LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022217\
Data File : BF093096.D
Acq On : 23 Feb 2017 00:50
Operator : SJ/MA
Sample : I1948-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP23-24-COMP17

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	3.733	141	144	151	rVB	37256	64903	1.55%	0.152%
2	4.327	194	196	209	rBV	658001	838553	20.06%	1.964%
3	5.001	252	255	265	rBV	1409332	2154870	51.55%	5.047%
4	5.436	290	293	295	rBV	3312679	3647690	87.26%	8.543%
5	6.476	381	384	386	rBV	3611968	4180355	100.00%	9.790%
6	6.602	392	395	397	rBV	3883760	3654924	87.43%	8.560%
7	6.830	413	415	418	rBV	1218138	1007456	24.10%	2.359%
8	6.990	426	429	431	rBV	3378552	3176850	75.99%	7.440%
9	7.402	462	465	467	rBV	2739340	2617750	62.62%	6.131%
10	8.122	525	528	530	rBV	1365730	1346607	32.21%	3.154%
11	9.196	619	622	624	rBV	4505907	4078379	97.56%	9.551%
12	9.585	654	656	659	rBV	225136	283054	6.77%	0.663%
13	9.802	673	675	676	rBV	65681	55113	1.32%	0.129%
14	9.871	679	681	683	rBV	1711665	1469261	35.15%	3.441%
15	10.305	715	719	720	rBV	118959	140228	3.35%	0.328%
16	10.522	735	738	741	rBV	42466	61794	1.48%	0.145%
17	10.659	747	750	753	rBV	2020310	1984084	47.46%	4.647%
18	10.773	757	760	765	rVB	303357	358733	8.58%	0.840%
19	11.094	786	788	793	rVB5	30064	52861	1.26%	0.124%
20	11.219	796	799	800	rBV	132583	138970	3.32%	0.325%
21	11.254	800	802	804	rVB	45448	55793	1.33%	0.131%
22	11.356	808	811	812	rBV	1548892	1530463	36.61%	3.584%
23	11.425	815	817	819	rVB	76408	89335	2.14%	0.209%
24	11.596	828	832	835	rBV6	24555	69940	1.67%	0.164%
25	11.642	835	836	839	rVV	47755	52405	1.25%	0.123%
26	11.859	852	855	856	rBV	44443	77032	1.84%	0.180%
27	11.882	856	857	859	rVV	97396	80980	1.94%	0.190%
28	11.962	863	864	869	rVB2	81836	144698	3.46%	0.339%
29	12.054	869	872	874	rBV3	27429	52331	1.25%	0.123%
30	12.145	878	880	882	rBV3	32934	44939	1.08%	0.105%
31	12.396	901	902	904	rBV	37037	56303	1.35%	0.132%
32	12.442	904	906	909	rVB	37216	52276	1.25%	0.122%
33	12.568	915	917	919	rBV	427274	466246	11.15%	1.092%
34	12.797	933	937	939	rBV2	327522	487427	11.66%	1.142%

LSC Area Percent Report

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Acq On : 23 Feb 2017 00:50
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Sample : I1948-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP23-24-COMP17

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
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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

35	12.842	939	941	944	rVB2	37286	60305	1.44%	0.141%
36	12.945	947	950	952	rVV	2816485	3809740	91.13%	8.922%
37	13.014	952	956	958	rVB2	34679	50226	1.20%	0.118%
38	13.117	962	965	967	rBV	50282	88123	2.11%	0.206%
39	13.162	967	969	972	rBV3	25692	55656	1.33%	0.130%
40	13.219	972	974	978	rBV2	48764	88249	2.11%	0.207%
41	13.414	989	991	994	rBV4	30250	47880	1.15%	0.112%
42	13.505	997	999	1001	rBV3	44821	76534	1.83%	0.179%
43	13.631	1008	1010	1012	rVB	47496	52872	1.26%	0.124%
44	13.734	1017	1019	1021	rBV2	27293	44395	1.06%	0.104%
45	13.837	1026	1028	1032	rVB	173455	279037	6.67%	0.653%
46	13.985	1037	1041	1046	rBV3	1053216	1581404	37.83%	3.704%
47	15.002	1128	1130	1134	rBV	101930	210590	5.04%	0.493%
48	15.071	1134	1136	1138	rVB	112789	119612	2.86%	0.280%
49	15.300	1154	1156	1159	rVB	52843	73932	1.77%	0.173%
50	15.357	1159	1161	1164	rVV	96521	142133	3.40%	0.333%
51	15.414	1164	1166	1175	rVB	737654	998206	23.88%	2.338%
52	15.837	1201	1203	1205	rBV	54905	79233	1.90%	0.186%
53	16.305	1242	1244	1250	rVB	51627	98253	2.35%	0.230%
54	16.808	1285	1288	1290	rBV2	35354	76561	1.83%	0.179%
55	17.231	1322	1325	1331	rVB2	36540	94150	2.25%	0.220%

Sum of corrected areas: 42699694

LSC Report - Integrated Chromatogram

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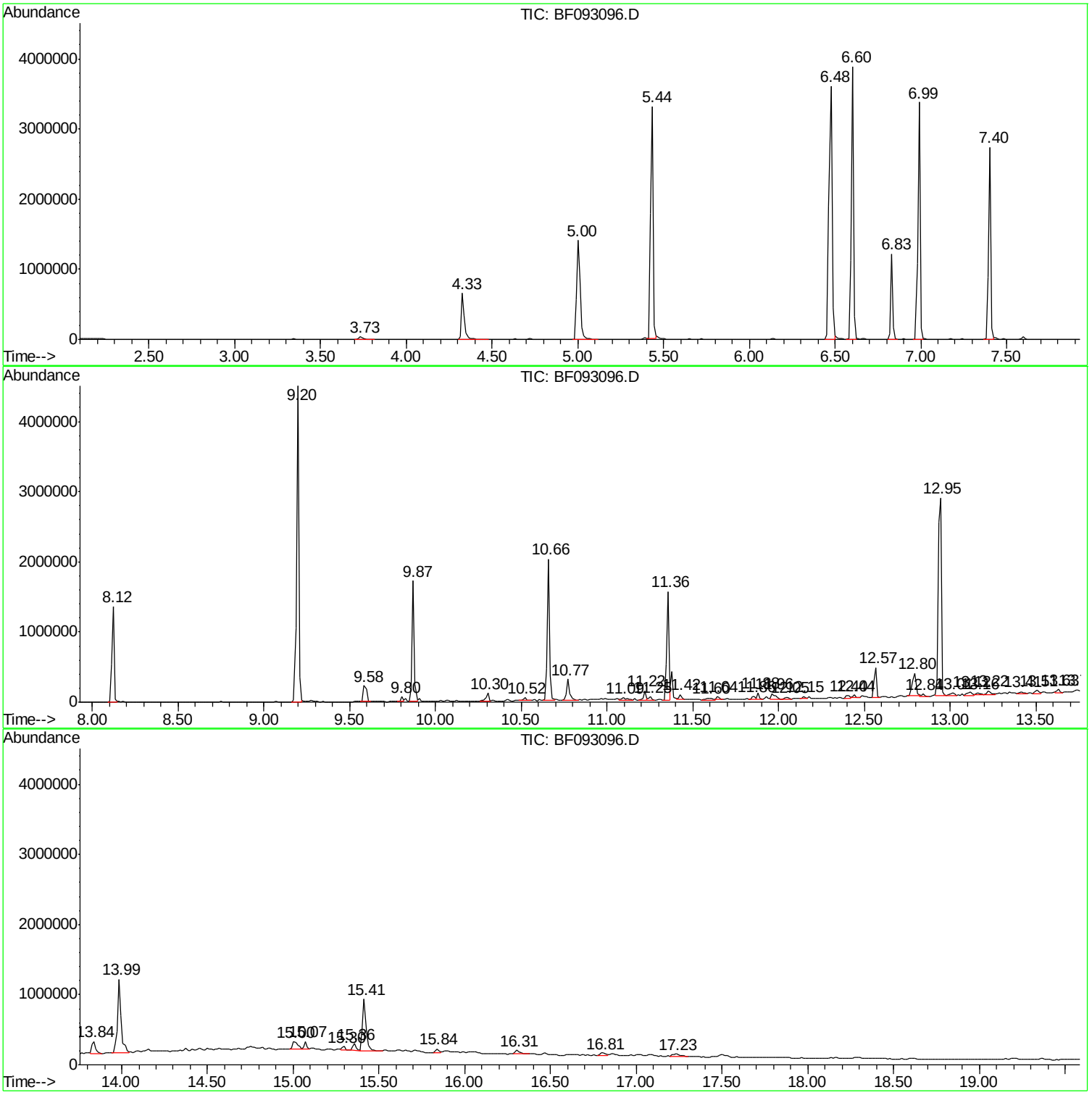
Data File : BF093096.D
Acq On : 23 Feb 2017 00:50
Operator : SJ/MA
Sample : I1948-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP23-24-COMP17

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF022217\
Data File : BF093096.D
Acq On : 23 Feb 2017 00:50
Operator : SJ/MA
Sample : I1948-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP23-24-COMP17

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

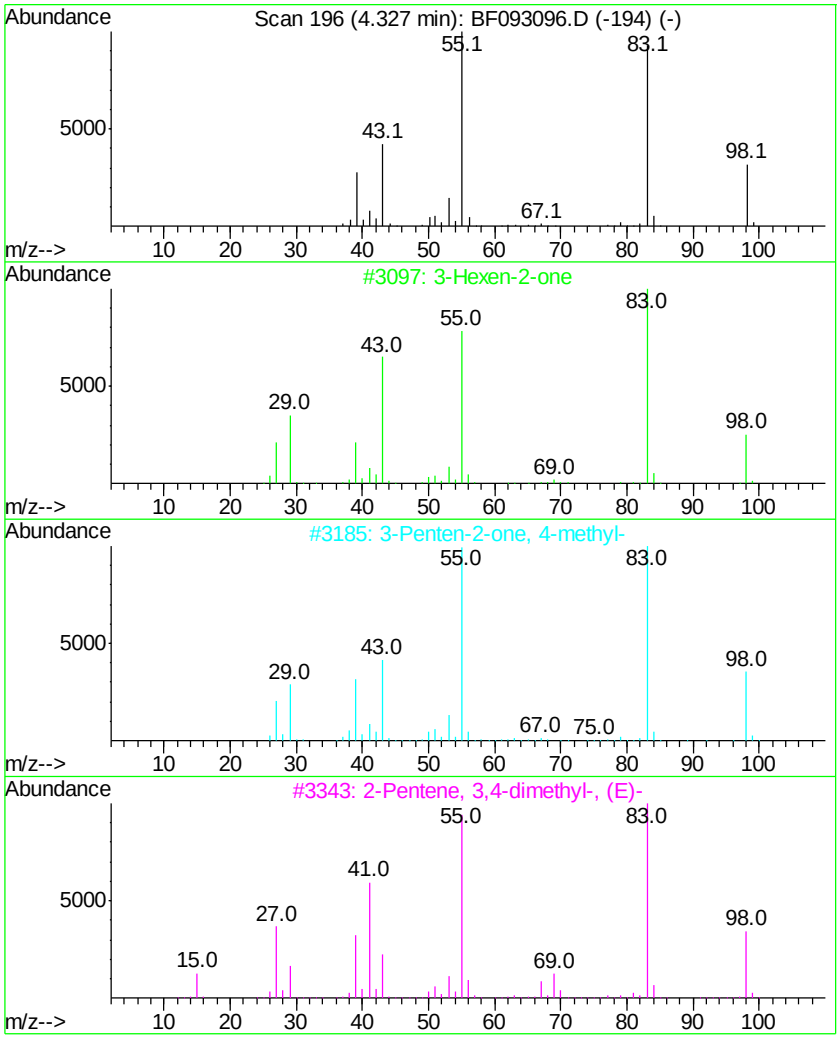
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

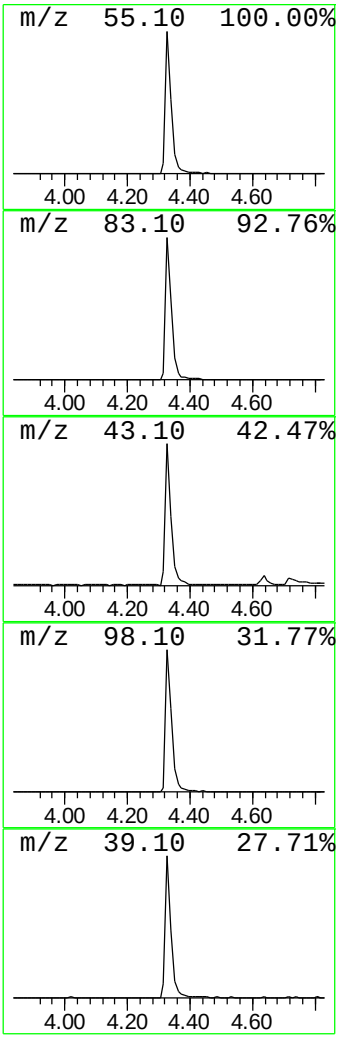
****

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	16.65 ng	838553	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022217\
Data File : BF093096.D
Acq On : 23 Feb 2017 00:50
Operator : SJ/MA
Sample : I1948-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP23-24-COMP17

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

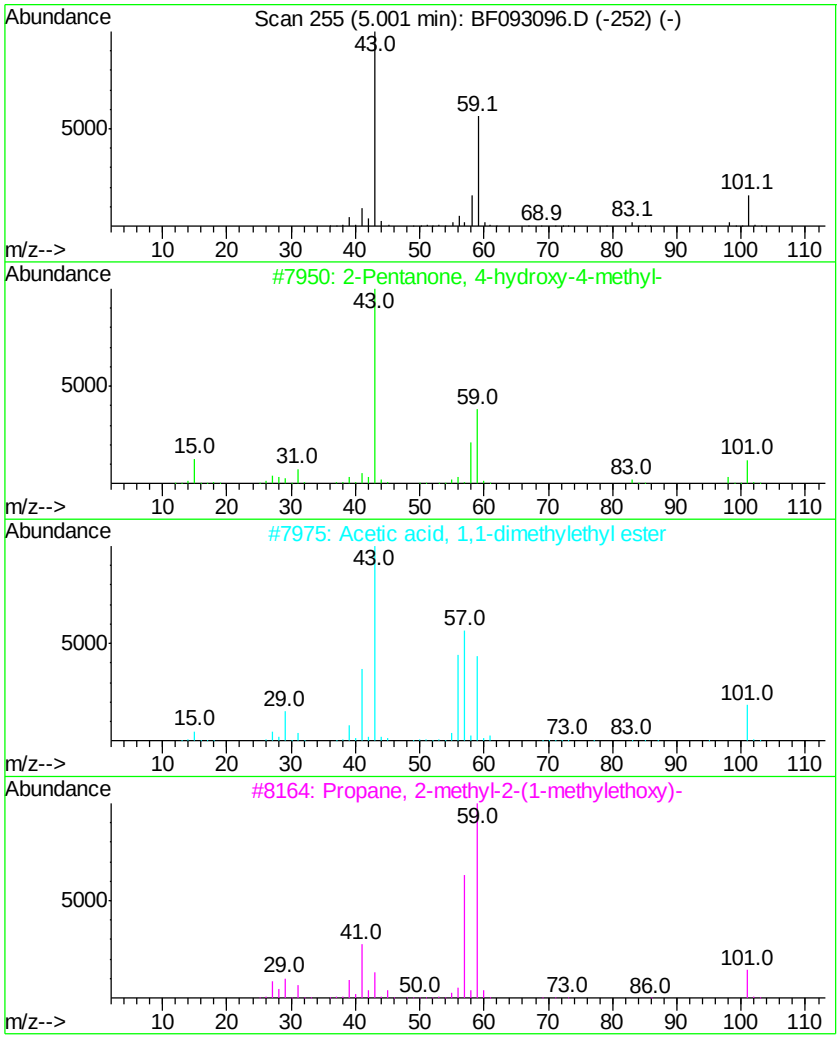
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

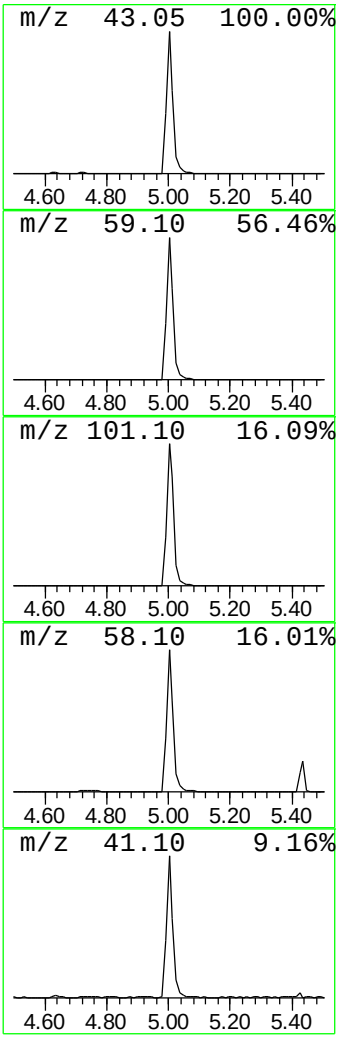
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	42.78 ng	2154870	1,4-Dichlorobenzene-d4	6.83

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	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022217\
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Acq On : 23 Feb 2017 00:50
Operator : SJ/MA
Sample : I1948-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP23-24-COMP17

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

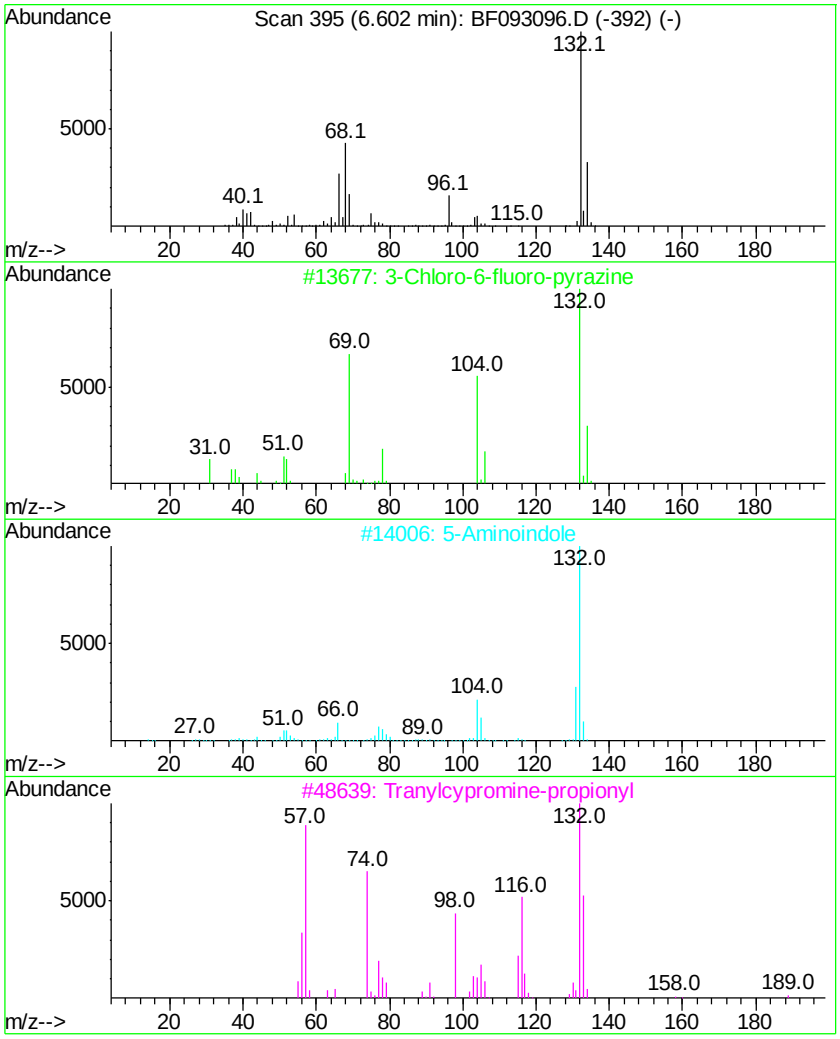
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

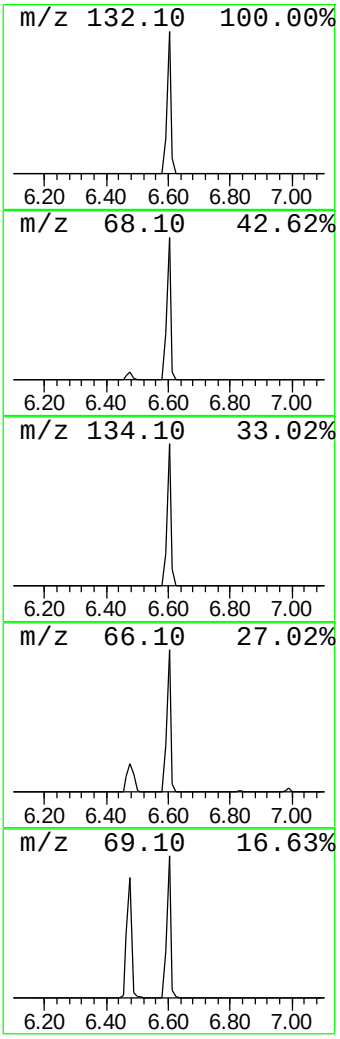
****

Peak Number 3 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	72.56 ng	3654920	1,4-Dichlorobenzene-d4	6.83

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	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Library Search Compound Report

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF013017.M
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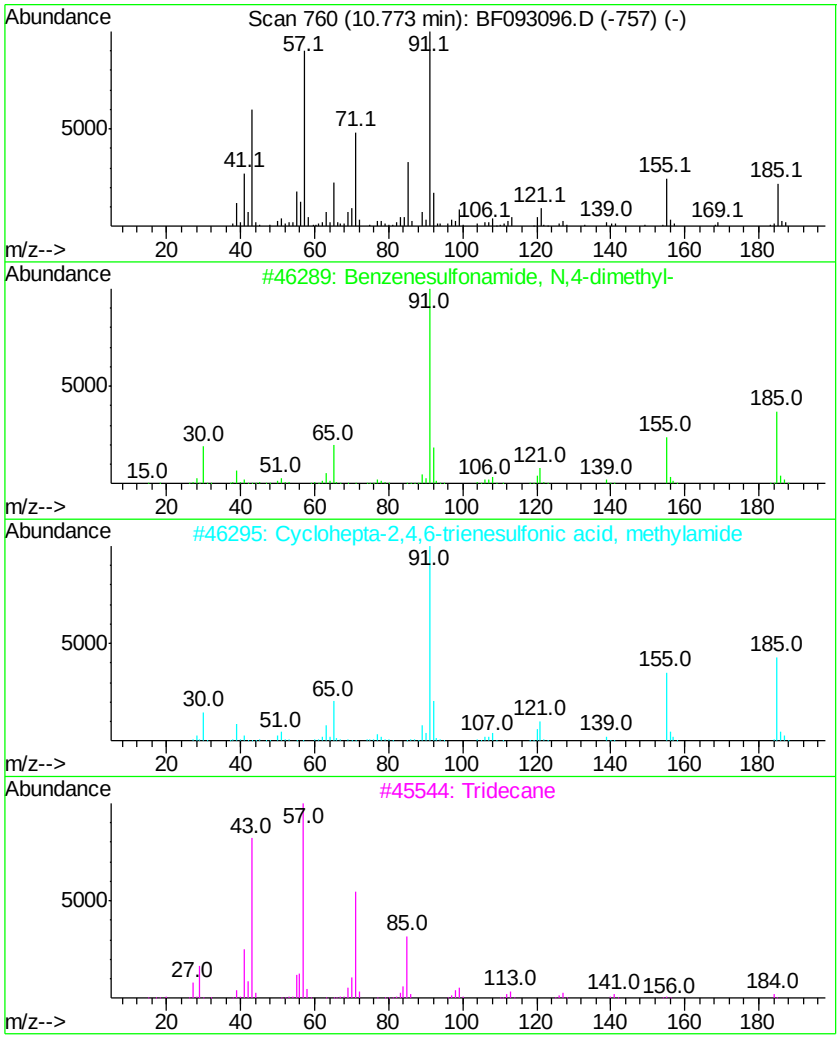
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

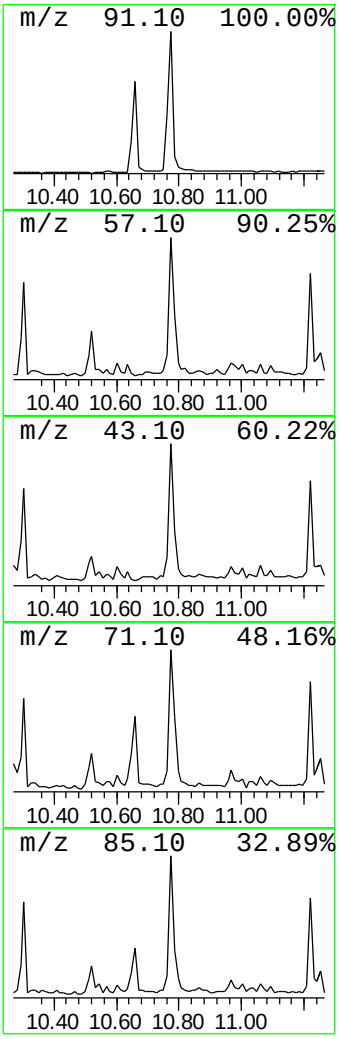
****

Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	4.69 ng	358733	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	87
2	Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	87
3	Tridecane	184	C13H28	000629-50-5	42
4	Eicosane	282	C20H42	000112-95-8	42
5	Hexadecane	226	C16H34	000544-76-3	38





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TIC Library : C:\DATABASE\NIST02.L
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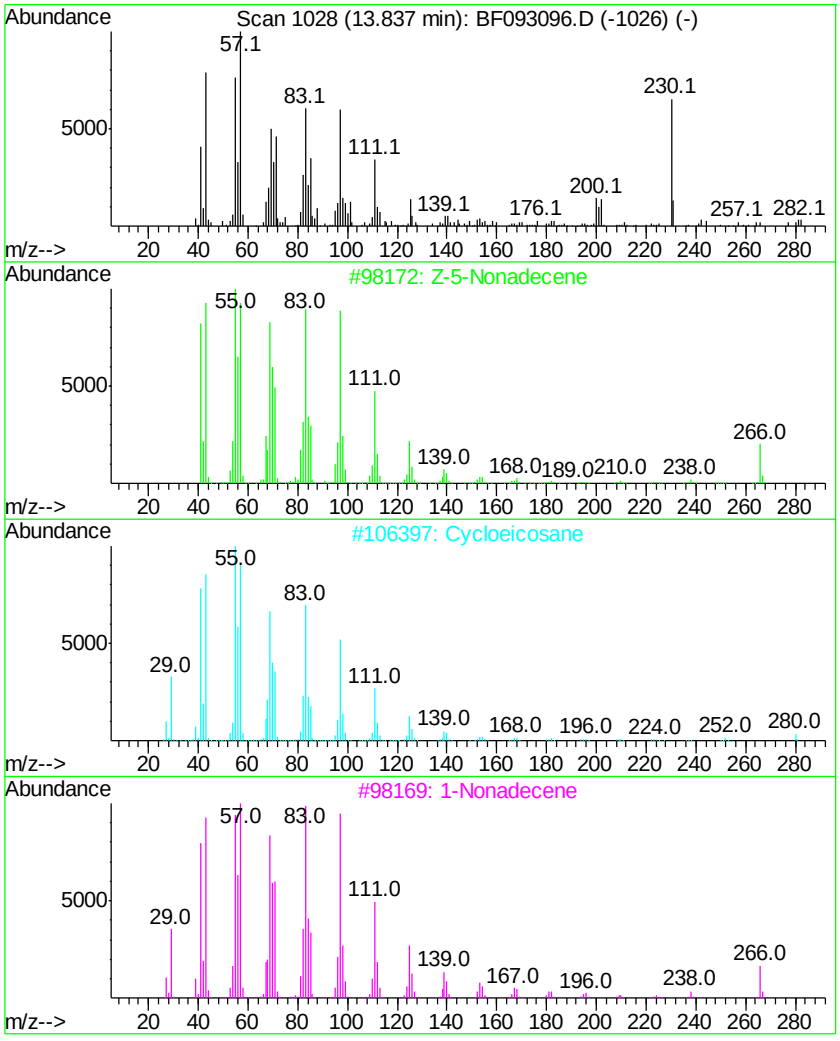
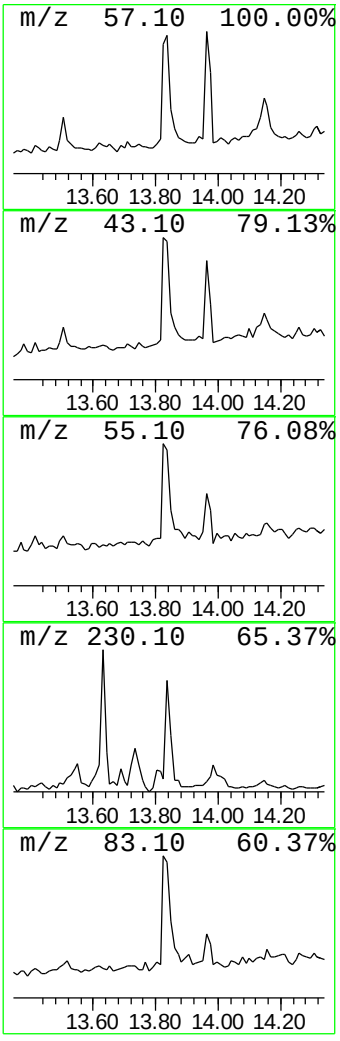
****

Peak Number 6 Z-5-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.53 ng	279037	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	95
2	Cycloeicosane	280	C20H40	000296-56-0	87
3	1-Nonadecene	266	C19H38	018435-45-5	86
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	86
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	83





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Sample : I1948-05
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ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP23-24-COMP17

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

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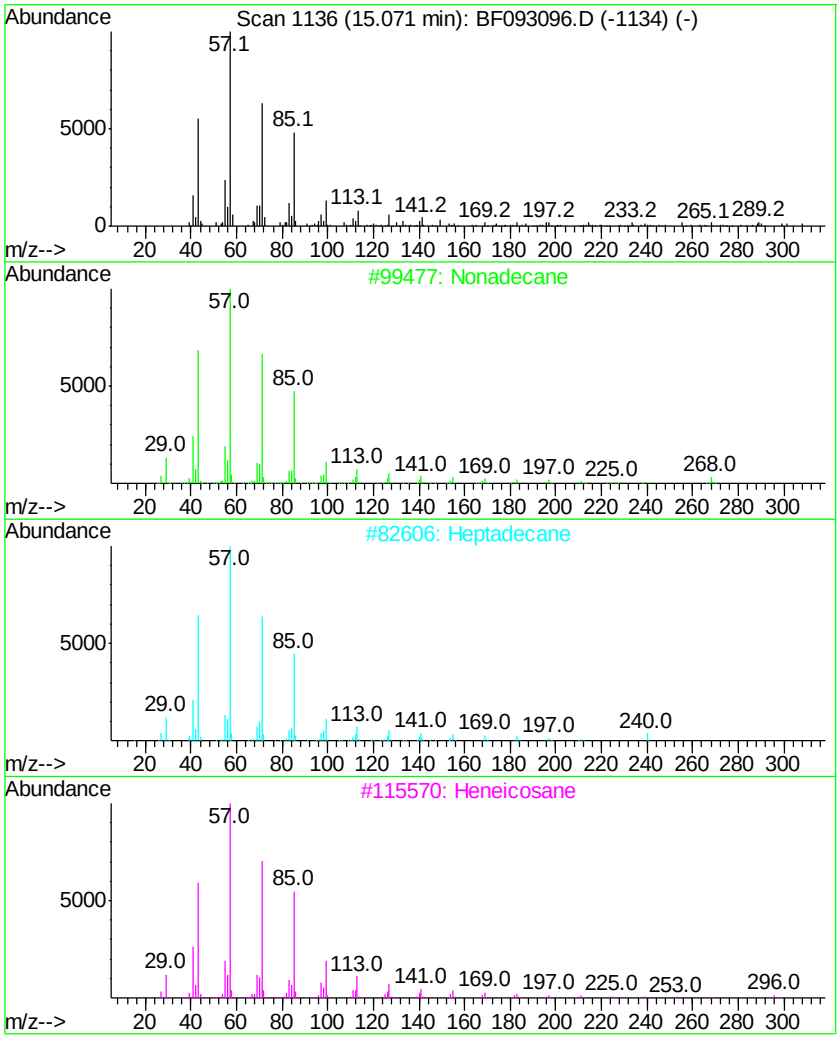
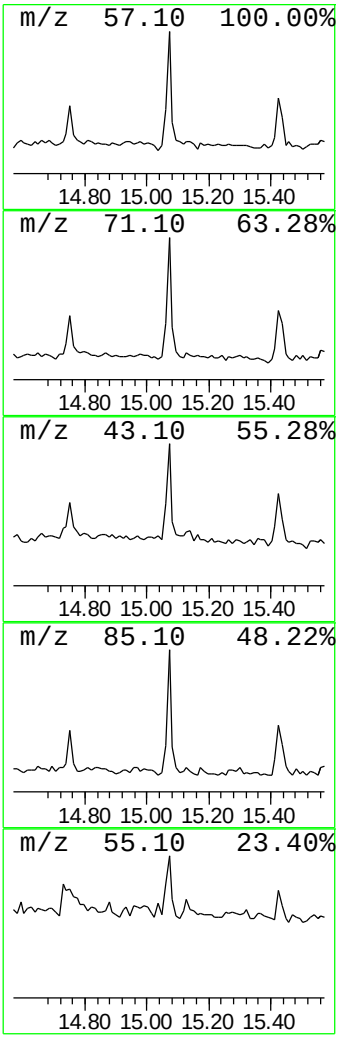
Peak Number 7 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.40 ng	119612	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Heptadecane	240	C17H36	000629-78-7	83
3	Heneicosane	296	C21H44	000629-94-7	83
4	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	80
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80





Tentatively Identified Compound (LSC) summary

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Data File : BF093096.D
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Sample : I1948-05
Misc :
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Instrument : BNA_F
ClientSampleId : TP23-24-COMP17

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
3-Hexen-2-one	4.33	16.6	ng	838553	1	6.83	1007460	20.0
2-Pentanone, 4-hy...	5.00	42.8	ng	2154870	1	6.83	1007460	20.0
unknown6.60	6.60	72.6	ng	3654920	1	6.83	1007460	20.0
Benzenesulfonamid...	10.77	4.7	ng	358733	4	11.36	1530460	20.0
Z-5-Nonadecene	13.84	3.5	ng	279037	5	13.99	1581400	20.0
Nonadecane	15.07	2.4	ng	119612	6	15.41	998206	20.0