LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044257.D
Acq On : 31 Jan 2020 13:03
Operator : CG/JU
Sample : L1319-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RAINEY-PARK-BH-01-C

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-BG013020.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	5.016	324	328	336	rVB	44194	66892	1.54%	0.288%
2	5.492	402	409	424	rBV	910403	1482499	34.04%	6.391%
3	7.084	672	680	691	rBV	979802	1705666	39.16%	7.353%
4	7.912	815	821	829	rBV	233716	398422	9.15%	1.718%
5	8.236	868	876	886	rBV	733346	1292801	29.68%	5.573%
6	9.070	1010	1018	1033	rBV	582965	1063377	24.41%	4.584%
7	10.715	1291	1298	1313	rBV	322102	608193	13.96%	2.622%
8	13.177	1709	1717	1728	rBV	1734272	2733048	62.75%	11.782%
9	14.005	1853	1858	1870	rBV	48634	81489	1.87%	0.351%
10	14.552	1944	1951	1961	rBV2	608403	996649	22.88%	4.296%
11	16.038	2198	2204	2220	rBV	1370717	2205050	50.63%	9.506%
12	17.296	2411	2418	2424	rBV	825914	1270496	29.17%	5.477%
13	17.689	2481	2485	2497	rBV5	19609	46931	1.08%	0.202%
14	19.346	2762	2767	2773	rBV	37718	59108	1.36%	0.255%
15	19.710	2822	2829	2835	rBV	36773	67972	1.56%	0.293%
16	19.910	2857	2863	2877	rBV	3237750	4355618	100.00%	18.777%
17	20.598	2973	2980	2988	rBV	290937	432131	9.92%	1.863%
18	21.215	3080	3085	3093	rBV3	170638	334038	7.67%	1.440%
19	21.544	3133	3141	3160	rVB	792618	1389936	31.91%	5.992%
20	21.749	3172	3176	3181	rVB	45920	64365	1.48%	0.277%
21	22.337	3272	3276	3285	rVB2	61601	105551	2.42%	0.455%
22	23.007	3385	3390	3398	rVB	77811	144759	3.32%	0.624%
23	23.195	3415	3422	3432	rVB	271108	501735	11.52%	2.163%
24	23.782	3516	3522	3531	rBV2	79905	167843	3.85%	0.724%
25	24.640	3658	3668	3687	rBV2	428264	1484418	34.08%	6.399%
26	25.786	3854	3863	3871	rVB3	47401	137861	3.17%	0.594%

Sum of corrected areas: 23196848

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
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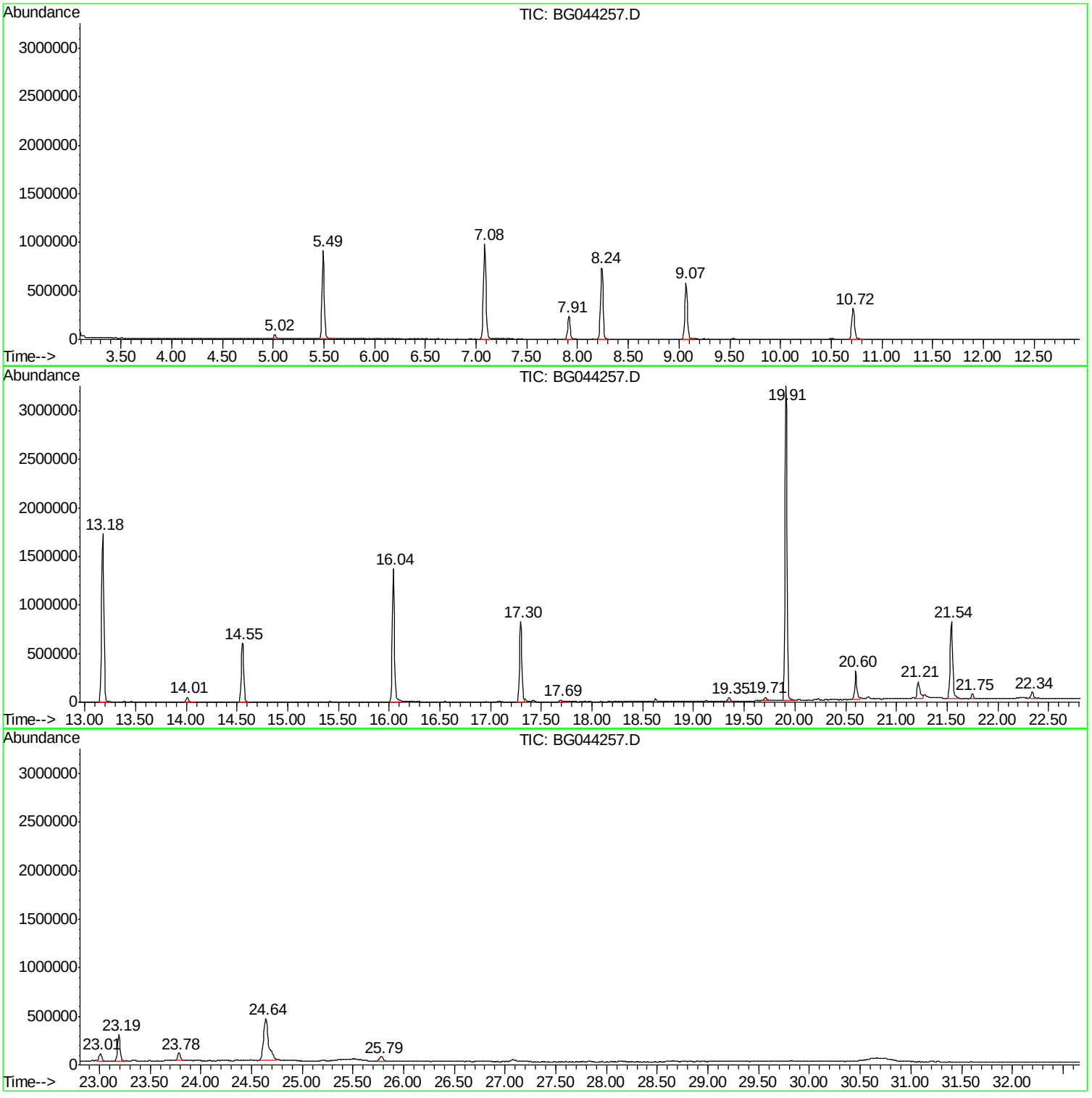
Operator : CG/JU
Sample : L1319-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RAINEY-PARK-BH-01-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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 G\DATA\BG013120\
Data File : BG044257.D
Acq On : 31 Jan 2020 13:03
Operator : CG/JU
Sample : L1319-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RAINEY-PARK-BH-01-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

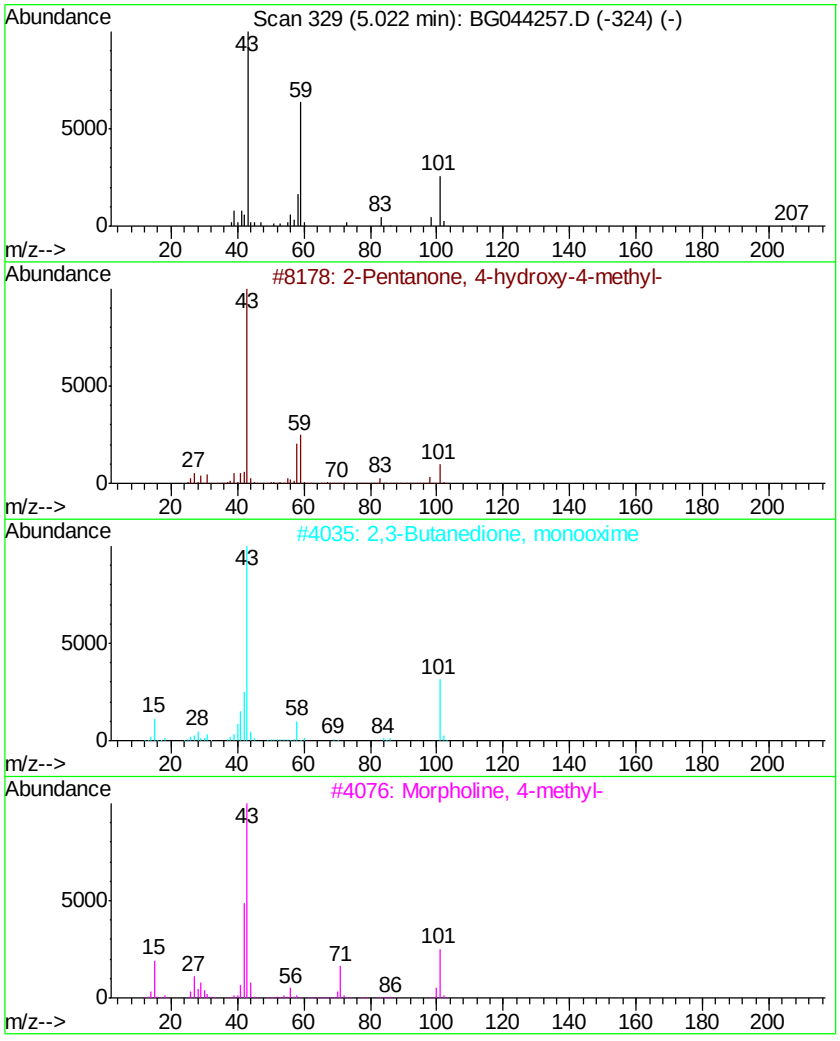
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

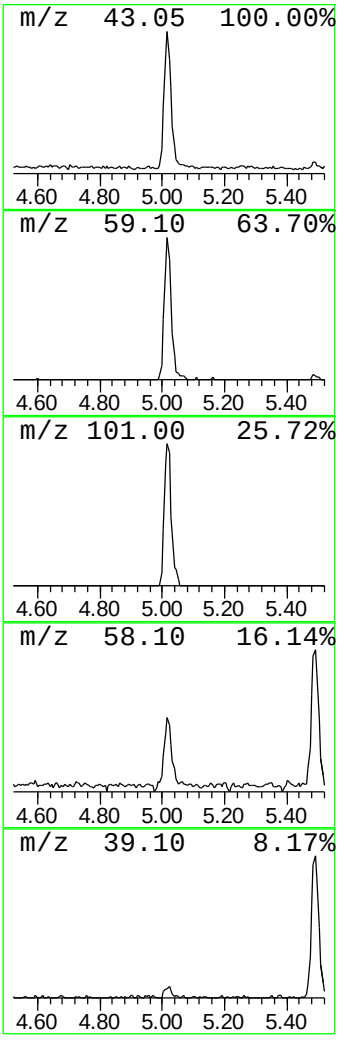
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.36 ng	66892	1,4-Dichlorobenzene-d4	7.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9





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Acq On : 31 Jan 2020 13:03
Operator : CG/JU
Sample : L1319-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RAINEY-PARK-BH-01-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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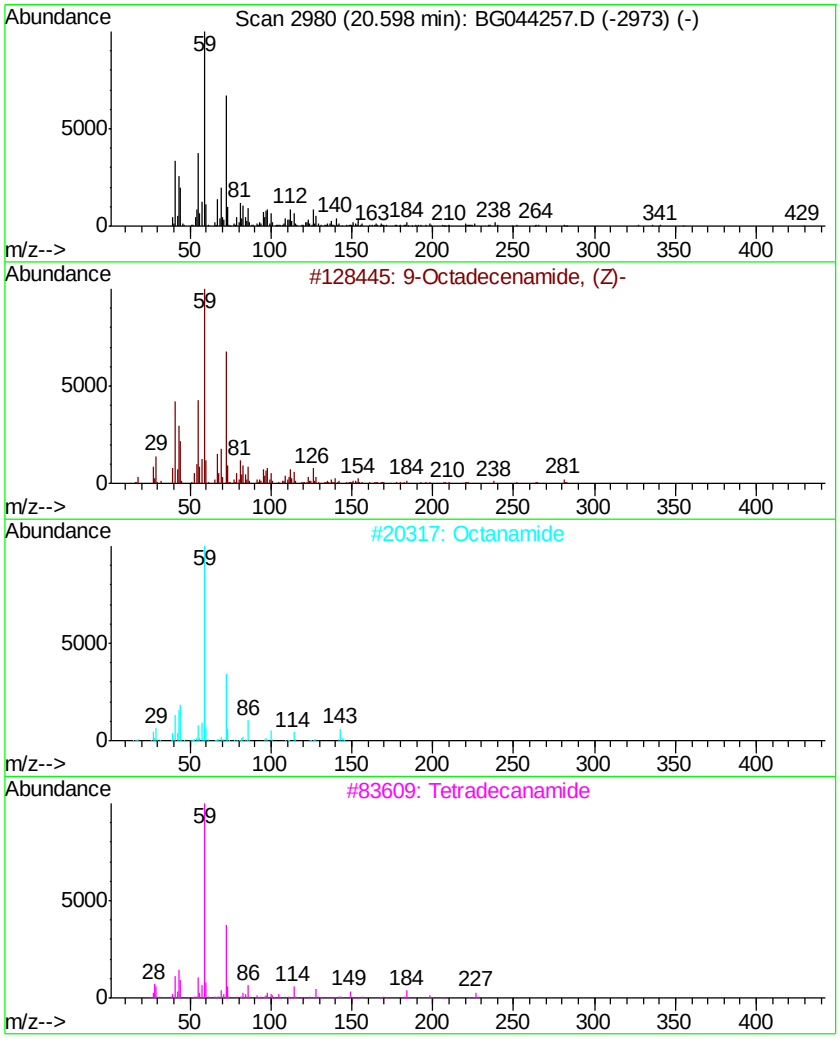
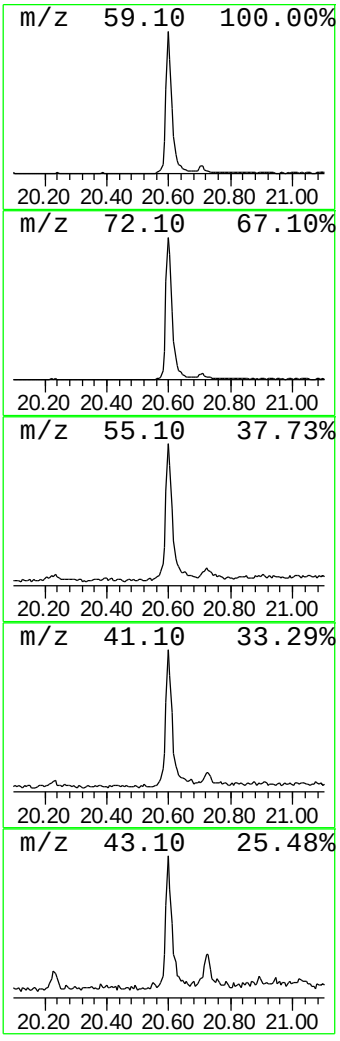
Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.60	6.22 ng	432131	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Octanamide	143	C8H17NO	000629-01-6	72
3	Tetradecanamide	227	C14H29NO	000638-58-4	64
4	Hexadecanamide	255	C16H33NO	000629-54-9	53
5	Butanamide, 3-methyl-	101	C5H11NO	000541-46-8	47





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044257.D
Acq On : 31 Jan 2020 13:03
Operator : CG/JU
Sample : L1319-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RAINEY-PARK-BH-01-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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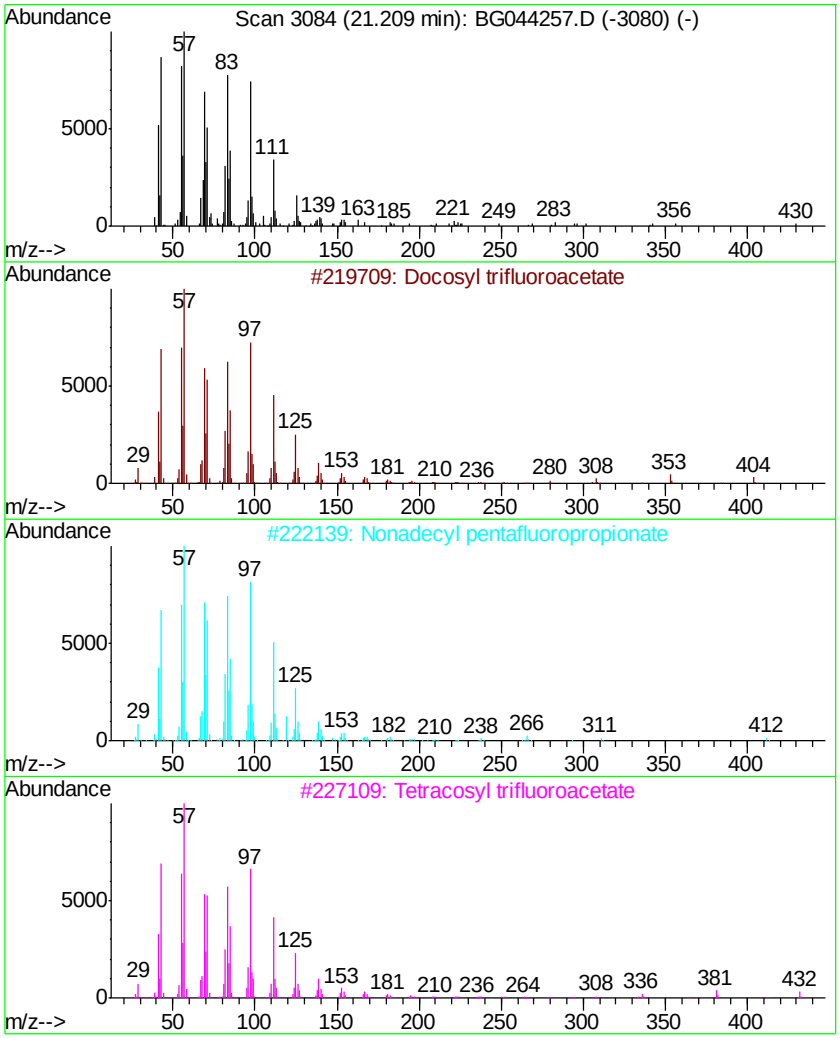
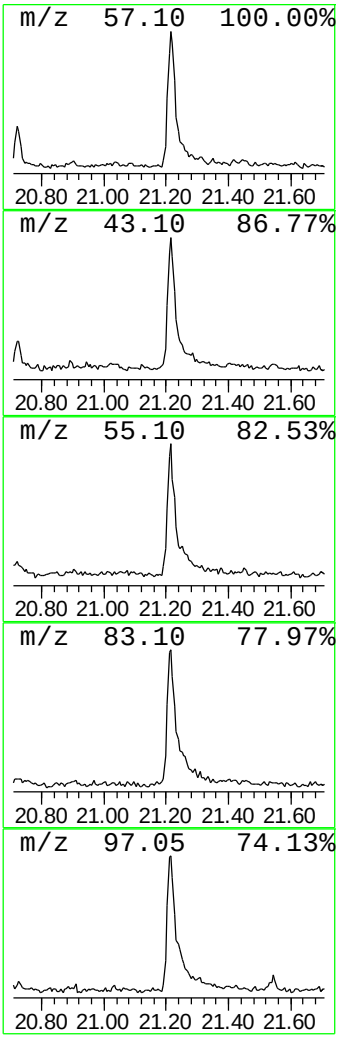
Peak Number 4 Docosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.21	4.81 ng	334038	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	91
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	Tetracosyl trifluoroacetate	450	C26H49F3O2	1000351-76-4	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044257.D
Acq On : 31 Jan 2020 13:03
Operator : CG/JU
Sample : L1319-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RAINEY-PARK-BH-01-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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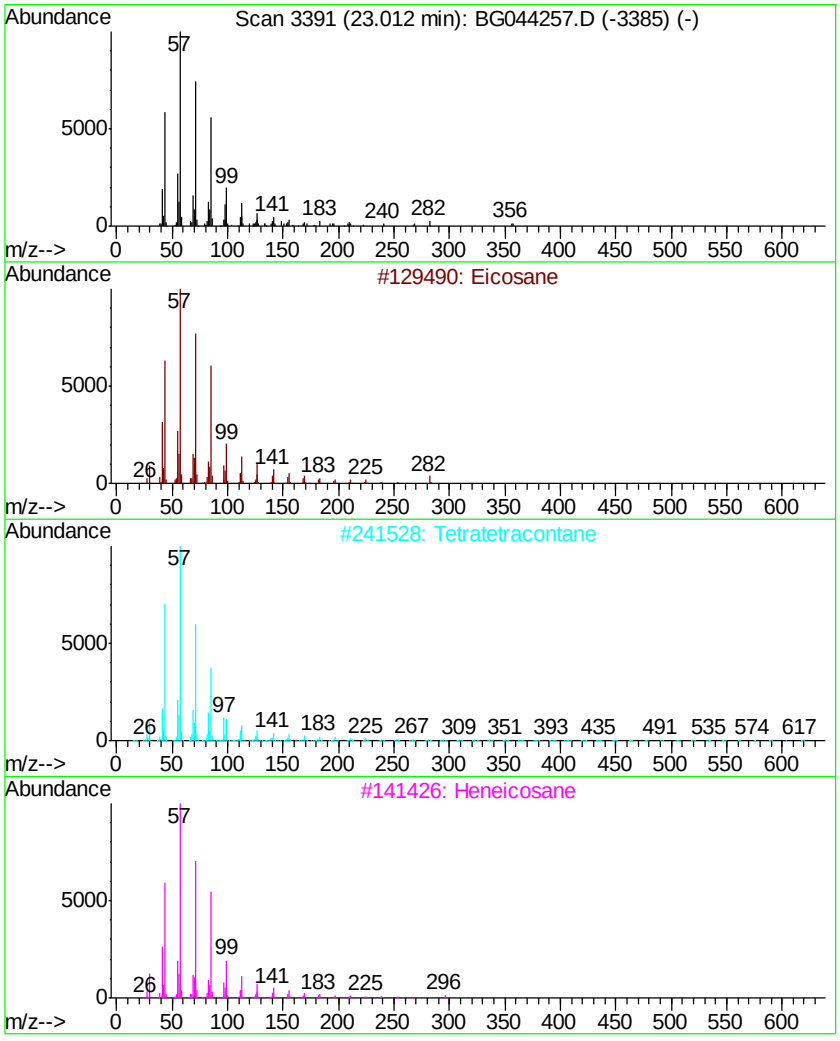
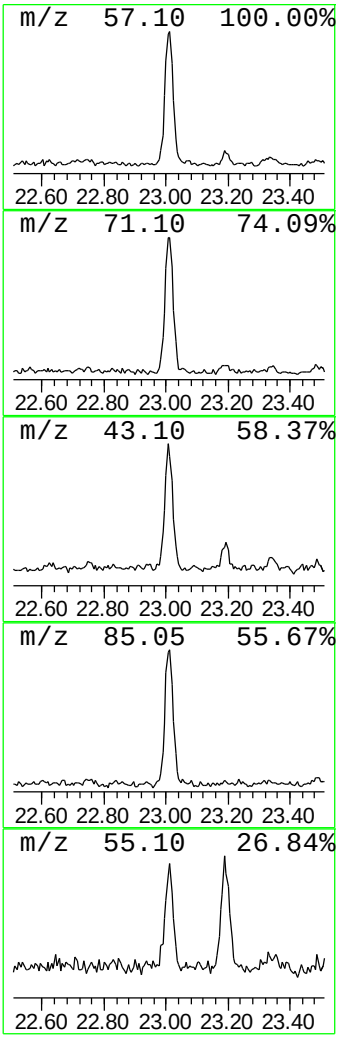
Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.01	2.08 ng	144759	Chrysene-d12	21.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Tetratetracontane	619	C44H90	007098-22-8	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
Data File : BG044257.D
Acq On : 31 Jan 2020 13:03
Operator : CG/JU
Sample : L1319-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RAINEY-PARK-BH-01-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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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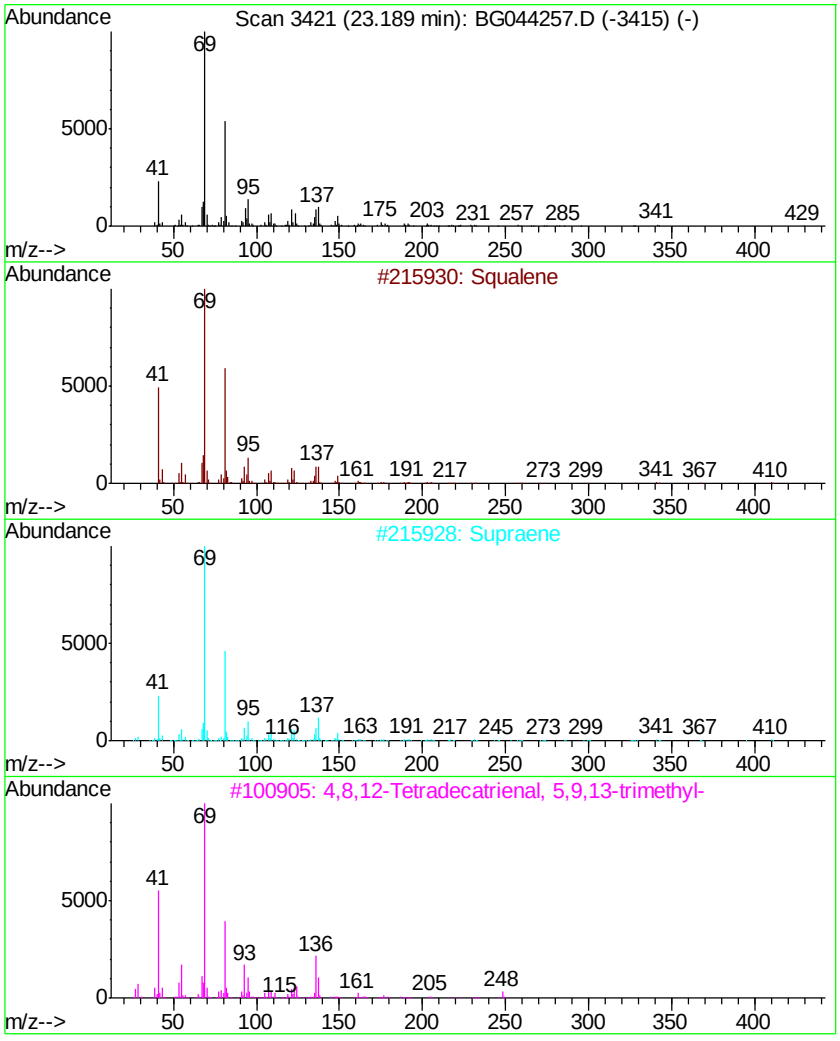
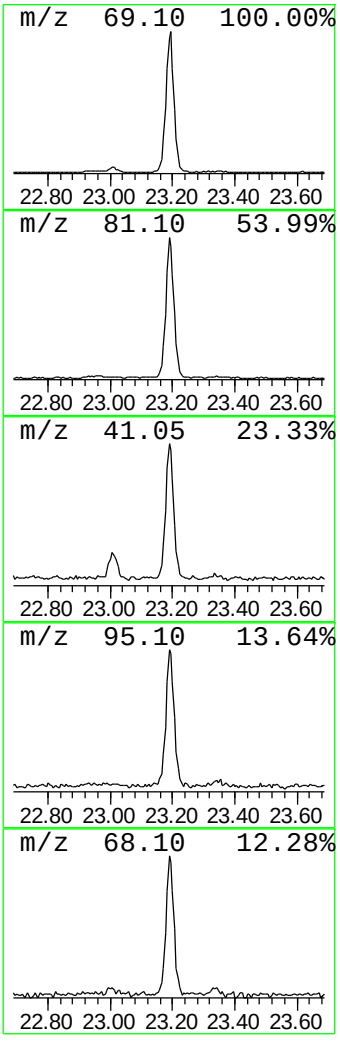
Peak Number 6 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	6.76 ng	501735	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
4	trans-Geranylgeraniol	290	C20H34O	024034-73-9	78
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG013120\
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Sample : L1319-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RAINEY-PARK-BH-01-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

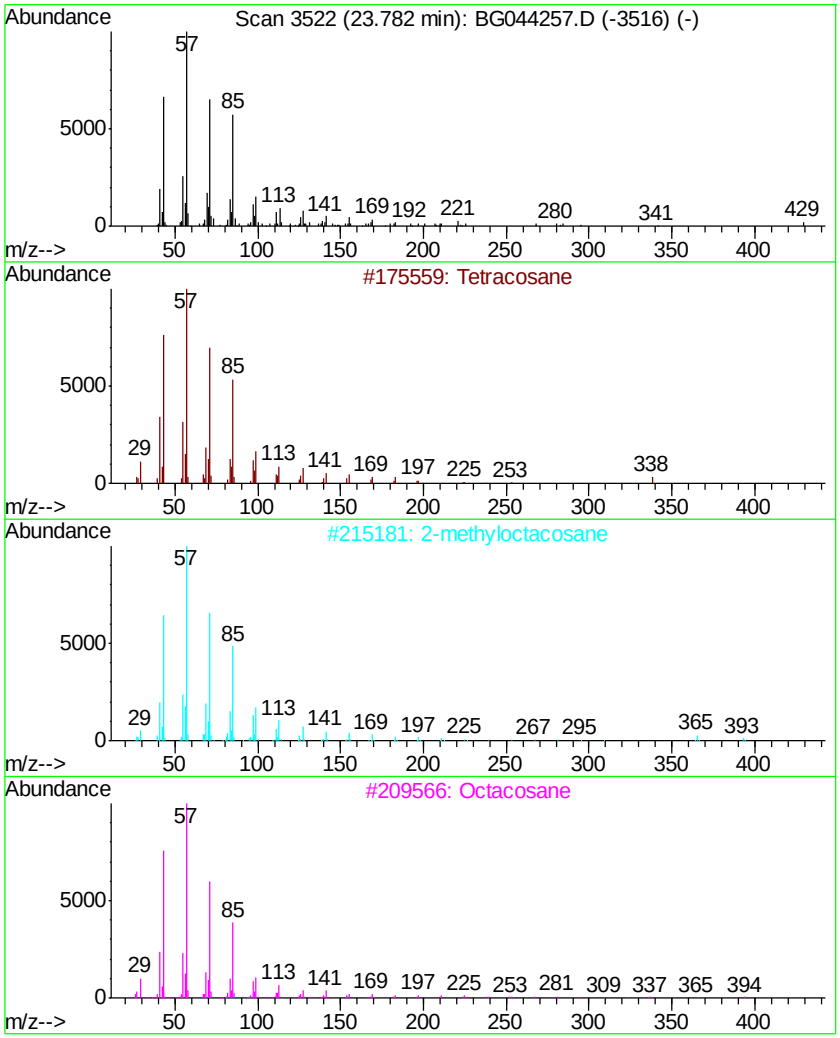
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

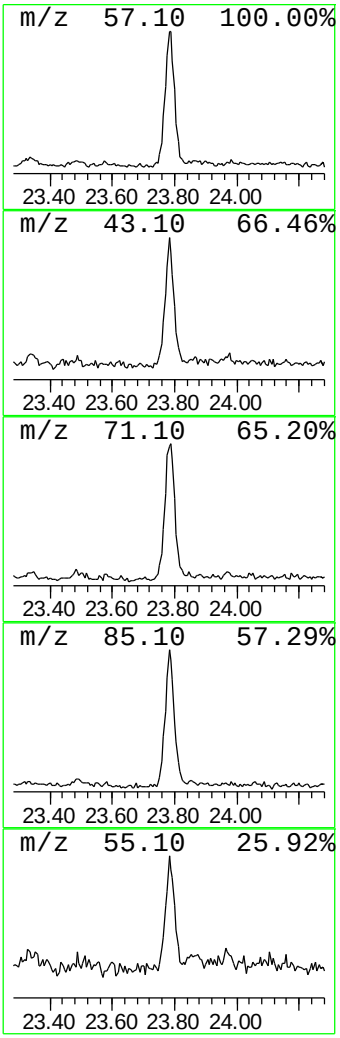
****

Peak Number 7 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.78	2.26 ng	167843	Perylene-d12	24.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG013120\
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Instrument :
BNA_G
ClientSampleId :
RAINEY-PARK-BH-01-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG013020.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
2-Pentanone, 4-hy...	5.02	3.4	ng	66892	1	7.92	398422	20.0
9-Octadecenamide,...	20.60	6.2	ng	432131	5	21.54	1389940	20.0
Docosyl trifluoro...	21.21	4.8	ng	334038	5	21.54	1389940	20.0
Eicosane	23.01	2.1	ng	144759	5	21.54	1389940	20.0
Squalene	23.19	6.8	ng	501735	6	24.64	1484420	20.0
Tetracosane	23.78	2.3	ng	167843	6	24.64	1484420	20.0