LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096333.D
Acq On : 30 Jun 2017 13:19
Operator : SJ/MA
Sample : I3883-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G44-1.5-3

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-BF062717.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	4.322	375	380	386	rVB	51924	60425	1.38%	0.165%
2	4.616	427	430	440	rBV	47006	61406	1.40%	0.167%
3	4.975	483	491	494	rBV	3086902	4387631	100.00%	11.957%
4	5.375	555	559	563	rVB	1240062	1161380	26.47%	3.165%
5	6.404	727	734	738	rBV	2858133	3063801	69.83%	8.349%
6	6.540	752	757	760	rBV	1871806	1679174	38.27%	4.576%
7	6.769	793	796	800	rBV	1008041	842448	19.20%	2.296%
8	6.840	804	808	811	rBV	598457	480003	10.94%	1.308%
9	6.928	819	823	827	rVB	2861105	2616753	59.64%	7.131%
10	7.328	883	891	894	rBV	2239184	2319481	52.86%	6.321%
11	7.381	897	900	903	rVV2	69689	65945	1.50%	0.180%
12	7.587	922	935	938	rVB6	25339	61950	1.41%	0.169%
13	7.751	958	963	966	rBV	72712	74771	1.70%	0.204%
14	8.051	1010	1014	1017	rBV	1440997	1235258	28.15%	3.366%
15	8.357	1059	1066	1068	rBV6	31833	50858	1.16%	0.139%
16	8.486	1084	1088	1093	rBV	80865	93750	2.14%	0.255%
17	8.657	1113	1117	1120	rBV	223603	184386	4.20%	0.502%
18	8.763	1130	1135	1138	rVB2	72639	86238	1.97%	0.235%
19	8.863	1149	1152	1156	rBV2	52920	59896	1.37%	0.163%
20	9.086	1188	1190	1193	rVB	81747	67554	1.54%	0.184%
21	9.133	1193	1198	1201	rBV	3363025	3380400	77.04%	9.212%
22	9.222	1208	1213	1216	rBV2	272880	251810	5.74%	0.686%
23	9.386	1239	1241	1247	rBV3	52390	84111	1.92%	0.229%
24	9.469	1251	1255	1257	rBV2	71319	80471	1.83%	0.219%
25	9.522	1261	1264	1266	rBV	591887	490594	11.18%	1.337%
26	9.545	1266	1268	1269	rVB	80075	57210	1.30%	0.156%
27	9.751	1300	1303	1307	rVB	305962	242225	5.52%	0.660%
28	9.804	1307	1312	1316	rBV	1211936	1136432	25.90%	3.097%
29	9.833	1316	1317	1320	rVB	62200	49926	1.14%	0.136%
30	9.910	1328	1330	1335	rVB3	35149	49191	1.12%	0.134%
31	9.980	1339	1342	1344	rVV3	38809	49134	1.12%	0.134%
32	10.010	1344	1347	1350	rVV	136935	129764	2.96%	0.354%
33	10.045	1350	1353	1355	rVV2	57030	61617	1.40%	0.168%
34	10.075	1355	1358	1361	rVB2	76571	79459	1.81%	0.217%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I3883-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G44-1.5-3

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-BF062717.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.216	1380	1382	1385	rBV3	32314	44074	1.00%	0.120%
36	10.245	1385	1387	1390	rVB	315876	274835	6.26%	0.749%
37	10.351	1402	1405	1407	rBV2	97761	92126	2.10%	0.251%
38	10.469	1421	1425	1429	rBV	239099	239801	5.47%	0.653%
39	10.551	1437	1439	1442	rBV2	74644	78239	1.78%	0.213%
40	10.586	1442	1445	1449	rVB3	223578	205751	4.69%	0.561%
41	10.722	1465	1468	1469	rBV	473134	408720	9.32%	1.114%
42	10.733	1469	1470	1474	rVB	485776	399199	9.10%	1.088%
43	10.951	1505	1507	1510	rVB2	59935	48909	1.11%	0.133%
44	11.004	1514	1516	1519	rBV2	60286	64379	1.47%	0.175%
45	11.169	1541	1544	1547	rBV	365555	312913	7.13%	0.853%
46	11.198	1547	1549	1554	rVB	358674	350853	8.00%	0.956%
47	11.286	1560	1564	1566	rBV	973933	828703	18.89%	2.258%
48	11.310	1566	1568	1571	rVV	617552	477553	10.88%	1.301%
49	11.357	1573	1576	1579	rVB2	224547	216565	4.94%	0.590%
50	11.510	1600	1602	1606	rBV3	57199	56610	1.29%	0.154%
51	11.551	1606	1609	1611	rVV	89842	79340	1.81%	0.216%
52	11.592	1613	1616	1619	rVV	289346	236886	5.40%	0.646%
53	11.786	1647	1649	1652	rBV	80372	67123	1.53%	0.183%
54	11.816	1652	1654	1658	rVB	231664	203585	4.64%	0.555%
55	11.857	1658	1661	1664	rBV2	58316	67007	1.53%	0.183%
56	11.898	1665	1668	1670	rBV2	165376	172682	3.94%	0.471%
57	11.974	1679	1681	1683	rBV2	48656	48512	1.11%	0.132%
58	11.998	1683	1685	1688	rVV	253885	218493	4.98%	0.595%
59	12.286	1732	1734	1739	rVB	110987	87983	2.01%	0.240%
60	12.339	1740	1743	1746	rBV2	139993	153856	3.51%	0.419%
61	12.392	1749	1752	1754	rVB	242539	235892	5.38%	0.643%
62	12.463	1762	1764	1766	rBV2	65367	58736	1.34%	0.160%
63	12.492	1766	1769	1773	rVV	636955	601380	13.71%	1.639%
64	12.721	1805	1808	1812	rVB	480779	407496	9.29%	1.110%
65	12.763	1812	1815	1817	rVB	206557	172299	3.93%	0.470%
66	12.874	1830	1834	1837	rBV	2393210	2332995	53.17%	6.358%
67	13.116	1873	1875	1878	rVB2	258884	223427	5.09%	0.609%
68	13.357	1913	1916	1922	rVB	693483	677304	15.44%	1.846%
69	13.457	1931	1933	1936	rBV2	190811	179166	4.08%	0.488%
70	13.774	1984	1987	1995	rVB3	319030	545489	12.43%	1.486%
71	13.916	2008	2011	2014	rBV2	743348	833140	18.99%	2.270%

LSC Area Percent Report

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Sample : I3883-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G44-1.5-3

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
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.104	2041	2043	2046	rVB	242199	199041	4.54%	0.542%

Sum of corrected areas: 36696514

LSC Report - Integrated Chromatogram

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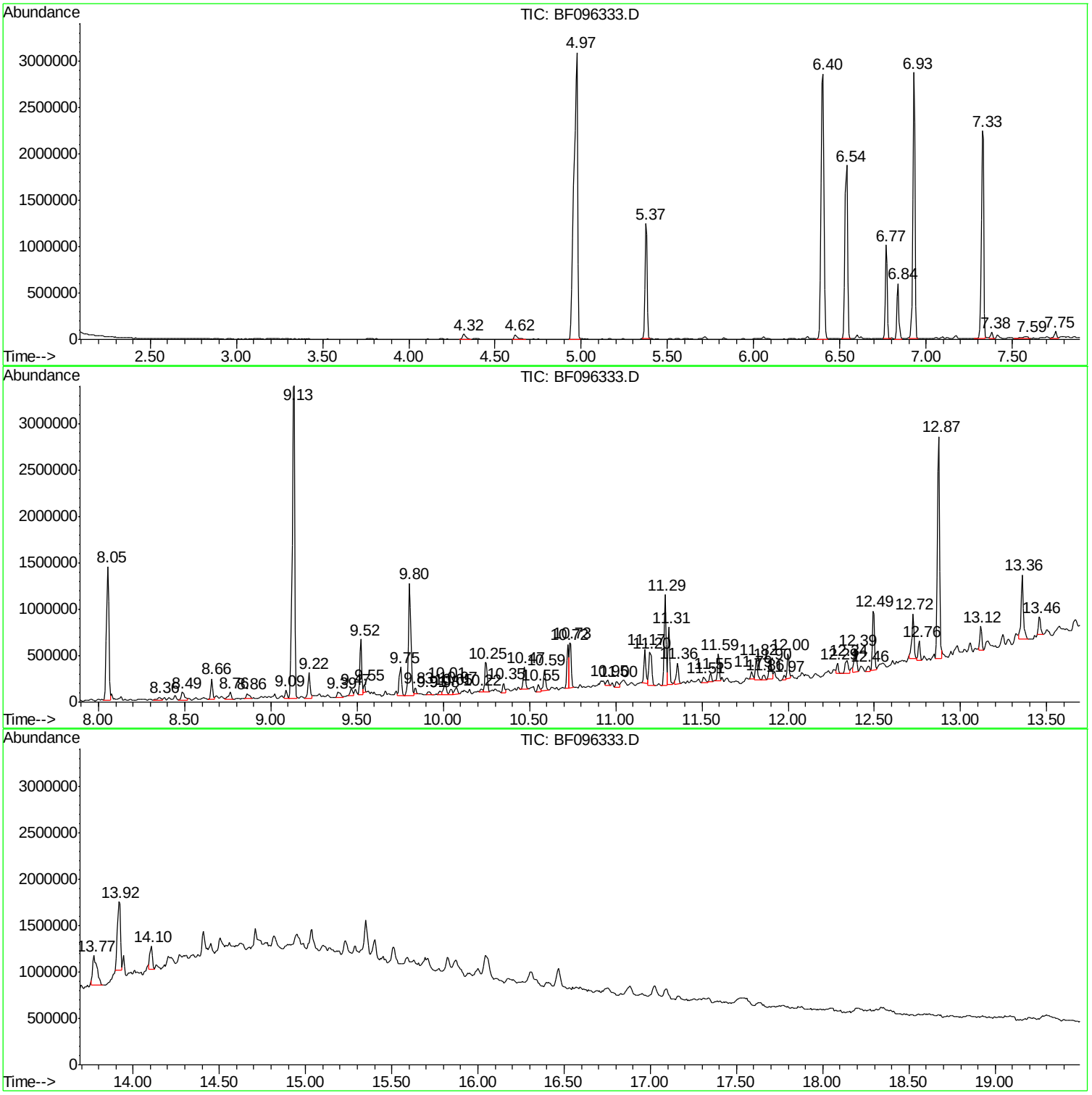
Sample : I3883-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G44-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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\BF063017\
Data File : BF096333.D
Acq On : 30 Jun 2017 13:19
Operator : SJ/MA
Sample : I3883-10
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ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G44-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

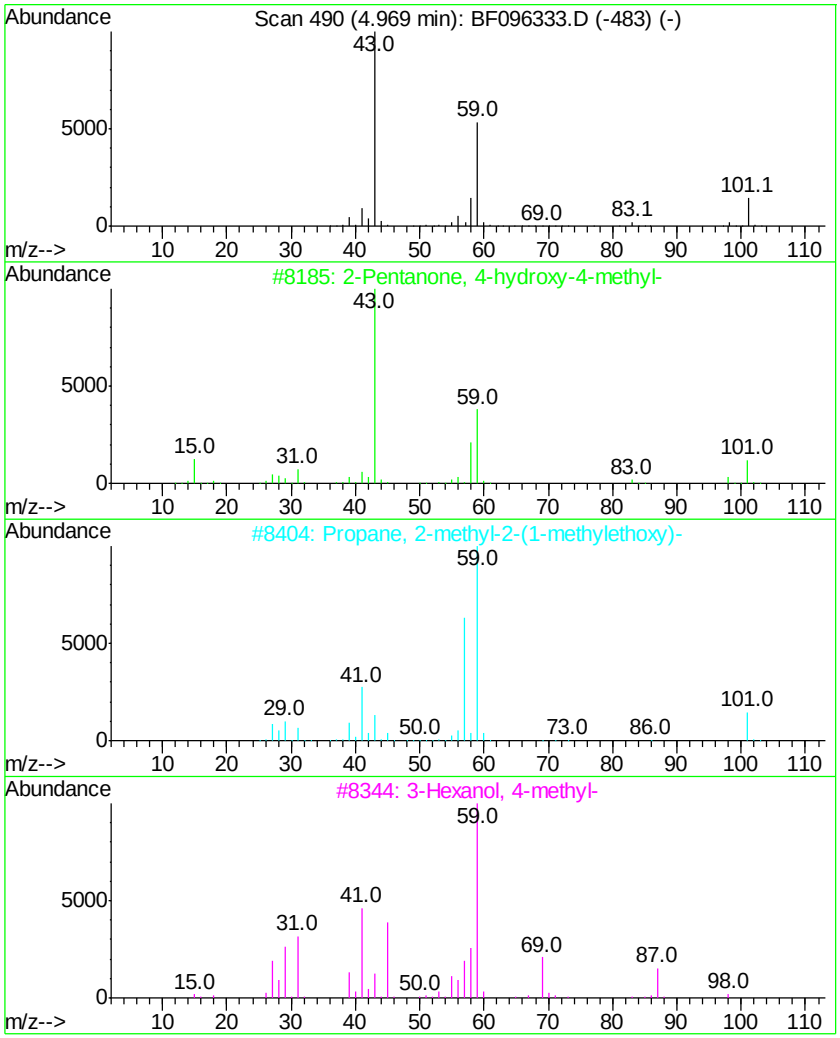
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

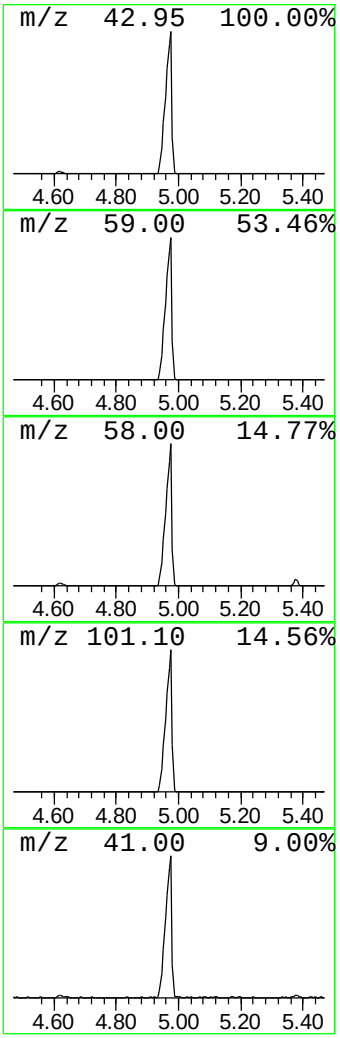
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	104.16 ng	4387630	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF063017\
Data File : BF096333.D
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Sample : I3883-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G44-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

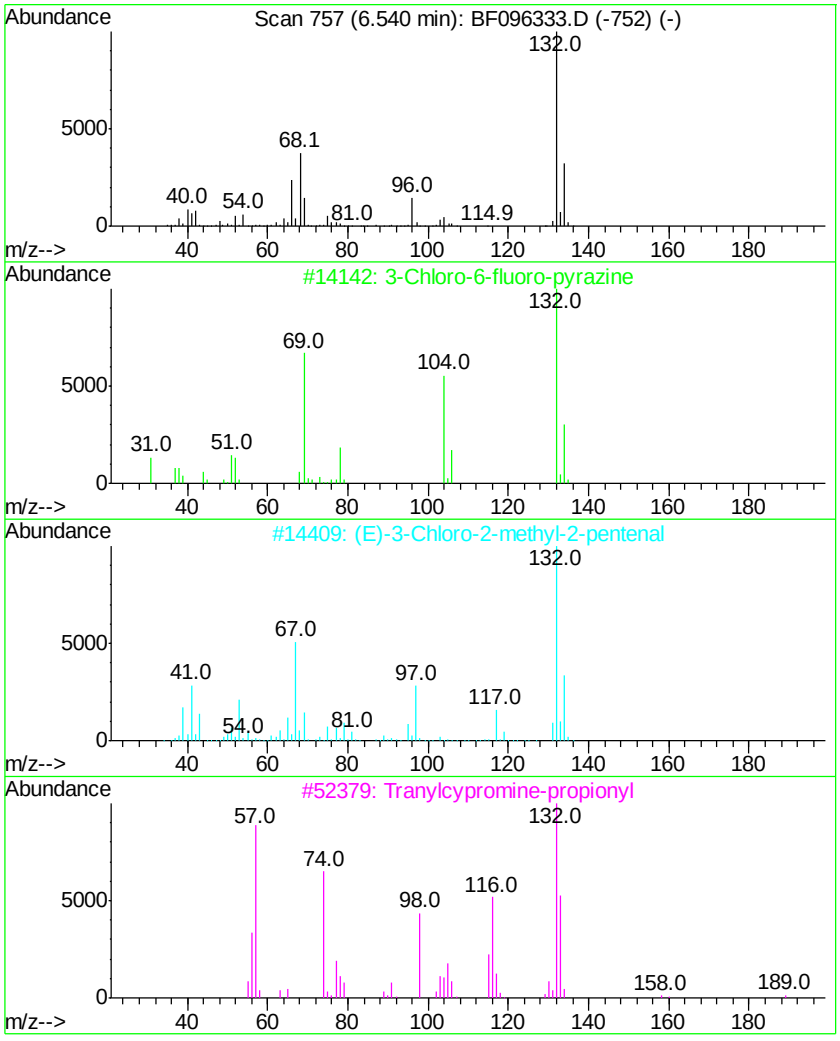
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

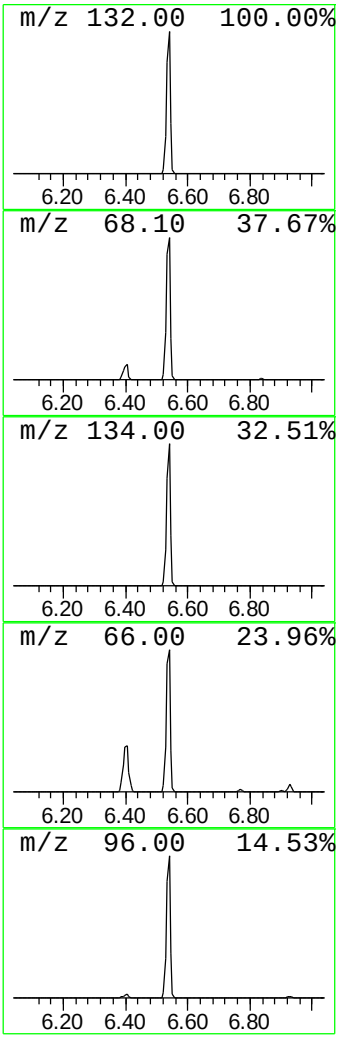
****

Peak Number 2 unknown6.54 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	39.86 ng	1679170	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Data File : BF096333.D
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Operator : SJ/MA
Sample : I3883-10
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G44-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

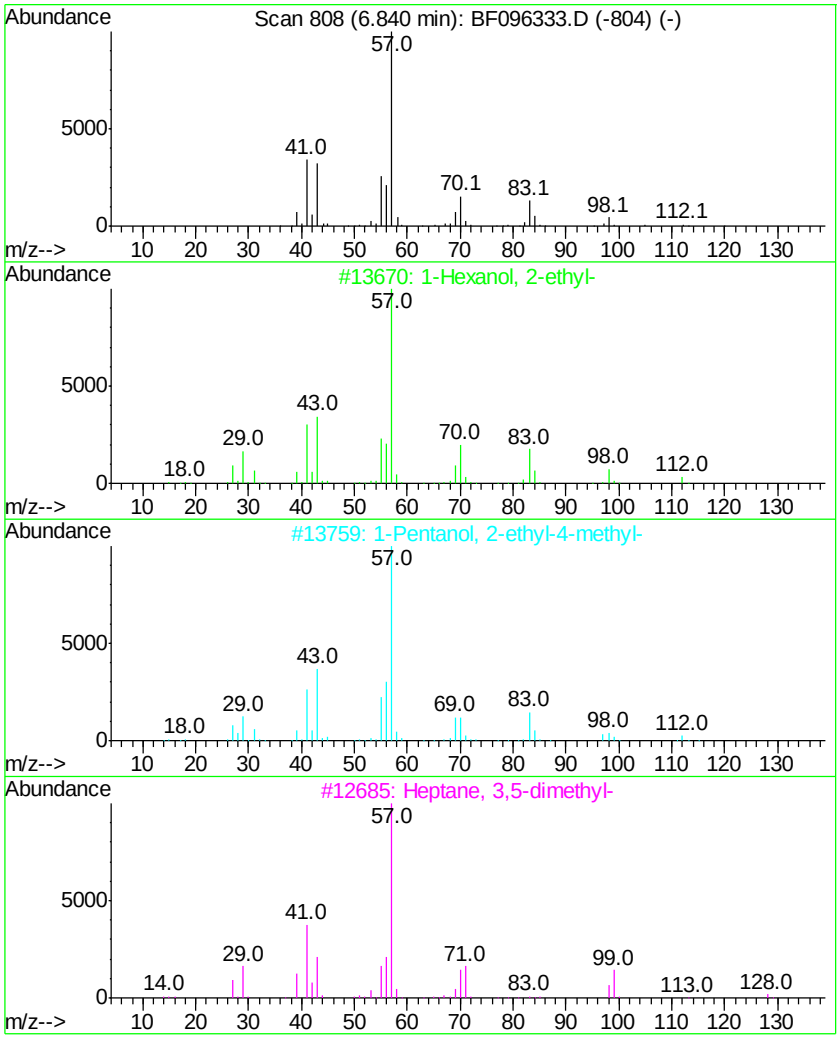
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

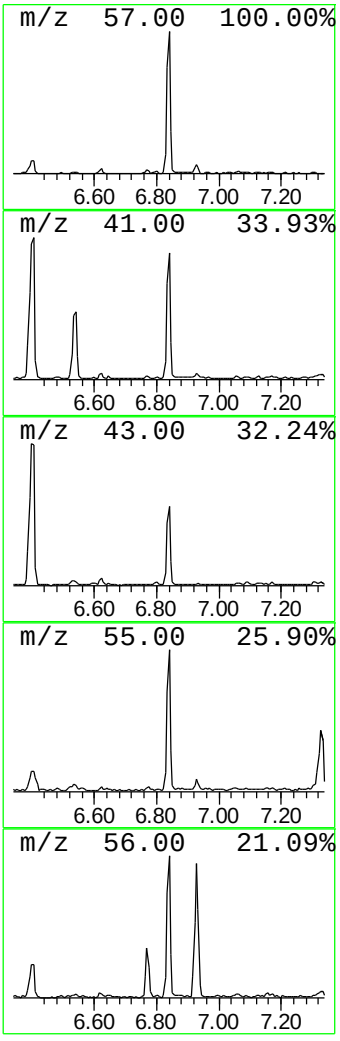
****

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.84	11.40 ng	480003	1,4-Dichlorobenzene-d4	6.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	53
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	45





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Instrument : BNA_F
ClientSampleId : G44-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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TIC Library : C:\DATABASE\NIST11.L
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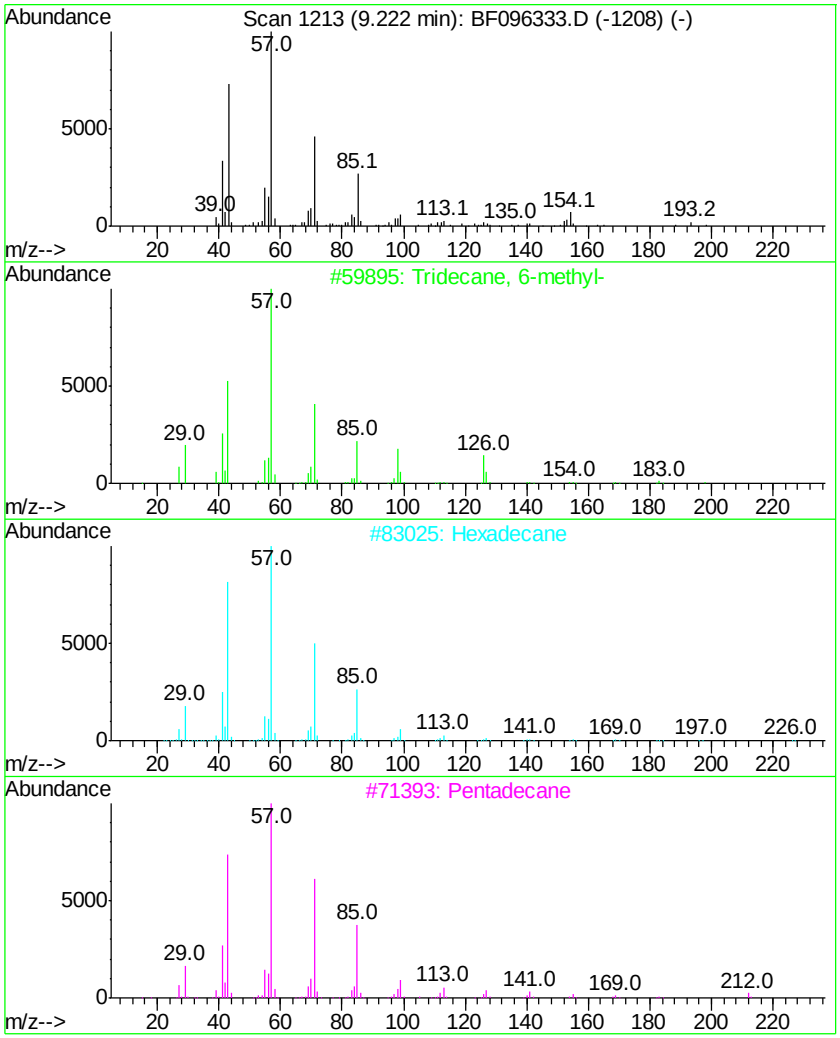
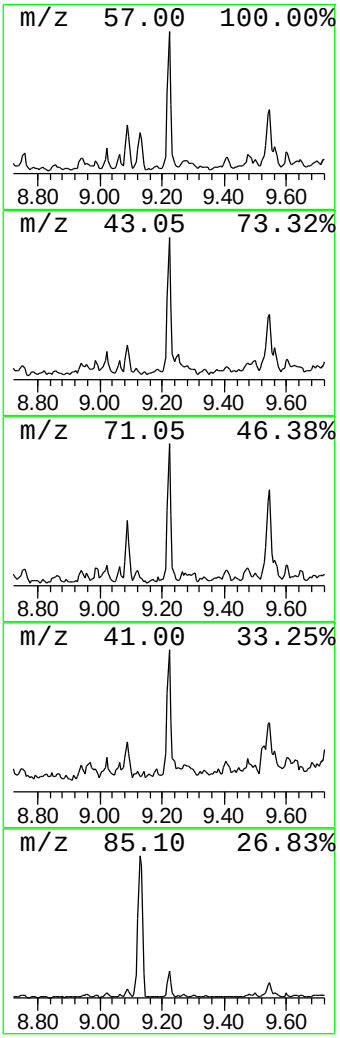
****

Peak Number 5 Tridecane, 6-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.22	4.43 ng	251810	Acenaphthene-d10	9.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 6-methyl-	198	C14H30	013287-21-3	90
2	Hexadecane	226	C16H34	000544-76-3	87
3	Pentadecane	212	C15H32	000629-62-9	86
4	Heneicosane	296	C21H44	000629-94-7	80
5	Undecane, 5-ethyl-	184	C13H28	017453-94-0	78





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Instrument : BNA_F
ClientSampleId : G44-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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TIC Library : C:\DATABASE\NIST11.L
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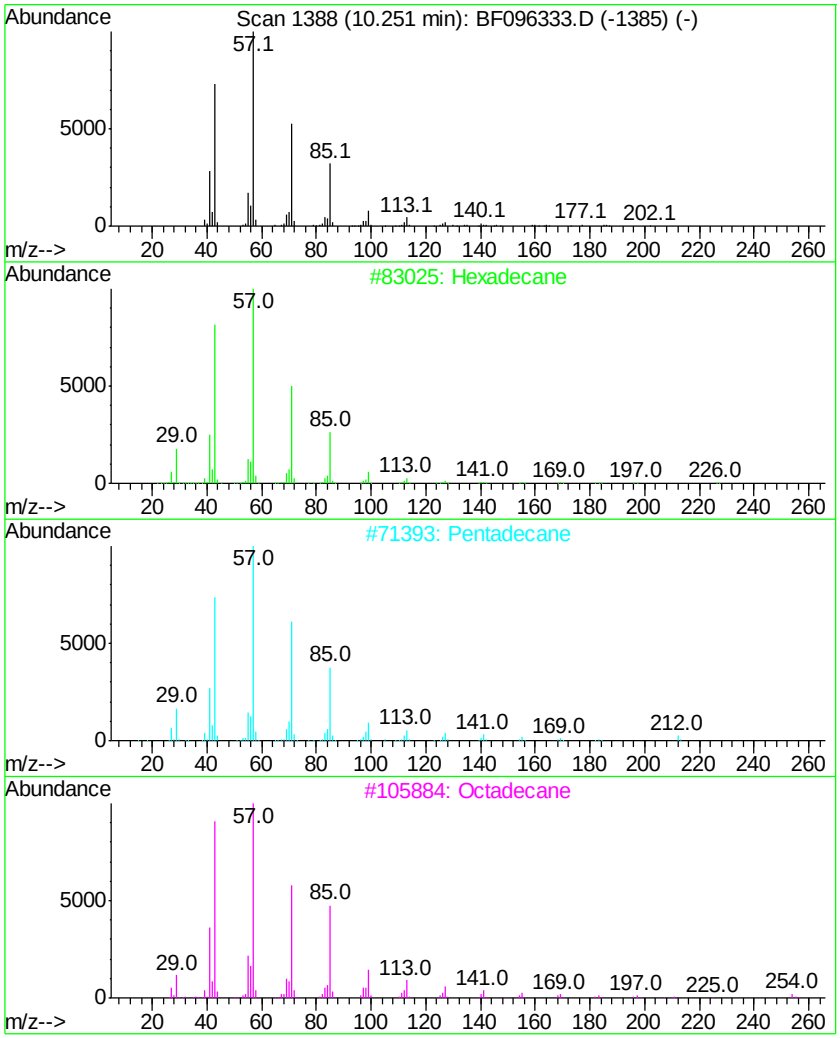
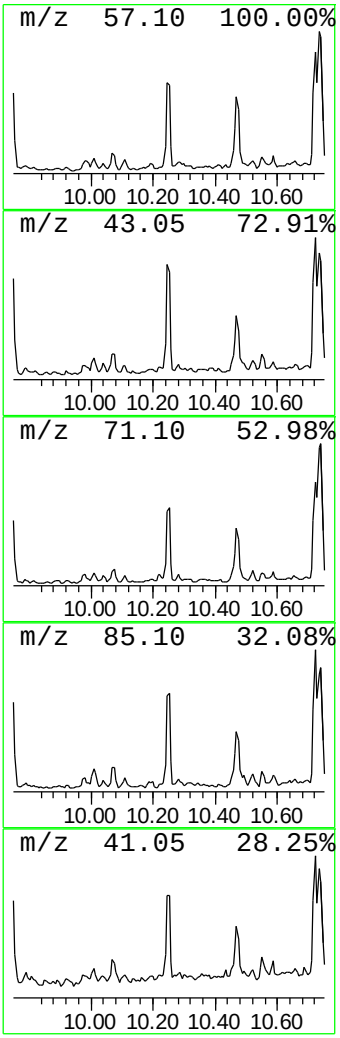
****

Peak Number 7 Pentadecane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.25	4.84 ng	274835	Acenaphthene-d10	9.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	97
2	Pentadecane	212	C15H32	000629-62-9	83
3	Octadecane	254	C18H38	000593-45-3	80
4	Heneicosane	296	C21H44	000629-94-7	80
5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	72





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Instrument : BNA_F
ClientSampleId : G44-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.M
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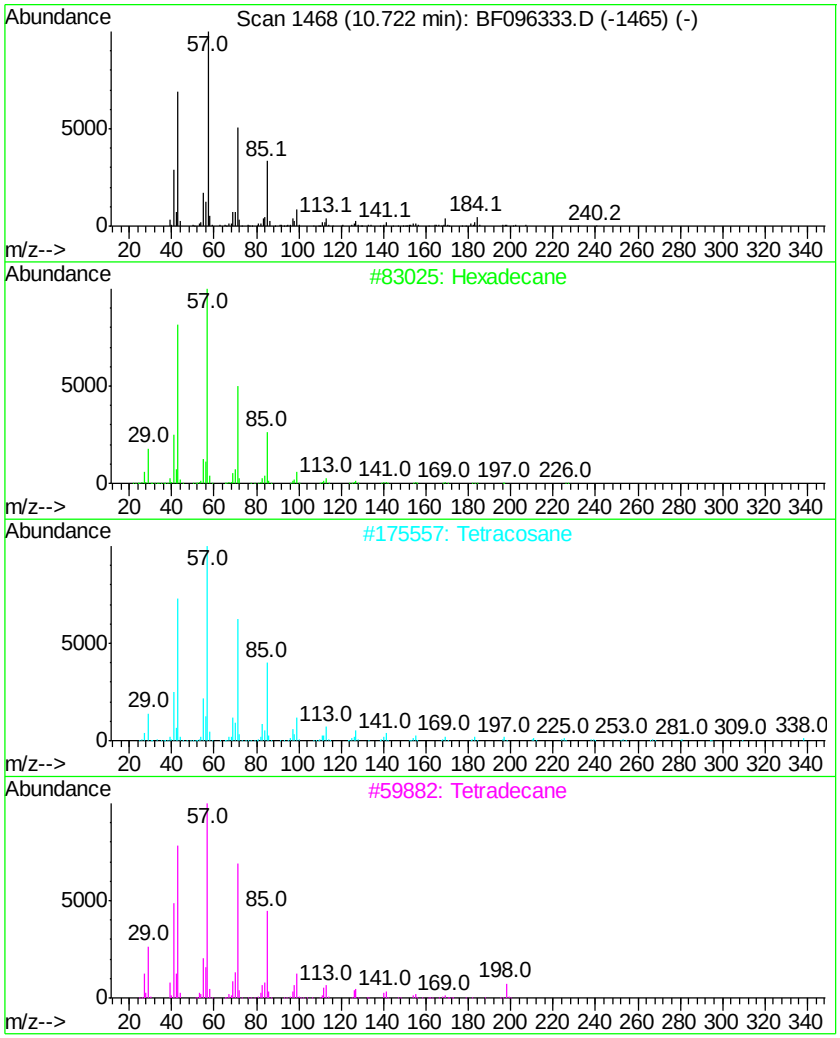
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

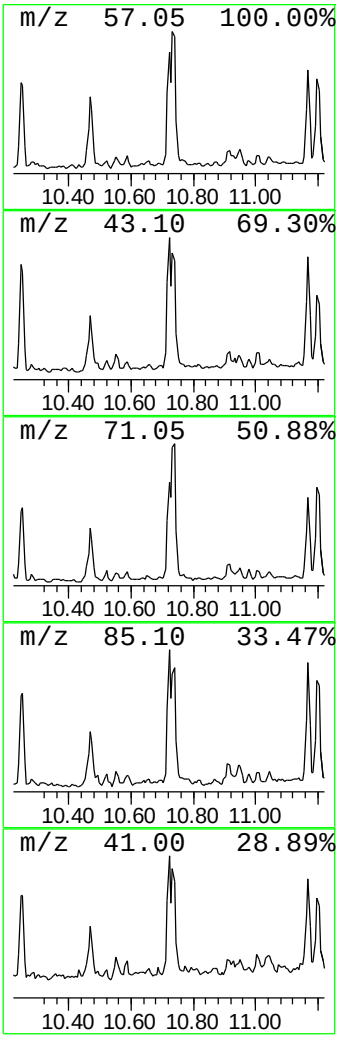
****

Peak Number 8 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	9.86 ng	408720	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Tetracosane	338	C24H50	000646-31-1	86
3	Tetradecane	198	C14H30	000629-59-4	80
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	76





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Instrument : BNA_F
ClientSampleId : G44-1.5-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF062717.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 9 Undecane, 3,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	9.63 ng	399199	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	78
2	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	78
3	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72
4	Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	59
5	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	59