LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF082217\
Data File : BF097967.D
Acq On : 22 Aug 2017 21:34
Operator : SJ/JU
Sample : I4900-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-STONE

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-BF081517.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	4.939	482	485	490	rBV	177032	195855	8.63%	1.232%
2	5.357	552	556	560	rBV	1649956	1655885	72.94%	10.414%
3	5.534	582	586	590	rBV	76048	76673	3.38%	0.482%
4	6.186	691	697	700	rBV	161884	168651	7.43%	1.061%
5	6.386	726	731	736	rBV	1946988	1894434	83.44%	11.914%
6	6.469	738	745	749	rBV2	68509	68911	3.04%	0.433%
7	6.516	749	753	757	rBV	1888351	1846615	81.34%	11.613%
8	6.751	789	793	796	rBV	958722	804303	35.43%	5.058%
9	6.904	815	819	823	rBV	1700247	1440659	63.46%	9.060%
10	6.963	827	829	834	rVB2	49295	57099	2.52%	0.359%
11	7.310	881	888	891	rBV	1220233	1112848	49.02%	6.999%
12	7.969	998	1000	1007	rVB2	52523	59035	2.60%	0.371%
13	8.033	1007	1011	1014	rBV	1218631	987962	43.52%	6.213%
14	8.392	1069	1072	1078	rBV4	83368	103869	4.58%	0.653%
15	8.463	1081	1084	1089	rVB6	36361	59487	2.62%	0.374%
16	8.751	1129	1133	1136	rBV2	312992	302683	13.33%	1.904%
17	8.880	1151	1155	1159	rBV3	59700	73570	3.24%	0.463%
18	8.963	1166	1169	1174	rBV5	37183	57615	2.54%	0.362%
19	9.110	1189	1194	1197	rBV	2705472	2270292	100.00%	14.278%
20	9.216	1210	1212	1216	rVB	140410	103829	4.57%	0.653%
21	9.404	1241	1244	1246	rBV	73829	68979	3.04%	0.434%
22	9.504	1257	1261	1265	rVB	301554	259679	11.44%	1.633%
23	9.786	1305	1309	1312	rBV	1040911	905931	39.90%	5.697%
24	10.204	1376	1380	1381	rBV2	78461	97293	4.29%	0.612%
25	10.574	1439	1443	1445	rBV	1114953	1048965	46.20%	6.597%
26	10.657	1455	1457	1459	rBV2	195781	179727	7.92%	1.130%

Sum of corrected areas: 15900849

LSC Report - Integrated Chromatogram

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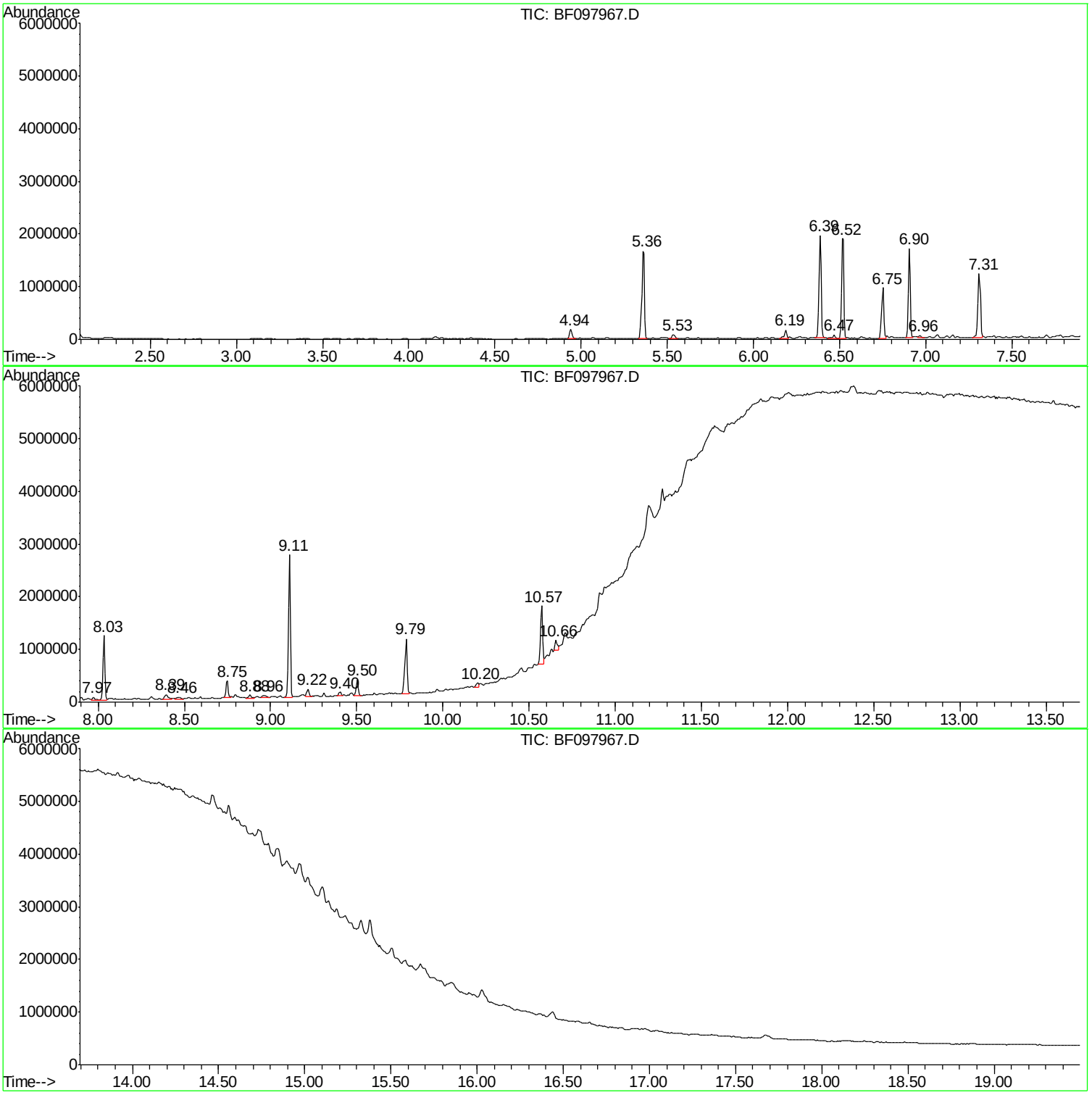
Operator : SJ/JU
Sample : I4900-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-STONE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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

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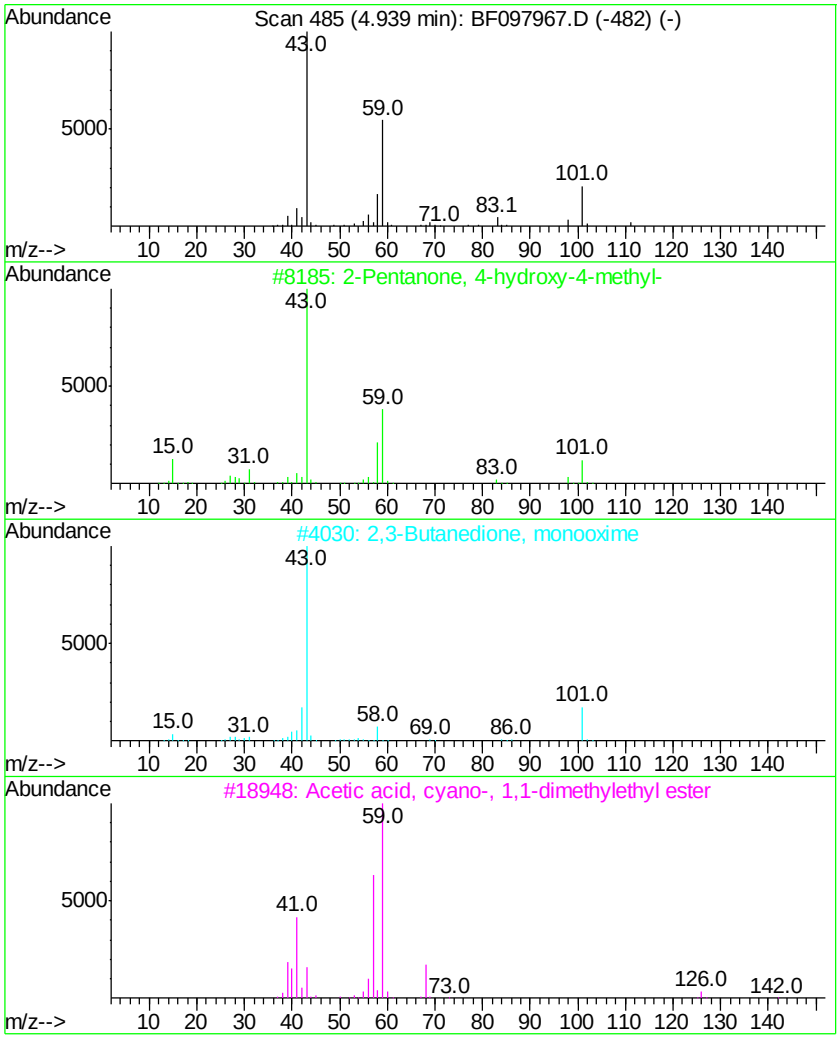
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

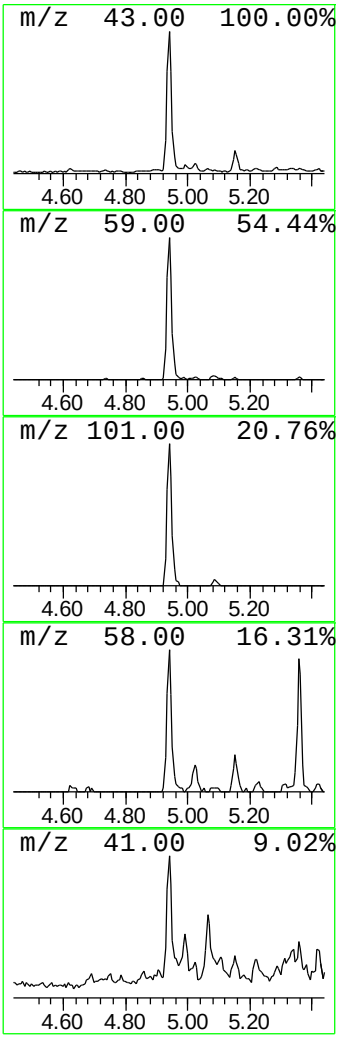
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	4.87 ng	195855	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	17
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Operator : SJ/JU
Sample : I4900-15
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Instrument : BNA_F
ClientSampleId : 220-1-STONE

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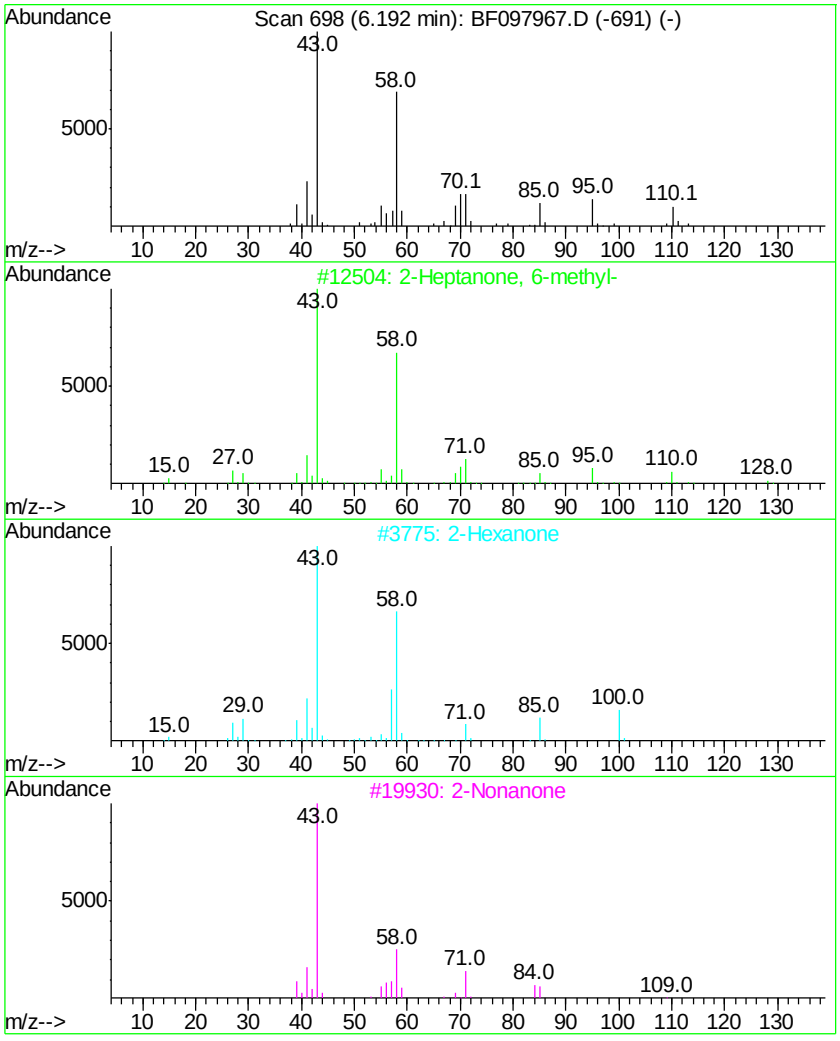
TIC Integration Parameters: LSCINT.P

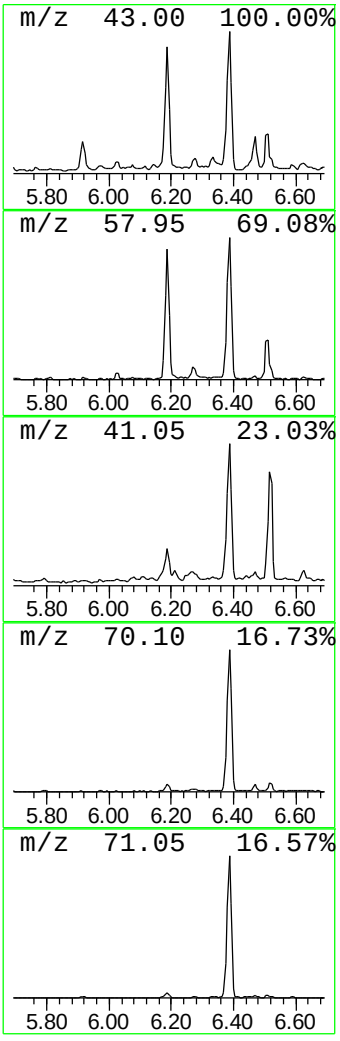
****

Peak Number 2 2-Heptanone, 6-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	4.19 ng	168651	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	83
2	2-Hexanone	100	C6H12O	000591-78-6	50
3	2-Nonanone	142	C9H18O	000821-55-6	37
4	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	36
5	2-Hexanone, 4-hydroxy-3-propyl-	158	C9H18O2	062338-17-4	36





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Operator : SJ/JU
Sample : I4900-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-STONE

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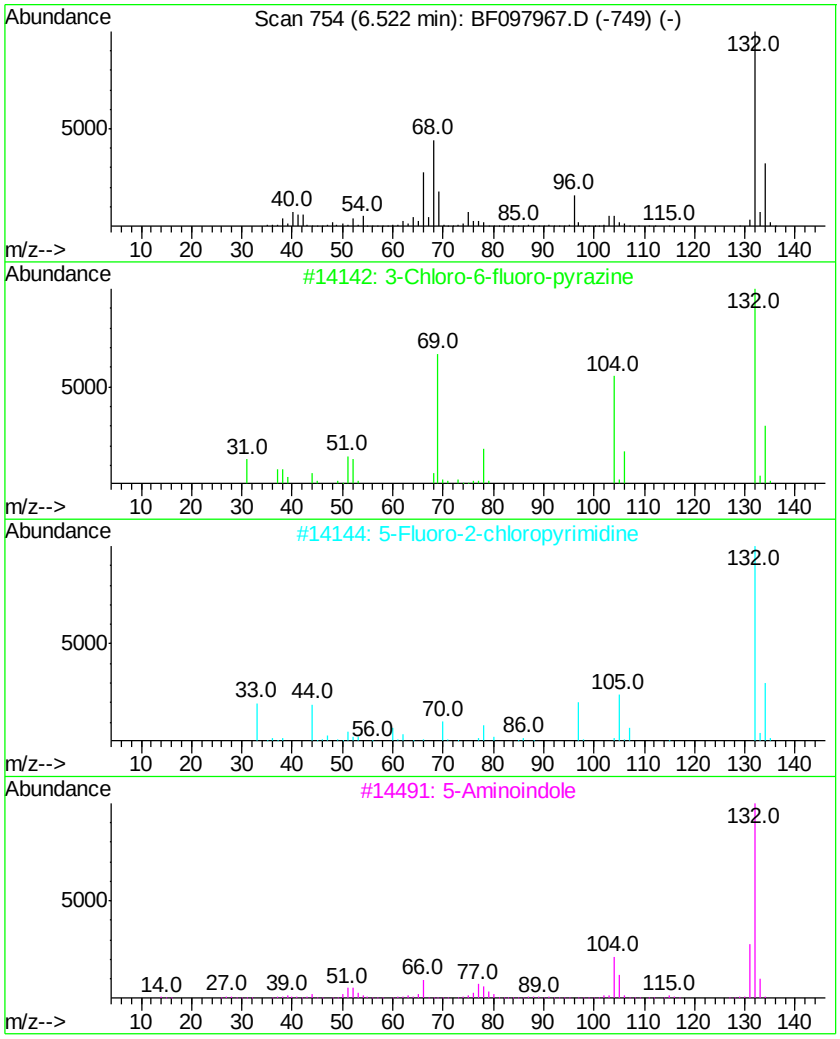
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

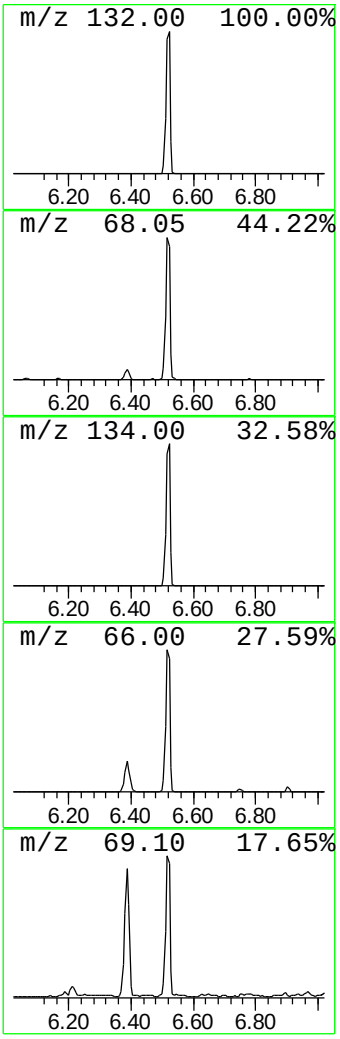
****

Peak Number 3 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	45.92 ng	1846620	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : 220-1-STONE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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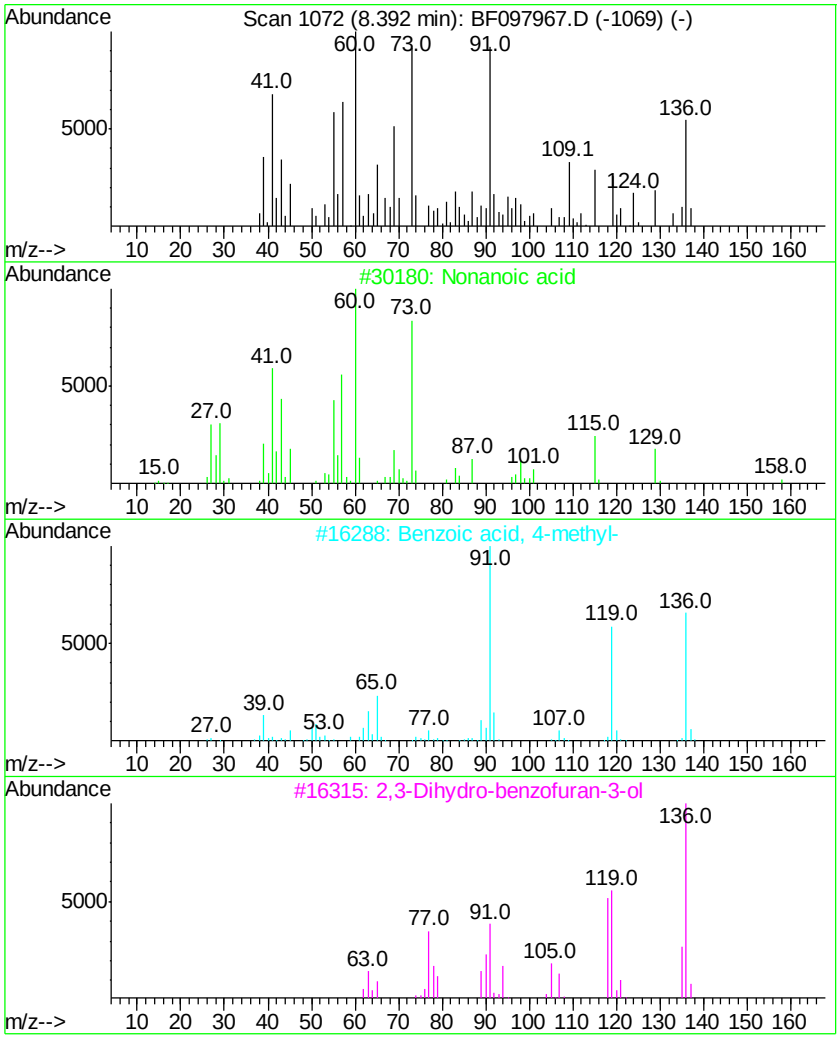
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

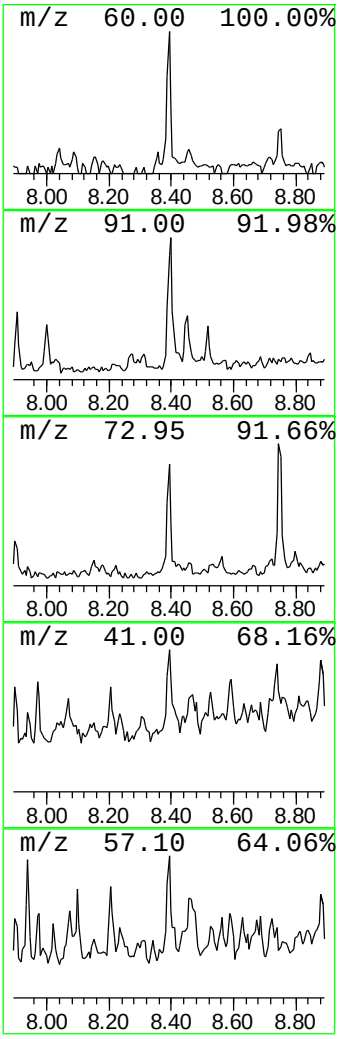
****

Peak Number 5 unknown8.39 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.39	2.10 ng	103869	Naphthalene-d8	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	38
2	Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	25
3	2,3-Dihydro-benzofuran-3-ol	136	C8H8O2	1000146-26-4	22
4	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	20
5	2-Purinol	136	C5H4N4O	002308-57-8	18





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Instrument : BNA_F
ClientSampleId : 220-1-STONE

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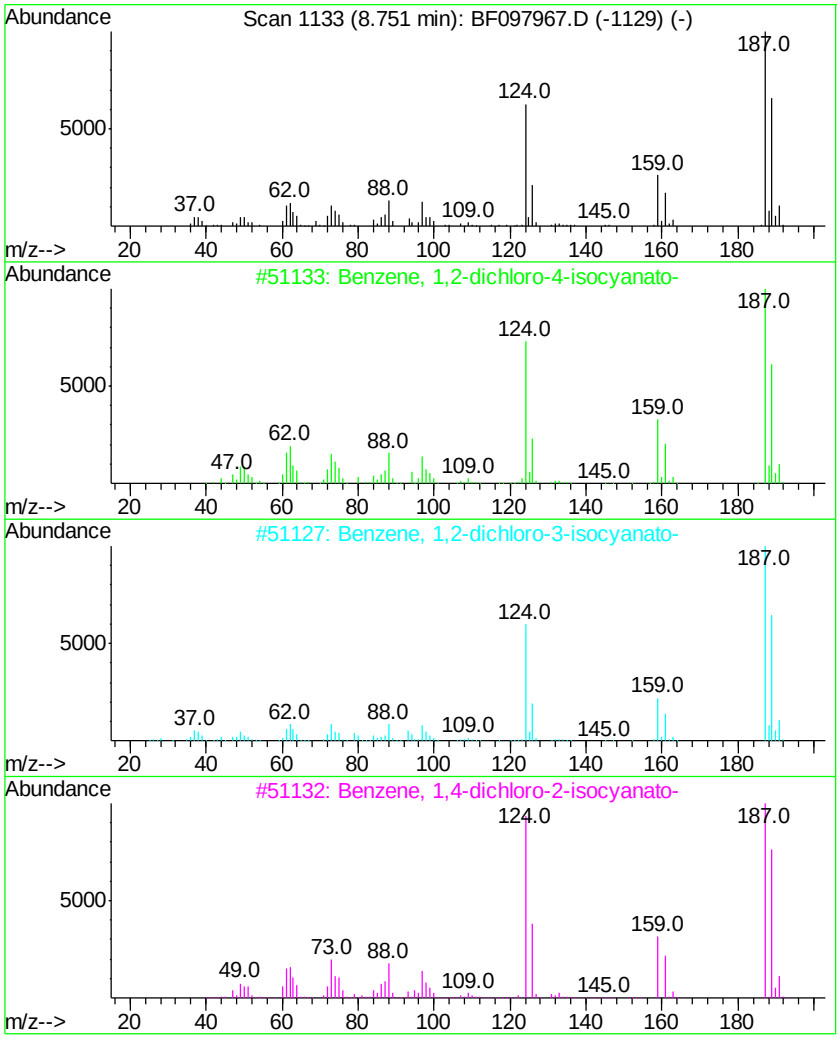
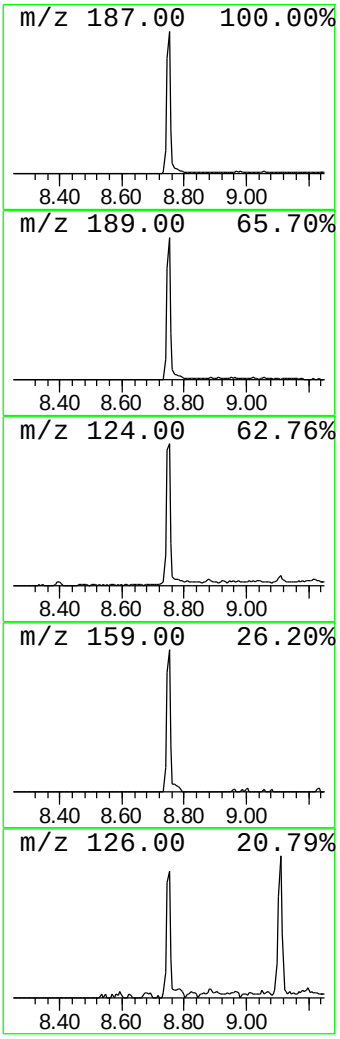
****

Peak Number 6 Benzene, 1,2-dichloro-4-iso... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.75	6.13 ng	302683	Naphthalene-d8	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-dichloro-4-isocyanato-	187	C7H3Cl2NO	000102-36-3	99
2	Benzene, 1,2-dichloro-3-isocyanato-	187	C7H3Cl2NO	041195-90-8	99
3	Benzene, 1,4-dichloro-2-isocyanato-	187	C7H3Cl2NO	005392-82-5	98
4	3,5-Dichlorophenyl isocyanate	187	C7H3Cl2NO	034893-92-0	97
5	Benzene, 1,3-dichloro-2-isocyanato-	187	C7H3Cl2NO	039920-37-1	96





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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-STONE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

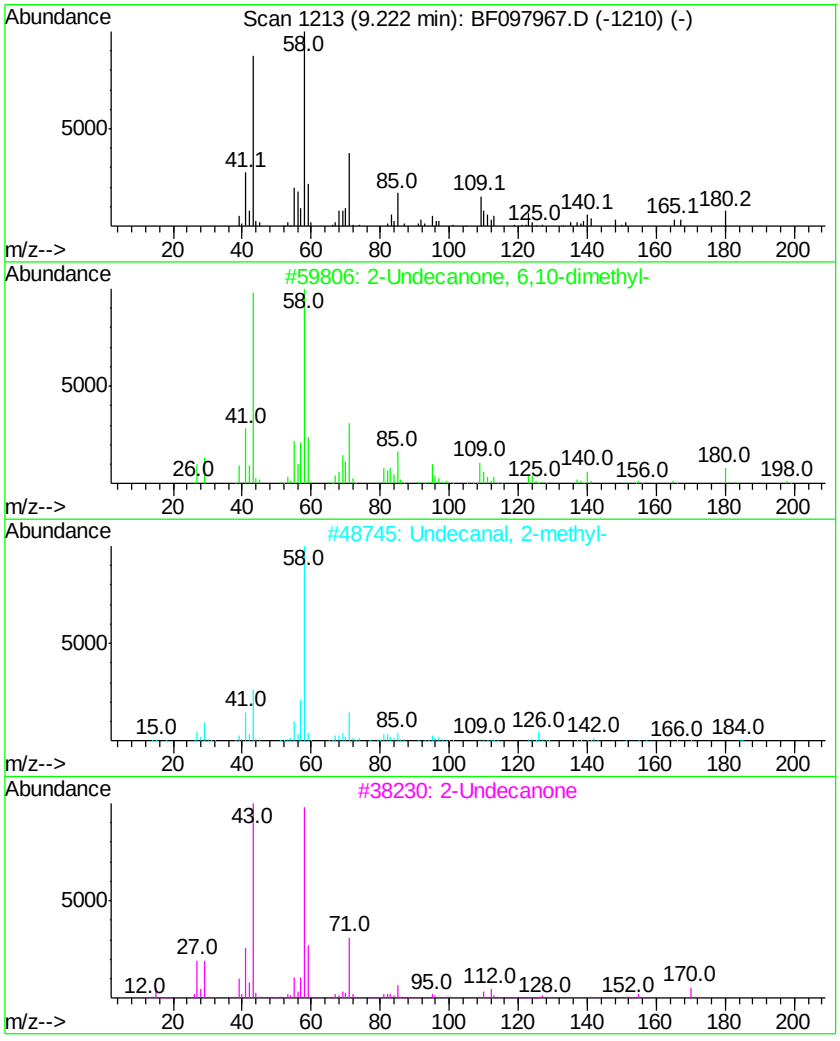
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

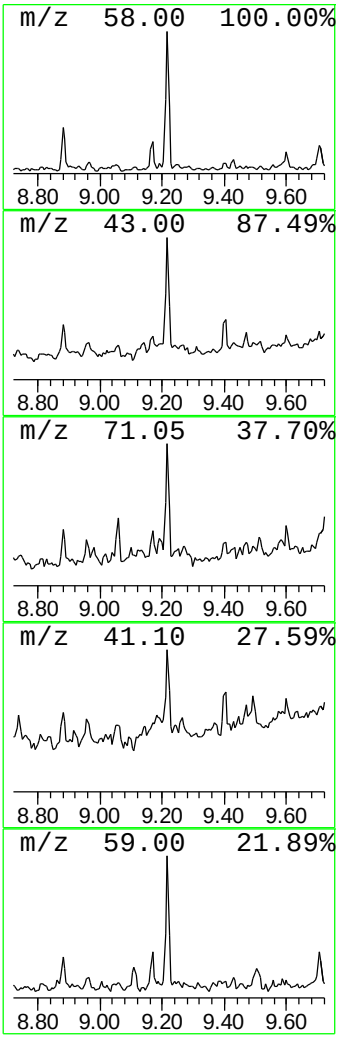
****

Peak Number 7 2-Undecanone, 6,10-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.22	2.29 ng	103829	Acenaphthene-d10	9.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Undecanone, 6,10-dimethyl-	198	C13H26O	001604-34-8	80
2	Undecanal, 2-methyl-	184	C12H24O	000110-41-8	59
3	2-Undecanone	170	C11H22O	000112-12-9	59
4	2-Nonadecanone	282	C19H38O	000629-66-3	59
5	2-Dodecanone	184	C12H24O	006175-49-1	47





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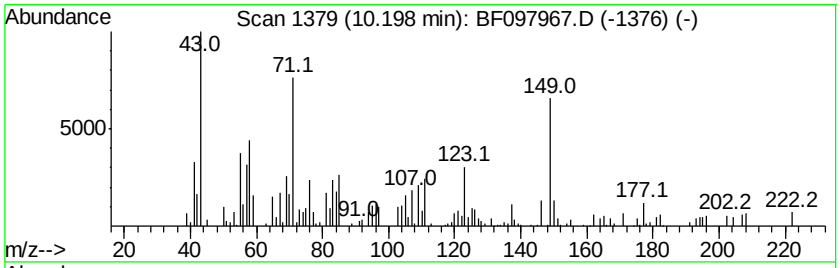
TIC Integration Parameters: LSCINT.P

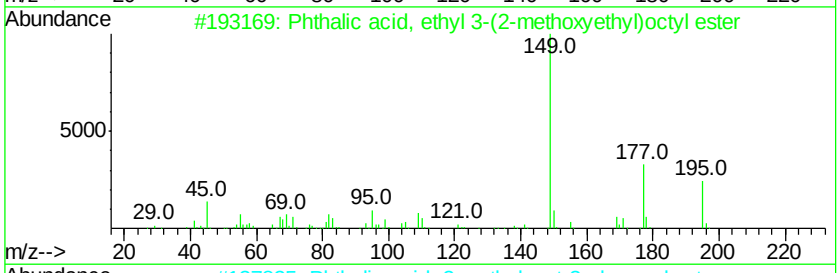
****

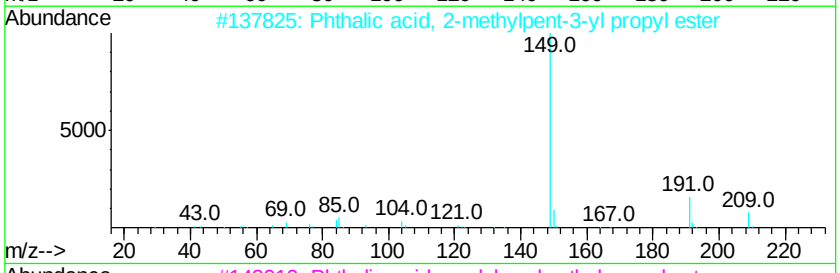
Peak Number 8 Phthalic acid, ethyl 3-(2-m... Concentration Rank 8

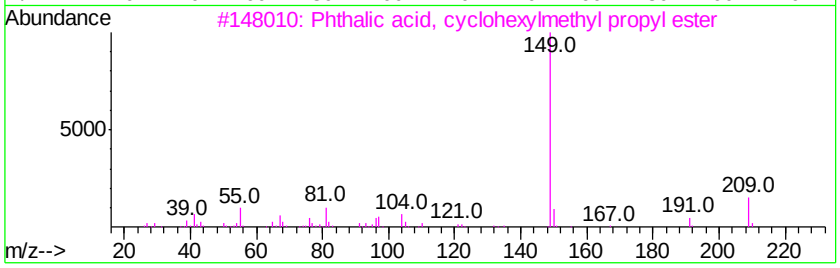
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.20	2.15 ng	97293	Acenaphthene-d10	9.79

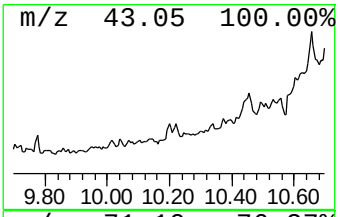
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, ethyl 3-(2-methox...	364	C21H32O5	1000315-40-1	50
2	Phthalic acid, 2-methylpent-3-yl...	292	C17H24O4	1000356-90-6	50
3	Phthalic acid, cyclohexylmethyl ...	304	C18H24O4	1000309-08-7	47
4	Diethyl Phthalate	222	C12H14O4	000084-66-2	47
5	Phthalic acid, ethyl 3-methylbut...	262	C15H18O4	1000315-44-5	47

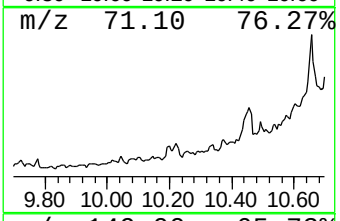


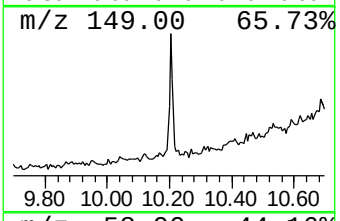


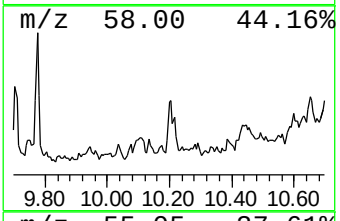


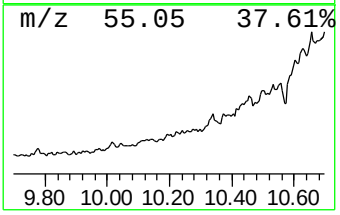












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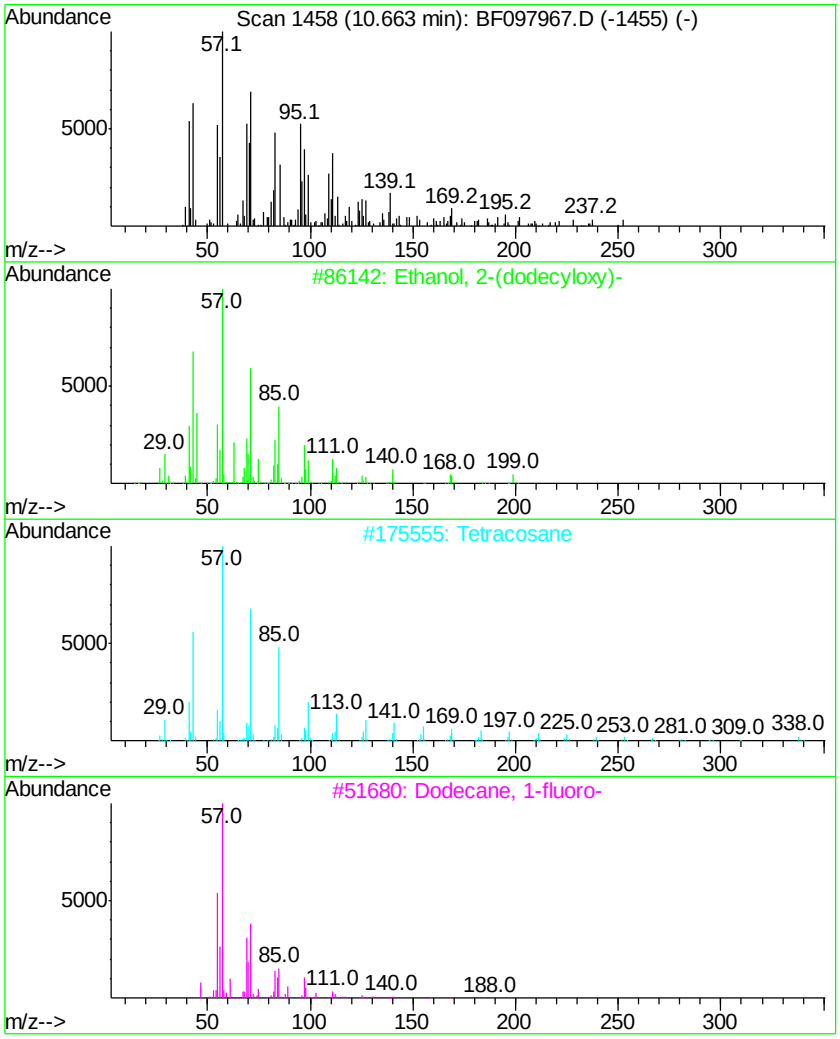
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

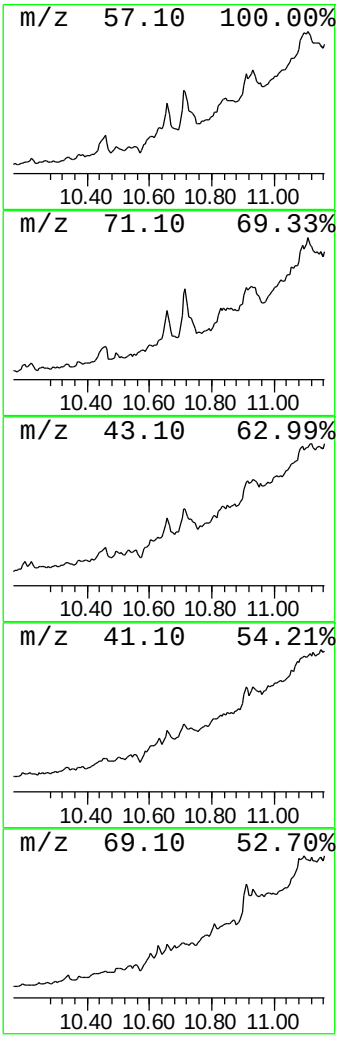
****

Peak Number 9 Ethanol, 2-(dodecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	20.00 ng	179727	Phenanthrene-d10	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	59
2	Tetracosane	338	C24H50	000646-31-1	50
3	Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	50
4	Octane, 2-methyl-	128	C9H20	003221-61-2	49
5	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	47





Tentatively Identified Compound (LSC) summary

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Sample : I4900-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 220-1-STONE

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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
2-Pentanone, 4-hy...	4.94	4.9	ng	195855	1	6.75	804303	20.0
2-Heptanone, 6-me...	6.19	4.2	ng	168651	1	6.75	804303	20.0
unknown6.52	6.52	45.9	ng	1846620	1	6.75	804303	20.0
unknown8.39	8.39	2.1	ng	103869	2	8.03	987962	20.0
Benzene, 1,2-dich...	8.75	6.1	ng	302683	2	8.03	987962	20.0
2-Undecanone, 6,1...	9.22	2.3	ng	103829	3	9.79	905931	20.0
Phthalic acid, et...	10.20	2.1	ng	97293	3	9.79	905931	20.0
Ethanol, 2-(dodec...	10.66	20.0	ng	179727	4	11.27	179727	20.0