LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017287.D
Acq On : 23 Oct 2018 16:35
Operator : MJ/SJ
Sample : PB114097BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PB114097BL

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_M\METHODS\8270-BM101718.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	4.828	308	313	319	rBV	372158	511584	2.99%	0.549%
2	5.281	382	390	399	rBV	4905841	6909956	40.37%	7.410%
3	6.846	647	656	672	rBV	4673118	7313406	42.73%	7.842%
4	7.199	708	716	724	rBV	4889809	7528464	43.99%	8.073%
5	7.657	787	794	802	rBV	1091668	1716232	10.03%	1.840%
6	7.975	839	848	856	rBV	3639793	5832927	34.08%	6.255%
7	8.810	980	990	1001	rBV	2707169	4544071	26.55%	4.873%
8	10.434	1258	1266	1273	rBV	1399589	2286940	13.36%	2.452%
9	12.916	1680	1688	1697	rBV	7396800	10628377	62.10%	11.397%
10	14.169	1884	1901	1917	rVV2	183631	681632	3.98%	0.731%
11	14.298	1917	1923	1933	rVB2	1971141	3079582	17.99%	3.302%
12	15.133	2059	2065	2076	rVB	205326	388555	2.27%	0.417%
13	15.798	2171	2178	2200	rBV	6549088	9058706	52.93%	9.714%
14	17.051	2385	2391	2401	rBV2	2736000	3955732	23.11%	4.242%
15	17.957	2540	2545	2554	rBV	512924	829212	4.84%	0.889%
16	19.245	2760	2764	2776	rBV	373174	626209	3.66%	0.671%
17	19.692	2834	2840	2850	rBV	14293682	17115578	100.00%	18.353%
18	21.245	3099	3104	3112	rBV	3841426	4874490	28.48%	5.227%
19	21.839	3202	3205	3208	rBV	148644	184010	1.08%	0.197%
20	22.298	3280	3283	3290	rVB2	236541	304281	1.78%	0.326%
21	22.797	3365	3368	3374	rVB	303205	413467	2.42%	0.443%
22	23.350	3459	3462	3470	rVB	344583	546409	3.19%	0.586%
23	23.456	3474	3480	3488	rVB	2163598	3927820	22.95%	4.212%

Sum of corrected areas: 93257640

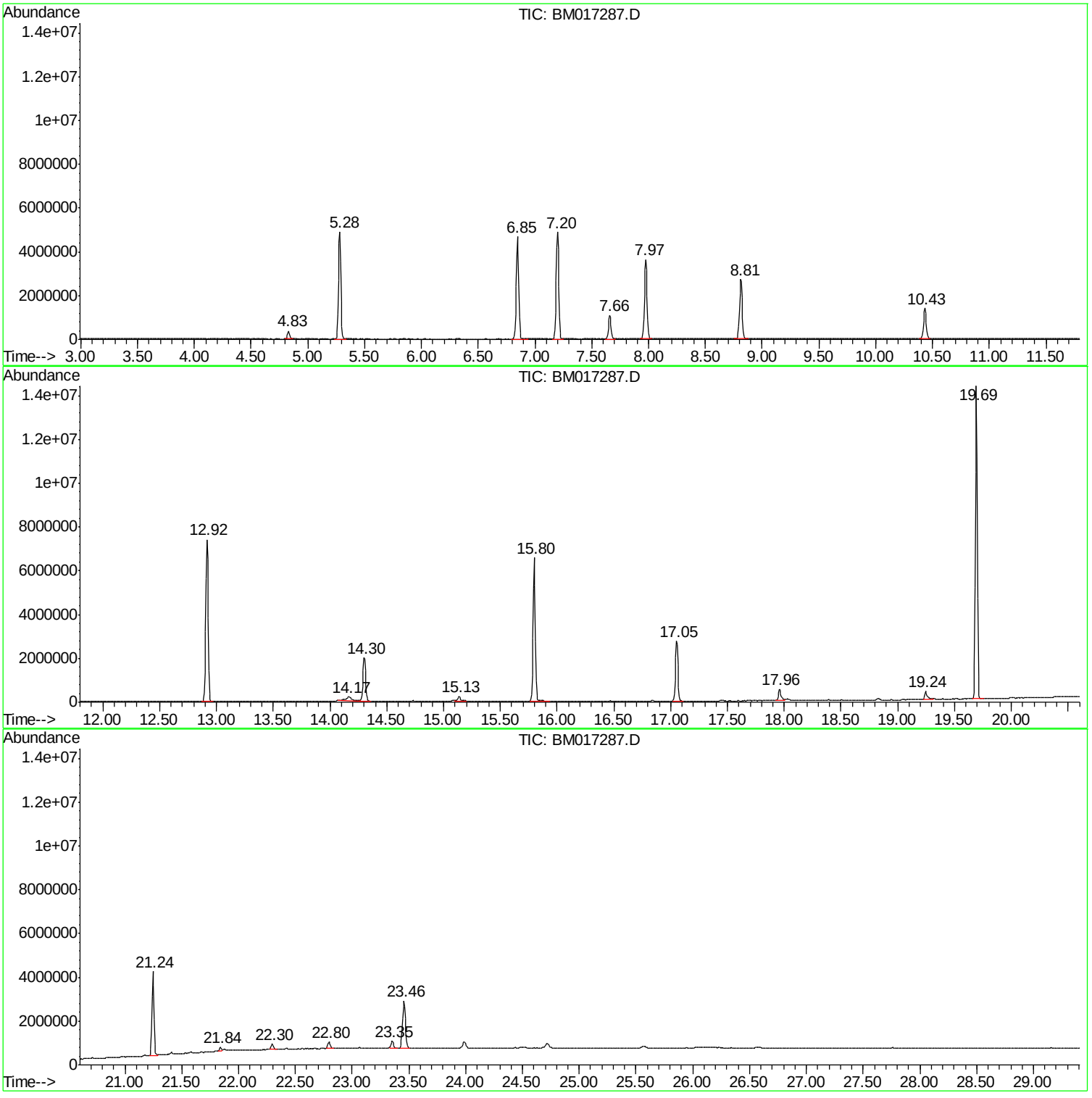
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017287.D
Acq On : 23 Oct 2018 16:35
Operator : MJ/SJ
Sample : PB114097BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PB114097BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017287.D
Acq On : 23 Oct 2018 16:35
Operator : MJ/SJ
Sample : PB114097BL
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Instrument : BNA_M
ClientSampleId : PB114097BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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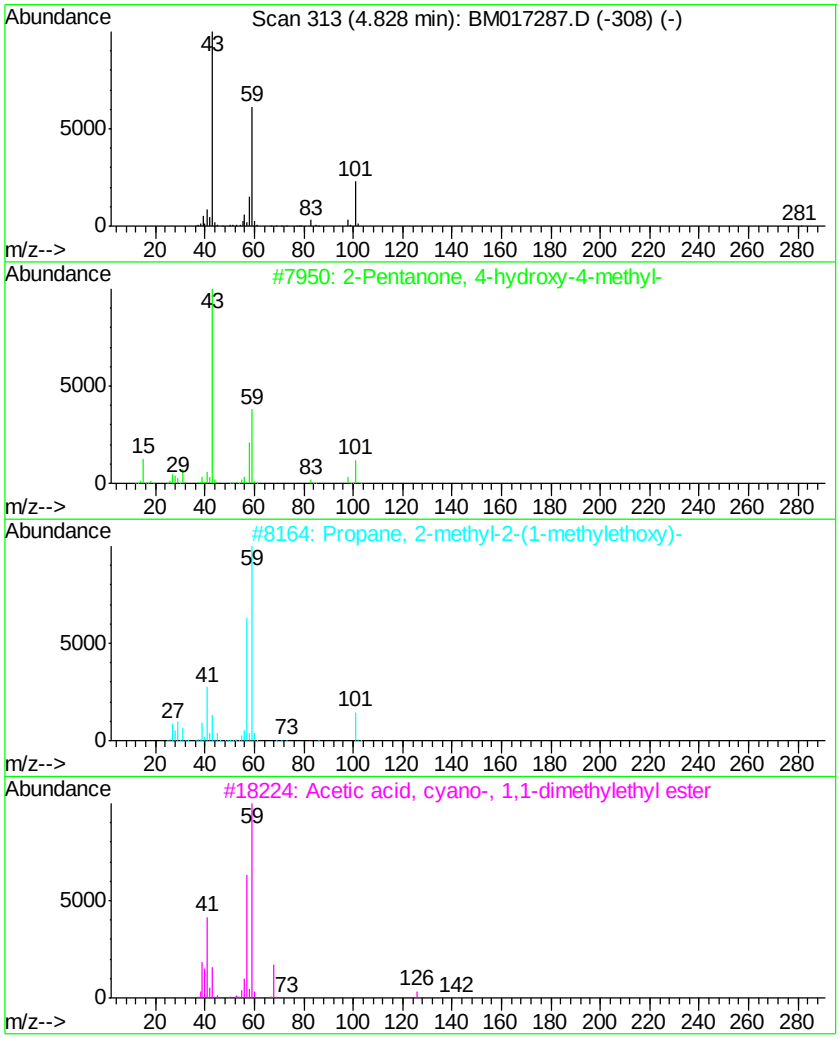
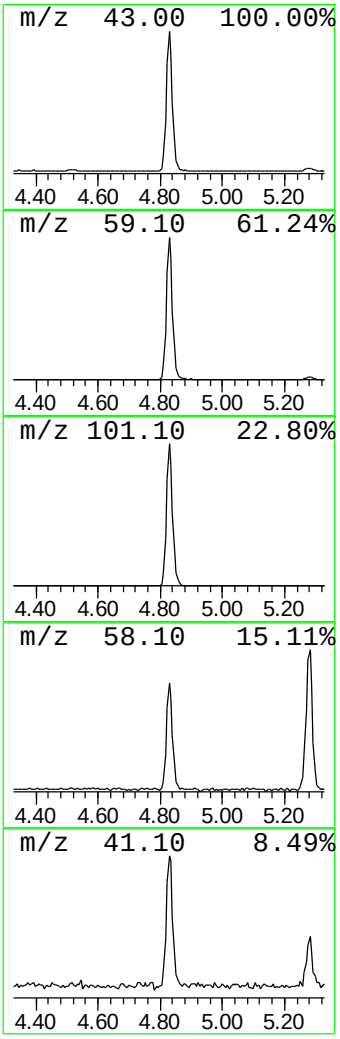
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	5.96 ng	511584	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017287.D
Acq On : 23 Oct 2018 16:35
Operator : MJ/SJ
Sample : PB114097BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PB114097BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

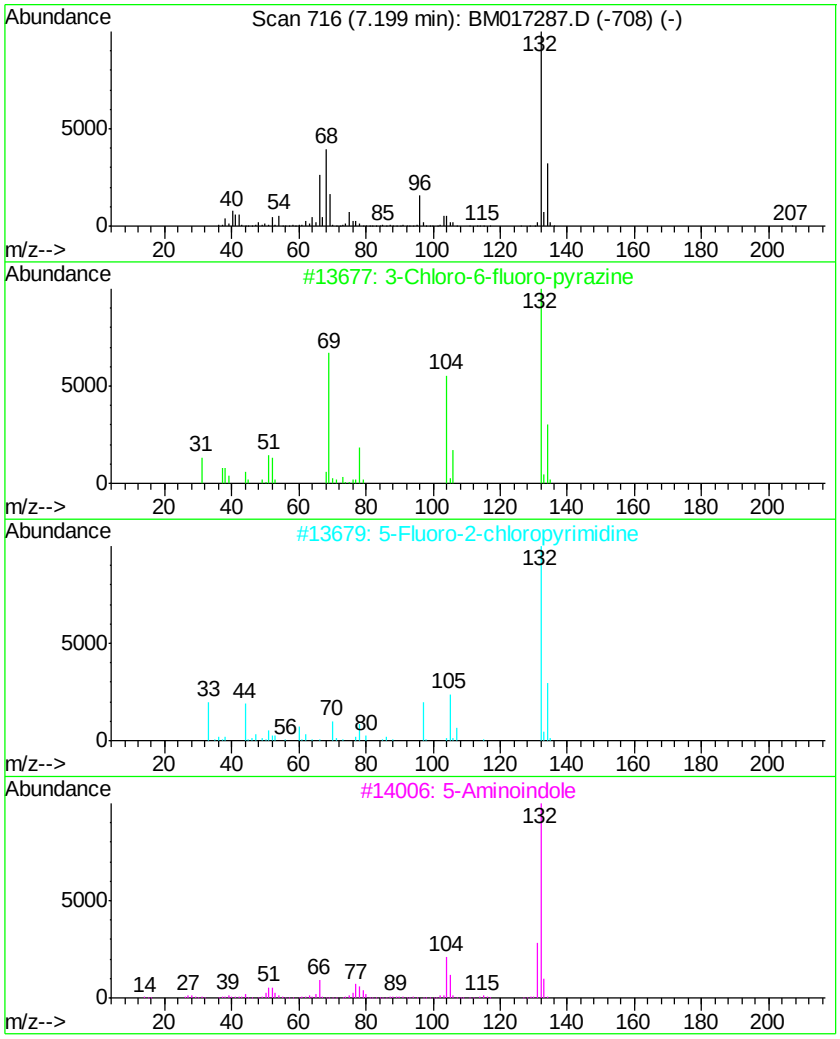
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

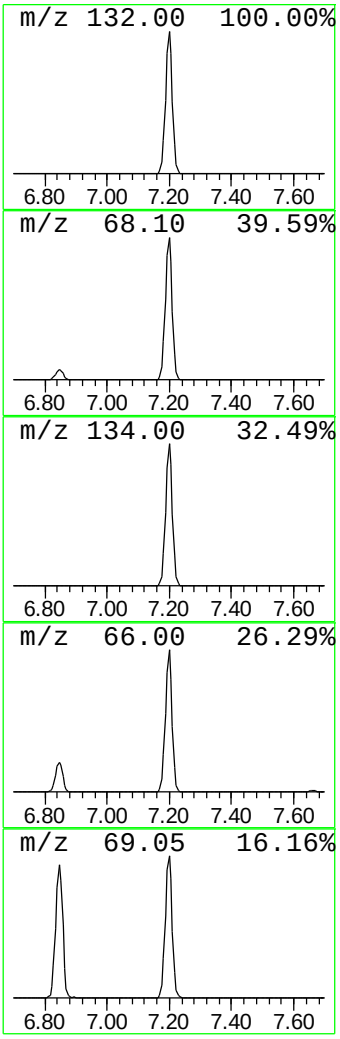
****

Peak Number 2 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	87.73 ng	7528460	1,4-Dichlorobenzene-d4	7.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017287.D
Acq On : 23 Oct 2018 16:35
Operator : MJ/SJ
Sample : PB114097BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PB114097BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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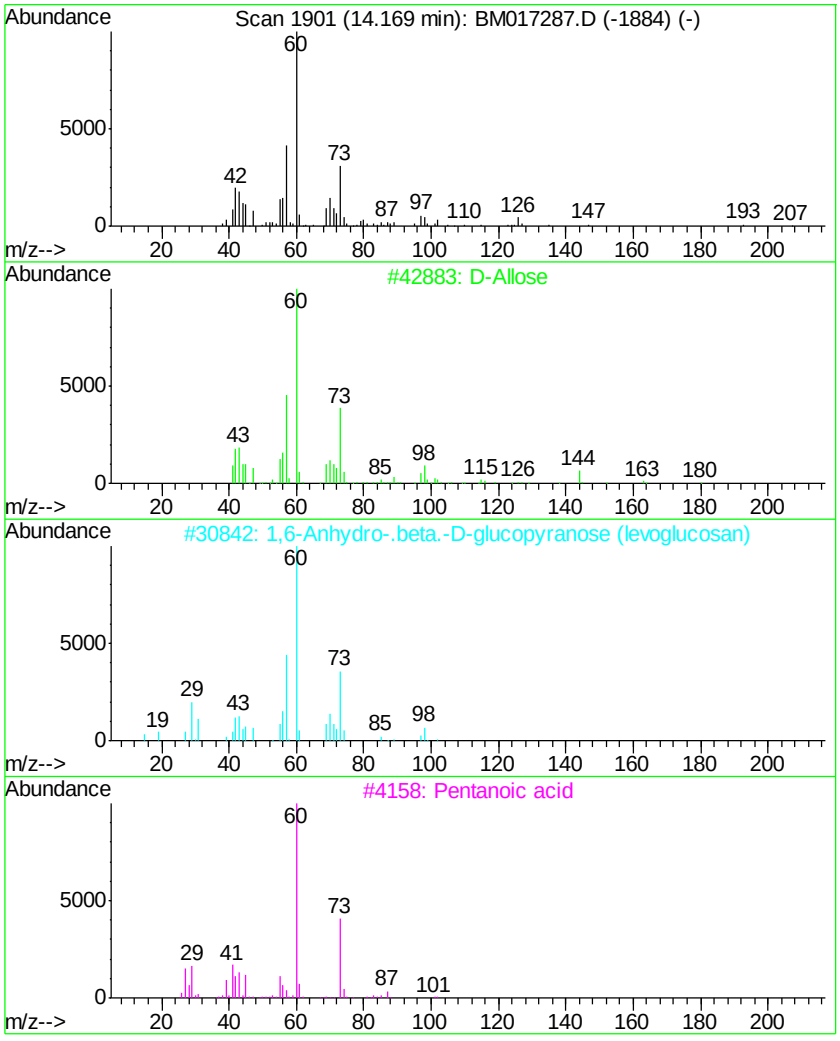
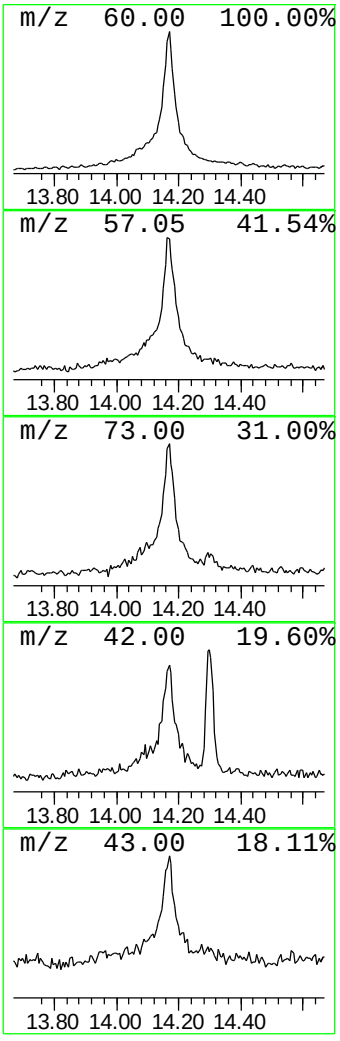
Peak Number 4 D-Allose Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	4.43 ng	681632	Acenaphthene-d10	14.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose	180	C6H12O6	002595-97-3	72
2	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	64
3	Pentanoic acid	102	C5H10O2	000109-52-4	47
4	3,4-Altrosan	162	C6H10O5	1000129-76-4	42
5	Butanoic acid	88	C4H8O2	000107-92-6	40





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017287.D
Acq On : 23 Oct 2018 16:35
Operator : MJ/SJ
Sample : PB114097BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PB114097BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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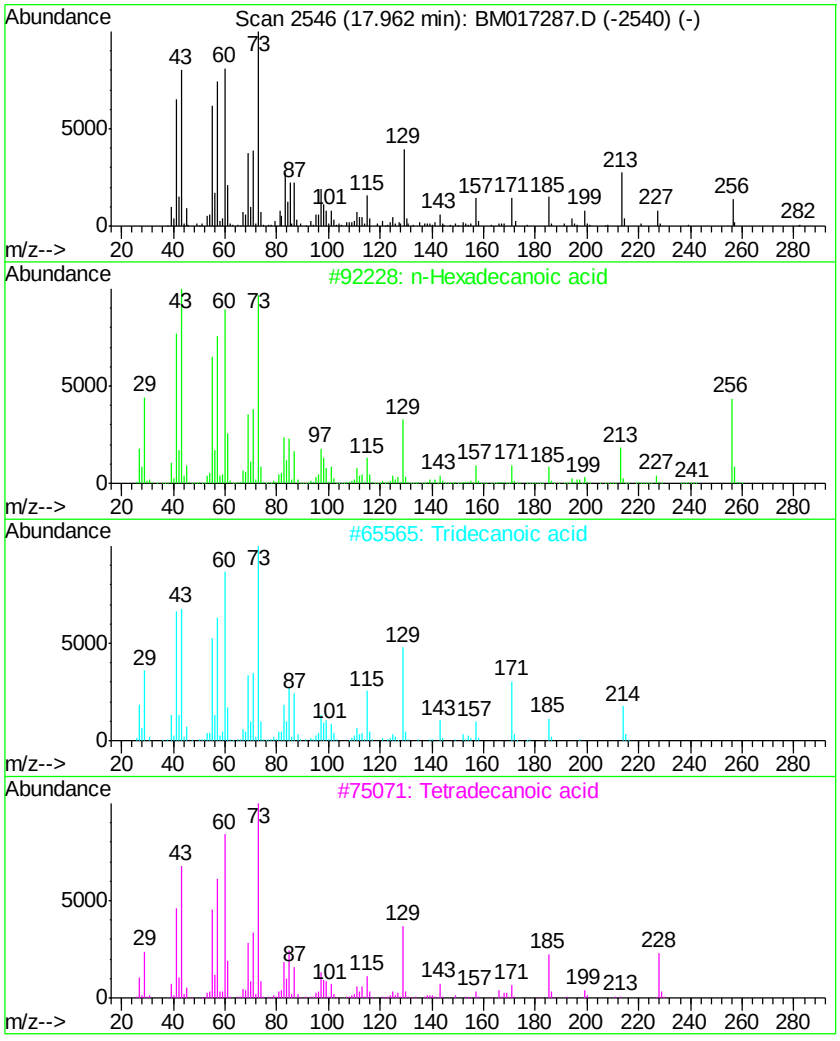
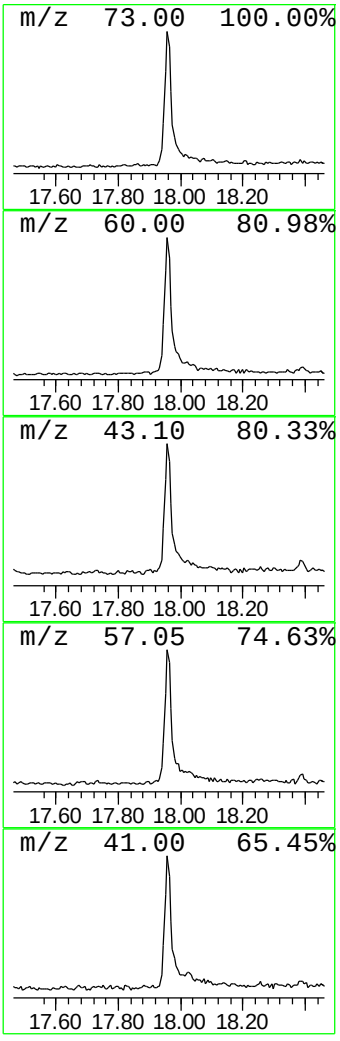
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	4.19 ng	829212	Phenanthrene-d10	17.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	97
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM102318\
Data File : BM017287.D
Acq On : 23 Oct 2018 16:35
Operator : MJ/SJ
Sample : PB114097BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : PB114097BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

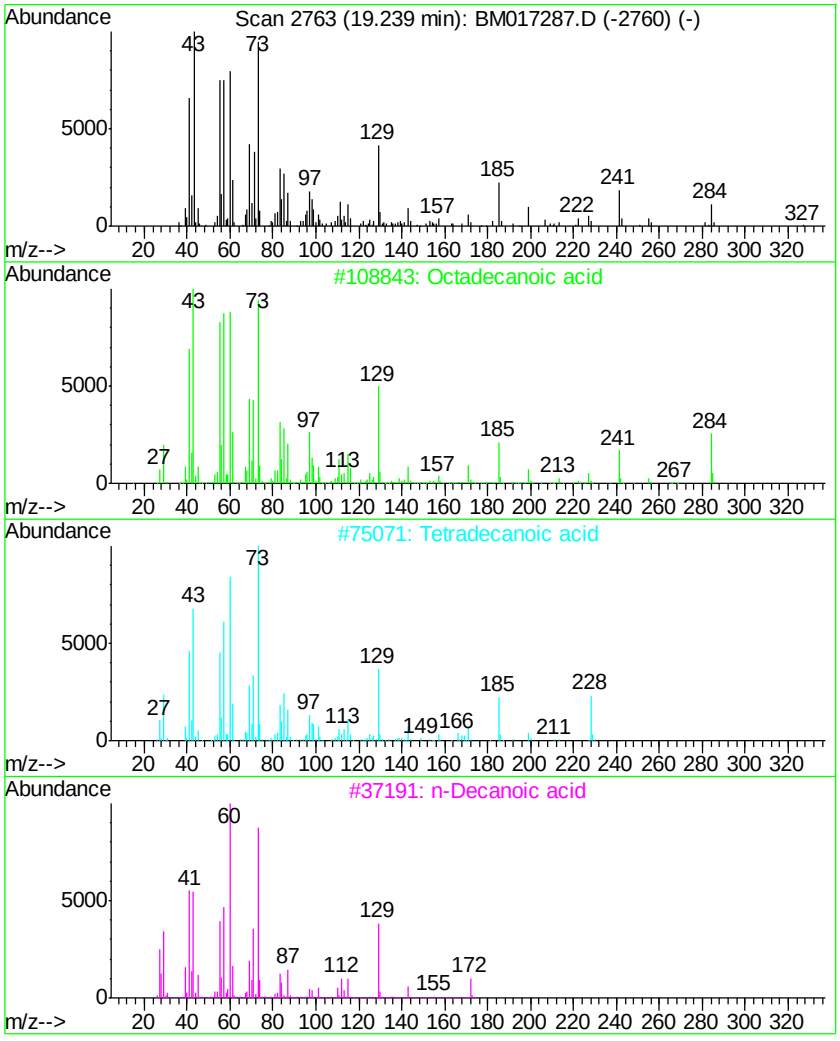
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

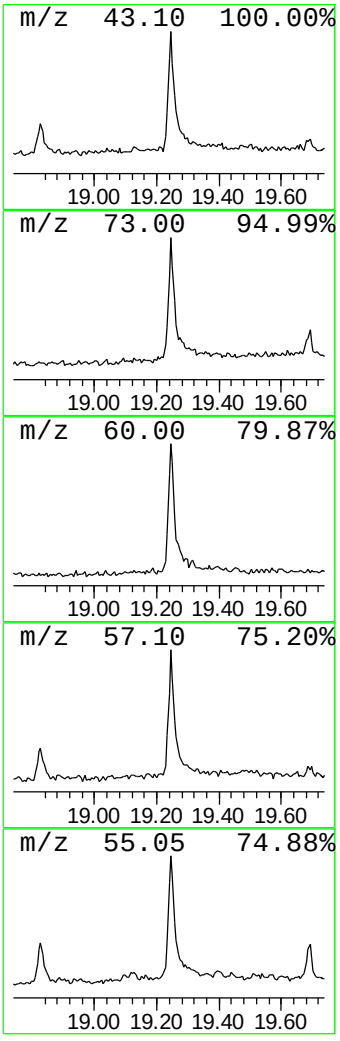
****

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.24	2.57 ng	626209	Chrysene-d12	21.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58





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ClientSampleId : PB114097BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

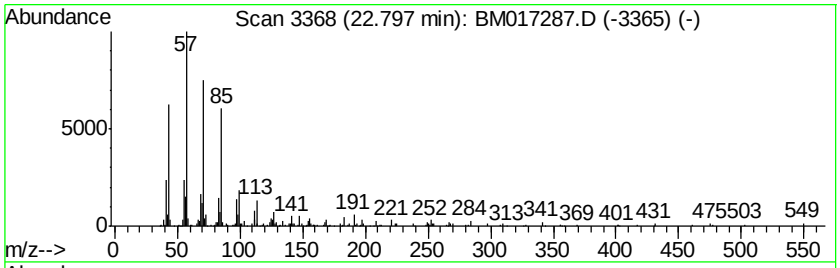
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

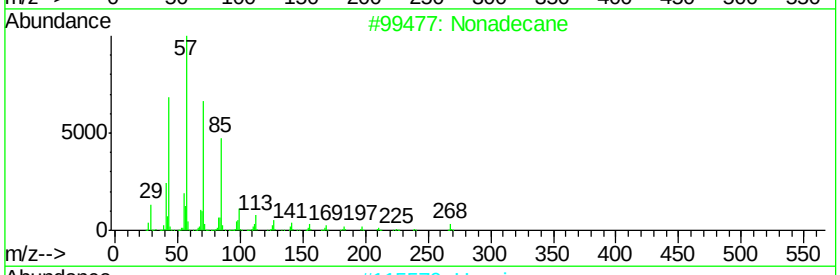
****

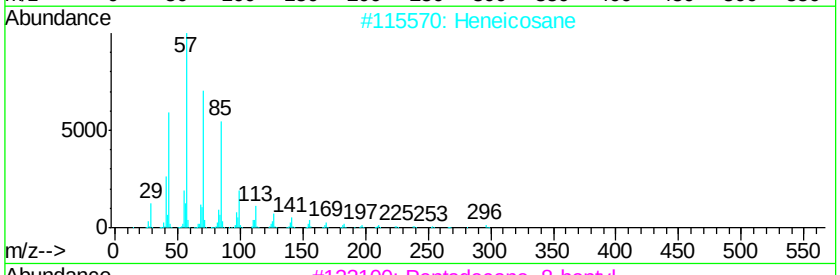
Peak Number 7 Nonadecane Concentration Rank 8

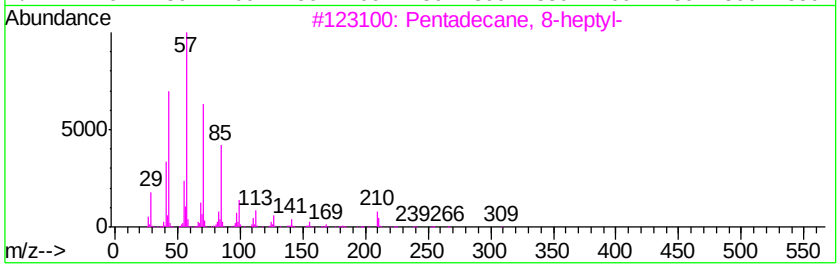
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.80	2.11 ng	413467	Perylene-d12	23.46

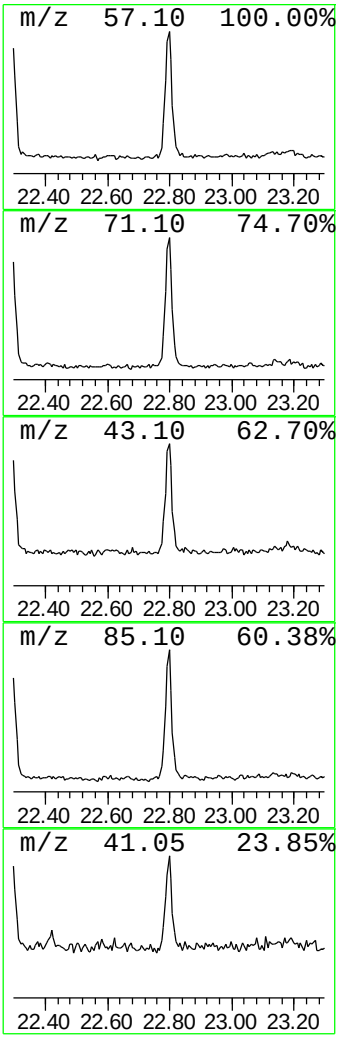
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91











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ClientSampleId : PB114097BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

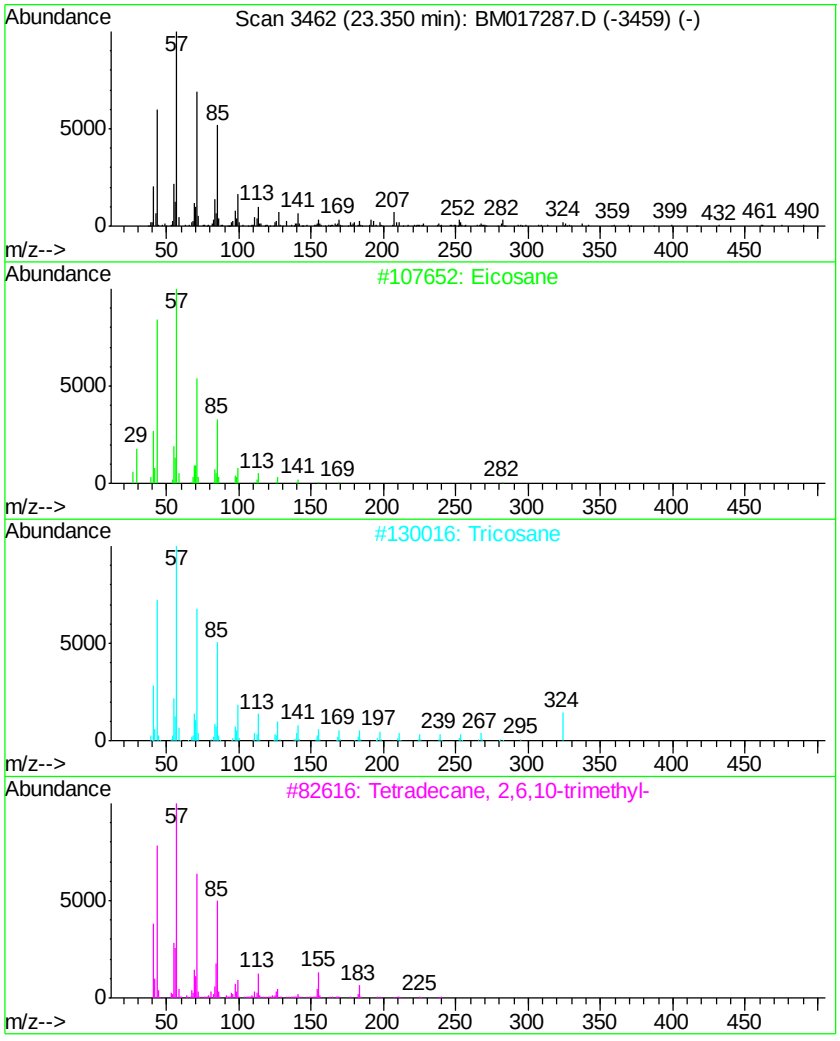
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

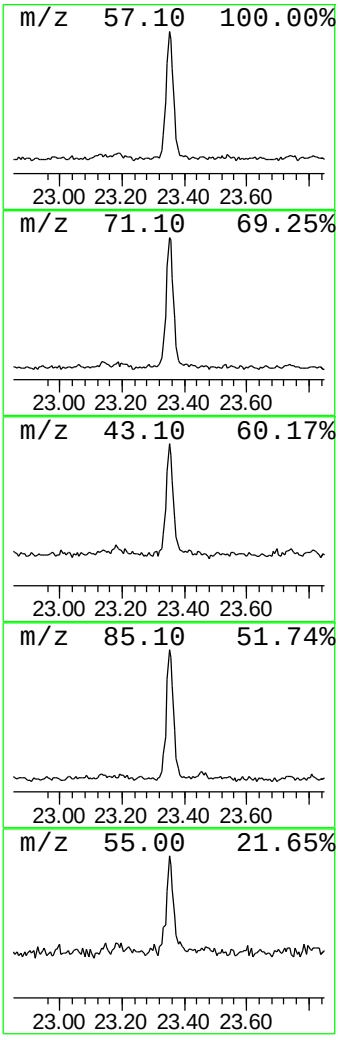
****

Peak Number 8 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	2.78 ng	546409	Perylene-d12	23.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Tricosane	324	C23H48	000638-67-5	93
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	91
4	Nonacosane	408	C29H60	000630-03-5	90
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\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	6.0	ng	511584	1	7.66	1716230	20.0
unknown7.20	7.20	87.7	ng	7528460	1	7.66	1716230	20.0
D-Allose	14.17	4.4	ng	681632	3	14.30	3079580	20.0
n-Hexadecanoic acid	17.96	4.2	ng	829212	4	17.05	3955730	20.0
Octadecanoic acid	19.24	2.6	ng	626209	5	21.24	4874490	20.0
Nonadecane	22.80	2.1	ng	413467	6	23.46	3927820	20.0
Eicosane	23.35	2.8	ng	546409	6	23.46	3927820	20.0