LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
Data File : BF089801.D
Acq On : 19 Aug 2016 17:47
Operator : UM/SJ
Sample : PB92975BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92975BL

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-BF081916.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	1.655	4	6	15	rBV	3440569	6216296	30.08%	3.950%
2	1.781	15	17	27	rVV	8372568	20664480	100.00%	13.131%
3	1.907	27	28	64	rVB2	770126	3966390	19.19%	2.520%
4	4.833	281	284	294	rVB	1874969	3360899	16.26%	2.136%
5	5.267	319	322	325	rBV	8696597	12842655	62.15%	8.161%
6	6.319	411	414	417	rBV	8896978	11478013	55.54%	7.294%
7	6.444	422	425	428	rBV	10001444	12670162	61.31%	8.051%
8	6.684	443	446	448	rBV	3515064	3237580	15.67%	2.057%
9	6.844	457	460	462	rBV	8407379	10688122	51.72%	6.792%
10	7.245	492	495	498	rBV	6635796	7495489	36.27%	4.763%
11	7.965	555	558	560	rBV	4898974	4248604	20.56%	2.700%
12	9.050	650	653	655	rBV	14029238	15610660	75.54%	9.920%
13	9.713	708	711	713	rBV	5595680	4931577	23.86%	3.134%
14	10.502	777	780	782	rBV	6067214	7402660	35.82%	4.704%
15	11.188	837	840	843	rBV	5399836	4818693	23.32%	3.062%
16	11.736	885	888	899	rBV2	506799	1053022	5.10%	0.669%
17	12.399	943	946	948	rBV	160430	240264	1.16%	0.153%
18	12.525	953	957	963	rVV	1856953	2996547	14.50%	1.904%
19	12.628	963	966	969	rVB	219855	378387	1.83%	0.240%
20	12.788	976	980	982	rBV	10283944	14610216	70.70%	9.284%
21	13.337	1025	1028	1030	rBV	353453	536942	2.60%	0.341%
22	13.714	1057	1061	1064	rBV	293547	437471	2.12%	0.278%
23	13.828	1069	1071	1074	rVB	3887287	4324064	20.93%	2.748%
24	15.280	1195	1198	1201	rBV	2816036	3158649	15.29%	2.007%

Sum of corrected areas: 157367842

LSC Report - Integrated Chromatogram

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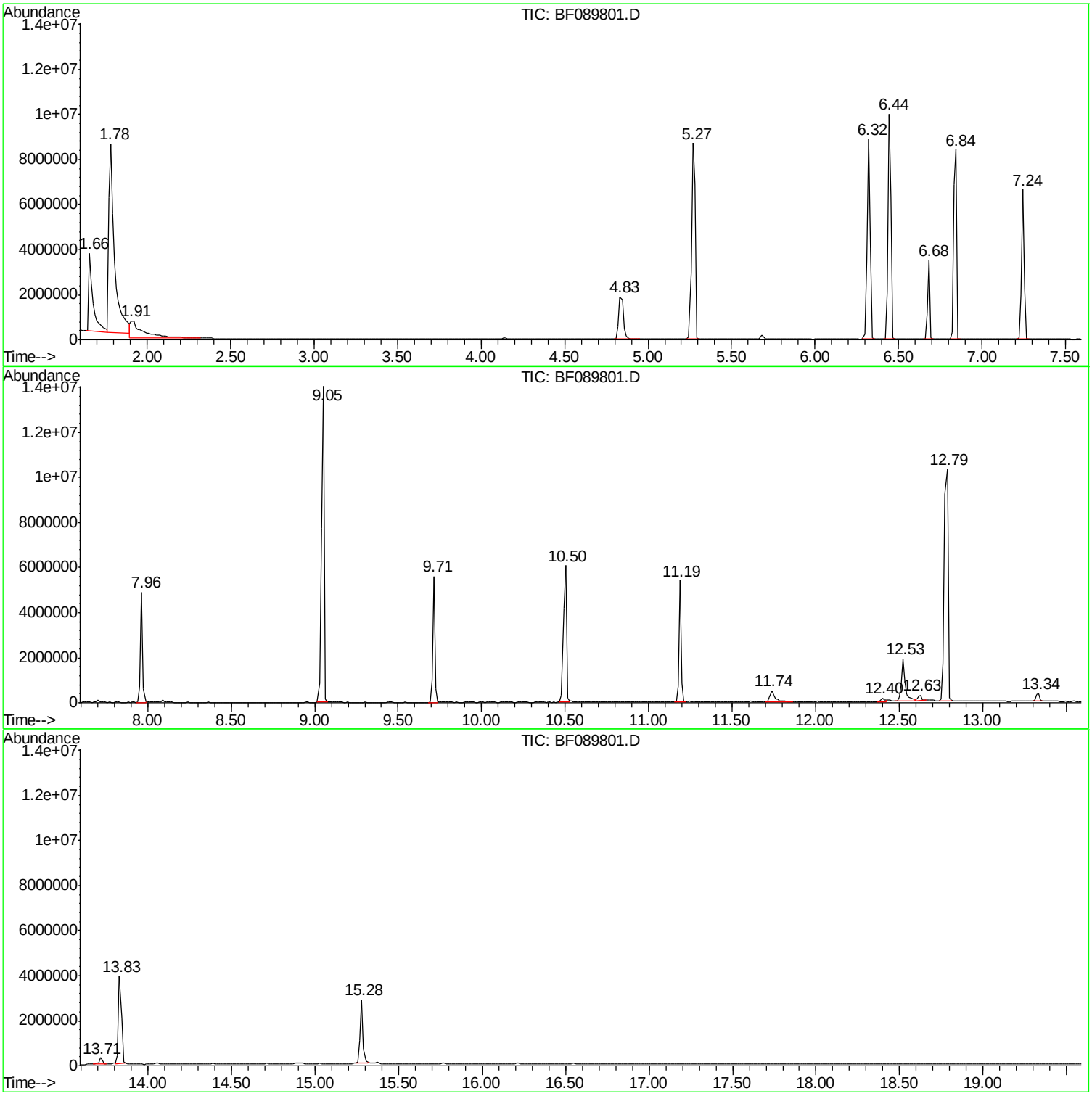
Operator : UM/SJ
Sample : PB92975BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92975BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
Data File : BF089801.D
Acq On : 19 Aug 2016 17:47
Operator : UM/SJ
Sample : PB92975BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92975BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

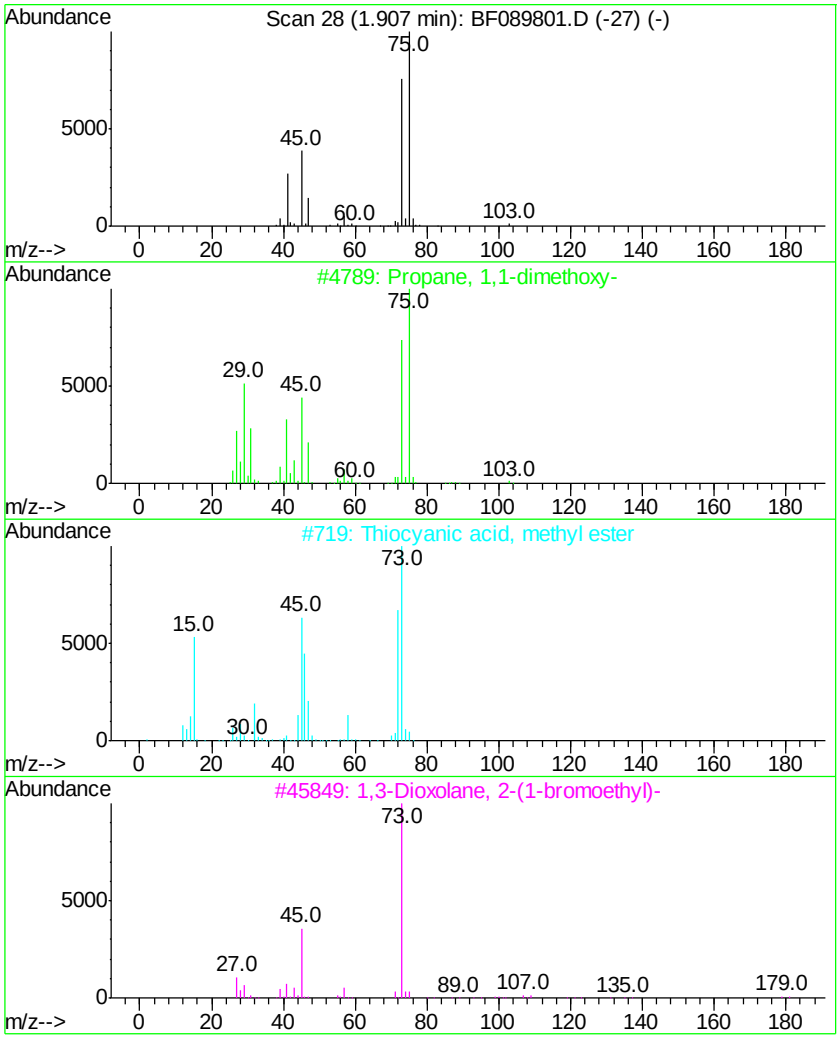
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

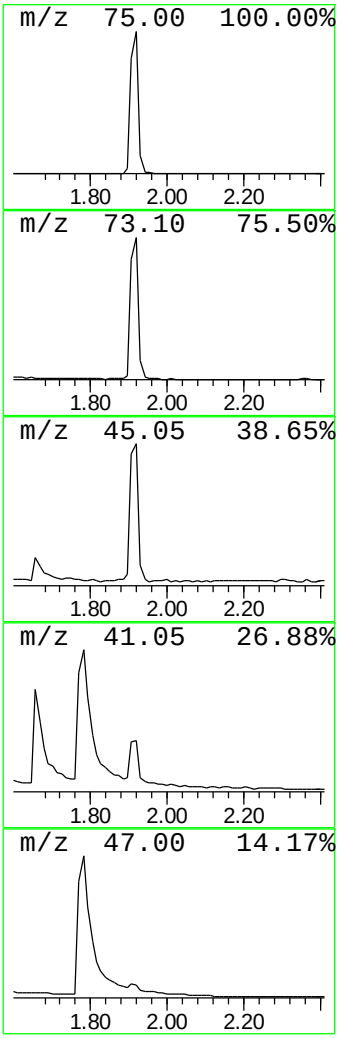
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.91	24.50 ng	3966390	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	38
3	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,1,3-Trimethoxypropane	134	C6H14O3	014315-97-0	9





Library Search Compound Report

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Sample : PB92975BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92975BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

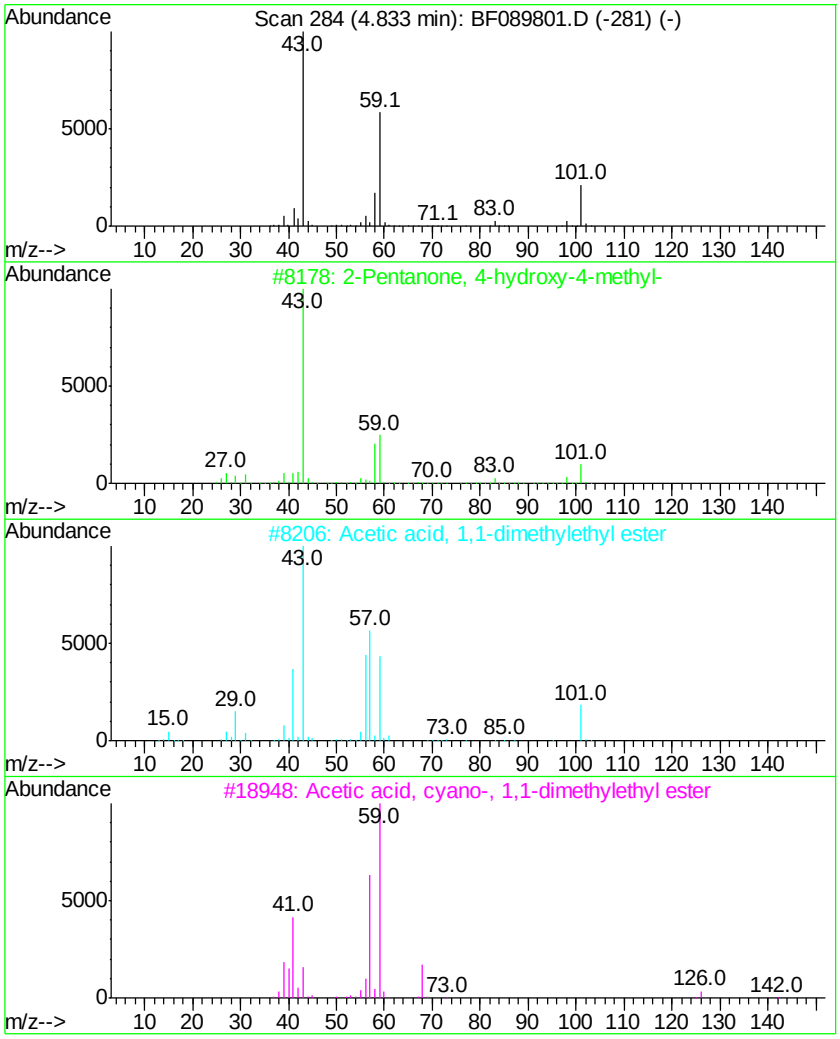
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

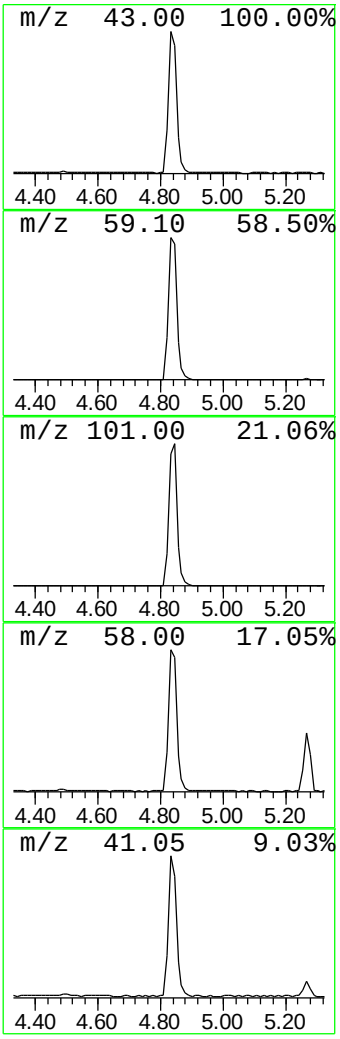
****

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	20.76 ng	3360900	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\
Data File : BF089801.D
Acq On : 19 Aug 2016 17:47
Operator : UM/SJ
Sample : PB92975BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92975BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

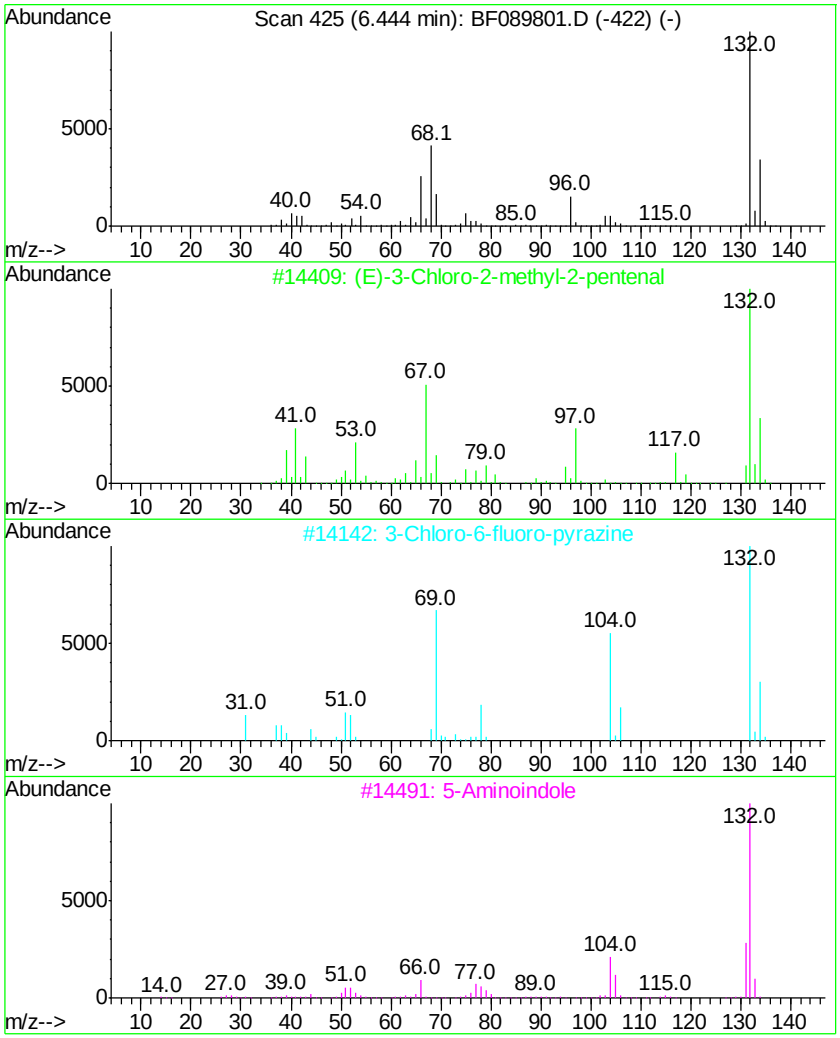
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

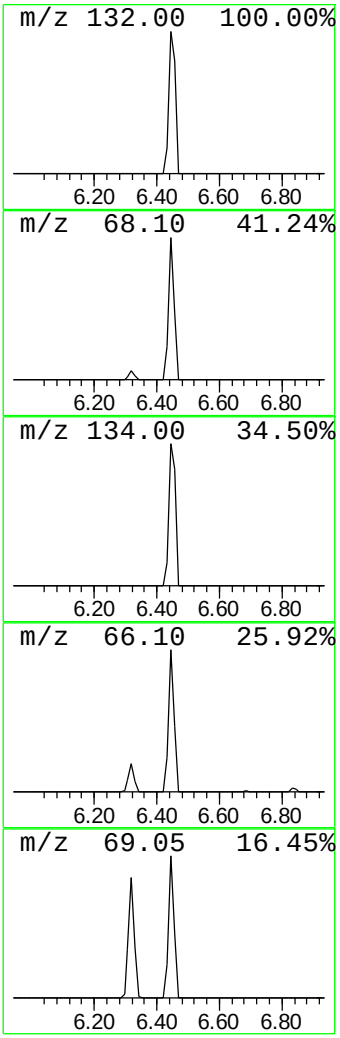
****

Peak Number 5 unknown6.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	78.27 ng	12670200	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Data File : BF089801.D
Acq On : 19 Aug 2016 17:47
Operator : UM/SJ
Sample : PB92975BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92975BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

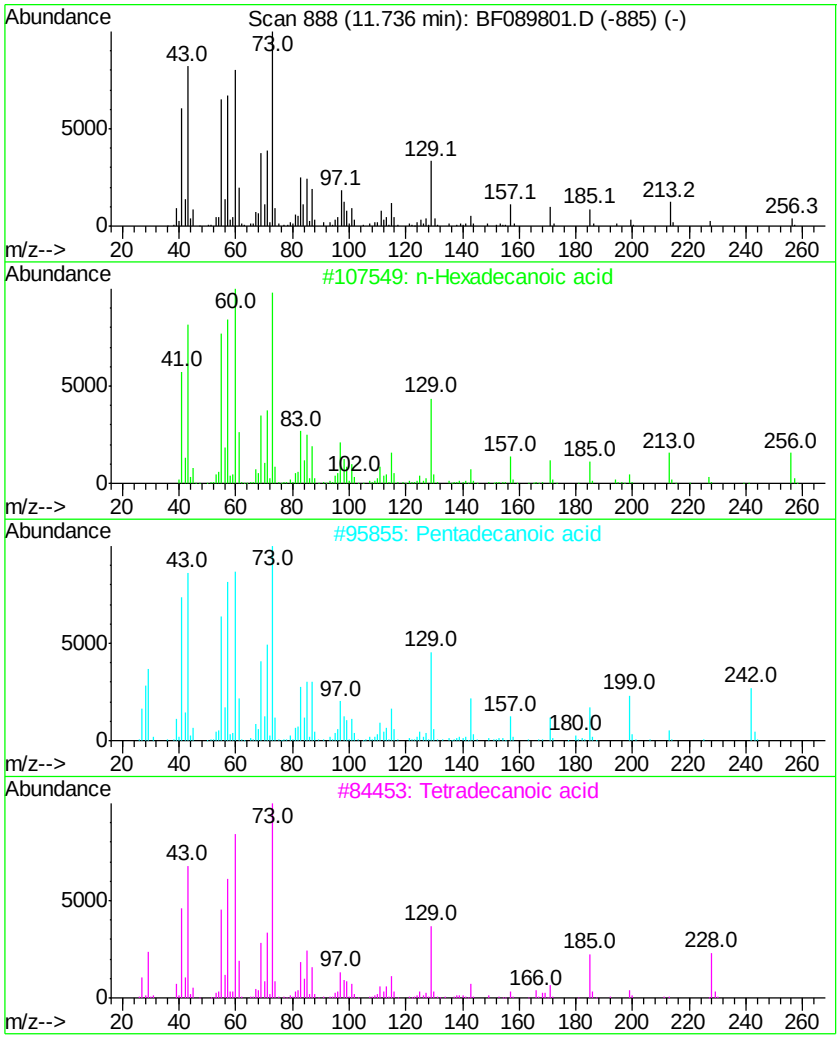
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

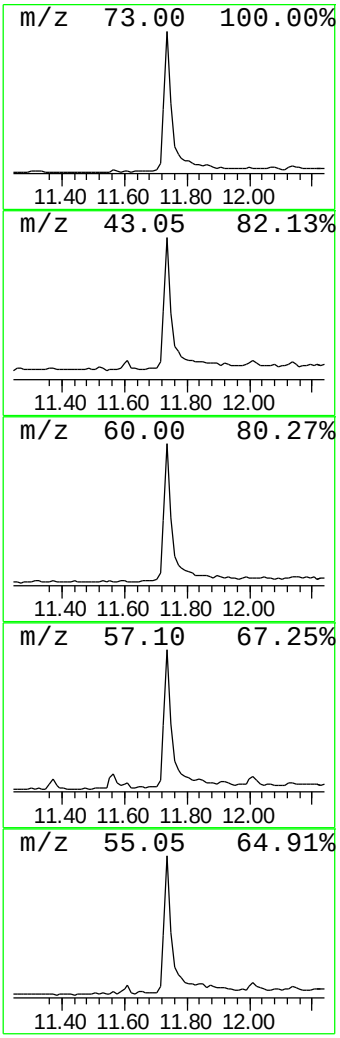
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	4.37 ng	1053020	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Library Search Compound Report

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Acq On : 19 Aug 2016 17:47
Operator : UM/SJ
Sample : PB92975BL
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB92975BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

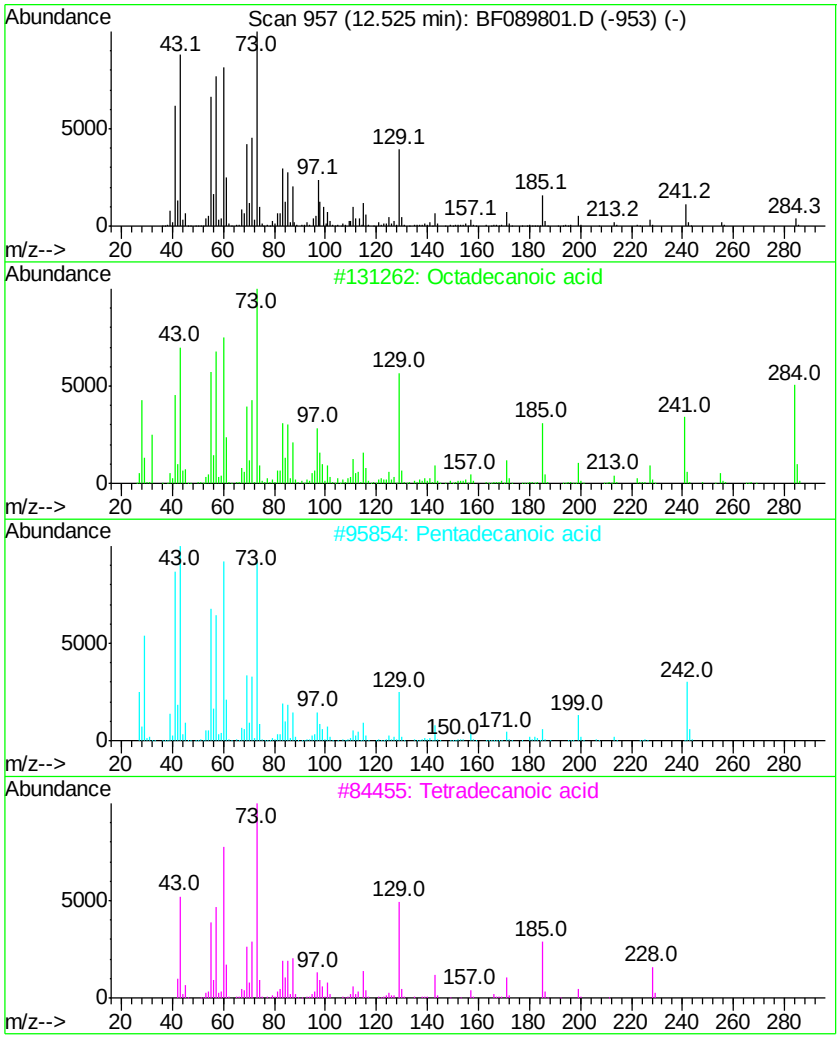
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

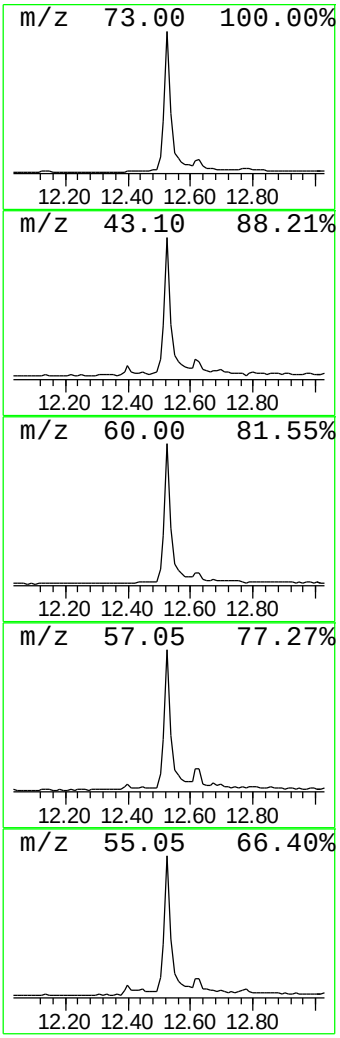
****

Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	13.86 ng	2996550	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25





Library Search Compound Report

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ALS Vial : 17 Sample Multiplier: 1

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BNA_F
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PB92975BL

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

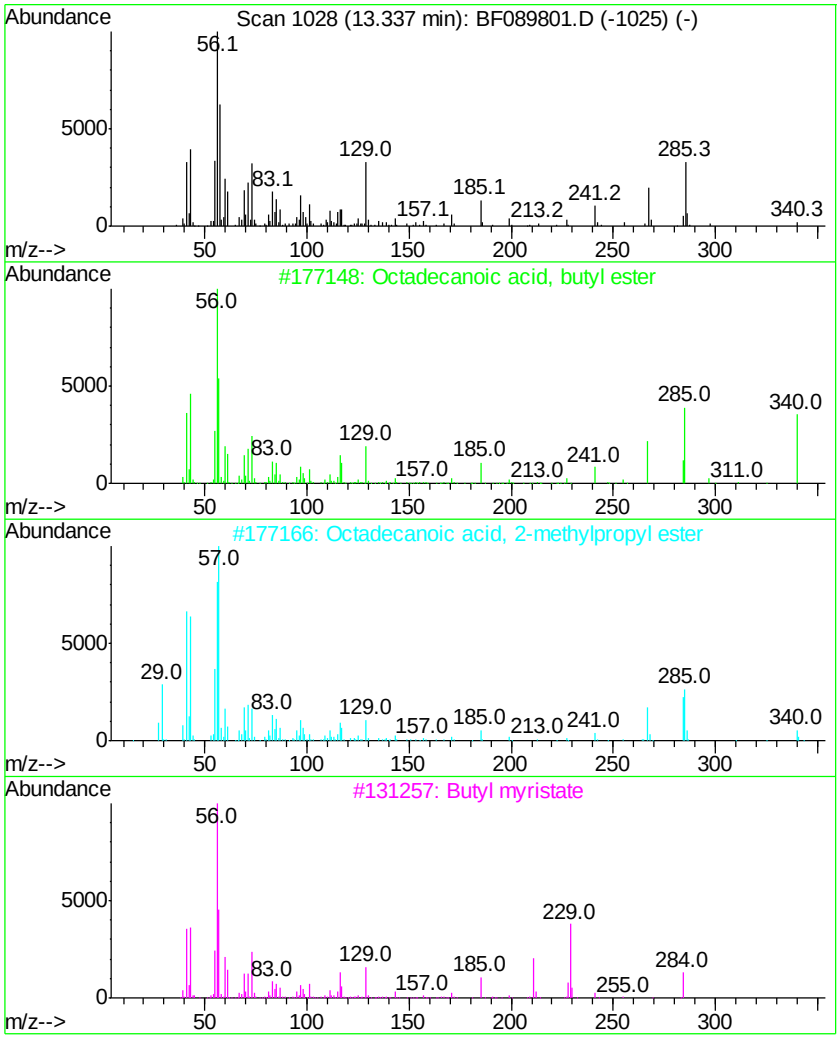
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

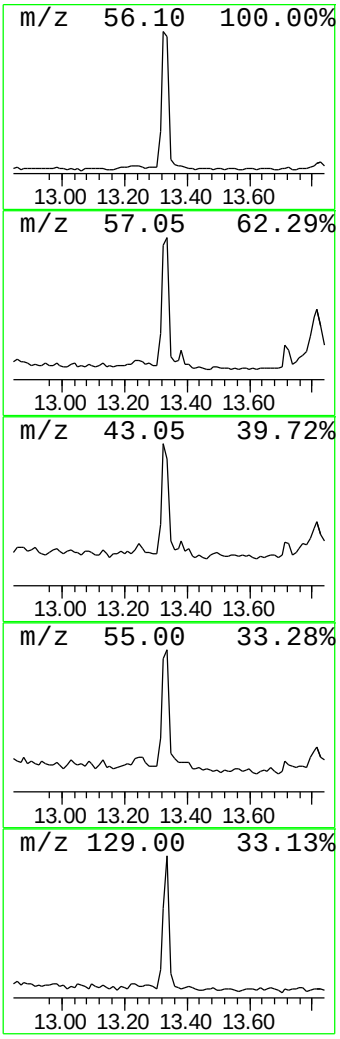
****

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	2.48 ng	536942	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	72
3	Butyl myristate	284	C18H36O2	000110-36-1	49
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27





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Operator : UM/SJ
Sample : PB92975BL
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

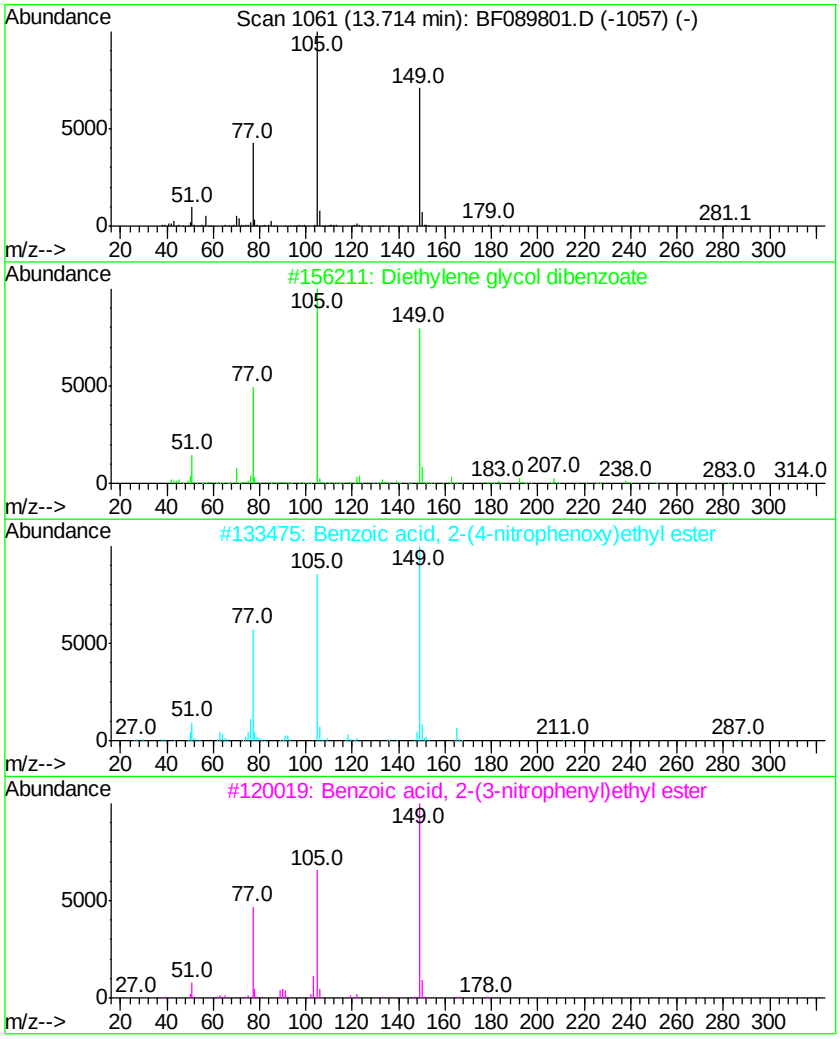
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

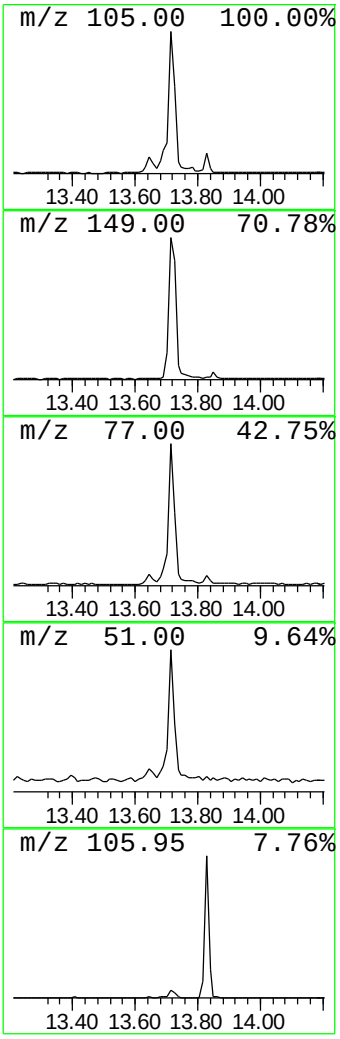
****

Peak Number 10 Diethylene glycol dibenzoate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	2.02 ng	437471	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	83
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
3	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	64
5	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	64





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Propane, 1,1-dime...	1.91	24.5	ng	3966390	1	6.68	3237580	20.0
2-Pentanone, 4-hy...	4.83	20.8	ng	3360900	1	6.68	3237580	20.0
unknown6.44	6.44	78.3	ng	12670200	1	6.68	3237580	20.0
n-Hexadecanoic acid	11.74	4.4	ng	1053020	4	11.19	4818690	20.0
Octadecanoic acid	12.53	13.9	ng	2996550	5	13.83	4324060	20.0
Octadecanoic acid...	13.34	2.5	ng	536942	5	13.83	4324060	20.0
Diethylene glycol...	13.71	2.0	ng	437471	5	13.83	4324060	20.0