LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 90THAVE-SB-16(0.5-6.0)

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-BF050916.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	1.735	11	13	56	rVB	4007955	8076851	100.00%	19.834%
2	4.753	275	277	289	rBV	704576	1091262	13.51%	2.680%
3	5.210	315	317	320	rBV	2737420	3485824	43.16%	8.560%
4	5.610	350	352	362	rVB	72190	83662	1.04%	0.205%
5	6.284	408	411	414	rBV	3198751	3447613	42.69%	8.466%
6	6.387	418	420	423	rBV	3844553	3561285	44.09%	8.745%
7	6.616	437	440	442	rBV	823890	994415	12.31%	2.442%
8	6.764	451	453	456	rBV	2497593	2640938	32.70%	6.485%
9	7.187	487	490	500	rVB	2402359	2408338	29.82%	5.914%
10	7.896	550	552	555	rBV	1060378	1198440	14.84%	2.943%
11	8.650	616	618	620	rBV	334553	345031	4.27%	0.847%
12	8.982	644	647	649	rBV	3797955	3542917	43.87%	8.700%
13	9.382	680	682	684	rBV	382596	327136	4.05%	0.803%
14	9.645	703	705	708	rBV	1134611	1219450	15.10%	2.995%
15	10.091	742	744	746	rVB	122885	94448	1.17%	0.232%
16	10.433	772	774	777	rBV2	1482428	1967235	24.36%	4.831%
17	10.559	783	785	790	rVB	135291	144354	1.79%	0.354%
18	11.039	825	827	830	rVB	82363	85877	1.06%	0.211%
19	11.131	833	835	837	rBV	835007	1019790	12.63%	2.504%
20	11.679	880	883	886	rBV	186577	219363	2.72%	0.539%
21	12.548	956	959	962	rBV2	63281	103492	1.28%	0.254%
22	12.708	971	973	976	rBV	2195158	2103665	26.05%	5.166%
23	13.622	1049	1053	1059	rBV2	202963	459754	5.69%	1.129%
24	13.748	1062	1064	1067	rBV	659023	927593	11.48%	2.278%
25	13.908	1076	1078	1084	rBV	170748	260123	3.22%	0.639%
26	15.120	1181	1184	1191	rVB	668430	913206	11.31%	2.243%

Sum of corrected areas: 40722062

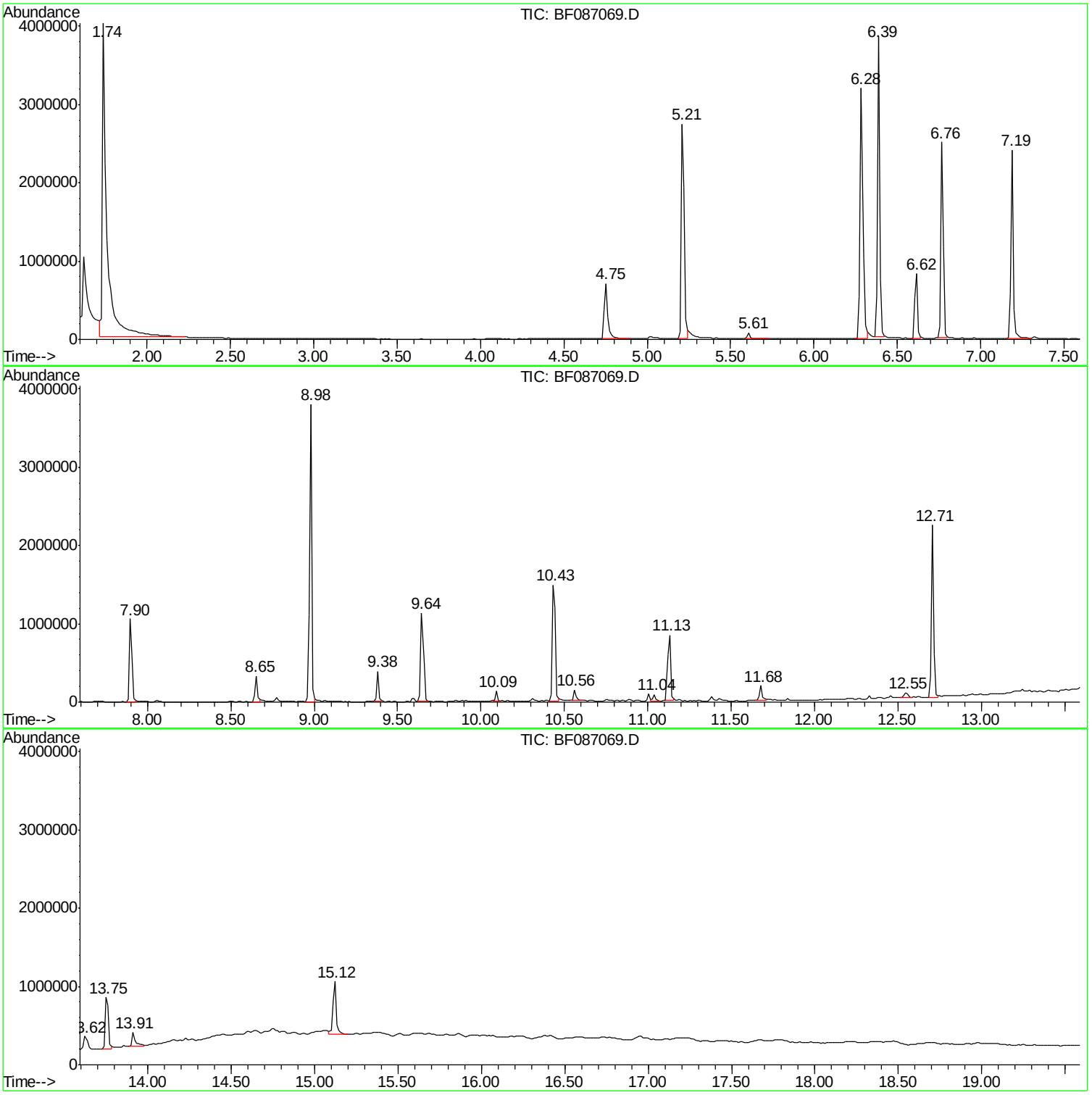
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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\BF051416\
Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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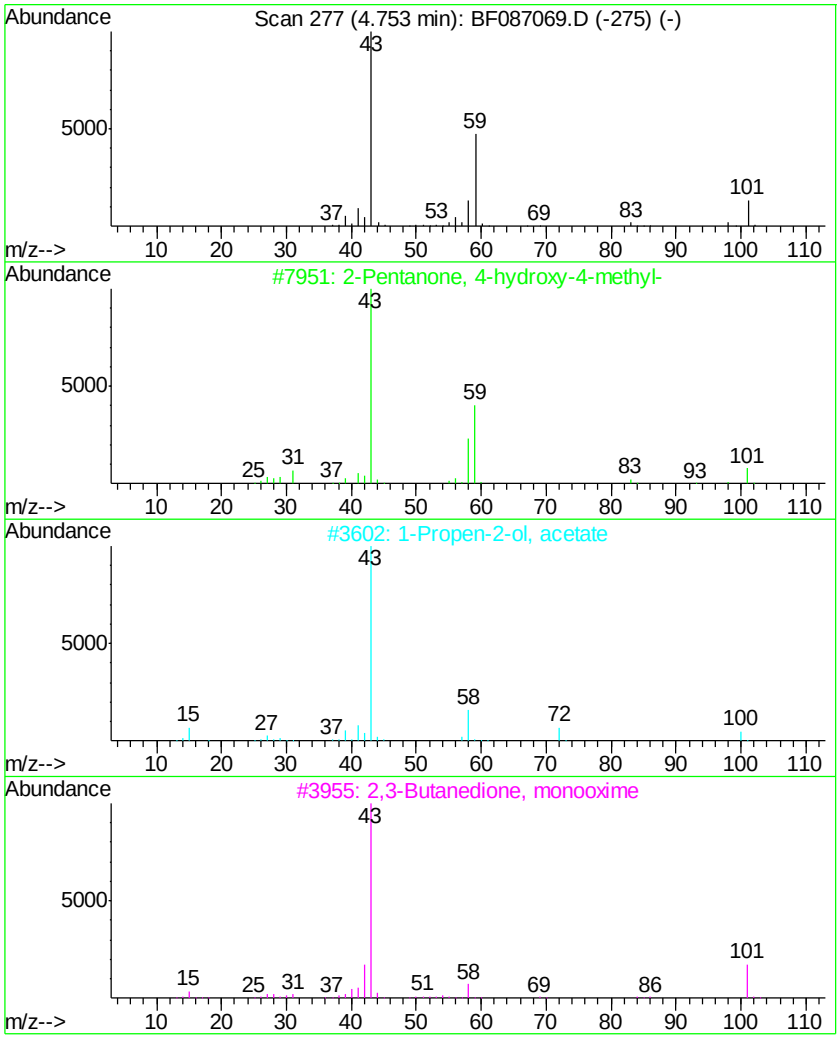
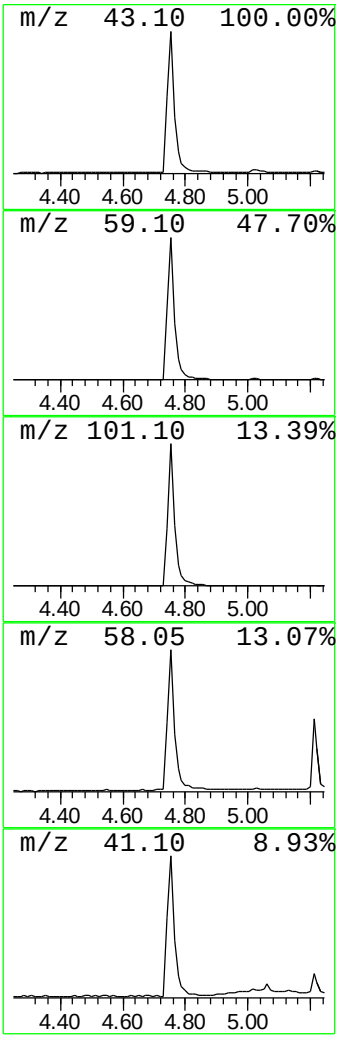
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.75	21.95 ng	1091260	1,4-Dichlorobenzene-d4	6.62

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	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7





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Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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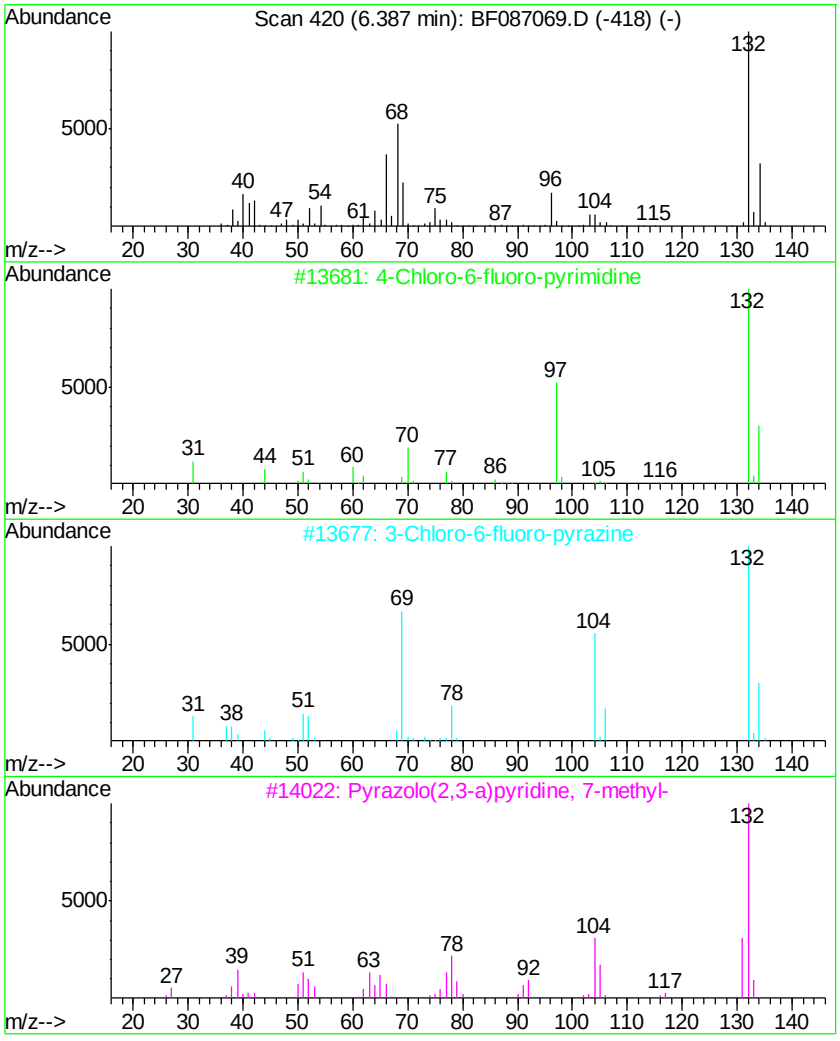
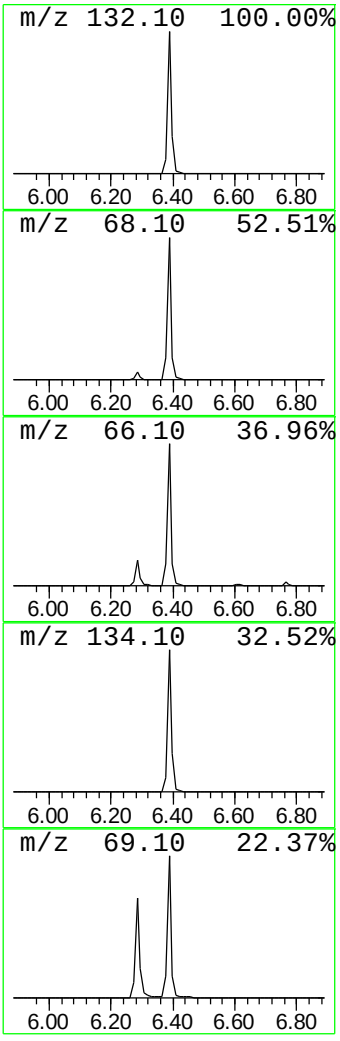
Peak Number 3 unknown6.39 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	71.63 ng	3561290	1,4-Dichlorobenzene-d4	6.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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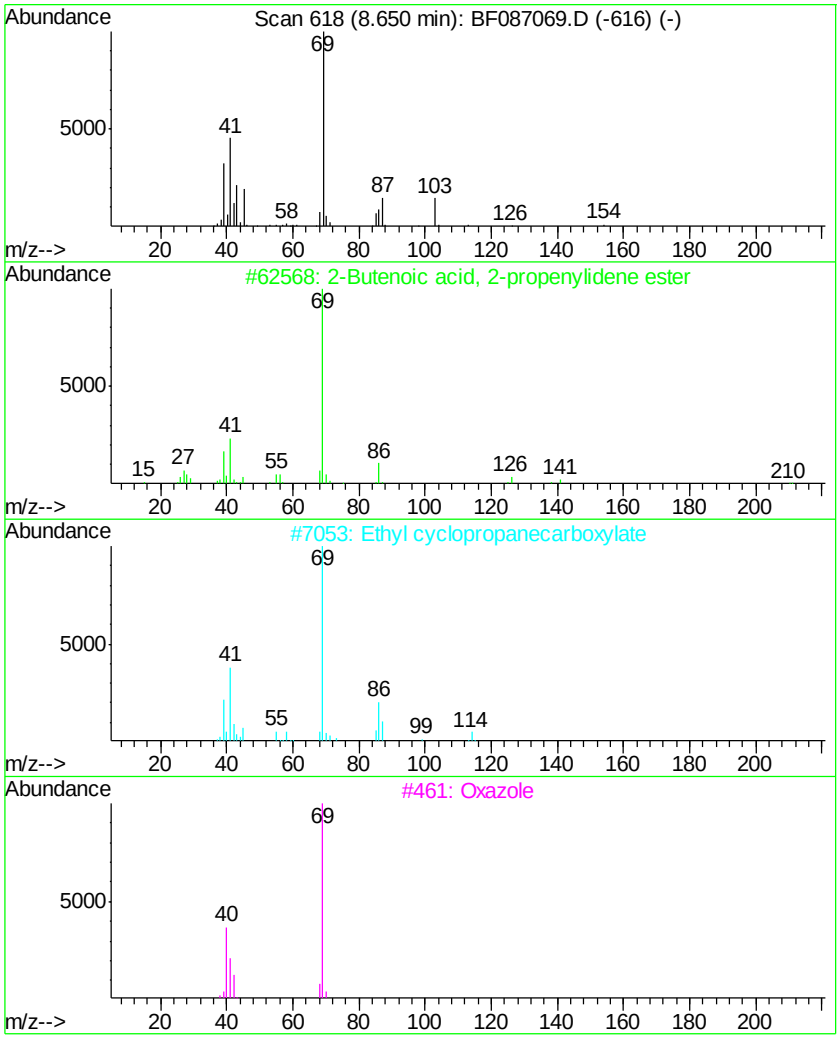
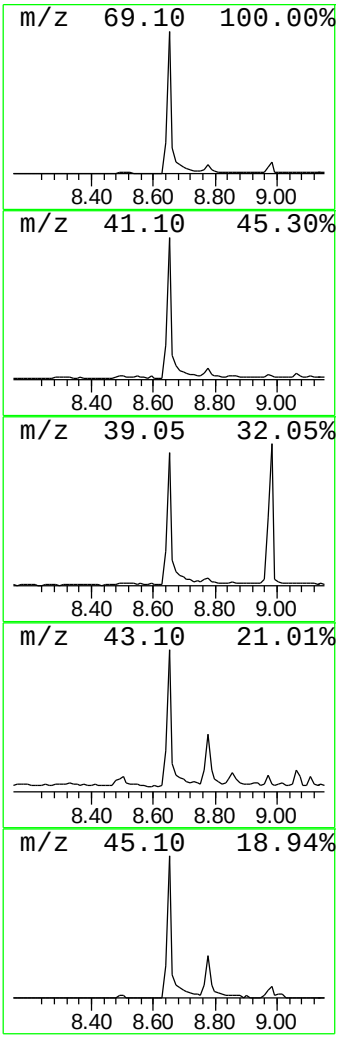
Peak Number 5 unknown8.65 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.65	5.76 ng	345031	Naphthalene-d8	7.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	42
2	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	40
3	Oxazole	69	C3H3NO	000288-42-6	36
4	Cyclopentane, bromo-	148	C5H9Br	000137-43-9	33
5	Isoxazole	69	C3H3NO	000288-14-2	33





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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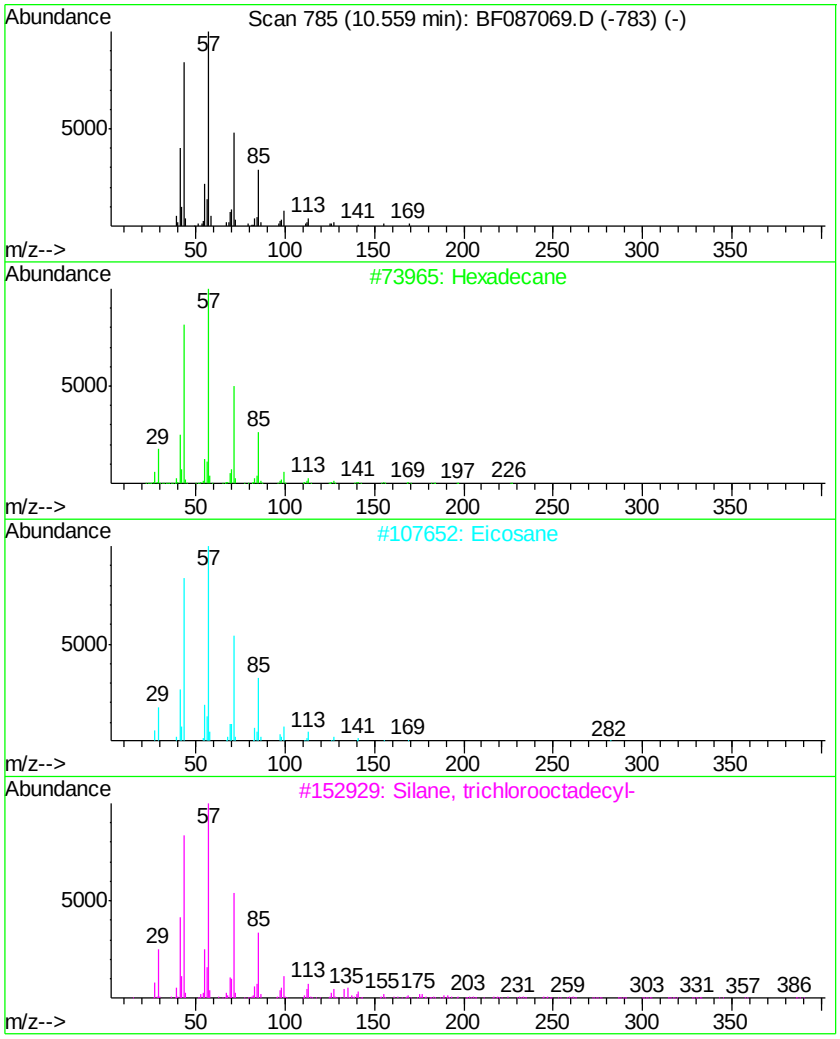
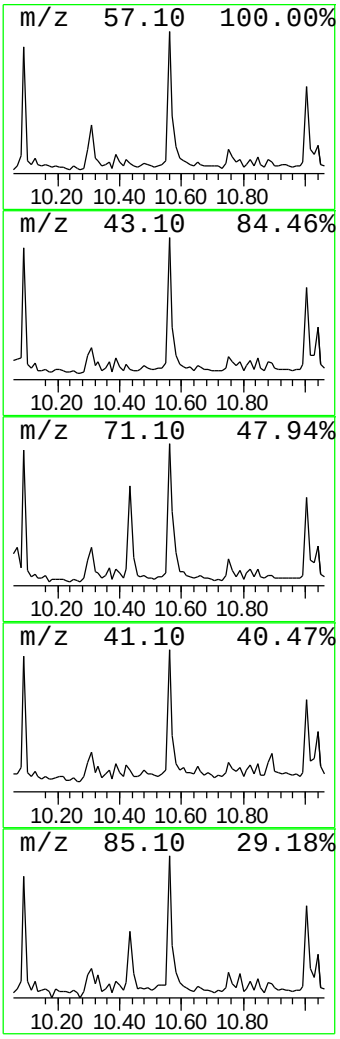
Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.56	2.83 ng	144354	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051416\
Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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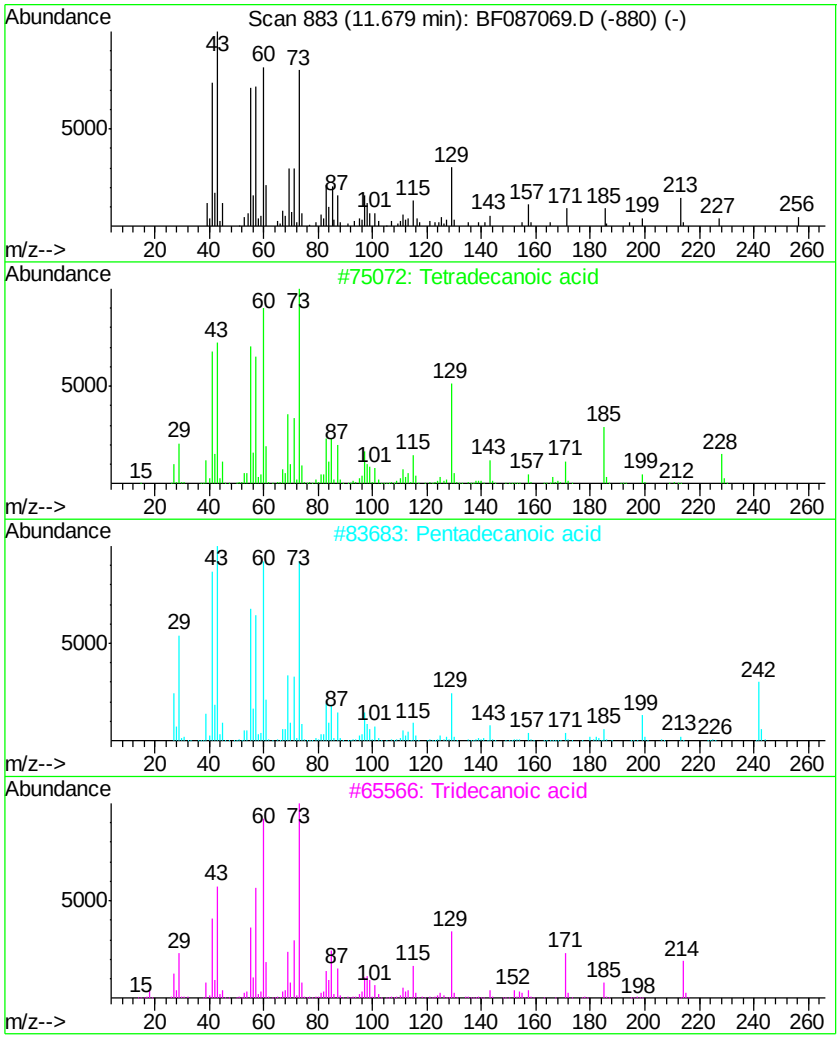
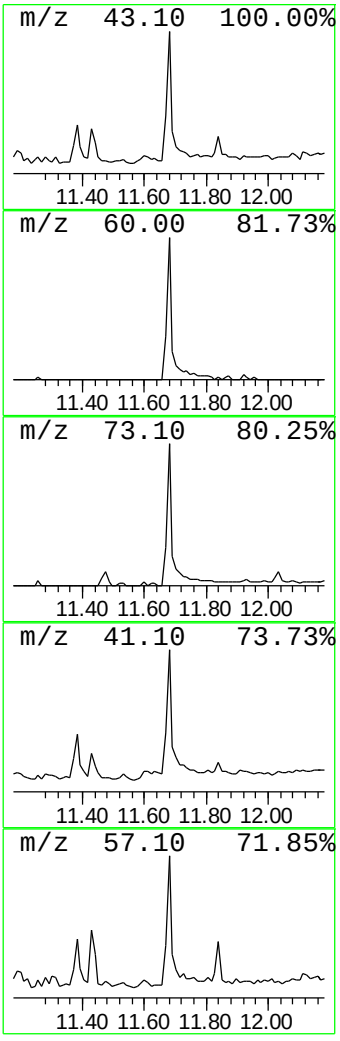
Peak Number 7 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.68	4.30 ng	219363	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





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Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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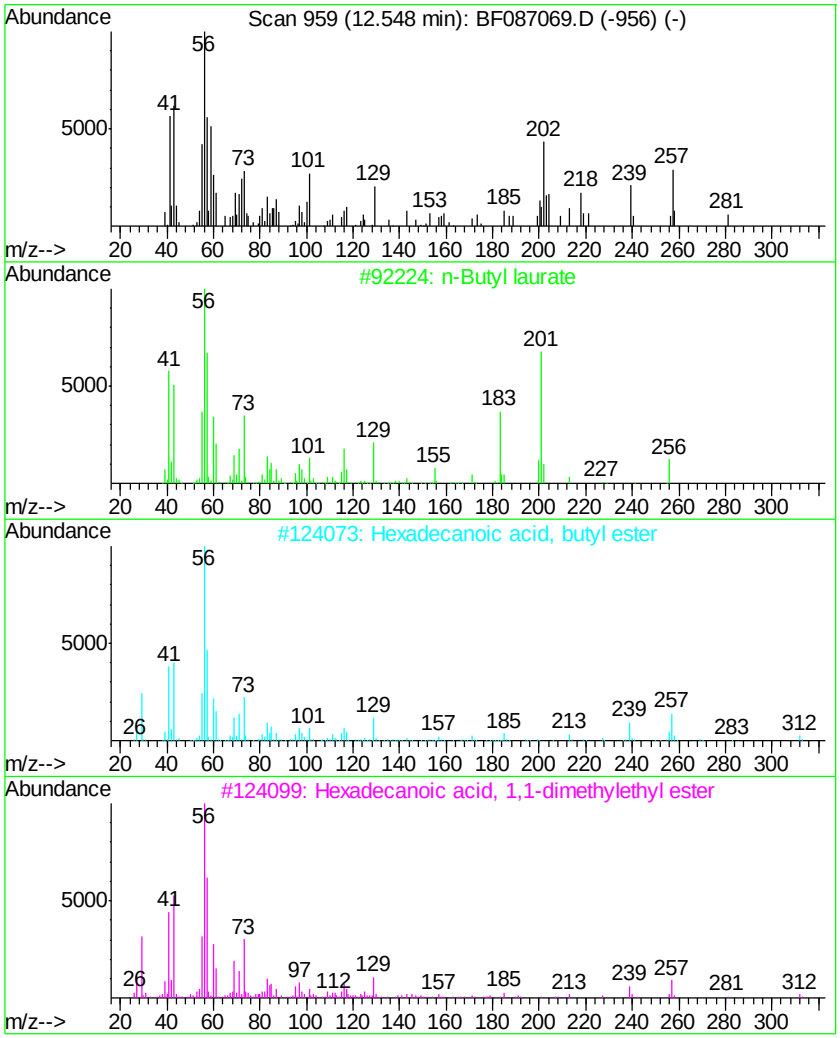
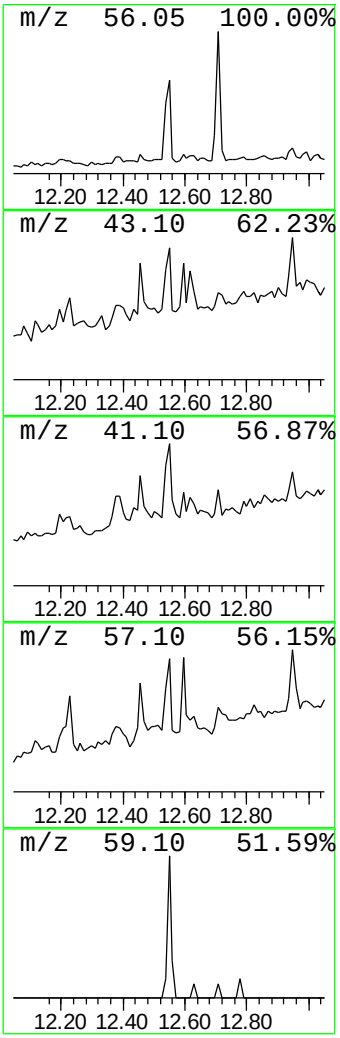
Peak Number 8 unknown12.55 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	2.23 ng	103492	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl laurate	256	C16H32O2	000106-18-3	43
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	43
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	35
4	Isobutyl laurate	256	C16H32O2	037811-72-6	27
5	5-Methyl-5-hexen-3-ol	114	C7H14O	067760-89-8	27





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Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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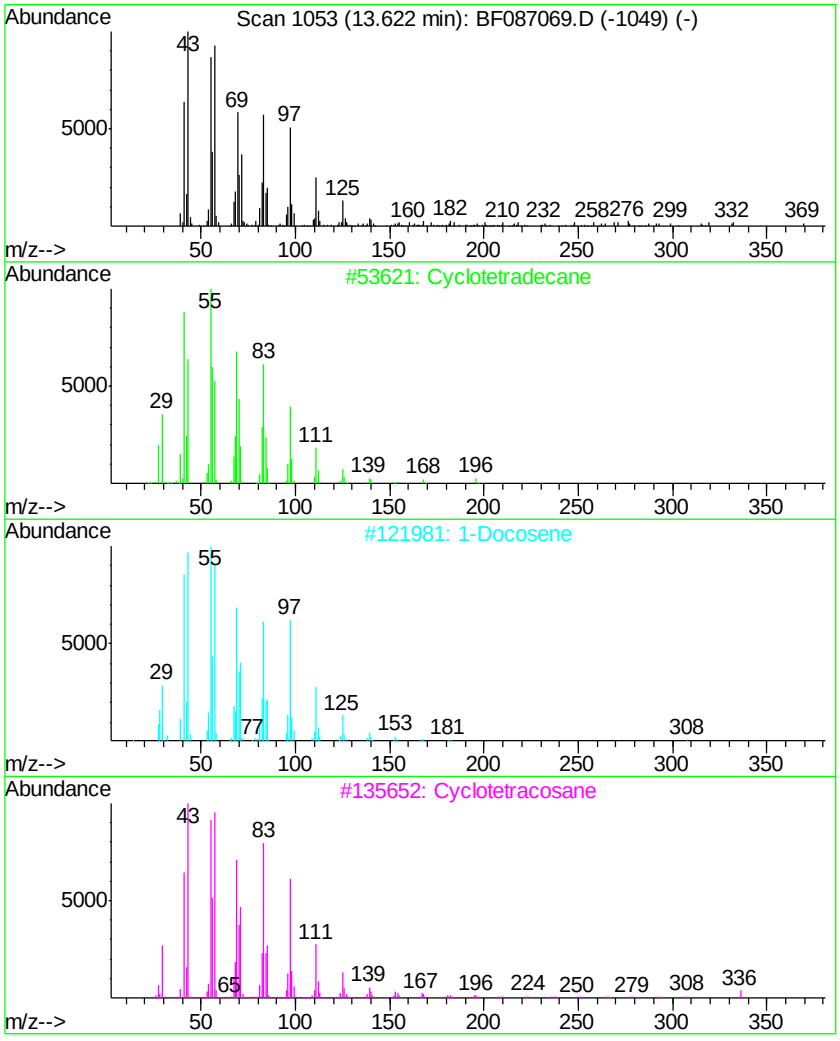
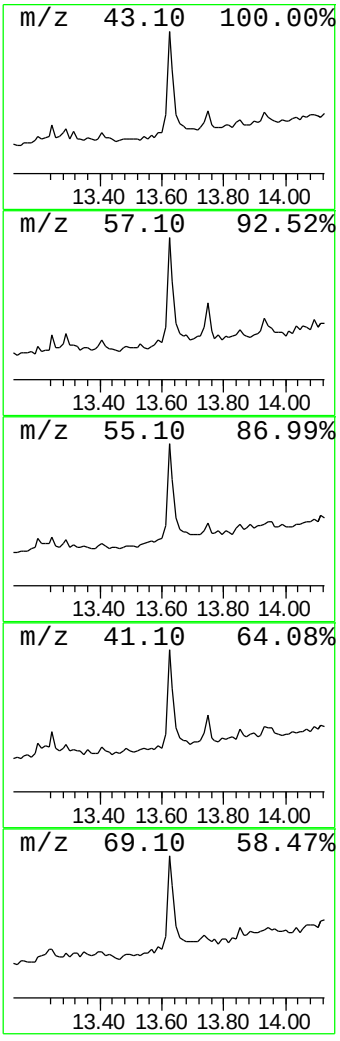
Peak Number 9 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.62	9.91 ng	459754	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	96
2	1-Docosene	308	C22H44	001599-67-3	95
3	Cyclotetracosane	336	C24H48	000297-03-0	95
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
5	Cycloeicosane	280	C20H40	000296-56-0	91





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Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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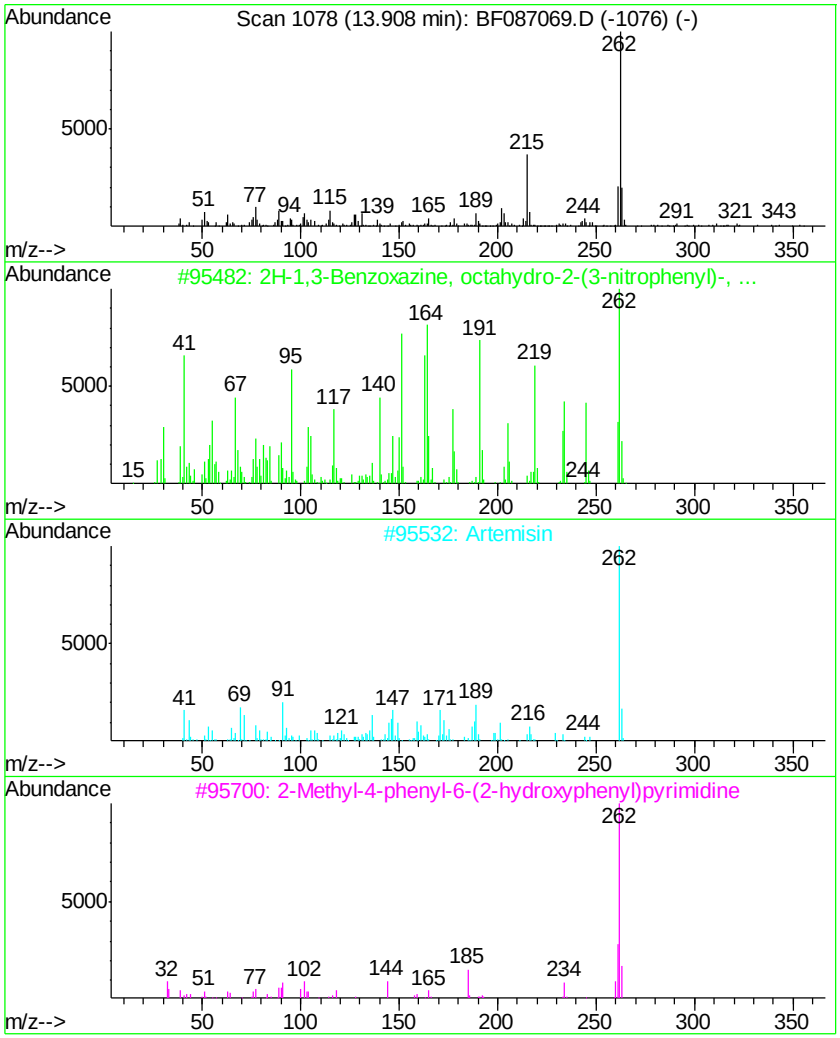
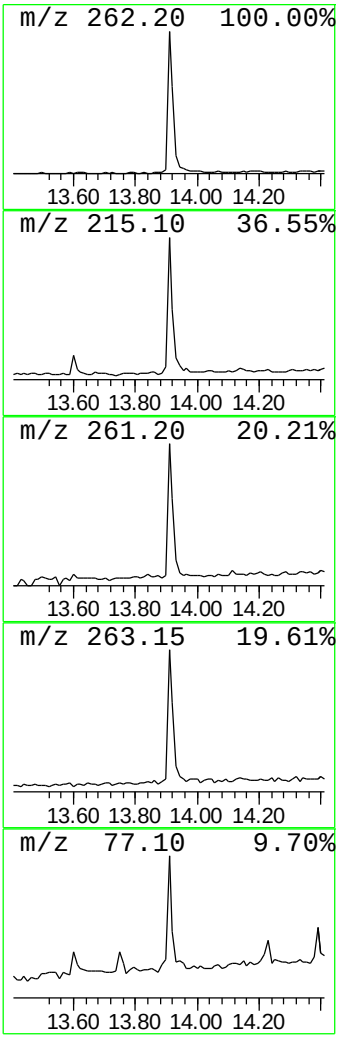
Peak Number 10 2H-1,3-Benzoxazine, octahyd... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	5.61 ng	260123	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-1,3-Benzoxazine, octahydro-2-...	262	C14H18N2O3	109086-79-5	92
2	Artemisin	262	C15H18O4	000481-05-0	50
3	2-Methyl-4-phenyl-6-(2-hydroxyph...	262	C17H14N2O	017432-80-3	50
4	Indigo	262	C16H10N2O2	000482-89-3	49
5	1-Naphthol, 2-(4-methylphenyl)azo-	262	C17H14N2O	1000196-25-6	49





Tentatively Identified Compound (LSC) summary

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Data File : BF087069.D
Acq On : 15 May 2016 14:59
Operator : UM/SJ
Sample : H2992-02
Misc :
ALS Vial : 88 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 90THAVE-SB-16(0.5-6.0)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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...	4.75	21.9	ng	1091260	1	6.62	994415	20.0
unknown6.39	6.39	71.6	ng	3561290	1	6.62	994415	20.0
unknown8.65	8.65	5.8	ng	345031	2	7.90	1198440	20.0
Hexadecane	10.56	2.8	ng	144354	4	11.13	1019790	20.0
Tetradecanoic acid	11.68	4.3	ng	219363	4	11.13	1019790	20.0
unknown12.55	12.55	2.2	ng	103492	5	13.76	927593	20.0
Cyclotetradecane	13.62	9.9	ng	459754	5	13.76	927593	20.0
2H-1,3-Benzoxazin...	13.91	5.6	ng	260123	5	13.76	927593	20.0