LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

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-BF110316.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	1.767	5	7	56	rVB	1905492	6198175	100.00%	10.268%
2	4.819	271	274	286	rBV	647722	1225608	19.77%	2.030%
3	5.207	306	308	310	rBV	52247	83114	1.34%	0.138%
4	5.264	310	313	316	rBV	4346200	4820918	77.78%	7.986%
5	6.327	403	406	413	rBV	4344744	5800134	93.58%	9.608%
6	6.442	413	416	418	rBV	5028073	5320918	85.85%	8.815%
7	6.670	434	436	438	rBV	1131017	1074540	17.34%	1.780%
8	6.830	447	450	452	rBV	3142377	4189239	67.59%	6.940%
9	7.242	483	486	488	rBV	3043060	3311464	53.43%	5.486%
10	7.950	546	548	551	rBV	1219249	1370844	22.12%	2.271%
11	9.036	640	643	646	rBV	5243797	5341125	86.17%	8.848%
12	9.436	675	678	680	rBV	963185	821649	13.26%	1.361%
13	9.710	699	702	704	rBV	1815760	1739901	28.07%	2.882%
14	10.122	736	738	740	rBV	41929	73593	1.19%	0.122%
15	10.156	740	741	743	rVB	125431	90330	1.46%	0.150%
16	10.373	757	760	763	rBV	51232	69584	1.12%	0.115%
17	10.499	768	771	774	rBV	3297174	3627046	58.52%	6.009%
18	10.625	780	782	786	rVB	171306	208430	3.36%	0.345%
19	11.071	820	821	823	rBV	141477	141524	2.28%	0.234%
20	11.185	829	831	835	rBV2	1385073	1777326	28.67%	2.944%
21	11.265	835	838	842	rVB3	59329	95683	1.54%	0.159%
22	11.448	849	854	856	rBV4	25123	68982	1.11%	0.114%
23	11.493	856	858	861	rBV	89152	129762	2.09%	0.215%
24	11.734	877	879	883	rVB4	28413	72671	1.17%	0.120%
25	11.802	883	885	890	rVB3	52678	88120	1.42%	0.146%
26	11.905	893	894	898	rVB	79657	68238	1.10%	0.113%
27	12.396	935	937	939	rBV	473489	435492	7.03%	0.721%
28	12.625	954	957	959	rBV	315881	405044	6.53%	0.671%
29	12.785	968	971	973	rBV	4367462	5635468	90.92%	9.336%
30	13.059	993	995	999	rVB2	35378	65368	1.05%	0.108%
31	13.677	1047	1049	1053	rVB	362174	469978	7.58%	0.779%
32	13.825	1059	1062	1063	rBV	1088152	1393735	22.49%	2.309%
33	14.317	1102	1105	1111	rBV2	130423	244490	3.94%	0.405%
34	14.648	1127	1134	1147	rVB2	309809	1711473	27.61%	2.835%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

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-BF110316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.820	1147	1149	1153	rBV	141238	230496	3.72%	0.382%
36	15.082	1170	1172	1175	rVB	58283	95293	1.54%	0.158%
37	15.151	1175	1178	1180	rBV	80337	122766	1.98%	0.203%
38	15.197	1180	1182	1185	rBV	756223	1079130	17.41%	1.788%
39	15.631	1217	1220	1221	rBV	41605	62429	1.01%	0.103%
40	15.665	1221	1223	1228	rVB3	74370	140692	2.27%	0.233%
41	15.814	1234	1236	1241	rVB2	59288	110989	1.79%	0.184%
42	16.191	1267	1269	1275	rVB3	44099	97179	1.57%	0.161%
43	16.488	1293	1295	1300	rVB2	52042	117503	1.90%	0.195%
44	16.877	1326	1329	1336	rBV	45341	138175	2.23%	0.229%

Sum of corrected areas: 60364618

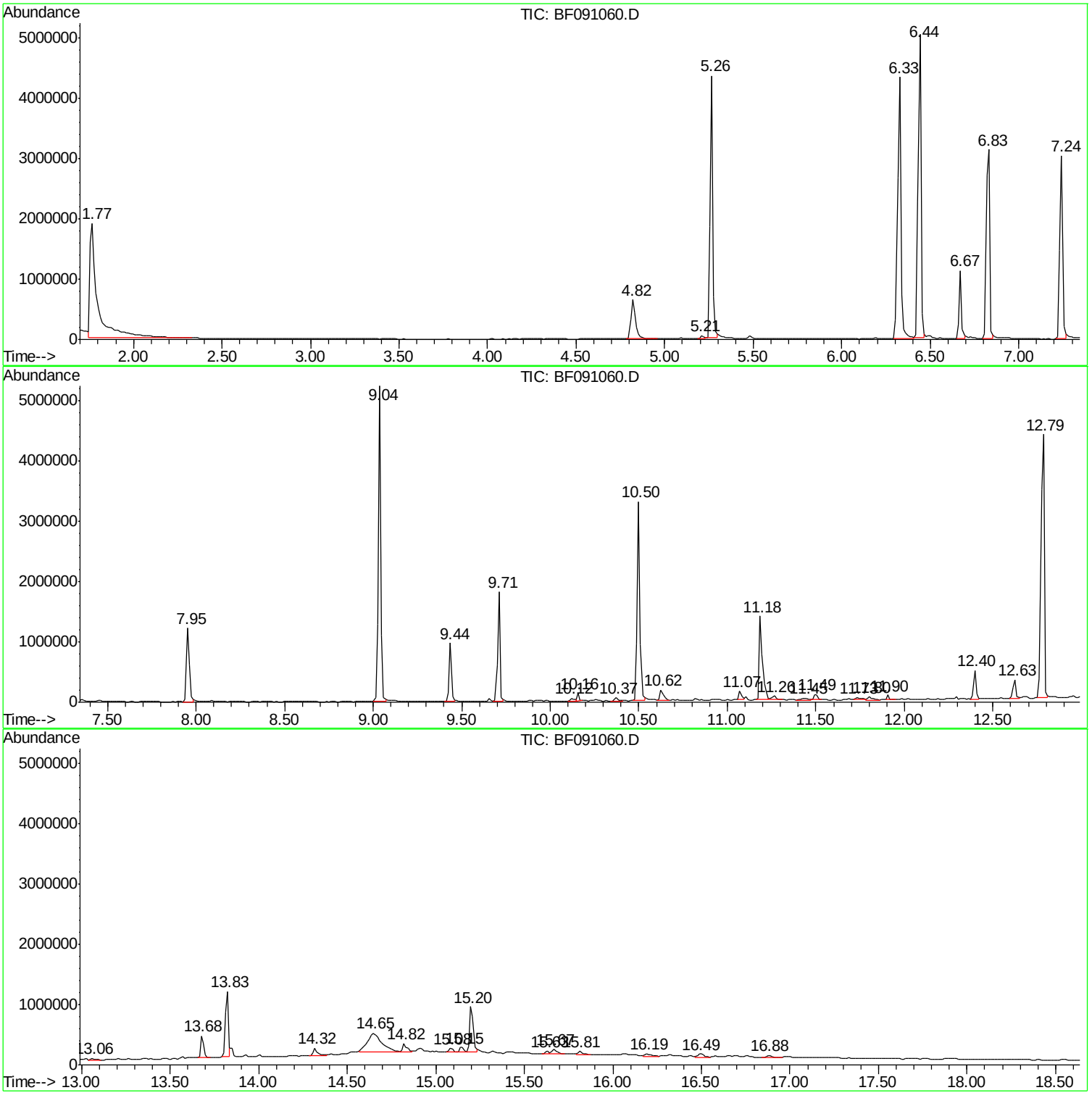
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

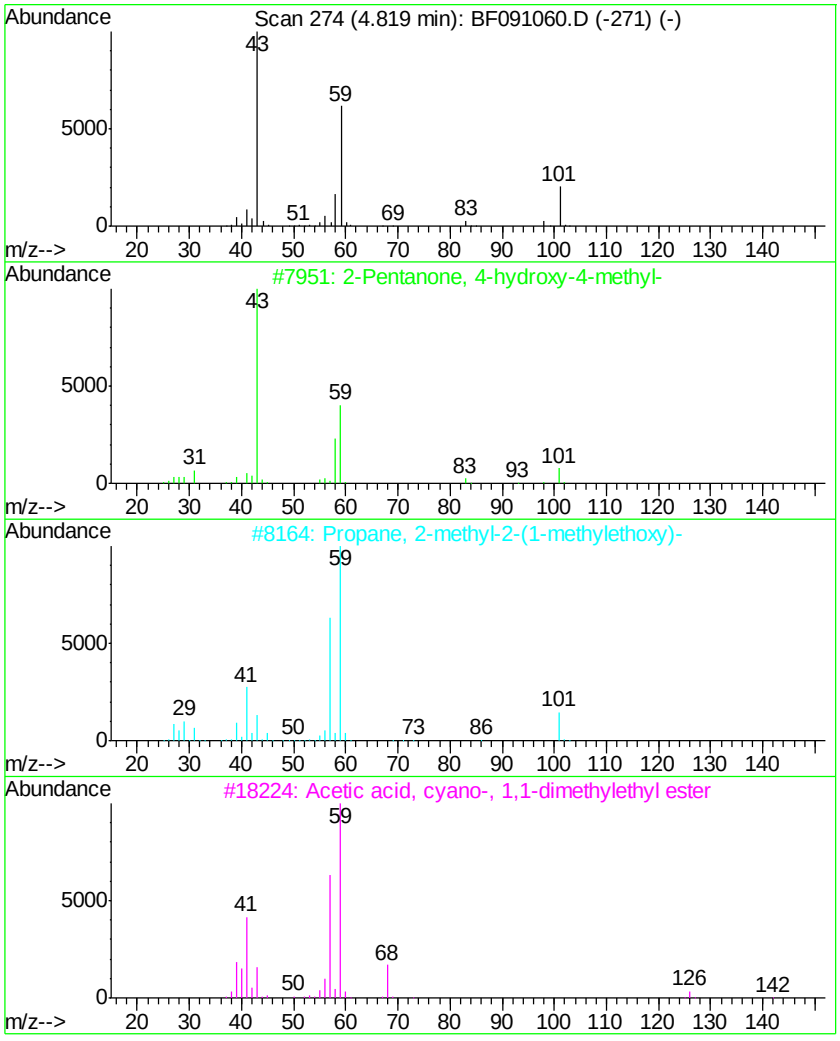
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

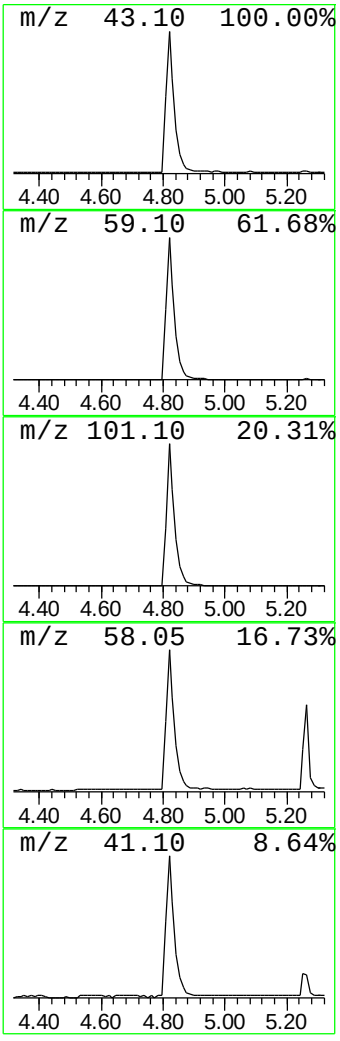
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	22.81 ng	1225610	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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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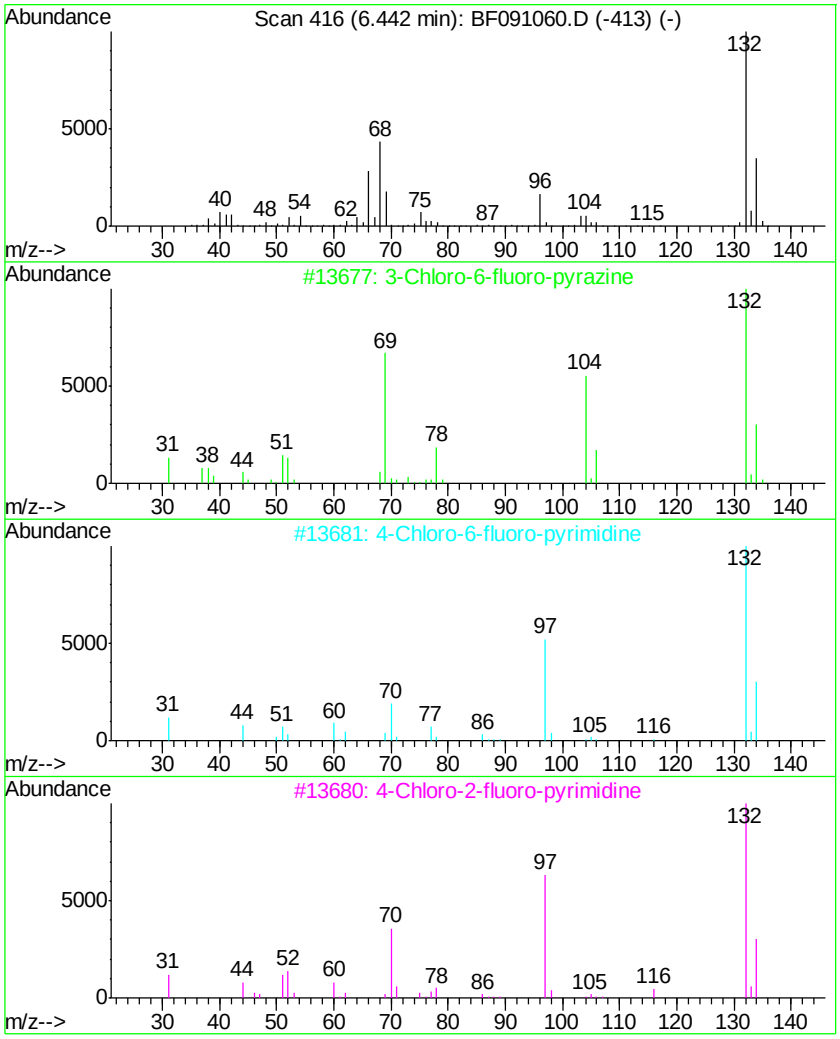
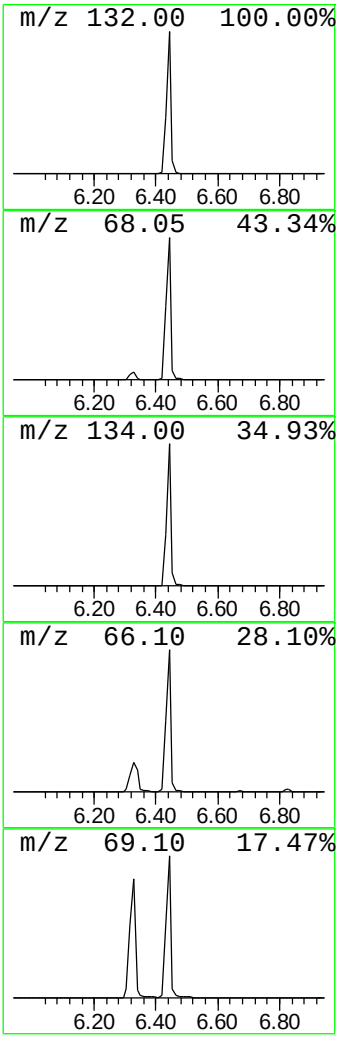
Peak Number 3 unknown6.44 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	99.04 ng	5320920	1,4-Dichlorobenzene-d4	6.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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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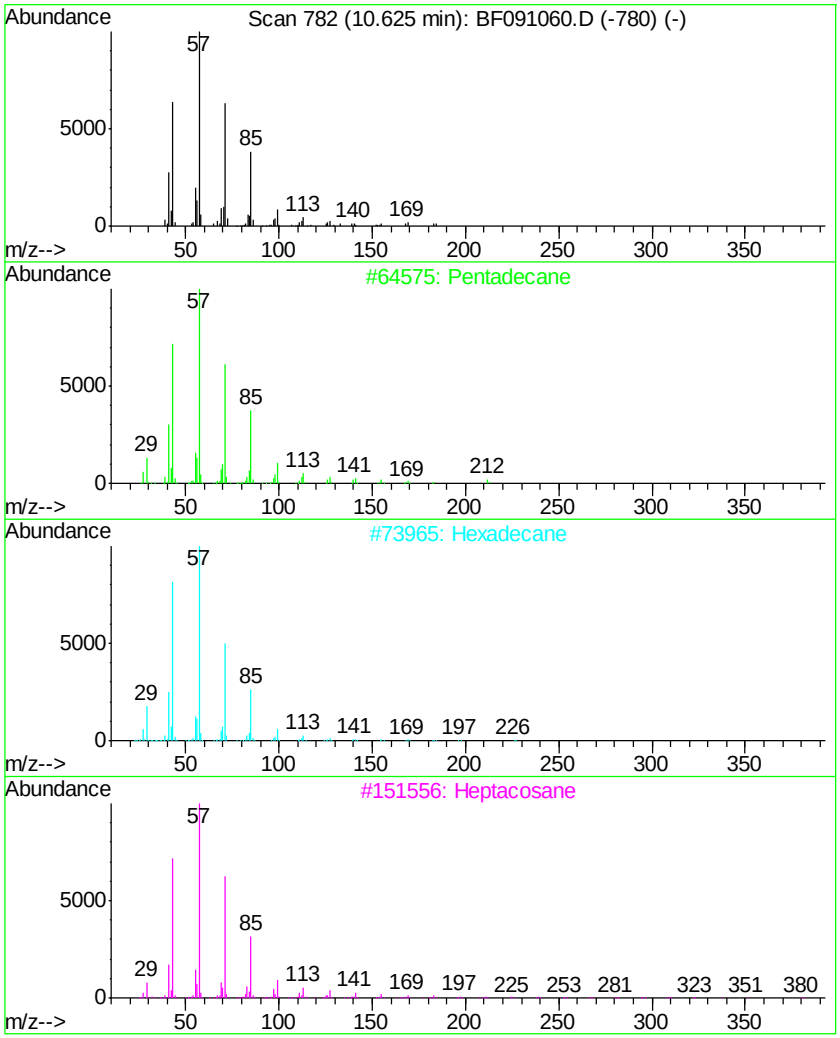
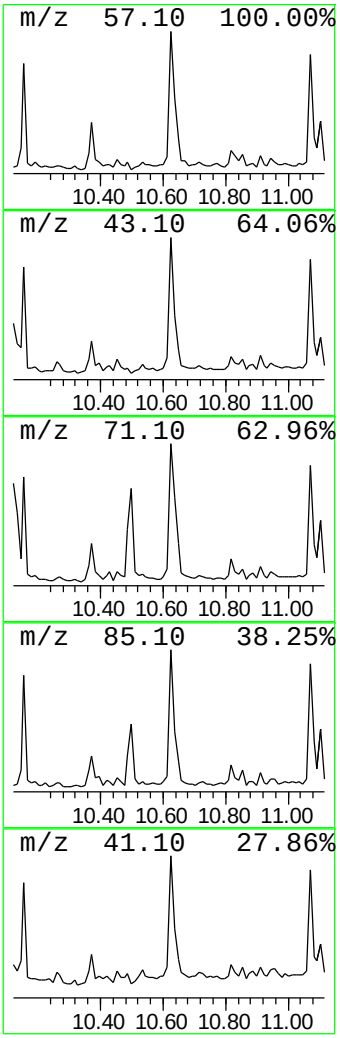
Peak Number 5 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	2.35 ng	208430	Phenanthrene-d10	11.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Heptadecane	240	C17H36	000629-78-7	83
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

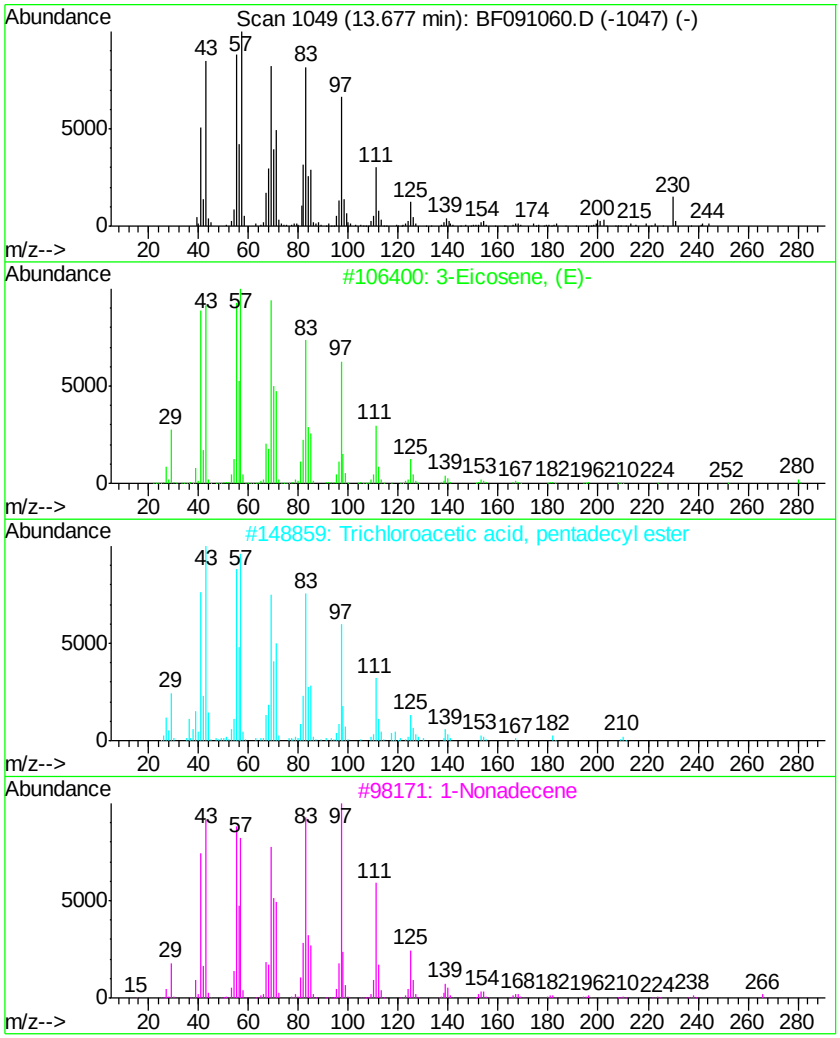
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

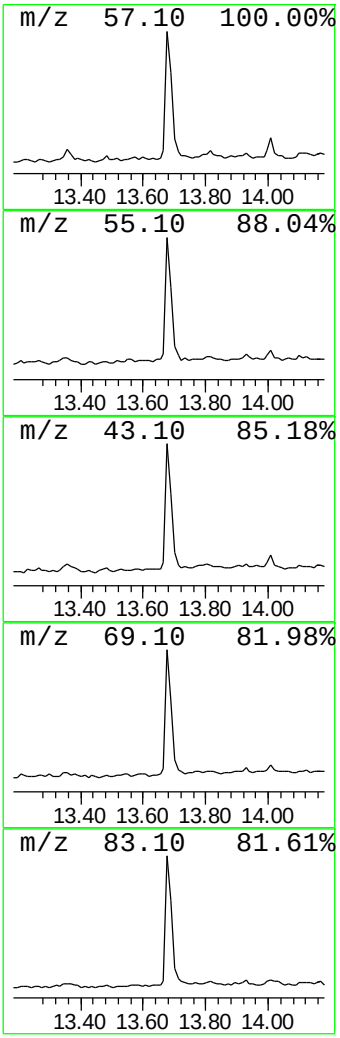
****

Peak Number 6 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	6.74 ng	469978	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

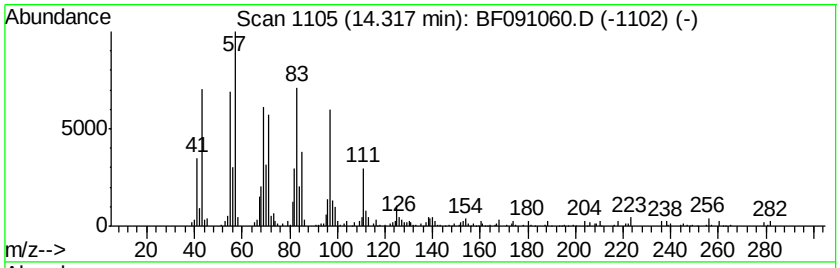
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

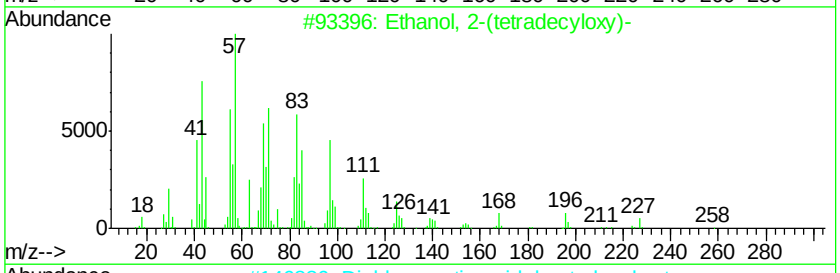
****

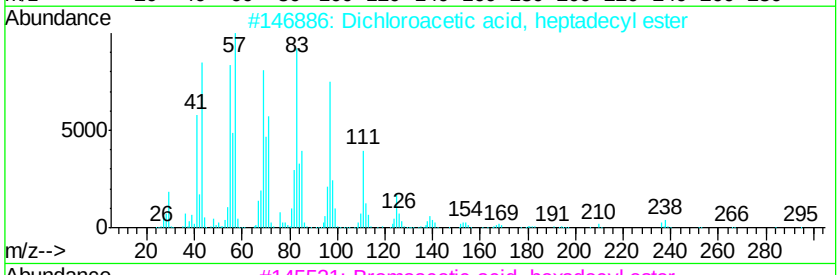
Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 7

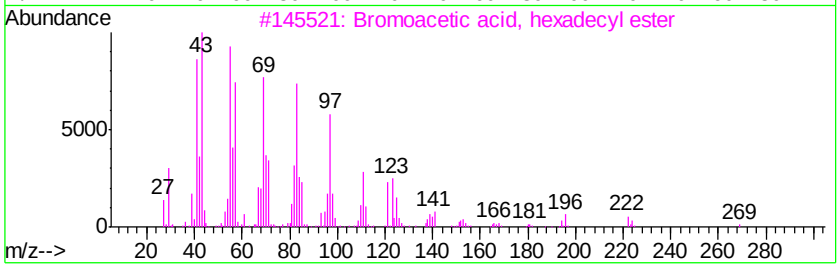
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	3.51 ng	244490	Chrysene-d12	13.83

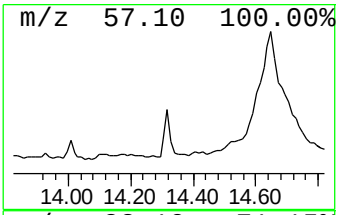
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	76
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76
5	1-Octadecanol	270	C18H38O	000112-92-5	76

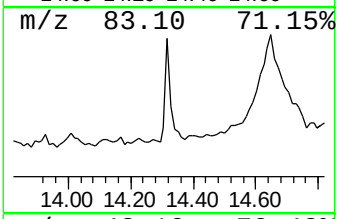


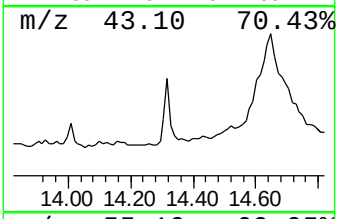


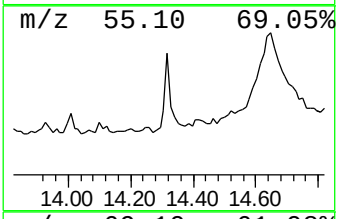


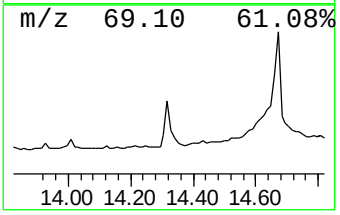












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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

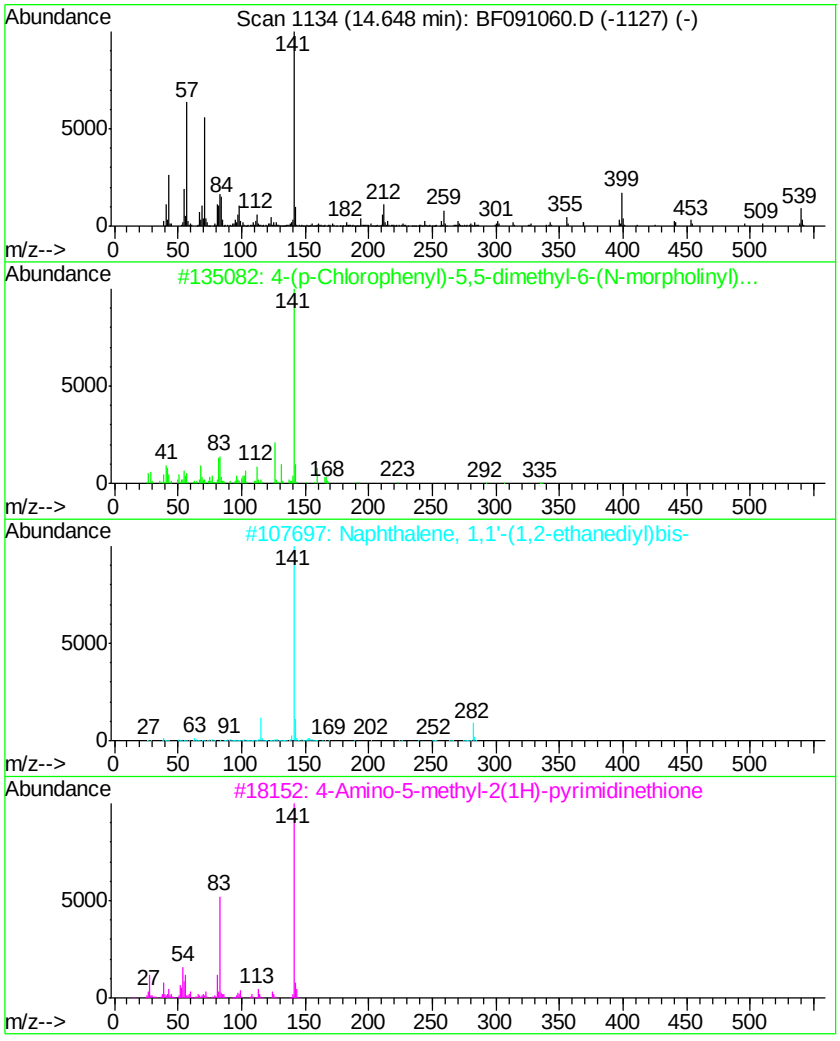
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

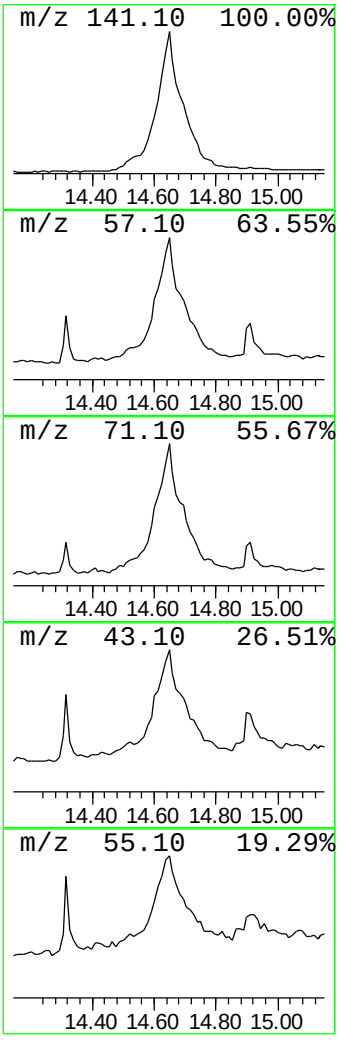
****

Peak Number 8 unknown14.65 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	31.72 ng	1711470	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(p-Chlorophenyl)-5,5-dimethyl-...	335	C18H22ClNO3	1000101-49-5	38
2	Naphthalene, 1,1'-(1,2-ethanediy...	282	C22H18	015374-45-5	38
3	4-Amino-5-methyl-2(1H)-pyrimidin...	141	C5H7N3S	007390-56-9	32
4	Piperidin-4-ol, 1,2,5-trimethyl-...	283	C19H25NO	329789-67-5	32
5	2-Fluorobenzoic acid, heptadecyl...	378	C24H39FO2	1000282-96-6	32





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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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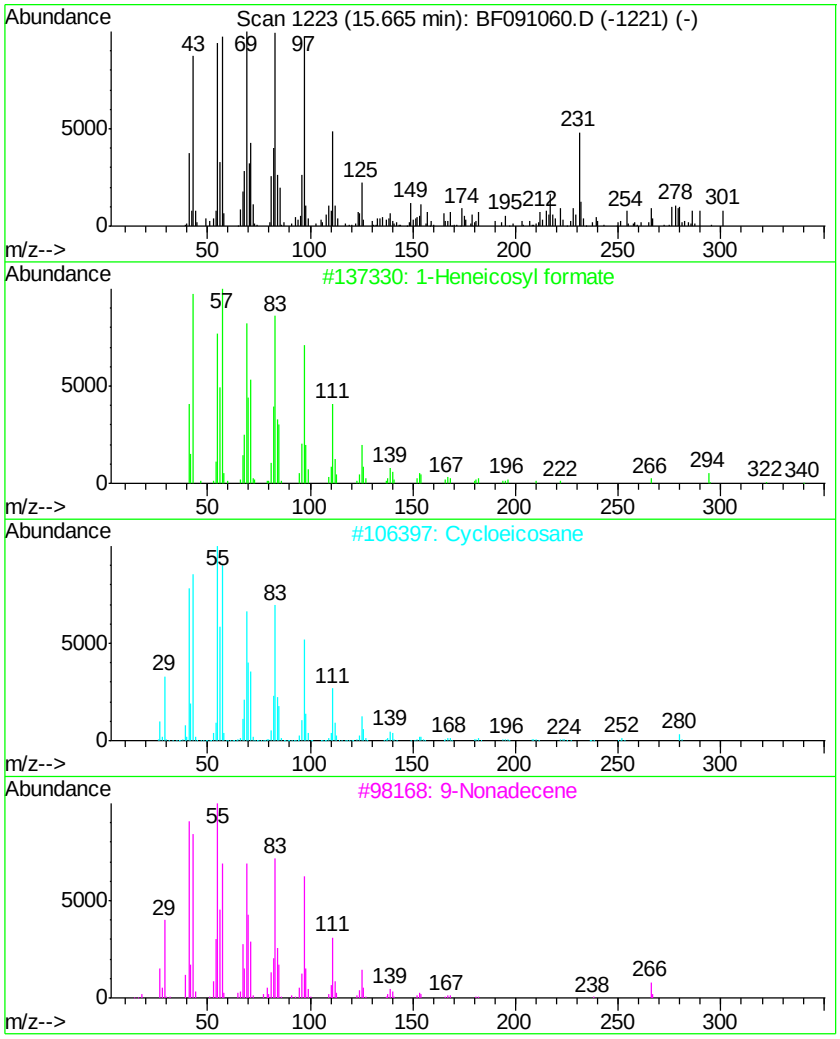
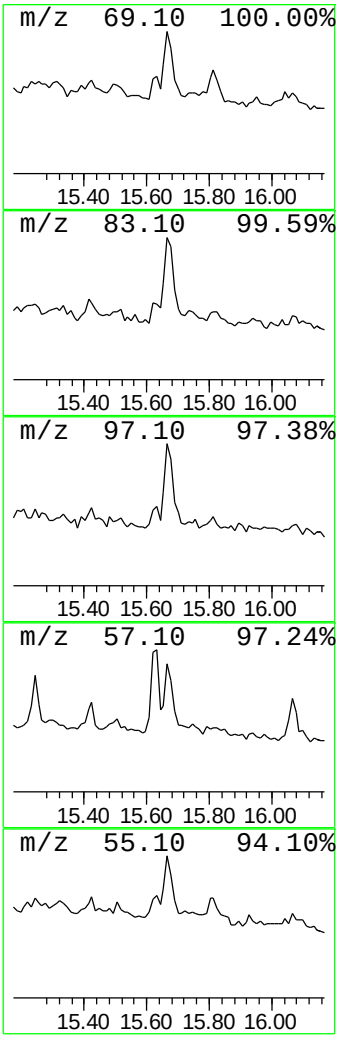
Peak Number 9 1-Heneicosyl formate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	2.61 ng	140692	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	68
2	Cycloeicosane	280	C20H40	000296-56-0	49
3	9-Nonadecene	266	C19H38	031035-07-1	49
4	3-Decene, 2,2-dimethyl-, (E)-	168	C12H24	055499-02-0	43
5	Cyclopentane, 1-butyl-2-propyl-	168	C12H24	062199-50-2	42





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Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

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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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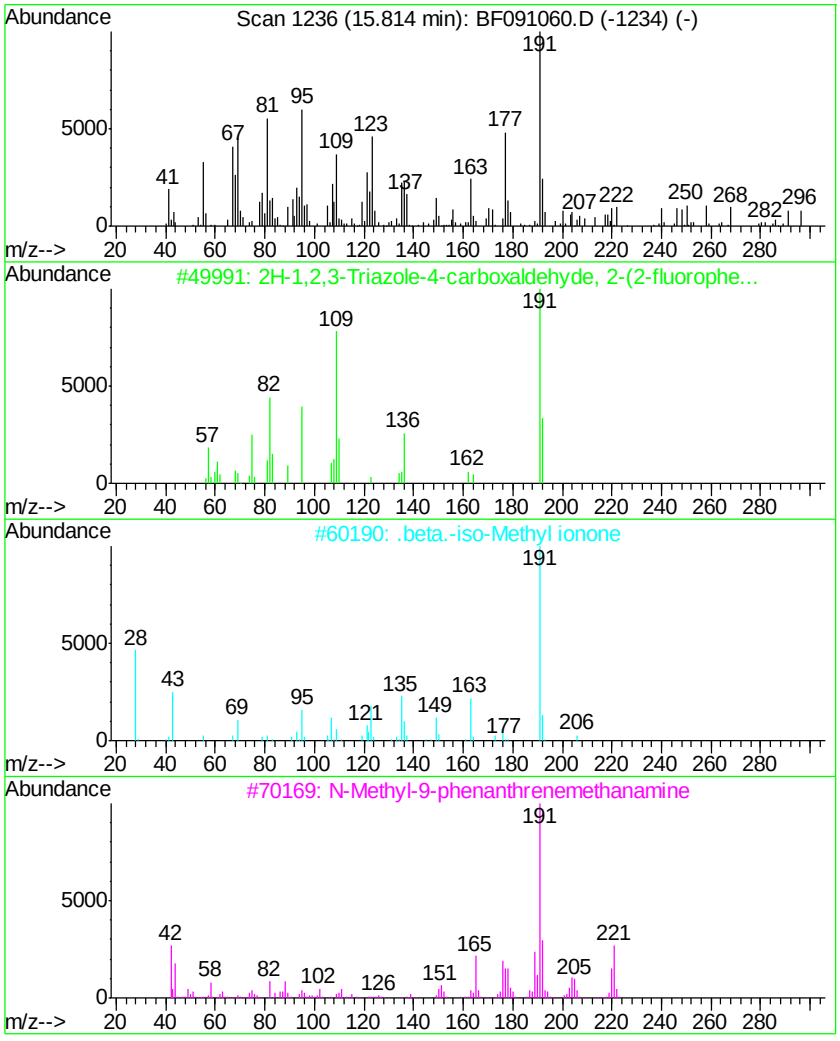
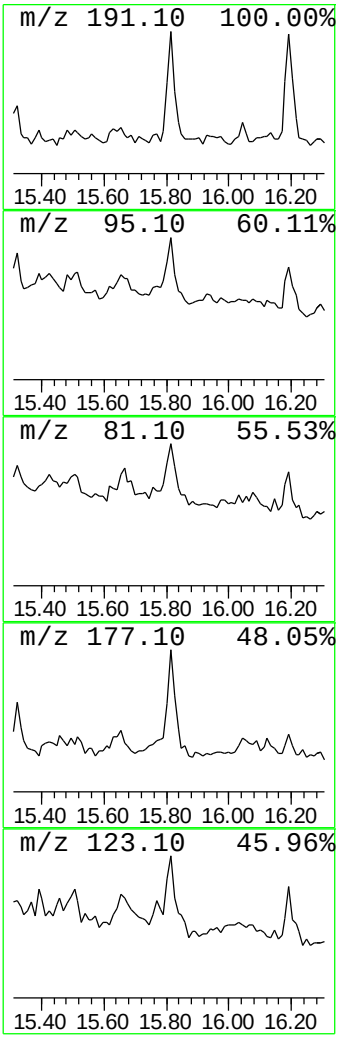
Peak Number 10 unknown15.81 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	2.06 ng	110989	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	35
2	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	30
3	N-Methyl-9-phenanthrenemethanamine	221	C16H15N	076532-36-0	27
4	1,4-Methanoazulen-9-one, decahyd...	220	C15H24O	000465-26-9	25
5	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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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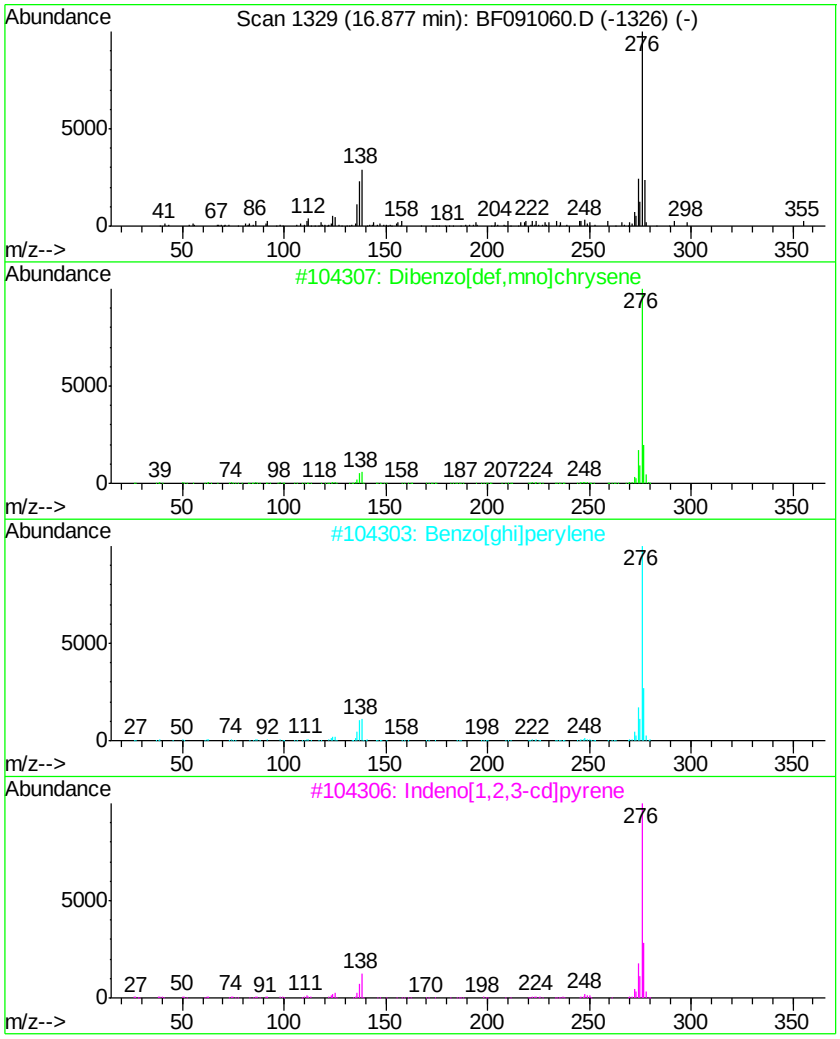
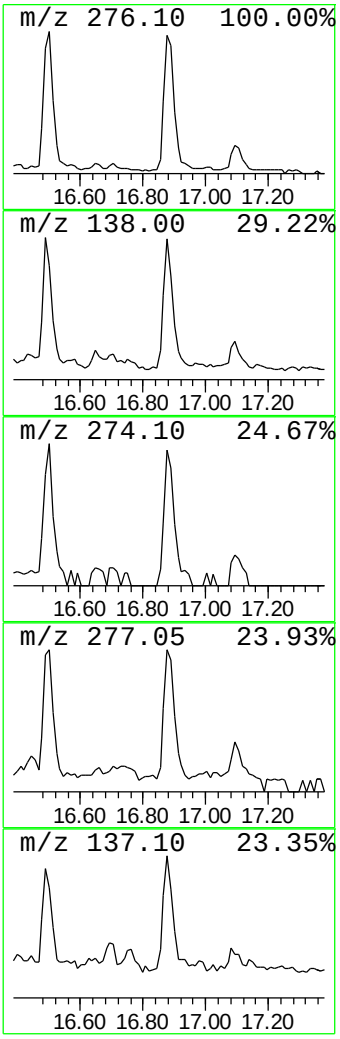
Peak Number 12 Dibenzo[def,mno]chrysene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.88	2.56 ng	138175	Perylene-d12	15.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	95
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	94
3	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	91
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	87
5	6H-Pyrido[4,3-b]carbazole, 9-met...	276	C18H16N2O	010371-86-5	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110716\
Data File : BF091060.D
Acq On : 7 Nov 2016 17:12
Operator : UM/SJ
Sample : H5539-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : V001-BF016-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110316.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...	4.82	22.8	ng	1225610	1	6.67	1074540	20.0
unknown6.44	6.44	99.0	ng	5320920	1	6.67	1074540	20.0
Pentadecane	10.62	2.4	ng	208430	4	11.18	1777330	20.0
3-Eicosene, (E)-	13.68	6.7	ng	469978	5	13.83	1393740	20.0
Ethanol, 2-(tetra...	14.32	3.5	ng	244490	5	13.83	1393740	20.0
unknown14.65	14.65	31.7	ng	1711470	6	15.20	1079130	20.0
1-Heneicosyl formate	15.67	2.6	ng	140692	6	15.20	1079130	20.0
unknown15.81	15.81	2.1	ng	110989	6	15.20	1079130	20.0
Dibenzo[def,mno]c...	16.88	2.6	ng	138175	6	15.20	1079130	20.0