LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118052.D
Acq On : 27 Nov 2019 20:28
Operator : JU
Sample : K5977-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-2-5-COMP-B5

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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	2.152	5	11	18	rVB	543504	676737	21.13%	2.179%
2	5.093	506	511	524	rVB	405418	478068	14.93%	1.540%
3	5.498	576	580	583	rBV	2697114	2431921	75.92%	7.832%
4	6.510	747	752	755	rBV	2741571	2594474	81.00%	8.355%
5	6.651	772	776	779	rBV	3144648	2762146	86.23%	8.895%
6	6.881	812	815	819	rBV	974758	842469	26.30%	2.713%
7	7.040	838	842	845	rBV	2678784	2179828	68.05%	7.020%
8	7.445	906	911	914	rBV	1863096	1624518	50.72%	5.232%
9	8.169	1030	1034	1037	rBV	1185579	1085815	33.90%	3.497%
10	8.192	1037	1038	1051	rVB	51733	42089	1.31%	0.136%
11	9.251	1213	1218	1221	rBV	3979233	3203112	100.00%	10.315%
12	9.645	1281	1285	1288	rVB	576006	481486	15.03%	1.551%
13	9.933	1330	1334	1337	rBV	1575666	1238232	38.66%	3.988%
14	9.969	1337	1340	1343	rVB	57329	52279	1.63%	0.168%
15	10.728	1465	1469	1472	rBV	2240413	1887573	58.93%	6.079%
16	11.427	1584	1588	1590	rBV	1401233	1127260	35.19%	3.630%
17	11.451	1590	1592	1595	rVV	506073	390192	12.18%	1.257%
18	11.504	1595	1601	1603	rVB2	80873	106725	3.33%	0.344%
19	11.657	1621	1627	1630	rBV2	40694	54256	1.69%	0.175%
20	11.951	1674	1677	1684	rVB2	221991	274182	8.56%	0.883%
21	12.045	1689	1693	1695	rBV	67343	76334	2.38%	0.246%
22	12.480	1761	1767	1770	rBV	31238	42925	1.34%	0.138%
23	12.569	1779	1782	1787	rVB2	37192	40933	1.28%	0.132%
24	12.645	1791	1795	1800	rBV	575859	469378	14.65%	1.512%
25	12.739	1808	1811	1814	rBV2	64640	72832	2.27%	0.235%
26	12.874	1828	1834	1839	rBV	445661	491633	15.35%	1.583%
27	12.927	1839	1843	1848	rVB2	26713	38171	1.19%	0.123%
28	13.016	1854	1858	1862	rBV	2857365	2539052	79.27%	8.177%
29	13.098	1867	1872	1875	rBV2	34919	56608	1.77%	0.182%
30	13.204	1884	1890	1893	rBV2	44341	66957	2.09%	0.216%
31	13.310	1904	1908	1911	rBV2	49624	51557	1.61%	0.166%
32	13.716	1974	1977	1981	rVB	43752	49937	1.56%	0.161%
33	13.827	1992	1996	1998	rBV2	41055	53272	1.66%	0.172%
34	13.916	2008	2011	2020	rVB3	184523	261839	8.17%	0.843%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118052.D
Acq On : 27 Nov 2019 20:28
Operator : JU
Sample : K5977-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-2-5-COMP-B5

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.080	2031	2039	2042	rBV2	1131298	1240370	38.72%	3.995%
36	14.104	2042	2043	2048	rVB	202653	143450	4.48%	0.462%
37	14.463	2102	2104	2107	rVB	50566	44760	1.40%	0.144%
38	14.539	2115	2117	2123	rBV3	51240	66510	2.08%	0.214%
39	14.857	2169	2171	2176	rVB	69028	63635	1.99%	0.205%
40	14.933	2182	2184	2187	rBV	40610	37876	1.18%	0.122%
41	15.139	2215	2219	2222	rBV	159347	249183	7.78%	0.802%
42	15.210	2228	2231	2234	rVB2	64872	74418	2.32%	0.240%
43	15.451	2269	2272	2279	rVB	103429	130353	4.07%	0.420%
44	15.515	2279	2283	2287	rVV	129245	157147	4.91%	0.506%
45	15.580	2289	2294	2304	rBV	694408	999323	31.20%	3.218%

Sum of corrected areas: 31051815

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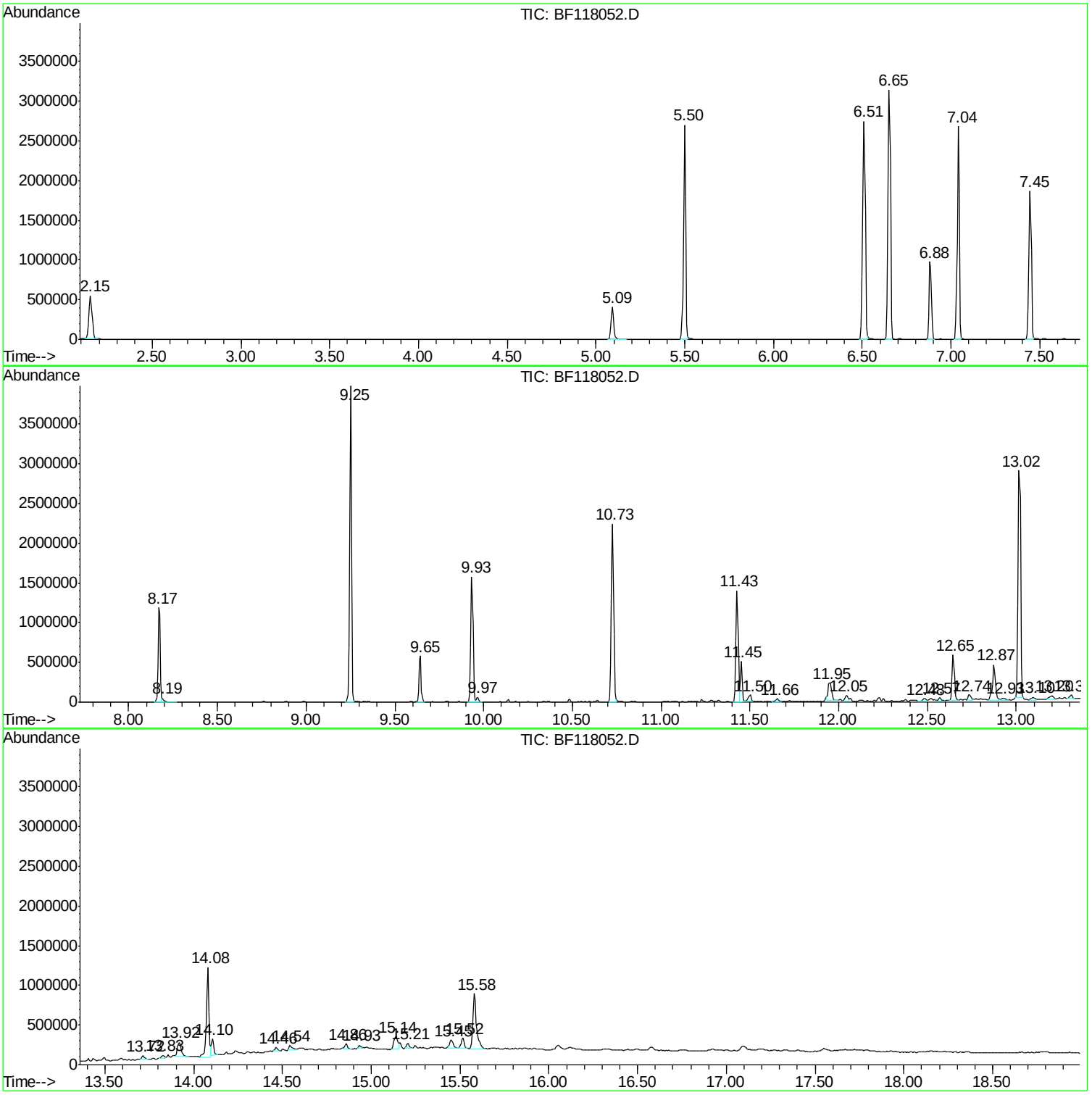
Instrument :
BNA_F
ClientSampleId :
WS-112119-2-5-COMP-B5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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Data File : BF118052.D
Acq On : 27 Nov 2019 20:28
Operator : JU
Sample : K5977-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-2-5-COMP-B5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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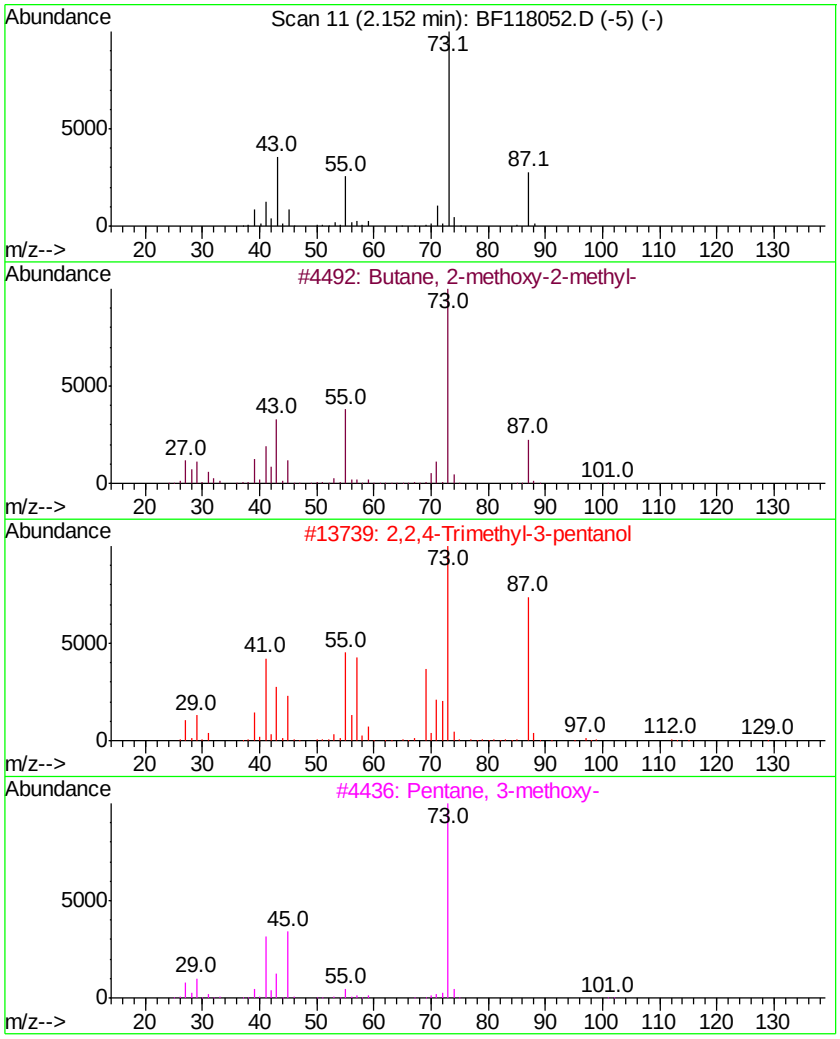
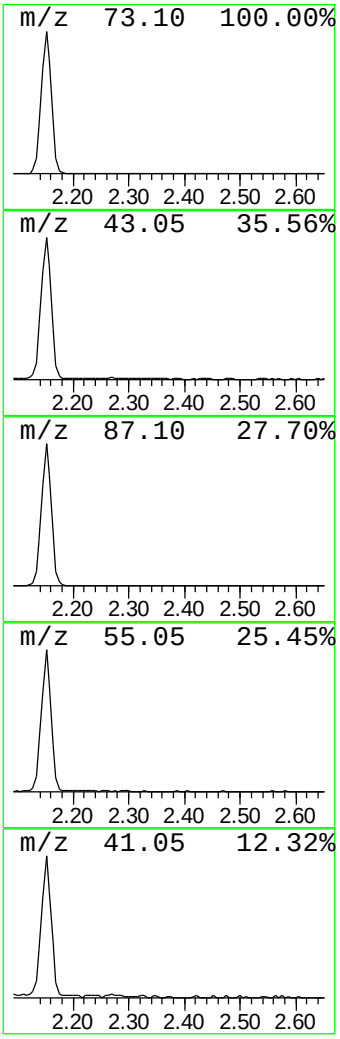
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	16.07 ng	676737	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Operator : JU
Sample : K5977-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-2-5-COMP-B5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

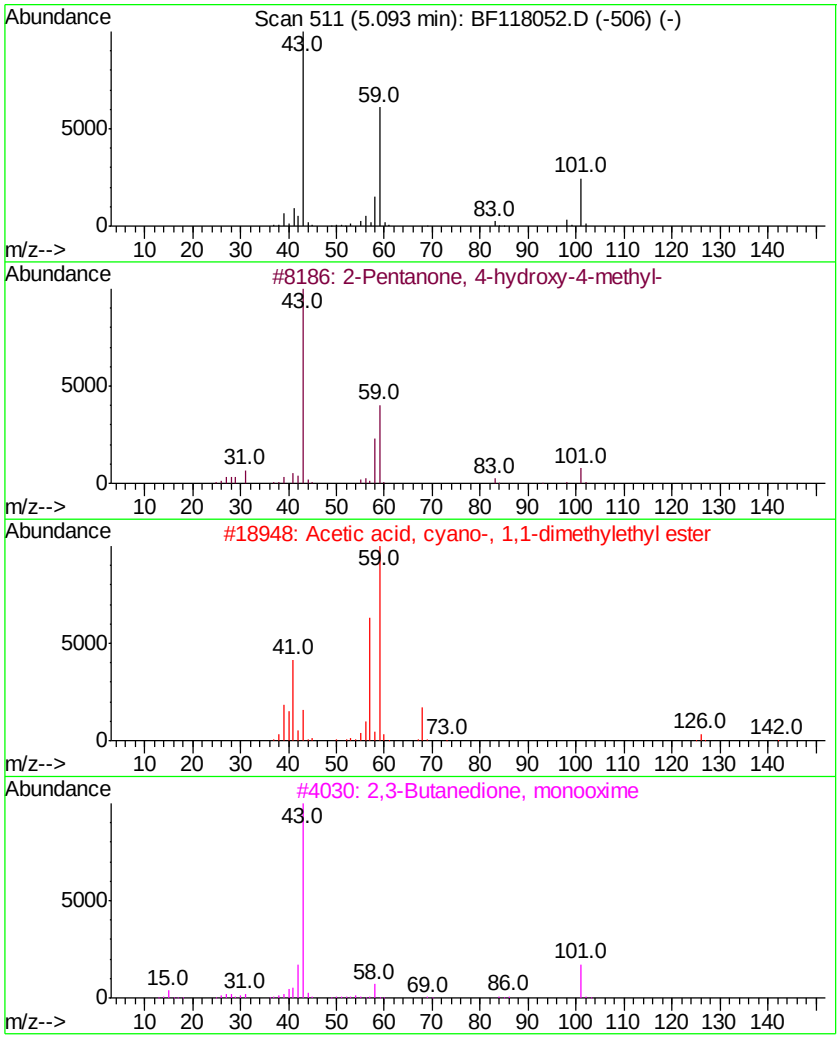
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

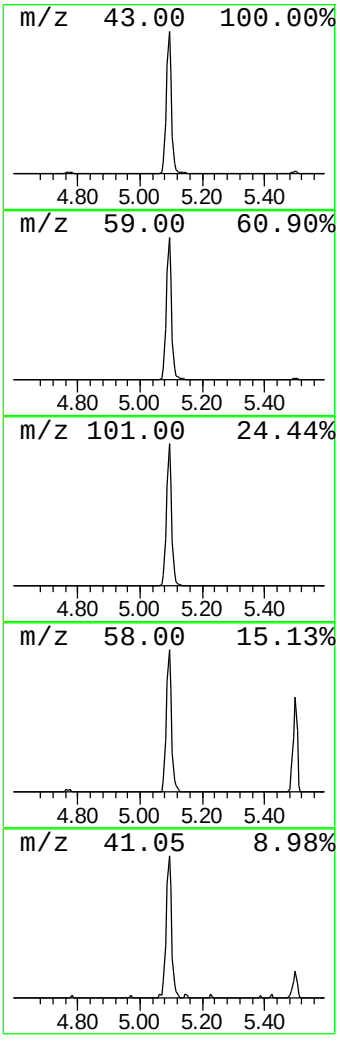
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	11.35 ng	478068	1,4-Dichlorobenzene-d4	6.89

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Data File : BF118052.D
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Operator : JU
Sample : K5977-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-2-5-COMP-B5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

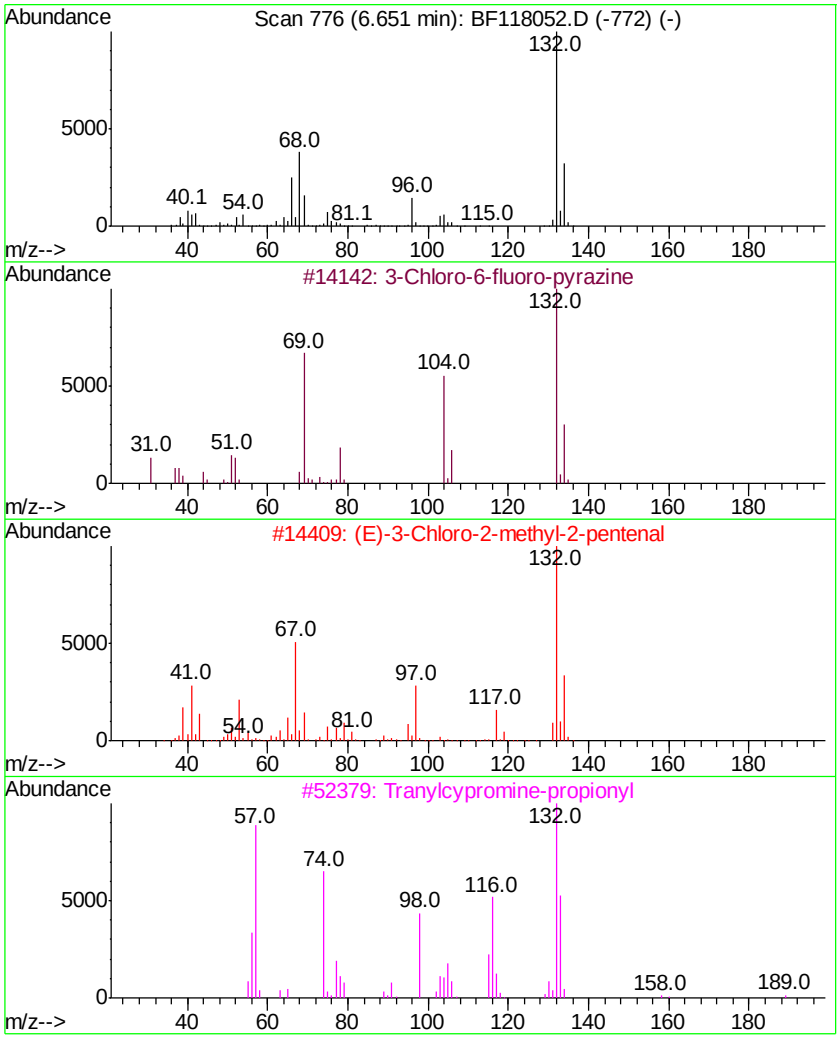
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

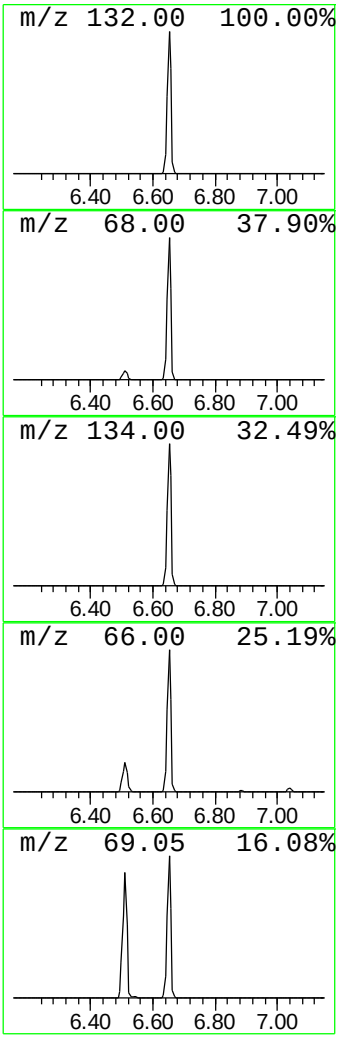
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	65.57 ng	2762150	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Library Search Compound Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-2-5-COMP-B5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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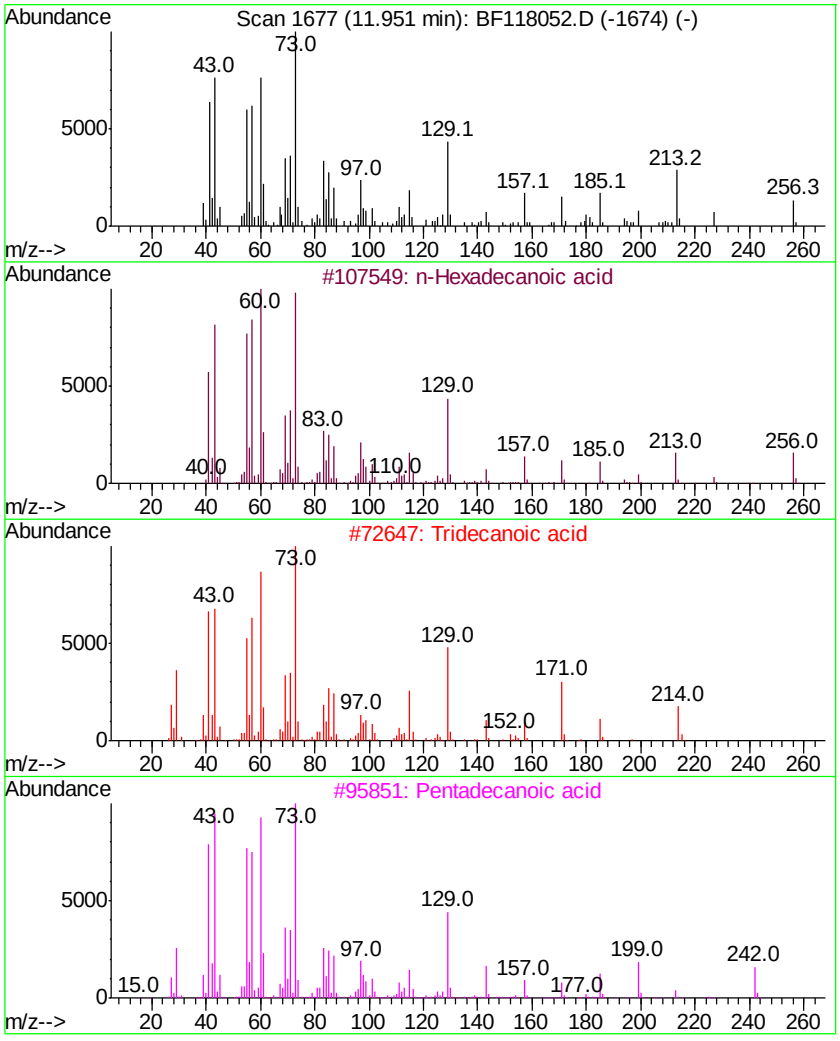
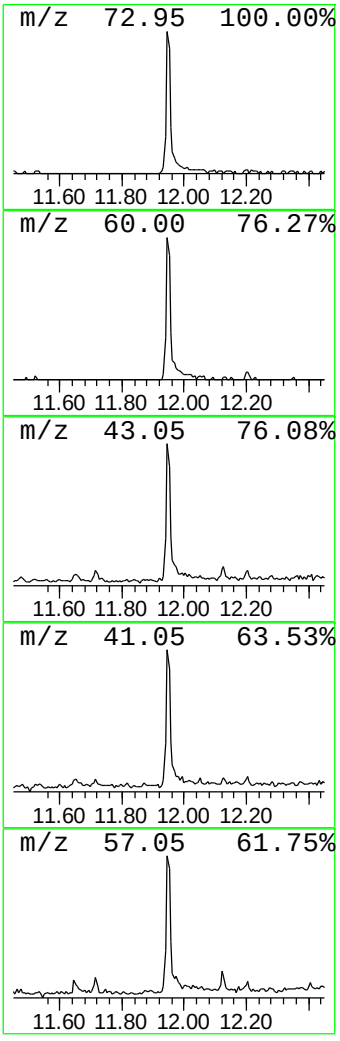
Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	4.86 ng	274182	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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Sample : K5977-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-2-5-COMP-B5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

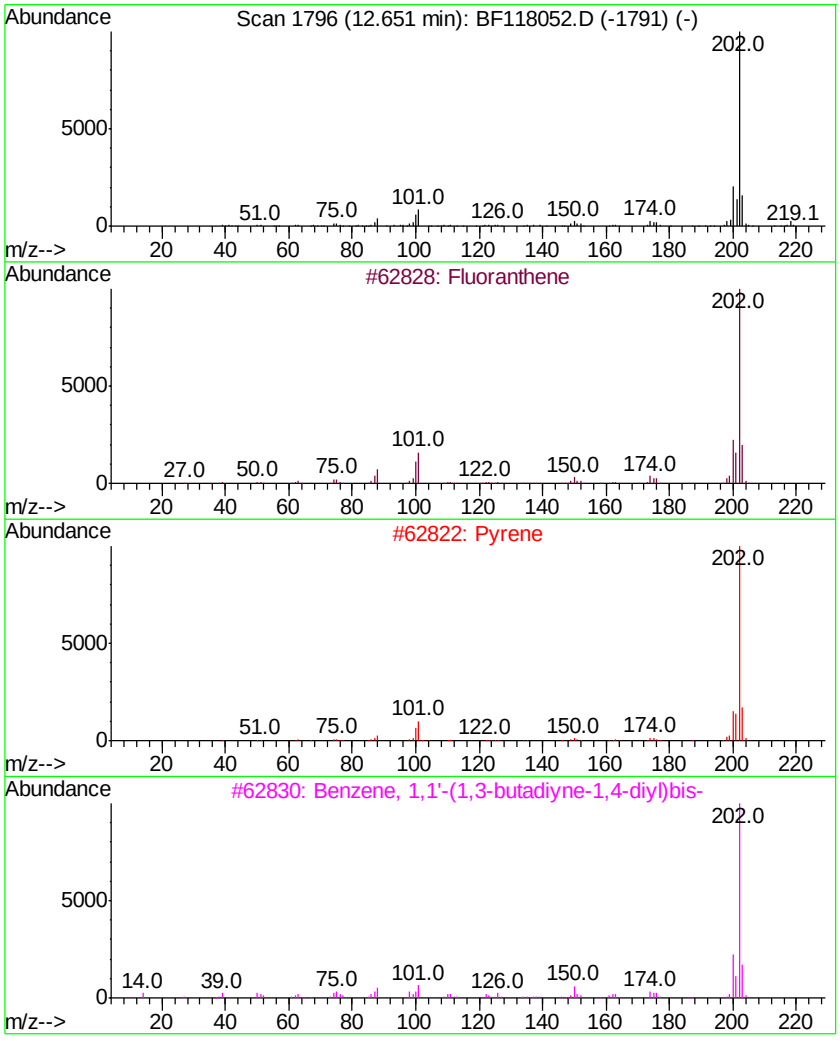
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

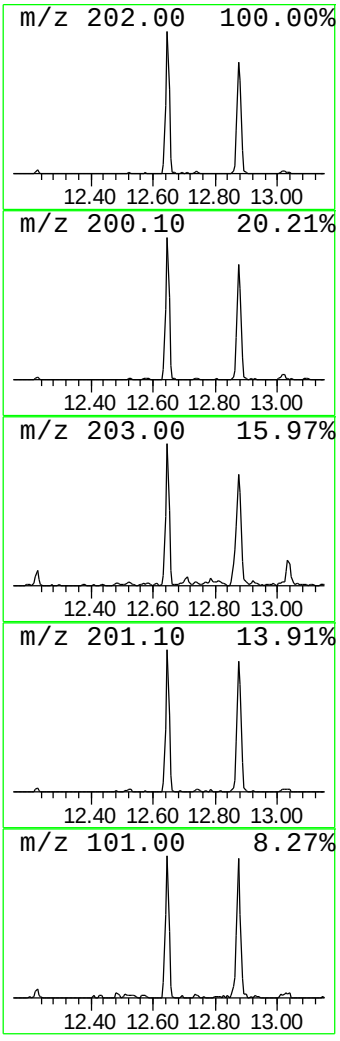
****

Peak Number 6 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	8.33 ng	469378	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	96
2	Pyrene	202	C16H10	000129-00-0	94
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
4	Pyrimidine, 2-phenyl-4-hydroxy-5...	202	C11H10N2O2	085386-21-6	9
5	4-Isothiazolecarbonitrile, 3,5-b...	202	C6H6N2S3	004886-13-9	9





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Instrument : BNA_F
ClientSampleId : WS-112119-2-5-COMP-B5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

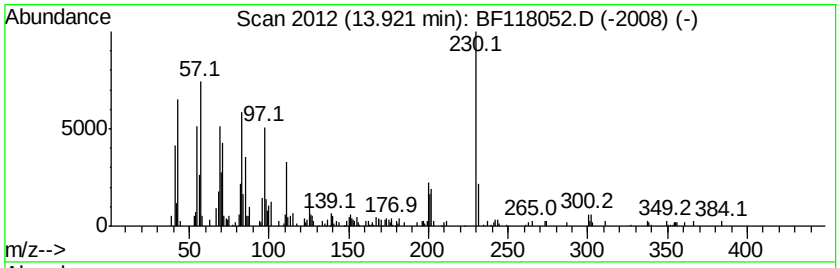
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

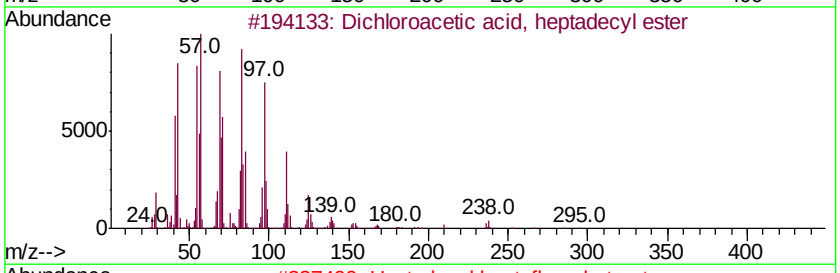
****

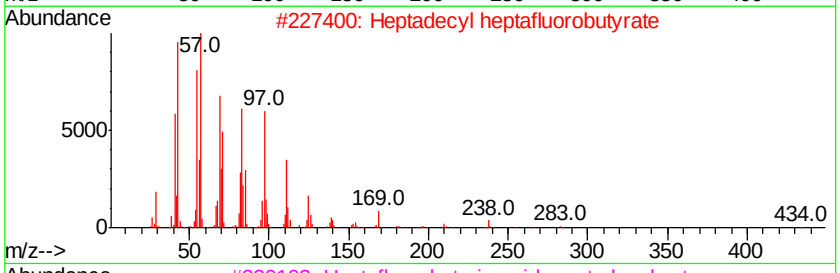
Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 7

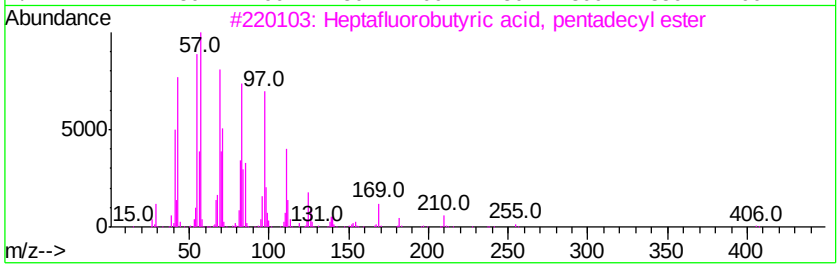
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	4.22 ng	261839	Chrysene-d12	14.08

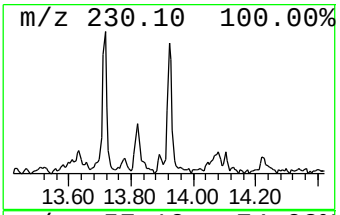
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	83
5	Behenic alcohol	326	C22H46O	000661-19-8	76

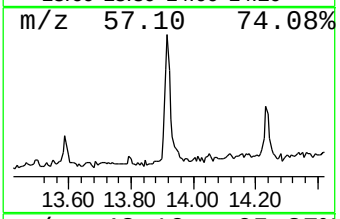


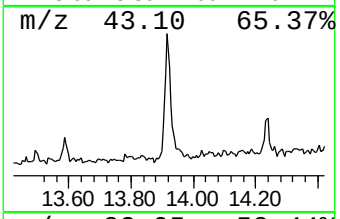


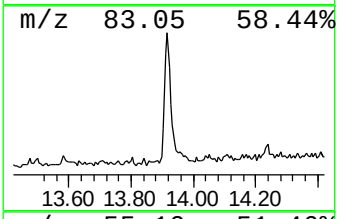


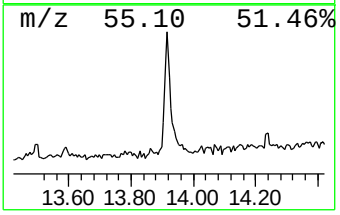












Library Search Compound Report

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Data File : BF118052.D
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Sample : K5977-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-112119-2-5-COMP-B5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

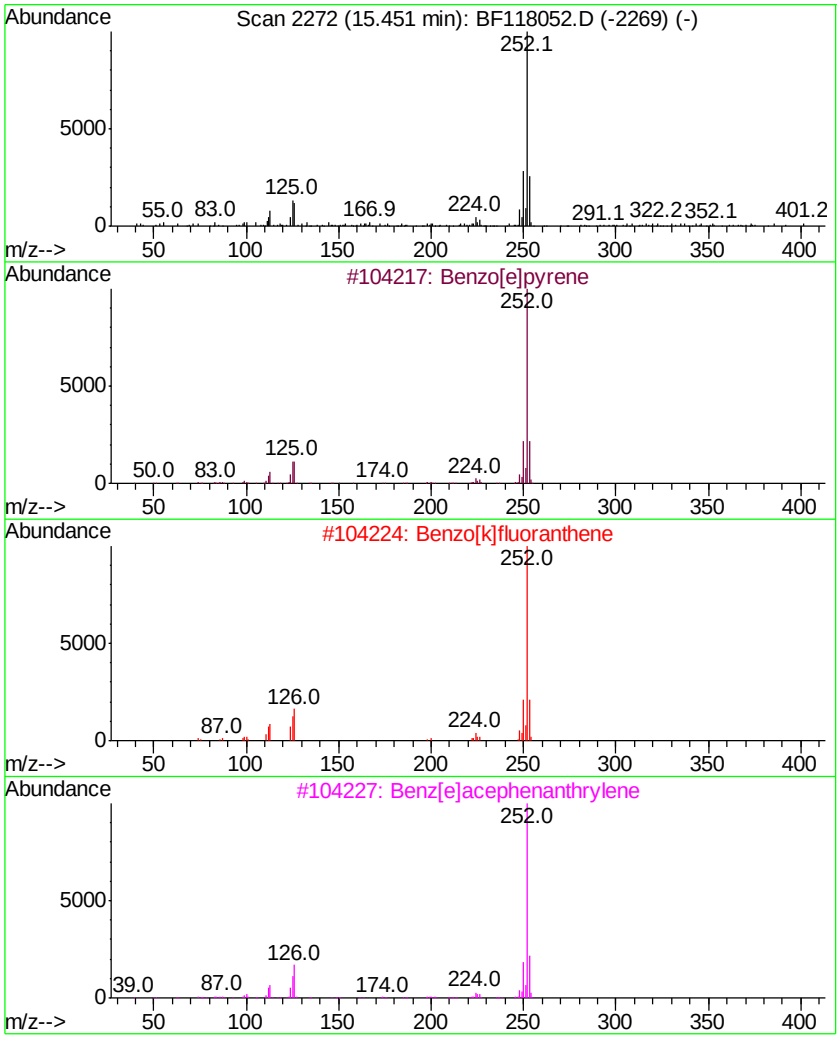
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

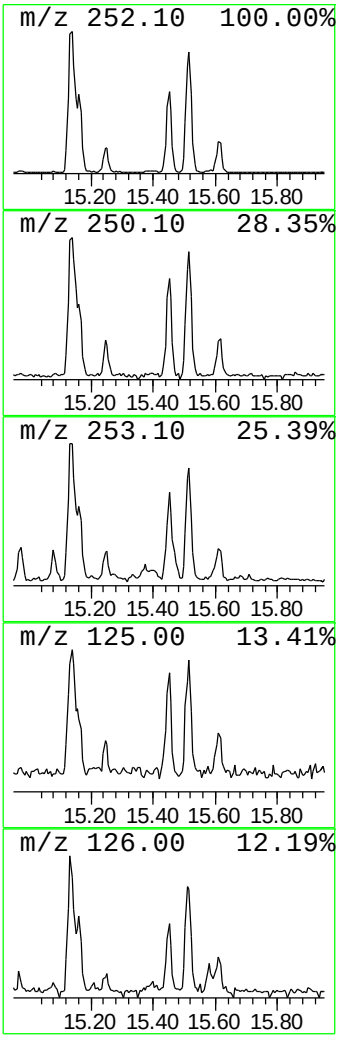
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	2.61 ng	130353	Perylene-d12	15.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	94
4	Benzo[a]pyrene	252	C20H12	000050-32-8	91
5	Perylene	252	C20H12	000198-55-0	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112719\
Data File : BF118052.D
Acq On : 27 Nov 2019 20:28
Operator : JU
Sample : K5977-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-2-5-COMP-B5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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...	2.15	16.1	ng	676737	1	6.89	842469	20.0
2-Pentanone, 4-hy...	5.09	11.4	ng	478068	1	6.89	842469	20.0
unknown6.65	6.65	65.6	ng	2762150	1	6.89	842469	20.0
n-Hexadecanoic acid	11.95	4.9	ng	274182	4	11.43	1127260	20.0
Benzene, 1,1'-(1,...	12.65	8.3	ng	469378	4	11.43	1127260	20.0
Dichloroacetic ac...	13.92	4.2	ng	261839	5	14.08	1240370	20.0
Benzo[e]pyrene	15.45	2.6	ng	130353	6	15.58	999323	20.0