LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098466.D
Acq On : 12 Sep 2017 22:38
Operator : SJ/JU
Sample : I5140-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

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-BF091117.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	3.593	247	256	264	rBV	343488	555714	11.79%	1.309%
2	4.851	466	470	489	rVB	473282	700226	14.86%	1.649%
3	5.275	538	542	557	rBV	4594375	4713580	100.00%	11.100%
4	6.316	714	719	731	rBV	4398570	4709634	99.92%	11.091%
5	6.440	735	740	743	rVV	4584007	4540542	96.33%	10.693%
6	6.663	774	778	783	rBV	1535230	1286320	27.29%	3.029%
7	6.816	800	804	808	rBV	3400086	3371561	71.53%	7.940%
8	7.234	870	875	878	rBV	3132130	2827845	59.99%	6.659%
9	7.263	878	880	884	rVB2	46004	53215	1.13%	0.125%
10	7.945	991	996	999	rBV	1950290	1645382	34.91%	3.875%
11	9.022	1173	1179	1182	rBV	4202389	3638953	77.20%	8.570%
12	9.104	1188	1193	1198	rBV3	39296	60554	1.28%	0.143%
13	9.416	1243	1246	1250	rVB	548115	460586	9.77%	1.085%
14	9.633	1279	1283	1286	rVB	57673	51865	1.10%	0.122%
15	9.692	1287	1293	1297	rBV	1565434	1476726	31.33%	3.478%
16	10.128	1364	1367	1370	rBV2	61150	57622	1.22%	0.136%
17	10.351	1402	1405	1411	rVB	90808	89893	1.91%	0.212%
18	10.486	1421	1428	1436	rBV	1931338	1865014	39.57%	4.392%
19	10.545	1436	1438	1445	rVV	142107	173999	3.69%	0.410%
20	10.604	1445	1448	1456	rVB	124907	187562	3.98%	0.442%
21	11.051	1521	1524	1526	rBV2	60231	52358	1.11%	0.123%
22	11.075	1526	1528	1533	rVB	69756	73922	1.57%	0.174%
23	11.175	1541	1545	1548	rBV	1435325	1313557	27.87%	3.093%
24	11.198	1548	1549	1553	rVV	397330	254839	5.41%	0.600%
25	11.251	1553	1558	1561	rVB	94416	113201	2.40%	0.267%
26	11.704	1633	1635	1640	rVB3	62441	58450	1.24%	0.138%
27	11.786	1646	1649	1652	rBV	90603	83642	1.77%	0.197%
28	12.227	1721	1724	1725	rBV	54906	54776	1.16%	0.129%
29	12.386	1747	1751	1754	rBV	730338	609622	12.93%	1.436%
30	12.616	1782	1790	1792	rBV	544380	668749	14.19%	1.575%
31	12.757	1810	1814	1818	rBV	2518697	2380129	50.50%	5.605%
32	12.939	1843	1845	1849	rVB	106328	108637	2.30%	0.256%
33	13.010	1852	1857	1859	rVV2	77847	109420	2.32%	0.258%
34	13.657	1964	1967	1975	rVB3	290833	348562	7.39%	0.821%

LSC Area Percent Report

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Acq On : 12 Sep 2017 22:38
Operator : SJ/JU
Sample : I5140-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.810	1988	1993	1996	rBV2	1298713	1460133	30.98%	3.439%
36	13.833	1996	1997	2004	rVB	294082	207055	4.39%	0.488%
37	14.286	2071	2074	2077	rBV2	149890	176811	3.75%	0.416%
38	14.815	2161	2164	2172	rBV	249191	389182	8.26%	0.917%
39	14.886	2174	2176	2178	rVB	126925	103926	2.20%	0.245%
40	15.098	2209	2212	2218	rVB	142648	173507	3.68%	0.409%
41	15.157	2218	2222	2227	rVV	209283	265233	5.63%	0.625%
42	15.210	2227	2231	2239	rVB	728050	894218	18.97%	2.106%
43	15.621	2299	2301	2305	rVB	89389	97094	2.06%	0.229%

Sum of corrected areas: 42463816

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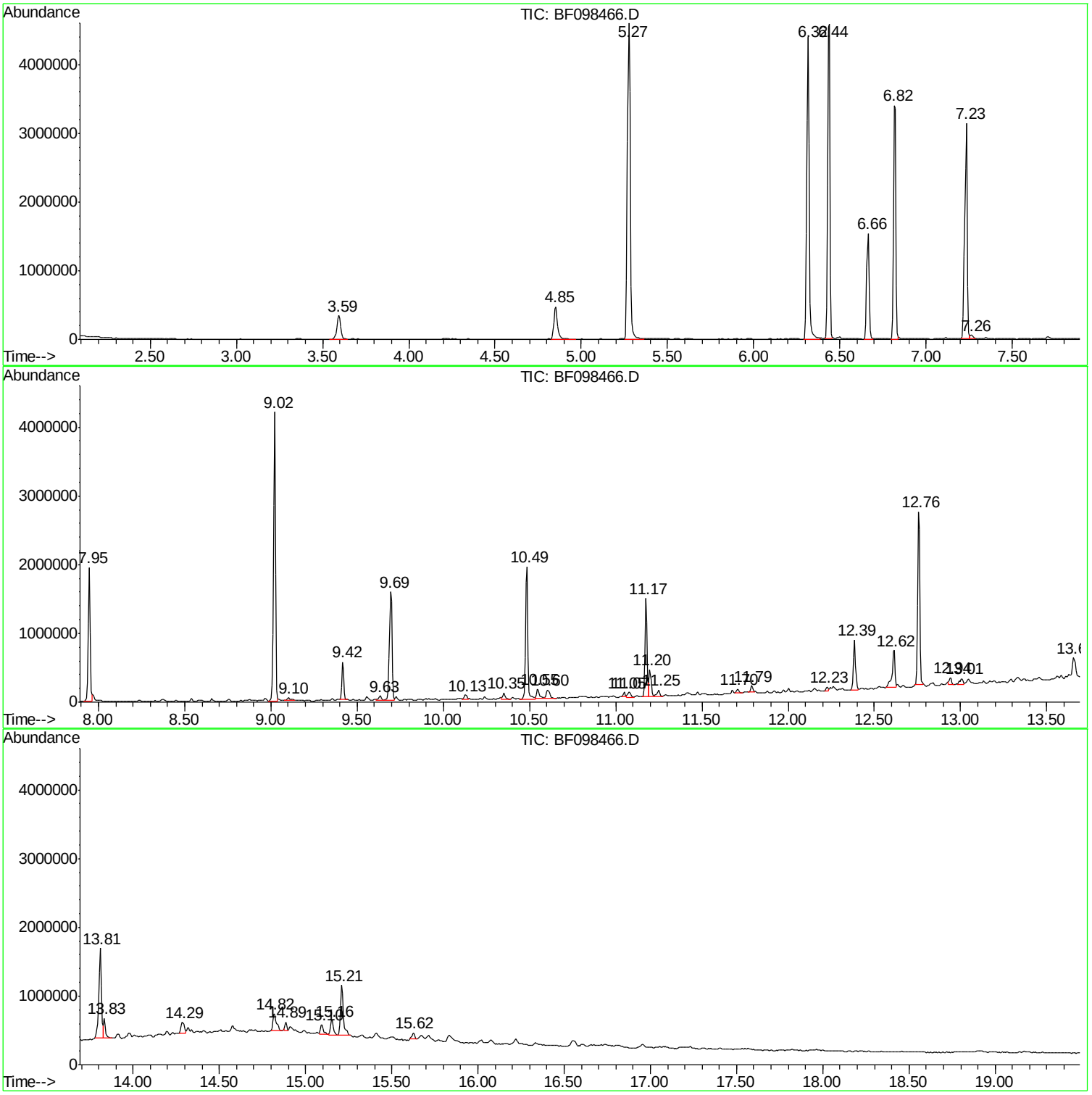
Instrument :
BNA_F
ClientSampleId :
RL-10-0-10.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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

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Data File : BF098466.D
Acq On : 12 Sep 2017 22:38
Operator : SJ/JU
Sample : I5140-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

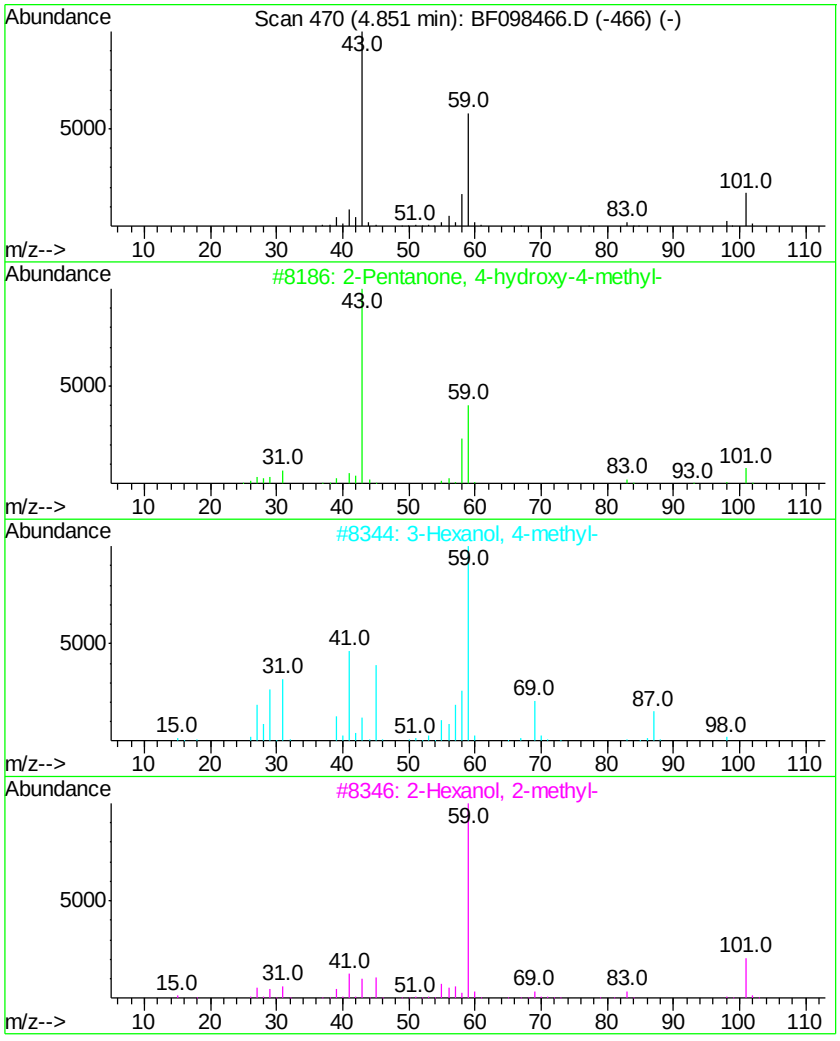
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

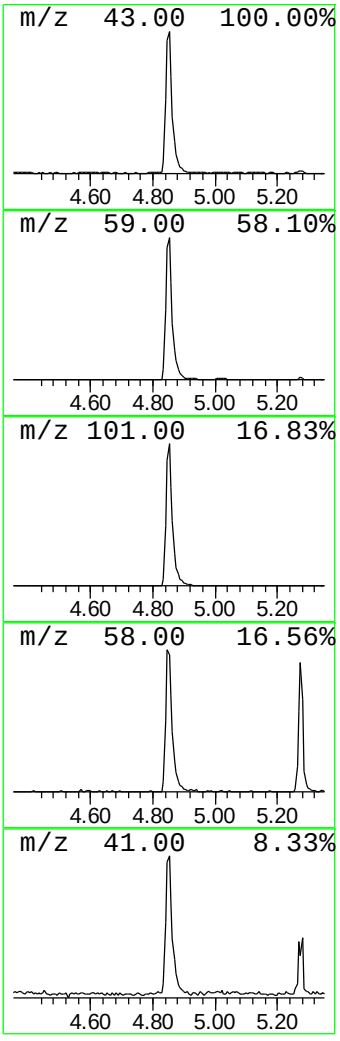
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	10.89 ng	700226	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33





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Operator : SJ/JU
Sample : I5140-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

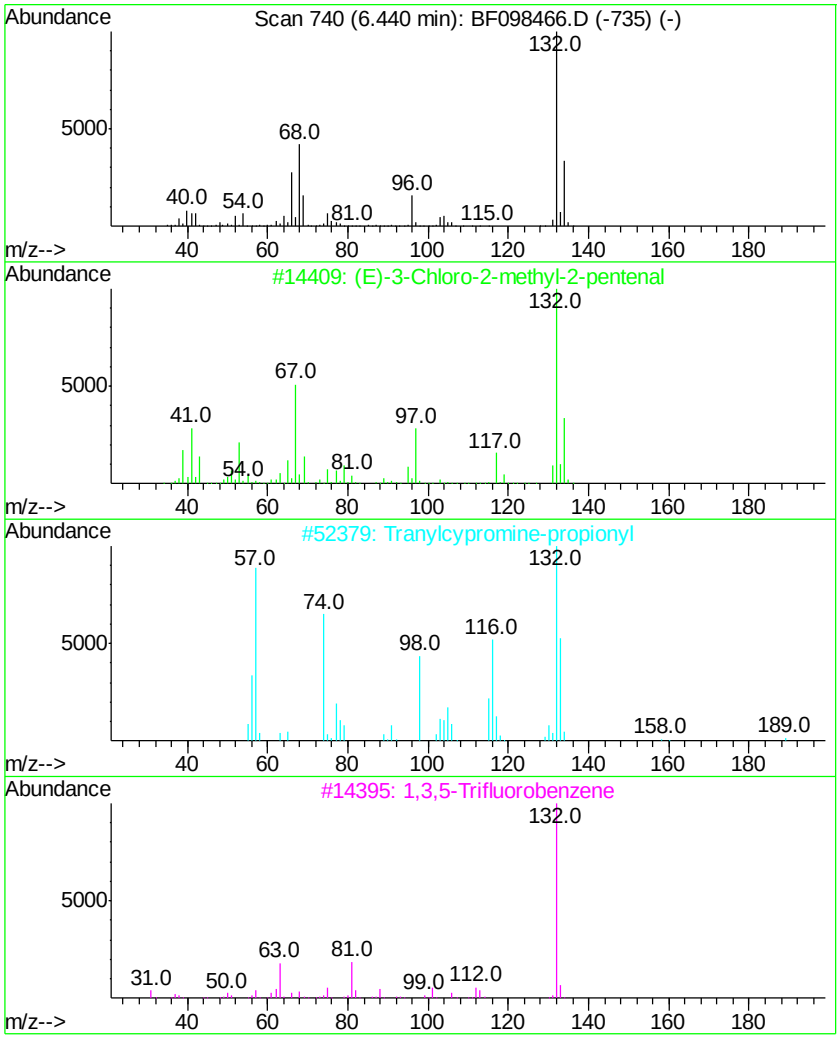
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

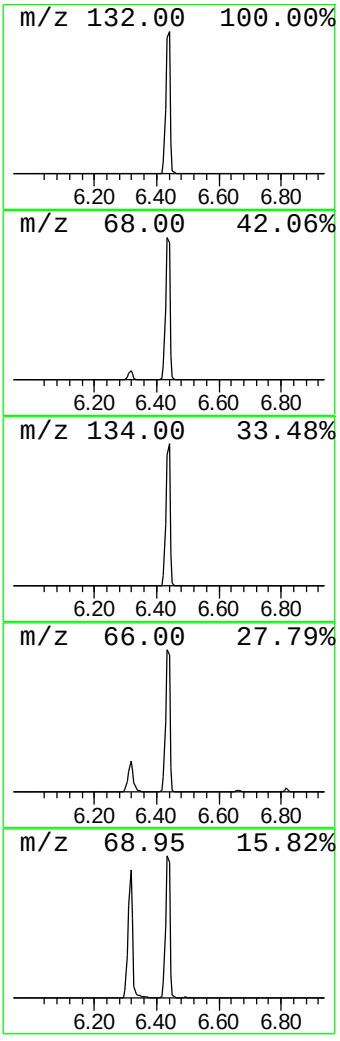
****

Peak Number 3 unknown6.44 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	70.60 ng	4540540	1,4-Dichlorobenzene-d4	6.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098466.D
Acq On : 12 Sep 2017 22:38
Operator : SJ/JU
Sample : I5140-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

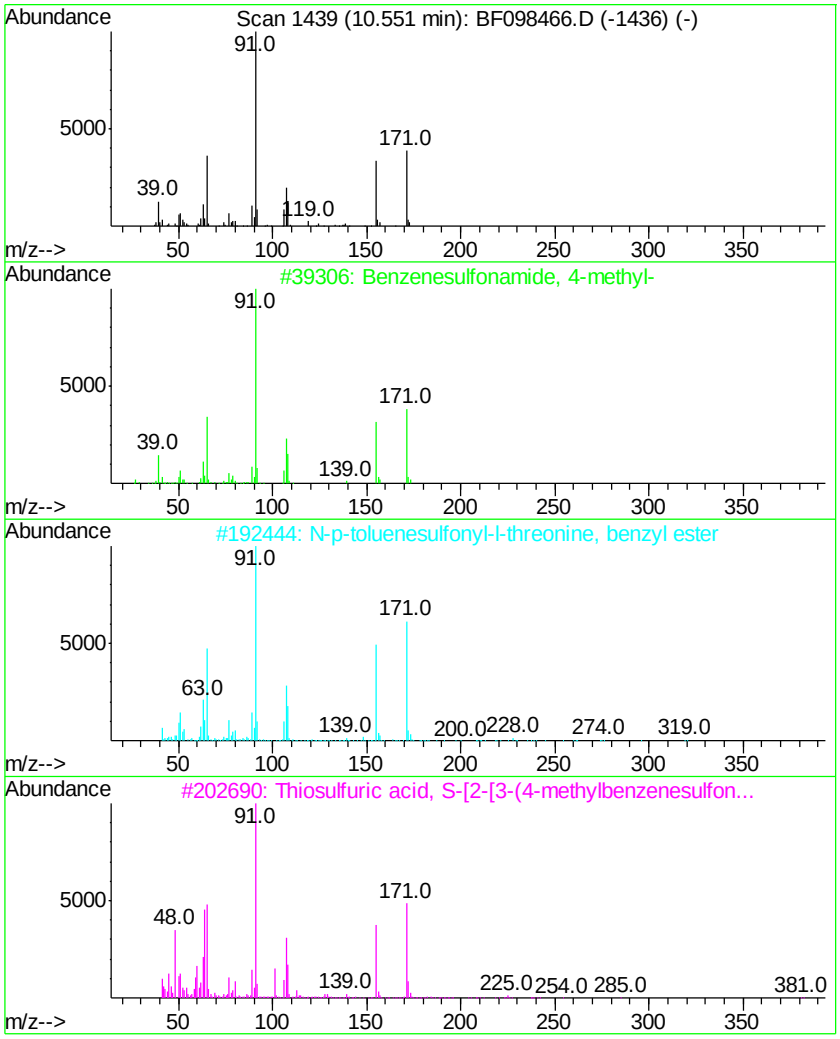
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

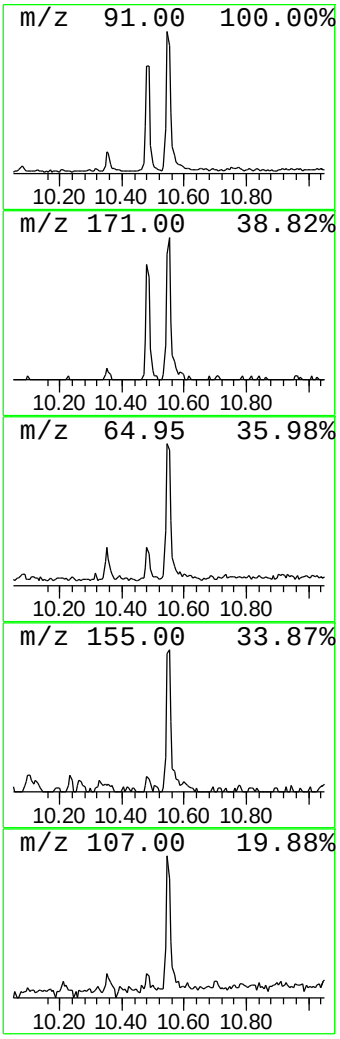
****

Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.55	2.65 ng	173999	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	83
3	Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	72
4	Tolbutamide	270	C12H18N2O3S	000064-77-7	64
5	N-(4H-1,2,4-Triazol-4-yl)-p-tolu...	238	C9H10N4O2S	032585-76-5	50





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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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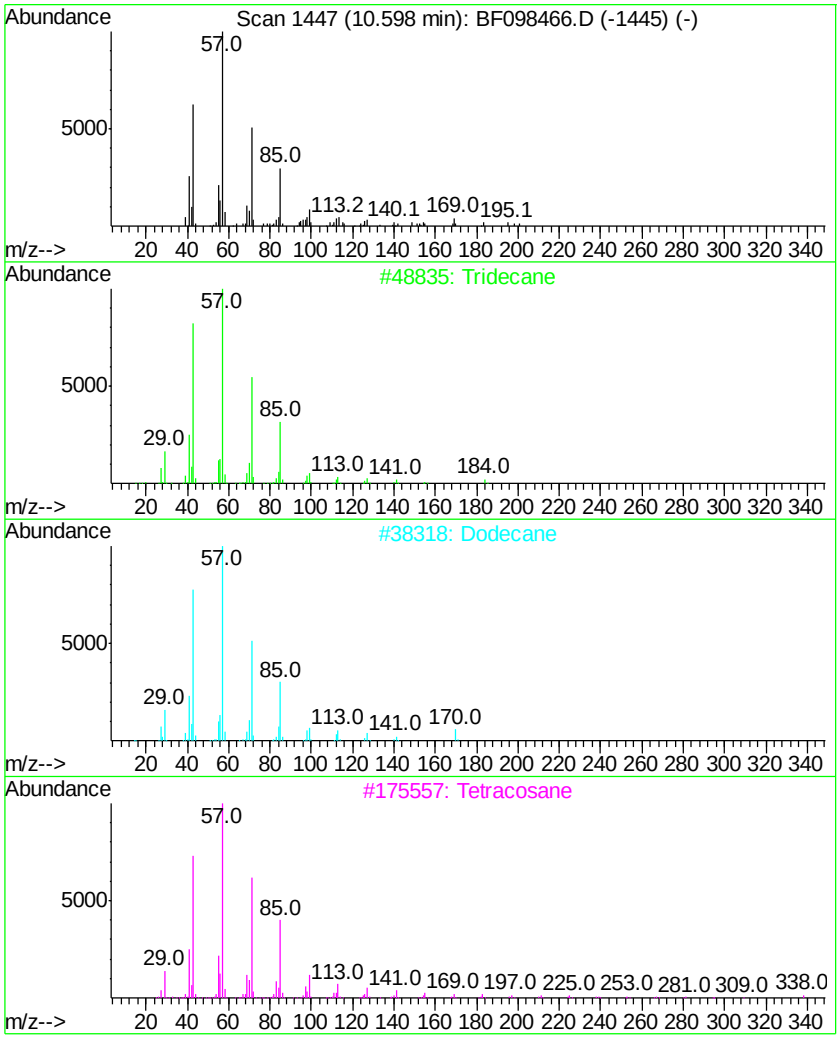
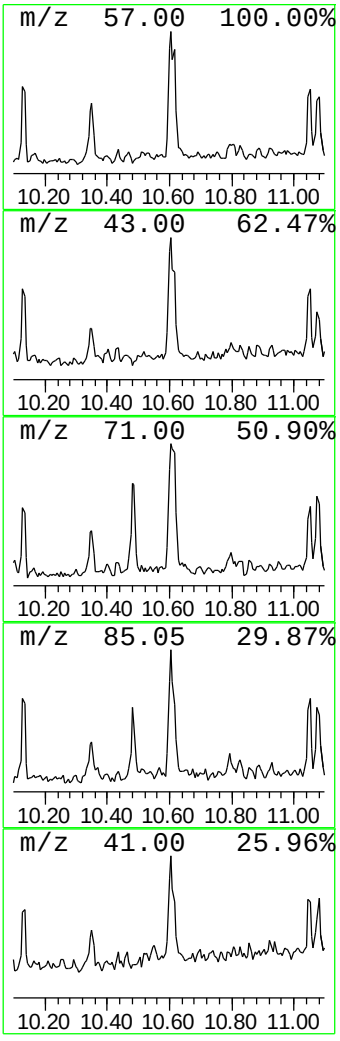
Peak Number 6 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.86 ng	187562	Phenanthrene-d10	11.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	87
2	Dodecane	170	C12H26	000112-40-3	87
3	Tetracosane	338	C24H50	000646-31-1	80
4	Octacosane	394	C28H58	000630-02-4	80
5	Hexadecane	226	C16H34	000544-76-3	80





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
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Operator : SJ/JU
Sample : I5140-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
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TIC Library : C:\DATABASE\NIST11.L
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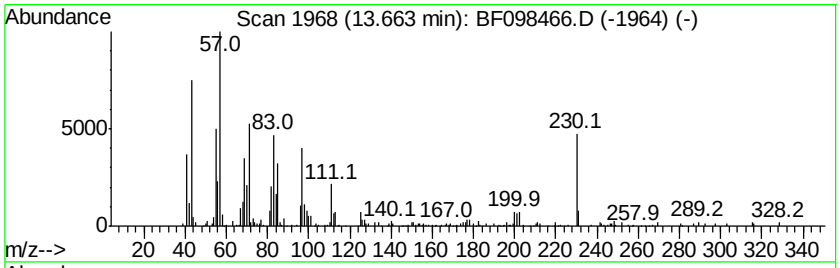
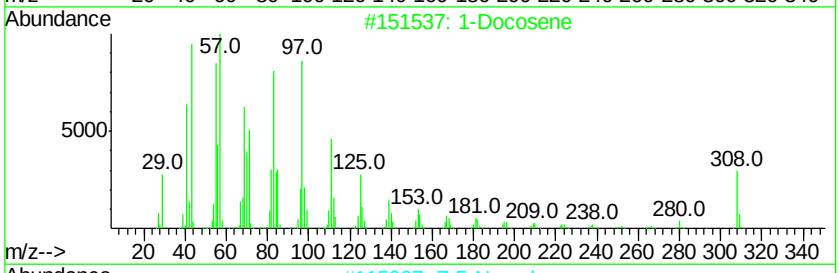
****

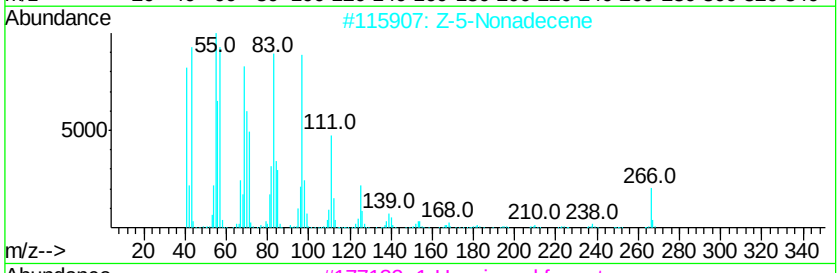
Peak Number 7 1-Docosene Concentration Rank 5

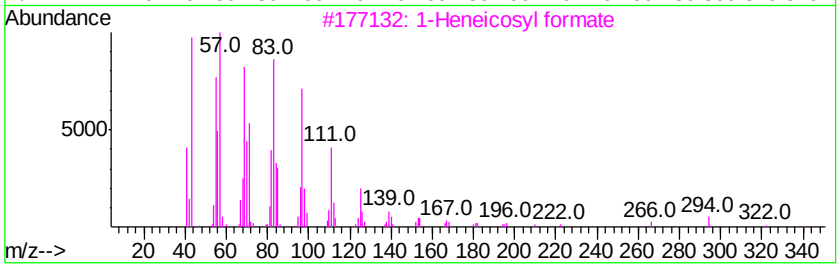
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	4.77 ng	348562	Chrysene-d12	13.81

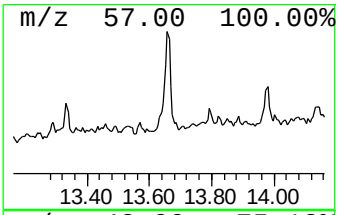
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	Z-5-Nonadecene	266	C19H38	1000131-11-8	90
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90

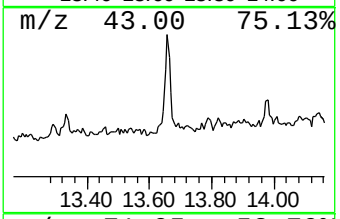


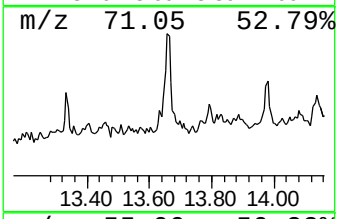


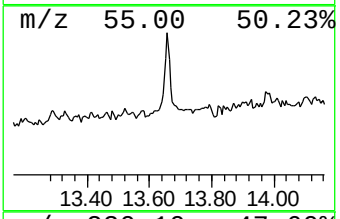


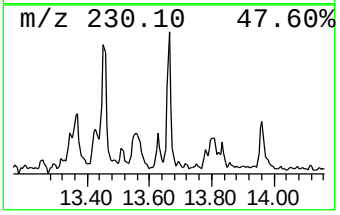












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

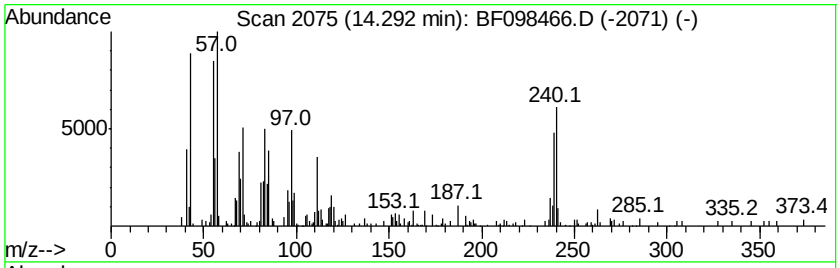
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

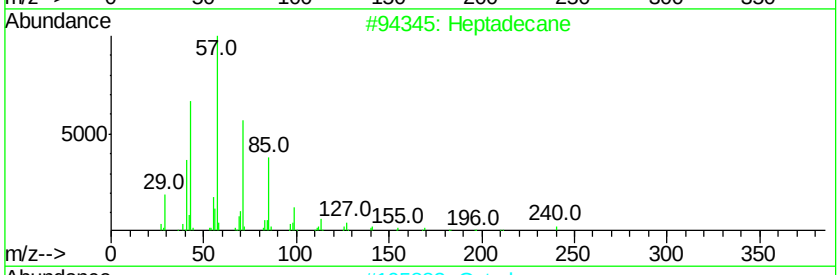
****

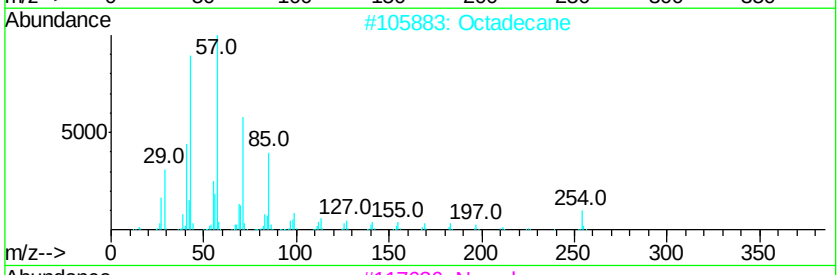
Peak Number 8 Heptadecane Concentration Rank 9

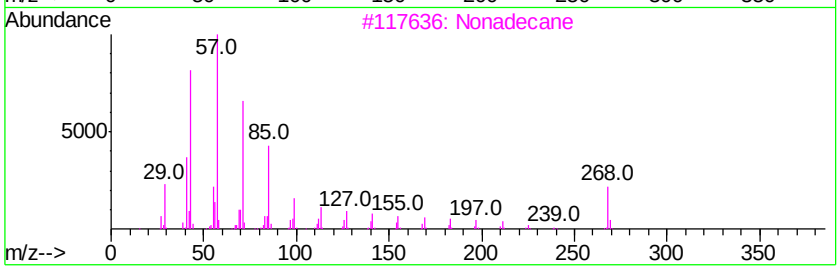
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.42 ng	176811	Chrysene-d12	13.81

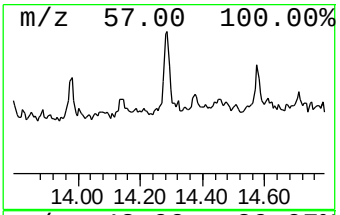
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	60
2	Octadecane	254	C18H38	000593-45-3	50
3	Nonadecane	268	C19H40	000629-92-5	46
4	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	46
5	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	46

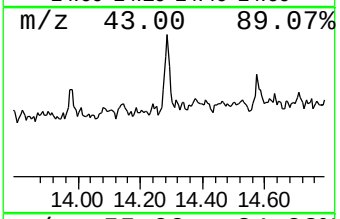


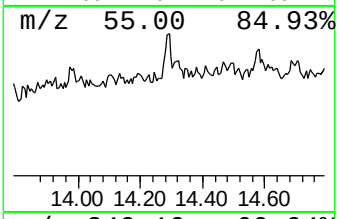


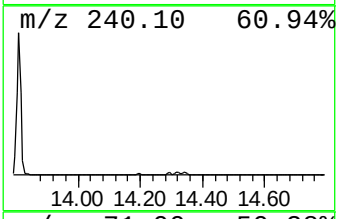


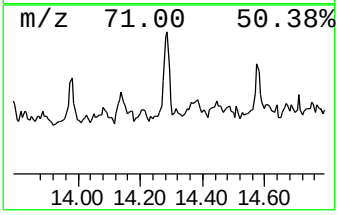












Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091217\
Data File : BF098466.D
Acq On : 12 Sep 2017 22:38
Operator : SJ/JU
Sample : I5140-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

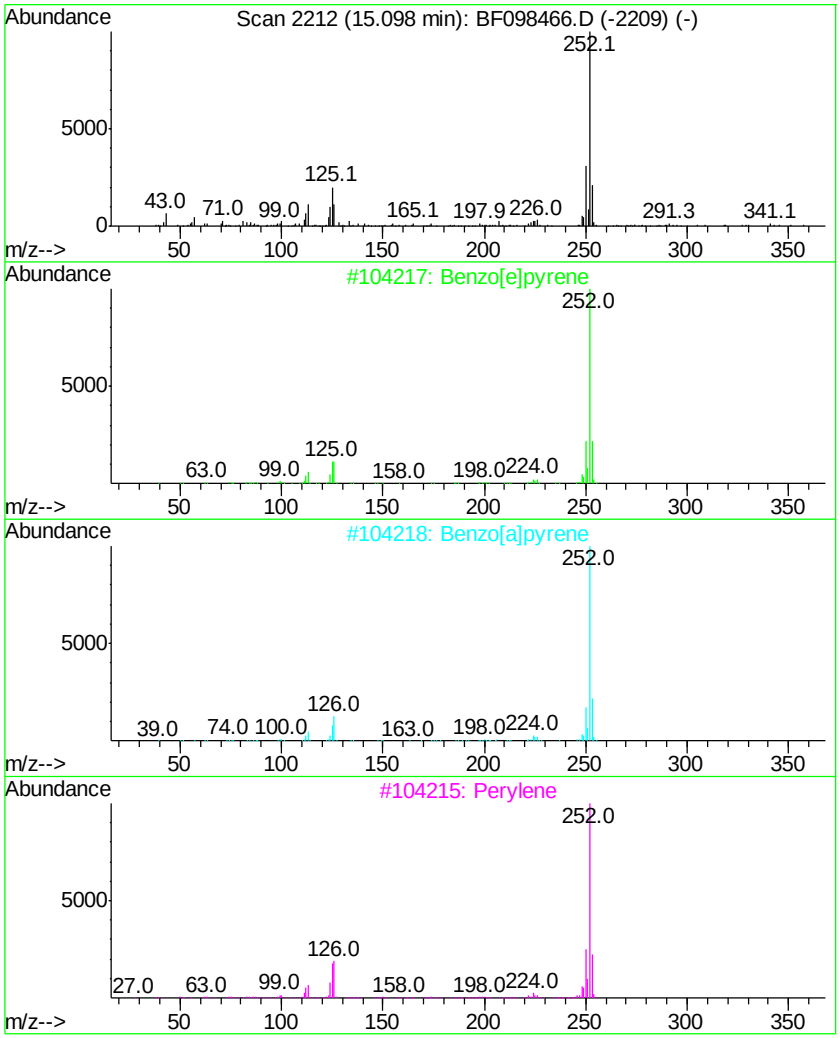
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

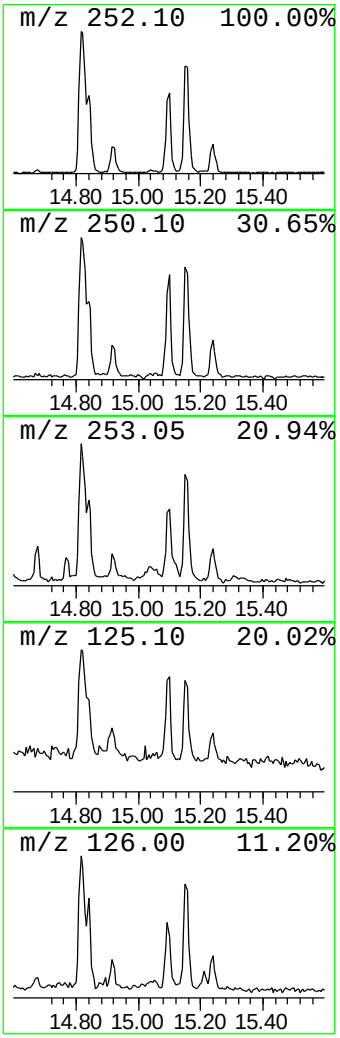
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	3.88 ng	173507	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benzo[a]pyrene	252	C20H12	000050-32-8	93
3	Perylene	252	C20H12	000198-55-0	90
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	89





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Data File : BF098466.D
Acq On : 12 Sep 2017 22:38
Operator : SJ/JU
Sample : I5140-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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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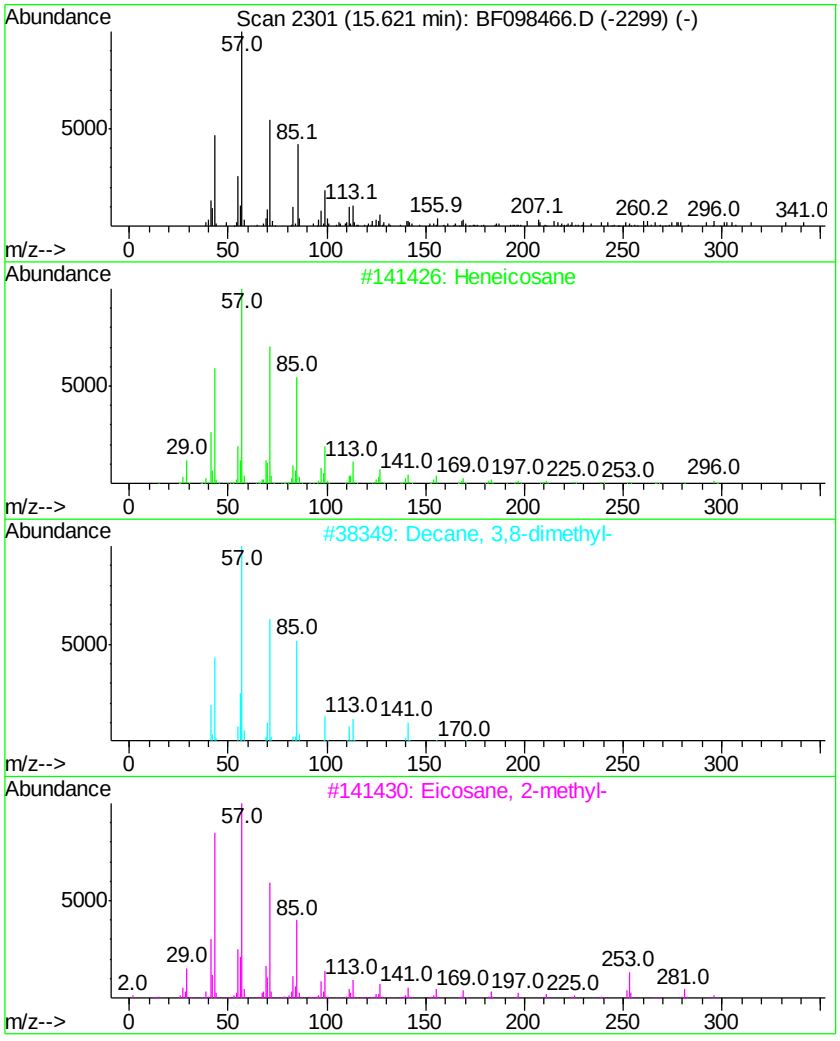
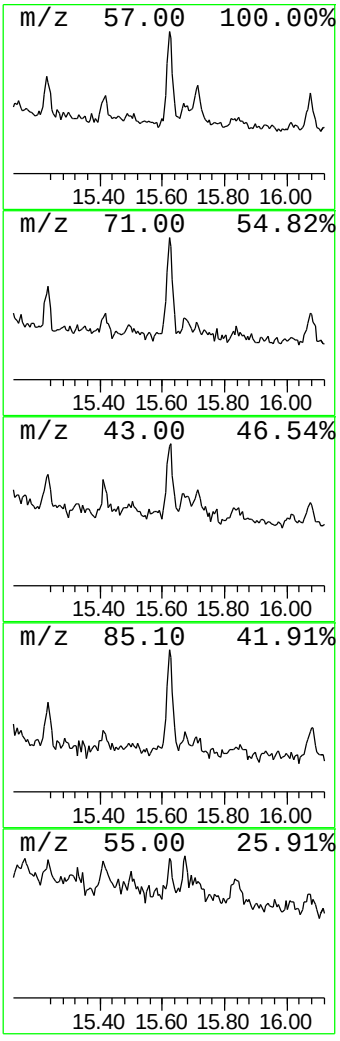
Peak Number 10 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	2.17 ng	97094	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
3	Eicosane, 2-methyl-	296	C21H44	001560-84-5	80
4	Hexadecane	226	C16H34	000544-76-3	72
5	Pentacosane	352	C25H52	000629-99-2	72





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF091217\
Data File : BF098466.D
Acq On : 12 Sep 2017 22:38
Operator : SJ/JU
Sample : I5140-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RL-10-0-10.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.85	10.9	ng	700226	1	6.66	1286320	20.0
unknown6.44	6.44	70.6	ng	4540540	1	6.66	1286320	20.0
Benzenesulfonamid...	10.55	2.6	ng	173999	4	11.17	1313560	20.0
Tridecane	10.60	2.9	ng	187562	4	11.17	1313560	20.0
1-Docosene	13.66	4.8	ng	348562	5	13.81	1460130	20.0
Heptadecane	14.29	2.4	ng	176811	5	13.81	1460130	20.0
Benzo[e]pyrene	15.10	3.9	ng	173507	6	15.21	894218	20.0
Heneicosane	15.62	2.2	ng	97094	6	15.21	894218	20.0