LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
Data File : BG040354.D
Acq On : 4 Apr 2019 10:35
Operator : JU/SJ
Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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	3.187	14	17	28	rVB	54040	106406	2.94%	0.572%
2	5.137	343	349	357	rBV	40390	69349	1.92%	0.373%
3	5.601	421	428	440	rBV	364435	589424	16.28%	3.168%
4	7.200	693	700	713	rBV	222212	396727	10.96%	2.133%
5	7.576	756	764	772	rBV	583501	1025291	28.32%	5.511%
6	8.046	836	844	856	rVB	204172	362090	10.00%	1.946%
7	8.369	891	899	908	rBV	779033	1371901	37.89%	7.375%
8	9.221	1035	1044	1054	rBV	625346	1136234	31.38%	6.108%
9	10.860	1315	1323	1328	rBV	258194	484840	13.39%	2.606%
10	13.298	1730	1738	1752	rBV	1597923	2535443	70.03%	13.629%
11	13.604	1784	1790	1798	rBV2	30622	56960	1.57%	0.306%
12	14.679	1965	1973	1986	rVB2	392288	661721	18.28%	3.557%
13	15.178	2052	2058	2072	rBV	214490	401992	11.10%	2.161%
14	16.166	2219	2226	2237	rBV	832222	1285090	35.50%	6.908%
15	17.423	2433	2440	2452	rVB2	547973	867146	23.95%	4.661%
16	17.999	2530	2538	2542	rBV6	31507	71145	1.97%	0.382%
17	18.275	2581	2585	2593	rBV2	57583	99454	2.75%	0.535%
18	18.416	2603	2609	2617	rBV2	79550	135121	3.73%	0.726%
19	19.009	2706	2710	2716	rBV5	25741	41568	1.15%	0.223%
20	19.550	2797	2802	2808	rBV6	33055	58808	1.62%	0.316%
21	20.020	2876	2882	2893	rVB	2637624	3620434	100.00%	19.461%
22	21.295	3095	3099	3105	rBV4	30823	50403	1.39%	0.271%
23	21.694	3160	3167	3175	rVB2	649221	1087292	30.03%	5.845%
24	21.835	3186	3191	3196	rBV4	30414	52058	1.44%	0.280%
25	22.441	3290	3294	3301	rVB	53312	86268	2.38%	0.464%
26	22.623	3321	3325	3330	rBV3	30269	54040	1.49%	0.290%
27	23.140	3405	3413	3421	rVB	85123	161845	4.47%	0.870%
28	23.945	3541	3550	3558	rBV3	94911	218882	6.05%	1.177%
29	24.891	3705	3711	3716	rBV2	79931	193231	5.34%	1.039%
30	24.967	3716	3724	3737	rVB2	375790	1104923	30.52%	5.939%
31	26.025	3897	3904	3913	rBV3	59155	173077	4.78%	0.930%
32	27.399	4132	4138	4140	rBV7	23927	44040	1.22%	0.237%

LSC Area Percent Report

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Acq On : 4 Apr 2019 10:35
Operator : JU/SJ
Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-TRACK-78-79

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

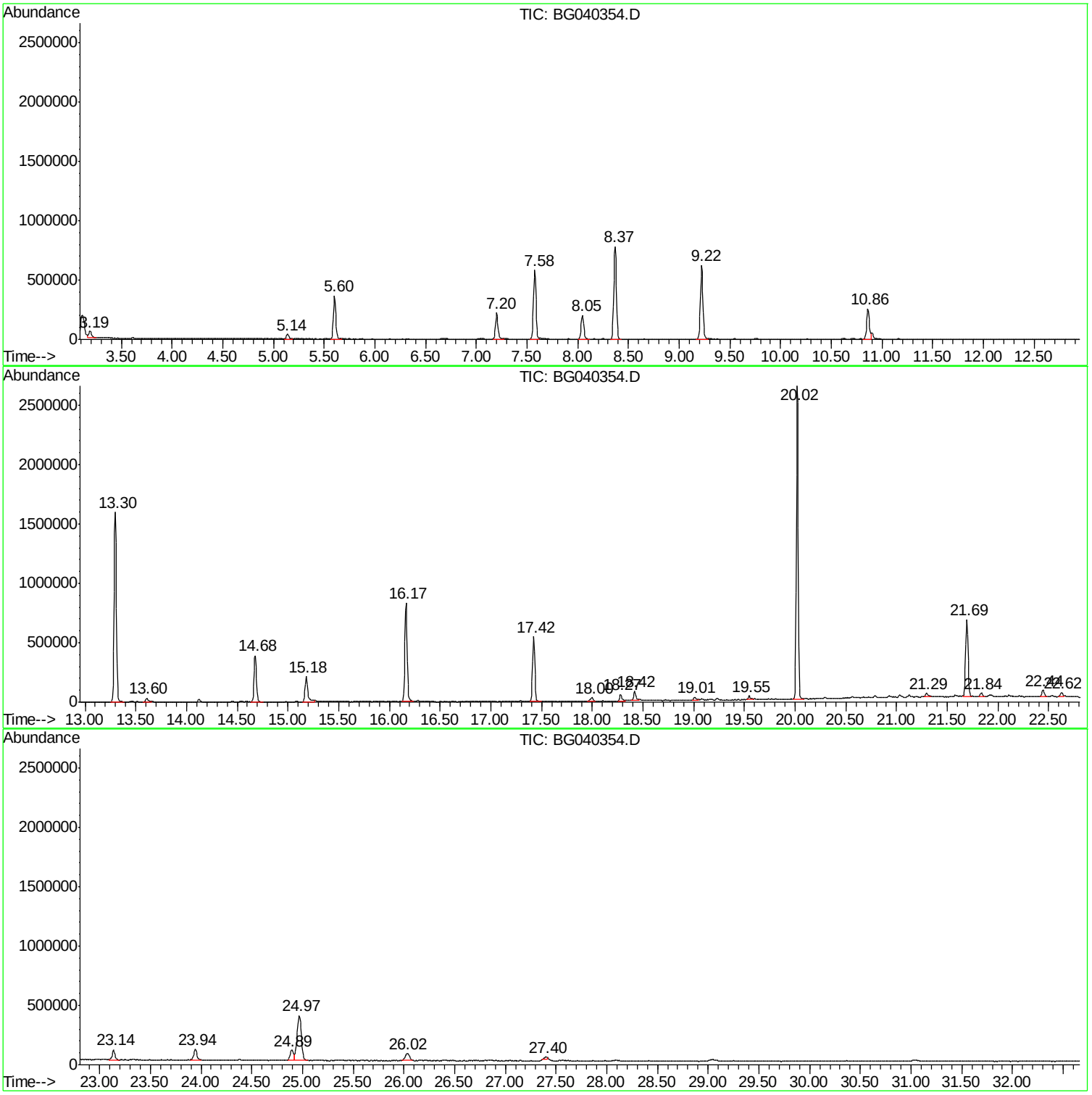
Sum of corrected areas: 18603203

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
Data File : BG040354.D
Acq On : 4 Apr 2019 10:35
Operator : JU/SJ
Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-TRACK-78-79

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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Data File : BG040354.D
Acq On : 4 Apr 2019 10:35
Operator : JU/SJ
Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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

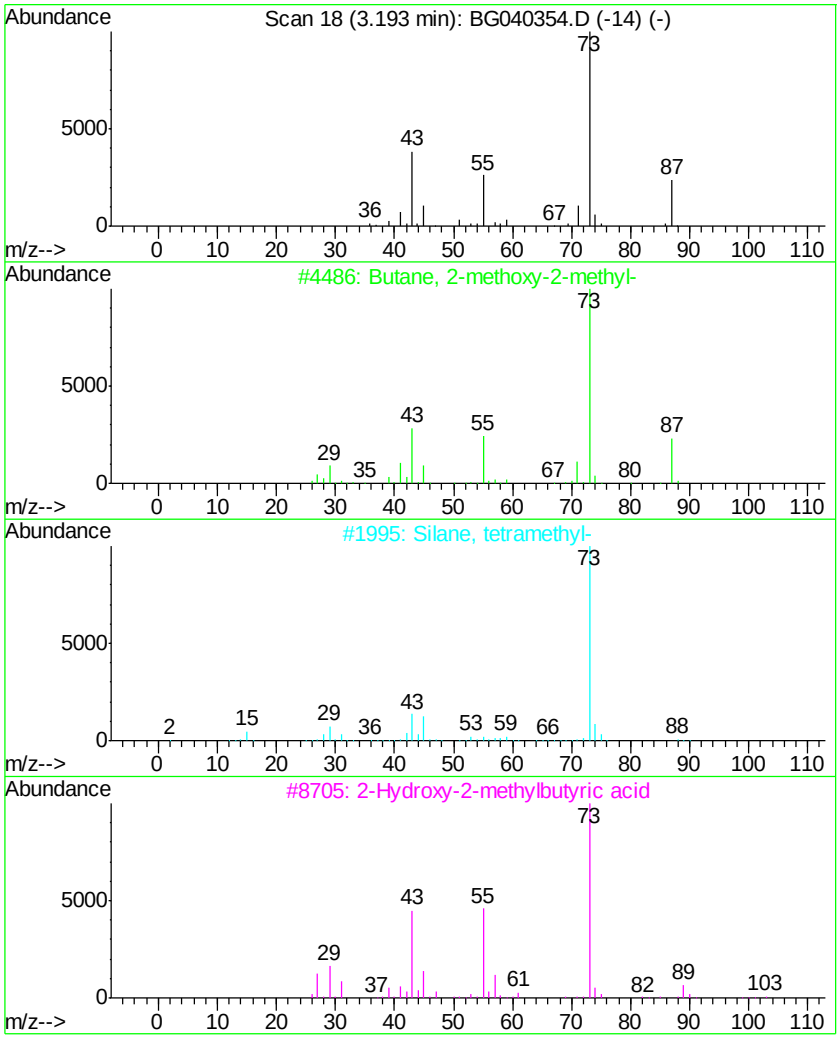
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

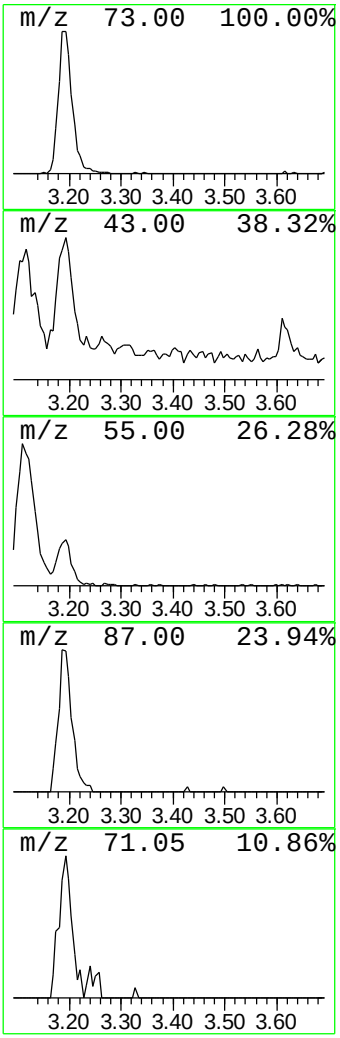
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	5.88 ng	106406	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	12
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	1,3-Dioxolane, 2-heptyl-	172	C10H20O2	004359-57-3	9





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Data File : BG040354.D
Acq On : 4 Apr 2019 10:35
Operator : JU/SJ
Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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

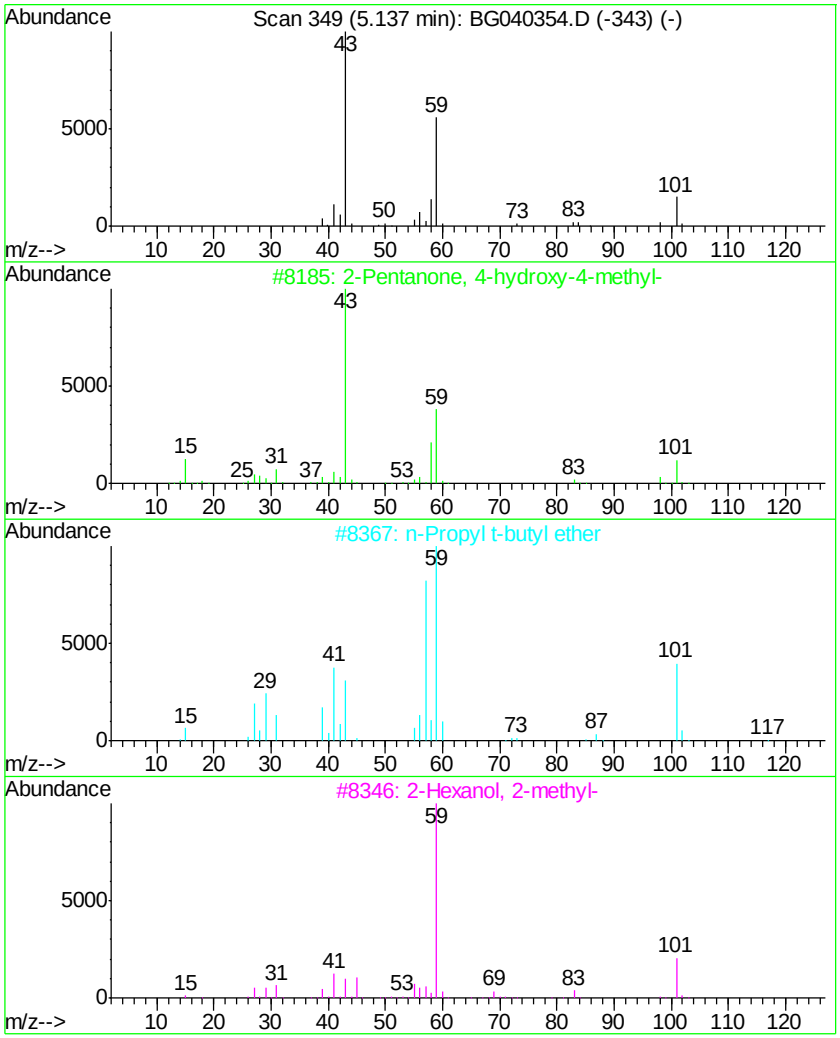
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

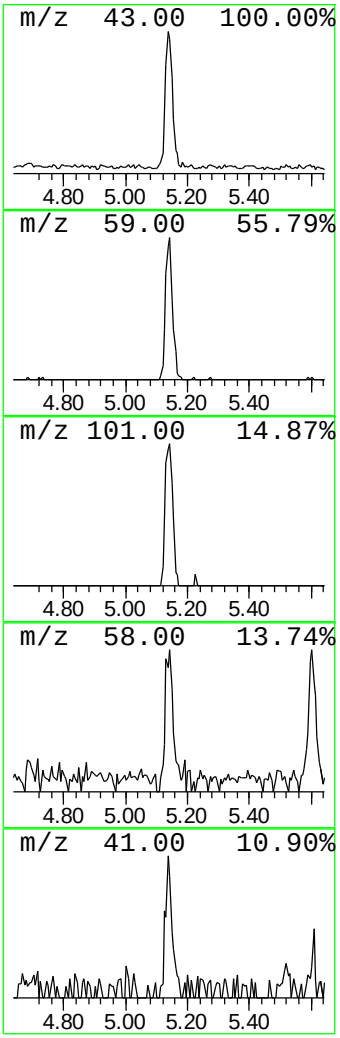
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	3.83 ng	69349	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5	Pentanal, oxime	101	C5H11NO	000628-79-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
Data File : BG040354.D
Acq On : 4 Apr 2019 10:35
Operator : JU/SJ
Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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

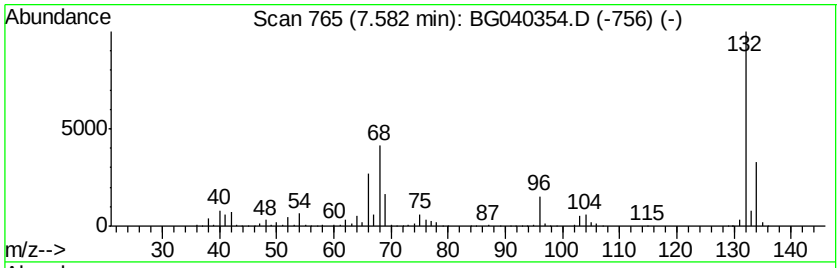
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

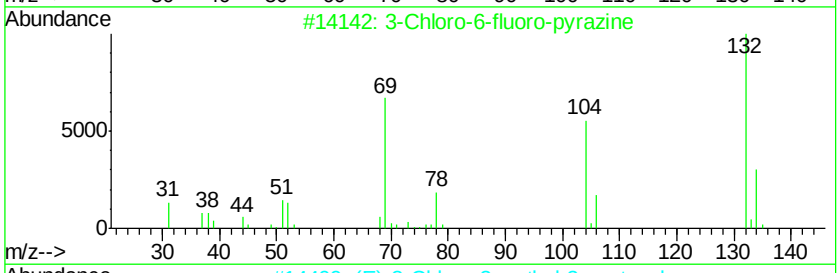
****

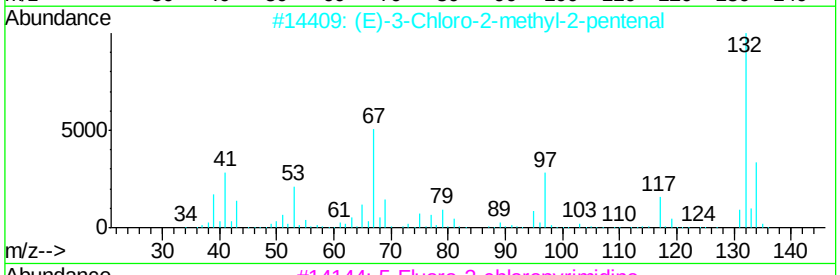
Peak Number 3 unknown7.58 Concentration Rank 2

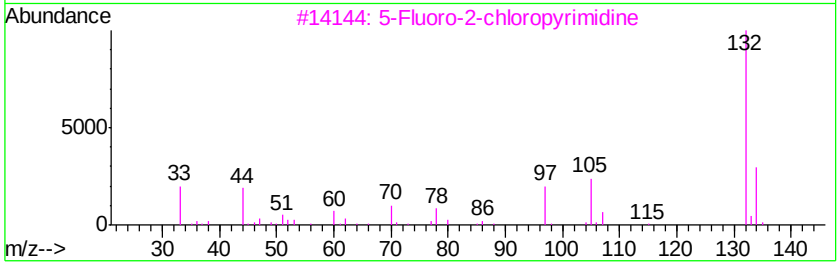
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	56.63 ng	1025290	1,4-Dichlorobenzene-d4	8.05

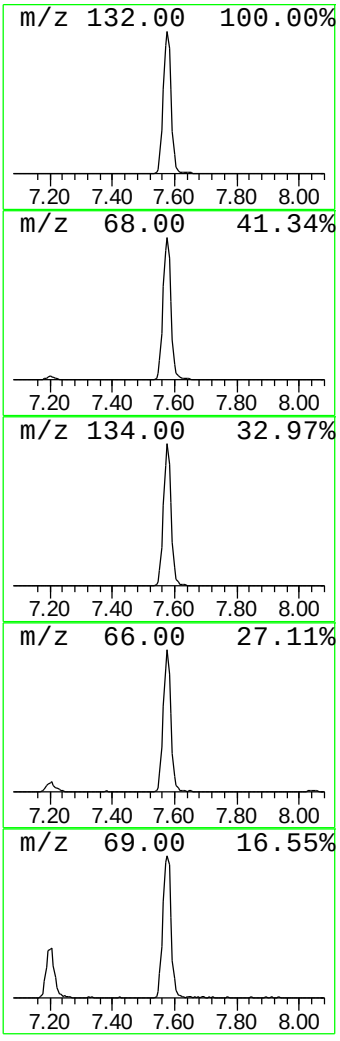
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Aminoindole	132	C8H8N2	005192-03-0	10











Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
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Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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

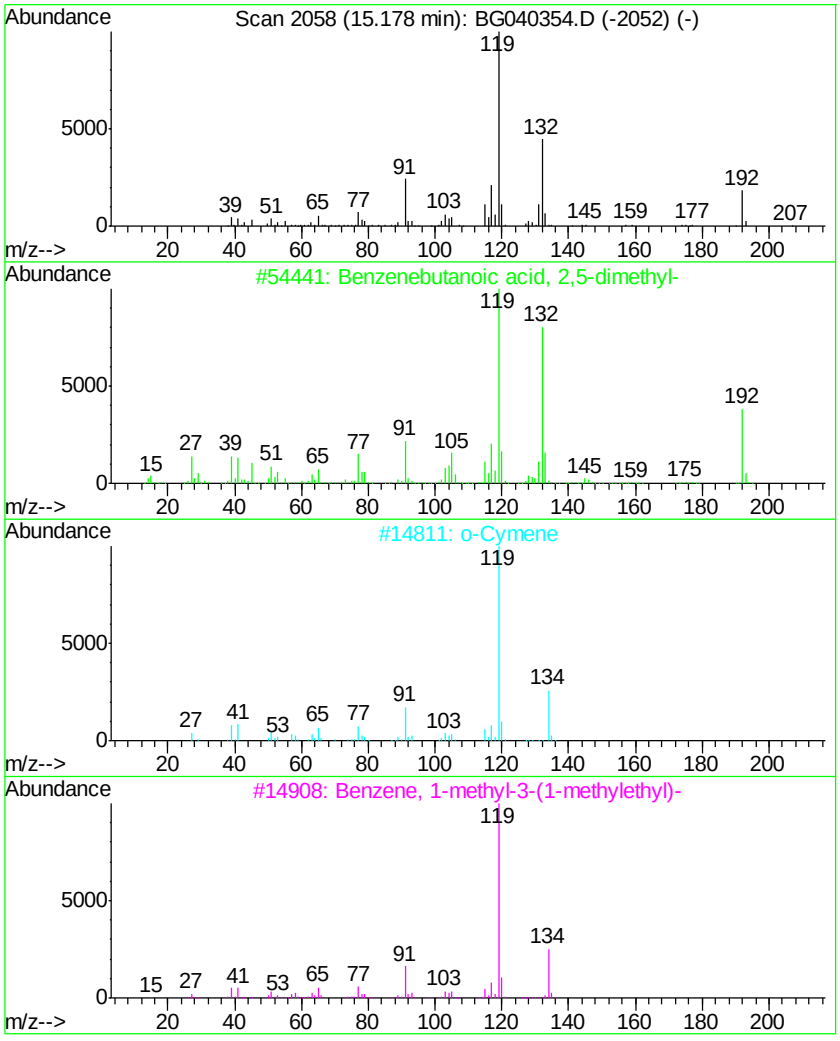
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

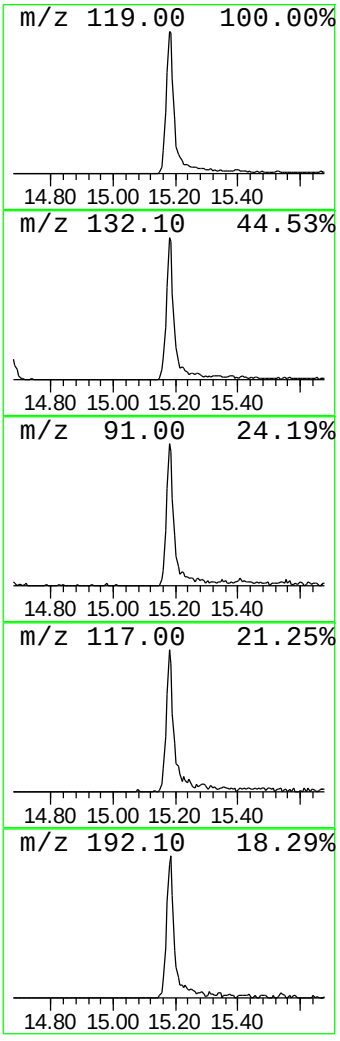
****

Peak Number 5 Benzenebutanoic acid, 2,5-d... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	12.15 ng	401992	Acenaphthene-d10	14.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenebutanoic acid, 2,5-dimethyl-	192	C12H16O2	001453-06-1	58
2	o-Cymene	134	C10H14	000527-84-4	46
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	46
4	Ethyl 3,5-dimethylphenylacetate	192	C12H16O2	105337-18-6	46
5	Ethyl 1,3-dithiane-2-carboxylate	192	C7H12O2S2	020462-00-4	38





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Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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
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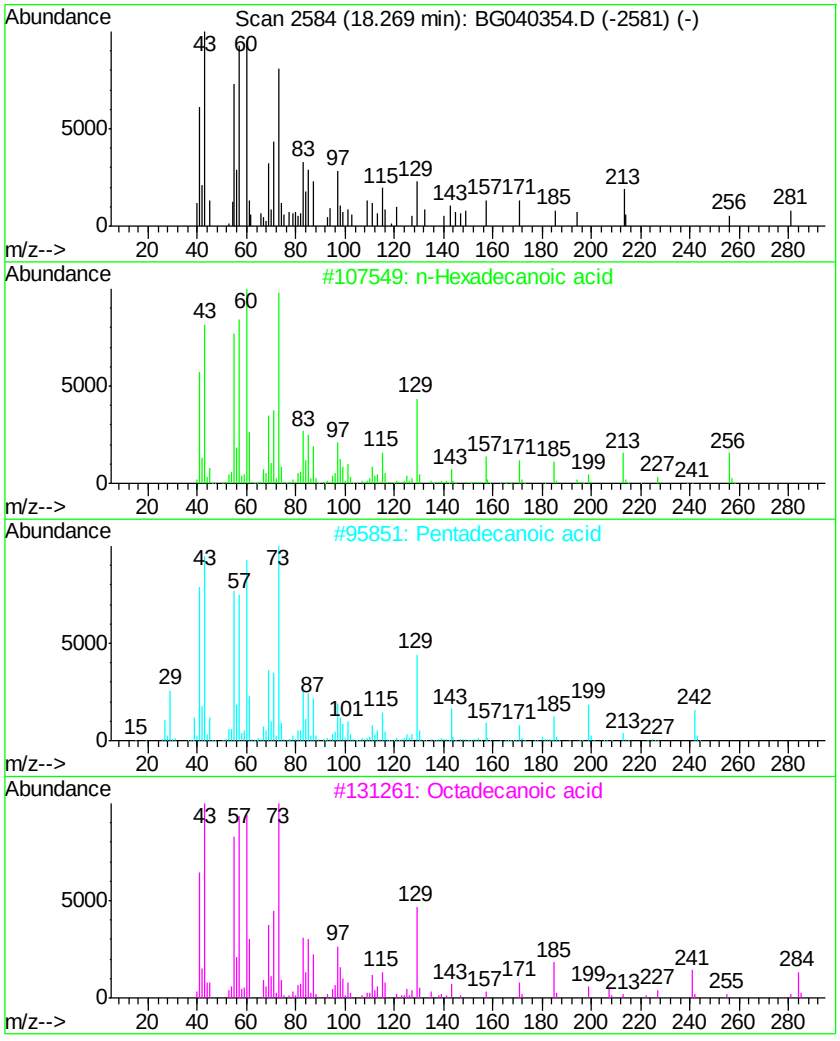
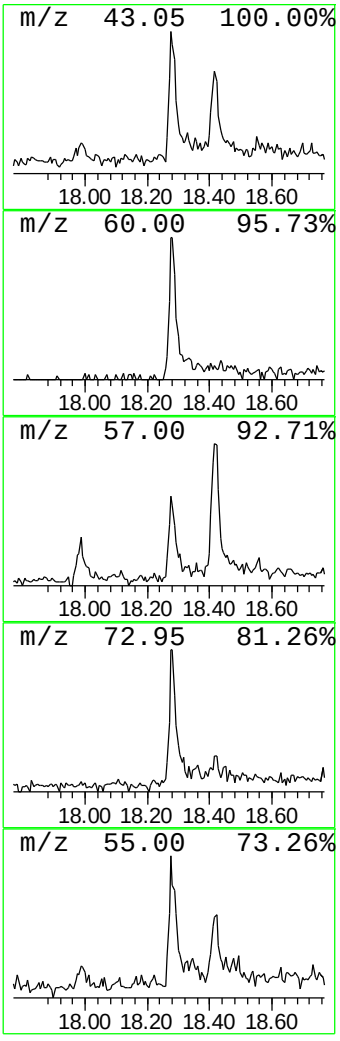
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	2.29 ng	99454	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Octadecanoic acid	284	C18H36O2	000057-11-4	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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

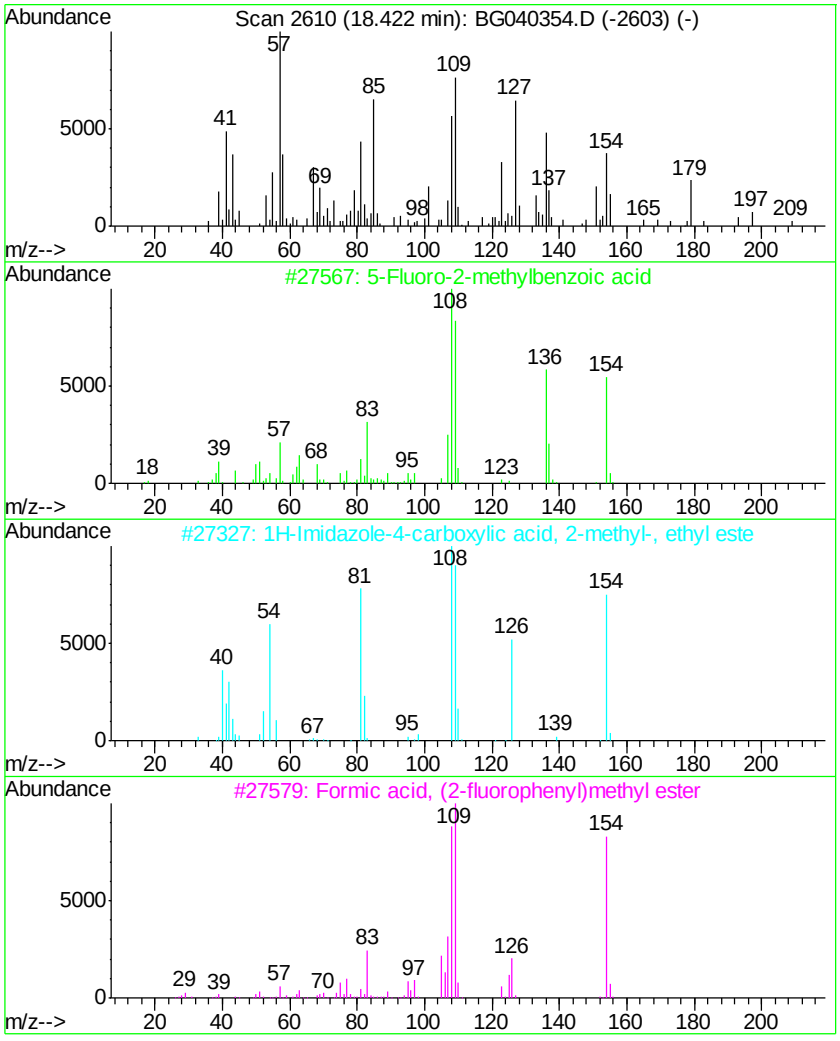
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

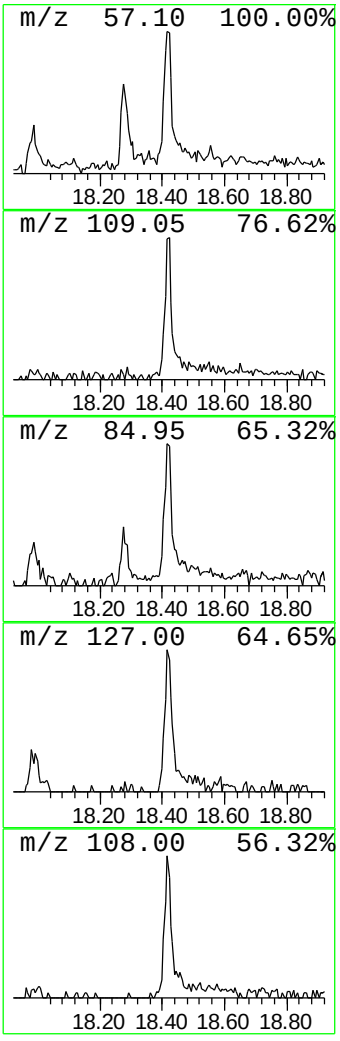
****

Peak Number 7 unknown18.42 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	3.12 ng	135121	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methylbenzoic acid	154	C8H7FO2	033184-16-6	45
2	1H-Imidazole-4-carboxylic acid, ...	154	C7H10N2O2	087326-25-8	38
3	Formic acid, (2-fluorophenyl)met...	154	C8H7FO2	1000368-73-6	38
4	Phenacetin	179	C10H13NO2	000062-44-2	25
5	o-Acetylphenetidine	179	C10H13NO2	000581-08-8	22





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

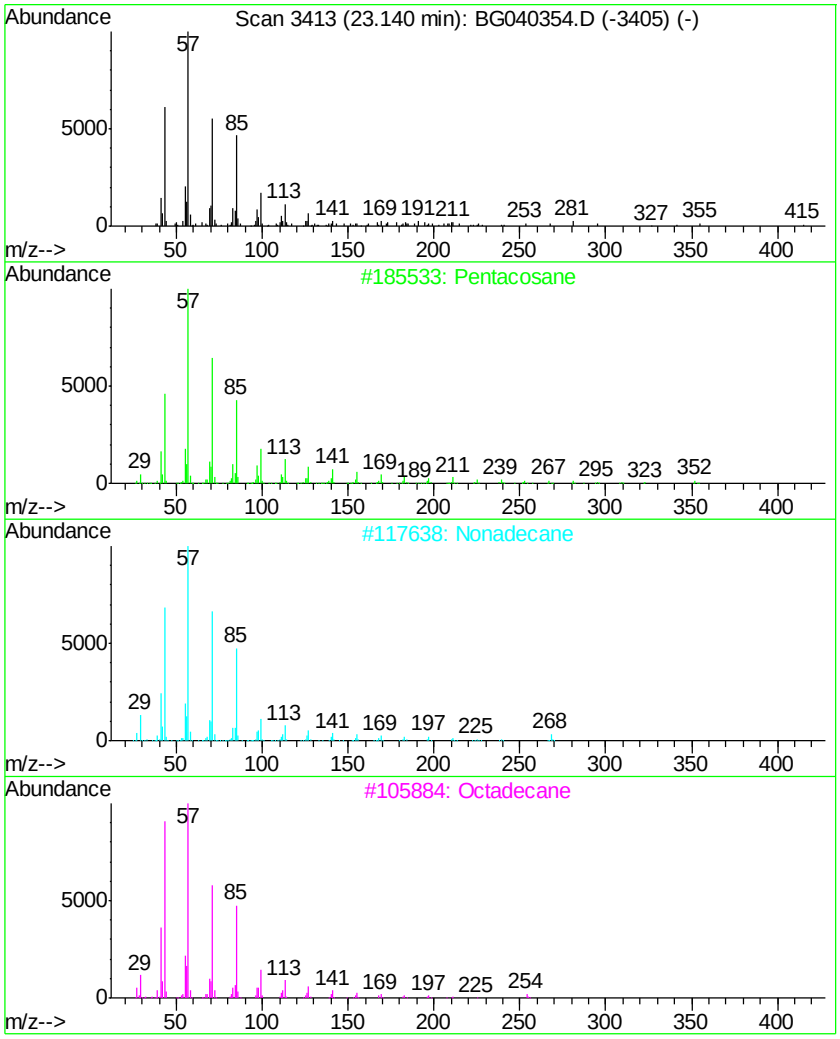
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

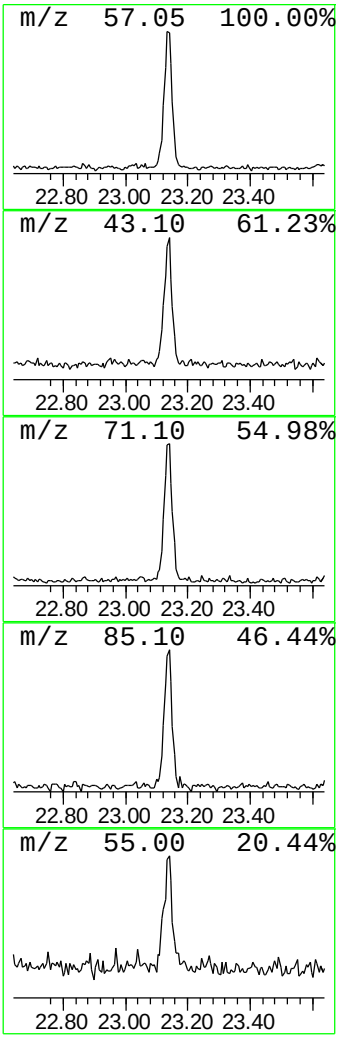
****

Peak Number 8 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	2.98 ng	161845	Chrysene-d12	21.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	87
2	Nonadecane	268	C19H40	000629-92-5	87
3	Octadecane	254	C18H38	000593-45-3	87
4	Eicosane	282	C20H42	000112-95-8	86
5	Heptadecane	240	C17H36	000629-78-7	86





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Data File : BG040354.D
Acq On : 4 Apr 2019 10:35
Operator : JU/SJ
Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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

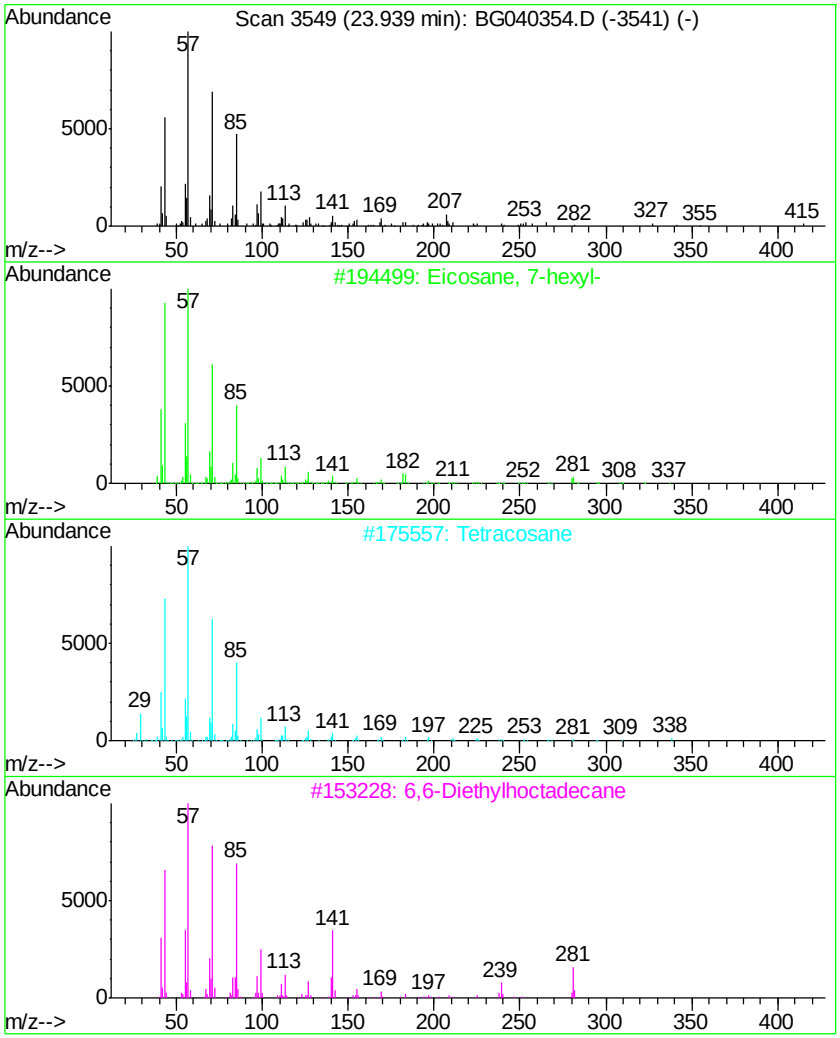
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

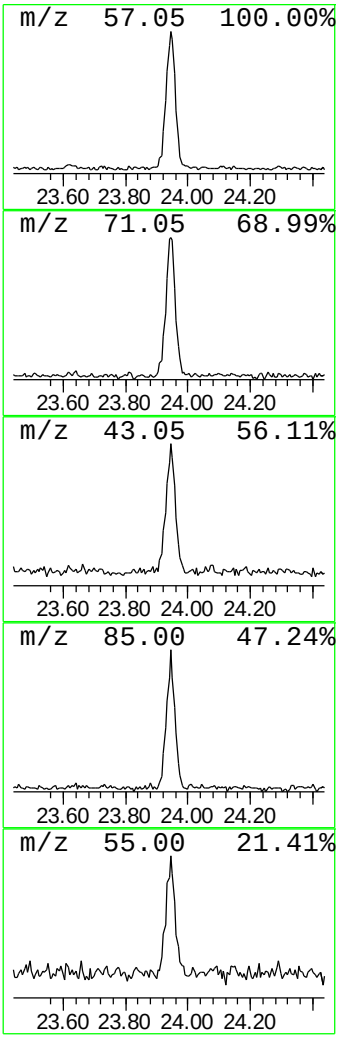
****

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.94	3.96 ng	218882	Perylene-d12	24.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
2	Tetracosane	338	C24H50	000646-31-1	86
3	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	86
4	Hexacosane	366	C26H54	000630-01-3	86
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	86





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Misc :
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Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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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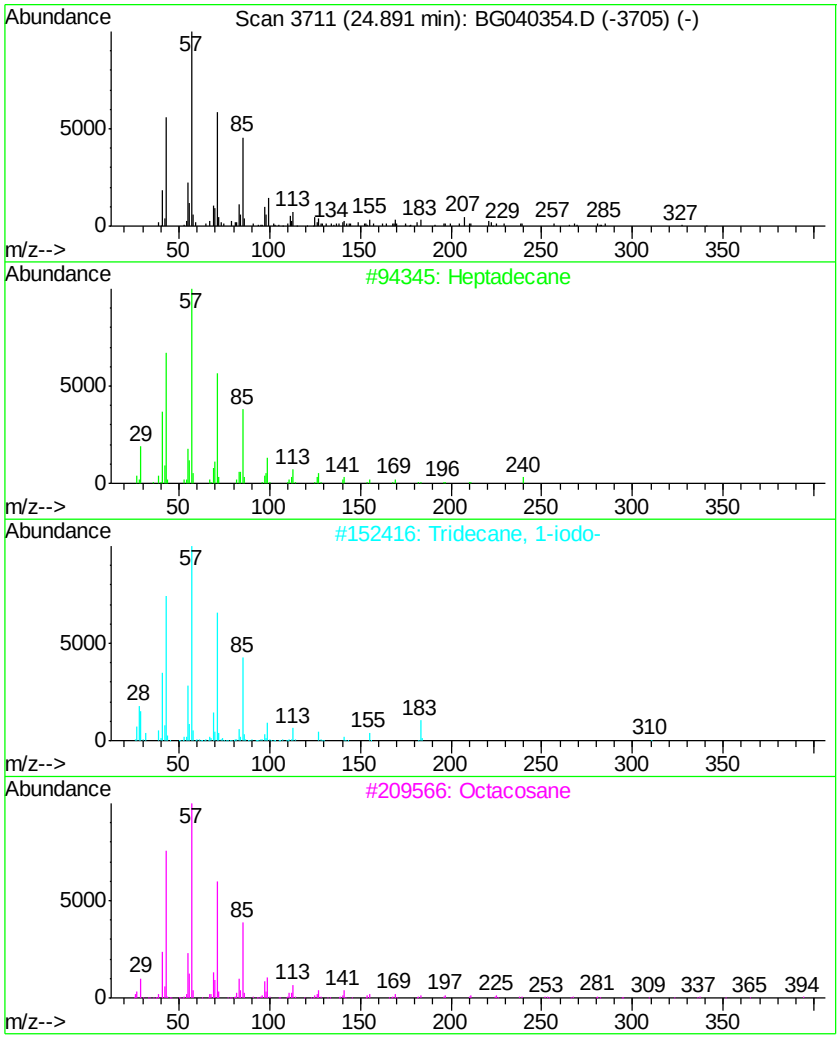
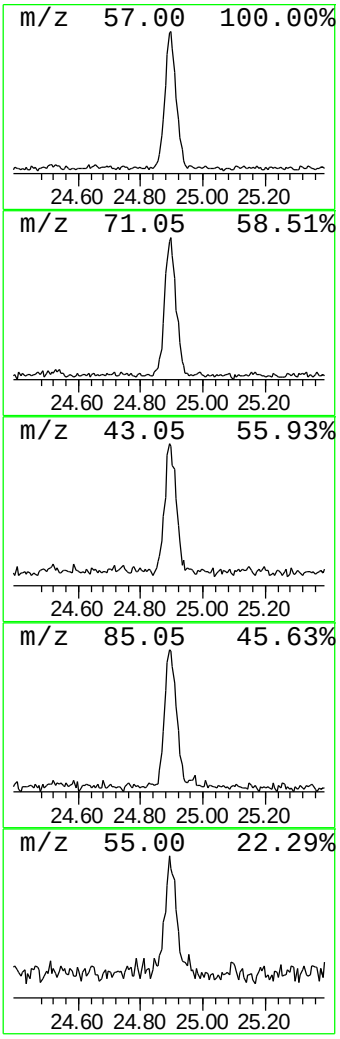
Peak Number 10 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.89	3.50 ng	193231	Perylene-d12	24.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	80
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
3	Octacosane	394	C28H58	000630-02-4	76
4	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	72
5	Hexadecane	226	C16H34	000544-76-3	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
Data File : BG040354.D
Acq On : 4 Apr 2019 10:35
Operator : JU/SJ
Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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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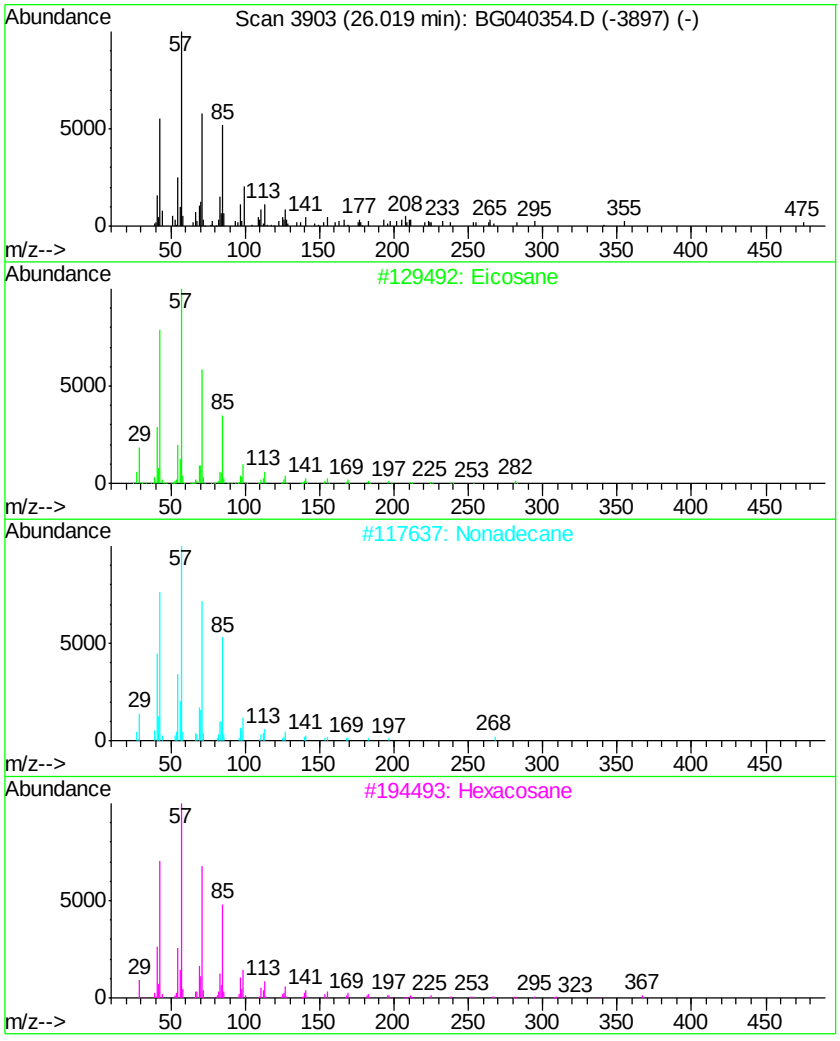
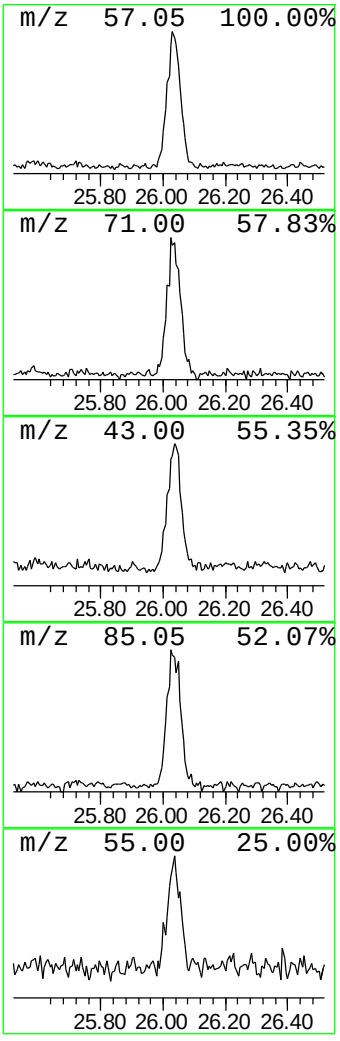
Peak Number 11 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.02	3.13 ng	173077	Perylene-d12	24.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	92
2	Nonadecane	268	C19H40	000629-92-5	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Tetracosane	338	C24H50	000646-31-1	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG040319\
Data File : BG040354.D
Acq On : 4 Apr 2019 10:35
Operator : JU/SJ
Sample : K2187-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-TRACK-78-79

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...	3.19	5.9	ng	106406	1	8.05	362090	20.0
2-Pentanone, 4-hy...	5.14	3.8	ng	69349	1	8.05	362090	20.0
unknown7.58	7.58	56.6	ng	1025290	1	8.05	362090	20.0
Benzenebutanoic a...	15.18	12.2	ng	401992	3	14.68	661721	20.0
n-Hexadecanoic acid	18.27	2.3	ng	99454	4	17.42	867146	20.0
unknown18.42	18.42	3.1	ng	135121	4	17.42	867146	20.0
Pentacosane	23.14	3.0	ng	161845	5	21.69	1087290	20.0
Eicosane, 7-hexyl-	23.94	4.0	ng	218882	6	24.97	1104920	20.0
Heptadecane	24.89	3.5	ng	193231	6	24.97	1104920	20.0
Eicosane	26.02	3.1	ng	173077	6	24.97	1104920	20.0