LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-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-BF122116.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	4.622	246	248	260	rBV	875754	1574573	31.60%	2.933%
2	5.102	288	290	305	rBV	3236840	3714810	74.56%	6.920%
3	6.187	382	385	392	rBV	3097814	4117485	82.64%	7.670%
4	6.290	392	394	397	rVV	3469184	3610578	72.47%	6.726%
5	6.347	397	399	403	rVB2	36240	77124	1.55%	0.144%
6	6.519	412	414	417	rBV	891427	818669	16.43%	1.525%
7	6.679	425	428	430	rBV	3133553	3292777	66.09%	6.134%
8	7.102	462	465	467	rBV	2070024	2489154	49.96%	4.637%
9	7.810	525	527	529	rBV	1205076	1120653	22.49%	2.088%
10	8.530	587	590	592	rVB	61472	74774	1.50%	0.139%
11	8.622	596	598	603	rVB2	43918	61343	1.23%	0.114%
12	8.896	619	622	624	rBV	3809385	4982465	100.00%	9.282%
13	8.988	624	630	632	rVV	46925	57008	1.14%	0.106%
14	9.148	642	644	649	rBV2	38181	71985	1.44%	0.134%
15	9.296	655	657	659	rBV	545060	570529	11.45%	1.063%
16	9.422	666	668	670	rBV	277527	348958	7.00%	0.650%
17	9.513	674	676	677	rBV	51842	54663	1.10%	0.102%
18	9.559	677	680	681	rVV	1501399	1565267	31.42%	2.916%
19	9.593	681	683	685	rVB	75162	107853	2.16%	0.201%
20	9.765	695	698	700	rVB	62679	65364	1.31%	0.122%
21	9.879	705	708	709	rBV2	31293	50137	1.01%	0.093%
22	9.982	713	717	718	rBV2	42514	88706	1.78%	0.165%
23	10.005	718	719	721	rVV2	129786	120761	2.42%	0.225%
24	10.096	726	727	731	rVB2	63492	110650	2.22%	0.206%
25	10.222	736	738	740	rBV3	43998	80570	1.62%	0.150%
26	10.348	746	749	751	rBV	2135829	2481989	49.81%	4.624%
27	10.474	758	760	764	rVB	146970	219107	4.40%	0.408%
28	10.919	798	799	804	rVB2	130148	223237	4.48%	0.416%
29	11.034	806	809	813	rBV2	1264788	2013335	40.41%	3.751%
30	11.102	813	815	818	rBV	280190	395648	7.94%	0.737%
31	11.148	818	819	822	rBV3	28505	54940	1.10%	0.102%
32	11.274	828	830	834	rBV2	70930	160019	3.21%	0.298%
33	11.354	834	837	839	rVB3	86419	152957	3.07%	0.285%
34	11.536	850	853	854	rBV	125429	144604	2.90%	0.269%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.559	854	855	856	rVV	167833	157215	3.16%	0.293%
36	11.616	856	860	861	rVV	571930	965707	19.38%	1.799%
37	11.639	861	862	867	rVV	263623	377660	7.58%	0.704%
38	11.754	870	872	875	rVV2	98538	129605	2.60%	0.241%
39	11.834	877	879	881	rVV	103102	166899	3.35%	0.311%
40	11.868	881	882	884	rVB	78583	76532	1.54%	0.143%
41	12.085	899	901	902	rBV	110963	124284	2.49%	0.232%
42	12.142	902	906	907	rVV3	91837	158183	3.17%	0.295%
43	12.177	907	909	910	rVB2	114430	115051	2.31%	0.214%
44	12.234	912	914	917	rBV	1279420	1605935	32.23%	2.992%
45	12.291	917	919	921	rBV2	32747	63142	1.27%	0.118%
46	12.337	921	923	925	rVB	117760	109692	2.20%	0.204%
47	12.382	925	927	931	rBV4	109182	282782	5.68%	0.527%
48	12.462	931	934	937	rBV	1649992	1803565	36.20%	3.360%
49	12.622	945	948	950	rVB	2760235	3181322	63.85%	5.926%
50	12.691	950	954	956	rBV2	90418	99939	2.01%	0.186%
51	12.794	960	963	965	rBV2	256684	465880	9.35%	0.868%
52	12.862	967	969	971	rVV	246485	264874	5.32%	0.493%
53	12.897	971	972	976	rVB2	210493	279859	5.62%	0.521%
54	13.022	981	983	984	rBV2	108247	107793	2.16%	0.201%
55	13.434	1015	1019	1020	rBV3	142474	357071	7.17%	0.665%
56	13.525	1025	1027	1029	rBV	145055	221392	4.44%	0.412%
57	13.662	1036	1039	1040	rBV2	1486143	2226783	44.69%	4.148%
58	14.668	1124	1127	1132	rBV	900624	1785790	35.84%	3.327%
59	14.920	1147	1149	1151	rVB	381174	421681	8.46%	0.786%
60	14.965	1151	1153	1156	rBV	638245	869548	17.45%	1.620%
61	15.023	1156	1158	1159	rBV	564154	628119	12.61%	1.170%
62	16.246	1262	1265	1274	rVB	314186	910987	18.28%	1.697%
63	16.600	1294	1296	1303	rVB	261669	650035	13.05%	1.211%

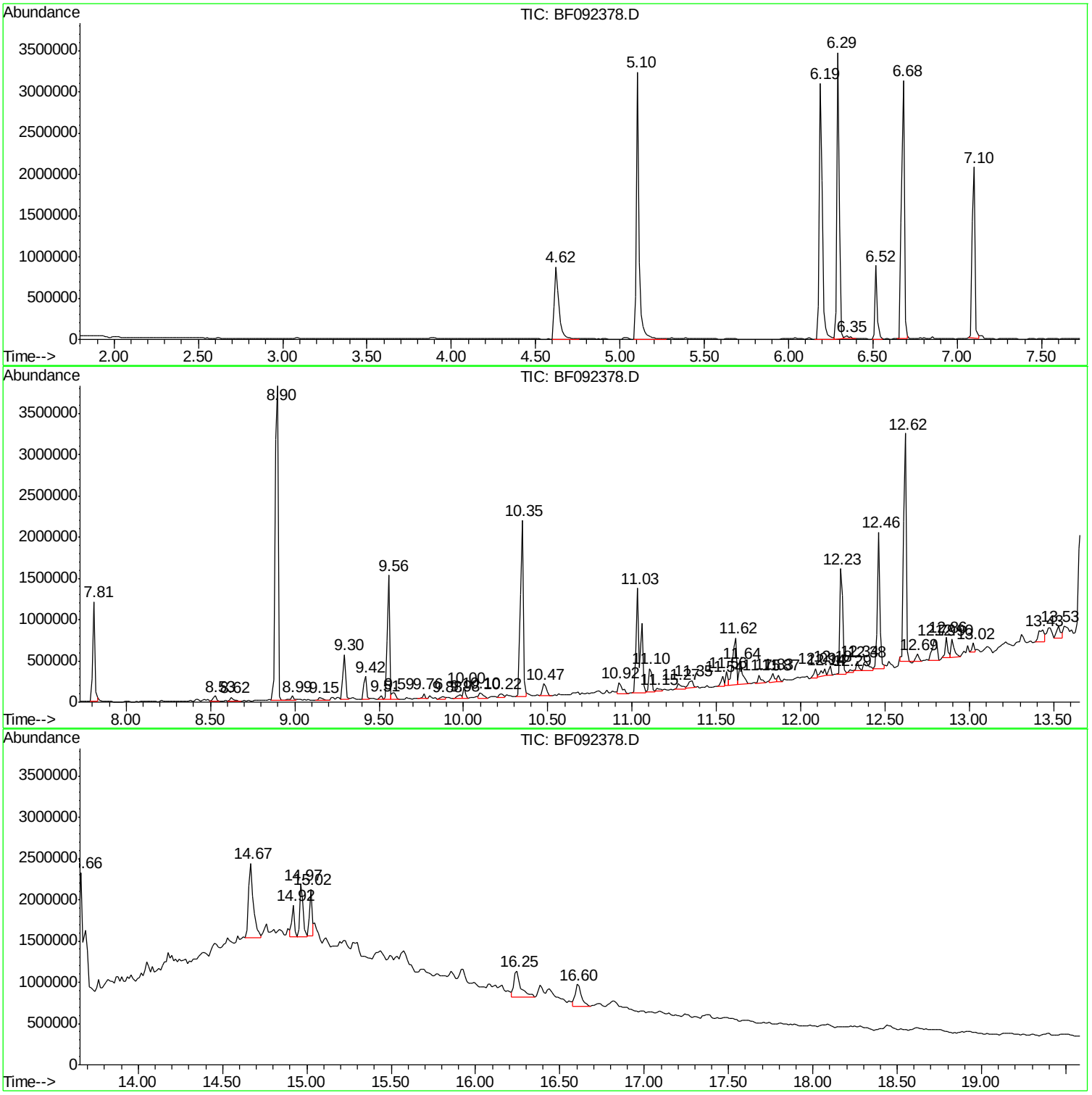
Sum of corrected areas: 53680017

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

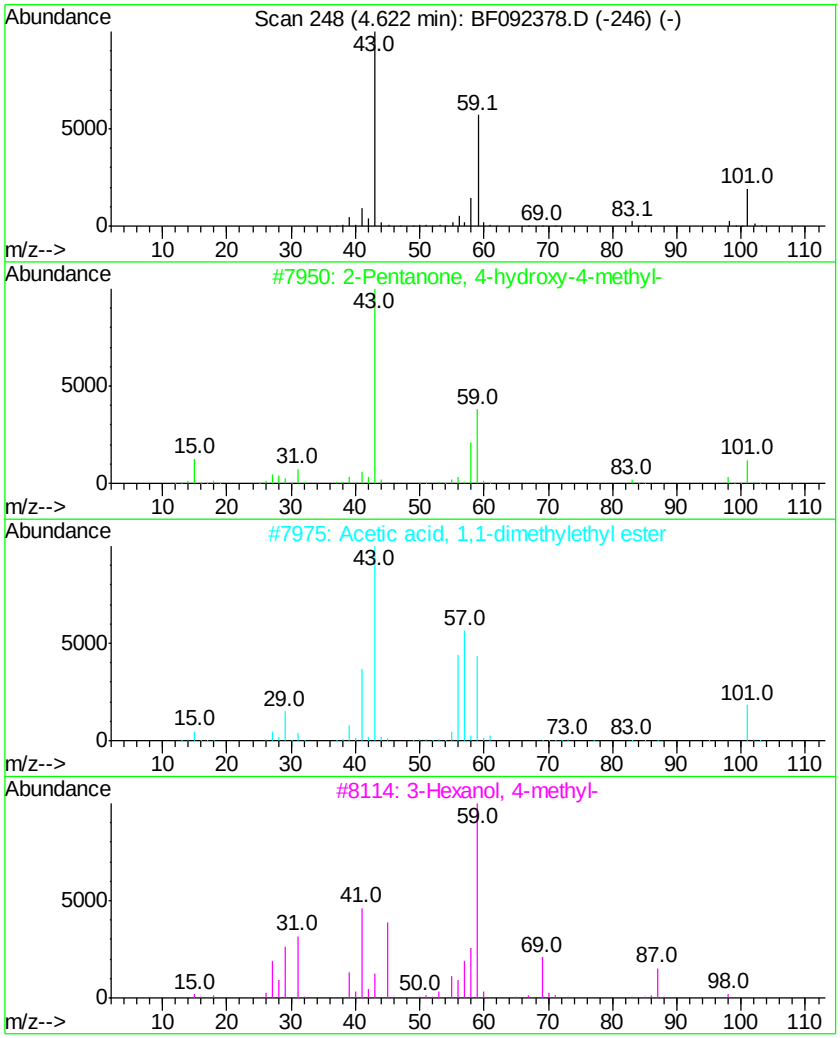
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

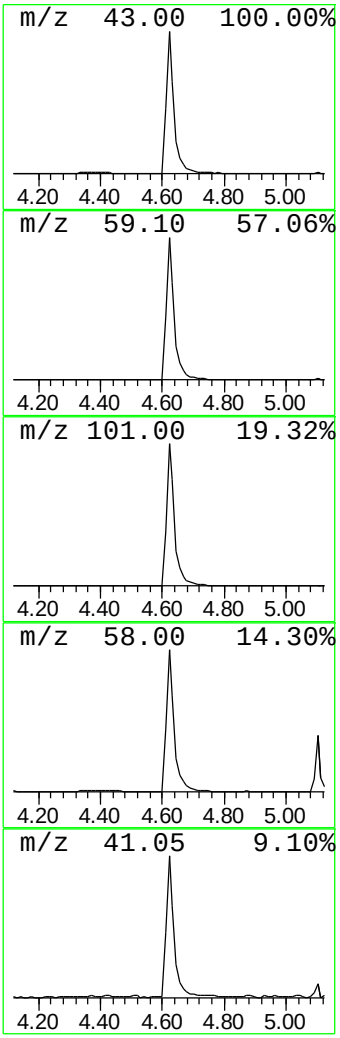
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	38.47 ng	1574570	1,4-Dichlorobenzene-d4	6.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

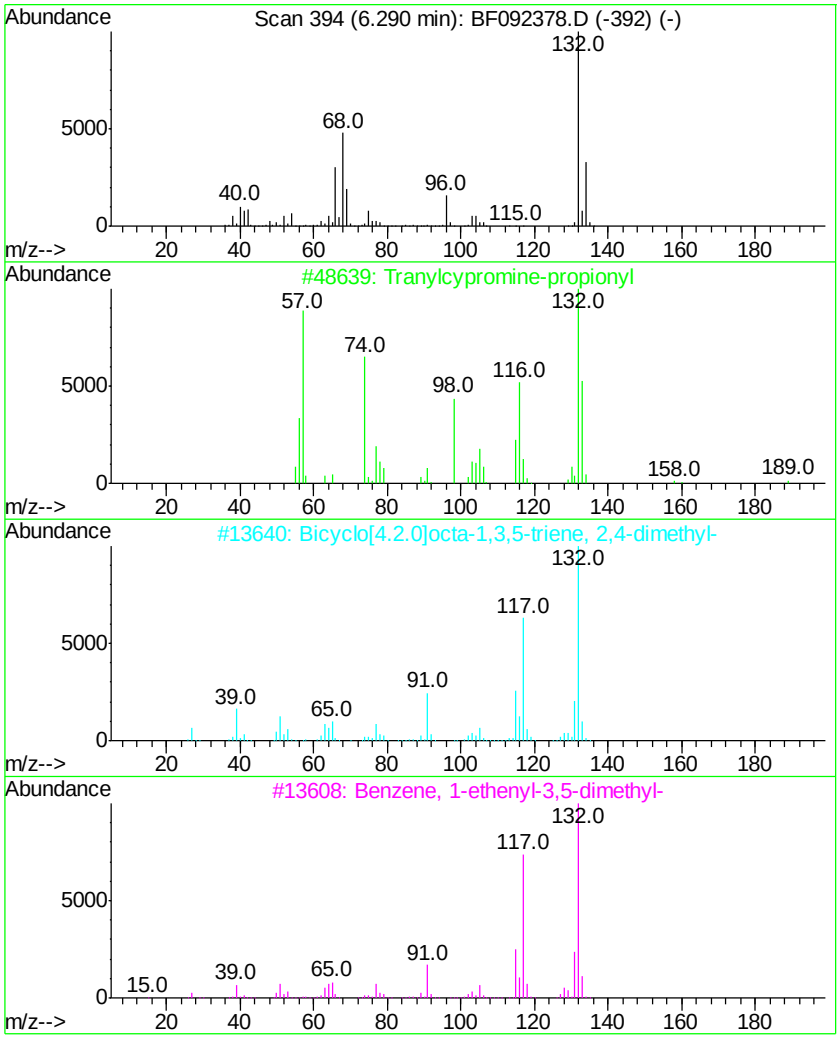
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

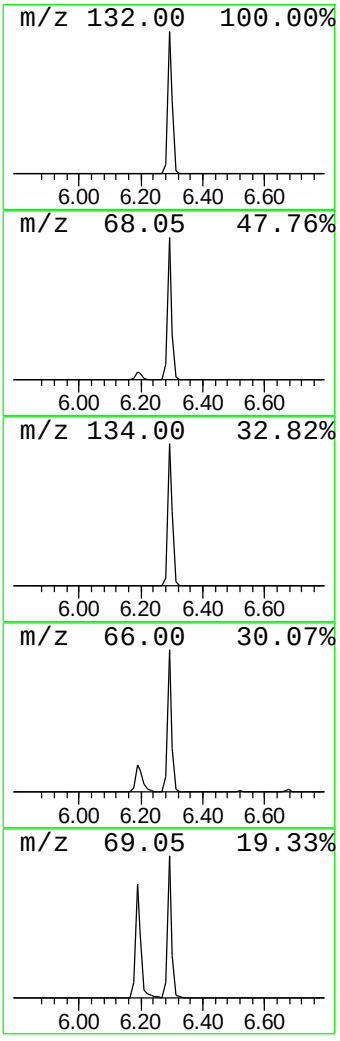
****

Peak Number 2 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	88.21 ng	3610580	1,4-Dichlorobenzene-d4	6.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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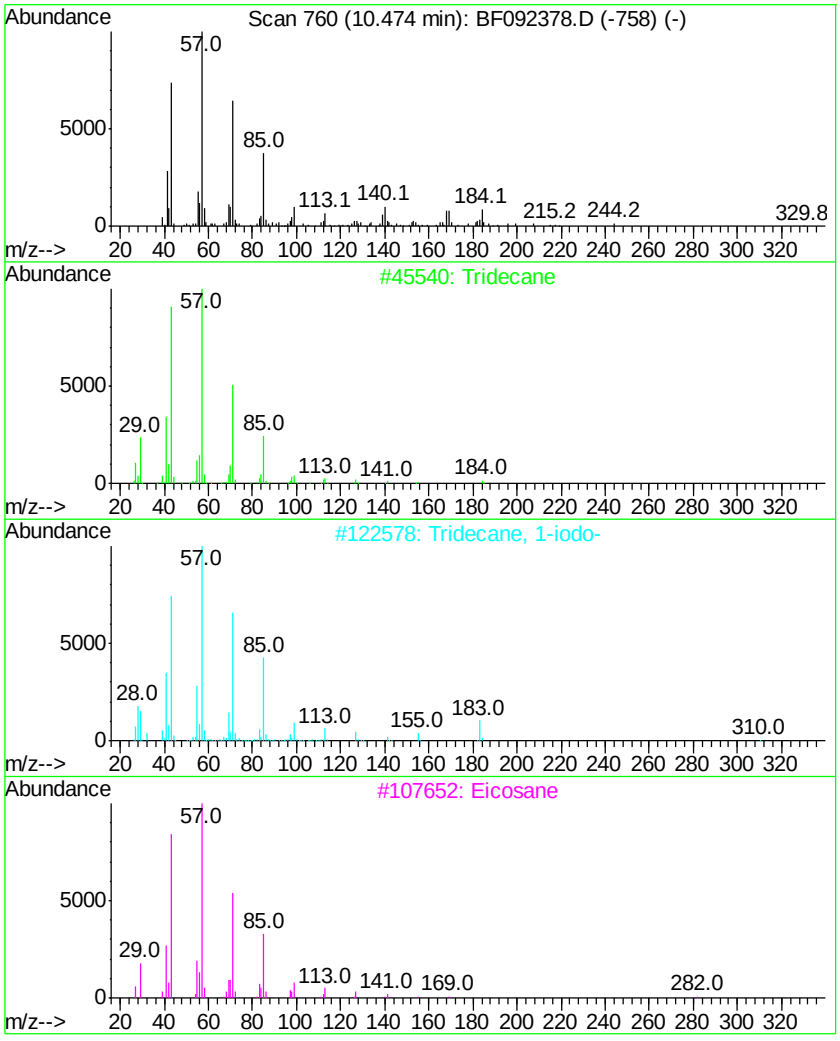
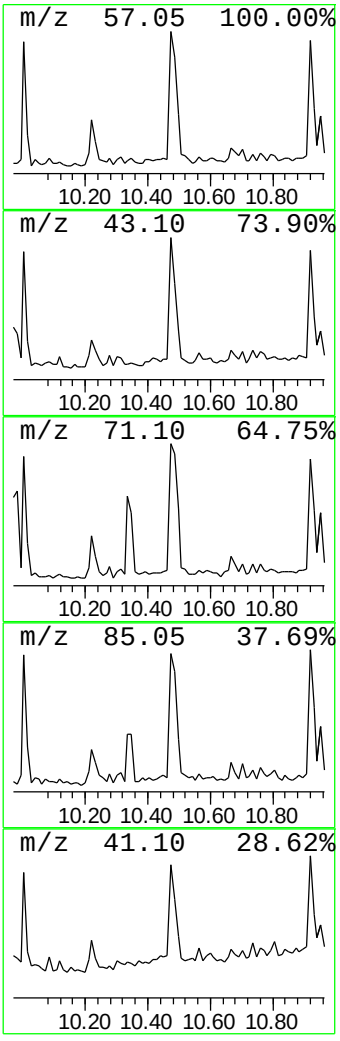
Peak Number 4 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.47	2.18 ng	219107	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
3	Eicosane	282	C20H42	000112-95-8	68
4	Tetradecane	198	C14H30	000629-59-4	64
5	5-Ethyldecane	170	C12H26	017302-36-2	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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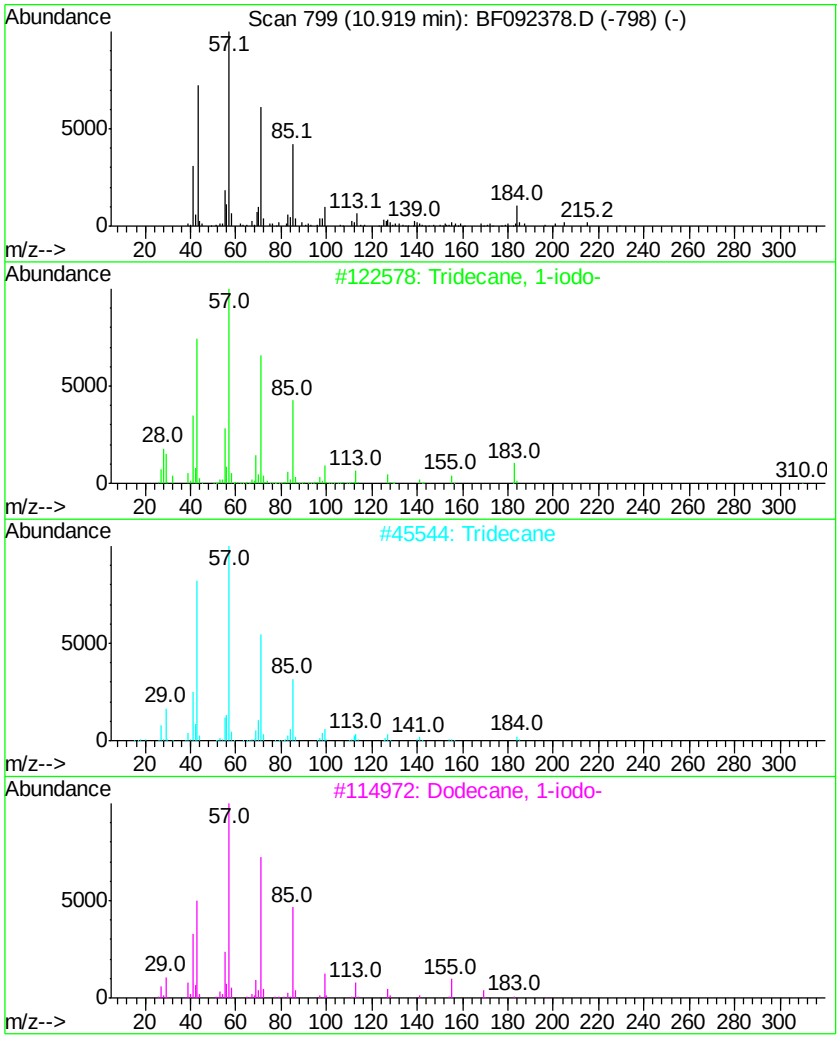
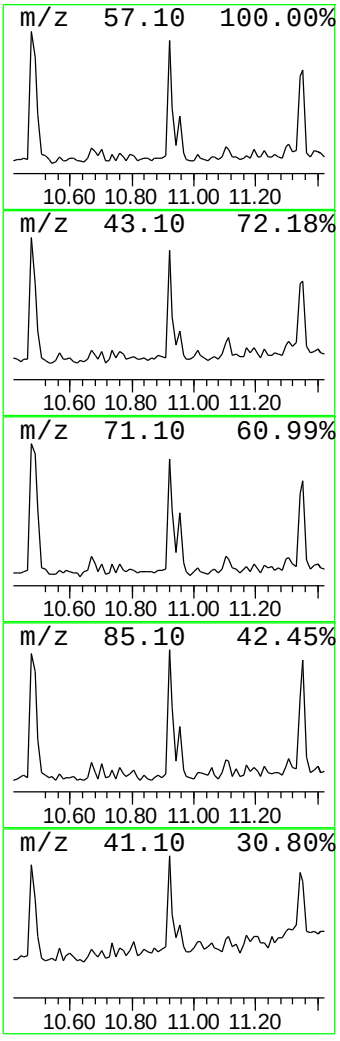
Peak Number 5 Tridecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.92	2.22 ng	223237	Phenanthrene-d10	11.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
2	Tridecane	184	C13H28	000629-50-5	86
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
5	Heptadecane	240	C17H36	000629-78-7	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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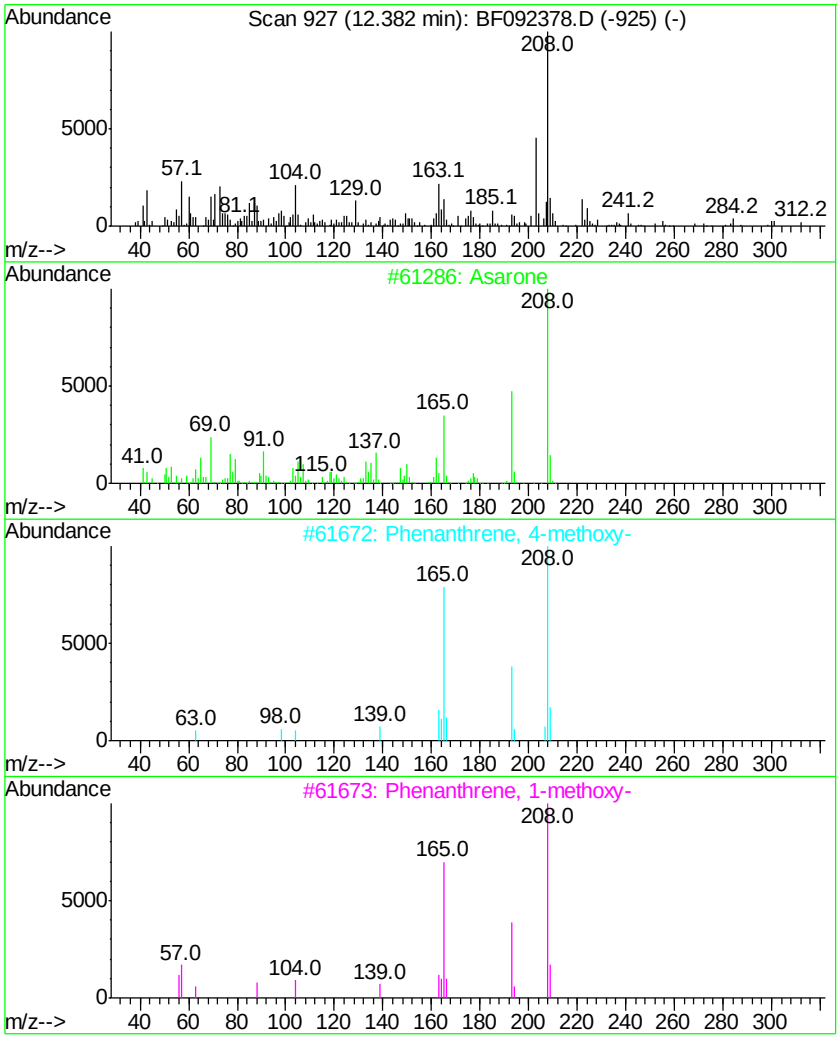
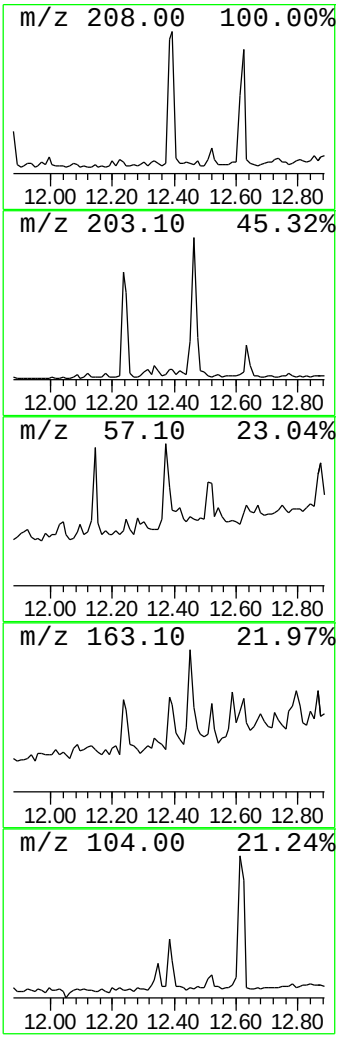
Peak Number 6 unknown12.38 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	2.54 ng	282782	Chrysene-d12	13.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Asarone	208	C12H16O3	002883-98-9	38
2	Phenanthrene, 4-methoxy-	208	C15H12O	015638-06-9	38
3	Phenanthrene, 1-methoxy-	208	C15H12O	000834-99-1	38
4	2,2-Dimethoxy-1-oxa-2-sila-1,2-d...	208	C10H12O3Si	073060-35-2	35
5	Anthracene, 1-methoxy-	208	C15H12O	054458-84-3	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

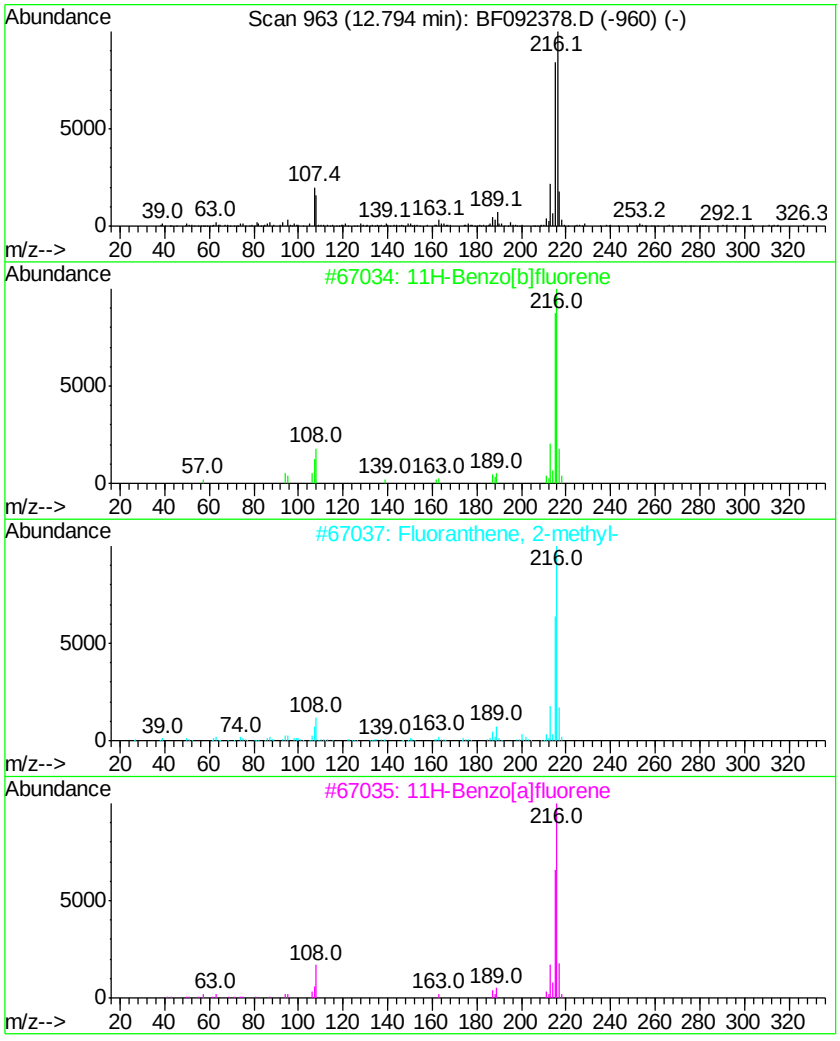
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

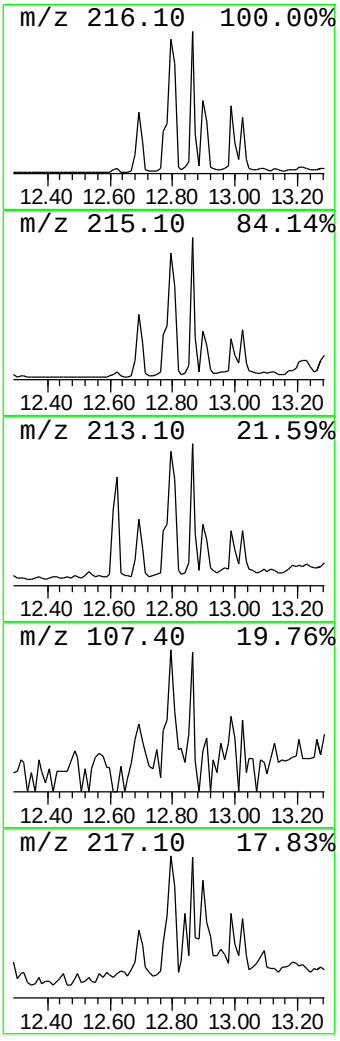
****

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	4.18 ng	465880	Chrysene-d12	13.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
4	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87
5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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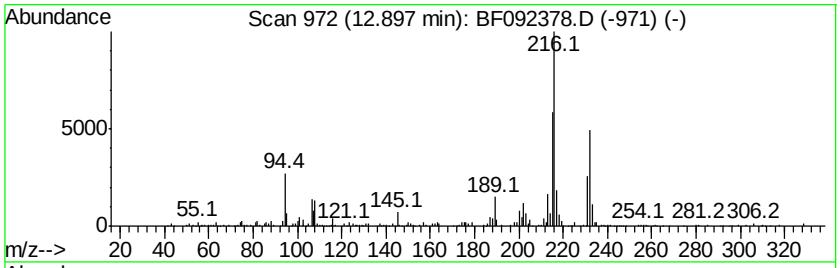
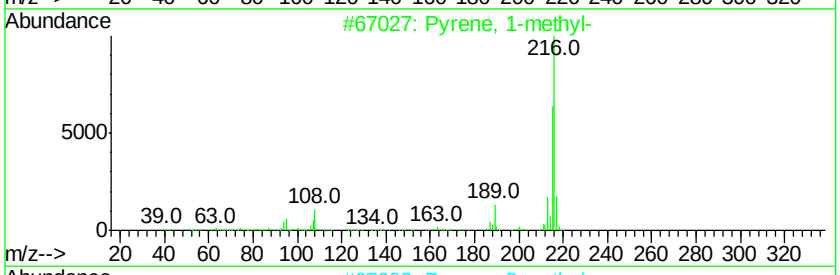
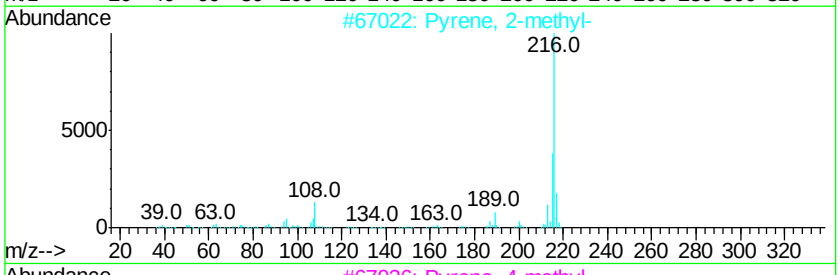
Peak Number 9 Pyrene, 1-methyl- Concentration Rank 7

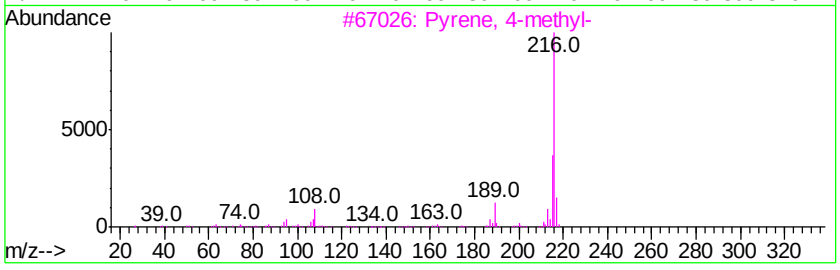
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.90	2.51 ng	279859	Chrysene-d12	13.66

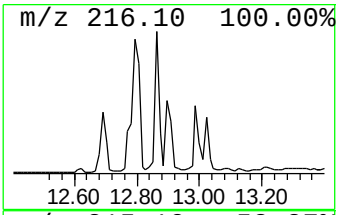
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	95
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
3	Pyrene, 4-methyl-	216	C17H12	003353-12-6	89
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	55

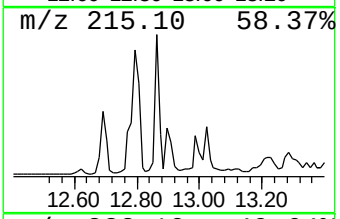


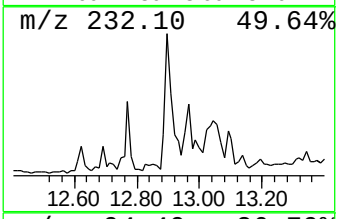


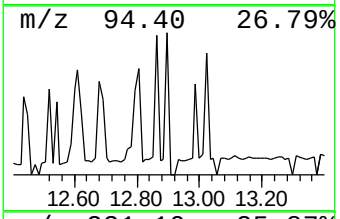


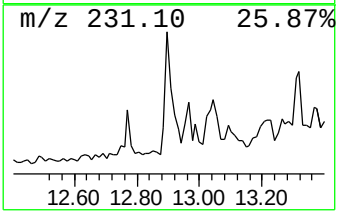












Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

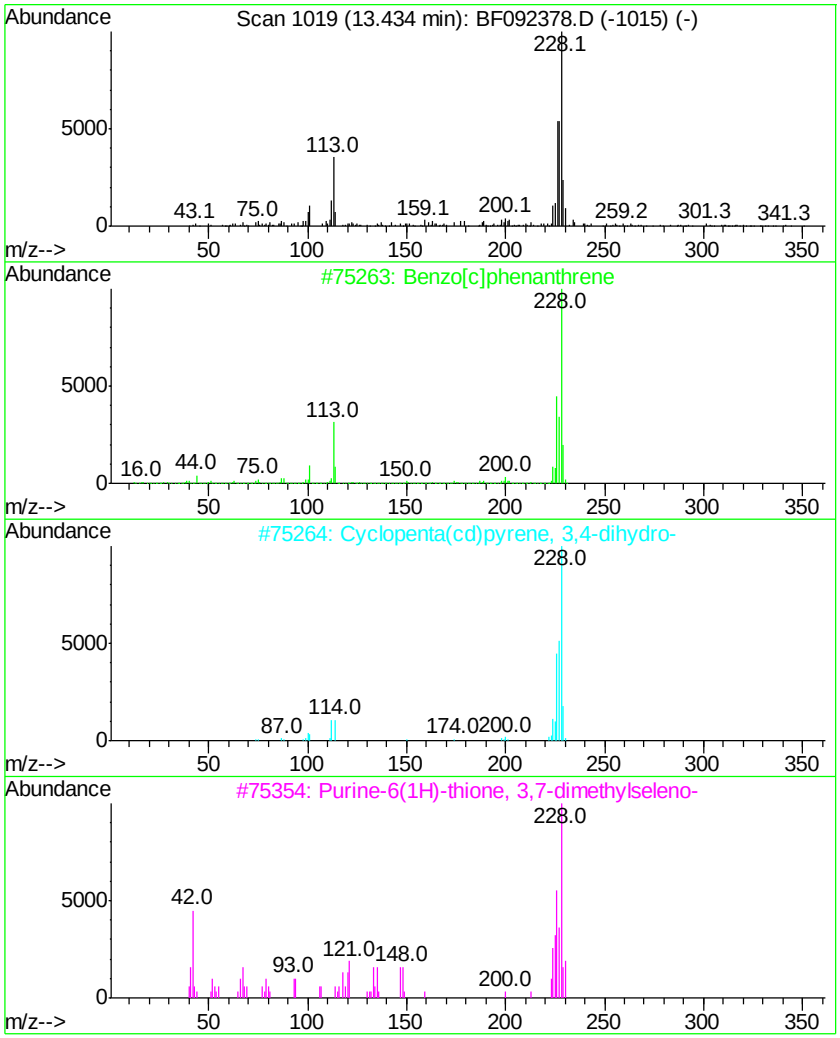
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

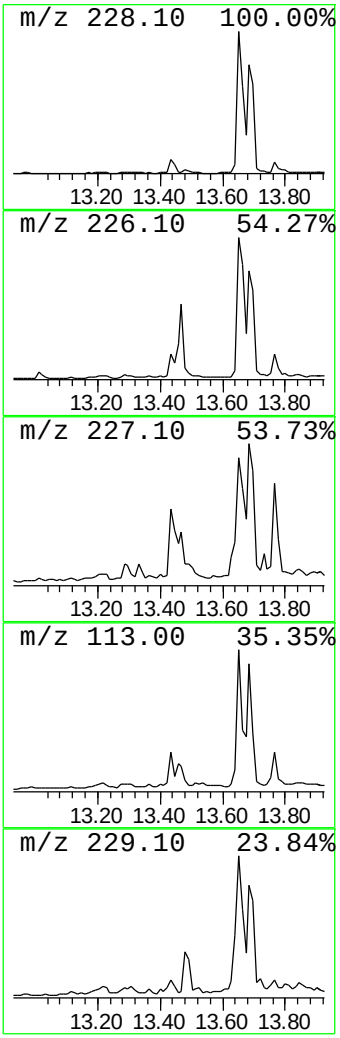
****

Peak Number 10 Benzo[c]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	3.21 ng	357071	Chrysene-d12	13.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]phenanthrene	228	C18H12	000195-19-7	60
2	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	53
3	Purine-6(1H)-thione, 3,7-dimethy...	228	C7H8N4Se	023663-58-3	52
4	Benz[a]anthracene	228	C18H12	000056-55-3	50
5	Triphenylene	228	C18H12	000217-59-4	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092378.D
Acq On : 20 Jan 2017 17:47
Operator : UM/SJ
Sample : I1265-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.62	38.5	ng	1574570	1	6.52	818669	20.0
unknown6.29	6.29	88.2	ng	3610580	1	6.52	818669	20.0
Tridecane	10.47	2.2	ng	219107	4	11.03	2013340	20.0
Tridecane, 1-iodo-	10.92	2.2	ng	223237	4	11.03	2013340	20.0
unknown12.38	12.38	2.5	ng	282782	5	13.66	2226780	20.0
11H-Benzo[b]fluorene	12.79	4.2	ng	465880	5	13.66	2226780	20.0
Pyrene, 1-methyl-	12.90	2.5	ng	279859	5	13.66	2226780	20.0
Benzo[c]phenanthrene	13.43	3.2	ng	357071	5	13.66	2226780	20.0