LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090319\
Data File : BF116766.D
Acq On : 3 Sep 2019 12:24
Operator : HP/JU
Sample : PB122720BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122720BL

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-BF083019.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	2.193	12	18	24	rVB	87453	134685	2.68%	0.339%
2	5.481	571	577	580	rBV	3968490	4071498	80.91%	10.244%
3	6.481	741	747	750	rBV	3703177	4335193	86.15%	10.907%
4	6.622	766	771	774	rBV	4438597	4336488	86.17%	10.910%
5	6.845	806	809	813	rBV	1092049	910587	18.09%	2.291%
6	7.004	832	836	840	rBV	3461468	3368573	66.94%	8.475%
7	7.410	899	905	908	rBV	2552954	2763330	54.91%	6.952%
8	8.127	1022	1027	1031	rBV	1392704	1195424	23.75%	3.008%
9	9.204	1204	1210	1213	rBV	5094415	5032349	100.00%	12.661%
10	9.880	1320	1325	1329	rBV	1652412	1385150	27.52%	3.485%
11	10.669	1454	1459	1462	rBV	2881151	2728834	54.23%	6.866%
12	11.363	1573	1577	1580	rBV	1631409	1352775	26.88%	3.404%
13	12.951	1841	1847	1850	rBV	4487493	4797994	95.34%	12.072%
14	13.992	2020	2024	2030	rVB	1238686	1054876	20.96%	2.654%
15	14.462	2099	2104	2108	rBV2	82251	90732	1.80%	0.228%
16	14.768	2151	2156	2160	rBV	145206	164665	3.27%	0.414%
17	15.104	2208	2213	2218	rBV	199850	245650	4.88%	0.618%
18	15.445	2266	2271	2274	rBV	711062	872674	17.34%	2.196%
19	15.480	2274	2277	2287	rVB	243210	317424	6.31%	0.799%
20	15.909	2344	2350	2361	rVB	195291	315457	6.27%	0.794%
21	16.409	2430	2435	2441	rVB	108117	188730	3.75%	0.475%
22	16.992	2530	2534	2544	rVB4	42144	83128	1.65%	0.209%

Sum of corrected areas: 39746216

LSC Report - Integrated Chromatogram

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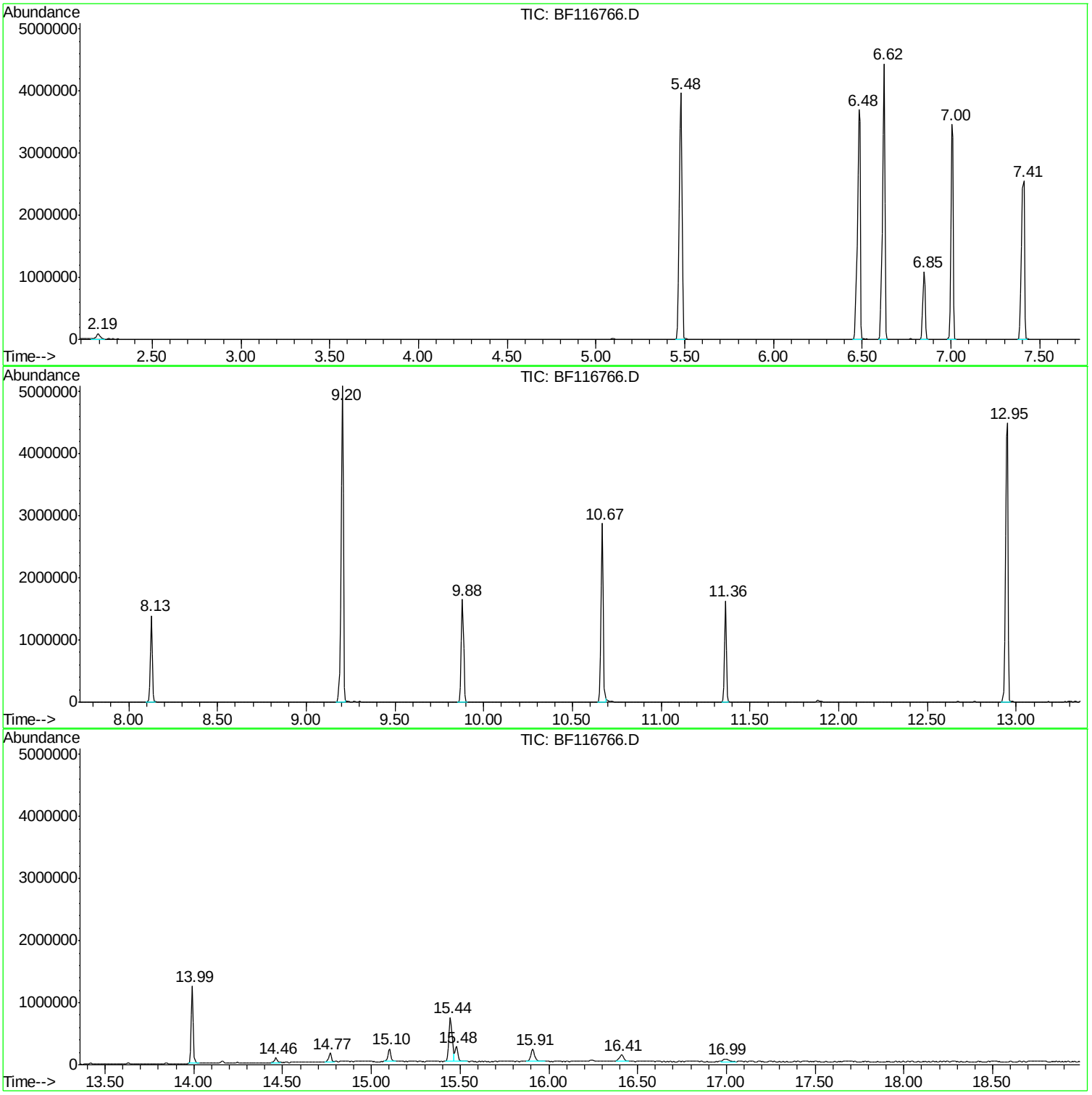
Sample : PB122720BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122720BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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\BF090319\
Data File : BF116766.D
Acq On : 3 Sep 2019 12:24
Operator : HP/JU
Sample : PB122720BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122720BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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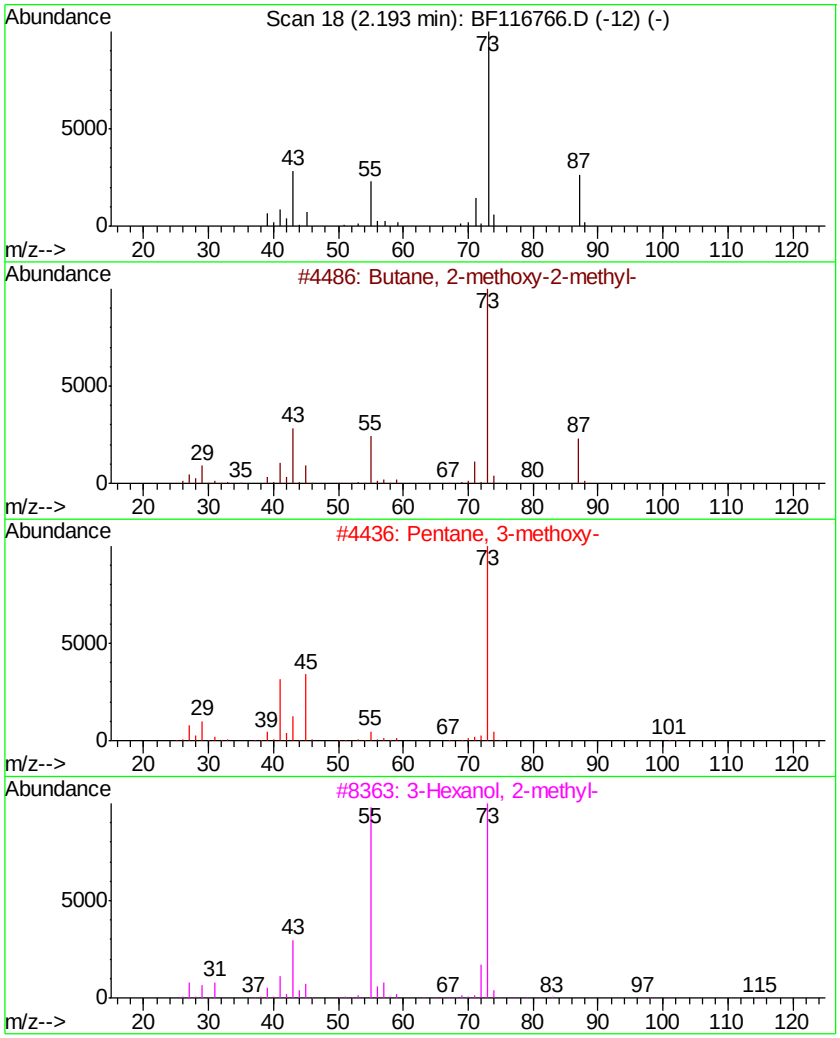
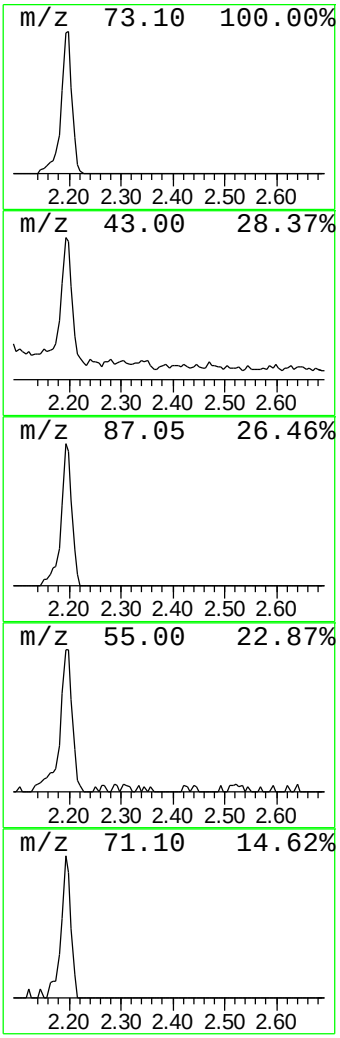
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	2.96 ng	134685	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





Library Search Compound Report

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Data File : BF116766.D
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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122720BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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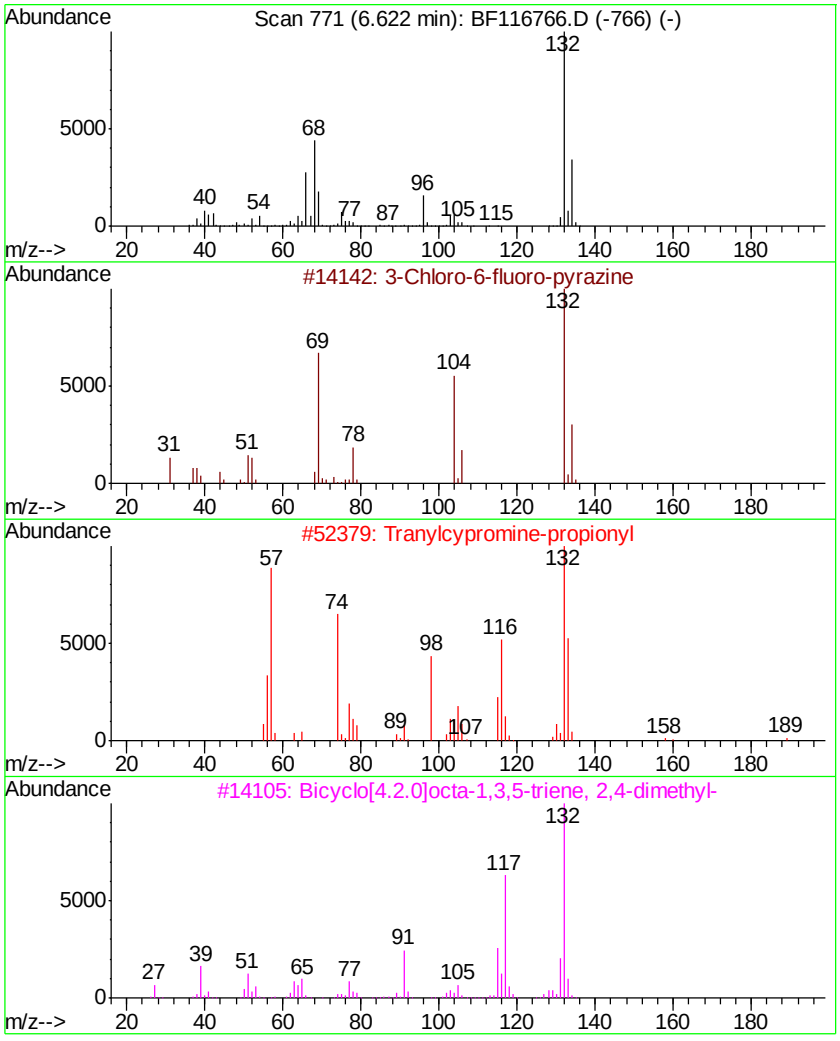
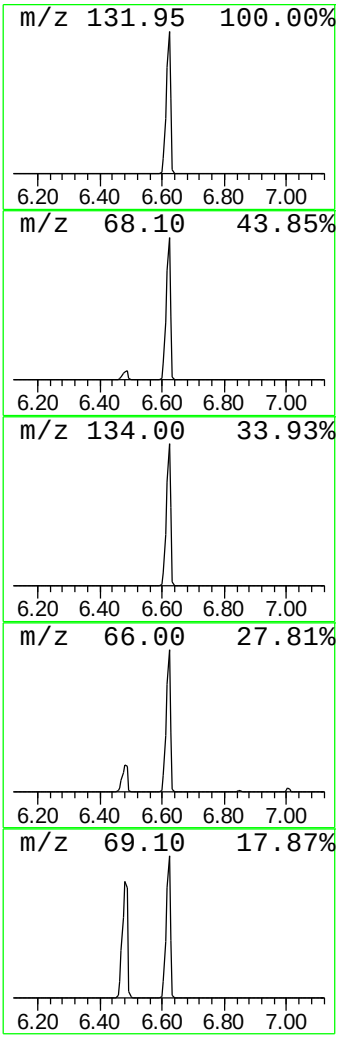
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	95.25 ng	4336490	1,4-Dichlorobenzene-d4	6.85

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	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	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\BF090319\
Data File : BF116766.D
Acq On : 3 Sep 2019 12:24
Operator : HP/JU
Sample : PB122720BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122720BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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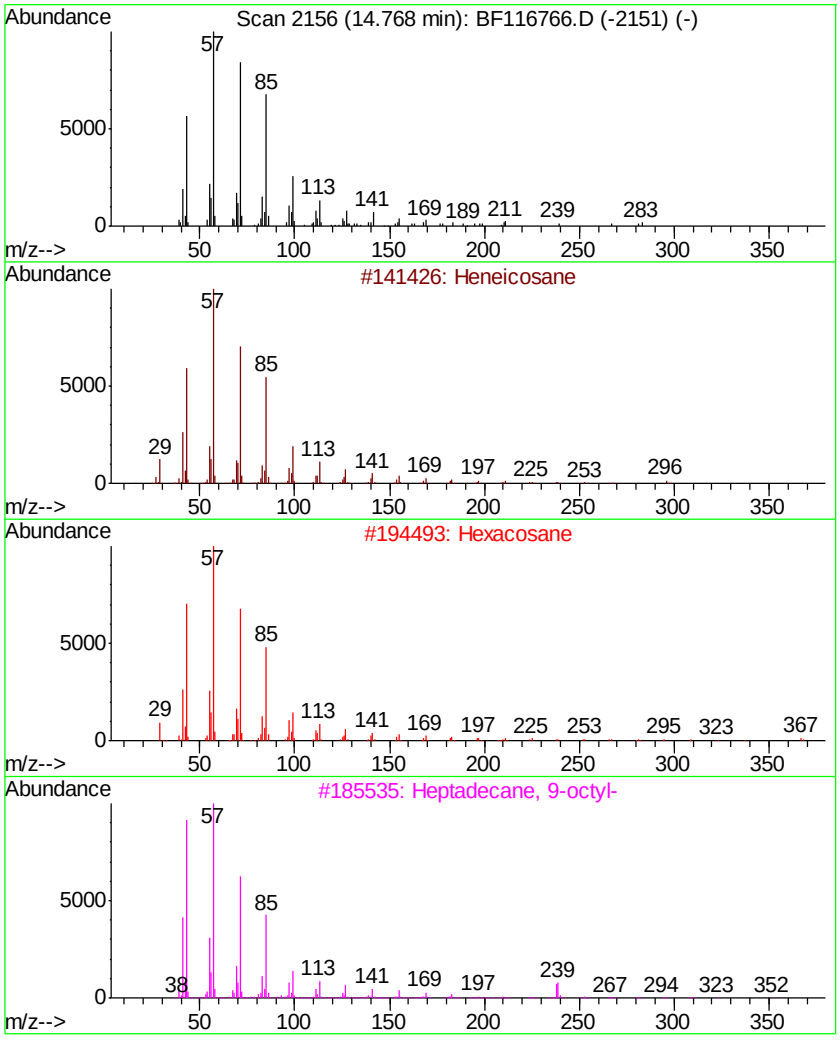
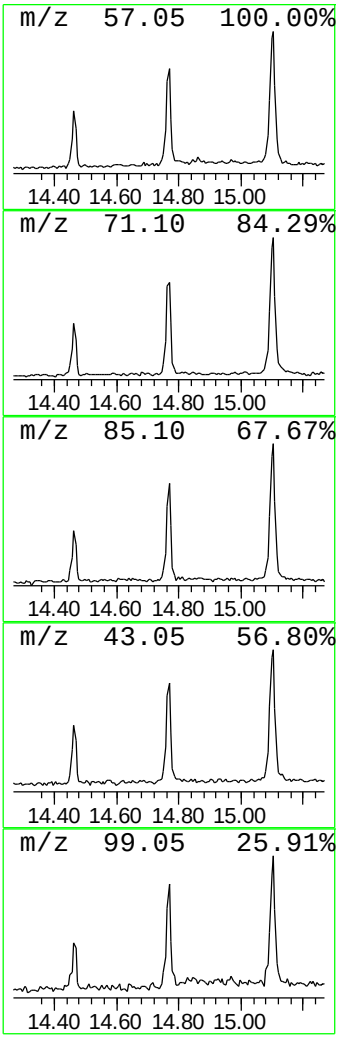
Peak Number 4 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	3.77 ng	164665	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Eicosane	282	C20H42	000112-95-8	86





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Data File : BF116766.D
Acq On : 3 Sep 2019 12:24
Operator : HP/JU
Sample : PB122720BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122720BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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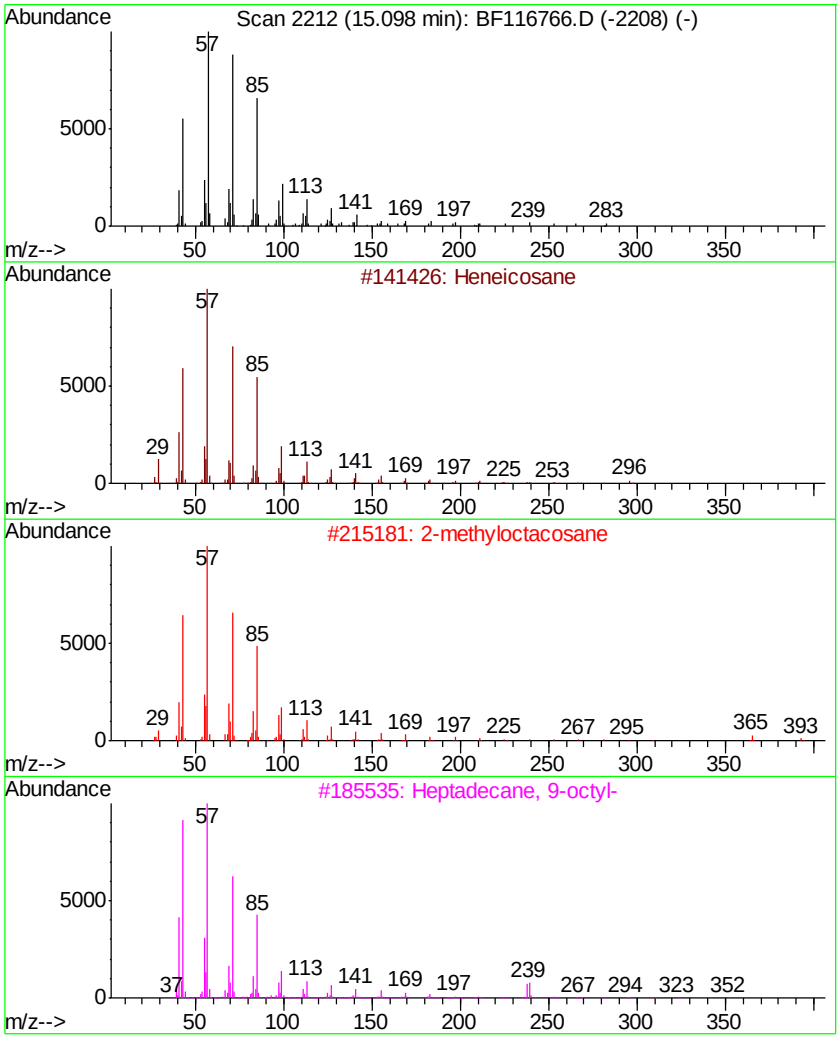
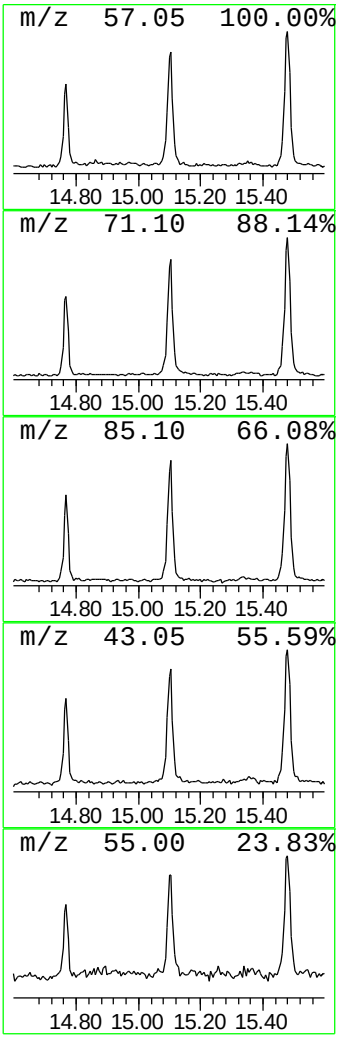
Peak Number 5 2-methyloctacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	5.63 ng	245650	Perylene-d12	15.44

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	87
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Hexadecane	226	C16H34	000544-76-3	80
5	Nonadecane	268	C19H40	000629-92-5	80





Library Search Compound Report

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Data File : BF116766.D
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Sample : PB122720BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122720BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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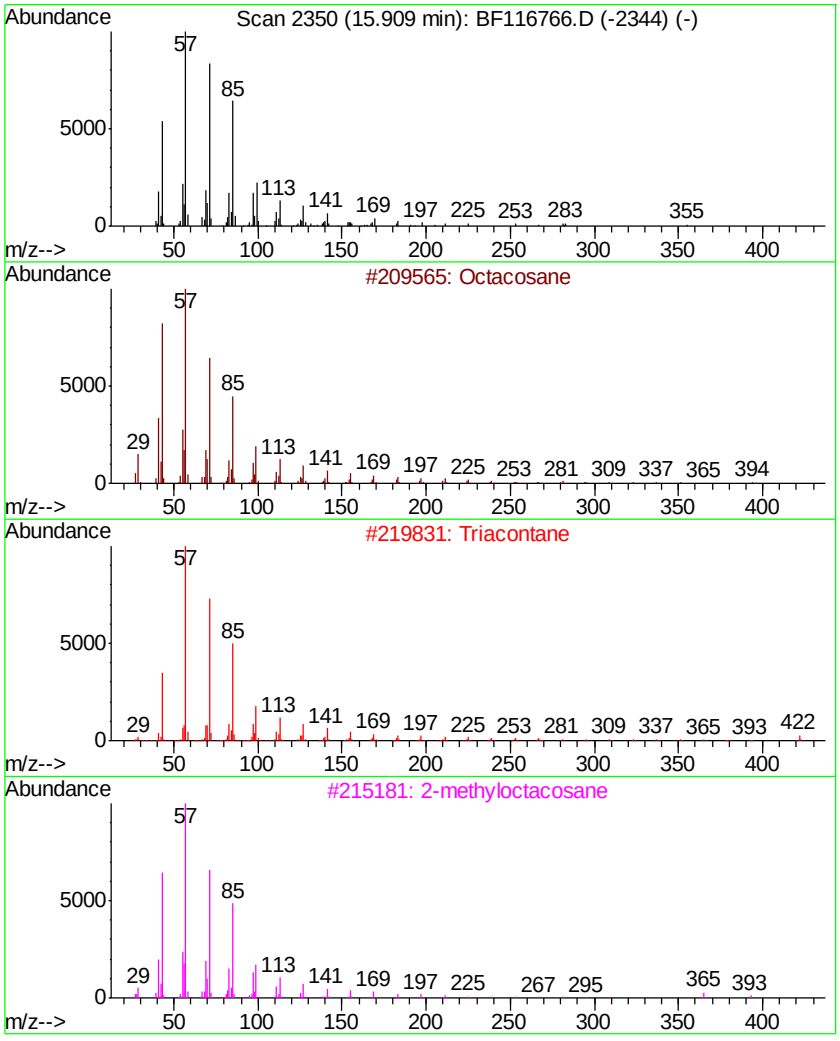
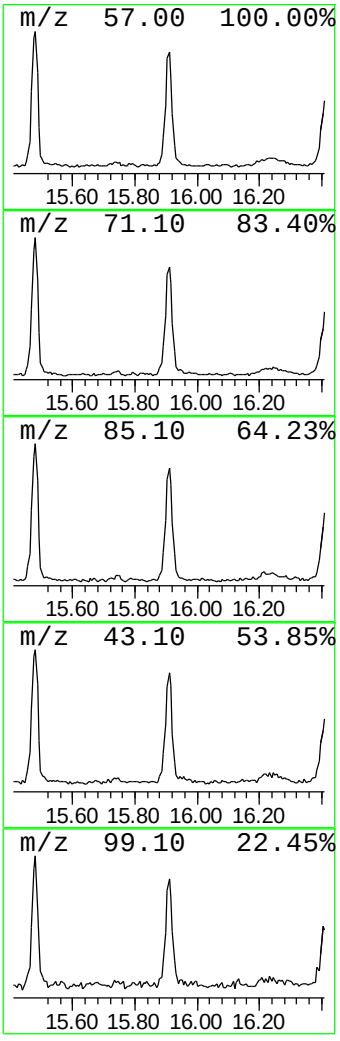
Peak Number 6 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	7.23 ng	315457	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Triacontane	422	C30H62	000638-68-6	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Heptacosane	380	C27H56	000593-49-7	91





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Operator : HP/JU
Sample : PB122720BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB122720BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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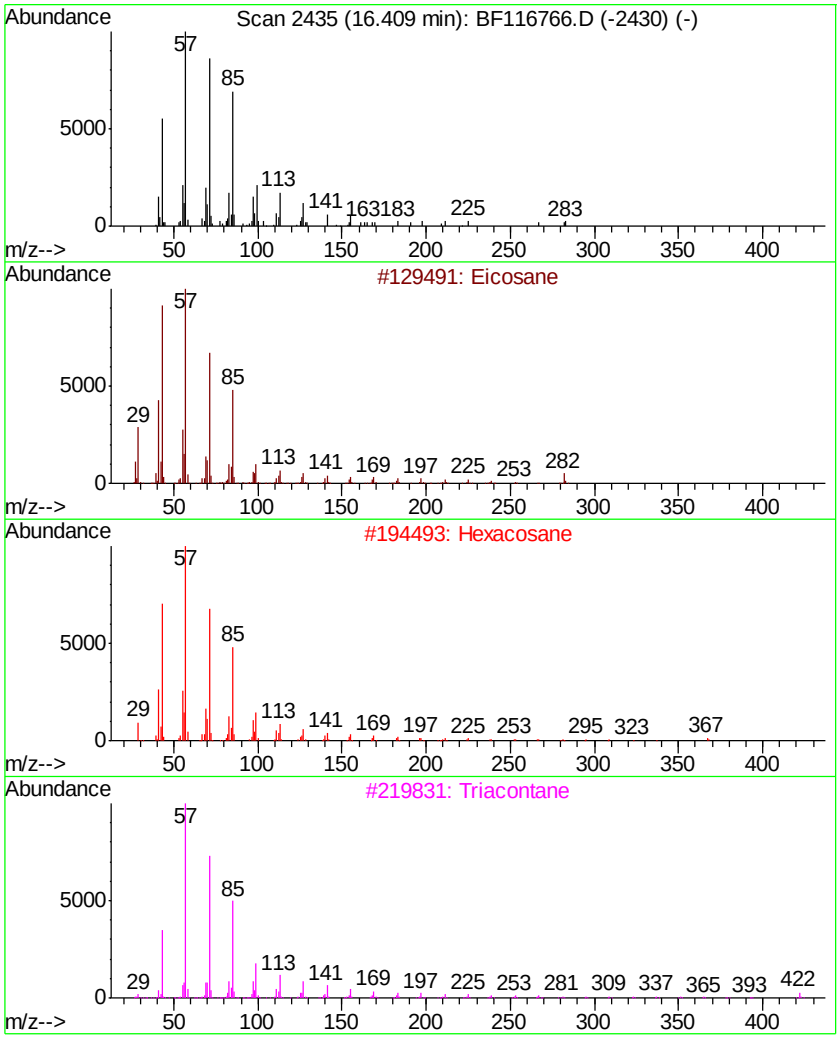
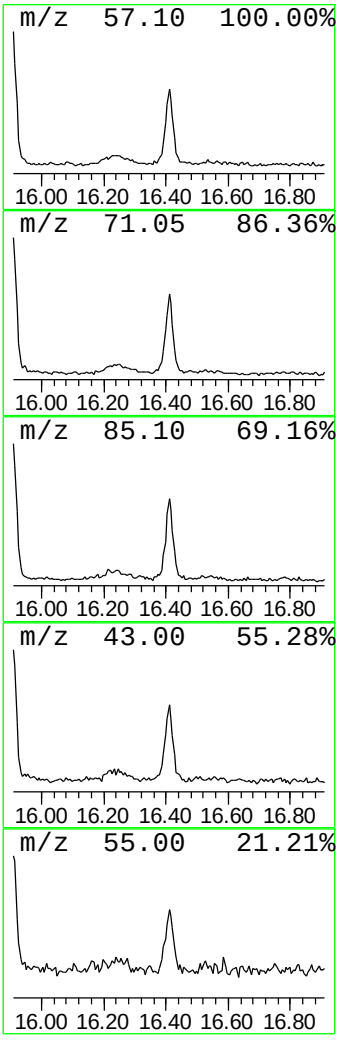
Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	4.33 ng	188730	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hexacosane	366	C26H54	000630-01-3	91
3	Triacontane	422	C30H62	000638-68-6	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heneicosane	296	C21H44	000629-94-7	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090319\
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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
Butane, 2-methoxy...	2.19	3.0	ng	134685	1	6.85	910587	20.0
unknown6.62	6.62	95.3	ng	4336490	1	6.85	910587	20.0
Heneicosane	14.77	3.8	ng	164665	6	15.44	872674	20.0
2-methyloctacosane	15.10	5.6	ng	245650	6	15.44	872674	20.0
Octacosane	15.91	7.2	ng	315457	6	15.44	872674	20.0
Eicosane	16.41	4.3	ng	188730	6	15.44	872674	20.0