LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102881.D
Acq On : 9 Feb 2018 11:50
Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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	2.128	3	7	16	rVB	217592	278964	13.62%	0.887%
2	5.098	509	512	518	rVB	58006	64417	3.14%	0.205%
3	5.498	573	580	583	rBV	2095257	2048787	100.00%	6.518%
4	6.504	747	751	757	rBV	2207148	1912422	93.34%	6.084%
5	6.651	772	776	779	rBV	2432750	2034004	99.28%	6.471%
6	6.710	783	786	790	rVB2	43041	40633	1.98%	0.129%
7	6.881	812	815	819	rBV	1148819	1063511	51.91%	3.383%
8	6.939	822	825	831	rVB2	30845	32742	1.60%	0.104%
9	7.039	838	842	845	rBV	1920811	1551891	75.75%	4.937%
10	7.063	845	846	849	rVB	66467	35280	1.72%	0.112%
11	7.198	865	869	876	rVB4	27219	37361	1.82%	0.119%
12	7.281	876	883	887	rBV4	17018	28444	1.39%	0.090%
13	7.416	902	906	907	rBV	30206	25443	1.24%	0.081%
14	7.445	907	911	914	rVV	1529211	1353242	66.05%	4.305%
15	7.475	914	916	920	rVV	30642	31184	1.52%	0.099%
16	7.516	920	923	928	rVB4	28496	33236	1.62%	0.106%
17	7.904	986	989	992	rVB2	28642	26505	1.29%	0.084%
18	8.139	1026	1029	1030	rBV	34697	26711	1.30%	0.085%
19	8.169	1030	1034	1036	rVV	1606531	1433024	69.94%	4.559%
20	8.186	1036	1037	1040	rVV	465719	307306	15.00%	0.978%
21	8.239	1044	1046	1050	rVB3	22483	27121	1.32%	0.086%
22	8.457	1078	1083	1086	rBV5	19524	28059	1.37%	0.089%
23	8.751	1130	1133	1137	rBV2	75067	68610	3.35%	0.218%
24	8.880	1152	1155	1159	rBV	263813	223779	10.92%	0.712%
25	8.933	1161	1164	1167	rVV	43179	43788	2.14%	0.139%
26	8.980	1167	1172	1175	rVB	172711	157159	7.67%	0.500%
27	9.110	1191	1194	1199	rBV4	25609	32671	1.59%	0.104%
28	9.180	1204	1206	1208	rVB	41965	27719	1.35%	0.088%
29	9.239	1212	1216	1219	rBV	2243053	1820053	88.84%	5.790%
30	9.316	1226	1229	1231	rBV	131719	102058	4.98%	0.325%
31	9.339	1231	1233	1238	rVB	63987	60331	2.94%	0.192%
32	9.392	1238	1242	1244	rVB4	28811	35319	1.72%	0.112%
33	9.433	1244	1249	1256	rBV	38567	51018	2.49%	0.162%
34	9.510	1257	1262	1266	rBV2	57571	79888	3.90%	0.254%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102881.D
Acq On : 9 Feb 2018 11:50
Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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	9.580	1267	1274	1276	rBV2	100917	130186	6.35%	0.414%
36	9.604	1276	1278	1280	rVB	41772	31221	1.52%	0.099%
37	9.633	1280	1283	1286	rBV2	216856	208545	10.18%	0.663%
38	9.698	1291	1294	1296	rBV2	52532	49765	2.43%	0.158%
39	9.780	1305	1308	1311	rBV	61286	65354	3.19%	0.208%
40	9.845	1314	1319	1322	rVB	216364	181801	8.87%	0.578%
41	9.922	1329	1332	1335	rBV2	1530098	1312544	64.06%	4.176%
42	9.957	1335	1338	1341	rVB	415859	349271	17.05%	1.111%
43	10.022	1346	1349	1354	rVB3	28079	37548	1.83%	0.119%
44	10.080	1354	1359	1361	rBV2	60404	81253	3.97%	0.258%
45	10.127	1361	1367	1370	rVB	214003	219775	10.73%	0.699%
46	10.163	1370	1373	1378	rBV3	66895	69070	3.37%	0.220%
47	10.204	1378	1380	1382	rVB	33417	23855	1.16%	0.076%
48	10.239	1383	1386	1388	rBV3	43710	46331	2.26%	0.147%
49	10.322	1397	1400	1402	rBV2	69441	85705	4.18%	0.273%
50	10.345	1402	1404	1407	rVB	267315	192426	9.39%	0.612%
51	10.469	1422	1425	1431	rBV	318739	288046	14.06%	0.916%
52	10.563	1438	1441	1444	rBV2	113240	124179	6.06%	0.395%
53	10.651	1454	1456	1460	rBV5	26690	34763	1.70%	0.111%
54	10.686	1460	1462	1463	rBV	31393	25975	1.27%	0.083%
55	10.710	1463	1466	1471	rVV	1169648	1101822	53.78%	3.505%
56	10.822	1482	1485	1486	rBV	266573	272686	13.31%	0.867%
57	10.886	1494	1496	1498	rBV2	43468	43243	2.11%	0.138%
58	11.016	1515	1518	1520	rBV4	55644	68436	3.34%	0.218%
59	11.104	1530	1533	1535	rBV	62249	52399	2.56%	0.167%
60	11.216	1550	1552	1555	rVB	62810	45932	2.24%	0.146%
61	11.269	1558	1561	1563	rVV	266384	230658	11.26%	0.734%
62	11.298	1563	1566	1572	rVB2	241609	300003	14.64%	0.954%
63	11.410	1582	1585	1587	rBV	1228866	1167360	56.98%	3.714%
64	11.439	1587	1590	1593	rVV	1198653	1142669	55.77%	3.635%
65	11.486	1595	1598	1601	rVB	284153	231615	11.30%	0.737%
66	11.639	1622	1624	1629	rVB2	151843	164622	8.04%	0.524%
67	11.692	1631	1633	1637	rVB2	142749	133576	6.52%	0.425%
68	11.910	1668	1670	1672	rBV	101342	110032	5.37%	0.350%
69	11.933	1672	1674	1680	rVB2	209818	285228	13.92%	0.907%
70	12.027	1687	1690	1692	rBV3	157763	163103	7.96%	0.519%
71	12.627	1789	1792	1796	rVB	1163077	944133	46.08%	3.004%

LSC Area Percent Report

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Acq On : 9 Feb 2018 11:50
Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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

72	12.857	1826	1831	1837	rBV	997500	1160247	56.63%	3.691%
73	12.998	1849	1855	1857	rBV	1106007	1278933	62.42%	4.069%
74	14.027	2027	2030	2031	rBV	486588	394929	19.28%	1.256%
75	14.057	2031	2035	2038	rVV2	935415	1282139	62.58%	4.079%
76	14.080	2038	2039	2043	rVB	409174	291290	14.22%	0.927%
77	15.104	2210	2213	2217	rBV	408549	592561	28.92%	1.885%
78	15.480	2275	2277	2283	rVB	338622	482071	23.53%	1.534%
79	15.551	2285	2289	2293	rBV	621790	814043	39.73%	2.590%

Sum of corrected areas: 31434023

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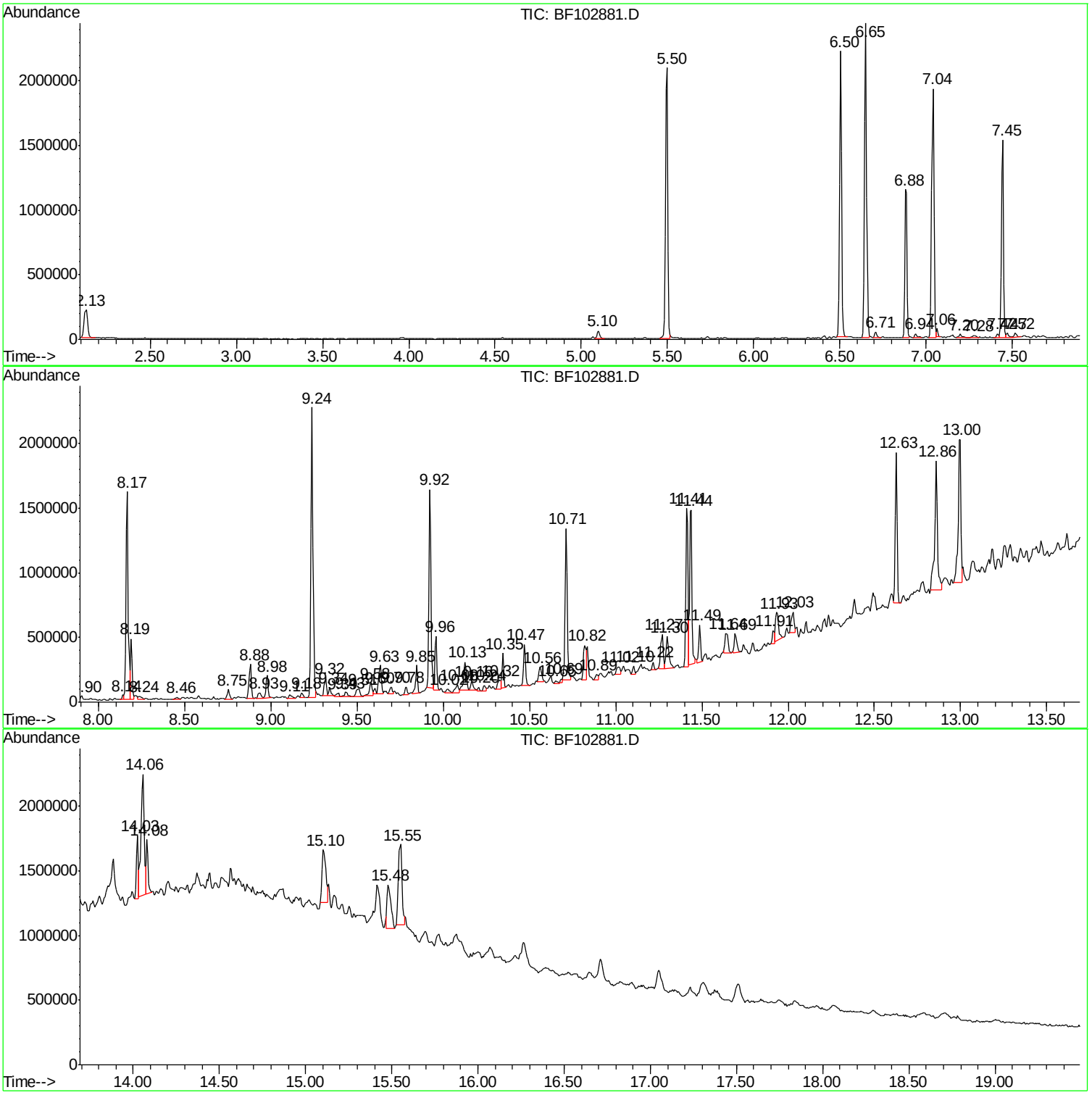
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102881.D
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Sample : J1485-01 2X
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

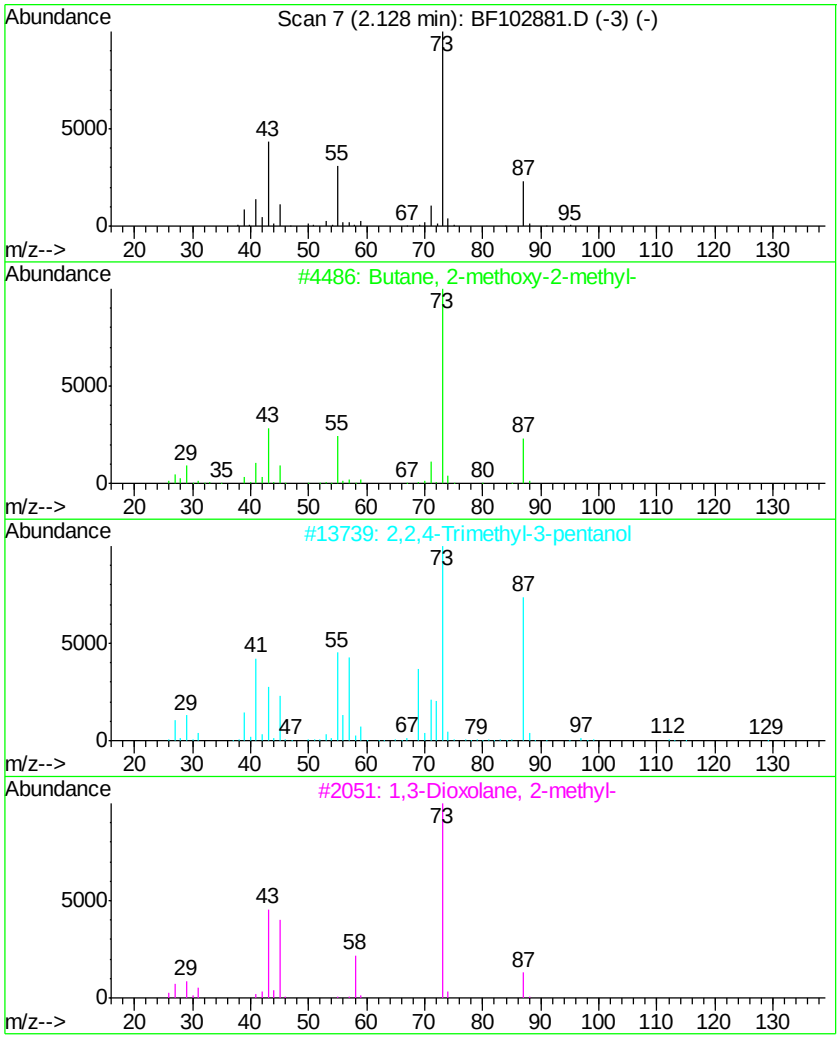
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

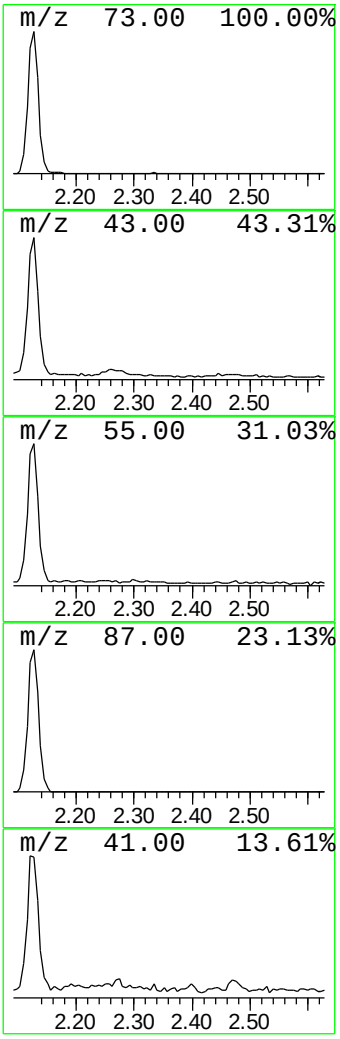
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	5.25 ng	278964	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102881.D
Acq On : 9 Feb 2018 11:50
Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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

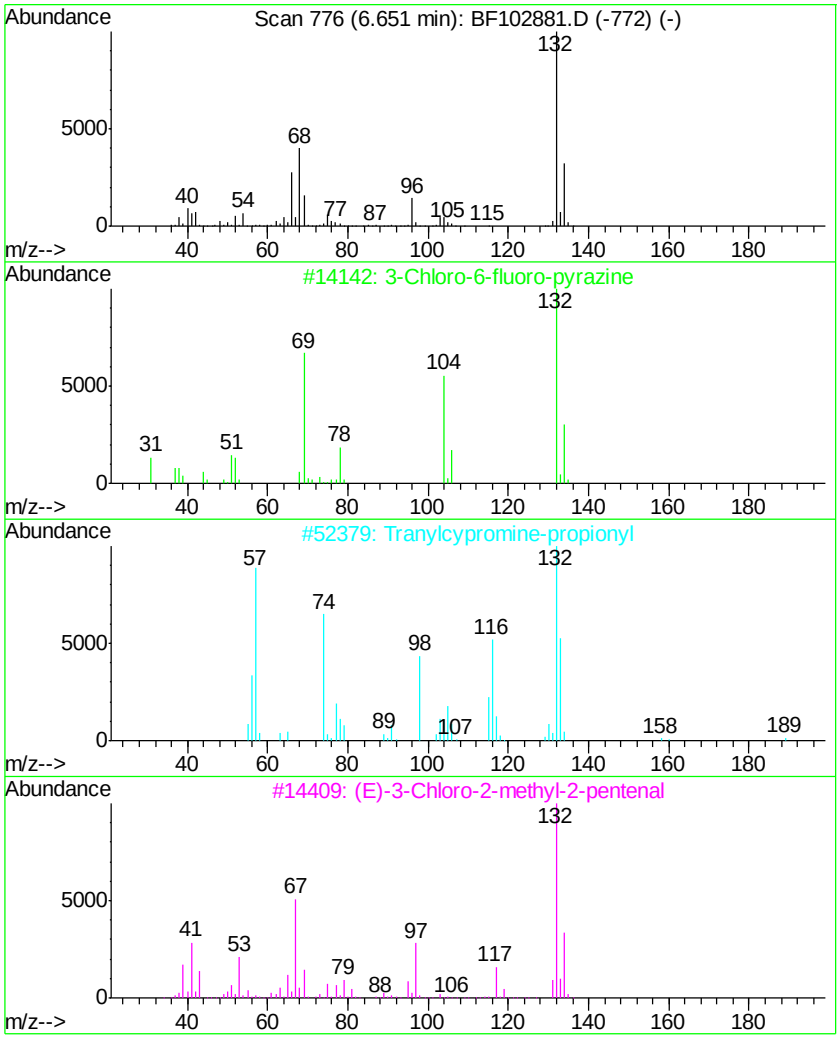
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

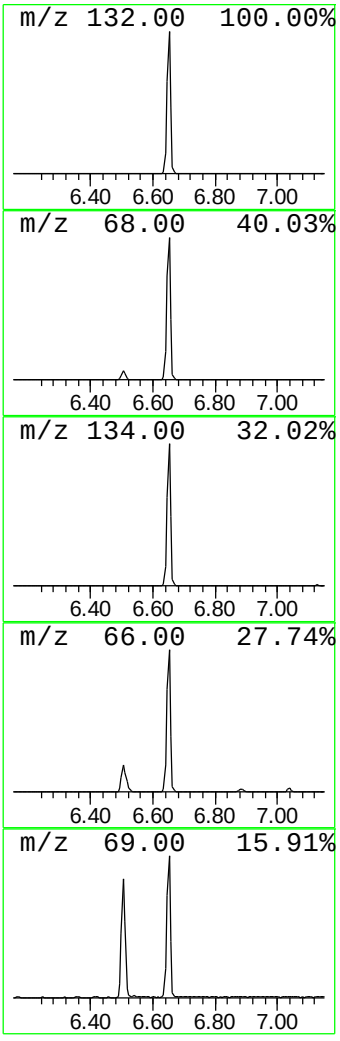
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	38.25 ng	2034000	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102881.D
Acq On : 9 Feb 2018 11:50
Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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

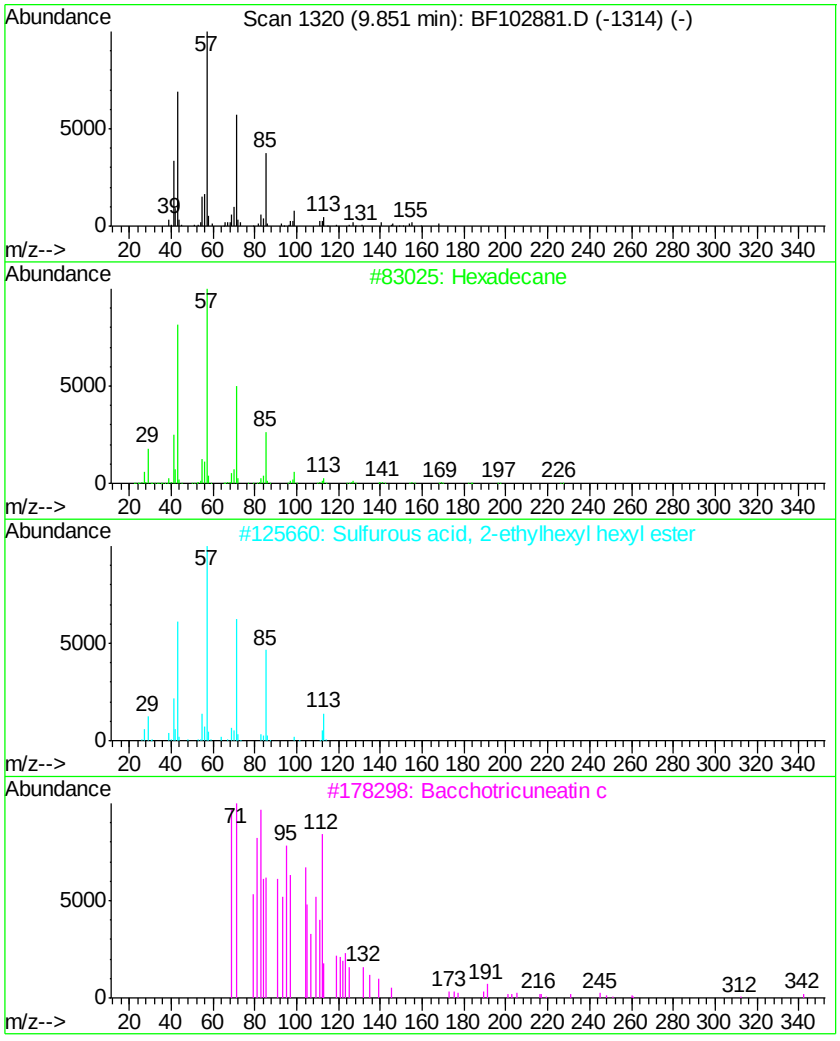
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

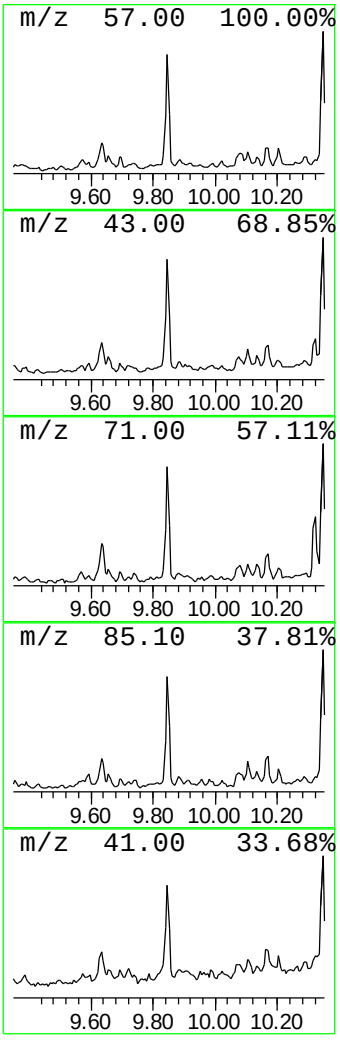
****

Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.77 ng	181801	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	Bacchotricuneatin c	342	C20H22O5	066563-30-2	74
4	Pentadecane	212	C15H32	000629-62-9	72
5	Tridecane	184	C13H28	000629-50-5	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
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Acq On : 9 Feb 2018 11:50
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Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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

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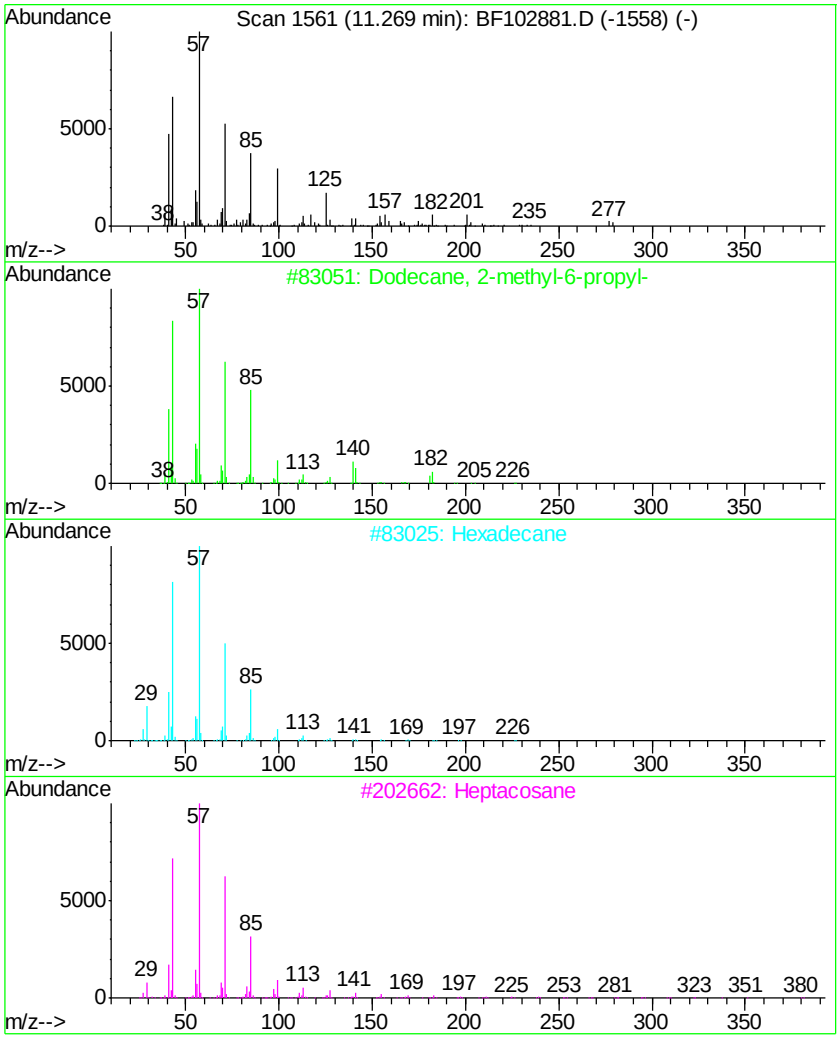
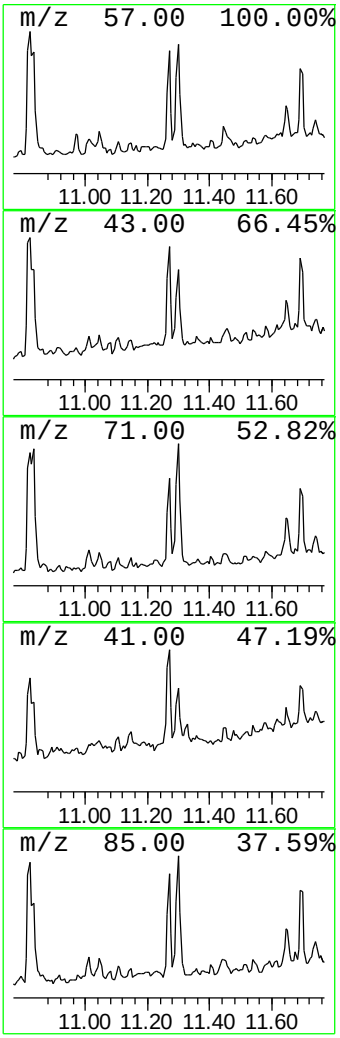
Peak Number 8 Dodecane, 2-methyl-6-propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.27	3.95 ng	230658	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	58
2	Hexadecane	226	C16H34	000544-76-3	52
3	Heptacosane	380	C27H56	000593-49-7	50
4	Tridecane	184	C13H28	000629-50-5	49
5	Undecane, 6-ethyl-	184	C13H28	017312-60-6	49





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102881.D
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Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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

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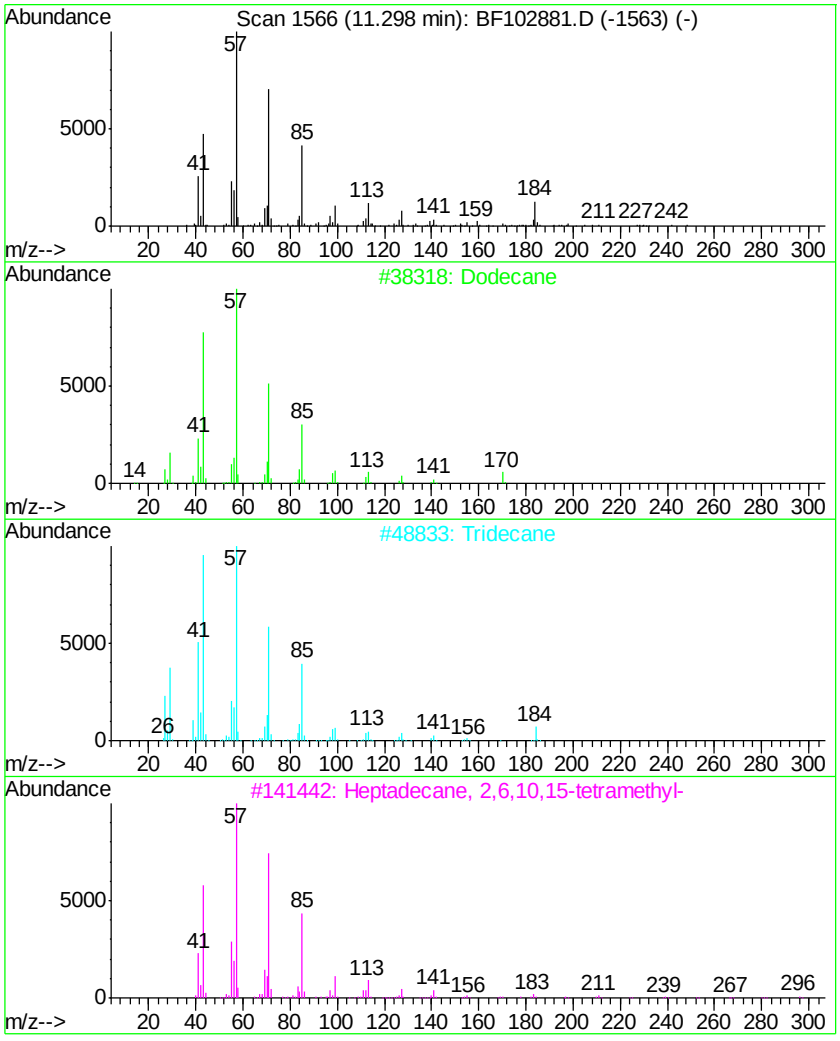
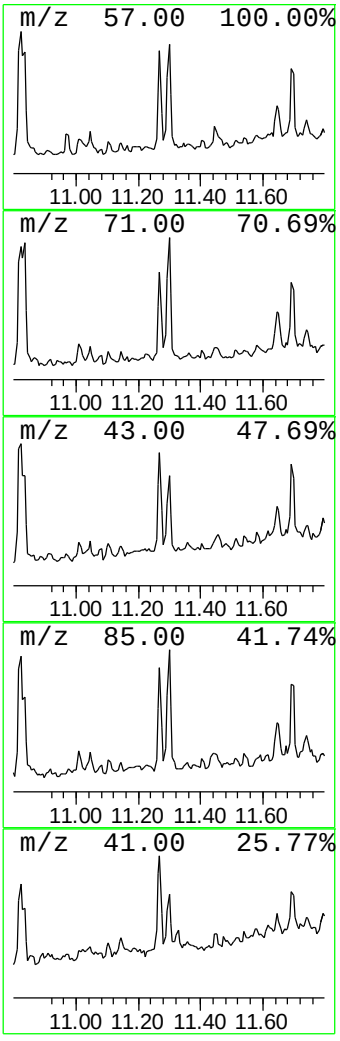
Peak Number 9 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	5.14 ng	300003	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	90
2	Tridecane	184	C13H28	000629-50-5	87
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4	Eicosane	282	C20H42	000112-95-8	86
5	Tetracosane	338	C24H50	000646-31-1	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102881.D
Acq On : 9 Feb 2018 11:50
Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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

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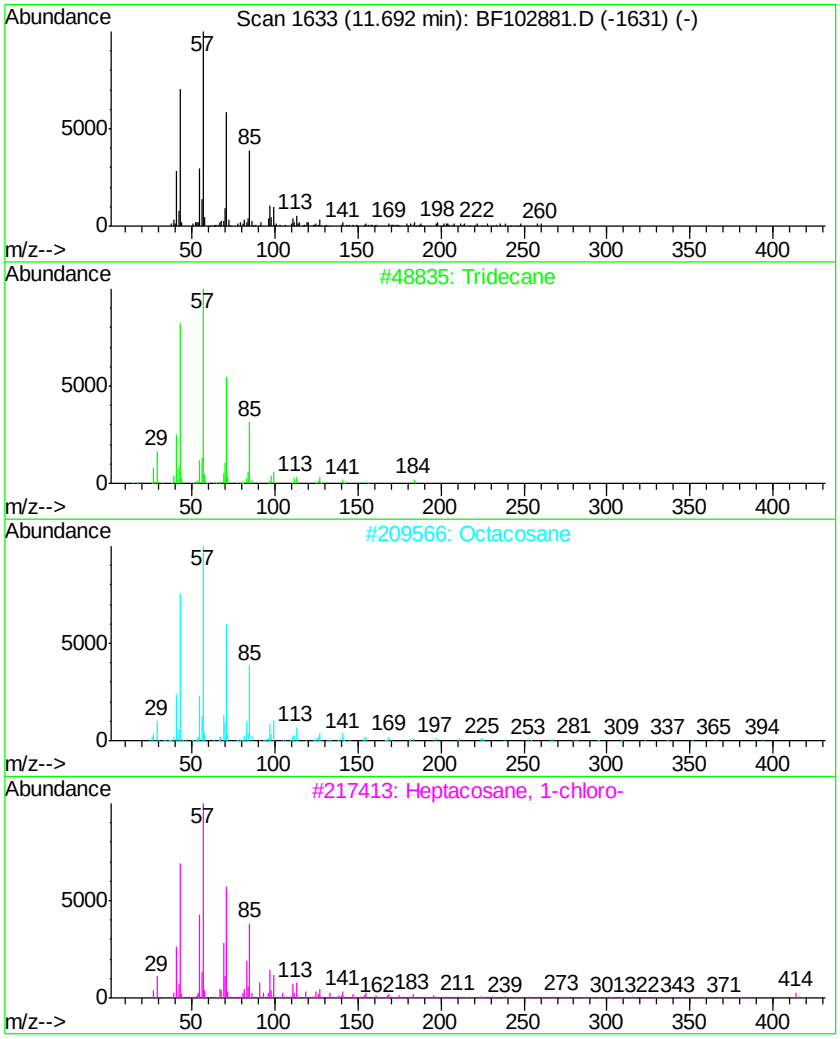
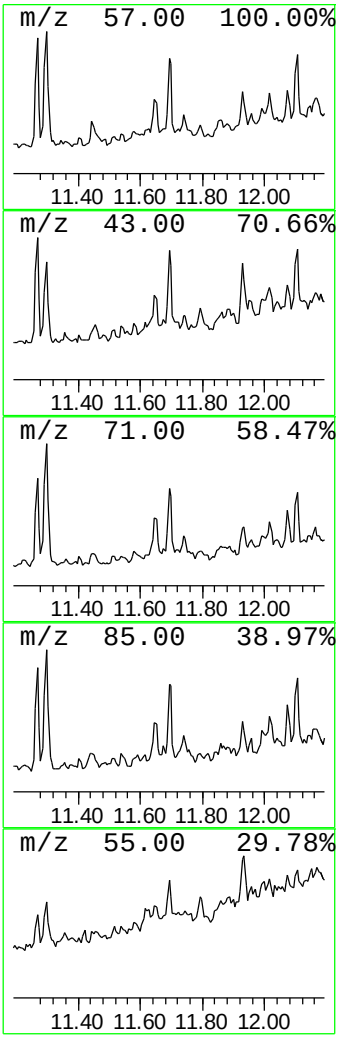
Peak Number 10 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	2.29 ng	133576	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	91
2	Octacosane	394	C28H58	000630-02-4	86
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
5	Tetradecane	198	C14H30	000629-59-4	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102881.D
Acq On : 9 Feb 2018 11:50
Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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

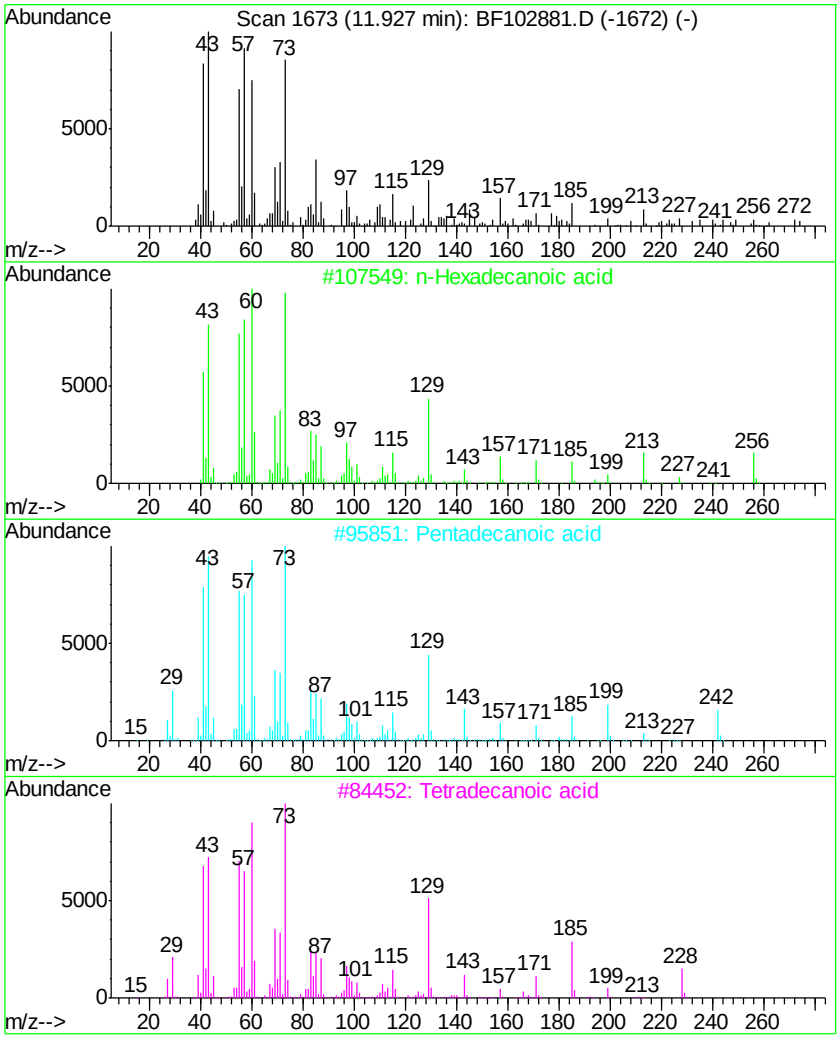
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

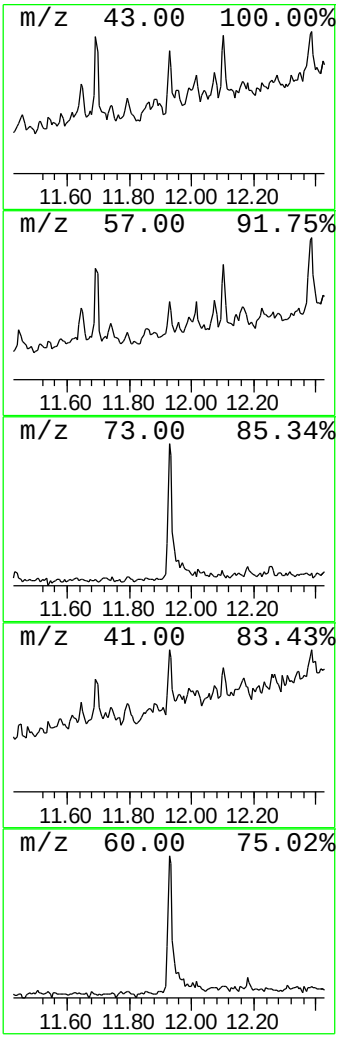
****

Peak Number 11 unknown11.93 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	4.89 ng	285228	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	45
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	41
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	38
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	35
5	Nonanoic acid	158	C9H18O2	000112-05-0	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF020918\
Data File : BF102881.D
Acq On : 9 Feb 2018 11:50
Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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

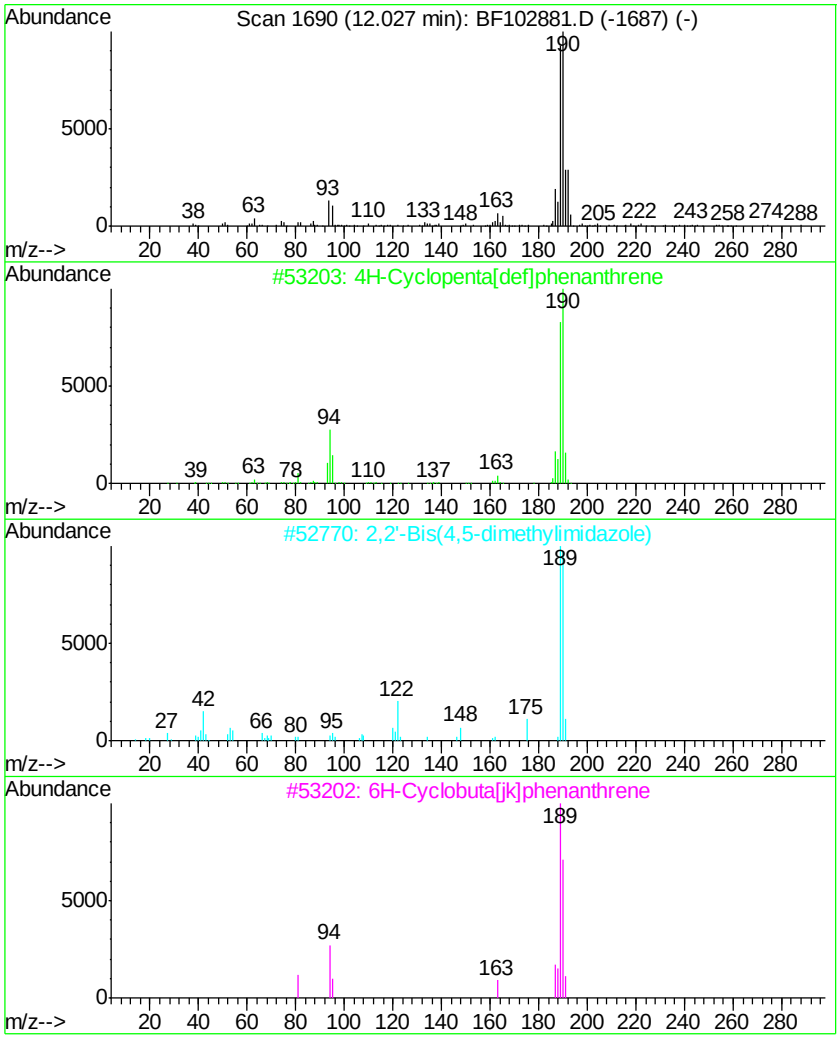
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

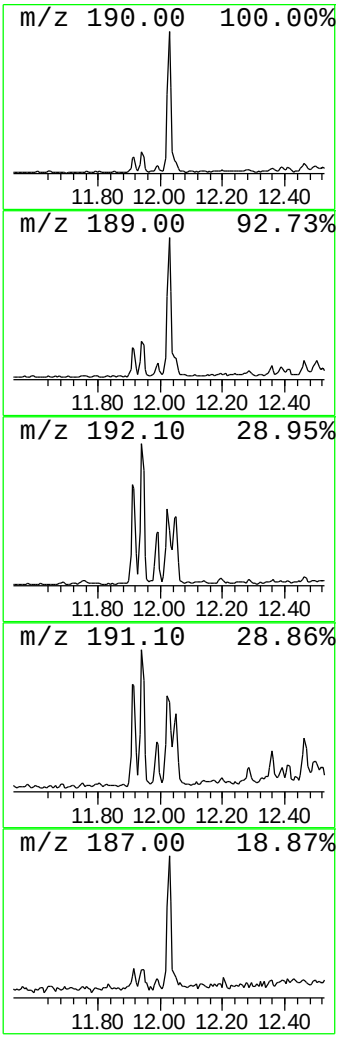
****

Peak Number 12 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	2.79 ng	163103	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	90
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	53
3	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	33
4	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	22
5	2-Naphthaldehyde, 1,2,3,4-tetrah...	190	C12H14O2	002472-02-8	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020918\
Data File : BF102881.D
Acq On : 9 Feb 2018 11:50
Operator : SJ/JU
Sample : J1485-01 2X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RO-201

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...	2.13	5.3	ng	278964	1	6.89	1063510	20.0
unknown6.65	6.65	38.3	ng	2034000	1	6.89	1063510	20.0
Hexadecane	9.85	2.8	ng	181801	3	9.92	1312540	20.0
Dodecane, 2-methy...	11.27	4.0	ng	230658	4	11.41	1167360	20.0
Dodecane	11.30	5.1	ng	300003	4	11.41	1167360	20.0
Tridecane	11.69	2.3	ng	133576	4	11.41	1167360	20.0
unknown11.93	11.93	4.9	ng	285228	4	11.41	1167360	20.0
4H-Cyclopenta[def...	12.03	2.8	ng	163103	4	11.41	1167360	20.0