LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

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-BF022218.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	2.146	5	10	16	rVB	255083	332256	9.74%	1.071%
2	5.110	512	514	525	rVB	83404	108445	3.18%	0.350%
3	5.504	576	581	594	rBV	3313968	3410092	100.00%	10.996%
4	6.516	748	753	768	rBV	2901043	3298837	96.74%	10.637%
5	6.645	771	775	779	rBV	3158923	3249999	95.31%	10.480%
6	6.875	810	814	822	rBV	1129089	923184	27.07%	2.977%
7	7.034	836	841	844	rBV	2669962	2582573	75.73%	8.328%
8	7.439	905	910	913	rBV	2164985	2133951	62.58%	6.881%
9	8.157	1028	1032	1051	rVB	1336416	1246700	36.56%	4.020%
10	8.651	1113	1116	1119	rVB	73112	57100	1.67%	0.184%
11	9.233	1210	1215	1218	rBV	3442166	3245947	95.19%	10.467%
12	9.569	1267	1272	1276	rVB	492258	469259	13.76%	1.513%
13	9.622	1276	1281	1289	rBV	322859	314667	9.23%	1.015%
14	9.775	1304	1307	1312	rBV	51278	49593	1.45%	0.160%
15	9.833	1312	1317	1320	rBV	91394	85031	2.49%	0.274%
16	9.916	1327	1331	1335	rBV	1287013	1128533	33.09%	3.639%
17	10.304	1394	1397	1399	rBV	75615	62025	1.82%	0.200%
18	10.327	1399	1401	1405	rVV	121467	107257	3.15%	0.346%
19	10.386	1405	1411	1414	rVB	332200	297911	8.74%	0.961%
20	10.551	1433	1439	1441	rBV	39108	48298	1.42%	0.156%
21	10.710	1462	1466	1475	rBV	1437133	1472087	43.17%	4.747%
22	10.804	1479	1482	1492	rVB	136007	157678	4.62%	0.508%
23	10.998	1510	1515	1519	rBV4	25199	42364	1.24%	0.137%
24	11.251	1555	1558	1561	rBV	83029	72479	2.13%	0.234%
25	11.404	1581	1584	1587	rBV	918158	896184	26.28%	2.890%
26	11.427	1587	1588	1595	rVV	175042	147727	4.33%	0.476%
27	11.486	1595	1598	1602	rVV	32185	35151	1.03%	0.113%
28	11.616	1617	1620	1626	rBV5	27990	35013	1.03%	0.113%
29	11.680	1628	1631	1637	rVB	73167	66338	1.95%	0.214%
30	11.780	1645	1648	1651	rBV	71151	59355	1.74%	0.191%
31	11.916	1667	1671	1673	rBV2	50464	66989	1.96%	0.216%
32	11.939	1673	1675	1679	rVB2	55878	50506	1.48%	0.163%
33	11.986	1679	1683	1685	rBV2	31132	38855	1.14%	0.125%
34	12.021	1686	1689	1691	rBV2	54892	53425	1.57%	0.172%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.086	1698	1700	1703	rBV	67981	57823	1.70%	0.186%
36	12.433	1756	1759	1761	rBV	83402	70844	2.08%	0.228%
37	12.469	1761	1765	1767	rVV3	133677	179956	5.28%	0.580%
38	12.492	1767	1769	1772	rVV3	135500	130893	3.84%	0.422%
39	12.551	1775	1779	1781	rBV4	25392	34306	1.01%	0.111%
40	12.574	1781	1783	1788	rVB	41707	39263	1.15%	0.127%
41	12.621	1788	1791	1795	rBV	196497	184525	5.41%	0.595%
42	12.851	1825	1830	1833	rBV	194544	239469	7.02%	0.772%
43	12.904	1837	1839	1842	rVB	39222	40631	1.19%	0.131%
44	12.992	1849	1854	1857	rBV	2247645	2105490	61.74%	6.789%
45	13.074	1864	1868	1872	rBV5	27911	54424	1.60%	0.175%
46	13.286	1902	1904	1908	rVB2	45238	40981	1.20%	0.132%
47	13.868	2000	2003	2007	rBV2	168261	188221	5.52%	0.607%
48	14.057	2031	2035	2038	rBV	783602	793500	23.27%	2.559%
49	15.562	2287	2291	2299	rVB	395858	505755	14.83%	1.631%

Sum of corrected areas: 31011890

LSC Report - Integrated Chromatogram

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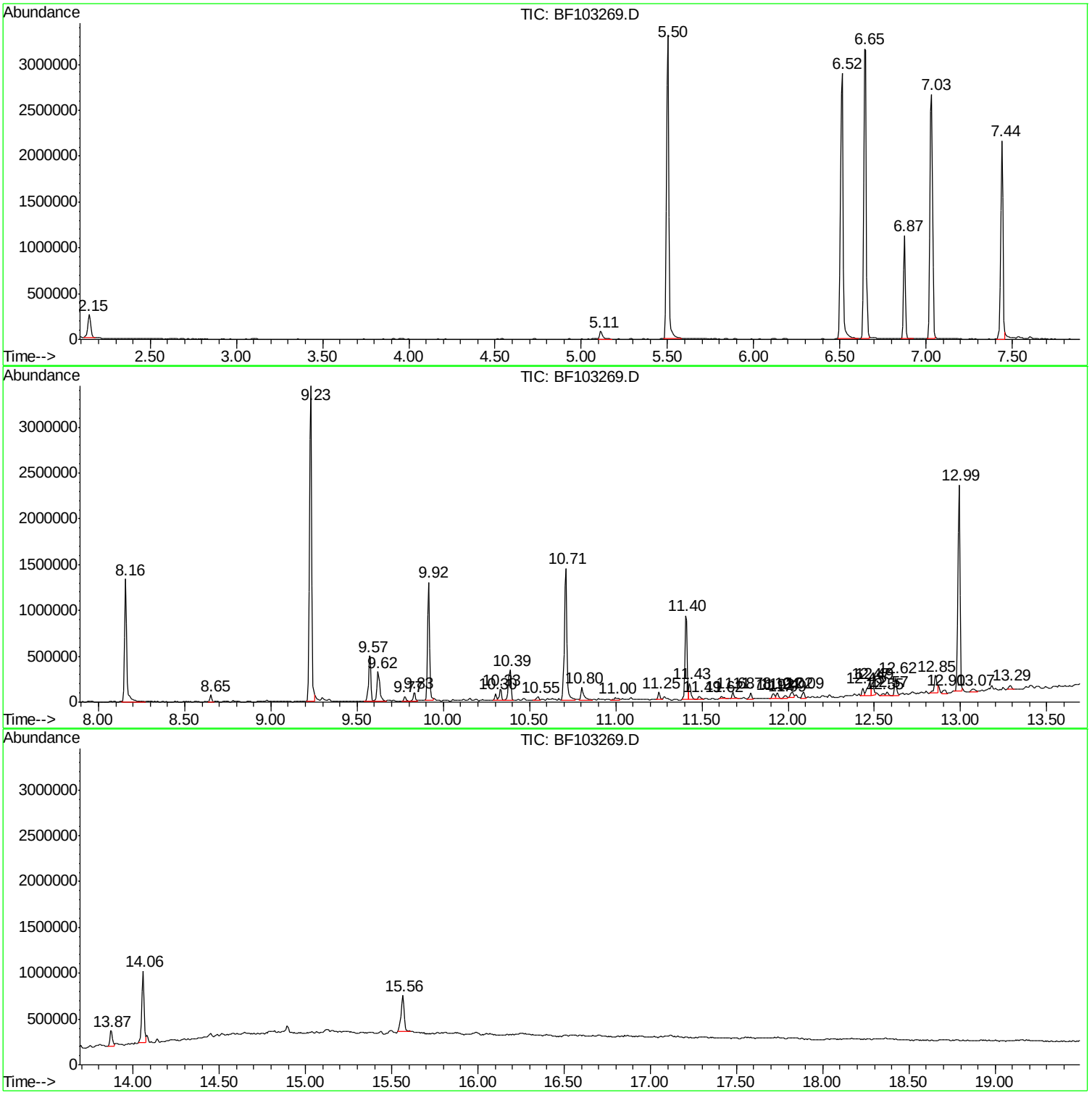
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

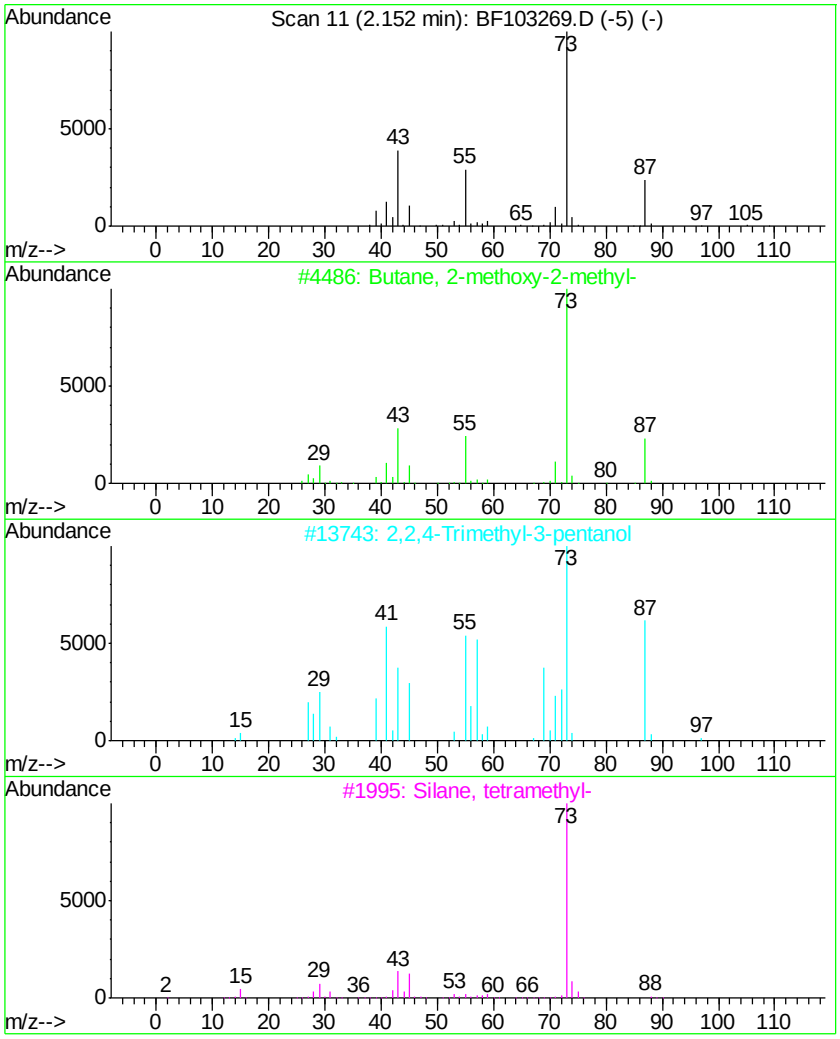
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

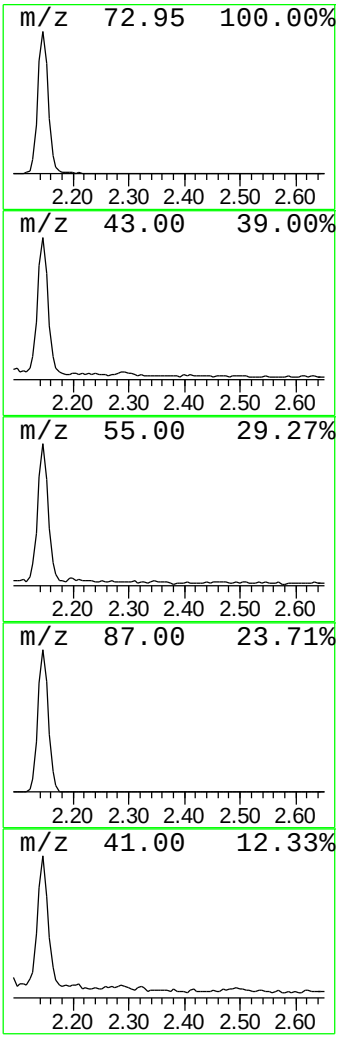
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	7.20 ng	332256	1,4-Dichlorobenzene-d4	6.87

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	35
4	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	28
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

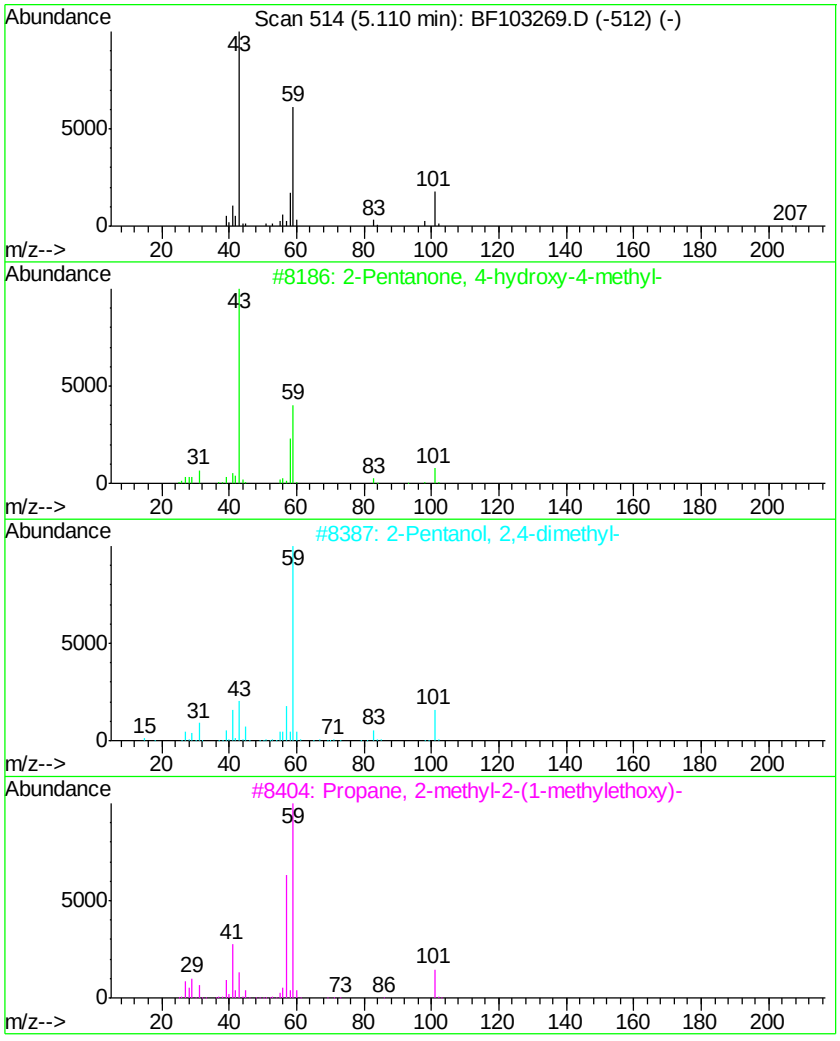
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

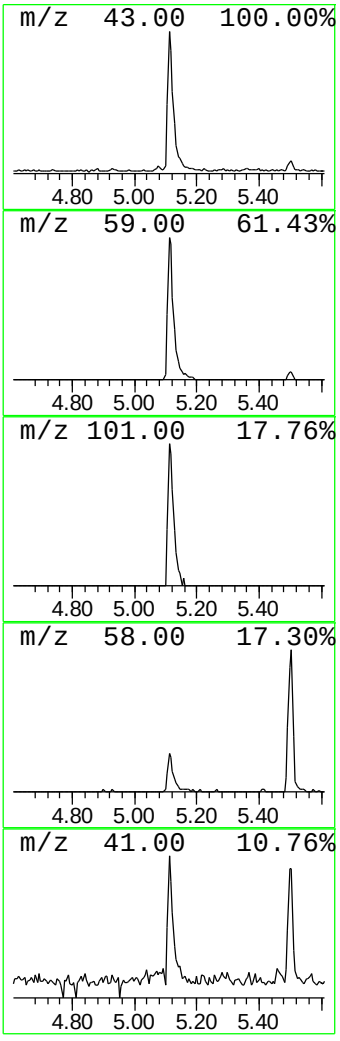
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	2.35 ng	108445	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
5	3-Octanol	130	C8H18O	000589-98-0	36





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

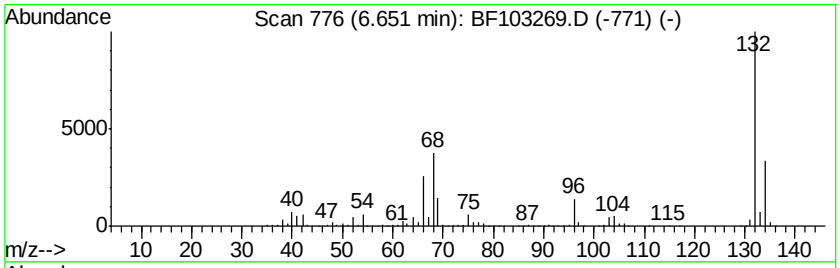
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

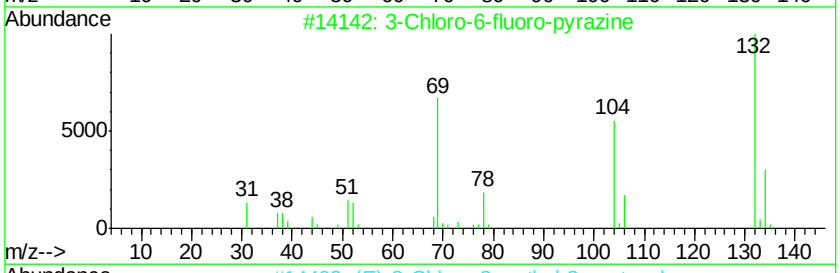
****

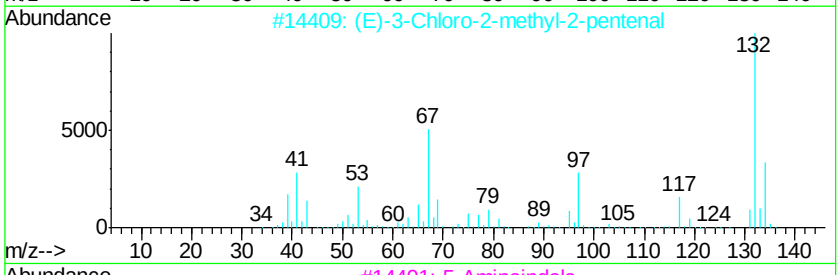
Peak Number 3 unknown6.65 Concentration Rank 1

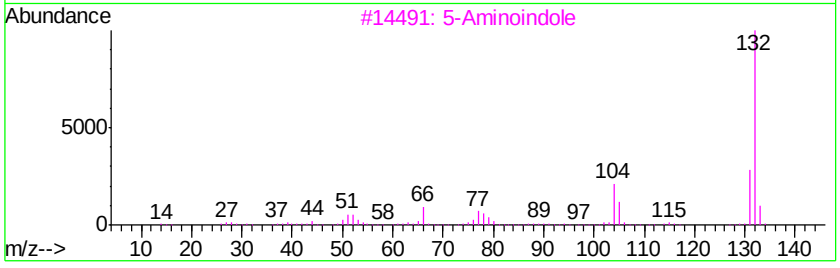
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	70.41 ng	3250000	1,4-Dichlorobenzene-d4	6.87

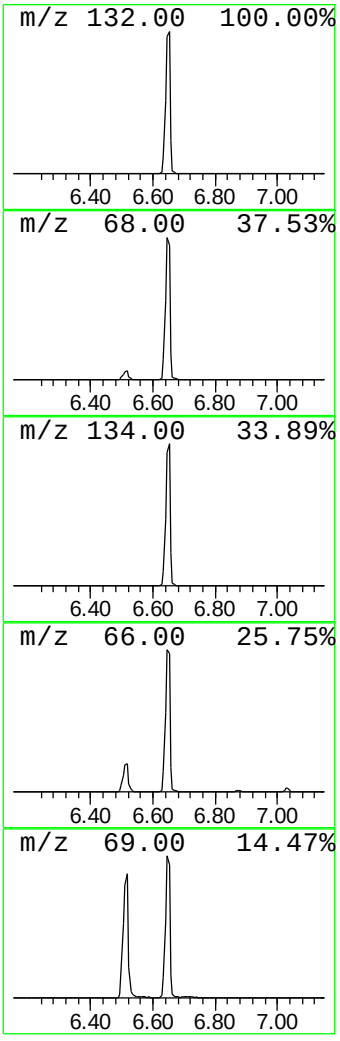
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9











Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

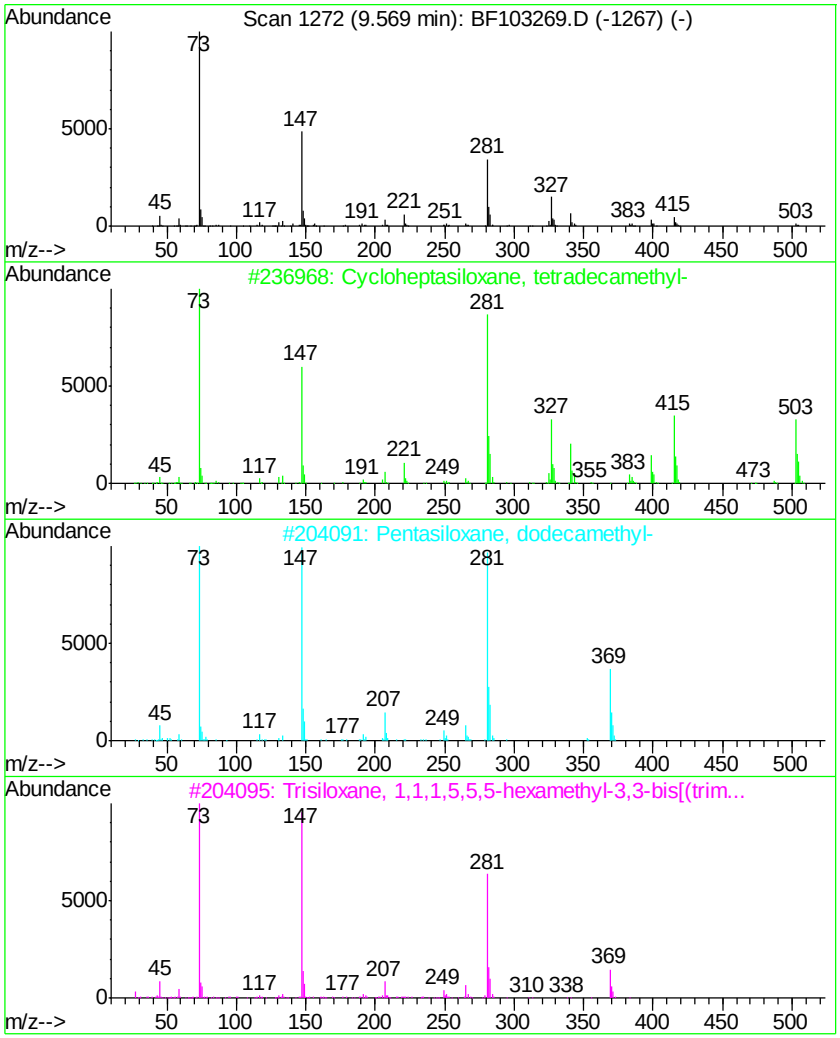
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

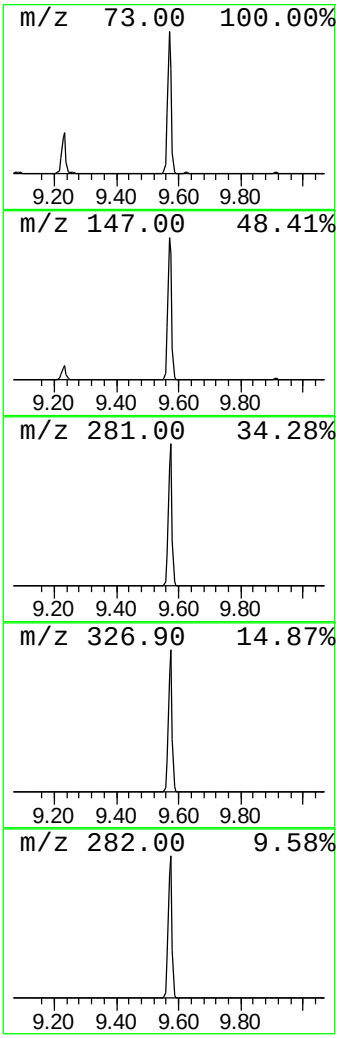
****

Peak Number 5 Cycloheptasiloxane, tetrade... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	8.32 ng	469259	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptasiloxane, tetradecamet...	518	C14H42O7Si7	000107-50-6	91
2	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	45
3	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	42
4	Ethanedioic acid, bis(trimethyls...	234	C8H18O4Si2	018294-04-7	32
5	Butanoic acid, 2-[(trimethylsily...	248	C10H24O3Si2	055133-93-2	32





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Misc :
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Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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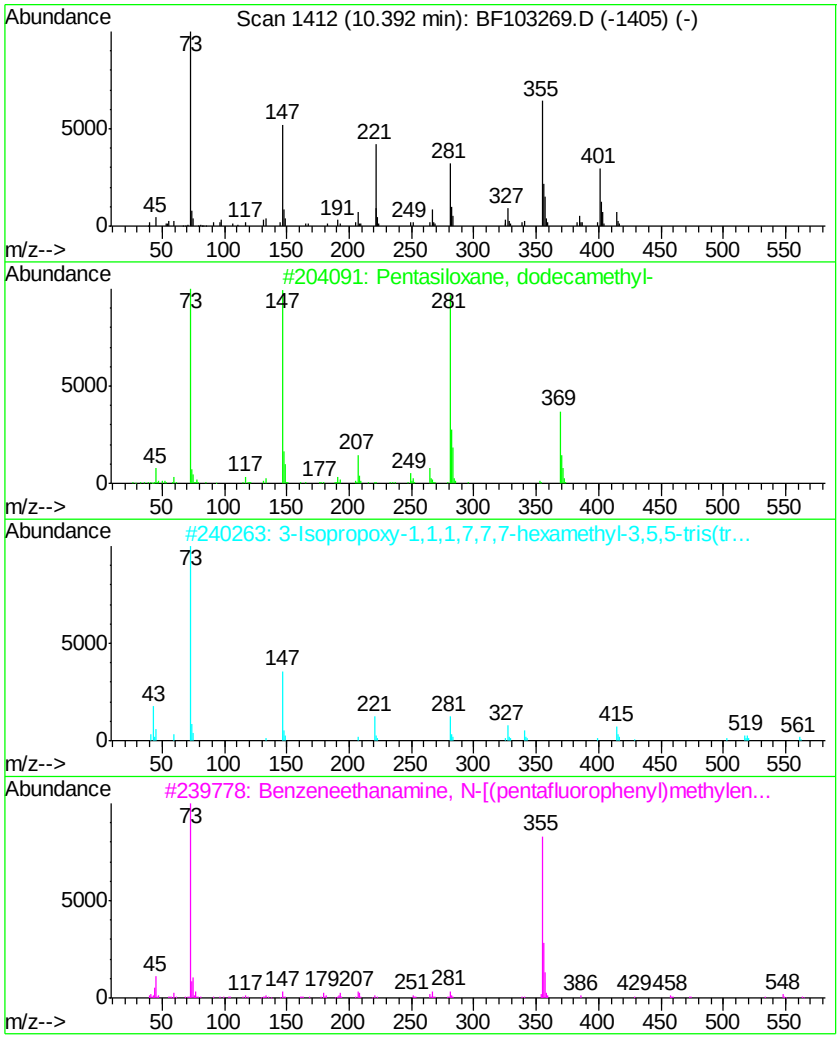
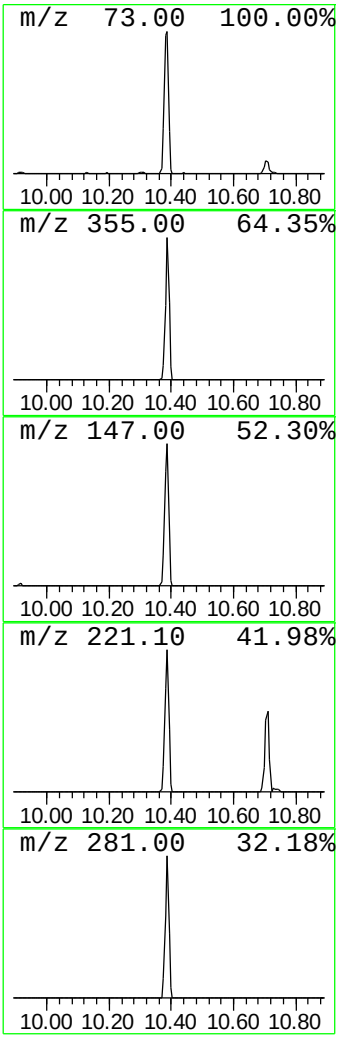
Peak Number 6 unknown10.39 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.39	5.28 ng	297911	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	35
2	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	23
3	Benzeneethanamine, N-[(pentafluo...	563	C24H34F5NO3Si3	055429-13-5	22
4	N-(Trifluoroacetyl)-N,O,O',O''-t...	553	C22H42F3NO4Si4	1000072-26-7	16
5	Phenethylamine, N-methyl-.beta.,...	399	C18H37NO3Si3	010538-85-9	12





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

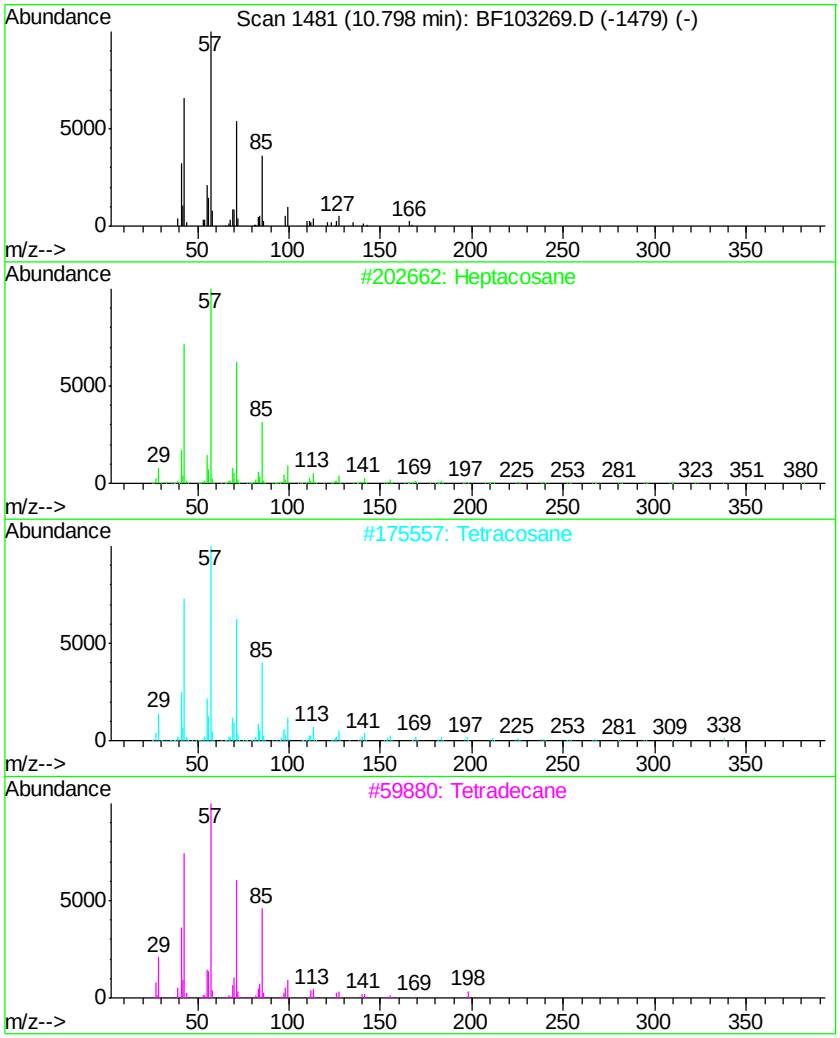
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

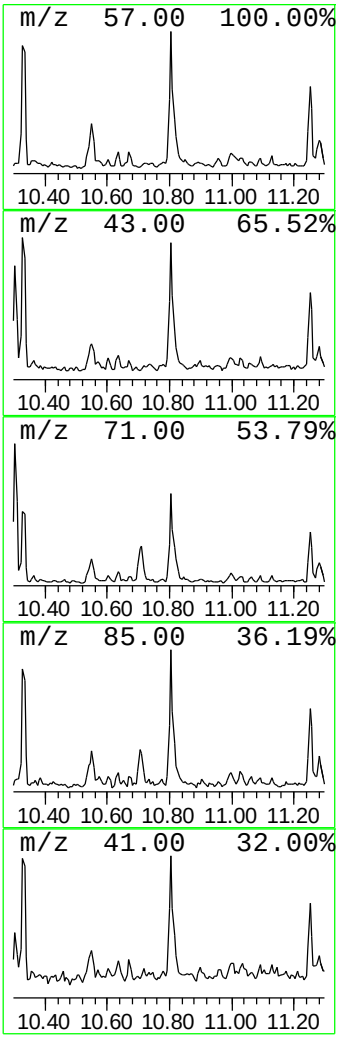
****

Peak Number 7 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	3.52 ng	157678	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Tetradecane	198	C14H30	000629-59-4	87
4	Heneicosane	296	C21H44	000629-94-7	86
5	Tritetracontane	605	C43H88	007098-21-7	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

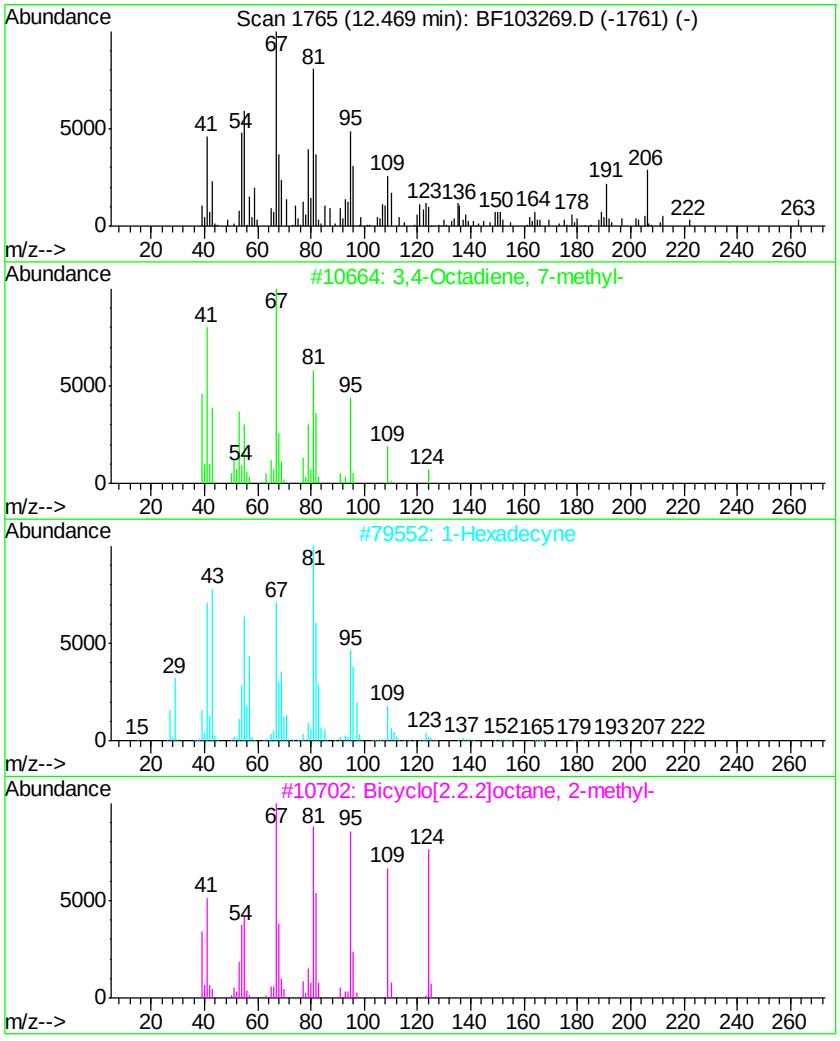
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

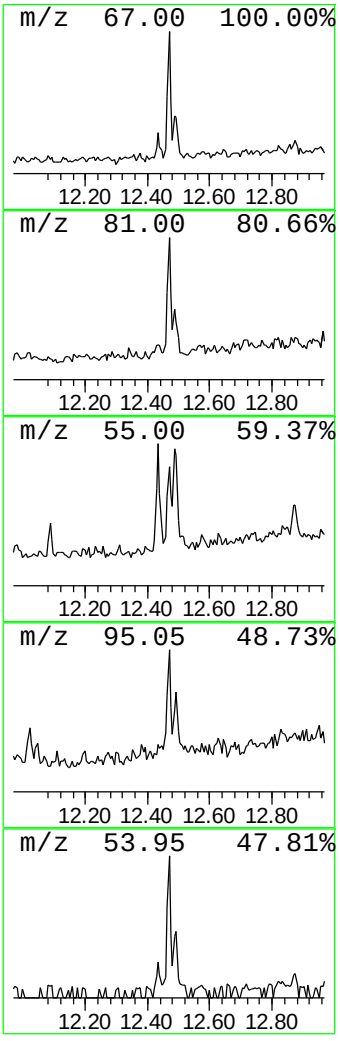
****

Peak Number 8 3,4-Octadiene, 7-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	4.02 ng	179956	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	86
2	1-Hexadecyne	222	C16H30	000629-74-3	83
3	Bicyclo[2.2.2]octane, 2-methyl-	124	C9H16	000766-53-0	62
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	52
5	11-Hexadecynal	236	C16H28O	086426-73-5	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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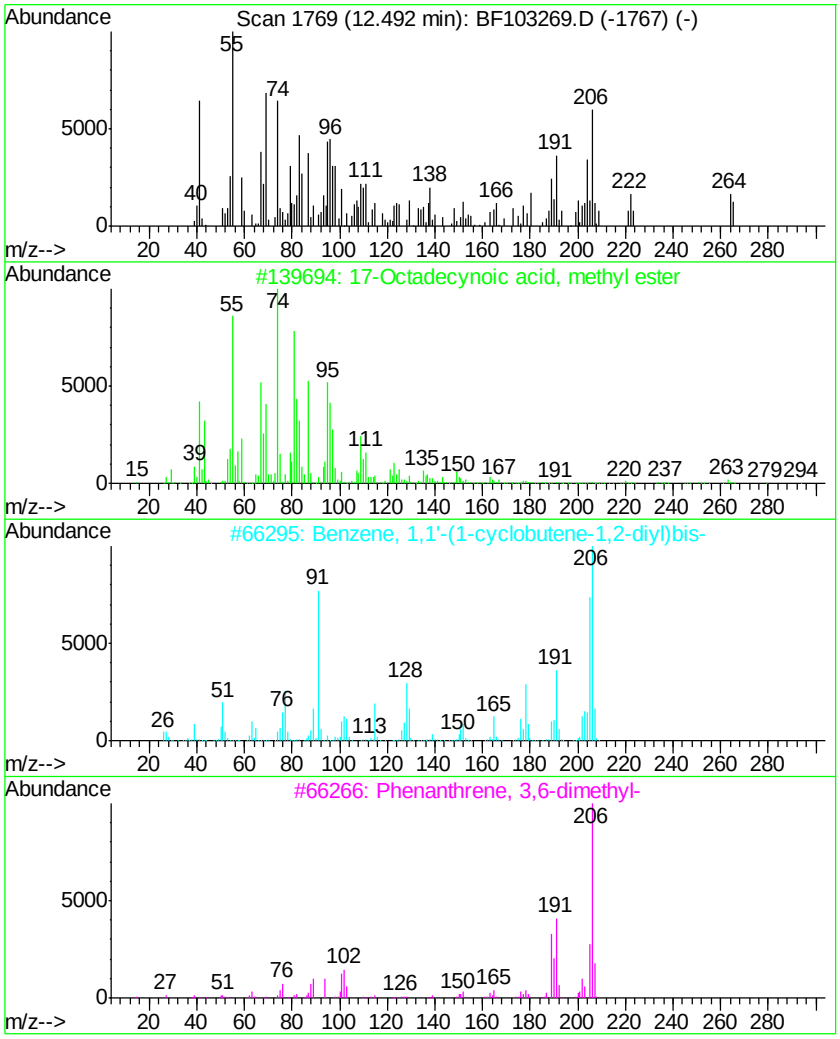
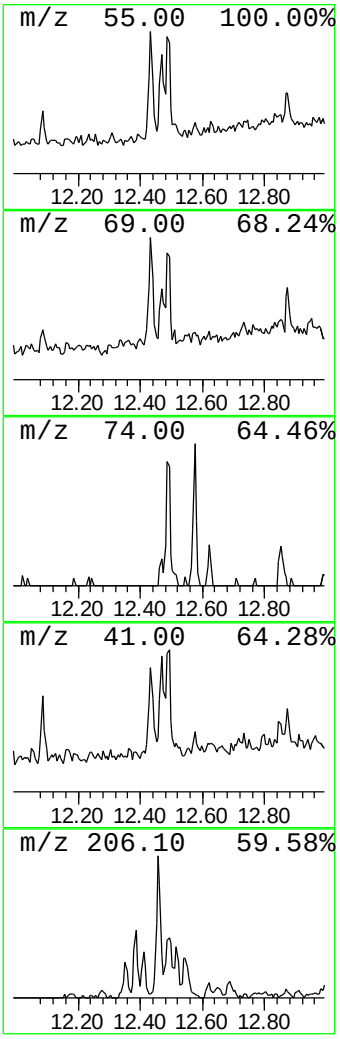
Peak Number 9 unknown12.49 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	2.92 ng	130893	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Octadecynoic acid, methyl ester	294	C19H34O2	1000333-54-0	38
2	Benzene, 1,1'-(1-cyclobutene-1,2...	206	C16H14	003306-02-3	35
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	30
4	4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	25
5	4H-1-Benzopyran-4-one, 5-hydroxy...	206	C11H10O4	000480-34-2	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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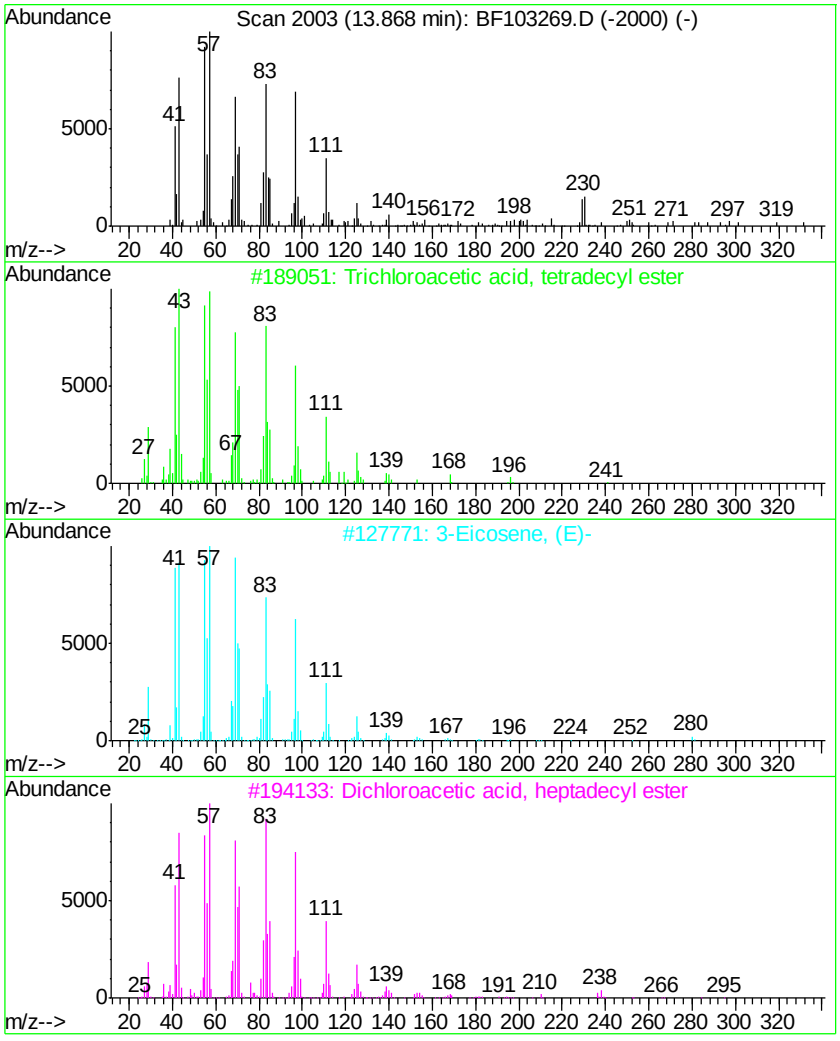
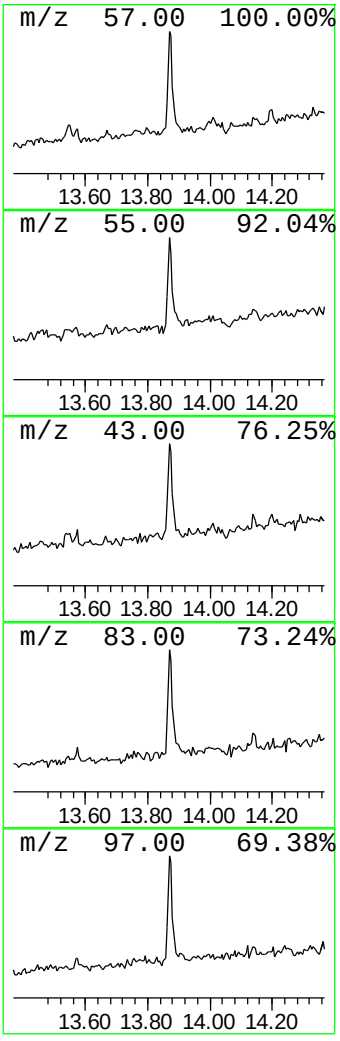
Peak Number 10 Trichloroacetic acid, tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	4.74 ng	188221	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
4	1-Docosene	308	C22H44	001599-67-3	87
5	1-Octadecene	252	C18H36	000112-88-9	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF022718\
Data File : BF103269.D
Acq On : 27 Feb 2018 18:02
Operator : SJ/JU
Sample : J1697-13
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-022318-C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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...	2.15	7.2	ng	332256	1	6.87	923184	20.0
2-Pentanone, 4-hy...	5.11	2.4	ng	108445	1	6.87	923184	20.0
unknown6.65	6.65	70.4	ng	3250000	1	6.87	923184	20.0
Cycloheptasiloxan...	9.57	8.3	ng	469259	3	9.92	1128530	20.0
unknown10.39	10.39	5.3	ng	297911	3	9.92	1128530	20.0
Heptacosane	10.80	3.5	ng	157678	4	11.40	896184	20.0
3,4-Octadiene, 7-...	12.47	4.0	ng	179956	4	11.40	896184	20.0
unknown12.49	12.49	2.9	ng	130893	4	11.40	896184	20.0
Trichloroacetic a...	13.87	4.7	ng	188221	5	14.06	793500	20.0