LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092115\
Data File : BF081717.D
Acq On : 21 Sep 2015 16:38
Operator : UM/IZ
Sample : G3717-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

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-BF090115.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	1.201	7	10	12	rBV	2308061	2459443	100.00%	15.099%
2	1.281	15	17	27	rVB2	11413	34775	1.41%	0.213%
3	1.441	30	31	37	rBV	45429	106812	4.34%	0.656%
4	1.521	37	38	82	rVB	646451	2320611	94.36%	14.247%
5	4.413	289	291	309	rBV	70353	200909	8.17%	1.233%
6	5.304	367	369	390	rBV	182192	501688	20.40%	3.080%
7	7.590	567	569	573	rBV	110880	256549	10.43%	1.575%
8	7.670	573	576	591	rVB	607556	1216770	49.47%	7.470%
9	8.162	615	619	626	rBB	148845	270607	11.00%	1.661%
10	8.482	643	647	659	rBB	649800	1112430	45.23%	6.829%
11	9.465	729	733	736	rBV	537332	952387	38.72%	5.847%
12	11.053	869	872	890	rBB	183555	336510	13.68%	2.066%
13	13.705	1099	1104	1107	rBV	1000919	1772146	72.05%	10.880%
14	14.768	1195	1197	1207	rBB	22602	47860	1.95%	0.294%
15	15.191	1230	1234	1243	rBB	190914	353109	14.36%	2.168%
16	17.100	1397	1401	1412	rBV	591399	1104905	44.93%	6.783%
17	18.700	1537	1541	1548	rBV	188581	367520	14.94%	2.256%
18	19.786	1633	1636	1639	rBV	28501	50241	2.04%	0.308%
19	20.460	1691	1695	1706	rBV	50537	107867	4.39%	0.662%
20	21.866	1816	1818	1826	rBV	33834	60700	2.47%	0.373%
21	21.980	1826	1828	1831	rBV	31410	45990	1.87%	0.282%
22	22.072	1832	1836	1839	rBV	1337295	1809953	73.59%	11.112%
23	22.883	1904	1907	1912	rBV2	109917	201621	8.20%	1.238%
24	23.318	1942	1945	1946	rBV	35090	52678	2.14%	0.323%
25	23.352	1946	1948	1951	rVB	222967	320360	13.03%	1.967%
26	24.781	2071	2073	2080	rVB	179264	224376	9.12%	1.377%

Sum of corrected areas: 16288817

LSC Report - Integrated Chromatogram

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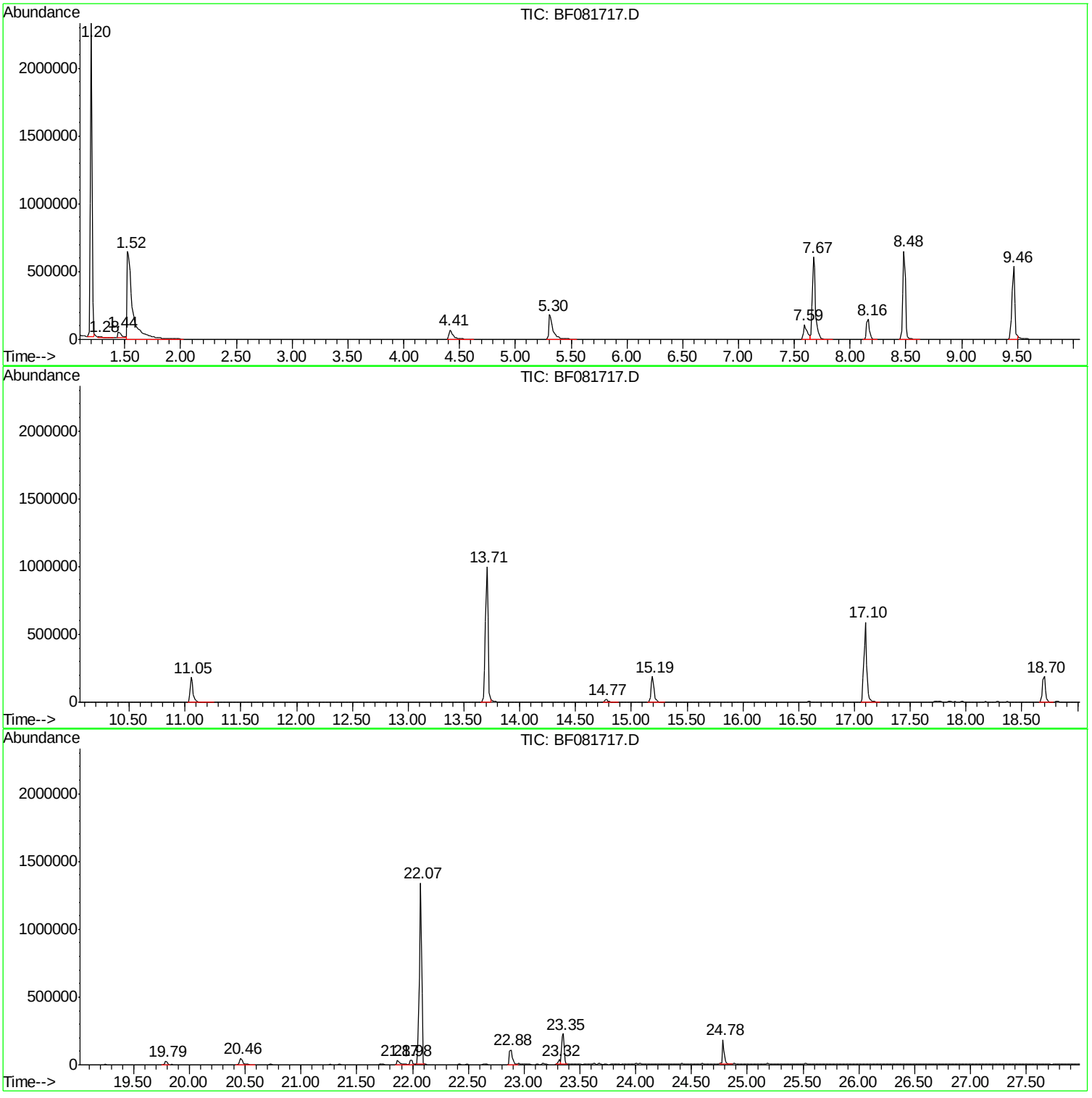
Operator : UM/IZ
Sample : G3717-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.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\BF092115\
Data File : BF081717.D
Acq On : 21 Sep 2015 16:38
Operator : UM/IZ
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Misc :
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Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

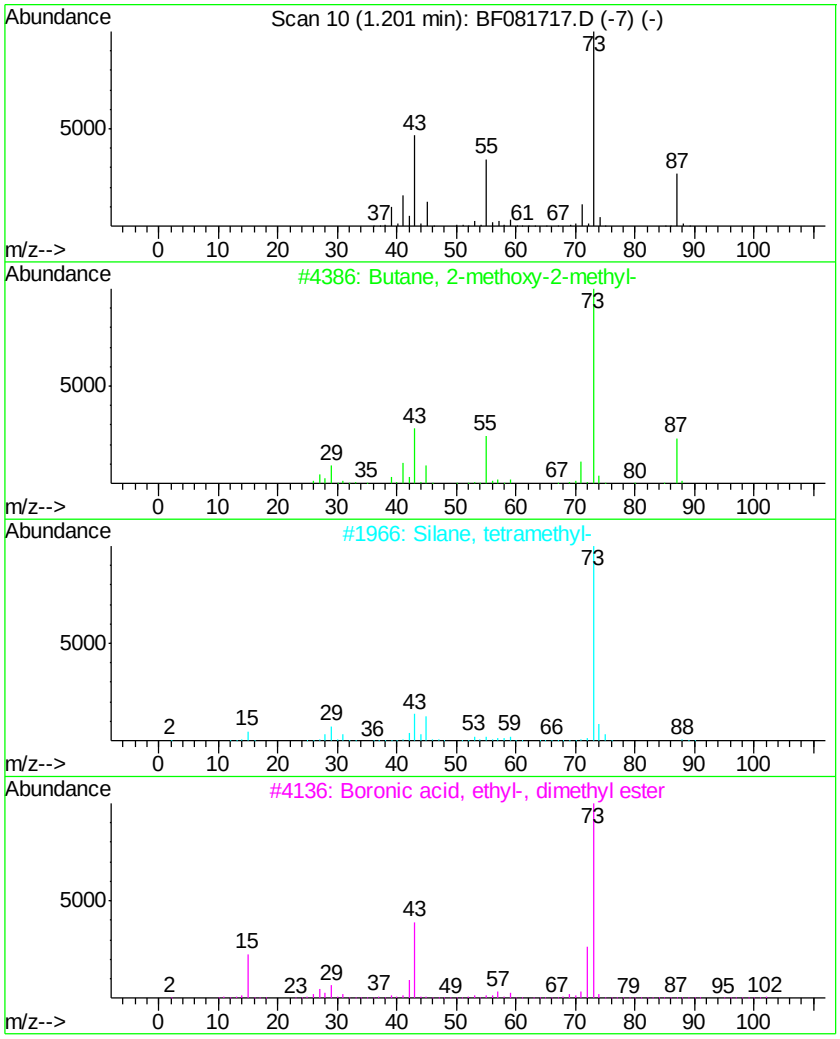
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

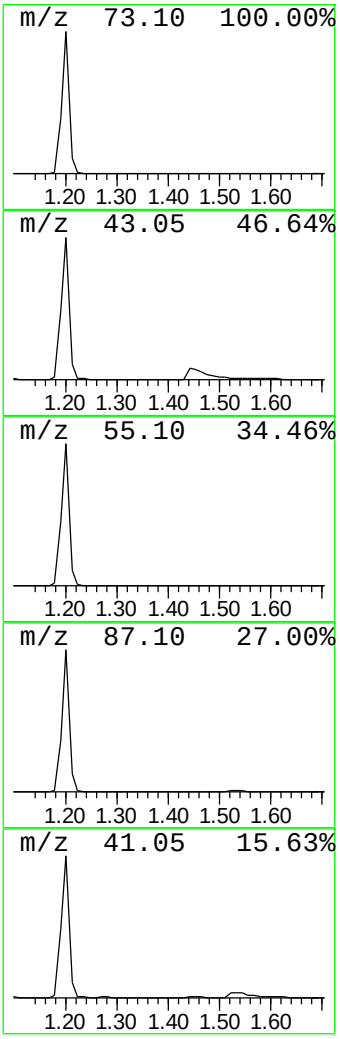
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.20	181.77 ng	2459440	1,4-Dichlorobenzene-d4	8.16

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	38
3	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	10
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Misc :
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Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

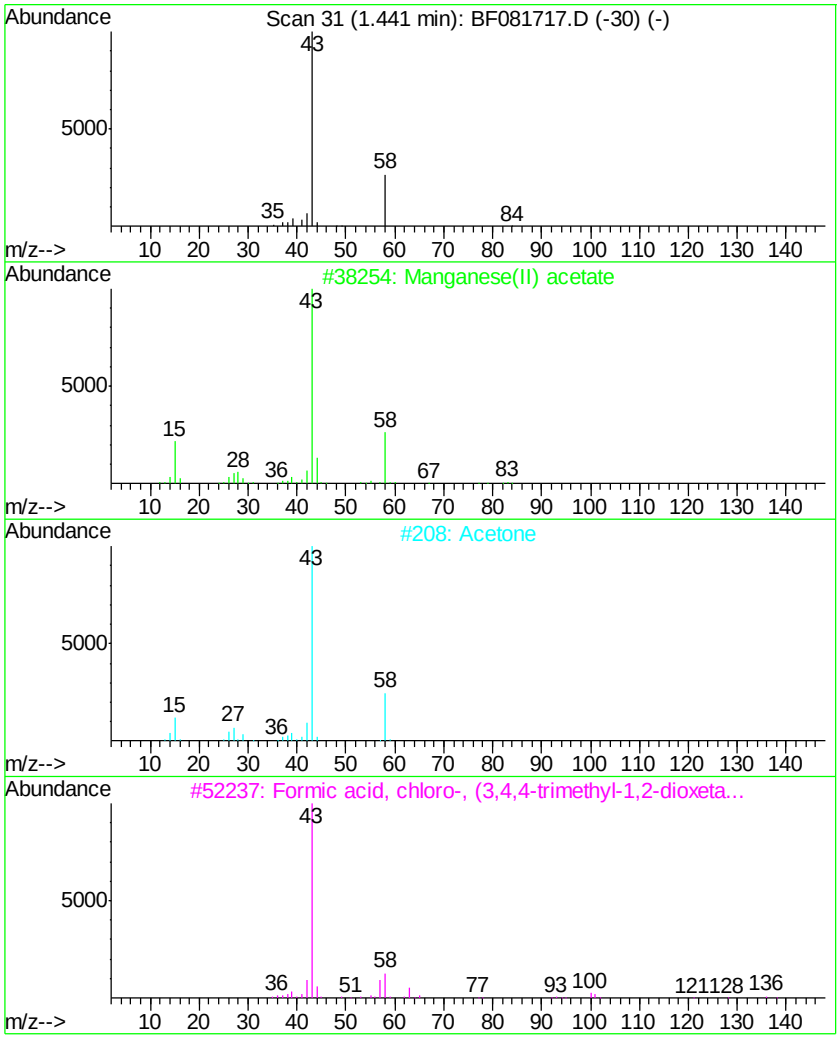
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

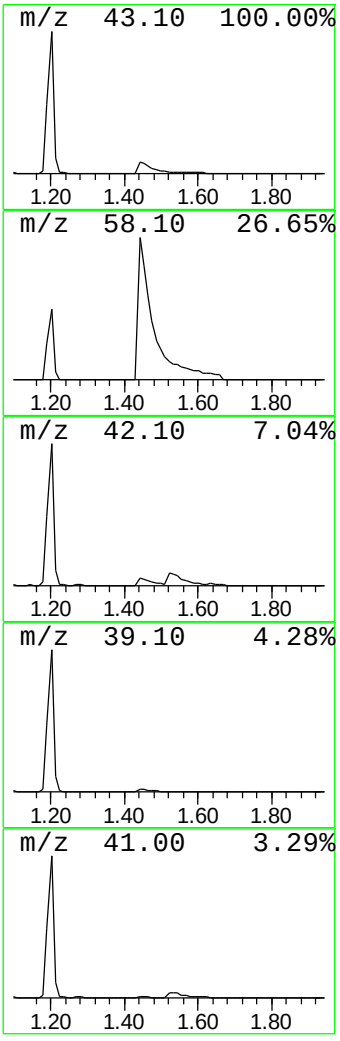
****

Peak Number 3 Manganese(II) acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.44	7.89 ng	106812	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Manganese(II) acetate	173	C4H6MnO4	006156-78-1	50
2	Acetone	58	C3H6O	000067-64-1	45
3	Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	9
4	Hydrogen azide	43	HN3	007782-79-8	4
5	Ethene, methoxy-	58	C3H6O	000107-25-5	3





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Data File : BF081717.D
Acq On : 21 Sep 2015 16:38
Operator : UM/IZ
Sample : G3717-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

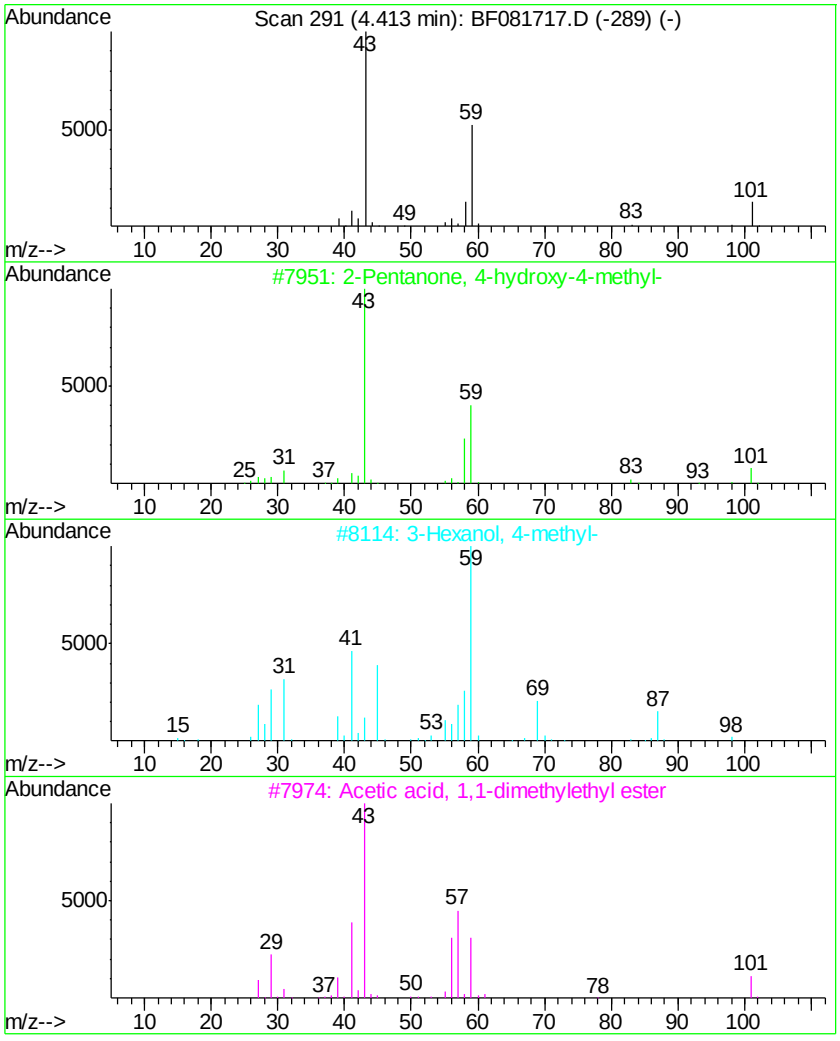
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

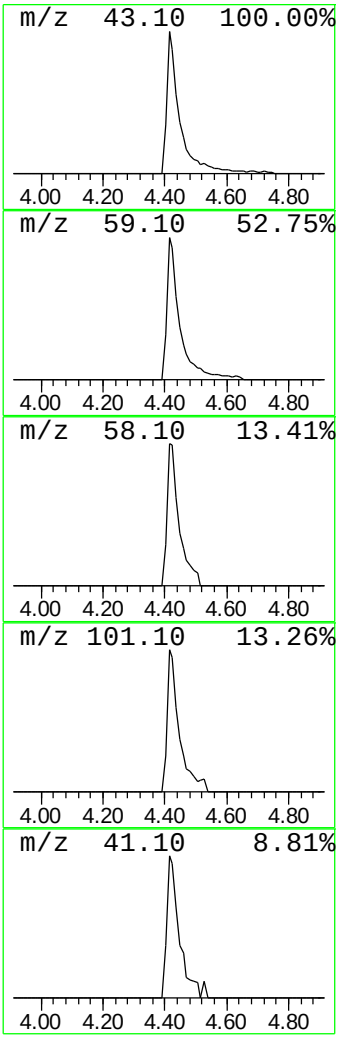
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	14.85 ng	200909	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Operator : UM/IZ
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Misc :
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Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

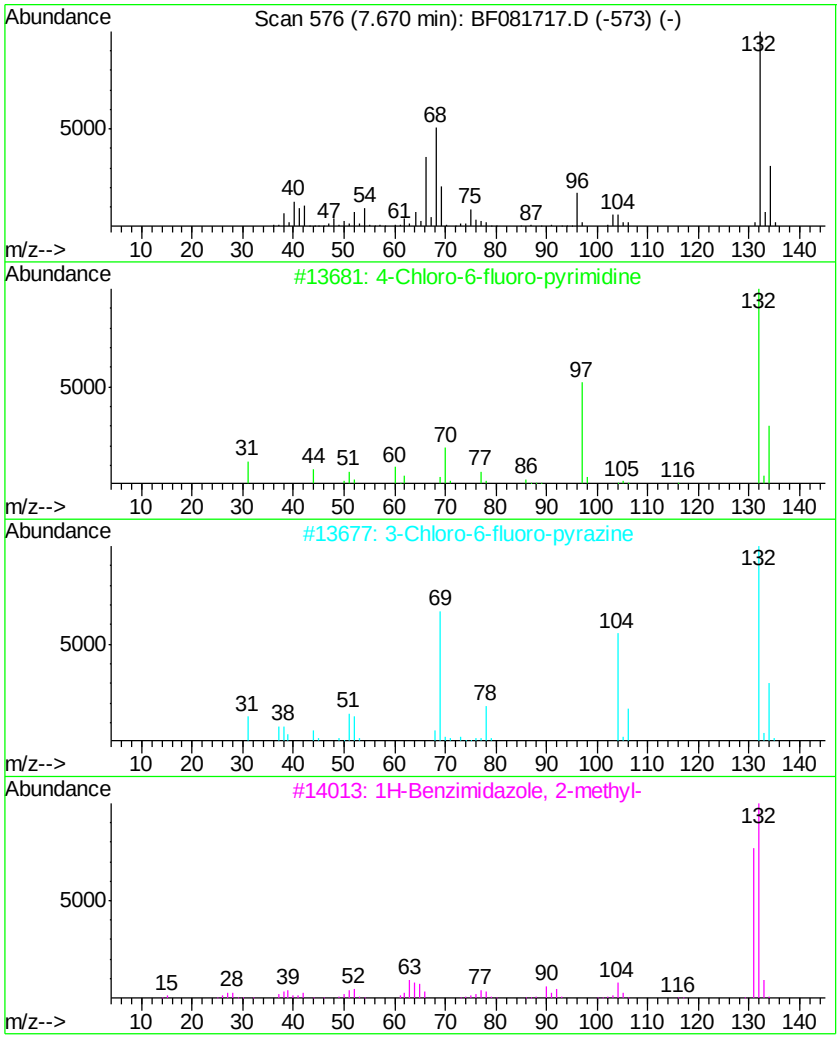
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

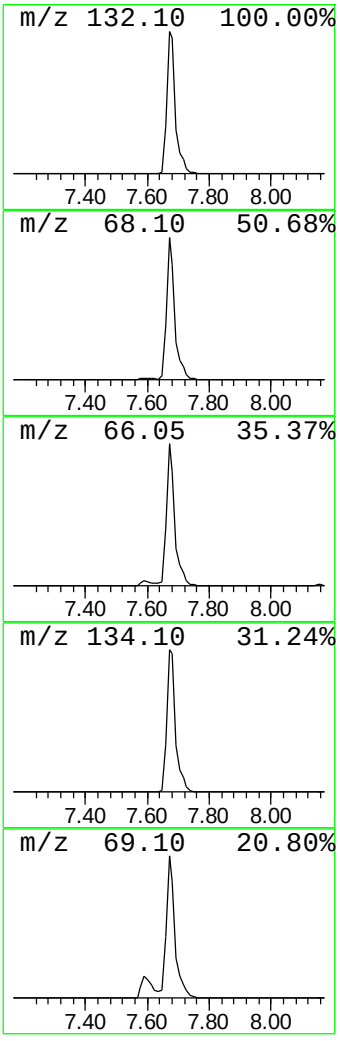
****

Peak Number 6 unknown7.67 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.67	89.93 ng	1216770	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Benzene, 1-methyl-4-(1-methyleth...	132	C10H12	001195-32-0	10





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Data File : BF081717.D
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Operator : UM/IZ
Sample : G3717-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
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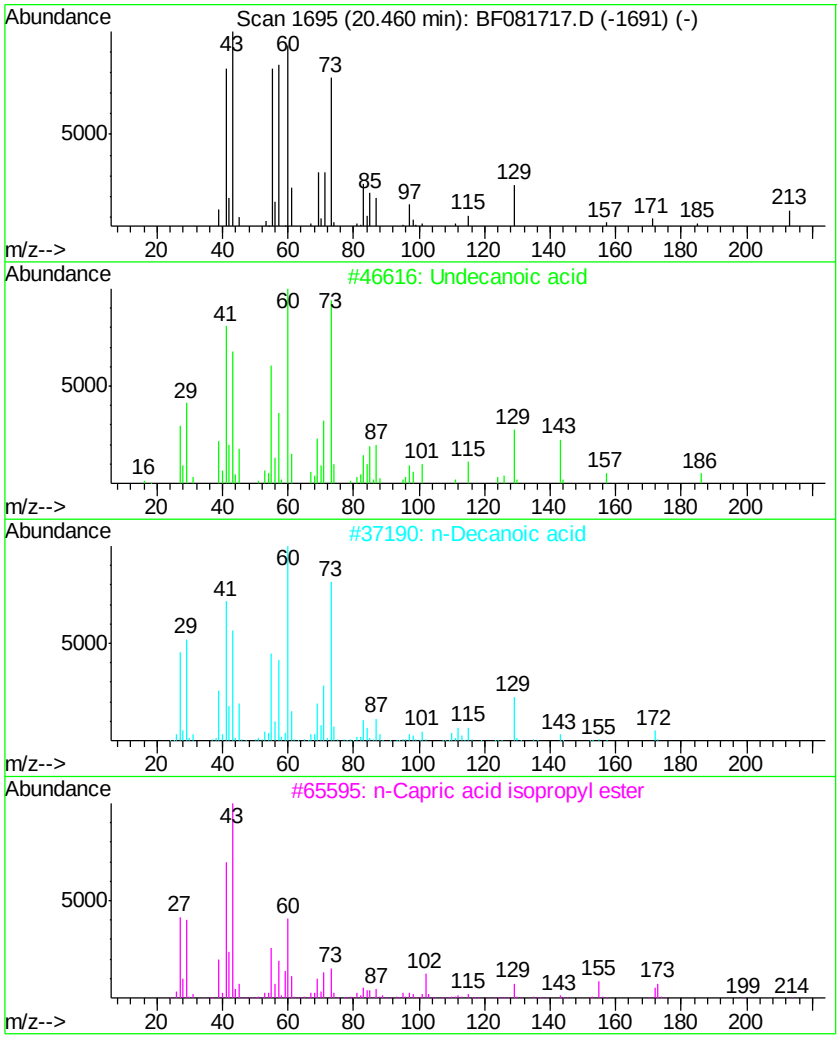
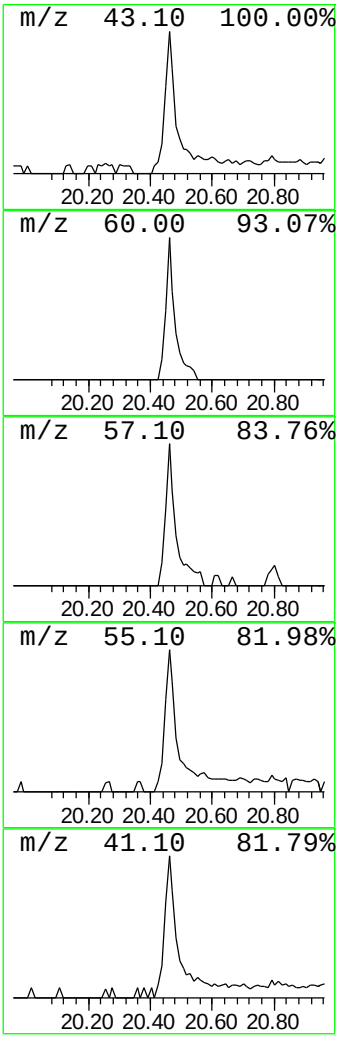
****

Peak Number 9 Undecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.46	5.87 ng	107867	Phenanthrene-d10	18.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	80
2	n-Decanoic acid	172	C10H20O2	000334-48-5	53
3	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
4	Dodecanoic acid	200	C12H24O2	000143-07-7	50
5	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	47





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Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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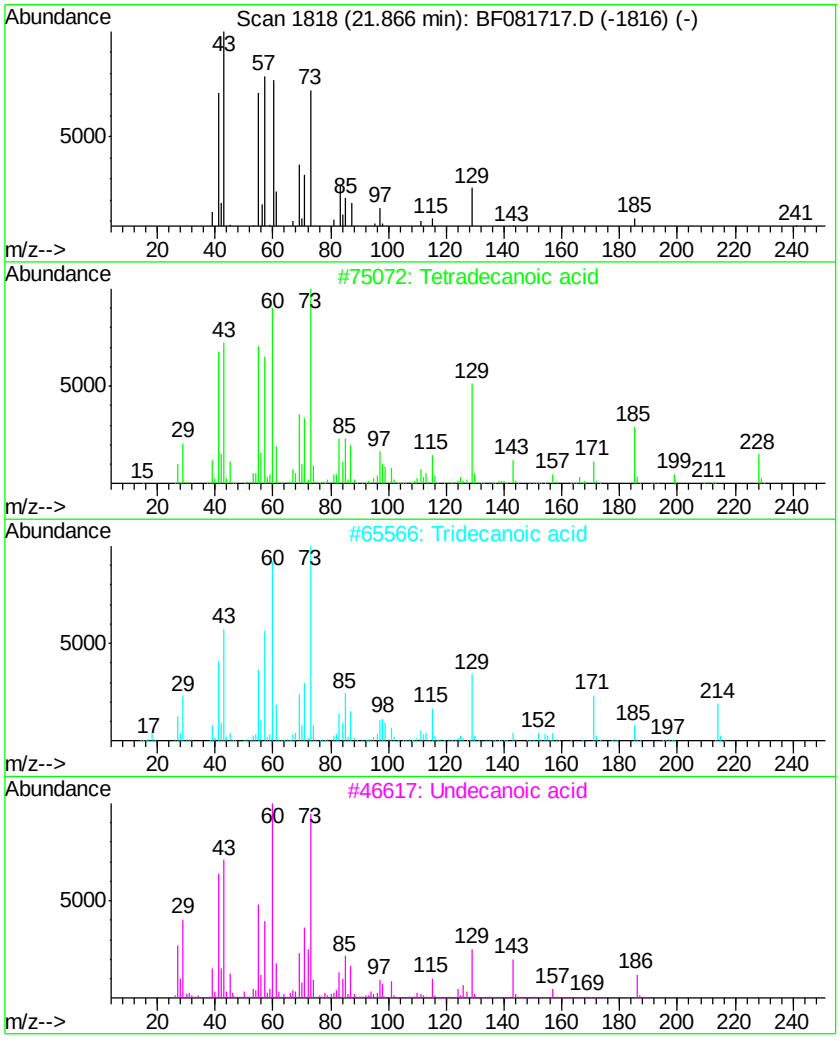
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

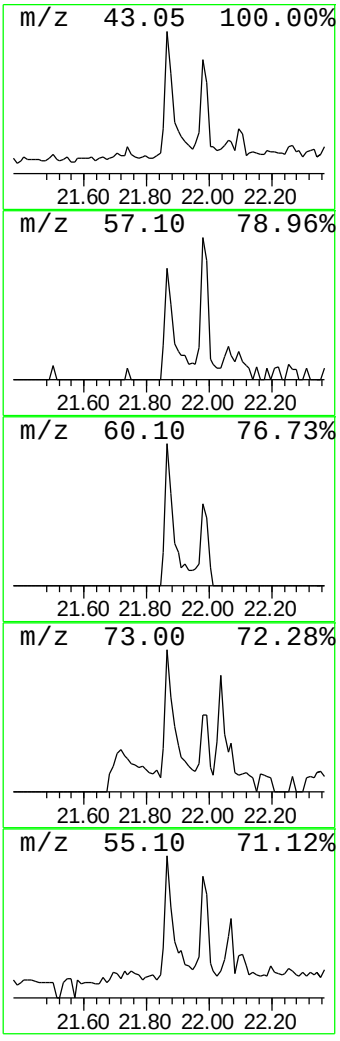
****

Peak Number 10 Tetradecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.87	3.79 ng	60700	Chrysene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Undecanoic acid	186	C11H22O2	000112-37-8	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47





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Misc :
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Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

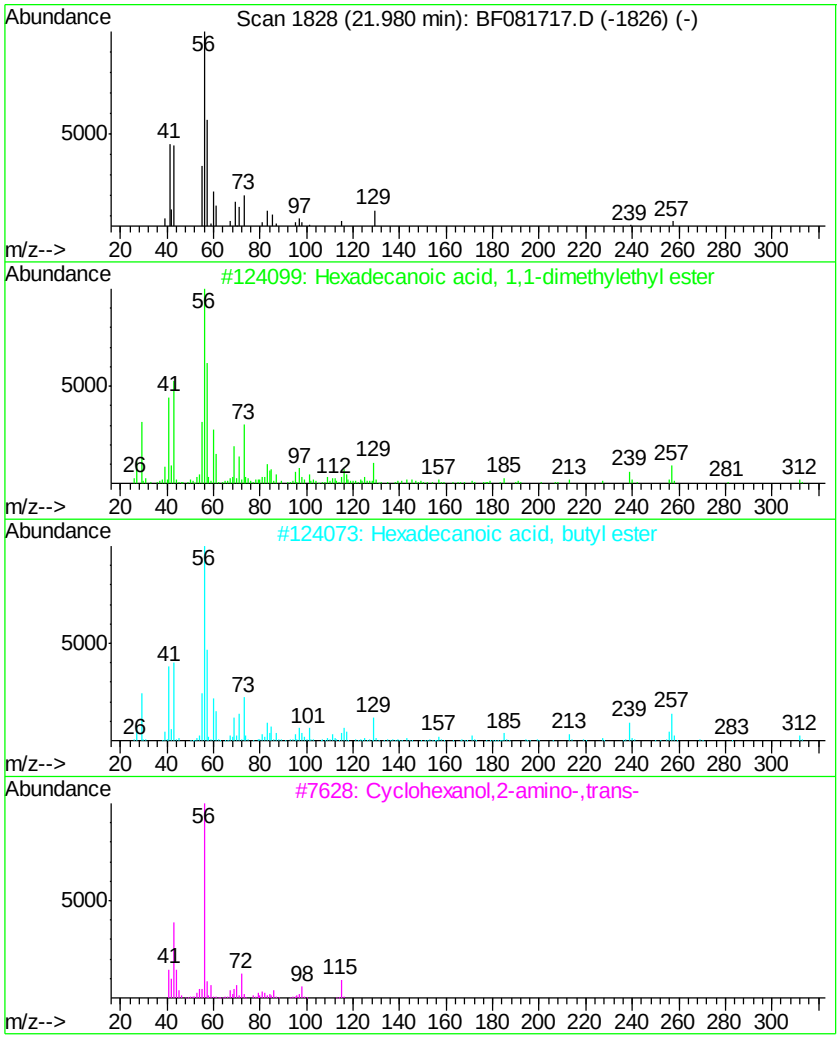
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

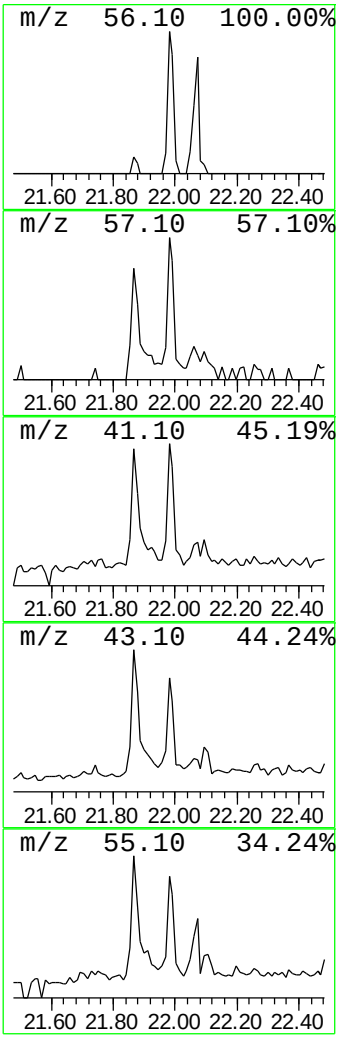
****

Peak Number 11 Hexadecanoic acid, 1,1-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.98	2.87 ng	45990	Chrysene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
3	Cyclohexanol,2-amino-,trans-	115	C6H13NO	006982-39-4	38
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	37
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	37





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Instrument : BNA_F
ClientSampleId : PZ-3-9-16-15

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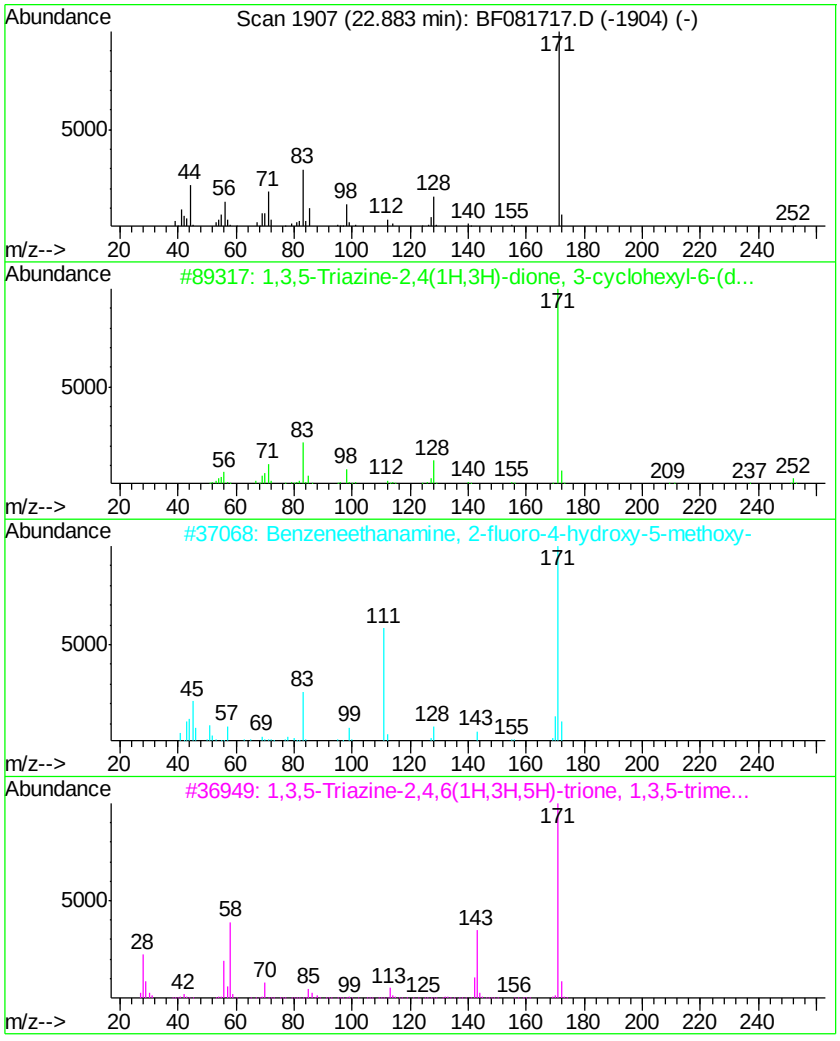
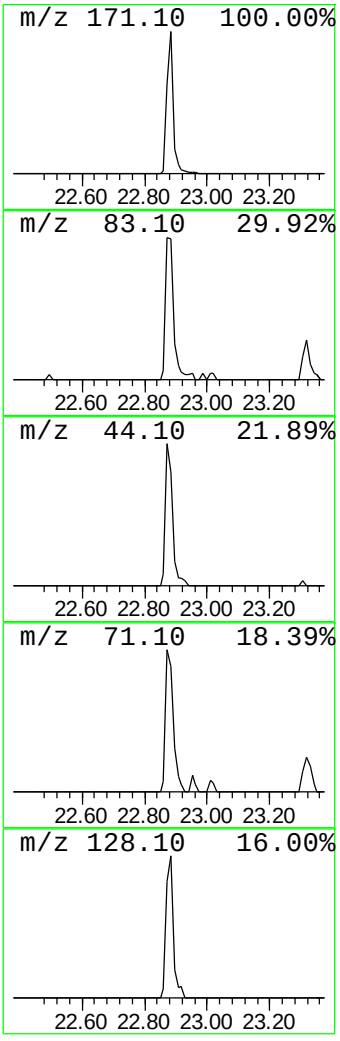
Peak Number 12 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.88	12.59 ng	201621	Chrysene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	95
2	Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FNO2	1000116-43-3	59
3	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	171	C6H9N3O3	000827-16-7	43
4	2,5-Difluorophenyl isothiocyanate	171	C7H3F2NS	206559-57-1	43
5	Pyrimidin-4(3H)-one, 6-amino-3-m...	171	C6H9N3OS	102363-06-4	33





Tentatively Identified Compound (LSC) summary

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Data File : BF081717.D
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Operator : UM/IZ
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	1.20	181.8	ng	2459440	1	8.16	270607	20.0
Manganese(II) ace...	1.44	7.9	ng	106812	1	8.16	270607	20.0
2-Pentanone, 4-hy...	4.41	14.9	ng	200909	1	8.16	270607	20.0
unknown7.67	7.67	89.9	ng	1216770	1	8.16	270607	20.0
Undecanoic acid	20.46	5.9	ng	107867	4	18.70	367520	20.0
Tetradecanoic acid	21.87	3.8	ng	60700	5	23.35	320360	20.0
Hexadecanoic acid...	21.98	2.9	ng	45990	5	23.35	320360	20.0
1,3,5-Triazine-2,...	22.88	12.6	ng	201621	5	23.35	320360	20.0