LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099593.D
Acq On : 17 Oct 2017 20:51
Operator : SJ/JU
Sample : I5869-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

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-BF092317.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	4.440	397	400	408	rBV	41287	50739	1.51%	0.196%
2	5.075	500	508	511	rBV	1697861	2972488	88.50%	11.488%
3	5.198	514	529	532	rBV2	53726	180677	5.38%	0.698%
4	5.269	538	541	545	rVB	73003	116297	3.46%	0.449%
5	5.398	547	563	566	rVB	61947	205647	6.12%	0.795%
6	5.469	571	575	592	rVB	2032022	1893769	56.38%	7.319%
7	6.475	742	746	757	rBV	1612170	1589479	47.32%	6.143%
8	6.604	763	768	771	rBV	2702865	2585421	76.97%	9.992%
9	6.828	802	806	809	rBV	732739	646463	19.25%	2.498%
10	6.887	812	816	823	rVB	63111	63402	1.89%	0.245%
11	6.987	828	833	836	rBV	2219353	2317477	69.00%	8.957%
12	7.398	897	903	906	rBV	1662983	1809221	53.86%	6.992%
13	8.104	1019	1023	1027	rBV	943037	902685	26.87%	3.489%
14	8.386	1067	1071	1074	rBV2	160139	182303	5.43%	0.705%
15	8.757	1131	1134	1140	rVB	53208	48012	1.43%	0.186%
16	8.810	1140	1143	1152	rBV	38867	50002	1.49%	0.193%
17	9.186	1200	1207	1210	rBV	3154607	3358852	100.00%	12.982%
18	9.245	1213	1217	1221	rBV2	40755	46365	1.38%	0.179%
19	9.575	1268	1273	1278	rBV	205832	158869	4.73%	0.614%
20	9.786	1303	1309	1312	rBV2	42747	46794	1.39%	0.181%
21	9.863	1317	1322	1326	rVB	1074438	976438	29.07%	3.774%
22	10.239	1380	1386	1389	rBV	44263	45529	1.36%	0.176%
23	10.275	1389	1392	1395	rVV3	52238	51052	1.52%	0.197%
24	10.622	1448	1451	1453	rBV	78179	66651	1.98%	0.258%
25	10.651	1453	1456	1460	rVV	1112085	1033053	30.76%	3.993%
26	11.351	1571	1575	1578	rBV	1017379	874939	26.05%	3.382%
27	11.380	1578	1580	1583	rVB2	76311	78589	2.34%	0.304%
28	12.933	1839	1844	1847	rBV	2477434	2274484	67.72%	8.791%
29	13.810	1990	1993	1998	rBV2	79884	90037	2.68%	0.348%
30	13.951	2014	2017	2020	rBV	47403	37132	1.11%	0.144%
31	13.992	2020	2024	2027	rBV	570871	542399	16.15%	2.096%
32	15.451	2266	2272	2281	rVB	447172	578828	17.23%	2.237%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099593.D
Acq On : 17 Oct 2017 20:51
Operator : SJ/JU
Sample : I5869-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 25874093

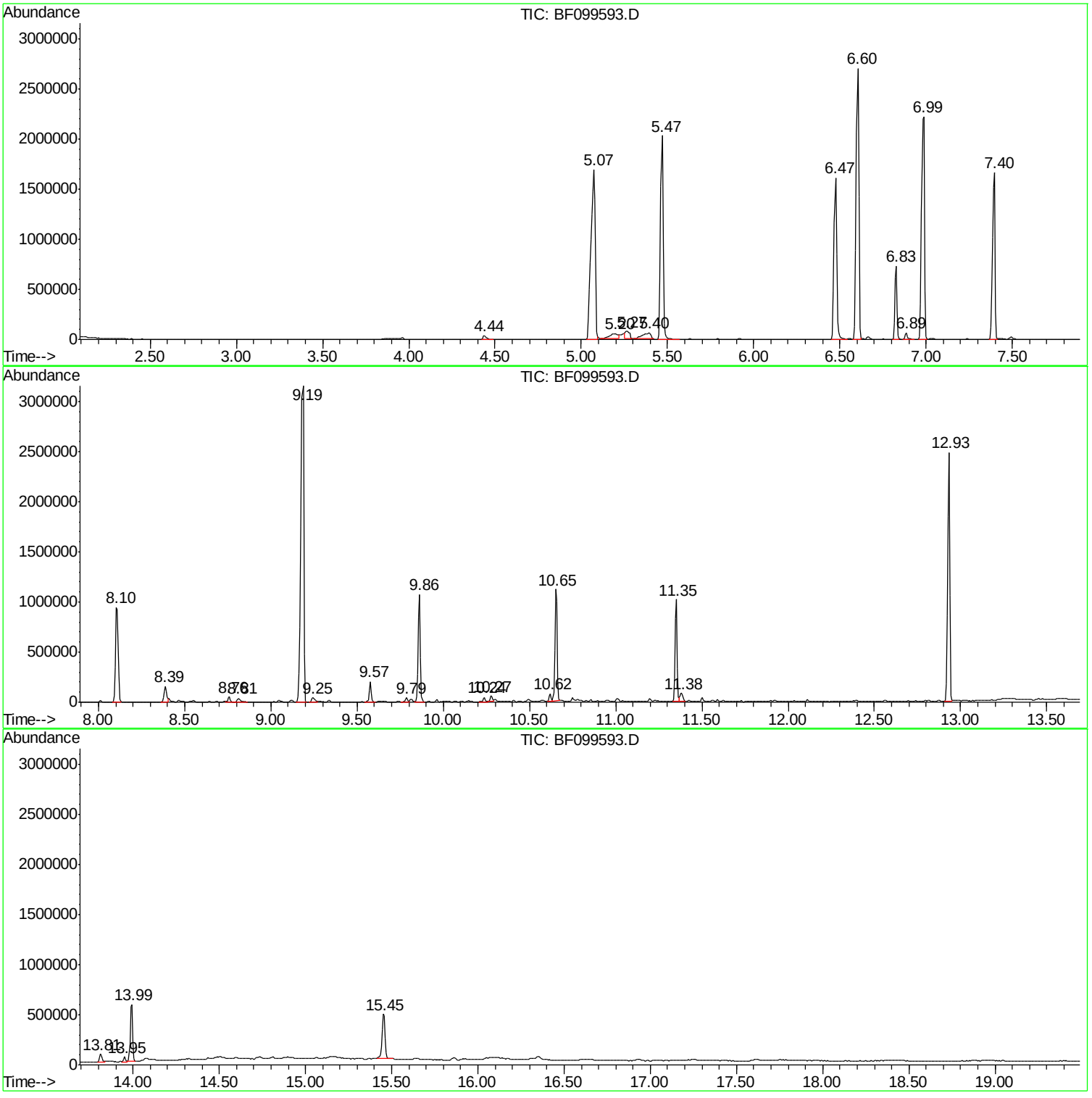
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099593.D
Acq On : 17 Oct 2017 20:51
Operator : SJ/JU
Sample : I5869-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099593.D
Acq On : 17 Oct 2017 20:51
Operator : SJ/JU
Sample : I5869-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

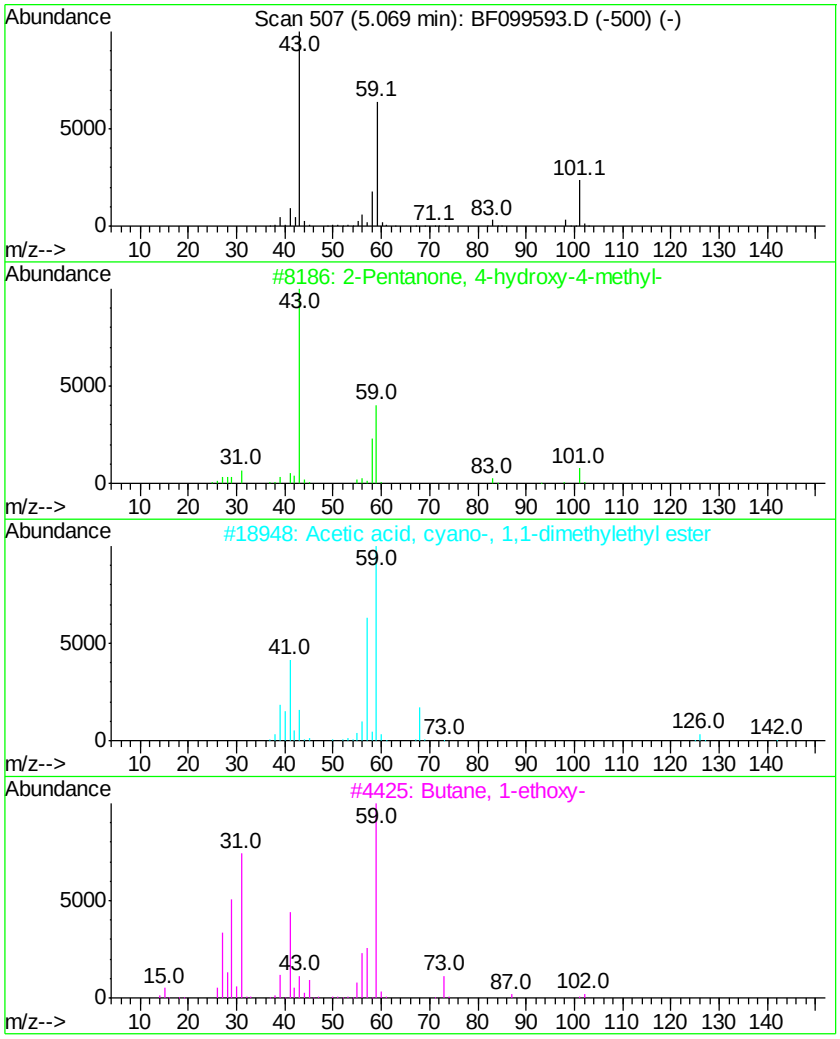
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

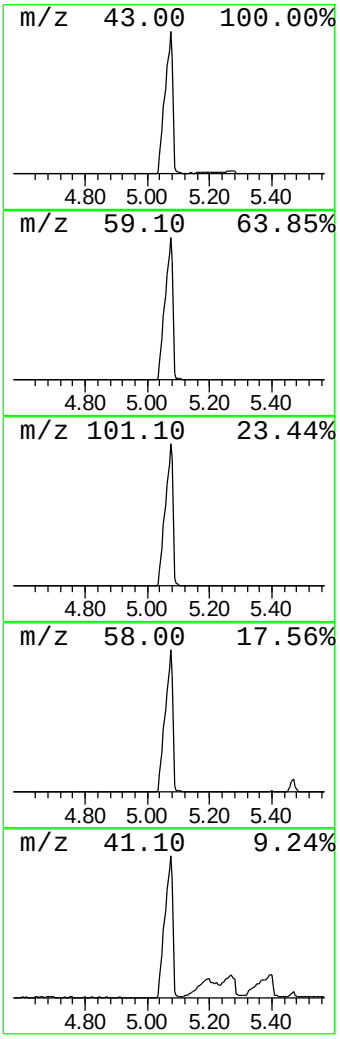
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	91.96 ng	2972490	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099593.D
Acq On : 17 Oct 2017 20:51
Operator : SJ/JU
Sample : I5869-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

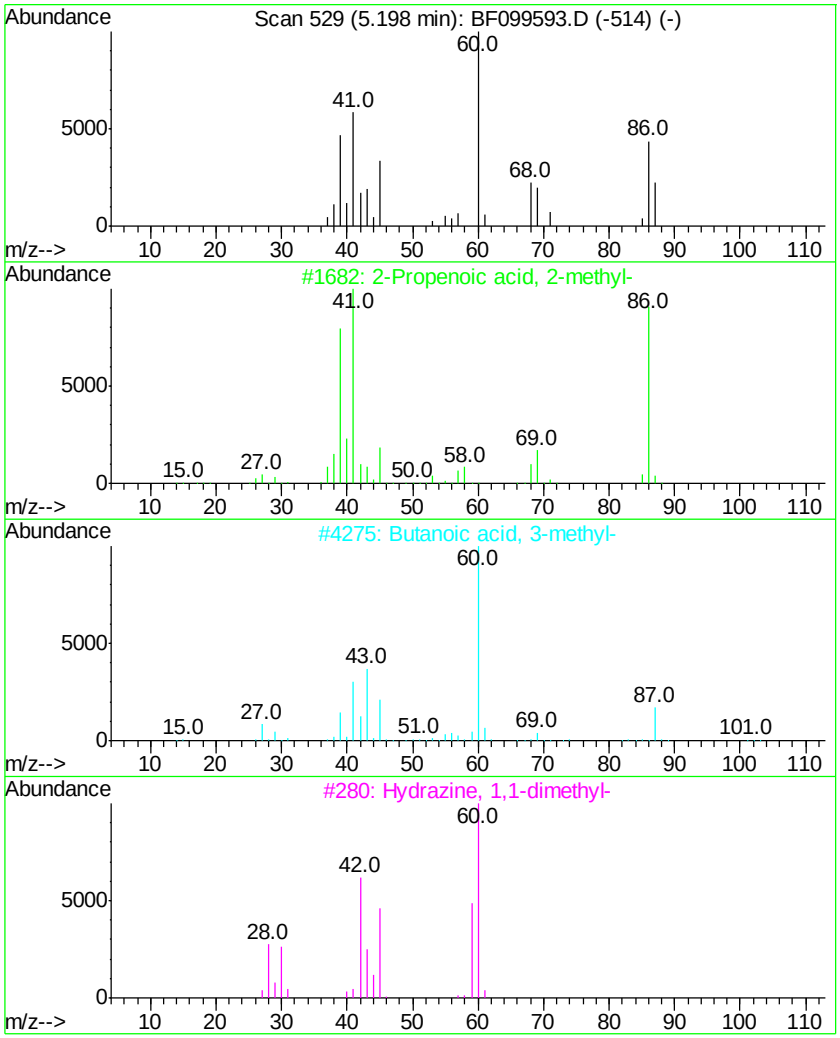
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

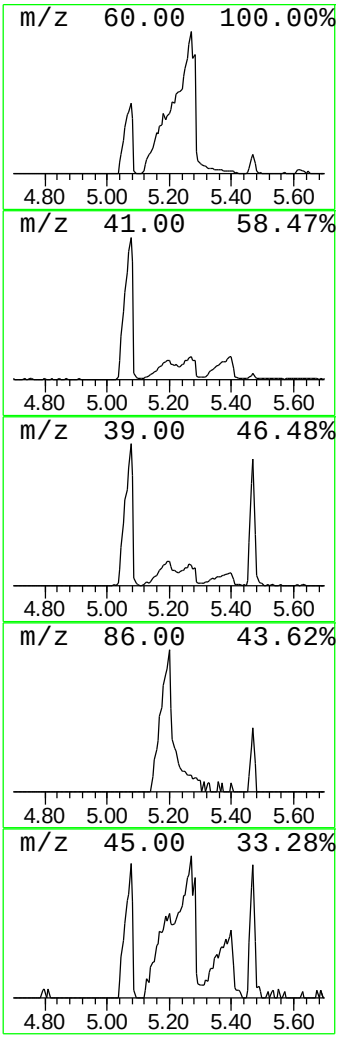
****

Peak Number 2 unknown5.20 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	5.59 ng	180677	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	38
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	17
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	16
4	Methacrolein	70	C4H6O	000078-85-3	10
5	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099593.D
Acq On : 17 Oct 2017 20:51
Operator : SJ/JU
Sample : I5869-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

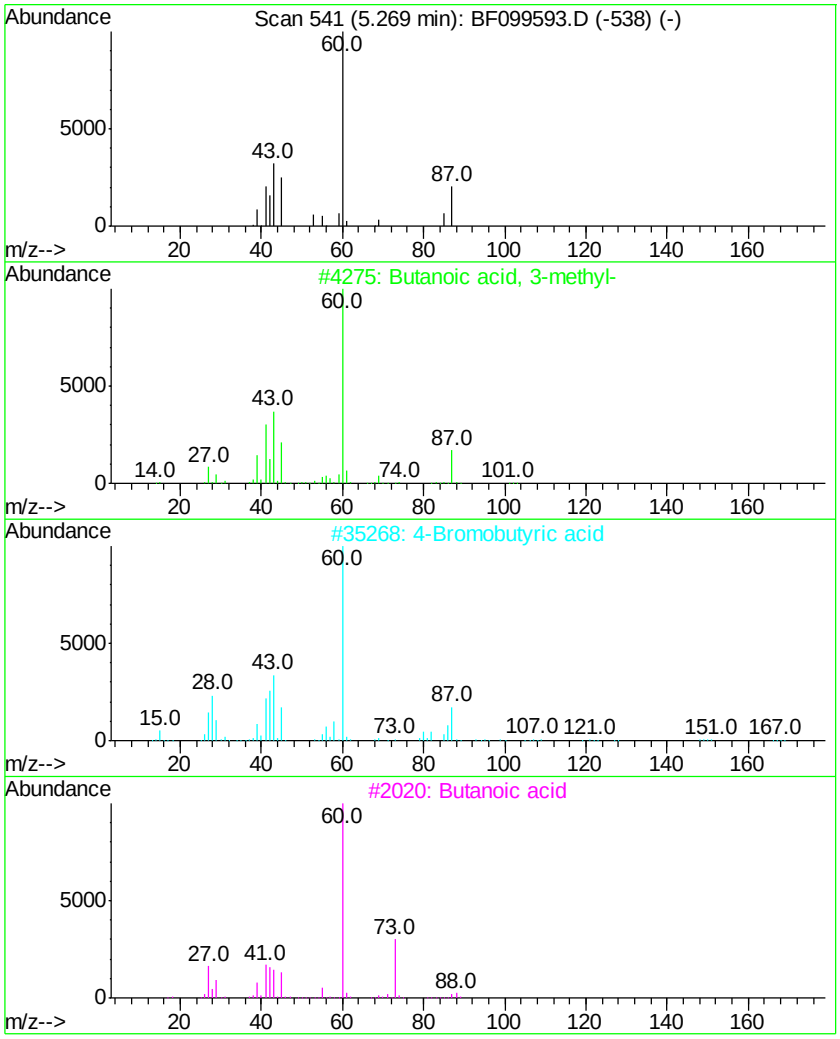
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

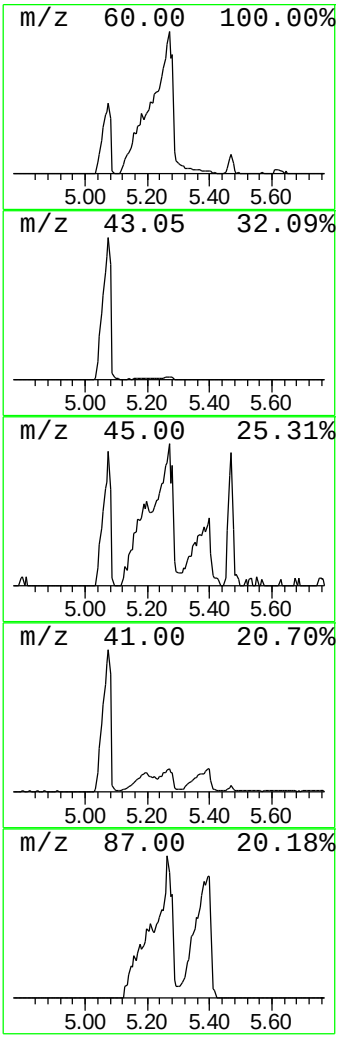
****

Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	3.60 ng	116297	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
2	4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	39
3	Butanoic acid	88	C4H8O2	000107-92-6	9
4	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	9
5	Hexanoic acid	116	C6H12O2	000142-62-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
Data File : BF099593.D
Acq On : 17 Oct 2017 20:51
Operator : SJ/JU
Sample : I5869-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

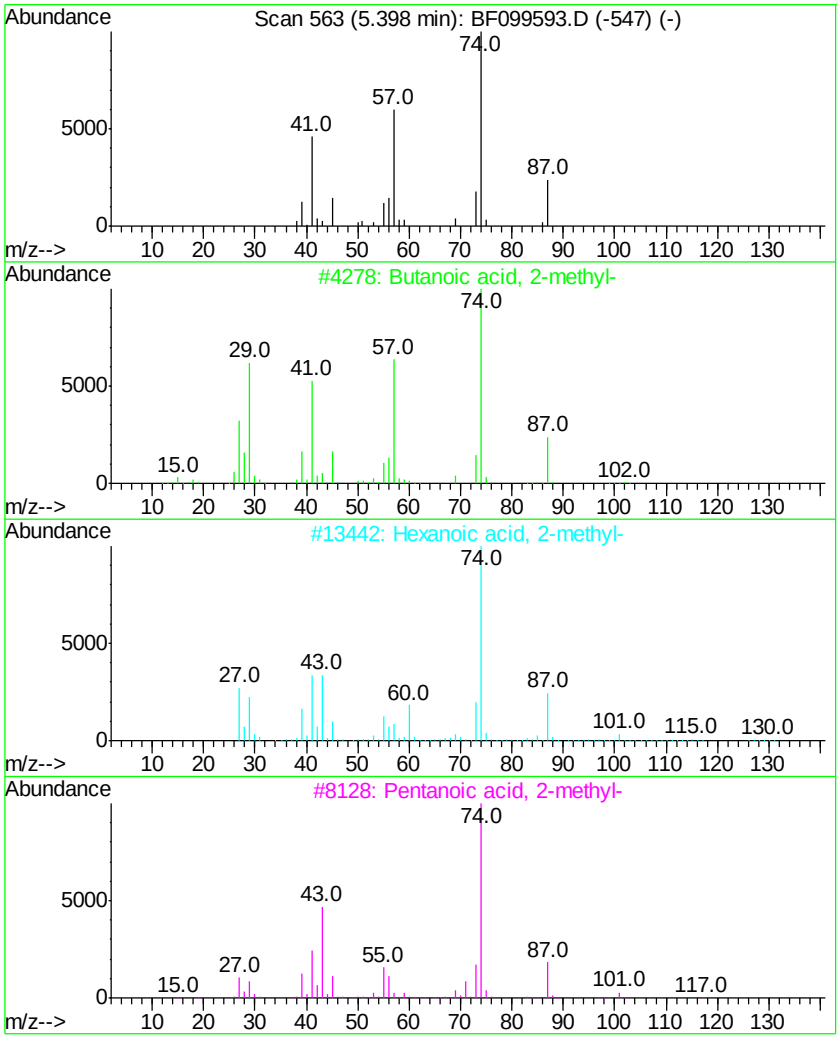
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

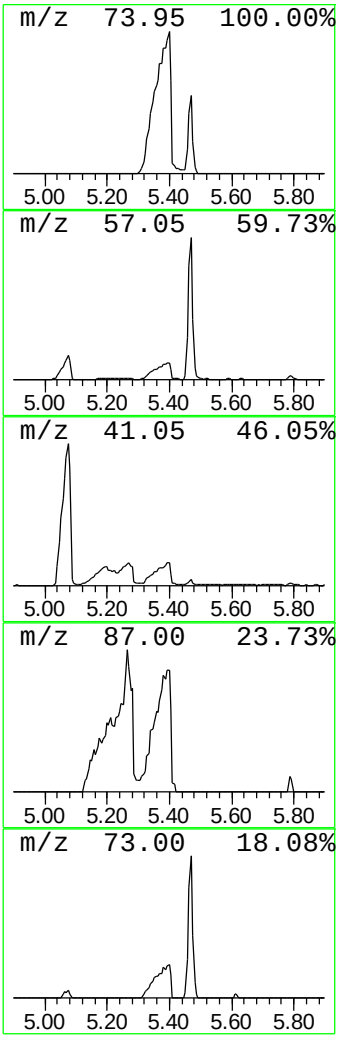
****

Peak Number 4 Butanoic acid, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.40	6.36 ng	205647	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
2	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	56
3	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	56
4	Morpholine	87	C4H9NO	000110-91-8	9
5	Propanoic acid	74	C3H6O2	000079-09-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101717\
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Acq On : 17 Oct 2017 20:51
Operator : SJ/JU
Sample : I5869-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

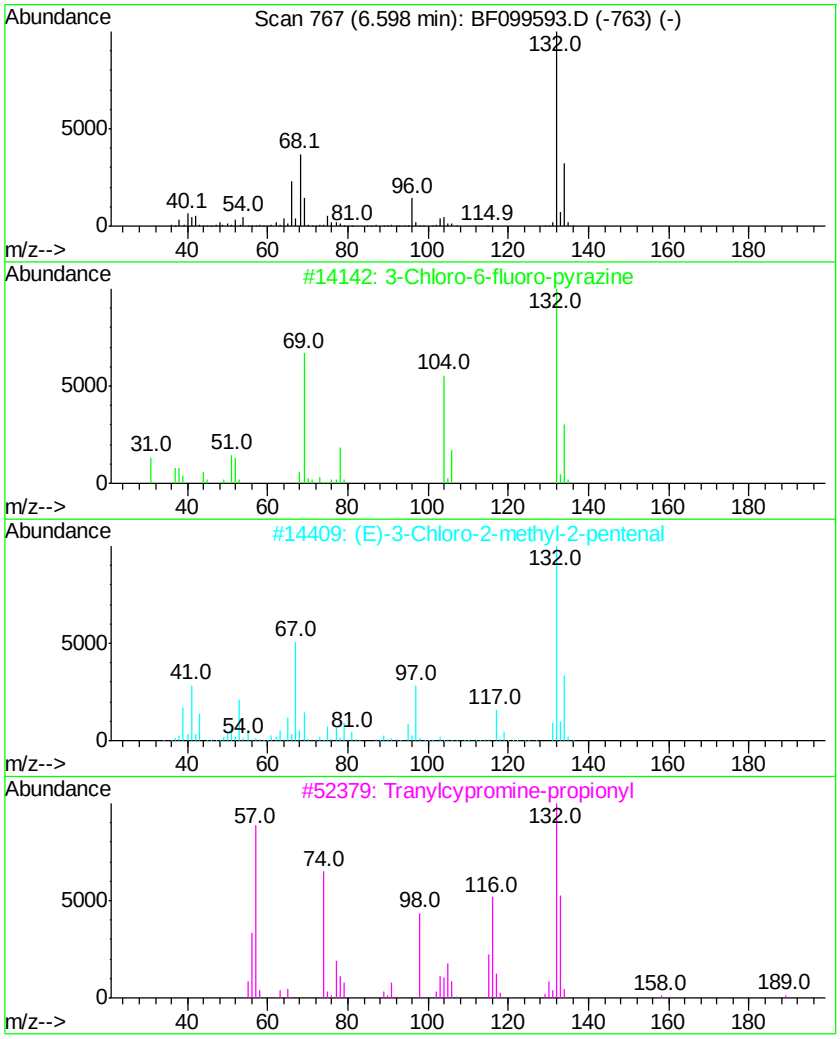
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

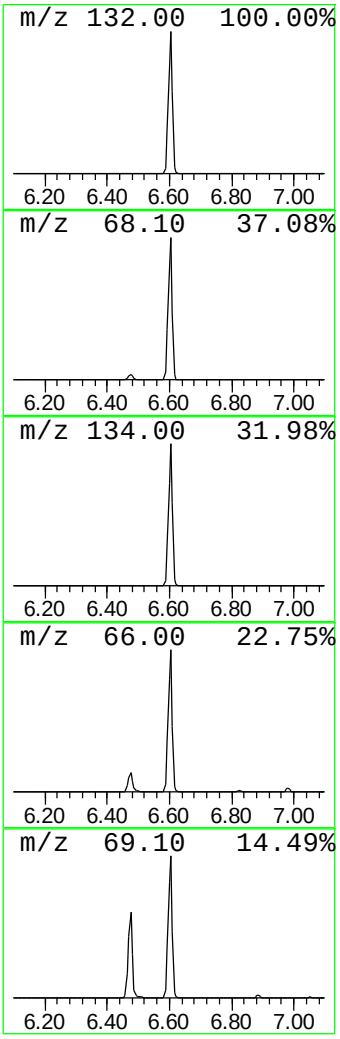
****

Peak Number 5 unknown6.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	79.99 ng	2585420	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Sample : I5869-01
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Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

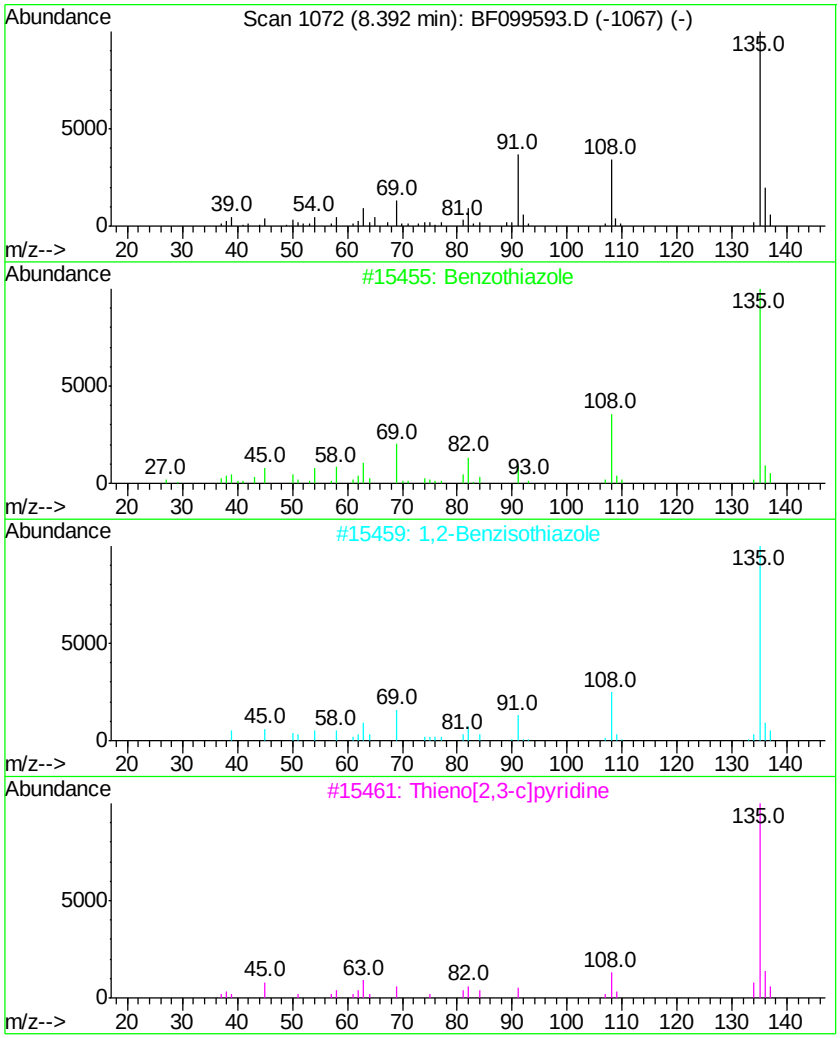
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

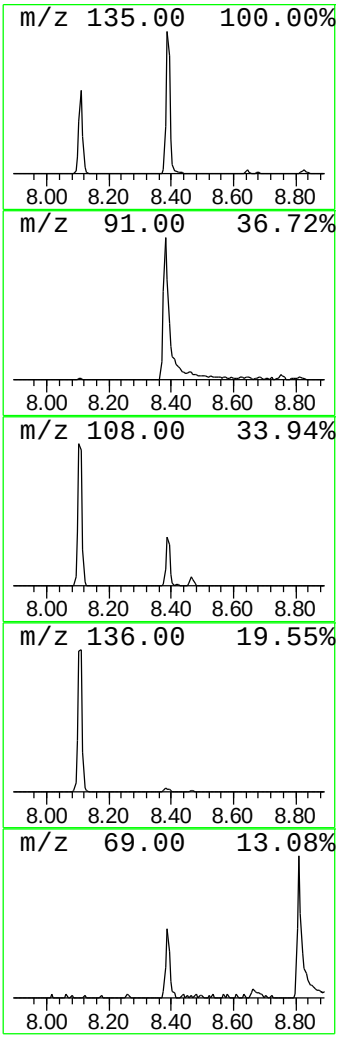
****

Peak Number 7 Benzothiazole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.39	4.04 ng	182303	Naphthalene-d8	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	93
2	1,2-Benzisothiazole	135	C7H5NS	000272-16-2	83
3	Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	72
4	3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
5	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	47





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Operator : SJ/JU
Sample : I5869-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-1-10-11-17

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

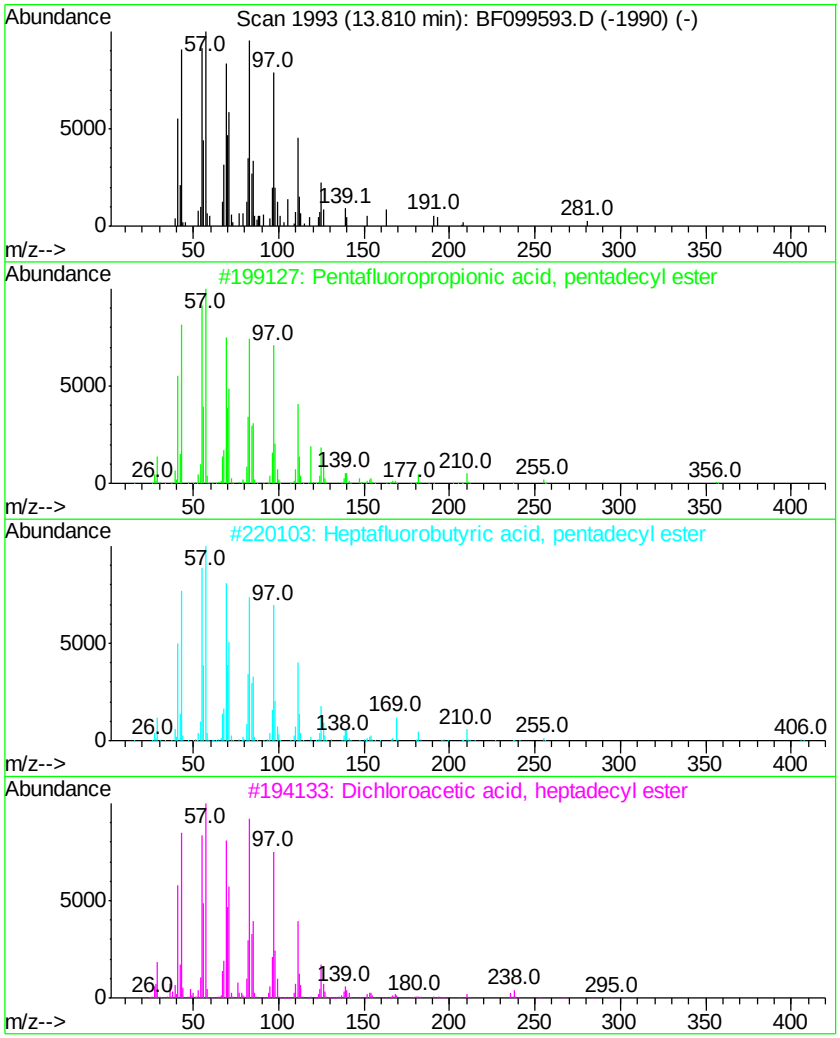
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

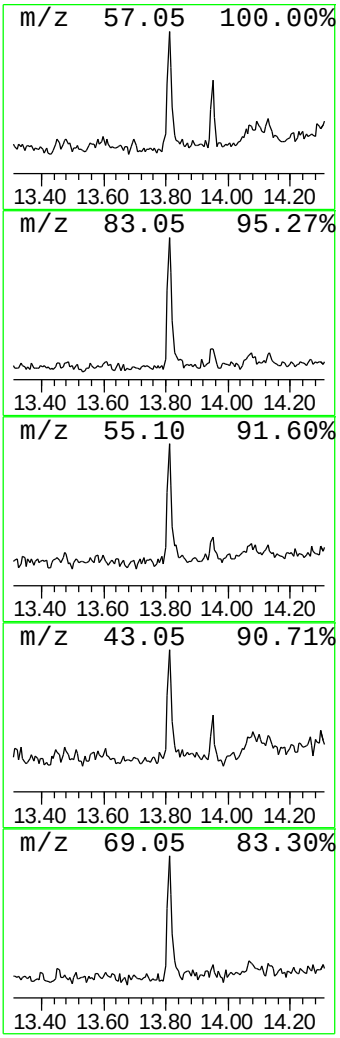
****

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.32 ng	90037	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101717\
Data File : BF099593.D
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
2-Pentanone, 4-hy...	5.07	92.0	ng	2972490	1	6.83	646463	20.0
unknown5.20	5.20	5.6	ng	180677	1	6.83	646463	20.0
Butanoic acid, 3-...	5.27	3.6	ng	116297	1	6.83	646463	20.0
Butanoic acid, 2-...	5.40	6.4	ng	205647	1	6.83	646463	20.0
unknown6.60	6.60	80.0	ng	2585420	1	6.83	646463	20.0
Benzothiazole	8.39	4.0	ng	182303	2	8.11	902685	20.0
Pentafluoropropio...	13.81	3.3	ng	90037	5	13.99	542399	20.0