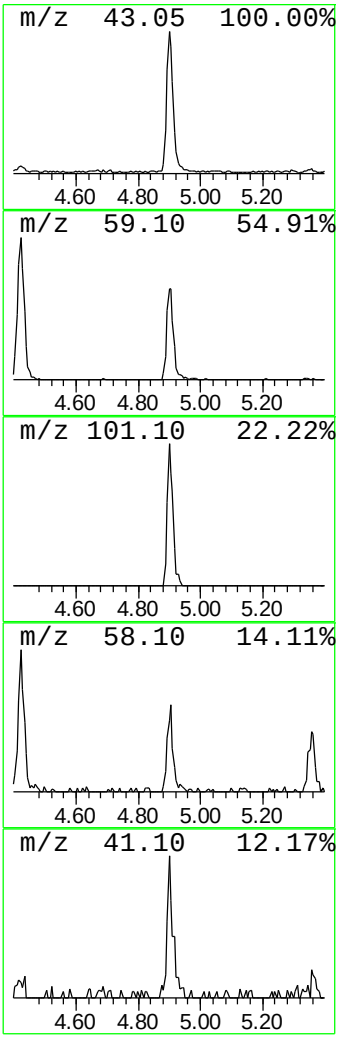
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	7.89 ng	224084	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	40
3	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
4	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	17
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17





Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009971.D
Acq On : 10 May 2017 15:21
Operator : SJ/MA
Sample : I3058-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DUP-0398-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

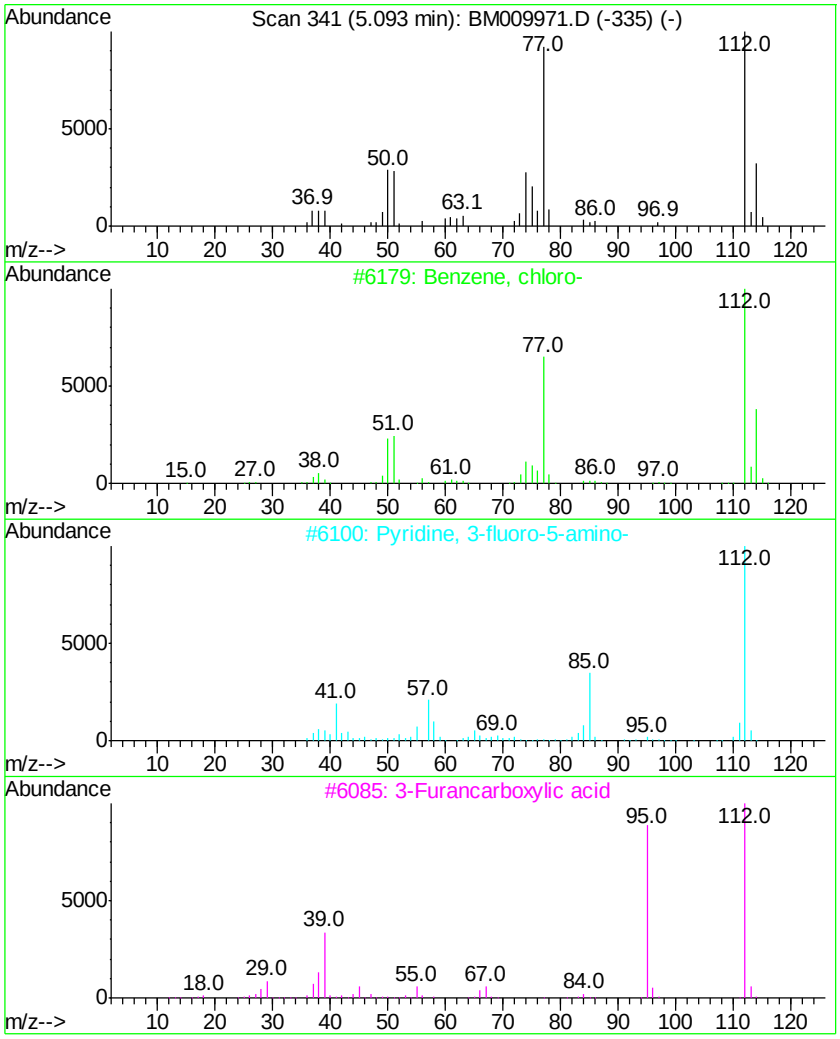
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

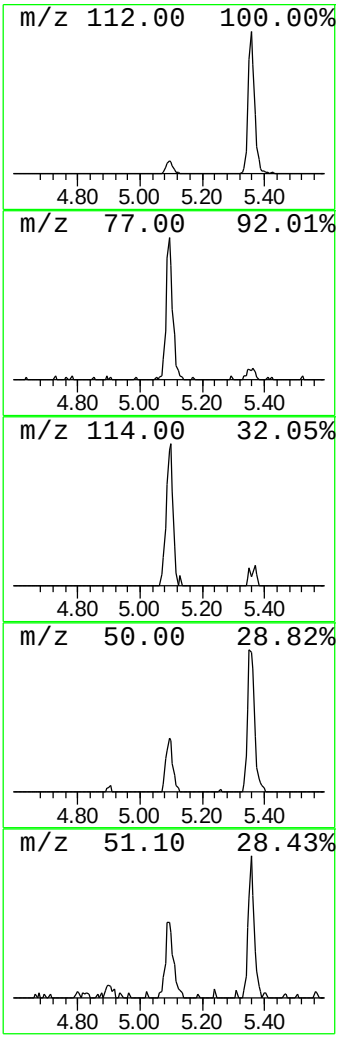
****

Peak Number 3 Benzene, chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	4.67 ng	132597	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, chloro-	112	C6H5Cl	000108-90-7	90
2	Pyridine, 3-fluoro-5-amino-	112	C5H5FN2	210169-05-4	14
3	3-Furancarboxylic acid	112	C5H4O3	000488-93-7	14
4	2-Furancarboxylic acid	112	C5H4O3	000088-14-2	14
5	Phosphonic acid, [2-methyl-1-[(1...	337	C13H32NO3PSi2	055108-68-4	10





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Data File : BM009971.D
Acq On : 10 May 2017 15:21
Operator : SJ/MA
Sample : I3058-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DUP-0398-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

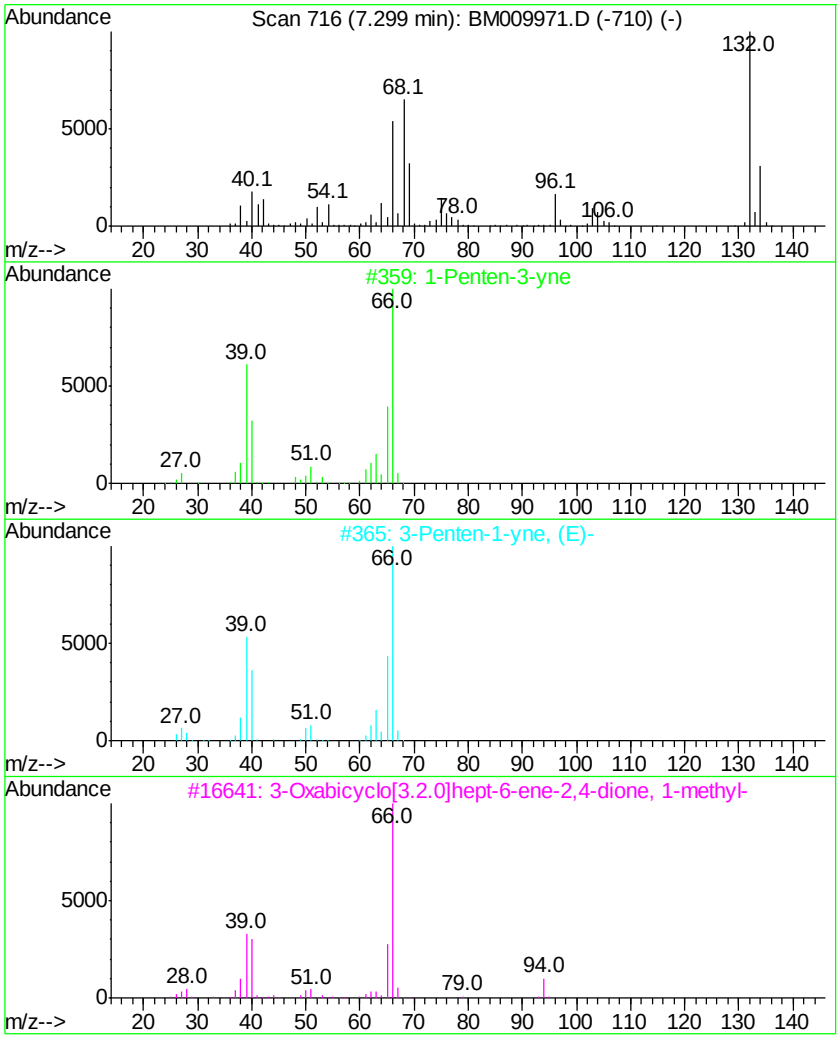
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

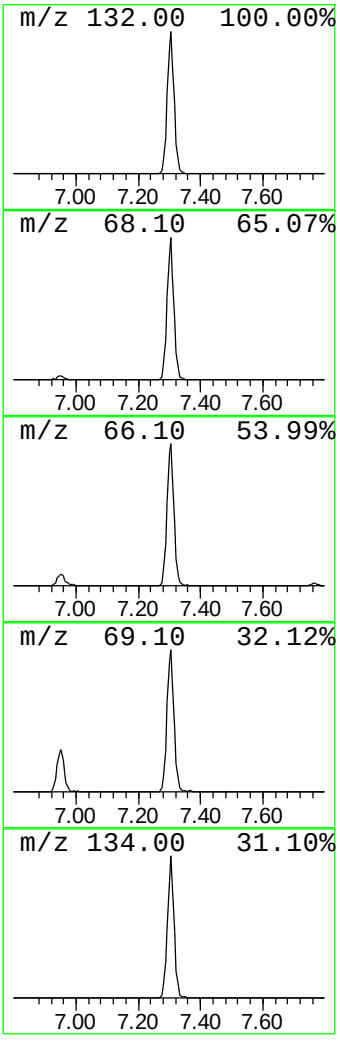
****

Peak Number 4 unknown7.30 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	102.40 ng	2907150	1,4-Dichlorobenzene-d4	7.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-yne	66	C5H6	000646-05-9	38
2	3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	35
3	3-Oxabicyclo[3.2.0]hept-6-ene-2,...	138	C7H6O3	064197-88-2	25
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	18





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051017\
Data File : BM009971.D
Acq On : 10 May 2017 15:21
Operator : SJ/MA
Sample : I3058-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DUP-0398-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

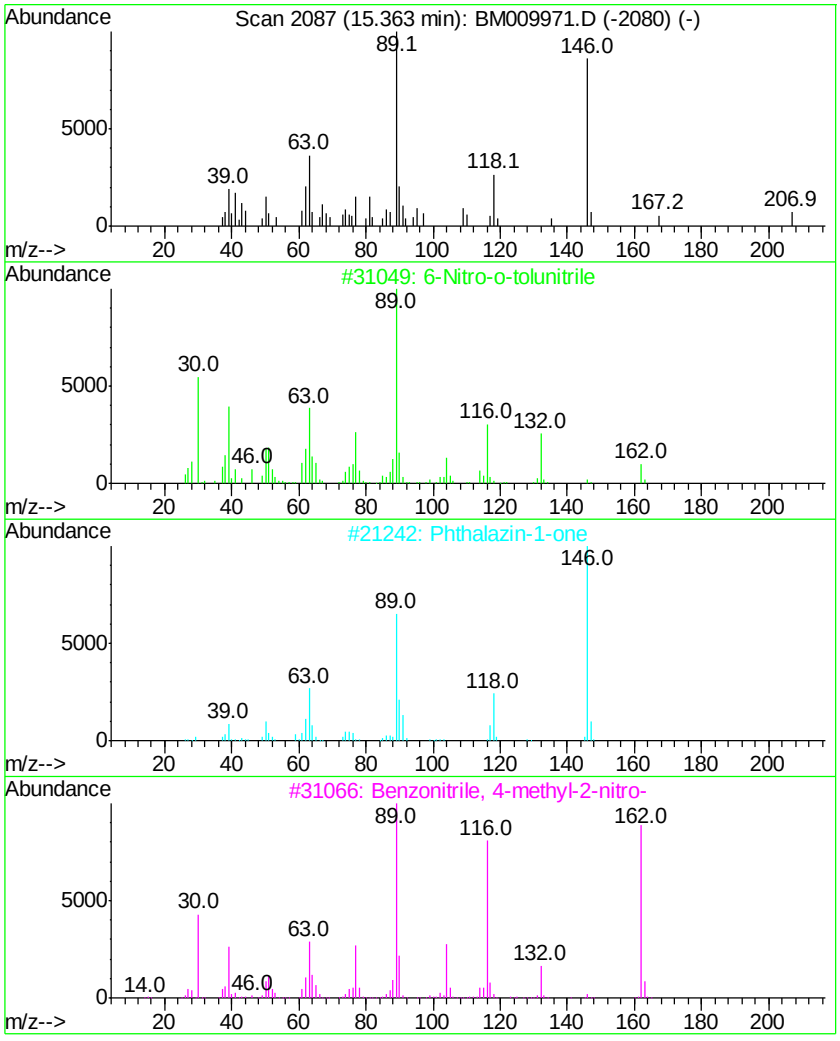
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

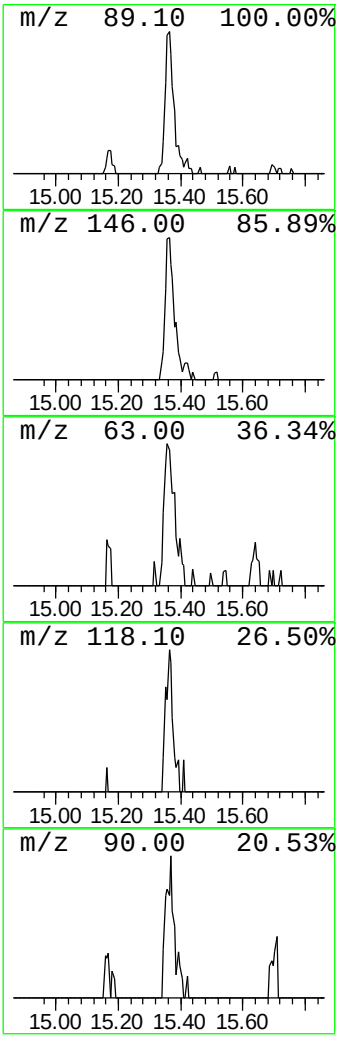
****

Peak Number 6 6-Nitro-o-tolunitrile Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	2.58 ng	127863	Acenaphthene-d10	14.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Nitro-o-tolunitrile	162	C8H6N2O2	001885-76-3	50
2	Phthalazin-1-one	146	C8H6N2O	000119-39-1	41
3	Benzonitrile, 4-methyl-2-nitro-	162	C8H6N2O2	026830-95-5	38
4	Cinnoline, 2-oxide	146	C8H6N2O	004215-44-5	38
5	Cinnoline, 1-oxide	146	C8H6N2O	001125-61-7	37





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Sample : I3058-06
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Instrument : BNA_M
ClientSampleId : DUP-0398-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

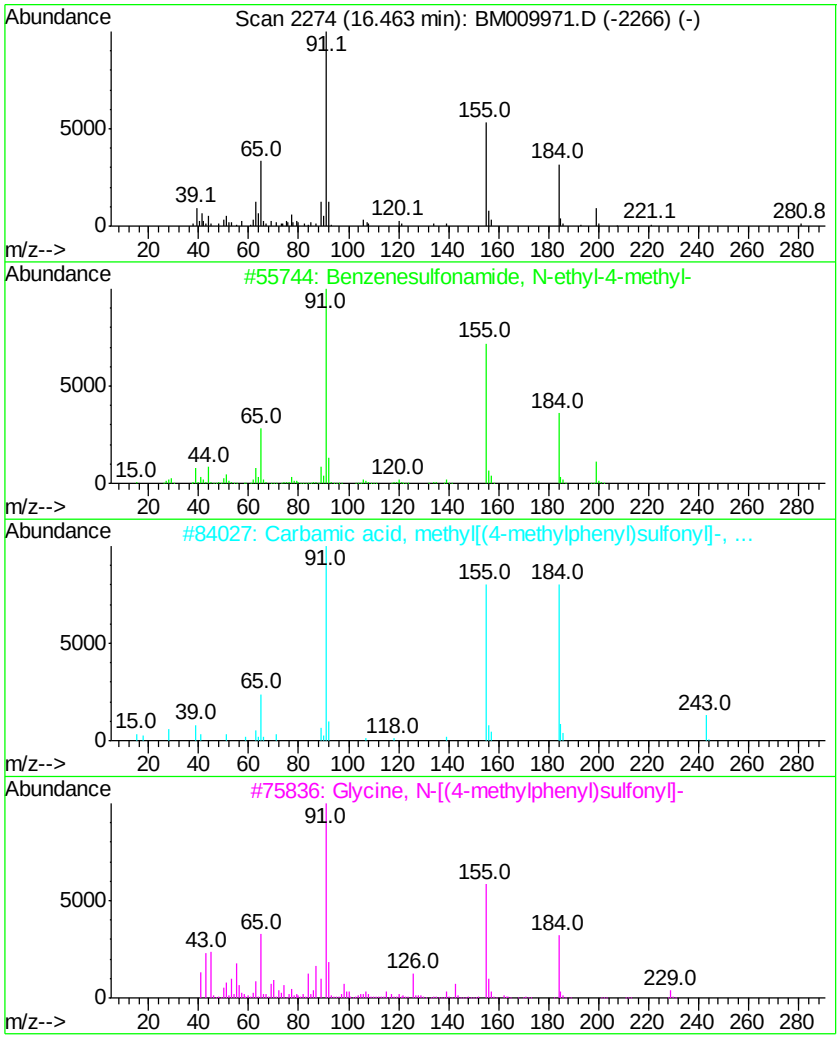
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

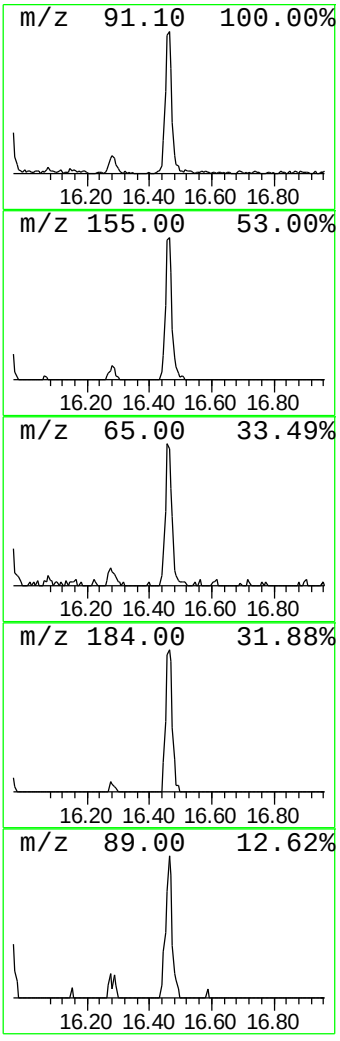
****

Peak Number 7 Benzenesulfonamide, N-ethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	3.62 ng	228603	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N-ethyl-4-me...	199	C9H13NO2S	000080-39-7	97
2	Carbamic acid, methyl[(4-methylp...	243	C10H13NO4S	032258-50-7	78
3	Glycine, N-[(4-methylphenyl)sulf...	229	C9H11NO4S	001080-44-0	78
4	Acetic acid, 2-(4-methylphenylsu...	243	C10H13NO4S	002645-02-5	78
5	(N-(p-Tolylsulfonyl)glycyl)hydra...	243	C9H13N3O3S	003619-20-3	78





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Sample : I3058-06
Misc :
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Instrument : BNA_M
ClientSampleId : DUP-0398-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

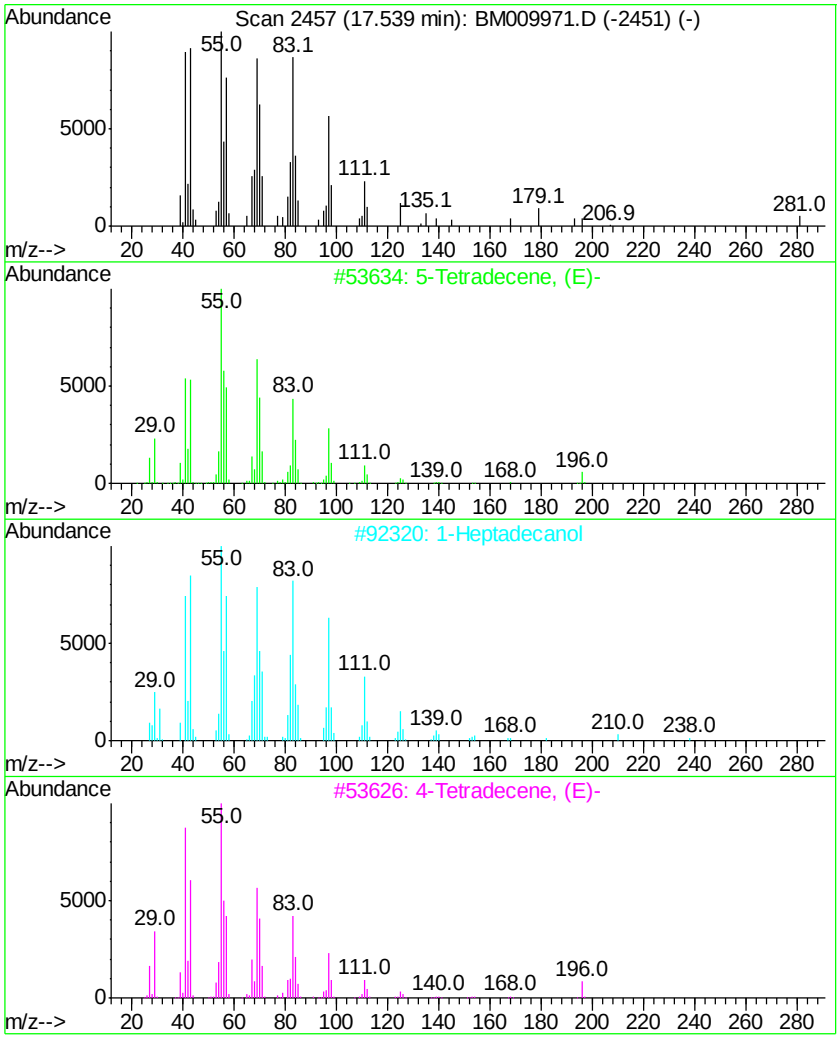
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

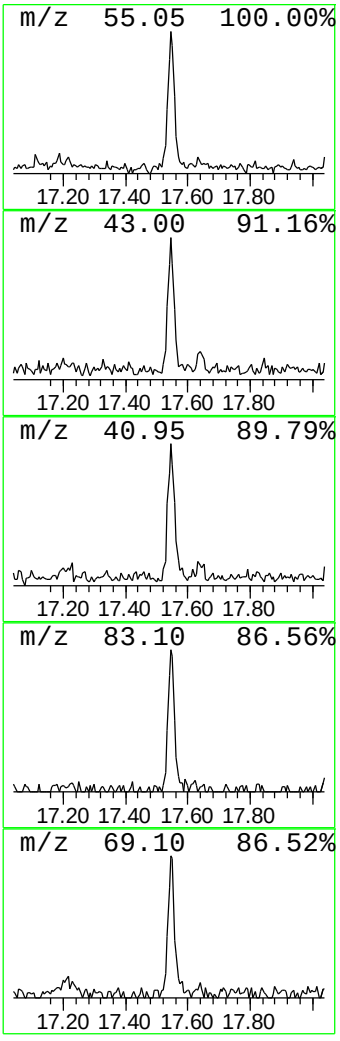
****

Peak Number 8 5-Tetradecene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.54	3.11 ng	196067	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Tetradecene, (E)-	196	C14H28	041446-66-6	94
2	1-Heptadecanol	256	C17H36O	001454-85-9	91
3	4-Tetradecene, (E)-	196	C14H28	041446-78-0	89
4	1-Tetradecene	196	C14H28	001120-36-1	86
5	2-Tetradecene, (E)-	196	C14H28	035953-53-8	86





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Data File : BM009971.D
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Sample : I3058-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DUP-0398-170508

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM050517.M
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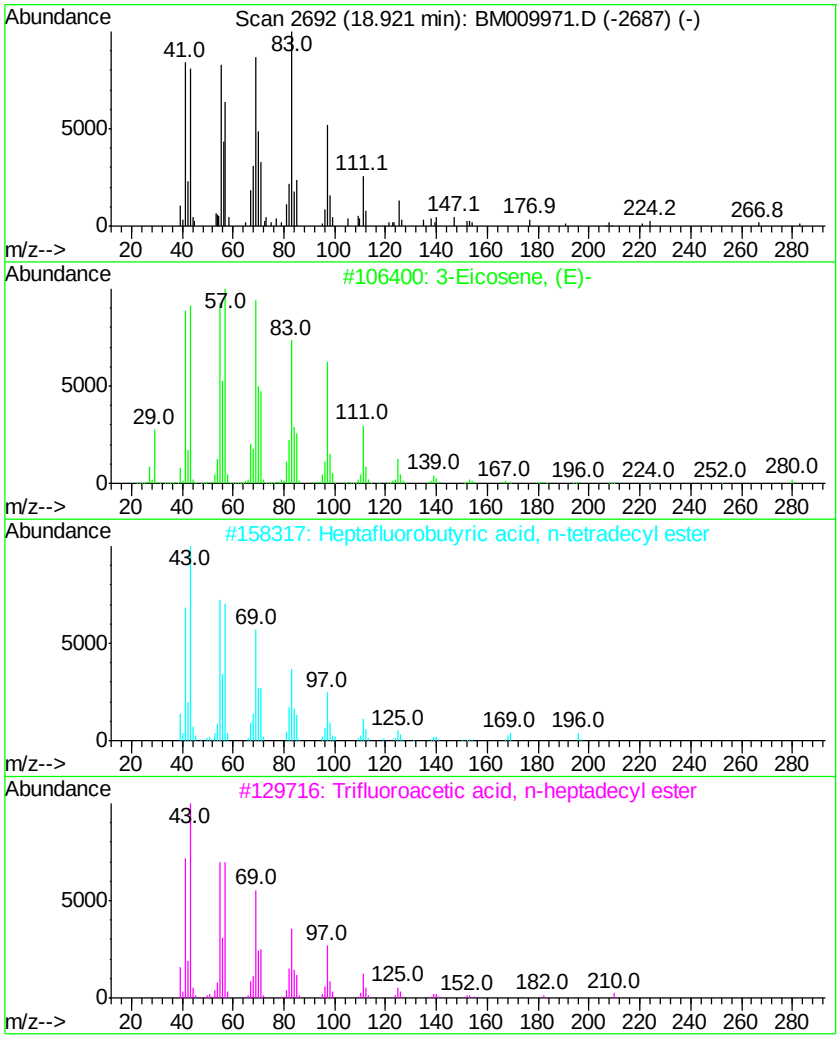
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

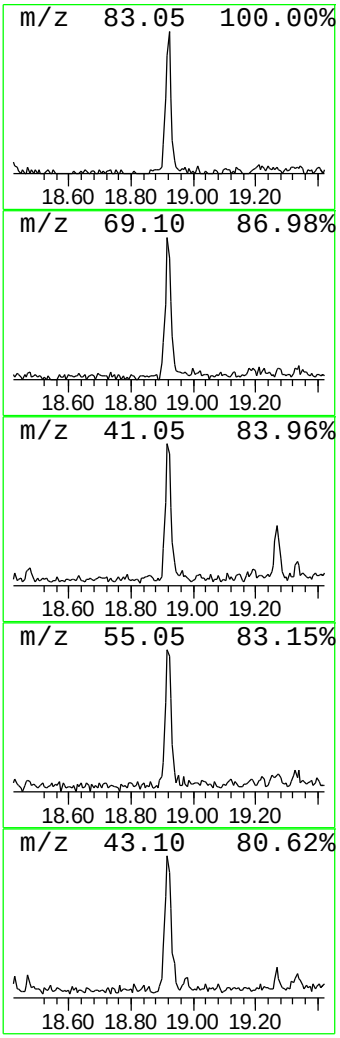
****

Peak Number 9 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.92	3.78 ng	238726	Phenanthrene-d10	17.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91





Tentatively Identified Compound (LSC) summary

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Data File : BM009971.D
Acq On : 10 May 2017 15:21
Operator : SJ/MA
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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
Hydrazinecarboxyl...	4.42	16.8	ng	477934	1	7.77	567816	20.0
2-Pentanone, 4-hy...	4.90	7.9	ng	224084	1	7.77	567816	20.0
Benzene, chloro-	5.09	4.7	ng	132597	1	7.77	567816	20.0
unknown7.30	7.30	102.4	ng	2907150	1	7.77	567816	20.0
6-Nitro-o-tolunit...	15.36	2.6	ng	127863	3	14.42	992358	20.0
Benzenesulfonamid...	16.46	3.6	ng	228603	4	17.17	1262330	20.0
5-Tetradecene, (E)-	17.54	3.1	ng	196067	4	17.17	1262330	20.0
3-Eicosene, (E)-	18.92	3.8	ng	238726	4	17.17	1262330	20.0