LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099897.D
Acq On : 28 Oct 2017 1:31
Operator : SJ/JU
Sample : I6029-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

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-BF102317.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	5.004	493	496	509	rBV	143548	212433	11.94%	1.241%
2	5.410	562	565	599	rBV	1173971	1408600	79.18%	8.229%
3	6.439	736	740	758	rBV	1406366	1480697	83.23%	8.651%
4	6.569	758	762	768	rVV	1631301	1503068	84.49%	8.781%
5	6.792	797	800	810	rBV	596608	515983	29.00%	3.015%
6	6.951	823	827	845	rBV	1170898	1154571	64.90%	6.745%
7	7.363	894	897	910	rBV	998811	901930	50.70%	5.269%
8	8.075	1015	1018	1029	rBV	826587	718124	40.37%	4.195%
9	8.639	1111	1114	1124	rBB	49847	52914	2.97%	0.309%
10	9.151	1198	1201	1205	rBV	1876229	1779054	100.00%	10.394%
11	9.551	1266	1269	1275	rVB	286610	237732	13.36%	1.389%
12	9.704	1290	1295	1298	rBV3	11231	19647	1.10%	0.115%
13	9.839	1314	1318	1321	rBV	844199	773846	43.50%	4.521%
14	9.869	1321	1323	1327	rVB	34998	33693	1.89%	0.197%
15	10.392	1408	1412	1417	rVB	25806	24609	1.38%	0.144%
16	10.551	1436	1439	1449	rVB	203440	162562	9.14%	0.950%
17	10.633	1449	1453	1464	rBV	970918	889883	50.02%	5.199%
18	11.333	1568	1572	1574	rBV	760008	716543	40.28%	4.186%
19	11.357	1574	1576	1579	rVV	281886	231768	13.03%	1.354%
20	11.410	1581	1585	1590	rVV	54853	52311	2.94%	0.306%
21	11.580	1610	1614	1619	rBV2	18858	23280	1.31%	0.136%
22	11.845	1654	1659	1661	rBV2	45026	74723	4.20%	0.437%
23	11.863	1661	1662	1668	rVB2	52783	46772	2.63%	0.273%
24	11.951	1673	1677	1679	rBV	53519	54603	3.07%	0.319%
25	12.127	1703	1707	1711	rVB	26044	26156	1.47%	0.153%
26	12.492	1763	1769	1775	rVB4	10940	21406	1.20%	0.125%
27	12.551	1775	1779	1784	rBV	363018	315707	17.75%	1.844%
28	12.704	1801	1805	1808	rBV	18602	21743	1.22%	0.127%
29	12.780	1812	1818	1824	rVV	317491	326286	18.34%	1.906%
30	12.915	1837	1841	1844	rBV	1422652	1246161	70.05%	7.280%
31	12.998	1851	1855	1861	rBV2	18531	31883	1.79%	0.186%
32	13.115	1868	1875	1878	rBV	32976	61220	3.44%	0.358%
33	13.215	1889	1892	1896	rVB3	22687	24416	1.37%	0.143%
34	13.310	1905	1908	1911	rBV2	19592	18396	1.03%	0.107%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099897.D
Acq On : 28 Oct 2017 1:31
Operator : SJ/JU
Sample : I6029-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

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-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.339	1911	1913	1917	rVV2	17403	18840	1.06%	0.110%
36	13.639	1959	1964	1965	rBV3	17539	21651	1.22%	0.126%
37	13.757	1978	1984	1987	rBV3	29370	45620	2.56%	0.267%
38	13.798	1987	1991	1997	rVV5	62754	108648	6.11%	0.635%
39	13.851	1997	2000	2004	rVB	23455	26314	1.48%	0.154%
40	13.939	2012	2015	2018	rBV	50471	48985	2.75%	0.286%
41	13.986	2018	2023	2026	rVV2	551022	654765	36.80%	3.825%
42	14.009	2026	2027	2031	rVB	117425	87657	4.93%	0.512%
43	14.092	2039	2041	2044	rBV	18730	18802	1.06%	0.110%
44	15.033	2197	2201	2204	rBV	95651	147429	8.29%	0.861%
45	15.339	2249	2253	2256	rBV	55850	70230	3.95%	0.410%
46	15.398	2260	2263	2269	rBV	87562	144602	8.13%	0.845%
47	15.456	2269	2273	2278	rVV	358579	456583	25.66%	2.667%
48	16.339	2420	2423	2429	rVB4	29140	46905	2.64%	0.274%
49	17.415	2602	2606	2612	rVB2	31142	56835	3.19%	0.332%

Sum of corrected areas: 17116586

LSC Report - Integrated Chromatogram

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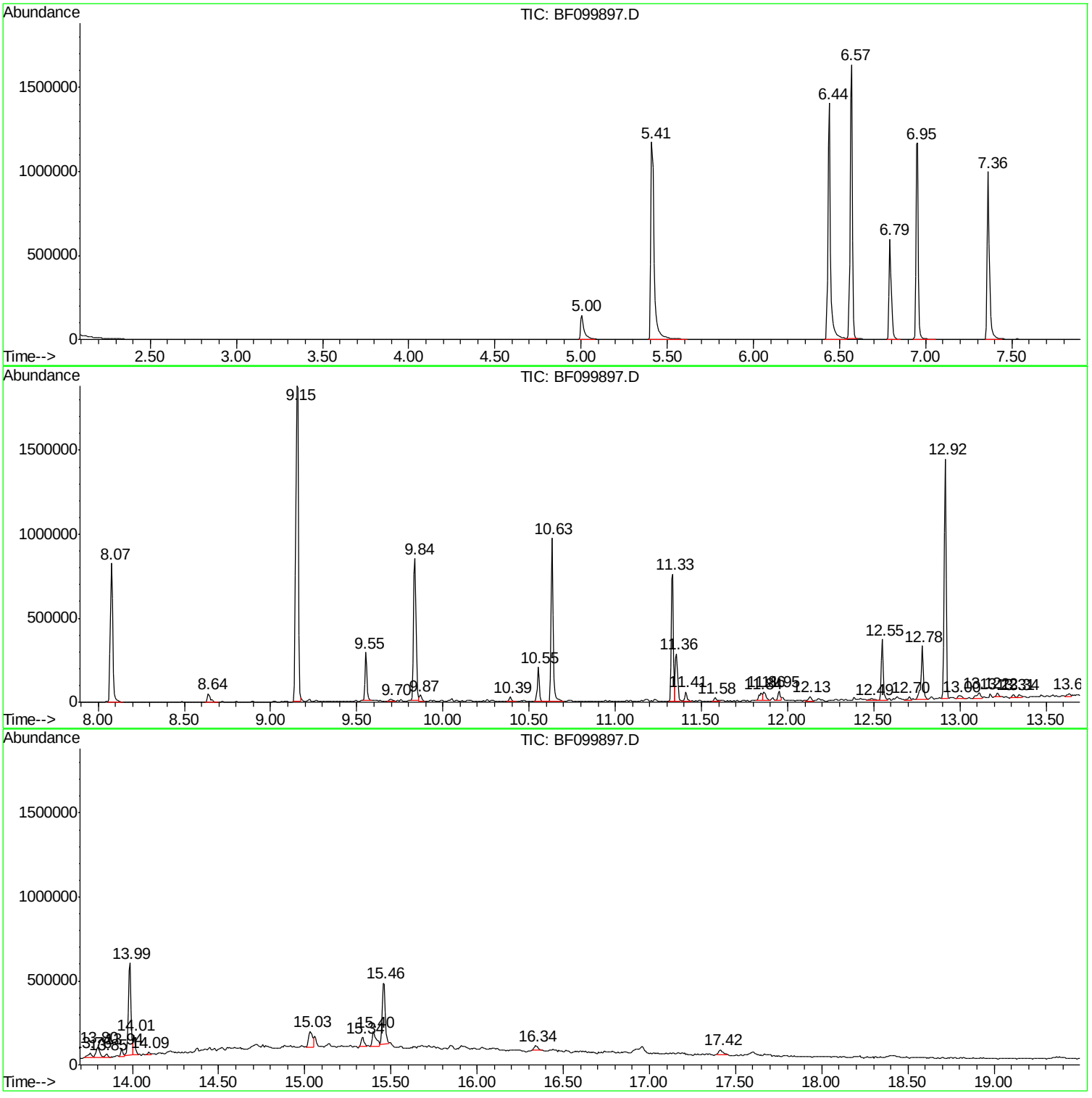
Operator : SJ/JU
Sample : I6029-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099897.D
Acq On : 28 Oct 2017 1:31
Operator : SJ/JU
Sample : I6029-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

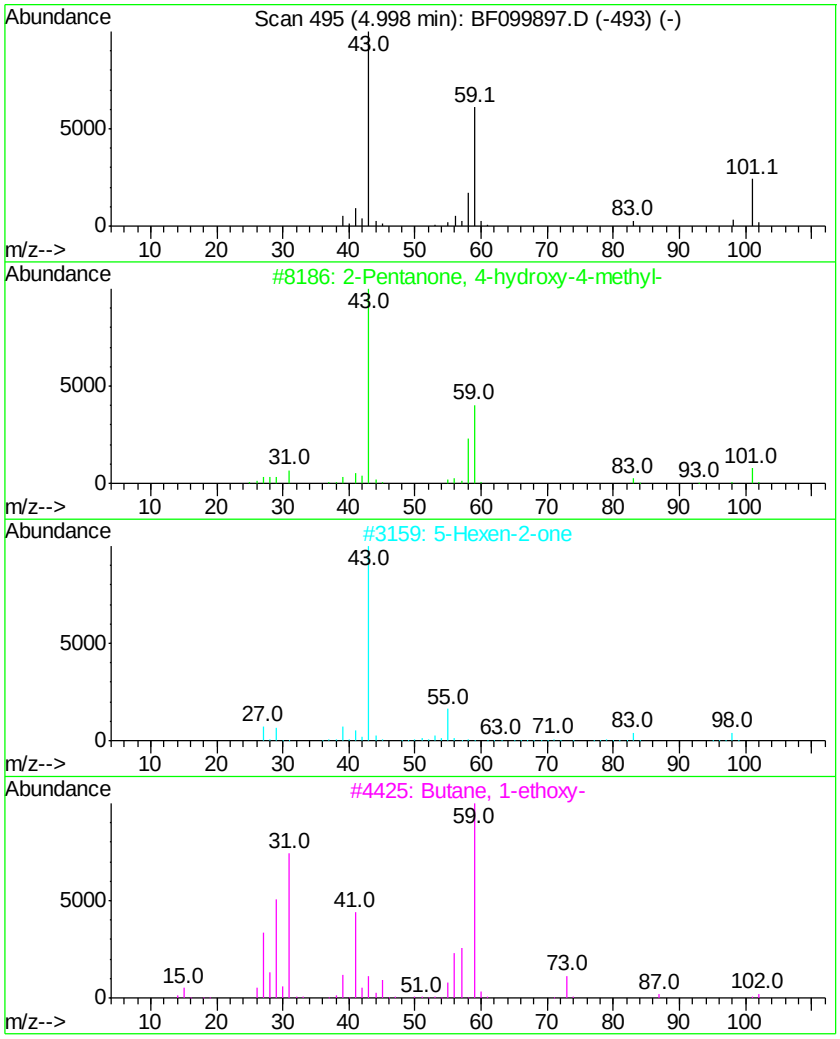
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

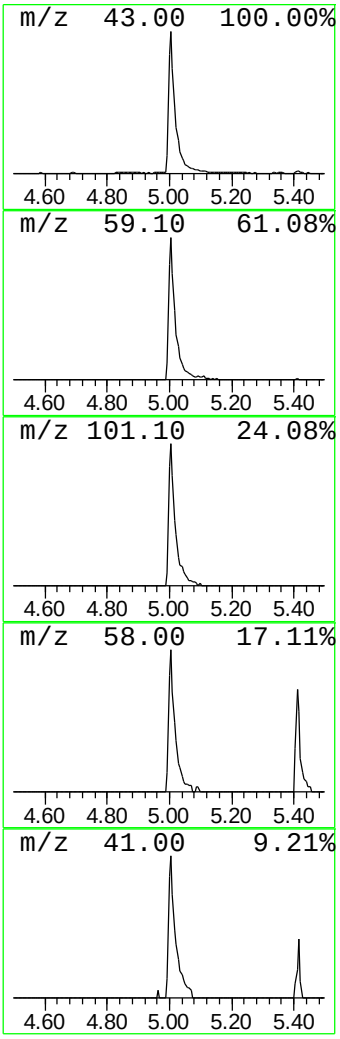
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	8.23 ng	212433	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
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Operator : SJ/JU
Sample : I6029-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

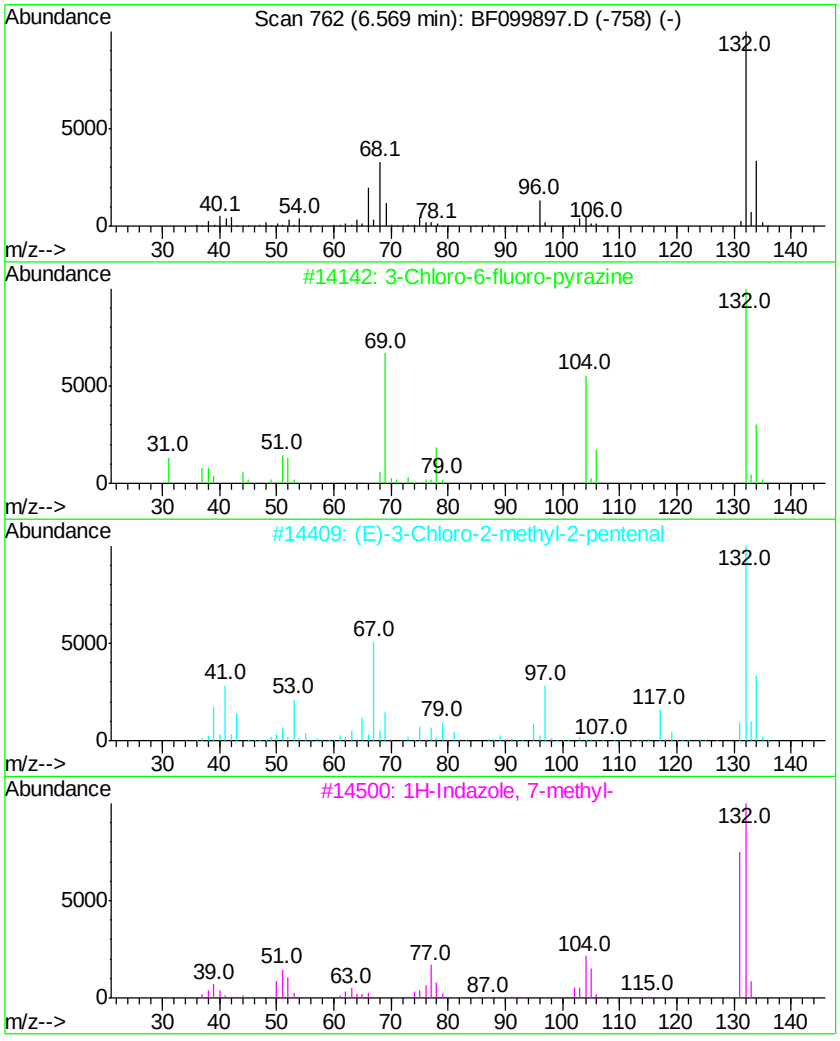
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

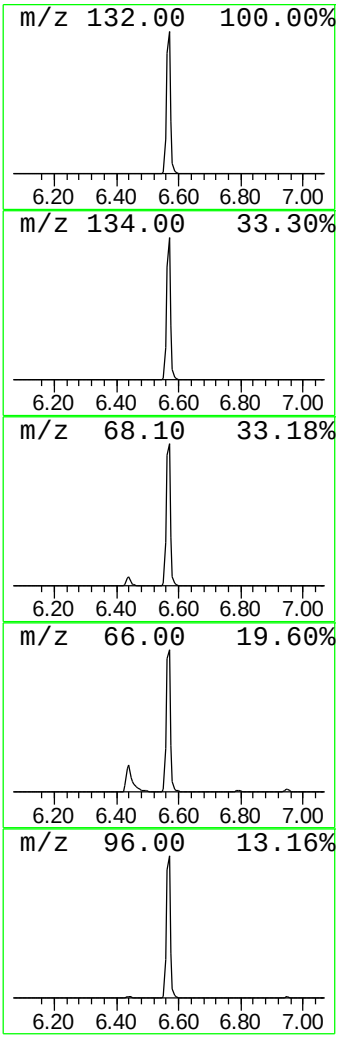
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	58.26 ng	1503070	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102717\
Data File : BF099897.D
Acq On : 28 Oct 2017 1:31
Operator : SJ/JU
Sample : I6029-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

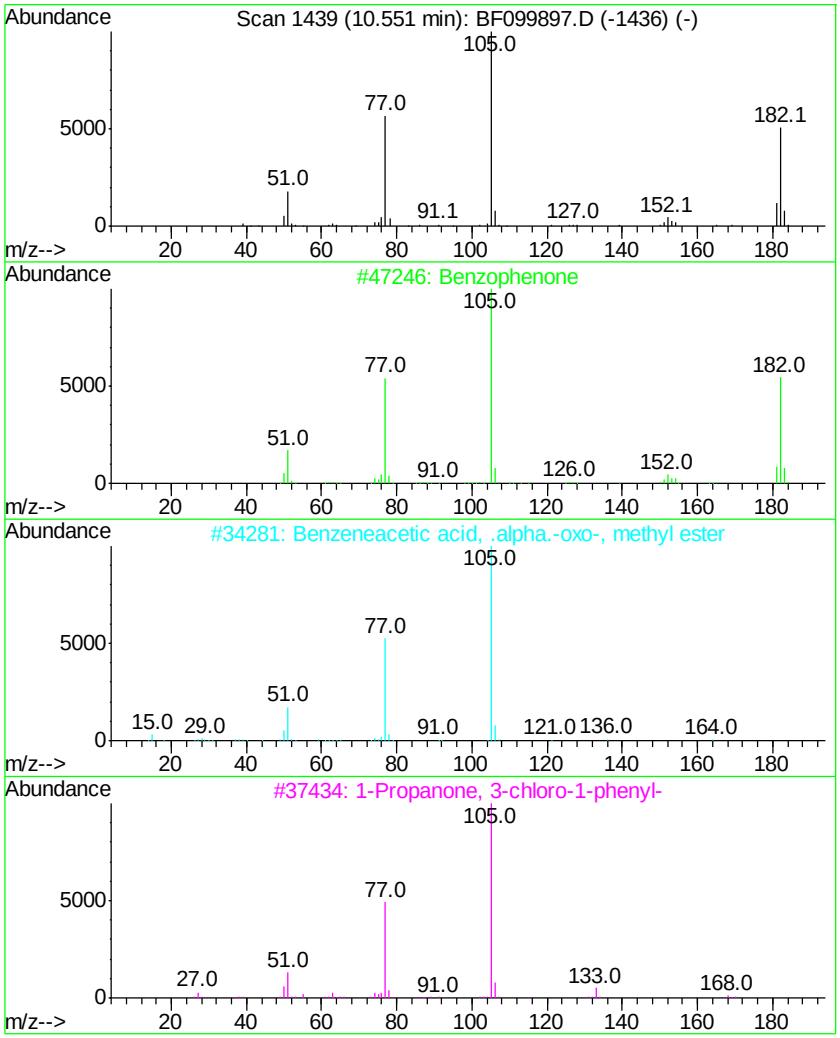
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

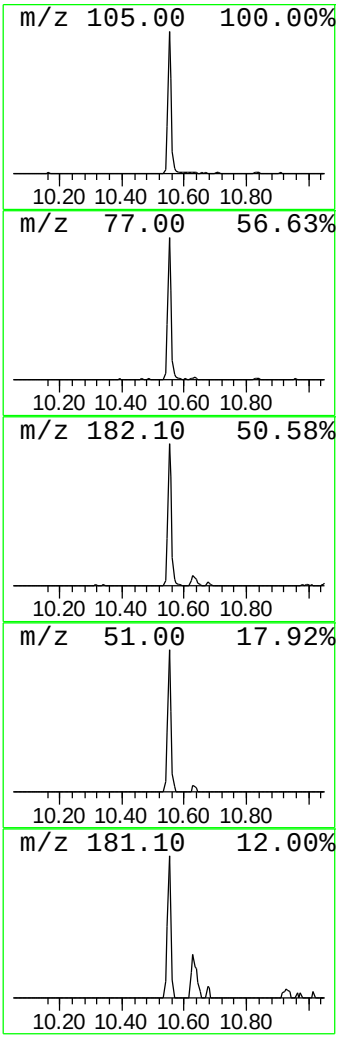
****

Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	4.20 ng	162562	Acenaphthene-d10	9.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	43
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	43
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
5	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43





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Sample : I6029-10
Misc :
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Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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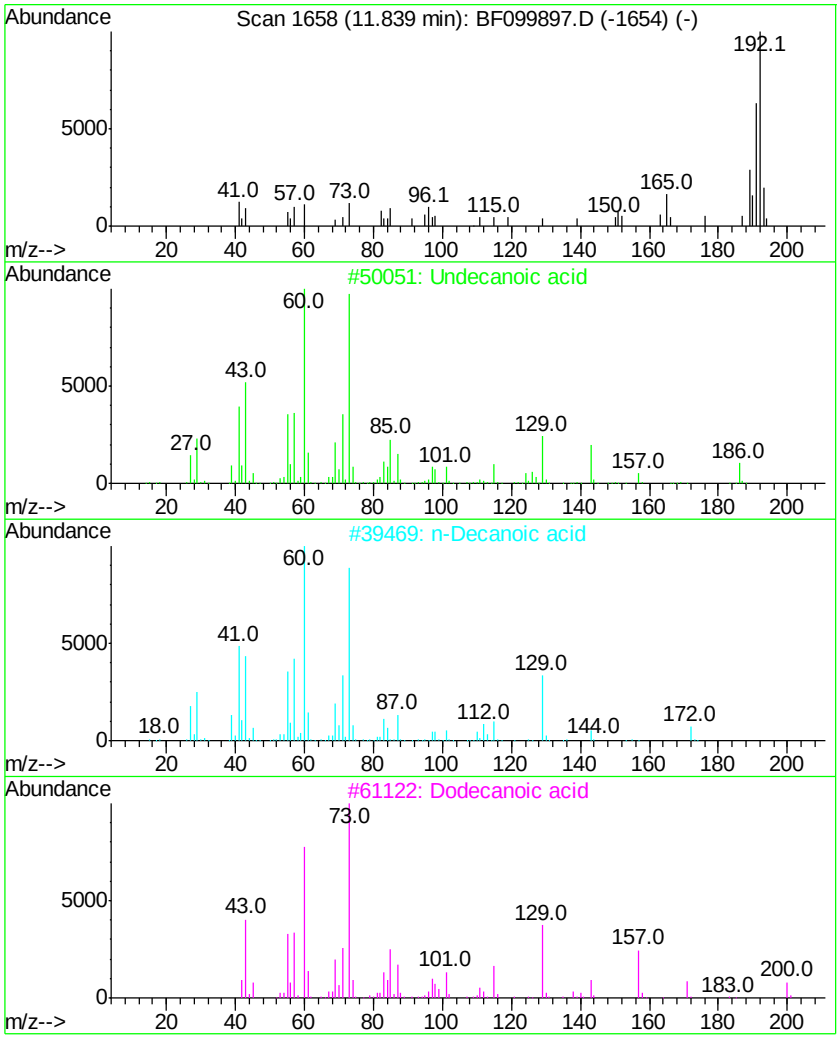
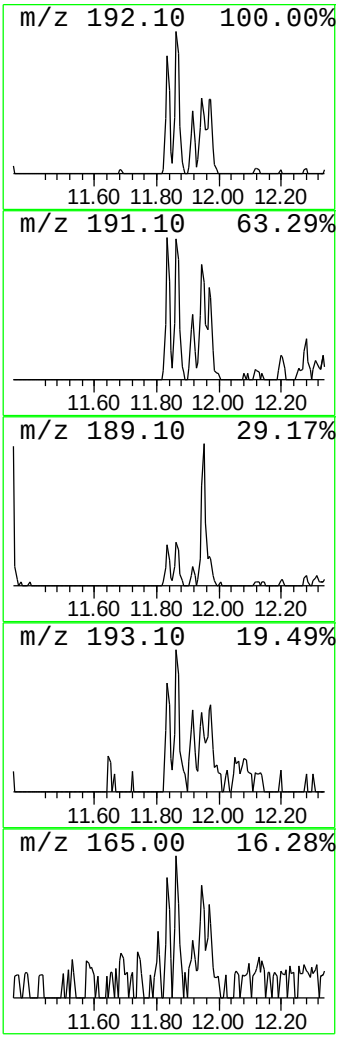
Peak Number 5 unknown11.84 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.09 ng	74723	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	38
2	n-Decanoic acid	172	C10H20O2	000334-48-5	38
3	Dodecanoic acid	200	C12H24O2	000143-07-7	38
4	Lactose	342	C12H22O11	000063-42-3	35
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	25





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Data File : BF099897.D
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Sample : I6029-10
Misc :
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Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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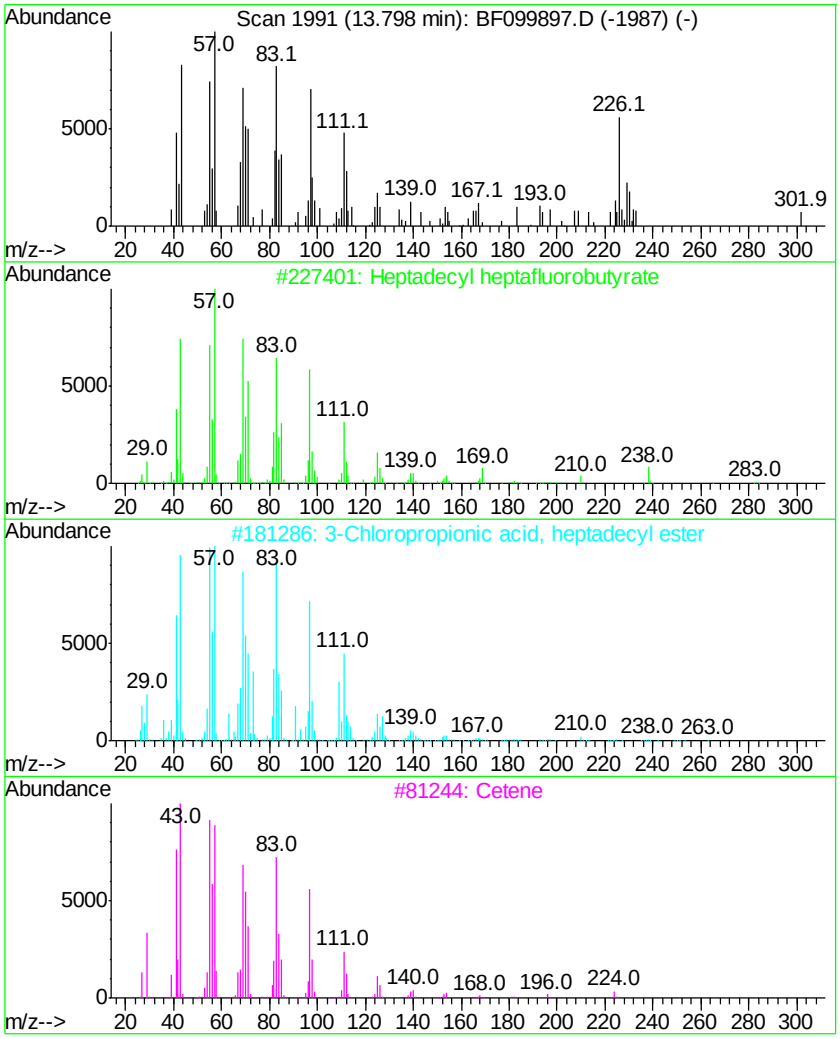
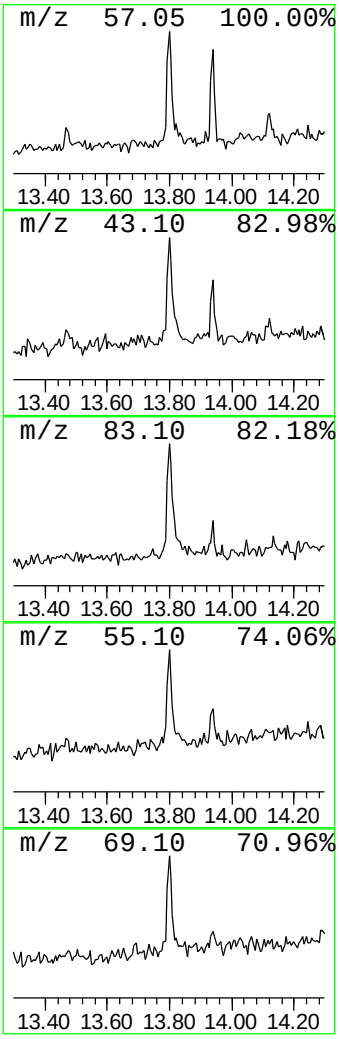
Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.32 ng	108648	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	64
3	Cetene	224	C16H32	000629-73-2	60
4	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	58
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	58





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Data File : BF099897.D
Acq On : 28 Oct 2017 1:31
Operator : SJ/JU
Sample : I6029-10
Misc :
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Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

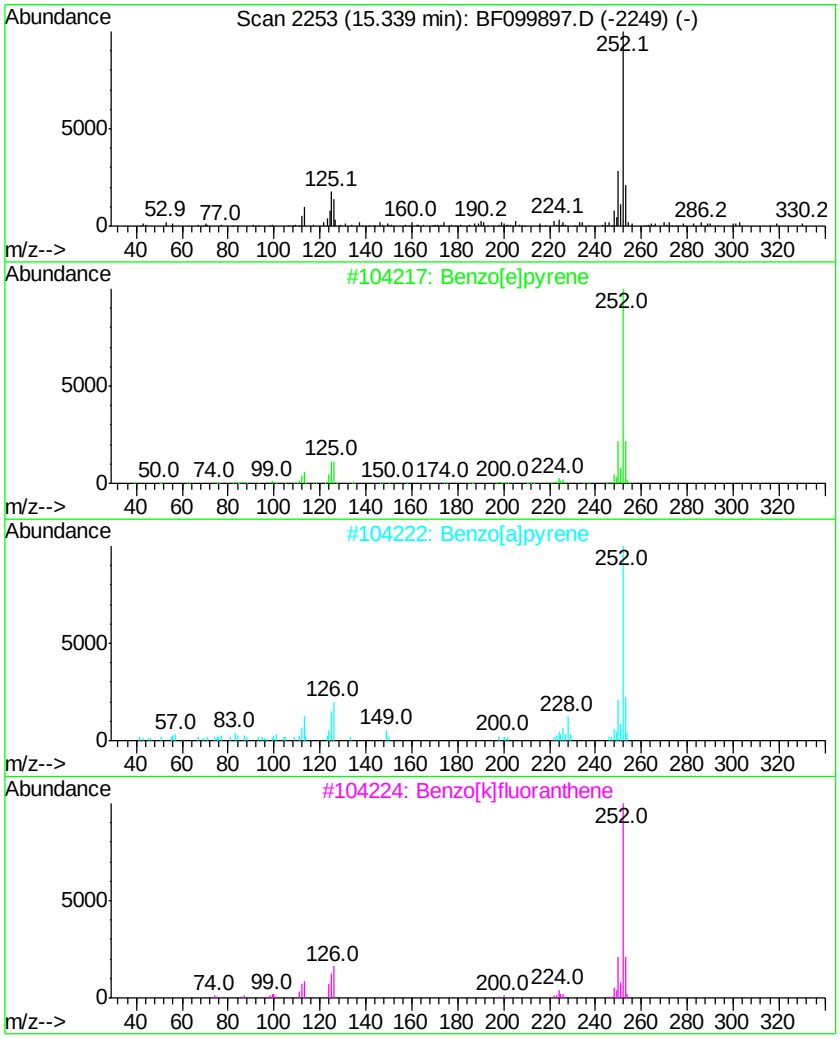
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

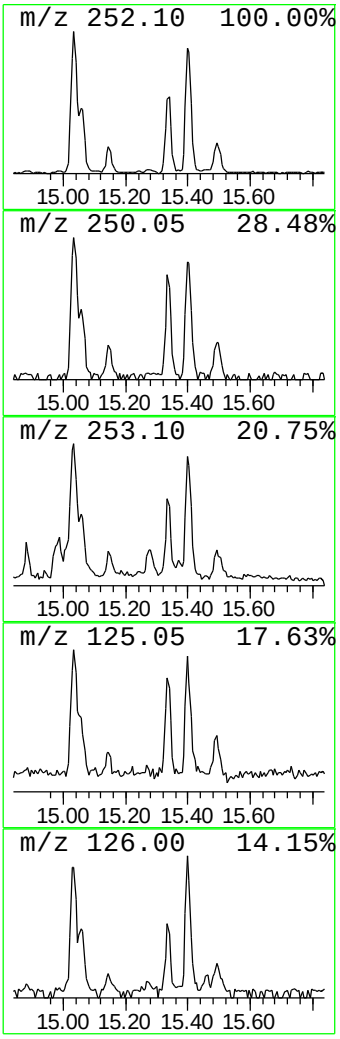
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	3.08 ng	70230	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[a]pyrene	252	C20H12	000050-32-8	91
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
4	Perylene	252	C20H12	000198-55-0	91
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	87





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Sample : I6029-10
Misc :
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Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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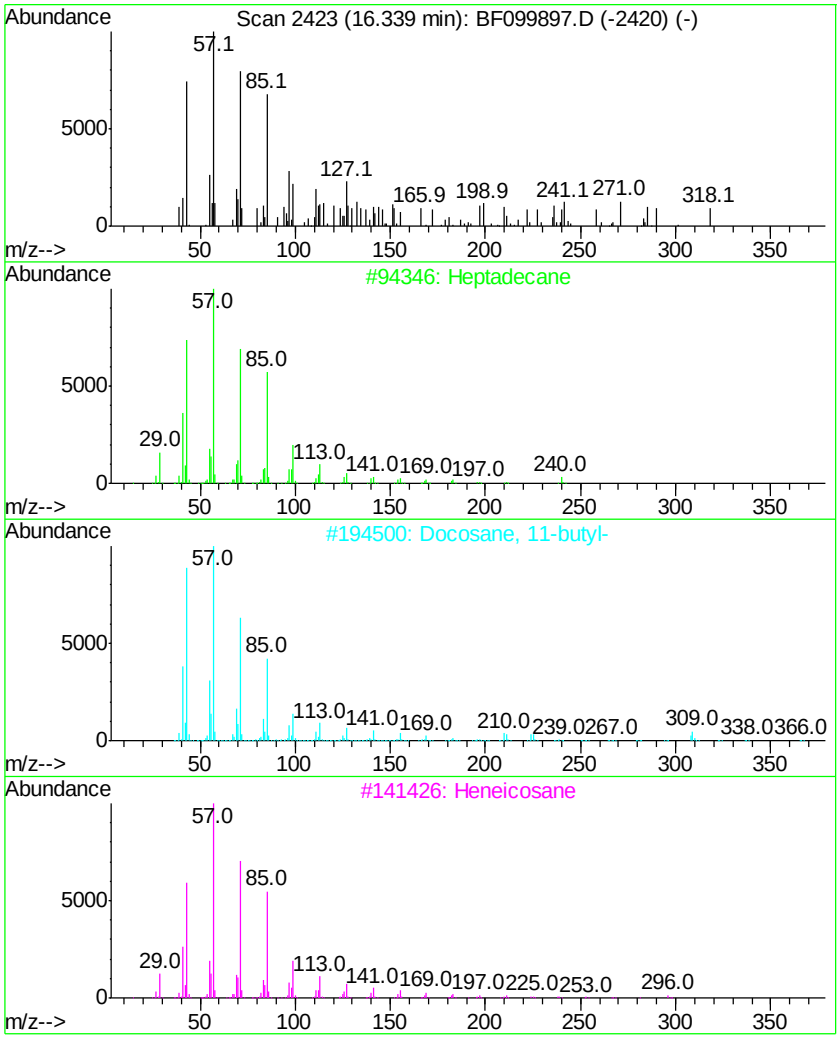
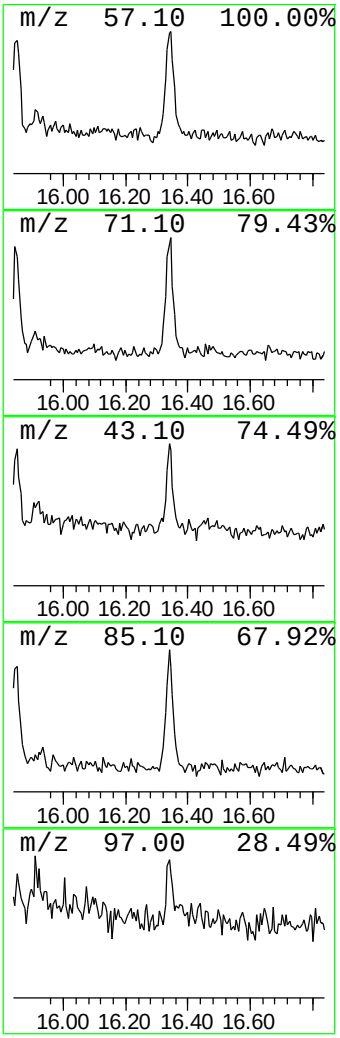
Peak Number 8 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	2.05 ng	46905	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	64
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	53
3	Heneicosane	296	C21H44	000629-94-7	50
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	50
5	Sulfurous acid, dodecyl pentyl e...	320	C17H36O3S	1000309-14-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF102717\
Data File : BF099897.D
Acq On : 28 Oct 2017 1:31
Operator : SJ/JU
Sample : I6029-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-116-6(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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
2-Pentanone, 4-hy...	5.00	8.2	ng	212433	1	6.79	515983	20.0
unknown6.57	6.57	58.3	ng	1503070	1	6.79	515983	20.0
Benzophenone	10.55	4.2	ng	162562	3	9.84	773846	20.0
unknown11.84	11.84	2.1	ng	74723	4	11.33	716543	20.0
Heptadecyl heptaf...	13.80	3.3	ng	108648	5	13.99	654765	20.0
Benzo[e]pyrene	15.34	3.1	ng	70230	6	15.46	456583	20.0
Heptadecane	16.34	2.0	ng	46905	6	15.46	456583	20.0