LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

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-BG071519.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	3.202	14	19	33	rVB	235125	470733	7.68%	1.067%
2	5.611	422	429	446	rVB	1287459	2074215	33.85%	4.704%
3	7.198	691	699	712	rBV	1349979	2339319	38.18%	5.305%
4	7.580	755	764	777	rBV	1287597	2241091	36.58%	5.082%
5	8.050	836	844	852	rBV	387541	684173	11.17%	1.551%
6	8.373	891	899	910	rVB	993074	1732761	28.28%	3.929%
7	9.201	1032	1040	1052	rBV	778465	1394639	22.76%	3.162%
8	10.852	1313	1321	1328	rBV	535921	957738	15.63%	2.172%
9	13.290	1729	1736	1746	rBV	2083810	3293793	53.76%	7.469%
10	13.561	1777	1782	1788	rBV2	46370	75220	1.23%	0.171%
11	14.007	1851	1858	1865	rVB	1568428	2251595	36.75%	5.106%
12	14.107	1865	1875	1888	rVB	267010	515669	8.42%	1.169%
13	14.389	1916	1923	1928	rBV2	38715	61422	1.00%	0.139%
14	14.513	1937	1944	1949	rBV3	38341	63929	1.04%	0.145%
15	14.665	1956	1970	1976	rBV2	796051	1717049	28.03%	3.894%
16	14.742	1976	1983	1986	rBV	45378	74452	1.22%	0.169%
17	14.924	2008	2014	2020	rBV	151769	226878	3.70%	0.514%
18	15.000	2020	2027	2034	rVB3	93544	173128	2.83%	0.393%
19	15.394	2088	2094	2100	rBV	509728	717714	11.71%	1.627%
20	15.658	2133	2139	2144	rBV4	42736	64601	1.05%	0.146%
21	15.999	2186	2197	2201	rBV3	70135	146575	2.39%	0.332%
22	16.040	2201	2204	2212	rVV2	72511	114198	1.86%	0.259%
23	16.140	2212	2221	2232	rVV	1950414	3090645	50.44%	7.008%
24	16.228	2232	2236	2244	rVB5	42628	80046	1.31%	0.182%
25	17.397	2425	2435	2447	rBV2	1123001	1774294	28.96%	4.023%
26	18.291	2581	2587	2603	rBV2	166130	360832	5.89%	0.818%
27	19.554	2798	2802	2813	rBV	61398	142822	2.33%	0.324%
28	20.000	2872	2878	2885	rBV	3707474	4780615	78.03%	10.841%
29	20.312	2926	2931	2938	rBV4	69981	139900	2.28%	0.317%
30	20.588	2974	2978	2982	rBV	85994	99282	1.62%	0.225%
31	20.688	2991	2995	3003	rBV4	44376	70448	1.15%	0.160%
32	20.952	3036	3040	3044	rBV	65062	82315	1.34%	0.187%
33	21.122	3062	3069	3083	rVB	4682427	6126812	100.00%	13.893%
34	21.322	3097	3103	3127	rBV2	140015	554719	9.05%	1.258%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

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-BG071519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.645	3152	3158	3169	rVB2	1228817	2006329	32.75%	4.550%
36	22.480	3295	3300	3302	rBV4	71499	120936	1.97%	0.274%
37	23.167	3413	3417	3426	rVB2	70040	147042	2.40%	0.333%
38	23.361	3444	3450	3457	rVB	140500	280407	4.58%	0.636%
39	23.984	3549	3556	3565	rBV	106321	244764	3.99%	0.555%
40	24.836	3691	3701	3711	rBV2	730309	2034252	33.20%	4.613%
41	24.936	3713	3718	3727	rVB3	60489	143420	2.34%	0.325%
42	26.075	3904	3912	3928	rVB	148548	428539	6.99%	0.972%

Sum of corrected areas: 44099311

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
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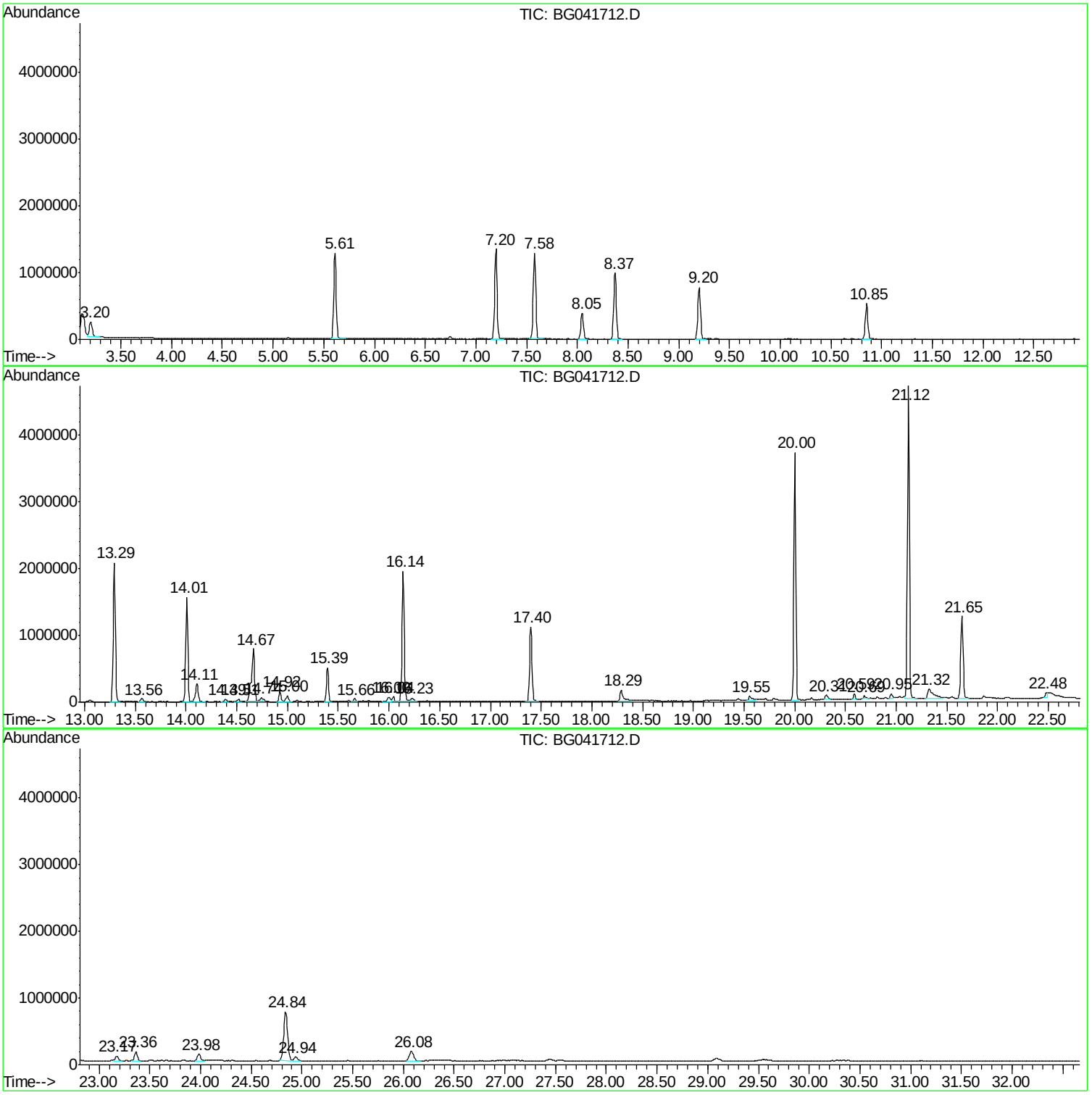
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

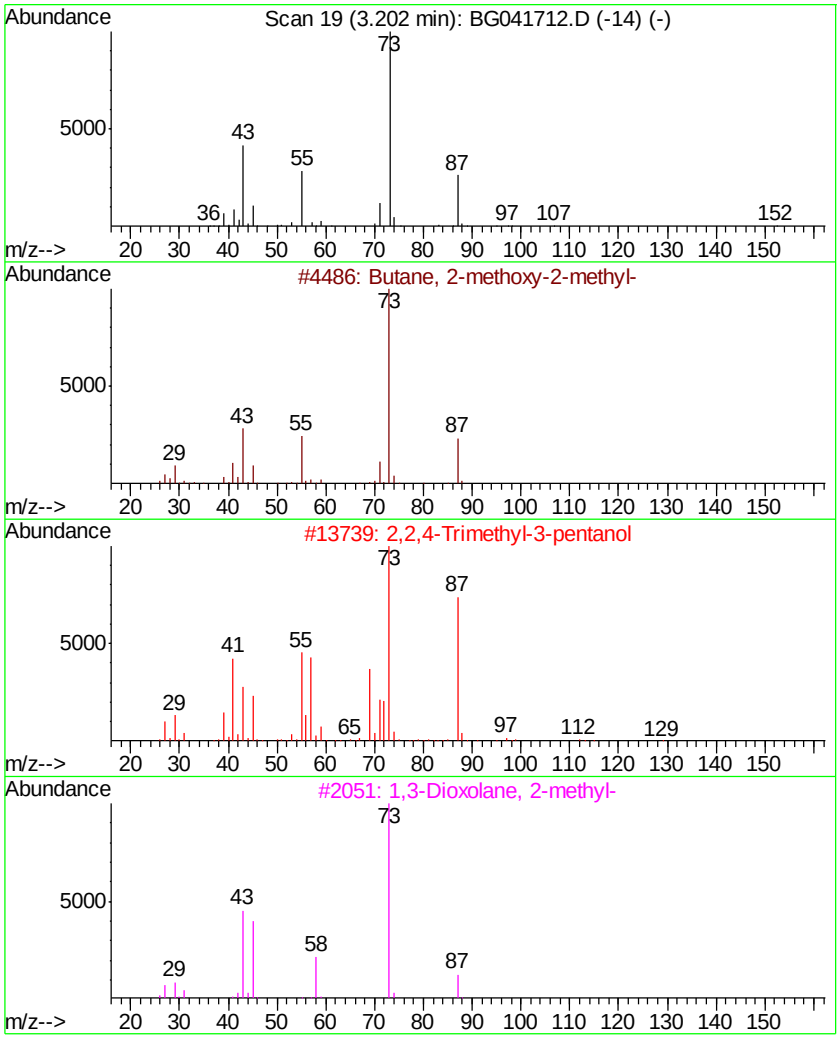
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

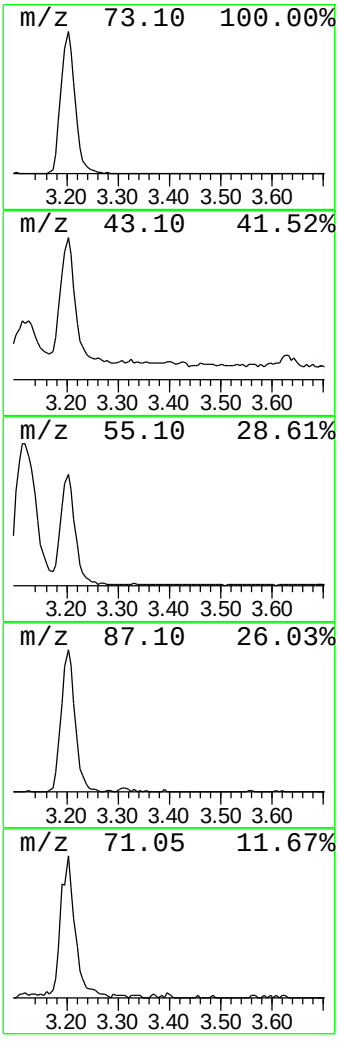
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	13.76 ng	470733	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	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

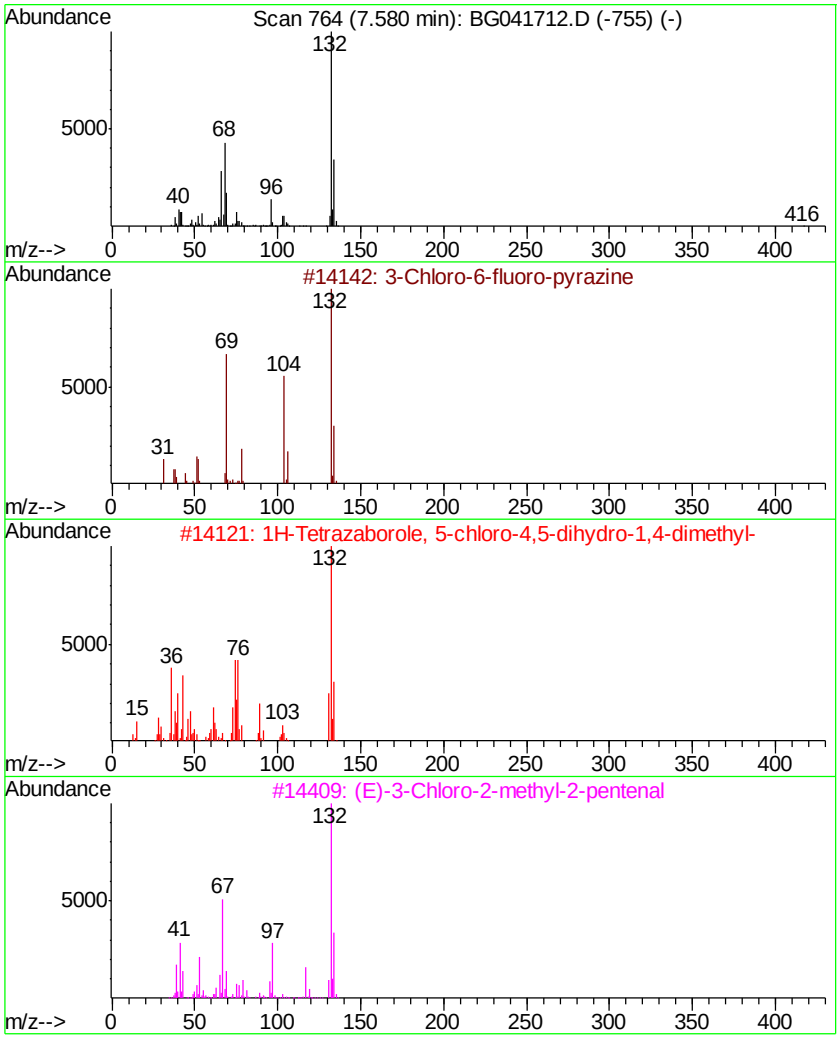
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

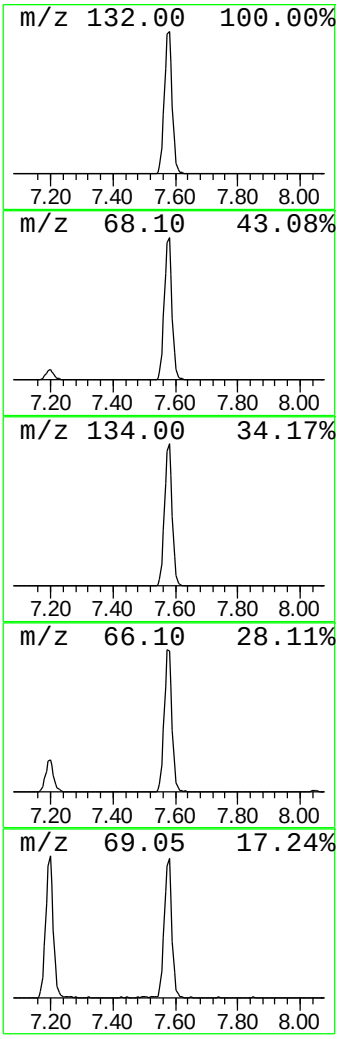
****

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	65.51 ng	2241090	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	1H-Tetrazaborole, 5-chloro-4,5-d...	132	C2H6BClN4	021960-49-6	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Amphetaminil	250	C17H18N2	017590-01-1	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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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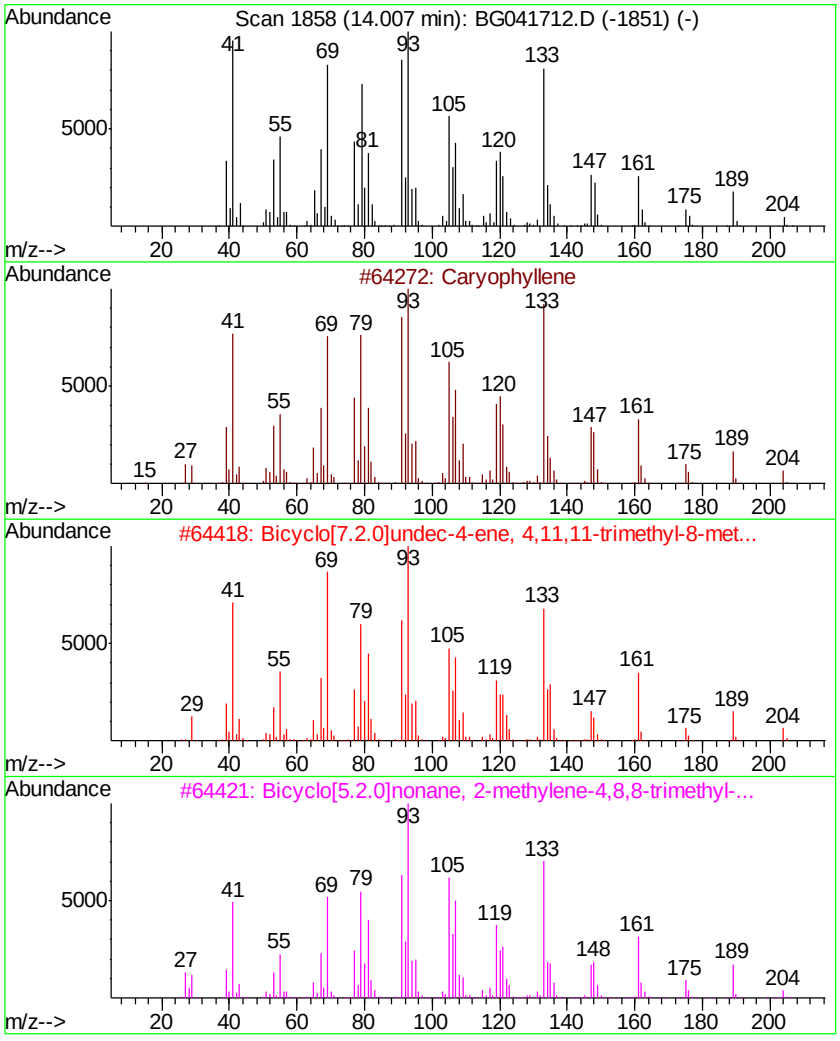
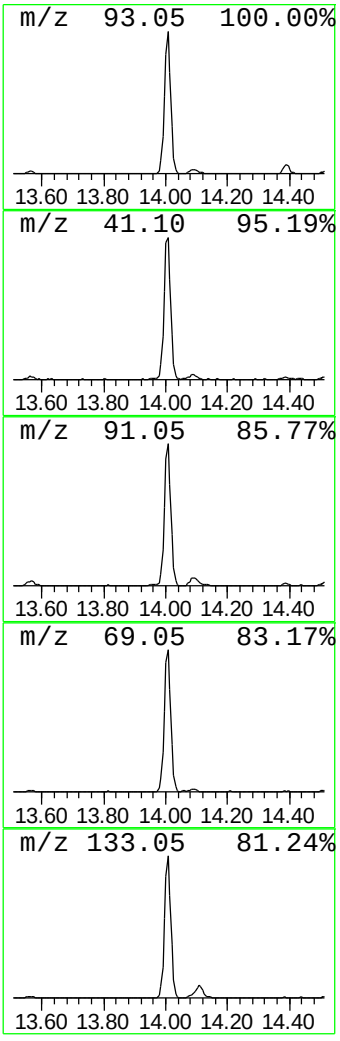
Peak Number 4 Caryophyllene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	26.23 ng	2251600	Acenaphthene-d10	14.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	99
2	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	93
3	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	93
4	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
5	1S,2S,5R-1,4,4-Trimethyltricyclo...	204	C15H24	1000140-07-5	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

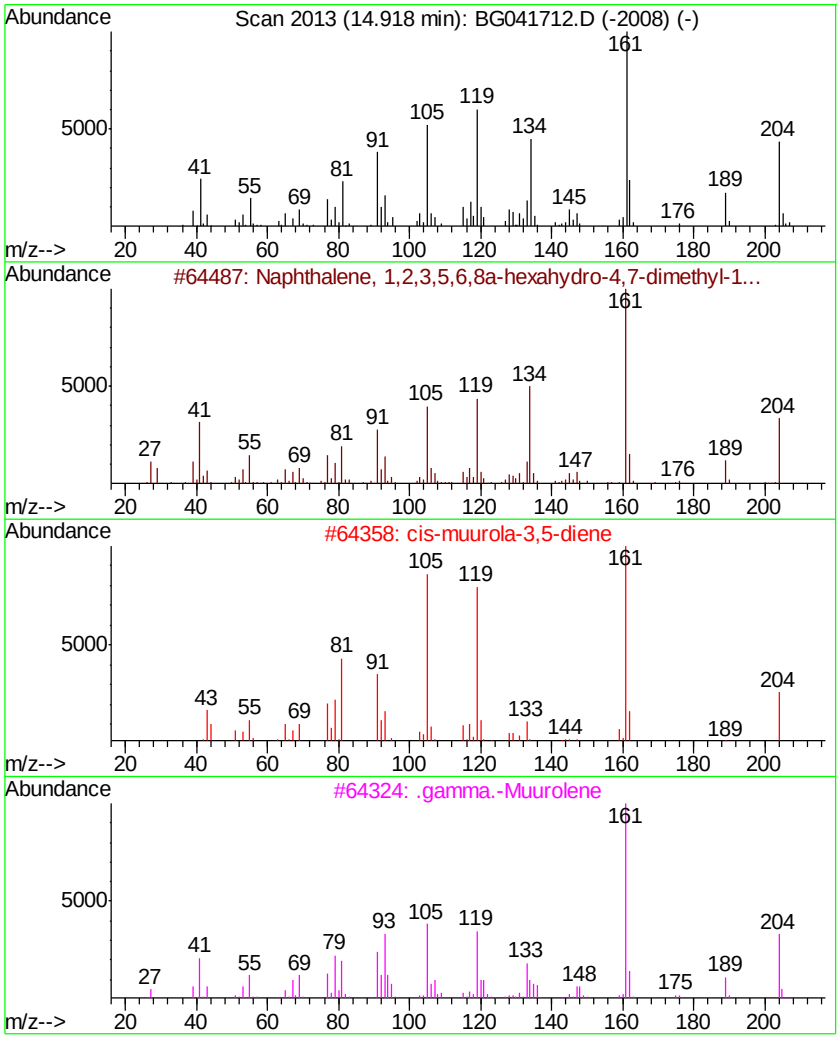
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

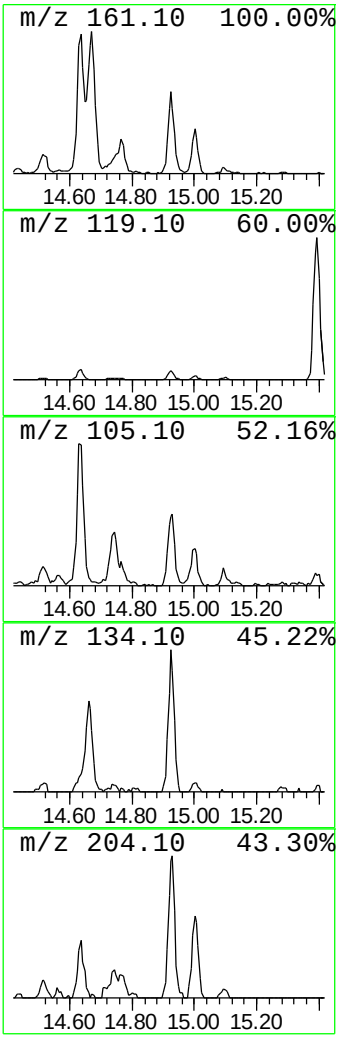
****

Peak Number 5 Naphthalene, 1,2,3,5,6,8a-h... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	2.64 ng	226878	Acenaphthene-d10	14.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	98
2	cis-muurola-3,5-diene	204	C15H24	1000365-95-4	70
3	.gamma.-Muurolene	204	C15H24	030021-74-0	70
4	.alpha.-Cubebene	204	C15H24	017699-14-8	70
5	Isoledene	204	C15H24	1000156-10-8	68





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

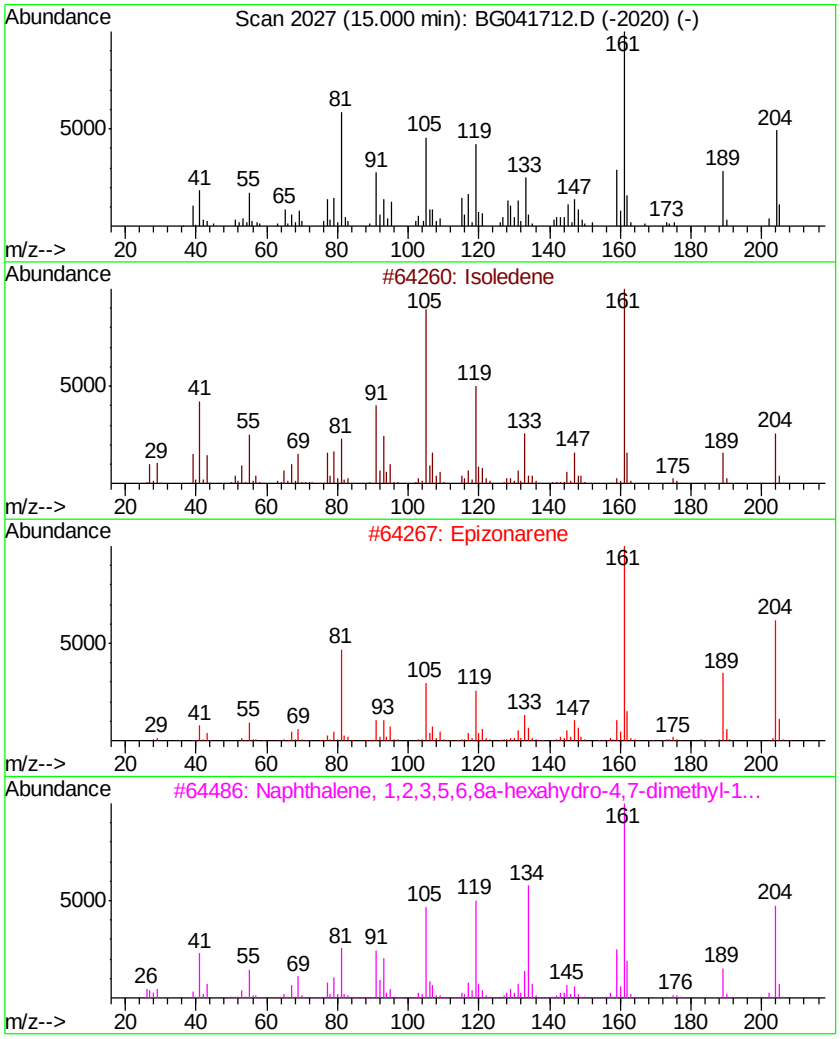
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

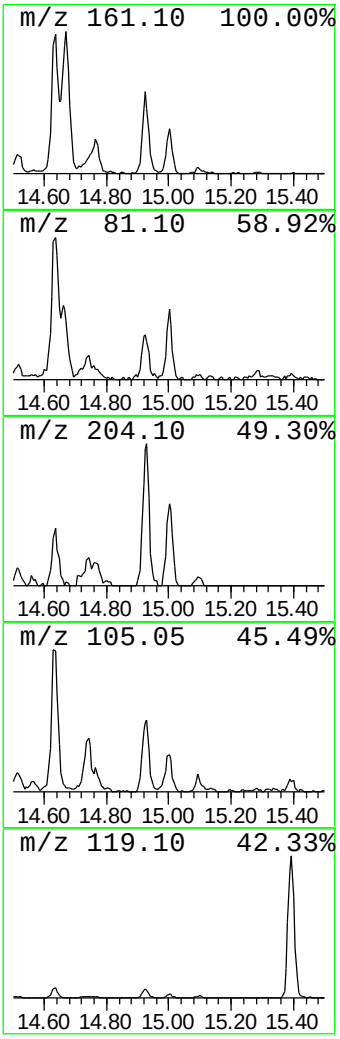
****

Peak Number 6 Isoledene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.02 ng	173128	Acenaphthene-d10	14.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoledene	204	C15H24	1000156-10-8	93
2	Epizonarene	204	C15H24	041702-63-0	93
3	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	90
4	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	83
5	Cyclohexene, 6-ethenyl-6-methyl-...	204	C15H24	005951-67-7	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

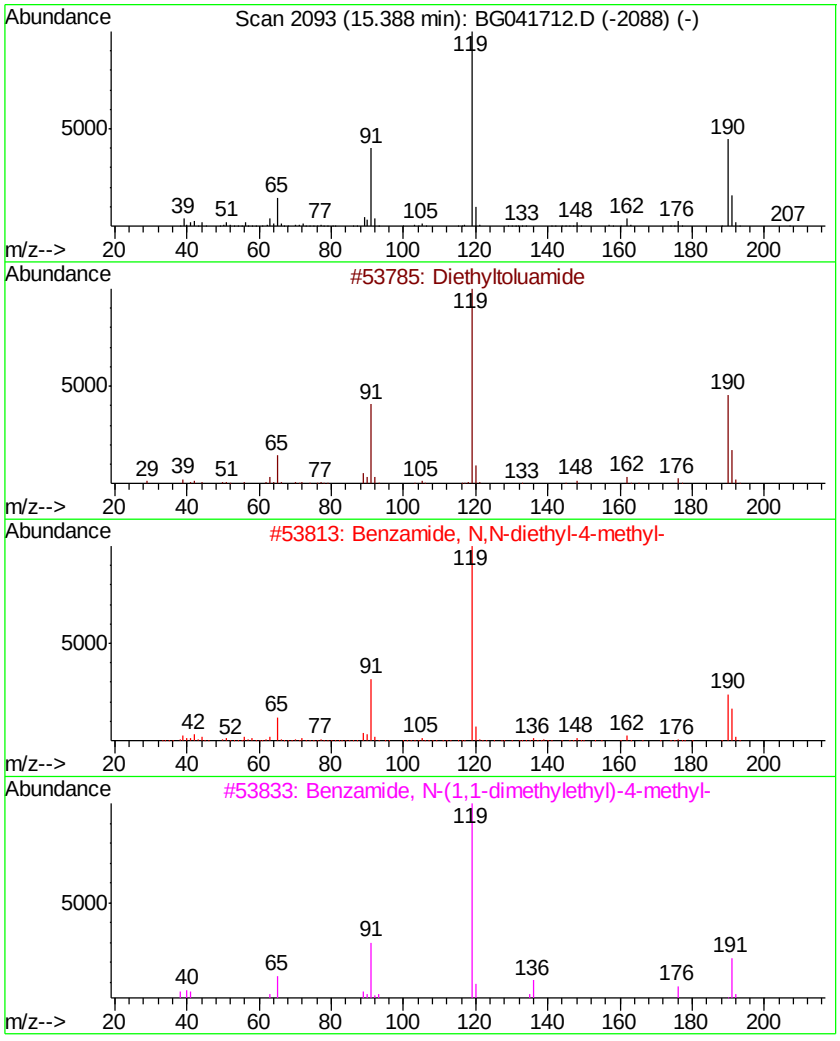
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

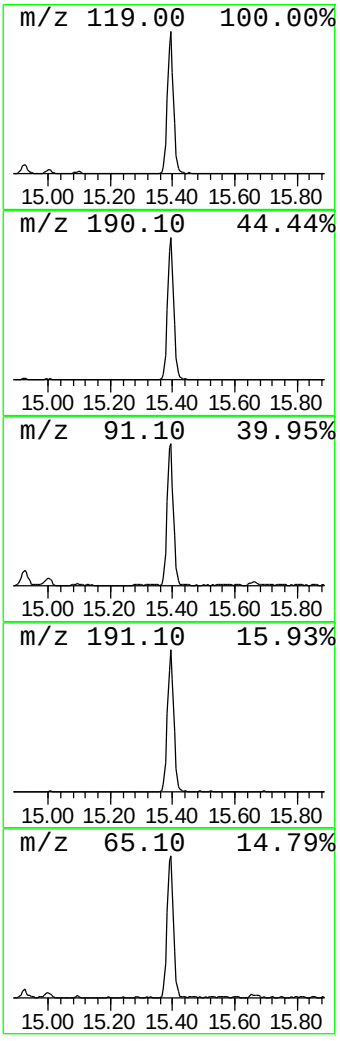
****

Peak Number 7 Diethyltoluamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	8.36 ng	717714	Acenaphthene-d10	14.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	96
2	Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	93
3	Benzamide, N-(1,1-dimethylethyl)...	191	C12H17NO	042498-32-8	58
4	N-Isopropyl-p-toluamide	177	C11H15NO	002144-17-4	50
5	Benzamide, N,N,3-trimethyl-	163	C10H13NO	006935-65-5	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

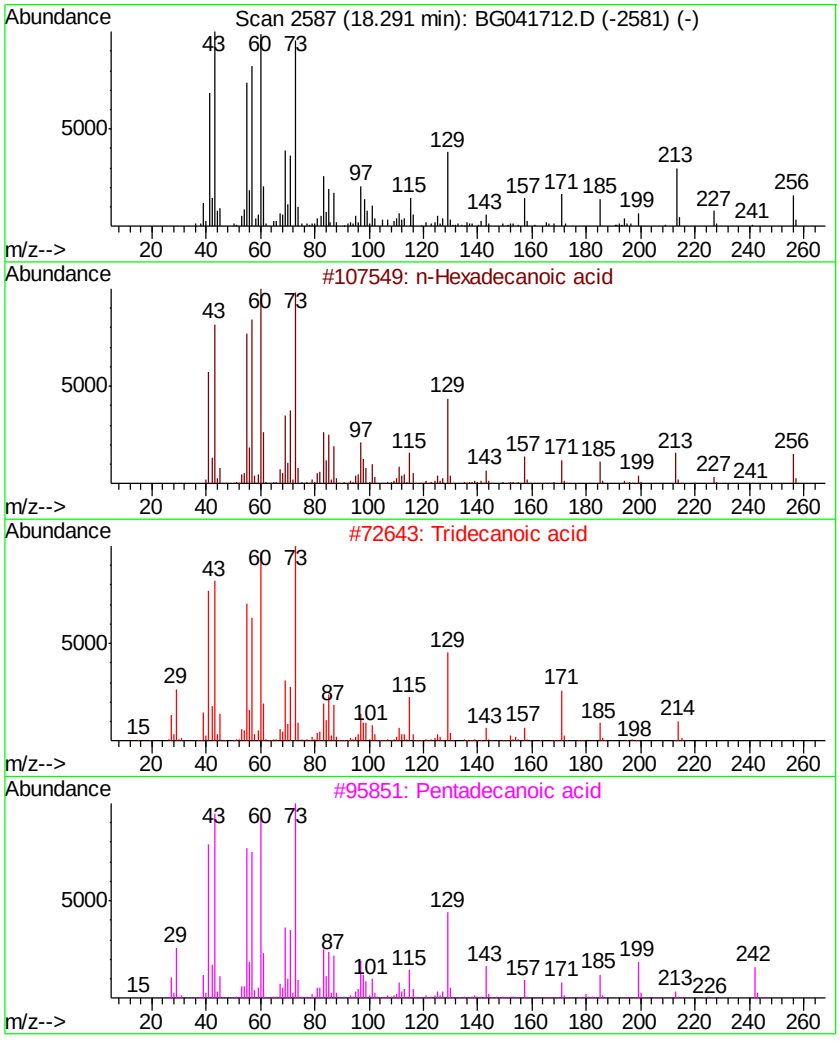
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

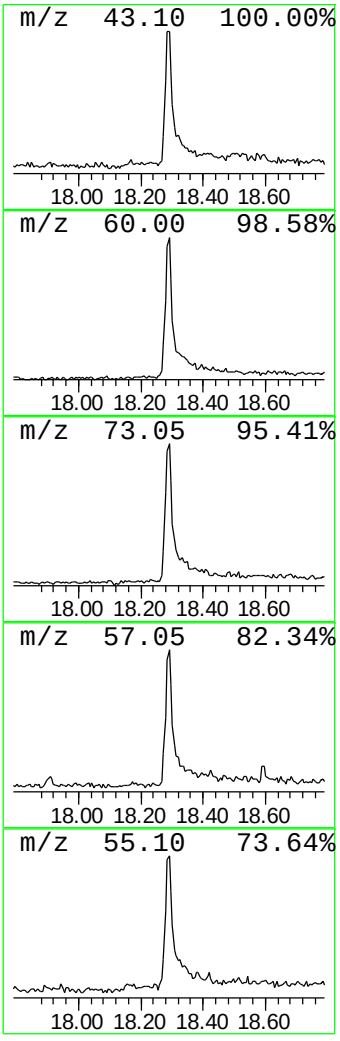
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	4.07 ng	360832	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

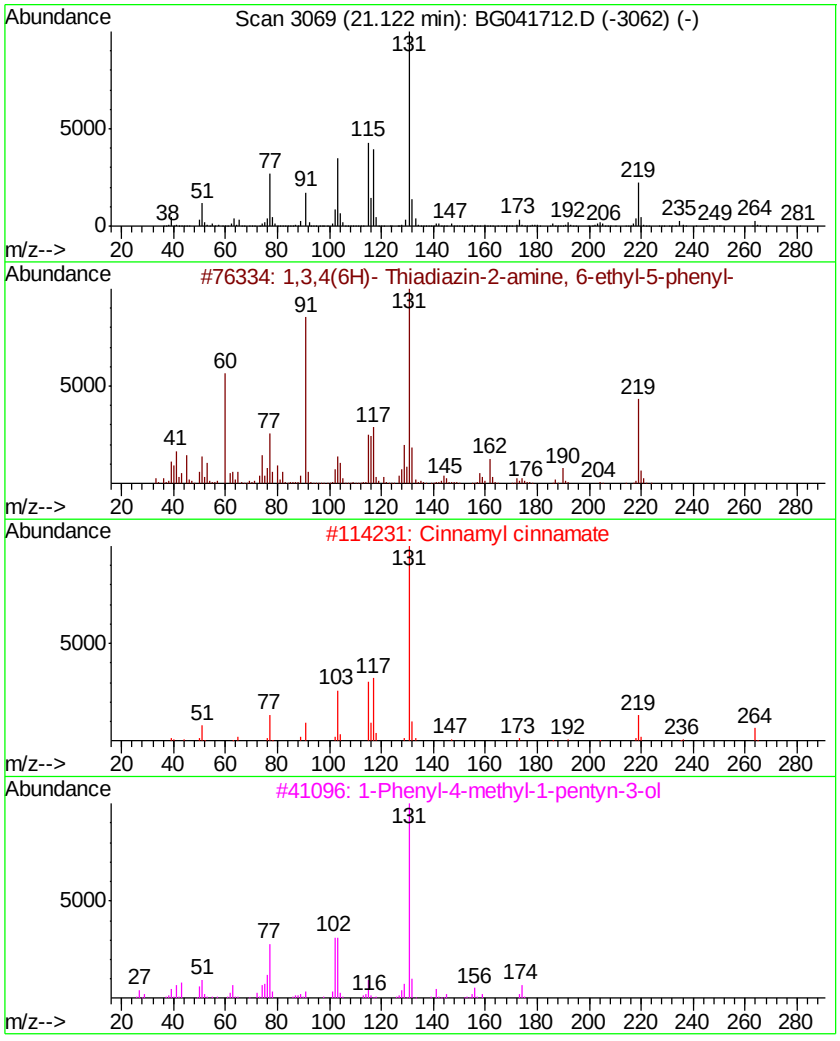
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

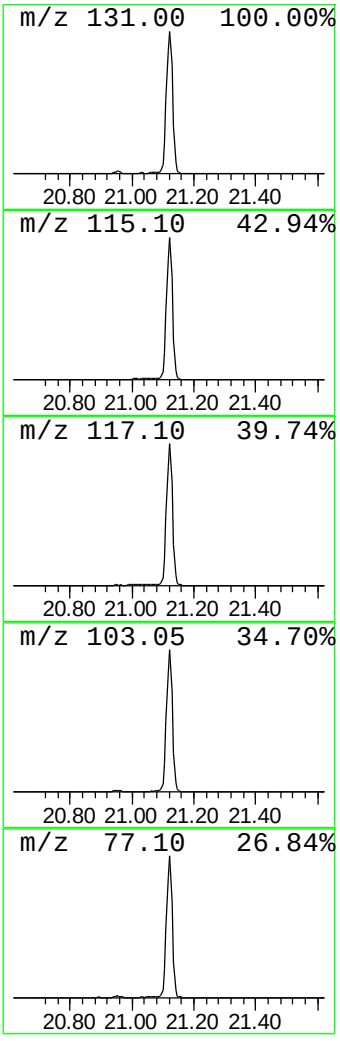
****

Peak Number 9 unknown21.12 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.12	61.07 ng	6126810	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,4(6H)- Thiadiazin-2-amine, 6...	219	C11H13N3S	054418-98-3	47
2	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	47
3	1-Phenyl-4-methyl-1-pentyn-3-ol	174	C12H14O	005923-02-4	43
4	Benzene, 1-(chloromethyl)-4-(2-p...	166	C10H11Cl	036875-10-2	40
5	1,3-Bis(cinnamoyloxymethyl)adama...	456	C30H32O4	303797-58-2	38





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Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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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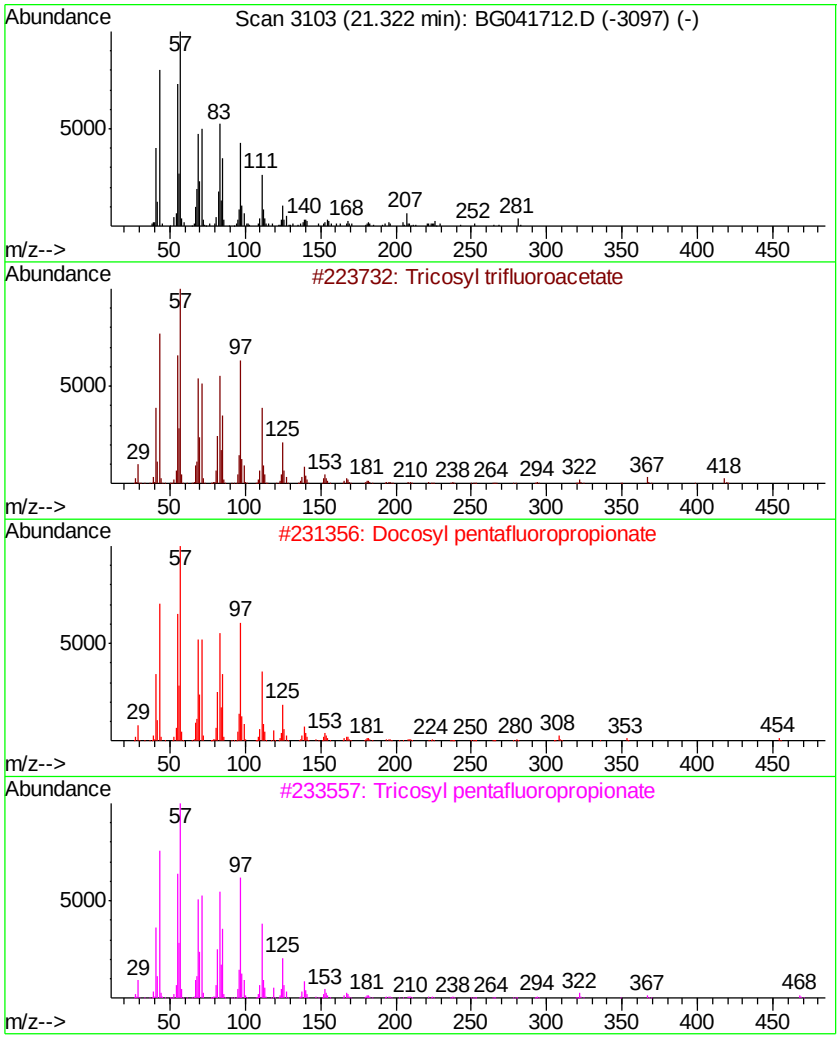
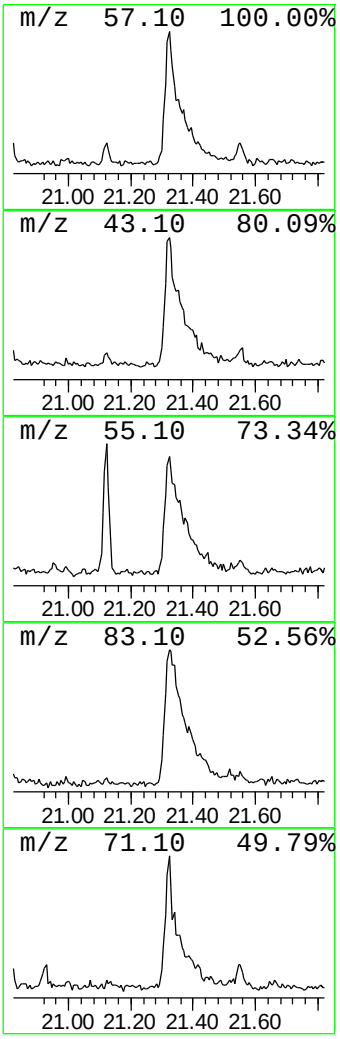
Peak Number 10 Tricosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	5.53 ng	554719	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
3	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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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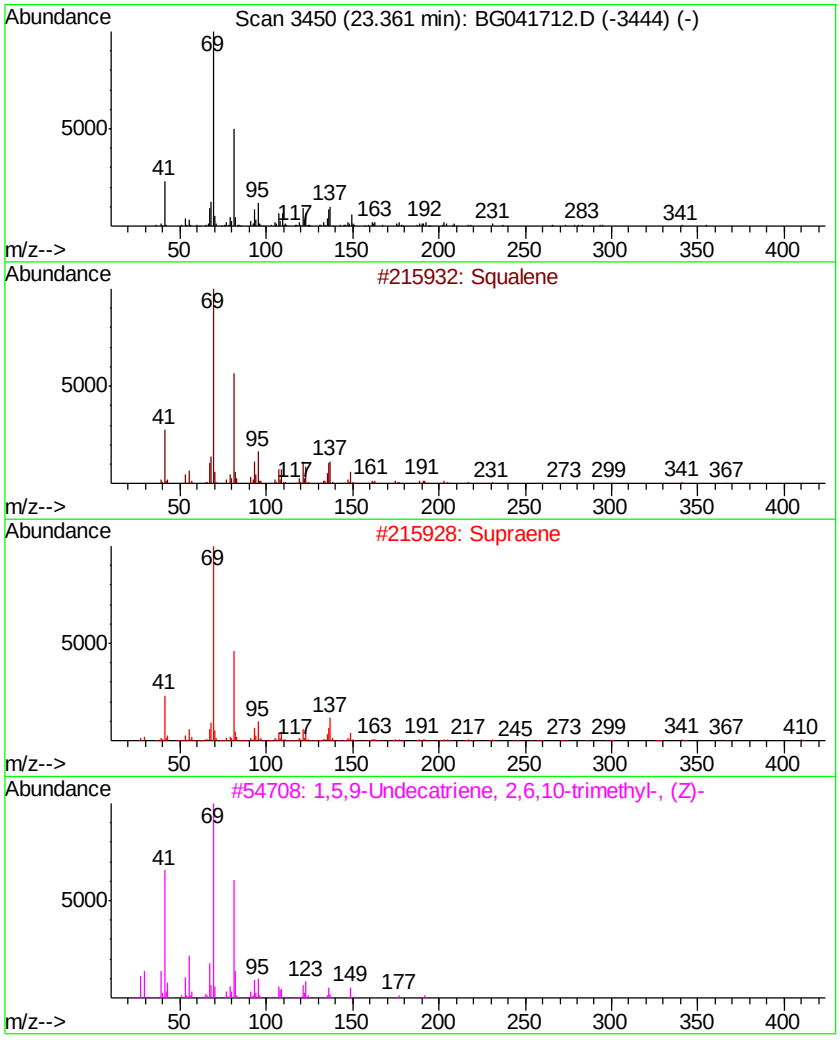
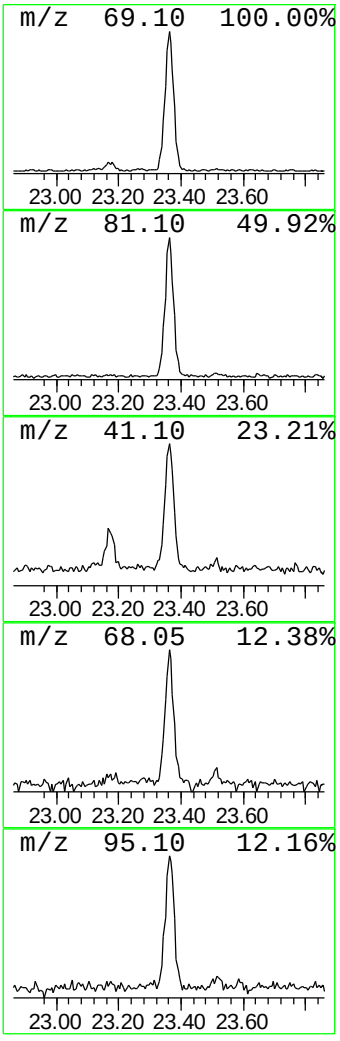
Peak Number 11 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.36	2.76 ng	280407	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
5	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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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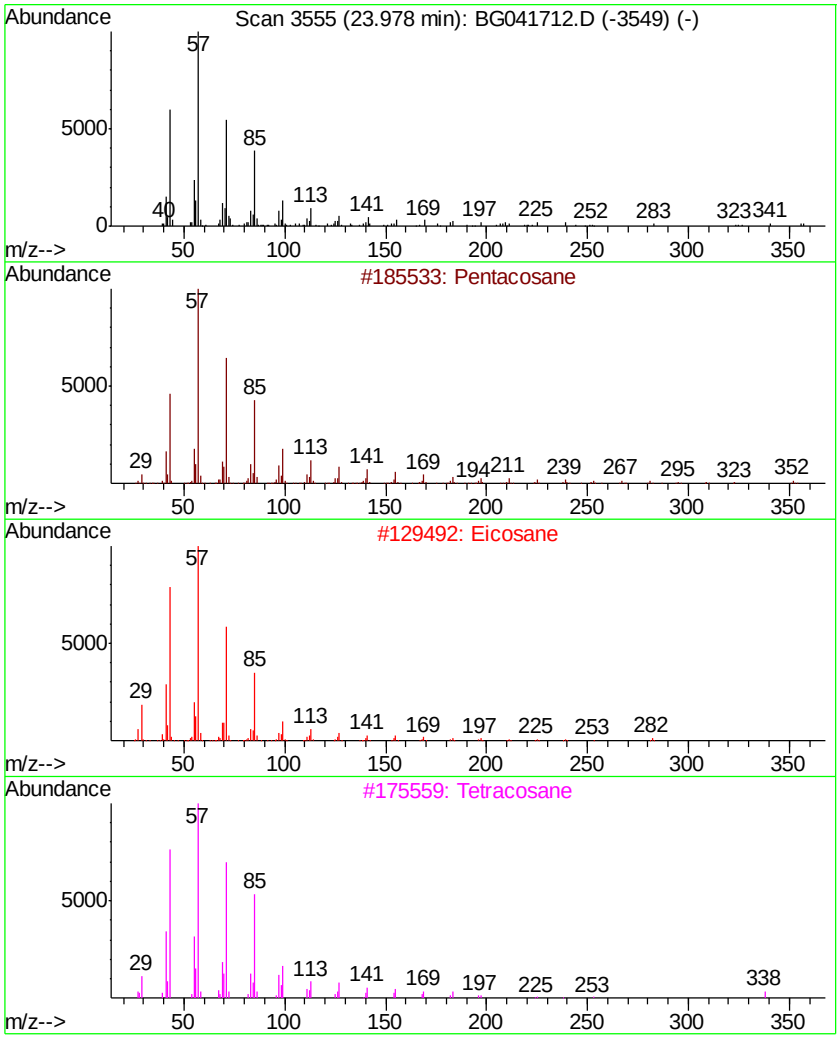
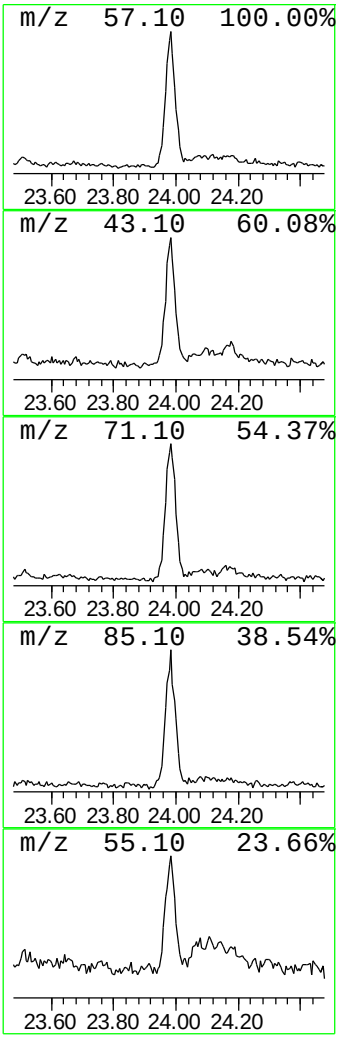
Peak Number 12 Pentacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.98	2.41 ng	244764	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	Nonadecane	268	C19H40	000629-92-5	89
5	Hexadecane	226	C16H34	000544-76-3	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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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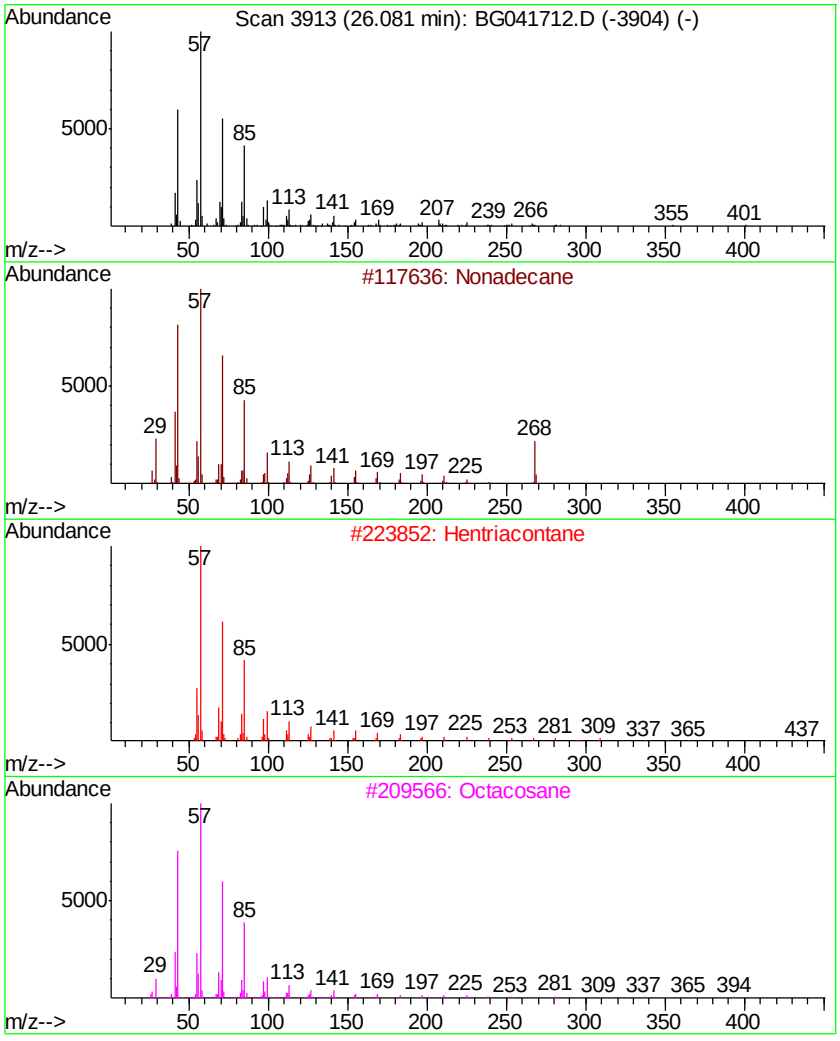
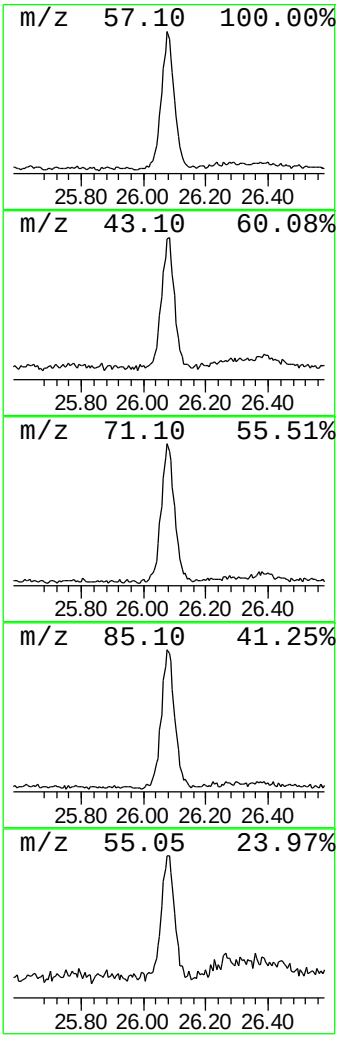
Peak Number 13 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.08	4.21 ng	428539	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Octacosane	394	C28H58	000630-02-4	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Hexacosane	366	C26H54	000630-01-3	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071819\
Data File : BG041712.D
Acq On : 18 Jul 2019 16:30
Operator : HP/JU
Sample : K3835-45
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-8(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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...	3.20	13.8	ng	470733	1	8.05	684173	20.0
unknown7.58	7.58	65.5	ng	2241090	1	8.05	684173	20.0
Caryophyllene	14.01	26.2	ng	2251600	3	14.67	1717050	20.0
Naphthalene, 1,2,...	14.92	2.6	ng	226878	3	14.67	1717050	20.0
Isoledene	15.00	2.0	ng	173128	3	14.67	1717050	20.0
Diethyltoluamide	15.39	8.4	ng	717714	3	14.67	1717050	20.0
n-Hexadecanoic acid	18.29	4.1	ng	360832	4	17.40	1774290	20.0
unknown21.12	21.12	61.1	ng	6126810	5	21.65	2006330	20.0
Tricosyl trifluor...	21.32	5.5	ng	554719	5	21.65	2006330	20.0
Squalene	23.36	2.8	ng	280407	6	24.84	2034250	20.0
Pentacosane	23.98	2.4	ng	244764	6	24.84	2034250	20.0
Nonadecane	26.08	4.2	ng	428539	6	24.84	2034250	20.0