LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041919\
Data File : BG040569.D
Acq On : 19 Apr 2019 19:46
Operator : JU/SJ
Sample : K2479-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-70-71

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-BG032719.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	3.171	11	14	24	rVB	58862	100064	2.67%	0.521%
2	5.122	341	346	354	rBV2	42417	64928	1.73%	0.338%
3	5.586	419	425	440	rBV	358939	609050	16.22%	3.170%
4	7.184	690	697	709	rBV	222197	405322	10.80%	2.110%
5	7.560	754	761	776	rBV	621417	1088229	28.99%	5.665%
6	8.030	834	841	852	rBV	244840	399024	10.63%	2.077%
7	8.353	888	896	906	rVB	843680	1469641	39.15%	7.650%
8	9.205	1032	1041	1055	rBV	704129	1296069	34.53%	6.747%
9	10.844	1310	1320	1330	rBV	274934	505136	13.46%	2.629%
10	13.283	1728	1735	1749	rBV	1787964	3013839	80.28%	15.689%
11	14.111	1871	1876	1884	rBV	47703	80851	2.15%	0.421%
12	14.663	1963	1970	1984	rBV2	423095	700382	18.66%	3.646%
13	16.150	2216	2223	2236	rBV	1074688	1762148	46.94%	9.173%
14	17.413	2431	2438	2447	rBV2	582965	920880	24.53%	4.794%
15	20.016	2874	2881	2894	rBV	2677299	3753963	100.00%	19.541%
16	21.679	3158	3164	3176	rVB2	605802	1041658	27.75%	5.422%
17	21.826	3185	3189	3194	rVB	34104	45809	1.22%	0.238%
18	22.425	3287	3291	3296	rBV2	53330	86018	2.29%	0.448%
19	23.118	3404	3409	3415	rVB2	75605	145489	3.88%	0.757%
20	23.312	3435	3442	3451	rBV	100431	208296	5.55%	1.084%
21	23.923	3539	3546	3554	rBV	71644	154440	4.11%	0.804%
22	24.881	3701	3709	3713	rBV2	55802	145719	3.88%	0.759%
23	24.957	3713	3722	3739	rVB	357346	1030590	27.45%	5.365%
24	26.015	3894	3902	3913	rVB4	40415	123135	3.28%	0.641%
25	27.372	4129	4133	4140	rVB6	22418	59687	1.59%	0.311%

Sum of corrected areas: 19210367

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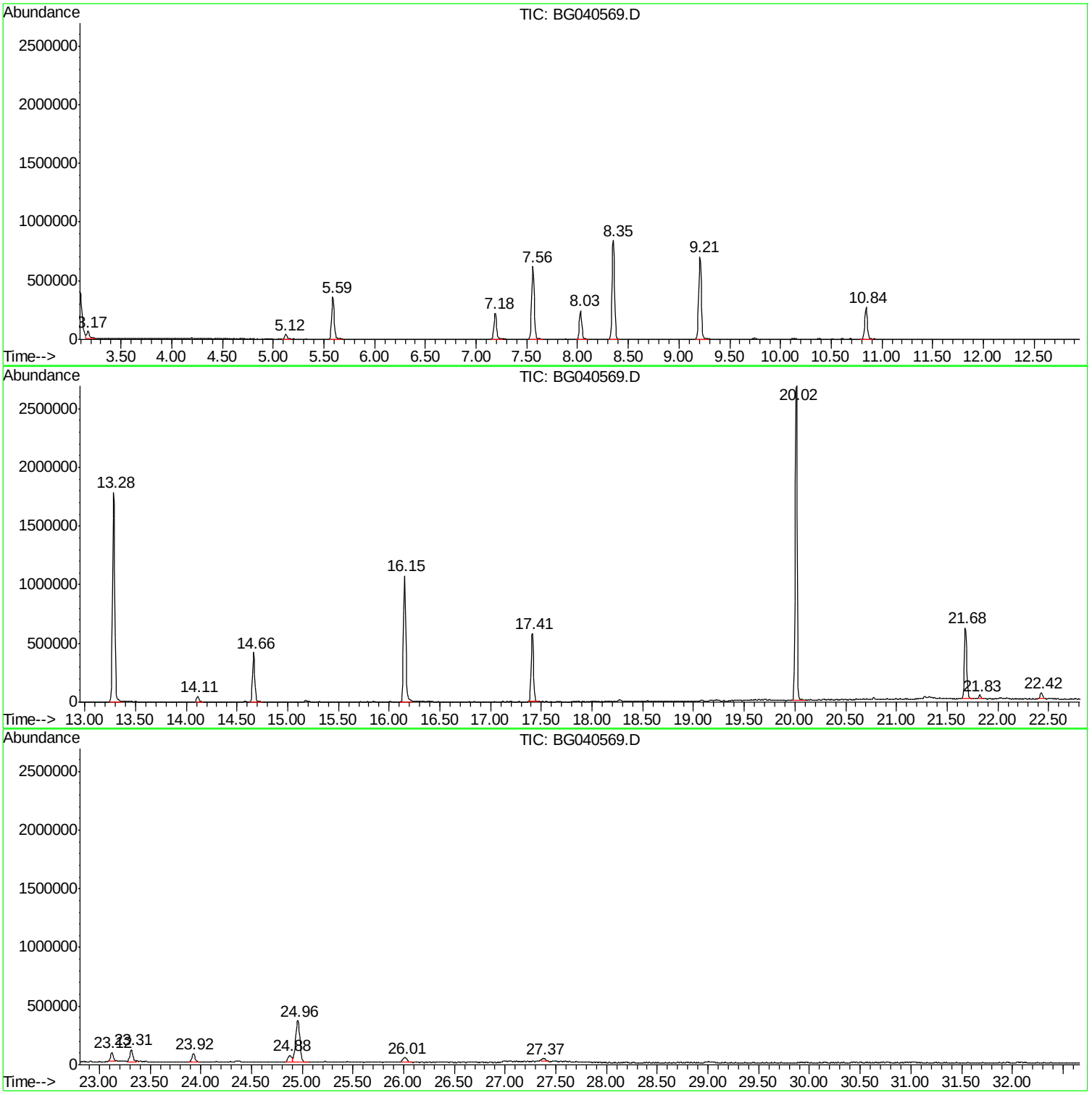
Acq On : 19 Apr 2019 19:46
Operator : JU/SJ
Sample : K2479-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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\BG041919\
Data File : BG040569.D
Acq On : 19 Apr 2019 19:46
Operator : JU/SJ
Sample : K2479-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

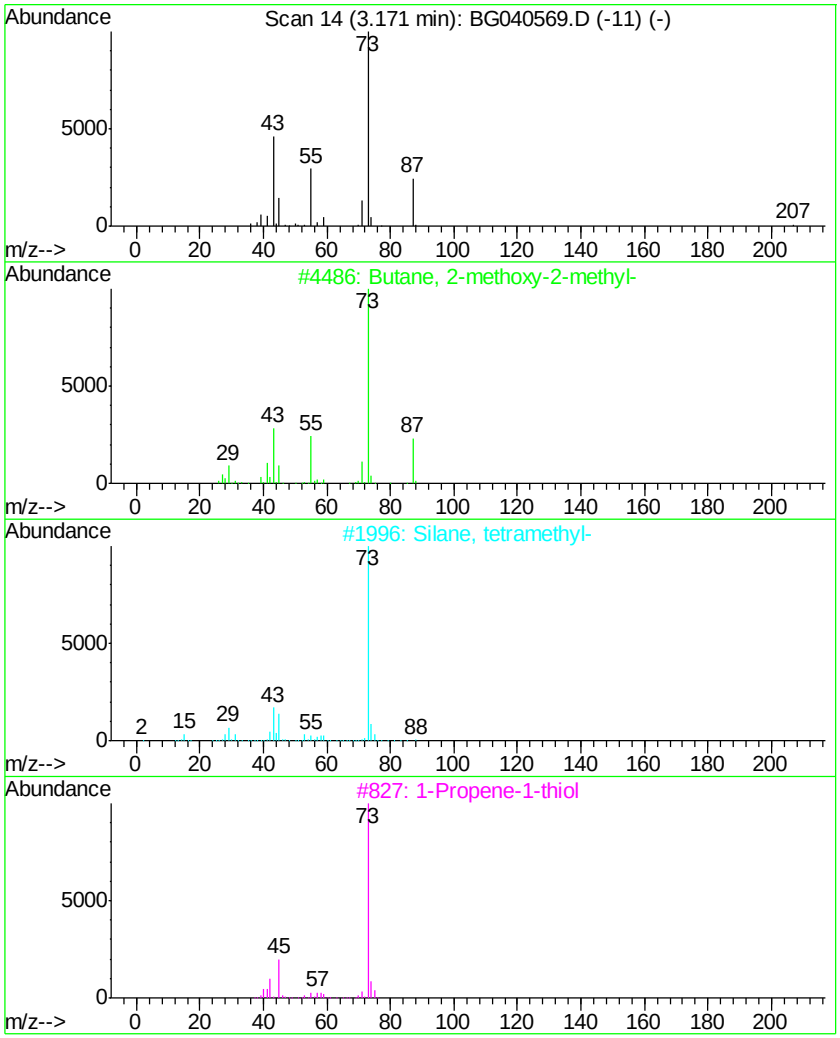
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

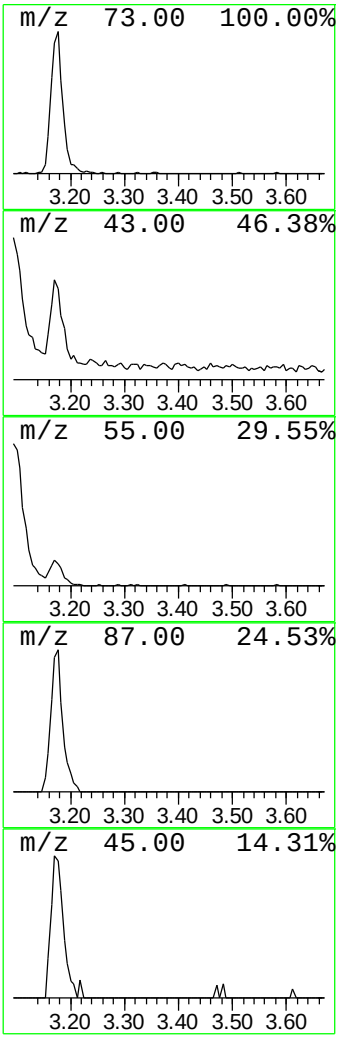
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	5.02 ng	100064	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
3	1-Propene-1-thiol	74	C3H6S	000925-89-3	9
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





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Data File : BG040569.D
Acq On : 19 Apr 2019 19:46
Operator : JU/SJ
Sample : K2479-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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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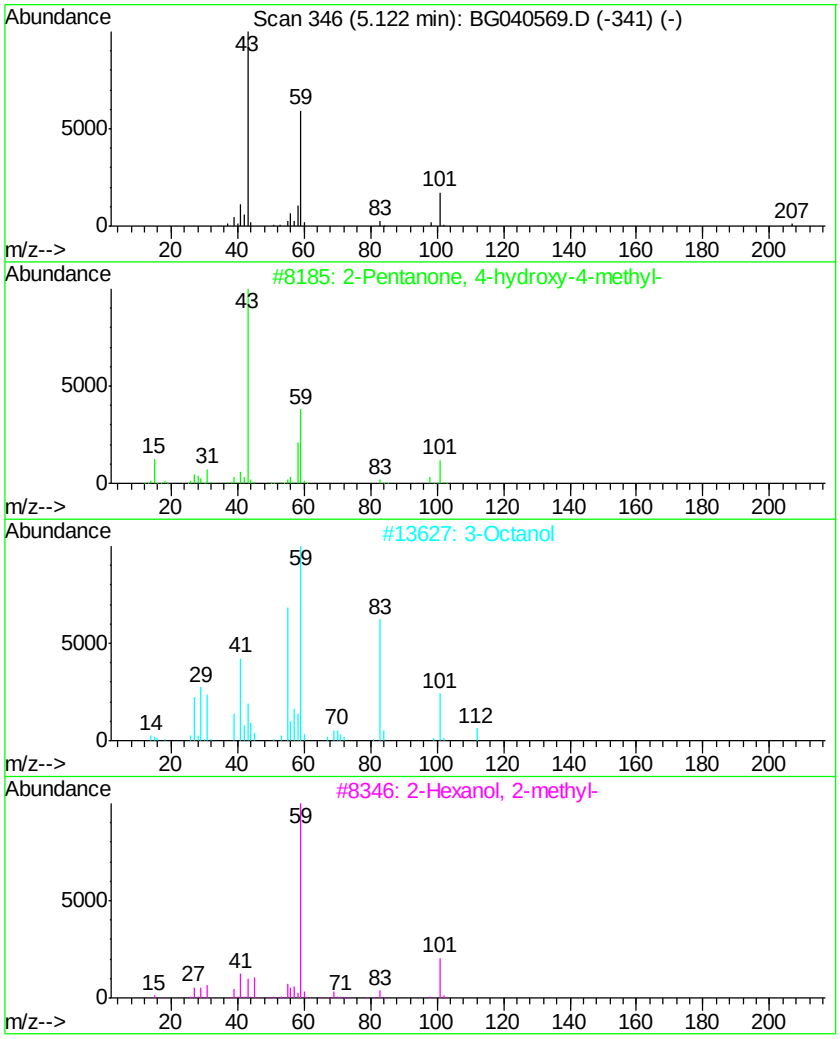
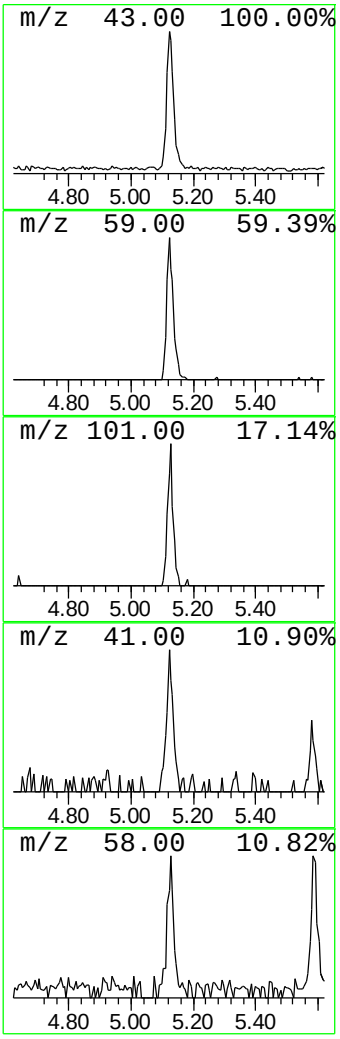
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.25 ng	64928	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Octanol	130	C8H18O	000589-98-0	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Data File : BG040569.D
Acq On : 19 Apr 2019 19:46
Operator : JU/SJ
Sample : K2479-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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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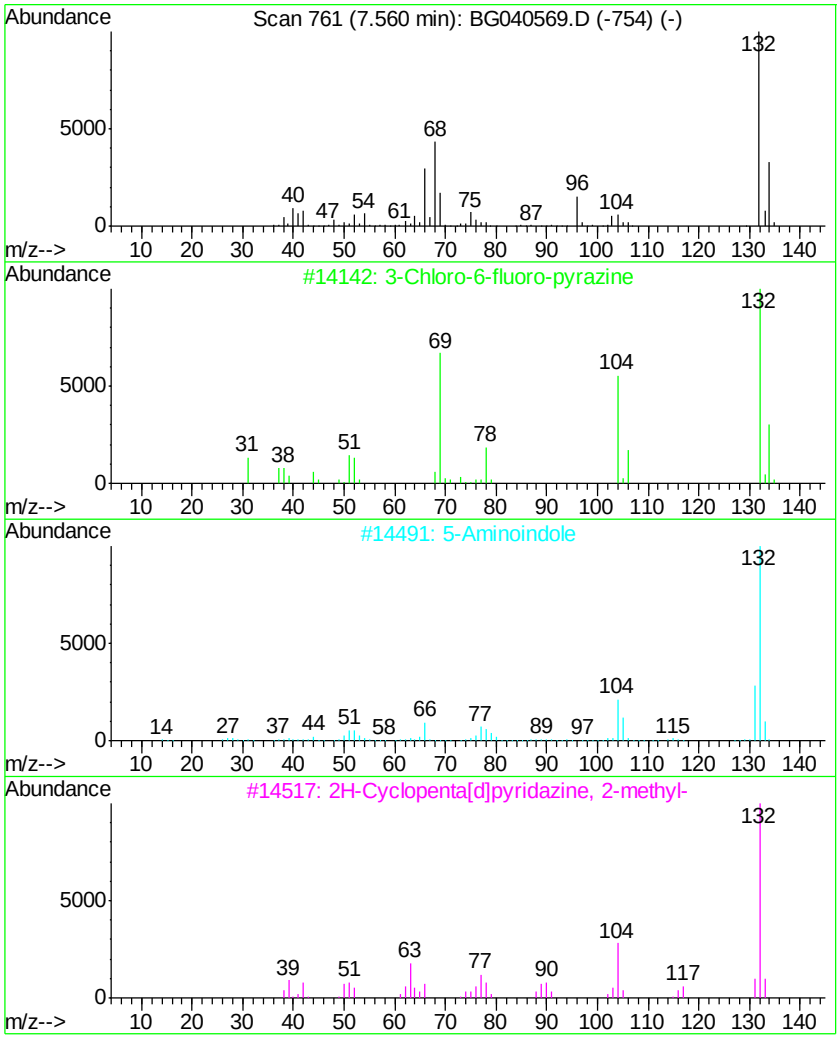
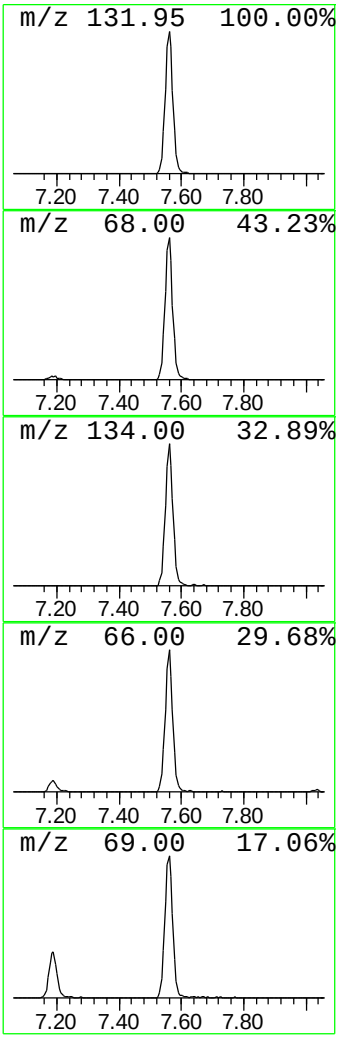
Peak Number 3 unknown7.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	54.54 ng	1088230	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	Xenon	132	Xe	007440-63-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041919\
Data File : BG040569.D
Acq On : 19 Apr 2019 19:46
Operator : JU/SJ
Sample : K2479-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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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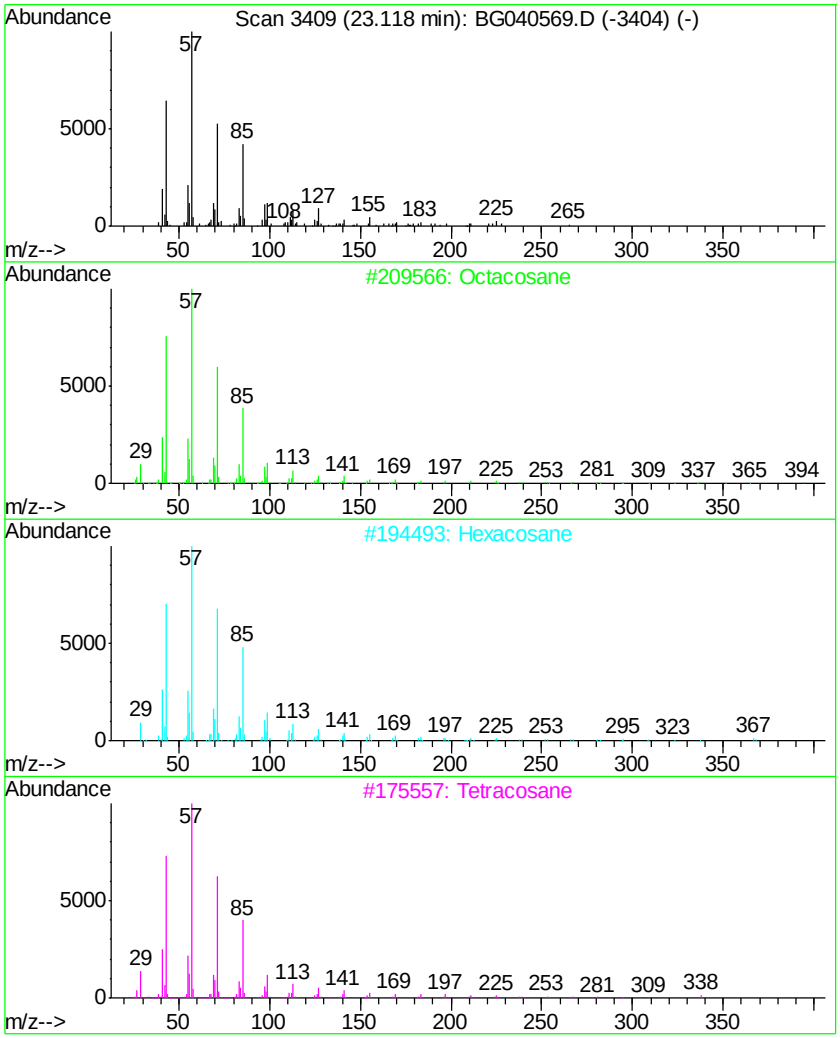
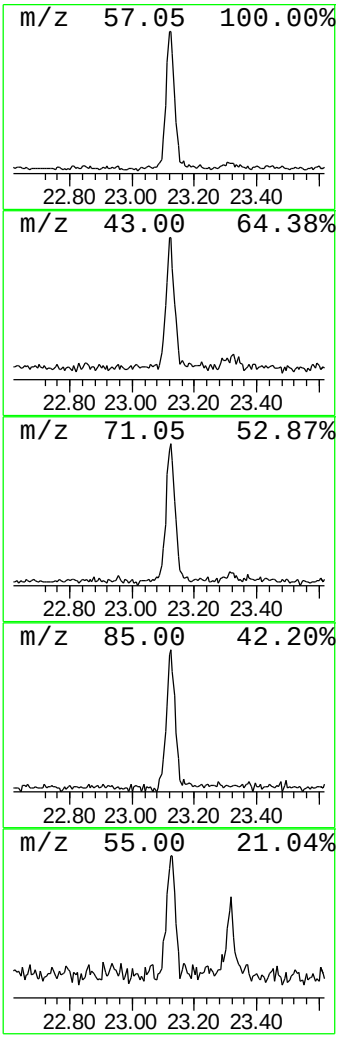
Peak Number 5 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.12	2.79 ng	145489	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Tetracosane	338	C24H50	000646-31-1	87
4	Heptadecane	240	C17H36	000629-78-7	86
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041919\
Data File : BG040569.D
Acq On : 19 Apr 2019 19:46
Operator : JU/SJ
Sample : K2479-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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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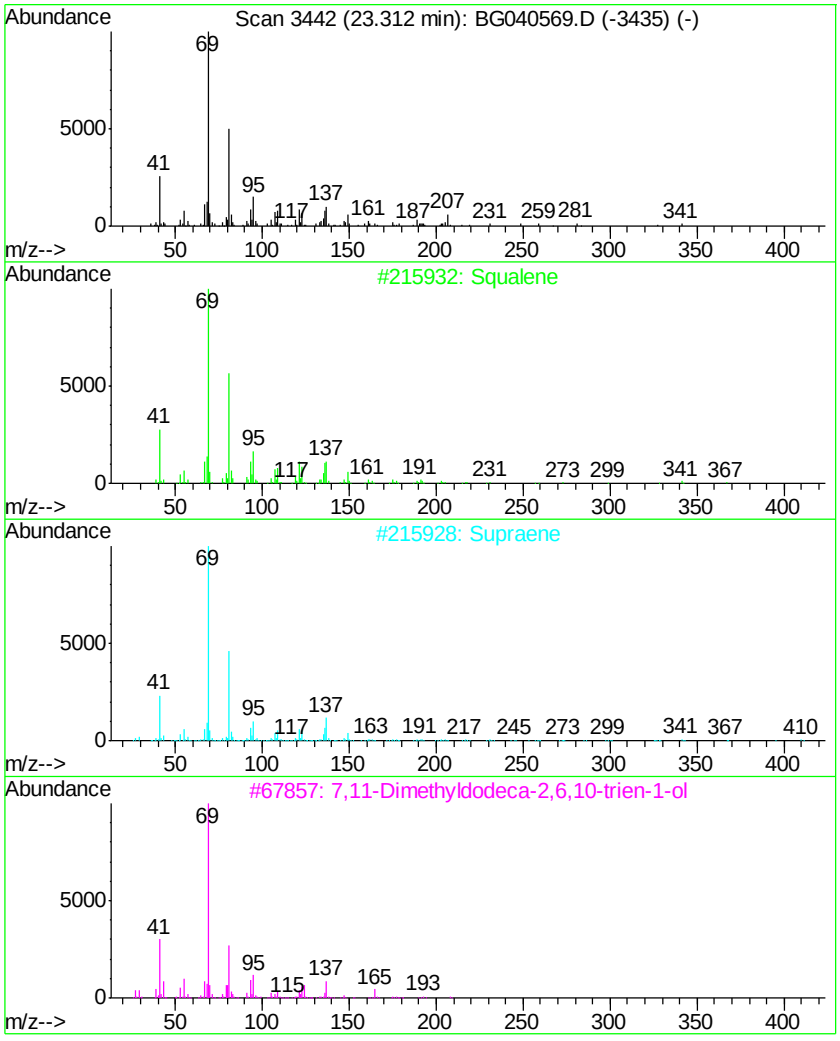
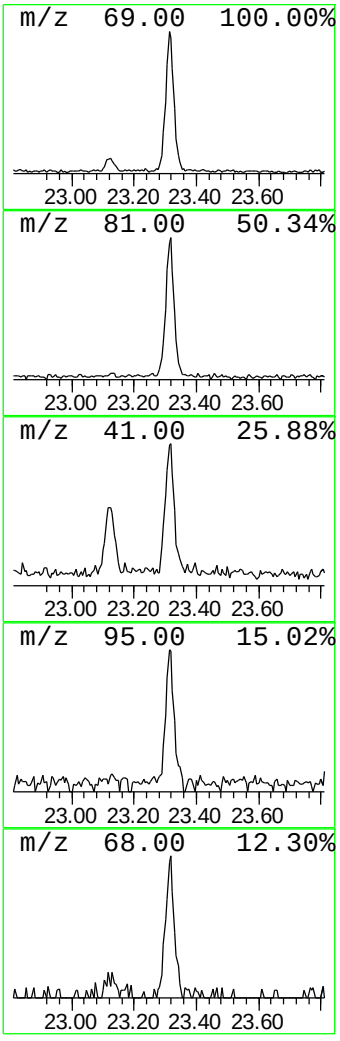
Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	4.00 ng	208296	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	83
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	trans-Farnesol	222	C15H26O	000106-28-5	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





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Operator : JU/SJ
Sample : K2479-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

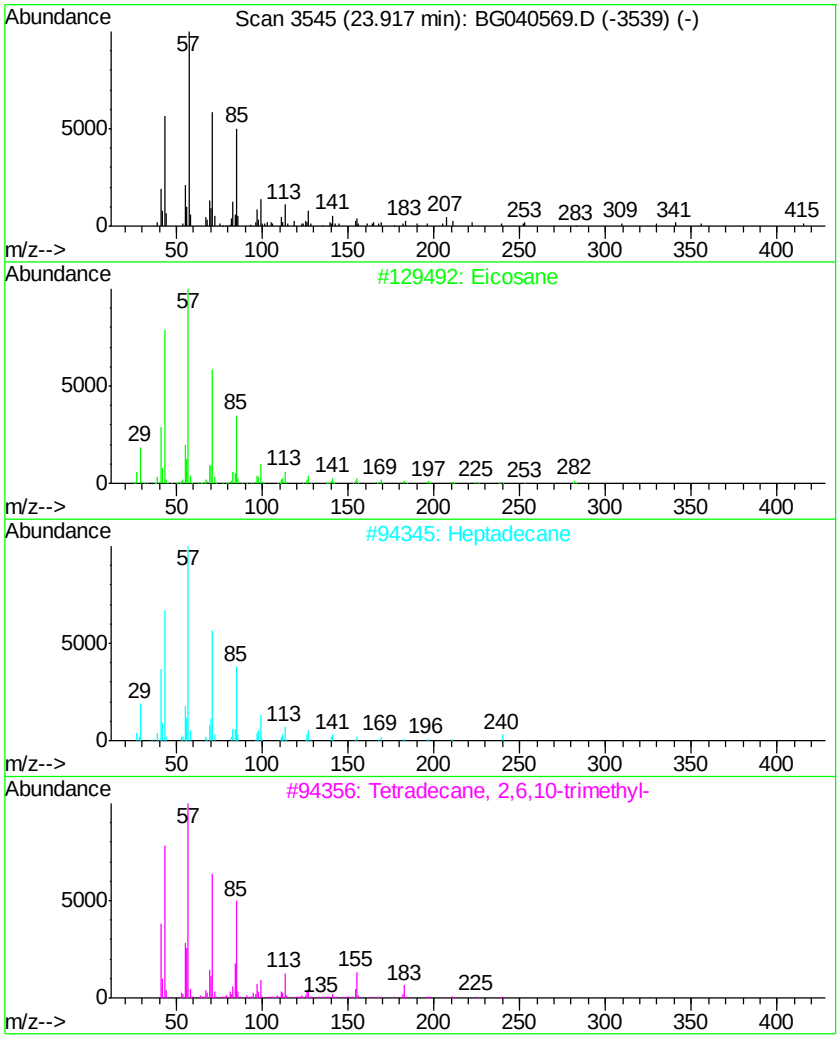
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

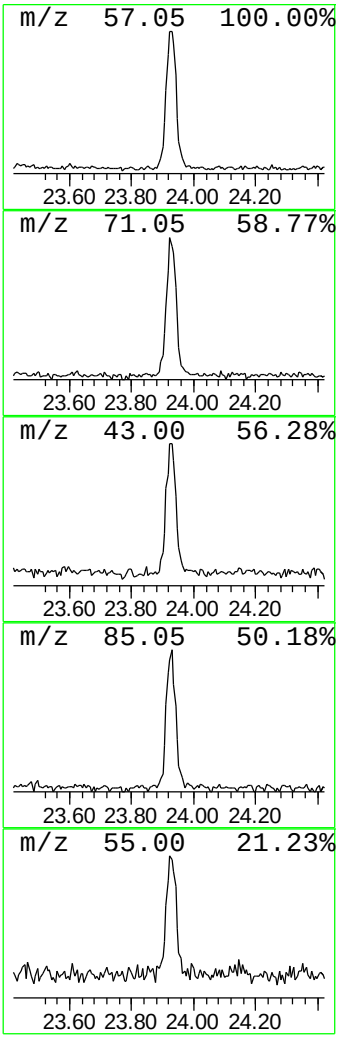
****

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	3.00 ng	154440	Perylene-d12	24.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Heptadecane	240	C17H36	000629-78-7	93
3	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heneicosane	296	C21H44	000629-94-7	90





Library Search Compound Report

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Operator : JU/SJ
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Misc :
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Instrument :
BNA_G
ClientSampleId :
TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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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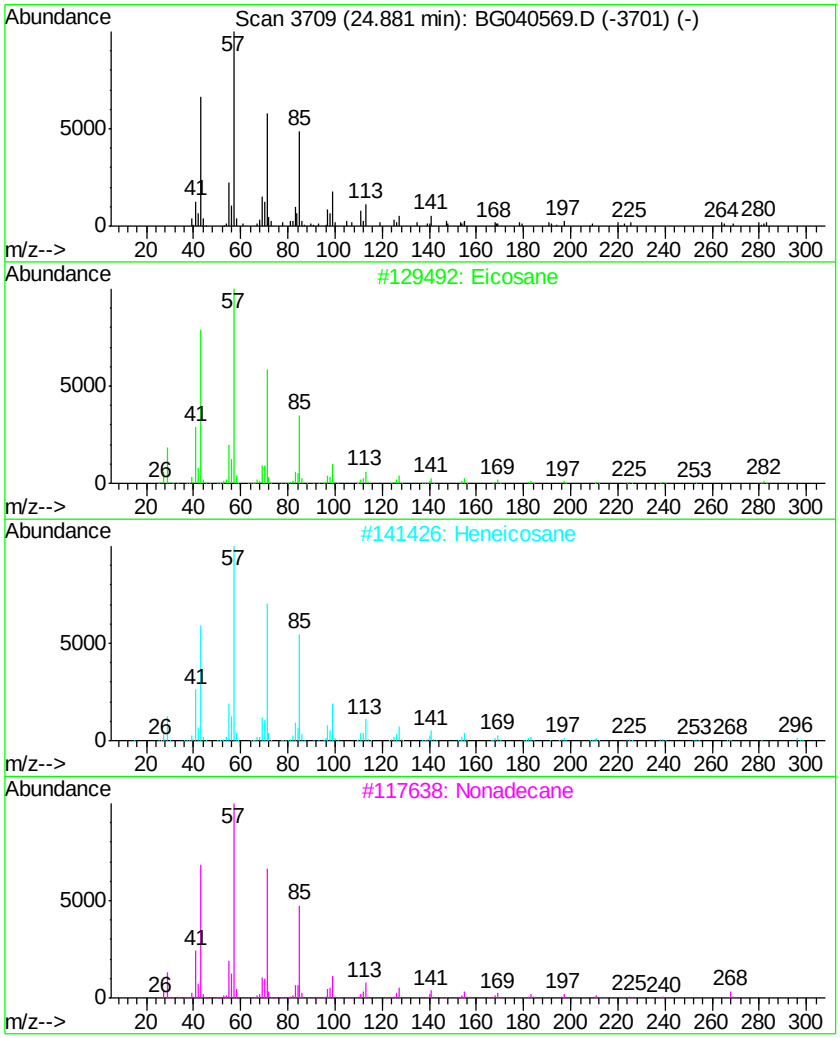
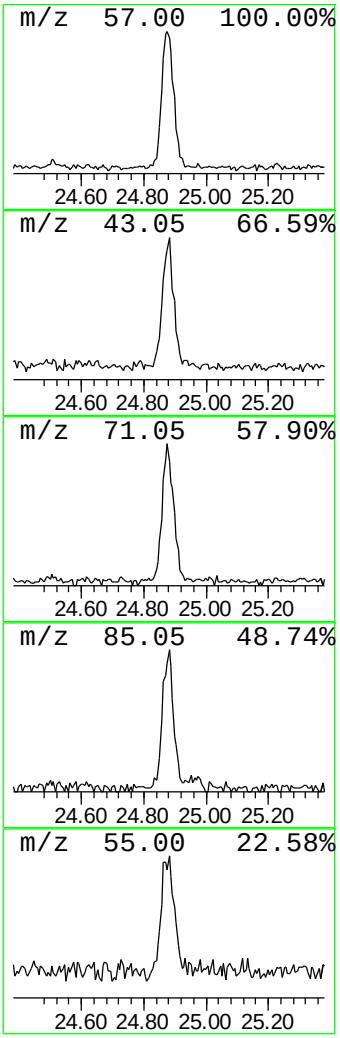
Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.88	2.83 ng	145719	Perylene-d12	24.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Nonadecane	268	C19H40	000629-92-5	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Hexacosane	366	C26H54	000630-01-3	87





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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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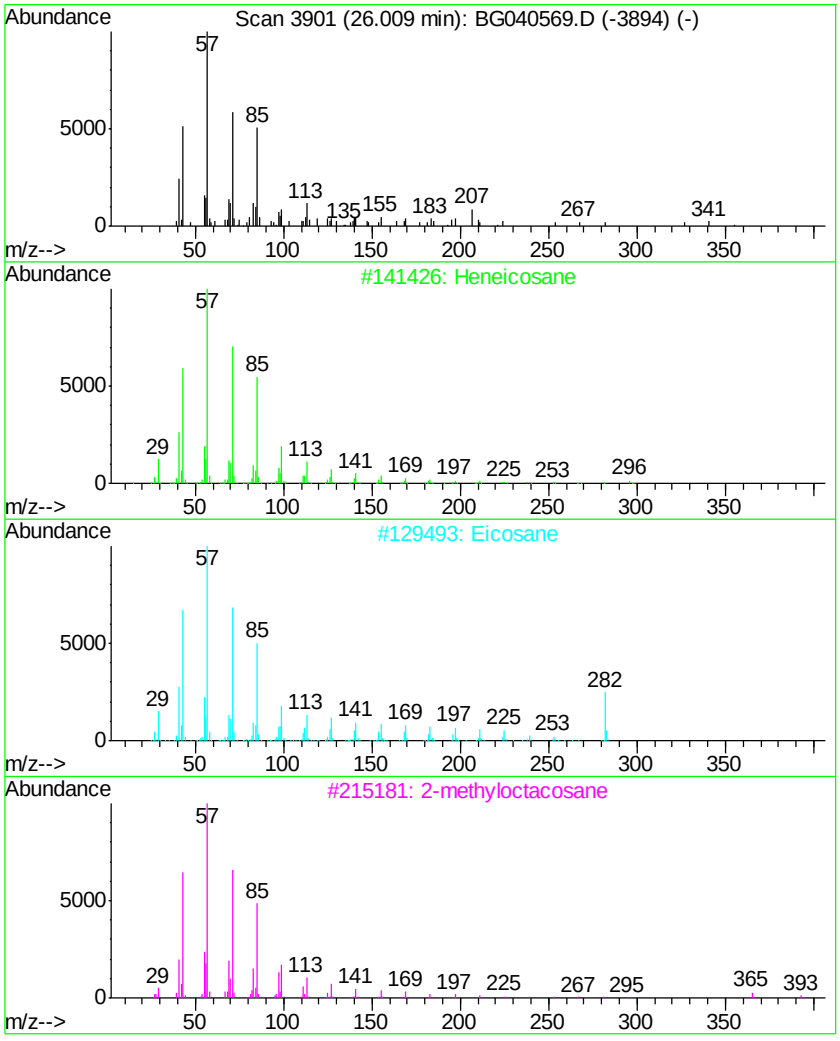
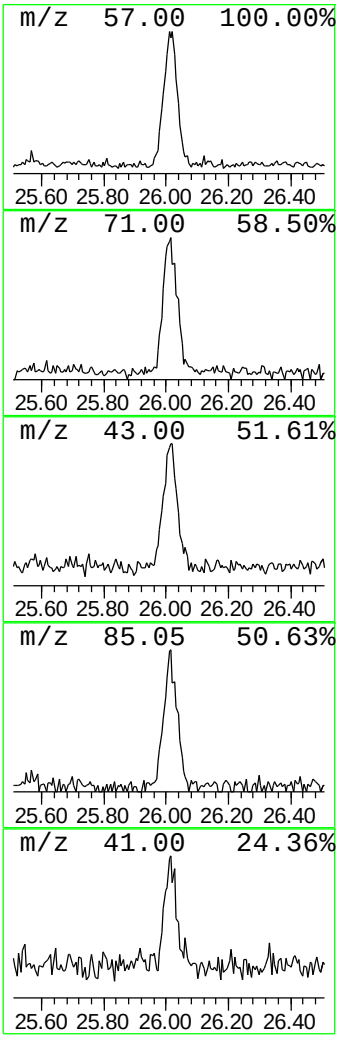
Peak Number 9 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.01	2.39 ng	123135	Perylene-d12	24.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Eicosane	282	C20H42	000112-95-8	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	86
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80
5	Octacosane	394	C28H58	000630-02-4	80





Tentatively Identified Compound (LSC) summary

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Data File : BG040569.D
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Operator : JU/SJ
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Misc :
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ClientSampleId : TP-TRACK-70-71

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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
Butane, 2-methoxy...	3.17	5.0	ng	100064	1	8.03	399024	20.0
2-Pentanone, 4-hy...	5.12	3.3	ng	64928	1	8.03	399024	20.0
unknown7.56	7.56	54.5	ng	1088230	1	8.03	399024	20.0
Octacosane	23.12	2.8	ng	145489	5	21.68	1041660	20.0
Squalene	23.31	4.0	ng	208296	5	21.68	1041660	20.0
Eicosane	23.92	3.0	ng	154440	6	24.96	1030590	20.0
Nonadecane	24.88	2.8	ng	145719	6	24.96	1030590	20.0
Heneicosane	26.01	2.4	ng	123135	6	24.96	1030590	20.0