LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
Data File : BF108826.D
Acq On : 6 Sep 2018 16:34
Operator : JU/SJ
Sample : PB112638BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112638BL

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	4.966	442	447	458	rBV	217292	345427	3.84%	0.456%
2	5.360	508	514	517	rBV	6051370	7419992	82.58%	9.786%
3	6.372	679	686	689	rBV	6062050	7731277	86.04%	10.196%
4	6.507	703	709	712	rBV	6757204	7582752	84.39%	10.000%
5	6.737	744	748	751	rBV	2214824	1948866	21.69%	2.570%
6	6.896	770	775	778	rBV	6123302	5969046	66.43%	7.872%
7	7.295	837	843	846	rBV	4372476	5176044	57.60%	6.826%
8	8.013	960	965	969	rBV	2544512	2528386	28.14%	3.335%
9	9.095	1142	1149	1152	rBV	8122655	8985694	100.00%	11.851%
10	9.766	1257	1263	1266	rBV	3193410	2919789	32.49%	3.851%
11	10.554	1389	1397	1400	rBV	5353657	5543854	61.70%	7.311%
12	11.242	1507	1514	1517	rBV	3598053	3026870	33.69%	3.992%
13	12.830	1777	1784	1787	rBV2	7711950	8831125	98.28%	11.647%
14	13.866	1956	1960	1964	rVB	3101348	2751970	30.63%	3.629%
15	14.360	2040	2044	2052	rVB	182001	168472	1.87%	0.222%
16	14.654	2088	2094	2102	rBV	381881	401921	4.47%	0.530%
17	14.977	2142	2149	2158	rBV	451886	576679	6.42%	0.761%
18	15.271	2194	2199	2203	rBV	1927791	2244540	24.98%	2.960%
19	15.330	2203	2209	2224	rVB	498148	672566	7.48%	0.887%
20	15.742	2272	2279	2286	rBV	344926	545435	6.07%	0.719%
21	16.213	2353	2359	2370	rVB	181430	336387	3.74%	0.444%
22	16.765	2448	2453	2458	rVB2	66800	117247	1.30%	0.155%

Sum of corrected areas: 75824339

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090618\
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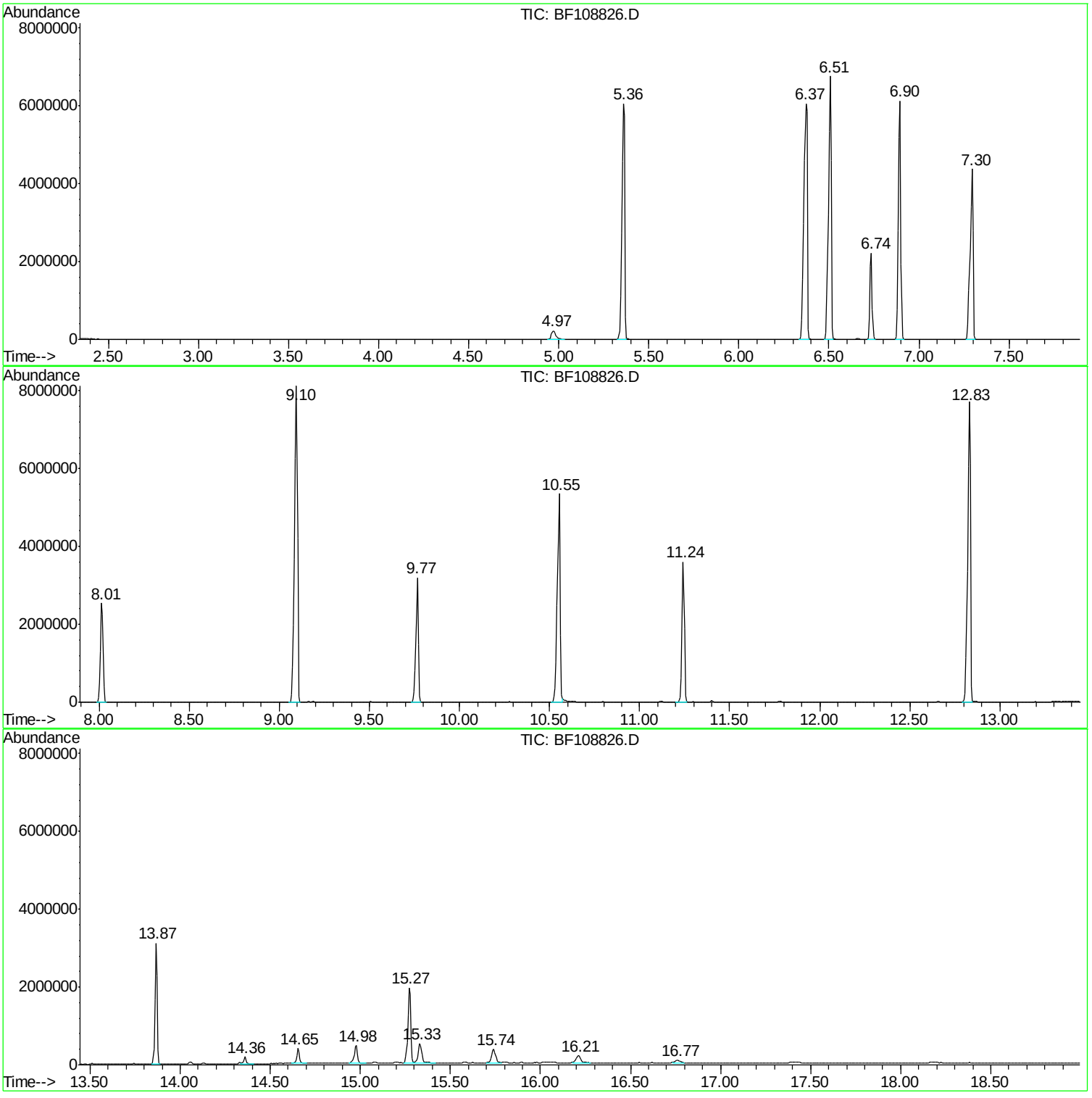
Acq On : 6 Sep 2018 16:34
Operator : JU/SJ
Sample : PB112638BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112638BL

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\BF090618\
Data File : BF108826.D
Acq On : 6 Sep 2018 16:34
Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : PB112638BL

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

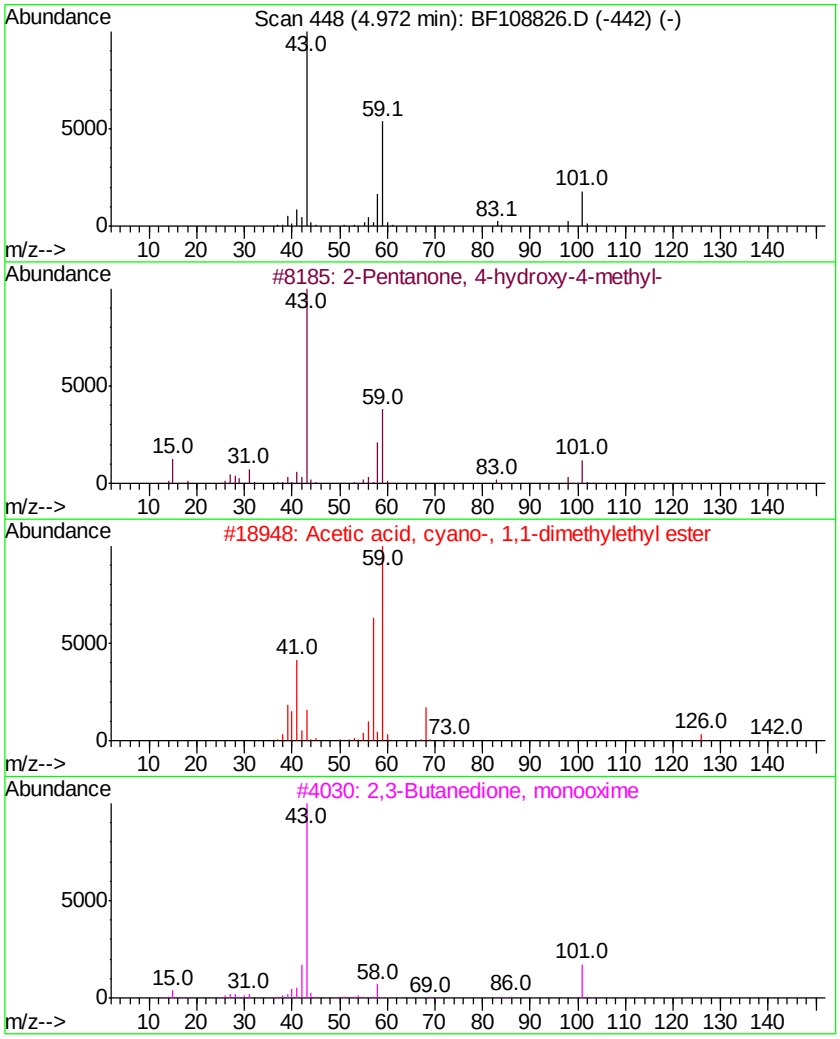
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

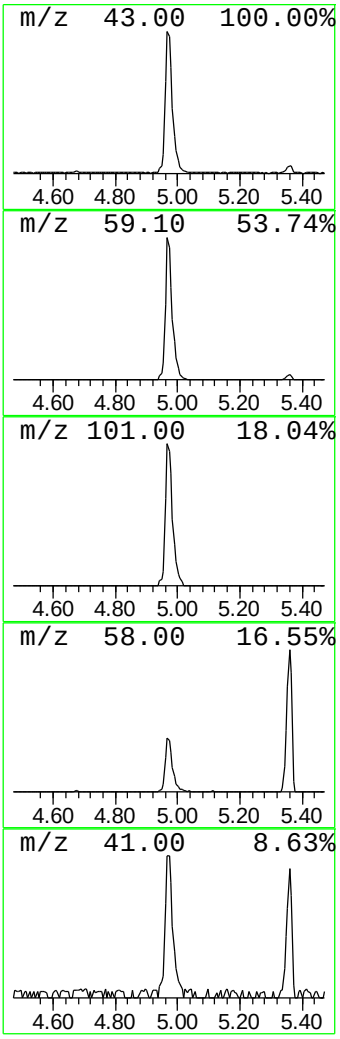
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.97	3.54 ng	345427	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	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Diacetamide	101	C4H7NO2	000625-77-4	9





Library Search Compound Report

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

Instrument : BNA_F
ClientSampleId : PB112638BL

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

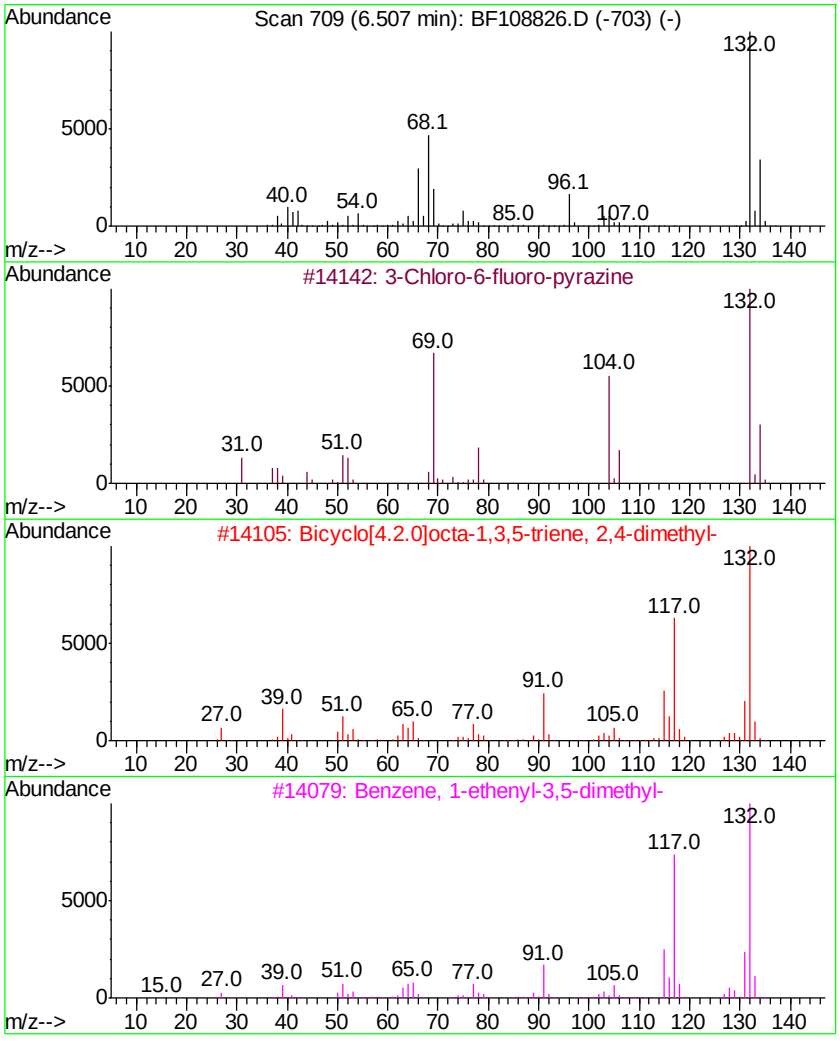
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

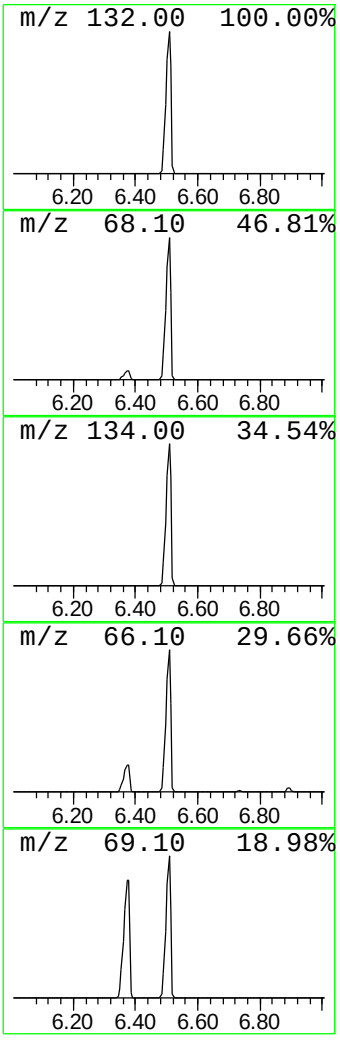
****

Peak Number 2 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	77.82 ng	7582750	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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Operator : JU/SJ
Sample : PB112638BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112638BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
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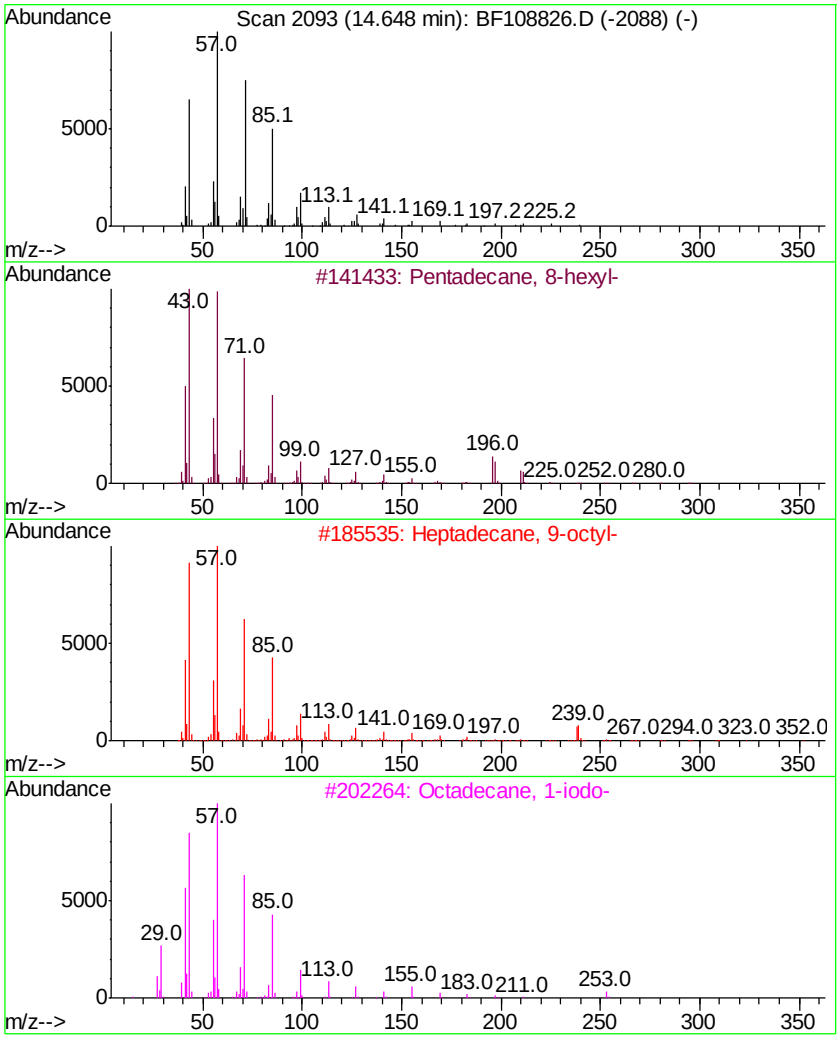
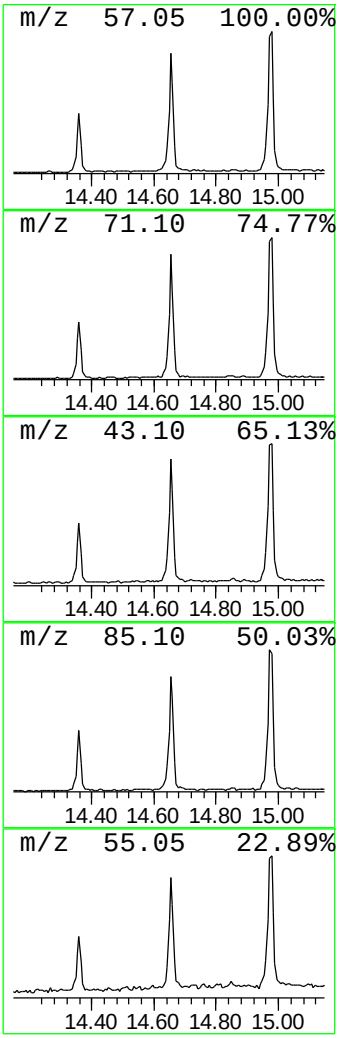
****

Peak Number 4 Pentadecane, 8-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	3.58 ng	401921	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4	Hexadecane	226	C16H34	000544-76-3	86
5	Tetracosane	338	C24H50	000646-31-1	83





Library Search Compound Report

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Data File : BF108826.D
Acq On : 6 Sep 2018 16:34
Operator : JU/SJ
Sample : PB112638BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112638BL

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

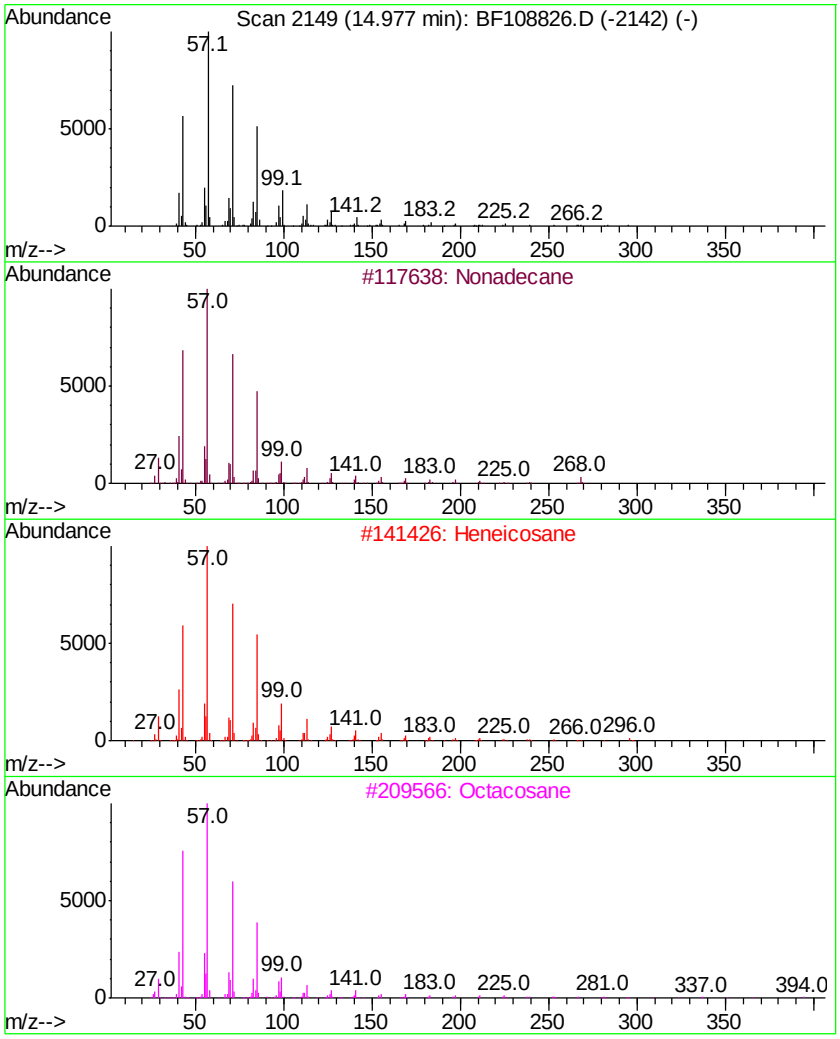
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

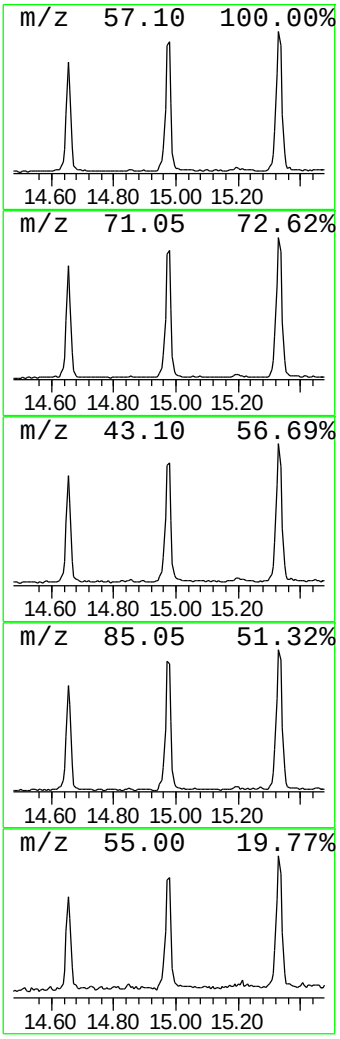
****

Peak Number 5 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	5.14 ng	576679	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90





Library Search Compound Report

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Sample : PB112638BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB112638BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.M
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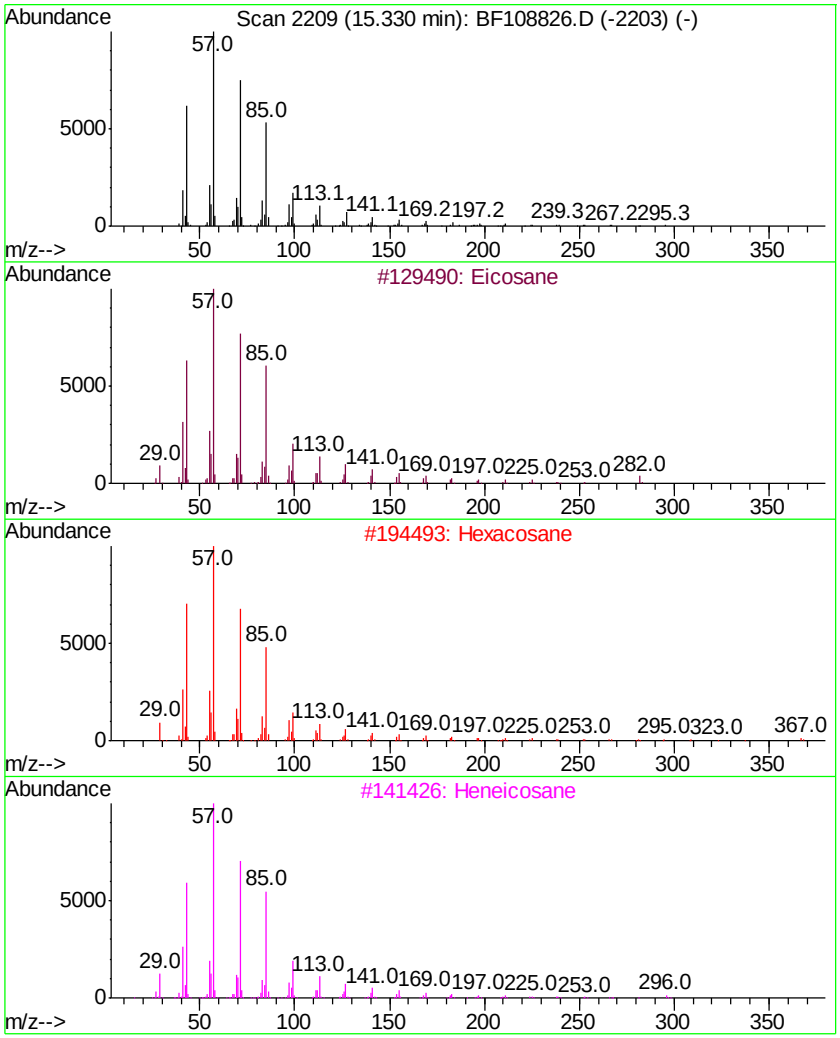
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

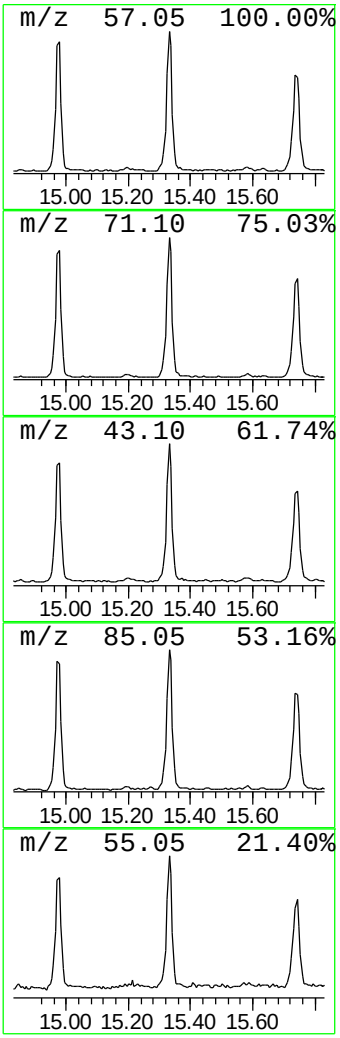
****

Peak Number 6 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	5.99 ng	672566	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Hexacosane	366	C26H54	000630-01-3	94
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : PB112638BL

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

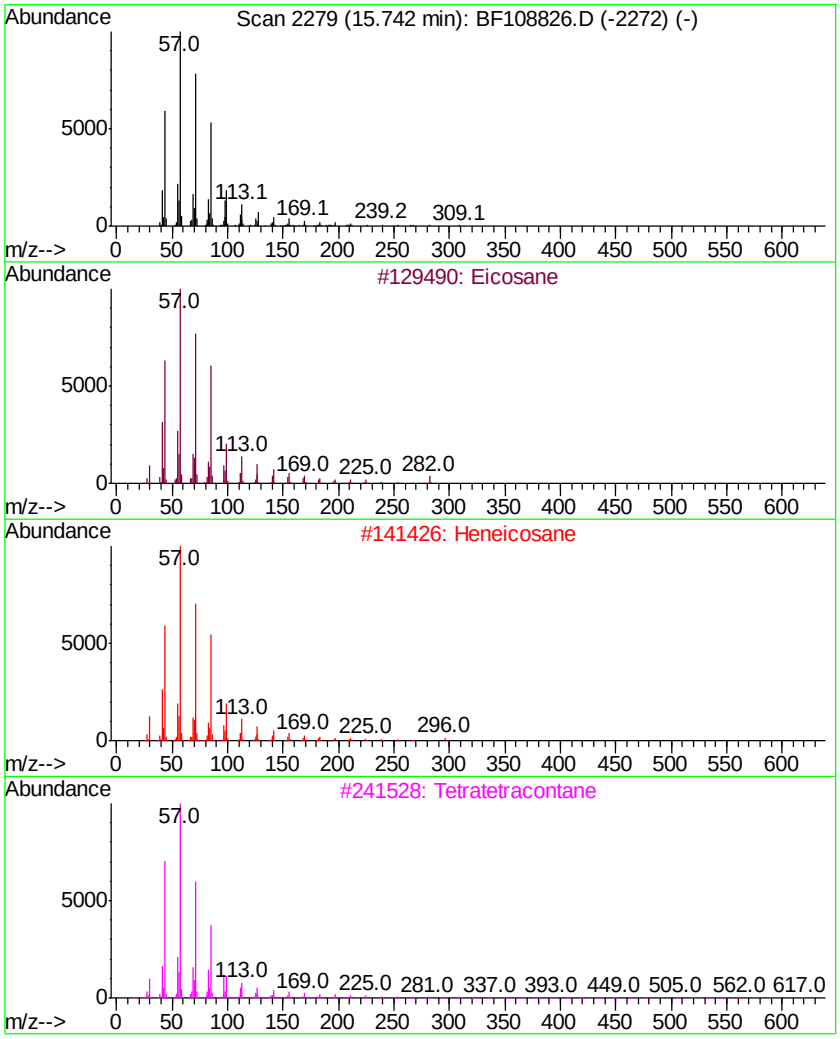
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

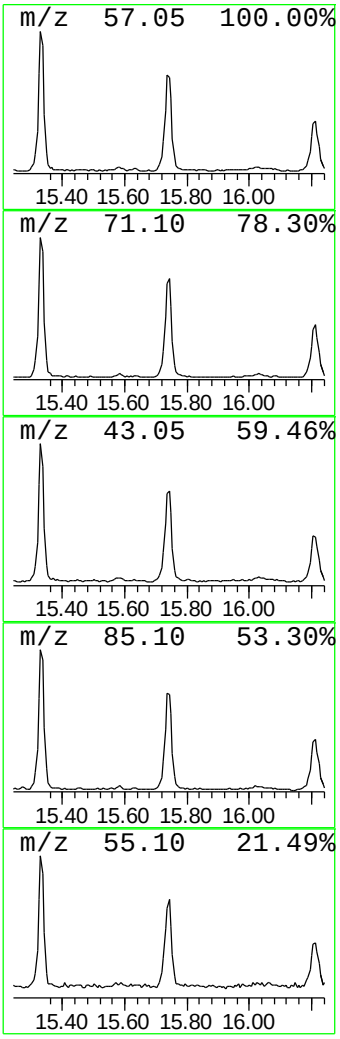
****

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	4.86 ng	545435	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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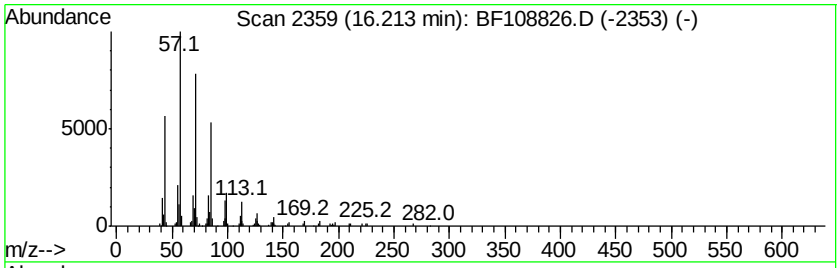
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

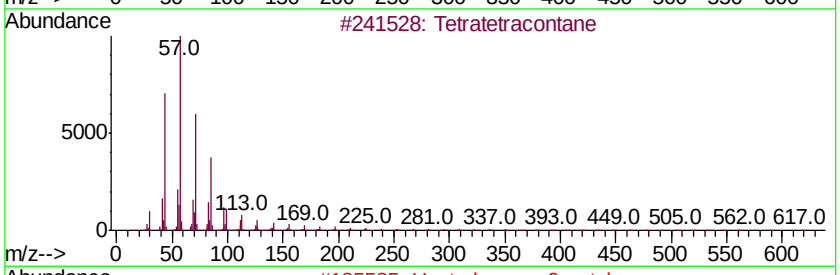
****

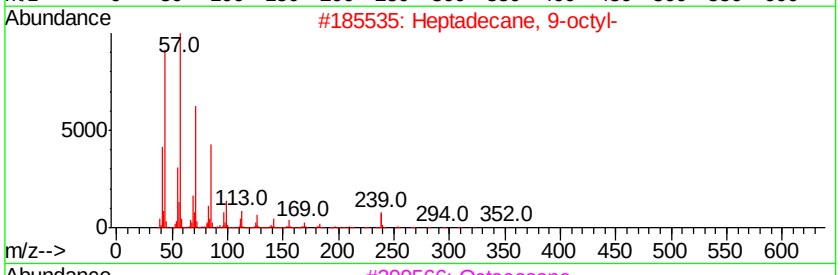
Peak Number 8 Tetratetracontane Concentration Rank 8

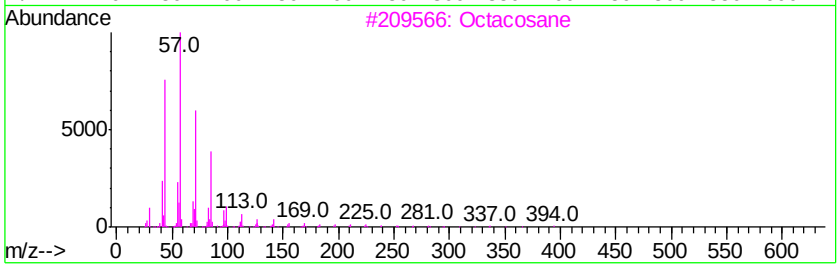
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	3.00 ng	336387	Perylene-d12	15.27

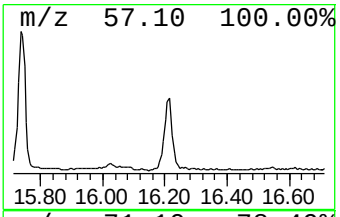
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Tetracosane	338	C24H50	000646-31-1	91

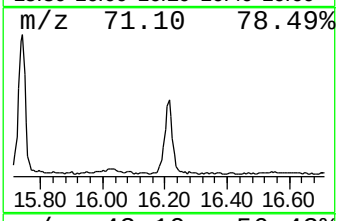


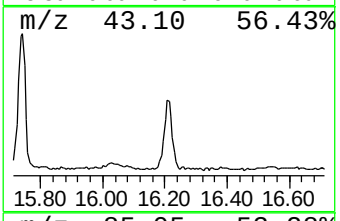


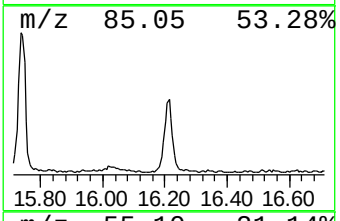


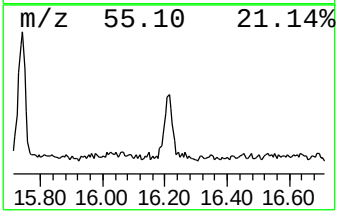












Tentatively Identified Compound (LSC) summary

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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...	4.97	3.5	ng	345427	1	6.74	1948870	20.0
unknown6.51	6.51	77.8	ng	7582750	1	6.74	1948870	20.0
Pentadecane, 8-he...	14.65	3.6	ng	401921	6	15.27	2244540	20.0
Nonadecane	14.98	5.1	ng	576679	6	15.27	2244540	20.0
Hexacosane	15.33	6.0	ng	672566	6	15.27	2244540	20.0
Eicosane	15.74	4.9	ng	545435	6	15.27	2244540	20.0
Tetratetracontane	16.21	3.0	ng	336387	6	15.27	2244540	20.0