LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114443.D
Acq On : 20 May 2019 17:22
Operator : JU/SJ
Sample : K2943-17
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-1

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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	5.463	570	574	592	rBV	3673404	3858232	91.94%	8.552%
2	6.475	741	746	764	rBV	3740619	4110944	97.96%	9.112%
3	6.604	764	768	789	rVB	4346951	3956016	94.27%	8.768%
4	6.828	802	806	814	rBV	1293491	1089363	25.96%	2.415%
5	6.987	829	833	848	rBV	3129043	3070002	73.16%	6.805%
6	7.387	897	901	916	rBV	2309091	2536859	60.45%	5.623%
7	8.110	1020	1024	1047	rBV	1442375	1411496	33.63%	3.129%
8	8.481	1083	1087	1097	rBV	44896	78086	1.86%	0.173%
9	8.728	1126	1129	1139	rVB	143373	142580	3.40%	0.316%
10	9.181	1202	1206	1218	rBV	4159105	4196560	100.00%	9.301%
11	9.575	1270	1273	1284	rBV	473243	499600	11.90%	1.107%
12	9.863	1313	1322	1332	rBV	1693438	1550788	36.95%	3.437%
13	10.657	1453	1457	1470	rBV	2407661	2593809	61.81%	5.749%
14	11.351	1571	1575	1589	rBV	1734017	1619505	38.59%	3.590%
15	11.875	1660	1664	1677	rBV2	158421	243897	5.81%	0.541%
16	12.657	1794	1797	1809	rBV2	93028	150558	3.59%	0.334%
17	12.933	1839	1844	1847	rBV	4197475	3963711	94.45%	8.785%
18	13.498	1935	1940	1946	rVB2	45468	72713	1.73%	0.161%
19	13.827	1992	1996	2011	rBV6	143144	365967	8.72%	0.811%
20	13.992	2020	2024	2032	rBV	1343145	1307895	31.17%	2.899%
21	14.139	2045	2049	2052	rBV	192239	171725	4.09%	0.381%
22	14.445	2096	2101	2105	rBV	441931	458779	10.93%	1.017%
23	14.745	2147	2152	2162	rBV	1008406	1115650	26.58%	2.473%
24	14.821	2162	2165	2168	rVB	55020	51688	1.23%	0.115%
25	15.080	2203	2209	2216	rVB	1186971	1425249	33.96%	3.159%
26	15.451	2266	2272	2286	rBV2	1809489	2681796	63.90%	5.944%
27	15.710	2314	2316	2321	rVB2	36190	44229	1.05%	0.098%
28	15.874	2338	2344	2355	rBV	825997	1331845	31.74%	2.952%
29	16.368	2422	2428	2437	rBV	382276	688556	16.41%	1.526%
30	16.951	2521	2527	2536	rVB2	108996	229533	5.47%	0.509%
31	17.627	2639	2642	2652	rVB5	40301	99514	2.37%	0.221%

Sum of corrected areas: 45117145

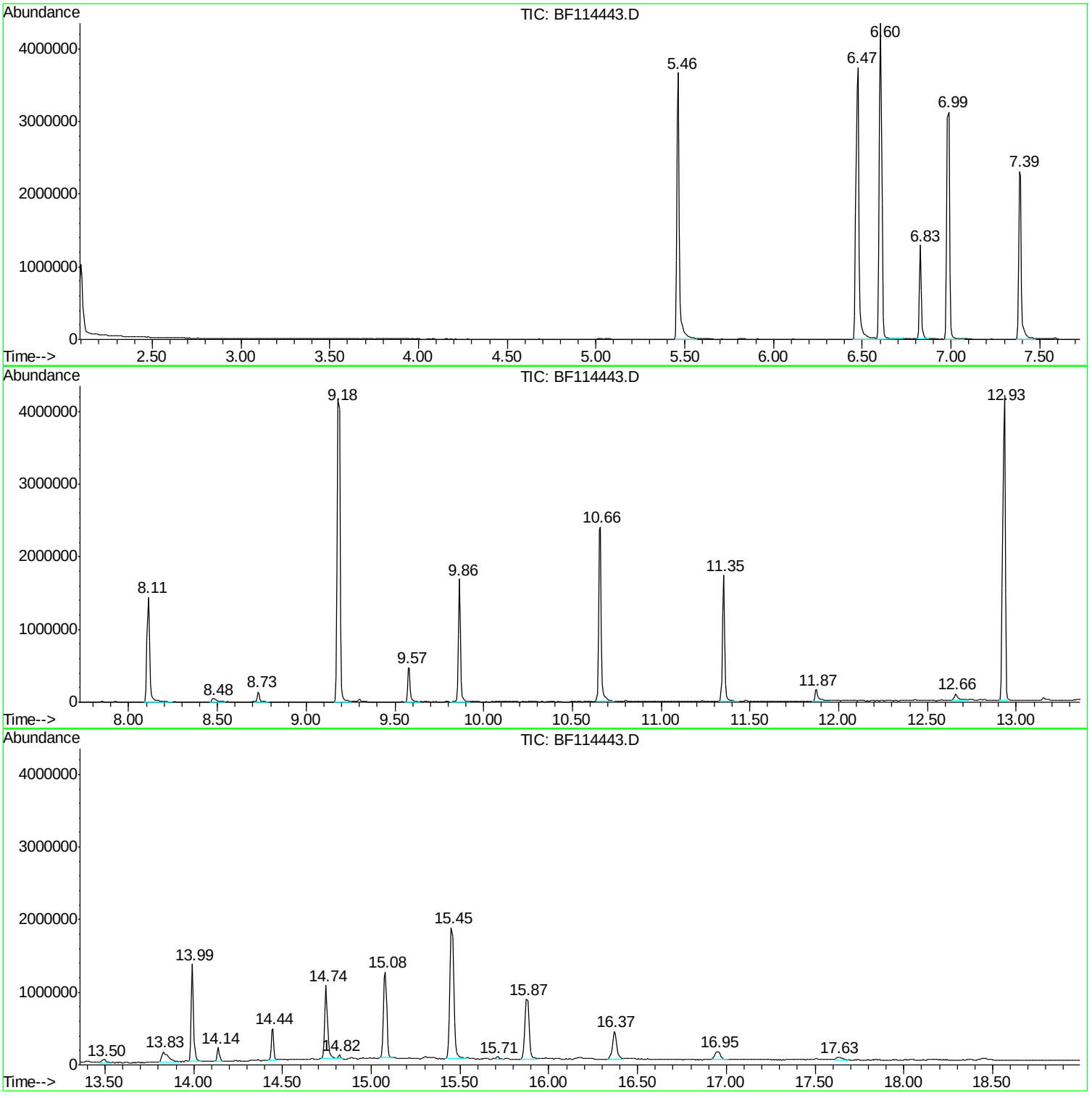
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114443.D
Acq On : 20 May 2019 17:22
Operator : JU/SJ
Sample : K2943-17
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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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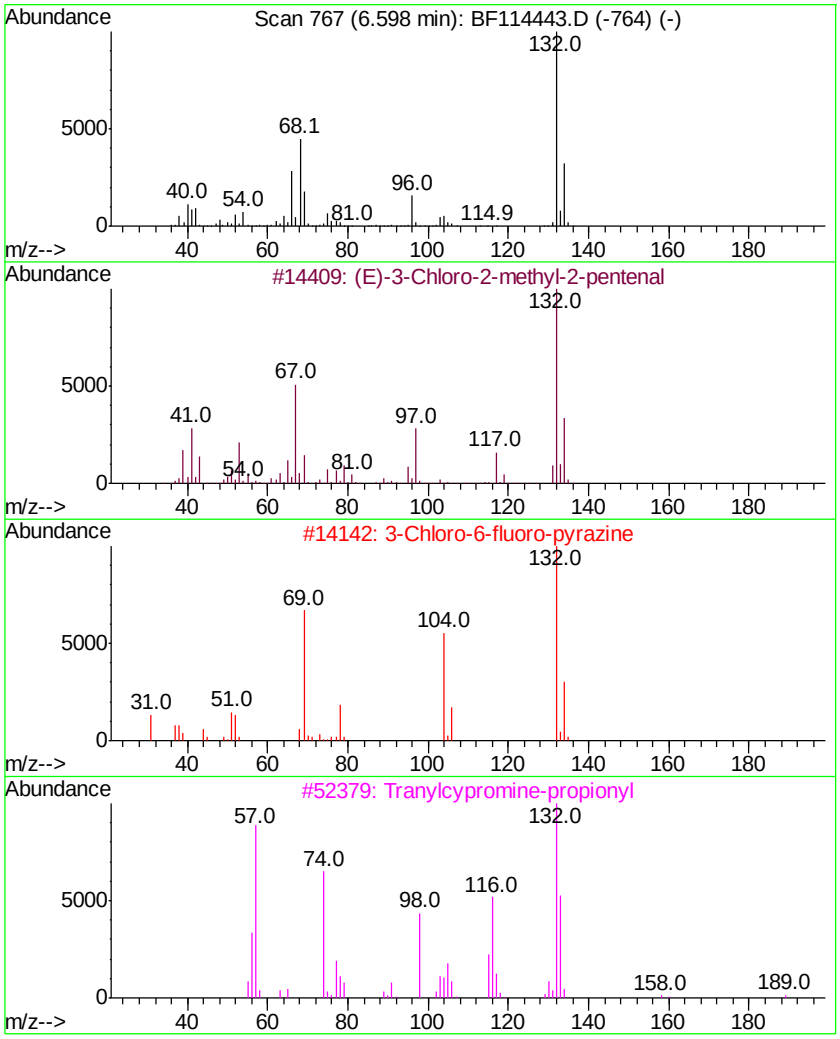
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

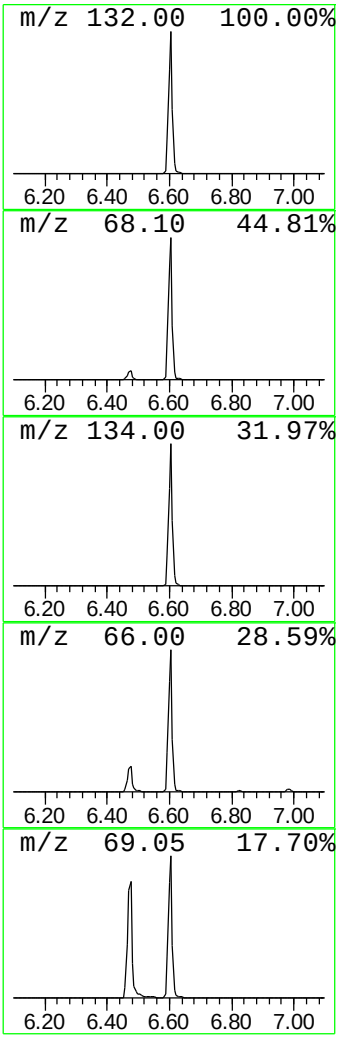
****

Peak Number 1 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	72.63 ng	3956020	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Instrument : BNA_F
ClientSampleId : DB-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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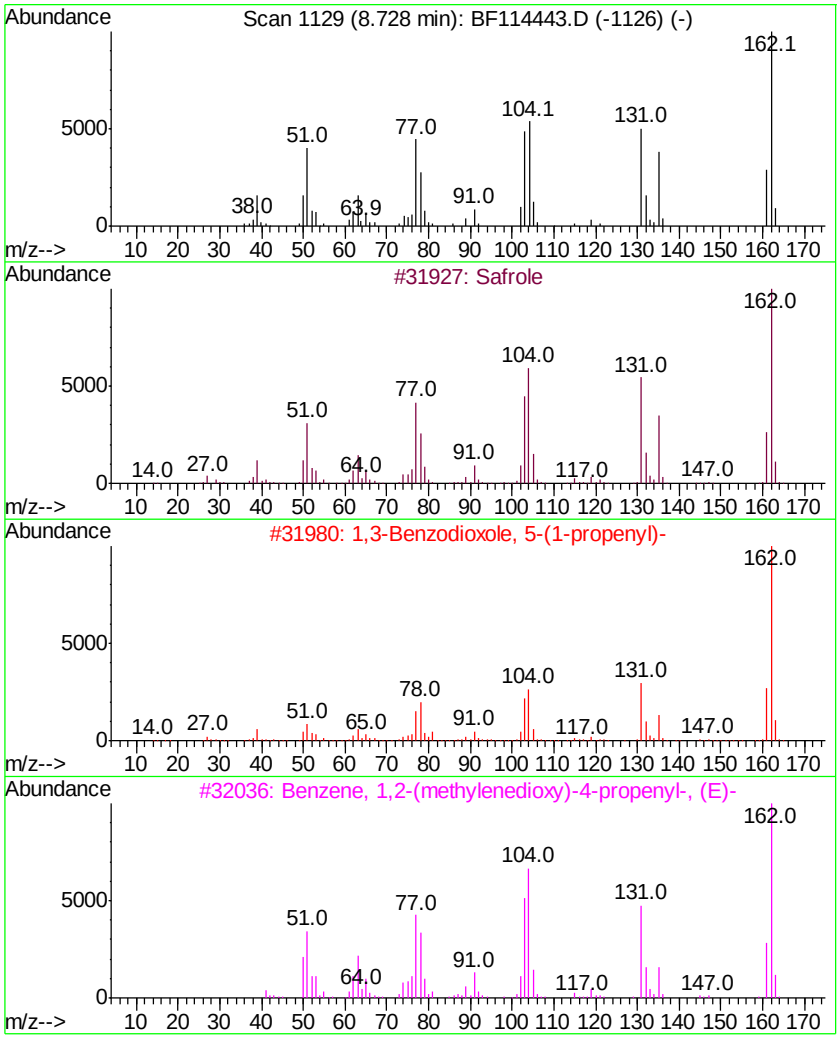
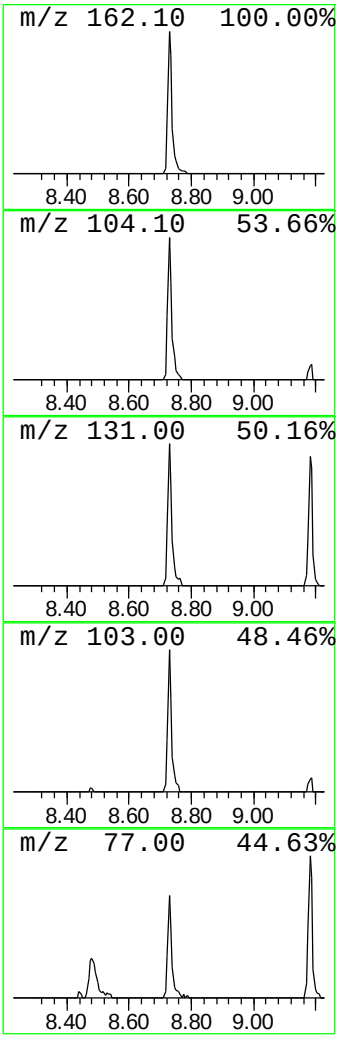
Peak Number 3 Safrole Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	2.02 ng	142580	Naphthalene-d8	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Safrole	162	C10H10O2	000094-59-7	98
2	1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	95
3	Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	74
4	2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	000103-26-4	58
5	1,3-Benzodioxole, 5-(1-propenyl)...	162	C10H10O2	017627-76-8	43





Library Search Compound Report

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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
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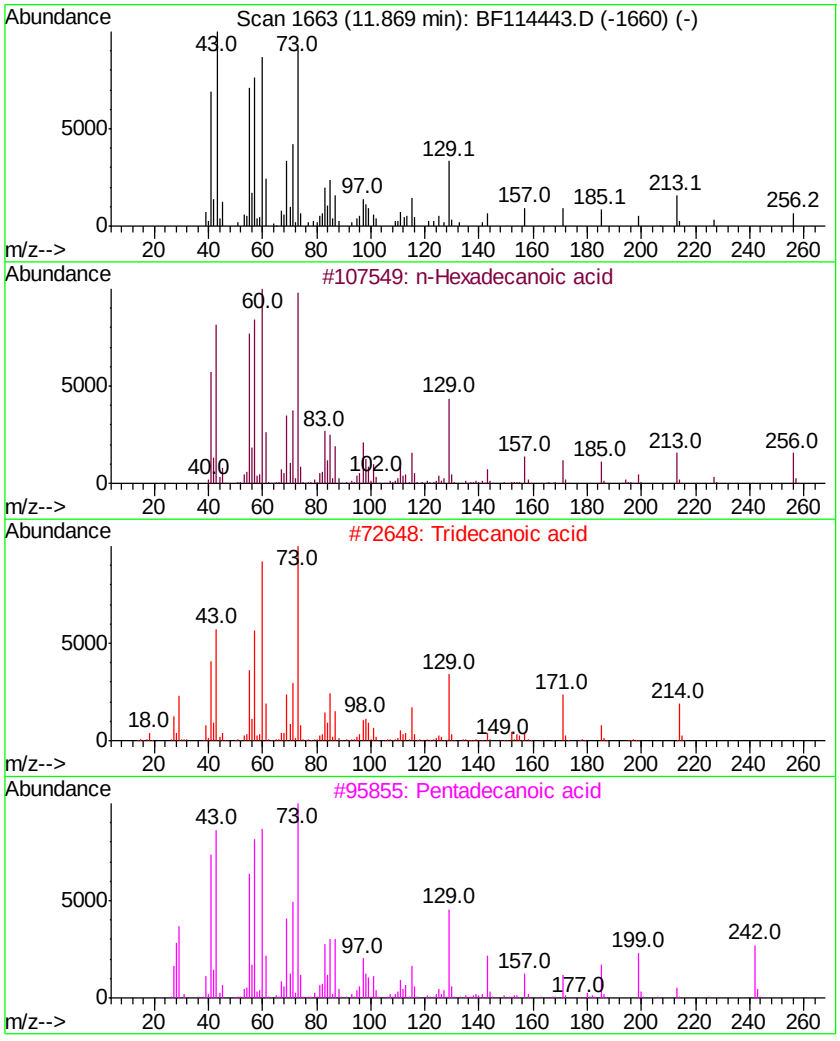
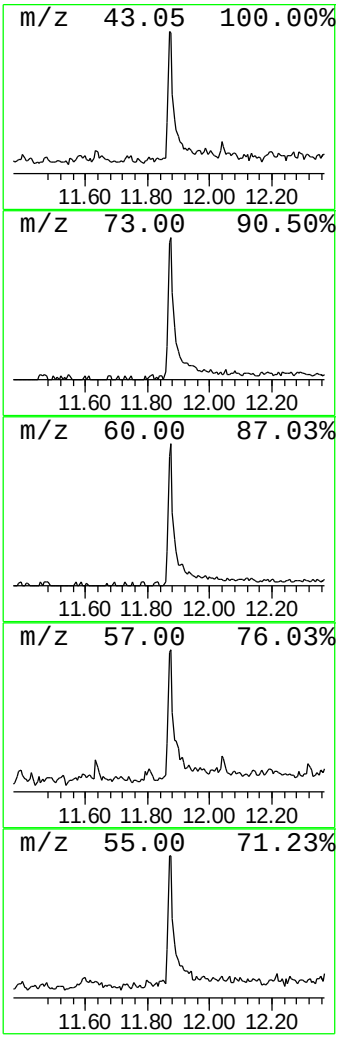
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.01 ng	243897	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
Data File : BF114443.D
Acq On : 20 May 2019 17:22
Operator : JU/SJ
Sample : K2943-17
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

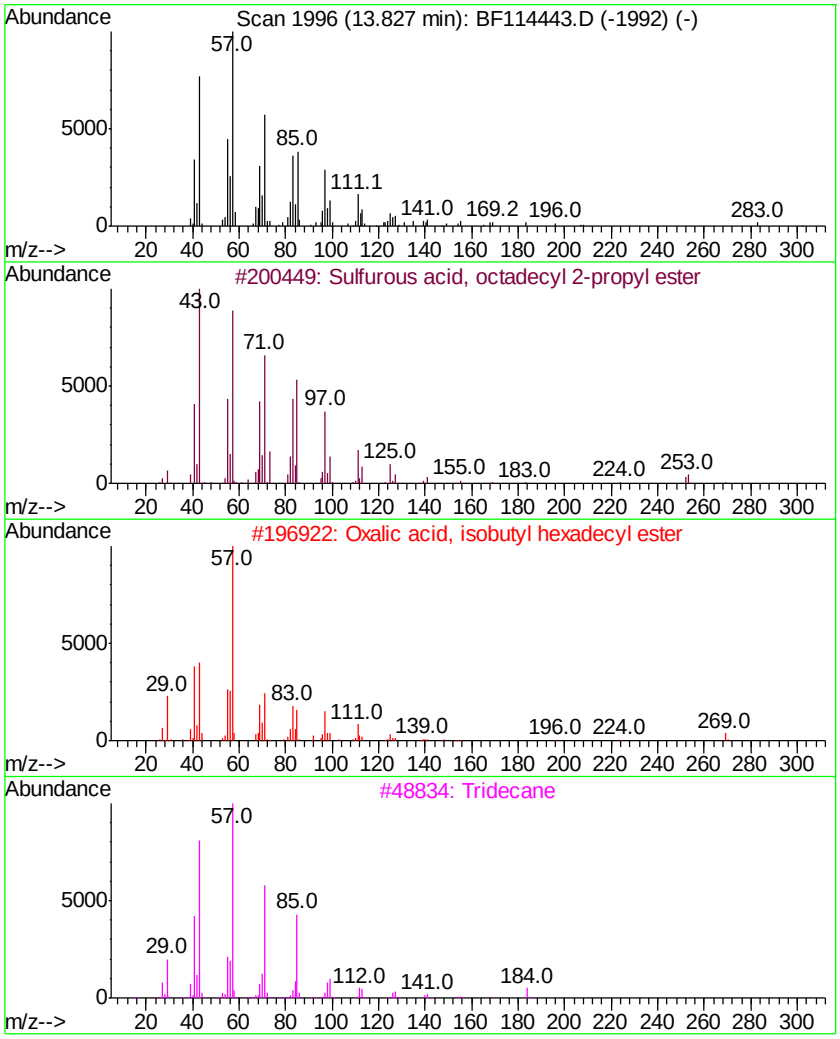
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

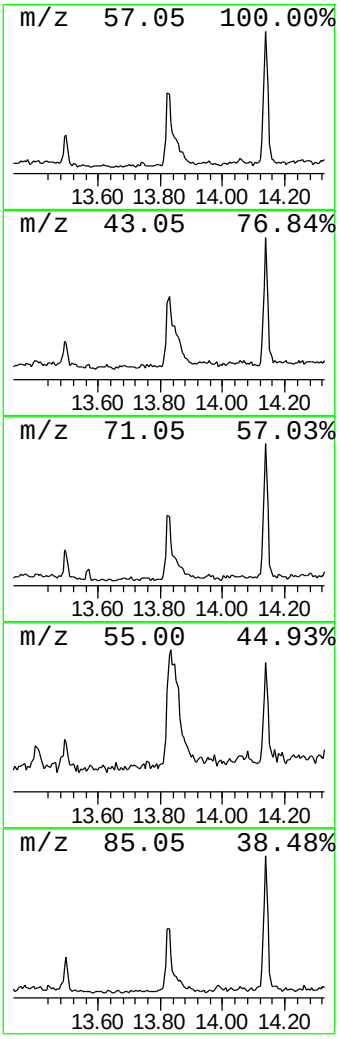
****

Peak Number 5 Sulfurous acid, octadecyl 2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.60 ng	365967	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
2	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	74
3	Tridecane	184	C13H28	000629-50-5	68
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	64
5	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	62





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF052019\
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Operator : JU/SJ
Sample : K2943-17
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

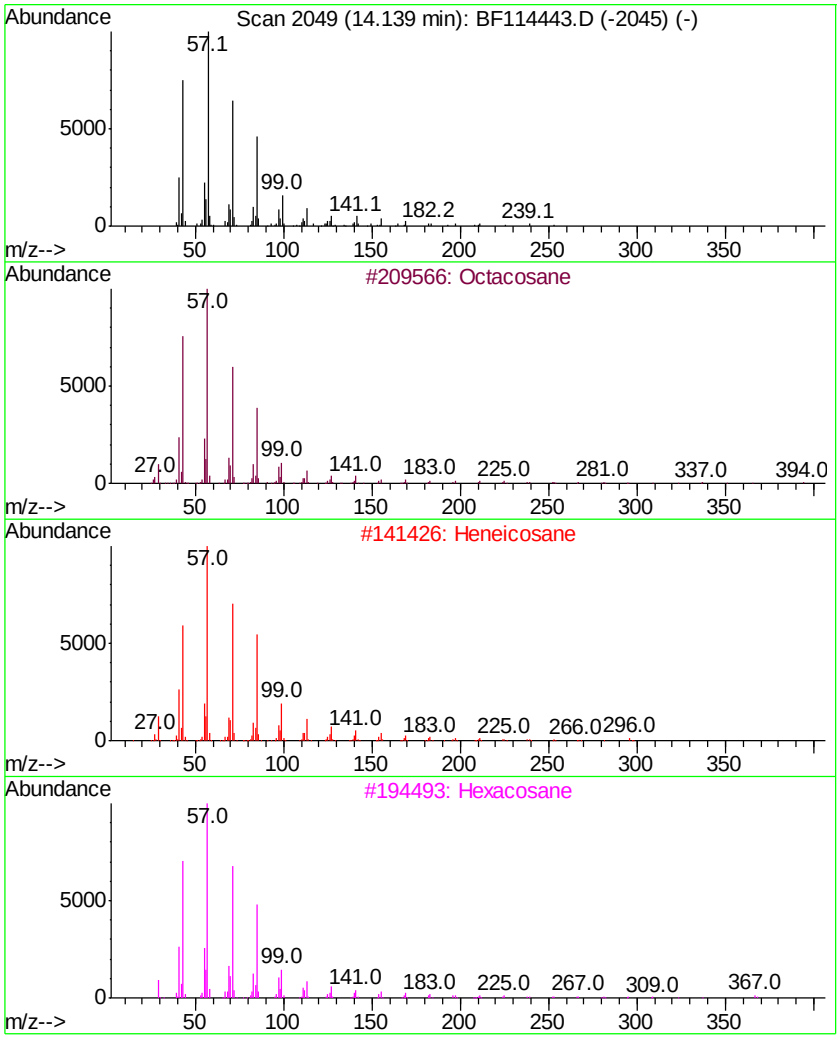
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

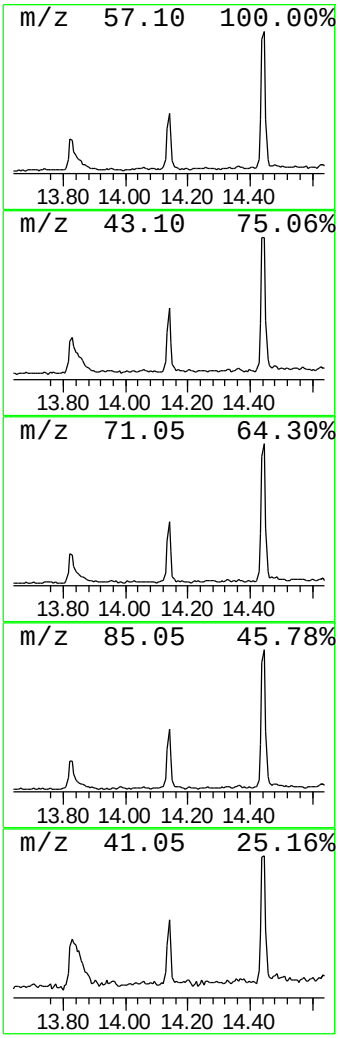
****

Peak Number 6 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.63 ng	171725	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Pentadecane	212	C15H32	000629-62-9	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Library Search Compound Report

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Operator : JU/SJ
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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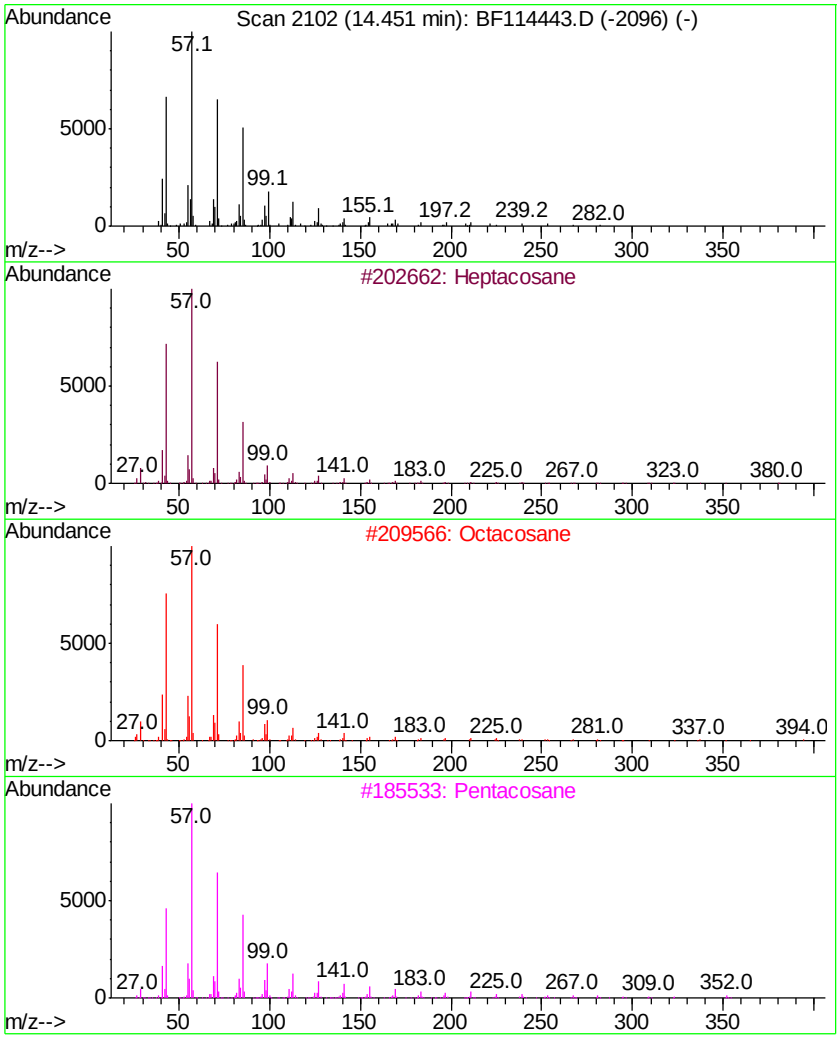
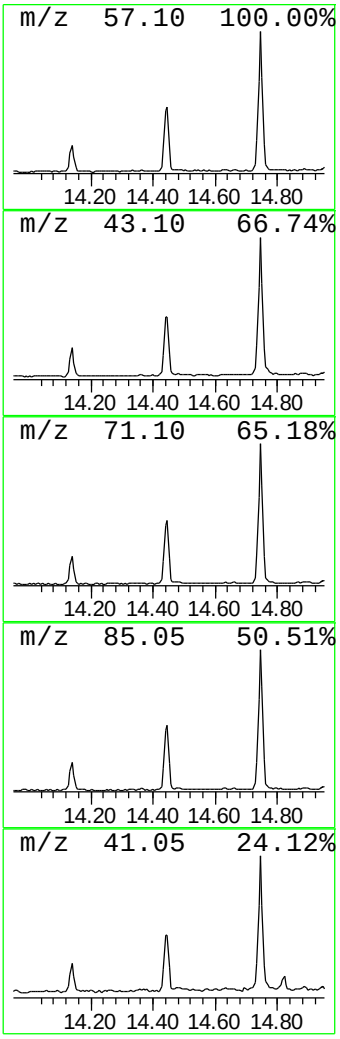
****

Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	7.02 ng	458779	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane	296	C21H44	000629-94-7	90





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Misc :
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Instrument : BNA_F
ClientSampleId : DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

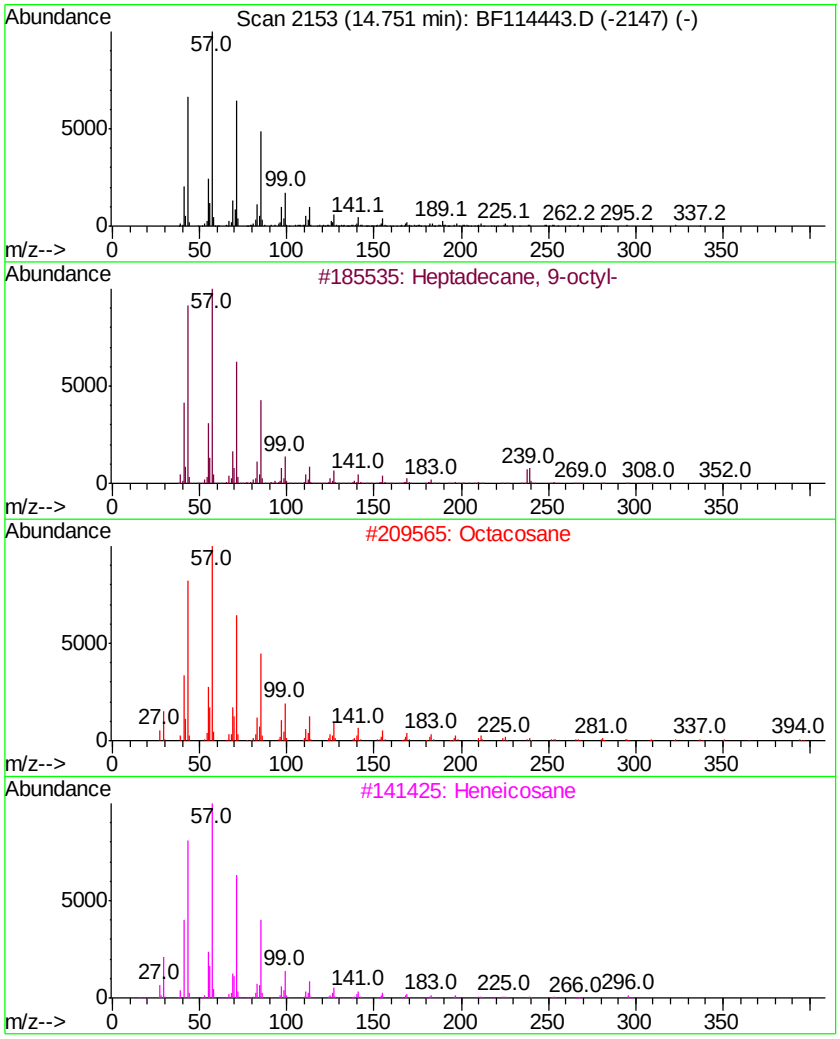
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

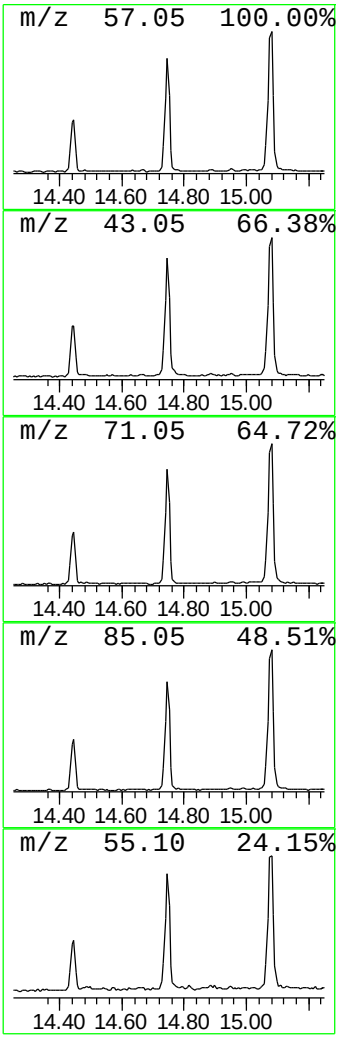
****

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	8.32 ng	1115650	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Tetracosane	338	C24H50	000646-31-1	91





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Instrument : BNA_F
ClientSampleId : DB-1

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TIC Library : C:\DATABASE\NIST11.L
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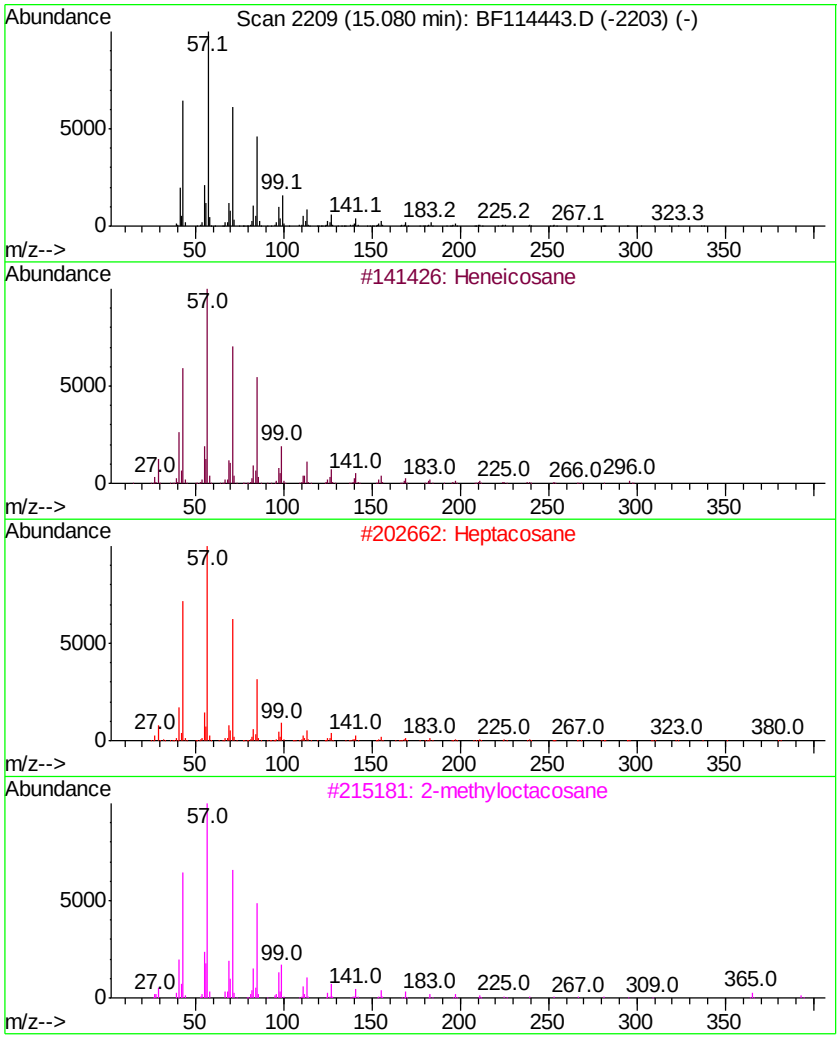
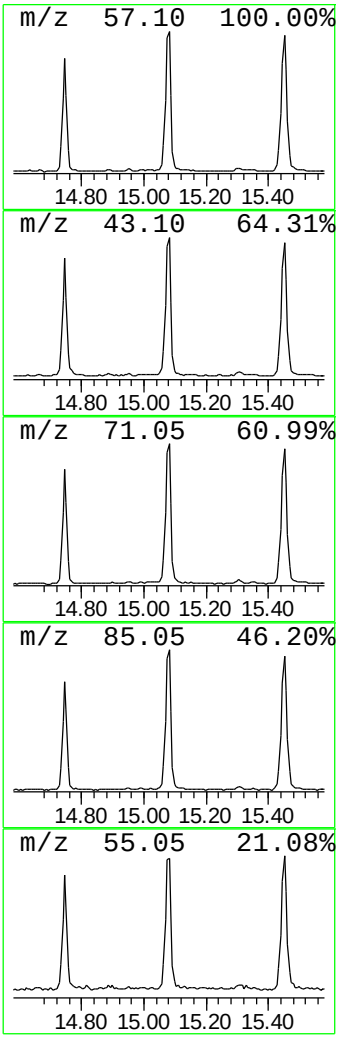
****

Peak Number 9 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	10.63 ng	1425250	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Triacontane	422	C30H62	000638-68-6	90
5	Pentadecane	212	C15H32	000629-62-9	87





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Instrument : BNA_F
ClientSampleId : DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

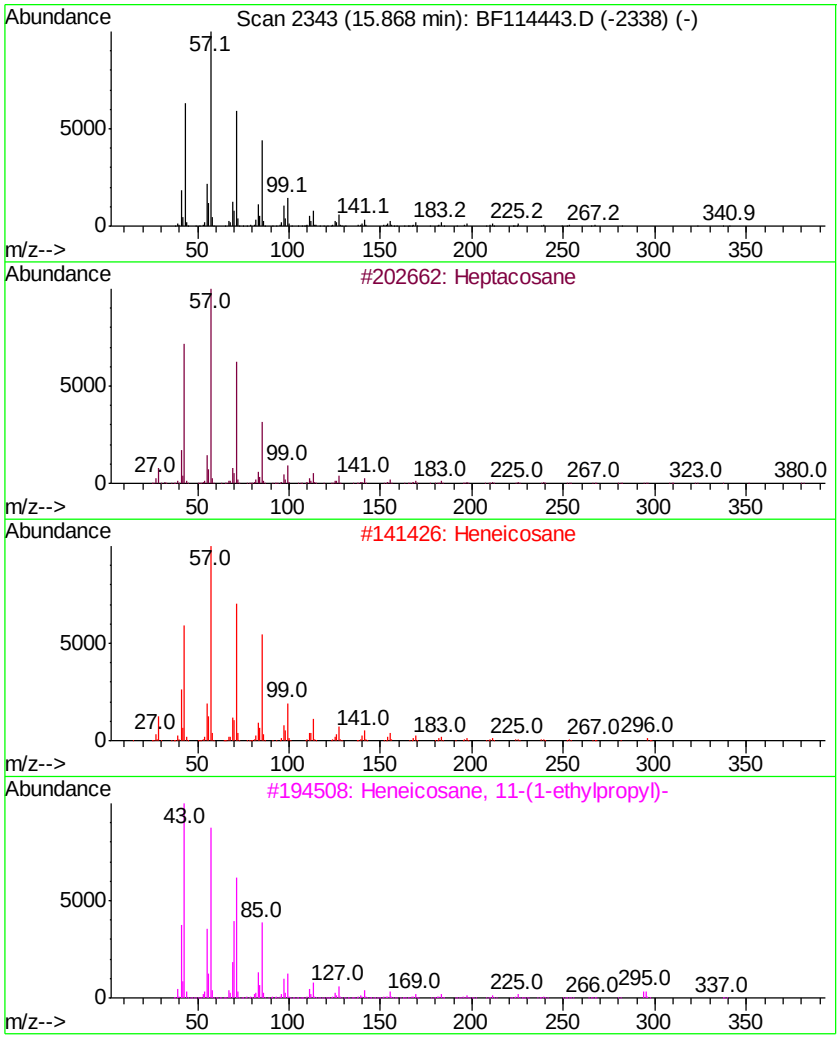
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

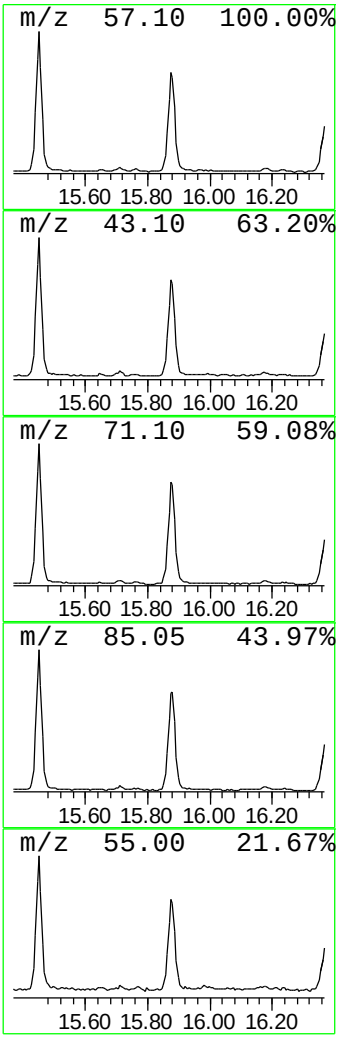
****

Peak Number 10 Heneicosane, 11-(1-ethylpro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	9.93 ng	1331850	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Hexacosane	366	C26H54	000630-01-3	90





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Instrument : BNA_F
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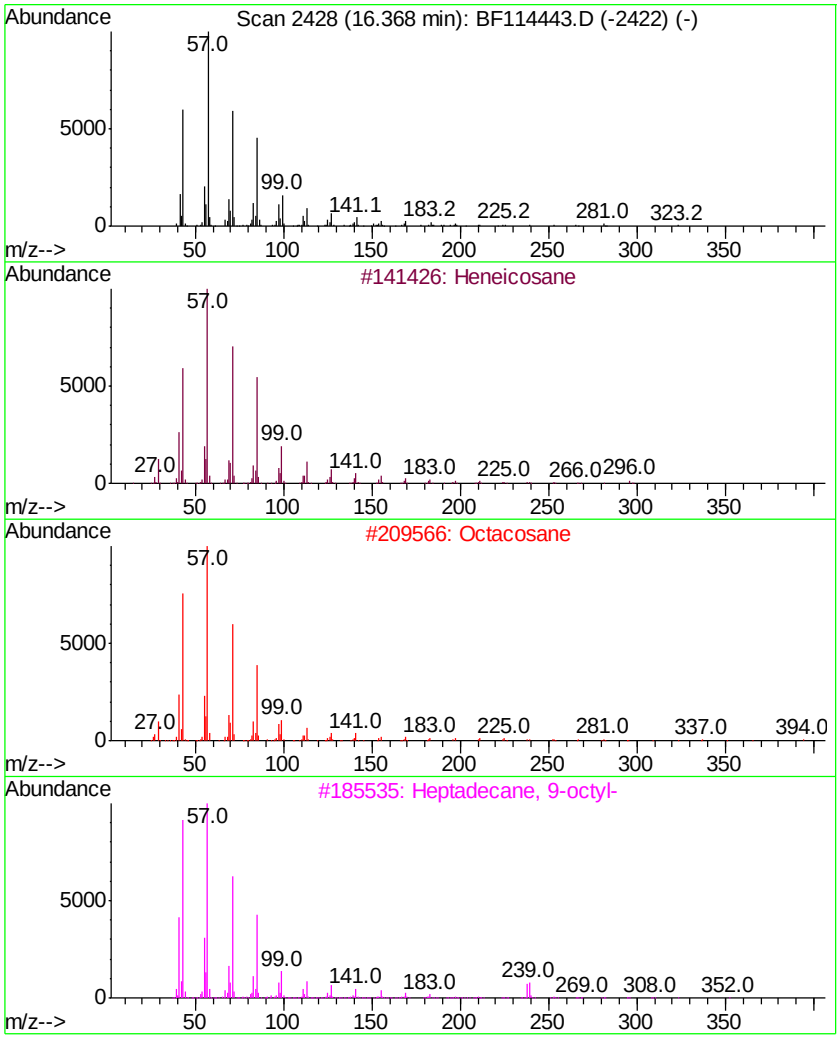
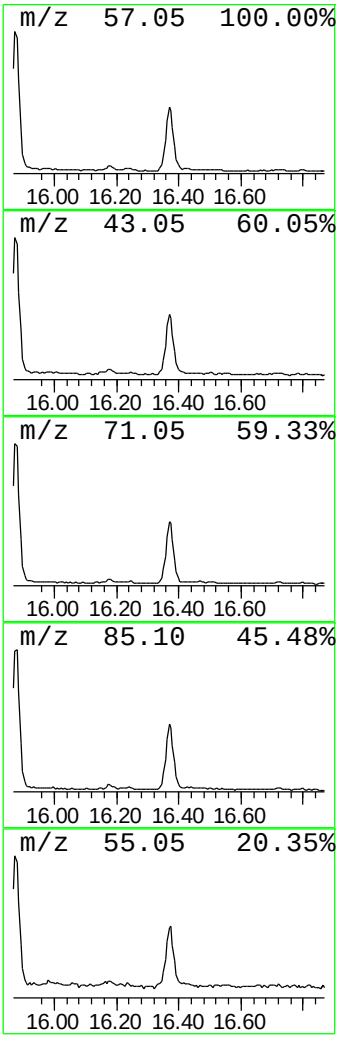
****

Peak Number 11 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	5.14 ng	688556	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Triacontane	422	C30H62	000638-68-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF052019\
Data File : BF114443.D
Acq On : 20 May 2019 17:22
Operator : JU/SJ
Sample : K2943-17
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DB-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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
unknown6.60	6.60	72.6	ng	3956020	1	6.83	1089360	20.0
Safrole	8.73	2.0	ng	142580	2	8.11	1411500	20.0
n-Hexadecanoic acid	11.87	3.0	ng	243897	4	11.35	1619510	20.0
Sulfurous acid, o...	13.83	5.6	ng	365967	5	13.99	1307900	20.0
Octacosane	14.14	2.6	ng	171725	5	13.99	1307900	20.0
Heptacosane	14.45	7.0	ng	458779	5	13.99	1307900	20.0
Heptadecane, 9-oc...	14.75	8.3	ng	1115650	6	15.46	2681800	20.0
Heneicosane	15.08	10.6	ng	1425250	6	15.46	2681800	20.0
Heneicosane, 11-(...	15.87	9.9	ng	1331850	6	15.46	2681800	20.0
2-methyloctacosane	16.37	5.1	ng	688556	6	15.46	2681800	20.0