LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118051.D
Acq On : 27 Nov 2019 20:00
Operator : JU
Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-0-2-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	6	11	21	rVB	551088	721752	28.38%	2.580%
2	5.093	507	511	521	rVB	370287	415108	16.32%	1.484%
3	5.498	576	580	584	rBV	2323983	2129064	83.71%	7.610%
4	6.510	747	752	755	rBV	2461595	2170756	85.35%	7.759%
5	6.651	772	776	780	rBV	2666700	2370696	93.21%	8.474%
6	6.887	812	816	819	rBV	845037	719095	28.27%	2.570%
7	7.039	838	842	846	rBV	2236232	1925153	75.70%	6.881%
8	7.445	907	911	914	rBV	1589852	1351789	53.15%	4.832%
9	8.169	1031	1034	1038	rBV	916101	836832	32.90%	2.991%
10	9.251	1214	1218	1221	rBV	3010953	2445549	96.16%	8.741%
11	9.645	1281	1285	1288	rBV	382971	341681	13.43%	1.221%
12	9.933	1330	1334	1338	rBV	1054920	844803	33.22%	3.020%
13	10.727	1465	1469	1472	rBV	1510686	1339421	52.66%	4.788%
14	11.292	1559	1565	1569	rBV4	34551	53360	2.10%	0.191%
15	11.427	1584	1588	1590	rBV	996364	788467	31.00%	2.818%
16	11.451	1590	1592	1596	rVV	223540	170195	6.69%	0.608%
17	11.504	1596	1601	1604	rVB	53102	58260	2.29%	0.208%
18	11.951	1670	1677	1684	rBV2	241994	335365	13.19%	1.199%
19	12.045	1689	1693	1695	rBV2	62064	66261	2.61%	0.237%
20	12.480	1764	1767	1770	rBV	34989	41201	1.62%	0.147%
21	12.569	1780	1782	1787	rBV3	44653	41371	1.63%	0.148%
22	12.645	1792	1795	1799	rBV	587873	517155	20.33%	1.849%
23	12.739	1808	1811	1814	rBV2	97770	97597	3.84%	0.349%
24	12.874	1828	1834	1840	rBV	527384	582020	22.88%	2.080%
25	12.927	1840	1843	1848	rVB3	31577	41490	1.63%	0.148%
26	13.016	1852	1858	1862	rBV	2675591	2543290	100.00%	9.091%
27	13.098	1867	1872	1876	rBV4	47224	80615	3.17%	0.288%
28	13.180	1883	1886	1888	rBV4	42332	51144	2.01%	0.183%
29	13.204	1888	1890	1893	rVB2	65757	61862	2.43%	0.221%
30	13.268	1899	1901	1904	rBV	30956	32207	1.27%	0.115%
31	13.310	1904	1908	1911	rBV2	69412	76472	3.01%	0.273%
32	13.404	1921	1924	1927	rBV	39757	35779	1.41%	0.128%
33	13.433	1927	1929	1933	rBV2	45541	48095	1.89%	0.172%
34	13.492	1936	1939	1942	rBV3	62764	63418	2.49%	0.227%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118051.D
Acq On : 27 Nov 2019 20:00
Operator : JU
Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-0-2-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	13.715	1974	1977	1981	rVB	63758	59059	2.32%	0.211%
36	13.827	1992	1996	1999	rBV2	61586	83962	3.30%	0.300%
37	13.857	1999	2001	2003	rVV	58765	52690	2.07%	0.188%
38	13.880	2003	2005	2008	rVV2	50743	66418	2.61%	0.237%
39	13.921	2008	2012	2021	rVB3	188303	300867	11.83%	1.075%
40	14.080	2034	2039	2042	rBV2	1201235	1351719	53.15%	4.832%
41	14.104	2042	2043	2049	rVB	327786	248968	9.79%	0.890%
42	14.186	2055	2057	2059	rBV	55274	44076	1.73%	0.158%
43	14.468	2103	2105	2107	rVB	72843	51687	2.03%	0.185%
44	14.545	2115	2118	2124	rBV4	76747	132040	5.19%	0.472%
45	14.857	2169	2171	2175	rVB2	73966	76838	3.02%	0.275%
46	15.139	2215	2219	2222	rBV	323679	468799	18.43%	1.676%
47	15.210	2228	2231	2235	rVB2	86656	97923	3.85%	0.350%
48	15.451	2269	2272	2279	rVB	170296	237142	9.32%	0.848%
49	15.515	2279	2283	2289	rVV	246175	313950	12.34%	1.122%
50	15.586	2290	2295	2306	rVB	615948	993537	39.07%	3.551%

Sum of corrected areas: 27976998

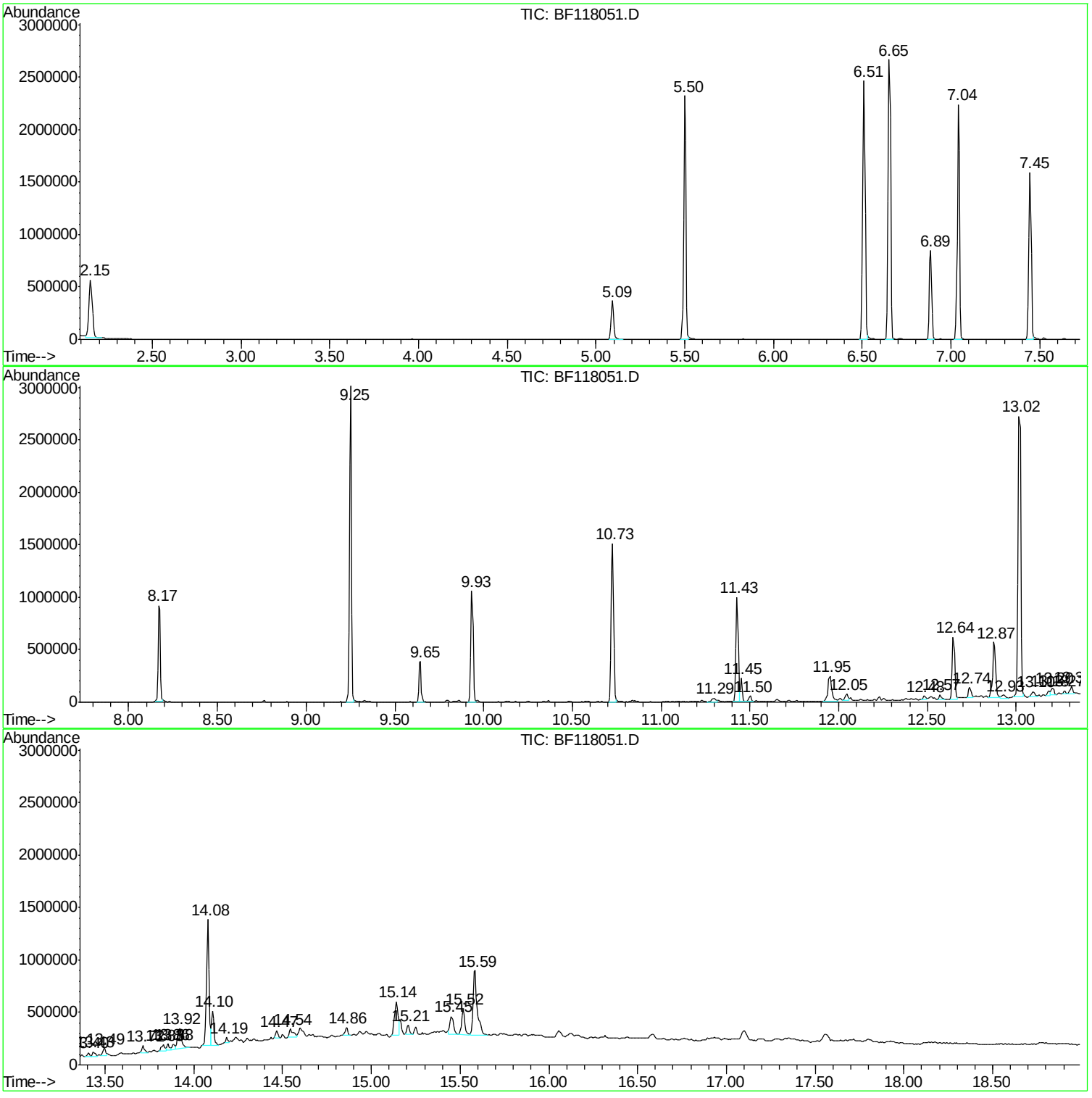
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118051.D
Acq On : 27 Nov 2019 20:00
Operator : JU
Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-112119-0-2-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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118051.D
Acq On : 27 Nov 2019 20:00
Operator : JU
Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-0-2-COMP-B5

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

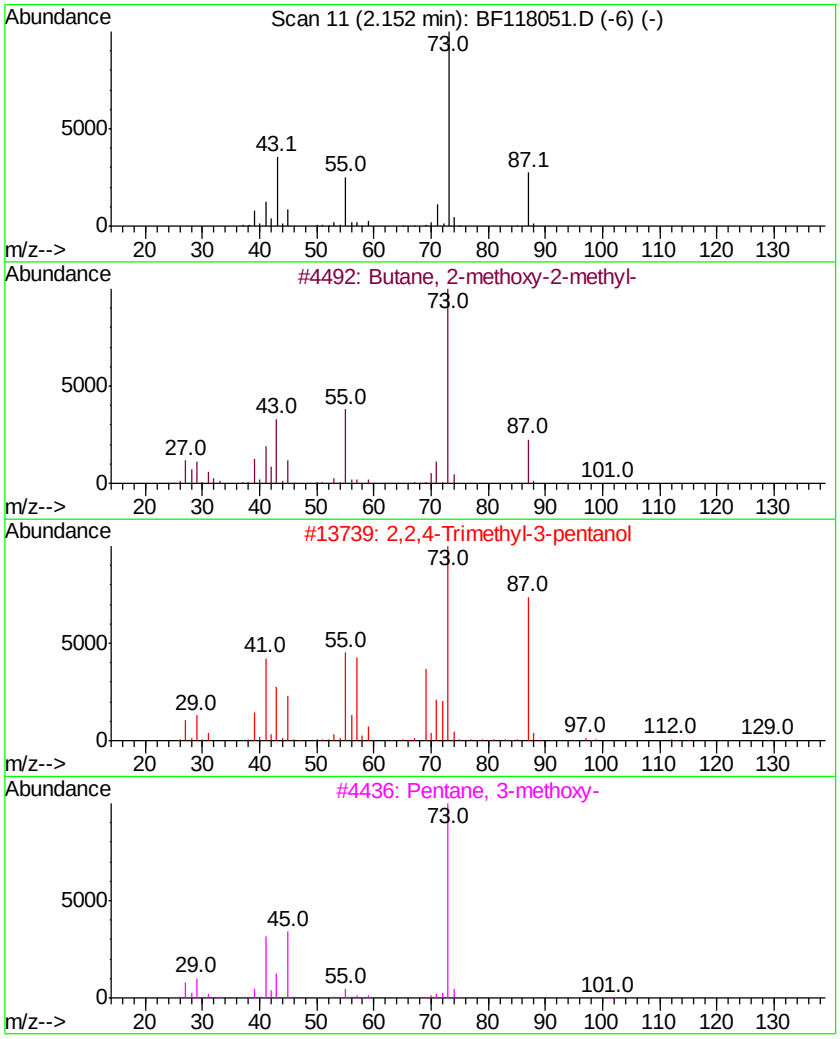
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

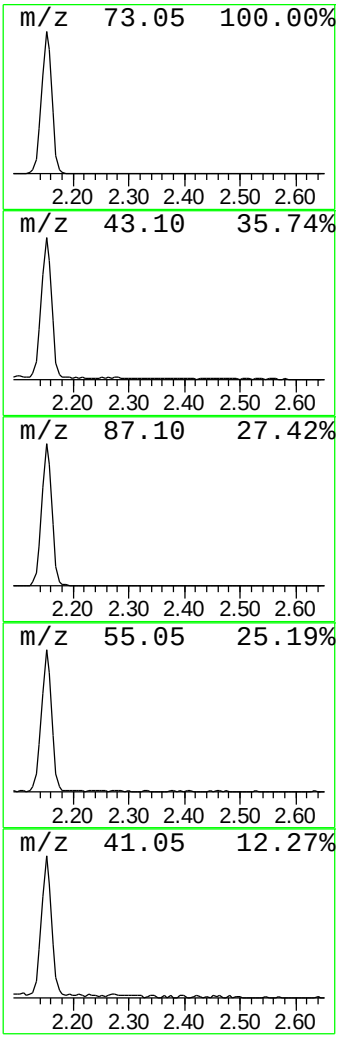
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	20.07 ng	721752	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	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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118051.D
Acq On : 27 Nov 2019 20:00
Operator : JU
Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-0-2-COMP-B5

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

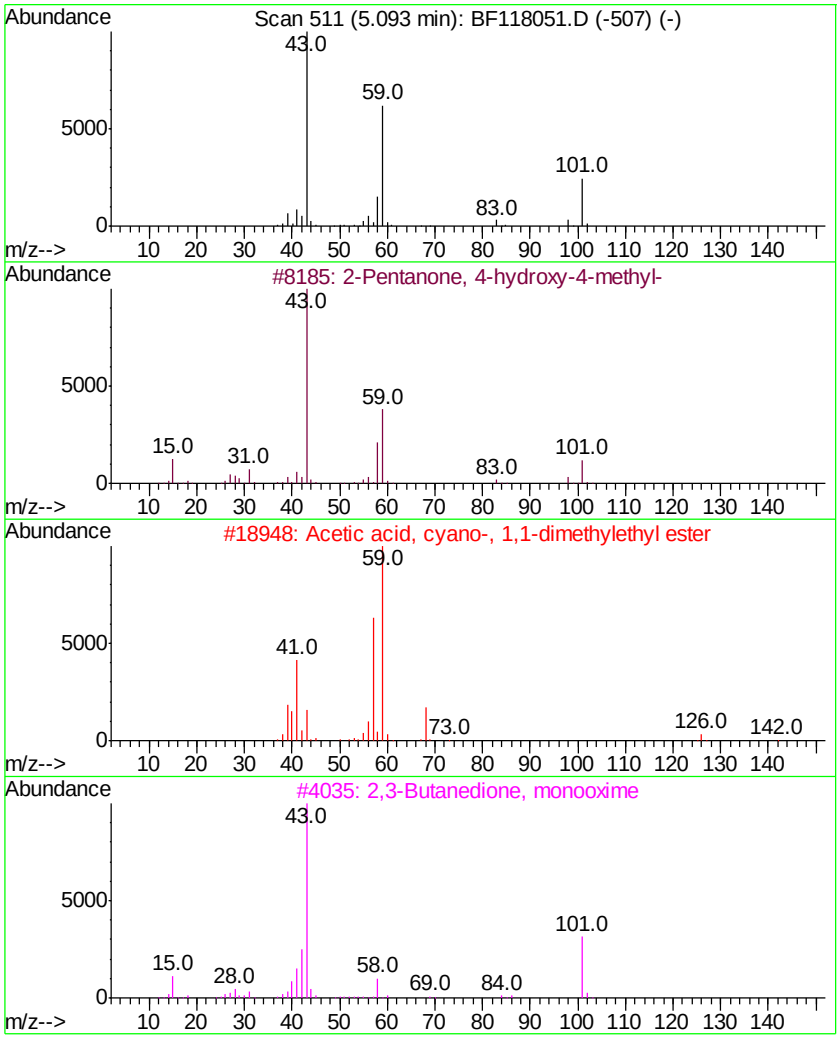
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

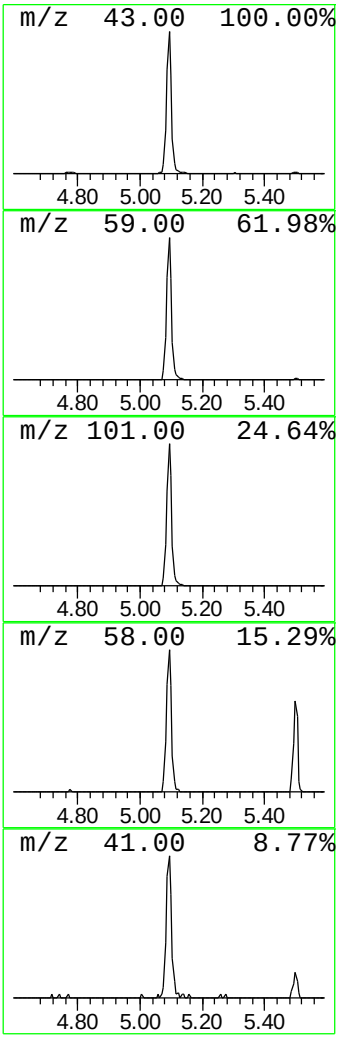
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	11.55 ng	415108	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	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118051.D
Acq On : 27 Nov 2019 20:00
Operator : JU
Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-0-2-COMP-B5

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

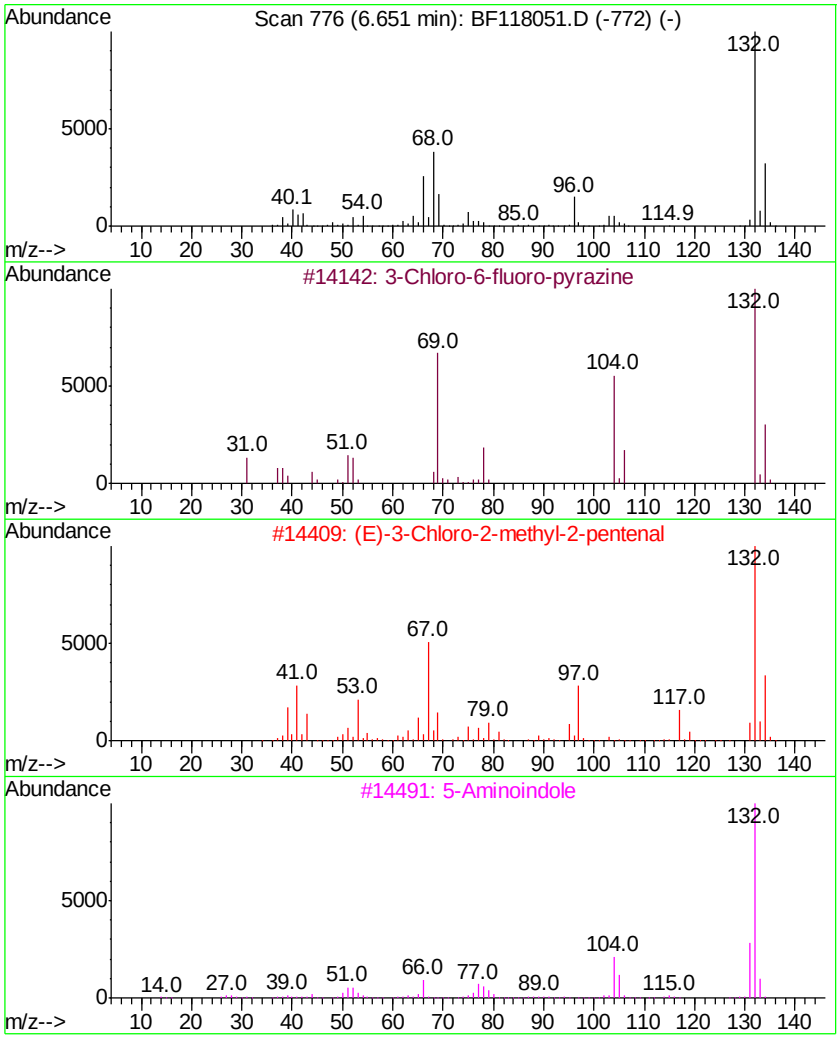
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

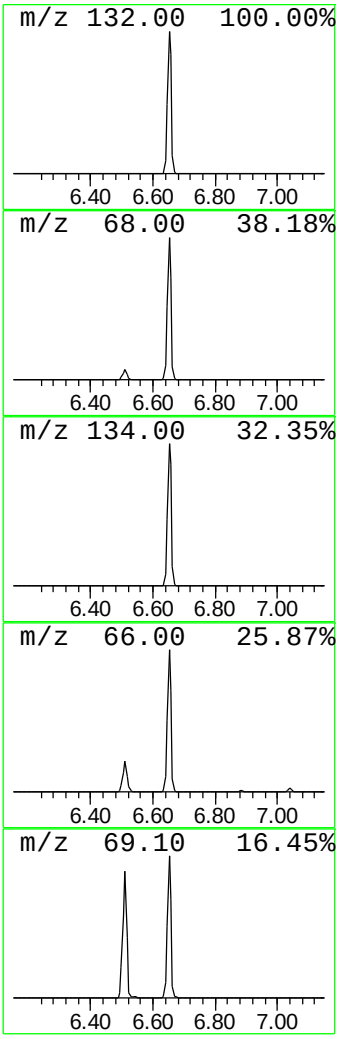
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	65.94 ng	2370700	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-112119-0-2-COMP-B5

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

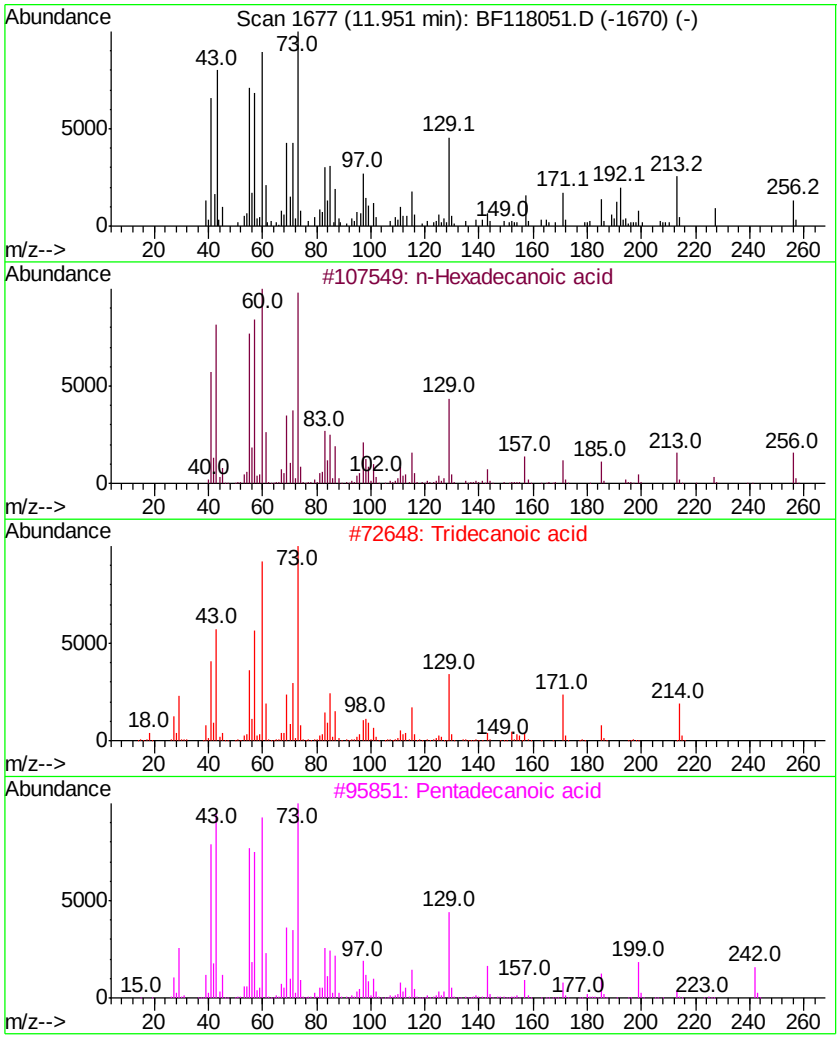
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

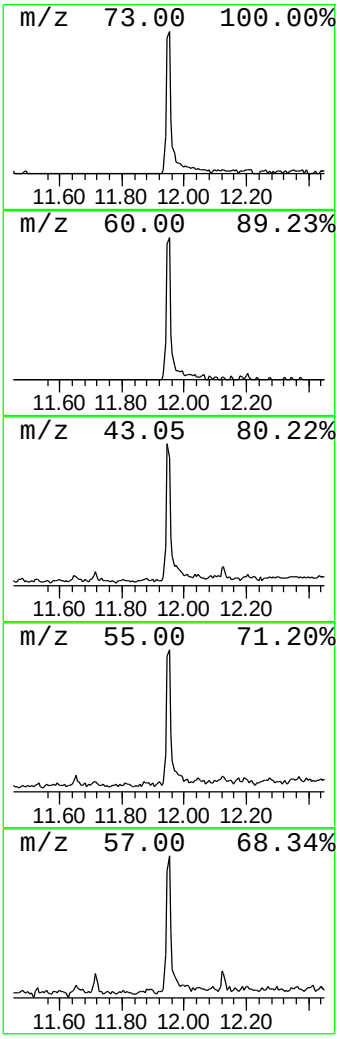
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	8.51 ng	335365	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





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Acq On : 27 Nov 2019 20:00
Operator : JU
Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-0-2-COMP-B5

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

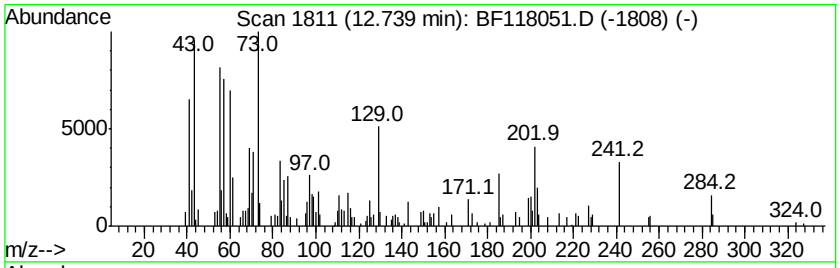
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

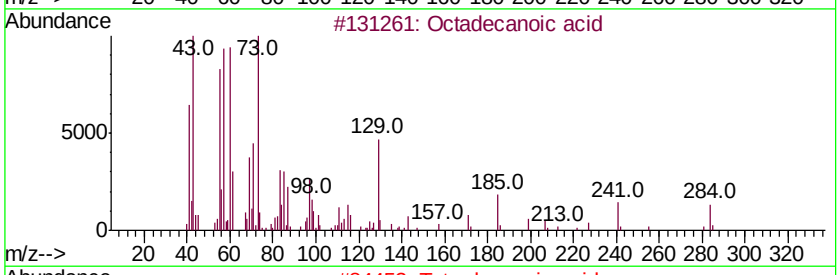
****

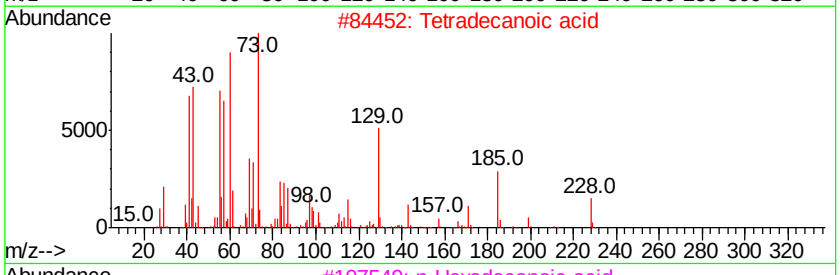
Peak Number 6 Octadecanoic acid Concentration Rank 8

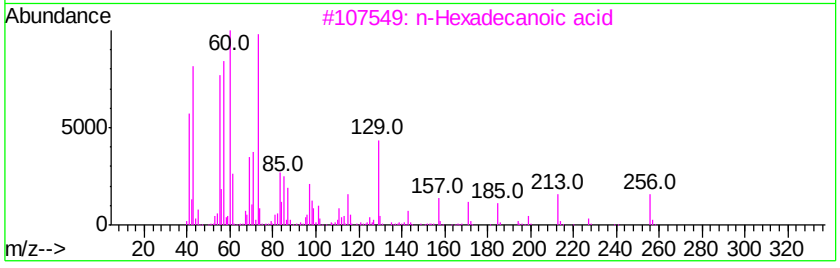
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.48 ng	97597	Phenanthrene-d10	11.43

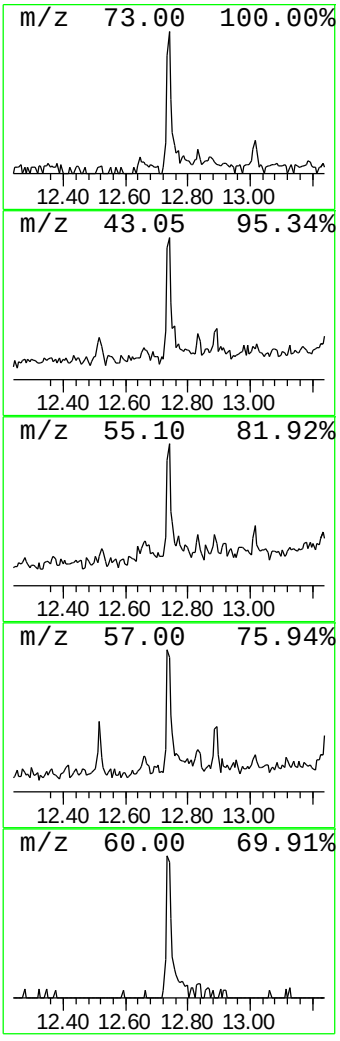
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	44











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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-0-2-COMP-B5

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

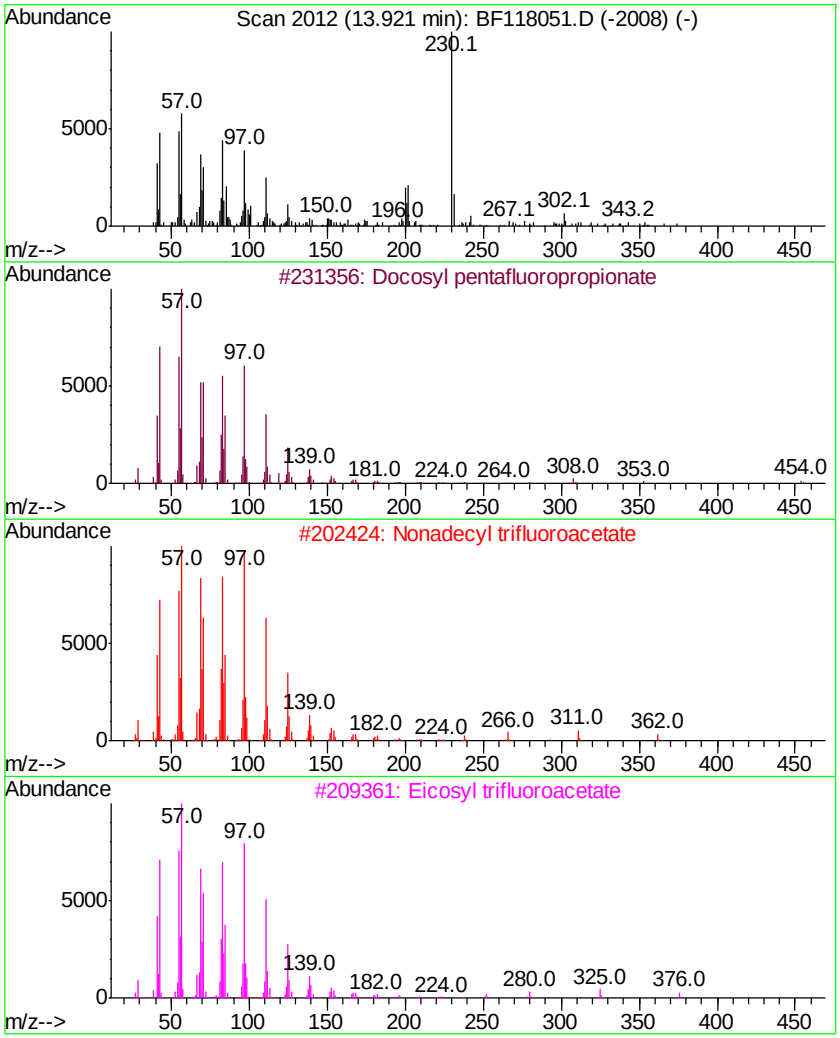
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

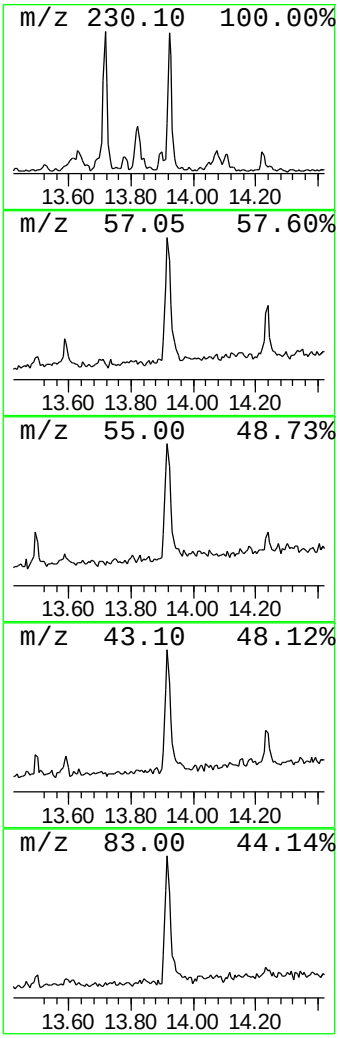
****

Peak Number 7 Docosyl pentafluoropropionate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	4.45 ng	300867	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	50
2	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	46
3	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	46
4	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	46
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	46





Library Search Compound Report

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Data File : BF118051.D
Acq On : 27 Nov 2019 20:00
Operator : JU
Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-0-2-COMP-B5

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

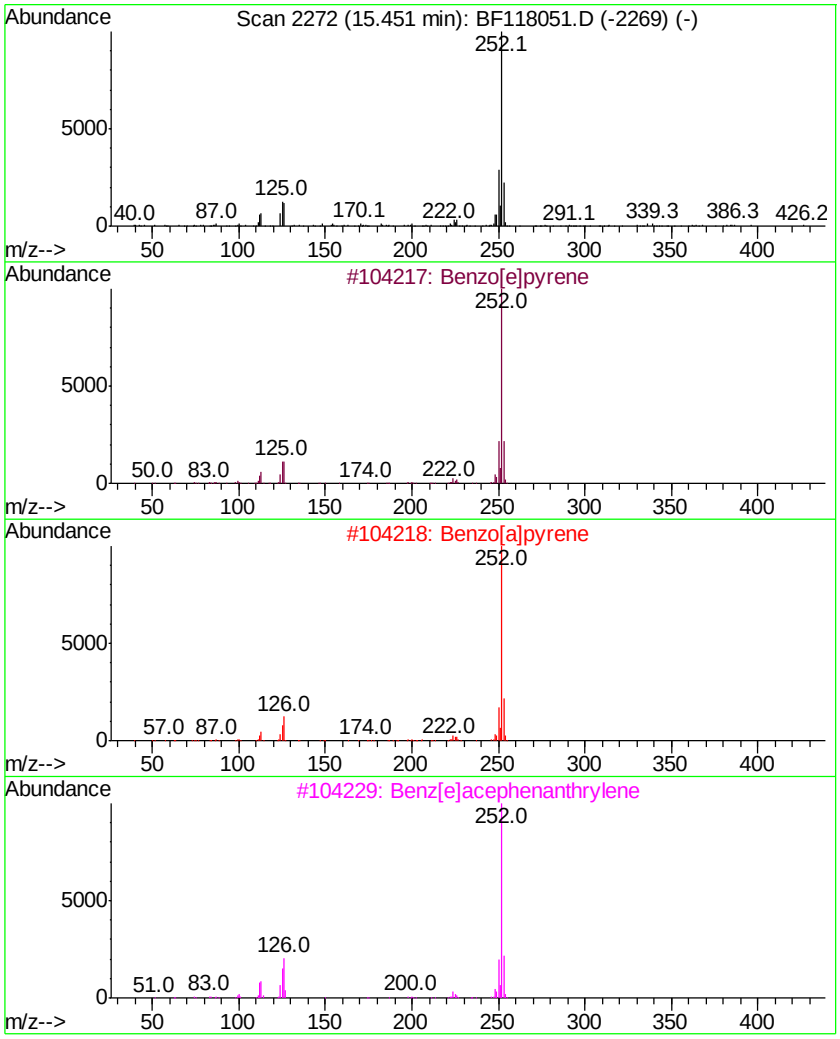
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

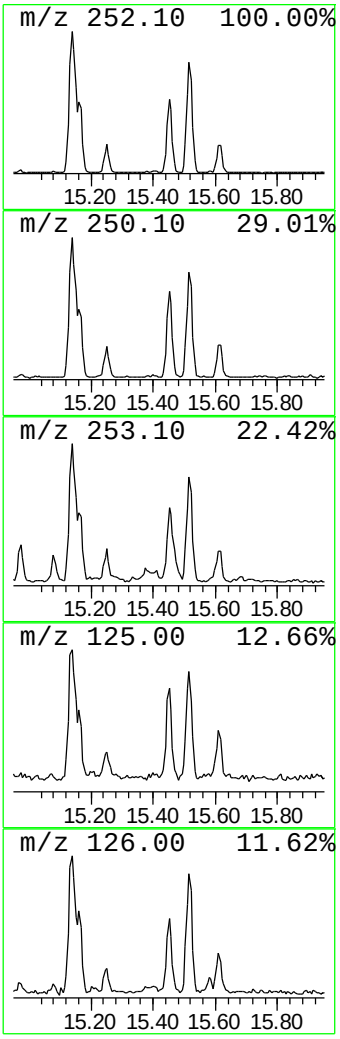
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.45	4.77 ng	237142	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	95
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
5	Perylene	252	C20H12	000198-55-0	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112719\
Data File : BF118051.D
Acq On : 27 Nov 2019 20:00
Operator : JU
Sample : K5977-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-112119-0-2-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	20.1	ng	721752	1	6.89	719095	20.0
2-Pentanone, 4-hy...	5.09	11.6	ng	415108	1	6.89	719095	20.0
unknown6.65	6.65	65.9	ng	2370700	1	6.89	719095	20.0
n-Hexadecanoic acid	11.95	8.5	ng	335365	4	11.43	788467	20.0
Octadecanoic acid	12.74	2.5	ng	97597	4	11.43	788467	20.0
Docosyl pentafluo...	13.92	4.5	ng	300867	5	14.08	1351720	20.0
Benzo[e]pyrene	15.45	4.8	ng	237142	6	15.59	993537	20.0