LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079073.D
Acq On : 9 May 2015 9:58
Operator : TP/IZ
Sample : G2151-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-9.0

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-BF043015.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	1.484	24	26	29	rVB	463311	498533	7.18%	1.758%
2	1.621	34	38	41	rVB	197720	411954	5.93%	1.453%
3	1.747	48	49	52	rBV	620417	834532	12.01%	2.943%
4	1.804	52	54	58	rVV	279472	406223	5.85%	1.433%
5	1.873	58	60	98	rVB	3410035	6947133	100.00%	24.503%
6	5.119	343	344	351	rVB	93696	130175	1.87%	0.459%
7	5.622	385	388	391	rBV	1945627	1940362	27.93%	6.844%
8	6.879	495	498	500	rBV	2263561	2027958	29.19%	7.153%
9	7.027	509	511	514	rBV	1924541	2004644	28.86%	7.070%
10	7.313	534	536	539	rBV	291312	393548	5.66%	1.388%
11	7.507	550	553	555	rBV	1652362	1540318	22.17%	5.433%
12	8.010	594	597	599	rBV	1410911	1250020	17.99%	4.409%
13	8.319	621	624	633	rVB	98164	182490	2.63%	0.644%
14	8.890	672	674	677	rBV	492473	536243	7.72%	1.891%
15	10.239	790	792	795	rBV	2527759	2275625	32.76%	8.026%
16	10.742	834	836	839	rBV	106532	95214	1.37%	0.336%
17	11.074	862	865	867	rBV	597303	601344	8.66%	2.121%
18	11.542	904	906	910	rBV	75286	83801	1.21%	0.296%
19	12.056	948	951	953	rBV2	1193296	1583994	22.80%	5.587%
20	12.914	1024	1026	1029	rBV	674781	643178	9.26%	2.268%
21	14.914	1198	1201	1203	rBV	2543551	2441648	35.15%	8.612%
22	16.091	1301	1304	1312	rBV	82059	150308	2.16%	0.530%
23	16.205	1312	1314	1317	rBV	621327	637664	9.18%	2.249%
24	17.360	1413	1415	1418	rBV	96804	113833	1.64%	0.401%
25	17.954	1464	1467	1470	rBV	437392	621886	8.95%	2.193%

Sum of corrected areas: 28352628

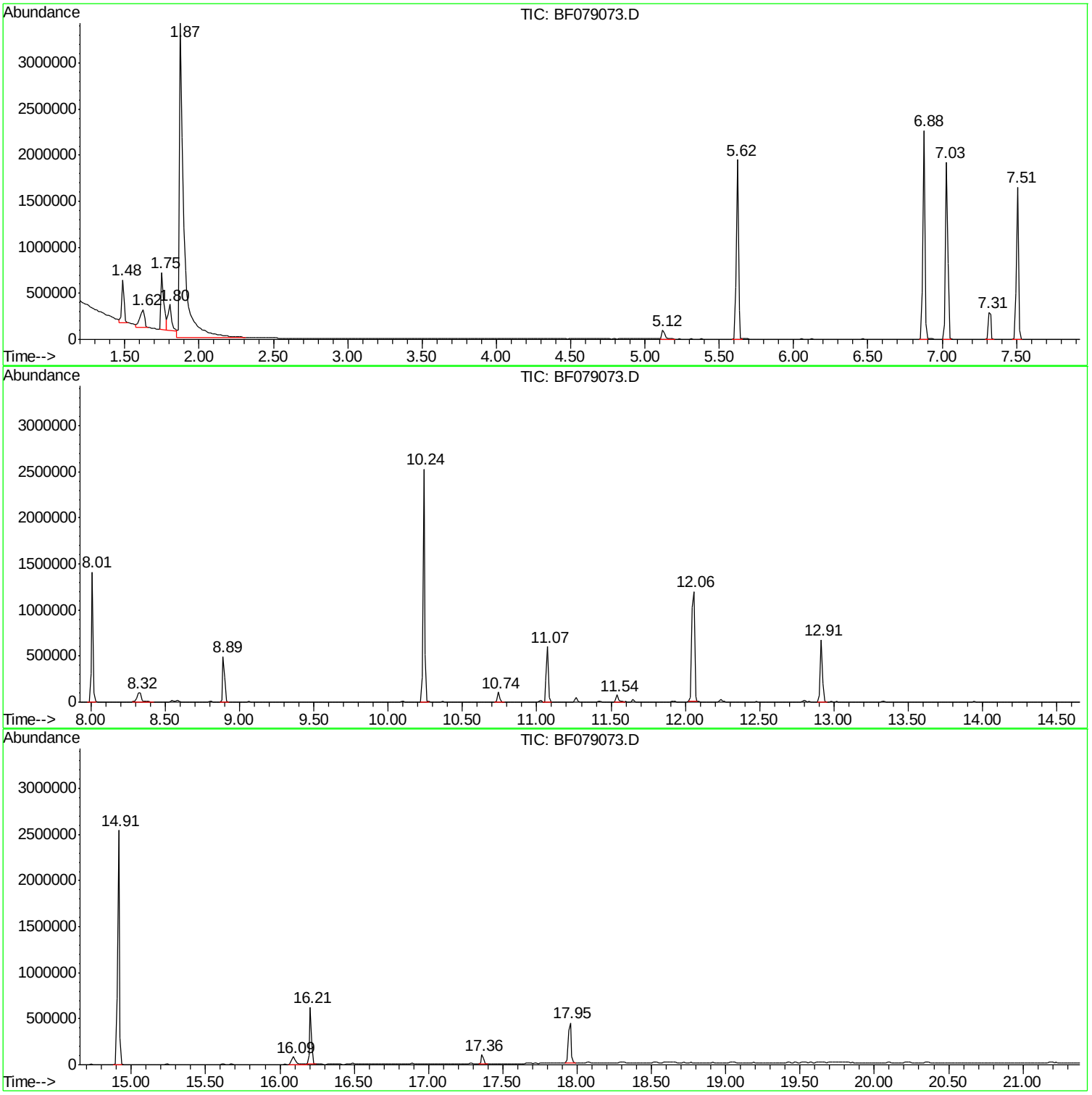
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079073.D
Acq On : 9 May 2015 9:58
Operator : TP/IZ
Sample : G2151-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-9.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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 F\DATA\BF050815\
Data File : BF079073.D
Acq On : 9 May 2015 9:58
Operator : TP/IZ
Sample : G2151-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-9.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

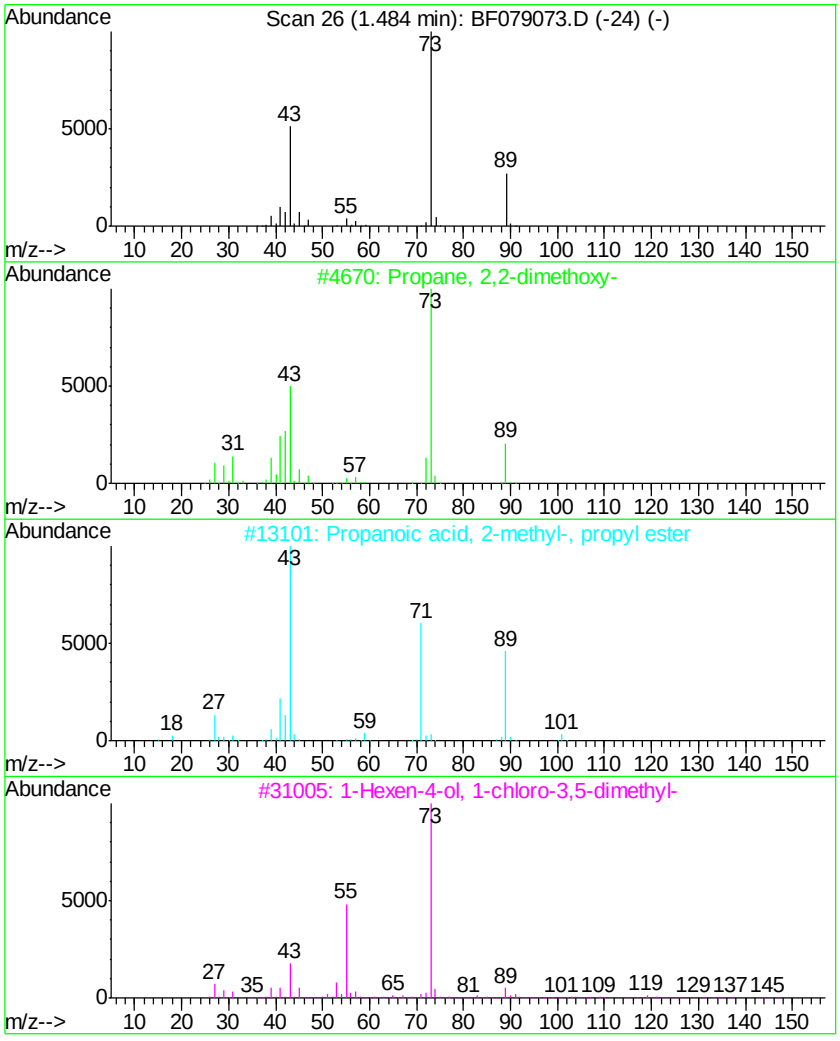
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

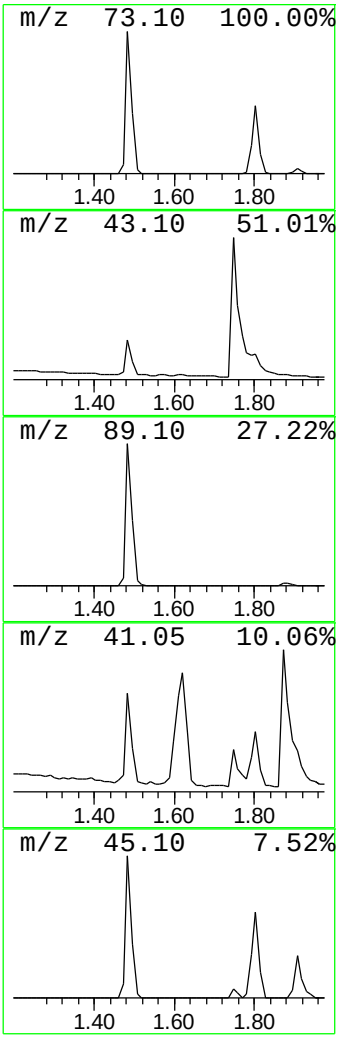
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	25.34 ng	498533	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
3	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	7





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Data File : BF079073.D
Acq On : 9 May 2015 9:58
Operator : TP/IZ
Sample : G2151-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-9.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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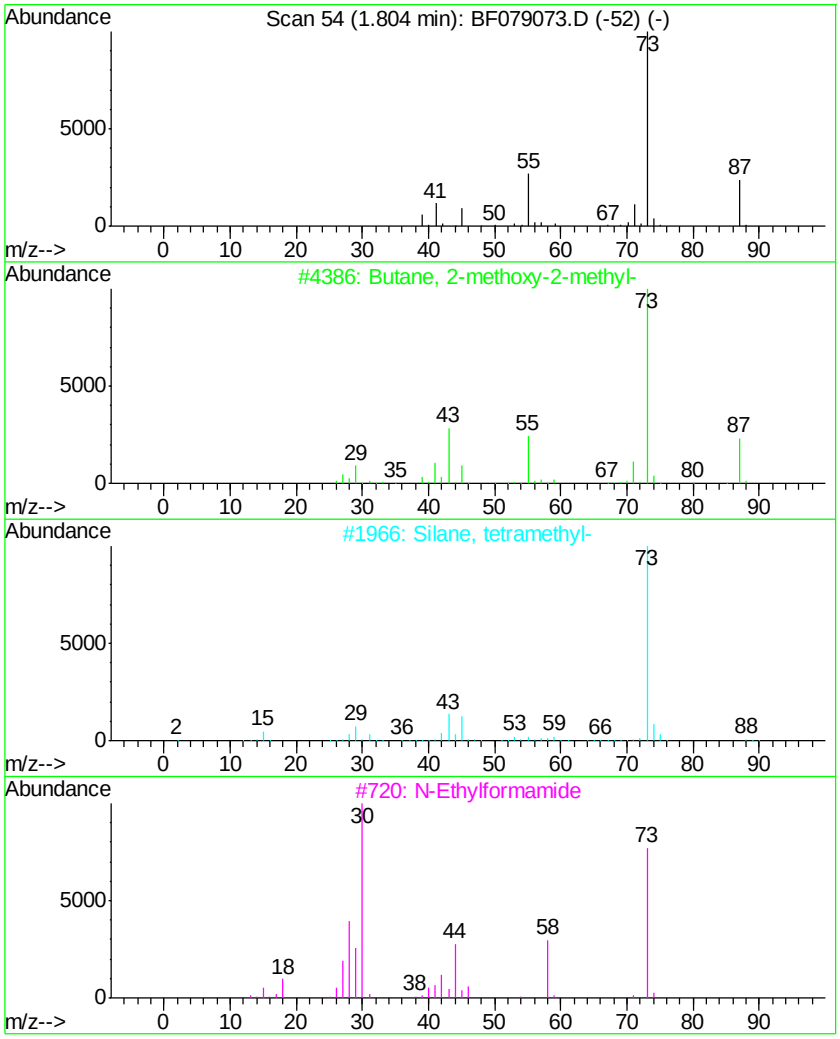
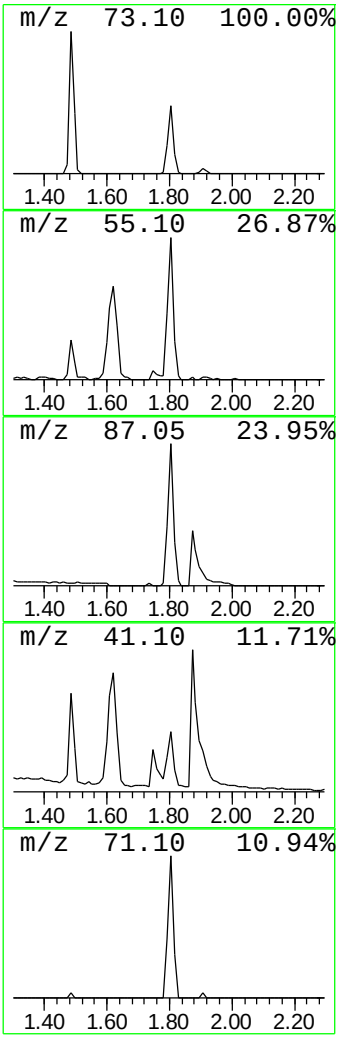
Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.80	20.64 ng	406223	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079073.D
Acq On : 9 May 2015 9:58
Operator : TP/IZ
Sample : G2151-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-9.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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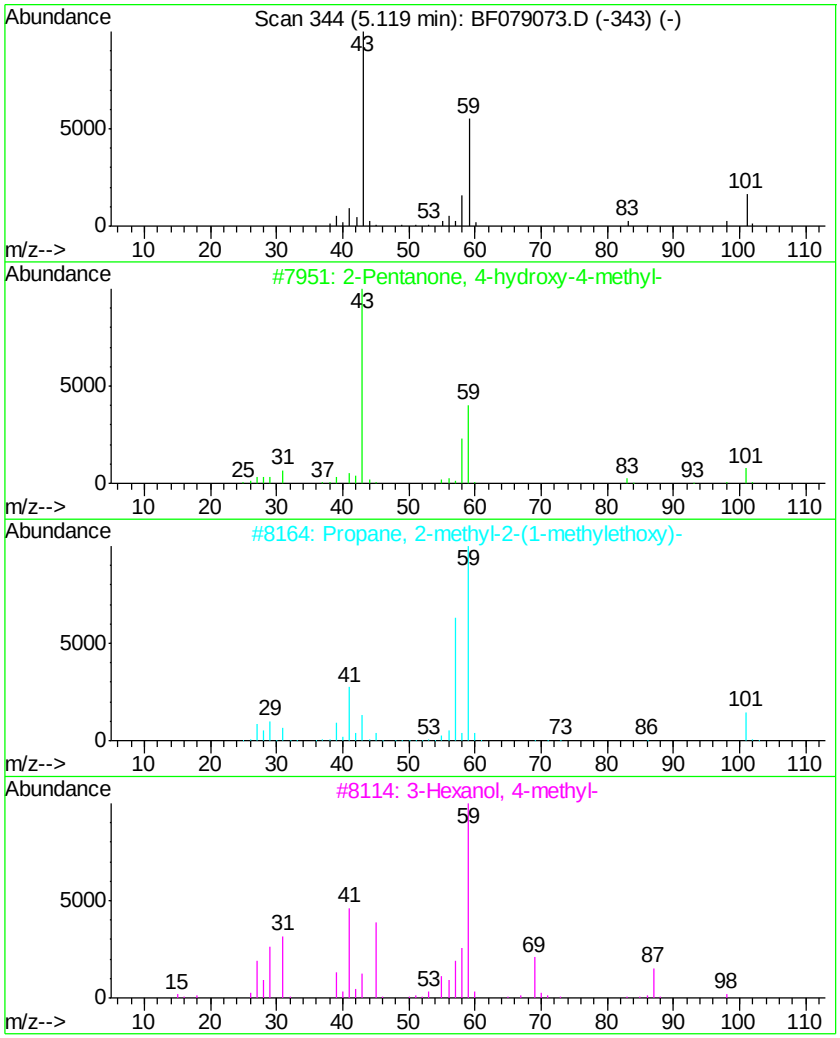
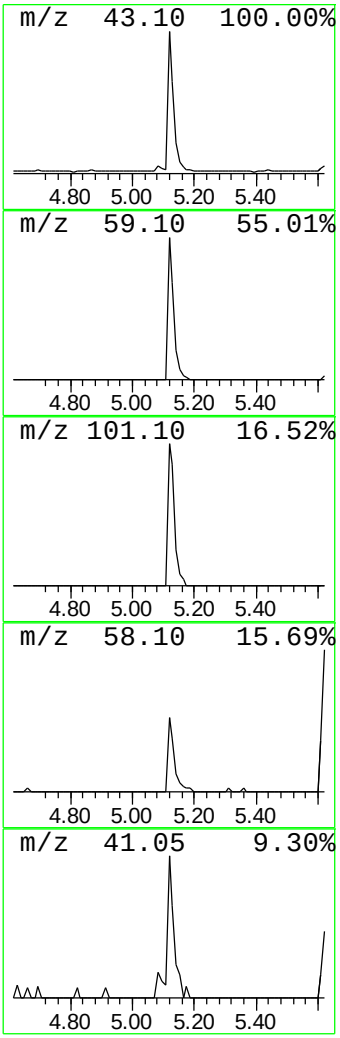
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	6.62 ng	130175	1,4-Dichlorobenzene-d4	7.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079073.D
Acq On : 9 May 2015 9:58
Operator : TP/IZ
Sample : G2151-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-9.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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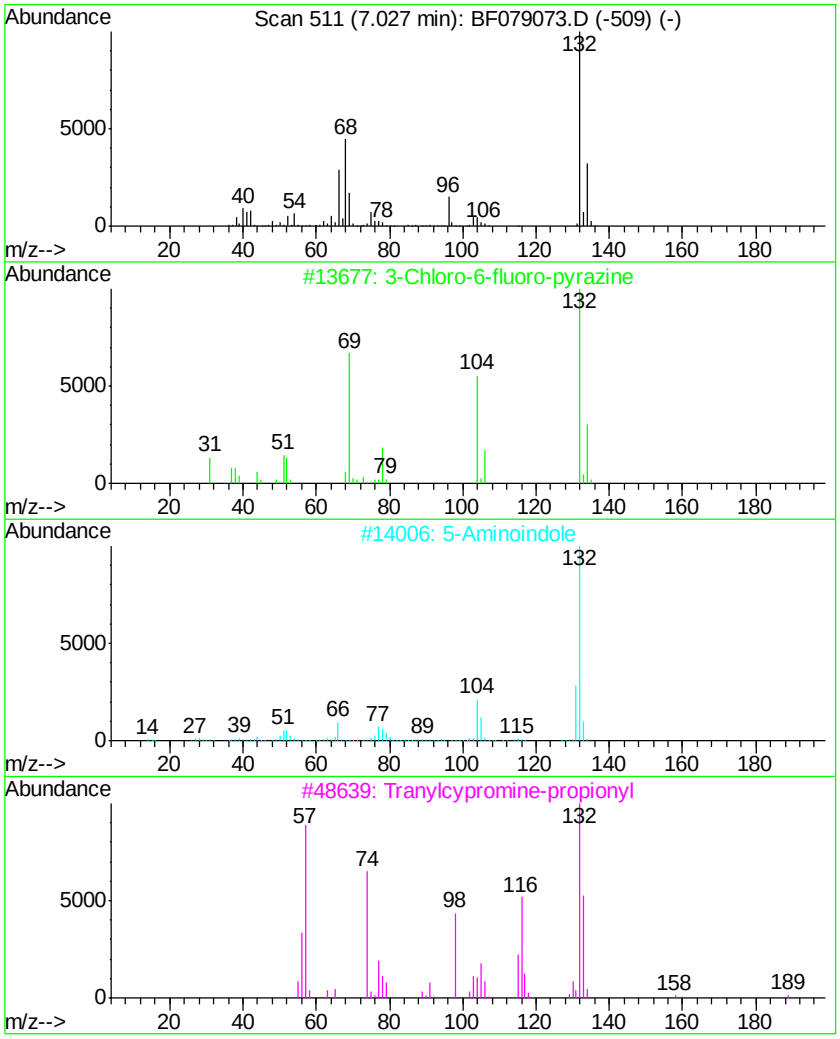
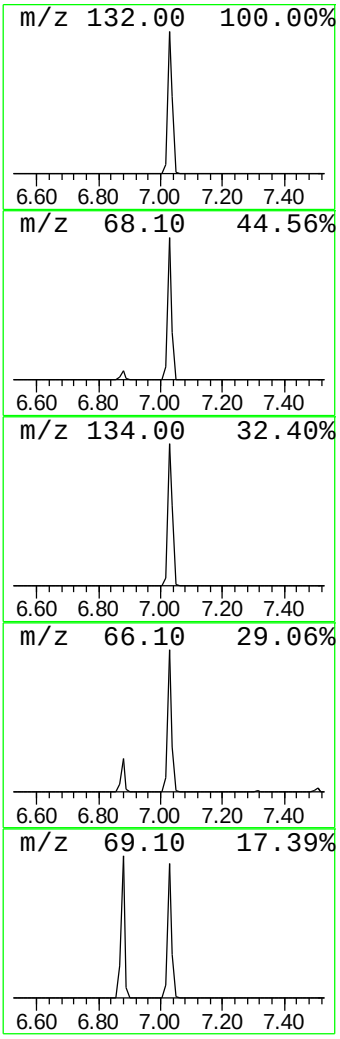
Peak Number 7 unknown7.03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	101.88 ng	2004640	1,4-Dichlorobenzene-d4	7.32

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF050815\
Data File : BF079073.D
Acq On : 9 May 2015 9:58
Operator : TP/IZ
Sample : G2151-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-9.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

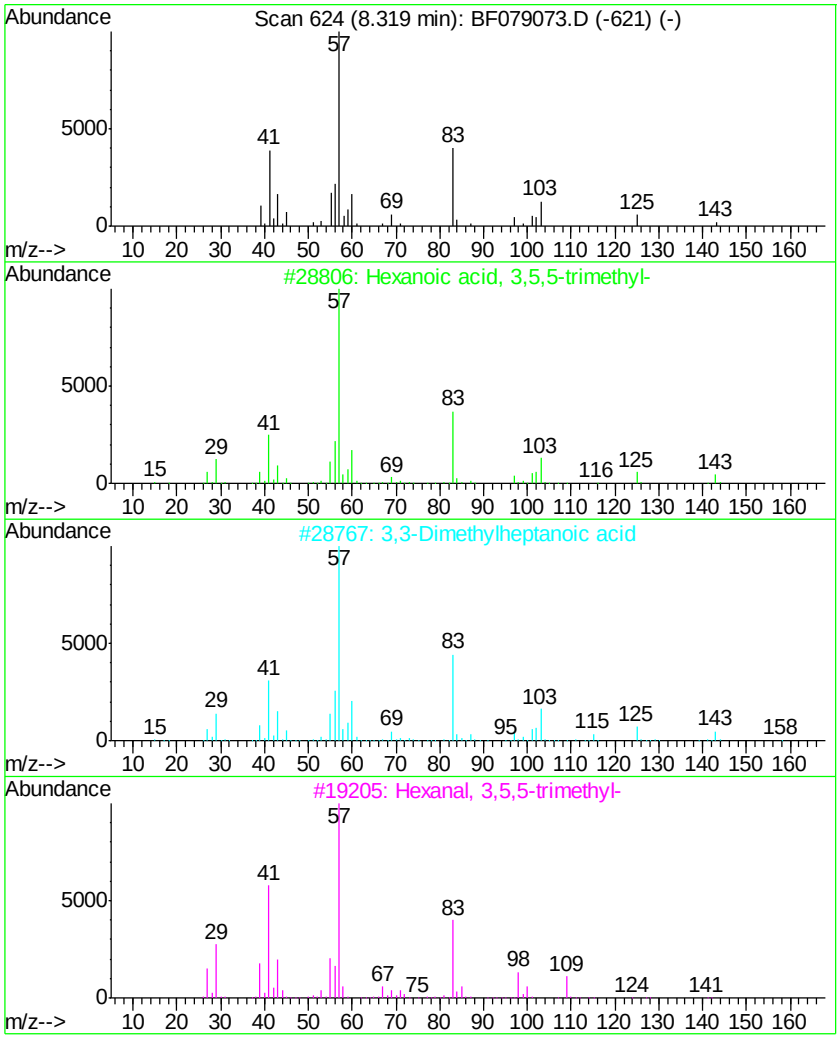
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

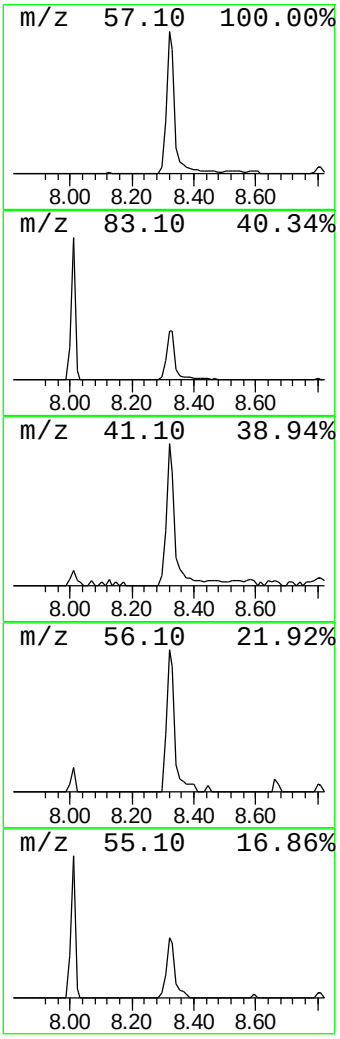
****

Peak Number 9 Hexanoic acid, 3,5,5-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.32	6.81 ng	182490	Naphthalene-d8	8.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3	Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	28
4	Propanoic acid, 2,2-dimethyl-, h...	186	C11H22O2	005434-57-1	16
5	Propanoic acid, 2,2-dimethyl-, h...	200	C12H24O2	017660-61-6	16





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Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-9.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

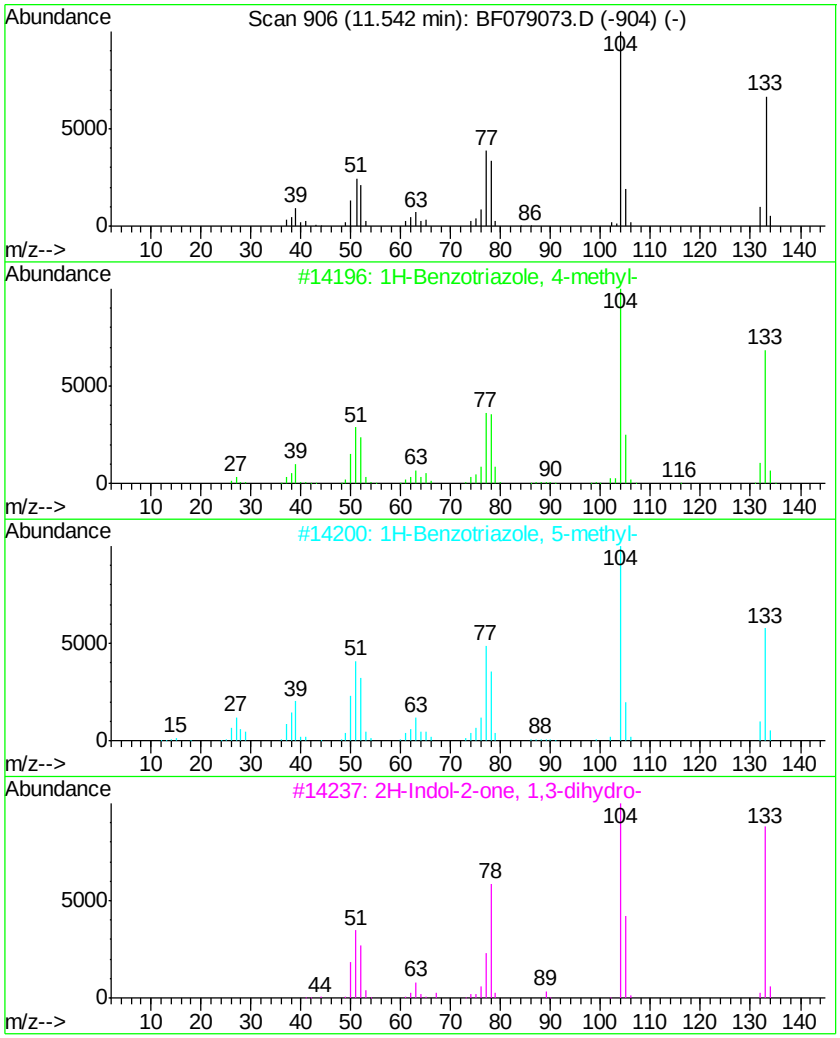
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

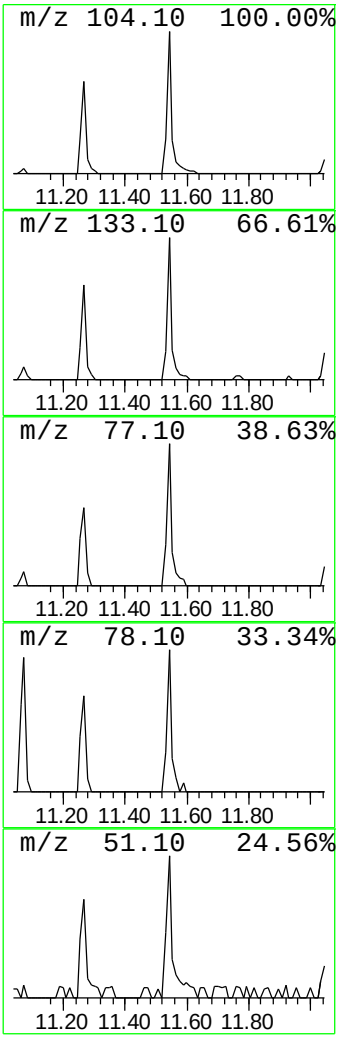
****

Peak Number 10 1H-Benzotriazole, 4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.79 ng	83801	Acenaphthene-d10	11.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	98
2	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	97
3	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	68
4	1H-Indol-5-ol	133	C8H7NO	001953-54-4	53
5	Benzene, 1-isocyanato-4-methyl-	133	C8H7NO	000622-58-2	50





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Operator : TP/IZ
Sample : G2151-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TU012-SB-16-9.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

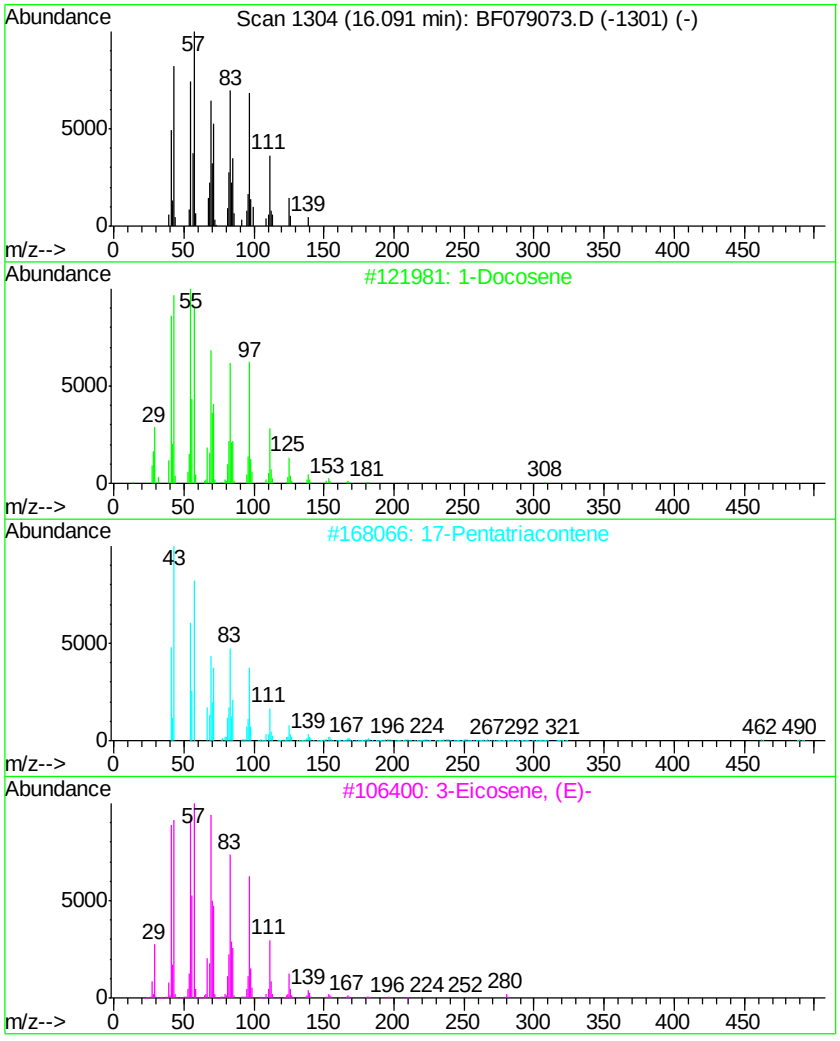
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

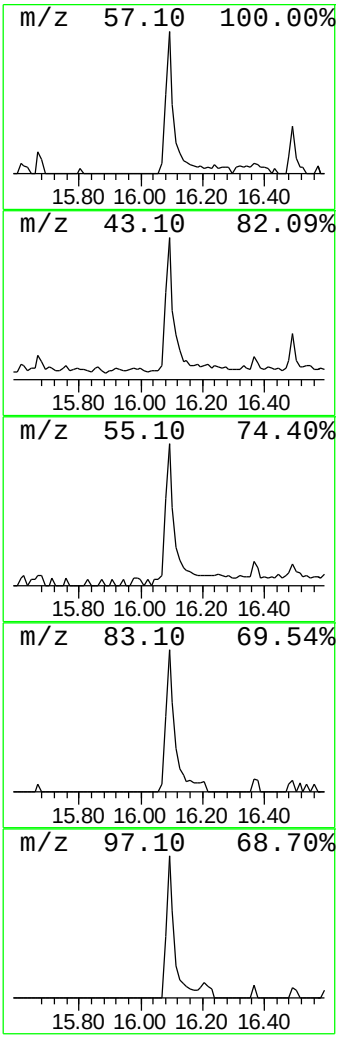
****

Peak Number 11 1-Docosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	4.71 ng	150308	Chrysene-d12	16.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	90
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	74
4	1-Hexacosanol	382	C26H54O	000506-52-5	72
5	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	64





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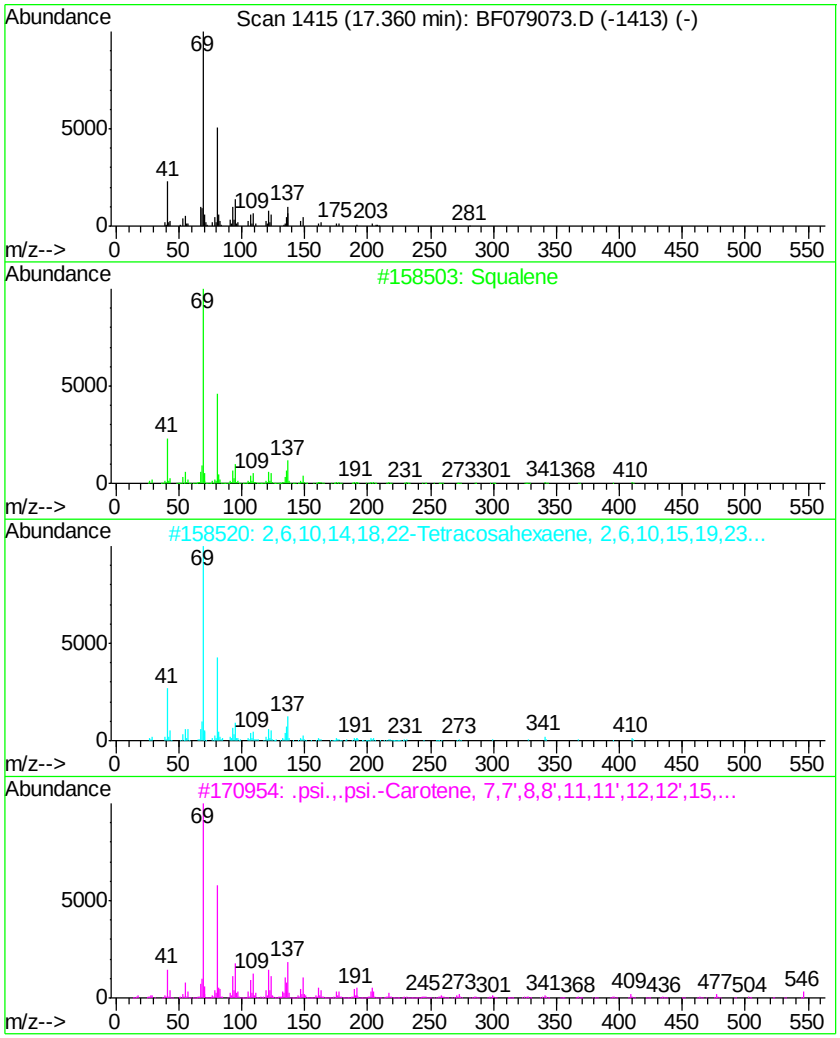
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

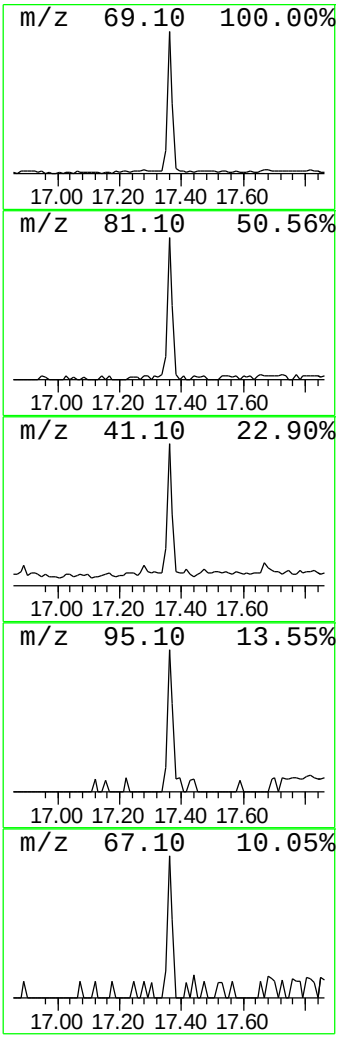
****

Peak Number 12 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.36	3.66 ng	113833	Perylene-d12	17.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	83
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050815\
Data File : BF079073.D
Acq On : 9 May 2015 9:58
Operator : TP/IZ
Sample : G2151-02
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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
Propane, 2,2-dime...	1.48	25.3	ng	498533	1	7.32	393548	20.0
Butane, 2-methoxy...	1.80	20.6	ng	406223	1	7.32	393548	20.0
2-Pentanone, 4-hy...	5.12	6.6	ng	130175	1	7.32	393548	20.0
unknown7.03	7.03	101.9	ng	2004640	1	7.32	393548	20.0
Hexanoic acid, 3,...	8.32	6.8	ng	182490	2	8.89	536243	20.0
1H-Benzotriazole,...	11.54	2.8	ng	83801	3	11.07	601344	20.0
1-Docosene	16.09	4.7	ng	150308	5	16.21	637664	20.0
Squalene	17.36	3.7	ng	113833	6	17.95	621886	20.0