LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092900.D
Acq On : 10 Feb 2017 23:07
Operator : SJ/MA
Sample : I1777-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-0-2

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-BF013017.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	4.418	201	204	209	rBV	62521	91414	2.28%	0.240%
2	5.070	258	261	272	rVB	1174556	1547368	38.63%	4.058%
3	5.493	295	298	301	rBV	2719372	2852966	71.23%	7.482%
4	6.533	386	389	392	rBV	3206642	3436848	85.80%	9.013%
5	6.659	398	400	403	rBV	2650972	3234941	80.76%	8.484%
6	6.887	418	420	423	rBV	701014	939196	23.45%	2.463%
7	7.047	432	434	437	rBV	2592470	2575874	64.31%	6.755%
8	7.459	467	470	473	rBV	2151857	2149033	53.65%	5.636%
9	8.179	530	533	536	rBV	1401757	1268868	31.68%	3.328%
10	9.253	624	627	630	rBV	3209488	3943554	98.46%	10.342%
11	9.653	660	662	664	rBV	213944	199943	4.99%	0.524%
12	9.859	676	680	684	rBV	79485	132549	3.31%	0.348%
13	9.939	684	687	689	rBV	1334159	1543276	38.53%	4.047%
14	10.362	723	724	726	rVB	144317	115481	2.88%	0.303%
15	10.579	741	743	747	rBV	42366	70617	1.76%	0.185%
16	10.728	753	756	758	rBV	1561938	1792958	44.76%	4.702%
17	10.842	764	766	770	rVB	131178	220832	5.51%	0.579%
18	11.025	780	782	787	rVB3	18934	47149	1.18%	0.124%
19	11.288	802	805	806	rBV	119472	132382	3.31%	0.347%
20	11.311	806	807	810	rVB	53097	56514	1.41%	0.148%
21	11.425	814	817	818	rBV	1443987	1629493	40.68%	4.273%
22	11.448	818	819	820	rVV	187479	140288	3.50%	0.368%
23	11.493	820	823	825	rVB	45675	59639	1.49%	0.156%
24	11.711	840	842	844	rBV	70897	61851	1.54%	0.162%
25	11.916	858	860	862	rBV	35525	48780	1.22%	0.128%
26	11.951	862	863	864	rVV	56522	41087	1.03%	0.108%
27	12.031	868	870	874	rVB	74582	127138	3.17%	0.333%
28	12.111	875	877	879	rVB	39850	55675	1.39%	0.146%
29	12.465	907	908	910	rVB	34408	41746	1.04%	0.109%
30	12.511	910	912	914	rBV	57820	79719	1.99%	0.209%
31	12.636	920	923	925	rVV	309753	371785	9.28%	0.975%
32	12.785	932	936	938	rBV3	22797	46051	1.15%	0.121%
33	12.865	940	943	946	rVV	278661	440976	11.01%	1.156%
34	13.014	953	956	958	rBV	3299903	4005424	100.00%	10.504%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092900.D
Acq On : 10 Feb 2017 23:07
Operator : SJ/MA
Sample : I1777-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-0-2

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.082	959	962	966	rBV4	43776	94397	2.36%	0.248%
36	13.185	968	971	973	rBV	60318	105729	2.64%	0.277%
37	13.231	973	975	976	rBV	44798	48689	1.22%	0.128%
38	13.288	978	980	982	rVB2	34370	48885	1.22%	0.128%
39	13.574	1003	1005	1008	rBV2	51774	89191	2.23%	0.234%
40	13.699	1013	1016	1020	rVB4	38746	84766	2.12%	0.222%
41	13.905	1031	1034	1037	rVB2	152663	261648	6.53%	0.686%
42	14.054	1044	1047	1054	rVB	1311956	1669252	41.67%	4.378%
43	14.214	1059	1061	1063	rBV2	31283	61487	1.54%	0.161%
44	14.522	1086	1088	1091	rBV3	35750	63391	1.58%	0.166%
45	14.900	1119	1121	1123	rBV2	29396	44270	1.11%	0.116%
46	15.082	1135	1137	1141	rBV	123965	229713	5.74%	0.602%
47	15.380	1161	1163	1166	rBV	62712	80286	2.00%	0.211%
48	15.437	1166	1168	1171	rVB	90291	130168	3.25%	0.341%
49	15.505	1171	1174	1184	rVB	833941	1168745	29.18%	3.065%
50	15.768	1194	1197	1208	rVB	143838	300711	7.51%	0.789%
51	16.934	1295	1299	1303	rVV2	35108	82265	2.05%	0.216%
52	17.357	1333	1336	1341	rVB2	31432	65746	1.64%	0.172%

Sum of corrected areas: 38130754

LSC Report - Integrated Chromatogram

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Data File : BF092900.D
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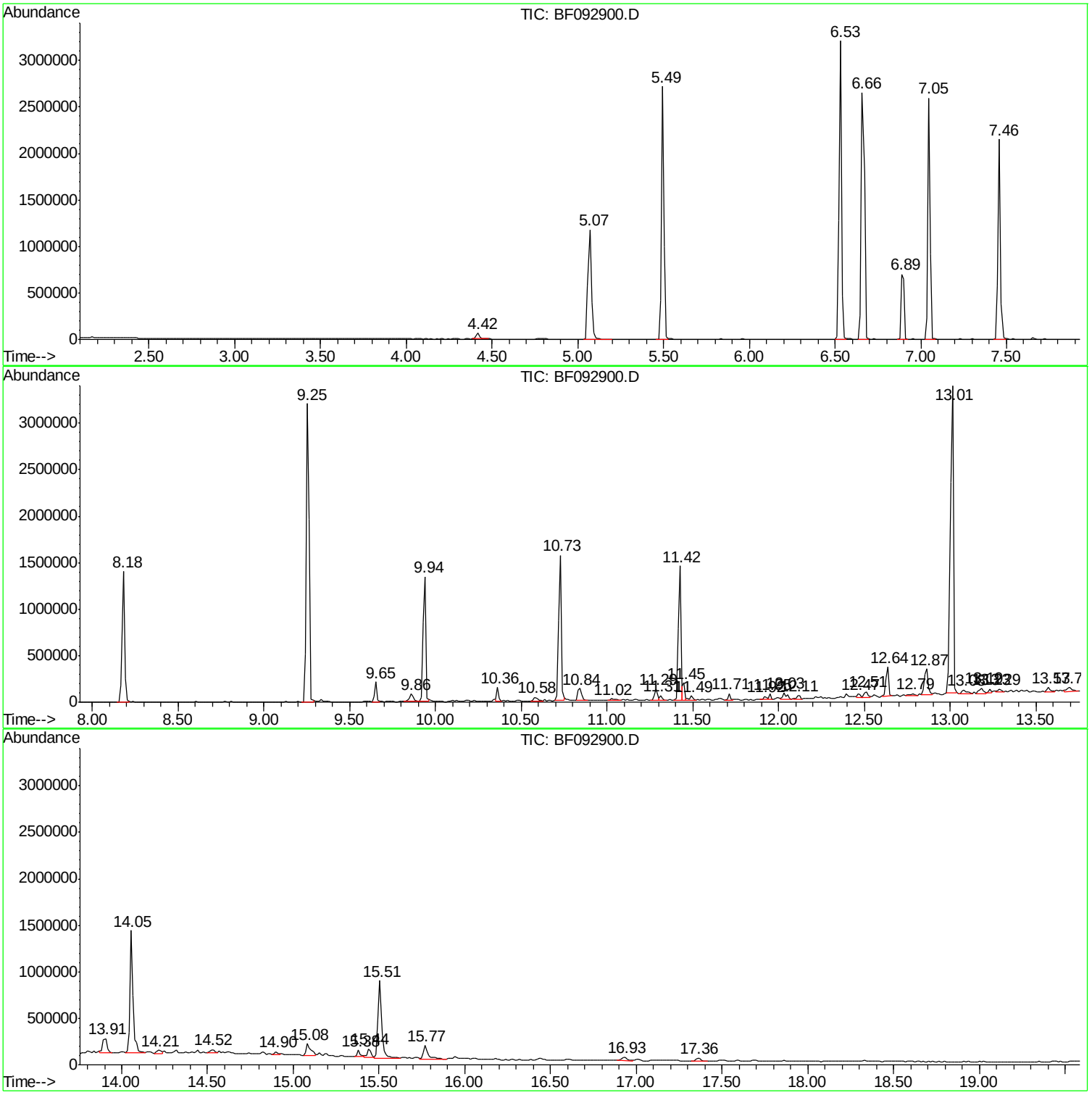
Operator : SJ/MA
Sample : I1777-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
38-SB-03-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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\BF021017\
Data File : BF092900.D
Acq On : 10 Feb 2017 23:07
Operator : SJ/MA
Sample : I1777-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
38-SB-03-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

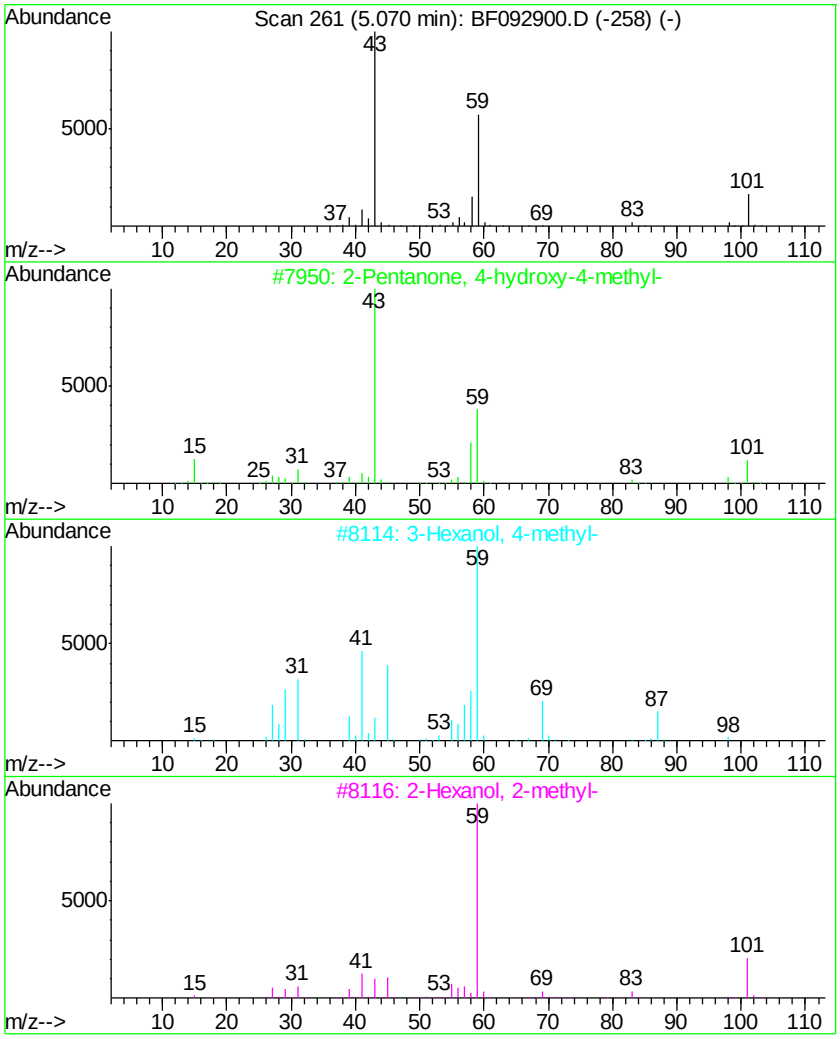
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

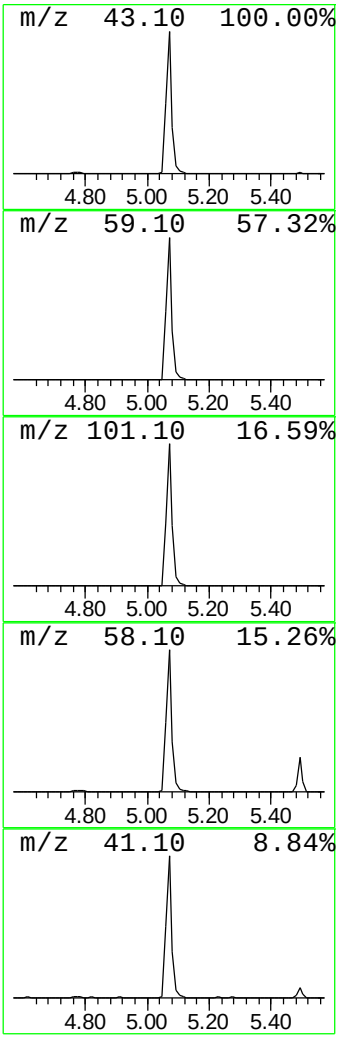
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	32.95 ng	1547370	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092900.D
Acq On : 10 Feb 2017 23:07
Operator : SJ/MA
Sample : I1777-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

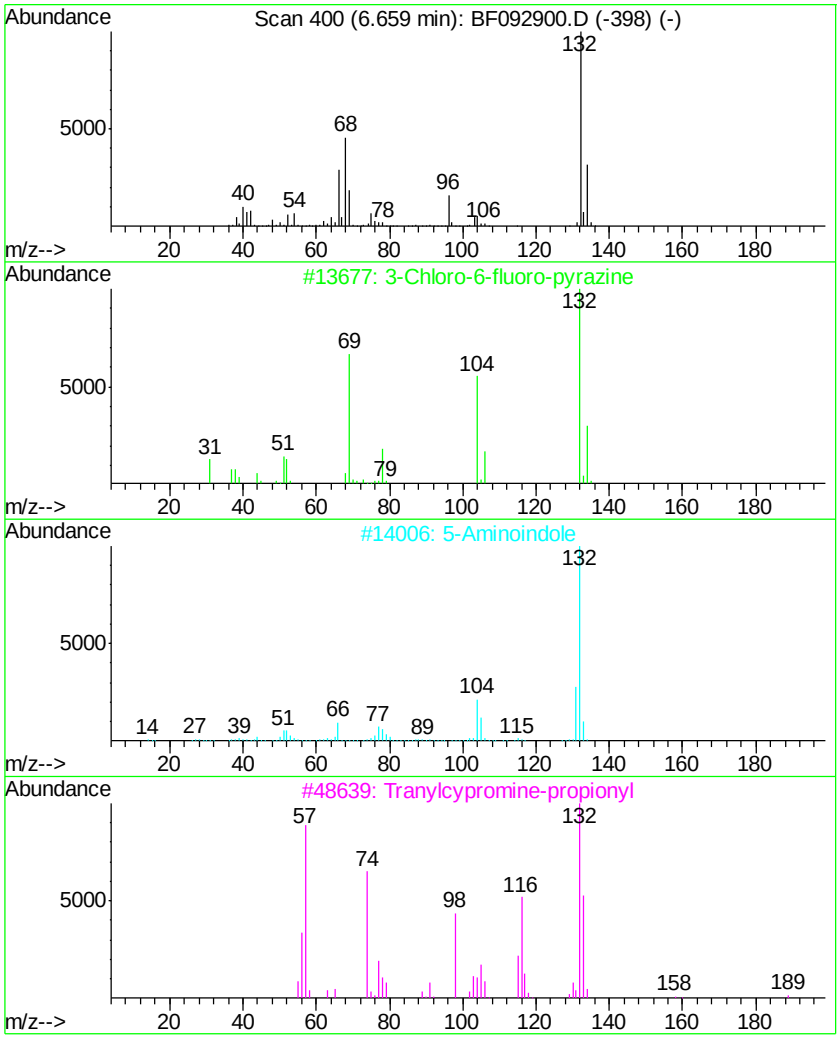
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

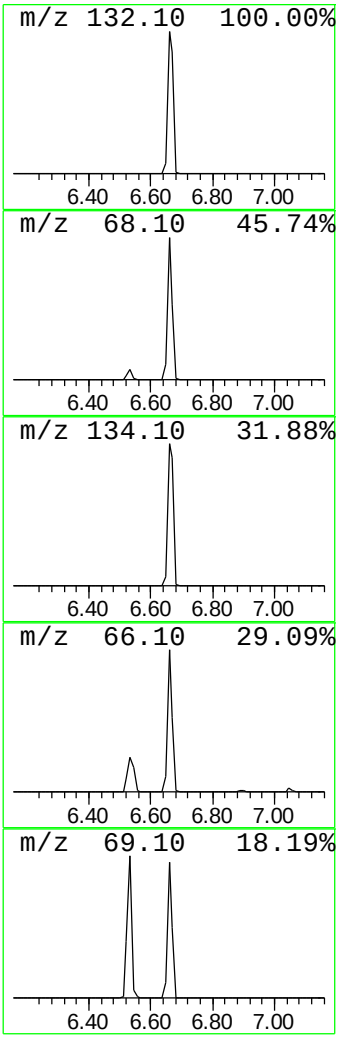
****

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	68.89 ng	3234940	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092900.D
Acq On : 10 Feb 2017 23:07
Operator : SJ/MA
Sample : I1777-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

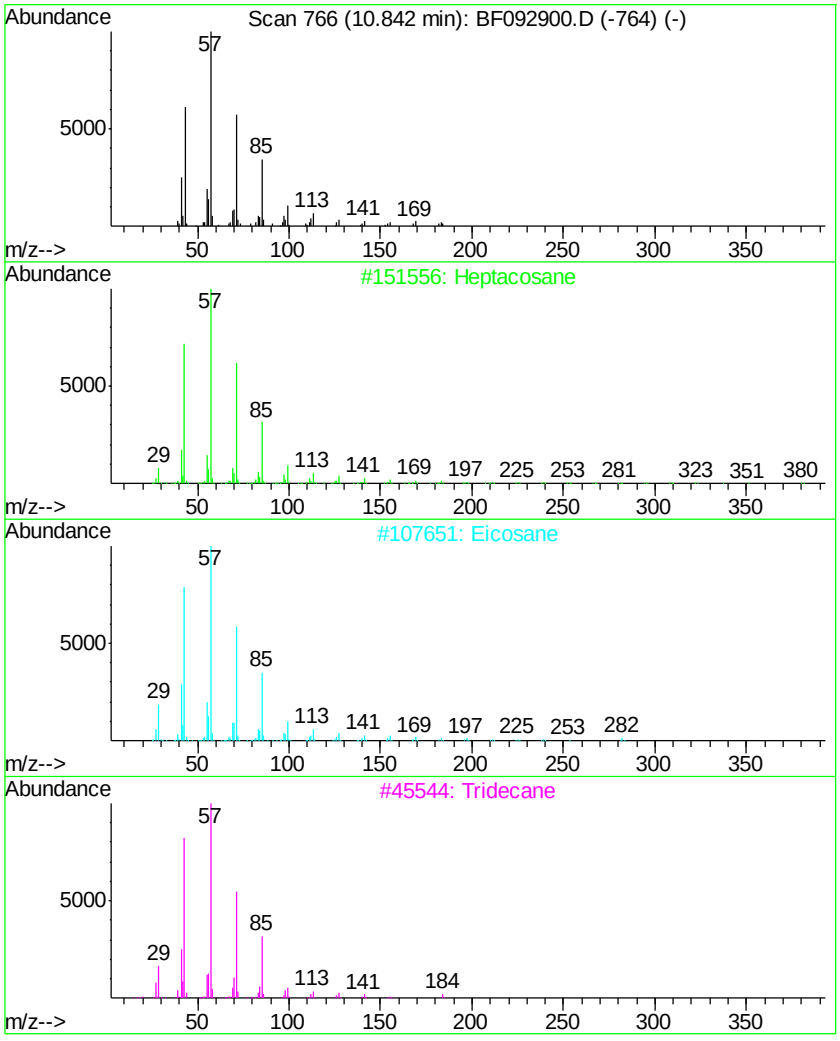
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

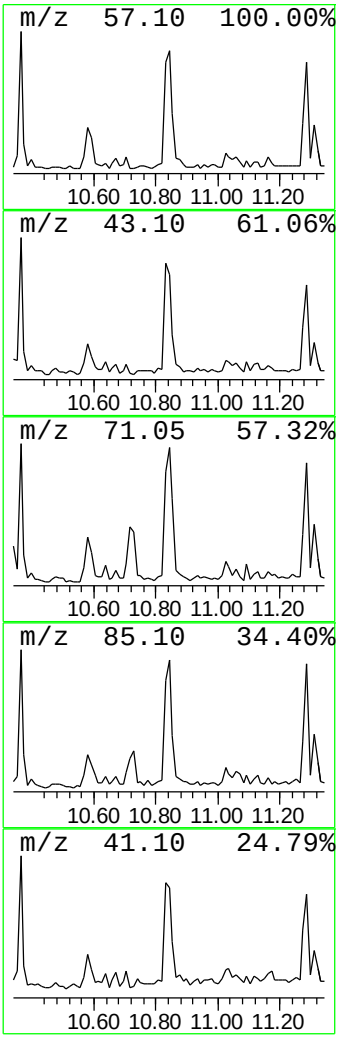
****

Peak Number 4 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	2.71 ng	220832	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Eicosane	282	C20H42	000112-95-8	90
3	Tridecane	184	C13H28	000629-50-5	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	87





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
Data File : BF092900.D
Acq On : 10 Feb 2017 23:07
Operator : SJ/MA
Sample : I1777-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

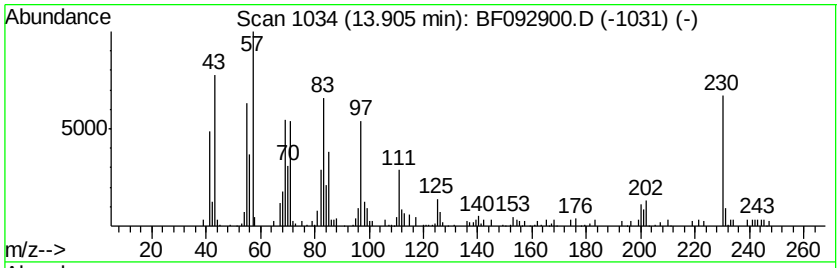
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

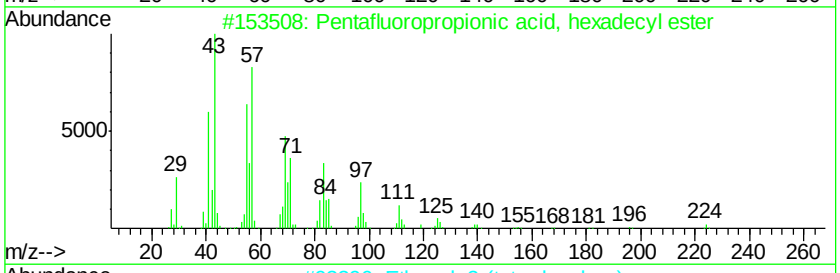
****

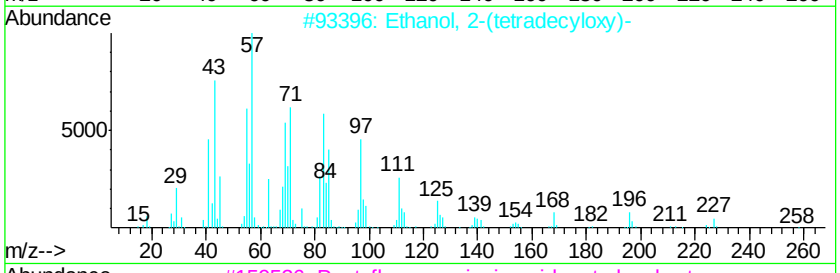
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 5

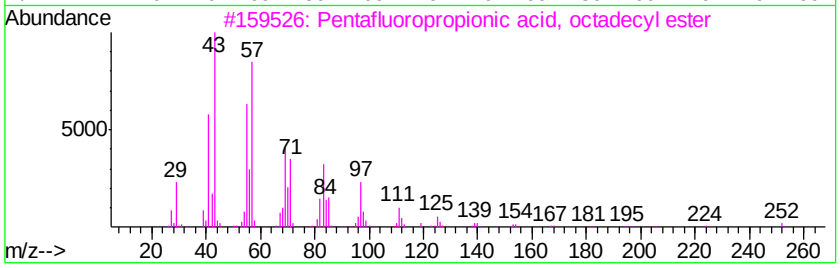
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	3.13 ng	261648	Chrysene-d12	14.05

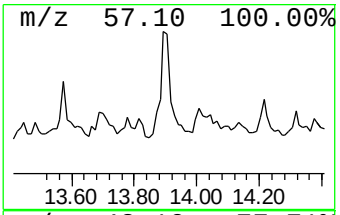
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	70
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	70
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	70
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	70
5	17-Pentatriacontene	491	C35H70	006971-40-0	70

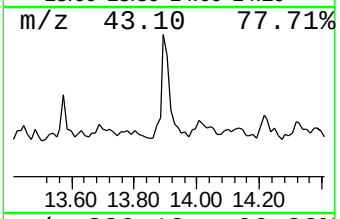


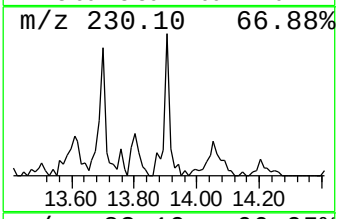


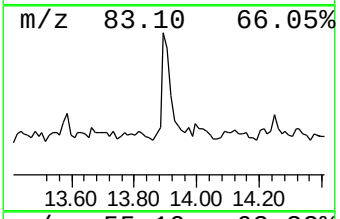


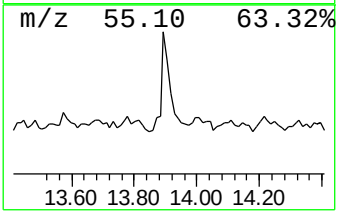












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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

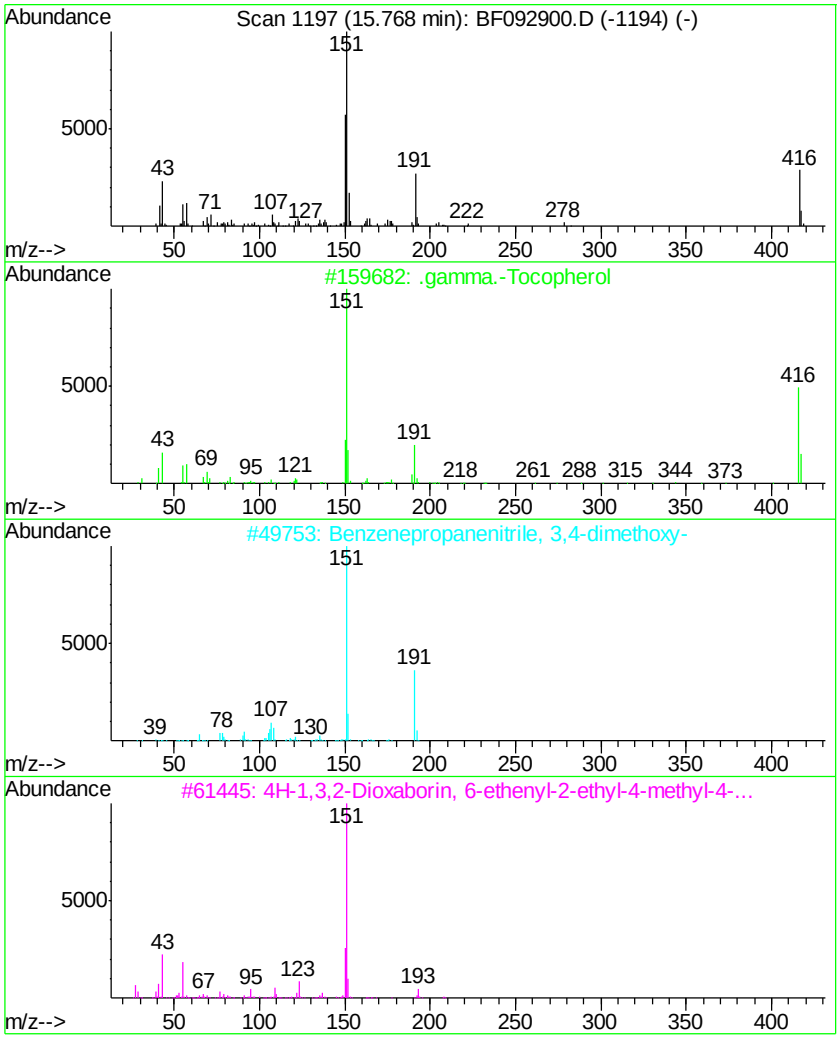
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

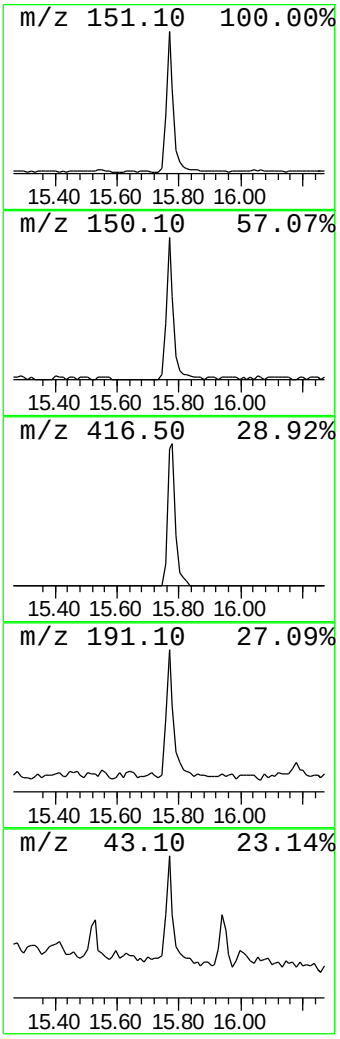
****

Peak Number 6 .gamma.-Tocopherol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.77	5.15 ng	300711	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	81
2	Benzenepropanenitrile, 3,4-dimet...	191	C11H13NO2	049621-56-9	49
3	4H-1,3,2-Dioxaborin, 6-ethenyl-2...	208	C12H21BO2	074630-05-0	43
4	4-Ethylbenzoic acid, octadecyl e...	402	C27H46O2	1000292-35-1	40
5	Dimethyl-(allyl)-silyloxybenzene	192	C11H16OSi	066998-68-3	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF021017\
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ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 38-SB-03-0-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.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...	5.07	33.0	ng	1547370	1	6.90	939196	20.0
unknown6.66	6.66	68.9	ng	3234940	1	6.90	939196	20.0
Heptacosane	10.84	2.7	ng	220832	4	11.42	1629490	20.0
Pentafluoropropio...	13.91	3.1	ng	261648	5	14.05	1669250	20.0
.gamma.-Tocopherol	15.77	5.2	ng	300711	6	15.51	1168750	20.0