LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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	2.146	4	10	21	rVB	1245550	1674223	24.32%	2.673%
2	5.487	574	578	600	rBV	5580714	5953451	86.48%	9.504%
3	6.498	744	750	753	rBV	5722882	6349061	92.23%	10.135%
4	6.628	767	772	775	rBV	6298047	5984440	86.93%	9.553%
5	6.845	806	809	817	rBV	1589755	1401684	20.36%	2.238%
6	7.004	832	836	840	rBV	4958212	4735970	68.80%	7.560%
7	7.410	900	905	908	rBV	3977555	4012730	58.29%	6.406%
8	8.128	1023	1027	1036	rBV	1878232	1774731	25.78%	2.833%
9	9.204	1205	1210	1213	rBV	6943072	6602758	95.91%	10.540%
10	9.592	1273	1276	1285	rBV	723369	731184	10.62%	1.167%
11	9.881	1321	1325	1330	rBV	2082969	1971047	28.63%	3.146%
12	10.675	1456	1460	1470	rBV	4283084	4298447	62.44%	6.862%
13	10.798	1476	1481	1484	rBV	103210	100679	1.46%	0.161%
14	11.263	1556	1560	1566	rVB3	77005	92715	1.35%	0.148%
15	11.369	1574	1578	1588	rBV	2405711	2310211	33.56%	3.688%
16	11.892	1661	1667	1675	rBV3	362544	437484	6.36%	0.698%
17	12.586	1782	1785	1789	rBV	109504	107814	1.57%	0.172%
18	12.680	1797	1801	1805	rBV4	51039	81537	1.18%	0.130%
19	12.816	1818	1824	1827	rBV	75510	107362	1.56%	0.171%
20	12.957	1843	1848	1851	rBV	6668226	6884057	100.00%	10.989%
21	13.421	1924	1927	1932	rVB2	139332	127564	1.85%	0.204%
22	13.845	1996	1999	2007	rVB	240799	306952	4.46%	0.490%
23	14.010	2023	2027	2038	rVB	1957462	2160413	31.38%	3.449%
24	14.168	2050	2054	2056	rBV	119362	114507	1.66%	0.183%
25	14.474	2102	2106	2113	rBV	214301	221345	3.22%	0.353%
26	14.780	2155	2158	2163	rVB	260127	273770	3.98%	0.437%
27	15.121	2212	2216	2220	rVB	318646	354248	5.15%	0.565%
28	15.492	2274	2279	2288	rBV2	1678186	2343678	34.05%	3.741%
29	15.933	2349	2354	2359	rVB	295255	431566	6.27%	0.689%
30	16.433	2434	2439	2446	rVB	203538	367792	5.34%	0.587%
31	17.021	2534	2539	2548	rVB2	99865	201891	2.93%	0.322%
32	17.715	2652	2657	2665	rVB3	55373	128316	1.86%	0.205%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

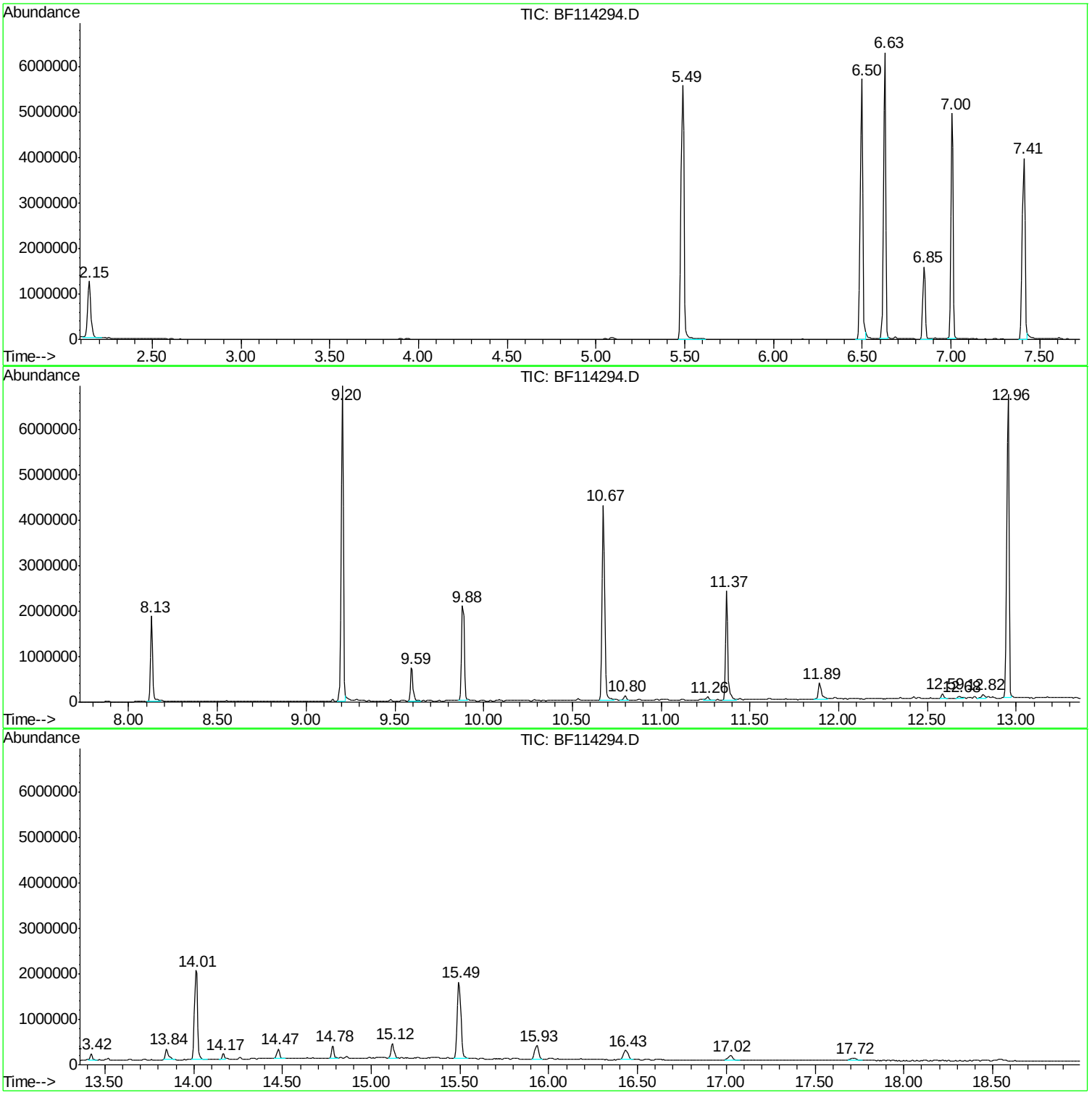
Sum of corrected areas: 62643627

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1(35-37)

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

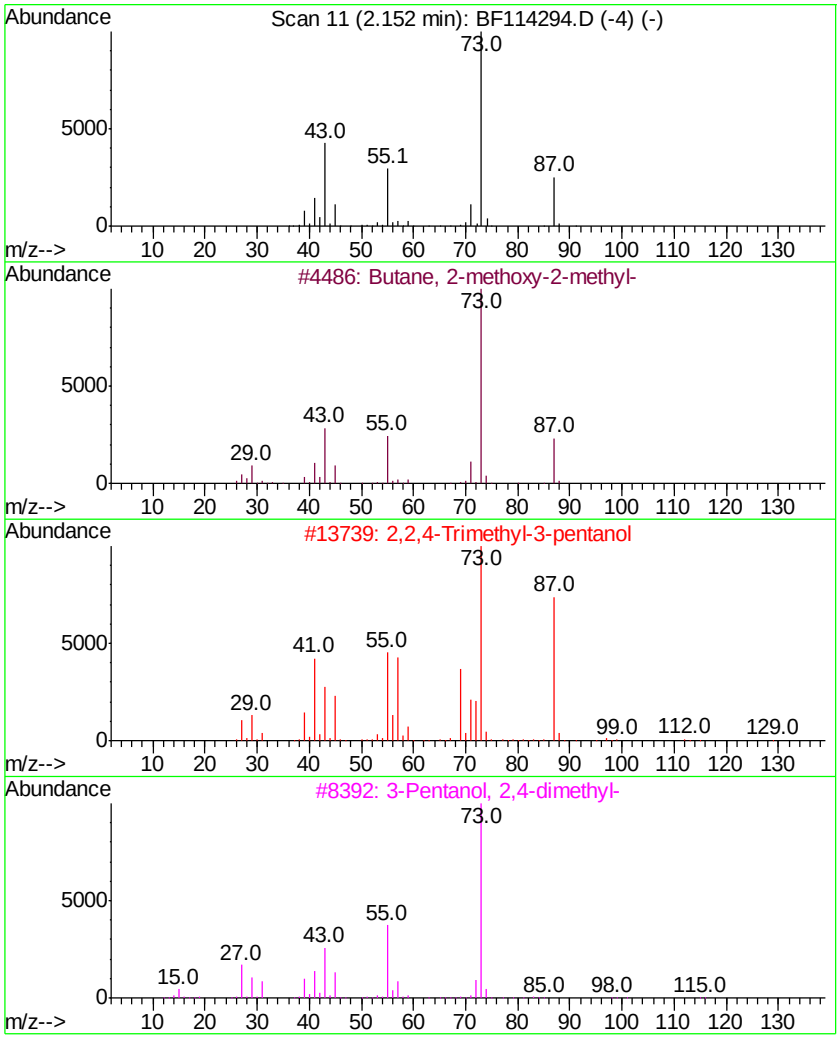
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

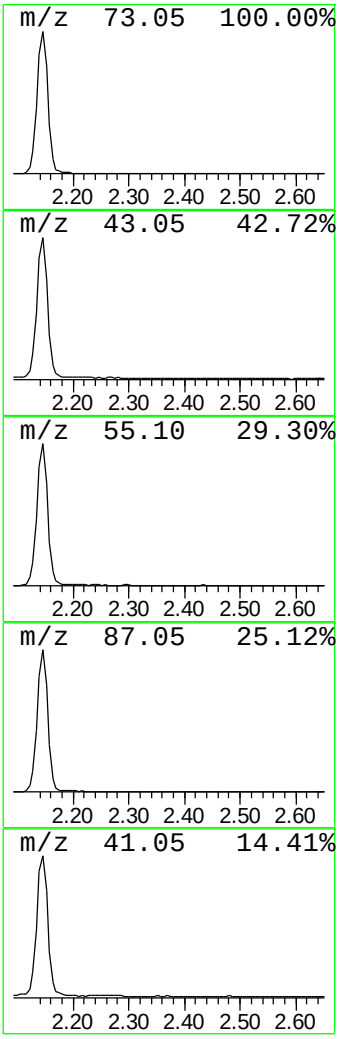
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	23.89 ng	1674220	1,4-Dichlorobenzene-d4	6.85

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

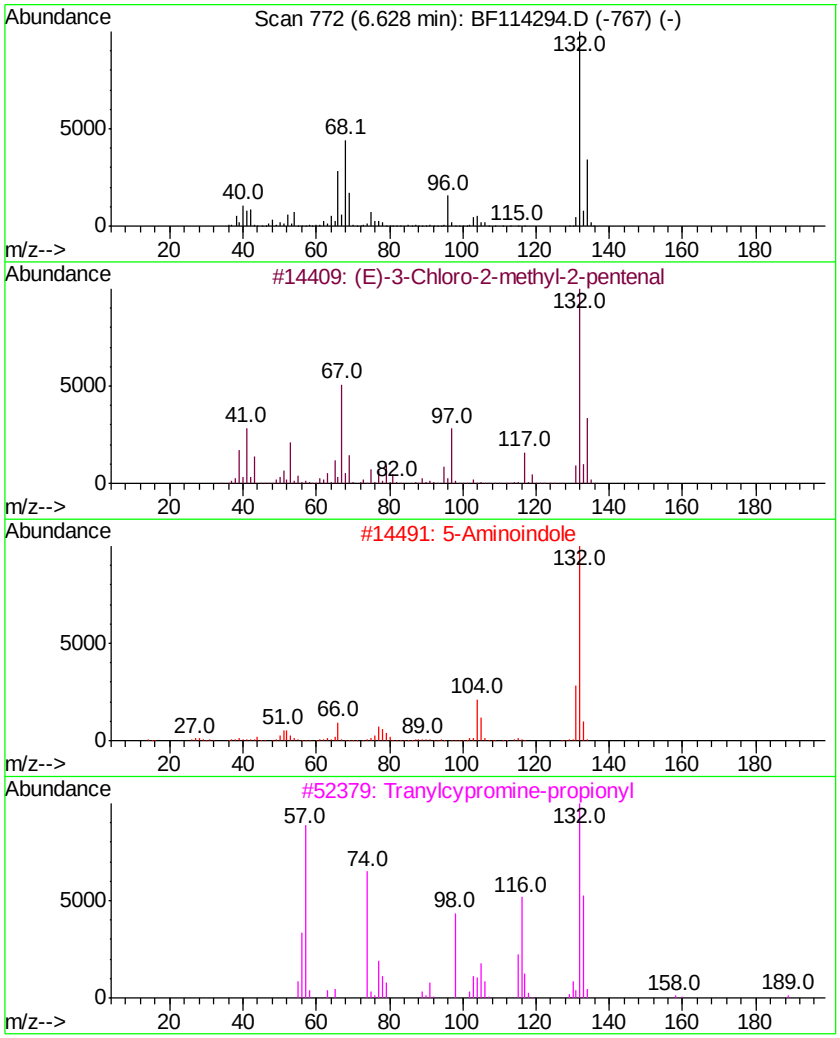
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

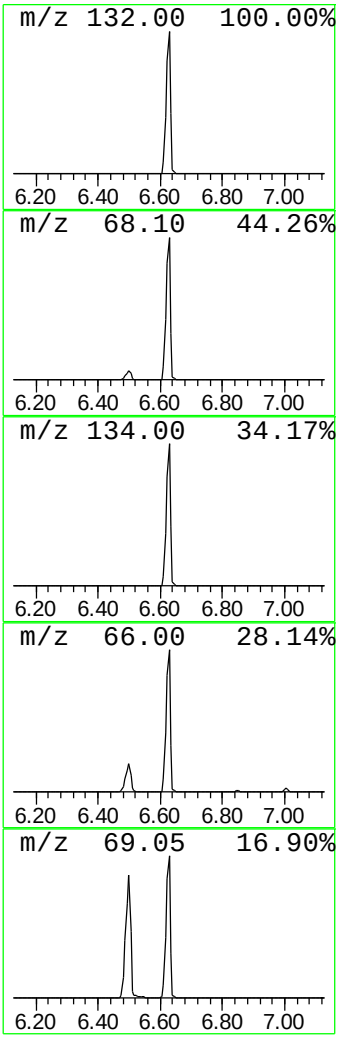
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	85.39 ng	5984440	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
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	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

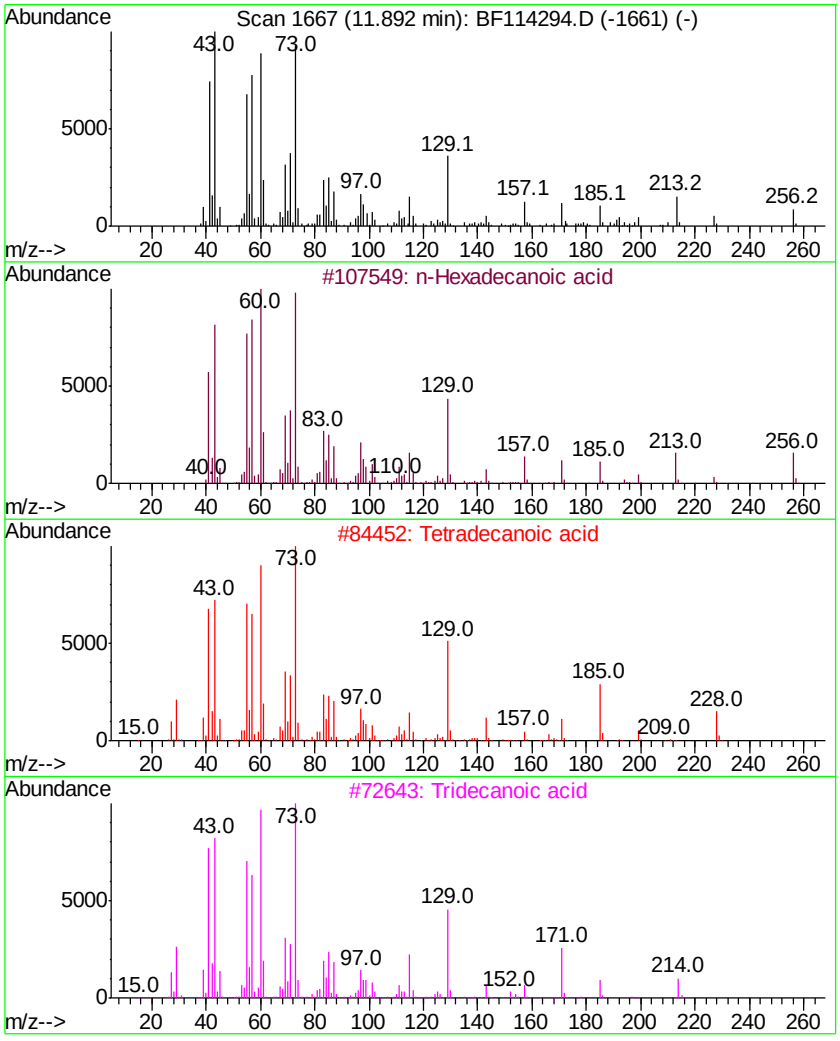
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

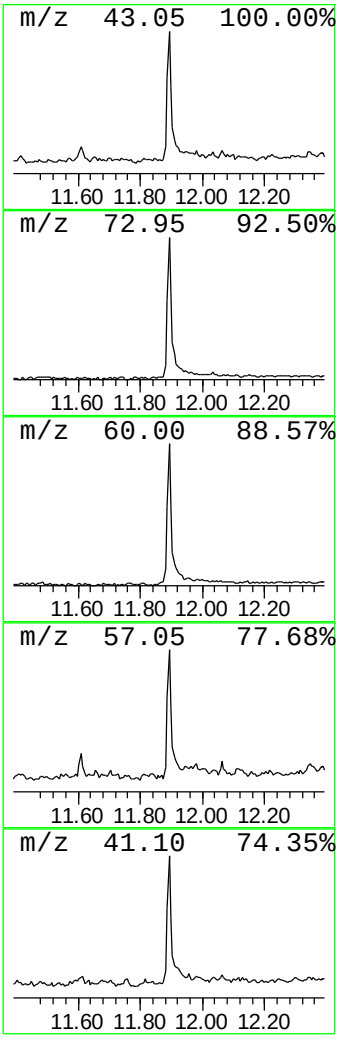
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	3.79 ng	437484	Phenanthrene-d10	11.37

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

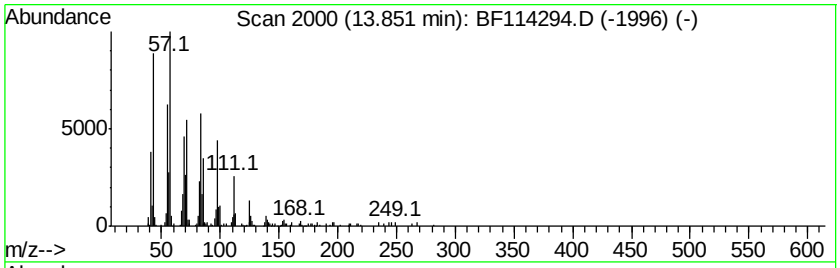
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

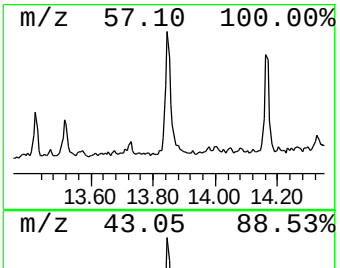
****

Peak Number 5 Oxalic acid, isobutyl hexad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.84 ng	306952	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
5	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
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Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

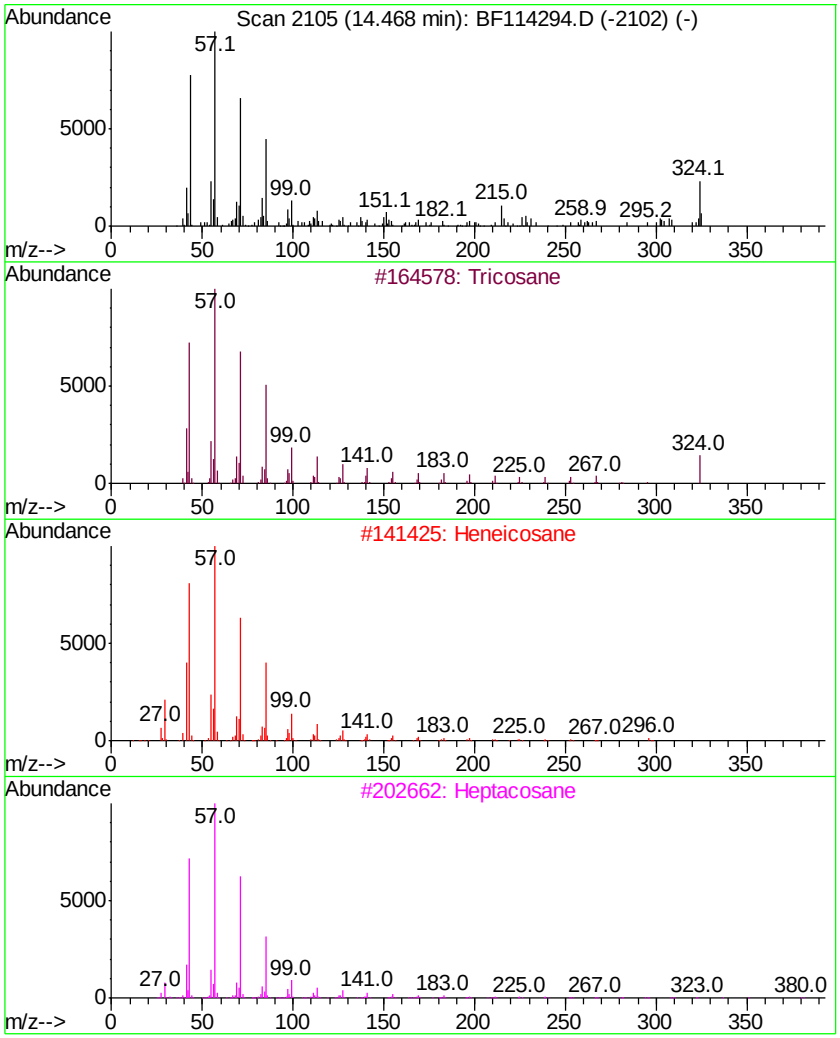
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

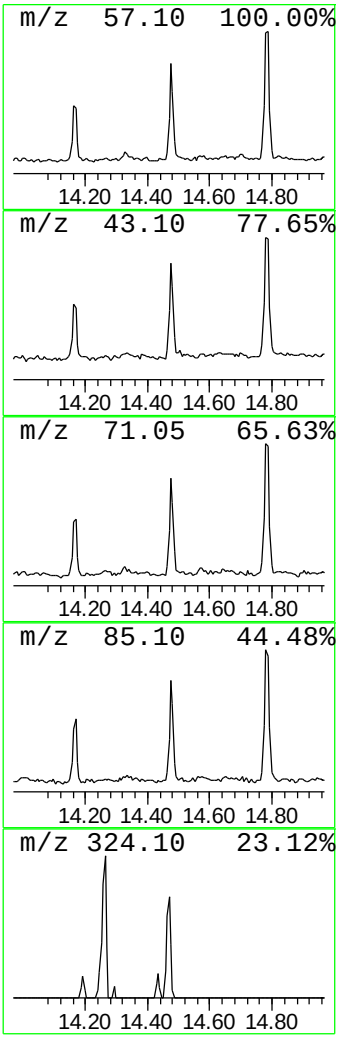
****

Peak Number 6 Tricosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.05 ng	221345	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Heneicosane	296	C21H44	000629-94-7	87
3	Heptacosane	380	C27H56	000593-49-7	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Hexacosane	366	C26H54	000630-01-3	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

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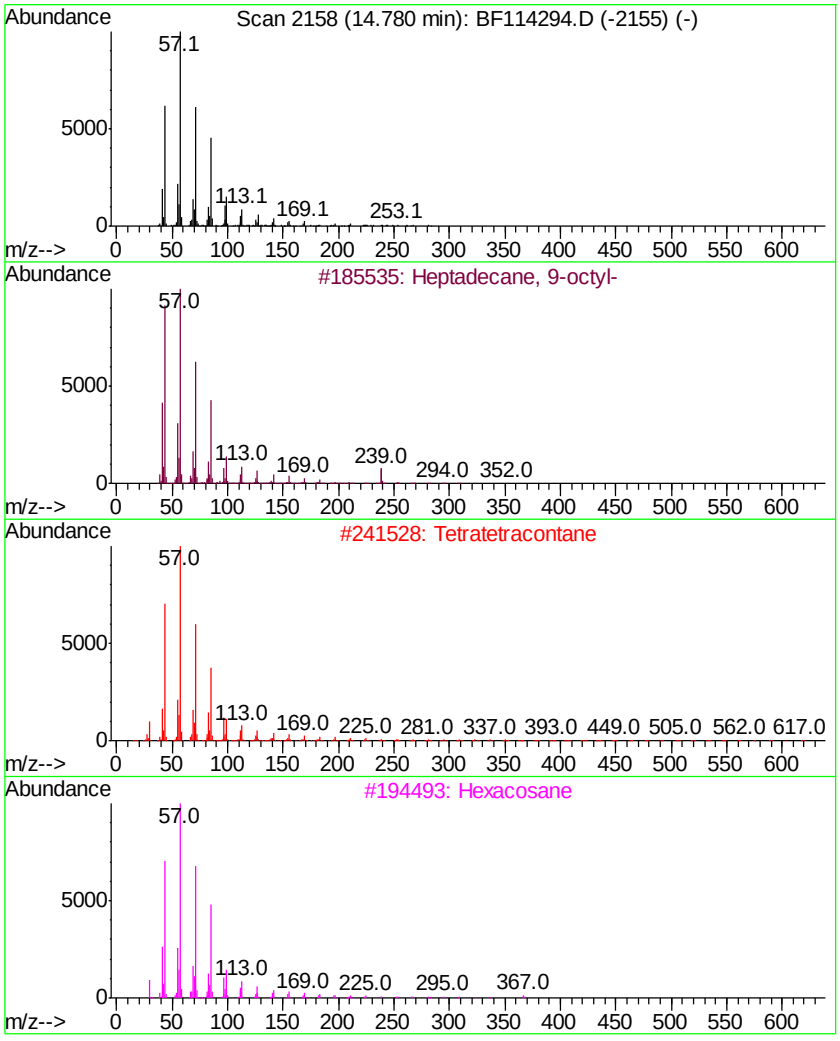
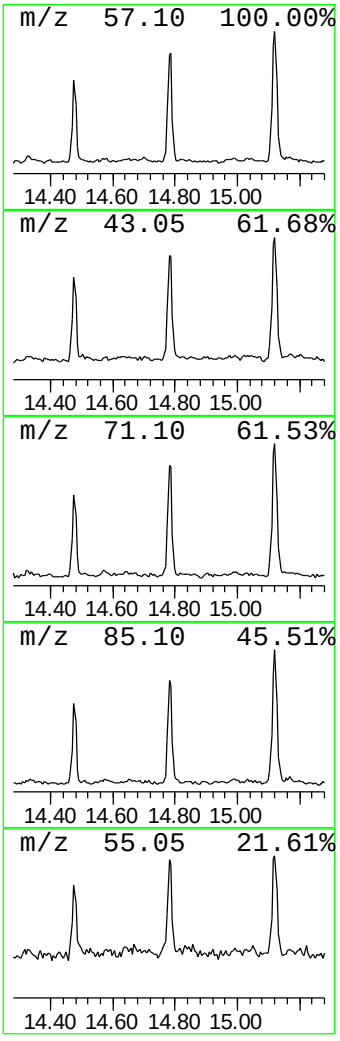
Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	2.34 ng	273770	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Triacontane	422	C30H62	000638-68-6	90
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

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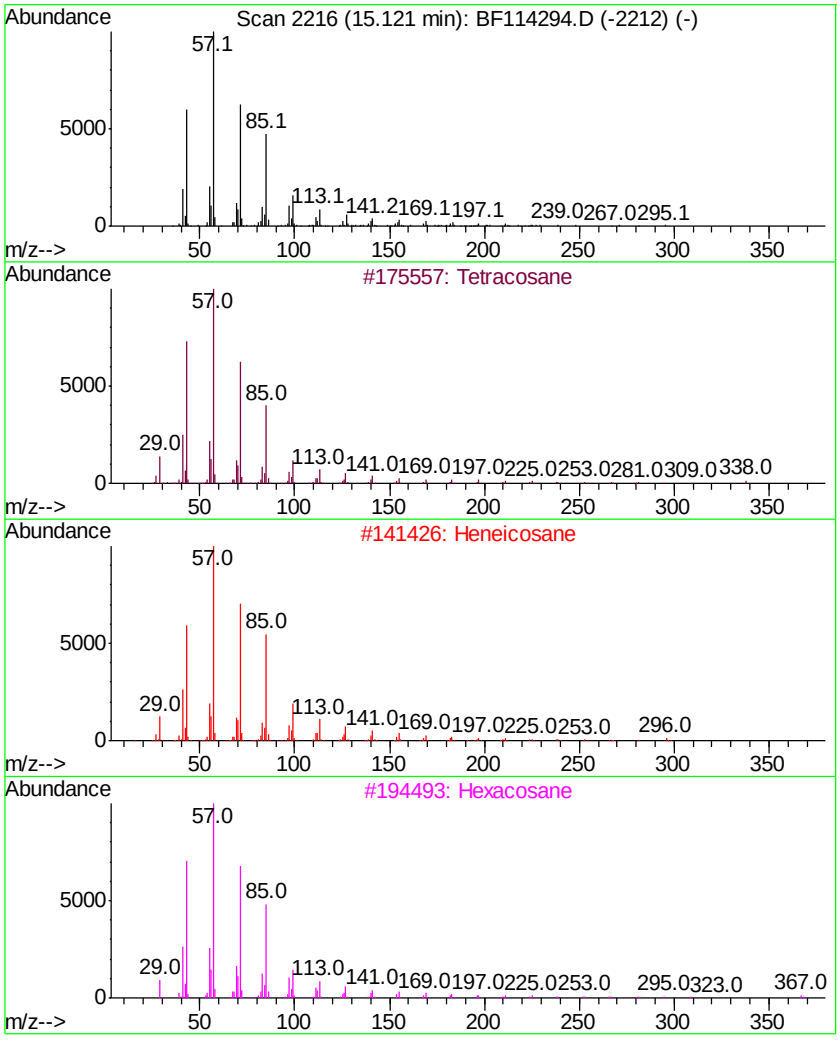
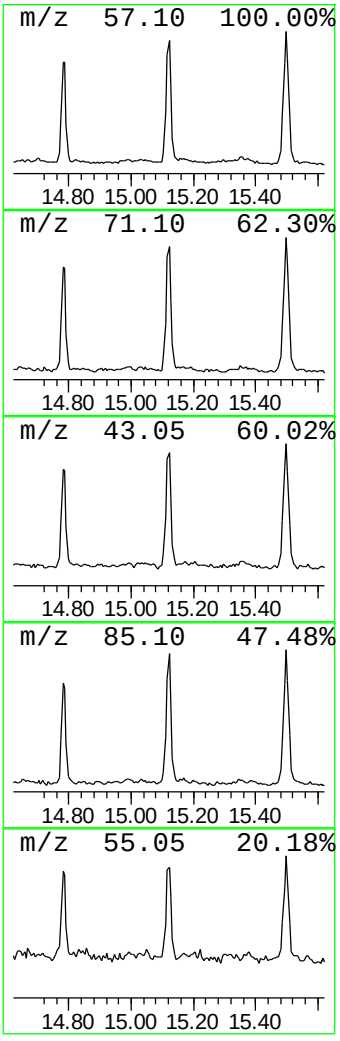
Peak Number 8 Tetracosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	3.02 ng	354248	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octadecane	254	C18H38	000593-45-3	87
5	Nonadecane	268	C19H40	000629-92-5	87





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Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

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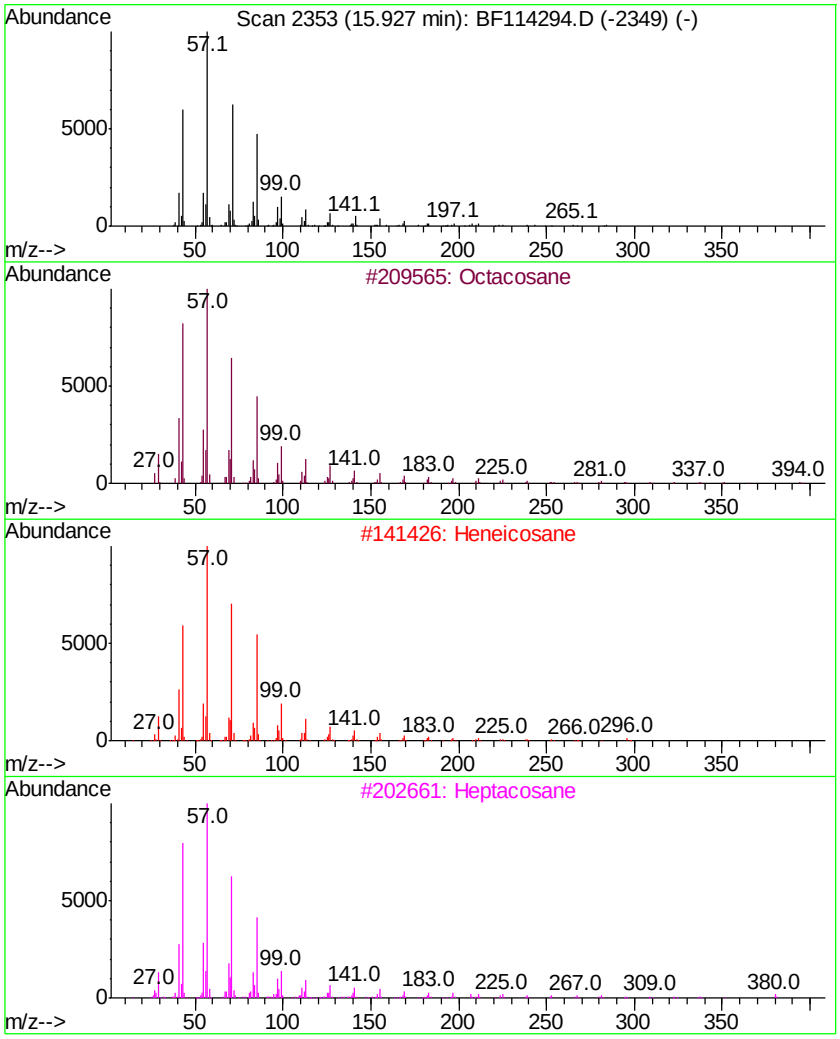
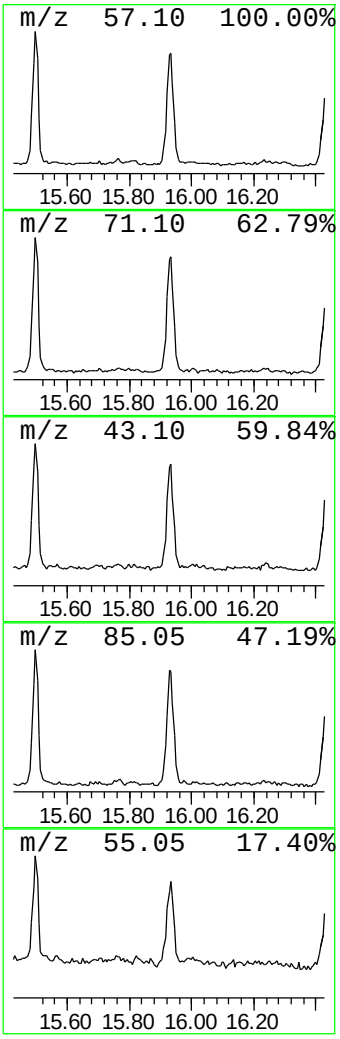
Peak Number 9 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	3.68 ng	431566	Perylene-d12	15.49

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	Heptacosane	380	C27H56	000593-49-7	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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

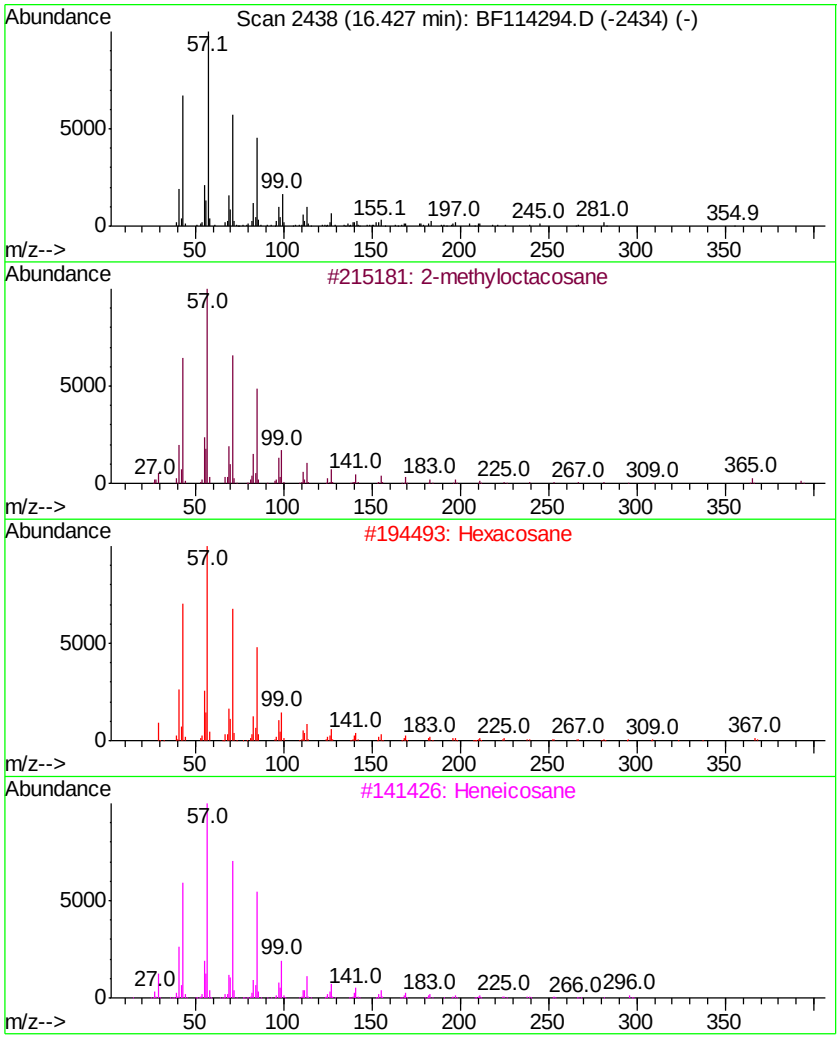
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

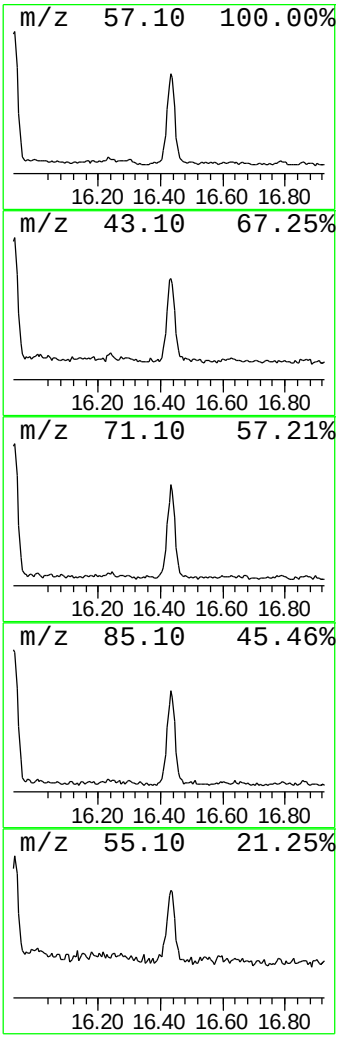
****

Peak Number 10 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	3.14 ng	367792	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Tetracosane	338	C24H50	000646-31-1	87
5	Docosane	310	C22H46	000629-97-0	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051519\
Data File : BF114294.D
Acq On : 15 May 2019 19:40
Operator : JU/SJ
Sample : K2704-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1(35-37)

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
Butane, 2-methoxy...	2.15	23.9	ng	1674220	1	6.85	1401680	20.0
unknown6.63	6.63	85.4	ng	5984440	1	6.85	1401680	20.0
n-Hexadecanoic acid	11.89	3.8	ng	437484	4	11.37	2310210	20.0
Oxalic acid, isob...	13.85	2.8	ng	306952	5	14.01	2160410	20.0
Tricosane	14.47	2.0	ng	221345	5	14.01	2160410	20.0
Heptadecane, 9-oc...	14.78	2.3	ng	273770	6	15.49	2343680	20.0
Tetracosane	15.12	3.0	ng	354248	6	15.49	2343680	20.0
Octacosane	15.93	3.7	ng	431566	6	15.49	2343680	20.0
2-methyloctacosane	16.43	3.1	ng	367792	6	15.49	2343680	20.0