LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088659.D
Acq On : 3 Jul 2016 20:54
Operator : UM/SJ
Sample : H3817-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BS-3C10.5-11FT

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-BF063016.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	1.644	3	5	7	rVB	4820013	6358925	100.00%	17.769%
2	2.021	35	38	41	rBV	74321	85392	1.34%	0.239%
3	3.050	123	128	138	rBV	146863	394965	6.21%	1.104%
4	4.959	292	295	301	rVB	179532	259641	4.08%	0.726%
5	5.381	329	332	334	rBV	2710750	2989353	47.01%	8.353%
6	6.422	420	423	425	rVB	2549836	2969854	46.70%	8.299%
7	6.547	431	434	437	rBV	2320915	3119073	49.05%	8.716%
8	6.787	452	455	456	rBV	518414	629096	9.89%	1.758%
9	6.936	466	468	471	rVB	1937948	2258100	35.51%	6.310%
10	7.347	501	504	506	rBV	1932208	2002325	31.49%	5.595%
11	8.067	564	567	569	rVB	1065467	921696	14.49%	2.576%
12	9.142	658	661	664	rBV	2495958	2907366	45.72%	8.124%
13	9.542	693	696	698	rBV	492303	506258	7.96%	1.415%
14	9.816	717	720	722	rBV	1143468	997621	15.69%	2.788%
15	10.205	751	754	755	rBV	1158125	1368150	21.52%	3.823%
16	10.605	786	789	791	rBV	2103906	2186392	34.38%	6.110%
17	11.176	837	839	841	rBV	120137	110319	1.73%	0.308%
18	11.291	847	849	851	rVB	1111982	962234	15.13%	2.689%
19	11.359	851	855	859	rVB4	33795	78597	1.24%	0.220%
20	11.599	875	876	879	rVB	79791	73481	1.16%	0.205%
21	12.879	985	988	990	rBV	2695982	2531436	39.81%	7.074%
22	13.817	1066	1070	1076	rBV	117581	265208	4.17%	0.741%
23	13.919	1076	1079	1081	rVB	878295	924583	14.54%	2.584%
24	14.457	1124	1126	1136	rBV	40573	98467	1.55%	0.275%
25	15.302	1197	1200	1203	rBV	473700	703504	11.06%	1.966%
26	17.554	1392	1397	1403	rBV3	22634	83647	1.32%	0.234%

Sum of corrected areas: 35785683

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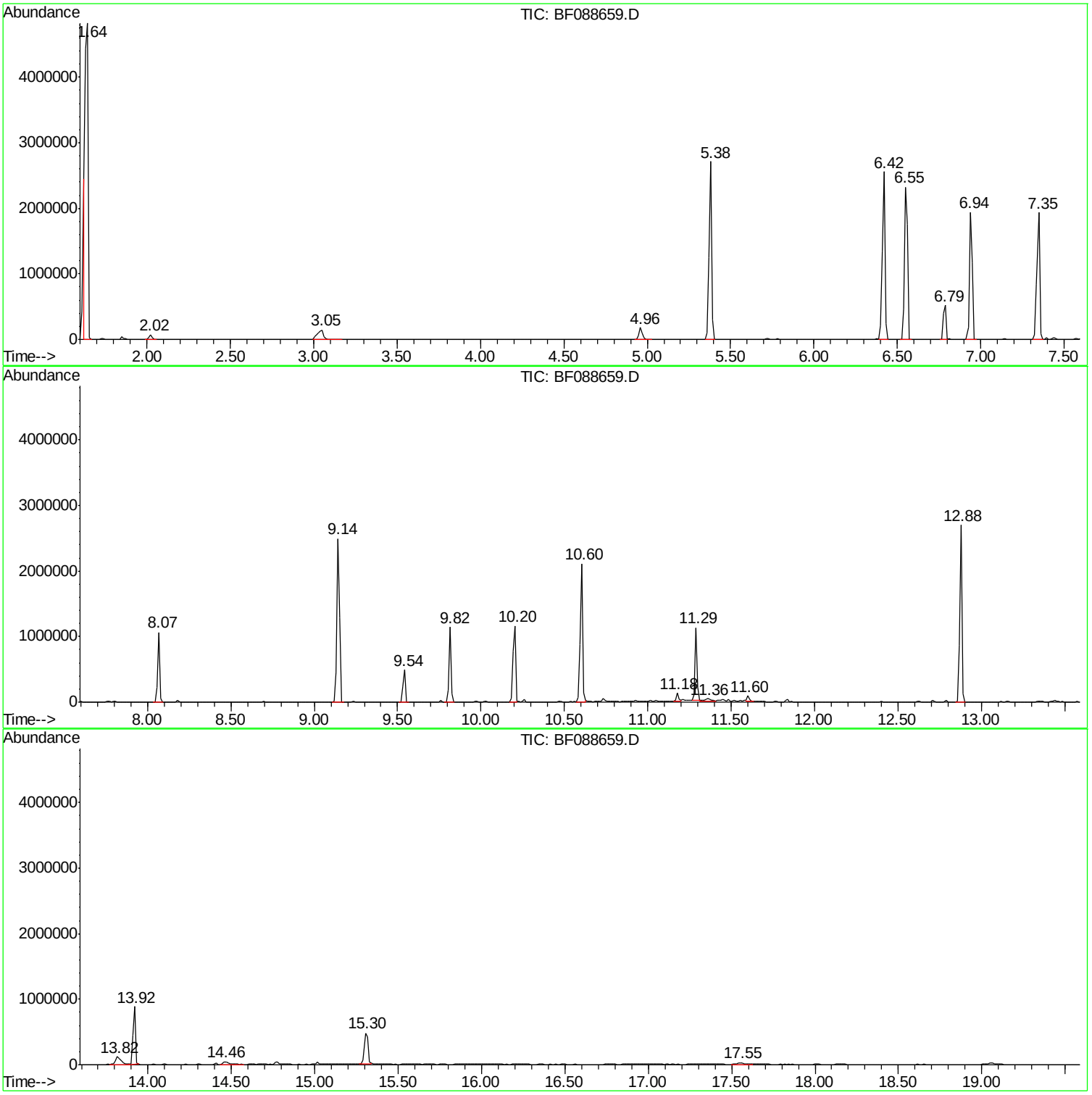
ClientSampleId : BS-3C10.5-11FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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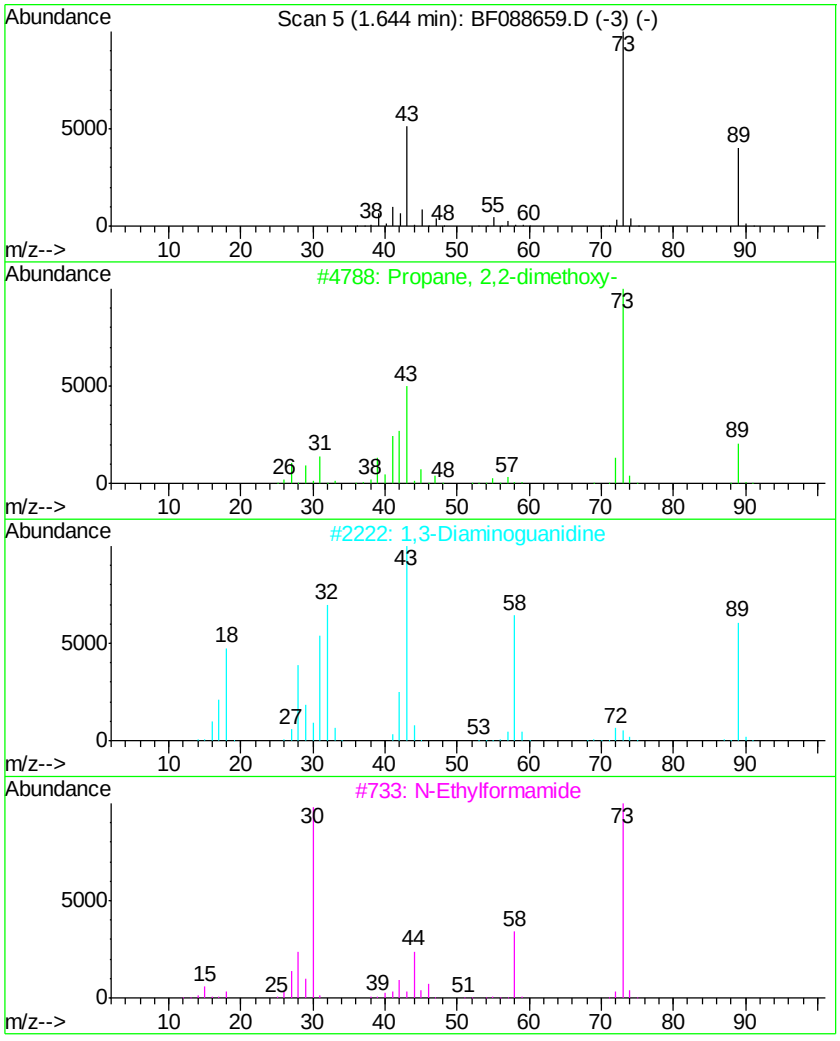
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

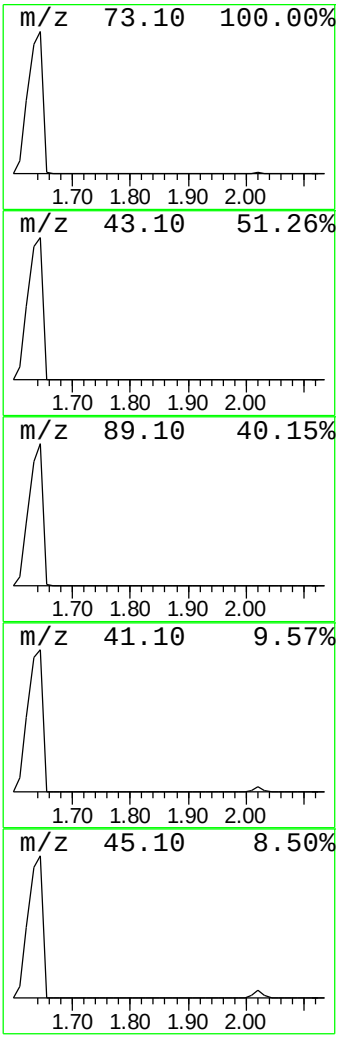
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.64	202.16 ng	6358930	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : BS-3C10.5-11FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

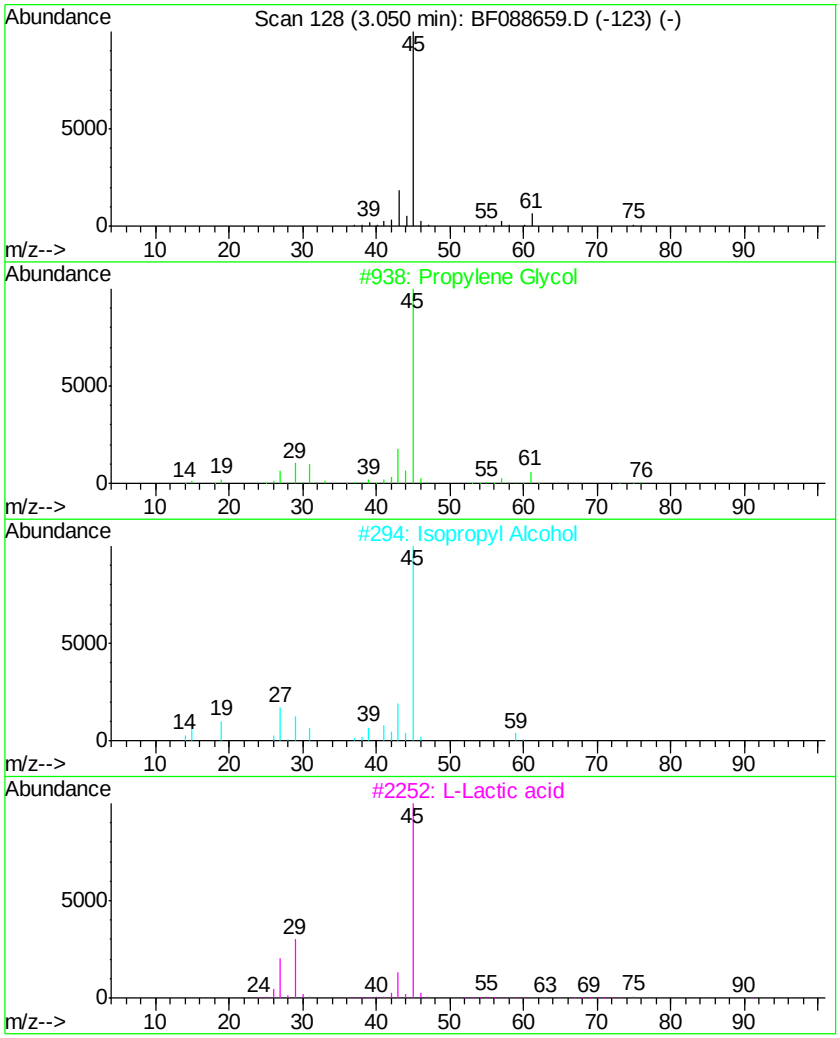
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

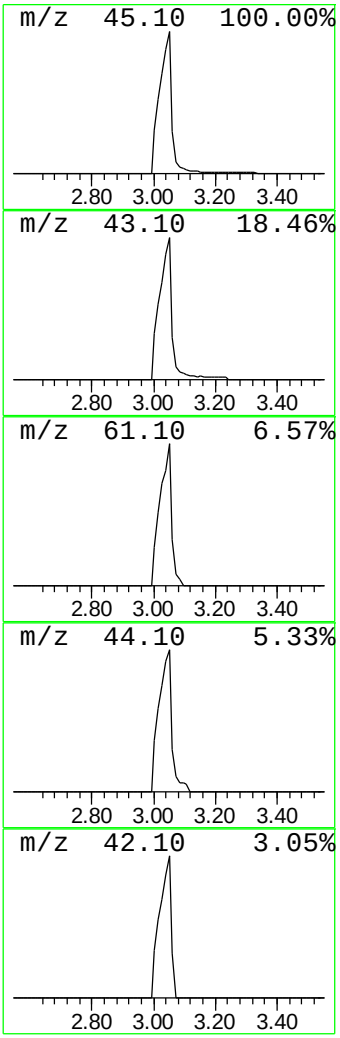
****

Peak Number 3 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.05	12.56 ng	394965	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	83
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3	L-Lactic acid	90	C3H6O3	000079-33-4	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	9





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Operator : UM/SJ
Sample : H3817-03
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Instrument : BNA_F
ClientSampleId : BS-3C10.5-11FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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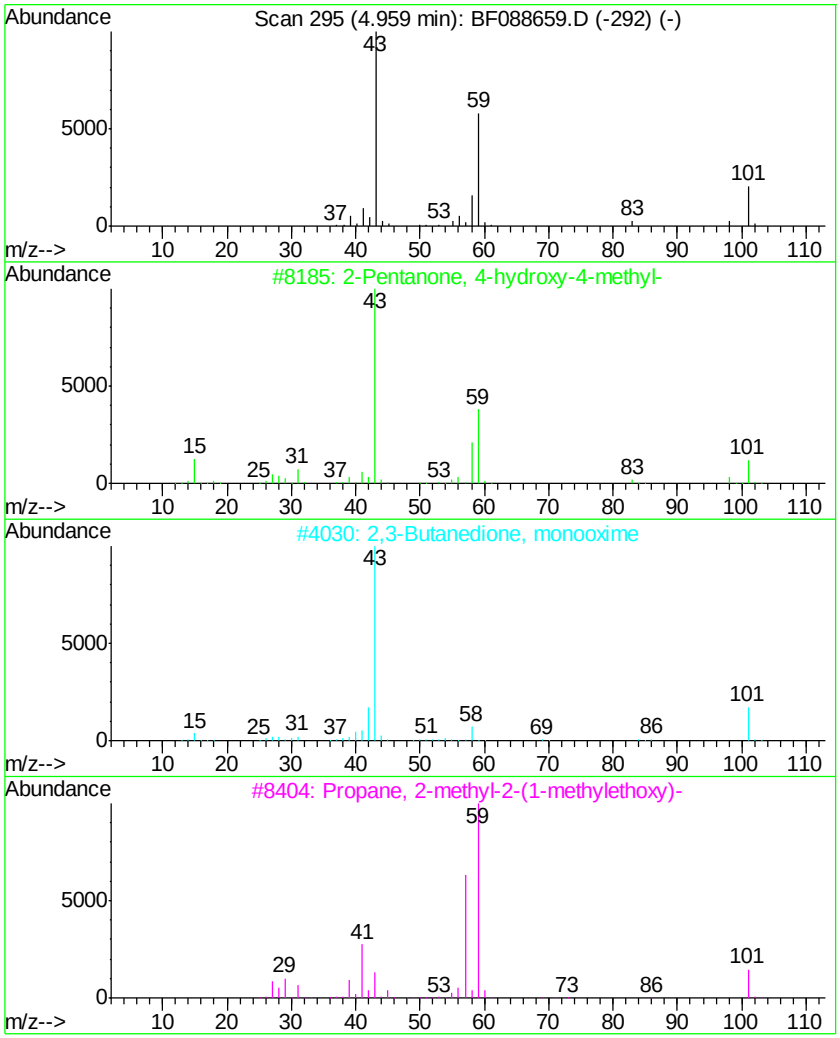
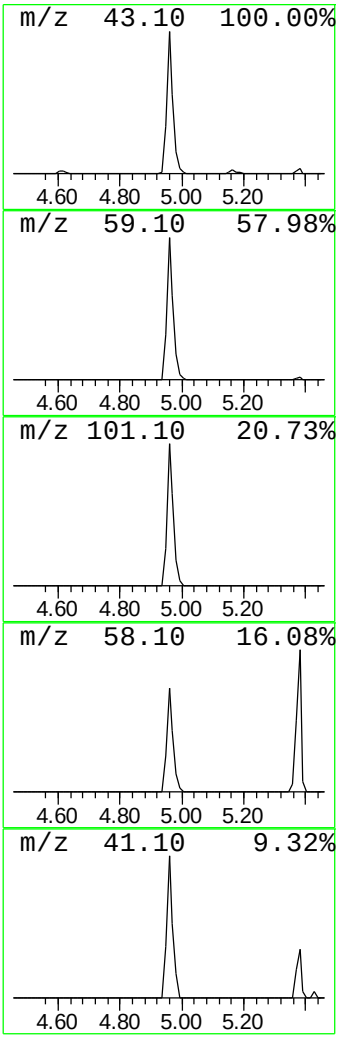
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	8.25 ng	259641	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Instrument : BNA_F
ClientSampleId : BS-3C10.5-11FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

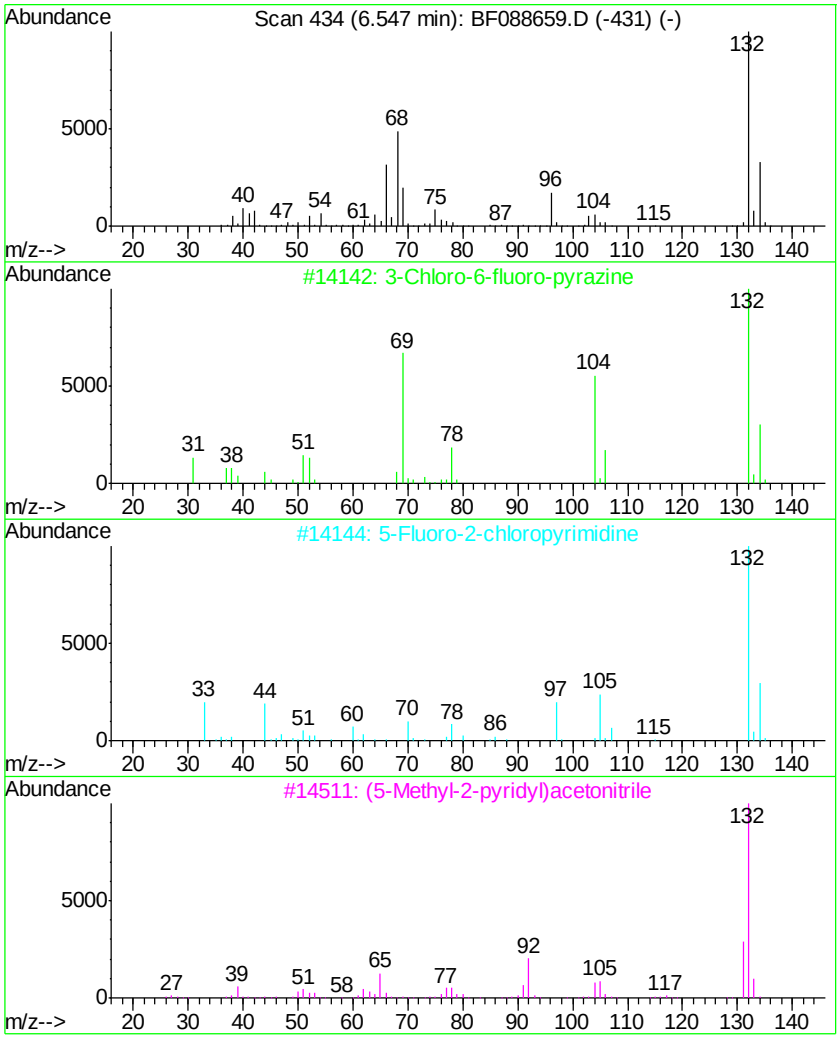
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

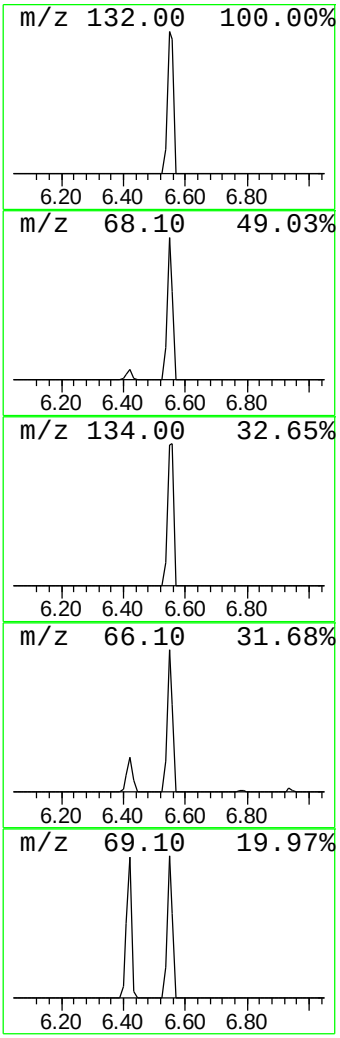
****

Peak Number 5 unknown6.55 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	99.16 ng	3119070	1,4-Dichlorobenzene-d4	6.79

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-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10





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Operator : UM/SJ
Sample : H3817-03
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BS-3C10.5-11FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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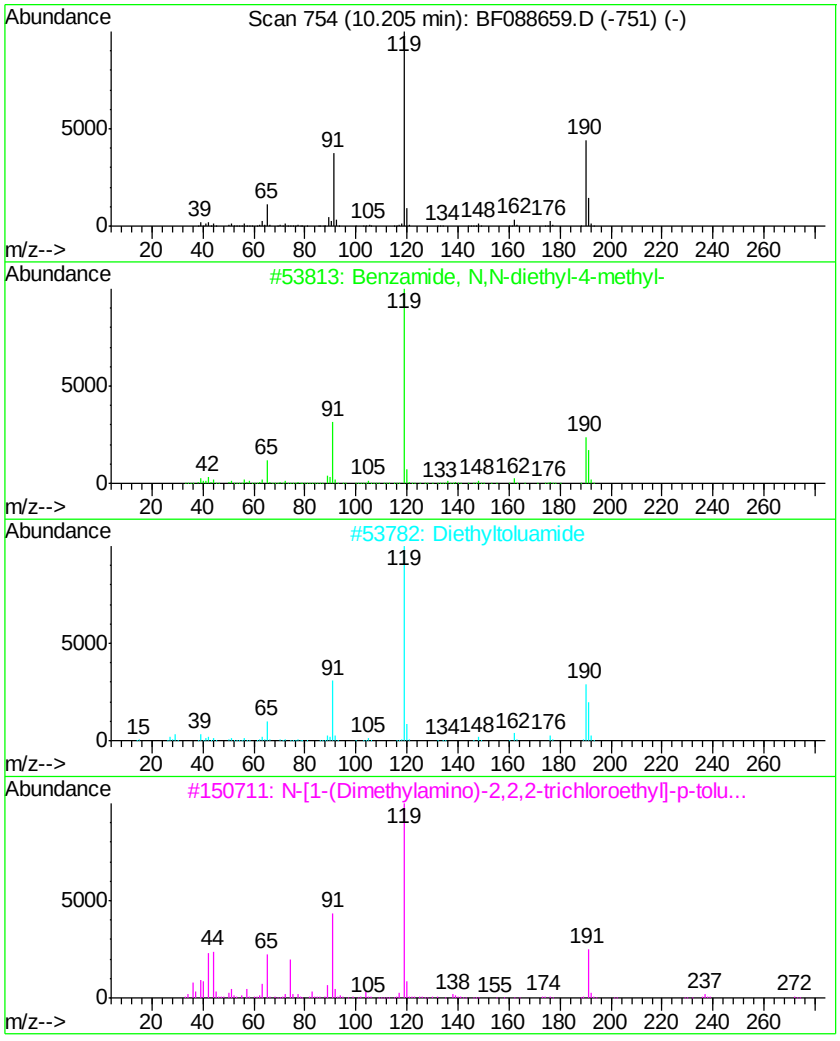
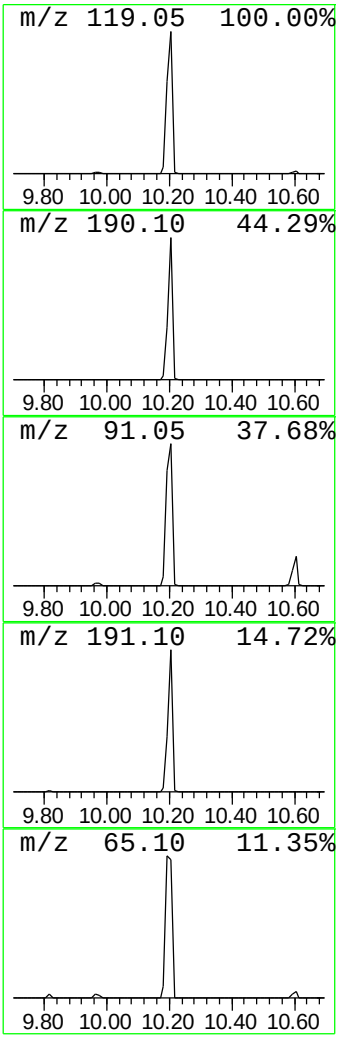
****

Peak Number 7 Benzamide, N,N-diethyl-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.20	27.43 ng	1368150	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	93
2	Diethyltoluamide	191	C12H17NO	000134-62-3	87
3	N-[1-(Dimethylamino)-2,2,2-trich...	308	C12H15Cl3N2O	300814-41-9	53
4	m-Toluic acid, 4-nitrophenyl ester	257	C14H11NO4	1000307-57-1	47
5	p-Toluic acid, 5-fluoro-2-nitrop...	275	C14H10FNO4	1000292-64-6	47





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Sample : H3817-03
Misc :
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Instrument : BNA_F
ClientSampleId : BS-3C10.5-11FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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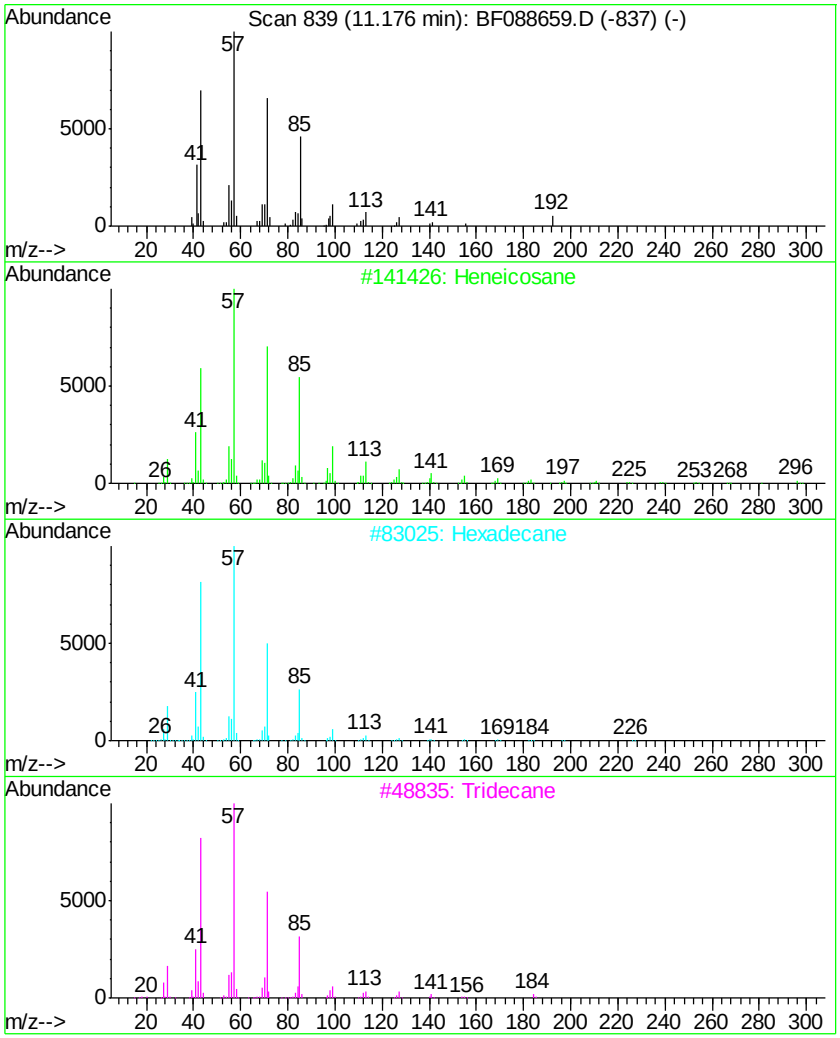
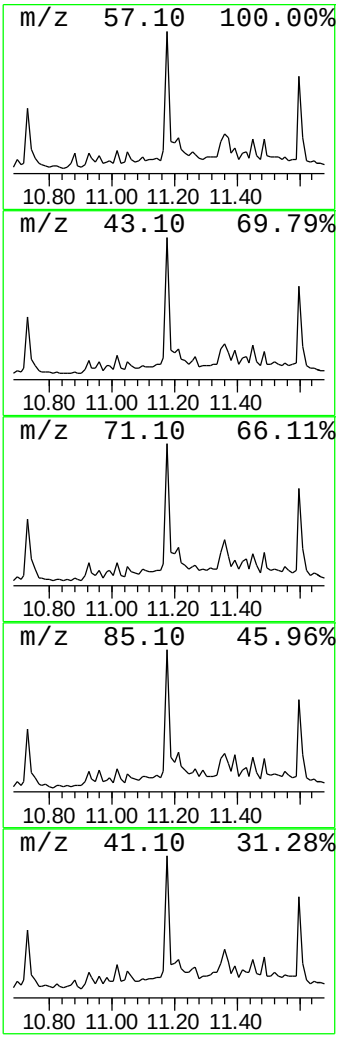
Peak Number 8 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	2.29 ng	110319	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
5	Hentriacontane	437	C31H64	000630-04-6	86





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Instrument : BNA_F
ClientSampleId : BS-3C10.5-11FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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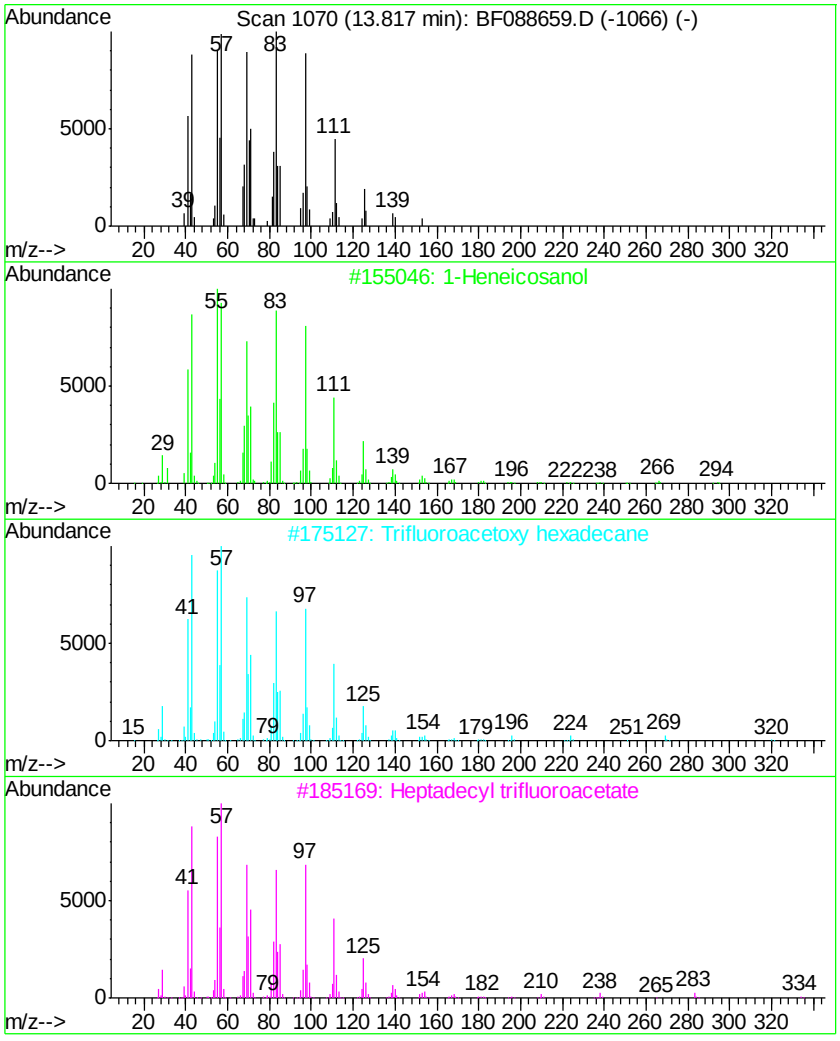
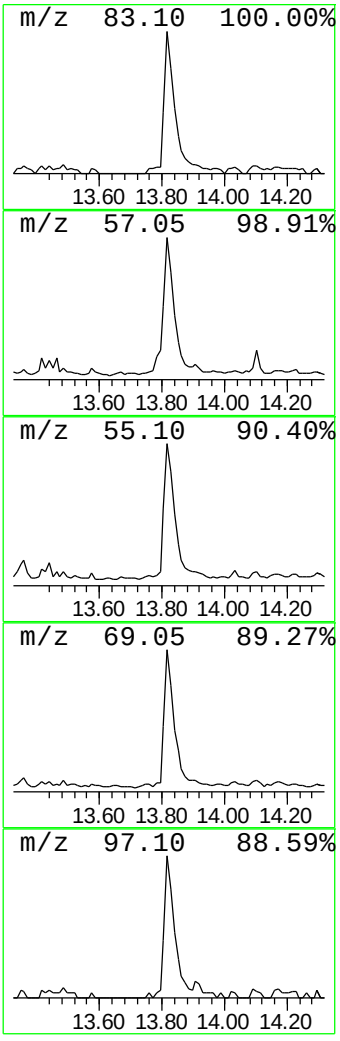
Peak Number 9 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	5.74 ng	265208	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	92
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





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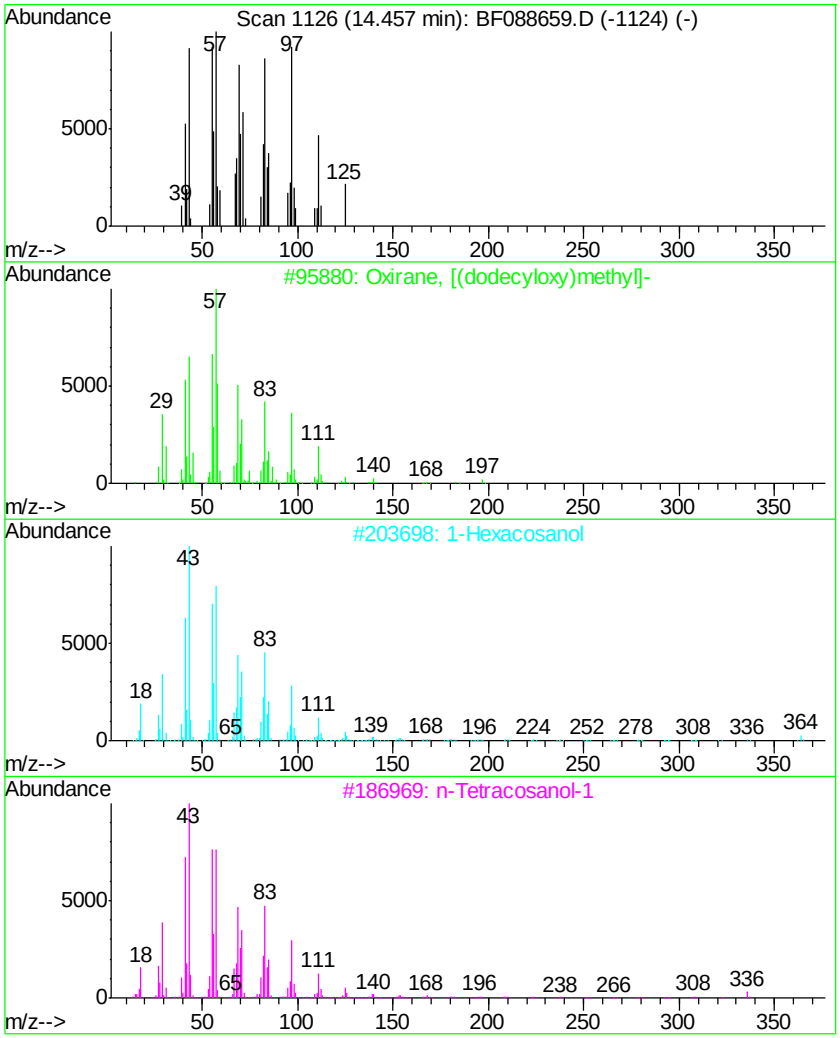
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

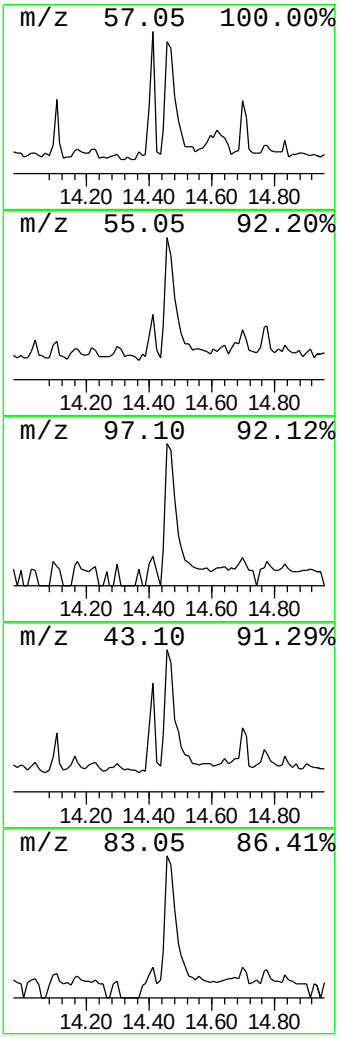
****

Peak Number 10 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.13 ng	98467	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	86
2	1-Hexacosanol	382	C26H54O	000506-52-5	83
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	81
4	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	64
5	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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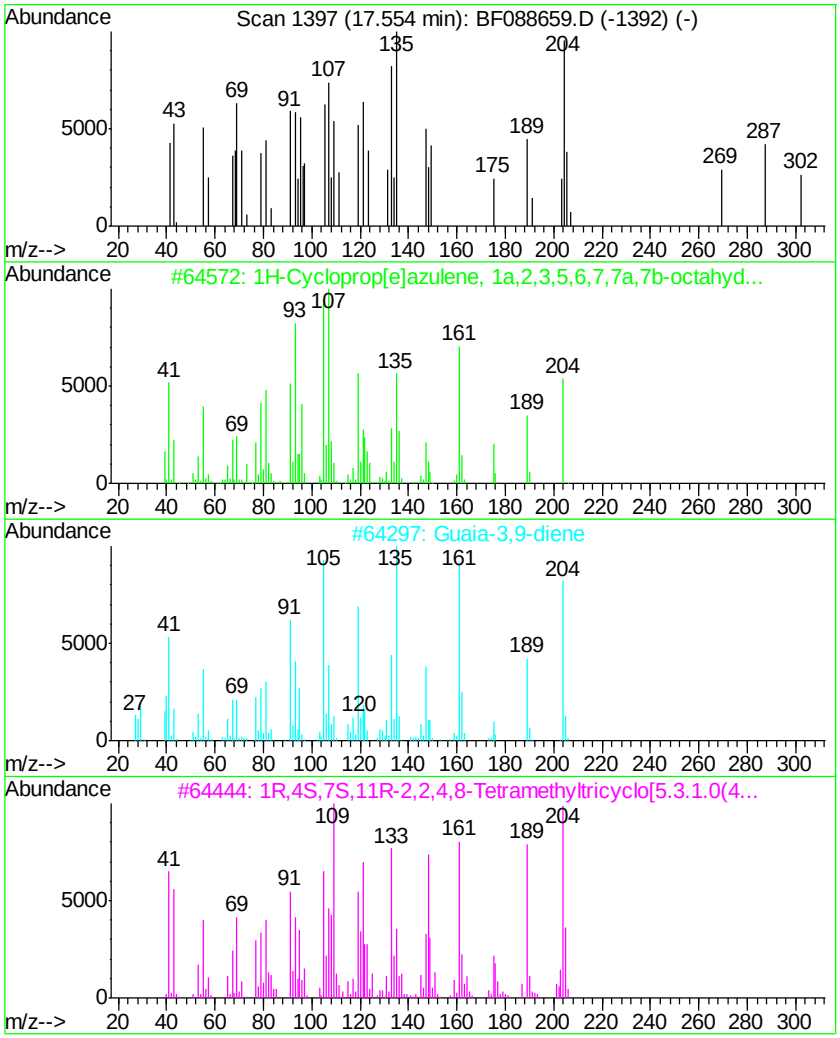
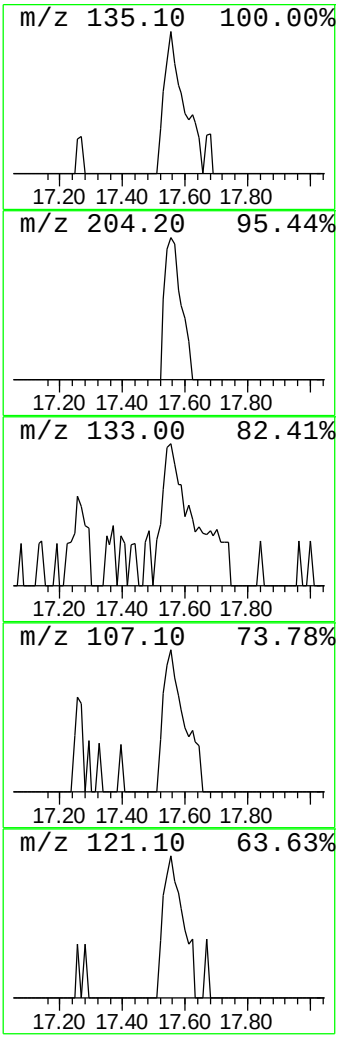
****

Peak Number 11 1H-Cycloprop[e]azulene, 1a,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.55	2.38 ng	83647	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	50
2	Guaia-3,9-diene	204	C15H24	000489-83-8	49
3	1R,4S,7S,11R-2,2,4,8-Tetramethyl...	204	C15H24	1000140-07-6	47
4	cis-Thujopsene	204	C15H24	000470-40-6	46
5	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	45





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
Propane, 2,2-dime...	1.64	202.2	ng	6358930	1	6.79	629096	20.0
Propylene Glycol	3.05	12.6	ng	394965	1	6.79	629096	20.0
2-Pentanone, 4-hy...	4.96	8.3	ng	259641	1	6.79	629096	20.0
unknown6.55	6.55	99.2	ng	3119070	1	6.79	629096	20.0
Benzamide, N,N-di...	10.20	27.4	ng	1368150	3	9.82	997621	20.0
Heneicosane	11.18	2.3	ng	110319	4	11.29	962234	20.0
1-Heneicosanol	13.82	5.7	ng	265208	5	13.92	924583	20.0
Oxirane, [(dodecy...	14.46	2.1	ng	98467	5	13.92	924583	20.0
1H-Cycloprop[e]az...	17.55	2.4	ng	83647	6	15.31	703504	20.0