LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100418\
Data File : BF109589.D
Acq On : 4 Oct 2018 16:22
Operator : JU/SJ
Sample : J5221-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

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-BF092218.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	4.887	473	476	489	rBV	80242	97759	2.90%	0.480%
2	5.316	545	549	564	rBV	711809	796256	23.60%	3.911%
3	6.339	720	723	739	rBV	417562	578345	17.14%	2.841%
4	6.475	742	746	758	rBV	1679181	1633811	48.42%	8.025%
5	6.704	781	785	795	rBV	587399	586159	17.37%	2.879%
6	6.863	808	812	815	rBV	2524628	2240505	66.40%	11.005%
7	7.269	876	881	902	rBV	1639261	1994135	59.10%	9.795%
8	7.986	999	1003	1022	rBV	736638	763733	22.63%	3.751%
9	9.063	1181	1186	1189	rBV	3545183	3374377	100.00%	16.574%
10	9.180	1203	1206	1215	rVB	142079	130204	3.86%	0.640%
11	9.451	1249	1252	1267	rBV	367344	305858	9.06%	1.502%
12	9.733	1296	1300	1317	rVB	958383	843124	24.99%	4.141%
13	10.521	1430	1434	1452	rBV	1121494	1213928	35.97%	5.963%
14	11.210	1548	1551	1566	rVB	760302	740099	21.93%	3.635%
15	12.798	1816	1821	1824	rBV	2510529	2406729	71.32%	11.821%
16	13.698	1971	1974	1980	rBV3	22084	45839	1.36%	0.225%
17	13.839	1994	1998	2008	rBV	610999	581146	17.22%	2.854%
18	14.321	2077	2080	2083	rVB	66893	60221	1.78%	0.296%
19	14.615	2126	2130	2133	rBV	149434	143990	4.27%	0.707%
20	14.927	2178	2183	2191	rVB	230083	273798	8.11%	1.345%
21	15.245	2232	2237	2240	rBV	450780	580052	17.19%	2.849%
22	15.274	2240	2242	2249	rVB	272549	330048	9.78%	1.621%
23	15.674	2305	2310	2316	rBV	215416	314544	9.32%	1.545%
24	16.139	2383	2389	2401	rVB	125977	242354	7.18%	1.190%
25	16.674	2476	2480	2488	rVB2	45271	82312	2.44%	0.404%

Sum of corrected areas: 20359326

LSC Report - Integrated Chromatogram

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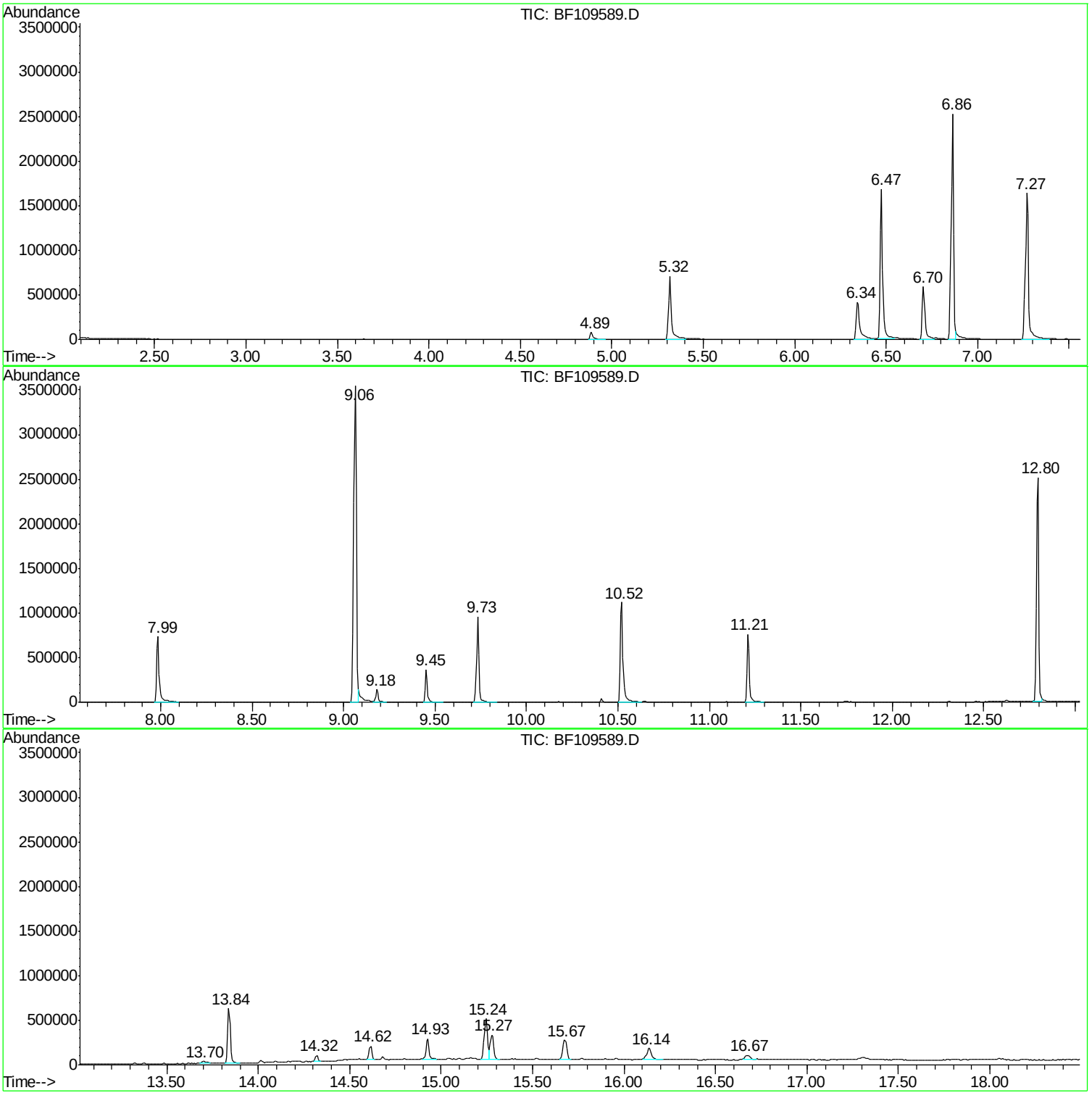
Operator : JU/SJ
Sample : J5221-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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Data File : BF109589.D
Acq On : 4 Oct 2018 16:22
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Sample : J5221-03
Misc :
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Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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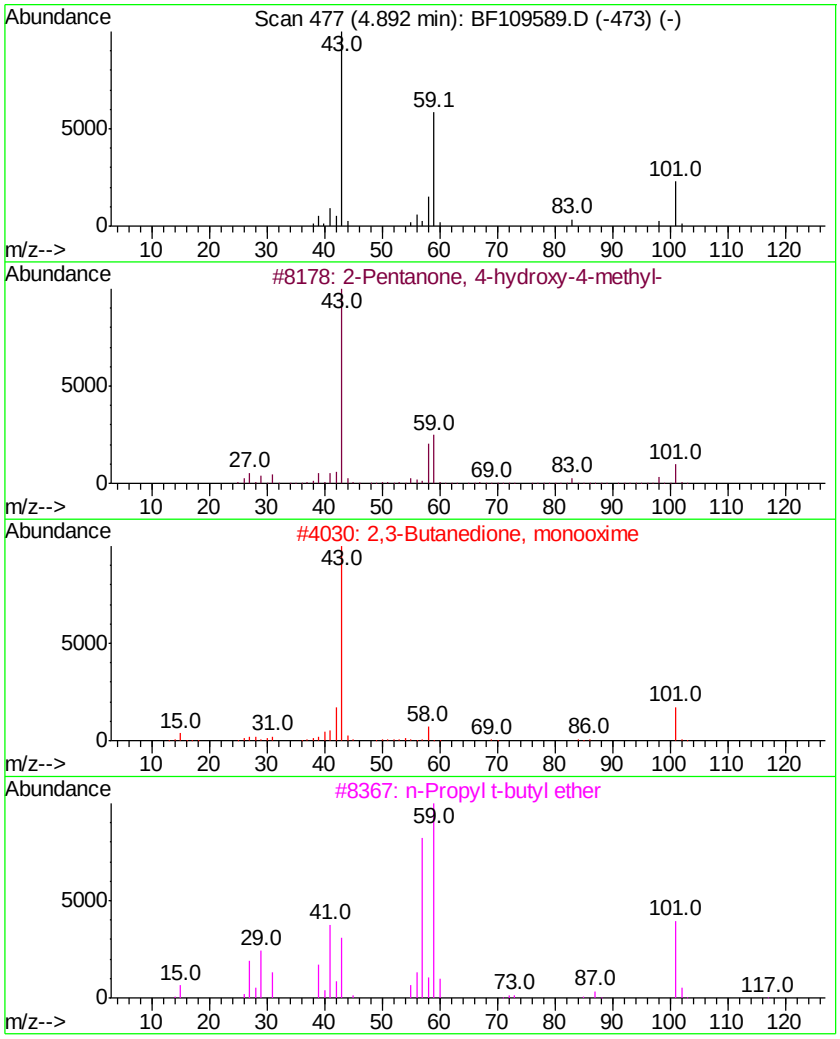
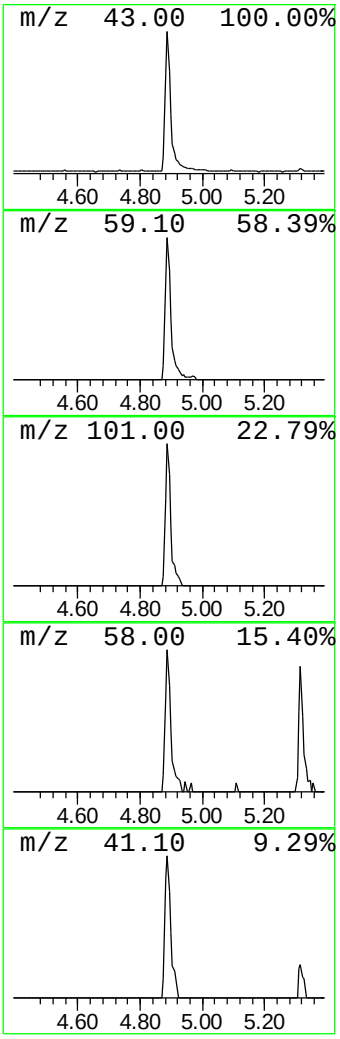
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	3.34 ng	97759	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100418\
Data File : BF109589.D
Acq On : 4 Oct 2018 16:22
Operator : JU/SJ
Sample : J5221-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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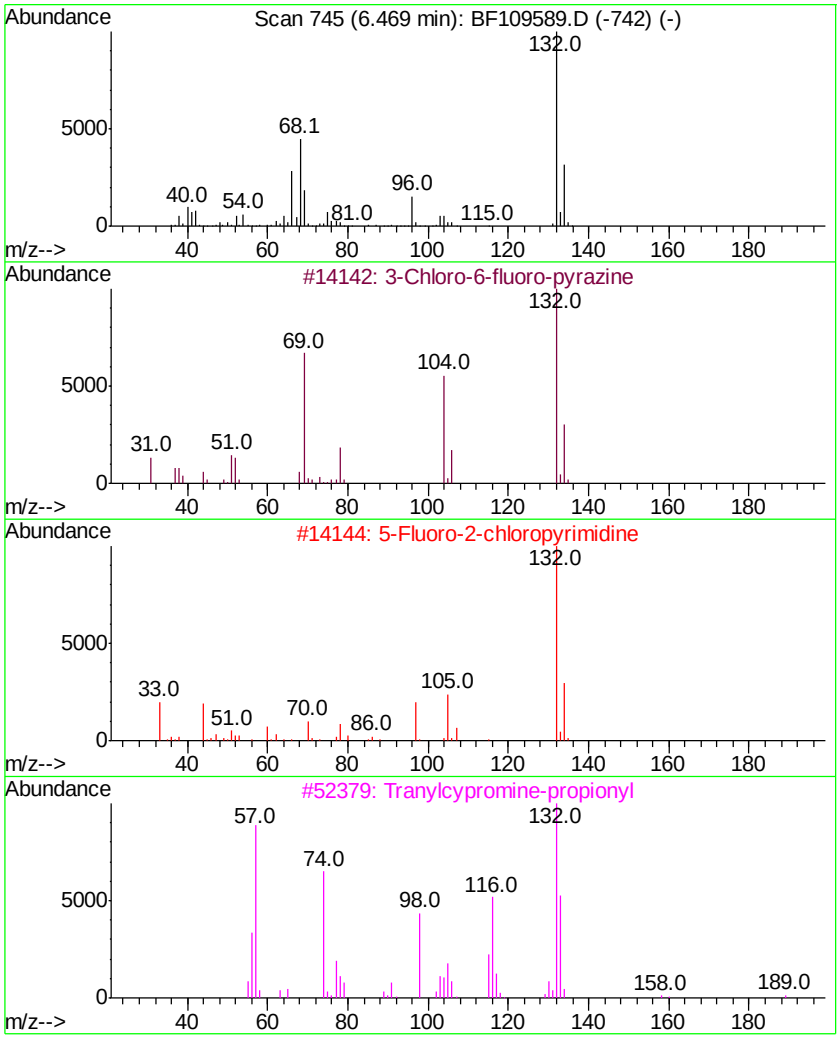
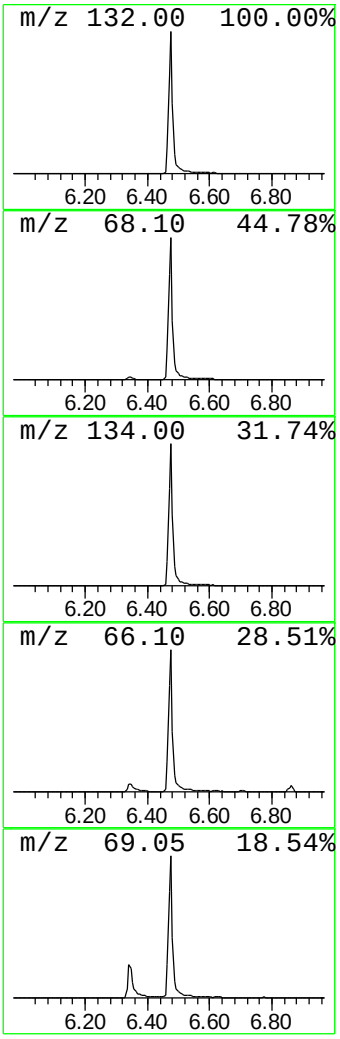
Peak Number 2 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	55.75 ng	1633810	1,4-Dichlorobenzene-d4	6.70

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	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100418\
Data File : BF109589.D
Acq On : 4 Oct 2018 16:22
Operator : JU/SJ
Sample : J5221-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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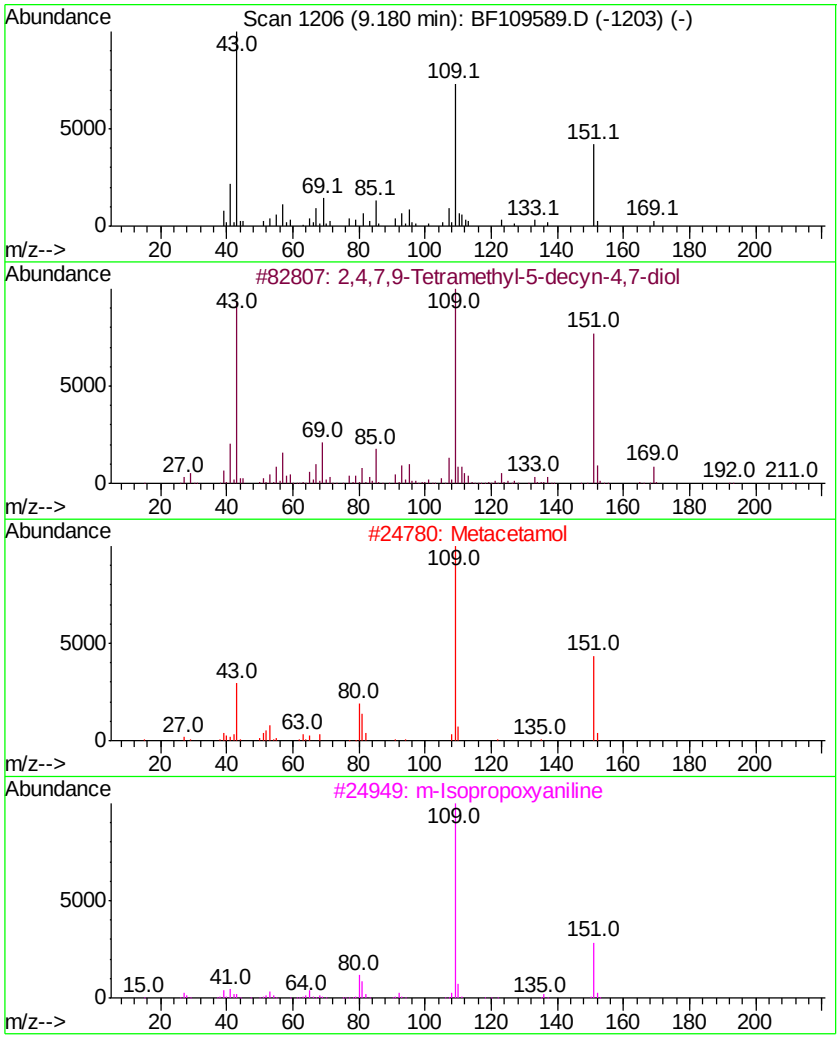
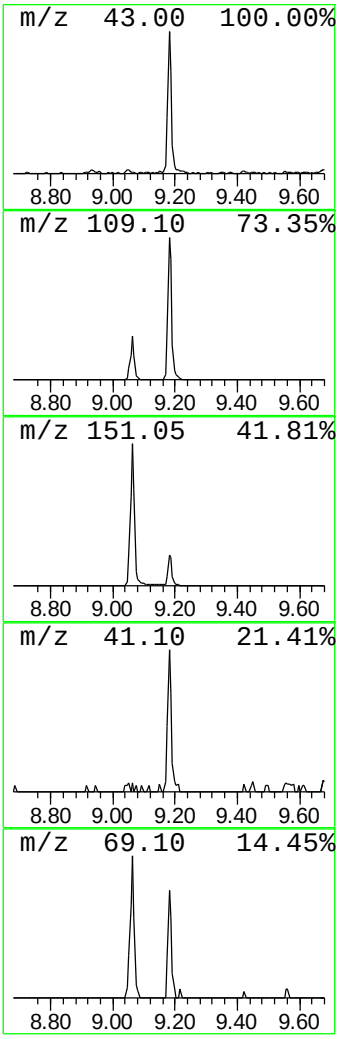
Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.18	3.09 ng	130204	Acenaphthene-d10	9.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	53
2	Metacetamol	151	C8H9NO2	000621-42-1	53
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	43
4	Cyclohexanol, 3,3,5-trimethyl-, ...	142	C9H18O	000767-54-4	38
5	1-(1,2,3-Trimethyl-cyclopent-2-e...	152	C10H16O	070987-81-4	38





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Data File : BF109589.D
Acq On : 4 Oct 2018 16:22
Operator : JU/SJ
Sample : J5221-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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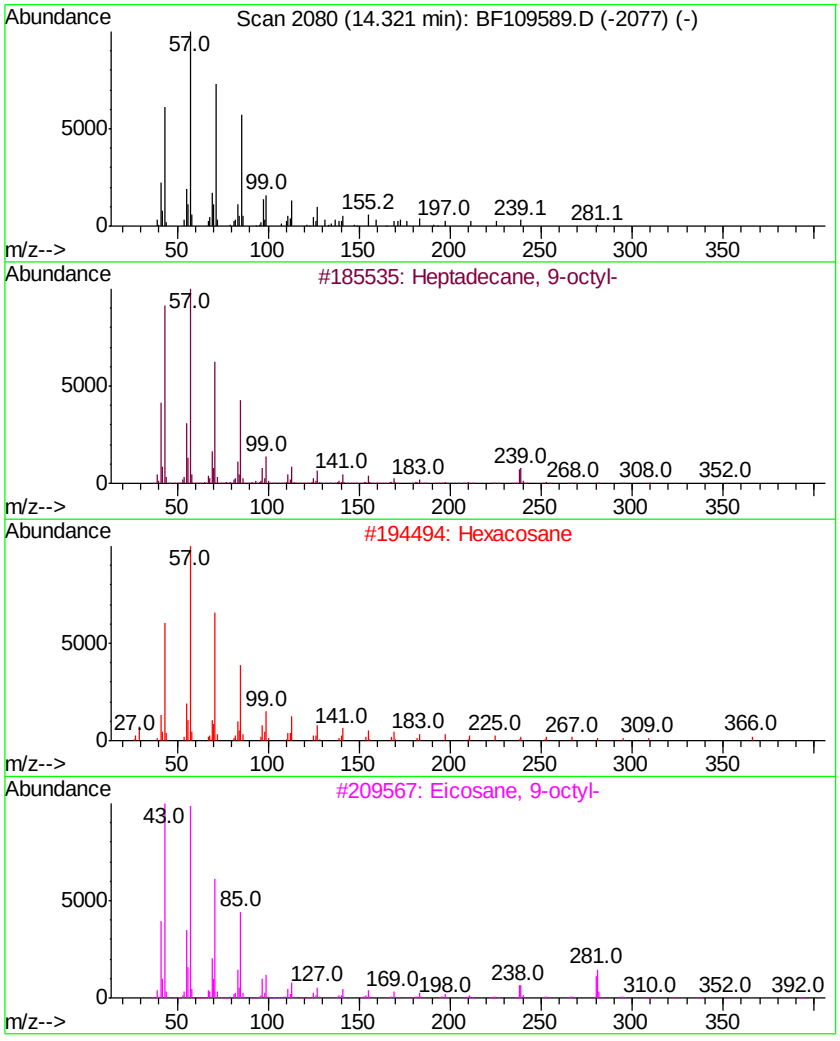
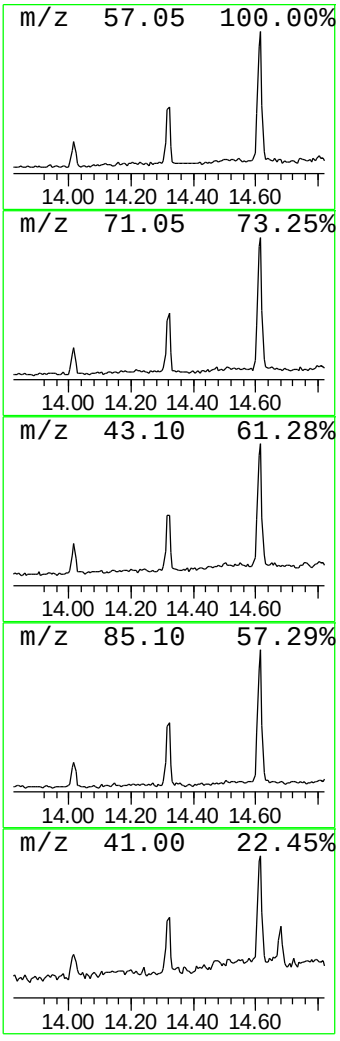
Peak Number 5 Eicosane, 9-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.07 ng	60221	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Eicosane, 9-octyl-	394	C28H58	013475-77-9	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100418\
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Acq On : 4 Oct 2018 16:22
Operator : JU/SJ
Sample : J5221-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

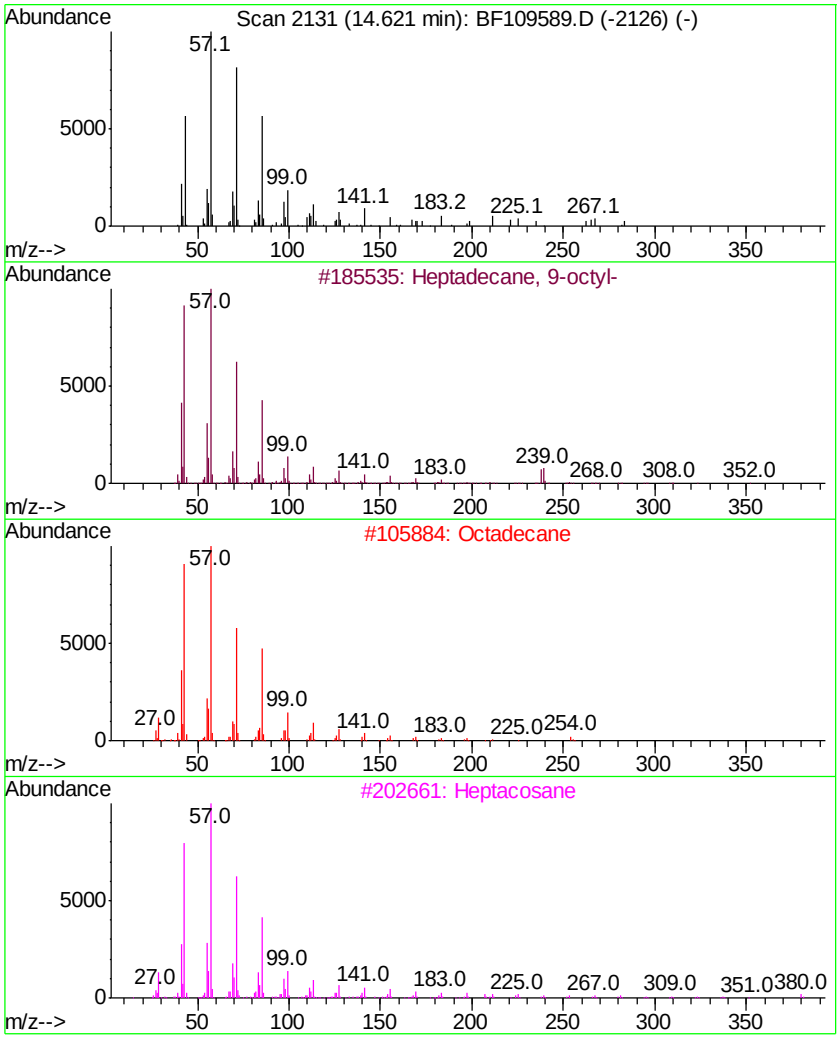
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

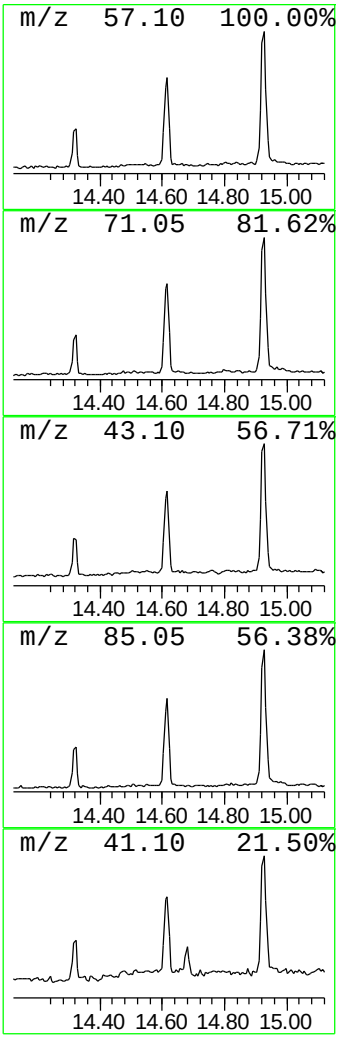
****

Peak Number 6 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	4.96 ng	143990	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2	Octadecane	254	C18H38	000593-45-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane	240	C17H36	000629-78-7	91





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Operator : JU/SJ
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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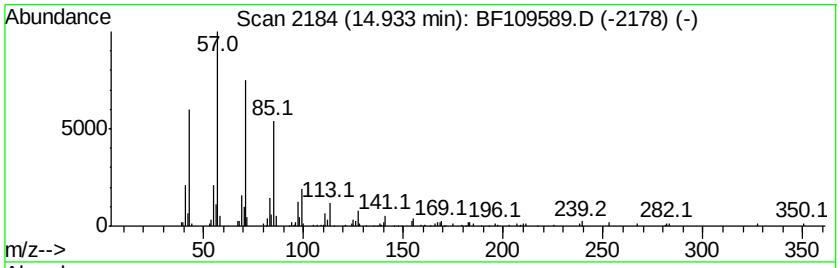
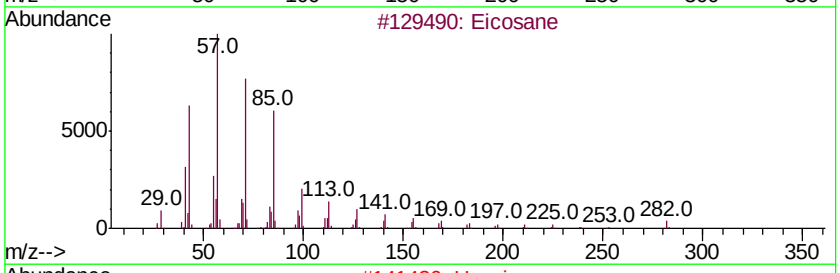
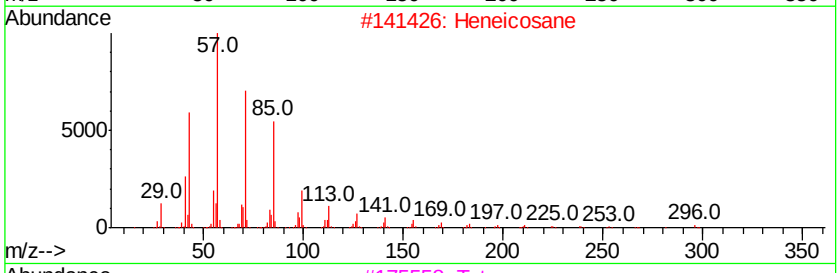
Peak Number 7 Eicosane Concentration Rank 4

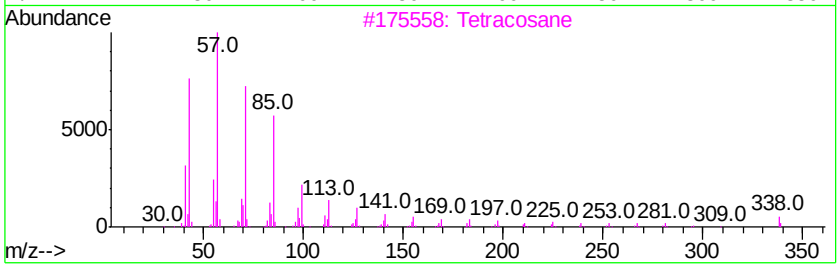
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	9.44 ng	273798	Perylene-d12	15.24

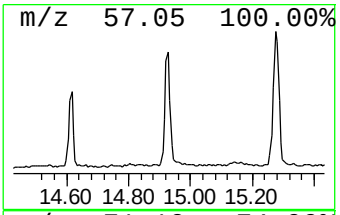
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octadecane	254	C18H38	000593-45-3	90
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90

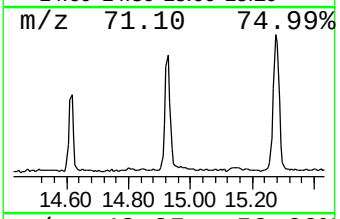


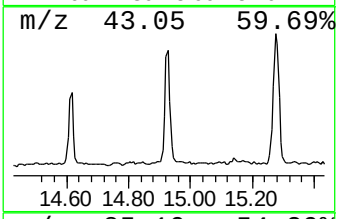


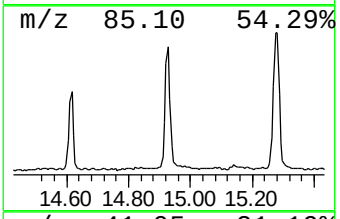


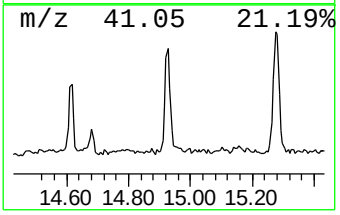












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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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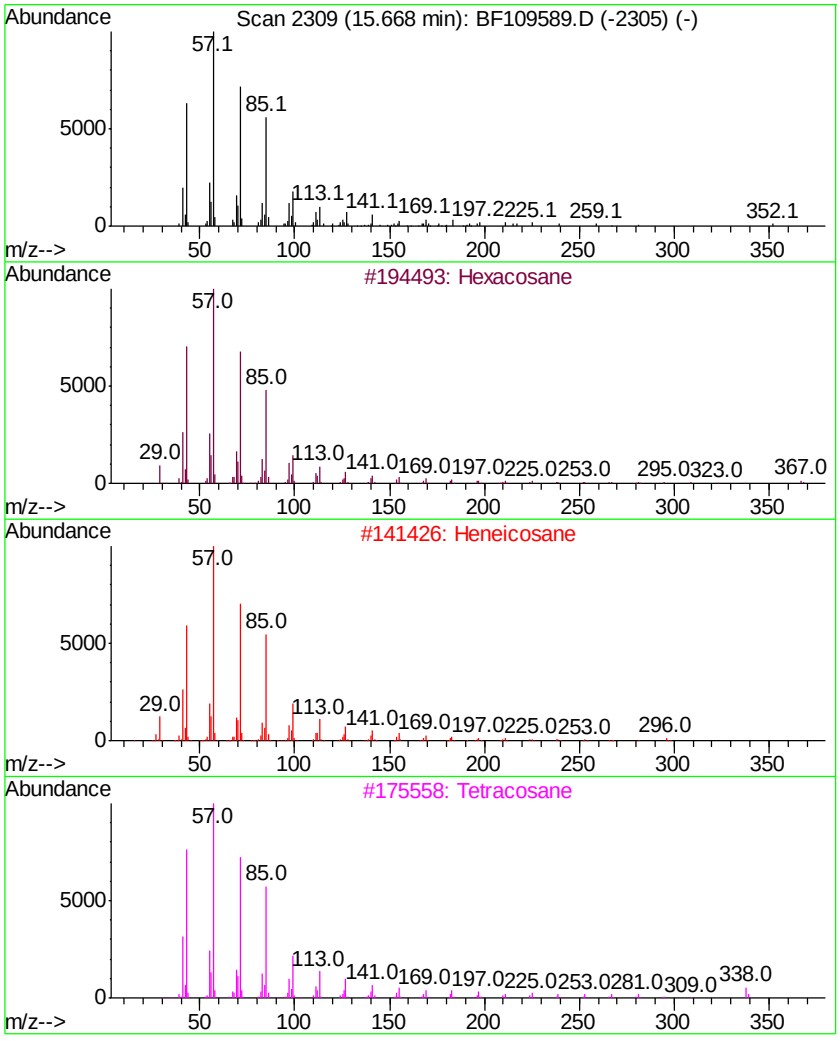
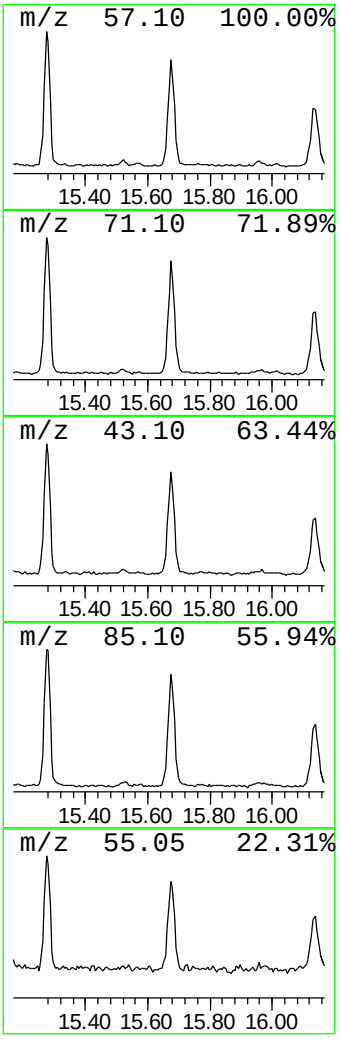
Peak Number 8 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	10.85 ng	314544	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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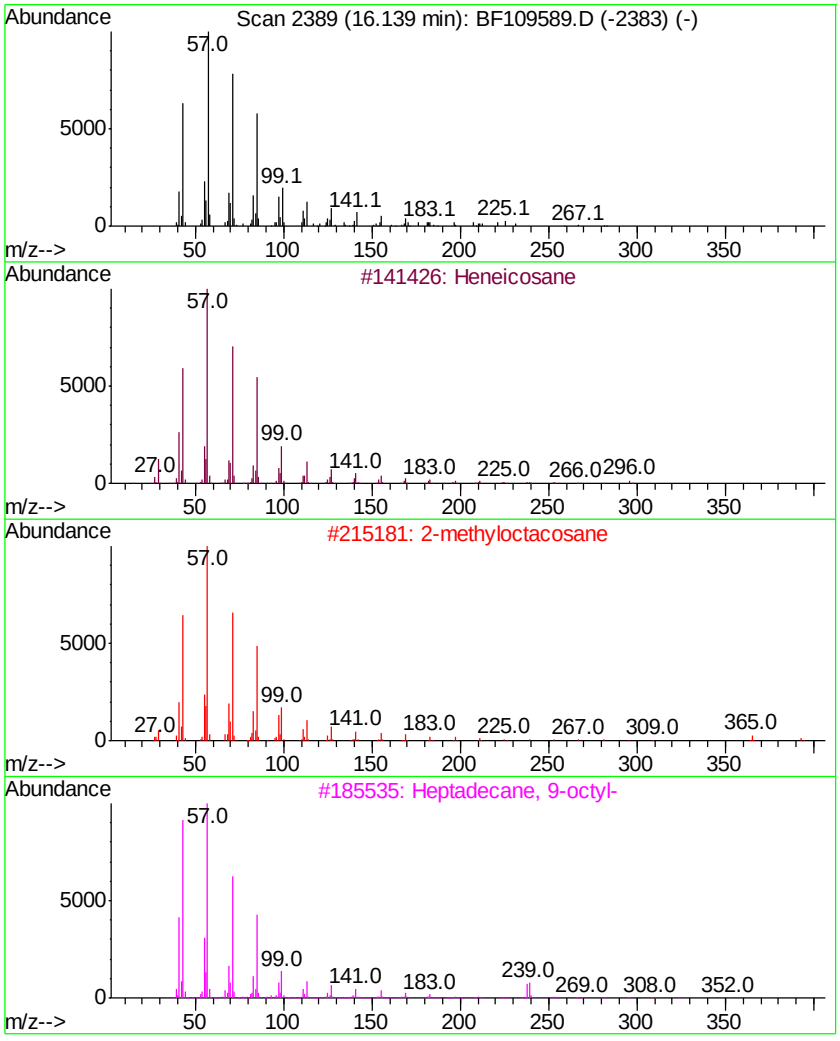
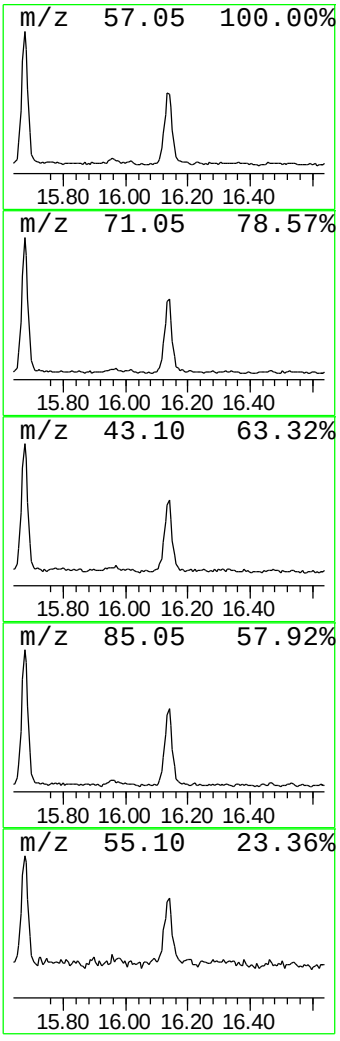
Peak Number 9 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	8.36 ng	242354	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Octacosane	394	C28H58	000630-02-4	91





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Data File : BF109589.D
Acq On : 4 Oct 2018 16:22
Operator : JU/SJ
Sample : J5221-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

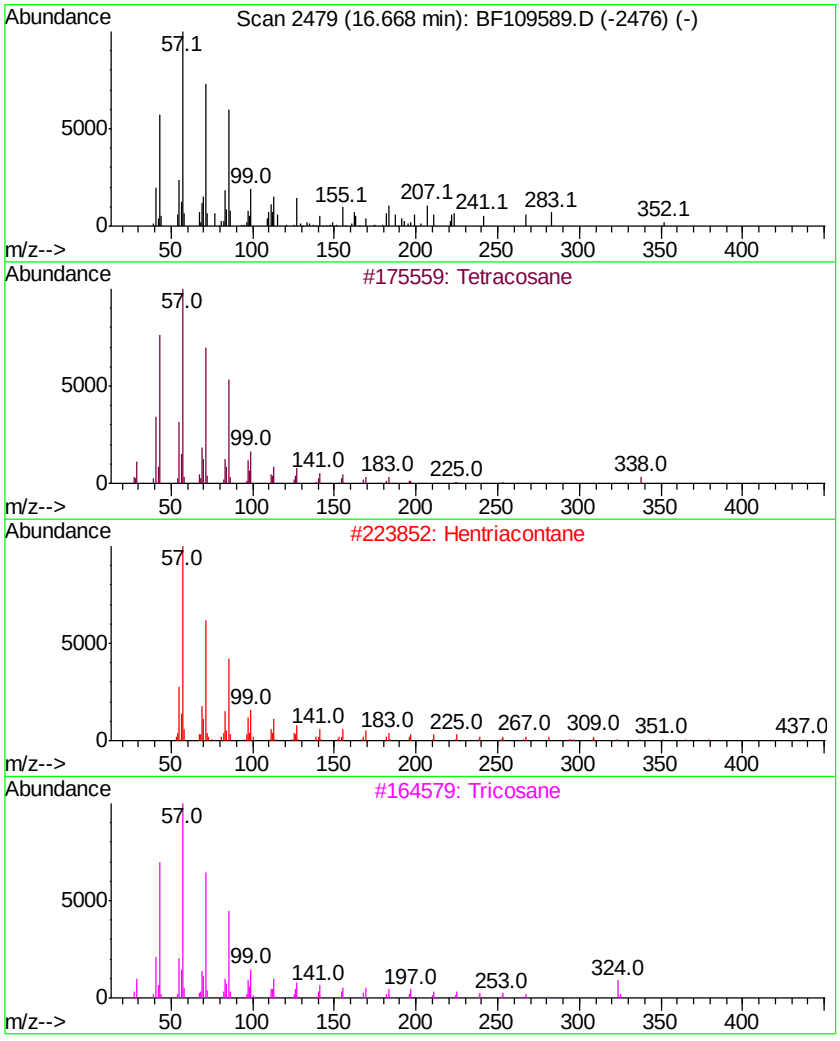
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

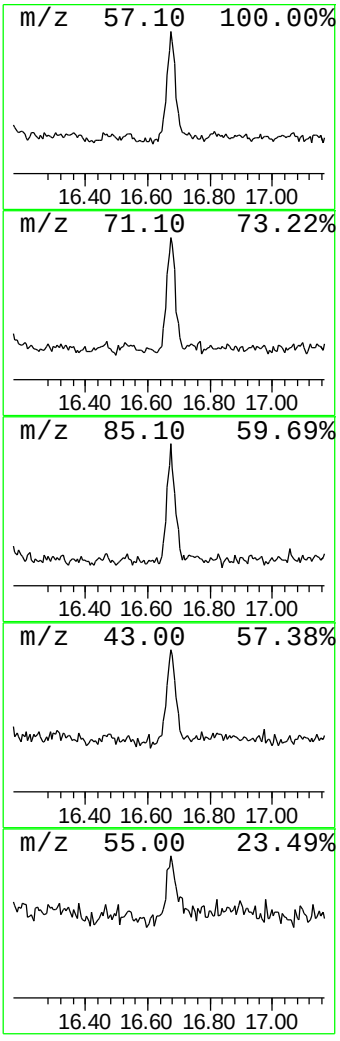
****

Peak Number 10 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	2.84 ng	82312	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	86
2	Hentriacontane	437	C31H64	000630-04-6	86
3	Tricosane	324	C23H48	000638-67-5	86
4	Heptacosane	380	C27H56	000593-49-7	83
5	Heneicosane	296	C21H44	000629-94-7	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100418\
Data File : BF109589.D
Acq On : 4 Oct 2018 16:22
Operator : JU/SJ
Sample : J5221-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 100118-JETT-E-U-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.89	3.3	ng	97759	1	6.70	586159	20.0
unknown6.47	6.47	55.8	ng	1633810	1	6.70	586159	20.0
2,4,7,9-Tetrameth...	9.18	3.1	ng	130204	3	9.73	843124	20.0
Eicosane, 9-octyl-	14.32	2.1	ng	60221	5	13.84	581146	20.0
Heptadecane, 9-oc...	14.62	5.0	ng	143990	6	15.24	580052	20.0
Eicosane	14.93	9.4	ng	273798	6	15.24	580052	20.0
Hexacosane	15.67	10.9	ng	314544	6	15.24	580052	20.0
Heneicosane	16.14	8.4	ng	242354	6	15.24	580052	20.0
Tetracosane	16.67	2.8	ng	82312	6	15.24	580052	20.0