LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

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-BF072018.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	5.207	484	488	503	rBV	518713	781996	15.38%	1.640%
2	5.607	551	556	584	rBV	3262762	4943433	97.26%	10.366%
3	6.601	721	725	744	rBV	3237977	4936423	97.12%	10.351%
4	6.743	744	749	772	rVB	4157541	5082898	100.00%	10.658%
5	6.966	784	787	809	rVB	1214473	1522003	29.94%	3.191%
6	7.125	809	814	830	rBV	3379853	3875559	76.25%	8.126%
7	7.531	879	883	907	rBV	2409057	3170098	62.37%	6.647%
8	8.248	1001	1005	1022	rBV	1678492	1867483	36.74%	3.916%
9	9.219	1168	1170	1179	rVB	46095	74508	1.47%	0.156%
10	9.325	1182	1188	1203	rBV	4782444	4822103	94.87%	10.111%
11	9.713	1251	1254	1262	rVB	231744	221683	4.36%	0.465%
12	9.872	1277	1281	1285	rBV2	52546	62336	1.23%	0.131%
13	10.007	1300	1304	1309	rBV	1719909	1650995	32.48%	3.462%
14	10.419	1366	1374	1379	rVB2	40617	59543	1.17%	0.125%
15	10.801	1435	1439	1452	rBV	2299737	2529804	49.77%	5.305%
16	10.889	1452	1454	1465	rVB3	50699	104748	2.06%	0.220%
17	11.501	1554	1558	1561	rBV	1457010	1484267	29.20%	3.112%
18	11.525	1561	1562	1570	rVB	437638	367165	7.22%	0.770%
19	11.654	1579	1584	1593	rVB10	18687	51825	1.02%	0.109%
20	12.007	1640	1644	1646	rBV	178734	201796	3.97%	0.423%
21	12.030	1646	1648	1653	rVB	173331	180802	3.56%	0.379%
22	12.113	1659	1662	1665	rBV2	138313	172947	3.40%	0.363%
23	12.136	1665	1666	1671	rVB	95531	87654	1.72%	0.184%
24	12.448	1713	1719	1722	rBV	48870	58545	1.15%	0.123%
25	12.477	1722	1724	1726	rBV	73172	59004	1.16%	0.124%
26	12.501	1726	1728	1733	rVB2	51907	51771	1.02%	0.109%
27	12.554	1733	1737	1740	rBV	169578	201629	3.97%	0.423%
28	12.636	1749	1751	1761	rVB4	62124	109199	2.15%	0.229%
29	12.719	1761	1765	1769	rBV	376626	353122	6.95%	0.740%
30	12.948	1798	1804	1810	rBV	408001	578740	11.39%	1.214%
31	13.001	1810	1813	1817	rVB	83461	84371	1.66%	0.177%
32	13.089	1823	1828	1837	rVV	3537097	3694549	72.69%	7.747%
33	13.166	1837	1841	1848	rVB6	66363	121983	2.40%	0.256%
34	13.342	1869	1871	1874	rBV	52199	57320	1.13%	0.120%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

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-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.383	1874	1878	1881	rVB	97523	103426	2.03%	0.217%
36	13.477	1891	1894	1896	rBV	73219	66590	1.31%	0.140%
37	13.507	1896	1899	1902	rVV	57608	53506	1.05%	0.112%
38	13.636	1917	1921	1924	rBV	72021	77483	1.52%	0.162%
39	13.789	1939	1947	1952	rBV3	49628	102982	2.03%	0.216%
40	13.971	1974	1978	1986	rVB4	164233	249983	4.92%	0.524%
41	14.154	2003	2009	2012	rBV	1291415	1559215	30.68%	3.269%
42	14.283	2028	2031	2033	rBV	67831	54719	1.08%	0.115%
43	14.536	2072	2074	2078	rVB	66475	57022	1.12%	0.120%
44	14.589	2078	2083	2088	rBV2	82702	125414	2.47%	0.263%
45	14.907	2135	2137	2140	rVB	70875	67288	1.32%	0.141%
46	14.989	2149	2151	2154	rVB	63560	63481	1.25%	0.133%
47	15.230	2188	2192	2194	rBV	64652	97110	1.91%	0.204%
48	15.260	2195	2197	2205	rVB3	77517	113579	2.23%	0.238%
49	15.548	2243	2246	2253	rVB	51464	70856	1.39%	0.149%
50	15.618	2254	2258	2262	rVV	68332	93286	1.84%	0.196%
51	15.683	2263	2269	2281	rVV	671165	1054786	20.75%	2.212%
52	16.136	2342	2346	2351	rVB4	39158	57652	1.13%	0.121%

Sum of corrected areas: 47690680

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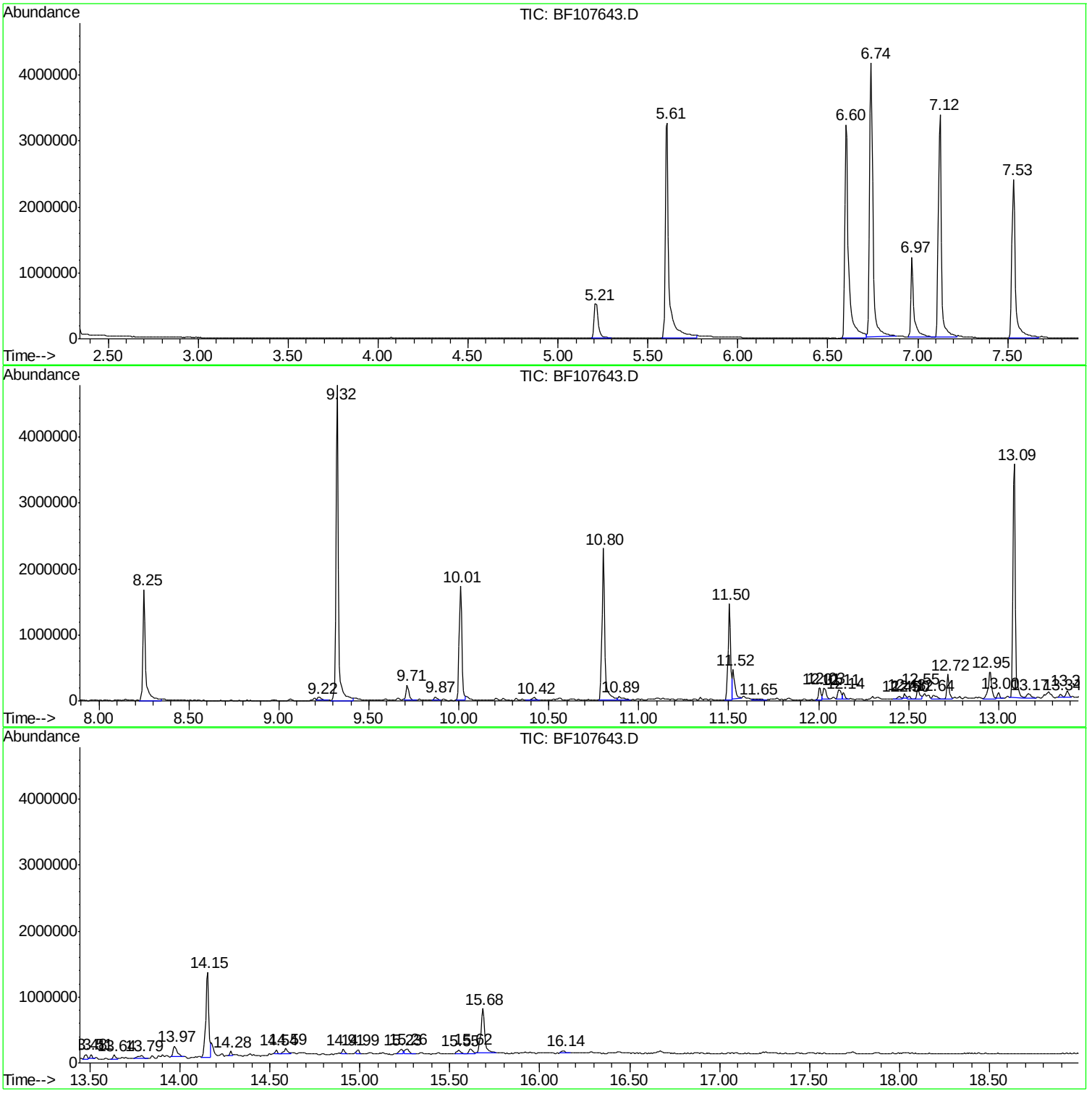
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ST-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

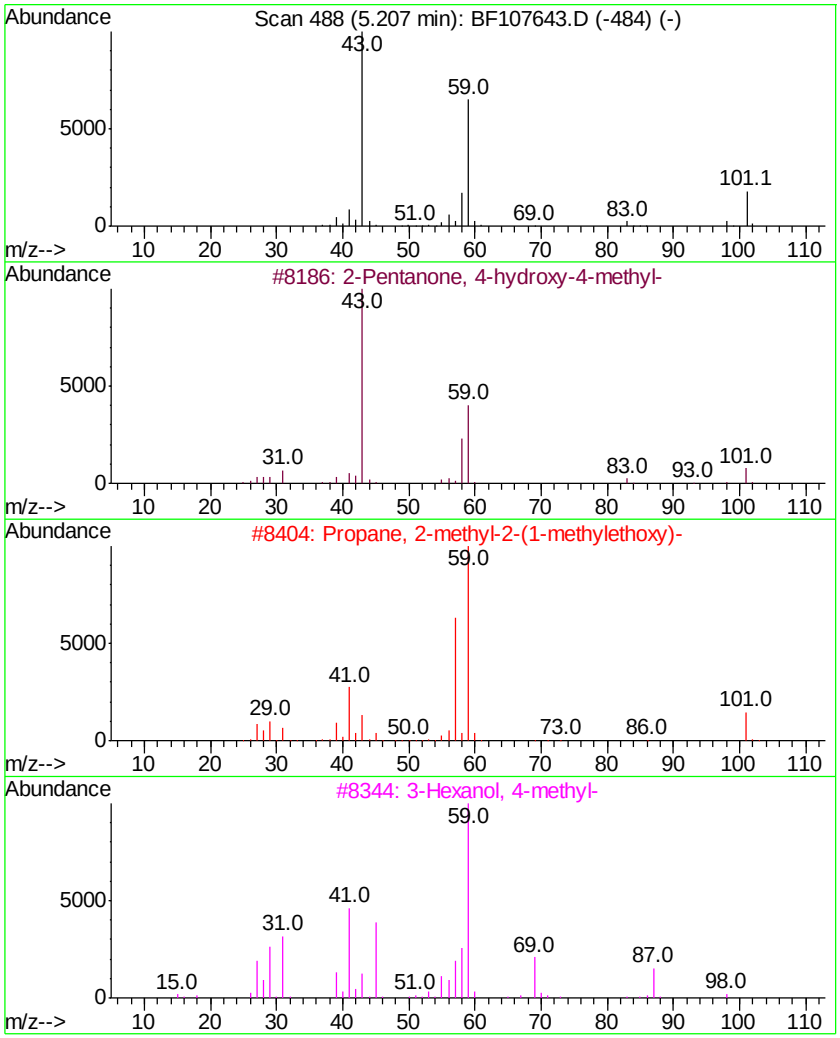
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

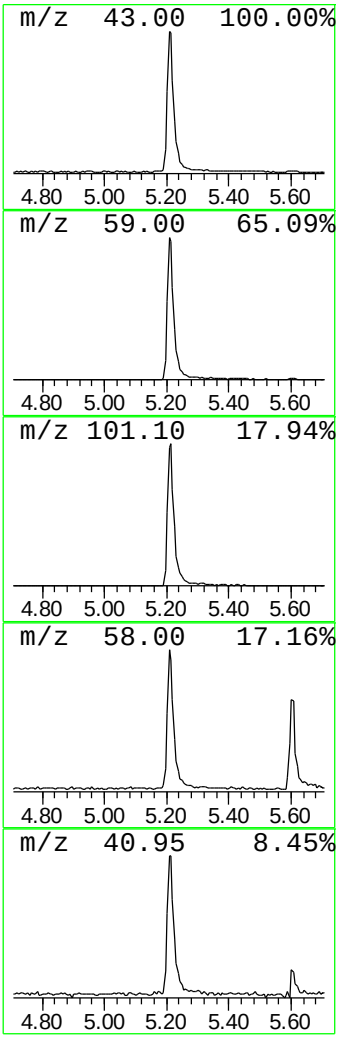
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	10.28 ng	781996	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

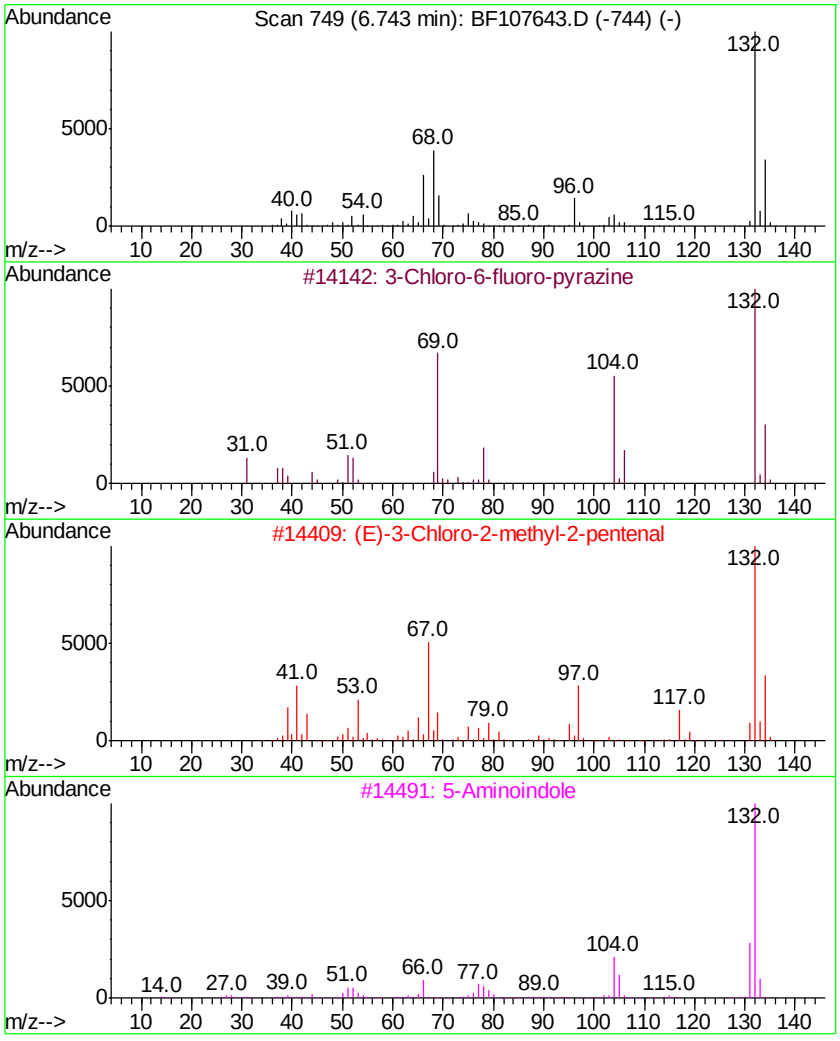
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

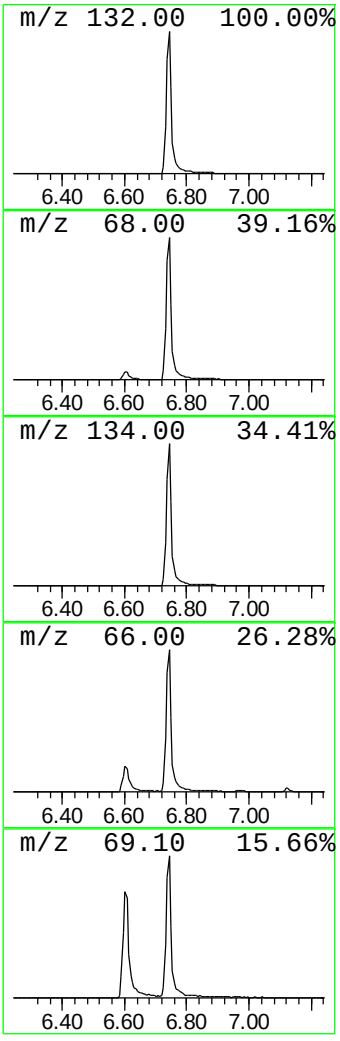
****

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	66.79 ng	5082900	1,4-Dichlorobenzene-d4	6.97

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

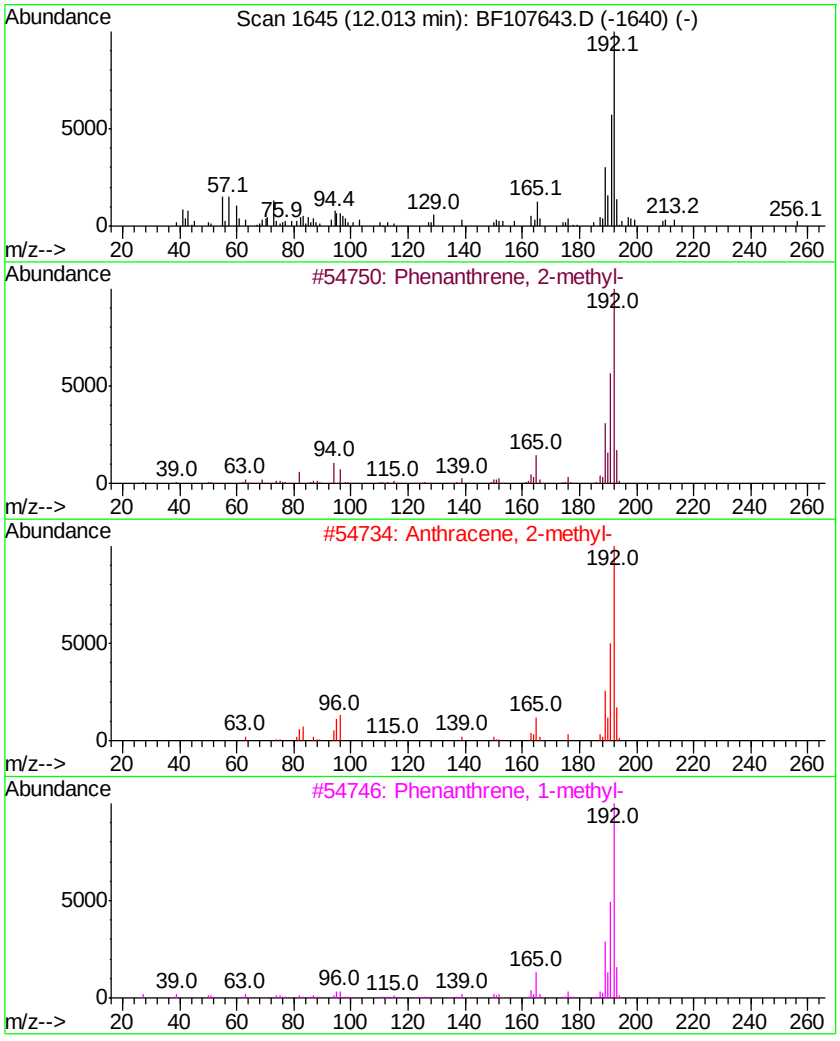
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

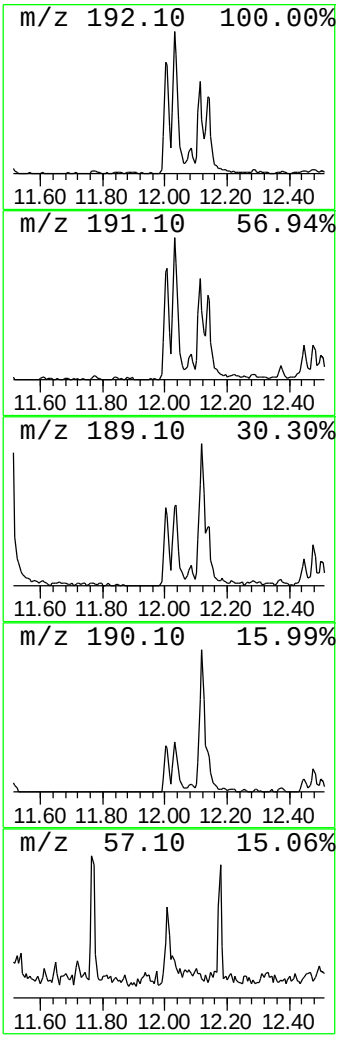
****

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	2.72 ng	201796	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	90
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	86
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	76
5	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072418\
Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

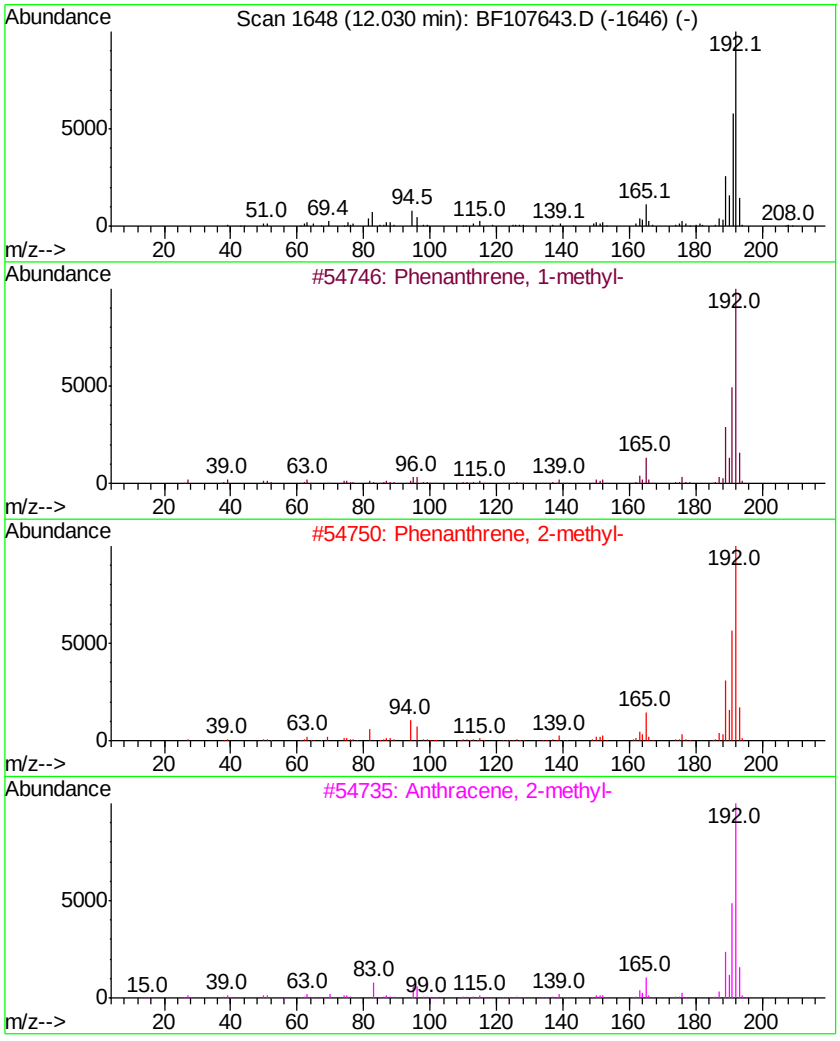
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

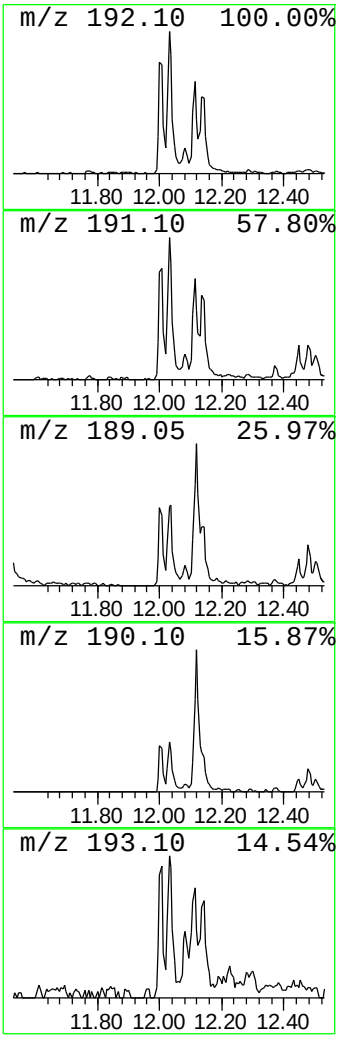
****

Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	2.44 ng	180802	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	91
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91





Library Search Compound Report

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Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

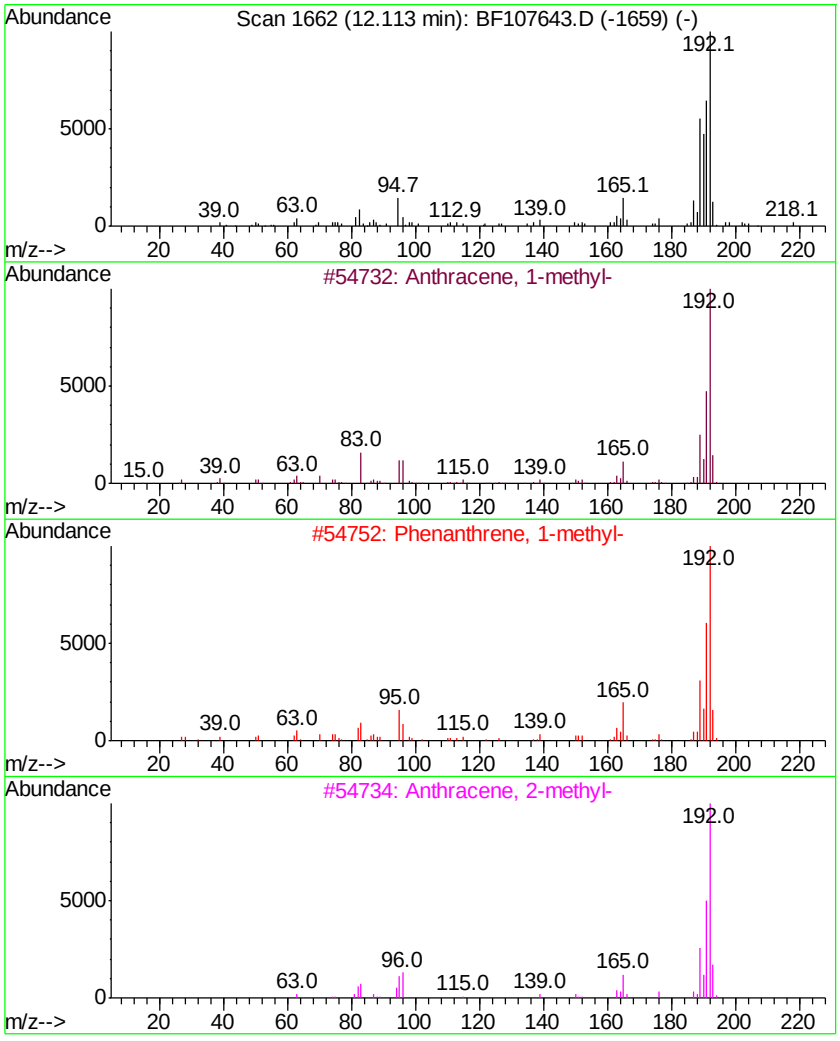
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

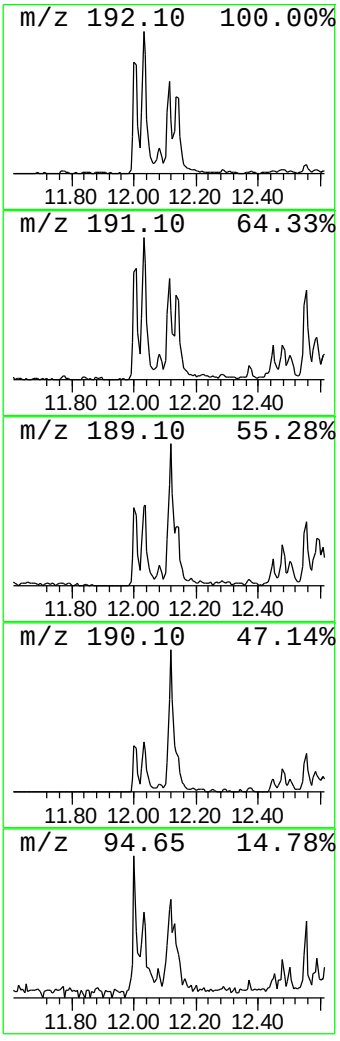
****

Peak Number 6 Anthracene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	2.33 ng	172947	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	64
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	64
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	60
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	55
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	53





Library Search Compound Report

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Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

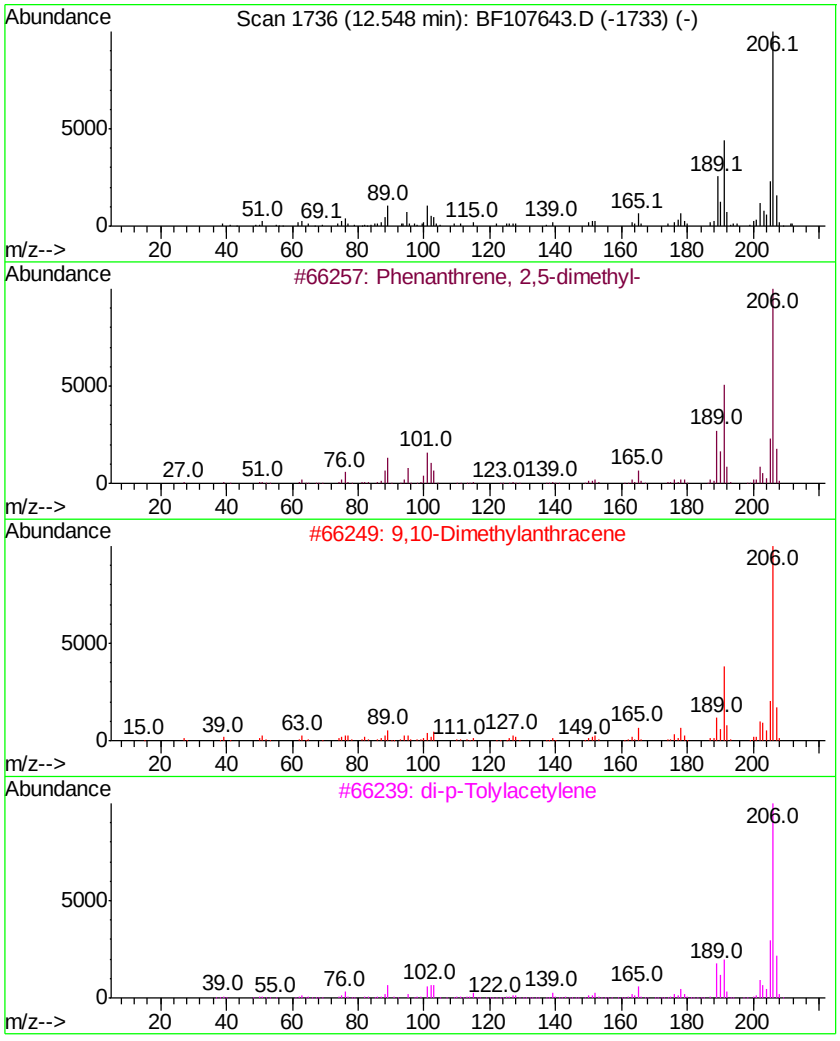
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

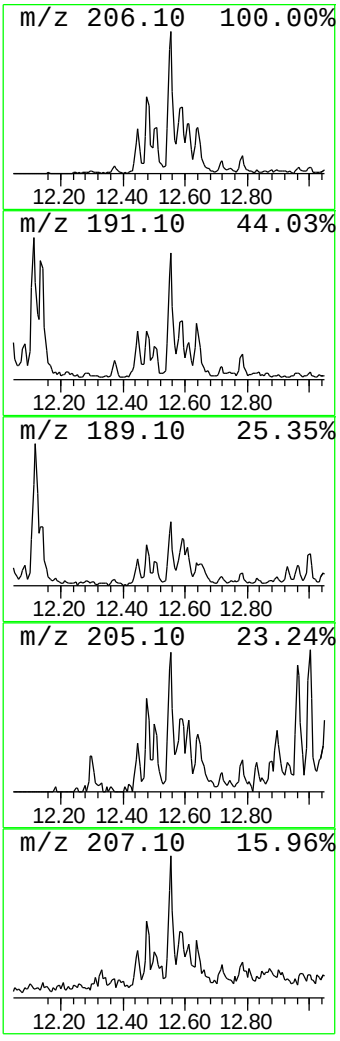
****

Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	2.72 ng	201629	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	97
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	96
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	96
4	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	94
5	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	90





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Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

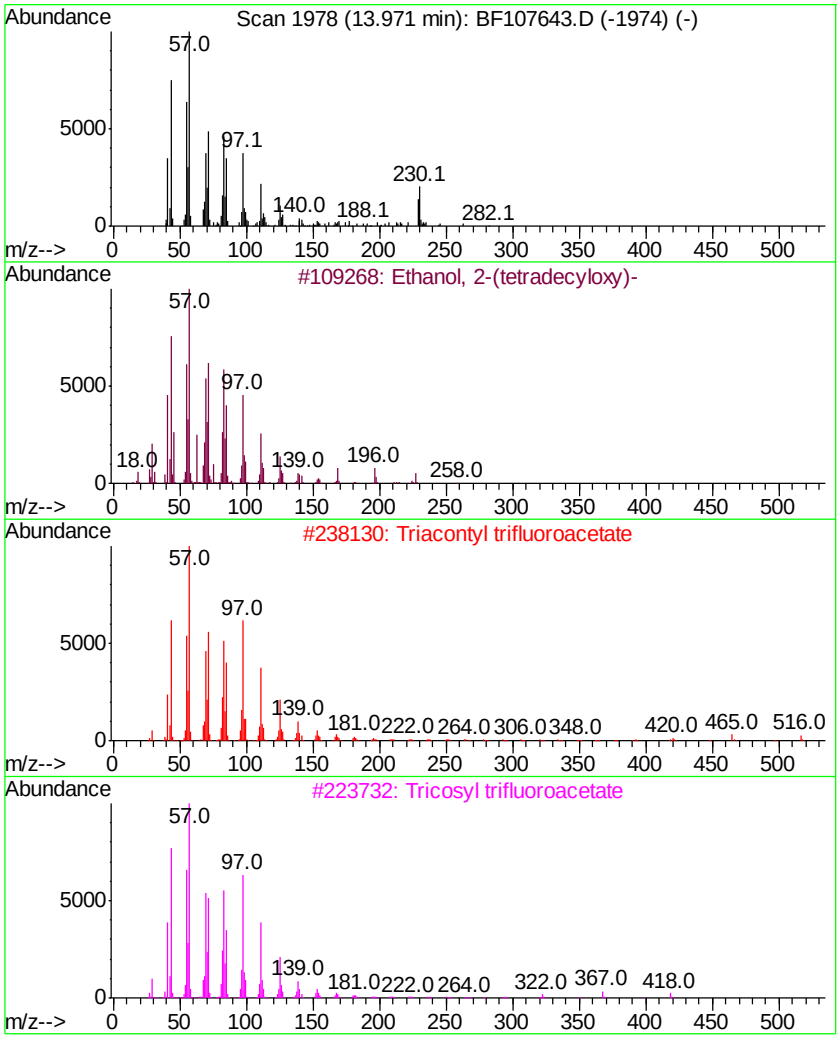
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

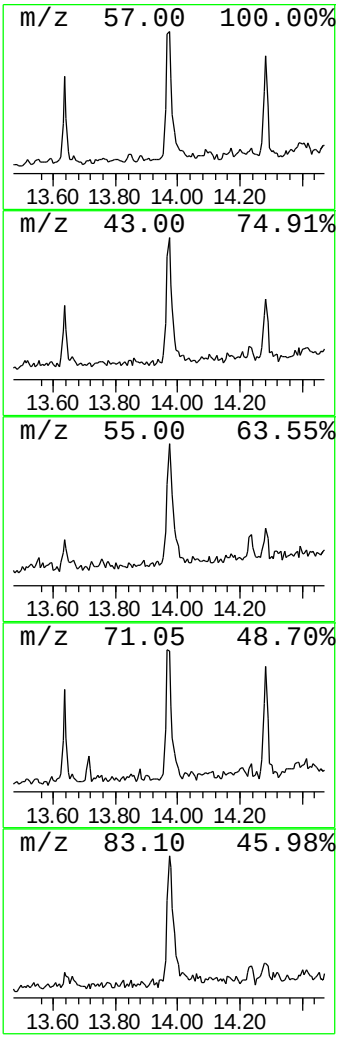
****

Peak Number 8 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.21 ng	249983	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	74
2	Triacontyl trifluoroacetate	534	C32H61F3O2	1000351-75-7	72
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	72
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	72
5	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072418\
Data File : BF107643.D
Acq On : 25 Jul 2018 3:58
Operator : JU/SJ
Sample : J4120-04
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ST-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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...	5.21	10.3	ng	781996	1	6.97	1522000	20.0
unknown6.74	6.74	66.8	ng	5082900	1	6.97	1522000	20.0
Phenanthrene, 2-m...	12.01	2.7	ng	201796	4	11.50	1484270	20.0
Phenanthrene, 1-m...	12.03	2.4	ng	180802	4	11.50	1484270	20.0
Anthracene, 1-met...	12.11	2.3	ng	172947	4	11.50	1484270	20.0
Phenanthrene, 2,5...	12.55	2.7	ng	201629	4	11.50	1484270	20.0
Ethanol, 2-(tetra...	13.97	3.2	ng	249983	5	14.15	1559220	20.0