LSC Area Percent Report

Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
Data File : BF102441.D
Acq On : 25 Jan 2018 23:19
Operator : SJ/JU
Sample : J1289-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

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-BF012218.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	4.934	480	484	490	rBV	71432	105488	2.94%	0.315%
2	5.339	547	553	556	rBV	3022444	3384103	94.22%	10.100%
3	6.369	722	728	744	rBV	3078512	3591723	100.00%	10.720%
4	6.492	744	749	752	rBV	3723413	3484007	97.00%	10.399%
5	6.716	784	787	795	rBV	917214	761772	21.21%	2.274%
6	6.875	809	814	816	rBV	3009986	2637749	73.44%	7.873%
7	6.892	816	817	828	rVB	171472	130106	3.62%	0.388%
8	7.286	879	884	887	rBV	2276461	2192021	61.03%	6.542%
9	7.998	1001	1005	1007	rBV	1141120	999497	27.83%	2.983%
10	8.022	1007	1009	1016	rVB	469121	389953	10.86%	1.164%
11	8.716	1123	1127	1133	rBV	54697	59352	1.65%	0.177%
12	9.074	1183	1188	1198	rBV	3461163	3487478	97.10%	10.409%
13	9.469	1251	1255	1263	rVB	553800	482034	13.42%	1.439%
14	9.751	1299	1303	1307	rBV2	1106292	1000424	27.85%	2.986%
15	9.786	1307	1309	1314	rVB	76797	66911	1.86%	0.200%
16	9.957	1333	1338	1343	rBV	44430	49693	1.38%	0.148%
17	10.298	1393	1396	1401	rVB	69936	61256	1.71%	0.183%
18	10.463	1420	1424	1431	rVB2	53729	65427	1.82%	0.195%
19	10.545	1434	1438	1448	rBV	1656570	1589800	44.26%	4.745%
20	11.239	1552	1556	1558	rBV	918869	823228	22.92%	2.457%
21	11.263	1558	1560	1563	rVV	563216	445845	12.41%	1.331%
22	11.315	1566	1569	1572	rVB	93492	92742	2.58%	0.277%
23	11.474	1591	1596	1601	rBV2	65680	97893	2.73%	0.292%
24	11.739	1638	1641	1643	rBV	60348	53040	1.48%	0.158%
25	11.768	1643	1646	1649	rVV	79615	70951	1.98%	0.212%
26	11.851	1657	1660	1662	rBV	98823	99290	2.76%	0.296%
27	12.063	1694	1696	1699	rBV2	47117	37210	1.04%	0.111%
28	12.292	1732	1735	1738	rBV3	37863	38765	1.08%	0.116%
29	12.380	1748	1750	1756	rVB	45769	51095	1.42%	0.153%
30	12.451	1759	1762	1767	rVB	701662	645317	17.97%	1.926%
31	12.680	1795	1801	1805	rBV	604751	603959	16.82%	1.803%
32	12.827	1819	1826	1829	rBV	2543391	2374887	66.12%	7.088%
33	13.009	1854	1857	1859	rVB	62135	56209	1.56%	0.168%
34	13.074	1866	1868	1870	rBV	54838	40965	1.14%	0.122%

LSC Area Percent Report

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Acq On : 25 Jan 2018 23:19
Operator : SJ/JU
Sample : J1289-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

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-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.109	1870	1874	1877	rBV	52122	58217	1.62%	0.174%
36	13.233	1893	1895	1899	rBV2	35150	42287	1.18%	0.126%
37	13.515	1941	1943	1948	rVB	52562	56984	1.59%	0.170%
38	13.627	1959	1962	1964	rBV	58192	53958	1.50%	0.161%
39	13.715	1974	1977	1982	rVB2	309635	329892	9.18%	0.985%
40	13.880	2000	2005	2007	rBV2	849597	997771	27.78%	2.978%
41	13.904	2007	2009	2018	rVB	314805	271579	7.56%	0.811%
42	13.968	2018	2020	2025	rBV2	88058	135571	3.77%	0.405%
43	14.898	2174	2178	2181	rBV	259541	367656	10.24%	1.097%
44	15.186	2224	2227	2233	rVV	140178	167738	4.67%	0.501%
45	15.245	2234	2237	2243	rVV	202980	239954	6.68%	0.716%
46	15.309	2244	2248	2259	rVB	487354	712763	19.84%	2.127%

Sum of corrected areas: 33504560

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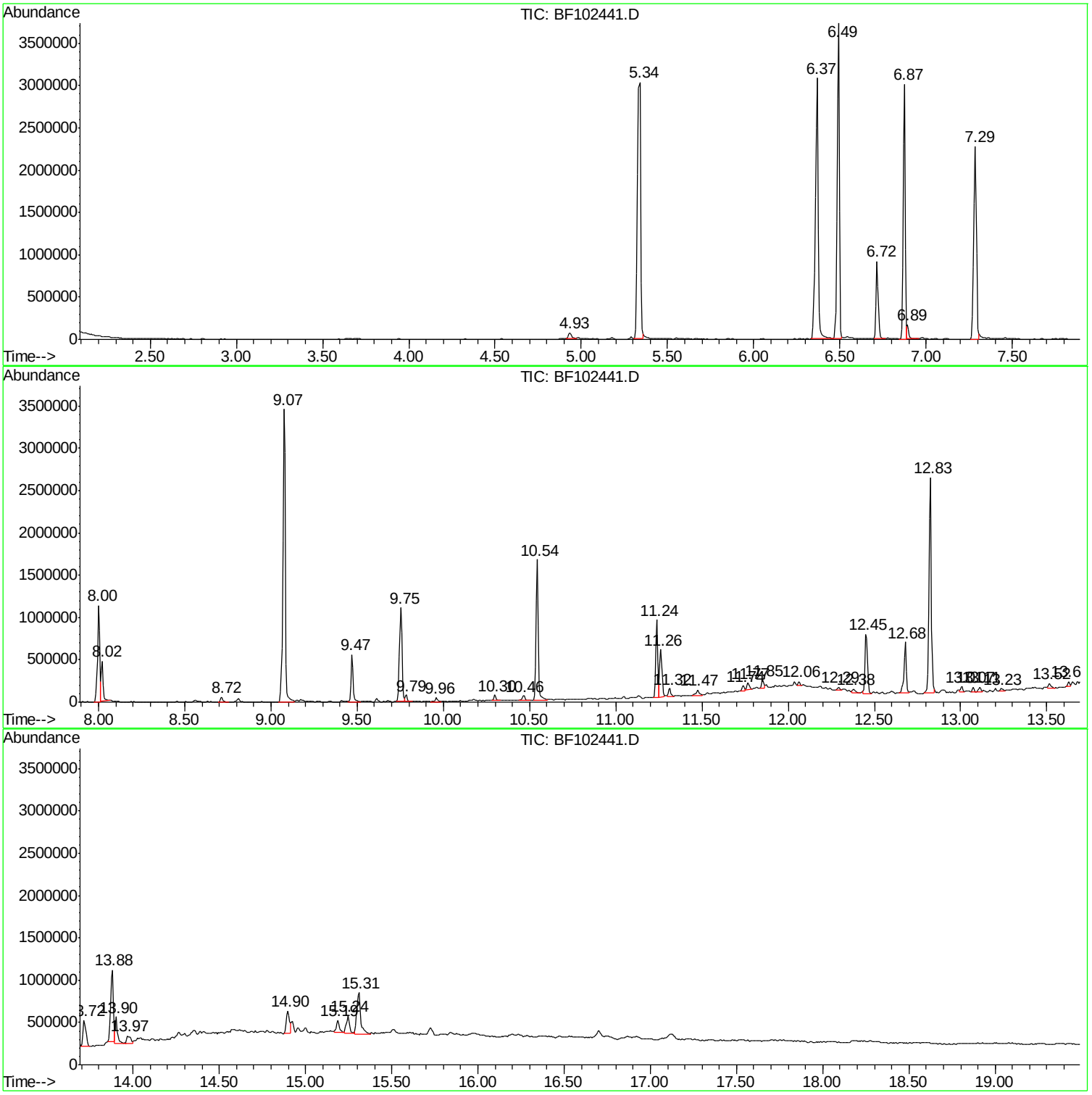
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
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Acq On : 25 Jan 2018 23:19
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Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

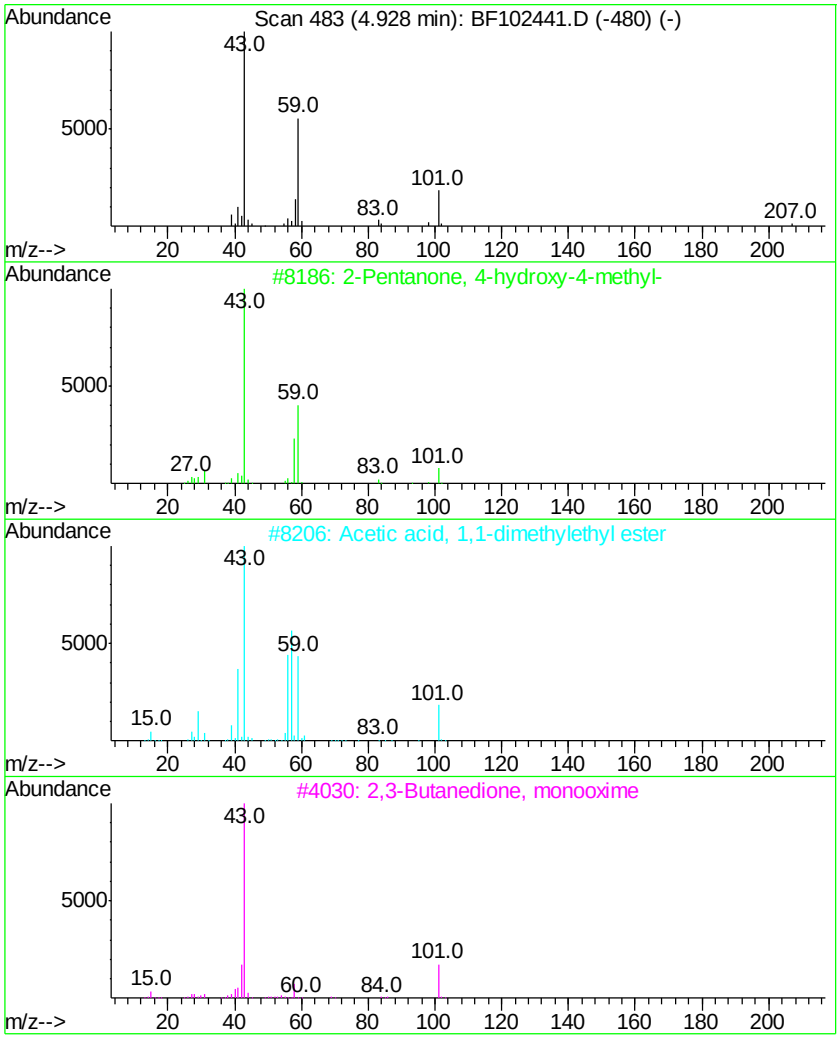
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

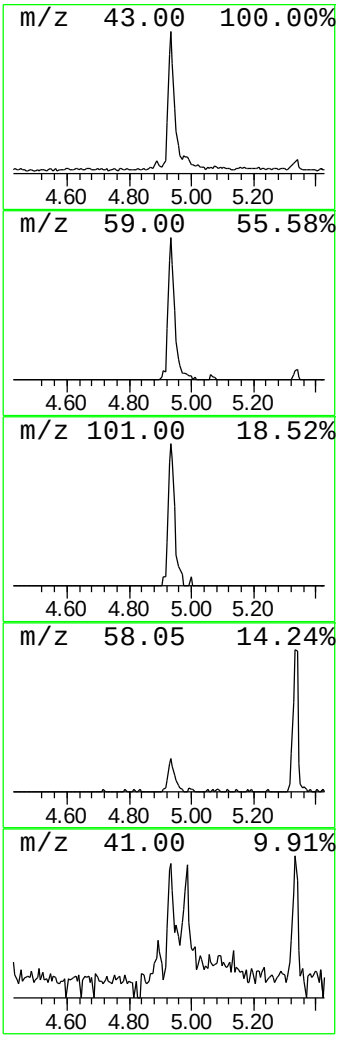
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.77 ng	105488	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane	58	C4H10	000106-97-8	9





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Operator : SJ/JU
Sample : J1289-07
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-11-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

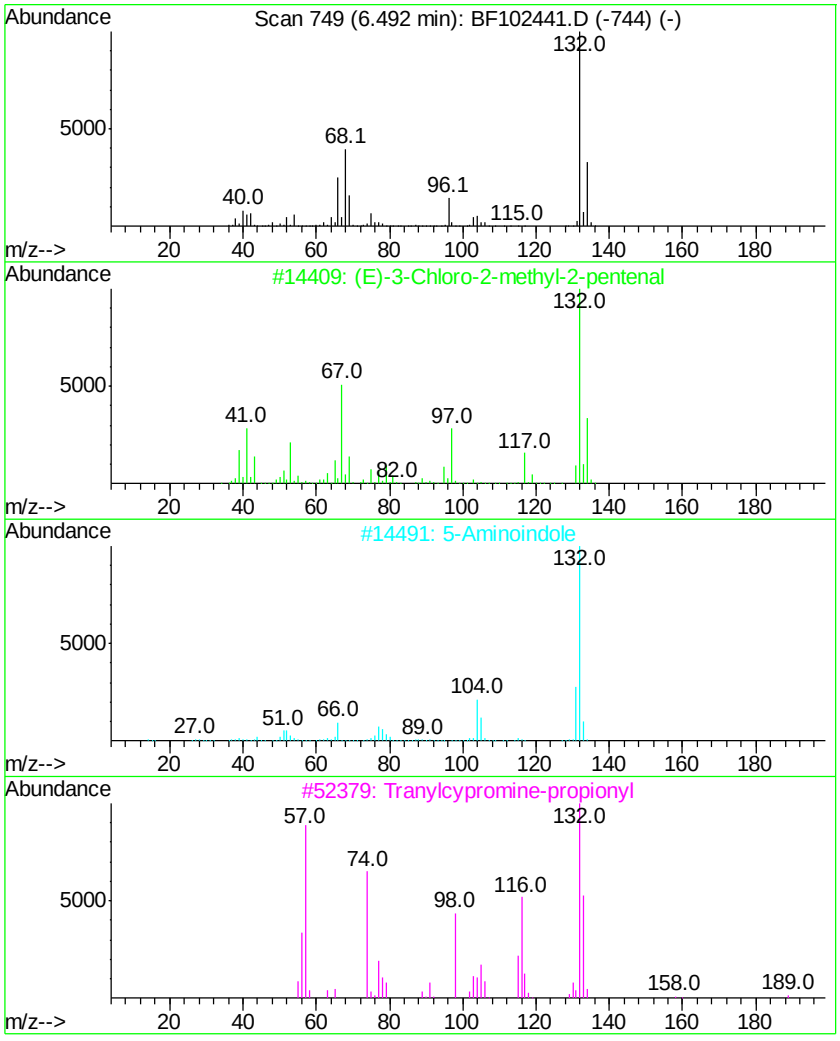
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

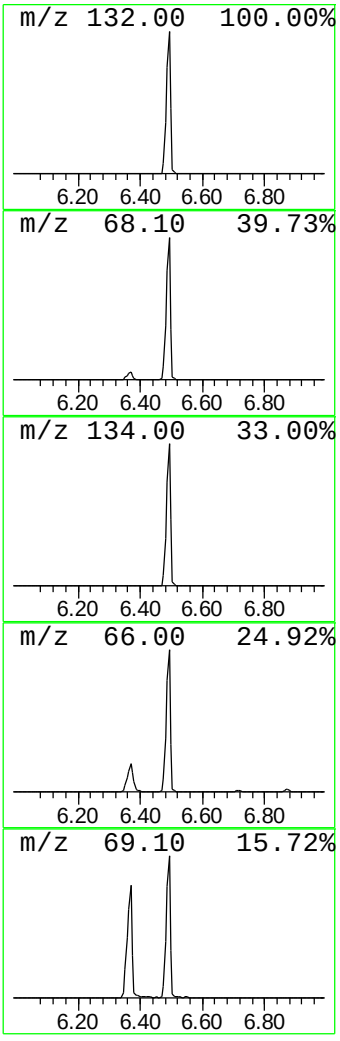
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	91.47 ng	3484010	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
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Acq On : 25 Jan 2018 23:19
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Sample : J1289-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

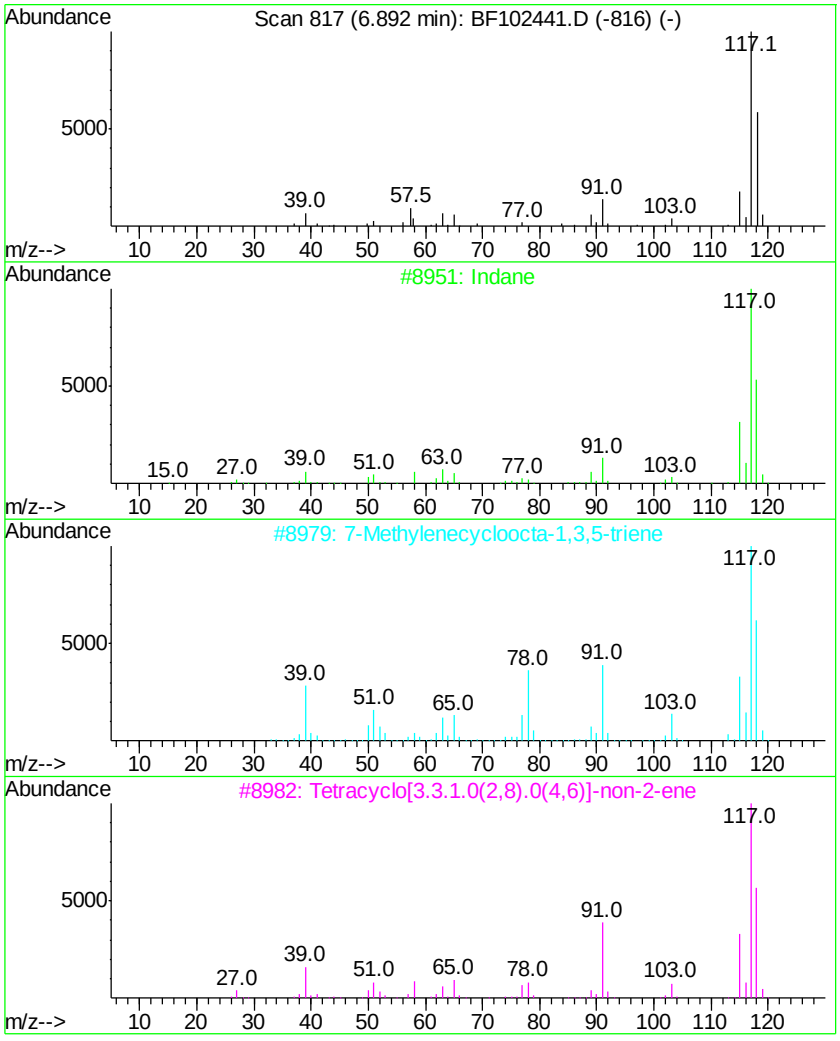
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

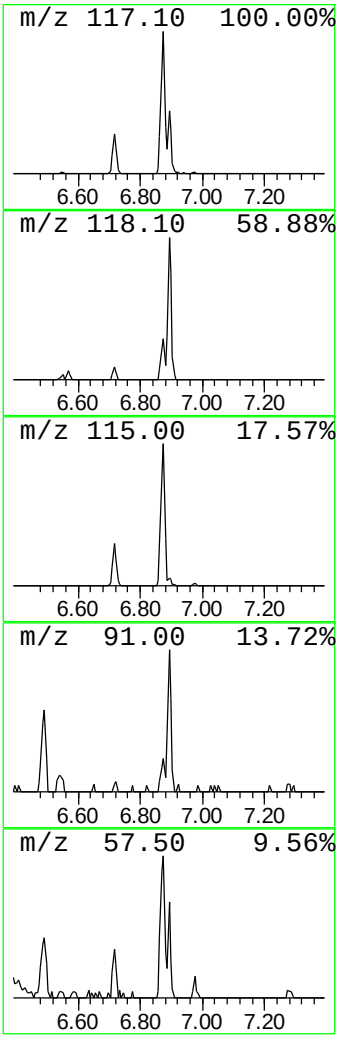
****

Peak Number 4 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.89	3.42 ng	130106	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	83
2	7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	64
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	59
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	47





Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
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Sample : J1289-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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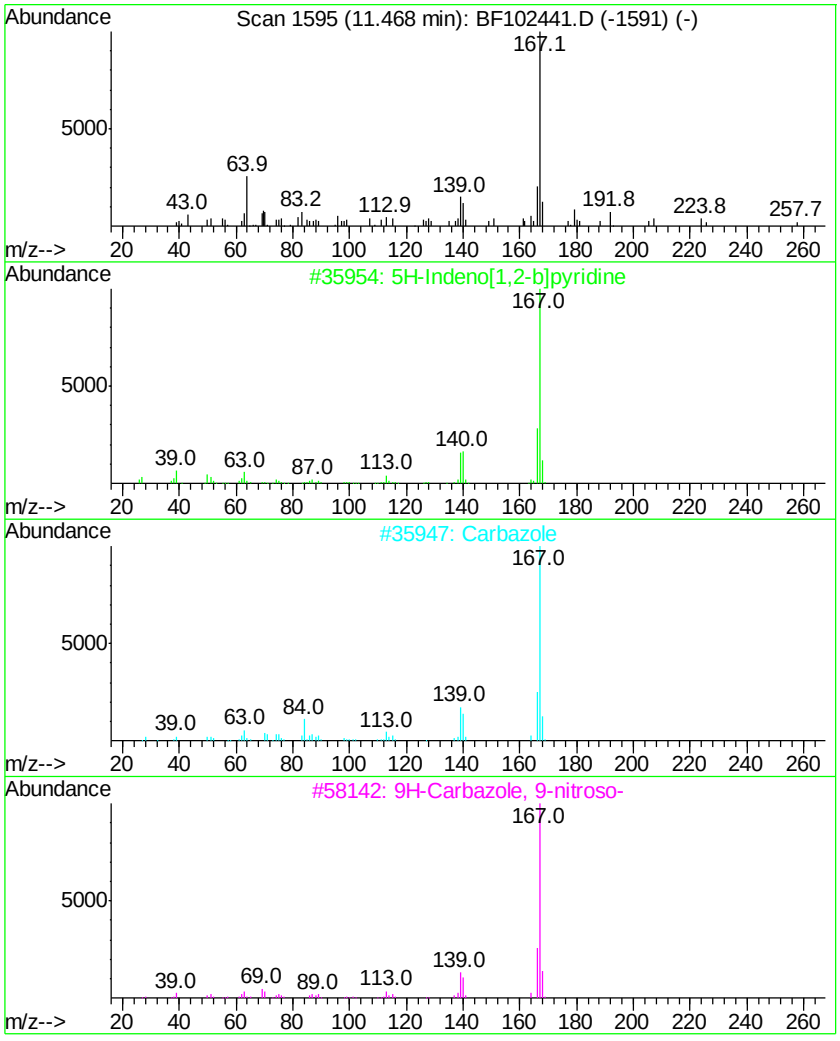
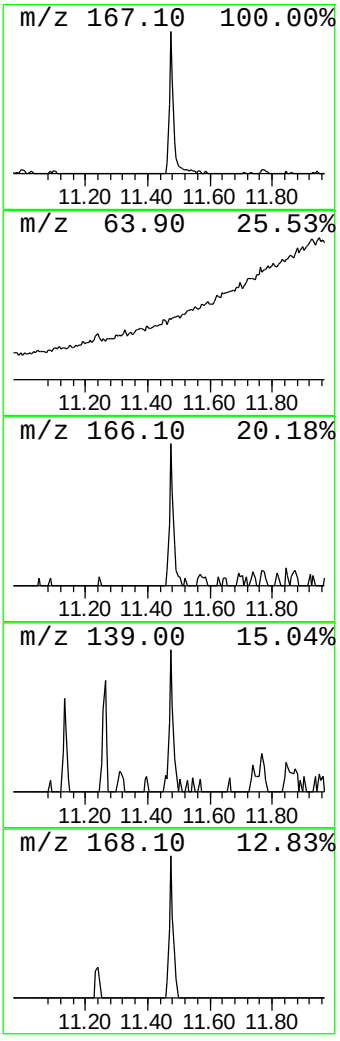
Peak Number 5 5H-Indeno[1,2-b]pyridine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	2.38 ng	97893	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	94
2	Carbazole	167	C12H9N	000086-74-8	90
3	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	87
4	9H-Carbazole-9-methanol	197	C13H11NO	002409-36-1	86
5	2-Azafluorene	167	C12H9N	000244-40-6	72





Data Path : U:\HPCHEM1\BNA F\DATA\BF012518\
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

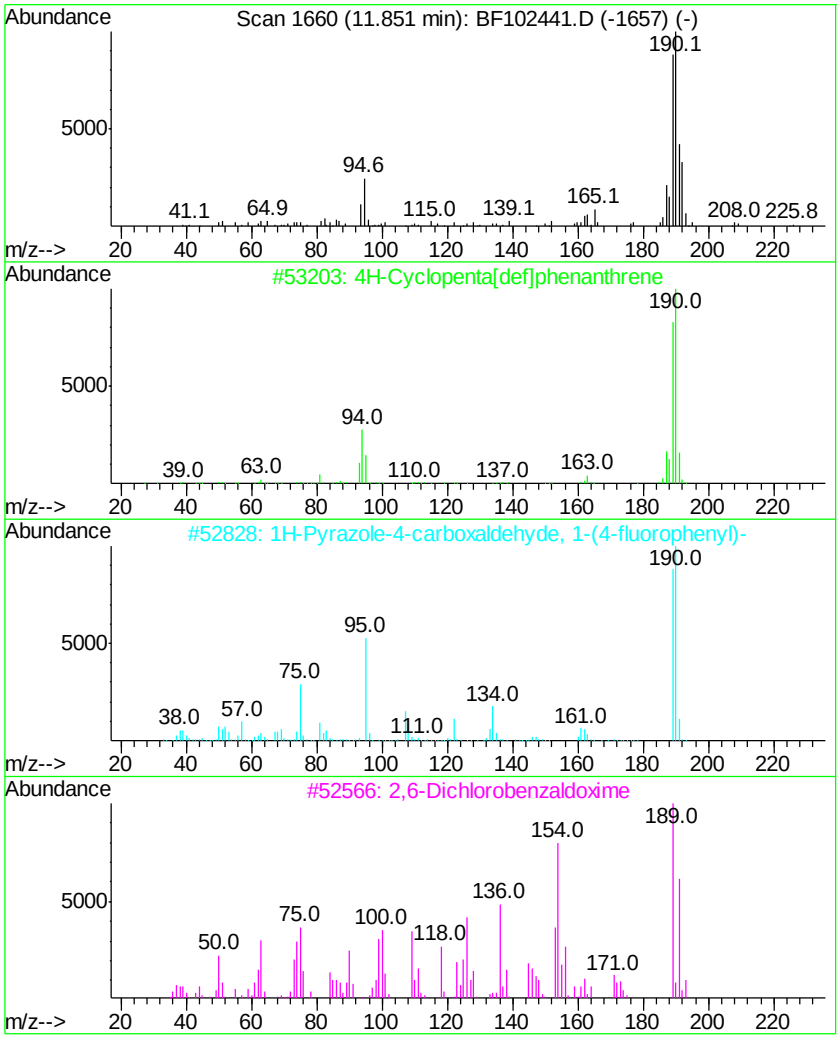
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

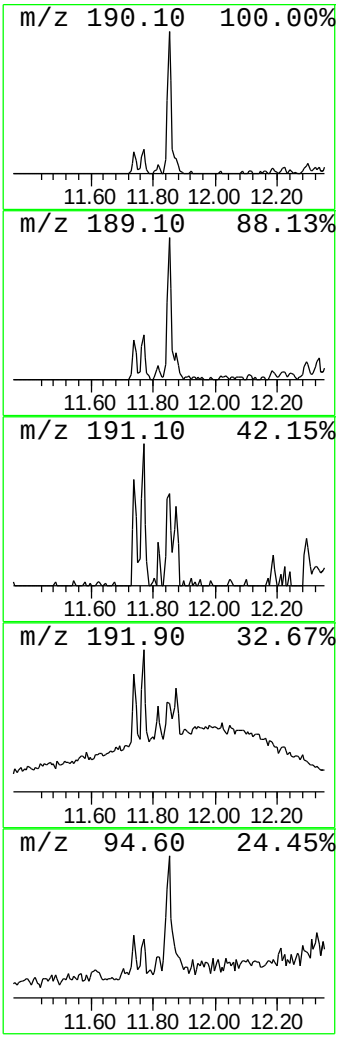
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.41 ng	99290	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	47
3	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	46
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	38
5	Methyl diselenide	190	C2H6Se2	007101-31-7	38





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Misc :
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Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

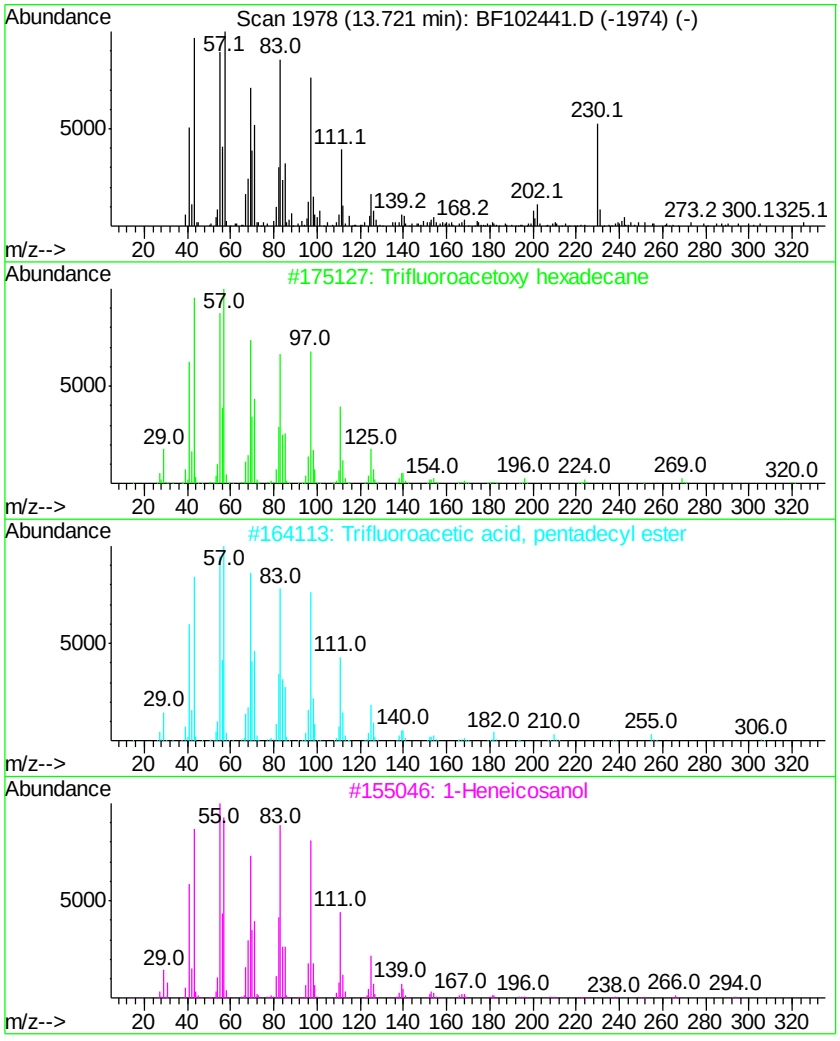
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

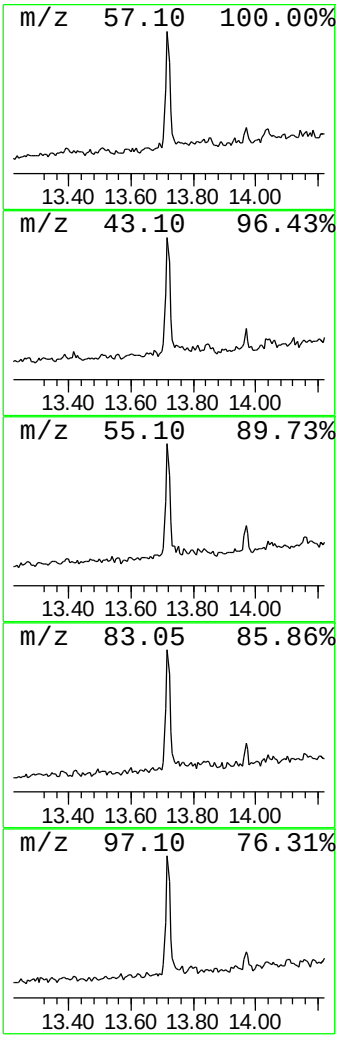
****

Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	6.61 ng	329892	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	Octacosanol	410	C28H58O	000557-61-9	91
5	1-Nonadecene	266	C19H38	018435-45-5	91





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Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

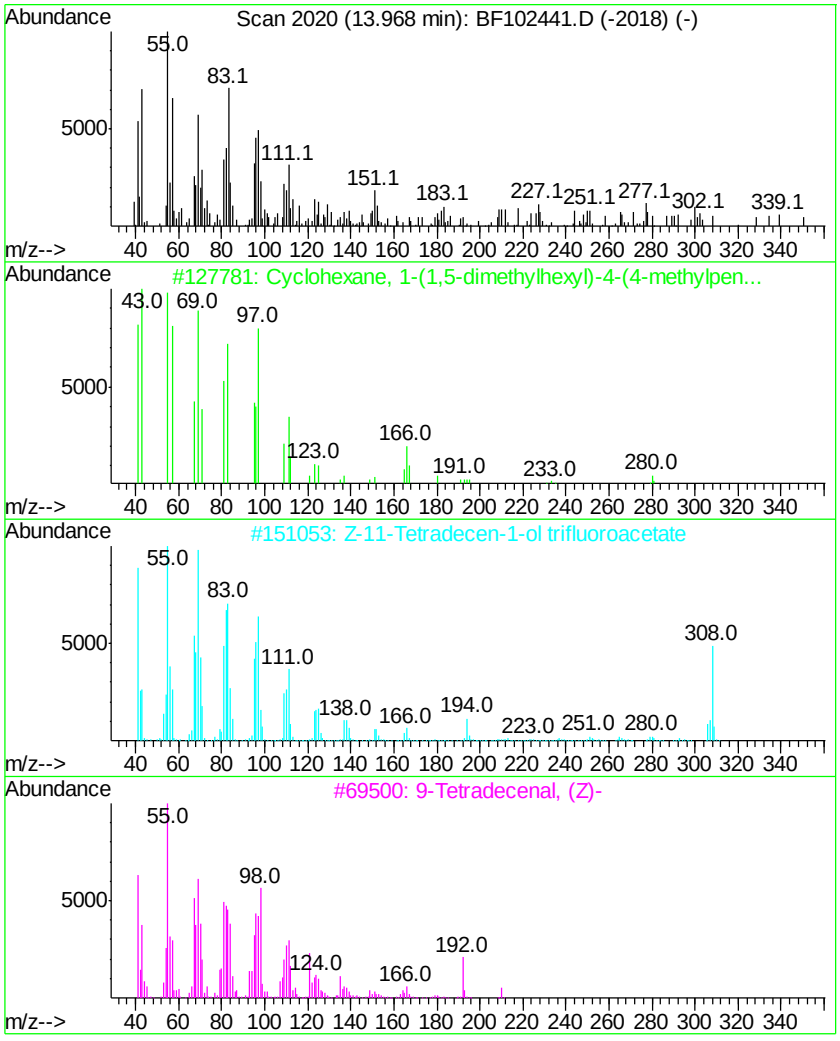
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

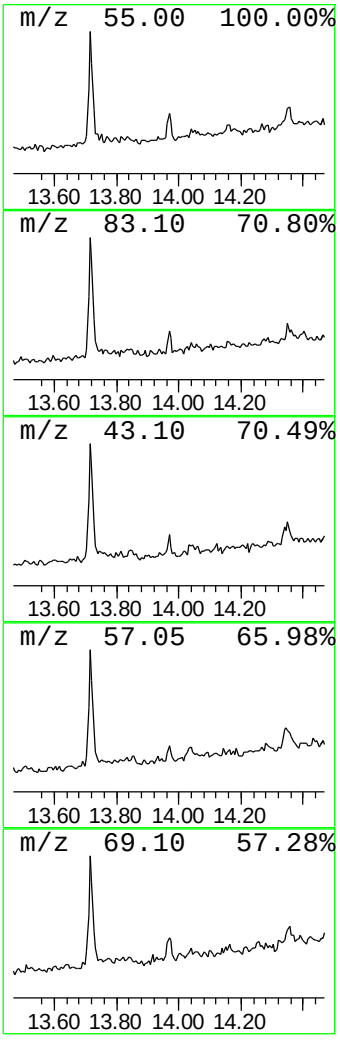
****

Peak Number 8 Cyclohexane, 1-(1,5-dimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.72 ng	135571	Chrysene-d12	13.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-(1,5-dimethylhexy...	280	C20H40	056009-20-2	90
2	Z-11-Tetradecen-1-ol trifluoroac...	308	C16H27F3O2	1000131-33-7	86
3	9-Tetradecenal, (Z)-	210	C14H26O	053939-27-8	76
4	Cyclohexadecane	224	C16H32	000295-65-8	70
5	Cyclopentadecane	210	C15H30	000295-48-7	55





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Data File : BF102441.D
Acq On : 25 Jan 2018 23:19
Operator : SJ/JU
Sample : J1289-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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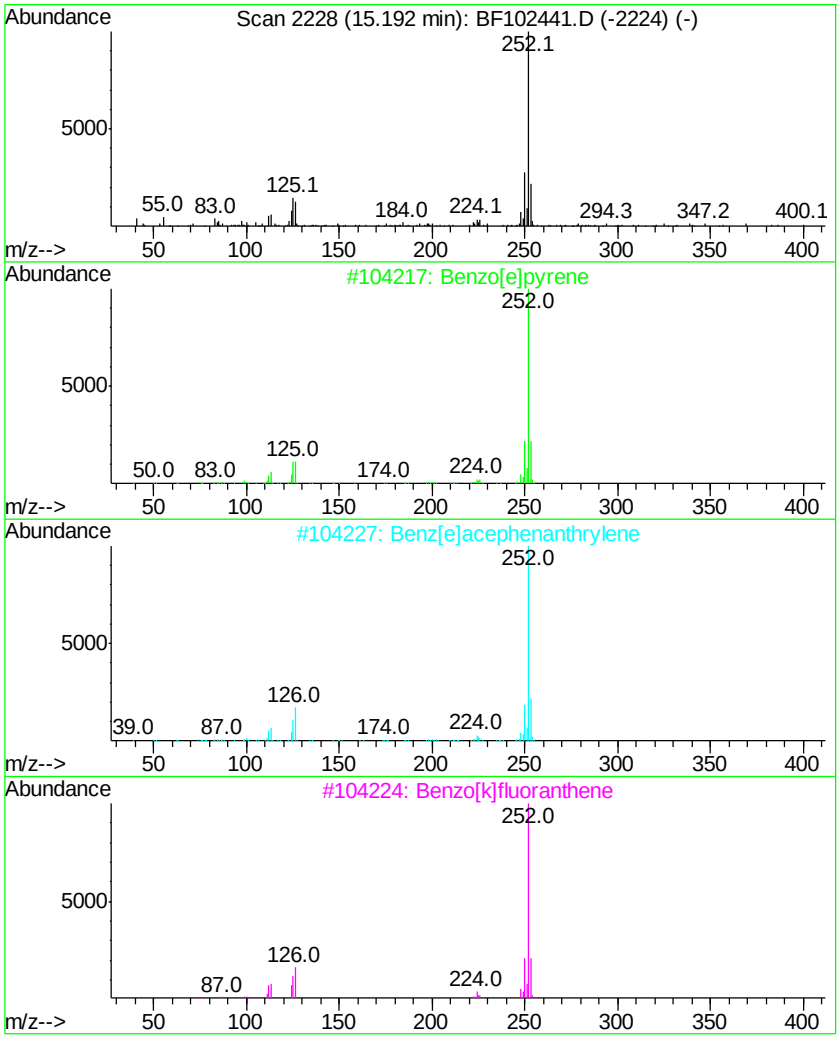
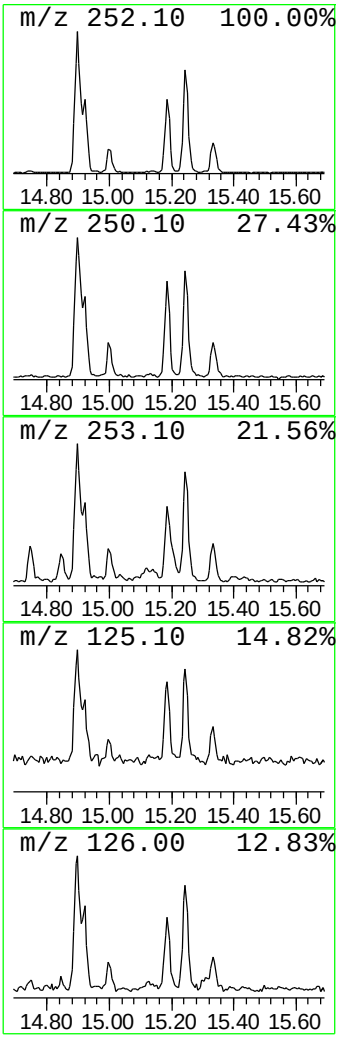
Peak Number 9 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	4.71 ng	167738	Perylene-d12	15.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	89
5	Perylene	252	C20H12	000198-55-0	81





Tentatively Identified Compound (LSC) summary

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Data File : BF102441.D
Acq On : 25 Jan 2018 23:19
Operator : SJ/JU
Sample : J1289-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-11-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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...	4.93	2.8	ng	105488	1	6.72	761772	20.0
unknown6.49	6.49	91.5	ng	3484010	1	6.72	761772	20.0
Indane	6.89	3.4	ng	130106	1	6.72	761772	20.0
5H-Indeno[1,2-b]p...	11.47	2.4	ng	97893	4	11.24	823228	20.0
4H-Cyclopenta[def...	11.85	2.4	ng	99290	4	11.24	823228	20.0
Trifluoroacetoxy ...	13.72	6.6	ng	329892	5	13.88	997771	20.0
Cyclohexane, 1-(1...	13.97	2.7	ng	135571	5	13.88	997771	20.0
Benzo[e]pyrene	15.19	4.7	ng	167738	6	15.31	712763	20.0