LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044120.D
Acq On : 21 Jan 2020 6:16
Operator : JU
Sample : L1176-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-2

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-BG123019.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	5.035	324	331	343	rBV	341930	551544	9.09%	1.600%
2	5.511	405	412	432	rBV	1553101	2536373	41.79%	7.360%
3	7.104	674	683	704	rBV	1670843	3087196	50.86%	8.958%
4	7.468	737	745	761	rBV	1613829	2862203	47.15%	8.305%
5	7.932	817	824	833	rBV	274558	468273	7.71%	1.359%
6	8.255	871	879	888	rBV	1210803	2119724	34.92%	6.151%
7	9.090	1012	1021	1033	rBV	968459	1781751	29.35%	5.170%
8	10.735	1292	1301	1319	rBV	372200	707600	11.66%	2.053%
9	13.191	1712	1719	1737	rBV	2693389	4429062	72.97%	12.852%
10	14.019	1854	1860	1876	rBV	130397	225325	3.71%	0.654%
11	14.571	1946	1954	1969	rBV	687866	1097817	18.09%	3.186%
12	16.058	2200	2207	2229	rBV	2135952	3465986	57.10%	10.057%
13	17.315	2412	2421	2433	rBV	749139	1248594	20.57%	3.623%
14	19.930	2859	2866	2880	rBV	4546464	6069855	100.00%	17.613%
15	21.234	3082	3088	3103	rBV	123781	319791	5.27%	0.928%
16	21.557	3137	3143	3162	rBV	779733	1292003	21.29%	3.749%
17	22.362	3275	3280	3287	rBV2	84812	162659	2.68%	0.472%
18	23.038	3389	3395	3401	rVB	97476	176939	2.92%	0.513%
19	23.220	3421	3426	3433	rVB3	39565	77345	1.27%	0.224%
20	23.813	3521	3527	3535	rVB	101639	205271	3.38%	0.596%
21	24.671	3663	3673	3681	rBV2	461943	1302966	21.47%	3.781%
22	25.823	3862	3869	3879	rBV2	62131	174601	2.88%	0.507%
23	27.139	4086	4093	4102	rVB6	31665	99998	1.65%	0.290%

Sum of corrected areas: 34462876

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
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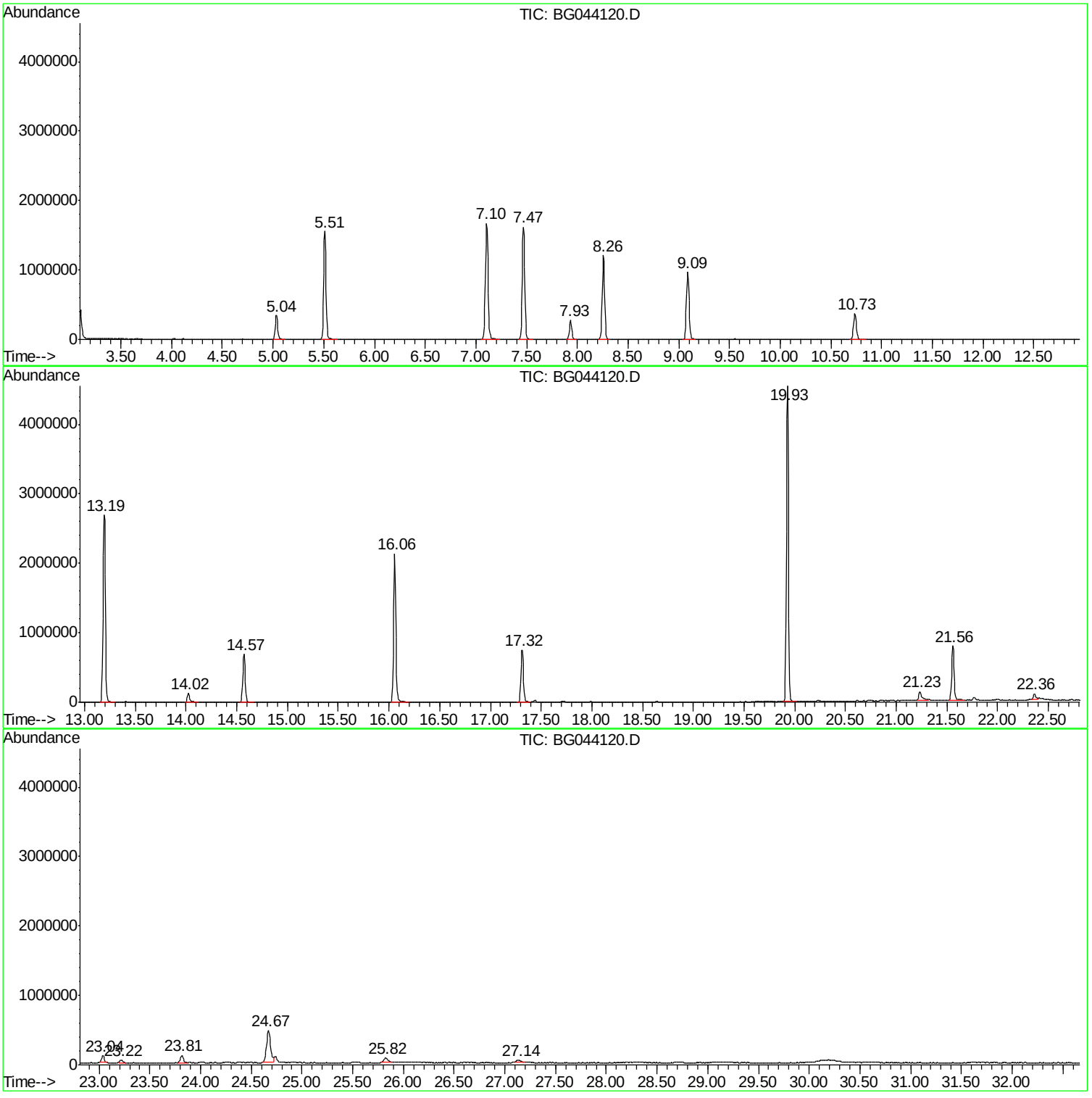
Sample : L1176-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
EP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044120.D
Acq On : 21 Jan 2020 6:16
Operator : JU
Sample : L1176-02
Misc :
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Instrument : BNA_G
ClientSampleId : EP-2

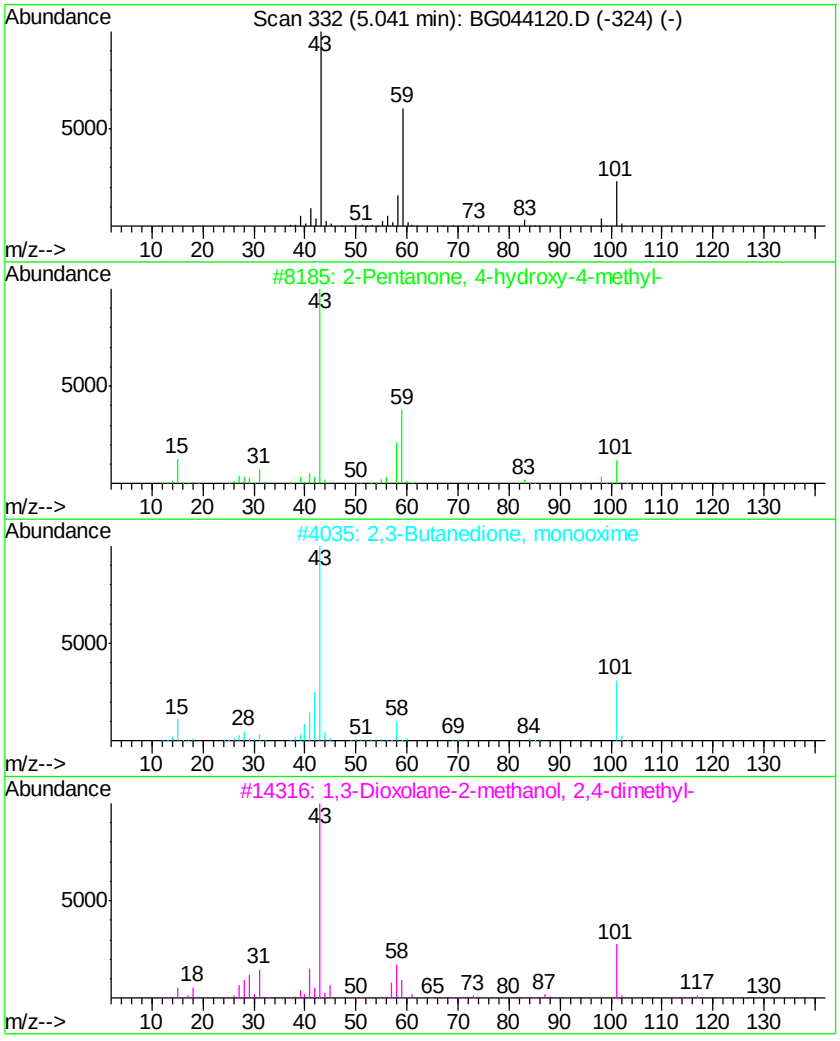
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

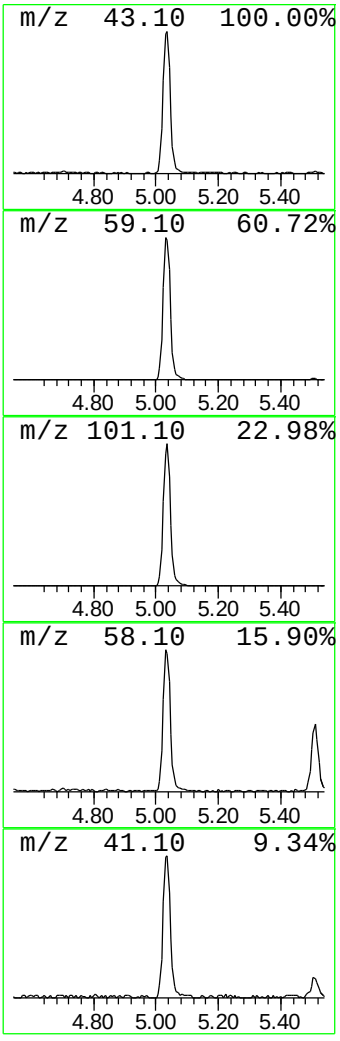
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	23.56 ng	551544	1,4-Dichlorobenzene-d4	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044120.D
Acq On : 21 Jan 2020 6:16
Operator : JU
Sample : L1176-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

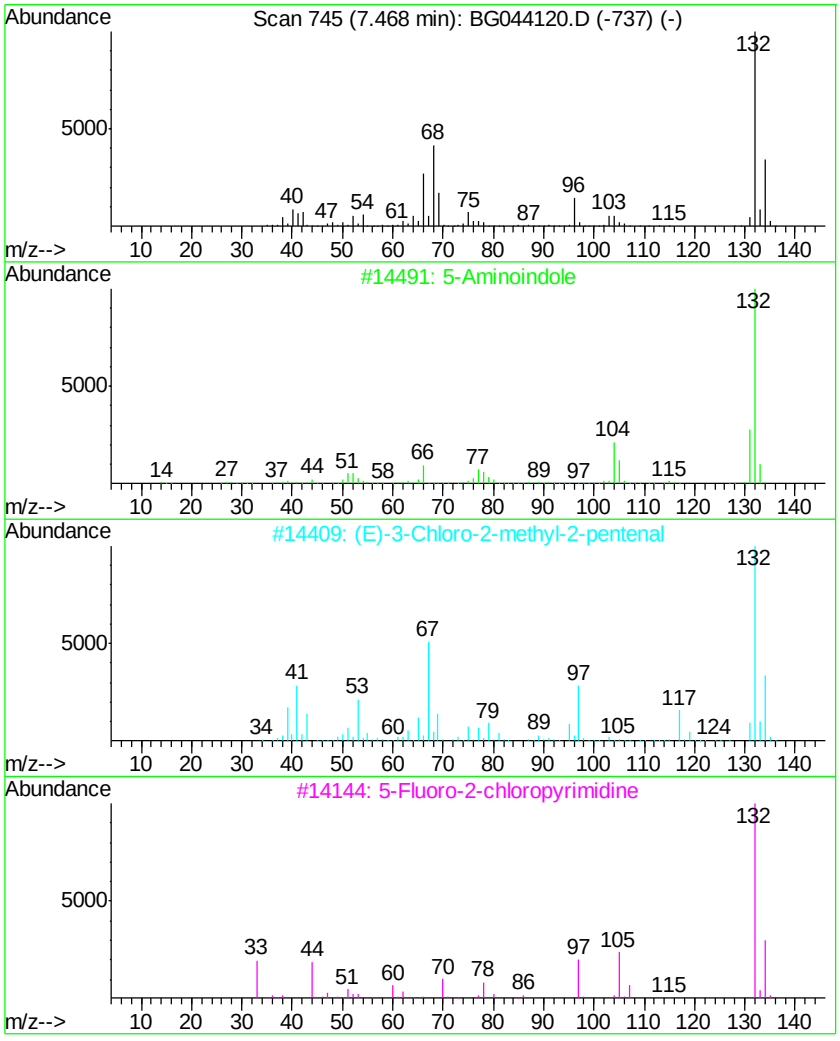
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

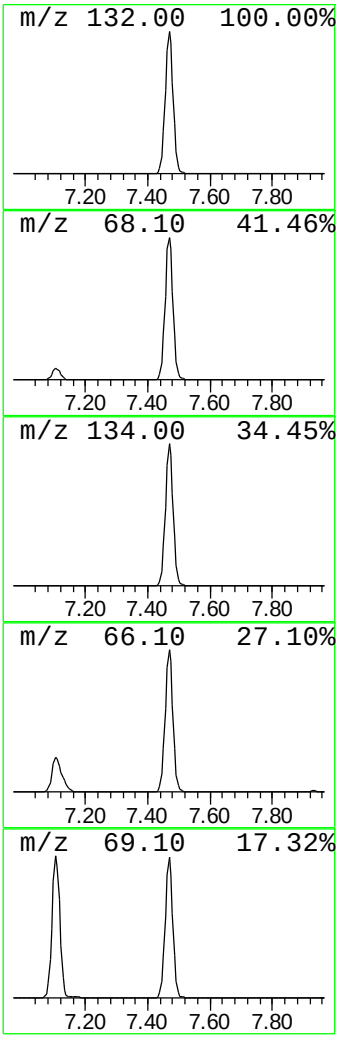
****

Peak Number 2 unknown7.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	122.25 ng	2862200	1,4-Dichlorobenzene-d4	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	22
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Amphetaminil	250	C17H18N2	017590-01-1	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044120.D
Acq On : 21 Jan 2020 6:16
Operator : JU
Sample : L1176-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

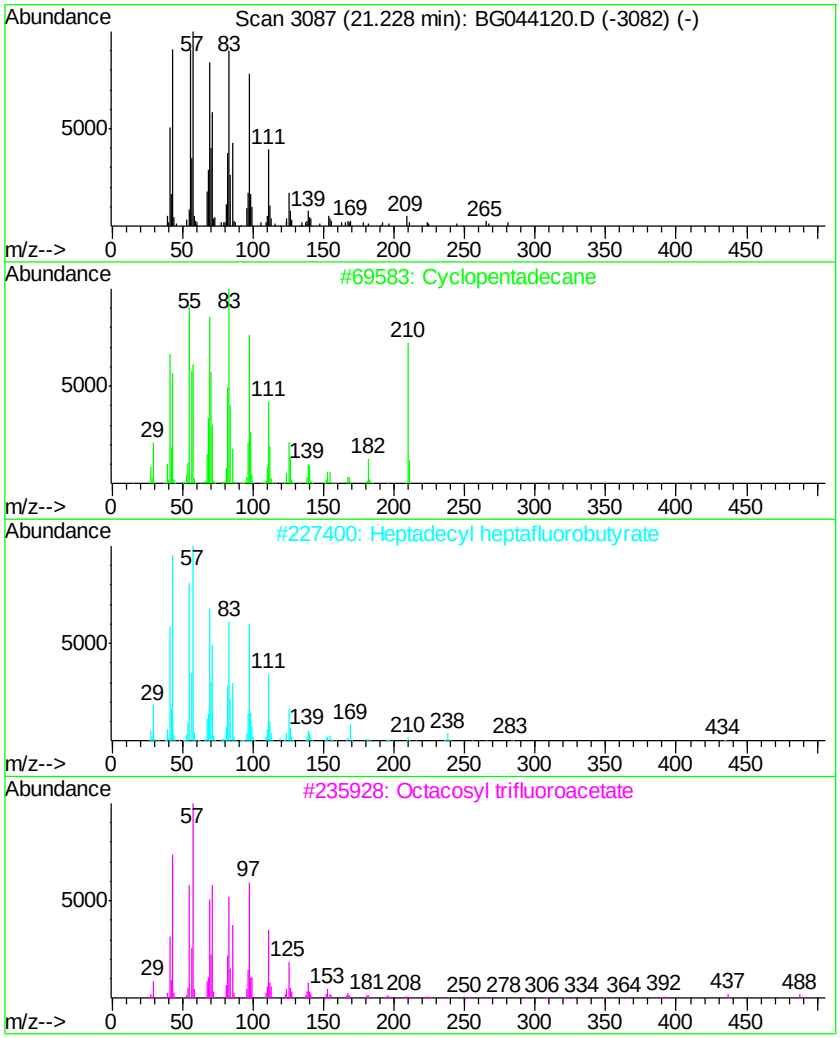
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

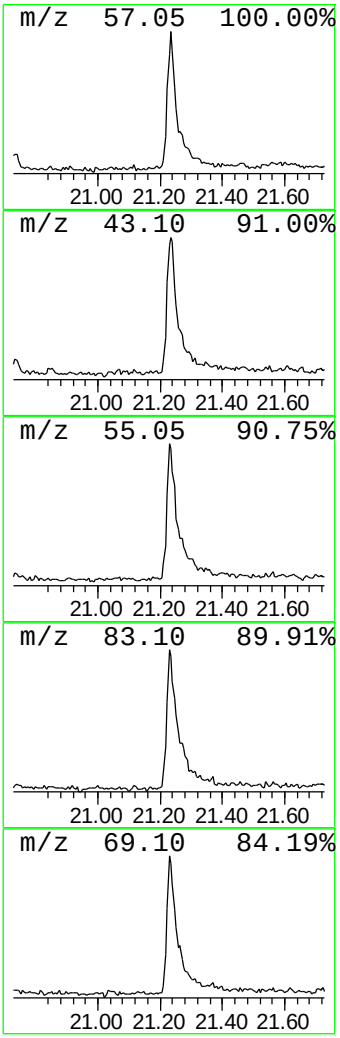
****

Peak Number 4 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.23	4.95 ng	319791	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	96
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044120.D
Acq On : 21 Jan 2020 6:16
Operator : JU
Sample : L1176-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

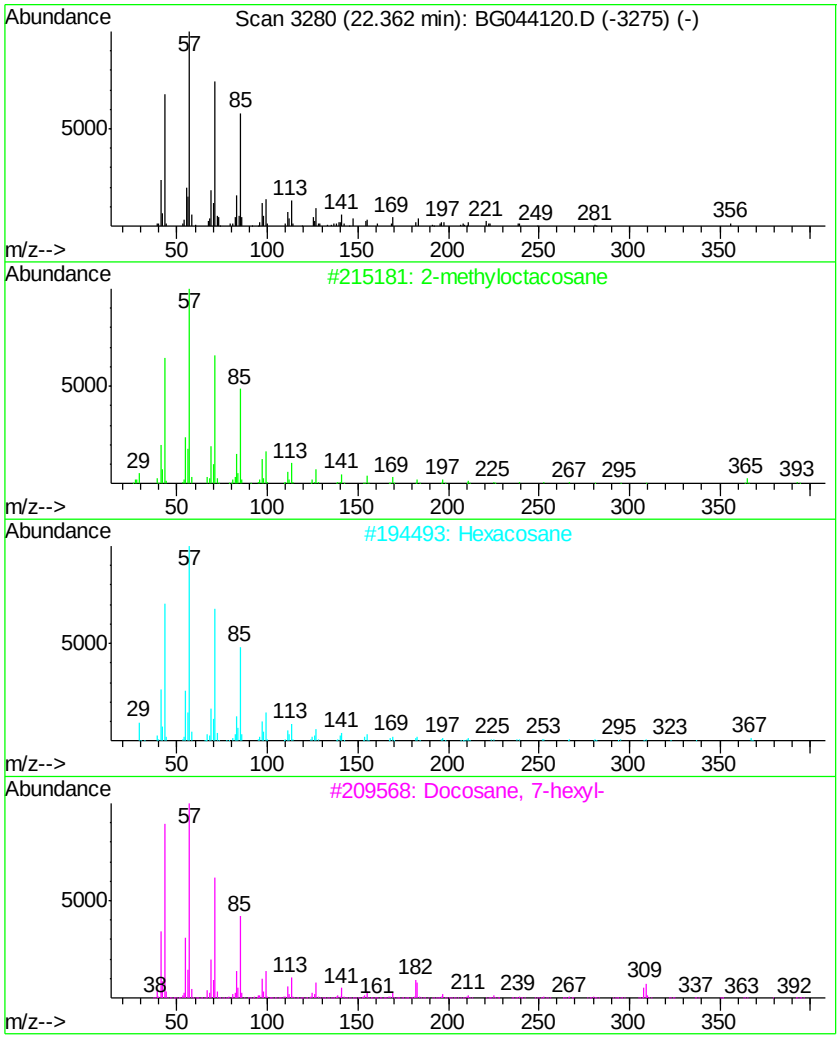
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

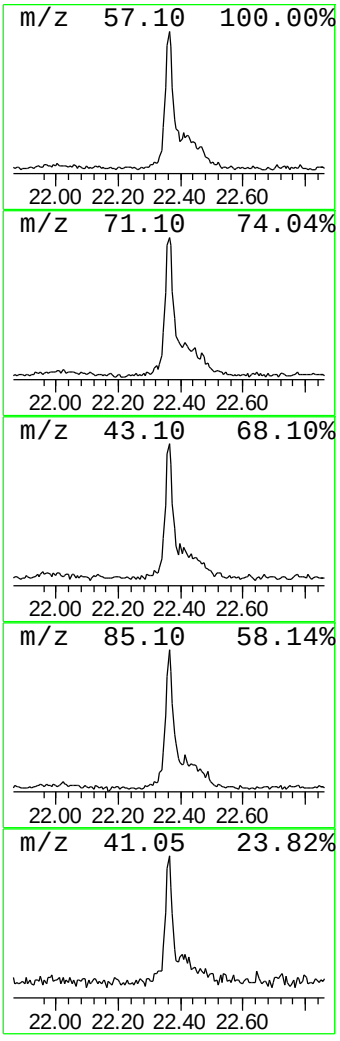
****

Peak Number 5 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.36	2.52 ng	162659	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044120.D
Acq On : 21 Jan 2020 6:16
Operator : JU
Sample : L1176-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

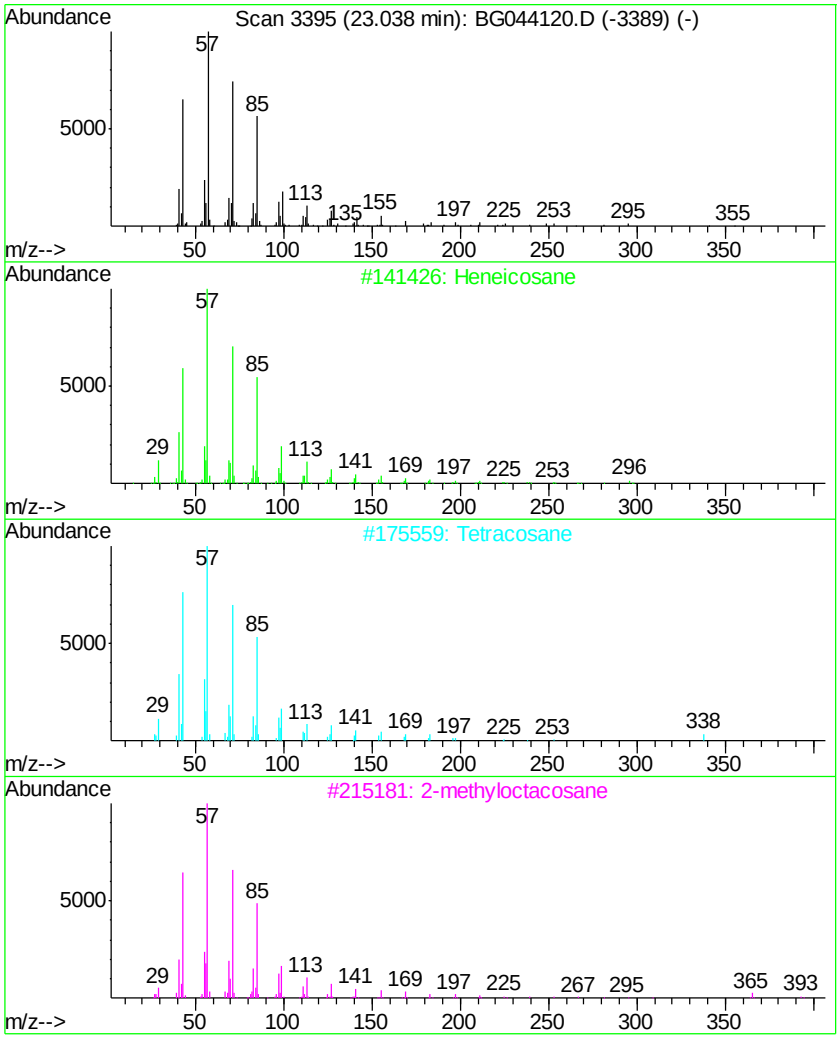
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

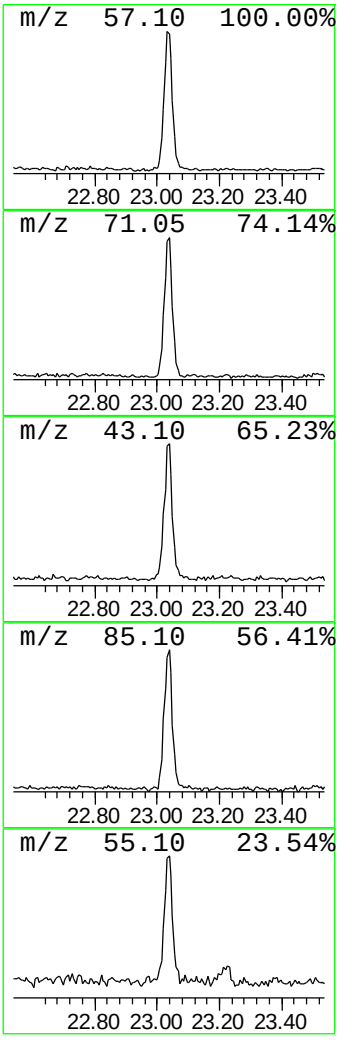
****

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.04	2.74 ng	176939	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG012020\
Data File : BG044120.D
Acq On : 21 Jan 2020 6:16
Operator : JU
Sample : L1176-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

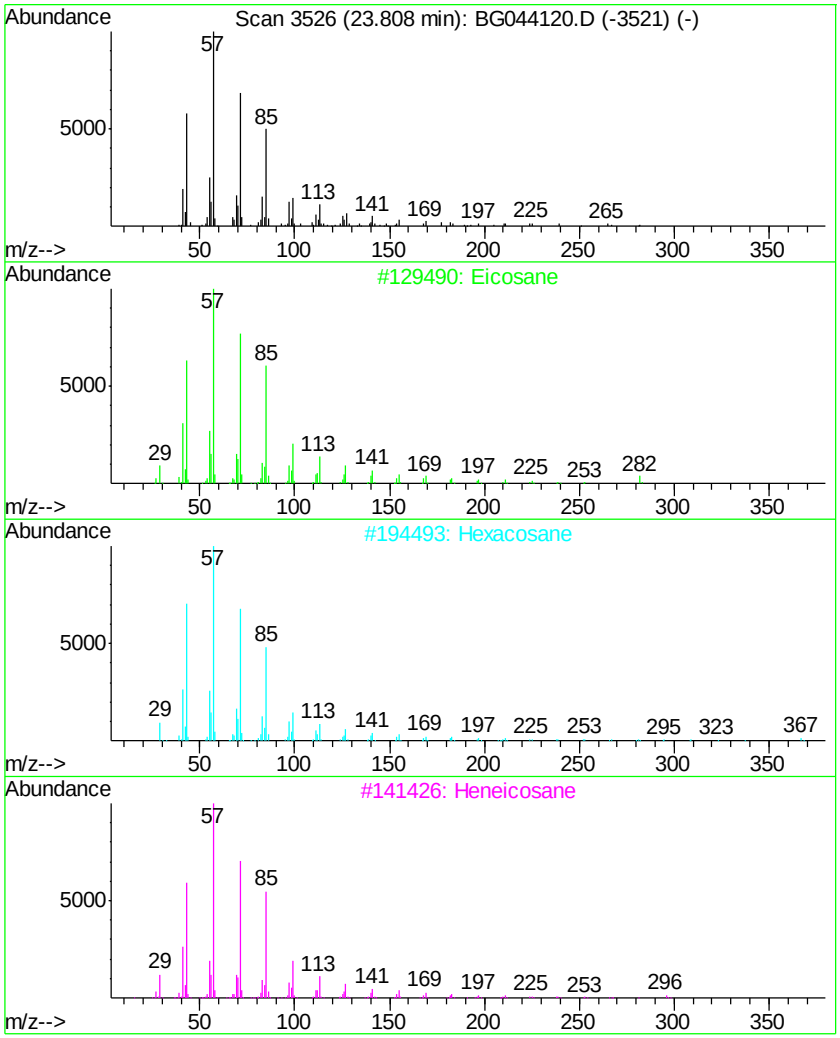
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

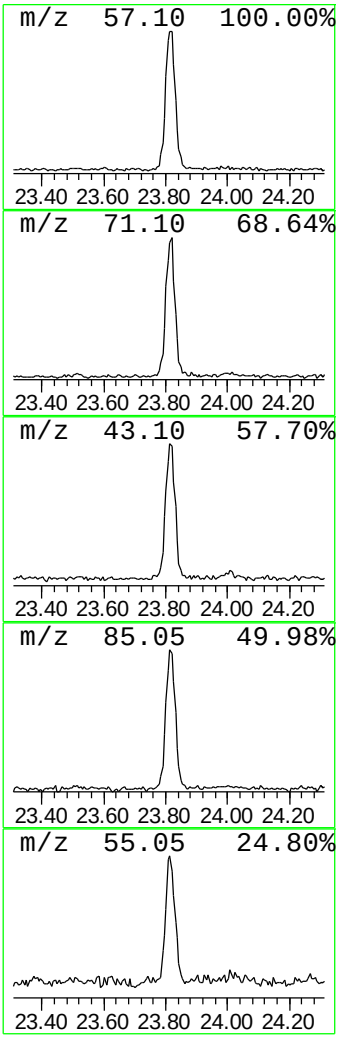
****

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.81	3.15 ng	205271	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Hexacosane	366	C26H54	000630-01-3	94
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane	394	C28H58	000630-02-4	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Library Search Compound Report

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

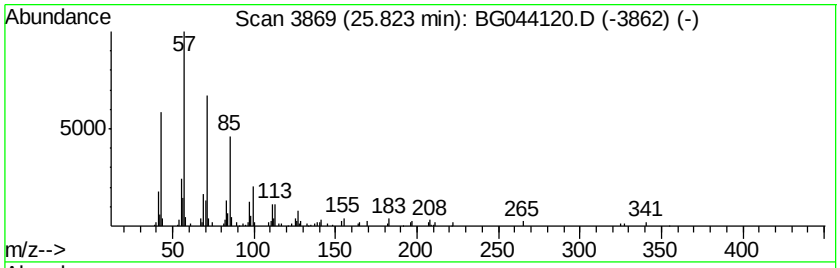
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

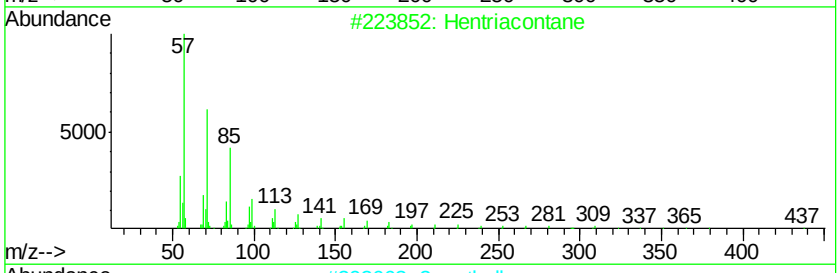
****

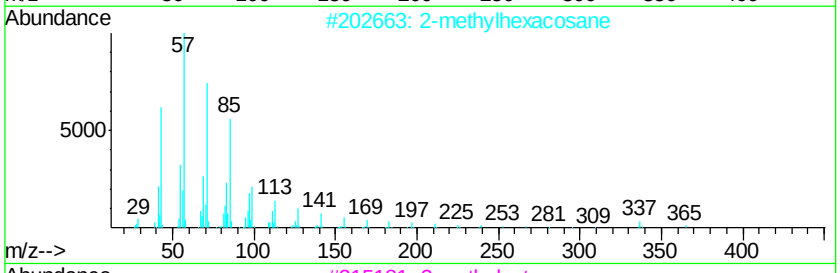
Peak Number 8 Hentriacontane Concentration Rank 7

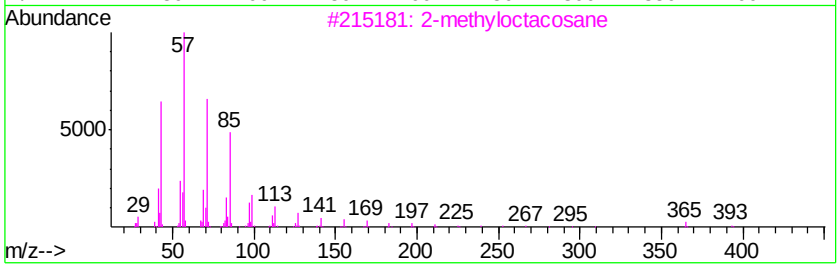
R.T.	EstConc	Area	Relative to ISTD	R.T.
25.82	2.68 ng	174601	Perylene-d12	24.67

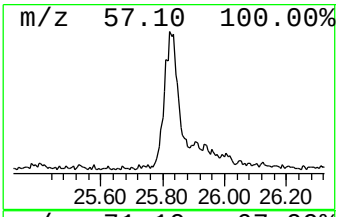
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	2-methylhexacosane	380	C27H56	1000376-72-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
5	Tetratetracontane	619	C44H90	007098-22-8	87

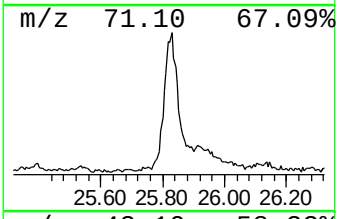


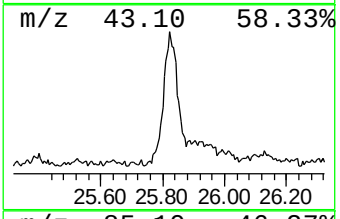


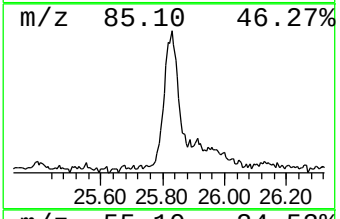


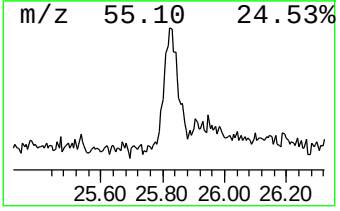












Tentatively Identified Compound (LSC) summary

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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...	5.04	23.6	ng	551544	1	7.93	468273	20.0
unknown7.47	7.47	122.3	ng	2862200	1	7.93	468273	20.0
Cyclopentadecane	21.23	5.0	ng	319791	5	21.56	1292000	20.0
2-methyloctacosane	22.36	2.5	ng	162659	5	21.56	1292000	20.0
Heneicosane	23.04	2.7	ng	176939	5	21.56	1292000	20.0
Eicosane	23.81	3.1	ng	205271	6	24.67	1302970	20.0
Hentriacontane	25.82	2.7	ng	174601	6	24.67	1302970	20.0