LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
Data File : BF104757.D
Acq On : 24 Apr 2018 15:40
Operator : JU/SJ
Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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	4.434	395	399	407	rVB	20860	27528	1.20%	0.111%
2	5.010	493	497	503	rBV	86187	114698	4.98%	0.463%
3	5.428	564	568	575	rBV	2157802	2069962	89.92%	8.347%
4	5.734	617	620	629	rVB2	24291	39858	1.73%	0.161%
5	6.239	701	706	711	rBV	19506	25275	1.10%	0.102%
6	6.451	737	742	745	rBV	2035566	1924932	83.62%	7.762%
7	6.581	760	764	767	rBV	2481490	2118438	92.02%	8.542%
8	6.675	777	780	788	rVB2	30479	36136	1.57%	0.146%
9	6.804	799	802	806	rBV	767087	668301	29.03%	2.695%
10	6.863	806	812	817	rVB5	14518	29239	1.27%	0.118%
11	6.963	825	829	832	rBV	2121471	1774953	77.10%	7.157%
12	7.169	861	864	869	rBV3	12930	25285	1.10%	0.102%
13	7.375	895	899	902	rBV	1477961	1262472	54.84%	5.091%
14	7.445	909	911	913	rBV	33086	29352	1.28%	0.118%
15	7.545	925	928	934	rVB	24526	27660	1.20%	0.112%
16	7.828	973	976	979	rBV2	33023	37889	1.65%	0.153%
17	7.969	997	1000	1003	rBV2	35526	36062	1.57%	0.145%
18	8.092	1017	1021	1024	rBV	978001	794302	34.50%	3.203%
19	8.122	1024	1026	1031	rVV3	32721	41066	1.78%	0.166%
20	8.169	1031	1034	1046	rVB	152109	159514	6.93%	0.643%
21	8.433	1076	1079	1081	rBV2	30325	32241	1.40%	0.130%
22	8.869	1150	1153	1161	rBV	34934	53641	2.33%	0.216%
23	8.998	1173	1175	1180	rBV	29219	34248	1.49%	0.138%
24	9.169	1199	1204	1207	rBV	2591193	2302068	100.00%	9.283%
25	9.239	1214	1216	1218	rVB	33663	25572	1.11%	0.103%
26	9.275	1218	1222	1226	rVV3	61132	69583	3.02%	0.281%
27	9.310	1226	1228	1234	rVB2	34390	32216	1.40%	0.130%
28	9.498	1257	1260	1262	rBV3	31451	26713	1.16%	0.108%
29	9.557	1268	1270	1273	rBV	158751	132639	5.76%	0.535%
30	9.651	1283	1286	1291	rBV6	20170	27976	1.22%	0.113%
31	9.751	1301	1303	1304	rBV	55743	45289	1.97%	0.183%
32	9.769	1304	1306	1310	rVB	99209	77360	3.36%	0.312%
33	9.845	1316	1319	1323	rBV	873448	815366	35.42%	3.288%
34	9.898	1326	1328	1333	rVB4	27743	29705	1.29%	0.120%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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	10.051	1351	1354	1358	rVB3	65539	61314	2.66%	0.247%
36	10.269	1384	1391	1394	rBV2	144131	221916	9.64%	0.895%
37	10.357	1404	1406	1410	rBV3	27178	25967	1.13%	0.105%
38	10.486	1425	1428	1431	rBV2	29470	33132	1.44%	0.134%
39	10.569	1439	1442	1446	rBV4	22503	29310	1.27%	0.118%
40	10.639	1450	1454	1463	rVV	1297105	1177726	51.16%	4.749%
41	10.716	1464	1467	1469	rVB	83559	67345	2.93%	0.272%
42	10.745	1469	1472	1476	rBV	111160	124541	5.41%	0.502%
43	10.833	1484	1487	1489	rBV2	30495	25142	1.09%	0.101%
44	10.886	1493	1496	1502	rVV4	170298	181344	7.88%	0.731%
45	10.998	1512	1515	1524	rBV	269711	264595	11.49%	1.067%
46	11.192	1545	1548	1551	rBV	83055	77775	3.38%	0.314%
47	11.280	1560	1563	1567	rBV3	43398	60155	2.61%	0.243%
48	11.339	1569	1573	1578	rVV	823034	793983	34.49%	3.202%
49	11.380	1578	1580	1583	rVB2	45685	44179	1.92%	0.178%
50	11.539	1604	1607	1609	rBV	60231	69411	3.02%	0.280%
51	11.616	1618	1620	1622	rVB	30159	25351	1.10%	0.102%
52	11.739	1639	1641	1645	rVB	37391	30587	1.33%	0.123%
53	11.869	1658	1663	1665	rBV	351509	360234	15.65%	1.453%
54	11.892	1665	1667	1670	rVB	73483	65405	2.84%	0.264%
55	12.027	1687	1690	1692	rBV2	62503	64790	2.81%	0.261%
56	12.739	1808	1811	1814	rBV2	98622	107958	4.69%	0.435%
57	12.816	1821	1824	1829	rVB	64185	82672	3.59%	0.333%
58	12.927	1839	1843	1846	rBV	2274290	2007257	87.19%	8.094%
59	13.398	1920	1923	1926	rBV	352875	294708	12.80%	1.188%
60	13.815	1991	1994	1997	rBV	304979	308290	13.39%	1.243%
61	13.957	2015	2018	2020	rBV	872032	733323	31.85%	2.957%
62	13.986	2020	2023	2026	rVB	691397	647864	28.14%	2.612%
63	15.092	2208	2211	2215	rVB	645432	655380	28.47%	2.643%
64	15.462	2272	2274	2287	rVB2	675243	1209769	52.55%	4.878%

Sum of corrected areas: 24798962

LSC Report - Integrated Chromatogram

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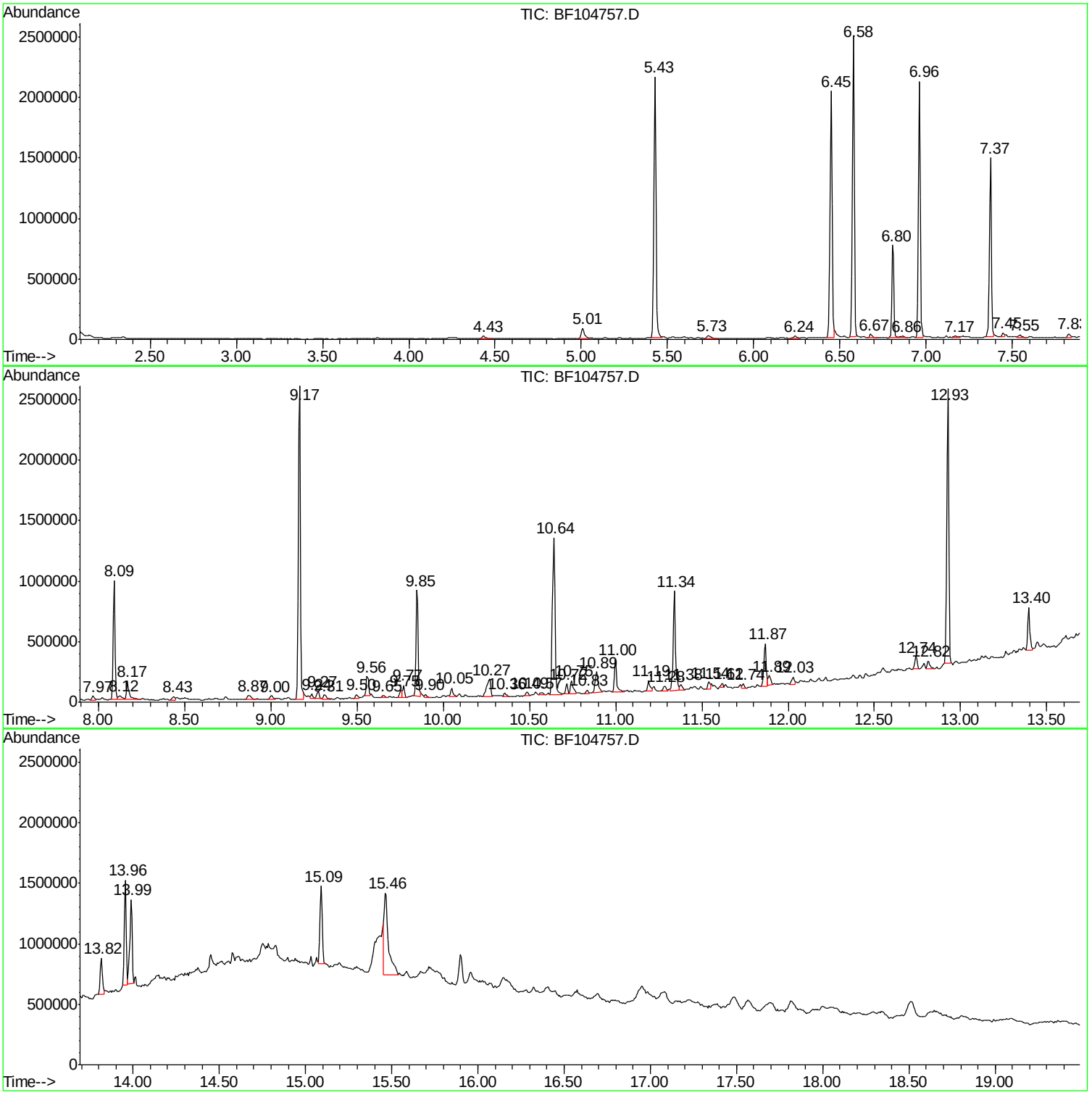
Data File : BF104757.D
Acq On : 24 Apr 2018 15:40
Operator : JU/SJ
Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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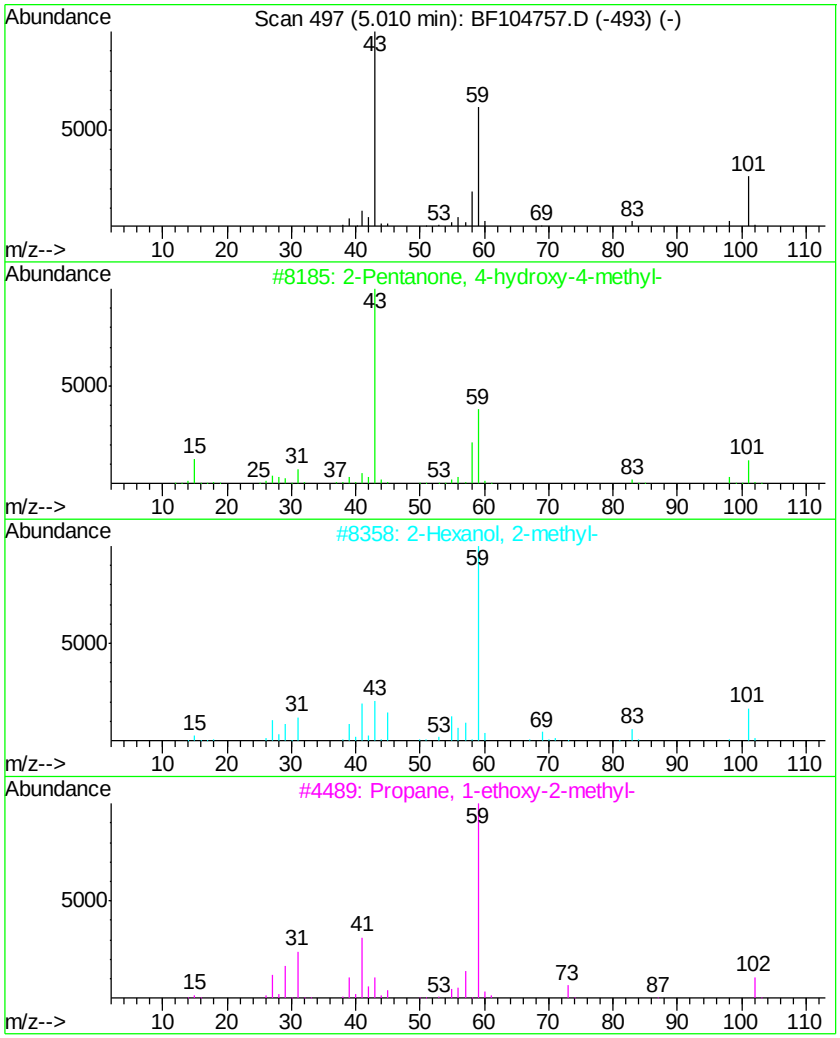
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

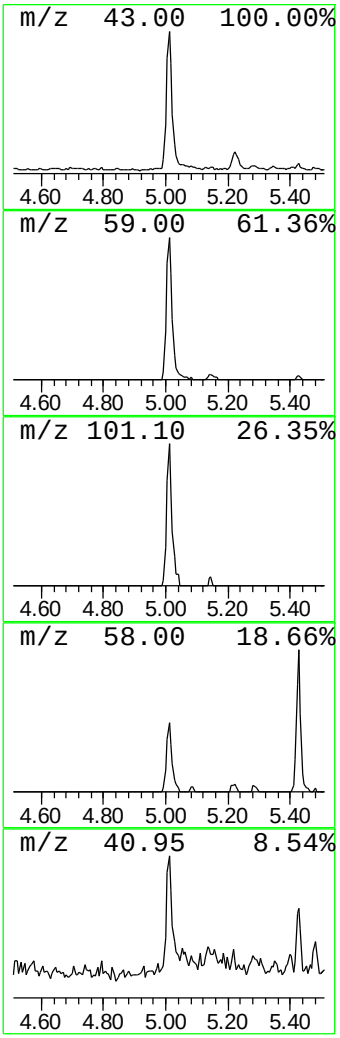
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	3.43 ng	114698	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-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	36
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
Data File : BF104757.D
Acq On : 24 Apr 2018 15:40
Operator : JU/SJ
Sample : J2461-04
Misc :
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Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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

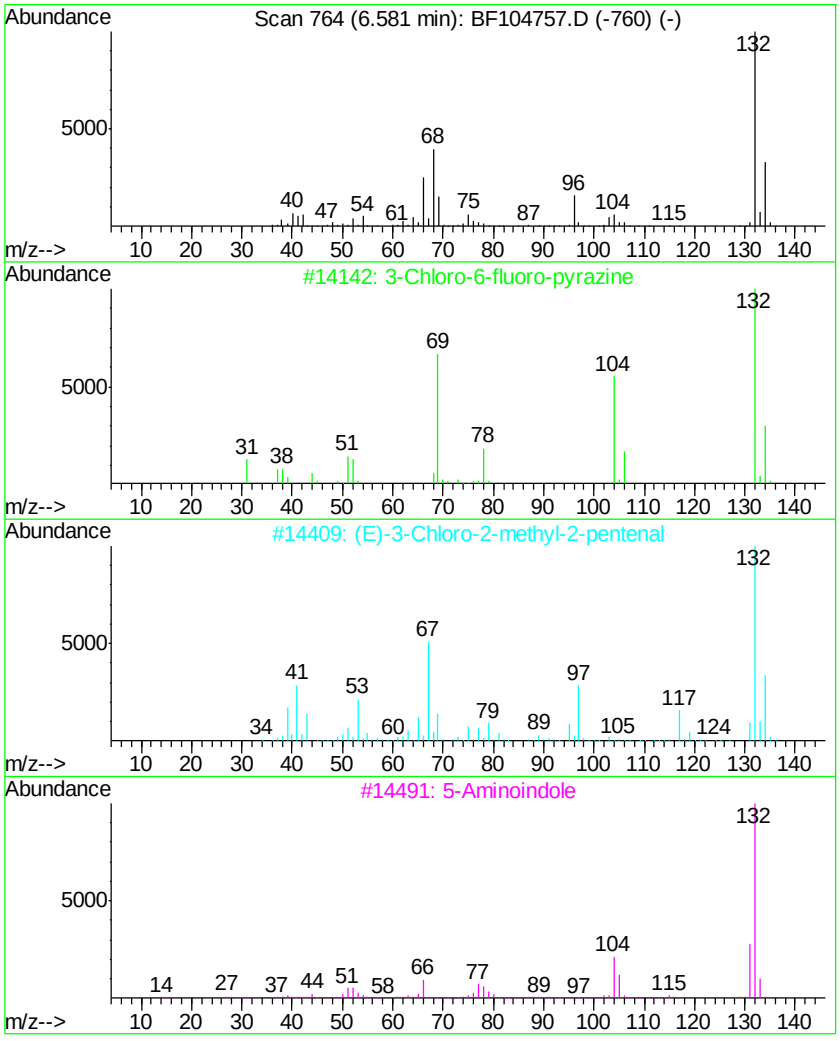
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

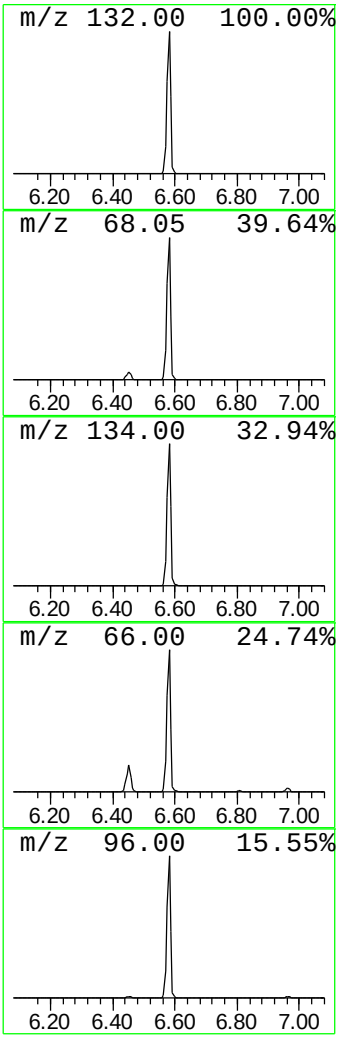
****

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	63.40 ng	2118440	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	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : J2461-04
Misc :
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Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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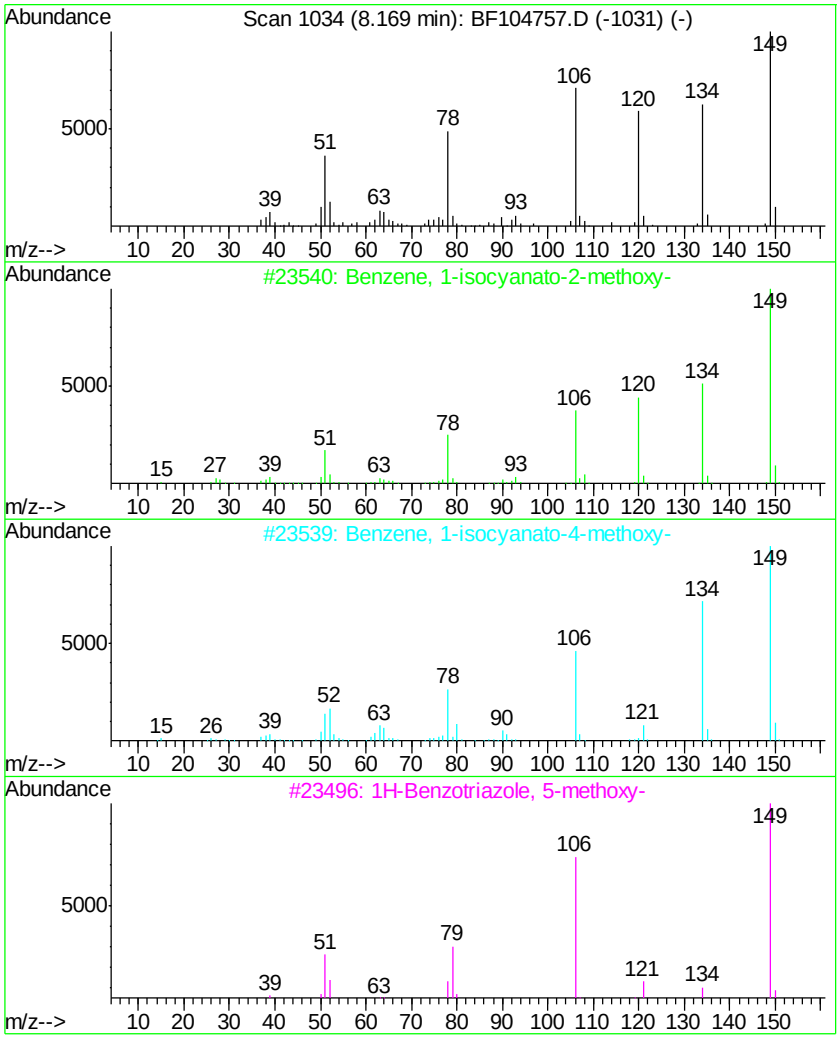
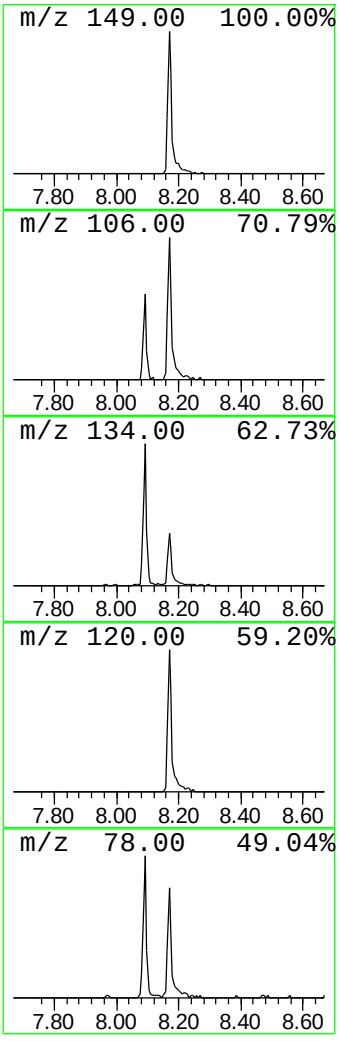
Peak Number 4 Benzene, 1-isocyanato-2-met... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	4.02 ng	159514	Naphthalene-d8	8.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-isocyanato-2-methoxy-	149	C8H7NO2	000700-87-8	94
2	Benzene, 1-isocyanato-4-methoxy-	149	C8H7NO2	005416-93-3	58
3	1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	46
4	Benzonitrile, 4-hydroxy-3-methoxy-	149	C8H7NO2	004421-08-3	45
5	Benzene, 1-isocyanato-3-methoxy-	149	C8H7NO2	018908-07-1	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
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Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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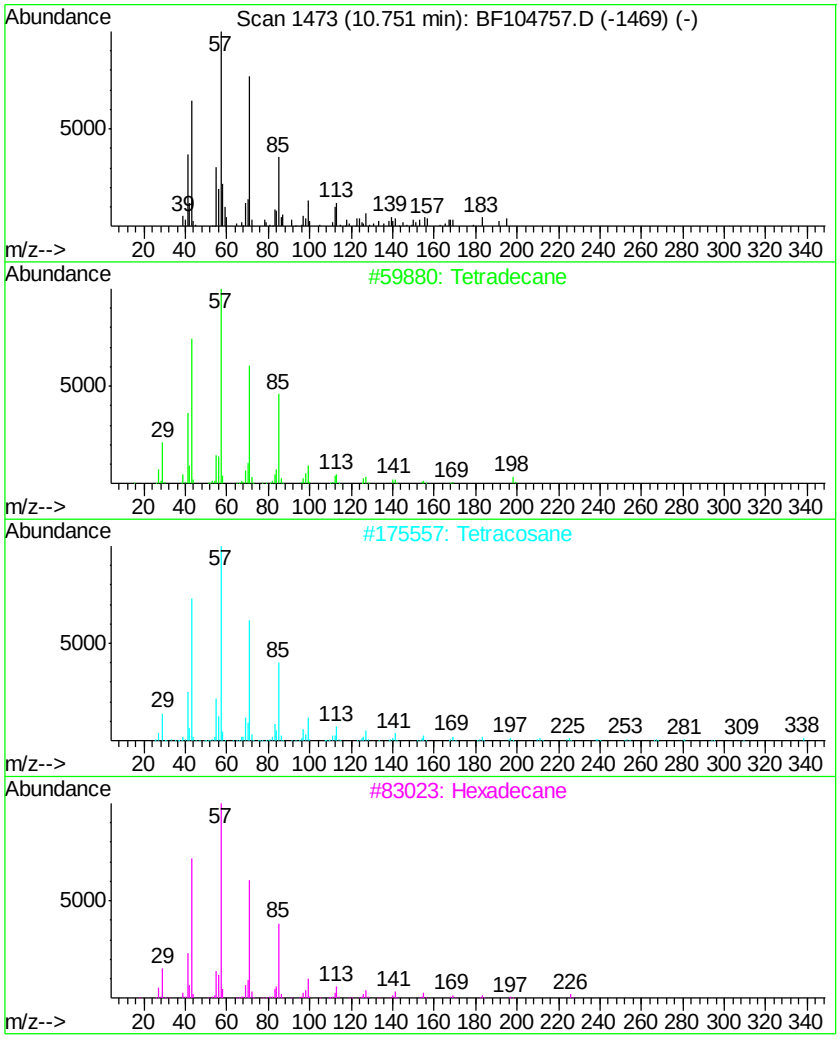
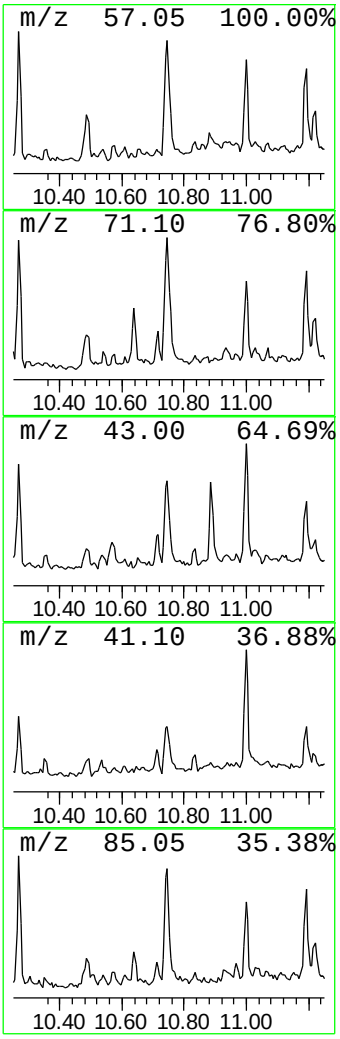
Peak Number 5 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	3.14 ng	124541	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tritetracontane	605	C43H88	007098-21-7	90
5	Eicosane	282	C20H42	000112-95-8	87





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Data File : BF104757.D
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Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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

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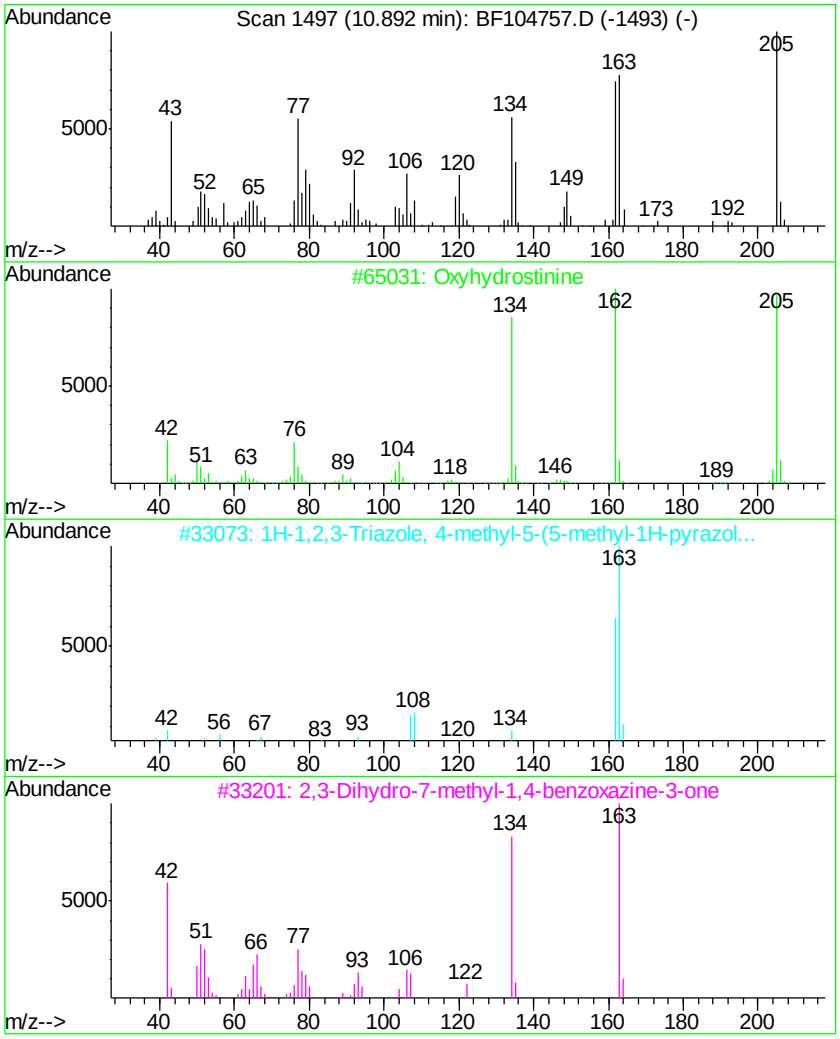
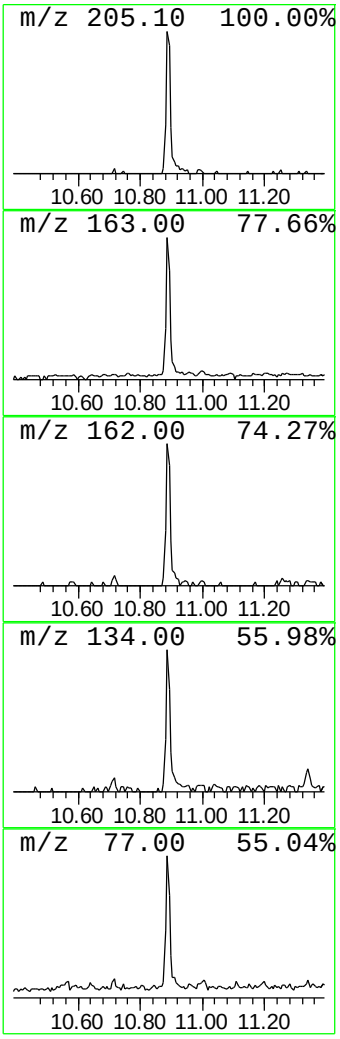
Peak Number 6 Oxyhydrostinine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.89	4.57 ng	181344	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxyhydrostinine	205	C11H11NO3	000552-29-4	50
2	1H-1,2,3-Triazole, 4-methyl-5-(5...	163	C7H9N5	051719-86-9	38
3	2,3-Dihydro-7-methyl-1,4-benzoxa...	163	C9H9NO2	039522-25-3	35
4	2-Hydroxy-3-methoxyphenylacetoni...	163	C9H9NO2	042973-56-8	30
5	Quinolin-2(1H)-one, 4-hydroxy-7-...	205	C11H11NO3	074798-86-0	30





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Sample : J2461-04
Misc :
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Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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

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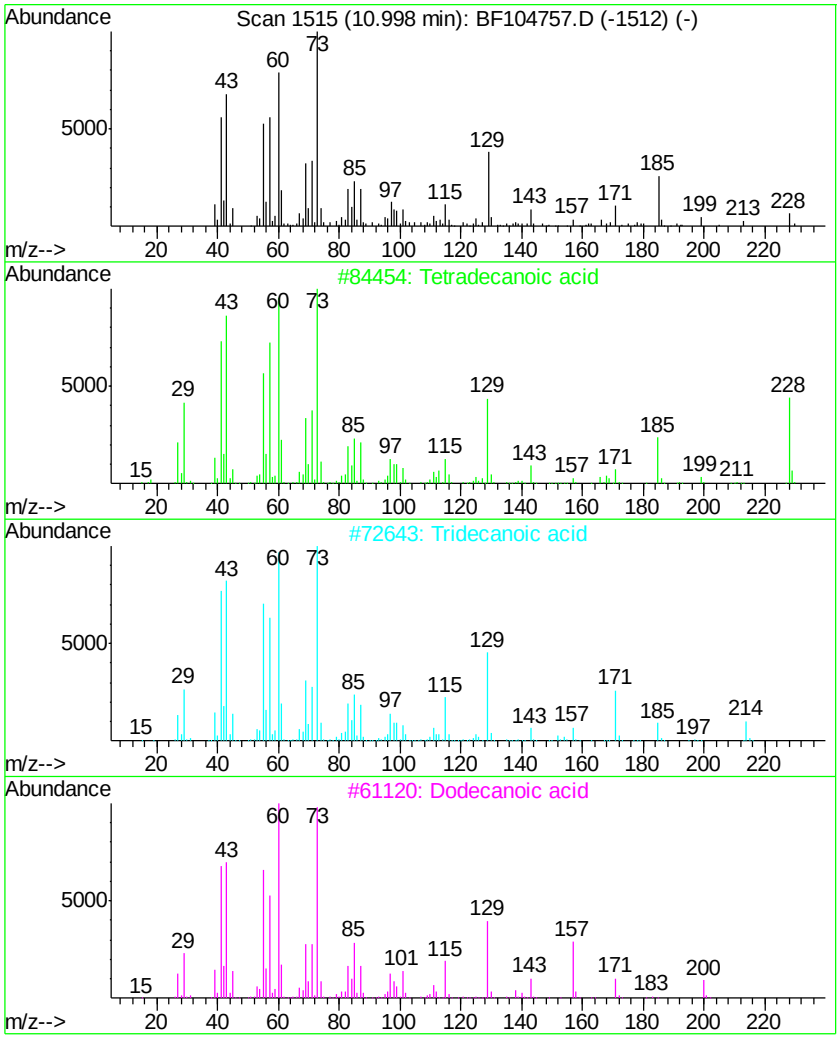
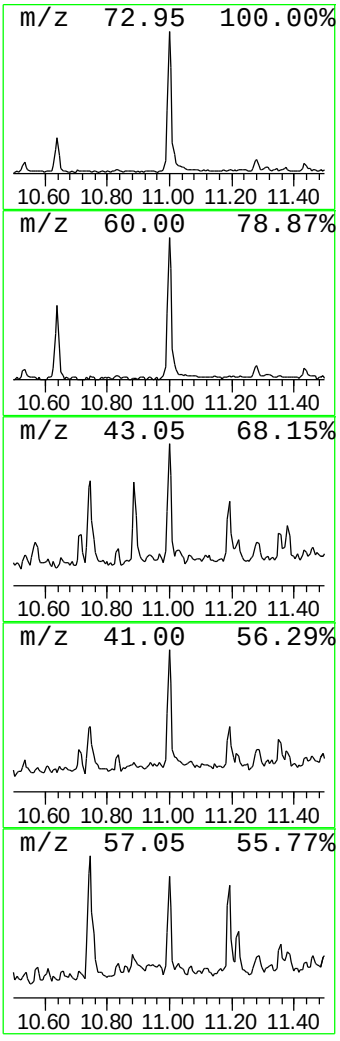
Peak Number 7 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	6.67 ng	264595	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Dodecanoic acid	200	C12H24O2	000143-07-7	78
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	Nonanoic acid	158	C9H18O2	000112-05-0	47





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Data File : BF104757.D
Acq On : 24 Apr 2018 15:40
Operator : JU/SJ
Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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

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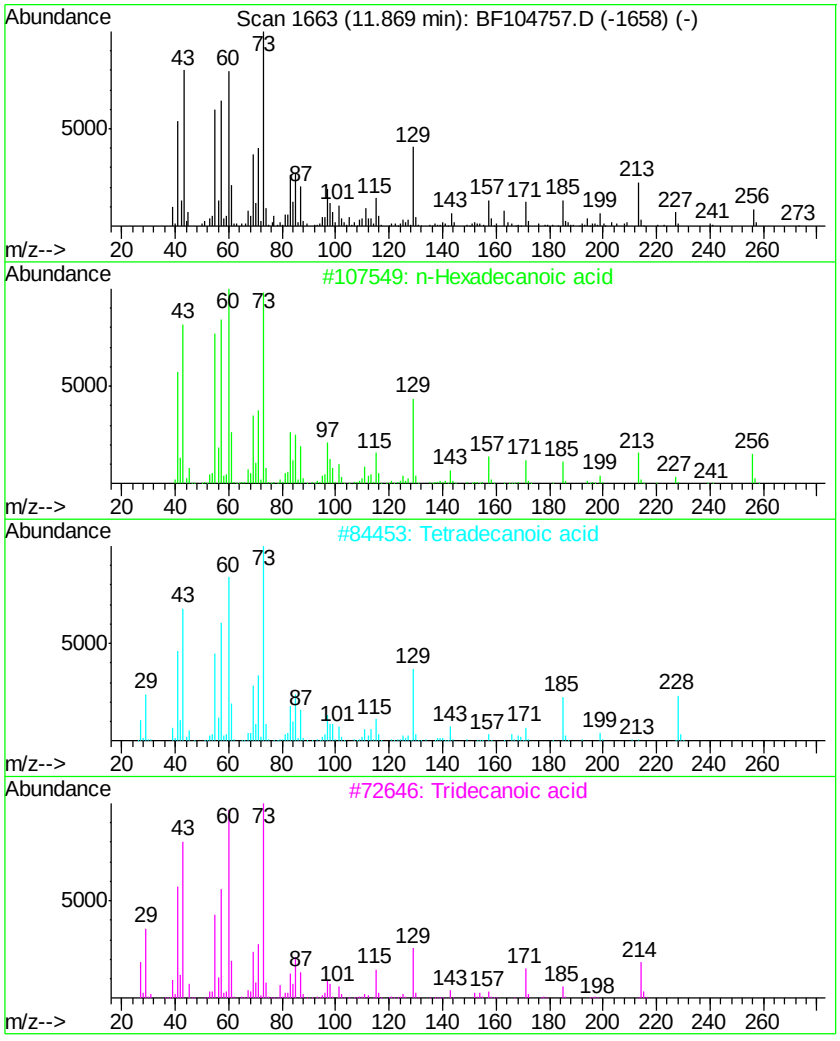
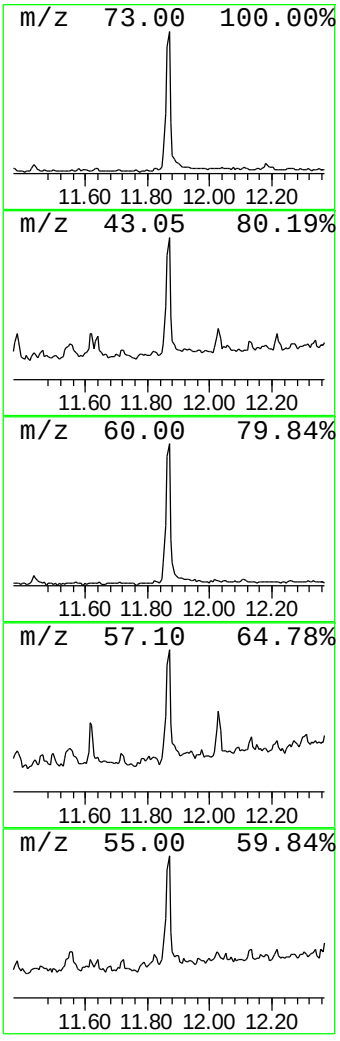
Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	9.07 ng	360234	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
Data File : BF104757.D
Acq On : 24 Apr 2018 15:40
Operator : JU/SJ
Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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

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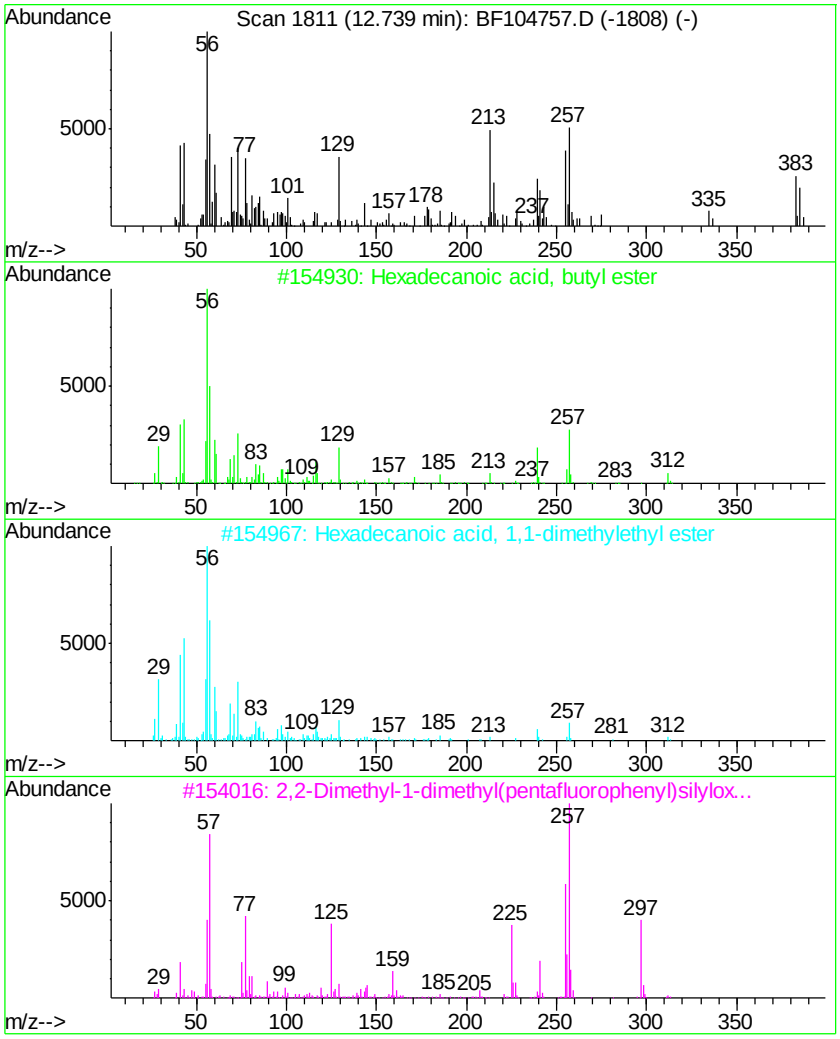
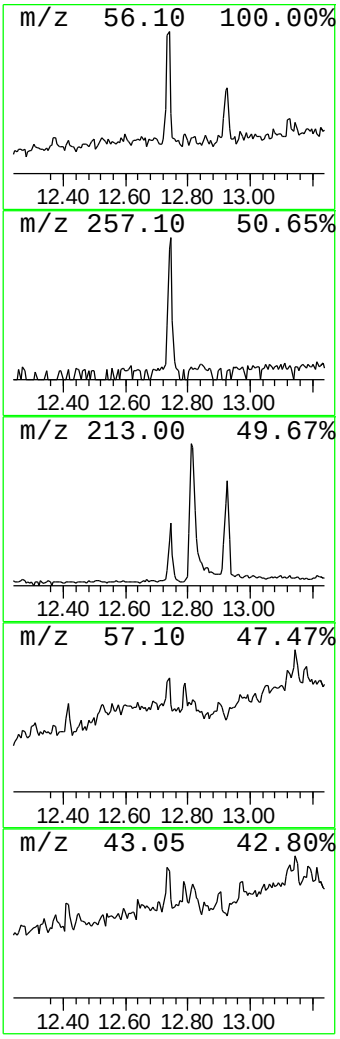
Peak Number 9 unknown12.74 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	3.33 ng	107958	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	38
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	22
3	2,2-Dimethyl-1-dimethyl(pentaflu...	312	C13H17F5OSi	062394-64-3	10
4	Benz[c]acridine, 7,10-dimethyl-	257	C19H15N	002381-40-0	9
5	Nordextromethorphan	257	C17H23NO	051195-74-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
Data File : BF104757.D
Acq On : 24 Apr 2018 15:40
Operator : JU/SJ
Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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

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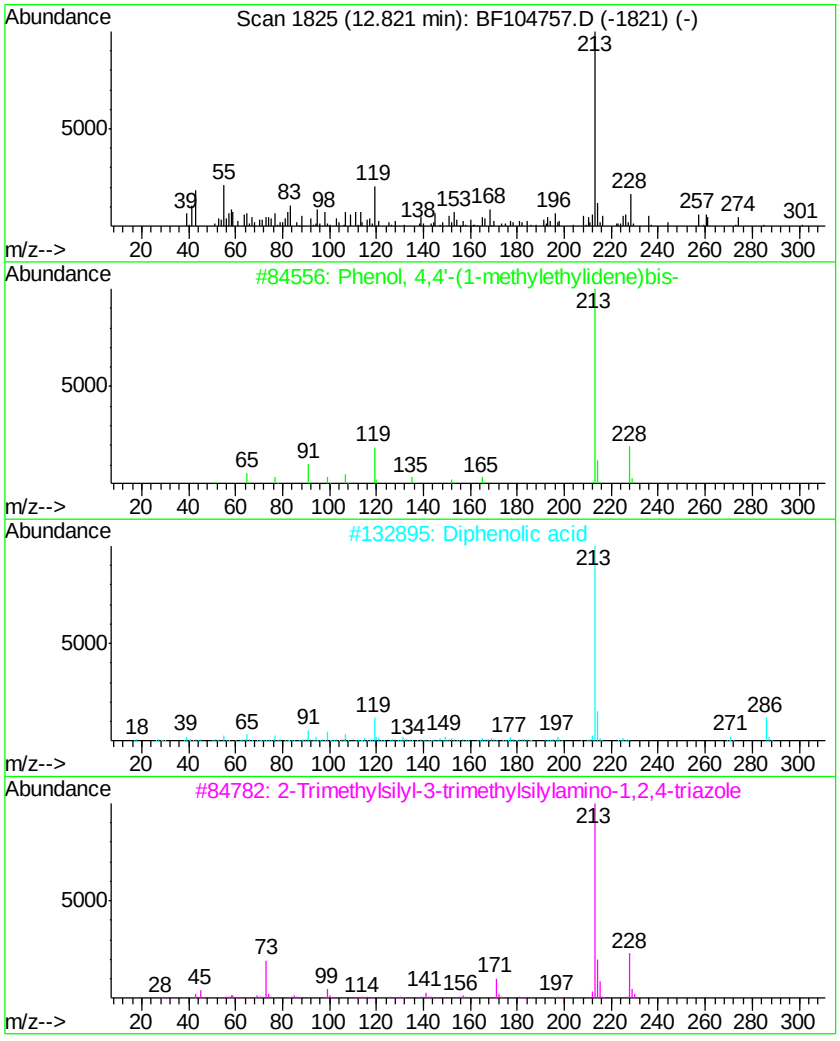
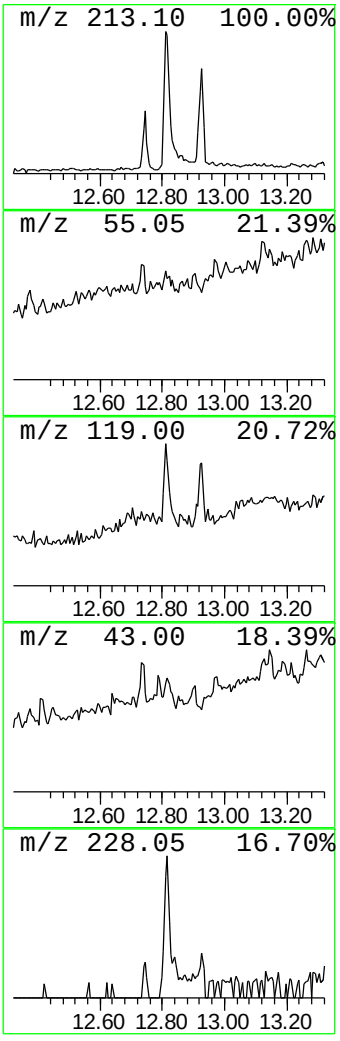
Peak Number 10 Phenol, 4,4'-(1-methylethyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	2.55 ng	82672	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2	Diphenolic acid	286	C17H18O4	000126-00-1	64
3	2-Trimethylsilyl-3-trimethylsily...	228	C8H20N4Si2	1000373-05-5	59
4	2,2-Bis-(4-hyxroxyphenyl)-butane	242	C16H18O2	000077-40-7	59
5	Bicyclo[2.2.1]heptan-3-one, 2-ph...	241	C16H19NO	1000197-48-0	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF042418\
Data File : BF104757.D
Acq On : 24 Apr 2018 15:40
Operator : JU/SJ
Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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

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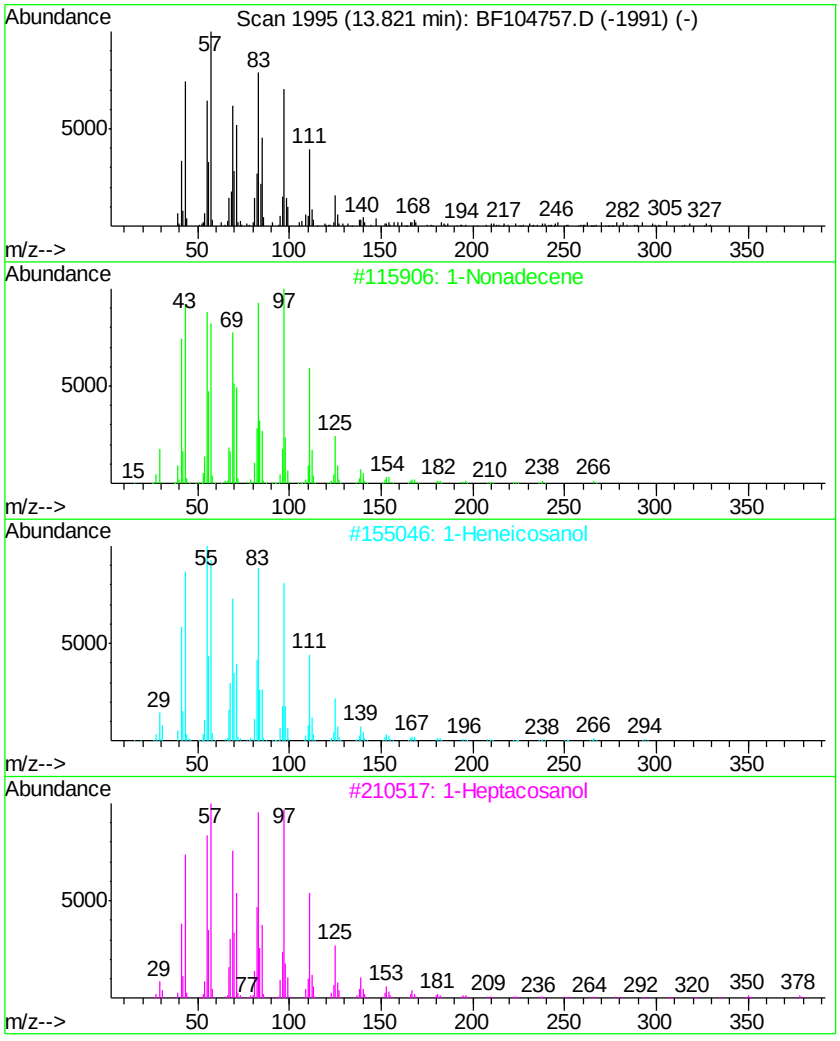
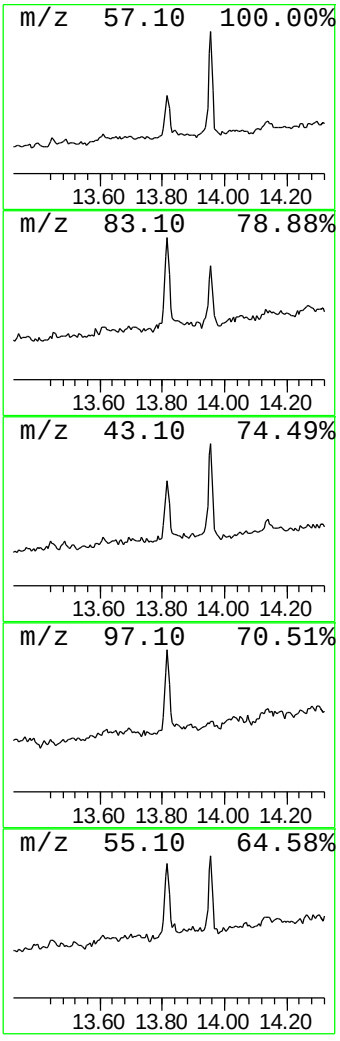
Peak Number 11 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	9.52 ng	308290	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	1-Docosene	308	C22H44	001599-67-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042418\
Data File : BF104757.D
Acq On : 24 Apr 2018 15:40
Operator : JU/SJ
Sample : J2461-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-P001-S002-0001-02

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	3.4	ng	114698	1	6.80	668301	20.0
unknown6.58	6.58	63.4	ng	2118440	1	6.80	668301	20.0
Benzene, 1-isocya...	8.17	4.0	ng	159514	2	8.09	794302	20.0
Tetradecane	10.75	3.1	ng	124541	4	11.34	793983	20.0
Oxyhydrostinine	10.89	4.6	ng	181344	4	11.34	793983	20.0
Tetradecanoic acid	11.00	6.7	ng	264595	4	11.34	793983	20.0
n-Hexadecanoic acid	11.87	9.1	ng	360234	4	11.34	793983	20.0
unknown12.74	12.74	3.3	ng	107958	5	13.99	647864	20.0
Phenol, 4,4'-(1-m...	12.82	2.5	ng	82672	5	13.99	647864	20.0
1-Nonadecene	13.82	9.5	ng	308290	5	13.99	647864	20.0