LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-MH-C02

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-BG012919.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	3.219	17	22	31	rBV	84950	175097	4.27%	0.688%
2	3.296	31	35	48	rVB2	58260	98833	2.41%	0.388%
3	3.842	122	128	137	rBV	53175	90109	2.20%	0.354%
4	5.710	439	446	460	rBV	1184670	1932014	47.06%	7.588%
5	7.314	709	719	734	rBV	1233754	2327270	56.69%	9.140%
6	7.696	775	784	792	rBV	1183179	2030627	49.47%	7.975%
7	8.166	857	864	875	rVB	198784	348905	8.50%	1.370%
8	8.489	911	919	929	rBV	818925	1450161	35.33%	5.696%
9	9.346	1056	1065	1073	rBV	706902	1273676	31.03%	5.002%
10	10.985	1337	1344	1354	rBV	279632	505595	12.32%	1.986%
11	11.990	1509	1515	1521	rBV2	42780	71775	1.75%	0.282%
12	13.412	1746	1757	1766	rBV	1848826	2971391	72.38%	11.670%
13	14.228	1890	1896	1903	rBV	118464	179847	4.38%	0.706%
14	14.792	1985	1992	1999	rBV2	457267	751377	18.30%	2.951%
15	16.278	2236	2245	2258	rBV	1677097	2652427	64.61%	10.417%
16	17.535	2451	2459	2464	rBV2	638298	1005997	24.51%	3.951%
17	17.571	2464	2465	2471	rVB	53066	60960	1.48%	0.239%
18	18.381	2598	2603	2611	rBV3	85575	138382	3.37%	0.543%
19	19.227	2743	2747	2755	rBV	30364	51535	1.26%	0.202%
20	19.574	2795	2806	2813	rVB	96304	160608	3.91%	0.631%
21	19.938	2864	2868	2876	rVB	86326	118075	2.88%	0.464%
22	20.126	2894	2900	2907	rBV	3121825	4105177	100.00%	16.123%
23	21.412	3114	3119	3134	rVB2	126961	264174	6.44%	1.038%
24	21.824	3180	3189	3194	rBV	626052	1157474	28.20%	4.546%
25	21.871	3194	3197	3204	rVB2	36929	57736	1.41%	0.227%
26	22.599	3316	3321	3325	rVB3	35397	52925	1.29%	0.208%
27	23.316	3437	3443	3453	rVB	44984	82656	2.01%	0.325%
28	24.156	3581	3586	3598	rVB4	53755	148035	3.61%	0.581%
29	25.201	3748	3764	3778	rBV2	347046	1135848	27.67%	4.461%
30	26.335	3950	3957	3963	rBV6	25136	62819	1.53%	0.247%

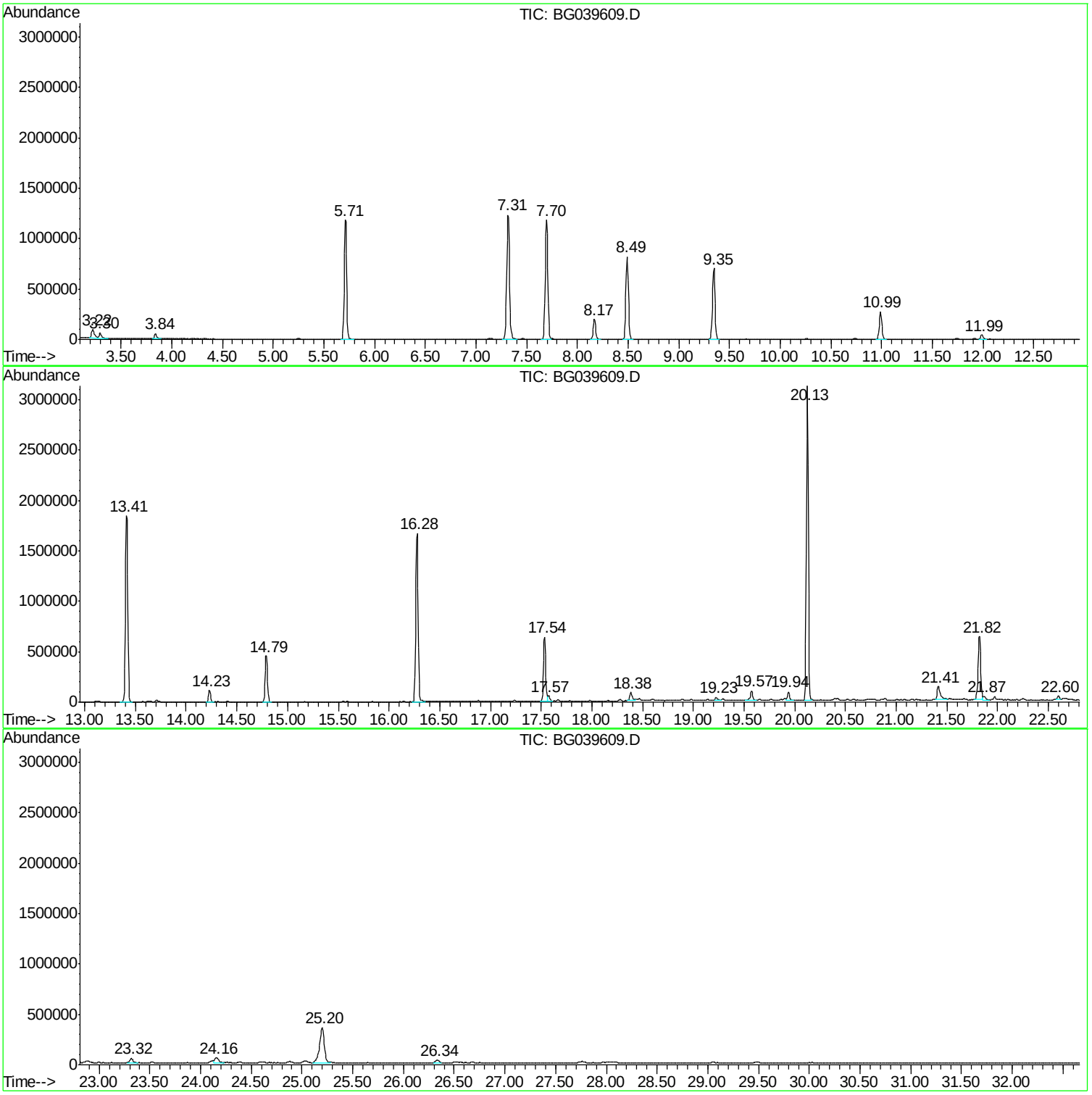
Sum of corrected areas: 25461505

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-MH-C02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-MH-C02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

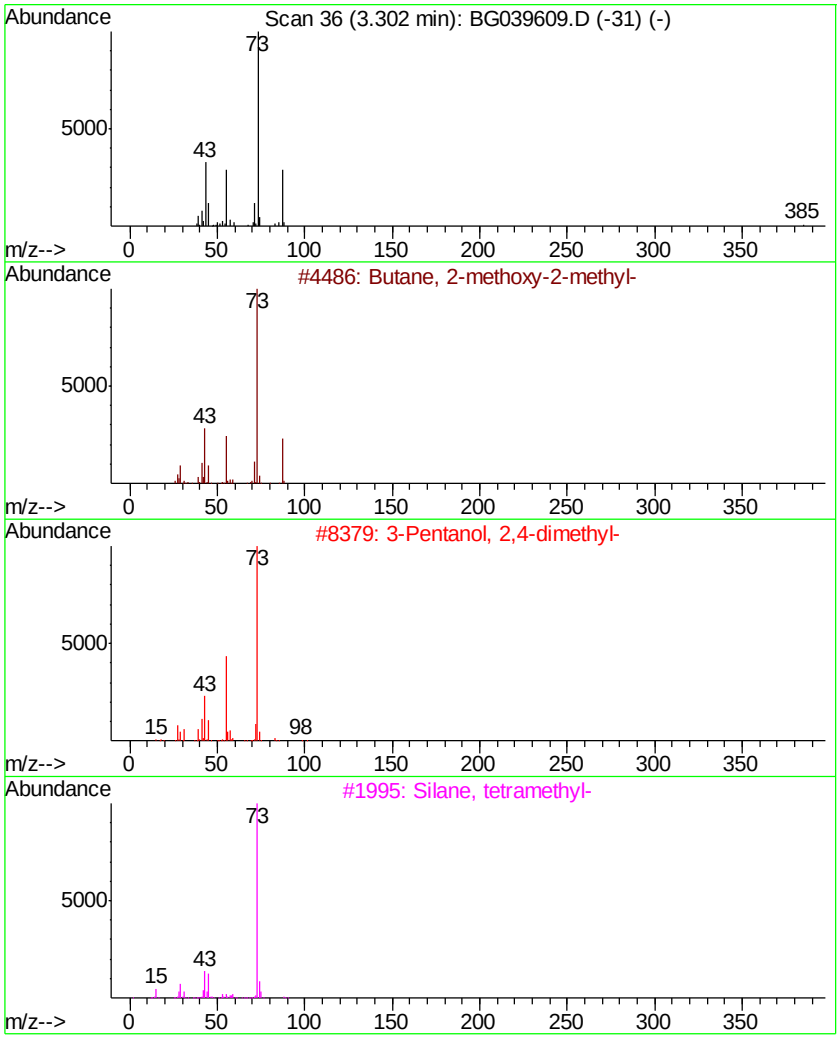
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

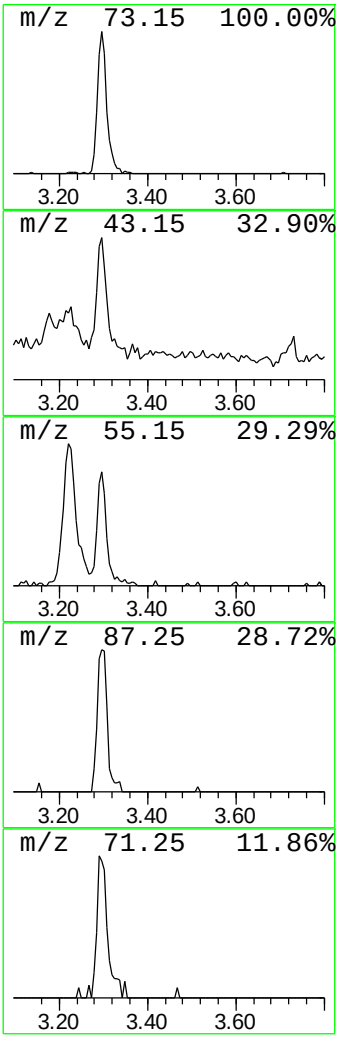
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.30	5.67 ng	98833	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-MH-C02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

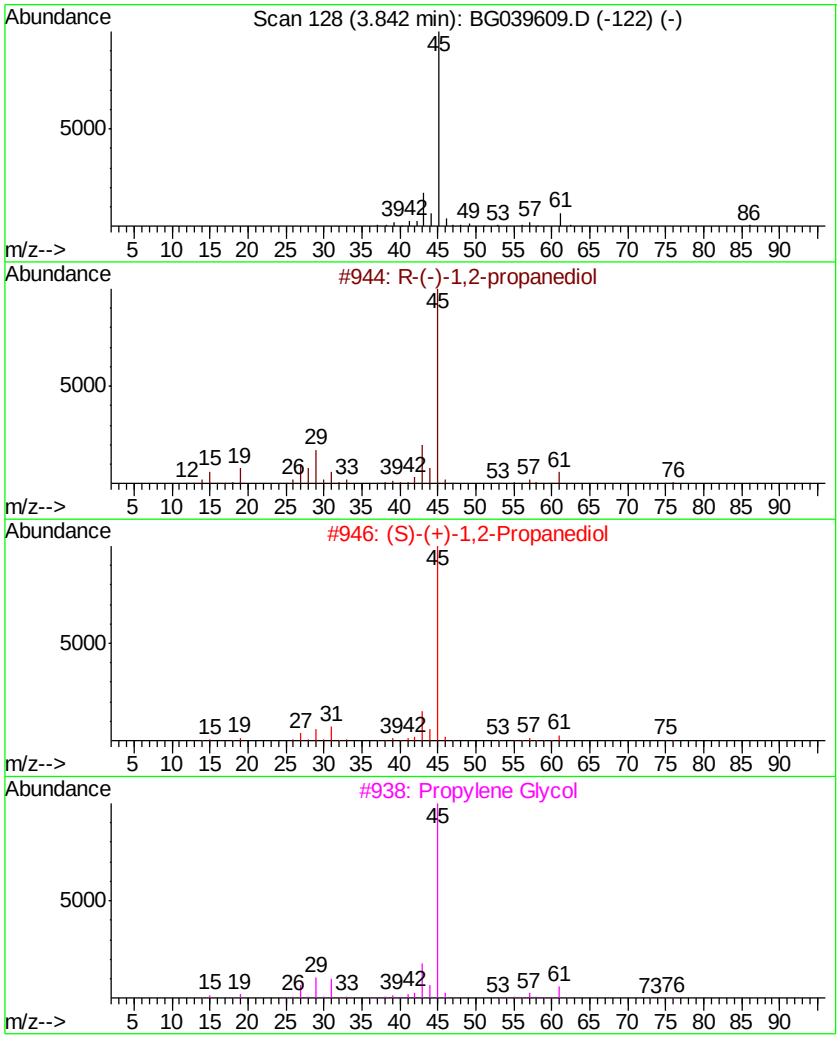
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

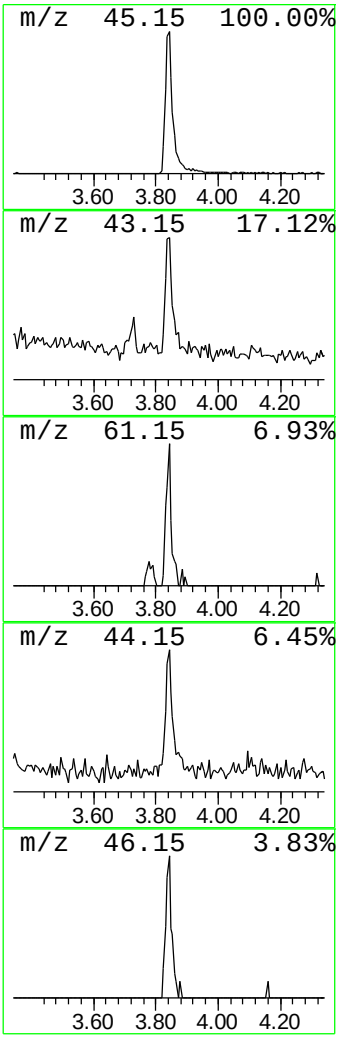
****

Peak Number 3 unknown3.84 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.84	5.17 ng	90109	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
3	Propylene Glycol	76	C3H8O2	000057-55-6	40
4	Methyltartronic acid	134	C4H6O5	000595-98-2	9
5	Formamide	45	CH3NO	000075-12-7	7





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-MH-C02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

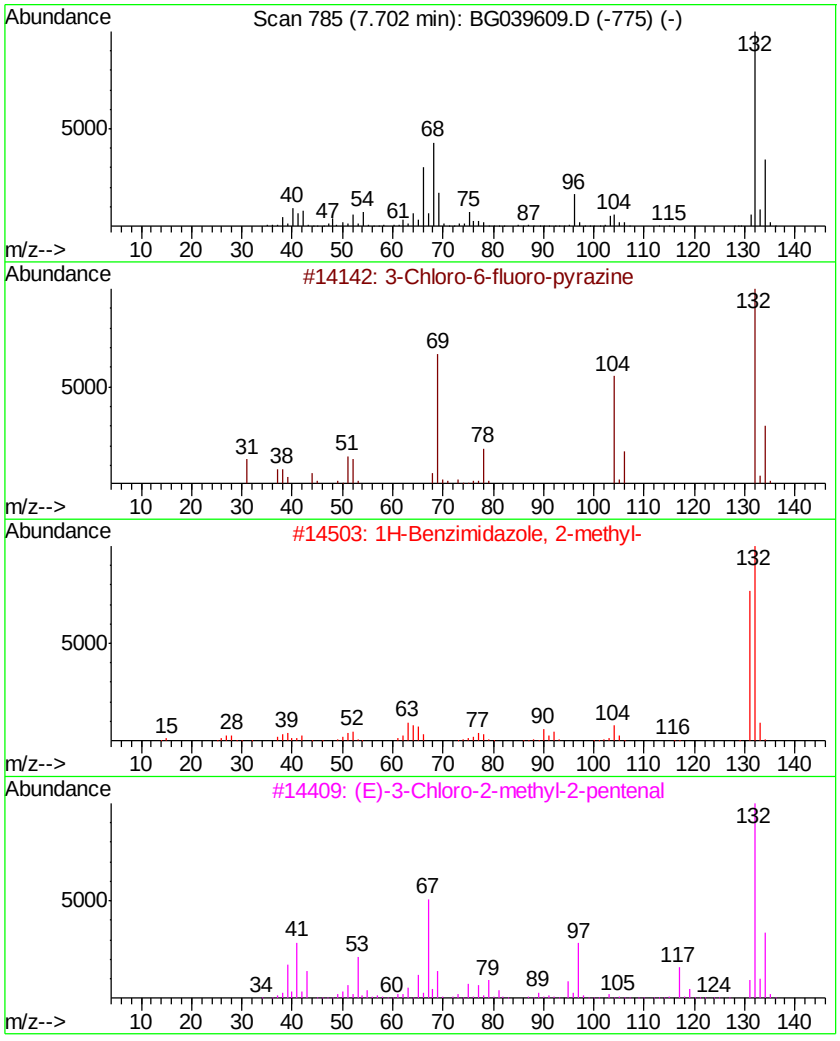
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

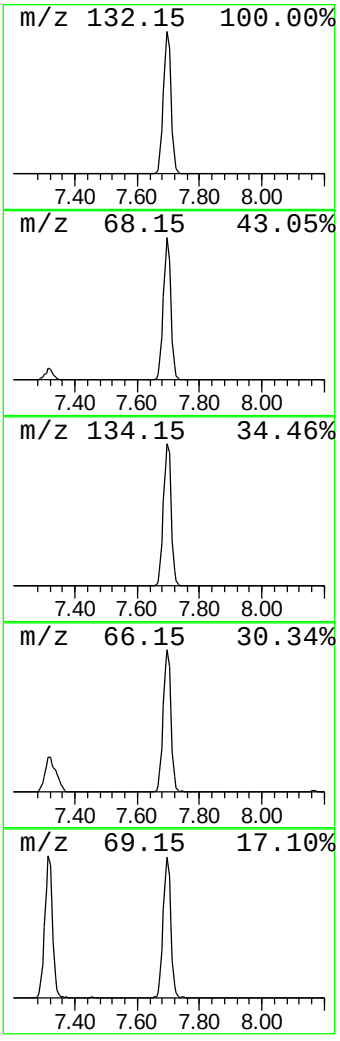
****

Peak Number 4 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	116.40 ng	2030630	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-MH-C02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

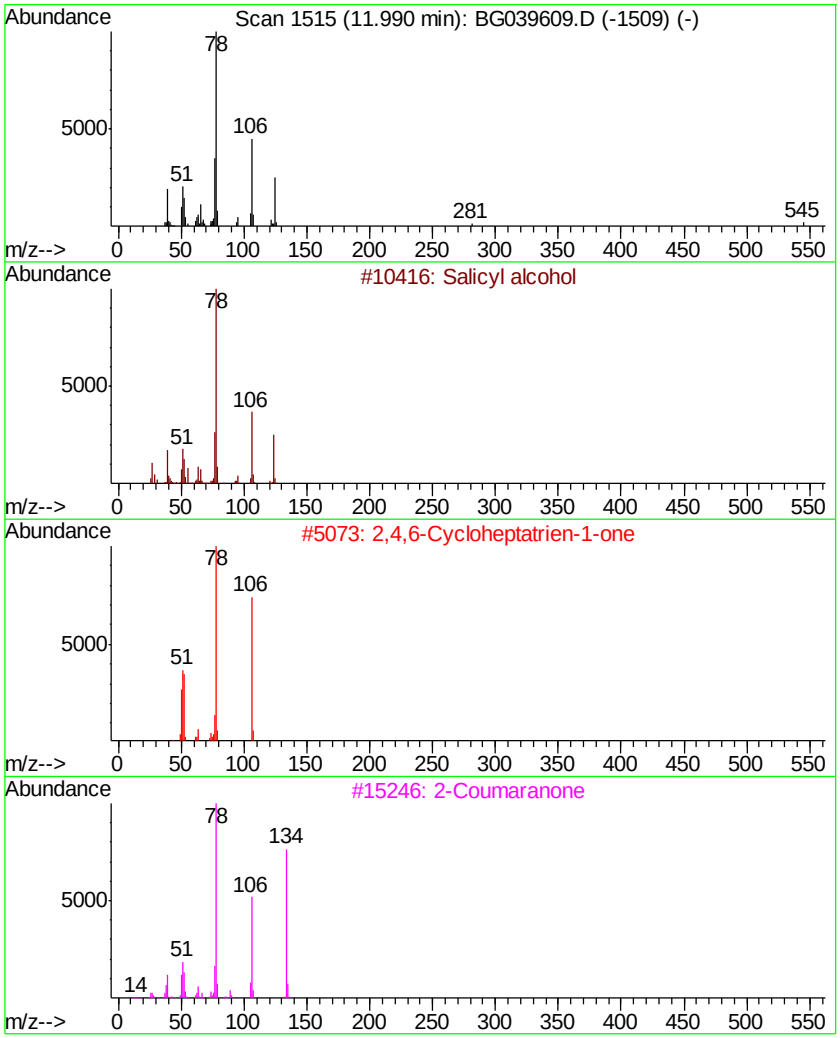
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

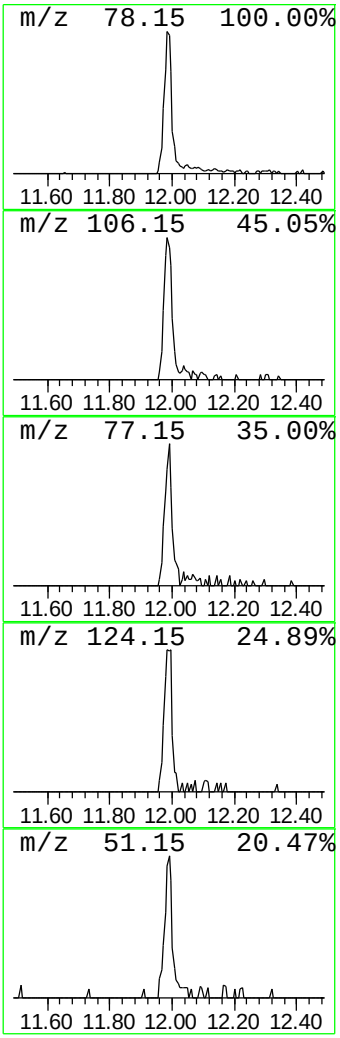
****

Peak Number 6 Salicyl alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.84 ng	71775	Naphthalene-d8	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Salicyl alcohol	124	C7H8O2	000090-01-7	91
2	2,4,6-Cycloheptatrien-1-one	106	C7H6O	000539-80-0	87
3	2-Coumaranone	134	C8H6O2	000553-86-6	78
4	Benzenemethanesulfonic acid, 2-h...	170	C7H6O3S	010284-44-3	72
5	Phenylphosphonous acid	142	C6H7O2P	001779-48-2	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-MH-C02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

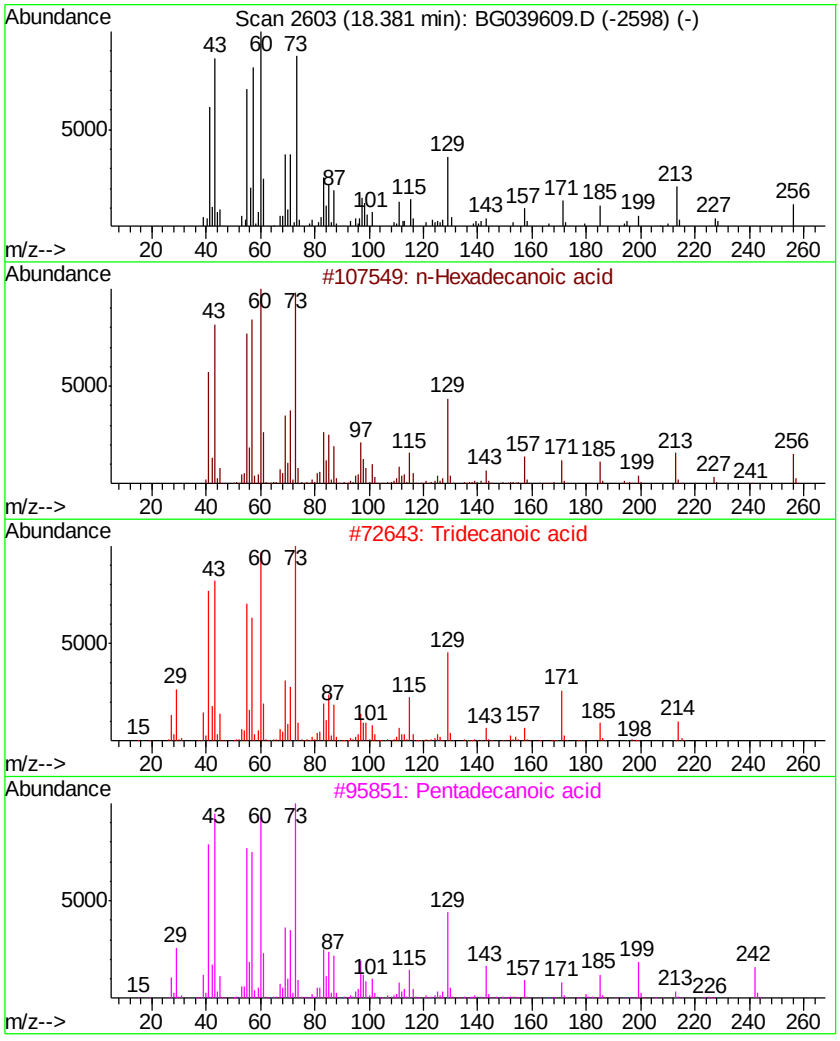
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

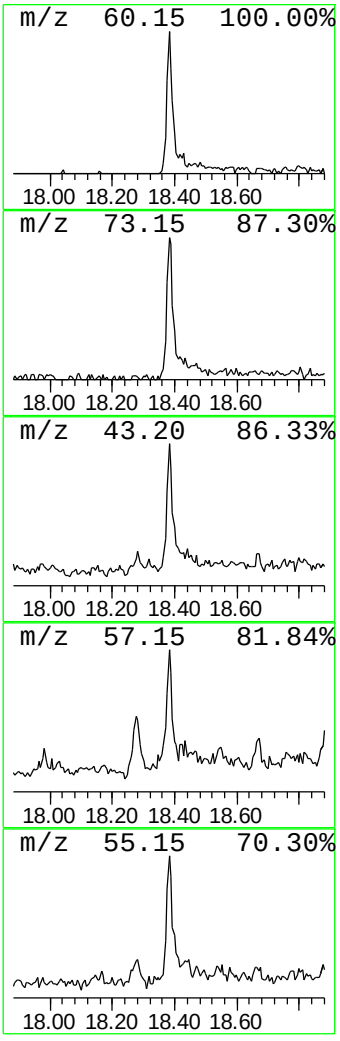
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	2.75 ng	138382	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-MH-C02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

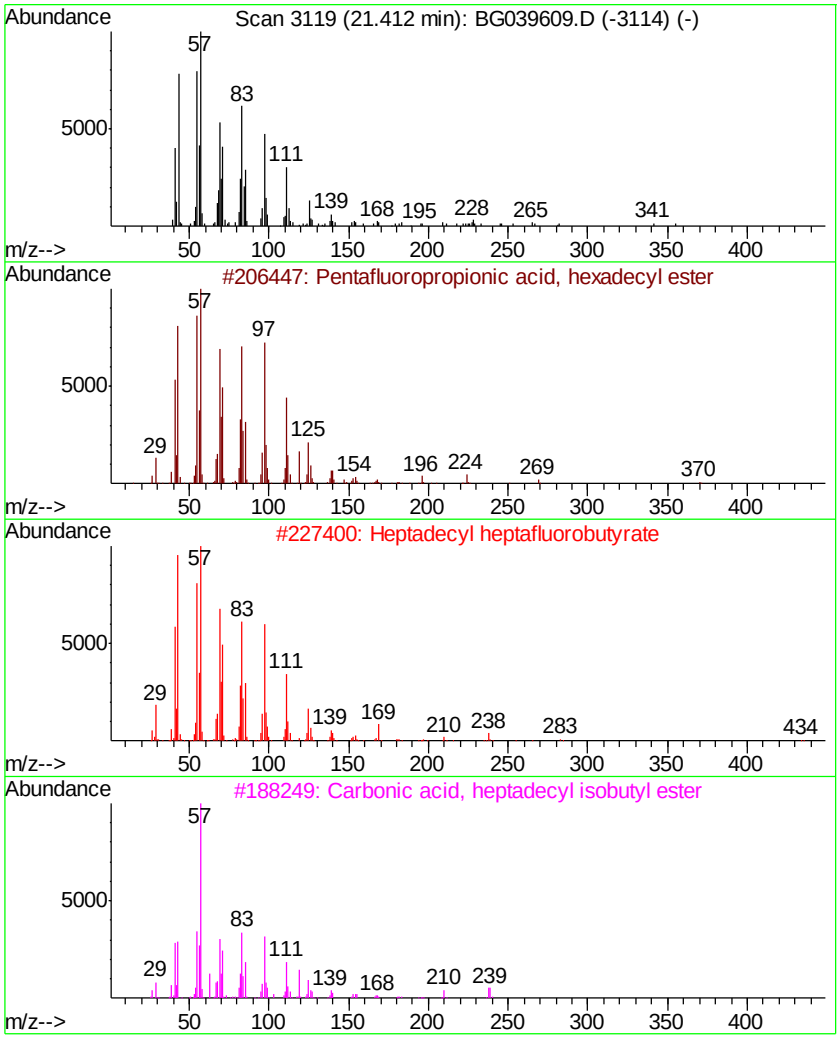
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

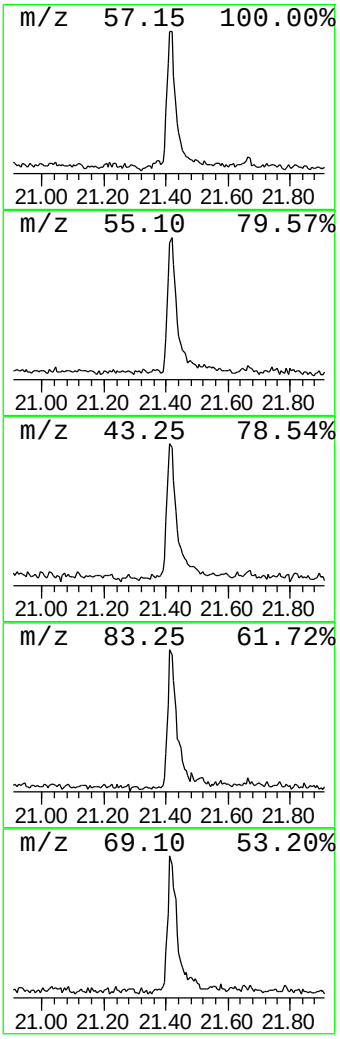
****

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	4.56 ng	264174	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-MH-C02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

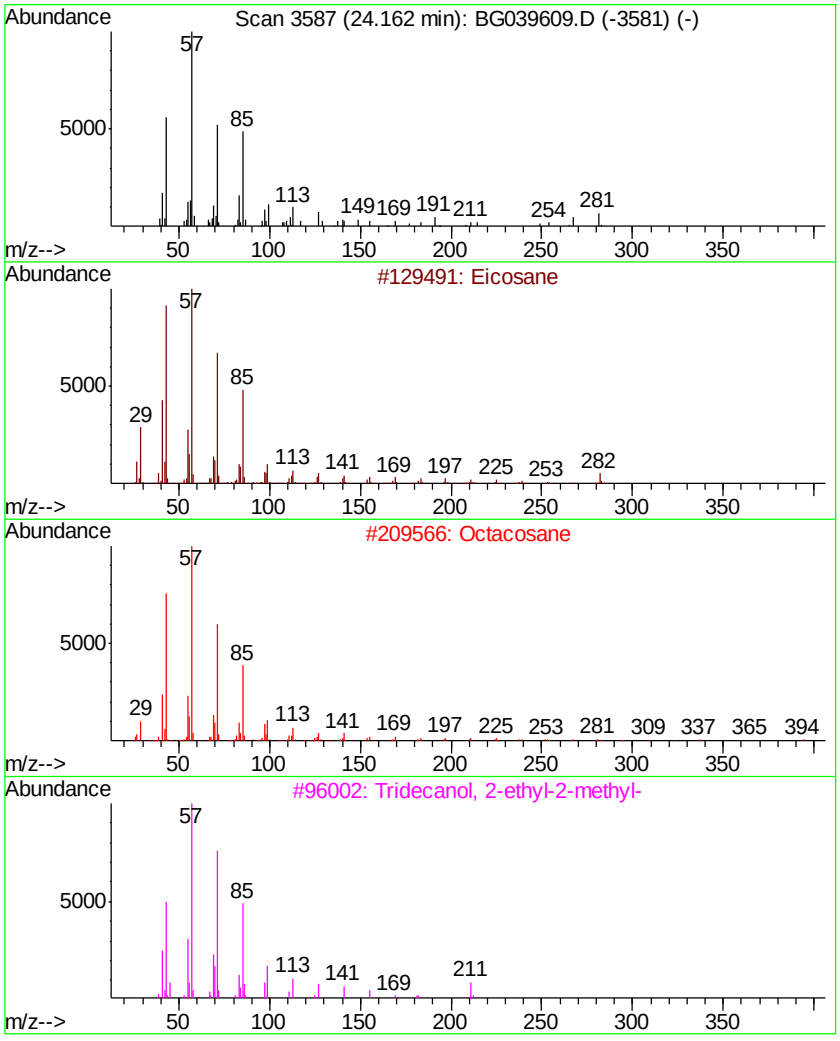
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

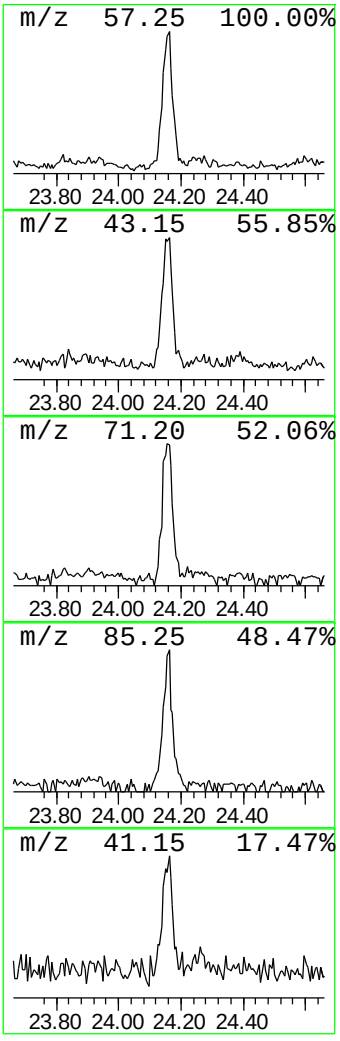
****

Peak Number 9 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.16	2.61 ng	148035	Perylene-d12	25.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Octacosane	394	C28H58	000630-02-4	83
3	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	83
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG022619\
Data File : BG039609.D
Acq On : 26 Feb 2019 20:39
Operator : JU/SJ
Sample : K1595-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-MH-C02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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...	3.30	5.7	ng	98833	1	8.17	348905	20.0
unknown3.84	3.84	5.2	ng	90109	1	8.17	348905	20.0
unknown7.70	7.70	116.4	ng	2030630	1	8.17	348905	20.0
Salicyl alcohol	11.99	2.8	ng	71775	2	10.99	505595	20.0
n-Hexadecanoic acid	18.38	2.8	ng	138382	4	17.54	1006000	20.0
Pentafluoropropio...	21.41	4.6	ng	264174	5	21.82	1157470	20.0
Eicosane	24.16	2.6	ng	148035	6	25.20	1135850	20.0