LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108929.D
Acq On : 11 Sep 2018 12:29
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112707BL

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	4.948	440	444	455	rBV	120787	167471	3.27%	0.413%
2	5.360	508	514	517	rBV	3775924	3859333	75.35%	9.512%
3	6.378	681	687	689	rBV	3677916	4019286	78.48%	9.906%
4	6.507	704	709	712	rBV	4006606	4027400	78.63%	9.926%
5	6.736	745	748	752	rBV	1240861	985384	19.24%	2.429%
6	6.895	771	775	778	rBV	3659522	3215389	62.78%	7.925%
7	7.295	838	843	846	rBV	2660413	2655460	51.85%	6.545%
8	8.019	961	966	969	rBV	1461013	1257162	24.55%	3.098%
9	9.095	1144	1149	1152	rBV	5043929	4835438	94.41%	11.917%
10	9.766	1258	1263	1267	rBV	1536433	1467099	28.64%	3.616%
11	10.554	1392	1397	1400	rBV	3222385	3022715	59.02%	7.450%
12	11.248	1510	1515	1518	rBV	1784667	1569719	30.65%	3.869%
13	12.830	1779	1784	1788	rBV	4868055	5121688	100.00%	12.623%
14	13.871	1957	1961	1965	rBV	1794410	1575982	30.77%	3.884%
15	14.359	2041	2044	2047	rVB	81126	70608	1.38%	0.174%
16	14.654	2088	2094	2098	rBV	158787	169410	3.31%	0.418%
17	14.977	2144	2149	2154	rBV	221450	248595	4.85%	0.613%
18	15.283	2195	2201	2205	rBV	1146151	1379568	26.94%	3.400%
19	15.336	2205	2210	2216	rVB	245077	332067	6.48%	0.818%
20	15.742	2273	2279	2285	rBV	207094	308806	6.03%	0.761%
21	16.212	2354	2359	2368	rVB2	113402	201912	3.94%	0.498%
22	16.765	2448	2453	2460	rVB3	39587	84749	1.65%	0.209%

Sum of corrected areas: 40575241

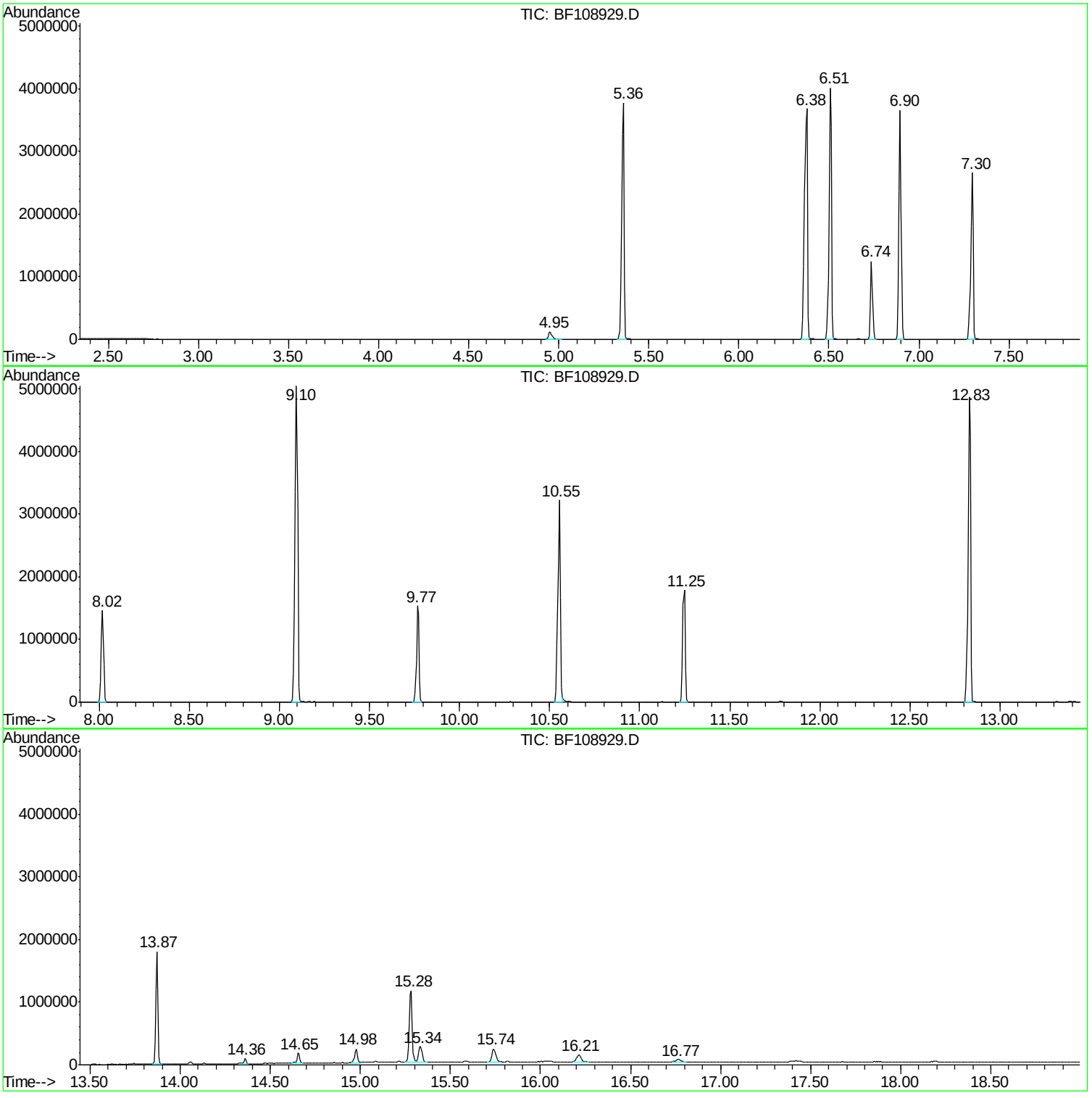
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108929.D
Acq On : 11 Sep 2018 12:29
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112707BL

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\BF091118\
Data File : BF108929.D
Acq On : 11 Sep 2018 12:29
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112707BL

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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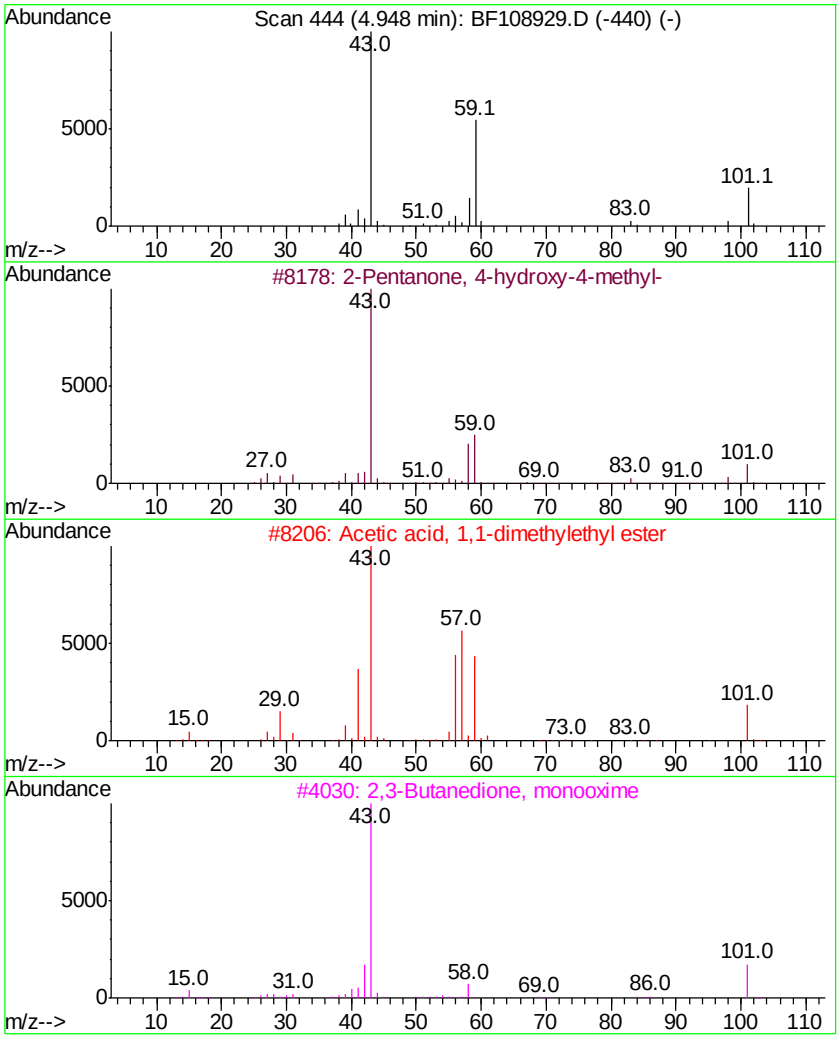
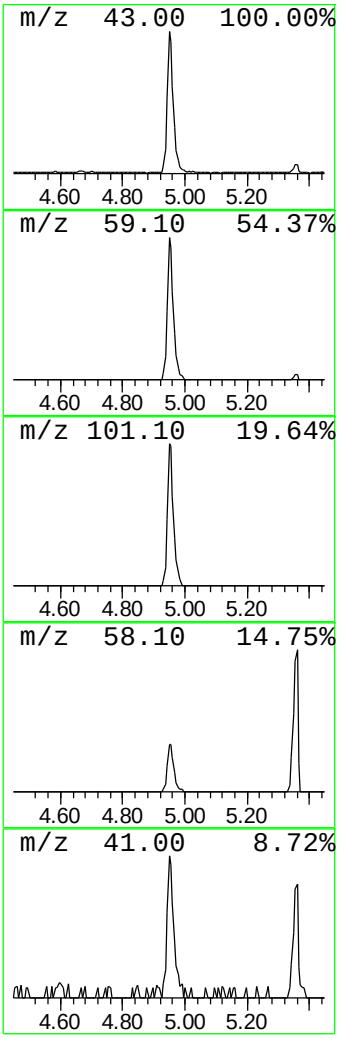
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	3.40 ng	167471	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	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	3-Hexanol	102	C6H14O	000623-37-0	28
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108929.D
Acq On : 11 Sep 2018 12:29
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112707BL

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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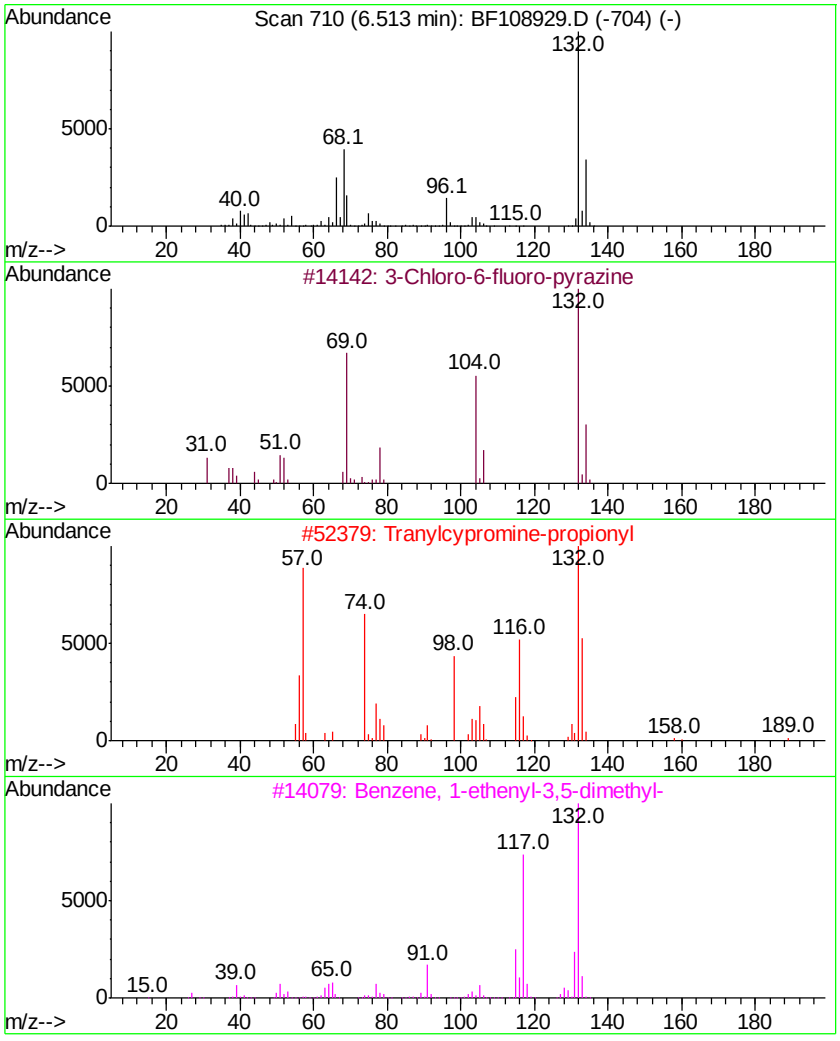
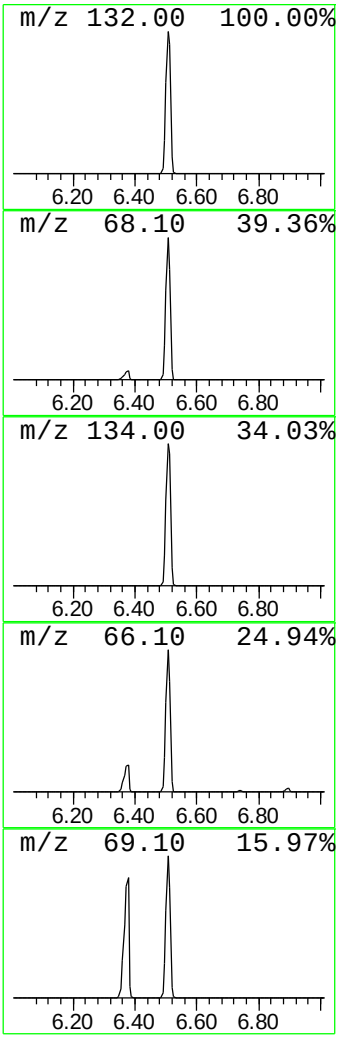
Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	81.74 ng	4027400	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	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108929.D
Acq On : 11 Sep 2018 12:29
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112707BL

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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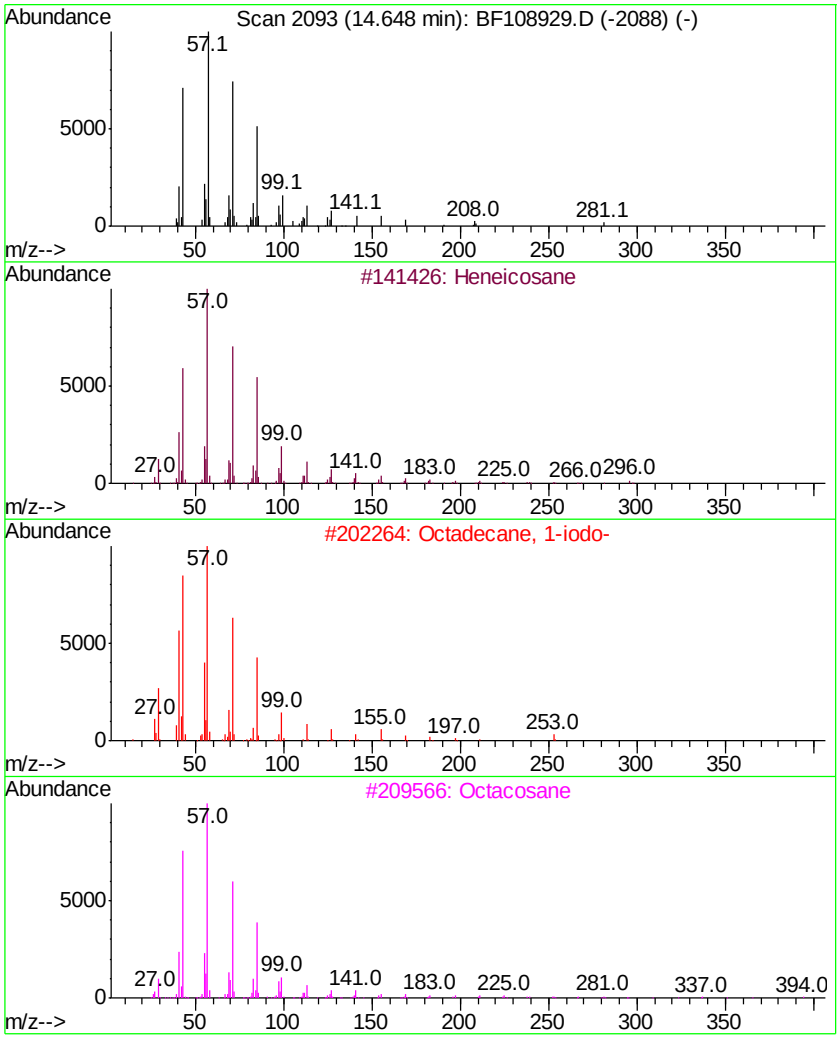
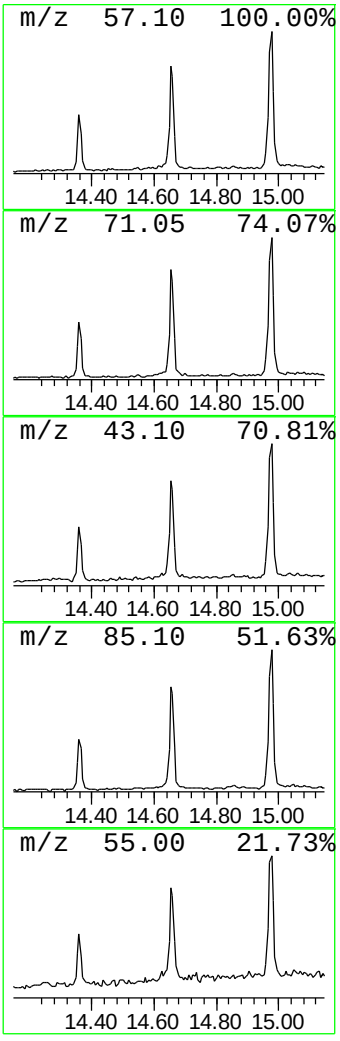
Peak Number 4 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.46 ng	169410	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
5	Octadecane	254	C18H38	000593-45-3	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108929.D
Acq On : 11 Sep 2018 12:29
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112707BL

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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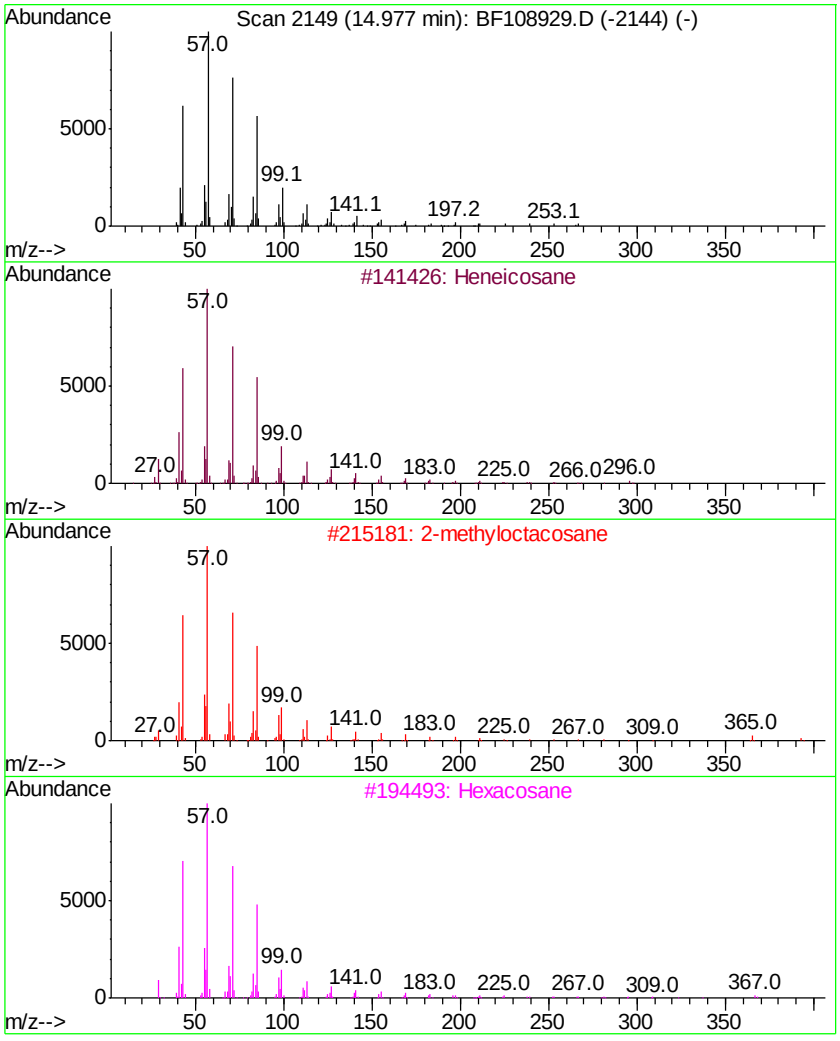
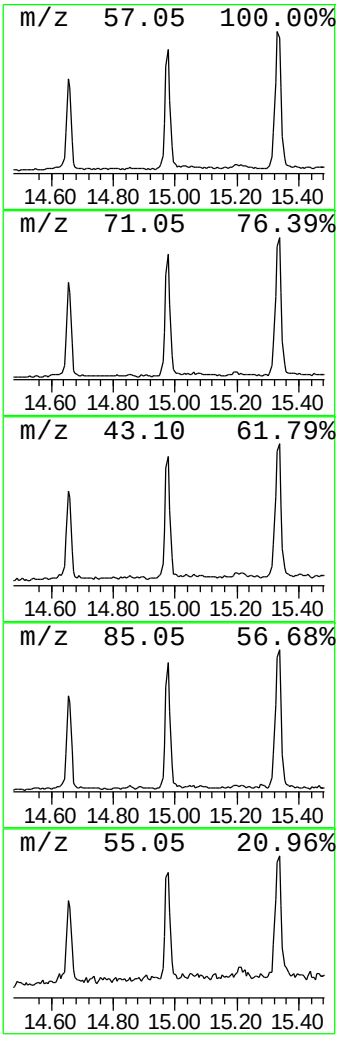
Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	3.60 ng	248595	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	Hexacosane	366	C26H54	000630-01-3	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptacosane	380	C27H56	000593-49-7	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
Data File : BF108929.D
Acq On : 11 Sep 2018 12:29
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112707BL

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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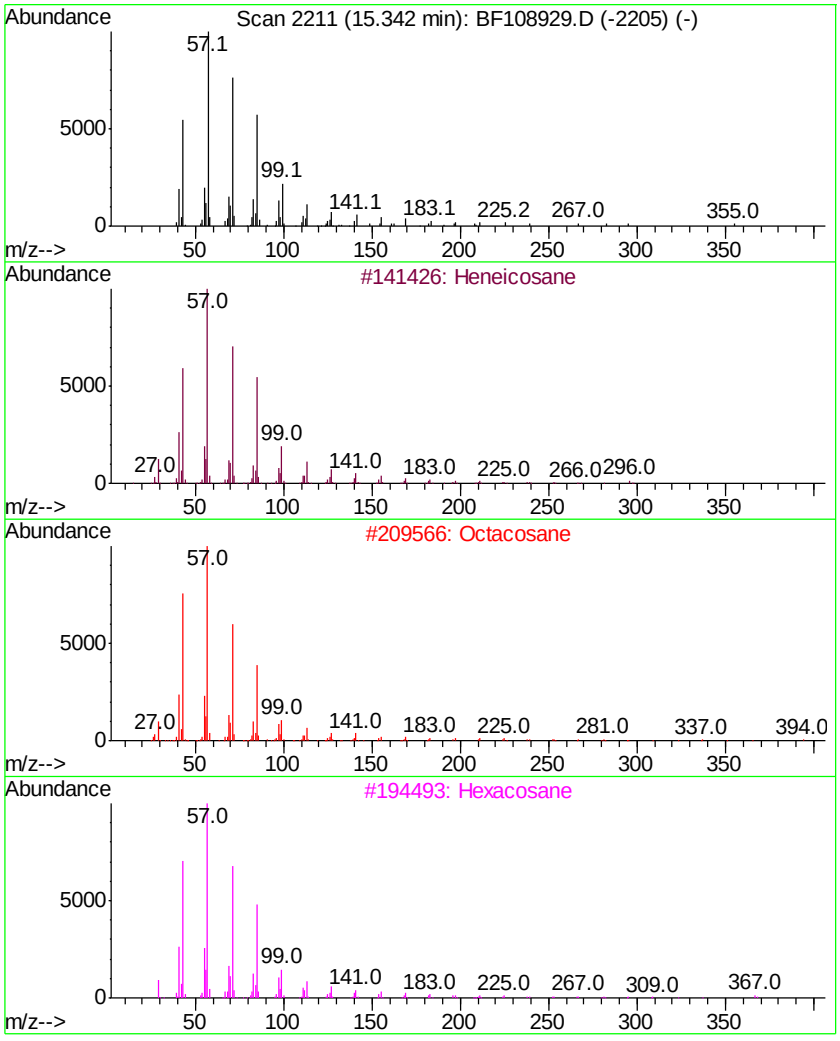
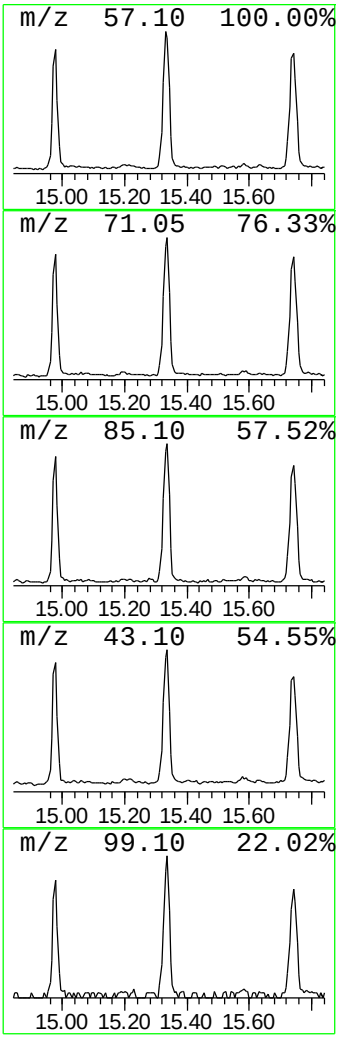
Peak Number 6 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	4.81 ng	332067	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	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Heptadecane	240	C17H36	000629-78-7	87





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Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112707BL

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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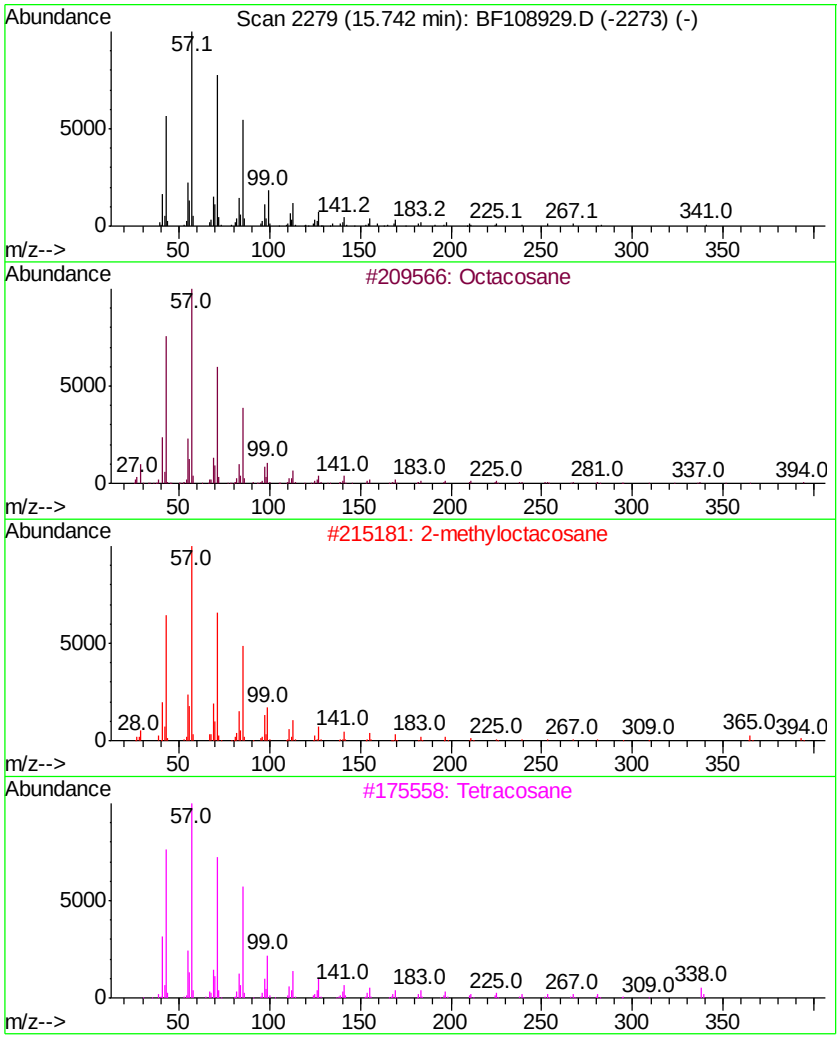
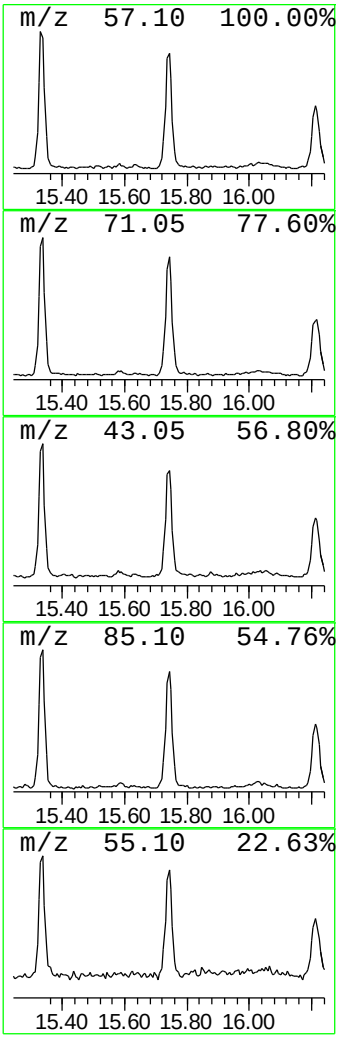
Peak Number 7 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	4.48 ng	308806	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptadecane	240	C17H36	000629-78-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091118\
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Acq On : 11 Sep 2018 12:29
Operator : JU/SJ
Sample : PB112707BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112707BL

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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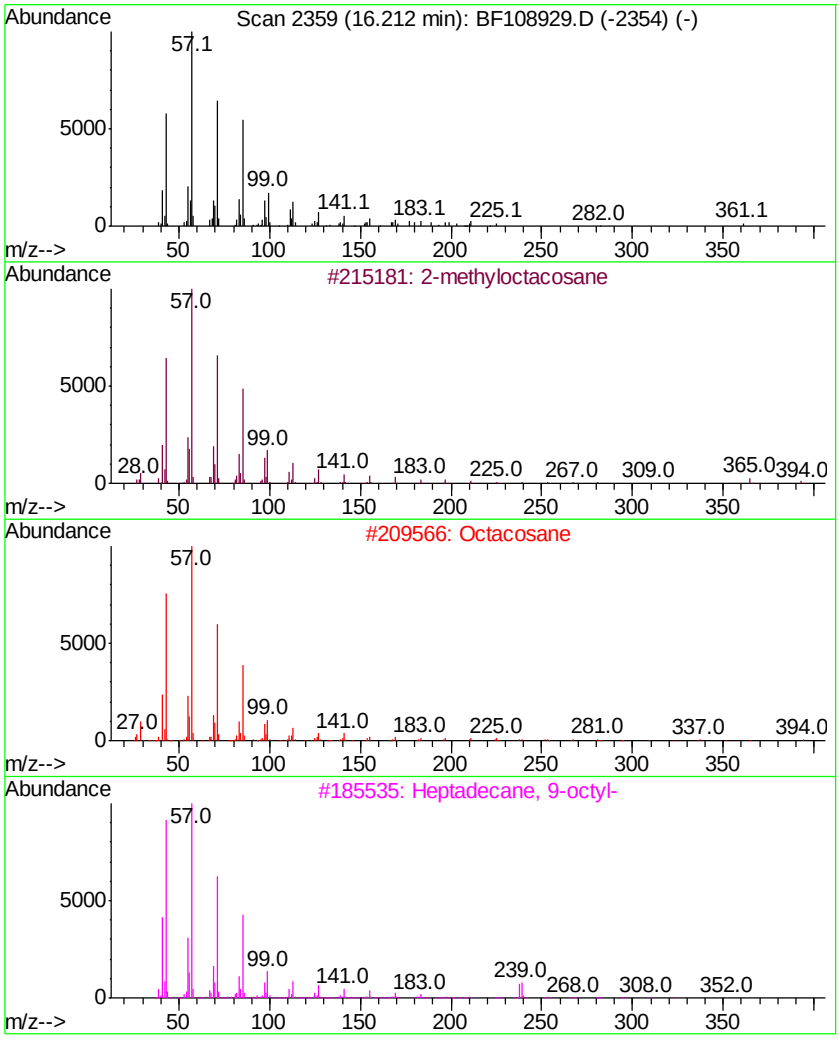
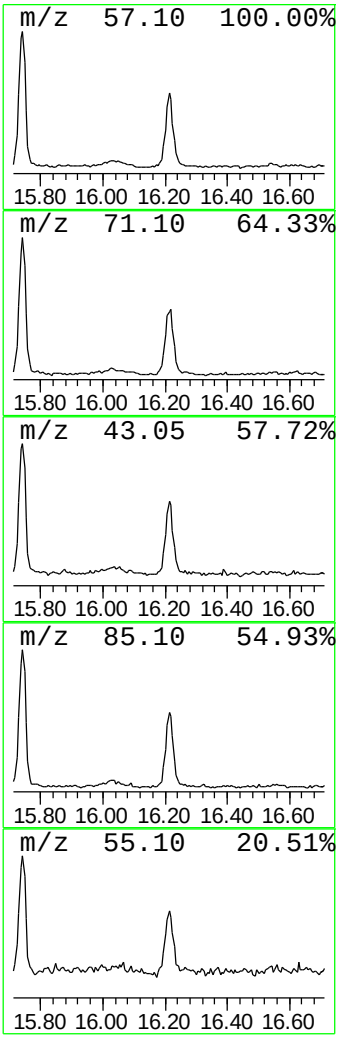
Peak Number 8 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	2.93 ng	201912	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Octadecane	254	C18H38	000593-45-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091118\
Data File : BF108929.D
Acq On : 11 Sep 2018 12:29
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
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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...	4.95	3.4	ng	167471	1	6.74	985384	20.0
unknown6.51	6.51	81.7	ng	4027400	1	6.74	985384	20.0
Heneicosane	14.65	2.5	ng	169410	6	15.28	1379570	20.0
Hexacosane	14.98	3.6	ng	248595	6	15.28	1379570	20.0
Heptadecane	15.34	4.8	ng	332067	6	15.28	1379570	20.0
Octacosane	15.74	4.5	ng	308806	6	15.28	1379570	20.0
2-methyloctacosane	16.21	2.9	ng	201912	6	15.28	1379570	20.0