LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021519\
Data File : BF112583.D
Acq On : 15 Feb 2019 17:19
Operator : JU/SJ
Sample : K1484-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2-D

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	5.040	498	502	517	rBV	56170	75330	2.74%	0.367%
2	5.463	571	574	596	rBV	1304141	1464210	53.18%	7.126%
3	6.481	743	747	765	rBV	1514295	1593927	57.89%	7.758%
4	6.610	765	769	780	rVB	1760236	1696649	61.62%	8.258%
5	6.828	803	806	816	rBV	563493	498984	18.12%	2.429%
6	6.987	829	833	849	rBV	1583335	1304075	47.36%	6.347%
7	7.392	898	902	915	rBV	1008454	1005474	36.52%	4.894%
8	8.116	1021	1025	1043	rBV	628872	658362	23.91%	3.204%
9	9.186	1203	1207	1217	rBV	2420477	2024468	73.52%	9.853%
10	9.581	1270	1274	1280	rBV	90869	80733	2.93%	0.393%
11	9.869	1319	1323	1337	rVB	941349	840700	30.53%	4.092%
12	10.663	1454	1458	1470	rBV	1542128	1582530	57.47%	7.702%
13	11.363	1573	1577	1585	rBV	1038910	973969	35.37%	4.740%
14	11.874	1661	1664	1682	rBV2	183954	241966	8.79%	1.178%
15	12.663	1794	1798	1803	rBV	59477	74788	2.72%	0.364%
16	12.945	1841	1846	1849	rBV	2991511	2753565	100.00%	13.402%
17	13.827	1993	1996	2004	rBV	148737	174678	6.34%	0.850%
18	14.010	2023	2027	2034	rBV	1178883	1172179	42.57%	5.705%
19	14.145	2047	2050	2054	rBV	82939	75839	2.75%	0.369%
20	14.451	2098	2102	2107	rBV	131807	137279	4.99%	0.668%
21	14.751	2150	2153	2158	rVB	162631	166214	6.04%	0.809%
22	14.827	2163	2166	2170	rVB	55837	53317	1.94%	0.259%
23	15.086	2206	2210	2216	rVB	192374	214339	7.78%	1.043%
24	15.463	2269	2274	2275	rBV	177408	228994	8.32%	1.115%
25	15.492	2275	2279	2287	rVB	845589	1075436	39.06%	5.234%
26	15.892	2342	2347	2353	rVB	150154	223253	8.11%	1.087%
27	16.386	2426	2431	2439	rVB	87781	155015	5.63%	0.754%

Sum of corrected areas: 20546273

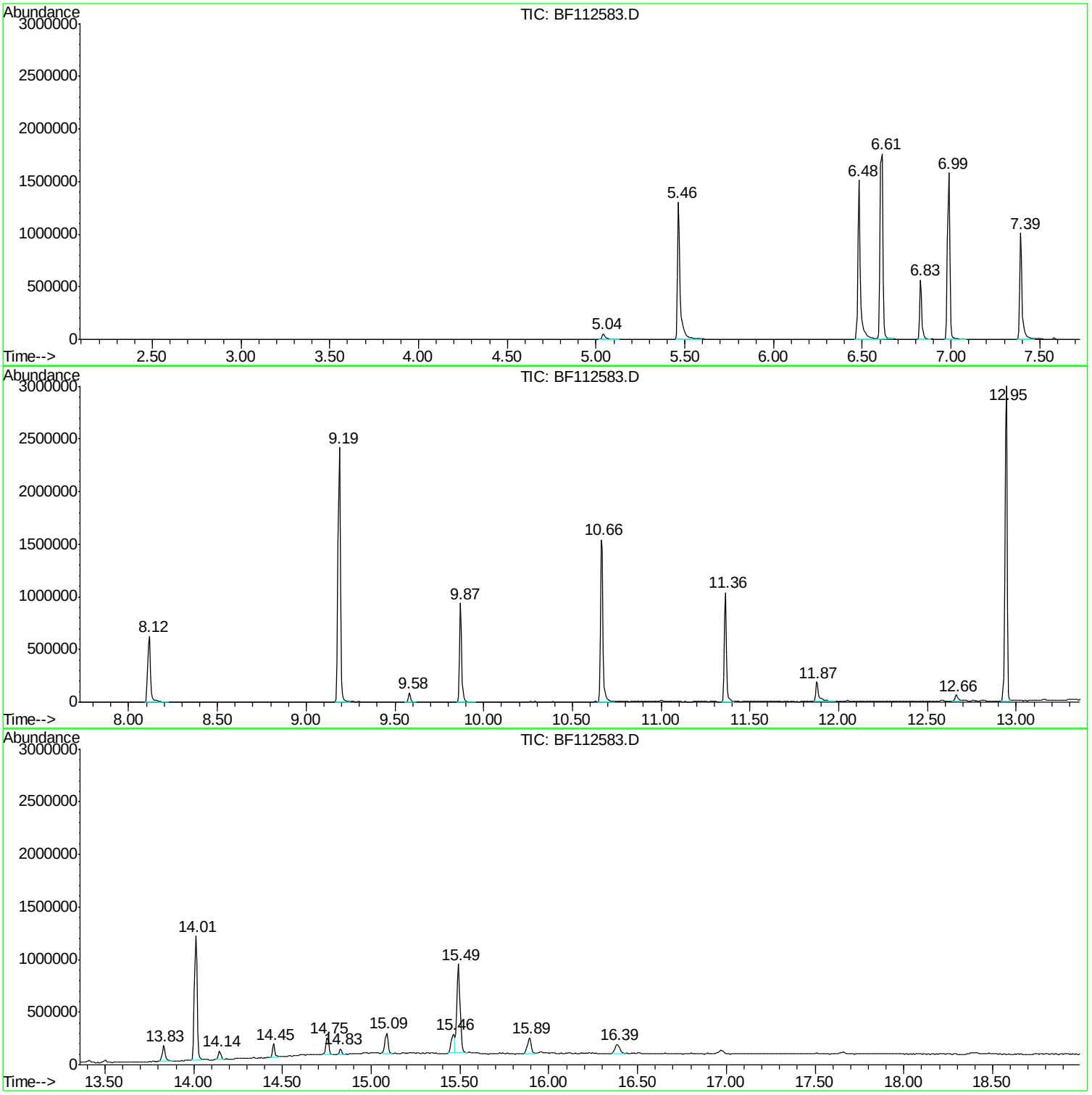
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021519\
Data File : BF112583.D
Acq On : 15 Feb 2019 17:19
Operator : JU/SJ
Sample : K1484-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2-D

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\BF021519\
Data File : BF112583.D
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Instrument : BNA_F
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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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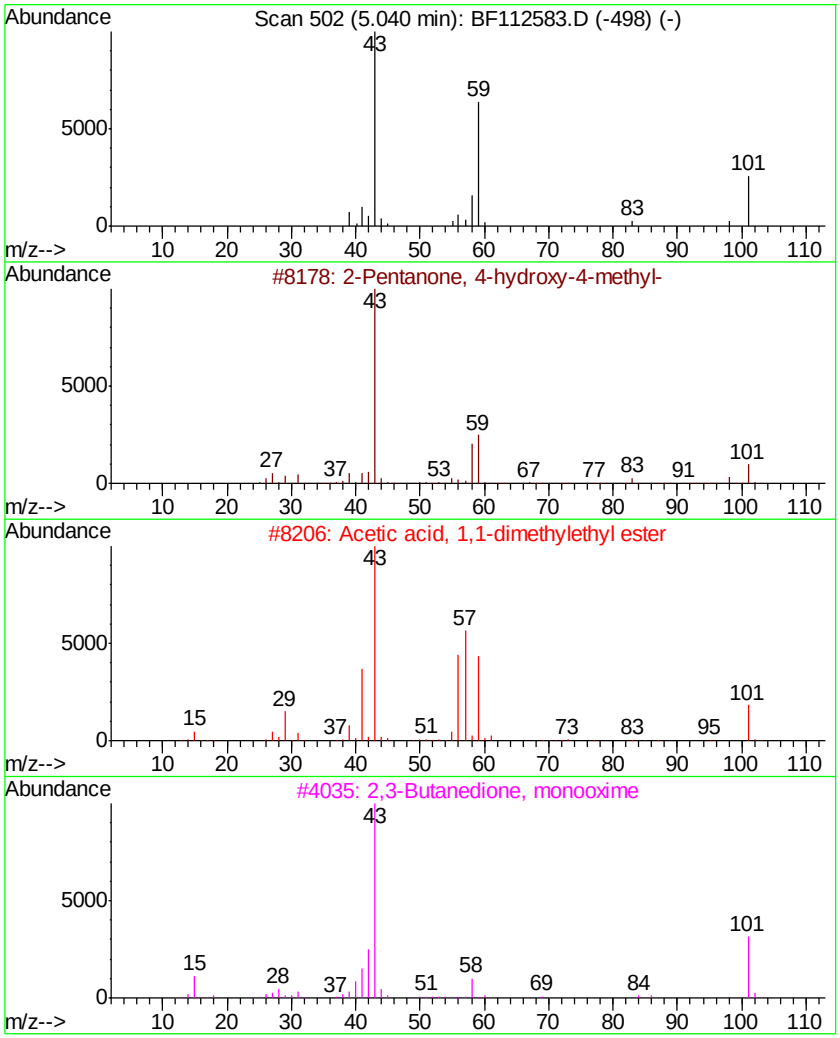
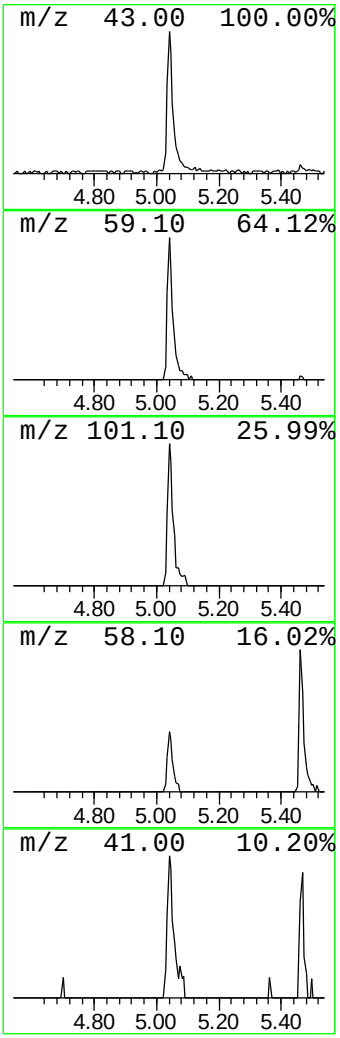
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	3.02 ng	75330	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	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25





Library Search Compound Report

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Data File : BF112583.D
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Operator : JU/SJ
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2-D

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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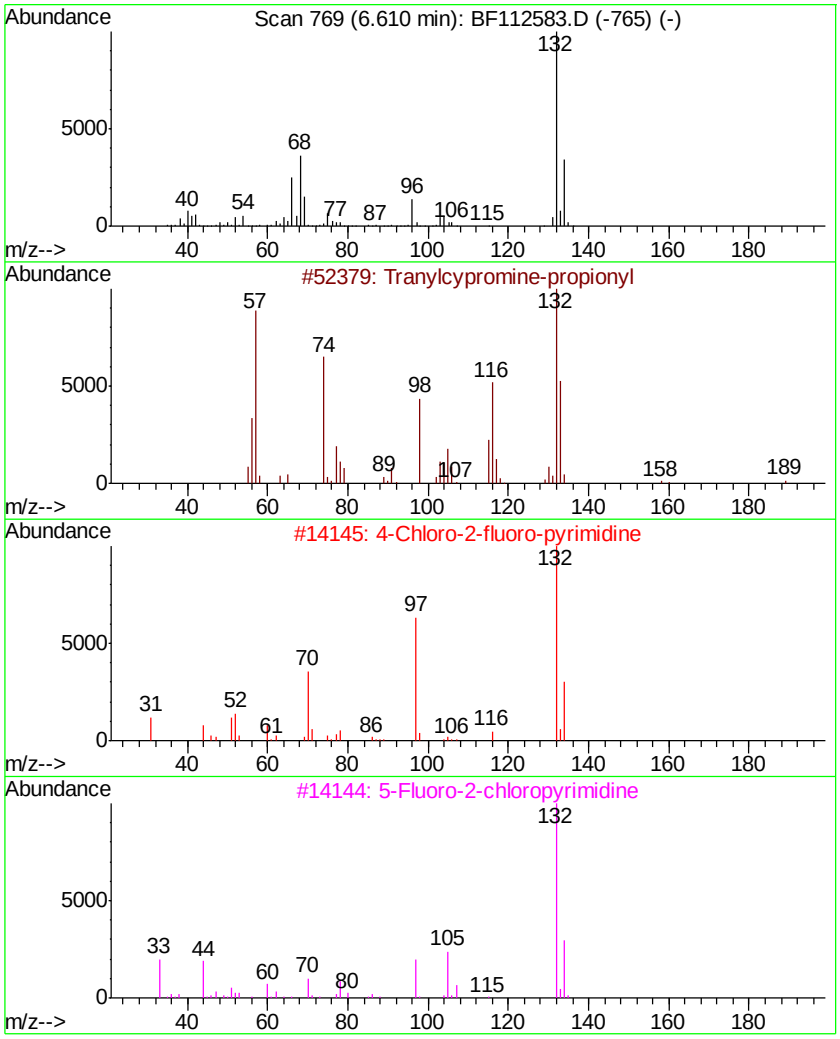
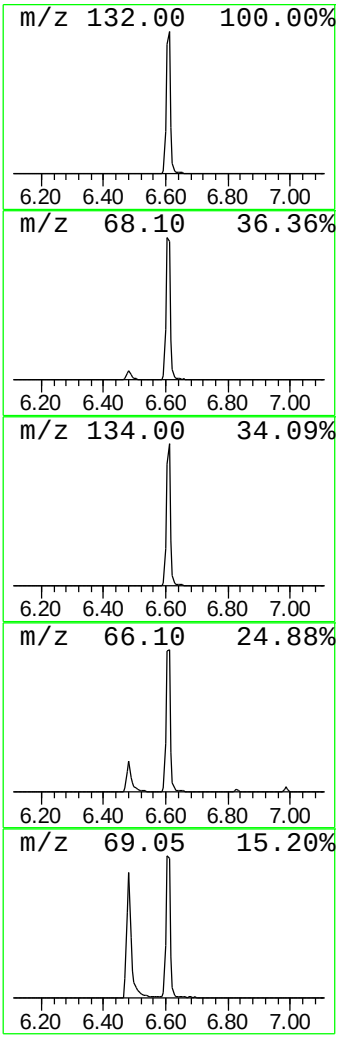
Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	68.00 ng	1696650	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
2	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Library Search Compound Report

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Data File : BF112583.D
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Operator : JU/SJ
Sample : K1484-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2-D

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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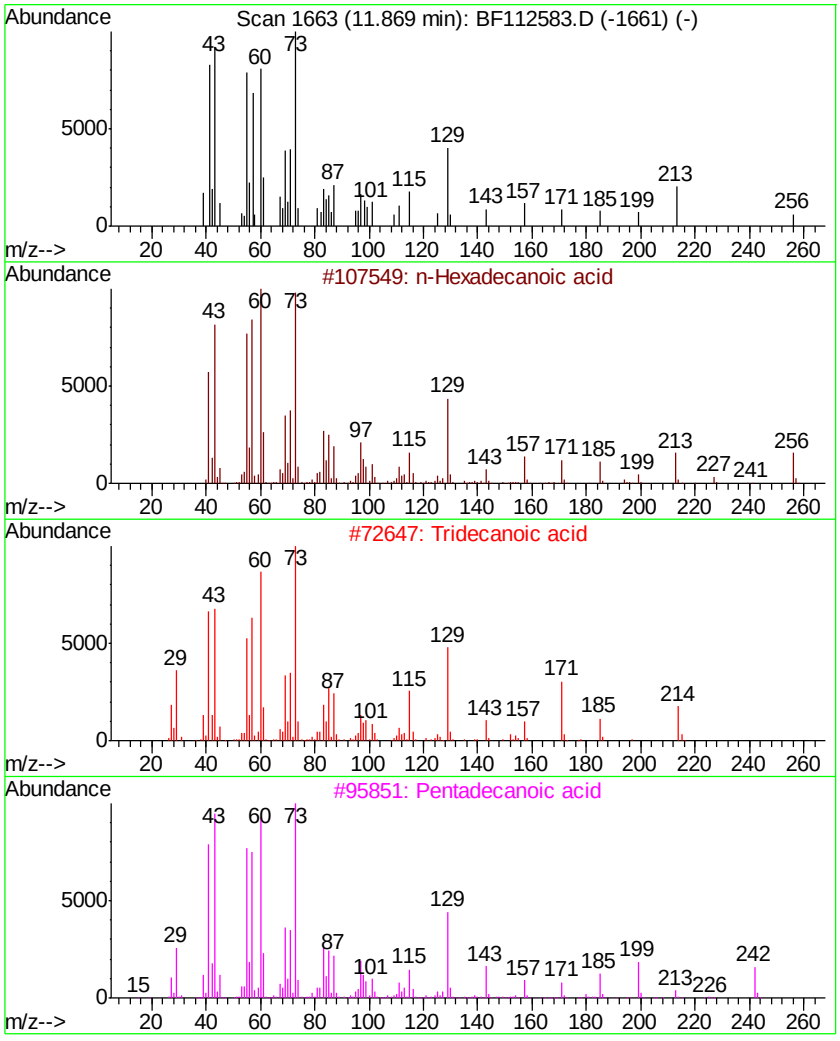
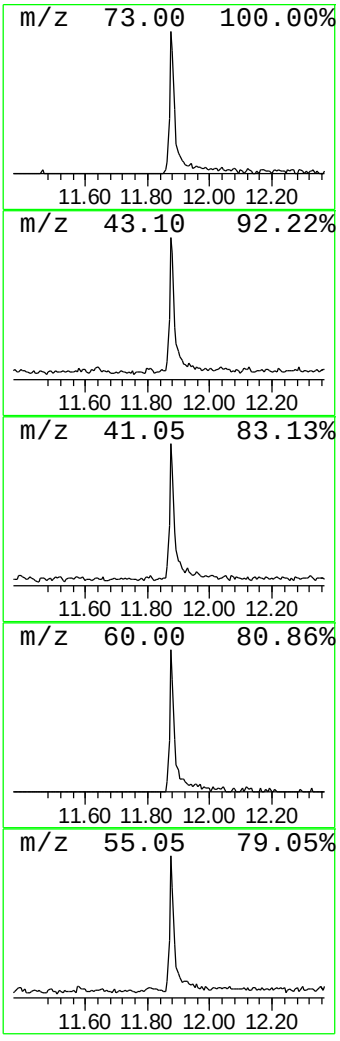
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	4.97 ng	241966	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	97
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Library Search Compound Report

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Data File : BF112583.D
Acq On : 15 Feb 2019 17:19
Operator : JU/SJ
Sample : K1484-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2-D

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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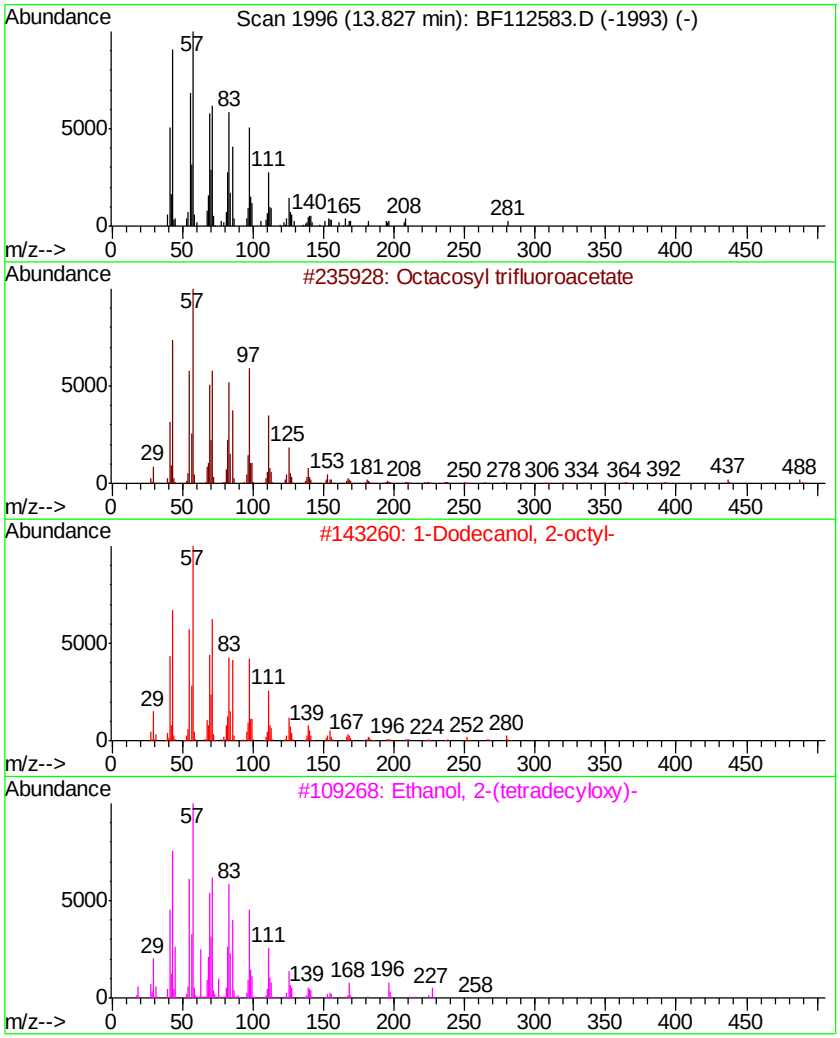
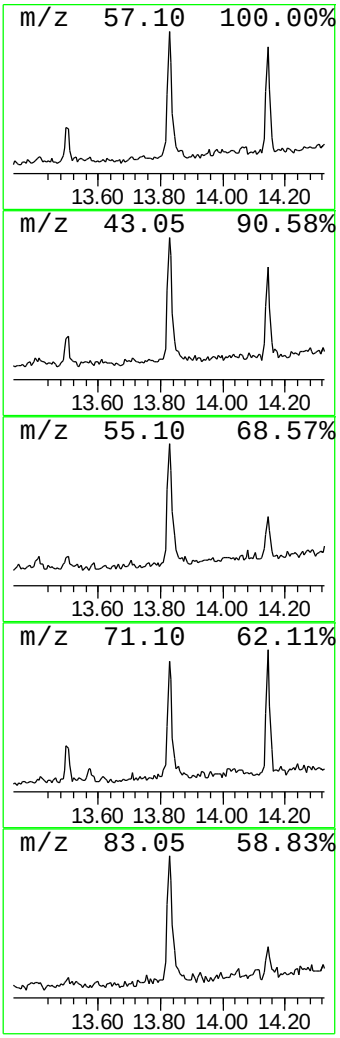
Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.98 ng	174678	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
4	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87
5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87





Library Search Compound Report

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Operator : JU/SJ
Sample : K1484-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2-D

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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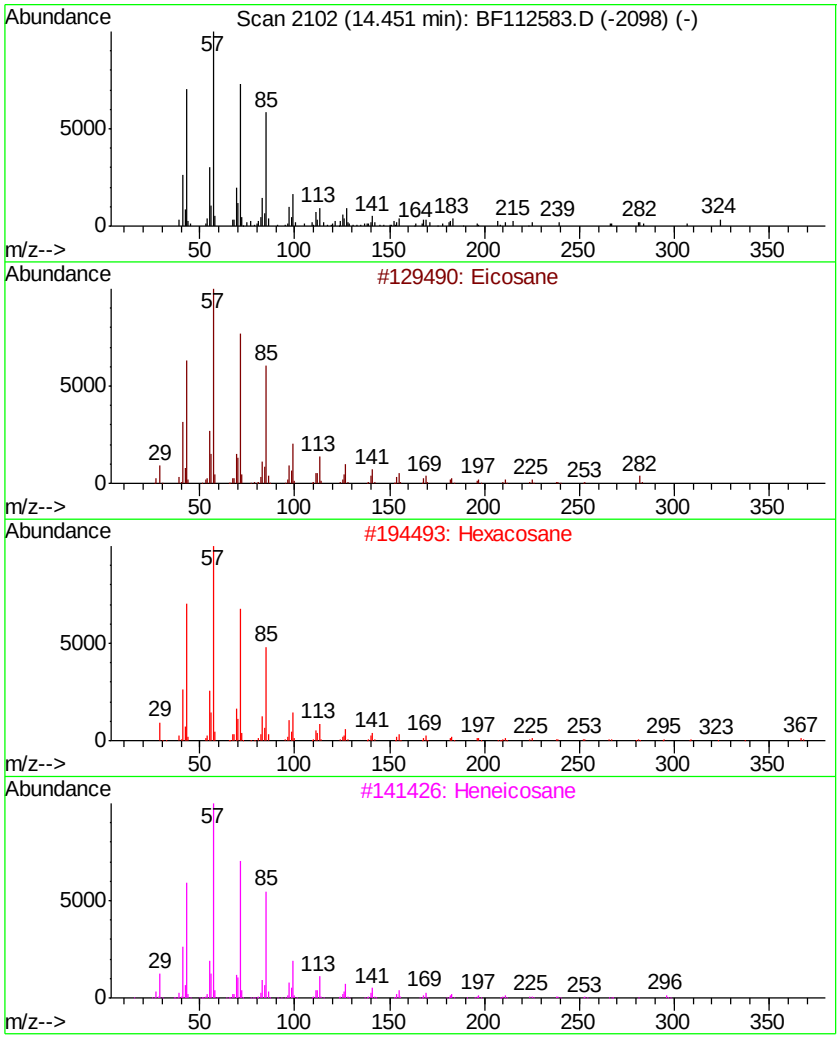
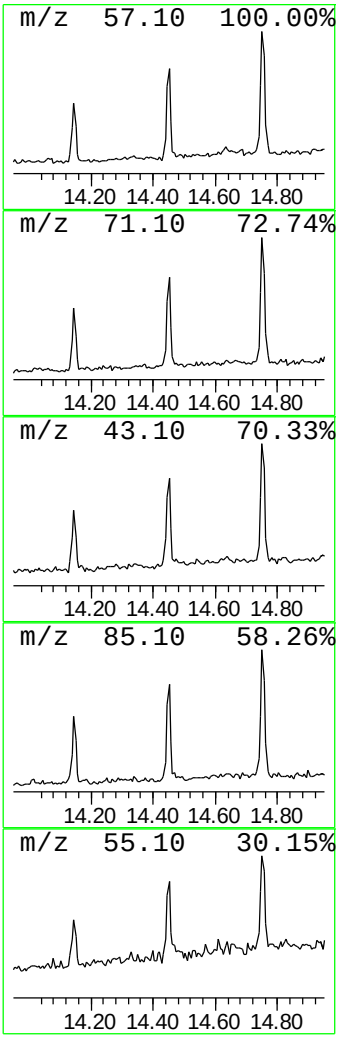
Peak Number 6 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.34 ng	137279	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2-D

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

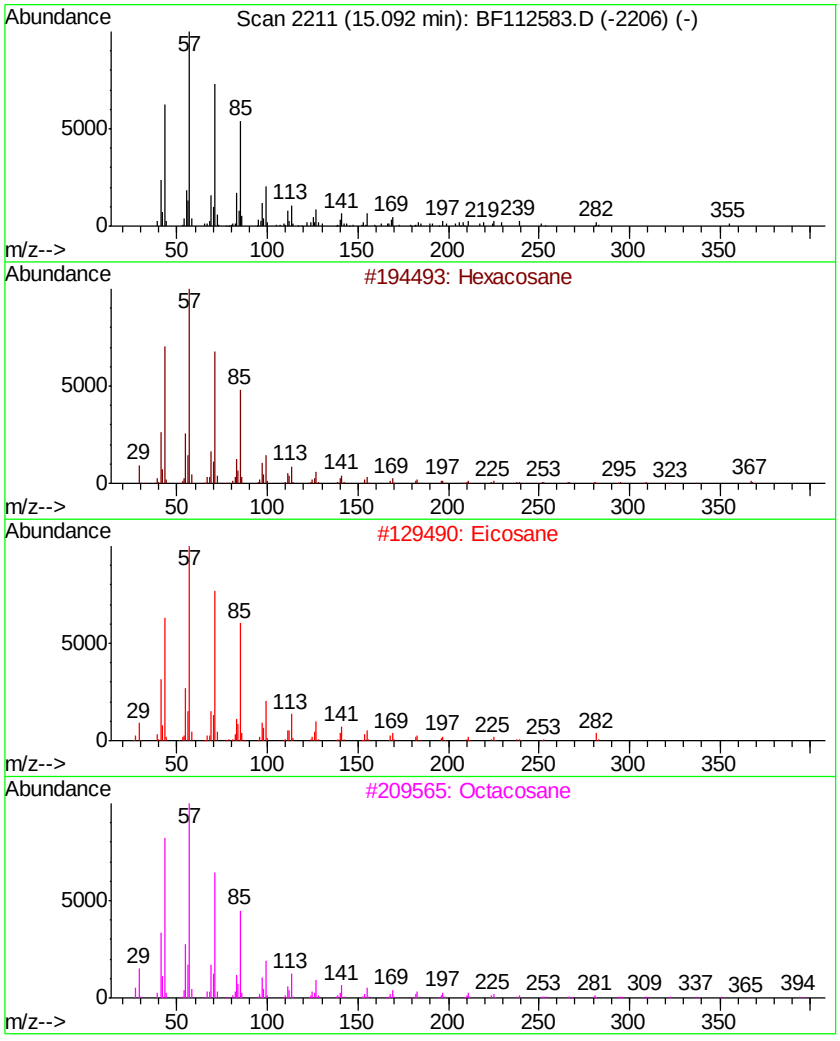
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

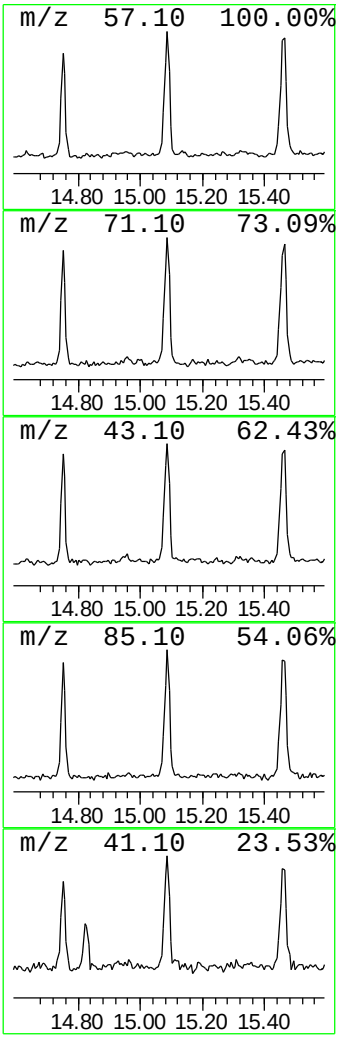
****

Peak Number 8 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	3.99 ng	214339	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Eicosane	282	C20H42	000112-95-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90





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Misc :
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Instrument : BNA_F
ClientSampleId : M-2-D

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

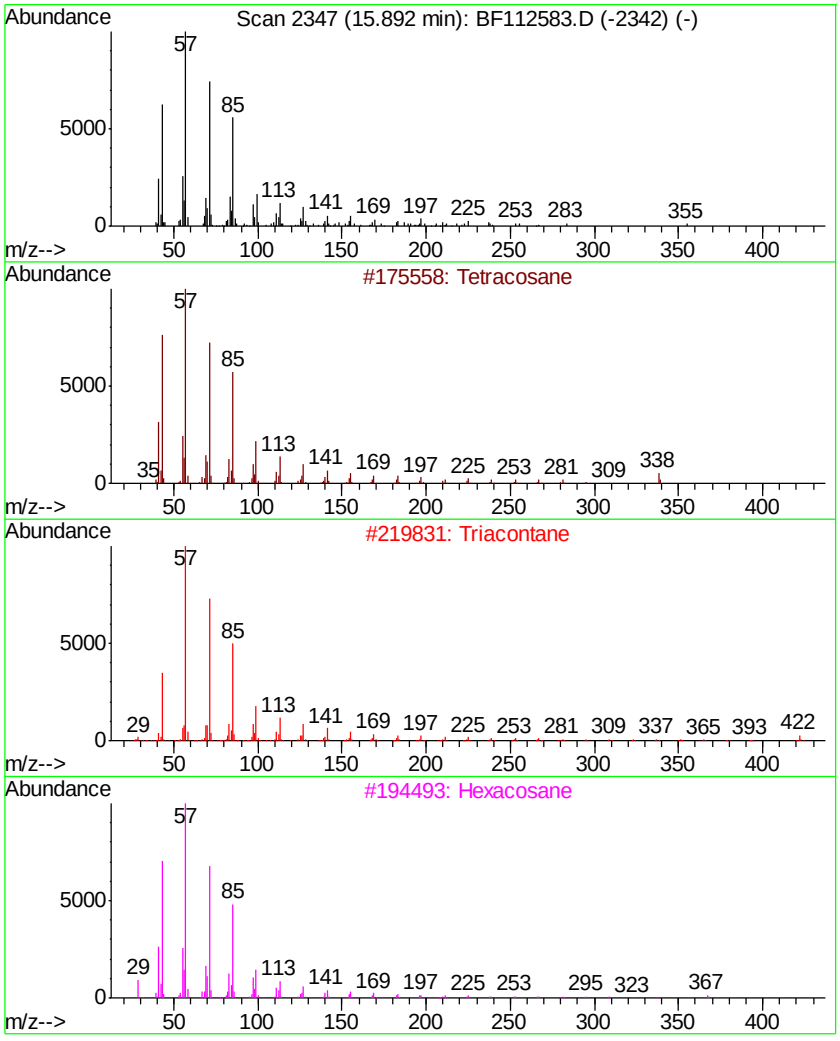
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

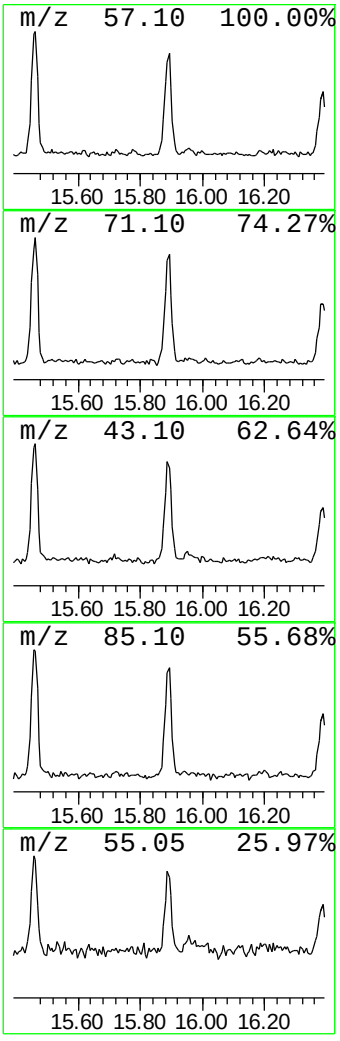
****

Peak Number 9 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.89	4.15 ng	223253	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Docosane	310	C22H46	000629-97-0	91





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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-2-D

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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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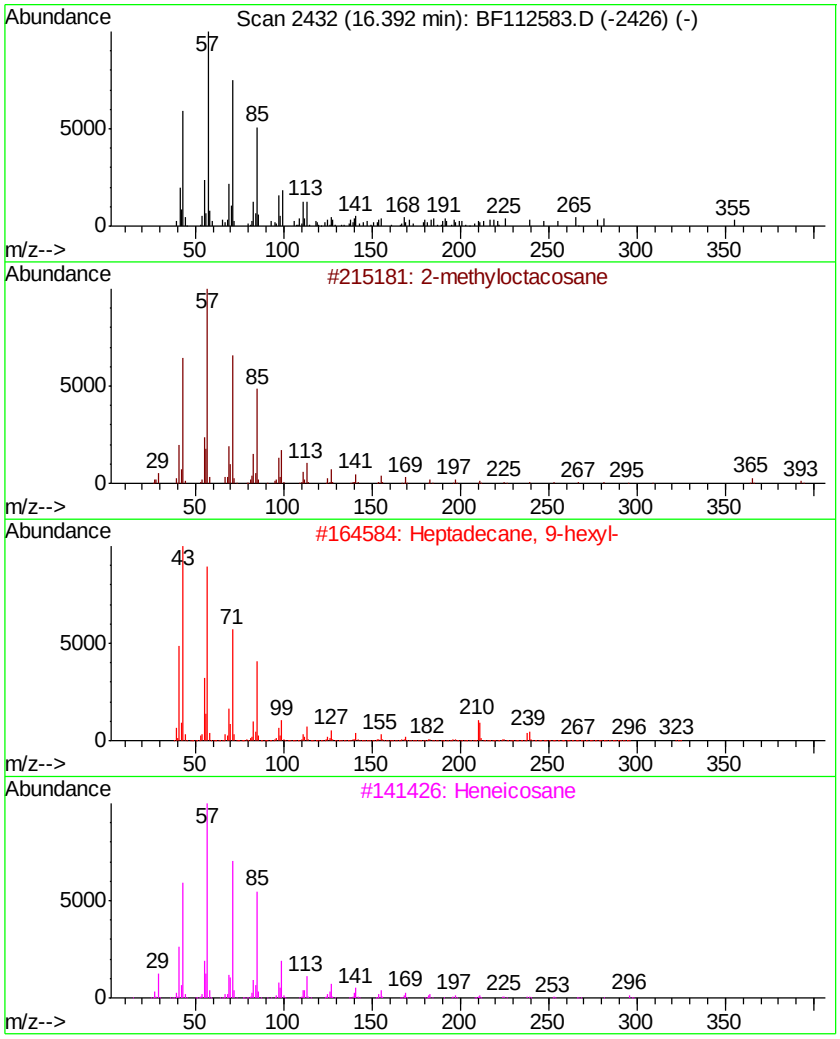
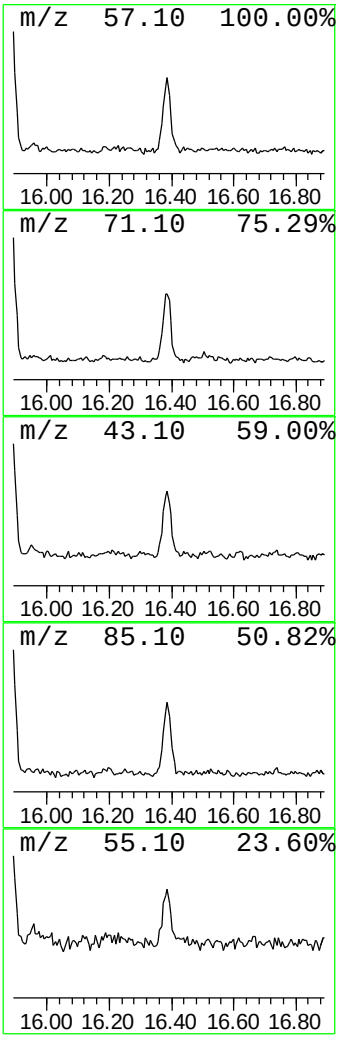
Peak Number 10 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.39	2.88 ng	155015	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	86
2	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	80
3	Heneicosane	296	C21H44	000629-94-7	72
4	Tetratetracontane	619	C44H90	007098-22-8	64
5	Heptadecane, 2-methyl-	254	C18H38	001560-89-0	64





Tentatively Identified Compound (LSC) summary

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Data File : BF112583.D
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Instrument : BNA_F
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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...	5.04	3.0	ng	75330	1	6.83	498984	20.0
unknown6.61	6.61	68.0	ng	1696650	1	6.83	498984	20.0
n-Hexadecanoic acid	11.87	5.0	ng	241966	4	11.36	973969	20.0
Octacosyl trifluo...	13.83	3.0	ng	174678	5	14.01	1172180	20.0
Eicosane	14.45	2.3	ng	137279	5	14.01	1172180	20.0
Hexacosane	15.09	4.0	ng	214339	6	15.49	1075440	20.0
Tetracosane	15.89	4.2	ng	223253	6	15.49	1075440	20.0
2-methyloctacosane	16.39	2.9	ng	155015	6	15.49	1075440	20.0