LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

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-BF092317.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	2.163	7	13	18	rVB	157403	204244	5.46%	0.617%
2	5.098	508	512	525	rVB	471942	663455	17.72%	2.005%
3	5.493	574	579	583	rBV	2920029	3246814	86.73%	9.814%
4	6.504	740	751	757	rBV	2853284	3425948	91.52%	10.356%
5	6.640	769	774	777	rBV	3392123	3327492	88.89%	10.058%
6	6.863	808	812	816	rBV	978933	756930	20.22%	2.288%
7	6.922	818	822	827	rBV	78156	68345	1.83%	0.207%
8	7.022	834	839	842	rBV	2965364	2677270	71.52%	8.093%
9	7.428	903	908	911	rBV	1949390	2164229	57.81%	6.542%
10	7.510	917	922	928	rBV3	37937	48013	1.28%	0.145%
11	8.145	1026	1030	1033	rBV	1272569	1004439	26.83%	3.036%
12	9.222	1207	1213	1216	rBV	3938997	3743538	100.00%	11.316%
13	9.486	1254	1258	1261	rBV2	83384	66458	1.78%	0.201%
14	9.610	1276	1279	1282	rBV	627504	470213	12.56%	1.421%
15	9.898	1319	1328	1332	rBV2	1244835	1068941	28.55%	3.231%
16	10.322	1397	1400	1403	rVB	61531	52205	1.39%	0.158%
17	10.533	1430	1436	1439	rBV2	66334	72121	1.93%	0.218%
18	10.692	1458	1463	1466	rBV	1829276	1827743	48.82%	5.525%
19	10.792	1477	1480	1488	rVB2	93049	114330	3.05%	0.346%
20	11.039	1520	1522	1526	rVB2	34892	38766	1.04%	0.117%
21	11.239	1553	1556	1558	rBV	68787	52176	1.39%	0.158%
22	11.386	1577	1581	1583	rBV	1093309	938446	25.07%	2.837%
23	11.410	1583	1585	1588	rVV	179272	148696	3.97%	0.449%
24	11.457	1590	1593	1596	rVB	42984	50494	1.35%	0.153%
25	11.592	1613	1616	1619	rBV	82853	93359	2.49%	0.282%
26	11.663	1626	1628	1634	rVB2	37773	45074	1.20%	0.136%
27	11.869	1660	1663	1665	rBV	69192	71065	1.90%	0.215%
28	11.904	1666	1669	1676	rVB3	247267	266014	7.11%	0.804%
29	12.069	1695	1697	1700	rBV	39996	38293	1.02%	0.116%
30	12.122	1700	1706	1710	rVV3	32934	70743	1.89%	0.214%
31	12.598	1784	1787	1791	rBV	268738	238109	6.36%	0.720%
32	12.686	1800	1802	1805	rBV2	59155	56611	1.51%	0.171%
33	12.827	1823	1826	1828	rBV	241957	241125	6.44%	0.729%
34	12.851	1828	1830	1842	rVB	393642	435515	11.63%	1.316%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.969	1846	1850	1854	rBV	2512653	2620423	70.00%	7.921%
36	13.069	1865	1867	1870	rVB2	77336	64979	1.74%	0.196%
37	13.445	1925	1931	1934	rBV	672324	673043	17.98%	2.034%
38	13.851	1997	2000	2005	rBV3	154553	163959	4.38%	0.496%
39	14.021	2025	2029	2032	rBV2	673017	706643	18.88%	2.136%
40	14.051	2032	2034	2036	rVB	92197	70245	1.88%	0.212%
41	15.063	2203	2206	2210	rBV	106095	162646	4.34%	0.492%
42	15.368	2256	2258	2264	rVB	67465	84874	2.27%	0.257%
43	15.433	2266	2269	2275	rBV	86833	112198	3.00%	0.339%
44	15.498	2276	2280	2285	rBV	500885	636671	17.01%	1.924%

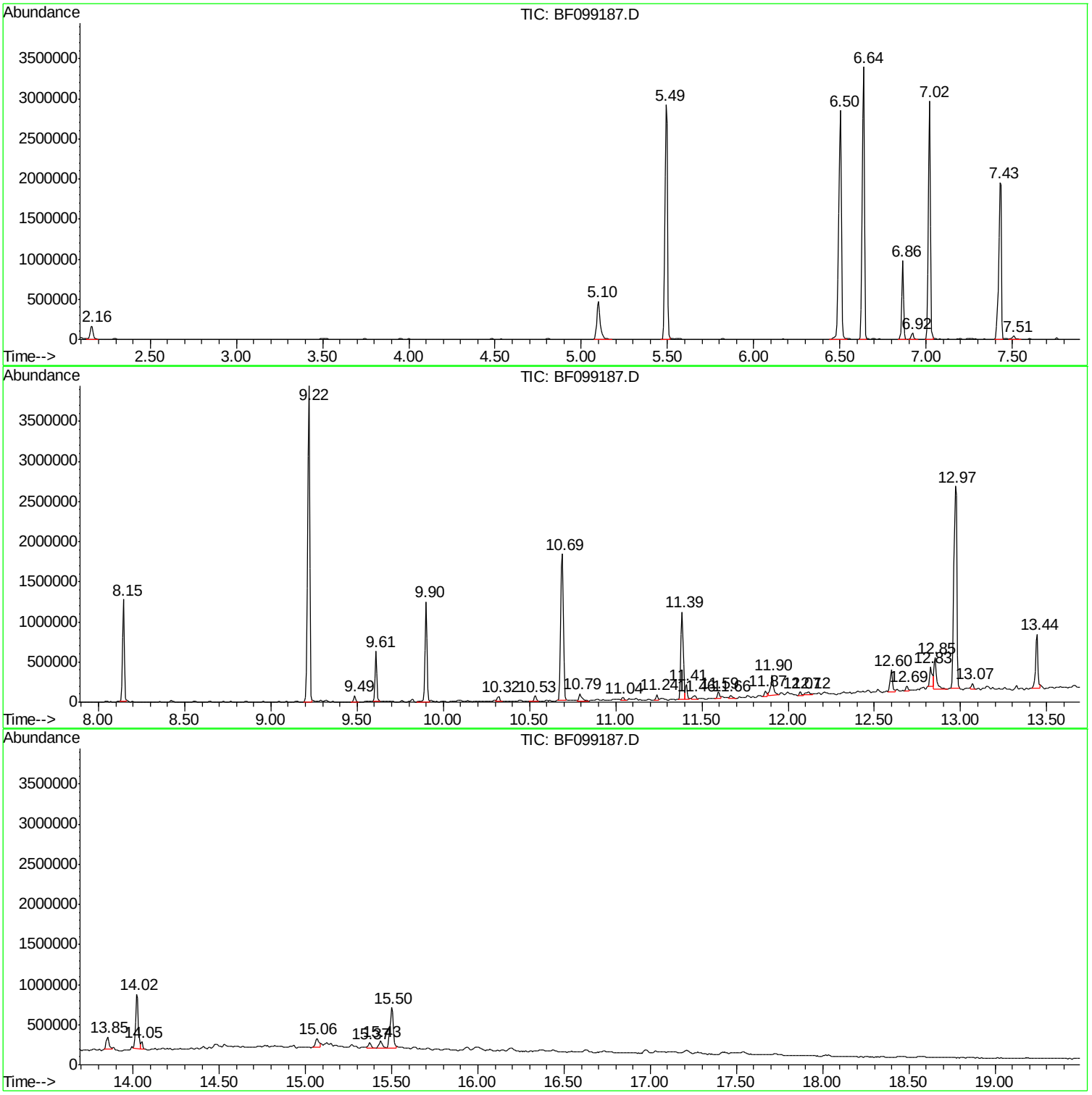
Sum of corrected areas: 33082895

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

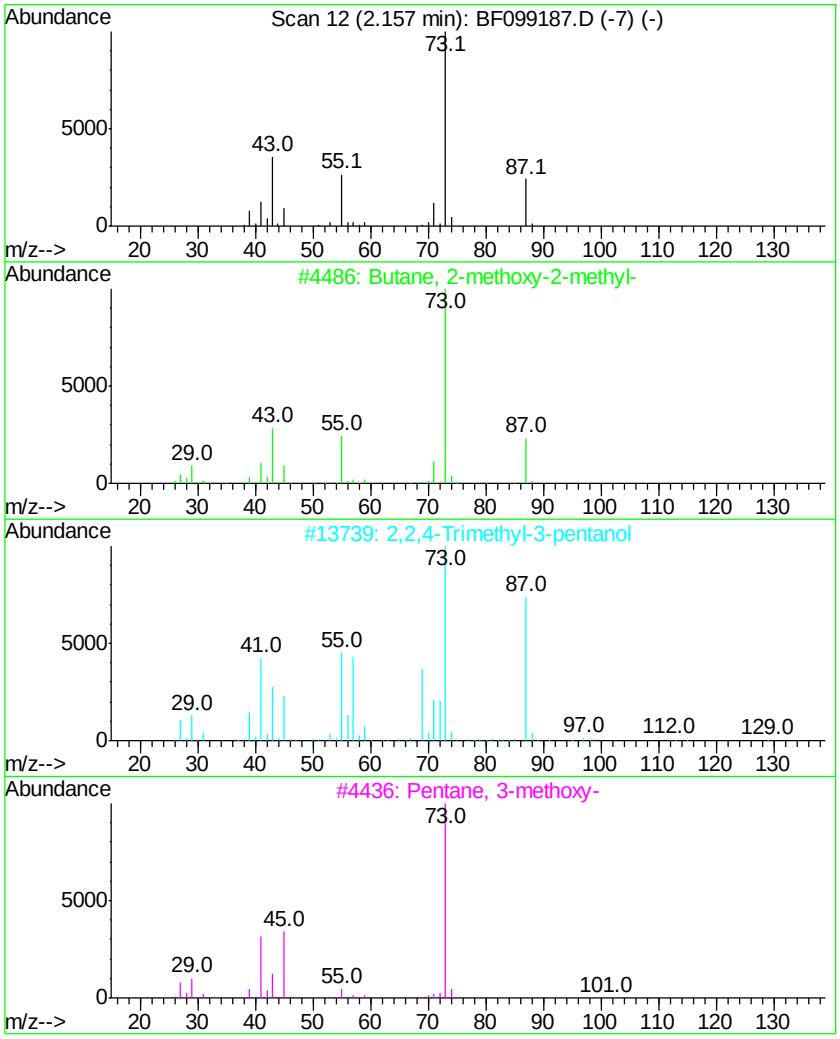
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

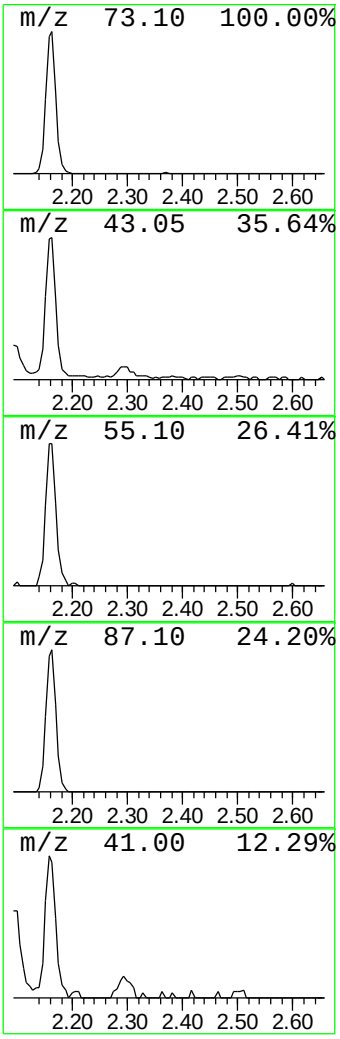
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	5.40 ng	204244	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

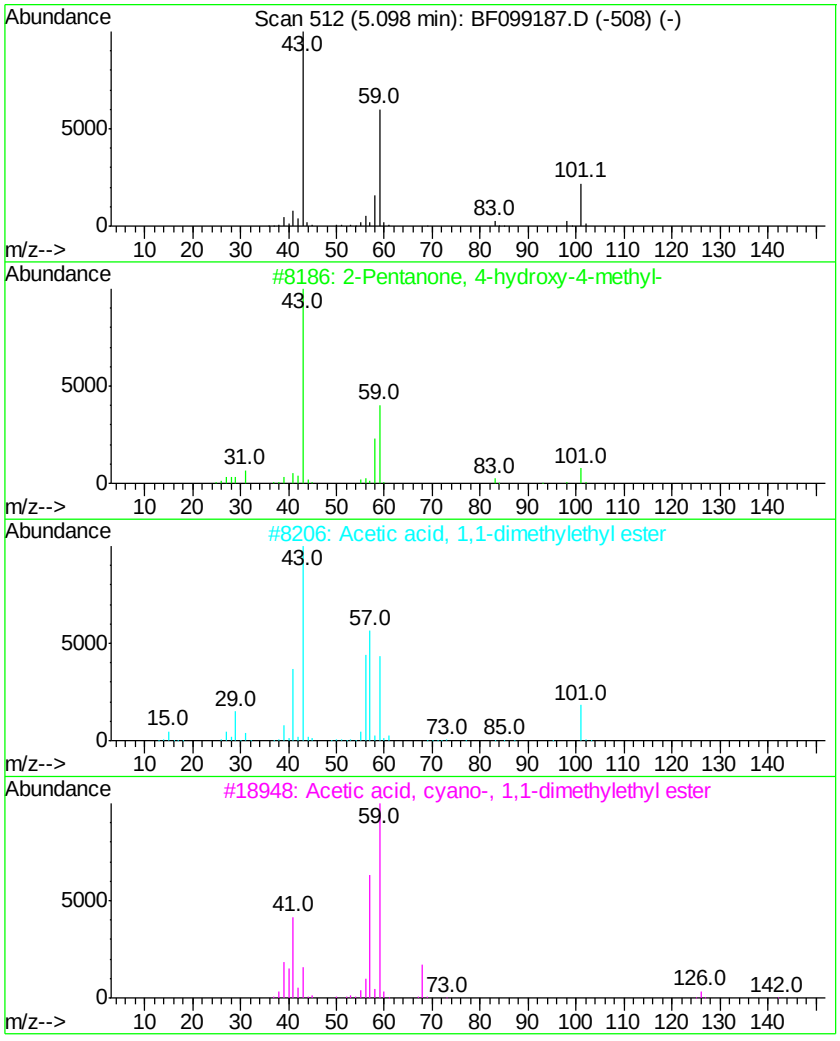
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

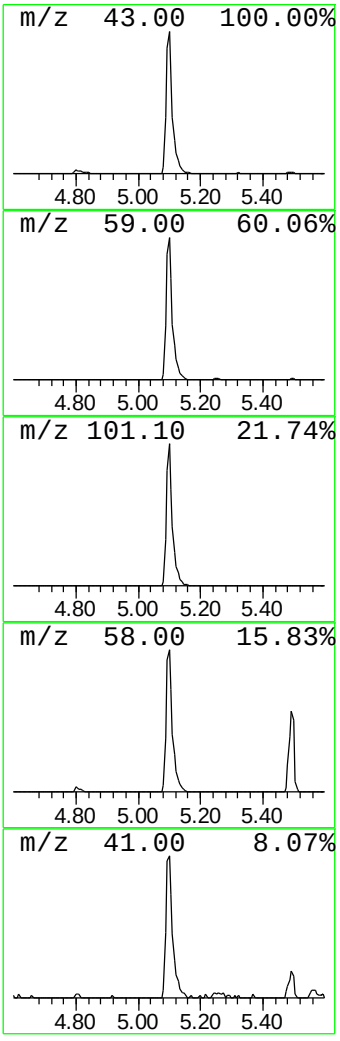
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	17.53 ng	663455	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Guanidine	59	CH5N3	000113-00-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

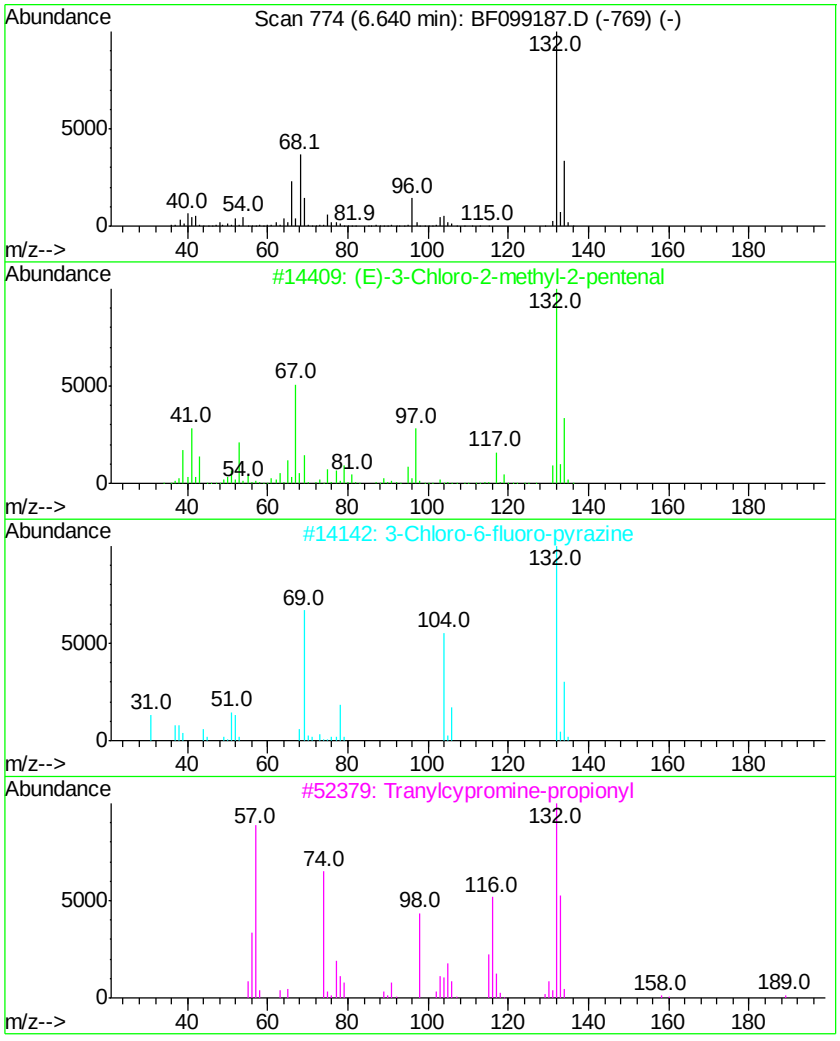
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

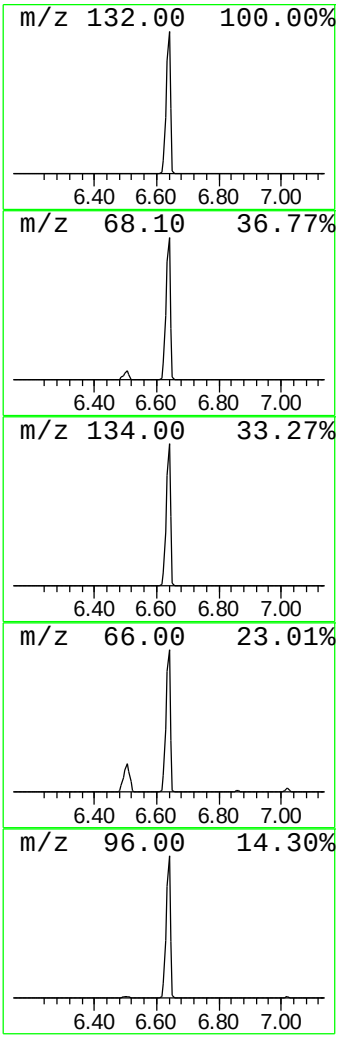
****

Peak Number 3 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	87.92 ng	3327490	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

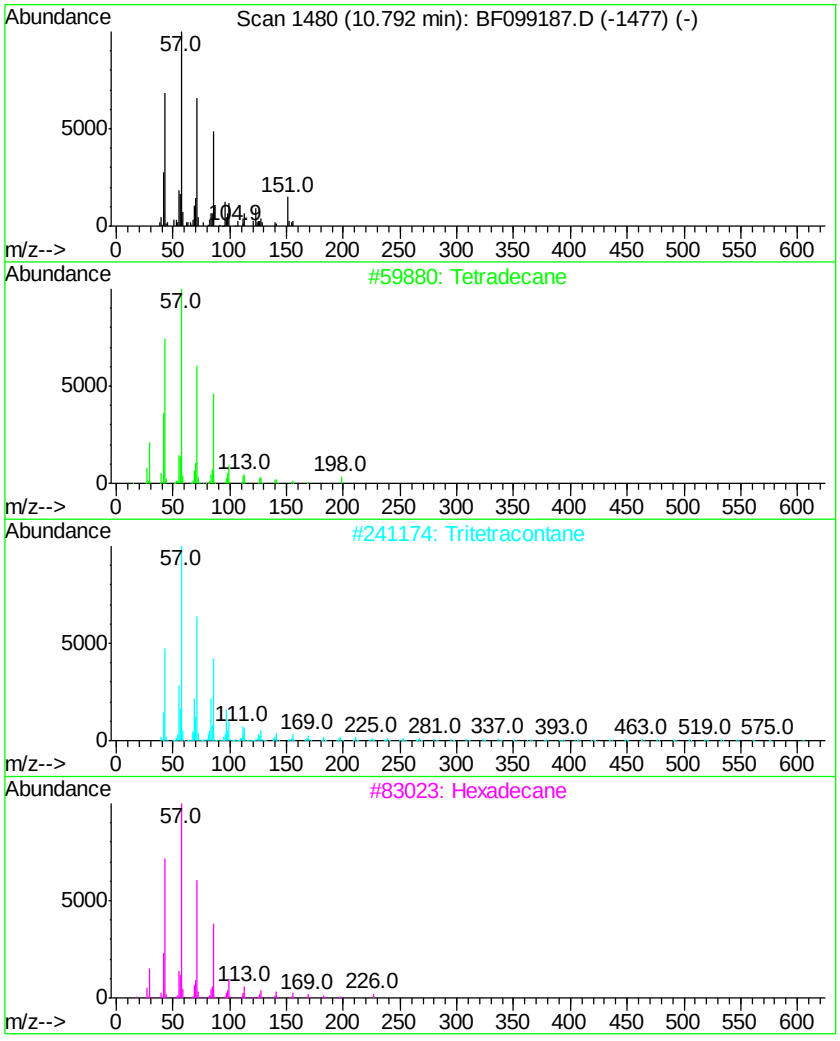
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

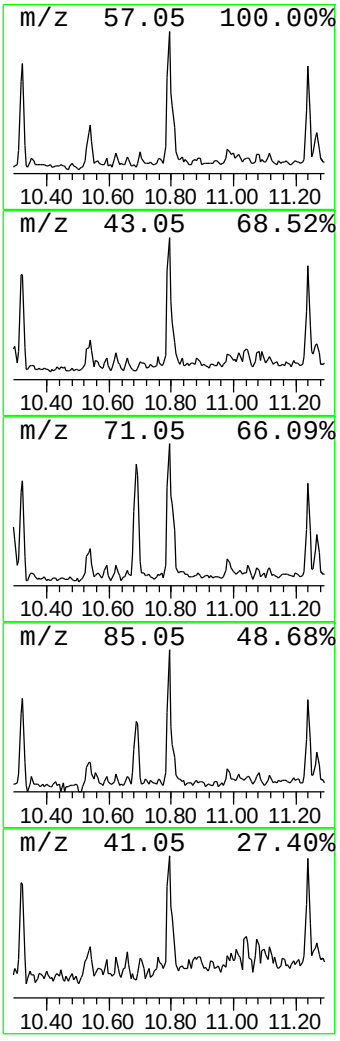
****

Peak Number 5 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	2.44 ng	114330	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	74
2	Tritetracontane	605	C43H88	007098-21-7	72
3	Hexadecane	226	C16H34	000544-76-3	72
4	Heneicosane	296	C21H44	000629-94-7	64
5	Pentadecane	212	C15H32	000629-62-9	64





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

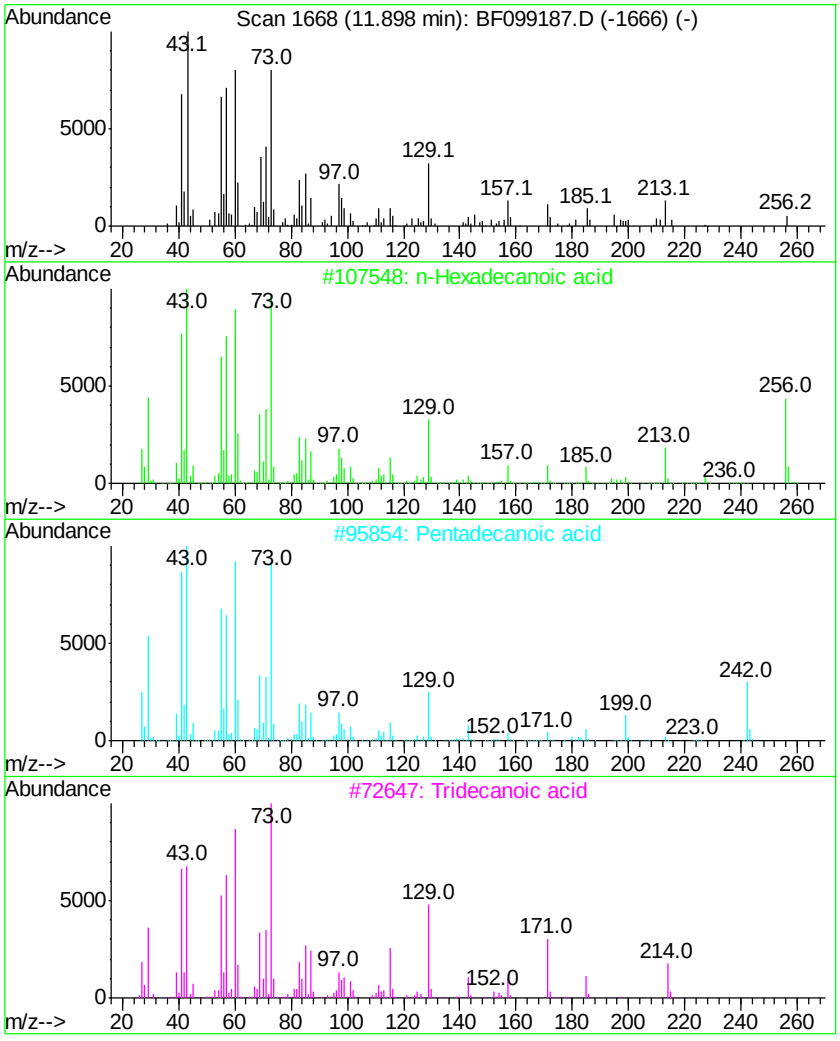
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

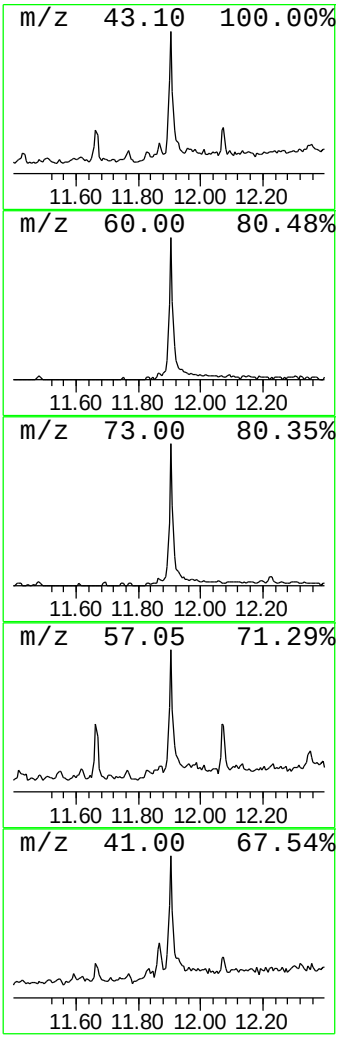
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	5.67 ng	266014	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Nonanoic acid	158	C9H18O2	000112-05-0	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

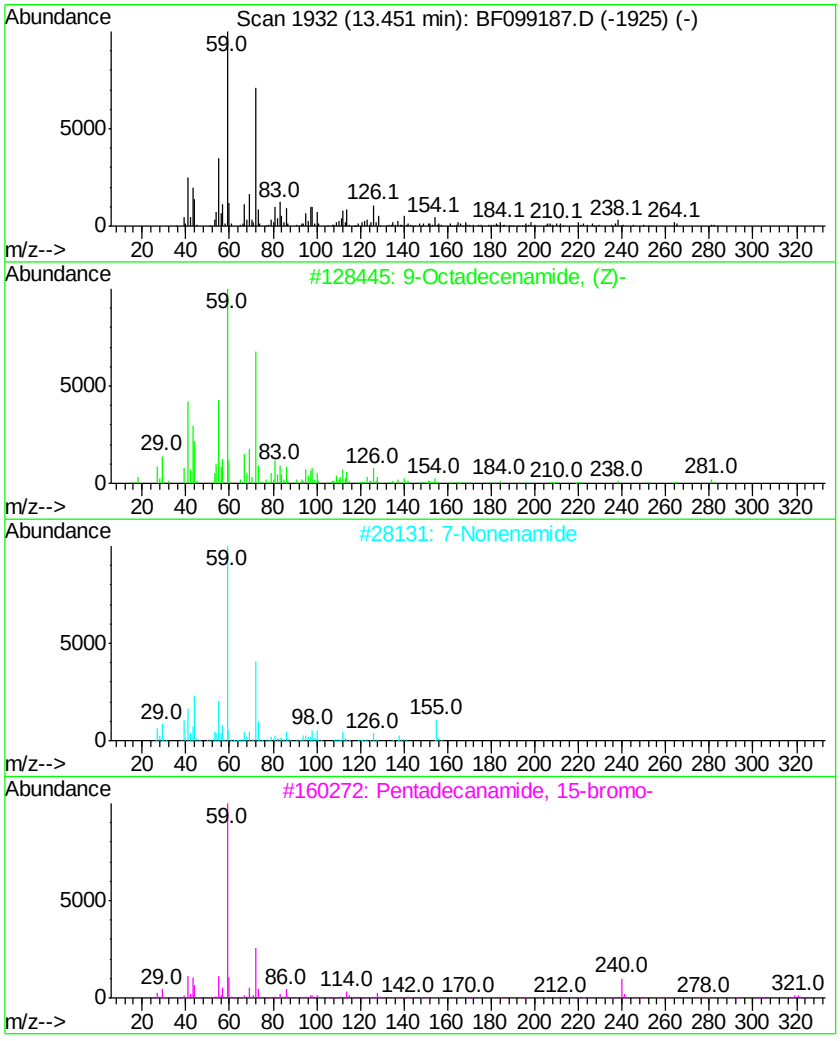
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

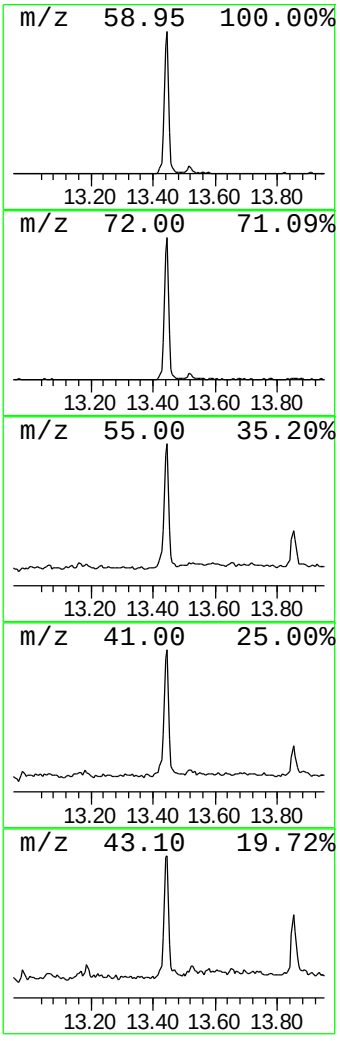
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	19.05 ng	673043	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	7-Nonenamide	155	C9H17NO	090949-53-4	78
3	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	59
4	Nonanamide	157	C9H19NO	001120-07-6	59
5	Octanamide	143	C8H17NO	000629-01-6	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

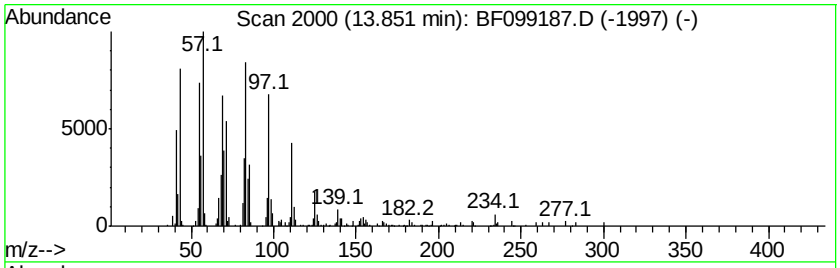
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

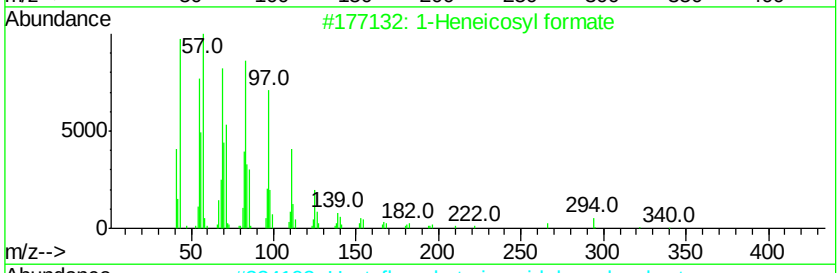
****

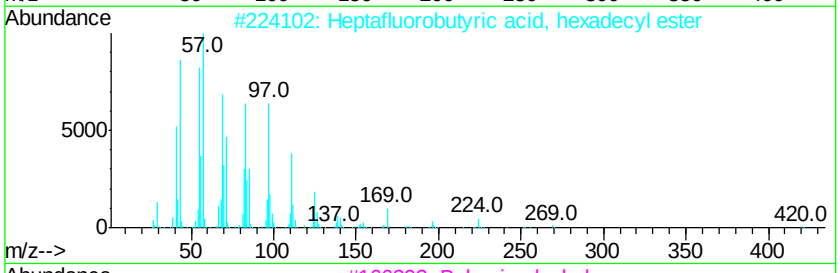
Peak Number 8 1-Heneicosyl formate Concentration Rank 7

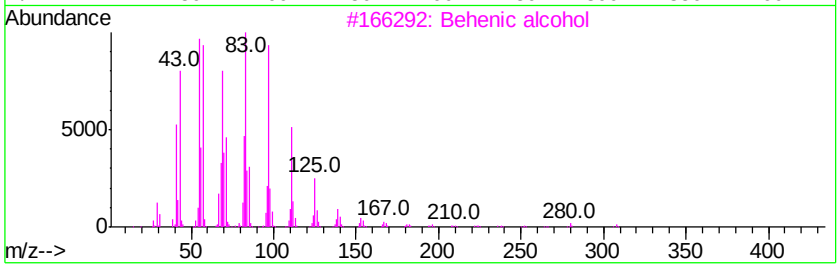
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	4.64 ng	163959	Chrysene-d12	14.03

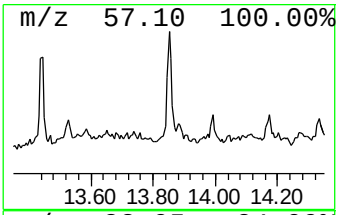
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Octadecanol	270	C18H38O	000112-92-5	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93

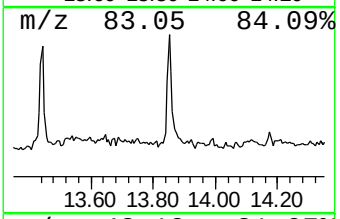


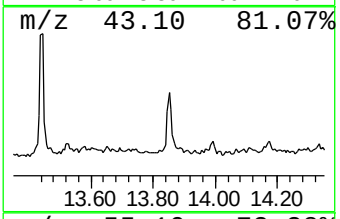


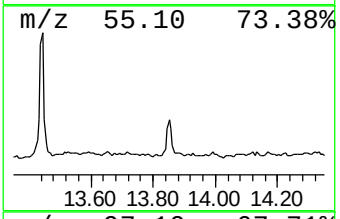


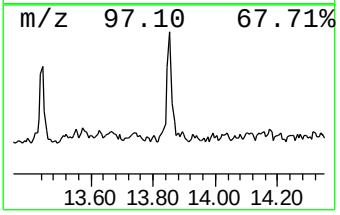












Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

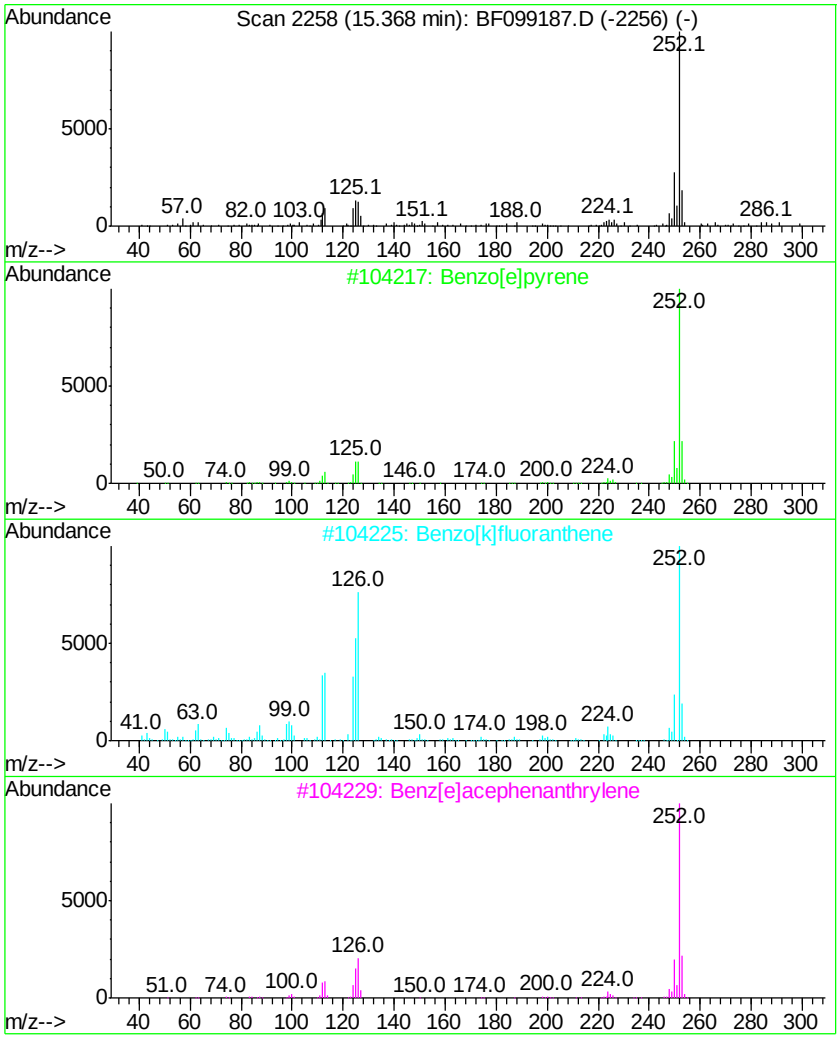
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

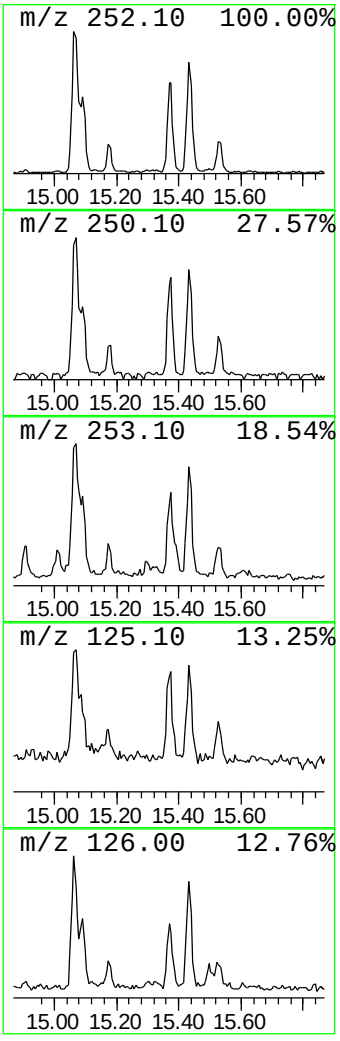
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	2.67 ng	84874	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100717\
Data File : BF099187.D
Acq On : 7 Oct 2017 11:53
Operator : SJ/JU
Sample : I5586-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G72-1-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.16	5.4	ng	204244	1	6.86	756930	20.0
2-Pentanone, 4-hy...	5.10	17.5	ng	663455	1	6.86	756930	20.0
unknown6.64	6.64	87.9	ng	3327490	1	6.86	756930	20.0
Tetradecane	10.79	2.4	ng	114330	4	11.39	938446	20.0
n-Hexadecanoic acid	11.90	5.7	ng	266014	4	11.39	938446	20.0
9-Octadecenamide,...	13.45	19.1	ng	673043	5	14.03	706643	20.0
1-Heneicosyl formate	13.85	4.6	ng	163959	5	14.03	706643	20.0
Benzo[e]pyrene	15.37	2.7	ng	84874	6	15.50	636671	20.0