LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

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-BF072517.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	1.887	15	17	32	rVB2	80541	169971	7.22%	0.720%
2	4.516	461	464	480	rBV	104006	217661	9.25%	0.922%
3	4.987	541	544	571	rBV	1414604	2174675	92.38%	9.215%
4	6.069	725	728	742	rBV	1956864	2353933	100.00%	9.975%
5	6.169	742	745	762	rVB	2116872	2233305	94.88%	9.463%
6	6.398	780	784	798	rBV	675052	709747	30.15%	3.007%
7	6.551	806	810	825	rBV	1478122	1500121	63.73%	6.357%
8	6.969	878	881	900	rBV	1413071	1470775	62.48%	6.232%
9	7.680	998	1002	1013	rBV	978314	991753	42.13%	4.202%
10	8.757	1181	1185	1198	rBV	2368756	2249664	95.57%	9.533%
11	9.163	1251	1254	1261	rBV	353542	322728	13.71%	1.368%
12	9.422	1294	1298	1302	rBV	1011423	923814	39.25%	3.915%
13	9.457	1302	1304	1308	rVB	56966	54398	2.31%	0.231%
14	9.874	1372	1375	1378	rVB	66265	57872	2.46%	0.245%
15	9.974	1389	1392	1398	rVB	36550	36974	1.57%	0.157%
16	10.098	1408	1413	1415	rBV	36803	48490	2.06%	0.205%
17	10.210	1429	1432	1448	rBV	1134426	1199796	50.97%	5.084%
18	10.345	1452	1455	1463	rBV	118788	160324	6.81%	0.679%
19	10.792	1528	1531	1534	rBV3	75383	73443	3.12%	0.311%
20	10.821	1534	1536	1539	rVB	31313	28260	1.20%	0.120%
21	10.898	1545	1549	1551	rBV	787211	758581	32.23%	3.214%
22	10.921	1551	1553	1558	rVV	304690	278302	11.82%	1.179%
23	10.980	1559	1563	1569	rVB	71719	81117	3.45%	0.344%
24	11.057	1573	1576	1582	rVB	49459	49031	2.08%	0.208%
25	11.151	1588	1592	1594	rBV2	32911	36470	1.55%	0.155%
26	11.216	1601	1603	1608	rVB2	26820	25922	1.10%	0.110%
27	11.433	1637	1640	1641	rBV	25836	24715	1.05%	0.105%
28	11.457	1641	1644	1646	rVV	91006	75465	3.21%	0.320%
29	11.510	1650	1653	1656	rBV	48855	42405	1.80%	0.180%
30	11.745	1691	1693	1705	rVB4	24327	40714	1.73%	0.173%
31	12.098	1750	1753	1758	rBV	362009	356468	15.14%	1.510%
32	12.233	1773	1776	1778	rBV2	32386	31346	1.33%	0.133%
33	12.321	1786	1791	1796	rBV	339754	380814	16.18%	1.614%
34	12.474	1811	1817	1821	rBV	1433181	1418540	60.26%	6.011%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.557	1827	1831	1835	rVB4	18661	27493	1.17%	0.116%
36	12.662	1846	1849	1853	rVB2	36683	39734	1.69%	0.168%
37	12.727	1857	1860	1863	rVV2	34038	32507	1.38%	0.138%
38	12.762	1863	1866	1874	rVB4	37142	52076	2.21%	0.221%
39	12.968	1896	1901	1907	rBV	282796	306412	13.02%	1.298%
40	13.180	1934	1937	1943	rVB	28539	31665	1.35%	0.134%
41	13.274	1949	1953	1954	rBV2	28309	28106	1.19%	0.119%
42	13.392	1969	1973	1980	rBV2	102595	144718	6.15%	0.613%
43	13.515	1988	1994	1997	rBV2	651776	801509	34.05%	3.396%
44	13.545	1997	1999	2007	rVB2	171333	188421	8.00%	0.798%
45	13.621	2009	2012	2017	rVB2	32919	36919	1.57%	0.156%
46	13.909	2057	2061	2064	rBV2	31538	40632	1.73%	0.172%
47	14.292	2121	2126	2130	rBV	125497	146432	6.22%	0.620%
48	14.515	2160	2164	2167	rBV	182008	225896	9.60%	0.957%
49	14.609	2177	2180	2184	rVB	25408	28806	1.22%	0.122%
50	14.762	2202	2206	2209	rBV	84992	89882	3.82%	0.381%
51	14.809	2211	2214	2218	rVB	122063	122650	5.21%	0.520%
52	14.856	2218	2222	2226	rBV	479836	512348	21.77%	2.171%
53	15.233	2283	2286	2291	rVB4	20679	27433	1.17%	0.116%
54	16.056	2421	2426	2432	rBV4	45826	88831	3.77%	0.376%
55	16.403	2481	2485	2490	rBV	30906	49412	2.10%	0.209%

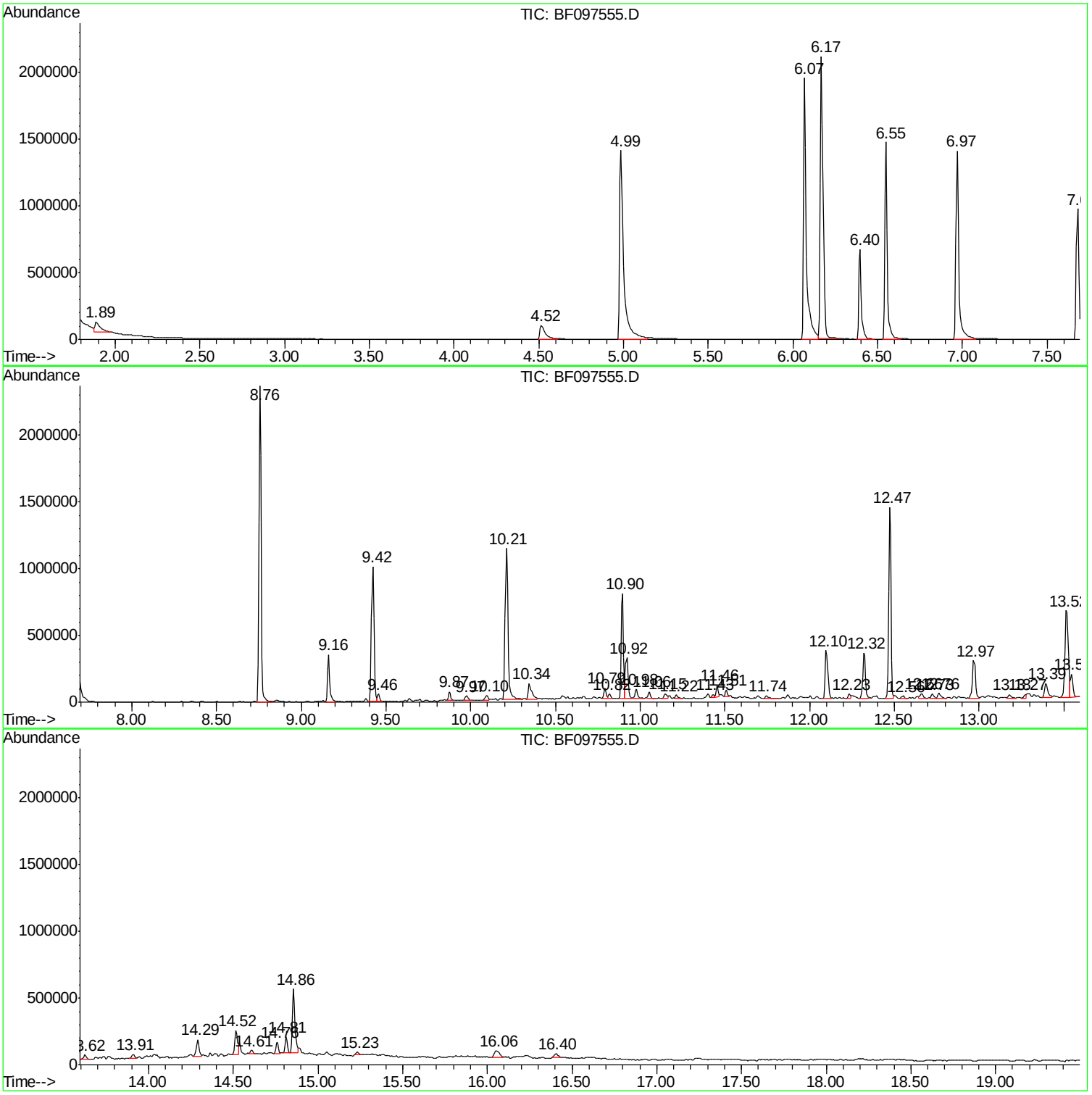
Sum of corrected areas: 23599476

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

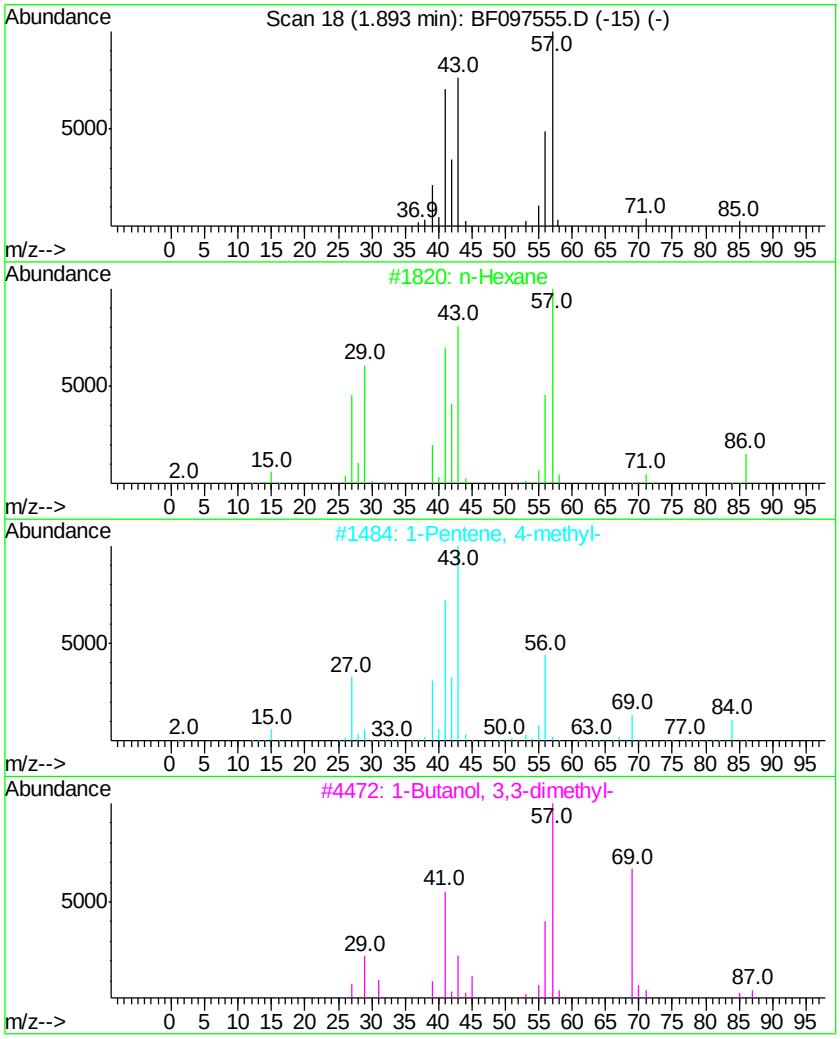
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

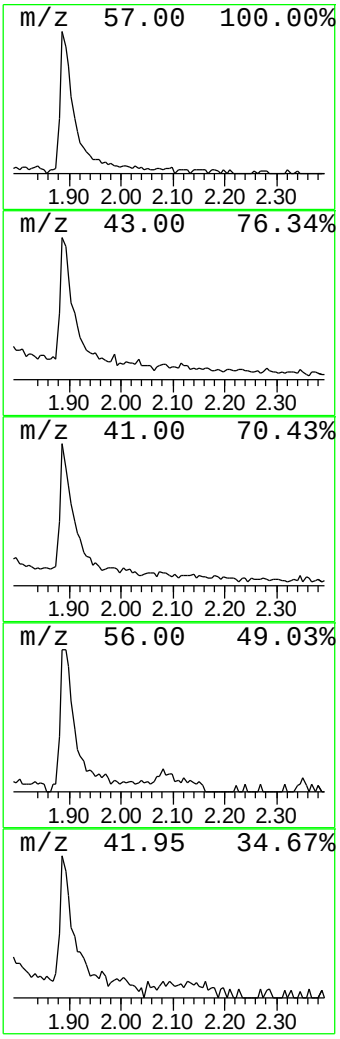
****

Peak Number 1 n-Hexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.89	4.79 ng	169971	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	78
2	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	42
3	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	39
4	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	28
5	Pentane, 3-methyl-	86	C6H14	000096-14-0	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

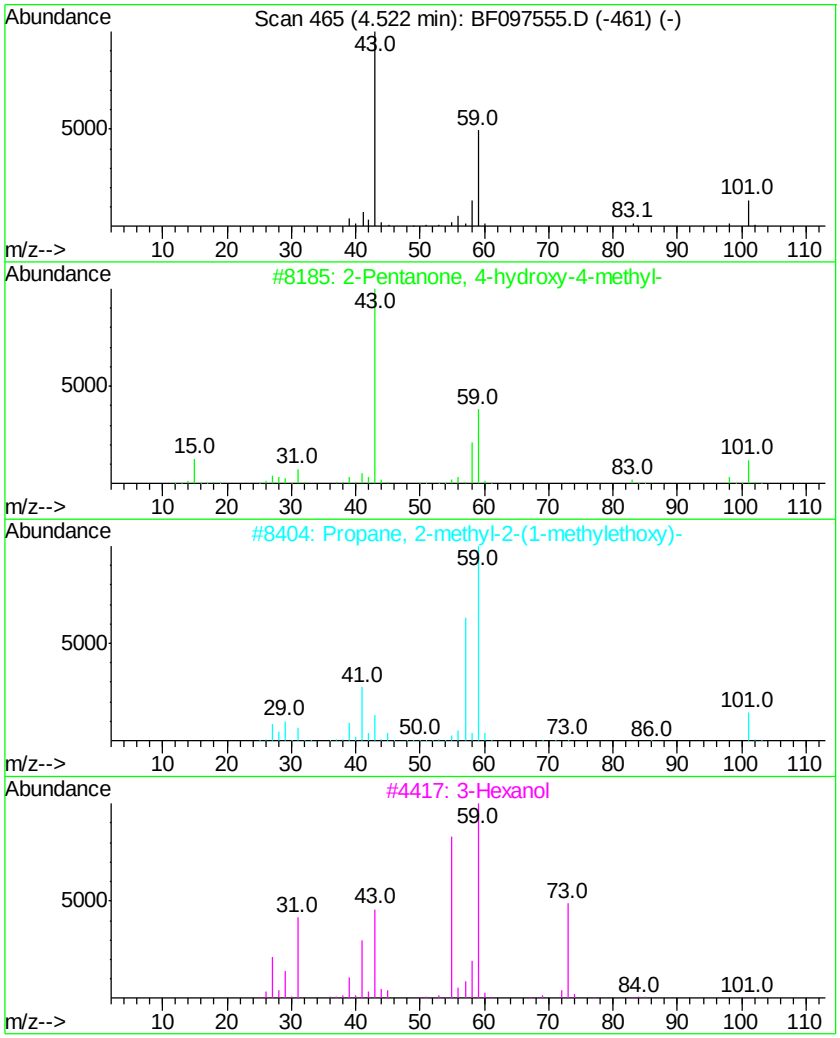
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

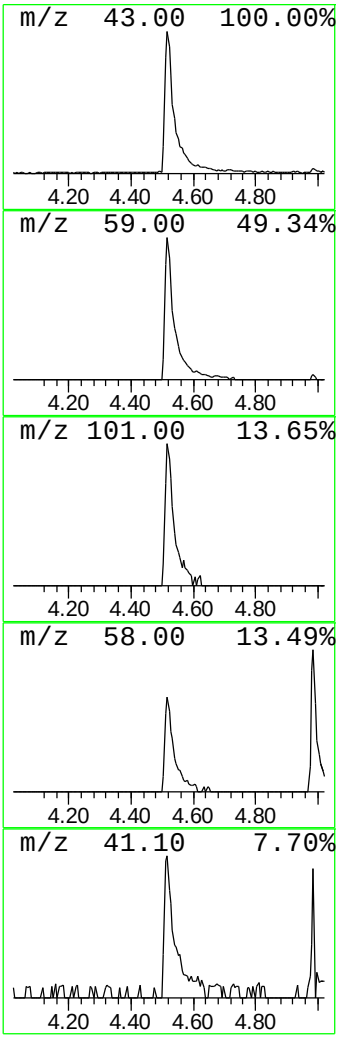
****

Peak Number 2 unknown4.52 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	6.13 ng	217661	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

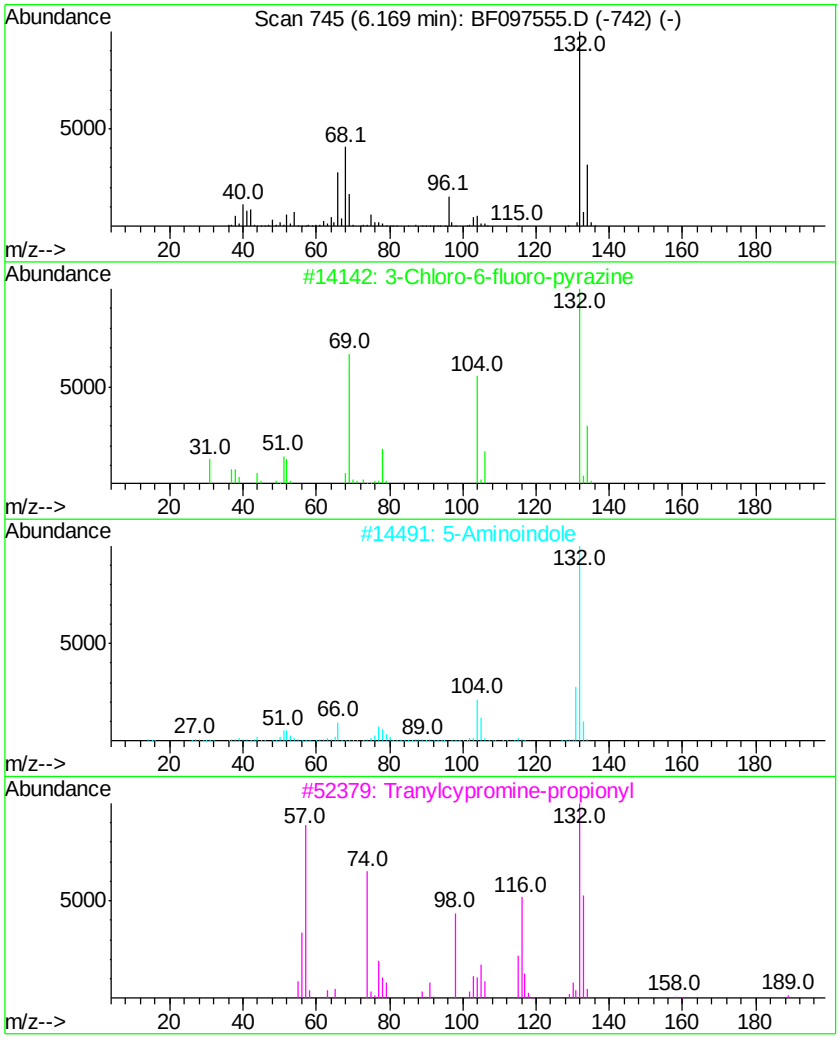
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

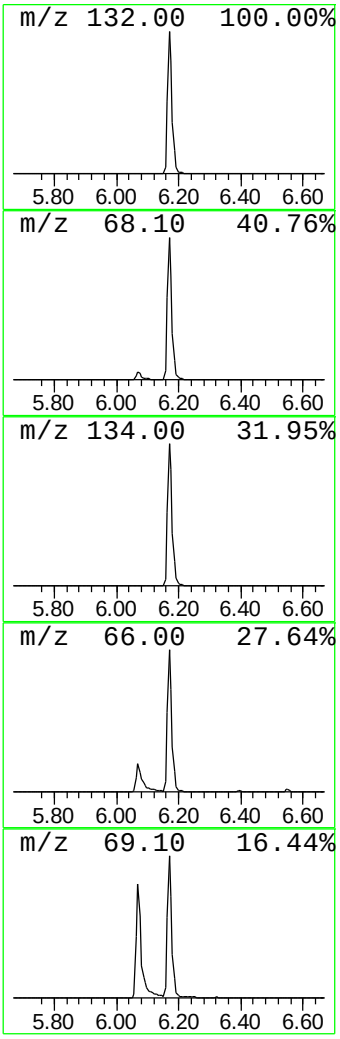
****

Peak Number 3 unknown6.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.17	62.93 ng	2233310	1,4-Dichlorobenzene-d4	6.40

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	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

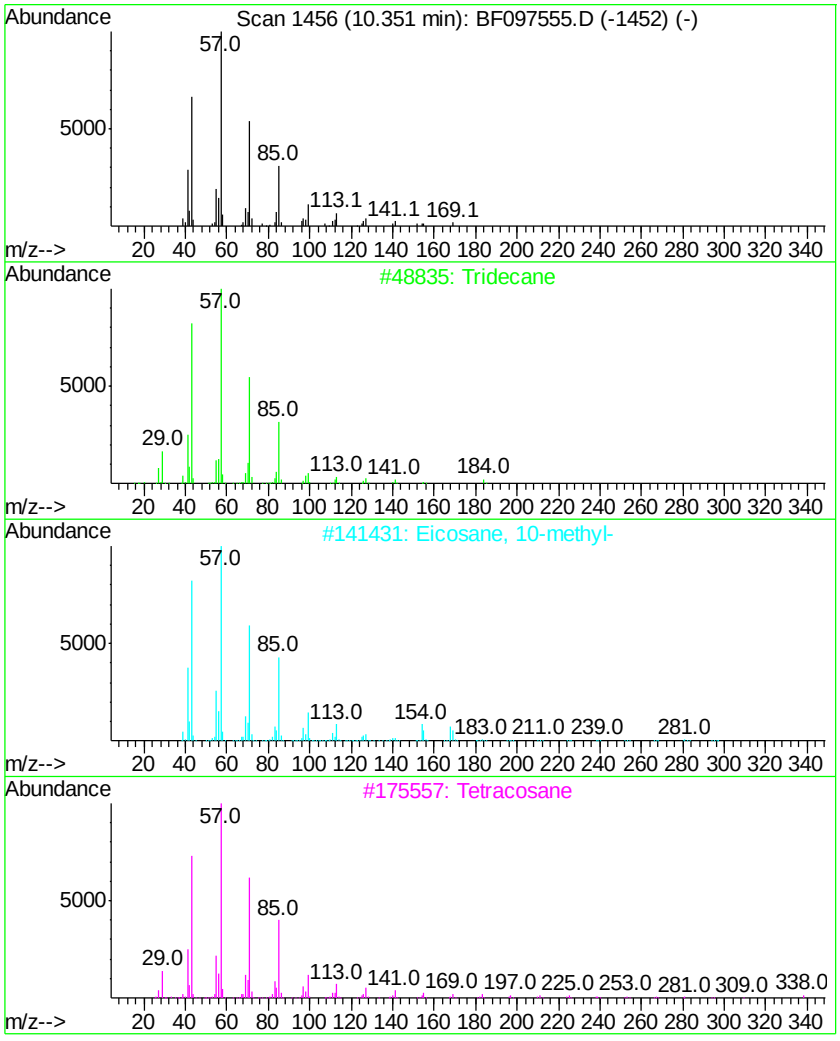
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

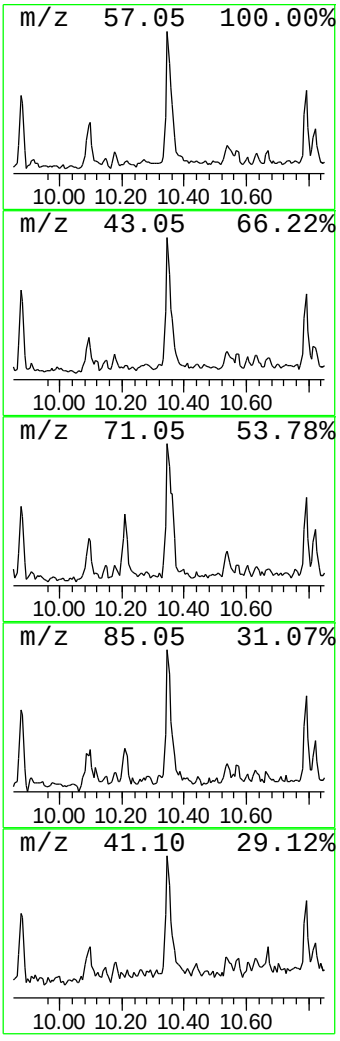
****

Peak Number 5 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	4.23 ng	160324	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Hexadecane	226	C16H34	000544-76-3	87
5	Heneicosane	296	C21H44	000629-94-7	83





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

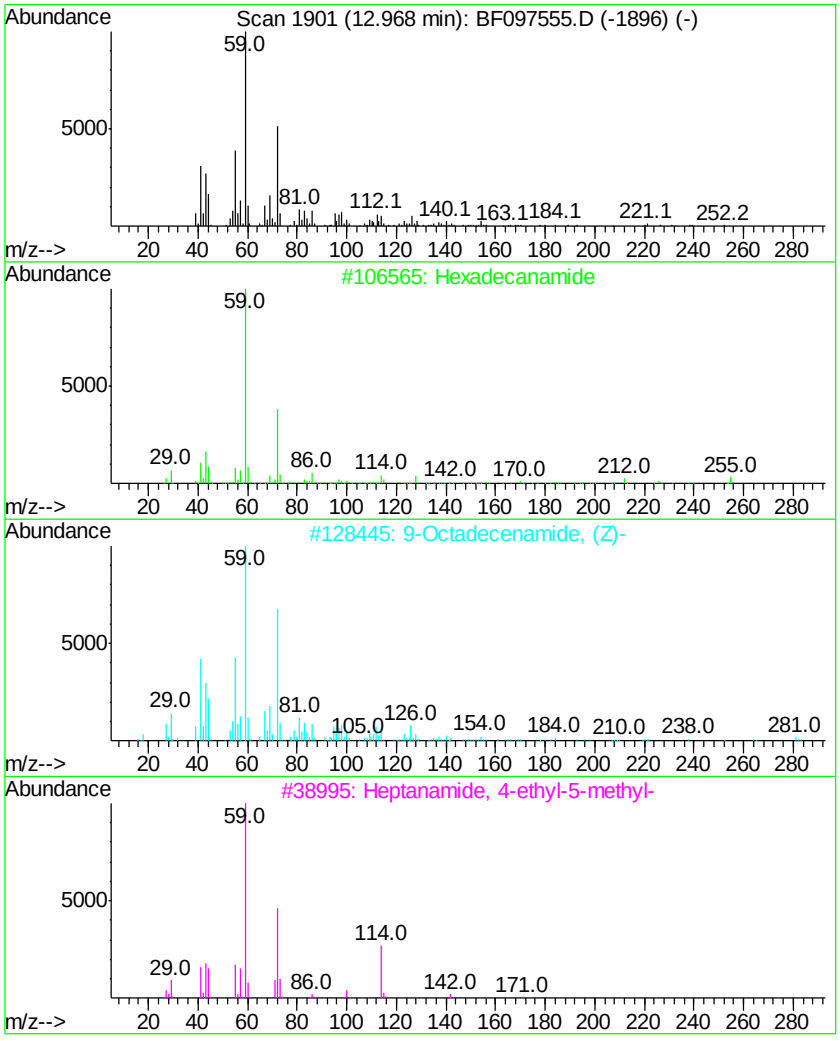
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

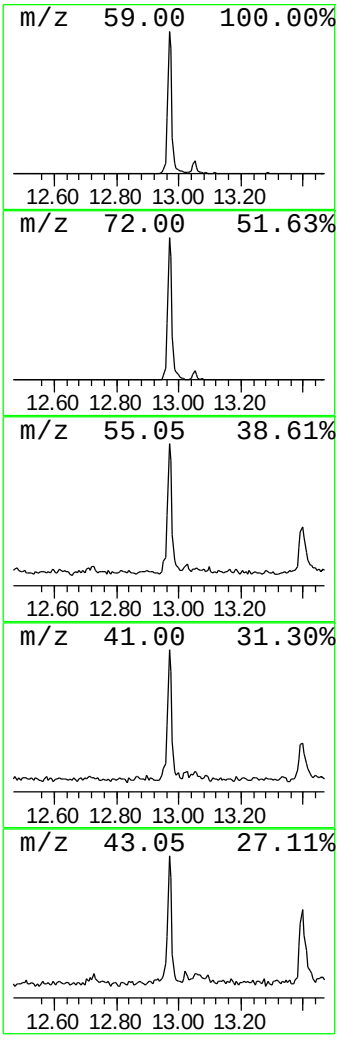
****

Peak Number 7 Hexadecanamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	7.65 ng	306412	Chrysene-d12	13.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanamide	255	C16H33NO	000629-54-9	78
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	76
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
4	Tridecanoic acid, thiophen-2-ylm...	322	C18H30N2OS	1000259-08-5	45
5	2-Hydroxy-2-methylundec-5-en-3-one	198	C12H22O2	1000191-46-2	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

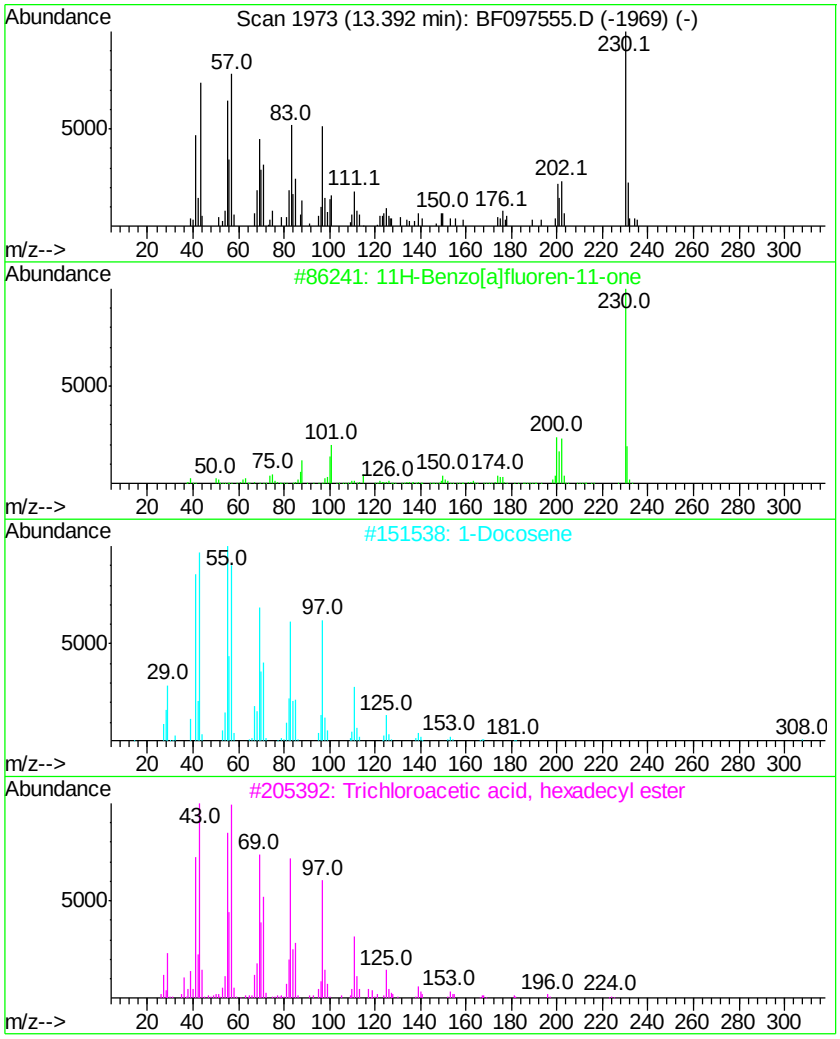
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

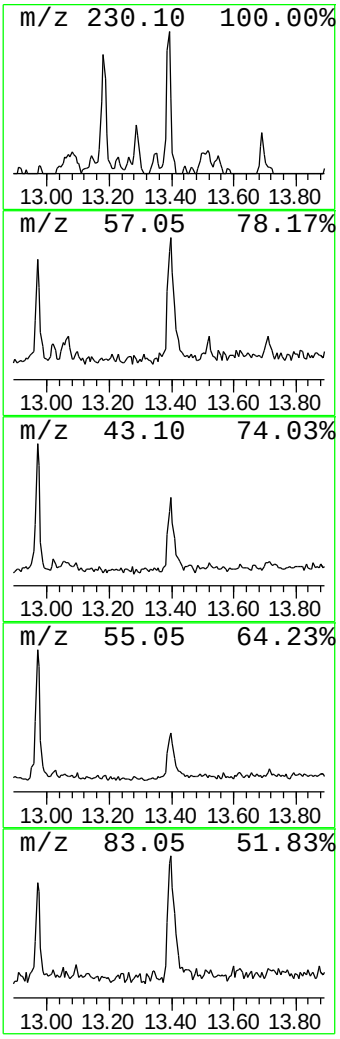
****

Peak Number 8 11H-Benzo[a]fluoren-11-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	3.61 ng	144718	Chrysene-d12	13.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	95
2	1-Docosene	308	C22H44	001599-67-3	72
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	70
4	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	64
5	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

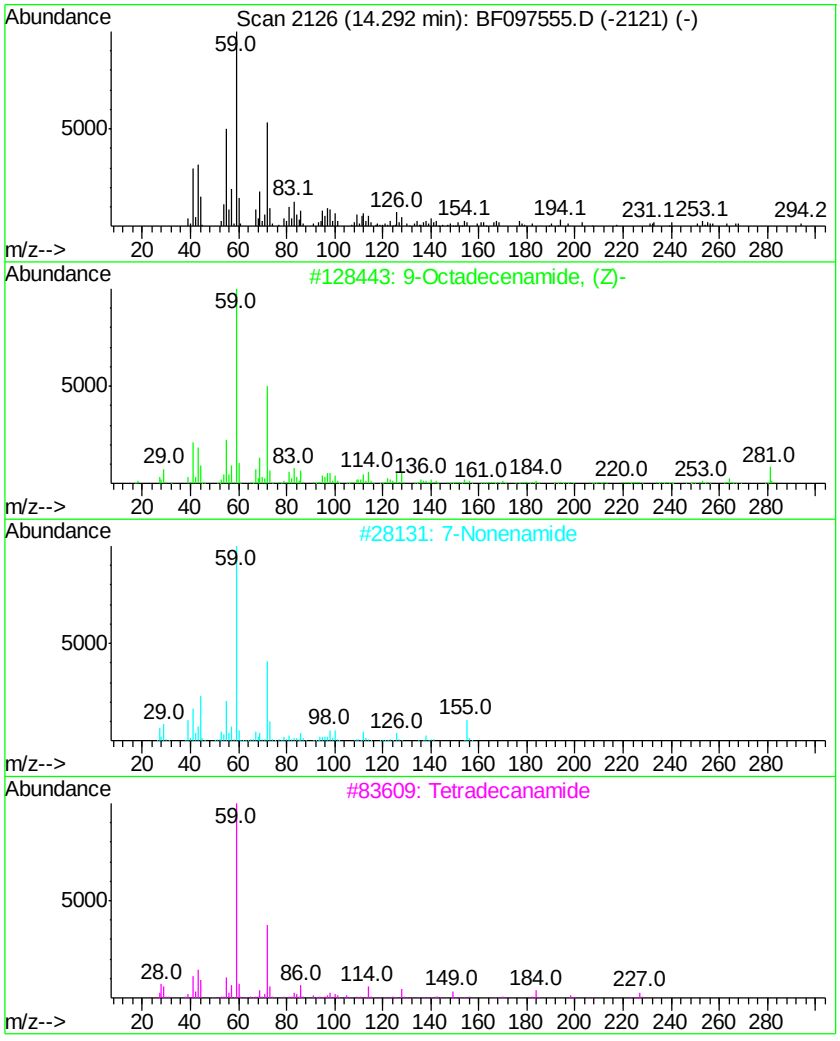
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

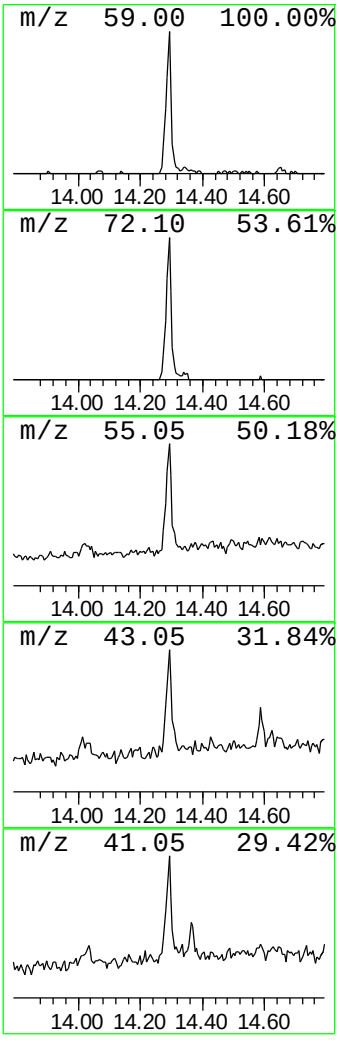
****

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	5.72 ng	146432	Perylene-d12	14.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	7-Nonenamide	155	C9H17NO	090949-53-4	81
3	Tetradecanamide	227	C14H29NO	000638-58-4	78
4	Dodecanamide	199	C12H25NO	001120-16-7	59
5	Octanamide	143	C8H17NO	000629-01-6	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080917\
Data File : BF097555.D
Acq On : 10 Aug 2017 11:38
Operator : SJ/JU
Sample : I4623-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S1COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
n-Hexane	1.89	4.8	ng	169971	1	6.40	709747	20.0
unknown4.52	4.52	6.1	ng	217661	1	6.40	709747	20.0
unknown6.17	6.17	62.9	ng	2233310	1	6.40	709747	20.0
Tridecane	10.35	4.2	ng	160324	4	10.90	758581	20.0
Hexadecanamide	12.97	7.7	ng	306412	5	13.52	801509	20.0
11H-Benzo[a]fluor...	13.39	3.6	ng	144718	5	13.52	801509	20.0
9-Octadecenamide,...	14.29	5.7	ng	146432	6	14.86	512348	20.0