LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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	5	7	11	rBV	57456	79740	4.04%	0.421%
2	1.735	11	13	15	rVV	28066	37728	1.91%	0.199%
3	1.781	15	17	24	rVV	578425	800942	40.62%	4.230%
4	1.884	24	26	40	rVB2	55077	148451	7.53%	0.784%
5	2.913	115	116	122	rBV	14301	36312	1.84%	0.192%
6	3.210	139	142	146	rVB	12916	25126	1.27%	0.133%
7	4.844	283	285	292	rBV	92763	123098	6.24%	0.650%
8	5.290	322	324	327	rBV	1710531	1715684	87.00%	9.061%
9	6.341	413	416	419	rBV2	1332636	1809341	91.75%	9.555%
10	6.456	424	426	429	rBV	1592780	1681652	85.28%	8.881%
11	6.684	444	446	449	rBV	634702	534526	27.11%	2.823%
12	6.844	457	460	462	rBV	1658662	1619875	82.14%	8.555%
13	7.256	493	496	498	rBV	1104377	1067898	54.15%	5.640%
14	7.382	501	507	512	rVB3	13055	26326	1.33%	0.139%
15	7.976	556	559	561	rBV	655094	684916	34.73%	3.617%
16	9.050	650	653	656	rBV	2055355	1972018	100.00%	10.414%
17	9.450	685	688	690	rBV	793461	660482	33.49%	3.488%
18	9.542	692	696	705	rVB	14971	30664	1.55%	0.162%
19	9.725	709	712	714	rBV	719913	667489	33.85%	3.525%
20	10.513	778	781	783	rBV	672187	762457	38.66%	4.027%
21	10.548	783	784	790	rVB	18241	23559	1.19%	0.124%
22	10.639	790	792	795	rBV2	24499	41747	2.12%	0.220%
23	11.085	829	831	832	rBV	27337	34618	1.76%	0.183%
24	11.199	839	841	844	rVB	662436	560318	28.41%	2.959%
25	11.451	859	863	866	rBV	21153	33988	1.72%	0.179%
26	11.508	866	868	870	rVV	38877	37753	1.91%	0.199%
27	12.102	919	920	924	rBV4	9967	20713	1.05%	0.109%
28	12.788	977	980	982	rBV	1665081	1701426	86.28%	8.985%
29	12.936	992	993	996	rVB3	19742	20847	1.06%	0.110%
30	13.119	1008	1009	1012	rBV3	24064	48147	2.44%	0.254%
31	13.188	1013	1015	1021	rVB6	25729	80257	4.07%	0.424%
32	13.268	1021	1022	1024	rVB2	27061	21106	1.07%	0.111%
33	13.314	1024	1026	1027	rBV2	24758	20068	1.02%	0.106%
34	13.371	1028	1031	1032	rBV2	34250	66560	3.38%	0.352%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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

35	13.519	1042	1044	1047	rBV2	52543	71906	3.65%	0.380%
36	13.634	1050	1054	1058	rBV	45680	105719	5.36%	0.558%
37	13.702	1058	1060	1063	rVV2	40930	64686	3.28%	0.342%
38	13.828	1069	1071	1074	rBV	541378	571019	28.96%	3.016%
39	13.885	1074	1076	1078	rVV2	27923	33371	1.69%	0.176%
40	13.931	1078	1080	1084	rVB	34847	40940	2.08%	0.216%
41	14.091	1092	1094	1095	rBV2	31775	34187	1.73%	0.181%
42	14.137	1095	1098	1102	rVV6	43998	109625	5.56%	0.579%
43	14.274	1107	1110	1112	rVV3	35338	54921	2.79%	0.290%
44	14.582	1135	1137	1141	rBV2	24457	57137	2.90%	0.302%
45	15.211	1190	1192	1198	rVB	333473	425124	21.56%	2.245%
46	17.828	1419	1421	1423	rVB2	36041	30932	1.57%	0.163%
47	18.080	1442	1443	1444	rBV	42221	30305	1.54%	0.160%
48	18.526	1480	1482	1487	rVB4	59923	109894	5.57%	0.580%

Sum of corrected areas: 18935598

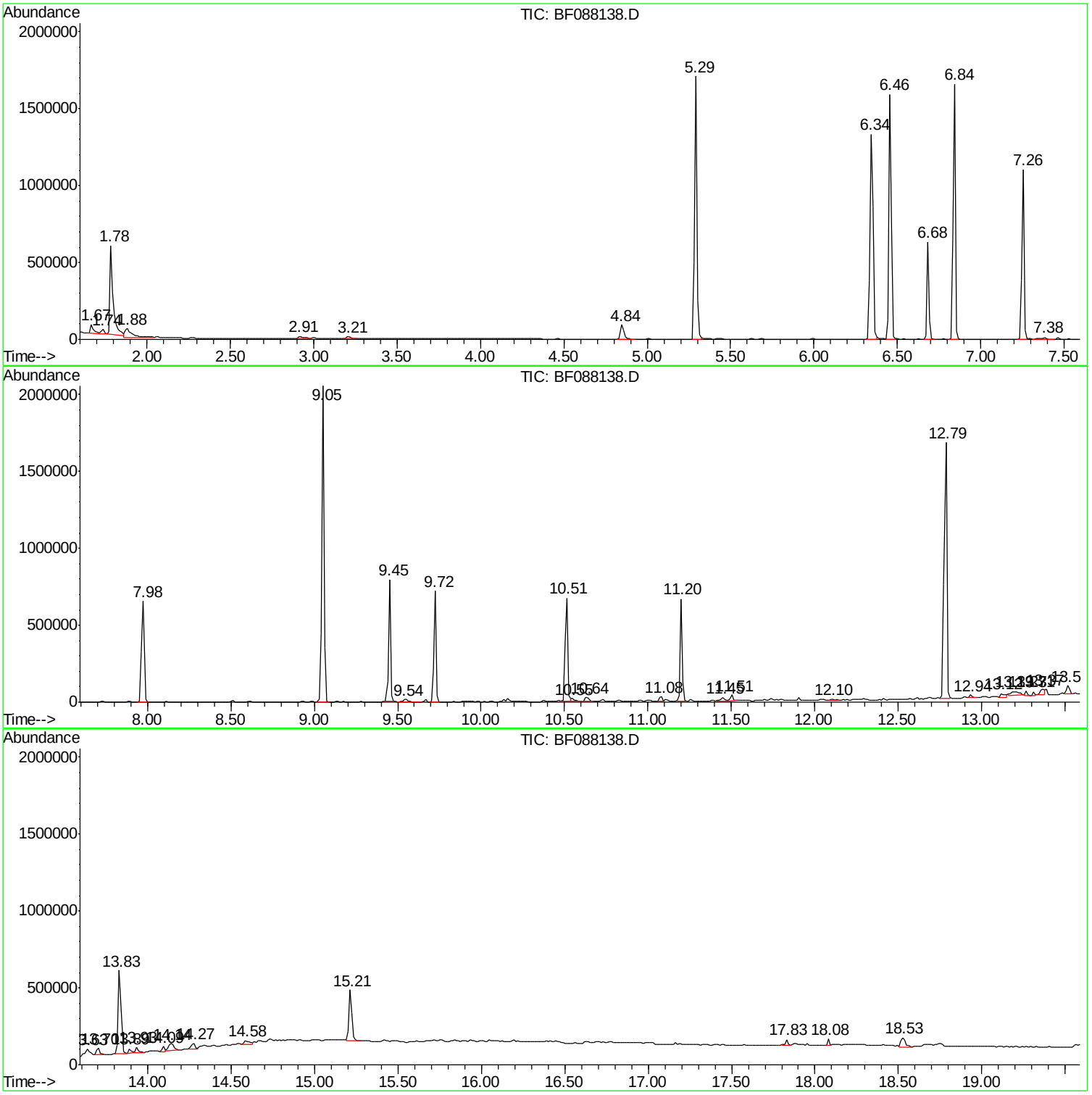
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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

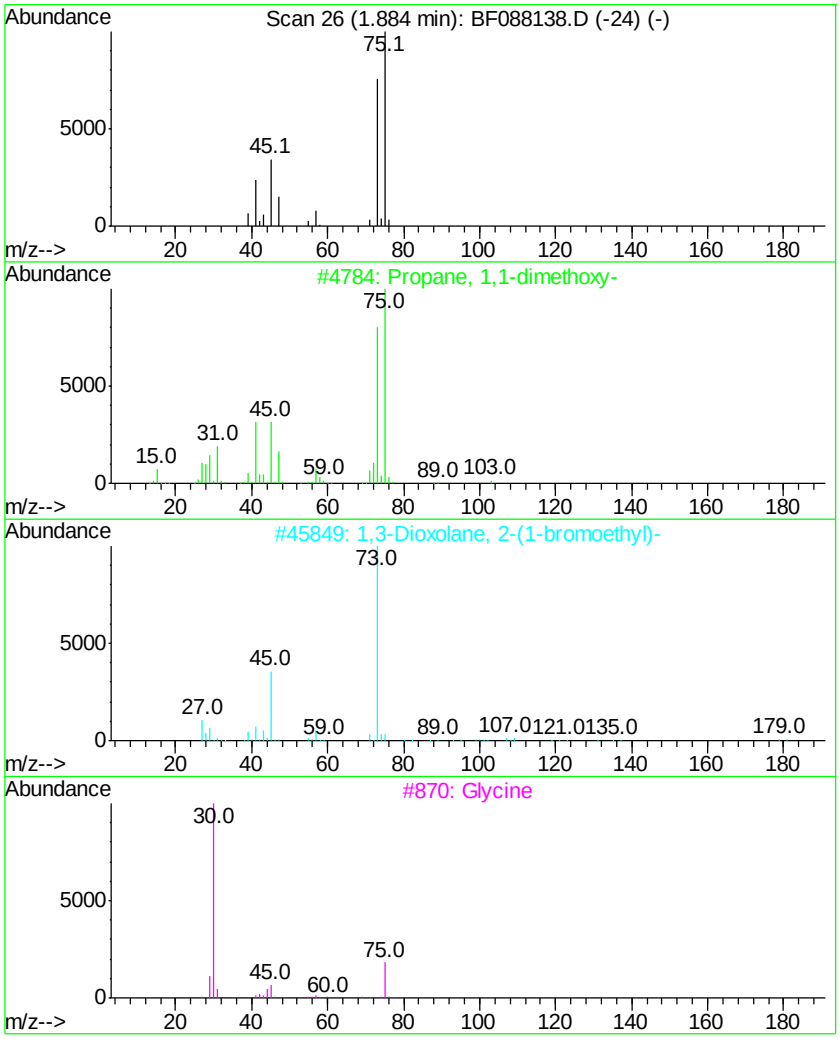
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

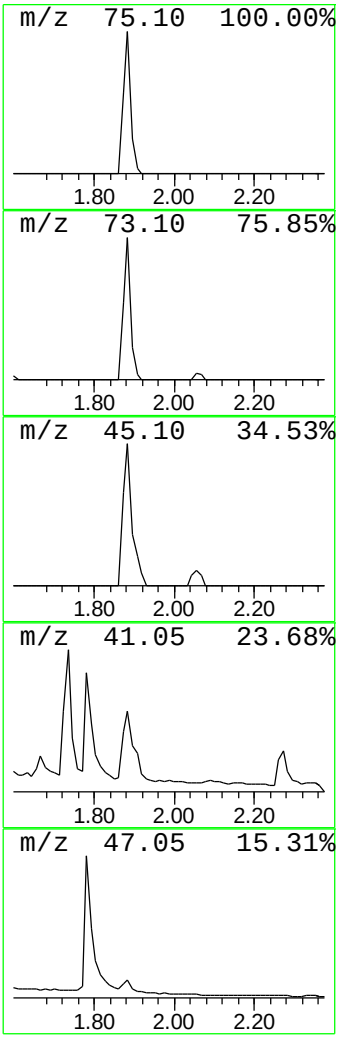
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.88	5.55 ng	148451	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
3	Glycine	75	C2H5NO2	000056-40-6	9
4	Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9
5	1-Butanamine	73	C4H11N	000109-73-9	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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

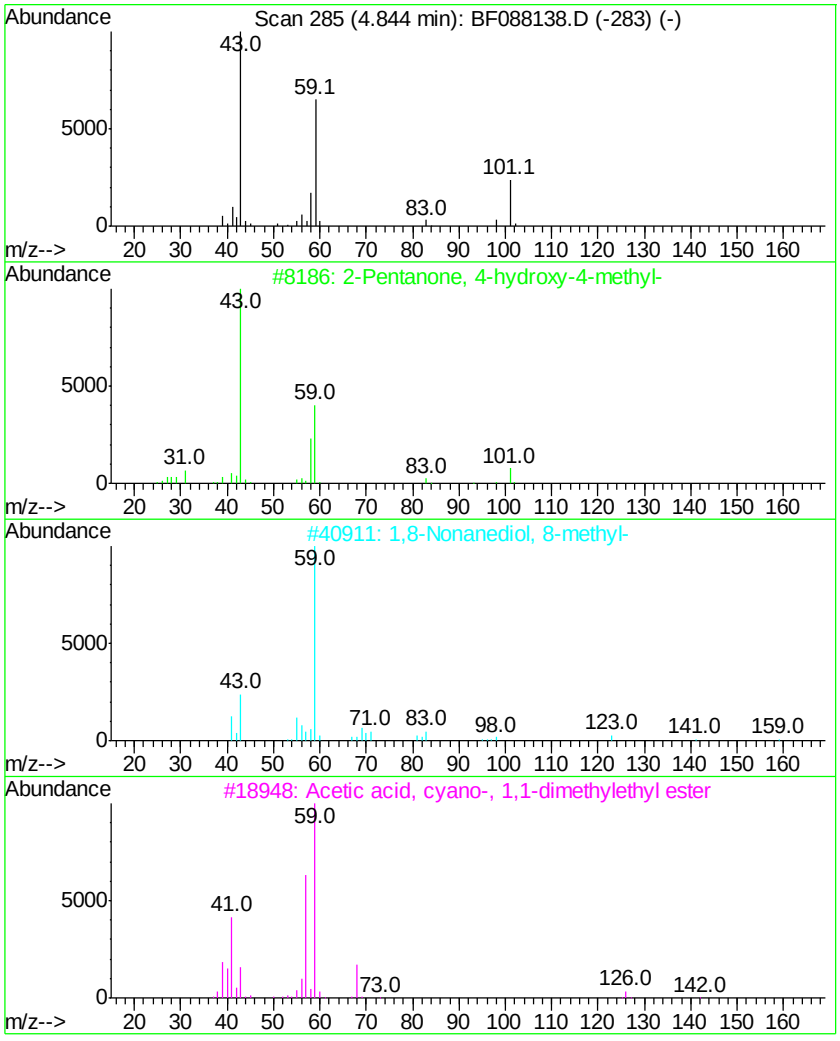
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

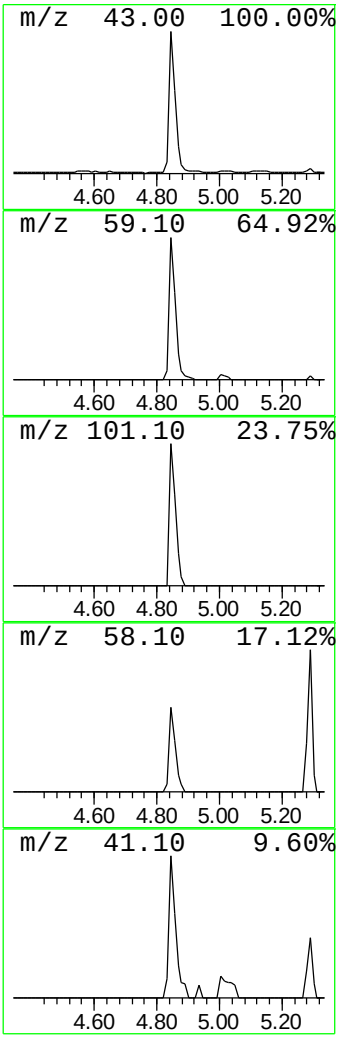
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	4.61 ng	123098	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	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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

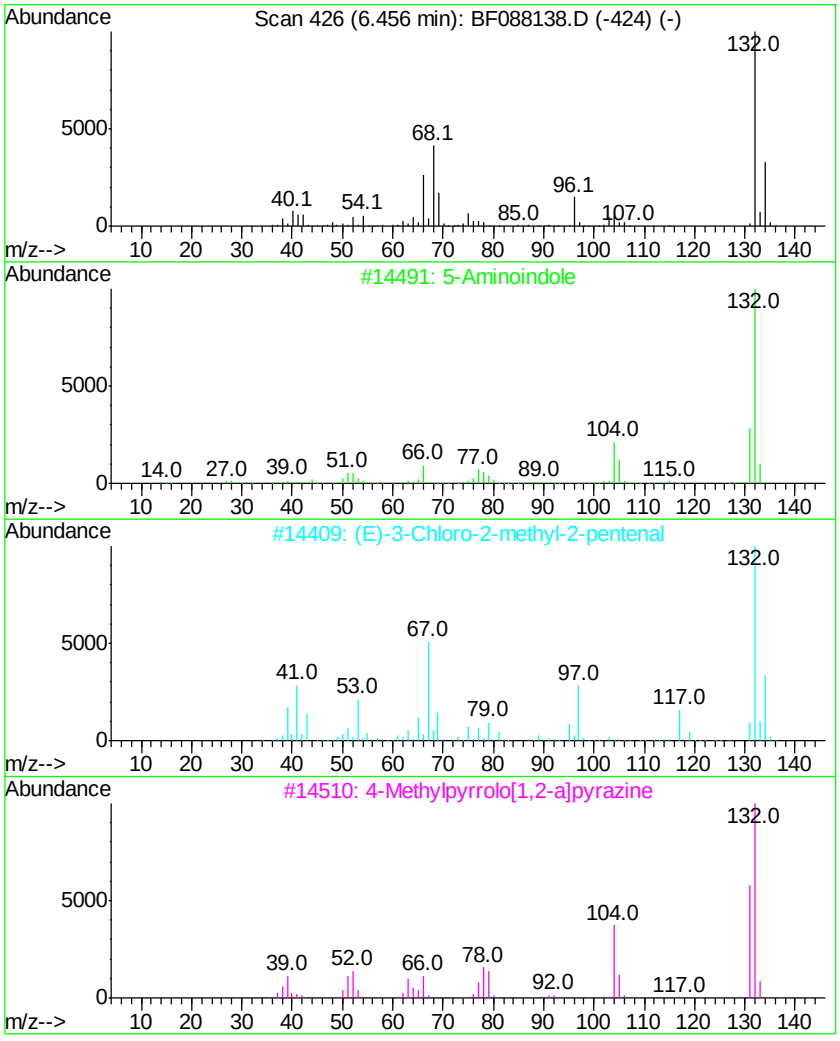
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

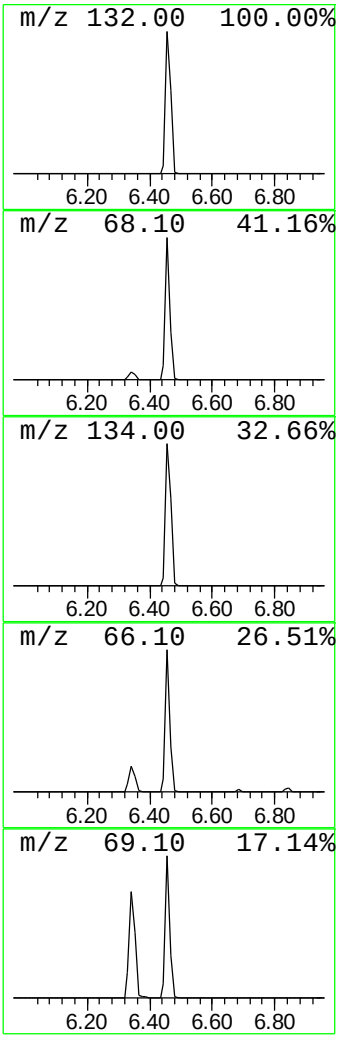
****

Peak Number 5 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	62.92 ng	1681650	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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

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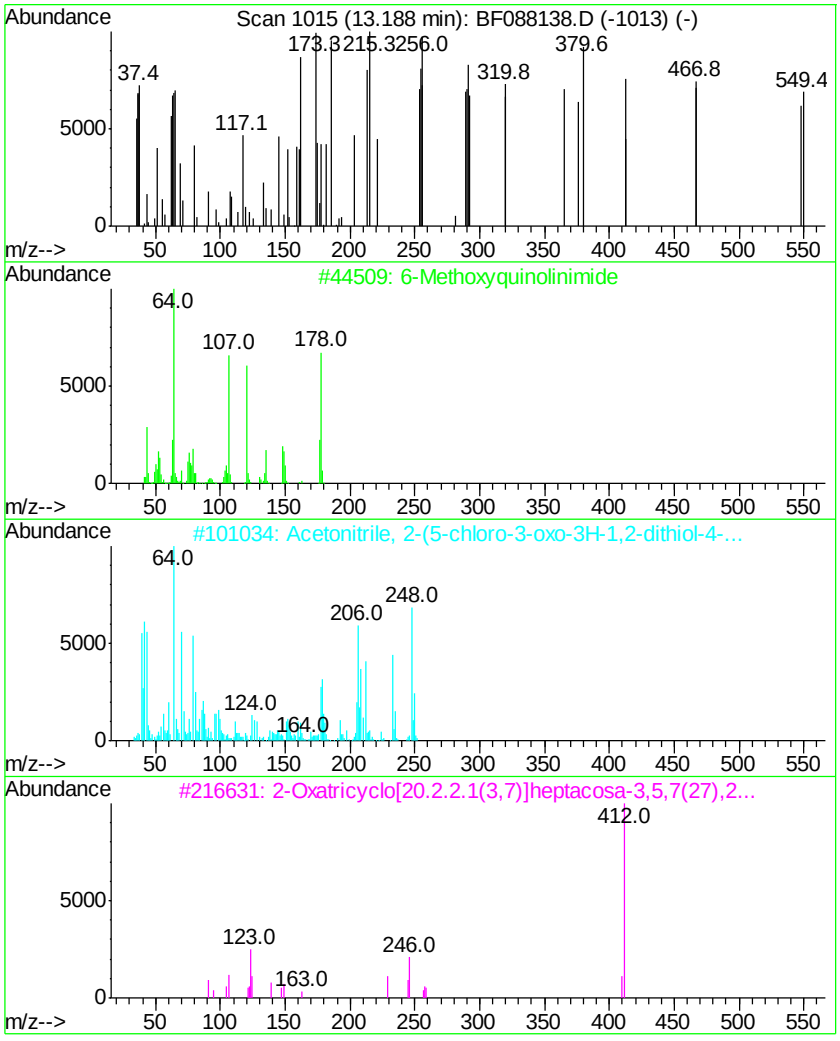
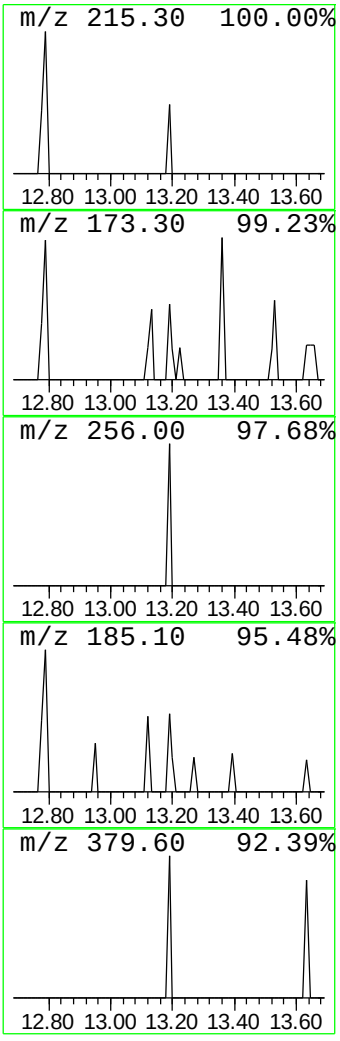
Peak Number 7 unknown13.19 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.81 ng	80257	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Methoxyquinolinimide	178	C8H6N2O3	1000214-53-5	25
2	Acetonitrile, 2-(5-chloro-3-oxo-...	248	C8H9ClN2OS2	1000269-94-4	10
3	2-Oxatricyclo[20.2.2.1(3,7)]hept...	412	C26H36O4	027825-37-2	10
4	Cyclic octaatomic sulfur	256	S8	010544-50-0	9
5	Benzenesulfonamide, 4-(2-hydroxy...	321	C13H11N3O5S	303214-10-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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

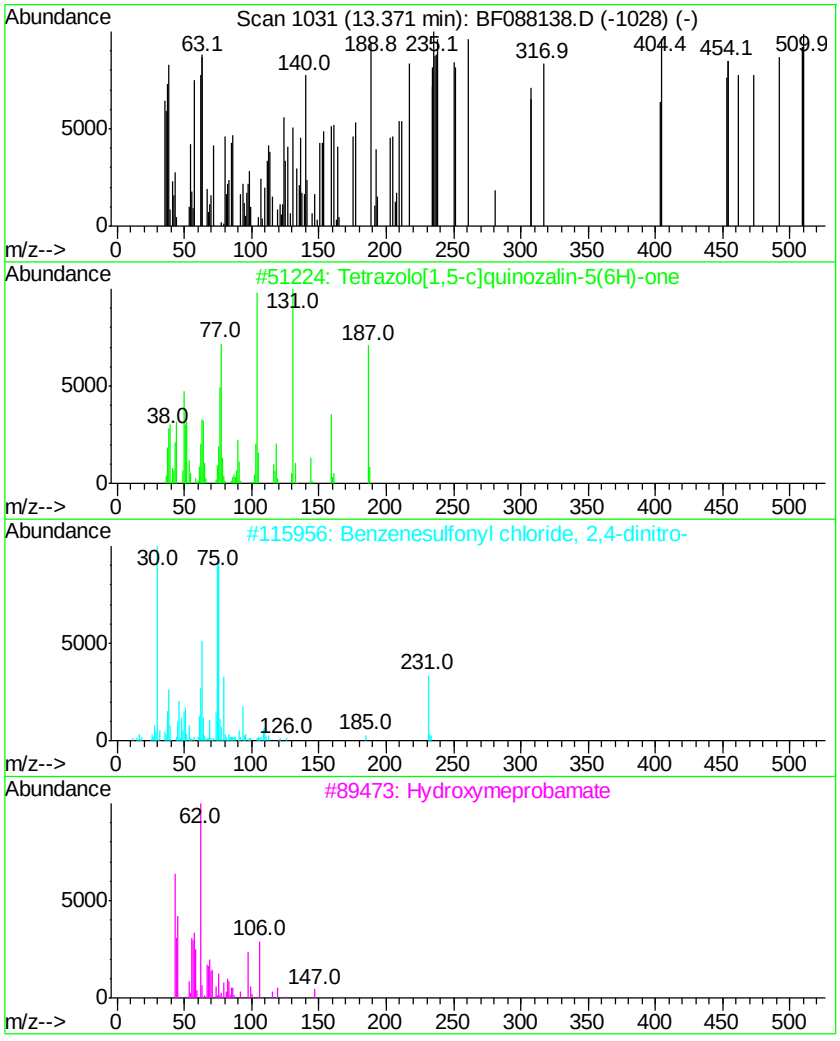
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

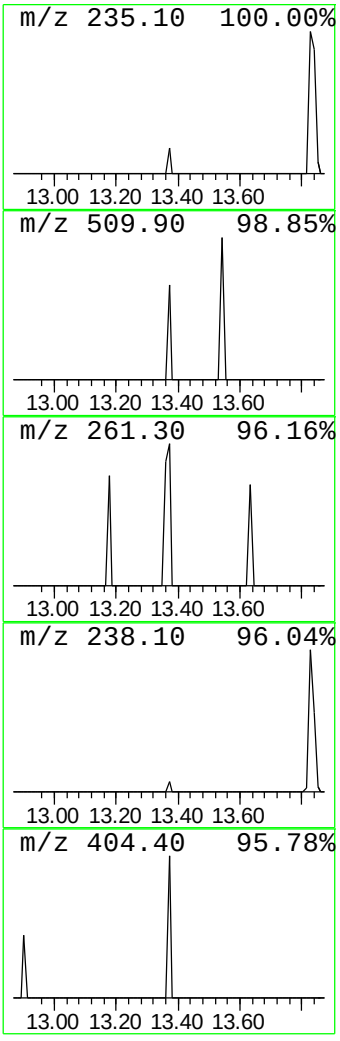
****

Peak Number 8 unknown13.37 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.37	2.33 ng	66560	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrazolo[1,5-c]quinozalin-5(6H)...	187	C8H5N5O	040595-12-8	32
2	Benzenesulfonyl chloride, 2,4-di...	266	C6H3ClN2O6S	001656-44-6	12
3	Hydroxymeprobamate	234	C9H18N2O5	003567-43-9	10
4	Pyridine, 2-chloro-4-nitro-, 1-o...	174	C5H3ClN2O3	014432-16-7	10
5	2-Chloroethyl 1-propynyl sulfoxide	150	C5H7ClOS	1000250-50-5	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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

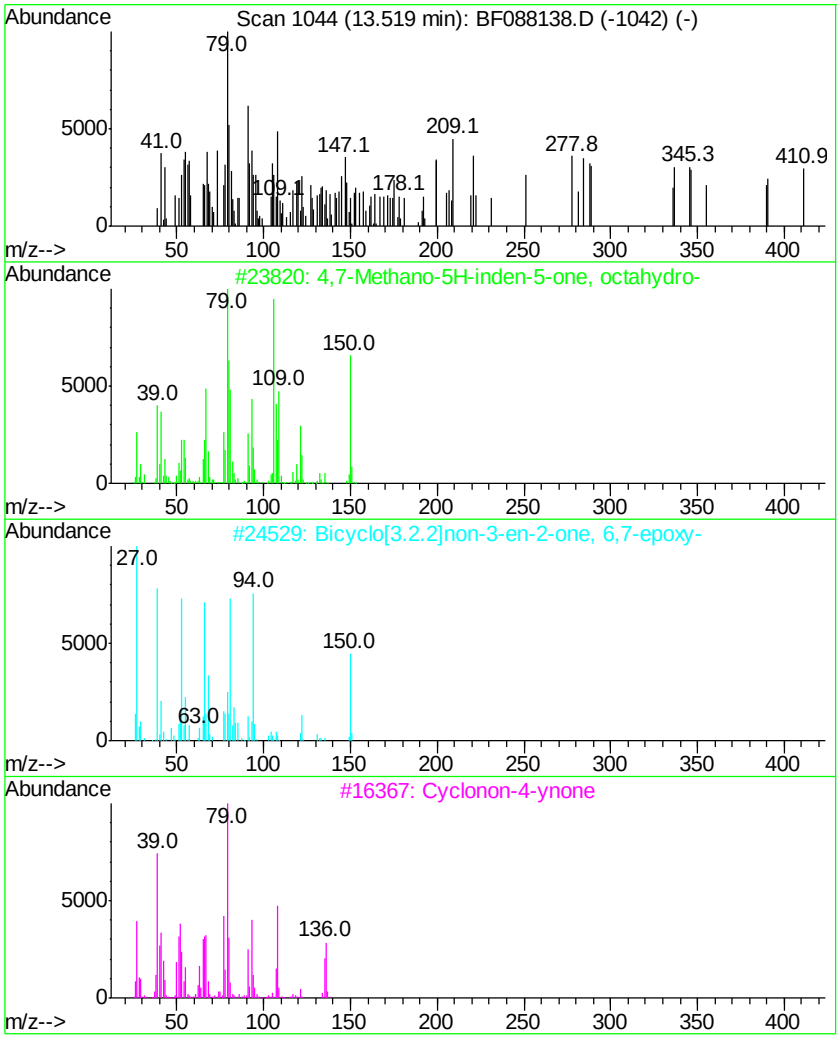
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

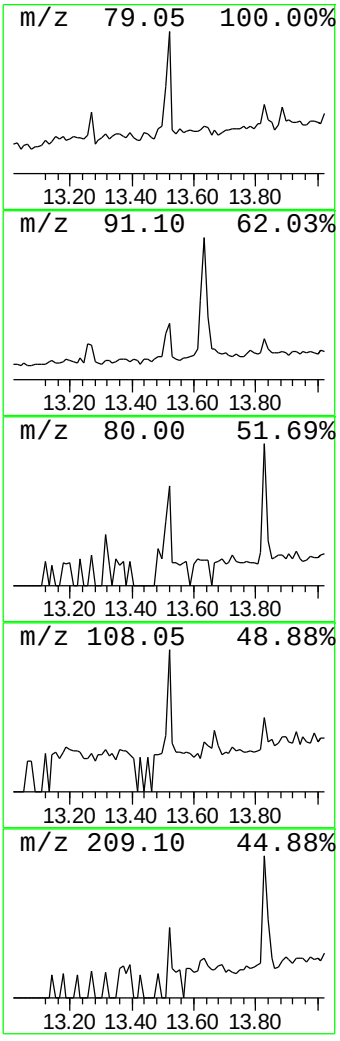
****

Peak Number 9 unknown13.52 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	2.52 ng	71906	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-5H-inden-5-one, octa...	150	C10H14O	013380-94-4	15
2	Bicyclo[3.2.2]non-3-en-2-one, 6,...	150	C9H10O2	1000155-95-4	11
3	Cyclonon-4-ynone	136	C9H12O	037079-60-0	11
4	Tetracyclo[3.3.1.1(3,7).0(4,6)]d...	148	C10H12O	052750-53-5	11
5	Tricyclo[2.2.1.0(2,6)]heptane, 3...	162	C7H8Cl2	1000327-37-7	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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

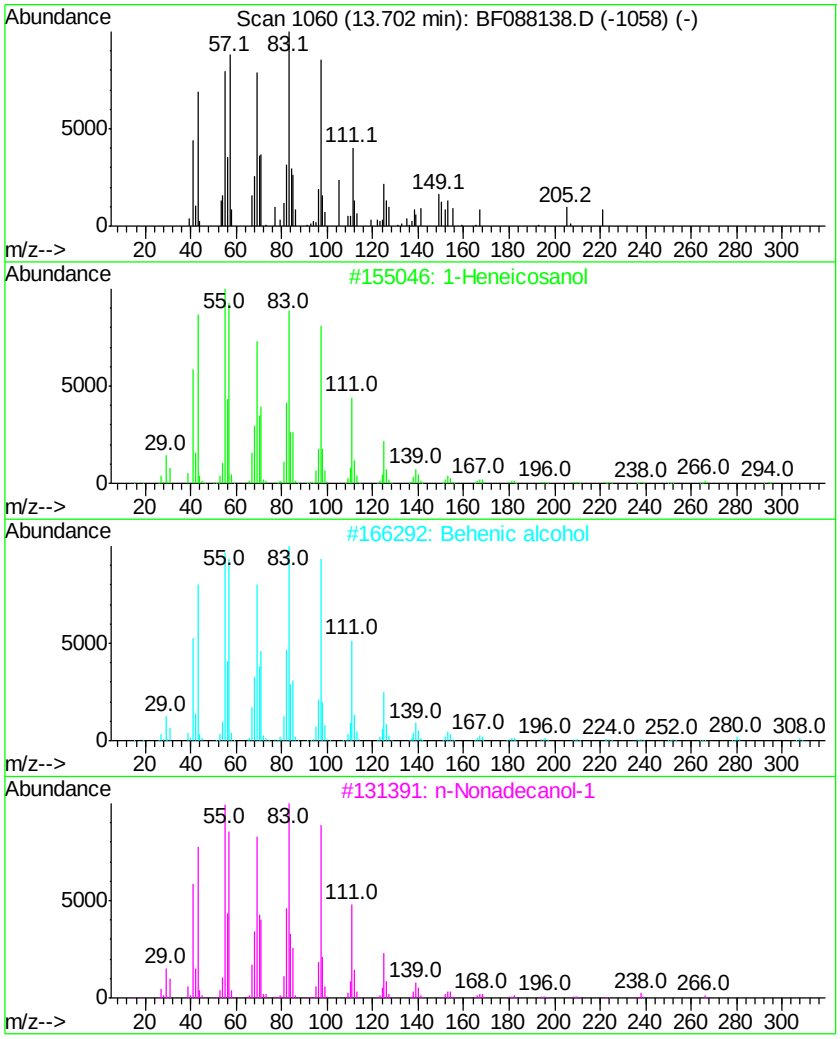
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

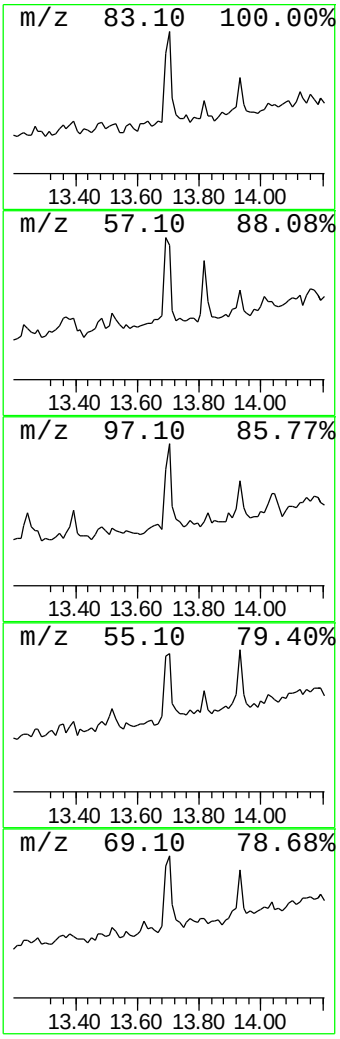
****

Peak Number 11 1-Heneicosanol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.27 ng	64686	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	87
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	81





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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

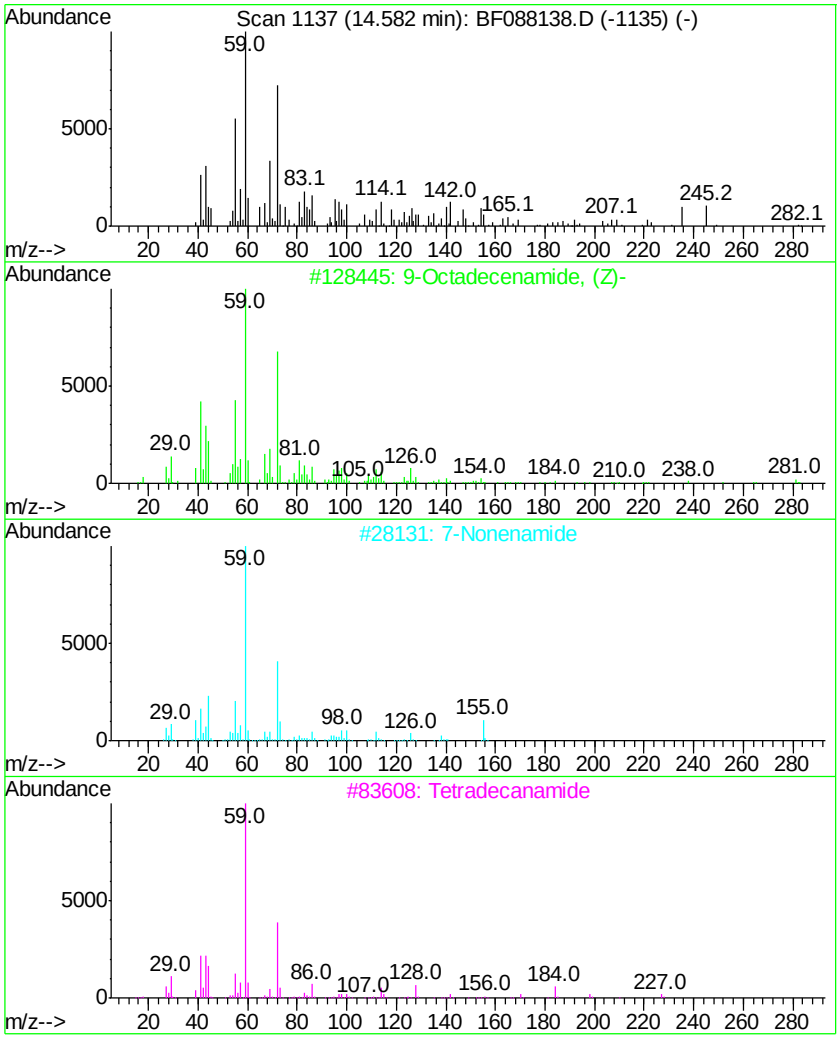
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

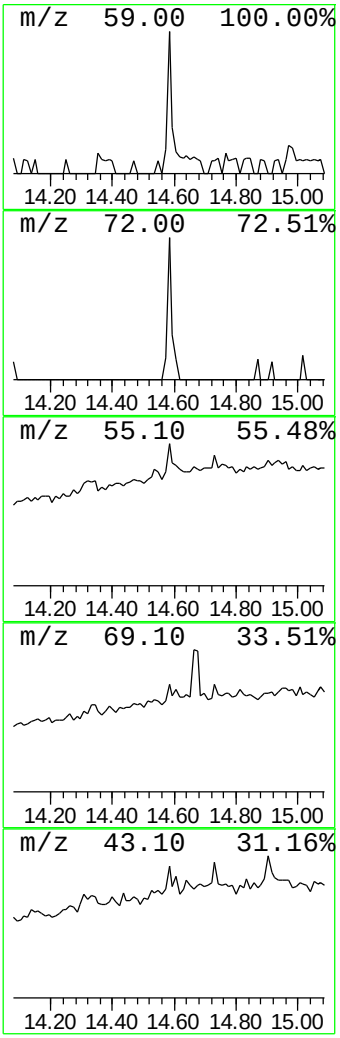
****

Peak Number 13 9-Octadecenamide, (Z)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	2.69 ng	57137	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
2	7-Nonenamide	155	C9H17NO	090949-53-4	58
3	Tetradecanamide	227	C14H29NO	000638-58-4	53
4	Decanamide-	171	C10H21NO	002319-29-1	53
5	8-Methyl-6-nonenamide	169	C10H19NO	1000293-20-9	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088138.D
Acq On : 18 Jun 2016 17:10
Operator : UM/SJ
Sample : H3501-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB11-1-3

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
Propane, 1,1-dime...	1.88	5.5	ng	148451	1	6.68	534526	20.0
2-Pentanone, 4-hy...	4.84	4.6	ng	123098	1	6.68	534526	20.0
unknown6.46	6.46	62.9	ng	1681650	1	6.68	534526	20.0
unknown13.19	13.19	2.8	ng	80257	5	13.83	571019	20.0
unknown13.37	13.37	2.3	ng	66560	5	13.83	571019	20.0
unknown13.52	13.52	2.5	ng	71906	5	13.83	571019	20.0
1-Heneicosanol	13.70	2.3	ng	64686	5	13.83	571019	20.0
9-Octadecenamide,...	14.58	2.7	ng	57137	6	15.21	425124	20.0