LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.205	16	20	30	rVB	264852	352551	7.09%	1.201%
2	5.128	514	517	527	rVB	216698	238413	4.80%	0.812%
3	5.522	580	584	588	rBV	1545921	1491555	30.01%	5.082%
4	6.528	750	755	758	rBV	1200662	994841	20.02%	3.389%
5	6.681	776	781	784	rBV	2898116	2643849	53.20%	9.008%
6	6.910	817	820	824	rBV	974599	819315	16.49%	2.791%
7	7.069	843	847	851	rBV	3516230	3393669	68.29%	11.562%
8	7.475	910	916	919	rBV	2529860	2852730	57.40%	9.719%
9	8.192	1034	1038	1042	rBV	1343701	1106871	22.27%	3.771%
10	9.210	1208	1211	1216	rVB	59345	51799	1.04%	0.176%
11	9.269	1216	1221	1225	rBV	4577711	4969514	100.00%	16.931%
12	9.657	1284	1287	1291	rBV3	166041	183871	3.70%	0.626%
13	9.951	1333	1337	1340	rVB	1363751	1170537	23.55%	3.988%
14	10.592	1439	1446	1453	rBV	82189	90787	1.83%	0.309%
15	10.739	1466	1471	1474	rBV	1973054	1873028	37.69%	6.382%
16	10.857	1486	1491	1498	rVB	108628	130390	2.62%	0.444%
17	11.433	1585	1589	1593	rBV	1298189	1108197	22.30%	3.776%
18	13.021	1854	1859	1862	rBV	3759640	3867088	77.82%	13.175%
19	14.074	2034	2038	2041	rBV	781349	695529	14.00%	2.370%
20	15.562	2285	2291	2303	rVB	515610	735394	14.80%	2.506%
21	16.021	2364	2369	2375	rBV	68202	100537	2.02%	0.343%
22	16.545	2452	2458	2466	rVB	77193	137408	2.77%	0.468%
23	17.156	2554	2562	2571	rBV3	59475	134564	2.71%	0.458%
24	17.880	2678	2685	2692	rVB3	50930	113715	2.29%	0.387%
25	18.745	2824	2832	2844	rVB5	30156	94746	1.91%	0.323%

Sum of corrected areas: 29350898

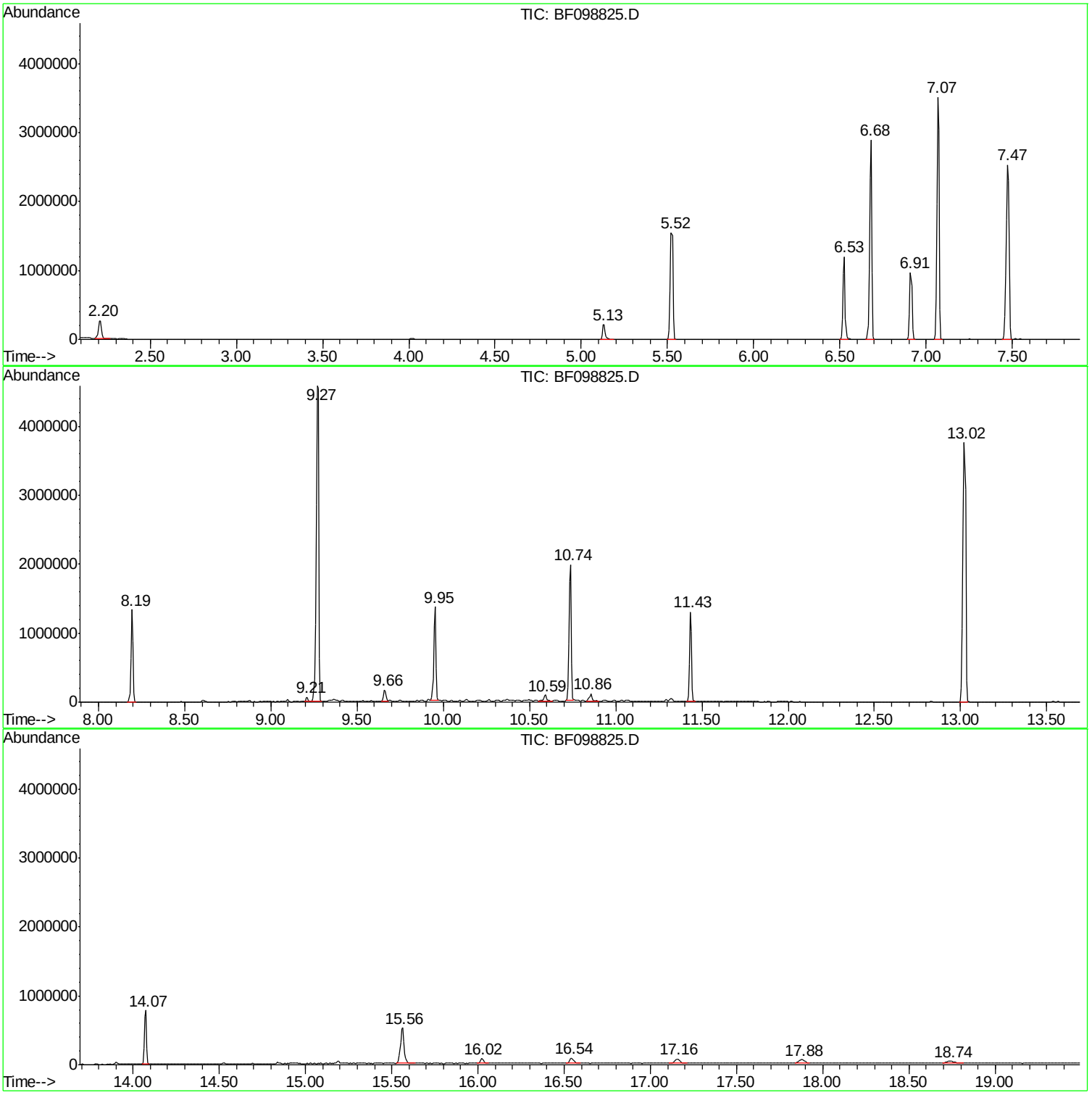
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

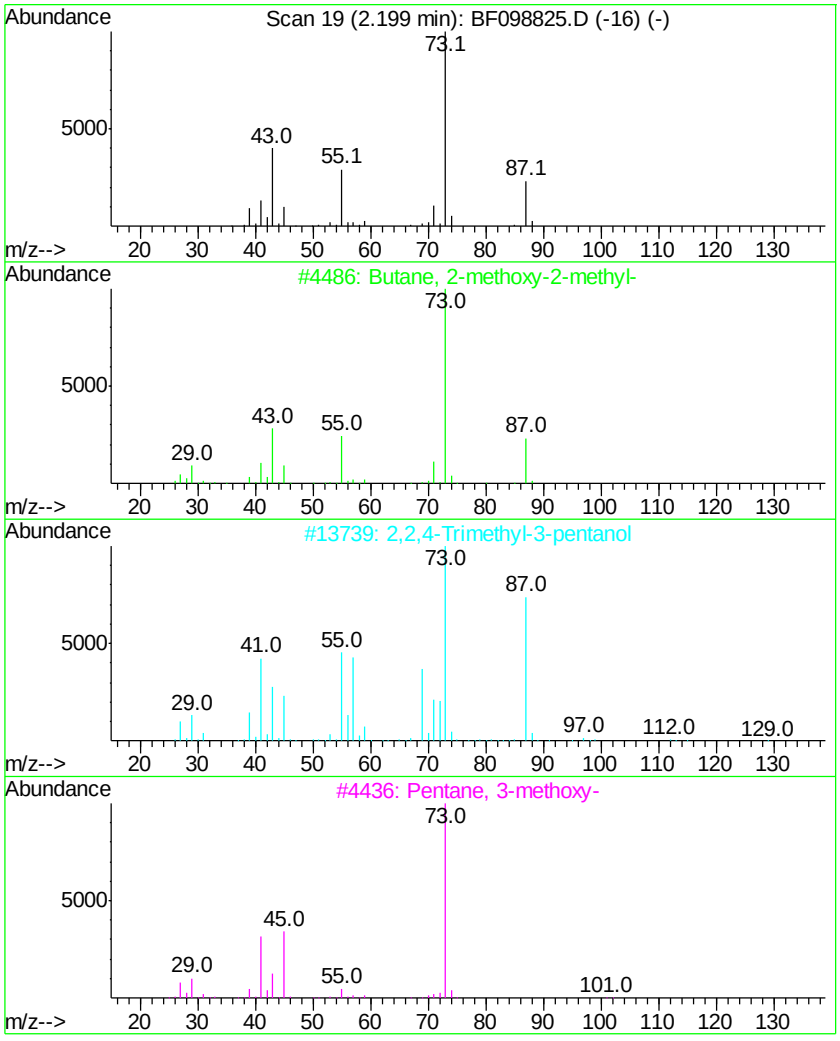
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

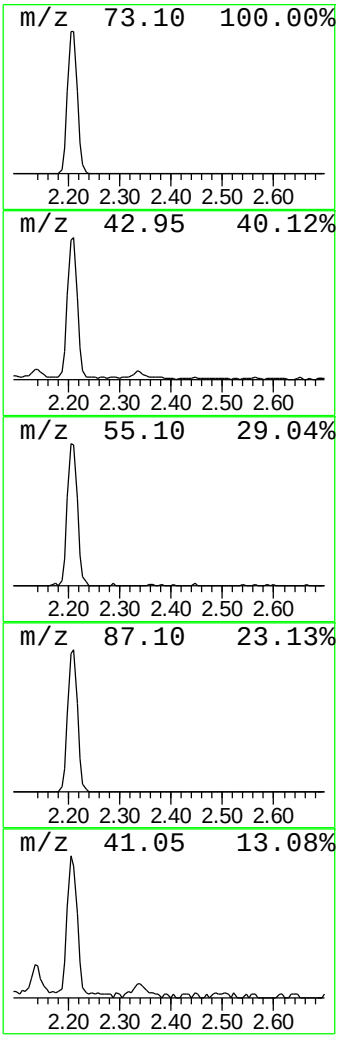
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	8.61 ng	352551	1,4-Dichlorobenzene-d4	6.91

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	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

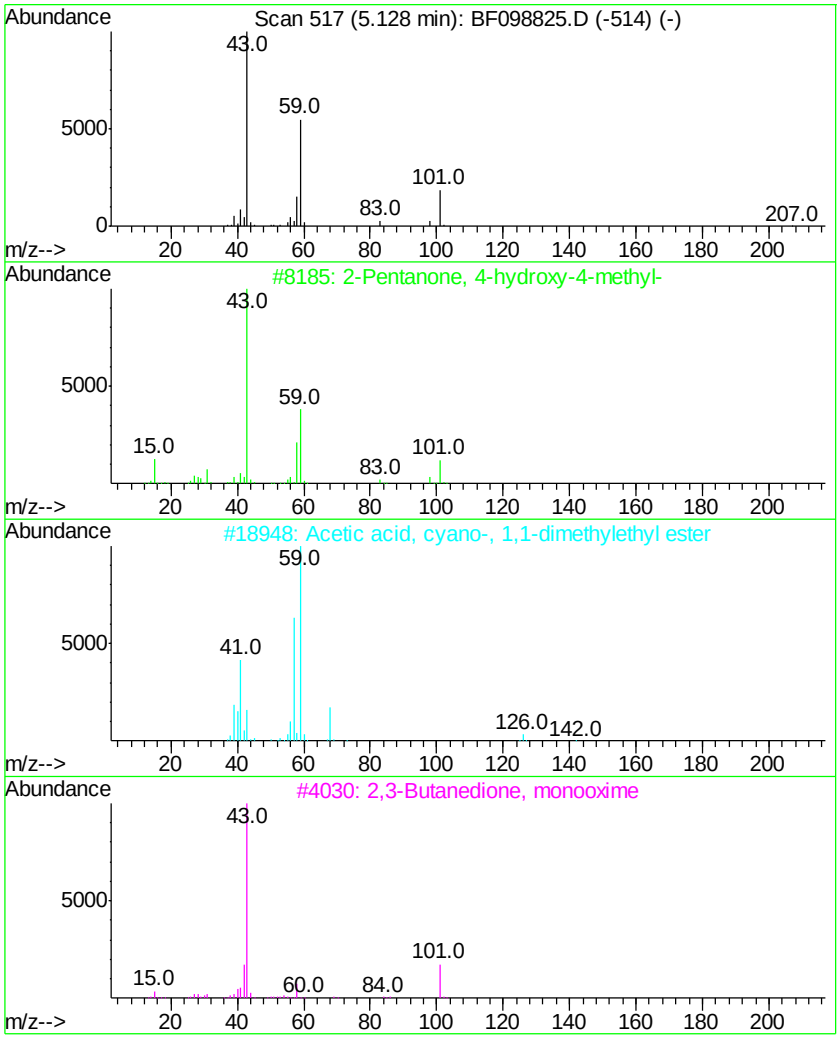
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

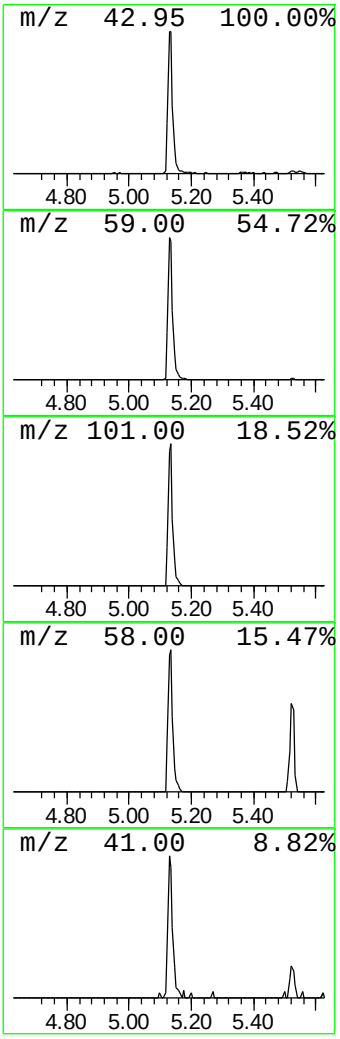
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	5.82 ng	238413	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

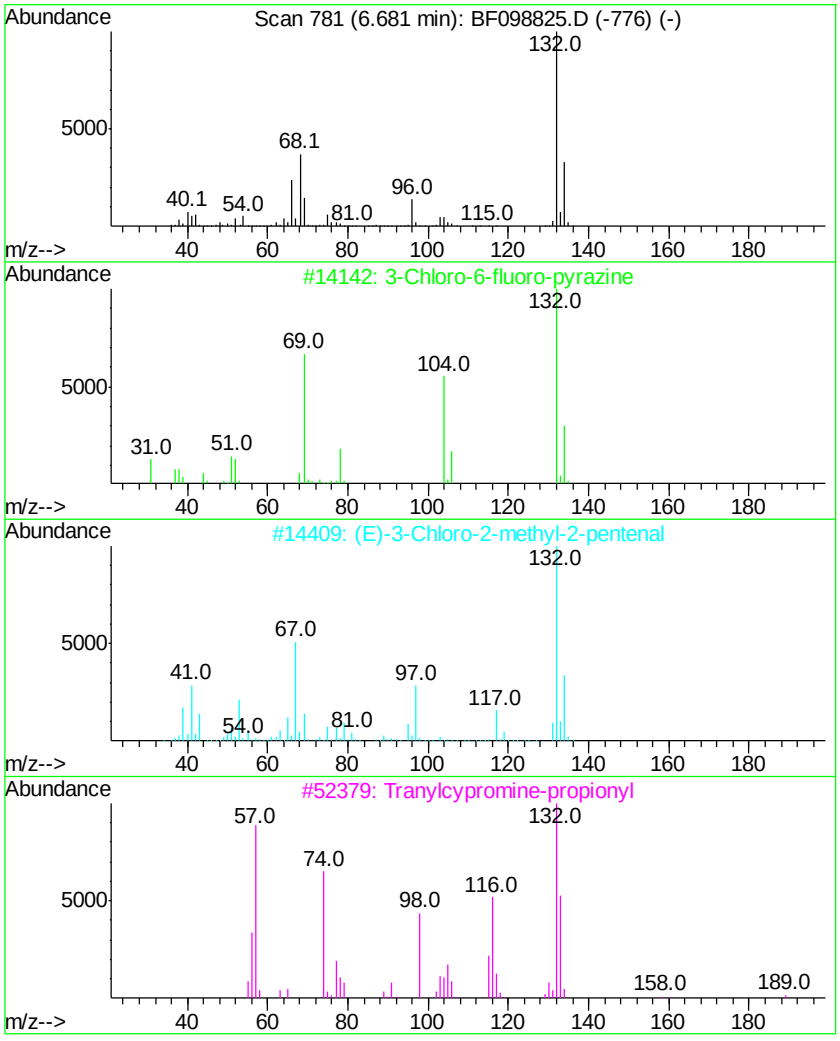
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

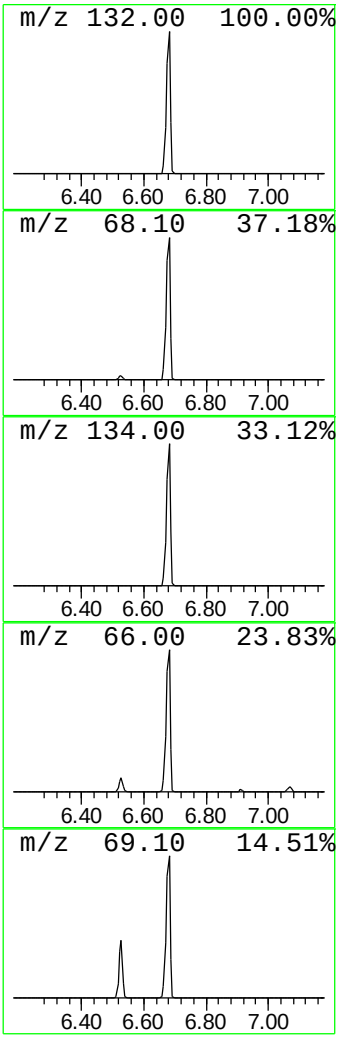
****

Peak Number 3 unknown6.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	64.54 ng	2643850	1,4-Dichlorobenzene-d4	6.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

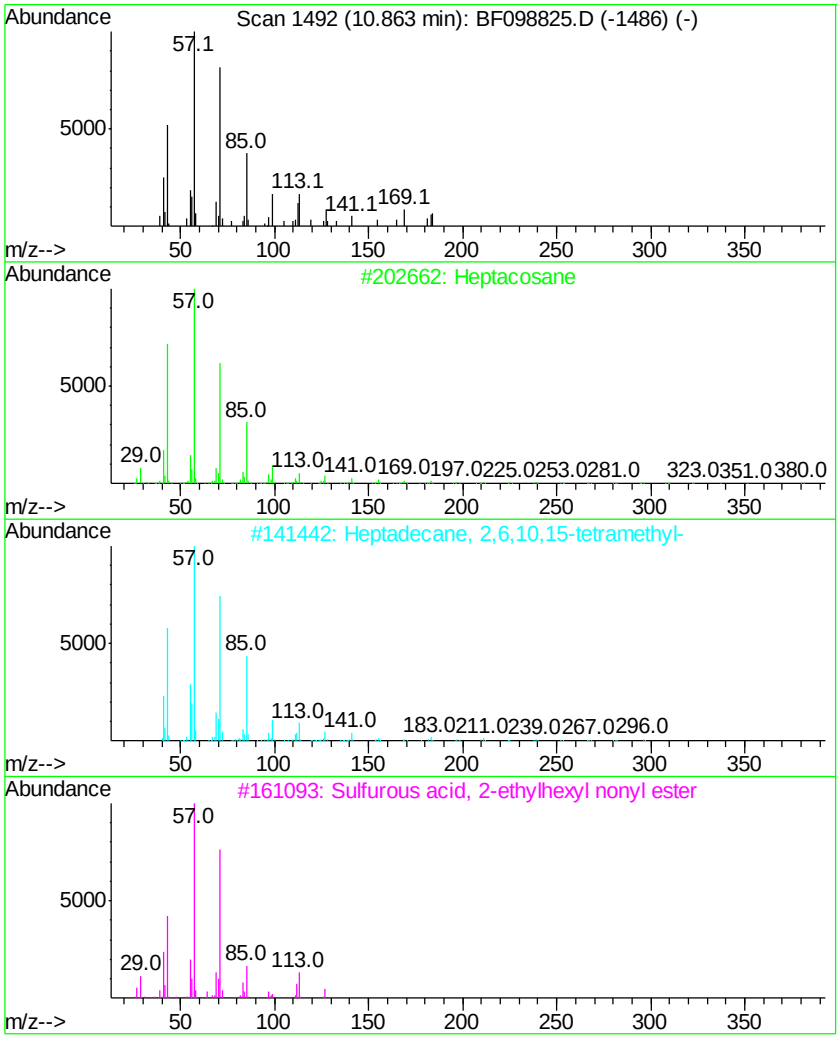
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

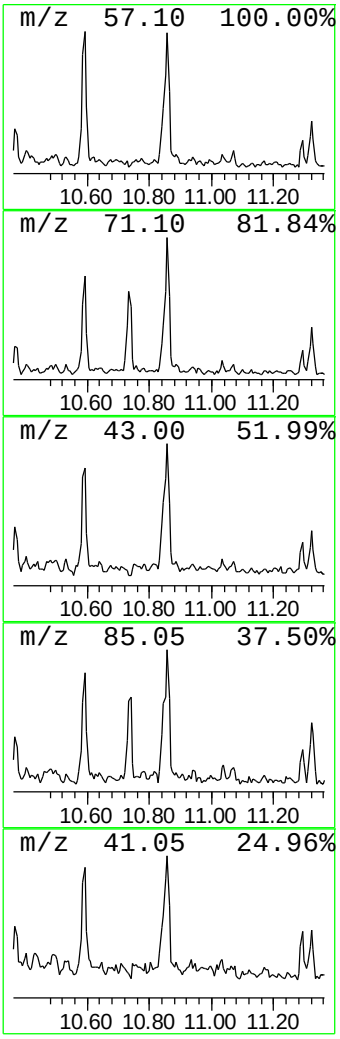
****

Peak Number 6 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	2.35 ng	130390	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	86
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
3	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1000309-19-2	64
4	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64
5	Sulfurous acid, dodecyl 2-ethylh...	362	C20H42O3S	1000309-19-5	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

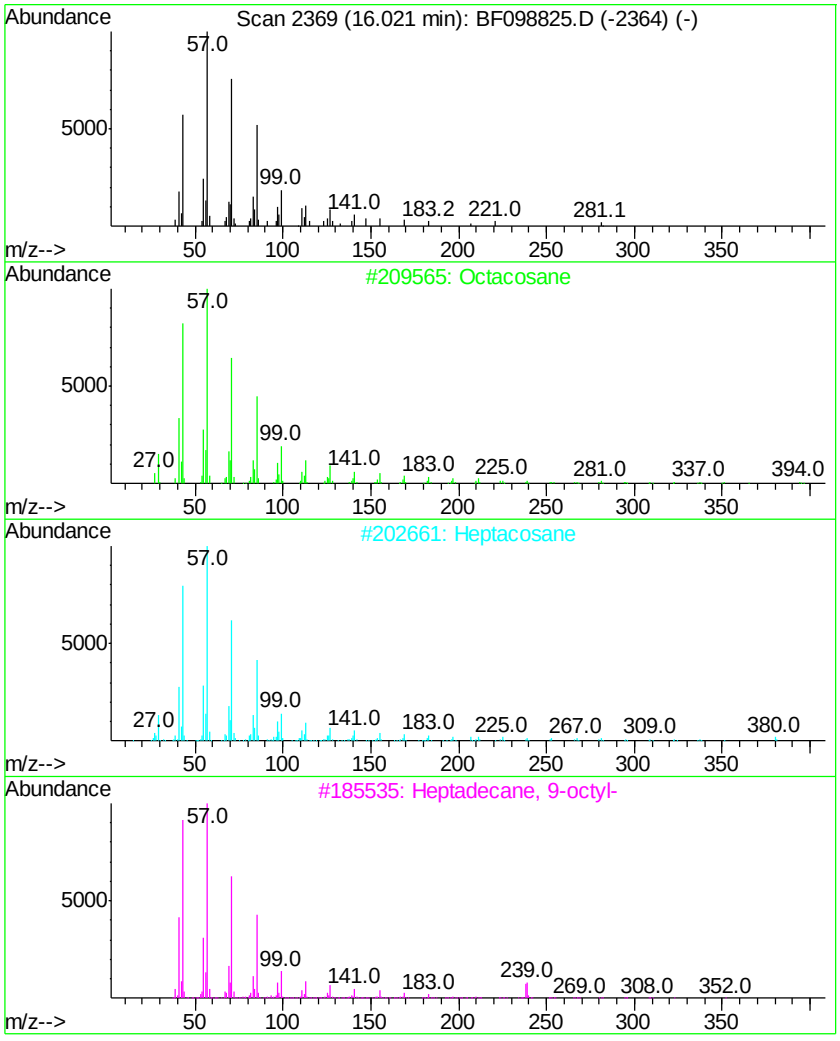
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

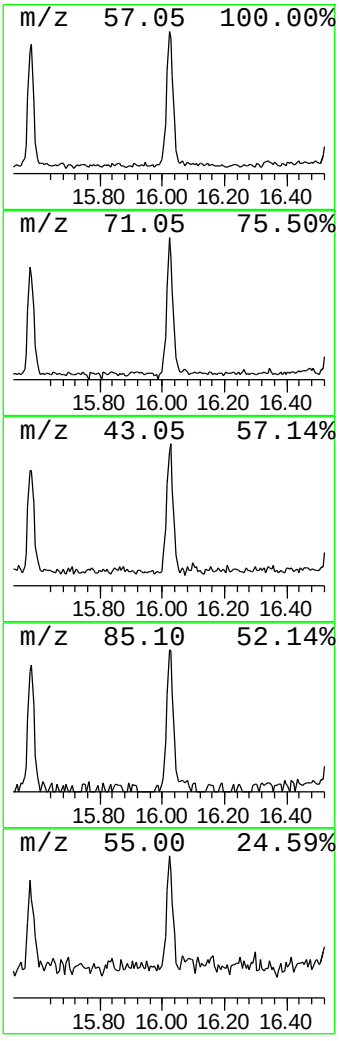
****

Peak Number 7 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.73 ng	100537	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Hexacosane	366	C26H54	000630-01-3	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

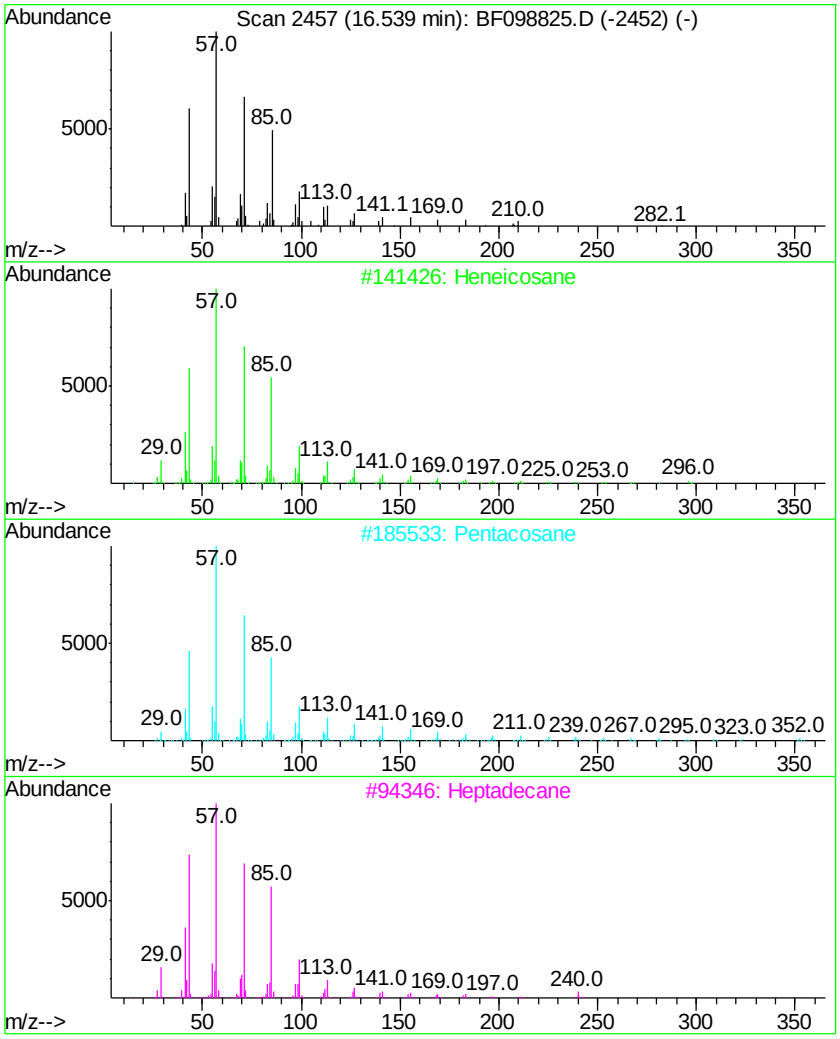
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

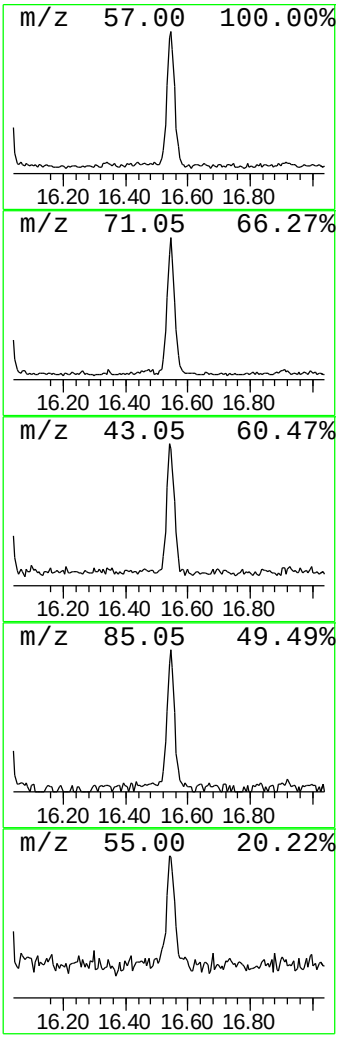
****

Peak Number 8 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.54	3.74 ng	137408	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

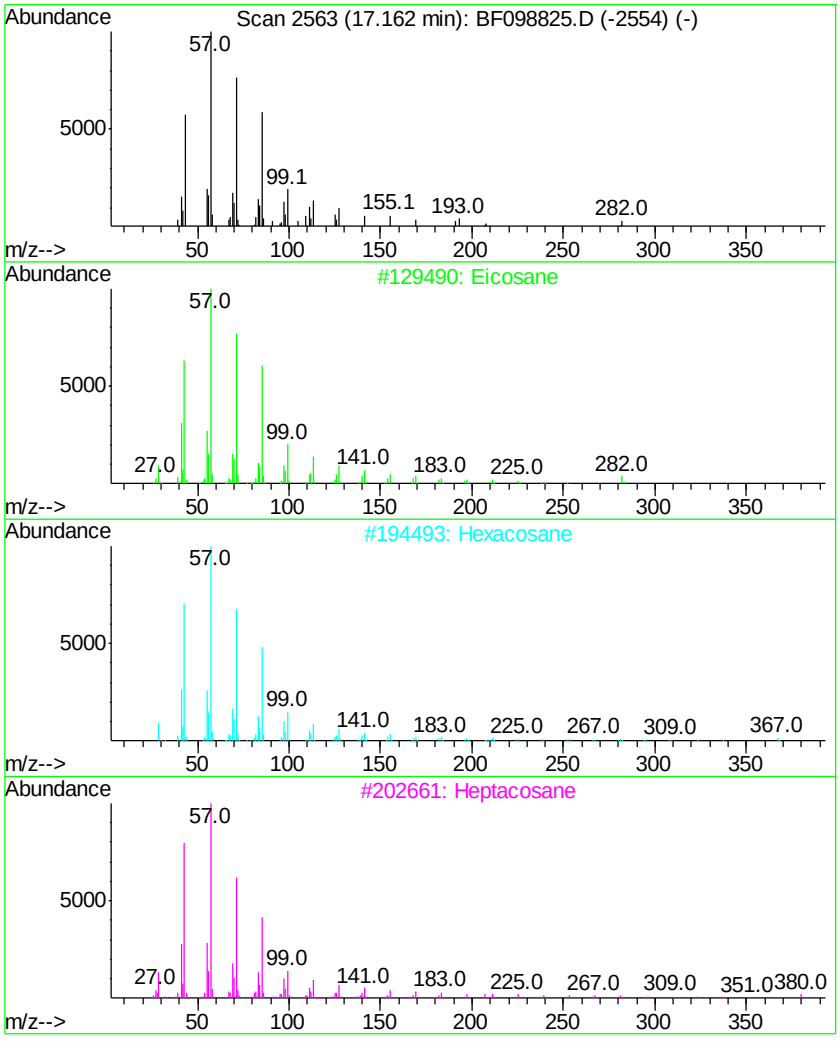
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

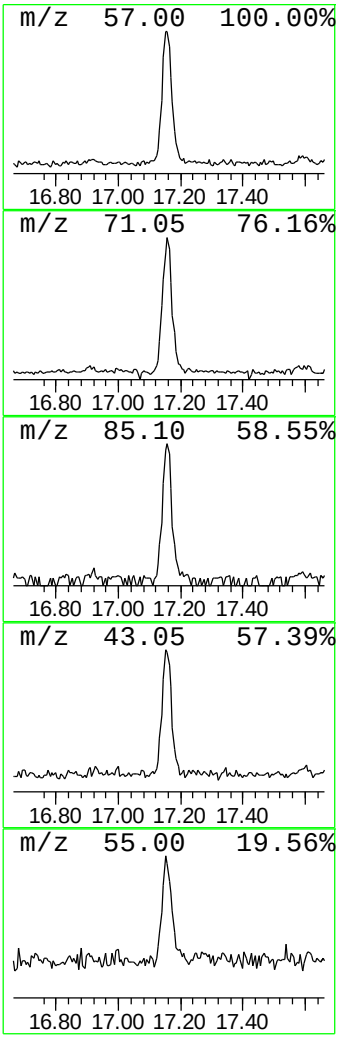
****

Peak Number 9 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	3.66 ng	134564	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Triacontane	422	C30H62	000638-68-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092517\
Data File : BF098825.D
Acq On : 26 Sep 2017 11:46
Operator : SJ/JU
Sample : I5385-08
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 092117-TIDO-F-U-M

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	2.20	8.6	ng	352551	1	6.91	819315	20.0
2-Pentanone, 4-hy...	5.13	5.8	ng	238413	1	6.91	819315	20.0
unknown6.68	6.68	64.5	ng	2643850	1	6.91	819315	20.0
Heptacosane	10.86	2.4	ng	130390	4	11.43	1108200	20.0
Octacosane	16.02	2.7	ng	100537	6	15.56	735394	20.0
Heneicosane	16.54	3.7	ng	137408	6	15.56	735394	20.0
Eicosane	17.16	3.7	ng	134564	6	15.56	735394	20.0