LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

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-BF020318.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	2.163	8	13	18	rVB	426078	587398	15.74%	1.600%
2	4.493	404	409	416	rBV	38610	46378	1.24%	0.126%
3	5.110	511	514	522	rVB	130474	170452	4.57%	0.464%
4	5.504	576	581	584	rBV	3775931	3713429	99.48%	10.118%
5	6.510	747	752	770	rVB	3298127	3732691	100.00%	10.170%
6	6.657	772	777	780	rBV	3561311	3564066	95.48%	9.711%
7	6.887	812	816	819	rBV	1303187	1121209	30.04%	3.055%
8	7.040	838	842	846	rBV	3062699	2838878	76.05%	7.735%
9	7.445	906	911	914	rBV	2557991	2366718	63.41%	6.448%
10	7.622	938	941	945	rVB	61716	54928	1.47%	0.150%
11	8.169	1030	1034	1037	rBV	1607137	1393626	37.34%	3.797%
12	9.239	1212	1216	1220	rBV	3632662	3498125	93.72%	9.531%
13	9.316	1226	1229	1231	rVB	65736	50052	1.34%	0.136%
14	9.633	1279	1283	1286	rBV	397828	360950	9.67%	0.983%
15	9.845	1315	1319	1322	rBV	205153	155976	4.18%	0.425%
16	9.922	1328	1332	1336	rBV	1503778	1324355	35.48%	3.608%
17	10.169	1371	1374	1378	rBV2	40989	45094	1.21%	0.123%
18	10.345	1401	1404	1407	rVB	231956	173766	4.66%	0.473%
19	10.563	1435	1441	1444	rBV	54966	74743	2.00%	0.204%
20	10.710	1463	1466	1477	rVB	1669967	1678959	44.98%	4.574%
21	10.816	1481	1484	1495	rVB	165992	194581	5.21%	0.530%
22	11.269	1557	1561	1563	rBV	75626	64537	1.73%	0.176%
23	11.298	1563	1566	1572	rVB4	26099	40236	1.08%	0.110%
24	11.410	1581	1585	1588	rBV	1226969	1127399	30.20%	3.072%
25	11.433	1588	1589	1596	rVB	194836	140991	3.78%	0.384%
26	11.927	1667	1673	1677	rBV2	53981	99601	2.67%	0.271%
27	12.022	1686	1689	1692	rBV2	49710	55678	1.49%	0.152%
28	12.233	1722	1725	1731	rVB	42236	40496	1.08%	0.110%
29	12.469	1761	1765	1768	rBV2	40940	48327	1.29%	0.132%
30	12.545	1776	1778	1783	rVB	43367	38805	1.04%	0.106%
31	12.622	1788	1791	1796	rVB	396151	367722	9.85%	1.002%
32	12.810	1820	1823	1825	rBV	53669	41949	1.12%	0.114%
33	12.857	1825	1831	1834	rBV	326408	354905	9.51%	0.967%
34	12.998	1843	1855	1858	rBV	2770836	2696343	72.24%	7.346%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.180	1884	1886	1890	rVB	37622	38879	1.04%	0.106%
36	13.469	1931	1935	1938	rBV4	29872	39549	1.06%	0.108%
37	13.686	1965	1972	1976	rBV2	30930	43996	1.18%	0.120%
38	13.804	1987	1992	1994	rBV3	34341	44113	1.18%	0.120%
39	13.880	2002	2005	2012	rVB2	260601	274861	7.36%	0.749%
40	14.021	2025	2029	2031	rBV	596696	509987	13.66%	1.390%
41	14.051	2031	2034	2037	rVV	1199247	1222849	32.76%	3.332%
42	14.074	2037	2038	2045	rVB	162993	136366	3.65%	0.372%
43	14.204	2056	2060	2069	rBV8	26210	41640	1.12%	0.113%
44	14.510	2109	2112	2115	rBV3	39315	49163	1.32%	0.134%
45	14.668	2136	2139	2145	rVB2	46638	54219	1.45%	0.148%
46	14.821	2162	2165	2169	rVB4	39505	42411	1.14%	0.116%
47	14.963	2187	2189	2193	rVB3	35916	38440	1.03%	0.105%
48	15.098	2208	2212	2216	rBV	132794	219935	5.89%	0.599%
49	15.163	2220	2223	2226	rVV	49086	52171	1.40%	0.142%
50	15.410	2261	2265	2269	rVB	79896	102801	2.75%	0.280%
51	15.474	2272	2276	2281	rVB	90618	118989	3.19%	0.324%
52	15.539	2282	2287	2299	rBV	769207	1049146	28.11%	2.859%
53	15.992	2360	2364	2369	rVB	64989	95941	2.57%	0.261%
54	16.515	2448	2453	2458	rBV3	32725	61924	1.66%	0.169%
55	17.033	2538	2541	2550	rVB3	31364	59300	1.59%	0.162%
56	17.121	2552	2556	2564	rVB2	42469	86018	2.30%	0.234%
57	17.492	2615	2619	2626	rVB2	27184	56573	1.52%	0.154%

Sum of corrected areas: 36702634

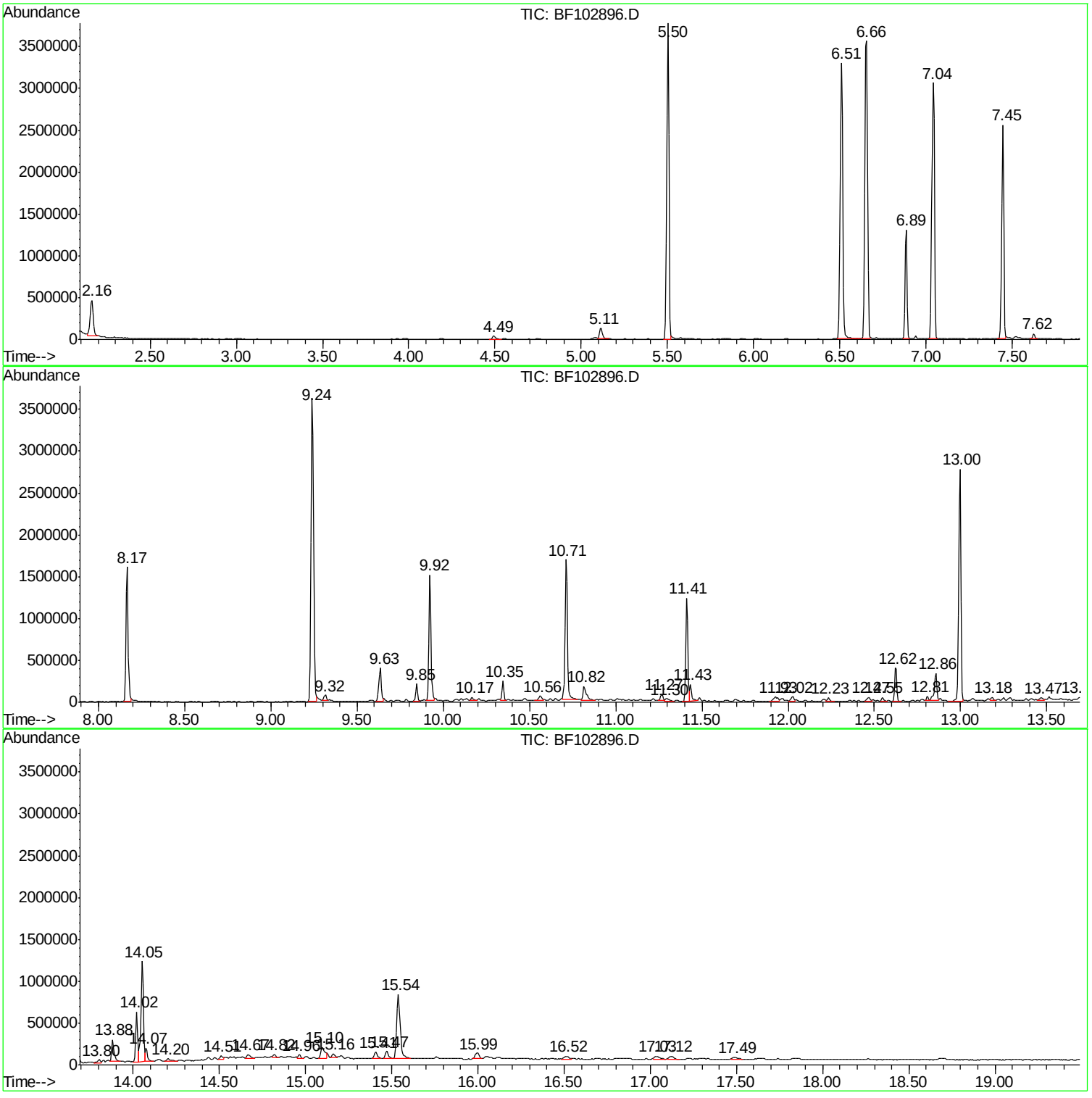
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

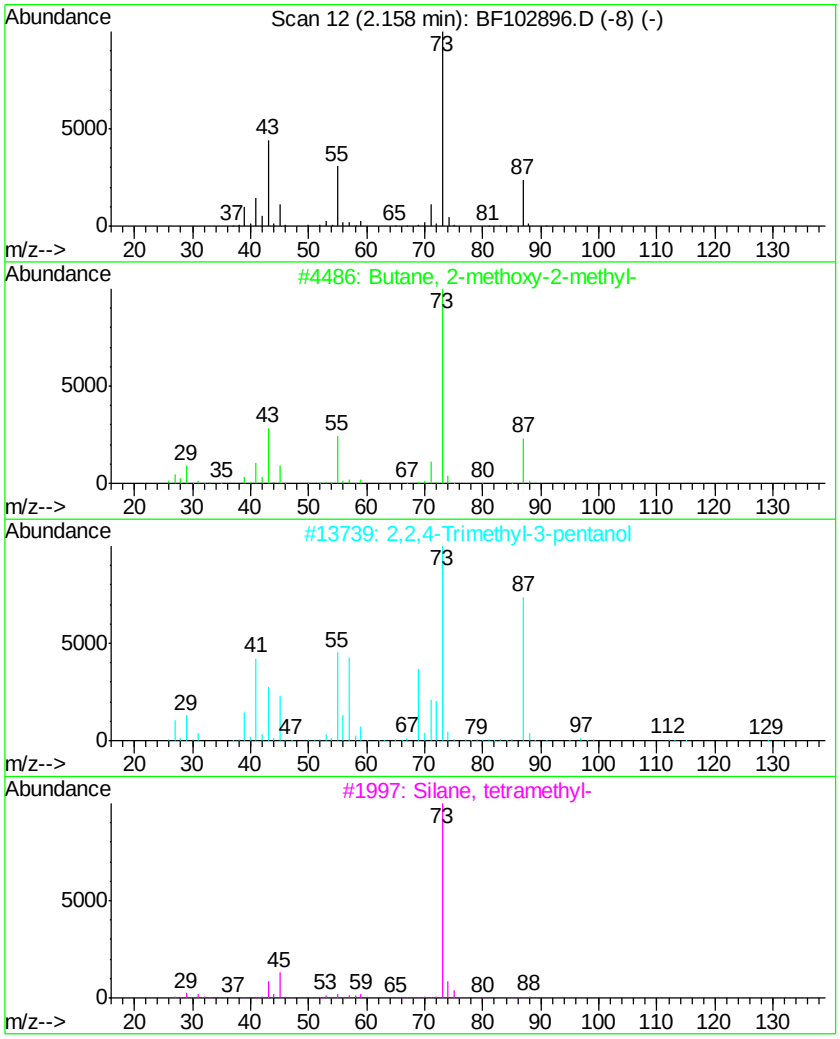
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

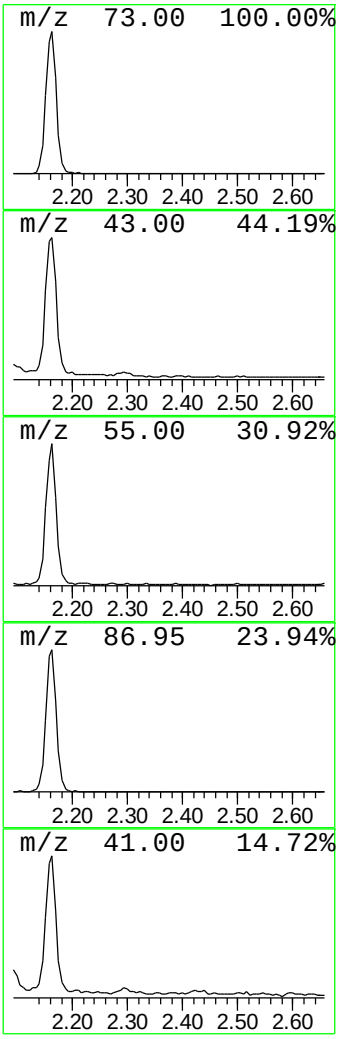
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	10.48 ng	587398	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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

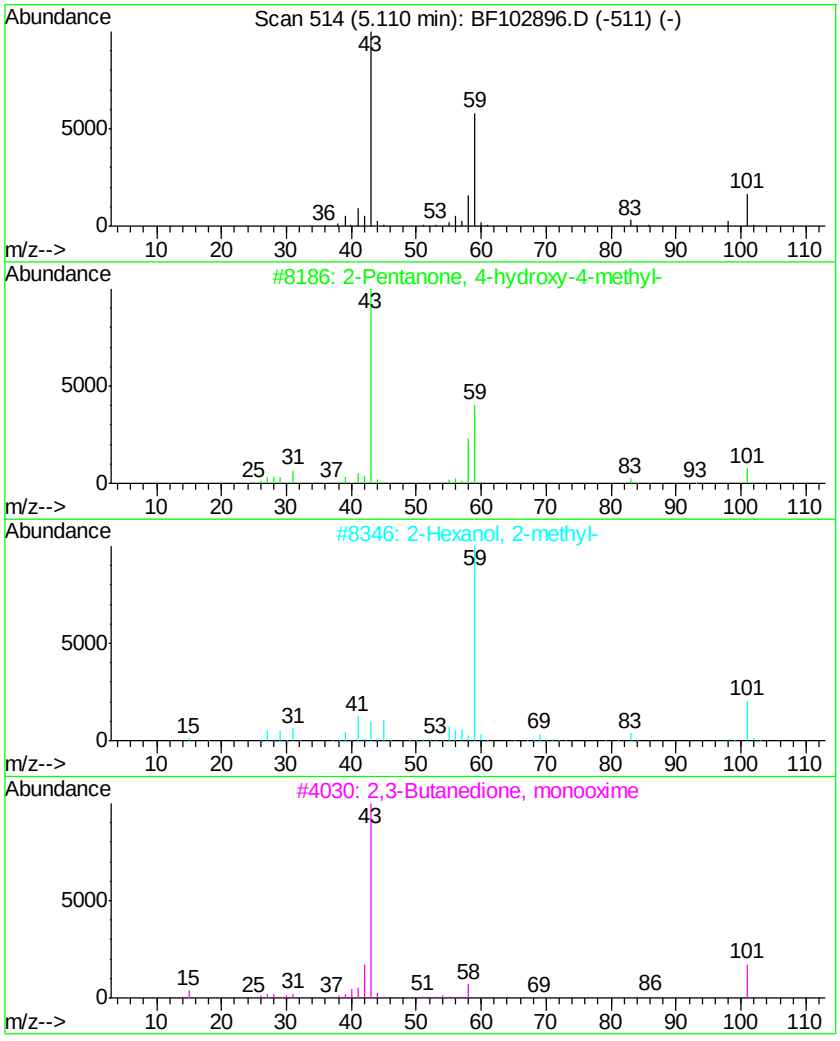
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

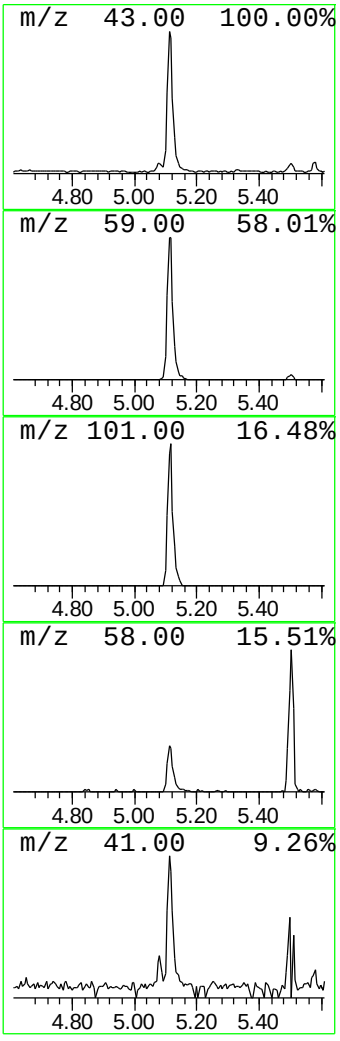
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	3.04 ng	170452	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	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Acetone	58	C3H6O	000067-64-1	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

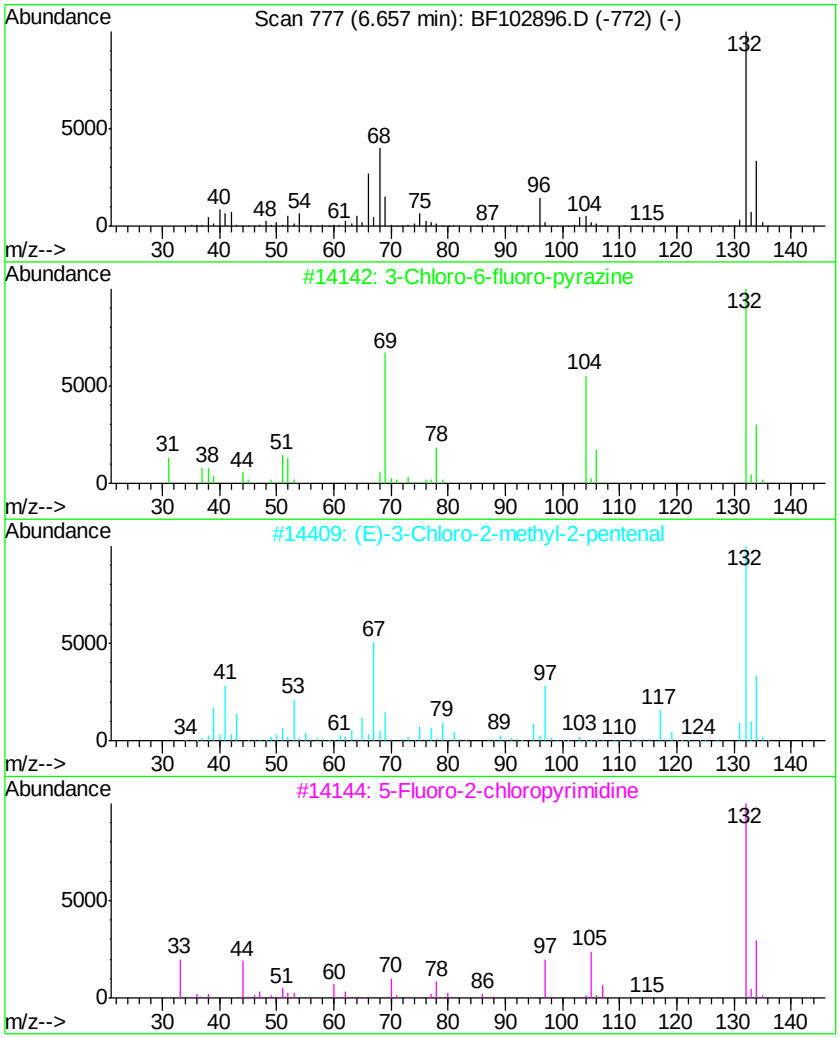
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

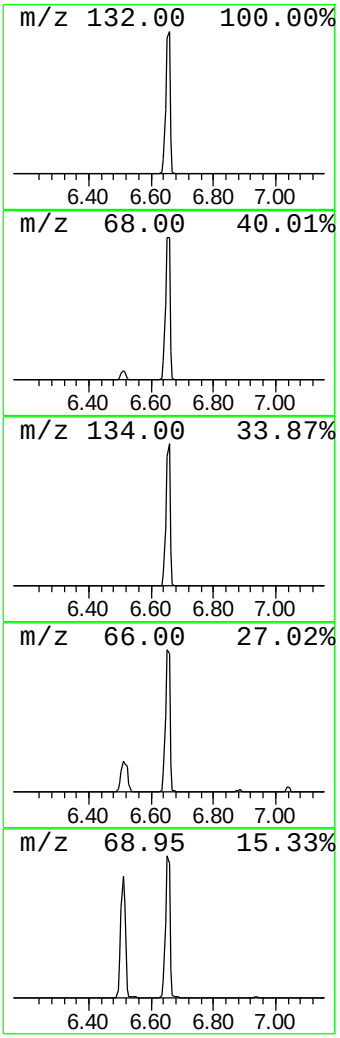
****

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	63.58 ng	3564070	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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

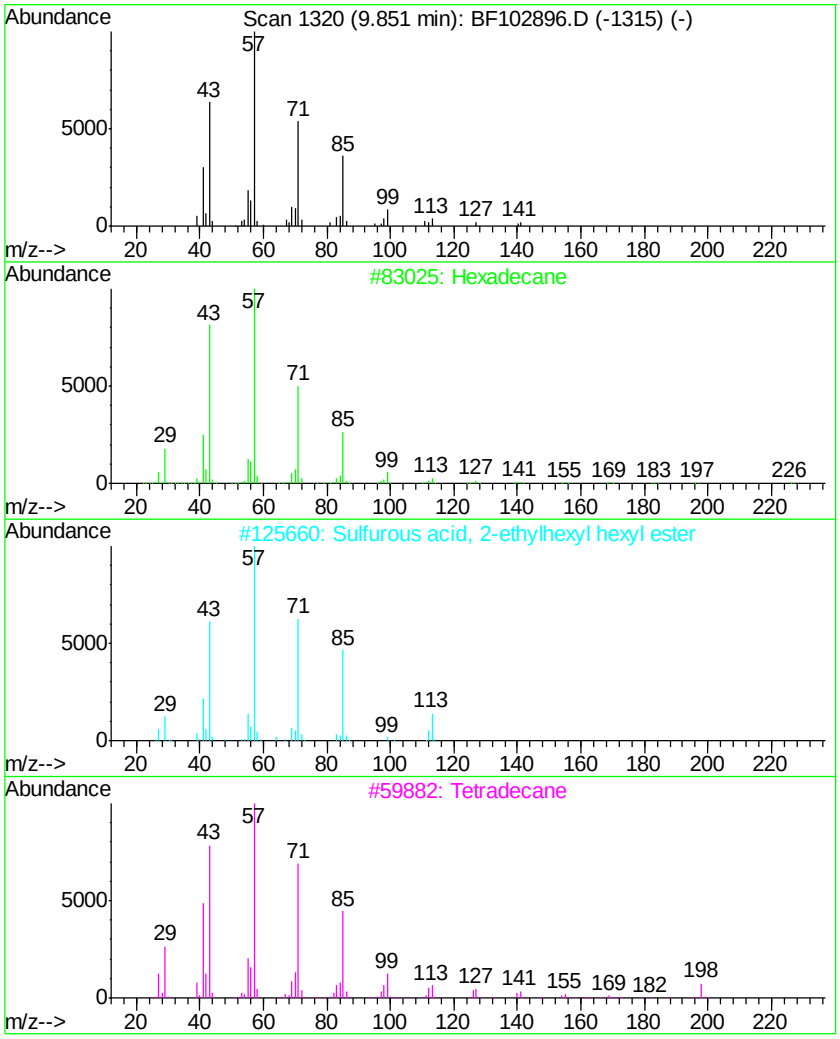
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

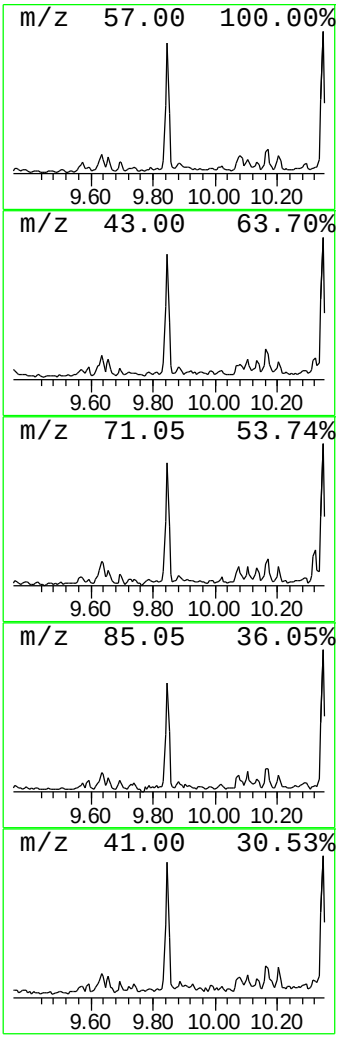
****

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.36 ng	155976	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
3	Tetradecane	198	C14H30	000629-59-4	80
4	Tridecane	184	C13H28	000629-50-5	78
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

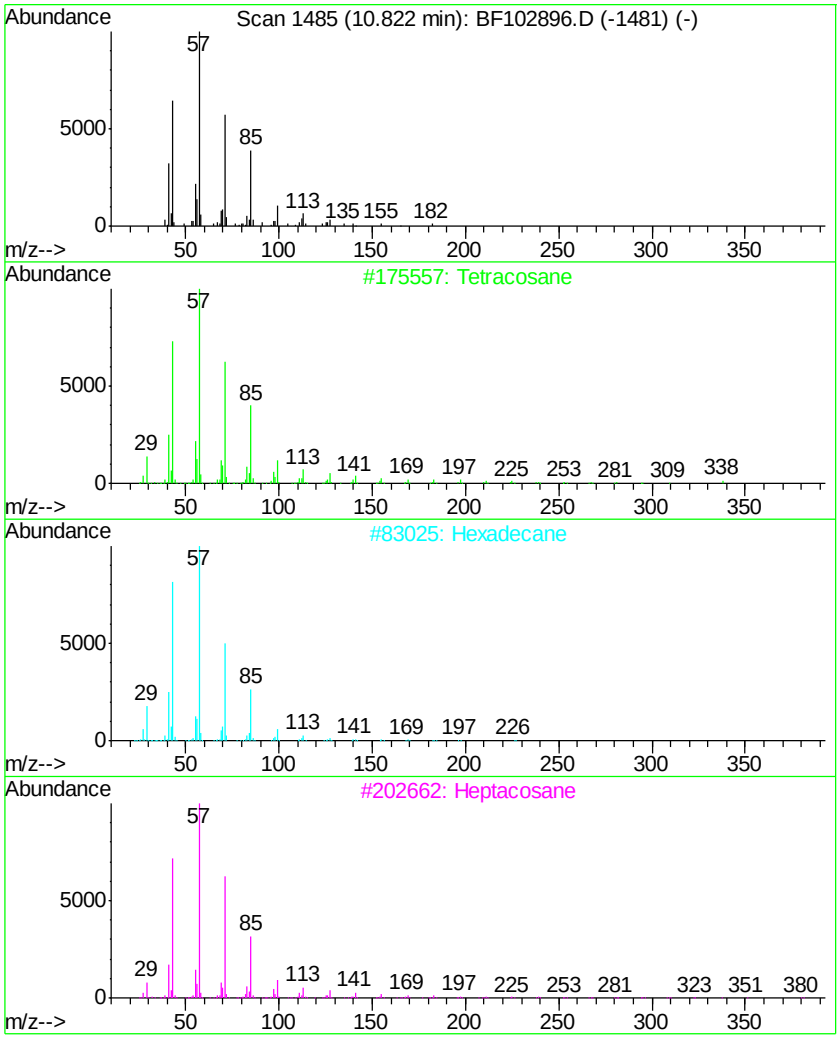
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

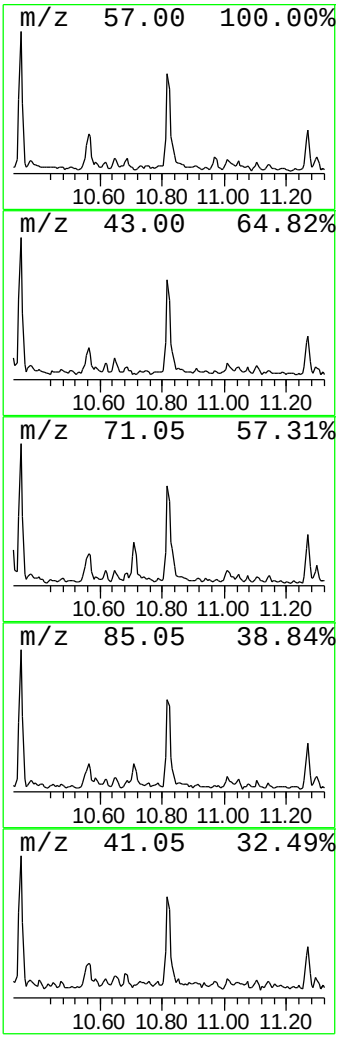
****

Peak Number 7 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.45 ng	194581	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

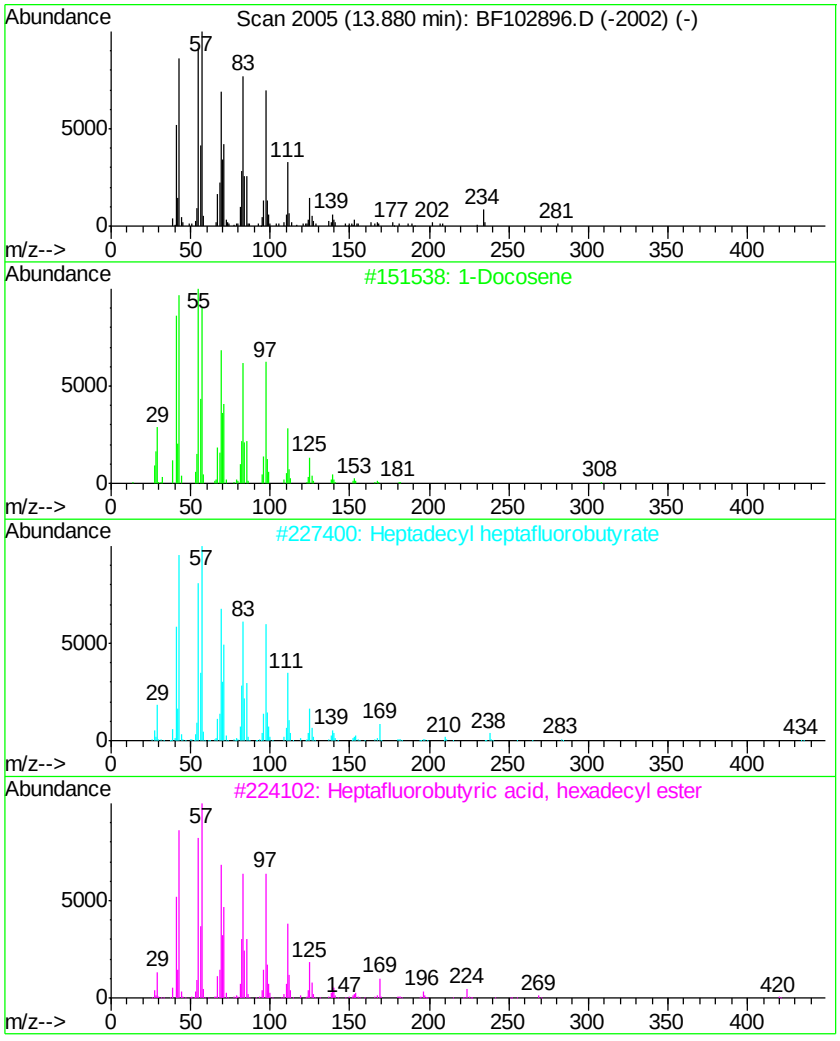
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

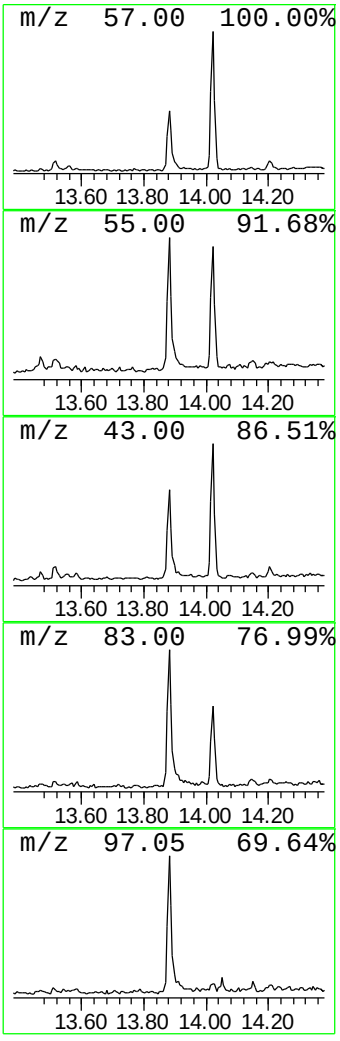
****

Peak Number 8 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	4.50 ng	274861	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
4	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102896.D
Acq On : 9 Feb 2018 18:38
Operator : SJ/JU
Sample : J1499-01
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-154

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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...	2.16	10.5	ng	587398	1	6.89	1121210	20.0
2-Pentanone, 4-hy...	5.11	3.0	ng	170452	1	6.89	1121210	20.0
unknown6.66	6.66	63.6	ng	3564070	1	6.89	1121210	20.0
Hexadecane	9.85	2.4	ng	155976	3	9.92	1324360	20.0
Tetracosane	10.82	3.5	ng	194581	4	11.41	1127400	20.0
1-Docosene	13.88	4.5	ng	274861	5	14.05	1222850	20.0