LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49C-9-11

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-BF041717.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	3.937	335	340	348	rBV	489761	583924	14.68%	1.652%
2	4.331	402	407	410	rBV	3312649	3257710	81.88%	9.218%
3	5.401	583	589	592	rBV	2877311	3572096	89.79%	10.107%
4	5.525	605	610	614	rBV	3275607	3581133	90.01%	10.133%
5	5.772	648	652	665	rBV	859916	744341	18.71%	2.106%
6	5.954	678	683	686	rBV	2647118	2705766	68.01%	7.656%
7	6.425	757	763	766	rBV	2133178	2205987	55.45%	6.242%
8	6.589	787	791	797	rBV	53829	70889	1.78%	0.201%
9	7.266	902	906	909	rBV	1093014	968203	24.34%	2.740%
10	8.589	1126	1131	1134	rBV	3804266	3907256	98.21%	11.056%
11	8.772	1159	1162	1167	rVB	45097	44781	1.13%	0.127%
12	9.089	1211	1216	1219	rBV	1222267	1071814	26.94%	3.033%
13	9.395	1264	1268	1273	rVB2	976237	950080	23.88%	2.688%
14	10.377	1429	1435	1438	rBV	1974025	2306282	57.97%	6.526%
15	10.577	1466	1469	1472	rBV	56555	57762	1.45%	0.163%
16	11.218	1573	1578	1581	rBV	1081026	1116434	28.06%	3.159%
17	11.571	1634	1638	1650	rBV	231887	346944	8.72%	0.982%
18	12.583	1806	1810	1824	rBV	1177695	1483153	37.28%	4.197%
19	13.201	1909	1915	1918	rBV	3338553	3978496	100.00%	11.257%
20	13.518	1965	1969	1972	rBV3	37471	62003	1.56%	0.175%
21	13.789	2009	2015	2020	rBV	167443	182134	4.58%	0.515%
22	13.918	2033	2037	2041	rVB3	38819	44157	1.11%	0.125%
23	14.371	2107	2114	2121	rBV2	128532	218822	5.50%	0.619%
24	14.459	2125	2129	2134	rVV	929490	960482	24.14%	2.718%
25	14.518	2134	2139	2144	rVB	118607	131998	3.32%	0.373%
26	15.324	2272	2276	2282	rBV	73784	79130	1.99%	0.224%
27	16.083	2401	2405	2415	rVB	655638	709499	17.83%	2.008%

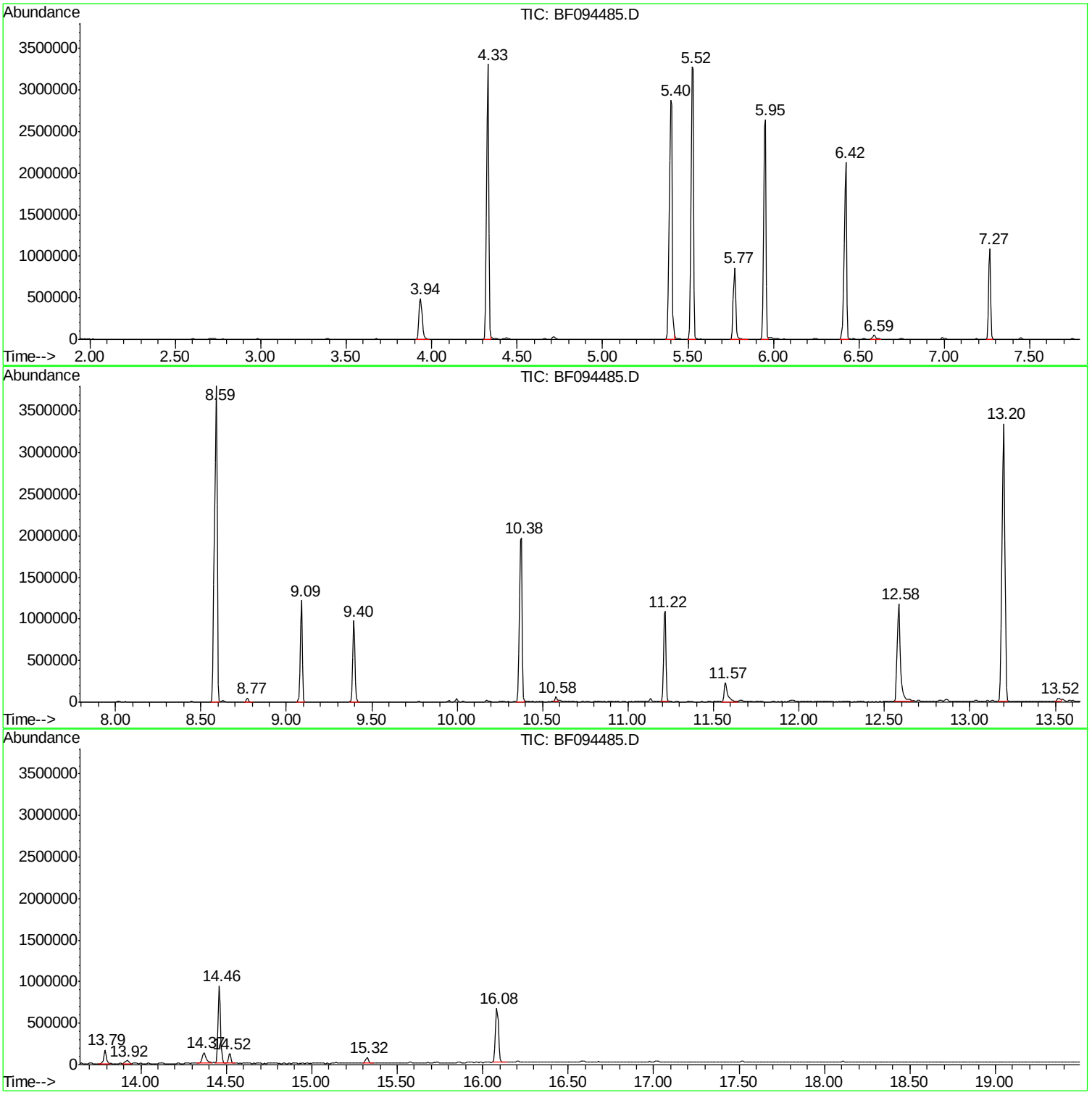
Sum of corrected areas: 35341276

Data Path : Z:\HPCHEM1\BNA F\Data\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
49C-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49C-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

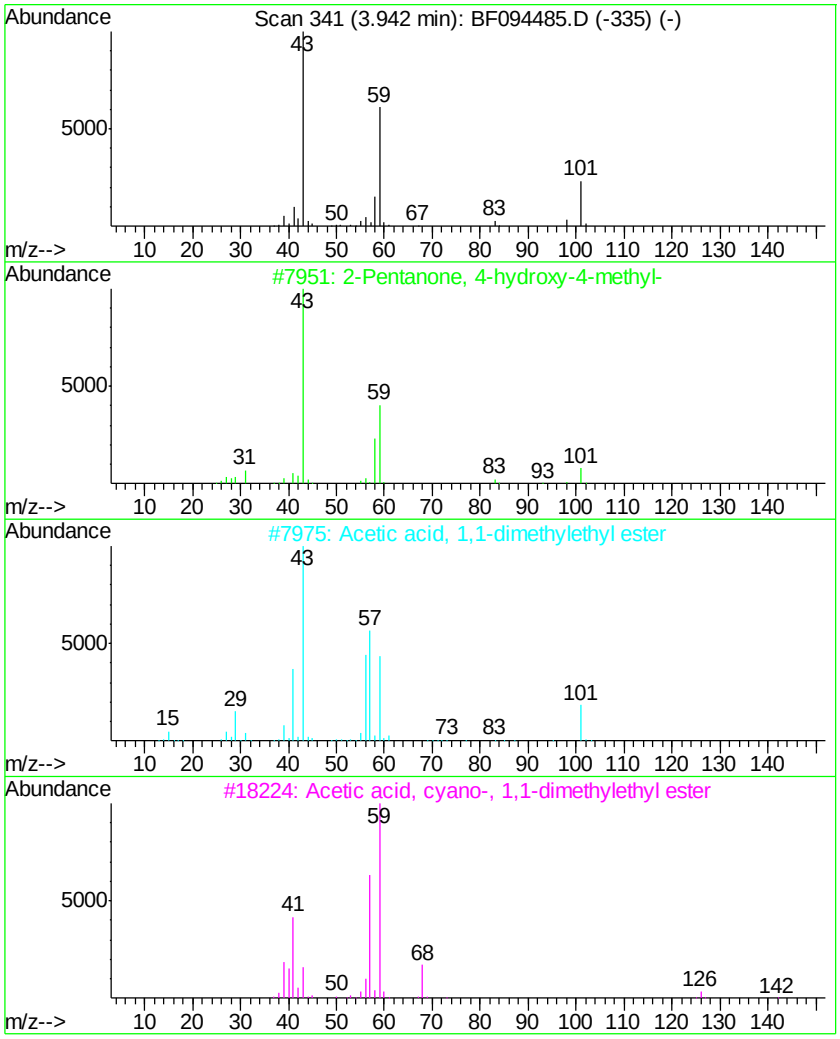
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

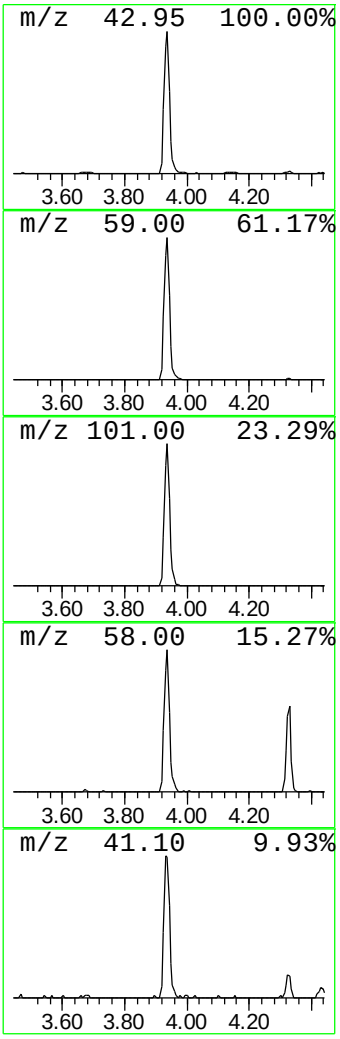
****

Peak Number 1 unknown3.94 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	15.69 ng	583924	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Data Path : Z:\HPCHEM1\BNA F\Data\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49C-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

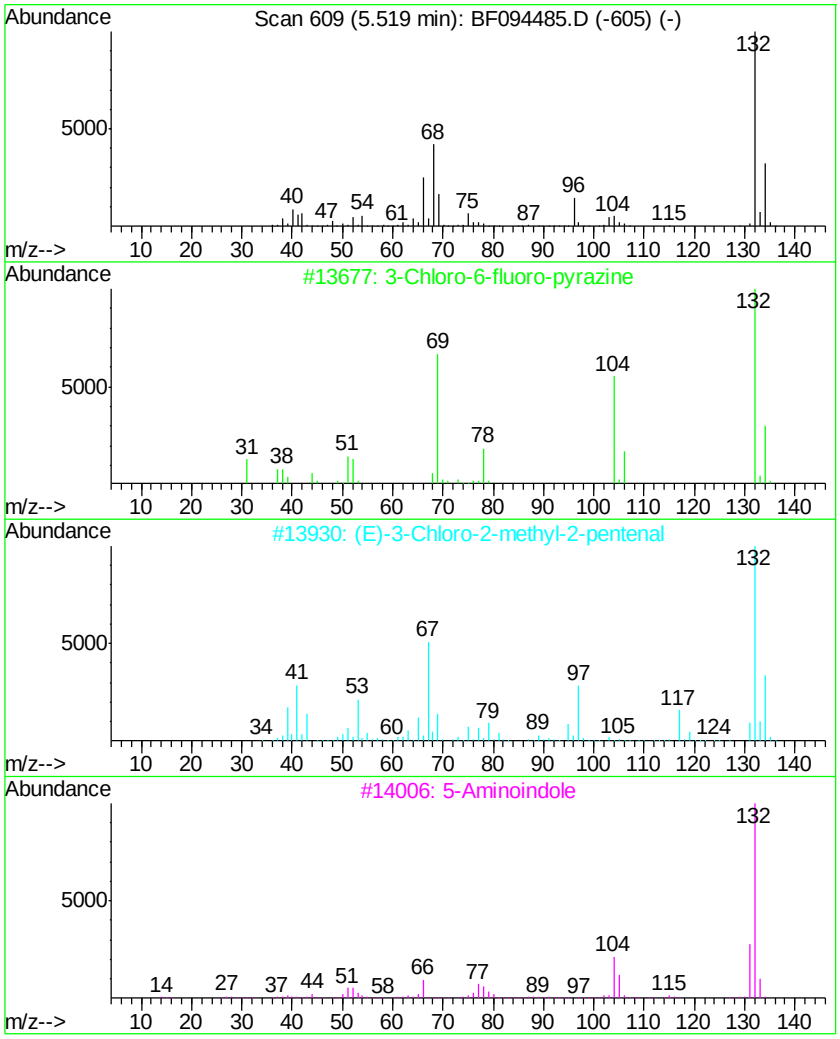
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

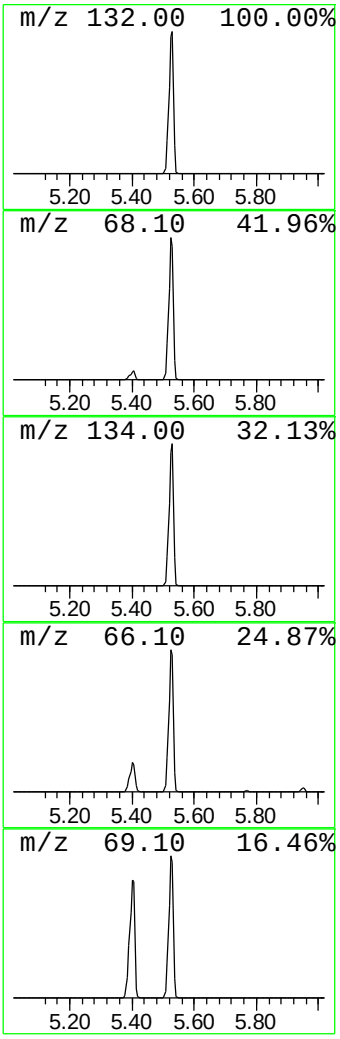
****

Peak Number 2 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	96.22 ng	3581130	1,4-Dichlorobenzene-d4	5.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49C-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

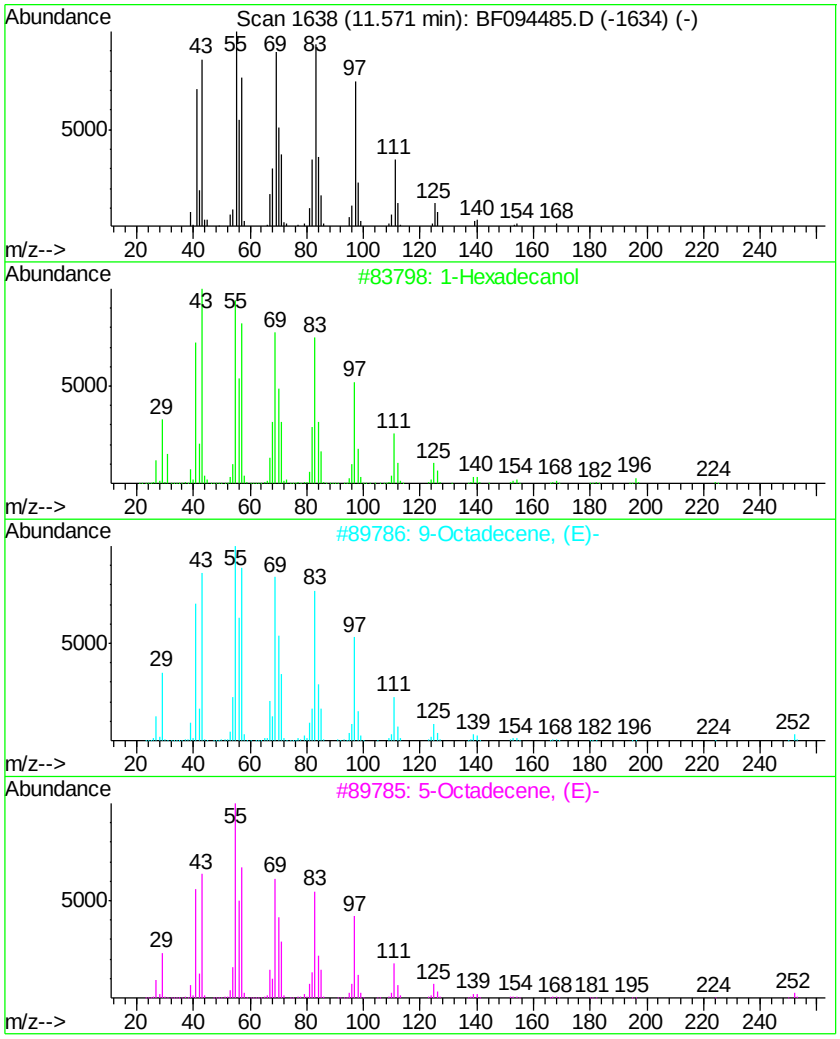
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

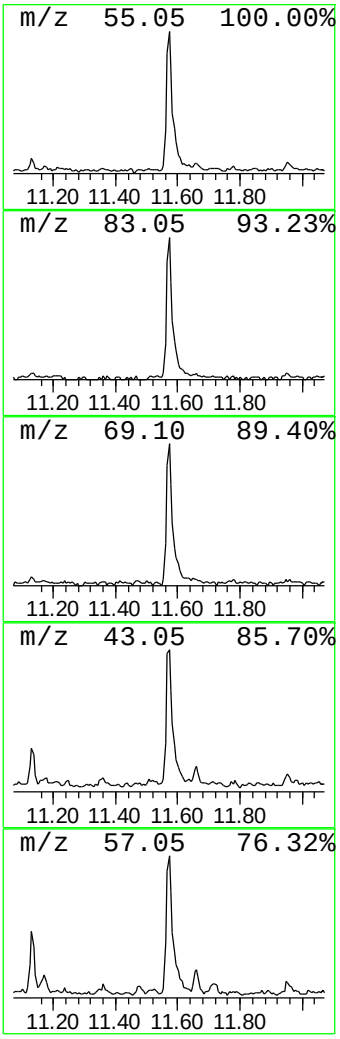
****

Peak Number 4 1-Hexadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	6.22 ng	346944	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	91
2	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
4	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91
5	1-Heptadecanol	256	C17H36O	001454-85-9	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49C-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

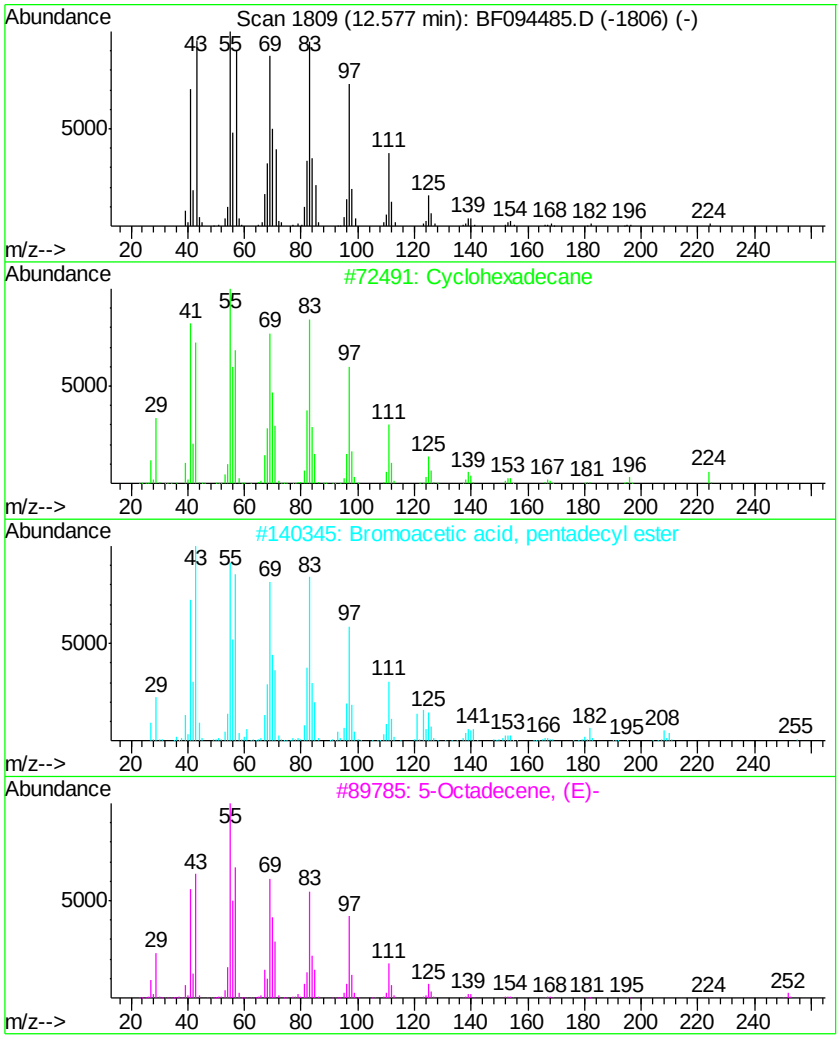
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

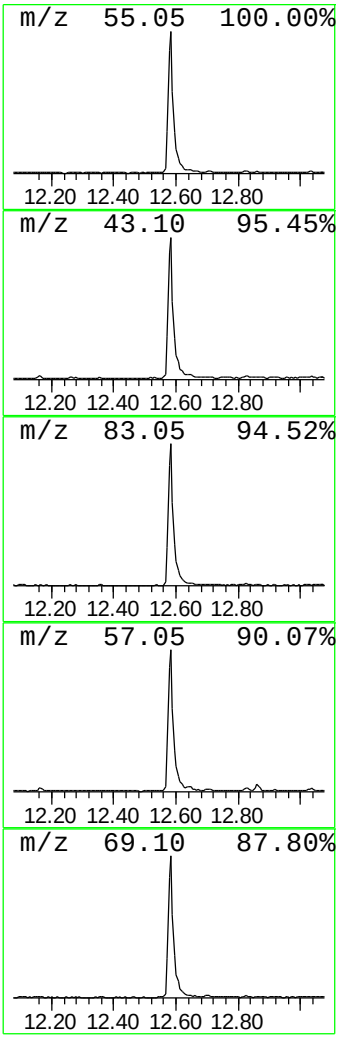
****

Peak Number 5 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	26.57 ng	1483150	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	94
2	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	1-Octadecanol	270	C18H38O	000112-92-5	91





Data Path : Z:\HPCHEM1\BNA F\Data\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49C-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

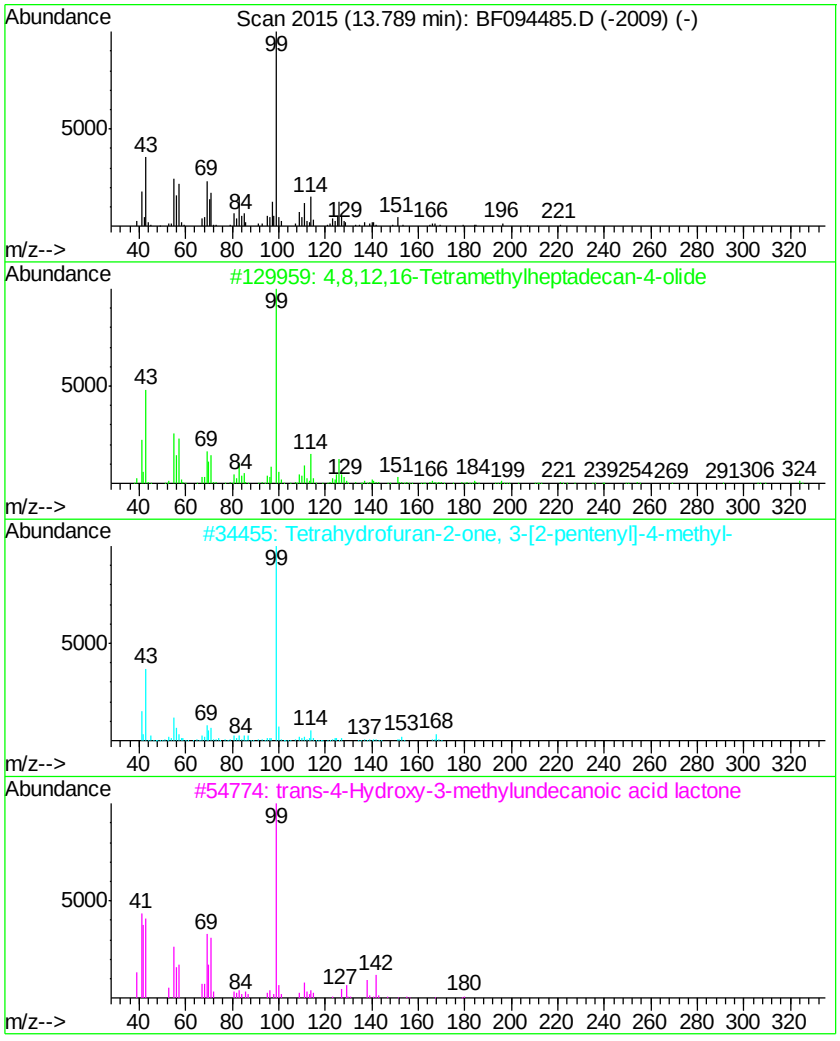
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

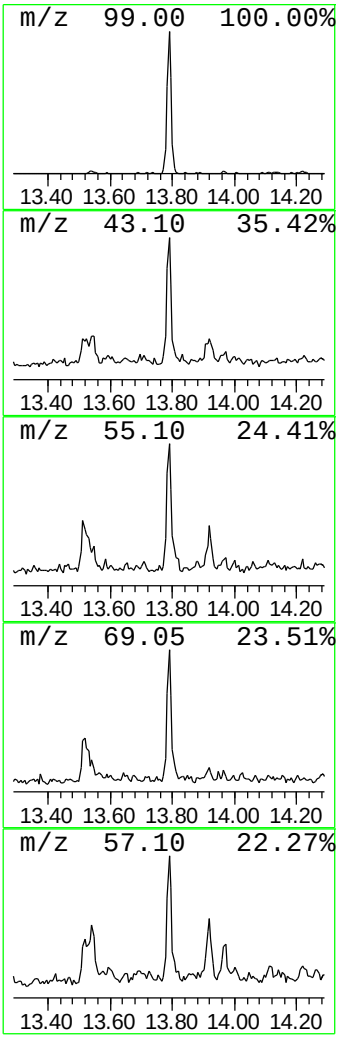
****

Peak Number 6 4,8,12,16-Tetramethylheptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.79 ng	182134	Chrysene-d12	14.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8,12,16-Tetramethylheptadecan-...	324	C21H40O2	096168-15-9	91
2	Tetrahydrofuran-2-one, 3-[2-pent...	168	C10H16O2	1000132-08-6	59
3	trans-4-Hydroxy-3-methylundecano...	198	C12H22O2	148806-10-4	53
4	Hexanoic acid, 4-hexadecyl ester	340	C22H44O2	1000282-83-8	53
5	Tripropyl phosphate	224	C9H21O4P	000513-08-6	50





Data Path : Z:\HPCHEM1\BNA F\Data\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49C-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

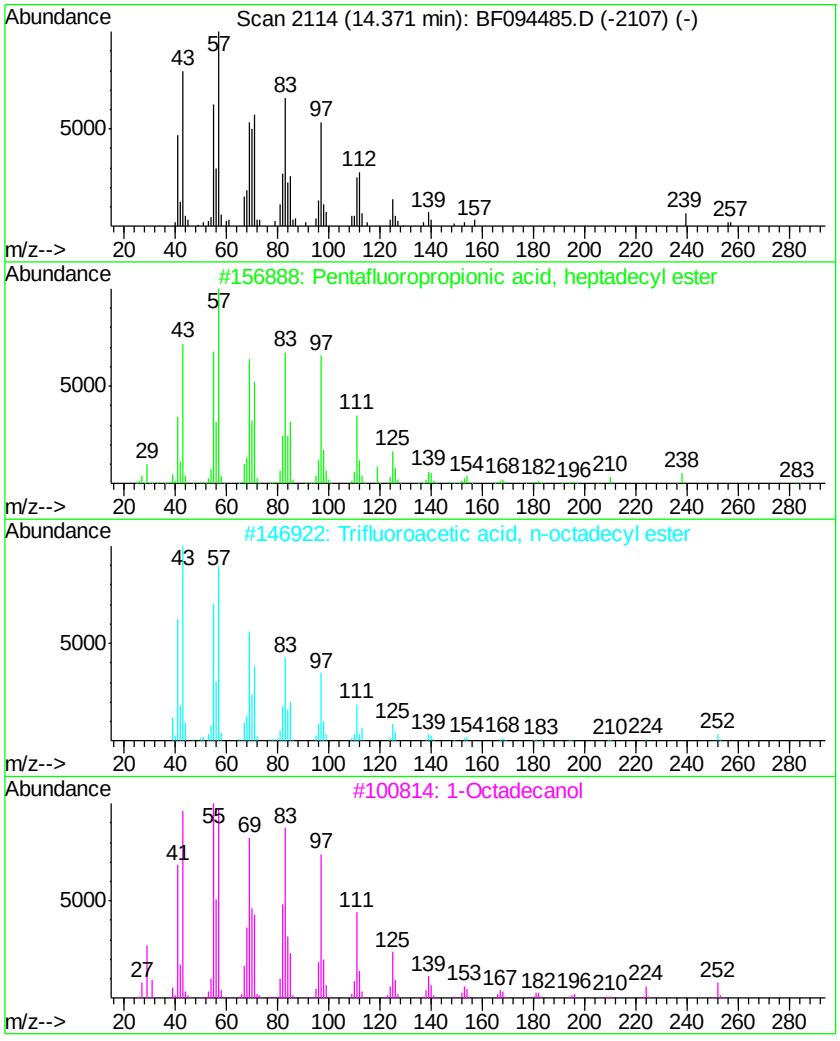
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

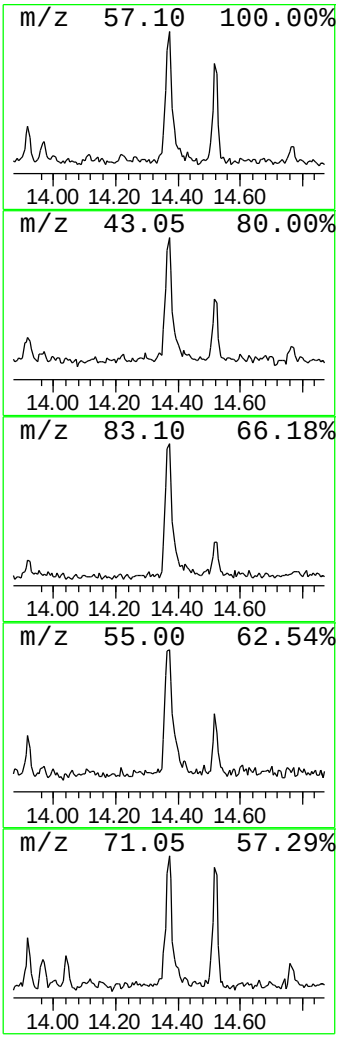
****

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	4.56 ng	218822	Chrysene-d12	14.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	83
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	80
3	1-Octadecanol	270	C18H38O	000112-92-5	76
4	17-Pentatriacontene	491	C35H70	006971-40-0	72
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	68





Data Path : Z:\HPCHEM1\BNA F\Data\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49C-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

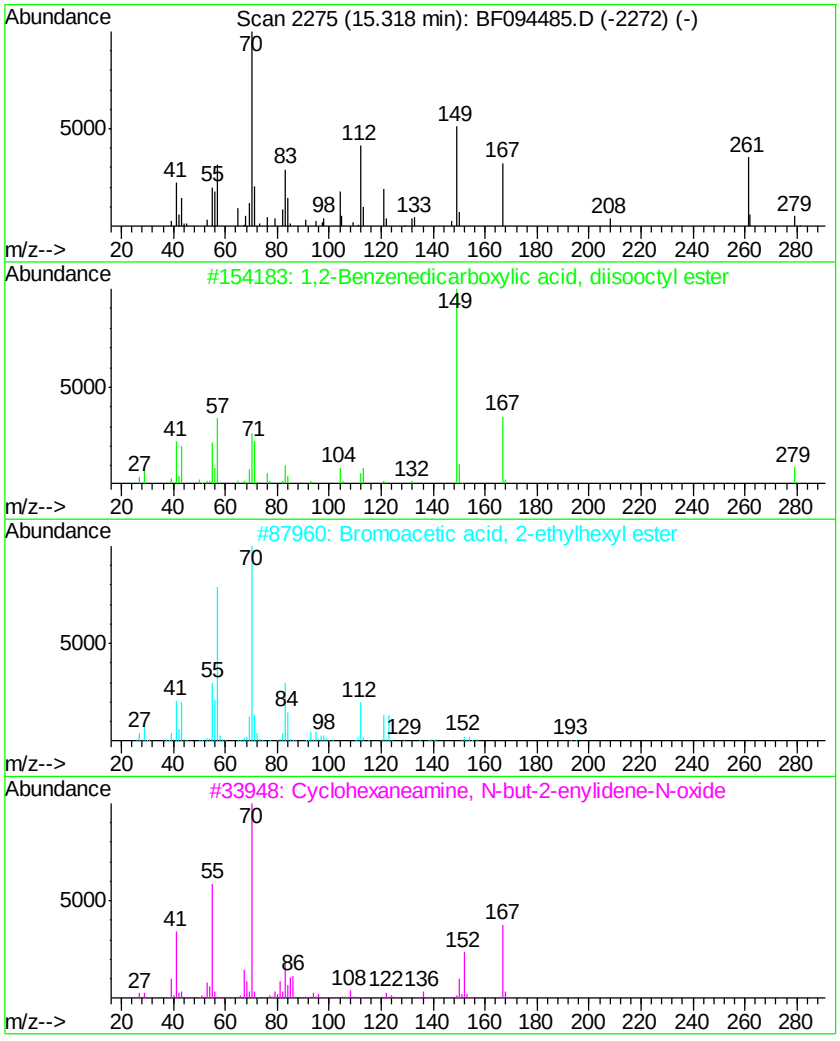
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

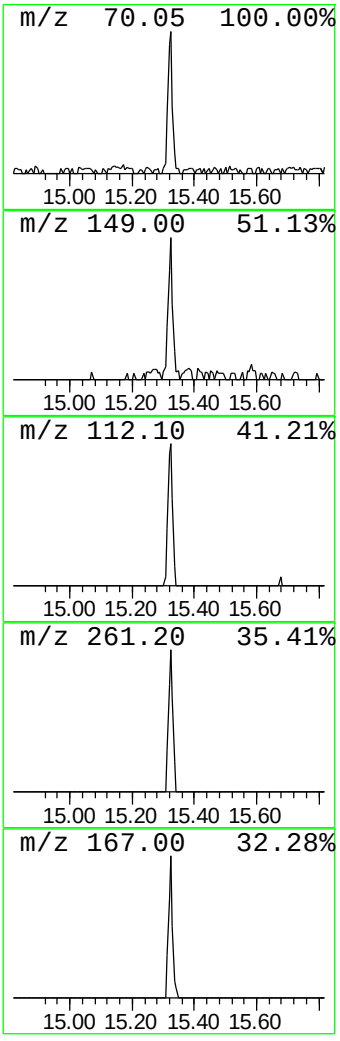
****

Peak Number 8 unknown15.32 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	2.23 ng	79130	Perylene-d12	16.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	37
2	Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	22
3	Cyclohexaneamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	17
4	2-Heptene, 3-methyl-	112	C8H16	003404-75-9	16
5	Benzoic acid, 3-(4-nitro-1-pyraz...	261	C12H11N3O4	1000273-84-4	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF041817\
Data File : BF094485.D
Acq On : 18 Apr 2017 14:24
Operator : SJ/MA
Sample : I2695-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 49C-9-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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
unknown3.94	3.94	15.7	ng	583924	1	5.77	744341	20.0
unknown5.52	5.52	96.2	ng	3581130	1	5.77	744341	20.0
1-Hexadecanol	11.57	6.2	ng	346944	4	11.22	1116430	20.0
Cyclohexadecane	12.58	26.6	ng	1483150	4	11.22	1116430	20.0
4,8,12,16-Tetrame...	13.79	3.8	ng	182134	5	14.46	960482	20.0
Pentafluoropropio...	14.37	4.6	ng	218822	5	14.46	960482	20.0
unknown15.32	15.32	2.2	ng	79130	6	16.08	709499	20.0