LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108924.D
Acq On : 11 Sep 2018 5:45
Operator : JU/SJ
Sample : J4830-14
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-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-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	451	rVB	133366	145673	2.96%	0.481%
2	5.343	507	511	515	rBV	1643479	1555955	31.57%	5.137%
3	6.366	681	685	694	rBV	1220041	1057999	21.47%	3.493%
4	6.507	704	709	712	rBV	3201752	2833779	57.50%	9.355%
5	6.737	745	748	752	rBV	1326054	1035031	21.00%	3.417%
6	6.895	771	775	778	rBV	4157323	3839036	77.89%	12.674%
7	7.301	838	844	847	rBV	3172211	3074810	62.39%	10.151%
8	8.019	962	966	969	rBV	1544346	1188223	24.11%	3.923%
9	9.095	1144	1149	1152	rBV	5207512	4928535	100.00%	16.271%
10	9.484	1212	1215	1226	rVB	625848	492528	9.99%	1.626%
11	9.766	1260	1263	1267	rBV	1245535	1113304	22.59%	3.675%
12	10.448	1376	1379	1382	rBV	84745	61904	1.26%	0.204%
13	10.548	1392	1396	1407	rBV	1676359	1647297	33.42%	5.438%
14	11.242	1511	1514	1518	rBV	1019951	957001	19.42%	3.159%
15	12.830	1779	1784	1787	rBV	4208503	3872526	78.57%	12.785%
16	13.742	1935	1939	1948	rBV2	55859	91121	1.85%	0.301%
17	13.871	1957	1961	1964	rBV	1283840	1116825	22.66%	3.687%
18	14.654	2091	2094	2098	rVB	55960	54491	1.11%	0.180%
19	14.724	2103	2106	2112	rVB	152171	145035	2.94%	0.479%
20	14.971	2145	2148	2152	rBV	69916	77887	1.58%	0.257%
21	15.277	2195	2200	2205	rBV	651533	753104	15.28%	2.486%
22	15.330	2205	2209	2214	rVV	70705	96691	1.96%	0.319%
23	15.742	2274	2279	2284	rBV2	57631	86147	1.75%	0.284%
24	16.213	2354	2359	2366	rVB	40804	65806	1.34%	0.217%

Sum of corrected areas: 30290708

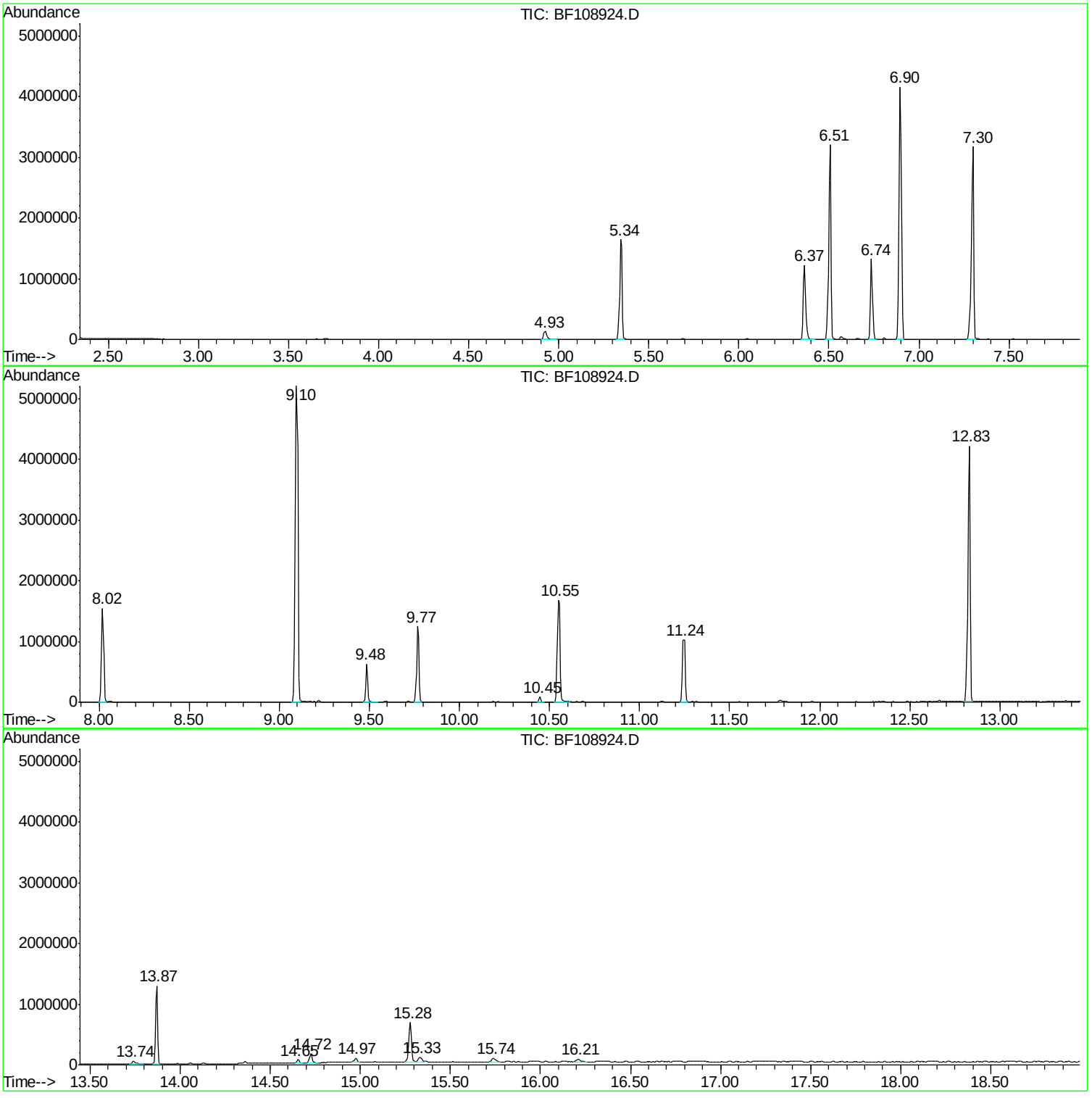
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108924.D
Acq On : 11 Sep 2018 5:45
Operator : JU/SJ
Sample : J4830-14
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-S

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 : BF108924.D
Acq On : 11 Sep 2018 5:45
Operator : JU/SJ
Sample : J4830-14
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-S

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

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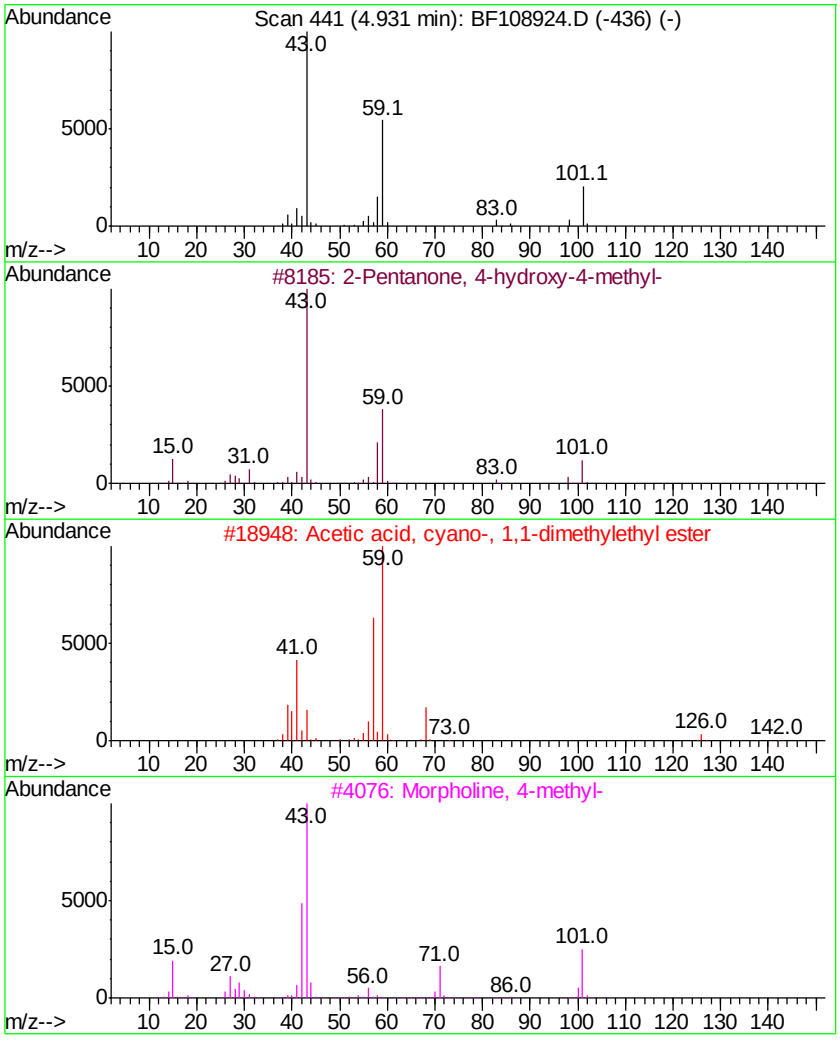
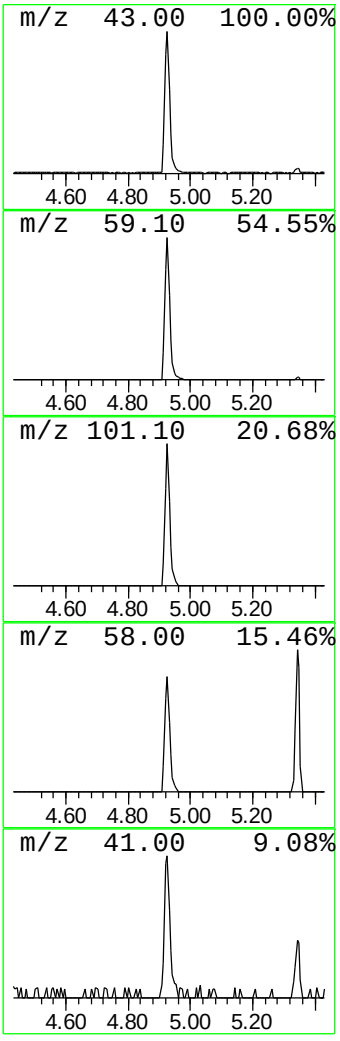
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.81 ng	145673	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	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108924.D
Acq On : 11 Sep 2018 5:45
Operator : JU/SJ
Sample : J4830-14
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
090618-DBRI-E-U-S

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

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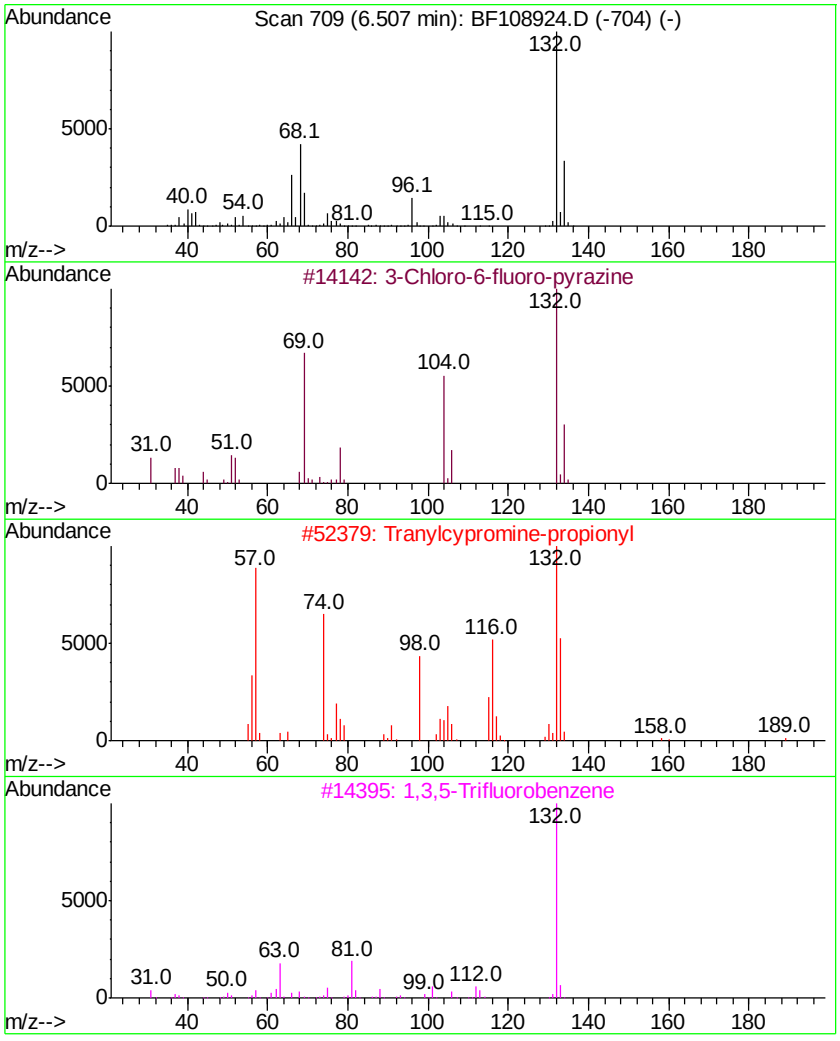
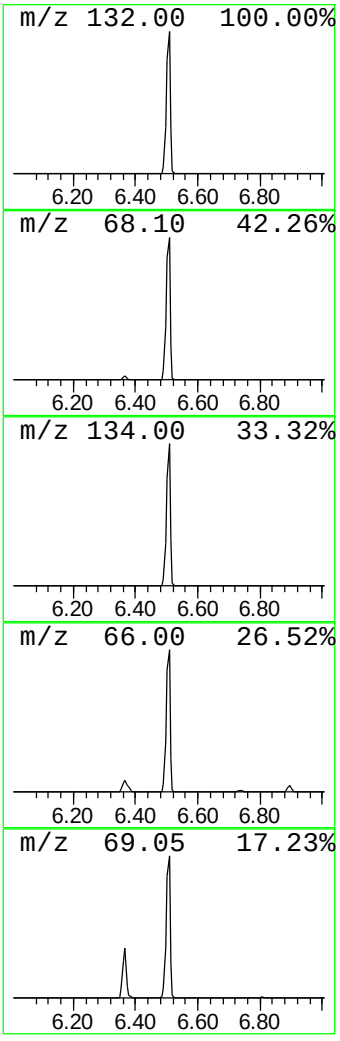
Peak Number 2 unknown6.51 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	54.76 ng	2833780	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108924.D
Acq On : 11 Sep 2018 5:45
Operator : JU/SJ
Sample : J4830-14
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-S

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

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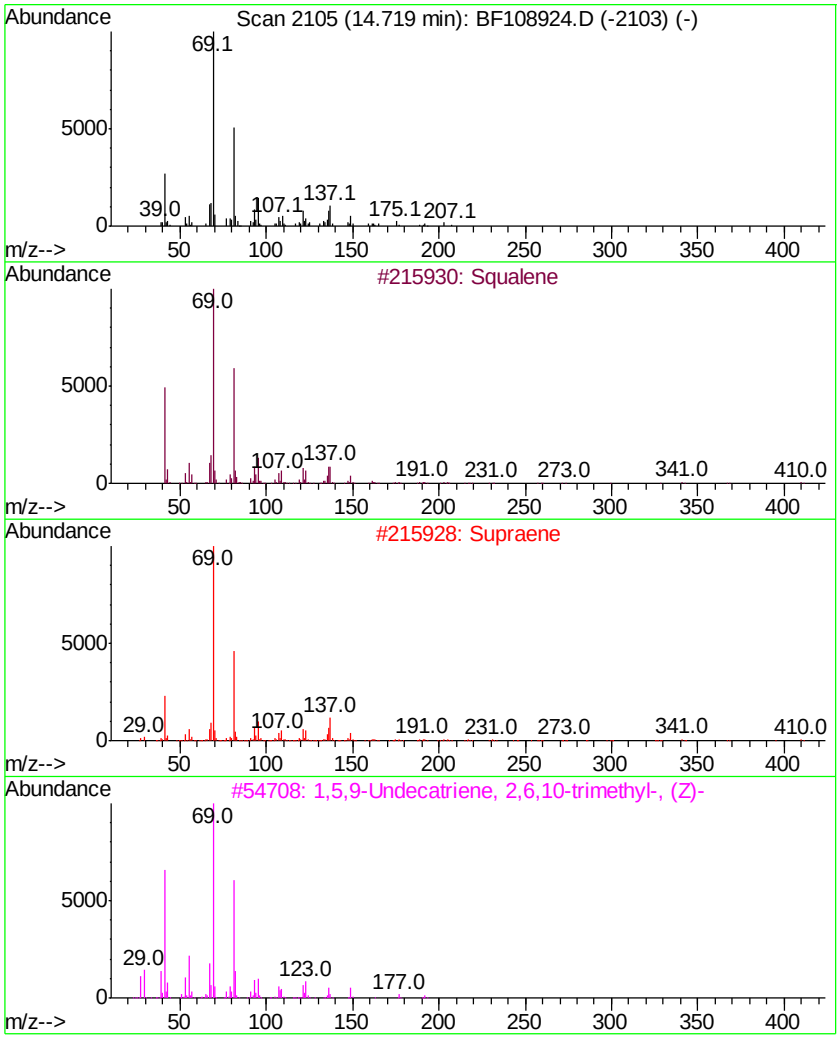
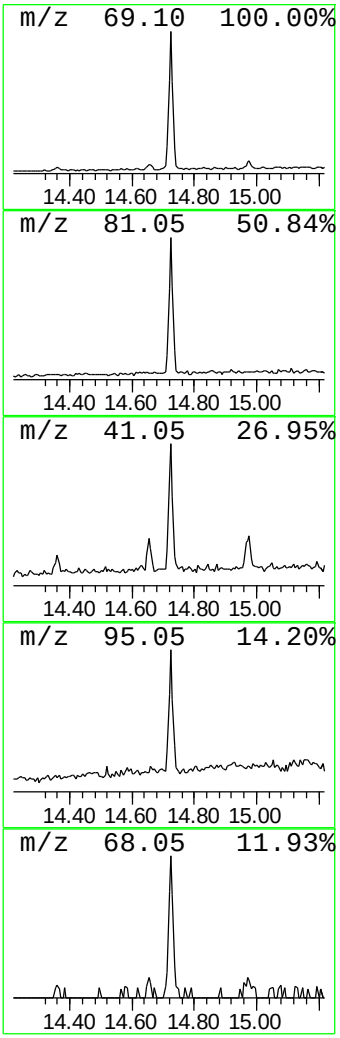
Peak Number 4 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.85 ng	145035	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	90
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108924.D
Acq On : 11 Sep 2018 5:45
Operator : JU/SJ
Sample : J4830-14
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-S

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

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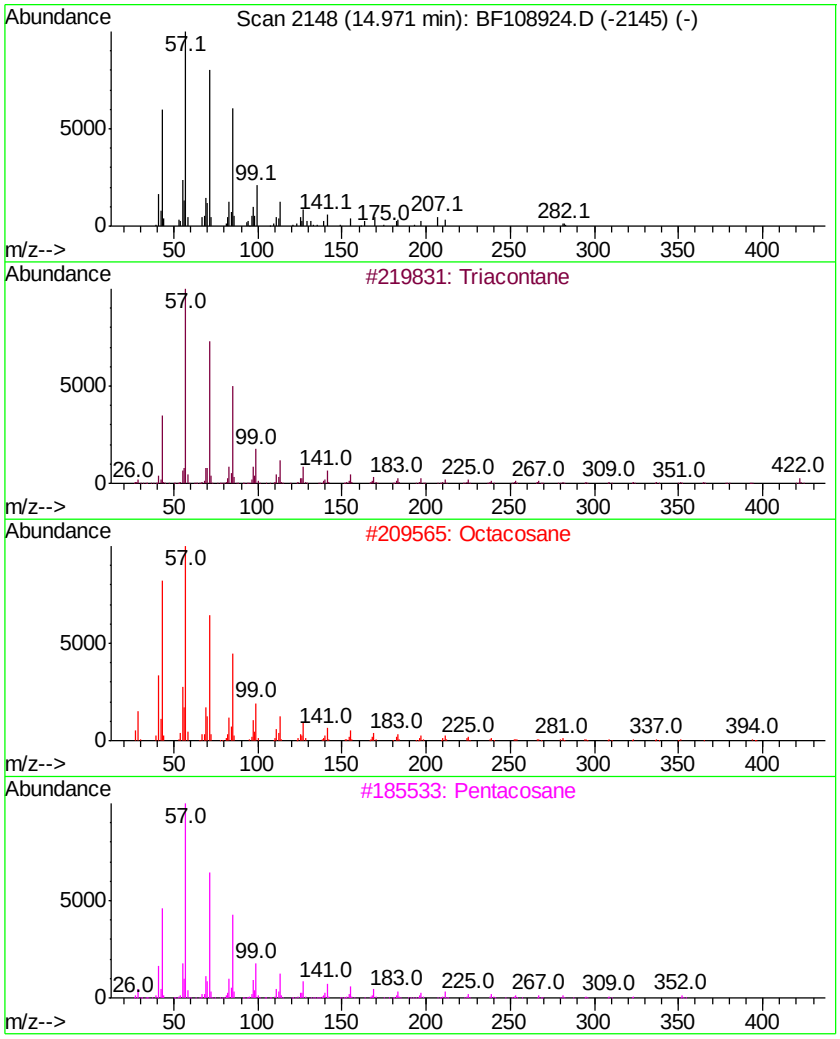
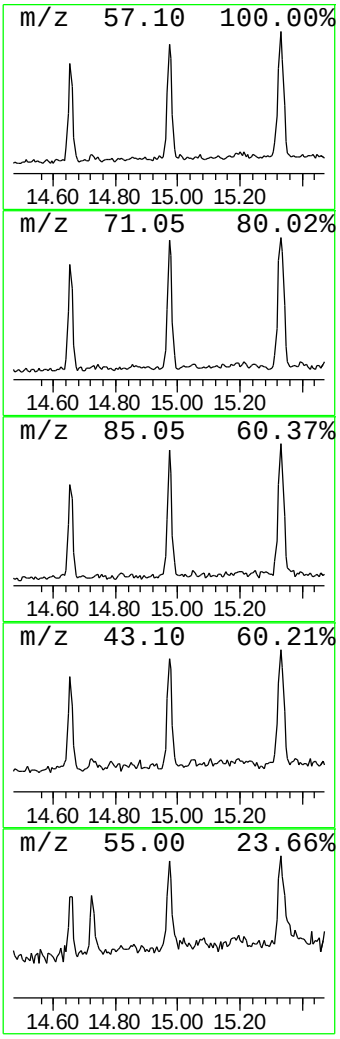
Peak Number 5 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.07 ng	77887	Perylene-d12	15.28

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	Pentacosane	352	C25H52	000629-99-2	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Tetracosane	338	C24H50	000646-31-1	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091018\
Data File : BF108924.D
Acq On : 11 Sep 2018 5:45
Operator : JU/SJ
Sample : J4830-14
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 090618-DBRI-E-U-S

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

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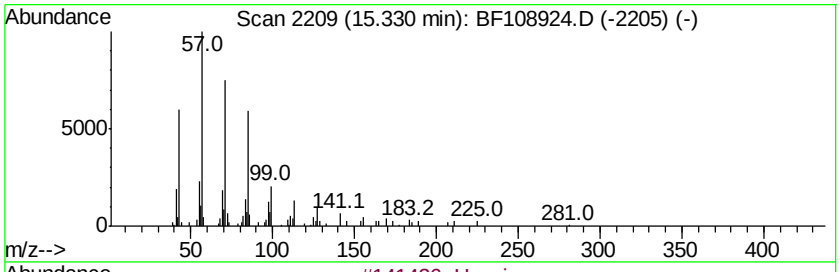
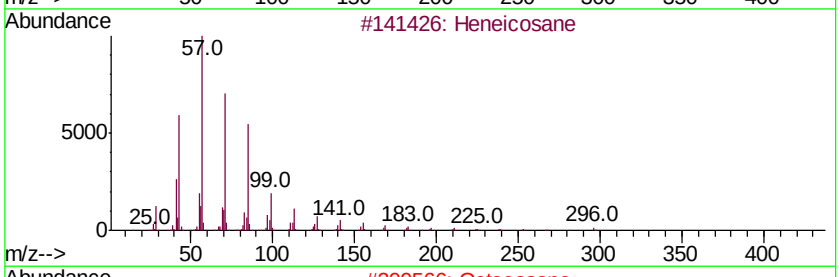
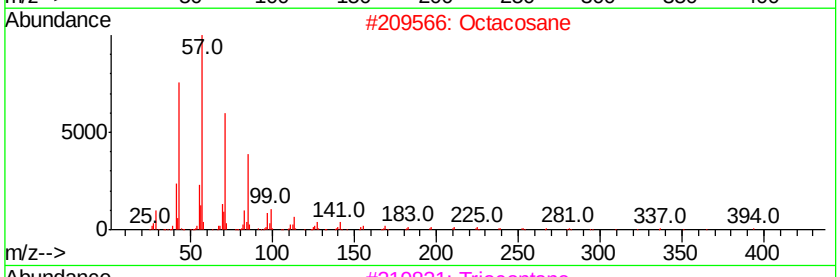
Peak Number 6 Heneicosane Concentration Rank 5

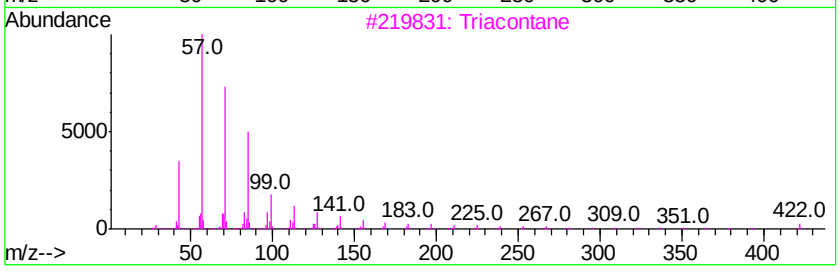
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	2.57 ng	96691	Perylene-d12	15.28

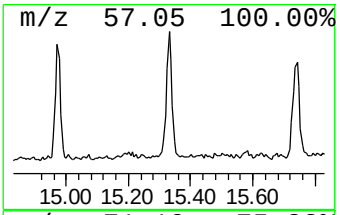
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Triacontane	422	C30H62	000638-68-6	91
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	91
5	Hexadecane	226	C16H34	000544-76-3	91

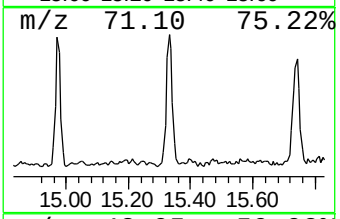


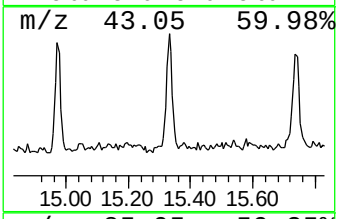


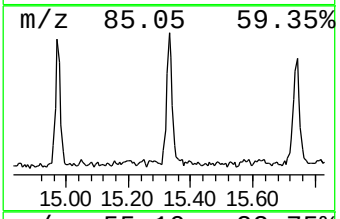


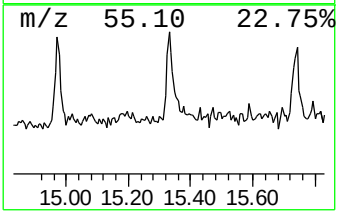












Library Search Compound Report

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090618-DBRI-E-U-S

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

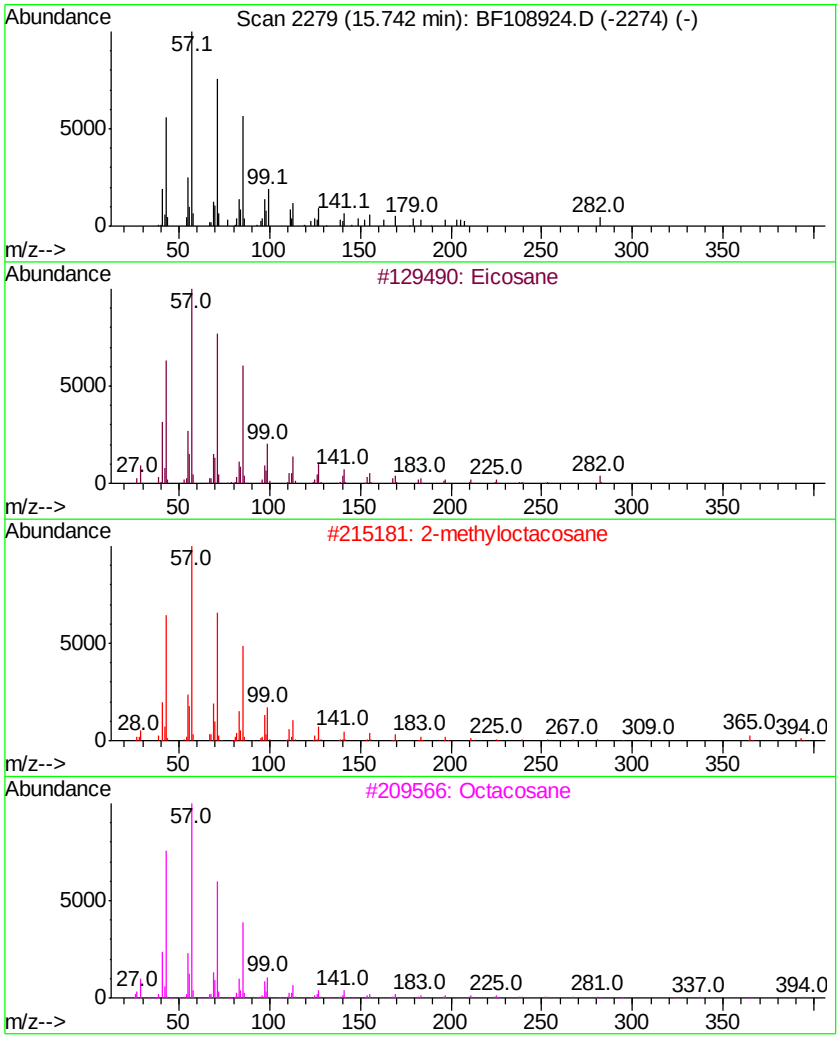
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

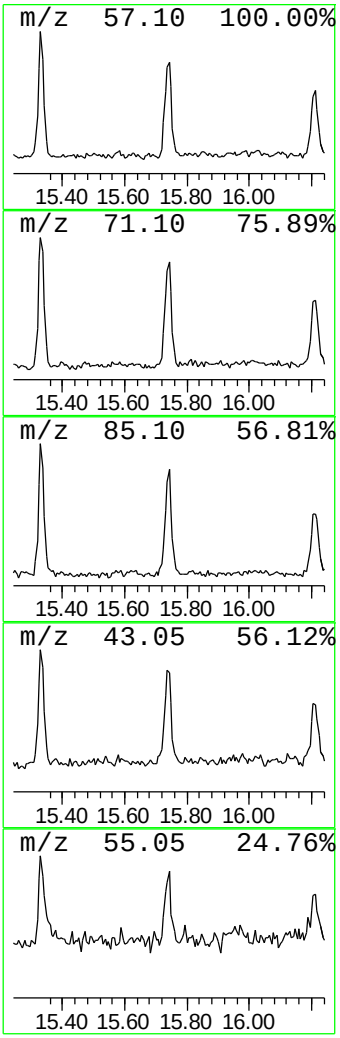
****

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	2.29 ng	86147	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Heneicosane	296	C21H44	000629-94-7	90





Tentatively Identified Compound (LSC) summary

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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...	4.93	2.8	ng	145673	1	6.74	1035030	20.0
unknown6.51	6.51	54.8	ng	2833780	1	6.74	1035030	20.0
Squalene	14.72	3.9	ng	145035	6	15.28	753104	20.0
Triacontane	14.97	2.1	ng	77887	6	15.28	753104	20.0
Heneicosane	15.33	2.6	ng	96691	6	15.28	753104	20.0
Eicosane	15.74	2.3	ng	86147	6	15.28	753104	20.0