LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
Data File : BF104522.D
Acq On : 14 Apr 2018 12:54
Operator : JU/SJ
Sample : J2368-16
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-SIDI-E-U-M

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-BF040618.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	5.004	493	496	504	rVB	111745	118183	2.75%	0.460%
2	5.422	563	567	570	rBV	1330118	1209874	28.13%	4.705%
3	6.028	668	670	681	rBV	103618	105539	2.45%	0.410%
4	6.434	736	739	751	rVB2	785628	813389	18.91%	3.163%
5	6.575	759	763	766	rBV	2507606	2266920	52.72%	8.816%
6	6.804	799	802	806	rBV	1054391	916437	21.31%	3.564%
7	6.963	825	829	833	rBV	3274805	3220315	74.89%	12.524%
8	7.375	893	899	902	rBV	2531910	2640697	61.41%	10.270%
9	7.457	909	913	920	rBV	40878	45804	1.07%	0.178%
10	8.092	1017	1021	1024	rBV	1376899	1181034	27.46%	4.593%
11	9.169	1198	1204	1207	rBV	4492058	4300322	100.00%	16.724%
12	9.557	1267	1270	1278	rBV	379333	333663	7.76%	1.298%
13	9.845	1314	1319	1328	rVB2	1411374	1211972	28.18%	4.713%
14	10.275	1388	1392	1395	rVB2	94839	85130	1.98%	0.331%
15	10.522	1431	1434	1436	rVB	162275	129957	3.02%	0.505%
16	10.633	1449	1453	1464	rVB	1500310	1409455	32.78%	5.482%
17	10.745	1470	1472	1482	rVB	98952	99043	2.30%	0.385%
18	11.333	1568	1572	1576	rBV	1174383	939090	21.84%	3.652%
19	12.739	1808	1811	1814	rVB	130298	99421	2.31%	0.387%
20	12.927	1838	1843	1846	rBV	3074411	2992465	69.59%	11.638%
21	13.445	1928	1931	1935	rBV	81661	65190	1.52%	0.254%
22	13.821	1989	1995	2005	rBV	55754	74963	1.74%	0.292%
23	13.974	2017	2021	2025	rBV	860623	807023	18.77%	3.139%
24	15.439	2265	2270	2282	rBV2	463625	647054	15.05%	2.516%

Sum of corrected areas: 25712940

LSC Report - Integrated Chromatogram

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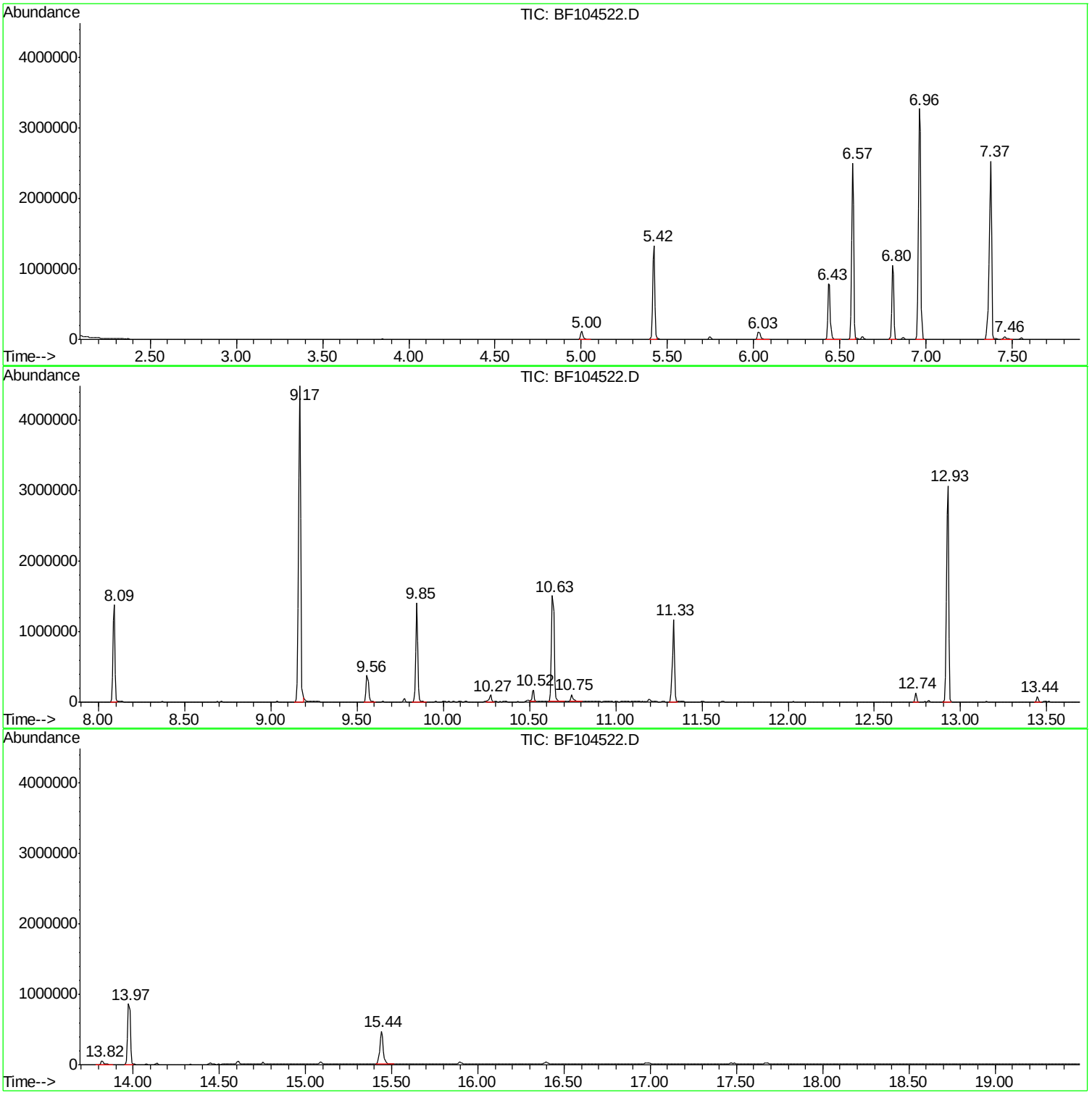
Instrument : BNA_F
ClientSampleId : 041118-SIDI-E-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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ClientSampleId : 041118-SIDI-E-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

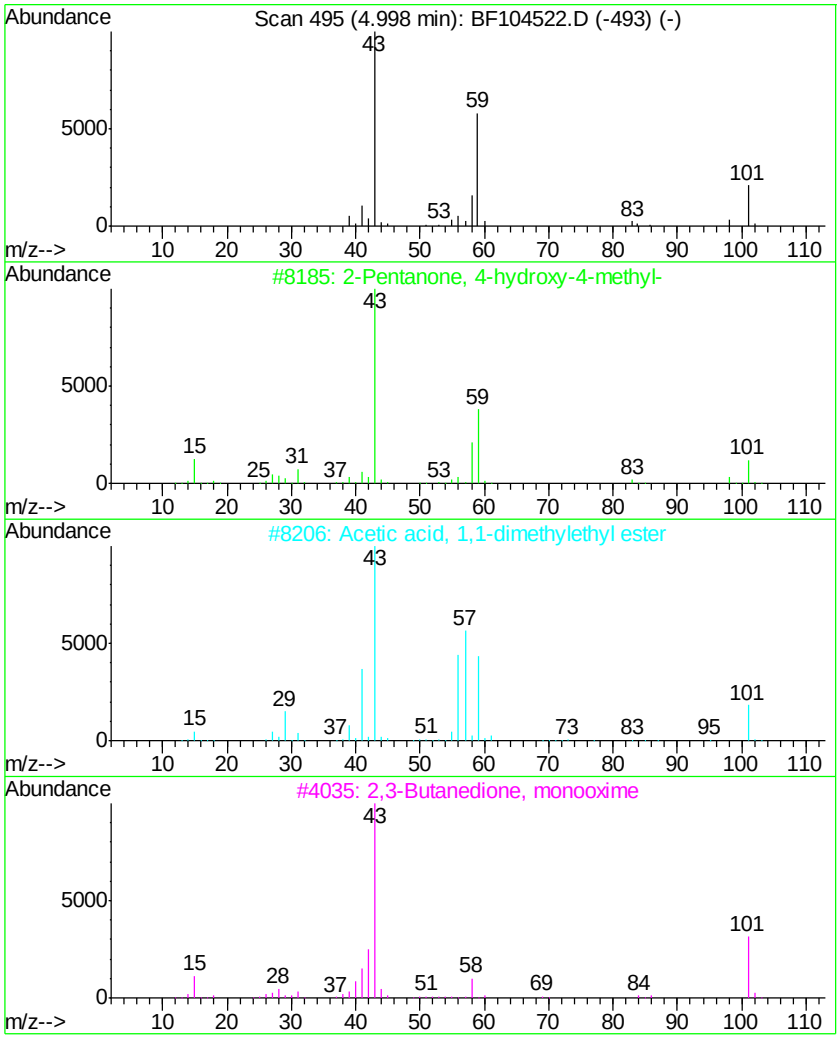
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

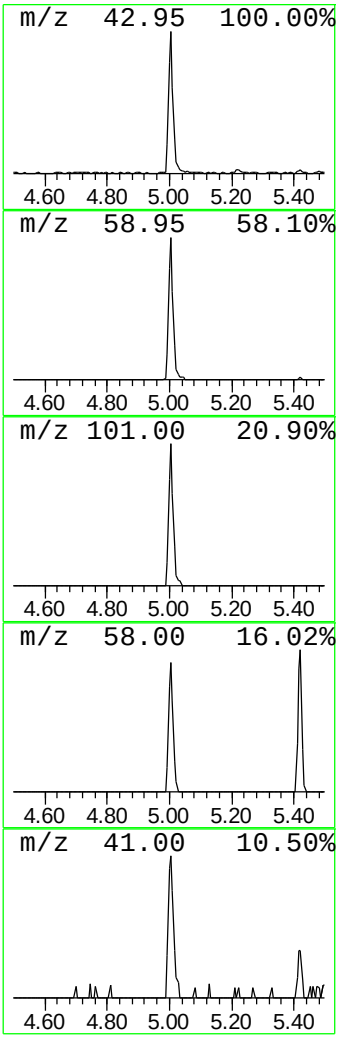
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	2.58 ng	118183	1,4-Dichlorobenzene-d4	6.80

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17





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Instrument : BNA_F
ClientSampleId : 041118-SIDI-E-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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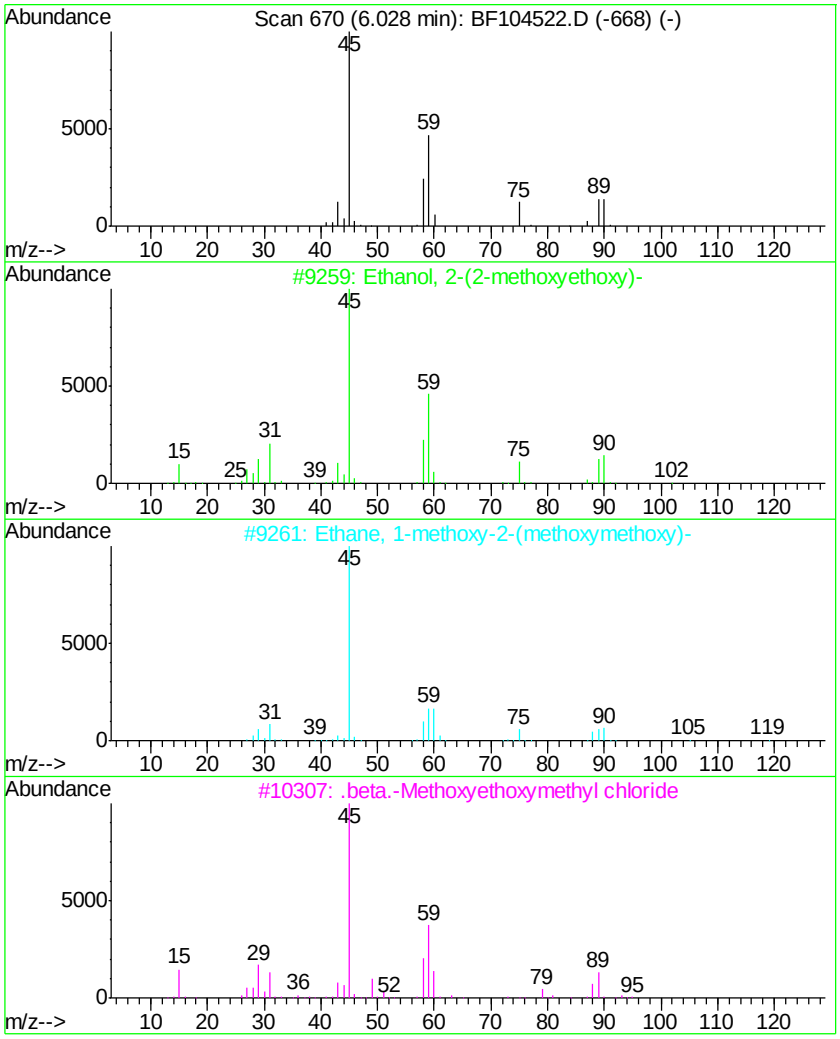
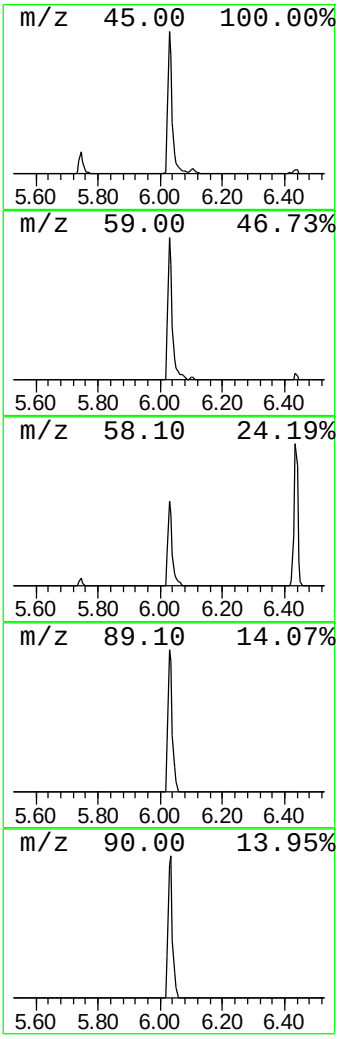
Peak Number 2 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.03	2.30 ng	105539	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	90
2	Ethane, 1-methoxy-2-(methoxymeth...	120	C5H12O3	074498-88-7	64
3	.beta.-Methoxyethoxymethyl chloride	124	C4H9ClO2	003970-21-6	50
4	Ethane, 1,2-dimethoxy-	90	C4H10O2	000110-71-4	43
5	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	36





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Data File : BF104522.D
Acq On : 14 Apr 2018 12:54
Operator : JU/SJ
Sample : J2368-16
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-SIDI-E-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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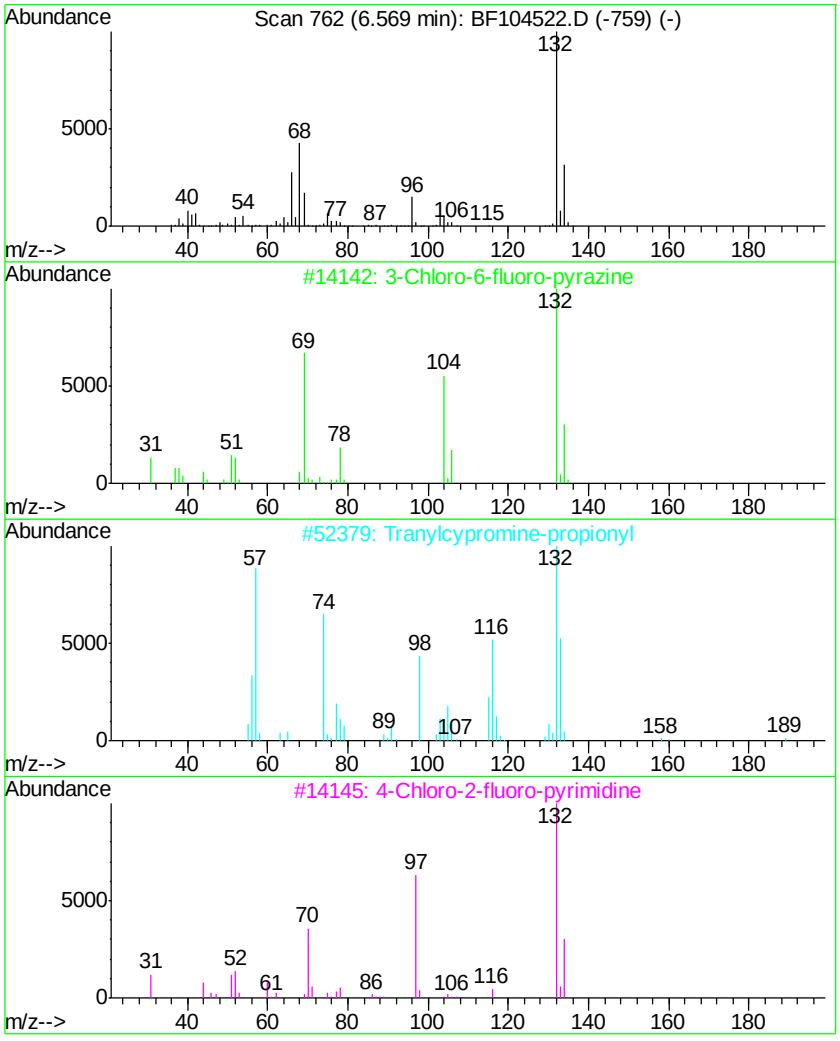
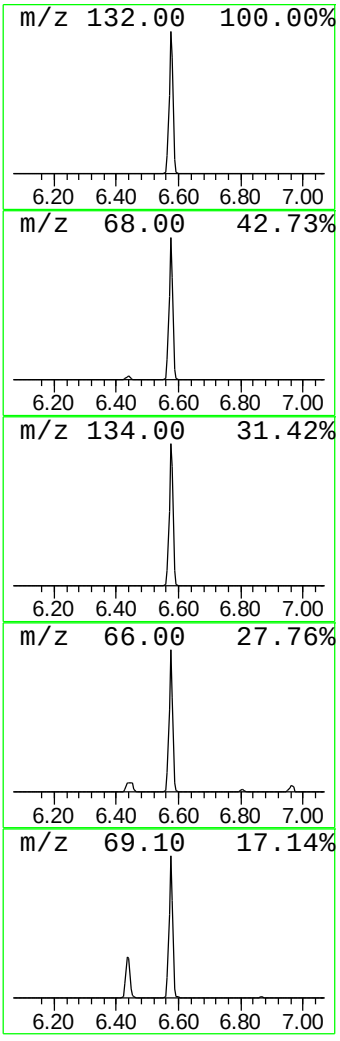
Peak Number 3 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	49.47 ng	2266920	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Misc :
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Instrument : BNA_F
ClientSampleId : 041118-SIDI-E-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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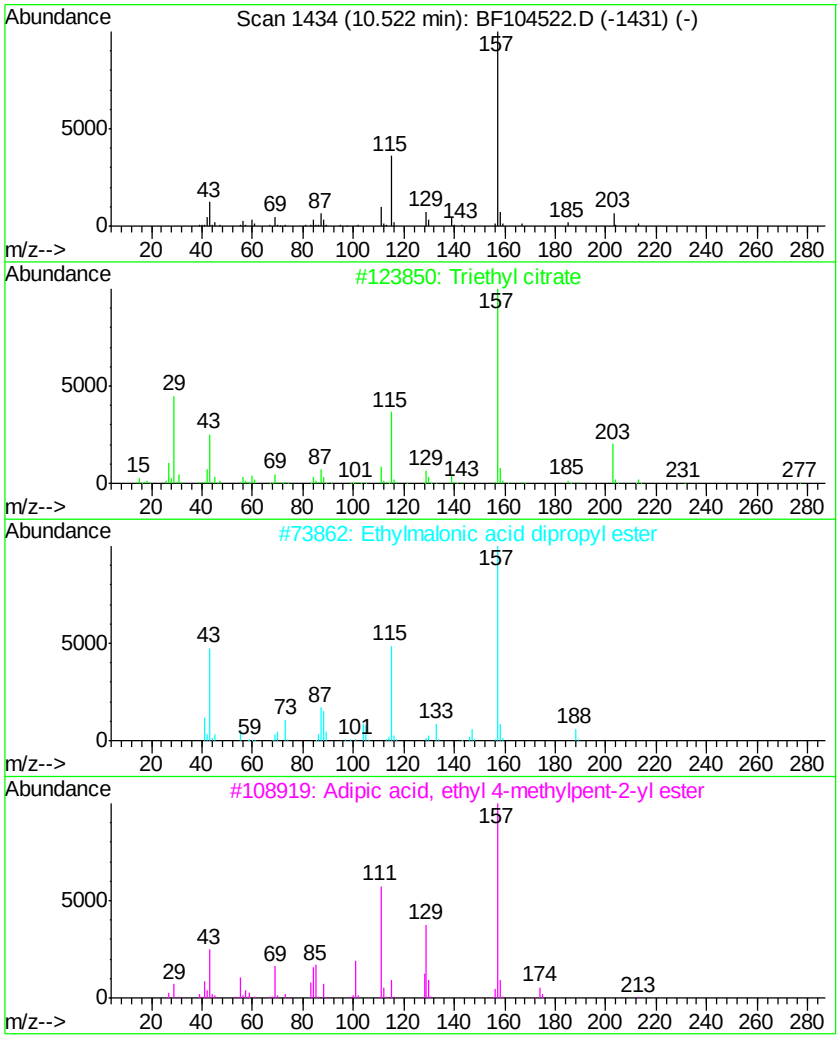
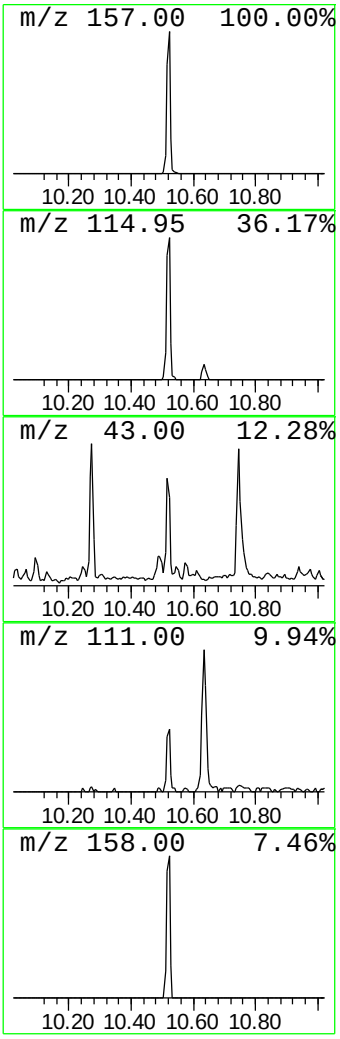
Peak Number 5 Triethyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.52	2.14 ng	129957	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	90
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	59
3	Adipic acid, ethyl 4-methylpent-...	258	C14H26O4	1000353-49-9	53
4	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	36
5	Quinoline, 2,4-dimethyl-	157	C11H11N	001198-37-4	36





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Instrument : BNA_F
ClientSampleId : 041118-SIDI-E-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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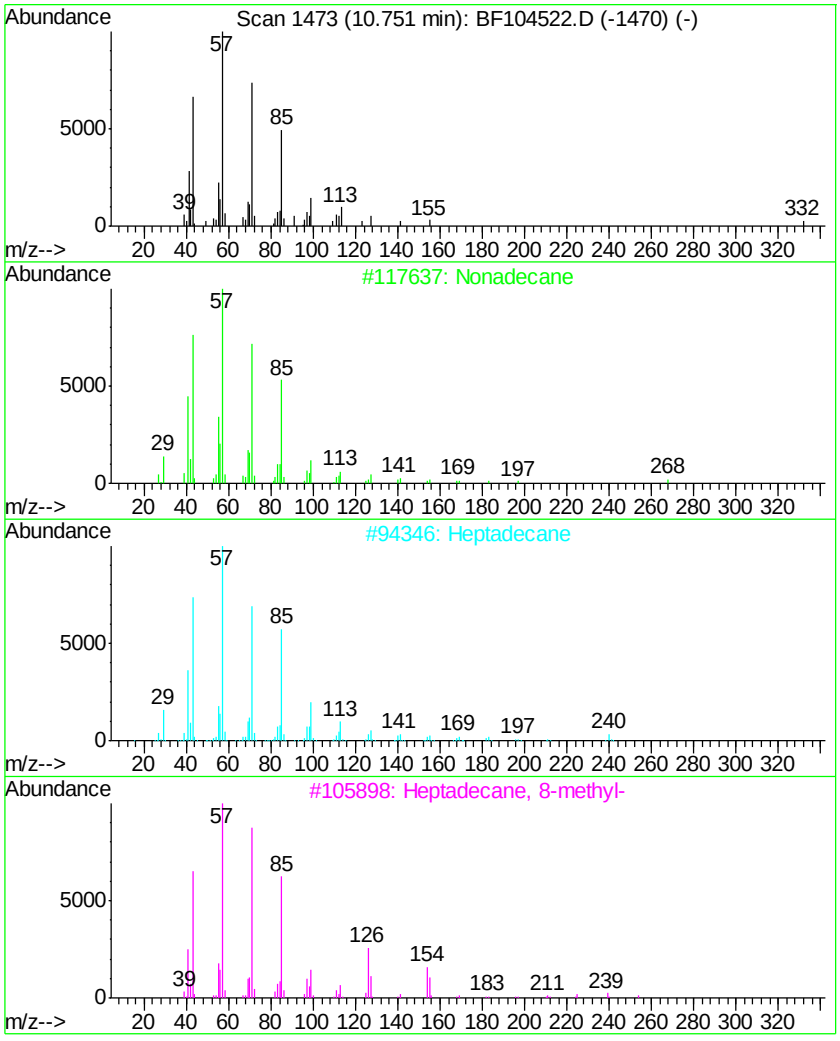
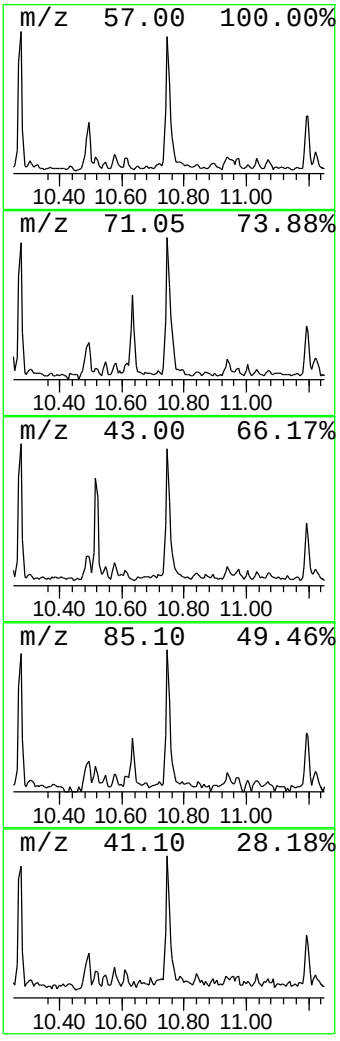
****

Peak Number 6 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.11 ng	99043	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	90
4	Tetradecane	198	C14H30	000629-59-4	87
5	Hexadecane	226	C16H34	000544-76-3	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\
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Operator : JU/SJ
Sample : J2368-16
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 041118-SIDI-E-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

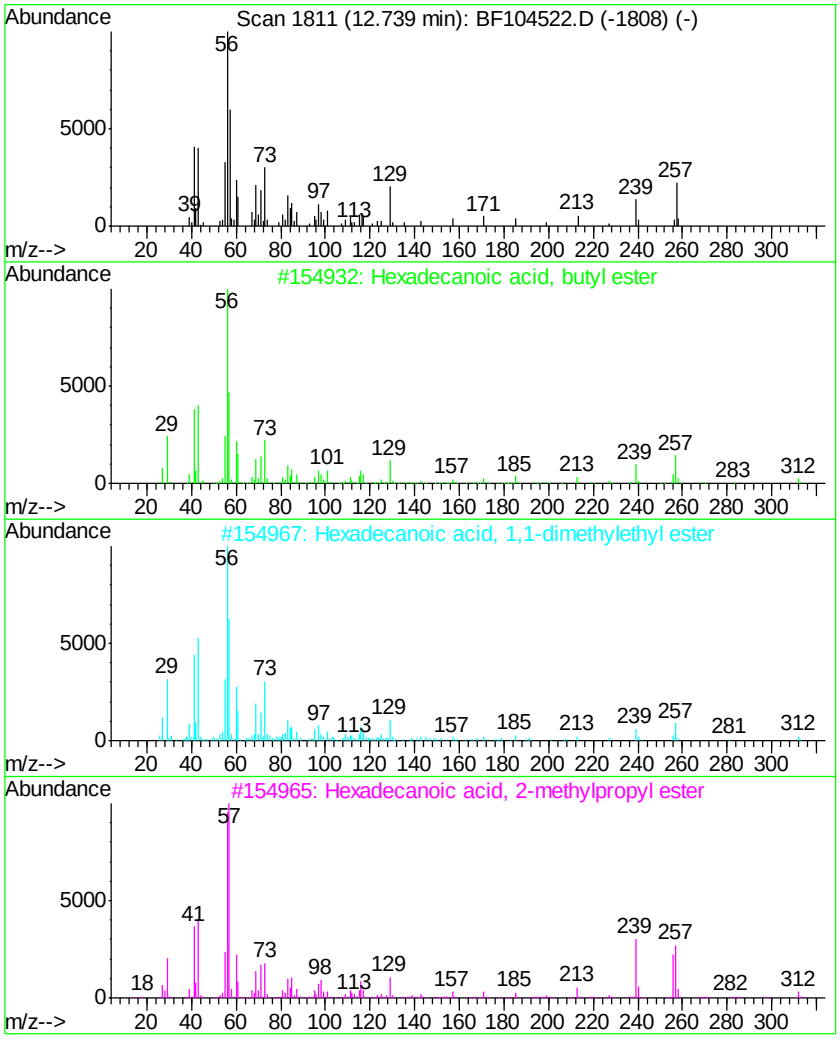
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

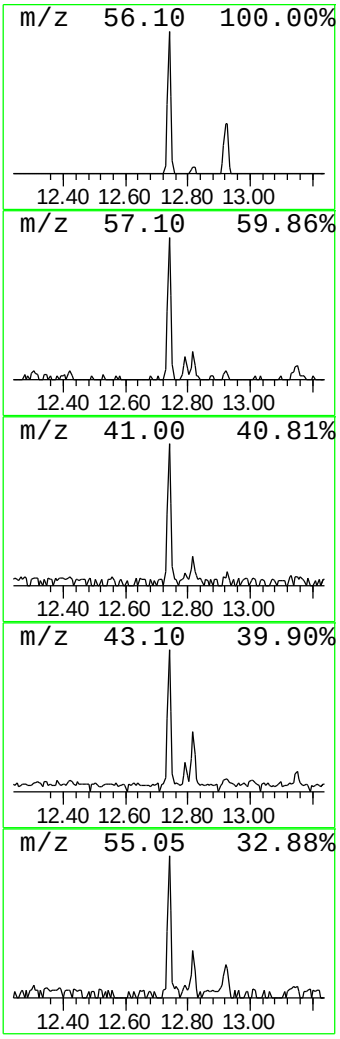
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.46 ng	99421	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	64
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	38
5	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35





Tentatively Identified Compound (LSC) summary

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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...	5.00	2.6	ng	118183	1	6.80	916437	20.0
Ethanol, 2-(2-met...	6.03	2.3	ng	105539	1	6.80	916437	20.0
unknown6.57	6.57	49.5	ng	2266920	1	6.80	916437	20.0
Triethyl citrate	10.52	2.1	ng	129957	3	9.85	1211970	20.0
Nonadecane	10.75	2.1	ng	99043	4	11.33	939090	20.0
Hexadecanoic acid...	12.74	2.5	ng	99421	5	13.97	807023	20.0