LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041919\
Data File : BG040568.D
Acq On : 19 Apr 2019 19:08
Operator : JU/SJ
Sample : K2479-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-8-9

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	3.175	11	15	26	rVB	61894	109369	2.97%	0.593%
2	5.126	342	347	355	rBV2	46895	72953	1.98%	0.396%
3	5.590	417	426	437	rBV	332407	553271	15.01%	3.002%
4	7.188	690	698	708	rBV	201570	366214	9.93%	1.987%
5	7.559	754	761	774	rBV	597811	1048558	28.44%	5.689%
6	8.029	835	841	848	rBV	251079	446413	12.11%	2.422%
7	8.352	888	896	905	rBV	1010665	1740148	47.20%	9.441%
8	9.204	1034	1041	1051	rBV	694974	1284411	34.84%	6.969%
9	10.843	1313	1320	1331	rBV	274733	487737	13.23%	2.646%
10	13.281	1728	1735	1750	rBV	1711584	2688869	72.94%	14.588%
11	14.110	1869	1876	1882	rBV	71252	109699	2.98%	0.595%
12	14.662	1963	1970	1981	rBV2	412484	677408	18.38%	3.675%
13	16.154	2218	2224	2241	rVB	885100	1369656	37.15%	7.431%
14	17.412	2432	2438	2451	rBV2	568314	886890	24.06%	4.812%
15	17.993	2530	2537	2542	rBV7	15294	38157	1.04%	0.207%
16	18.270	2580	2584	2592	rVB4	26140	46675	1.27%	0.253%
17	20.015	2874	2881	2888	rBV	2791706	3686550	100.00%	20.001%
18	21.572	3141	3146	3151	rBV6	24227	40684	1.10%	0.221%
19	21.683	3158	3165	3175	rVB	691164	1147149	31.12%	6.224%
20	21.824	3186	3189	3196	rVB2	37290	46589	1.26%	0.253%
21	22.435	3288	3293	3298	rVB	50655	88565	2.40%	0.481%
22	23.123	3404	3410	3423	rVB2	59309	122283	3.32%	0.663%
23	23.317	3437	3443	3452	rVB	78987	150846	4.09%	0.818%
24	23.928	3542	3547	3557	rVB3	55470	117184	3.18%	0.636%
25	24.885	3702	3710	3713	rBV5	35822	87282	2.37%	0.474%
26	24.956	3713	3722	3734	rVB2	316847	940764	25.52%	5.104%
27	26.019	3896	3903	3916	rVB4	28427	77330	2.10%	0.420%

Sum of corrected areas: 18431654

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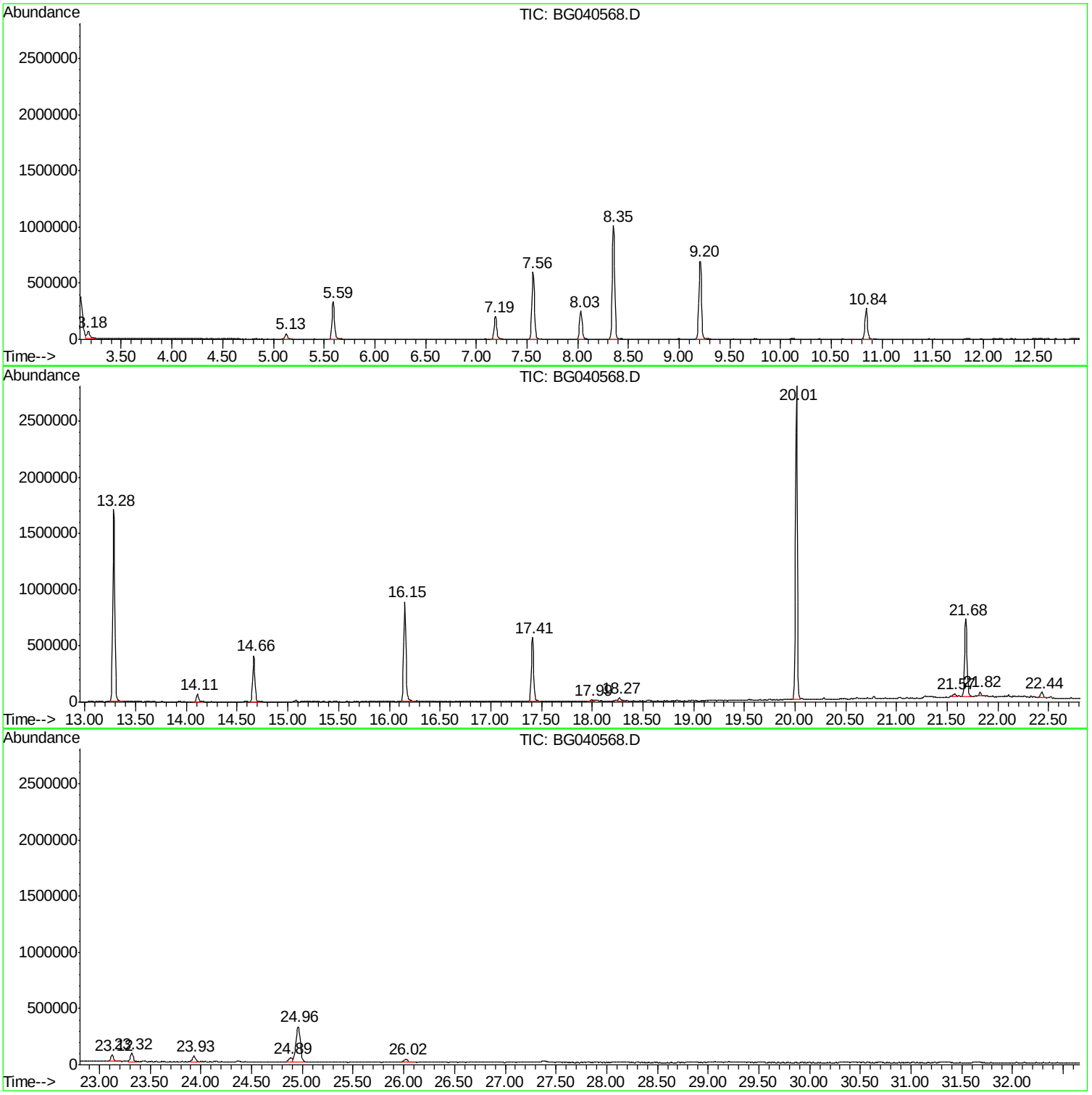
Instrument :
BNA_G
ClientSampleId :
TP-TRACK-8-9

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

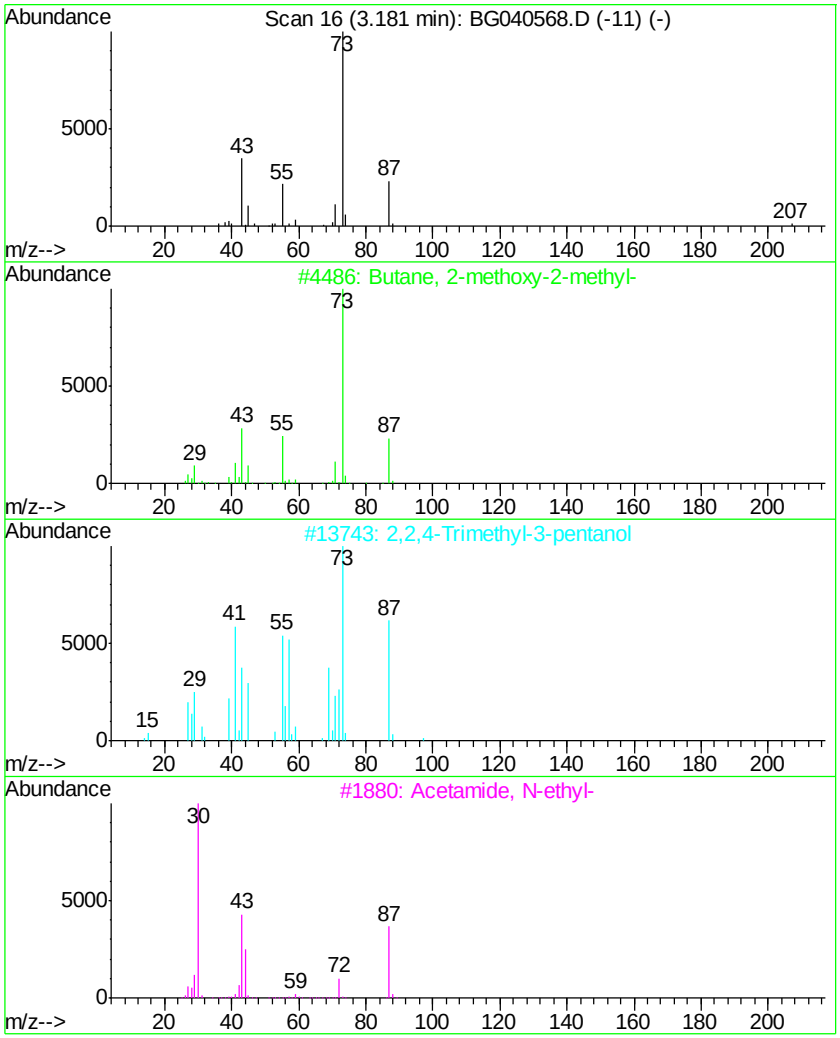
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

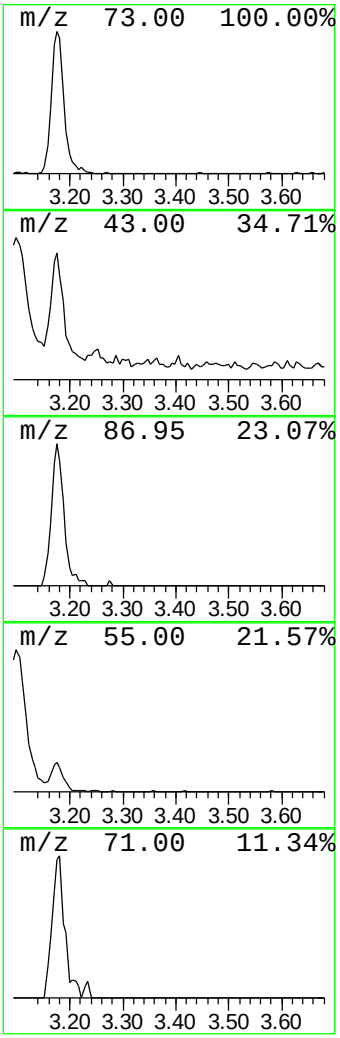
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	4.90 ng	109369	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	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





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Operator : JU/SJ
Sample : K2479-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-8-9

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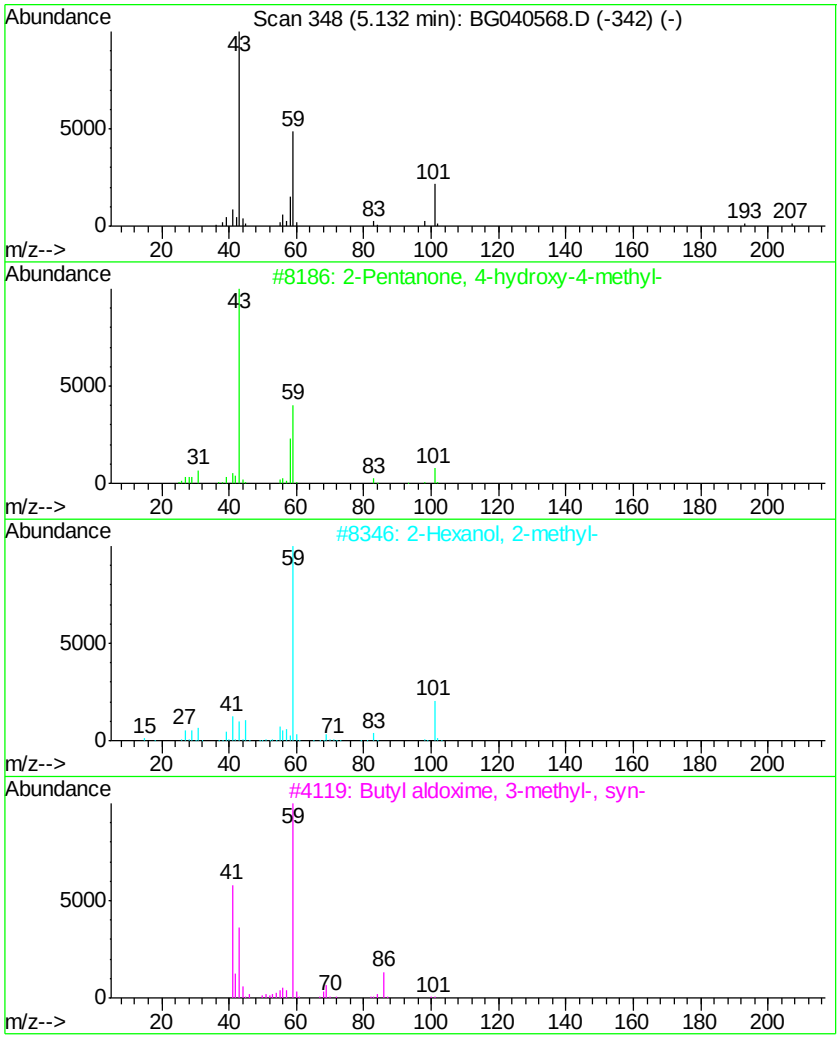
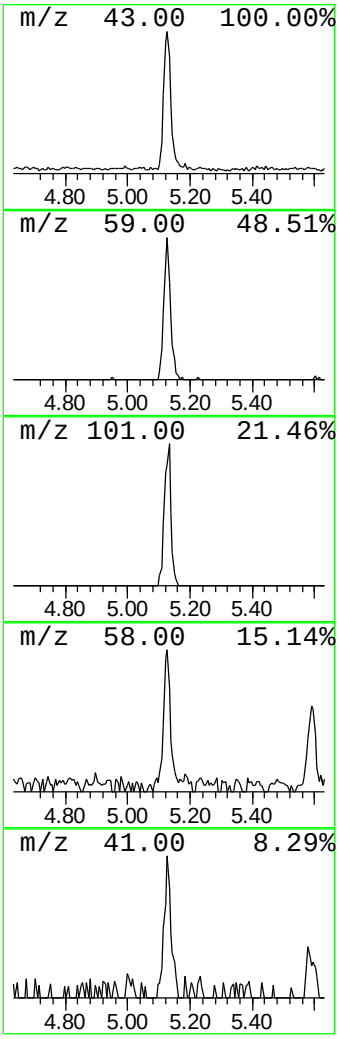
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	3.27 ng	72953	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Operator : JU/SJ
Sample : K2479-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-8-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
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TIC Library : C:\Database\NIST11.L
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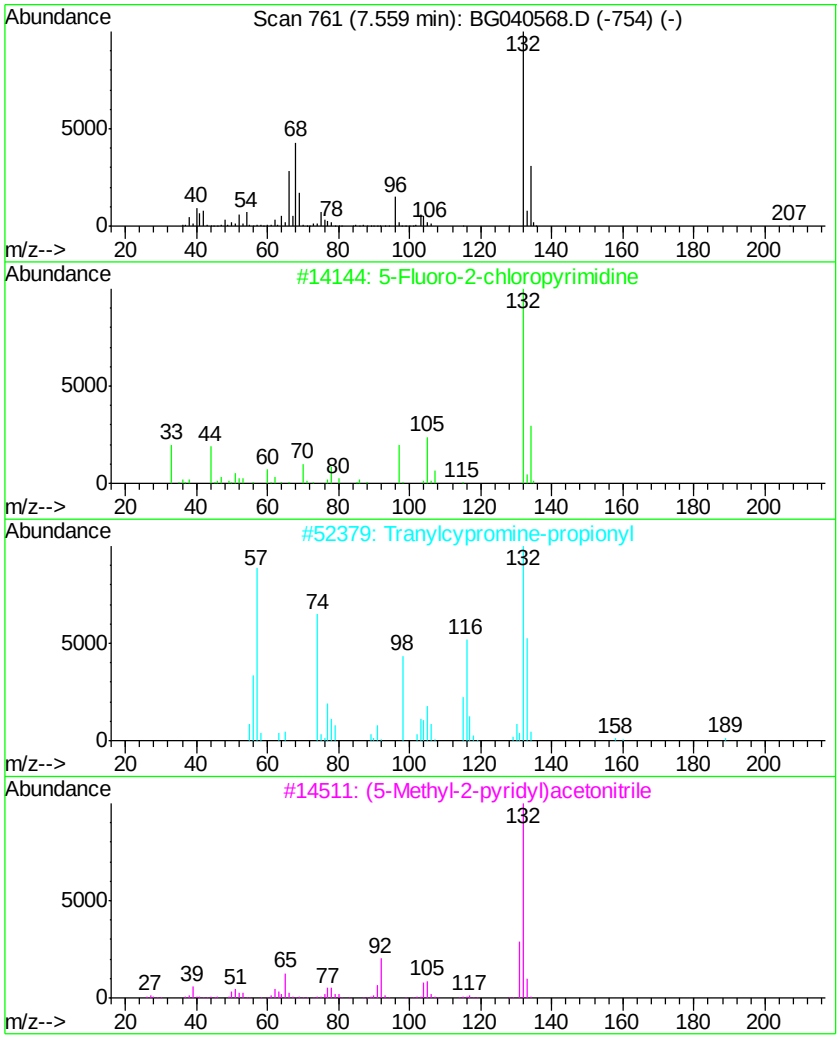
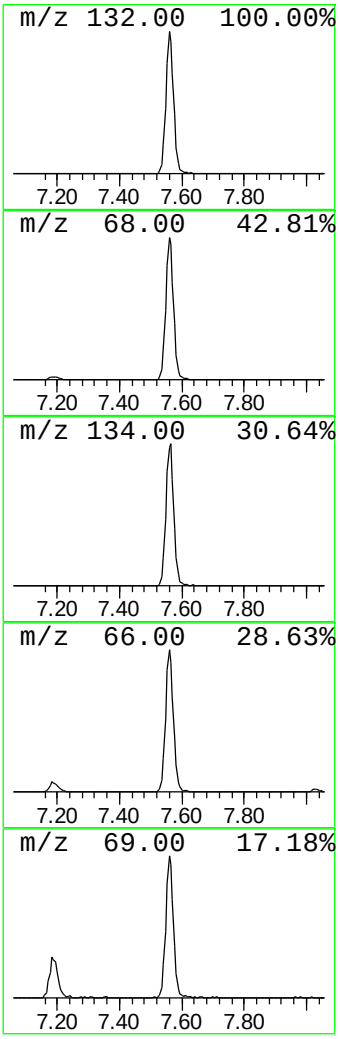
Peak Number 3 unknown7.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	46.98 ng	1048560	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041919\
Data File : BG040568.D
Acq On : 19 Apr 2019 19:08
Operator : JU/SJ
Sample : K2479-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
TP-TRACK-8-9

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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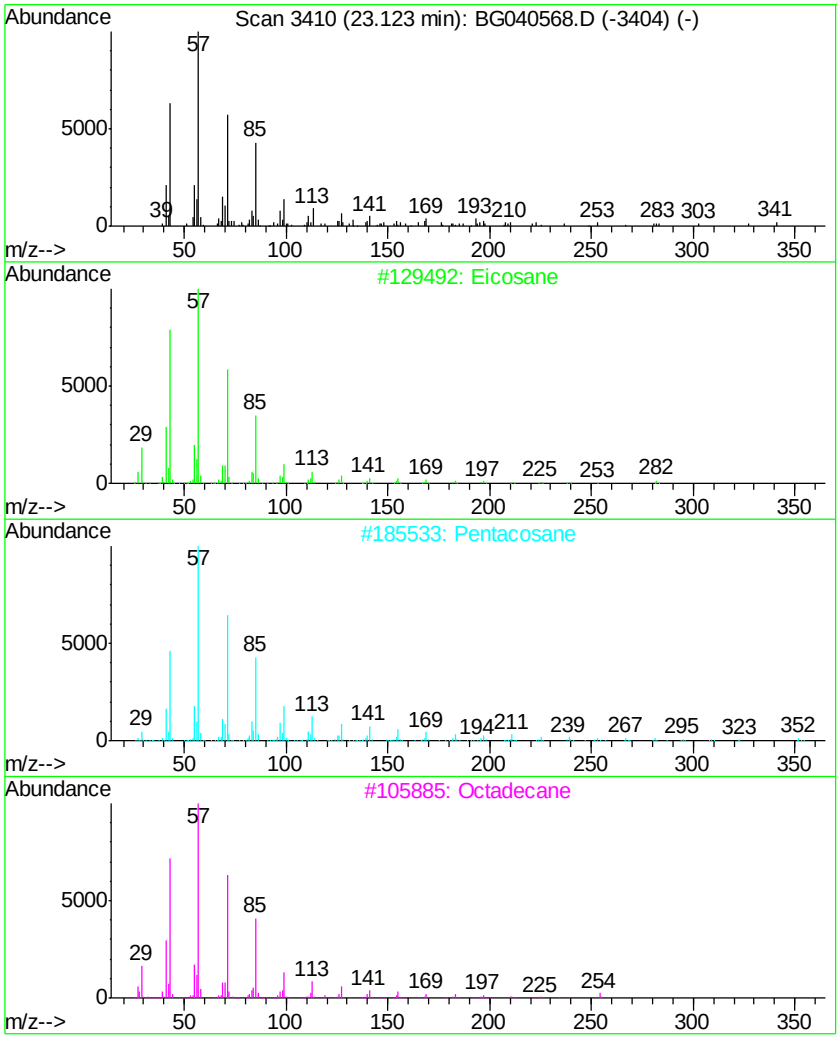
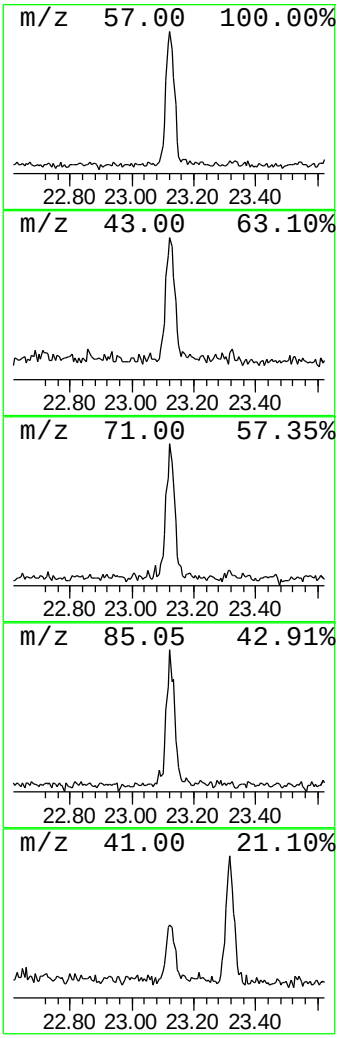
Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.12	2.13 ng	122283	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Pentacosane	352	C25H52	000629-99-2	90
3	Octadecane	254	C18H38	000593-45-3	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Triacontane	422	C30H62	000638-68-6	87





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Operator : JU/SJ
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-8-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
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TIC Library : C:\Database\NIST11.L
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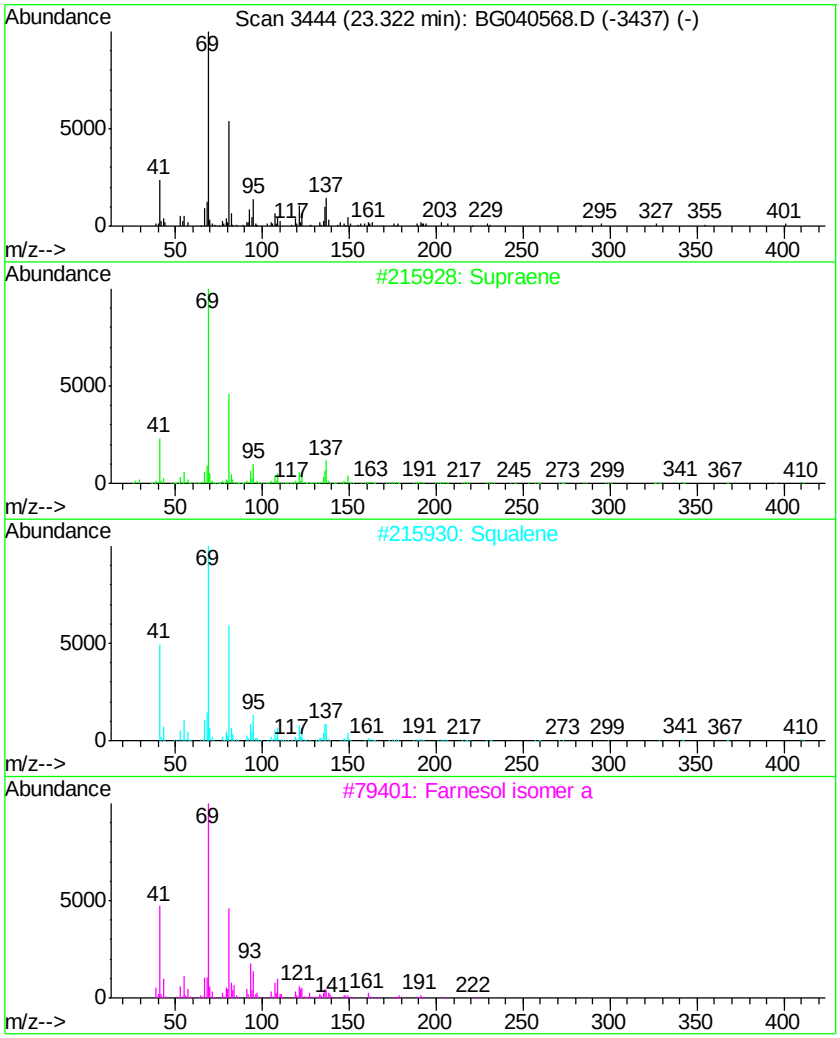
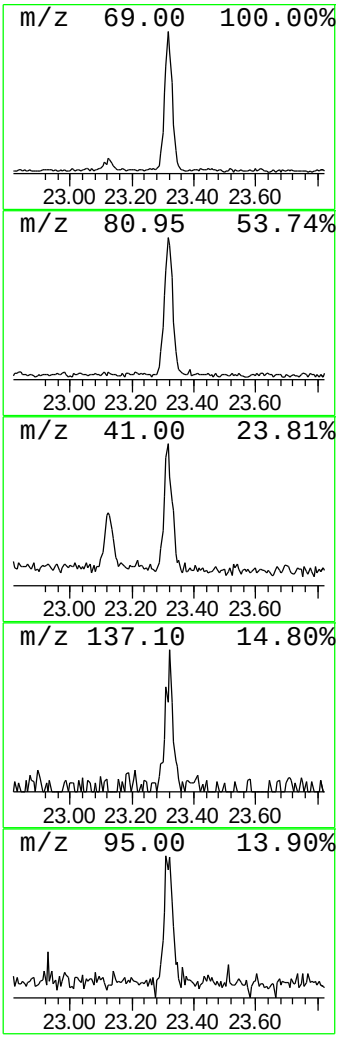
Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.32	2.63 ng	150846	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	Farnesol isomer a	222	C15H26O	1000108-92-4	91
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5	Carbonic acid, methyl ester, [(E...	280	C17H28O3	1000164-38-7	72





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Instrument : BNA_G
ClientSampleId : TP-TRACK-8-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
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TIC Library : C:\Database\NIST11.L
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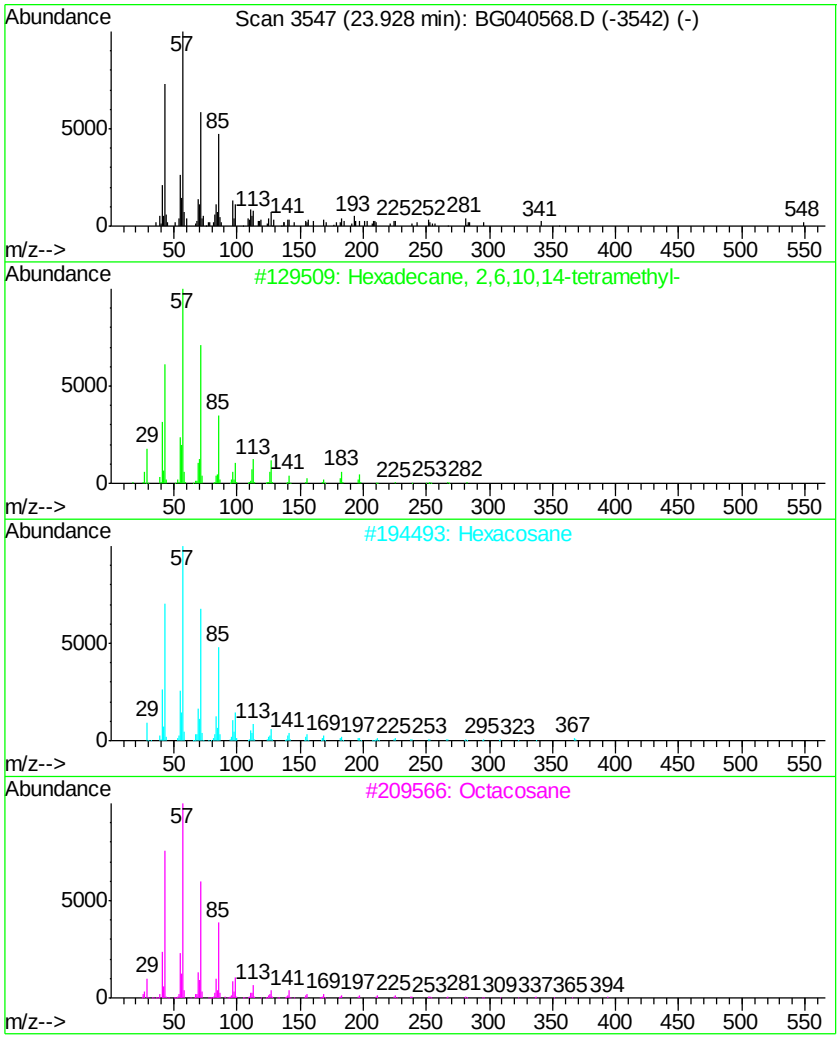
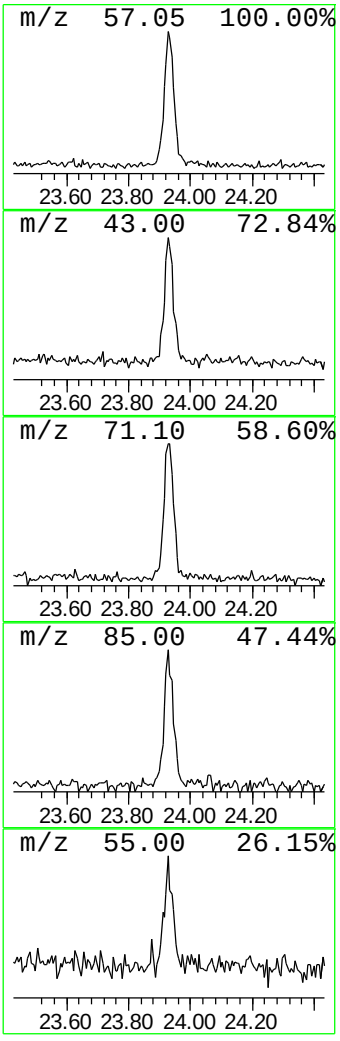
****

Peak Number 7 Hexadecane, 2,6,10,14-tetra... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.93	2.49 ng	117184	Perylene-d12	24.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	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
Butane, 2-methoxy...	3.18	4.9	ng	109369	1	8.03	446413	20.0
2-Pentanone, 4-hy...	5.13	3.3	ng	72953	1	8.03	446413	20.0
unknown7.56	7.56	47.0	ng	1048560	1	8.03	446413	20.0
Eicosane	23.12	2.1	ng	122283	5	21.68	1147150	20.0
Supraene	23.32	2.6	ng	150846	5	21.68	1147150	20.0
Hexadecane, 2,6,1...	23.93	2.5	ng	117184	6	24.96	940764	20.0