LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083749.D
Acq On : 14 Dec 2015 00:32
Operator : UM/IZ
Sample : G4759-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K210-35-37

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-BF121315.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	2.224	10	12	29	rVB4	50760	160521	4.78%	0.539%
2	5.116	262	265	271	rBV	497780	713528	21.23%	2.397%
3	5.527	298	301	303	rBV	2729665	2869668	85.38%	9.639%
4	6.544	387	390	392	rBV	2615882	2829641	84.19%	9.505%
5	6.681	399	402	405	rBV	2474841	3115783	92.70%	10.466%
6	6.922	420	423	425	rBV	635228	731580	21.77%	2.457%
7	7.070	434	436	439	rVB	1890668	2357974	70.16%	7.921%
8	7.482	469	472	474	rBV	1461922	2107125	62.69%	7.078%
9	8.202	532	535	537	rBV	1102772	1020877	30.37%	3.429%
10	9.276	626	629	631	rBV	3550473	3361032	100.00%	11.290%
11	9.665	661	663	665	rBV	796846	659510	19.62%	2.215%
12	9.893	681	683	686	rBV	42846	35993	1.07%	0.121%
13	9.950	686	688	691	rVB	1218436	1095365	32.59%	3.679%
14	10.396	723	727	728	rBV	44388	57813	1.72%	0.194%
15	10.739	754	757	759	rBV	2140199	2267971	67.48%	7.618%
16	10.865	765	768	772	rBV	74625	92059	2.74%	0.309%
17	11.311	805	807	808	rBV	57583	46106	1.37%	0.155%
18	11.436	815	818	820	rBV	834132	1050870	31.27%	3.530%
19	12.842	939	941	944	rBV2	205041	184816	5.50%	0.621%
20	12.922	944	948	950	rVB2	49933	62731	1.87%	0.211%
21	13.014	953	956	959	rBV	2925218	2788638	82.97%	9.367%
22	13.551	1001	1003	1005	rBV	99576	120315	3.58%	0.404%
23	13.596	1005	1007	1011	rVB2	46446	60222	1.79%	0.202%
24	13.905	1032	1034	1045	rBV2	167491	271362	8.07%	0.912%
25	14.054	1045	1047	1050	rVV	756208	732712	21.80%	2.461%
26	14.237	1060	1063	1069	rVB	70134	67618	2.01%	0.227%
27	14.545	1088	1090	1092	rBV	46464	57530	1.71%	0.193%
28	14.842	1113	1116	1119	rBV	46544	47426	1.41%	0.159%
29	14.922	1120	1123	1125	rVB	26886	36817	1.10%	0.124%
30	15.174	1142	1145	1150	rBV	33663	43806	1.30%	0.147%
31	15.494	1170	1173	1176	rBV	524778	633657	18.85%	2.128%
32	16.477	1254	1259	1268	rVB2	14223	38282	1.14%	0.129%
33	17.757	1364	1371	1382	rVB3	11176	50890	1.51%	0.171%

LSC Area Percent Report

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Data File : BF083749.D
Acq On : 14 Dec 2015 00:32
Operator : UM/IZ
Sample : G4759-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K210-35-37

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-BF121315.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 29770238

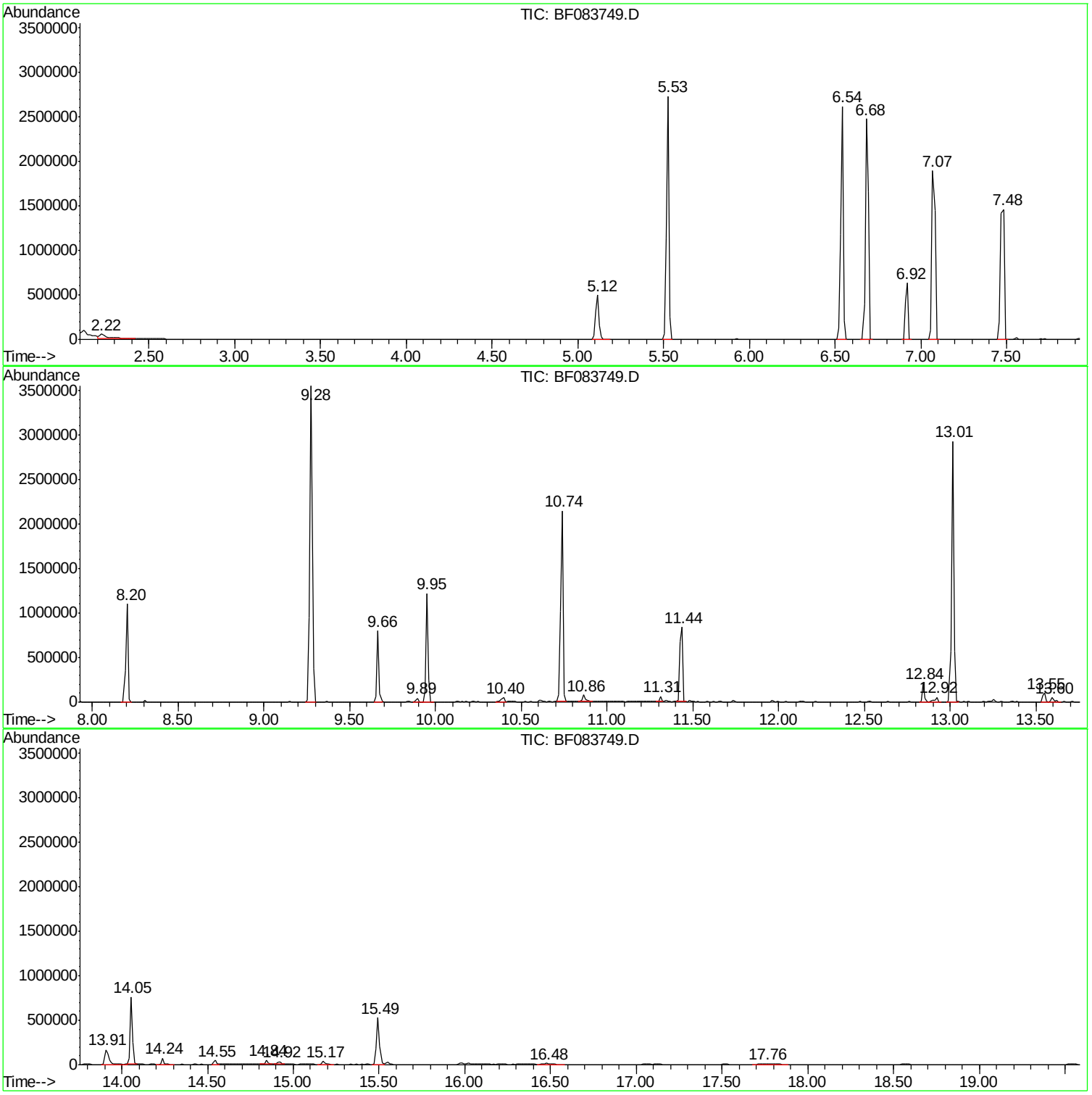
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083749.D
Acq On : 14 Dec 2015 00:32
Operator : UM/IZ
Sample : G4759-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K210-35-37

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083749.D
Acq On : 14 Dec 2015 00:32
Operator : UM/IZ
Sample : G4759-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K210-35-37

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

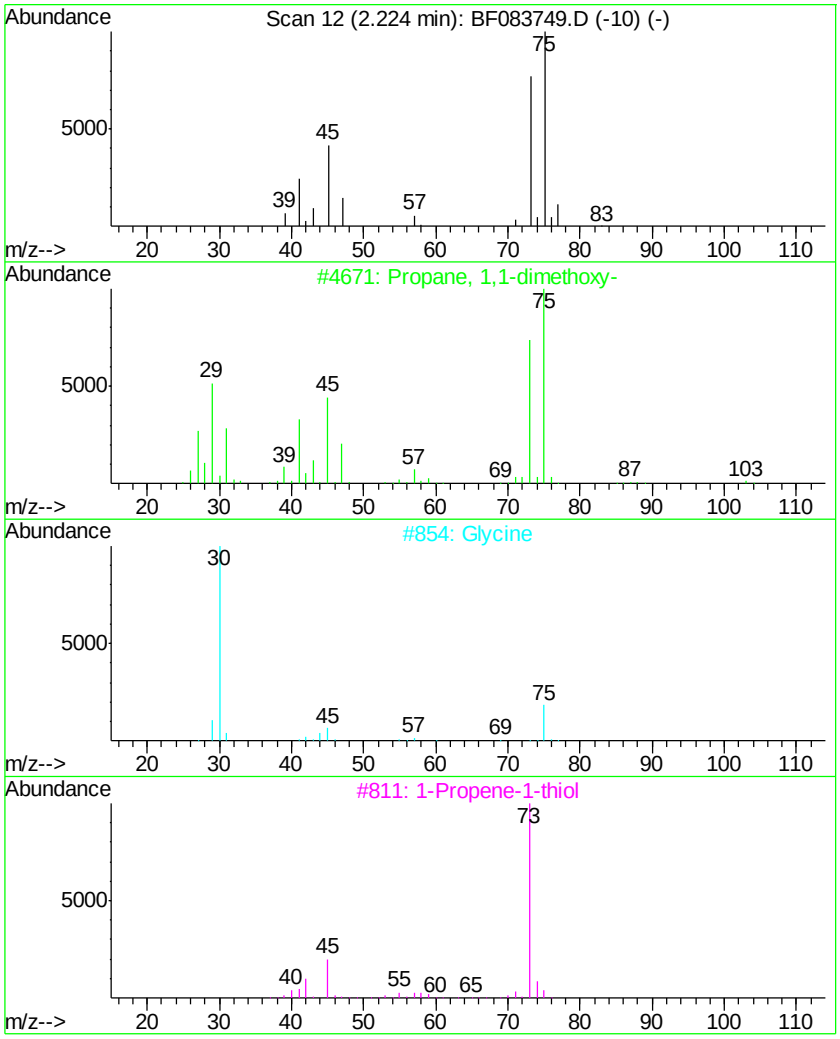
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

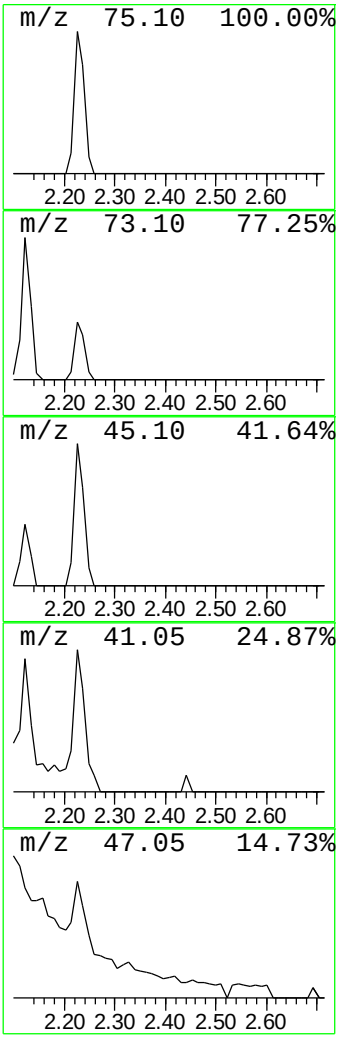
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	4.39 ng	160521	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	Glycine	75	C2H5NO2	000056-40-6	7
3	1-Propene-1-thiol	74	C3H6S	000925-89-3	4
4	Methane, nitroso-	45	CH3NO	000865-40-7	4
5	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083749.D
Acq On : 14 Dec 2015 00:32
Operator : UM/IZ
Sample : G4759-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K210-35-37

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

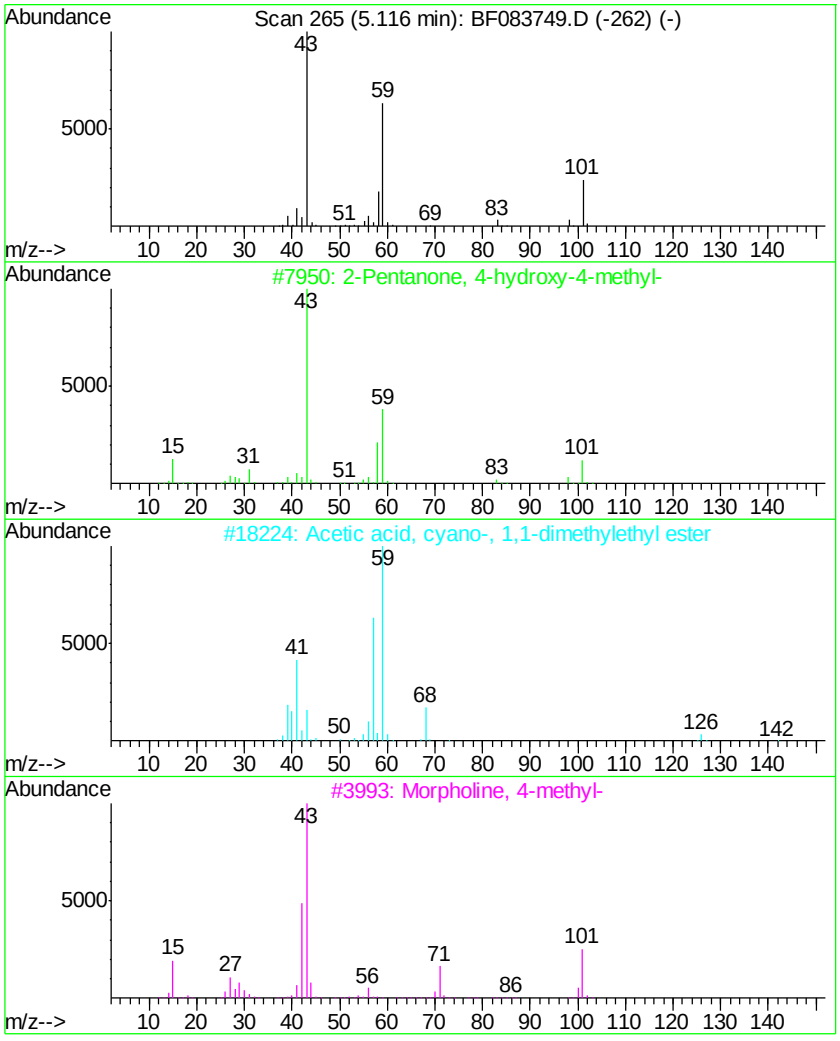
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

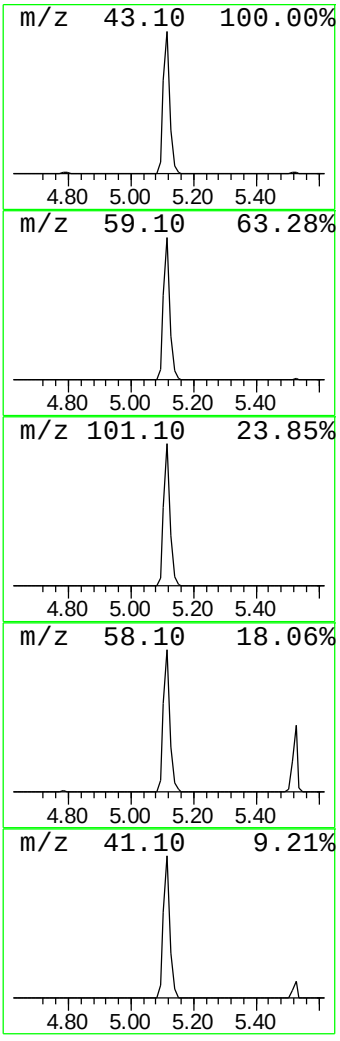
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	19.51 ng	713528	1,4-Dichlorobenzene-d4	6.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF121315\
Data File : BF083749.D
Acq On : 14 Dec 2015 00:32
Operator : UM/IZ
Sample : G4759-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K210-35-37

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

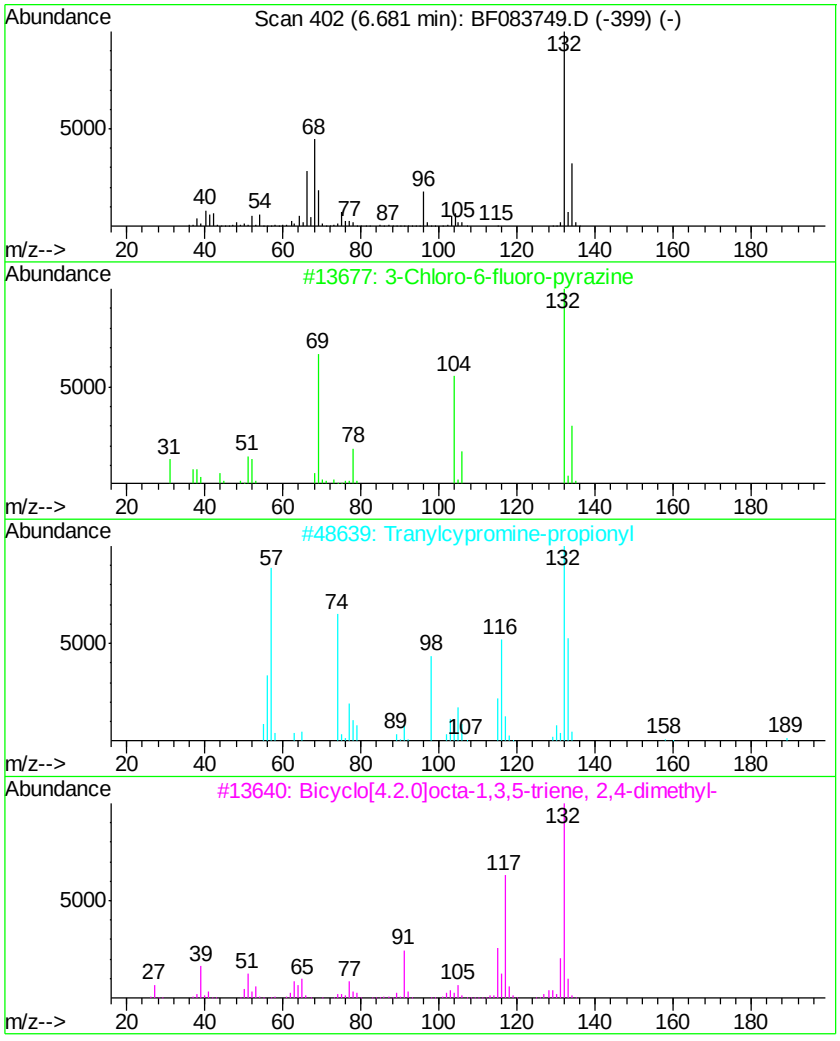
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

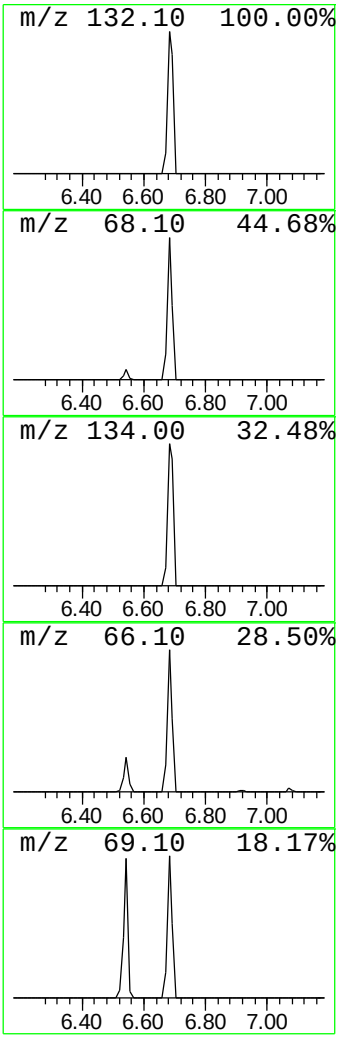
****

Peak Number 3 unknown6.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	85.18 ng	3115780	1,4-Dichlorobenzene-d4	6.92

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Data File : BF083749.D
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Operator : UM/IZ
Sample : G4759-08
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K210-35-37

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

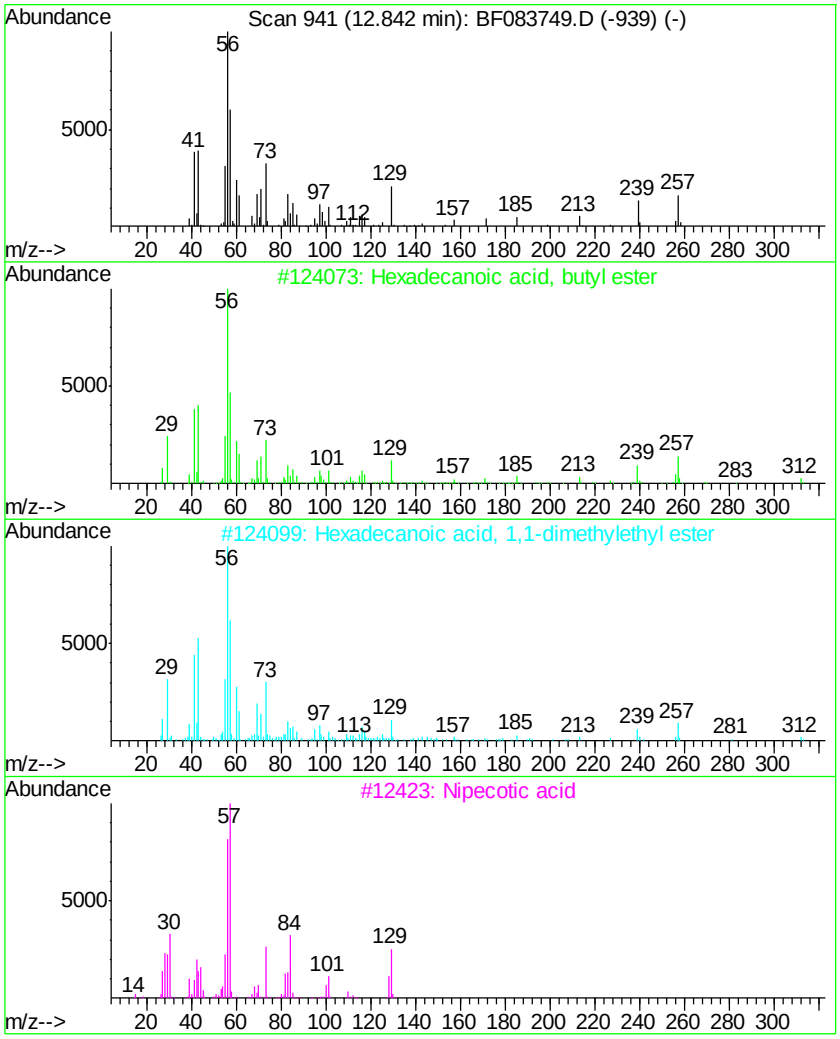
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

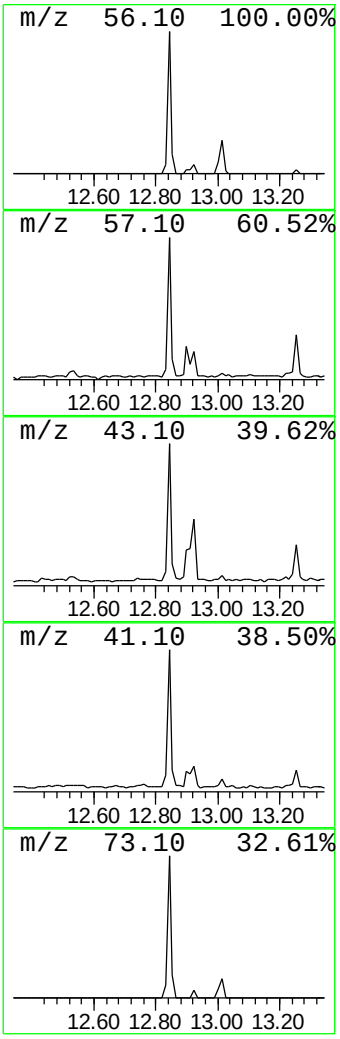
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	5.04 ng	184816	Chrysene-d12	14.05

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	74
3	Nipecotic acid	129	C6H11NO2	000498-95-3	43
4	Piperidin-4-carboxylic acid	129	C6H11NO2	000498-94-2	38
5	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35





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Operator : UM/IZ
Sample : G4759-08
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ALS Vial : 41 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : K210-35-37

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

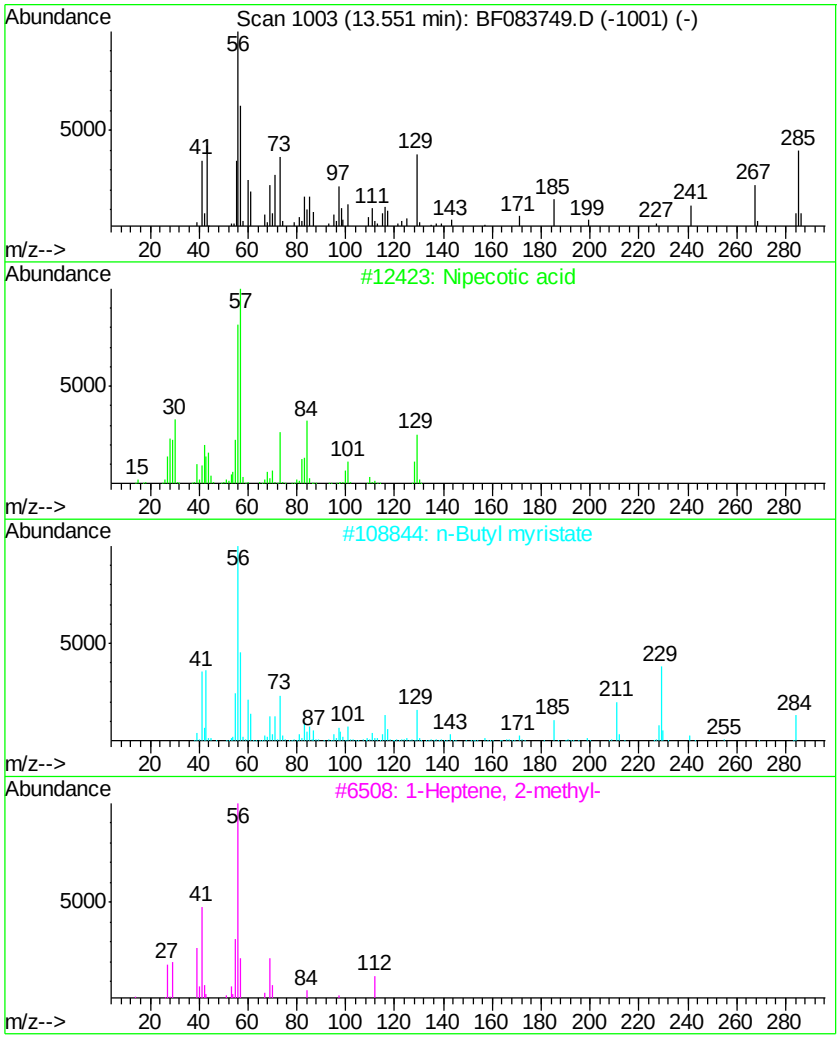
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

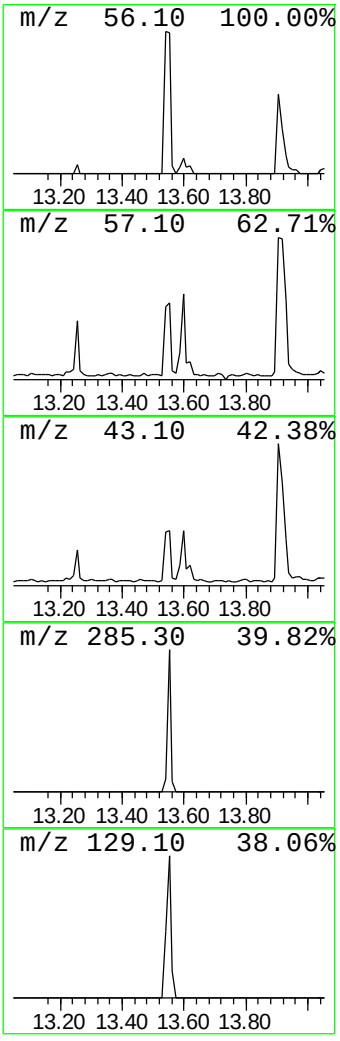
****

Peak Number 6 unknown13.55 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	3.28 ng	120315	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nipecotic acid	129	C6H11NO2	000498-95-3	38
2	n-Butyl myristate	284	C18H36O2	000110-36-1	38
3	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	18
4	Cyclohexanamine	99	C6H13N	000108-91-8	18
5	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	14





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Sample : G4759-08
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
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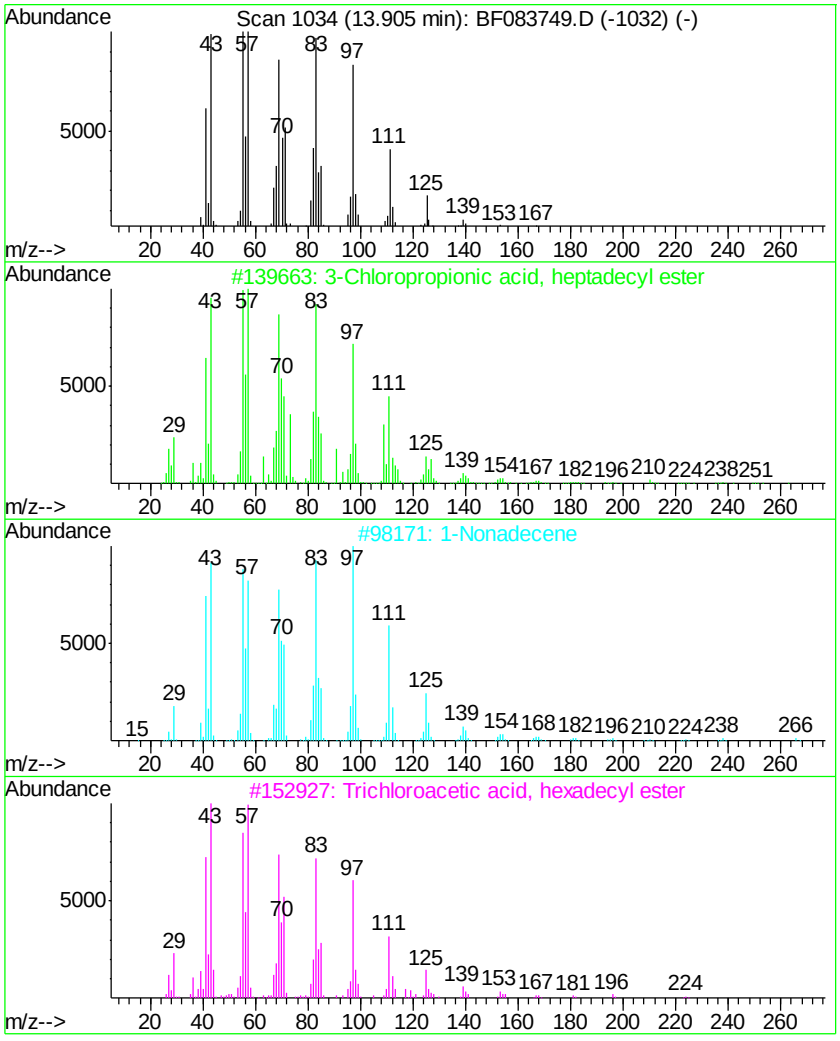
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

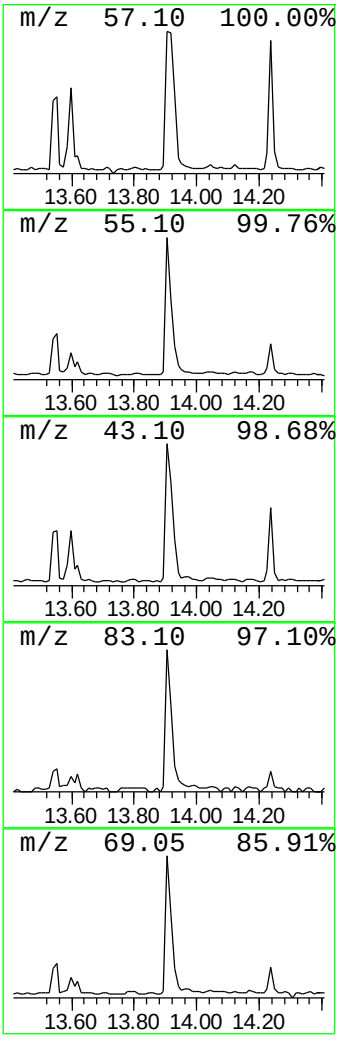
****

Peak Number 7 3-Chloropropionic acid, hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	7.41 ng	271362	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	90
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121315\
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Acq On : 14 Dec 2015 00:32
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Misc :
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Instrument : BNA_F
ClientSampleId : K210-35-37

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 1,1-dime...	2.22	4.4	ng	160521	1	6.92	731580	20.0
2-Pentanone, 4-hy...	5.12	19.5	ng	713528	1	6.92	731580	20.0
unknown6.68	6.68	85.2	ng	3115780	1	6.92	731580	20.0
Hexadecanoic acid...	12.84	5.0	ng	184816	5	14.05	732712	20.0
unknown13.55	13.55	3.3	ng	120315	5	14.05	732712	20.0
3-Chloropropionic...	13.91	7.4	ng	271362	5	14.05	732712	20.0