LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100119\
Data File : BG042979.D
Acq On : 1 Oct 2019 22:50
Operator : JU
Sample : K4946-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-5_(1-3)

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_G\METHODS\8270-BG092519.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	3.181	10	16	25	rBV2	75494	177103	3.73%	0.671%
2	3.258	25	29	38	rVB	72589	115239	2.43%	0.437%
3	5.185	352	357	366	rVB	29744	49615	1.05%	0.188%
4	5.655	429	437	447	rBV	1022574	1686287	35.53%	6.390%
5	7.241	699	707	719	rBV	1130770	2054094	43.28%	7.784%
6	7.606	762	769	783	rVB	1071198	1882259	39.66%	7.133%
7	8.070	841	848	855	rBV2	256121	447260	9.42%	1.695%
8	8.393	895	903	911	rBV	833237	1468702	30.95%	5.566%
9	9.227	1037	1045	1062	rBV	654677	1210332	25.50%	4.587%
10	10.872	1316	1325	1337	rBV	321685	608143	12.81%	2.305%
11	13.316	1733	1741	1752	rBV	1823335	2908733	61.29%	11.023%
12	14.139	1874	1881	1887	rBV	252396	383436	8.08%	1.453%
13	14.685	1968	1974	1982	rBV	537613	895643	18.87%	3.394%
14	16.172	2220	2227	2238	rBV	1718688	2654274	55.93%	10.059%
15	17.429	2435	2441	2446	rBV2	725765	1144225	24.11%	4.336%
16	17.470	2446	2448	2454	rVB	71984	98692	2.08%	0.374%
17	18.317	2587	2592	2597	rBV3	168539	242471	5.11%	0.919%
18	19.480	2785	2790	2795	rVB	89318	127550	2.69%	0.483%
19	19.838	2842	2851	2857	rBV	95976	163973	3.46%	0.621%
20	20.038	2879	2885	2896	rBV	3565458	4745589	100.00%	17.984%
21	21.348	3104	3108	3124	rBV2	149541	381035	8.03%	1.444%
22	21.701	3161	3168	3174	rBV	814584	1408954	29.69%	5.339%
23	24.926	3706	3717	3730	rBV2	508553	1534739	32.34%	5.816%

Sum of corrected areas: 26388348

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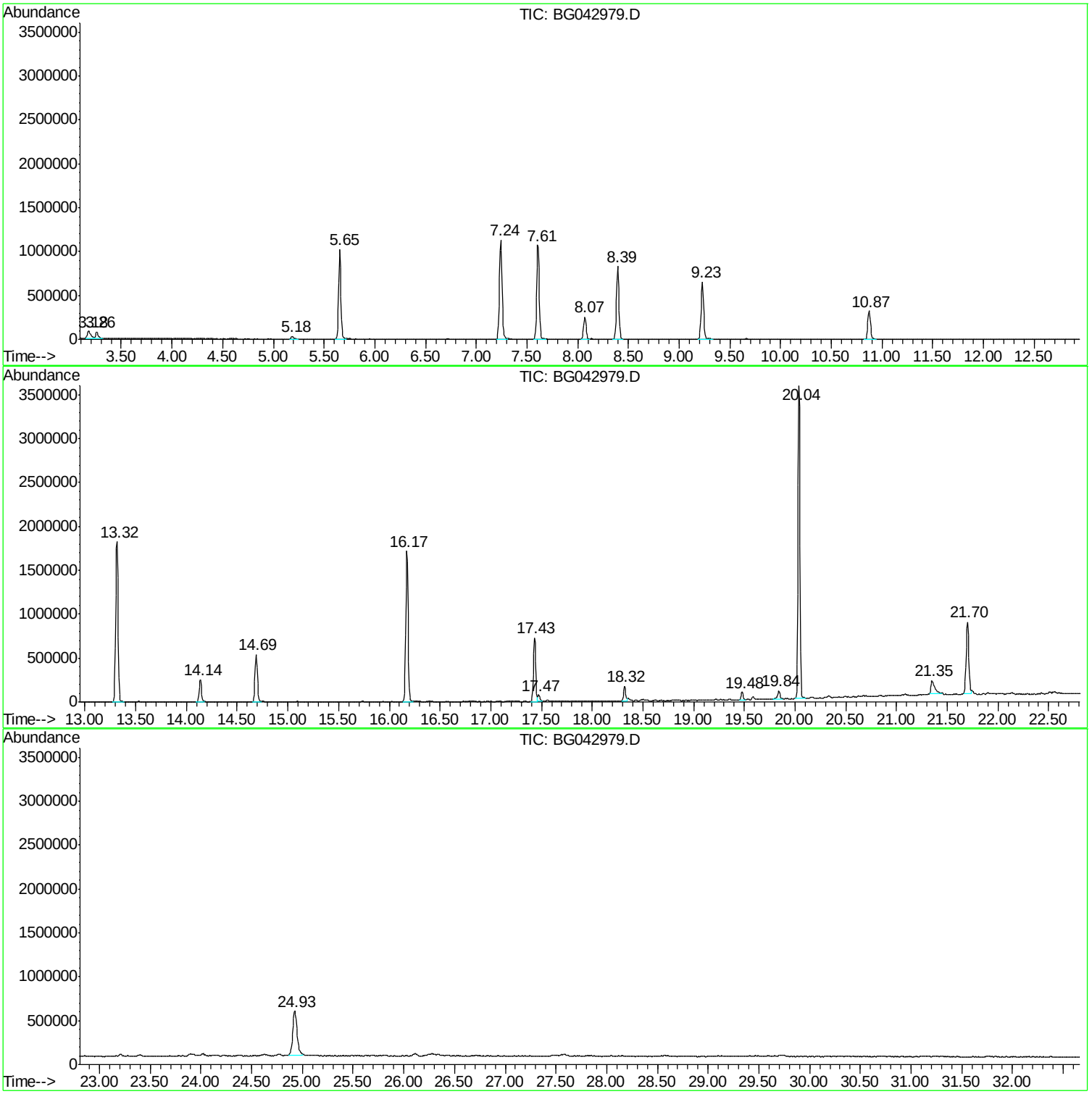
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GP-5_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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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Data File : BG042979.D
Acq On : 1 Oct 2019 22:50
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Sample : K4946-10
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Instrument : BNA_G
ClientSampleId : GP-5_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

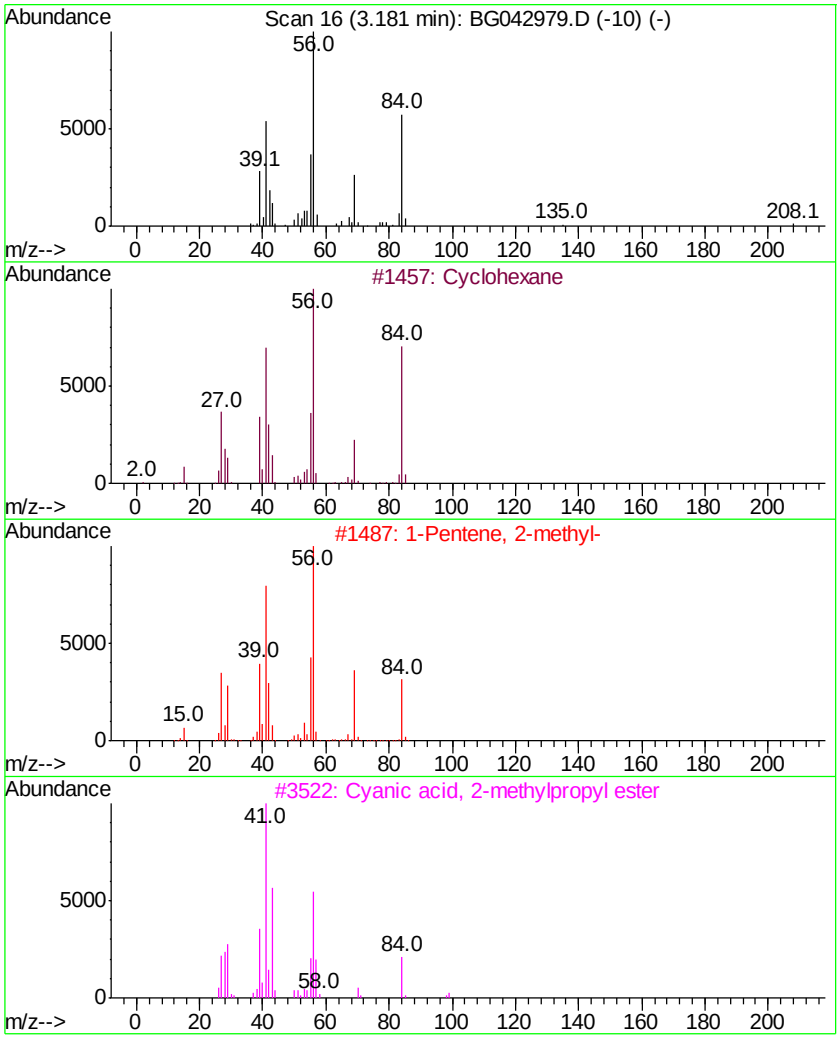
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

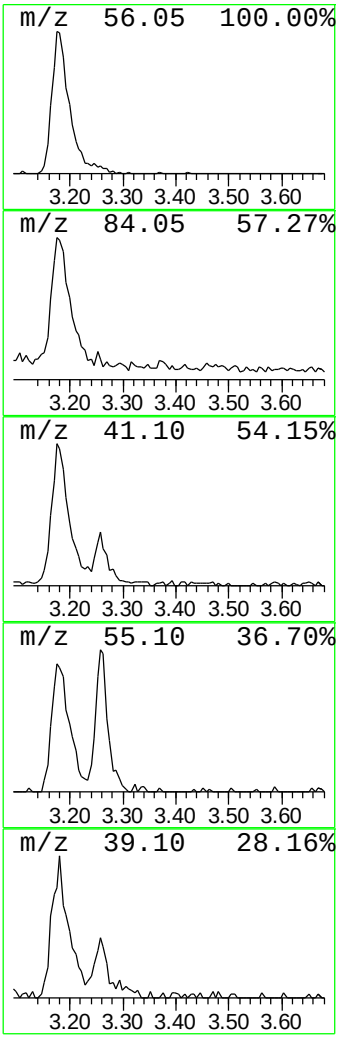
****

Peak Number 1 1-Pentene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	7.92 ng	177103	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	78
3	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	72
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	47





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Data File : BG042979.D
Acq On : 1 Oct 2019 22:50
Operator : JU
Sample : K4946-10
Misc :
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Instrument : BNA_G
ClientSampleId : GP-5_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

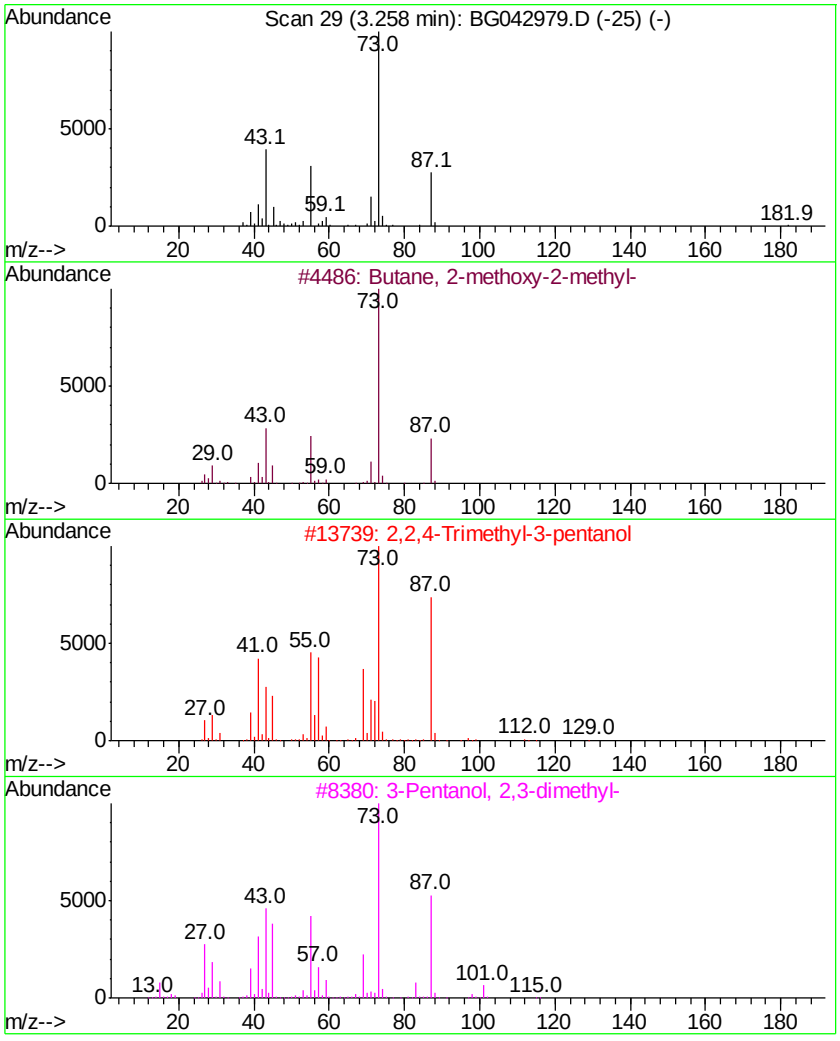
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

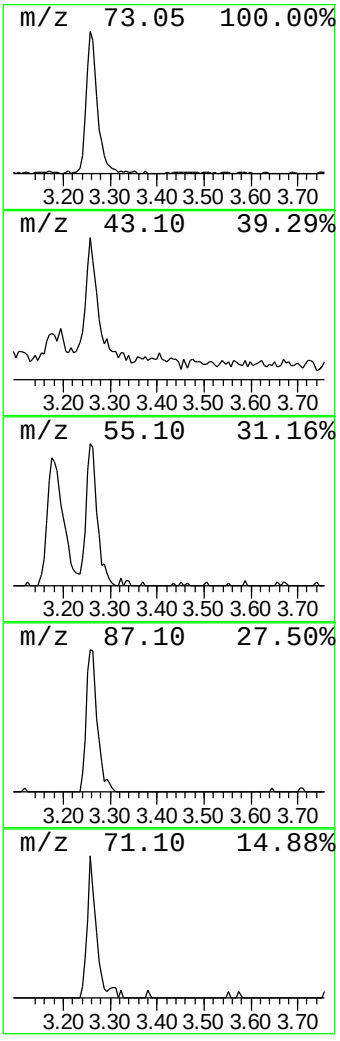
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	5.15 ng	115239	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	33
4	2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	28
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100119\
Data File : BG042979.D
Acq On : 1 Oct 2019 22:50
Operator : JU
Sample : K4946-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-5_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

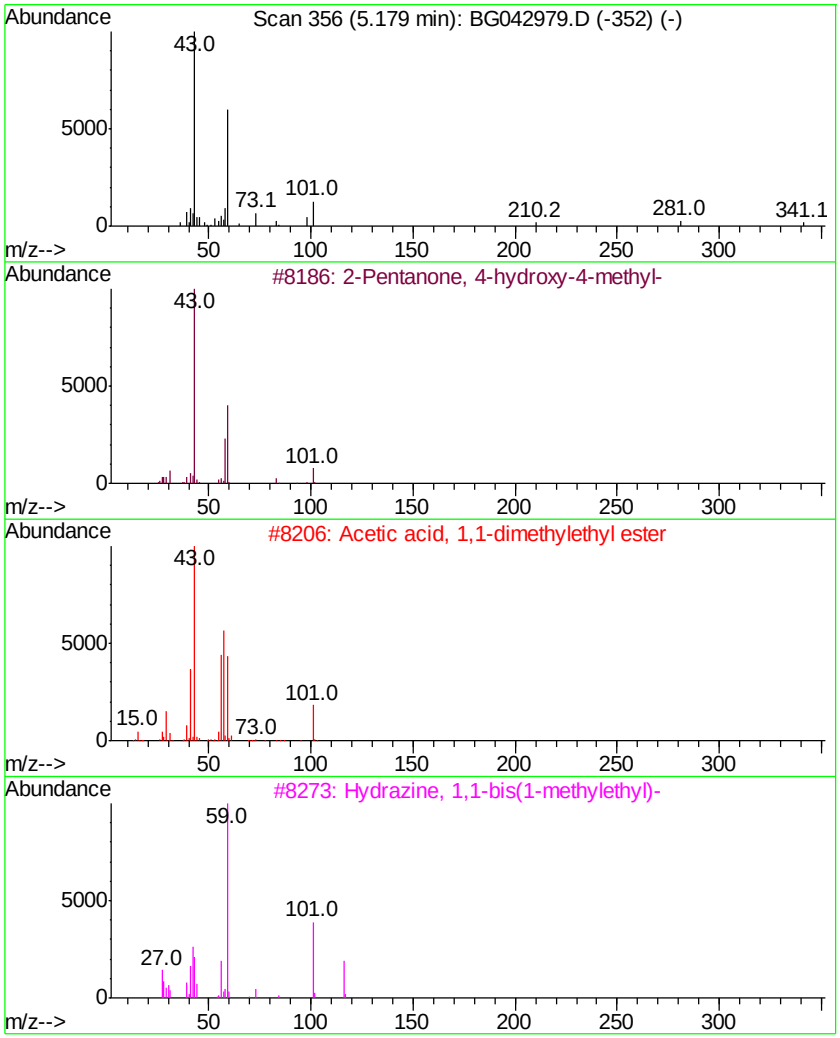
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

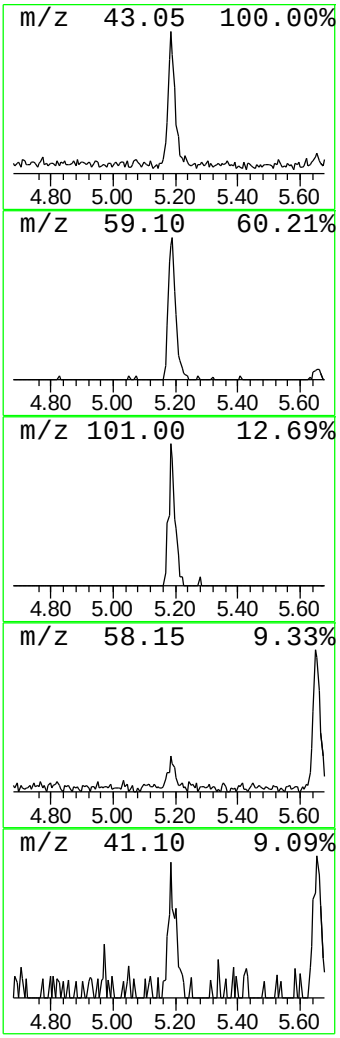
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	2.22 ng	49615	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

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Data File : BG042979.D
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Operator : JU
Sample : K4946-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-5_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

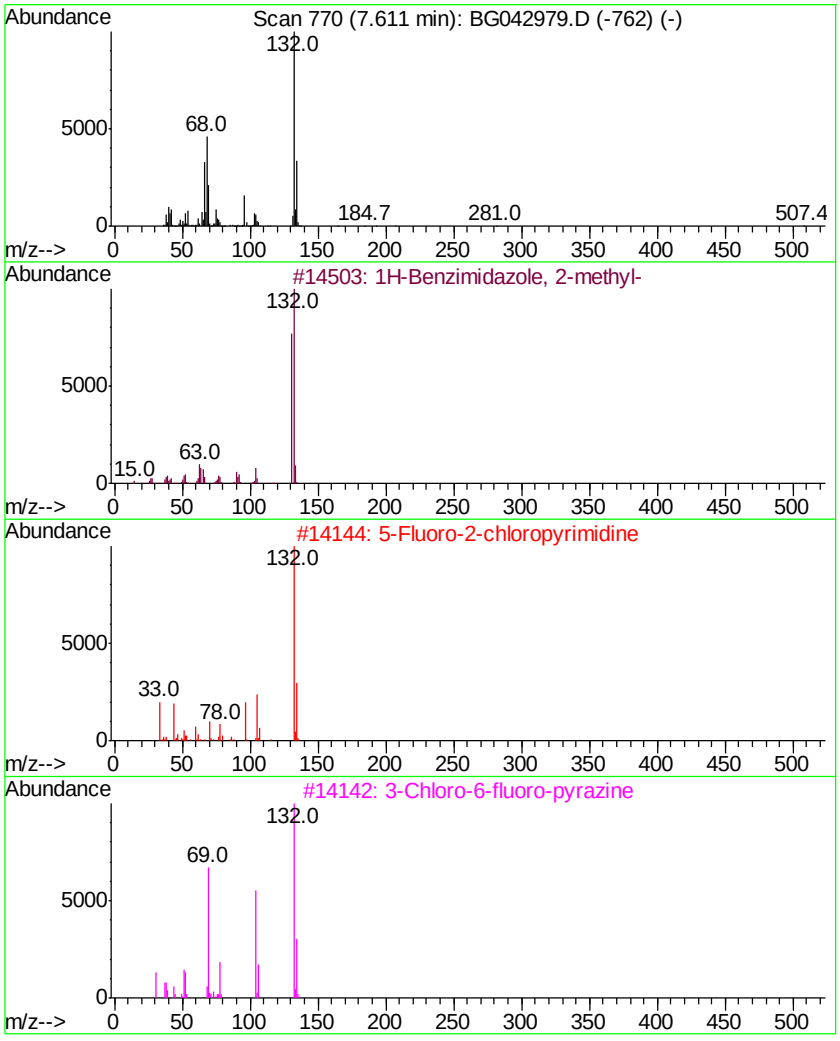
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

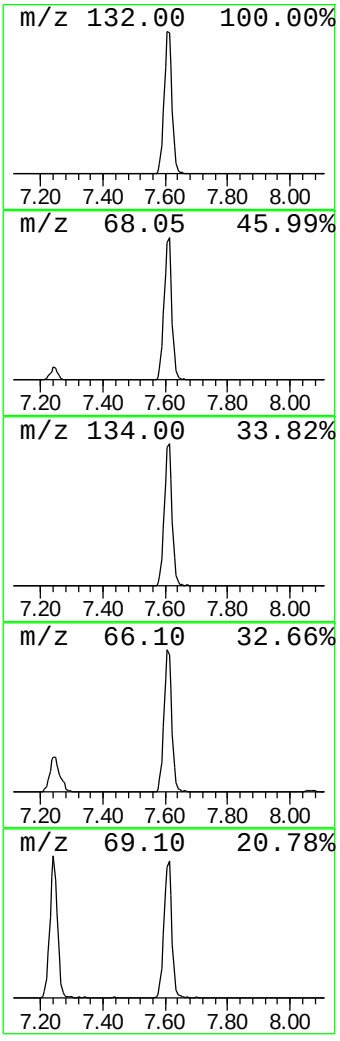
****

Peak Number 4 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	84.17 ng	1882260	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG100119\
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Operator : JU
Sample : K4946-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-5_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

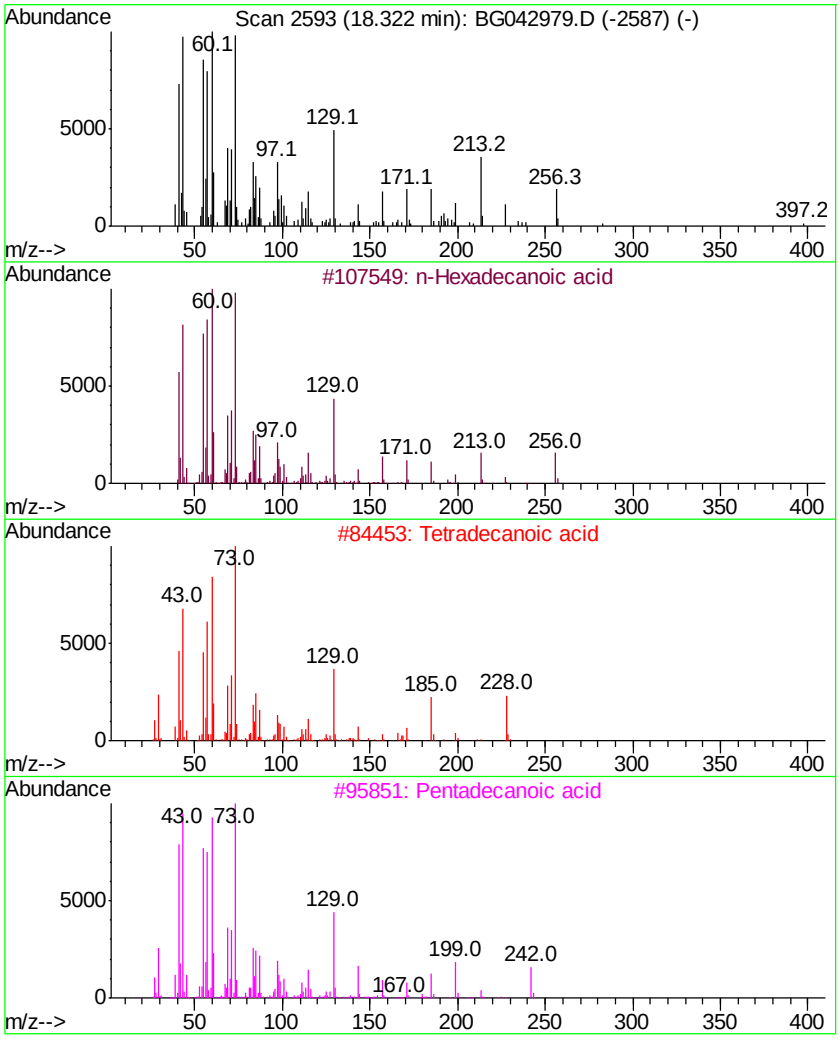
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

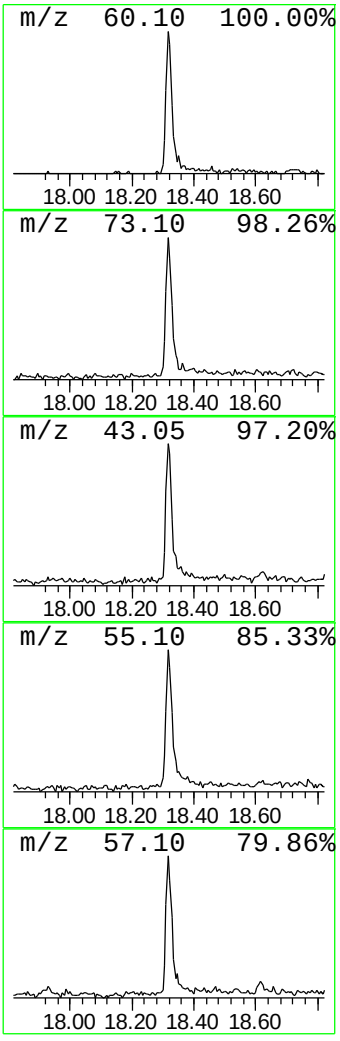
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	4.24 ng	242471	Phenanthrene-d10	17.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : GP-5_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

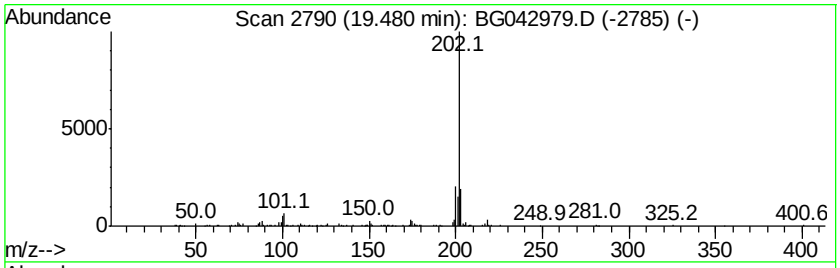
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

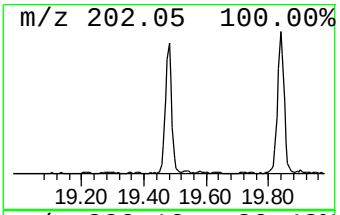
****

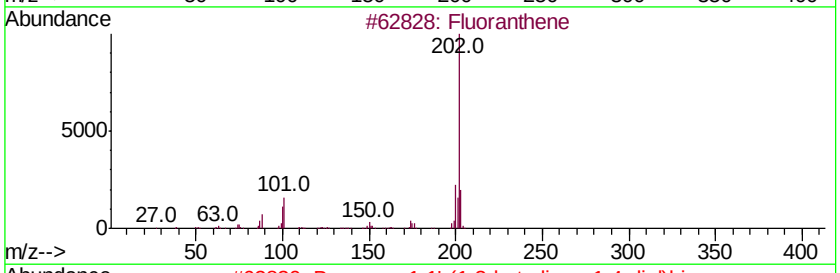
Peak Number 7 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 7

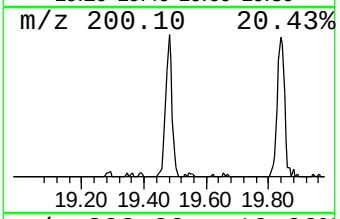
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.48	2.23 ng	127550	Phenanthrene-d10	17.43

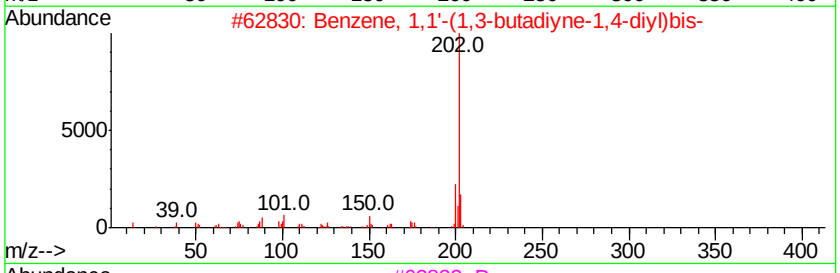
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	95
2	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
3	Pyrene	202	C16H10	000129-00-0	70
4	1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	43
5	Furan-2-one, 2,5-dihydro-5-(4-me...	202	C12H10O3	024962-84-3	40

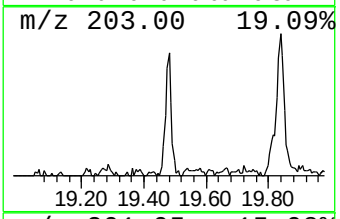


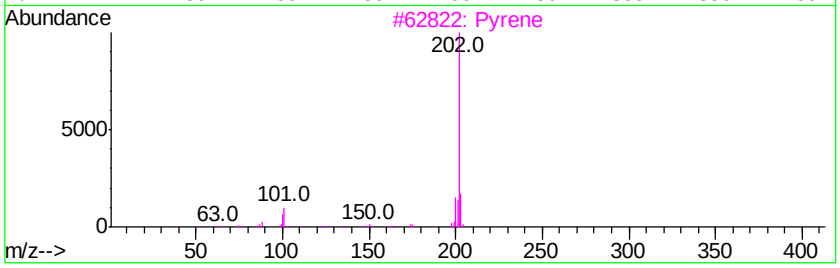


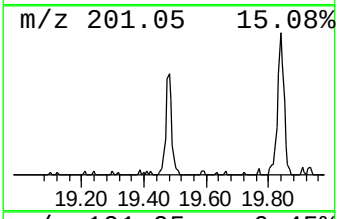


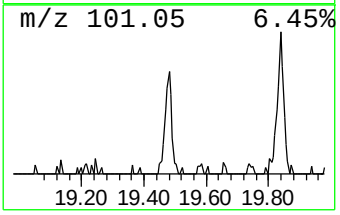












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

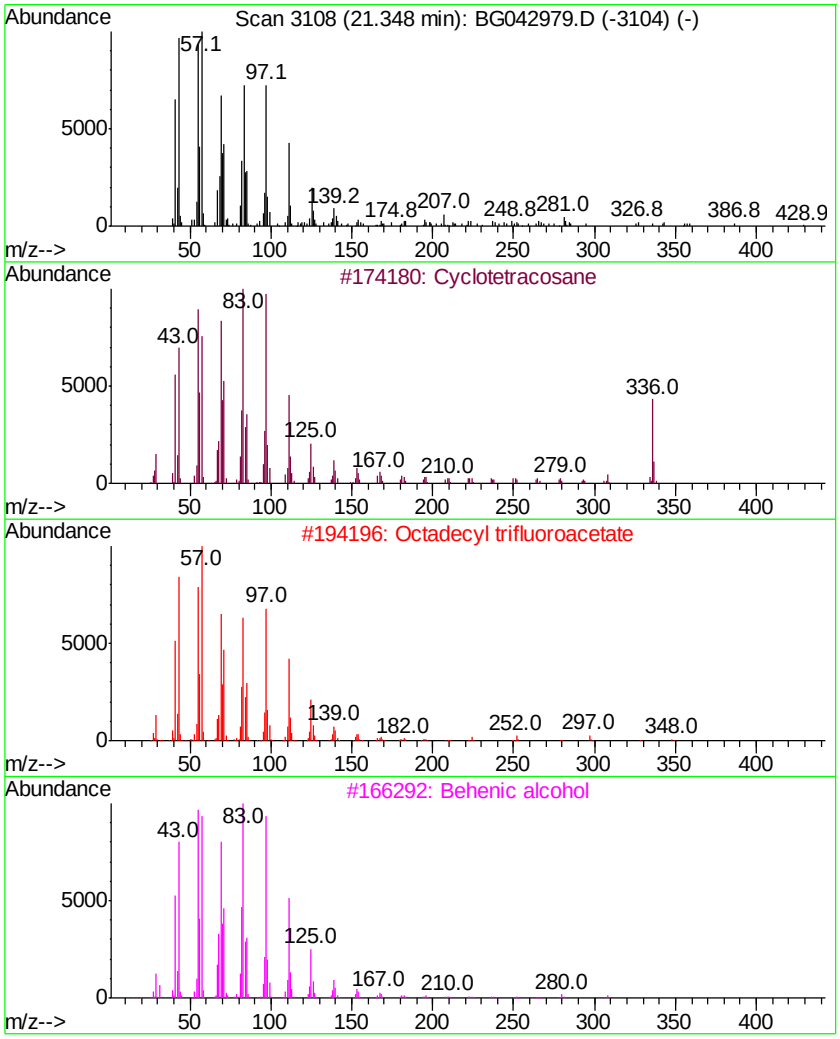
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

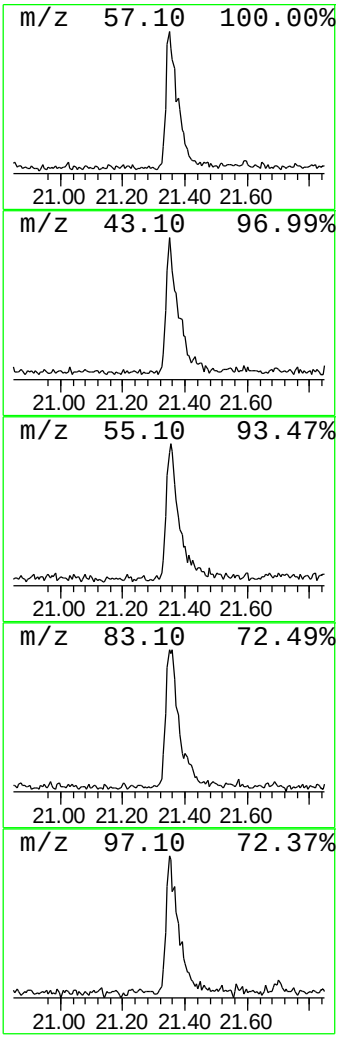
****

Peak Number 8 Cyclotetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	5.41 ng	381035	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	97
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	94





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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
1-Pentene, 2-methyl-	3.18	7.9	ng	177103	1	8.07	447260	20.0
Butane, 2-methoxy...	3.26	5.2	ng	115239	1	8.07	447260	20.0
2-Pentanone, 4-hy...	5.18	2.2	ng	49615	1	8.07	447260	20.0
unknown7.61	7.61	84.2	ng	1882260	1	8.07	447260	20.0
n-Hexadecanoic acid	18.32	4.2	ng	242471	4	17.43	1144230	20.0
Benzene, 1,1'-(1,...	19.48	2.2	ng	127550	4	17.43	1144230	20.0
Cyclotetracosane	21.35	5.4	ng	381035	5	21.70	1408950	20.0