LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
Data File : BF103290.D
Acq On : 28 Feb 2018 4:14
Operator : SJ/JU
Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

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	2.140	4	9	17	rVB	1109269	1431469	39.50%	4.682%
2	5.093	509	511	523	rBV	102802	136780	3.77%	0.447%
3	5.498	576	580	593	rBV	2074821	2321123	64.05%	7.592%
4	6.504	747	751	768	rBV	1373643	1512647	41.74%	4.947%
5	6.645	770	775	778	rBV	3800795	3604747	99.46%	11.790%
6	6.869	810	813	819	rBV	1086897	1036518	28.60%	3.390%
7	7.028	836	840	844	rBV	3368161	3479164	96.00%	11.379%
8	7.439	905	910	913	rBV	2822087	2936690	81.03%	9.605%
9	8.157	1028	1032	1049	rBV	1320130	1304293	35.99%	4.266%
10	9.228	1210	1214	1218	rBV	3480230	3624179	100.00%	11.854%
11	9.622	1276	1281	1289	rBV	143827	149402	4.12%	0.489%
12	9.828	1313	1316	1320	rBV	83406	68340	1.89%	0.224%
13	9.910	1326	1330	1340	rVB2	1000517	1006518	27.77%	3.292%
14	10.322	1396	1400	1405	rBV	1065177	861250	23.76%	2.817%
15	10.545	1433	1438	1441	rBV	32352	43389	1.20%	0.142%
16	10.704	1461	1465	1474	rBV	1614845	1675537	46.23%	5.480%
17	10.804	1479	1482	1488	rVB	94930	98851	2.73%	0.323%
18	11.404	1580	1584	1592	rBV	893461	842924	23.26%	2.757%
19	12.792	1817	1820	1825	rBV	62527	50264	1.39%	0.164%
20	12.986	1849	1853	1857	rBV	2366801	2521211	69.57%	8.246%
21	13.498	1937	1940	1943	rBV	52621	41715	1.15%	0.136%
22	13.868	1999	2003	2015	rBV	167708	220903	6.10%	0.723%
23	14.051	2030	2034	2044	rBV	761394	759527	20.96%	2.484%
24	14.804	2160	2162	2167	rVB	34590	36570	1.01%	0.120%
25	15.151	2217	2221	2224	rVB	34306	40850	1.13%	0.134%
26	15.551	2282	2289	2297	rBV	345445	582848	16.08%	1.906%
27	15.974	2357	2361	2365	rVB	43014	58758	1.62%	0.192%
28	16.492	2444	2449	2453	rBV3	39099	68573	1.89%	0.224%
29	17.098	2548	2552	2561	rVB5	30286	59422	1.64%	0.194%

Sum of corrected areas: 30574462

LSC Report - Integrated Chromatogram

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Data File : BF103290.D
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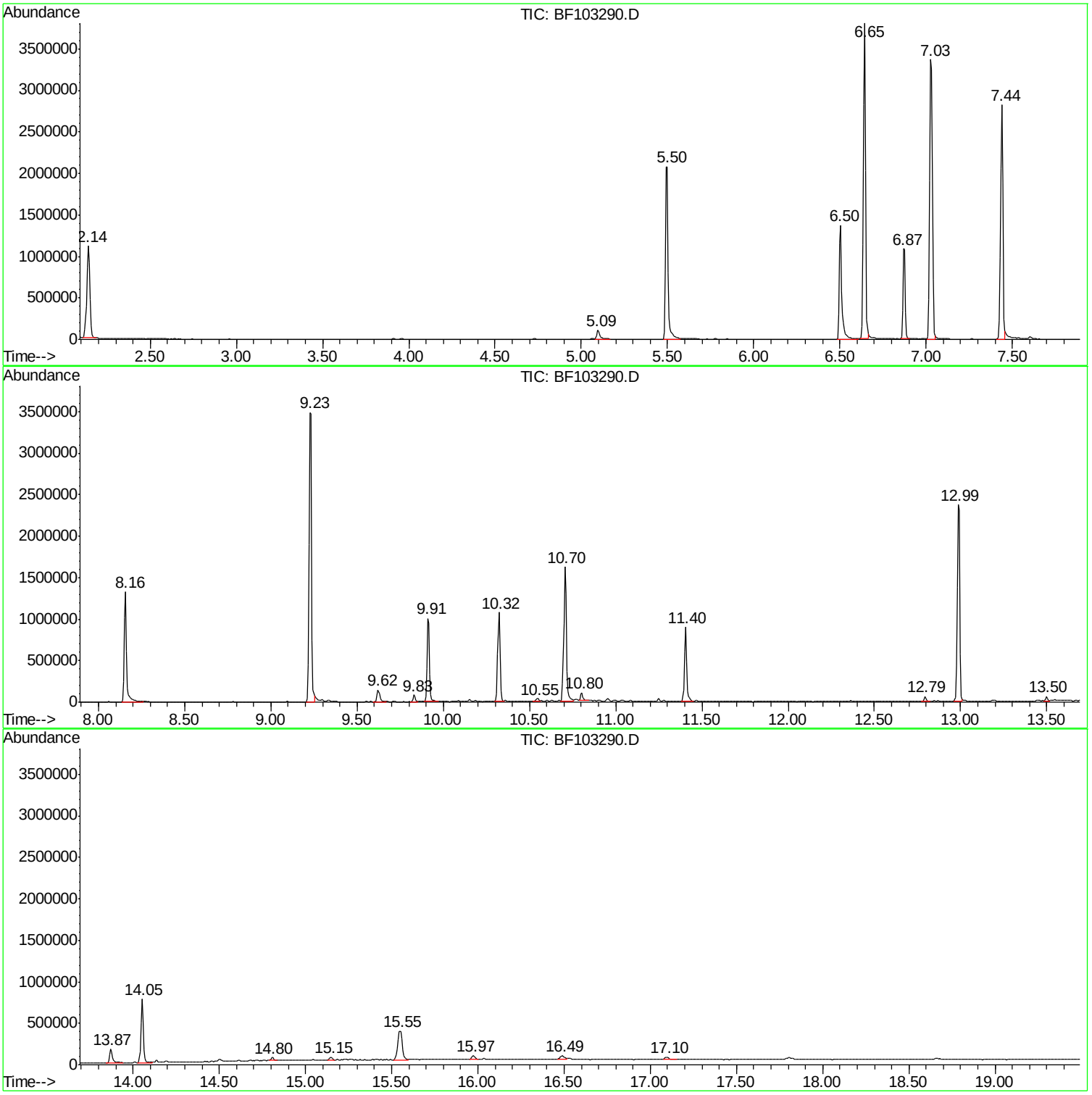
Operator : SJ/JU
Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

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



Library Search Compound Report

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Data File : BF103290.D
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Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

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

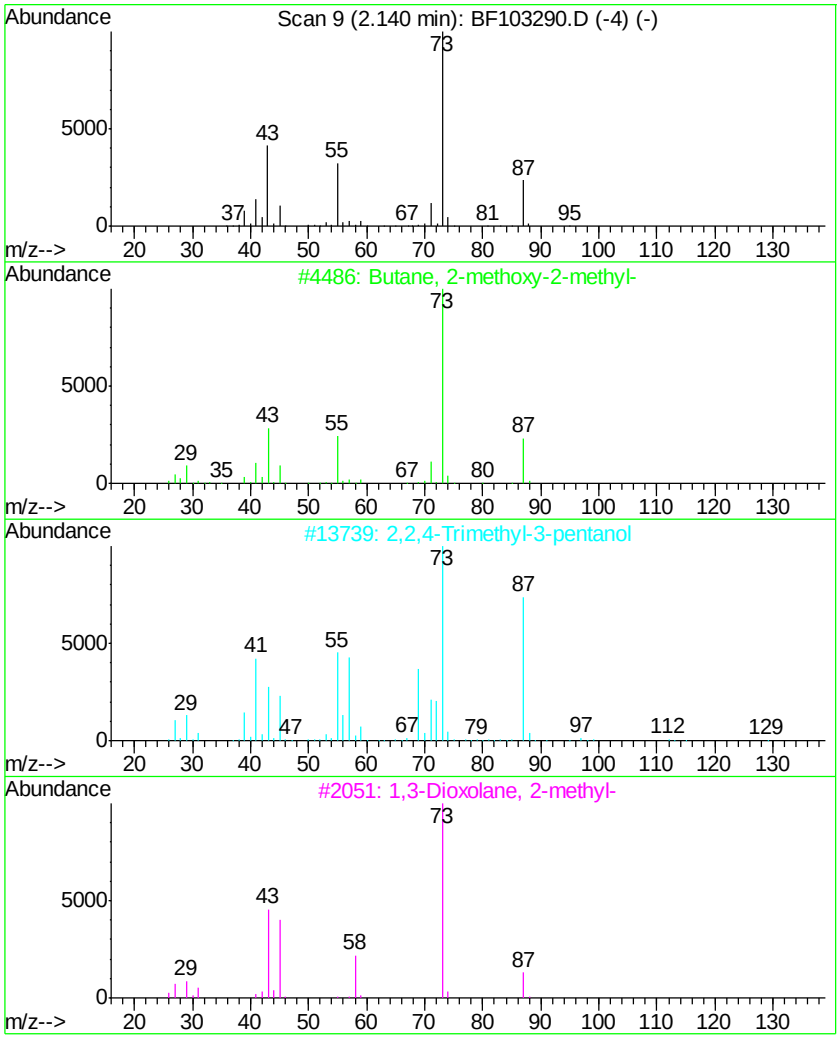
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

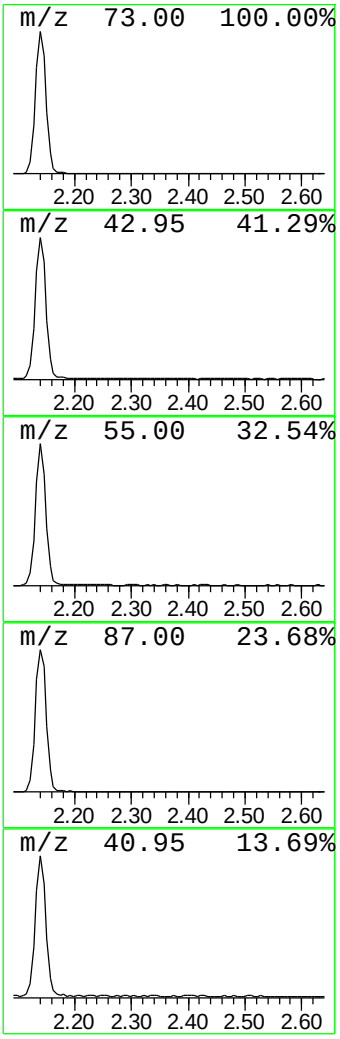
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	27.62 ng	1431470	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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Library Search Compound Report

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Acq On : 28 Feb 2018 4:14
Operator : SJ/JU
Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

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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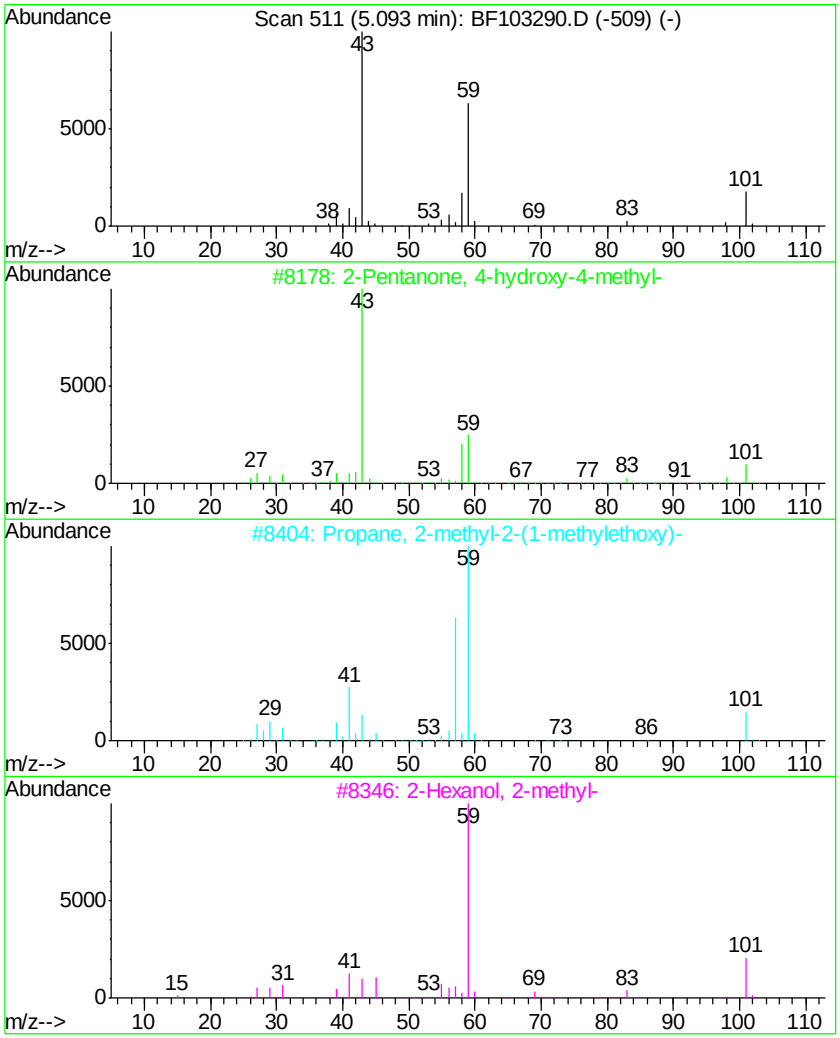
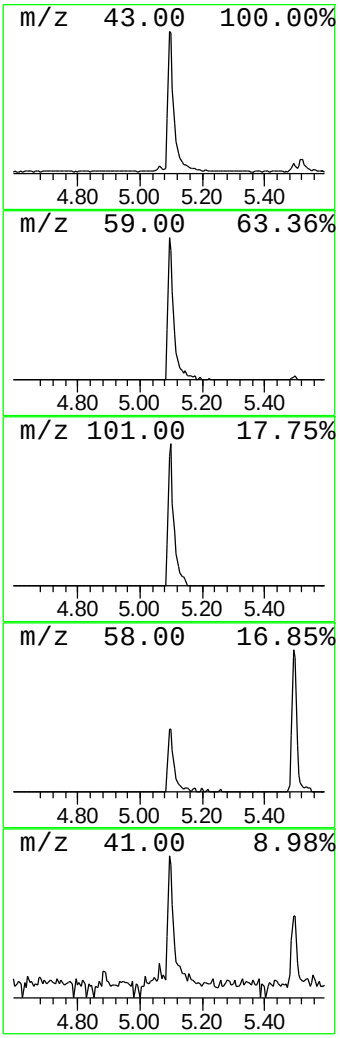
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.64 ng	136780	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	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	40
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
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Operator : SJ/JU
Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

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

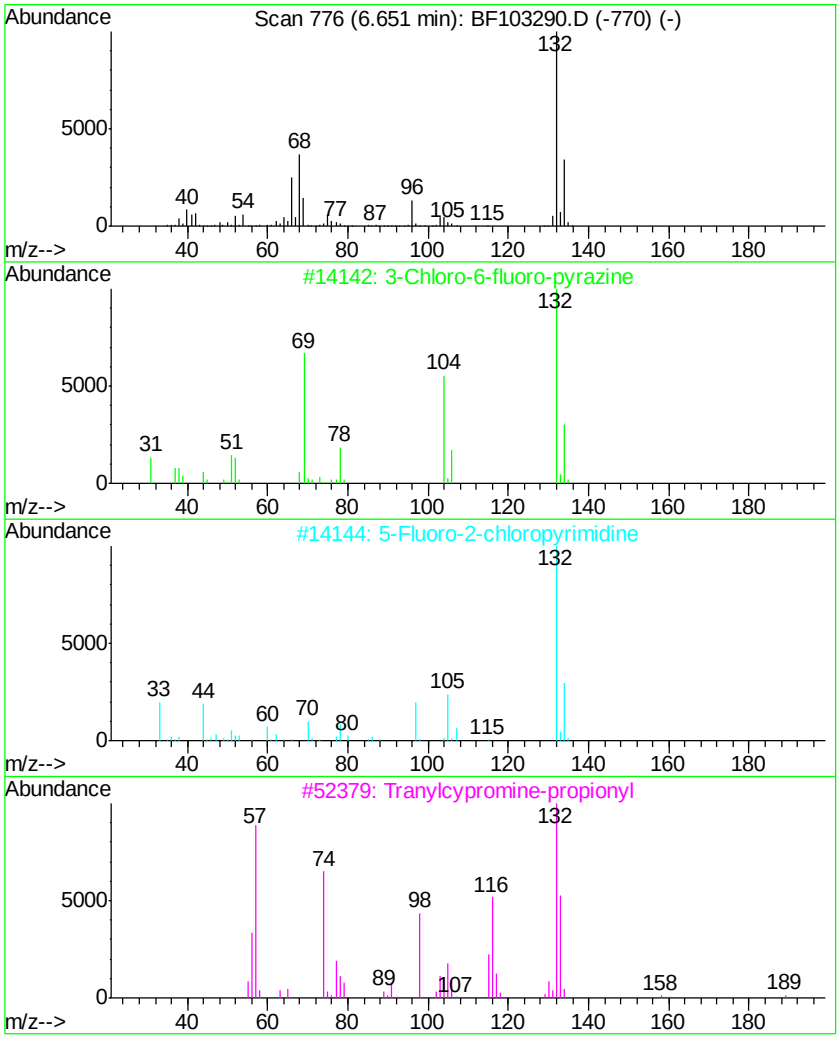
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

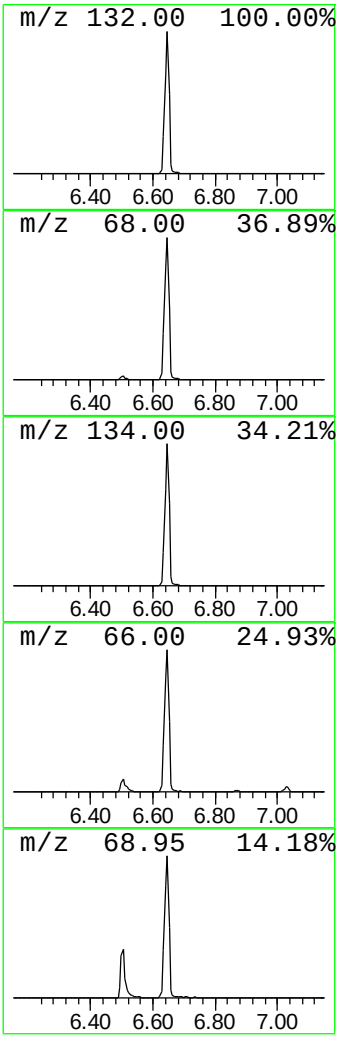
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	69.55 ng	3604750	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF022718\
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Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

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

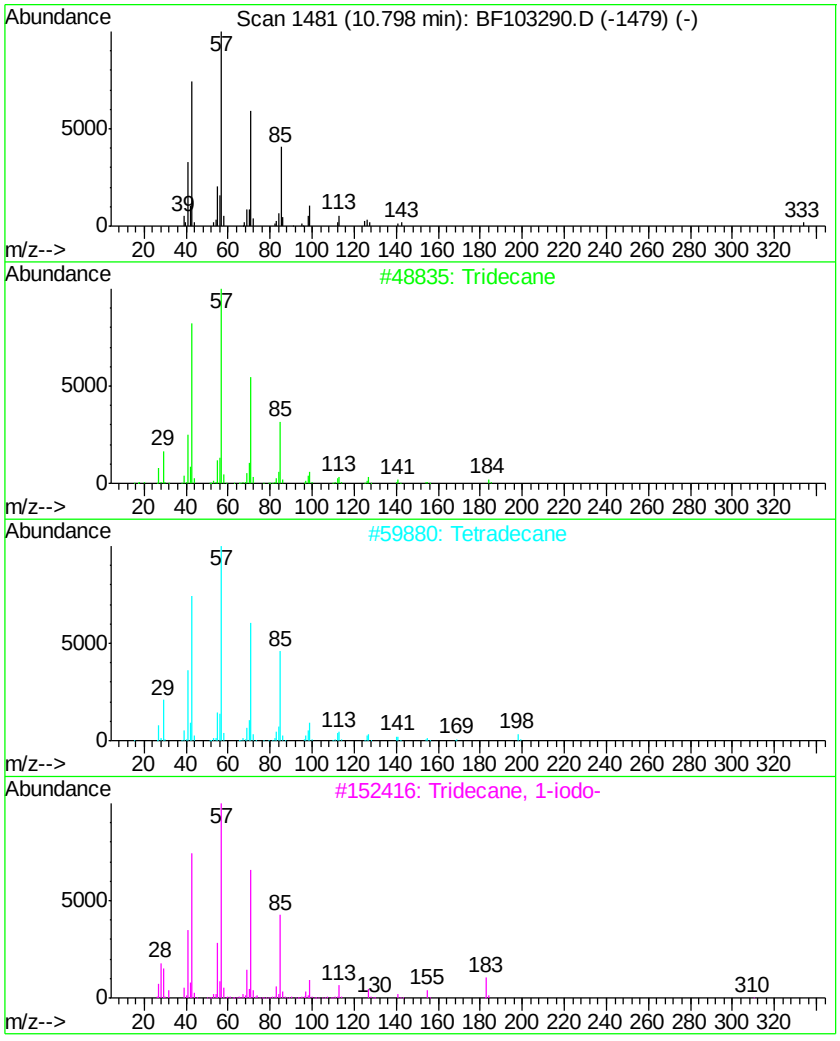
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

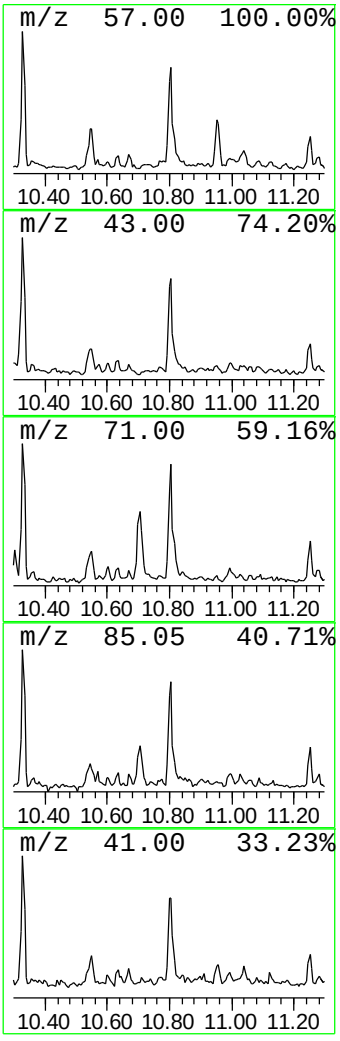
****

Peak Number 5 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.35 ng	98851	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	78
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
5	Hexadecane	226	C16H34	000544-76-3	59





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Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
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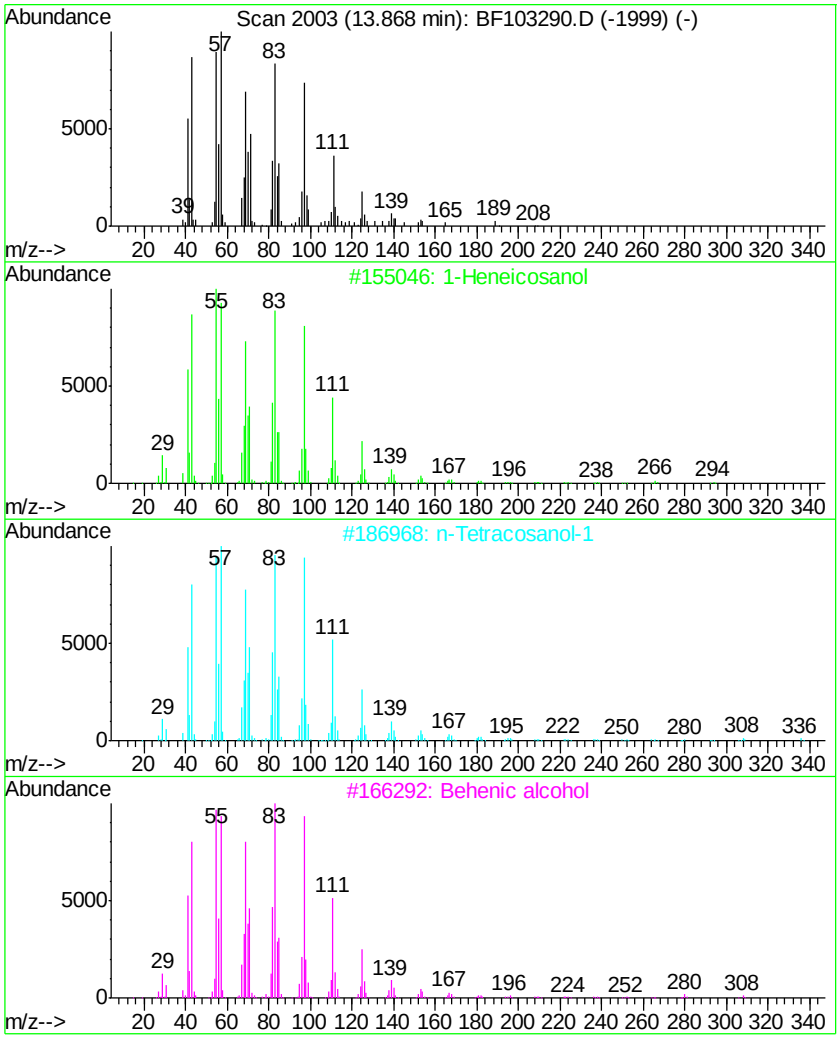
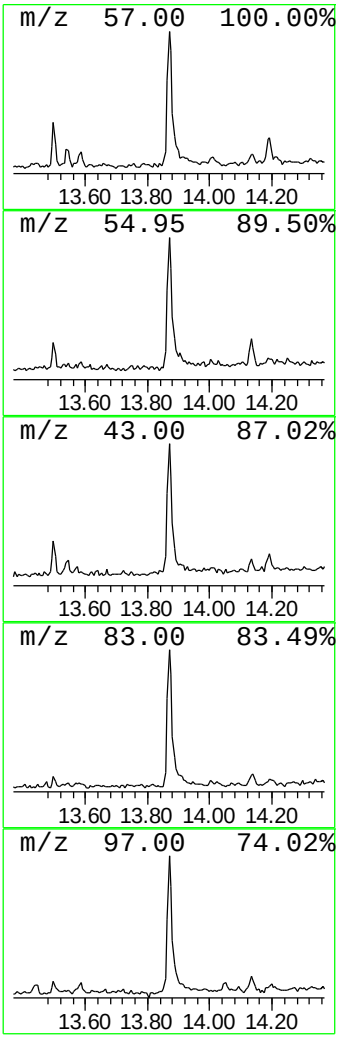
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	5.82 ng	220903	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





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Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

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

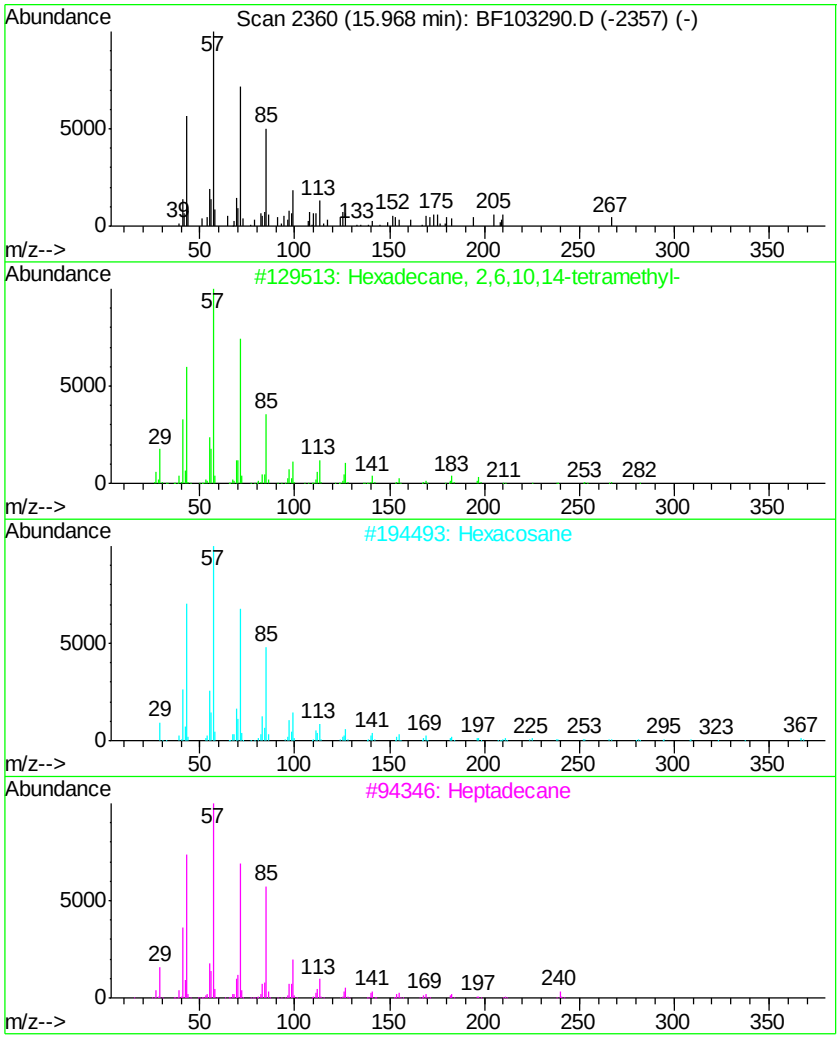
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

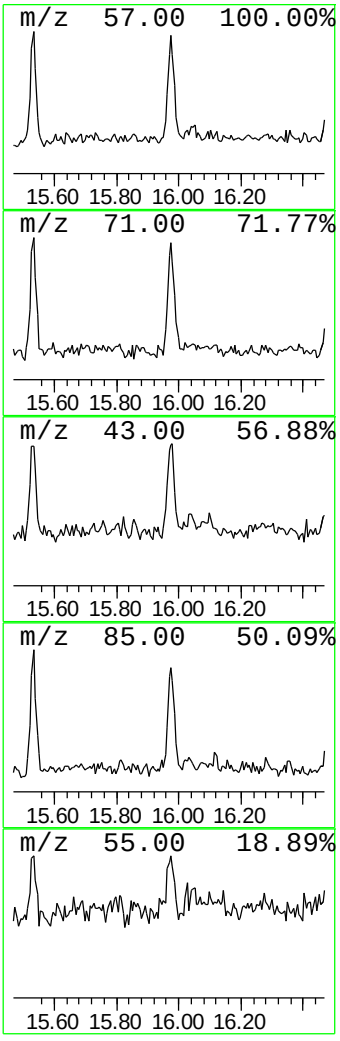
****

Peak Number 7 Hexadecane, 2,6,10,14-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.02 ng	58758	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2	Hexacosane	366	C26H54	000630-01-3	74
3	Heptadecane	240	C17H36	000629-78-7	74
4	Pentacosane	352	C25H52	000629-99-2	72
5	Tetracosane	338	C24H50	000646-31-1	72





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Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

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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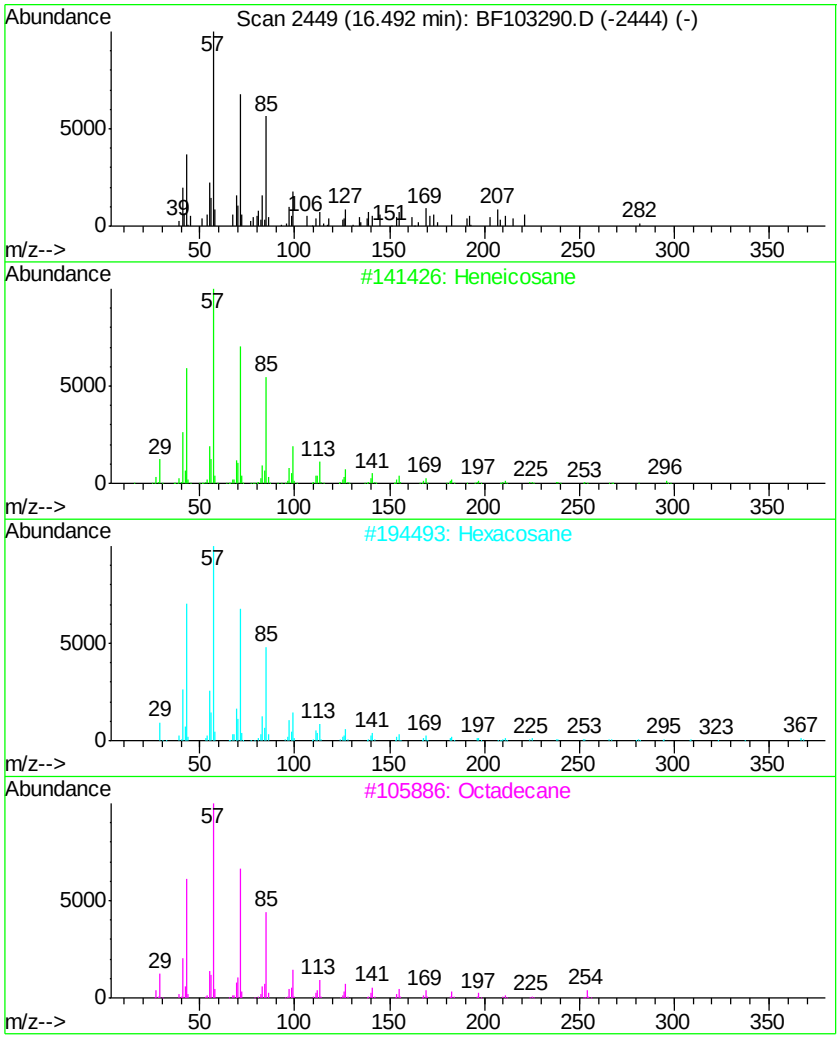
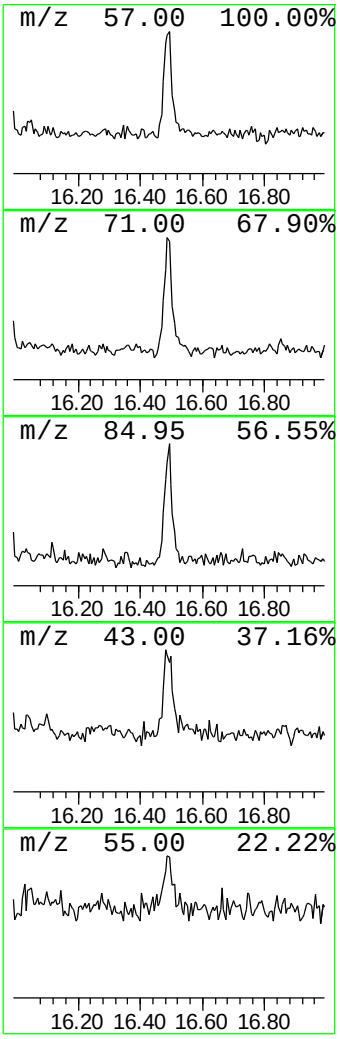
Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.35 ng	68573	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	83
2	Hexacosane	366	C26H54	000630-01-3	83
3	Octadecane	254	C18H38	000593-45-3	80
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5	Octacosane	394	C28H58	000630-02-4	80





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ALS Vial : 34 Sample Multiplier: 1

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

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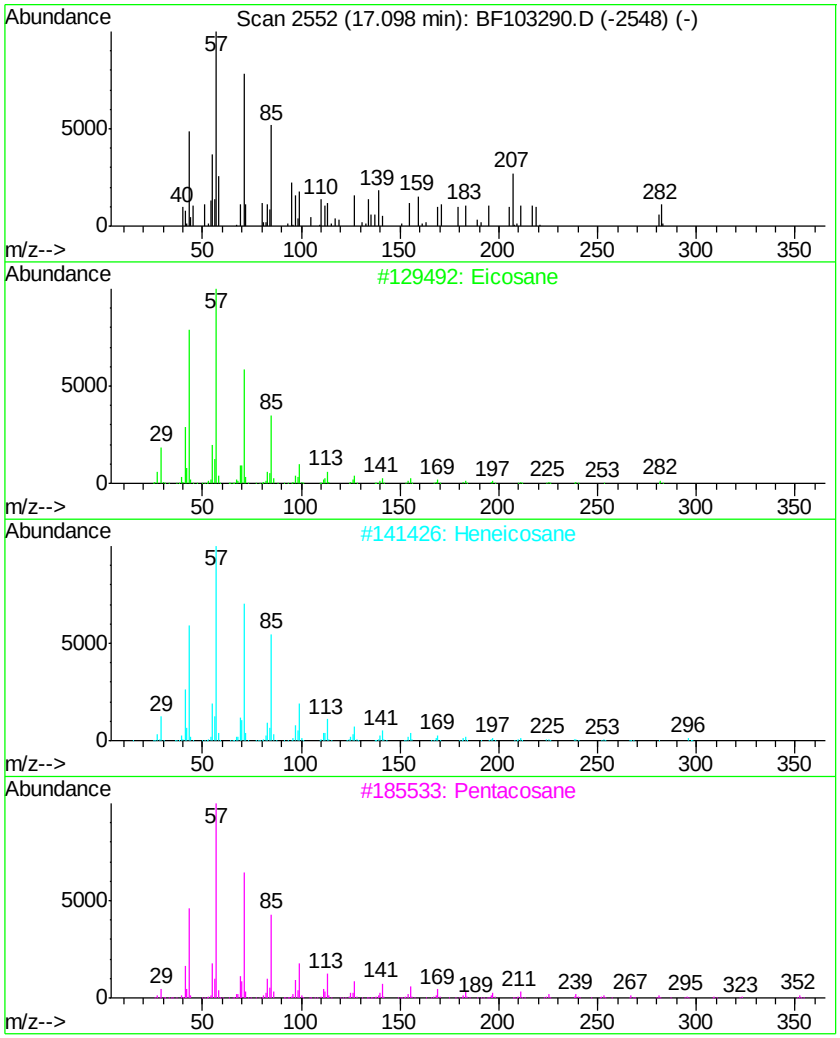
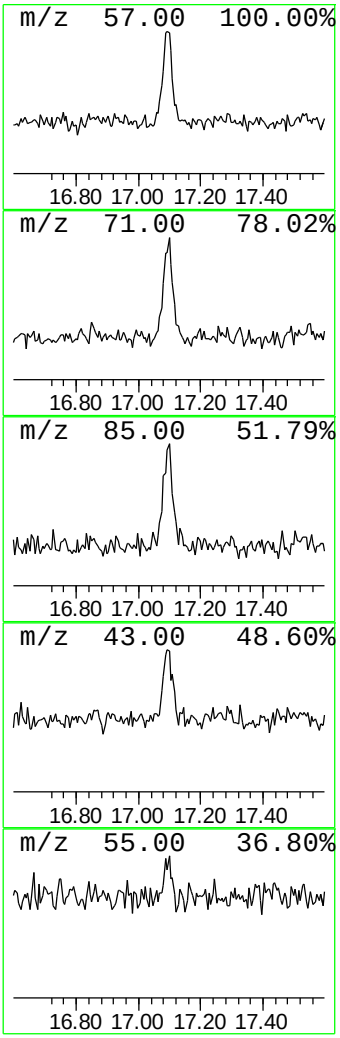
Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.10	2.04 ng	59422	Perylene-d12	15.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	78
2	Heneicosane	296	C21H44	000629-94-7	46
3	Pentacosane	352	C25H52	000629-99-2	46
4	Octacosane	394	C28H58	000630-02-4	46
5	Tetracontane	563	C40H82	004181-95-7	43





Tentatively Identified Compound (LSC) summary

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Data File : BF103290.D
Acq On : 28 Feb 2018 4:14
Operator : SJ/JU
Sample : J1683-04
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RFK-RMAB-MW11-GW

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...	2.14	27.6	ng	1431470	1	6.87	1036520	20.0
2-Pentanone, 4-hy...	5.09	2.6	ng	136780	1	6.87	1036520	20.0
unknown6.65	6.65	69.5	ng	3604750	1	6.87	1036520	20.0
Tridecane	10.80	2.4	ng	98851	4	11.40	842924	20.0
1-Heneicosanol	13.87	5.8	ng	220903	5	14.05	759527	20.0
Hexadecane, 2,6,1...	15.97	2.0	ng	58758	6	15.55	582848	20.0
Heneicosane	16.49	2.4	ng	68573	6	15.55	582848	20.0
Eicosane	17.10	2.0	ng	59422	6	15.55	582848	20.0