LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF082815\
Data File : BF081258.D
Acq On : 28 Aug 2015 2:41
Operator : UM/IZ
Sample : G3430-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB2(24-25)

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-BF081715.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	3.805	179	181	187	rBB	19470	33196	2.09%	0.234%
2	4.606	246	251	264	rVB	595714	1192688	75.21%	8.404%
3	5.063	289	291	294	rBV	1103118	1422096	89.68%	10.020%
4	5.497	327	329	331	rBV	23551	33001	2.08%	0.233%
5	6.160	384	387	389	rBV	1393170	1459958	92.07%	10.287%
6	6.274	394	397	399	rBV	1475890	1585754	100.00%	11.173%
7	6.503	415	417	419	rBV	314518	251353	15.85%	1.771%
8	6.663	428	431	433	rBV	1125523	1101881	69.49%	7.764%
9	7.074	465	467	470	rBV	832294	893816	56.37%	6.298%
10	7.794	528	530	532	rBV	291660	314800	19.85%	2.218%
11	8.869	622	624	627	rBV	1410156	1395366	87.99%	9.832%
12	9.269	657	659	661	rBV	196892	152947	9.65%	1.078%
13	9.532	680	682	684	rBV	446157	372842	23.51%	2.627%
14	10.320	748	751	753	rBV	793252	1041265	65.66%	7.337%
15	10.458	761	763	768	rVB	24001	26785	1.69%	0.189%
16	10.903	797	802	803	rBV	23600	21630	1.36%	0.152%
17	10.995	808	810	813	rVB	377742	376595	23.75%	2.654%
18	11.566	857	860	862	rBV	76160	106313	6.70%	0.749%
19	12.584	946	949	952	rBV	1441820	1425788	89.91%	10.046%
20	13.178	995	1001	1005	rBV	8499	16058	1.01%	0.113%
21	13.498	1026	1029	1037	rBV	133112	221552	13.97%	1.561%
22	13.612	1037	1039	1041	rBV	344312	369994	23.33%	2.607%
23	14.115	1081	1083	1090	rBV2	7168	19842	1.25%	0.140%
24	14.469	1112	1114	1116	rVB	38572	36622	2.31%	0.258%
25	14.938	1152	1155	1157	rBV	185439	249748	15.75%	1.760%
26	15.395	1192	1195	1203	rBV4	11336	37219	2.35%	0.262%
27	18.093	1425	1431	1439	rVB3	4067	16660	1.05%	0.117%
28	18.996	1504	1510	1516	rBV2	3790	16541	1.04%	0.117%

Sum of corrected areas: 14192310

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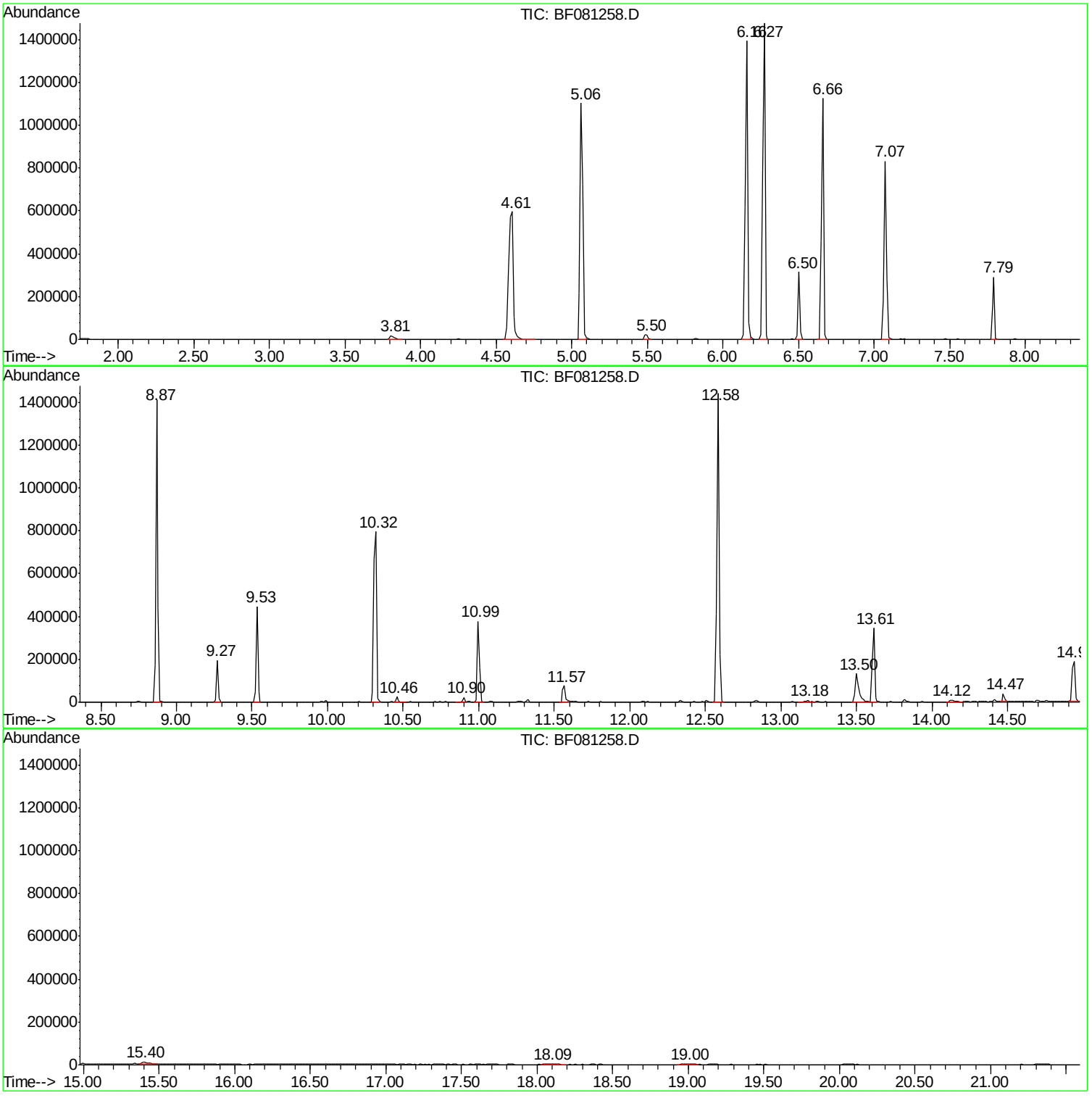
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB2(24-25)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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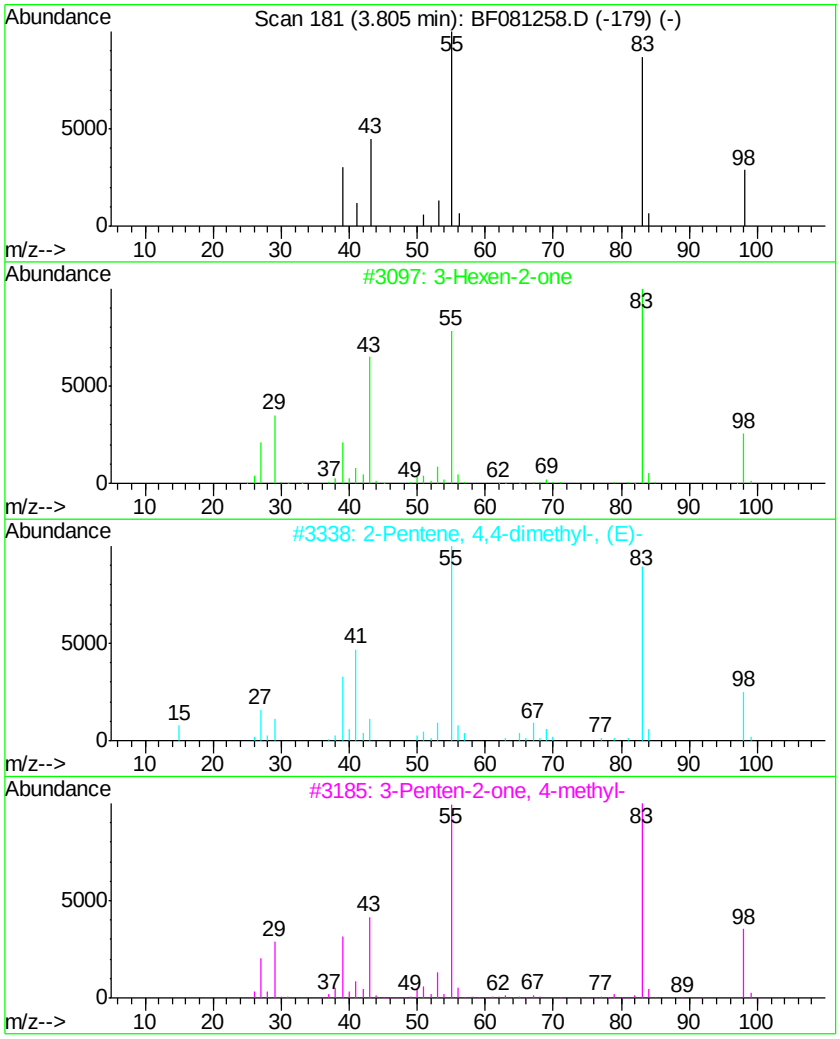
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

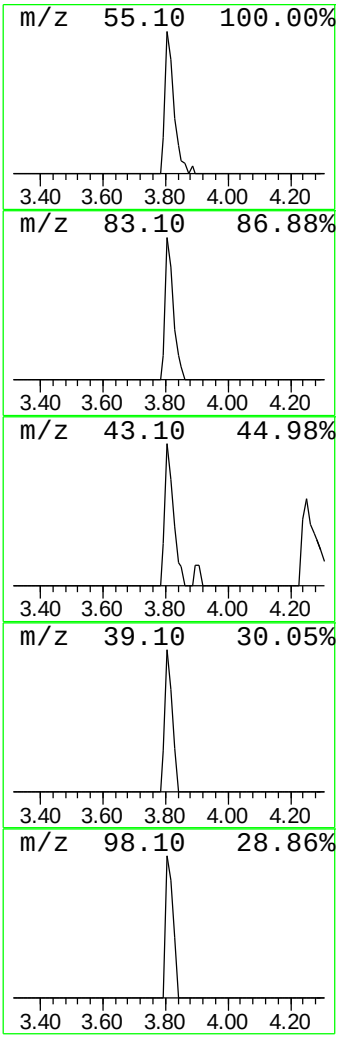
****

Peak Number 1 3-Hexen-2-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.81	2.64 ng	33196	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	90
2	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	90
3	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
4	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	83
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	83





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Sample : G3430-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB2(24-25)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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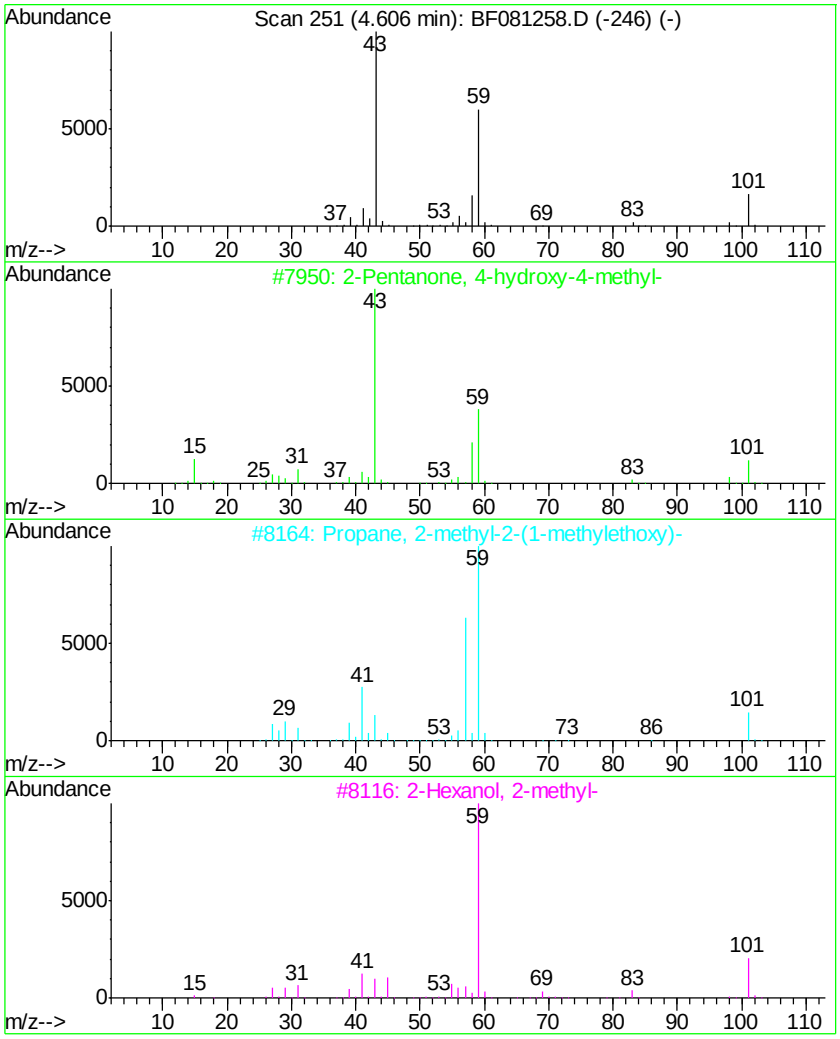
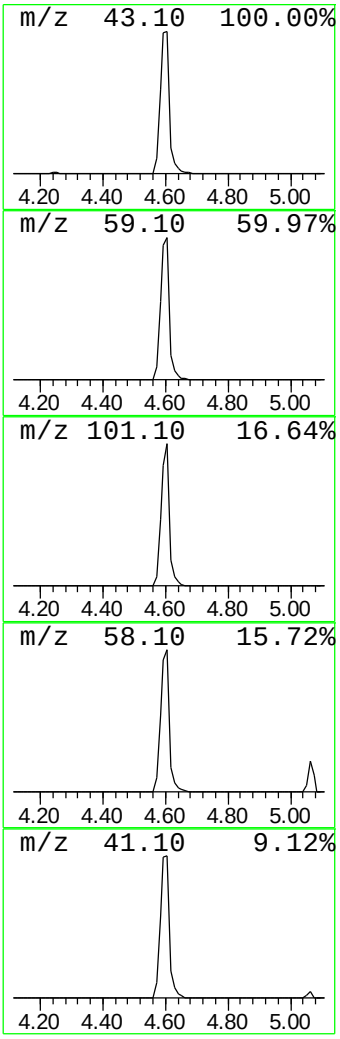
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	94.90 ng	1192690	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Operator : UM/IZ
Sample : G3430-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB2(24-25)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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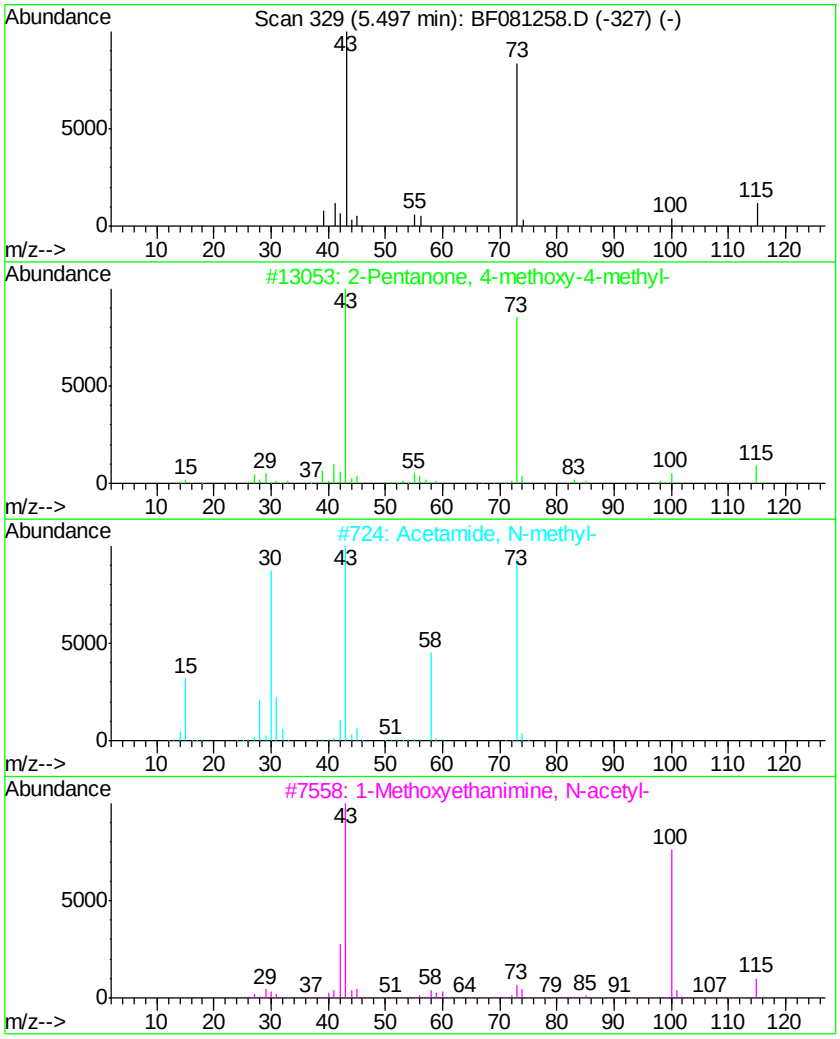
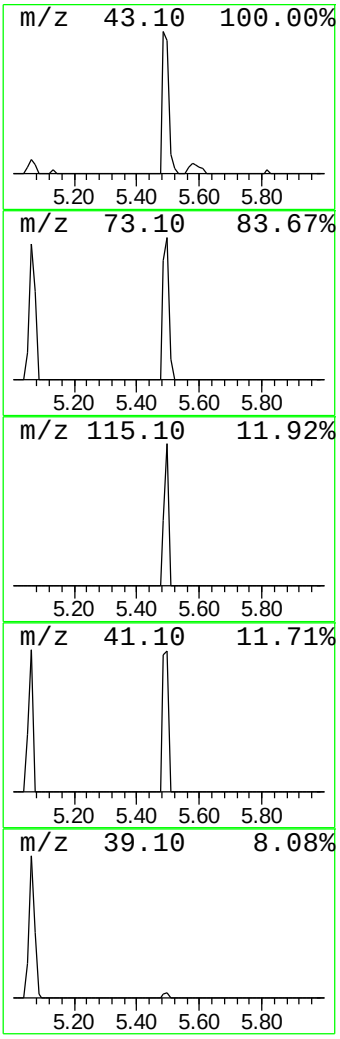
Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.50	2.63 ng	33001	1,4-Dichlorobenzene-d4	6.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
3	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9
4	5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9





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Acq On : 28 Aug 2015 2:41
Operator : UM/IZ
Sample : G3430-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB2(24-25)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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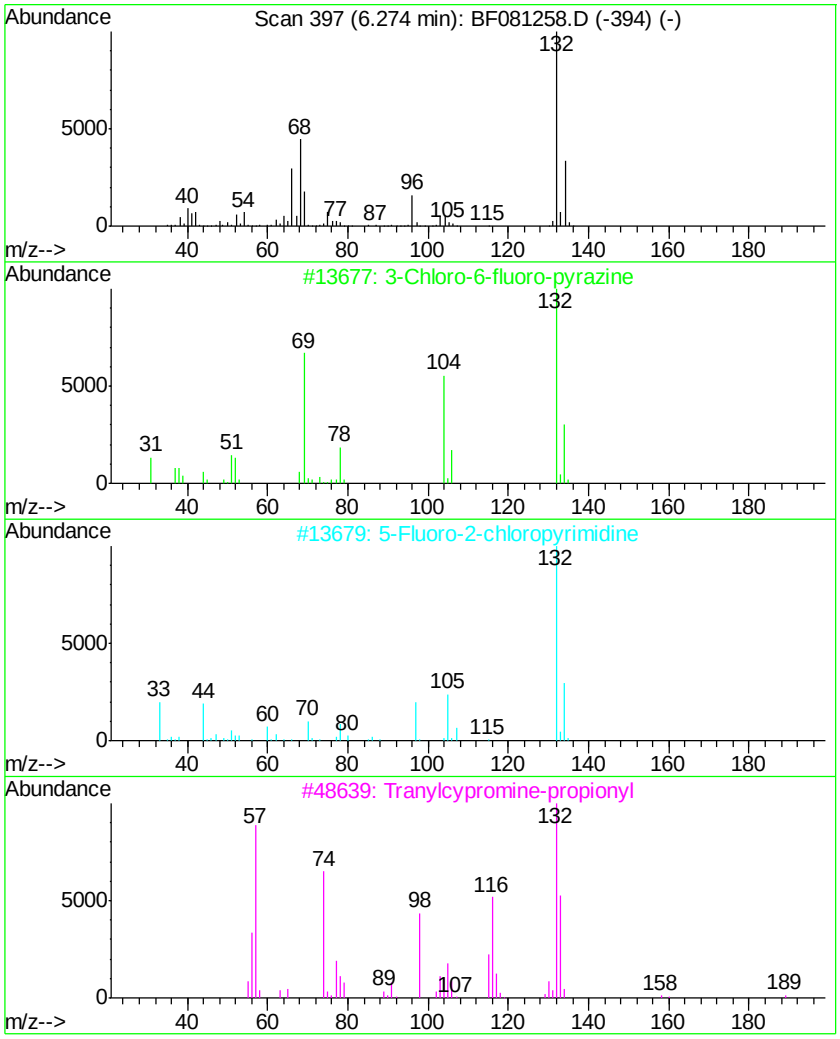
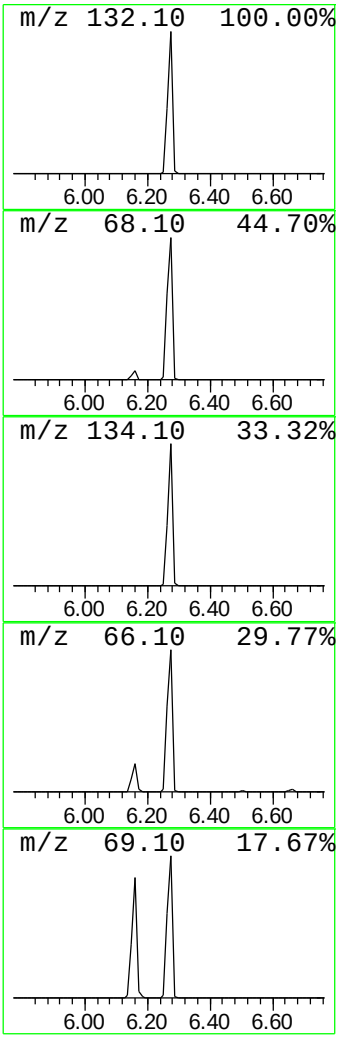
Peak Number 4 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	126.18 ng	1585750	1,4-Dichlorobenzene-d4	6.50

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Acq On : 28 Aug 2015 2:41
Operator : UM/IZ
Sample : G3430-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB2(24-25)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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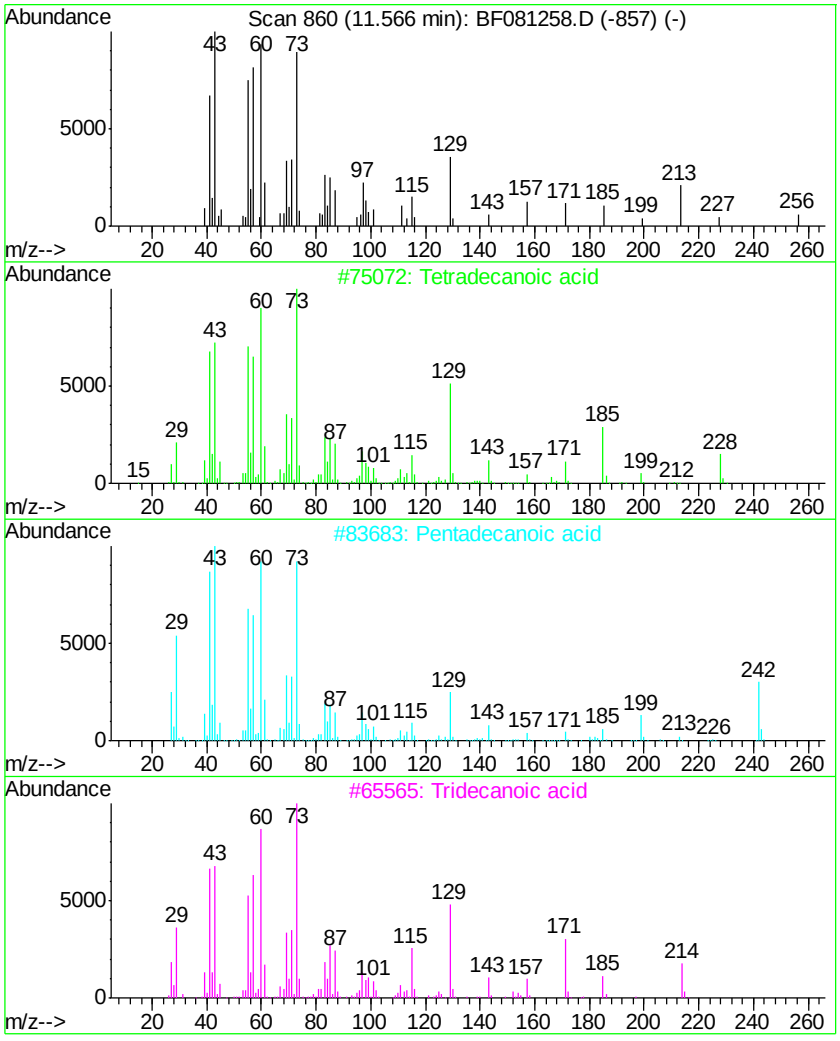
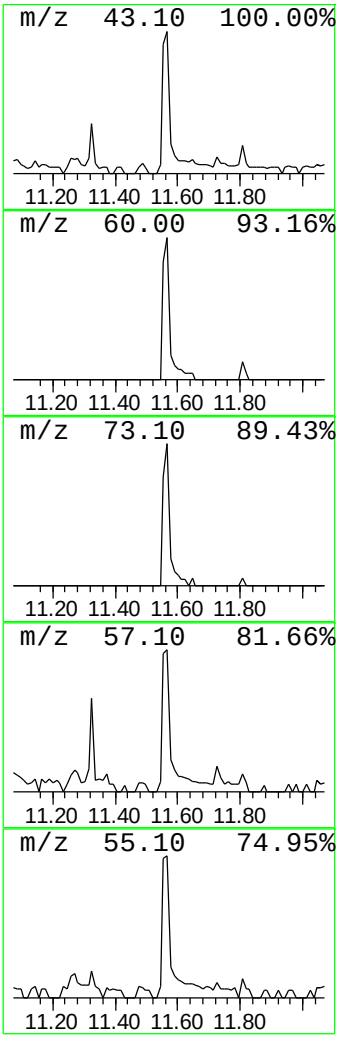
Peak Number 6 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	5.65 ng	106313	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





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Sample : G3430-04
Misc :
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Instrument : BNA_F
ClientSampleId : SB2(24-25)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.M
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TIC Library : C:\DATABASE\NIST02.L
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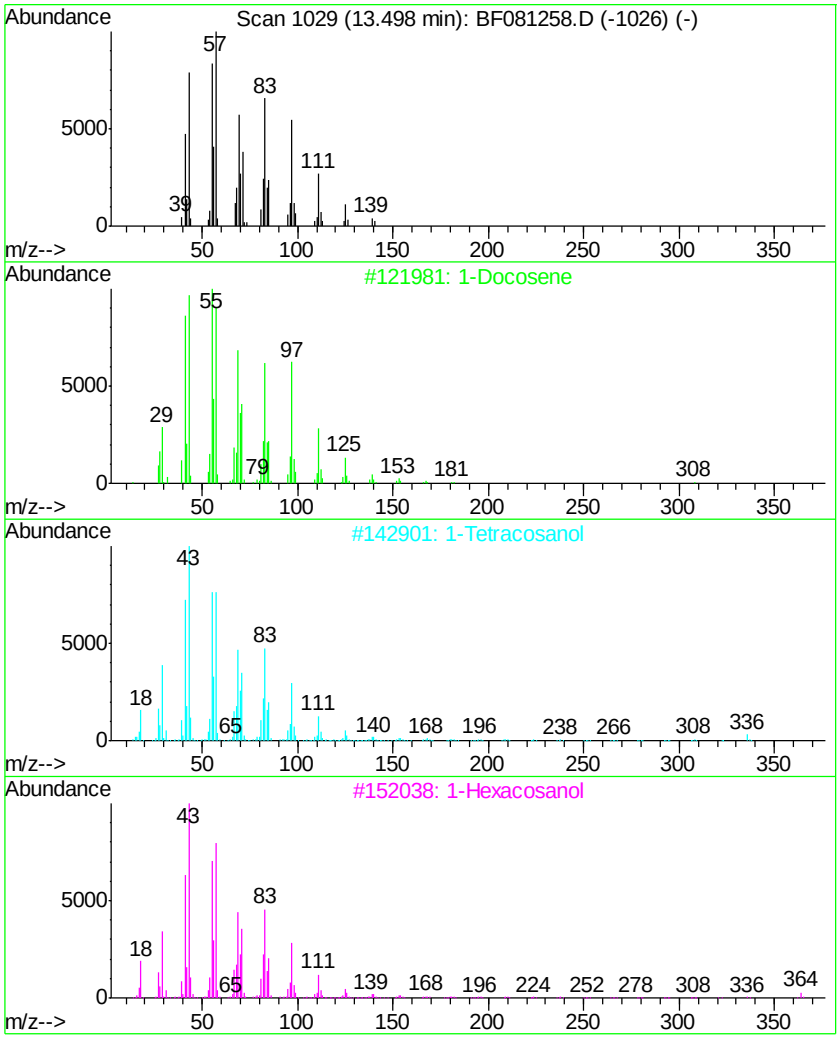
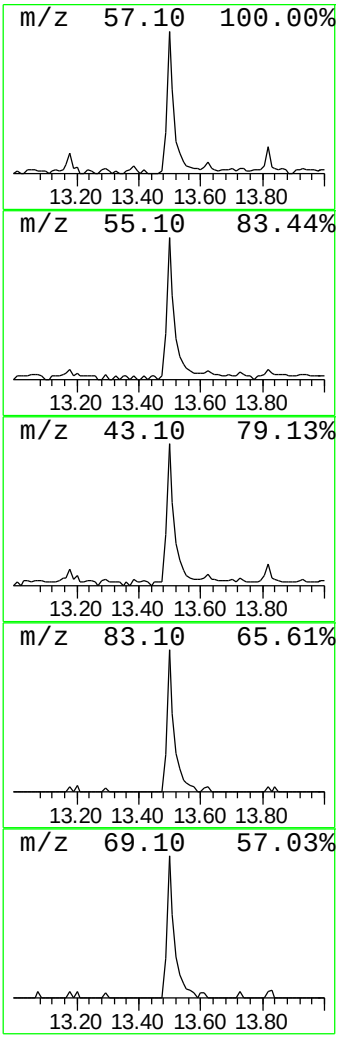
Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	11.98 ng	221552	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Tetracosanol	354	C24H50O	000506-51-4	83
3	1-Hexacosanol	382	C26H54O	000506-52-5	80
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	72
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	72





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Sample : G3430-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB2(24-25)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081715.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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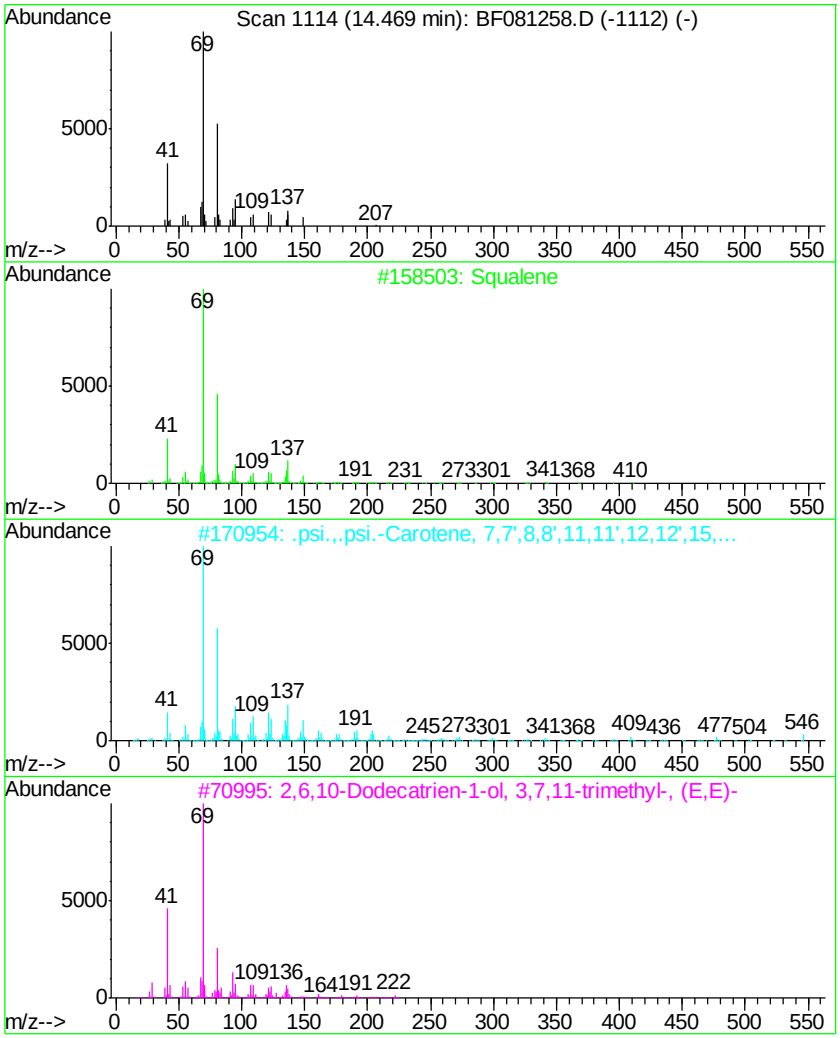
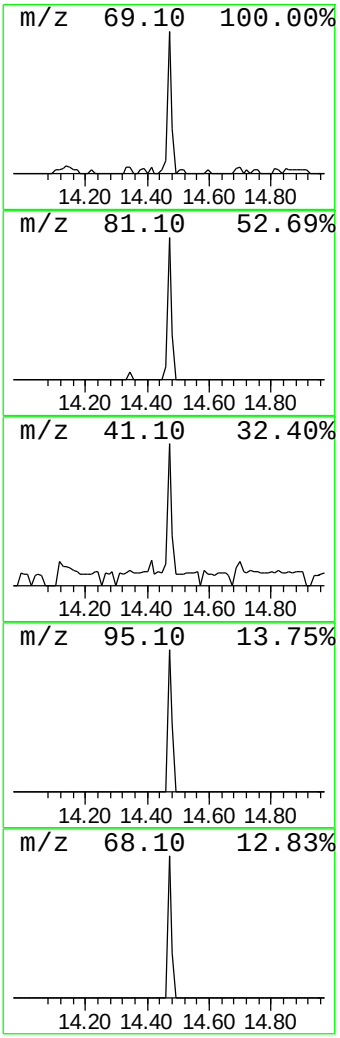
Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.93 ng	36622	Perylene-d12	14.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	90
2	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST02.L
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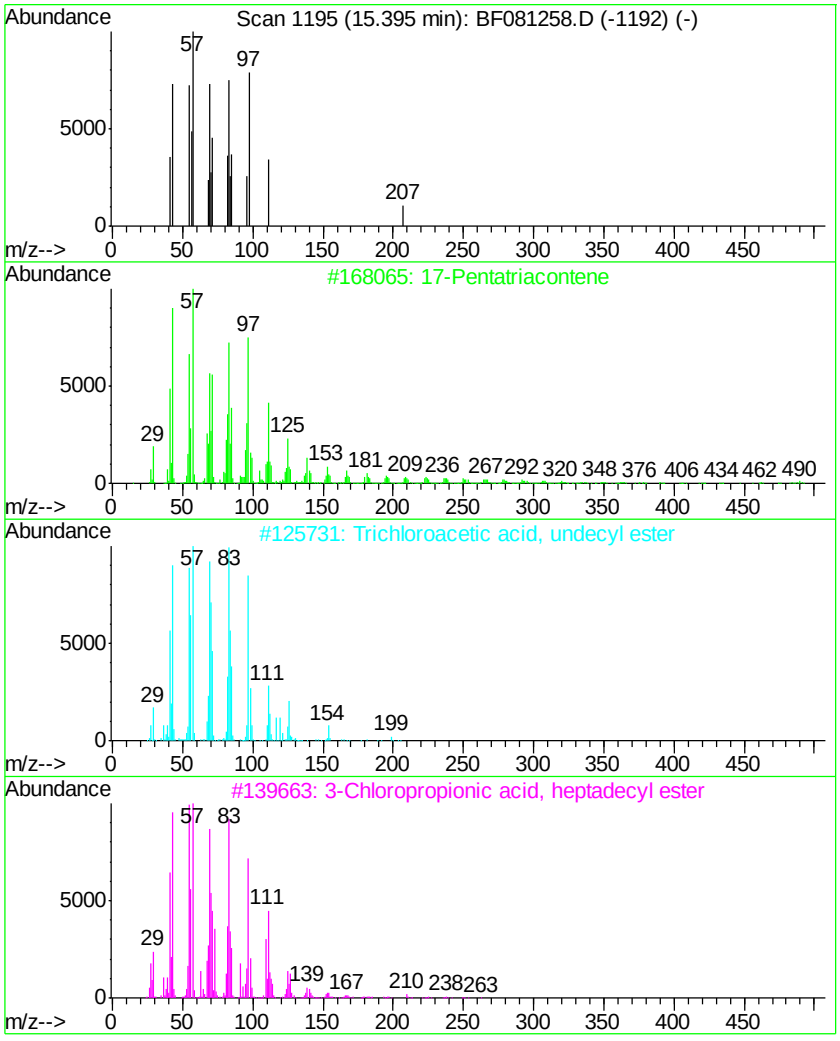
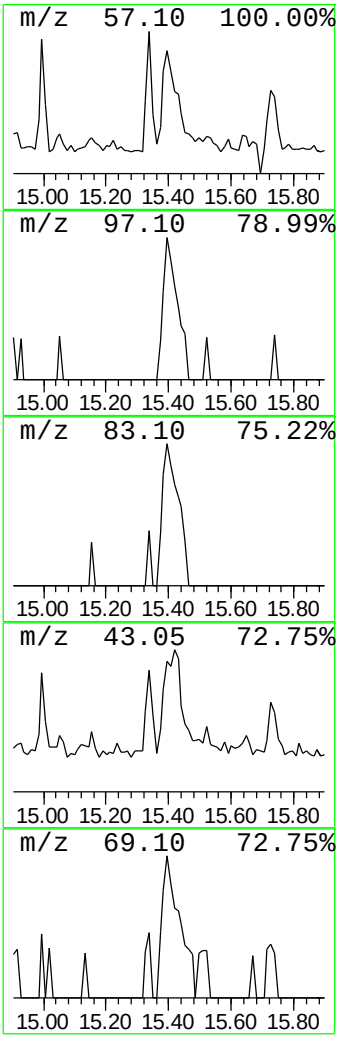
Peak Number 9 17-Pentatriacontene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.40	2.98 ng	37219	Perylene-d12	14.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	80
2	Trichloroacetic acid, undecyl ester	316	C13H23Cl3O2	074339-49-4	72
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	64
4	1-Tetracosanol	354	C24H50O	000506-51-4	59
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	59





Tentatively Identified Compound (LSC) summary

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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
3-Hexen-2-one	3.81	2.6	ng	33196	1	6.50	251353	20.0
2-Pentanone, 4-hy...	4.61	94.9	ng	1192690	1	6.50	251353	20.0
2-Pentanone, 4-me...	5.50	2.6	ng	33001	1	6.50	251353	20.0
unknown6.27	6.27	126.2	ng	1585750	1	6.50	251353	20.0
Tetradecanoic acid	11.57	5.7	ng	106313	4	10.99	376595	20.0
1-Docosene	13.50	12.0	ng	221552	5	13.61	369994	20.0
Squalene	14.47	2.9	ng	36622	6	14.94	249748	20.0
17-Pentatriacontene	15.40	3.0	ng	37219	6	14.94	249748	20.0