LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090984.D
Acq On : 2 Nov 2016 17:18
Operator : UM/SJ
Sample : H5509-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-87-8.4-16.0

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-BF102616.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	2.178	3	8	15	rBV	2802251	15698560	100.00%	26.761%
2	3.561	125	129	145	rBV	341191	746279	4.75%	1.272%
3	4.327	194	196	206	rVB	230280	344242	2.19%	0.587%
4	4.876	242	244	258	rBV	503630	691582	4.41%	1.179%
5	5.321	280	283	285	rBV	3159540	3356346	21.38%	5.722%
6	5.653	310	312	315	rBV	184462	194492	1.24%	0.332%
7	6.361	372	374	383	rBV	1802006	2627554	16.74%	4.479%
8	6.487	383	385	388	rVV	3885840	4399725	28.03%	7.500%
9	6.579	391	393	400	rVB	121745	167997	1.07%	0.286%
10	6.716	403	405	408	rBV	852950	989812	6.31%	1.687%
11	6.876	416	419	422	rBV	4160023	4052892	25.82%	6.909%
12	7.287	452	455	458	rBV	2641463	3747446	23.87%	6.388%
13	7.779	494	498	506	rVB3	80375	216590	1.38%	0.369%
14	8.007	516	518	526	rVB	1034011	987619	6.29%	1.684%
15	9.093	609	613	615	rBV	4836939	5118830	32.61%	8.726%
16	9.482	645	647	649	rBV	162830	163877	1.04%	0.279%
17	9.756	669	671	674	rBV	887511	1157409	7.37%	1.973%
18	10.556	738	741	743	rBV	2904510	3113690	19.83%	5.308%
19	11.242	797	801	804	rBV2	1307515	1506721	9.60%	2.569%
20	12.842	937	941	943	rBV	3764297	5469606	34.84%	9.324%
21	13.882	1029	1032	1034	rBV	743117	986880	6.29%	1.682%
22	14.728	1100	1106	1108	rBV3	173216	637026	4.06%	1.086%
23	14.911	1120	1122	1127	rVB2	116068	250109	1.59%	0.426%
24	15.277	1151	1154	1158	rVB	736538	1127955	7.19%	1.923%
25	15.471	1169	1171	1173	rBV2	94241	225326	1.44%	0.384%
26	16.248	1238	1239	1243	rVB	119475	195432	1.24%	0.333%
27	16.362	1246	1249	1252	rVV2	87181	192962	1.23%	0.329%
28	17.163	1316	1319	1322	rBV3	83028	294114	1.87%	0.501%

Sum of corrected areas: 58661073

LSC Report - Integrated Chromatogram

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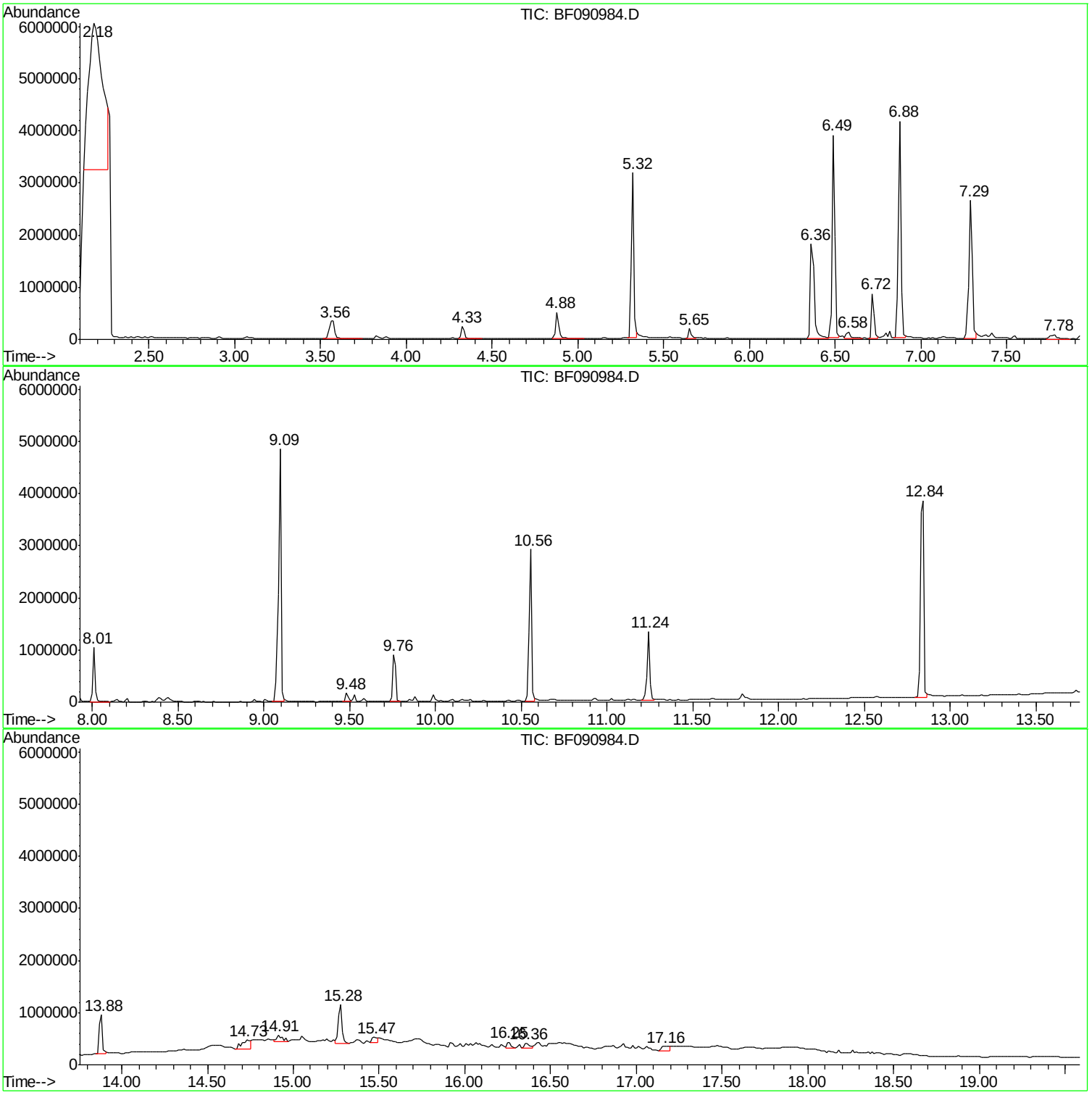
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GW-87-8.4-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-87-8.4-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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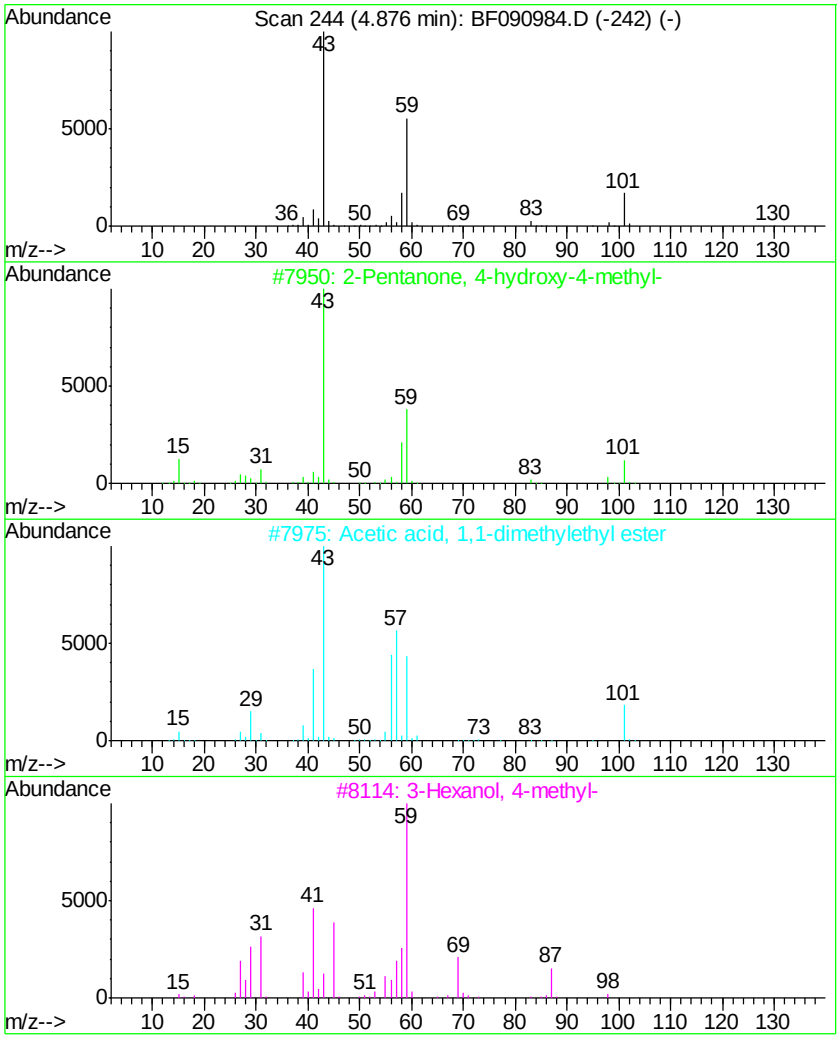
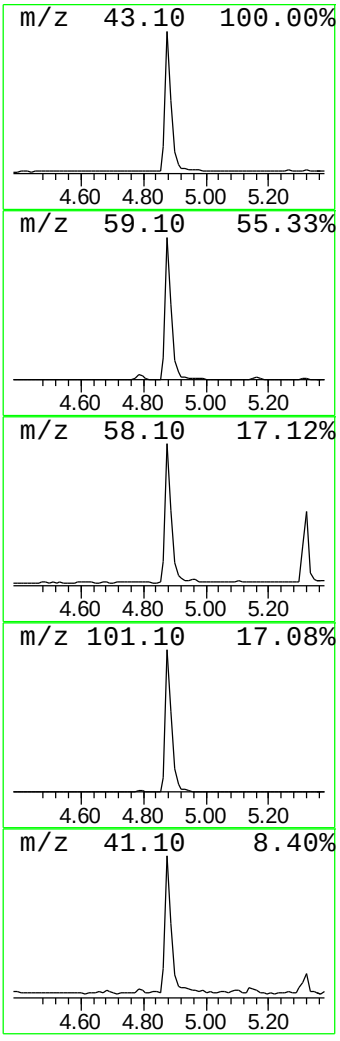
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	13.97 ng	691582	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Sample : H5509-18
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Instrument : BNA_F
ClientSampleId : GW-87-8.4-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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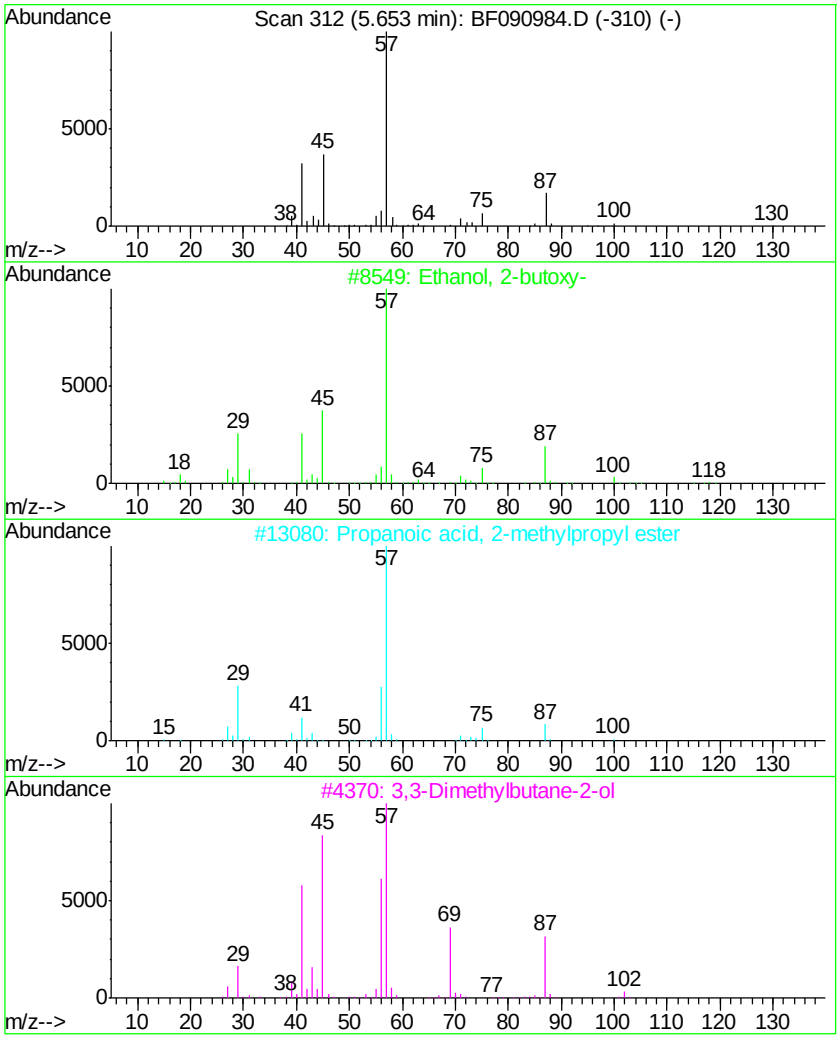
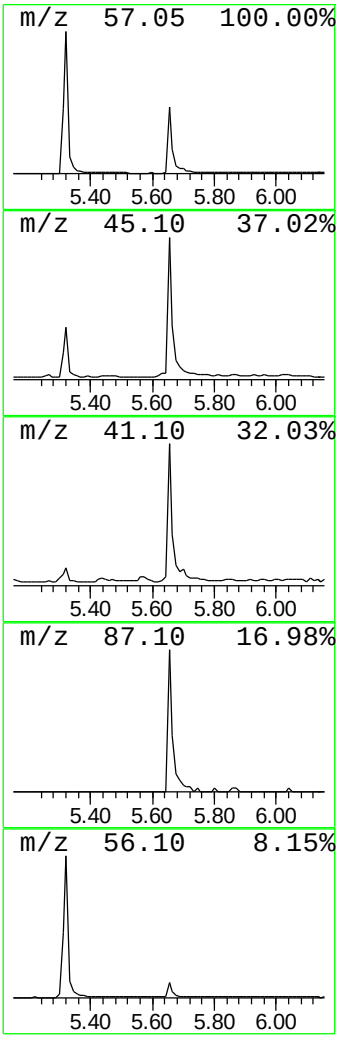
Peak Number 5 Ethanol, 2-butoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.65	3.93 ng	194492	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2	Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	37
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	33
4	n-Butyl ether	130	C8H18O	000142-96-1	32
5	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	23





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Instrument : BNA_F
ClientSampleId : GW-87-8.4-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
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TIC Library : C:\DATABASE\NIST02.L
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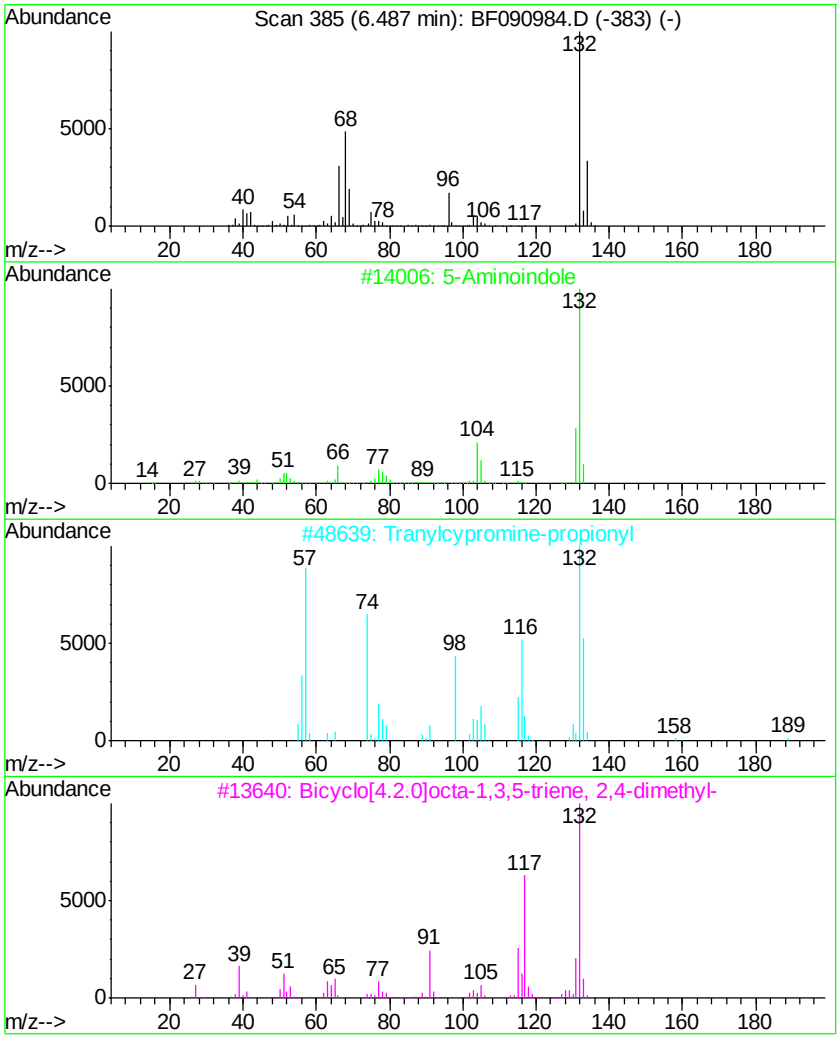
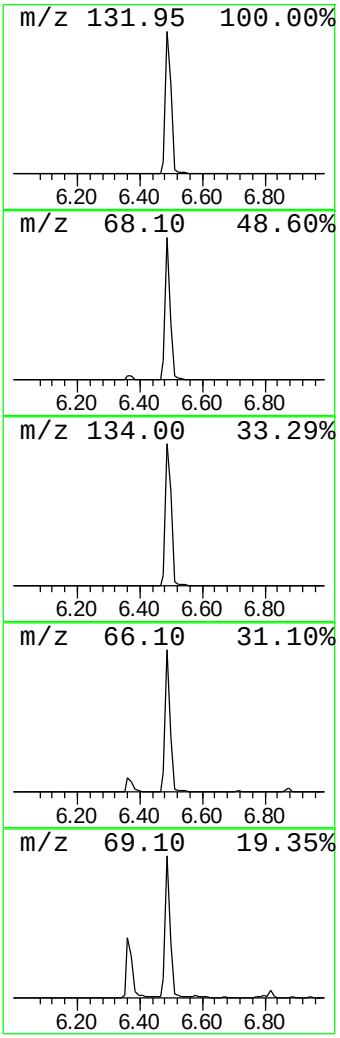
Peak Number 6 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	88.90 ng	4399730	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	9





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Misc :
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Instrument : BNA_F
ClientSampleId : GW-87-8.4-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
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TIC Library : C:\DATABASE\NIST02.L
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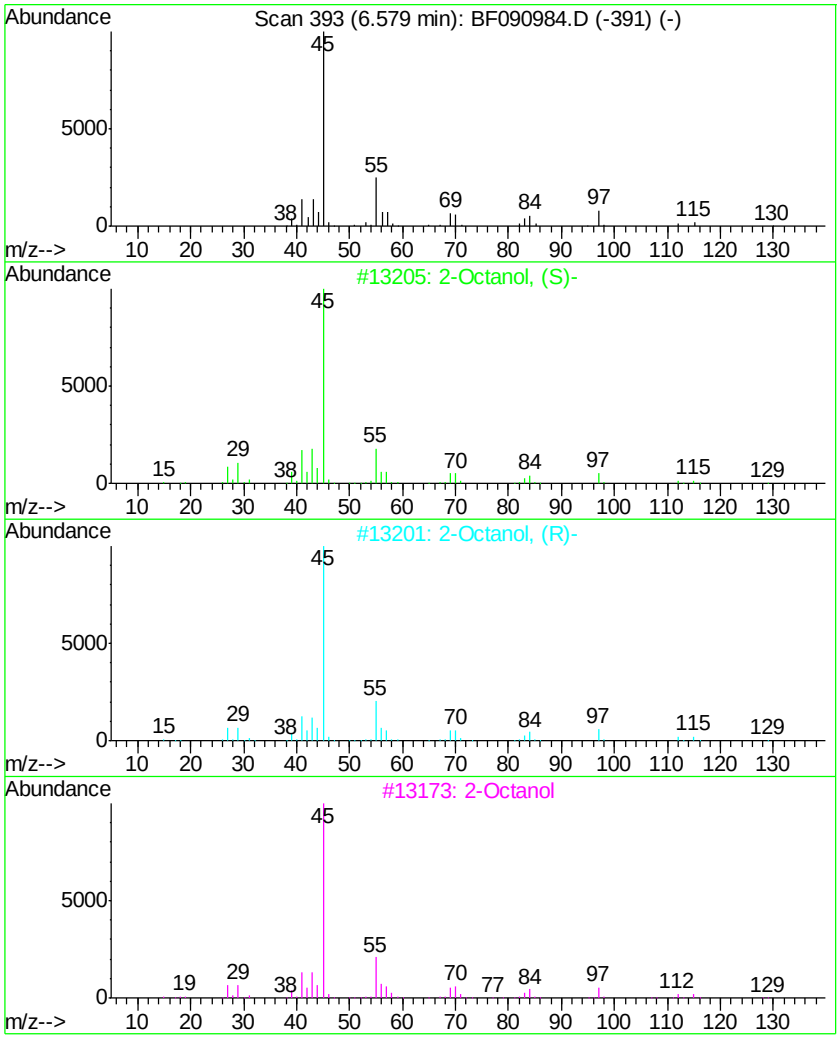
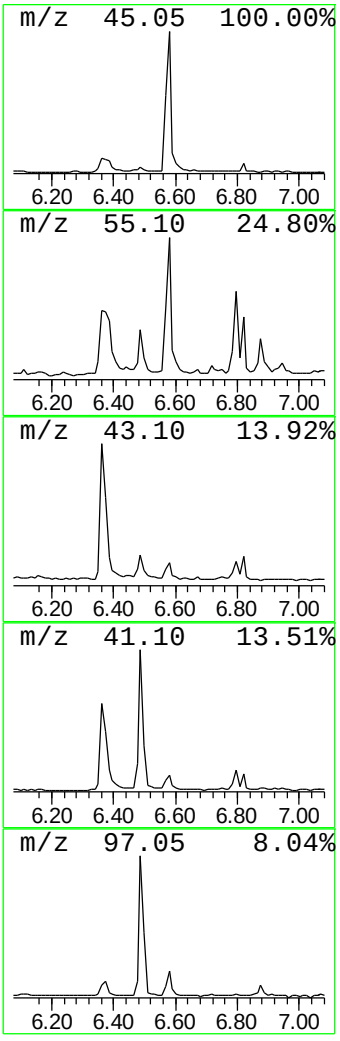
Peak Number 7 2-Octanol, (S)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	3.39 ng	167997	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol, (S)-	130	C8H18O	006169-06-8	83
2	2-Octanol, (R)-	130	C8H18O	005978-70-1	83
3	2-Octanol	130	C8H18O	000123-96-6	83
4	2-Heptanol, 6-methyl-	130	C8H18O	004730-22-7	78
5	2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	72





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Instrument : BNA_F
ClientSampleId : GW-87-8.4-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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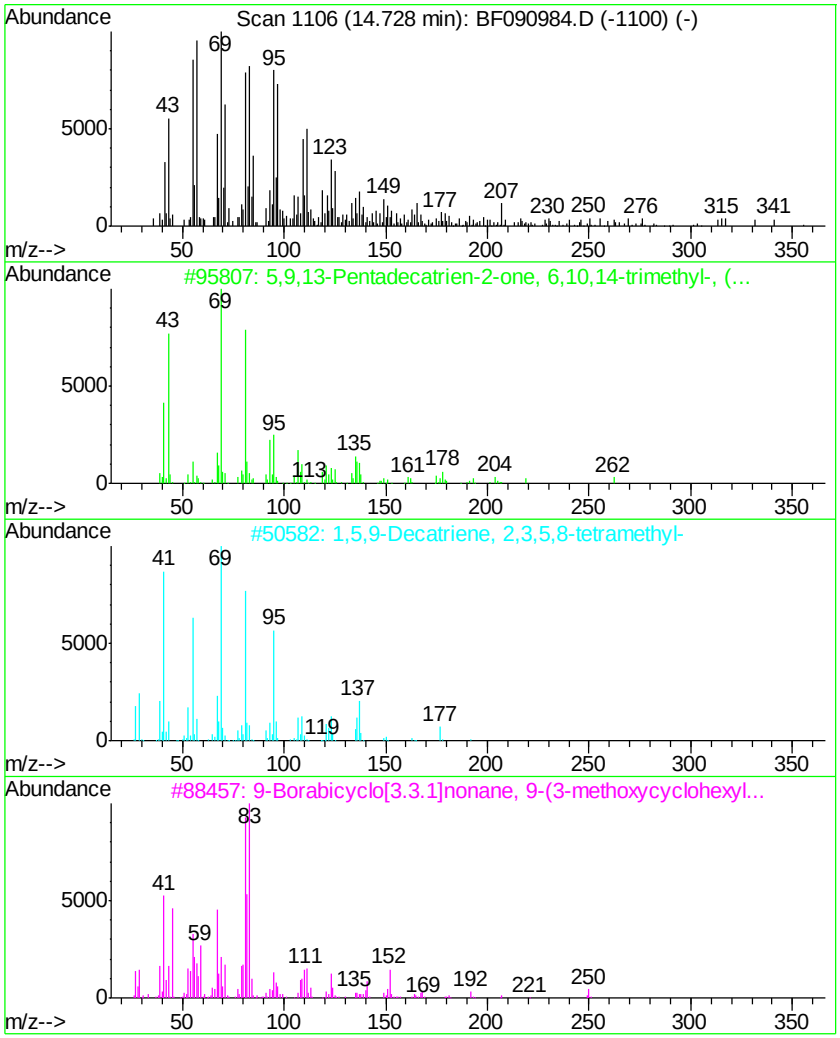
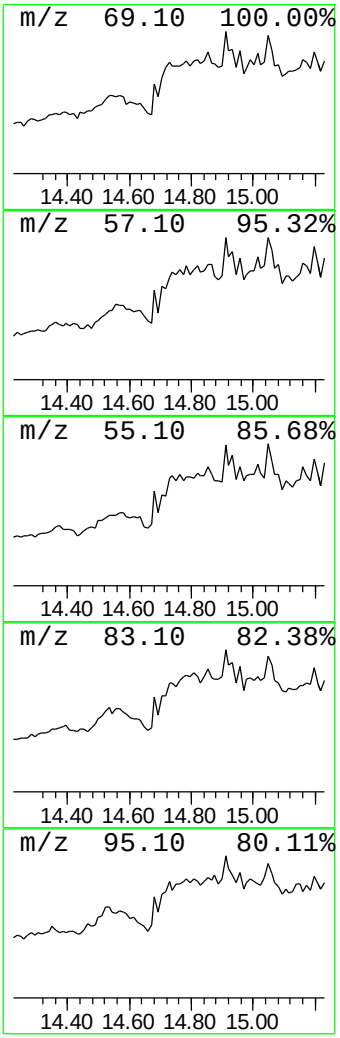
Peak Number 9 5,9,13-Pentadecatrien-2-one... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	11.30 ng	637026	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	52
2	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	46
3	9-Borabicyclo[3.3.1]nonane, 9-(3...	250	C15H27BO2	1000150-57-9	30
4	2,2,4-Trimethyl-3-(3,8,12,16-tet...	428	C30H52O	1000194-01-4	30
5	Oxirane, 2-decyl-3-(5-methylhexy...	282	C19H38O	057457-72-4	30





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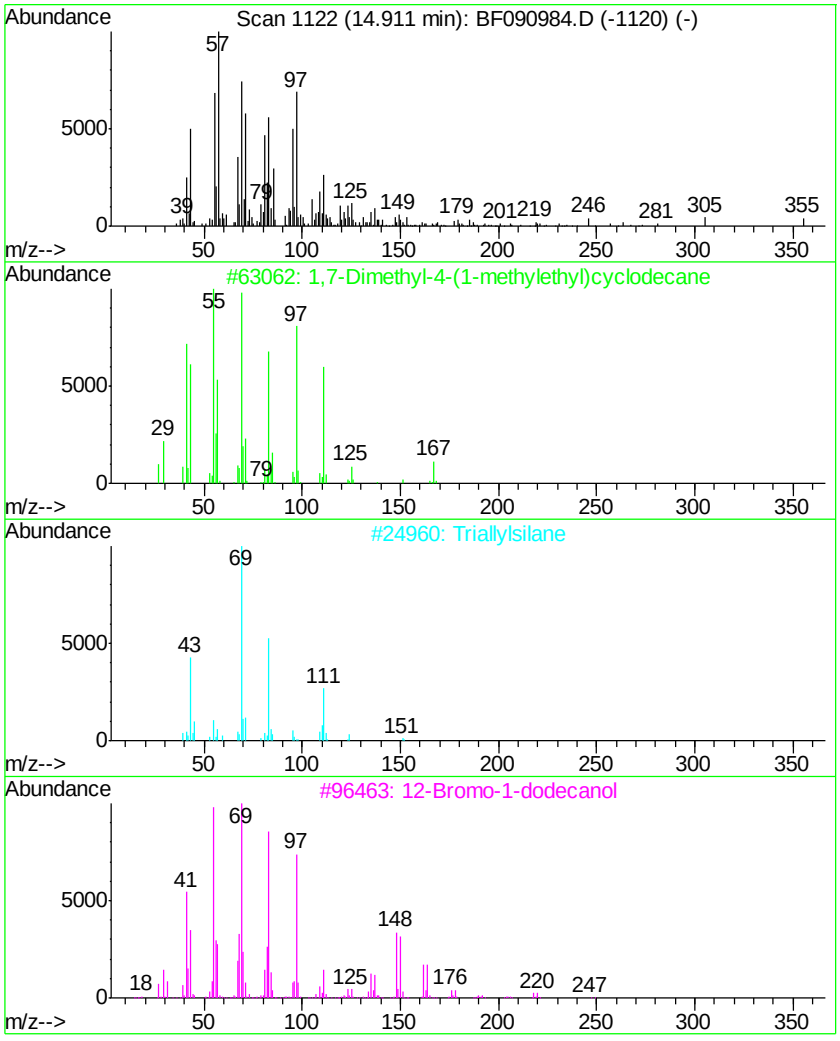
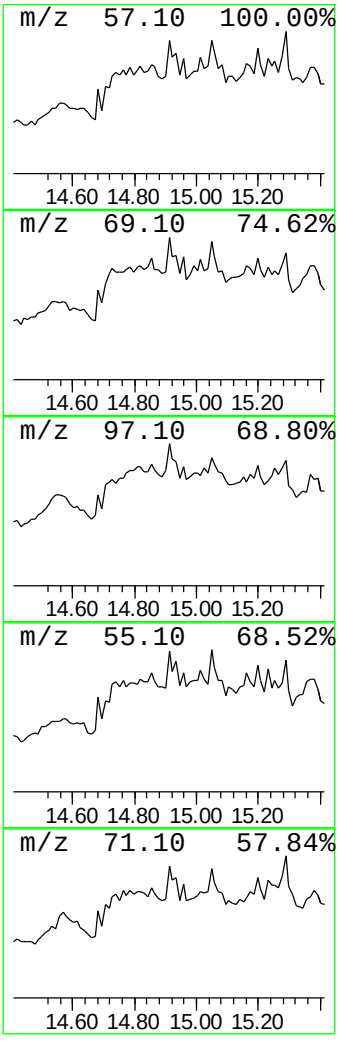
Peak Number 10 unknown14.91 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	4.43 ng	250109	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	49
2	Triallylsilane	152	C9H16Si	001116-62-7	45
3	12-Bromo-1-dodecanol	264	C12H25BrO	003344-77-2	43
4	Vinyltris(cyclopropyl)silane	178	C11H18Si	1000109-97-3	38
5	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	30





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TIC Library : C:\DATABASE\NIST02.L
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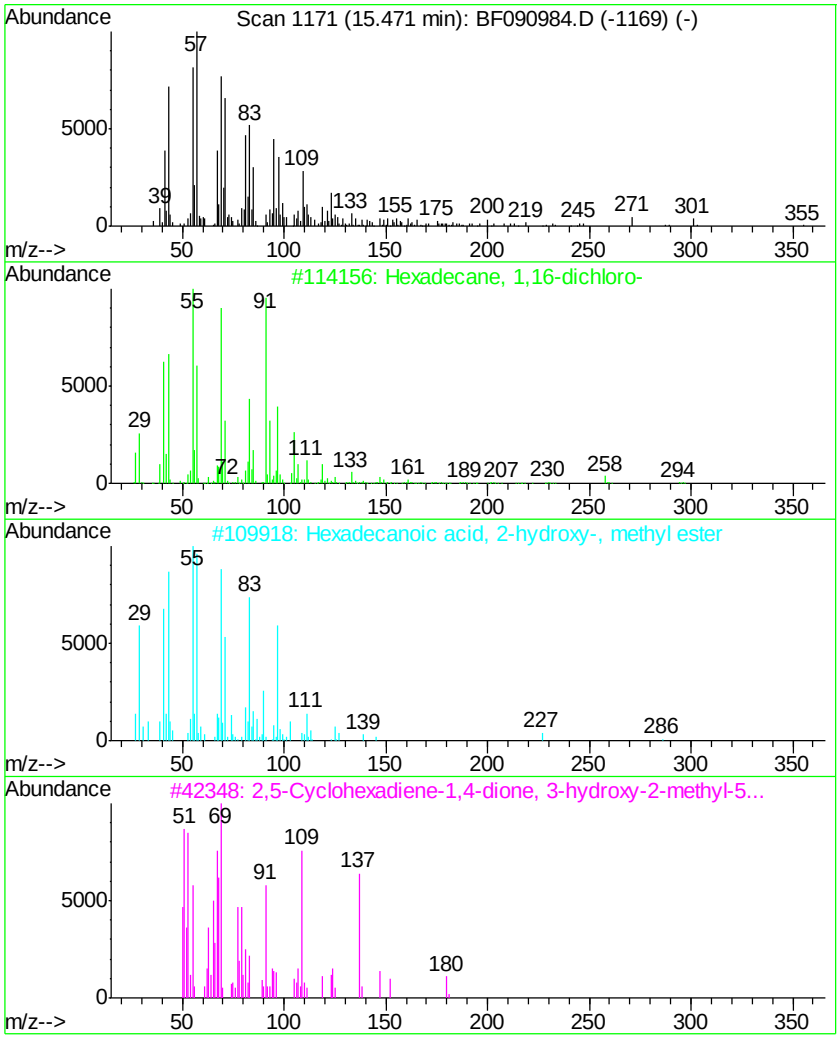
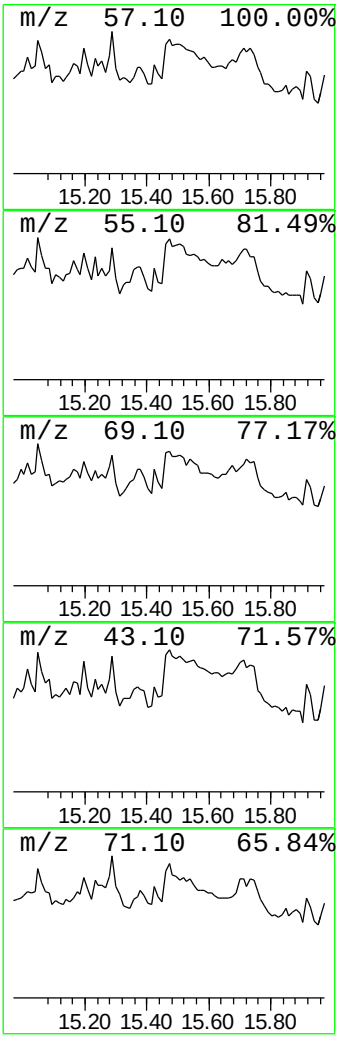
Peak Number 11 unknown15.47 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	4.00 ng	225326	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1,16-dichloro-	294	C16H32Cl2	007735-39-9	46
2	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	43
3	2,5-Cyclohexadiene-1,4-dione, 3-...	180	C10H12O3	004586-58-7	35
4	(-)-trans-Pinane	138	C10H18	033626-25-4	30
5	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	25





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TIC Library : C:\DATABASE\NIST02.L
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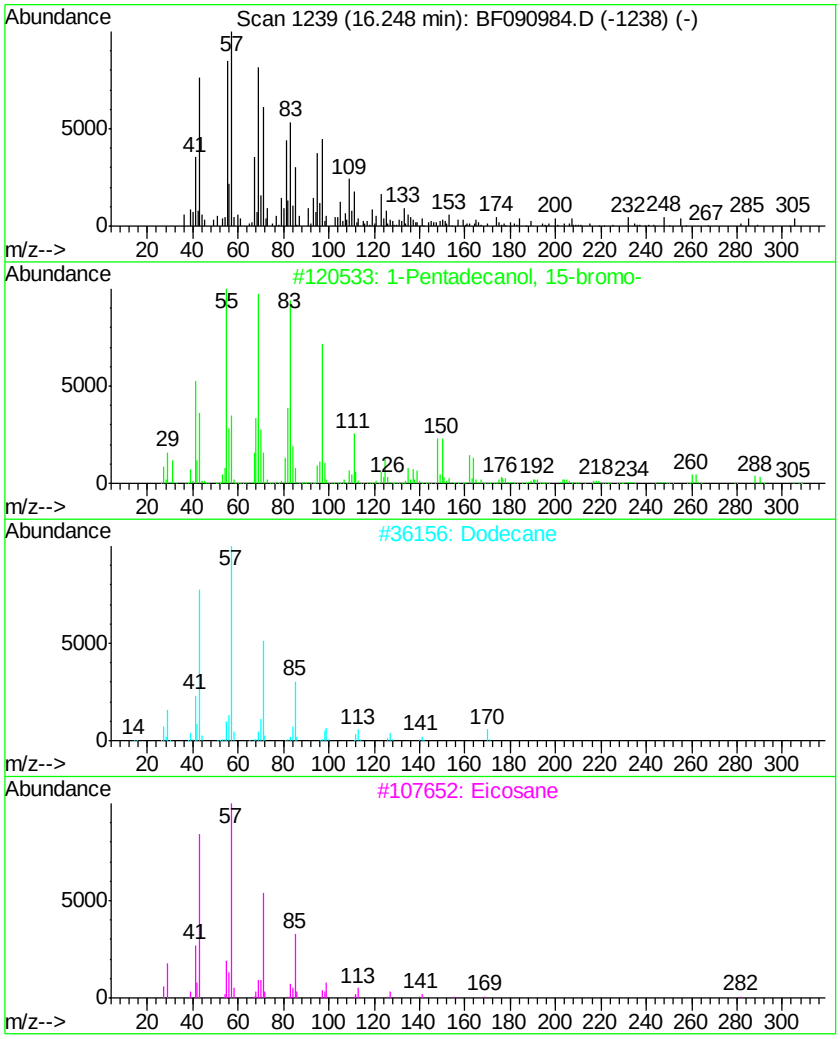
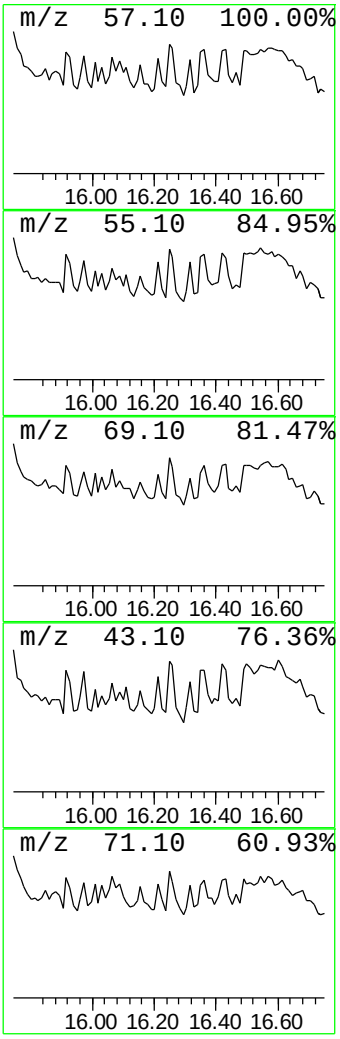
Peak Number 12 unknown16.25 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.25	3.47 ng	195432	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanol, 15-bromo-	306	C15H31BrO	059101-27-8	49
2	Dodecane	170	C12H26	000112-40-3	25
3	Eicosane	282	C20H42	000112-95-8	25
4	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	25
5	1-Hexyl-2-nitrocyclohexane	213	C12H23NO2	118252-04-3	22





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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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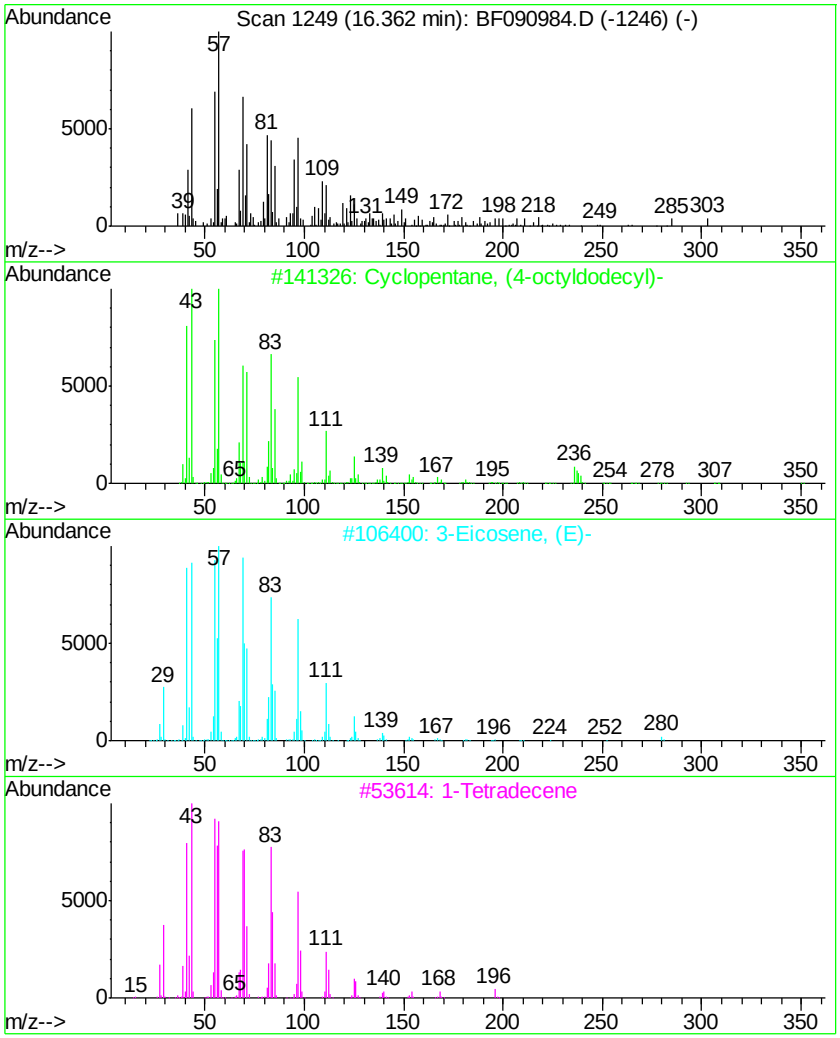
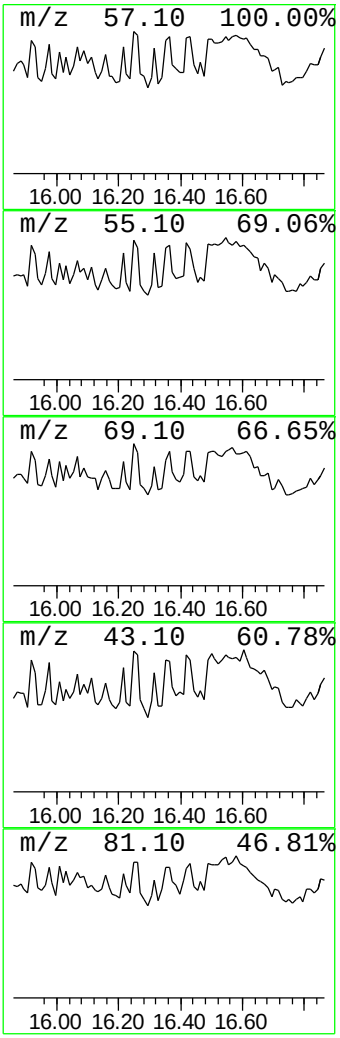
Peak Number 13 Cyclopentane, (4-octyldodec... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	3.42 ng	192962	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	59
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	58
3	1-Tetradecene	196	C14H28	001120-36-1	46
4	2-Tetradecene, (E)-	196	C14H28	035953-53-8	46
5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	38





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ClientSampleId : GW-87-8.4-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

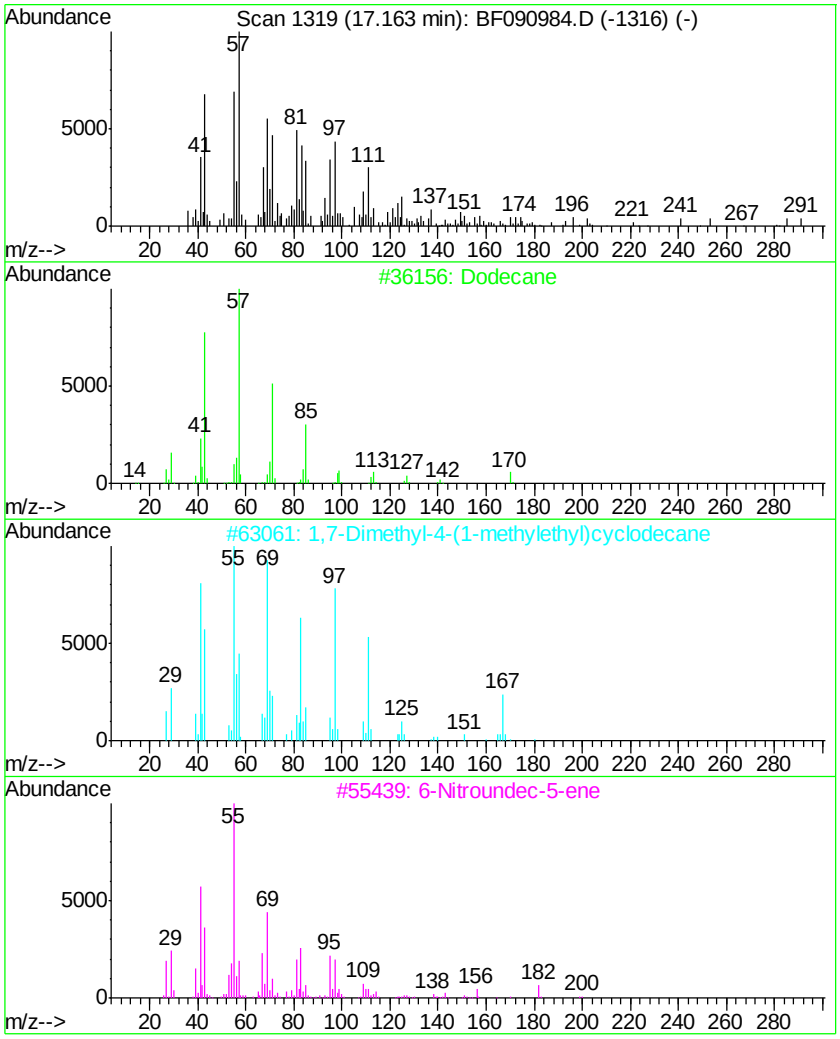
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

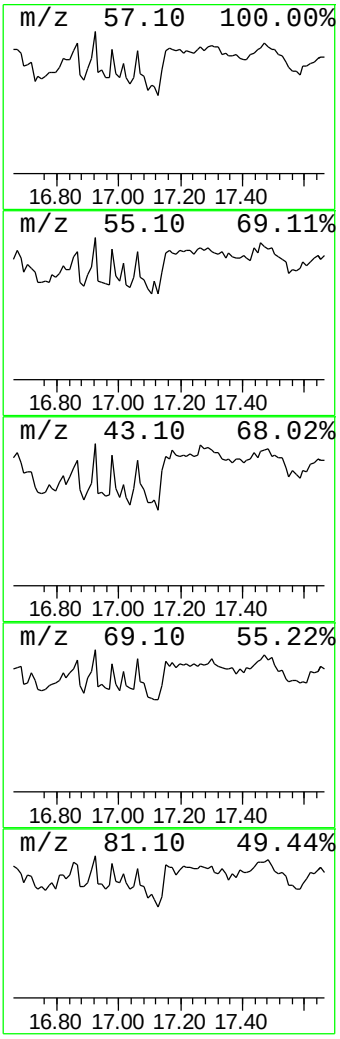
****

Peak Number 14 Dodecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	5.22 ng	294114	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	60
2	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	49
3	6-Nitroundec-5-ene	199	C11H21NO2	1000192-40-3	43
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	30
5	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF110216\
Data File : BF090984.D
Acq On : 2 Nov 2016 17:18
Operator : UM/SJ
Sample : H5509-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-87-8.4-16.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102616.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...	4.88	14.0	ng	691582	1	6.72	989812	20.0
Ethanol, 2-butoxy-	5.65	3.9	ng	194492	1	6.72	989812	20.0
unknown6.49	6.49	88.9	ng	4399730	1	6.72	989812	20.0
2-Octanol, (S)-	6.58	3.4	ng	167997	1	6.72	989812	20.0
5,9,13-Pentadecat...	14.73	11.3	ng	637026	6	15.28	1127960	20.0
unknown14.91	14.91	4.4	ng	250109	6	15.28	1127960	20.0
unknown15.47	15.47	4.0	ng	225326	6	15.28	1127960	20.0
unknown16.25	16.25	3.5	ng	195432	6	15.28	1127960	20.0
Cyclopentane, (4-...	16.36	3.4	ng	192962	6	15.28	1127960	20.0
Dodecane	17.16	5.2	ng	294114	6	15.28	1127960	20.0