LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110411.D
Acq On : 2 Nov 2018 14:50
Operator : JU/SJ
Sample : J5794-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10B-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-BF102318.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	2.275	27	32	47	rVB	249797	366315	22.22%	2.511%
2	5.192	524	528	536	rBV	58070	82014	4.98%	0.562%
3	5.581	589	594	597	rBV	1491089	1409001	85.48%	9.657%
4	6.581	759	764	779	rBV	1528975	1564499	94.92%	10.723%
5	6.722	784	788	792	rBV	1628635	1552962	94.22%	10.644%
6	6.957	824	828	834	rBV	524712	465849	28.26%	3.193%
7	7.110	850	854	863	rBV	1396793	1169181	70.93%	8.014%
8	7.516	918	923	947	rBV	977637	960004	58.24%	6.580%
9	8.239	1042	1046	1058	rBV	562684	580216	35.20%	3.977%
10	9.310	1223	1228	1239	rBV	1900073	1648283	100.00%	11.298%
11	9.704	1291	1295	1303	rBV	165059	178519	10.83%	1.224%
12	9.998	1341	1345	1354	rVB	585807	565423	34.30%	3.875%
13	10.786	1475	1479	1492	rBV	816275	763643	46.33%	5.234%
14	11.486	1595	1598	1607	rBV	475503	472110	28.64%	3.236%
15	11.821	1652	1655	1659	rBV	15230	18470	1.12%	0.127%
16	11.992	1679	1684	1687	rBV2	41659	42903	2.60%	0.294%
17	12.033	1687	1691	1696	rVB	14662	20818	1.26%	0.143%
18	12.939	1840	1845	1848	rBV2	17774	25739	1.56%	0.176%
19	13.068	1863	1867	1870	rBV	1453704	1242164	75.36%	8.514%
20	13.951	2013	2017	2021	rBV	88722	113269	6.87%	0.776%
21	14.133	2044	2048	2056	rBV	534729	534564	32.43%	3.664%
22	14.268	2068	2071	2075	rBV3	19927	21350	1.30%	0.146%
23	14.568	2120	2122	2131	rVB2	32470	55747	3.38%	0.382%
24	14.886	2174	2176	2180	rVB	37600	35514	2.15%	0.243%
25	14.968	2186	2190	2195	rVB	84039	94864	5.76%	0.650%
26	15.239	2233	2236	2241	rVB	54785	64866	3.94%	0.445%
27	15.656	2301	2307	2316	rVB	298025	471839	28.63%	3.234%
28	16.092	2378	2381	2386	rVB2	44603	69612	4.22%	0.477%

Sum of corrected areas: 14589738

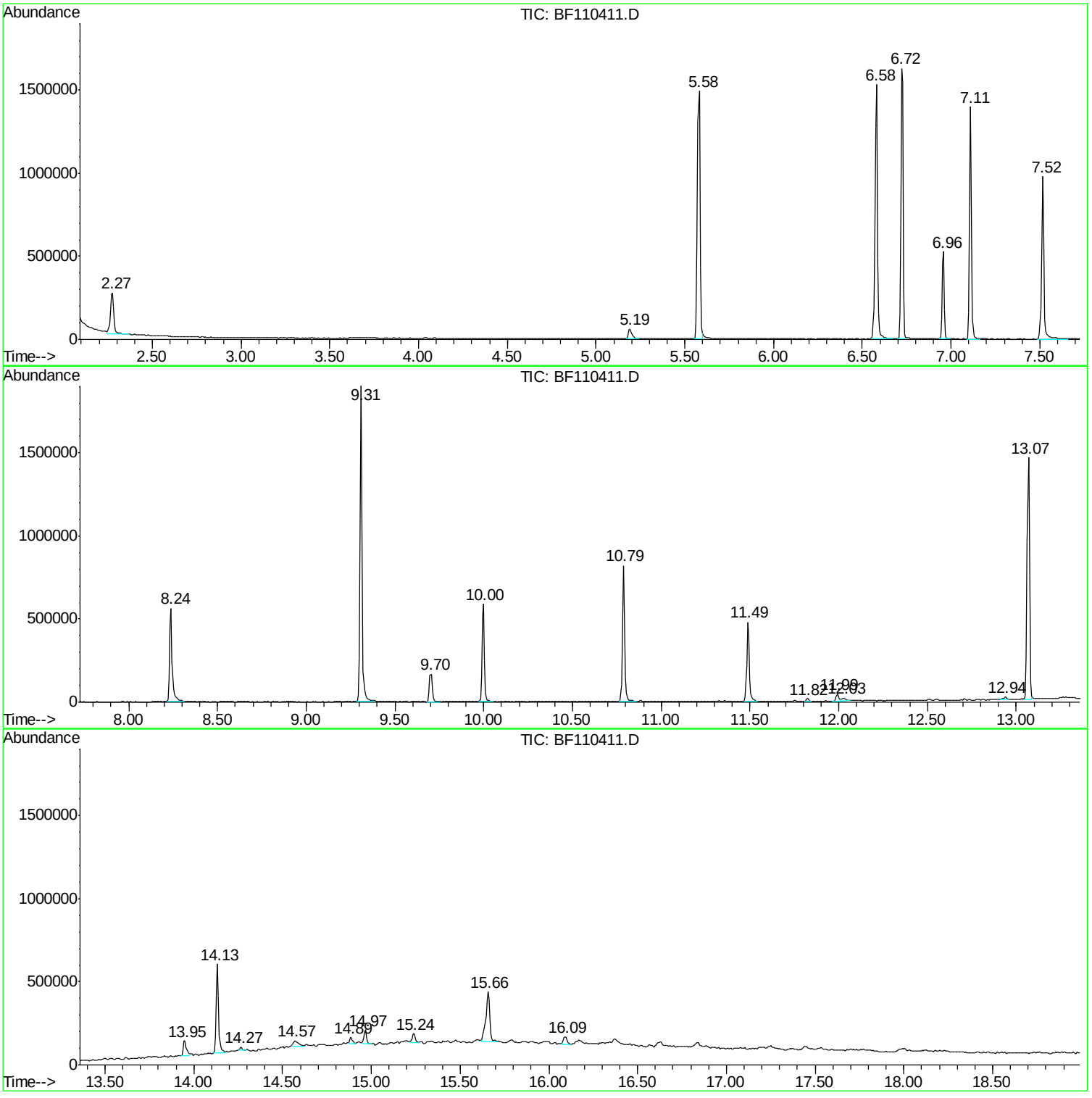
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110411.D
Acq On : 2 Nov 2018 14:50
Operator : JU/SJ
Sample : J5794-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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

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Data File : BF110411.D
Acq On : 2 Nov 2018 14:50
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : TP-10B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

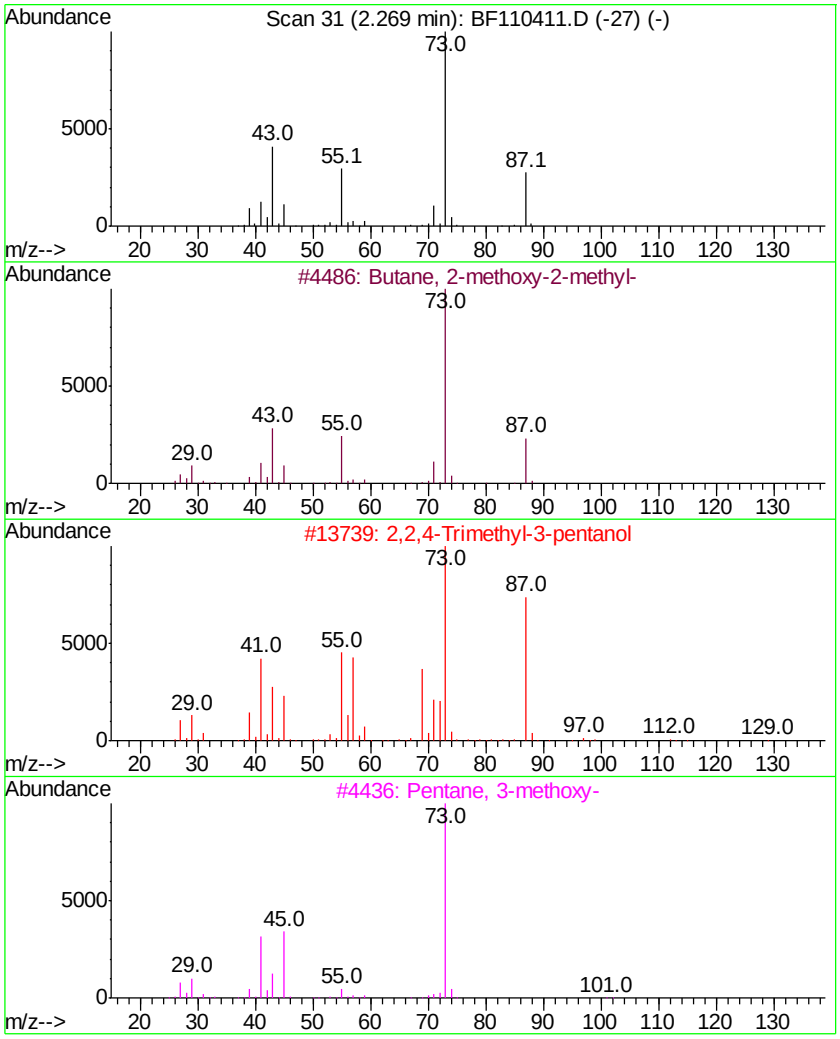
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

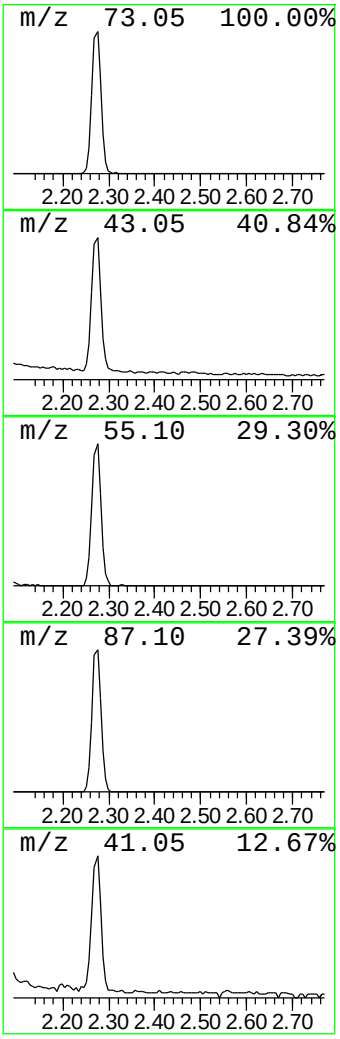
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	15.73 ng	366315	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J5794-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

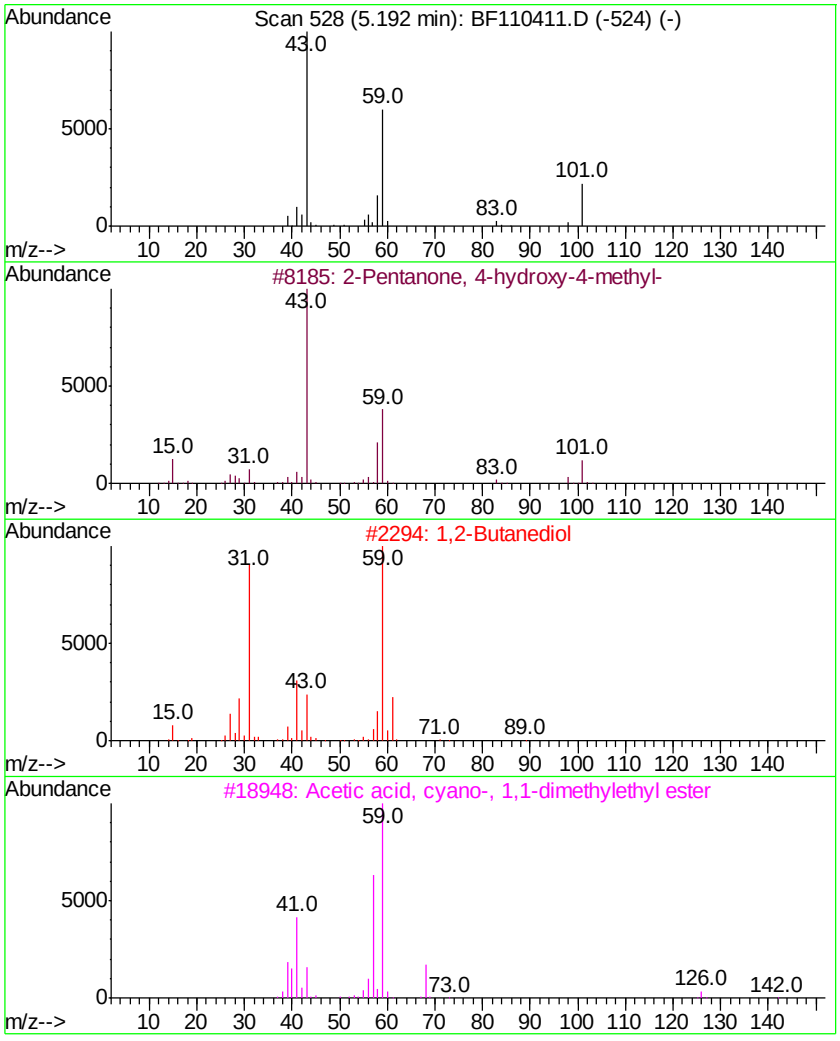
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

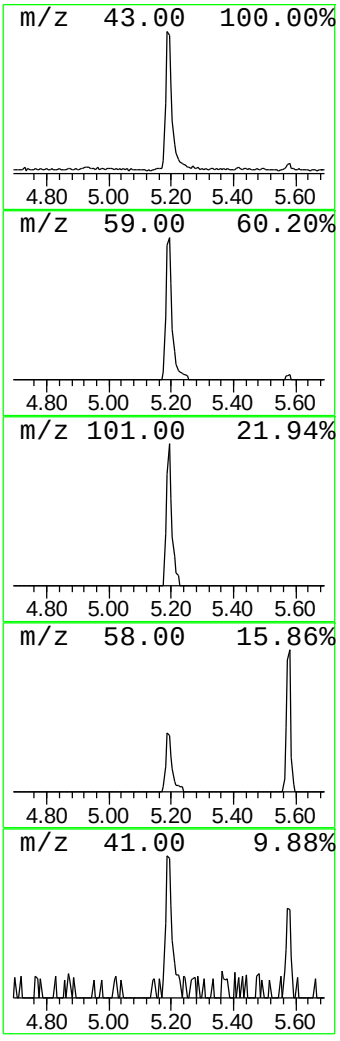
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.52 ng	82014	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	1,2-Butanediol	90	C4H10O2	000584-03-2	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	9
5	Hexanamide	115	C6H13NO	000628-02-4	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J5794-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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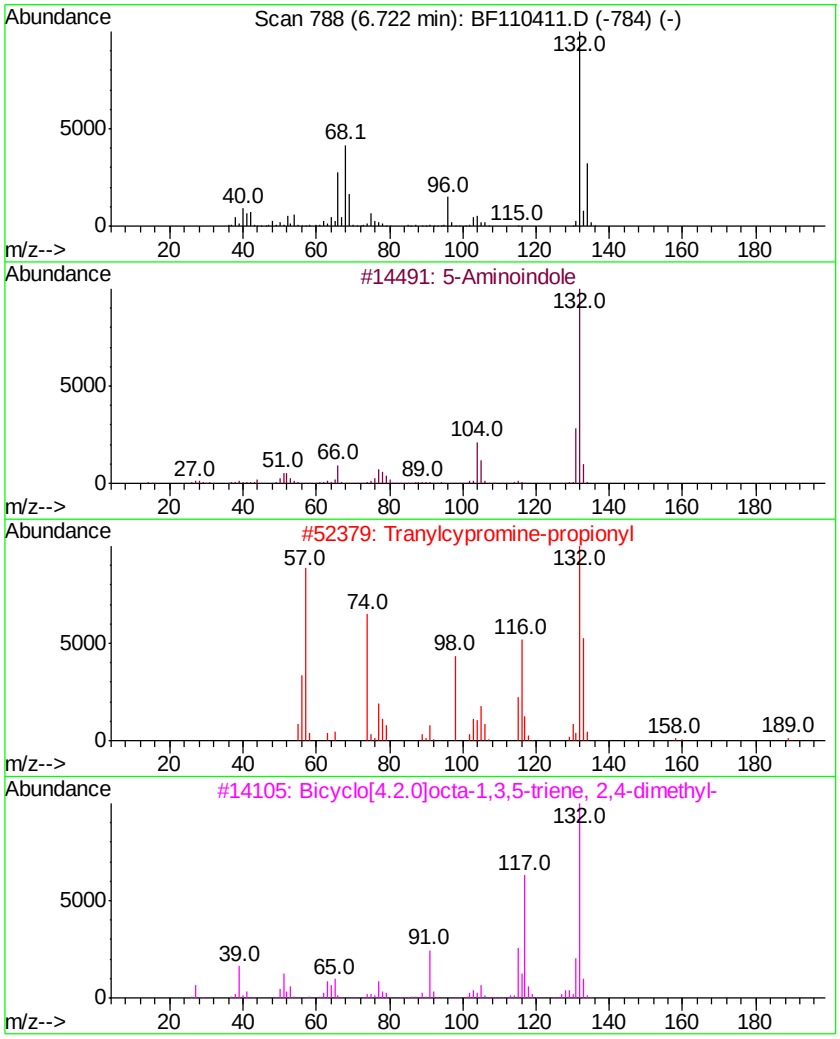
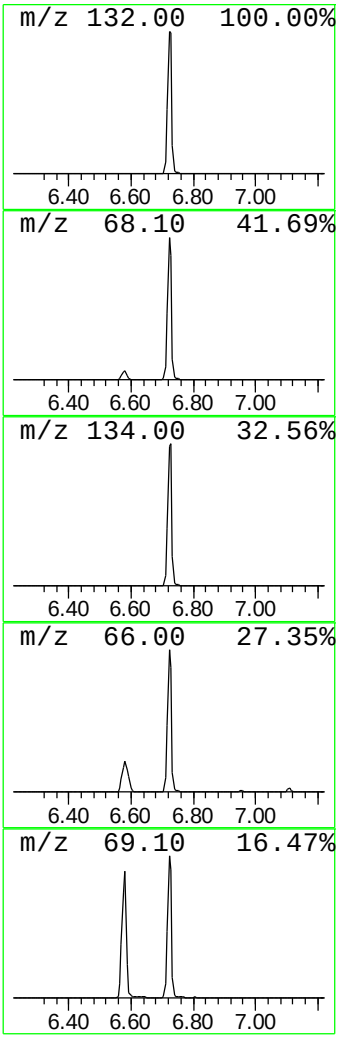
Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	66.67 ng	1552960	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
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Operator : JU/SJ
Sample : J5794-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

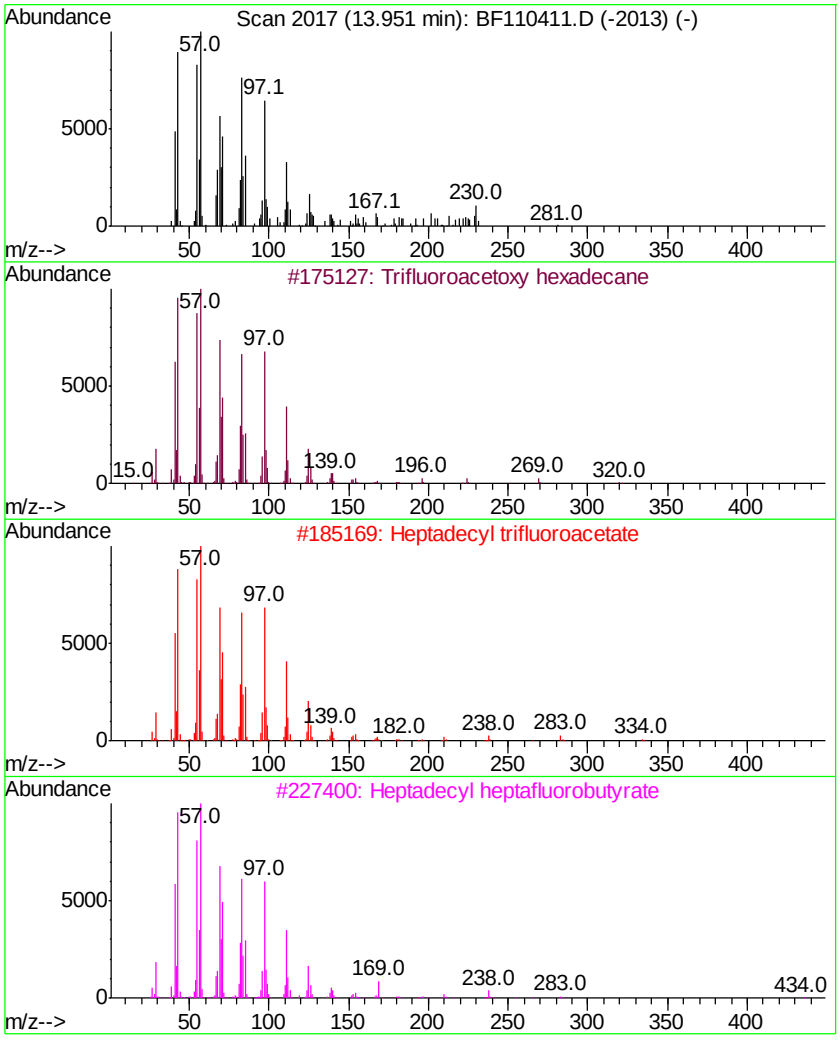
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

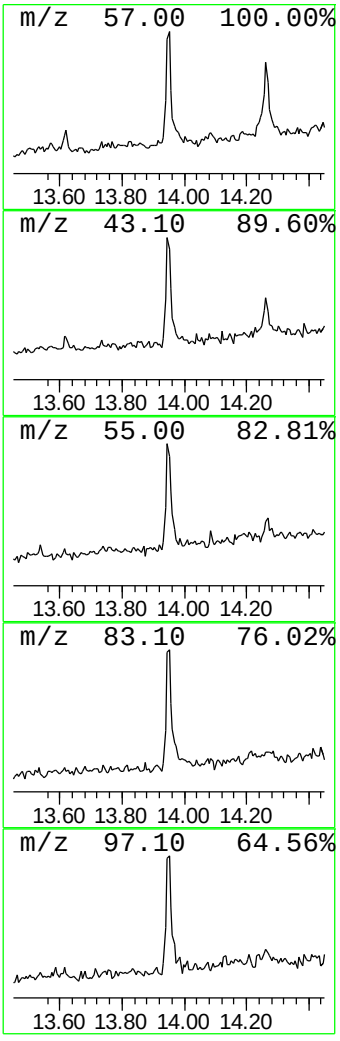
****

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.24 ng	113269	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





Library Search Compound Report

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Operator : JU/SJ
Sample : J5794-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-10B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

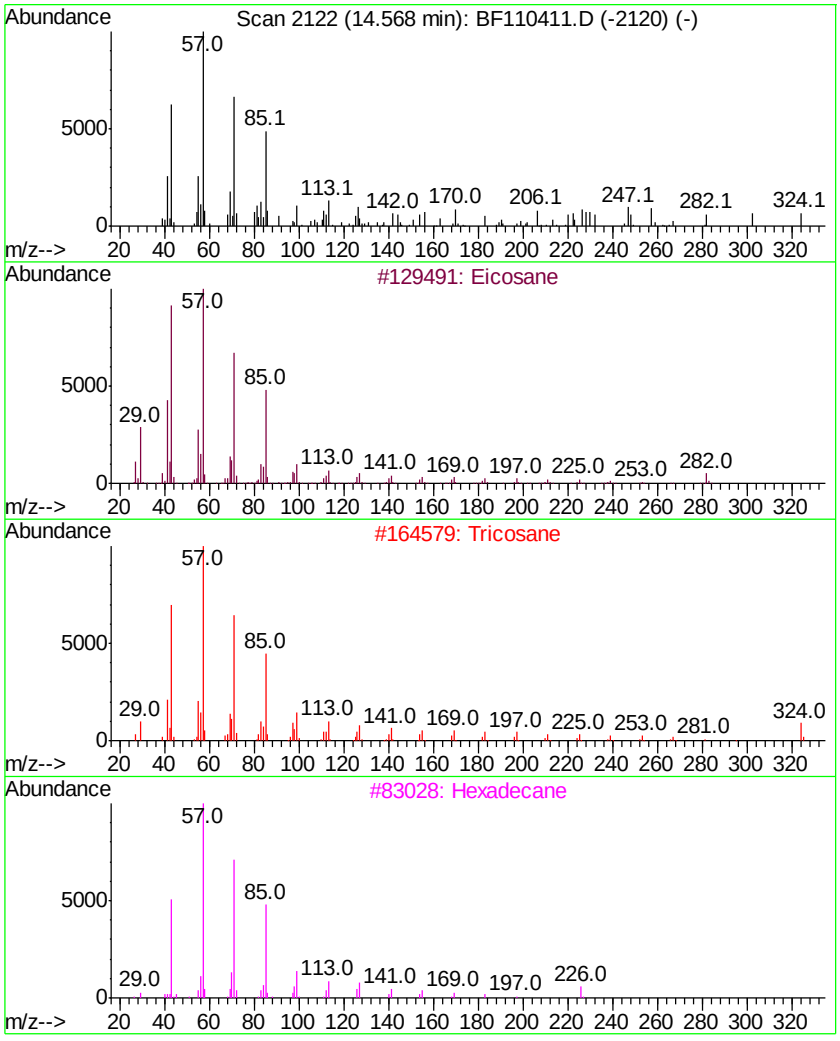
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

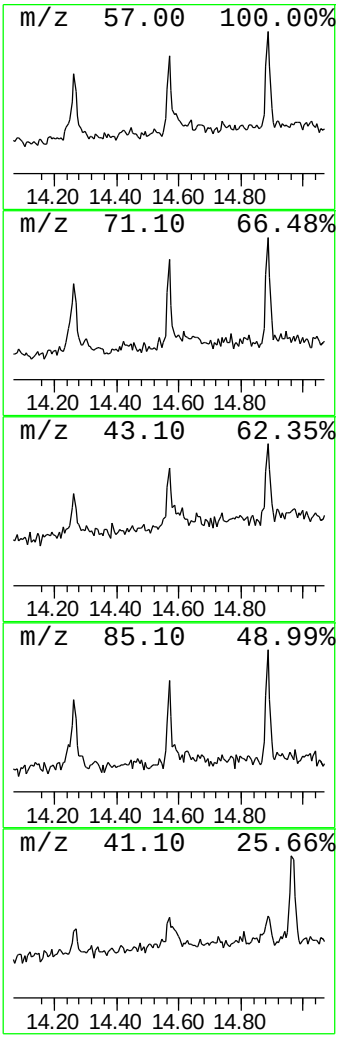
****

Peak Number 6 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.09 ng	55747	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	64
2	Tricosane	324	C23H48	000638-67-5	58
3	Hexadecane	226	C16H34	000544-76-3	53
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	49
5	Hentriacontane	437	C31H64	000630-04-6	49





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-10B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

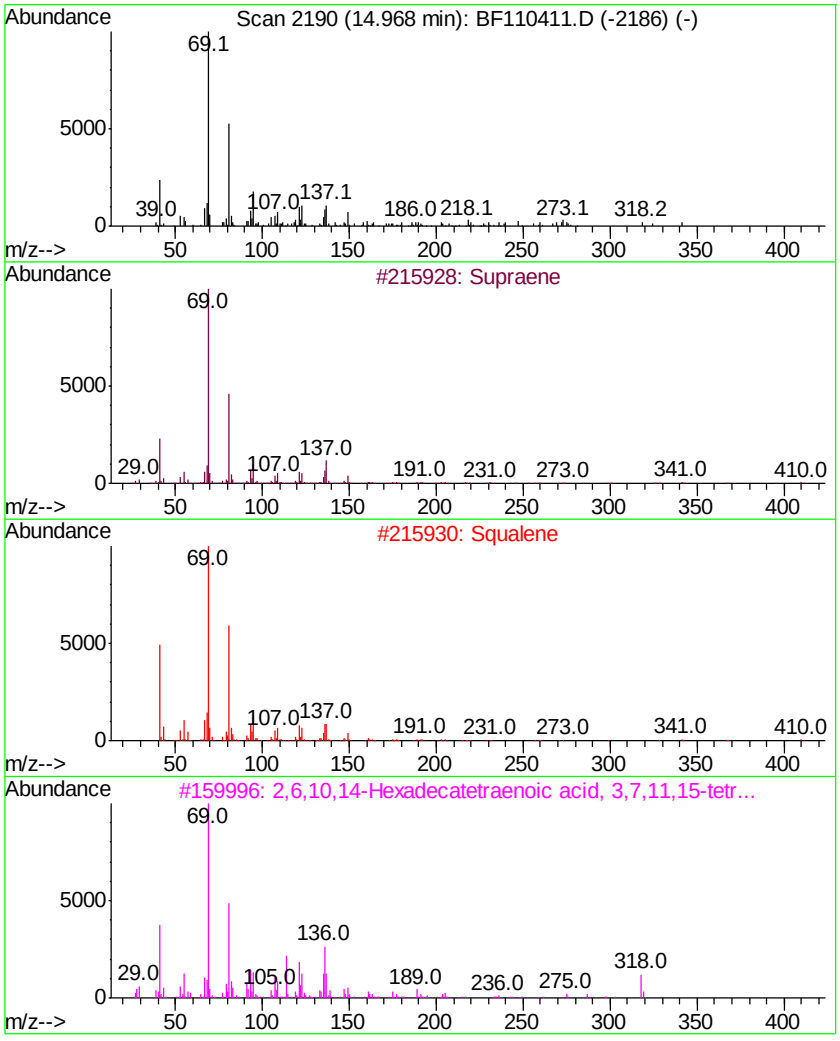
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

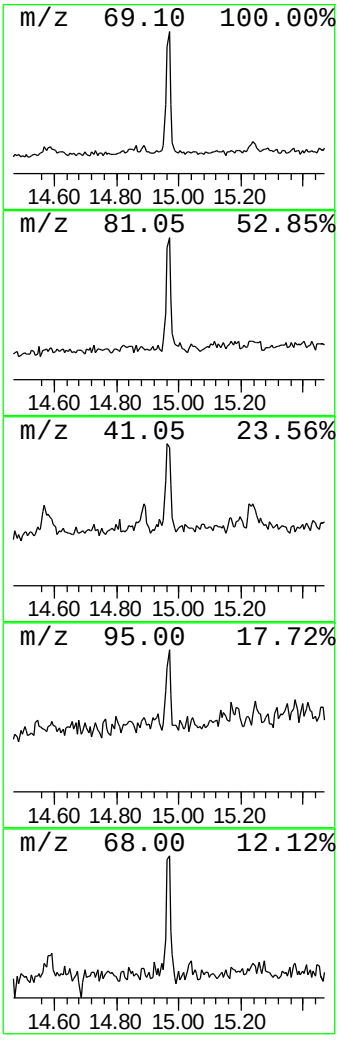
****

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	4.02 ng	94864	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	Squalene	410	C30H50	000111-02-4	87
3	2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	80
4	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : TP-10B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

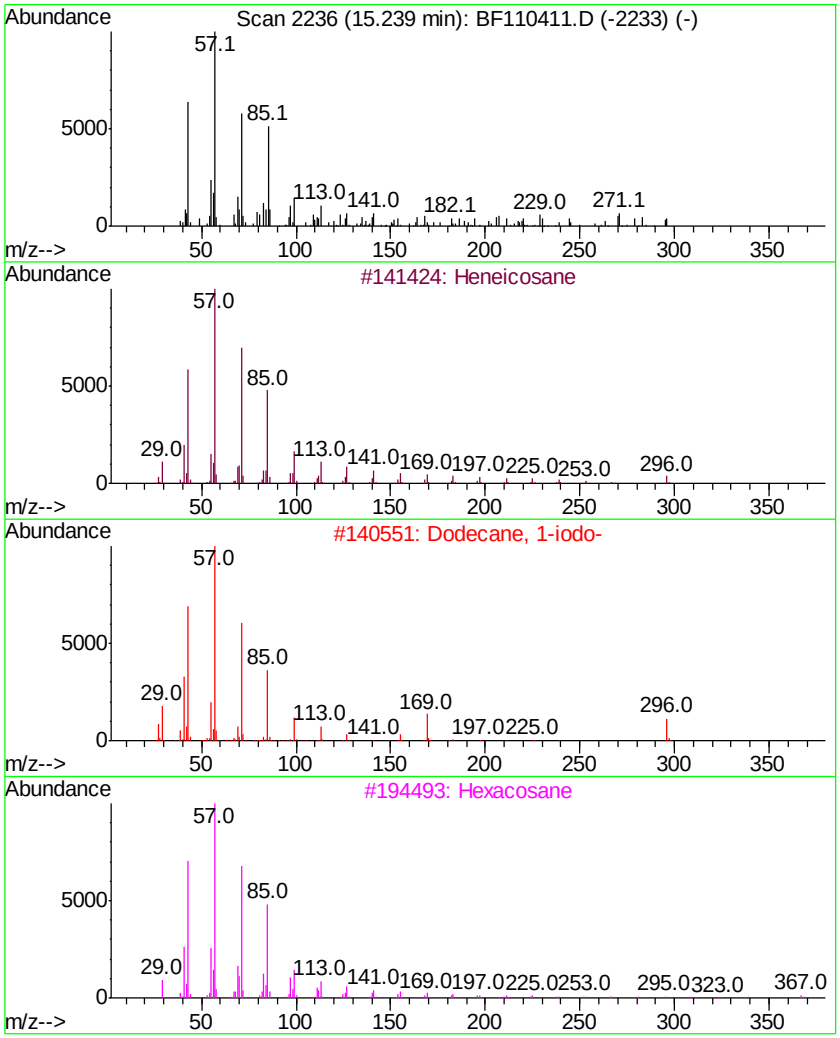
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

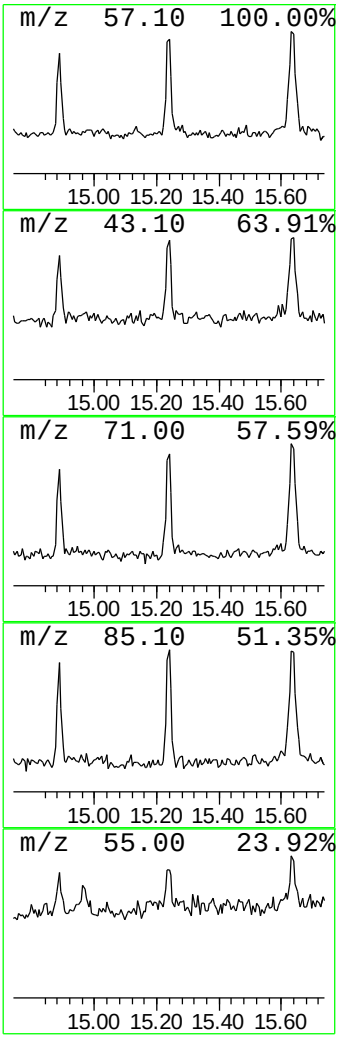
****

Peak Number 8 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	2.75 ng	64866	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	70
3	Hexacosane	366	C26H54	000630-01-3	64
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	58
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	58





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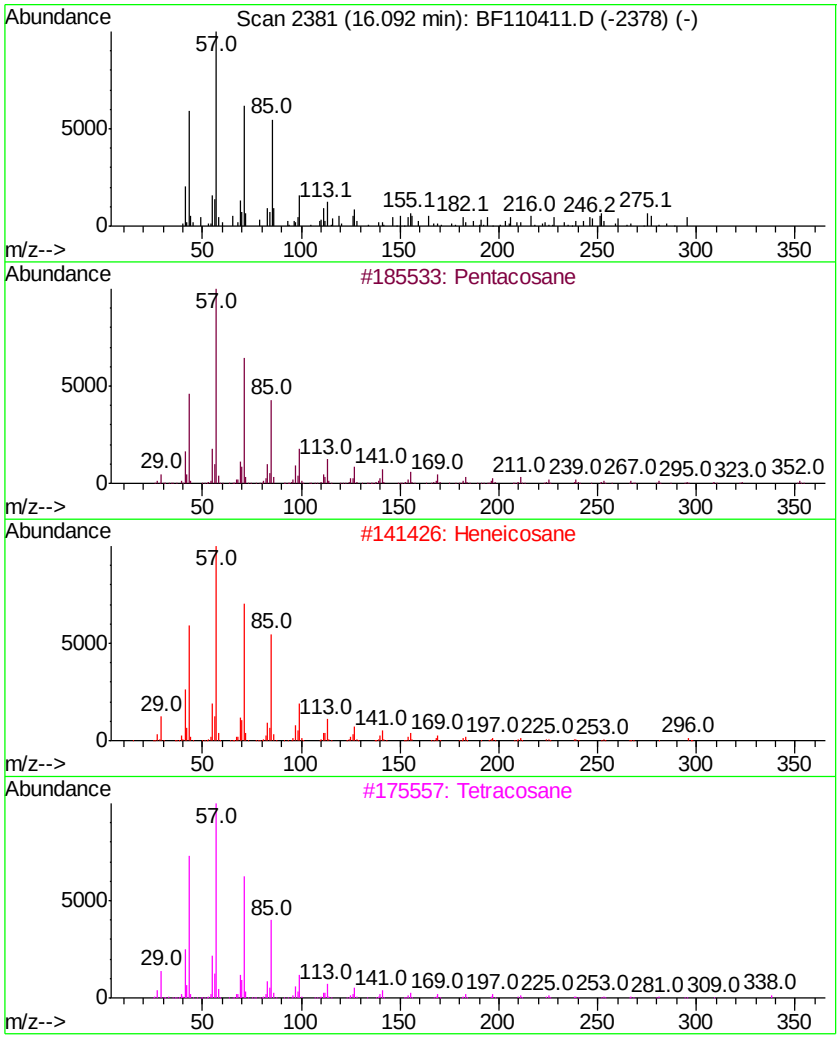
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

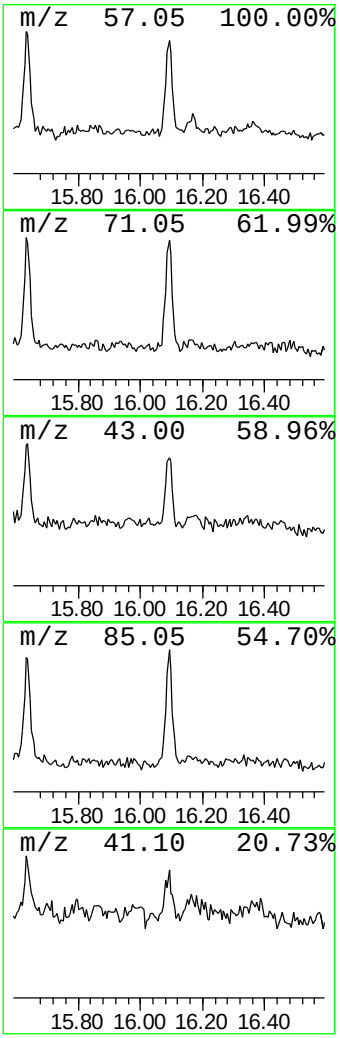
****

Peak Number 9 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	2.95 ng	69612	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	58
2	Heneicosane	296	C21H44	000629-94-7	52
3	Tetracosane	338	C24H50	000646-31-1	52
4	Hexadecane	226	C16H34	000544-76-3	50
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110218\
Data File : BF110411.D
Acq On : 2 Nov 2018 14:50
Operator : JU/SJ
Sample : J5794-11
Misc :
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Instrument : BNA_F
ClientSampleId : TP-10B-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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
Butane, 2-methoxy...	2.27	15.7	ng	366315	1	6.96	465849	20.0
2-Pentanone, 4-hy...	5.19	3.5	ng	82014	1	6.96	465849	20.0
unknown6.72	6.72	66.7	ng	1552960	1	6.96	465849	20.0
Trifluoroacetoxy ...	13.95	4.2	ng	113269	5	14.13	534564	20.0
Eicosane	14.57	2.1	ng	55747	5	14.13	534564	20.0
Supraene	14.97	4.0	ng	94864	6	15.66	471839	20.0
Heneicosane	15.24	2.8	ng	64866	6	15.66	471839	20.0
Pentacosane	16.09	3.0	ng	69612	6	15.66	471839	20.0