LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088907.D
Acq On : 11 Jul 2016 18:56
Operator : UM/SJ
Sample : H3915-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q6-B2-0-11-C

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-BF063016.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	1.678	6	8	14	rVV	130755	195836	11.64%	1.113%
2	1.758	14	15	17	rVV	25462	26244	1.56%	0.149%
3	1.793	17	18	28	rVB	909139	1591367	94.61%	9.047%
4	2.890	111	114	121	rBV	25198	55773	3.32%	0.317%
5	4.170	224	226	229	rVB	19999	28746	1.71%	0.163%
6	4.867	285	287	292	rBB	85134	127510	7.58%	0.725%
7	5.313	323	326	328	rBV	1204476	1682091	100.00%	9.563%
8	6.353	414	417	420	rVB	1374600	1492873	88.75%	8.487%
9	6.479	425	428	430	rBV	1771012	1625959	96.66%	9.244%
10	6.707	446	448	450	rBB	425654	397348	23.62%	2.259%
11	6.867	459	462	464	rBB	1474014	1265244	75.22%	7.193%
12	7.279	495	498	500	rBV	1163307	1165857	69.31%	6.628%
13	7.725	534	537	543	rBB2	29273	50151	2.98%	0.285%
14	7.999	558	561	563	rBV	569015	542639	32.26%	3.085%
15	9.073	652	655	657	rBV	1871091	1633228	97.10%	9.285%
16	9.473	687	690	692	rVB	350878	383314	22.79%	2.179%
17	9.748	711	714	716	rBV	503311	518392	30.82%	2.947%
18	10.193	751	753	754	rVB	22953	20740	1.23%	0.118%
19	10.525	780	782	785	rBV2	900340	948281	56.38%	5.391%
20	10.662	790	794	799	rBV	34254	43495	2.59%	0.247%
21	11.108	831	833	834	rBV	32525	29315	1.74%	0.167%
22	11.222	841	843	844	rBV	445582	450522	26.78%	2.561%
23	11.531	868	870	872	rVB	22285	18254	1.09%	0.104%
24	12.422	946	948	950	rVB	71986	58617	3.48%	0.333%
25	12.685	964	971	979	rBV2	521023	835797	49.69%	4.752%
26	12.799	979	981	984	rVB	1144940	1132451	67.32%	6.438%
27	13.702	1058	1060	1064	rVB2	94495	116617	6.93%	0.663%
28	13.839	1069	1072	1076	rBV	508155	515017	30.62%	2.928%
29	14.342	1113	1116	1120	rBV2	19552	40399	2.40%	0.230%
30	14.754	1150	1152	1154	rBV2	16592	18619	1.11%	0.106%
31	14.834	1156	1159	1163	rVV	41512	72137	4.29%	0.410%
32	15.097	1180	1182	1185	rVB	23739	33358	1.98%	0.190%
33	15.154	1185	1187	1189	rBV	26610	29570	1.76%	0.168%
34	15.211	1189	1192	1195	rBV	297524	339452	20.18%	1.930%

LSC Area Percent Report

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Misc :
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Instrument :
BNA_F
ClientSampleId :
Q6-B2-0-11-C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.645	1228	1230	1232	rBV	10642	18819	1.12%	0.107%
36	15.691	1232	1234	1238	rVB3	14189	31258	1.86%	0.178%
37	16.491	1302	1304	1309	rVB2	13332	30892	1.84%	0.176%
38	16.880	1335	1338	1342	rBV	11965	23716	1.41%	0.135%

Sum of corrected areas: 17589898

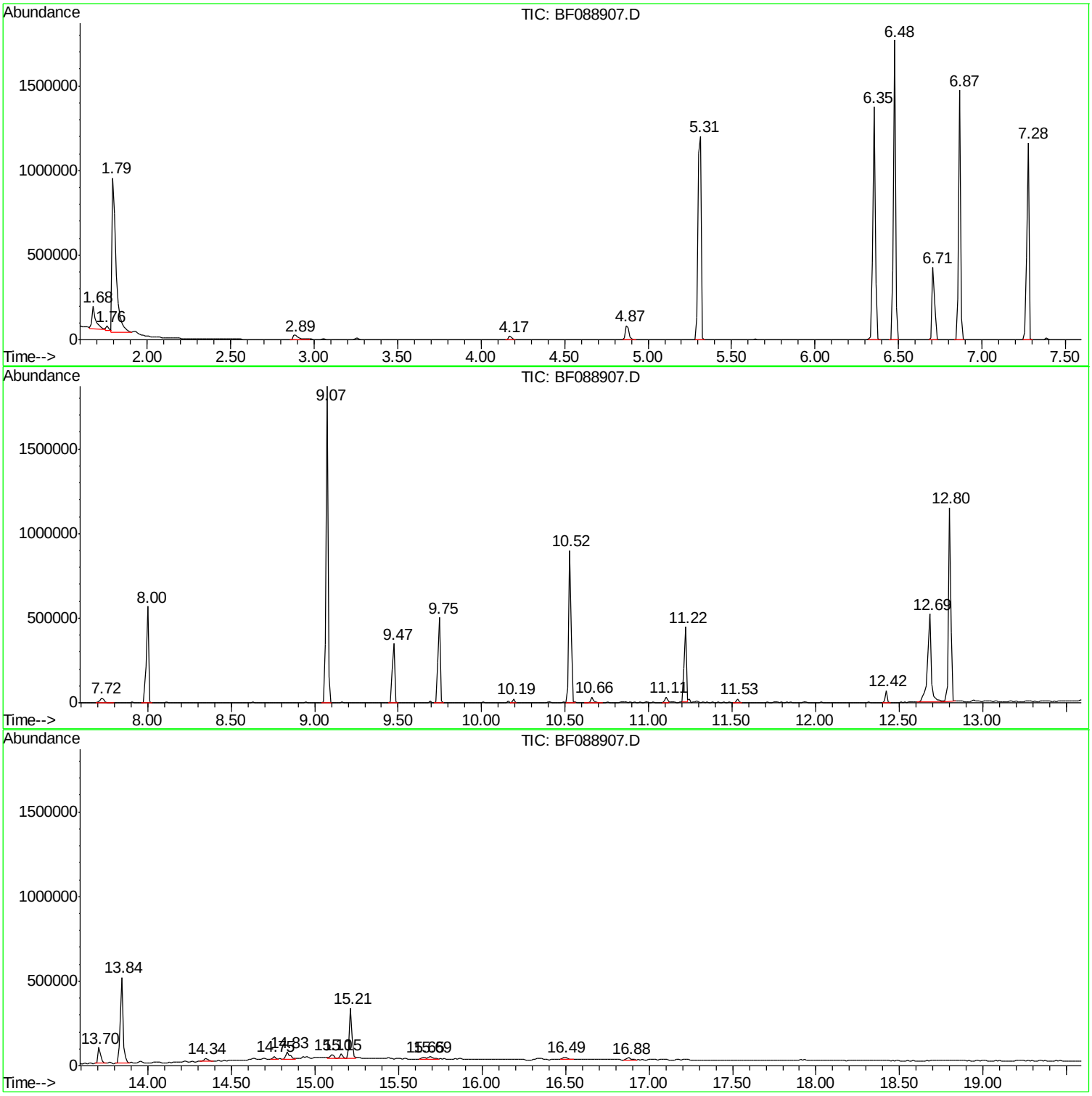
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088907.D
Acq On : 11 Jul 2016 18:56
Operator : UM/SJ
Sample : H3915-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q6-B2-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088907.D
Acq On : 11 Jul 2016 18:56
Operator : UM/SJ
Sample : H3915-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q6-B2-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

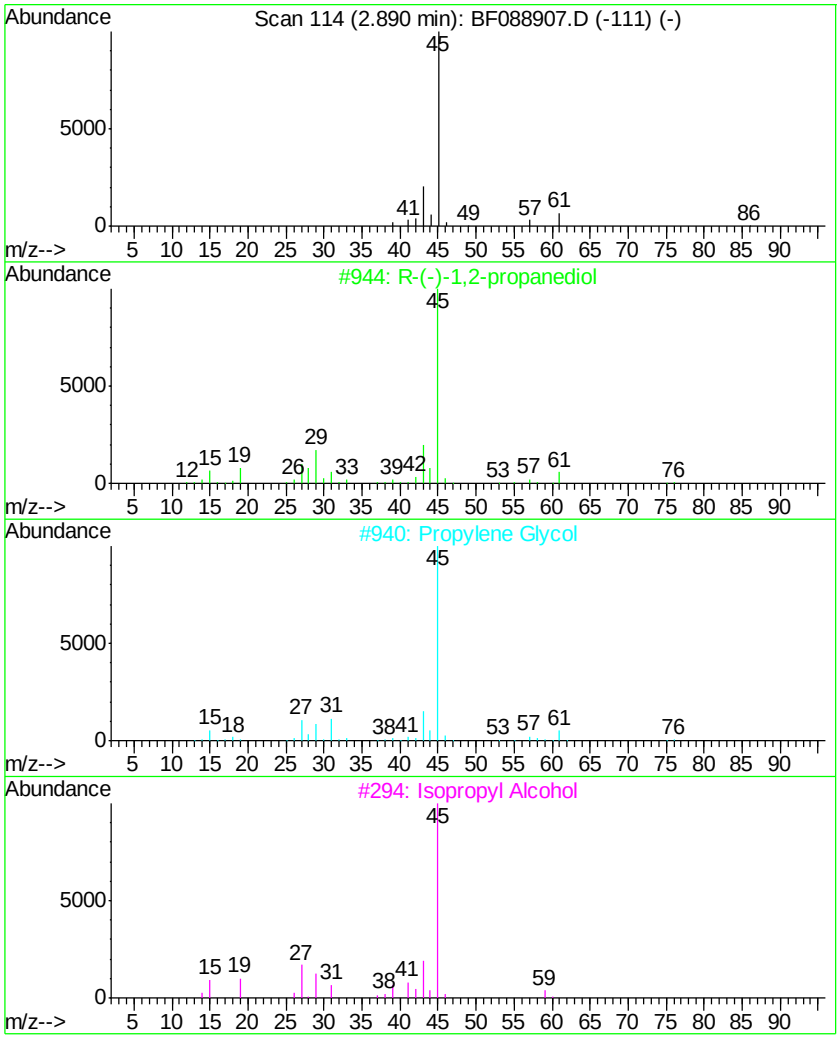
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

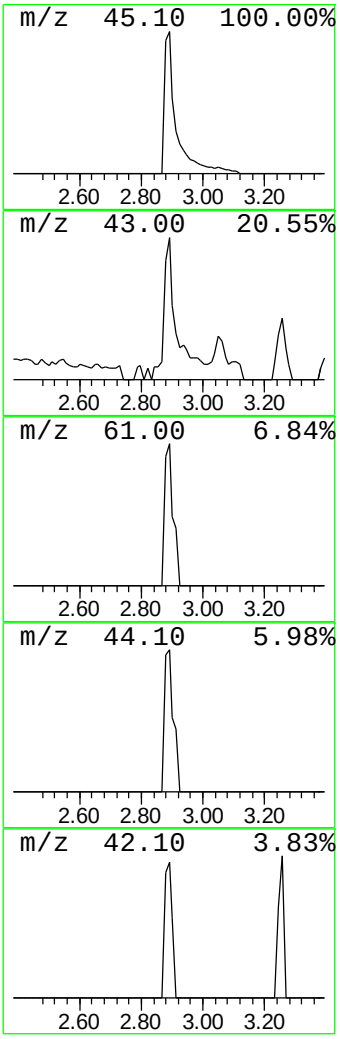
****

Peak Number 3 R-(-)-1,2-propanediol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	2.81 ng	55773	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5	Formamide	45	CH3NO	000075-12-7	5





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
Data File : BF088907.D
Acq On : 11 Jul 2016 18:56
Operator : UM/SJ
Sample : H3915-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q6-B2-0-11-C

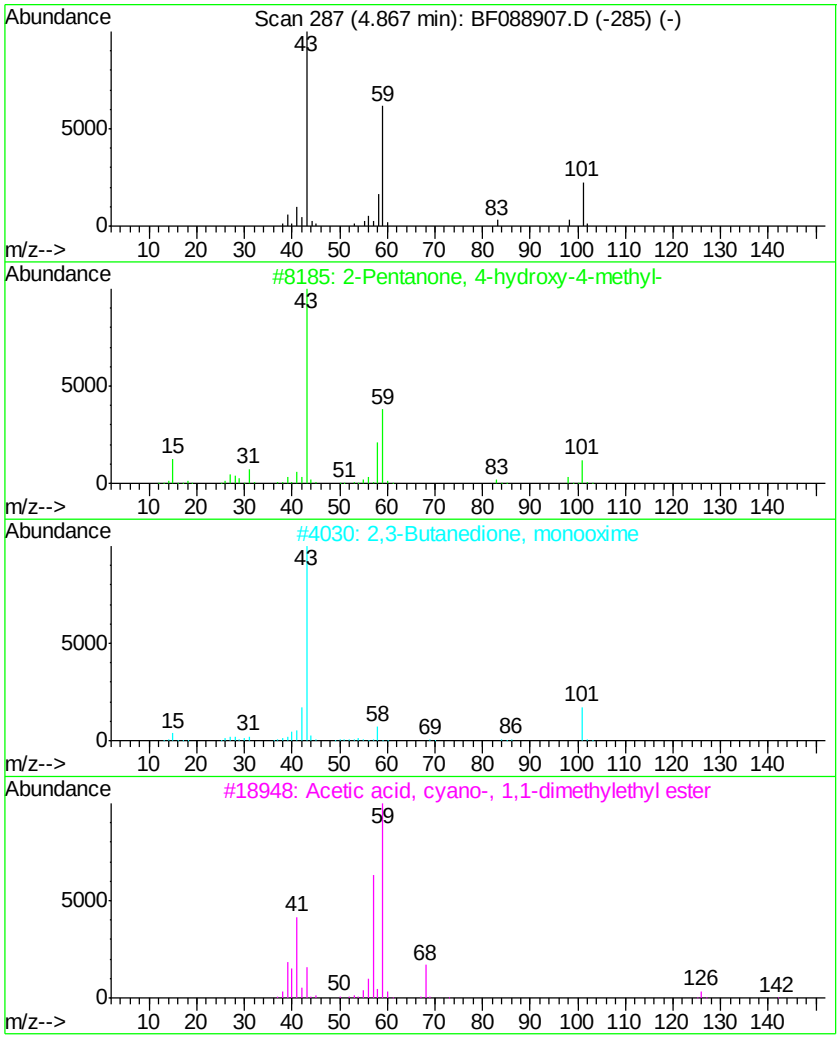
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

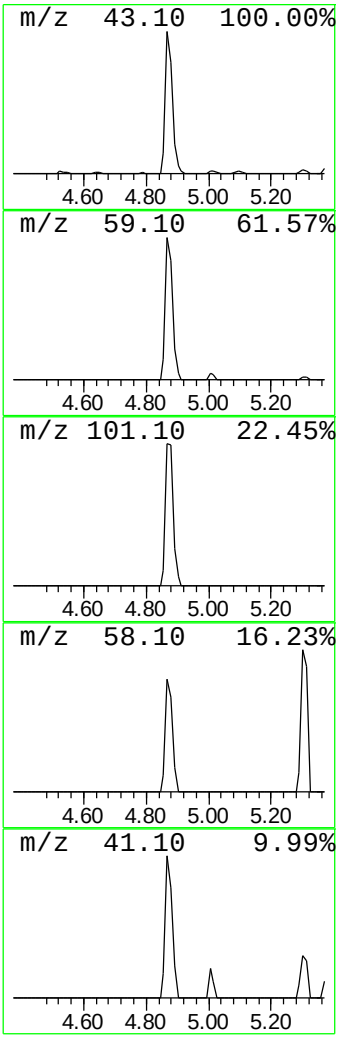
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	6.42 ng	127510	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071116\
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Sample : H3915-05
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Instrument :
BNA_F
ClientSampleId :
Q6-B2-0-11-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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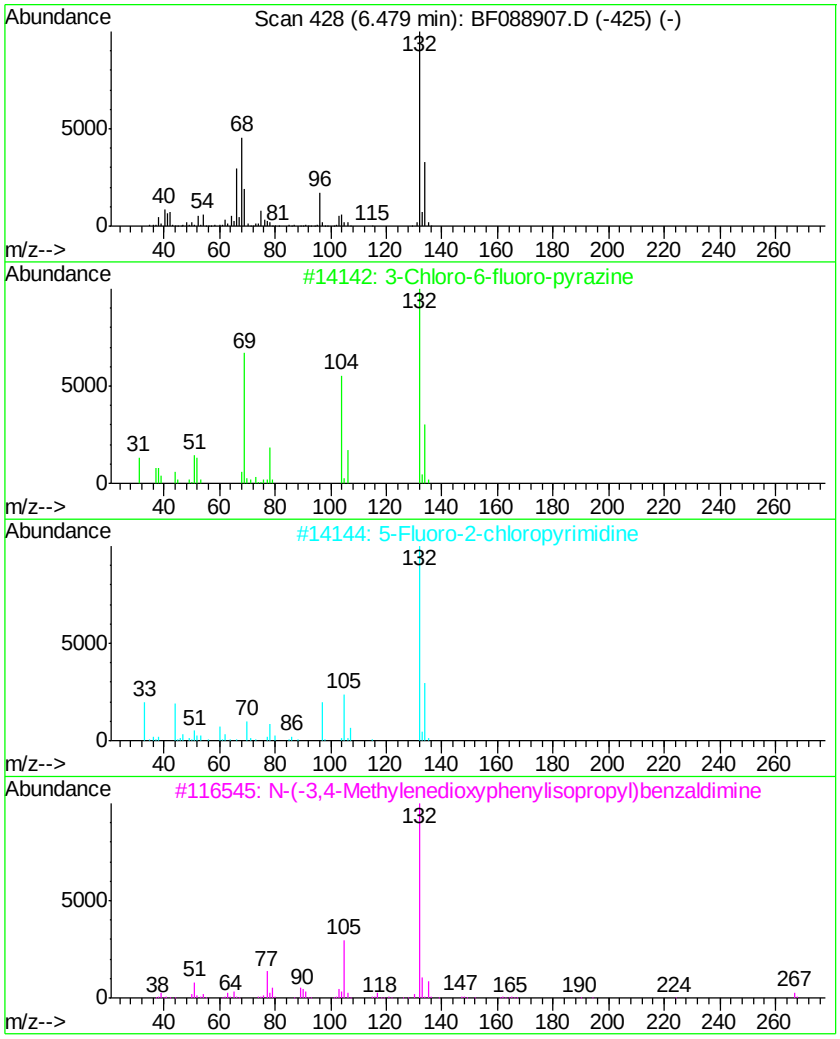
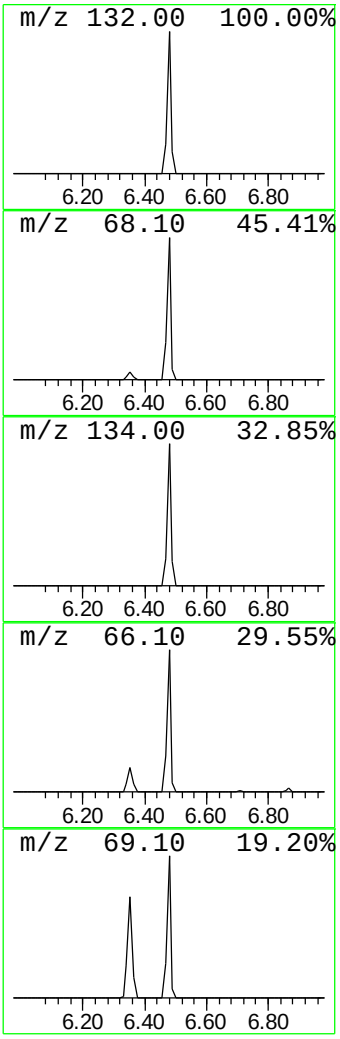
****
Peak Number 5 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	81.84 ng	1625960	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Q6-B2-0-11-C

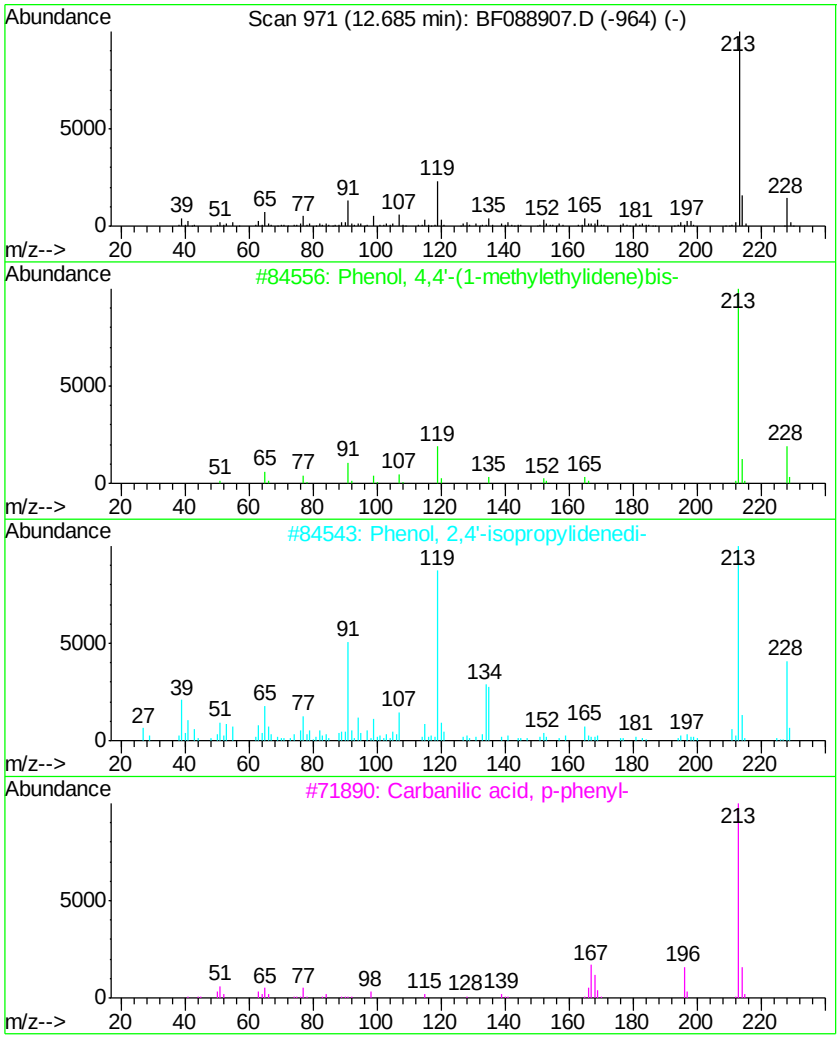
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

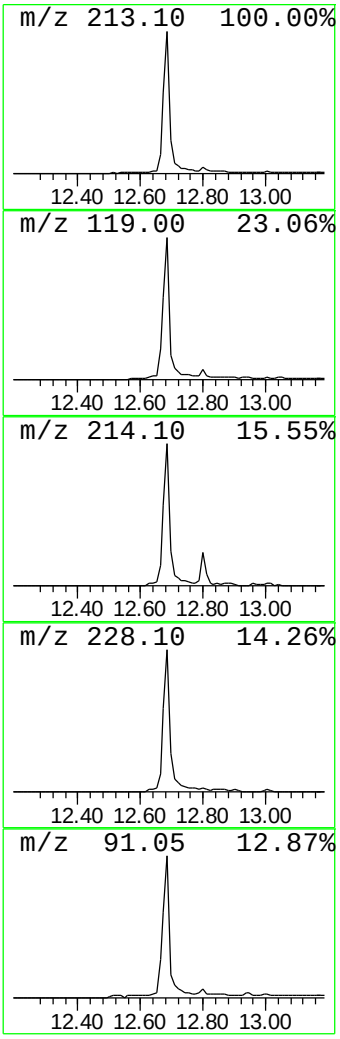
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	32.46 ng	835797	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	50
3	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	47
4	2,4(1H,3H)-Pyrimidinedione, 1,3-...	228	C9H16N2O3Si	089447-84-7	42
5	1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	40





Library Search Compound Report

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BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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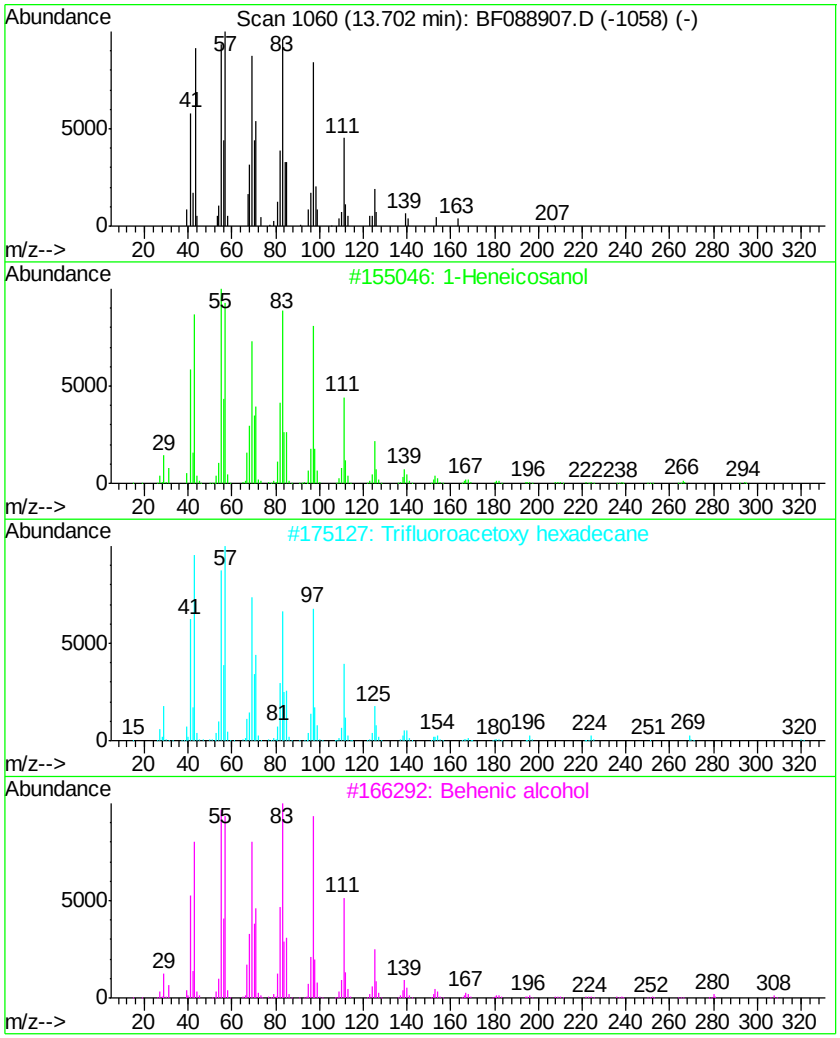
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

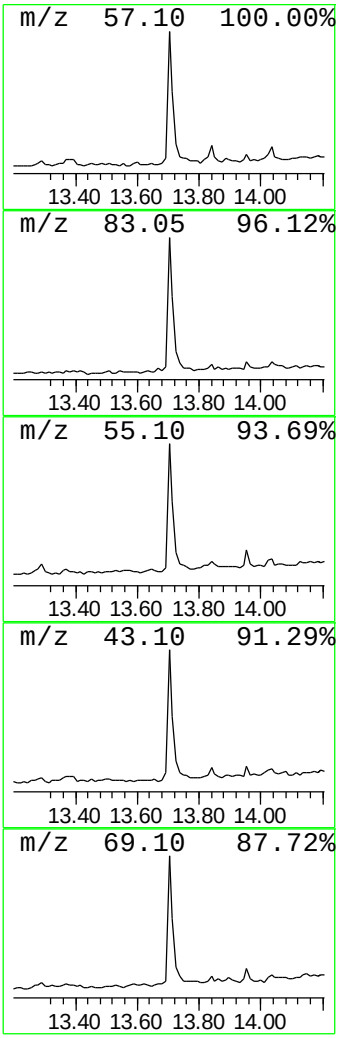
****

Peak Number 8 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	4.53 ng	116617	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
R-(-)-1,2-propane...	2.89	2.8	ng	55773	1	6.71	397348	20.0
2-Pentanone, 4-hy...	4.87	6.4	ng	127510	1	6.71	397348	20.0
unknown6.48	6.48	81.8	ng	1625960	1	6.71	397348	20.0
Phenol, 4,4'-(1-m...	12.69	32.5	ng	835797	5	13.84	515017	20.0
1-Heneicosanol	13.70	4.5	ng	116617	5	13.84	515017	20.0