LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051915\
Data File : BF079370.D
Acq On : 20 May 2015 6:52
Operator : TP/IZ
Sample : G2289-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35S

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-BF043015.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	1.278	5	8	10	rVB	2823936	3437149	100.00%	15.128%
2	1.393	15	18	27	rVB	62977	150845	4.39%	0.664%
3	1.564	30	33	36	rVB	137409	202780	5.90%	0.892%
4	1.644	39	40	48	rBV	302671	488188	14.20%	2.149%
5	1.758	48	50	89	rVB	1625986	3024494	87.99%	13.312%
6	4.879	321	323	330	rBV	261169	341907	9.95%	1.505%
7	5.416	367	370	373	rBV	1280619	1341422	39.03%	5.904%
8	6.707	480	483	485	rBV	1312568	1447214	42.11%	6.370%
9	6.845	492	495	497	rBV	1209030	1465987	42.65%	6.452%
10	7.130	518	520	522	rBV	265721	269352	7.84%	1.185%
11	7.313	534	536	539	rBV	1245583	1123174	32.68%	4.943%
12	7.828	578	581	583	rBV	740763	879388	25.58%	3.870%
13	8.708	655	658	660	rBV	324075	368316	10.72%	1.621%
14	10.056	773	776	778	rBV	1454667	1777922	51.73%	7.825%
15	10.559	818	820	822	rBV	116519	101422	2.95%	0.446%
16	10.879	846	848	850	rBV	326799	400388	11.65%	1.762%
17	11.851	931	933	936	rBV2	827290	1139749	33.16%	5.016%
18	12.720	1006	1009	1010	rBV	369445	433396	12.61%	1.907%
19	12.742	1010	1011	1013	rVV	159093	137947	4.01%	0.607%
20	12.811	1013	1017	1020	rVV	24248	35621	1.04%	0.157%
21	14.217	1138	1140	1142	rBV	136817	144064	4.19%	0.634%
22	14.503	1162	1165	1167	rVB	114354	146591	4.26%	0.645%
23	14.708	1181	1183	1186	rBV	1534344	1999689	58.18%	8.801%
24	15.897	1284	1287	1293	rBV2	94129	164907	4.80%	0.726%
25	16.011	1293	1297	1299	rVV	501533	633962	18.44%	2.790%
26	16.046	1299	1300	1306	rVB2	57602	90977	2.65%	0.400%
27	17.337	1410	1413	1419	rBV	48789	119389	3.47%	0.525%
28	17.657	1439	1441	1445	rBV	31038	65228	1.90%	0.287%
29	17.726	1445	1447	1450	rVV	55312	68926	2.01%	0.303%
30	17.794	1450	1453	1458	rVV	424758	554166	16.12%	2.439%
31	18.434	1504	1509	1515	rBV4	25601	103237	3.00%	0.454%
32	19.177	1572	1574	1580	rBV3	24652	63077	1.84%	0.278%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051915\
Data File : BF079370.D
Acq On : 20 May 2015 6:52
Operator : TP/IZ
Sample : G2289-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35S

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-BF043015.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 22720874

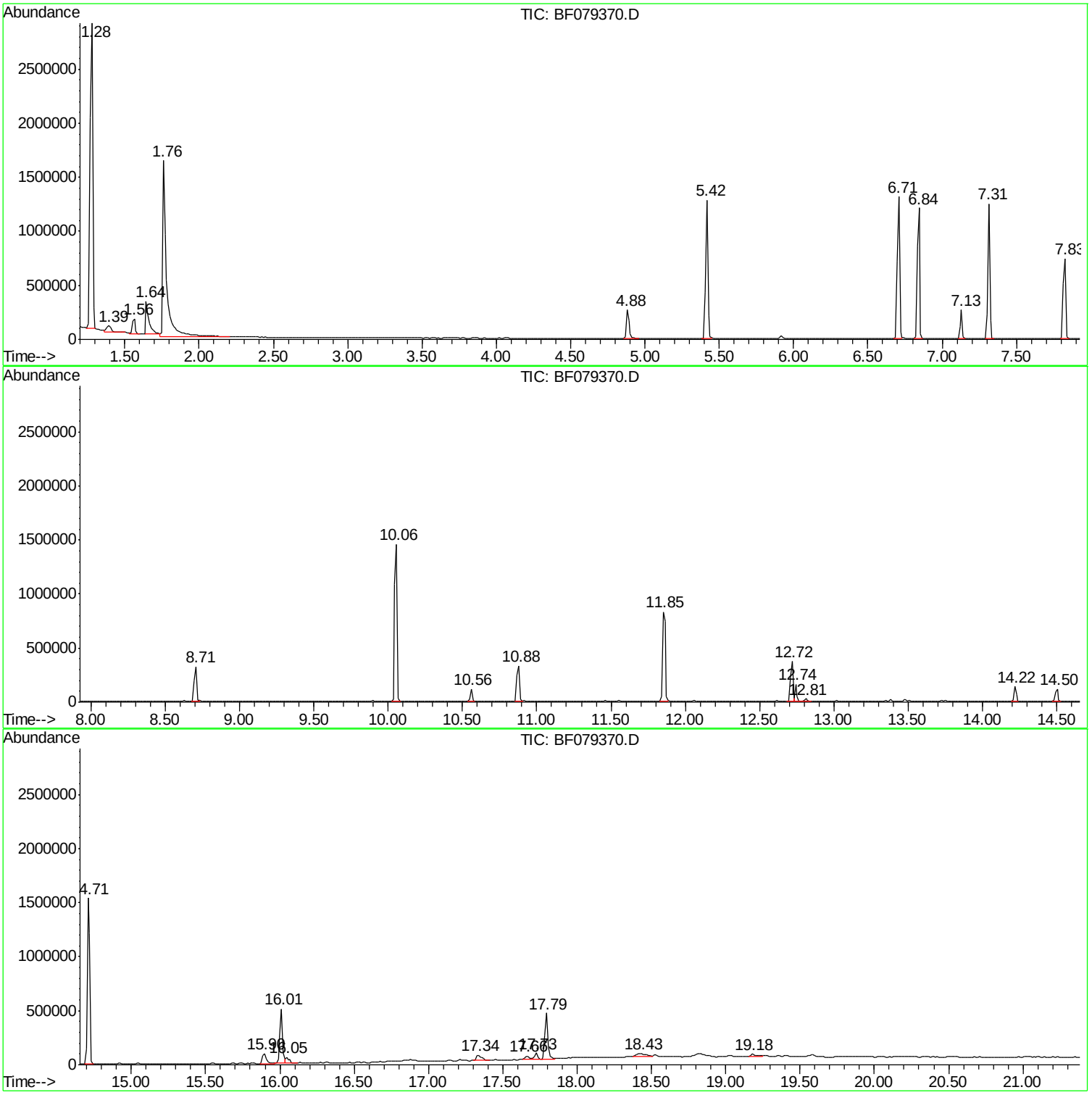
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051915\
Data File : BF079370.D
Acq On : 20 May 2015 6:52
Operator : TP/IZ
Sample : G2289-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051915\
Data File : BF079370.D
Acq On : 20 May 2015 6:52
Operator : TP/IZ
Sample : G2289-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

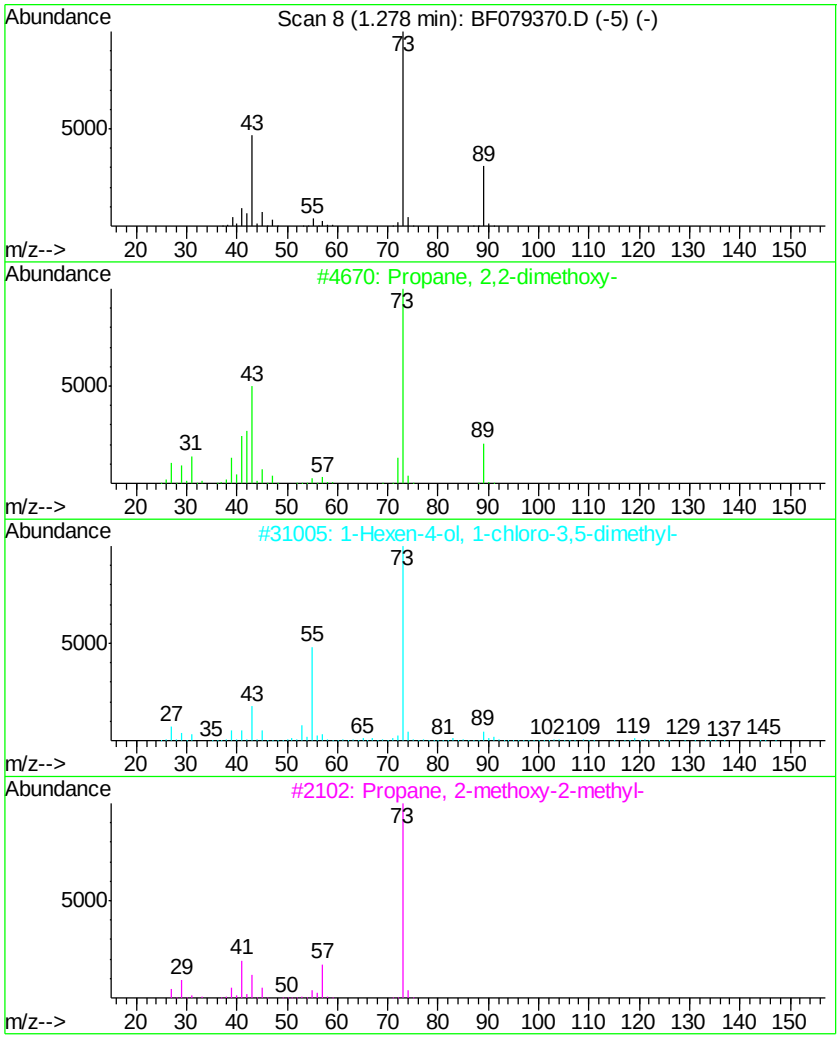
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

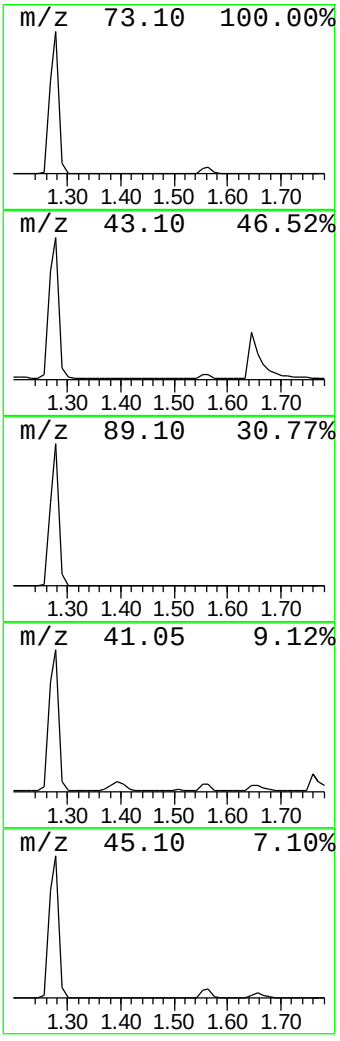
****

Peak Number 1 unknown1.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	255.22 ng	3437150	1,4-Dichlorobenzene-d4	7.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051915\
Data File : BF079370.D
Acq On : 20 May 2015 6:52
Operator : TP/IZ
Sample : G2289-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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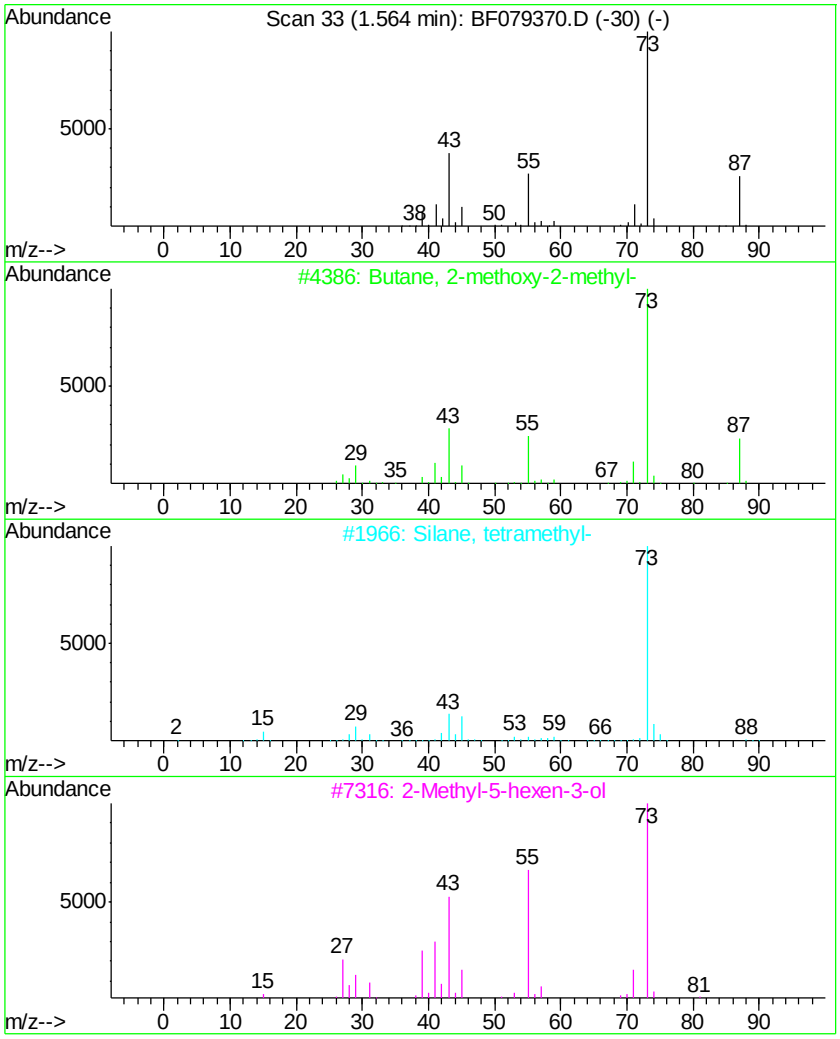
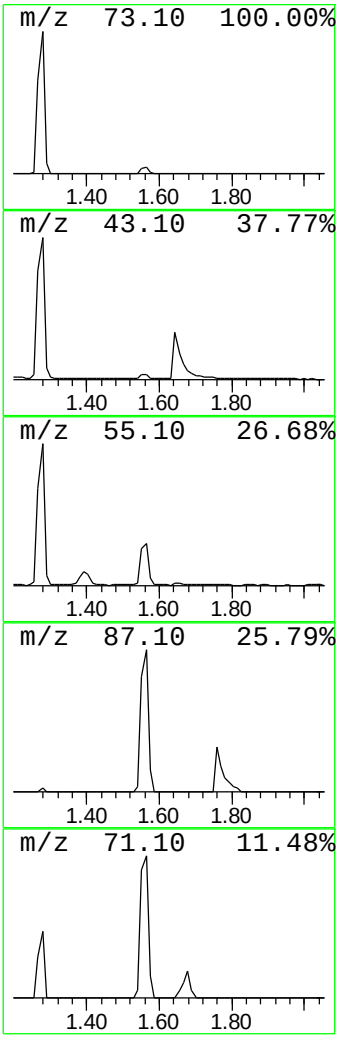
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.56	15.06 ng	202780	1,4-Dichlorobenzene-d4	7.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051915\
Data File : BF079370.D
Acq On : 20 May 2015 6:52
Operator : TP/IZ
Sample : G2289-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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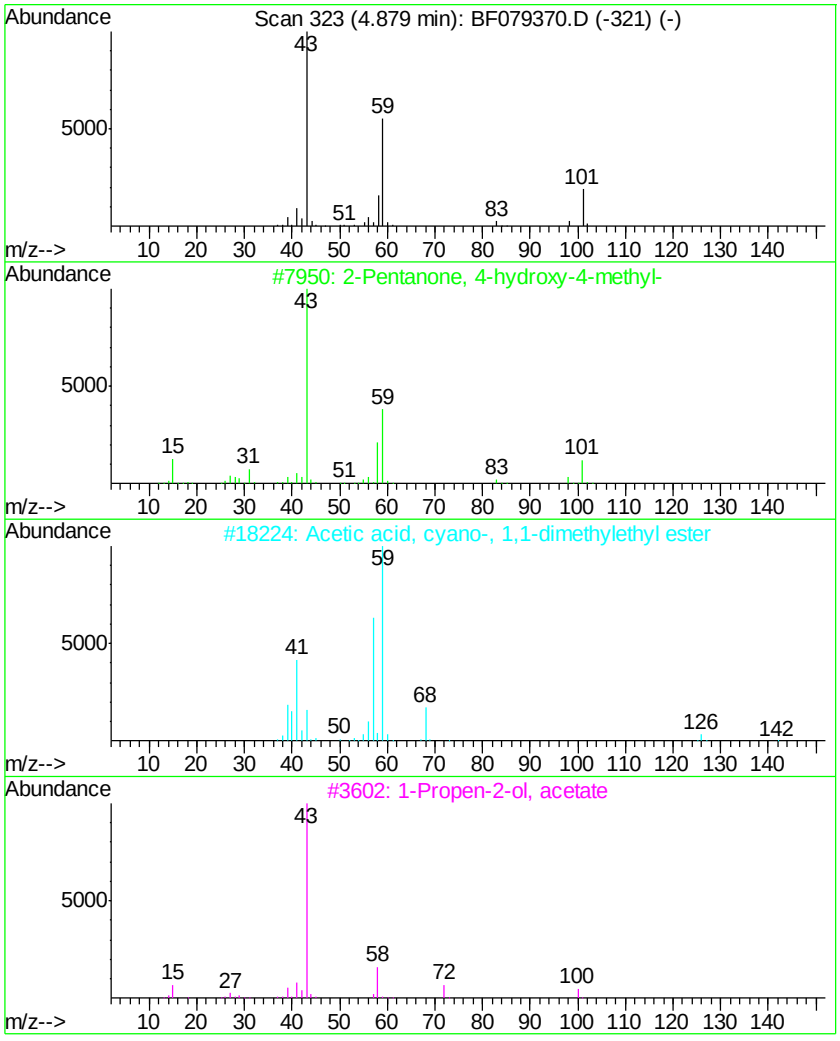
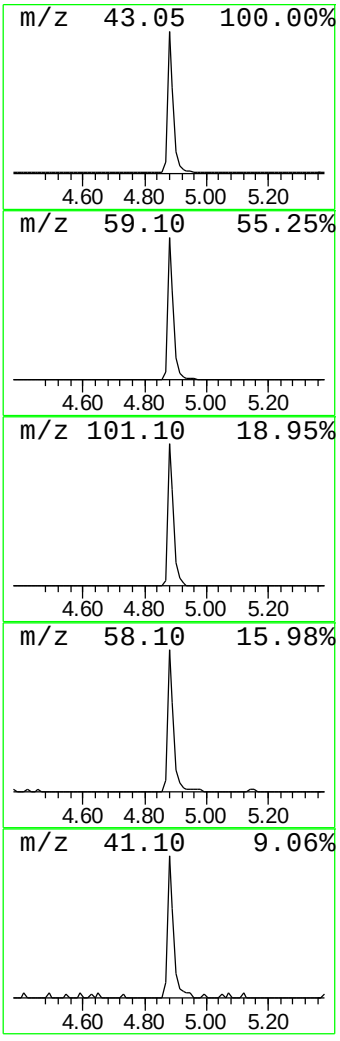
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	25.39 ng	341907	1,4-Dichlorobenzene-d4	7.13

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051915\
Data File : BF079370.D
Acq On : 20 May 2015 6:52
Operator : TP/IZ
Sample : G2289-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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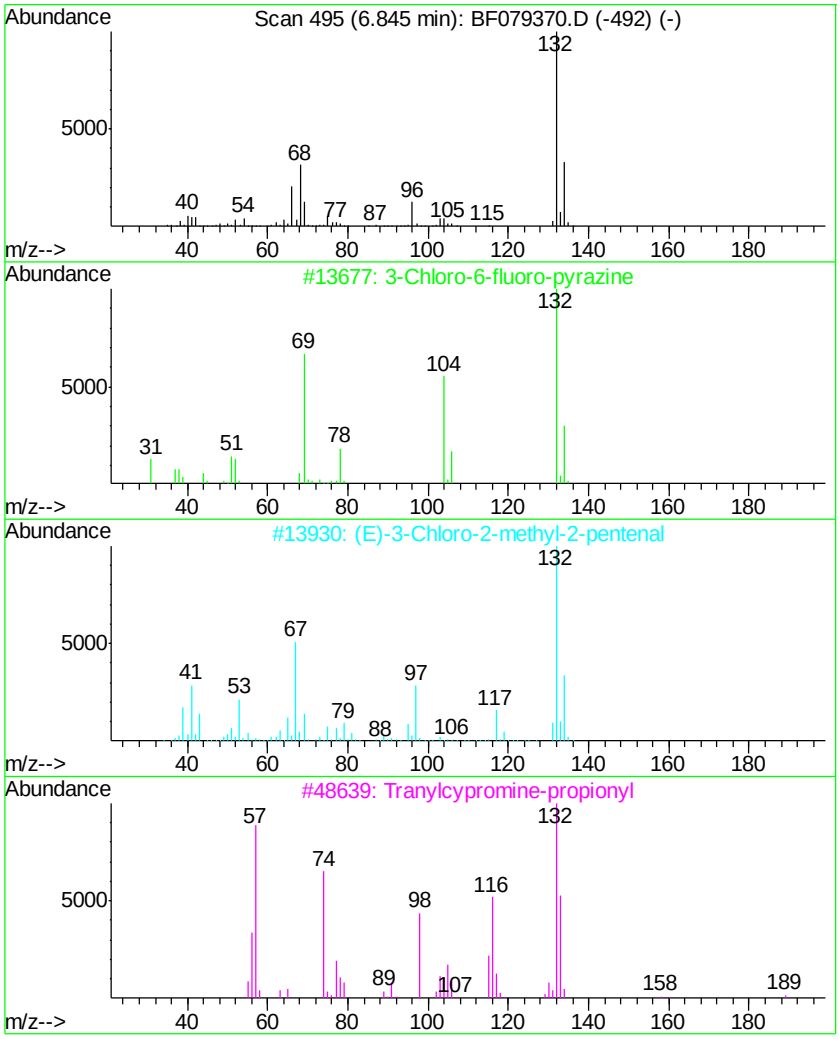
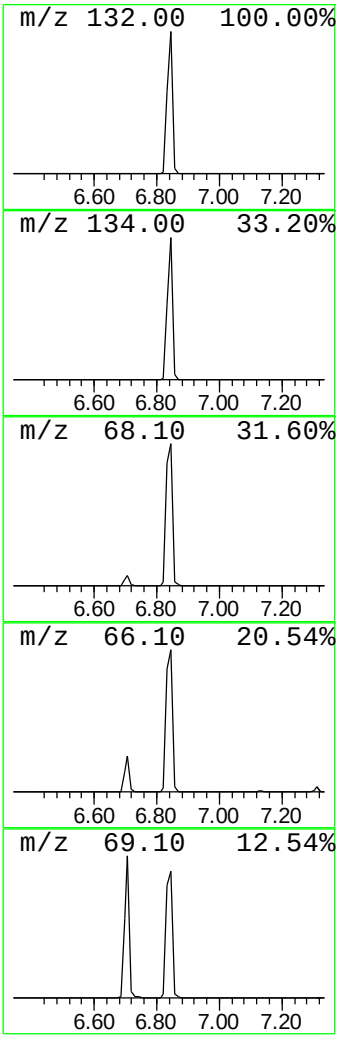
Peak Number 7 unknown6.84 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.84	108.85 ng	1465990	1,4-Dichlorobenzene-d4	7.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Xenon	132	Xe	007440-63-3	9





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Sample : G2289-04
Misc :
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Instrument : BNA_F
ClientSampleId : SB-35S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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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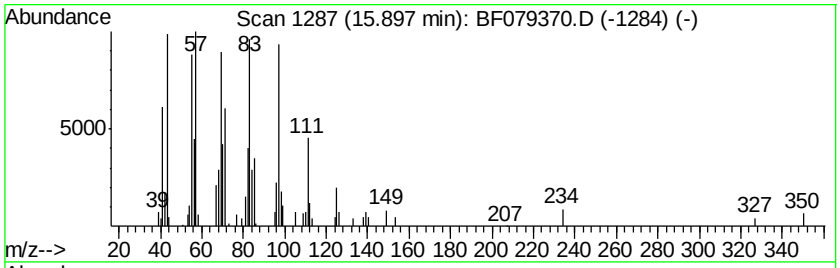
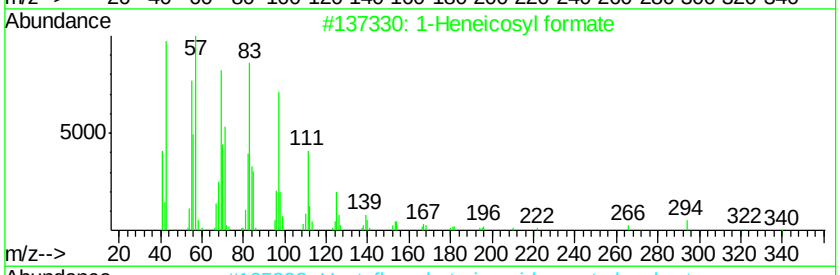
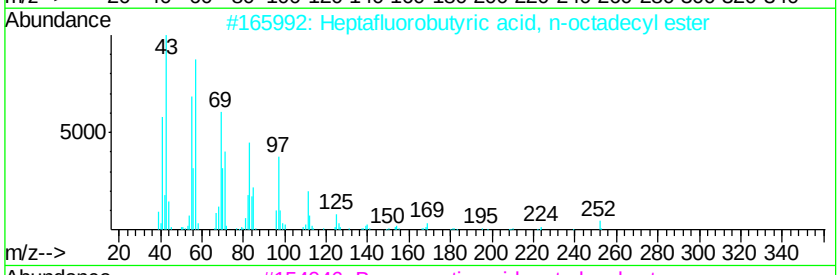
Peak Number 9 1-Heneicosyl formate Concentration Rank 9

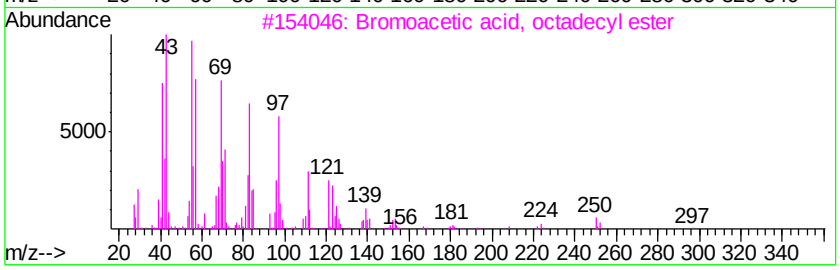
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	5.20 ng	164907	Chrysene-d12	16.01

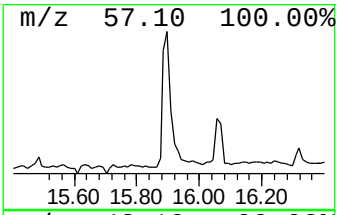
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
5	Cyclohexadecane	224	C16H32	000295-65-8	87

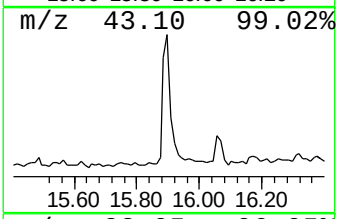


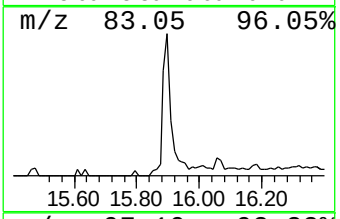


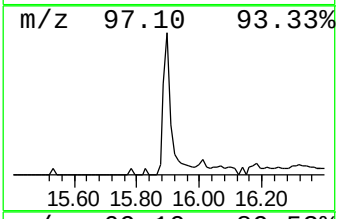


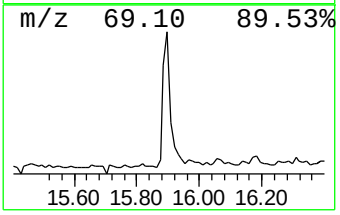












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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

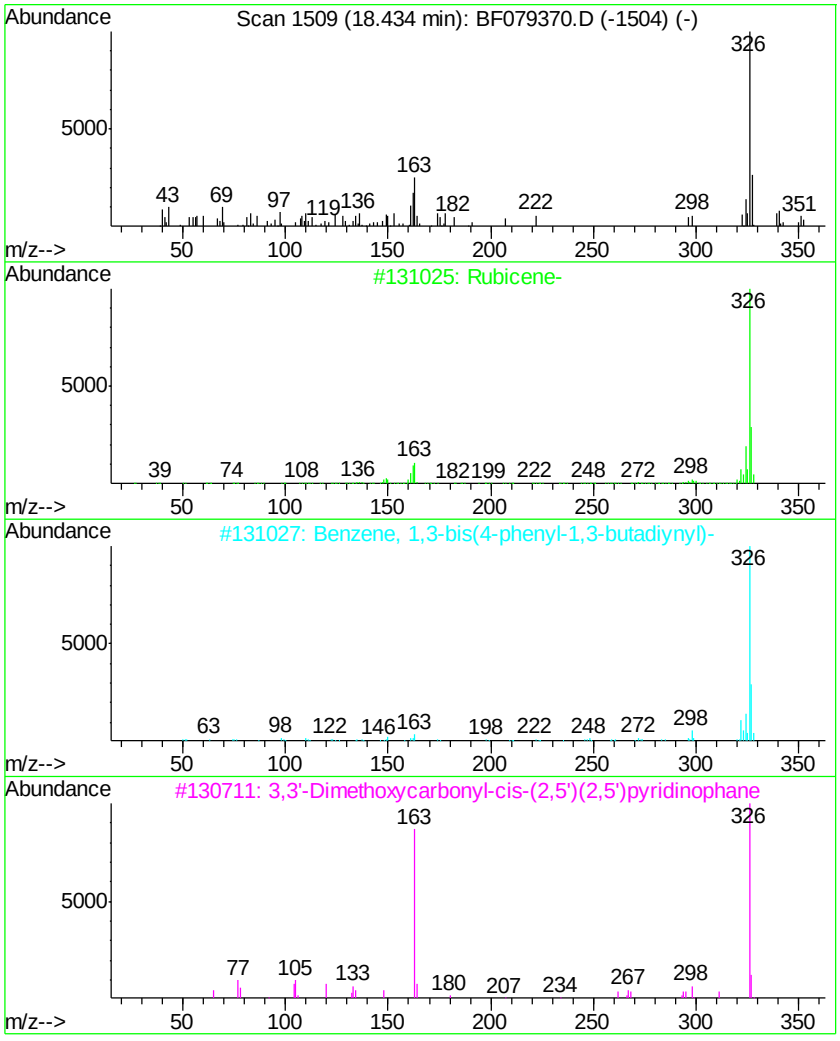
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

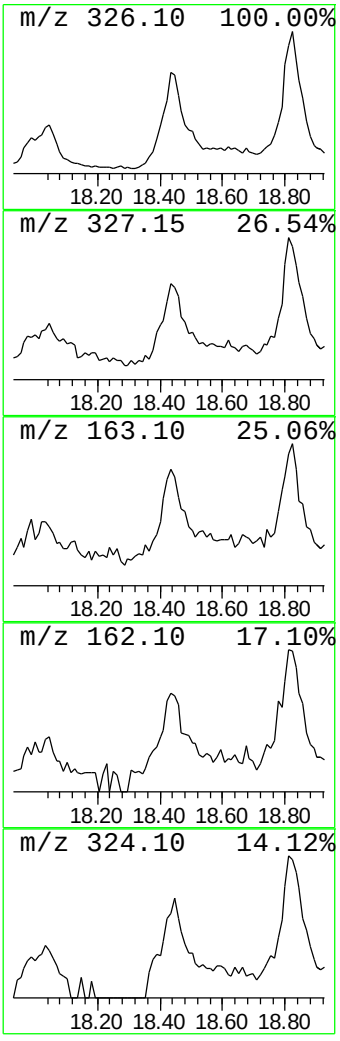
****

Peak Number 11 Rubicene- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	3.73 ng	103237	Perylene-d12	17.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Rubicene-	326	C26H14	000197-61-5	68
2	Benzene, 1,3-bis(4-phenyl-1,3-bu...	326	C26H14	037902-13-9	64
3	3,3'-Dimethoxycarbonyl-cis-(2,5'...	326	C18H18N2O4	1000148-86-9	52
4	Silane, (estra-1,3,5(10),16-tetr...	326	C21H30OSi	069688-27-3	50
5	Ajmaline	326	C20H26N2O2	004360-12-7	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051915\
Data File : BF079370.D
Acq On : 20 May 2015 6:52
Operator : TP/IZ
Sample : G2289-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.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
unknown1.28	1.28	255.2	ng	3437150	1	7.13	269352	20.0
Butane, 2-methoxy...	1.56	15.1	ng	202780	1	7.13	269352	20.0
2-Pentanone, 4-hy...	4.88	25.4	ng	341907	1	7.13	269352	20.0
unknown6.84	6.84	108.8	ng	1465990	1	7.13	269352	20.0
1-Heneicosyl formate	15.90	5.2	ng	164907	5	16.01	633962	20.0
Rubicene-	18.43	3.7	ng	103237	6	17.79	554166	20.0