LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045564.D
Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-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	5.543	409	418	427	rBV	655550	1140299	37.03%	4.428%
2	7.153	684	692	702	rBV	732992	1340821	43.54%	5.206%
3	7.952	821	828	837	rBV	290446	505953	16.43%	1.964%
4	8.275	876	883	894	rBV	671337	1208619	39.25%	4.693%
5	9.115	1017	1026	1036	rBV	491741	944924	30.68%	3.669%
6	10.759	1298	1306	1314	rBV	370899	709175	23.03%	2.754%
7	13.215	1717	1724	1733	rBV	1480128	2362744	76.73%	9.174%
8	13.750	1809	1815	1819	rBV3	22215	37913	1.23%	0.147%
9	13.873	1829	1836	1841	rBV3	76713	121369	3.94%	0.471%
10	13.920	1841	1844	1852	rVB6	37601	61573	2.00%	0.239%
11	14.043	1857	1865	1875	rBV	256920	411483	13.36%	1.598%
12	14.125	1875	1879	1888	rVB4	23345	37947	1.23%	0.147%
13	14.319	1903	1912	1918	rVB6	18444	40819	1.33%	0.158%
14	14.425	1926	1930	1937	rVB5	23934	39651	1.29%	0.154%
15	14.496	1937	1942	1948	rVB3	49315	76640	2.49%	0.298%
16	14.595	1948	1959	1967	rBV	697702	1137982	36.95%	4.419%
17	15.265	2068	2073	2079	rVB2	26759	41991	1.36%	0.163%
18	15.882	2173	2178	2185	rVB2	75292	118998	3.86%	0.462%
19	16.088	2202	2213	2224	rBV	1089470	1768324	57.42%	6.866%
20	16.745	2319	2325	2334	rBV9	29058	81522	2.65%	0.317%
21	17.345	2420	2427	2432	rBV	736939	1163752	37.79%	4.519%
22	17.386	2432	2434	2441	rVB	106876	134123	4.36%	0.521%
23	17.486	2446	2451	2454	rVB	22465	33981	1.10%	0.132%
24	17.727	2488	2492	2495	rBV6	23456	39684	1.29%	0.154%
25	18.220	2573	2576	2581	rVV4	20360	46679	1.52%	0.181%
26	18.267	2582	2584	2590	rVB2	29051	38635	1.25%	0.150%
27	18.420	2605	2610	2613	rBV4	33387	53807	1.75%	0.209%
28	19.266	2749	2754	2760	rBV3	47638	106909	3.47%	0.415%
29	19.342	2761	2767	2772	rBV	476954	665196	21.60%	2.583%
30	19.401	2772	2777	2783	rVB	276216	402363	13.07%	1.562%
31	19.759	2828	2838	2846	rBV	247977	463979	15.07%	1.802%
32	19.959	2866	2872	2885	rBV	2332741	3079441	100.00%	11.957%
33	20.253	2918	2922	2928	rVB3	54168	96968	3.15%	0.377%
34	20.440	2952	2954	2959	rVB3	42108	47368	1.54%	0.184%

LSC Area Percent Report

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Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-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	20.605	2977	2982	2986	rBV2	283310	378243	12.28%	1.469%
36	20.646	2986	2989	2998	rVB	179613	245329	7.97%	0.953%
37	21.263	3090	3094	3102	rVB4	174799	311996	10.13%	1.211%
38	21.498	3130	3134	3141	rVB	140566	214156	6.95%	0.832%
39	21.604	3144	3152	3157	rVV3	725128	1407327	45.70%	5.464%
40	21.651	3157	3160	3173	rVB	124919	234973	7.63%	0.912%
41	21.803	3183	3186	3192	rVB3	63758	91362	2.97%	0.355%
42	22.403	3283	3288	3306	rVB7	125934	408583	13.27%	1.586%
43	23.754	3512	3518	3526	rBV	112943	346610	11.26%	1.346%
44	23.865	3532	3537	3543	rVB2	224009	420455	13.65%	1.633%
45	24.600	3657	3662	3672	rVB	85326	226783	7.36%	0.881%
46	24.752	3679	3688	3704	rVB	405233	1272018	41.31%	4.939%
47	25.299	3775	3781	3790	rVB9	75592	221532	7.19%	0.860%
48	25.898	3873	3883	3895	rVB2	369644	1122104	36.44%	4.357%
49	26.021	3897	3904	3915	rBV8	80024	291792	9.48%	1.133%

Sum of corrected areas: 25754895

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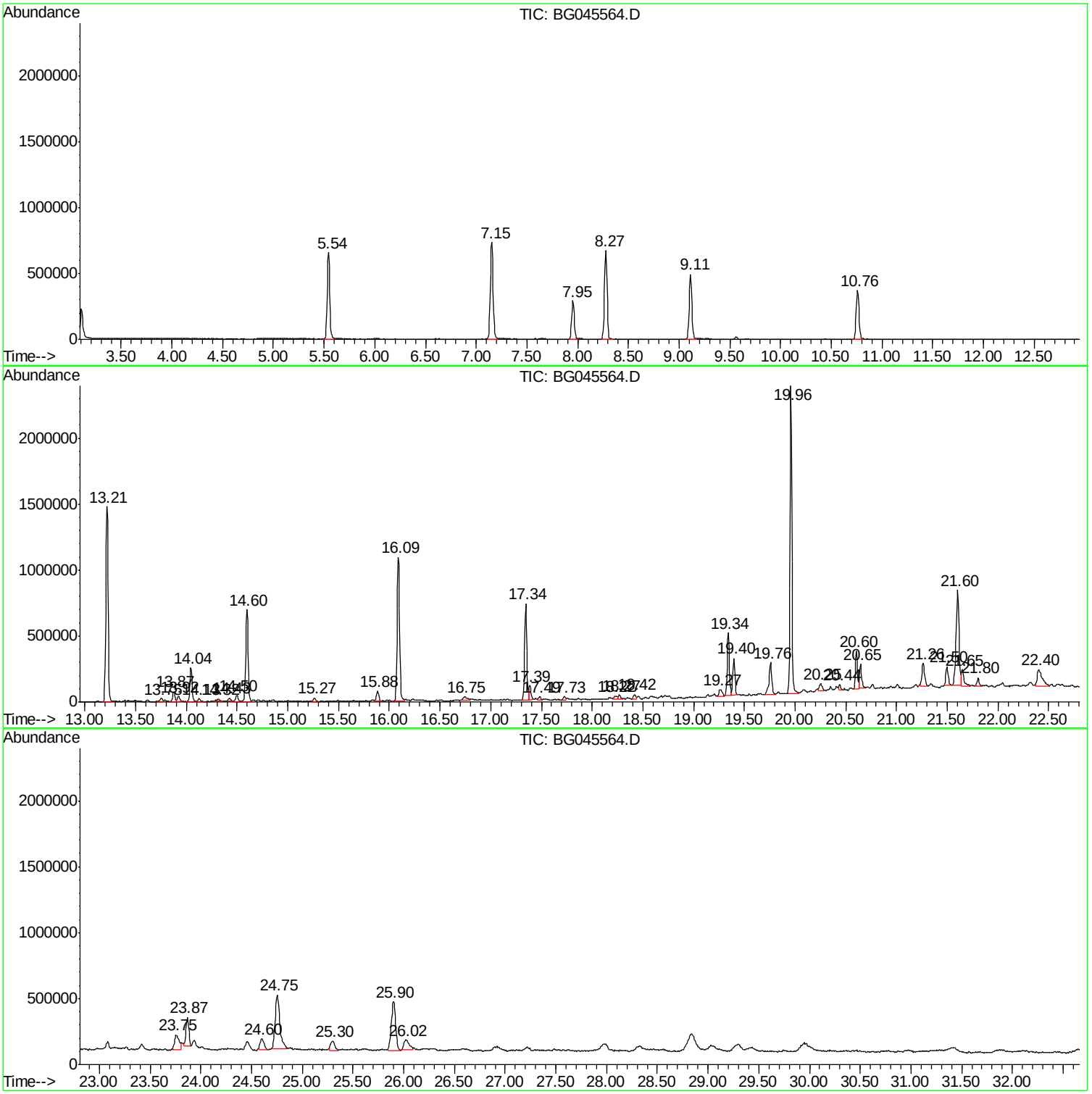
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NM57-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

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Data File : BG045564.D
Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-COMP-2020-0-6

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

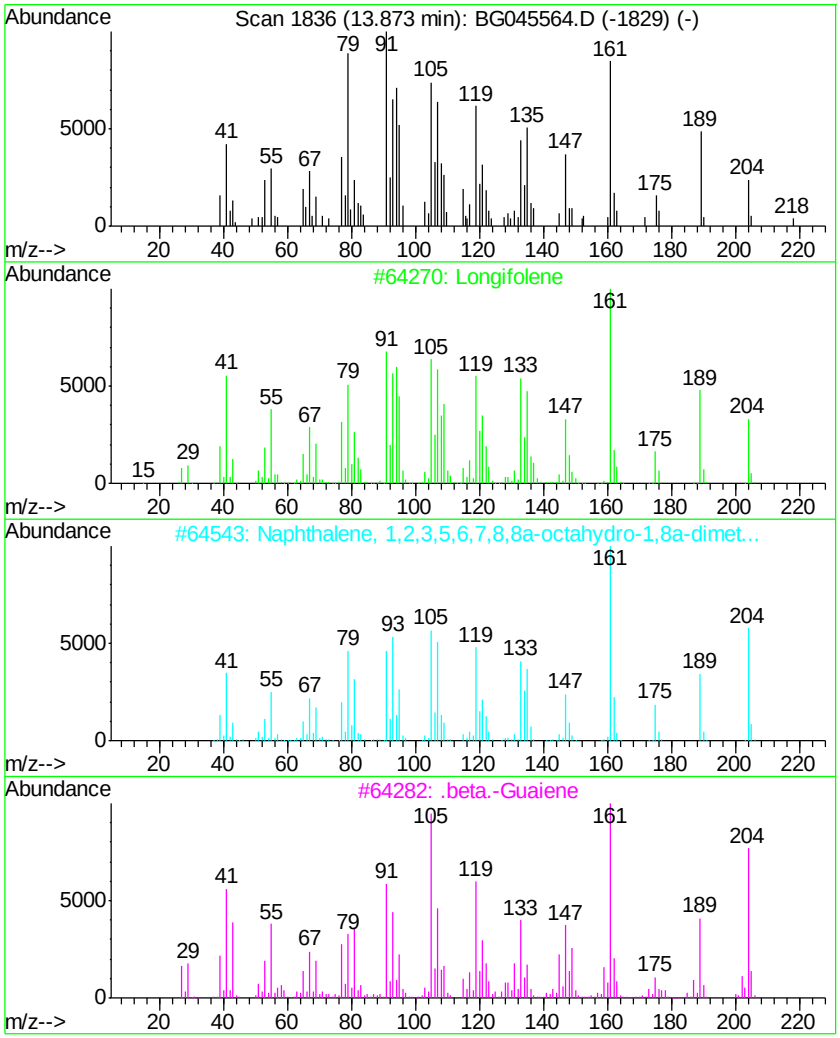
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

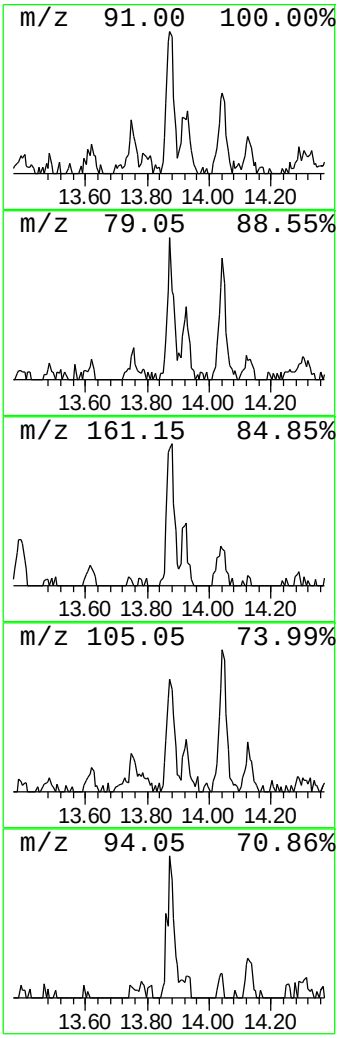
****

Peak Number 2 Longifolene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.13 ng	121369	Acenaphthene-d10	14.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Longifolene	204	C15H24	000475-20-7	89
2	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	83
3	.beta.-Guaiene	204	C15H24	000088-84-6	70
4	Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	70
5	2H-2,4a-Methanonaphthalene, 1,3,...	204	C15H24	001135-66-6	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045564.D
Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-COMP-2020-0-6

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

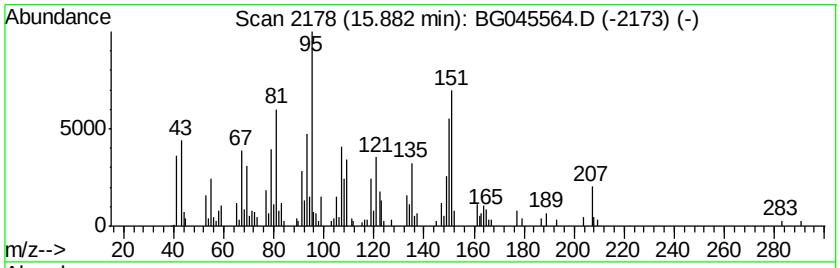
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

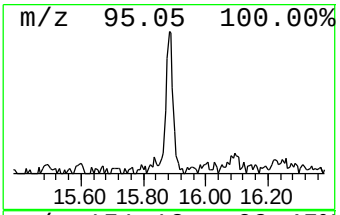
****

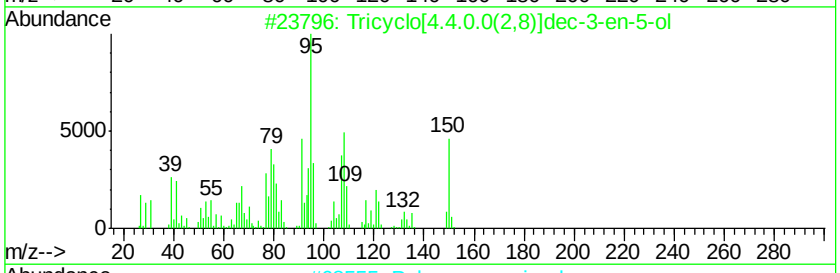
Peak Number 3 unknown15.88 Concentration Rank 13

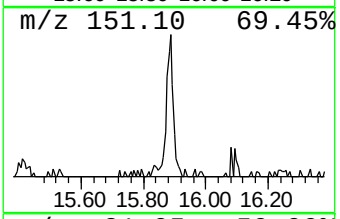
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	2.09 ng	118998	Acenaphthene-d10	14.60

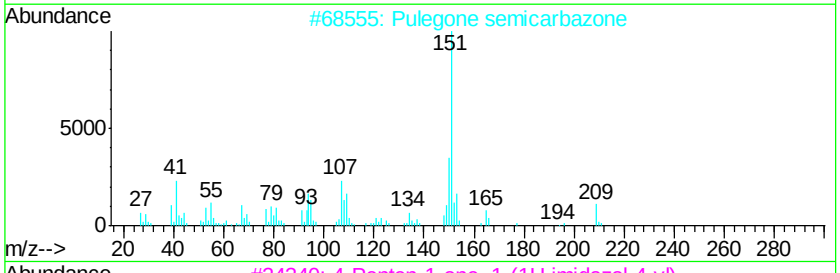
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[4.4.0.0(2,8)]dec-3-en-5-ol	150	C10H14O	1000193-38-7	46
2	Pulegone semicarbazone	209	C11H19N3O	023733-71-3	43
3	4-Penten-1-one, 1-(1H-imidazol-4...	150	C8H10N2O	069393-39-1	38
4	Methanone, cyclobutyl-1H-imidazo...	150	C8H10N2O	069393-27-7	38
5	Aminocarb	208	C11H16N2O2	002032-59-9	35

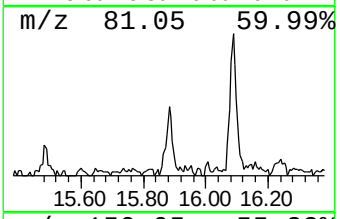


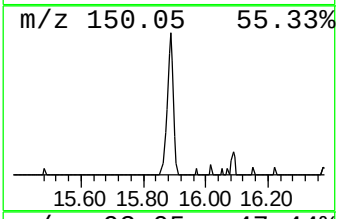


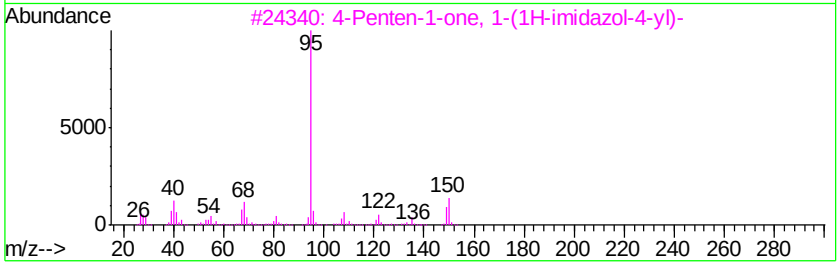


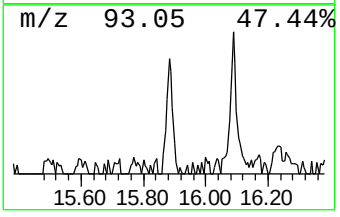












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045564.D
Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-COMP-2020-0-6

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

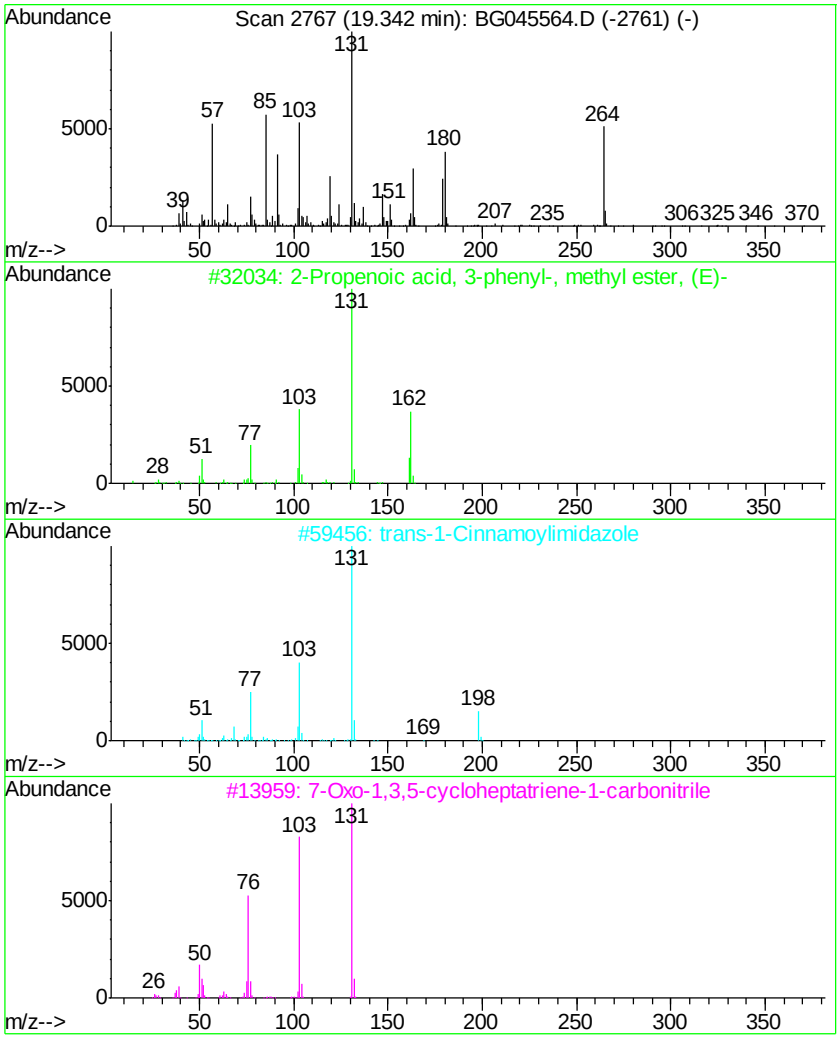
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

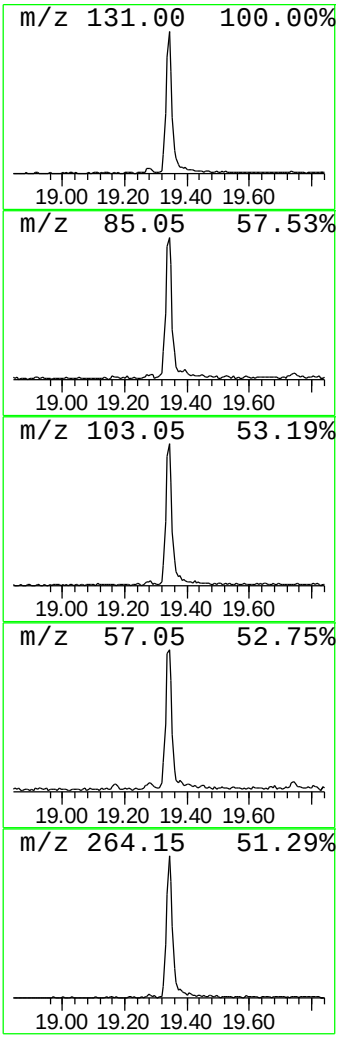
****

Peak Number 4 unknown19.34 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	11.43 ng	665196	Phenanthrene-d10	17.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	001754-62-7	30
2	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	22
3	7-Oxo-1,3,5-cycloheptatriene-1-c...	131	C8H5NO	000934-19-0	22
4	3-Butenoic acid, 2-oxo-4-phenyl-	176	C10H8O3	1000142-21-0	22
5	Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
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Sample : L2798-07
Misc :
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Instrument : BNA_G
ClientSampleId : NM57-COMP-2020-0-6

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

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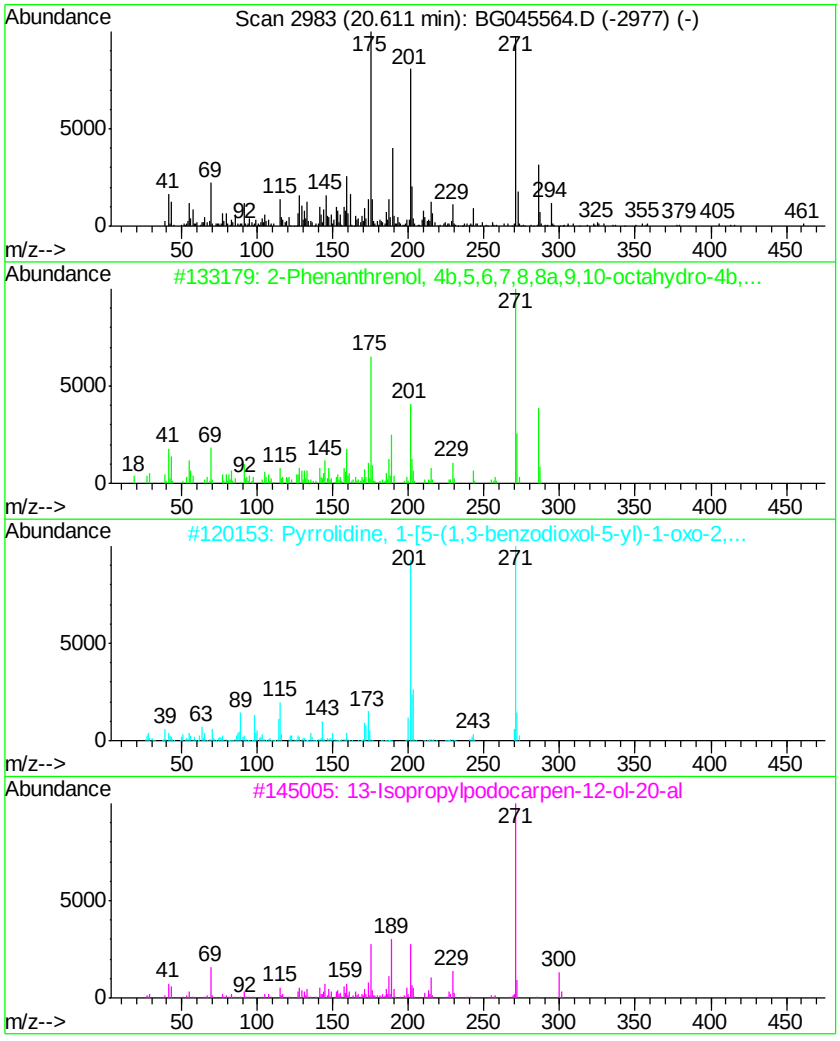
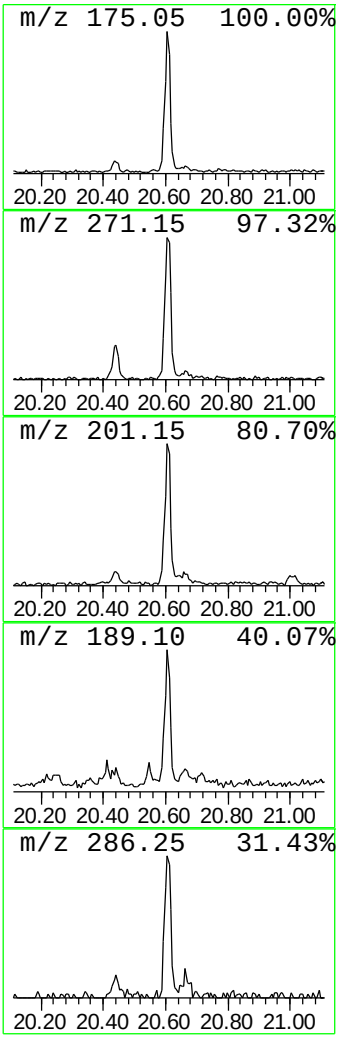
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.61	5.38 ng	378243	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	38
3	13-Isopropylpodocarpen-12-ol-20-al	300	C20H28O2	024035-37-8	35
4	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	27
5	Silane, dimethyl(2-chlorophenoxy...	286	C14H23ClO2Si	1000347-07-3	22





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ClientSampleId : NM57-COMP-2020-0-6

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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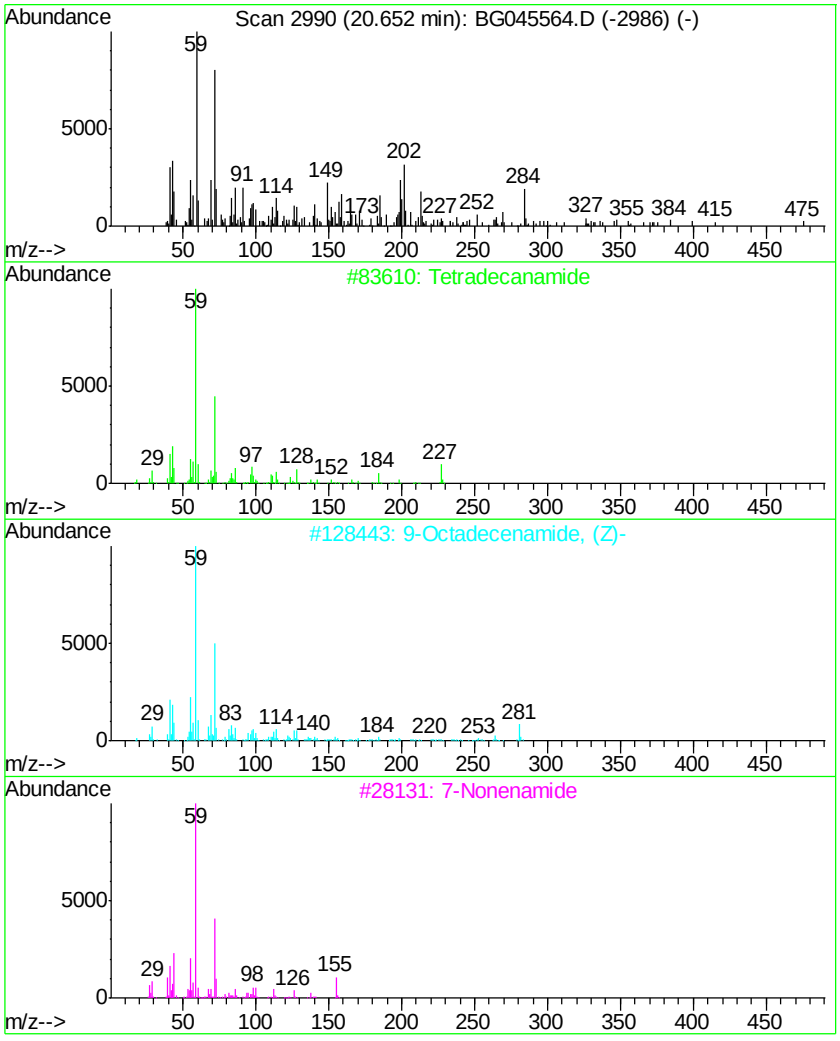
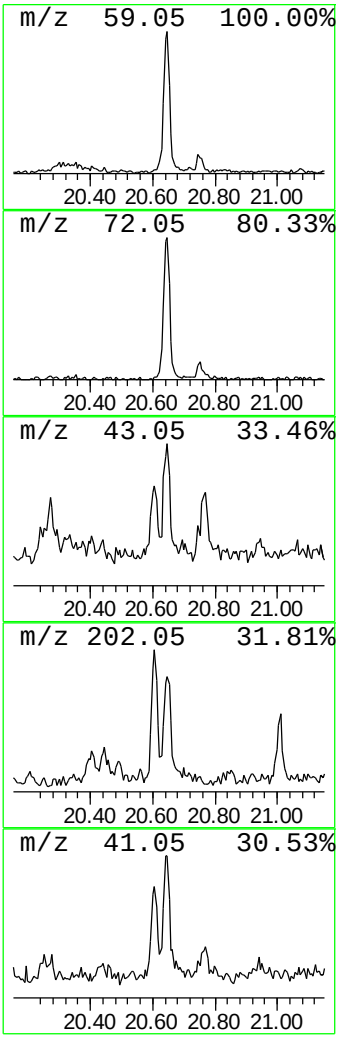
****

Peak Number 6 Tetradecanamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.65	3.49 ng	245329	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanamide	227	C14H29NO	000638-58-4	62
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	52
3	7-Nonenamide	155	C9H17NO	090949-53-4	43
4	Promethazine	284	C17H20N2S	000060-87-7	38
5	N-Ethylpiperazine	114	C6H14N2	005308-25-8	25





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Data File : BG045564.D
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Misc :
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Instrument : BNA_G
ClientSampleId : NM57-COMP-2020-0-6

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

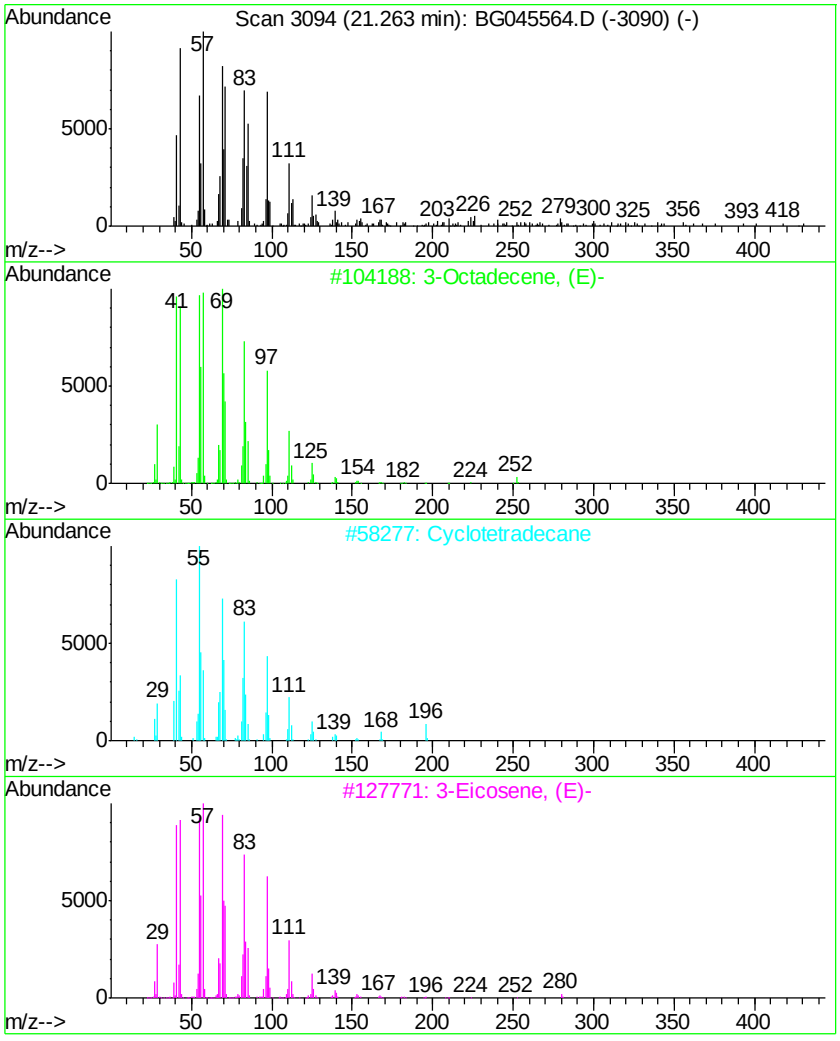
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

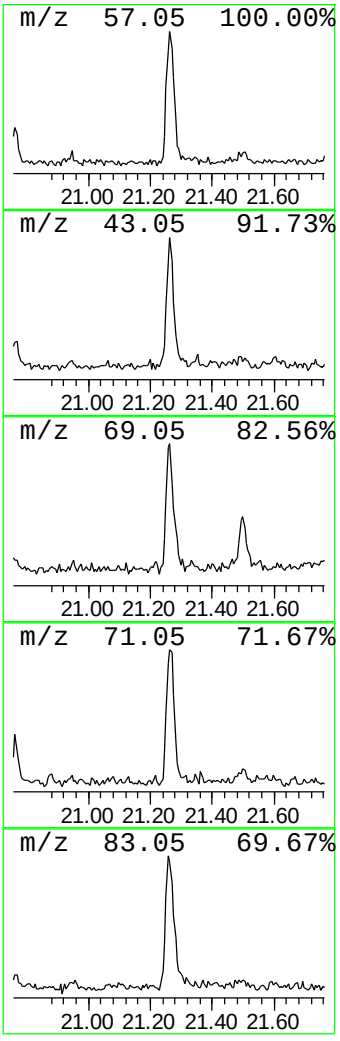
****

Peak Number 7 3-Octadecene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.26	4.43 ng	311996	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	95
2	Cyclotetradecane	196	C14H28	000295-17-0	95
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	92
4	Cyclohexadecane	224	C16H32	000295-65-8	90
5	Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	90





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

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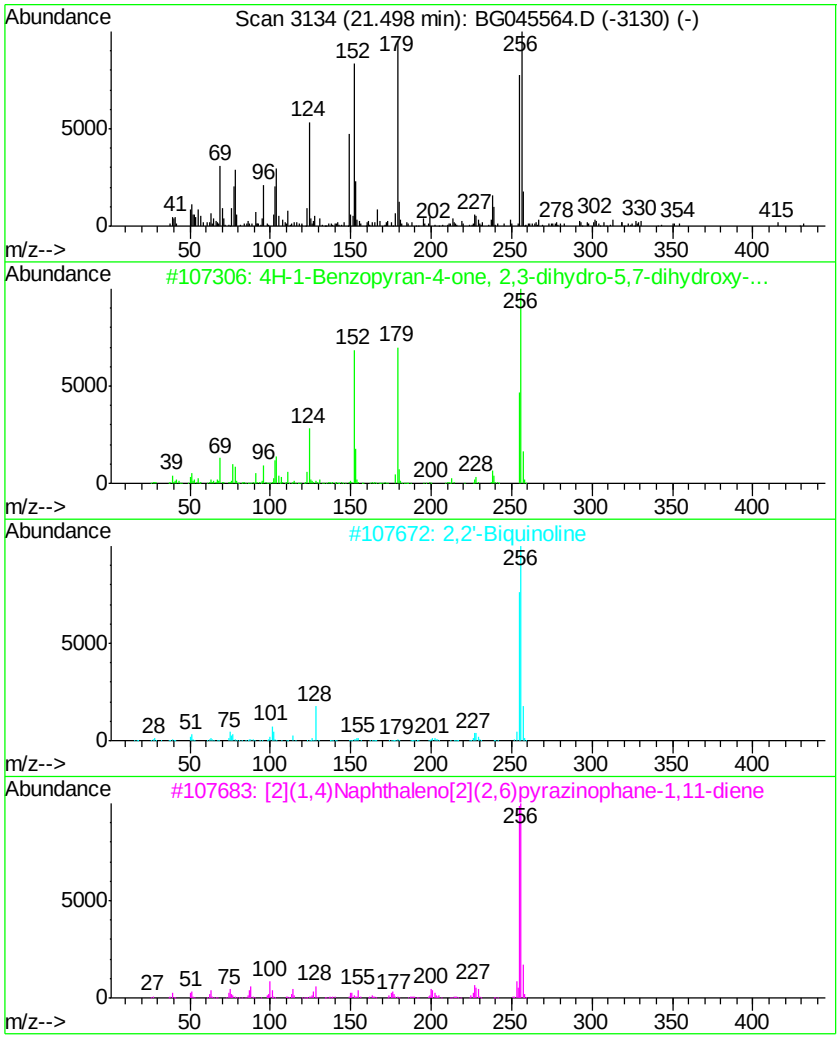
TIC Integration Parameters: LSCINT.P

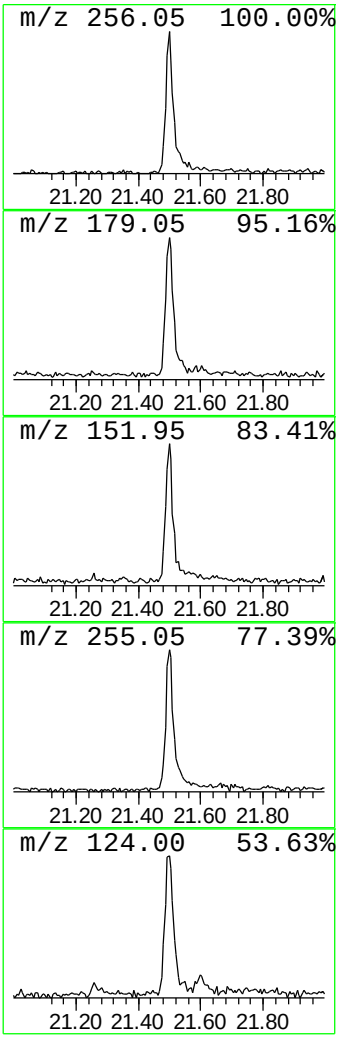
****

Peak Number 8 4H-1-Benzopyran-4-one, 2,3-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	3.04 ng	214156	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1-Benzopyran-4-one, 2,3-dihyd...	256	C15H12O4	000480-39-7	94
2	2,2'-Biquinoline	256	C18H12N2	000119-91-5	38
3	[2](1,4)Naphthaleno[2](2,6)pyraz...	256	C18H12N2	100762-12-7	25
4	Benzonitrile, 3-(2,2-dicyanoethe...	179	C11H5N3	060595-33-7	22
5	2-Isoquinolin-3-ylquinoline	256	C18H12N2	1000220-86-8	22





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Data File : BG045564.D
Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-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

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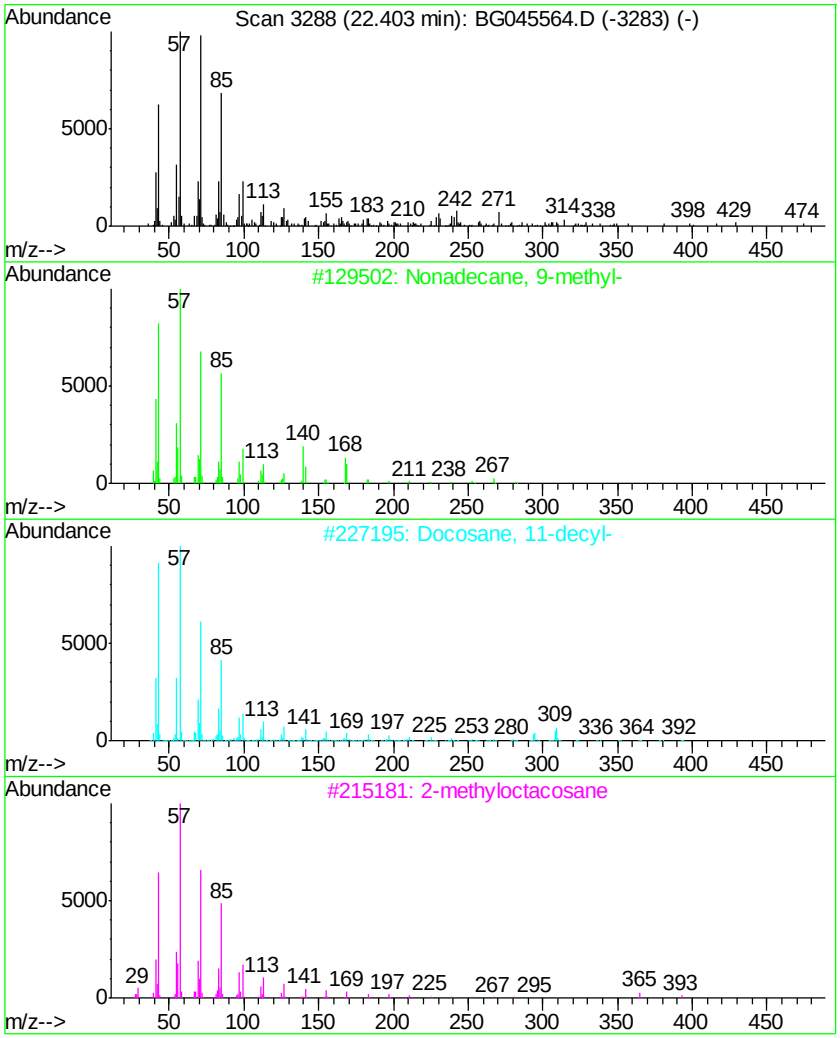
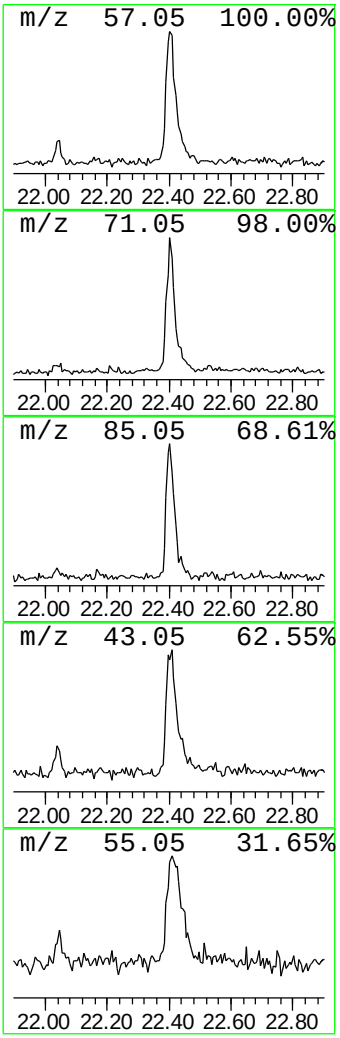
Peak Number 9 Nonadecane, 9-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.40	5.81 ng	408583	Chrysene-d12	21.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80
2	Docosane, 11-decyl-	451	C32H66	055401-55-3	80
3	2-methyloctacosane	408	C29H60	1000376-72-8	80
4	Tetracosane	338	C24H50	000646-31-1	80
5	Hexacosane	366	C26H54	000630-01-3	80





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Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-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

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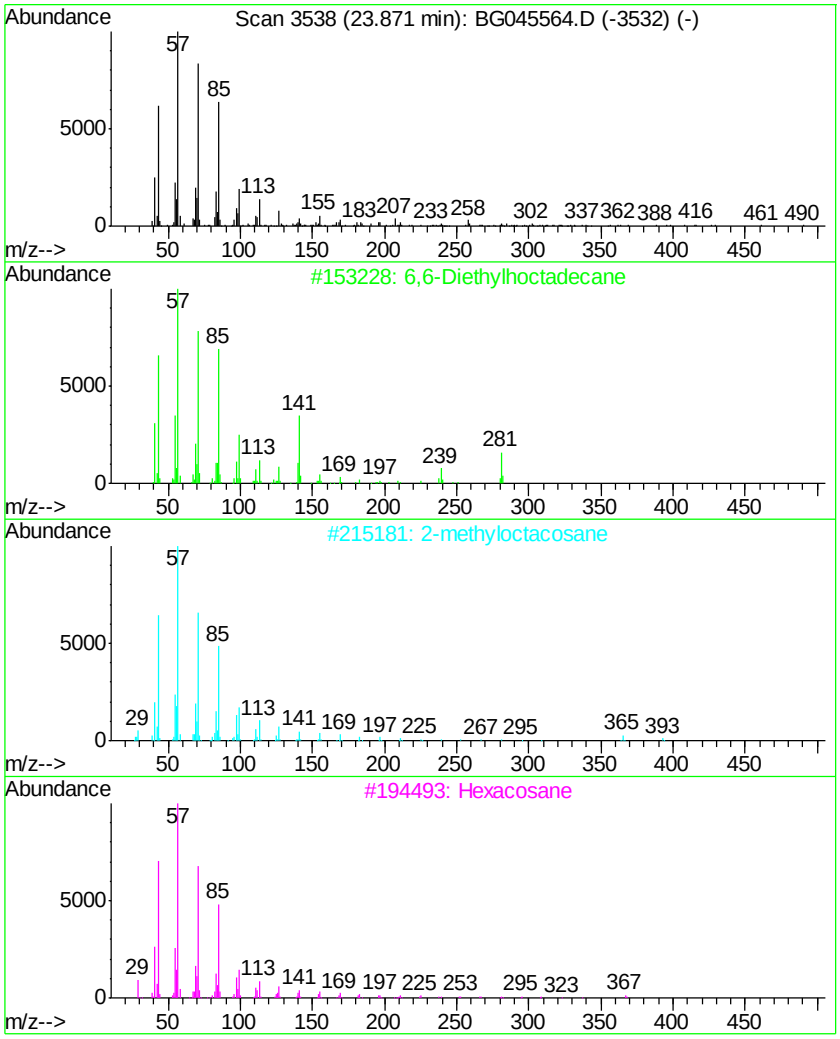
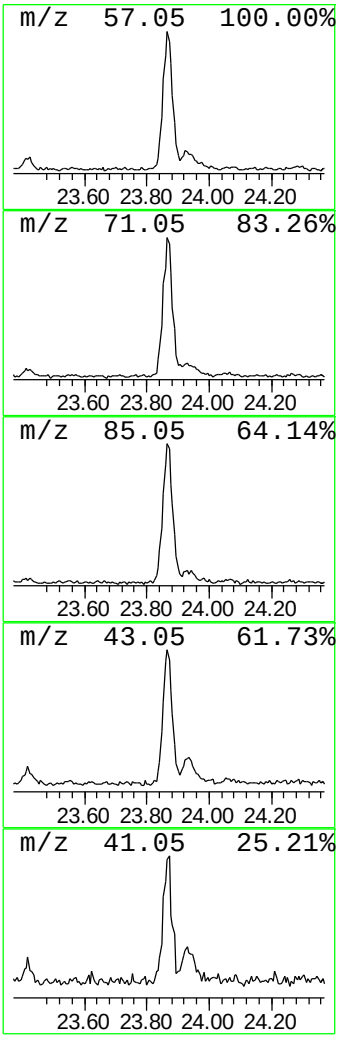
Peak Number 10 6,6-Diethylhoctadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.87	6.61 ng	420455	Perylene-d12	24.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
5	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045564.D
Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-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

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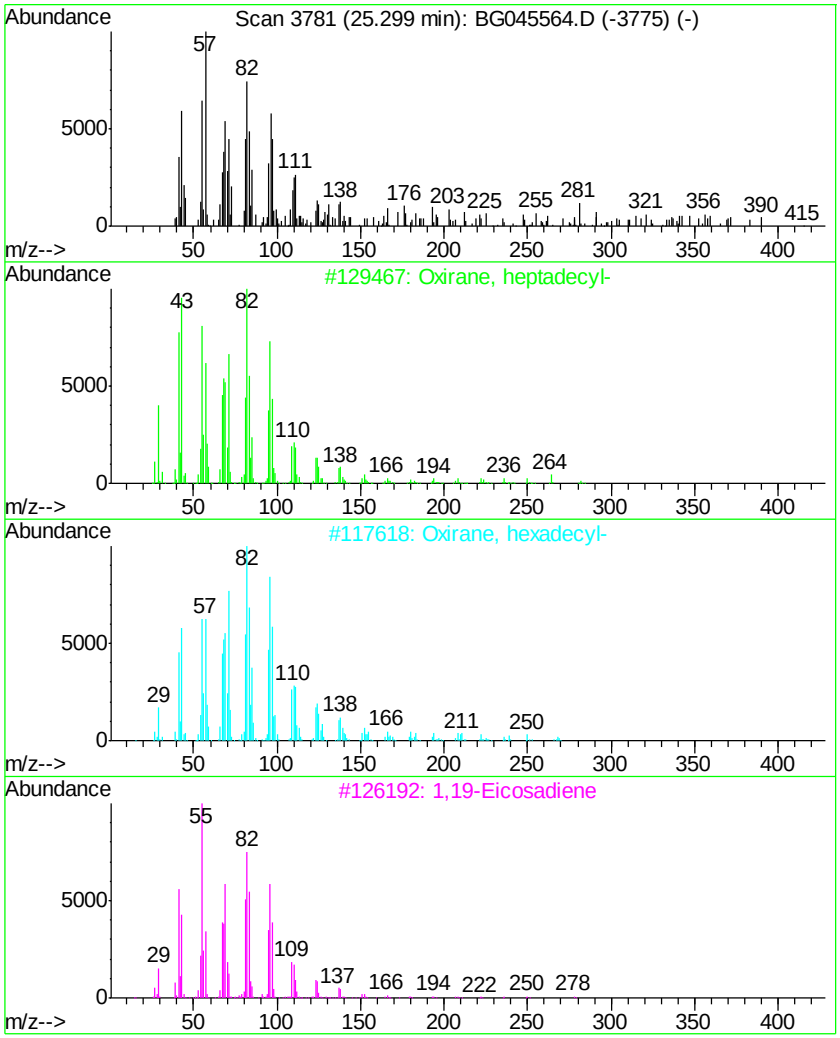
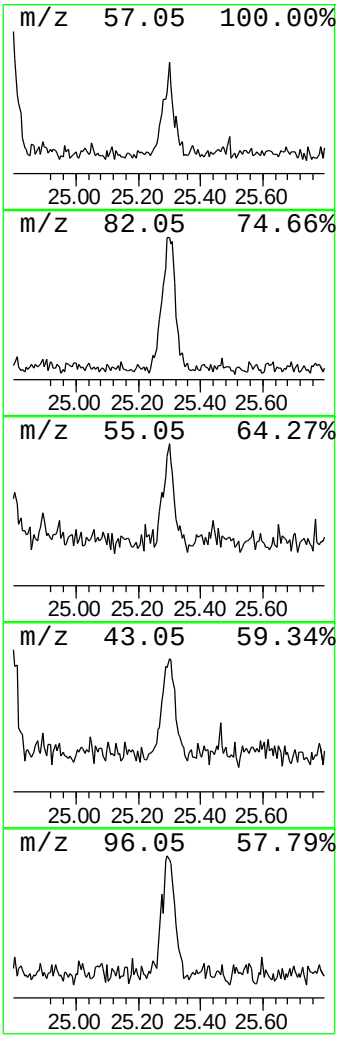
Peak Number 11 Oxirane, heptadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.30	3.48 ng	221532	Perylene-d12	24.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	93
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	87
3	1,19-Eicosadiene	278	C20H38	014811-95-1	80
4	Z-11,13-Dimethyl-11-tetradecen-1...	282	C18H34O2	1000131-36-6	70
5	Z-9-Hexadecen-1-ol acetate	282	C18H34O2	1000130-89-2	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045564.D
Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-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

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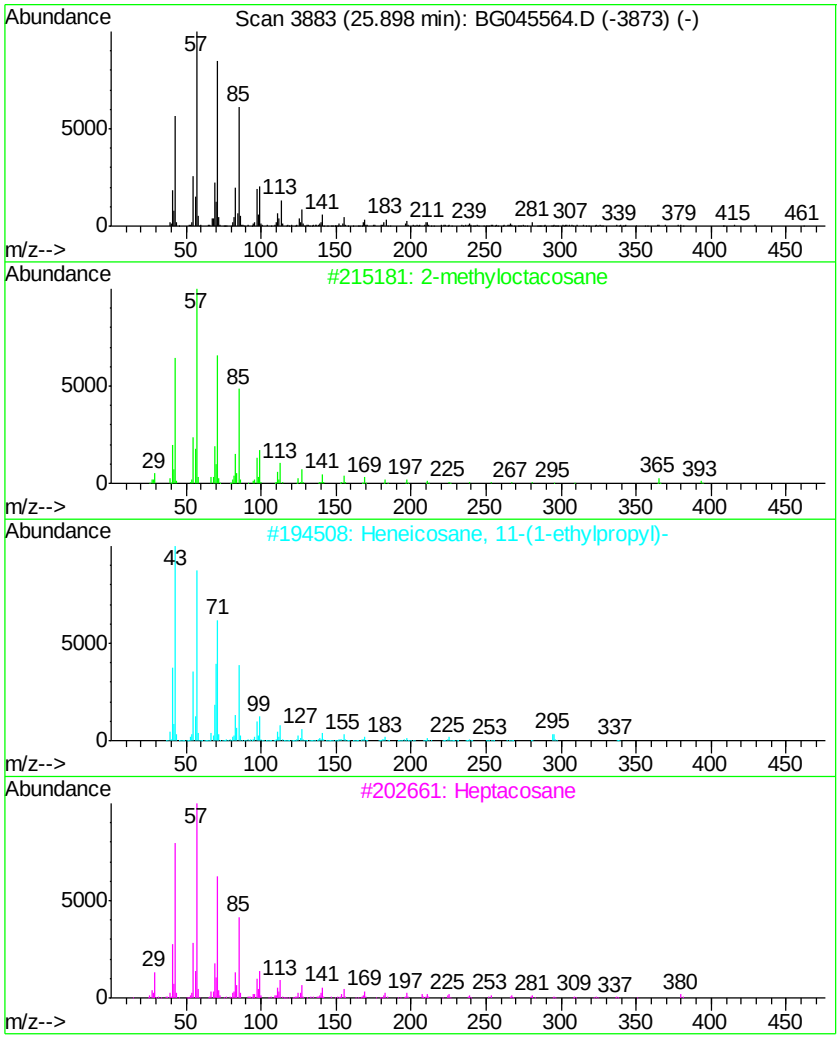
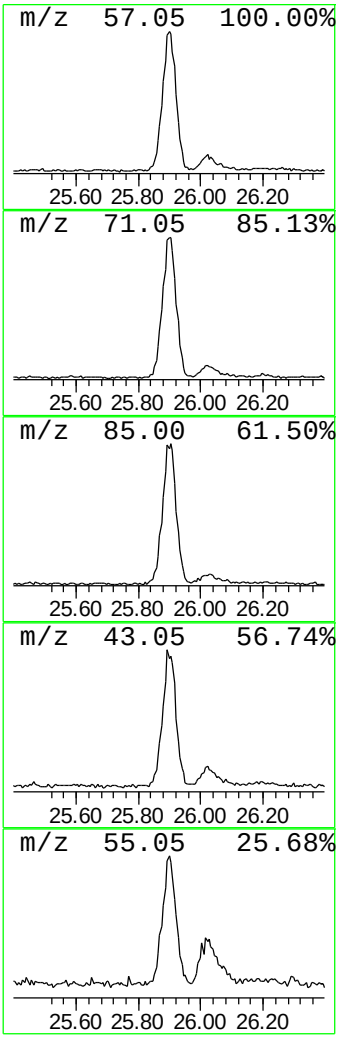
Peak Number 12 2-methyloctacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.90	17.64 ng	1122100	Perylene-d12	24.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3	Heptacosane	380	C27H56	000593-49-7	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetracosane	338	C24H50	000646-31-1	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG060120\
Data File : BG045564.D
Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-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

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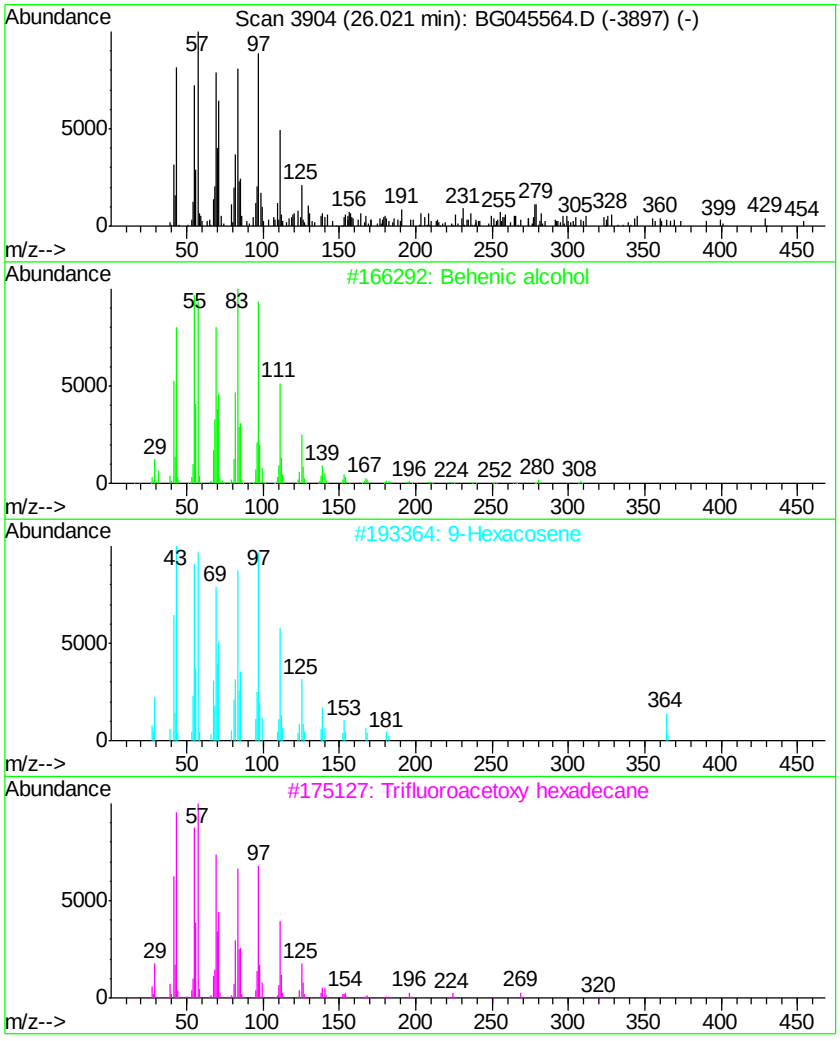
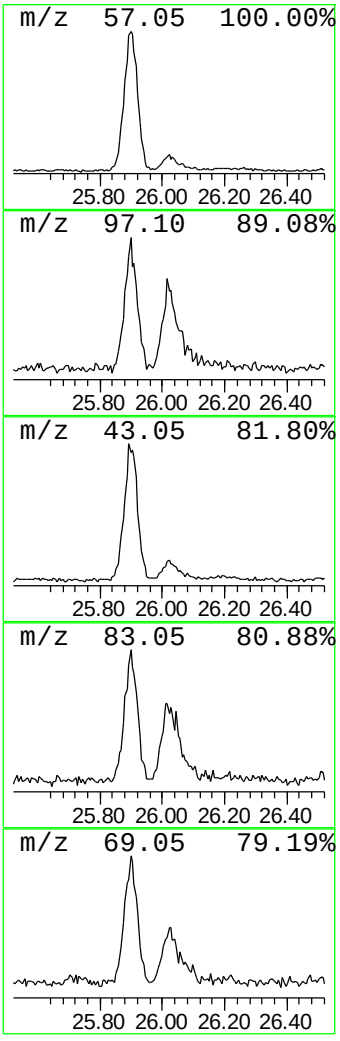
Peak Number 13 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.02	4.59 ng	291792	Perylene-d12	24.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	87
2	9-Hexacosene	364	C26H52	071502-22-2	86
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	83
4	1-Docosene	308	C22H44	001599-67-3	83
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG060120\
Data File : BG045564.D
Acq On : 1 Jun 2020 20:36
Operator : CG/JU
Sample : L2798-07
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : NM57-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
Longifolene	13.87	2.1	ng	121369	3	14.60	1137980	20.0
unknown15.88	15.88	2.1	ng	118998	3	14.60	1137980	20.0
unknown19.34	19.34	11.4	ng	665196	4	17.34	1163750	20.0
2-Phenanthrenol, ...	20.61	5.4	ng	378243	5	21.60	1407330	20.0
Tetradecanamide	20.65	3.5	ng	245329	5	21.60	1407330	20.0
3-Octadecene, (E)-	21.26	4.4	ng	311996	5	21.60	1407330	20.0
4H-1-Benzopyran-4...	21.50	3.0	ng	214156	5	21.60	1407330	20.0
Nonadecane, 9-met...	22.40	5.8	ng	408583	5	21.60	1407330	20.0
6,6-Diethylhoctad...	23.87	6.6	ng	420455	6	24.75	1272020	20.0
Oxirane, heptadecyl-	25.30	3.5	ng	221532	6	24.75	1272020	20.0
2-methyloctacosane	25.90	17.6	ng	1122100	6	24.75	1272020	20.0
Behenic alcohol	26.02	4.6	ng	291792	6	24.75	1272020	20.0