LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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	4.925	436	440	448	rVB	132065	142657	3.23%	0.513%
2	5.348	507	512	515	rBV	1449449	1354866	30.72%	4.876%
3	6.366	681	685	694	rBV	1208959	987947	22.40%	3.556%
4	6.507	705	709	712	rVB	2891893	2425088	54.99%	8.728%
5	6.737	745	748	752	rBV	1154335	930199	21.09%	3.348%
6	6.895	771	775	779	rBV	3757182	3363300	76.26%	12.105%
7	7.301	838	844	847	rBV	2777730	2672437	60.60%	9.619%
8	8.019	962	966	970	rBV	1356367	1079413	24.47%	3.885%
9	9.095	1145	1149	1152	rBV	4864416	4410296	100.00%	15.874%
10	9.483	1212	1215	1222	rBV	304693	255489	5.79%	0.920%
11	9.772	1260	1264	1268	rBV	1149215	1054052	23.90%	3.794%
12	10.448	1376	1379	1382	rBV	134445	96623	2.19%	0.348%
13	10.554	1393	1397	1407	rBV	1649003	1504127	34.10%	5.414%
14	11.248	1511	1515	1518	rBV	1085230	929315	21.07%	3.345%
15	12.830	1779	1784	1787	rBV	4215650	3789715	85.93%	13.640%
16	13.742	1935	1939	1946	rBV3	45217	68846	1.56%	0.248%
17	13.871	1957	1961	1965	rBV	1336546	1081881	24.53%	3.894%
18	14.654	2091	2094	2098	rBV	78455	77958	1.77%	0.281%
19	14.724	2102	2106	2110	rBV	371350	369711	8.38%	1.331%
20	14.977	2145	2149	2154	rBV	106995	119385	2.71%	0.430%
21	15.277	2196	2200	2205	rBV	615446	733007	16.62%	2.638%
22	15.336	2206	2210	2217	rVB	102143	137219	3.11%	0.494%
23	15.742	2275	2279	2284	rVB	85911	116685	2.65%	0.420%
24	16.212	2355	2359	2365	rVB2	50175	83460	1.89%	0.300%

Sum of corrected areas: 27783676

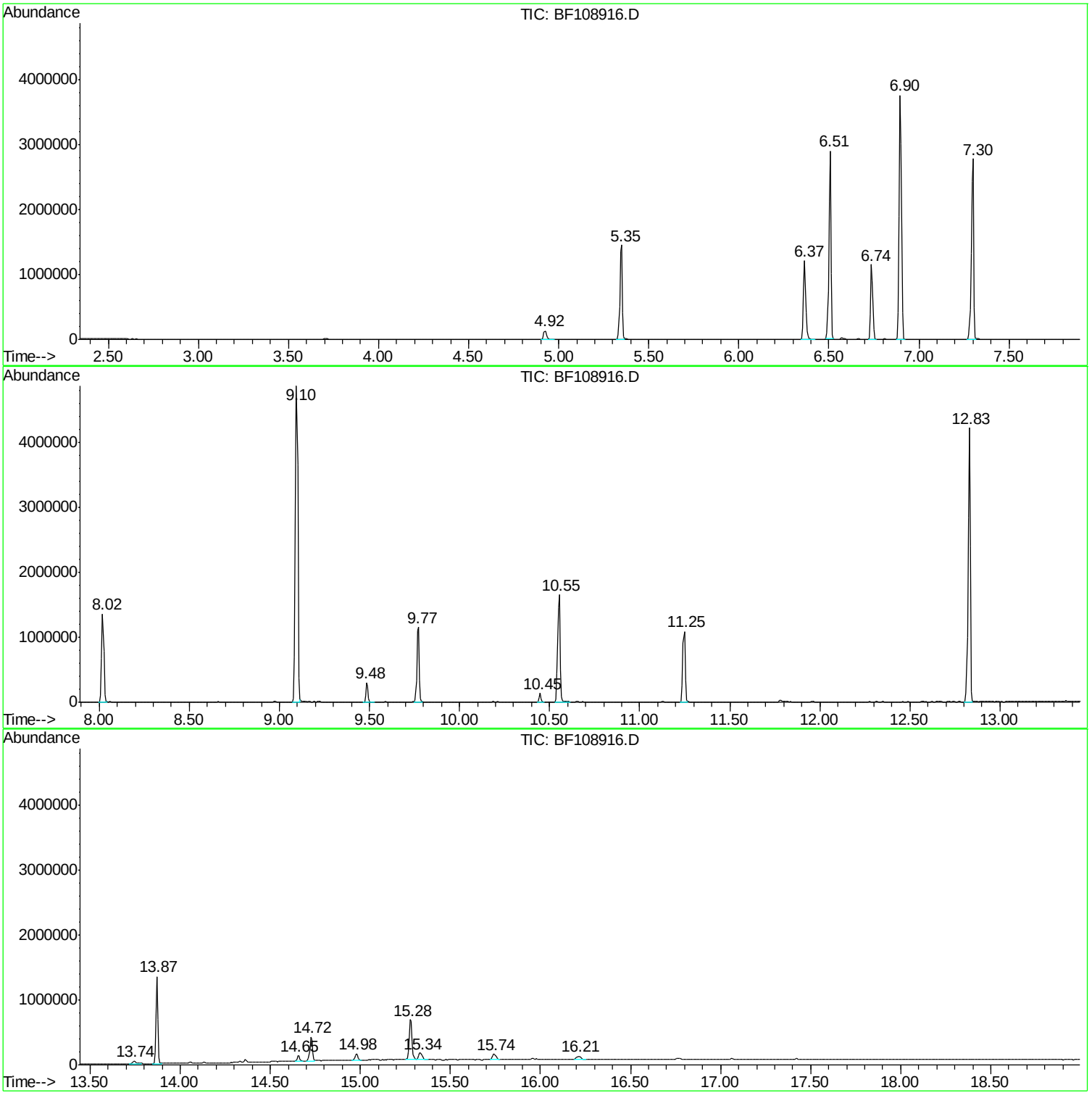
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

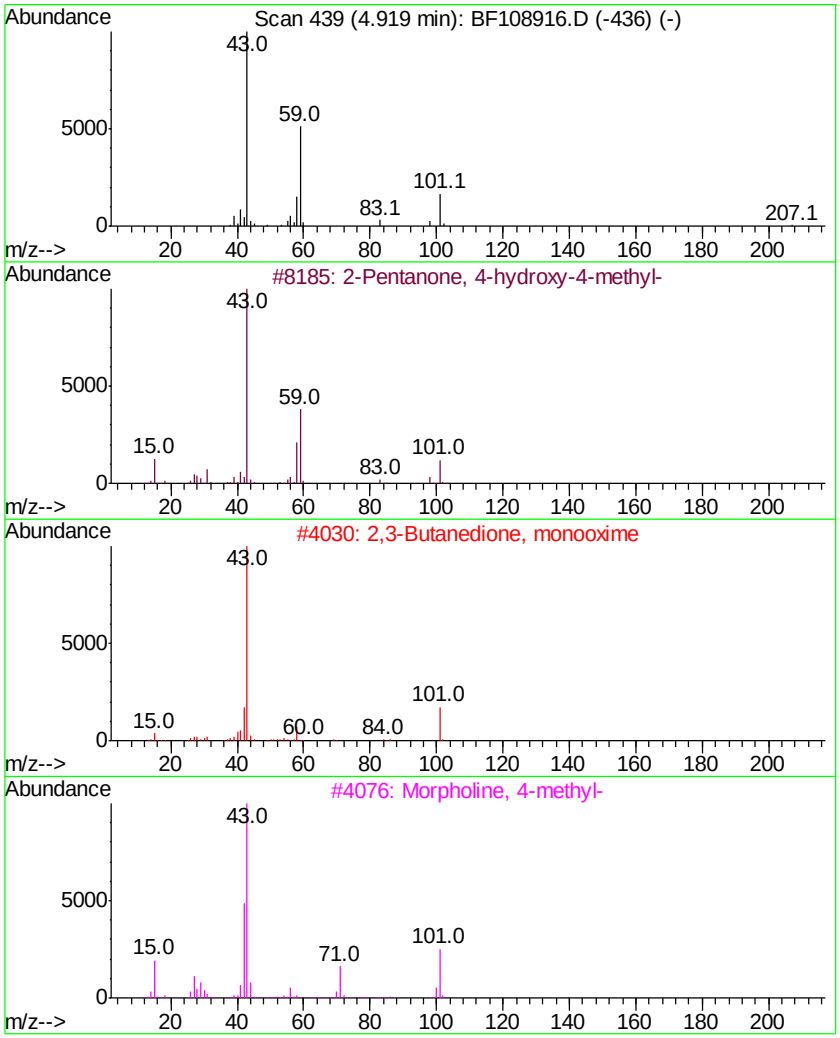
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

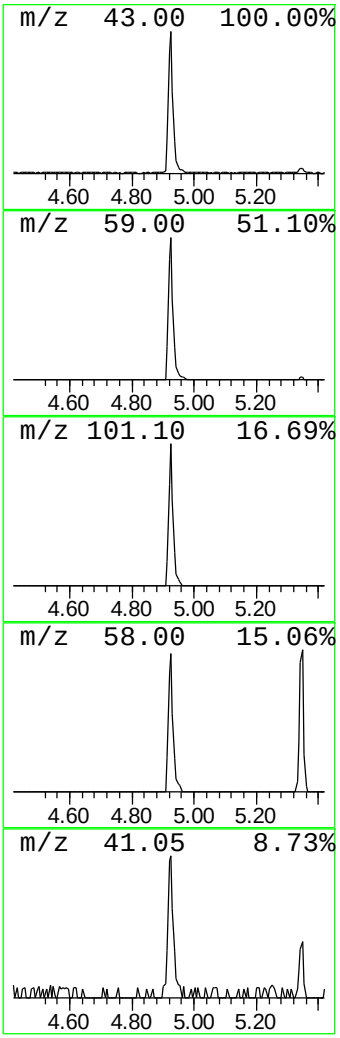
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.07 ng	142657	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

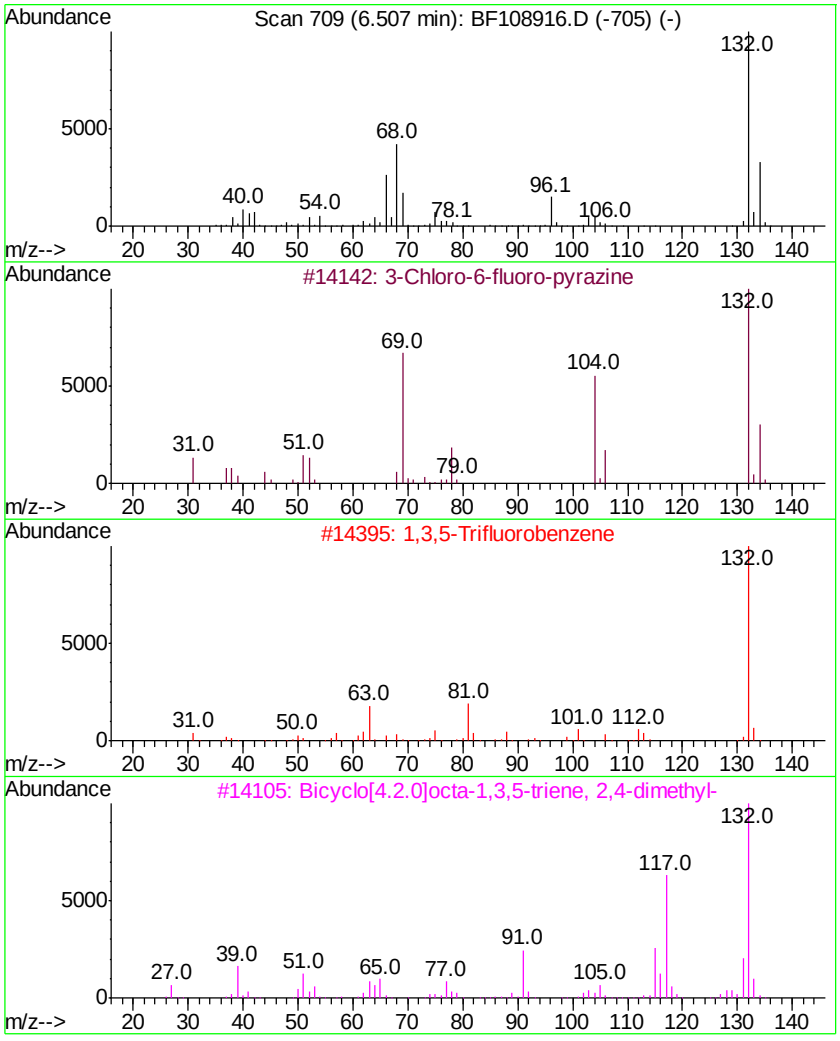
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

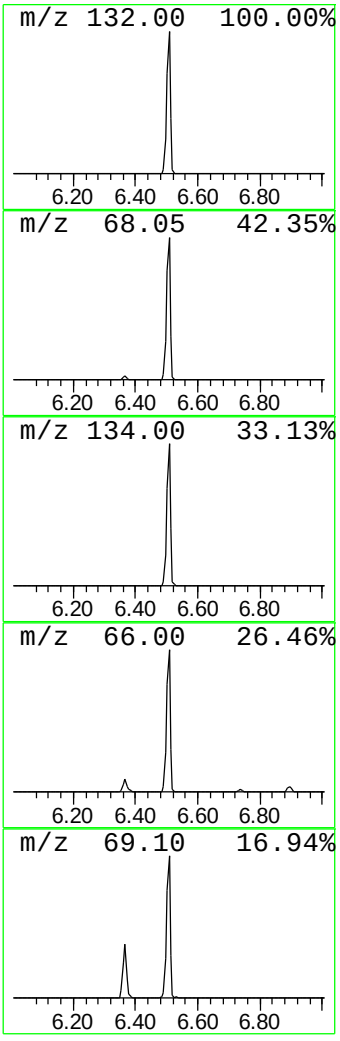
****

Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	52.14 ng	2425090	1,4-Dichlorobenzene-d4	6.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

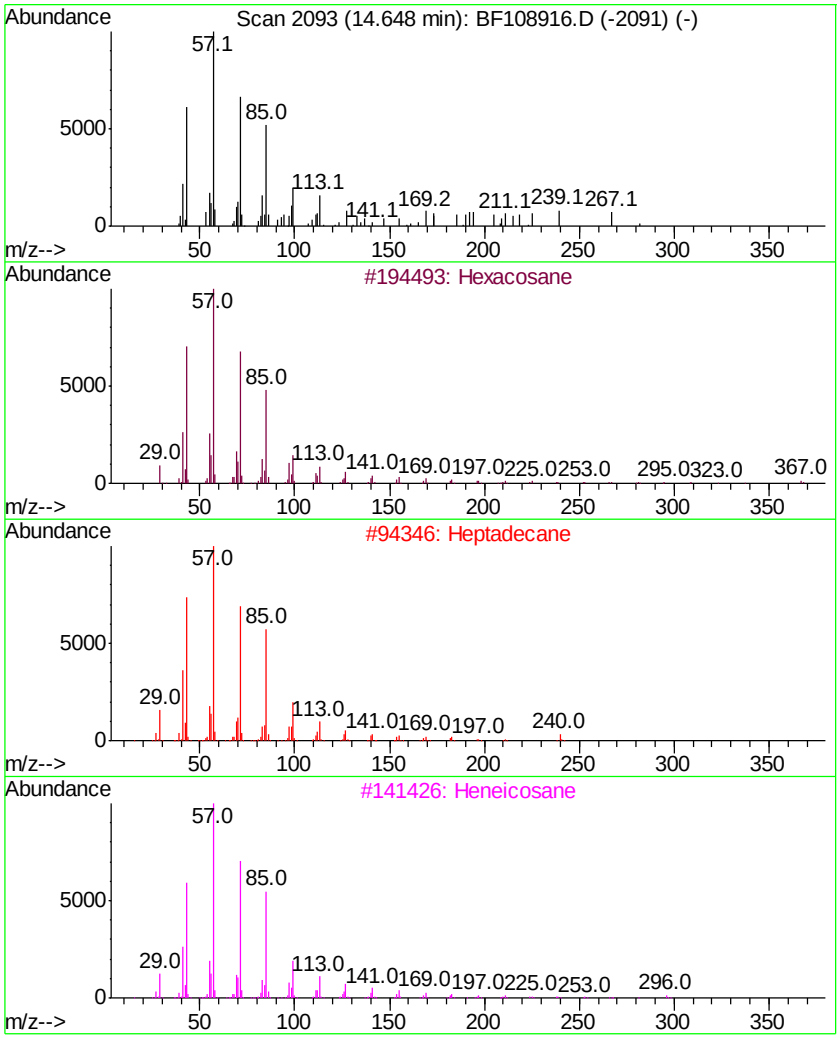
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

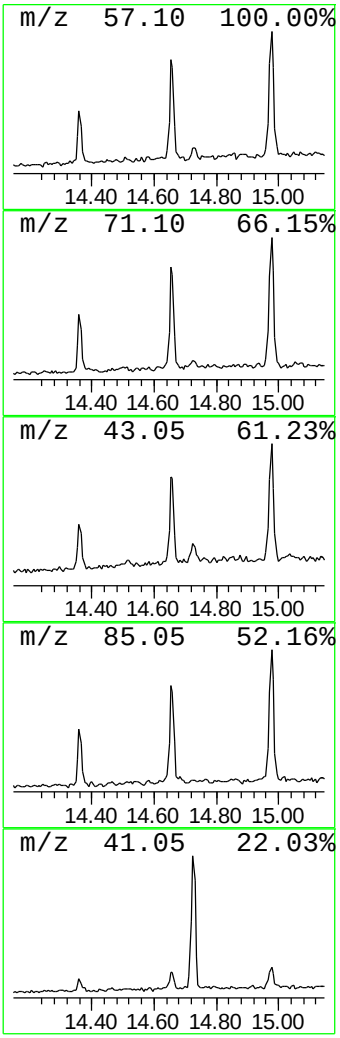
****

Peak Number 4 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.13 ng	77958	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Octacosane	394	C28H58	000630-02-4	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

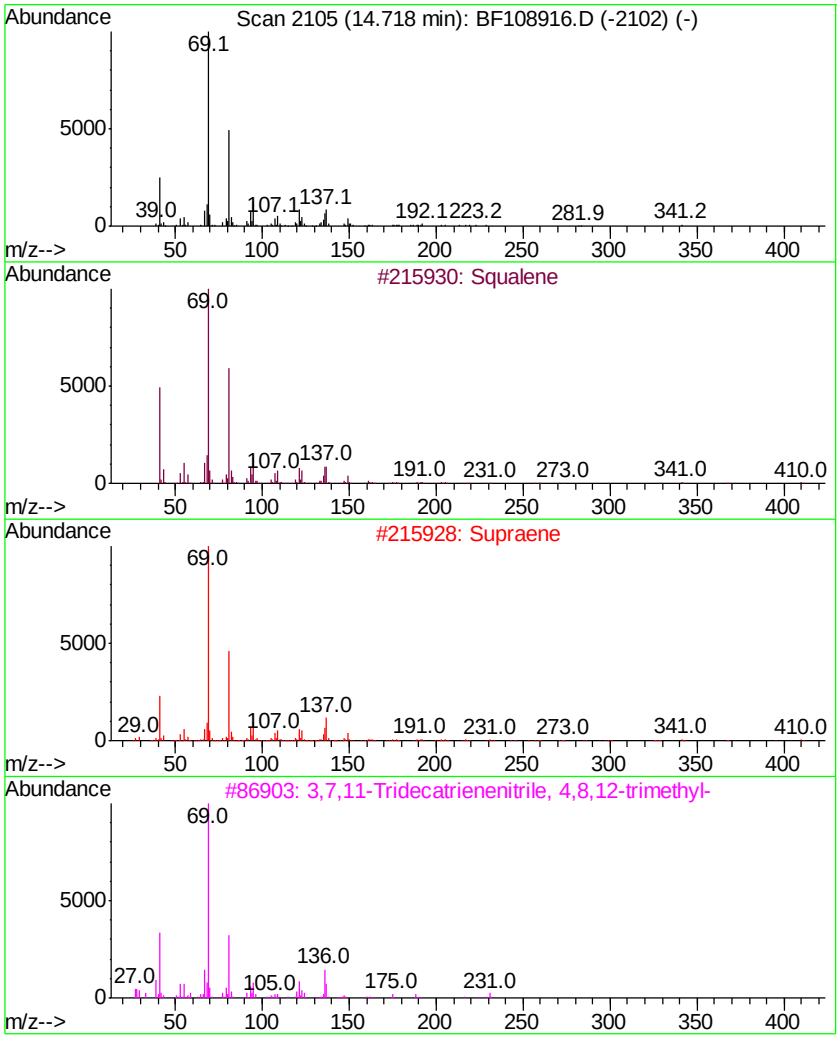
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

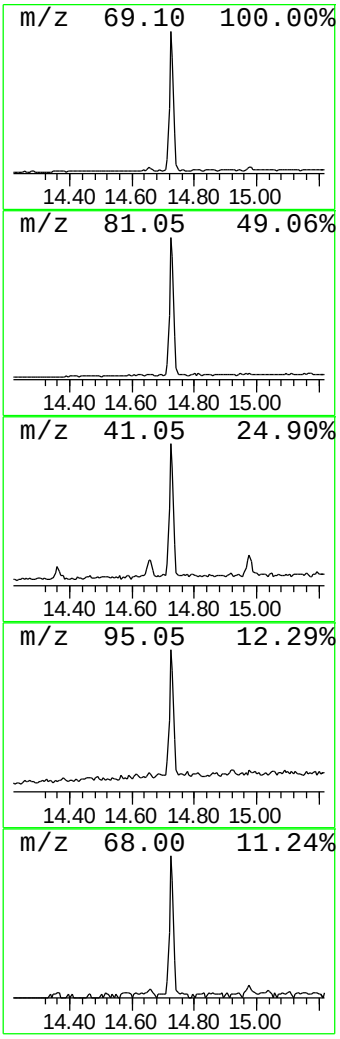
****

Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	10.09 ng	369711	Perylene-d12	15.28

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	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
090618-SIDI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

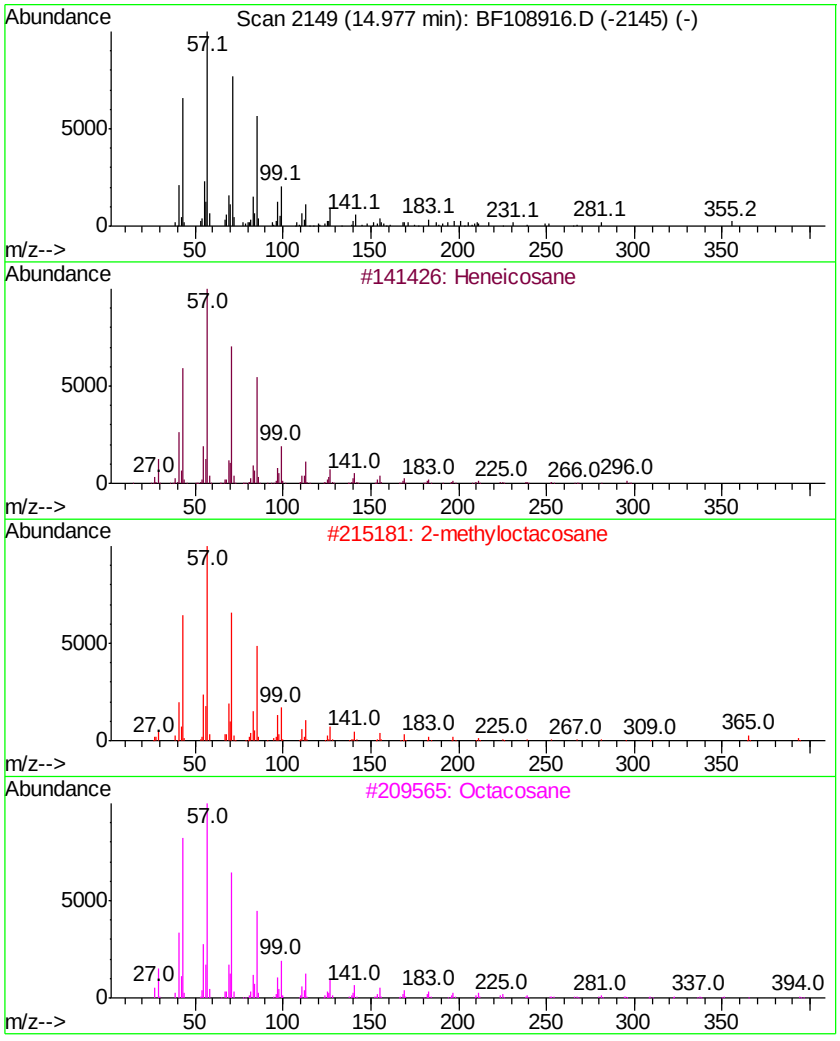
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

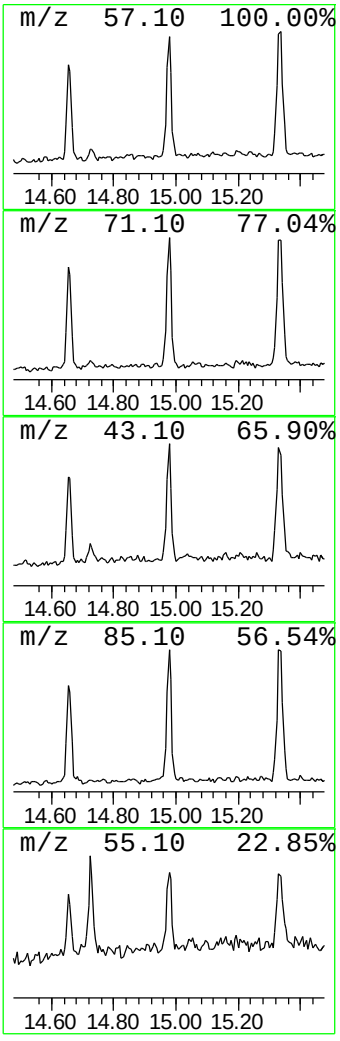
****

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	3.26 ng	119385	Perylene-d12	15.28

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	Octacosane	394	C28H58	000630-02-4	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

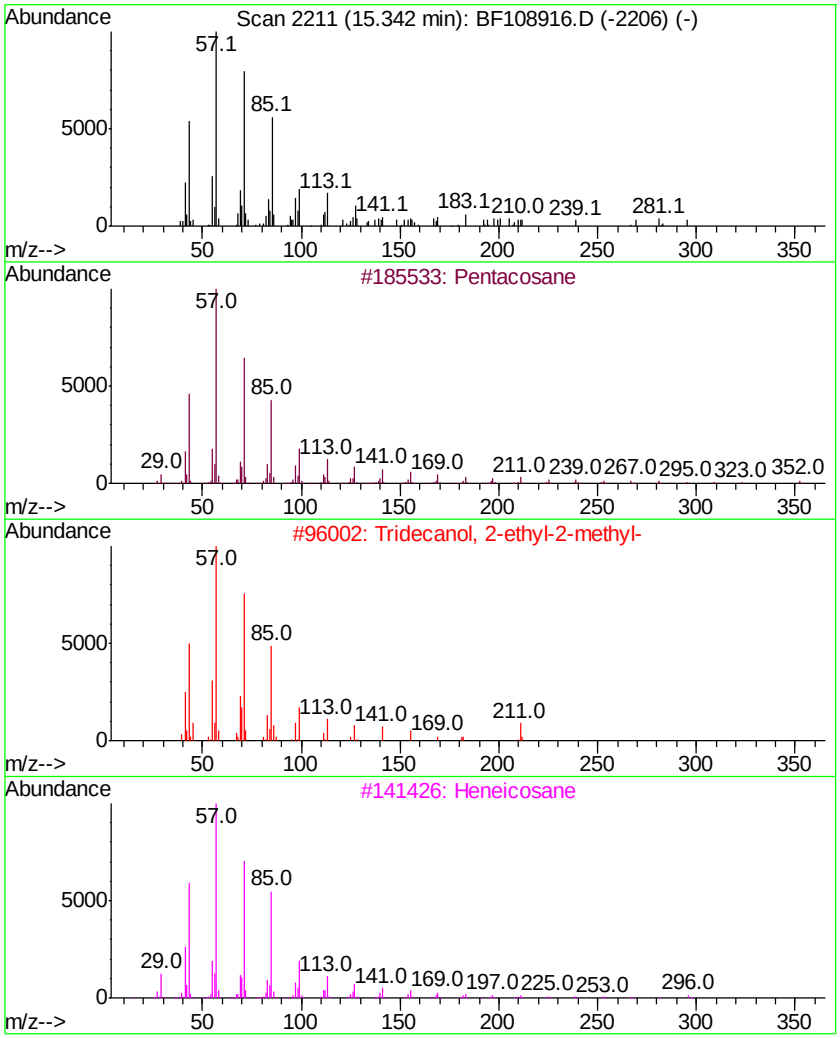
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

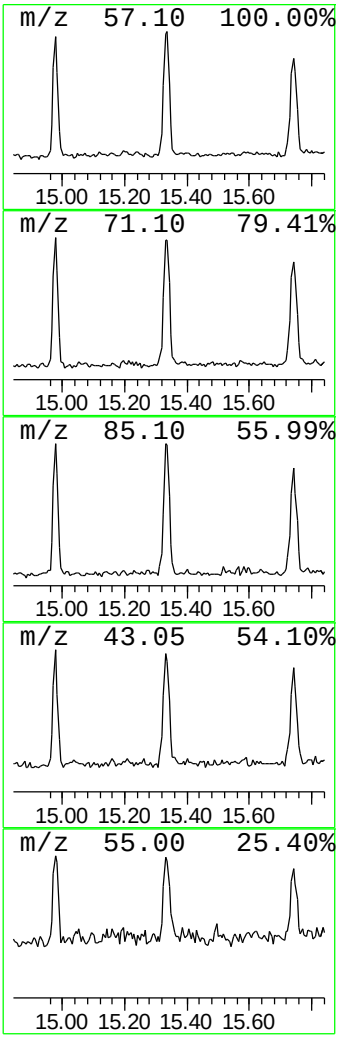
****

Peak Number 7 Pentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	3.74 ng	137219	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Triacontane	422	C30H62	000638-68-6	86
5	Octacosane	394	C28H58	000630-02-4	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

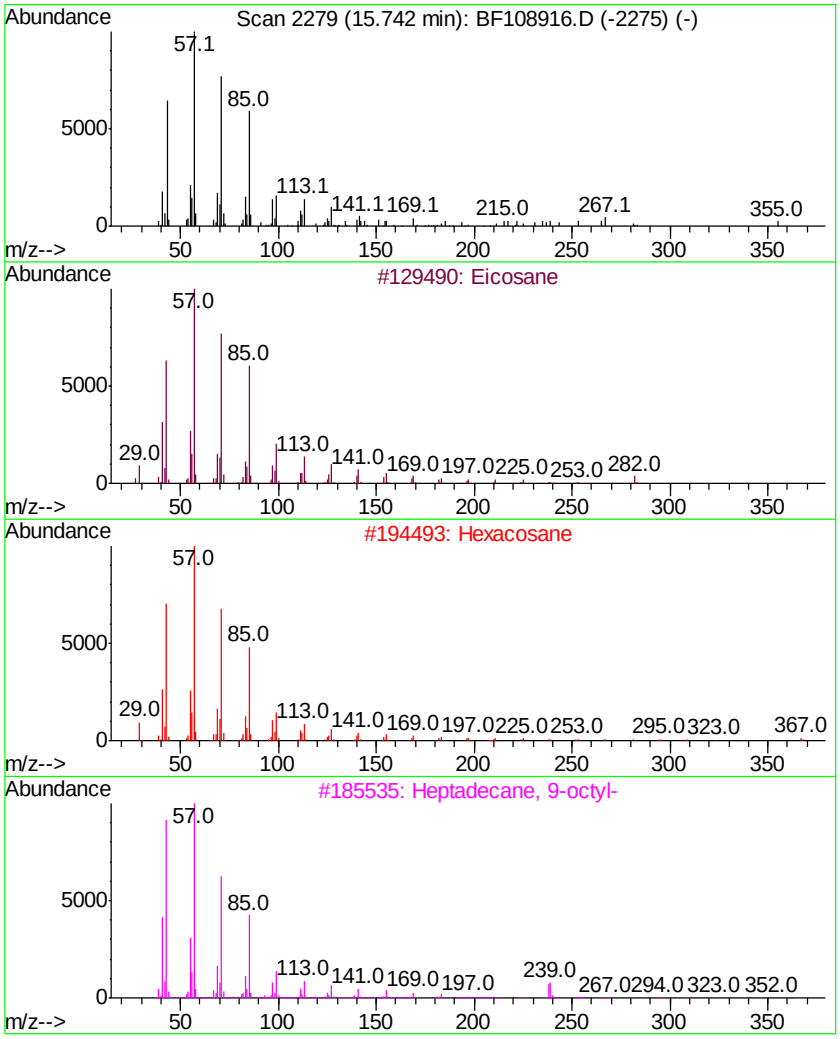
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

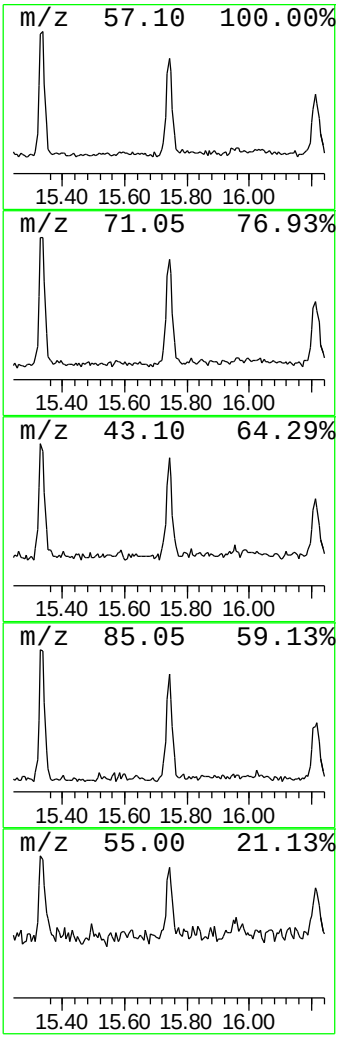
****

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	3.18 ng	116685	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091018\
Data File : BF108916.D
Acq On : 11 Sep 2018 2:11
Operator : JU/SJ
Sample : J4830-02
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-SIDI-F-D-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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...	4.92	3.1	ng	142657	1	6.74	930199	20.0
unknown6.51	6.51	52.1	ng	2425090	1	6.74	930199	20.0
Hexacosane	14.65	2.1	ng	77958	6	15.28	733007	20.0
Squalene	14.72	10.1	ng	369711	6	15.28	733007	20.0
Heneicosane	14.98	3.3	ng	119385	6	15.28	733007	20.0
Pentacosane	15.34	3.7	ng	137219	6	15.28	733007	20.0
Eicosane	15.74	3.2	ng	116685	6	15.28	733007	20.0