LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042618\
Data File : BF104842.D
Acq On : 26 Apr 2018 17:34
Operator : JU/SJ
Sample : J2155-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-042418-A

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-BF040618.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	5.016	494	498	506	rBV	90162	112534	4.41%	0.451%
2	5.422	562	567	570	rBV	2480738	2369882	92.85%	9.489%
3	6.445	735	741	744	rBV	2372878	2346732	91.95%	9.397%
4	6.575	758	763	766	rBV	2525861	2498927	97.91%	10.006%
5	6.798	797	801	804	rBV	817996	656671	25.73%	2.629%
6	6.951	823	827	831	rBV	2056654	1964597	76.97%	7.866%
7	7.363	892	897	908	rBV	1431009	1557022	61.01%	6.234%
8	8.081	1015	1019	1035	rVB	935468	868043	34.01%	3.476%
9	9.157	1198	1202	1205	rBV	2891684	2552285	100.00%	10.220%
10	9.551	1264	1269	1277	rBV	187683	176244	6.91%	0.706%
11	9.757	1302	1304	1309	rVB	46594	40125	1.57%	0.161%
12	9.839	1314	1318	1326	rBV	1015378	927122	36.33%	3.712%
13	10.257	1386	1389	1393	rVB2	82964	73124	2.87%	0.293%
14	10.480	1421	1427	1429	rBV	22383	29205	1.14%	0.117%
15	10.633	1449	1453	1463	rBV	1621384	1538342	60.27%	6.160%
16	10.733	1467	1470	1476	rVB	72001	72852	2.85%	0.292%
17	11.327	1567	1571	1574	rBV	903653	813150	31.86%	3.256%
18	11.351	1574	1575	1581	rVB	103485	73416	2.88%	0.294%
19	11.710	1633	1636	1640	rVB	95240	79192	3.10%	0.317%
20	12.398	1747	1753	1755	rBV2	285166	261515	10.25%	1.047%
21	12.422	1755	1757	1762	rVB	212068	185709	7.28%	0.744%
22	12.504	1769	1771	1774	rVB	46702	36834	1.44%	0.147%
23	12.545	1774	1778	1782	rBV	339501	286090	11.21%	1.146%
24	12.774	1811	1817	1823	rBV	313672	311382	12.20%	1.247%
25	12.916	1834	1841	1844	rBV	2269982	2094277	82.05%	8.386%
26	12.998	1850	1855	1859	rBV3	29018	49976	1.96%	0.200%
27	13.104	1865	1873	1876	rBV2	45884	94967	3.72%	0.380%
28	13.204	1887	1890	1893	rBV2	33722	40449	1.58%	0.162%
29	13.298	1904	1906	1909	rBV	25505	29129	1.14%	0.117%
30	13.616	1957	1960	1963	rVB	42298	37596	1.47%	0.151%
31	13.727	1976	1979	1981	rBV	32237	28984	1.14%	0.116%
32	13.774	1985	1987	1989	rBV2	39241	34363	1.35%	0.138%
33	13.804	1989	1992	1994	rVV3	145898	136574	5.35%	0.547%
34	13.974	2016	2021	2024	rBV2	788656	921944	36.12%	3.692%

LSC Area Percent Report

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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-042418-A

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.004	2024	2026	2032	rVB	229870	212249	8.32%	0.850%
36	14.445	2098	2101	2106	rVB5	34255	42774	1.68%	0.171%
37	15.015	2195	2198	2202	rBV	179236	268028	10.50%	1.073%
38	15.321	2246	2250	2252	rBV	124394	162680	6.37%	0.651%
39	15.380	2257	2260	2266	rVB	193095	284739	11.16%	1.140%
40	15.445	2267	2271	2275	rBV	483066	616602	24.16%	2.469%
41	16.904	2515	2519	2523	rBV2	54896	88088	3.45%	0.353%

Sum of corrected areas: 24974414

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042618\
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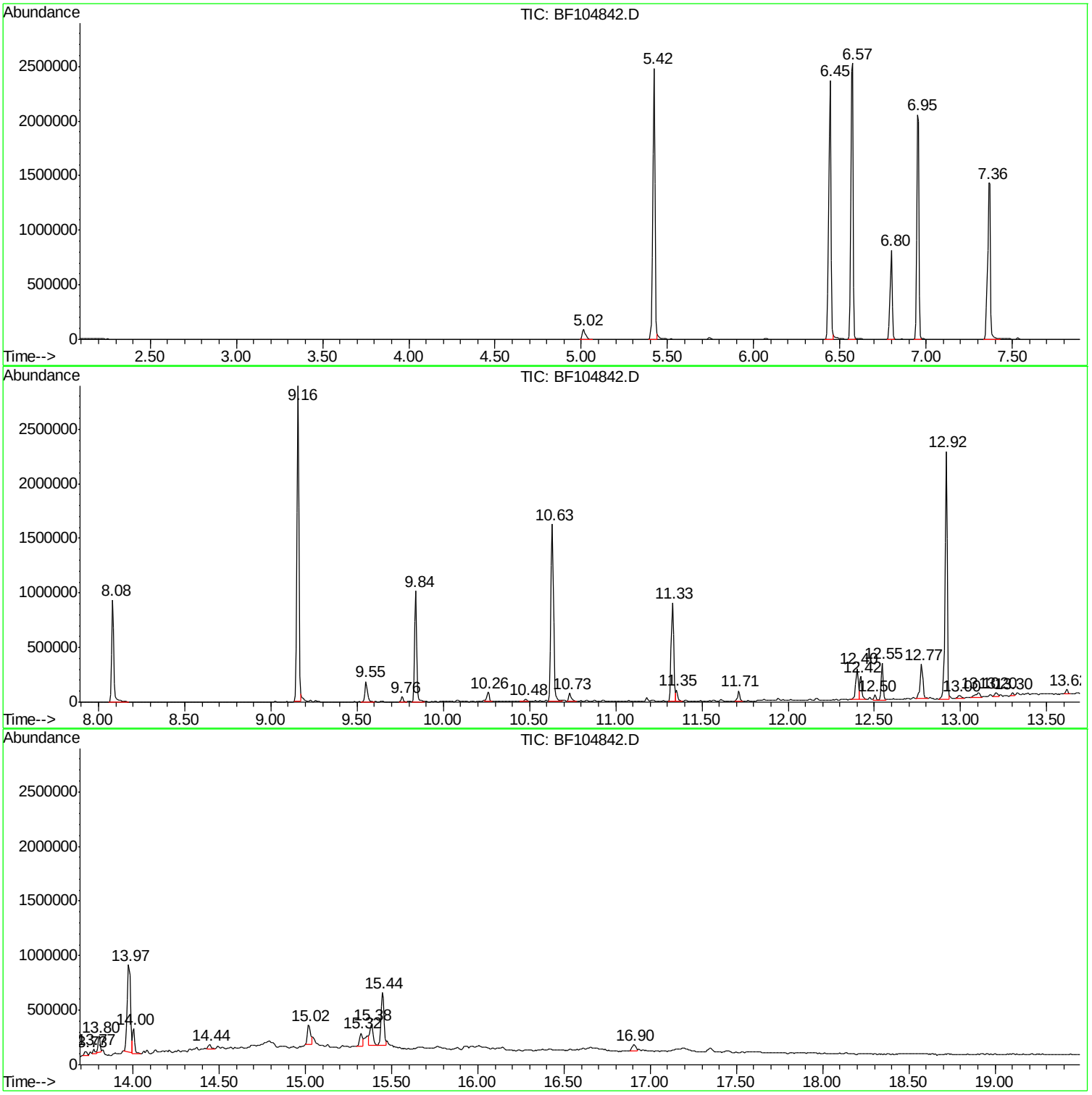
Operator : JU/SJ
Sample : J2155-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-042418-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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:\HPCHEM1\BNA F\DATA\BF042618\
Data File : BF104842.D
Acq On : 26 Apr 2018 17:34
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Sample : J2155-07
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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-042418-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

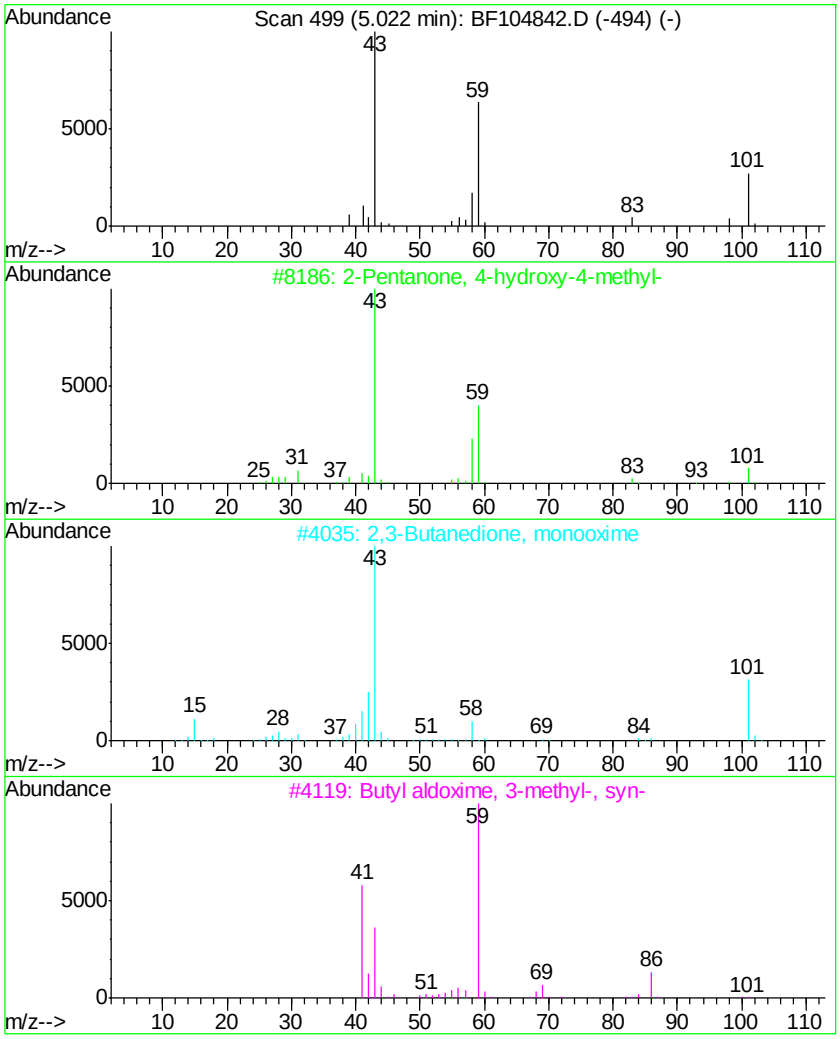
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

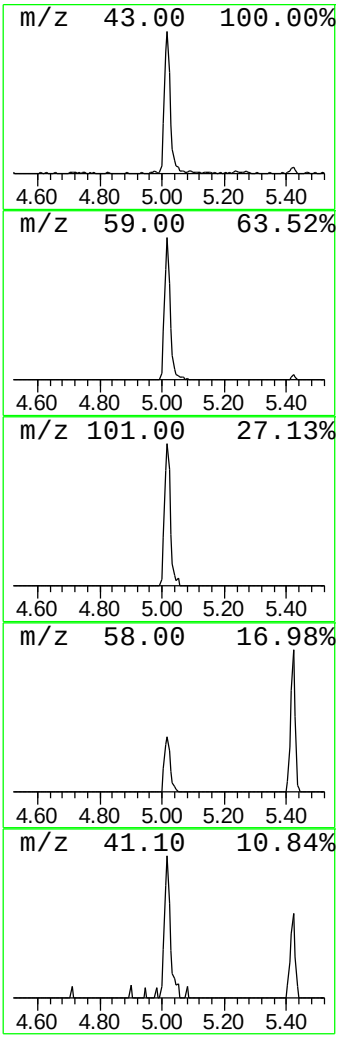
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.43 ng	112534	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	1,2-Butanediol	90	C4H10O2	000584-03-2	23
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042618\
Data File : BF104842.D
Acq On : 26 Apr 2018 17:34
Operator : JU/SJ
Sample : J2155-07
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NB-08-042418-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

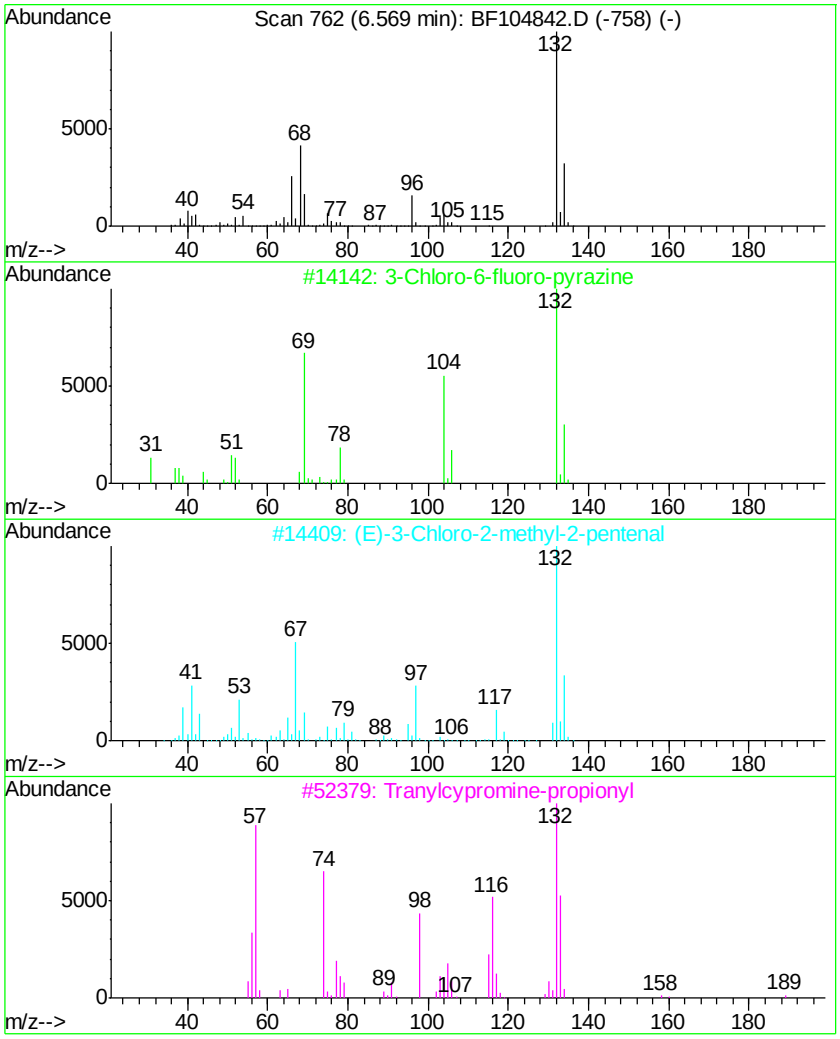
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

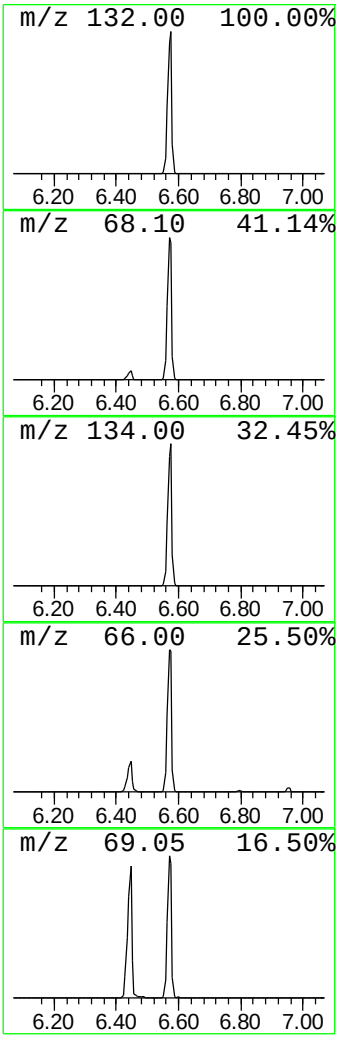
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	76.11 ng	2498930	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Instrument : BNA_F
ClientSampleId : NB-08-042418-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

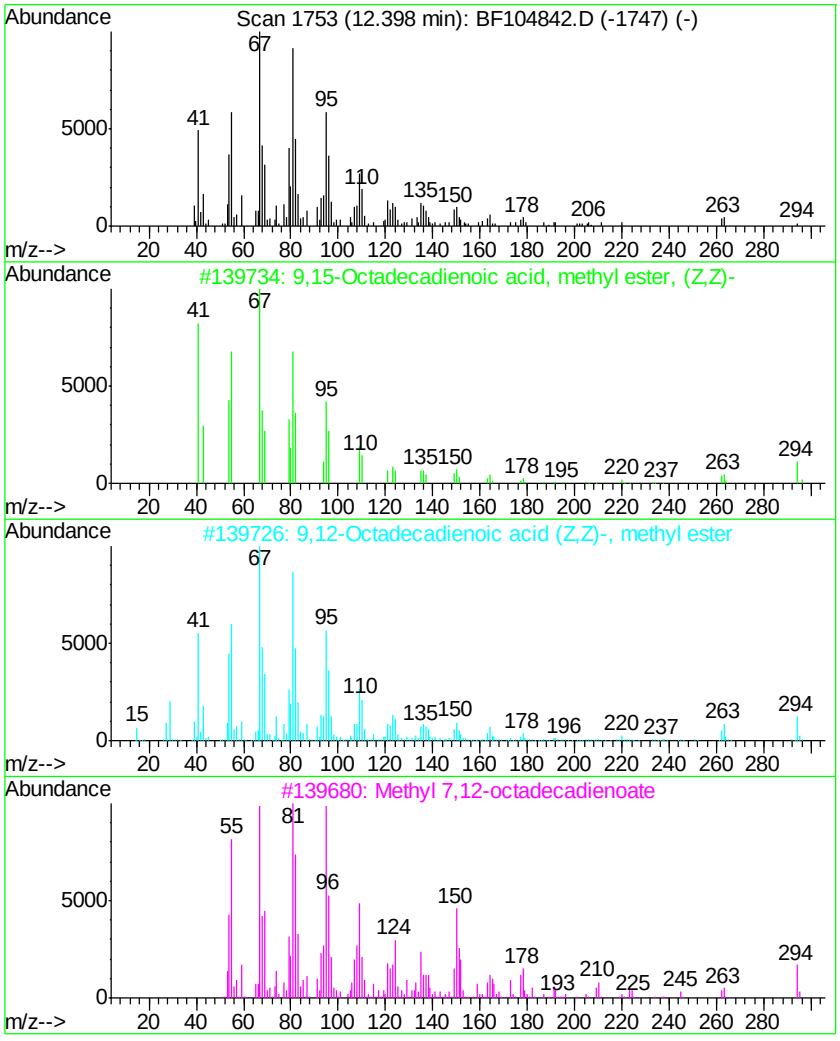
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

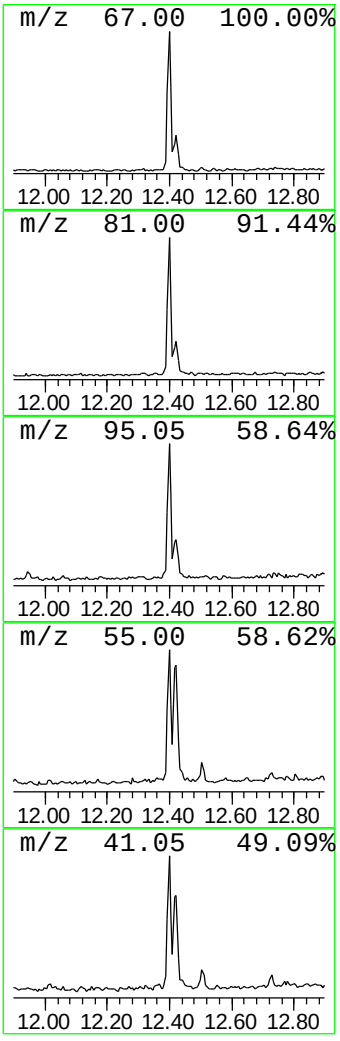
****

Peak Number 4 9,15-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	6.43 ng	261515	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,15-Octadecadienoic acid, methv...	294	C19H34O2	017309-05-6	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	Methyl 7,12-octadecadienoate	294	C19H34O2	1000336-43-8	97
4	9,12-Octadecadienoic acid, methv...	294	C19H34O2	002566-97-4	96
5	12,15-Octadecadienoic acid, meth...	294	C19H34O2	057156-97-5	96





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Sample : J2155-07
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Instrument : BNA_F
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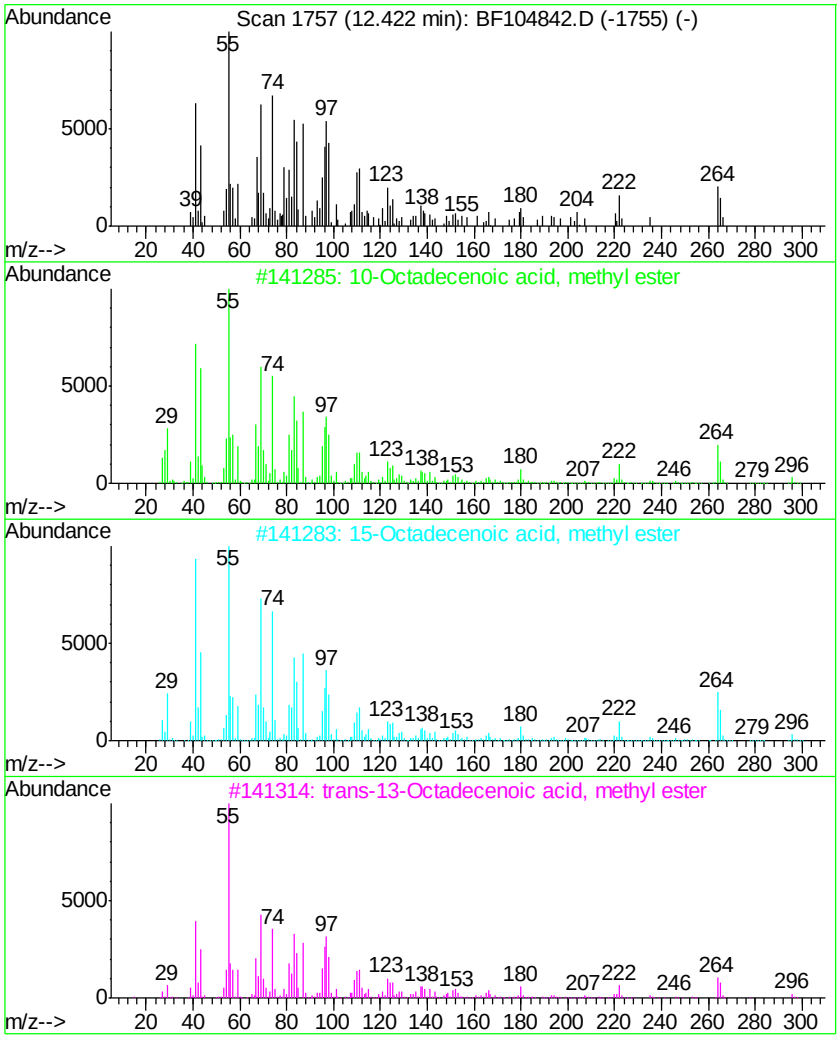
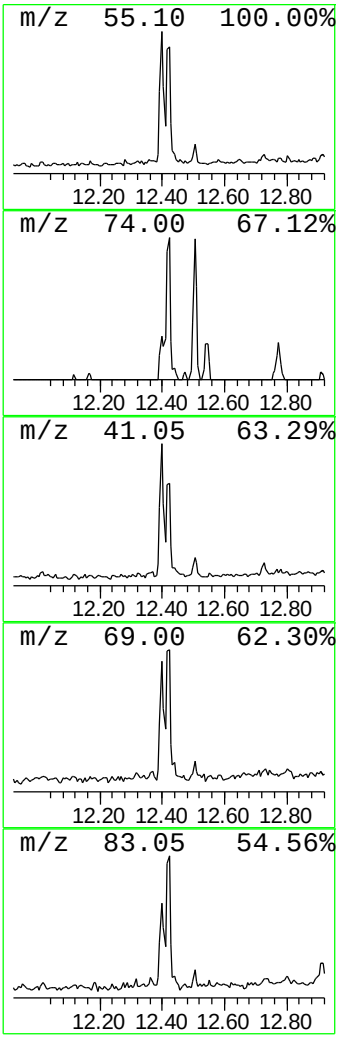
****

Peak Number 5 10-Octadecenoic acid, methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	4.57 ng	185709	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	91
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
5	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90





Library Search Compound Report

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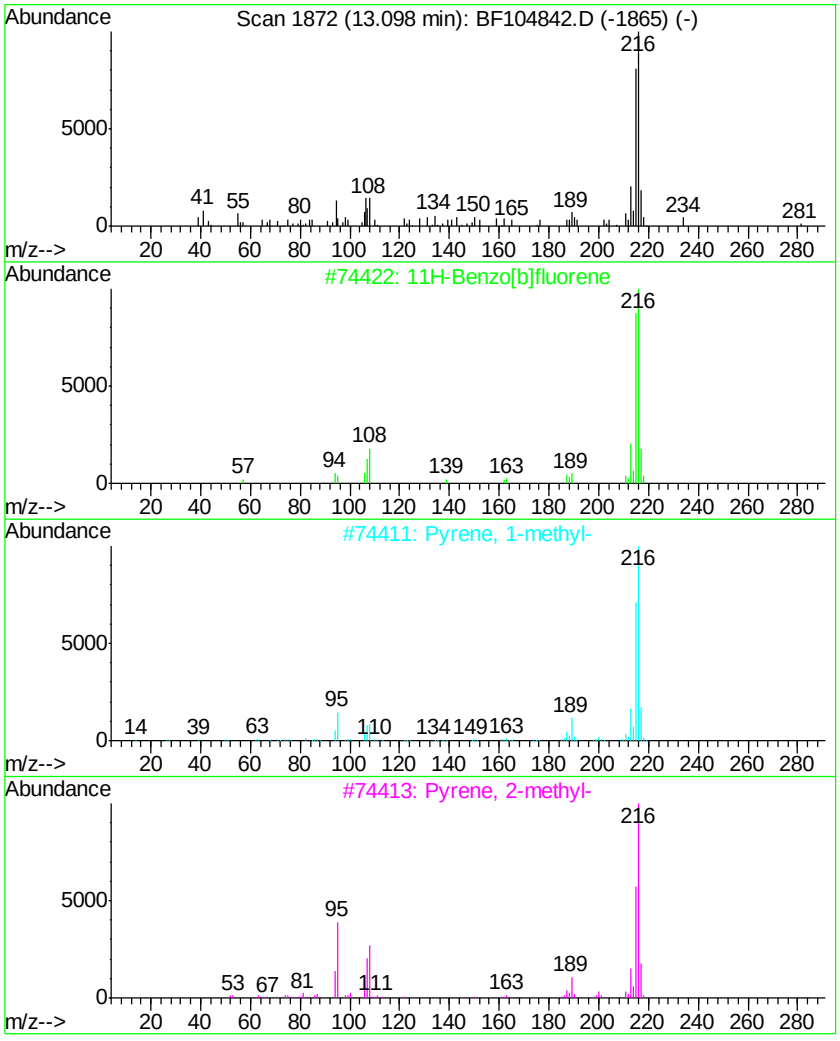
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

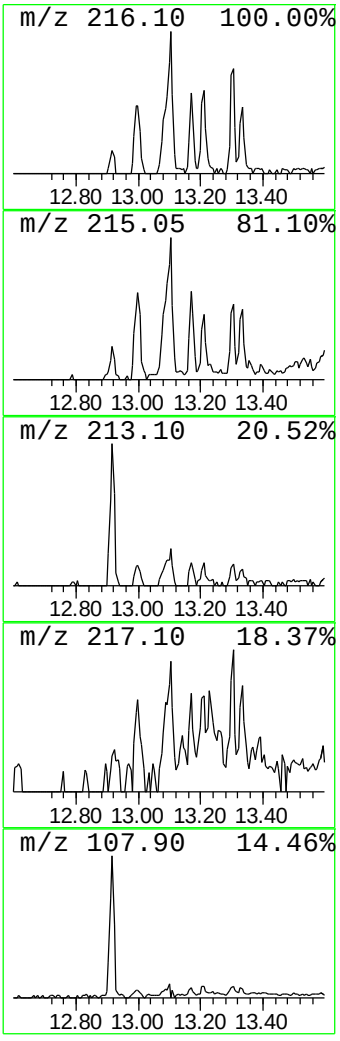
****

Peak Number 6 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.10	2.06 ng	94967	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	96
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	90
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	86





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

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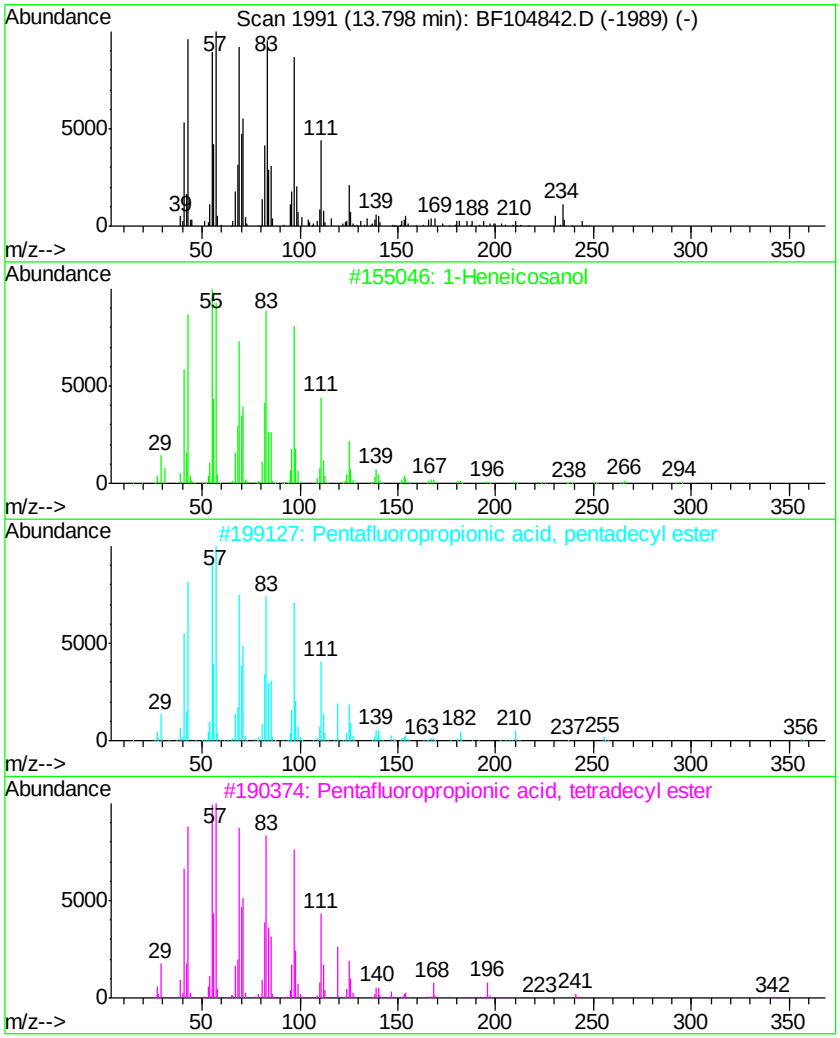
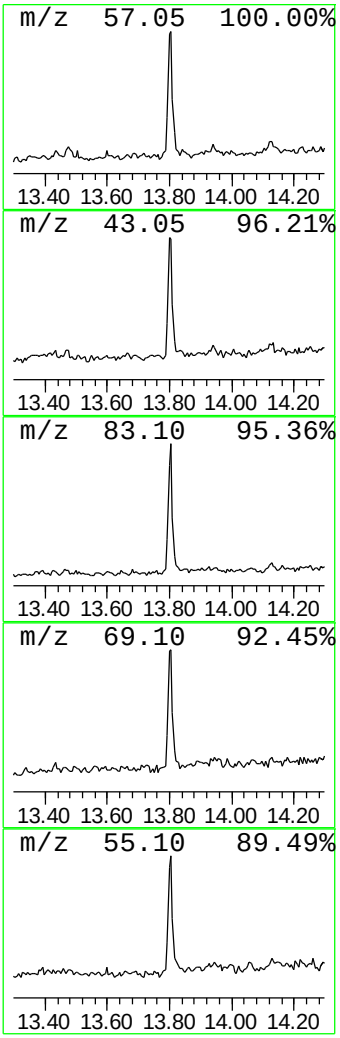
Peak Number 7 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	2.96 ng	136574	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





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...	5.02	3.4	ng	112534	1	6.80	656671	20.0
unknown6.57	6.57	76.1	ng	2498930	1	6.80	656671	20.0
9,15-Octadecadien...	12.40	6.4	ng	261515	4	11.33	813150	20.0
10-Octadecenoic a...	12.42	4.6	ng	185709	4	11.33	813150	20.0
11H-Benzo[b]fluorene	13.10	2.1	ng	94967	5	13.97	921944	20.0
1-Heneicosanol	13.80	3.0	ng	136574	5	13.97	921944	20.0