LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-1K

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-BF050916.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	4.841	238	241	249	rBV	396745	614036	16.64%	1.853%
2	5.287	277	280	282	rBV	3214734	3687269	99.93%	11.126%
3	5.687	313	315	324	rVB	50239	79742	2.16%	0.241%
4	6.350	370	373	375	rBV	2705818	3689899	100.00%	11.133%
5	6.453	380	382	385	rBV	3096070	3529564	95.65%	10.650%
6	6.682	400	402	409	rBV	1121837	1035036	28.05%	3.123%
7	6.842	413	416	418	rBV	3169822	3132963	84.91%	9.453%
8	7.253	450	452	455	rBV	2104327	2235070	60.57%	6.744%
9	7.973	512	515	517	rBV	1195517	1167957	31.65%	3.524%
10	9.047	607	609	612	rBV	3606649	3417461	92.62%	10.311%
11	9.448	642	644	648	rBV	418476	388193	10.52%	1.171%
12	9.665	660	663	665	rBV	112133	108594	2.94%	0.328%
13	9.722	665	668	670	rBV	1161925	1146031	31.06%	3.458%
14	9.893	679	683	687	rBV2	26937	65789	1.78%	0.199%
15	10.156	704	706	708	rVB	228425	186881	5.06%	0.564%
16	10.373	722	725	729	rBV	71888	124388	3.37%	0.375%
17	10.511	734	737	739	rBV	1489379	1837534	49.80%	5.544%
18	10.625	746	747	752	rBV	201864	267997	7.26%	0.809%
19	10.819	762	764	766	rBV	30957	39849	1.08%	0.120%
20	11.071	784	786	792	rVB	83656	139589	3.78%	0.421%
21	11.196	795	797	801	rBV	1044901	924949	25.07%	2.791%
22	11.745	843	845	850	rBV2	18087	37617	1.02%	0.114%
23	12.682	926	927	930	rBV	50336	59405	1.61%	0.179%
24	12.774	933	935	938	rBV	2093462	2688321	72.86%	8.111%
25	13.014	954	956	962	rBV	36724	70648	1.91%	0.213%
26	13.471	994	996	999	rBV	67465	81568	2.21%	0.246%
27	13.699	1013	1016	1022	rBV	118195	249609	6.76%	0.753%
28	13.825	1024	1027	1029	rBV	830153	848856	23.00%	2.561%
29	14.271	1063	1066	1070	rBV	205896	351466	9.53%	1.060%
30	14.900	1119	1121	1122	rBV	38130	50800	1.38%	0.153%
31	15.197	1144	1147	1153	rVB	577591	713275	19.33%	2.152%
32	15.608	1181	1183	1186	rVB	26064	37296	1.01%	0.113%
33	16.294	1240	1243	1247	rVB2	28349	56261	1.52%	0.170%
34	17.003	1302	1305	1310	rVB5	28375	78542	2.13%	0.237%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-1K

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-BF050916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

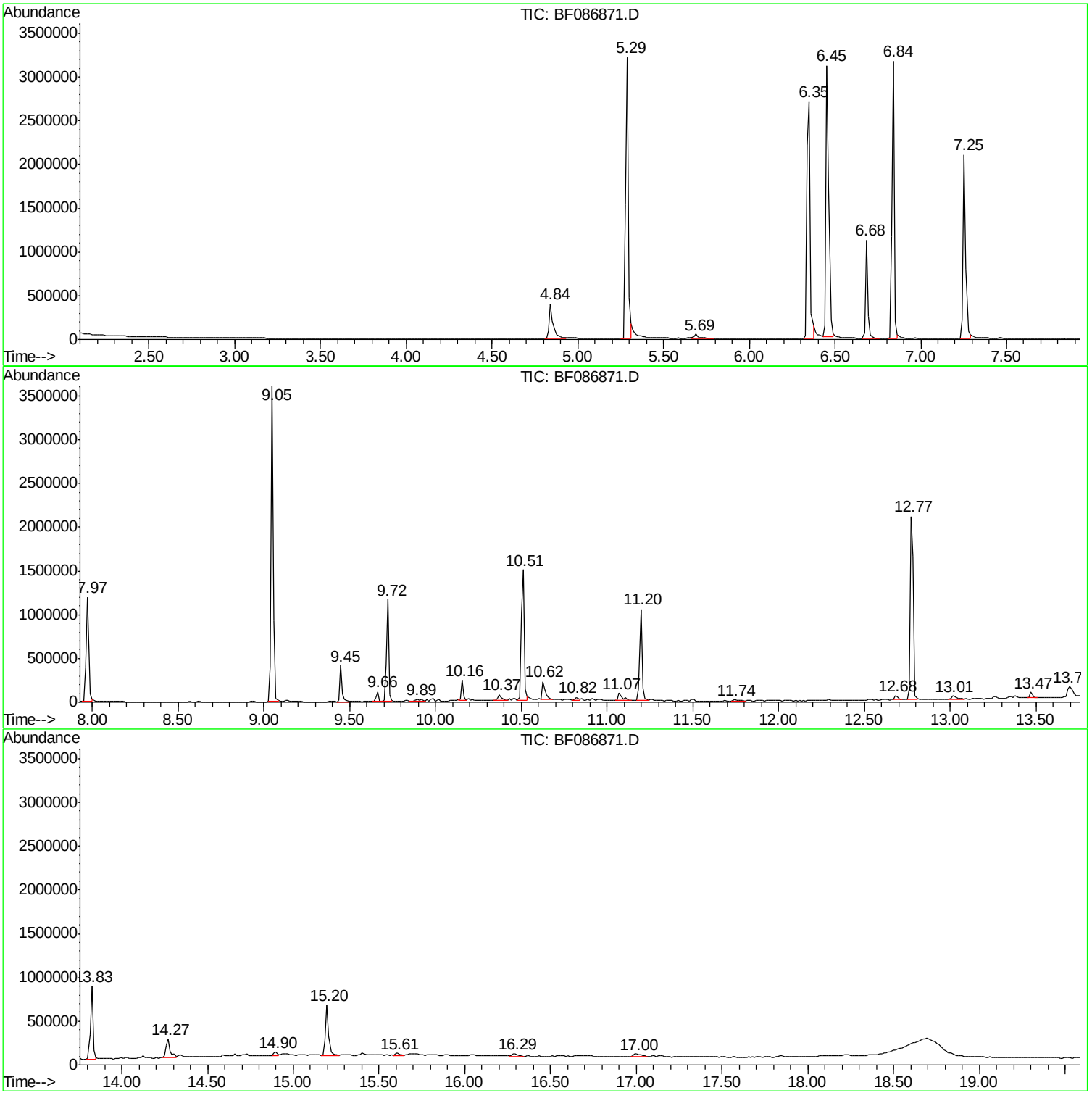
Sum of corrected areas: 33142455

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-1K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-1K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

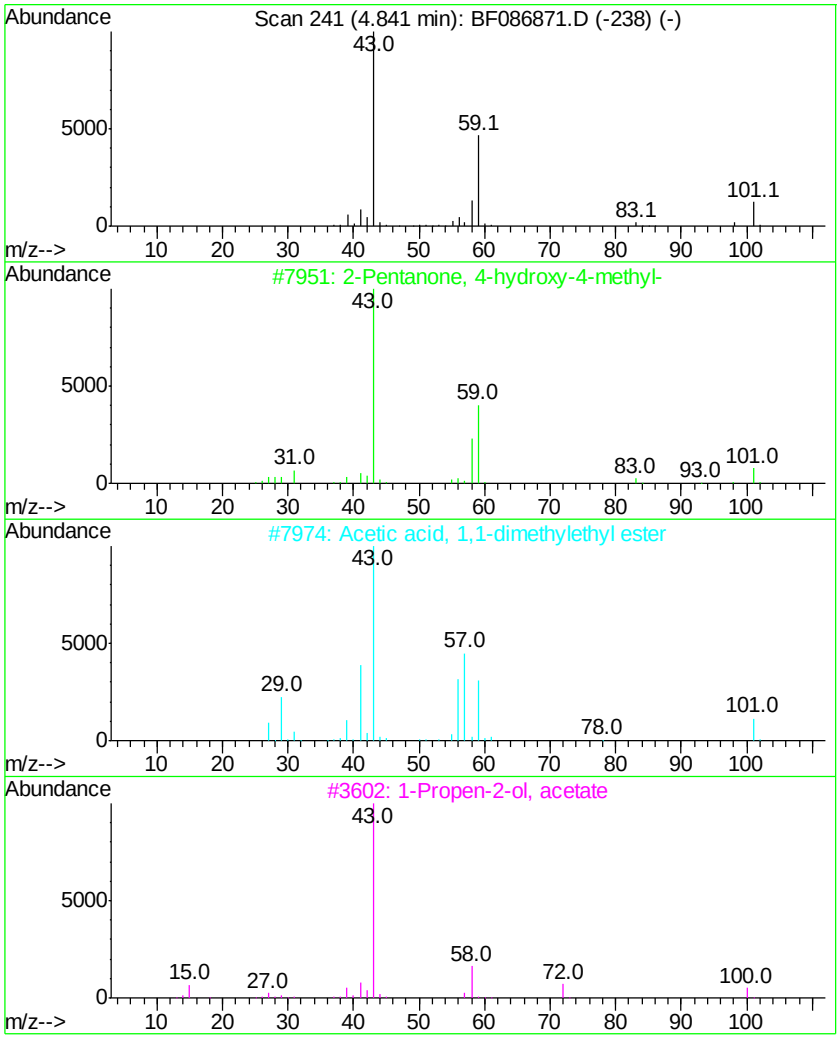
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

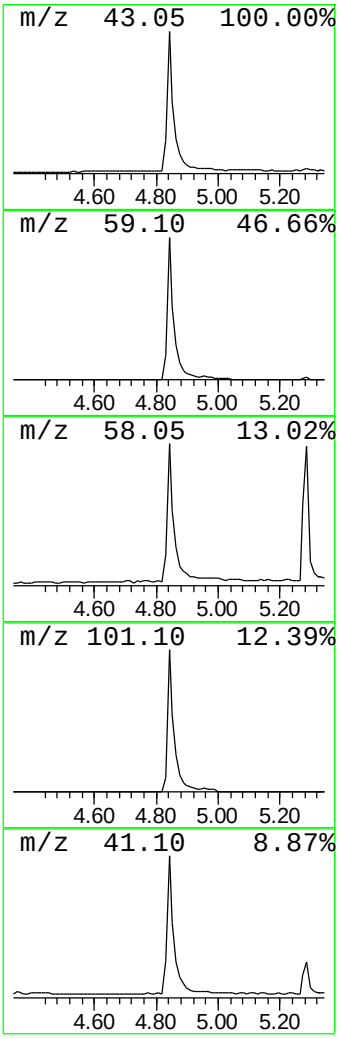
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	11.87 ng	614036	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-1K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

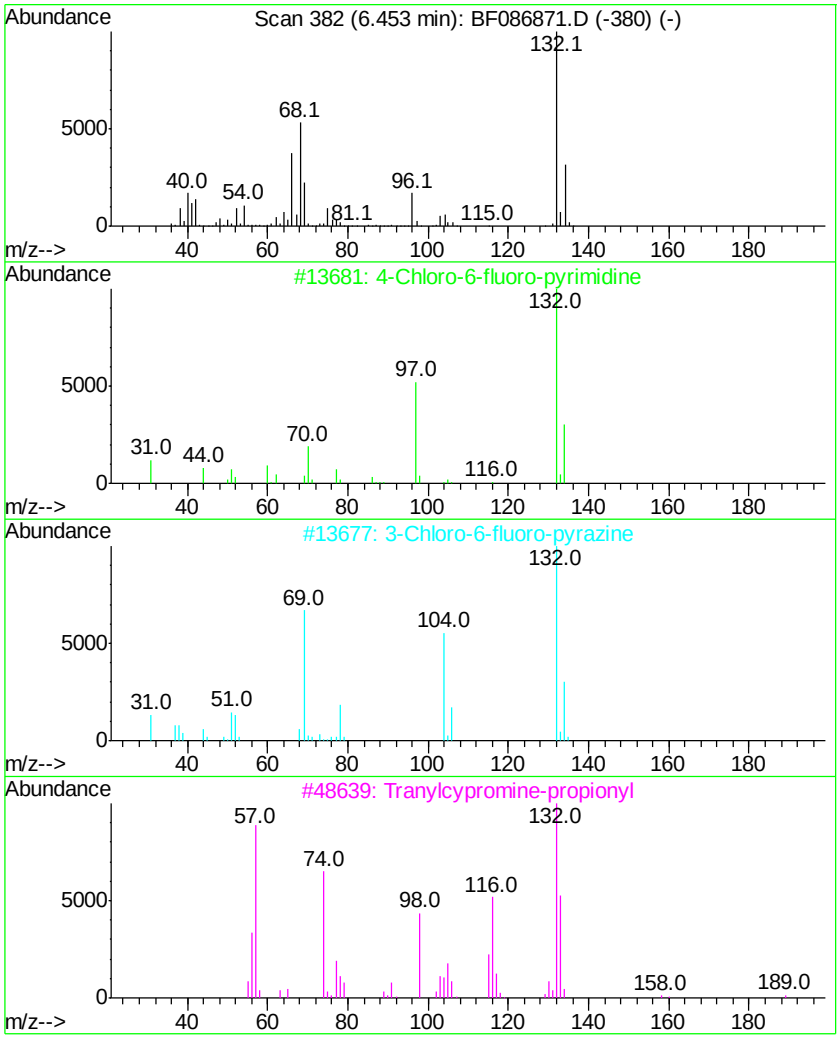
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

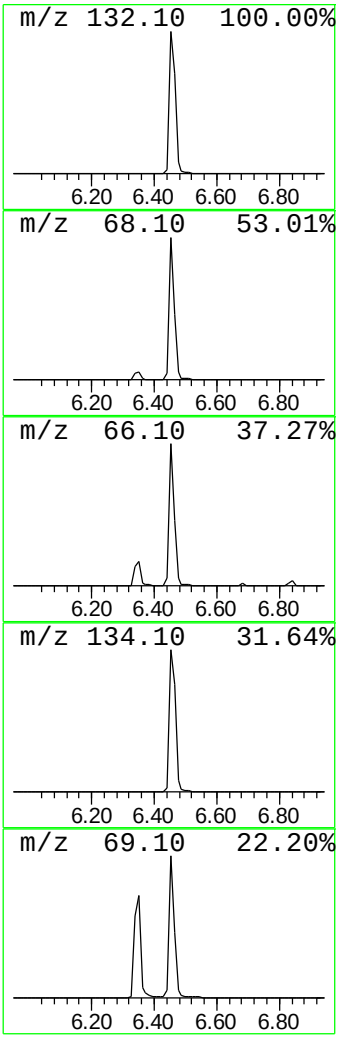
****

Peak Number 2 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	68.20 ng	3529560	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-1K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

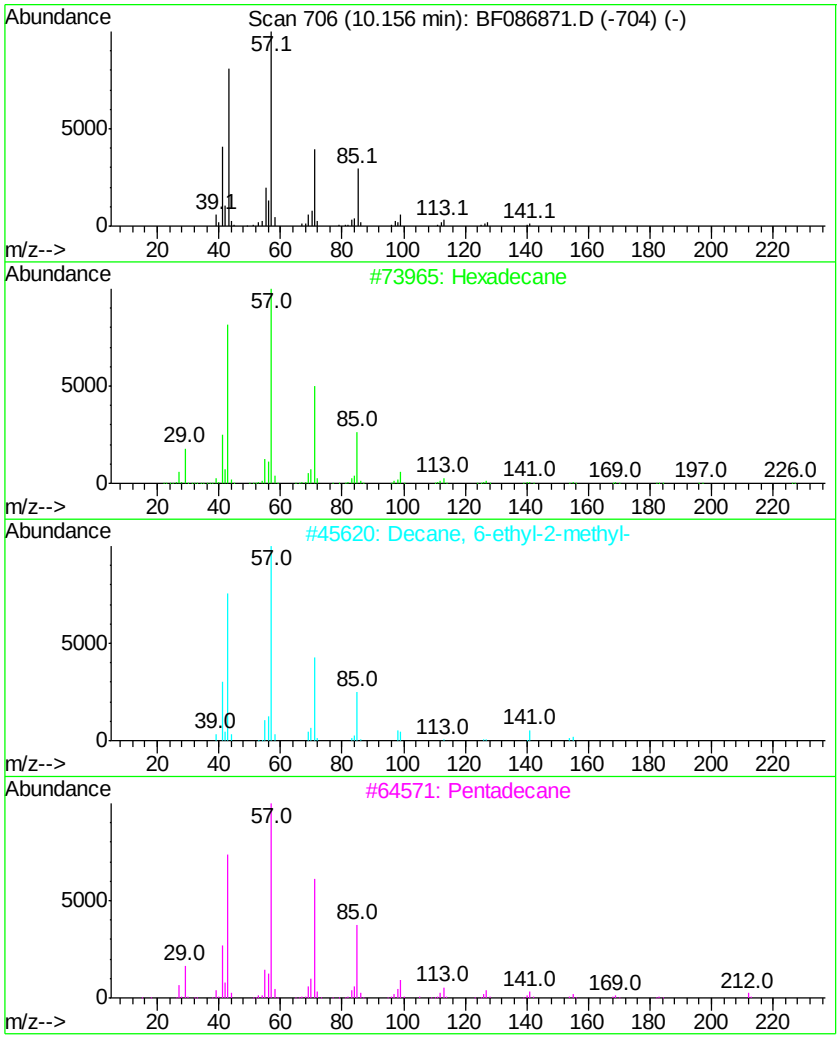
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

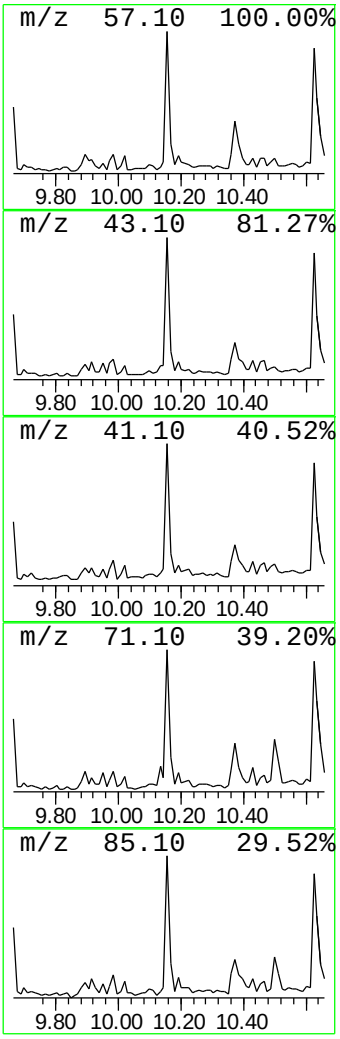
****

Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	3.26 ng	186881	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	83
3	Pentadecane	212	C15H32	000629-62-9	78
4	Nonane	128	C9H20	000111-84-2	72
5	Octadecane	254	C18H38	000593-45-3	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-1K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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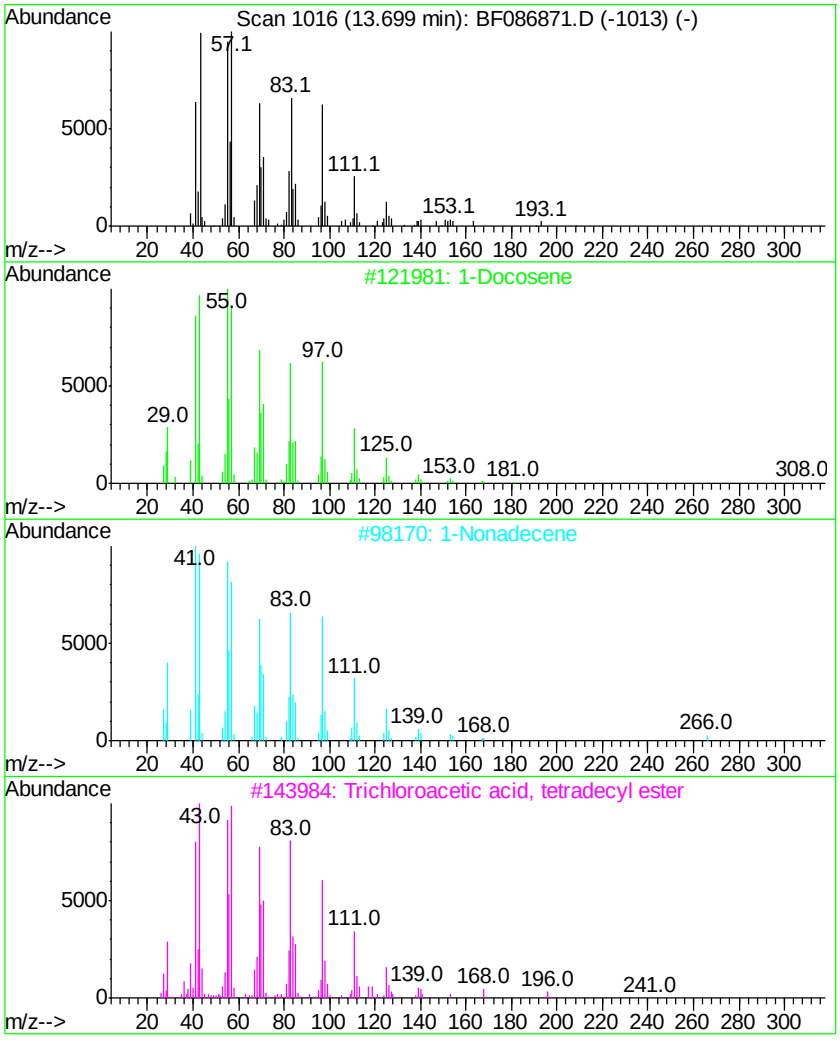
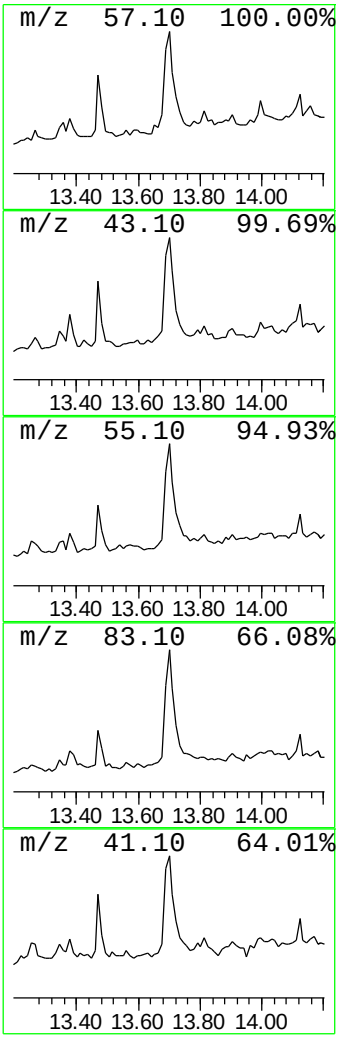
Peak Number 8 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	5.88 ng	249609	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	87
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-1K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

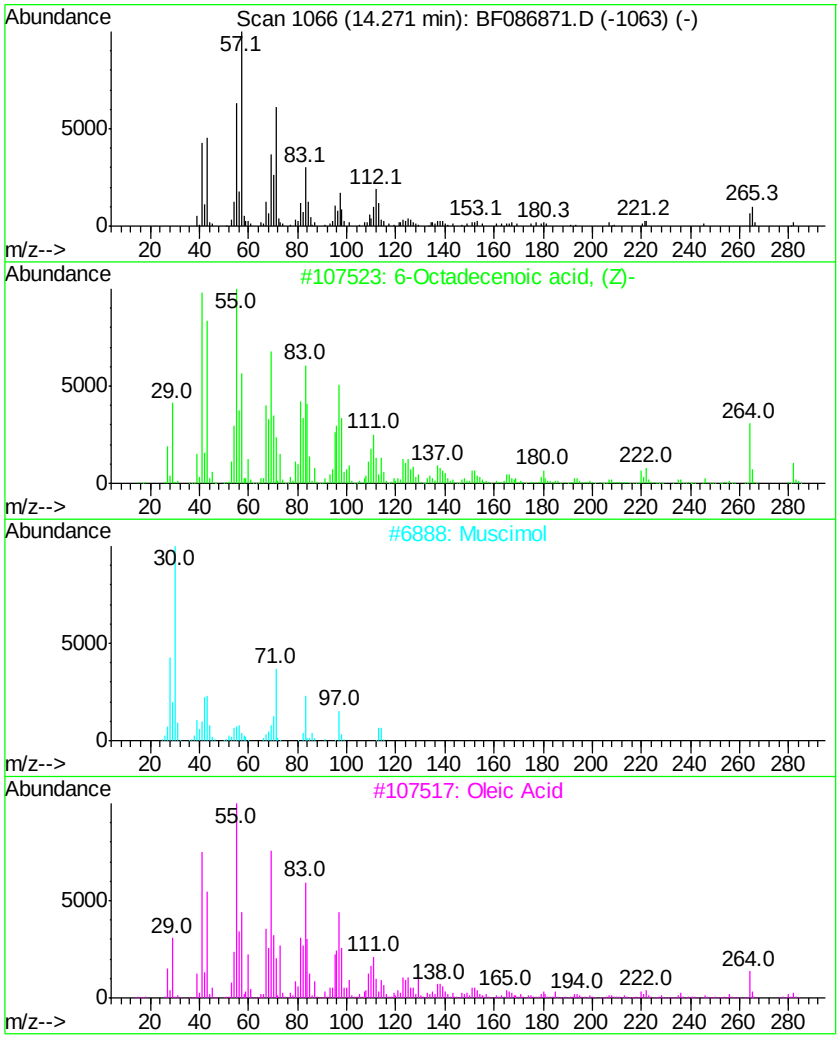
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

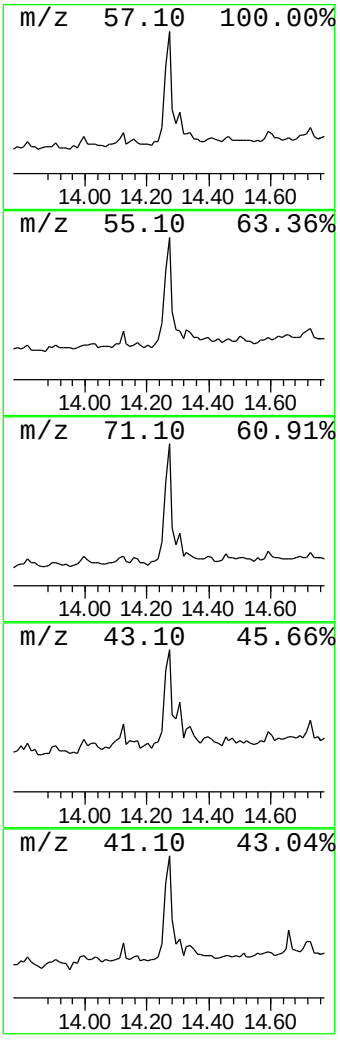
****

Peak Number 9 6-Octadecenoic acid, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	8.28 ng	351466	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	70
2	Muscimol	114	C4H6N2O2	002763-96-4	38
3	Oleic Acid	282	C18H34O2	000112-80-1	30
4	Z-8-Methyl-9-tetradecenoic acid	240	C15H28O2	1000130-84-5	25
5	Z-5-Nonadecene	266	C19H38	1000131-11-8	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-1K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

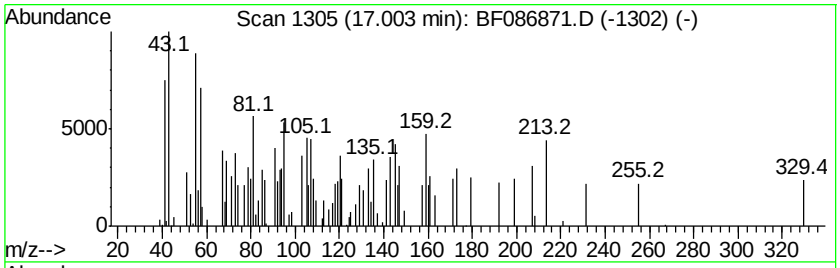
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

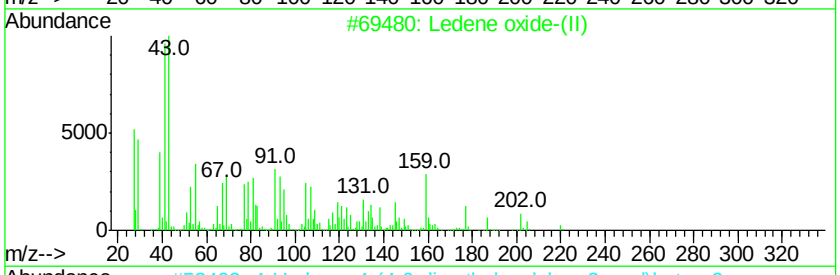
****

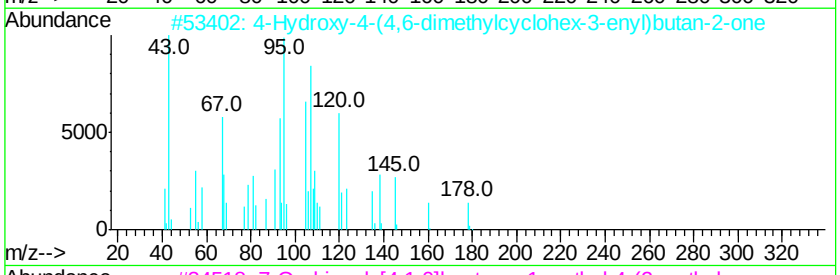
Peak Number 10 unknown17.00 Concentration Rank 9

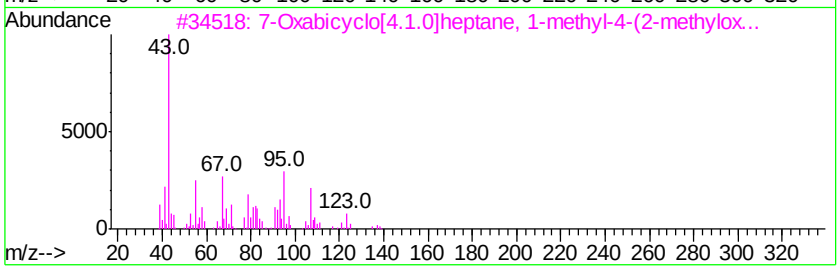
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.00	2.20 ng	78542	Perylene-d12	15.20

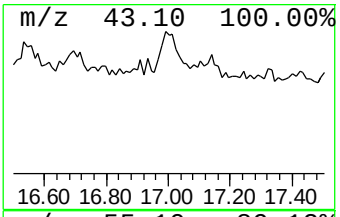
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ledene oxide-(II)	220	C15H24O	1000159-36-7	12
2	4-Hydroxy-4-(4,6-dimethylcyclohe...	196	C12H20O2	002316-79-2	10
3	7-Oxabicyclo[4.1.0]heptane, 1-me...	168	C10H16O2	000096-08-2	10
4	2,3-Di(2,2-dimethylethyl)thiophe...	228	C12H20O2S	128788-12-5	9
5	Tetracyclo[6.1.0.0(2,4).0(5,7)]n...	204	C15H24	1000151-74-7	9

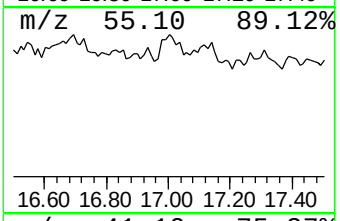


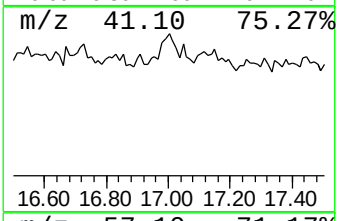


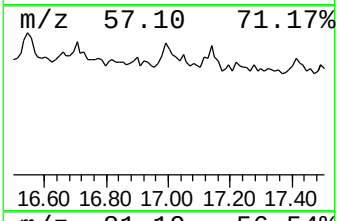


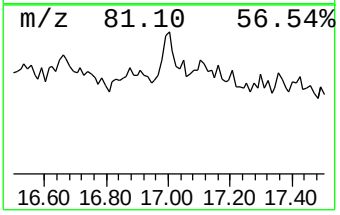












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
Data File : BF086871.D
Acq On : 10 May 2016 20:39
Operator : UM/SJ
Sample : H2916-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-1K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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...	4.84	11.9	ng	614036	1	6.68	1035040	20.0
unknown6.45	6.45	68.2	ng	3529560	1	6.68	1035040	20.0
Hexadecane	10.16	3.3	ng	186881	3	9.72	1146030	20.0
1-Docosene	13.70	5.9	ng	249609	5	13.83	848856	20.0
6-Octadecenoic ac...	14.27	8.3	ng	351466	5	13.83	848856	20.0
unknown17.00	17.00	2.2	ng	78542	6	15.20	713275	20.0