LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048949.D
Acq On : 14 Jun 2021 14:43
Operator : CG/JU
Sample : M2678-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0243-AMND-COMPOSITE-H

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-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048949.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.170	16	22	36	rVB	186137	325602	6.87%	2.210%
2	3.287	38	42	52	rVB	82768	120708	2.55%	0.819%
3	4.592	258	264	280	rBV	565338	889187	18.77%	6.034%
4	5.214	361	370	376	rBV	2642439	4736630	100.00%	32.144%
5	5.661	441	446	455	rBV	30895	52608	1.11%	0.357%
6	5.737	455	459	468	rVB2	21609	48432	1.02%	0.329%
7	7.259	711	718	727	rBV	182248	317530	6.70%	2.155%
8	8.123	858	865	871	rBV	142511	253496	5.35%	1.720%
9	9.286	1056	1063	1073	rVB	401195	738632	15.59%	5.012%
10	10.702	1298	1304	1313	rBV	109827	193972	4.10%	1.316%
11	10.943	1337	1345	1352	rVB	187434	349283	7.37%	2.370%
12	13.387	1752	1761	1767	rBV	925563	1492803	31.52%	10.130%
13	14.762	1986	1995	2002	rBV	315780	493114	10.41%	3.346%
14	16.160	2228	2233	2238	rBV2	51736	72275	1.53%	0.490%
15	17.512	2457	2463	2473	rBV	408433	629372	13.29%	4.271%
16	20.121	2900	2907	2912	rBV	1804689	2431761	51.34%	16.502%
17	21.443	3126	3132	3138	rBV3	72164	138455	2.92%	0.940%
18	21.689	3170	3174	3179	rVB	44761	64770	1.37%	0.440%
19	21.801	3186	3193	3203	rBV2	384017	672817	14.20%	4.566%
20	23.035	3397	3403	3408	rBV6	27453	56439	1.19%	0.383%
21	25.138	3751	3761	3772	rBV3	220431	657990	13.89%	4.465%

Sum of corrected areas: 14735876

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
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Acq On : 14 Jun 2021 14:43
Operator : CG/JU
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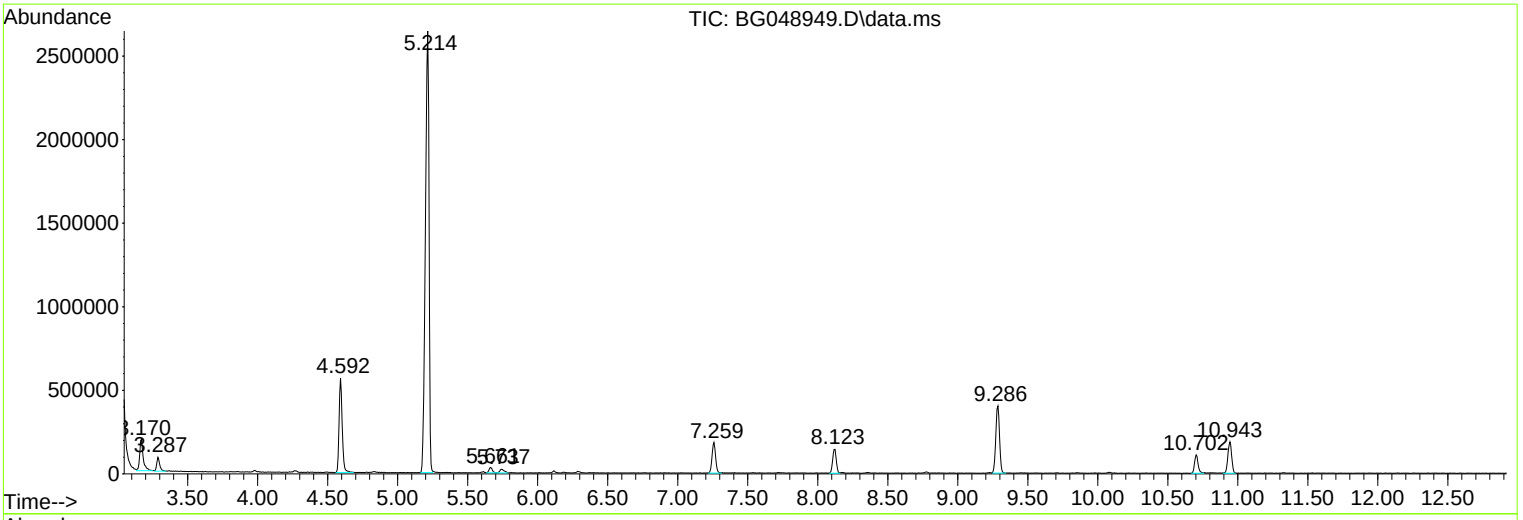
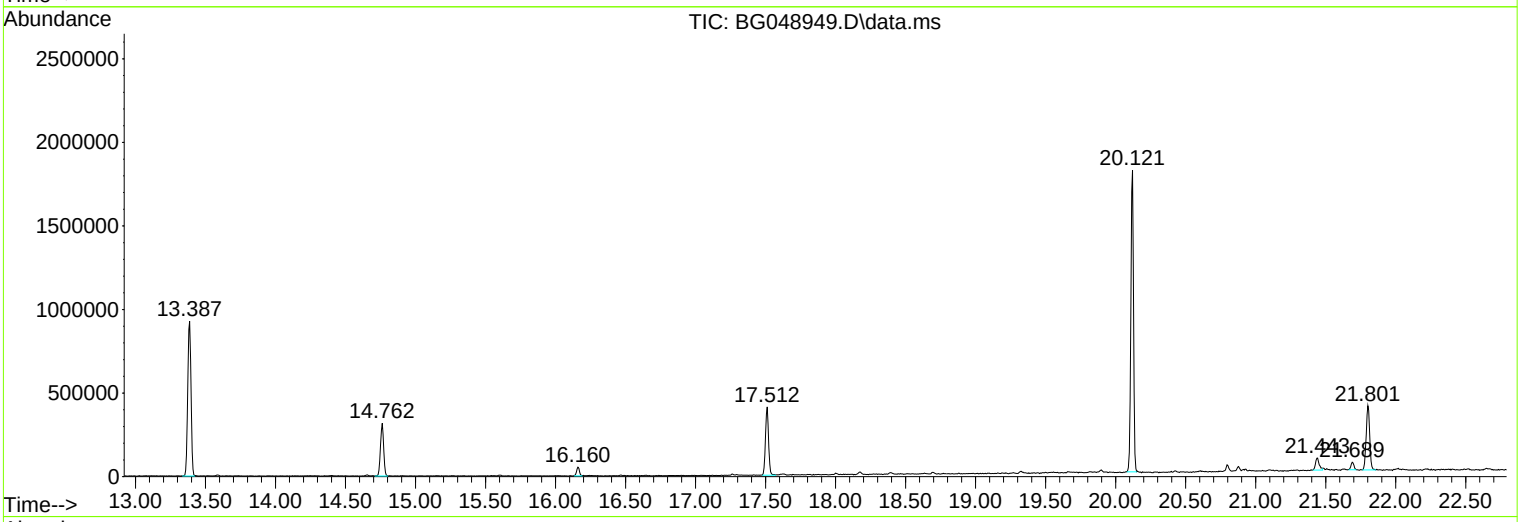
Misc :
ALS Vial : 8 Sample Multiplier: 1

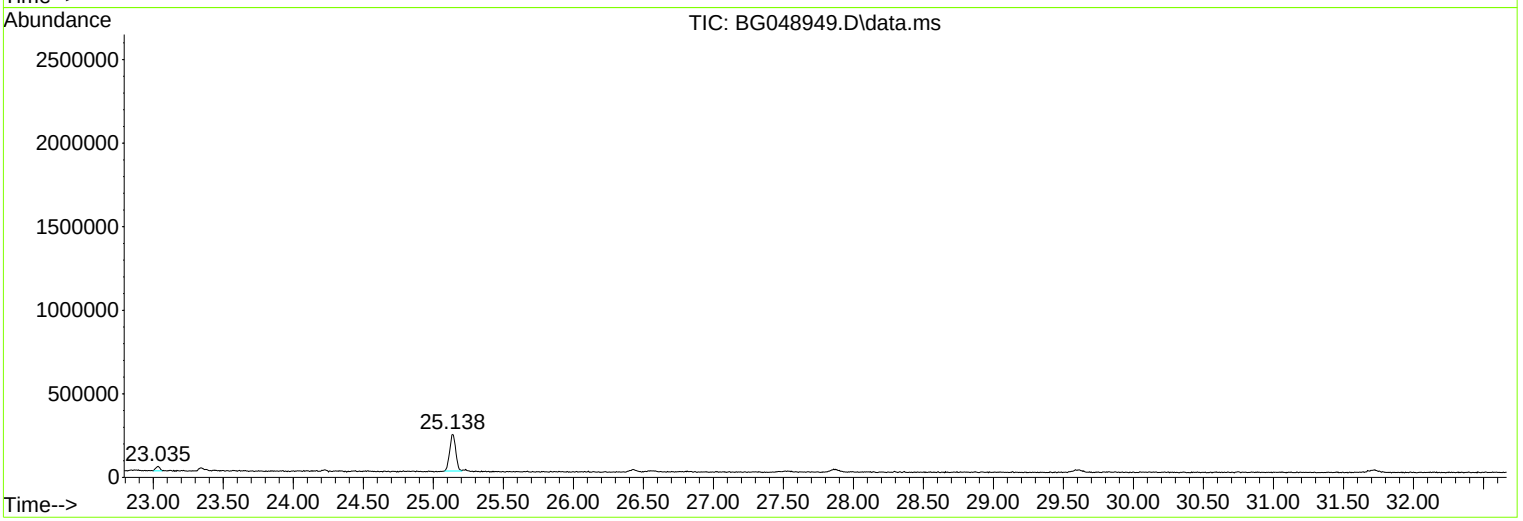
Instrument :
BNA_G
ClientSampleId :
0243-AMND-COMPOSITE-H

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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 : BG048949.D
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Instrument :
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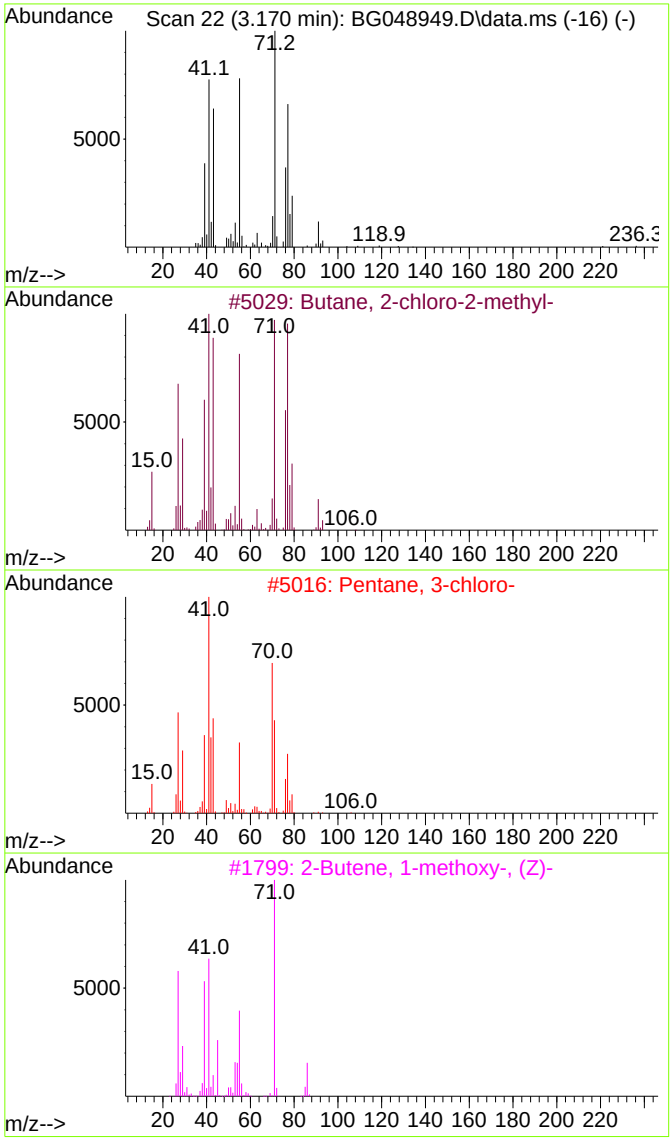
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

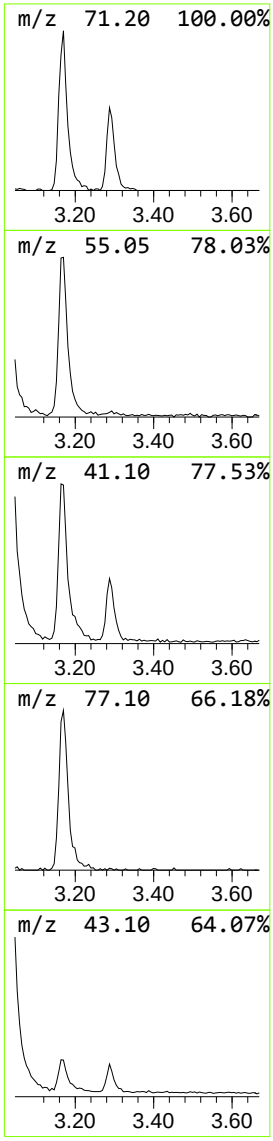
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-chloro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.170	25.69 ng	325602	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	72
2	Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	42
3	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	32
4	3-Chloro-2-buten-1-ol	106	C4H7ClO	040605-42-3	23
5	Allyl chloride	76	C3H5Cl	000107-05-1	14





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Data File : BG048949.D
Acq On : 14 Jun 2021 14:43
Operator : CG/JU
Sample : M2678-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0243-AMND-COMPOSITE-H

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

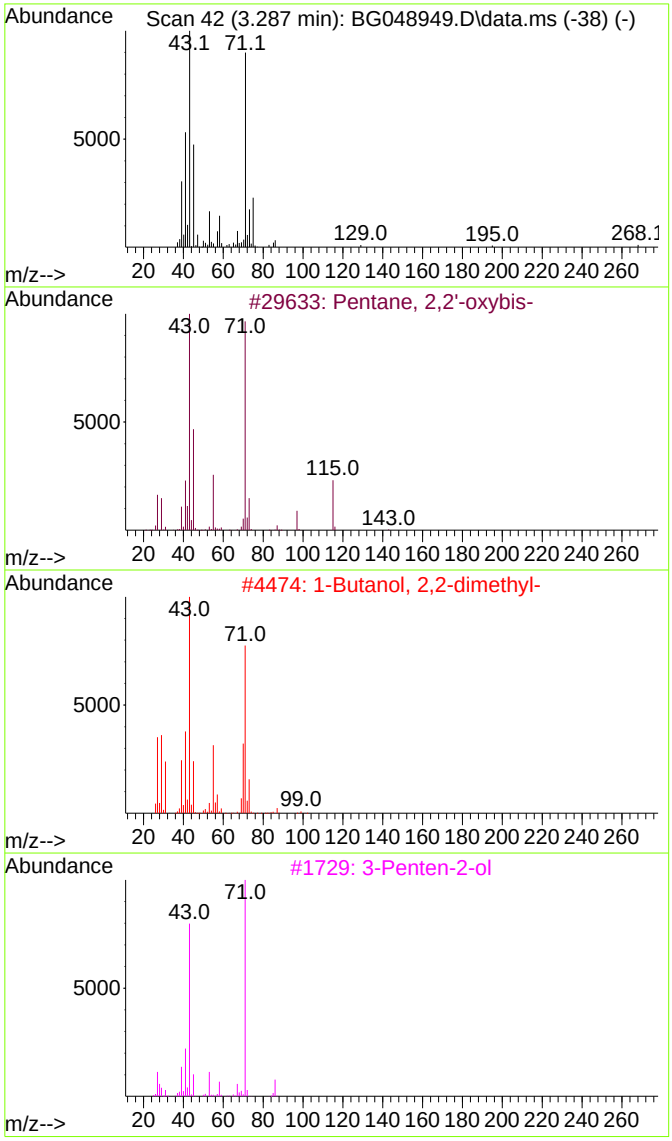
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

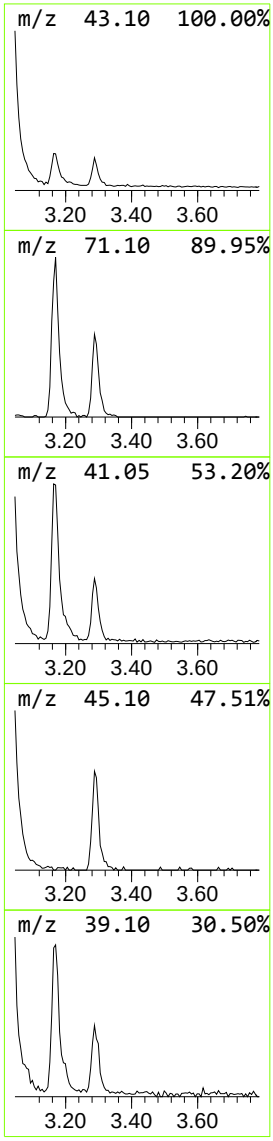
****

Peak Number 2 Pentane, 2,2'-oxybis- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.287	9.52 ng	120708	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	53
2	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	40
3	3-Penten-2-ol	86	C5H10O	001569-50-2	38
4	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	38
5	2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	37





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Data File : BG048949.D
Acq On : 14 Jun 2021 14:43
Operator : CG/JU
Sample : M2678-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0243-AMND-COMPOSITE-H

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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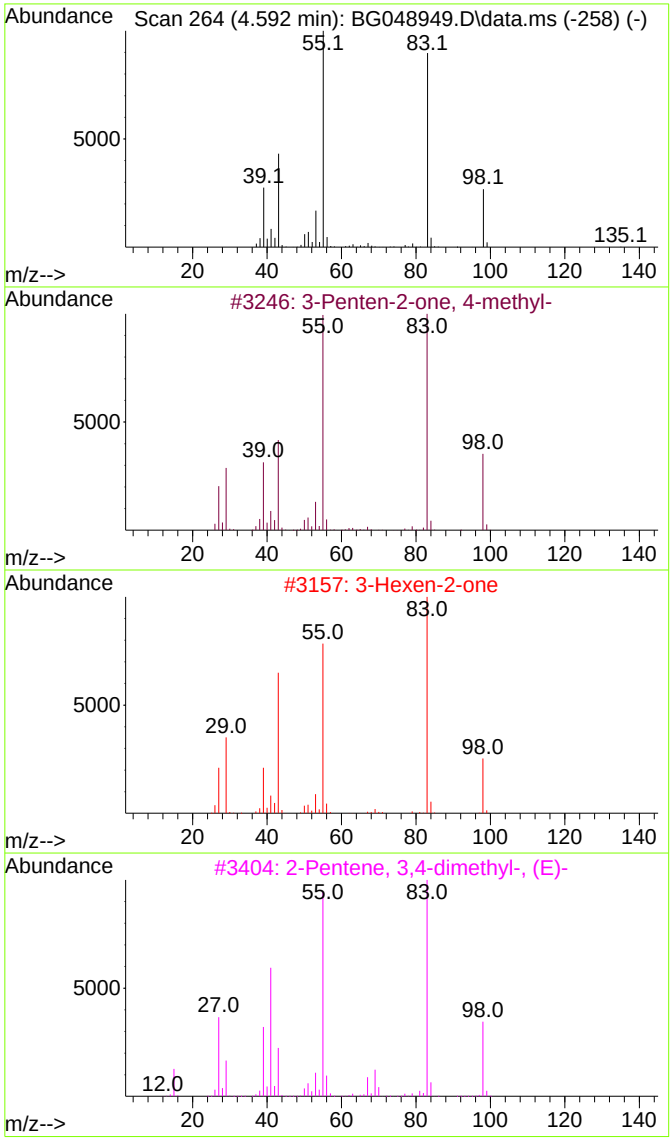
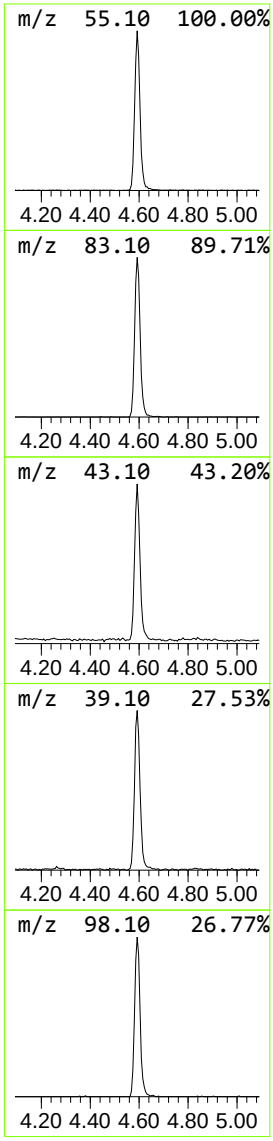
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.592	70.15 ng	889187	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048949.D
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Operator : CG/JU
Sample : M2678-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0243-AMND-COMPOSITE-H

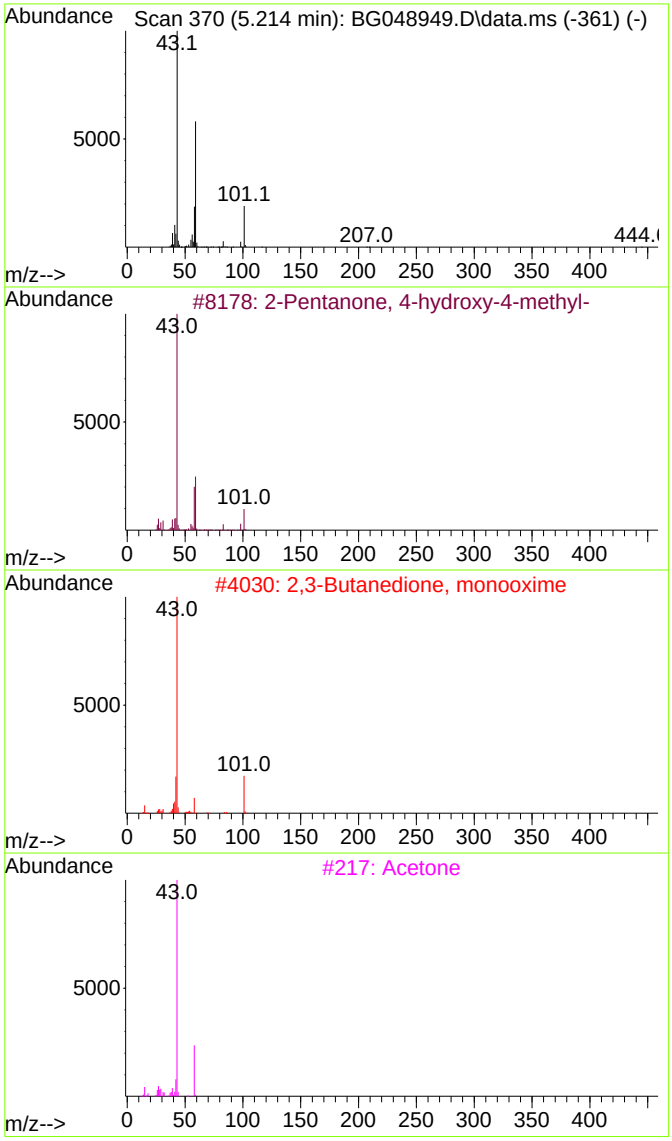
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

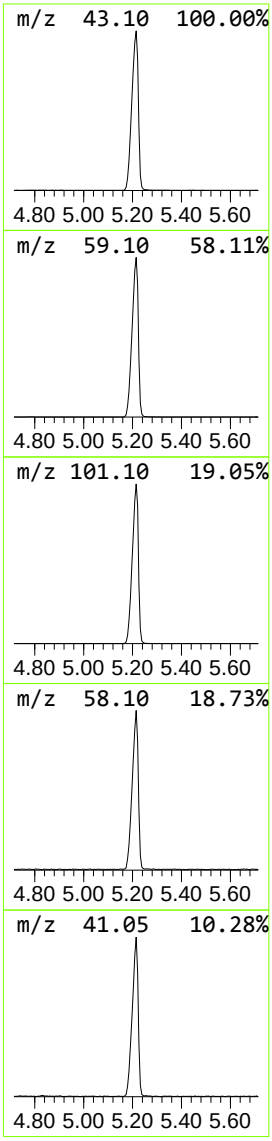
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.214	373.70 ng	4736630	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
3	Acetone	58	C3H6O	000067-64-1	10
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9





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Sample : M2678-10
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0243-AMND-COMPOSITE-H

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

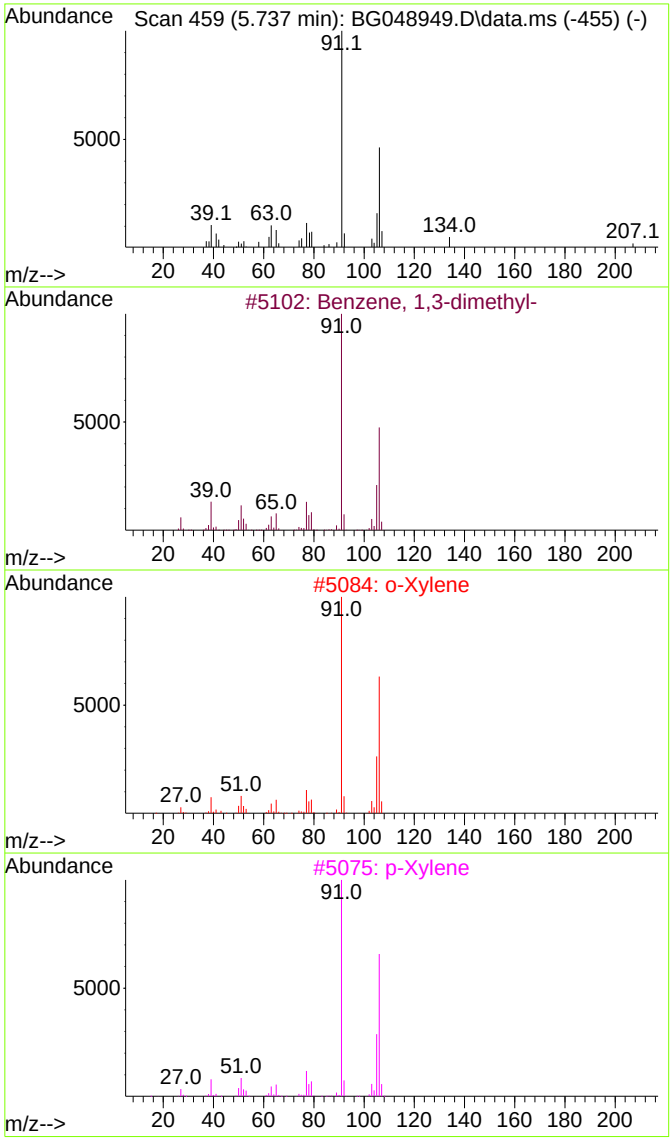
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

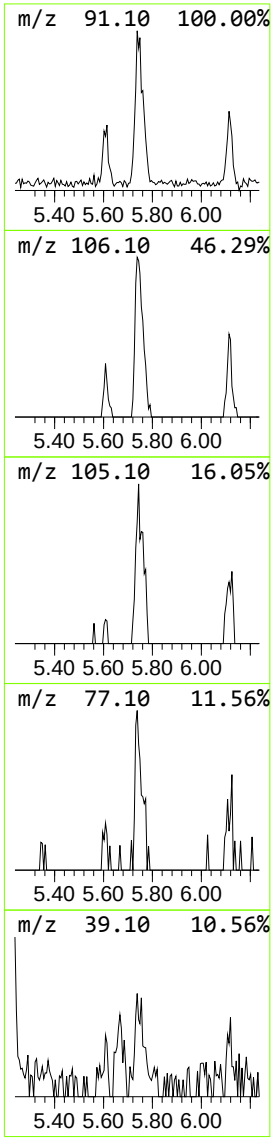
****

Peak Number 5 Benzene, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.737	3.82 ng	48432	1,4-Dichlorobenzene-d4	8.123

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	90
2	o-Xylene	106	C8H10	000095-47-6	90
3	p-Xylene	106	C8H10	000106-42-3	83
4	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	80
5	Ethylbenzene	106	C8H10	000100-41-4	64





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Instrument :
BNA_G
ClientSampleId :
0243-AMND-COMPOSITE-H

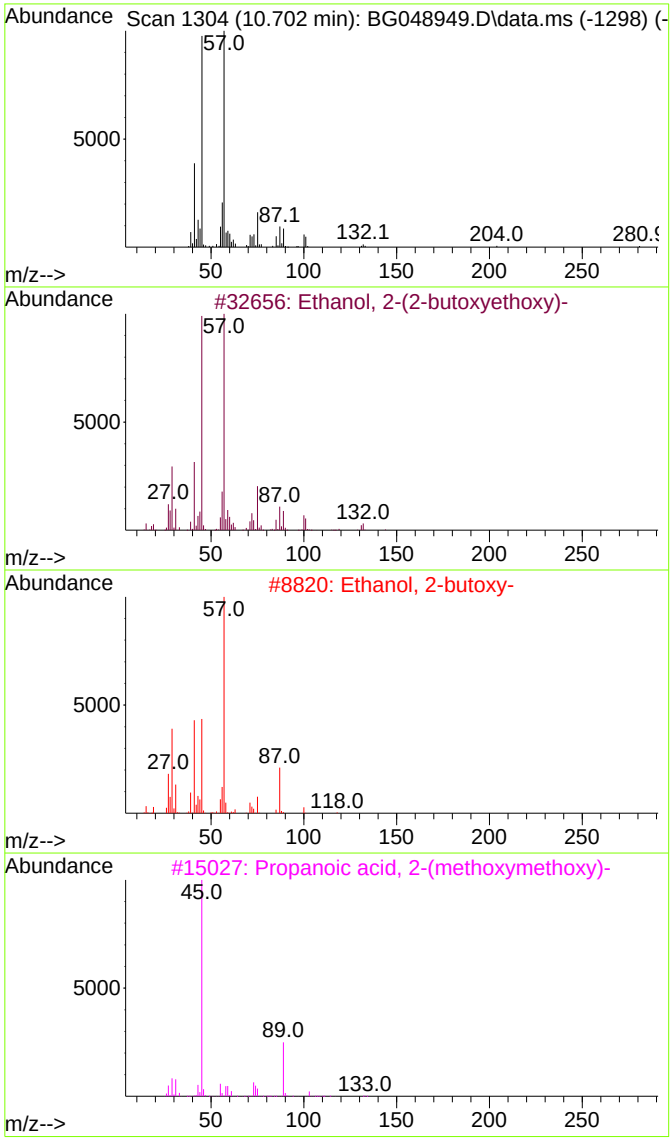
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

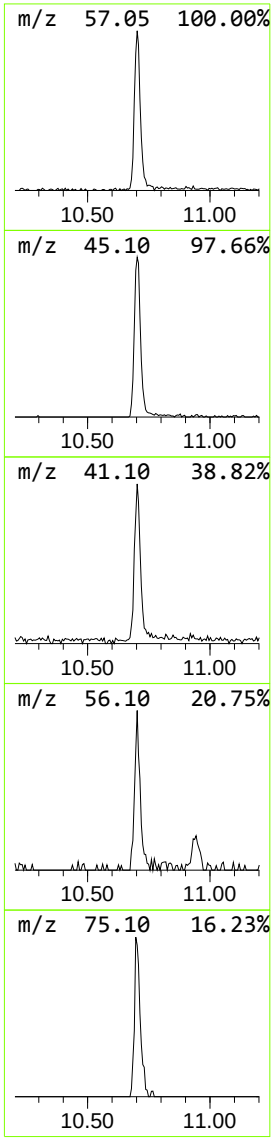
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.702	11.11 ng	193972	Naphthalene-d8	10.943

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
2	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	59
3	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	43
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	43
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	38





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BNA_G
ClientSampleId :
0243-AMND-COMPOSITE-H

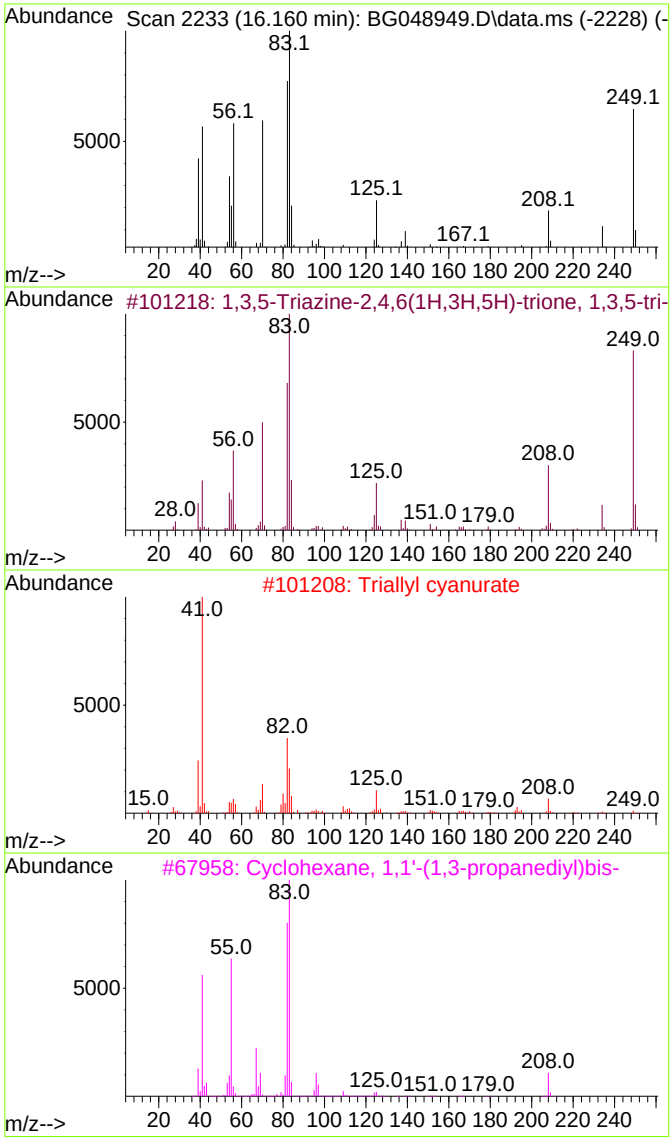
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

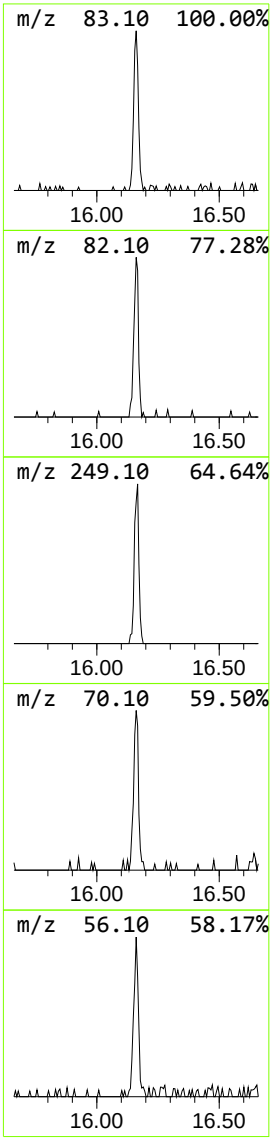
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.160	2.30 ng	72275	Phenanthrene-d10	17.512

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	97
2	Triallyl cyanurate	249	C12H15N3O3	000101-37-1	43
3	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	32
4	Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	32
5	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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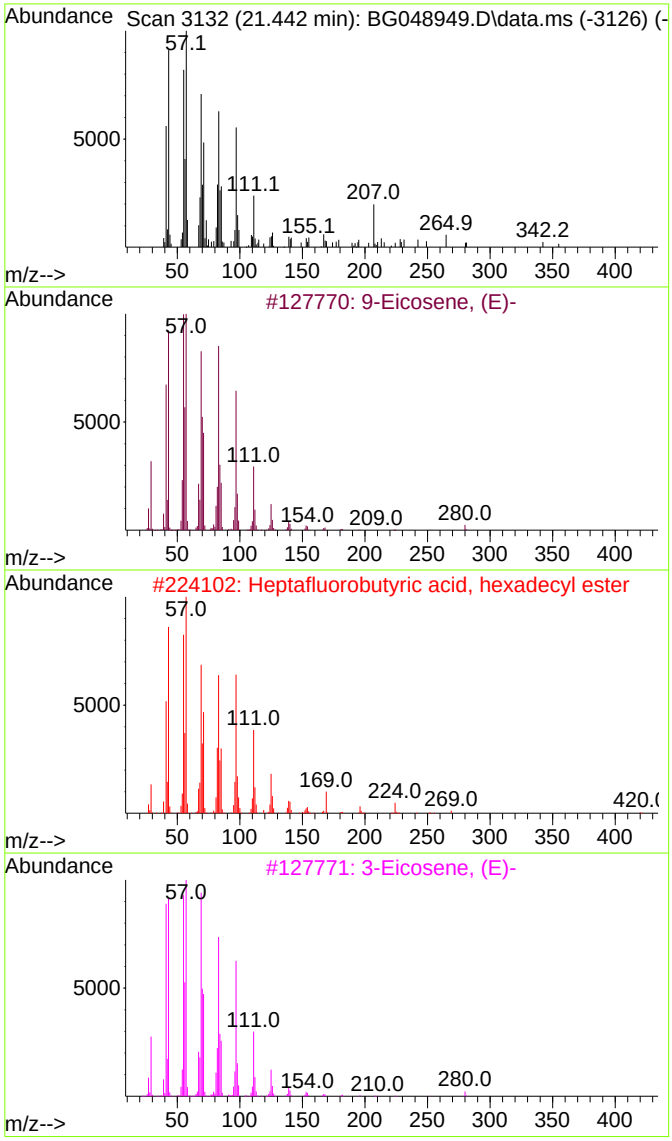
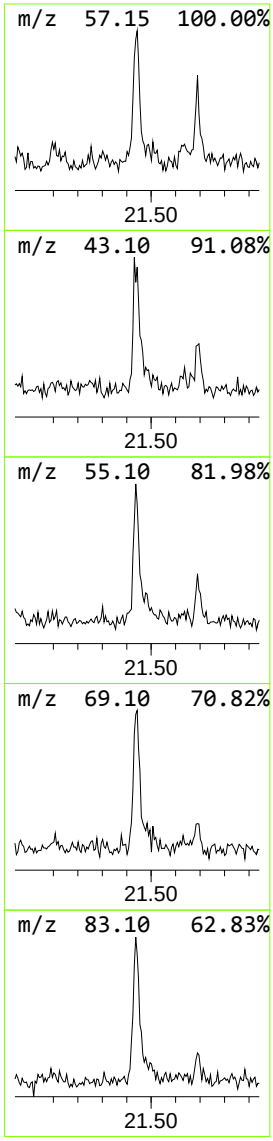
****

Peak Number 8 9-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.442	4.12 ng	138455	Chrysene-d12	21.801

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048949.D
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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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-chlor...	3.170	25.7	ng	325602	1	8.123	253496	20.0
Pentane, 2,2'-o...	3.287	9.5	ng	120708	1	8.123	253496	20.0
3-Penten-2-one,...	4.592	70.2	ng	889187	1	8.123	253496	20.0
2-Pentanone, 4-...	5.214	373.7	ng	4736630	1	8.123	253496	20.0
Benzene, 1,3-di...	5.737	3.8	ng	48432	1	8.123	253496	20.0
Ethanol, 2-(2-b...	10.702	11.1	ng	193972	2	10.943	349283	20.0
1,3,5-Triazine-...	16.160	2.3	ng	72275	4	17.512	629372	20.0
9-Eicosene, (E)-	21.442	4.1	ng	138455	5	21.801	672817	20.0