LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF063018\
Data File : BF107026.D
Acq On : 30 Jun 2018 20:24
Operator : JU/SJ
Sample : J3638-02 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.184	480	484	498	rBV	45264	52893	5.32%	0.438%
2	5.595	550	554	568	rBV	713444	739622	74.39%	6.128%
3	6.595	720	724	743	rBV	802225	763606	76.80%	6.326%
4	6.731	743	747	750	rBV	901203	754401	75.88%	6.250%
5	6.954	781	785	788	rBV	479818	395282	39.76%	3.275%
6	7.107	807	811	815	rBV	750593	618838	62.24%	5.127%
7	7.513	877	880	895	rBV	429245	418598	42.10%	3.468%
8	8.236	999	1003	1022	rVB	502032	462747	46.54%	3.834%
9	9.307	1181	1185	1194	rBV	974448	819042	82.38%	6.785%
10	9.701	1246	1252	1257	rBV	85082	82198	8.27%	0.681%
11	9.901	1282	1286	1289	rBV	22732	18736	1.88%	0.155%
12	9.995	1298	1302	1306	rBV	518827	455065	45.77%	3.770%
13	10.025	1306	1307	1311	rVB	21533	14761	1.48%	0.122%
14	10.401	1368	1371	1374	rVB	34023	25029	2.52%	0.207%
15	10.542	1392	1395	1401	rVB	11224	13243	1.33%	0.110%
16	10.619	1405	1408	1413	rBV3	11700	14786	1.49%	0.122%
17	10.789	1433	1437	1446	rBV	521662	477340	48.01%	3.955%
18	10.877	1448	1452	1457	rBV	28883	36562	3.68%	0.303%
19	11.324	1525	1528	1530	rBV	23512	17245	1.73%	0.143%
20	11.489	1552	1556	1558	rBV	580812	501482	50.44%	4.155%
21	11.513	1558	1560	1564	rVV	192116	153274	15.42%	1.270%
22	11.566	1565	1569	1573	rVB	35773	32090	3.23%	0.266%
23	11.724	1594	1596	1598	rBV	18175	12919	1.30%	0.107%
24	11.748	1598	1600	1603	rVB2	13800	10948	1.10%	0.091%
25	11.989	1637	1641	1643	rBV	25360	24099	2.42%	0.200%
26	12.018	1643	1646	1651	rVB2	33002	30543	3.07%	0.253%
27	12.107	1657	1661	1663	rBV2	37673	43427	4.37%	0.360%
28	12.124	1663	1664	1667	rVB	20111	13532	1.36%	0.112%
29	12.160	1667	1670	1674	rBV3	11963	14589	1.47%	0.121%
30	12.283	1688	1691	1694	rBV	15692	15112	1.52%	0.125%
31	12.318	1694	1697	1702	rVB	22022	22670	2.28%	0.188%
32	12.424	1712	1715	1720	rBV5	17514	26072	2.62%	0.216%
33	12.542	1731	1735	1738	rBV2	19358	26340	2.65%	0.218%
34	12.636	1747	1751	1754	rBV2	20529	27546	2.77%	0.228%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J3638-02 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.707	1759	1763	1766	rBV	480988	395559	39.79%	3.277%
36	12.765	1770	1773	1777	rBV3	9493	11681	1.17%	0.097%
37	12.860	1783	1789	1791	rBV2	19188	26603	2.68%	0.220%
38	12.918	1795	1799	1800	rBV2	88451	87849	8.84%	0.728%
39	12.936	1800	1802	1807	rVV	389298	358683	36.08%	2.972%
40	12.983	1807	1810	1814	rVB2	16667	20444	2.06%	0.169%
41	13.071	1820	1825	1828	rBV	1096057	994239	100.00%	8.237%
42	13.101	1828	1830	1832	rVB	27319	23473	2.36%	0.194%
43	13.160	1835	1840	1843	rBV2	27199	51522	5.18%	0.427%
44	13.265	1851	1858	1863	rBV2	59043	94148	9.47%	0.780%
45	13.330	1866	1869	1871	rBV	40810	34387	3.46%	0.285%
46	13.371	1871	1876	1878	rBV2	34904	41552	4.18%	0.344%
47	13.465	1890	1892	1894	rVB	23431	18433	1.85%	0.153%
48	13.495	1894	1897	1900	rBV	30530	30881	3.11%	0.256%
49	13.618	1915	1918	1920	rBV3	21465	25775	2.59%	0.214%
50	13.777	1942	1945	1949	rVB	40119	37303	3.75%	0.309%
51	13.889	1961	1964	1966	rBV	43813	37522	3.77%	0.311%
52	13.912	1966	1968	1971	rVV	35913	33393	3.36%	0.277%
53	13.948	1971	1974	1979	rVV4	112594	143402	14.42%	1.188%
54	13.989	1979	1981	1984	rVB	32359	30267	3.04%	0.251%
55	14.142	2002	2007	2010	rBV2	587438	743620	74.79%	6.161%
56	14.165	2010	2011	2014	rVB	232780	158717	15.96%	1.315%
57	14.248	2023	2025	2027	rBV	35006	33240	3.34%	0.275%
58	14.536	2072	2074	2076	rVB	41597	31036	3.12%	0.257%
59	15.054	2159	2162	2167	rBV3	39691	49599	4.99%	0.411%
60	15.224	2187	2191	2194	rBV	206705	310604	31.24%	2.573%
61	15.342	2208	2211	2215	rVB	40399	44454	4.47%	0.368%
62	15.548	2242	2246	2253	rVB	131122	173032	17.40%	1.434%
63	15.612	2253	2257	2262	rBV	162463	217662	21.89%	1.803%
64	15.683	2265	2269	2272	rBV	234878	284490	28.61%	2.357%
65	17.253	2531	2536	2544	rVB	96947	214196	21.54%	1.775%
66	17.736	2613	2618	2632	rVB	79948	178088	17.91%	1.475%

Sum of corrected areas: 12070491

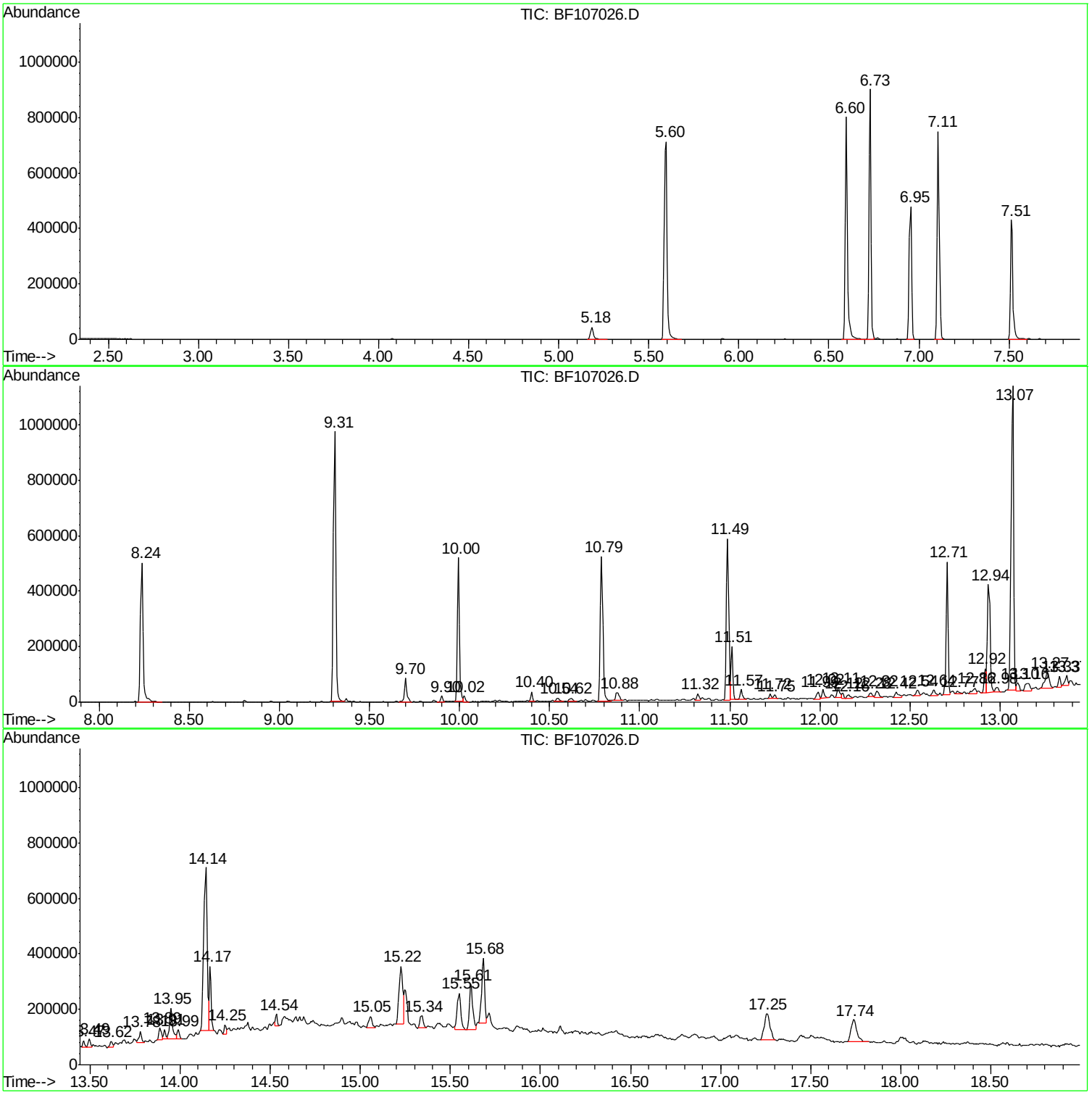
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF063018\
Data File : BF107026.D
Acq On : 30 Jun 2018 20:24
Operator : JU/SJ
Sample : J3638-02 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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\BF063018\
Data File : BF107026.D
Acq On : 30 Jun 2018 20:24
Operator : JU/SJ
Sample : J3638-02 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

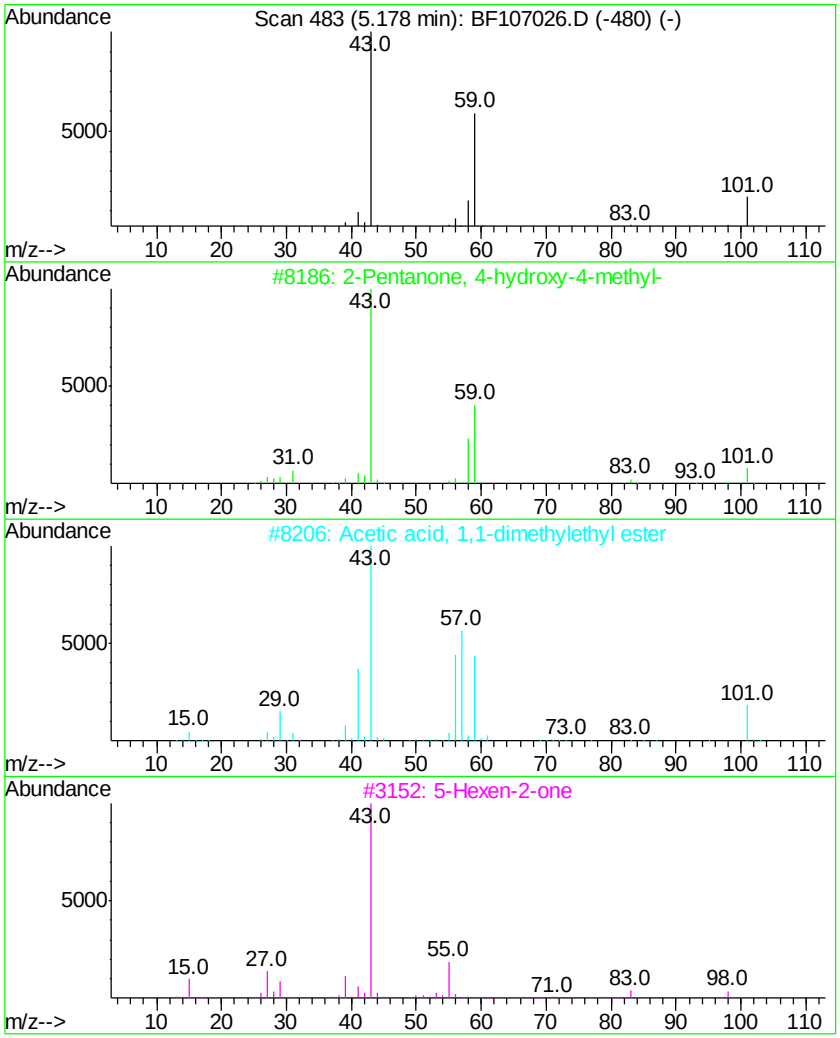
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

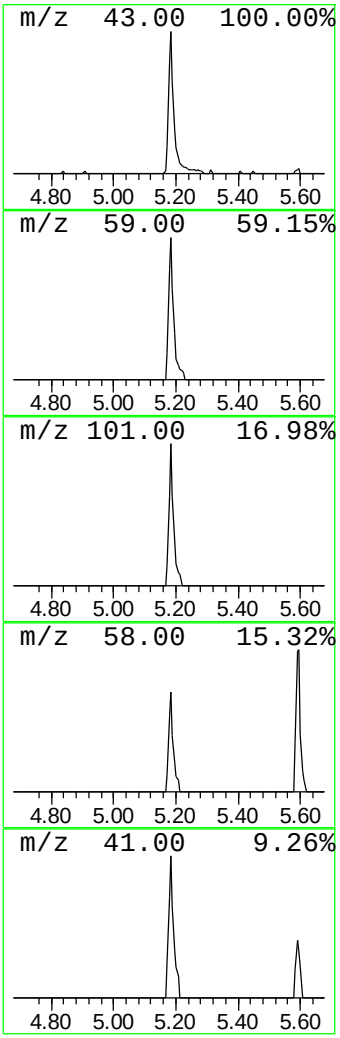
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	2.68 ng	52893	1,4-Dichlorobenzene-d4	6.95

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9





Library Search Compound Report

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Acq On : 30 Jun 2018 20:24
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Sample : J3638-02 2X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

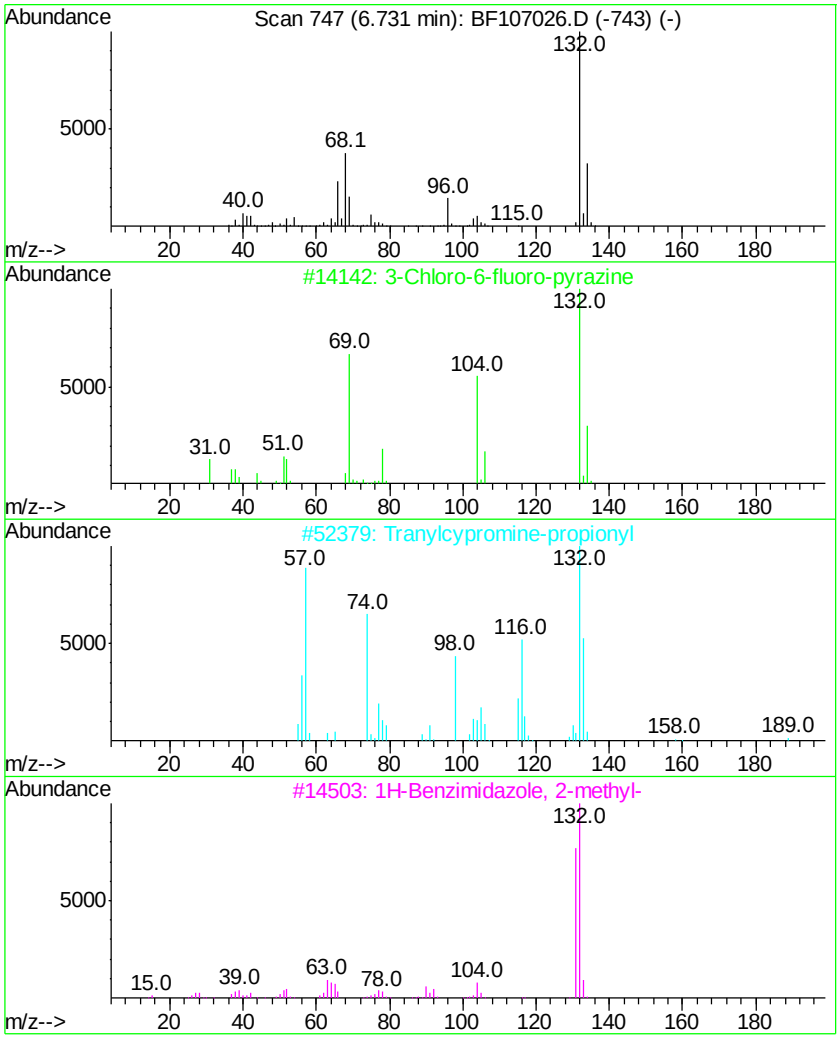
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

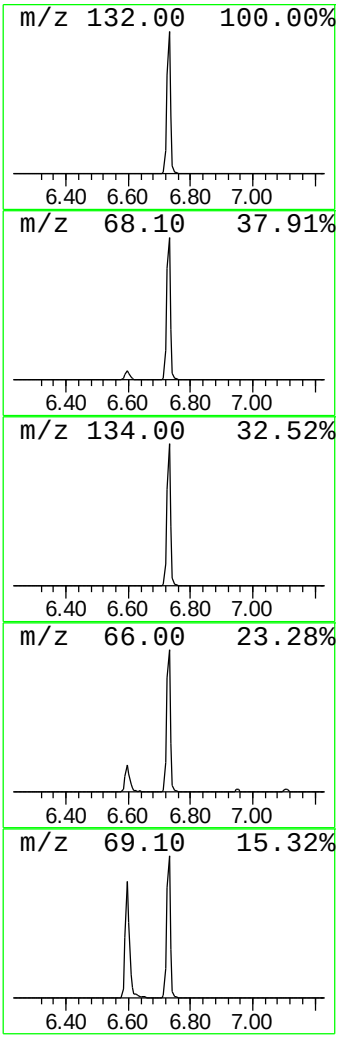
****

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	38.17 ng	754401	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF063018\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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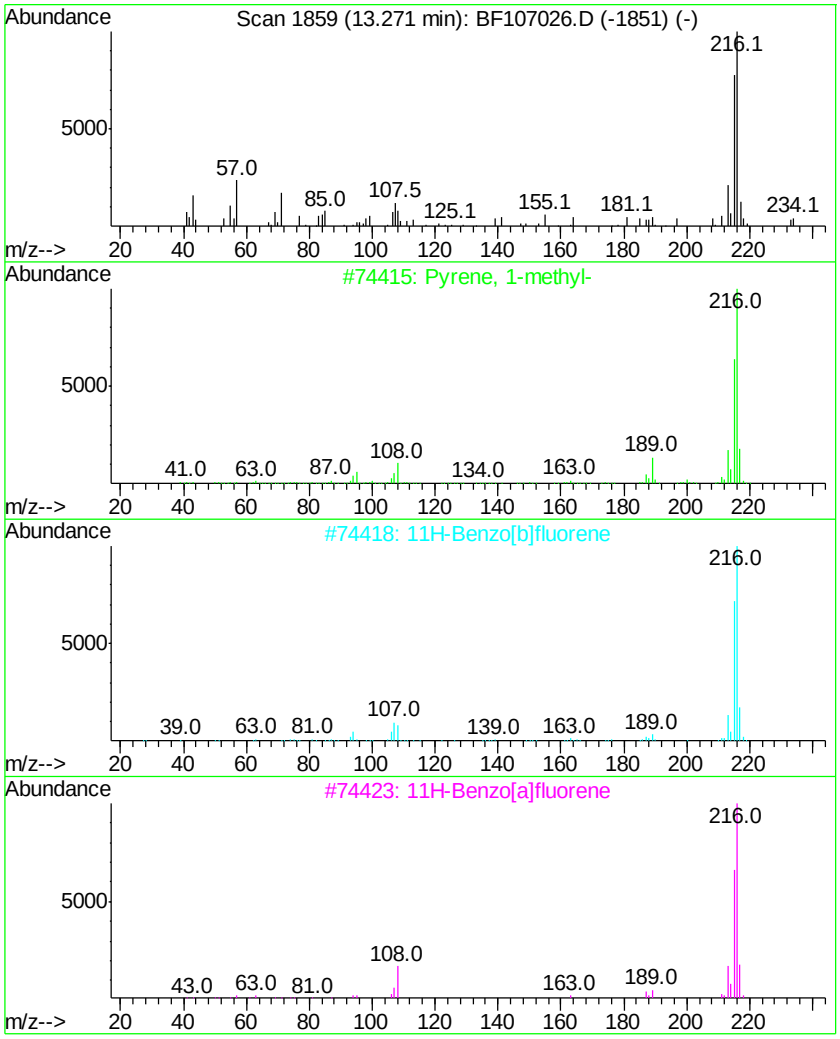
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

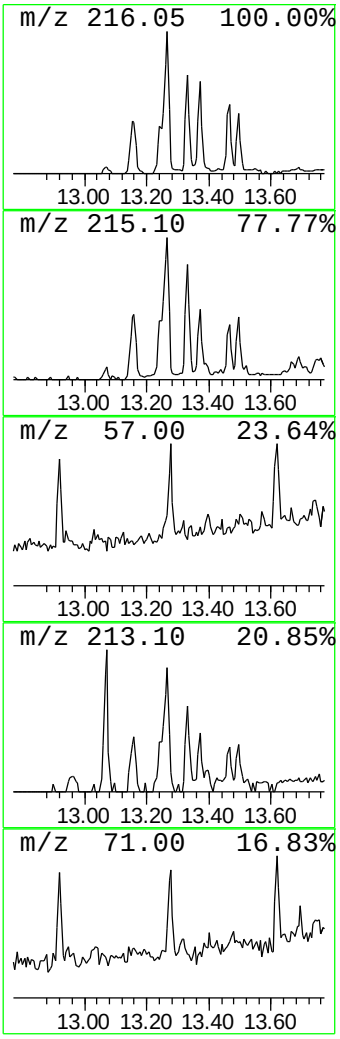
****

Peak Number 4 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	2.53 ng	94148	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	87
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF063018\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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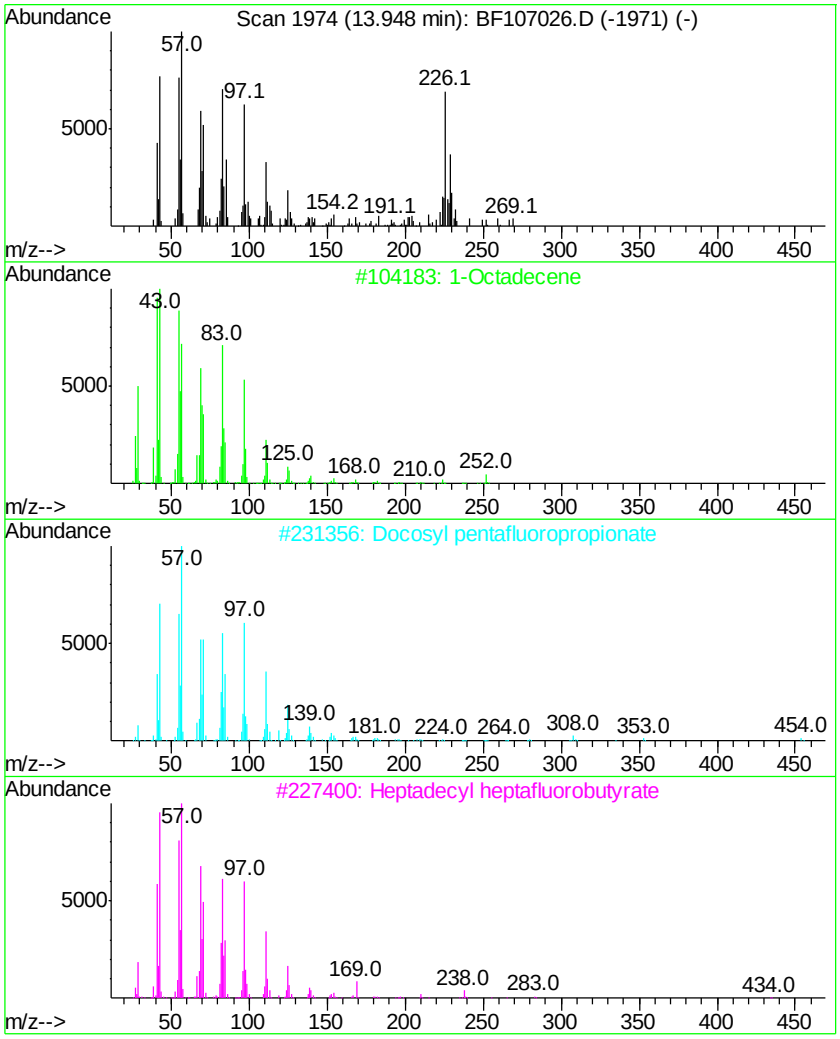
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

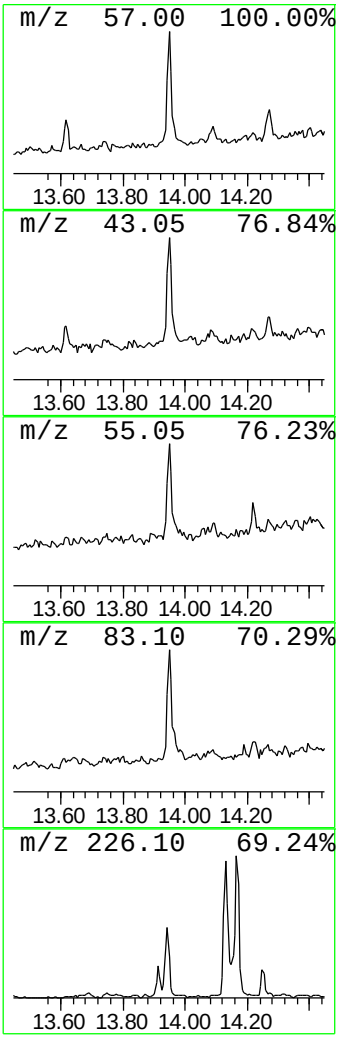
****

Peak Number 5 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.86 ng	143402	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	89
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	70
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	64
5	1-Hentetracontanol	593	C41H84O	040710-42-7	62





Library Search Compound Report

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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : P-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

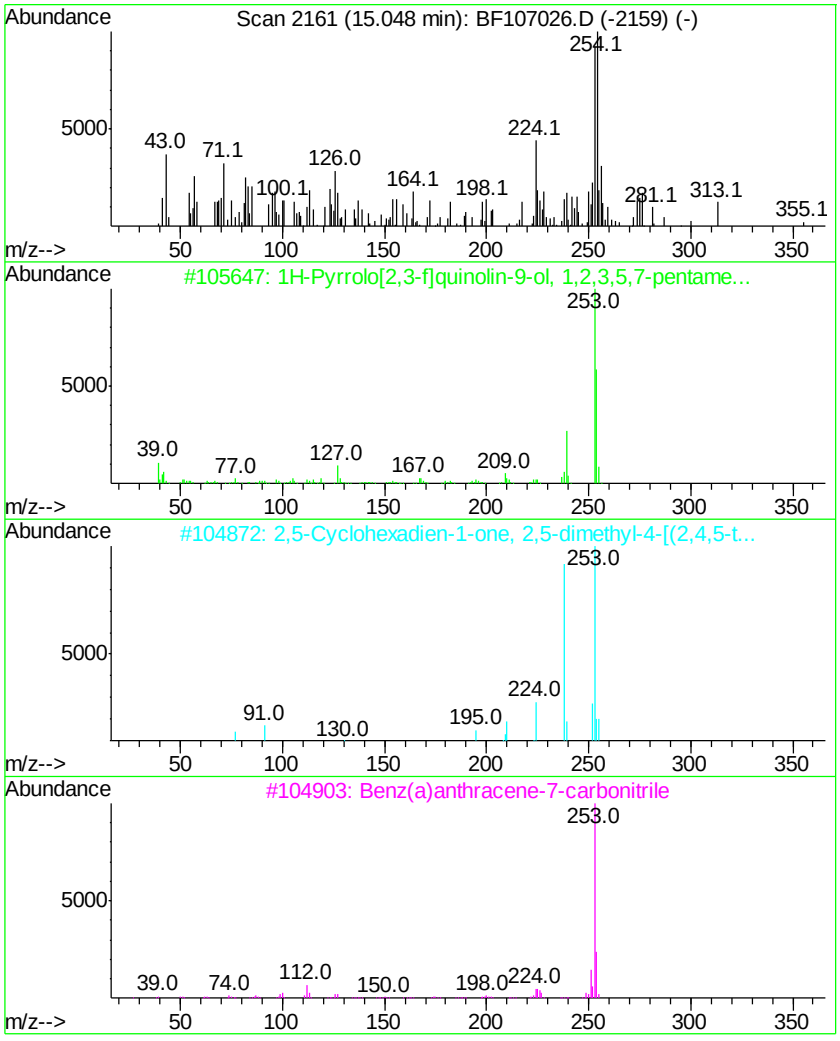
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

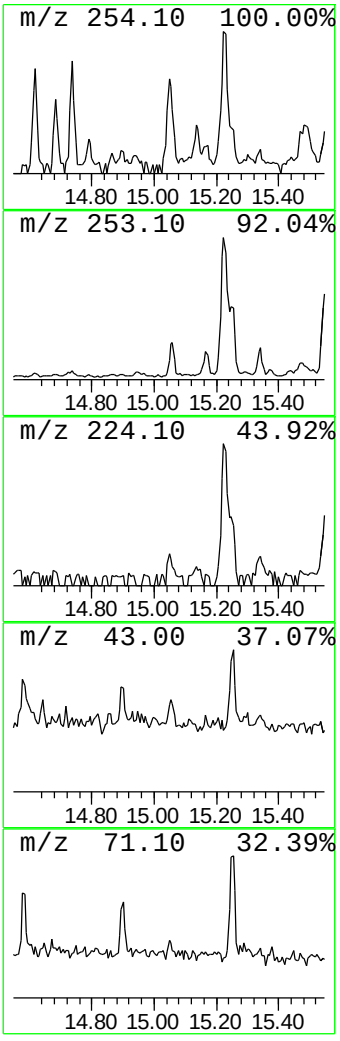
****

Peak Number 6 unknown15.05 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	3.49 ng	49599	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrrolo[2,3-f]quinolin-9-ol, ...	254	C16H18N2O	1000303-71-9	38
2	2,5-Cyclohexadien-1-one, 2,5-dim...	253	C17H19NO	054245-93-1	37
3	Benz(a)anthracene-7-carbonitrile	253	C19H11N	007476-08-6	35
4	4-Propyl-10H-acridine-9-thione	253	C16H15NS	1000211-07-8	32
5	10-Oxo-5,5-dimethyl-5-sila-5,10-...	254	C14H14N2OSi	089052-45-9	27





Tentatively Identified Compound (LSC) summary

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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...	5.18	2.7	ng	52893	1	6.95	395282	20.0
unknown6.73	6.73	38.2	ng	754401	1	6.95	395282	20.0
Pyrene, 1-methyl-	13.27	2.5	ng	94148	5	14.14	743620	20.0
1-Octadecene	13.95	3.9	ng	143402	5	14.14	743620	20.0
unknown15.05	15.05	3.5	ng	49599	6	15.68	284490	20.0