LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090515\
Data File : BF081477.D
Acq On : 5 Sep 2015 21:59
Operator : UM/IZ
Sample : G3555-02
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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-BF090115.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	3.530	168	170	177	rBV	15513	34351	1.75%	0.202%
2	4.410	243	247	266	rVB	678649	1316625	67.22%	7.748%
3	4.913	288	291	293	rBV	1459374	1852429	94.57%	10.901%
4	6.033	386	389	391	rBV	1449761	1958694	100.00%	11.526%
5	6.124	395	397	399	rBV	1873443	1714322	87.52%	10.088%
6	6.353	415	417	420	rVB	372644	341804	17.45%	2.011%
7	6.513	429	431	433	rBV	1566819	1363403	69.61%	8.023%
8	6.936	465	468	470	rBV	1199659	1197720	61.15%	7.048%
9	7.645	528	530	532	rBV	526813	437430	22.33%	2.574%
10	8.730	622	625	627	rBV	2119761	1942959	99.20%	11.433%
11	9.130	658	660	663	rBV	336942	284071	14.50%	1.672%
12	9.382	680	682	685	rVB	463365	436344	22.28%	2.568%
13	9.828	718	721	722	rBV2	22544	22833	1.17%	0.134%
14	10.170	748	751	753	rBV	1186003	1151551	58.79%	6.776%
15	10.319	762	764	767	rBV	26269	29564	1.51%	0.174%
16	10.845	808	810	813	rBV	440582	443672	22.65%	2.611%
17	11.428	859	861	866	rBV	40302	57505	2.94%	0.338%
18	12.296	934	937	939	rVB	75840	90534	4.62%	0.533%
19	12.434	946	949	952	rBV	1584178	1564096	79.85%	9.204%
20	12.994	996	998	1000	rBV	68693	65501	3.34%	0.385%
21	13.359	1028	1030	1036	rBV	43895	100856	5.15%	0.593%
22	13.451	1036	1038	1041	rVB	334198	329382	16.82%	1.938%
23	13.679	1056	1058	1060	rBV	18332	20208	1.03%	0.119%
24	14.765	1151	1153	1155	rBV	198100	237854	12.14%	1.400%

Sum of corrected areas: 16993708

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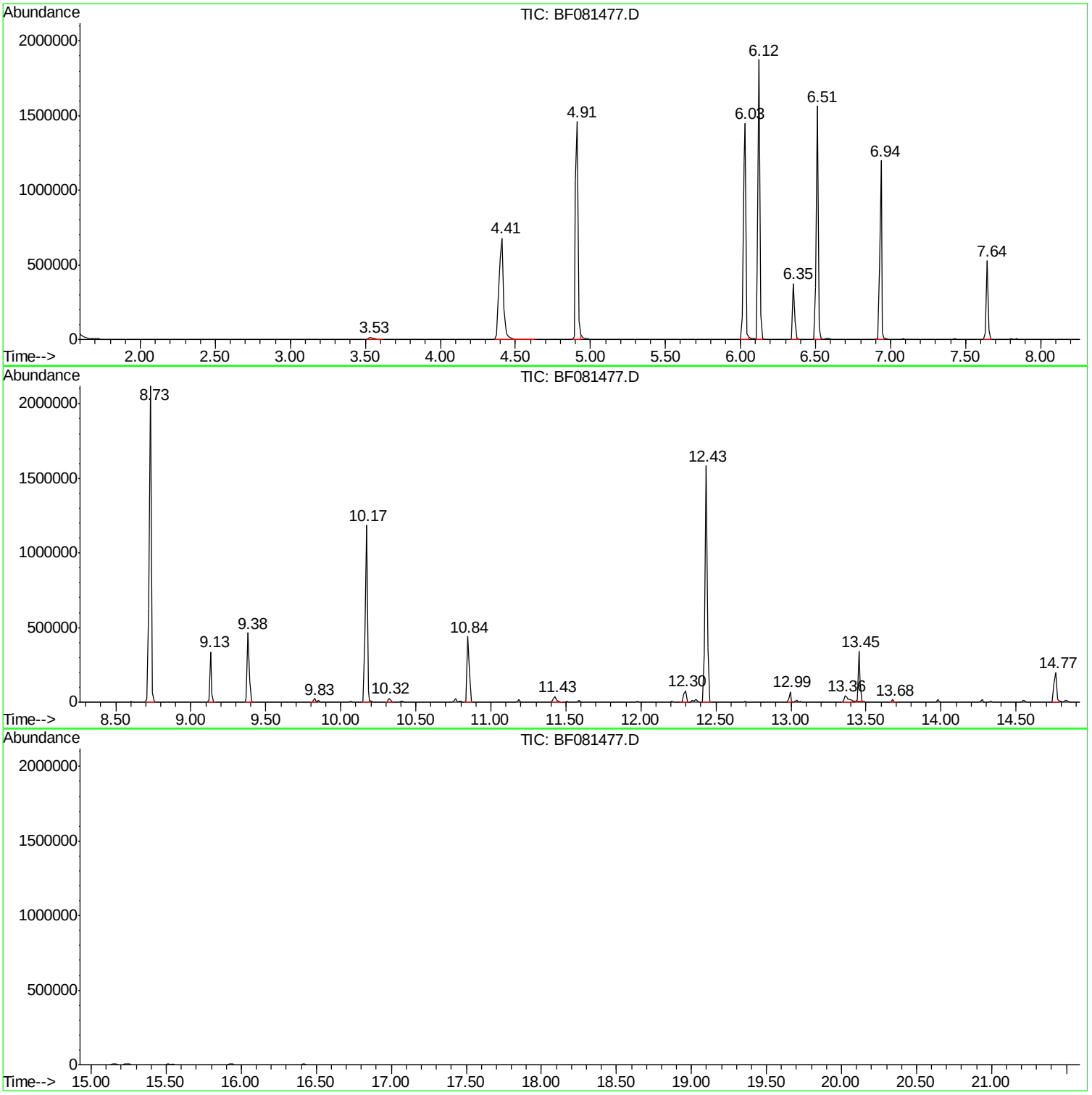
Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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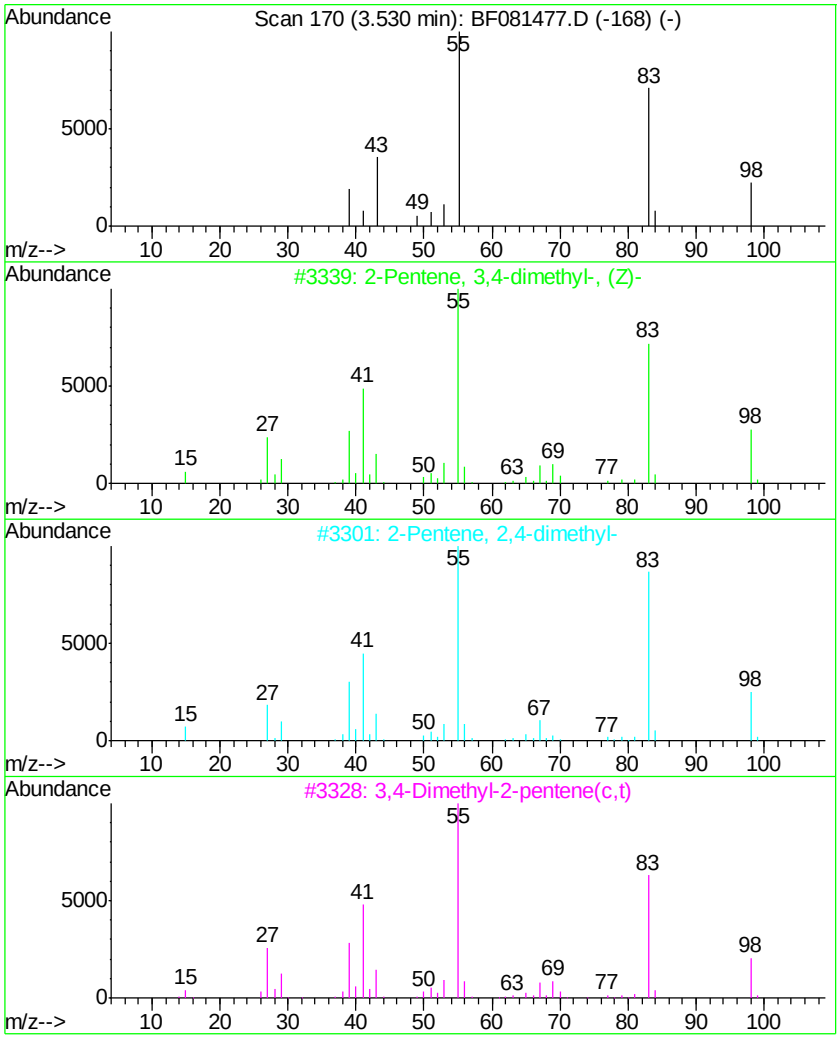
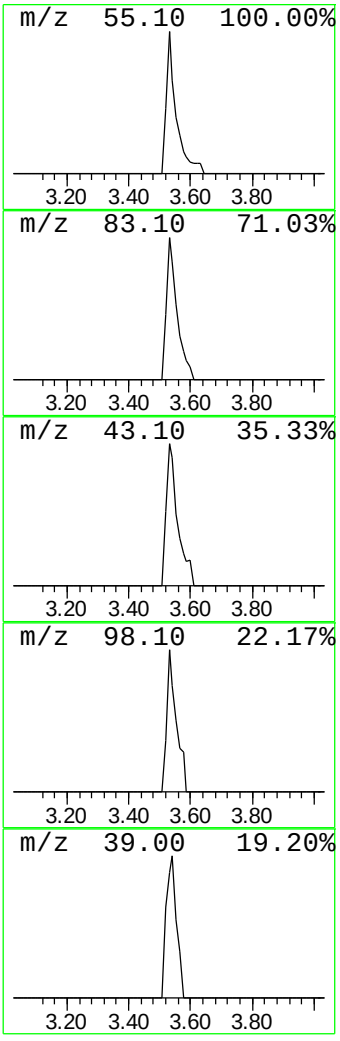
Peak Number 1 2-Pentene, 3,4-dimethyl-, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	2.01 ng	34351	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	83
2	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	83
3	3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	83
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	83
5	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	83





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Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
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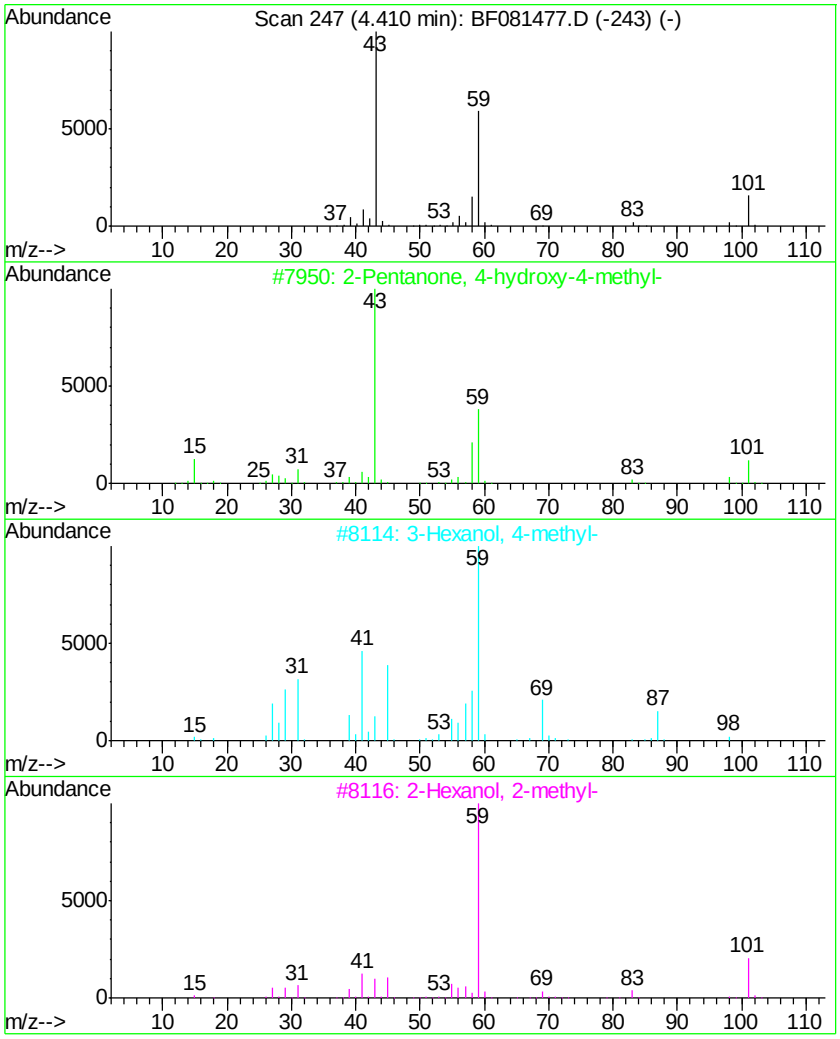
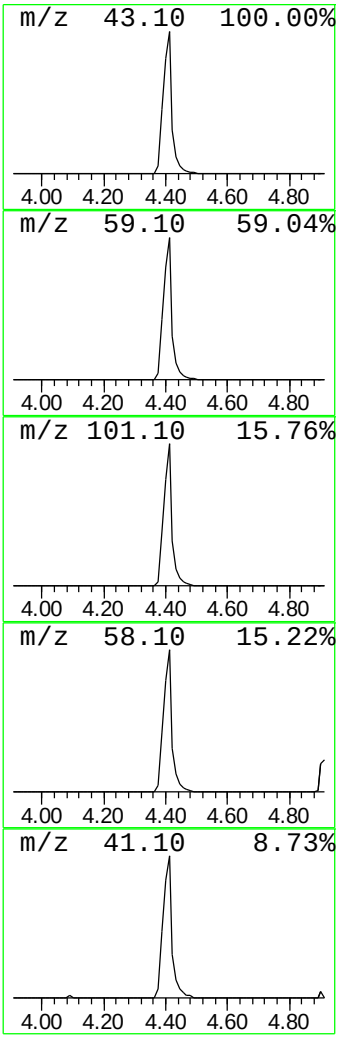
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	77.04 ng	1316630	1,4-Dichlorobenzene-d4	6.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : G3555-02
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
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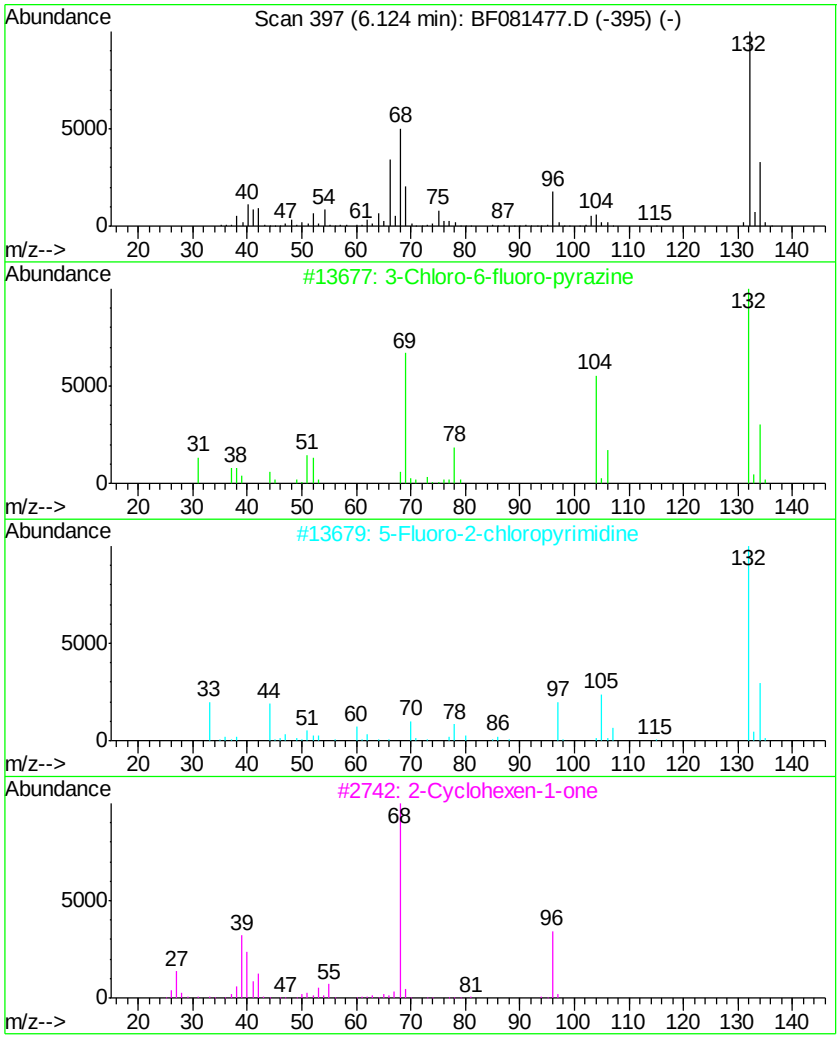
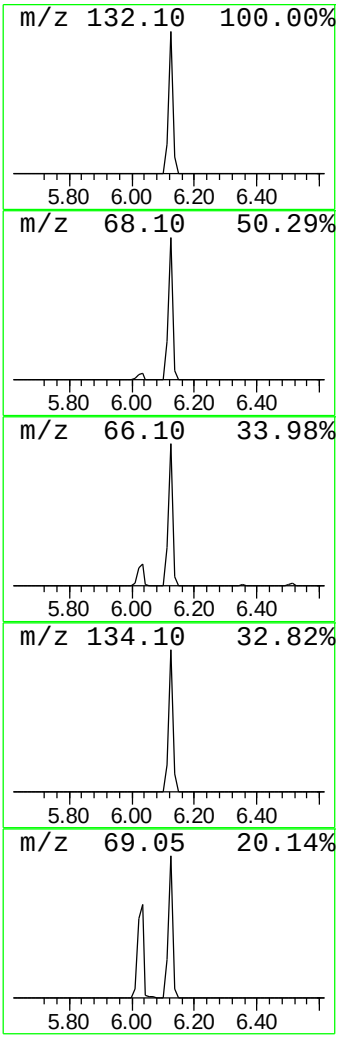
Peak Number 3 unknown6.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.12	100.31 ng	1714320	1,4-Dichlorobenzene-d4	6.35

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	16
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





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Operator : UM/IZ
Sample : G3555-02
Misc :
ALS Vial : 54 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2

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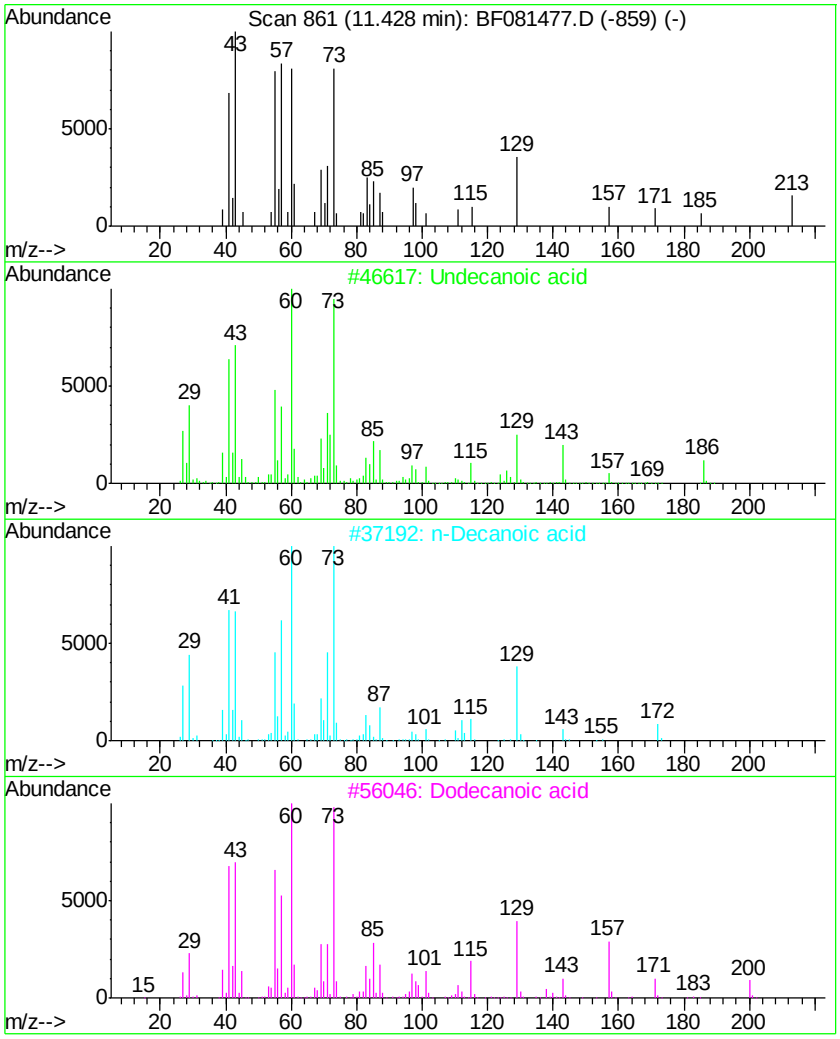
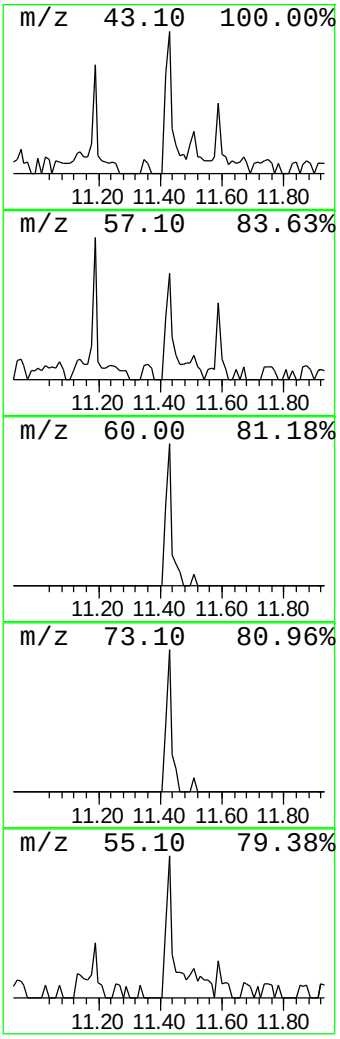
Peak Number 5 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	2.59 ng	57505	Phenanthrene-d10	10.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	59
2	n-Decanoic acid	172	C10H20O2	000334-48-5	47
3	Dodecanoic acid	200	C12H24O2	000143-07-7	45
4	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	42
5	.beta.-D-Glucopyranoside, methyl...	292	C14H28O6	1000157-04-9	38





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Sample : G3555-02
Misc :
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Instrument : BNA_F
ClientSampleId : SB-2

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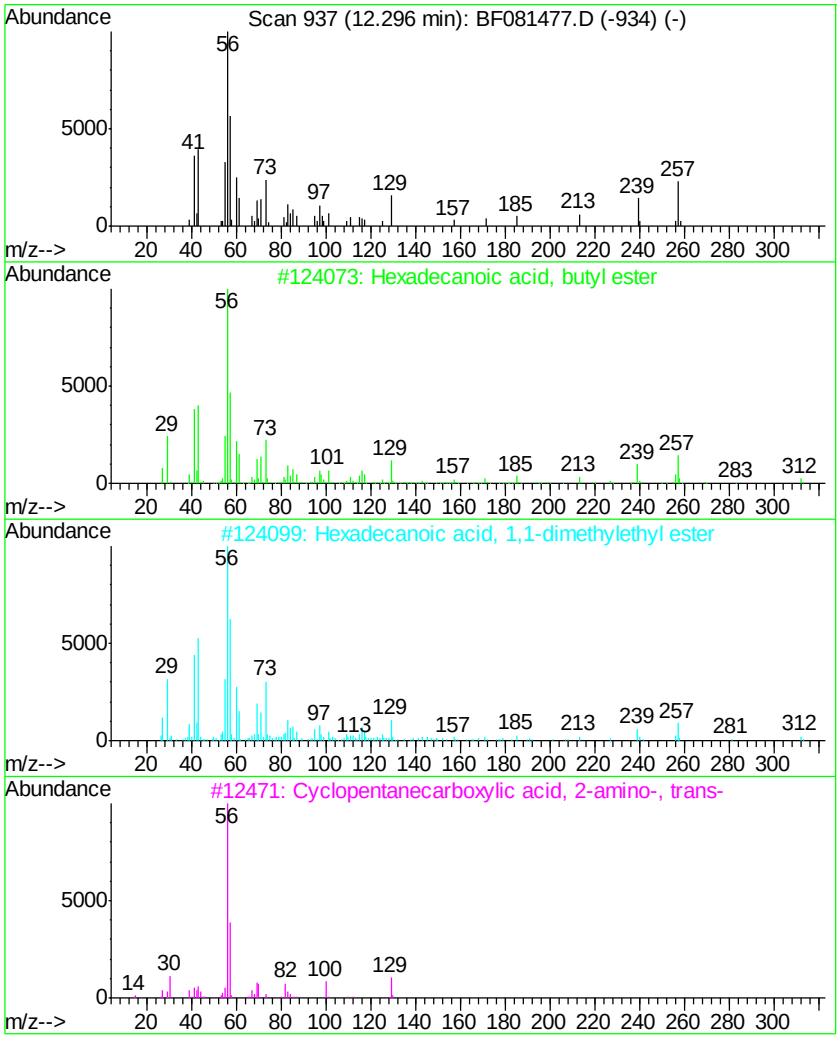
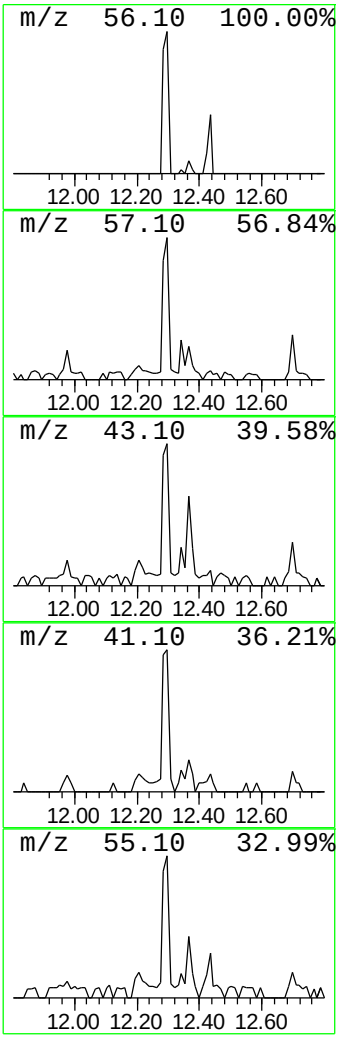
Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	5.50 ng	90534	Chrysene-d12	13.45

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	43
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
4	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35





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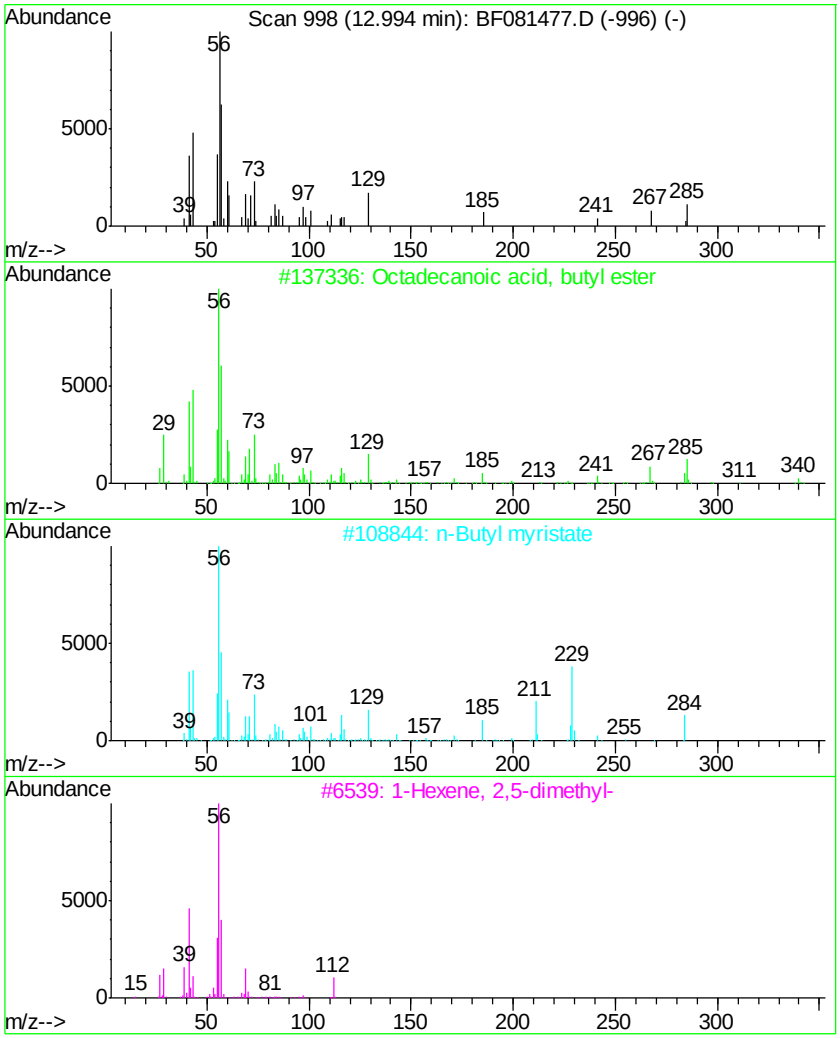
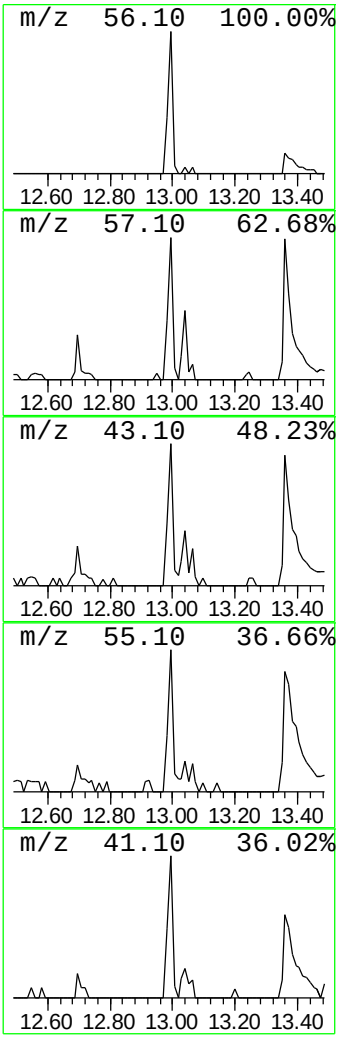
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.99	3.98 ng	65501	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	n-Butyl myristate	284	C18H36O2	000110-36-1	72
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	35
5	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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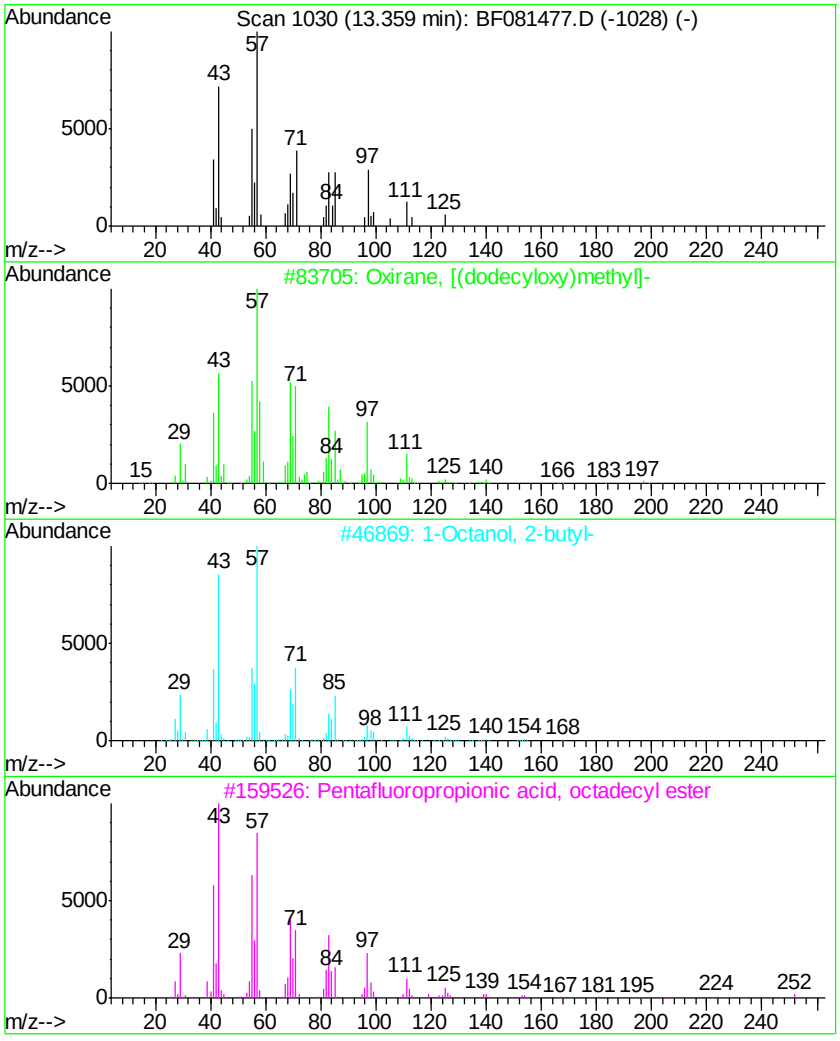
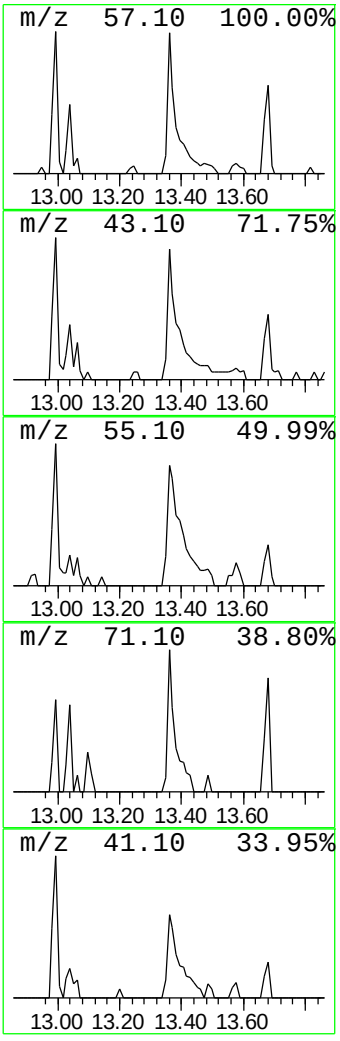
Peak Number 8 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	6.12 ng	100856	Chrysene-d12	13.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	53
2	1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	53
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	50
4	Dotriacontane	451	C32H66	000544-85-4	50
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	50





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentene, 3,4-di...	3.53	2.0	ng	34351	1	6.35	341804	20.0
2-Pentanone, 4-hy...	4.41	77.0	ng	1316630	1	6.35	341804	20.0
unknown6.12	6.12	100.3	ng	1714320	1	6.35	341804	20.0
Undecanoic acid	11.43	2.6	ng	57505	4	10.84	443672	20.0
Hexadecanoic acid...	12.30	5.5	ng	90534	5	13.45	329382	20.0
Octadecanoic acid...	12.99	4.0	ng	65501	5	13.45	329382	20.0
Oxirane, [(dodecy...	13.36	6.1	ng	100856	5	13.45	329382	20.0