LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087275.D
Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

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-BF051716.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	1.701	8	10	23	rVB	3091673	4792935	100.00%	11.677%
2	4.684	269	271	286	rBV	253554	512181	10.69%	1.248%
3	5.153	310	312	333	rBV	2244795	3731660	77.86%	9.091%
4	6.227	404	406	409	rBV	2655479	3652972	76.22%	8.899%
5	6.330	413	415	418	rVV	3934453	3670422	76.58%	8.942%
6	6.559	432	435	441	rVB	698787	925668	19.31%	2.255%
7	6.707	446	448	451	rBV	2818232	2615018	54.56%	6.371%
8	7.130	483	485	488	rBV	2056184	2246157	46.86%	5.472%
9	7.839	545	547	550	rBV	1097314	1238937	25.85%	3.018%
10	8.925	639	642	644	rBV	4516121	4326177	90.26%	10.539%
11	9.325	675	677	681	rBV	454374	417785	8.72%	1.018%
12	9.530	693	695	698	rBV	122649	125007	2.61%	0.305%
13	9.588	698	700	703	rVV	1590636	1404523	29.30%	3.422%
14	10.033	735	739	740	rBV	216348	206406	4.31%	0.503%
15	10.250	755	758	761	rBV	64936	106712	2.23%	0.260%
16	10.376	767	769	772	rBV2	2110716	2370507	49.46%	5.775%
17	10.502	778	780	784	rBV	211924	239887	5.01%	0.584%
18	10.696	795	797	801	rVB	26824	48577	1.01%	0.118%
19	10.948	817	819	820	rBV	96041	88737	1.85%	0.216%
20	11.062	827	829	832	rBV	1237074	1253669	26.16%	3.054%
21	12.479	951	953	956	rBV	444415	377078	7.87%	0.919%
22	12.559	959	960	962	rVB	92769	66891	1.40%	0.163%
23	12.651	965	968	970	rBV	3667596	3691962	77.03%	8.994%
24	13.176	1012	1014	1016	rBV2	179358	237081	4.95%	0.578%
25	13.222	1016	1018	1020	rBV	74134	82055	1.71%	0.200%
26	13.554	1045	1047	1054	rBV	149979	223461	4.66%	0.544%
27	13.691	1057	1059	1062	rVB	1017272	969074	20.22%	2.361%
28	13.862	1072	1074	1077	rBV	66350	78902	1.65%	0.192%
29	14.171	1097	1101	1103	rBV	67793	87039	1.82%	0.212%
30	14.457	1123	1126	1129	rBV2	68803	133031	2.78%	0.324%
31	14.525	1130	1132	1136	rVB	49470	54312	1.13%	0.132%
32	14.754	1149	1152	1154	rBV	48715	65994	1.38%	0.161%
33	15.039	1175	1177	1185	rBV	562970	845952	17.65%	2.061%
34	15.417	1207	1210	1213	rBV	47549	70912	1.48%	0.173%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087275.D
Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

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-BF051716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.817	1242	1245	1252	rVB2	46119	89834	1.87%	0.219%

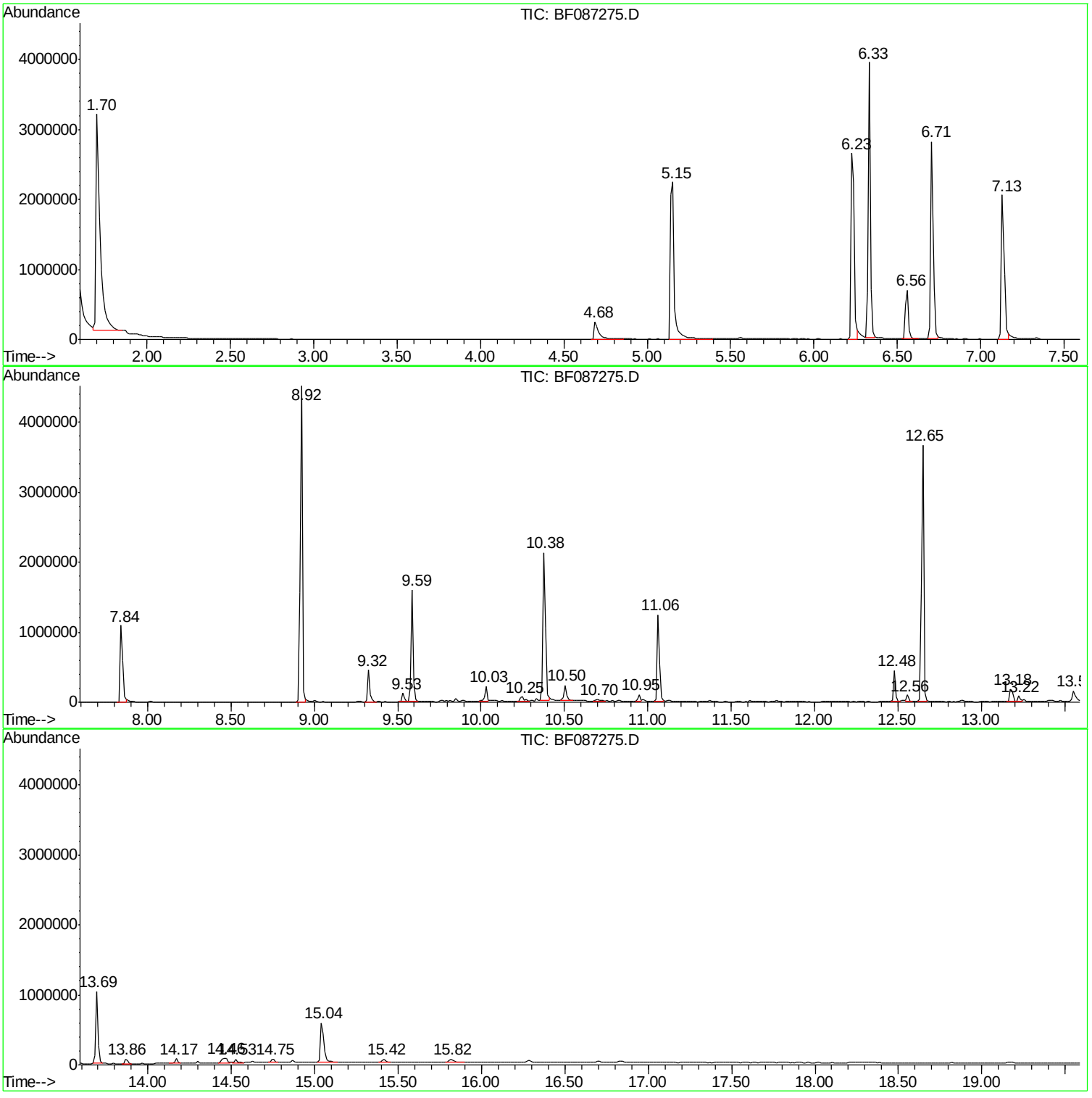
Sum of corrected areas: 41047515

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087275.D
Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087275.D
Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

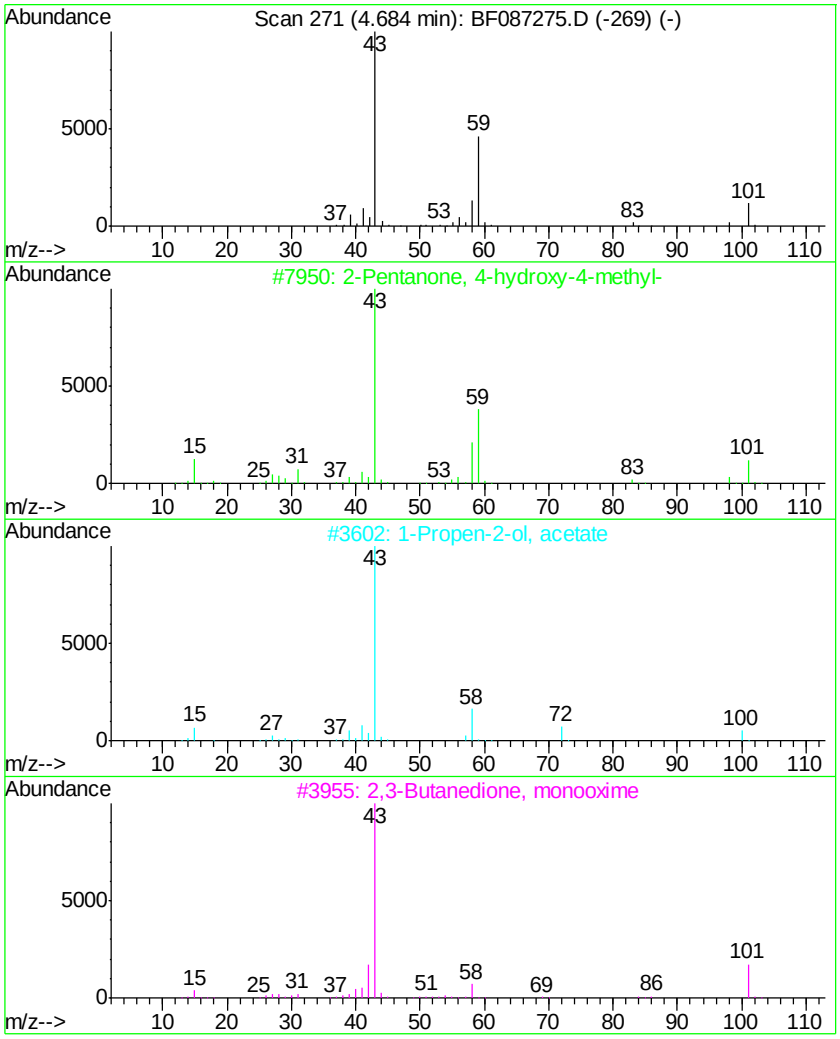
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

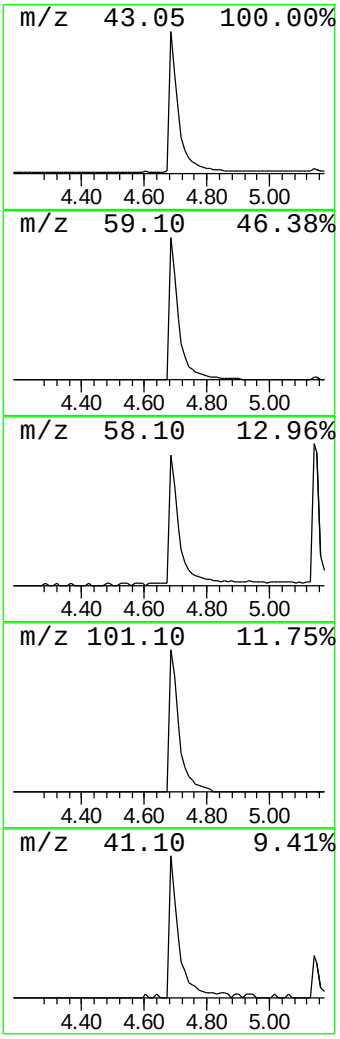
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	11.07 ng	512181	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087275.D
Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

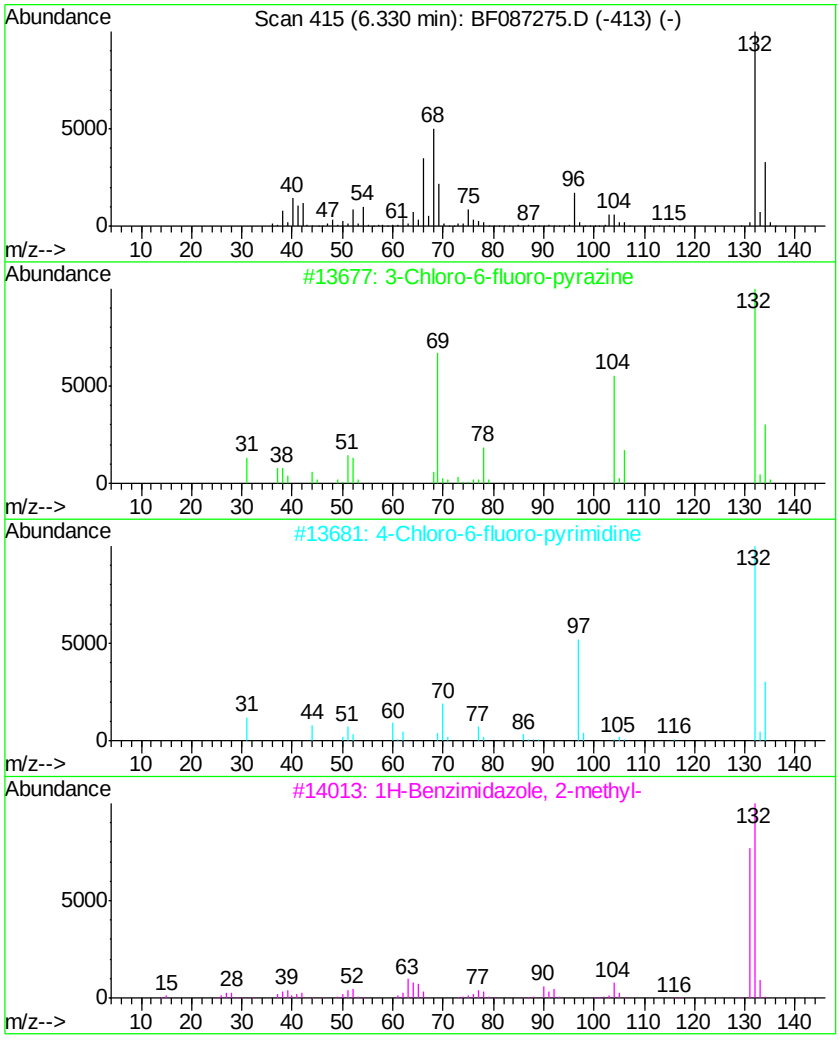
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

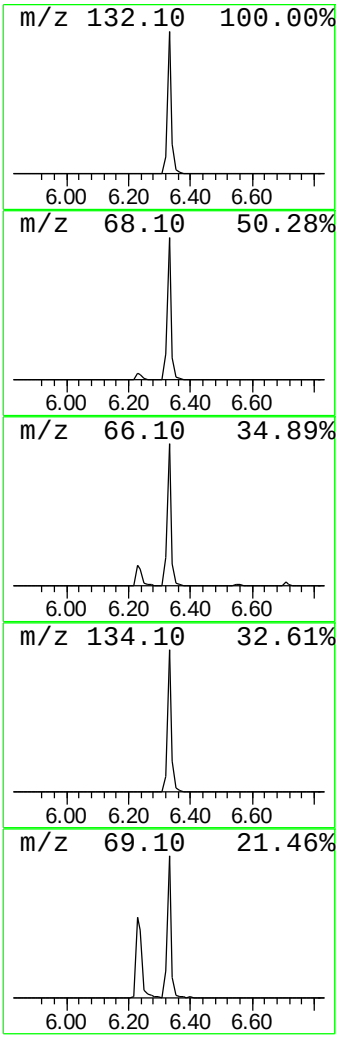
****

Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	79.30 ng	3670420	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087275.D
Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

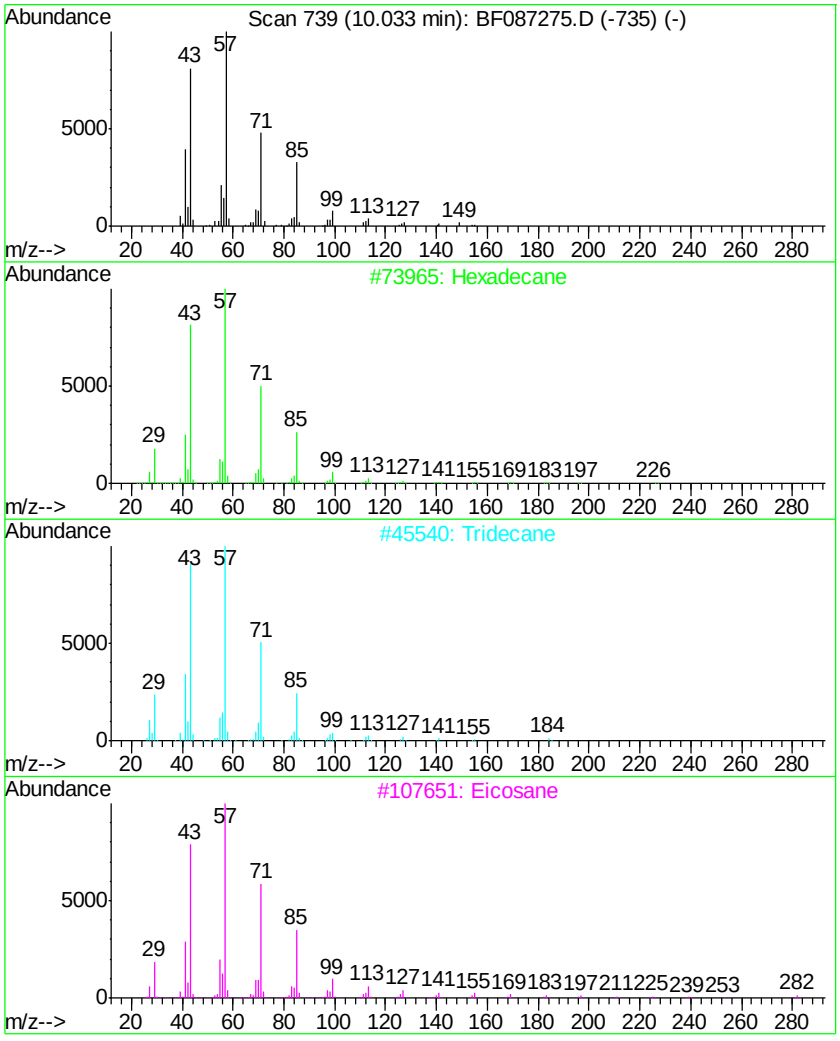
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

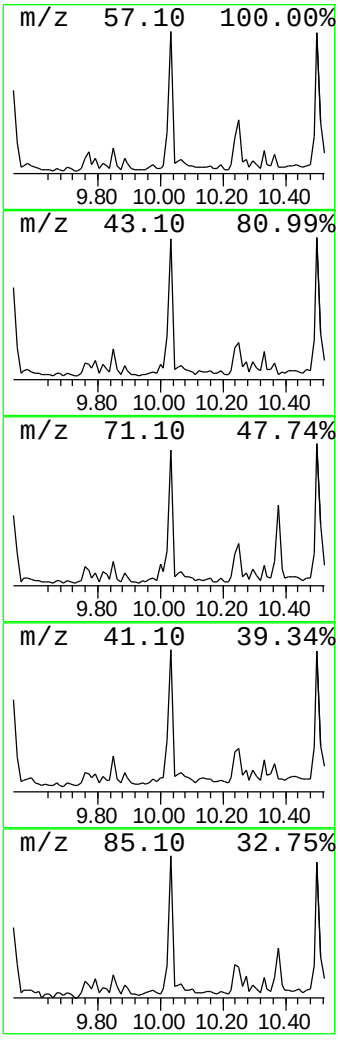
****

Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	2.94 ng	206406	Acenaphthene-d10	9.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tridecane	184	C13H28	000629-50-5	90
3	Eicosane	282	C20H42	000112-95-8	86
4	Tetradecane	198	C14H30	000629-59-4	80
5	Decane, 3-bromo-	220	C10H21Br	030571-71-2	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
Data File : BF087275.D
Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

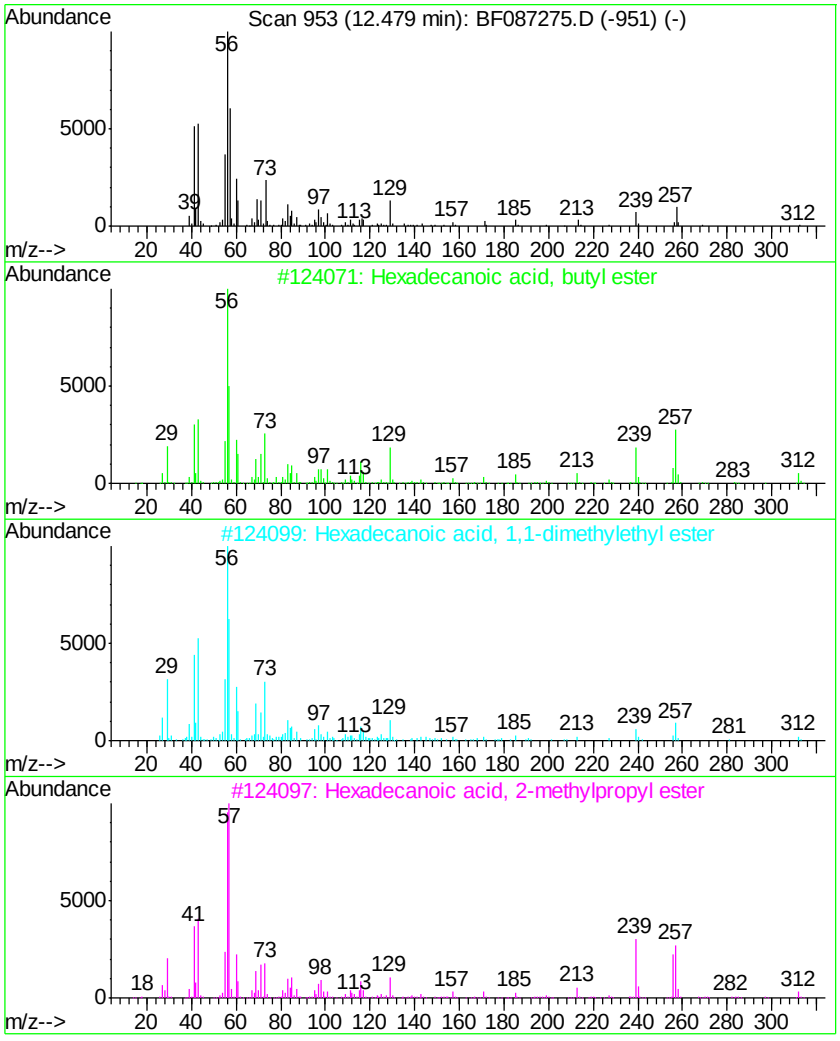
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

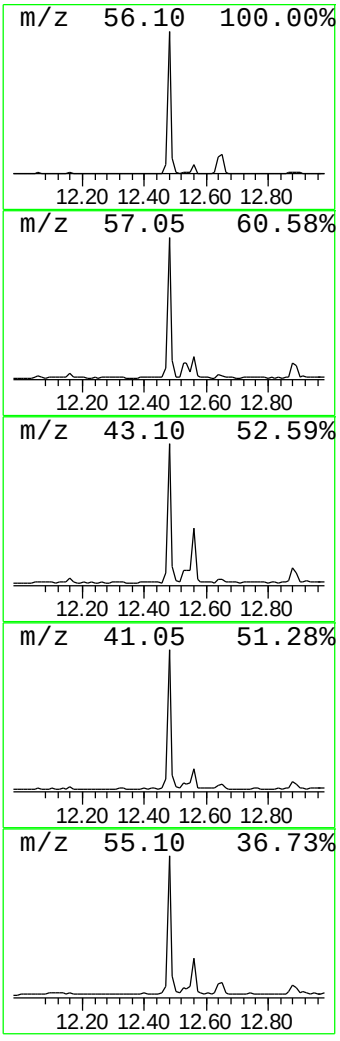
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	7.78 ng	377078	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	38
4	Eicosanoic acid	312	C20H40O2	000506-30-9	38
5	2-Isopropyl-3-vinyloxirane	112	C7H12O	070777-23-0	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
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Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

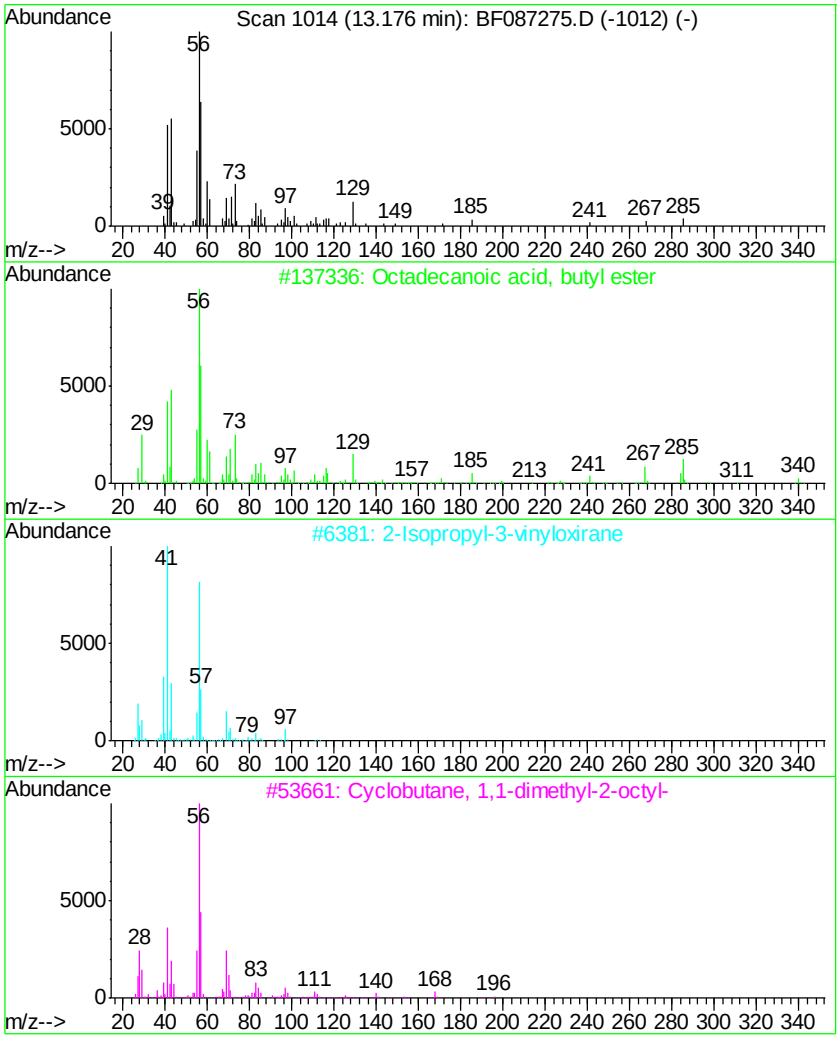
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

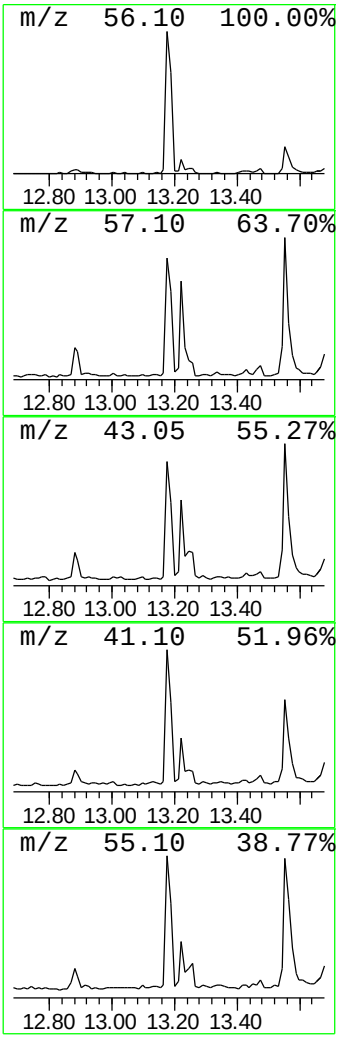
****

Peak Number 8 unknown13.18 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	4.89 ng	237081	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	47
2	2-Isopropyl-3-vinyloxirane	112	C7H12O	070777-23-0	43
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4	Chloromethyl 2-chloroundecanoate	268	C12H22Cl2O2	080418-88-8	37
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	37





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Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

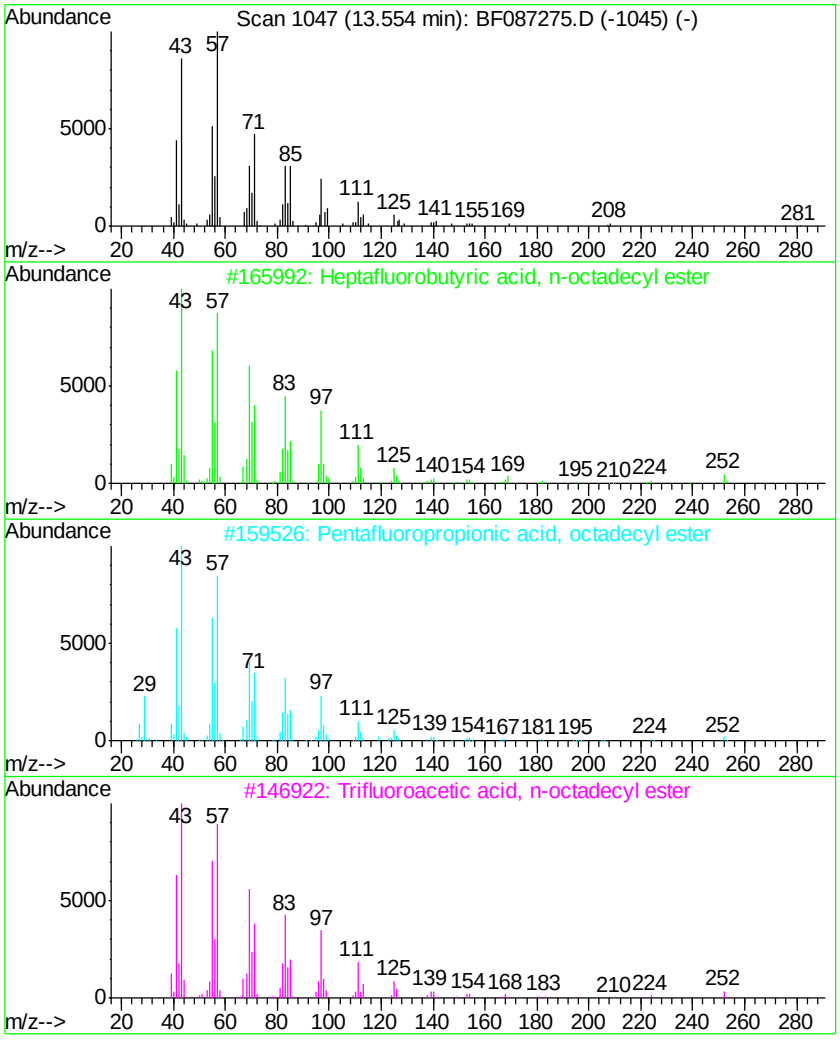
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

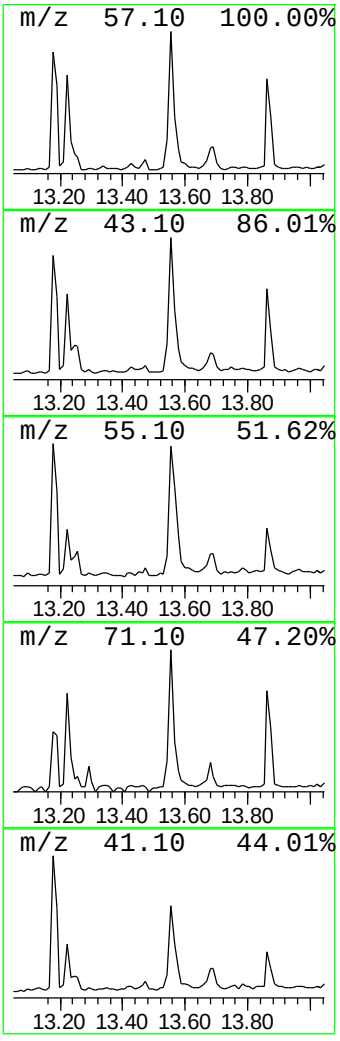
****

Peak Number 9 Heptafluorobutyric acid, n-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	4.61 ng	223461	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	62
2	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	58
3	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	58
4	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	53
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	53





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Acq On : 21 May 2016 16:22
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Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.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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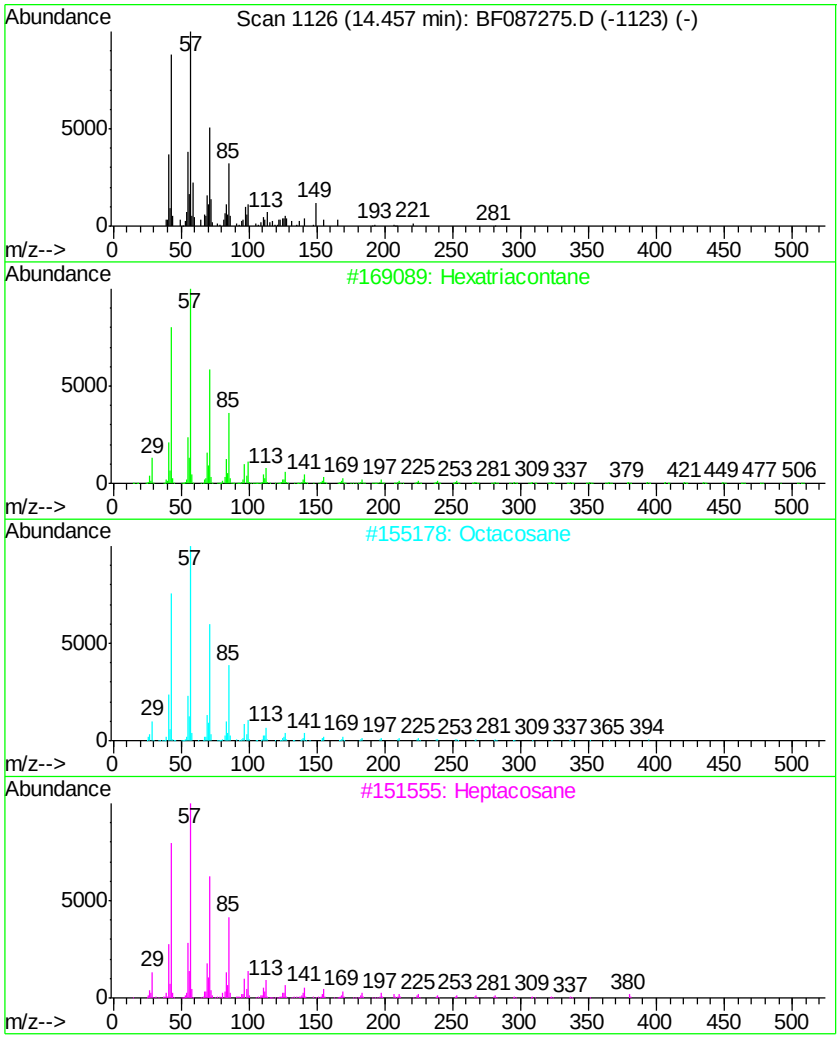
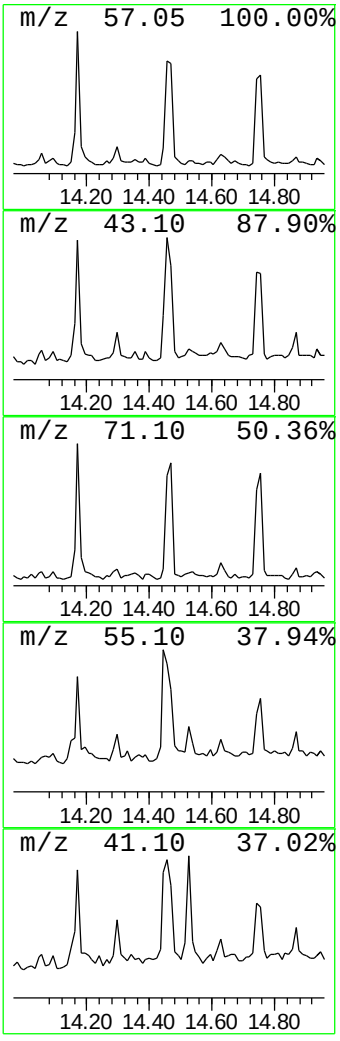
Peak Number 10 Hexatriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	3.15 ng	133031	Perylene-d12	15.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexatriacontane	507	C36H74	000630-06-8	70
2	Octacosane	394	C28H58	000630-02-4	62
3	Heptacosane	380	C27H56	000593-49-7	62
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	58
5	Tetracosane	338	C24H50	000646-31-1	58





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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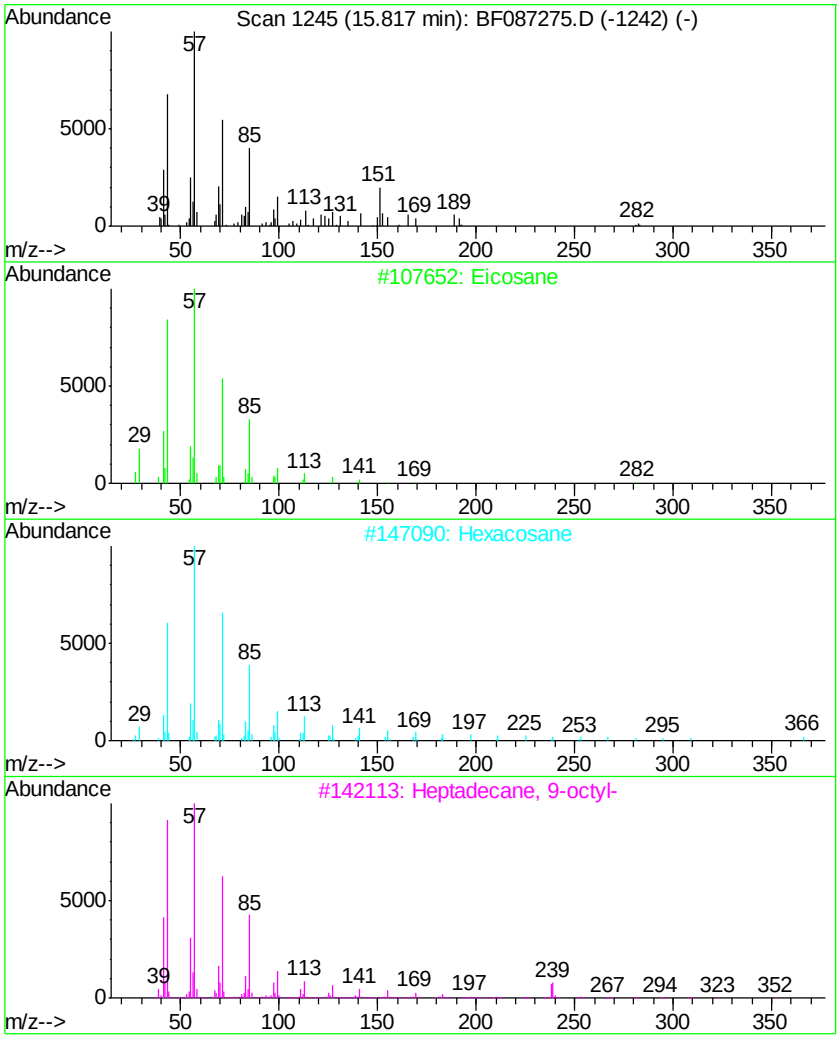
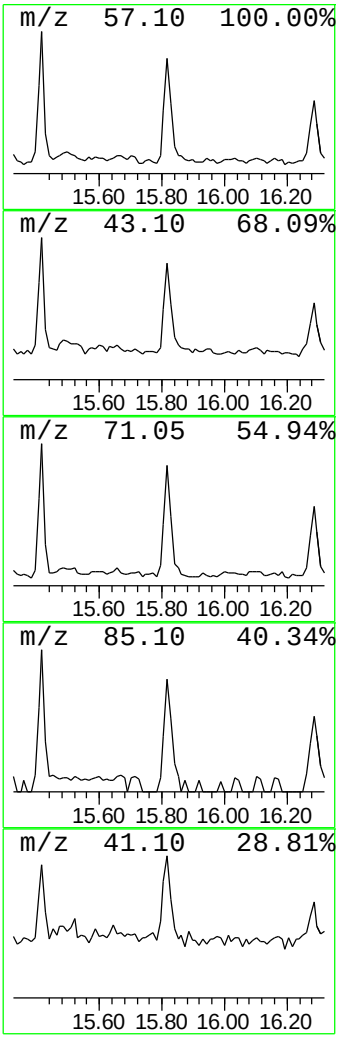
Peak Number 11 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.82	2.12 ng	89834	Perylene-d12	15.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Hexacosane	366	C26H54	000630-01-3	64
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64
4	Heptadecane	240	C17H36	000629-78-7	64
5	Triacontane	422	C30H62	000638-68-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052016\
Data File : BF087275.D
Acq On : 21 May 2016 16:22
Operator : UM/SJ
Sample : H3168-02
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-40-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
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
2-Pentanone, 4-hy...	4.68	11.1	ng	512181	1	6.56	925668	20.0
unknown6.33	6.33	79.3	ng	3670420	1	6.56	925668	20.0
Hexadecane	10.03	2.9	ng	206406	3	9.59	1404520	20.0
Hexadecanoic acid...	12.48	7.8	ng	377078	5	13.69	969074	20.0
unknown13.18	13.18	4.9	ng	237081	5	13.69	969074	20.0
Heptafluorobutyri...	13.55	4.6	ng	223461	5	13.69	969074	20.0
Hexatriacontane	14.46	3.1	ng	133031	6	15.04	845952	20.0
Eicosane	15.82	2.1	ng	89834	6	15.04	845952	20.0