LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

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-BF121716.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	4.247	187	189	192	rBV	85753	111276	1.49%	0.186%
2	4.921	246	248	251	rBV	849191	1016273	13.56%	1.695%
3	5.367	284	287	289	rBV	2979416	3186415	42.53%	5.313%
4	6.407	376	378	380	rBV	2064271	1992018	26.59%	3.322%
5	6.533	386	389	391	rBV	5599514	5687675	75.91%	9.484%
6	6.761	407	409	410	rVV	1151307	1335064	17.82%	2.226%
7	6.784	410	411	413	rVB	172377	119124	1.59%	0.199%
8	6.853	413	417	418	rBV	47835	87304	1.17%	0.146%
9	6.921	420	423	425	rVB	3731546	5113255	68.25%	8.526%
10	7.036	430	433	437	rVB	196869	323017	4.31%	0.539%
11	7.104	437	439	442	rBV	184400	273686	3.65%	0.456%
12	7.207	444	448	452	rVB3	107970	262969	3.51%	0.439%
13	7.276	452	454	456	rBV2	87289	148135	1.98%	0.247%
14	7.333	456	459	461	rVV	3002106	4708669	62.85%	7.852%
15	7.402	463	465	467	rVB3	72436	80419	1.07%	0.134%
16	7.516	474	475	478	rVB2	74948	142933	1.91%	0.238%
17	7.687	488	490	492	rVB2	75744	103970	1.39%	0.173%
18	7.756	492	496	497	rBV4	35070	89393	1.19%	0.149%
19	7.790	497	499	501	rVV2	97565	134713	1.80%	0.225%
20	7.950	508	513	515	rBV5	54125	158277	2.11%	0.264%
21	8.042	518	521	523	rBV	1865288	1825821	24.37%	3.045%
22	8.247	538	539	543	rVB2	61258	106692	1.42%	0.178%
23	8.339	543	547	548	rBV3	71377	128605	1.72%	0.214%
24	8.396	548	552	554	rBV4	68051	153983	2.06%	0.257%
25	8.487	557	560	564	rVV3	105871	287923	3.84%	0.480%
26	8.590	567	569	571	rVV2	111156	133910	1.79%	0.223%
27	8.933	597	599	600	rBV	67320	86474	1.15%	0.144%
28	9.070	610	611	613	rVB	191426	205880	2.75%	0.343%
29	9.127	613	616	618	rBV	6672111	7492357	100.00%	12.493%
30	9.207	620	623	625	rBV2	147258	273284	3.65%	0.456%
31	9.253	625	627	631	rVV5	59828	175680	2.34%	0.293%
32	9.367	636	637	638	rBV	92312	118618	1.58%	0.198%
33	9.527	648	651	652	rBV3	261721	446017	5.95%	0.744%
34	9.665	661	663	665	rBV3	94078	176503	2.36%	0.294%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

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-BF121716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.710	665	667	668	rVB2	139811	156686	2.09%	0.261%
36	9.790	672	674	677	rVV	1625429	2285080	30.50%	3.810%
37	9.836	677	678	681	rVB3	55223	81615	1.09%	0.136%
38	10.065	696	698	700	rBV2	52435	92011	1.23%	0.153%
39	10.316	718	720	721	rVB	76391	75131	1.00%	0.125%
40	10.590	741	744	746	rBV	4168408	4895065	65.33%	8.163%
41	10.705	753	754	757	rVB	138784	217657	2.91%	0.363%
42	11.276	802	804	807	rVB	2138181	1884980	25.16%	3.143%
43	11.813	849	851	853	rBV3	72444	93524	1.25%	0.156%
44	12.865	940	943	946	rBV	5274061	7290775	97.31%	12.157%
45	13.654	1010	1012	1016	rBV4	43185	90948	1.21%	0.152%
46	13.768	1020	1022	1023	rBV2	57785	86702	1.16%	0.145%
47	13.905	1032	1034	1037	rBV	1639171	1897993	25.33%	3.165%
48	14.545	1088	1090	1094	rVB	132167	154791	2.07%	0.258%
49	15.334	1154	1159	1167	rVB2	1384140	3407699	45.48%	5.682%
50	15.745	1193	1195	1198	rVB	80987	108522	1.45%	0.181%
51	16.202	1233	1235	1241	rVB	85663	162520	2.17%	0.271%
52	16.740	1279	1282	1285	rBV	68246	138216	1.84%	0.230%
53	17.380	1334	1338	1345	rVB	59823	163806	2.19%	0.273%

Sum of corrected areas: 59970053

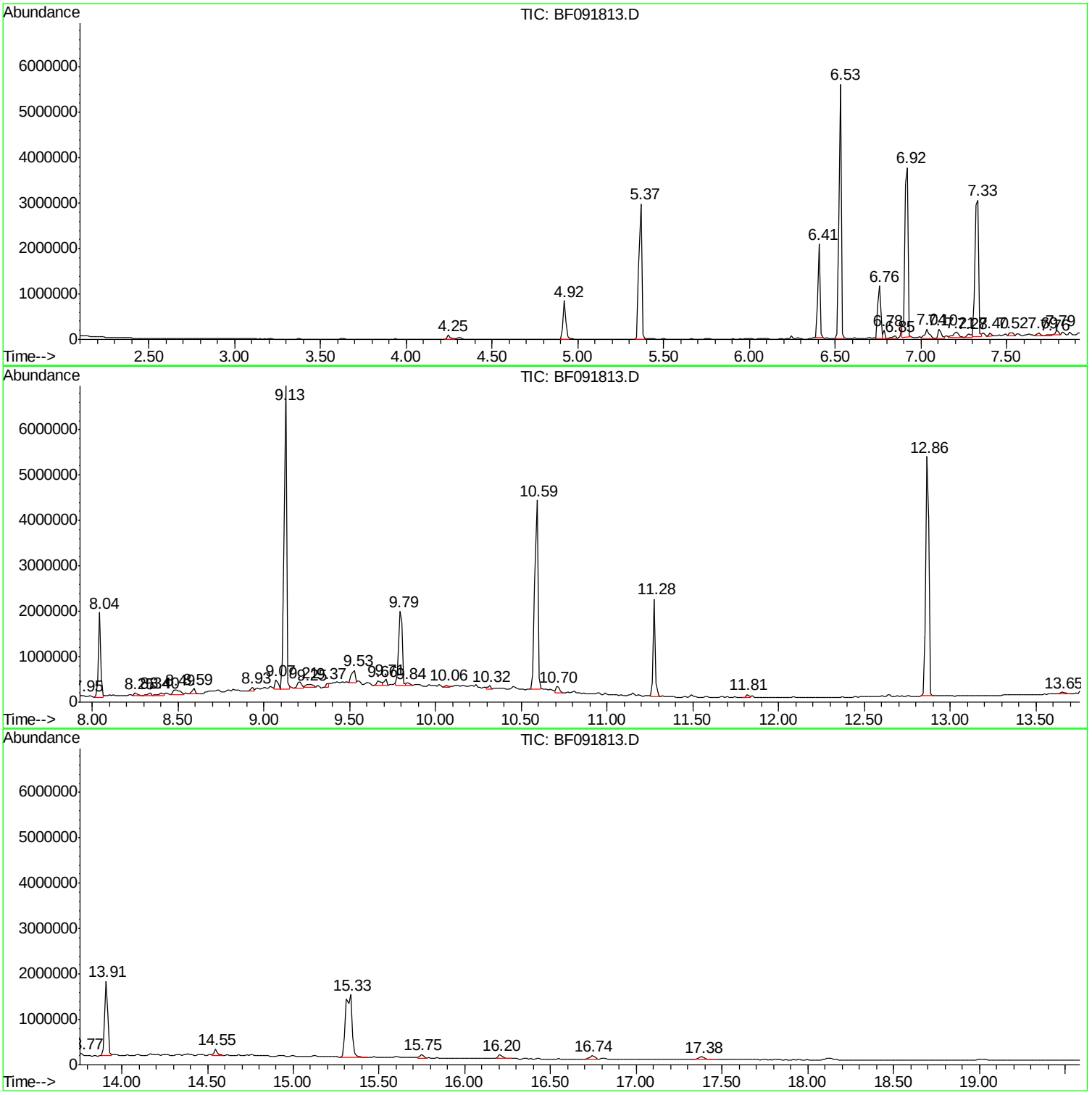
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

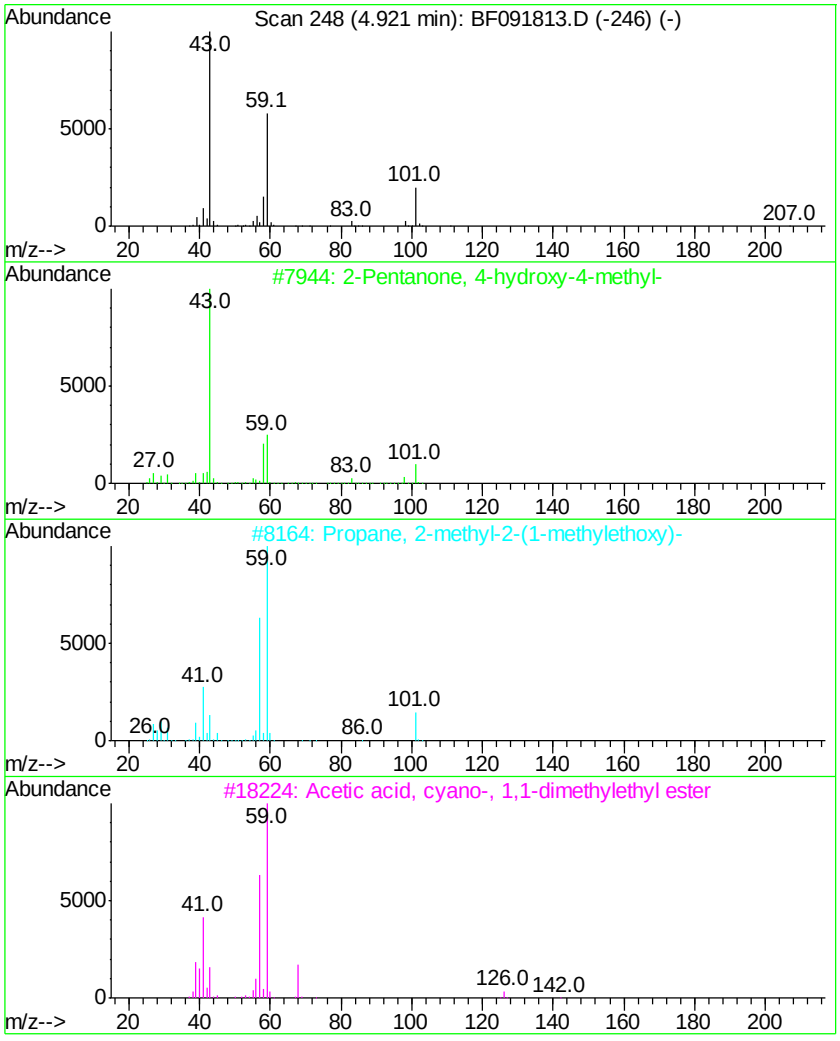
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

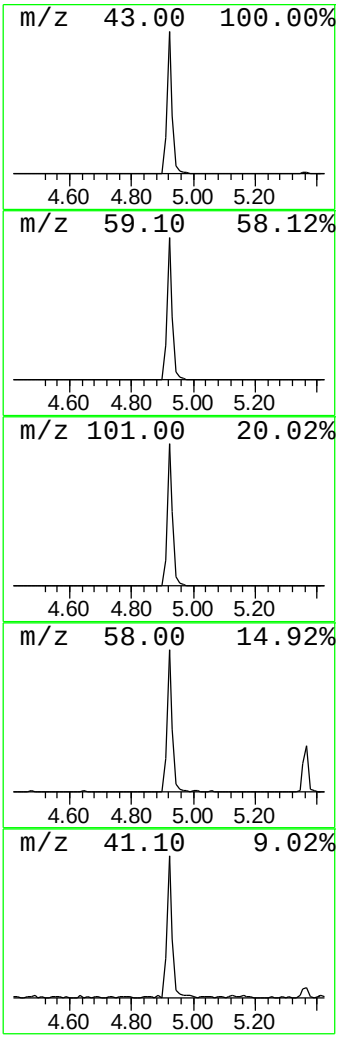
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	15.22 ng	1016270	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

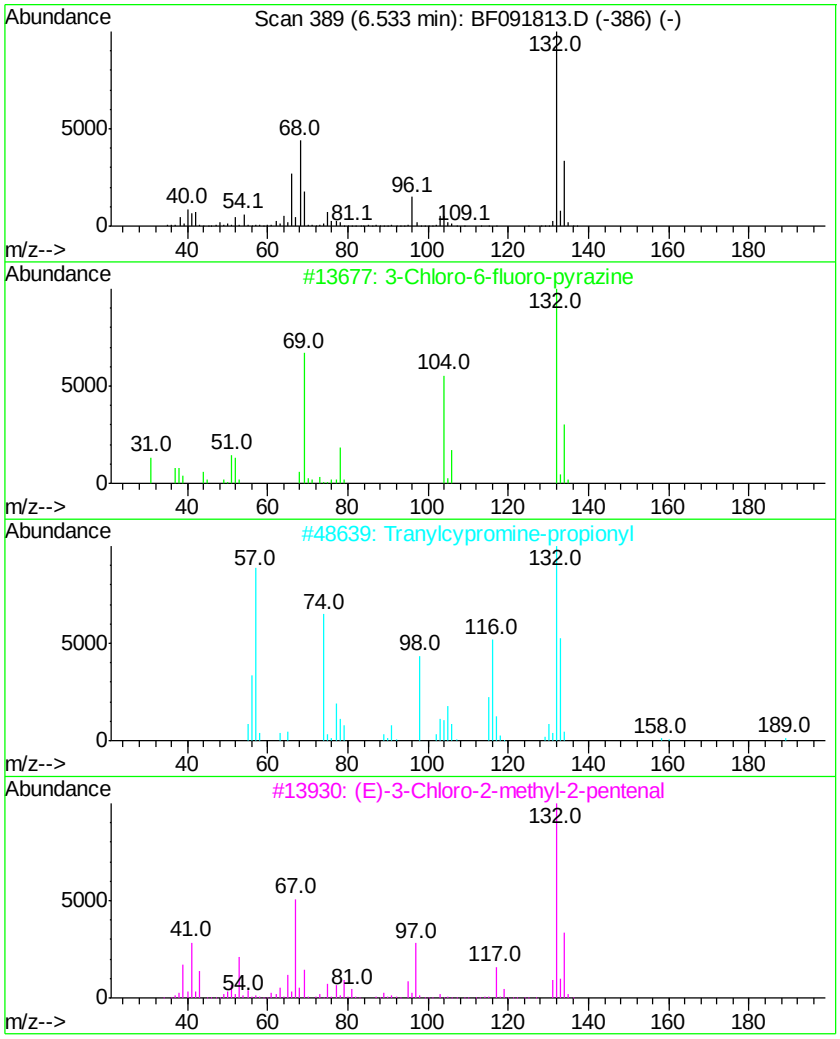
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

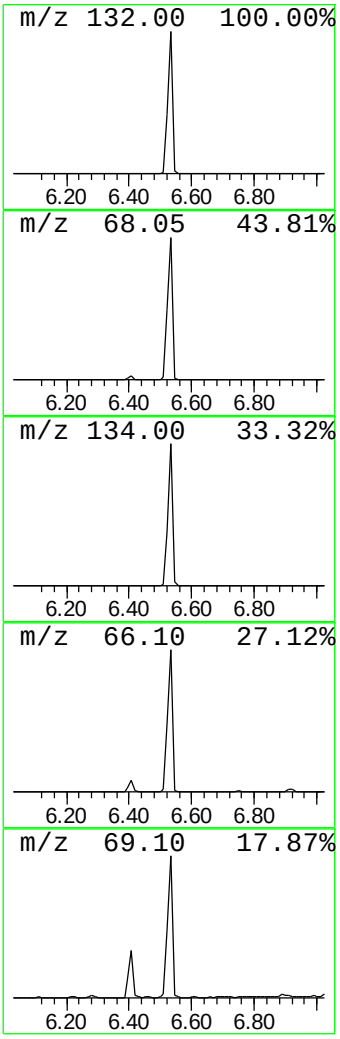
****

Peak Number 2 unknown6.53 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	85.20 ng	5687680	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

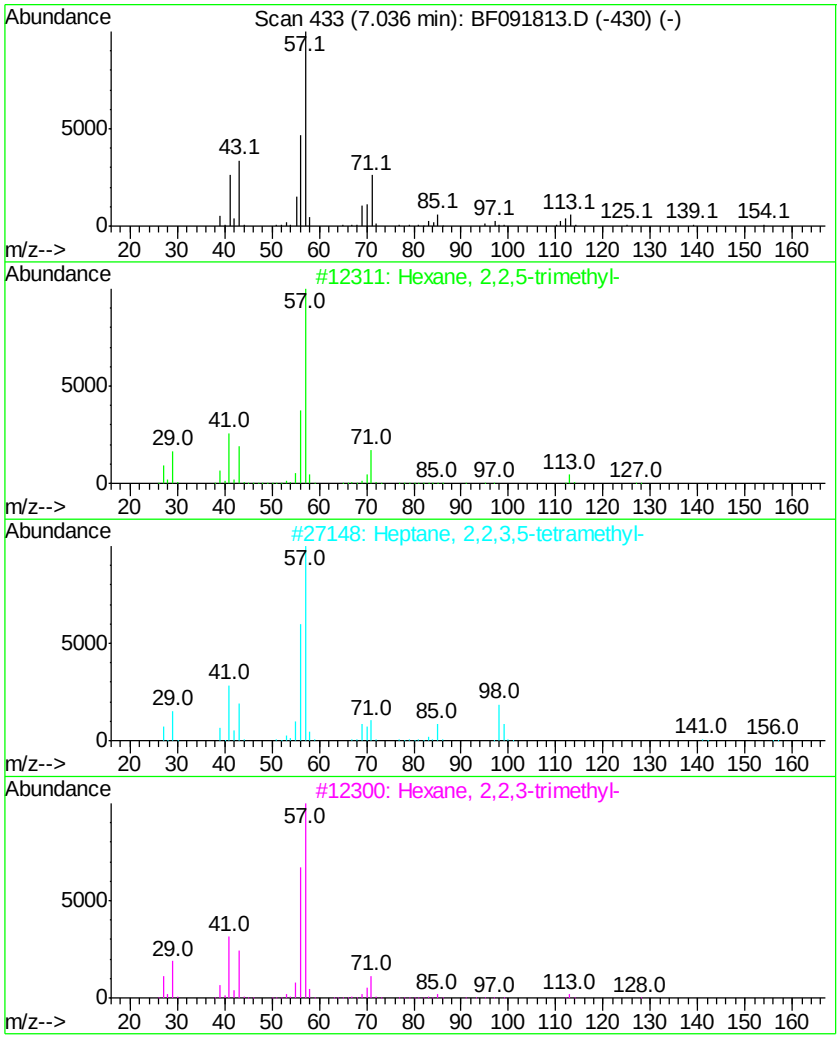
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

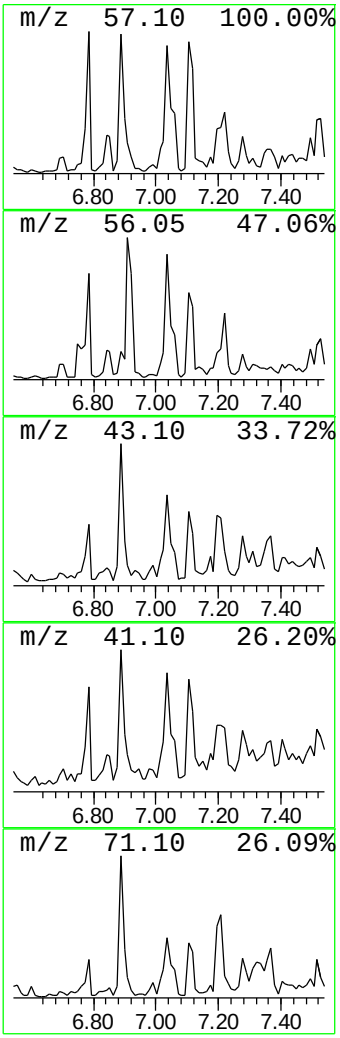
****

Peak Number 4 Hexane, 2,2,5-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	4.84 ng	323017	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64
2	Heptane, 2,2,3,5-tetramethyl-	156	C11H24	061868-42-6	64
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	59
4	Heptane, 5-ethyl-2,2,3-trimethyl-	170	C12H26	062199-06-8	59
5	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

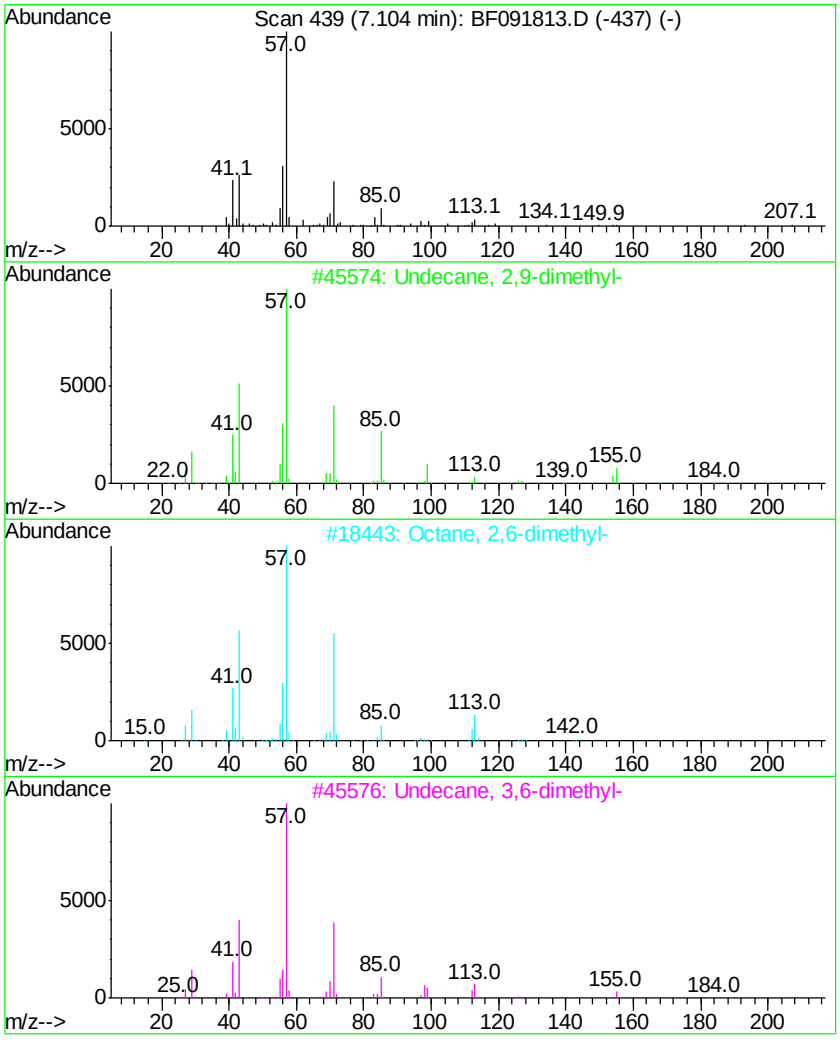
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

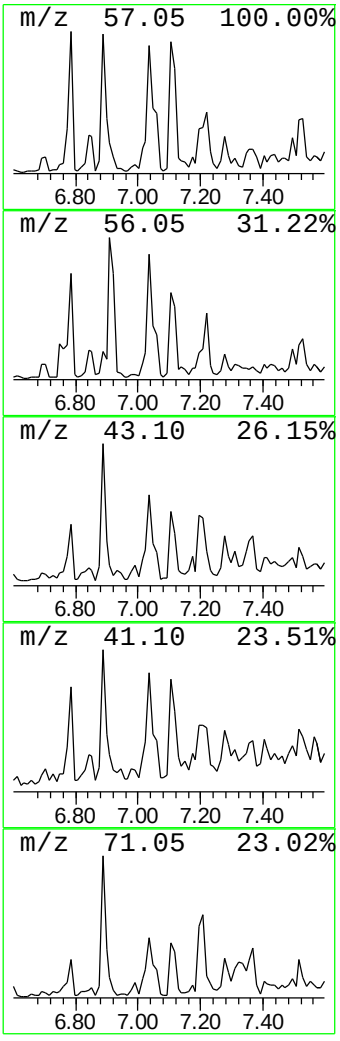
****

Peak Number 5 Undecane, 2,9-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	4.10 ng	273686	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	64
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	53
4	Tridecane, 3-methyl-	198	C14H30	006418-41-3	50
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

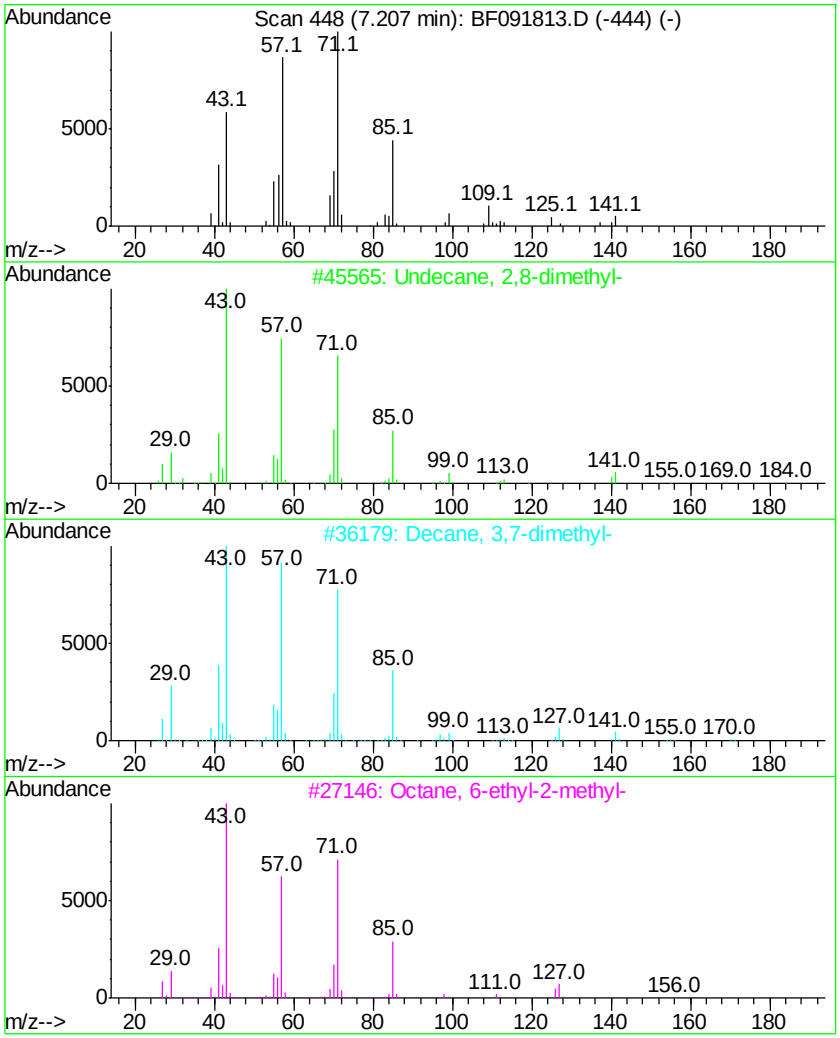
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

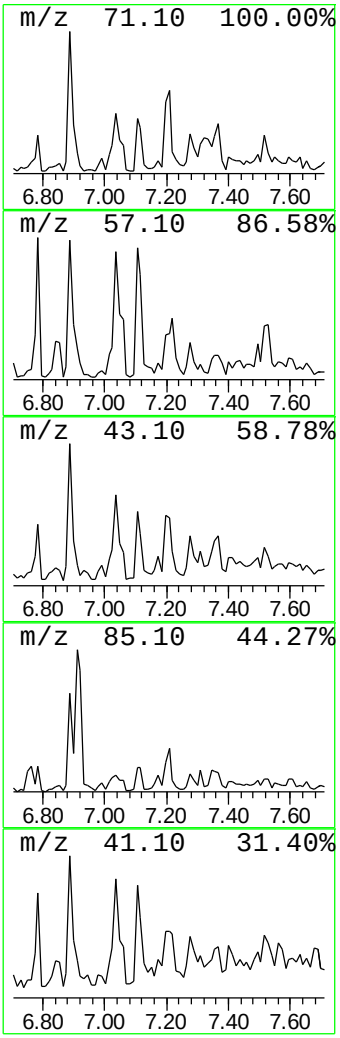
****

Peak Number 6 Undecane, 2,8-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	3.94 ng	262969	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,8-dimethyl-	184	C13H28	017301-25-6	72
2	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	72
3	Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	64
4	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	59
5	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

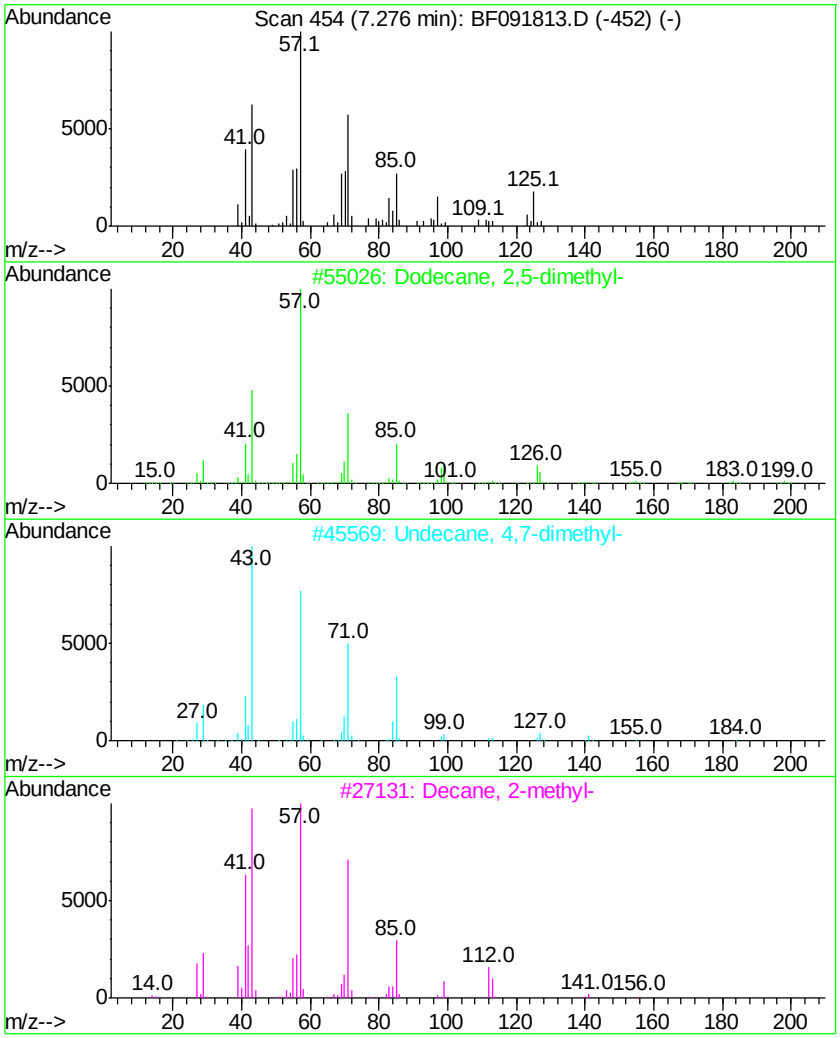
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

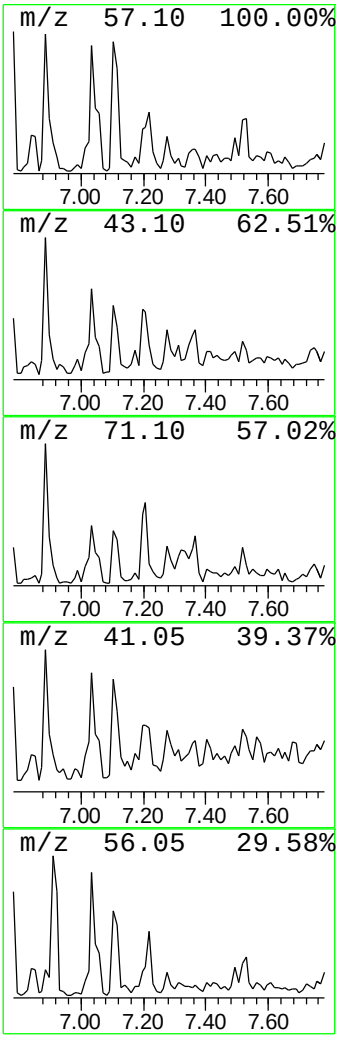
****

Peak Number 7 Dodecane, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	2.22 ng	148135	1,4-Dichlorobenzene-d4	6.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,5-dimethyl-	198	C14H30	056292-65-0	53
2	Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	50
3	Decane, 2-methyl-	156	C11H24	006975-98-0	50
4	Undecane	156	C11H24	001120-21-4	50
5	Eicosane	282	C20H42	000112-95-8	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

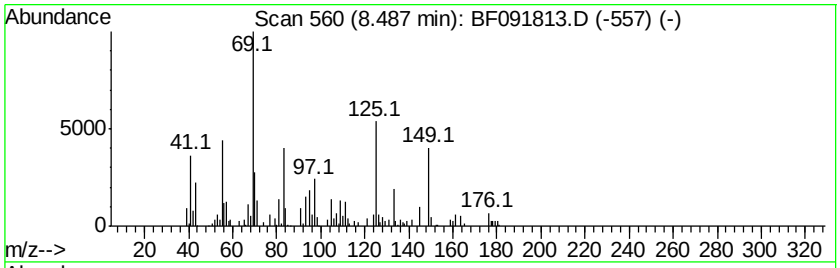
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

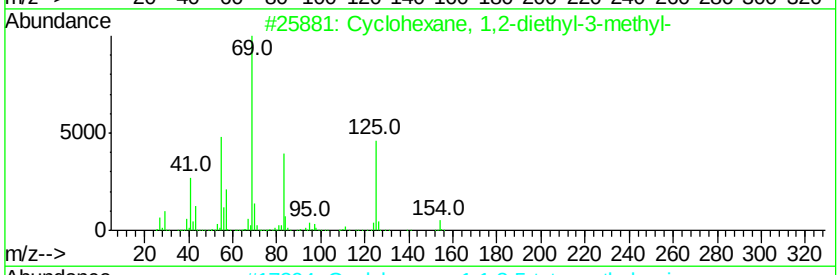
****

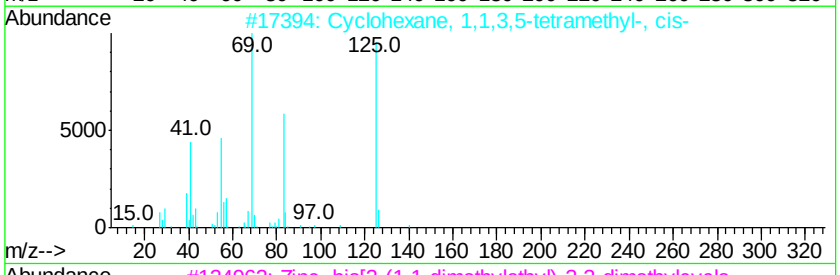
Peak Number 8 unknown8.49 Concentration Rank 7

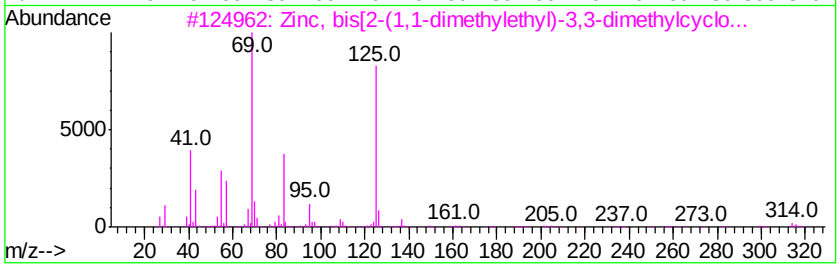
R.T.	EstConc	Area	Relative to ISTD	R.T.
8.49	3.15 ng	287923	Naphthalene-d8	8.04

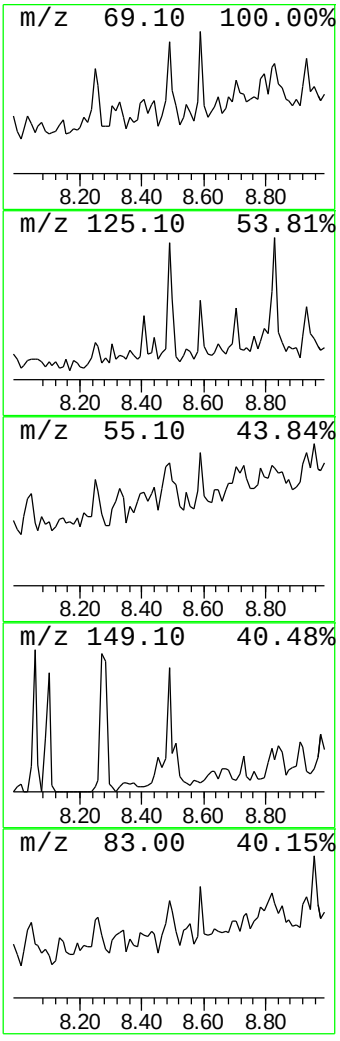
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-diethyl-3-methyl-	154	C11H22	061141-80-8	47
2	Cyclohexane, 1,1,3,5-tetramethyl...	140	C10H20	050876-32-9	47
3	Zinc, bis[2-(1,1-dimethylethyl)-...	314	C18H34Zn	074793-36-5	38
4	Triallylsilane	152	C9H16Si	001116-62-7	38
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	22











Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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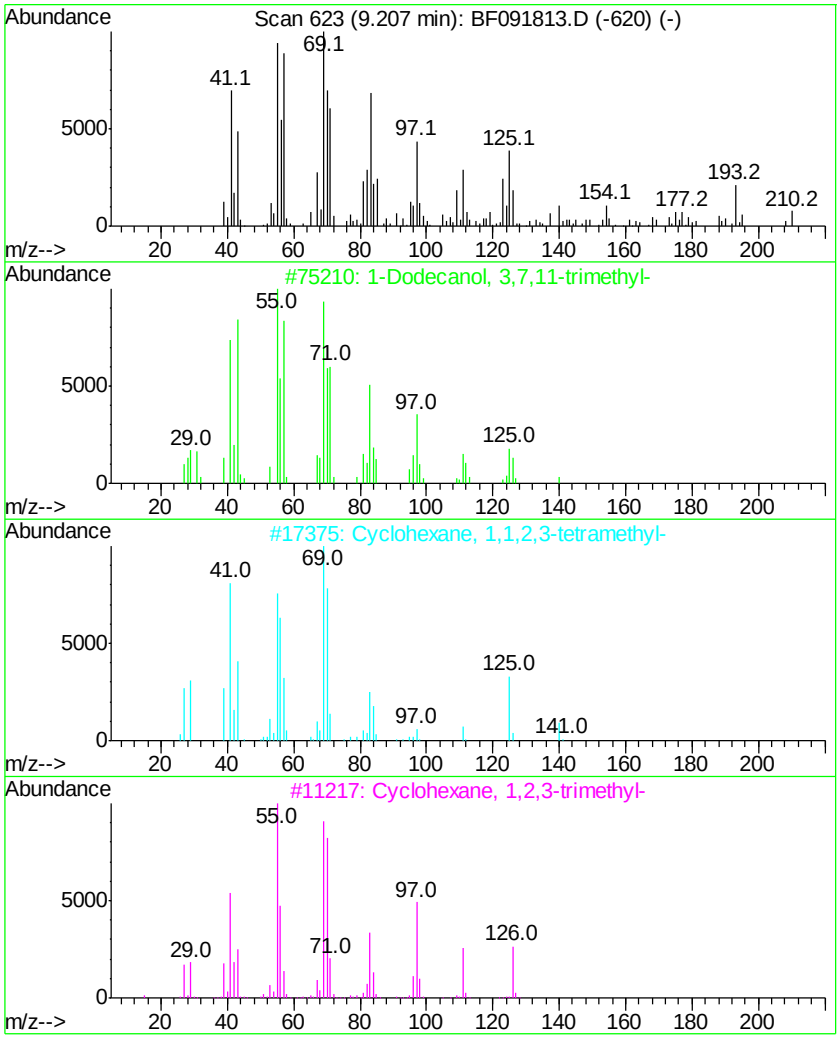
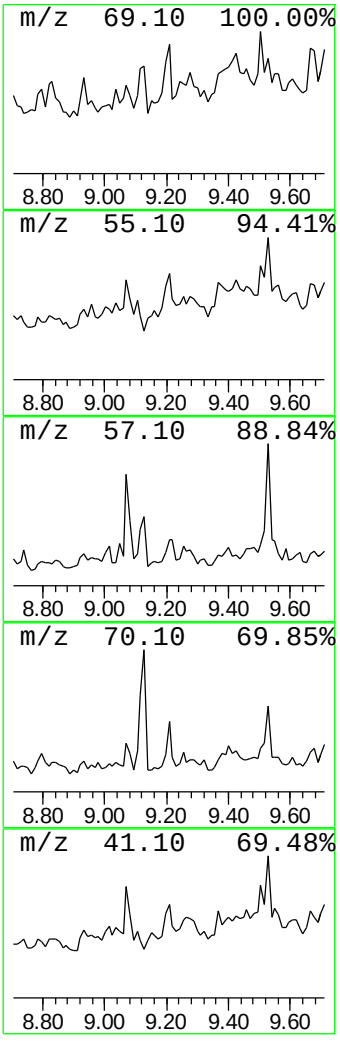
Peak Number 9 1-Dodecanol, 3,7,11-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.21	2.39 ng	273284	Acenaphthene-d10	9.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	006750-34-1	58
2	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	50
3	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	50
4	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	43
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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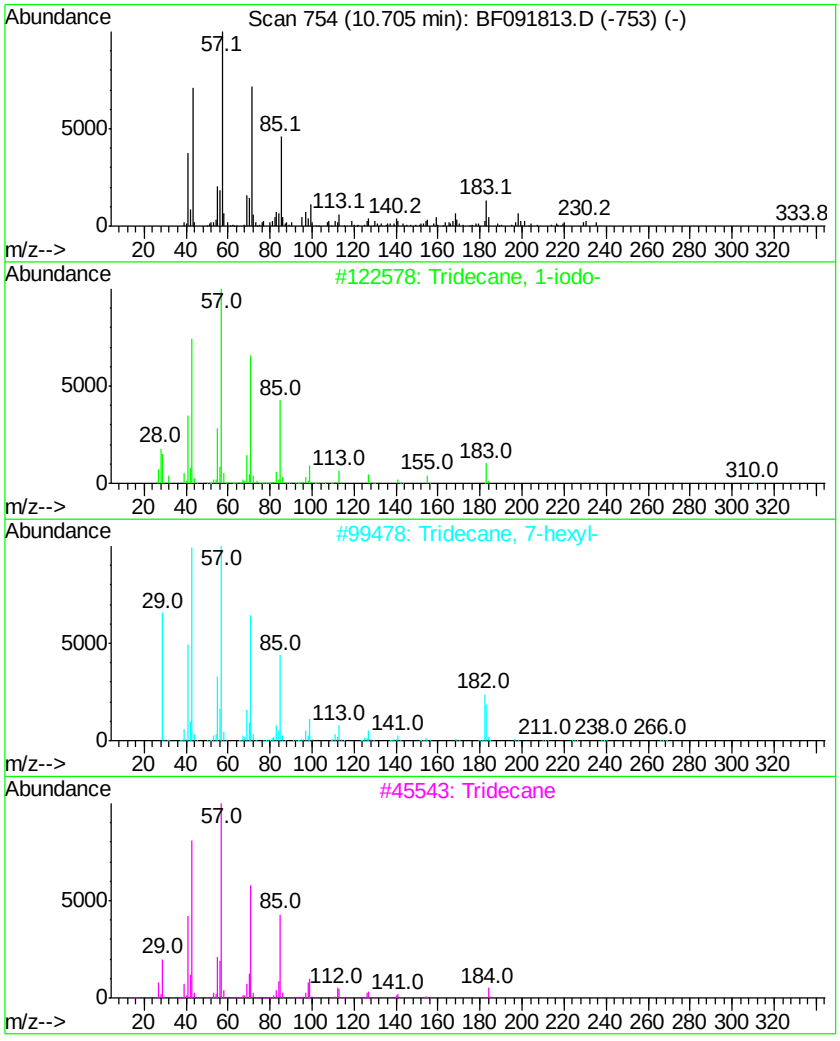
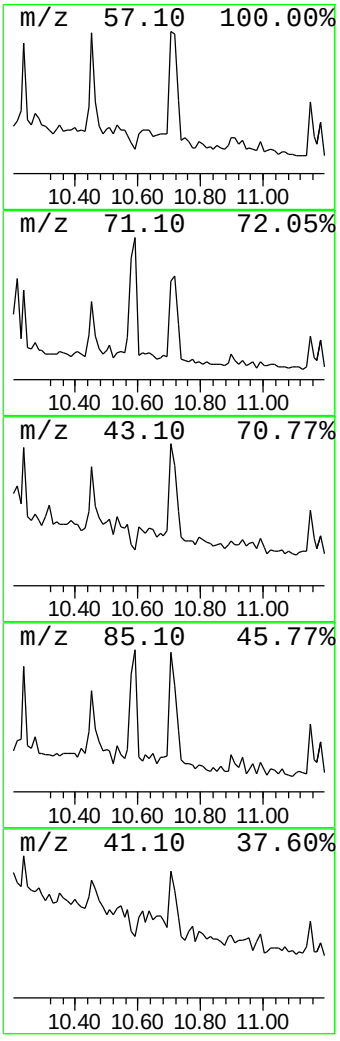
Peak Number 10 Tridecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	2.31 ng	217657	Phenanthrene-d10	11.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
2	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	86
3	Tridecane	184	C13H28	000629-50-5	81
4	Tetradecane	198	C14H30	000629-59-4	81
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF122016\
Data File : BF091813.D
Acq On : 20 Dec 2016 12:04
Operator : UM/SJ
Sample : H6147-05
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-30

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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...	4.92	15.2	ng	1016270	1	6.76	1335060	20.0
unknown6.53	6.53	85.2	ng	5687680	1	6.76	1335060	20.0
Hexane, 2,2,5-tri...	7.04	4.8	ng	323017	1	6.76	1335060	20.0
Undecane, 2,9-dim...	7.10	4.1	ng	273686	1	6.76	1335060	20.0
Undecane, 2,8-dim...	7.21	3.9	ng	262969	1	6.76	1335060	20.0
Dodecane, 2,5-dim...	7.28	2.2	ng	148135	1	6.76	1335060	20.0
unknown8.49	8.49	3.1	ng	287923	2	8.04	1825820	20.0
1-Dodecanol, 3,7,...	9.21	2.4	ng	273284	3	9.80	2285080	20.0
Tridecane, 1-iodo-	10.70	2.3	ng	217657	4	11.28	1884980	20.0