LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109125.D
Acq On : 19 Sep 2018 5:10
Operator : JU/SJ
Sample : J4930-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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	4.901	433	436	443	rBV	118034	123347	3.66%	0.585%
2	5.325	504	508	520	rBV	1176105	1051342	31.21%	4.984%
3	6.348	678	682	695	rVB	881357	745112	22.12%	3.532%
4	6.489	702	706	709	rBV	2152692	1833180	54.42%	8.690%
5	6.719	742	745	749	rBV	859665	686735	20.39%	3.256%
6	6.878	768	772	775	rBV	2893986	2553442	75.81%	12.105%
7	7.284	836	841	844	rBV	2182059	2037269	60.48%	9.658%
8	8.001	959	963	978	rBV	987457	777373	23.08%	3.685%
9	9.078	1142	1146	1149	rBV	3679199	3368376	100.00%	15.968%
10	9.472	1209	1213	1220	rVB	111320	98361	2.92%	0.466%
11	9.748	1257	1260	1270	rVB	806887	758794	22.53%	3.597%
12	10.536	1390	1394	1409	rBV	1246902	1206814	35.83%	5.721%
13	11.224	1508	1511	1515	rBV	728413	666020	19.77%	3.157%
14	12.813	1776	1781	1784	rBV	3386801	3100725	92.05%	14.699%
15	13.724	1932	1936	1946	rVB3	32985	42284	1.26%	0.200%
16	13.854	1954	1958	1962	rBV	936025	811867	24.10%	3.849%
17	14.636	2088	2091	2096	rVB	52750	51923	1.54%	0.246%
18	14.707	2099	2103	2108	rVB	134549	127061	3.77%	0.602%
19	14.954	2141	2145	2152	rVB	72602	79114	2.35%	0.375%
20	15.260	2192	2197	2202	rBV	563054	655461	19.46%	3.107%
21	15.312	2202	2206	2212	rVB	77886	101904	3.03%	0.483%
22	15.712	2269	2274	2281	rBV	68933	100755	2.99%	0.478%
23	16.183	2349	2354	2362	rVB	44655	80609	2.39%	0.382%
24	16.724	2442	2446	2453	rVB3	20728	36528	1.08%	0.173%

Sum of corrected areas: 21094396

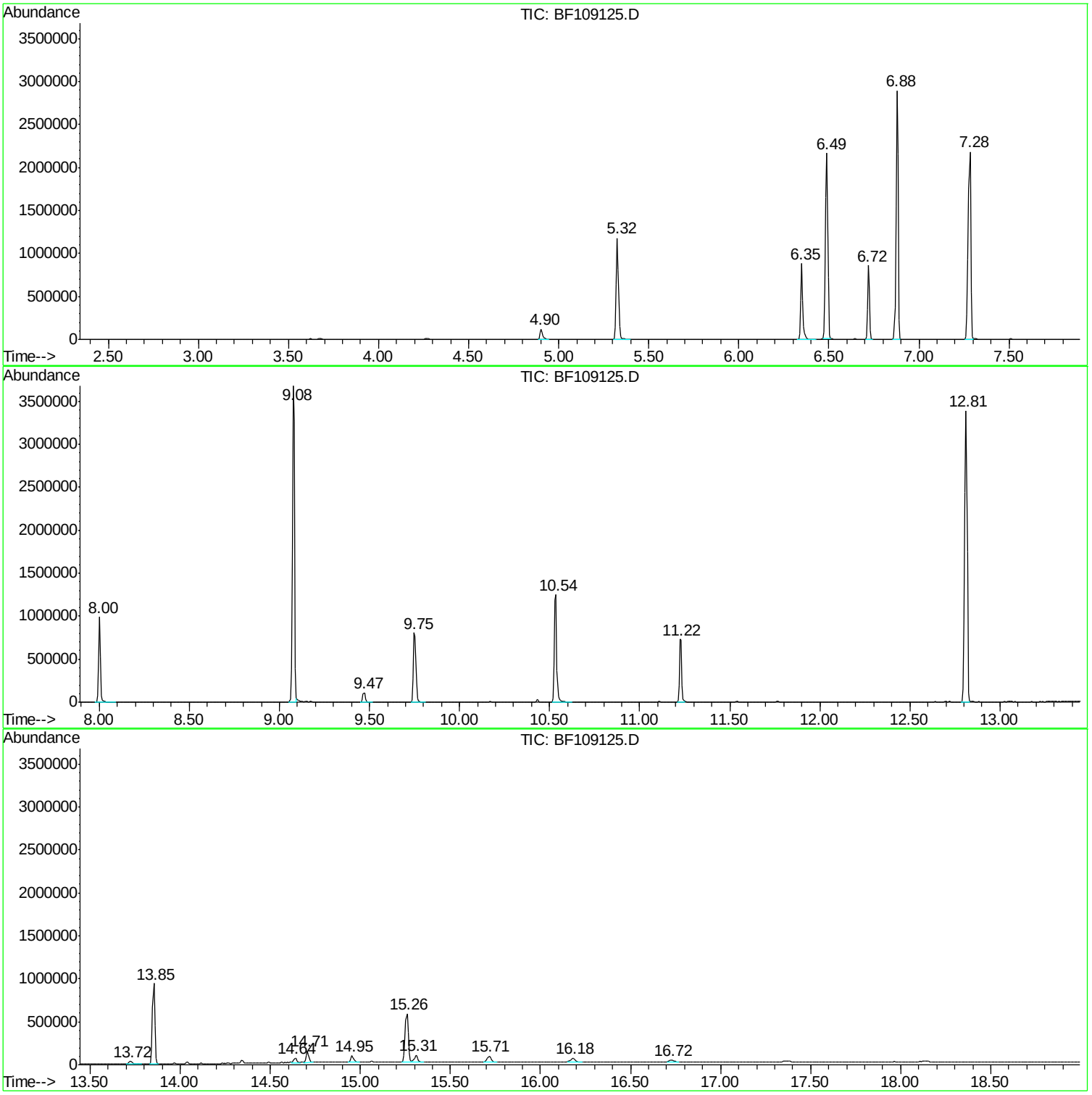
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109125.D
Acq On : 19 Sep 2018 5:10
Operator : JU/SJ
Sample : J4930-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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\BF091818\
Data File : BF109125.D
Acq On : 19 Sep 2018 5:10
Operator : JU/SJ
Sample : J4930-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

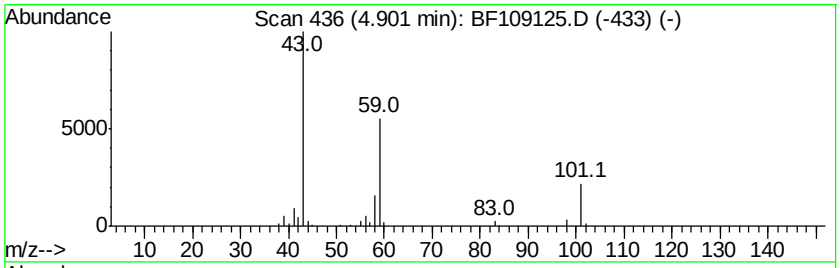
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

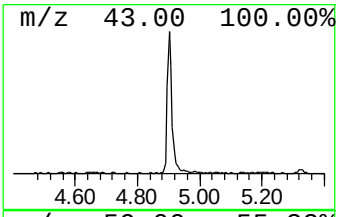
****

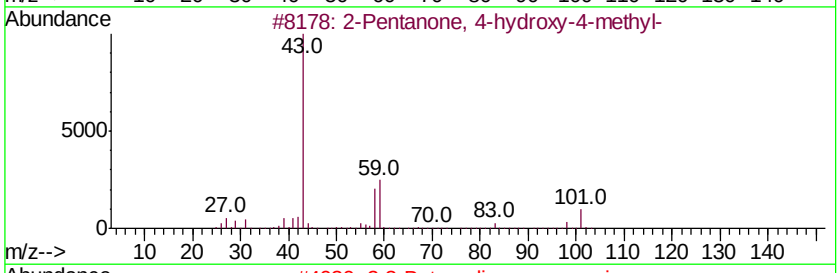
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

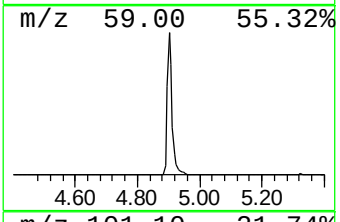
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	3.59 ng	123347	1,4-Dichlorobenzene-d4	6.72

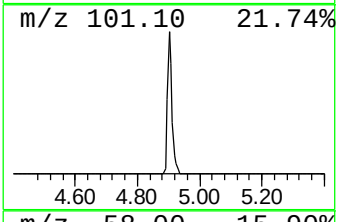
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9

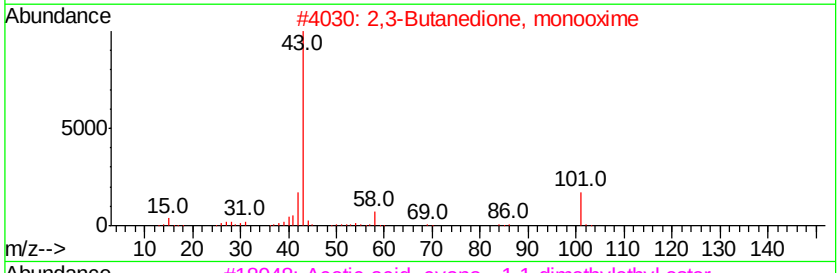


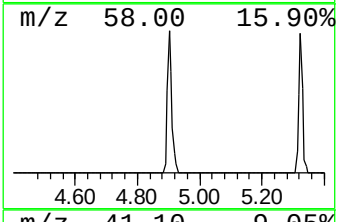


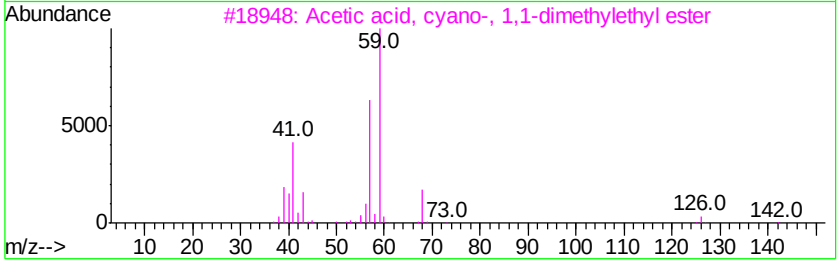


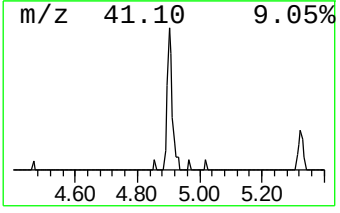












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109125.D
Acq On : 19 Sep 2018 5:10
Operator : JU/SJ
Sample : J4930-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

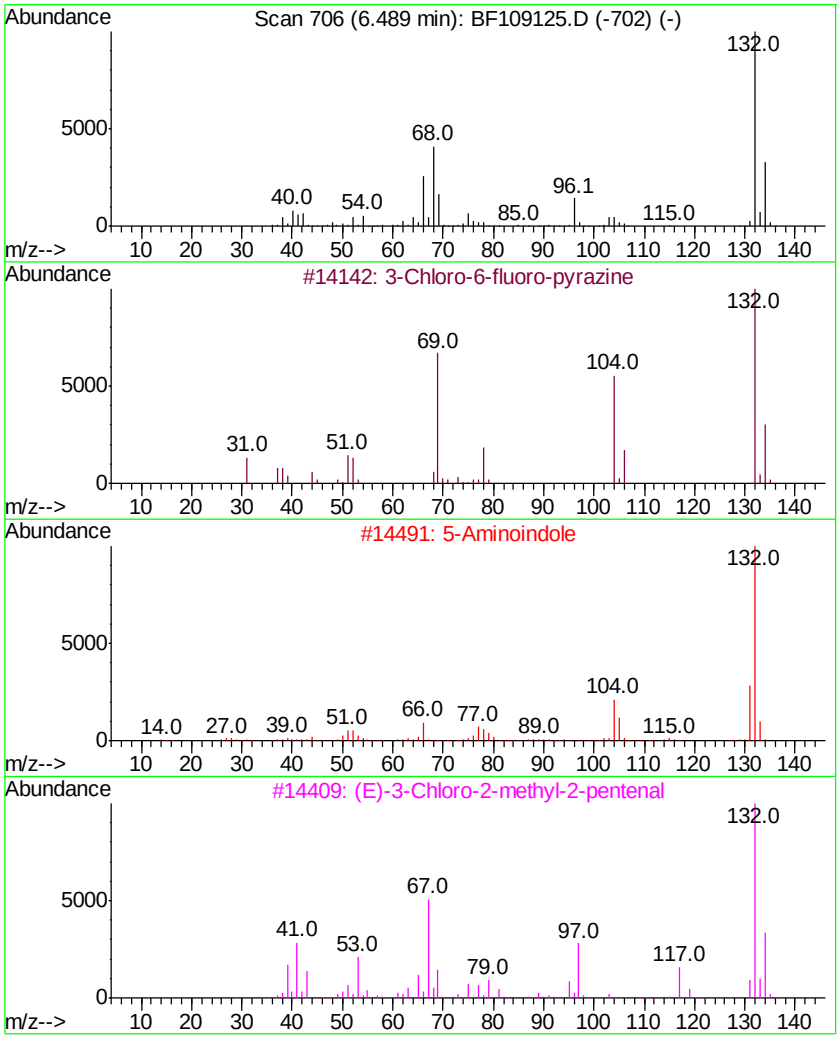
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

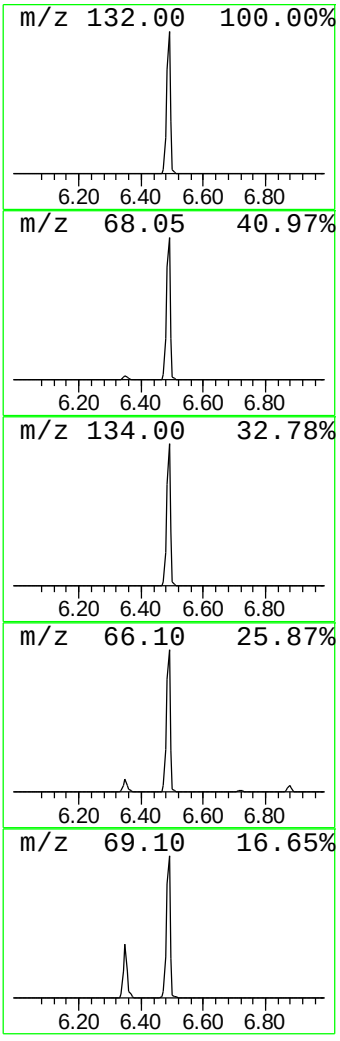
****

Peak Number 2 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	53.39 ng	1833180	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109125.D
Acq On : 19 Sep 2018 5:10
Operator : JU/SJ
Sample : J4930-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

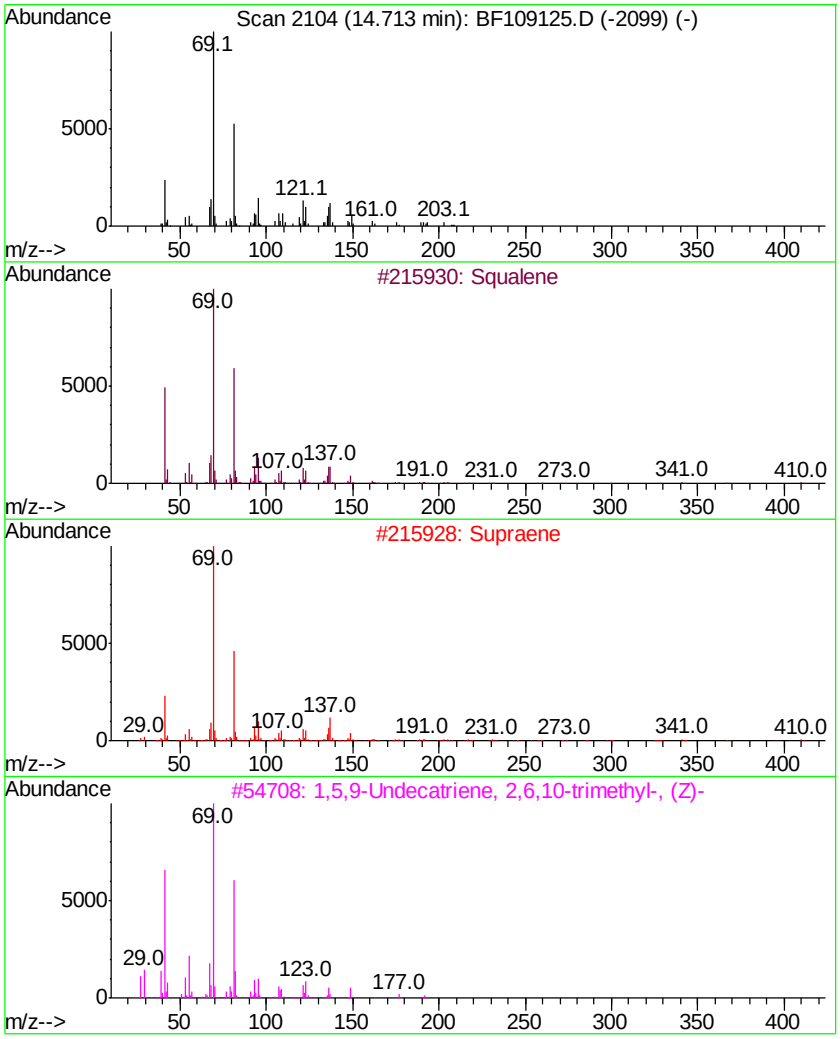
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

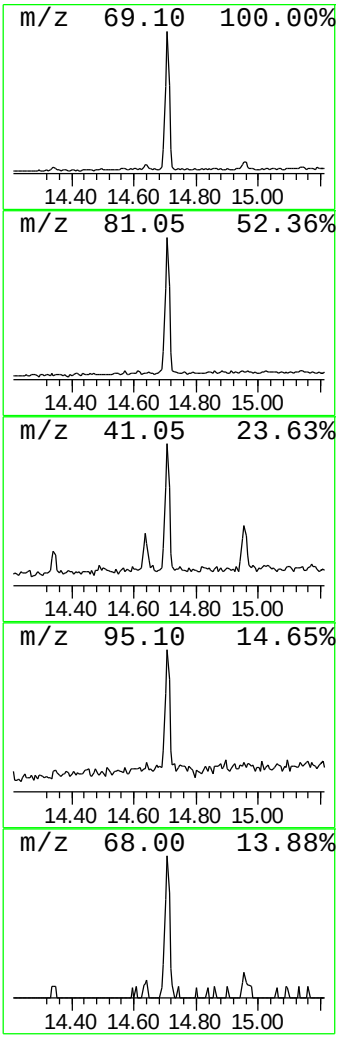
****

Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.88 ng	127061	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	87
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4	1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109125.D
Acq On : 19 Sep 2018 5:10
Operator : JU/SJ
Sample : J4930-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

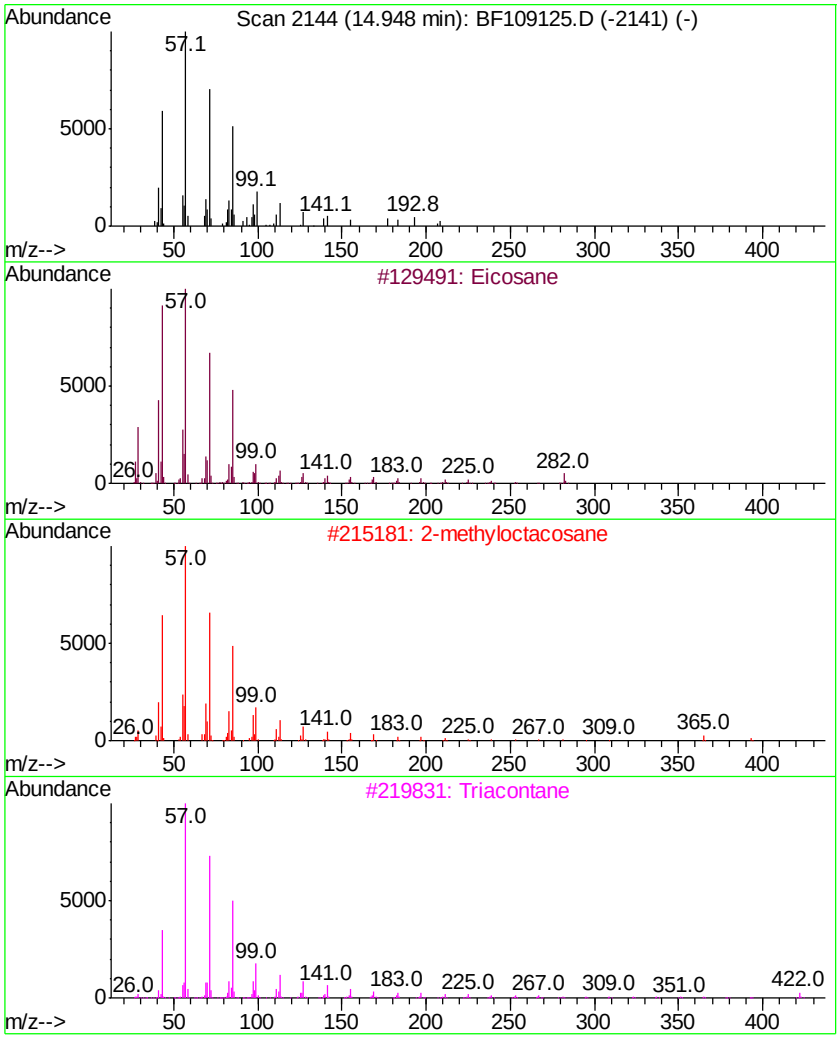
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

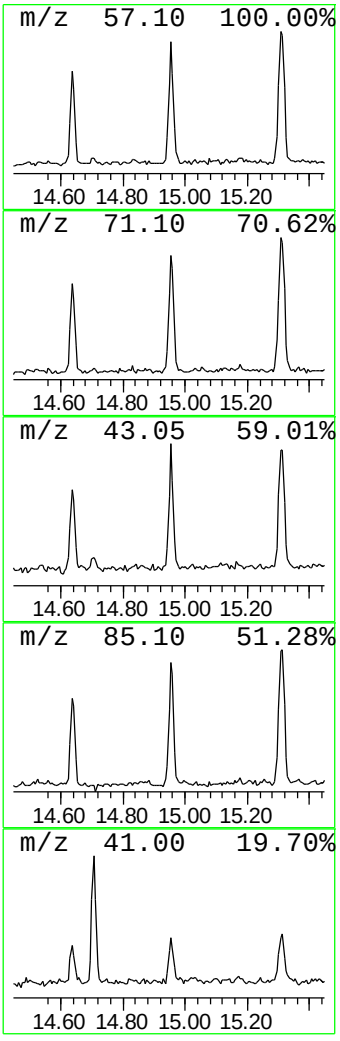
****

Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.41 ng	79114	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Pentacosane	352	C25H52	000629-99-2	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109125.D
Acq On : 19 Sep 2018 5:10
Operator : JU/SJ
Sample : J4930-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

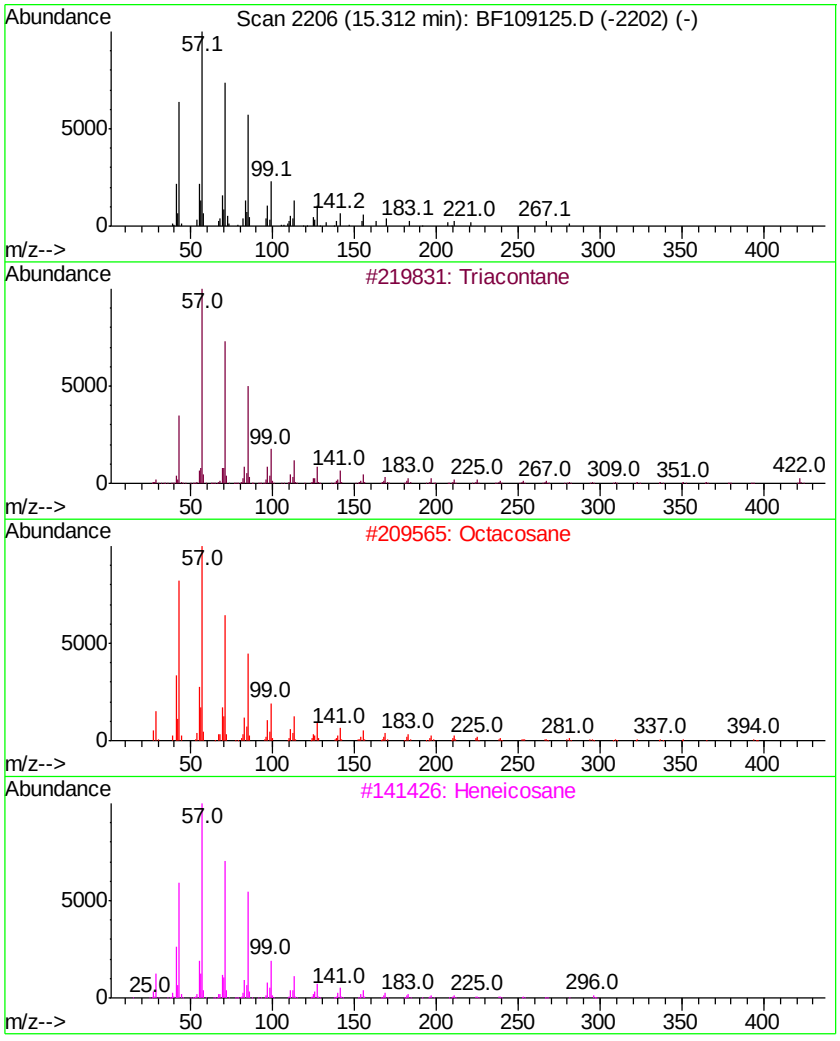
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

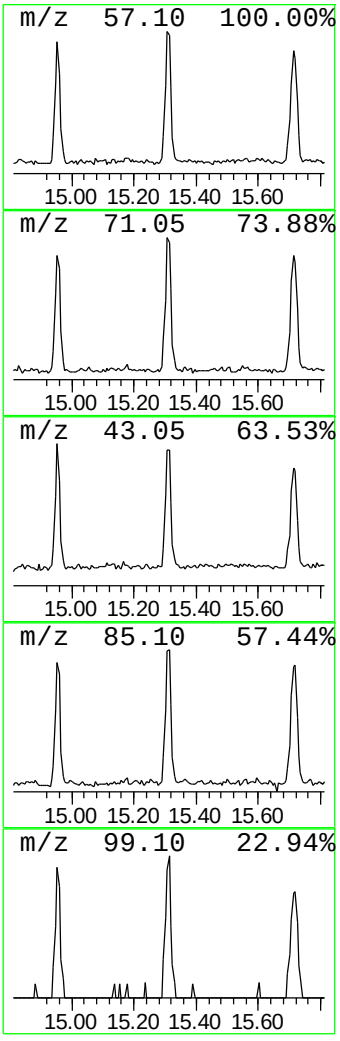
****

Peak Number 6 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	3.11 ng	101904	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	90
5	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109125.D
Acq On : 19 Sep 2018 5:10
Operator : JU/SJ
Sample : J4930-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

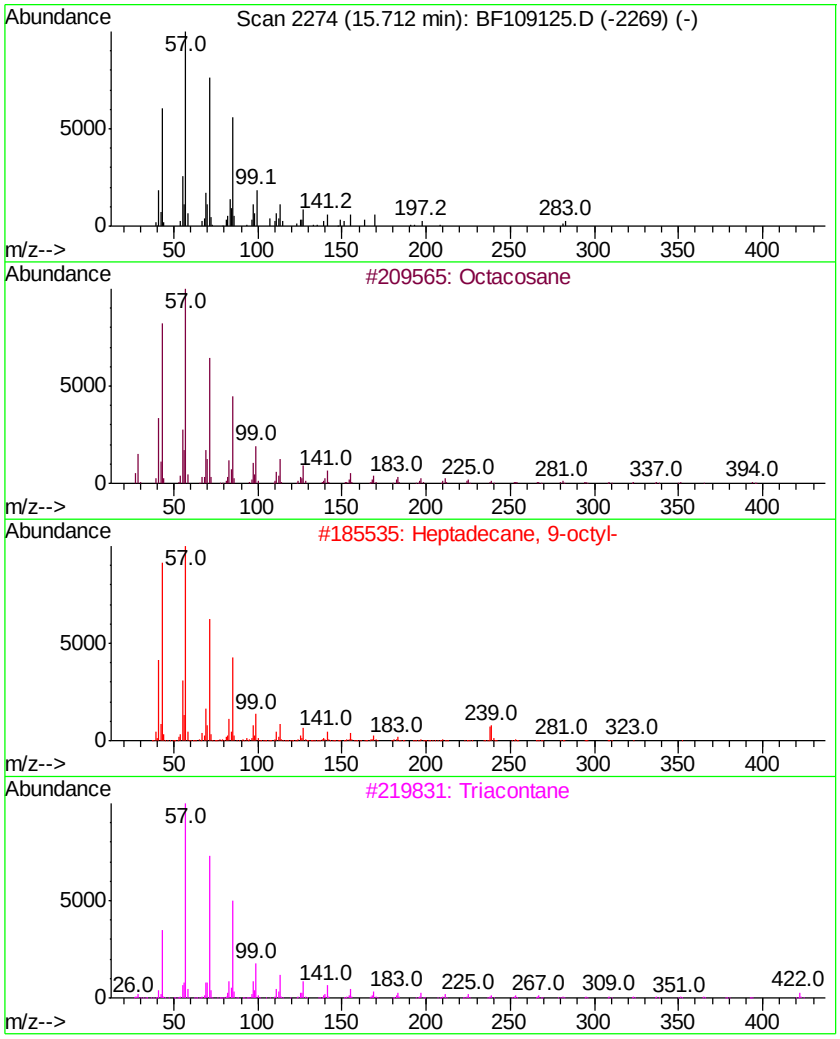
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

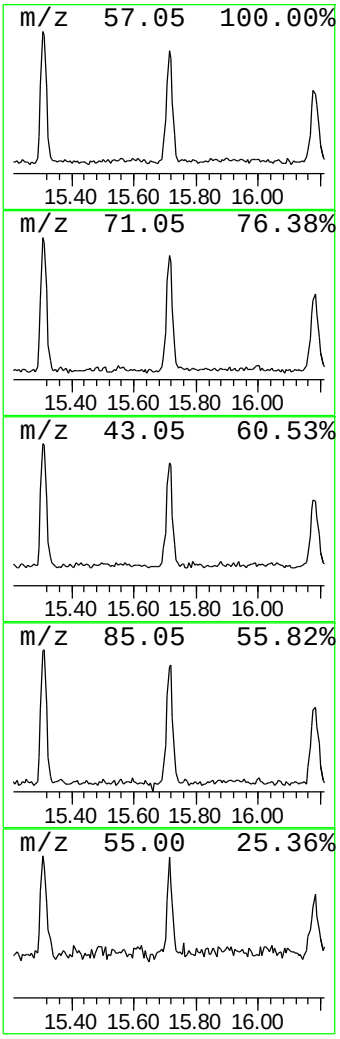
****

Peak Number 7 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.07 ng	100755	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane	240	C17H36	000629-78-7	90
5	Hexacosane	366	C26H54	000630-01-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091818\
Data File : BF109125.D
Acq On : 19 Sep 2018 5:10
Operator : JU/SJ
Sample : J4930-09
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 091318-DBRI-E-U-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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...	4.90	3.6	ng	123347	1	6.72	686735	20.0
unknown6.49	6.49	53.4	ng	1833180	1	6.72	686735	20.0
Squalene	14.71	3.9	ng	127061	6	15.26	655461	20.0
Eicosane	14.95	2.4	ng	79114	6	15.26	655461	20.0
Triacontane	15.31	3.1	ng	101904	6	15.26	655461	20.0
Octacosane	15.71	3.1	ng	100755	6	15.26	655461	20.0