LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112438.D
Acq On : 7 Feb 2019 15:18
Operator : JU/SJ
Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

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-BF012519.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	2.134	4	8	20	rVB	131336	209919	5.53%	0.626%
2	5.057	502	505	521	rVB	105186	156588	4.12%	0.467%
3	5.469	572	575	594	rBV	2851454	3090458	81.35%	9.221%
4	6.487	743	748	765	rBV	2960887	3383231	89.06%	10.095%
5	6.610	765	769	772	rBV	3901021	3407385	89.70%	10.167%
6	6.834	803	807	815	rBV	939180	886281	23.33%	2.645%
7	6.987	829	833	837	rBV	2858953	2633065	69.31%	7.857%
8	7.398	898	903	914	rBV	2113240	2078787	54.72%	6.203%
9	8.116	1021	1025	1044	rVB	1176806	1160543	30.55%	3.463%
10	9.186	1202	1207	1218	rBV	3927575	3798763	100.00%	11.335%
11	9.581	1271	1274	1280	rBV	274744	248903	6.55%	0.743%
12	9.869	1318	1323	1332	rVB	1442638	1316826	34.66%	3.929%
13	10.663	1454	1458	1471	rBV	2651298	2443505	64.32%	7.291%
14	11.357	1572	1576	1587	rBV	1424933	1272101	33.49%	3.796%
15	11.704	1630	1635	1638	rBV2	39810	56283	1.48%	0.168%
16	11.874	1659	1664	1673	rBV3	167780	268934	7.08%	0.802%
17	12.574	1779	1783	1787	rBV	163599	169571	4.46%	0.506%
18	12.663	1795	1798	1802	rBV4	32641	43585	1.15%	0.130%
19	12.804	1816	1822	1825	rBV	172247	205233	5.40%	0.612%
20	12.939	1840	1845	1848	rBV	3494437	3124376	82.25%	9.323%
21	13.504	1937	1941	1943	rBV2	46698	50685	1.33%	0.151%
22	13.827	1992	1996	2004	rVB2	234136	307038	8.08%	0.916%
23	13.998	2021	2025	2029	rBV	1054835	1075821	28.32%	3.210%
24	14.145	2047	2050	2060	rBV	110471	147724	3.89%	0.441%
25	14.451	2099	2102	2107	rVB	133103	132867	3.50%	0.396%
26	14.751	2150	2153	2156	rVB	131972	128863	3.39%	0.385%
27	14.827	2163	2166	2169	rVB	204879	179107	4.71%	0.534%
28	15.045	2200	2203	2206	rBV	68633	101904	2.68%	0.304%
29	15.080	2206	2209	2213	rVB2	150787	198012	5.21%	0.591%
30	15.410	2263	2265	2268	rVB	52243	55996	1.47%	0.167%
31	15.468	2270	2275	2288	rVB	700823	1062402	27.97%	3.170%
32	15.892	2343	2347	2351	rVB2	83369	118931	3.13%	0.355%

LSC Area Percent Report

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Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 33513687

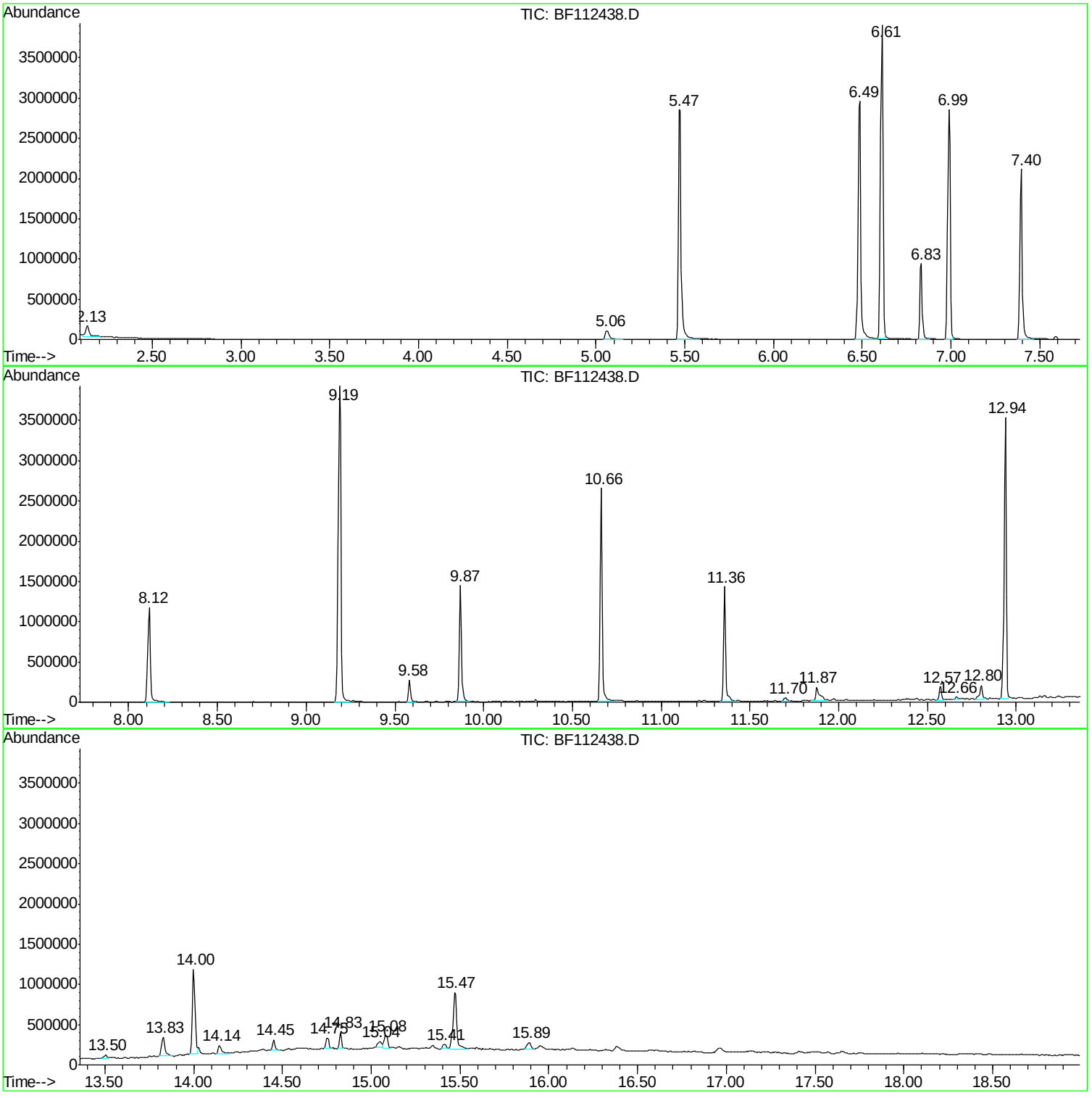
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112438.D
Acq On : 7 Feb 2019 15:18
Operator : JU/SJ
Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112438.D
Acq On : 7 Feb 2019 15:18
Operator : JU/SJ
Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

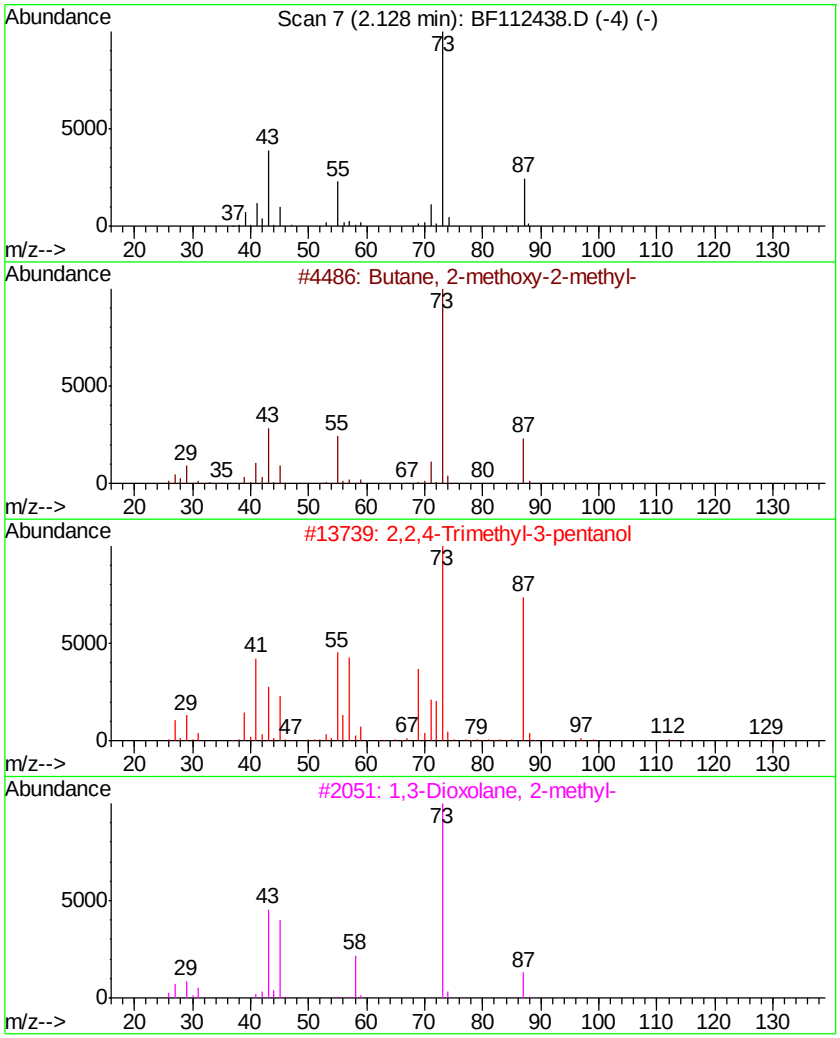
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

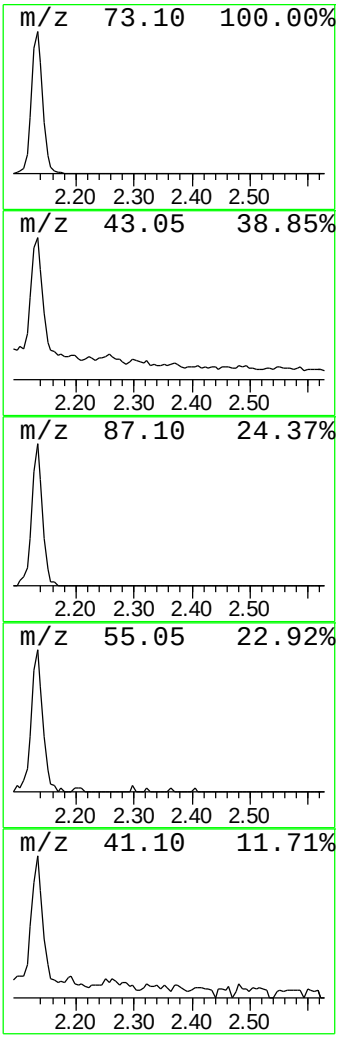
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	4.74 ng	209919	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
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	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112438.D
Acq On : 7 Feb 2019 15:18
Operator : JU/SJ
Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

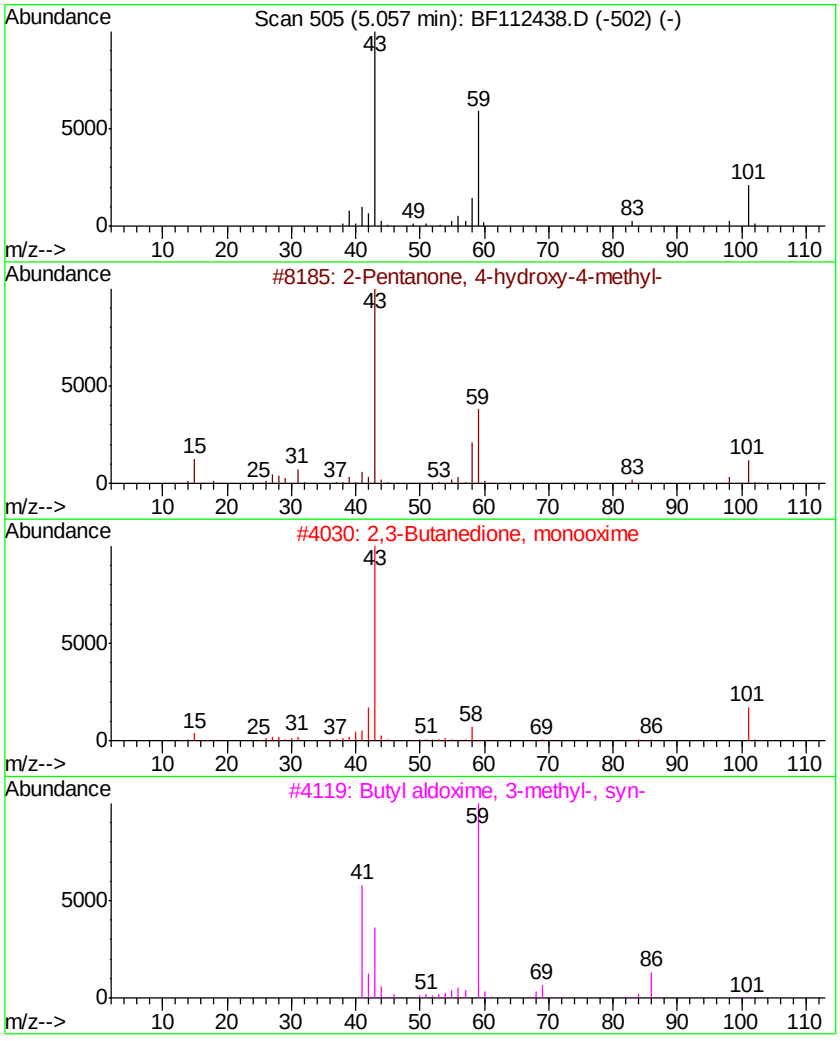
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

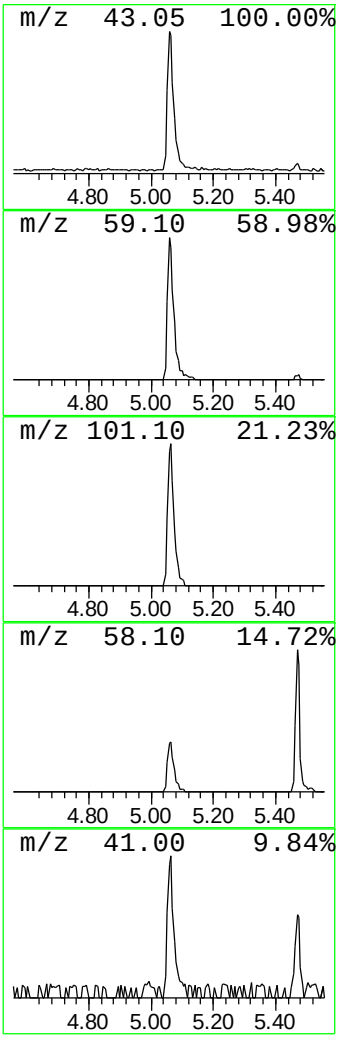
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	3.53 ng	156588	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112438.D
Acq On : 7 Feb 2019 15:18
Operator : JU/SJ
Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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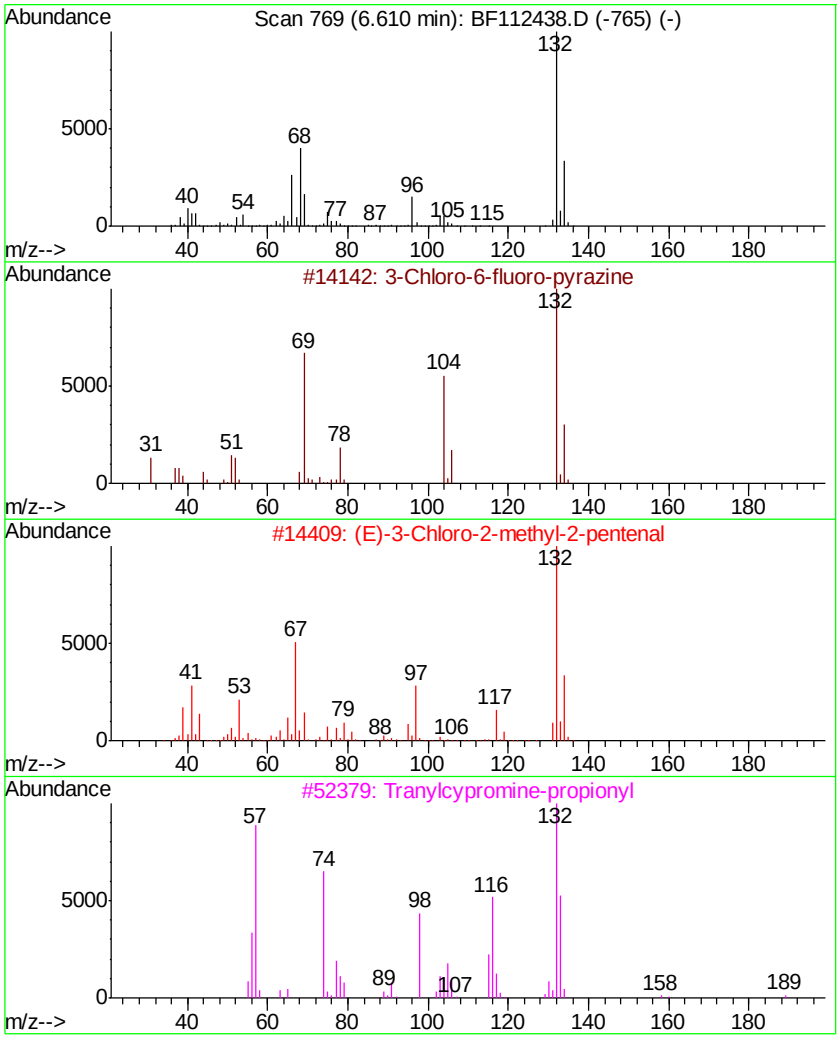
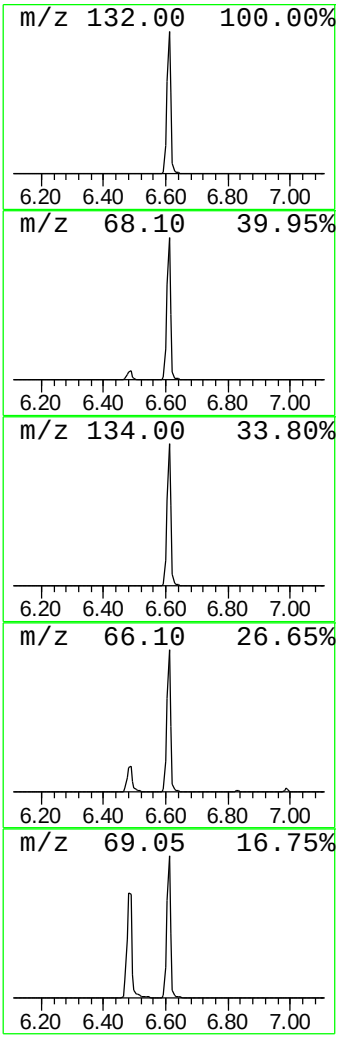
Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	76.89 ng	3407390	1,4-Dichlorobenzene-d4	6.83

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	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\BF020719\
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Operator : JU/SJ
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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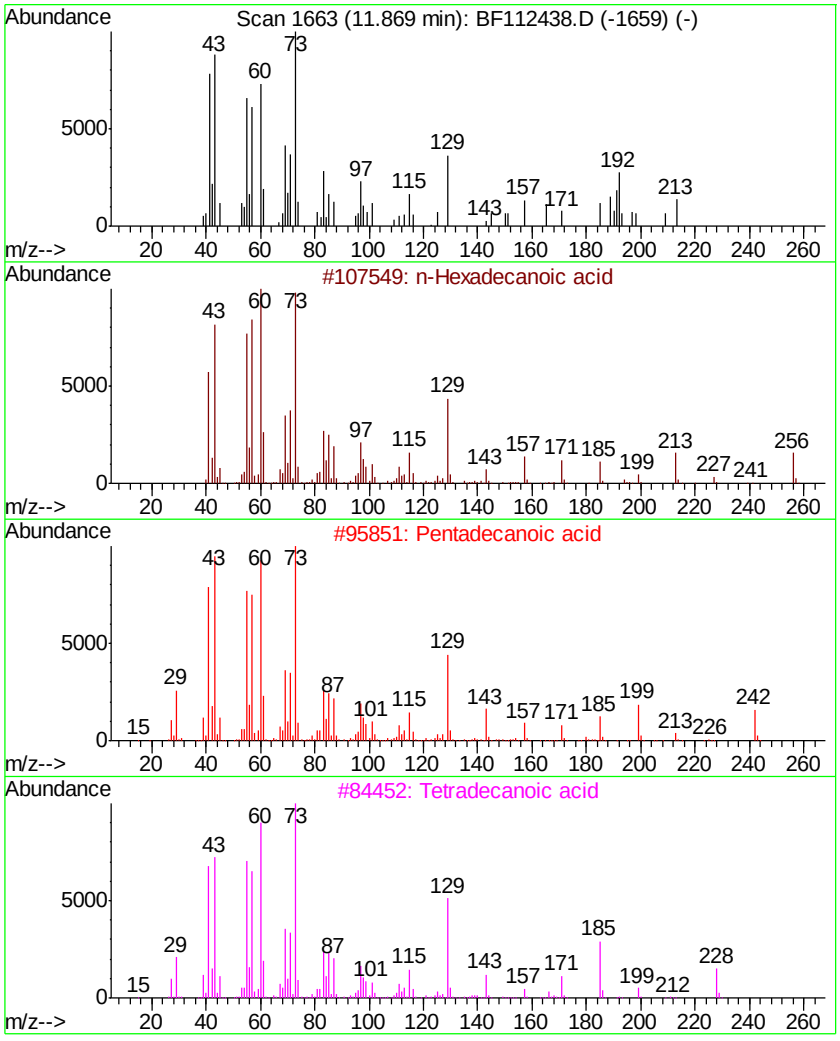
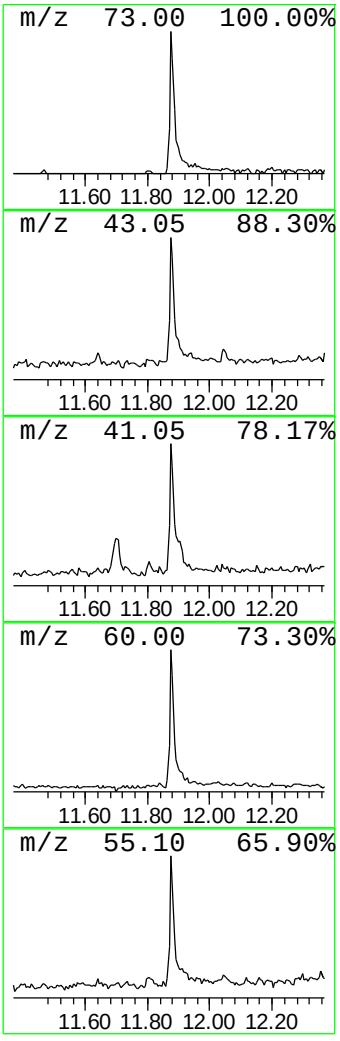
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	4.23 ng	268934	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	50





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Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

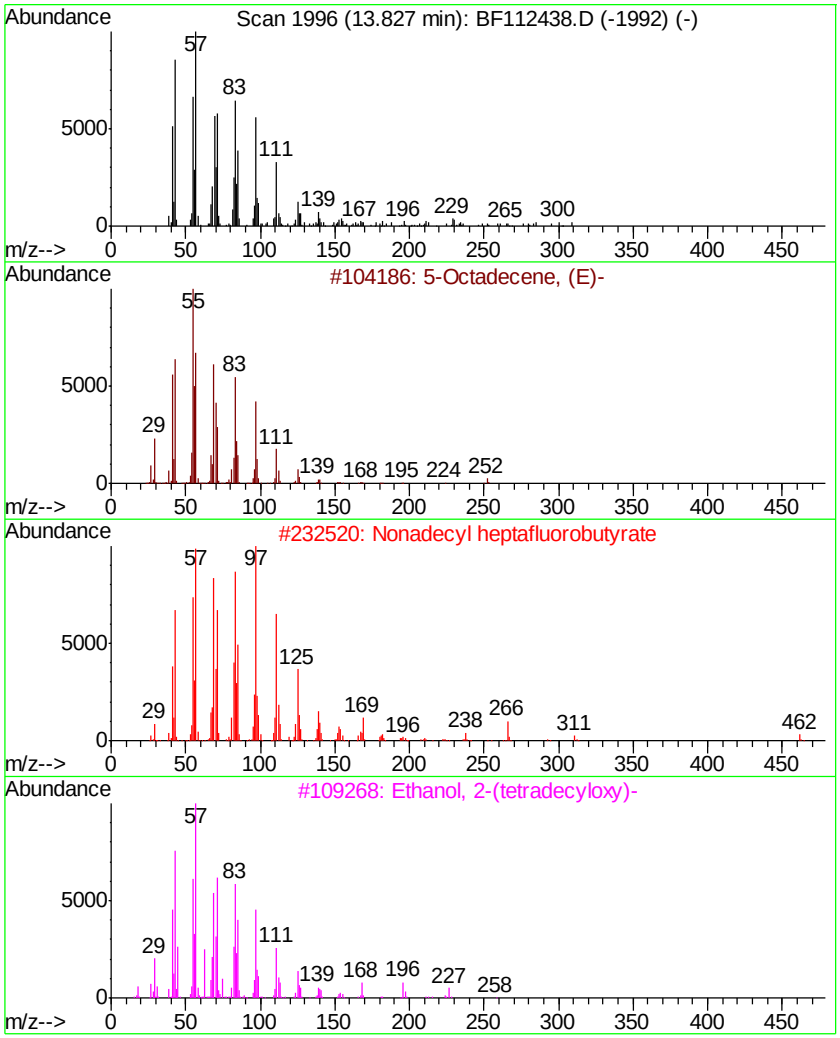
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

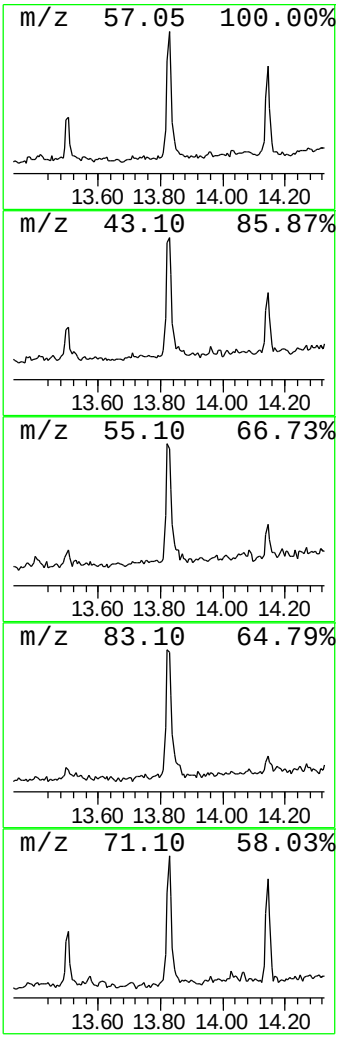
****

Peak Number 6 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	5.71 ng	307038	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
2	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





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Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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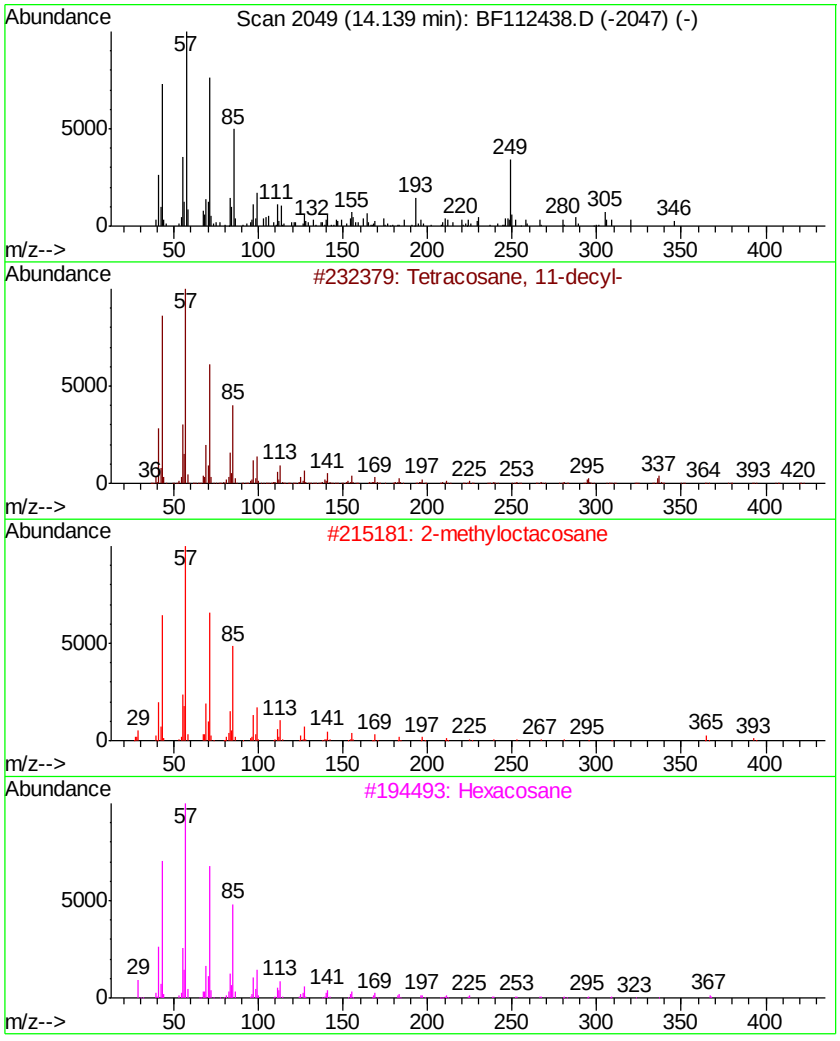
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

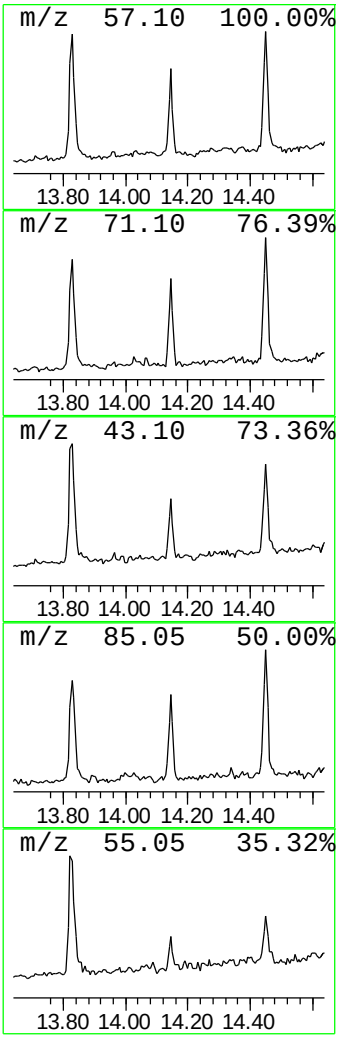
****

Peak Number 7 Tetracosane, 11-decyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.75 ng	147724	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	64
2	2-methyloctacosane	408	C29H60	1000376-72-8	64
3	Hexacosane	366	C26H54	000630-01-3	64
4	Tetracosane	338	C24H50	000646-31-1	58
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	58





Library Search Compound Report

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Acq On : 7 Feb 2019 15:18
Operator : JU/SJ
Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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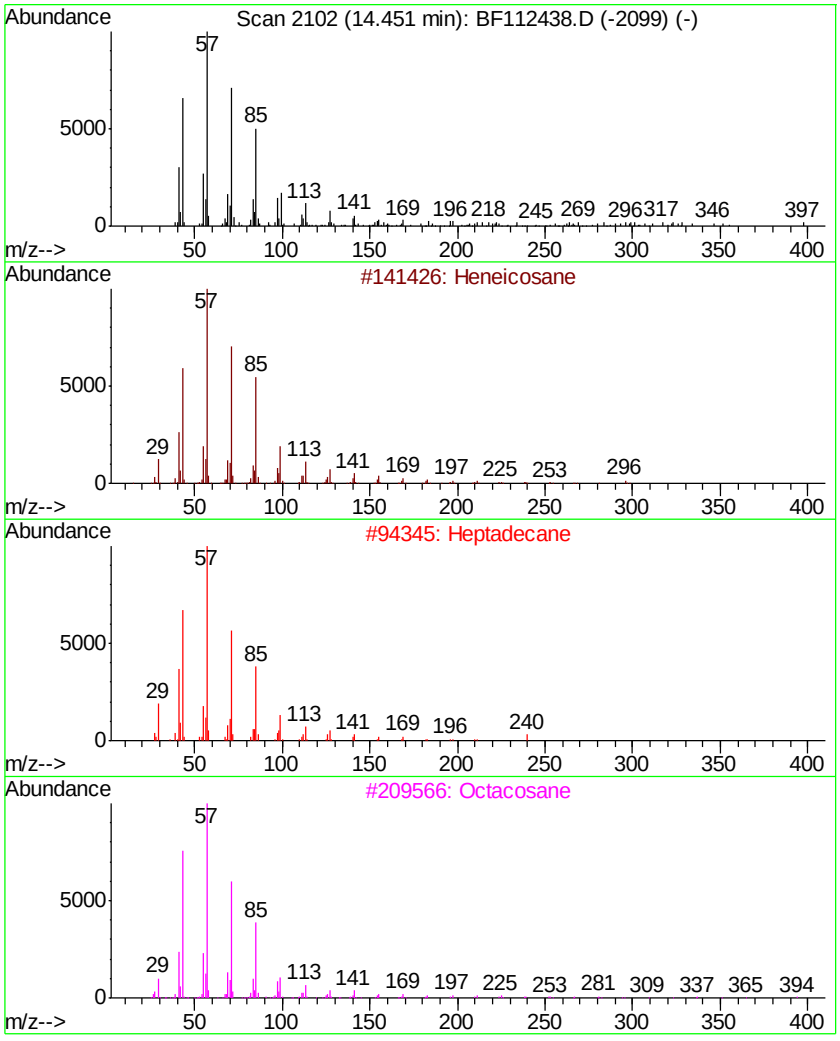
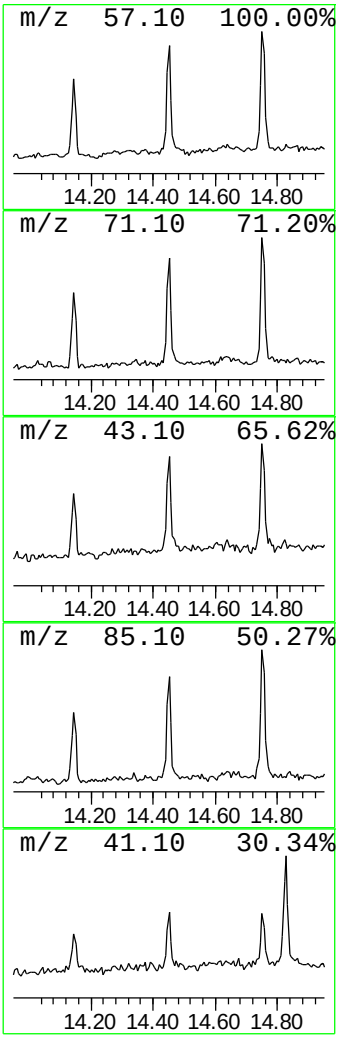
Peak Number 8 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.47 ng	132867	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	99
2	Heptadecane	240	C17H36	000629-78-7	93
3	Octacosane	394	C28H58	000630-02-4	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





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Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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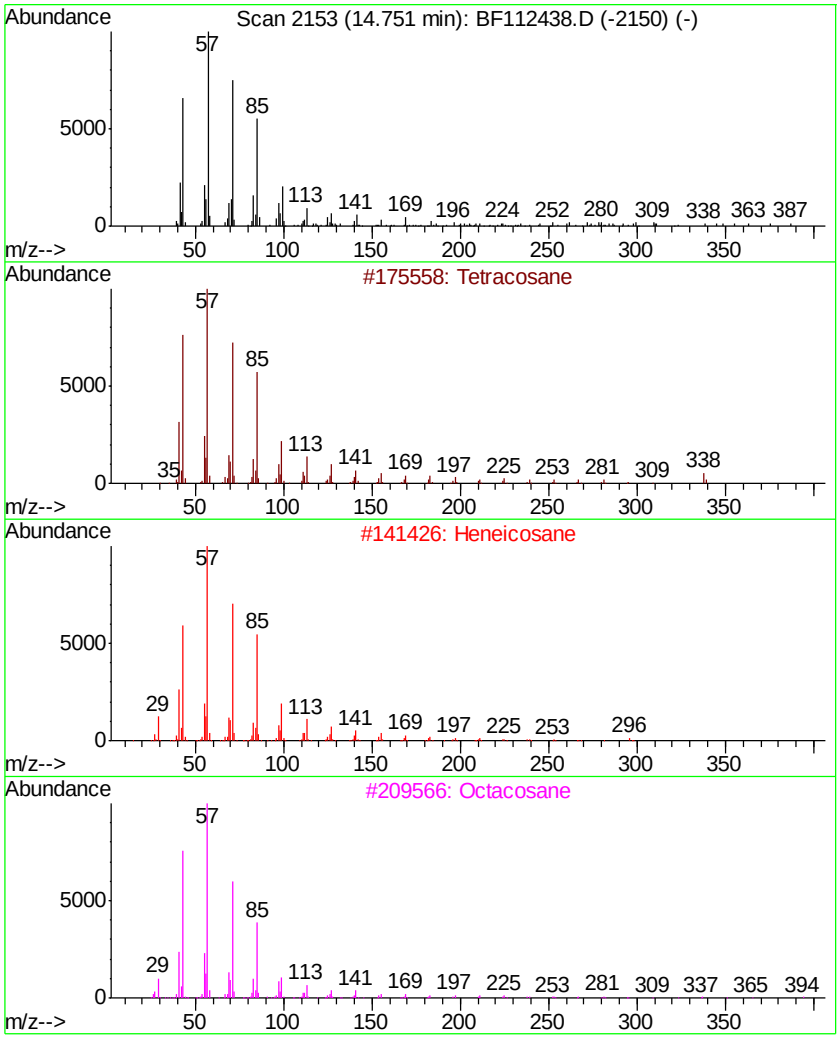
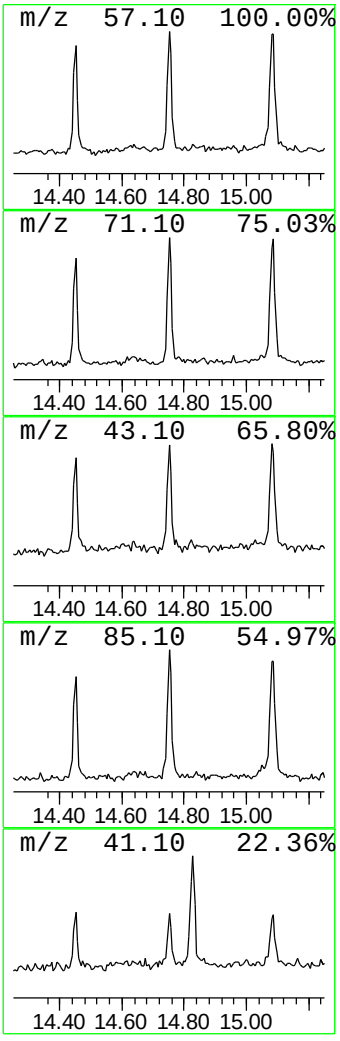
Peak Number 9 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.43 ng	128863	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	86
4	Hexacosane	366	C26H54	000630-01-3	86
5	Hexadecane	226	C16H34	000544-76-3	80





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112438.D
Acq On : 7 Feb 2019 15:18
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Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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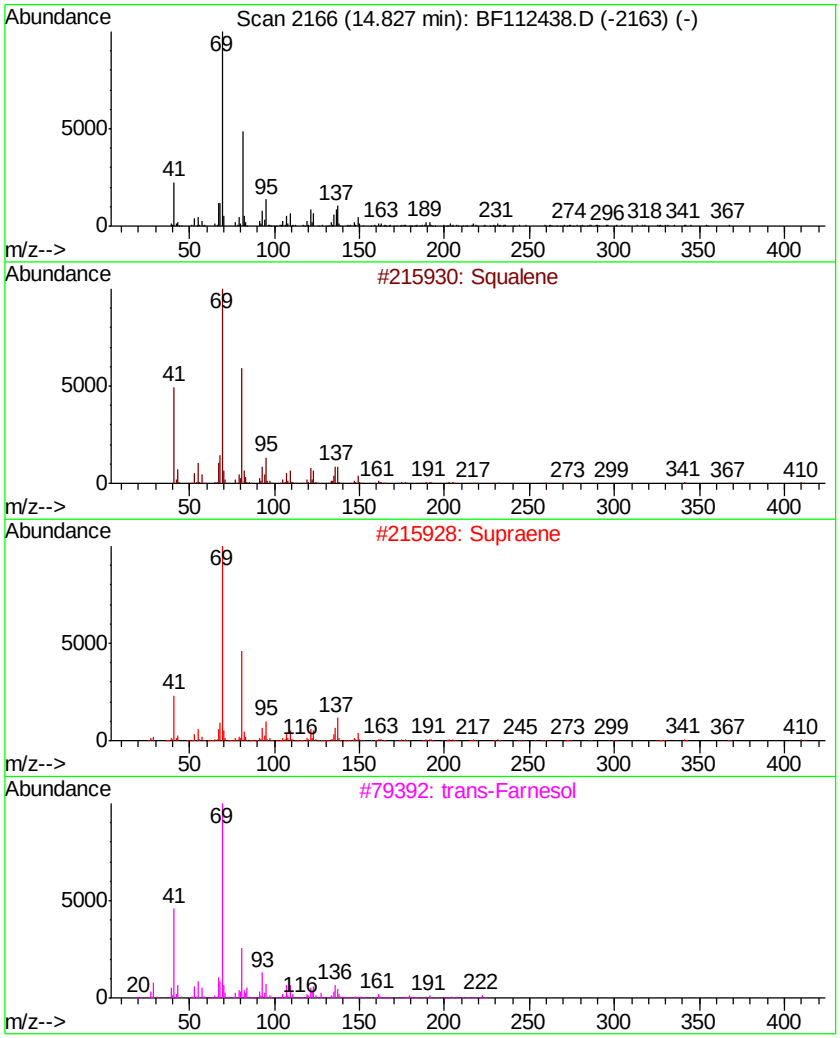
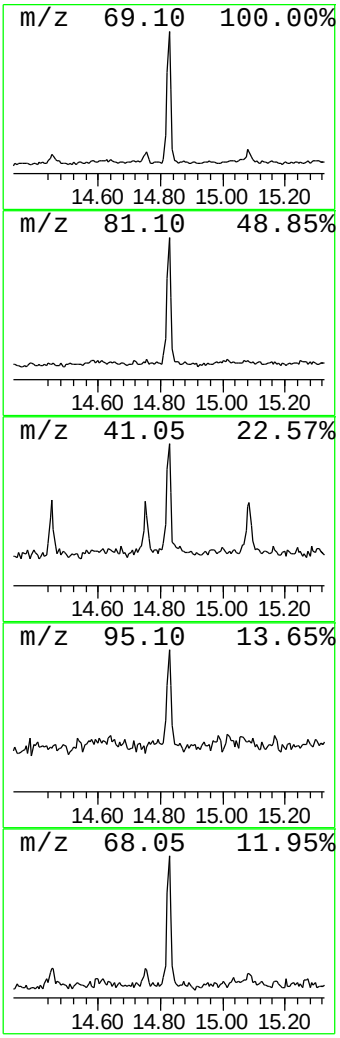
Peak Number 10 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.37 ng	179107	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	trans-Farnesol	222	C15H26O	000106-28-5	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020719\
Data File : BF112438.D
Acq On : 7 Feb 2019 15:18
Operator : JU/SJ
Sample : K1389-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-5S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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...	2.13	4.7	ng	209919	1	6.83	886281	20.0
2-Pentanone, 4-hy...	5.06	3.5	ng	156588	1	6.83	886281	20.0
unknown6.61	6.61	76.9	ng	3407390	1	6.83	886281	20.0
n-Hexadecanoic acid	11.87	4.2	ng	268934	4	11.36	1272100	20.0
5-Octadecene, (E)-	13.83	5.7	ng	307038	5	14.00	1075820	20.0
Tetracosane, 11-d...	14.14	2.8	ng	147724	5	14.00	1075820	20.0
Heneicosane	14.45	2.5	ng	132867	5	14.00	1075820	20.0
Tetracosane	14.75	2.4	ng	128863	6	15.47	1062400	20.0
Squalene	14.83	3.4	ng	179107	6	15.47	1062400	20.0