LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

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-BF020318.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	2.181	8	16	23	rVB	758069	991227	23.47%	2.558%
2	4.492	405	409	417	rBV	588172	685212	16.23%	1.768%
3	5.116	509	515	527	rVB	1985321	2555273	60.51%	6.593%
4	5.510	577	582	585	rBV	3629329	3400827	80.53%	8.775%
5	6.516	748	753	756	rBV	3797388	3999069	94.70%	10.318%
6	6.657	772	777	780	rBV	3846276	3540525	83.84%	9.135%
7	6.886	812	816	819	rBV	1484297	1214591	28.76%	3.134%
8	7.045	838	843	846	rBV	3676250	3480684	82.42%	8.981%
9	7.451	906	912	915	rBV	2916433	2898742	68.64%	7.479%
10	8.169	1030	1034	1037	rBV	1800060	1531000	36.25%	3.950%
11	9.245	1211	1217	1220	rBV	4466422	4223102	100.00%	10.896%
12	9.633	1279	1283	1291	rBV	302168	280256	6.64%	0.723%
13	9.845	1315	1319	1323	rBV	134546	104144	2.47%	0.269%
14	9.921	1328	1332	1341	rVV	1442557	1419061	33.60%	3.661%
15	10.345	1401	1404	1407	rVB	230650	166617	3.95%	0.430%
16	10.563	1435	1441	1444	rBV	66630	92255	2.18%	0.238%
17	10.710	1463	1466	1475	rBV	948614	906597	21.47%	2.339%
18	10.821	1482	1485	1490	rBV	172451	202612	4.80%	0.523%
19	10.968	1507	1510	1513	rVB	54038	50490	1.20%	0.130%
20	11.268	1557	1561	1563	rBV	86402	77292	1.83%	0.199%
21	11.298	1563	1566	1572	rVB	52314	64666	1.53%	0.167%
22	11.410	1582	1585	1589	rBV	1112847	1076128	25.48%	2.777%
23	11.445	1589	1591	1596	rVB2	43252	52138	1.23%	0.135%
24	12.810	1820	1823	1825	rBV	64636	52525	1.24%	0.136%
25	12.998	1851	1855	1858	rBV	2956387	2744773	64.99%	7.082%
26	13.468	1933	1935	1940	rVB	61930	56231	1.33%	0.145%
27	13.880	2002	2005	2010	rBV	680673	642321	15.21%	1.657%
28	14.051	2031	2034	2038	rBV	970525	958804	22.70%	2.474%
29	14.515	2110	2113	2117	rVB2	48837	51089	1.21%	0.132%
30	14.892	2175	2177	2183	rVB	79531	88371	2.09%	0.228%
31	15.162	2220	2223	2226	rVB	46084	46878	1.11%	0.121%
32	15.539	2282	2287	2298	rVB	654533	918641	21.75%	2.370%
33	15.998	2361	2365	2368	rVB3	51827	74847	1.77%	0.193%
34	16.051	2370	2374	2380	rVB3	64163	109799	2.60%	0.283%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 38756787

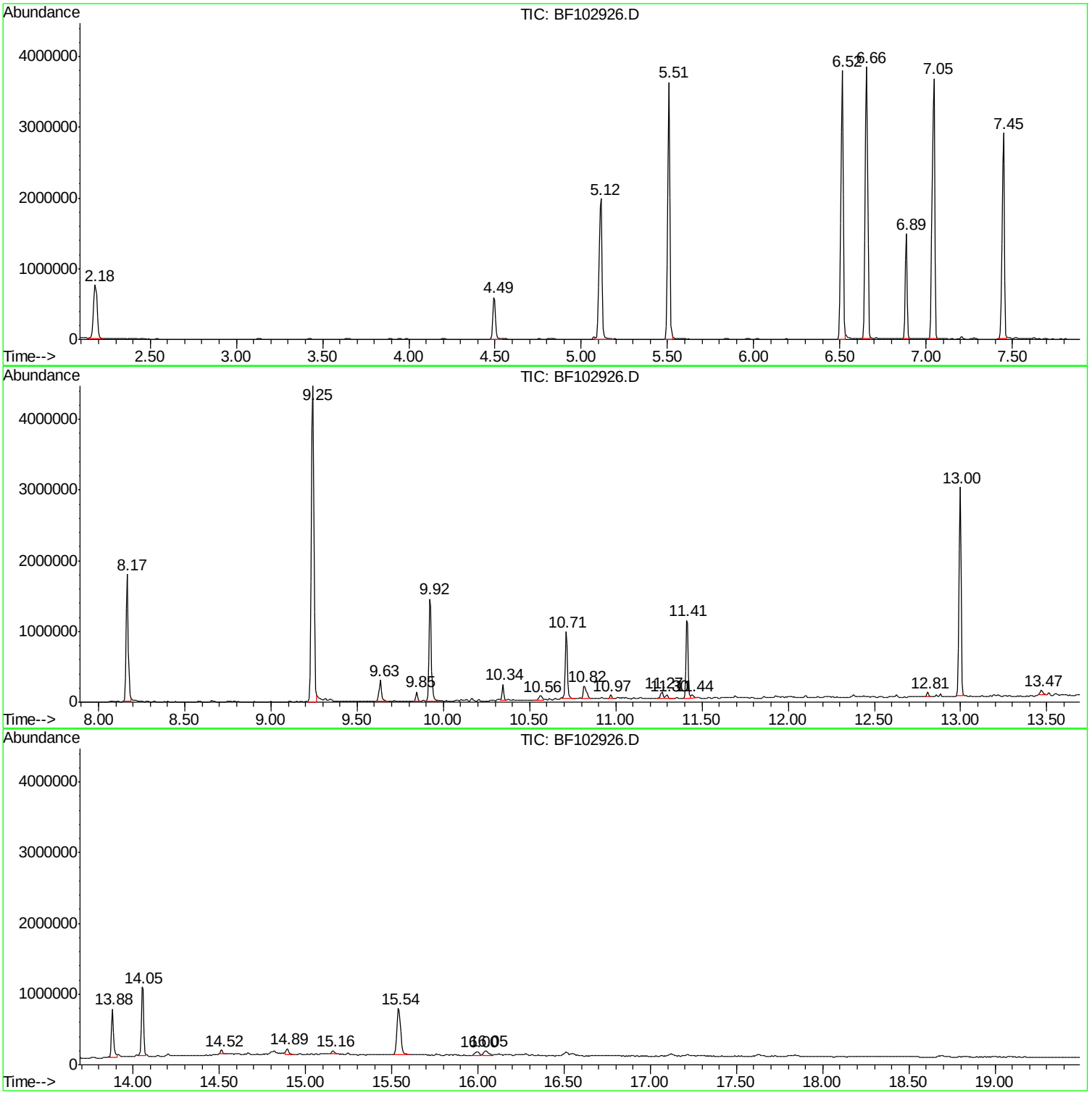
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CO-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

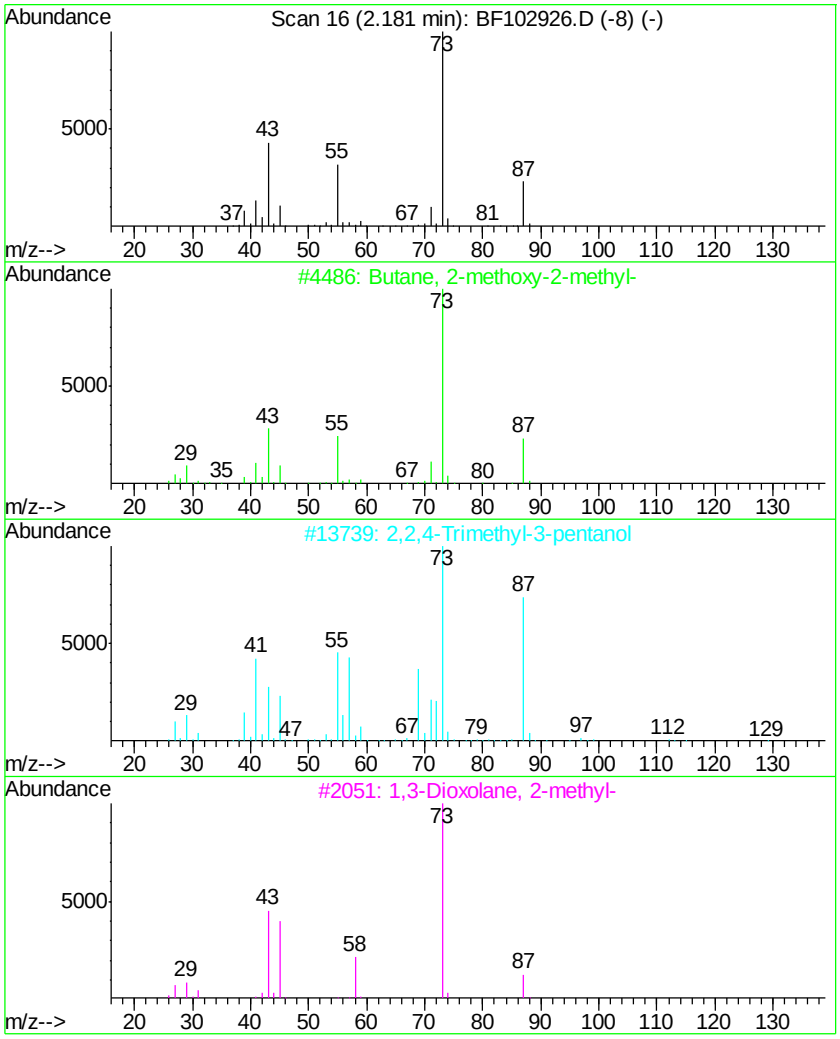
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

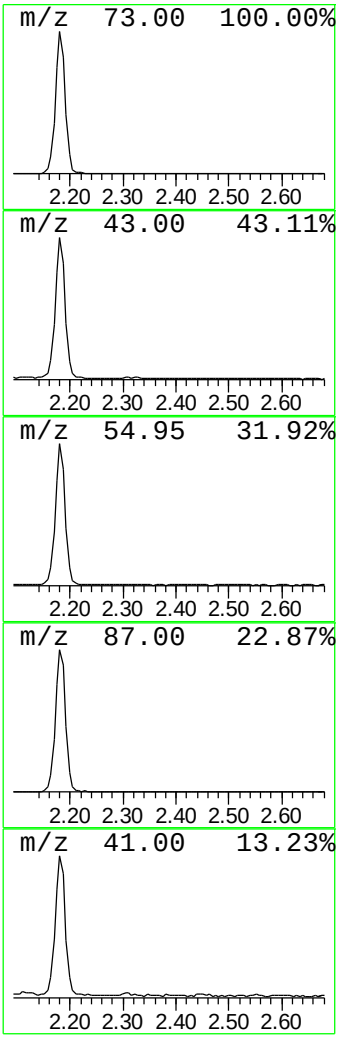
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	16.32 ng	991227	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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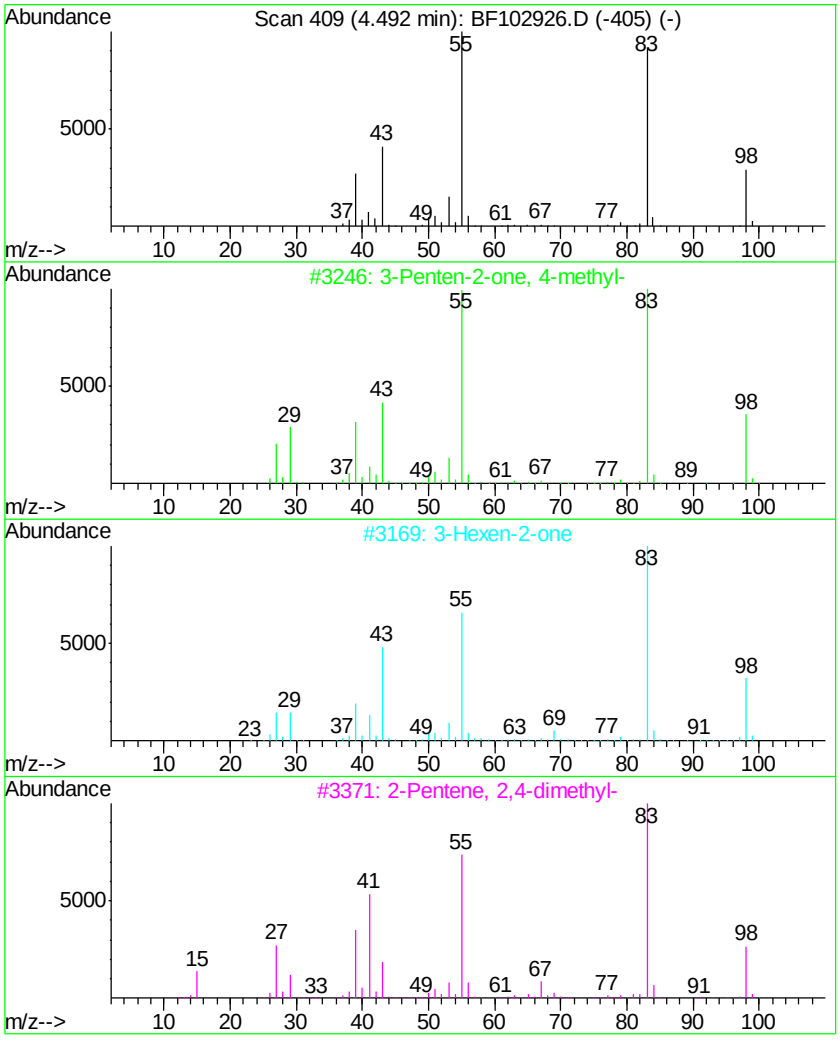
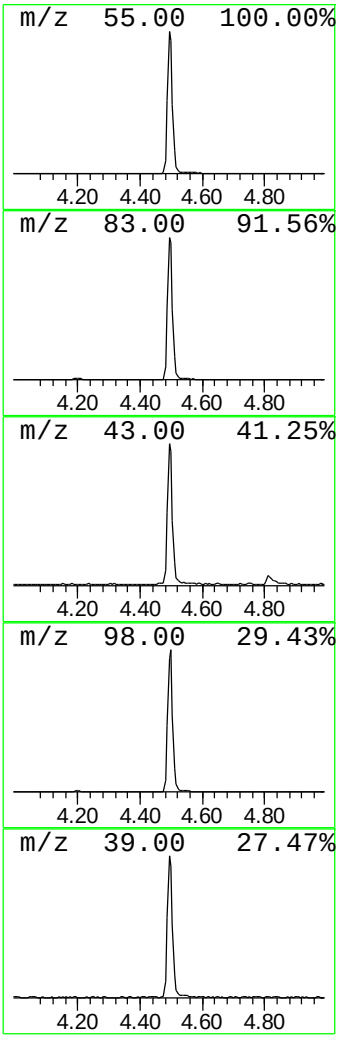
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	11.28 ng	685212	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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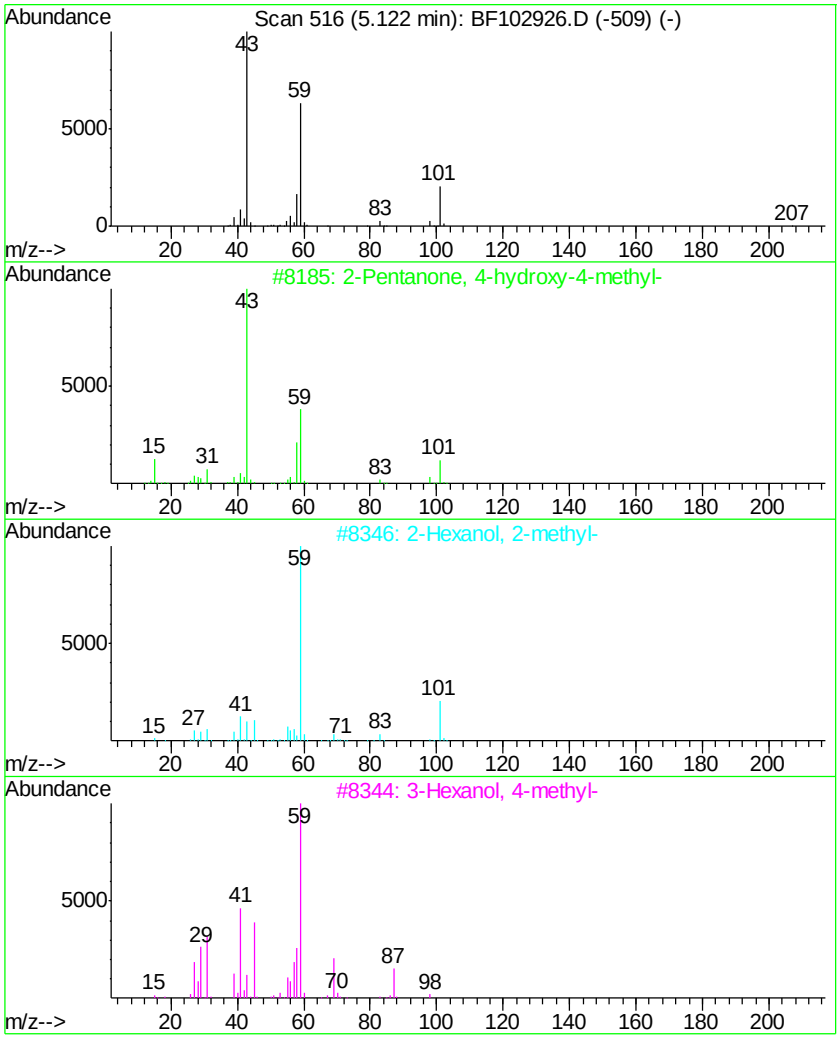
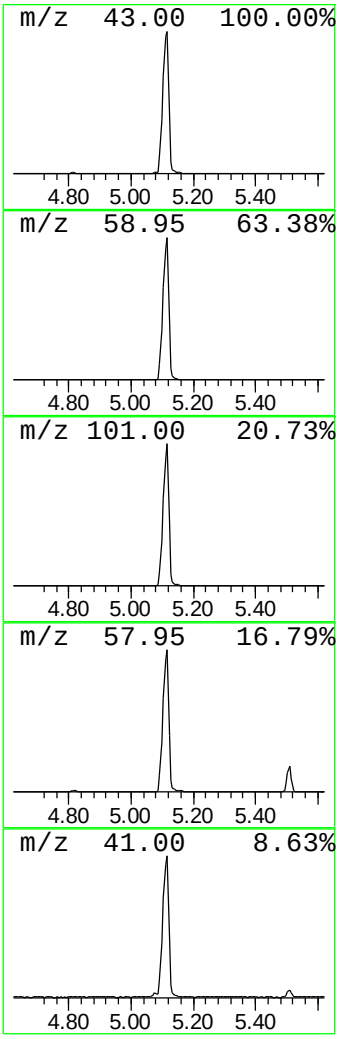
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	42.08 ng	2555270	1,4-Dichlorobenzene-d4	6.89

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





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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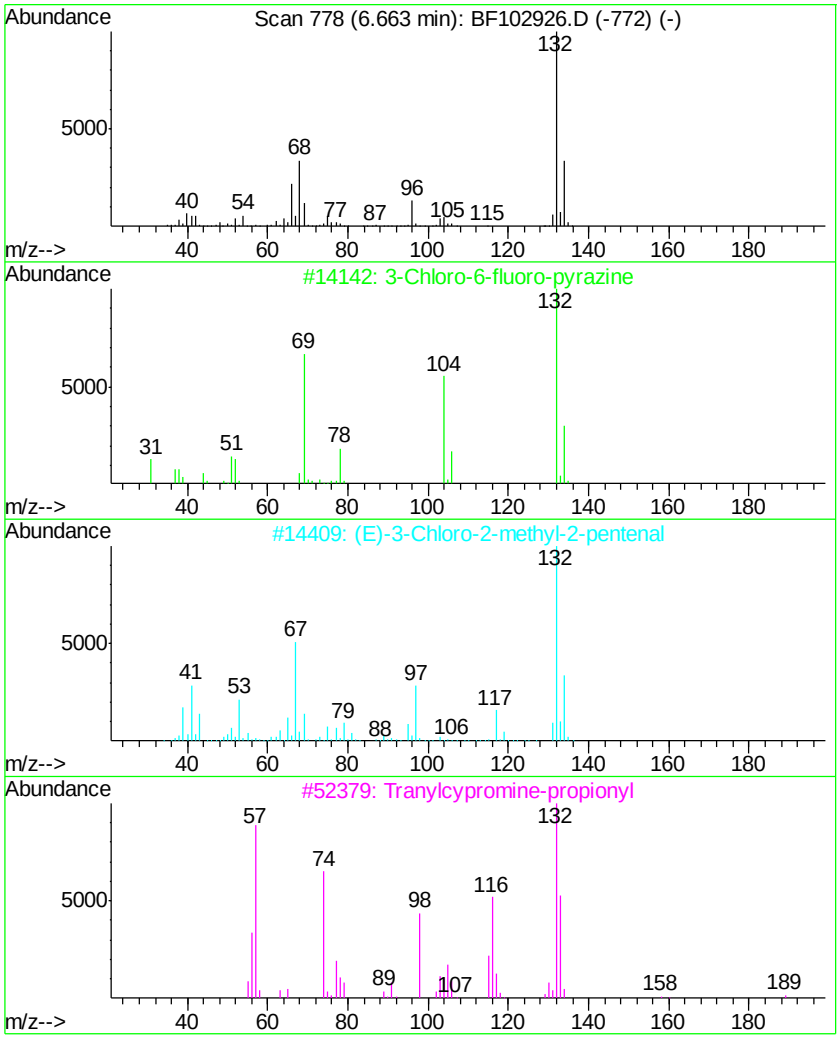
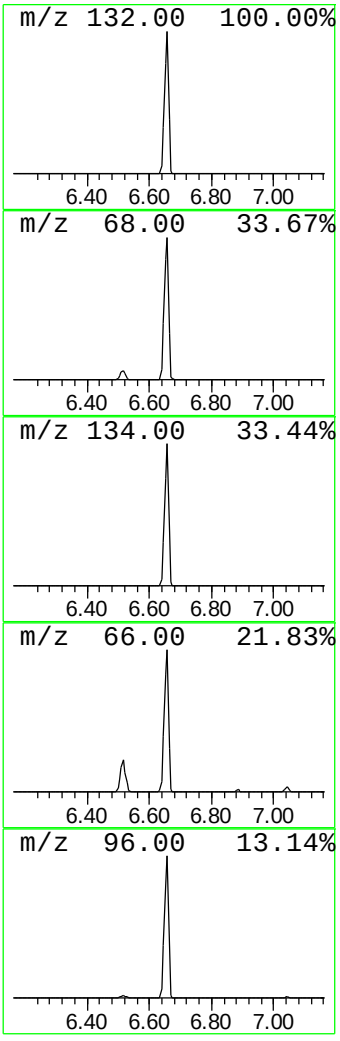
Peak Number 4 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	58.30 ng	3540530	1,4-Dichlorobenzene-d4	6.89

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	17
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	Xenon	132	Xe	007440-63-3	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

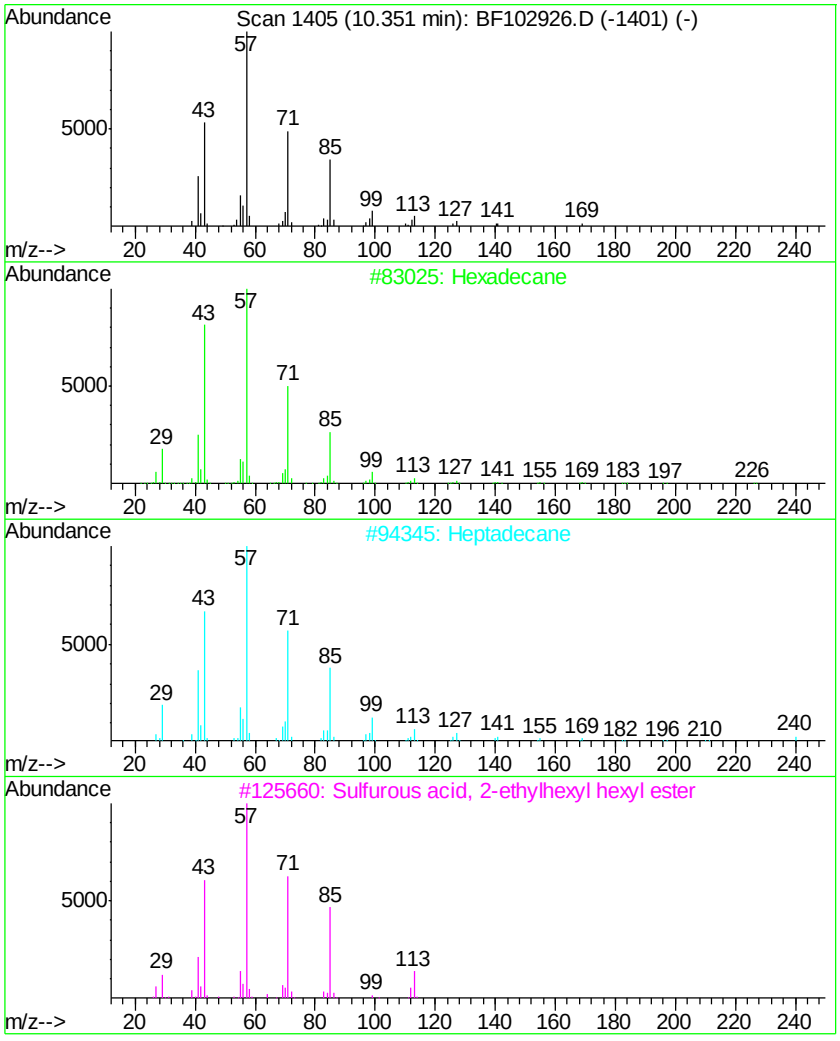
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

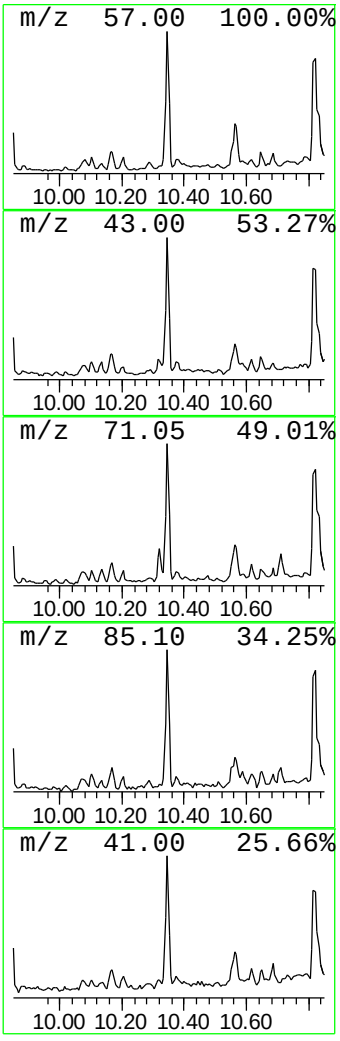
****

Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.35 ng	166617	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Heptadecane	240	C17H36	000629-78-7	86
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	78





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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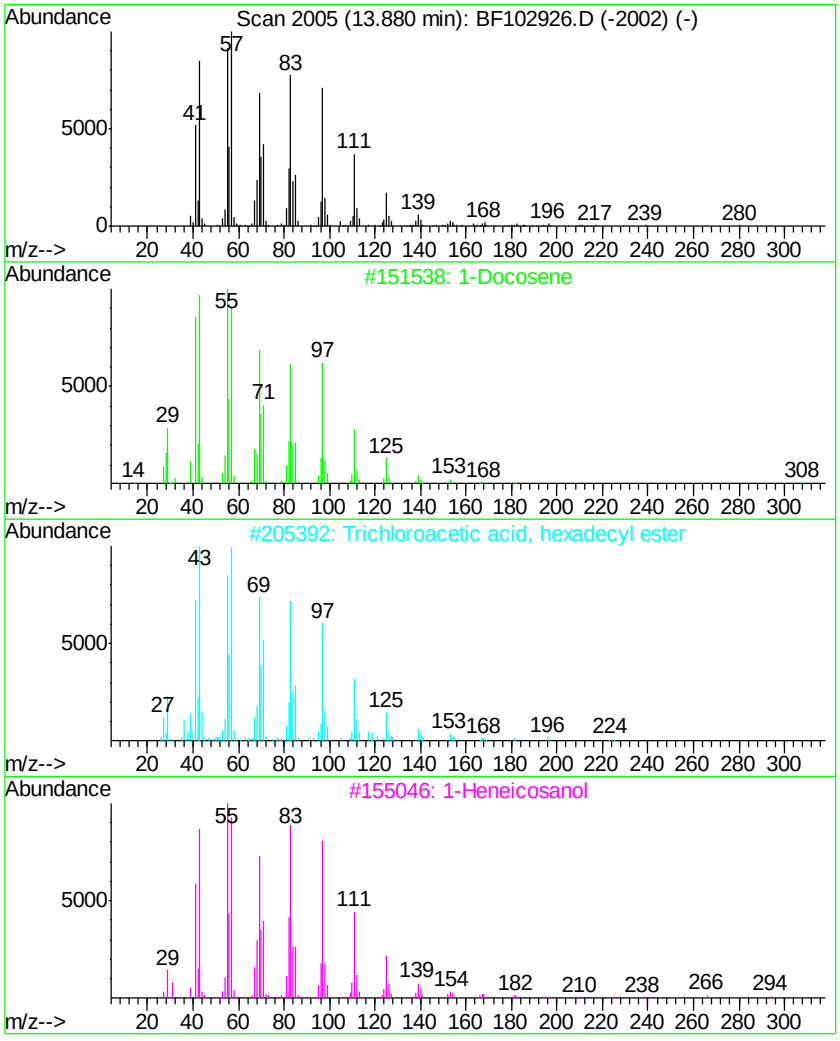
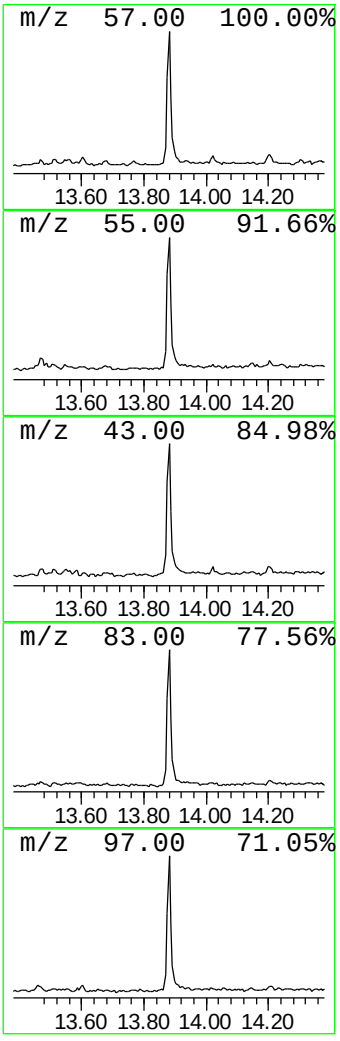
Peak Number 8 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	13.40 ng	642321	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

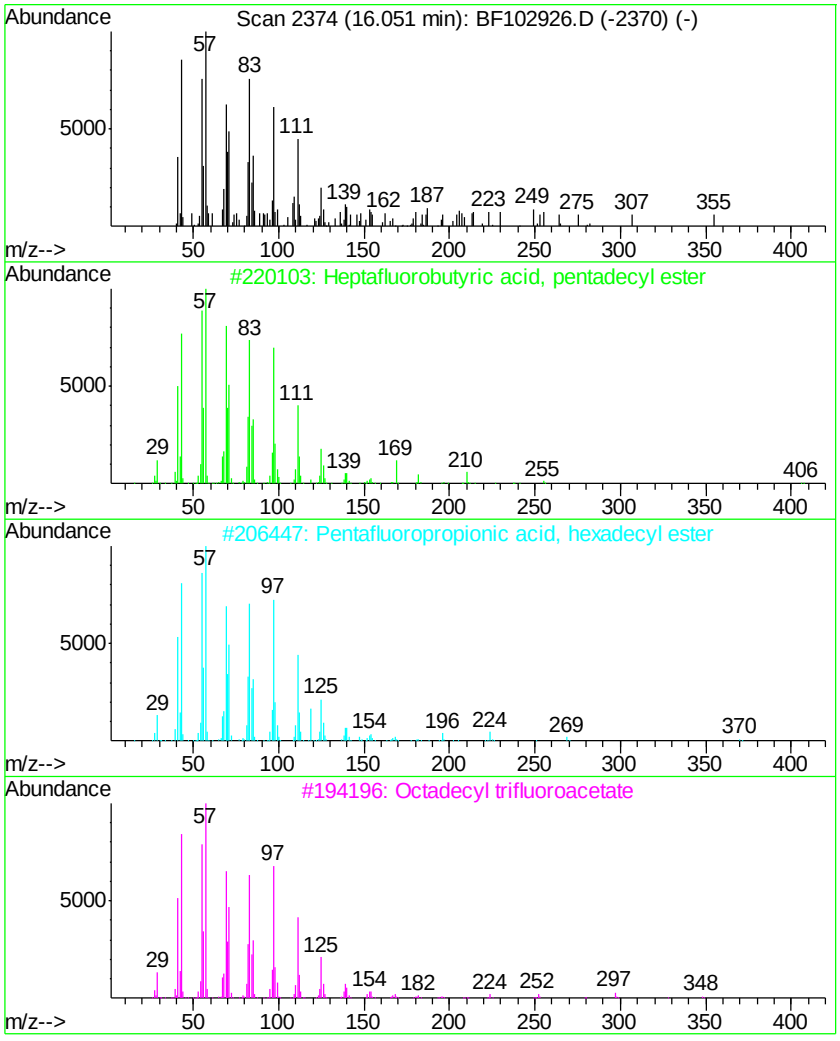
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

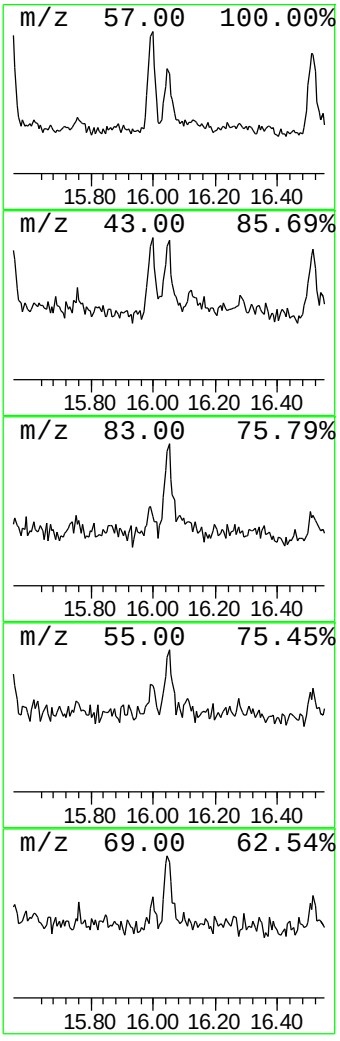
****

Peak Number 9 Heptafluorobutyric acid, pe... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	2.39 ng	109799	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF021218\
Data File : BF102926.D
Acq On : 12 Feb 2018 17:49
Operator : SJ/JU
Sample : J1517-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CO-E

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.18	16.3	ng	991227	1	6.89	1214590	20.0
3-Penten-2-one, 4...	4.49	11.3	ng	685212	1	6.89	1214590	20.0
2-Pentanone, 4-hy...	5.12	42.1	ng	2555270	1	6.89	1214590	20.0
unknown6.66	6.66	58.3	ng	3540530	1	6.89	1214590	20.0
Hexadecane	10.35	2.4	ng	166617	3	9.92	1419060	20.0
1-Docosene	13.88	13.4	ng	642321	5	14.06	958804	20.0
Heptafluorobutyri...	16.05	2.4	ng	109799	6	15.54	918641	20.0