LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
Data File : BF112485.D
Acq On : 11 Feb 2019 17:16
Operator : JU/SJ
Sample : K1453-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-8-S

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	2.122	3	6	13	rVB	128960	174461	3.86%	0.515%
2	5.063	502	506	516	rBV	116200	176813	3.91%	0.522%
3	5.475	572	576	595	rBV	3580127	3592372	79.52%	10.603%
4	6.487	743	748	765	rBV	3451236	3781684	83.72%	11.162%
5	6.610	765	769	773	rBV	4154005	4005064	88.66%	11.821%
6	6.834	803	807	816	rBV	861859	798178	17.67%	2.356%
7	6.992	829	834	837	rBV	3279069	3149960	69.73%	9.297%
8	7.398	898	903	906	rBV	2461196	2366910	52.40%	6.986%
9	8.116	1021	1025	1039	rBV	969967	1004992	22.25%	2.966%
10	9.186	1202	1207	1219	rBV	4488909	4517317	100.00%	13.333%
11	9.580	1270	1274	1283	rBV	278780	270278	5.98%	0.798%
12	9.869	1319	1323	1338	rVB	1175940	1063812	23.55%	3.140%
13	10.663	1454	1458	1472	rBV	2575019	2417818	53.52%	7.136%
14	11.357	1572	1576	1585	rBV	952901	896930	19.86%	2.647%
15	11.874	1661	1664	1675	rBV2	153912	197149	4.36%	0.582%
16	12.663	1795	1798	1802	rBV3	36762	48938	1.08%	0.144%
17	12.939	1840	1845	1848	rBV	3549325	3107769	68.80%	9.173%
18	13.827	1992	1996	2004	rBV	250744	364943	8.08%	1.077%
19	14.004	2022	2026	2037	rBV	787420	800334	17.72%	2.362%
20	14.145	2047	2050	2052	rBV2	55654	53398	1.18%	0.158%
21	14.445	2098	2101	2108	rBV2	76907	111780	2.47%	0.330%
22	14.751	2150	2153	2156	rVB	83191	75768	1.68%	0.224%
23	15.080	2206	2209	2214	rVB	84940	101241	2.24%	0.299%
24	15.474	2270	2276	2283	rVB	577020	803075	17.78%	2.370%

Sum of corrected areas: 33880984

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
Data File : BF112485.D
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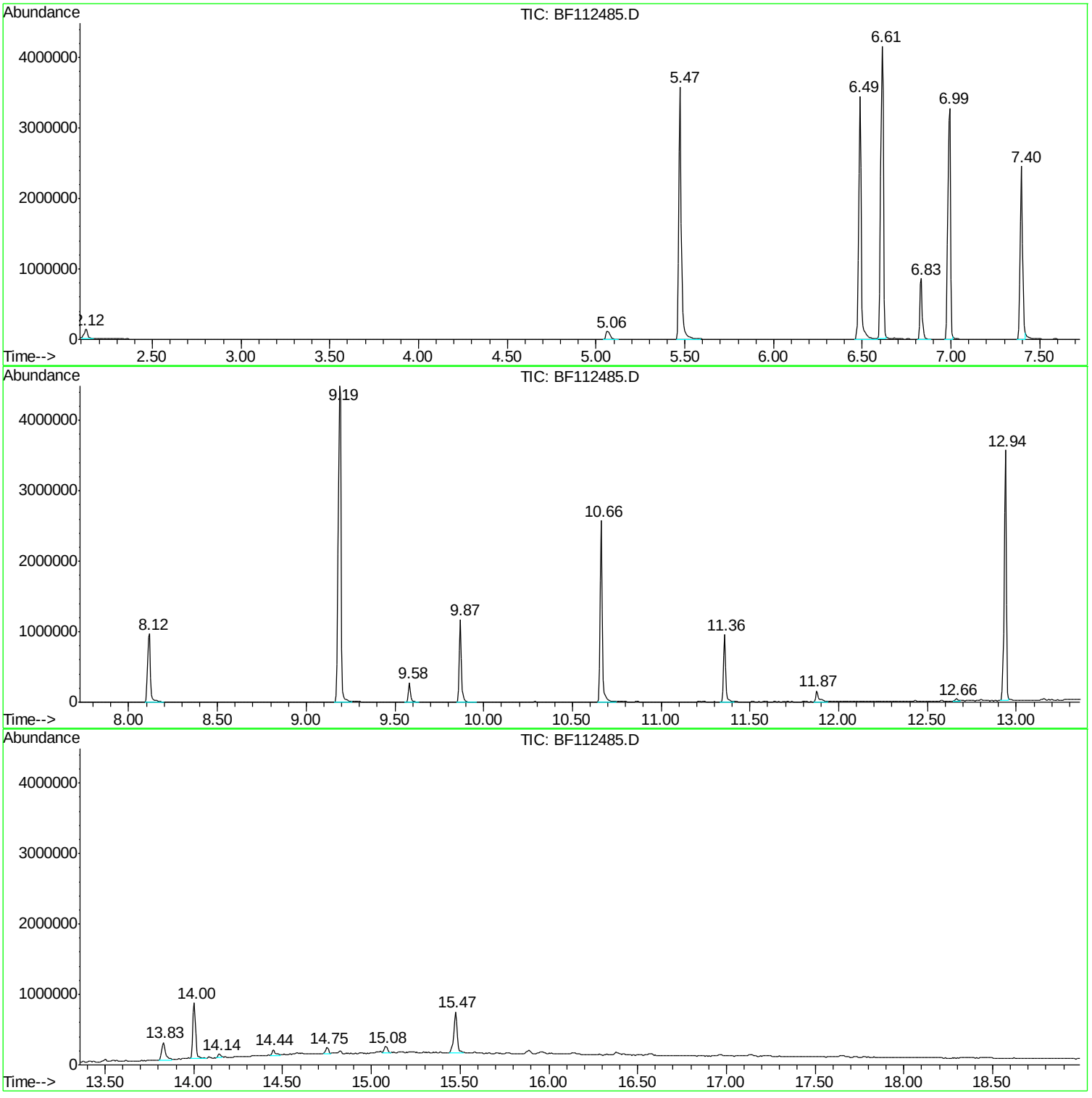
Operator : JU/SJ
Sample : K1453-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-8-S

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
Data File : BF112485.D
Acq On : 11 Feb 2019 17:16
Operator : JU/SJ
Sample : K1453-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-8-S

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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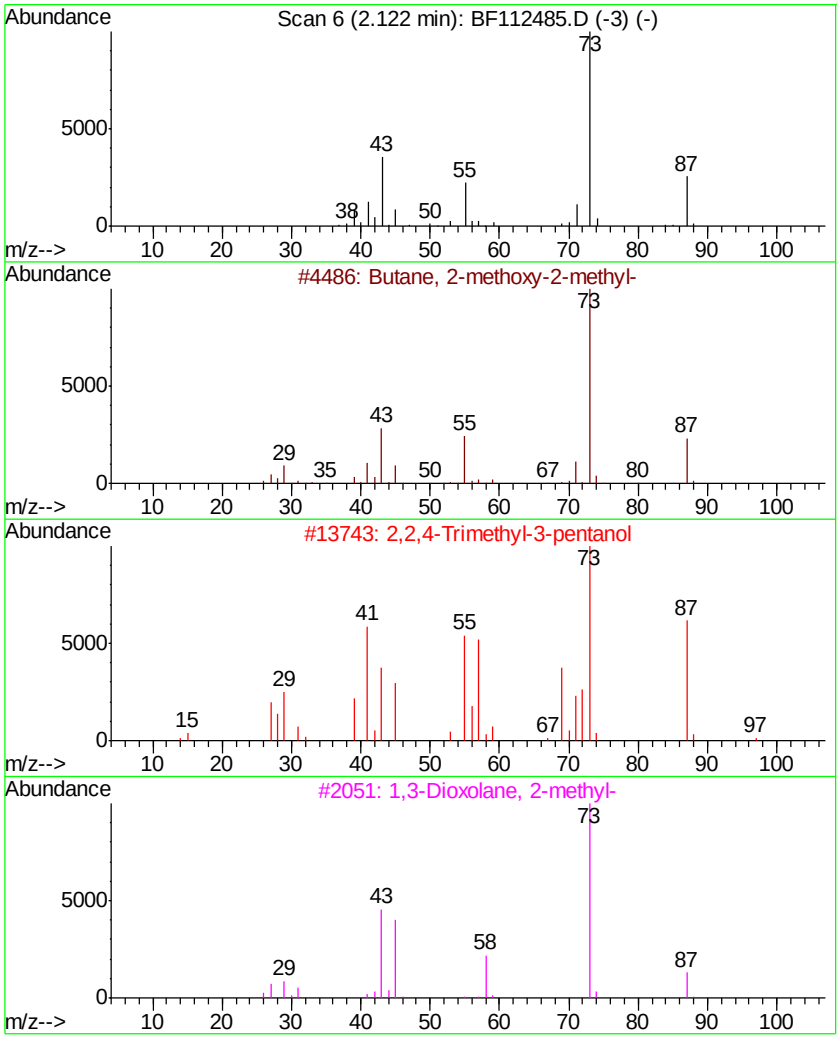
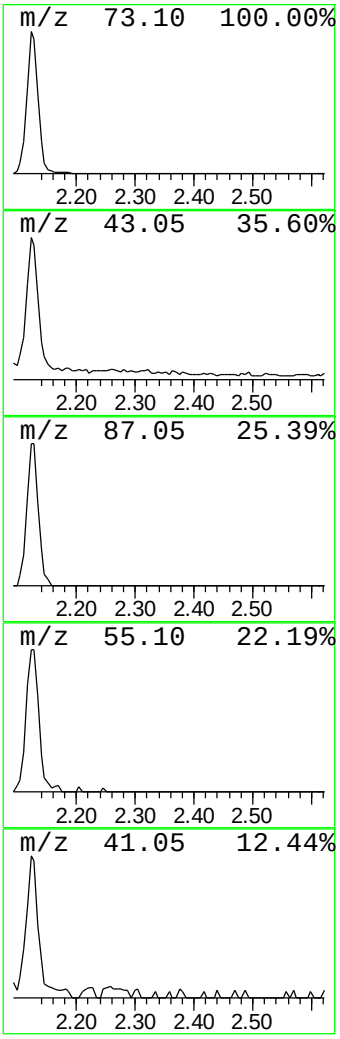
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	4.37 ng	174461	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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
Data File : BF112485.D
Acq On : 11 Feb 2019 17:16
Operator : JU/SJ
Sample : K1453-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-8-S

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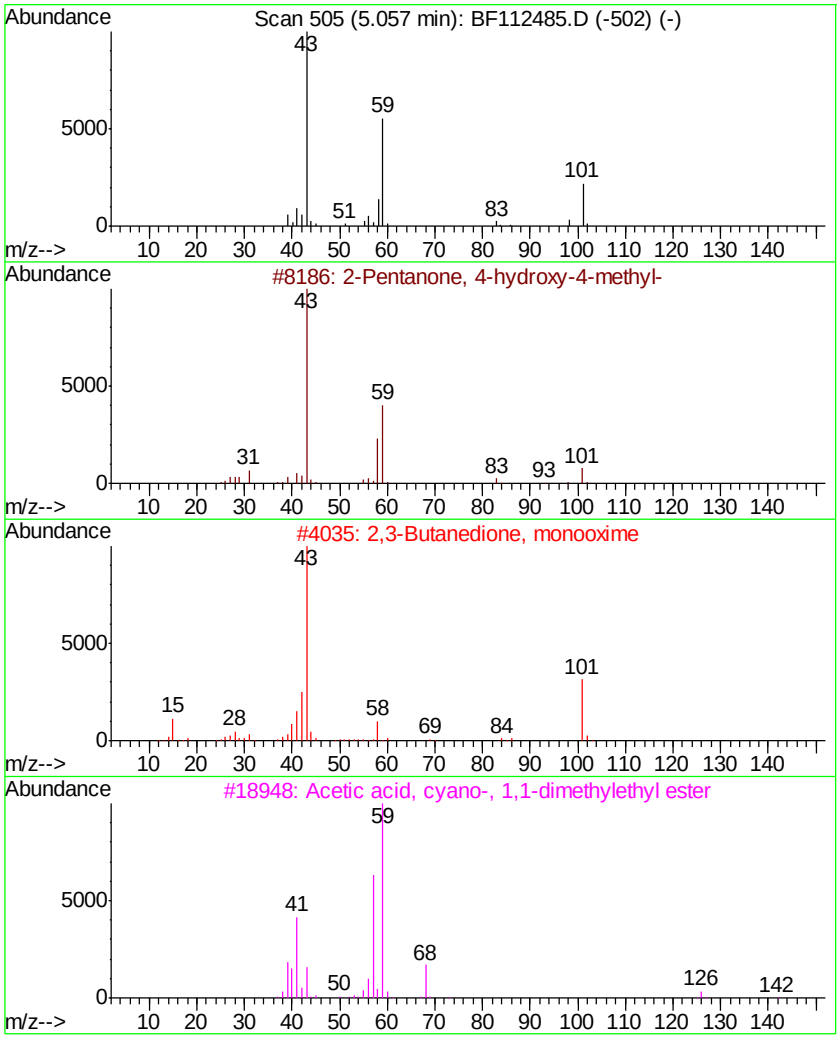
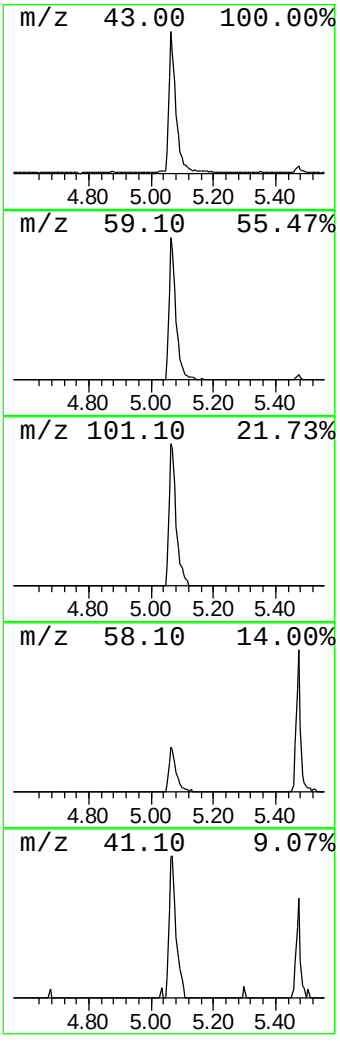
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	4.43 ng	176813	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	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
Data File : BF112485.D
Acq On : 11 Feb 2019 17:16
Operator : JU/SJ
Sample : K1453-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-8-S

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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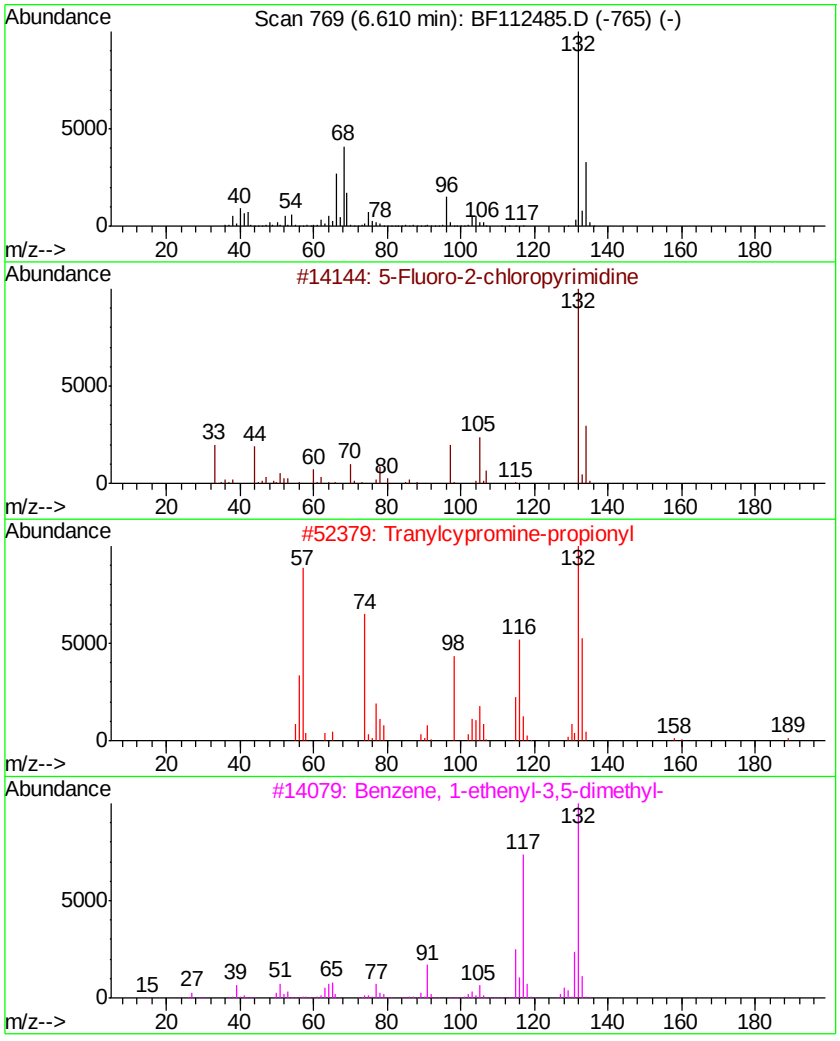
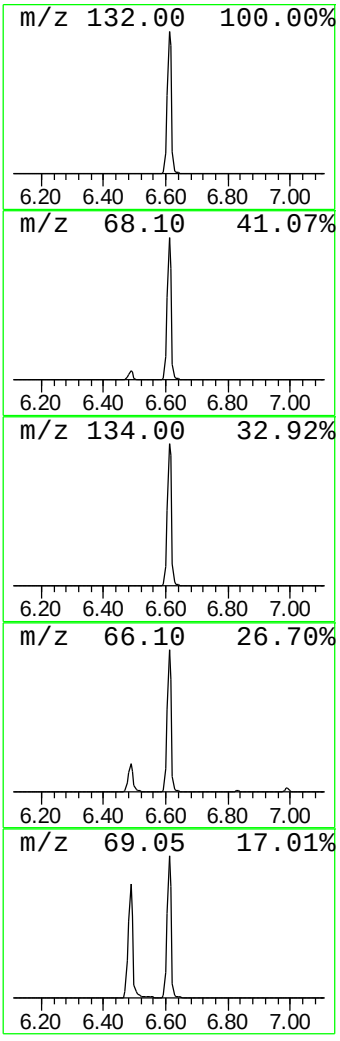
Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	100.36 ng	4005060	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
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Operator : JU/SJ
Sample : K1453-03
Misc :
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Instrument : BNA_F
ClientSampleId : M-8-S

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

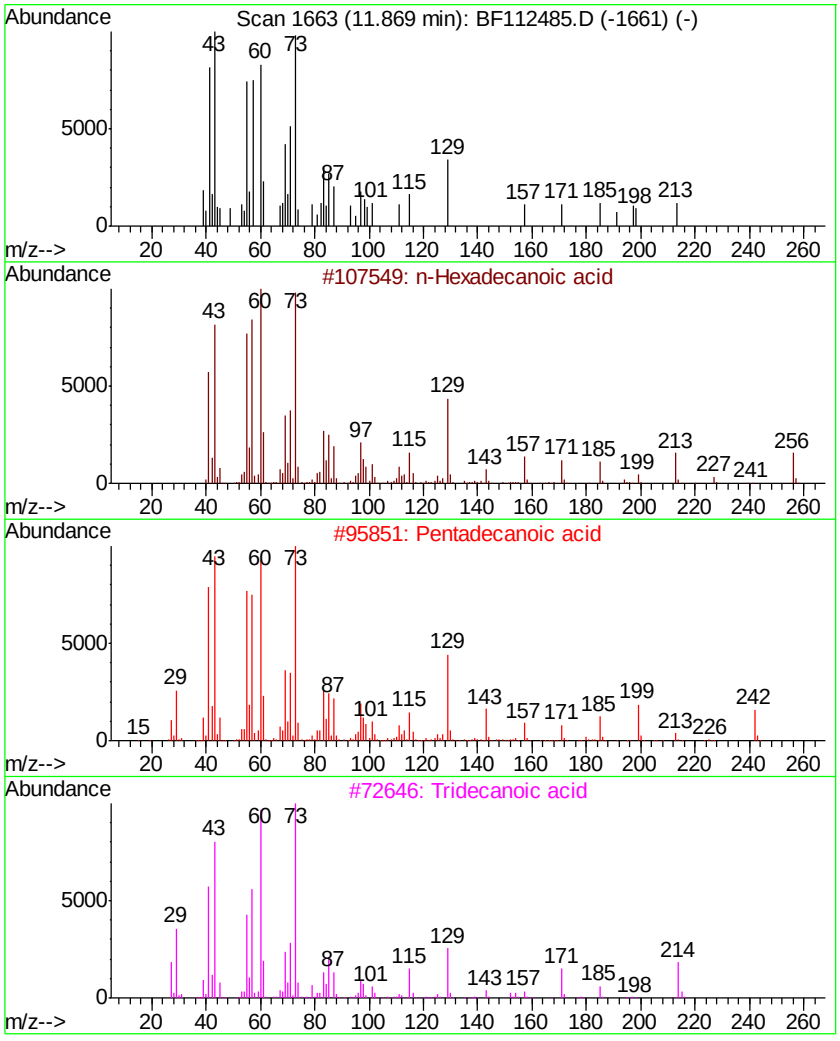
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

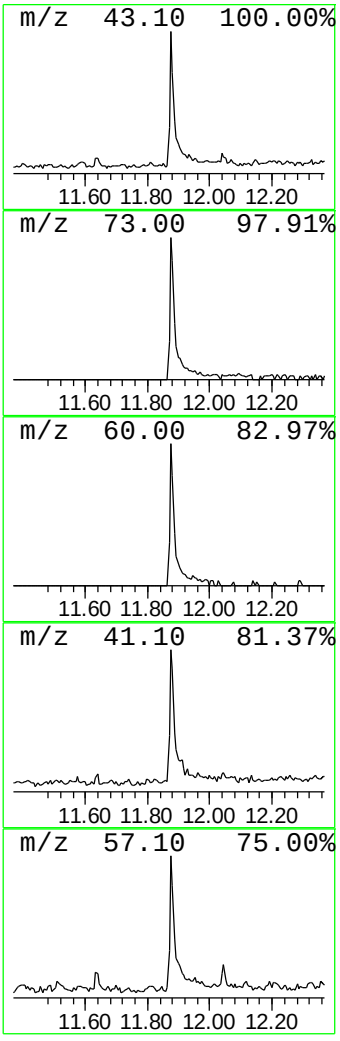
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	4.40 ng	197149	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021119\
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Operator : JU/SJ
Sample : K1453-03
Misc :
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Instrument : BNA_F
ClientSampleId : M-8-S

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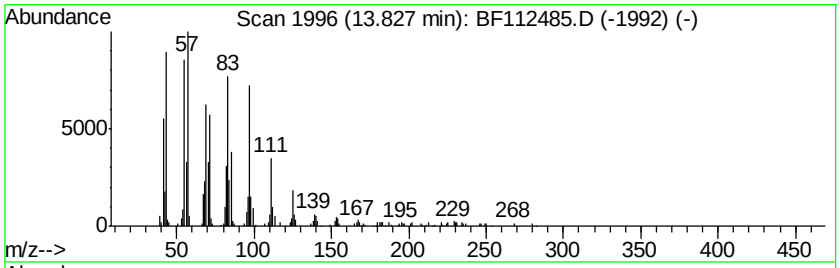
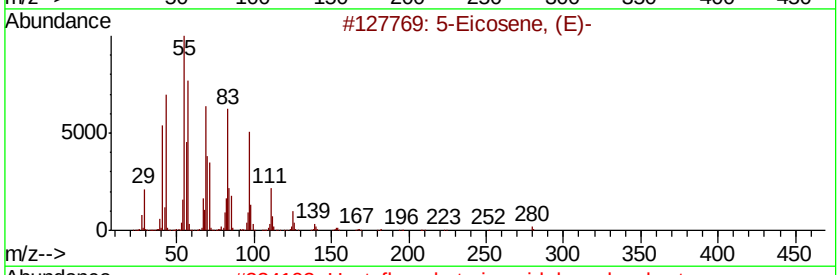
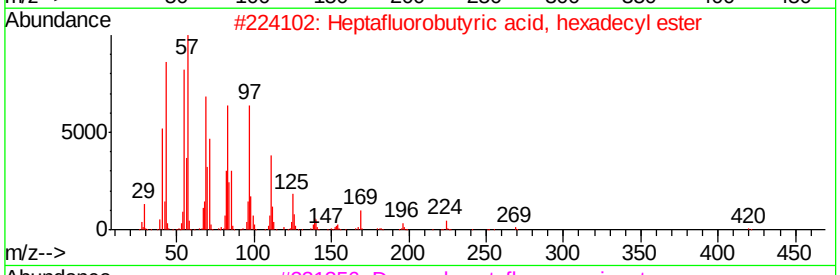
Peak Number 6 5-Eicosene, (E)- Concentration Rank 3

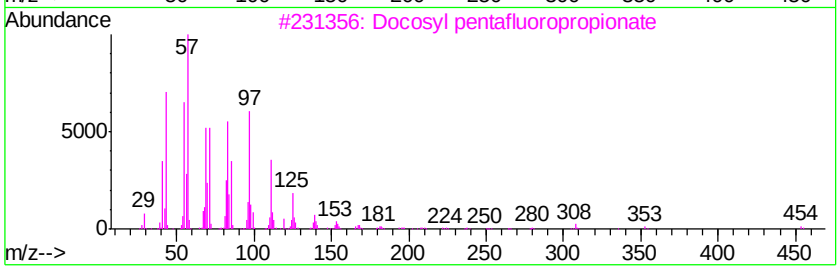
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	9.12 ng	364943	Chrysene-d12	14.00

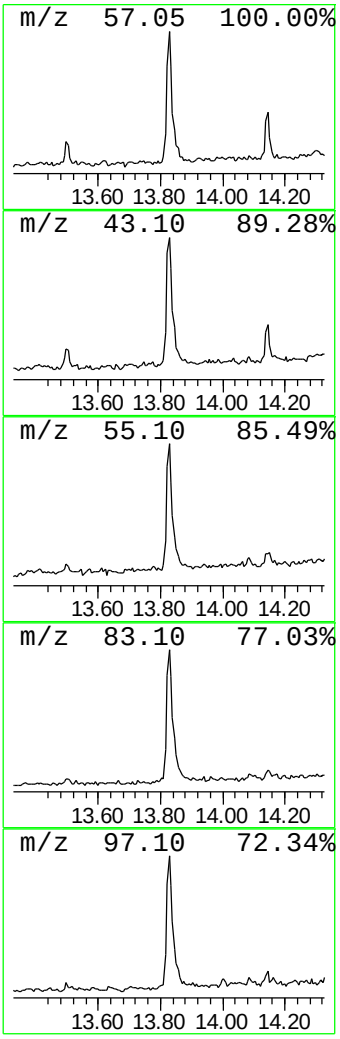
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93











Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : M-8-S

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

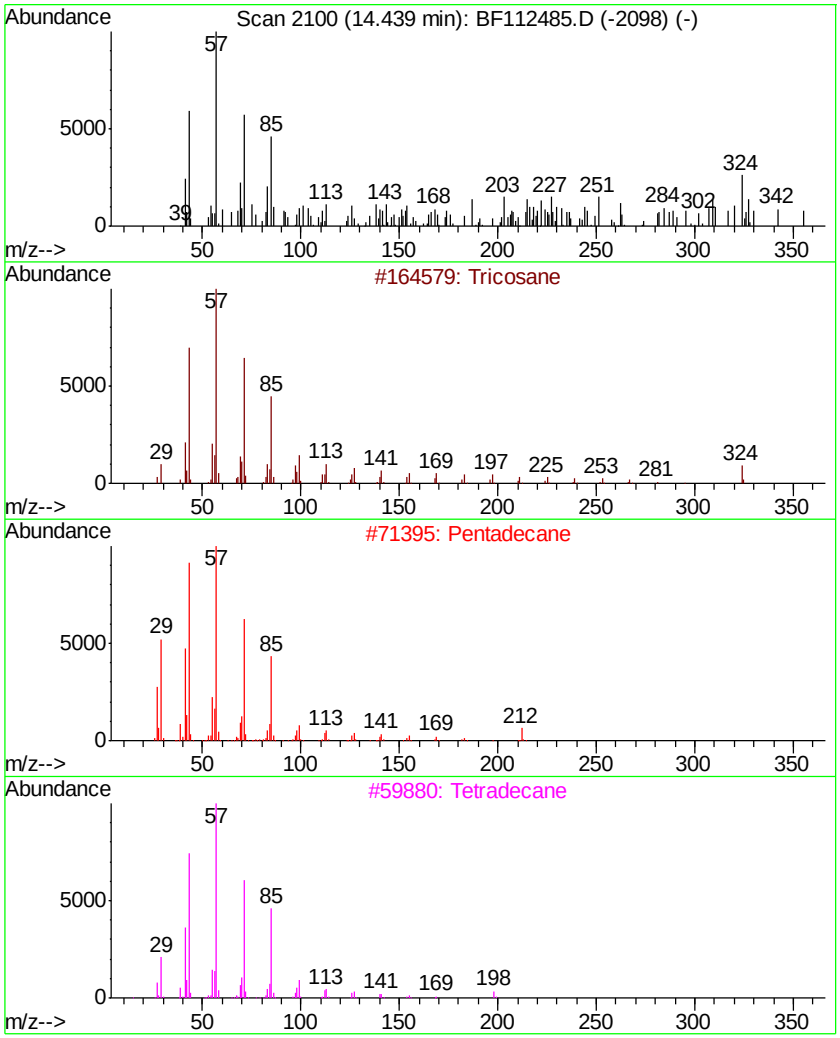
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

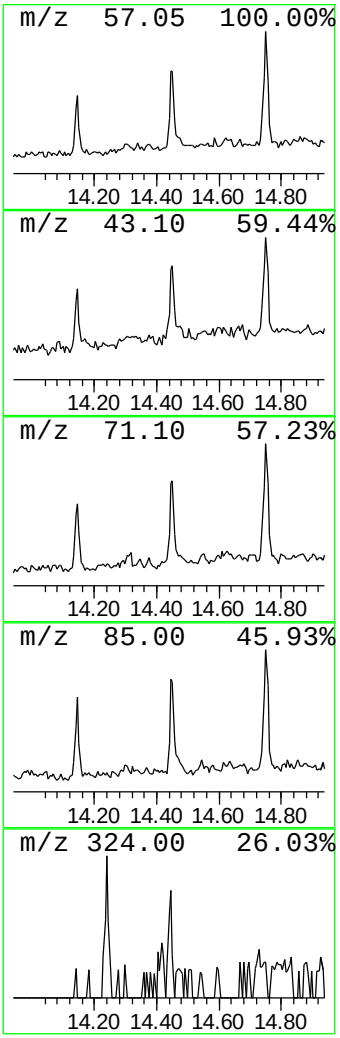
****

Peak Number 7 Tricosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	2.79 ng	111780	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	91
2	Pentadecane	212	C15H32	000629-62-9	60
3	Tetradecane	198	C14H30	000629-59-4	60
4	Heptadecane	240	C17H36	000629-78-7	53
5	Octadecane	254	C18H38	000593-45-3	53





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Sample : K1453-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-8-S

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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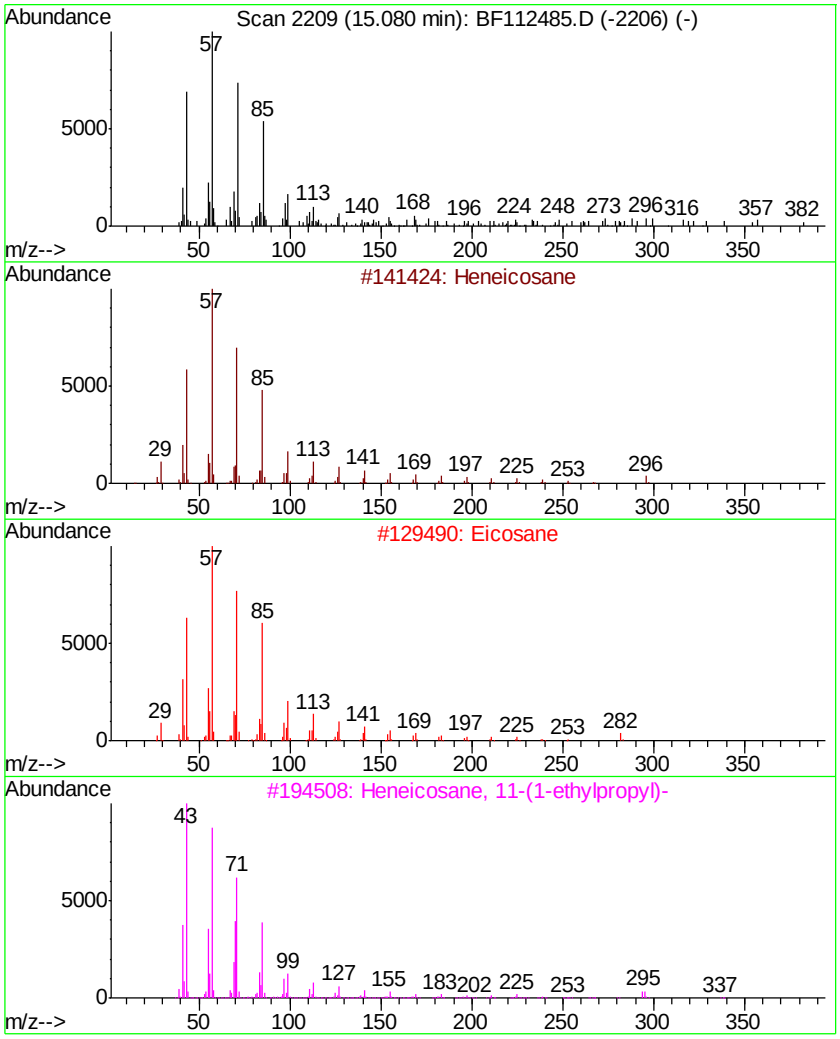
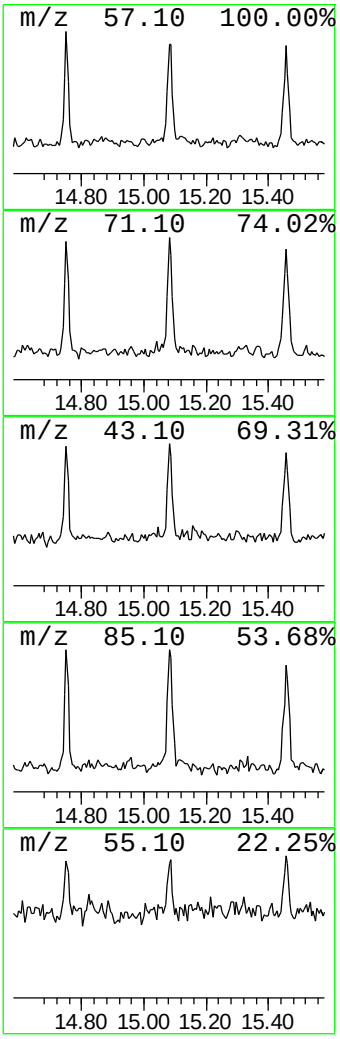
Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.08	2.52 ng	101241	Perylene-d12	15.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	Eicosane	282	C20H42	000112-95-8	90
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	80





Tentatively Identified Compound (LSC) summary

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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...	2.12	4.4	ng	174461	1	6.83	798178	20.0
2-Pentanone, 4-hy...	5.06	4.4	ng	176813	1	6.83	798178	20.0
unknown6.61	6.61	100.4	ng	4005060	1	6.83	798178	20.0
n-Hexadecanoic acid	11.87	4.4	ng	197149	4	11.36	896930	20.0
5-Eicosene, (E)-	13.83	9.1	ng	364943	5	14.00	800334	20.0
Tricosane	14.44	2.8	ng	111780	5	14.00	800334	20.0
Heneicosane	15.08	2.5	ng	101241	6	15.47	803075	20.0