LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098822.D
Acq On : 26 Sep 2017 10:23
Operator : SJ/JU
Sample : I5385-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-SIDI-F-D-B

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	2.199	15	19	38	rVB	262877	472687	10.68%	1.829%
2	5.128	514	517	527	rVB	194150	193279	4.37%	0.748%
3	5.522	580	584	588	rBV	1396124	1245098	28.13%	4.818%
4	6.522	751	754	758	rBV	867336	774582	17.50%	2.997%
5	6.681	776	781	784	rBV	2411302	2278853	51.48%	8.818%
6	6.910	817	820	824	rBV	962018	783105	17.69%	3.030%
7	7.069	843	847	850	rBV	3164458	2917604	65.91%	11.290%
8	7.475	910	916	919	rBV	2425532	2443573	55.20%	9.456%
9	8.192	1034	1038	1042	rBV	1282648	1076051	24.31%	4.164%
10	9.269	1216	1221	1224	rBV	4446190	4426484	100.00%	17.129%
11	9.657	1283	1287	1290	rBV	205900	150859	3.41%	0.584%
12	9.951	1333	1337	1341	rVB	1311860	1142576	25.81%	4.421%
13	10.739	1466	1471	1474	rBV	1675086	1622678	36.66%	6.279%
14	10.857	1486	1491	1494	rBV	62387	80081	1.81%	0.310%
15	11.433	1585	1589	1593	rBV	1160872	1059564	23.94%	4.100%
16	12.833	1823	1827	1830	rBV	269348	206630	4.67%	0.800%
17	13.021	1854	1859	1862	rBV	3413408	3287802	74.28%	12.723%
18	13.539	1943	1947	1950	rBV	165453	138348	3.13%	0.535%
19	13.904	2005	2009	2018	rBV2	55308	74787	1.69%	0.289%
20	14.074	2034	2038	2041	rVB	746290	677156	15.30%	2.620%
21	15.562	2285	2291	2304	rVB	517428	686663	15.51%	2.657%
22	16.545	2453	2458	2466	rVB3	31338	57335	1.30%	0.222%
23	17.886	2680	2686	2693	rVB5	19554	46599	1.05%	0.180%

Sum of corrected areas: 25842394

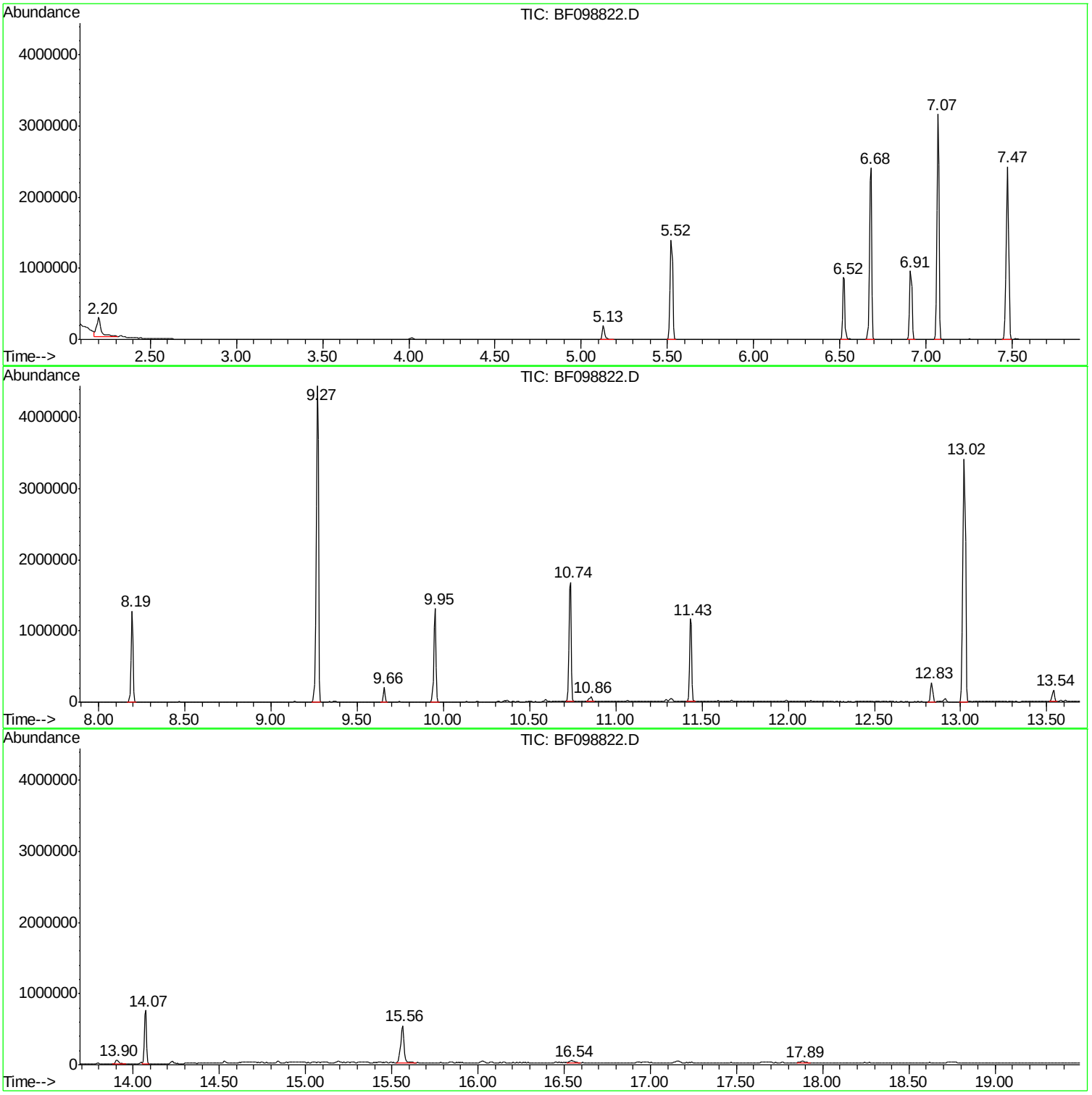
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098822.D
Acq On : 26 Sep 2017 10:23
Operator : SJ/JU
Sample : I5385-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-SIDI-F-D-B

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\BF092517\
Data File : BF098822.D
Acq On : 26 Sep 2017 10:23
Operator : SJ/JU
Sample : I5385-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-SIDI-F-D-B

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

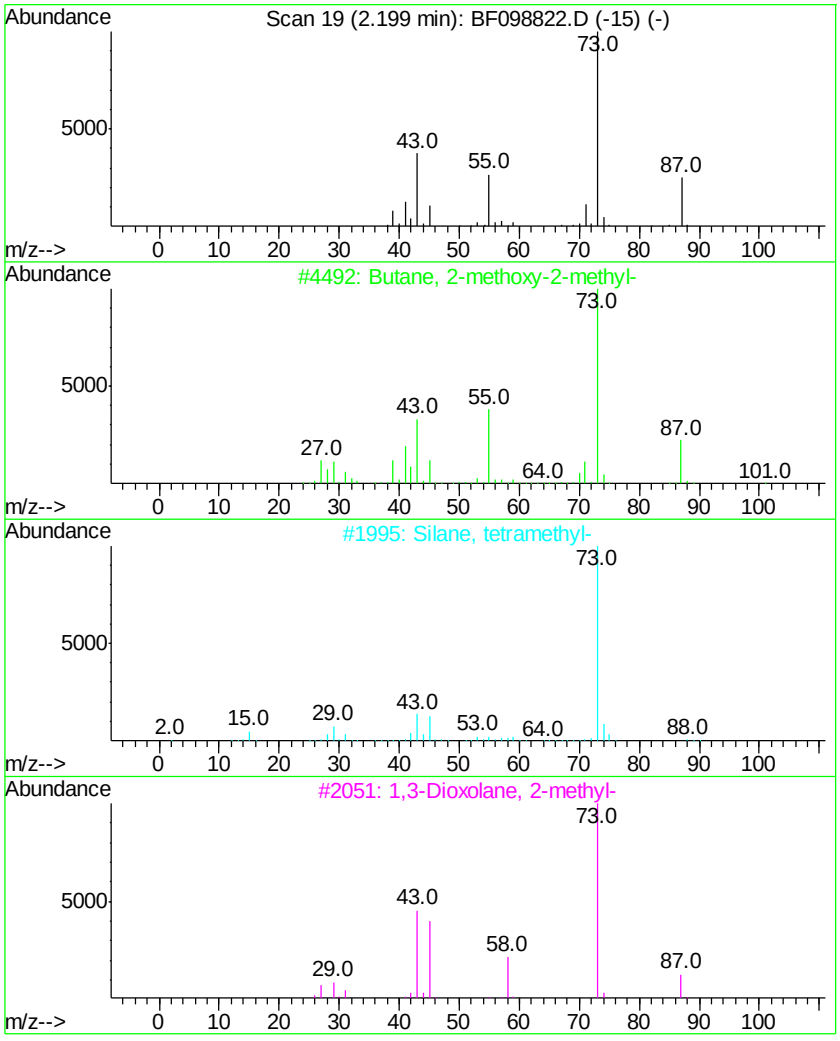
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

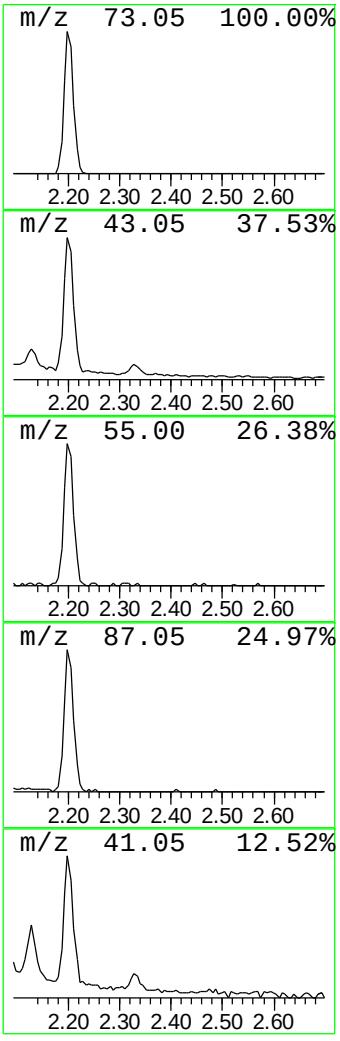
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	12.07 ng	472687	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	37
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098822.D
Acq On : 26 Sep 2017 10:23
Operator : SJ/JU
Sample : I5385-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-SIDI-F-D-B

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

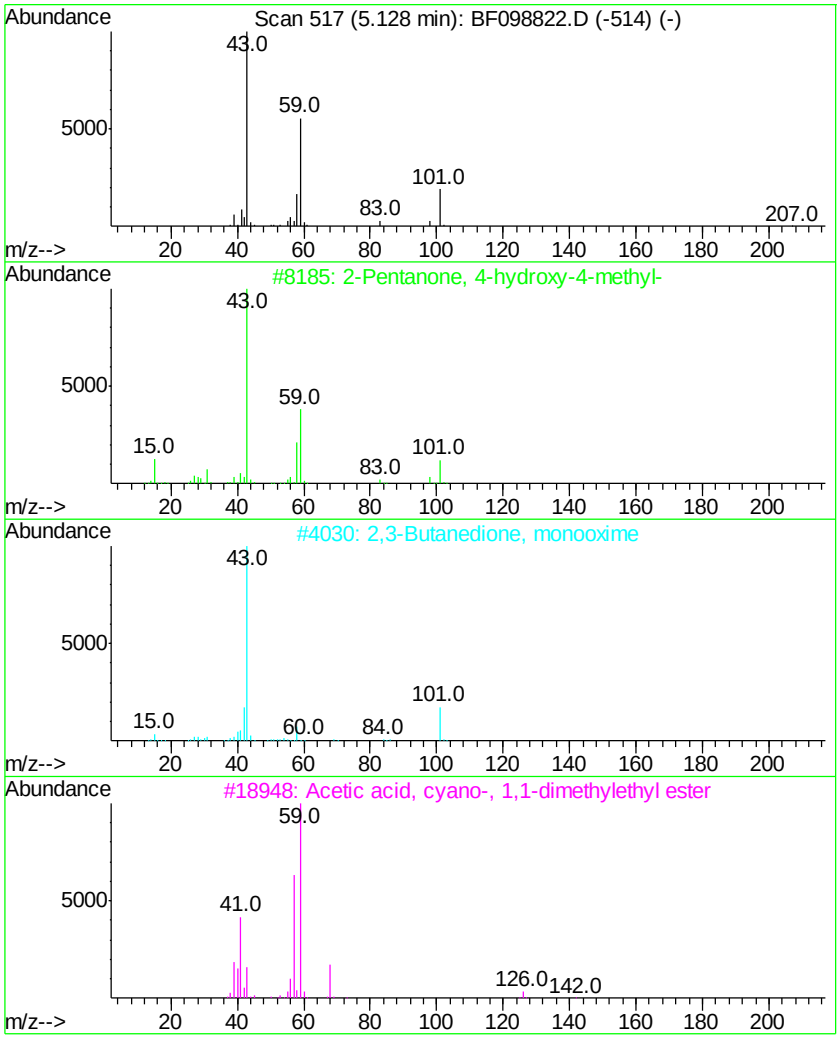
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

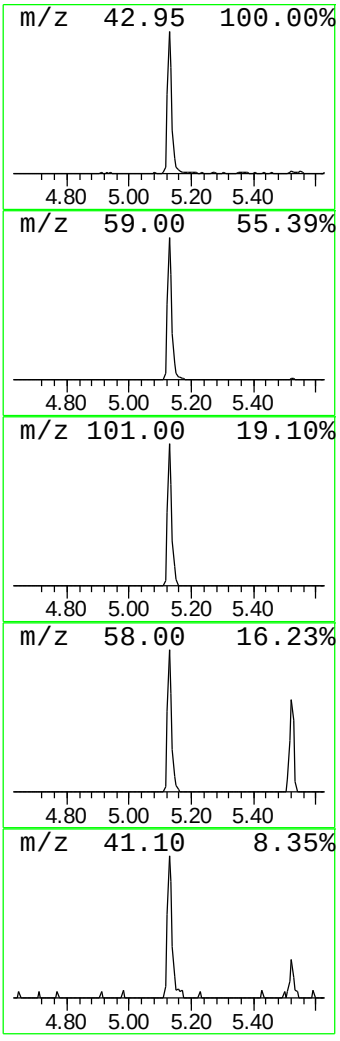
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	4.94 ng	193279	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098822.D
Acq On : 26 Sep 2017 10:23
Operator : SJ/JU
Sample : I5385-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-SIDI-F-D-B

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

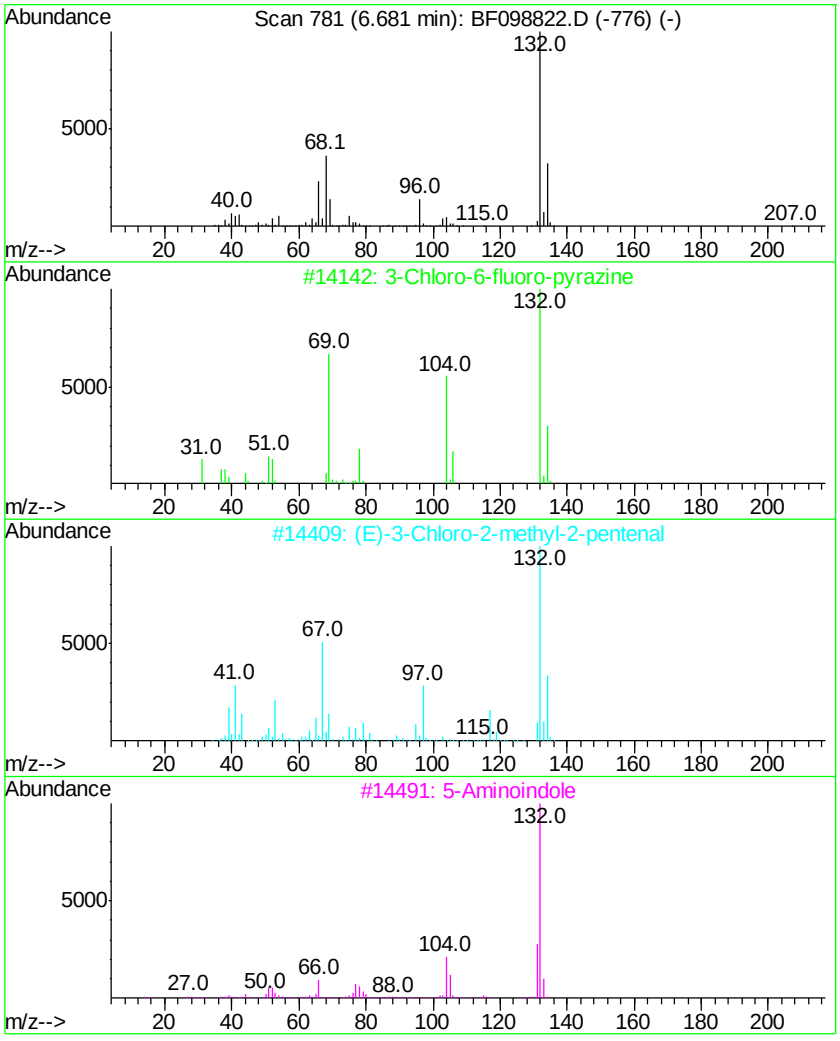
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

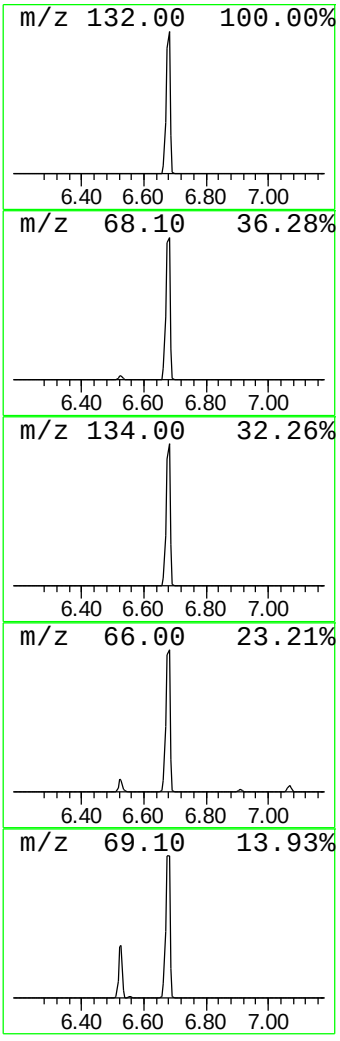
****

Peak Number 3 unknown6.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	58.20 ng	2278850	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098822.D
Acq On : 26 Sep 2017 10:23
Operator : SJ/JU
Sample : I5385-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-SIDI-F-D-B

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

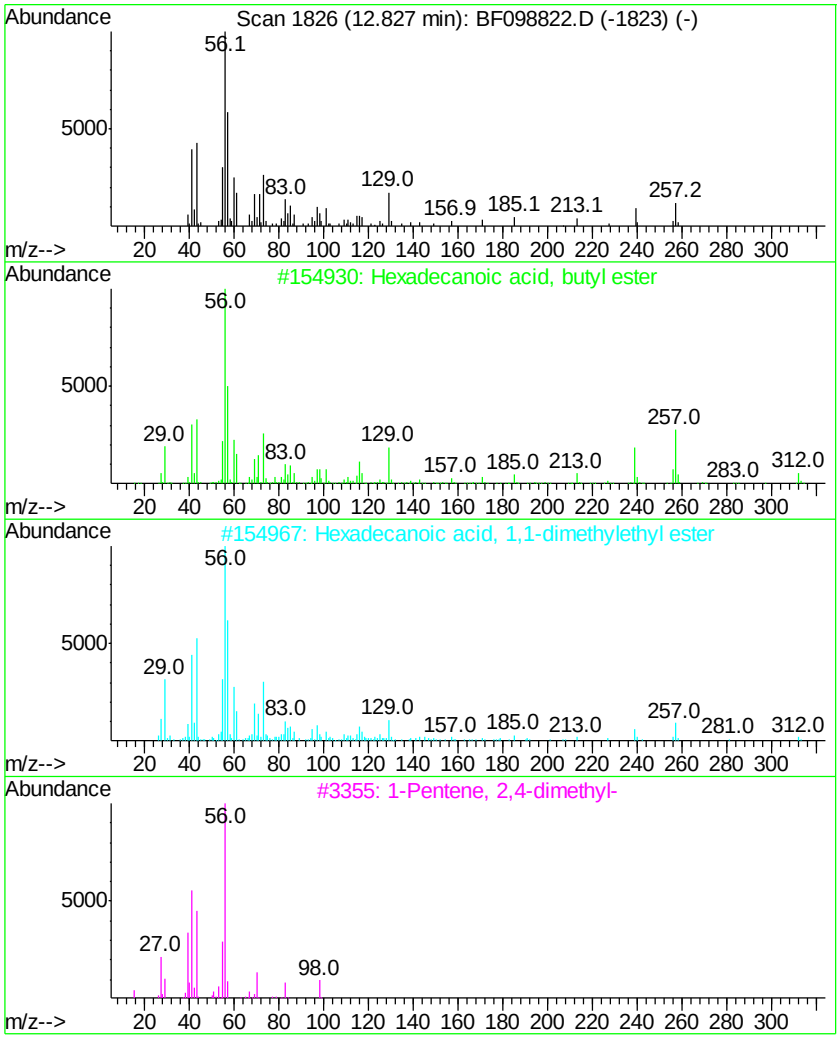
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

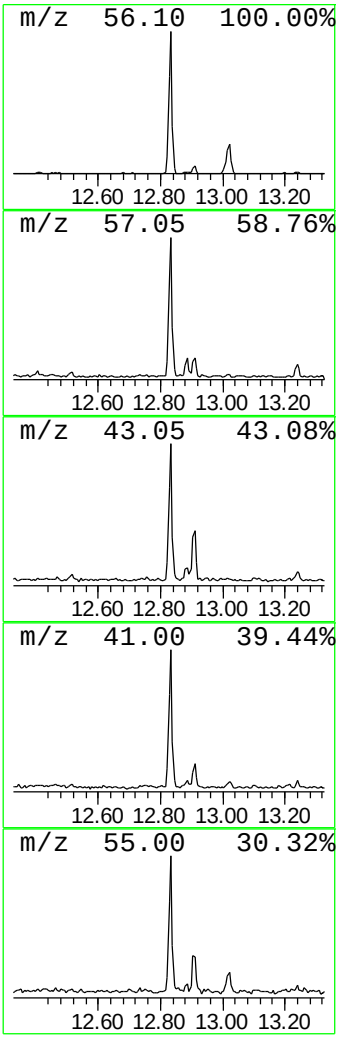
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	6.10 ng	206630	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098822.D
Acq On : 26 Sep 2017 10:23
Operator : SJ/JU
Sample : I5385-01
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-SIDI-F-D-B

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

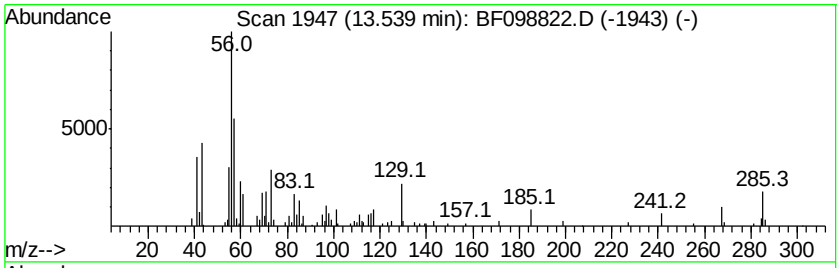
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

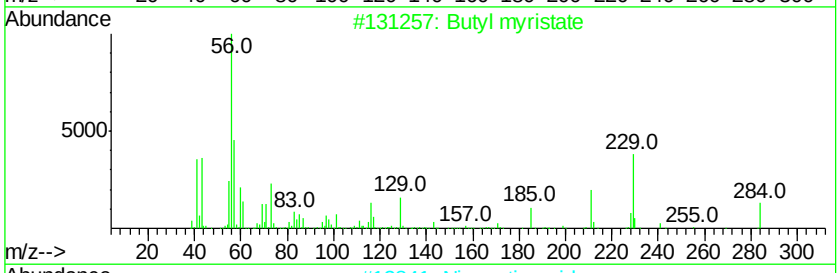
****

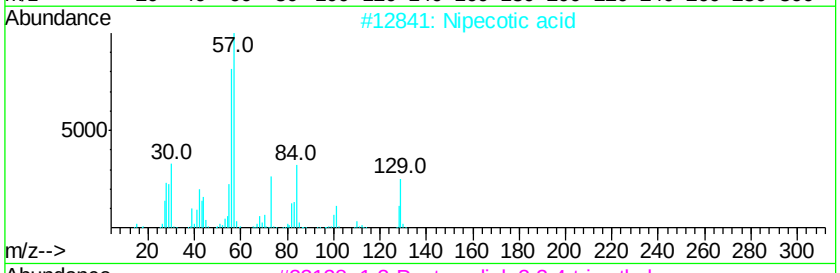
Peak Number 6 Butyl myristate Concentration Rank 6

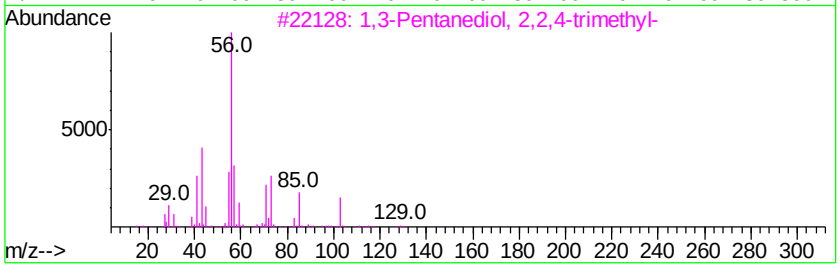
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	4.09 ng	138348	Chrysene-d12	14.07

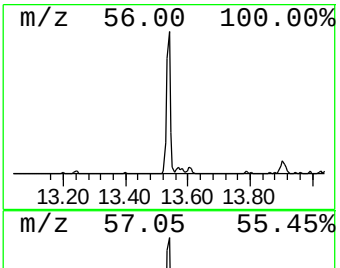
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	59
2	Nipecotic acid	129	C6H11NO2	000498-95-3	38
3	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	37
4	Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	35
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35

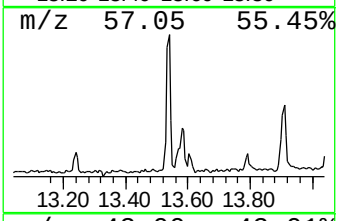


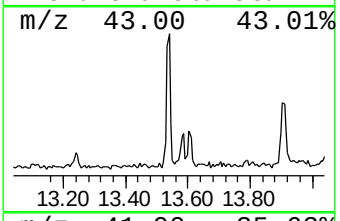


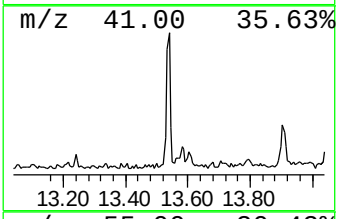


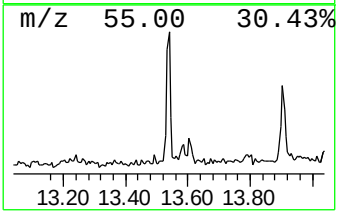












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

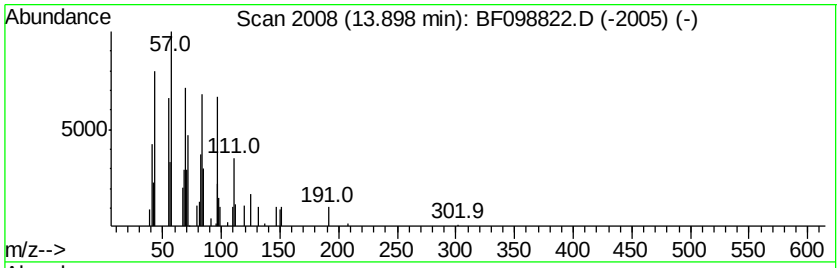
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

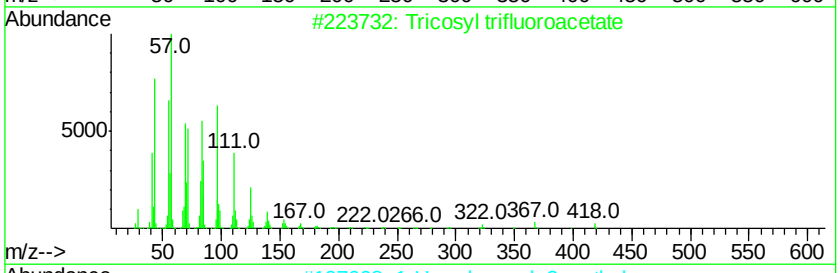
****

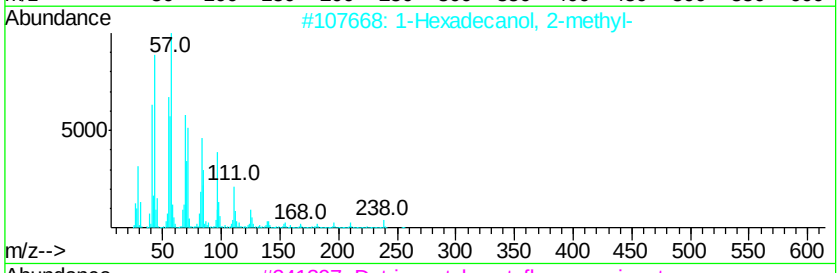
Peak Number 7 Tricosyl trifluoroacetate Concentration Rank 7

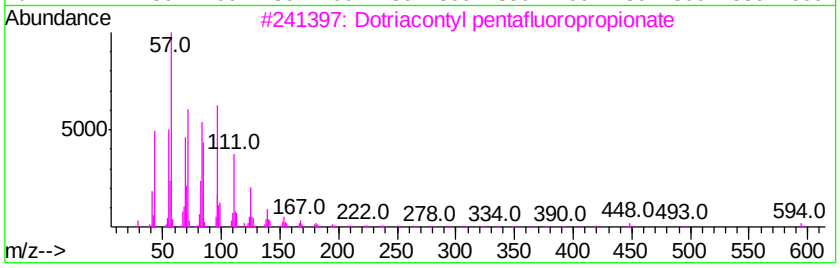
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	2.21 ng	74787	Chrysene-d12	14.07

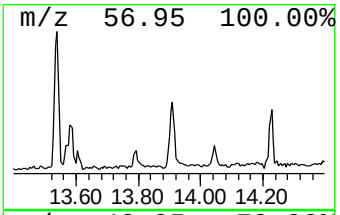
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	91
3	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	90
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	90

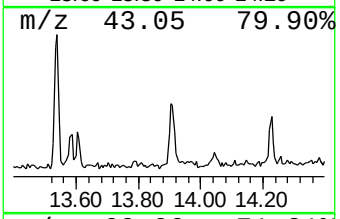


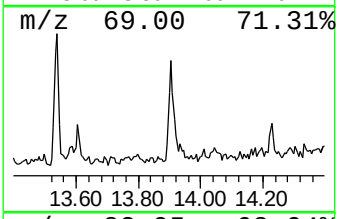


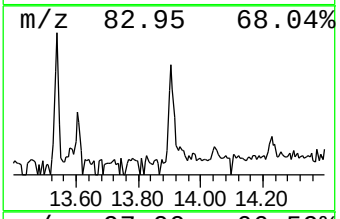


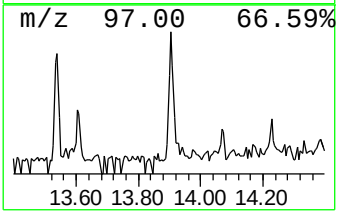












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098822.D
Acq On : 26 Sep 2017 10:23
Operator : SJ/JU
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Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-SIDI-F-D-B

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
Butane, 2-methoxy...	2.20	12.1	ng	472687	1	6.91	783105	20.0
2-Pentanone, 4-hy...	5.13	4.9	ng	193279	1	6.91	783105	20.0
unknown6.68	6.68	58.2	ng	2278850	1	6.91	783105	20.0
Hexadecanoic acid...	12.83	6.1	ng	206630	5	14.07	677156	20.0
Butyl myristate	13.54	4.1	ng	138348	5	14.07	677156	20.0
Tricosyl trifluor...	13.90	2.2	ng	74787	5	14.07	677156	20.0