LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

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-BG051520.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	5.058	330	335	342	rBV2	32408	54022	1.14%	0.154%
2	5.558	413	420	435	rBV	1034265	1784808	37.71%	5.084%
3	6.644	599	605	616	rVB	335308	579625	12.25%	1.651%
4	7.173	687	695	708	rBV	1175697	2066752	43.67%	5.888%
5	7.960	822	829	837	rBV	383140	663642	14.02%	1.891%
6	8.283	876	884	893	rBV	1097665	1911284	40.38%	5.445%
7	9.123	1018	1027	1036	rBV	799229	1507200	31.84%	4.294%
8	10.081	1182	1190	1198	rBV4	33458	66530	1.41%	0.190%
9	10.768	1299	1307	1315	rBV	516777	948404	20.04%	2.702%
10	13.224	1716	1725	1735	rBV	2386190	3732563	78.86%	10.633%
11	13.758	1811	1816	1822	rBV4	32869	56014	1.18%	0.160%
12	13.882	1826	1837	1841	rVV2	119113	199250	4.21%	0.568%
13	13.929	1841	1845	1851	rVB4	43674	76021	1.61%	0.217%
14	14.052	1858	1866	1875	rBV	334387	515743	10.90%	1.469%
15	14.604	1951	1960	1967	rBV	854086	1405168	29.69%	4.003%
16	15.891	2173	2179	2185	rVB2	86802	127533	2.69%	0.363%
17	16.096	2205	2214	2228	rBV	1802753	2847944	60.17%	8.113%
18	17.353	2418	2428	2432	rBV	956723	1608552	33.99%	4.582%
19	17.389	2432	2434	2441	rVB	216464	299094	6.32%	0.852%
20	17.483	2446	2450	2457	rVB	40892	77256	1.63%	0.220%
21	18.423	2604	2610	2614	rBV2	62687	109338	2.31%	0.311%
22	19.210	2739	2744	2749	rVV4	60448	92495	1.95%	0.263%
23	19.280	2752	2756	2762	rVV5	34295	58838	1.24%	0.168%
24	19.345	2762	2767	2772	rVV	226959	334103	7.06%	0.952%
25	19.404	2772	2777	2782	rVB	455348	679252	14.35%	1.935%
26	19.762	2828	2838	2847	rBV	426986	834160	17.62%	2.376%
27	19.967	2867	2873	2885	rVB	3417340	4733066	100.00%	13.483%
28	20.103	2891	2896	2903	rVB3	97876	144472	3.05%	0.412%
29	20.255	2918	2922	2927	rVB2	75942	112580	2.38%	0.321%
30	20.355	2936	2939	2943	rBV	42596	58023	1.23%	0.165%
31	20.443	2951	2954	2961	rVB2	108077	151141	3.19%	0.431%
32	20.614	2977	2983	2986	rBV2	578150	820418	17.33%	2.337%
33	20.672	2986	2993	3006	rVB3	454686	1014491	21.43%	2.890%
34	21.266	3090	3094	3103	rVB4	218659	373394	7.89%	1.064%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

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-BG051520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.606	3144	3152	3157	rBV2	953311	1886302	39.85%	5.373%
36	21.653	3157	3160	3169	rVB	183163	308153	6.51%	0.878%
37	21.806	3183	3186	3191	rBV3	48184	77078	1.63%	0.220%
38	22.329	3270	3275	3281	rVB2	147595	272552	5.76%	0.776%
39	23.768	3513	3520	3527	rBV2	136275	417304	8.82%	1.189%
40	23.874	3535	3538	3543	rVB2	74302	122130	2.58%	0.348%
41	24.608	3657	3663	3673	rVB2	119626	316092	6.68%	0.900%
42	24.761	3679	3689	3706	rBV2	525802	1661073	35.10%	4.732%

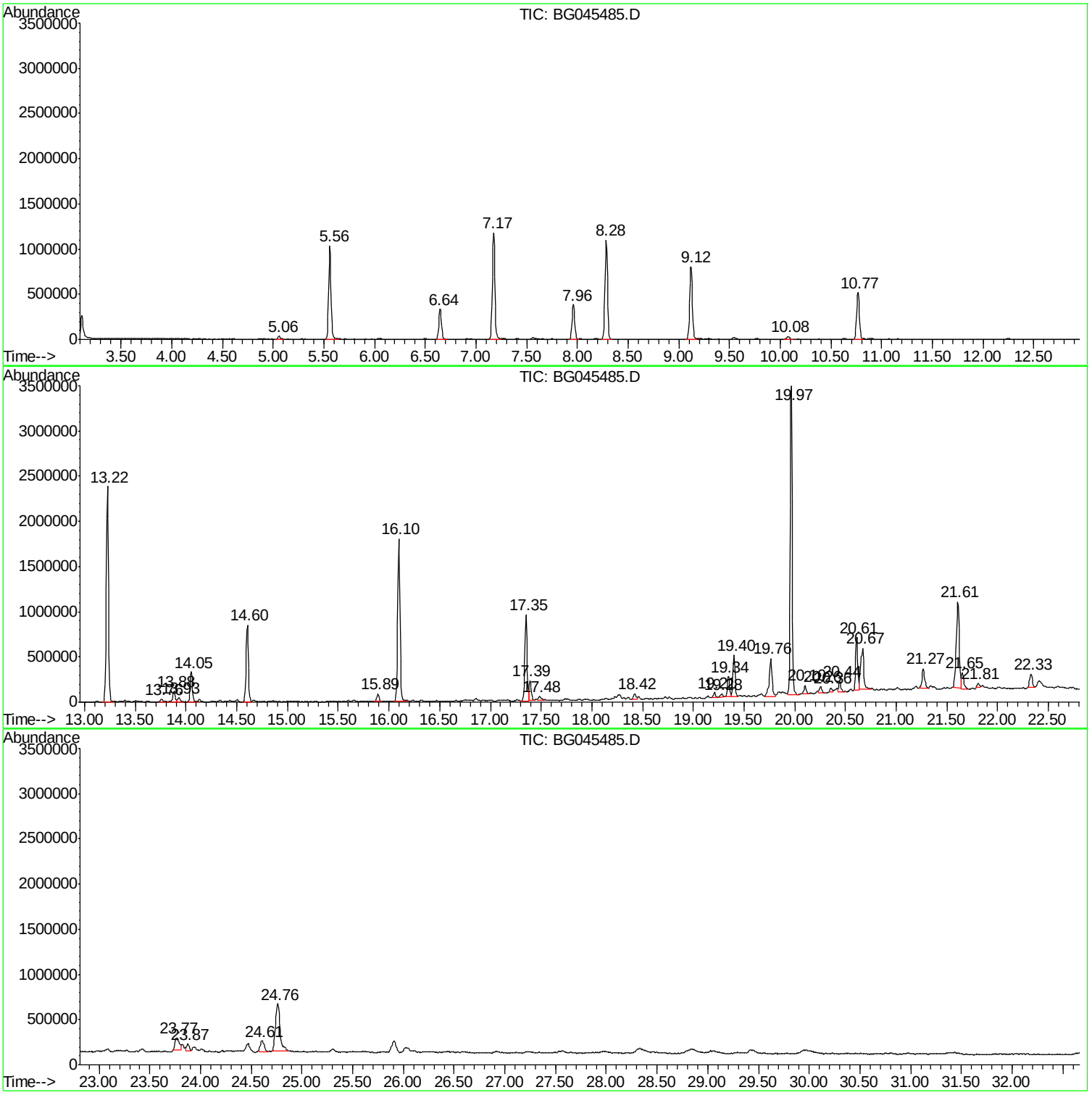
Sum of corrected areas: 35103860

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NMDUP03-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

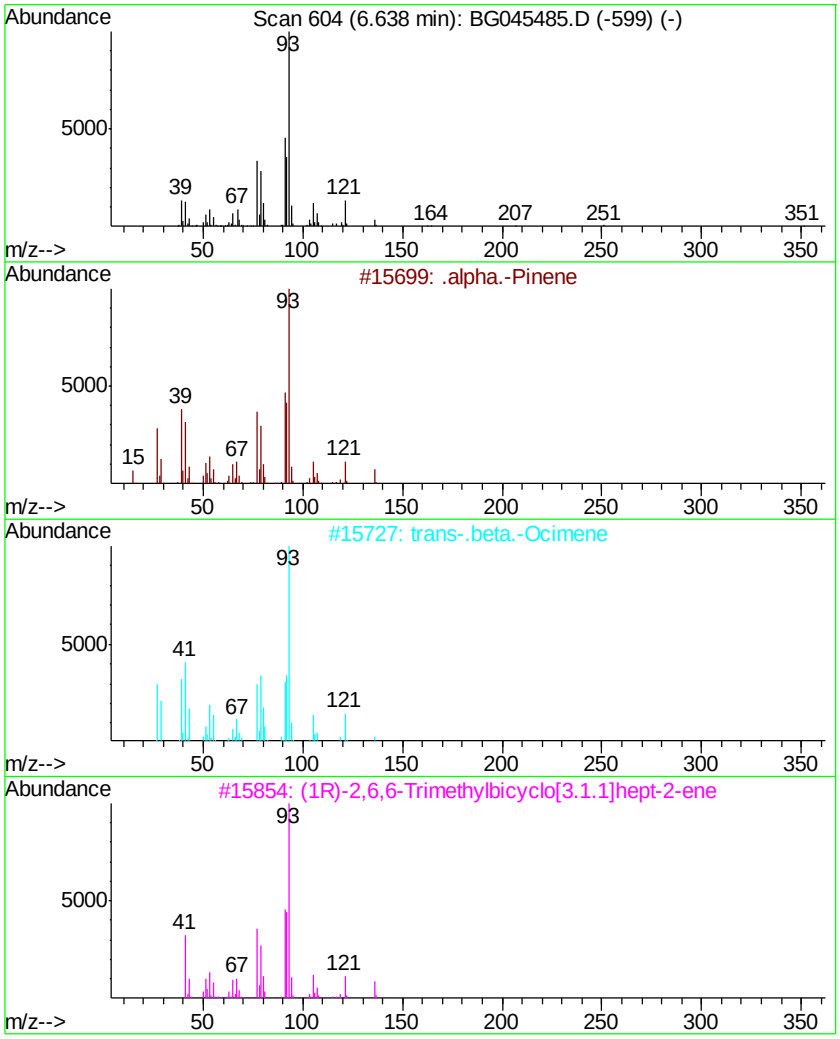
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

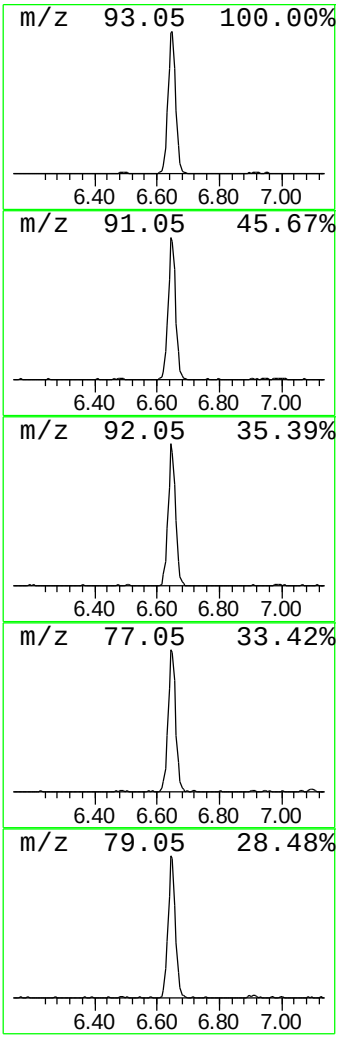
****

Peak Number 1 .alpha.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	17.47 ng	579625	1,4-Dichlorobenzene-d4	7.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	95
2	trans-.beta.-Ocimene	136	C10H16	003779-61-1	94
3	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	94
4	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
5	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

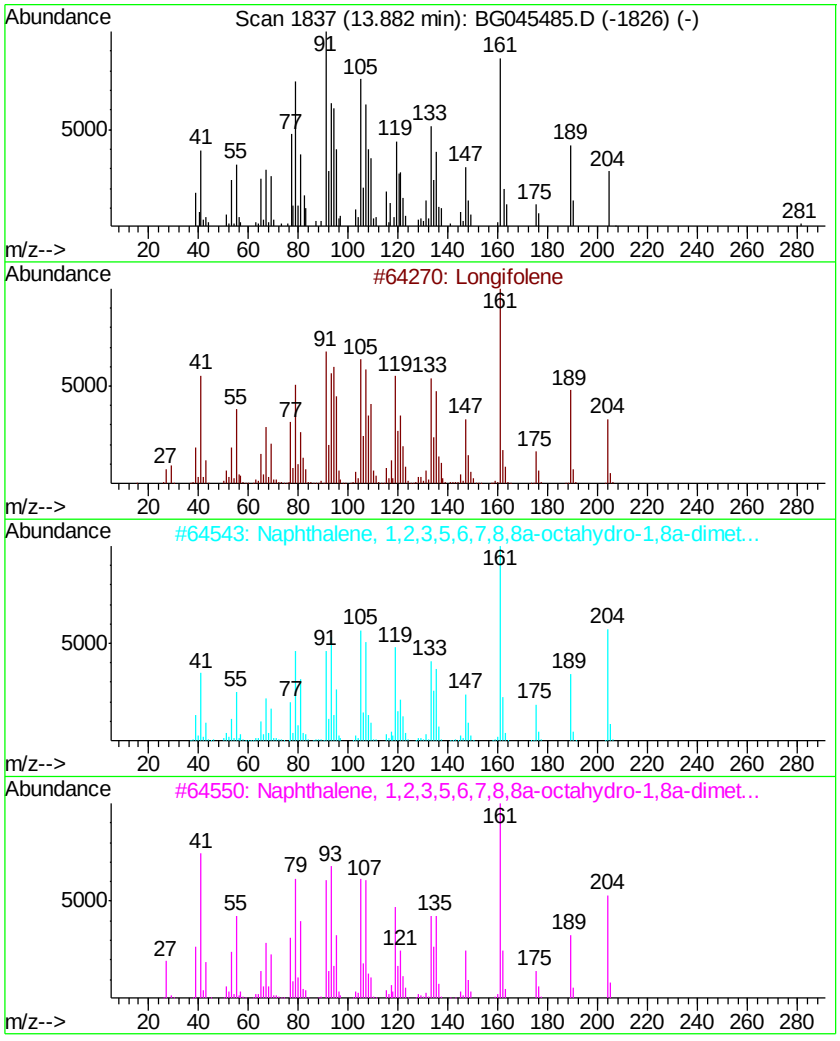
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

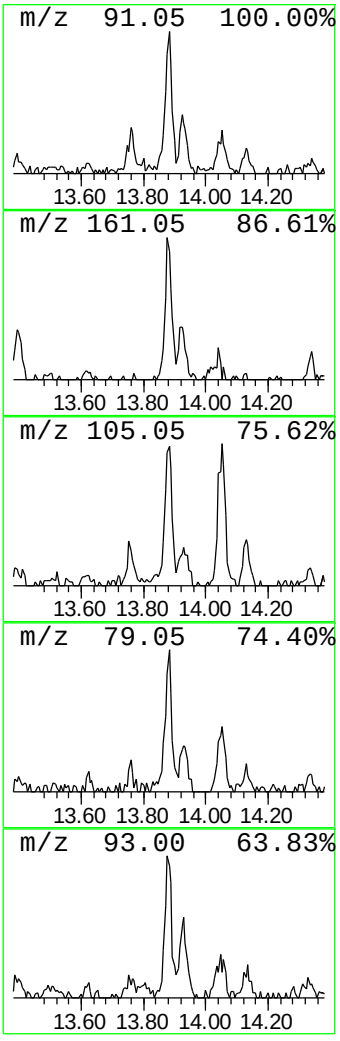
****

Peak Number 3 Longifolene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	2.84 ng	199250	Acenaphthene-d10	14.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Longifolene	204	C15H24	000475-20-7	99
2	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	98
3	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	97
4	4,5-di-epi-aristolochene	204	C15H24	1000374-17-1	76
5	Caryophyllene-(I1)	204	C15H24	1000158-18-5	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

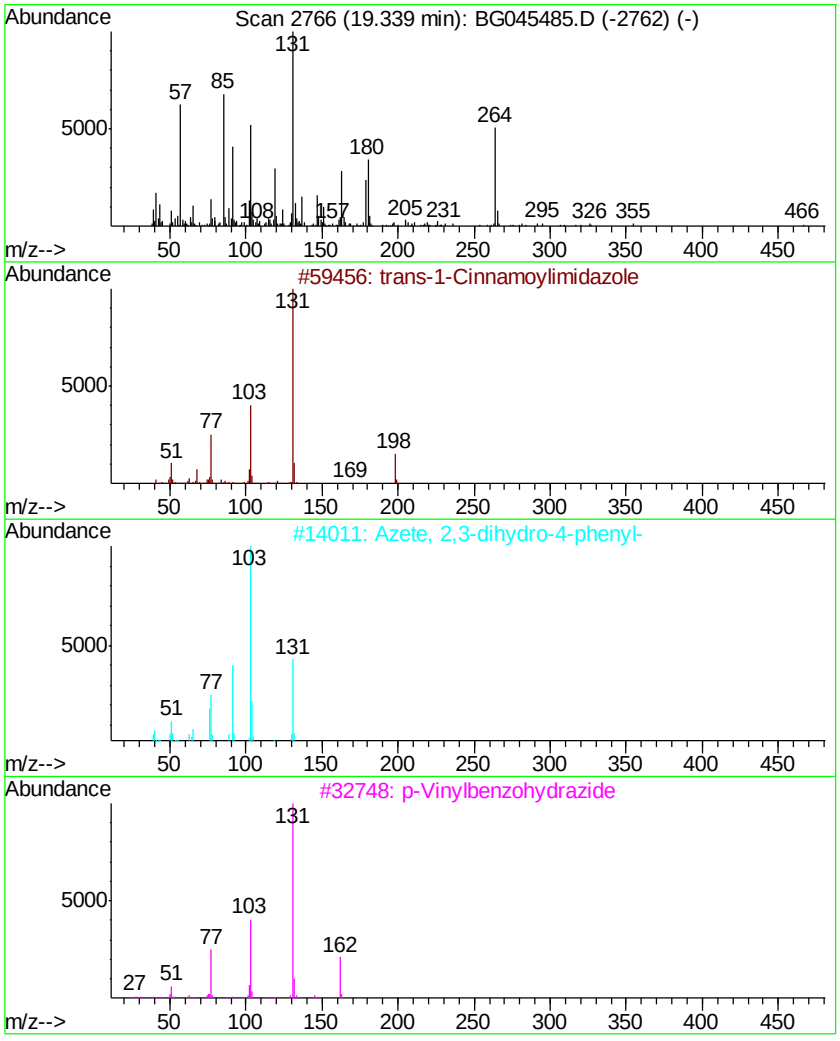
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

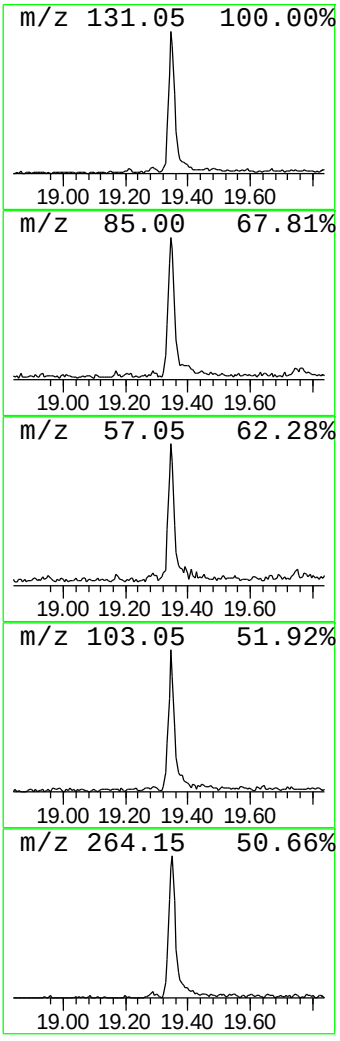
****

Peak Number 4 unknown19.34 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	4.15 ng	334103	Phenanthrene-d10	17.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	27
2	Azete, 2,3-dihydro-4-phenyl-	131	C9H9N	033720-74-0	27
3	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	27
4	Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	27
5	Succinoic acid, 2-hydroxy-3-meth...	204	C9H16O5	1000196-85-6	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

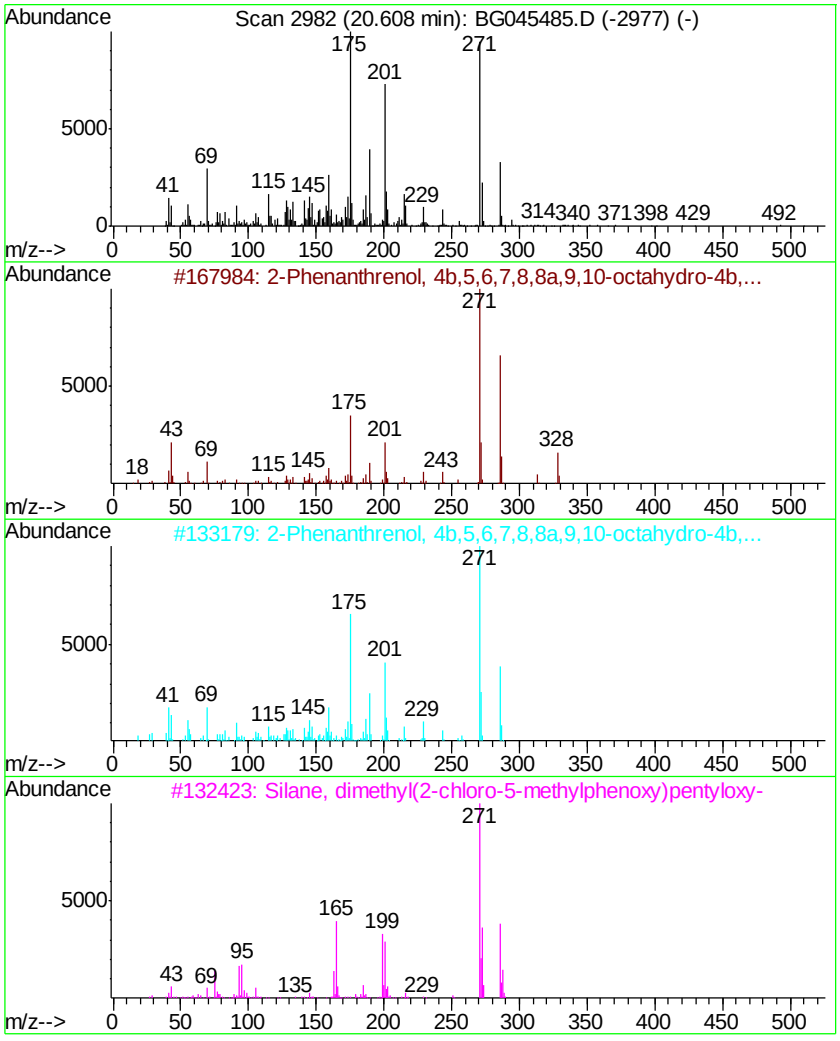
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

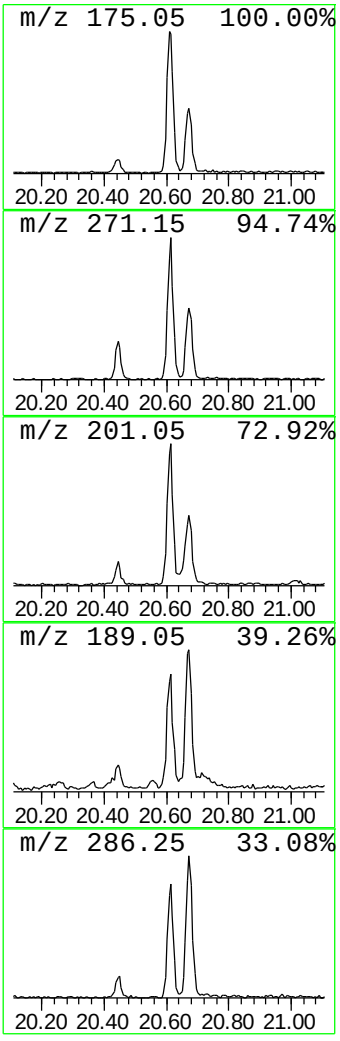
****

Peak Number 5 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.61	8.70 ng	820418	Chrysene-d12	21.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	90
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	70
3	Silane, dimethyl(2-chloro-5-meth...	286	C14H23ClO2Si	1000347-54-6	41
4	Crinan-1-ol, 2,3-didehydro-,(1.a...	271	C16H17NO3	1000111-31-3	22
5	Crinan-1-one	271	C16H17NO3	098301-98-5	20





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

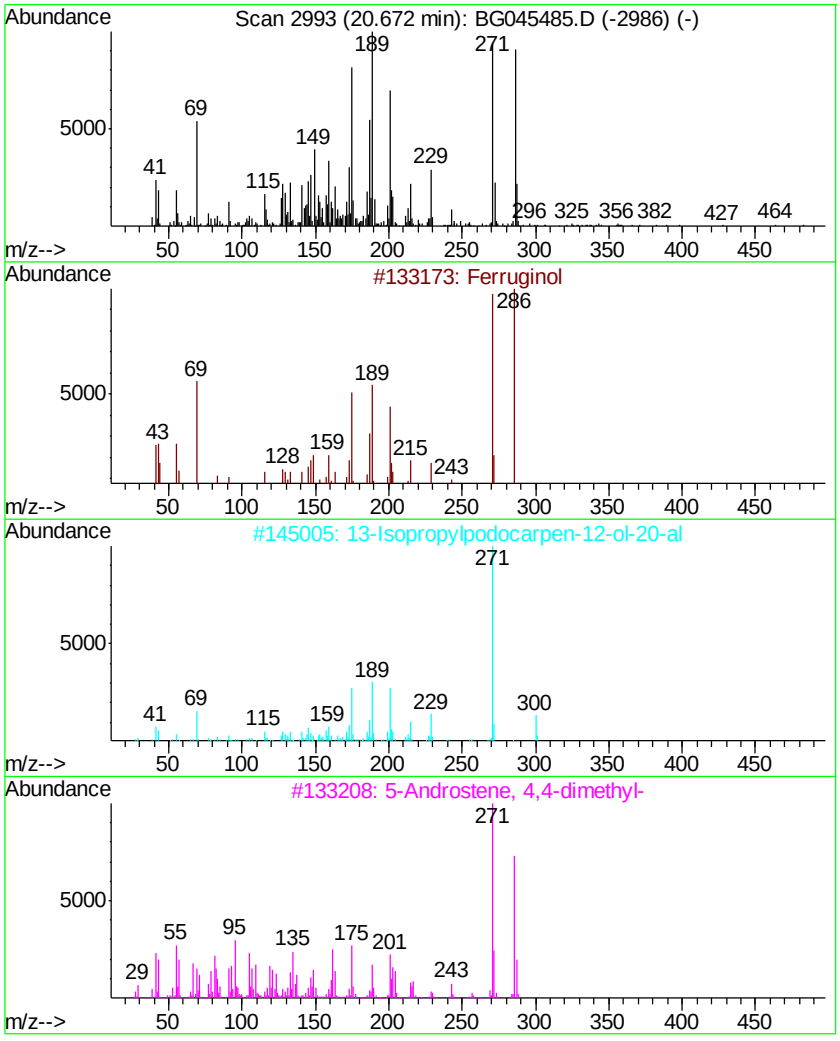
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

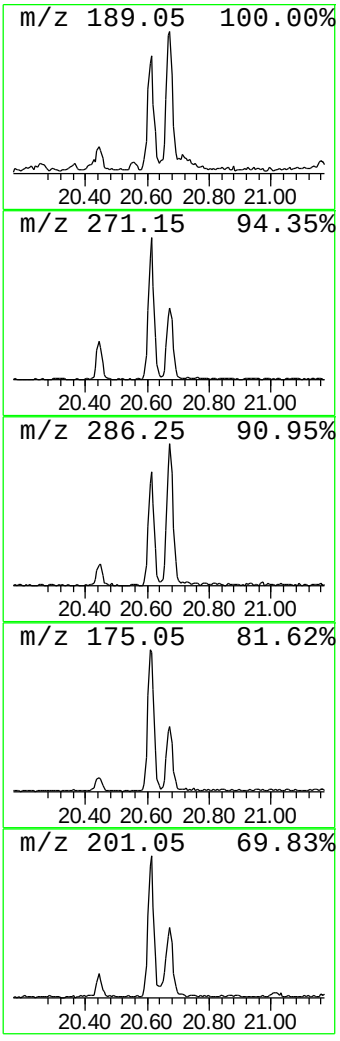
****

Peak Number 6 Ferruginol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.67	10.76 ng	1014490	Chrysene-d12	21.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ferruginol	286	C20H30O	000514-62-5	96
2	13-Isopropylpodocarpen-12-ol-20-al	300	C20H28O2	024035-37-8	91
3	5-Androstene, 4,4-dimethyl-	286	C21H34	1000194-15-4	43
4	Dinaphtho[2,1-b:1',2'-d]thiophen...	286	C20H14S	016587-62-5	25
5	1',2'-Dihydro-2,2'-dimethyl-4,4'...	286	C20H18N2	1000326-82-8	18





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

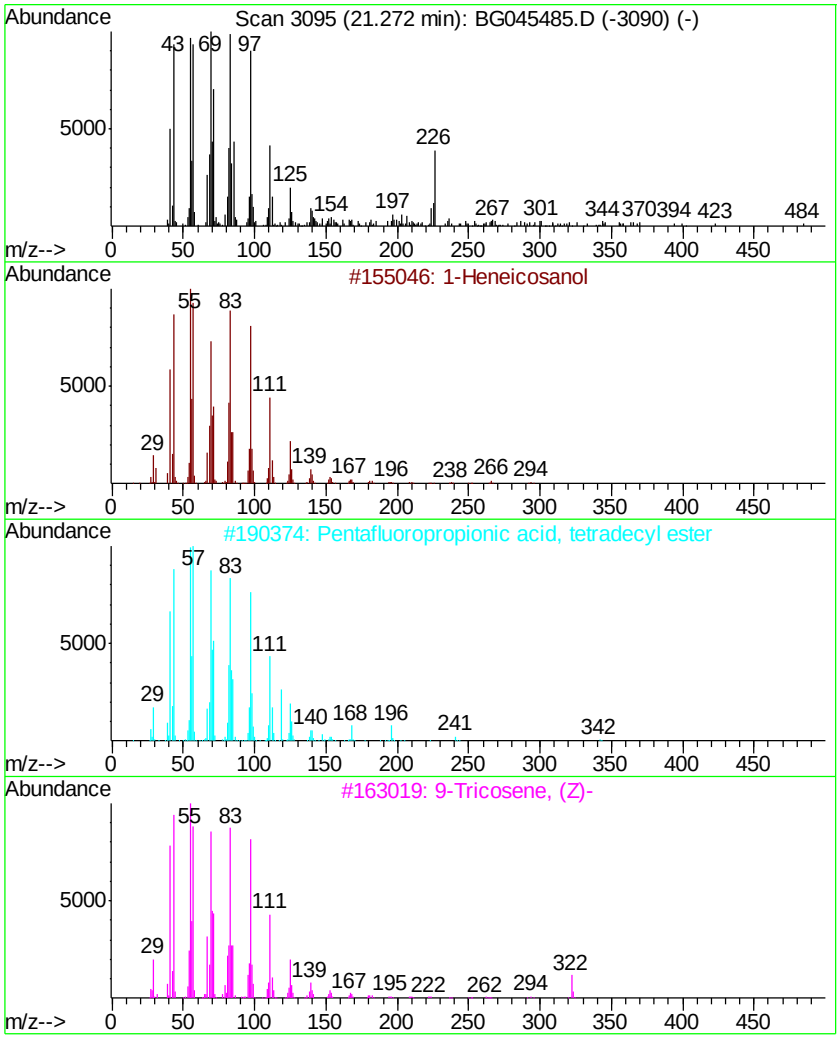
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

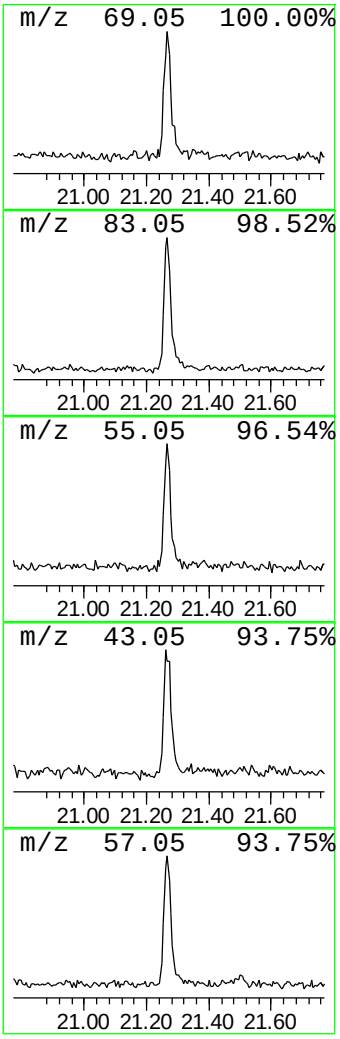
****

Peak Number 7 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	3.96 ng	373394	Chrysene-d12	21.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	87
4	1-Nonadecene	266	C19H38	018435-45-5	86
5	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

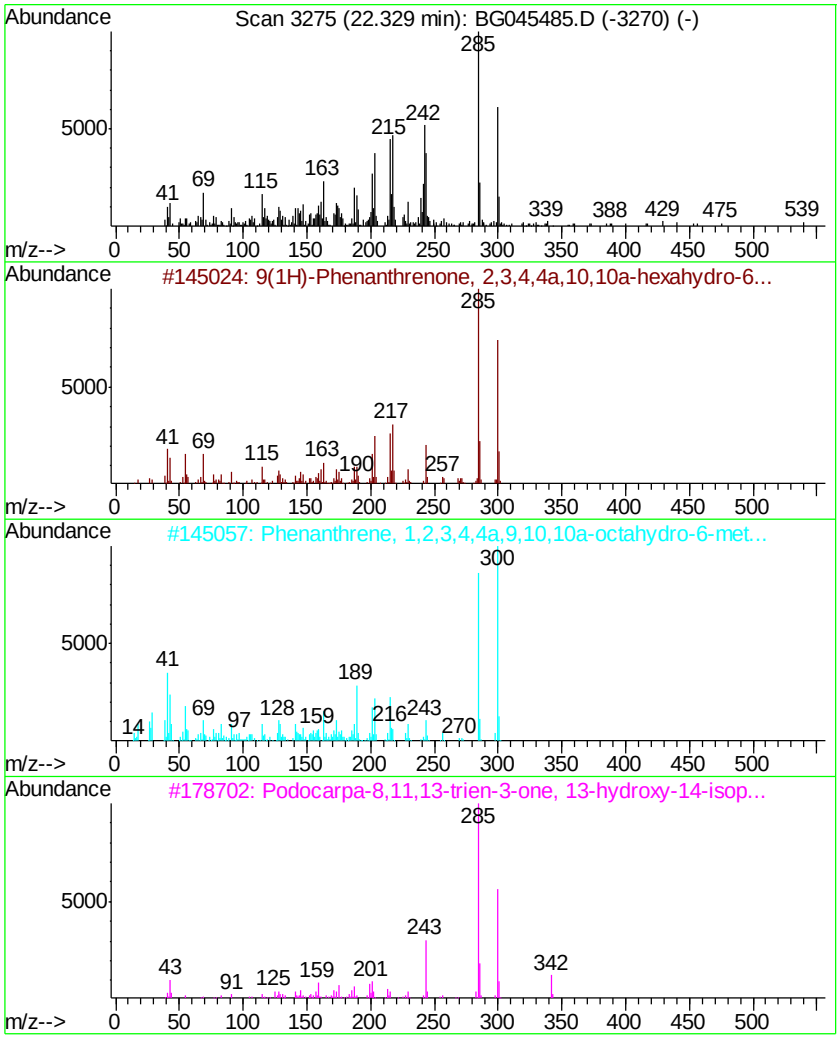
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

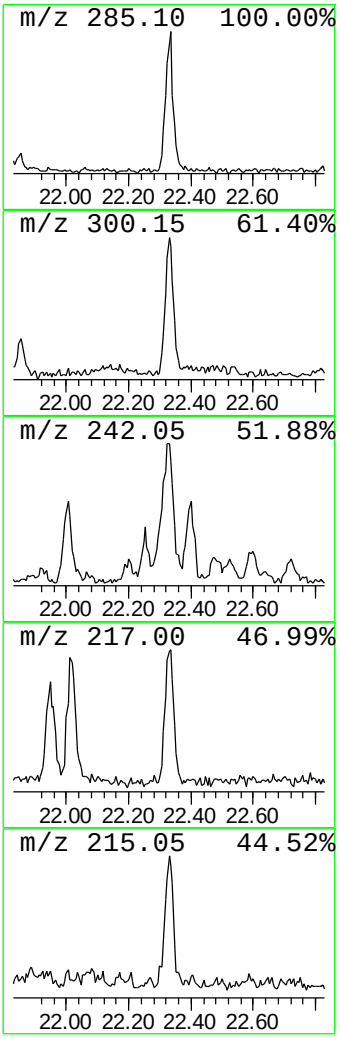
****

Peak Number 8 9(1H)-Phenanthrenone, 2,3,4... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.33	2.89 ng	272552	Chrysene-d12	21.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9(1H)-Phenanthrenone, 2,3,4,4a,1...	300	C20H28O2	000511-05-7	93
2	Phenanthrene, 1,2,3,4,4a,9,10,10...	300	C21H32O	010064-26-3	53
3	Podocarpa-8,11,13-trien-3-one, 1...	342	C22H30O3	018468-20-7	46
4	Benzonitrile, 4-(6-butyl-2-napht...	285	C21H19N	087633-72-5	45
5	Phenanthrene, 1,2,3,4,4a,9,10,10...	300	C21H32O	015340-83-7	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052720\
Data File : BG045485.D
Acq On : 27 May 2020 20:59
Operator : CG/JU
Sample : L2746-09
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NMDUP03-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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
.alpha.-Pinene	6.64	17.5	ng	579625	1	7.96	663642	20.0
Longifolene	13.88	2.8	ng	199250	3	14.60	1405170	20.0
unknown19.34	19.34	4.2	ng	334103	4	17.35	1608550	20.0
2-Phenanthrenol, ...	20.61	8.7	ng	820418	5	21.61	1886300	20.0
Ferruginol	20.67	10.8	ng	1014490	5	21.61	1886300	20.0
1-Heneicosanol	21.27	4.0	ng	373394	5	21.61	1886300	20.0
9(1H)-Phenanthren...	22.33	2.9	ng	272552	5	21.61	1886300	20.0