LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088168.D
Acq On : 19 Jun 2016 8:07
Operator : UM/SJ
Sample : H3628-13
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-18

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-BF060716.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	1.667	6	7	15	rVV	38564	62863	2.75%	0.375%
2	1.781	15	17	45	rVB	507487	871511	38.12%	5.193%
3	4.833	282	284	290	rBV	53212	66974	2.93%	0.399%
4	5.279	321	323	326	rBV	1028226	996173	43.57%	5.936%
5	6.342	414	416	418	rBV	488901	618599	27.06%	3.686%
6	6.456	424	426	428	rBV	1929359	1751212	76.59%	10.434%
7	6.684	444	446	448	rBV	614747	542695	23.74%	3.234%
8	6.844	457	460	462	rVB	1573686	1823019	79.73%	10.862%
9	7.256	493	496	498	rBV	1354727	1372808	60.04%	8.180%
10	7.965	556	558	561	rBV	467128	623433	27.27%	3.715%
11	8.605	613	614	616	rVB	28673	31351	1.37%	0.187%
12	8.708	621	623	630	rBV2	23601	52734	2.31%	0.314%
13	9.050	650	653	655	rBV	2487395	2286444	100.00%	13.624%
14	9.450	686	688	690	rBV	38360	39805	1.74%	0.237%
15	9.725	709	712	713	rBV	458331	593633	25.96%	3.537%
16	9.748	713	714	717	rVB	25852	26676	1.17%	0.159%
17	9.896	724	727	730	rBV	28043	49579	2.17%	0.295%
18	10.159	748	750	752	rVB	38175	31529	1.38%	0.188%
19	10.239	752	757	762	rVB	16686	30247	1.32%	0.180%
20	10.376	767	769	772	rVB	249825	213090	9.32%	1.270%
21	10.513	778	781	783	rBV2	838767	1060913	46.40%	6.321%
22	10.571	785	786	789	rVV	203429	229777	10.05%	1.369%
23	10.628	789	791	795	rVB	30704	42155	1.84%	0.251%
24	11.199	838	841	843	rBV	614945	523965	22.92%	3.122%
25	12.411	945	947	948	rBV	37048	35588	1.56%	0.212%
26	12.571	958	961	963	rBV	19221	24719	1.08%	0.147%
27	12.616	963	965	968	rVV2	26917	44774	1.96%	0.267%
28	12.788	977	980	982	rBV	1457993	1863348	81.50%	11.103%
29	13.702	1057	1060	1065	rVB	18723	29764	1.30%	0.177%
30	13.828	1068	1071	1074	rBV	518292	481256	21.05%	2.868%
31	15.211	1189	1192	1198	rBV	296712	362276	15.84%	2.159%

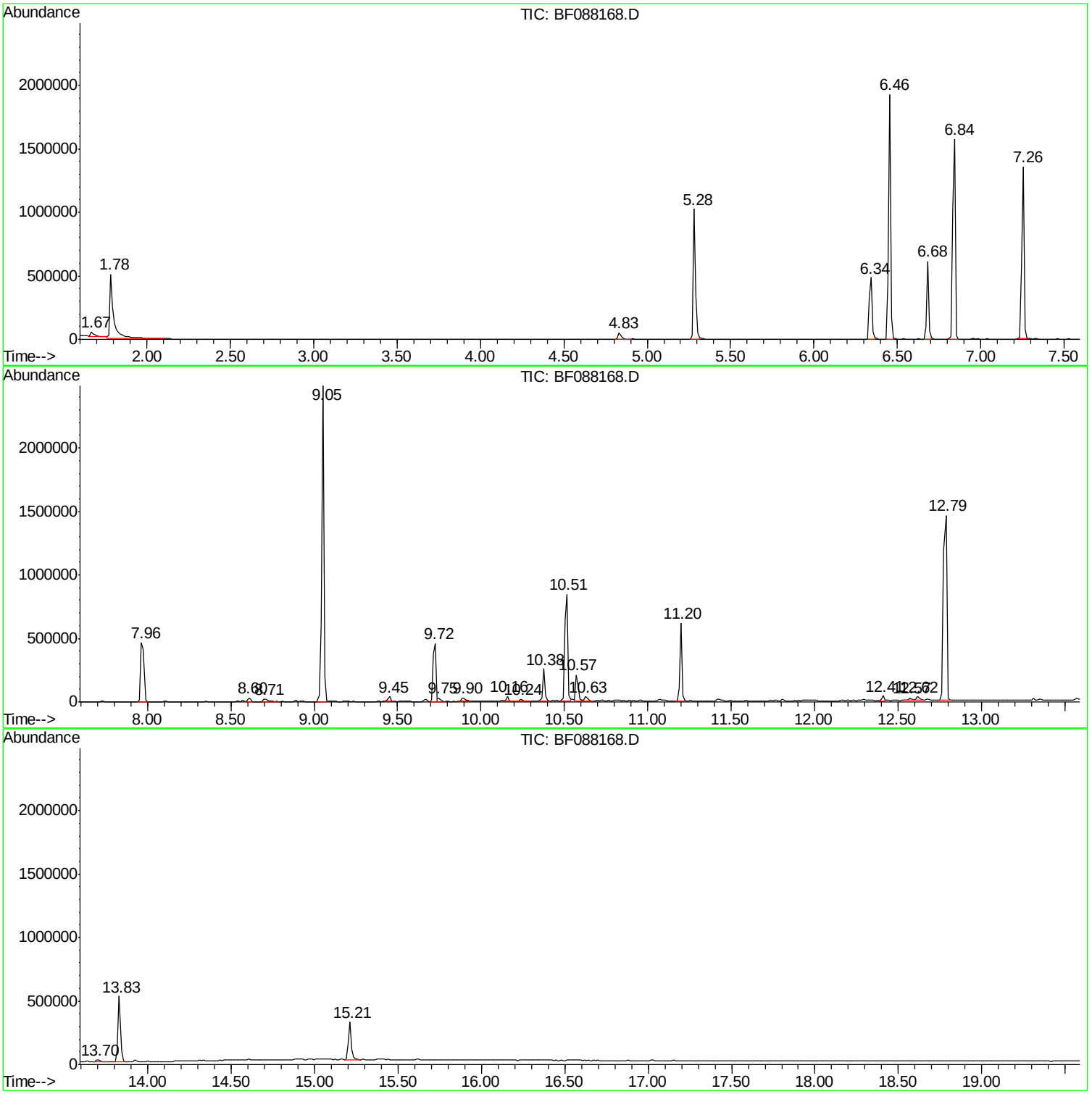
Sum of corrected areas: 16782910

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088168.D
Acq On : 19 Jun 2016 8:07
Operator : UM/SJ
Sample : H3628-13
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF061816\
Data File : BF088168.D
Acq On : 19 Jun 2016 8:07
Operator : UM/SJ
Sample : H3628-13
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

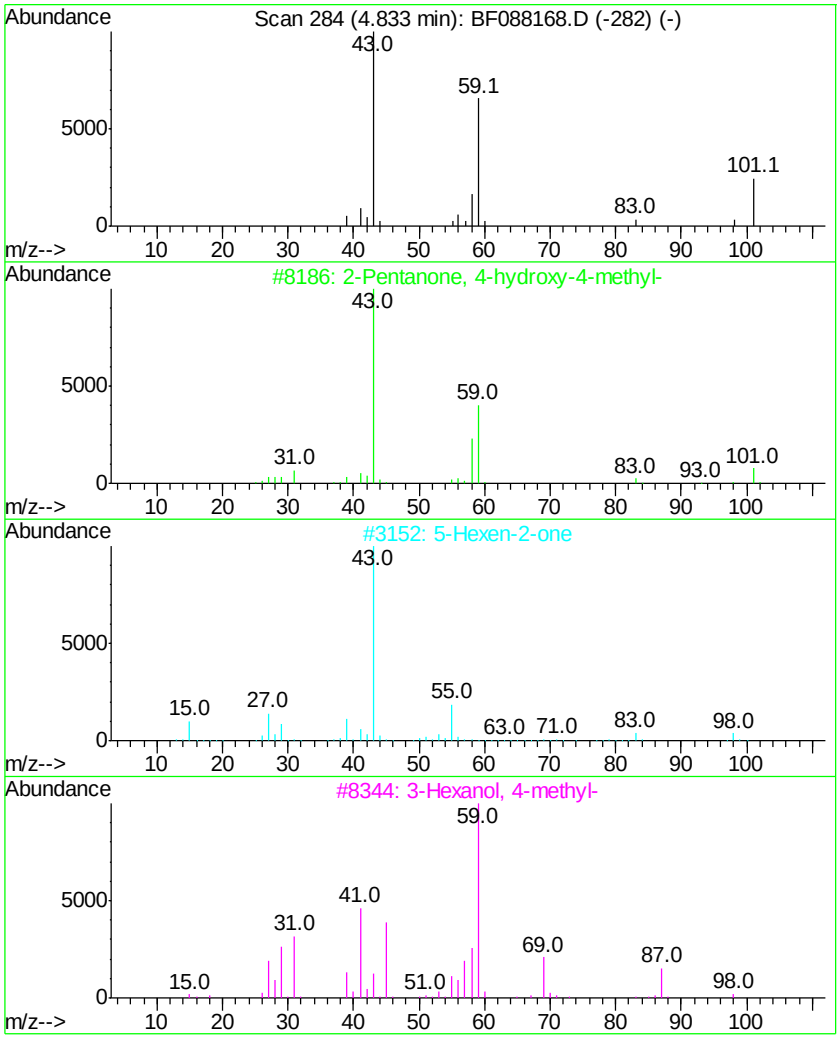
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

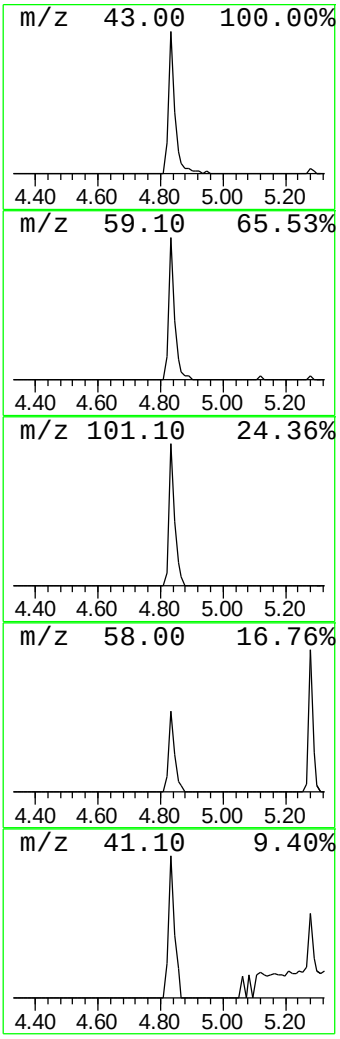
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	2.47 ng	66974	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088168.D
Acq On : 19 Jun 2016 8:07
Operator : UM/SJ
Sample : H3628-13
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

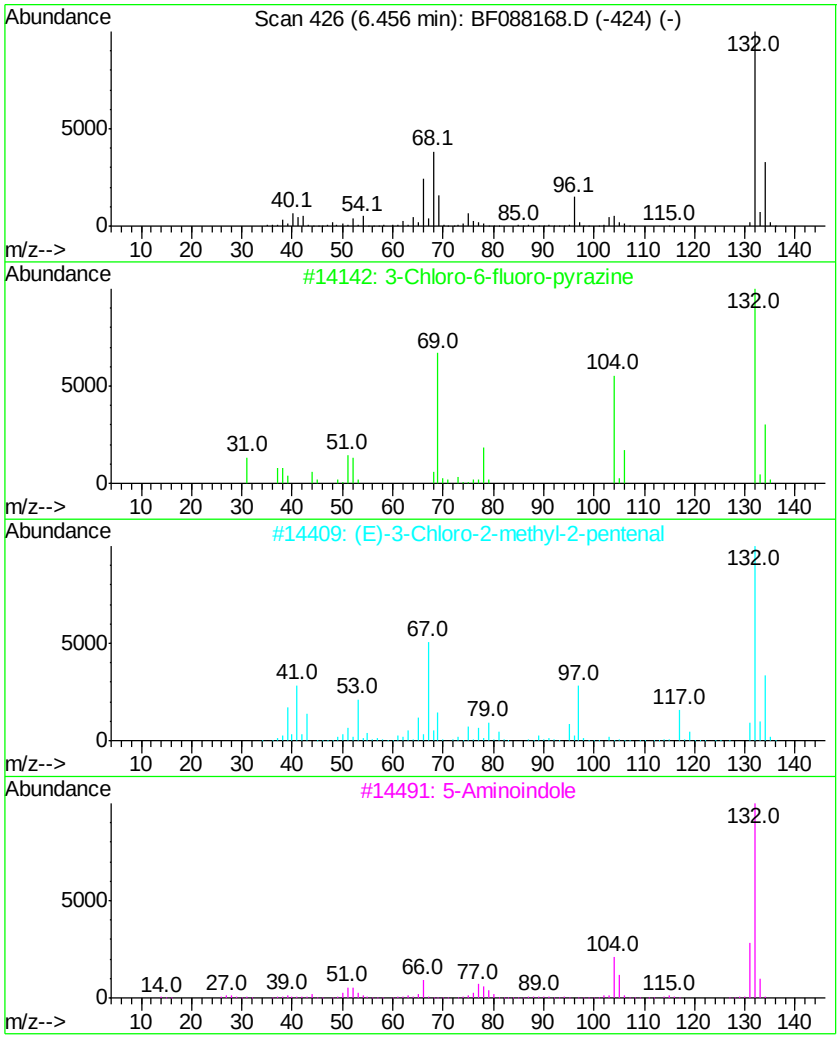
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

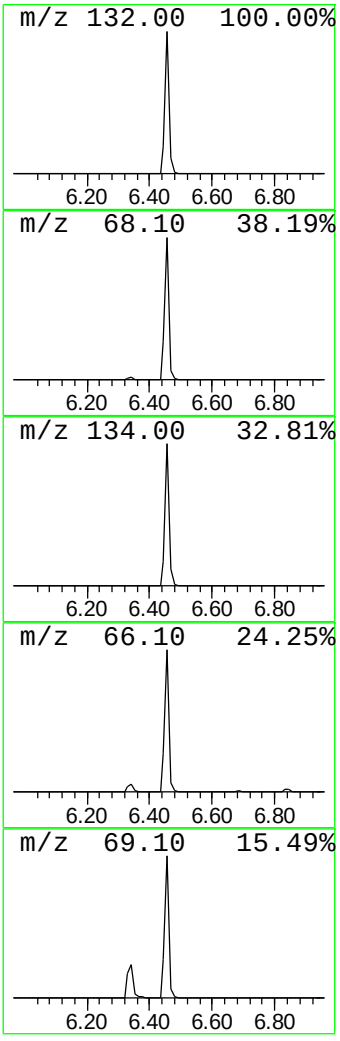
****

Peak Number 4 unknown6.46 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	64.54 ng	1751210	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088168.D
Acq On : 19 Jun 2016 8:07
Operator : UM/SJ
Sample : H3628-13
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

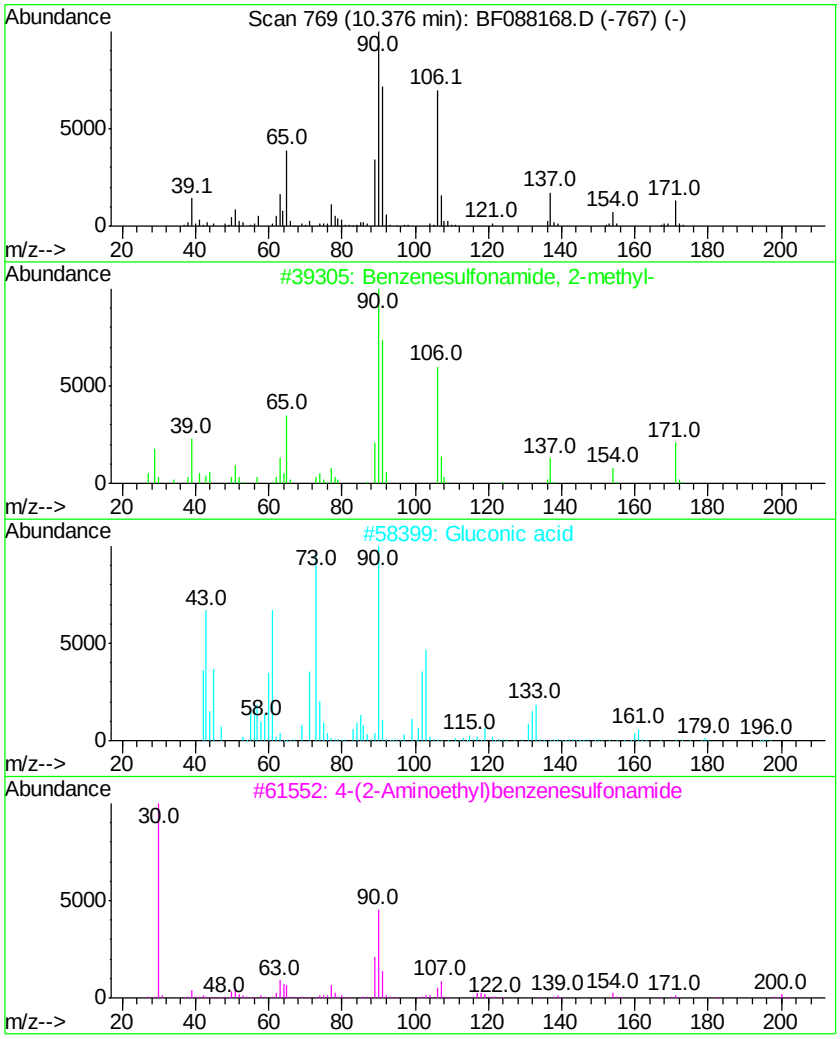
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

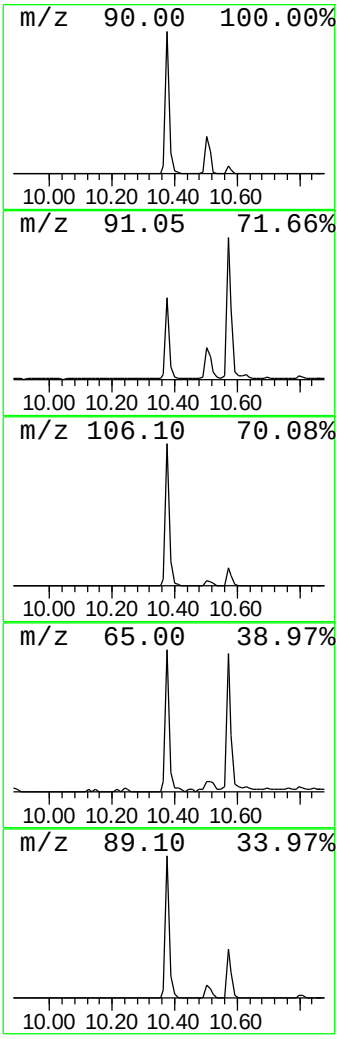
****

Peak Number 6 Benzenesulfonamide, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	7.18 ng	213090	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	96
2	Gluconic acid	196	C6H12O7	000526-95-4	43
3	4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	38
4	2,4-Octadiyne	106	C8H10	002809-71-4	25
5	Thiourea, methyl-	90	C2H6N2S	000598-52-7	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088168.D
Acq On : 19 Jun 2016 8:07
Operator : UM/SJ
Sample : H3628-13
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

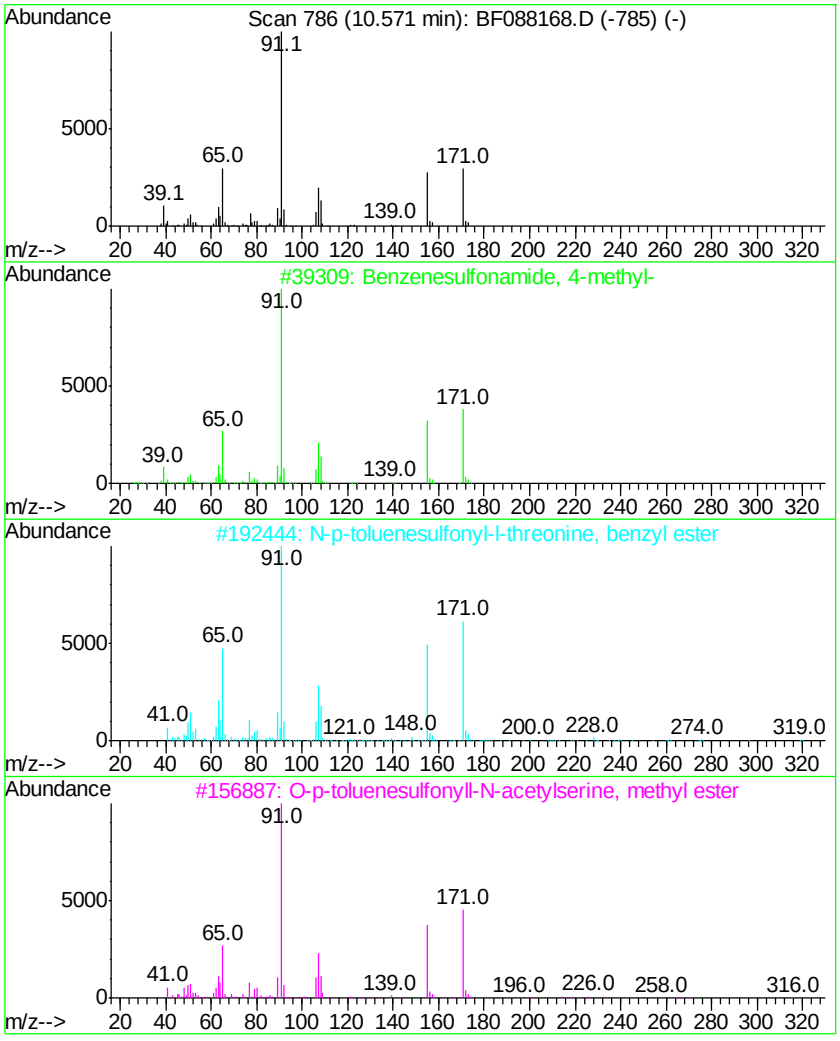
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

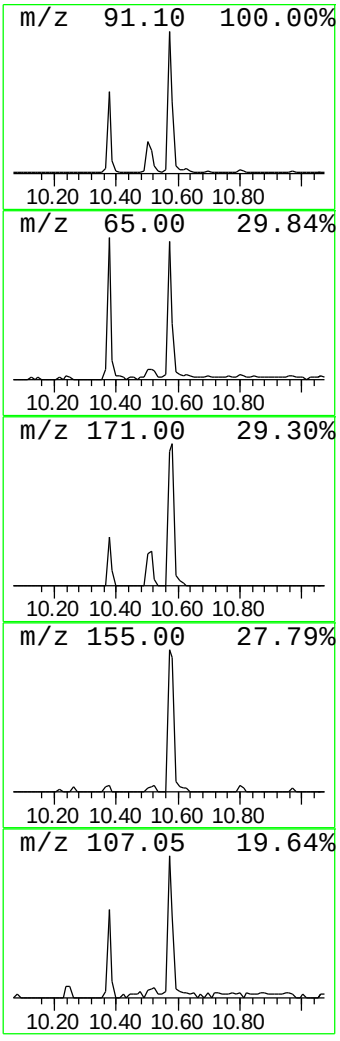
****

Peak Number 7 Benzenesulfonamide, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	8.77 ng	229777	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	83
3	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	64
4	Benzenemethanesulfonamide	171	C7H9NO2S	004563-33-1	47
5	1-Hydroxytricyclo[4.3.0.0(4,9)]n...	308	C16H20O4S	201992-83-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088168.D
Acq On : 19 Jun 2016 8:07
Operator : UM/SJ
Sample : H3628-13
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	2.5	ng	66974	1	6.68	542695	20.0
unknown6.46	6.46	64.5	ng	1751210	1	6.68	542695	20.0
Benzenesulfonamid...	10.38	7.2	ng	213090	3	9.72	593633	20.0
Benzenesulfonamid...	10.57	8.8	ng	229777	4	11.20	523965	20.0